# An enantioselective four-component reaction via assembling two reaction intermediates

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## 1. General Information

**General.** Unless noted all solvents were purified and dried using standard procedures. All reactions were carried out under an inert atmosphere in oven-dried Schlenk tubes with magnetic stirring using freshly distilled solvents. Analytical thin layer chromatography (TLC) plates were purchased from EM Science (silica gel 60 F254 plates). All NMR spectra were recorded on a Bruker spectrometer at 400 or 500 MHz ($^{1}$H NMR), 101 or 126 MHz ($^{13}$C NMR) and 376 or 471 MHz ($^{19}$F NMR). Chemical shifts (δ value) were reported in ppm with the solvent signals as reference (in $CDCl_3$ as solvent) and coupling constants (*J*) are given in Hertz (Hz). The peak information was described as: br = broad singlet, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, comp = composite of magnetically non-equivalent protons, down field from internal tetramethylsilane (TMS). Syringe pump was purchased from Longerpump. Needle filters were purchased from Anpel. Single-crystal X-ray diffraction data (**21** & **S28**) were collected in a Rikagu XtaLAB Synergy. The optical rotation data were collected in a Anton Paar MCP 100/150. HRMS (ESI) Mass Spectra were recorded on SHIMADZU LCMS-IT-TOF mass spectrometer. Liquid chromatography–mass spectrometry (LC-MS) was recorded on WATERS ACQUITY UPLC. HPLC analysis was performed on WATERS e2695. NMR tube experiments were handled by Demen Ultrasonic cleaning machine JP-040S.

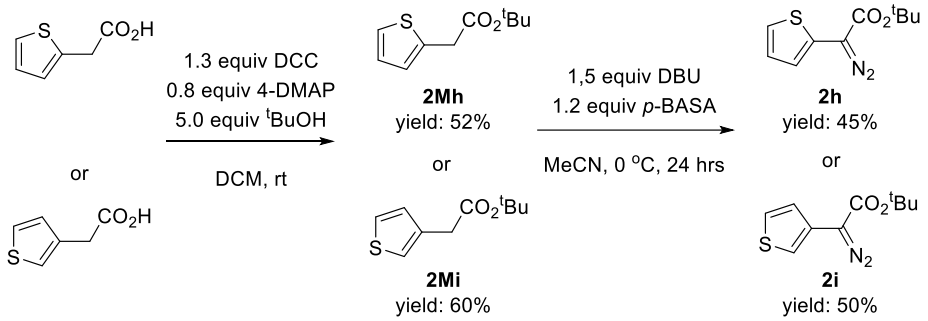
**Materials.** Alcohol **1**(except cinnamyl alcohol and alkynol), arylacetic acids, indole **3A-3G**, aldehyde **4,** amine **5** and all dry solvents except toluene (99.9%, Extra Dry, with molecular sieves, Water ≤ 50 ppm (by K.F.), EnergySeal) were purchased from Energy Chemical. All catalysts including JohnphosAu(MeCN)$SbF_6$, $[PdCl(2\text{-butenyl})]_2$ and $Rh_2(TFA)_4$ were purchased from Laajoo. $Cu(MeCN)_4PF_6$, CuOTf, $[PdCl(allyl)]_2$, $Rh_2(Oct)_4$, $[PdCl(cinnyl)]_2$, $[Ir(COD)Cl]_2$, Cp*Ru(COD)Cl were purchased from

Energy Chemical. $Rh_2(OAc)_4$, $Rh_2(esp)_2$ were purchased from Sigma-Aldrich. enamine **3**,[1] chiral BINOL phosphoric acids **S6b-S6e**, **S6h-S6j**, **6b**, **6c** were prepared according to the literature procedures.[3] $[PdOAc(allyl)]_2$,[2] $[PdTFA(allyl)]_2$,[2] chiral BINOL phosphoric acid **S6a**, chiral SPINOL phosphoric acids (*S*)-**S6f-S6g, S6k, 6a** were purchased from Daicel Chiral Technologies (China) Co., LTD, diazo compounds,[4-5] cinnamyl alcohol,[6] alkynol,[7] arylpropiolaldehyde,[8] olefine aldehyde[9], indole **3H-3I**[10-11] were prepared according to the literature procedures. Anhydrous toluene was distilled from Na under an atmosphere of argon. All other chemicals were obtained from commercial sources and used as received without further purification.

## 2. Experimental Procedures

### 2.1 Preparation of diazo compounds 2h-2i.

Aryldiazoacetates **2a-2g**[4] were prepared according to the literature procedures. Alkyldiazoacetates **2j-2l**[5] were prepared according to the literature procedures. **2h** and **2i** were synthesized via the same literature procedure as follow.[12]



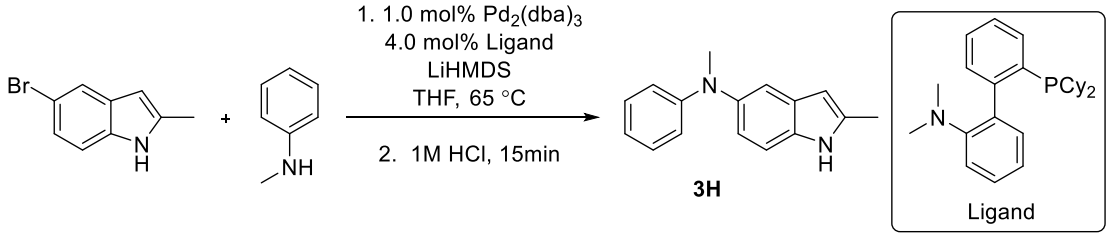

To a flame-dried 250-mL flask charged with a magnetic stirring bar, 2-(thiophen-2-yl)acetic acid or 2-(thiophen-3-yl)acetic acid (2.84 g, 20.0 mmol, 1.0 equiv.), tert-butanol (7.41 g, 100.0 mmol, 5.0 equiv.) and 4-DMAP (1.7 g, 14.0 mmol, 0.7 equiv.) in 50 mL dichloromethane at 0 °C was added DCC (5.36 g, 26.0 mmol, 1.3 equiv.) slowly. The resulting mixture was warmed up slowly to room temperature and stirred overnight. The solid was filtered off and washed with hexanes. The filtrate was

concentrated in vacuo and products were purified by column chromatography (eluent: PE/EA = 50:1 ~ 30:1, v/v) to afford the pure product **2Mh** (2.06 g, 52% yield) or **2Mi** (2.38 g, 60% yield).

To a flame-dried 50-mL Schlenk flask charged with a magnetic stirring bar, *p*-ABSA (3.12 g, 13.0 mmol, 1.3 equiv.), **2Mh** or **2Mi** (1.98g, 10.0 mmol, 1.0 equiv.) in 8.0 mL MeCN were sequentially added at 0 °C. DBU (1.83 g, 12.0 mmol, 1.5 equiv.) dissolved in MeCN (2.0 mL) were added over 10.0 mins. The resulting mixture was warmed up slowly to room temperature and stirred overnight. The reaction solution was slowly added saturated $NH_4Cl$(aq) before extracted with diethyl ether (15 x 3 mL). The organic layers were washed with brine. After drying over $MgSO_4$ and concentration in vacuo, the crude product was purified by flash chromatography on silica gel (eluent: PE/EA = 20:1, v/v) to afford the pure product **2h** (1.01 g, 45% yield) or **2i** (1.12 g, 50% yield).

**2.2 Preparation of indole compounds 3H-3I.**

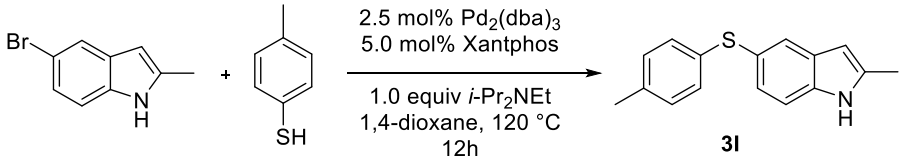
**1) Procedure for Synthesis of 3H**




$Pd_2(dba)_3$ (45.8 mg, 0.05 mmol), 2- dicyclohexylphosphino-2′-(N,N-dimethylamino)biphenyl (78.7 mg, 0.2 mmol) and 5-bromo-2-methyl-1*H*-indole (1.04 g, 5.0 mmol) were added to an oven dried vacuum schlenk tube under argon. The solids were dissolved in THF (5.0 mL). Lithium bis(trimethylsilyl)amide 1.0 M solution in THF (11.0 mL, 11.0 mmol) and the corresponding amine (6.0 mmol) were added to the solution. The reaction mixture was heated during 24 h at 65 °C. After reaction go to

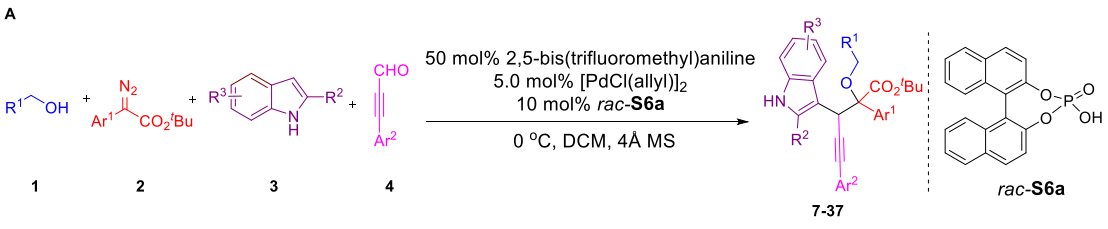
complete (monitored by TLC), the system was cooled to room temperature and 1 M HCl (10.0 mL) was added to the reaction and the mixture was stirred for 15 min. The reaction crude was poured into a separatory funnel and diluted with saturated $NaHCO_3$ (20 mL). The aqueous phase was extracted with ethyl acetate (3 x 20 mL). The combined organic extracts were washed with brine (50 mL), dried over $Na_2SO_4$ and the solvent was removed under vacuum. The residue was purified by column chromatography (Petroleum Ether: EtOAc = 40: 1) to give N,2-dimethyl-N-phenyl-1*H*-indol-5-amine **3H** (885.5 mg, 75% yield) as brown solid.

## 2) Procedure for Synthesis of 3I

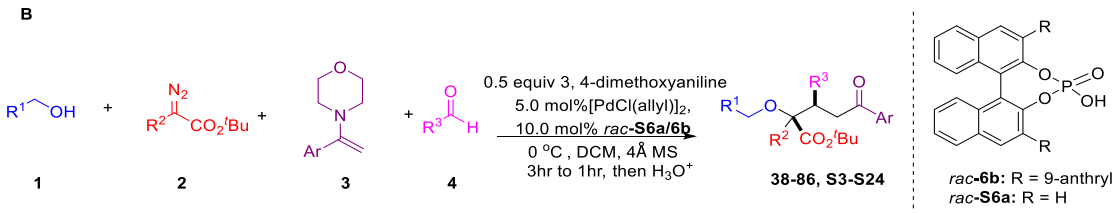



5-Bromo-2-methyl-1H-indole (1.04 g, 5.0 mmol), 4-methylbenzenethiol (682.2 mg, 5.5 mmol), $Pd_2(dba)_3$ (114.5 mg, 0.125 mmol), Xantphos (289.3 mg, 0.25 mmol), *i*-Pr2NEt (646.2 mg, 5.0 mmol) were dissolved in 1,4-dioxane (20.0 mL), the mixture was stirred at 120 °C for 12 hrs. After reaction go to complete (monitored by TLC), the solution was cooled to room temperature, the mixture was filtered through a plug of silica/sand/celite. The residue was purified by silica-gel column chromatography (Petroleum Ether: EtOAc = 60: 1) to give 2-methyl-5-(p-tolylthio)-1H-indole **3I** (911.1 mg, 72% yield) as yellow solid.

## 2.3 General Procedure for Racemic Four-component Reactions



To a flame-dried 10-mL Schlenk flask charged with a magnetic stirring bar, alcohol **1** (0.15 mmol), aldehyde **4** (0.15 mmol), 2,5-bis(trifluoromethyl)aniline **5a** (50 mol%), $[PdCl(allyl)]_2$ (5 mol%), *rac*-**S6a** (10 mol%) and 4Å MS (70 mg) in DCM (1.0 mL), was added a mixture of diazoacetate **2** (0.075 mmol) and indole **3** (0.05 mmol) in DCM (1.0 mL) for 1.0 h via a syringe pump at 0 °C. The mixture was stirred for additional 6 hrs under these conditions. After the completion of the reaction, the reaction mixture was filtrated and the filtrate was evaporated in vacuo to give the crude product. And then the crude product was purified by flash chromatography on silica gel (eluent: PE: EA = 20 : 1) to afford the pure products.




To a flame-dried 10-mL Schlenk flask charged with a magnetic stirring bar, 3,4-dimethoxyaniline **5b** (0.10 mmol), 5.0 mol% $[PdCl(allyl)]_2$, 10.0 mol% *rac*-**S6a** or *rac*-**6b**, alcohol **1**(0.24 mmol), aldehyde **4** (0.20 mmol) and 100 mg 4 Å MS in 2.0 mL DCM were sequentially added at 0 °C. Diazoacetate **2** (0.24 mmol) and enamine **3**(0.24 mmol) dissolved in DCM (1.0 mL) were added by syringe pump over 180 mins. The mixture was stirred for 1.0 hr at 0 °C. After the completion of the reaction, the reaction mixture was filtrated and the filtrate was evaporated in vacuo to give the crude product. And then the crude product was purified by flash chromatography on silica gel (eluent: PE/EA = 50:1 ~ 30:1, v/v) to give the mixed products containing *anti*-product and *syn*-product or *syn*-product.

## 2.4 General Procedure and Substrate Scope of Enantioselective Four-component Reactions of Alcohol, Diazoester, Indole/Enamine and Aldehyde Derivatives

## Procedure A under the condition A

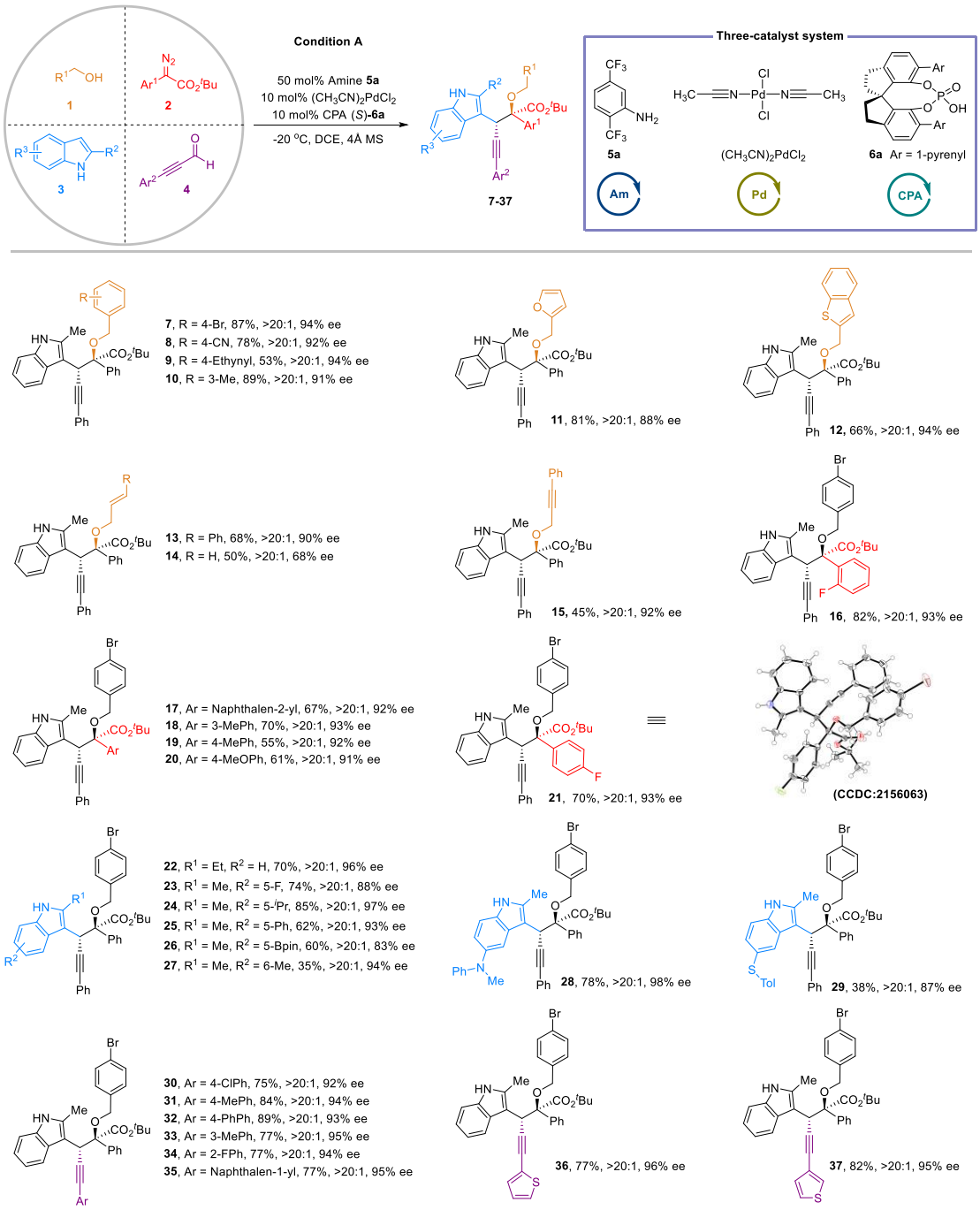



**Figure S1. Substrate scope of enantioselective four-component reactions of alcohol, diazoester, indole and aldehyde derivatives.**

To a flame-dried 10-mL Schlenk flask charged with a magnetic stirring bar, alcohol **1** (0.6 mmol), aldehyde **4** (0.6 mmol), 2,5-bis(trifluoromethyl)aniline **5a** (50 mol%), Pd $(CH_3CN)_2Cl_2$ (10 mol%), (*S*)-**6a** (10 mol%) and 4Å MS (100 mg) in DCE (4.0 mL),

was added a mixture of diazoacetate **2** (0.3 mmol) and indole **3** (0.2mmol) in DCE (4.0 mL) for 1.0 h via a syringe pump at -20 °C. The mixture was stirred for additional 12 hrs under these conditions. After the completion of the reaction, the reaction mixture was filtrated and the filtrate was evaporated in vacuo to give the crude product. And then the crude product was purified by flash chromatography on silica gel (eluent: PE: EA = 20 : 1) to afford the pure products.

## Procedure B under the condition B

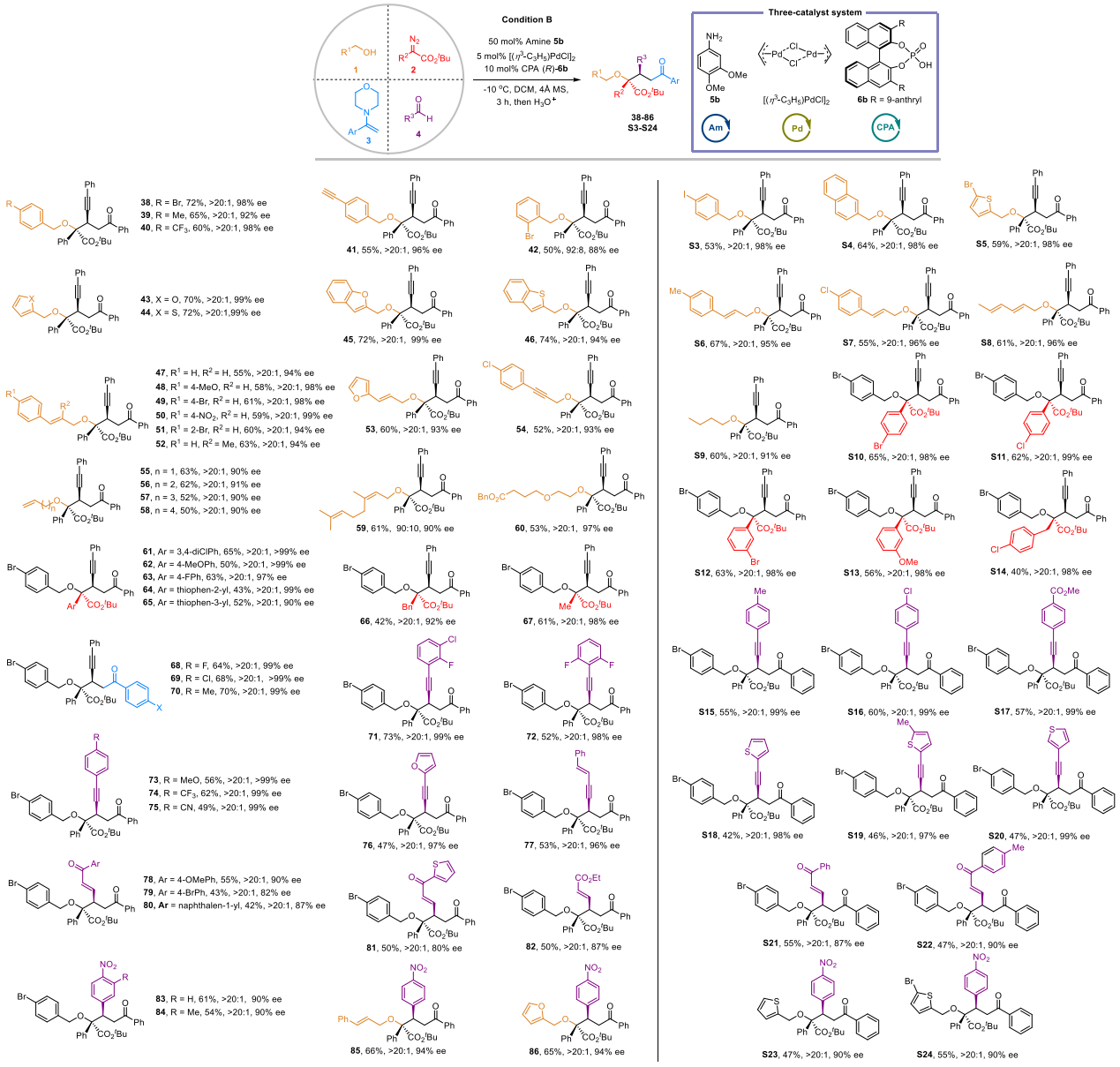


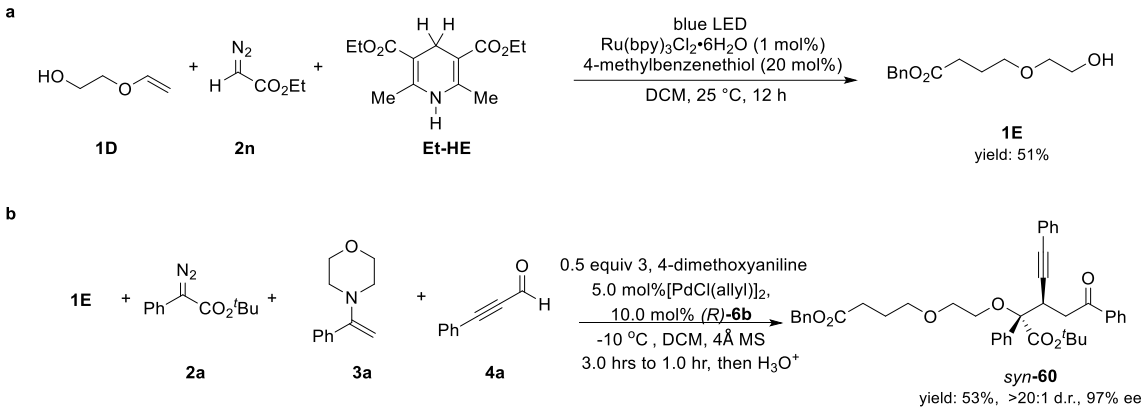

**Figure S2. Substrate scope of enantioselective four-component reactions of alcohol, diazoester, enamine and**

**aldehyde derivatives.**

To a flame-dried 10-mL Schlenk flask charged with a magnetic stirring bar, 3,4-dimethoxyaniline **5b** (0.075 mmol), 5.0 mol% $[PdCl(allyl)]_2$, 10.0 mol% *(R)*-**6b**, alcohol **1**(0.18 mmol), aldehyde **4** (0.15 mmol) and 100 mg 4 Å MS in 2 mL DCM were sequentially added at -10 °C. Diazoacetate **2** (0.18 mmol) and enamine **3** (0.18 mmol) dissolved in DCM (1.5 mL) were added by syringe pump over 180 mins. The mixture was stirred for 1.0 hr at -10 °C. After the completion of the reaction, the reaction mixture was filtrated and the filtrate was evaporated in vacuo to give the crude product. And then the crude product was purified by flash chromatography on silica gel (eluent: PE/EA = 50:1 ~ 30:1, v/v) to give the pure product (If the reaction was carried out on more than 0.15 mmol scale, the decreased ee value of corresponding product might be detected).

## 2.5 Procedure for Synthesis of 60. [13]

***Stepwise Synthesis***



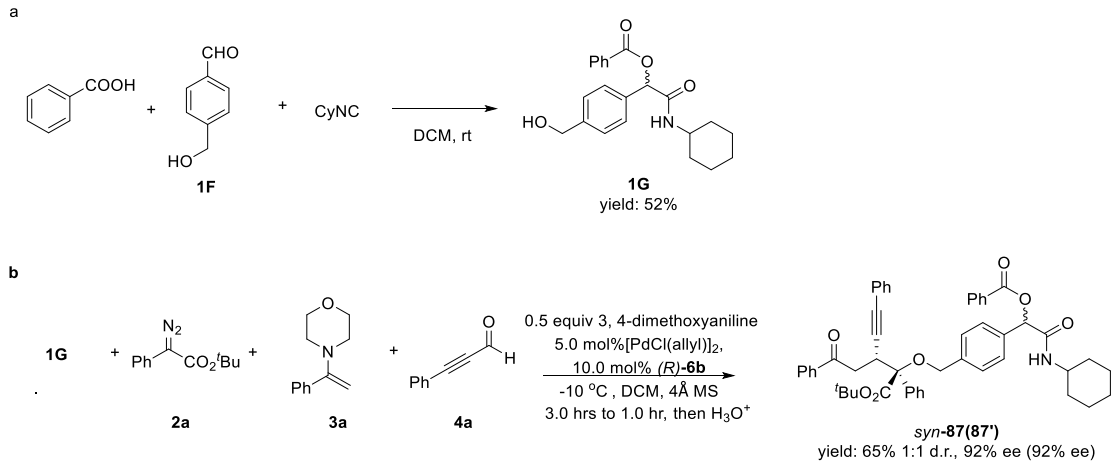

To a 10-ml glass tube equipped with a magnetic stir bar were added **Et-HE** (202.4 mg, 0.8 mmol, 2.0 equiv.), $Ru(bpy)_3Cl_2•6H_2O$ (3.0 mg, 0.004 mmol, 1.0 mol%), and 4-methylbenzenethiol (10.0 mg, 0.08 mmol, 20.0 mol%). The tube was capped. After evacuation and backfilling with argon three times, anhydrous DCM (2.0 mL, 0.2 M) was added via a syringe, followed by the addition of **1D** (0.4 mmol, 1.0 equiv.), and **2n** (0.8 mmol, 2.0 equiv.). The resulting solution was irradiated by a 50 W blue LED with

stirring at a distance of ~15 cm (with cooling by the fan) at 25°C for about 12 h until the diazo compound was consumed completely, as monitored by TLC analysis. The reaction mixture was filtered, and the filtrate were concentrated, the crude product was purified by flash chromatography on silica gel (eluent: PE/EA = 5:1 ~ 2:1, v/v) to afford the pure product **1E (**48.6 mg, 51% yield, colorless oil).

The procedure of reaction **b** refers to Section **2.3** (The reaction was carried out on 0.05 mmol scale). Product **60** (53% yield, 17.5 mg, >20:1 d.r., 97% ee, Colorless oil).

## 2.6 Procedure for Synthesis of 87.

***Stepwise Synthesis***

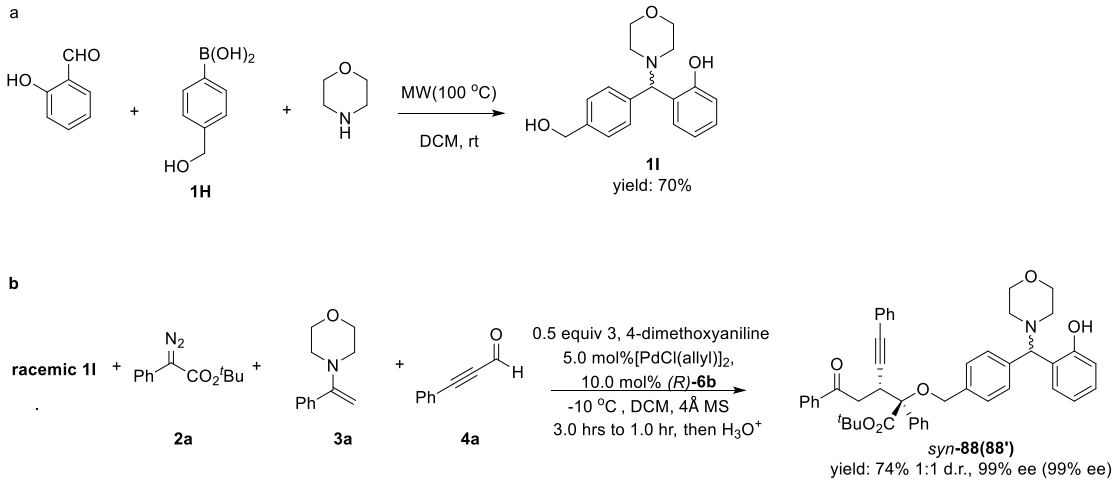



To a flame-dried 25-mL Schlenk flask charged with a magnetic stirring bar, acid (550 mg, 4.5 mmol, 1.5 equiv.), aldehyde **1F** (408.5 mg, 3.0 mmol, 1.0 equiv.), isocyanide (982.6 mg, 9.0 mmol, 3.0 equiv.) in 10 mL DCM. The mixture was stirred at room temperature for overnight. The mixture was concentrated, the crude product was purified by flash chromatography on silica gel (eluent: PE/EA = 5:1 ~ 2:1, v/v) to afford the pure product **1G (**573.2 mg, 52% yield, white solid).

The procedure of reaction **b** refers to Section **2.3** (The reaction was carried out on 0.05 mmol scale). Product **87** (total 65% yield, 25.6 mg, 1:1 d.r., 92% ee, 92% ee, white solid).

## 2.7 Procedure for Synthesis of 88. [14]

***Stepwise Synthesis***



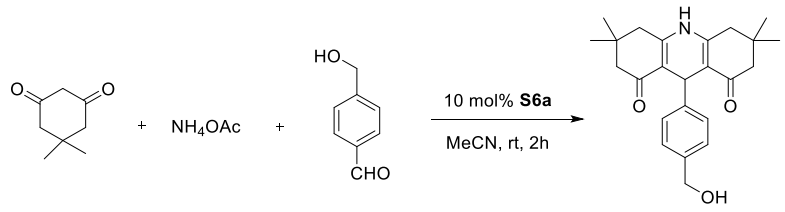

Aldehyde (122.1 mg, 1.0 mmol, 1.0 equiv.), morpholine (87.1 mg, 1 mmol, 1.0 equiv.) and boronic acid **1H** (152.0 mg, 1.0 mmol, 1.0 equiv.) were mixed in a 10 mL microwave vial and heated to 100 ºC with microwave irradiation for 1 hr. The crude product was purified by flash chromatography on silica gel (eluent: PE/EA = 3:1 ~ 1:1, v/v) to afford the pure product **1I (**209.6 mg, 70% yield, colorless oil).

The procedure of reaction **b** refers to Section **2.3** (The reaction was carried out on 0.05 mmol scale). Product **88** (total 74% yield, 26.7 mg, 1:1 d.r., 99% ee, 99% ee, white solid).

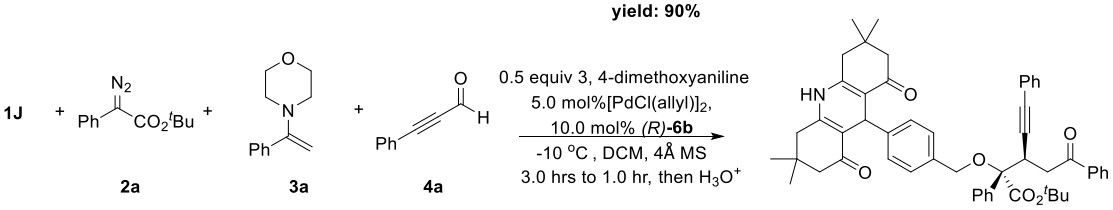
## 2.8 Procedure for Synthesis of 89. [15]

***Stepwise Synthesis***

a




b

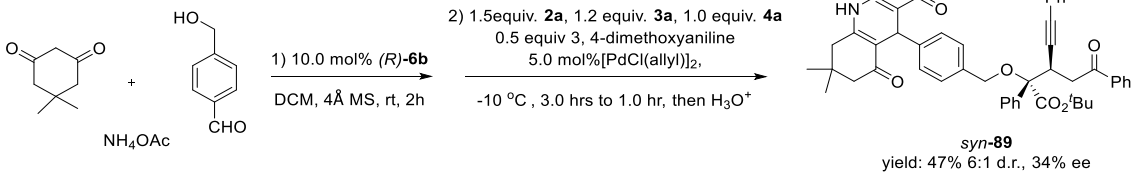



*syn*-**89**
yield: 64% 10:1 d.r., 96% ee

To a flame-dried 10-mL Schlenk flask charged with a magnetic stirring bar, aldehyde (27.2 mg, 0.2 mmol, 1.0 equiv.), dimedone (61.7 mg, 0.44mmol, 2.2 equiv.), $NH_4OAc$ (15.4 mg, 0.2 mmol, 1.0 equiv.), and 10 mol% racemic **S6a** were dissolved in 3.0 mL MeCN. The mixture was stirred for 2.0 hrs at room temperature. The mixture was concentrated, the crude product was purified by flash chromatography on silica gel (eluent: PE/EA = 5:1 ~ 2:1, v/v) to afford the pure product **1J (**68.2 mg, 90% yield, colorless oil).

The procedure of reaction **b** refers to Section **2.3** (The reaction was carried out on 0.05 mmol scale). Product **89** (64% yield, 25.6 mg, 10:1 d.r., 96% ee, white solid).

***One-pot Cascade Synthesis***

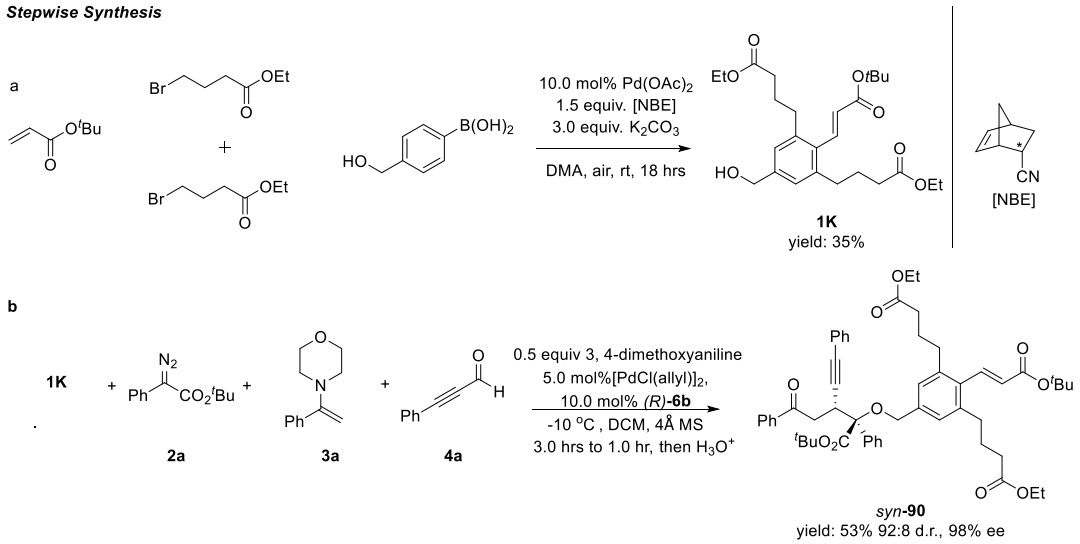



*syn*-**89**
yield: 47% 6:1 d.r., 34% ee

To a flame-dried 10-mL Schlenk flask charged with a magnetic stirring bar, aldehyde (0.05 mmol, 1.0 equiv.), dimedone (0.11mmol, 2.2 equiv.), $NH_4OAc$ (0.05 mmol, 1.0 equiv.), 10 mol% **6b**, and 100 mg 4 Å MS were dissolved in 1.0 mL DCM. The mixture

was stirred for 2.0 hrs at room temperature. Then 3, 4-dimethoxyaniline **5b** (0.025 mmol, 0.5 equiv.), 5.0 mol% $[PdCl(allyl)]_2$, aldehyde **4a** (0.05 mmol, 1.0 equiv.) were sequentially added at -10 °C. Diazoacetate **2a** (0.75 mmol) and enamine **3a** (0.06 mmol, 1.2 equiv.) dissolved in DCM (0.5 mL) were added by syringe pump over 180 mins. The mixture was stirred for 1.0 hr at -10 °C. After the completion of the reaction, the reaction mixture was filtrated and the filtrate was evaporated in vacuo to give the crude product. And then the crude product was purified by flash chromatography on silica gel (eluent: PE/EA = 10:1 ~ 5:1, v/v) to give the pure product **89**.

## 2.9 Procedure for Synthesis of 90.[16]



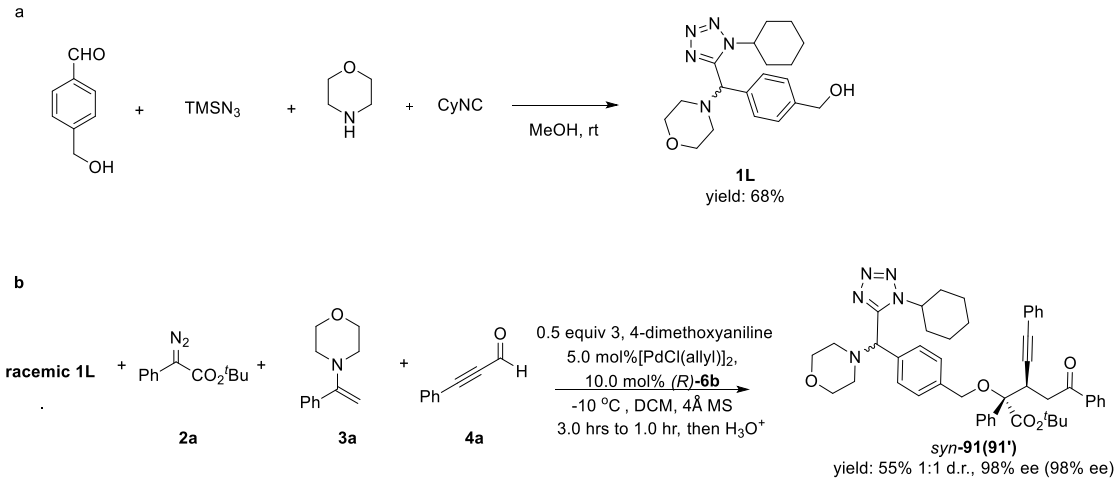

To a flame-dried 10-mL Schlenk flask charged with a magnetic stirring bar, aryl boron (1.5 mmol, 228mg, 1.5 equiv.), $Pd(OAc)_2$ (23 mg, 0.10 mmol, 0.1 equiv.), $K_2CO_3$ (414 mg, 3.0 mmol, 3.0 equiv.) alkyl bromide (466 mg, 1.2 mmol, 1.2 equiv.), olefin (141 mg, 1.0 mmol, 1.0 equiv.), 5-norbornene-2-carbonitrile (179 mg, 1.5 mmol, 1.5 equiv.) and DMA (1 mL) under air. The reaction was stirred at room temperature for 18 hrs. Then the mixture was filtered through a thin pad of celite eluting with ethyl acetate (30 mL), and the filtrate was sequentially washed with water, brine, dried over $Na_2SO_4$. After concentrated *in vacuo*, the crude product was purified by flash chromatography

on silica gel (eluent: PE/EA = 10:1 ~ 5:1, v/v) to afford the pure product **1K (**161.7 mg, 35% yield).

The procedure of reaction **b** refers to Section **2.3** (The reaction was carried out on 0.05 mmol scale). Product **90** (53% yield, 23.5 mg, 92:8 d.r., 98% ee, colorless oil).

## 2.10 Procedure for Synthesis of 91. [17]

***Stepwise Synthesis***

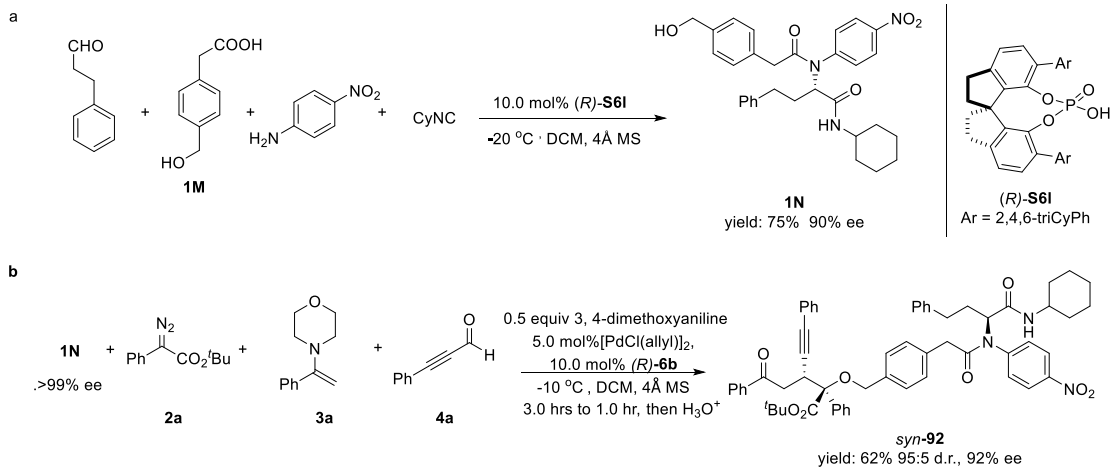



To a flame-dried 25-mL Schlenk flask charged with a magnetic stirring bar, morpholine (261.4 mg, 3.0 mmol, 1.0 equiv.), aldehyde (408.5 mg, 3.0 mmol, 1.0 equiv.) in 6 mL MeOH, the resulting solution was stirred for 15 mins at room temperature and then a solution of isocyanide (327.5 mg, 3.0 mmol, 1.0 equiv.), and $TMSN_3$ (345.6 mg, 3.0 mmol, 1.0 equiv.) in MeOH (2.0 mL) was added to the mixture in one portion. The mixture was stirred at room temperature for overnight. The mixture was concentrated, the crude product was purified by flash chromatography on silica gel (eluent: PE/EA = 5:1 ~ 2:1, v/v) to afford the pure product **1L (**243 mg, 68% yield, colorless oil).

The procedure of reaction **b** refers to Section **2.3** (The reaction was carried out on 0.05 mmol scale). Product **91** (total 55% yield, 21.4 mg, 1:1 d.r., 98% ee, 98% ee, white solid).

## 2.11 Procedure for Synthesis of 92. [18]

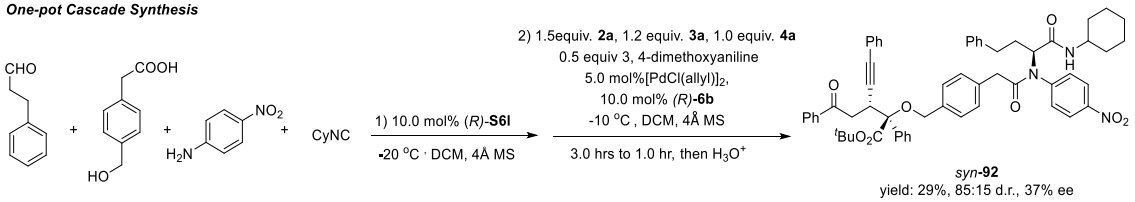
***Stepwise Synthesis***




To a flame-dried 10-mL Schlenk flask charged with a magnetic stirring bar, amine (18.0 mg, 0.13 mmol, 1.3 equiv.), acid (16.6 mg, 0.1 mmol, 1.0 equiv.), 10.0 mol% (*R*)-**S6l**, and dry DCM (1.0 mL) under argon. The resulting solution was stirred for 15 mins at -20 °C and then a solution of aldehyde (17.4 mg, 0.13 mmol, 1.3 equiv.) in DCM (0.5 mL) was added to the mixture in one portion. After 15 mins, a solution of isocyanide (14.1 mg, 0.13 mmol) in DCM (0.5 mL) was added to the mixture in one portion. Then the mixture was stirred at -20 °C for 12 hrs. The mixture was concentrated, the crude product was purified by flash chromatography on silica gel (eluent: PE/EA = 5:1 ~ 2:1, v/v) to afford the pure product **1N (**39.7 mg, 75% yield, 90% ee, yellow solid).

The procedure of reaction **b** refers to Section **2.3** (The reaction was carried out on 0.05 mmol scale). Product **92** (62% yield, 29.5 mg, 95:5 d.r., 92% ee, yellow solid).

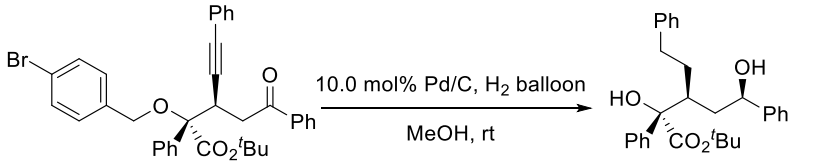
***One-pot Cascade Synthesis***




To a flame-dried 10-mL Schlenk flask charged with a magnetic stirring bar, amine

(0.065 mmol, 1.3 equiv.), acid (0.05 mmol, 1.0 equiv.), 10.0 mol% (*R*)-**S6l**, and dry DCM (1.0 mL) under argon. The resulting solution was stirred for 15 mins at -20 °C and then a solution of aldehyde (0.065 mmol) in DCM (0.5 mL) was added to the mixture in one portion. After 15 mins, a solution of isocyanide (0.065 mmol) in DCM (0.5 mL) was added to the mixture in one portion. Then the mixture was stirred at -20 °C for 12 hrs. Then 3, 4-dimethoxyaniline **5b** (0.025 mmol, 0.5 equiv.), 5.0 mol% $[PdCl(allyl)]_2$, 10.0 mol% **6b**, aldehyde **4a** (0.05 mmol, 1.0 equiv.) were sequentially added at -10 °C. Diazoacetate **2a** (0.075 mmol) and enamine **3a** (0.06 mmol, 1.2 equiv.) dissolved in DCM (0.5 mL) were added by syringe pump over 180 mins. The mixture was stirred for 1.0 hr at -10 °C. After the completion of the reaction, the reaction mixture was filtrated and the filtrate was evaporated in vacuo to give the crude product. And then the crude product was purified by flash chromatography on silica gel (eluent: PE/EA = 10:1 ~ 5:1, v/v) to give the pure product **92**.

**2.12 Procedure for Synthesis of 93 from 38.**




**38**
>20:1 d.r., 94 % ee

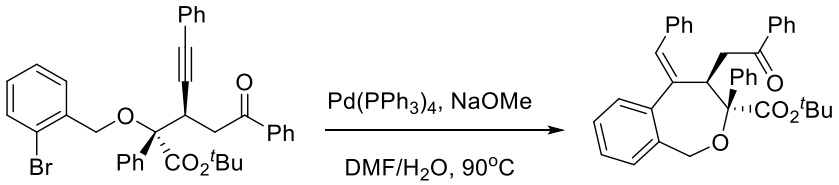
**93**
>20:1 d.r., 92% ee

The half a gram-scale synthesis of product **38** refer to Section **2.3** (The reaction was carried out on 2.0 mmol scale). Product **38** (60% yield, 731.5 mg, >20:1 d.r., 94% ee, Colorless oil).

To a flame-dried 10-mL Schlenk flask charged with a magnetic stirring bar, **38** (60.8 mg, 0.10mmol), Pd/C (1.1 mg, 10.0 mol%) in 4.0mL MeOH were sequentially added and stirred for overnight with a hydrogen-filled balloon. The reaction mixture the

reaction mixture was filtered, and the filtrate were concentrated, the crude product was purified by flash chromatography on silica gel (eluent: PE/EA = 30:1 ~ 10:1, v/v) to afford the pure product **93 (**38.4 mg, 86% yield, >20:1 d.r., 92% ee, colorless oil).

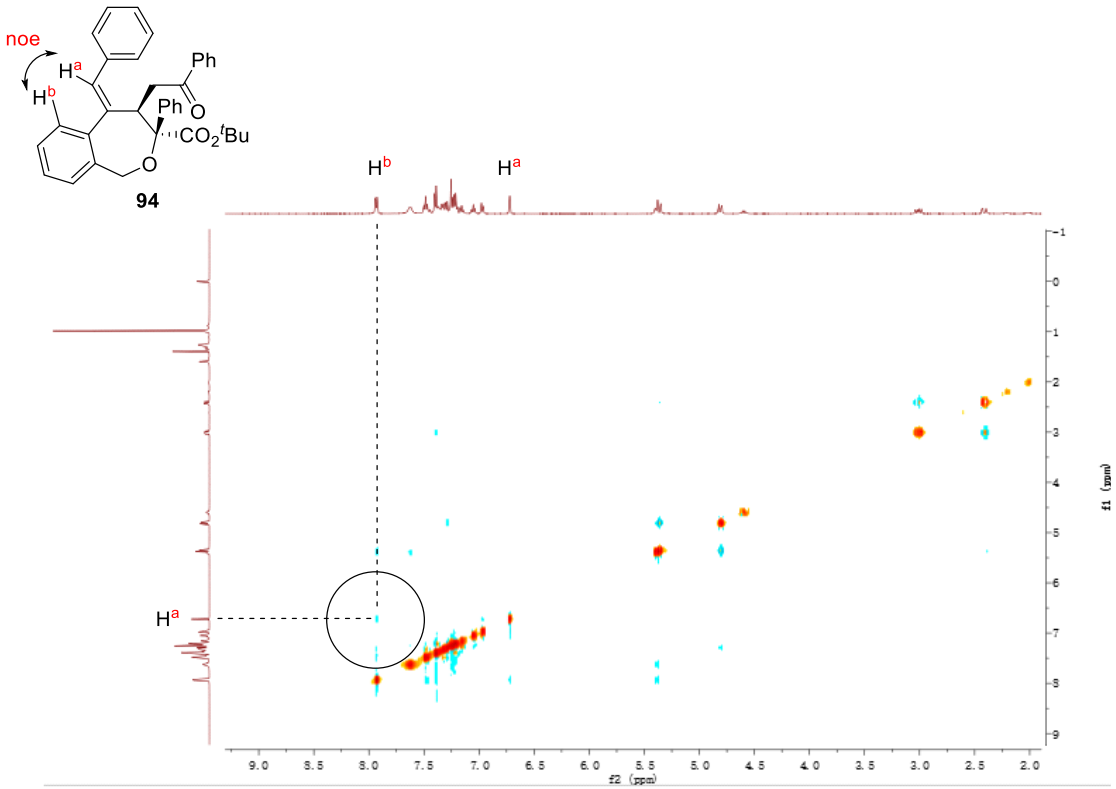
**2.13 Procedure for Synthesis of 94 from 42.** [19]



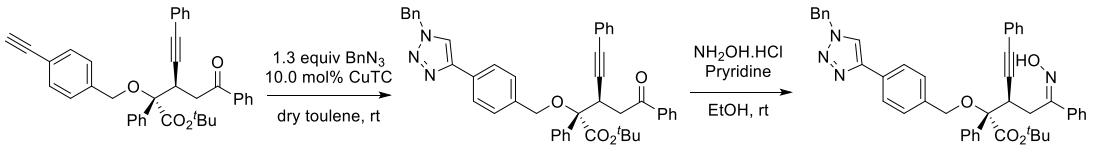

**42**
92:8 d.r., 88 % ee

**94**
92:8 d.r., 88% ee

To a flame-dried 10-mL Schlenk flask charged with a magnetic stirring bar, **42** (61.0 mg, 0.1 mmol, 1.0 equiv.), 0.5 mol% $Pd(PPh_3)_4$ (5.8 mg), NaOMe (16.2 mg, 0.3 mmol, 3.0 equiv.) in 5.0 mL DMF and $H_2O$ ($v_{DMF}$ : $v_{H2O}$ =7:1) under argon, and the flask was heated to 90 °C under argon for 4.0 hrs. The mixture was extracted with ethyl acetate and the combined organic layers were washed with 2N HCl (× 3) and brine, dried with $Na_2SO_4$, the mixture was then cooled down and partitioned by $CH_2Cl_2$ and water, and the aqueous layer was extracted with $CH_2Cl_2$ (4.0 mL x 3). The organic layers were combined together and dried over $Na_2SO_4$. After filtration, the solvent was removed under vacuum, the crude product was purified by by flash chromatography on silica gel (eluent: PE/EA = 2:1 ~ 10:1, v/v) to afford the product **94 (**38.2 mg, 75% yield, 92:8 d.r., 88% ee, colorless oil).




## 2.14 Procedure for Synthesis of S26, S28 from 41. [20]




**41**
>20:1 d.r., 96% ee

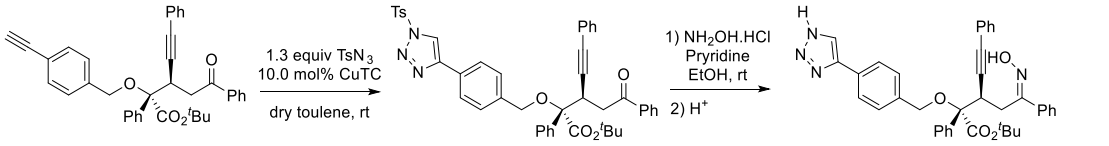
**S27**
yield: 88%, >20:1 d.r., 94% ee

**S28**
yield: 90%, >20:1 d.r., 94% ee

To a flame-dried 10-mL Schlenk flask charged with a magnetic stirring bar, 10.0 mol% CuTC, **41** (55.4 mg, 0.10 mmol) in 2.0 mL of dry toluene under a dinitrogen atmosphere was at room temperature. $BnN_3$ (17.3mg, 0.13 mmol) in dry toluene (1.0 mL) were introduced by syringe pump over 10.0 mins and the reaction solution was stirred for another 2.0 hr. The reaction was concentrated in vacuo, the crude product was purified by flash chromatography on silica gel (eluent: PE/EA = 10:1 ~ 5:1, v/v) to afford the pure product **S27** (60.4 mg, 88% yield, 10:1 d.r, >20:1 d.r., 94% ee, colorless oil).

To a flame-dried 10-mL Schlenk flask charged with a magnetic stirring bar, **S27** (34.4 mg, 0.05 mmol, 1.0 equiv.) in ethanol was added pyridine (15.8 mg, 0.2 mmol, 4.0

equiv.) and hydroxylamine hydrochloride (13.9 mg, 0.2 mmol, 4.0 equiv.) at room temperature. The mixture was stirred overnight. The mixture was extracted with ethyl acetate and the combined organic layers were washed with 2.0 N HCl (× 3) and brine, dried with $Na_2SO_4$, the reaction mixture the reaction mixture was filtered, and the filtrate were concentrated, the crude product was purified by flash chromatography on silica gel (eluent: PE/EA = 5:1 ~ 2:1, v/v) to afford the pure product **S28 (**31.6 mg, 90% yield, >20:1 d.r., 94% ee, white solid).




**41**
>20:1 d.r., 96% ee

**S25**
yield: 86%, >20:1 d.r., 94% ee

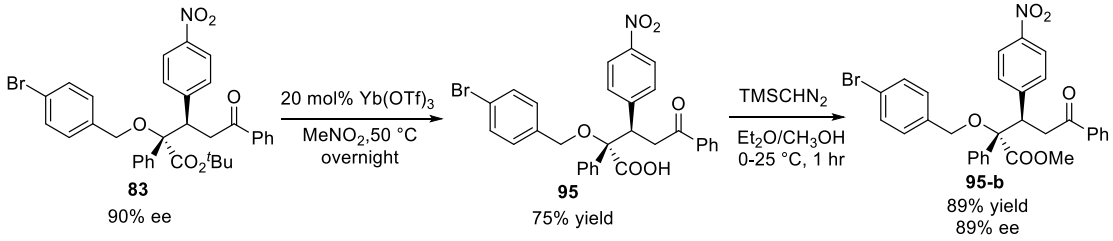
**S26**
yield: 75%, >20:1 d.r., 92% ee

To a flame-dried 10-mL Schlenk flask charged with a magnetic stirring bar, 10.0 mol% CuTC, **41** (55.4 mg, 0.10 mmol) in 2.0 mL of dry toluene under a dinitrogen atmosphere was at room temperature. $TsN_3$ (25.6 mg, 0.13 mmol) in dry toluene (1.0 mL) were introduced by syringe pump over 10.0 mins and the reaction solution was stirred for another 2.0 hr. The reaction was concentrated in vacuo, the crude product was purified by flash chromatography on silica gel (eluent: PE/EA = 10:1 ~ 5:1, v/v) to afford the pure product **S25** (64.6mg, 86% yield, 10:1 d.r, >20:1 d.r., 94% ee, colorless oil).

To a flame-dried 10-mL Schlenk flask charged with a magnetic stirring bar, **S25** (37.6 mg, 0.05 mmol, 1.0 equiv.) in ethanol was added pyridine (15.8 mg, 0.2 mmol, 4.0 equiv.) and hydroxylamine hydrochloride (13.9 mg, 0.2 mmol, 4.0 equiv.) at room temperature. The mixture was stirred overnight. The mixture was extracted with ethyl acetate and the combined organic layers were washed with 2.0 N HCl (× 3) and brine, dried with $Na_2SO_4$, The reaction mixture the reaction mixture was filtered, and the filtrate were concentrated, the crude product was purified by flash chromatography on

silica gel (eluent: PE/EA = 5:1 ~ 2:1, v/v) to afford the pure product **S26 (**23.0 mg, 75% yield, >20:1 d.r., 92% ee, white solid).

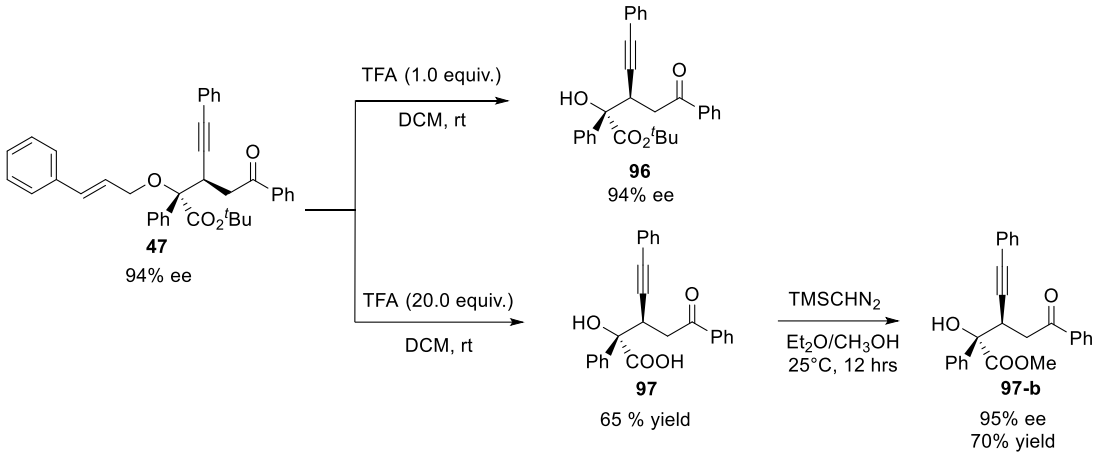
### 2.15 Procedure for Synthesis of 95 and 95-b.




To a flame-dried 10-mL Schlenk flask charged with a magnetic stirring bar, **83** (62.9 mg, 0.1 mmol, 1.0 equiv.), 20.0 mol% $Yb(OTf)_3$ in 3 mL $MeNO_2$. The mixture was stirred at 50 °C for overnight. The mixture was concentrated, the crude product was purified by flash chromatography on silica gel (eluent: PE/EA = 2:1 ~ 1:2, v/v) to afford the pure product **95 (**43.1 mg, 75% yield).

To a flame-dried 10-mL Schlenk flask charged with a magnetic stirring bar, **95** (57.44 mg, 0.10 mmol) in 1.0 mL $Et_2O$/MeOH (v : v=1:1) at room temperature. $TMSCHN_2$ (3.0 equiv.) was added to the reaction slowly for 5.0 mins. The reaction solution was stirred for 1 hr. The reaction solution was slowly added saturated $NaHCO_3$(aq) before extracted with EtOAc (5 x 3 mL). The organic layers were washed with brine. After drying over $MgSO_4$ and concentration in vacuo, the crude product was purified by flash chromatography on silica gel (eluent: DCM/MeOH = 40:1 ~ 20:1, v/v) to afford the pure product **95-b (**52.4 mg, 70% yield, 89% ee, colorless oil).

### 2.16 Procedure for Synthesis of 96, 97, and 97-b.




The half a gram-scale synthesis of product **47** refer to Section **2.3** (The reaction was carried out on 2.0 mmol scale). Product **47** (52% yield, 579.0 mg, >20:1 d.r., 94% ee, Colorless oil).

To a flame-dried 10-mL Schlenk flask charged with a magnetic stirring bar, **47** 55.6 mg (0.10 mmol) in 4.0 mL DCM at room temperature. TFA (1.0 equiv.) was added to the reaction slowly for 2.0 mins. The reaction solution was stirred for overnight. The reaction solution was slowly added saturated $NaHCO_3$(aq) before extracted with EtOAc (5 x 3 mL). The organic layers were washed with brine. After drying over $MgSO_4$ and concentration in vacuo, the crude product was purified by flash chromatography on silica gel (eluent: PE/EA = 30:1 ~ 10:1, v/v) to afford the pure product **96 (**26.4 mg, 60% yield, >20:1 d.r., 94% ee, colorless oil).

To a flame-dried 10-mL Schlenk flask charged with a magnetic stirring bar, **47** 55.6 mg (0.10 mmol) in 4.0 mL DCM at room temperature. TFA (20.0 equiv.) was added to the reaction slowly for 2.0 mins. The reaction solution was stirred for overnight. The reaction solution was slowly added saturated $NH_4Cl$(aq) before extracted with EtOAc (5 x 3 mL). The organic layers were washed with brine. After drying over $MgSO_4$ and concentration in vacuo, the crude product was purified by flash chromatography on

silica gel (eluent: PE/EA = 20:1 ~ 10:1, v/v) to afford the pure product **97 (**25.0 mg, 65% yield, >20:1 d.r., colorless oil).

To a flame-dried 10-mL Schlenk flask charged with a magnetic stirring bar, **97** 38.4 mg (0.10 mmol) in 1.0 mL $Et_2O$/MeOH (v : v=1:1) at room temperature. $TMSCHN_2$ (3.0 equiv.) was added to the reaction slowly for 5.0 mins. The reaction solution was stirred for 12 hrs. The reaction solution was slowly added saturated $NaHCO_3$(aq) before extracted with EtOAc (5 x 3 mL). The organic layers were washed with brine. After drying over $MgSO_4$ and concentration in vacuo, the crude product was purified by flash chromatography on silica gel (eluent: DCM/MeOH = 40:1 ~ 20:1, v/v) to afford the pure product **97-b (**27.9 mg, 70% yield, >20:1 d.r., 95% ee, colorless oil).

**2.17 Conclusion of 6CRs/7CRs design and synthetic applications.**

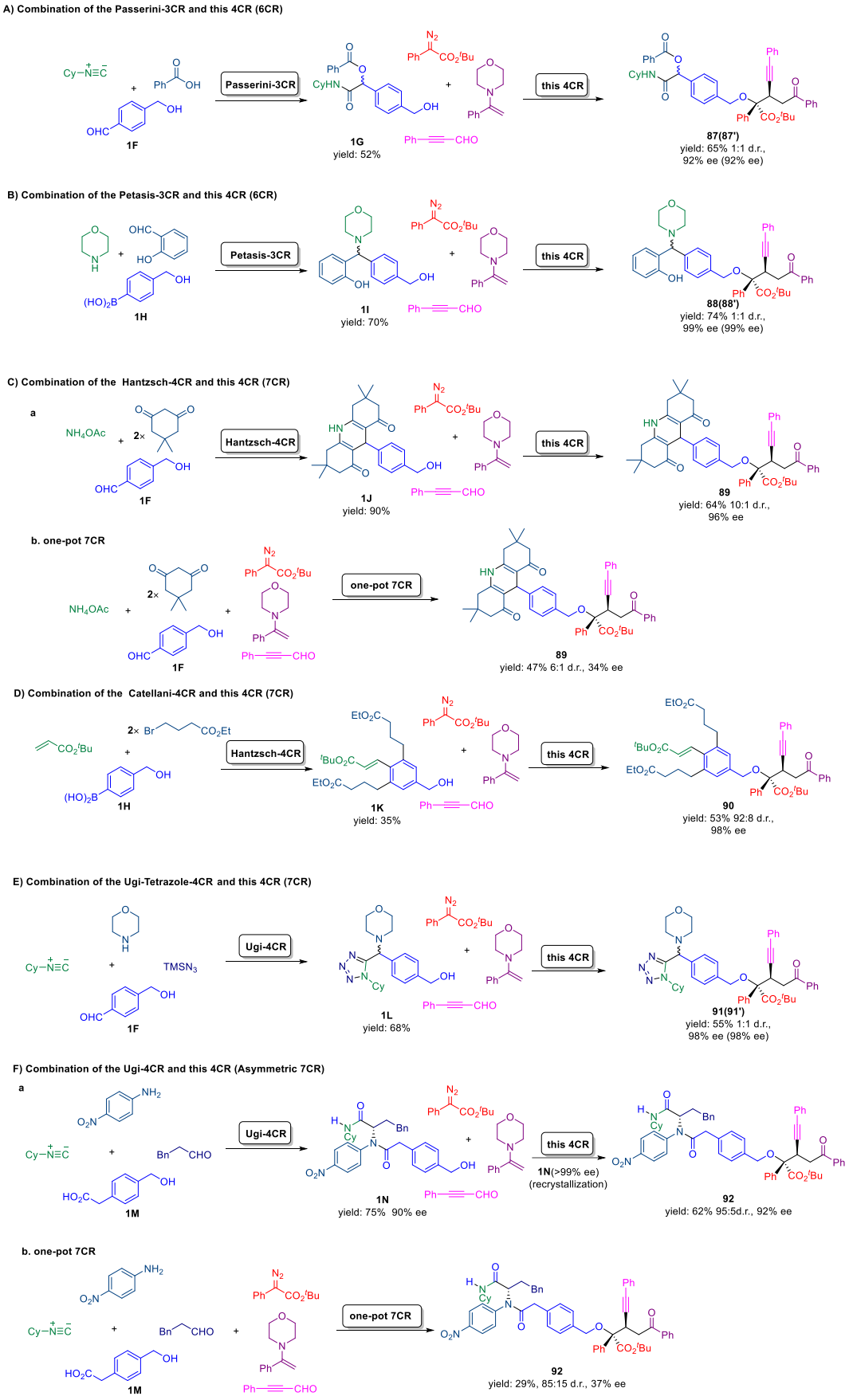



**Figure S3. Higher-order MCRs design**

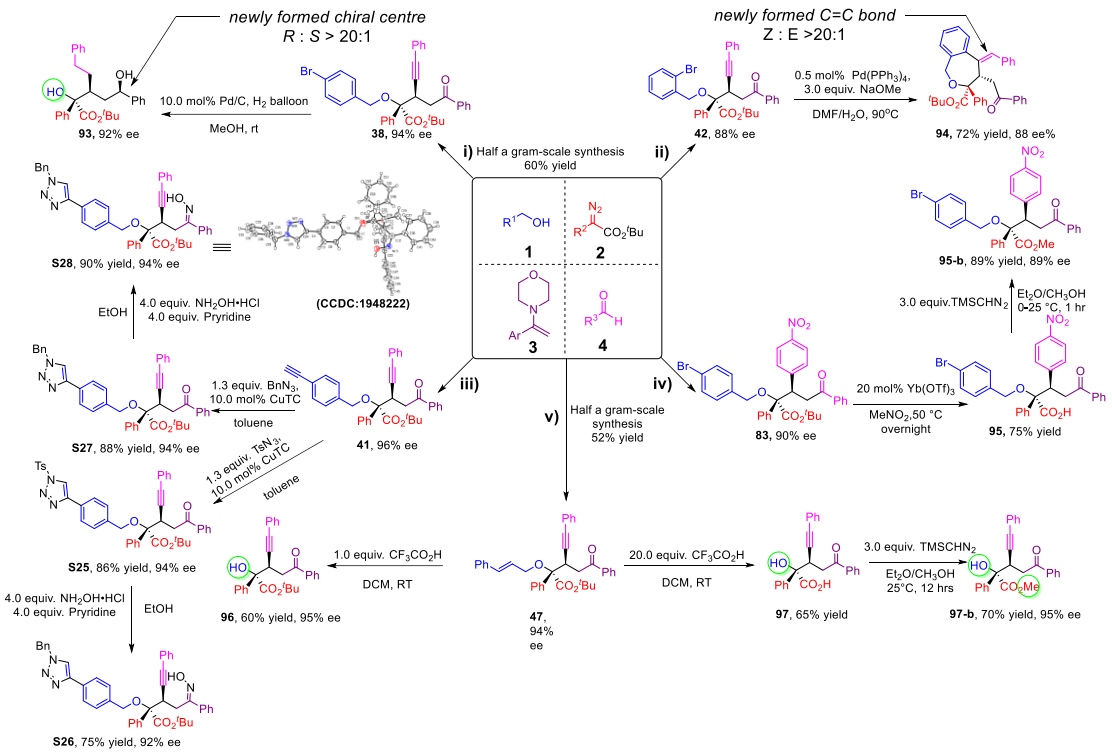
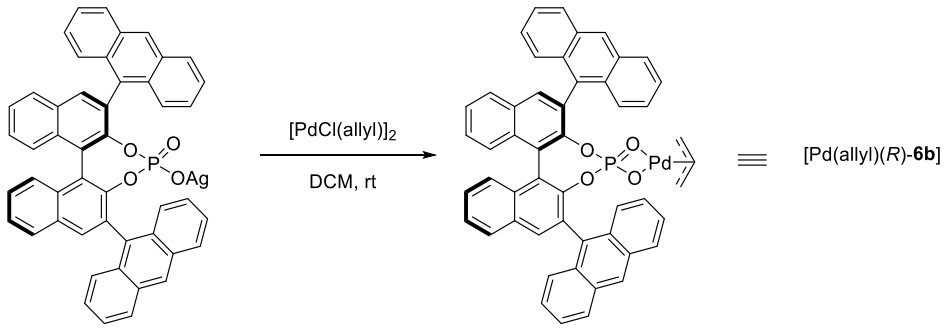



**Figure S4. Synthetic application.**

## 2.18 Preparation of [Pd(allyl)(*R*)-6b].[21]

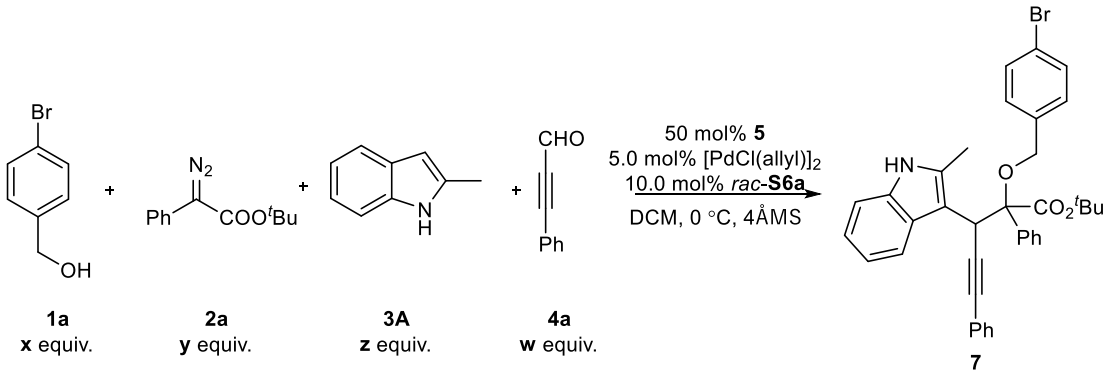
The silver salt of phosphate was were prepared according to the literature procedures.



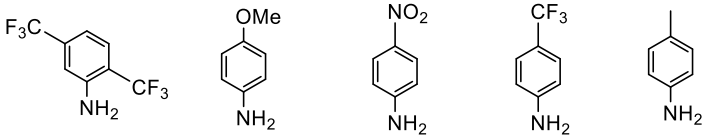

To a flame-dried 25-mL Schlenk flask charged with a magnetic stirring bar, silver phosphate (161.5 mg, 0.2 mmol, 1.0 equiv.) was dissolved in 5.0 mL DCM and then Schlenk flask was placed in dark. Subsequently $[PdCl(allyl)]_2$ (161.5 mg, 0.2 mmol, 1.0 equiv.) was added. The resulting mixture was stirred overnight at room temperature. The mixture was filtered and the filtrate was concentrated to give a fluffy yellowish powder [Pd(allyl)(*R*)-**6b**] (118.47 mg, 70% yield).

## 3. Table S1-S2 for Detailed Racemic Condition Optimizations

**Table S1 Condition Optimization of Racemic Four-component Reaction** [a]




**S5**




| Entry | **III-5** | **x** (equiv.) | **y** (equiv.) | **z** (equiv.) | **w** (equiv.) | dr[b] | Yield (%)[c] |
|---|---|---|---|---|---|---|---|
| 1 | **5a** | 1.2 | 1.5 | 1.2 | 1.0 | >20:1 | 25.0 |
| 2 | **S5b** | 1.2 | 1.5 | 1.2 | 1.0 | - | ND |
| 3 | **S5c** | 1.2 | 1.5 | 1.2 | 1.0 | - | ND |
| 4 | **S5d** | 1.2 | 1.5 | 1.2 | 1.0 | - | ND |
| 5 | **S5e** | 1.2 | 1.5 | 1.2 | 1.0 | - | ND |
| 6 | **5a** | 1.2 | 2.0 | 1.2 | 1.0 | >20:1 | 20.0 |
| 7 | **5a** | 1.2 | 1.5 | 1.0 | 3.0 | >20:1 | 44.0 |
| 8 | **5a** | 1.2 | 1.5 | 1.0 | 4.0 | >20:1 | 42.0 |
| 9 | **5a** | 1.5 | 1.5 | 1.0 | 3.0 | >20:1 | 42.0 |
| 10 | **5a** | 2.0 | 1.5 | 1.0 | 3.0 | >20:1 | 54.0 |
| 11 | **5a** | 3.0 | 1.5 | 1.0 | 3.0 | >20:1 | 63.0 |

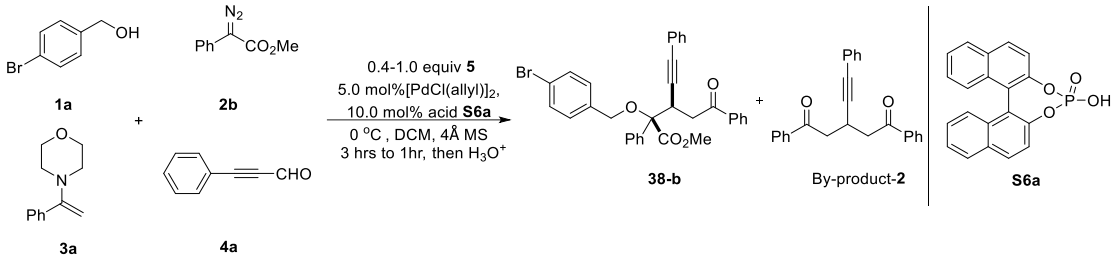
| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 12 | **5a** | 4.0 | 1.5 | 1.0 | 3.0 | >20:1 | 56.0 |

[a] Standard conditions: **2b** and **3A** in 1.0 mL DCM was added into a solution of **1a**, **4a**, **5**, $[Pd(allyl)Cl]_2$ (5 mol%), *rac*-**S6a** (10 mol%) and 4 Å MS (70 mg) in 1.0 mL DCM via a syringe pump for 60 mins, and the resulting mixture was stirred for another 6 hr. [b] Determined by $^1H$ NMR spectroscopy analyses. [c] Determined by $^1H$ NMR spectroscopy analyses using 1, 3, 5-trimethoxybenzene as an internal standard.

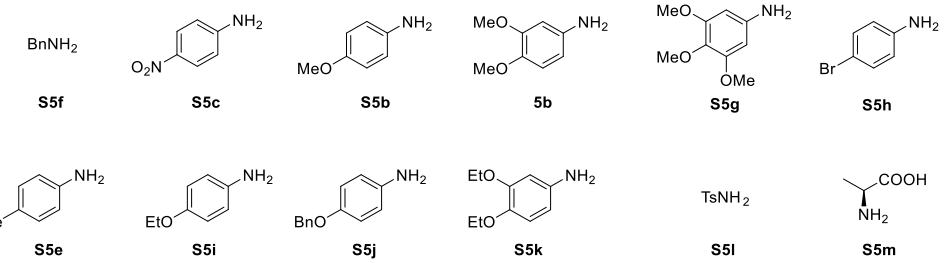
**Procedure**

To a flame-dried 10-mL Schlenk flask charged with a magnetic stirring bar, alcohol **1a** (0.15 mmol), aldehyde **4a** (0.15 mmol), **5** (50 mol%), $[PdCl(allyl)]_2$ (5 mol%), *rac*-**S6a** (10 mol%) and 4Å MS (70 mg) in DCM (1.0 mL), was added a mixture of diazoacetate **2a** (0.075 mmol) and indole **3A** (0.05 mmol) in DCM (1.0 mL) for 1.0 h via a syringe pump at 0 °C. The mixture was stirred for additional 6 hrs under these conditions. After the completion of the reaction, the reaction mixture was filtrated and the filtrate was evaporated in vacuo to give the crude product. And then the crude product was purified by flash chromatography on silica gel (eluent: PE: EA = 20 : 1) to afford the pure products **7**.

**Table S2 Racemic Condition Optimization [a]**




**S5**:




| entry | **S5(equiv.)** | Acid | Yield of **7-b**/%[b] | d.r.[c] | Yield of by-product-**2**/%[b] |
|---|---|---|---|---|---|
| 1 | **S5f**(0.5) | **S6a** | 0 | ND | 81 |
| 2 | **S5c**(0.5) | **S6a** | 13 | 3:1 | 70 |
| 3 | **S5b**(0.5) | **S6a** | 32 | 3:1 | 47 |
| 4 | **5b**(0.5) | **S6a** | 45 | 3:1 | 39 |
| 5 | **S5g**(0.5) | **S6a** | 35 | 3:1 | 41 |
| 6 | **S5h**(0.5) | **S6a** | 16 | 3:1 | 62 |
| 7 | **S5e**(0.5) | **S6a** | 31 | 3:1 | 52 |
| 8 | **S5i**(0.5) | **S6a** | 33 | 3:1 | 46 |
| 9 | **S5j**(0.5) | **S6a** | 36 | 3:1 | 42 |
| 10 | **S5k**(0.5) | **S6a** | 35 | 3:1 | 41 |
| 11 | **S5l**(0.5) | **S6a** | 33 | 4:1 | 45 |
| 12 | **S5m**(0.5) | **S6a** | 39 | 2:1 | 45 |
| 13 | **5b**(0.5) | TsOH | 7 | ND | 61 |
| 14 | **5b**(0.5) | TFOH | 0 | ND | < 5 |
| 15 | **5b**(0.5) | HCOOH | 13(14)[d] | 3:1 | 64(69)[e] |
| 16 | **5b**(0.5) | EtCOOH | 10 | 3:1 | 67 |

| | | | | | |
|---|---|---|---|---|---|
| 17 | **5a**(0.5) | 4-$NO_2$PhCOOH | 14 | 3:1 | 63 |
| 18 | **5a**(0.4) | **S6a** | 30 | 3:1 | 43 |
| 19 | **5a**(1.0) | **S6a** | 39 | 3:1 | 40 |

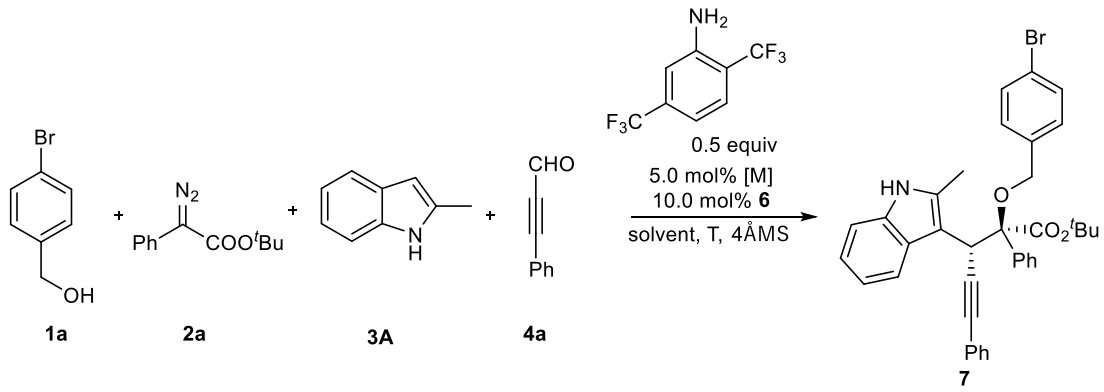
[a] Standard condition: **1a**/**2b**/**3a**/**4a**/**5**/[PdCl(allyl)]$_2$/acid = 0.18/0.18/0.18/0.15/0.06-0.15/0.0075/0.015-0.03 mmol, **2b** and **3a** in 1.0 mL dry DCM were added into a solution of **1a**, **4a**, [PdCl(allyl)]$_2$, acid, **5** and 100 mg 4 Å MS in 2.0 mL dry DCM via a syringe pump under a dinitrogen atmosphere for 180 mins, and the resulting mixture was stirred for another 1.0 hr. [b] Isolated yield. [c] Determined by $^1$H NMR spectroscopy analyses. [d] Adding amount of HCOOH is 50.0 mol%.

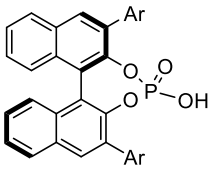
## Procedure

To a flame-dried 10-mL Schlenk flask charged with a magnetic stirring bar, **5** (0.075 mmol), 5.0 mol% [PdCl(allyl)]$_2$, 10.0-50.0 mol% acid, alcohol **1a** (0.18 mmol), aldehyde **4a** (0.15 mmol) and 100 mg 4 Å MS in 2.0 mL DCM were sequentially added at 0 ºC. Diazoacetate **2b** (0.18 mmol) and enamine **3a** (0.18 mmol) dissolved in DCM (1.0 mL) were added by syringe pump over 180 mins. The mixture was stirred for 1.0 hr at 0 ºC. After the completion of the reaction, the reaction mixture was filtrated and the filtrate was evaporated in vacuo to give the crude product. And then the crude product was purified by flash chromatography on silica gel (eluent: PE/EA = 50:1 ~ 30:1, v/v) to give the mixed products **38-b** containing *anti*-product and *syn*-product or *anti*-product.

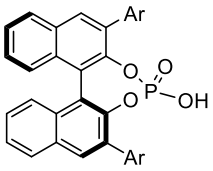
## 4. Table S3-S4 for Detailed Condition Optimizations

**Table S3 Condition Optimization of Asymmetric Four-component Reaction [a]**

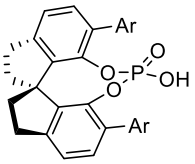



*(R)*-**6c**: Ar=$C_6H_5$
*(R)*-**6b**: Ar=9-anthryl
*(R)*-**S6b**: Ar=4-$CF_3$-$C_6H_4$




*(S)*-**S6c**: Ar=4-OMe-$C_6H_4$
*(S)*-**S6d**: Ar=$SiPh_3$
*(S)*-**S6e**: Ar=9-phenanthryl




*(S)*-**S6f**: Ar=$SiPh_3$
*(S)*-**S6g**: Ar=9-anthryl
*(S)*-**6a**: Ar=1-pyrenyl

| Entry | **6** | [M] | Solvent | T/°C | dr[b] | Yield (%)[c] | ee (%)[d] |
|---|---|---|---|---|---|---|---|
| 1 | (*R*)-**6c** | $[PdCl(allyl)]_2$ | DCM | 0 | >20:1 | 68 | -36 |
| 2 | (*R*)-**6b** | $[PdCl(allyl)]_2$ | DCM | 0 | >20:1 | 70 | -60 |
| 3 | (*R*)-**S6b** | $[PdCl(allyl)]_2$ | DCM | 0 | >20:1 | 73 | -53 |
| 4 | *(S)*-**S6c** | $[PdCl(allyl)]_2$ | DCM | 0 | >20:1 | 40 | 47 |
| 5 | *(S)*-**S6d** | $[PdCl(allyl)]_2$ | DCM | 0 | - | ND | - |
| 6 | *(S)*-**S6e** | $[PdCl(allyl)]_2$ | DCM | 0 | >20:1 | 69 | 84 |
| 7 | *(S)*-**S6f** | $[PdCl(allyl)]_2$ | DCM | 0 | - | ND | - |
| 8 | *(S)*-**S6g** | $[PdCl(allyl)]_2$ | DCM | 0 | >20:1 | 51 | 87 |
| 9 | *(S)*-**6a** | $[PdCl(allyl)]_2$ | DCM | 0 | >20:1 | 50 | 92 |
| 10 | *(S)*-**6a** | $[PdCl(2\text{-butenyl})]_2$ | DCM | 0 | >20:1 | 52 | 93 |
| 11 | *(S)*-**6a** | $[PdCl(cinnyl)]_2$ | DCM | 0 | >20:1 | 56 | 93 |
| 12 | *(S)*-**6a** | $Pd(CH_3CN)_2Cl_2$ | DCM | 0 | >20:1 | 64 | 93 |
| 13 | *(S)*-**6a** | $Pd(C_6H_5CN)_2Cl_2$ | DCM | 0 | >20:1 | 59 | 92 |

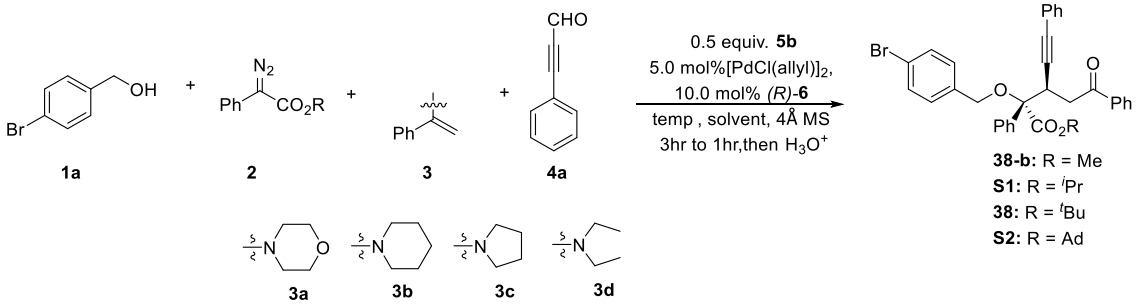
| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 14 | *(S)*-**6a** | $Pd(CH_3CN)_2Cl_2$ | DCE | 0 | >20:1 | 71 | 93 |
| 15 | *(S)*-**6a** | $Pd(CH_3CN)_2Cl_2$ | PhCl | 0 | >20:1 | 60 | 90 |
| 16 | *(S)*-**6a** | $Pd(CH_3CN)_2Cl_2$ | MTBE | 0 | - | ND | - |
| 17[e] | *(S)*-**6a** | $Pd(CH_3CN)_2Cl_2$ | DCE | -10 | >20:1 | 78 | 94 |
| 18[e] | *(S)*-**6a** | $Pd(CH_3CN)_2Cl_2$ | DCE | -20 | >20:1 | 83 | 94 |
| 19[e] | *(S)*-**6a** | $Pd(CH_3CN)_2Cl_2$ | DCE | -30 | >20:1 | 78 | 93 |

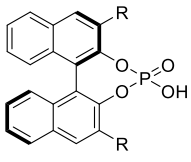
[a] Standard conditions: **1a**/**2a**/**3**A/**4a/5a/[M]/6** = 0.15/0.075/0.05/0.15/0.025/0.0025//0.005 mol, **2a, 3A** in 1.0 mL solvent was added into a solution of **1a**, **4a**, **5a** (50 mol%), [M] (5 mol%), and 4 Å MS (70 mg) in 1.0 mL solvent via a syringe pump for 60 mins, and the resulting mixture was stirred for another 12 hr. [b] Determined by $^1$H NMR spectroscopy analyses. [c] Determined by $^1$H NMR spectroscopy analyses using 1, 3, 5-trimethoxybenzene as an internal standard. [d] Determined by HPLC analyses using a chiral stationary phase. [e] 10 mol% $Pd(CH_3CN)_2Cl_2$

**Procedure**

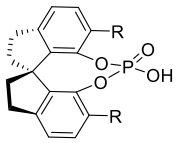
To a flame-dried 10-mL Schlenk flask charged with a magnetic stirring bar, alcohol **1a** (0.6 mmol), aldehyde **4a** (0.6 mmol), 2,5-bis(trifluoromethyl)aniline **5a** (50 mol%), [Pd] (10 mol%), **6** (10 mol%) and 4Å MS (100 mg) in solvent (4.0 mL), was added a mixture of diazoacetate **2a** (0.3 mmol) and indole **3A** (0.2mmol) in solvent (4.0 mL) for 1.0 h via a syringe pump at -20 ~ 0 ℃. The mixture was stirred for additional 12 hrs under these conditions. After the completion of the reaction, the reaction mixture was filtrated and the filtrate was evaporated in vacuo to give the crude product. And then the crude product was purified by flash chromatography on silica gel (eluent: PE: EA = 20 : 1) to afford the pure products.

**Table S4 Condition Optimization for Four-component Reactions [a]**



**S6a**: R = H
**S6d**: R = $SiPh_3$
**S6h**: R = 2,4,6-($i$Pr)$_3C_6H_2$
**S6i**: R = 3,5-$Cl_2C_6H_3$
**6b**: R = 9-anthryl
**S6e**: R = 9-phenanthryl
**S6b**: R = 4-$CF_3C_6H_4$
**S6j**: R = 3,5-$(CF_3)_2C_6H_3$



**S6g**: R = 9-anthryl
**S6k**: R = 9-phenanthryl

| entry | S6 | R | Temp/$^{o}$C | Solvent | 3 | Product | Yield/%[b] | d.r.[c] | ee/%[d] |
|---|---|---|---|---|---|---|---|---|---|
| 1 | **S6a** | Me | 0 | DCM | **3a** | **38-b** | 55 | 86:14 | 5 |
| 2 | **S6d** | Me | 0 | DCM | **3a** | **38-b** | 46 | 94:6 | 25 |
| 3 | **S6h** | Me | 0 | DCM | **3a** | **38-b** | 41 | 94:6 | 27 |
| 4 | **S6i** | Me | 0 | DCM | **3a** | **38-b** | 57 | 94:6 | 23 |
| 5 | **6b** | Me | 0 | DCM | **3a** | **38-b** | 60 | 96:4 | 52 |
| 6 | **S6e** | Me | 0 | DCM | **3a** | **38-b** | 51 | 96:4 | 53 |
| 7 | **S6b** | Me | 0 | DCM | **3a** | **38-b** | 60 | 95:5 | 33 |
| 8 | **S6j** | Me | 0 | DCM | **3a** | **38-b** | 42 | 90:10 | 11 |
| 9 | **S6g** | Me | 0 | DCM | **3a** | **38-b** | 46 | 90:10 | 13 |
| 10 | **S6k** | Me | 0 | DCM | **3a** | **38-b** | 43 | 98:2 | 38 |
| 11 | **6b** | Me | -10 | DCM | **3a** | **38-b** | 67 | 94:6 | 46 |
| 12 | **6b** | $^{i}$Pr | -10 | DCM | **3a** | **S1** | 63 | 96:4 | 80 |
| 13 | **6b** | $^{t}$Bu | -10 | DCM | **3a** | **38** | 72 | 98:2 | 98 |
| 14 | **6b** | Ad | -10 | DCM | **3a** | **S2** | 55 | 94:6 | 94 |
| 15 | **6b** | $^{t}$Bu | -20 | DCM | **3a** | **38** | 46 | 95:5 | 98 |
| 16 | **6b** | $^{t}$Bu | -10 | DCE | **3a** | **38** | 53 | 95:5 | 98 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 17 | **6b** | $^t$Bu | -10 | toluene | **3a** | **38** | 62 | 96:4 | 98 |
| 18 | **6b** | $^t$Bu | -10 | $CHCl_3$ | **3a** | **38** | 44 | 98:2 | 95 |
| 19 | **6b** | $^t$Bu | -10 | DCM | **3b** | **38** | 8 | 81:29 | 46 |
| 20 | **6b** | $^t$Bu | -10 | DCM | **3c** | **38** | < 5 | - | - |
| 21 | **6b** | $^t$Bu | -10 | DCM | **3d** | **38** | < 5 | - | - |

[a] Standard condition: **1a**/**2**/**3a**/**4a**/**5b**/$[PdCl(allyl)]_2$/**6** = 0.18/0.18/0.18/0.15/0.075/0.0075/0.015 mmol, **2** and **3a** in 1.0 mL dry solvent were added into a solution of **1a**, **4a**, $[PdCl(allyl)]_2$, **6**, aniline **5b** and 100 mg 4 Å MS in 1.5 mL dry solvent via a syringe pump under a dinitrogen atmosphere for 180 mins, and the resulting mixture was stirred for another 1.0 hr. [b] Isolated yield. [c] Determined by $^1$H NMR spectroscopy analyses or HPLC. [d] Determined by HPLC analyses using a chiral stationary phase.

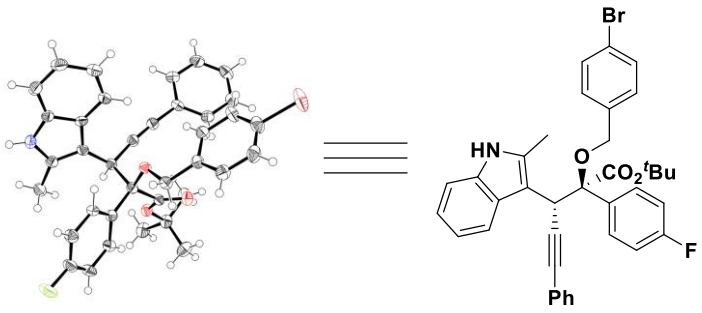
**Procedure**

To a flame-dried 10-mL Schlenk flask charged with a magnetic stirring bar, 3,4-dimethoxyaniline **5b** (0.10 mmol), 5.0 mol% $[PdCl(allyl)]_2$, 10.0 mol% *(R)*-**6**, alcohol **1a** (0.24 mmol), aldehyde **4a** (0.20 mmol) and 100 mg 4 Å MS in 2.0 mL of solent were sequentially added at -20～0 ºC. Diazoacetate **2** (0.24 mmol) and enamine **3**(0.24 mmol) dissolved in solvent (1.0 mL) were added by syringe pump over 180 mins. The mixture was stirred for 1.0 hr at -20～0 ºC. After the completion of the reaction, the reaction mixture was filtrated and the filtrate was evaporated in vacuo to give the crude product. And then the crude product was purified by flash chromatography on silica gel (eluent: PE/EA = 50:1 ~ 30:1, v/v) to give the product.

## 5. X-ray Diffraction Parameters and Data

### 1) X-ray Diffraction Parameters and Data of 21

**CCDC: 2156063**




---

Bond precision: C-C = 0.0079 A Wavelength=1.54184

Cell: a=11.9443(1) b=18.1049(3) c=31.5163(4)
alpha=90 beta=90 gamma=90
Temperature: 100 K

| | Calculated | Reported |
|---|---|---|
| Volume | 6815.41(15) | 6815.41(15) |
| Space group | P 21 21 21 | P 21 21 21 |
| Hall group | P 2ac 2ab | P 2ac 2ab |
| Moiety formula | 2(C37 H33 Br F N O3), C H Cl3 | 2(C37 H33 Br F N O3), C H Cl3 |
| Sum formula | C75 H67 Br2 Cl3 F2 N2 O6 | C75 H67 Br2 Cl3 F2 N2 O6 |
| Mr | 1396.46 | 1396.47 |
| Dx,g cm-3 | 1.361 | 1.361 |
| Z | 4 | 4 |
| Mu (mm-1) | 3.068 | 3.068 |
| F000 | 2872.0 | 2872.0 |
| F000' | 2878.12 | |
| h,k,lmax | 15,23,40 | 15,23,39 |
| Nref | 14768[ 8107] | 14446 |
| Tmin,Tmax | 0.604,0.736 | 0.621,1.000 |
| Tmin' | 0.516 | |

Correction method= # Reported T Limits: Tmin=0.621 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.78/0.98 Theta(max)= 79.235

R(reflections)= 0.0564( 12951) wR2(reflections)= 0.1596( 14446)

S = 1.051 Npar= 819

```
 Alert level C
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00787 Ang.
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N00E     --H00E     .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N00F     --H00F     .     Please Check
PLAT601_ALERT_2_C Unit Cell Contains Solvent Accessible VOIDS of .        71 Ang**3
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..         1 Check

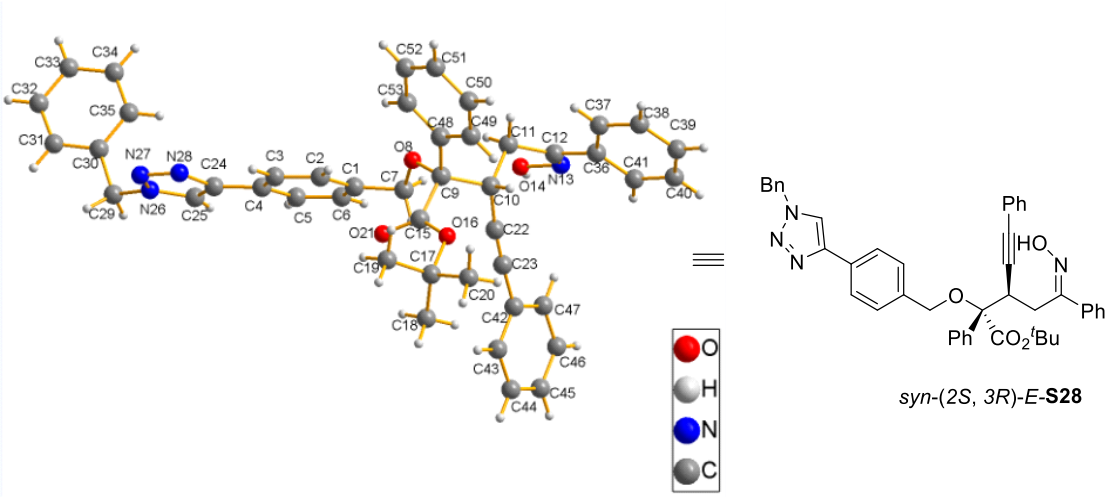
 Alert level G
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............         2 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      5.09 Why ?
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C00O     - C00V     .      1.44 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C00P     - C01K     .      1.43 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact Br02     ..Cl2      .      3.47 Ang.
                                        1-x,-1/2+y,1/2-z  =     3_645 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........       154 Note
PLAT791_ALERT_4_G Model has Chirality at C00J        (Sohnke SpGr)        R Verify
PLAT791_ALERT_4_G Model has Chirality at C00M        (Sohnke SpGr)        R Verify
PLAT791_ALERT_4_G Model has Chirality at C00X        (Sohnke SpGr)        R Verify
PLAT791_ALERT_4_G Model has Chirality at C016        (Sohnke SpGr)        R Verify
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600       86 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.        2 Info

   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   5 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  12 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   8 ALERT type 2 Indicator that the structure model may be wrong or deficient
   2 ALERT type 3 Indicator that the structure quality may be low
   6 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

## 2) X-ray Diffraction Parameters and Data of S28

## CCDC: 1948222




The structure and absolute stereochemistry of ketoxime **S28** was confirmed by X-ray crystallographic analysis, which also could determine the structure and absolute stereochemistry of **41**.

Bond precision: C-C = 0.0047 A Wavelength=1.54184

Cell: a=11.2326(2) b=15.9229(2) c=21.1892(3)
alpha=90 beta=90 gamma=90
Temperature: 100 K

| | Calculated | Reported |
|---|---|---|
| Volume | 3789.81(10) | 3789.81(10) |
| Space group | P 21 21 21 | P 21 21 21 |
| Hall group | P 2ac 2ab | P 2ac 2ab |
| Moiety formula | C45 H42 N4 O4 | C45 H42 N4 O4 |
| Sum formula | C45 H42 N4 O4 | C45 H42 N4 O4 |
| Mr | 702.83 | 702.82 |
| Dx,g cm-3 | 1.232 | 1.232 |
| Z | 4 | 4 |
| Mu (mm-1) | 0.631 | 0.631 |
| F000 | 1488.0 | 1488.0 |
| F000' | 1492.30 | |
| h,k,lmax | 14,20,26 | 13,19,26 |
| Nref | 8021[ 4470] | 7799 |
| Tmin,Tmax | 0.939,0.939 | 0.685,1.000 |
| Tmin' | 0.939 | |

Correction method= # Reported T Limits: Tmin=0.685 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.74/0.97 Theta(max)= 77.092

R(reflections)= 0.0439( 6912) wR2(reflections)= 0.1199( 7799)

S = 1.044 Npar= 482

**Alert level C**

| | |
|---|---|
| PLAT340_ALERT_3_C | Low Bond Precision on C-C Bonds ..... 0.00465 Ang. |

**Alert level G**

| | | |
|---|---|---|
| PLAT007_ALERT_5_G | Number of Unrefined Donor-H Atoms ..... | 1 Report |
| PLAT371_ALERT_2_G | Long C(sp2)-C(sp1) Bond C23 - C42 . | 1.43 Ang. |
| PLAT791_ALERT_4_G | Model has Chirality at C9 (Chiral SPGR) | S Verify |
| PLAT791_ALERT_4_G | Model has Chirality at C10 (Chiral SPGR) | R Verify |
| PLAT883_ALERT_1_G | No Info/Value for _atom_sites_solution_primary . | Please Do ! |
| PLAT912_ALERT_4_G | Missing # of FCF Reflections Above STh/L= 0.600 | 58 Note |
| PLAT978_ALERT_2_G | Number C-C Bonds with Positive Residual Density. | 5 Info |
| PLAT992_ALERT_5_G | Repd & Actual _reflns_number_gt Values Differ by | 1 Check |

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
8 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

## 6. ECD Parameters and Data of 93

The calculated and experimental ECD spectra are shown as below (to get better accuracy, the experimental data are not processed). Obviously, the calculated ECD spectra for the SSR diastereomer are more consistent with the experimental data. Therefore, we think the SSR one is more likely to be the actual product.

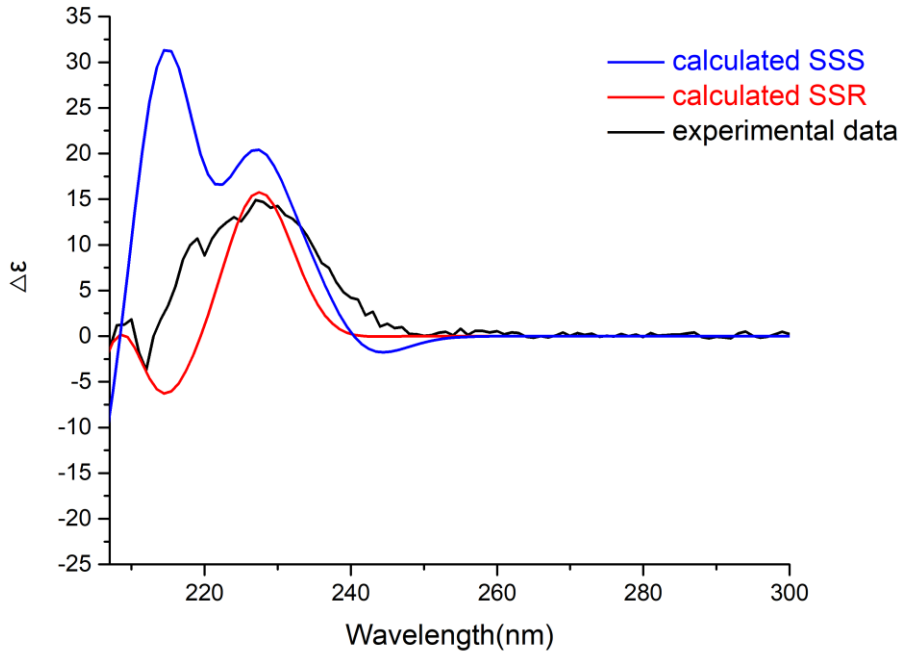


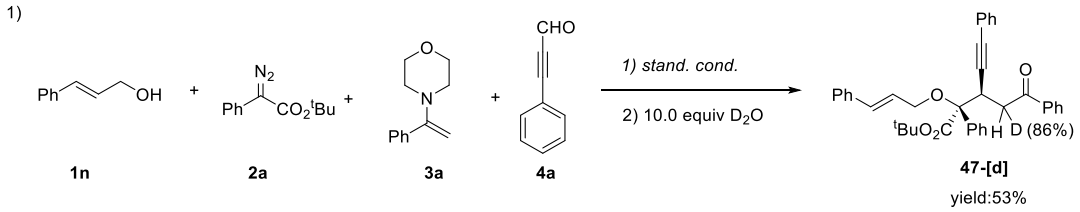

**Figure. S1 Comparision of B3LPY/6-311G(d,p)-calculated ECD with the experimental data in MeOH.**

**Computational Methods.**

MMFF and DFT/TDDFT calculations were perform with the molclus[22] software package and Gaussion 09[23] software package. The MMFF calculation was to do the conformational search and obtain 10 of the lowest configurations. Their geometries were then optimized at the B3LYP[242]/6-311G(d,p) level of theory combined with the SMD[25] model in MeOH. The TDDFT calculation were performed with the same level to get the ECD data. Finally, the Boltzmann weighted summation of spectra data were form by using SpecDis[26] software.

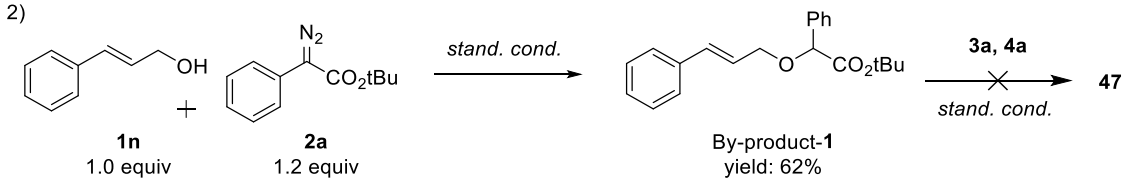
## 7. Control Experiments

### 7.1 Control Experiment 1




To a flame-dried 10-mL Schlenk flask charged with a magnetic stirring bar, 3,4-dimethoxyaniline (0.10 mmol), 5.0 mol% $[PdCl(allyl)]_2$, 10.0 mol% *(R)*- **6b**, alcohol **1n** (0.24 mmol), aldehyde **4a** (0.20 mmol) and 100 mg 4 Å MS in 2.0 mL DCM were sequentially added at -10 ºC. Diazoacetate **2a** (0.24 mmol) and enamine **3a** (0.24 mmol) dissolved in DCM (1.0 mL) were added by syringe pump over 60 mins. The mixture was stirred for 1.0 hr at -10 ºC. After the completion of the reaction, $D_2O$ (10.0 equiv.) was added in one portionthe and stirred for 2.0 hrs. The reaction mixture was filtrated and the filtrate was evaporated in vacuo to give the crude product. And then the crude product was purified by flash chromatography on silica gel (eluent: PE/EA = 50:1 ~ 30:1, v/v) to give the product **47**-[d] (59.0 mg, 53% yield). The yield of deuterated product **47**-[d] was detected by $^1$H NMR (86%).

### 7.2 Control Experiment 2

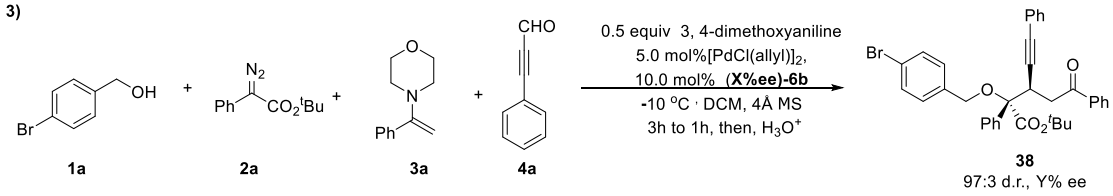



To a flame-dried 10-mL Schlenk flask charged with a magnetic stirring bar, 2.0 mol% $Rh_2(OAc)_4$, cinnamyl alcohol **1n** (0.24 mmol) and 100 mg 4 Å MS in 2.0 mL DCM were sequentially added at -10 ºC. Diazoacetate **2a** (0.24 mmol) dissolved in DCM (1.0 mL) were added by syringe pump over 60 mins. The mixture was stirred for 1.0 hr at -

10 °C. After the completion of the reaction, the reaction mixture was filtrated and the filtrate was evaporated in vacuo to give the crude product. And then the crude product was purified by flash chromatography on silica gel (eluent: PE/EA = 50:1 ~ 30:1, v/v) to give the pure By-product-**1**.

To a flame-dried 10-mL Schlenk flask charged with a magnetic stirring bar, 3,4-dimethoxyaniline (0.10 mmol), 5.0 mol% $[PdCl(allyl)]_2$, 10.0 mol% *(R)*-**6b**, By-product-**1** (0.24 mmol), aldehyde **4a** (0.20 mmol) and 100 mg 4 Å MS in 2.0 mL DCM were sequentially added at -10 °C. Enamine **3a** (0.24 mmol) dissolved in DCM (1.0 mL) were added by syringe pump over 60 mins. The mixture was stirred for 1.0 hr at -10 °C. After the completion of the reaction, the target **47** could not be detected by LC-MS.

### 7.3 Control Experiment 3

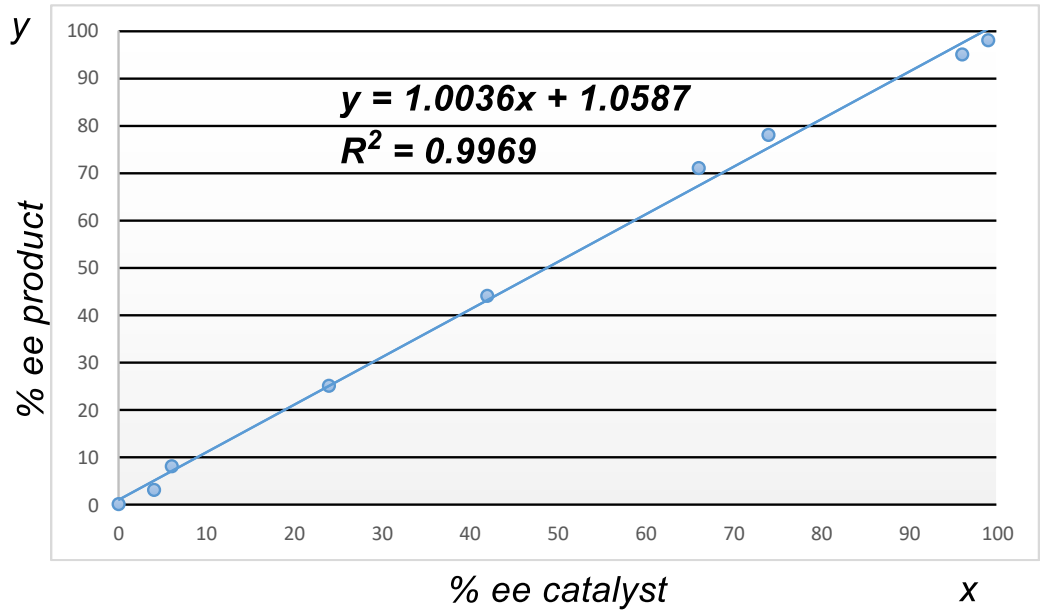



To a flame-dried 10-mL Schlenk flask charged with a magnetic stirring bar, 3,4-dimethoxyaniline **5b** (0.10 mmol), 5.0 mol% $[PdCl(allyl)]_2$, 10.0 mol% *(*X%ee*)*-**6b**, alcohol **1a** (0.24 mmol), aldehyde **4a** (0.20 mmol) and 100 mg 4 Å MS in 2.0 mL DCM were sequentially added at -10 °C. Diazoacetate **2a** (0.24 mmol) and enamine **3a** (0.24 mmol) dissolved in DCM (1.0 mL) were added by syringe pump over 60 mins. The mixture was stirred for 1.0 hr at -10 °C. After the completion of the reaction, the ee value of **38** was determined by HPLC analyses using a chiral stationary phase. The linear effect result: $y = 1.0036x + 1.0587$, $R^2 = 0.9969$.

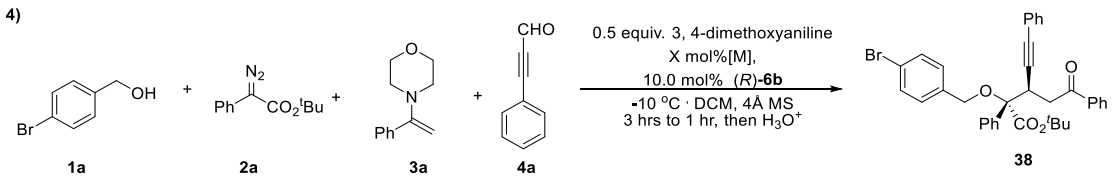
**Result:**

| Entry | x | y |
|---|---|---|

| | *ee* of CPA-**6b**/% | *ee* of product **38**/% |
|---|---|---|
| 1 | 0 | 0 |
| 2 | 4 | 3 |
| 3 | 6 | 8 |
| 4 | 24 | 25 |
| 5 | 42 | 44 |
| 6 | 66 | 71 |
| 7 | 74 | 78 |
| 8 | 96 | 95 |
| 9 | 99 | 98 |




### 7.4 Control Experiment 4




To a flame-dried 10-mL Schlenk flask charged with a magnetic stirring bar, 3,4-dimethoxyaniline **5b** (0.10 mmol), x mol% [M], 10.0 mol% *(R)*-**6b**, alcohol **1a** (0.24 mmol), aldehyde **4a** (0.20 mmol) and 100 mg 4 Å MS in 2.0 mL DCM were sequentially added at -10 ºC. Diazoacetate **2a** (0.24 mmol) and enamine **3a** (0.24 mmol) dissolved

in DCM (1.0 mL) were added by syringe pump over 180 mins. The mixture was stirred for 1.0 hr at -10 °C. After the completion of the reaction, he reaction mixture was filtrated and the filtrate was evaporated in vacuo to give the crude product. And then the crude product was purified by flash chromatography on silica gel (eluent: PE/EA = 50:1 ~ 30:1, v/v) to give the product **38**, and d.r and ee value of **38** were determined by HPLC analyses using a chiral stationary phase.

**Result:**

| Entry | [M]/mol% | yield of **38**/% | d.r. of **38** | ee of **38**/% |
|---|---|---|---|---|
| 1 | $[PdCl(allyl)]_2$/(5.0) | 72 | 98:2 | 98 |
| 2 | $[PdCl(2\text{-butenyl})]_2$/(5.0) | 55 | 98:2 | 98 |
| 3 | $[PdCl(cinnyl)]_2$/(5.0) | 61 | 96:4 | 96 |
| 4 | $[PdOAc(allyl)]_2$/(5.0) | 40 | 80:20 | 39 |
| 5 | $[PdTFA(allyl)]_2$/(5.0) | 53 | 90:10 | 60 |
| 6 | $Rh_2(OAc)_4$/(2.0) | 37 | 98:2 | 98 |
| 7 | $Rh_2(Oct)_4$/(2.0) | 28 | 98:2 | 98 |
| 8 | $Rh_2(esp)_2$/(1.0) | 30 | 98:2 | 98 |
| 9 | $[Ir(COD)Cl]_2$/(5.0) | 0 | ND | ND |
| 10 | CP*Ru(COD)Cl/(5.0) | 0 | ND | ND |
| 11 | CuOTf/(5.0) | 0 | ND | ND |
| 12 | $Cu(MeCN)_4PF_6$/(5.0) | 0 | ND | ND |

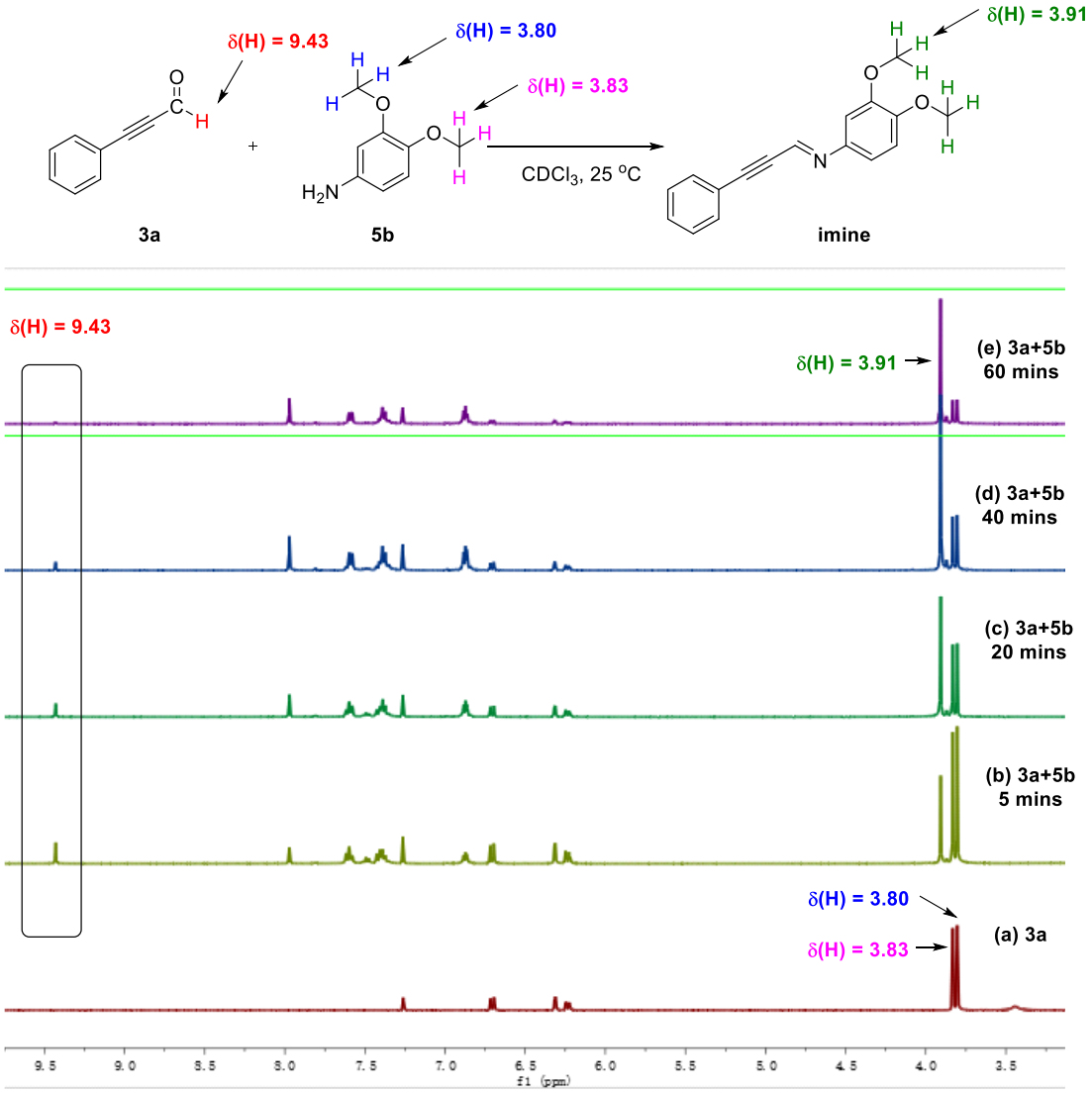
### 7.5 NMR Tube Experiments

(1) **The effect of CPA for the formation of imines**

**a. Absence of 6b(CPA)**

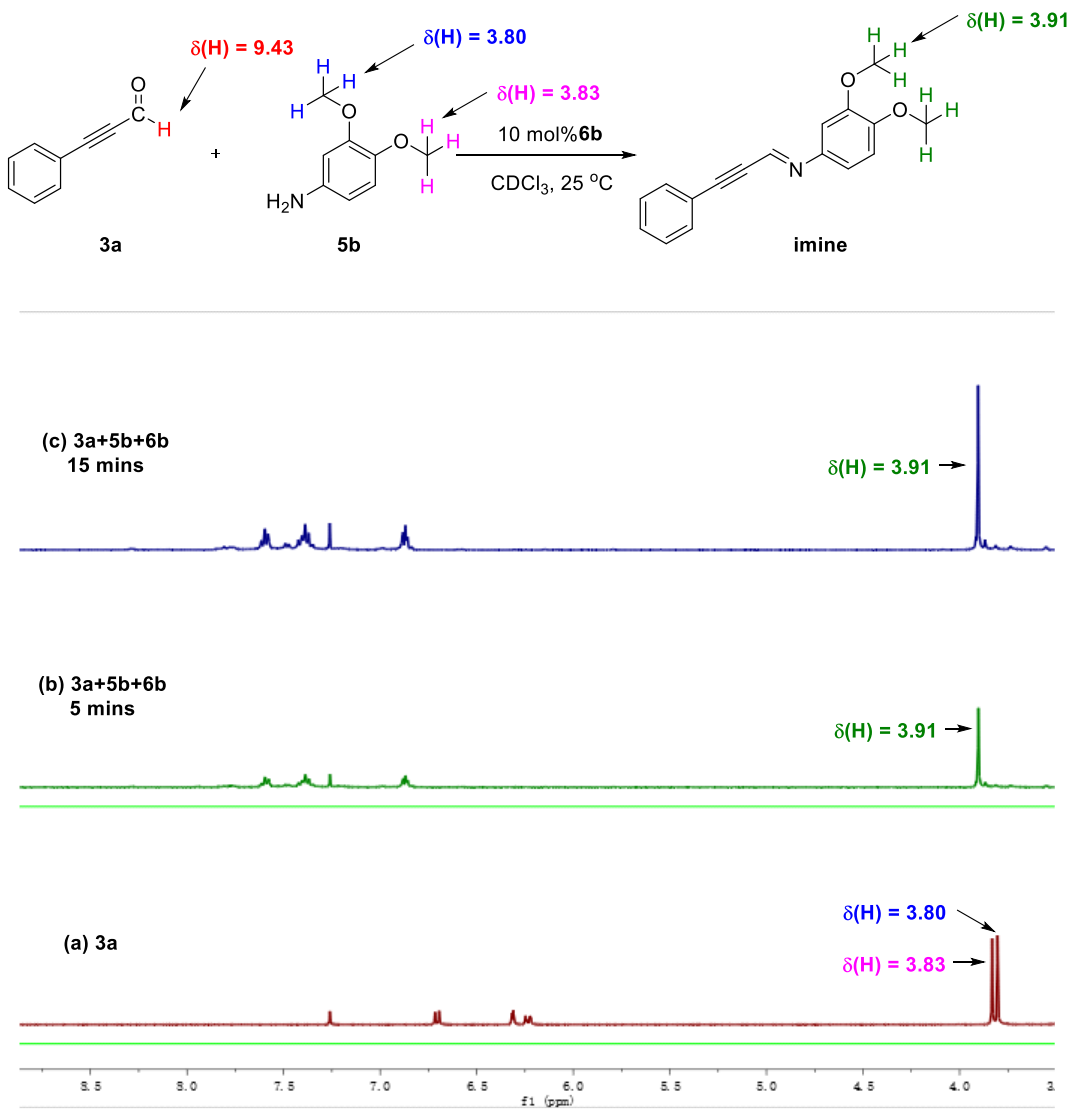
To a flame-dried NMR tube charged with 0.1 mmol **3a**, 0.1 mmol **5b** in 1.0 mL of

$CD_2Cl_2$. The mixture was shocked by ultrasonic cleaning machine for several times. The reaction progress was monitoring at 5 mins, 20 mins, 40 mins, 60 mins by $^1H$ NMR respectively.




**b. Presence of 6b (CPA)**

To a flame-dried NMR tube charged with 0.1 mmol **3a**, 0.1 mmol **5b,** 0.01 mmol **6b** in 1.0 mL of $CD_2Cl_2$. The mixture was shocked by ultrasonic cleaning machine for several times. The reaction progress was monitoring at 5 mins, 15 mins by $^1H$ NMR respectively.



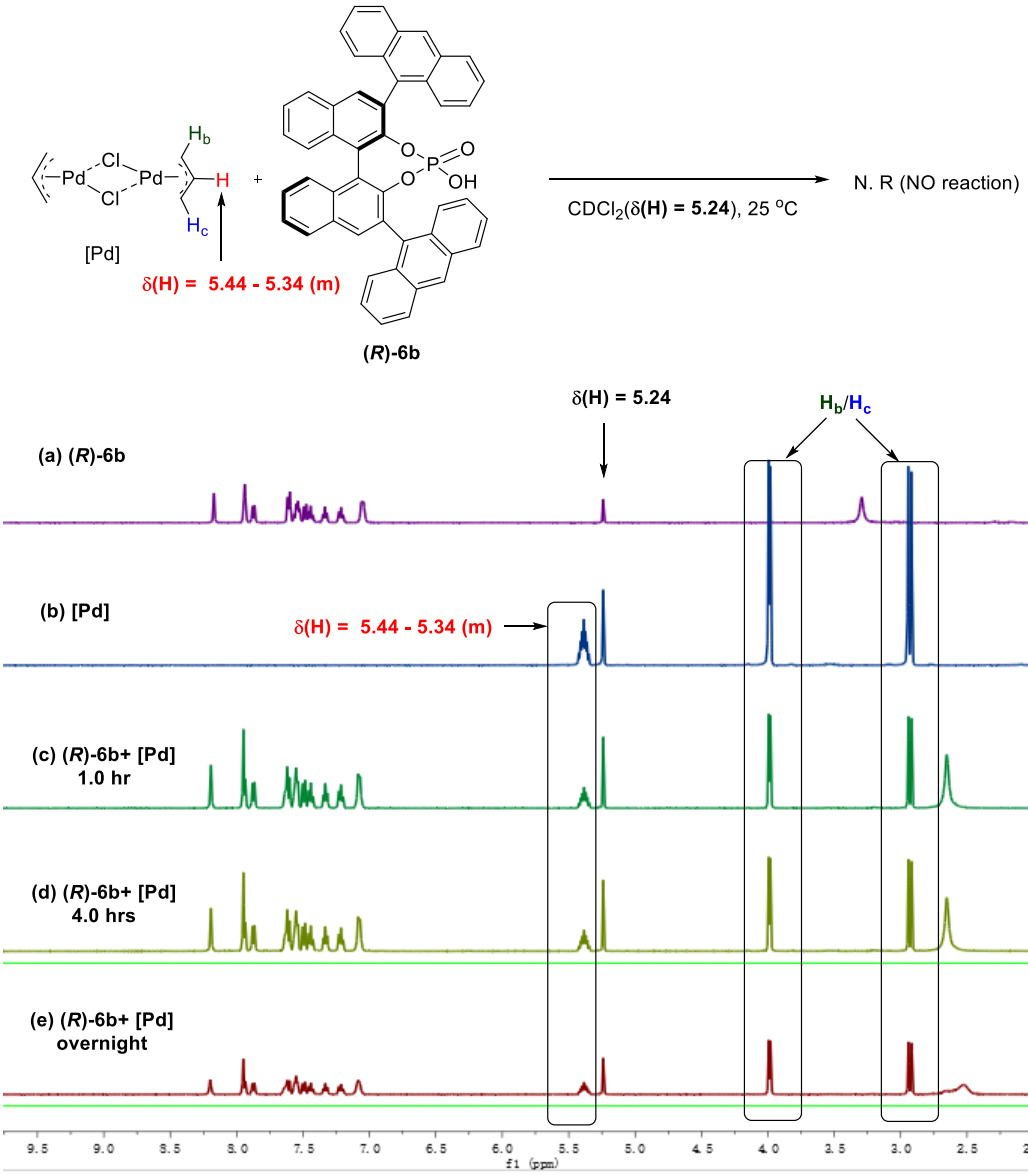

**(2) The reaction of [Pd], CPA, imine**

**a. Absence of imines**

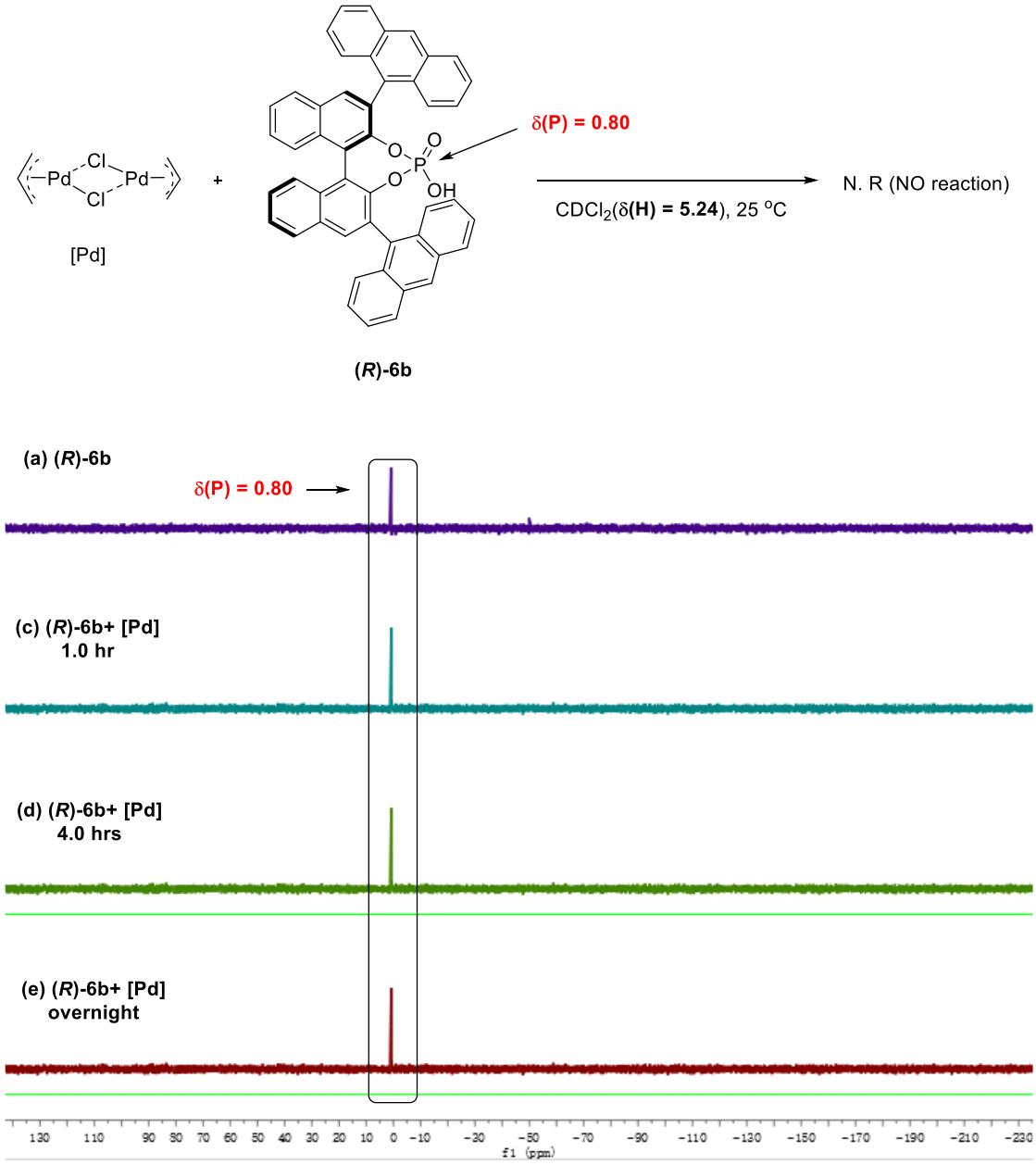
To a flame-dried NMR tube charged with 0.01 mmol $[PdCl(allyl)]_2$, 0.01 mmol *(R)*-**6b** in 1.0 mL of $CD_2Cl_2$. The mixture was shocked by ultrasonic cleaning machine for several times. The reaction progress was monitoring at 1.0 hr, 4.0 hrs and overnight by $^1H$ NMR and $^{31}P$ NMR respectively.

**Result**:

$^1H$ NMR


Pd
Cl
Pd
H
$H_b$
$H_c$
[Pd]
δ(H) = 5.44 - 5.34 (m)
O
P
O
OH
(R)-6b
CDCl2(δ(H) = 5.24), 25 °C
N. R (NO reaction)
δ(H) = 5.24
$H_b$/$H_c$
(a) (R)-6b
(b) [Pd]
δ(H) = 5.44 - 5.34 (m)
(c) (R)-6b+ [Pd]
1.0 hr
(d) (R)-6b+ [Pd]
4.0 hrs
(e) (R)-6b+ [Pd]
overnight
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0
f1 (ppm)

$^{31}$P NMR




Results of both $^{1}H$ NMR and $^{31}P$ NMR illustrated that no chiral palladium(II) phosphate complex existed.

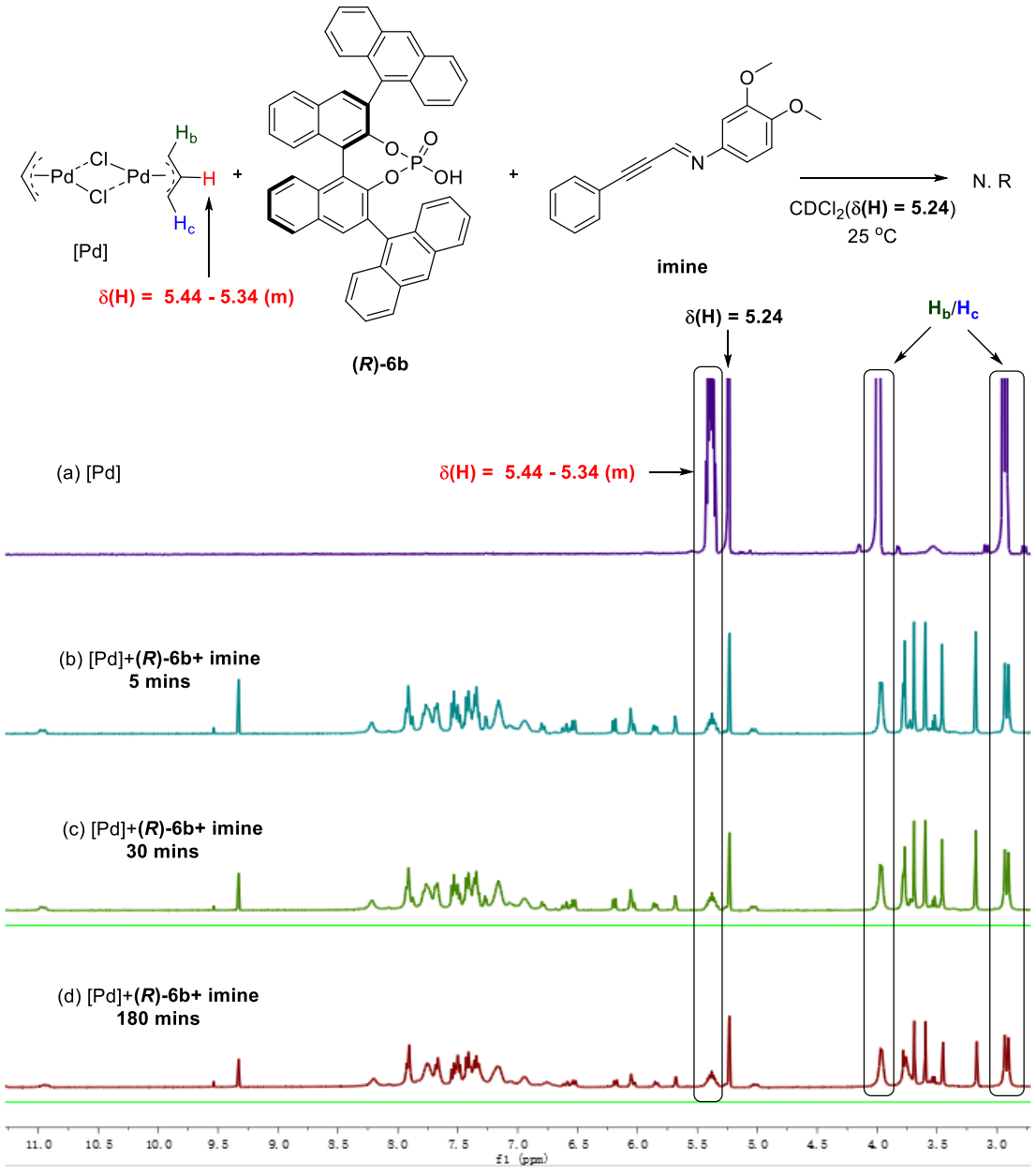
**b. Presence of imines**

To a flame-dried NMR tube charged with 0.01 mmol $[PdCl(allyl)]_2$, 0.01 mmol *(R)*-**6b**, 0.03 mmol **4a**, 0.03 mmol **5b** in 1.0 mL of $CD_2Cl_2$. The mixture was shocked by ultrasonic cleaning machine for several times. The reaction progress was monitoring at

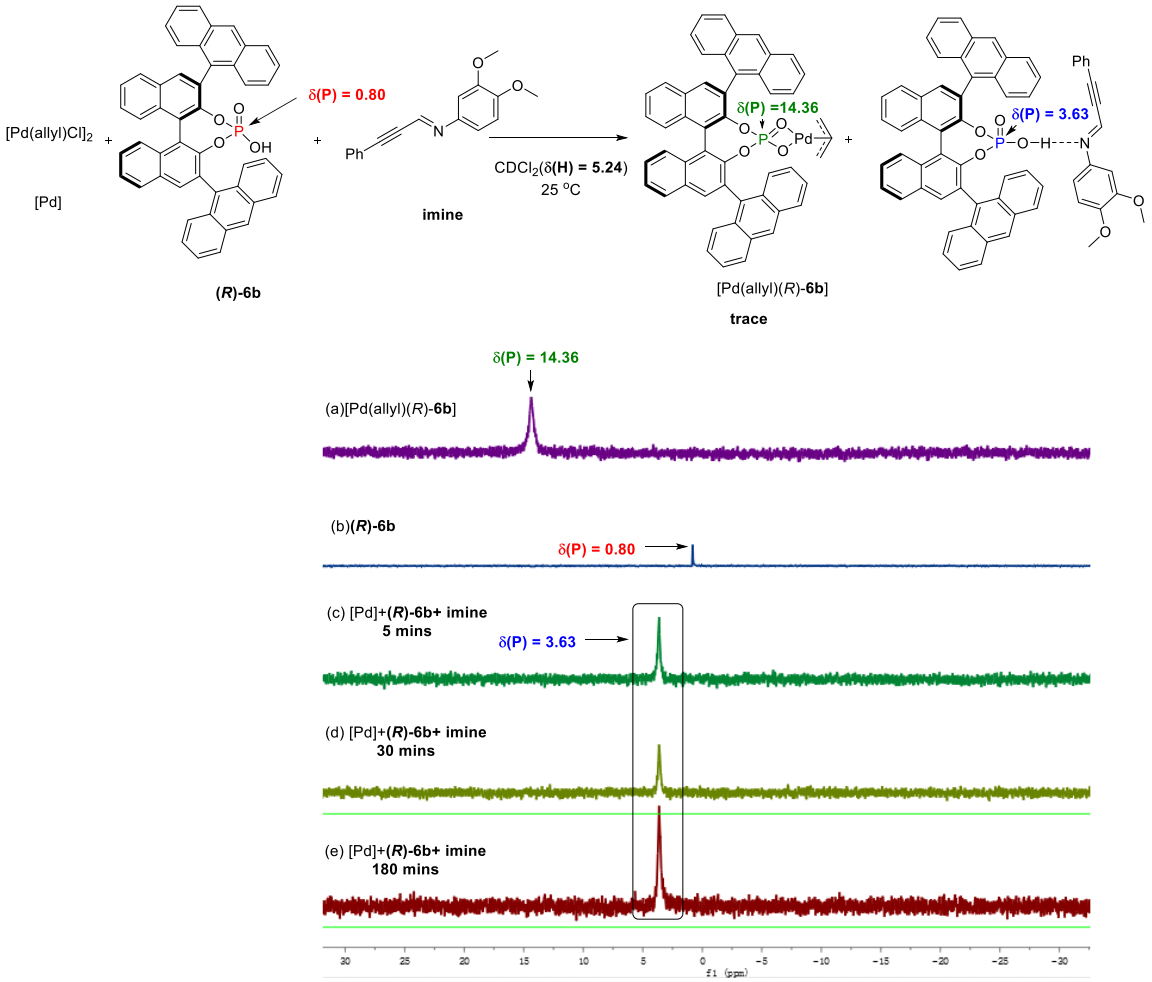
5 mins, 30 mins, 60 mins by $^{1}$H NMR and $^{31}$P NMR respectively.

**Result**:

$^{1}$H NMR



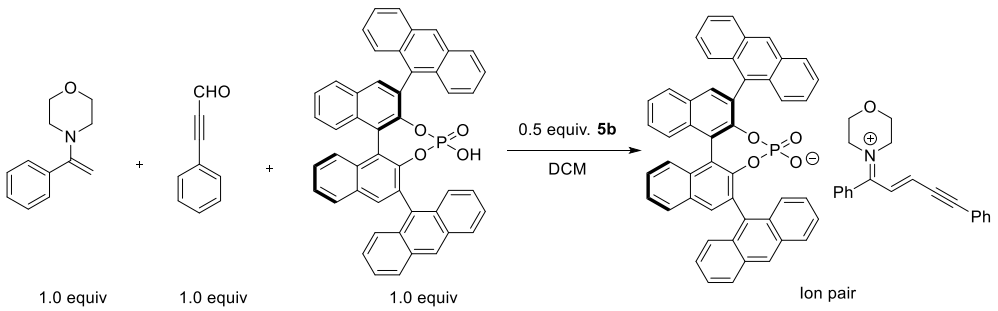

$^{31}$P NMR

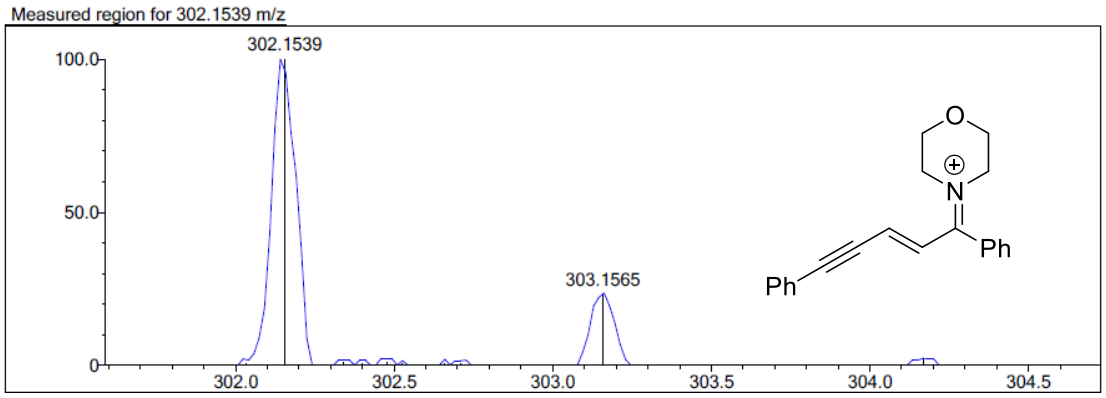


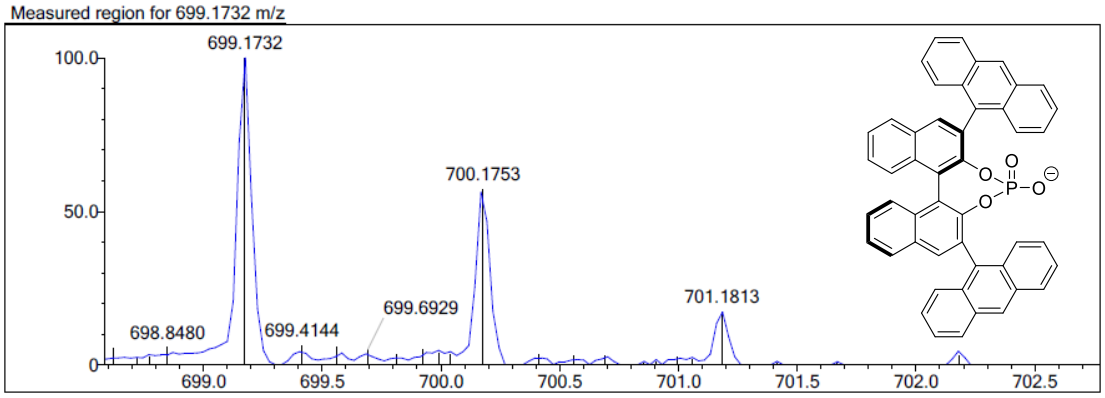

Results of both $^{1}H$ NMR and $^{31}P$ NMR illustrated that no chiral palladium(II) phosphate complex existed in the both absence and presence of imines.

## 7.6 High-resolution Mass Spectrometry (HRMS) Analysis

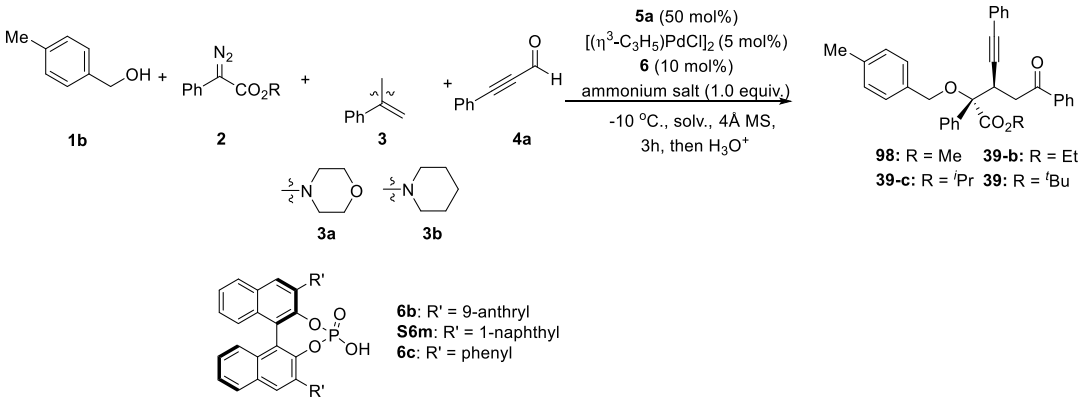
In order to deeply investigate the reaction mechanism, the follow reaction was analyzed by High-resolution mass spectrometry. The result illustrated that ion pair existed.






## 7.7 Control Experiments for DFT

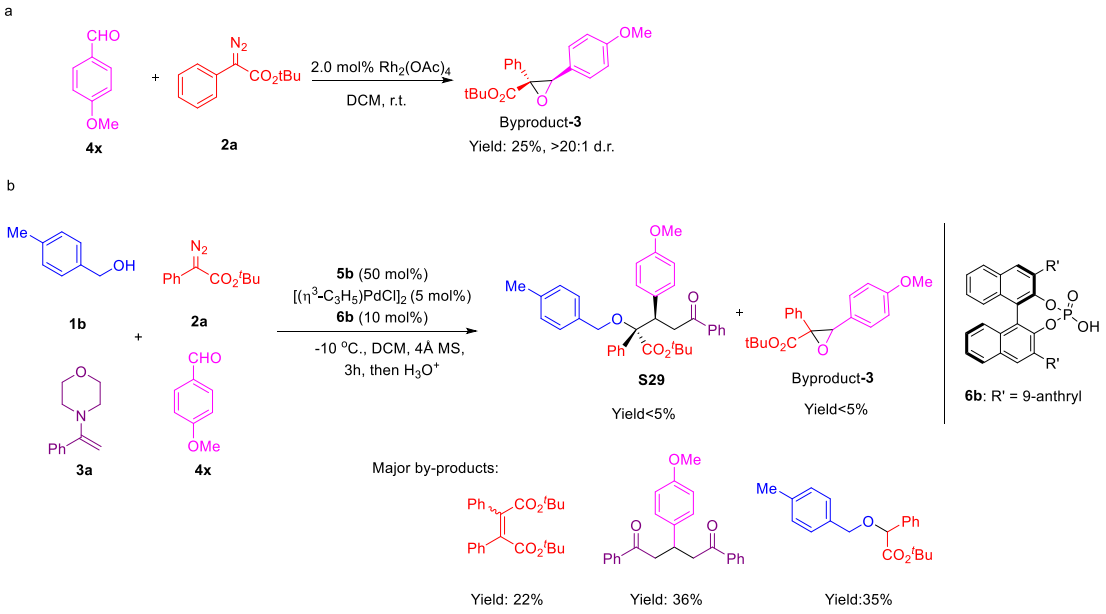



| entry | R | 6 | Solvent | Ammonium salt (1.0 equiv.) | 3 | Product | Yield/%[b] | d.r.[c] | ee/%[d] |
|---|---|---|---|---|---|---|---|---|---|
| 1 | Me | **6b** | DCM | - | **3a** | **98** | 53 | 83:17 | 21 |
| 2 | Et | **6b** | DCM | - | **3a** | **39-b** | 50 | 85:15 | 33 |
| 3 | $^{i}$Pr | **6b** | DCM | - | **3a** | **39-c** | 54 | 89:11 | 56 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 4 | $^t$Bu | **6b** | DCM | - | **3a** | **39** | 65 | 94:6 | 92 |
| 5 | $^t$Bu | **S6m** | DCM | - | **3a** | **39** | 43 | 89:11 | 67 |
| 6 | $^t$Bu | **6c** | DCM | - | **3a** | **39** | 47 | 84:16 | 6 |
| 7 | $^t$Bu | **6b** | DCE | - | **3a** | **39** | 42 | 90:10 | 92 |
| 8 | $^t$Bu | **6b** | $CHCl_3$ | - | **3a** | **39** | 35 | 90:10 | 92 |
| 9 | $^t$Bu | **6b** | toluene | - | **3a** | **39** | 53 | 90:10 | 94 |
| 10 | $^t$Bu | **6b** | EA | - | **3a** | **39** | 30 | 92:8 | 97 |
| 11 | $^t$Bu | **6b** | MeOH | - | **3a** | **39** | < 5 | | |
| 12 | $^t$Bu | **6b** | DMF | - | **3a** | **39** | < 5 | | |
| 13 | $^t$Bu | **6b** | THF | - | **3a** | **39** | 8 | 92:8 | 95 |
| 14 | $^t$Bu | **6b** | DCM/THF (1:9) | - | **3a** | **39** | 22 | 91:9 | 96 |
| 15 | $^t$Bu | **6b** | DCM/THF (1:4) | - | **3a** | **39** | 25 | 95:5 | 97 |
| 16 | $^t$Bu | **6b** | DCM/MeOH (1:9) | - | **3a** | **39** | 6 | 99:1 | 94 |
| 17 | $^t$Bu | **6b** | DCM | $(^n Bu)_4N^+Br^-$ | **3a** | **39** | 27 | 80:20 | 56 |
| 18 | $^t$Bu | **6b** | DCM | - | **3b** | **39** | 11 | 80:20 | 46 |

[a] Standard condition: **1a**/**2**/**3a**/**4a**/**5**/[PdCl(allyl)]$_2$/**6** = 0.18/0.18/0.18/0.15/0.075/0.0075/0.015 mmol, **2** and **3a** in 1.0 mL dry solvent were added into a solution of **1a**, **4a**, [PdCl(allyl)]$_2$, PA**6**, aniline **5b** and 100 mg 4 Å MS in 1.5 mL dry solvent via a syringe pump under a dinitrogen atmosphere for 180 mins, and the resulting mixture was stirred for another 1.0 hr. [b] Isolated yield. [c] Determined by $^1$H NMR spectroscopy analyses or HPLC. [d] Determined by HPLC analyses using a chiral stationary phase.

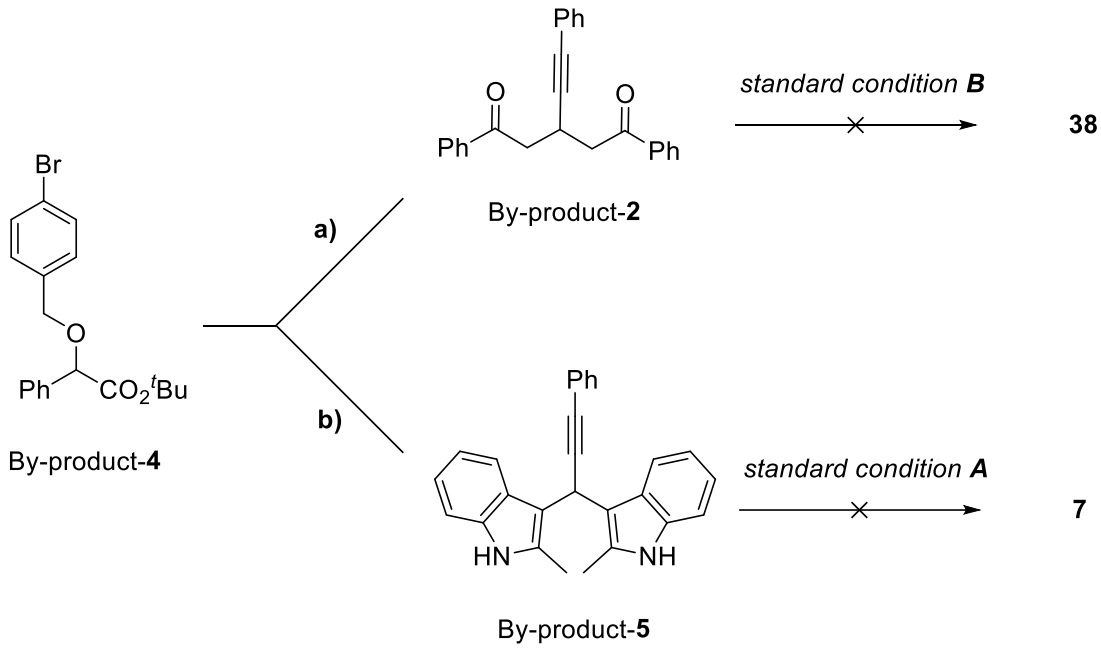
## 7.8 Control Experiment of Investigation Pathway of 4x.[27]




To a flame-dried 10-mL Schlenk flask charged with a magnetic stirring bar, 2.0 mol% $Rh_2(OAc)_4$, **4x** (0.20 mmol) and 100 mg 4 Å MS in 2.0 mL DCM were sequentially added at room temperature. Diazoacetate **2a** (0.24 mmol) dissolved in DCM (1.0 mL) were added by syringe pump over 60 mins. The mixture was stirred for 5.0 hrs. After the completion of the reaction, the reaction mixture was filtrated and the filtrate was evaporated in vacuo to give the crude product. And then the crude product was purified by flash chromatography on silica gel (eluent: PE/EA = 20:1 ~ 10:1, v/v) to give the by-product-**3** (25% yield, > 20:1 d.r.)

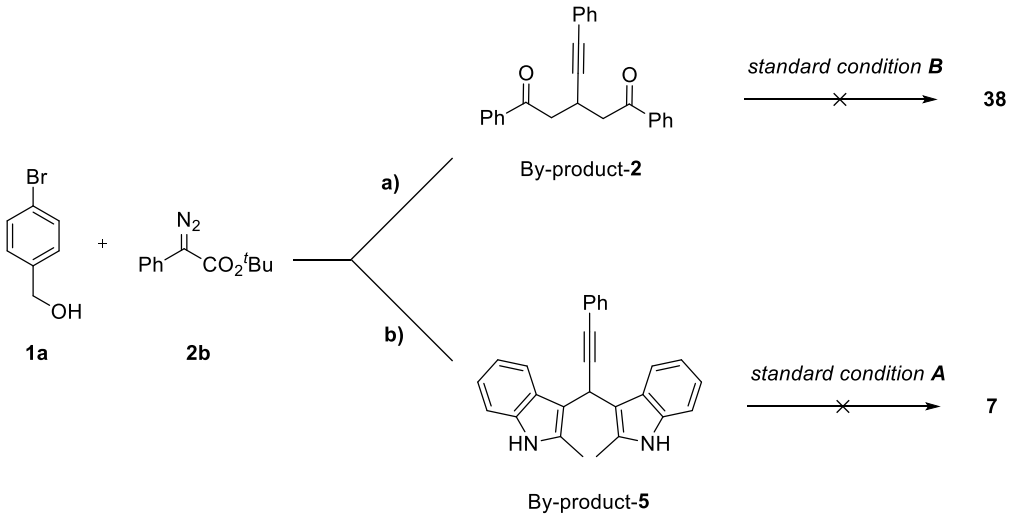
To a flame-dried 10-mL Schlenk flask charged with a magnetic stirring bar, 3,4-dimethoxyaniline (0.10 mmol), 5.0 mol% $[PdCl(allyl)]_2$, 10.0 mol% *(R)*-**6b**, **1b** (0.12 mmol), aldehyde **4x** (0.10 mmol) and 100 mg 4 Å MS in 1.0 mL DCM were sequentially added at -10 °C. Enamine **3a** (0.12 mmol), and **2a** (0.12 mmol) dissolved in DCM (1.0 mL) were added by syringe pump over 180 mins. The mixture was stirred for 1.0 hr at -10 °C. After the completion of the reaction, the target **S29** could not be detected by LC-MS and $^1$H NMR.

## 7.9 Control Experiments




To a flame-dried 10-mL Schlenk flask charged with a magnetic stirring bar, By-product-**4** (0.1 mmol), and By-product-**2** (0.1 mmol) or By-product-5 (0.1 mmol) were dissolved in 1.0 mL solvent. The mixture was conducted under the condition A or B. After the completion of the reaction, neither the target **7** or **38** could not be detected by LC-MS.

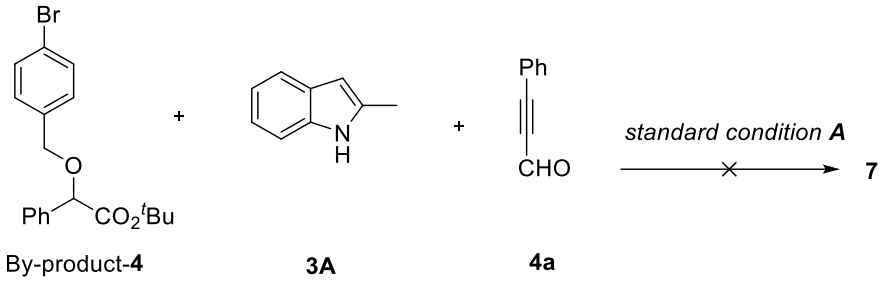
## 7.10 Control Experiments




To a flame-dried 10-mL Schlenk flask charged with a magnetic stirring bar, By-product-**1a** (0.12 mmol), and By-product-**2** (0.1 mmol) or By-product-5 (0.1 mmol) were

dissolved in 1.0 mL solvent. Diazoacetate **2a** (0.12 mmol) dissolved in solvent (1.0 mL) were added by syringe pump over 180 mins. The mixture was conducted under the condition A or B. After the completion of the reaction, neither the target **38** or **7** could not be detected by LC-MS.

### 7.11 Control Experiment




The procedure of reaction refers to Section **7.2**. The mixture was conducted under the condition B. After the completion of the reaction, neither the target **7** could not be detected by LC-MS.

## 8. DFT Calculation

DFT calculations on the mechanism and stereoselectivity of this four-component reaction have been conducted with Gaussian 09.[28] Geometry optimizations were carried out at the B3LYP level of theory[29,30] ,and LANL2DZ pseudo-potential[31,32] was used for Pd and 6-31G(d) basis set (5D keyword used) for all the other atoms in dichloromethane using the CPCM solvation model.[33-35] Vibrational frequencies were computed at the same level to verify that optimized structures are local minima or transition states and to evaluate zero-point vibrational energies and thermal corrections at 298 K, 1 atm. For transition states, intrinsic reaction coordinate (IRC)[36] was calculated to confirm that they indeed connected between correct minima. Single-point energy calculations were performed at the M06-2X level of theory[37] with SDD[38] for Pd and the 6-311+G(d,p) basis set (5D keyword used) for other atoms using the CPCM solvation model. The

three-dimensional structures were visualized utilizing CYLview.[39]

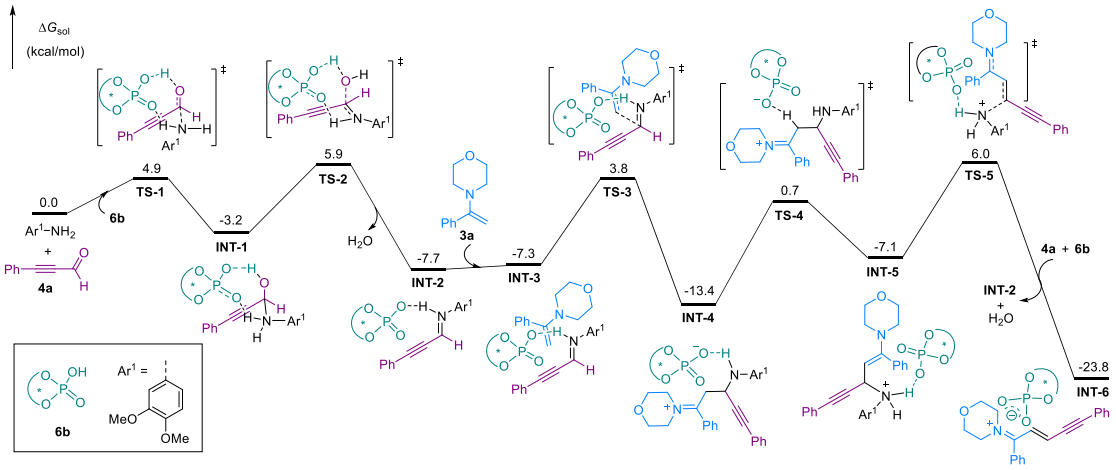



**Figure S5.** Free energy profiles for the CPA catalyzed iminium formation. The Gibbs free energies were computed with CPCM(DCM)-M06-2X/6-311+G(d,p)//CPCM(DCM)-B3LYP/6-31G(d).

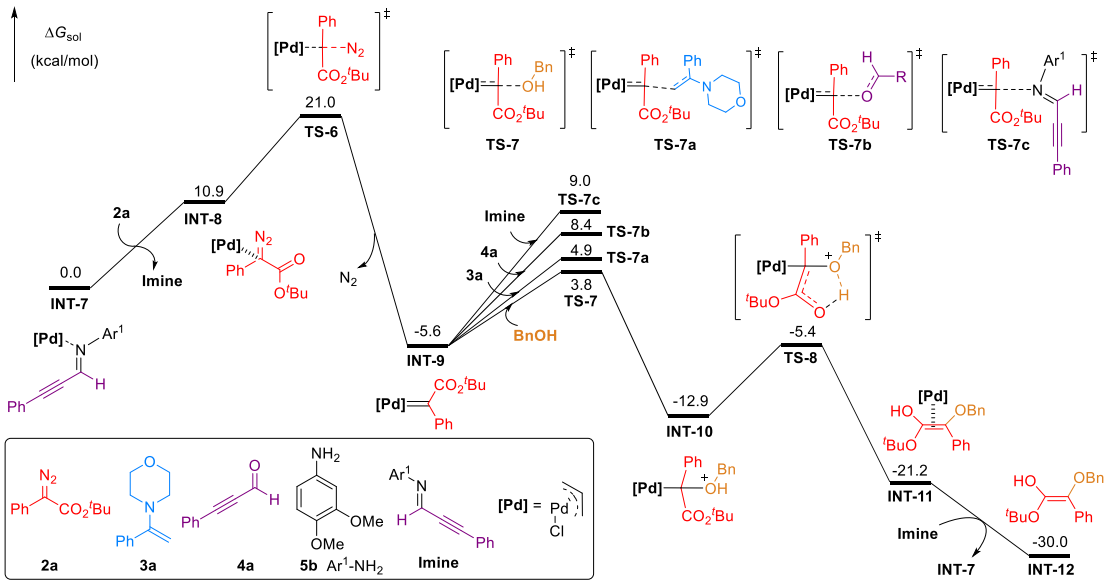



**Figure S6.** Free energy profiles for the palladium catalyzed enol formation. The Gibbs free energies were computed with CPCM(DCM)-M06-2X/6-311+G(d,p)[SDD for Pd]// CPCM(DCM)-B3LYP/6-31G(d)[LANL2DZ for Pd].

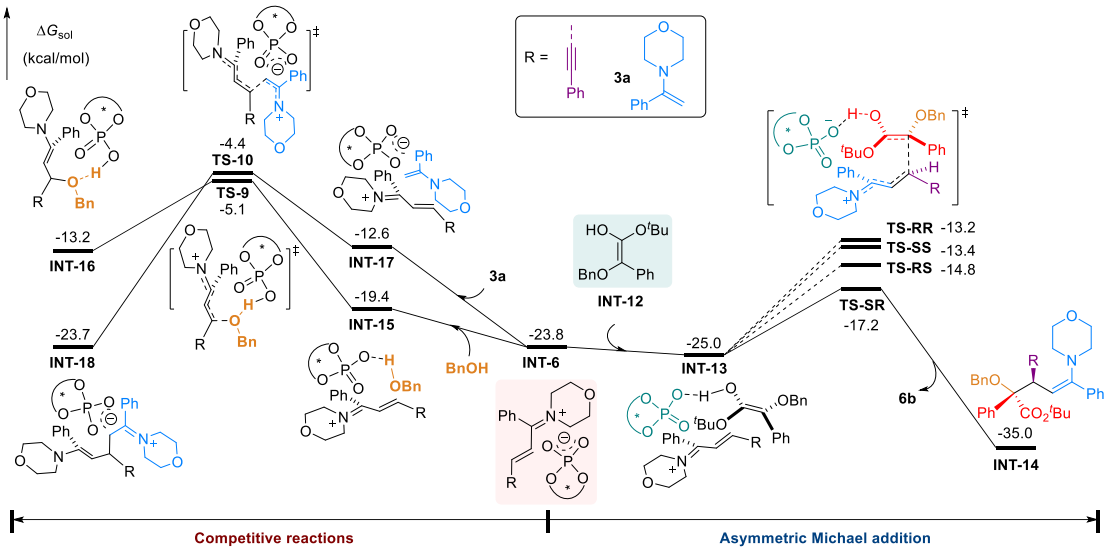



**Figure S7.** Free energy profiles for the asymmetric Michael addition and competitive side reactions. The Gibbs free energies were computed with CPCM(DCM)-M06-2X/6-311+G(d,p)//CPCM(DCM)-B3LYP/6-31G(d).

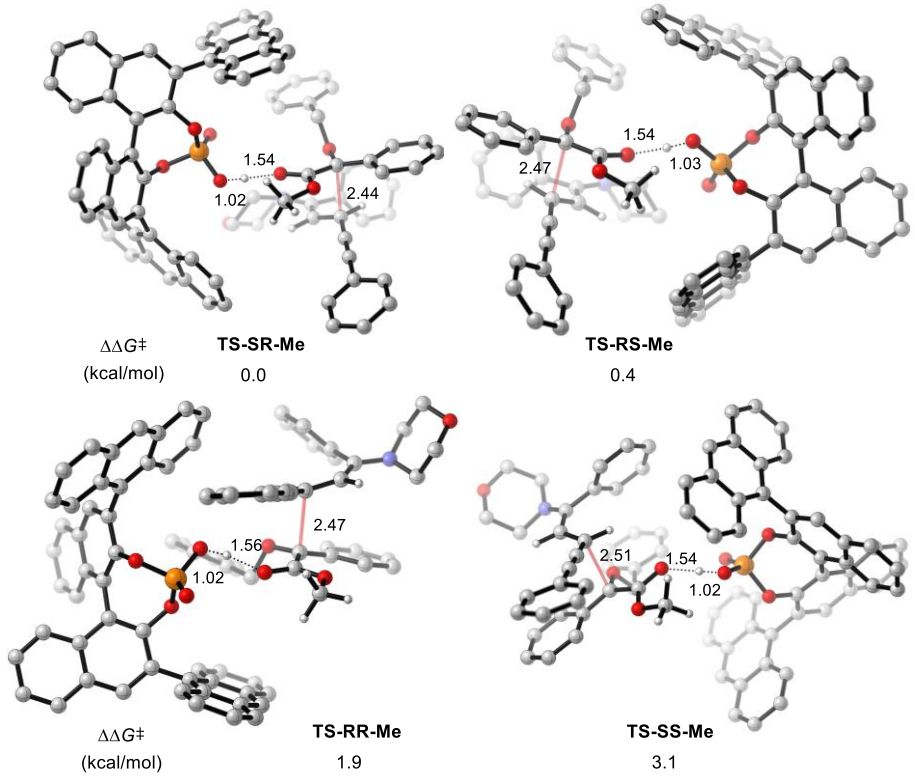



**Figure S8.** Optimized transition state geometries of symmetric Michael addition using CPA **6b** and diazoester **2b**. The Gibbs free energies were computed with CPCM(DCM)-M06-2X/6-311+G(d,p)//CPCM(DCM)-B3LYP/6-31G(d).

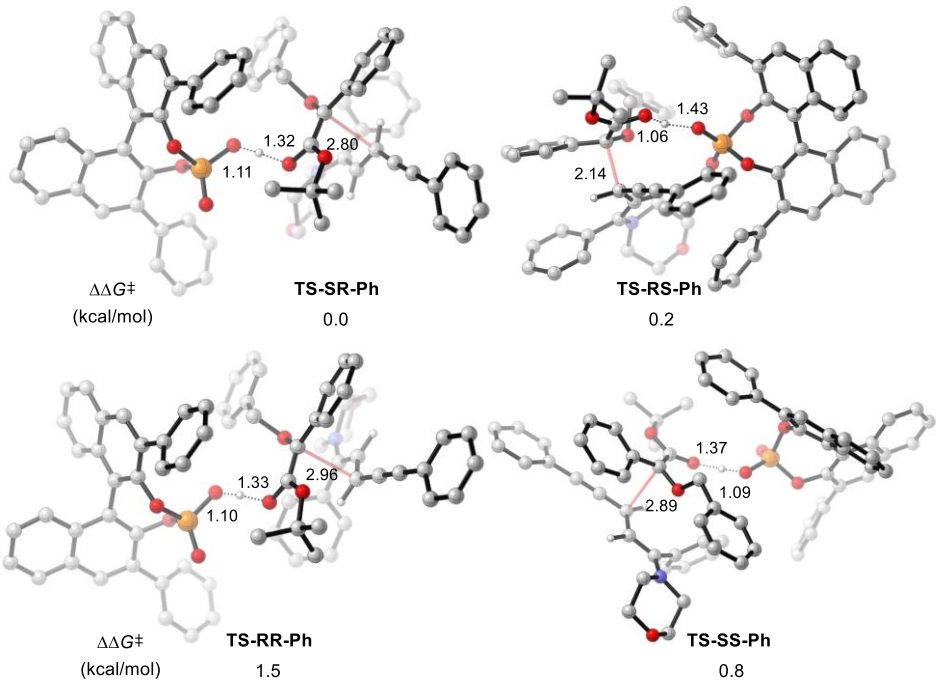



**Figure S9.** Optimized transition state geometries of symmetric Michael addition using CPA **6c** and diazoester **2a**. The Gibbs free energies were computed with CPCM(DCM)-M06-2X/6-311+G(d,p)//CPCM(DCM)-B3LYP/6-31G(d).

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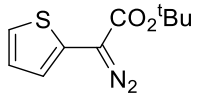
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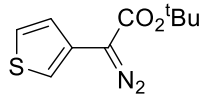
39. CYLview, 1.0b; Legault, C. Y., Université de Sherbrooke, 2009 (http://www.cylview.org).

## 10. Analytical Data for the Products



**2h**

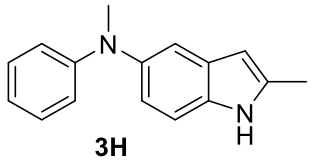
$^1$H NMR (400 MHz, $CDCl_3$) δ 7.30 (dd, *J* = 5.2, 1.2 Hz, 1H), 7.02 (dd, *J* = 5.2, 3.7 Hz, 1H), 6.76 (dd, *J* = 3.7, 1.2 Hz, 1H), 1.55 (s, 1H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 164.4, 126.8, 125.4, 120.3, 82.9, 55.8, 34.9, 28.4, 25.5.



**2i**

$^1$H NMR (400 MHz, $CDCl_3$) δ 7.39 – 7.34 (m, 2H), 7.01 (dd, *J* = 5.0, 1.4 Hz, 1H), 1.55 (s, 9H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 164.8, 126.2, 123.8, 122.5, 117.5, 37.2, 28.4, 28.1.

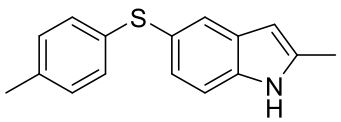
### N,2-Dimethyl-N-phenyl-1*H*-indol-5-amine (3H)



**3H**

Brown solid, mp: 91.8 – 92.3 °C; 885.5 mg, 75% yield; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.77 (s, 1H), 7.32 (d, *J* = 1.6 Hz, 1H), 7.23 (d, *J* = 8.6 Hz, 1H), 7.19 – 7.12 (m, 2H), 6.93 (dd, *J* = 8.5, 2.0 Hz, 1H), 6.78 – 6.67 (m, 3H), 6.17 (s, 1H), 3.30 (s, 3H), 2.41 (s, 3H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 150.6, 141.8, 136.0, 133.8, 130.0, 128.8, 120.4, 117.3, 117.2, 114.5, 111.1, 100.6, 40.9, 13.8. HRMS(ESI) $[M + H]^+$ calcd for $C_{16}H_{17}N_2^+$, 237.1386, found 237.1388.

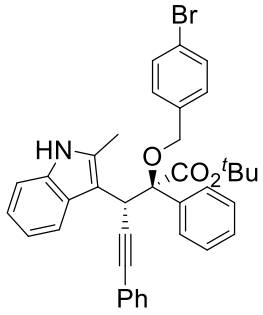
### 2-Methyl-5-(*p*-tolylthio)-1*H*-indole (3I)



**3l**

Yellow solid, mp: 116.6 – 117.5 ℃; 911.1 mg, 72% yield; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.89 (s, 1H), 7.66 (s, 1H), 7.22 – 7.19 (m, 2H), 7.09 (d, *J* = 8.2 Hz, 2H), 7.01 (d, *J* = 8.1 Hz, 2H), 6.18 (s, 1H), 2.42 (s, 3H), 2.27 (s, 3H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 136.1, 136.0, 135.8, 135.3, 130.0, 129.6, 128.4, 126.8, 125.6, 123.6, 111.2, 100.5, 21.0, 13.7. HRMS(ESI) $[M + H]^+$ calcd for $C_{16}H_{16}NS^+$, 254.0998, found 254.1001.

***tert*-Butyl (2*R*,3*R*)-2-((4-bromobenzyl)oxy)-3-(2-methyl-1*H*-indol-3-yl)-2,5-diphenylpent-4-ynoate (7)**



Yellow oil; 107.7 mg, 87% yield, >20:1 d.r., 94% *ee*, $[\alpha]_D^{20}$ = 3.76 (c = 0.033, MeOH); $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 5.6 Hz, 1H), 7.62 (s, 1H), 7.46 – 7.42 (m, 2H), 7.34 (d, *J* = 8.3 Hz, 2H), 7.28 (s, 4H), 7.22 – 7.14 (m, 3H), 7.08 (d, *J* = 4.3 Hz, 4H), 7.06 – 7.01 (m, 1H), 6.91 (t, *J* = 7.5 Hz, 1H), 4.81 (d, *J* = 13.0 Hz, 1H), 4.74 (s, 1H), 4.29 (d, *J* = 13.0 Hz, 1H), 1.57 (s, 3H), 1.53 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 170.9, 139.3, 136.1, 135.0, 134.3, 131.7, 131.0, 128.9, 128.5, 128.3, 128.0, 127.9, 127.7, 127.5, 124.1, 120.8, 120.3, 119.1, 109.8, 105.9, 89.7, 89.6, 83.2, 83.0, 67.7, 41.6, 28.2, 11.2. HRMS(ESI) $[M+Na]^+$ calcd for $C_{37}H_{34}BrNO_3Na^+$, 642.1614, found 642.1614. (Chiral IA, λ= 254 nm, *n*-hexane/2-propanol = 98/2, Flow rate = 1.0 mL/min), $t_R$ = 17.637 min, 20.256 min (major).

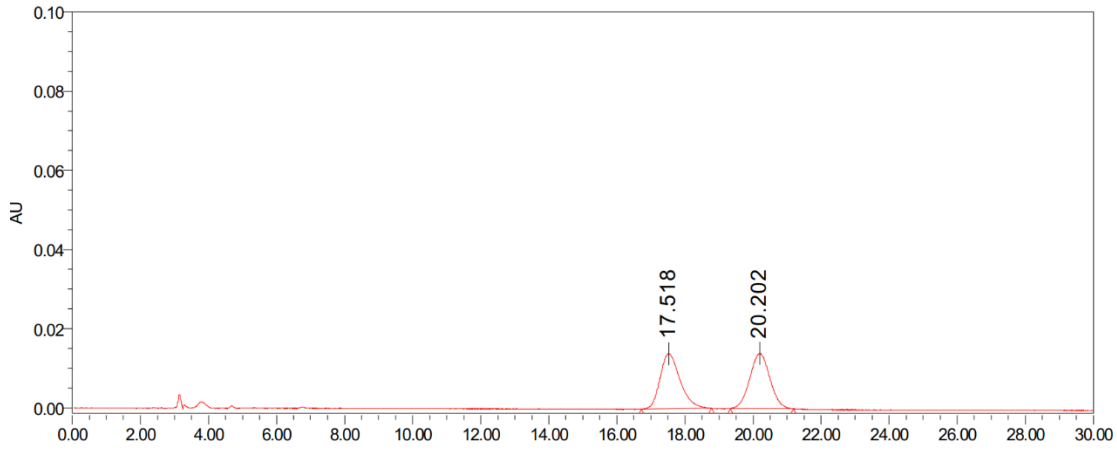
**HPLC chromatogram of racemic 7**

Condition: n-hexane/2-propanol = 98:2

Flow rate = 1.0 mL/min

λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 17.518 | 566658 | 13898 | 49.97 |
| 2 | 20.202 | 567229 | 13895 | 50.03 |

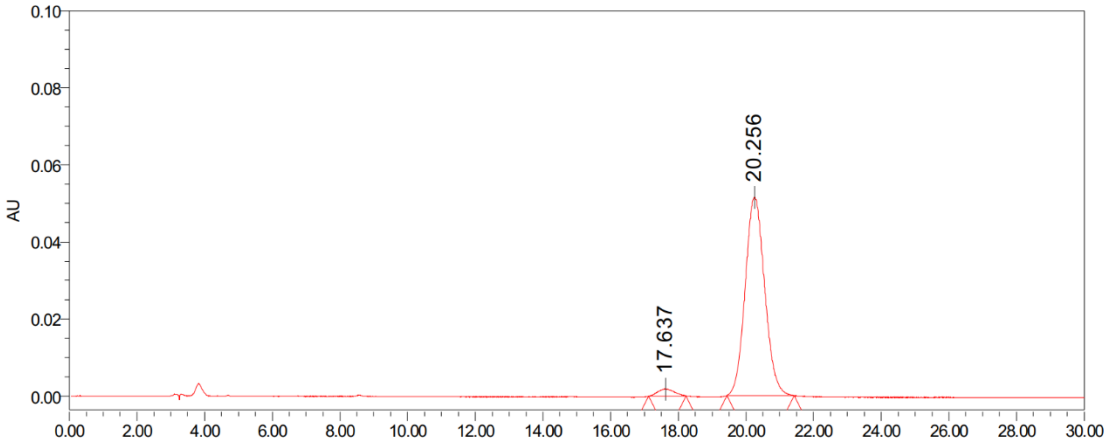
**HPLC chromatogram of chiral 7**

Condition: n-hexane/2-propanol = 98:2

Flow rate = 1.0 mL/min

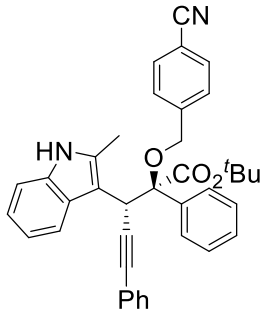
λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 17.637 | 61443 | 1816 | 2.92 |
| 2 | 20.256 | 2040876 | 51444 | 97.08 |

***tert*-Butyl (2*R*,3*R*)-2-((4-cyanobenzyl)oxy)-3-(2-methyl-1*H*-indol-3-yl)-2,5-diphenylpent-4-ynoate (8)**




**8**

Yellow oil; 88.3 mg, 78% yield, >20:1 d.r., 92% *ee*, $[\alpha]_D^{20}$ = -15.48 (c = 0.033, MeOH); $^1$H NMR (400 MHz, $CDCl_3$) δ 7.95 (s, 1H), 7.72 (s, 1H), 7.47 (ddd, *J* = 9.6, 9.1, 5.2 Hz, 6H), 7.32 – 7.28 (m, 3H), 7.21 (dd, *J* = 12.9, 7.3 Hz, 2H), 7.10 (t, *J* = 7.6 Hz, 2H), 7.08 – 7.02 (m, 3H), 6.92 (t, *J* = 7.4 Hz, 1H), 4.89 (d, *J* = 14.2 Hz, 1H), 4.74 (s, 1H), 4.40 (d, *J* = 14.2 Hz, 1H), 1.53 (s, 12H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 170.8, 146.1, 135.9, 135.1, 134.4, 131.8, 131.6, 128.8, 128.3, 128.2, 127.9, 127.8, 127.6, 127.1, 123.9, 121.7, 120.9, 119.4, 119.1, 110.2, 109.9, 105.7, 89.9, 89.5, 83.3, 83.2, 67.7, 41.5, 28.2, 11.0.

HRMS(ESI) $[M + Na]^+$ calcd for $C_{38}H_{34}N_2O_3Na^+$, 589.2462, found 589.2465. (Chiral IA, λ = 254 nm, *n*-hexane/2-propanol = 95/5, Flow rate = 1.0 mL/min), $t_R$ =17.555 min, 19.020 min (major).

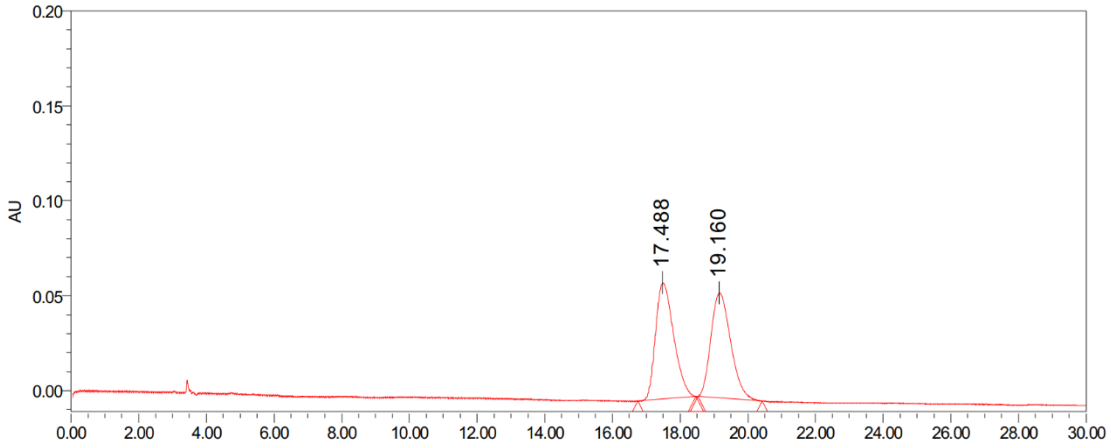
**HPLC chromatogram of racemic 8**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 17.488 | 2270400 | 61235 | 50.30 |
| 2 | 19.160 | 2243630 | 55219 | 49.70 |

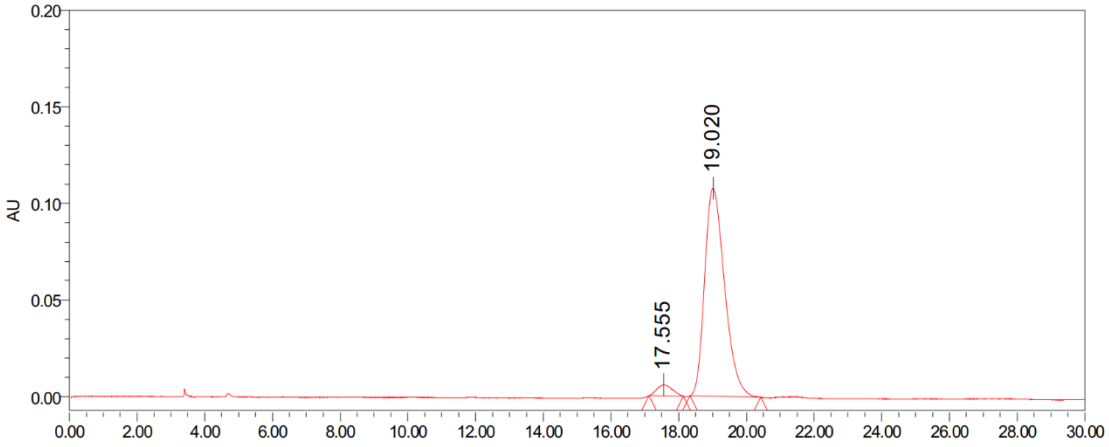
**HPLC chromatogram of chiral 8**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

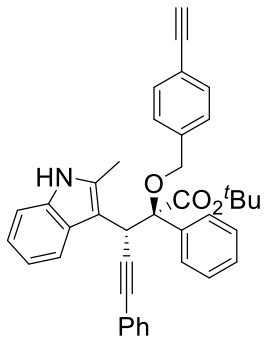
λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 17.555 | 182943 | 5711 | 3.95 |
| 2 | 19.020 | 4444458 | 107820 | 96.05 |

**_tert_-Butyl (2*R*,3*R*)-2-((4-ethynylbenzyl)oxy)-3-(2-methyl-1*H*-indol-3-yl)-2,5-diphenylpent-4-ynoate (9)**




**9**

Yellow oil; 59.9 mg, 53% yield, >20:1 d.r., 94% *ee*, $[\alpha]_D^{20}$ = -15.37 (c = 0.033, MeOH); $^1$H NMR (500 MHz, $CDCl_3$) δ 7.90 (s, 1H), 7.64 (s, 1H), 7.45 (d, *J* = 6.7 Hz, 2H), 7.37 (s, 4H), 7.29 (d, *J* = 6.2 Hz, 3H), 7.23 – 7.15 (m, 2H), 7.09 (d, *J* = 3.8 Hz, 4H), 7.03 (t, *J* = 7.5 Hz, 1H), 6.91 (t, *J* = 7.5 Hz, 1H), 4.86 (d, *J* = 13.3 Hz, 1H), 4.75 (s, 1H), 4.36 (d, *J* = 13.3 Hz, 1H), 3.03 (s, 1H), 1.59 (s, 3H), 1.51 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 171.0, 141.3, 136.2, 135.0, 134.3, 131.8, 131.7, 128.9, 128.2, 128.0, 127.9, 127.7, 127.4, 126.6, 124.1, 120.8, 120.1, 119.1, 109.7, 106.0, 89.7, 89.6, 84.1, 83.1,

83.0, 76.6, 68.0, 41.6, 28.2, 11.2. HRMS(ESI) $[M+Na]^+$ calcd for $C_{39}H_{35}NO_3Na^+$, 588.2509, found 588.2512. (Chiral IA, λ = 254 nm, *n*-hexane/2-propanol = 90/10, Flow rate = 1.0 mL/min), $t_R$ = 5.332 min, 5.933 min (major).

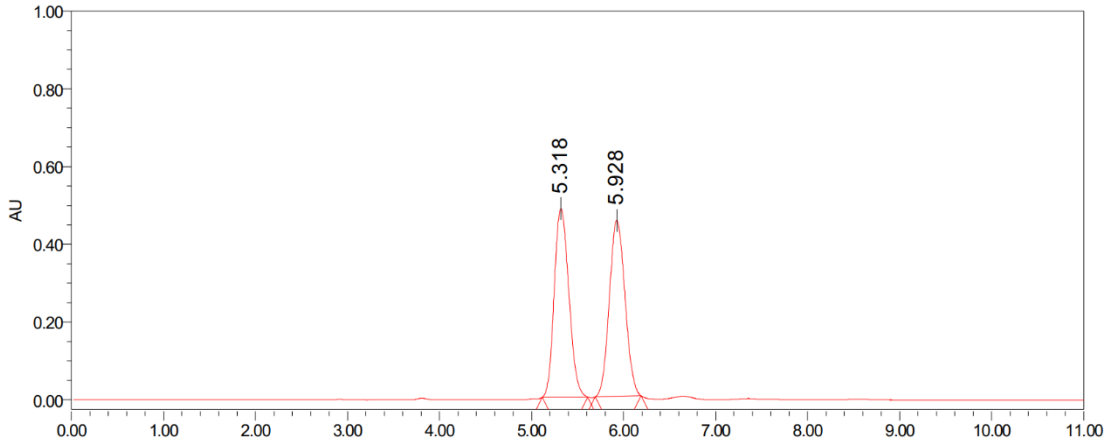
**HPLC chromatogram of racemic 9**

Condition: n-hexane/2-propanol = 90:10

Flow rate = 1.0 mL/min

λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 5.318 | 5362827 | 485056 | 50.02 |
| 2 | 5.928 | 5359577 | 452626 | 49.98 |

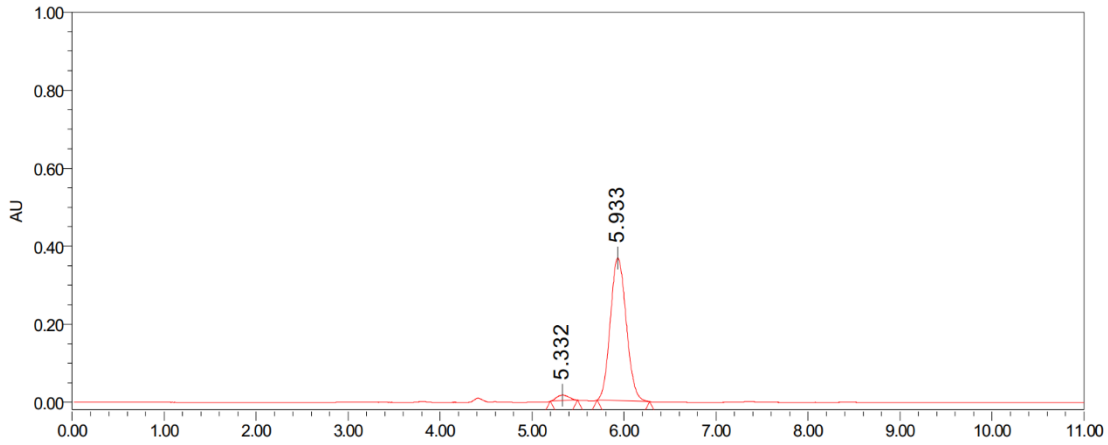
**HPLC chromatogram of chiral 9**

Condition: n-hexane/2-propanol = 90:10

Flow rate = 1.0 mL/min

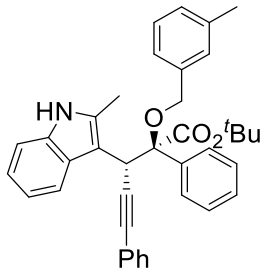
λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 5.332 | 134818 | 14395 | 2.97 |
| 2 | 5.933 | 4406257 | 365597 | 97.03 |

**_tert_-Butyl (2*R*,3*R*)-3-(2-methyl-1*H*-indol-3-yl)-2-((3-methylbenzyl)oxy)-2,5-diphenylpent-4-ynoate (10)**




**10**

Yellow oil; 98.8 mg, 89% yield, >20:1 d.r., 91% *ee*, $[\alpha]_D^{20}$ = 30.22 (c = 0.033, MeOH); $^1$H NMR (500 MHz, $CDCl_3$) δ 7.89 (s, 1H), 7.62 (s, 1H), 7.45 (d, *J* = 7.0 Hz, 2H), 7.26 (d, *J* = 5.9 Hz, 3H), 7.21 – 7.12 (m, 6H), 7.09 (dd, *J* = 14.4, 7.2 Hz, 3H), 7.01 (dd, *J* = 13.6, 6.6 Hz, 2H), 6.89 (t, *J* = 7.5 Hz, 1H), 4.88 (d, *J* = 12.6 Hz, 1H), 4.78 (s, 1H), 4.35 (d, *J* = 12.6 Hz, 1H), 2.21 (s, 3H), 1.61 (s, 3H), 1.52 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 171.1, 140.1, 137.4, 136.4, 135.0, 134.4, 131.8, 128.9, 128.2, 128.0, 127.9, 127.7, 127.6, 127.4, 127.3, 124.3, 123.8, 120.7, 119.1, 109.7, 106.1, 89.8, 89.5, 83.1,

82.8, 68.3, 41.6, 28.2, 21.4, 11.3. HRMS(ESI) $[M+Na]^+$ calcd for $C_{38}H_{37}NO_3Na^+$, 578.2666, found 578.2665. (Chiral IA, λ = 254 nm, *n*-hexane/2-propanol = 90/10, Flow rate = 1.0 mL/min), $t_R$ =4.869 min, 11.056 min (major).

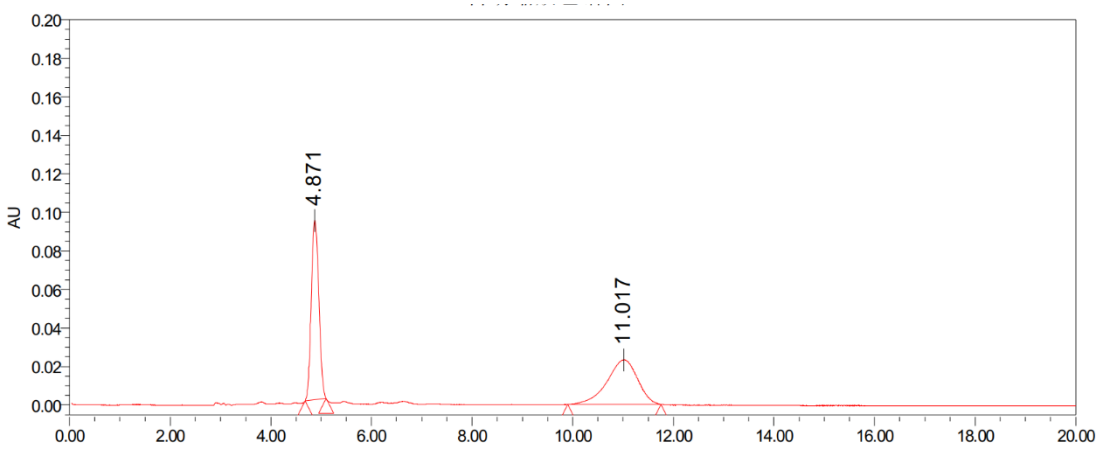
**HPLC chromatogram of racemic 10**

Condition: n-hexane/2-propanol = 90:10

Flow rate = 1.0 mL/min

λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 4.871 | 971838 | 93046 | 50.06 |
| 2 | 11.017 | 969335 | 23124 | 49.94 |

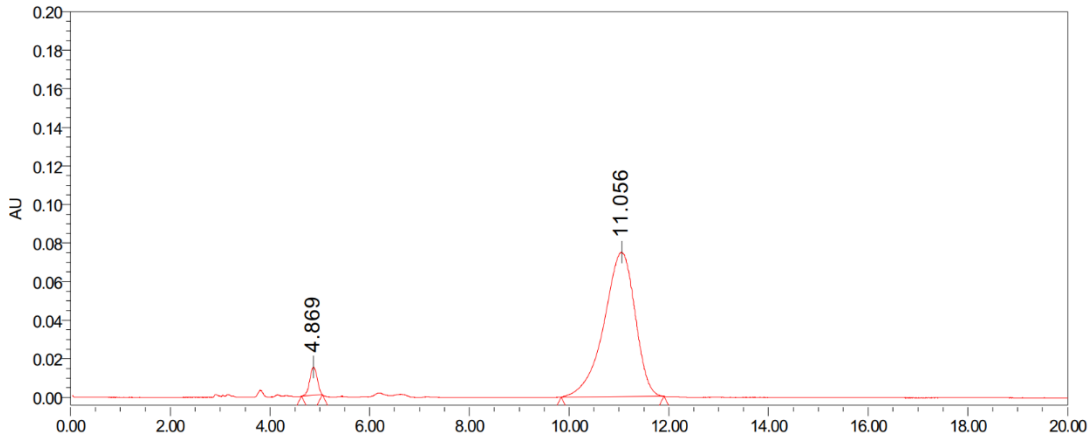
**HPLC chromatogram of chiral 10**

Condition: n-hexane/2-propanol = 90:10

Flow rate = 1.0 mL/min

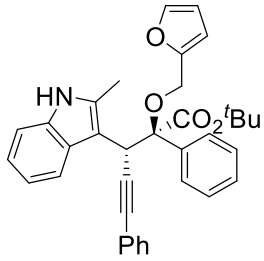
λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 4.869 | 153051 | 14659 | 4.52 |
| 2 | 11.056 | 3234379 | 74842 | 95.48 |

**_tert_-Butyl (2*R*,3*R*)-2-(furan-2-ylmethoxy)-3-(2-methyl-1*H*-indol-3-yl)-2,5-diphenylpent-4-ynoate (11)**




**11**

Yellow oil; 86.1 mg, 81% yield, >20:1 d.r., 88% *ee*, $[\alpha]_D^{20}$ = 63.29 (c = 0.033, MeOH); $^1$H NMR (500 MHz, $CDCl_3$) δ 7.67 (s, 1H), 7.63 (s, 1H), 7.41 – 7.38 (m, 2H), 7.28 (s, 1H), 7.25 (dt, *J* = 8.5, 4.3 Hz, 3H), 7.20 – 7.17 (m, 1H), 7.15 (d, *J* = 7.9 Hz, 3H), 7.09 (t, *J* = 7.6 Hz, 2H), 7.00 (t, *J* = 7.5 Hz, 1H), 6.84 (t, *J* = 7.5 Hz, 1H), 6.26 (s, 1H), 6.18 (d, *J* = 3.0 Hz, 1H), 4.97 (d, *J* = 12.5 Hz, 1H), 4.70 (s, 1H), 4.25 (d, *J* = 12.5 Hz, 1H), 1.67 (s, 3H), 1.63 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 171.1, 153.0, 141.7, 136.0, 134.8, 134.3, 131.7, 129.0, 128.1, 127.9, 127.5, 127.4, 124.3, 120.5, 118.9, 110.1, 109.4,

108.0, 106.1, 89.6, 89.4, 82.9, 82.8, 61.3, 41.4, 28.3, 11.3. HRMS(ESI) $[M+Na]^+$ calcd for $C_{35}H_{33}NO_4Na^+$, 554.2302, found 554.2300. (Chiral IA, λ = 254 nm, *n*-hexane/2-propanol = 95/5, Flow rate = 1.0 mL/min), $t_R$ =7.959 min, 13.869 min (major).

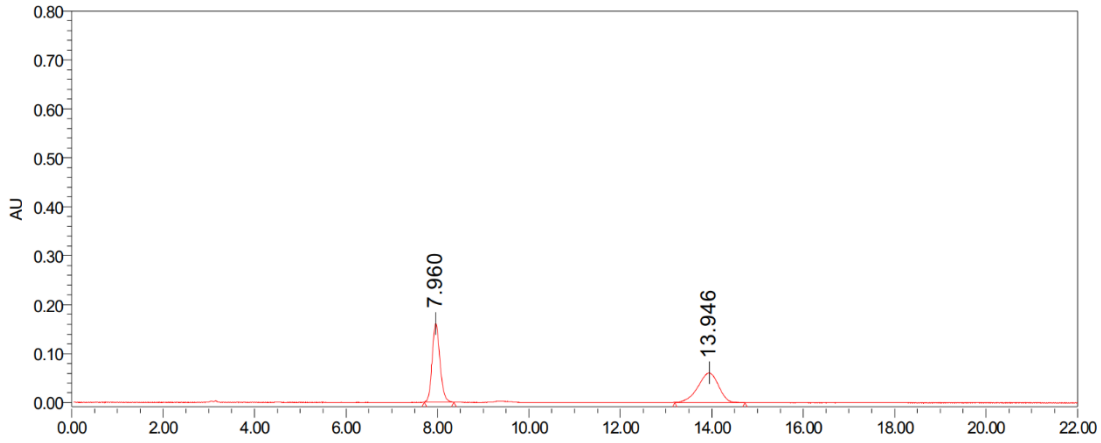
**HPLC chromatogram of racemic 11**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 7.960 | 1888114 | 160626 | 49.90 |
| 2 | 13.946 | 1895507 | 60340 | 50.10 |

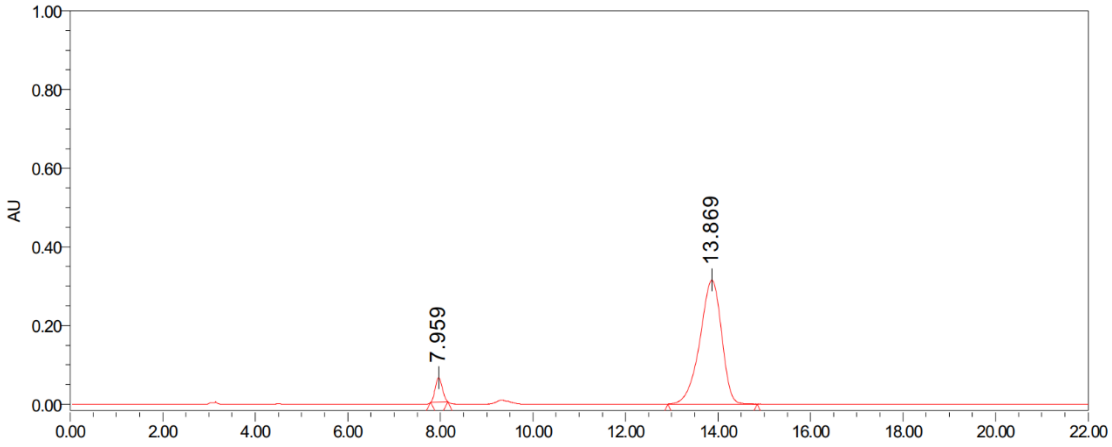
**HPLC chromatogram of chiral 11**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

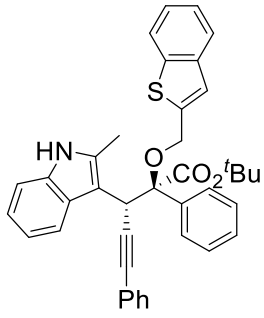
λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 7.959 | 653936 | 61580 | 5.98 |
| 2 | 13.869 | 10276348 | 315178 | 94.02 |

**_tert_-Butyl (2*R*,3*R*)-2-(benzo[b]thiophen-2-ylmethoxy)-3-(2-methyl-1*H*-indol-3-yl)-2,5-diphenylpent-4-ynoate (12)**




**12**

Brown solid, mp: 91.9 – 92.8 °C; 78.8 mg, 66% yield, >20:1 d.r., 94% *ee*, $[\alpha]_D^{20}$ = -3.59 (c = 0.033, MeOH); $^1$H NMR (500 MHz, $CDCl_3$) δ 7.92 (s, 1H), 7.75 (d, *J* = 7.6 Hz, 1H), 7.61 (s, 1H), 7.56 (d, *J* = 7.5 Hz, 1H), 7.49 (d, *J* = 4.0 Hz, 2H), 7.27 (d, *J* = 5.0 Hz, 4H), 7.23 – 7.07 (m, 8H), 7.02 (t, *J* = 7.4 Hz, 1H), 6.87 (t, *J* = 7.4 Hz, 1H), 5.13 (d, *J* = 13.0 Hz, 1H), 4.76 (s, 1H), 4.57 (d, *J* = 13.1 Hz, 1H), 1.64 (s, 3H), 1.59 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 170.9, 143.9, 139.9, 139.7, 136.0, 135.0, 134.4, 131.8, 129.0, 128.2, 128.1, 127.8, 127.63, 127.55, 124.2, 123.9, 123.6, 123.2, 122.2, 120.9,

120.7, 119.2, 109.7, 105.9, 89.8, 89.5, 83.2, 83.1, 64.9, 41.5, 28.3, 11.4. HRMS(ESI) $[M+Na]^+$ calcd for $C_{39}H_{35}NO_3SNa^+$, 620.2230, found 620.2231. (Chiral IA, λ = 254 nm, *n*-hexane/2-propanol = 95/5, Flow rate = 1.0 mL/min), $t_R$ = 9.245 min, 11.002 min (major).

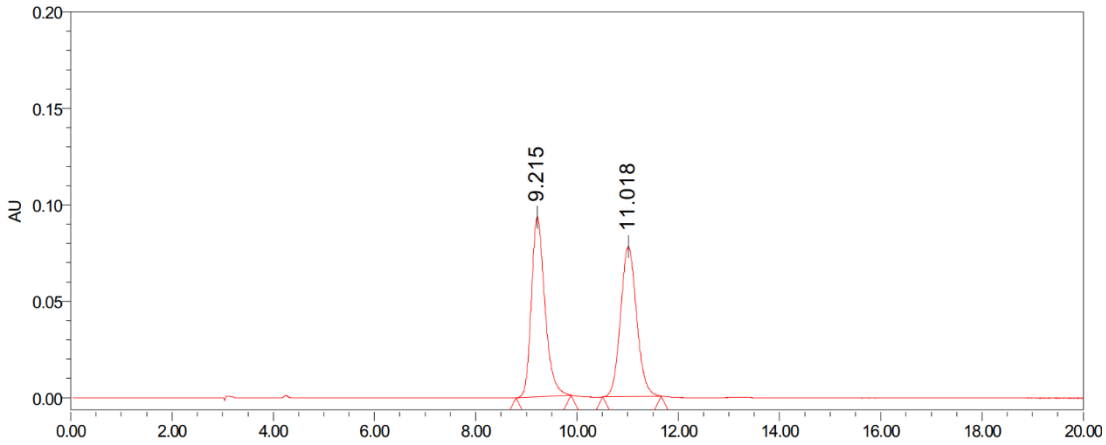
**HPLC chromatogram of racemic 12**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 9.215 | 1708962 | 93171 | 50.04 |
| 2 | 11.018 | 1706154 | 77828 | 49.96 |

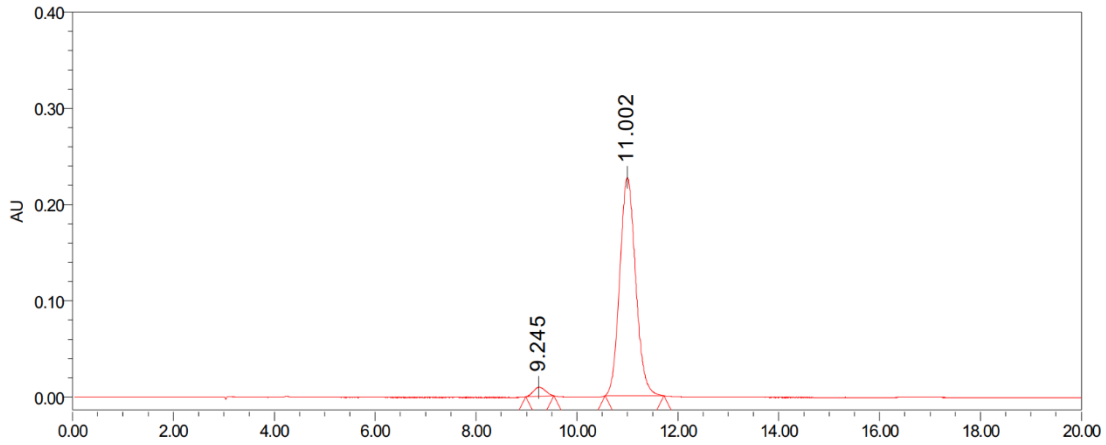
**HPLC chromatogram of chiral 12**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

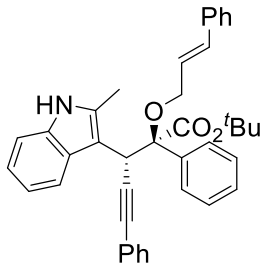
λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 9.245 | 156854 | 9561 | 3.08 |
| 2 | 11.002 | 4940033 | 226728 | 96.92 |

***tert*-Butyl (2*R*,3*R*)-2-(cinnamyloxy)-3-(2-methyl-1*H*-indol-3-yl)-2,5-diphenylpent-4-ynoate (13)**




**13**

Yellow oil; 77.1 mg, 68% yield, >20:1 d.r., 90% *ee*, $[\alpha]_D^{20}$ = -6.77 (c = 0.033, MeOH); $^1$H NMR (500 MHz, $CDCl_3$) δ 8.05 (s, 1H), 7.62 (s, 1H), 7.43 (dd, *J* = 6.5, 3.0 Hz, 2H), 7.24 (dd, *J* = 9.7, 5.1 Hz, 5H), 7.18 (dd, *J* = 6.3, 5.2 Hz, 5H), 7.12 – 7.05 (m, 5H), 7.01 (t, *J* = 7.4 Hz, 1H), 6.59 (d, *J* = 16.0 Hz, 1H), 6.20 (dt, *J* = 16.0, 4.8 Hz, 1H), 4.70 (s, 1H), 4.56 (ddd, *J* = 14.1, 4.6, 1.5 Hz, 1H), 3.94 (ddd, *J* = 14.2, 4.8, 1.4 Hz, 1H), 1.63 (s, 9H), 1.56 (s, 3H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 171.3, 137.6, 136.5, 135.1, 134.3,

131.8, 129.9, 129.1, 128.5, 128.2, 127.9, 127.84, 127.78, 127.6, 127.4, 127.1, 126.4, 124.3, 120.8, 119.1, 109.9, 106.2, 89.8, 89.7, 83.0, 82.9, 67.5, 41.6, 28.4, 11.1. HRMS(ESI) $[M+Na]^+$ calcd for $C_{39}H_{37}NO_3Na^+$, 590.2666, found 590.2665. (Chiral IA, λ = 254 nm, *n*-hexane/2-propanol = 98/2, Flow rate = 1.0 mL/min), $t_R$ = 23.652 min, 27.172 min (major).

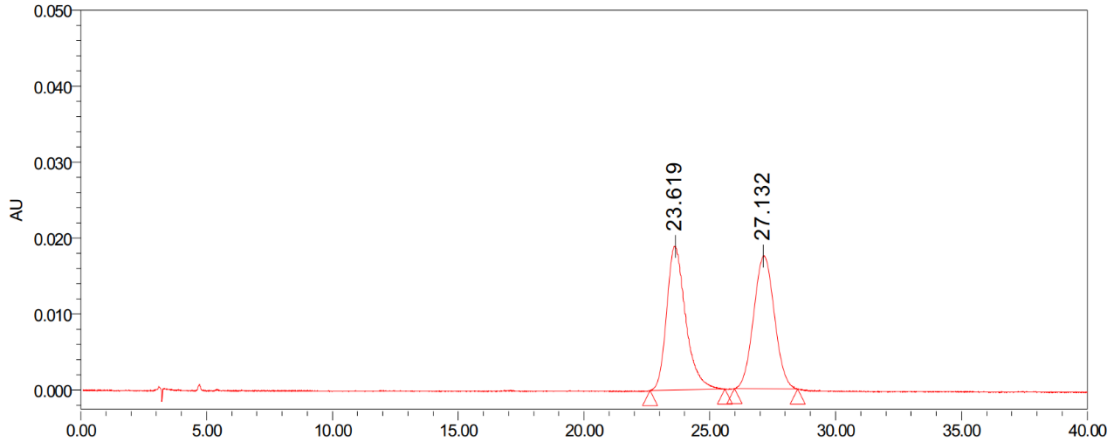
**HPLC chromatogram of racemic 13**

Condition: n-hexane/2-propanol = 98:2

Flow rate = 1.0 mL/min

λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 23.619 | 1003153 | 18908 | 50.00 |
| 2 | 27.132 | 1003050 | 17482 | 50.00 |

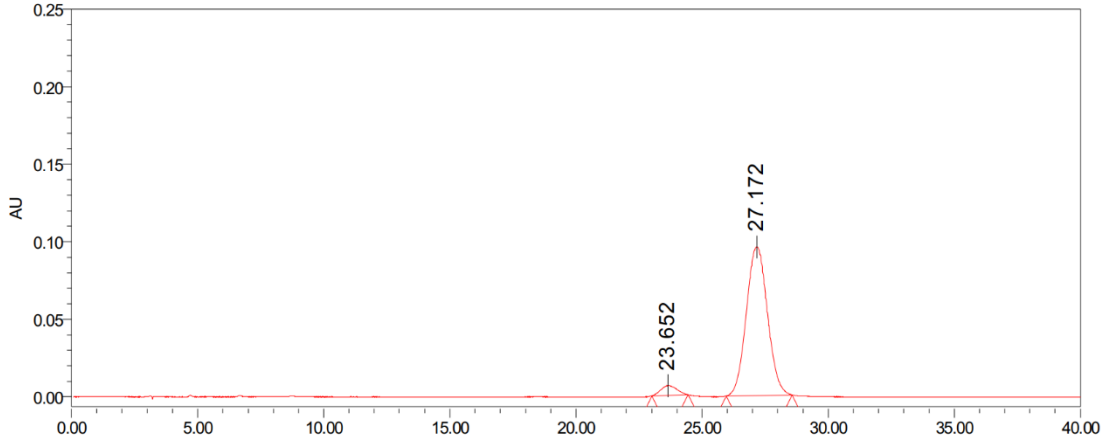
**HPLC chromatogram of chiral 13**

Condition: n-hexane/2-propanol = 98:2

Flow rate = 1.0 mL/min

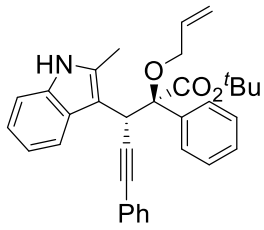
λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 23.652 | 279299 | 6244 | 4.80 |
| 2 | 27.172 | 5534956 | 95859 | 95.20 |

**_tert_-Butyl (2*R*,3*R*)-2-(allyloxy)-3-(2-methyl-1*H*-indol-3-yl)-2,5-diphenylpent-4-ynoate (14)**




**14**

Yellow solid, mp: 117.4 – 118.4 ℃; 49.1 mg, 50% yield, >20:1 d.r., 68% *ee*, $[\alpha]_D^{20}$ = 45.29 (c = 0.033, MeOH); $^1$H NMR (500 MHz, $CDCl_3$) δ 7.92 (s, 1H), 7.64 (s, 1H), 7.43 – 7.39 (m, 2H), 7.28 – 7.22 (m, 3H), 7.18 (dd, *J* = 10.0, 6.6 Hz, 2H), 7.06 (dd, *J* = 15.5, 6.2 Hz, 5H), 6.99 (t, *J* = 7.4 Hz, 1H), 5.98 – 5.81 (m, 1H), 5.26 (dd, *J* = 17.3, 1.8 Hz, 1H), 5.03 (dd, *J* = 10.6, 1.6 Hz, 1H), 4.69 (s, 1H), 4.36 (ddd, *J* = 13.4, 2.8, 1.9 Hz, 1H), 3.82 – 3.75 (m, 1H), 1.64 (s, 3H), 1.62 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ

171.1, 136.5, 136.0, 135.0, 134.2, 131.7, 129.0, 128.1, 127.9, 127.8, 127.5, 127.3, 124.3, 120.7, 119.0, 115.0, 109.6, 106.3, 89.7, 89.3, 82.8, 82.7, 67.9, 41.4, 28.3, 11.3. HRMS(ESI) $[M+Na]^+$ calcd for $C_{33}H_{33}NO_3Na^+$, 514.2353, found 514.2352. (Chiral IA, λ = 254 nm, *n*-hexane/2-propanol = 95/5, Flow rate = 1.0 mL/min), $t_R$ = 6.917 min, 9.166 min (major).

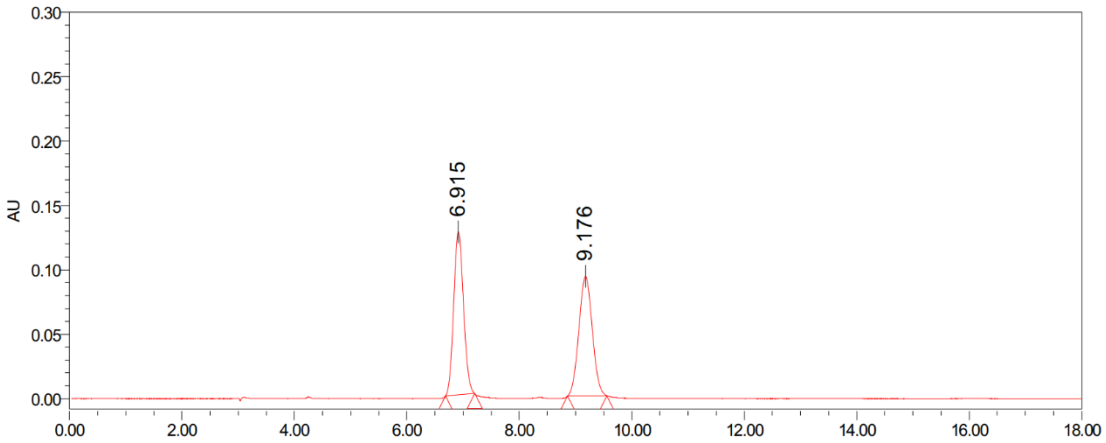
**HPLC chromatogram of racemic 14**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 6.915 | 1537068 | 126405 | 49.91 |
| 2 | 9.176 | 1542638 | 92762 | 50.09 |

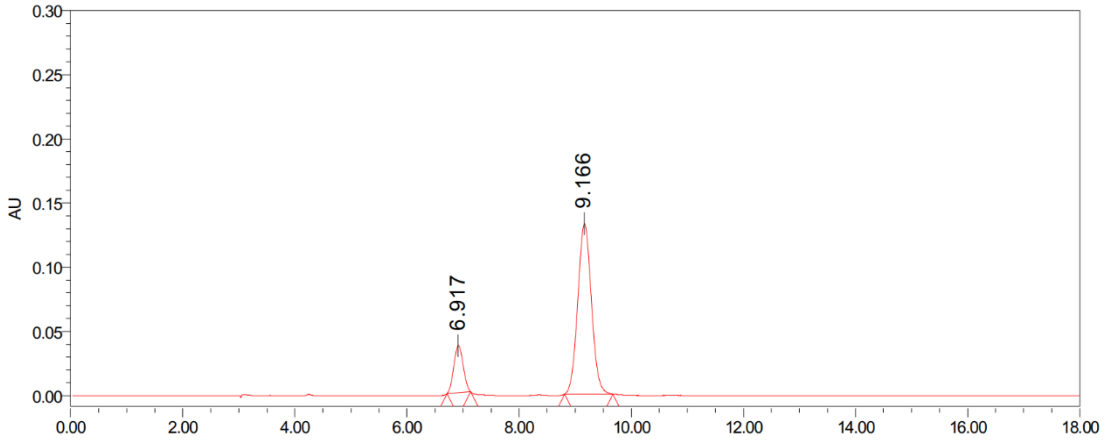
**HPLC chromatogram of chiral 14**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

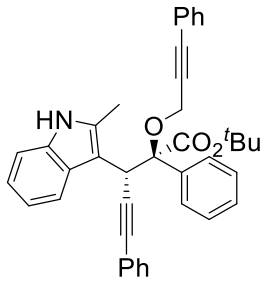
λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 6.917 | 426024 | 36603 | 15.91 |
| 2 | 9.166 | 2251782 | 132731 | 84.09 |

***tert*-Butyl (2*R*,3*R*)-3-(2-methyl-1*H*-indol-3-yl)-2,5-diphenyl-2-((3-phenylprop-2-yn-1-yl)oxy)pent-4-ynoate (15)**




**15**

Yellow oil; 50.9 mg, 45% yield, >20:1 d.r., 92% *ee*, $[\alpha]_D^{20}$ = 15.74 (c = 0.033, MeOH); $^1$H NMR (500 MHz, $CDCl_3$) δ 7.92 (s, 1H), 7.64 (s, 1H), 7.45 – 7.42 (m, 2H), 7.30 – 7.26 (m, 5H), 7.26 – 7.22 (m, 3H), 7.16 (dd, *J* = 9.6, 4.9 Hz, 4H), 7.08 (t, *J* = 7.6 Hz, 2H), 7.02 (t, *J* = 7.4 Hz, 1H), 6.96 (t, *J* = 7.4 Hz, 1H), 4.86 (d, *J* = 15.6 Hz, 1H), 4.69 (s, 1H), 4.10 (d, *J* = 15.6 Hz, 1H), 1.78 (s, 3H), 1.64 (s, 9H). $^{13}$C NMR (126 MHz,

$CDCl_3$) δ 171.0, 135.8, 134.9, 134.3, 131.8, 131.6, 129.0, 128.13, 128.08, 128.03, 127.96, 127.7, 127.5, 124.2, 123.3, 120.6, 119.1, 109.5, 106.1, 89.9, 89.5, 87.0, 85.2, 83.0, 82.8, 56.0, 41.3, 28.3, 11.5. HRMS(ESI) $[M+Na]^+$ calcd for $C_{39}H_{35}NO_3Na^+$, 588.2509, found 588.2513. (Chiral IA, λ = 254 nm, *n*-hexane/2-propanol = 95/5, Flow rate = 1.0 mL/min), $t_R$ = 9.774 min, 13.980 min (major).

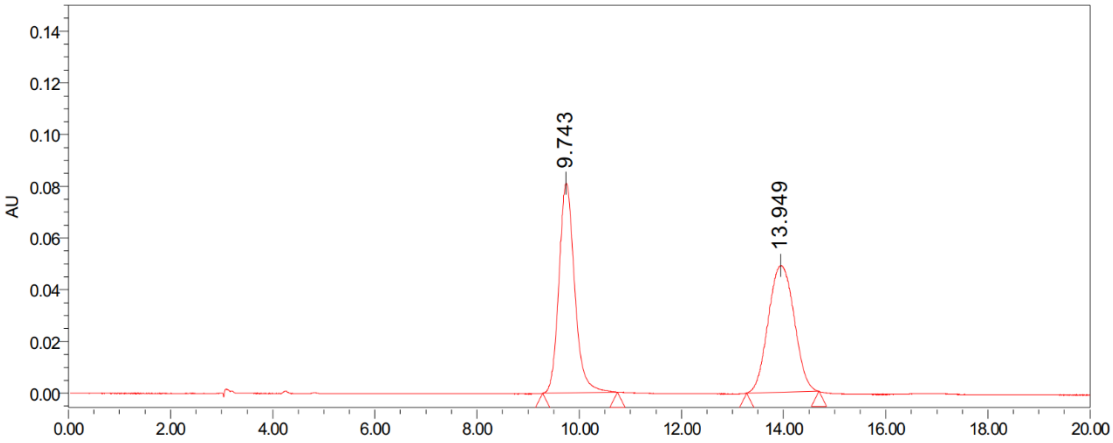
**HPLC chromatogram of racemic 15**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 9.743 | 1731460 | 80994 | 50.09 |
| 2 | 13.949 | 1725249 | 48998 | 49.91 |

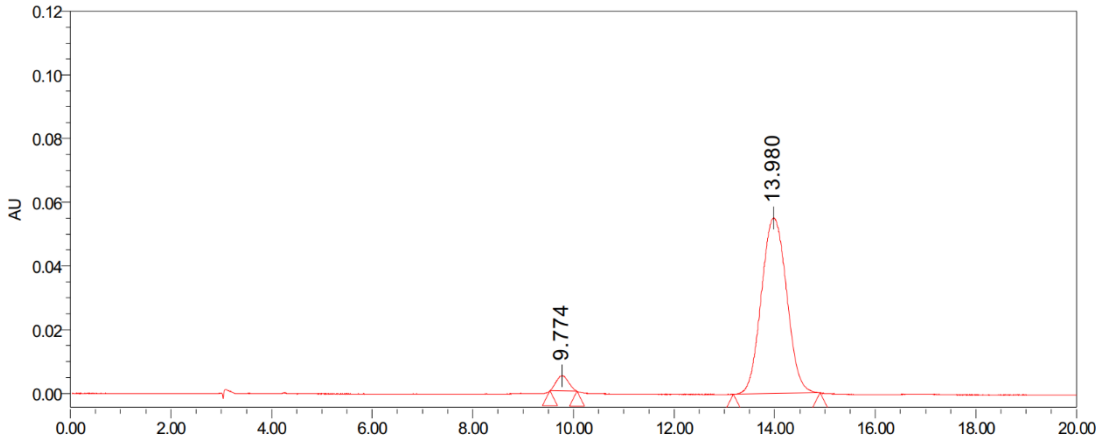
**HPLC chromatogram of chiral 15**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

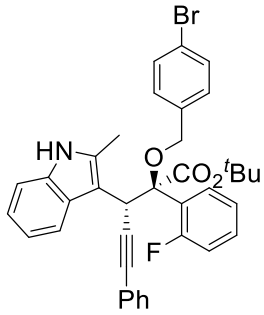
λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 9.774 | 80948 | 4809 | 4.03 |
| 2 | 13.980 | 1926825 | 55178 | 95.97 |

***tert*-Butyl (2*R*,3*R*)-2-((4-bromobenzyl)oxy)-2-(2-fluorophenyl)-3-(2-methyl-1*H*-indol-3-yl)-5-phenylpent-4-ynoate (16)**




**16**

Yellow oil; 104.5 mg, 82% yield, >20:1 d.r., 93% *ee*, $[\alpha]_D^{20}$ = 27.69 (c = 0.033, MeOH); $^1$H NMR (500 MHz, $CDCl_3$) δ 7.60 (s, 1H), 7.49 (d, *J* = 8.0 Hz, 1H), 7.41 (d, *J* = 8.4 Hz, 2H), 7.37 (s, 2H), 7.37 – 7.35 (m, 2H), 7.29 – 7.26 (m, 3H), 7.25 (s, 1H), 7.14 (dd, *J* = 10.4, 4.3 Hz, 1H), 7.10 (d, *J* = 8.0 Hz, 1H), 6.97 (t, *J* = 7.5 Hz, 1H), 6.89 (t, *J* = 7.6 Hz, 1H), 6.80 (t, *J* = 7.5 Hz, 1H), 6.74 (dd, *J* = 11.3, 8.3 Hz, 1H), 5.17 (s, 1H), 5.00 (d,

$J$ = 12.2 Hz, 1H), 4.60 (d, $J$ = 12.2 Hz, 1H), 2.10 (s, 3H), 1.39 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 168.6, δ 160.1 (d, $J$ = 247.0 Hz), 138.2, 134.9, 133.7, 131.6, 131.3, 129.52 (d, $J$ = 23.9 Hz), 129.50 (d, $J$ = 11.3 Hz), 129.0, 128.5, 128.2, 127.6, 126.4 (d, $J$ = 11.3 Hz), 124.2, 123.2 (d, $J$ = 2.5 Hz), 121.0, 120.7, 120.5, 118.8, 115.3 (d, $J$ = 22.7 Hz), 109.5, 106.8, 89.6, 85.7, 83.2, 82.7, 67.3, 37.6, 27.8, 12.2. $^{19}$F NMR (376 MHz, $CDCl_3$) δ -109.74. HRMS(ESI) $[M+Na]^+$ calcd for $C_{37}H_{33}BrFNO_3Na^+$, 660.1520, found 660.1524. (Chiral IC, λ = 254 nm, *n*-hexane/2-propanol = 98/2, Flow rate = 1.0 mL/min), $t_R$ = 7.585 min, 12.561 min (major).

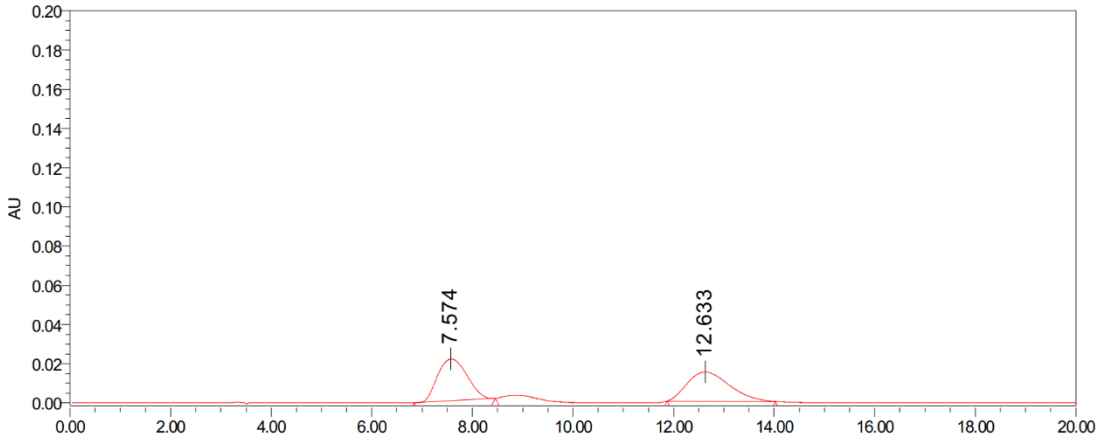
**HPLC chromatogram of racemic 16**

Condition: n-hexane/2-propanol = 98:2

Flow rate = 1.0 mL/min

λ = 254 nm

Chiral IC




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 7.574 | 871264 | 21326 | 49.96 |
| 2 | 12.633 | 872552 | 14880 | 50.04 |

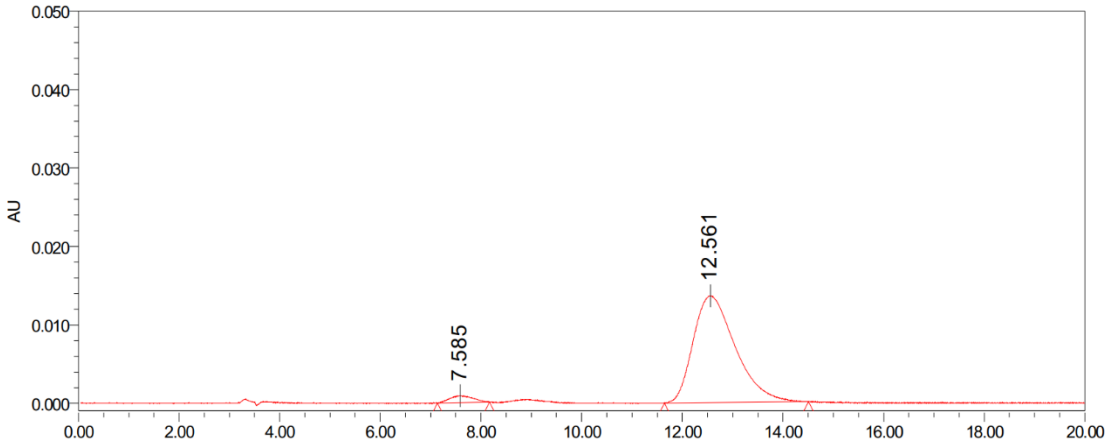
**HPLC chromatogram of chiral 16**

Condition: n-hexane/2-propanol = 98:2

Flow rate = 1.0 mL/min

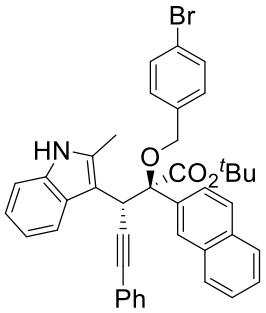
λ = 254 nm

Chiral IC




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 7.585 | 27962 | 862 | 3.42 |
| 2 | 12.561 | 788644 | 13587 | 96.58 |

***tert*-Butyl (2*R*,3*R*)-2-((4-bromobenzyl)oxy)-3-(2-methyl-1*H*-indol-3-yl)-2-(naphthalen-2-yl)-5-phenylpent-4-ynoate (17)**




**17**

Yellow solid, mp: 99.1 – 99.9 °C; 89.7 mg, 67% yield, >20:1 d.r., 92% *ee*, $[\alpha]_D^{20}$ = 42.19 (c = 0.033, MeOH); $^1$H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 6.9 Hz, 1H), 7.87

(s, 1H), 7.73 – 7.69 (m, 1H), 7.68 – 7.64 (m, 1H), 7.58 (s, 1H), 7.43 (ddd, $J$ = 6.5, 5.4, 2.9 Hz, 5H), 7.34 (d, $J$ = 8.4 Hz, 2H), 7.30 – 7.25 (m, 5H), 7.18 (d, $J$ = 8.0 Hz, 1H), 7.04 (t, $J$ = 7.3 Hz, 1H), 6.89 (dd, $J$ = 13.8, 7.3 Hz, 2H), 4.85 (s, 1H), 4.82 (d, $J$ = 13.3 Hz, 1H), 4.30 (d, $J$ = 12.9 Hz, 1H), 1.57 (s, 9H), 1.40 (s, 3H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 171.0, 139.2, 135.1, 134.1, 134.1, 132.8, 132.6, 131.7, 131.0, 128.8, 128.6, 128.5, 128.3, 127.8, 127.4, 127.3, 126.5, 126.4, 125.9, 125.8, 124.1, 120.9, 120.3, 119.2, 109.8, 106.1, 89.8, 89.6, 83.3, 83.1, 67.9, 41.7, 28.3, 11.2. HRMS(ESI) $[M+Na]^+$ calcd for $C_{41}H_{36}BrNO_3Na^+$, 692.1771, found 692.1770. (Chiral IA, λ = 254 nm, *n*-hexane/2-propanol = 95/5, Flow rate = 1.0 mL/min), $t_R$ = 8.828 min, 9.773 min (major).

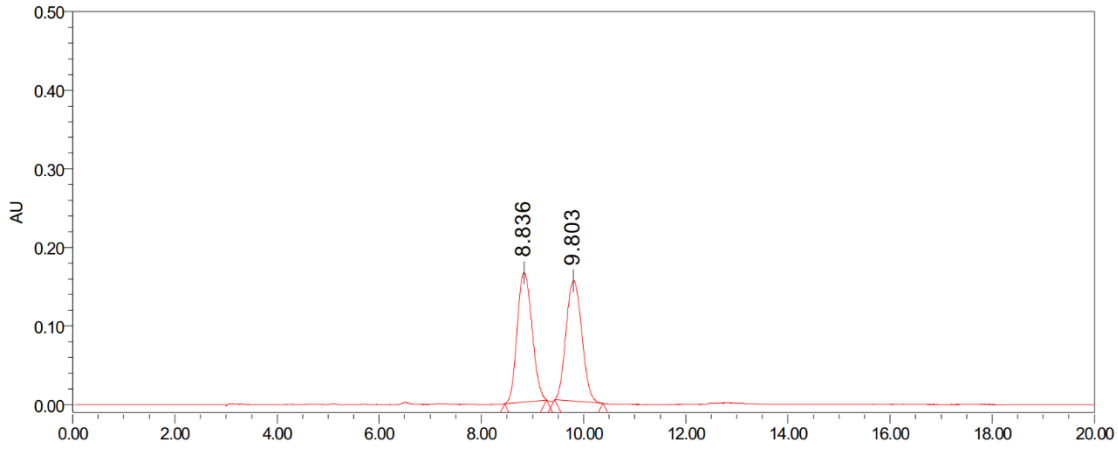
**HPLC chromatogram of racemic 17**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 8.836 | 3298871 | 164440 | 49.93 |
| 2 | 9.803 | 3308060 | 153201 | 50.07 |

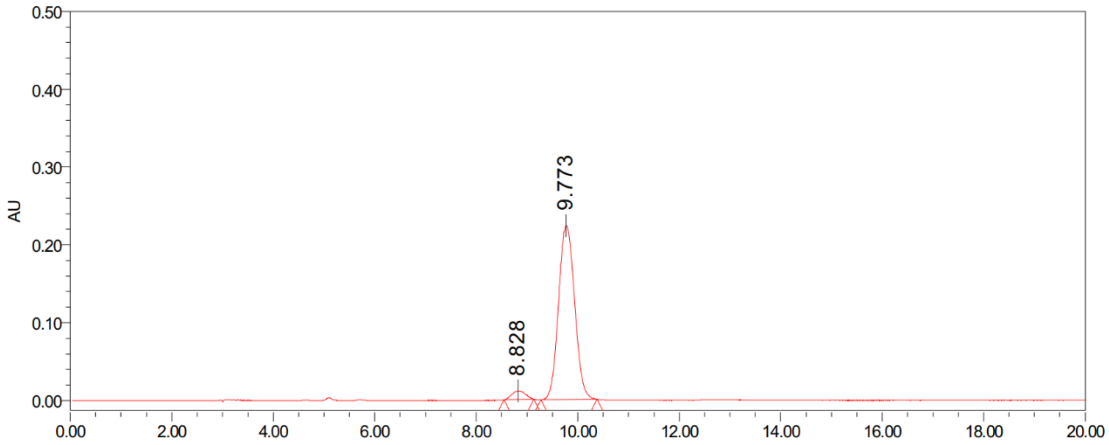
**HPLC chromatogram of chiral 17**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

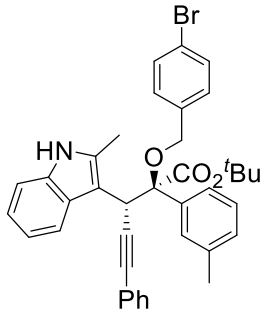
λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 8.828 | 202709 | 10981 | 3.94 |
| 2 | 9.773 | 4936347 | 223403 | 96.06 |

***tert*-Butyl (2*R*,3*R*)-2-((4-bromobenzyl)oxy)-3-(2-methyl-1*H*-indol-3-yl)-5-phenyl-2-(*m*-tolyl)pent-4-ynoate (18)**




**18**

Yellow oil; 88.6 mg, 70% yield, >20:1 d.r., 93% *ee*, $[\alpha]_D^{20}$ = -6.24 (c = 0.033, MeOH);

$^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 5.5 Hz, 1H), 7.66 (s, 1H), 7.46 – 7.42 (m, 2H), 7.34 (d, *J* = 8.4 Hz, 2H), 7.31 – 7.25 (m, 5H), 7.18 (d, *J* = 8.0 Hz, 1H), 7.00 (ddd, *J* = 18.3, 13.3, 7.3 Hz, 3H), 6.88 (dd, *J* = 15.9, 8.2 Hz, 3H), 4.81 (d, *J* = 13.0 Hz, 1H), 4.73 (s, 1H), 4.29 (d, *J* = 13.0 Hz, 1H), 2.10 (s, 3H), 1.65 (s, 3H), 1.53 (s,9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 171.0, 139.4, 137.0, 136.0, 135.0, 134.3, 131.6, 130.9, 129.0, 128.7, 128.58, 128.55, 128.2, 127.7, 127.3, 125.0, 124.1, 120.7, 120.2, 119.1, 109.7, 106.1, 89.7, 89.6, 83.1, 82.9, 67.7, 41.4, 28.2, 21.5, 11.3. HRMS(ESI) $[M+Na]^+$ calcd for $C_{38}H_{36}BrNO_3Na^+$, 656.1771, found 656.1771. (Chiral IA, λ = 254 nm, *n*-hexane/2-propanol = 95/5, Flow rate = 1.0 mL/min), $t_R$ =6.970 min, 8.280 min (major).

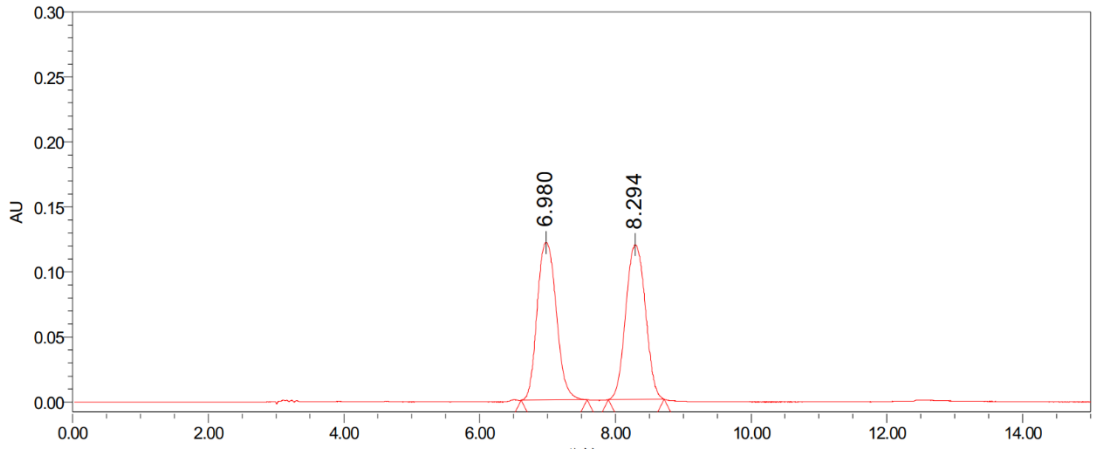
**HPLC chromatogram of racemic 18**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 6.980 | 2374601 | 121233 | 49.92 |
| 2 | 8.294 | 2382686 | 118785 | 50.08 |

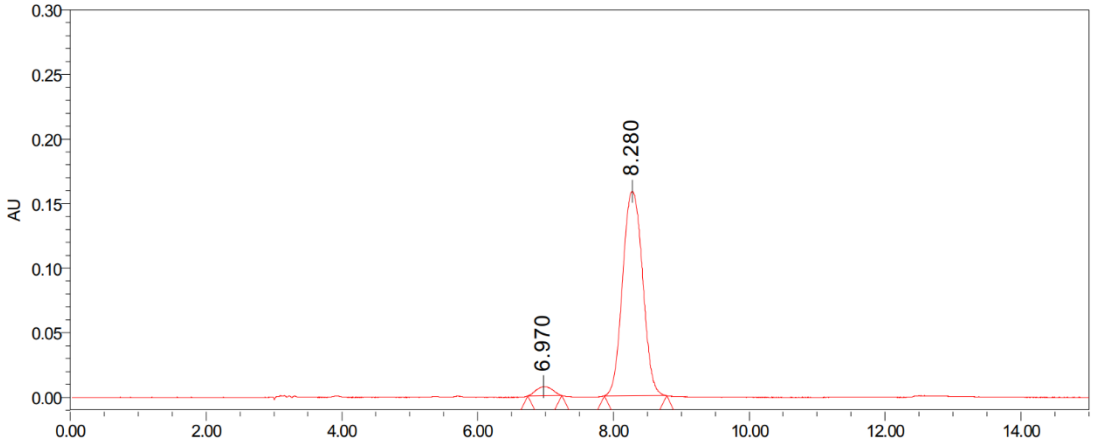
**HPLC chromatogram of chiral 18**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

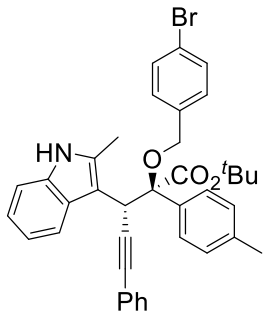
λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 6.970 | 117329 | 6866 | 3.51 |
| 2 | 8.280 | 3228799 | 158349 | 96.49 |

***tert*-Butyl (2*R*,3*R*)-2-((4-bromobenzyl)oxy)-3-(2-methyl-1*H*-indol-3-yl)-5-phenyl-2-(*p*-tolyl)pent-4-ynoate (19)**




**19**

Yellow oil; 69.7 mg, 55% yield, >20:1 d.r., 92% *ee*, $[\alpha]_D^{20}$ = 6.58 (c = 0.033, MeOH); $^1$H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 7.0 Hz, 1H), 7.67 (s, 1H), 7.44 (dd, *J* = 7.0, 2.4 Hz, 2H), 7.33 (d, *J* = 8.4 Hz, 2H), 7.28 (dd, *J* = 9.2, 5.4 Hz, 5H), 7.19 (d, *J* = 8.0 Hz, 1H), 7.04 (t, *J* = 7.4 Hz, 1H), 6.96 (d, *J* = 8.0 Hz, 2H), 6.91 (t, *J* = 7.1 Hz, 3H), 4.79 (d, *J* = 13.0 Hz, 1H), 4.72 (s, 1H), 4.28 (d, *J* = 13.0 Hz, 1H), 2.27 (s, 3H), 1.59 (s, 3H), 1.53 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 171.1, 155.3, 139.4, 137.7, 135.0, 134.3, 133.1, 131.6, 130.9, 128.9, 128.5, 128.2, 128.1, 127.8, 127.7, 124.1, 120.7, 120.2, 119.1, 109.7, 106.1, 89.7, 89.6, 83.0, 82.8, 67.6, 41.6, 28.2, 21.1, 11.2. HRMS(ESI) $[M+Na]^+$ calcd for $C_{38}H_{36}BrNO_3Na^+$, 656.1771, found 656.1772. (Chiral IA, λ = 254 nm, *n*-hexane/2-propanol = 98/2, Flow rate = 1.0 mL/min), $t_R$ = 16.428 min, 19.302 min (major).

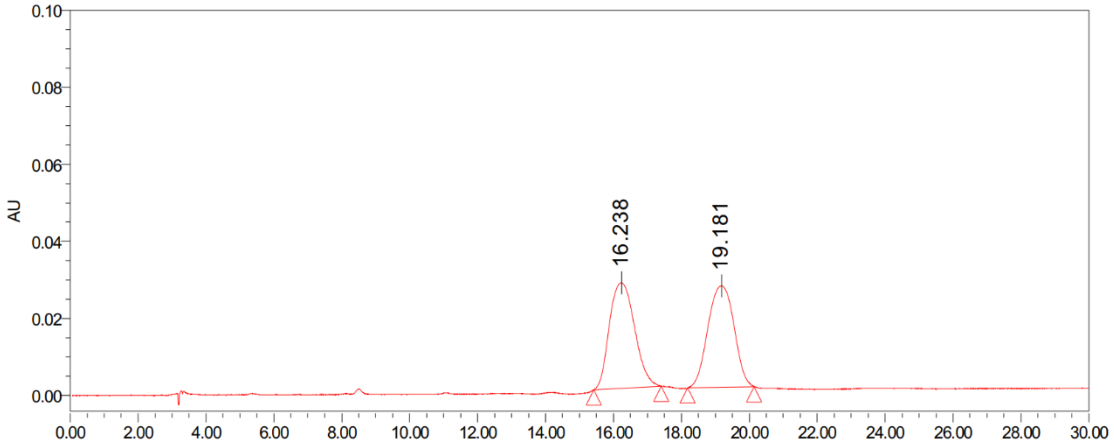
**HPLC chromatogram of racemic 19**

Condition: n-hexane/2-propanol = 98:2

Flow rate = 1.0 mL/min

λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 16.238 | 1412539 | 27362 | 50.02 |
| 2 | 19.181 | 1411551 | 26327 | 49.98 |

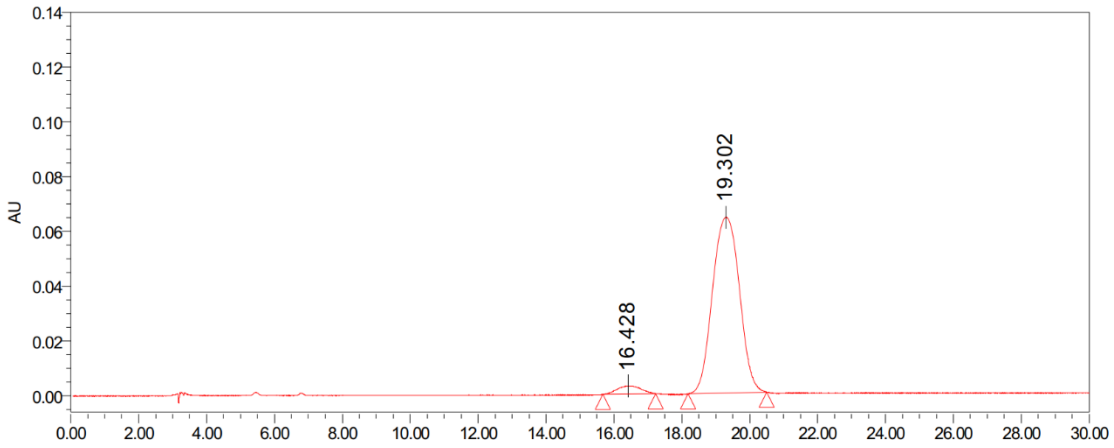
**HPLC chromatogram of chiral 19**

Condition: n-hexane/2-propanol = 98:2

Flow rate = 1.0 mL/min

λ = 254 nm

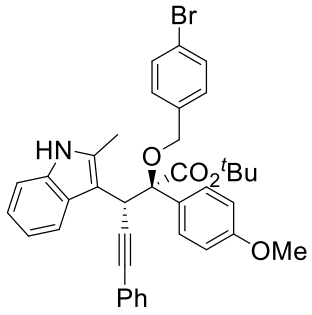
Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| 1 | 16.428 | 144041 | 2950 | 3.90 |
| 2 | 19.302 | 3549106 | 64172 | 96.10 |

***tert*-Butyl (2*R*,3*R*)-2-((4-bromobenzyl)oxy)-2-(4-methoxyphenyl)-3-(2-methyl-1*H*-indol-3-yl)-5-phenylpent-4-ynoate (20)**




**20**

Yellow solid, mp: 94.7 - 95.6 °C; 79.2 mg, 61% yield, >20:1 d.r., 91% *ee*, $[\alpha]_D^{20}$ = 15.87 (c = 0.033, MeOH); $^1$H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 6.0 Hz, 1H), 7.67 (s, 1H), 7.46 – 7.42 (m, 2H), 7.33 (d, *J* = 8.4 Hz, 2H), 7.30 – 7.27 (m, 5H), 7.17 (d, *J* = 8.0 Hz, 1H), 7.04 (t, *J* = 7.3 Hz, 1H), 6.98 (d, *J* = 8.5 Hz, 2H), 6.91 (t, *J* = 7.5 Hz, 1H), 6.62 (d, *J* = 9.0 Hz, 2H), 4.78 (d, *J* = 13.0 Hz, 1H), 4.70 (s, 1H), 4.25 (d, *J* = 13.0 Hz, 1H), 3.72 (s, 3H), 1.62 (s, 3H), 1.54 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 171.2, 159.4, 139.3, 135.0, 134.3, 131.7, 130.9, 129.2, 128.8, 128.5, 128.3, 128.2, 127.7, 124.1, 120.8, 120.2, 119.1, 112.7, 109.8, 106.0, 89.7, 89.3, 83.1, 82.9, 67.5, 55.3, 41.6, 28.2, 11.3. HRMS(ESI) $[M+Na]^+$ calcd for $C_{38}H_{36}BrNO_4Na^+$, 672.1720, found 672.1724. (Chiral IA, λ = 254 nm, *n*-hexane/2-propanol = 95/5, Flow rate = 1.0 mL/min), $t_R$ = 10.092 min, 10.901 min (major).

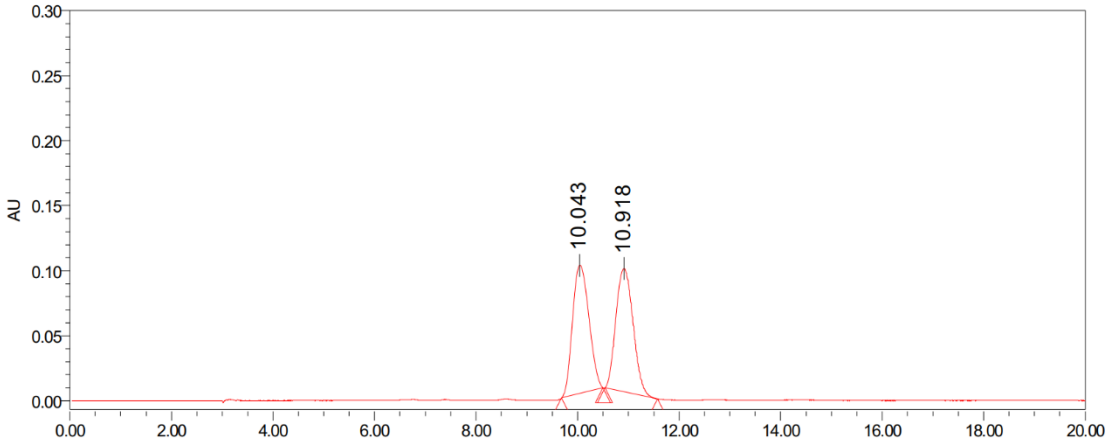
**HPLC chromatogram of racemic 20**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 10.043 | 2222108 | 98520 | 49.96 |
| 2 | 10.918 | 2225835 | 94643 | 50.04 |

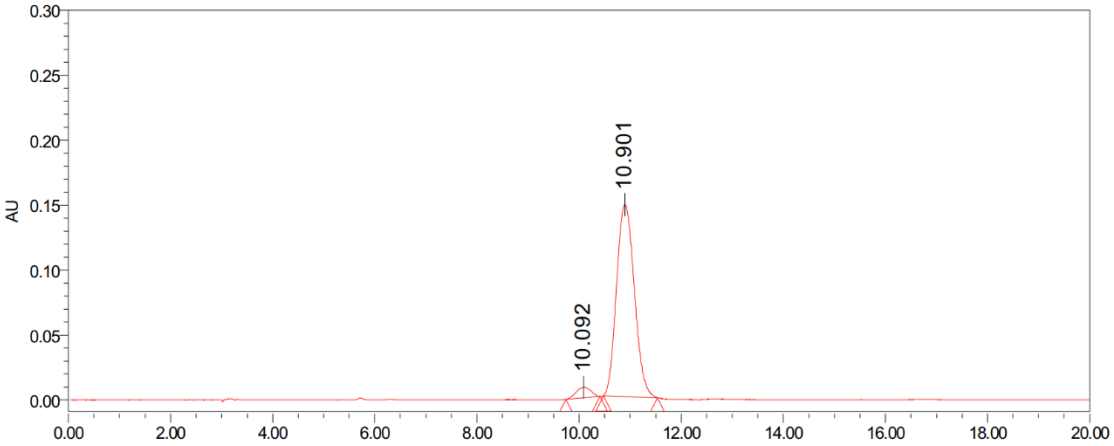
**HPLC chromatogram of chiral 20**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

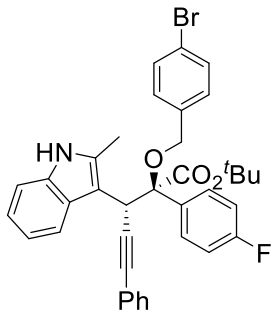
λ = 254 nm

Chiral IA



| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 10.092 | 166761 | 8170 | 4.47 |
| 2 | 10.901 | 3565018 | 147644 | 95.53 |

**_tert_-Butyl (2*R*,3*R*)-2-((4-bromobenzyl)oxy)-2-(4-fluorophenyl)-3-(2-methyl-1*H*-indol-3-yl)-5-phenylpent-4-ynoate (21)**




**21**

White solid, mp: 135.5 – 136.4 ℃; 89.2 mg, 70% yield, >20:1 d.r., 93% *ee*, $[\alpha]_D^{20}$ = 12.38 (c = 0.033, MeOH); $^1$H NMR (500 MHz, $CDCl_3$) δ 7.84 (s, 1H), 7.66 (s, 1H), 7.43 (s, 2H), 7.35 (s, 3H), 7.28 (s, 4H), 7.17 (d, *J* = 4.2 Hz, 1H), 7.06 (s, 3H), 6.91 (d, *J* = 2.5 Hz, 1H), 6.78 (s, 2H), 4.79 (d, *J* = 12.7 Hz, 1H), 4.72 (s, 1H), 4.24 (d, *J* = 9.7 Hz, 1H), 1.66 (s, 3H), 1.53 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 170.8, δ 162.6 (d, *J* = 247.0 Hz), 138.9, 135.0, 134.3, 132.0, 131.6, 131.0, 129.8 (d, *J* = 8.8 Hz), 128.7, 128.6, 128.3, 127.8, 124.0, 120.9, 120.4, 119.2, 114.2 (d, *J* = 20.2 Hz), 109.9, 105.8, 89.2, 89.1, 83.4, 83.2, 67.7, 41.6, 28.2, 11.3. $^{19}$F NMR (376 MHz, $CDCl_3$) δ -114.12. HRMS(ESI) $[M+Na]^+$ calcd for $C_{37}H_{33}BrFNO_3Na^+$, 660.1520, found 660.1522. (Chiral IA, λ = 254 nm, *n*-hexane/2-propanol = 95/5, Flow rate = 1.0 mL/min), $t_R$ = 7.466 min, 8.638 min (major).

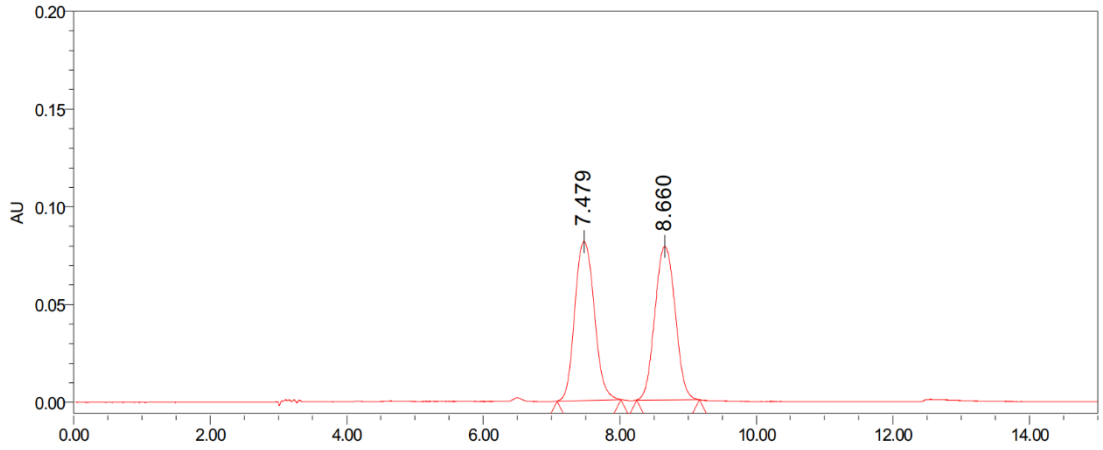
**HPLC chromatogram of racemic 21**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 7.479 | 1614729 | 81105 | 50.01 |
| 2 | 8.660 | 1613921 | 78487 | 49.99 |

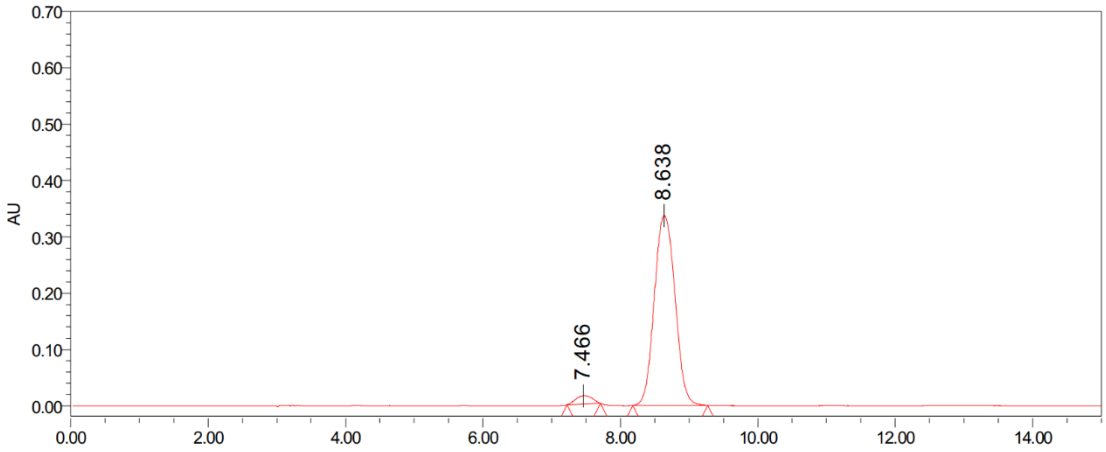
**HPLC chromatogram of chiral 21**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

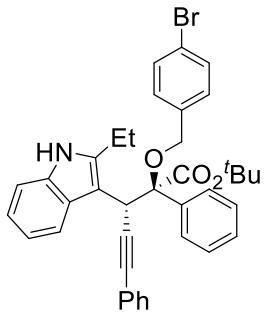
λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 7.466 | 251734 | 14895 | 3.47 |
| 2 | 8.638 | 7001045 | 336533 | 96.53 |

***tert*-Butyl (2*R*,3*R*)-2-((4-bromobenzyl)oxy)-3-(2-ethyl-1*H*-indol-3-yl)-2,5-diphenylpent-4-ynoate (22)**




**22**

Yellow oil; 88.6 mg, 70% yield, >20:1 d.r., 96% *ee*, $[\alpha]_D^{20}$ = 6.33 (c = 0.033, MeOH); $^1$H NMR (500 MHz, $CDCl_3$) δ 7.89 (s, 1H), 7.72 (s, 1H), 7.47 – 7.41 (m, 2H), 7.35 (d, *J* = 8.3 Hz, 2H), 7.32 – 7.26 (m, 5H), 7.22 – 7.15 (m, 2H), 7.10 – 7.01 (m, 5H), 6.90 (t, *J* = 7.4 Hz, 1H), 4.78 (d, *J* = 14.6 Hz, 2H), 4.29 (d, *J* = 13.0 Hz, 1H), 2.24 – 2.13 (m, 1H), 1.98 – 1.79 (m, 1H), 1.53 (s, 9H), 0.85 (t, *J* = 7.5 Hz, 3H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 171.0, 139.5, 139.3, 136.1, 135.1, 131.7, 131.0, 128.7, 128.6, 128.3, 128.0, 127.9, 127.7, 127.5, 124.1, 120.8, 120.3, 119.2, 109.9, 105.3, 89.8, 89.7, 82.99, 82.97,

67.7, 41.3, 28.2, 18.5, 12.9. HRMS(ESI) $[M+Na]^+$ calcd for $C_{38}H_{36}BrNO_3Na^+$, 656.1771, found 656.1771. (Chiral IA, λ = 254 nm, *n*-hexane/2-propanol = 95/5, Flow rate = 1.0 mL/min), $t_R$ = 6.171 min, 6.733 min (major).

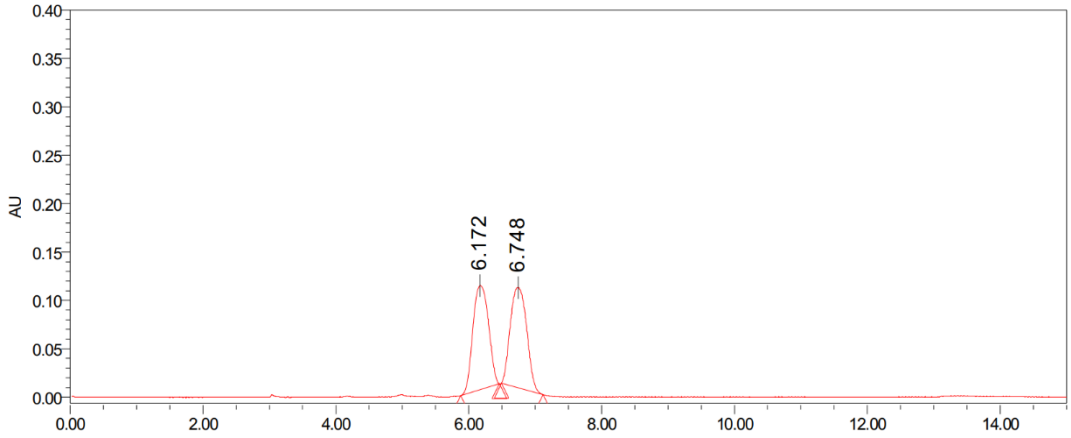
**HPLC chromatogram of racemic 22**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 6.172 | 1765567 | 107679 | 49.96 |
| 2 | 6.748 | 1768302 | 103663 | 50.04 |

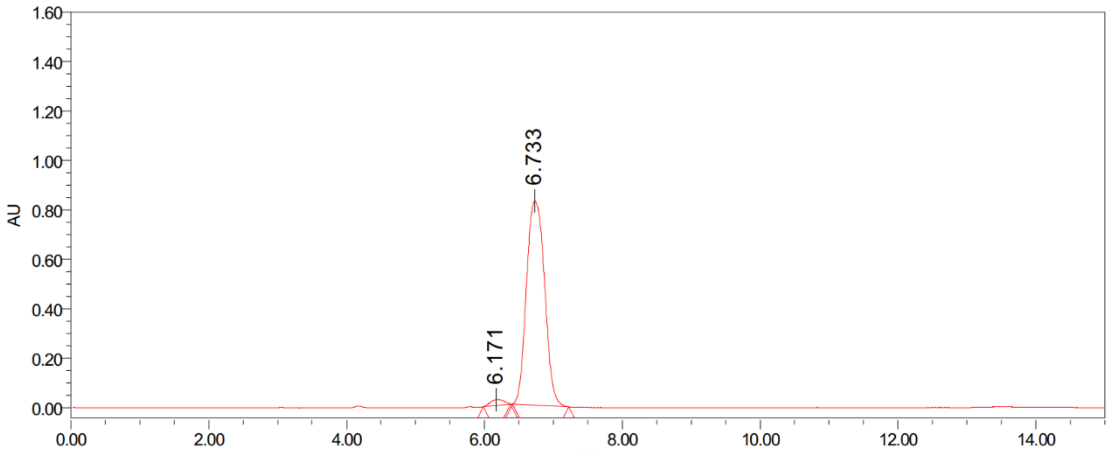
**HPLC chromatogram of chiral 22**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

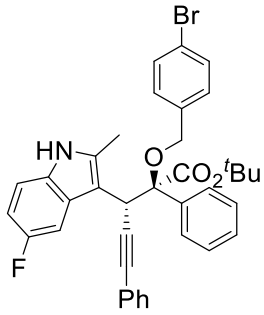
λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 6.171 | 308901 | 22565 | 2.03 |
| 2 | 6.733 | 14913309 | 825029 | 97.97 |

**_tert_-Butyl (2*R*,3*R*)-2-((4-bromobenzyl)oxy)-3-(5-fluoro-2-methyl-1*H*-indol-3-yl)-2,5-diphenylpent-4-ynoate (23)**




**23**

White solid, mp: 133.3 – 134.1 °C; 94.3 mg, 74% yield, >20:1 d.r., 88% *ee*, $[\alpha]_D^{20}$ = -6.25 (c = 0.033, MeOH); $^1$H NMR (500 MHz, $CDCl_3$) δ 7.57 (s, 1H), 7.45 (d, *J* = 7.3 Hz, 1H), 7.35 (dd, *J* = 7.2, 2.3 Hz, 2H), 7.28 (s, 1H), 7.26 (s, 1H), 7.23 – 7.19 (m, 3H), 7.17 (d, *J* = 8.3 Hz, 2H), 7.15 – 7.10 (m, 1H), 7.04 – 6.98 (m, 4H), 6.95 (dd, *J* = 8.7, 4.4 Hz, 1H), 6.67 (td, *J* = 9.0, 2.5 Hz, 1H), 4.75 (d, *J* = 12.8 Hz, 1H), 4.60 (s, 1H), 4.21 (d, *J* = 12.8 Hz, 1H), 1.47 (s, 3H), 1.45 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 170.8, δ 157.5 (d, *J* = 233.1 Hz), 139.0, 136.3, 136.0, 131.6, 131.4, 131.0, 129.4 (d, *J* = 10.1

Hz), 128.6, 128.3, 128.1, 127.9, 127.8, 127.5, 123.8, 120.5, 110.2 (d, $J$ = 8.8 Hz), 108.9 (d, $J$ = 26.5 Hz), 106.3 (d, $J$ = 5.0 Hz), 89.6, 89.1, 83.4, 83.1, 67.9, 41.5, 28.2, 11.3. $^{19}$F NMR (376 MHz, $CDCl_3$) δ -125.10. HRMS(ESI) $[M+Na]^+$ calcd for $C_{37}H_{33}BrFNO_3Na^+$, 660.1520, found 660.1519. (Chiral IF-3, λ = 254 nm, *n*-hexane/2-propanol = 95/5, Flow rate = 1.0 mL/min), $t_R$ = 6.931 min, 8.017 min (major).

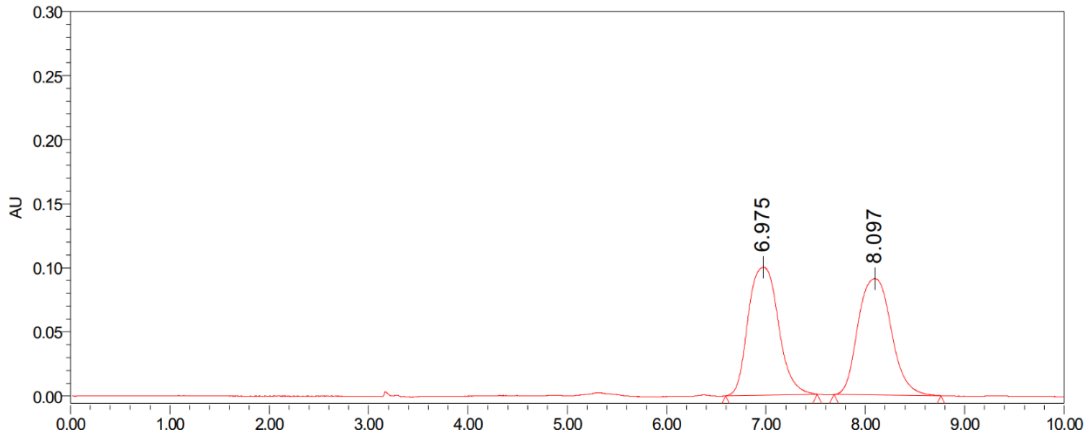
**HPLC chromatogram of racemic 23**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

λ = 254 nm

Chiral IF-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 6.975 | 2111947 | 99711 | 50.04 |
| 2 | 8.097 | 2108204 | 90715 | 49.96 |

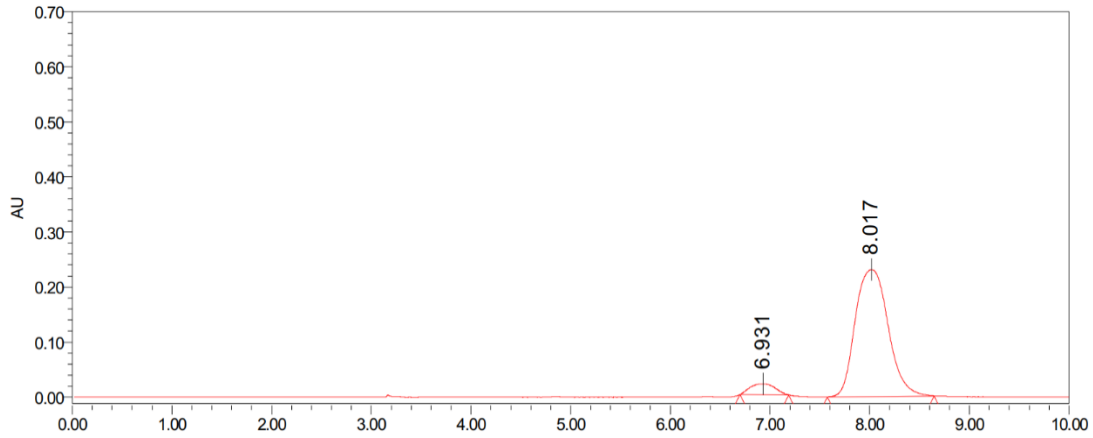
**HPLC chromatogram of chiral 23**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

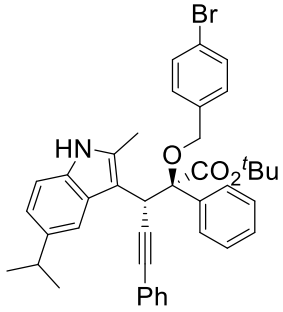
λ = 254 nm

Chiral IF-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 6.931 | 342597 | 19463 | 6.10 |
| 2 | 8.017 | 5270484 | 229930 | 93.90 |

***tert*-Butyl (2*R*,3*R*)-2-((4-bromobenzyl)oxy)-3-(5-isopropyl-2-methyl-1*H*-indol-3-yl)-2,5-diphenylpent-4-ynoate (24):**




**24**

Yellow oil; 117.7 mg, 89% yield, >20:1 d.r., 97% *ee*, $[\alpha]_D^{20}$ = -21.34 (c = 0.033, MeOH); $^1$H NMR (400 MHz, $CDCl_3$) δ 7.74 (s, 1H), 7.55 (s, 1H), 7.47 (d, *J* = 4.7 Hz, 2H), 7.34 (s, 4H), 7.29 (d, *J* = 4.7 Hz, 3H), 7.20 (d, *J* = 4.8 Hz, 1H), 7.13 – 7.05 (m, 5H), 6.91 (d, *J* = 8.1 Hz, 1H), 4.78 (d, *J* = 12.7 Hz, 1H), 4.70 (s, 1H), 4.27 (d, *J* = 12.7 Hz, 1H), 2.75 (dt, *J* = 13.2, 6.5 Hz, 1H), 1.55 (s, 12H), 1.08 (d, *J* = 6.7 Hz, 3H), 1.02 (d, *J* = 6.7 Hz, 3H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 171.0, 139.5, 139.4, 136.0, 134.5, 133.6, 131.6,

131.0, 129.0, 128.6, 128.2, 128.00, 127.98, 127.7, 127.4, 124.2, 120.3, 120.0, 109.4, 105.7, 89.8, 89.6, 83.2, 83.0, 67.6, 41.7, 34.2, 28.3, 24.51, 24.46, 11.2. HRMS(ESI) $[M+Na]^+$ calcd for $C_{40}H_{40}BrNO_3Na^+$, 684.2084, found 684.2083. (Chiral IA, λ = 254 nm, *n*-hexane/2-propanol = 95/5, Flow rate = 1.0 mL/min), $t_R$ = 6.140 min (major), 6.886 min.

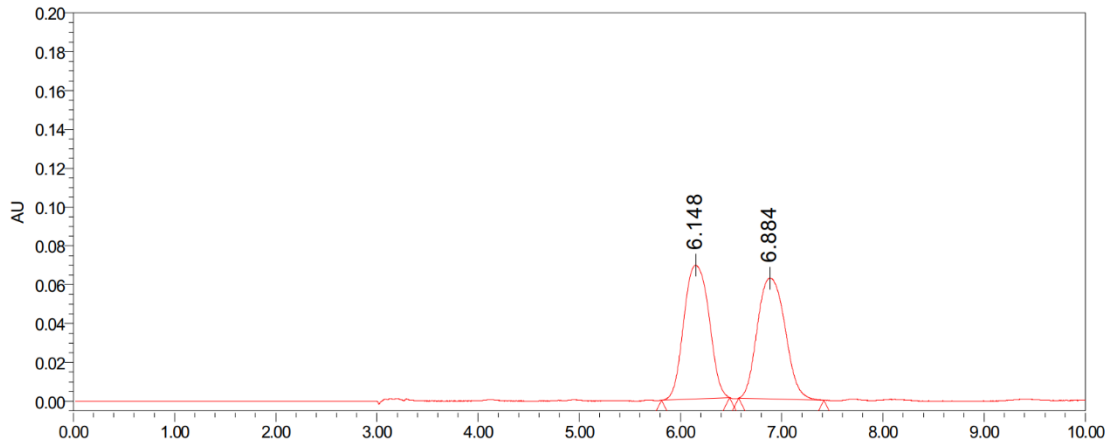
**HPLC chromatogram of racemic 24**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 6.148 | 1195845 | 68821 | 50.09 |
| 2 | 6.884 | 1191637 | 62268 | 49.91 |

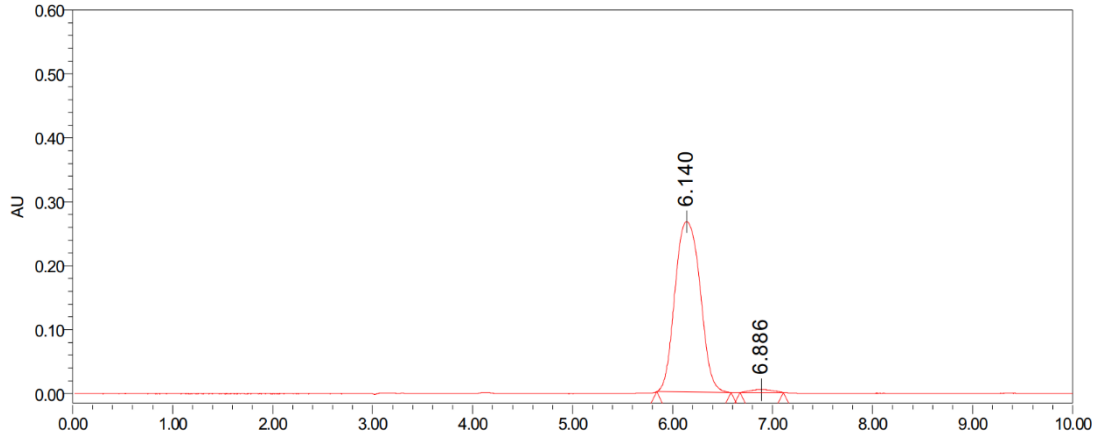
**HPLC chromatogram of chiral 24**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

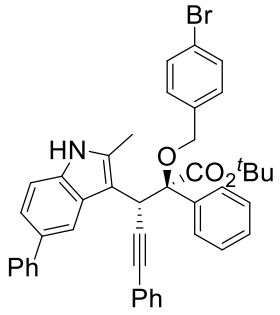
λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 6.140 | 4677048 | 266246 | 98.55 |
| 2 | 6.886 | 68585 | 4332 | 1.45 |

***tert*-Butyl (2*R*,3*R*)-2-((4-bromobenzyl)oxy)-3-(2-methyl-5-phenyl-1*H*-indol-3-yl)-2,5-diphenylpent-4-ynoate (25)**




**25**

Yellow oil; 86.2 mg, 62% yield, >20:1 d.r., 93% *ee*, $[\alpha]_D^{20}$ = -96.31 (c = 0.033, MeOH); $^1$H NMR (400 MHz, $CDCl_3$) δ 8.21 (s, 1H), 7.55 (s, 1H), 7.34 – 7.29 (m, 2H), 7.21 (t, *J* = 8.5 Hz, 6H), 7.18 – 7.08 (m, 10H), 7.04 (d, *J* = 3.8 Hz, 4H), 4.70 (d, *J* = 12.5 Hz, 1H), 4.62 (s, 1H), 4.18 (d, *J* = 12.5 Hz, 1H), 1.48 (s, 9H), 1.42 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 171.0, 142.6, 139.0, 135.9, 135.0, 134.7, 132.4, 131.7, 131.0, 129.3,

128.8, 128.5, 128.2, 128.1, 128.0, 127.8, 127.5, 127.1, 126.0, 123.9, 120.5, 120.4, 110.0, 106.4, 89.7, 89.6, 83.5, 83.1, 67.7, 41.9, 28.3, 11.0. HRMS(ESI) $[M+Na]^+$ calcd for $C_{43}H_{38}BrNO_3Na^+$, 718.1927, found 718.1929. (Chiral IA, λ = 254 nm, *n*-hexane/2-propanol = 95/5, Flow rate = 1.0 mL/min), $t_R$ = 12.060 min, 20.226 min (major).

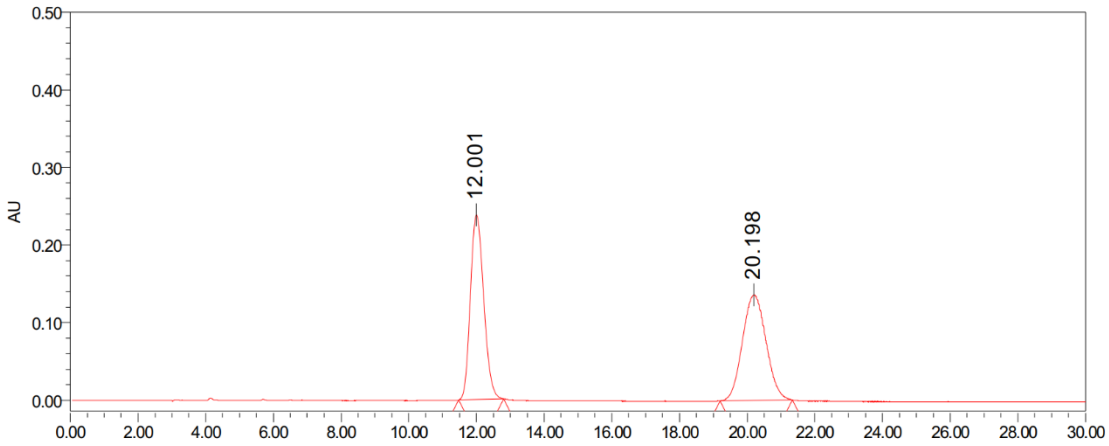
**HPLC chromatogram of racemic 25**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 12.001 | 6528807 | 237595 | 50.03 |
| 2 | 20.198 | 6521436 | 135809 | 49.97 |

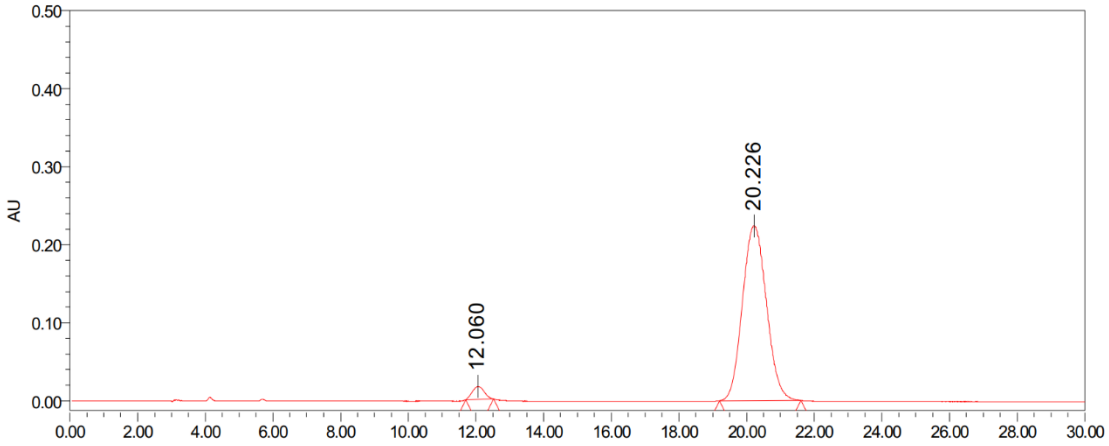
**HPLC chromatogram of chiral 25**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

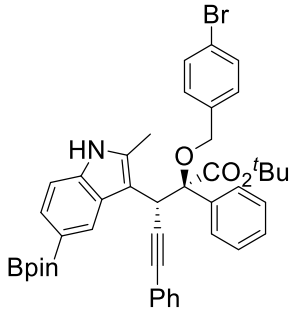
λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 12.060 | 399221 | 16434 | 3.51 |
| 2 | 20.226 | 10971568 | 223996 | 96.49 |

**_tert_-Butyl (2*R*,3*R*)-2-((4-bromobenzyl)oxy)-3-(2-methyl-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1*H*-indol-3-yl)-2,5-diphenylpent-4-ynoate (26)**




**26**

Yellow oil; 89.4 mg, 60% yield, >20:1 d.r., 83% *ee*, $[\alpha]_D^{20}$ = -48.49 (c = 0.033, MeOH); $^1$H NMR (400 MHz, $CDCl_3$) δ 8.74 (s, 1H), 7.73 (s, 1H), 7.65 – 7.60 (m, 2H), 7.51 (d, *J* = 8.1 Hz, 1H), 7.35 – 7.28 (m, 7H), 7.25 – 7.18 (m, 1H), 7.15 (d, *J* = 8.1 Hz, 1H), 7.09 (d, *J* = 4.3 Hz, 4H), 4.76 (d, *J* = 13.4 Hz, 1H), 4.72 (s, 1H), 4.33 (d, *J* = 13.4 Hz, 1H), 1.51 (s, 9H), 1.47 (s, 3H), 1.32 (s, 6H), 1.26 (s, 6H). $^{13}$C NMR (126 MHz, $CDCl_3$)

δ 171.0, 139.4, 137.2, 136.2, 134.3, 131.9, 130.8, 128.5, 128.3, 128.1, 128.0, 127.9, 127.7, 127.4, 127.0, 124.2, 120.0, 109.3, 106.3, 89.7, 89.6, 83.6, 83.1, 83.0, 67.7, 41.7, 28.2, 25.0, 24.8, 10.9. HRMS(ESI) $[M+Na]^+$ calcd for $C_{43}H_{45}BBrNO_5Na^+$, 768.2474, found 768.2475. (Chiral IA, λ = 254 nm, *n*-hexane/2-propanol = 95/5, Flow rate = 1.0 mL/min), $t_R$ = 5.973 min (major), 7.064 min.

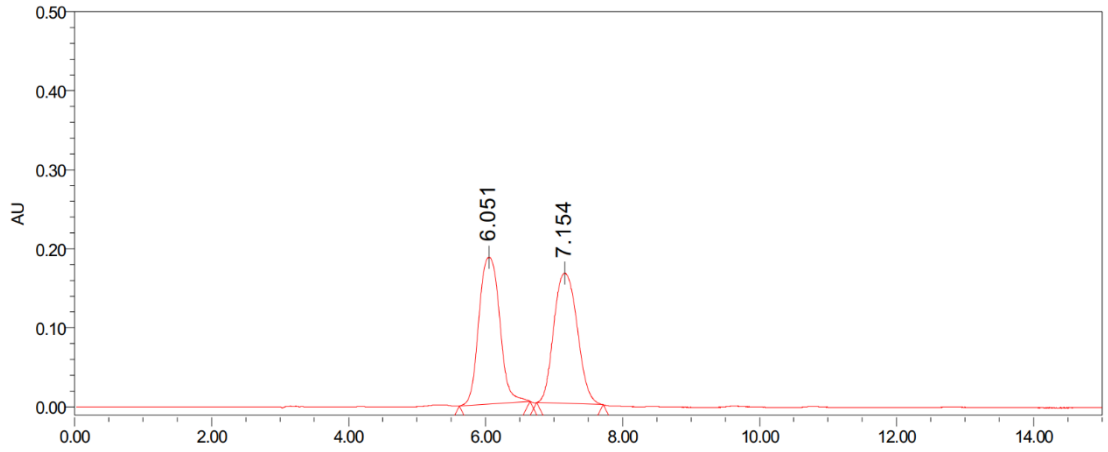
**HPLC chromatogram of racemic 26**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 6.051 | 3938892 | 185725 | 50.03 |
| 2 | 7.154 | 3934803 | 164784 | 49.97 |

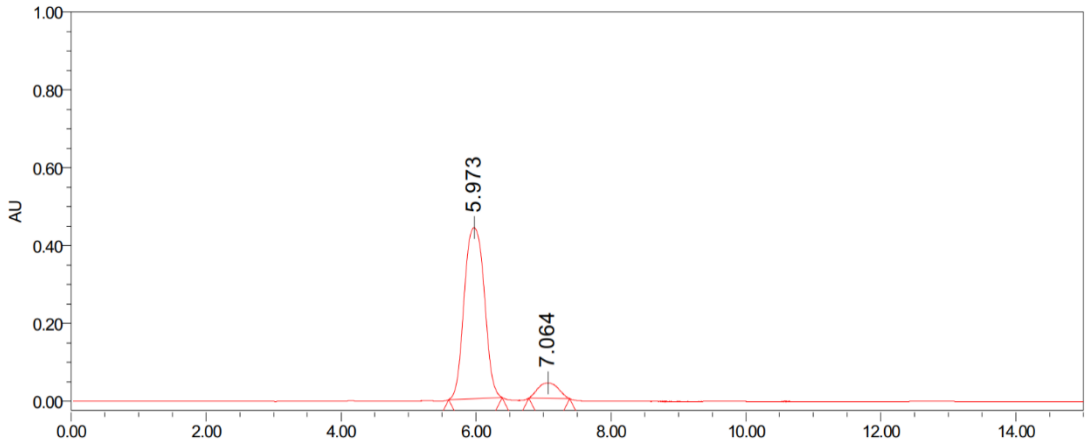
**HPLC chromatogram of chiral 26**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

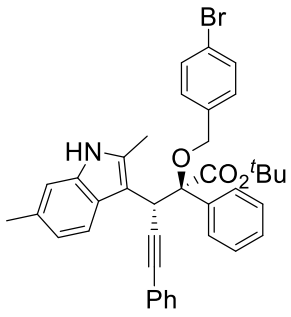
λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 5.973 | 9118990 | 438707 | 91.51 |
| 2 | 7.064 | 845605 | 39943 | 8.49 |

***tert*-Butyl (2*R*,3*R*)-2-((4-bromobenzyl)oxy)-3-(2,6-dimethyl-1*H*-indol-3-yl)-2,5-diphenylpent-4-ynoate (27)**




**27**

Yellow oil; 44.3 mg, 35% yield, >20:1 d.r., 94% *ee*, $[\alpha]_D^{20}$ = -3.18 (c = 0.033, MeOH); $^1$H NMR (500 MHz, $CDCl_3$) δ 7.82 (d, *J* = 6.3 Hz, 1H), 7.52 (s, 1H), 7.45 (dd, *J* = 7.3, 2.0 Hz, 2H), 7.35 (d, *J* = 8.4 Hz, 2H), 7.32 – 7.28 (m, 5H), 7.22 (t, *J* = 6.8 Hz, 1H), 7.14 – 7.08 (m, 4H), 6.99 (s, 1H), 6.76 (d, *J* = 8.1 Hz, 1H), 4.79 (d, *J* = 13.0 Hz, 1H), 4.70 (s, 1H), 4.30 (d, *J* = 13.0 Hz, 1H), 2.41 (s, 3H), 1.53 (s, 12H). $^{13}$C NMR (126 MHz,

$CDCl_3$) δ 170.9, 139.3, 136.2, 135.5, 133.5, 131.6, 130.9, 130.4, 128.5, 128.20, 127.93, 127.89, 127.7, 127.4, 126.7, 124.1, 120.8, 120.2, 109.7, 105.8, 89.7, 89.6, 83.0, 82.9, 67.7, 41.6, 28.2, 21.7, 11.0. HRMS(ESI) $[M+Na]^+$ calcd for $C_{38}H_{36}BrNO_3Na^+$, 656.1771, found 656.1770. (Chiral IA, λ = 254 nm, *n*-hexane/2-propanol = 95/5, Flow rate = 1.0 mL/min), $t_R$ =10.696 min, 11.494 min (major).

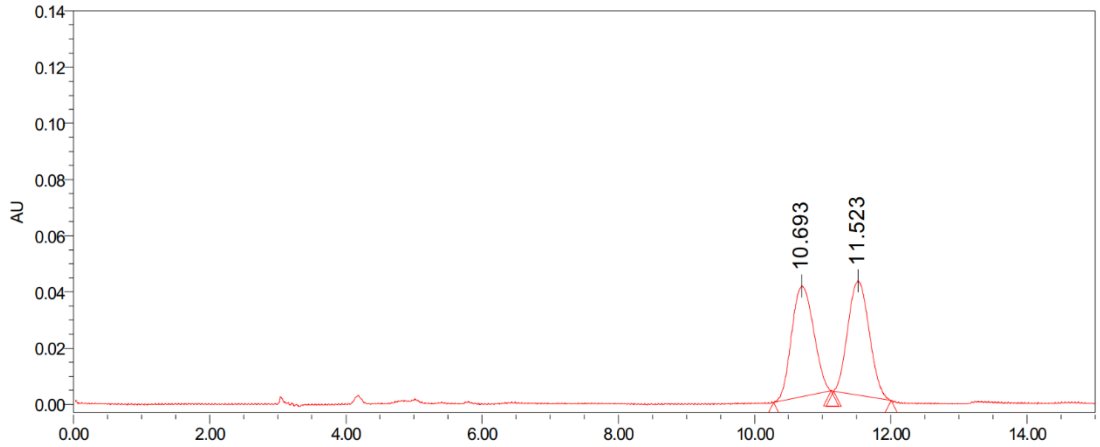
**HPLC chromatogram of racemic 27**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 10.693 | 882614 | 39485 | 49.99 |
| 2 | 11.523 | 882923 | 40622 | 50.01 |

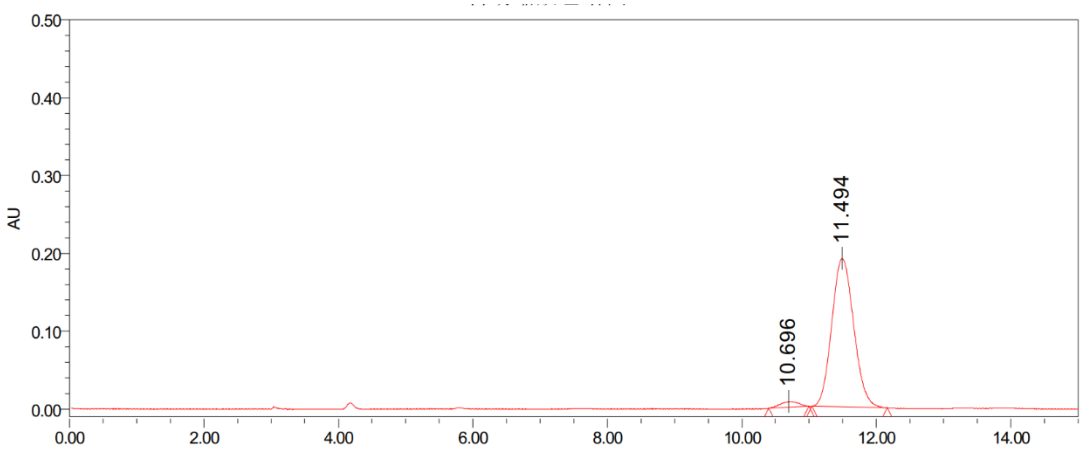
**HPLC chromatogram of chiral 27**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

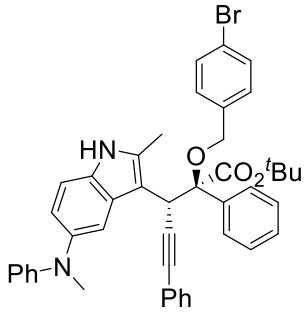
λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 10.696 | 135962 | 7299 | 3.05 |
| 2 | 11.494 | 4328022 | 190371 | 96.95 |

**_tert_-Butyl (2*R*,3*R*)-2-((4-bromobenzyl)oxy)-3-(2-methyl-5-(methyl(phenyl)amino)-1*H*-indol-3-yl)-2,5-diphenylpent-4-ynoate (28)**




**28**

Yellow oil; 113.0 mg, 78% yield, >20:1 d.r., 98% *ee*, $[\alpha]_D^{20}$ = 96.58 (c = 0.033, MeOH); $^1$H NMR (400 MHz, $CDCl_3$) δ 7.65 (s, 1H), 7.30 (d, *J* = 7.1 Hz, 2H), 7.25 (s, 4H), 7.20 (dt, *J* = 14.2, 7.0 Hz, 5H), 7.12 (d, *J* = 5.8 Hz, 5H), 7.06 (t, *J* = 7.8 Hz, 2H), 6.84 (d, *J* = 8.2 Hz, 1H), 6.65 (t, *J* = 7.8 Hz, 3H), 4.78 (d, *J* = 12.7 Hz, 1H), 4.69 (s, 1H), 4.27 (d, *J* = 12.7 Hz, 1H), 2.94 (s, 3H), 1.65 (s, 3H), 1.52 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$)

δ 170.9, 150.6, 141.1, 139.1, 136.0, 135.3, 132.7, 131.6, 131.1, 123.0, 128.7, 128.6, 128.3, 128.1, 127.9, 127.7, 127.5, 123.8, 120.4, 117.0, 114.5, 110.5, 106.2, 89.43, 89.38, 83.3, 83.1, 67.7, 41.6, 40.5, 28.2, 11.4. HRMS(ESI) $[M+Na]^+$ calcd for $C_{44}H_{41}BrN_2O_3Na^+$, 747.2193, found 747.2195. (Chiral IA, λ = 254 nm, *n*-hexane/2-propanol = 95/5, Flow rate = 1.0 mL/min), $t_R$ = 8.621 min (major), 27.352 min.

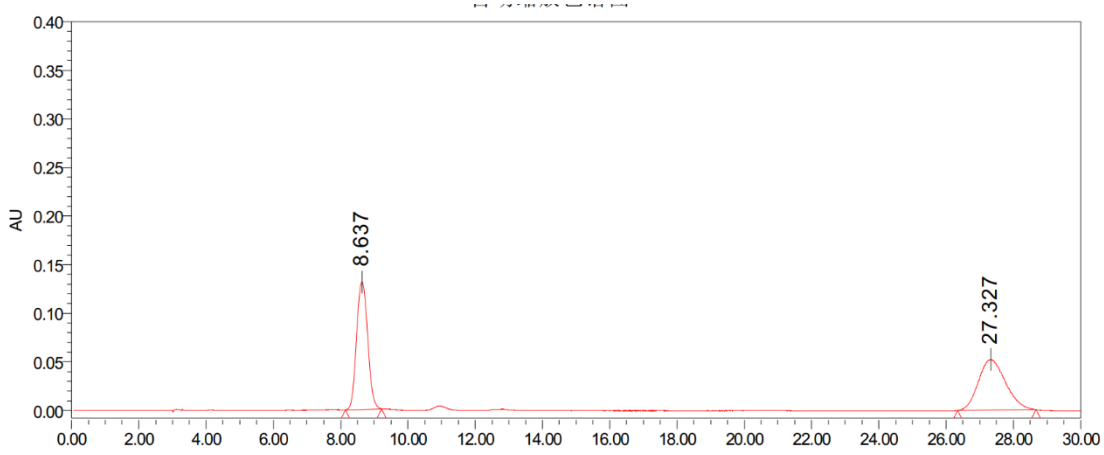
**HPLC chromatogram of racemic 28**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 8.637 | 3023567 | 130993 | 50.93 |
| 2 | 27.327 | 2912808 | 52055 | 49.07 |

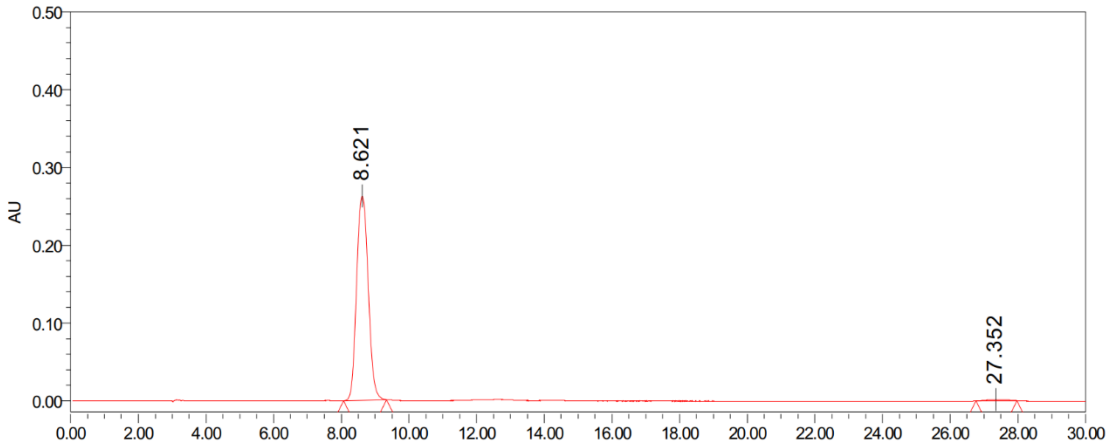
**HPLC chromatogram of chiral 28**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

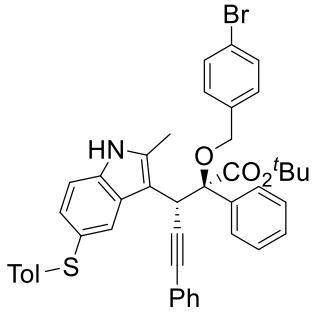
λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 8.621 | 6282115 | 262286 | 98.99 |
| 2 | 27.352 | 64273 | 1609 | 1.01 |

**_tert_-Butyl (2_R_,3_R_)-2-((4-bromobenzyl)oxy)-3-(2-methyl-5-(_p_-tolyl_thio_)-1_H_-indol-3-yl)-2,5-diphenylpent-4-ynoate (29)**




**29**

Yellow oil; 56.3 mg, 38% yield, >20:1 d.r., 87% *ee*, $[\alpha]_D^{20}$ = 75.26 (c = 0.033, MeOH); $^1$H NMR (400 MHz, $CDCl_3$) δ 8.14 (s, 1H), 7.77 (s, 1H), 7.37 – 7.33 (m, 2H), 7.30 (d, *J* = 8.4 Hz, 2H), 7.26 – 7.15 (m, 6H), 7.14 (d, *J* = 1.5 Hz, 2H), 7.10 (d, *J* = 4.3 Hz, 4H), 6.96 (d, *J* = 8.2 Hz, 2H), 6.87 (d, *J* = 8.0 Hz, 2H), 4.84 (d, *J* = 12.8 Hz, 1H), 4.75 (s, 1H), 4.28 (d, *J* = 12.8 Hz, 1H), 2.22 (s, 3H), 1.63 (s, 3H), 1.53 (s, 9H). $^{13}$C NMR (126

MHz, $CDCl_3$) δ 170.8, 138.8, 136.4, 136.1, 135.4, 134.8, 134.7, 131.6, 131.0, 129.8, 129.4, 128.5, 128.2, 128.1, 127.8, 127.74, 127.71, 127.5, 127.1, 123.7, 122.5, 120.4, 110.9, 106.3, 89.5, 89.2, 83.4, 83.1, 67.9, 41.5, 28.2, 21.0, 11.3. HRMS(ESI) $[M+Na]^+$ calcd for $C_{44}H_{40}BrNO_3SNa^+$, 764.1804, found 764.1803. (Chiral IA, λ = 254 nm, *n*-hexane/2-propanol = 95/5, Flow rate = 1.0 mL/min), $t_R$ = 9.819 min (major), 12.248 min.

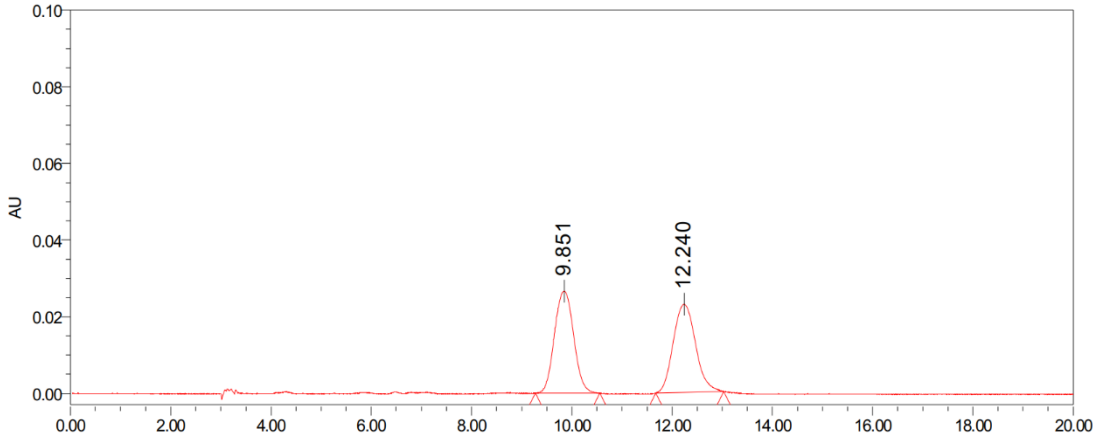
**HPLC chromatogram of racemic 29**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 9.851 | 712557 | 26653 | 50.01 |
| 2 | 12.240 | 712298 | 23027 | 49.99 |

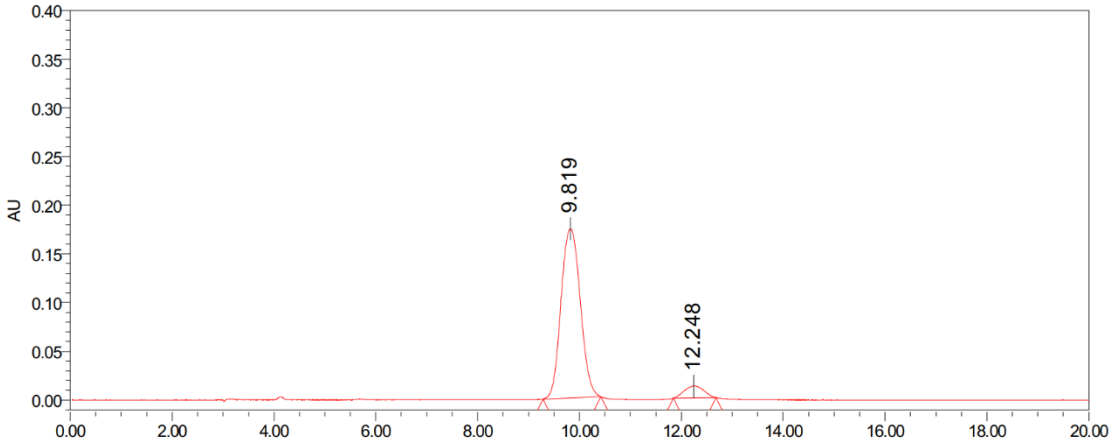
**HPLC chromatogram of chiral 29**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

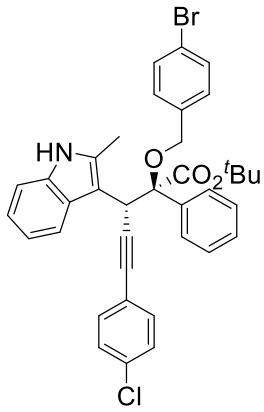
λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 9.819 | 4579504 | 173870 | 93.44 |
| 2 | 12.248 | 321292 | 12113 | 6.56 |

***tert*-Butyl (2*R*,3*R*)-2-((4-bromobenzyl)oxy)-5-(4-chlorophenyl)-3-(2-methyl-1*H*-indol-3-yl)-2-phenylpent-4-ynoate (30)**




**30**

Yellow oil; 98.0 mg, 75% yield, >20:1 d.r., 92% *ee*, $[\alpha]_D^{20}$ = 18.39 (c = 0.033, MeOH); $^1$H NMR (500 MHz, $CDCl_3$) δ 7.87 (s, 1H), 7.66 (s, 1H), 7.36 – 7.32 (m, 4H), 7.25 (t, *J* = 8.2 Hz, 4H), 7.22 – 7.18 (m, 1H), 7.17 (d, *J* = 8.0 Hz, 1H), 7.07 (td, *J* = 15.3, 7.8

Hz, 5H), 6.91 (t, $J$ = 7.5 Hz, 1H), 4.81 (d, $J$ = 12.9 Hz, 1H), 4.72 (s, 1H), 4.28 (d, $J$ = 12.9 Hz, 1H), 1.56 (s, 3H), 1.53 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 170.9, 139.2, 136.0, 135.0, 134.4, 133.7, 132.9, 131.0, 128.8, 128.61, 128.55, 128.1, 127.9, 127.5, 122.5, 120.9, 120.4, 119.2, 109.9, 105.7, 90.8, 89.6, 83.1, 82.0, 67.8, 41.6, 28.2, 11.1. HRMS(ESI) $[M+Na]^+$ calcd for $C_{37}H_{33}BrClNO_3Na^+$, 676.1225, found 676.1228. (Chiral IA, λ = 254 nm, *n*-hexane/2-propanol = 95/5, Flow rate = 1.0 mL/min), $t_R$ = 9.207 min, 10.215 min (major).

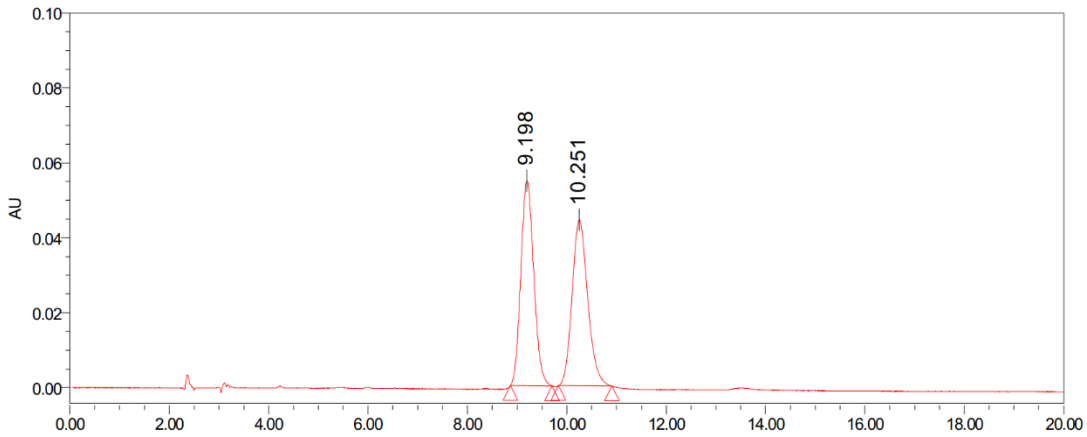
**HPLC chromatogram of racemic 30**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 9.198 | 977570 | 54746 | 50.09 |
| 2 | 10.251 | 973947 | 44326 | 49.91 |

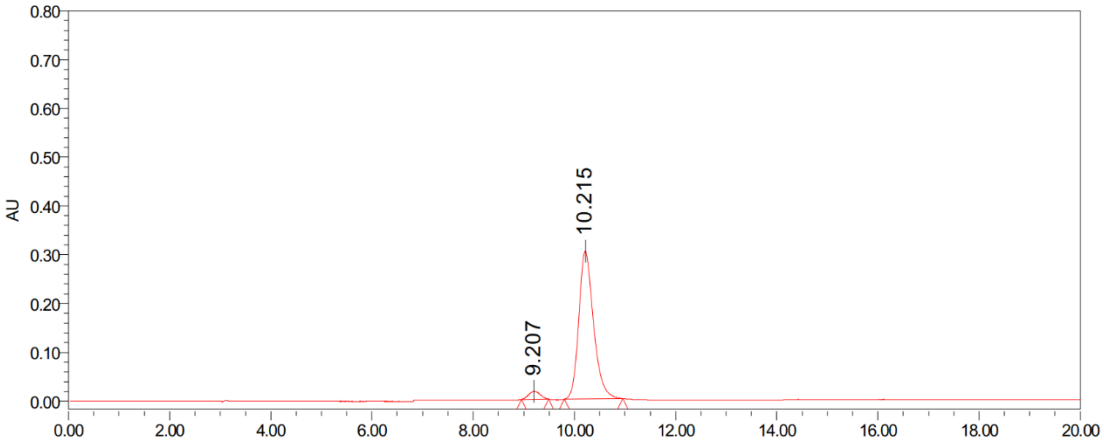
**HPLC chromatogram of chiral 30**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

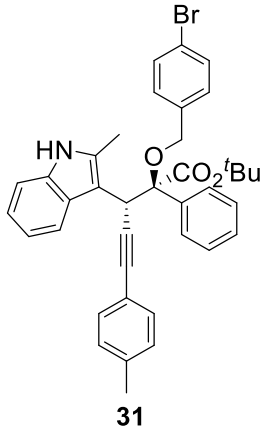
λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 9.207 | 254822 | 16285 | 3.98 |
| 2 | 10.215 | 6146368 | 303188 | 96.02 |

**_tert_-Butyl (2*R*,3*R*)-2-((4-bromobenzyl)oxy)-3-(2-methyl-1*H*-indol-3-yl)-2-phenyl-5-(*p*-tolyl)pent-4-ynoate (31)**




**31**

Yellow oil; 106.4 mg, 84% yield, >20:1 d.r., 94% *ee*, $[\alpha]_D^{20}$ = 12.27 (c = 0.033, MeOH);

$^{1}$H NMR (500 MHz, $CDCl_3$) δ 7.89 (s, 1H), 7.63 (s, 1H), 7.34 (d, *J* = 7.9 Hz, 4H), 7.28 (d, *J* = 8.1 Hz, 2H), 7.20 (dd, *J* = 9.3, 5.1 Hz, 1H), 7.16 (d, *J* = 8.0 Hz, 1H), 7.12 – 7.06 (m, 6H), 7.03 (t, *J* = 7.5 Hz, 1H), 6.90 (t, *J* = 7.5 Hz, 1H), 4.80 (d, *J* = 13.0 Hz, 1H), 4.73 (s, 1H), 4.29 (d, *J* = 13.0 Hz, 1H), 2.33 (s, 3H), 1.57 (s, 3H), 1.53 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 171.0, 139.3, 137.7, 136.2, 135.0, 134.3, 131.5, 130.9, 129.0, 128.9, 128.5, 128.0, 127.9, 127.4, 121.0, 120.8, 120.3, 119.1, 109.7, 106.0, 89.7, 88.8, 83.2, 83.0, 67.7, 41.6, 28.2, 21.5, 11.2. HRMS(ESI) $[M+Na]^+$ calcd for $C_{38}H_{36}BrNO_3Na^+$, 656.1771, found 656.1771. (Chiral IA, λ = 254 nm, *n*-hexane/2-propanol = 95/5, Flow rate = 1.0 mL/min), $t_R$ = 8.939 min, 11.703 min (major).

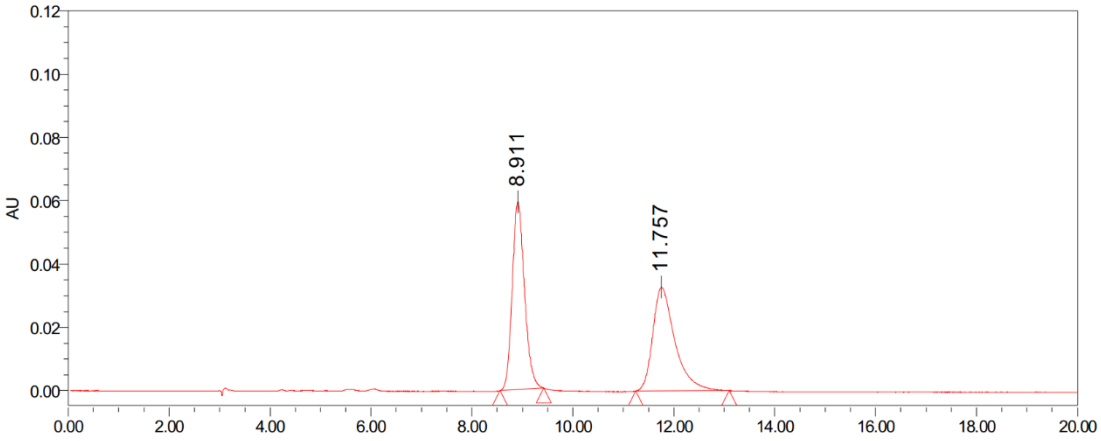
**HPLC chromatogram of racemic 31**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 8.911 | 996920 | 59333 | 49.93 |
| 2 | 11.757 | 999586 | 32728 | 50.07 |

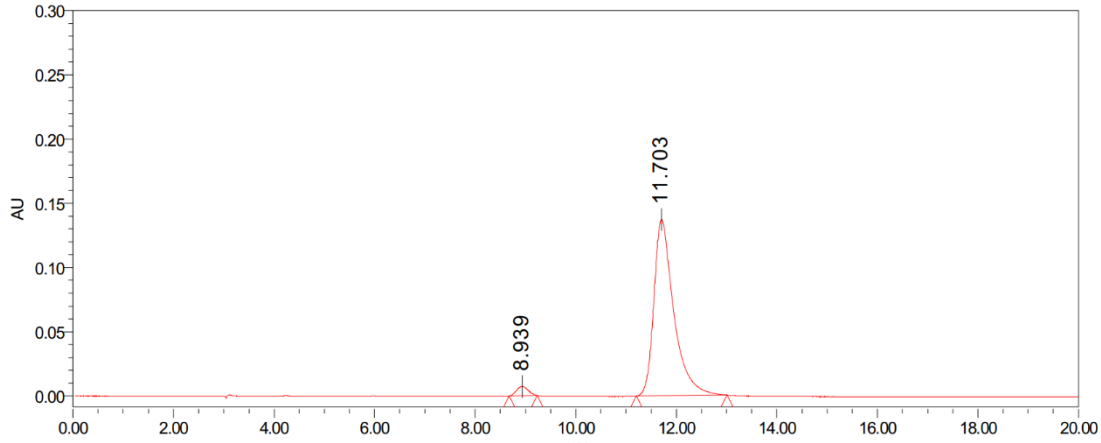
**HPLC chromatogram of chiral 31**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

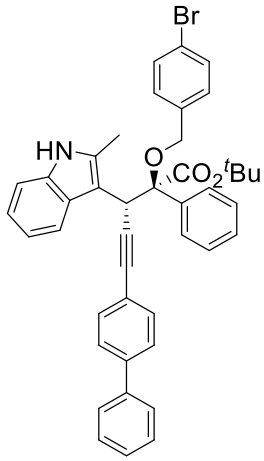
λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 8.939 | 115788 | 7387 | 2.98 |
| 2 | 11.703 | 3768296 | 137193 | 97.02 |

***tert*-Butyl (2*R*,3*R*)-5-([1,1'-biphenyl]-4-yl)-2-((4-bromobenzyl)oxy)-3-(2-methyl-1*H*-indol-3-yl)-2-phenylpent-4-ynoate (32)**




**32**

Yellow oil; 123.7 mg, 89% yield, >20:1 d.r., 93% *ee*, $[\alpha]_D^{20}$ = 45.81 (c = 0.033, MeOH); $^1$H NMR (500 MHz, $CDCl_3$) δ 7.91 (s, 1H), 7.63 (s, 1H), 7.58 (d, *J* = 7.6 Hz, 2H), 7.52 (q, *J* = 8.2 Hz, 4H), 7.42 (t, *J* = 7.6 Hz, 2H), 7.32 (dt, *J* = 16.0, 8.2 Hz, 5H), 7.19 (d, *J* = 3.7 Hz, 1H), 7.16 (d, *J* = 8.0 Hz, 1H), 7.09 (d, *J* = 4.1 Hz, 4H), 7.04 (t, *J* = 7.5 Hz, 1H), 6.92 (t, *J* = 7.5 Hz, 1H), 4.83 (d, *J* = 13.0 Hz, 1H), 4.77 (s, 1H), 4.30 (d, *J* = 13.0 Hz, 1H), 1.58 (s, 3H), 1.55 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 171.0, 140.6, 140.4, 139.3, 136.2, 135.1, 134.4, 132.1, 131.0, 128.9, 128.6, 128.0, 127.9, 127.6, 127.5, 127.1, 127.0, 123.1, 120.8, 120.3, 119.2, 109.8, 106.0, 90.4, 89.7, 83.0, 67.8, 41.7, 28.3, 11.2. HRMS(ESI) $[M+Na]^+$ calcd for $C_{43}H_{38}BrNO_3Na^+$, 718.1927, found 718.1926. (Chiral IA, λ = 254 nm, *n*-hexane/2-propanol = 95/5, Flow rate = 1.0 mL/min), $t_R$ = 12.425 min, 18.333 min (major).

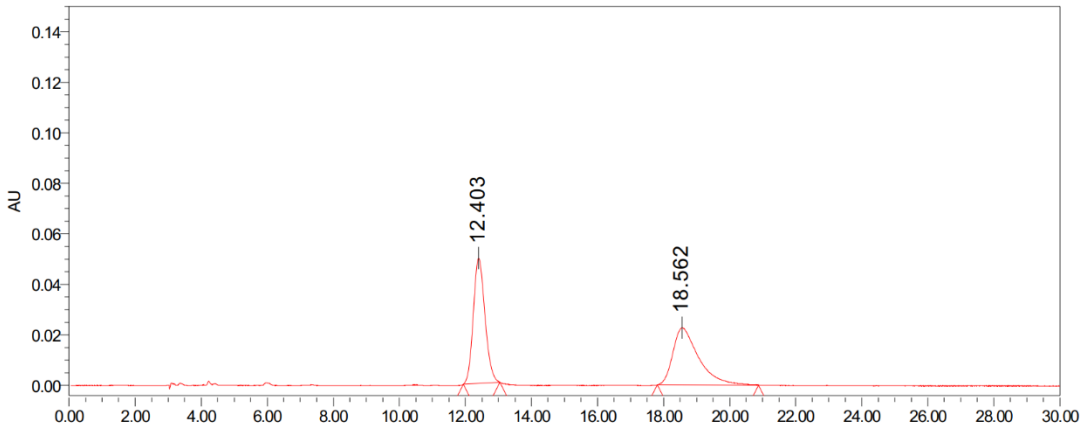
**HPLC chromatogram of racemic 32**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 12.403 | 1220788 | 49556 | 50.04 |
| 2 | 18.562 | 1218617 | 22597 | 49.96 |

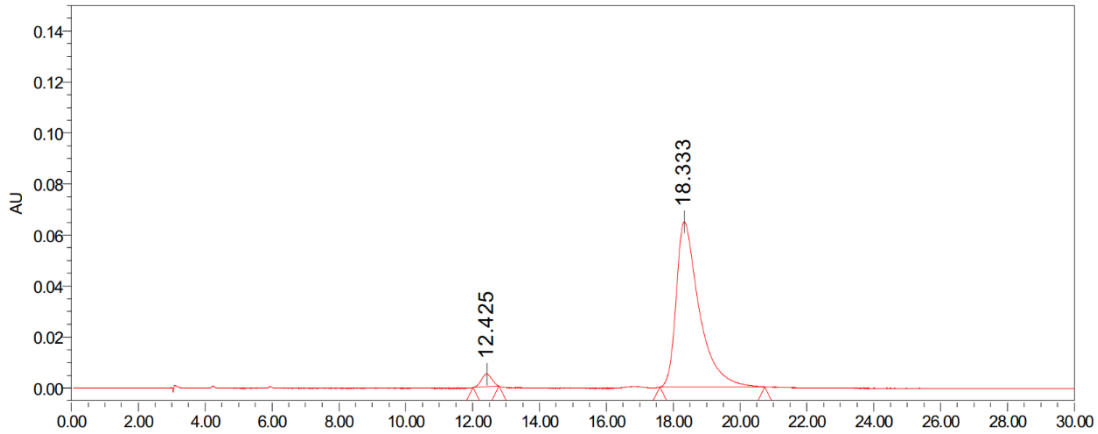
**HPLC chromatogram of chiral 32**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

λ = 254 nm

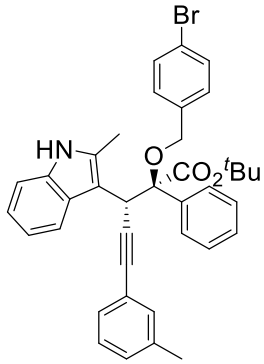
Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 12.425 | 110267 | 5022 | 3.44 |

| | | | | |
|---|---|---|---|---|
| 2 | 18.333 | 3099510 | 64842 | 96.56 |

***tert*-Butyl (2*R*,3*R*)-2-((4-bromobenzyl)oxy)-3-(2-methyl-1*H*-indol-3-yl)-2-phenyl-5-(*m*-tolyl)pent-4-ynoate (33)**




**33**

Yellow oil; 97.5 mg, 77% yield, >20:1 d.r., 95% *ee*, $[\alpha]_D^{20}$ = 6.83 (c = 0.033, MeOH); $^1$H NMR (500 MHz, $CDCl_3$) δ 7.88 (s, 1H), 7.64 (s, 1H), 7.34 (d, *J* = 8.0 Hz, 2H), 7.27 (dd, *J* = 17.0, 8.8 Hz, 4H), 7.22 – 7.14 (m, 3H), 7.08 (d, *J* = 2.9 Hz, 5H), 7.03 (t, *J* = 7.4 Hz, 1H), 6.90 (t, *J* = 7.4 Hz, 1H), 4.81 (d, *J* = 13.0 Hz, 1H), 4.74 (s, 1H), 4.30 (d, *J* = 13.0 Hz, 1H), 2.31 (s, 3H), 1.57 (s, 3H), 1.53 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 170.9, 139.3, 137.8, 136.2, 135.0, 134.3, 132.3, 131.0, 128.9, 128.7, 128.6, 128.6, 128.2, 128.0, 127.9, 127.5, 123.9, 120.8, 120.3, 119.1, 109.8, 106.0, 89.7, 89.2, 83.3, 83.0, 67.7, 41.5, 28.2, 21.3, 11.2. HRMS(ESI) $[M+Na]^+$ calcd for $C_{38}H_{36}BrNO_3Na^+$, 656.1771, found 656.1771. (Chiral IA, λ = 254 nm, *n*-hexane/2-propanol = 95/5, Flow rate = 1.0 mL/min), $t_R$ = 7.470 min, 8.958 min (major).

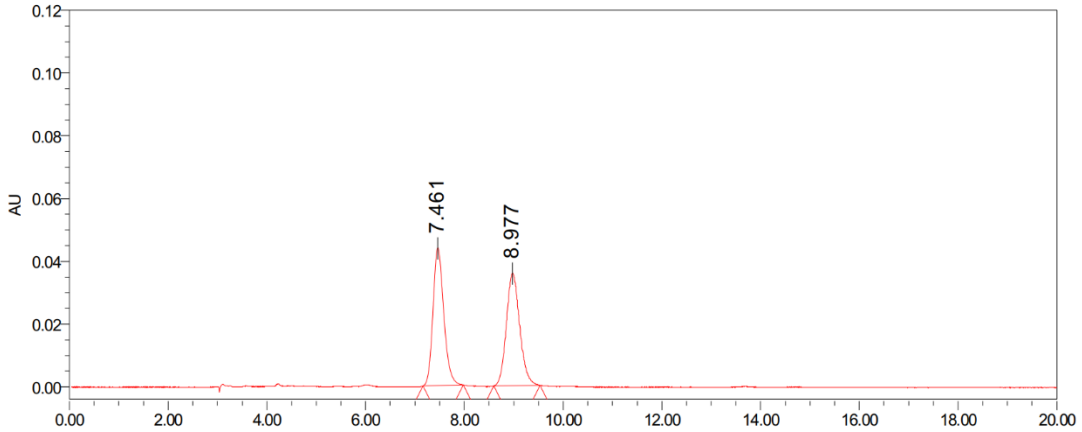
**HPLC chromatogram of racemic 33**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 7.461 | 669454 | 43804 | 50.09 |
| 2 | 8.977 | 667011 | 35772 | 49.91 |

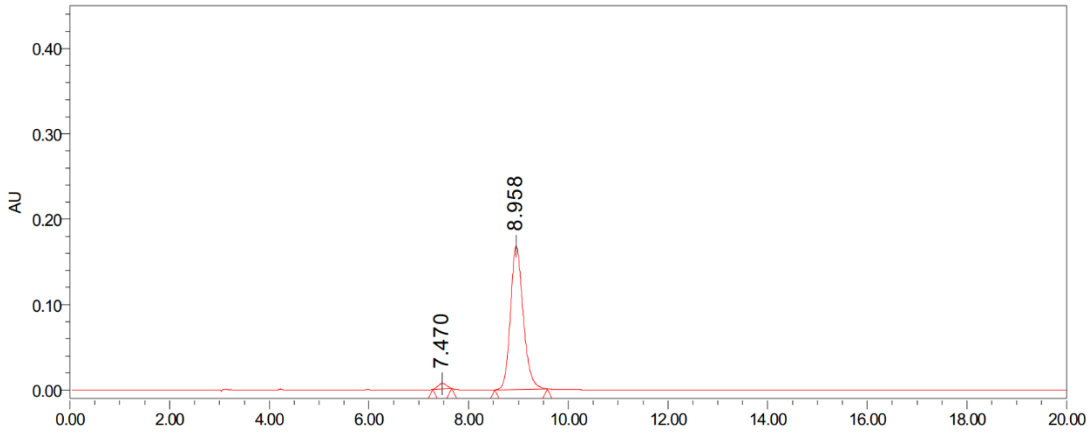
**HPLC chromatogram of chiral 33**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

λ = 254 nm

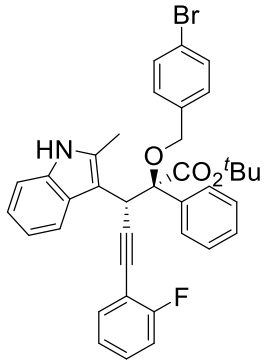
Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 7.470 | 75358 | 6271 | 2.48 |

| | | | | |
|---|---|---|---|---|
| 2 | 8.958 | 2959512 | 167864 | 97.52 |

***tert*-Butyl (2*R*,3*R*)-2-((4-bromobenzyl)oxy)-5-(2-fluorophenyl)-3-(2-methyl-1*H*-indol-3-yl)-2-phenylpent-4-ynoate (34)**




**34**

Yellow oil; 86.7 mg, 68% yield, >20:1 d.r., 94% *ee*, $[\alpha]_D^{20}$ = 9.58 (c = 0.033, MeOH); $^1$H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 5.7 Hz, 1H), 7.64 (s, 1H), 7.44 – 7.35 (m, 3H), 7.31 (d, *J* = 8.4 Hz, 2H), 7.28 – 7.24 (m, 1H), 7.23 – 7.19 (m, 1H), 7.17 (d, *J* = 8.0 Hz, 1H), 7.12 – 7.07 (m, 4H), 7.06 (d, *J* = 8.1 Hz, 2H), 7.02 (d, *J* = 7.6 Hz, 1H), 6.89 (t, *J* = 7.4 Hz, 1H), 4.82 (d, *J* = 14.1 Hz, 2H), 4.32 (d, *J* = 12.9 Hz, 1H), 1.61 (s, 3H), 1.51 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 170.9, δ 141.7 (d, *J* = 192.8 Hz), 139.2, 136.1, 135.0, 134.4, 133.9, 130.9, 129.4 (d, *J* = 7.6 Hz), 128.8, 128.6, 128.0, 127.9, 127.4, 123.8 (d, *J* = 3.8 Hz), 120.8, 120.3, 119.1, 115.5 (d, *J* = 21.4 Hz), 112.5 (d, *J* = 16.4 Hz), 109.7, 105.7, 94.8, 89.5, 83.1, 76.6, 67.8, 41.6, 28.1, 11.2. $^{19}$F NMR (376 MHz, $CDCl_3$) δ -109.85. HRMS(ESI) $[M+Na]^+$ calcd for $C_{37}H_{33}BrFNO_3Na^+$, 660.1520, found 660.1522. (Chiral IA, λ = 254 nm, *n*-hexane/2-propanol = 98/2, Flow rate = 1.0 mL/min), $t_R$ = 17.431 min, 19.478 min (major).

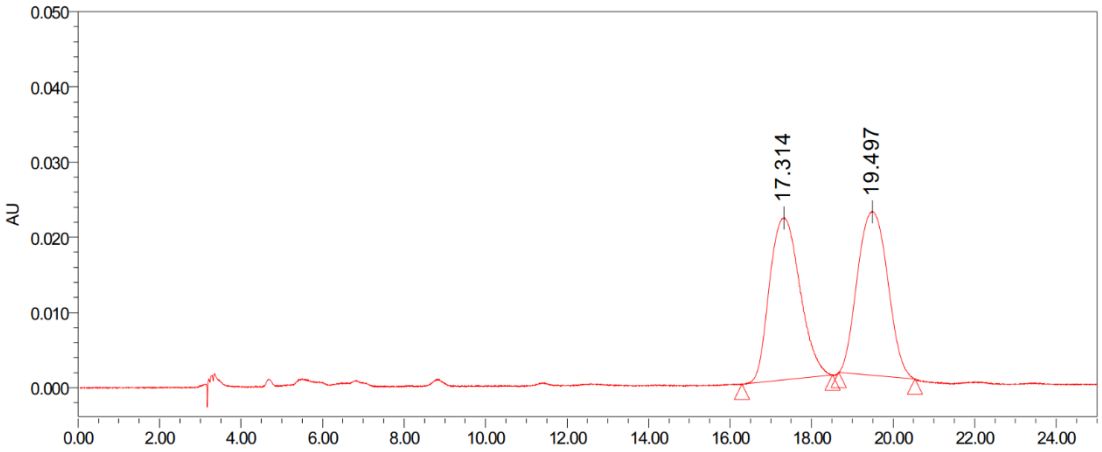
**HPLC chromatogram of racemic 34**

Condition: n-hexane/2-propanol = 98:2

Flow rate = 1.0 mL/min

λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 17.314 | 1120039 | 21525 | 49.94 |
| 2 | 19.497 | 1122854 | 21773 | 50.06 |

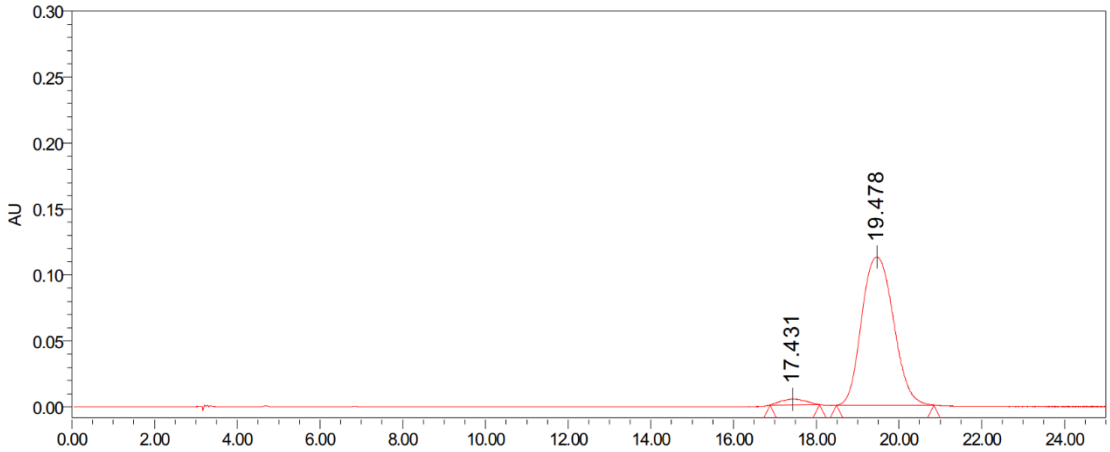
**HPLC chromatogram of chiral 34**

Condition: n-hexane/2-propanol = 98:2

Flow rate = 1.0 mL/min

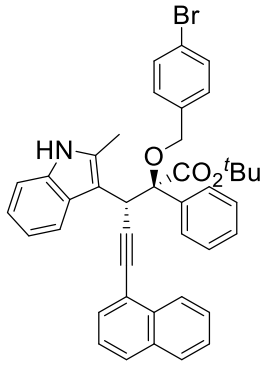
λ = 254 nm

Chiral IA



| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 17.431 | 179090 | 4259 | 2.90 |
| 2 | 19.478 | 5991215 | 112243 | 97.10 |

***tert*-Butyl (2*R*,3*R*)-2-((4-bromobenzyl)oxy)-3-(2-methyl-1*H*-indol-3-yl)-5-(naphthalen-1-yl)-2-phenylpent-4-ynoate (35)**




**35**

Yellow oil; 103.1 mg, 77% yield, >20:1 d.r., 95% *ee*, $[\alpha]_D^{20}$ = 54.41 (c = 0.033, MeOH); $^1$H NMR (500 MHz, $CDCl_3$) δ 8.48 (d, *J* = 8.4 Hz, 1H), 7.94 (s, 1H), 7.81 (d, *J* = 8.2 Hz, 1H), 7.76 (d, *J* = 8.2 Hz, 1H), 7.64 (s, 1H), 7.61 (d, *J* = 7.1 Hz, 1H), 7.47 (t, *J* = 7.5 Hz, 1H), 7.36 (dd, *J* = 14.9, 7.4 Hz, 3H), 7.33 – 7.27 (m, 3H), 7.21 (dd, *J* = 7.2, 4.7 Hz, 1H), 7.17 (d, *J* = 8.0 Hz, 1H), 7.14 – 7.09 (m, 4H), 7.03 (t, *J* = 7.5 Hz, 1H), 6.88 (t, *J* = 7.5 Hz, 1H), 4.92 (s, 1H), 4.88 (d, *J* = 12.5 Hz, 1H), 4.32 (d, *J* = 12.5 Hz, 1H), 1.63 (s, 3H), 1.48 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 171.1, 138.9, 136.1, 135.0, 134.5, 133.8, 133.2, 131.1, 130.2, 129.0, 128.8, 128.09, 128.06, 128.05, 128.0, 127.5, 127.1, 126.5, 126.3, 125.3, 121.8, 120.9, 120.5, 119.1, 109.8, 106.0, 94.4, 89.8, 83.1, 81.4, 68.0, 41.8, 28.2, 11.3. HRMS(ESI) $[M+Na]^+$ calcd for $C_{41}H_{36}BrNO_3Na^+$, 692.1771, found 692.1770. (Chiral IC, λ = 254 nm, *n*-hexane/2-propanol = 95/5, Flow rate = 1.0 mL/min), $t_R$ = 4.731 min, 5.691 min (major).

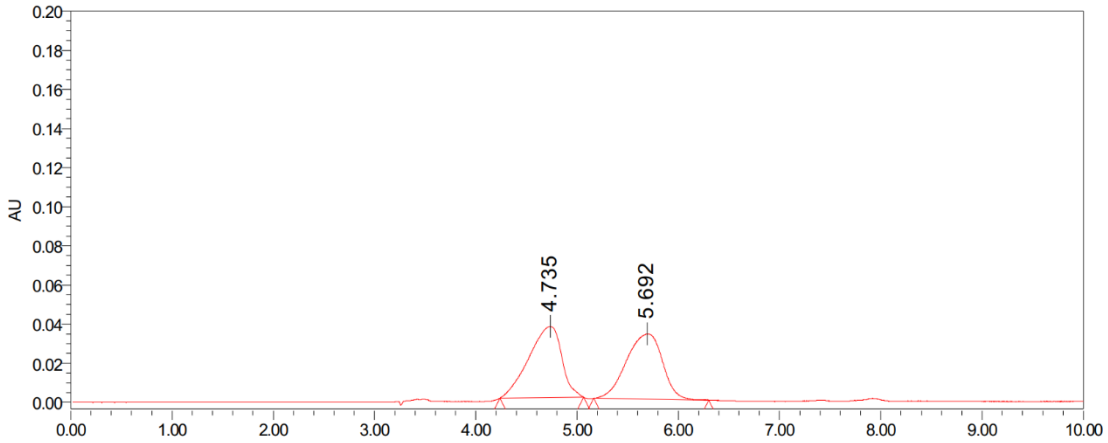
**HPLC chromatogram of racemic 35**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

λ = 254 nm

Chiral IC




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 4.735 | 823336 | 36408 | 49.94 |
| 2 | 5.692 | 825343 | 33356 | 50.06 |

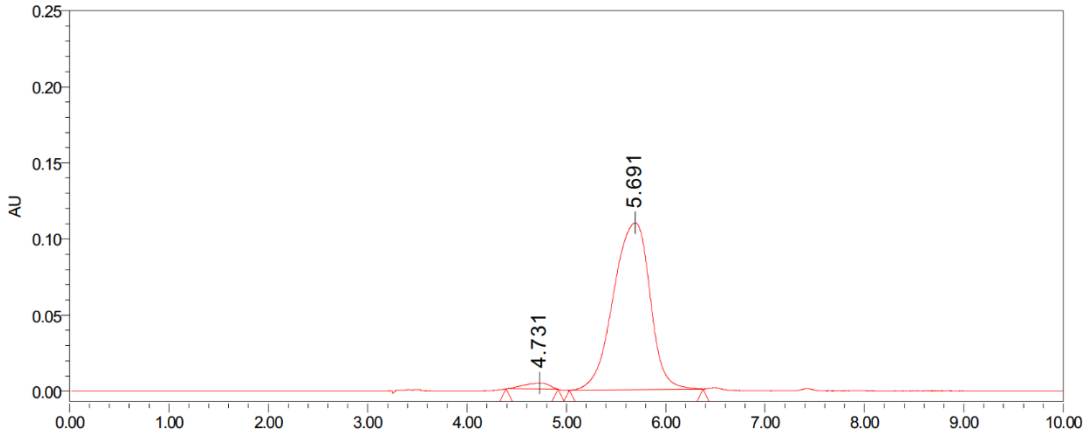
**HPLC chromatogram of chiral 35**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

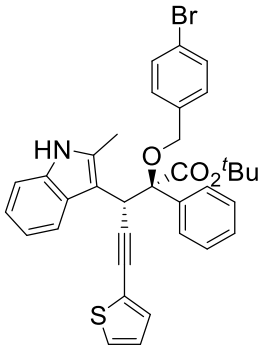
λ = 254 nm

Chiral IC




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 4.731 | 71946 | 4014 | 2.50 |
| 2 | 5.691 | 2801541 | 109530 | 97.50 |

**_tert_-Butyl (2*R*,3*R*)-2-((4-bromobenzyl)oxy)-3-(2-methyl-1*H*-indol-3-yl)-2-phenyl-5-(thiophen-2-yl)pent-4-ynoate (36)**




**36**

Yellow oil; 96.3 mg, 77% yield, >20:1 d.r., 96% *ee*, $[\alpha]_D^{20}$ = -9.36 (c = 0.033, MeOH); $^1$H NMR (500 MHz, $CDCl_3$) δ 7.83 (s, 1H), 7.64 (s, 1H), 7.37 (d, *J* = 8.2 Hz, 2H), 7.28 (d, *J* = 8.2 Hz, 2H), 7.22 – 7.17 (m, 2H), 7.14 (dd, *J* = 10.5, 5.7 Hz, 2H), 7.10 – 7.05 (m, 4H), 7.02 (t, *J* = 7.5 Hz, 1H), 6.95 – 6.92 (m, 1H), 6.90 (t, *J* = 7.5 Hz, 1H), 4.78 (d, *J* = 13.1 Hz, 1H), 4.75 (s, 1H), 4.30 (d, *J* = 13.1 Hz, 1H), 1.57 (s, 3H), 1.53 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 170.9, 139.3, 136.0, 135.0, 134.4, 131.2, 131.0, 128.8, 128.5,

128.1, 127.9, 127.5, 126.9, 126.3, 124.2, 120.8, 120.3, 119.2, 109.8, 105.6, 93.7, 89.6, 83.1, 76.5, 67.7, 41.9, 28.2, 11.2. HRMS(ESI) $[M+Na]^+$ calcd for $C_{35}H_{32}BrNO_3SNa^+$, 648.1178, found 648.1175. (Chiral IA, λ = 254 nm, *n*-hexane/2-propanol = 99/1, Flow rate = 1.0 mL/min), $t_R$ = 39.538 min, 43.205 min (major).

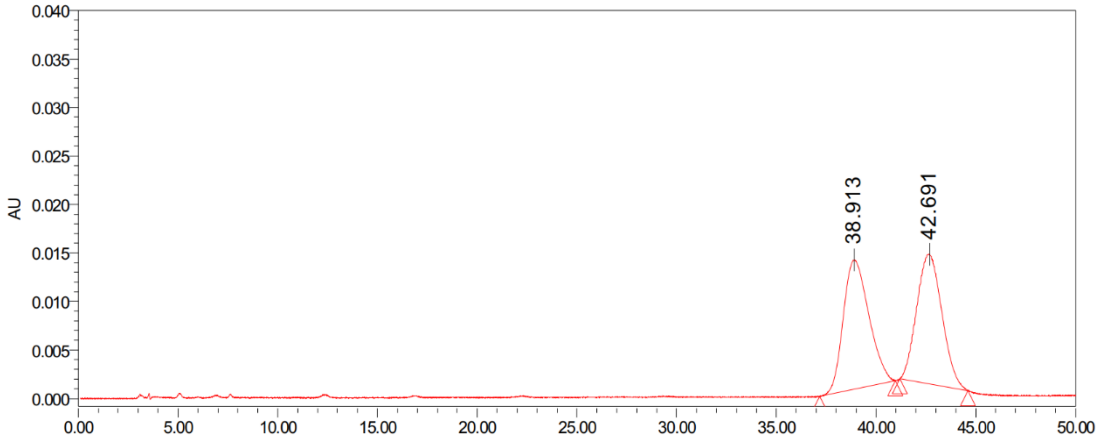
**HPLC chromatogram of racemic 36**

Condition: n-hexane/2-propanol = 99:1

Flow rate = 1.0 mL/min

λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 38.913 | 1184311 | 13330 | 50.03 |
| 2 | 42.691 | 1183023 | 13360 | 49.97 |

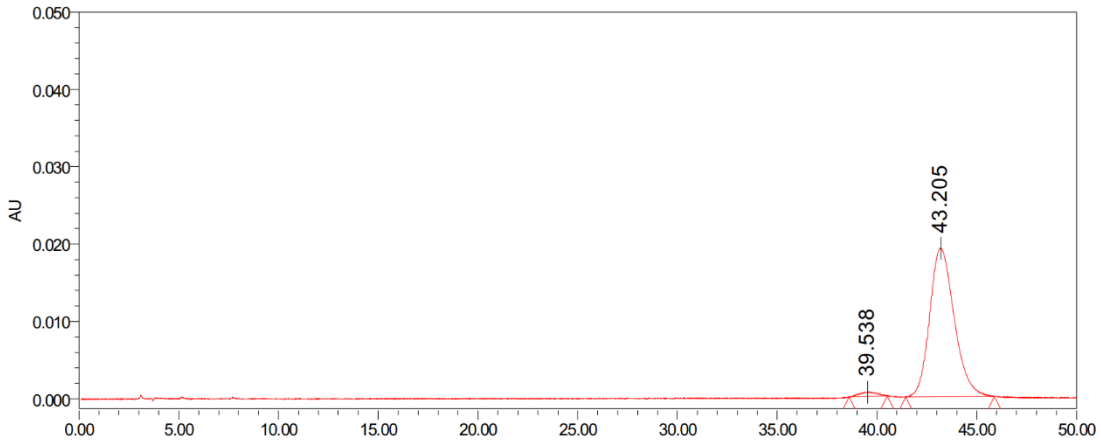
**HPLC chromatogram of chiral 36**

Condition: n-hexane/2-propanol = 99:1

Flow rate = 1.0 mL/min

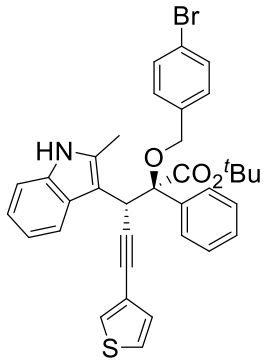
λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 39.538 | 34253 | 548 | 2.04 |
| 2 | 43.205 | 1647070 | 19207 | 97.96 |

**_tert_-Butyl (2*R*,3*R*)-2-((4-bromobenzyl)oxy)-3-(2-methyl-1*H*-indol-3-yl)-2-phenyl-5-(thiophen-3-yl)pent-4-ynoate (37)**




**37**

Yellow oil; 102.5 mg, 82% yield, >20:1 d.r., 95% *ee*, $[\alpha]_D^{20}$ = -12.15 (c = 0.033, MeOH); $^1$H NMR (500 MHz, $CDCl_3$) δ 7.88 (s, 1H), 7.64 (s, 1H), 7.34 (d, *J* = 8.6 Hz, 3H), 7.25 (d, *J* = 8.1 Hz, 2H), 7.23 – 7.21 (m, 1H), 7.18 (d, *J* = 8.0 Hz, 1H), 7.15 (d, *J* = 8.0 Hz, 1H), 7.11 – 7.06 (m, 5H), 7.03 (t, *J* = 7.5 Hz, 1H), 6.90 (t, *J* = 7.5 Hz, 1H), 4.81 (d, *J* = 13.0 Hz, 1H), 4.71 (s, 1H), 4.28 (d, *J* = 13.0 Hz, 1H), 1.55 (s, 3H), 1.53 (s, 9H). $^{13}$C

NMR (126 MHz, $CDCl_3$) δ 171.0, 139.3, 136.1, 135.1, 134.3, 130.9, 130.0, 128.8, 128.5, 128.0, 127.87, 127.86, 127.5, 125.1, 123.1, 120.8, 120.3, 119.1, 109.8, 105.8, 89.7, 89.0, 83.0, 78.4, 67.7, 41.6, 28.2, 11.1. HRMS(ESI) $[M+Na]^+$ calcd for $C_{35}H_{32}BrNO_3SNa^+$, 648.1178, found 648.1179. (Chiral IA, λ = 254 nm, *n*-hexane/2-propanol = 95/5, Flow rate = 1.0 mL/min), $t_R$ = 10.349 min, 12.001 min (major).

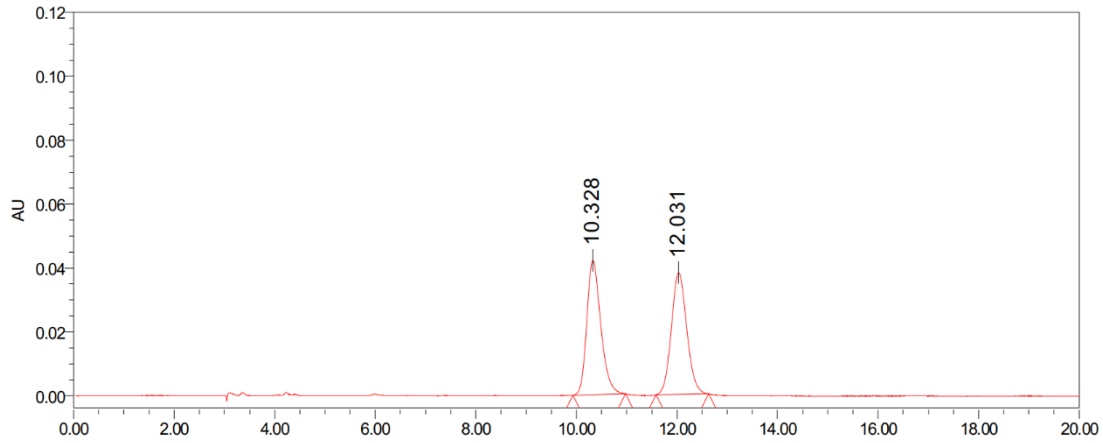
**HPLC chromatogram of racemic 37**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 10.328 | 813577 | 42019 | 50.07 |
| 2 | 12.031 | 811280 | 37995 | 49.93 |

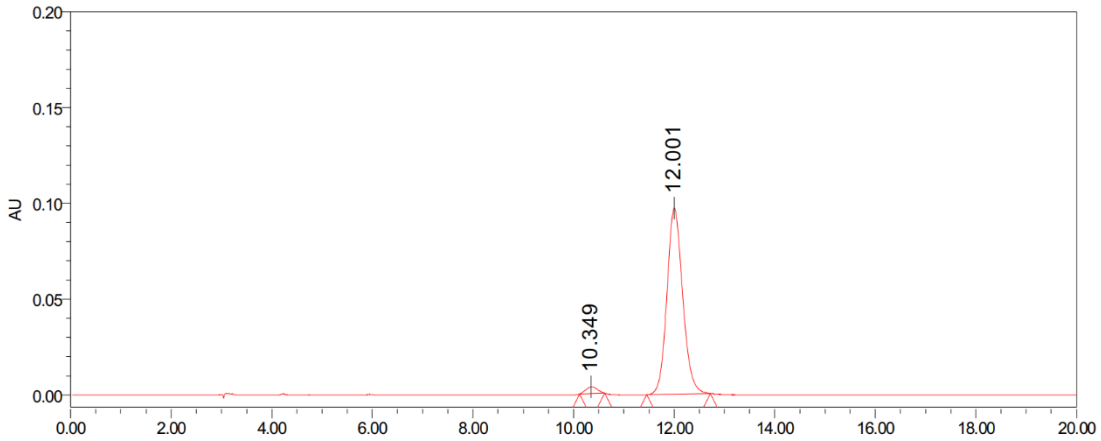
**HPLC chromatogram of chiral 37**

Condition: n-hexane/2-propanol = 95:5

Flow rate = 1.0 mL/min

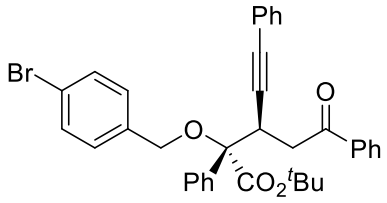
λ = 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 10.349 | 54960 | 3473 | 2.53 |
| 2 | 12.001 | 2117462 | 97155 | 97.47 |

**Tert-butyl (2S,3R)-2-((4-bromobenzyl)oxy)-3-(2-oxo-2-phenylethyl)-2,5-diphenylpent-4-ynoate(38)**




**38**

Colorless oil; 65.7 mg, 72% yield, 98:2 d.r., 98% *ee*, $[\alpha]_D^{20}$ = -14.66 (c = 0.1, $CH_2Cl_2$); $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.87 – 7.82 (m, 2H), 7.71 – 7.67 (m, 2H), 7.56 – 7.50 (m, 1H), 7.49 – 7.46 (m, 2H), 7.42 (d, *J* = 7.9 Hz, 2H), 7.38 (d, *J* = 8.5 Hz, 3H), 7.35 – 7.31 (m, 2H), 7.24 (d, *J* = 8.2 Hz, 5H), 5.05 (d, *J* = 11.7 Hz, 1H), 4.90 (d, *J* = 11.7 Hz, 1H), 4.41 (dd, *J* = 10.2, 3.1 Hz, 1H), 3.32 (dd, *J* = 16.6, 10.2 Hz, 1H), 3.09 (dd, *J* = 16.6, 3.1 Hz, 1H), 1.51 (s, 9H). $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 197.4, 169.4, 138.3,

138.1, 136.9, 133.1, 131.4, 129.2, 128.6, 128.6, 128.3, 128.3, 128.3, 128.2, 127.9, 126.7, 123.4, 121.2, 89.7, 85.9, 84.1, 83.0, 68.0, 39.2, 36.6, 28.1. HRMS (ESI) $[M+Na]^+$ calcd for $C_{36}H_{33}O_4BrNa^+$, 631.1454, found 631.1455. (Chiral IA, λ= 254 nm, *n*-hexane/2-propanol= 49/1, Flow rate = 1.0 mL/min), $t_R$ = 10.370 min(major), 18.293 min.

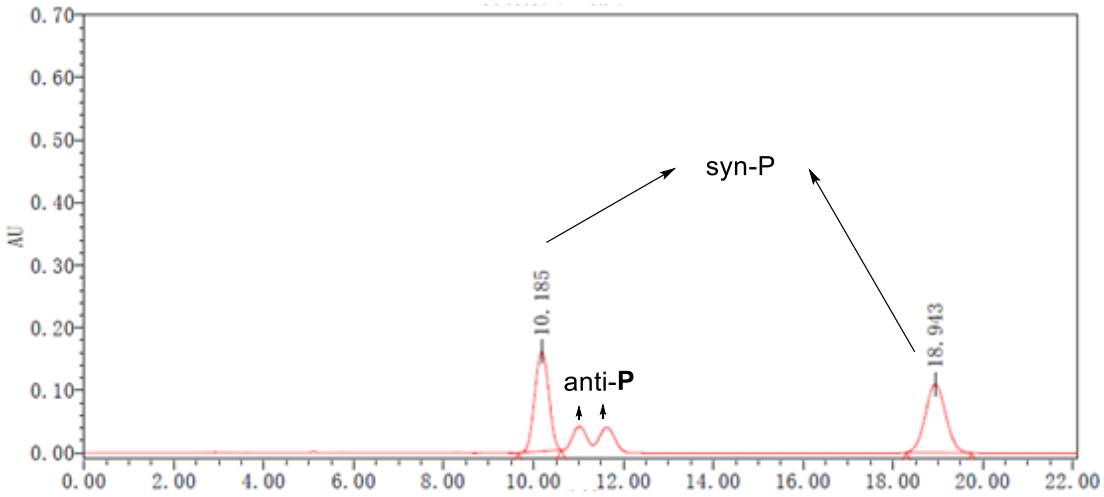
**HPLC chromatogram of racemic 38**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 10.185 | 3452482 | 159302 | 49.84 |
| 2 | 18.943 | 3475146 | 109538 | 50.16 |

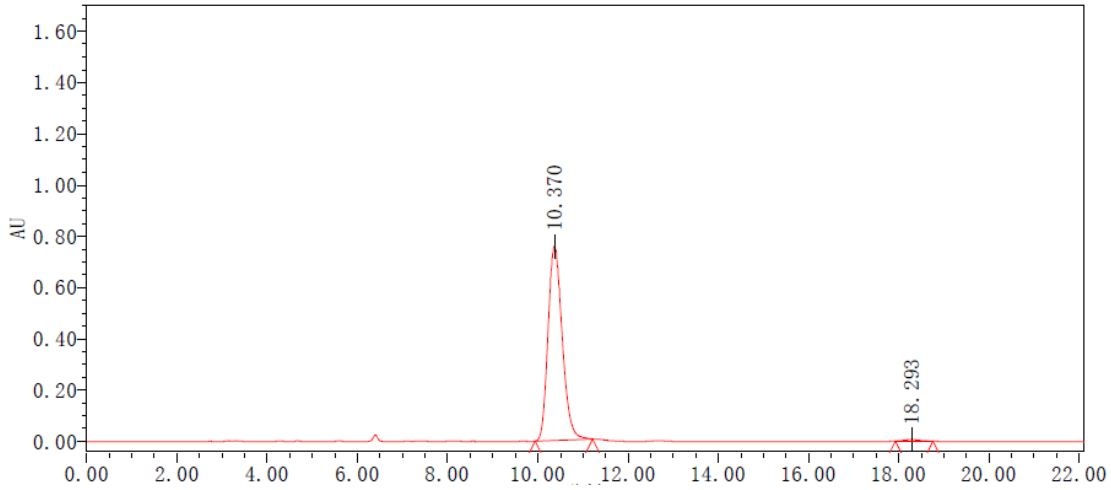
**HPLC chromatogram of chiral 38**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 10.370 | 16665235 | 756830 | 99.11 |
| 2 | 18.293 | 150064 | 5601 | 0.89 |

**HPLC chromatogram of 7 (half a gram-scale synthesis)**

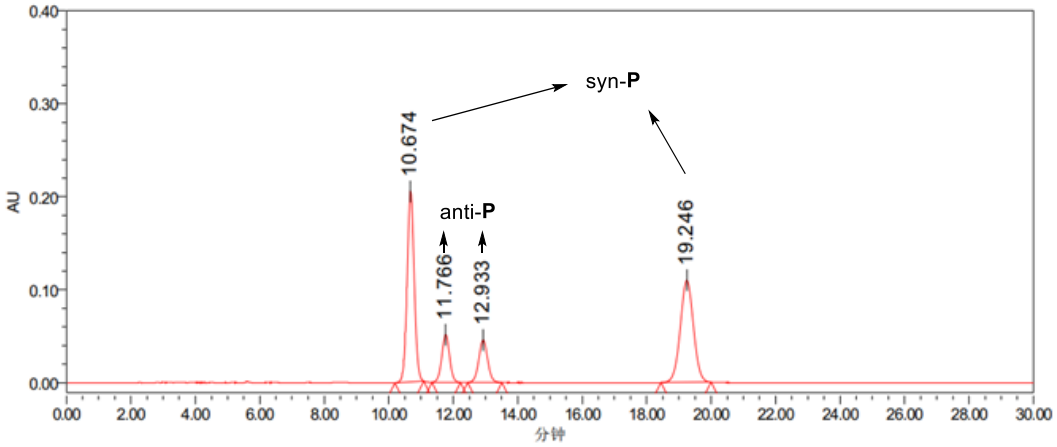
**HPLC chromatogram of racemic 38**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 10.674 | 3126283 | 204889 | 38.60 |
| 2 | 11.766 | 867633 | 51348 | 10.72 |
| 3 | 12.933 | 884701 | 45933 | 10.92 |
| 4 | 19.246 | 3130920 | 109766 | 38.66 |

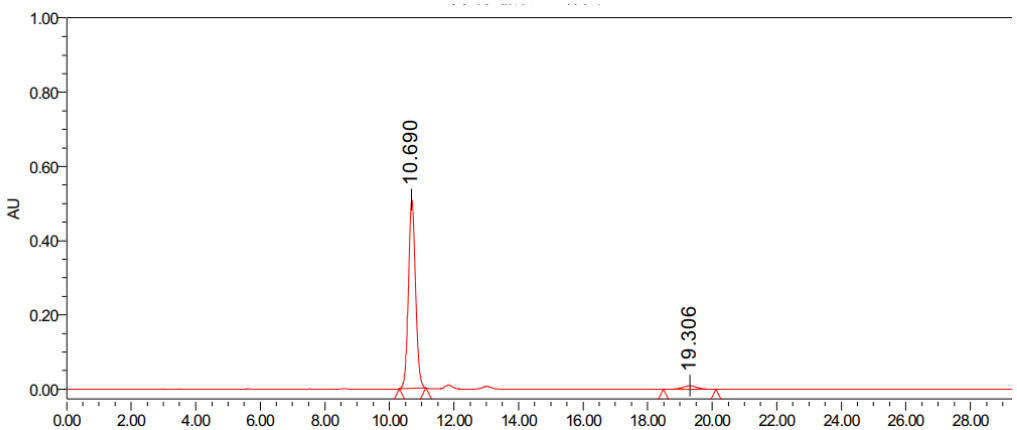
**HPLC chromatogram of chiral 38**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

λ= 254 nm

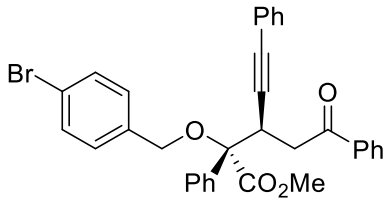
Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 10.690 | 7766989 | 508858 | 96.74 |

| | | | | |
|---|---|---|---|---|
| 2 | 19.306 | 262150 | 9198 | 3.26 |

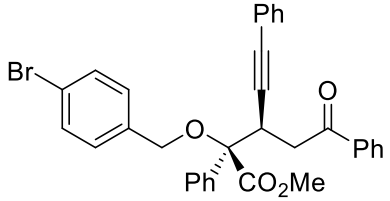
**Methyl (2*S*,3*R*)-2-((4-bromobenzyl)oxy)-3-(2-oxo-2-phenylethyl)-2,5-diphenylpent-4-ynoate(syn-38-b)**




*syn*-**38-b**

Colorless oil; 56.9 mg, 67% yield, 94:6 d.r., 46% *ee*; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.86 – 7.82 (m, 2H), 7.68 – 7.64 (m, 2H), 7.53 (t, *J* = 7.4 Hz, 1H), 7.47 (dd, *J* = 8.5, 4.0 Hz, 2H), 7.42 – 7.34 (m, 7H), 7.24 (d, *J* = 6.0 Hz, 5H), 5.03 (d, *J* = 11.6 Hz, 1H), 4.83 (d, *J* = 11.6 Hz, 1H), 4.48 (dd, *J* = 10.0, 3.2 Hz, 1H), 3.85 (s, 3H), 3.29 (dd, *J* = 16.7, 10.0 Hz, 1H), 3.18 – 3.11 (m, 1H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ $^{13}$C NMR (101 MHz, $CDCl_3$) δ 197.2, 171.2, 137.7, 136.8, 133.2, 131.5, 131.5, 129.3, 128.8, 128.6, 128.5, 128.2, 128.2, 128.2, 128.0, 126.7, 123.2, 121.4, 89.0, 86.2, 84.5, 68.2, 52.6, 39.3, 36.5. HRMS (ESI) $[M+Na]^+$ calcd for $C_{33}H_{27}O_4BrNa^+$, 589.0985, found 589.0985. (Chiral IA-3, λ= 254 nm, *n*-hexane/2-propanol= 49/1, Flow rate = 1.0 mL/min), $t_R$ = 23.807 min(major), 35.090 min.

**Methyl (2R,3R)-2-((4-bromobenzyl)oxy)-3-(2-oxo-2-phenylethyl)-2,5-diphenylpent-4-ynoate(anti-38-b)**




*anti*-**38-b**

$^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.88 – 7.84 (m, 2H), 7.61 (dd, *J* = 8.0, 1.6 Hz, 2H), 7.52

(t, *J* = 7.4 Hz, 1H), 7.45 (d, *J* = 8.4 Hz, 2H), 7.42 (d, *J* = 8.0 Hz, 3H), 7.39 (d, *J* = 1.9 Hz, 2H), 7.26 – 7.22 (m, 7H), 4.57 (d, *J* = 12.1 Hz, 1H), 4.49 (d, *J* = 12.4 Hz, 1H), 3.83 (s, 3H), 3.54 (s, 1H), 3.15 (d, *J* = 5.3 Hz, 2H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 197.3, 171.0, 137.2, 136.9, 135.5, 133.1, 131.5, 131.4, 128.8, 128.7, 128.6, 128.5, 128.4, 128.2, 128.1, 128.0, 123.2, 121.3, 88.6, 87.1, 84.3, 67.4, 52.6, 39.7, 37.3. HRMS (ESI) $[M+Na]^+$ calcd for $C_{33}H_{27}O_4BrNa^+$, 589.0985, found 589.0985.

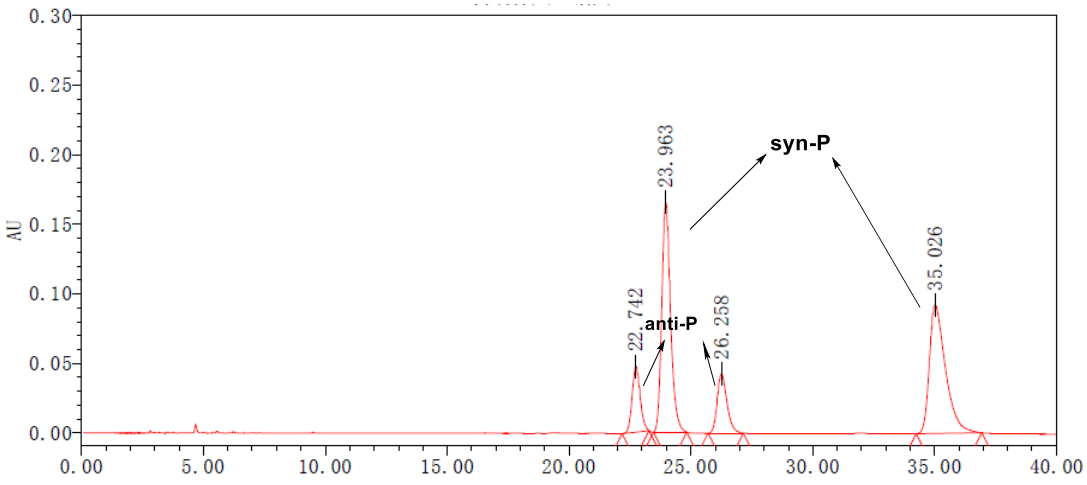
**HPLC chromatogram of racemic 38-b**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 22.742 | 1103292 | 47006 | 10.22 |
| 2 | 23.963 | 4220677 | 165268 | 39.10 |
| 3 | 26.258 | 1201744 | 42685 | 11.13 |
| 4 | 35.026 | 4267537 | 92238 | 39.54 |

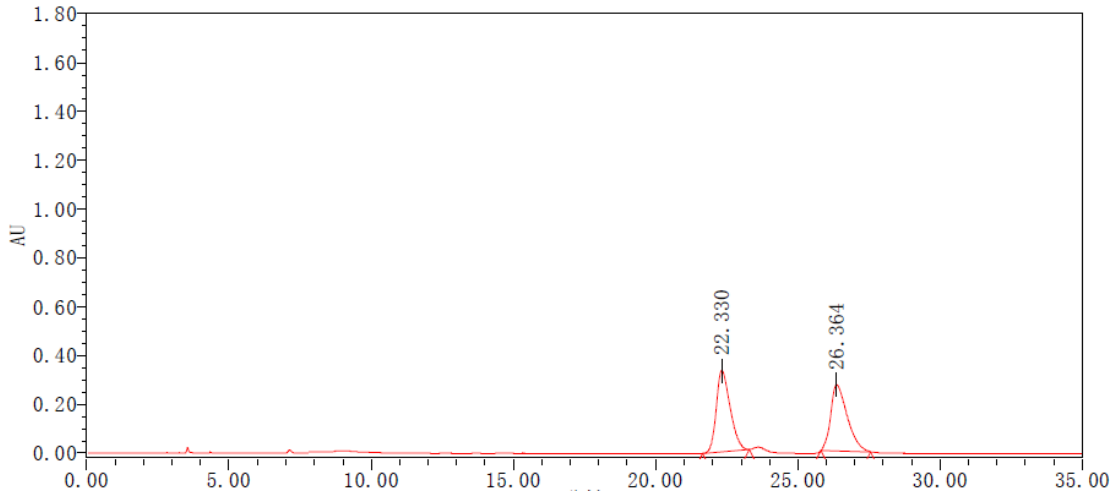
**HPLC chromatogram of racemic anti-38-b**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 22.330 | 11113205 | 333082 | 50.34 |
| 2 | 26.364 | 10962316 | 271172 | 49.66 |

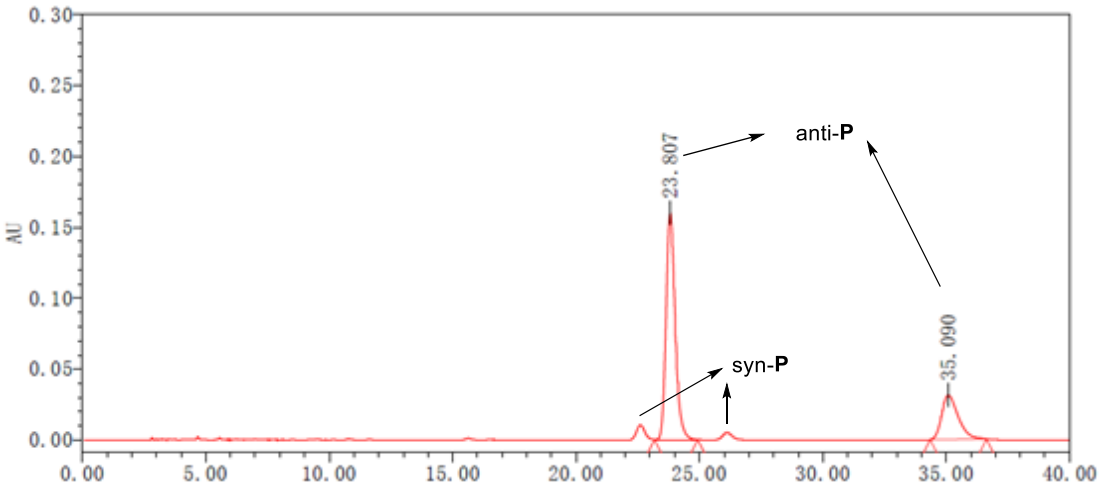
**HPLC chromatogram of chiral 38-b**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

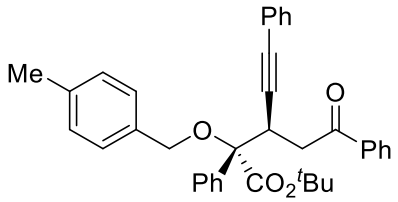
λ= 254 nm

Chiral IA-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 23.807 | 4122942 | 160048 | 73.78 |
| 2 | 35.090 | 1464980 | 31383 | 26.22 |

**Tert-butyl (2S,3R)-2-((4-methylbenzyl)oxy)-3-(2-oxo-2-phenylethyl)-2,5-diphenylpent-4-ynoate (39)**




**39**

Colorless oil; 53.0 mg, 65% yield, >20:1 d.r., 92% *ee*, $[\alpha]_D^{20}$ = -12.61 (c = 0.1, $CH_2Cl_2$); $^1$H NMR (500 MHz, $CDCl_3$) δ 7.85 (d, *J* = 7.5 Hz, 2H), 7.71 (d, *J* = 7.6 Hz, 2H), 7.52 (t, *J* = 7.3 Hz, 1H), 7.43 – 7.39 (m, 3H), 7.37 (d, *J* = 6.6 Hz, 1H), 7.35 (d, *J* = 7.8 Hz, 2H), 7.30 (d, *J* = 7.3 Hz, 2H), 7.26 – 7.22 (m, 4H), 7.18 (d, *J* = 7.8 Hz, 2H), 5.08 (d, *J* = 11.1 Hz, 1H), 4.92 (d, *J* = 11.1 Hz, 1H), 4.40 (dd, *J* = 10.3, 2.7 Hz, 1H), 3.36 (dd, *J* = 16.7, 10.4 Hz, 1H), 3.10 (dd, *J* = 16.6, 2.6 Hz, 1H), 2.36 (s, 3H), 1.52 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 197.6, 169.6, 138.7, 137.1, 136.0, 136.0, 133.0, 131.4, 129.0, 128.5, 128.2, 128.2, 128.2, 128.1, 127.8, 127.7, 126.8, 123.5, 89.9, 85.7, 84.1, 82.7,

68.5, 39.2, 36.6, 28.1, 21.3. HRMS (ESI) $[M+Na]^+$ calcd for $C_{37}H_{36}O_4Na^+$, 567.2506, found 567.2509. (Chiral IE-3, λ= 254 nm, *n*-hexane/2-propanol= 97/3, Flow rate = 1.0 mL/min), $t_R$ = 13.596 min(major), 30.967 min.

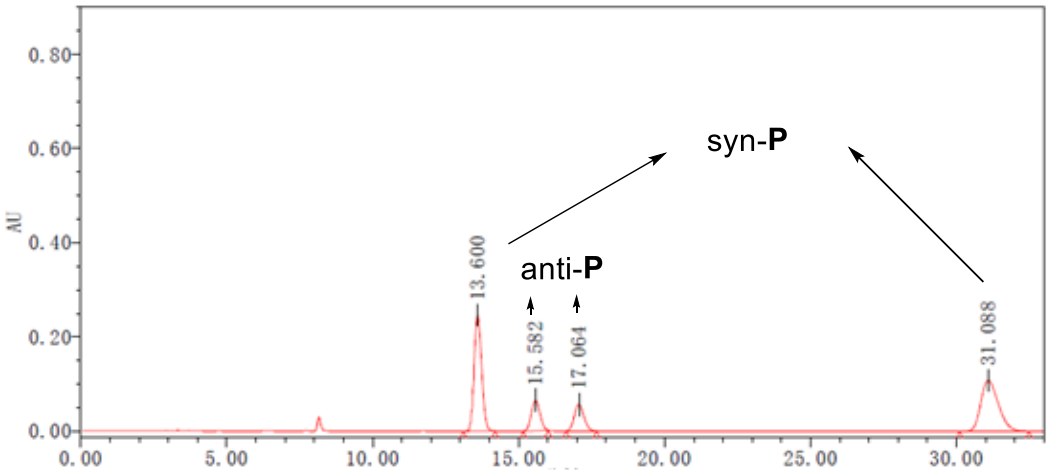
**HPLC chromatogram of racemic 39**

Condition: n-hexane/2-propanol =97:3

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 13.600 | 4423931 | 246453 | 38.31 |
| 2 | 15.582 | 1316349 | 64450 | 11.40 |
| 3 | 17.064 | 1316626 | 56624 | 11.40 |
| 4 | 31.088 | 4489356 | 108334 | 38.88 |

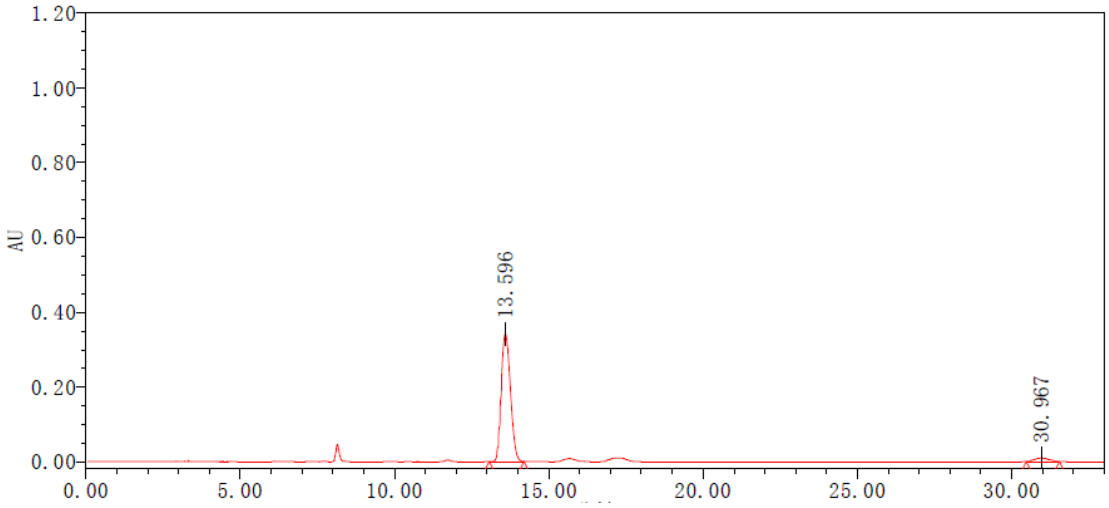
**HPLC chromatogram of chiral 39**

Condition: n-hexane/2-propanol =97:3

Flow rate =1.0 mL/min

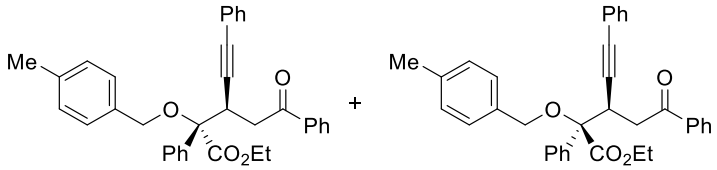
λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 13.596 | 7092744 | 341401 | 95.97 |
| 2 | 30.967 | 297822 | 8763 | 4.03 |

**Ethyl (2S,3R)-2-((4-methylbenzyl)oxy)-3-(2-oxo-2-phenylethyl)-2,5-diphenylpent-4-ynoate (*syn*-39-b)**




*syn*-**39-b**(major) *anti*-**39-b**(minor)

Colorless oil; Combined in 50% yield (35.6mg), 85:15 d.r, 33% ee. Composite NMR signals of *syn*-**39-b** (major) and *anti*-**39-b** (minor) (The ratio of two diasteroisomers in $^1$H NMR is *syn*-**39-b** : *anti*-**39-b** (minor) = 3.00 : 0.60).$^1$H NMR (500 MHz, $CDCl_3$) δ 7.85 (comp, 2.47H), 7.70 (d, *J* = 7.6 Hz, 2.06H), 7.66 (d, *J* = 7.4 Hz, 0.43H), 7.52 (comp, 1.35H), 7.39 (comp, 7.58H), 7.33 – 7.28 (comp, 1.54H), 7.23 (comp, 6.53H), 7.18 (d, *J* = 7.8 Hz, 2.07H), 7.15 (d, *J* = 7.9 Hz, 0.42H), 5.08 (d, *J* = 11.1 Hz, 1H), 4.88 (d, *J* = 11.1 Hz, 1H), 4.55 (q, *J* = 11.4 Hz, 0.43H), 4.46 (dd, *J* = 10.3, 2.7 Hz, 1H), 4.38 – 4.28

(comp, 2.52H), 3.33 (dd, *J* = 16.6, 10.3 Hz, 1.02H), 3.21 (dd, *J* = 16.5, 3.1 Hz, 0.21H), 3.13 (dd, *J* = 16.7, 2.9 Hz, 1.01H), 3.04 (dd, *J* = 16.5, 10.3 Hz, 0.21H), 2.36 (s, 3H), 2.34 (s, 0.6H), 1.32 (comp, 3.60H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 197.5, 170.8, 138.2, 137.2, 136.9, 135.7, 133.1, 131.5, 131.5, 129.0, 128.5, 128.3, 128.3, 128.2, 128.1, 127.9, 127.7, 127.3, 126.8, 123.4, 89.4, 86.6, 85.8, 84.3, 69.4, 68.5, 67.9, 61.7, 39.3, 36.6, 29.7, 21.2, 14.3. HRMS (ESI) $[M+Na]^+$ calcd for $C_{35}H_{32}O_4Na^+$, 539.2193, found 539.2197. (Chiral IA, λ= 254 nm, *n*-hexane/2-propanol= 19/1, Flow rate = 1.0 mL/min), $t_R$ = 12.128 min (major), 16.115 min.

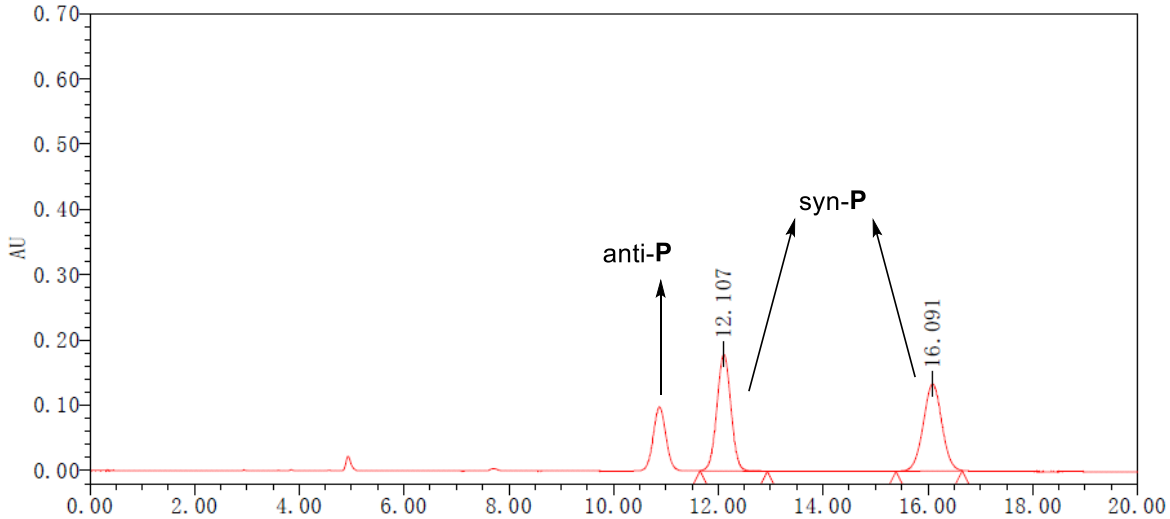
**HPLC chromatogram of racemic 39-b**

Condition: n-hexane/2-propanol = 19:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 12.107 | 3290381 | 178678 | 50.06 |
| 2 | 16.091 | 3282907 | 133193 | 49.94 |

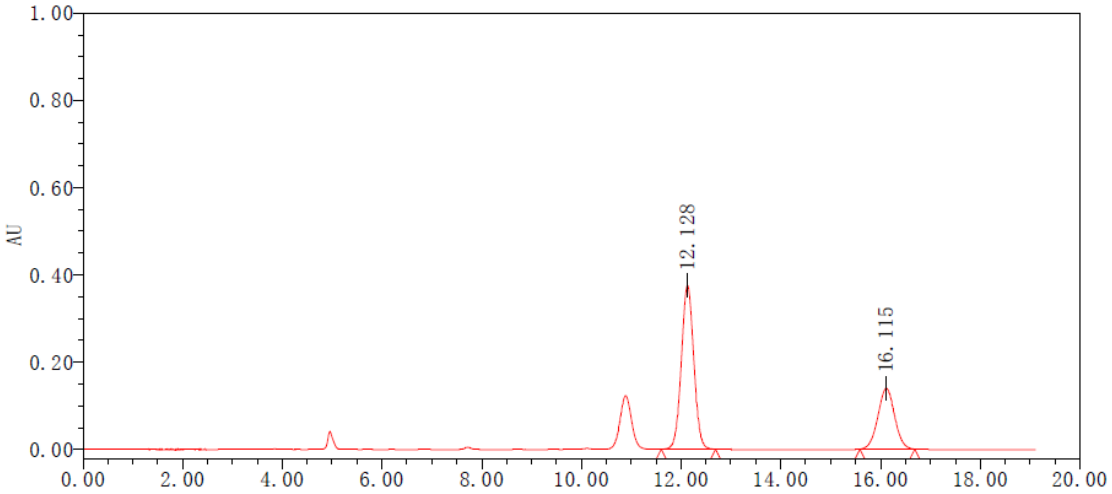
**HPLC chromatogram of chiral 39-b**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

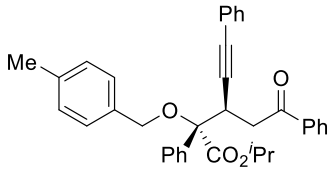
λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 12.128 | 6442648 | 375471 | 66.50 |
| 2 | 16.115 | 3244931 | 139136 | 33.50 |

**Isopropyl (2S,3R)-2-((4-methylbenzyl)oxy)-3-(2-oxo-2-phenylethyl)-2,5-diphenylpent-4-ynoate (*syn*-39-c)**




*syn*-**39-c**

Colorless oil; 54% yield (32.2mg), 89:11 d.r, 60% ee. $^1$H NMR (500 MHz, $CDCl_3$) δ 7.85 (d, *J* = 7.7 Hz, 2H), 7.71 (d, *J* = 7.5 Hz, 2H), 7.51 (t, *J* = 7.4 Hz, 1H), 7.42 (d, *J* = 5.4 Hz, 2H), 7.40 (d, *J* = 4.9 Hz, 2H), 7.37 (d, *J* = 7.1 Hz, 1H), 7.34 (d, *J* = 7.8 Hz, 2H), 7.30 (d, *J* = 7.1 Hz, 1H), 7.25 – 7.22 (m, 4H), 7.18 (d, *J* = 7.8 Hz, 2H), 5.21 (dt, *J* =

12.5, 6.3 Hz, 1H), 5.09 (d, *J* = 11.1 Hz, 1H), 4.92 (d, *J* = 11.1 Hz, 1H), 4.45 (dd, *J* = 10.3, 2.9 Hz, 1H), 3.35 (dd, *J* = 16.7, 10.4 Hz, 1H), 3.10 (dd, *J* = 16.7, 2.9 Hz, 1H), 2.37 (s, 3H), 1.31 (d, *J* = 6.3 Hz, 3H), 1.29 (d, *J* = 6.1 Hz, 3H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 197.5, 170.1, 138.4, 137.2, 135.8, 133.1, 131.4, 129.0, 128.5, 128.2, 128.1, 127.9, 127.8, 127.3, 126.8, 123.4, 89.6, 85.6, 84.2, 69.6, 68.7, 39.3, 36.5, 21.8, 21.8, 21.2. HRMS (ESI) $[M+Na]^+$ calcd for $C_{36}H_{34}O_4Na^+$, 553.2349, found 553.2351. (Chiral IA, λ= 254 nm, *n*-hexane/2-propanol= 49/1, Flow rate = 1.0 mL/min), $t_R$ = 15.207 min (major), 26.479 min.

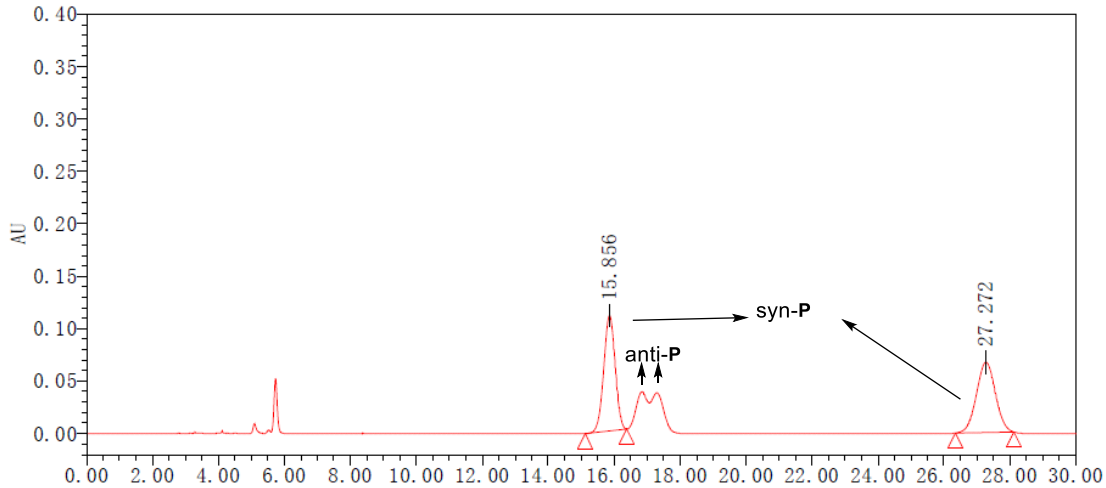
**HPLC chromatogram of racemic 39-c**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 15.856 | 2647839 | 110026 | 49.75 |
| 2 | 27.272 | 2674916 | 66984 | 50.25 |

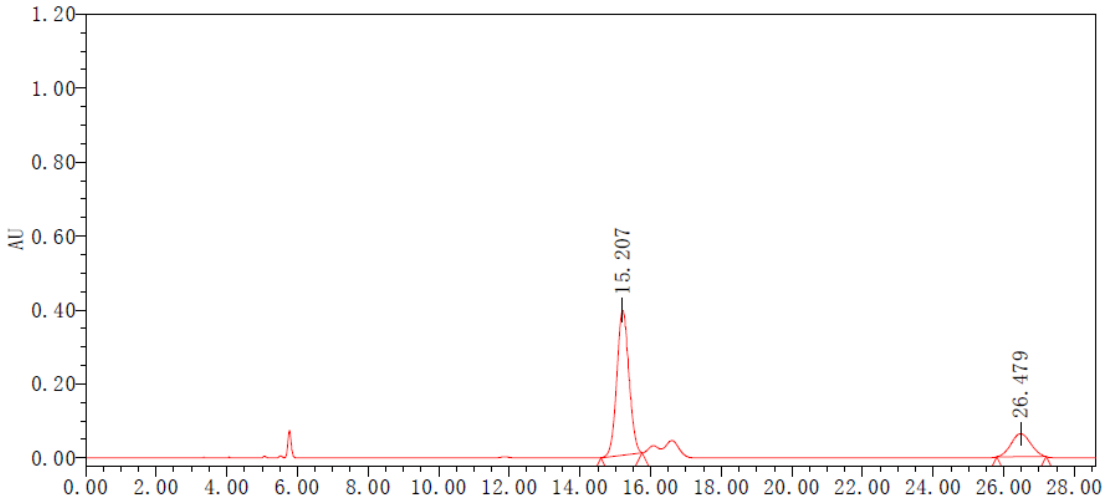
**HPLC chromatogram of chiral 39-c**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

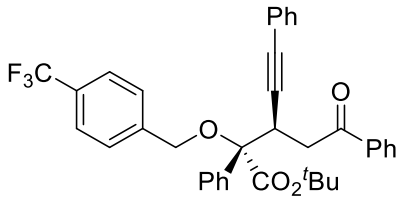
λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 15.207 | 9413437 | 391747 | 79.70 |
| 2 | 26.479 | 2398163 | 62428 | 20.30 |

**Tert-butyl (2S,3R)-3-(2-oxo-2-phenylethyl)-2,5-diphenyl-2-((4-(trifluoromethyl)benzyl)oxy)pent-4-ynoate(40)**




**40**

Colorless oil; 53.9 mg, 60% yield, >20:1 d.r., 98% *ee*, $[\alpha]_D^{20}$ = -13.91 (c = 0.1, $CH_2Cl_2$);

$^1$H NMR (400 MHz, $CDCl_3$) δ 7.87 – 7.83 (m, 2H), 7.72 – 7.68 (m, 2H), 7.64 – 7.59

(m, 4H), 7.53 (t, *J* = 7.4 Hz, 1H), 7.44 – 7.36 (m, 4H), 7.33 (d, *J* = 7.1 Hz, 1H), 7.25 (d, *J* = 6.3 Hz, 5H), 5.16 (d, *J* = 12.3 Hz, 1H), 5.02 (d, *J* = 12.2 Hz, 1H), 4.44 (dd, *J* = 10.1, 3.1 Hz, 1H), 3.34 (dd, *J* = 16.7, 10.1 Hz, 1H), 3.11 (dd, *J* = 16.7, 3.0 Hz, 1H), 1.51 (s, 9H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 197.3, 169.4, 143.1, 137.5 (d, *J* = 130.6 Hz), 133.2, 131.4, 131.4, 128.6, 128.5, 128.4, 128.2, 128.2, 128.0, 128.0, 127.5, 126.7, 125.2 (q, *J* = 3.7 Hz), 123.3, 89.6, 86.0, 84.2, 83.1, 68.0, 39.2, 36.6, 28.1. $^{19}$F NMR (376 MHz, $CDCl_3$) δ -62.38. HRMS (ESI) $[M+Na]^+$ calcd for $C_{37}H_{33}O_4F_3Na^+$, 621.2223, found 621.2225. (Chiral IA, λ= 254 nm, *n*-hexane/2-propanol= 19/1, Flow rate = 1.0 mL/min), $t_R$ = 9.784 min(major), 15.402 min.

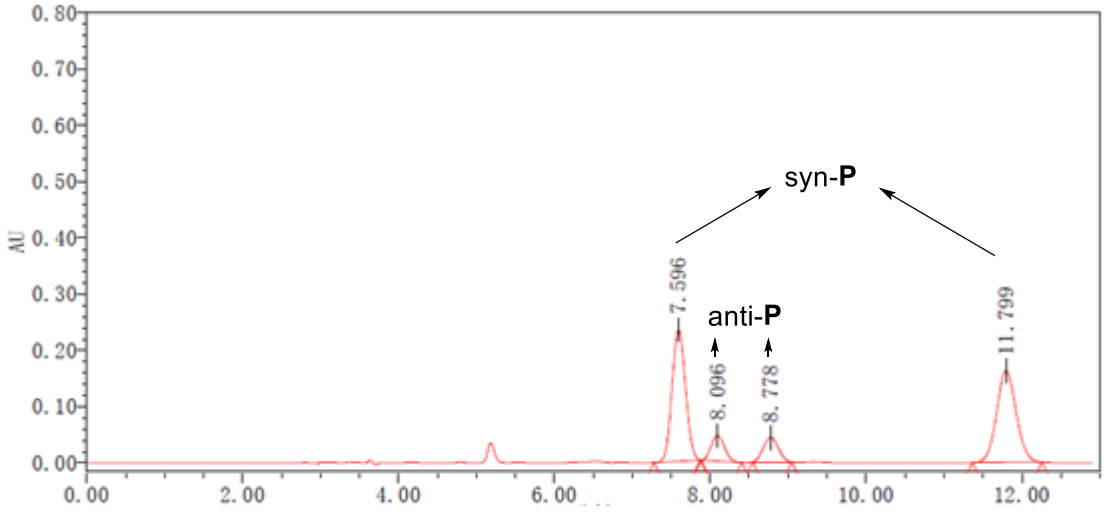
**HPLC chromatogram of racemic 40**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 7.596 | 2821506 | 233593 | 41.39 |
| 2 | 8.096 | 550314 | 45273 | 8.07 |

| | | | | |
|---|---|---|---|---|
| 3 | 8.778 | 584575 | 43290 | 8.58 |
| 4 | 11.799 | 2860608 | 162948 | 41.96 |

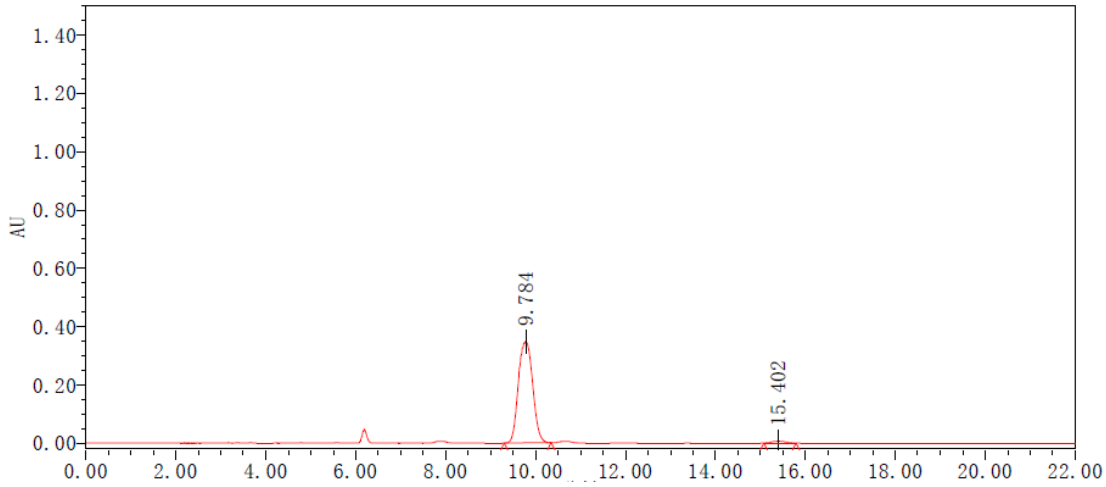
**HPLC chromatogram of chiral 40**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

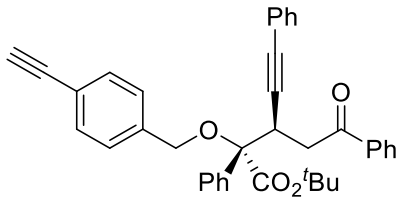
λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 9.784 | 7756472 | 347620 | 98.21 |
| 2 | 15.402 | 141404 | 6245 | 1.79 |

**Tert-butyl (2S,3R)-2-((4-ethynylbenzyl)oxy)-3-(2-oxo-2-phenylethyl)-2,5-diphenylpent-4-ynoate (41)**




**41**

Colorless oil; 45.6 mg, 55% yield, >20:1 d.r., 96% *ee*, $[\alpha]_D^{20}$ = -12.11 (c = 0.1, $CH_2Cl_2$); $^1$H NMR (400 MHz, $CDCl_3$) δ 7.86 – 7.81 (m, 2H), 7.72 – 7.68 (m, 2H), 7.53 – 7.49 (m, 1H), 7.47 (d, *J* = 4.7 Hz, 3H), 7.43 – 7.34 (m, 5H), 7.32 (d, *J* = 7.1 Hz, 1H), 7.24 (d, *J* = 9.1 Hz, 5H), 5.10 (d, *J* = 12.1 Hz, 1H), 4.95 (d, *J* = 12.1 Hz, 1H), 4.41 (dd, *J* = 10.1, 3.1 Hz, 1H), 3.33 (dd, *J* = 16.6, 10.2 Hz, 1H), 3.10 (dd, *J* = 16.6, 3.1 Hz, 1H), 3.07 (s, 1H), 1.51 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 197.5, 169.4, 139.9, 138.3, 136.9, 133.1, 132.1, 131.4, 128.5, 128.3, 128.2, 128.2, 128.2, 127.9, 127.3, 126.7, 123.4, 121.0, 89.7, 85.9, 84.1, 83.7, 82.9, 68.3, 39.2, 36.7, 28.1. HRMS (ESI) $[M+Na]^+$ calcd for $C_{38}H_{34}O_4Na^+$, 577.2349, found 577.2346. (Chiral IA-3, λ= 254 nm, *n*-hexane/2-propanol= 49/1, Flow rate = 1.0 mL/min), $t_R$ = 12.667 min(major), 26.065 min.

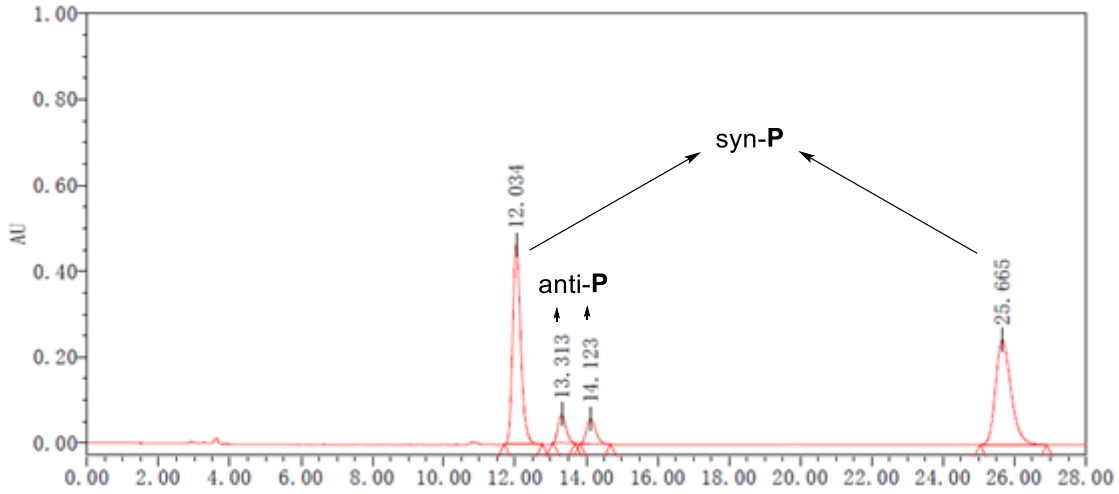
**HPLC chromatogram of racemic 41**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 12.034 | 7234797 | 465971 | 43.58 |
| 2 | 13.313 | 1048221 | 66826 | 6.31 |
| 3 | 14.123 | 1047789 | 58802 | 6.31 |
| 4 | 25.665 | 7269537 | 244342 | 43.79 |

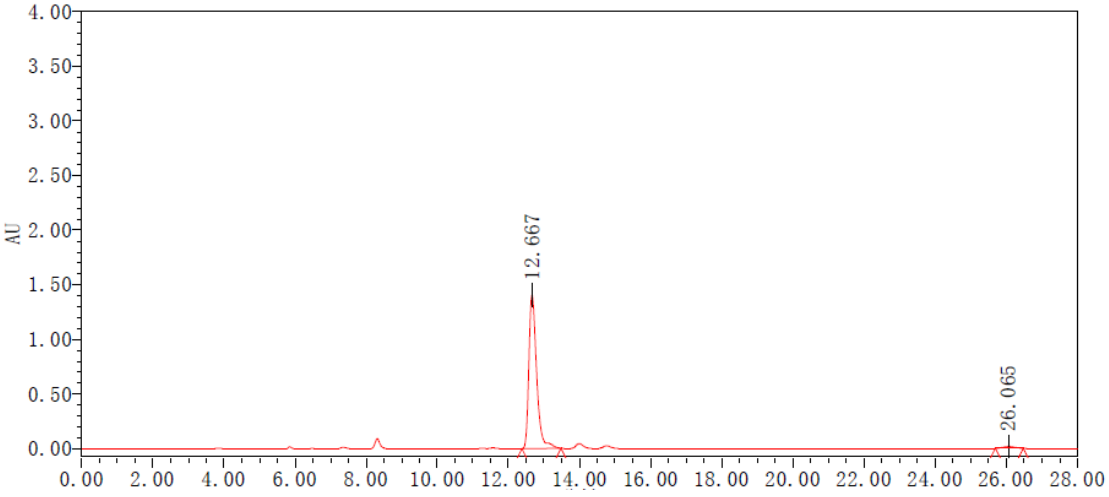
**HPLC chromatogram of chiral 41**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

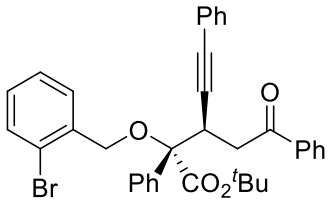
λ= 254 nm

Chiral IA-3



| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 12.667 | 20886858 | 1407348 | 98.01 |
| 2 | 26.065 | 424180 | 17606 | 1.99 |

**Tert-butyl (2S,3R)-2-((2-bromobenzyl)oxy)-3-(2-oxo-2-phenylethyl)-2,5-diphenylpent-4-ynoate (42)**




**42**

Colorless oil; 45.6 mg, 50% yield, 92:8 d.r., 88% *ee*, $[\alpha]_D^{20}$ = -13.11 (c = 0.1, $CH_2Cl_2$); $^1$H NMR (500 MHz, $CDCl_3$) δ 7.92 – 7.84 (m, 3H), 7.74 (d, *J* = 7.5 Hz, 2H), 7.55 – 7.50 (m, 2H), 7.43 – 7.36 (m, 5H), 7.34 (d, *J* = 6.3 Hz, 1H), 7.31 (dd, *J* = 7.5, 2.6 Hz, 2H), 7.23 (dt, *J* = 2.6, 2.2 Hz, 3H), 7.16 (t, *J* = 8.3 Hz, 1H), 5.27 (d, *J* = 13.1 Hz, 1H), 5.04 (d, *J* = 13.1 Hz, 1H), 4.44 (dd, *J* = 10.2, 3.0 Hz, 1H), 3.45 (dd, *J* = 16.8, 10.3 Hz, 1H), 3.10 (dd, *J* = 16.7, 2.9 Hz, 1H), 1.48 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 197.5, 169.3, 138.5, 138.4, 136.9, 133.1, 132.2, 131.6, 129.0, 128.6, 128.5, 128.3, 128.2, 128.1, 128.1, 127.8, 127.5, 126.6, 123.4, 121.9, 89.7, 86.1, 84.3, 82.9, 68.2, 39.2, 36.7, 28.0. HRMS (ESI) $[M+Na]^+$ calcd for $C_{36}H_{33}O_4BrNa^+$, 631.1454, found 631.1459. (Chiral IE-3, λ= 254 nm, *n*-hexane/2-propanol= 97/3, Flow rate = 1.0 mL/min), $t_R$ = 14.832 min(major), 33.652 min.

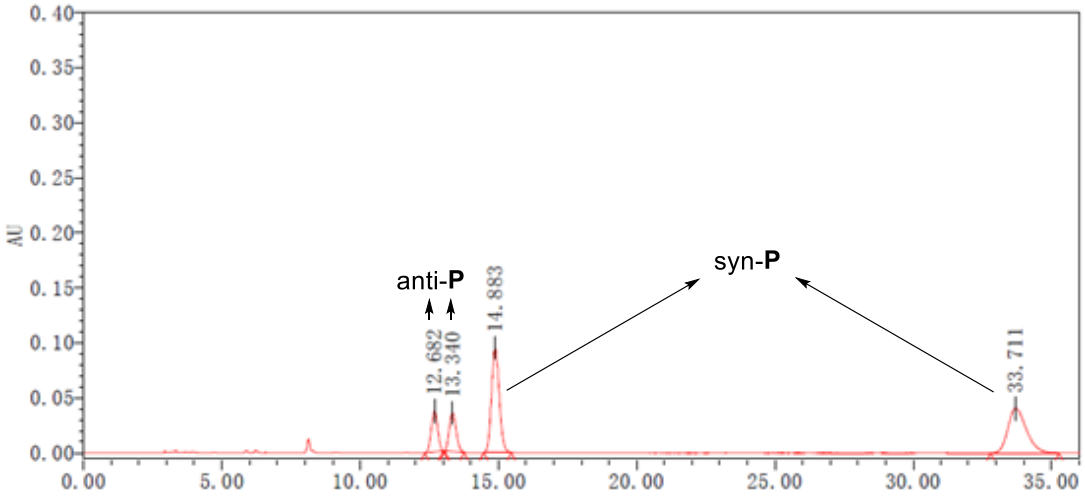
**HPLC chromatogram of racemic 42**

Condition: n-hexane/2-propanol =97:3

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 12.682 | 596062 | 37195 | 11.95 |
| 2 | 13.340 | 602382 | 34973 | 12.08 |
| 3 | 14.883 | 1894469 | 95327 | 38.00 |
| 4 | 33.711 | 1893011 | 40773 | 37.97 |

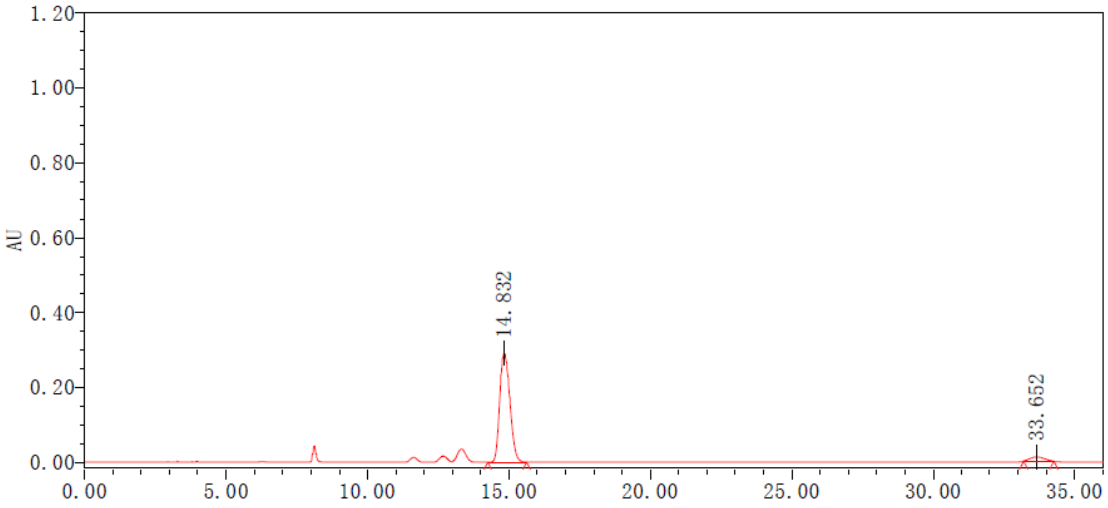
**HPLC chromatogram of chiral 42**

Condition: n-hexane/2-propanol =97:3

Flow rate =1.0 mL/min

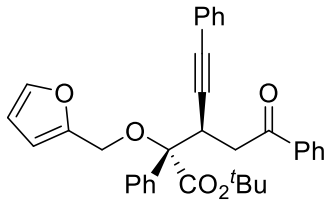
λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 14.832 | 6906065 | 290795 | 94.12 |
| 2 | 33.652 | 431065 | 11047 | 5.88 |

**Tert-butyl (2S,3R)-2-(furan-2-ylmethoxy)-3-(2-oxo-2-phenylethyl)-2,5-diphenylpent-4-ynoate(43)**




**43**

Colorless oil; 54.6 mg, 70% yield, >20:1 d.r., 99% *ee*; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 7.4 Hz, 2H), 7.70 (d, *J* = 7.4 Hz, 2H), 7.53 (t, *J* = 7.3 Hz, 1H), 7.42 (dd, *J* = 13.2, 5.4 Hz, 3H), 7.35 (t, *J* = 7.4 Hz, 2H), 7.30 (d, *J* = 7.1 Hz, 1H), 7.24 (d, *J* = 13.0 Hz, 5H), 6.38 (dd, *J* = 9.0, 2.3 Hz, 2H), 5.16 (d, *J* = 12.1 Hz, 1H), 4.91 (d, *J* = 12.1 Hz, 1H), 4.38 (dd, *J* = 10.3, 2.7 Hz, 1H), 3.46 (dd, *J* = 16.7, 10.4 Hz, 1H), 3.08 (dd, *J* = 16.7, 2.7 Hz, 1H), 1.53 (s, 9H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 197.6, 169.3, 152.3, 142.6, 138.3, 137.0, 133.1, 131.4, 128.5, 128.3, 128.2, 128.2, 128.1, 127.8, 126.8, 123.4, 110.3, 108.9, 89.8, 85.5, 84.1, 82.9, 61.2, 39.0, 36.5, 28.1. HRMS (ESI) $[M+Na]^+$ calcd

for $C_{34}H_{32}O_5Na^+$, 543.2140, found 543.2142. (Chiral IA, λ= 254 nm, *n*-hexane/2-propanol= 19/1, Flow rate = 1.0 mL/min), $t_R$ = 7.586 min(major), 15.075 min.

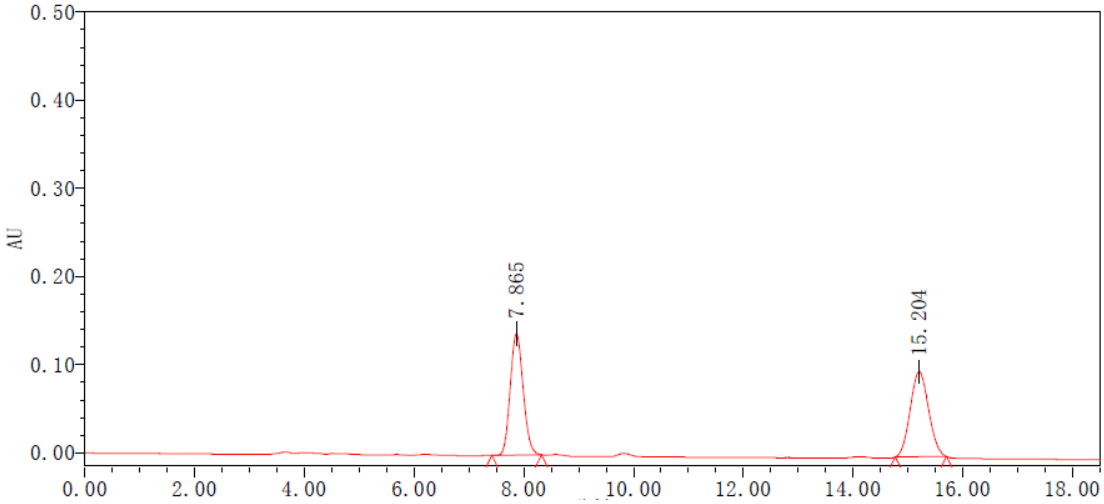
**HPLC chromatogram of racemic 43**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 7.865 | 2225887 | 137741 | 49.74 |
| 2 | 15.204 | 2249077 | 96528 | 50.26 |

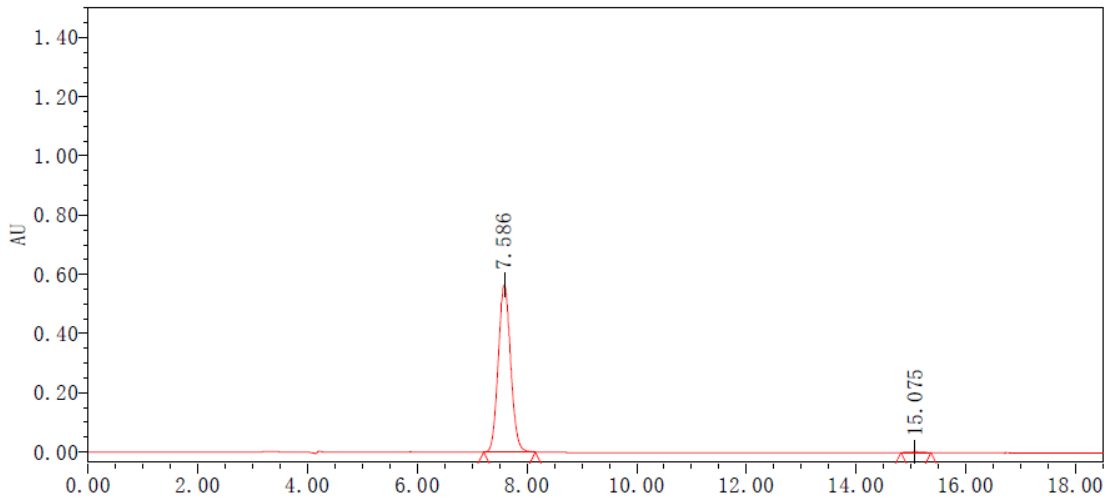
**HPLC chromatogram of chiral 43**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

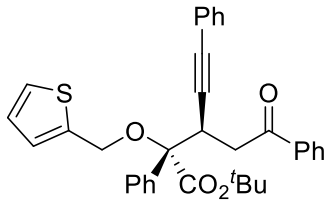
λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 7.586 | 8927372 | 564755 | 99.51 |
| 2 | 15.075 | 44057 | 2263 | 0.49 |

**Tert-butyl (2S,3R)-3-(2-oxo-2-phenylethyl)-2,5-diphenyl-2-(thiophen-2-ylmethoxy)pent-4-ynoate (44)**




**44**

Colorless oil; 57.7 mg, 72% yield, >20:1 d.r., 99% *ee*; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.91 – 7.84 (m, 2H), 7.77 – 7.68 (m, 2H), 7.52 (t, *J* = 7.4 Hz, 1H), 7.44 – 7.33 (m, 4H), 7.32 – 7.29 (m, 2H), 7.26 – 7.19 (m, 5H), 7.06 (d, *J* = 2.7 Hz, 1H), 6.99 (dd, *J* = 5.0, 3.5 Hz, 1H), 5.37 (d, *J* = 11.7 Hz, 1H), 5.14 (d, *J* = 11.7 Hz, 1H), 4.41 (dd, *J* = 10.4, 2.8 Hz, 1H), 3.42 (dd, *J* = 16.8, 10.4 Hz, 1H), 3.09 (dd, *J* = 16.8, 2.8 Hz, 1H), 1.53 (s, 9H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 197.5, 169.3, 141.9, 138.4, 136.9, 133.1, 131.4, 128.6, 128.3, 128.3, 128.2, 128.2, 127.9, 126.7, 126.5, 125.6, 125.5, 123.4, 89.7, 85.9,

84.1, 83.0, 64.1, 39.2, 36.5, 28.1. HRMS (ESI) $[M+Na]^+$ calcd for $C_{34}H_{32}O_4SNa^+$, 559.1914, found 559.1910. (Chiral IE-3, λ= 254 nm, *n*-hexane/2-propanol= 19/1, Flow rate = 1.0 mL/min), $t_R$ = 10.844 min(major), 26.285 min.

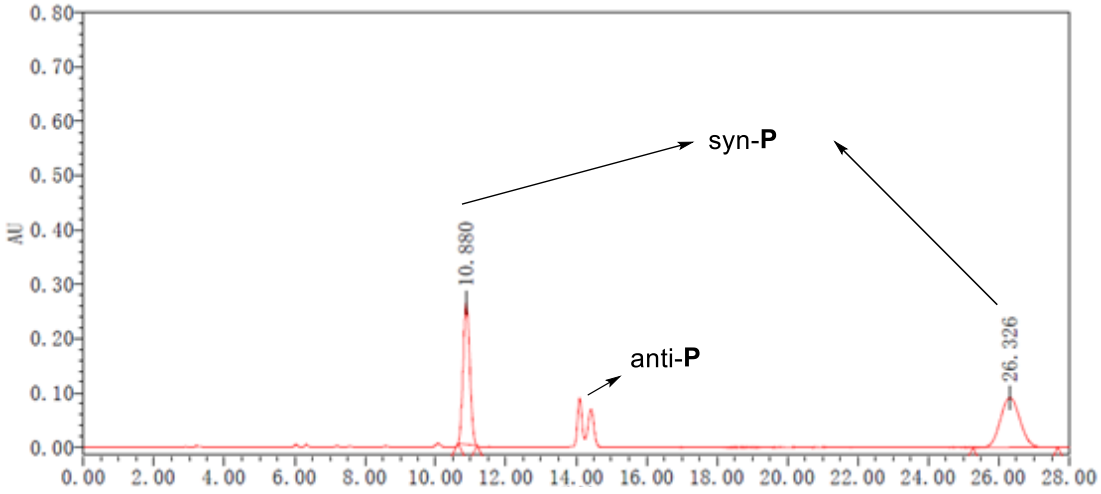
**HPLC chromatogram of racemic 44**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 10.880 | 3522490 | 261335 | 50.08 |
| 2 | 26.326 | 3511789 | 91478 | 49.92 |

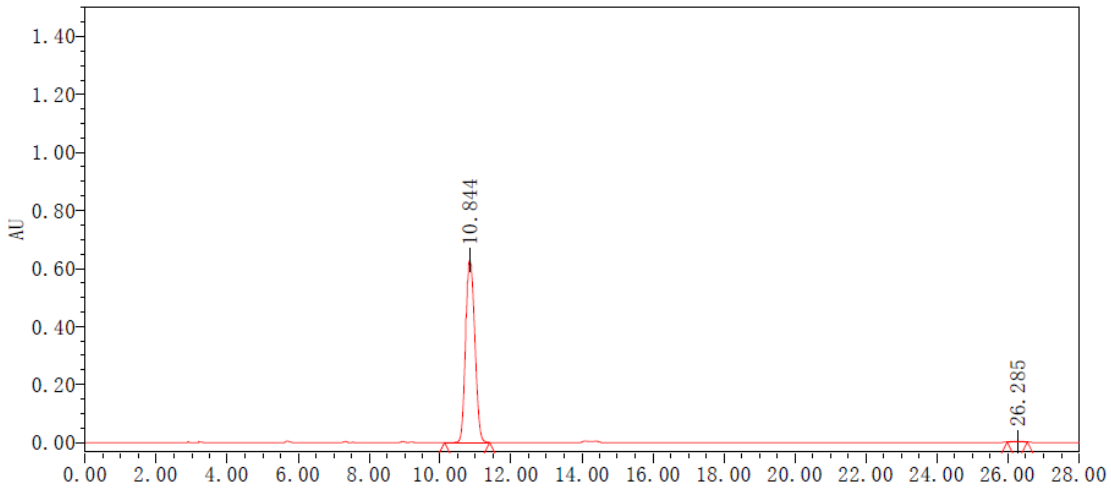
**HPLC chromatogram of chiral 44**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

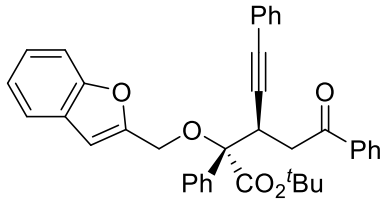
λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 10.844 | 11578063 | 628323 | 99.72 |
| 2 | 26.285 | 31953 | 1475 | 0.28 |

**Tert-butyl (2S,3R)-2-(benzofuran-2-ylmethoxy)-3-(2-oxo-2-phenylethyl)-2,5-diphenylpent-4-ynoate(45)**




**45**

Colorless oil; 61.5 mg, 72% yield, >20:1 d.r., 99% *ee*; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.96 – 7.91 (m, 2H), 7.80 – 7.71 (m, 2H), 7.60 (dd, *J* = 7.6, 0.7 Hz, 1H), 7.53 (ddd, *J* = 10.8, 10.3, 3.5 Hz, 2H), 7.41 (dd, *J* = 15.7, 7.9 Hz, 4H), 7.36 – 7.31 (m, 2H), 7.30 – 7.24 (m, 6H), 6.83 (s, 1H), 5.40 (d, *J* = 12.6 Hz, 1H), 5.14 (d, *J* = 12.6 Hz, 1H), 4.47 (dd, *J* = 10.3, 2.9 Hz, 1H), 3.58 (dd, *J* = 16.8, 10.3 Hz, 1H), 3.13 (dd, *J* = 16.7, 2.9 Hz, 1H), 1.59 (s, 9H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 197.6, 169.3, 155.1, 138.2, 137.0, 133.1, 131.4, 128.5, 128.4, 128.3, 128.3, 128.3, 128.2, 128.1, 127.9, 126.8, 124.2, 123.4, 122.7, 121.1, 111.3, 105.2, 89.7, 85.8, 84.2, 83.0, 61.9, 39.0, 36.7, 28.1. HRMS (ESI)

[M+Na]$^+$ calcd for $C_{38}H_{34}O_5Na^+$, 593.2298, found 593.2293. (Chiral IE-3, λ= 254 nm, *n*-hexane/2-propanol= 19/1, Flow rate = 1.0 mL/min), $t_R$ = 10.681 min(major), 22.058 min.

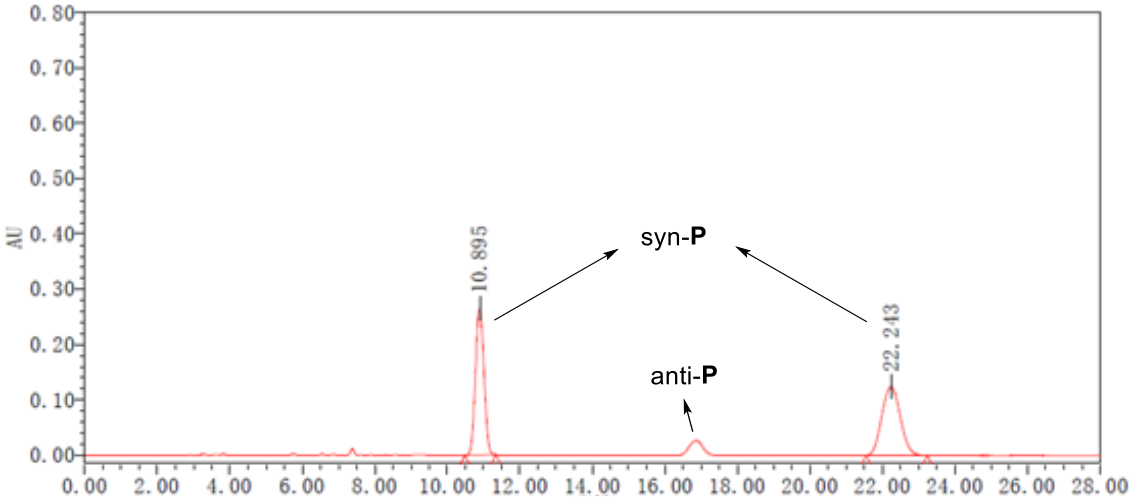
**HPLC chromatogram of racemic 45**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 10.895 | 4418288 | 264820 | 50.13 |
| 2 | 22.243 | 4395186 | 123830 | 49.87 |

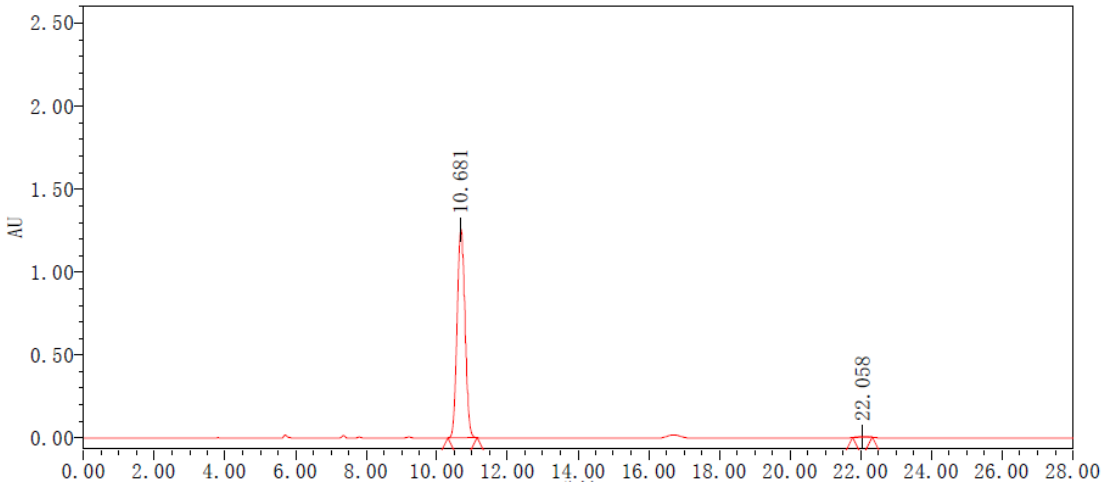
**HPLC chromatogram of chiral 45**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

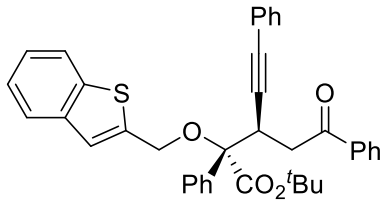
λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 10.681 | 19757193 | 1256331 | 99.51 |
| 2 | 22.058 | 96684 | 4552 | 0.49 |

**Tert-butyl (2S,3R)-2-(benzo[b]thiophen-2-ylmethoxy)-3-(2-oxo-2-phenylethyl)-2,5-diphenylpent-4-ynoate (46)**




**46**

Colorless oil; 60.2 mg, 74% yield, >20:1 d.r., 94% *ee*; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.88 – 7.81 (m, 3H), 7.76 – 7.69 (m, 3H), 7.53 – 7.47 (m, 1H), 7.41 – 7.36 (m, 4H), 7.34 (dd, *J* = 3.8, 1.6 Hz, 1H), 7.33 – 7.30 (m, 2H), 7.28 – 7.23 (m, 6H), 5.47 (d, *J* = 12.2 Hz, 1H), 5.25 (d, *J* = 12.1 Hz, 1H), 4.44 (dd, *J* = 10.4, 2.9 Hz, 1H), 3.45 (dd, *J* = 16.7, 10.4 Hz, 1H), 3.08 (dd, *J* = 16.7, 2.9 Hz, 1H), 1.54 (s, 9H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 197.5, 169.3, 143.0, 140.2, 139.5, 138.2, 136.9, 133.1, 131.5, 128.5, 128.4, 128.3, 128.3, 128.2, 128.1, 127.9, 126.7, 124.2, 124.1, 123.5, 123.4, 122.4, 121.7, 89.7,

86.0, 84.2, 83.1, 64.9, 39.1, 36.6, 28.1. HRMS (ESI) $[M+Na]^+$ calcd for $C_{38}H_{34}O_4SNa^+$, 609.2070, found 609.2065. (Chiral IA, λ= 254 nm, *n*-hexane/2-propanol= 49/1, Flow rate = 1.0 mL/min), $t_R$ = 13.028 min(major), 25.316 min.

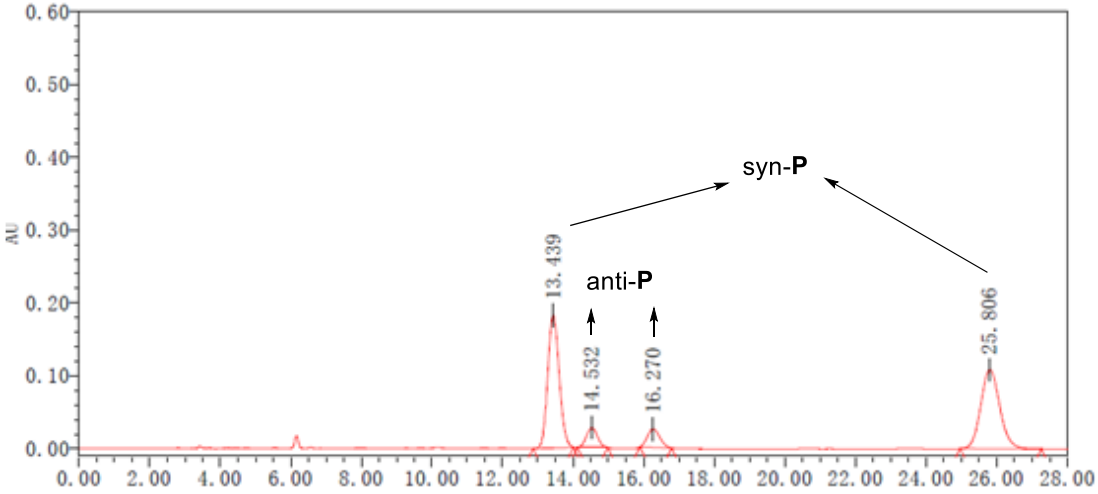
**HPLC chromatogram of racemic 46**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 13.439 | 4072895 | 183009 | 43.59 |
| 2 | 14.532 | 608324 | 27386 | 6.51 |
| 3 | 16.270 | 623506 | 25297 | 6.67 |
| 4 | 25.806 | 4039690 | 108681 | 43.23 |

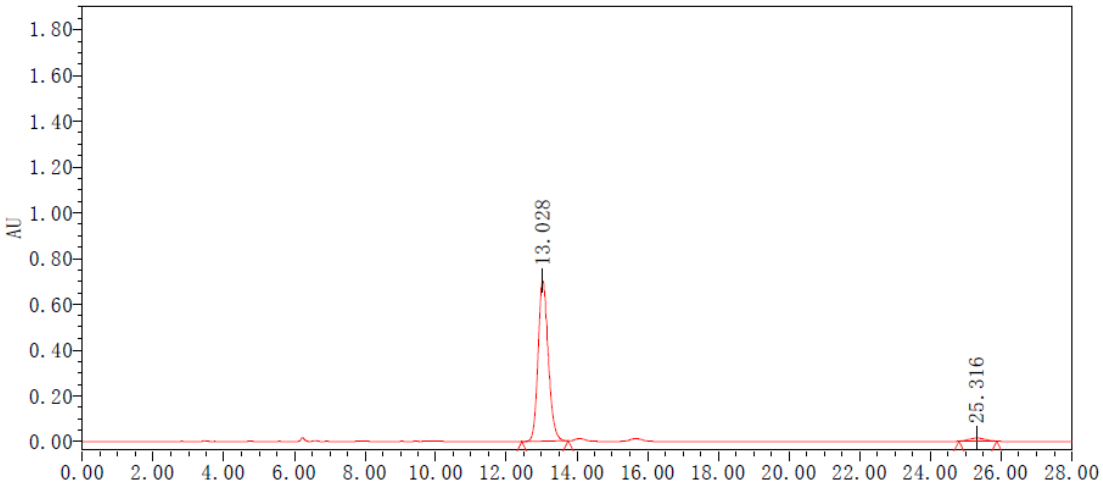
**HPLC chromatogram of chiral 46**

Condition: n-hexane/2-propanol = 49:1

Flow rate =1.0 mL/min

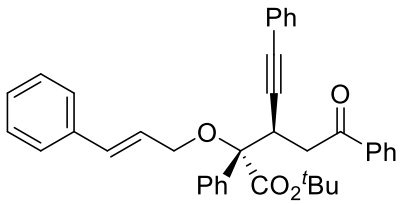
λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 13.028 | 14190254 | 701421 | 96.96 |
| 2 | 25.316 | 444194 | 13487 | 3.04 |

**Tert-butyl (2S,3R)-2-(cinnamyloxy)-3-(2-oxo-2-phenylethyl)-2,5-diphenylpent-4-ynoate (47)**




**47**

Colorless oil; 45.9 mg, 55% yield, >20:1 d.r., 94% *ee*, $[\alpha]_D^{20}$ = -12.79 (c = 0.1, $CH_2Cl_2$); $^1$H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 7.4 Hz, 2H), 7.71 (d, *J* = 7.3 Hz, 2H), 7.51 (t, *J* = 7.4 Hz, 1H), 7.38 (dd, *J* = 15.2, 8.2 Hz, 6H), 7.31 (t, *J* = 7.3 Hz, 3H), 7.26 – 7.20 (m, 6H), 6.71 (d, *J* = 15.9 Hz, 1H), 6.42 (dt, *J* = 15.9, 5.6 Hz, 1H), 4.70 (dd, *J* = 12.7, 5.8 Hz, 1H), 4.55 (dd, *J* = 12.6, 5.0 Hz, 1H), 4.37 (dd, *J* = 10.1, 2.9 Hz, 1H), 3.38 (dd,

*J* = 16.6, 10.2 Hz, 1H), 3.15 (dd, *J* = 16.6, 2.8 Hz, 1H), 1.53 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 197.6, 169.6, 138.6, 137.0, 137.0, 133.1, 131.5, 131.4, 128.5, 128.3, 128.2, 128.2, 128.2, 127.8, 127.6, 126.8, 126.7, 126.5, 123.5, 89.7, 85.8, 84.0, 82.8, 67.6, 39.3, 36.7, 28.1. HRMS (ESI) $[M+Na]^+$ calcd for $C_{38}H_{36}O_4Na^+$, 579.2506, found 579.2504. (Chiral IE-3, λ= 254 nm, *n*-hexane/2-propanol= 19/1, Flow rate = 1.0 mL/min), $t_R$ = 11.529 min(major), 22.634 min.

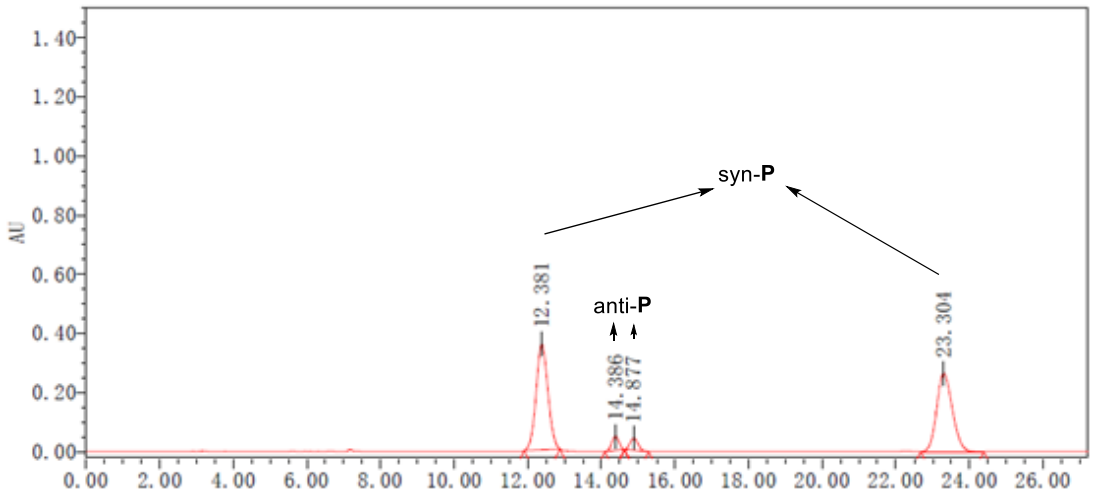
**HPLC chromatogram of racemic 47**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 12.381 | 7891813 | 358649 | 46.27 |
| 2 | 14.386 | 650976 | 48062 | 3.82 |
| 3 | 14.877 | 633398 | 41112 | 3.71 |
| 4 | 23.304 | 7880382 | 265218 | 46.20 |

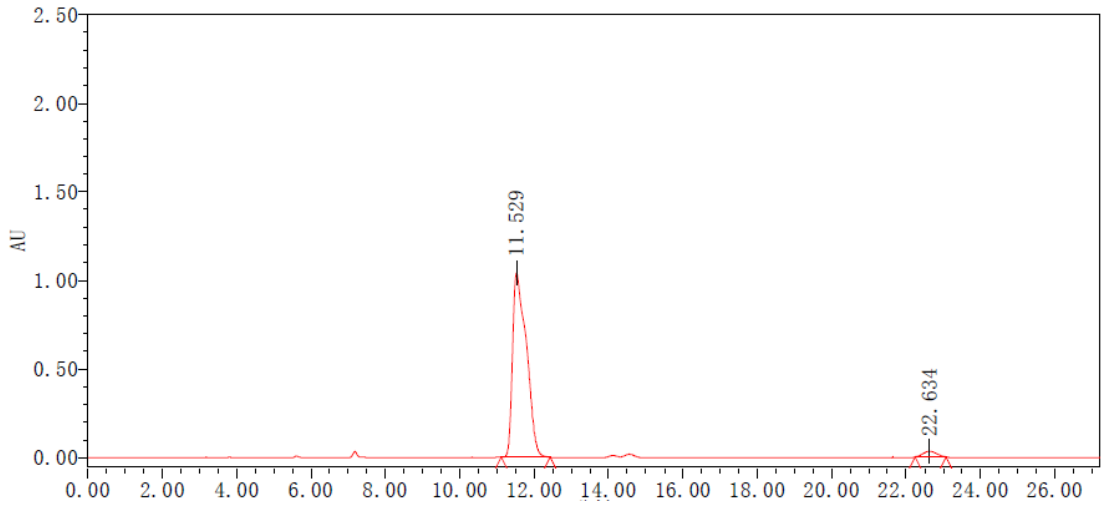
**HPLC chromatogram of chiral 47**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

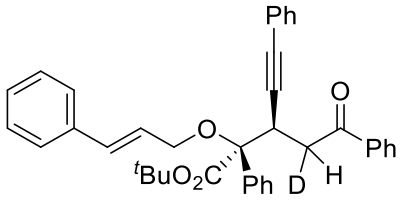
λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 11.529 | 26532083 | 1040734 | 97.06 |
| 2 | 22.634 | 803670 | 31828 | 2.94 |

**Tert-butyl (2S,3R)-2-(cinnamyloxy)-3-(2-oxo-2-phenylethyl-1-d)-2,5-diphenylpent-4-ynoate(47-[D])**

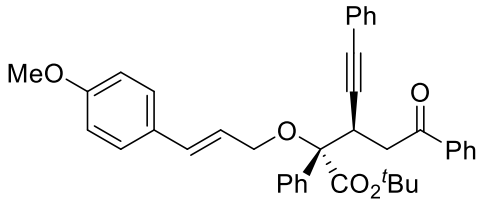



**47-[D]**

$^1$H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 7.8 Hz, 2H), 7.71 (d, *J* = 7.8 Hz, 2H), 7.50 (d, *J* = 7.1 Hz, 1H), 7.38 (dd, *J* = 14.3, 7.6 Hz, 6H), 7.31 (t, *J* = 7.4 Hz, 3H), 7.23 (d, *J*

= 7.7 Hz, 6H), 6.71 (d, *J* = 15.9 Hz, 1H), 6.42 (dt, *J* = 15.9, 5.6 Hz, 1H), 4.68 (d, *J* = 6.0 Hz, 1H), 4.55 (dd, *J* = 12.4, 4.9 Hz, 1H), 4.36 (d, *J* = 2.4 Hz, 1H), 3.38 (dd, *J* = 16.6, 10.3 Hz, 0.14H), 3.14 (dd, *J* = 15.0, 4.7 Hz, 1H), 1.53 (s, 9H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 197.7, 169.6, 138.6, 137.1, 137.0, 133.1, 131.5, 131.4, 128.5, 128.3, 128.2, 128.2, 128.1, 127.8, 127.6, 126.8, 126.7, 126.5, 123.5, 89.7, 85.8, 84.0, 82.8, 67.6, 39.3, 39.2, 39.0, 36.7, 28.1. HRMS (ESI) $[M+Na]^+$ calcd for $C_{38}H_{35}DO_4Na^+$, 580.2569, found 580.2566.

**Tert-butyl (2S,3R)-2-(((E)-3-(4-methoxyphenyl)allyl)oxy)-3-(2-oxo-2-phenylethyl)-2,5-diphenylpent-4-ynoate (48)**




**48**

Colorless oil; 51.0 mg, 58% yield, >20:1 d.r., 98% *ee*; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 7.7 Hz, 1H), 7.90 (d, *J* = 7.7 Hz, 2H), 7.71 (d, *J* = 7.7 Hz, 2H), 7.50 (dd, *J* = 15.4, 7.7 Hz, 2H), 7.41 – 7.36 (m, 3H), 7.35 – 7.31 (m, 3H), 7.25 – 7.21 (m, 4H), 6.85 (d, *J* = 8.4 Hz, 2H), 6.64 (d, *J* = 15.8 Hz, 1H), 6.29 (dt, *J* = 15.8, 5.8 Hz, 1H), 4.67 (dd, *J* = 12.2, 6.3 Hz, 1H), 4.53 (dd, *J* = 12.1, 5.3 Hz, 1H), 4.36 (dd, *J* = 10.0, 2.7 Hz, 1H), 3.80 (s, 3H), 3.38 (dd, *J* = 16.5, 10.2 Hz, 1H), 3.15 (dd, *J* = 16.6, 2.6 Hz, 1H), 1.53 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 197.7, 169.6, 159.2, 138.6, 137.0, 133.3, 133.1, 131.7, 131.4, 131.3, 129.8, 128.7, 128.5, 128.3, 128.3, 128.2, 128.1, 128.1, 127.8, 127.7, 126.8, 124.4, 123.5, 114.0, 89.8, 85.7, 84.0, 82.7, 67.9, 55.3, 39.3, 36.7, 28.1. HRMS (ESI) $[M+Na]^+$ calcd for $C_{39}H_{38}O_5Na^+$, 609.2611, found 609.2610. (Chiral IA, λ= 254 nm, *n*-hexane/2-propanol= 19/1, Flow rate = 1.0 mL/min), $t_R$ = 9.753 min(major), 17.375 min.

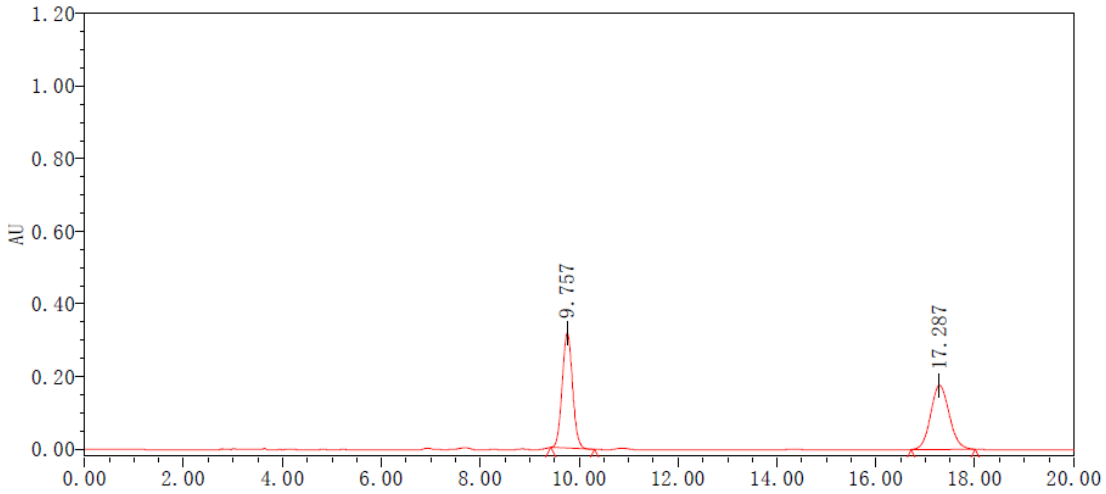
**HPLC chromatogram of racemic 48**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 9.757 | 4594856 | 317072 | 49.98 |
| 2 | 17.287 | 4599083 | 176656 | 50.02 |

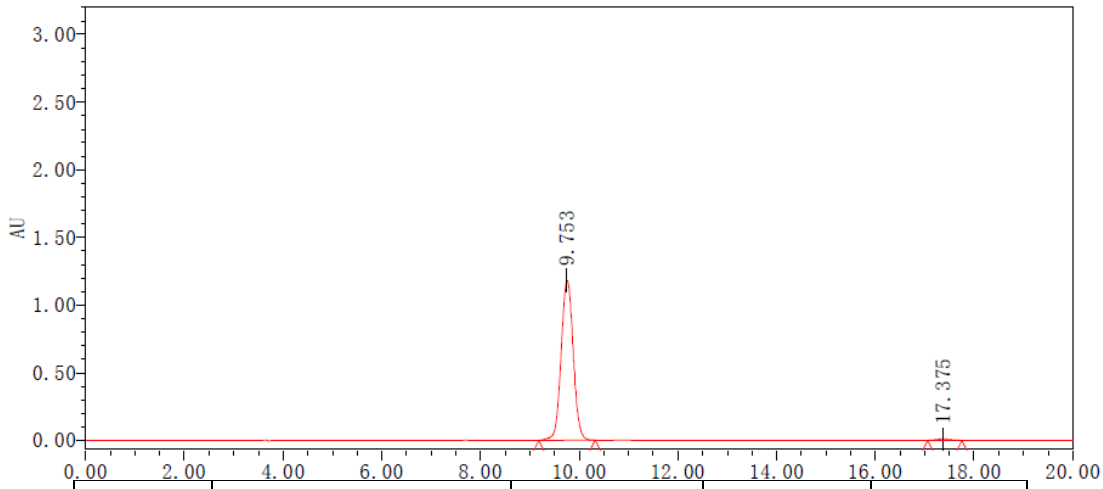
**HPLC chromatogram of chiral 48**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

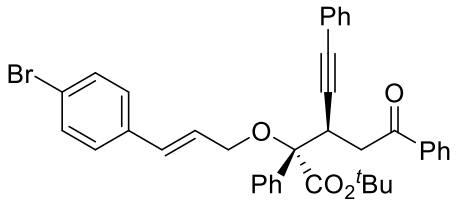
λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 9.753 | 20121122 | 1180943 | 98.96 |
| 2 | 17.375 | 210450 | 9580 | 1.04 |

**Tert-butyl (2S,3R)-2-(((E)-3-(4-bromophenyl)allyl)oxy)-3-(2-oxo-2-phenylethyl)-2,5-diphenylpent-4-ynoate (49)**




**49**

Colorless oil; 58.0 mg, 61% yield, >20:1 d.r., 98% *ee*; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 7.9 Hz, 2H), 7.70 (d, *J* = 8.0 Hz, 2H), 7.52 (t, *J* = 7.3 Hz, 1H), 7.44 – 7.35 (m, 6H), 7.32 (d, *J* = 7.0 Hz, 1H), 7.25 – 7.20 (m, 7H), 6.65 (d, *J* = 15.9 Hz, 1H), 6.40 (dt, *J* = 15.9, 5.4 Hz, 1H), 4.66 (dd, *J* = 12.9, 5.8 Hz, 1H), 4.53 (dd, *J* = 12.9, 5.0 Hz, 1H), 4.37 (dd, *J* = 10.0, 2.8 Hz, 1H), 3.35 (dd, *J* = 16.6, 10.1 Hz, 1H), 3.16 (dd, *J* = 16.5, 2.8 Hz, 1H), 1.53 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 197.5, 169.5, 138.4, 137.0, 136.0, 133.1, 131.6, 131.4, 130.2, 128.6, 128.2, 128.2, 128.2, 128.1, 127.9, 127.6, 126.8, 123.5, 121.3, 89.7, 85.8, 84.0, 82.8, 67.4, 39.3, 36.7, 28.1. HRMS (ESI) $[M+Na]^+$ calcd for $C_{38}H_{35}O_4BrNa^+$, 657.1611, found 657.1606. (Chiral IE-3, λ= 254 nm, *n*-

hexane/2-propanol= 19/1, Flow rate = 1.0 mL/min), $t_R$ = 11.987 min(major), 23.436 min.

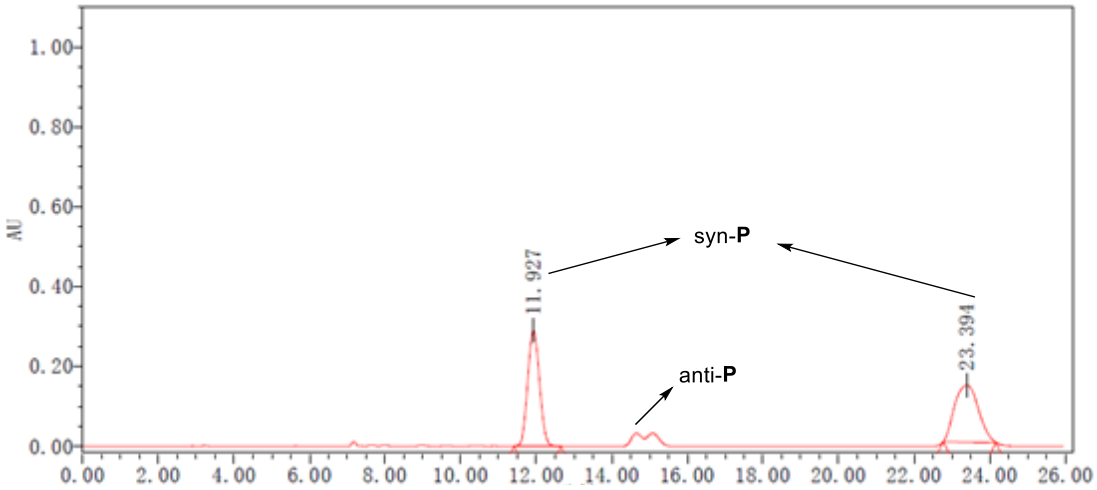
**HPLC chromatogram of racemic 49**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 11.927 | 6199542 | 290636 | 49.91 |
| 2 | 23.394 | 6222741 | 142333 | 50.09 |

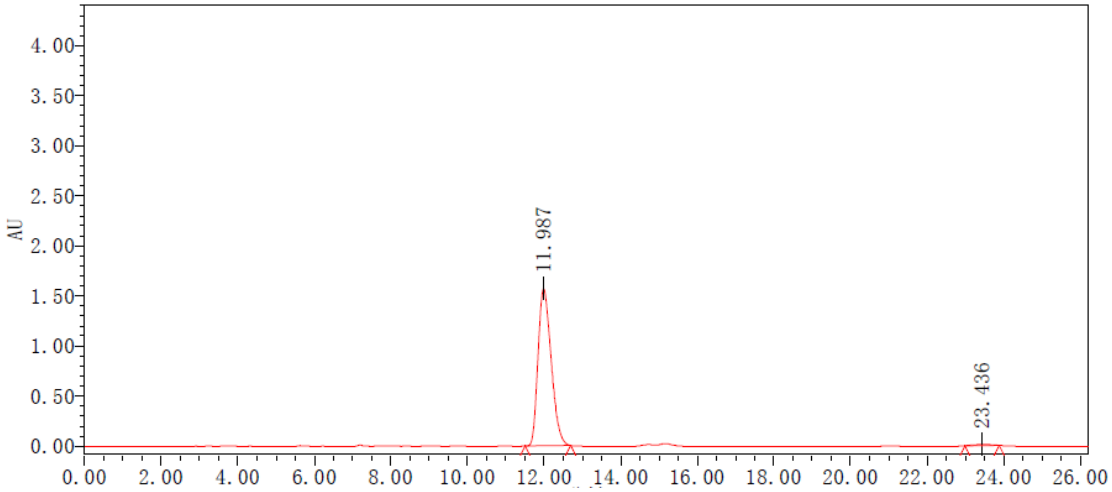
**HPLC chromatogram of chiral 49**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

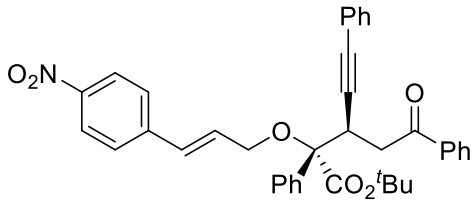
λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 11.987 | 37048978 | 1569398 | 98.95 |
| 2 | 23.436 | 394238 | 11754 | 1.05 |

**Tert-butyl (2S,3R)-2-(((E)-3-(4-nitrophenyl)allyl)oxy)-3-(2-oxo-2-phenylethyl)-2,5-diphenylpent-4-ynoate (50)**




**50**

Colorless oil; 53.2 mg, 59% yield, >20:1 d.r., 99% *ee*; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, *J* = 8.8 Hz, 2H), 7.94 – 7.86 (m, 2H), 7.73 – 7.66 (m, 2H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.48 (d, *J* = 8.8 Hz, 2H), 7.41 (dd, *J* = 16.2, 7.9 Hz, 4H), 7.36 – 7.32 (m, 1H), 7.25 (d, *J* = 9.4 Hz, 5H), 6.81 (d, *J* = 16.0 Hz, 1H), 6.57 (dt, *J* = 16.0, 5.1 Hz, 1H), 4.71 (ddd, *J* = 13.9, 5.4, 1.3 Hz, 1H), 4.58 (dd, *J* = 13.9, 3.3 Hz, 1H), 4.40 (dd, *J* = 9.9, 3.2 Hz, 1H), 3.35 (dd, *J* = 16.7, 9.9 Hz, 1H), 3.18 (dd, *J* = 16.7, 3.2 Hz, 1H), 1.54 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 197.4, 169.4, 146.9, 143.6, 138.1, 136.9, 133.2, 131.9, 131.4, 128.8, 128.6, 128.4, 128.3, 128.2, 128.2, 127.9, 127.0, 126.8, 124.0, 89.5, 85.9, 84.1,

83.0, 66.9, 39.3, 36.7, 28.1. HRMS (ESI) $[M+Na]^+$ calcd for $C_{38}H_{35}O_6Na^+$, 624.2357, found 624.2352. (Chiral IA, λ= 254 nm, *n*-hexane/2-propanol= 19/1, Flow rate = 1.0 mL/min), $t_R$ = 20.694 min(major), 37.037 min.

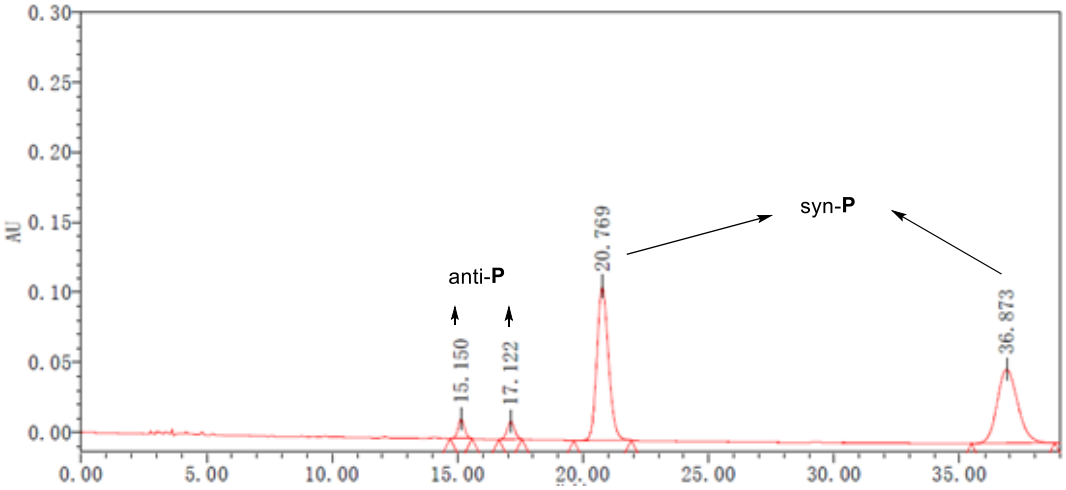
**HPLC chromatogram of racemic 50**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 15.150 | 266982 | 14198 | 3.79 |
| 2 | 17.122 | 265085 | 12700 | 3.77 |
| 3 | 20.769 | 3491967 | 109886 | 49.63 |
| 4 | 36.873 | 3012578 | 52919 | 42.81 |

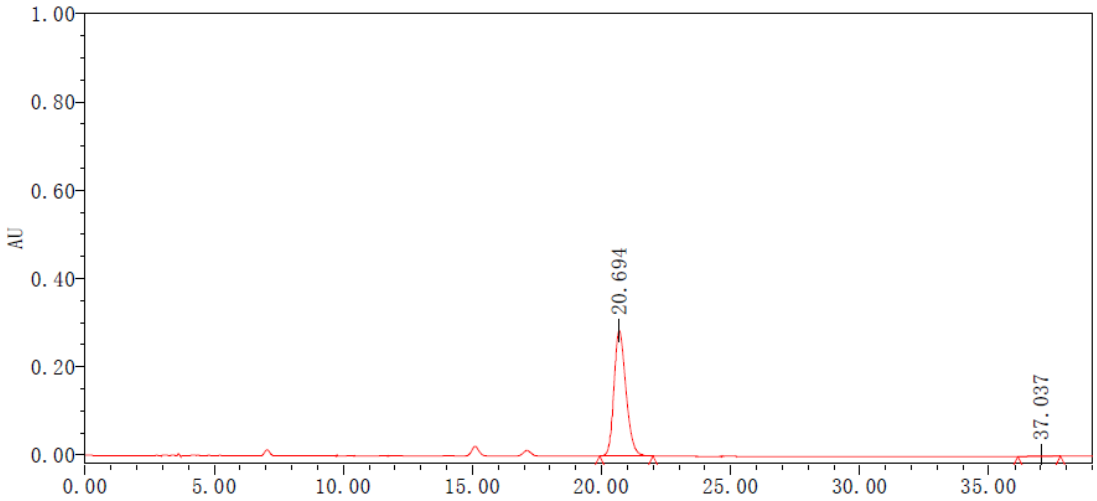
**HPLC chromatogram of chiral 50**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

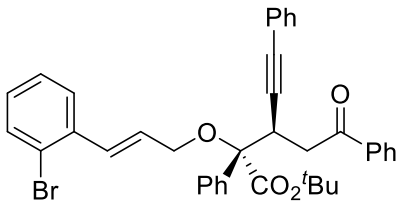
λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 20.694 | 9076478 | 284505 | 99.50 |
| 2 | 37.037 | 45354 | 927 | 0.50 |

**Tert-butyl (2S,3R)-2-(((E)-3-(2-bromophenyl)allyl)oxy)-3-(2-oxo-2-phenylethyl)-2,5-diphenylpent-4-ynoate (51)**




**51**

Colorless oil; 51.3 mg, 60% yield, >20:1 d.r., 94% *ee*; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 7.6 Hz, 2H), 7.72 (d, *J* = 7.7 Hz, 2H), 7.50 (dd, *J* = 14.9, 7.8 Hz, 2H), 7.38 (dd, *J* = 14.4, 7.5 Hz, 4H), 7.32 (d, *J* = 7.2 Hz, 1H), 7.26 – 7.19 (m, 5H), 7.15 (dd, *J* = 8.2, 3.0 Hz, 3H), 6.92 (d, *J* = 15.8 Hz, 1H), 6.32 (dt, *J* = 15.8, 5.7 Hz, 1H), 4.72 (dd, *J* = 12.5, 6.0 Hz, 1H), 4.55 (dd, *J* = 12.5, 5.1 Hz, 1H), 4.36 (dd, *J* = 10.1, 2.9 Hz, 1H),

3.39 (dd, *J* = 16.6, 10.2 Hz, 1H), 3.16 (dd, *J* = 16.5, 2.8 Hz, 1H), 2.31 (s, 3H), 1.54 (s, 9H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 197.6, 169.6, 138.6, 137.0, 136.0, 135.5, 133.1, 131.4, 130.3, 129.3, 128.5, 128.2, 128.2, 128.2, 128.1, 128.0, 127.8, 127.5, 126.9, 126.1, 125.8, 123.5, 89.8, 85.8, 84.0, 82.7, 67.9, 39.4, 36.8, 28.1, 19.8. HRMS (ESI) $[M+Na]^+$ calcd for $C_{38}H_{35}O_4BrNa^+$, 657.1611, found 657.1609. (Chiral IE-3, λ= 254 nm, *n*-hexane/2-propanol= 19/1, Flow rate = 1.0 mL/min), $t_R$ = 10.751 min(major), 22.224 min.

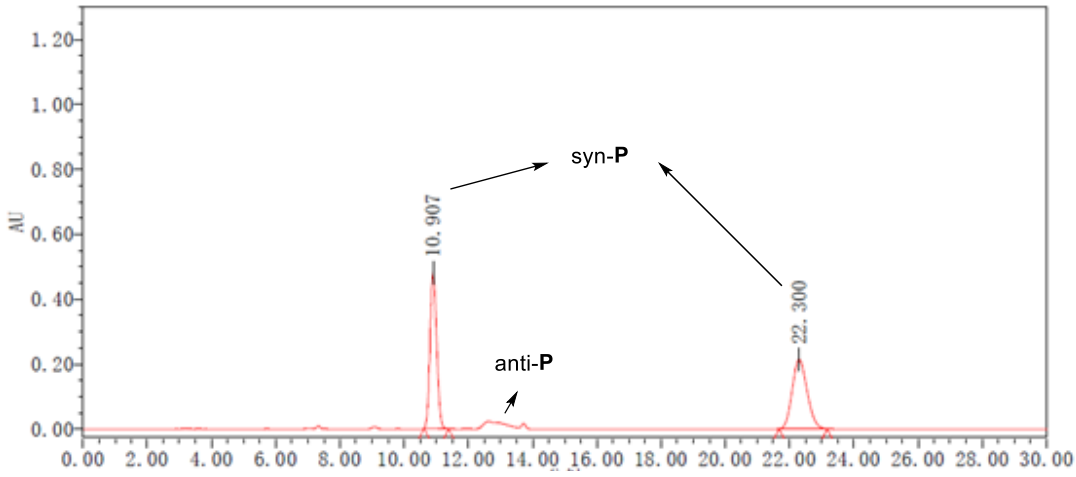
**HPLC chromatogram of racemic 51**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 10.907 | 7022469 | 479488 | 50.28 |
| 2 | 22.300 | 6944345 | 213967 | 49.72 |

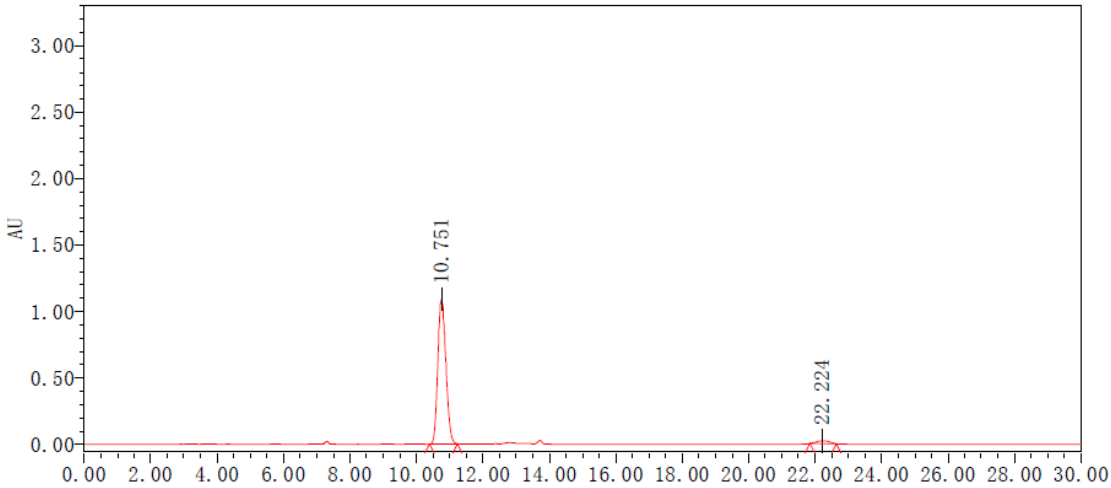
**HPLC chromatogram of chiral 51**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

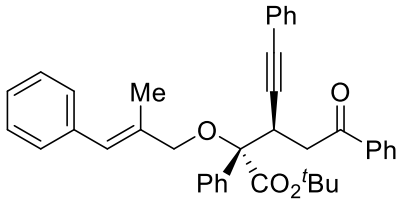
λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 10.751 | 18803712 | 1090492 | 96.92 |
| 2 | 22.224 | 597231 | 22671 | 3.08 |

**Tert-butyl (2S,3R)-2-(((E)-2-methyl-3-phenylallyl)oxy)-3-(2-oxo-2-phenylethyl)-2,5-diphenylpent-4-ynoate (52)**




**52**

Colorless oil; 53.9 mg, 63% yield, >20:1 d.r., 94% *ee*; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.92 – 7.87 (m, 2H), 7.76 – 7.71 (m, 2H), 7.51 (dd, *J* = 10.5, 4.2 Hz, 1H), 7.42 – 7.35 (m, 4H), 7.33 – 7.28 (m, 5H), 7.26 – 7.19 (m, 6H), 6.67 (s, 1H), 4.63 (d, *J* = 12.0 Hz,

1H), 4.46 – 4.35 (m, 2H), 3.50 – 3.36 (m, 1H), 3.16 (dd, *J* = 16.6, 3.0 Hz, 1H), 1.99 (d, *J* = 0.9 Hz, 3H), 1.53 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 197.6, 169.5, 138.7, 137.8, 137.0, 135.6, 133.1, 131.4, 129.0, 128.6, 128.2, 128.2, 128.2, 128.1, 127.8, 126.8, 126.4, 126.0, 123.5, 89.8, 85.5, 84.0, 82.7, 72.1, 39.4, 36.6, 28.1, 15.8. HRMS (ESI) $[M+Na]^+$ calcd for $C_{39}H_{38}O_4Na^+$, 593.2662, found 593.2662. (Chiral IC, λ= 254 nm, *n*-hexane/2-propanol= 49/1, Flow rate = 1.0 mL/min), $t_R$ = 7.560 min(major), 11.924 min.

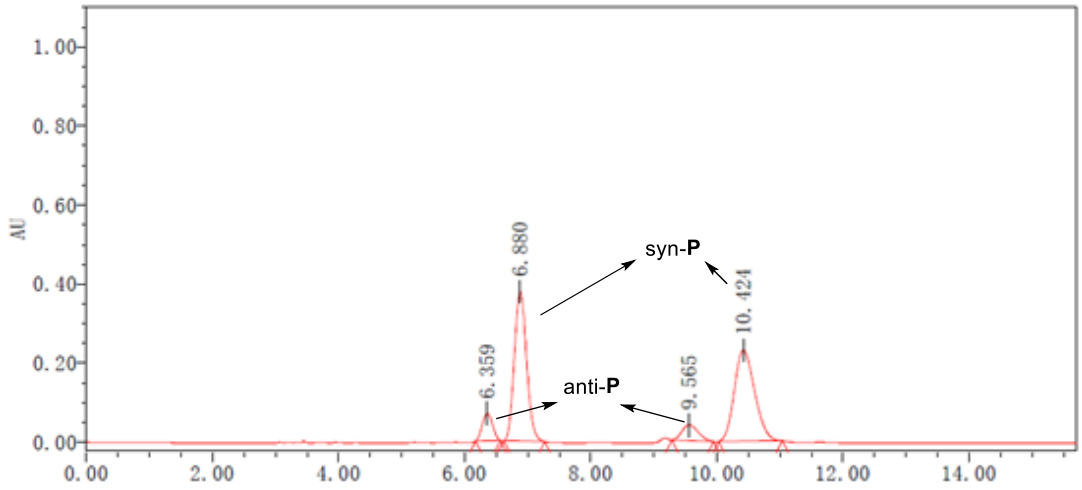
**HPLC chromatogram of racemic 52**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IC




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 6.359 | 781102 | 69069 | 6.61 |
| 2 | 6.880 | 5154728 | 378200 | 43.63 |
| 3 | 9.565 | 722113 | 39855 | 6.11 |
| 4 | 10.424 | 5155801 | 230506 | 43.64 |

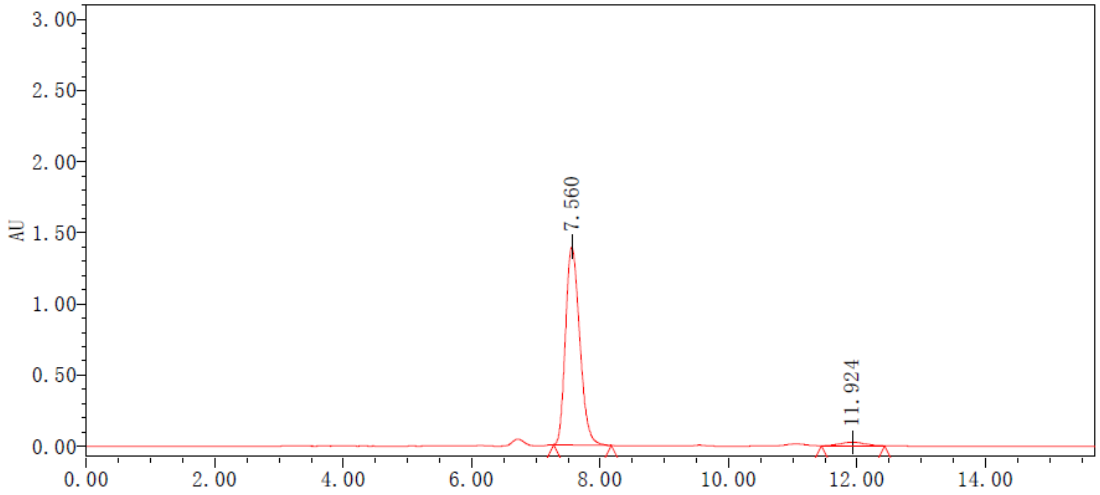
**HPLC chromatogram of chiral 52**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

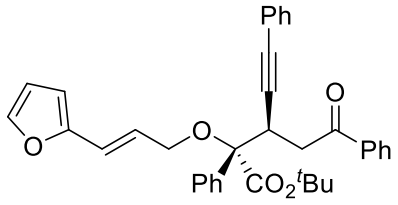
λ= 254 nm

Chiral IC




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 7.560 | 21270615 | 1391012 | 97.02 |
| 2 | 11.924 | 653961 | 24333 | 2.98 |

**Tert-butyl (2S,3R)-2-(((E)-3-(furan-2-yl)allyl)oxy)-3-(2-oxo-2-phenylethyl)-2,5-diphenylpent-4-ynoate (53)**




**53**

Colorless oil; 48.7 mg, 55% yield, >20:1 d.r., 96% *ee*; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 7.8 Hz, 2H), 7.70 (d, *J* = 7.8 Hz, 2H), 7.52 (t, *J* = 7.4 Hz, 1H), 7.44 – 7.34

(m, 1H), 7.31 (d, *J* = 7.0 Hz, 5H), 7.24 (d, *J* = 10.5 Hz, 1H), 6.57 (d, *J* = 15.9 Hz, 5H), 6.35 (dt, *J* = 18.9, 5.5 Hz, 1H), 6.21 (d, *J* = 3.1 Hz, 2H), 4.68 (dd, *J* = 13.3, 5.7 Hz, 1H), 4.52 (dd, *J* = 13.3, 4.9 Hz, 1H), 4.34 (dd, *J* = 10.1, 2.9 Hz, 1H), 3.37 (dd, *J* = 16.6, 10.2 Hz, 1H), 3.14 (dd, *J* = 16.5, 2.8 Hz, 1H), 1.52 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 197.6, 169.5, 152.7, 141.9, 138.5, 137.0, 133.1, 131.4, 128.5, 128.2, 128.2, 128.2, 128.1, 127.8, 126.8, 125.4, 123.5, 119.6, 111.3, 107.78, 89.7, 85.7, 84.0, 82.8, 67.0, 39.3, 36.8, 28.1. HRMS (ESI) $[M+Na]^+$ calcd for $C_{36}H_{34}O_5Na^+$, 569.2298, found 569.2294. (Chiral IE-3, λ= 254 nm, *n*-hexane/2-propanol= 19/1, Flow rate = 1.0 mL/min), $t_R$ = 11.457 min(major), 22.875 min.

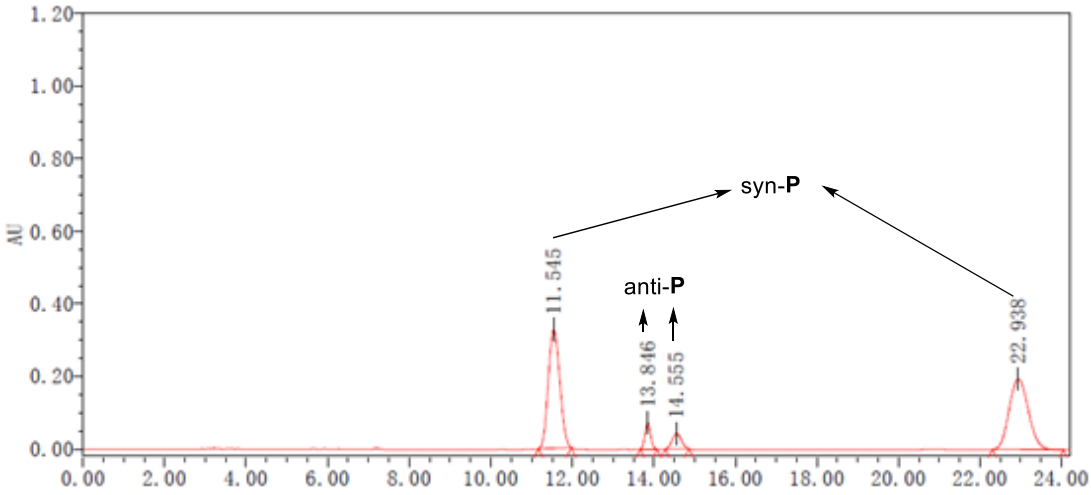
**HPLC chromatogram of racemic 53**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 11.545 | 6404622 | 326793 | 45.35 |
| 2 | 13.846 | 699675 | 73171 | 4.95 |

| | | | | |
|---|---|---|---|---|
| 3 | 14.555 | 673424 | 42324 | 4.77 |
| 4 | 22.938 | 6345621 | 194513 | 44.93 |

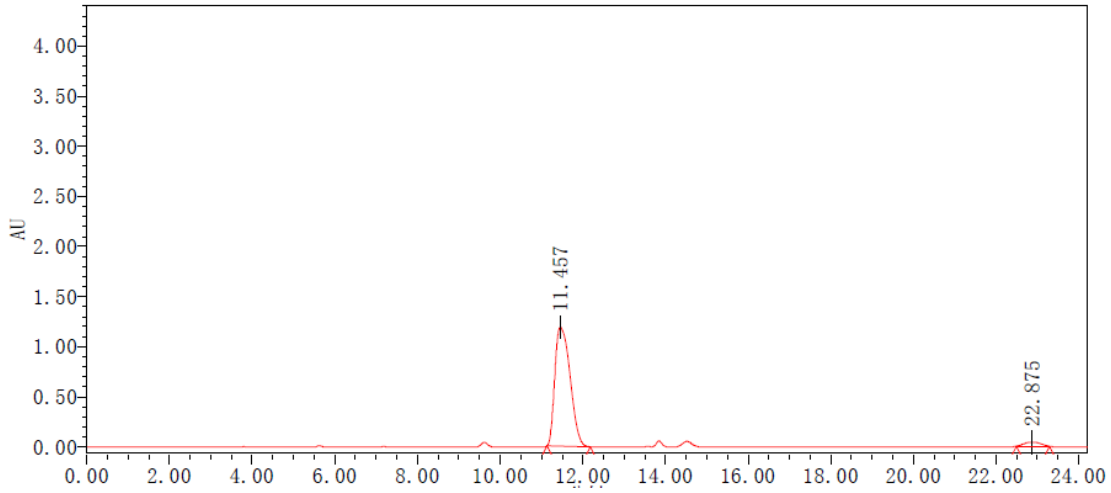
**HPLC chromatogram of chiral 53**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

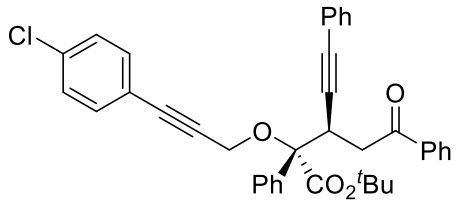
λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 11.457 | 30481356 | 1184631 | 96.50 |
| 2 | 22.875 | 1105463 | 41600 | 3.50 |

**Tert-butyl (2S,3R)-2-((3-(4-chlorophenyl)prop-2-yn-1-yl)oxy)-3-(2-oxo-2-phenylethyl)-2,5-diphenylpent-4-ynoate (54)**




**54**

Colorless oil; 45.9 mg, 52% yield, >20:1 d.r., 93% *ee*; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.93 – 7.87 (m, 2H), 7.74 – 7.69 (m, 2H), 7.51 (t, *J* = 7.4 Hz, 1H), 7.38 (dd, *J* = 5.8, 4.1 Hz, 2H), 7.36 – 7.31 (m, 5H), 7.27 – 7.24 (m, 4H), 7.24 – 7.20 (m, 3H), 5.07 (d, *J* = 15.7 Hz, 1H), 4.79 (d, *J* = 15.7 Hz, 1H), 4.40 (dd, *J* = 10.5, 2.8 Hz, 1H), 3.62 (dd, *J* = 16.9, 10.5 Hz, 1H), 3.05 (dd, *J* = 16.8, 2.8 Hz, 1H), 1.52 (s, 9H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 197.6, 169.2, 137.9, 137.0, 134.4, 133.1, 133.1, 131.5, 128.6, 128.5, 128.4, 128.2, 128.2, 127.9, 126.7, 123.3, 121.4, 89.4, 87.5, 86.2, 84.7, 84.0, 83.1, 56.3, 39.1, 36.4, 28.0. Peak overlapping was observed. HRMS (ESI) $[M+Na]^+$ calcd for $C_{38}H_{33}O_4ClNa^+$, 611.1960, found 611.1960. (Chiral IA, λ= 254 nm, *n*-hexane/2-propanol= 19/1, Flow rate = 1.0 mL/min), $t_R$ = 7.254 min(major), 14.901 min.

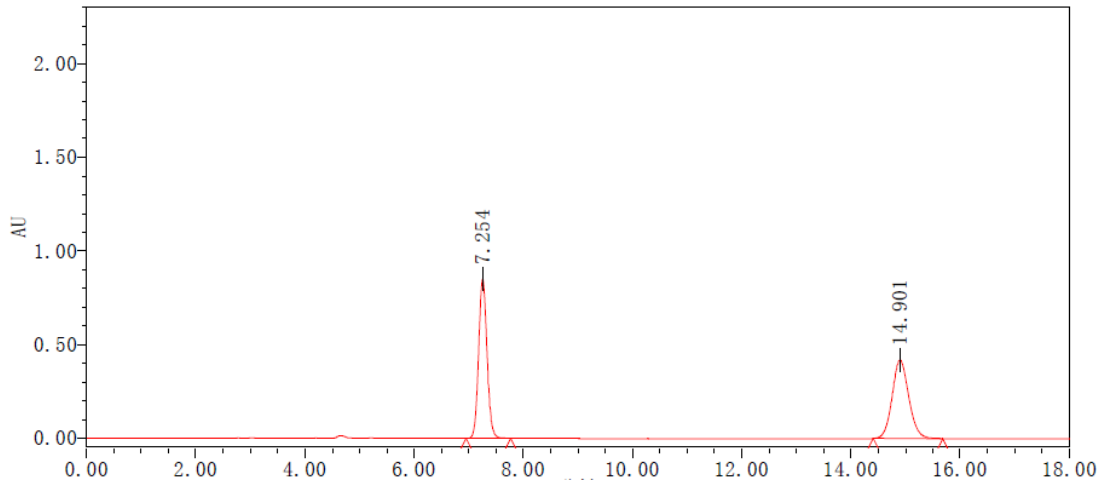
**HPLC chromatogram of racemic 54**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 7.254 | 7.254 | 851140 | 50.28 |
| 2 | 14.901 | 14.901 | 419548 | 49.72 |

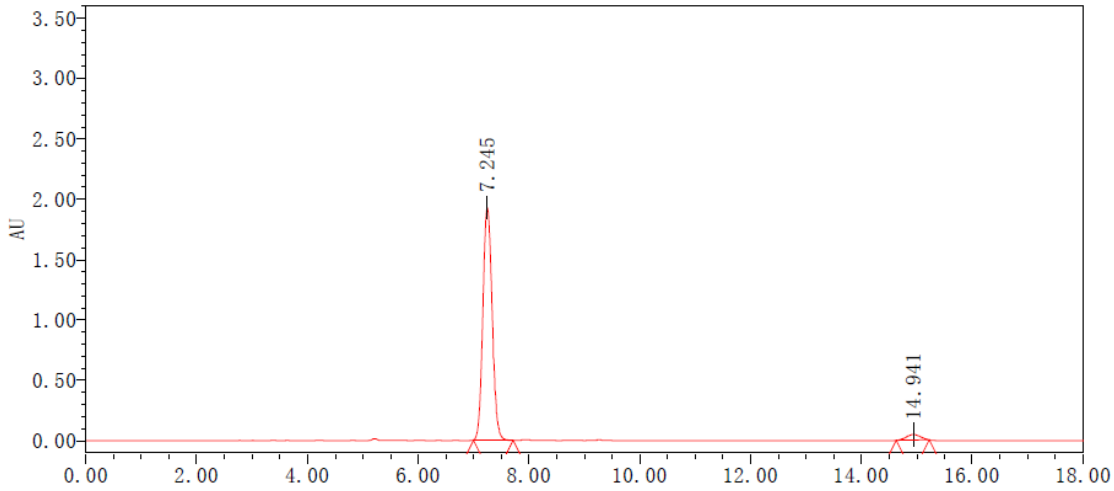
**HPLC chromatogram of chiral 54**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

λ= 254 nm

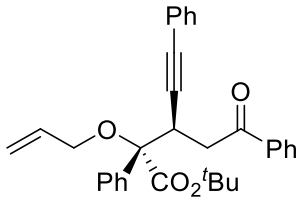
Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| 1 | 7.245 | 22158810 | 1925063 | 96.47 |
| 2 | 14.941 | 810673 | 45317 | 3.53 |

**Tert-butyl (2S,3R)-2-(allyloxy)-3-(2-oxo-2-phenylethyl)-2,5-diphenylpent-4-ynoate (55)**




**55**

Colorless oil; 45.3 mg, 63% yield, >20:1 d.r., 90% *ee*; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 7.9 Hz, 2H), 7.68 (d, *J* = 8.0 Hz, 2H), 7.53 (t, *J* = 7.3 Hz, 1H), 7.42 (t, *J* = 7.6 Hz, 2H), 7.36 (t, *J* = 7.4 Hz, 2H), 7.31 (d, *J* = 7.1 Hz, 1H), 7.24 (d, *J* = 13.6 Hz, 5H), 6.05 (ddd, *J* = 16.0, 10.3, 5.1 Hz, 1H), 5.41 (d, *J* = 17.2 Hz, 1H), 5.20 (d, *J* = 10.4 Hz, 1H), 4.54 (dd, *J* = 12.7, 5.2 Hz, 1H), 4.35 (ddd, *J* = 13.1, 11.6, 3.6 Hz, 2H), 3.34 (dd, *J* = 16.6, 10.2 Hz, 1H), 3.13 (dd, *J* = 16.6, 2.7 Hz, 1H), 1.51 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 197.6, 169.5, 138.6, 137.0, 135.2, 133.1, 131.4, 128.5, 128.2, 128.2, 128.1, 127.8, 126.8, 123.5, 116.0, 89.7, 85.6, 83.9, 82.7, 67.7, 39.3, 36.7, 28.1. HRMS (ESI) $[M+Na]^+$ calcd for $C_{32}H_{32}O_4Na^+$, 503.2193, found 503.2189. (Chiral IE-3, λ= 254 nm, *n*-hexane/2-propanol= 19/1, Flow rate = 1.0 mL/min), $t_R$ = 8.725 min(major), 19.158 min.

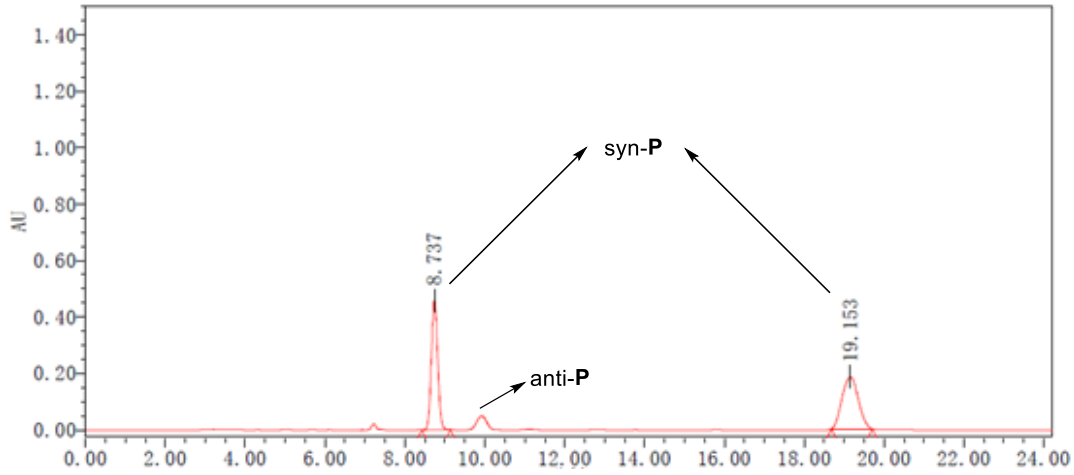
**HPLC chromatogram of racemic 55**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 8.737 | 5225981 | 459523 | 49.91 |
| 2 | 19.153 | 5244627 | 184171 | 50.09 |

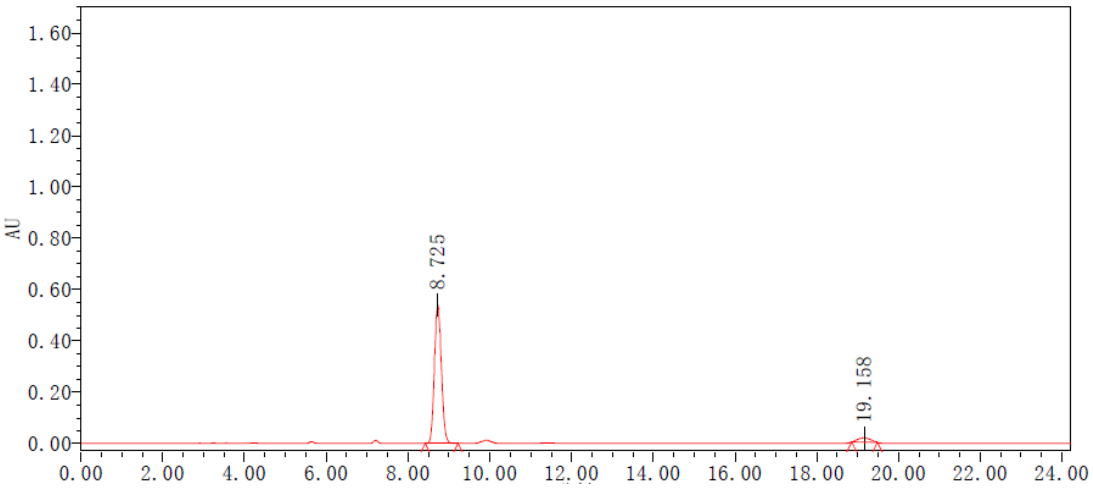
**HPLC chromatogram of chiral 55**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

λ= 254 nm

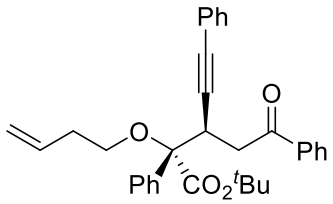
Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| 1 | 8.725 | 6624480 | 539623 | 94.78 |
| 2 | 19.158 | 365027 | 16480 | 5.22 |

**Tert-butyl (2S,3R)-2-(but-3-en-1-yloxy)-3-(2-oxo-2-phenylethyl)-2,5-diphenylpent-4-ynoate (56)**




**56**

Colorless oil; 45.2 mg, 62% yield, >20:1 d.r., 91% *ee*; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 7.6 Hz, 2H), 7.66 (d, *J* = 7.7 Hz, 2H), 7.53 (t, *J* = 7.3 Hz, 1H), 7.42 (t, *J* = 7.6 Hz, 2H), 7.35 (t, *J* = 7.5 Hz, 2H), 7.30 (d, *J* = 7.1 Hz, 1H), 7.24 (d, *J* = 12.9 Hz, 5H), 5.95 (ddt, *J* = 17.0, 10.2, 6.7 Hz, 1H), 5.14 (d, *J* = 17.2 Hz, 1H), 5.06 (d, *J* = 10.5 Hz, 1H), 4.31 (dd, *J* = 10.0, 2.8 Hz, 1H), 4.05 (dd, *J* = 15.3, 6.8 Hz, 1H), 3.88 (dd, *J* = 15.2, 6.7 Hz, 1H), 3.29 (dd, *J* = 16.6, 10.1 Hz, 1H), 3.12 (dd, *J* = 16.6, 2.8 Hz, 1H), 2.48 (dd, *J* = 13.1, 6.5 Hz, 2H), 1.51 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 197.7, 169.5, 138.8, 137.0, 135.6, 133.1, 131.4, 128.5, 128.2, 128.1, 128.1, 128.0, 127.7, 126.7, 123.6, 116.4, 89.8, 85.3, 83.9, 82.6, 65.8, 35.0, 28.1. HRMS (ESI) $[M+Na]^+$ calcd for $C_{33}H_{34}O_4Na^+$, 517.2349, found 517.2346. (Chiral IA, λ= 254 nm, *n*-hexane/2-propanol= 49/1, Flow rate = 1.0 mL/min), $t_R$ = 7.426 min(major), 14.607 min.

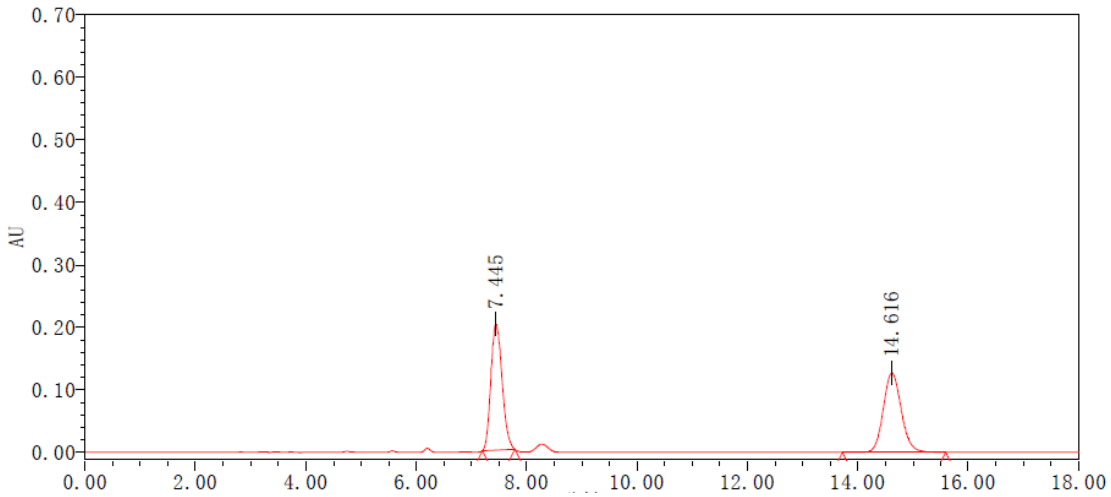
**HPLC chromatogram of racemic 56**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 7.445 | 2893437 | 201301 | 50.30 |
| 2 | 14.616 | 2858742 | 127090 | 49.70 |

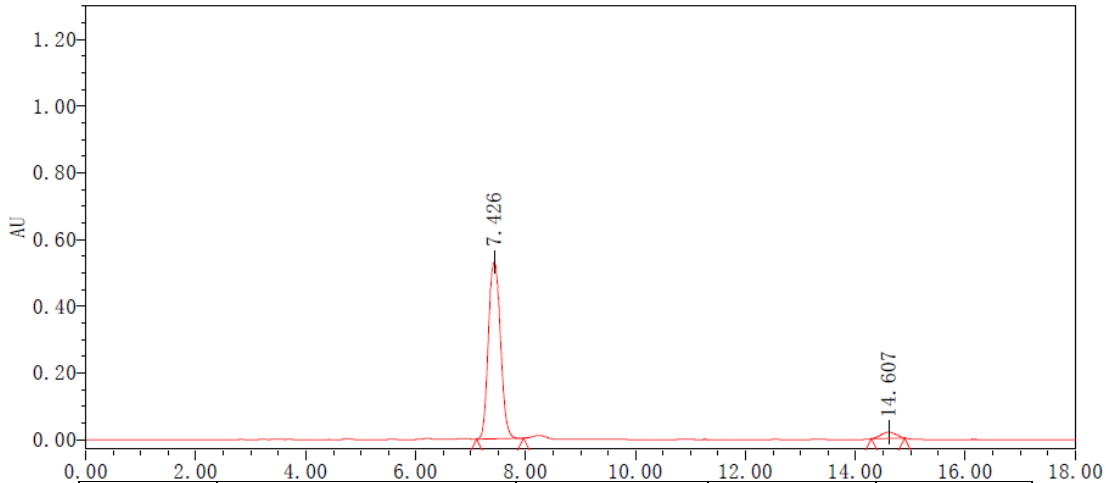
**HPLC chromatogram of chiral 56**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

λ= 254 nm

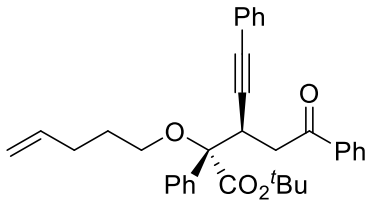
Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| 1 | 7.426 | 8186509 | 529686 | 95.95 |
| 2 | 14.607 | 345935 | 18208 | 4.05 |

**Tert-butyl (2S,3R)-3-(2-oxo-2-phenylethyl)-2-(pent-4-en-1-yloxy)-2,5-diphenylpent-4-ynoate (57)**




**57**

Colorless oil; 45.2 mg, 52% yield, >20:1 d.r., 90% *ee*; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.92 – 7.87 (m, 2H), 7.69 – 7.64 (m, 2H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.43 (t, *J* = 7.6 Hz, 2H), 7.36 (t, *J* = 7.4 Hz, 2H), 7.30 (d, *J* = 7.2 Hz, 1H), 7.24 (d, *J* = 14.6 Hz, 5H), 5.87 (ddt, *J* = 16.9, 10.2, 6.6 Hz, 1H), 5.04 (ddd, *J* = 17.1, 3.3, 1.6 Hz, 1H), 4.96 (dd, *J* = 10.2, 1.8 Hz, 1H), 4.31 (dd, *J* = 10.1, 3.2 Hz, 1H), 3.98 (dt, *J* = 8.8, 6.6 Hz, 1H), 3.81 (dt, *J* = 8.9, 6.4 Hz, 1H), 3.27 (dd, *J* = 16.6, 10.1 Hz, 1H), 3.12 (dd, *J* = 16.6, 3.1 Hz, 1H), 2.24 (dd, *J* = 14.2, 7.4 Hz, 2H), 1.89 – 1.73 (m, 2H), 1.50 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 197.7, 169.6, 138.9, 138.6, 137.0, 133.0, 131.4, 128.5, 128.2, 128.1, 128.1, 128.0, 127.7, 126.8, 123.6, 114.7, 89.8, 85.2, 83.9, 82.5, 65.8, 39.3, 36.3, 30.5, 29.73, 28.1. HRMS (ESI) $[M+Na]^+$ calcd for $C_{34}H_{36}O_4Na^+$, 531.2509, found 531.2506. (Chiral IC, λ= 254 nm, *n*-hexane/2-propanol= 49/1, Flow rate = 1.0 mL/min), $t_R$ = 7.432 min(major), 12.362 min.

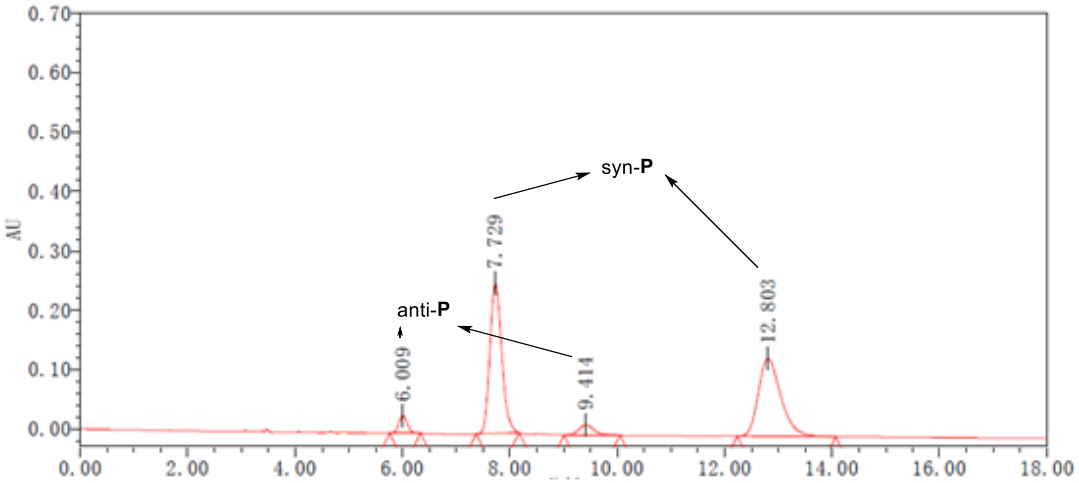
**HPLC chromatogram of racemic 57**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IC




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 6.009 | 336436 | 29596 | 4.03 |
| 2 | 7.729 | 3848417 | 252827 | 46.12 |
| 3 | 9.414 | 342179 | 16979 | 4.10 |
| 4 | 12.803 | 3817076 | 131176 | 45.75 |

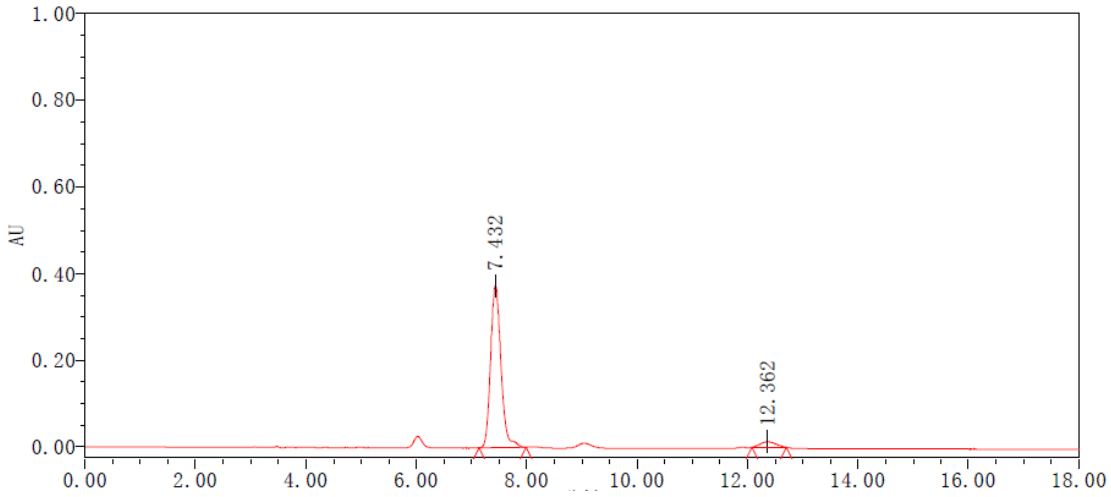
**HPLC chromatogram of chiral 57**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

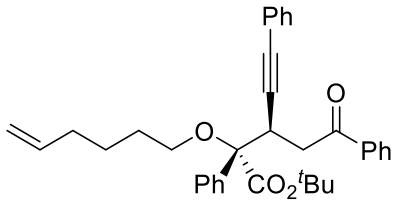
λ= 254 nm

Chiral IC




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 7.432 | 4948850 | 373399 | 95.02 |
| 2 | 12.362 | 259610 | 12978 | 4.98 |

**Tert-butyl (2S,3R)-2-(hex-5-en-1-yloxy)-3-(2-oxo-2-phenylethyl)-2,5-diphenylpent-4-ynoate (58)**




**58**

Colorless oil; 39.2 mg, 50% yield, >20:1 d.r., 90% *ee*; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.92 – 7.88 (m, 2H), 7.68 – 7.64 (m, 2H), 7.56 – 7.50 (m, 1H), 7.43 (t, *J* = 7.6 Hz, 2H), 7.36 (t, *J* = 7.4 Hz, 2H), 7.30 (d, *J* = 7.2 Hz, 1H), 7.24 (d, *J* = 14.4 Hz, 5H), 5.81 (ddt, *J* = 16.9, 10.2, 6.6 Hz, 1H), 5.00 (ddd, *J* = 17.1, 3.4, 1.6 Hz, 1H), 4.94 (dd, *J* = 10.2, 1.0 Hz, 1H), 4.30 (dd, *J* = 9.8, 3.3 Hz, 1H), 3.96 (dt, *J* = 8.8, 6.5 Hz, 1H), 3.26 (dd, *J* = 16.6, 9.9 Hz, 1H), 3.15 (dd, *J* = 16.6, 3.3 Hz, 1H), 2.10 (dd, *J* = 14.4, 7.1 Hz, 2H), 1.71 (dt, *J* = 12.7, 6.6 Hz, 2H), 1.61 – 1.56 (m, 2H), 1.51 (s, 9H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 197.7, 169.7, 138.9, 138.9, 137.0, 133.0, 131.4, 128.5, 128.2, 128.1, 128.0,

128.0, 127.7, 126.8, 123.6, 114.5, 89.8, 85.2, 83.8, 82.5, 66.2, 39.4, 36.4, 33.7, 30.0, 28.1, 25.6. HRMS (ESI) $[M+Na]^+$ calcd for $C_{35}H_{38}O_4Na^+$, 545.2662, found 545.2663. (Chiral IC, λ= 254 nm, *n*-hexane/2-propanol/EtOH= 197/1/2, Flow rate = 1.0 mL/min), $t_R$ = 6.752 min(major), 14.838 min.

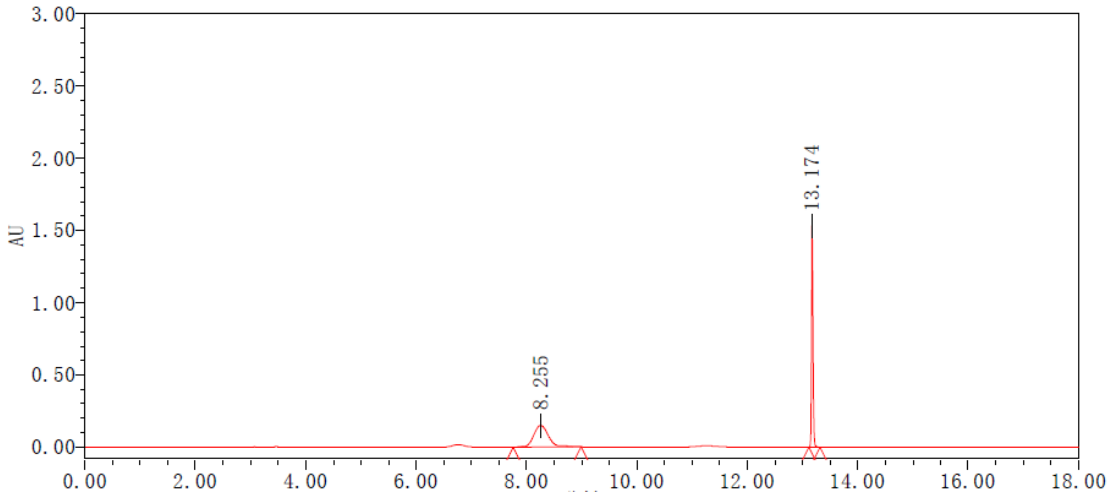
**HPLC chromatogram of racemic 58**

Condition: n-hexane/2-propanol/EtOH = 197:1:2

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IC




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 8.255 | 2783408 | 149850 | 50.23 |
| 2 | 13.174 | 2758327 | 1532847 | 49.77 |

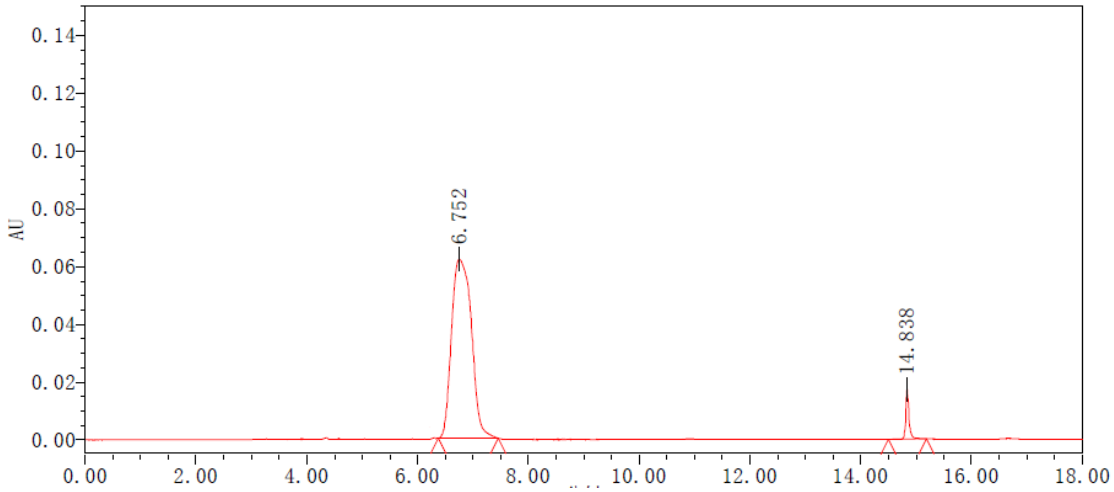
**HPLC chromatogram of chiral 58**

Condition: n-hexane/2-propanol/EtOH = 197:1:2

Flow rate =1.0 mL/min

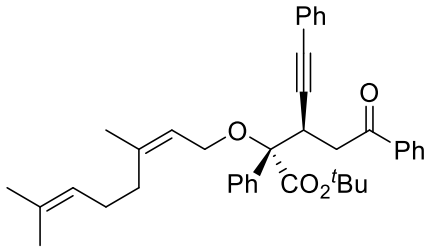
λ= 254 nm

Chiral IC




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 6.752 | 1545035 | 61969 | 95.66 |
| 2 | 14.838 | 70082 | 17161 | 4.34 |

**Tert-butyl (2S,3R)-2-(((Z)-3,8-dimethylnona-2,7-dien-1-yl)oxy)-3-(2-oxo-2-phenylethyl)-2,5-diphenylpent-4-ynoate (59)**




**59**

Colorless oil; 52.7 mg, 61% yield, 9:1 d.r., 90% *ee*; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.92 – 7.88 (m, 2H), 7.70 – 7.65 (m, 2H), 7.52 (dd, *J* = 10.5, 4.2 Hz, 1H), 7.42 (t, *J* = 7.6 Hz, 2H), 7.35 (dd, *J* = 8.2, 6.6 Hz, 2H), 7.29 (d, *J* = 7.2 Hz, 1H), 7.24 – 7.19 (m, 5H), 5.51 (t, *J* = 6.1 Hz, 1H), 5.02 (dd, *J* = 6.4, 5.2 Hz, 1H), 4.55 (dd, *J* = 11.1, 6.9 Hz, 1H), 4.35 – 4.25 (m, 2H), 3.32 (dd, *J* = 16.7, 10.2 Hz, 1H), 3.15 (dd, *J* = 16.7, 3.0 Hz, 1H), 2.07

(td, *J* = 8.7, 4.5 Hz, 3H), 2.02 (d, *J* = 3.3 Hz, 1H), 1.77 (t, *J* = 2.5 Hz, 3H), 1.61 (s, 1H), 1.59 (s, 3H), 1.55 (s, 3H), 1.51 (s, 9H), 1.35 (dd, *J* = 30.2, 12.4 Hz, 1H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 197.7, 169.7, 139.5, 138.8, 137.1, 133.0, 131.8, 131.4, 128.5, 128.2, 128.1, 128.0, 127.7, 126.9, 123.9, 123.6, 122.4, 121.6, 100.1, 89.8, 85.4, 83.9, 82.5, 63.4, 39.4, 36.5, 32.5, 28.1, 28.0, 26.8, 25.7, 23.5, 17.7. HRMS (ESI) $[M+Na]^+$ calcd for $C_{39}H_{44}O_4Na^+$, 599.3132, found 599.3128. (Chiral ID-3, λ= 254 nm, *n*-hexane/2-propanol= 49/1, Flow rate = 1.0 mL/min), $t_R$ = 7.648 min(major), 20.584 min.

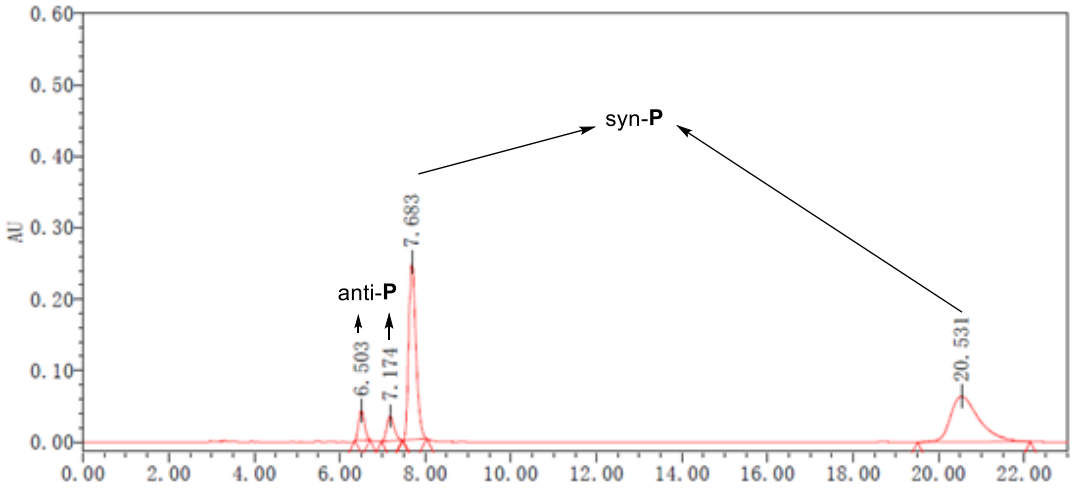
**HPLC chromatogram of racemic 59**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral ID-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 6.503 | 410294 | 42068 | 6.12 |
| 2 | 7.174 | 411303 | 34923 | 6.13 |
| 3 | 7.683 | 2945133 | 247583 | 43.92 |
| 4 | 20.531 | 2938239 | 63610 | 43.82 |

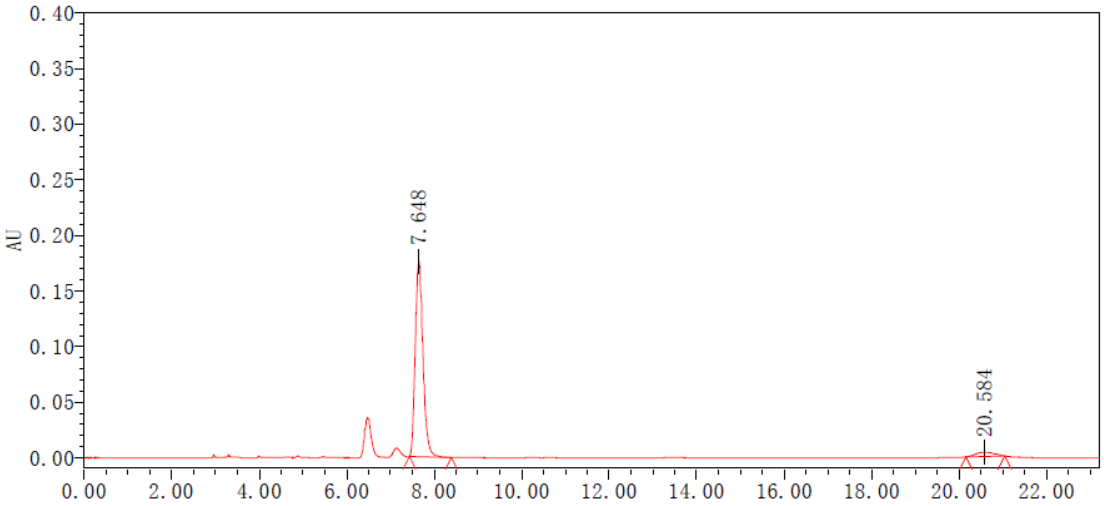
**HPLC chromatogram of chiral 59**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

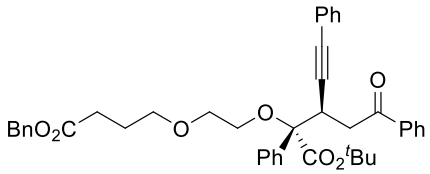
λ= 254 nm

Chiral ID-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 7.648 | 2200522 | 175662 | 95.25 |
| 2 | 20.584 | 109760 | 3728 | 4.75 |

**Tert-butyl (2S,3R)-2-(2-(4-(benzyloxy)-4-oxobutoxy)ethoxy)-3-(2-oxo-2-phenylethyl)-2,5-diphenylpent-4-ynoate (*syn*-60)**




*syn*-**60**

Colorless oil; 53% yield (17.5 mg), >20:1 d.r., 97% ee. $^1$H NMR (500 MHz, $CDCl_3$) δ 7.91 (d, *J* = 7.5 Hz, 2H), 7.68 (d, *J* = 7.6 Hz, 2H), 7.50 (t, *J* = 7.3 Hz, 1H), 7.41 (dd, *J* = 15.8, 7.8 Hz, 3H), 7.36 – 7.30 (m, 8H), 7.21 (d, *J* = 2.5 Hz, 4H), 5.08 (s, 2H), 4.32

(dd, *J* = 10.2, 2.8 Hz, 1H), 4.19 (dd, *J* = 9.5, 5.1 Hz, 1H), 4.03 – 3.95 (m, 1H), 3.70 (dd, *J* = 11.8, 7.2 Hz, 1H), 3.56 (t, *J* = 6.2 Hz, 2H), 3.41 (dd, *J* = 16.7, 10.3 Hz, 1H), 3.08 (dd, *J* = 16.7, 2.6 Hz, 1H), 2.46 (dd, *J* = 13.5, 7.2 Hz, 2H), 1.93 (dd, *J* = 12.3, 6.1 Hz, 2H), 1.50 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 197.7, 173.4, 173.3, 169.4, 138.6, 137.0, 136.1, 133.1, 131.4, 128.6, 128.5, 128.4, 128.3, 128.2, 128.2, 128.2, 128.1, 128.1, 128.1, 127.8, 127.2, 126.8, 123.5, 89.9, 85.3, 82.7, 81.7, 81.6, 70.6, 70.2, 70.1, 68.8, 66.2, 65.9, 39.0, 31.0, 28.1, 27.9, 25.2. HRMS (ESI) $[M+Na]^+$ calcd for $C_{42}H_{44}O_7Na^+$, 683.2979, found 683.2975. (Chiral IA-3, λ= 254 nm, *n*-hexane/2-propanol= 9/1, Flow rate = 1.0 mL/min), $t_R$ = 7.954 min (major), 13.564 min.

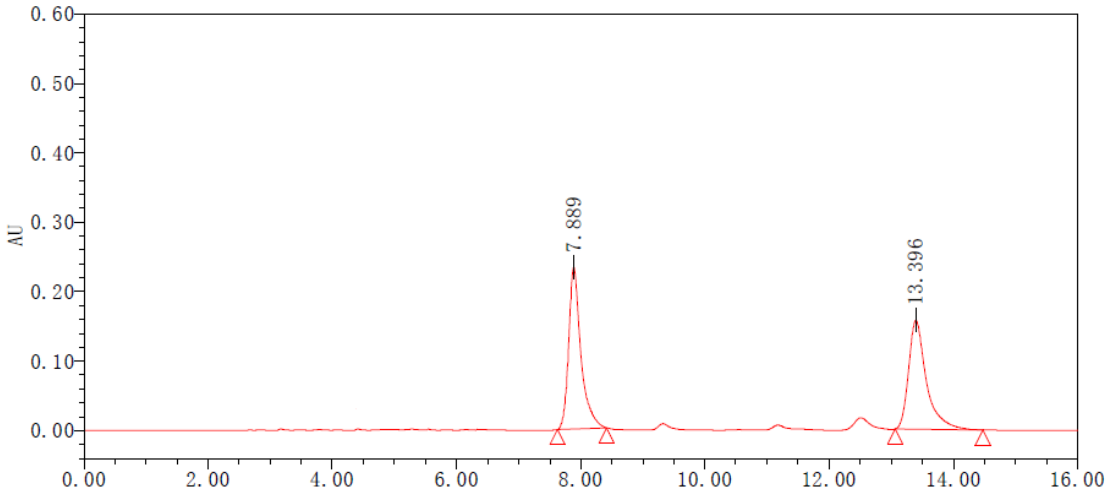
**HPLC chromatogram of racemic 60**

Condition: n-hexane/2-propanol =9:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 7.889 | 3170989 | 232747 | 50.19 |

| | | | | |
|---|---|---|---|---|
| 2 | 13.396 | 3146358 | 157120 | 49.81 |

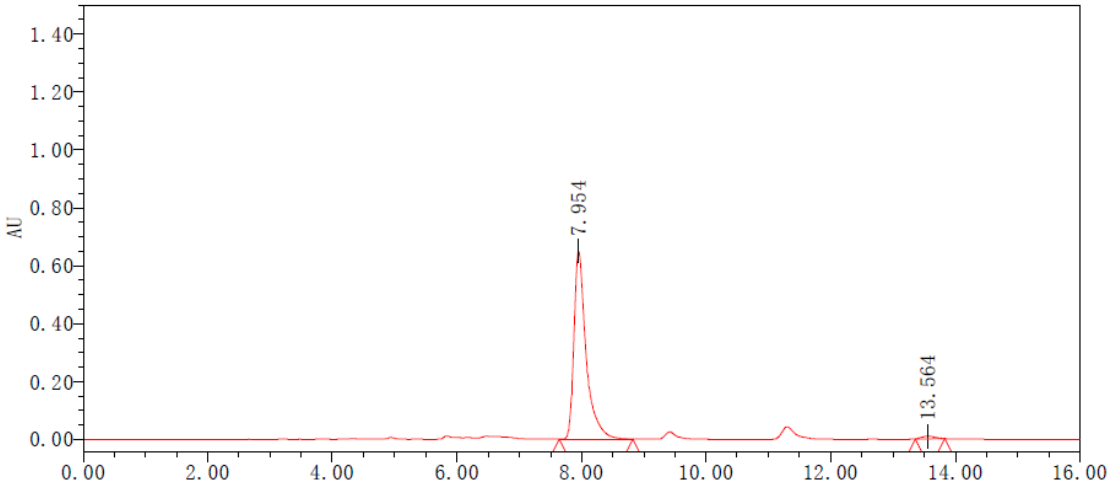
**HPLC chromatogram of chiral 60**

Condition: n-hexane/2-propanol =9:1

Flow rate =1.0 mL/min

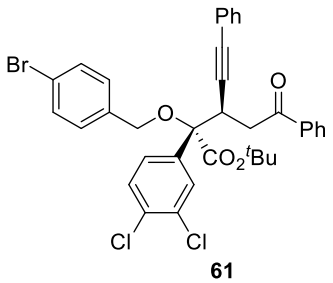
λ= 254 nm

Chiral IA-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 7.954 | 8774656 | 650002 | 98.53 |
| 2 | 13.564 | 130850 | 9043 | 1.47 |

**Tert-butyl (2S,3R)-2-((4-bromobenzyl)oxy)-2-(3,4-dichlorophenyl)-3-(2-oxo-2-phenylethyl)-5-phenylpent-4-ynoate (61)**




**61**

Colorless oil; 65.9 mg, 65% yield, >20:1 d.r., >99% *ee*, $[\alpha]_D^{20}$ = -12.36 (c = 0.1, $CH_2Cl_2$); $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 7.6 Hz, 3H), 7.55 (t, *J* = 8.3 Hz, 1H), 7.52 (s, 1H), 7.49 (d, *J* = 8.5 Hz, 2H), 7.46 – 7.41 (m, 3H), 7.34 (d, *J* = 8.2 Hz, 2H), 7.26 (d, *J* = 9.1 Hz, 5H), 4.99 (d, *J* = 11.5 Hz, 1H), 4.87 (d, *J* = 11.5 Hz, 1H), 4.35 (dd, *J* = 9.7, 3.2 Hz, 1H), 3.31 (dd, *J* = 16.7, 9.8 Hz, 1H), 3.09 (dd, *J* = 16.7, 3.1 Hz, 1H), 1.52 (s, 9H). $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 197.0, 168.5, 138.7, 137.3, 136.7, 133.3, 132.6, 131.5, 131.4, 130.2, 129.3, 128.7, 128.3, 128.2, 128.2, 126.1, 123.0, 121.6, 88.8, 85.1, 84.6, 83.7, 68.2, 39.1, 36.6, 28.1, 28.0. HRMS (ESI) $[M+Na]^+$ calcd for $C_{36}H_{31}O_4Cl_2BrNa^+$, 699.0675, found 699.0674. (Chiral IE-3, λ= 254 nm, *n*-hexane/2-propanol= 97/3, Flow rate = 1.0 mL/min), $t_R$ = 7.401 min(major), 10.092 min.

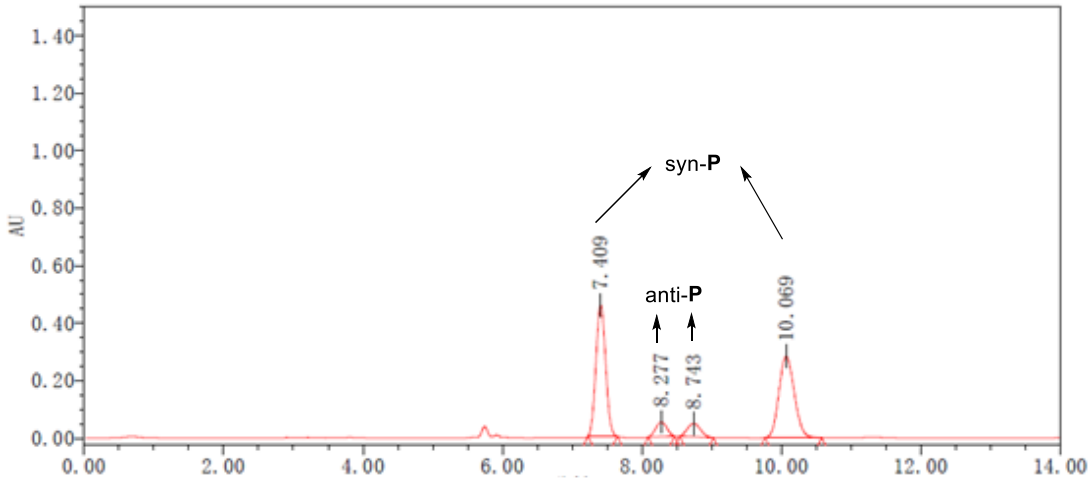
**HPLC chromatogram of racemic 61**

Condition: n-hexane/2-propanol =97:3

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 7.409 | 4374540 | 458002 | 44.26 |

| | | | | |
|---|---|---|---|---|
| 2 | 8.277 | 559177 | 50697 | 5.66 |
| 3 | 8.743 | 613385 | 46416 | 6.21 |
| 4 | 10.069 | 4337024 | 283557 | 43.88 |

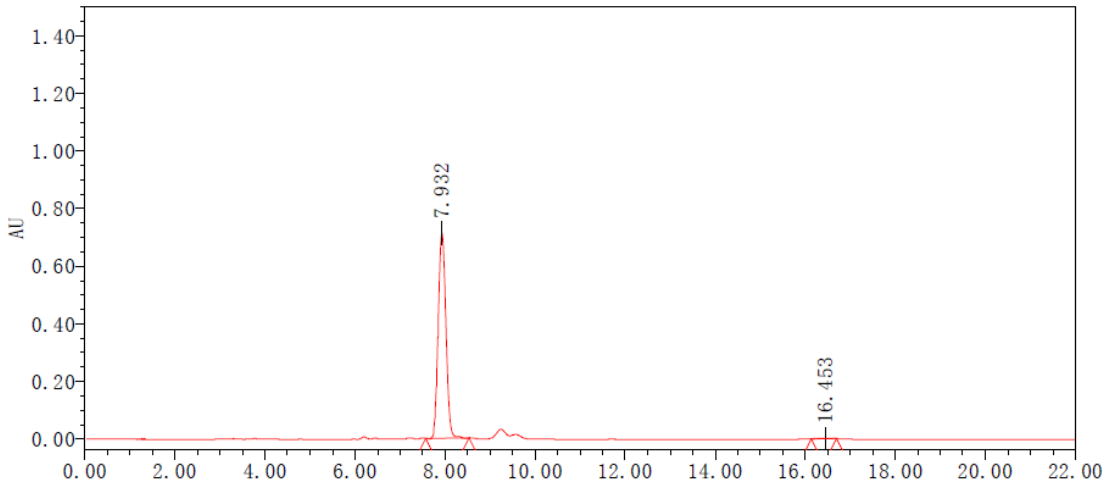
**HPLC chromatogram of chiral 61**

Condition: n-hexane/2-propanol =97:3

Flow rate =1.0 mL/min

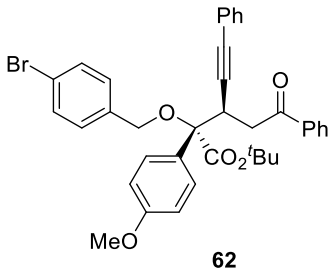
λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 7.932 | 8397971 | 711773 | 99.76 |
| 2 | 16.453 | 19993 | 970 | 0.24 |

**Tert-butyl (2S,3R)-2-((4-bromobenzyl)oxy)-2-(4-methoxyphenyl)-3-(2-oxo-2-phenylethyl)-5-phenylpent-4-ynoate (62)**




**62**

Colorless oil; 47.9 mg, 50% yield, >20:1 d.r., >99% *ee*, $[\alpha]_D^{20}$ = -12.98 (c = 0.1, $CH_2Cl_2$); $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 7.3 Hz, 2H), 7.60 (d, *J* = 8.9 Hz, 2H), 7.53 (t, *J* = 7.4 Hz, 1H), 7.47 (d, *J* = 8.4 Hz, 2H), 7.42 (d, *J* = 7.8 Hz, 2H), 7.38 (t, *J* = 6.9 Hz, 2H), 7.25 (d, *J* = 9.0 Hz, 5H), 6.88 (d, *J* = 9.0 Hz, 2H), 5.02 (d, *J* = 11.8 Hz, 1H), 4.88 (d, *J* = 11.8 Hz, 1H), 4.38 (dd, *J* = 10.1, 3.0 Hz, 1H), 3.80 (s, 3H), 3.32 (dd, *J* = 16.7, 10.1 Hz, 1H), 3.11 (dd, *J* = 16.6, 3.0 Hz, 1H), 1.51 (s, 9H). $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 197.5, 169.6, 159.4, 138.1, 136.9, 133.1, 132.4, 131.4, 130.2, 129.2, 128.6, 128.2, 128.2, 128.0, 127.9, 123.4, 121.2, 113.6, 89.8, 85.6, 82.8, 67.9, 55.3, 39.2, 36.6, 28.1. HRMS (ESI) $[M+Na]^+$ calcd for $C_{37}H_{35}O_5BrNa^+$, 661.1560, found 661.1560. (Chiral IB-3, λ= 254 nm, *n*-hexane/2-propanol= 19/1, Flow rate = 1.0 mL/min), $t_R$ = 14.080 min(major), 33.833 min.

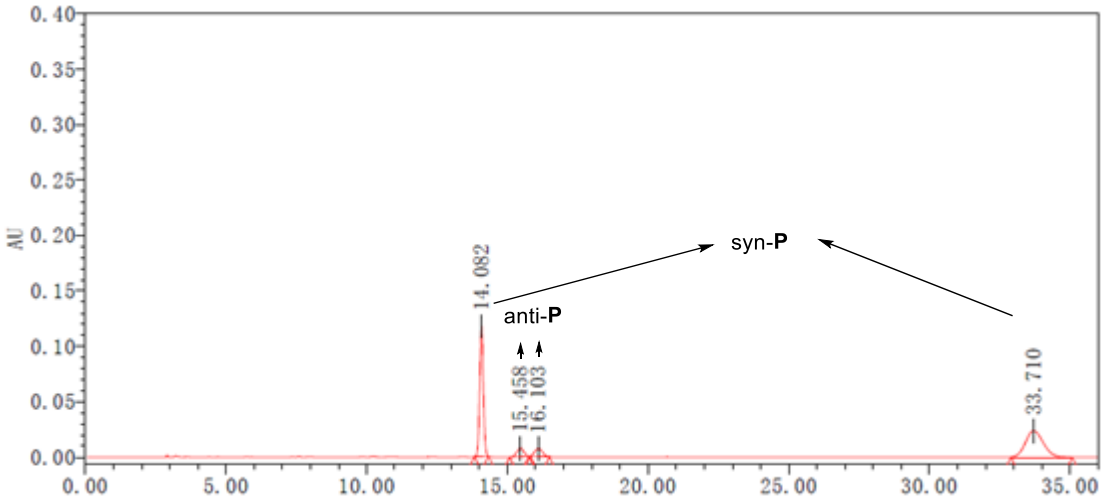
**HPLC chromatogram of racemic 62**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IB-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 14.082 | 1057188 | 117486 | 44.60 |
| 2 | 15.458 | 132000 | 7632 | 5.57 |
| 3 | 16.103 | 131926 | 7025 | 5.57 |
| 4 | 33.710 | 1049386 | 23871 | 44.27 |

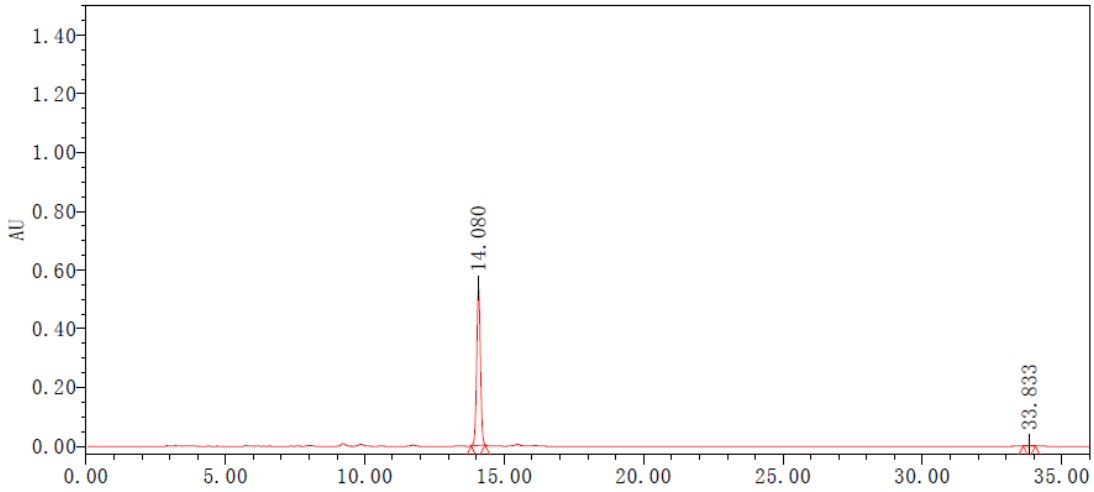
**HPLC chromatogram of chiral 62**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

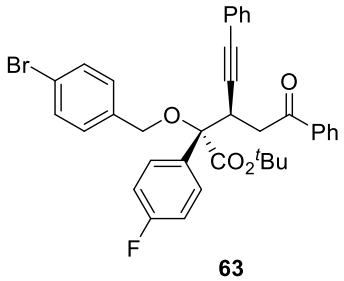
λ= 254 nm

Chiral IB-3



| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 14.080 | 4949393 | 536766 | 99.92 |
| 2 | 33.833 | 4088 | 257 | 0.08 |

**Tert-butyl (2S,3R)-2-((4-bromobenzyl)oxy)-2-(4-fluorophenyl)-3-(2-oxo-2-phenylethyl)-5-phenylpent-4-ynoate (63)**




**63**

Colorless oil; 59.2 mg, 63% yield, >20:1 d.r., 97% *ee*; $^{1}$H NMR (500 MHz, $CDCl_3$) δ 7.85 (d, *J* = 7.4 Hz, 2H), 7.67 (dd, *J* = 8.8, 5.3 Hz, 2H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.48 (d, *J* = 8.3 Hz, 2H), 7.42 (t, *J* = 7.7 Hz, 2H), 7.37 (d, *J* = 8.3 Hz, 2H), 7.25 (d, *J* = 6.8 Hz, 5H), 7.05 (t, *J* = 8.7 Hz, 2H), 5.02 (d, *J* = 11.6 Hz, 1H), 4.89 (d, *J* = 11.6 Hz, 1H), 4.40 (dd, *J* = 9.9, 3.0 Hz, 1H), 3.32 (dd, *J* = 16.7, 10.0 Hz, 1H), 3.09 (dd, *J* = 16.7, 2.9 Hz, 1H), 1.51 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 197.3, 169.2, 162.5 (d, *J* = 247.6 Hz), 137.8, 136.8, 134.2, 134.1, 133.2, 131.5, 131.4, 129.2, 128.7 (d, *J* = 8.2 Hz), 128.2, 128.2, 128.0, 122.3 (d, *J* = 230.4 Hz), 115.3, 115.1, 89.4, 85.5, 84.3, 83.2, 68.0, 39.2, 36.5, 28.1. $^{19}$F NMR (471 MHz, $CDCl_3$) δ -113.92. HRMS (ESI) $[M+Na]^+$ calcd for $C_{36}H_{32}O_4FBrNa^+$, 649.1560, found 649.1356. (Chiral IE-3, λ= 254 nm, *n*-hexane/2-propanol= 97/3, Flow rate = 1.0 mL/min), $t_R$ = 9.275 min(major), 24.098 min.

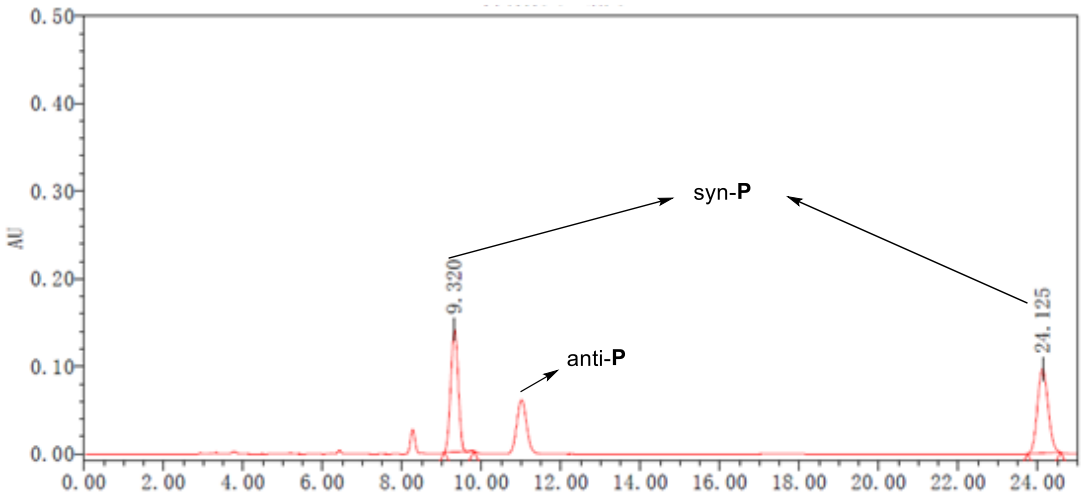
**HPLC chromatogram of racemic 63**

Condition: n-hexane/2-propanol =97:3

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 9.320 | 1813011 | 140041 | 50.29 |
| 2 | 24.125 | 1792365 | 96391 | 49.71 |

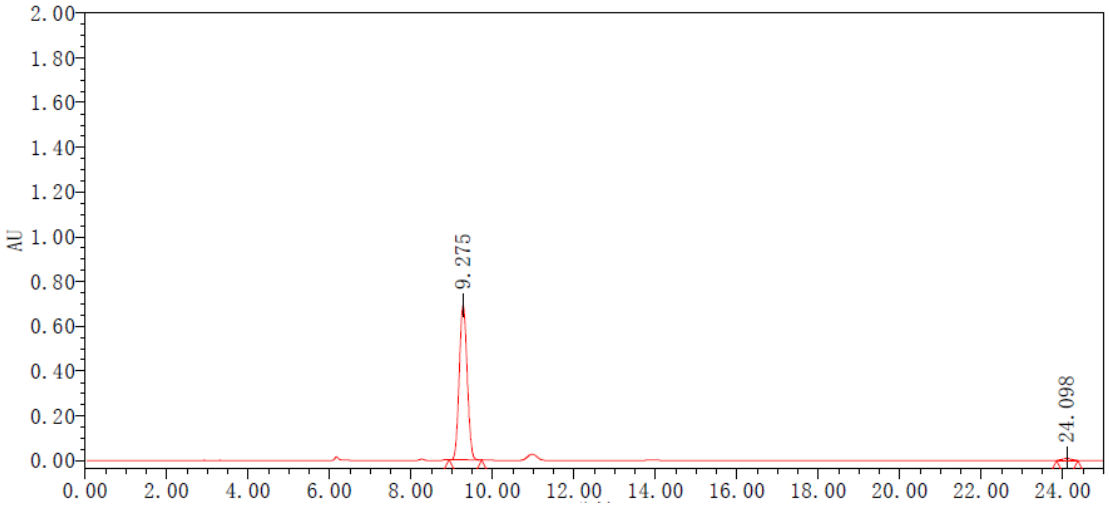
**HPLC chromatogram of chiral 63**

Condition: n-hexane/2-propanol =97:3

Flow rate =1.0 mL/min

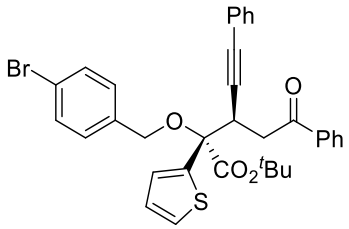
λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 9.275 | 9168282 | 689687 | 98.58 |
| 2 | 24.098 | 131642 | 8103 | 1.42 |

**Tert-butyl (2R,3R)-2-((4-bromobenzyl)oxy)-3-(2-oxo-2-phenylethyl)-5-phenyl-2-(thiophen-2-yl)pent-4-ynoate (64)**




**64**

Colorless oil; 39.6 mg, 43% yield, >20:1 d.r., 99% *ee*; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.91 – 7.85 (m, 2H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.43 (dd, *J* = 15.7, 7.9 Hz, 4H), 7.35 (d, *J* = 8.4 Hz, 2H), 7.30 (dd, *J* = 5.1, 1.1 Hz, 1H), 7.28 – 7.22 (m, 6H), 6.99 (dd, *J* = 5.1, 3.7 Hz, 1H), 4.94 (d, *J* = 11.9 Hz, 1H), 4.85 (d, *J* = 11.9 Hz, 1H), 4.29 (dd, *J* = 8.4, 4.7 Hz, 1H), 3.34 (dd, *J* = 6.5, 4.5 Hz, 2H), 1.56 (s, 9H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 197.2, 168.4, 141.7, 137.8, 136.9, 133.1, 131.5, 131.3, 129.0, 128.6, 128.2, 128.2, 128.0, 126.6, 126.4, 123.2, 121.1, 112.7, 93.2, 88.8, 85.0, 83.5, 81.1, 77.3, 77.0, 76.7, 69.4, 67.9, 51.3,

39.1, 39.2, 38.3, 28.0, 25.0. HRMS (ESI) $[M+Na]^+$ calcd for $C_{34}H_{31}O_4SBrNa^+$, 637.1019, found 637.1019. (Chiral ID-3, λ= 254 nm, *n*-hexane/2-propanol= 49/1, Flow rate = 1.0 mL/min), $t_R$ = 9.650 min(major), 22.555 min.

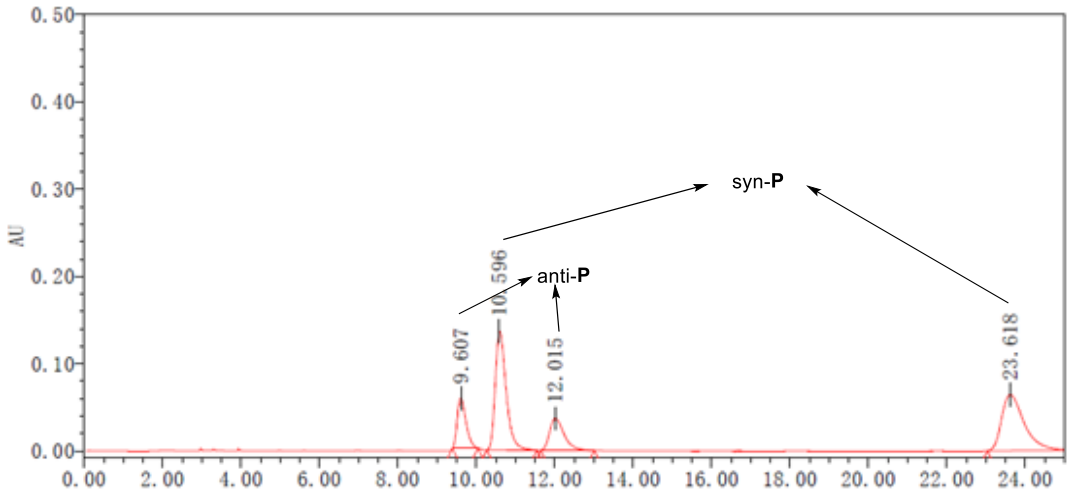
**HPLC chromatogram of racemic 64**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral ID-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 9.607 | 909105 | 57501 | 12.93 |
| 2 | 10.596 | 2610966 | 135845 | 37.14 |
| 3 | 12.015 | 926181 | 36593 | 13.17 |
| 4 | 23.618 | 2584403 | 64137 | 36.76 |

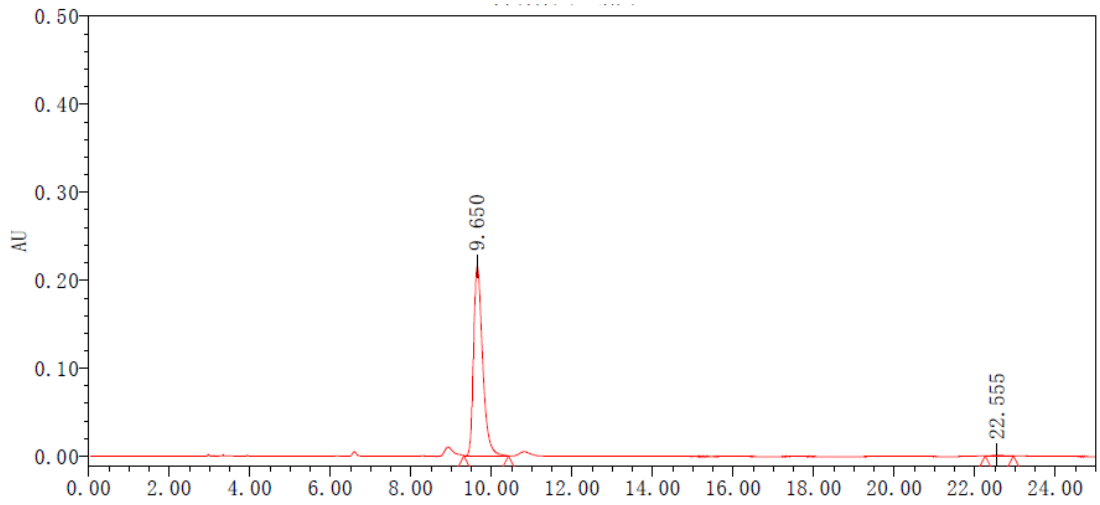
**HPLC chromatogram of chiral 64**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

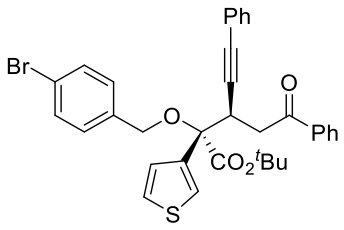
λ= 254 nm

Chiral ID-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 9.650 | 3331433 | 214864 | 99.72 |
| 2 | 22.555 | 9234 | 350 | 0.28 |

**Tert-butyl (2S,3R)-2-((4-bromobenzyl)oxy)-3-(2-oxo-2-phenylethyl)-5-phenyl-2-(thiophen-3-yl)pent-4-ynoate (65)**




**65**

Colorless oil; 47.9 mg, 52% yield, >20:1 d.r., 90% *ee*; $^{1}$H NMR (500 MHz, $CDCl_3$) δ 7.87 (d, *J* = 7.5 Hz, 2H), 7.58 – 7.51 (m, 2H), 7.48 – 7.39 (m, 4H), 7.34 (d, *J* = 7.7 Hz, 2H), 7.26 (d, *J* = 15.8 Hz, 4H), 7.24 (d, *J* = 4.3 Hz, 4H), 4.93 (d, *J* = 11.8 Hz, 1H), 4.81 (d, *J* = 11.8 Hz, 1H), 4.29 (d, *J* = 8.5 Hz, 1H), 3.34 (dd, *J* = 16.6, 9.6 Hz, 1H), 3.21 (dd, *J* = 33.2, 12.4 Hz, 1H), 1.54 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 197.4, 169.1, 139.5,

138.0, 136.9, 133.1, 131.4, 131.4, 129.1, 128.6, 128.2, 127.9, 126.8, 125.6, 124.2, 123.3, 121.2, 89.2, 84.8, 84.2, 83.04, 67.8, 39.1, 37.6, 28.1, 28.1. Peak overlapping was observed. HRMS (ESI) $[M+Na]^+$ calcd for $C_{34}H_{31}O_4SBrNa^+$, 637.1019, found 637.1017. (Chiral IE-3, λ= 254 nm, *n*-hexane/2-propanol= 49/1, Flow rate = 1.0 mL/min), $t_R$ = 16.568 min(major), 36.556 min.

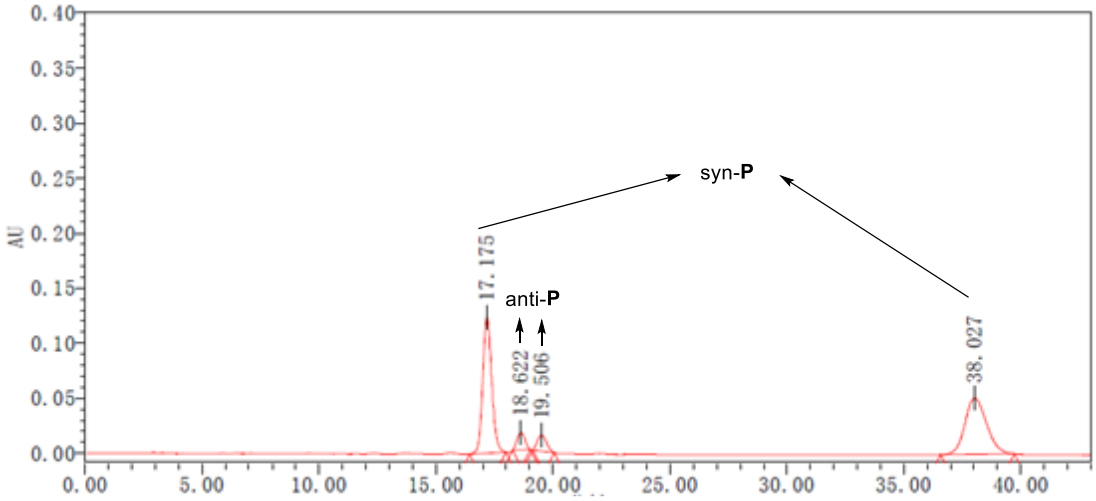
**HPLC chromatogram of racemic 65**

Condition: n-hexane/2-propanol = 49:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 17.175 | 3318551 | 123719 | 45.02 |
| 2 | 18.622 | 379526 | 16077 | 5.15 |
| 3 | 19.506 | 385317 | 14468 | 5.23 |
| 4 | 38.027 | 3287821 | 51212 | 44.60 |

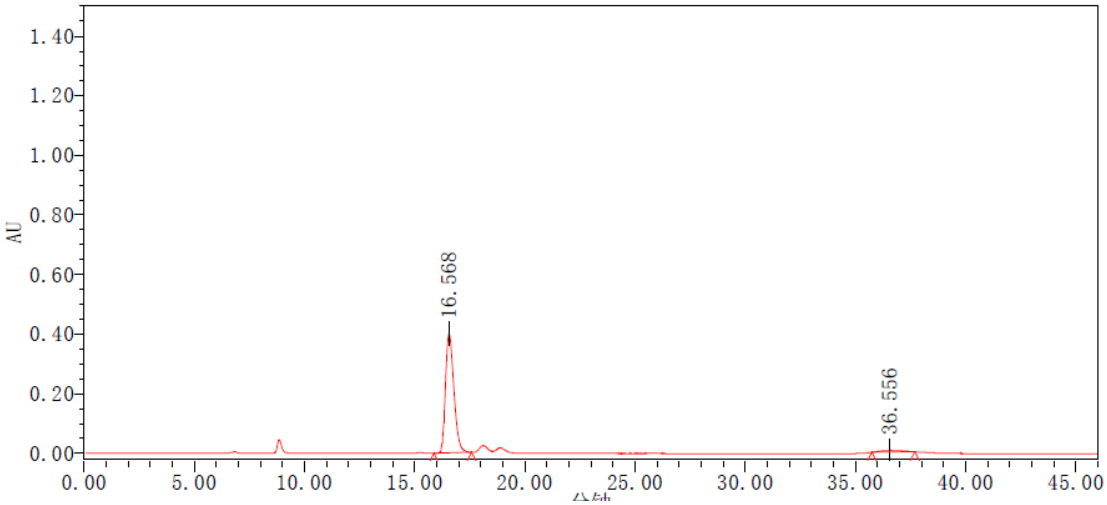
**HPLC chromatogram of chiral 65**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

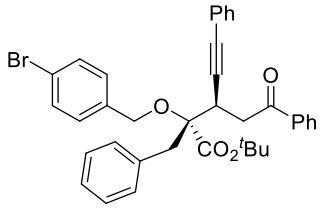
λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 16.568 | 10475819 | 399381 | 96.15 |
| 2 | 36.556 | 419706 | 6221 | 3.85 |

**Tert-butyl (2R,3R)-2-benzyl-2-((4-bromobenzyl)oxy)-3-(2-oxo-2-phenylethyl)-5-phenylpent-4-ynoate (66)**




**66**

Colorless oil; 39.2 mg, 42% yield, >20:1 d.r., 92% *ee*; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.96 – 7.89 (m, 2H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.47 – 7.42 (m, 5H), 7.36 – 7.32 (m, 4H), 7.30 – 7.28 (m, 5H), 7.23 (d, *J* = 8.4 Hz, 2H), 4.98 (d, *J* = 11.4 Hz, 1H), 4.75 (d, *J* =

11.4 Hz, 1H), 3.96 (dd, *J* = 8.8, 3.9 Hz, 1H), 3.67 (dd, *J* = 17.0, 3.9 Hz, 1H), 3.39 (dd, *J* = 16.9, 8.0 Hz, 2H), 3.36 – 3.32 (m, 1H), 1.50 (s, 9H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 197.6, 169.9, 137.4, 137.0, 135.7, 133.1, 131.5, 131.3, 130.7, 129.1, 128.6, 128.2, 128.2, 128.1, 128.0, 126.9, 123.2, 121.2, 91.8, 89.2, 88.2, 84.6, 83.1, 82.5, 66.8, 39.7, 39.1, 36.1, 34.2, 28.2. HRMS (ESI) $[M+Na]^+$ calcd for $C_{37}H_{35}O_4BrNa^+$, 645.1611, found 645.1614. (Chiral IA-3, λ= 254 nm, *n*-hexane/2-propanol= 49/1, Flow rate = 1.0 mL/min), $t_R$ = 10.805 min(major), 14.844 min.

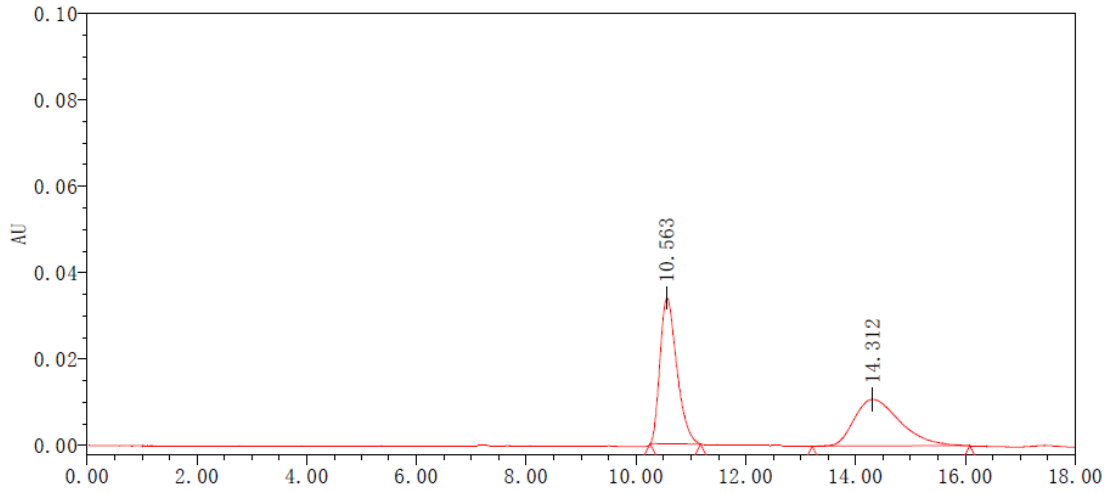
**HPLC chromatogram of racemic 66**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 10.563 | 668100 | 33750 | 50.42 |
| 2 | 14.312 | 667613 | 10779 | 49.58 |

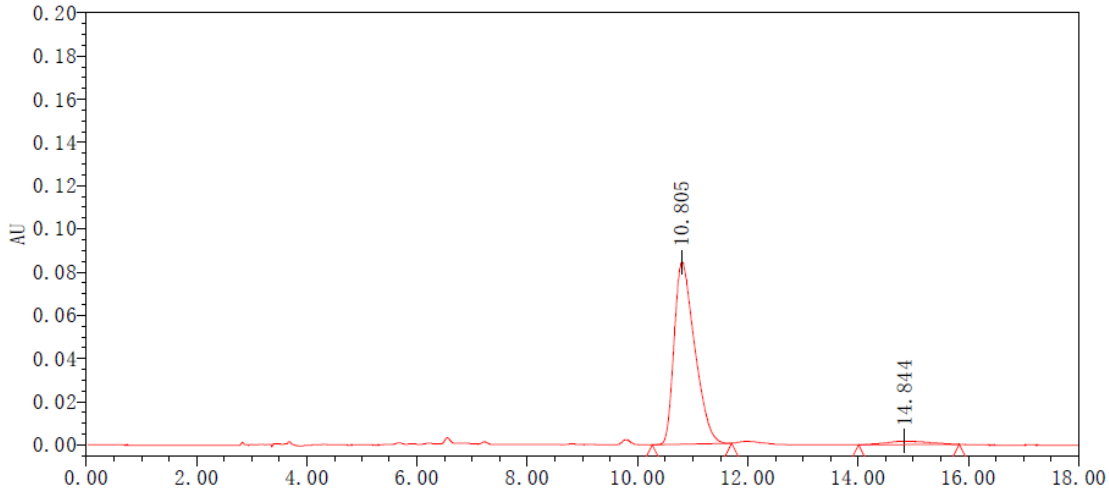
**HPLC chromatogram of chiral 66**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

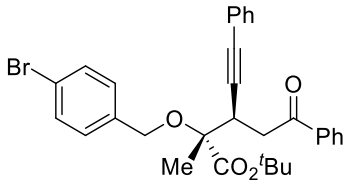
λ= 254 nm

Chiral IA-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 10.805 | 2191029 | 84327 | 96.20 |
| 2 | 14.844 | 86562 | 1602 | 3.80 |

**Tert-butyl (2R,3R)-2-((4-bromobenzyl)oxy)-2-methyl-3-(2-oxo-2-phenylethyl)-5-phenylpent-4-ynoate (67)**




**67**

Colorless oil; 50.0 mg, 61% yield, >20:1 d.r., 98% *ee*; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.98 – 7.93 (m, 2H), 7.58 – 7.52 (m, 1H), 7.43 (t, *J* = 6.7 Hz, 2H), 7.40 – 7.36 (m, 2H), 7.31 – 7.27 (m, 2H), 7.26 – 7.20 (m, 5H), 4.58 – 4.44 (m, 2H), 3.87 (dd, *J* = 8.8, 4.2 Hz, 1H), 3.61 (dd, *J* = 16.7, 4.2 Hz, 1H), 3.28 (dd, *J* = 16.7, 8.8 Hz, 1H), 1.67 (s, 3H),

1.52 (s, 9H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 197.8, 170.9, 137.5, 137.1, 133.0, 131.6, 131.3, 129.1, 128.5, 128.3, 128.1, 127.9, 123.4, 121.2, 88.7, 83.6, 82.1, 81.9, 66.4, 39.2, 37.2, 29.7, 28.1, 20.8. HRMS (ESI) $[M+Na]^+$ calcd for $C_{31}H_{31}O_4BrNa^+$, 569.1299, found 569.1298. (Chiral IA-3, λ= 254 nm, *n*-hexane/2-propanol= 99/1, Flow rate = 1.0 mL/min), $t_R$ = 11.569 min(major), 13.093 min.

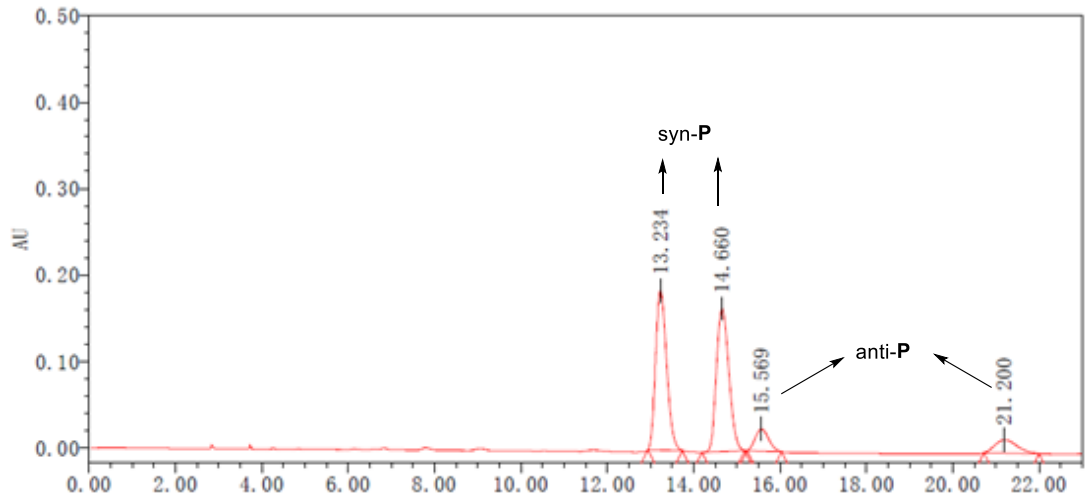
**HPLC chromatogram of racemic 67**

Condition: n-hexane/2-propanol =99:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 13.234 | 13.234 | 184637 | 43.12 |
| 2 | 14.660 | 14.660 | 165217 | 42.71 |
| 3 | 15.569 | 15.569 | 25358 | 7.17 |
| 4 | 21.200 | 21.200 | 15303 | 7.00 |

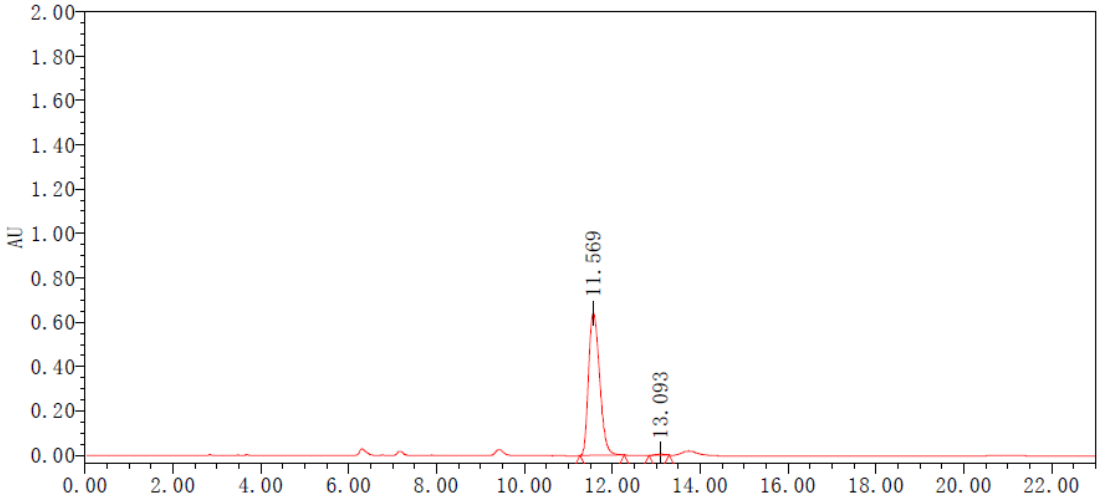
**HPLC chromatogram of chiral 67**

Condition: n-hexane/2-propanol =99:1

Flow rate =1.0 mL/min

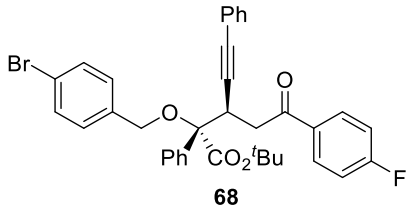
λ= 254 nm

Chiral IA-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 11.569 | 11115192 | 642444 | 99.27 |
| 2 | 13.093 | 82114 | 5594 | 0.73 |

**Tert-butyl (2S,3R)-2-((4-bromobenzyl)oxy)-3-(2-(4-fluorophenyl)-2-oxoethyl)-2,5-diphenylpent-4-ynoate (68)**




**68**

Colorless oil; 60.1 mg, 64% yield, >20:1 d.r., 99% *ee*, $[\alpha]_D^{20}$ = -14.39 (c = 0.1, $CH_2Cl_2$); $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.89 – 7.83 (m, 2H), 7.70 – 7.66 (m, 2H), 7.50 – 7.46 (m, 2H), 7.37 (dd, *J* = 7.8, 5.3 Hz, 4H), 7.32 (d, *J* = 7.1 Hz, 1H), 7.25 (d, *J* = 4.0 Hz, 1H), 7.24 (s, 4H), 7.10 – 7.04 (m, 2H), 5.04 (d, *J* = 11.7 Hz, 1H), 4.89 (d, *J* = 11.7 Hz,

1H), 4.38 (dd, *J* = 10.1, 3.2 Hz, 1H), 3.26 (dd, *J* = 16.5, 10.1 Hz, 1H), 3.13 – 3.00 (m, 1H), 1.51 (s, 9H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 195.9, 169.4, 165.8 (d, *J* = 254.8 Hz), 138.2 (d, *J* = 22.7 Hz), 133.3 (d, *J* = 2.8 Hz), 131.4 (d, *J* = 4.5 Hz), 130.9, 130.8, 129.2, 128.3, 128.2, 128.0, 126.7, 123.3, 121.3, 115.8, 115.5, 89.5, 85.9, 84.2, 83.0, 68.0, 39.1, 36.7, 28.1. Peak overlapping was observed. $^{19}$F NMR (376 MHz, $CDCl_3$) δ -105.15. HRMS (ESI) $[M+Na]^+$ calcd for $C_{36}H_{32}O_4FBrNa^+$, 649.1360, found 649.1356. (Chiral IE-3, λ= 254 nm, *n*-hexane/2-propanol= 19/1, Flow rate = 1.0 mL/min), $t_R$ = 10.750 min(major), 16.307 min.

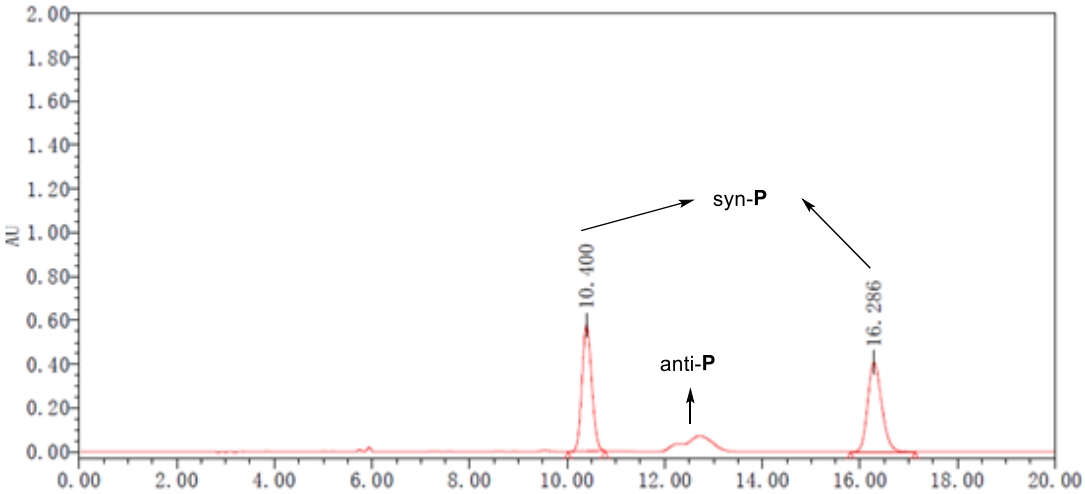
**HPLC chromatogram of racemic 68**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 10.400 | 8098660 | 577025 | 49.91 |
| 2 | 16.286 | 8129458 | 408821 | 50.09 |

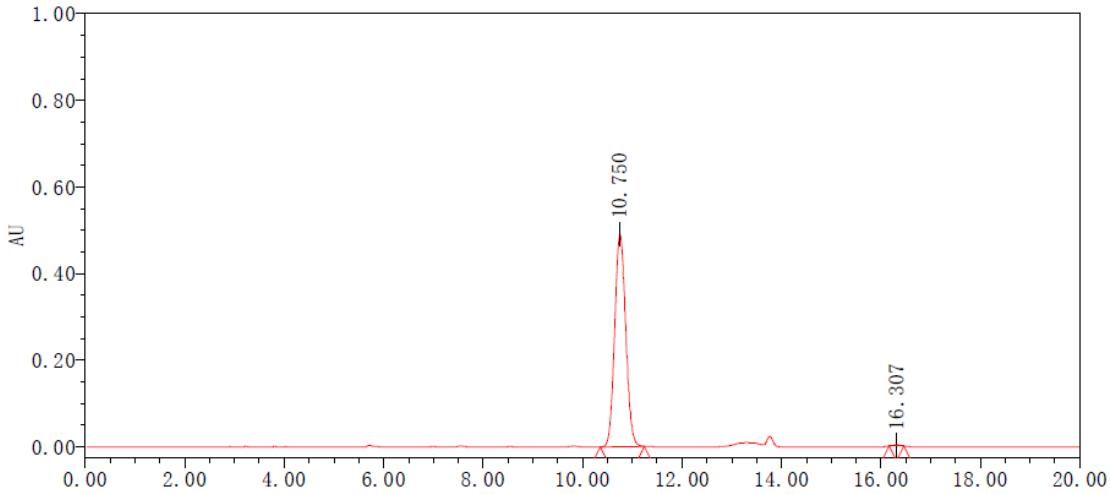
**HPLC chromatogram of chiral 68**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

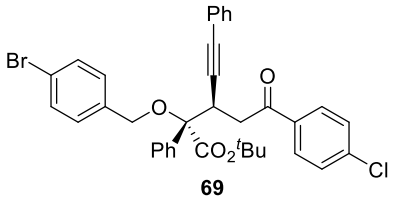
λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 10.750 | 7559970 | 489917 | 99.66 |
| 2 | 16.307 | 25774 | 2317 | 0.34 |

**Tert-butyl (2S,3R)-2-((4-bromobenzyl)oxy)-3-(2-(4-chlorophenyl)-2-oxoethyl)-2,5-diphenylpent-4-ynoate (69)**




**69**

Colorless oil; 65.5 mg, 68% yield, >20:1 d.r., >99% *ee*; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.78 – 7.74 (m, 2H), 7.70 – 7.65 (m, 2H), 7.48 (d, *J* = 8.4 Hz, 2H), 7.38 (d, *J* = 1.4 Hz, 3H), 7.36 (d, *J* = 1.1 Hz, 2H), 7.33 (dd, *J* = 6.5, 1.8 Hz, 1H), 7.25 (d, *J* = 5.6 Hz, 6H),

5.03 (d, *J* = 11.7 Hz, 1H), 4.88 (d, *J* = 11.7 Hz, 1H), 4.37 (dd, *J* = 10.0, 3.3 Hz, 1H), 3.25 (dd, *J* = 16.5, 10.0 Hz, 1H), 3.08 (dd, *J* = 16.5, 3.2 Hz, 1H), 1.51 (s, 9H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 197.0, 169.4, 143.9, 138.4, 138.1, 134.5, 131.4, 129.2, 128.3, 128.3, 128.2, 128.2, 127.9, 126.7, 123.4, 121.2, 89.8, 85.9, 84.1, 82.9, 68.0, 39.1, 36.6, 28.1, 21.7. Peak overlapping was observed. HRMS (ESI) $[M+Na]^+$ calcd for $C_{36}H_{32}O_4ClBrNa^+$, 665.1065, found 665.1069. (Chiral IE-3, λ= 254 nm, *n*-hexane/2-propanol= 19/1, Flow rate = 1.0 mL/min), $t_R$ = 7.401 min(major), 10.092 min.

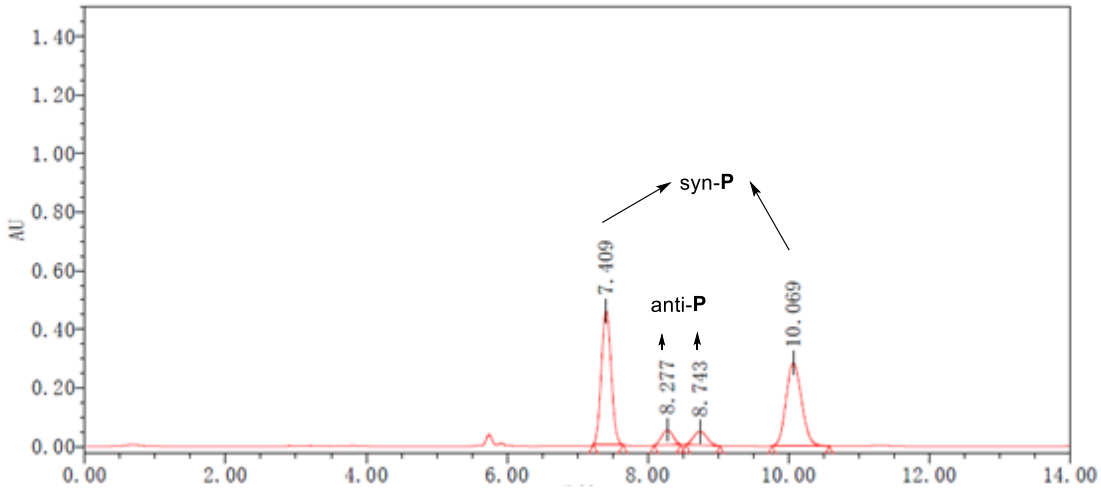
**HPLC chromatogram of racemic 69**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 7.409 | 4374540 | 458002 | 44.26 |
| 2 | 8.277 | 559177 | 50697 | 5.66 |
| 3 | 8.743 | 613385 | 46416 | 6.21 |
| 4 | 10.069 | 4337024 | 283557 | 43.88 |

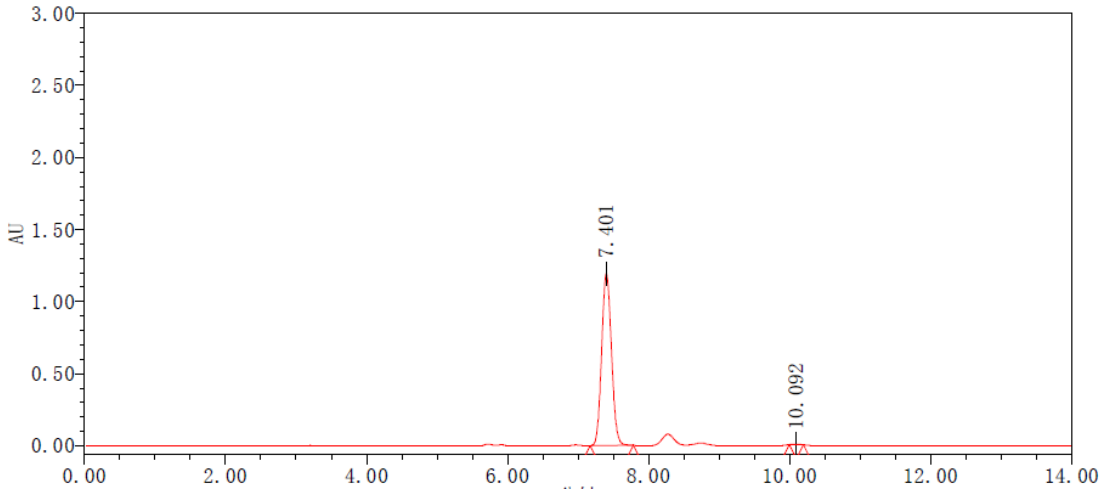
**HPLC chromatogram of chiral 69**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

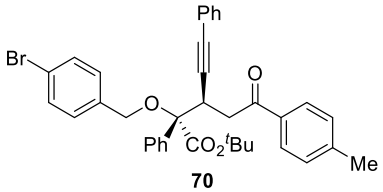
λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 7.401 | 11401645 | 1193220 | 99.73 |
| 2 | 10.092 | 30567 | 3945 | 0.27 |

**Tert-butyl (2S,3R)-2-((4-bromobenzyl)oxy)-3-(2-oxo-2-(p-tolyl)ethyl)-2,5-diphenylpent-4-ynoate (70)**




**70**

Colorless oil; 87.1 mg, 70% yield, >20:1 d.r., 99% *ee*; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 8.2 Hz, 2H), 7.71 – 7.66 (m, 2H), 7.48 (d, *J* = 8.4 Hz, 2H), 7.40 – 7.36 (m,

3H), 7.35 – 7.29 (m, 2H), 7.24 (d, *J* = 8.4 Hz, 5H), 7.20 (d, *J* = 8.0 Hz, 2H), 5.05 (d, *J* = 11.7 Hz, 1H), 4.91 (d, *J* = 11.7 Hz, 1H), 4.41 (dd, *J* = 10.2, 3.0 Hz, 1H), 3.30 (dd, *J* = 16.6, 10.2 Hz, 1H), 3.06 (dd, *J* = 16.5, 3.0 Hz, 1H), 2.38 (s, 3H), 1.51 (s, 9H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 197.0, 169.4, 143.9, 138.4, 138.1, 134.5, 131.4, 129.2, 128.3, 128.3, 128.2, 128.2, 127.9, 126.7, 123.4, 121.2, 89.8, 85.9, 84.1, 82.9, 68.0, 39.1, 36.6, 28.1, 21.7. Peak overlapping was observed. HRMS (ESI) $[M+Na]^+$ calcd for $C_{37}H_{35}O_4BrNa^+$, 645.1611, found 645.1610. (Chiral IE-3, λ= 254 nm, *n*-hexane/2-propanol= 19/1, Flow rate = 1.0 mL/min), $t_R$ = 7.581 min(major), 11.439 min.

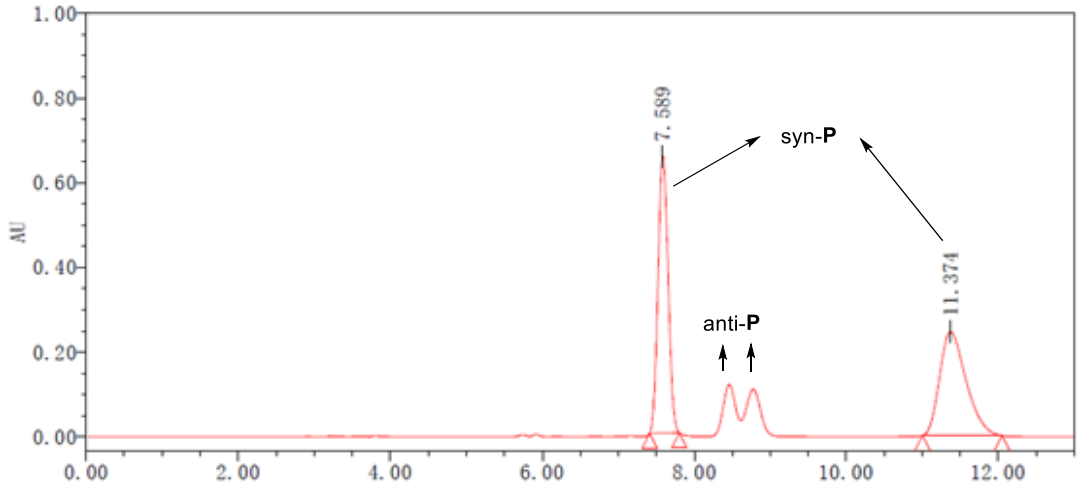
**HPLC chromatogram of racemic 70**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 7.589 | 5946947 | 654224 | 50.04 |
| 2 | 11.374 | 5936607 | 245522 | 49.96 |

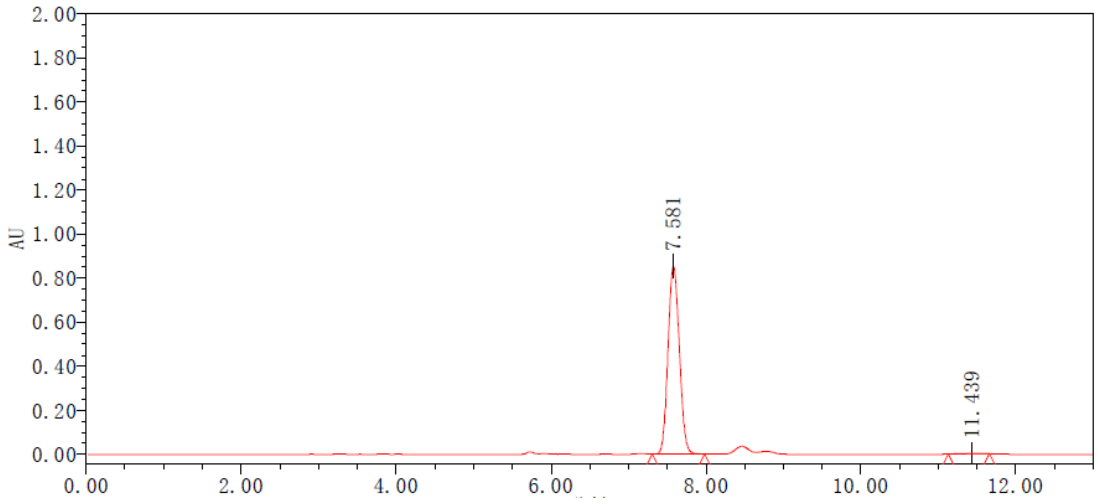
**HPLC chromatogram of chiral 70**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

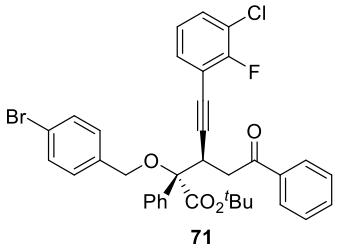
λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 7.581 | 8606054 | 852567 | 99.59 |
| 2 | 11.439 | 35308 | 1514 | 0.41 |

**Tert-butyl (2S,3R)-2-((4-bromobenzyl)oxy)-5-(3-chloro-2-fluorophenyl)-3-(2-oxo-2-phenylethyl)-2-phenylpent-4-ynoate (71)**




71

Colorless oil; 72.2 mg, 73% yield, >20:1 d.r., 99% *ee*, $[\alpha]_D^{20}$ = -12.68 (c = 0.1, $CH_2Cl_2$);

$^1$H NMR (500 MHz, $CDCl_3$) δ 7.86 – 7.81 (m, 2H), 7.68 (d, *J* = 7.5 Hz, 2H), 7.53 (t, *J*

= 7.4 Hz, 1H), 7.49 (d, *J* = 8.3 Hz, 2H), 7.43 – 7.38 (m, 5H), 7.36 (d, *J* = 7.8 Hz, 1H), 7.32 (d, *J* = 7.2 Hz, 1H), 7.30 – 7.26 (m, 1H), 7.16 – 7.12 (m, 1H), 6.95 (t, *J* = 7.9 Hz, 1H), 5.07 (d, *J* = 11.8 Hz, 1H), 4.92 (d, *J* = 11.8 Hz, 1H), 4.46 (dd, *J* = 10.2, 2.8 Hz, 1H), 3.35 (dd, *J* = 16.9, 10.2 Hz, 1H), 3.10 (dd, *J* = 16.9, 2.8 Hz, 1H), 1.50 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 197.1, 169.3, 158.5 (d, *J* = 253.0 Hz), 138.1 (d, *J* = 26.7 Hz), 136.7, 133.2, 131.7, 131.4, 130.3, 129.1, 128.6, 128.4, 128.4, 128.2, 126.6, 124.2, 124.2, 121.4, 121.2 (d, *J* = 3.8 Hz), 113.4, 96.5, 96.4, 85.8, 83.2, 68.1, 39.1, 36.6, 28.0. $^{19}$F NMR (471 MHz, $CDCl_3$) δ -112.4. HRMS (ESI) $[M+Na]^+$ calcd for $C_{36}H_{31}O_4FClBrNa^+$, 683.0970, found 683.0967. (Chiral IA-3, λ= 254 nm, *n*-hexane/2-propanol/EtOH= 98/1/1, Flow rate = 1.0 mL/min), $t_R$ = 9.178 min(major), 10.953 min.

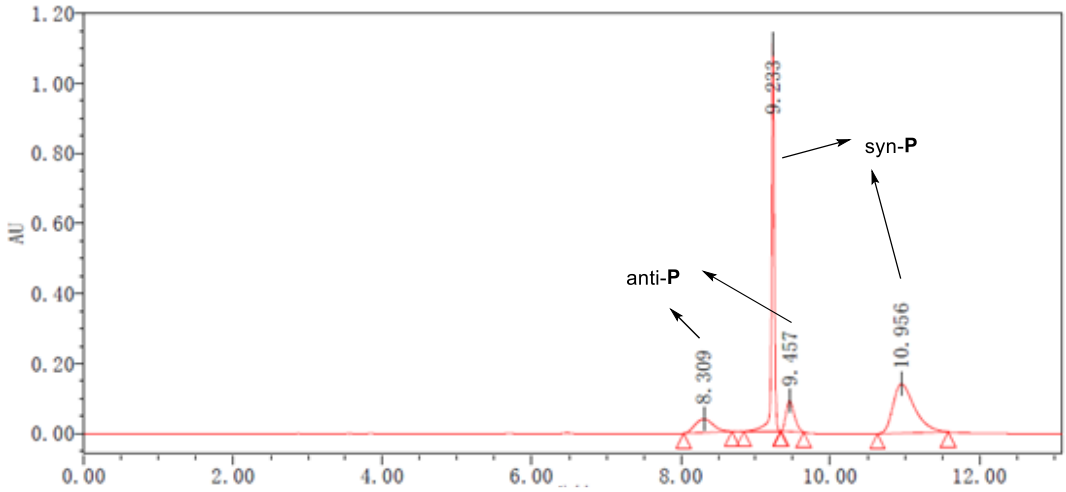
**HPLC chromatogram of racemic 71**

Condition: n-hexane/2-propanol/EtOH = 98:1:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| 1 | 8.309 | 658634 | 38234 | 9.44 |
| 2 | 9.233 | 2810523 | 1109878 | 40.26 |
| 3 | 9.457 | 688344 | 88087 | 9.86 |
| 4 | 10.956 | 2822567 | 139899 | 40.44 |

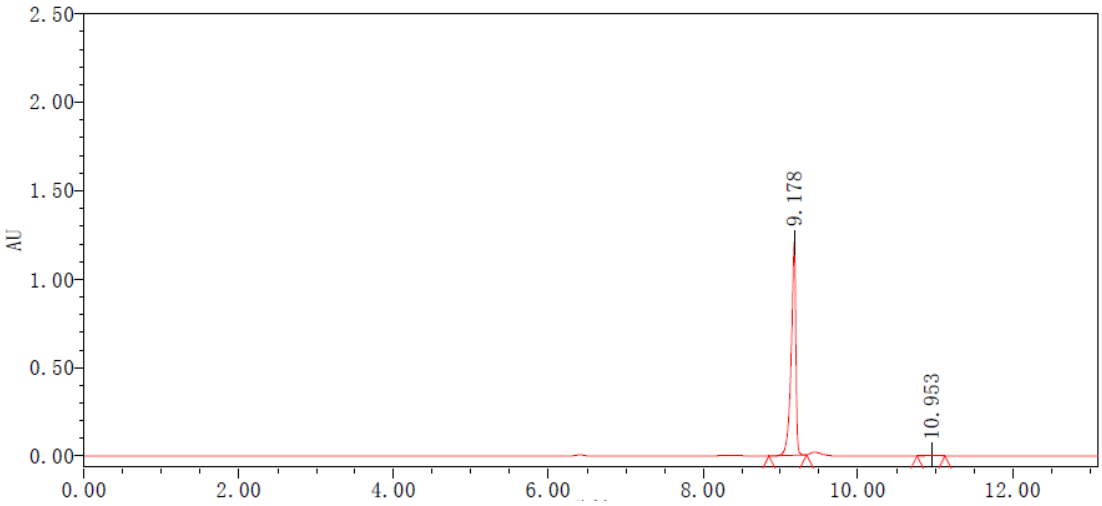
**HPLC chromatogram of chiral 71**

Condition: n-hexane/2-propanol/EtOH = 98:1:1

Flow rate =1.0 mL/min

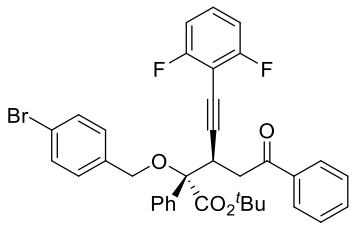
λ= 254 nm

Chiral IA-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 9.178 | 4898082 | 1206046 | 99.53 |
| 2 | 10.953 | 23259 | 1895 | 0.47 |

**Tert-butyl (2S,3R)-2-((4-bromobenzyl)oxy)-5-(2,6-difluorophenyl)-3-(2-oxo-2-phenylethyl)-2-phenylpent-4-ynoate (72)**




**72**

Colorless oil; 52.3 mg, 52% yield, >20:1 d.r., 98% *ee*, $[\alpha]_D^{20}$ = -14.33 (c = 0.1, $CH_2Cl_2$); $^1$H NMR (400 MHz, $CDCl_3$) δ 7.85 – 7.79 (m, 2H), 7.72 – 7.66 (m, 2H), 7.53 (d, *J* = 7.4 Hz, 1H), 7.51 – 7.47 (m, 2H), 7.41 (d, *J* = 8.7 Hz, 3H), 7.39 – 7.34 (m, 2H), 7.31 (d, *J* = 7.1 Hz, 1H), 7.26 (s, 1H), 7.19 (tt, *J* = 8.4, 6.3 Hz, 1H), 6.87 – 6.79 (m, 1H), 5.11 (d, *J* = 11.9 Hz, 1H), 4.98 (d, *J* = 11.8 Hz, 1H), 4.52 (dd, *J* = 10.1, 3.0 Hz, 1H), 3.36 (dd, *J* = 17.0, 10.1 Hz, 1H), 3.07 (dd, *J* = 17.0, 3.0 Hz, 1H), 1.49 (s, 9H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 197.1, 169.2, 138.2 (d, *J* = 22.7 Hz), 136.8, 133.1, 131.4, 129.28, 129.1, 128.5, 128.4, 128.3, 128.2, 128.2, 126.5, 121.2, 111.2 (d, *J* = 5.7 Hz), 111.2 (d, *J* = 5.7 Hz), 100.0, 85.7, 83.2, 68.2, 39.1, 36.5, 27.9. $^{19}$F NMR (376 MHz, $CDCl_3$) δ -107.72. HRMS (ESI) $[M+Na]^+$ calcd for $C_{36}H_{31}O_4F_2BrNa^+$, 667.1266, found 667.1269. (Chiral IA-3, λ= 254 nm, *n*-hexane/2-propanol/EtOH= 197/1/2, Flow rate = 1.0 mL/min), $t_R$ = 12.593 min(major), 14.042 min.

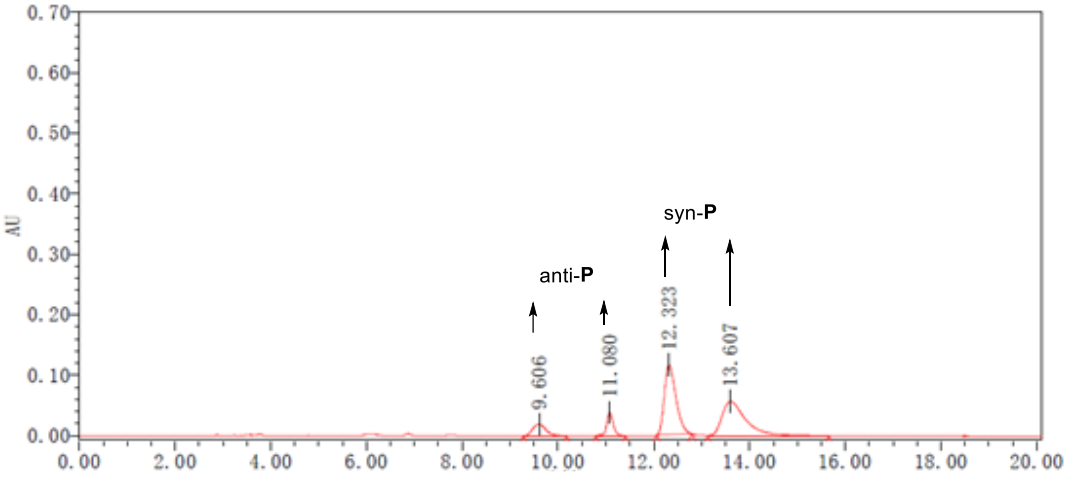
**HPLC chromatogram of racemic 72**

Condition: n-hexane/2-propanol/EtOH =197:1:2

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 9.606 | 367764 | 19093 | 7.96 |
| 2 | 11.080 | 367126 | 38276 | 7.94 |
| 3 | 12.323 | 1949814 | 115556 | 42.18 |
| 4 | 13.607 | 1937580 | 56523 | 41.92 |

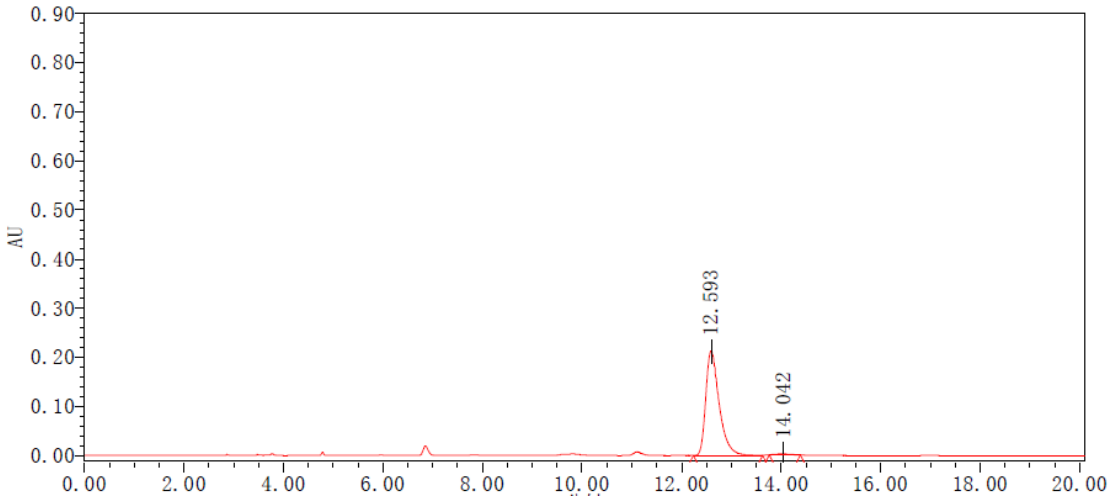
**HPLC chromatogram of chiral 72**

Condition: n-hexane/2-propanol/EtOH =197:1:2

Flow rate =1.0 mL/min

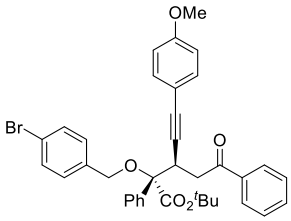
λ= 254 nm

Chiral IA-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 12.593 | 3997058 | 212561 | 99.02 |
| 2 | 14.042 | 39426 | 1713 | 0.98 |

**Tert-butyl (2S,3R)-2-((4-bromobenzyl)oxy)-5-(4-methoxyphenyl)-3-(2-oxo-2-phenylethyl)-2-phenylpent-4-ynoate (73)**




73

Colorless oil; 53.6 mg, 56% yield, >20:1 d.r., >99% *ee*; $^{1}$H NMR (500 MHz, $CDCl_3$) δ 7.83 (d, *J* = 7.4 Hz, 2H), 7.69 (d, *J* = 7.8 Hz, 2H), 7.52 (t, *J* = 7.1 Hz, 1H), 7.48 (d, *J* = 7.2 Hz, 2H), 7.37 (dd, *J* = 16.0, 8.1 Hz, 7H), 7.17 (d, *J* = 7.7 Hz, 2H), 6.76 (d, *J* = 7.7 Hz, 2H), 5.06 (d, *J* = 11.8 Hz, 1H), 4.91 (d, *J* = 11.8 Hz, 1H), 4.39 (d, *J* = 9.8 Hz, 1H), 3.76 (s, 3H), 3.31 (dd, *J* = 16.4, 10.2 Hz, 1H), 3.06 (d, *J* = 16.4 Hz, 1H), 1.51 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 197.5, 169.5, 159.3, 138.4, 138.1, 137.0, 133.1, 132.7, 131.4, 129.2, 128.5, 128.3, 128.2, 126.7, 126.7, 121.2, 115.6, 113.8, 88.1, 85.9, 840, 82.9, 68.0, 55.3, 39.3, 36.6, 28.1. HRMS (ESI) $[M+Na]^+$ calcd for $C_{37}H_{35}O_5BrNa^+$,

661.1560, found 661.1558. (Chiral IA, λ= 254 nm, *n*-hexane/2-propanol= 19/1, Flow rate = 1.0 mL/min), $t_R$ = 10.250 min(major), 19.466 min.

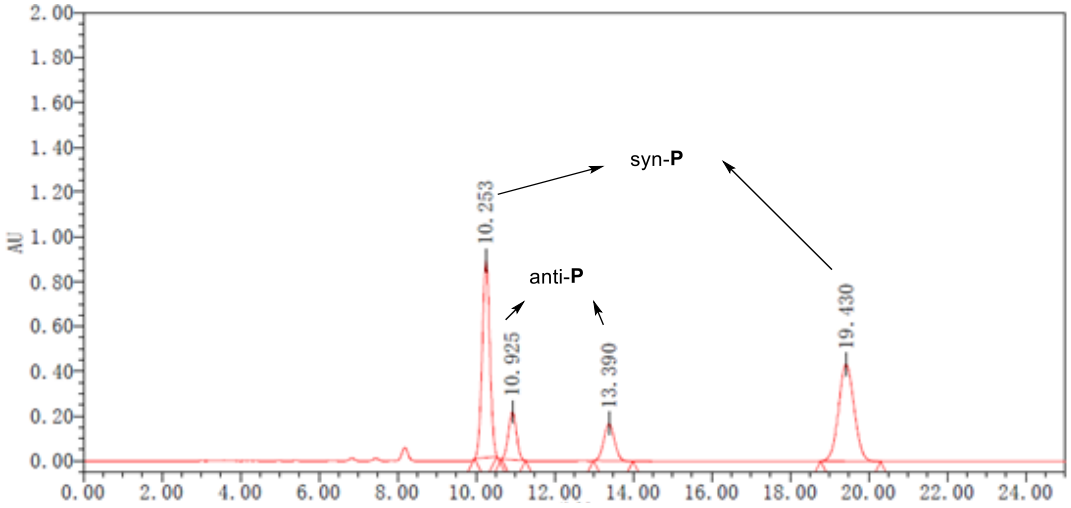
**HPLC chromatogram of racemic 73**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 10.253 | 12066968 | 880501 | 39.96 |
| 2 | 10.925 | 3086483 | 213067 | 10.22 |
| 3 | 13.390 | 3125223 | 165652 | 10.35 |
| 4 | 19.430 | 11917599 | 433062 | 39.47 |

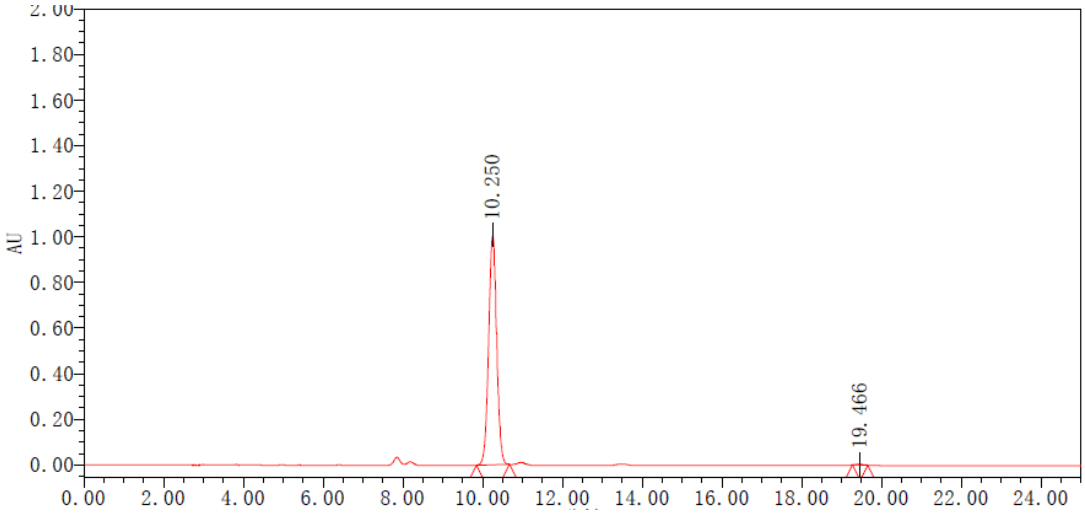
**HPLC chromatogram of chiral 73**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

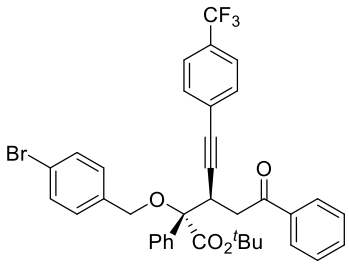
λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 10.250 | 14322650 | 1007259 | 99.76 |
| 2 | 19.466 | 34586 | 2328 | 0.24 |

**Tert-butyl (2S,3R)-2-((4-bromobenzyl)oxy)-3-(2-oxo-2-phenylethyl)-2-phenyl-5-(4-(trifluoromethyl)phenyl)pent-4-ynoate (74)**




**74**

Colorless oil; 65.0 mg, 62% yield, >20:1 d.r., 99% *ee*; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.88 – 7.84 (m, 2H), 7.68 – 7.64 (m, 2H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.50 – 7.45 (m, 4H), 7.43 (d, *J* = 7.8 Hz, 2H), 7.39 (d, *J* = 7.1 Hz, 2H), 7.36 (t, *J* = 2.5 Hz, 2H), 7.33 (d, *J* = 2.3 Hz, 1H), 7.30 (d, *J* = 8.3 Hz, 2H), 4.99 (d, *J* = 11.7 Hz, 1H), 4.80 (d, *J* = 11.6 Hz, 1H), 4.41 (dd, *J* = 10.1, 3.1 Hz, 1H), 3.33 (dd, *J* = 16.7, 10.1 Hz, 1H), 3.18 (dd, *J* = 16.7, 3.1 Hz, 1H), 1.52 (s, 9H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 197.2, 169.3, 137.9 (d,

*J* = 14.8 Hz), 136.8, 133.3, 131.6, 131.4, 129.1, 128.6, 128.6, 128.5, 128.4, 128.4, 128.2, 127.21 (d, *J* = 11.6 Hz), 126.8, 125.2 (q, *J* = 3.7 Hz), 121.3, 92.5, 85.9, 83.1, 67.9, 39.1, 36.9, 28.1. $^{19}$F NMR (376 MHz, $CDCl_3$) δ -62.80. HRMS (ESI) $[M+Na]^+$ calcd for $C_{37}H_{32}O_4F_3BrNa^+$, 699.1328, found 699.1328. (Chiral IA, λ= 254 nm, *n*-hexane/2-propanol= 19/1, Flow rate = 1.0 mL/min), $t_R$ = 6.894 min (major), 11.067 min.

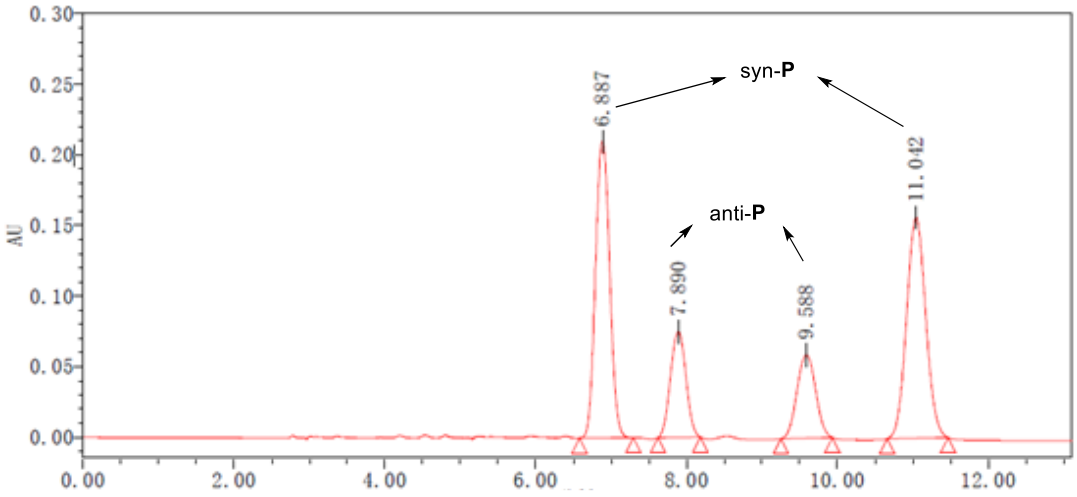
**HPLC chromatogram of racemic 74**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 6.887 | 2774985 | 210225 | 36.38 |
| 2 | 7.890 | 1075225 | 75013 | 14.10 |
| 3 | 9.588 | 1014480 | 59184 | 13.30 |
| 4 | 11.042 | 2763395 | 156333 | 36.23 |

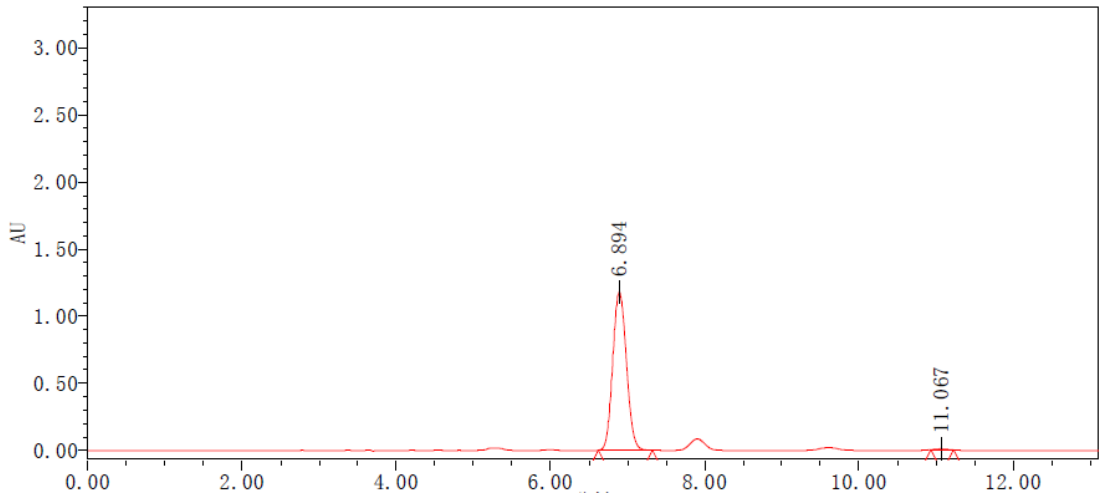
**HPLC chromatogram of chiral 74**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

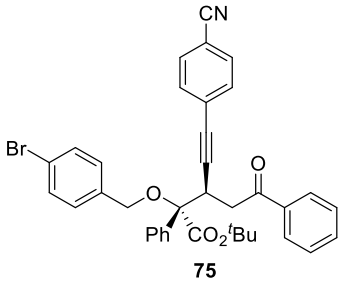
λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 6.894 | 14644587 | 1176627 | 99.49 |
| 2 | 11.067 | 74337 | 6962 | 0.51 |

**Tert-butyl (2S,3R)-2-((4-bromobenzyl)oxy)-5-(4-cyanophenyl)-3-(2-oxo-2-phenylethyl)-2-phenylpent-4-ynoate (75)**




**75**

Colorless oil; 46.7 mg, 49% yield, >20:1 d.r., 99% *ee*; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.88 – 7.83 (m, 2H), 7.64 (d, *J* = 7.1 Hz, 2H), 7.57 – 7.53 (m, 1H), 7.52 – 7.47 (m, 3H), 7.45 (d, *J* = 4.2 Hz, 2H), 7.42 (d, *J* = 7.7 Hz, 2H), 7.38 (d, *J* = 7.7 Hz, 2H), 7.32 (d, *J* =

8.3 Hz, 2H), 7.26 (d, *J* = 7.6 Hz, 2H), 4.95 (d, *J* = 11.6 Hz, 1H), 4.74 (d, *J* = 11.6 Hz, 1H), 4.40 (dd, *J* = 9.8, 3.3 Hz, 1H), 3.32 (dd, *J* = 16.7, 9.9 Hz, 1H), 3.23 (dd, *J* = 16.7, 3.3 Hz, 1H), 1.52 (s, 9H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 197.0, 169.3, 137.8, 137.7, 136.7, 133.3, 131.9, 131.9, 131.4, 129.1, 128.6, 128.5, 128.4, 128.3, 128.2, 126.8, 121.4, 118.5, 111.3, 94.7, 85.9, 83.2, 82.6, 67.9, 39.1, 37.1, 28.1. HRMS (ESI) $[M+Na]^+$ calcd for $C_{37}H_{32}NO_4BrNa^+$, 656.1407, found 656.1411. (Chiral IA-3, λ= 254 nm, *n*-hexane/2-propanol= 19/1, Flow rate = 1.0 mL/min), $t_R$ = 13.971 min(major), 27.226 min.

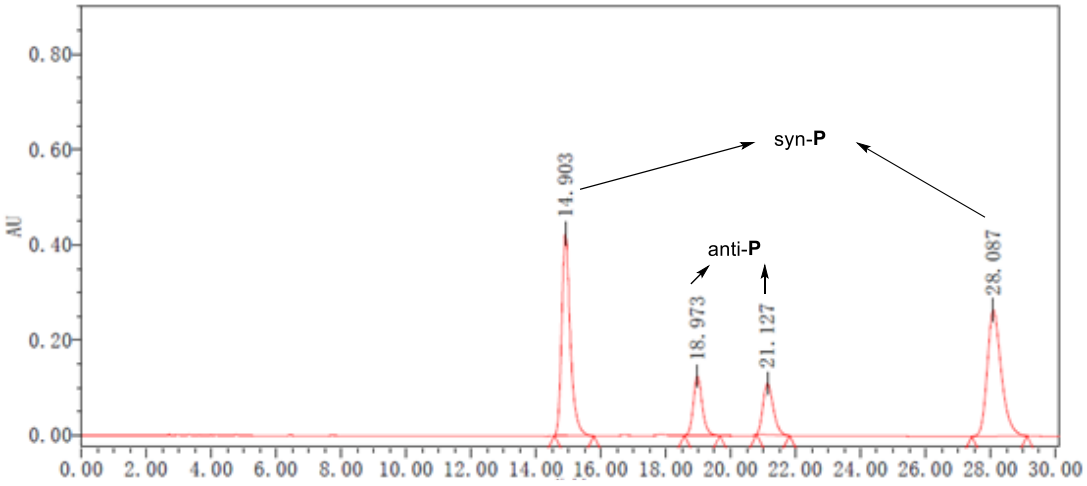
**HPLC chromatogram of racemic 75**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 14.903 | 7931507 | 424450 | 38.32 |
| 2 | 18.973 | 2414402 | 124514 | 11.67 |
| 3 | 21.127 | 2348469 | 107737 | 11.35 |
| 4 | 28.087 | 8001633 | 264366 | 38.66 |

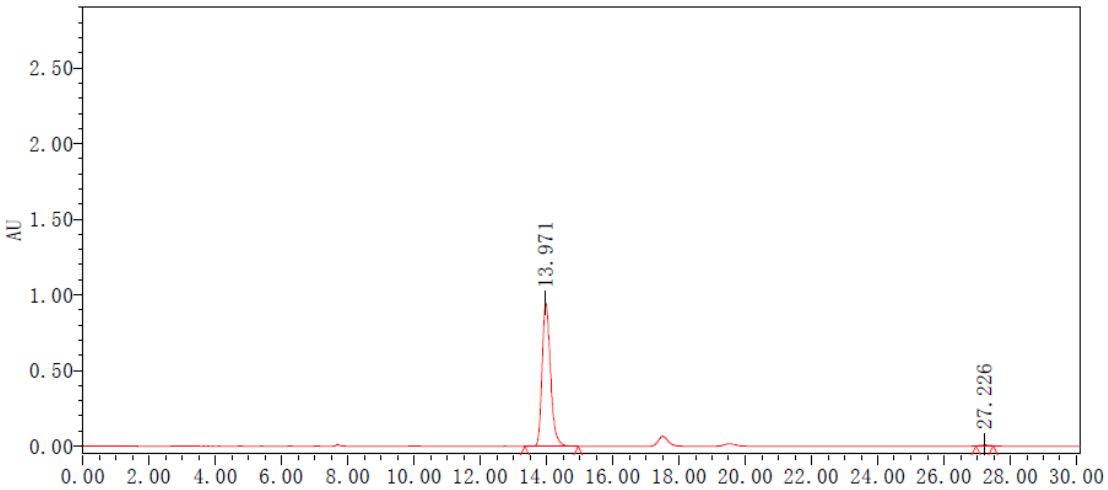
**HPLC chromatogram of chiral 75**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

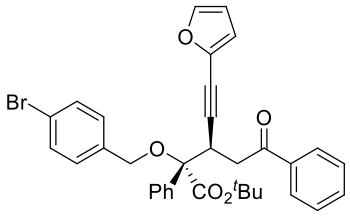
λ= 254 nm

Chiral IA-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 13.971 | 16765775 | 944933 | 99.48 |
| 2 | 27.226 | 87866 | 4621 | 0.52 |

**Tert-butyl (2S,3R)-2-((4-bromobenzyl)oxy)-5-(furan-2-yl)-3-(2-oxo-2-phenylethyl)-2-phenylpent-4-ynoate (76)**




**76**

Colorless oil; 39.6 mg, 47% yield, >20:1 d.r., 97% *ee*; $^{1}$H NMR (500 MHz, $CDCl_3$) δ

7.82 (d, *J* = 7.4 Hz, 2H), 7.66 (d, *J* = 7.5 Hz, 2H), 7.52 (t, *J* = 7.4 Hz, 1H), 7.48 (d, *J* = 8.3 Hz, 2H), 7.42 – 7.39 (m, 3H), 7.38 (t, *J* = 3.6 Hz, 1H), 7.35 (d, *J* = 7.8 Hz, 2H), 7.31 (d, *J* = 7.2 Hz, 1H), 7.29 (d, *J* = 1.2 Hz, 1H), 6.39 (d, *J* = 3.3 Hz, 1H), 6.31 (dd, *J* = 3.2, 1.9 Hz, 1H), 5.00 (d, *J* = 11.7 Hz, 1H), 4.86 (d, *J* = 11.7 Hz, 1H), 4.45 (dd, *J* = 10.0, 2.9 Hz, 1H), 3.31 (dd, *J* = 17.1, 10.1 Hz, 1H), 3.10 (dd, *J* = 17.1, 2.8 Hz, 1H), 1.53 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 196.9, 169.2, 143.1, 138.1, 138.0, 137.1, 136.7, 133.2, 131.4, 129.3, 128.6, 128.4, 128.3, 128.2, 126.6, 121.3, 114.4, 110.7, 94.0, 85.7, 83.2, 74.5, 68.0, 39.0, 36.4, 28.0. HRMS (ESI) $[M+Na]^+$ calcd for $C_{34}H_{31}O_5BrNa^+$, 621.1247, found 621.1247. (Chiral IE-3, λ= 254 nm, *n*-hexane/2-propanol= 19/1, Flow rate = 1.0 mL/min), $t_R$ = 11.605 min(major), 27.521 min.

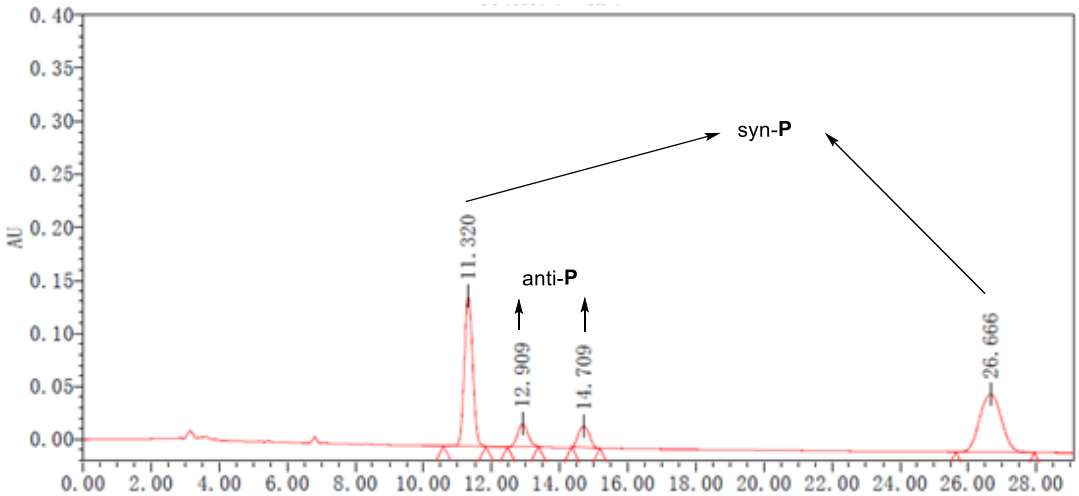
**HPLC chromatogram of racemic 76**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 11.320 | 2444372 | 141407 | 42.33 |

| | | | | |
|---|---|---|---|---|
| 2 | 12.909 | 459230 | 21538 | 7.95 |
| 3 | 14.709 | 449122 | 19961 | 7.78 |
| 4 | 26.666 | 2421323 | 54570 | 41.93 |

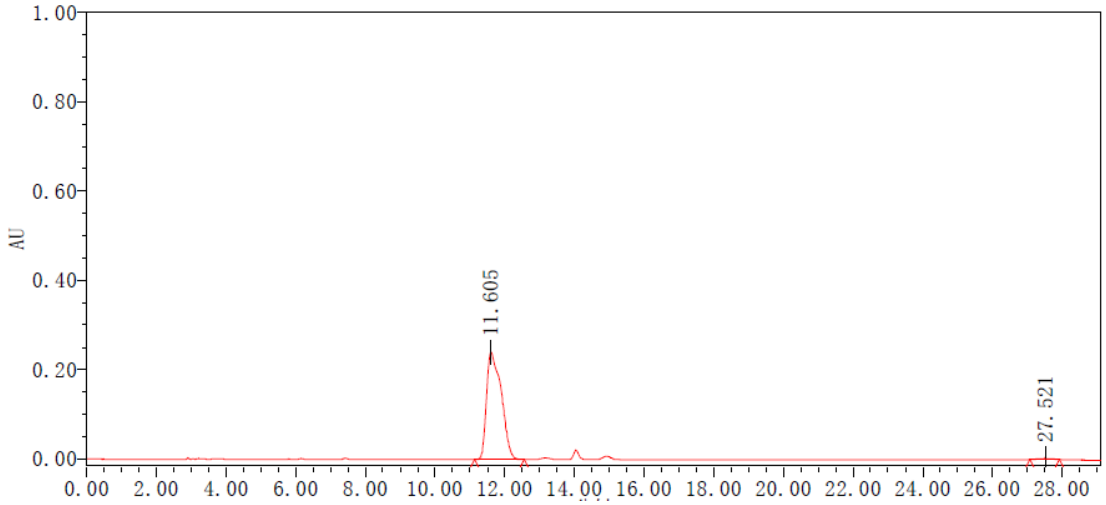
**HPLC chromatogram of chiral 76**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

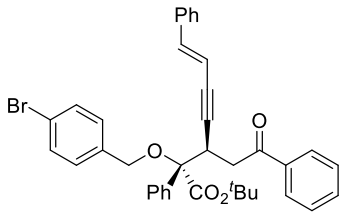
λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 11.605 | 6999862 | 240744 | 99.06 |
| 2 | 27.521 | 66662 | 2155 | 0.94 |

**Tert-butyl (2S,3R,E)-2-((4-bromobenzyl)oxy)-3-(2-oxo-2-phenylethyl)-2,7-diphenylhept-6-en-4-ynoate (77)**




**46**

Colorless oil; 50.4 mg, 53% yield, >20:1 d.r., 96% *ee*; $^{1}$H NMR (500 MHz, $CDCl_3$) δ 7.86 – 7.82 (m, 2H), 7.67 (d, *J* = 7.5 Hz, 2H), 7.53 (t, *J* = 7.4 Hz, 1H), 7.49 (d, *J* = 8.4 Hz, 2H), 7.43 – 7.34 (m, 6H), 7.34 – 7.27 (m, 5H), 7.26 – 7.24 (m, 1H), 6.71 (d, *J* = 16.2 Hz, 1H), 6.07 (dd, *J* = 16.2, 2.0 Hz, 1H), 5.01 (d, *J* = 11.7 Hz, 1H), 4.87 (d, *J* = 11.7 Hz, 1H), 4.44 – 4.32 (m, 1H), 3.28 (dd, *J* = 16.8, 10.3 Hz, 1H), 3.08 (dd, *J* = 16.8, 2.9 Hz, 1H), 1.53 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 197.4, 169.4, 140.7, 138.3, 138.1, 136.8, 136.3, 133.2, 131.4, 129.2, 128.7, 128.6, 128.5, 128.3, 128.3, 128.2, 126.7, 126.1, 121.3, 108.3, 91.9, 85.9, 83.4, 83.0, 67.9, 39.2, 36.7, 28.1. HRMS (ESI) $[M+Na]^+$ calcd for $C_{38}H_{35}O_4BrNa^+$, 657.1611, found 657.1612. (Chiral IE-3, λ= 254 nm, *n*-hexane/2-propanol= 19/1, Flow rate = 1.0 mL/min), $t_R$ = 15.071 min(major), 21.541 min.

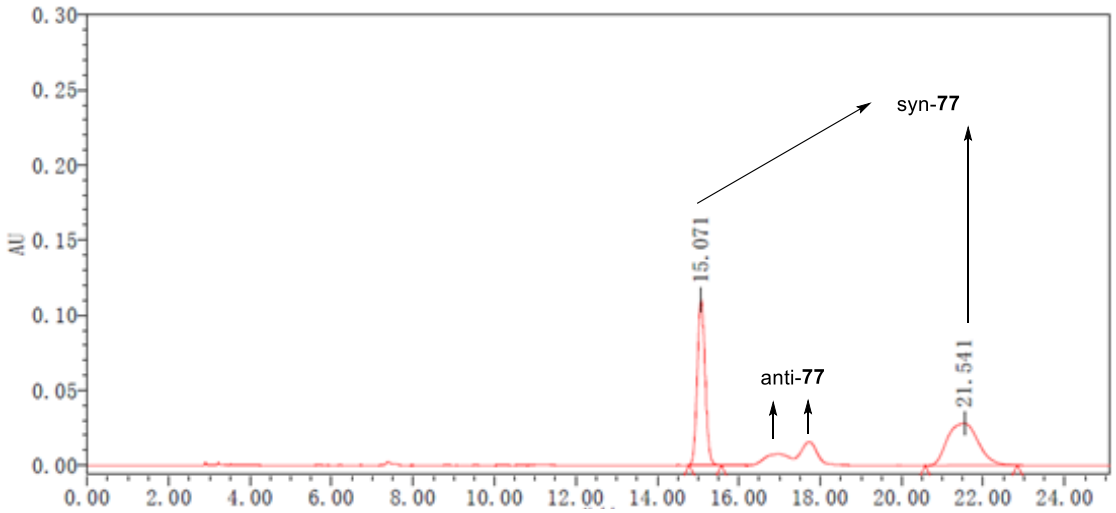
**HPLC chromatogram of racemic 77**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 15.071 | 1489715 | 110158 | 50.18 |
| 2 | 21.541 | 1478921 | 28046 | 49.82 |

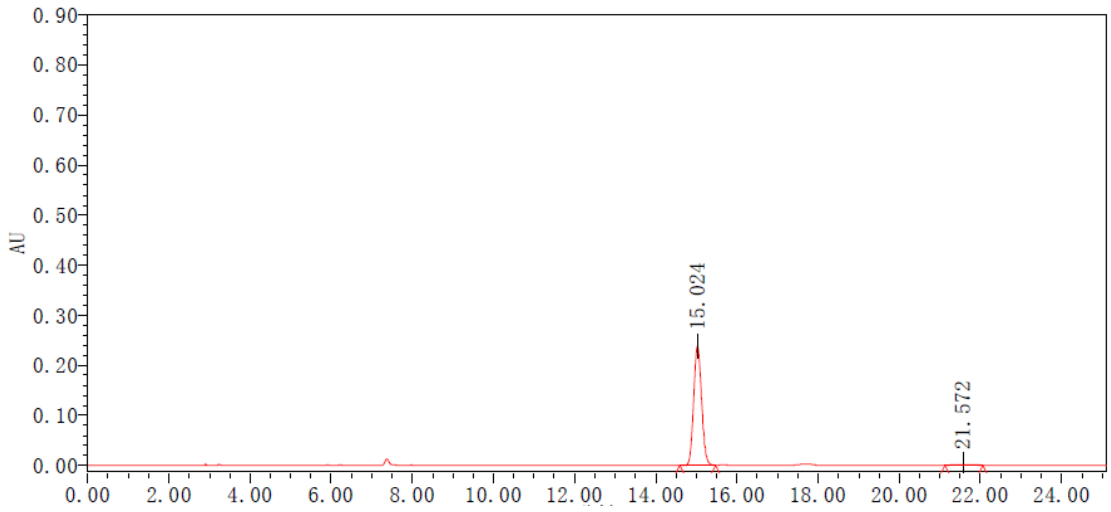
**HPLC chromatogram of chiral 77**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

λ= 254 nm

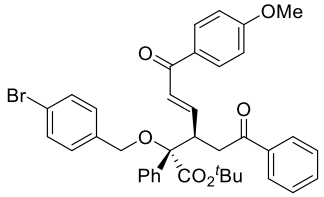
Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| 1 | 15.024 | 3211828 | 238201 | 98.98 |
| 2 | 21.572 | 33087 | 901 | 1.02 |

**Tert-butyl (2S,3R,E)-2-((4-bromobenzyl)oxy)-6-(4-methoxyphenyl)-6-oxo-3-(2-oxo-2-phenylethyl)-2-phenylhex-4-enoate (78)**



78

Colorless oil; 55.1 mg, 55% yield, >20:1 d.r., 90% *ee*; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 7.2 Hz, 2H), 7.71 (d, *J* = 8.9 Hz, 2H), 7.57 (t, *J* = 7.0 Hz, 3H), 7.47 – 7.41 (m, 5H), 7.36 (dd, *J* = 14.5, 7.4 Hz, 2H), 7.22 (d, *J* = 8.3 Hz, 2H), 6.94 (dd, *J* = 15.5, 8.4 Hz, 1H), 6.87 (d, *J* = 8.9 Hz, 2H), 6.70 (d, *J* = 15.6 Hz, 1H), 4.73 (d, *J* = 11.8 Hz, 1H), 4.30 (d, *J* = 11.8 Hz, 1H), 4.09 – 3.99 (m, 1H), 3.87 (s, 3H), 3.57 (dd, *J* = 16.7, 2.7 Hz, 1H), 3.15 (dd, *J* = 16.7, 9.6 Hz, 1H), 1.57 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 197.9, 188.8, 169.8, 163.2, 145.6, 137.8, 137.3, 136.9, 133.2, 131.3, 130.9, 130.6, 128.9, 128.6, 128.5, 128.3, 128.1, 127.7, 121.1, 113.6, 87.1, 83.4, 67.4, 55.5, 48.2, 38.7, 29.7, 28.2. HRMS (ESI) $[M+Na]^+$ calcd for $C_{38}H_{36}O_6BrNa^+$, 691.1666, found 691.1662. (Chiral IA, λ= 254 nm, *n*-hexane/2-propanol= 9/1, Flow rate = 1.0 mL/min), $t_R$ = 20.334 min(major), 24.716 min.

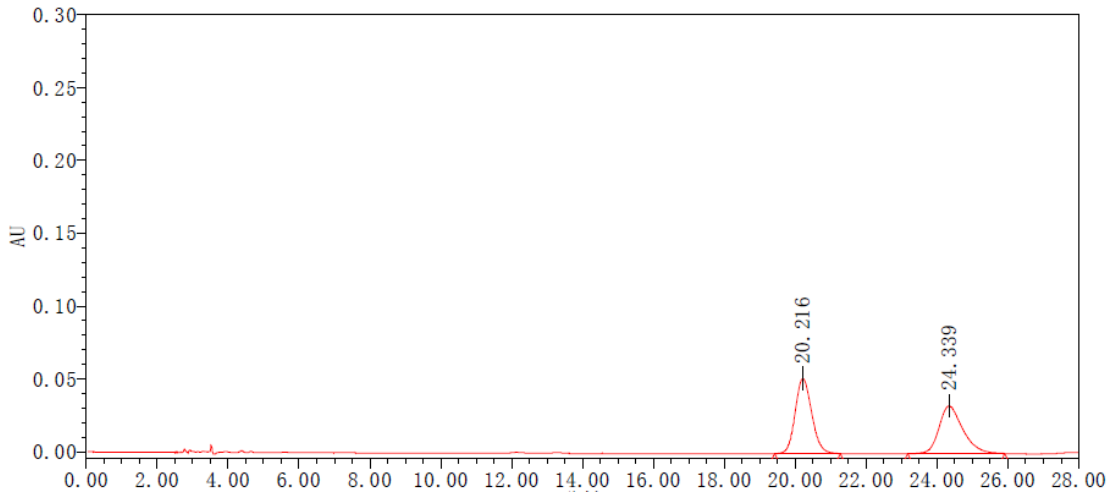
**HPLC chromatogram of racemic 78**

Condition: n-hexane/2-propanol =9:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 20.216 | 1602120 | 51569 | 50.40 |
| 2 | 24.339 | 1592157 | 32701 | 49.60 |

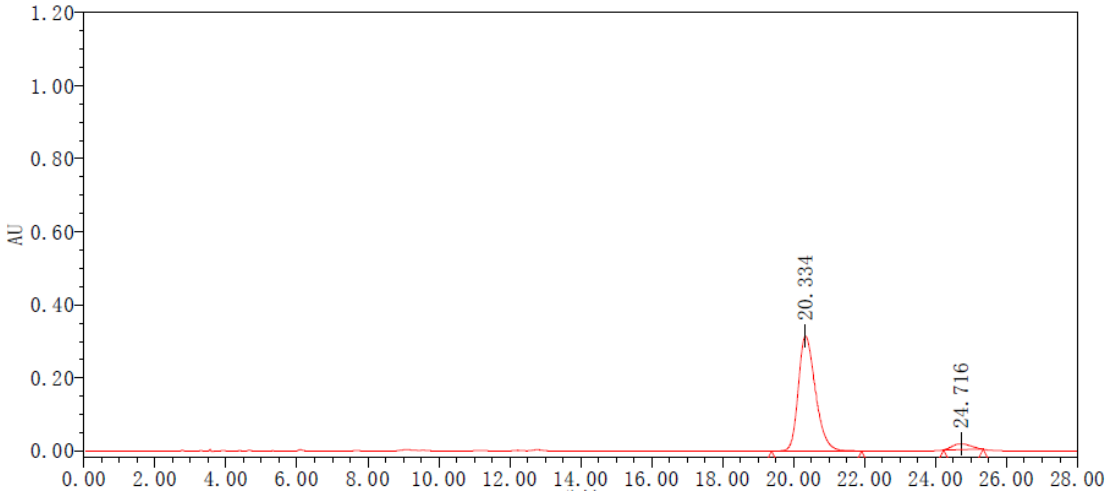
**HPLC chromatogram of chiral 78**

Condition: n-hexane/2-propanol =9:1

Flow rate =1.0 mL/min

λ= 254 nm

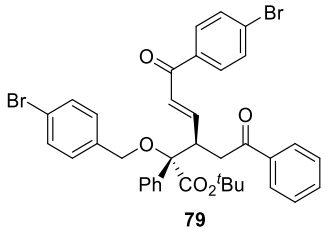
Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| 1 | 20.334 | 10474346 | 314667 | 94.83 |
| 2 | 24.716 | 570770 | 15766 | 5.17 |

**Tert-butyl (2S,3R,E)-2-((4-bromobenzyl)oxy)-6-(4-bromophenyl)-6-oxo-3-(2-oxo-2-phenylethyl)-2-phenylhex-4-enoate (79)**



79

Colorless oil; 46.2 mg, 43% yield, >20:1 d.r., 82% *ee*; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 7.4 Hz, 1H), 7.66 (d, *J* = 8.5 Hz, 1H), 7.58 – 7.48 (m, 5H), 7.45 – 7.34 (m, 5H), 7.18 (d, *J* = 8.3 Hz, 1H), 6.92 (dd, *J* = 15.6, 8.4 Hz, 1H), 6.57 (d, *J* = 15.6 Hz, 1H), 4.70 (d, *J* = 11.8 Hz, 1H), 4.25 (d, *J* = 11.8 Hz, 1H), 3.99 (t, *J* = 8.1 Hz, 1H), 3.59 (dd, *J* = 16.7, 2.6 Hz, 1H), 3.12 (dd, *J* = 16.7, 9.7 Hz, 1H), 1.55 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 197.7, 189.7, 180.0, 169.7, 165.4, 147.4, 145.2, 137.7, 136.4, 133.3, 131.7, 131.4, 130.1, 128.9, 128.7, 128.6, 128.2, 128.1, 127.7, 122.4, 121.1, 87.1, 83.5, 67.5, 48.5, 38.6, 28.2. HRMS (ESI) $[M+Na]^+$ calcd for $C_{37}H_{35}O_5Br_2Na^+$, 739.0665, found 739.0660. (Chiral IC, λ= 254 nm, *n*-hexane/2-propanol= 9/1, Flow rate = 1.0 mL/min), $t_R$ = 15.663 min(major), 16.958 min.

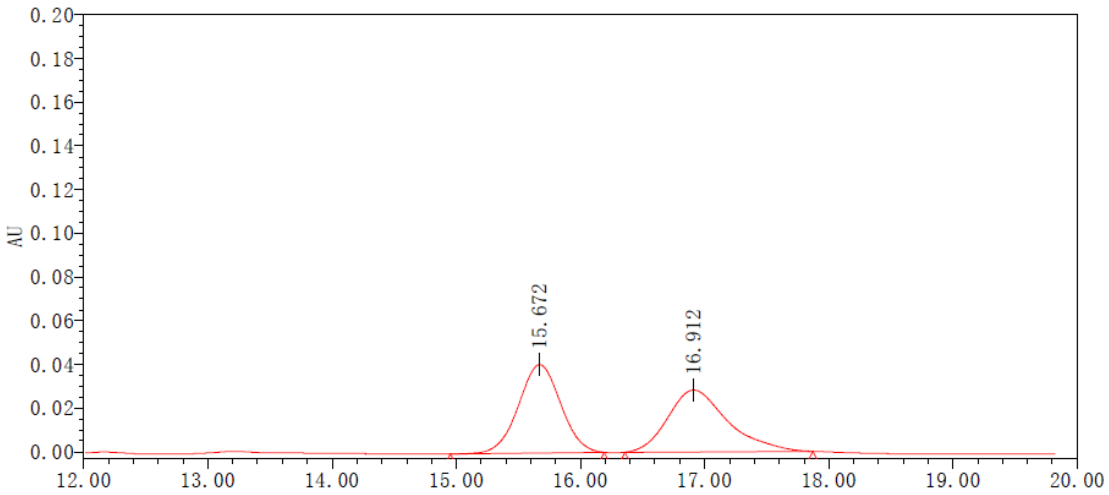
**HPLC chromatogram of racemic 79**

Condition: n-hexane/2-propanol =9:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IC




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 15.672 | 953526 | 40431 | 50.22 |
| 2 | 16.912 | 945207 | 28267 | 49.78 |

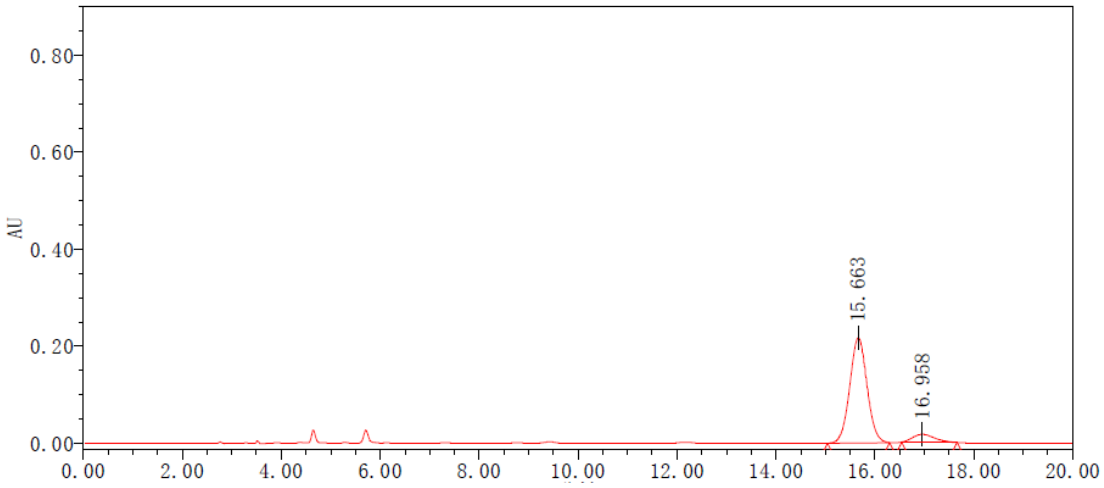
**HPLC chromatogram of chiral 79**

Condition: n-hexane/2-propanol =9:1

Flow rate =1.0 mL/min

λ= 254 nm

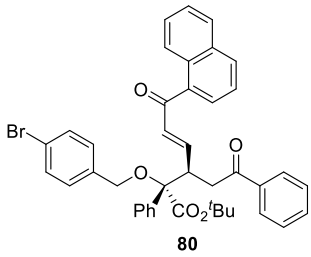
Chiral IC




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| 1 | 15.663 | 5262189 | 216676 | 91.12 |
| 2 | 16.958 | 512656 | 16602 | 8.88 |

**Tert-butyl (2S,3R,E)-2-((4-bromobenzyl)oxy)-6-(naphthalen-1-yl)-6-oxo-3-(2-oxo-2-phenylethyl)-2-phenylhex-4-enoate (80)**




**80**

Colorless oil; 43.3 mg, 42% yield, >20:1 d.r., 87% *ee*; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.11 (s, 1H), 7.90 (d, *J* = 7.2 Hz, 2H), 7.87 – 7.78 (m, 4H), 7.55 (p, *J* = 6.9 Hz, 6H), 7.41 (dd, *J* = 7.2, 5.0 Hz, 4H), 7.36 (d, *J* = 7.1 Hz, 1H), 7.20 (d, *J* = 8.3 Hz, 2H), 7.00 (dd, *J* = 15.6, 8.4 Hz, 2H), 6.79 (d, *J* = 15.6 Hz, 1H), 4.73 (d, *J* = 11.9 Hz, 1H), 4.29 (d, *J* = 11.8 Hz, 1H), 4.10 – 4.03 (m, 1H), 3.60 (dd, *J* = 16.7, 2.7 Hz, 1H), 3.16 (dd, *J* = 16.7, 9.6 Hz, 1H), 1.55 (s, 9H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 197.8, 190.5, 169.8, 146.7, 137.8, 137.3, 136.9, 135.4, 135.0, 133.2, 132.4, 131.3, 130.7, 130.2, 129.5, 128.9, 128.7, 128.6, 128.6, 128.3, 128.3, 128.2, 127.9, 127.8, 126.6, 124.5, 121.1, 87.2, 83.5, 67.5, 48.4, 38.7, 29.7, 28.2. HRMS (ESI) $[M+Na]^+$ calcd for $C_{41}H_{37}O_5Na^+$, 711.1717, found 711.1716. (Chiral IA, λ= 254 nm, *n*-hexane/2-propanol= 9/1, Flow rate = 1.0 mL/min), $t_R$ = 17.147 min(major), 27.484 min.

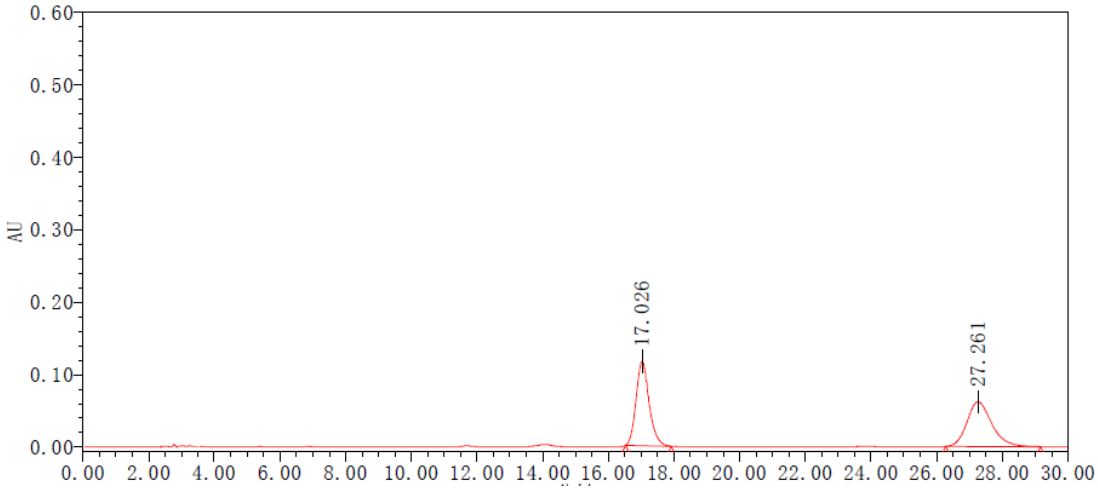
**HPLC chromatogram of racemic 80**

Condition: n-hexane/2-propanol =9:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 17.026 | 3239325 | 116348 | 49.98 |
| 2 | 27.261 | 3242134 | 61685 | 50.02 |

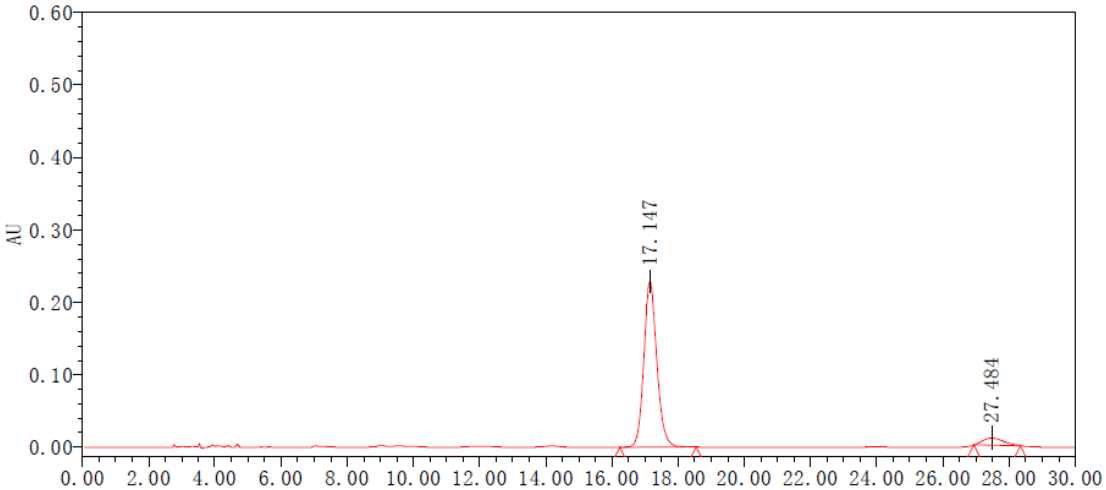
**HPLC chromatogram of chiral 80**

Condition: n-hexane/2-propanol =9:1

Flow rate =1.0 mL/min

λ= 254 nm

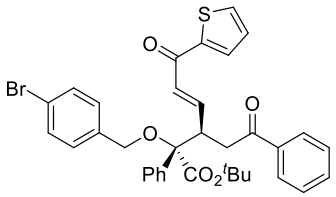
Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| 1 | 17.147 | 6289544 | 228806 | 93.51 |
| 2 | 27.484 | 436666 | 9969 | 6.49 |

**Tert-butyl (2S,3R,E)-2-((4-bromobenzyl)oxy)-6-oxo-3-(2-oxo-2-phenylethyl)-2-phenyl-6-(thiophen-2-yl)hex-4-enoate (81)**




81

Colorless oil; 48.3 mg, 50% yield, >20:1 d.r., 80% *ee*; $^{1}$H NMR (500 MHz, $CDCl_3$) δ 7.87 (d, *J* = 7.8 Hz, 2H), 7.60 – 7.56 (m, 1H), 7.54 (dd, *J* = 13.6, 7.4 Hz, 3H), 7.48 (d, *J* = 3.6 Hz, 1H), 7.44 – 7.36 (m, 6H), 7.33 (d, *J* = 7.0 Hz, 1H), 7.19 (d, *J* = 7.8 Hz, 2H), 7.06 (t, *J* = 3.9 Hz, 1H), 7.02 (dd, *J* = 15.5, 8.3 Hz, 1H), 6.60 (d, *J* = 15.4 Hz, 1H), 4.71 (d, *J* = 11.8 Hz, 1H), 4.28 (d, *J* = 11.8 Hz, 1H), 4.02 (t, *J* = 8.6 Hz, 1H), 3.56 (d, *J* = 16.5 Hz, 1H), 3.13 (dd, *J* = 16.7, 9.6 Hz, 1H), 1.56 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 197.8, 182.0, 169.7, 146.1, 145.0, 137.8, 137.2, 136.8, 133.8, 133.2, 132.1, 131.3, 128.9, 128.6, 128.6, 128.5, 128.1, 128.1, 127.8, 127.7, 121.1, 87.1, 83.5, 67.5, 48.0, 38.7, 28.2. HRMS (ESI) $[M+Na]^+$ calcd for $C_{35}H_{33}O_5SBrNa^+$, 667.1124, found 667.1128. (Chiral IC, λ= 254 nm, *n*-hexane/2-propanol= 9/1, Flow rate = 1.0 mL/min), $t_R$ = 18.306 min, 23.095 min (major).

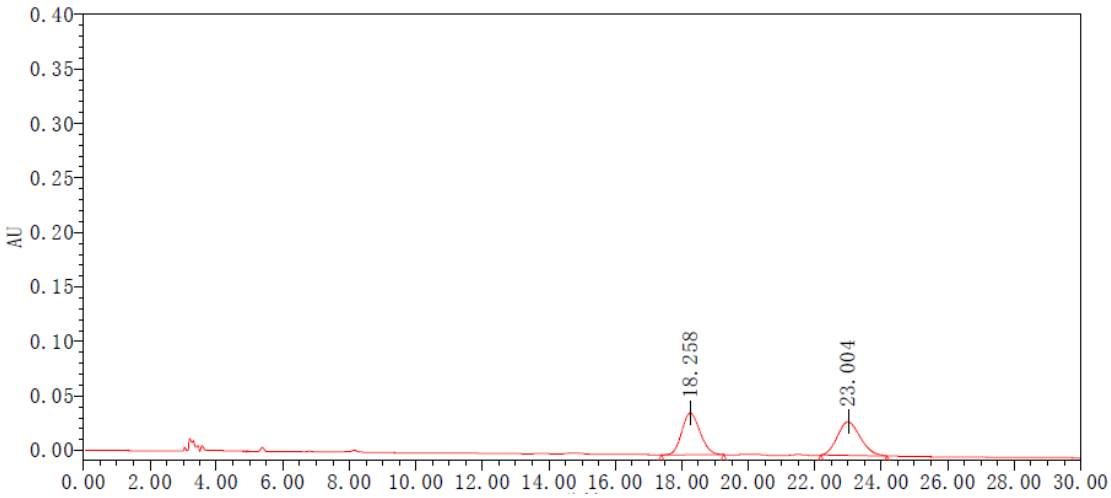
**HPLC chromatogram of racemic 81**

Condition: n-hexane/2-propanol =9:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IC




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 18.258 | 1464581 | 38159 | 49.79 |
| 2 | 23.004 | 1477072 | 30848 | 50.21 |

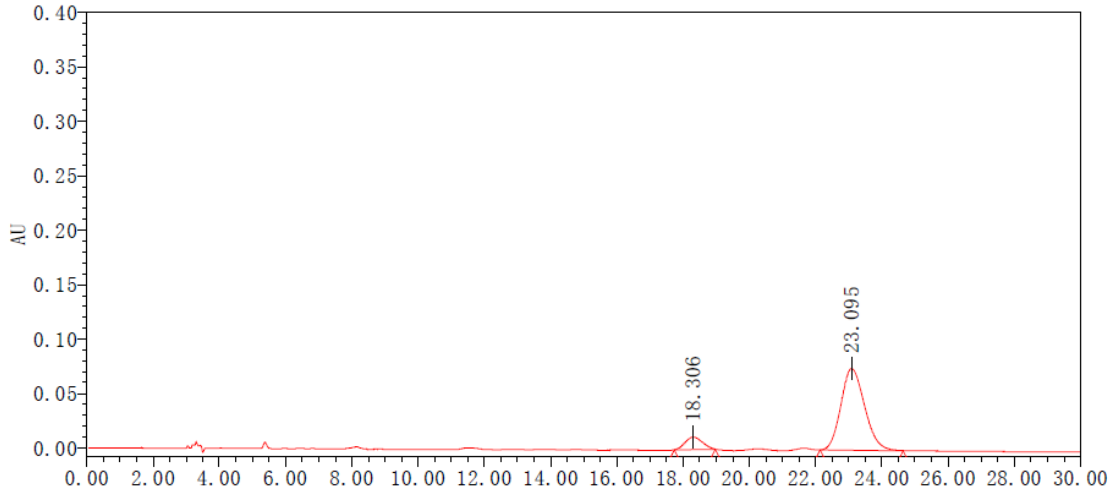
**HPLC chromatogram of chiral 81**

Condition: n-hexane/2-propanol =9:1

Flow rate =1.0 mL/min

λ= 254 nm

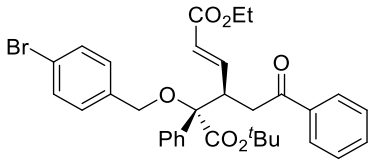
Chiral IC




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| 1 | 18.306 | 406258 | 11289 | 9.82 |
| 2 | 23.095 | 3730119 | 75142 | 90.18 |

**6-(tert-butyl) 1-ethyl (4R,5S,E)-5-((4-bromobenzyl)oxy)-4-(2-oxo-2-phenylethyl)-5-phenylhex-2-enedioate (82)**




**82**

Colorless oil; 45.5 mg, 50% yield, >20:1 d.r., 87% *ee*; $^{1}$H NMR (500 MHz, $CDCl_3$) δ 7.86 (d, *J* = 7.3 Hz, 2H), 7.54 (d, *J* = 7.5 Hz, 1H), 7.49 (d, *J* = 7.3 Hz, 2H), 7.43 – 7.40 (m, 4H), 7.35 (dd, *J* = 16.3, 7.4 Hz, 3H), 7.18 (d, *J* = 8.3 Hz, 2H), 6.94 (dd, *J* = 15.8, 8.0 Hz, 1H), 5.66 (d, *J* = 15.8 Hz, 1H), 4.68 (d, *J* = 11.8 Hz, 1H), 4.23 (d, *J* = 11.8 Hz, 1H), 4.08 (q, *J* = 7.2 Hz, 2H), 3.94 (d, *J* = 8.8 Hz, 1H), 3.51 (dd, *J* = 17.0, 2.6 Hz, 1H), 3.06 (dd, *J* = 17.0, 9.5 Hz, 1H), 1.56 (s, 9H), 1.20 (t, *J* = 7.1 Hz, 3H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 197.5, 169.7, 166.2, 146.7, 137.8, 137.1, 136.7, 133.2, 131.3, 128.9, 128.6, 128.5, 128.4, 128.1, 127.6, 123.5, 121.1, 86.9, 83.4, 67.3, 60.2, 38.4, 28.2, 14.2. HRMS (ESI) $[M+Na]^+$ calcd for $C_{33}H_{35}O_6BrNa^+$, 629.1509, found 629.1507. (Chiral IA-3, λ= 254 nm, *n*-hexane/2-propanol= 19/1, Flow rate = 1.0 mL/min), $t_R$ = 11.584 min(major), 15.677 min.

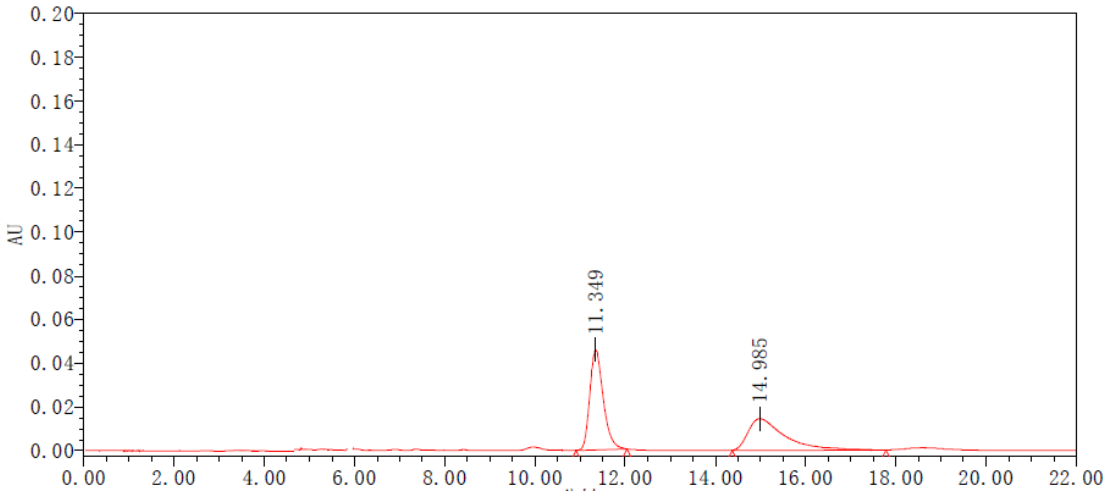
**HPLC chromatogram of racemic 82**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 11.349 | 883243 | 45701 | 50.08 |
| 2 | 14.985 | 882743 | 14418 | 49.92 |

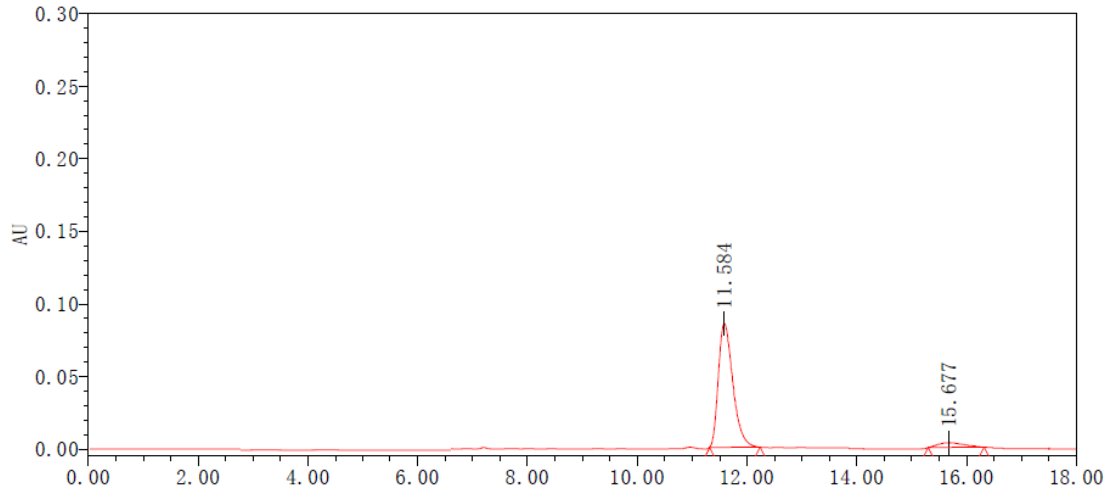
**HPLC chromatogram of chiral 82**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

λ= 254 nm

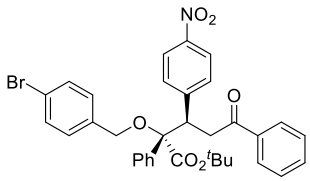
Chiral IA-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| 1 | 11.584 | 1565221 | 85549 | 93.50 |
| 2 | 15.677 | 108861 | 3232 | 6.50 |

**Tert-butyl (2*R*,3*S*)-2-((4-bromobenzyl)oxy)-3-(4-nitrophenyl)-5-oxo-2,5-diphenylpentanoate (83)**




**83**

Colorless oil; 57.6 mg, 61% yield, >20:1 d.r., 90% *ee*, $[\alpha]_D^{20}$ = -12.45 (c = 0.1, $CH_2Cl_2$); $^1$H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 8.8 Hz, 2H), 7.71 (d, *J* = 7.3 Hz, 2H), 7.55 – 7.47 (m, 5H), 7.42 (d, *J* = 8.7 Hz, 2H), 7.39 – 7.33 (m, 5H), 7.26 (d, *J* = 7.4 Hz, 2H), 4.86 (d, *J* = 12.4 Hz, 1H), 4.51 (d, *J* = 12.4 Hz, 1H), 4.27 (dd, *J* = 10.0, 3.7 Hz, 1H), 3.53 (qd, *J* = 17.2, 6.9 Hz, 2H), 1.37 (s, 9H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 197.4, 169.5, 147.8, 146.8, 137.9, 136.6, 136.4, 133.2, 131.6, 131.4, 128.6, 128.5, 128.5, 128.4, 127.9, 127.8, 122.6, 121.3, 87.9, 83.5, 67.7, 51.3, 39.6, 28.0. HRMS (ESI) $[M+Na]^+$ calcd for $C_{34}H_{32}NO_6BrNa^+$, 652.1305, found 652.1303. HPLC (Chiral IA, λ= 254 nm, *n*-hexane/2-propanol= 9/1, Flow rate = 1.0 mL/min), $t_R$ = 12.087 min (major), 10.037 min.

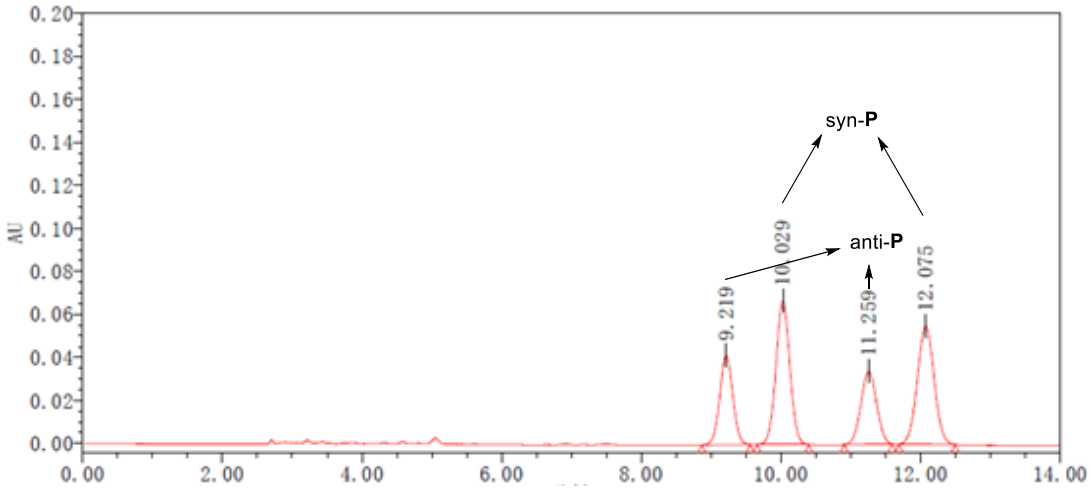
**HPLC chromatogram of racemic 83**

Condition: n-hexane/2-propanol =9:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 9.219 | 541702 | 41400 | 18.58 |
| 2 | 10.029 | 926669 | 66778 | 31.79 |
| 3 | 11.259 | 527070 | 33905 | 18.08 |
| 4 | 12.075 | 919516 | 54869 | 31.54 |

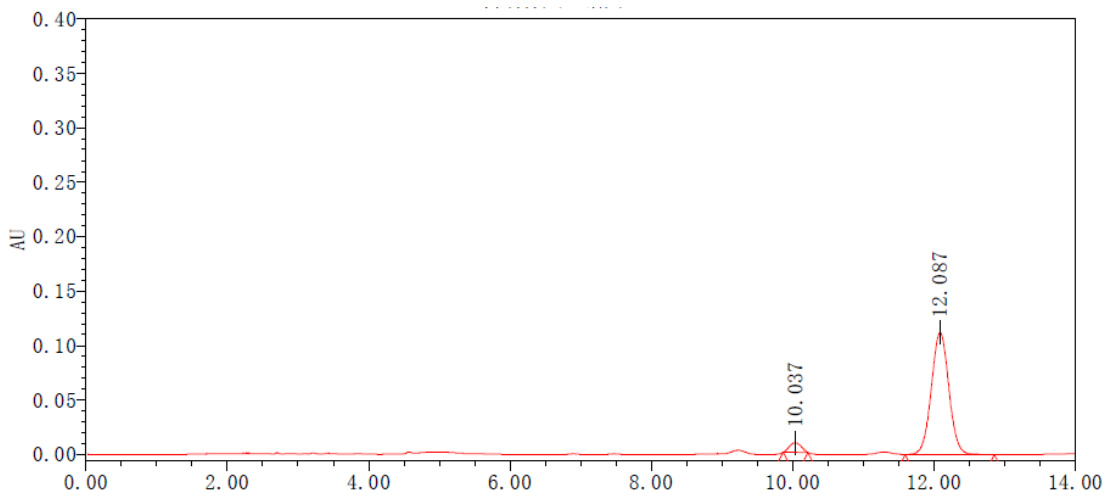
**HPLC chromatogram of chiral 83**

Condition: n-hexane/2-propanol =9:1

Flow rate =1.0 mL/min

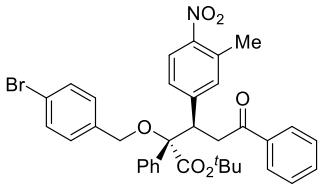
λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 10.037 | 102657 | 8926 | 5.06 |
| 2 | 12.087 | 1924279 | 112089 | 94.94 |

**Tert-butyl (2S,3R)-2-((4-bromobenzyl)oxy)-3-(3-methyl-4-nitrophenyl)-5-oxo-2,5-diphenylpentanoate (84)**




**84**

Colorless oil; 52.1 mg, 54% yield, >20:1 d.r., 90% *ee*, $[\alpha]_D^{20}$ = -13.78 (c = 0.1, $CH_2Cl_2$); $^1$H NMR (500 MHz, $CDCl_3$) δ 7.81 (d, *J* = 8.3 Hz, 1H), 7.73 (d, *J* = 7.5 Hz, 2H), 7.51 (t, *J* = 6.2 Hz, 5H), 7.41 – 7.36 (m, 3H), 7.35 (d, *J* = 1.3 Hz, 2H), 7.27 – 7.25 (m, 2H), 7.21 (d, *J* = 10.1 Hz, 2H), 4.83 (d, *J* = 12.4 Hz, 1H), 4.52 (d, *J* = 12.4 Hz, 1H), 4.20 (dd, *J* = 10.0, 3.4 Hz, 1H), 3.54 (dd, *J* = 17.2, 10.1 Hz, 1H), 3.47 (dd, *J* = 17.2, 3.5 Hz, 1H), 2.49 (s, 3H), 1.37 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 197.5, 169.5, 147.7, 145.8, 137.9, 136.7, 136.5, 135.2, 133.2, 132.7, 131.6, 128.7, 128.6, 128.6, 128.4, 128.3, 127.9, 127.9, 123.9, 121.2, 87.9, 83.3, 67.6, 51.0, 39.4, 28.0, 20.7. HRMS (ESI) $[M+Na]^+$ calcd for $C_{35}H_{34}NO_6BrNa^+$, 666.1462, found 666.1459. HPLC (Chiral IA, λ= 254 nm,

*n*-hexane/2-propanol= 19/1, Flow rate = 1.0 mL/min), $t_R$ = 9.344 min, 11.525 min(major).

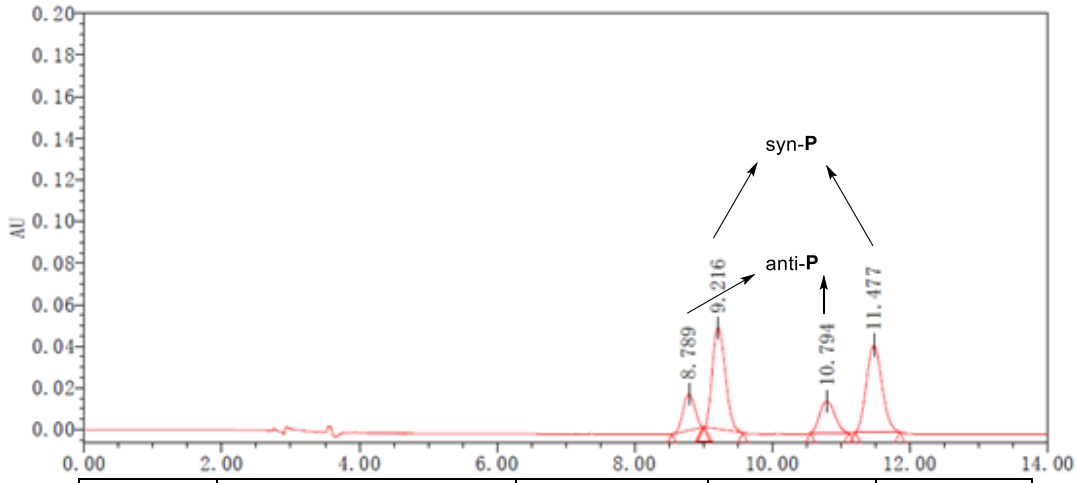
**HPLC chromatogram of racemic 84**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 8.789 | 208251 | 17259 | 11.94 |
| 2 | 9.216 | 644543 | 48750 | 36.95 |
| 3 | 10.794 | 230009 | 15158 | 13.19 |
| 4 | 11.477 | 661659 | 41630 | 37.93 |

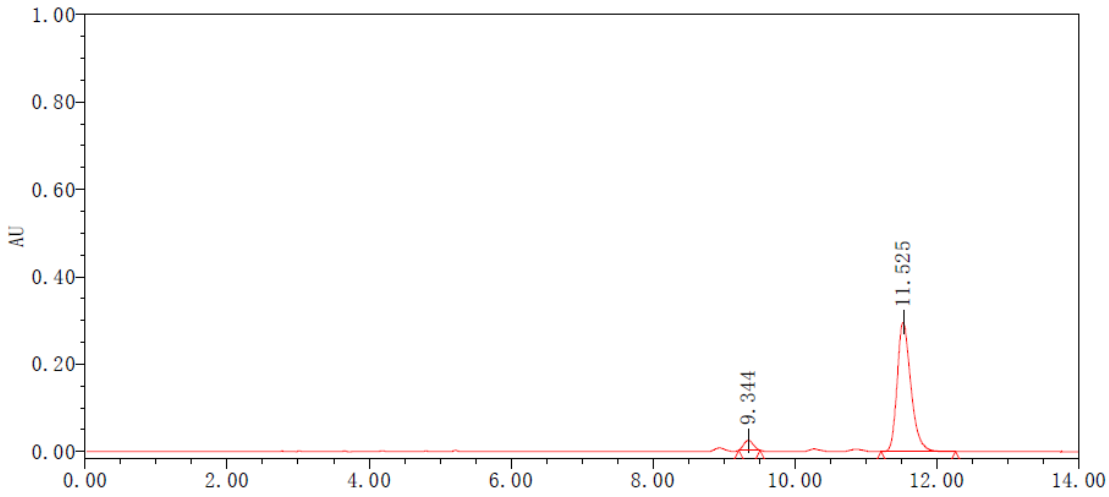
**HPLC chromatogram of chiral 84**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

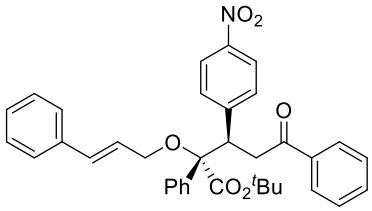
λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 9.344 | 206914 | 22766 | 4.94 |
| 2 | 11.525 | 3978778 | 295461 | 95.06 |

**Tert-butyl (2S,3R)-2-(cinnamyloxy)-3-(4-nitrophenyl)-5-oxo-2,5-diphenylpentanoate (85)**




**85**

Colorless oil; 57.1 mg, 66% yield, >20:1 d.r., 94% *ee*, $[\alpha]_D^{20}$ = -11.09 (c = 0.1, $CH_2Cl_2$); $^1$H NMR (500 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.7 Hz, 2H), 7.74 (d, *J* = 7.5 Hz, 2H), 7.57 (d, *J* = 7.3 Hz, 2H), 7.50 (dd, *J* = 7.7, 5.8 Hz, 3H), 7.44 (d, *J* = 7.5 Hz, 2H), 7.41 – 7.33 (m, 7H), 7.28 (t, *J* = 7.3 Hz, 1H), 6.69 (d, *J* = 16.0 Hz, 1H), 6.40 (dt, *J* = 15.9, 5.4 Hz, 1H), 4.52 (dd, *J* = 7.3, 6.1 Hz, 1H), 4.22 (td, *J* = 10.2, 4.6 Hz, 2H), 3.60 (dd, *J* = 17.3, 10.6 Hz, 1H), 3.46 (dd, *J* = 17.2, 3.1 Hz, 1H), 1.37 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 197.6, 169.7, 148.1, 146.8, 136.9, 136.8, 136.7, 133.2, 131.4, 131.2, 128.7, 128.6,

128.3, 128.30, 127.9, 127.8, 127.7, 126.6, 126.5, 122.6, 87.8, 83.2, 67.7, 51.5, 39.6, 28.0. HRMS (ESI) $[M+Na]^+$ calcd for $C_{36}H_{35}NO_6Na^+$, 600.2357, found 600.2358. HPLC (Chiral IE-3, λ= 254 nm, *n*-hexane/2-propanol= 17/3, Flow rate = 1.0 mL/min), $t_R$ = 9.798 min, 16.248 min(major).

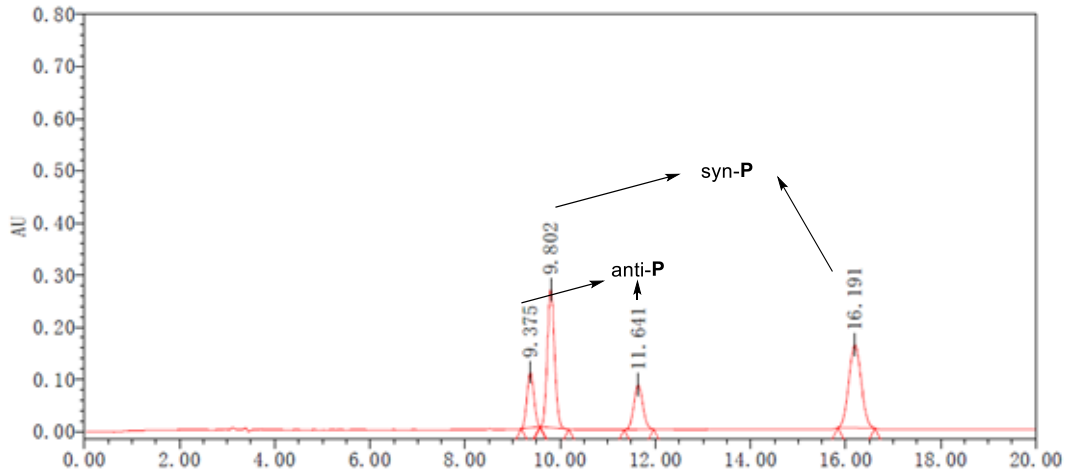
**HPLC chromatogram of racemic 85**

Condition: n-hexane/2-propanol =17:3

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 9.375 | 1070069 | 106241 | 13.49 |
| 2 | 9.802 | 2859038 | 264703 | 36.03 |
| 3 | 11.641 | 1108093 | 85549 | 13.97 |
| 4 | 16.191 | 2897132 | 159691 | 36.51 |

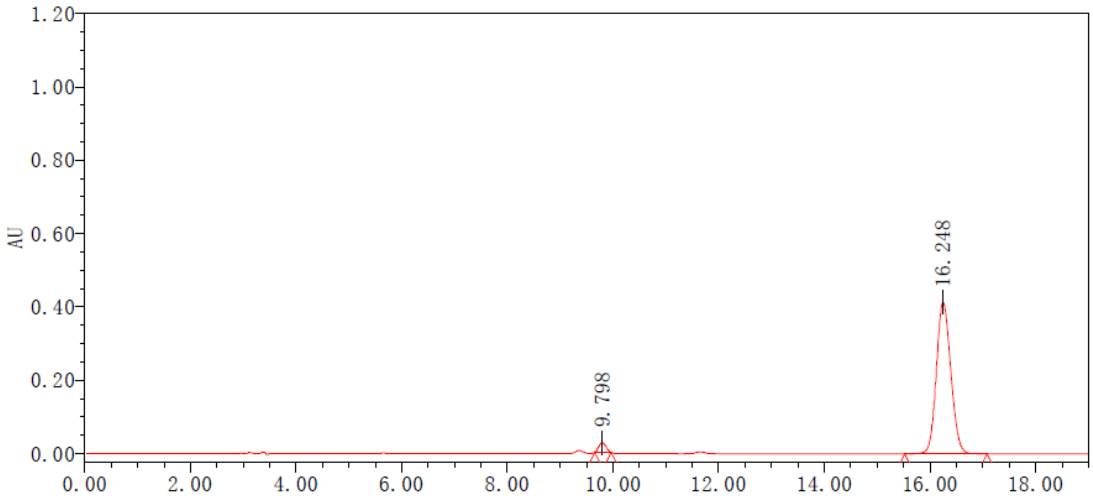
**HPLC chromatogram of chiral 85**

Condition: n-hexane/2-propanol =17:3

Flow rate =1.0 mL/min

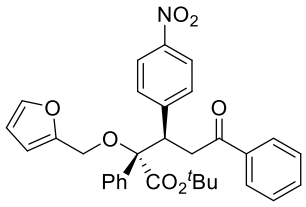
λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 9.798 | 255068 | 26006 | 3.15 |
| 2 | 16.248 | 7853260 | 413978 | 96.85 |

**Tert-butyl (2S,3R)-2-(furan-2-ylmethoxy)-3-(4-nitrophenyl)-5-oxo-2,5-diphenylpentanoate (86)**




**86**

Colorless oil; 52.7 mg, 65% yield, >20:1 d.r., 94% *ee*, $[\alpha]_D^{20}$ = -14.12 (c = 0.1, $CH_2Cl_2$); $^1H$ NMR (400 MHz, $CDCl_3$) δ 8.06 – 7.95 (m, 2H), 7.73 – 7.63 (m, 4H), 7.54 – 7.49 (m, 3H), 7.49 – 7.45 (m, 1H), 7.43 – 7.31 (m, 5H), 6.48 – 6.30 (m, 2H), 4.95 (d, *J* = 12.4 Hz, 1H), 4.55 (d, *J* = 12.4 Hz, 1H), 4.15 (dd, *J* = 10.5, 3.2 Hz, 1H), 3.54 (dd, *J* = 17.3, 10.5 Hz, 1H), 3.41 (dd, *J* = 17.3, 3.2 Hz, 1H), 1.36 (s, 9H). $^{13}C$ NMR (126 MHz, $CDCl_3$) δ 197.7, 169.6, 152.3, 148.3, 146.8, 142.7, 136.7, 136.6, 133.1, 131.4, 128.5,

128.4, 128.4, 127.9, 127.7, 122.5, 110.4, 108.6, 87.6, 83.4, 61.3, 51.5, 39.5, 27.9. HRMS (ESI) $[M+Na]^+$ calcd for $C_{32}H_{31}NO_7Na^+$, 564.1993, found 564.1996. (Chiral IA, λ= 254 nm, *n*-hexane/2-propanol= 49/1, Flow rate = 1.0 mL/min), $t_R$ = 16.664 min, 24.094 min(major)

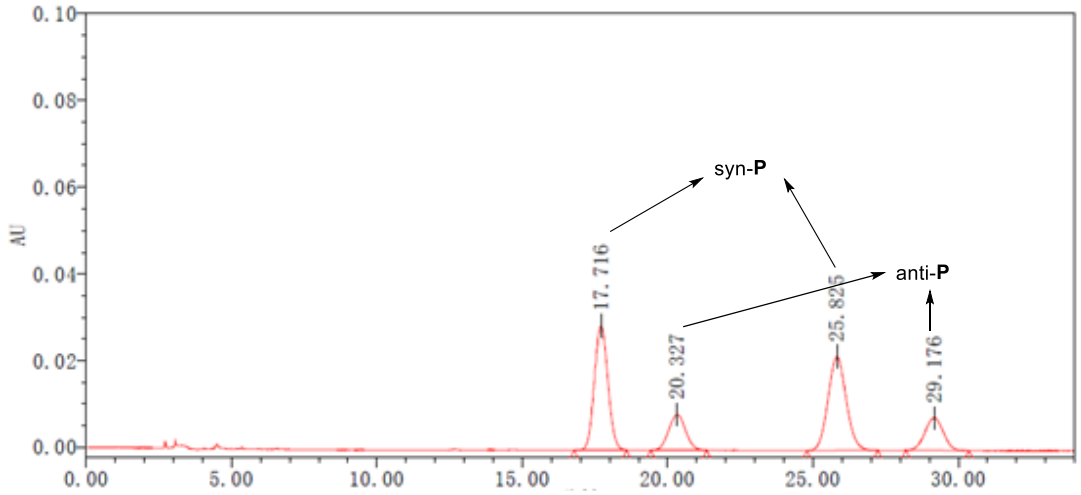
**HPLC chromatogram of racemic 86**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 17.716 | 932158 | 28631 | 36.63 |
| 2 | 20.327 | 335866 | 8223 | 13.20 |
| 3 | 25.825 | 944625 | 21582 | 37.12 |
| 4 | 29.176 | 332399 | 7539 | 13.06 |

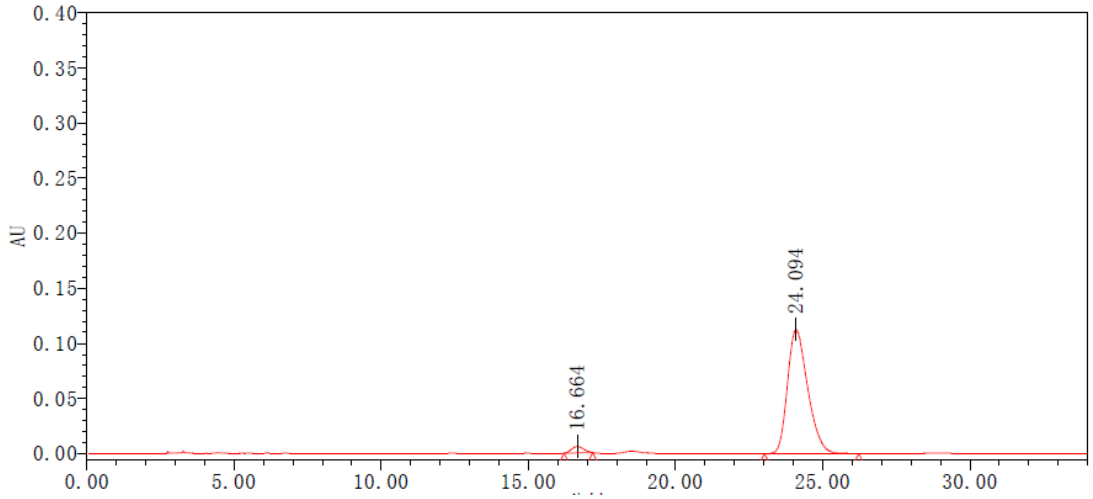
**HPLC chromatogram of chiral 86**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

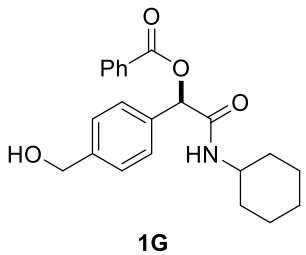
λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 16.664 | 168212 | 5826 | 3.03 |
| 2 | 24.094 | 5381329 | 112554 | 96.97 |

**2-(Cyclohexylamino)-1-(4-(hydroxymethyl)phenyl)-2-oxoethyl benzoate (racemic-1G)**

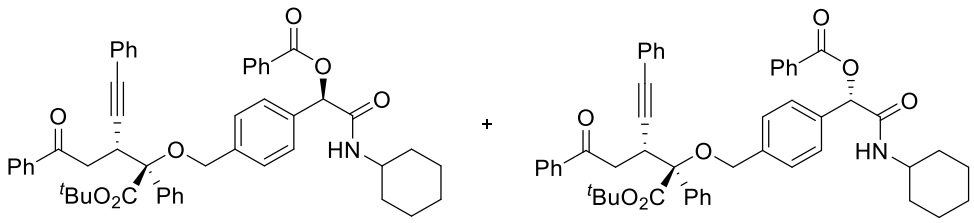



**1G**

White solid; 52% yield (572.5 mg). $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.12 – 8.05 (m, 2H), 7.61 (t, *J* = 7.4 Hz, 1H), 7.50 (d, *J* = 4.9 Hz, 1H), 7.48 (d, *J* = 4.4 Hz, 2H), 7.44 (d, *J* = 14.9 Hz, 1H), 7.36 (d, *J* = 8.1 Hz, 2H), 6.28 (s, 1H), 6.15 (d, *J* = 8.1 Hz, 1H), 4.66 (s, 2H), 3.82 (ddd, *J* = 21.0, 11.3, 7.2 Hz, 1H), 2.33 (s, 1H), 1.94 – 1.86 (m, 2H), 1.67 (t,

*J* = 11.9 Hz, 2H), 1.62 – 1.57 (m, 2H), 1.38 – 1.32 (m, 2H), 1.18 – 1.13 (m, 2H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 167.4, 165.0, 142.0, 135.0, 133.7, 129.8, 129.3, 128.7, 127.6, 127.3, 126.1, 75.7, 64.8, 48.3, 32.9, 32.8, 25.4, 24.7, 24.7. HRMS (ESI) $[M+H]^+$ calcd for $C_{22}H_{26}O_4^+$, 368.1856, found 368.1856.

**1-(4-((((2S,3R)-1-(tert-butoxy)-1-oxo-3-(2-oxo-2-phenylethyl)-2,5-diphenylpent-4-yn-2-yl)oxy)methyl)phenyl)-2-(cyclohexylamino)-2-oxoethyl benzoate (87)**




***syn*-87** ***syn*-87'**

White solid; 65% yield (25.6 mg), 1:1 d.r., 92% ee, 92% ee. Composite NMR signals of *syn*-**87** and *syn*-**87'** (All spectral peaks of two diasteroisomers *syn*-**87** and *syn*-**87'** are overlapping in $^1$H NMR and $^{13}$C NMR). $^1$H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, *J* = 8.2 Hz, 2H), 7.85 (d, *J* = 7.3 Hz, 2H), 7.70 (d, *J* = 7.5 Hz, 2H), 7.58 (d, *J* = 7.3 Hz, 2H), 7.54 (d, *J* = 5.1 Hz, 2H), 7.51 – 7.43 (m, 5H), 7.41 – 7.33 (m, 6H), 7.22 (d, *J* = 2.9 Hz, 3H), 6.32 (s, 1H), 6.11 (d, *J* = 8.1 Hz, 1H), 5.13 (d, *J* = 11.6 Hz, 1H), 4.96 (d, *J* = 11.7 Hz, 1H), 4.41 (dd, *J* = 10.2, 2.8 Hz, 1H), 3.85 – 3.79 (m, 1H), 3.36 (dd, *J* = 16.6, 10.2 Hz, 1H), 3.11 (dd, *J* = 16.6, 2.9 Hz, 1H), 1.93 (dd, *J* = 32.9, 16.4 Hz, 2H), 1.67 (dd, *J* = 13.2, 11.1 Hz, 4H), 1.51 (s, 9H), 1.32 (dd, *J* = 10.9, 5.1 Hz, 2H), 1.16 (dd, *J* = 16.2, 7.9 Hz, 2H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 197.5, 169.4, 167.4, 165.0, 139.9, 138.4, 136.9, 134.9, 133.7, 133.1, 131.4, 129.8, 128.7, 128.6, 128.5, 128.3, 128.2, 128.2, 127.8, 127.6, 127.5, 127.5, 127.3, 126.8, 123.4, 89.8, 85.8, 84.1, 82.9, 75.9, 70.6, 68.2, 48.3, 39.2, 33.0, 32.9, 28.1, 27.9, 25.5, 24.8, 24.7. HRMS (ESI) $[M+Na]^+$ calcd for $C_{51}H_{51}NO_7Na^+$, 812.3558, found 812.3562. (Chiral IC, λ= 254 nm, *n*-hexane/2-propanol= 4/1, Flow rate = 1.0 mL/min), $t_R$ = 17.339 min (major), 24.262 min; $t_{R'}$ =

31.982 min (major), 45.486 min.

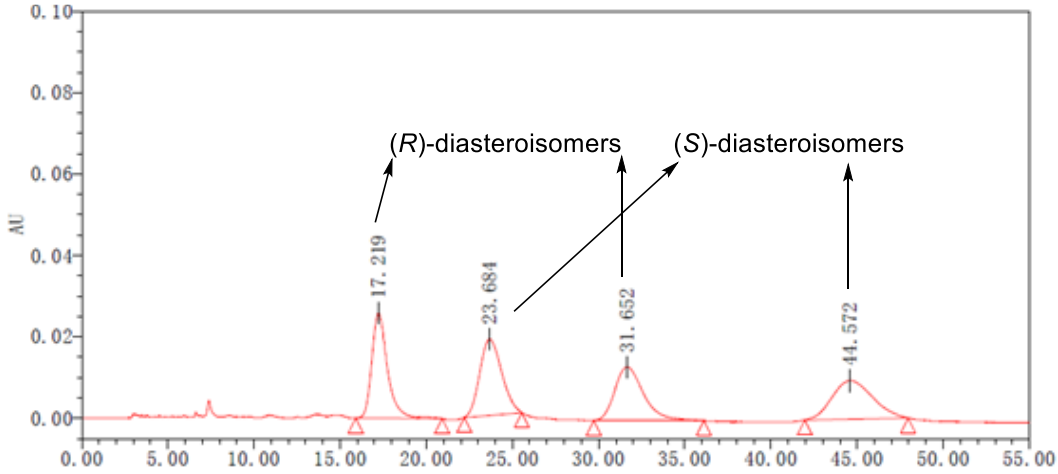
**HPLC chromatogram of racemic 87**

Condition: n-hexane/2-propanol =4:1

Flow rate =1.0 mL/min

λ= 254.0 nm

Chiral IC




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 17.219 | 1645637 | 25910 | 25.86 |
| 2 | 23.684 | 1657749 | 18758 | 26.05 |
| 3 | 31.652 | 1524635 | 13187 | 23.96 |
| 4 | 44.572 | 1535964 | 9468 | 24.14 |

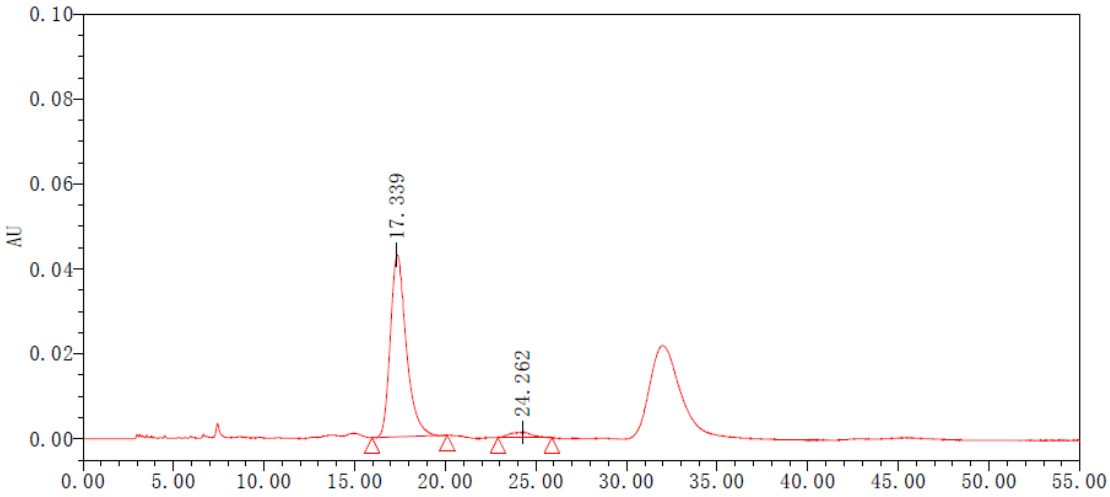
**HPLC chromatogram of chiral 87 and 87'**

Condition: n-hexane/2-propanol =4:1

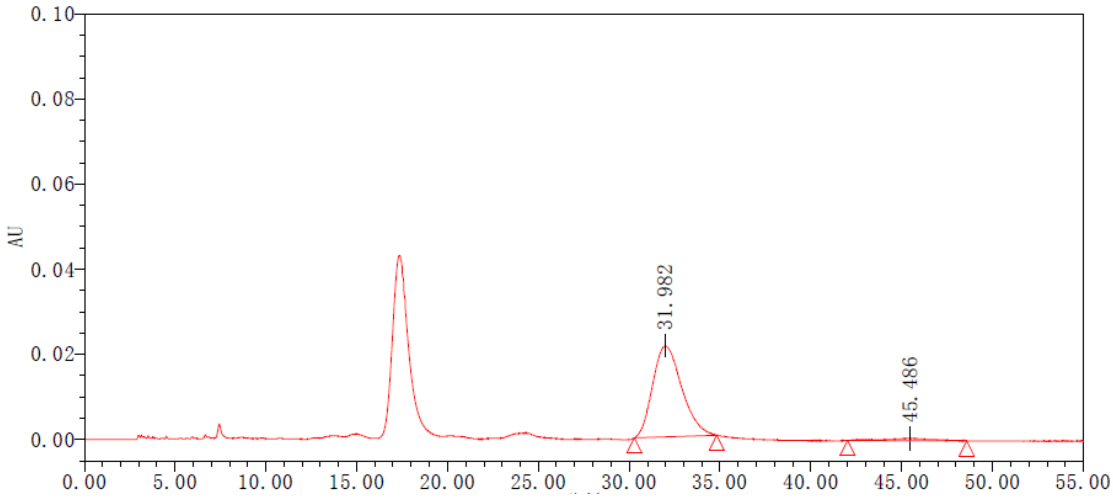
Flow rate =1.0 mL/min

λ= 254.0 nm

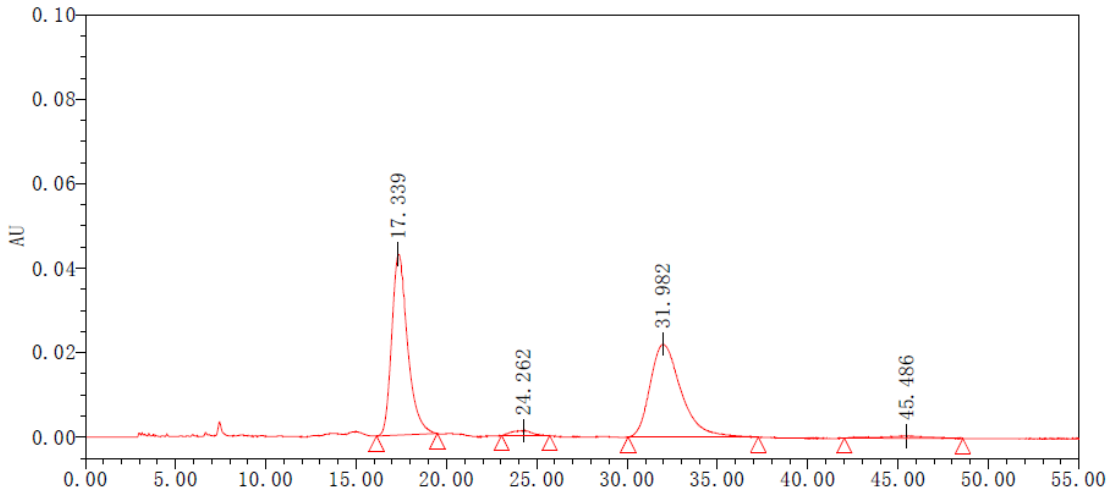
Chiral IC




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 17.339 | 2641026 | 42907 | 96.09 |
| 2 | 24.262 | 107348 | 1285 | 3.91 |

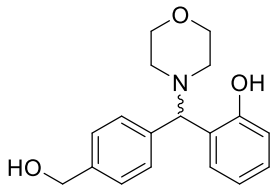



| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 31.982 | 2381648 | 21429 | 96.25 |
| 2 | 45.486 | 92669 | 485 | 3.75 |




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 17.339 | 2631702 | 42882 | 48.36 |
| 2 | 24.262 | 93357 | 1201 | 1.72 |
| 3 | 31.982 | 2624189 | 22021 | 48.22 |
| 4 | 45.486 | 92669 | 485 | 1.70 |

**2-((4-(Hydroxymethyl)phenyl)(morpholino)methyl)phenol (racemic-1I)**

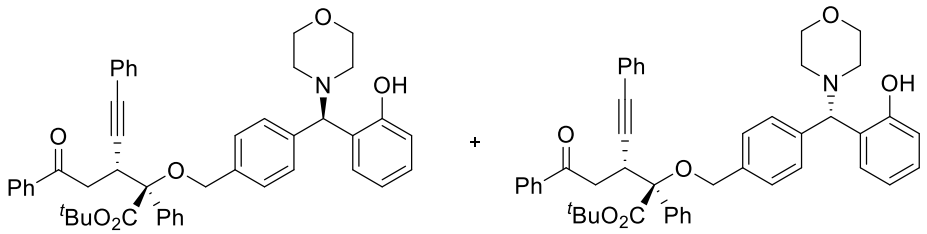



**1I**

Colorless oil; 70% yield (210 mg). $^{1}$H NMR (400 MHz, $CDCl_3$) δ 11.72 (s, 1H), 7.39 (d, *J* = 7.8 Hz, 2H), 7.27 (d, *J* = 8.3 Hz, 2H), 7.12 – 7.05 (m, 1H), 6.91 (dd, *J* = 7.6, 1.3 Hz, 1H), 6.83 (dd, *J* = 8.1, 0.7 Hz, 1H), 6.69 (td, *J* = 7.5, 1.0 Hz, 1H), 4.58 (s, 2H), 4.38 (s, 1H), 3.69 (dd, *J* = 10.9, 6.0 Hz, 4H), 2.62 – 2.35 (m, 4H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 156.0, 141.0, 138.6, 129.3, 128.8, 127.6, 124.8, 119.7, 117.1, 76.5, 66.9, 64.7, 52.2. HRMS (ESI) $[M+H]^+$ calcd for $C_{18}H_{22}NO_3^+$, 300.1594, found 300.1593.

**Tert-butyl (2S,3R)-2-((4-((R)-(2-hydroxyphenyl)(morpholino)methyl)benzyl)oxy)-3-(2-oxo-2-phenylethyl)-2,5-**

**diphenylpent-4-ynoate (*syn*-88)**

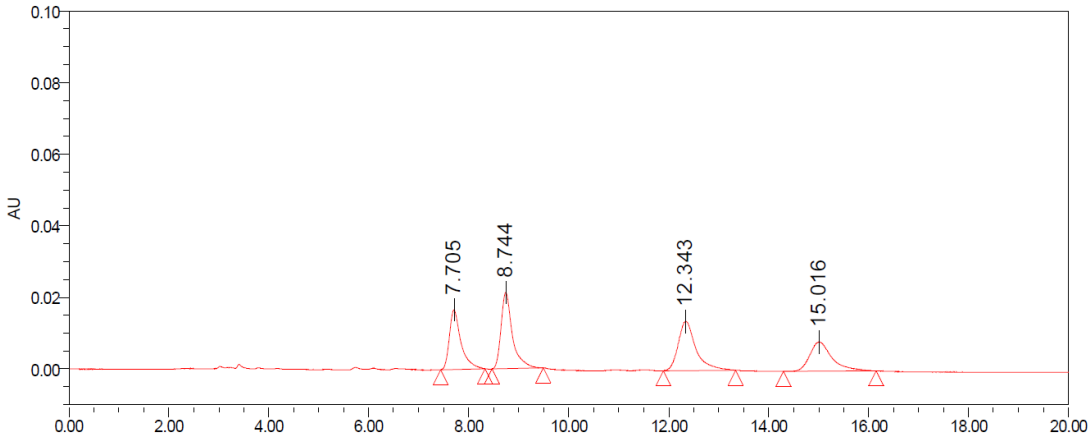



***syn*-88** ***syn*-88'**

White solid; 74% yield (26.7 mg), 1:1 d.r., 99% ee, 99% ee. Composite NMR signals of *syn*-**88** and *syn*-**88'** (All spectral peaks of two diasteroisomers *syn*-**88** and *syn*-**88'** are overlapping in $^1$H NMR and $^{13}$C NMR). $^1$H NMR (500 MHz, $CDCl_3$) δ 11.69 (s, 1H), 7.84 (d, *J* = 7.5 Hz, 2H), 7.69 (d, *J* = 7.7 Hz, 2H), 7.51 (t, *J* = 6.9 Hz, 1H), 7.45 (t, *J* = 8.8 Hz, 3H), 7.40 – 7.33 (m, 6H), 7.30 (d, *J* = 7.2 Hz, 1H), 7.24 (d, *J* = 6.6 Hz, 1H), 7.23 (d, *J* = 7.7 Hz, 3H), 7.12 (t, *J* = 7.7 Hz, 1H), 6.95 (d, *J* = 6.9 Hz, 1H), 6.86 (d, *J* = 8.1 Hz, 1H), 6.73 (t, *J* = 7.4 Hz, 1H), 5.06 (d, *J* = 11.7 Hz, 1H), 4.91 (d, *J* = 11.6 Hz, 1H), 4.42 (s, 1H), 4.41 (dd, *J* = 11.4, 4.0 Hz, 1H), 3.75 (d, *J* = 3.9 Hz, 4H), 3.33 (dd, *J* = 16.7, 10.3 Hz, 1H), 3.17 – 3.06 (m, 1H), 2.54 (d, *J* = 61.0 Hz, 4H), 1.50 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 197.4, 169.4, 156.1, 139.0, 138.4, 136.9, 133.1, 131.5, 131.4, 129.4, 128.7, 128.5, 128.5, 128.3, 128.2, 128.2, 128.2, 128.1, 128.1, 128.0, 127.9, 126.8, 124.9, 123.4, 119.6, 117.1, 89.7, 85.8, 84.1, 82.9, 76.6, 68.2, 66.9, 39.3, 36.5, 28.1. HRMS (ESI) $[M+Na]^+$ calcd for $C_{47}H_{47}NO_6Na^+$, 744.3296, found 744.3298. (Chiral IA-3, λ= 254 nm, *n*-hexane/2-propanol= 17/3, Flow rate = 1.0 mL/min), $t_R$ = 7.732 min (major), 12.434 min; $t_{R'}$ = 8.782 min (major), 15.130 min.

**HPLC chromatogram of racemic 88**

Condition: n-hexane/2-propanol =17:3
Flow rate =1.0 mL/min
λ= 254.0 nm
Chiral IA-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 7.705 | 267422 | 16613 | 22.37 |
| 2 | 8.744 | 337897 | 21296 | 28.26 |
| 3 | 12.343 | 336987 | 13741 | 28.19 |
| 4 | 15.016 | 253249 | 8181 | 21.18 |

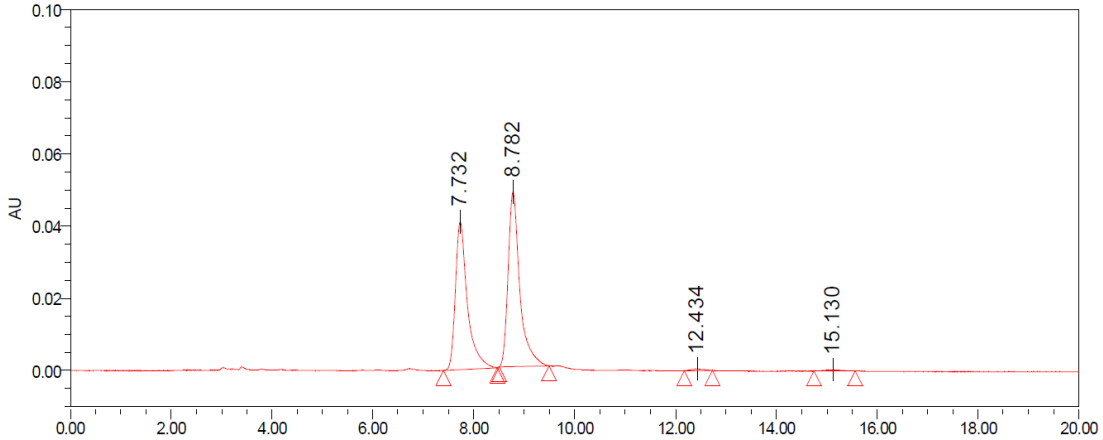
**HPLC chromatogram of chiral 88 and 88'**

Condition: n-hexane/2-propanol =17:3

Flow rate =1.0 mL/min

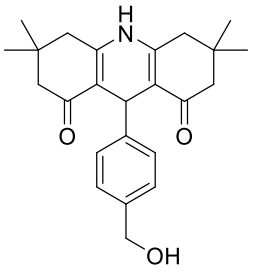
λ= 254.0 nm

Chiral IA-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 7.732 | 675372 | 40954 | 45.96 |
| 2 | 8.782 | 777546 | 48362 | 52.92 |
| 3 | 12.434 | 7977 | 464 | 0.54 |
| 4 | 15.130 | 8465 | 365 | 0.58 |

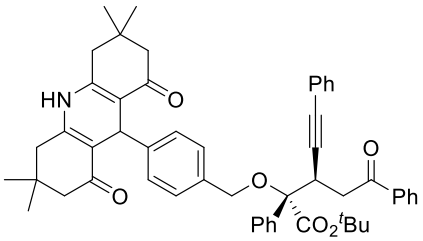
**9-(4-(Hydroxymethyl)phenyl)-3,3,6,6-tetramethyl-3,4,6,7,9,10-hexahydroacridine-1,8(2H,5H)-dione(1J)**




**1J**

Colorless oil; 90% yield (68.2 mg).$^{1}$H NMR (400 MHz, $CDCl_3$) δ 11.89 (s, 1H), 7.23 (d, *J* = 8.1 Hz, 2H), 7.05 (d, *J* = 7.9 Hz, 2H), 5.50 (s, 1H), 5.26 (s, 1H), 4.56 (s, 2H), 2.37 (dq, *J* = 35.3, 17.8 Hz, 8H), 1.21 (s, 6H), 1.08 (s, 6H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 190.6, 189.5, 138.7, 137.3, 127.0, 126.9, 115.6, 64.7, 47.0, 46.4, 32.6, 31.4, 29.6, 27.4. HRMS (ESI) $[M+Na]^+$ calcd for $C_{24}H_{29}NO_3Na^+$, 402.2040, found 402.2040.

**Tert-butyl (2S,3R)-3-(2-oxo-2-phenylethyl)-2,5-diphenyl-2-((4-(3,3,6,6-tetramethyl-1,8-dioxo-1,2,3,4,5,6,7,8,9,10-decahydroacridin-9-yl)benzyl)oxy)pent-4-ynoate (*syn*-89)**




*syn*-**89**

Colorless oil; 64% yield (25.6 mg), 10:1 d.r., 96% ee. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 11.96 (s, 1H), 7.86 (d, *J* = 7.5 Hz, 2H), 7.71 (d, *J* = 7.5 Hz, 2H), 7.52 (t, *J* = 7.3 Hz, 1H), 7.45 – 7.39 (m, 4H), 7.38 (d, *J* = 4.0 Hz, 1H), 7.35 (d, *J* = 7.8 Hz, 2H), 7.30 (d, *J* = 7.4 Hz, 1H), 7.23 (d, *J* = 2.5 Hz, 4H), 7.10 (d, *J* = 8.1 Hz, 2H), 5.54 (s, 1H), 5.08 (d, *J* = 11.4 Hz, 1H), 4.94 (d, *J* = 11.4 Hz, 1H), 4.39 (dd, *J* = 10.3, 2.7 Hz, 1H), 3.37 (dd,

*J* = 16.7, 10.3 Hz, 1H), 3.09 (dd, *J* = 16.7, 2.6 Hz, 1H), 2.51 – 2.27 (m, 8H), 1.50 (s, 9H), 1.24 (s, 6H), 1.10 (s, 6H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 197.6, 190.5, 189.4, 169.5, 138.6, 137.2, 136.9, 136.5, 133.1, 131.5, 131.4, 128.5, 128.5, 128.3, 128.2, 128.2, 128.2, 128.1, 127.8, 127.7, 127.5, 126.8, 123.5, 115.7, 115.6, 89.9, 85.7, 84.0, 82.8, 68.3, 47.1, 46.5, 39.2, 36.6, 32.6, 31.4, 29.7, 28.1, 27.4. HRMS (ESI) $[M+Na]^+$ calcd for $C_{53}H_{55}NO_6Na^+$, 802.4102, found 802.4104. (Chiral IA-3, λ= 254 nm, *n*-hexane/2-propanol= 4/1, Flow rate = 1.0 mL/min), $t_R$ = 11.547 min (major), 20.882 min.

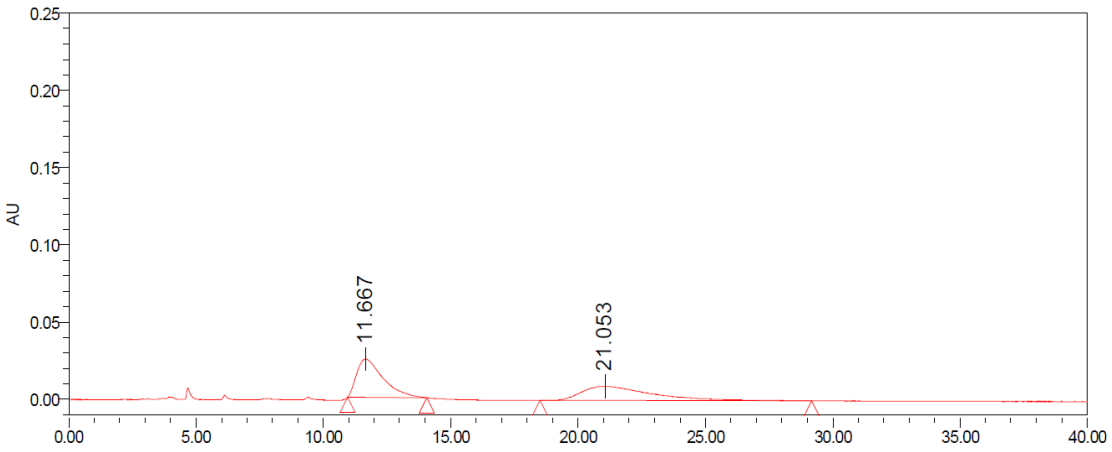
**HPLC chromatogram of racemic 89**

Condition: n-hexane/2-propanol =4:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 11.667 | 1802681 | 24754 | 50.56 |
| 2 | 21.053 | 1762595 | 9139 | 49.44 |

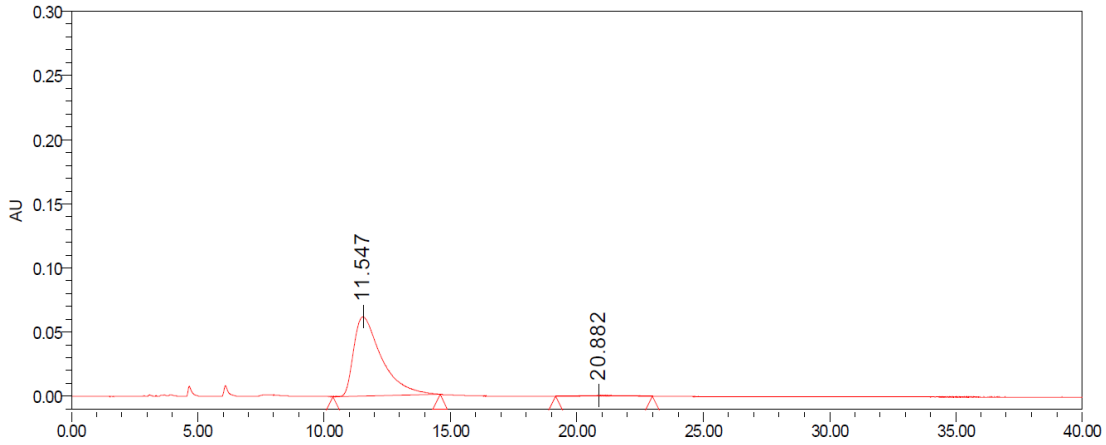
**HPLC chromatogram of chiral 89**

Condition: n-hexane/2-propanol =4:1

Flow rate =1.0 mL/min

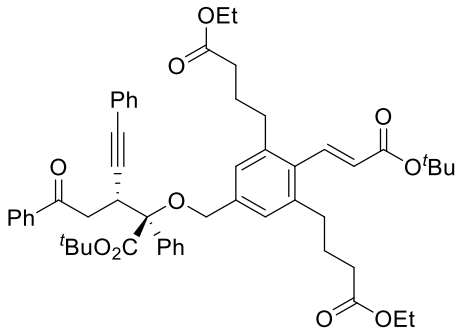
λ= 254 nm

Chiral IA-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 11.547 | 4709094 | 61522 | 98.33 |
| 2 | 20.882 | 79826 | 675 | 1.67 |

**Diethyl 4,4'-(5-((((2S,3R)-1-(tert-butoxy)-1-oxo-3-(2-oxo-2-phenylethyl)-2,5-diphenylpent-4-yn-2-yl)oxy)methyl)-2-((E)-3-(tert-butoxy)-3-oxoprop-1-en-1-yl)-1,3-phenylene)dibutyrate (*syn*-90)**




*syn*-**90**

Colorless oil; 53% yield (25.3 mg), 92:8 d.r., 98% ee. $^1$H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 7.5 Hz, 2H), 7.75 (d, *J* = 9.8 Hz, 1H), 7.71 (d, *J* = 7.6 Hz, 2H), 7.52 (t, *J* = 7.1 Hz, 1H), 7.43 – 7.36 (m, 4H), 7.32 (d, *J* = 7.2 Hz, 1H), 7.27 – 7.19 (m, 7H), 5.91 (d, *J* = 16.3 Hz, 1H), 5.05 (d, *J* = 11.6 Hz, 1H), 4.90 (d, *J* = 11.6 Hz, 1H), 4.42 (dd, *J* = 10.1, 2.6 Hz, 1H), 4.10 (q, *J* = 7.1 Hz, 4H), 3.35 (dd, *J* = 16.6, 10.2 Hz, 1H), 3.13 (dd, *J* = 20.6, 4.2 Hz, 1H), 2.68 – 2.61 (m, 4H), 2.29 (t, *J* = 7.4 Hz, 4H), 1.90 – 1.80 (m, 4H), 1.55 (s, 9H), 1.52 (s, 9H), 1.22 (t, *J* = 7.1 Hz, 6H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 197.5, 173.3, 169.4, 165.7, 142.0, 139.9, 138.5, 137.0, 133.4, 133.1, 131.5, 131.4, 128.5,

128.5, 128.2, 128.2, 128.2, 127.8, 126.8, 126.5, 89.8, 85.8, 84.1, 82.8, 80.7, 68.3, 60.3, 39.3, 36.5, 33.9, 33.0, 28.2, 28.1, 26.1, 14.3. HRMS (ESI) $[M+Na]^+$ calcd for $C_{55}H_{64}O_{10}Na^+$, 907.4392, found 907.4392. (Chiral IC, λ= 254 nm, *n*-hexane/2-propanol= 9/1, Flow rate = 1.0 mL/min), $t_R$ = 17.577 min (major), 29.700 min.

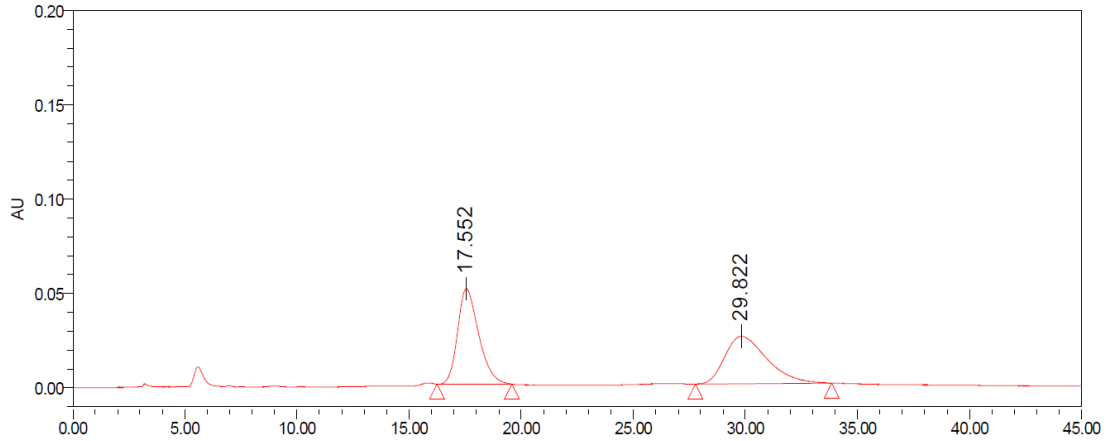
**HPLC chromatogram of racemic 90**

Condition: n-hexane/2-propanol =9:1

Flow rate =1.0 mL/min

λ= 254.0 nm

Chiral IC




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 17.552 | 3321391 | 50547 | 50.36 |
| 2 | 29.822 | 3273941 | 25125 | 49.64 |

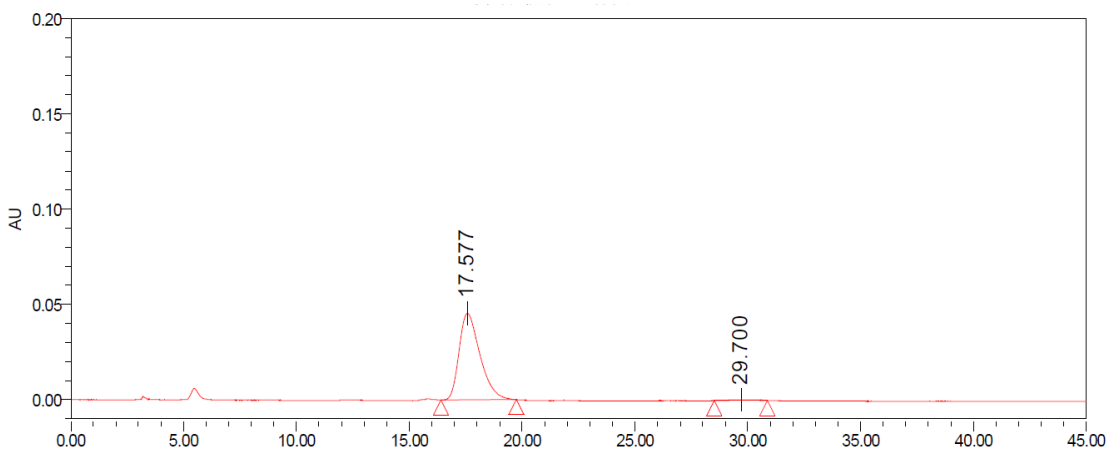
**HPLC chromatogram of chiral 90**

Condition: n-hexane/2-propanol =9:1

Flow rate =1.0 mL/min

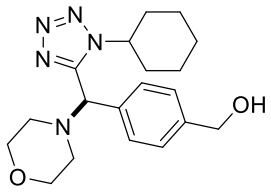
λ= 254.0 nm

Chiral IC




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 17.577 | 2934094 | 45448 | 99.17 |
| 2 | 29.700 | 24603 | 327 | 0.83 |

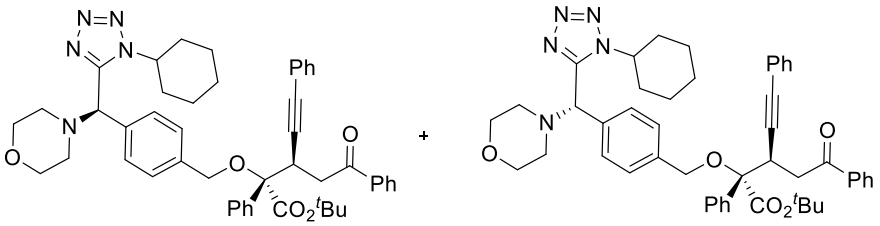
**(4-((1-Cyclohexyl-1H-tetrazol-5-yl)(morpholino)methyl)phenyl)methanol (racemic-1L)**




**1L**

Colorless oil; 68% yield (243 mg). $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.39 (d, *J* = 8.2 Hz, 2H), 7.35 (d, *J* = 8.2 Hz, 2H), 4.96 (s, 1H), 4.67 (s, 2H), 4.60 – 4.52 (m, 1H), 4.03 (s, 1H), 3.69 (t, *J* = 4.5 Hz, 4H), 2.57 (dd, *J* = 11.0, 4.5 Hz, 2H), 2.44 – 2.33 (m, 2H), 1.86 (dd, *J* = 9.8, 7.2 Hz, 4H), 1.74 (d, *J* = 7.9 Hz, 2H), 1.59 (d, *J* = 10.0 Hz, 1H), 1.44 – 1.19 (m, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 153.3, 142.2, 133.4, 128.7, 127.2, 66.7, 65.0, 63.9, 58.0, 51.6, 32.8, 32.7, 25.3, 25.2, 24.7. HRMS (ESI) $[M+H]^+$ calcd for $C_{19}H_{28}N_5O_2^+$, 358.2238, found 358.2236.

**Tert-butyl (2S,3R)-2-((4-((R)-(1-cyclohexyl-1H-tetrazol-5-yl)(morpholino)methyl)benzyl)oxy)-3-(2-oxo-2-phenylethyl)-2,5-diphenylpent-4-ynoate (*syn*-91)**




*syn*-**91** *syn*-**91'**

White solid; 55% yield (21.4 mg), 1:1 d.r., 98% ee, 98% ee. Composite NMR signals of *syn*-**91** and *syn*-**91'** (All spectral peaks of two diasteroisomers *syn*-**91** and *syn*-**91'** are overlapping in $^{1}$H NMR and $^{13}$C NMR). $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 7.7 Hz, 2H), 7.68 (d, *J* = 7.7 Hz, 2H), 7.53 – 7.48 (m, 3H), 7.45 – 7.38 (m, 6H), 7.37 – 7.32 (m, 4H), 7.26 – 7.21 (m, 6H), 5.07 (d, *J* = 11.7 Hz, 1H), 4.94 (d, *J* = 4.3 Hz, 1H), 4.93 – 4.89 (m, 1H), 4.53 (d, *J* = 8.1 Hz, 1H), 4.42 (d, *J* = 8.3 Hz, 1H), 3.75 (s, 4H), 3.33 (dd, *J* = 16.7, 10.2 Hz, 1H), 3.13 (dd, *J* = 14.2, 5.3 Hz, 1H), 2.71 – 2.58 (m, 2H), 2.43 – 2.34 (m, 2H), 1.89 (dd, *J* = 10.6, 8.2 Hz, 4H), 1.69 (dd, *J* = 24.5, 5.7 Hz, 4H), 1.52 (d, *J* = 1.5 Hz, 2H), 1.51 (s, 9H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 197.4, 169.4, 153.2, 139.8, 138.3, 136.9, 133.9, 133.2, 133.1, 131.5, 131.4, 128.6, 128.6, 128.5, 128.4, 128.3, 128.2, 128.2, 128.1, 128.0, 127.9, 126.7, 123.4, 89.6, 85.8, 82.9, 68.0, 66.9, 65.5, 58.1, 52.0, 39.3, 36.5, 32.8, 29.7, 28.1, 25.5, 25.4, 24.8. HRMS (ESI) $[M+Na]^+$ calcd for $C_{48}H_{53}N_5O_5Na^+$, 802.3939, found 802.3944. (Chiral IA-3, λ= 254 nm, *n*-hexane/2-propanol=19/1, Flow rate = 1.0 mL/min), (*R*)- 102 (98% ee) and 102' (98% ee): $t_R$ = 43.447 min (major), 102.904 min, $t_{R'}$ = 55.800 min (major), 113.780 min. (*S*)- 102 (98% ee) and 102' (98% ee): $t_R$ = 44.192 min, 103.376 min(major), $t_{R'}$ = 57.050 min, 114.206 min (major).

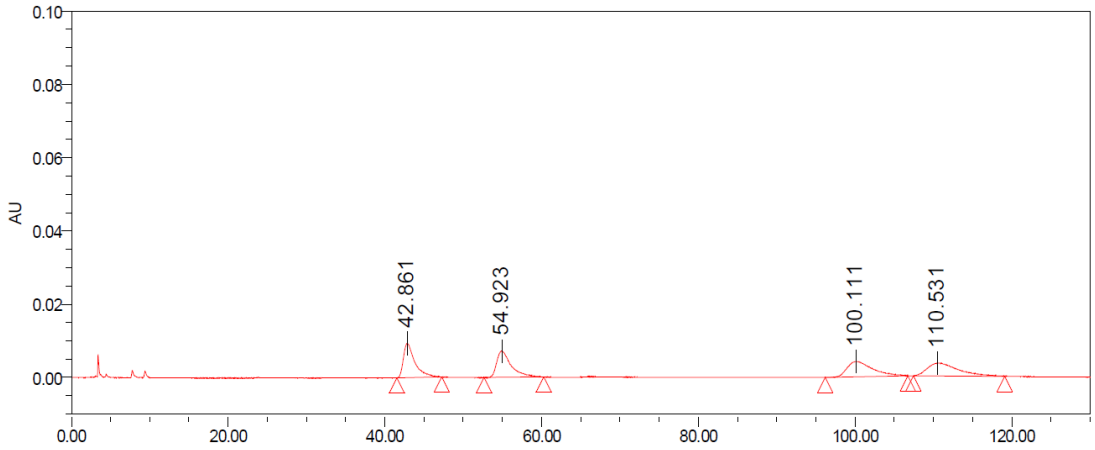
**HPLC chromatogram of racemic 91**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 42.861 | 947265 | 9351 | 25.29 |
| 2 | 54.923 | 929508 | 7204 | 24.82 |
| 3 | 100.111 | 936319 | 4180 | 25.00 |
| 4 | 110.531 | 931922 | 3459 | 24.88 |

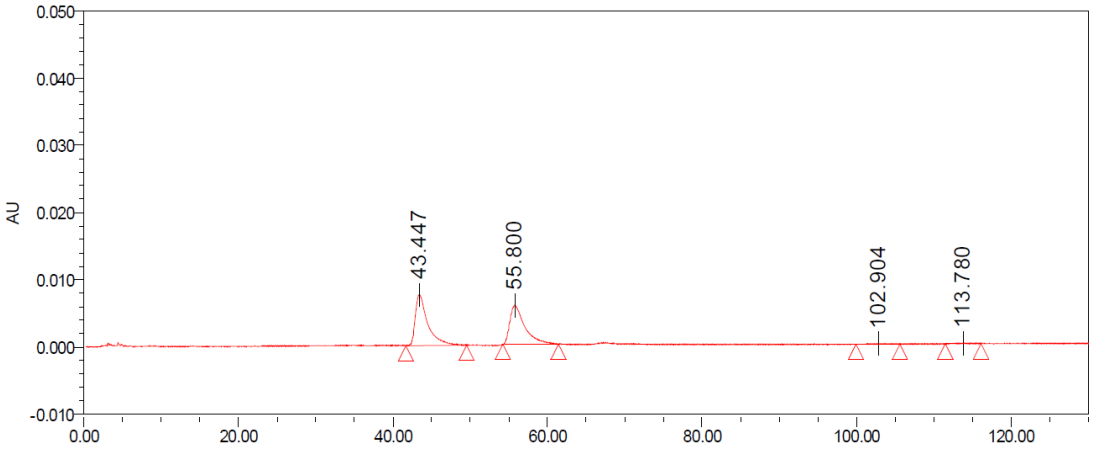
**HPLC chromatogram of (*R*)- 91 and 91'**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 43.447 | 826278 | 7549 | 50.99 |
| 2 | 55.800 | 772051 | 5763 | 47.64 |
| 3 | 102.904 | 13469 | 100 | 0.83 |
| 4 | 113.780 | 8814 | 80 | 0.54 |

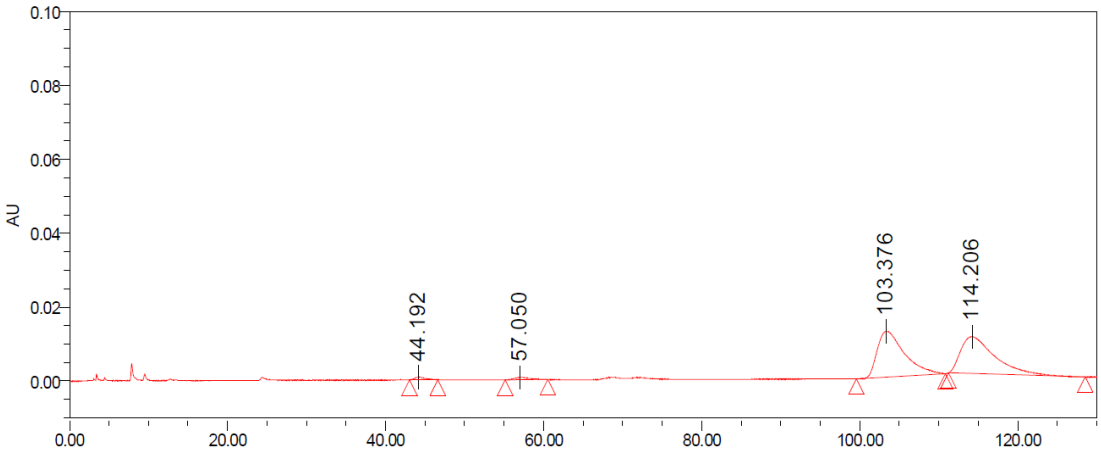
**HPLC chromatogram of (*S*)-91 and 91'**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

λ= 254 nm

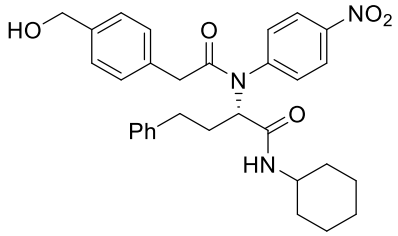
Chiral IA-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 44.192 | 66773 | 743 | 1.09 |

| | | | | |
|---|---|---|---|---|
| 2 | 57.050 | 81867 | 639 | 1.34 |
| 3 | 103.376 | 2951437 | 12376 | 48.14 |
| 4 | 114.206 | 3030941 | 10015 | 49.44 |

**(S)-N-cyclohexyl-2-(2-(4-(hydroxymethyl)phenyl)-N-(4-nitrophenyl)acetamido)-4-phenylbutanamide (1N)**

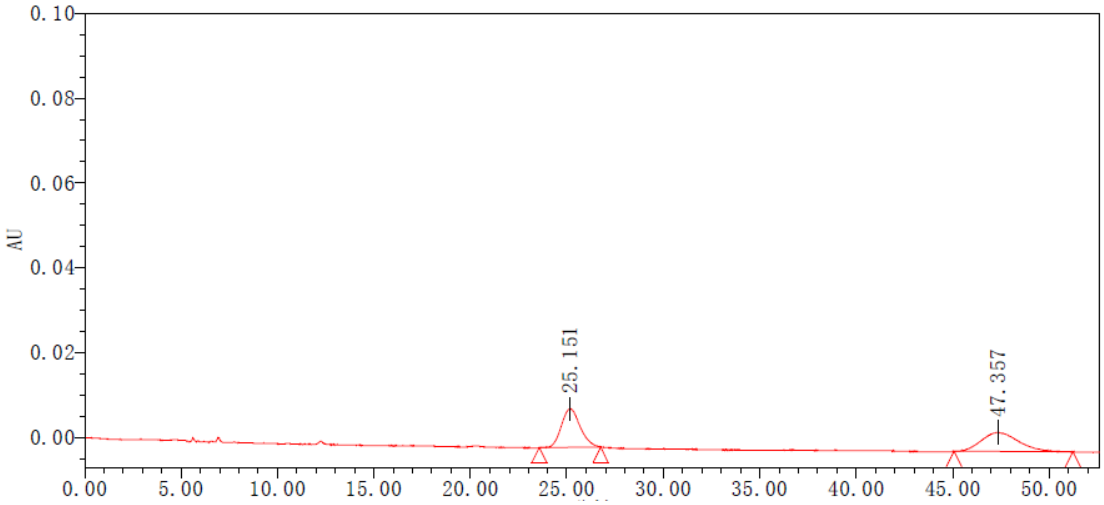



**1N**

Yellow solid; 75% yield (39.7 mg), 90% ee. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.20 (d, *J* = 9.0 Hz, 2H), 7.31 (d, *J* = 9.0 Hz, 2H), 7.26 – 7.21 (m, 4H), 7.18 (d, *J* = 7.2 Hz, 1H), 7.06 (d, *J* = 7.0 Hz, 2H), 6.93 (d, *J* = 8.0 Hz, 2H), 6.43 (d, *J* = 7.5 Hz, 1H), 5.01 (dd, *J* = 9.4, 5.8 Hz, 1H), 4.64 (s, 2H), 3.82 – 3.71 (m, 1H), 3.49 – 3.35 (m, 2H), 2.62 (ddd, *J* = 14.8, 9.6, 5.5 Hz, 1H), 2.54 – 2.45 (ddd, *J* = 14.8, 9.6, 5.5 Hz, 1H), 1.92 – 1.83 (m, 3H), 1.75 – 1.63 (m, 2H), 1.60 – 1.51 (m, 2H), 1.40 – 1.32 (m, 2H), 1.23 – 1.16 (m, 2H), 1.13 – 1.05 (m, 1H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 171.5, 168.9, 147.5, 144.5, 140.5, 140.0, 133.2, 131.0, 129.5, 128.9, 128.6, 128.4, 127.2, 126.3, 124.5, 64.7, 58.2, 48.4, 41.7, 32.9, 32.8, 32.4, 31.0, 25.5, 24.7. HRMS (ESI) $[M+Na]^+$ calcd for $C_{31}H_{35}N_3O_5Na^+$, 530.2649, found 530.2648. (Chiral IC, λ= 254 nm, *n*-hexane/2-propanol= 4/1, Flow rate = 1.0 mL/min), $t_R$ = 25.257 min (major), 47.611 min.

**HPLC chromatogram of racemic 1N**

Condition: n-hexane/2-propanol =4:1
Flow rate =1.0 mL/min
λ= 224.5 nm
Chiral IC




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 25.151 | 613419 | 9096 | 49.99 |
| 2 | 47.357 | 613670 | 4506 | 50.01 |

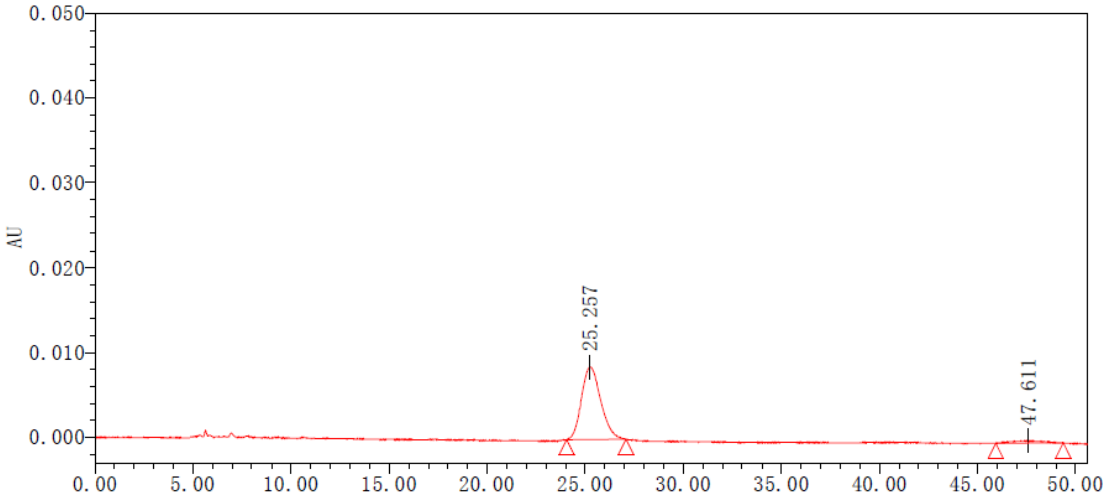
**HPLC chromatogram of chiral 1N**

Condition: n-hexane/2-propanol =4:1

Flow rate =1.0 mL/min

λ= 224.5 nm

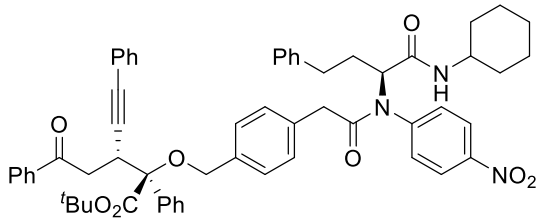
Chiral IC




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 25.257 | 583278 | 8532 | 94.95 |
| 2 | 47.611 | 31052 | 279 | 5.05 |

**Tert-butyl (2S,3R)-2-((4-(2-(((S)-1-(cyclohexylamino)-1-oxo-4-phenylbutan-2-**

**yl)(4-nitrophenyl)amino)-2-oxoethyl)benzyl)oxy)-3-(2-oxo-2-phenylethyl)-2,5-diphenylpent-4-ynoate (*syn*-92)**




*syn*-**92**

Yellow solid; 62% yield (29.5 mg), 95:5 d.r., 92% ee. $^{1}$H NMR (500 MHz, $CDCl_3$) δ 8.21 (d, *J* = 9.0 Hz, 2H), 7.86 (d, *J* = 7.7 Hz, 2H), 7.68 (d, *J* = 7.5 Hz, 2H), 7.52 (t, *J* = 7.4 Hz, 1H), 7.41 (t, *J* = 7.8 Hz, 2H), 7.39 – 7.35 (m, 4H), 7.33 – 7.28 (m, 3H), 7.25 – 7.22 (m, 7H), 7.17 (t, *J* = 7.3 Hz, 1H), 7.06 (d, *J* = 7.2 Hz, 2H), 6.94 (d, *J* = 8.0 Hz, 2H), 6.41 (s, 1H), 5.04 (td, *J* = 11.6, 4.9 Hz, 2H), 4.90 (d, *J* = 11.4 Hz, 1H), 4.41 (dd, *J* = 10.3, 2.8 Hz, 1H), 3.85 – 3.69 (m, 1H), 3.49 – 3.39 (m, 2H), 3.34 (dd, *J* = 16.5, 10.4 Hz, 1H), 3.10 (d, *J* = 16.0 Hz, 1H), 2.68 – 2.59 (m, 1H), 2.55 – 2.46 (m, 1H), 1.88 (td, *J* = 9.4, 4.7 Hz, 2H), 1.82 (d, *J* = 15.8 Hz, 1H), 1.59 (dd, *J* = 20.8, 14.8 Hz, 4H), 1.51 (s, 9H), 1.37 – 1.31 (m, 4H), 0.88 (t, *J* = 6.9 Hz, 1H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 197.4, 171.5, 169.4, 168.9, 147.5, 144.6, 140.5, 138.4, 138.1, 136.9, 133., 131.5, 131.4, 131.0, 128.7, 128.7, 128.6, 128.5, 128.4, 128.2, 128.2, 128.2, 128.2, 128.1, 127.9, 127.8, 127.8, 127.3, 126.7, 126.3, 124.5, 123.4, 89.7, 85.8, 84.1, 82.8, 68.2, 58.2, 48.3, 41.7, 39.2, 36.5, 32.9, 32.8, 32.4, 31.9, 31.6, 31.5, 30.9, 30.3, 30.2, 29.7, 29.7, 29.4, 28.1, 25.5, 24.7, 22.7, 14.1. HRMS (ESI) $[M+Na]^+$ calcd for $C_{60}H_{61}N_3O_7Na^+$, 974.4351, found 974.4355. (Chiral IA-3, λ= 254 nm, *n*-hexane/2-propanol= 17/3, Flow rate = 1.0 mL/min), $t_R$ = 23.126 min (major), 41.012 min.

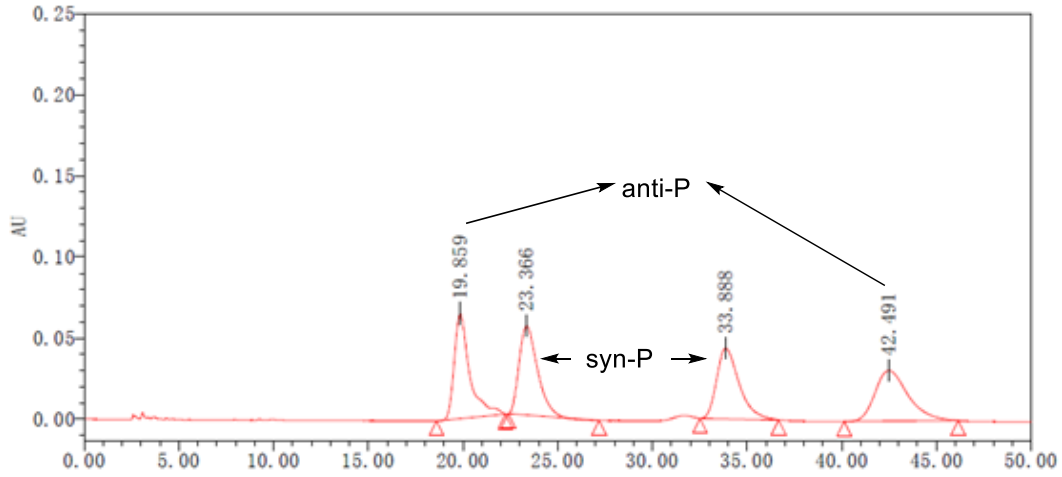
**HPLC chromatogram of racemic 92**

Condition: n-hexane/2-propanol =17:3

Flow rate =1.0 mL/min

λ= 254.0 nm

Chiral IA-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 19.859 | 3732170 | 64728 | 25.10 |
| 2 | 23.366 | 3743187 | 55078 | 25.17 |
| 3 | 33.888 | 3593935 | 43530 | 24.17 |
| 4 | 42.491 | 3799582 | 31233 | 25.55 |

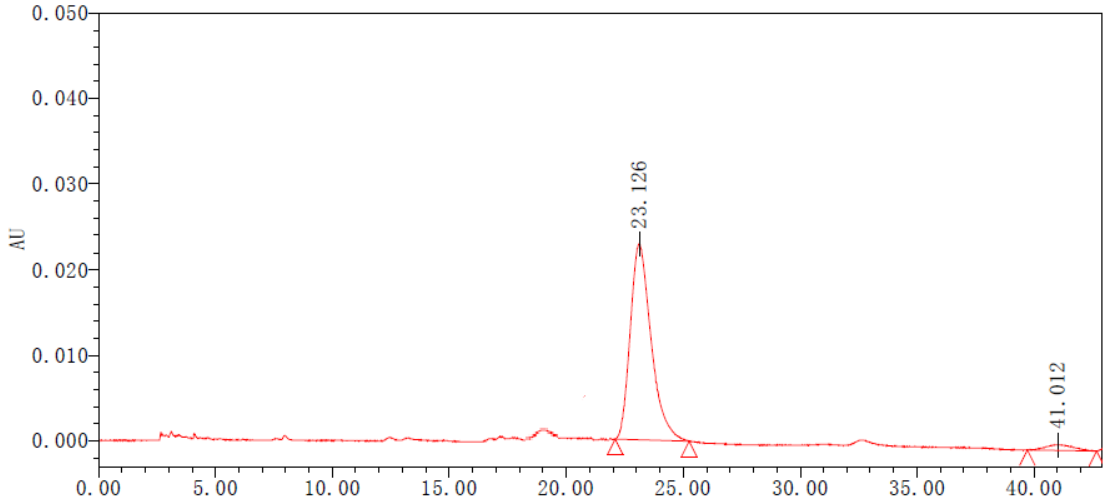
**HPLC chromatogram of chiral 92**

Condition: n-hexane/2-propanol =17:3

Flow rate =1.0 mL/min

λ= 254.0 nm

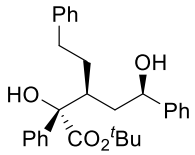
Chiral IA-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 23.126 | 1416957 | 22886 | 96.24 |

| | | | | |
|---|---|---|---|---|
| 2 | 41.012 | 55343 | 657 | 3.76 |

**Tert-butyl (2S,3S,5R)-2,5-dihydroxy-3-phenethyl-2,5-diphenylpentanoate(93)**




**93**

Colorless oil, 38.4 mg, 86% yield, >20:1 d.r., 92% ee. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, *J* = 7.2 Hz, 2H), 7.36 (dd, *J* = 8.4, 6.6 Hz, 2H), 7.33 (d, *J* = 7.3 Hz, 2H), 7.29 (d, *J* = 6.9 Hz, 1H), 7.25 – 7.20 (m, 5H), 7.14 (t, *J* = 7.3 Hz, 1H), 6.95 (d, *J* = 7.1 Hz, 2H), 3.86 (s, 1H), 2.92 – 2.82 (m, 1H), 2.69 (ddd, *J* = 13.7, 10.3, 6.7 Hz, 1H), 2.61 – 2.51 (m, 1H), 2.43 (dd, *J* = 13.1, 8.4 Hz, 1H), 2.32 – 2.22 (m, 1H), 1.98 – 1.87 (m, 1H), 1.79 – 1.70 (m, 1H), 1.70 – 1.62 (m, 1H), 1.54 (ddd, *J* = 14.4, 8.5, 4.4 Hz, 1H), 1.45 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 174.8, 142.8, 142.6, 141.6, 128.5, 128.4, 128.3, 128.2, 128.0, 127.5, 126.0, 125.9, 125.6, 83.42, 82.02, 44.44, 34.40, 34.14, 32.86, 30.87, 27.77. HRMS (ESI) $[M+Na]^+$ calcd for $C_{29}H_{34}O_4Na^+$, 469.2377, found 469.2377. (Chiral IE-3, λ= 254 nm, *n*-hexane/2-propanol= 99/1, Flow rate = 1.0 mL/min), $t_R$ = 14.319 min, 15.178 min (major).

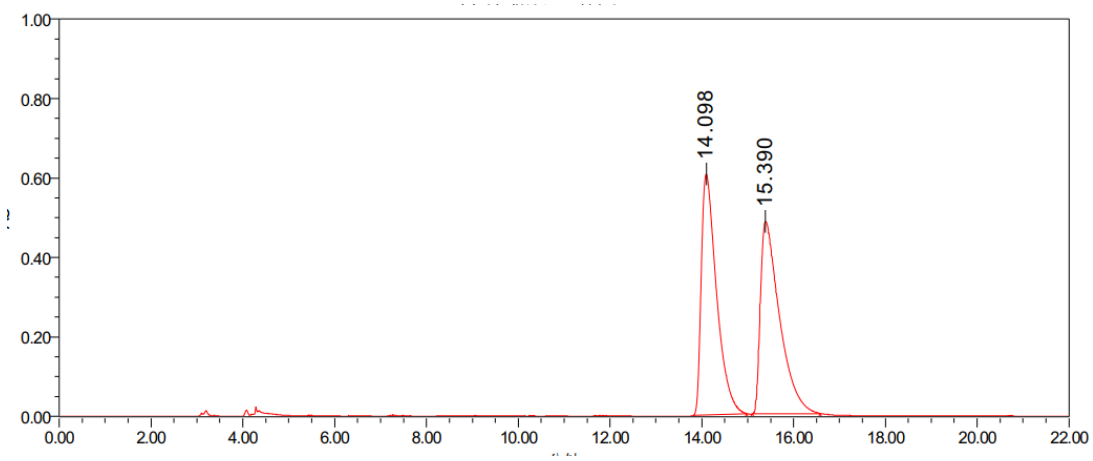
**HPLC chromatogram of racemic 93**

Condition: n-hexane/2-propanol = 99:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 14.098 | 14012053 | 605562 | 49.91 |
| 2 | 15.390 | 14065380 | 484444 | 50.09 |

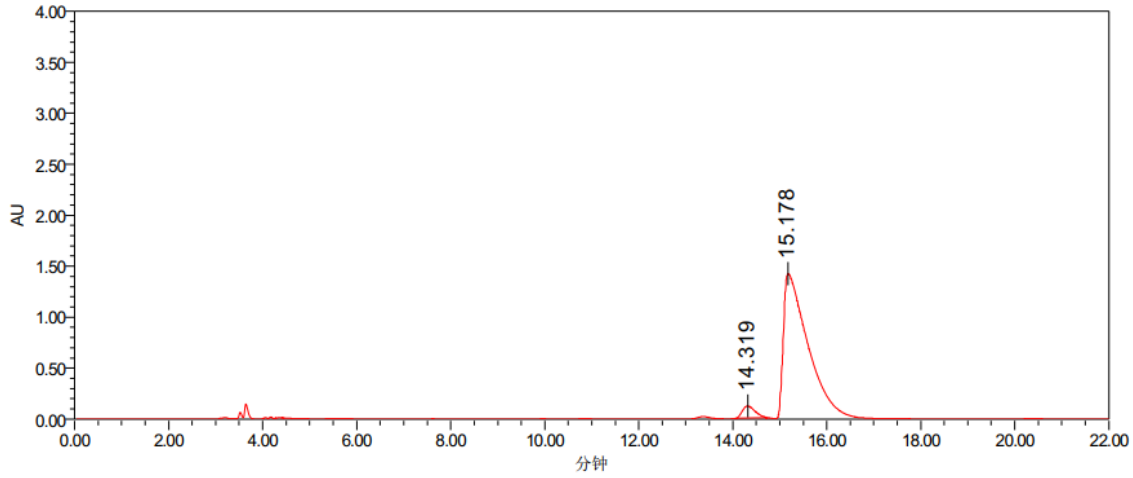
**HPLC chromatogram of chiral 93**

Condition: n-hexane/2-propanol =99:1

Flow rate =1.0 mL/min

λ= 254 nm

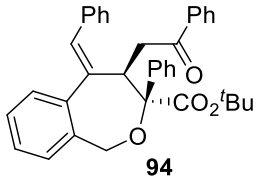
Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| 1 | 14.319 | 2147628 | 116439 | 4.00 |
| 2 | 15.178 | 51512268 | 142107 | 96.00 |

**Tert-butyl (3S,4R)-5-((E)-benzylidene)-4-(2-oxo-2-phenylethyl)-3-phenyl-1,3,4,5-tetrahydrobenzo[c]oxepine-3-carboxylate (94)**




**94**

Colorless oil; 38.2 mg, 72% yield, 92:8 d.r., 88% *ee*; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, *J* = 7.6 Hz, 2H), 7.62 (d, *J* = 7.1 Hz, 2H), 7.48 (t, *J* = 7.7 Hz, 2H), 7.40 (d, *J* = 8.1 Hz, 3H), 7.37 – 7.27 (m, 3H), 7.24 – 7.14 (m, 5H), 7.05 (t, *J* = 7.4 Hz, 1H), 6.97 (d, *J* = 6.9 Hz, 1H), 6.72 (s, 1H), 5.48 – 5.30 (m, 2H), 4.90 – 4.73 (m, 1H), 3.01 (dd, *J* = 17.5, 9.9 Hz, 1H), 2.41 (dd, *J* = 17.5, 3.5 Hz, 1H), 0.98 (s, 9H).$^{13}$C NMR (101 MHz, $CDCl_3$) δ 199.8, 169.8, 143.9, 140.6, 140.05, 138.0, 137.3, 136.2, 134.0, 132.6, 130.5, 129.7, 128.5, 128.4, 128.1, 128.1, 127.9, 127.58, 127.5, 127.3, 127.1, 126.0, 100.0, 88.1, 82.2, 70.2, 40.3, 37.9, 29.7, 27.2. HRMS (ESI) $[M+Na]^+$ calcd for $C_{36}H_{34}O_4Na^+$, 553.2349, found 553.2349. (Chiral IE-3, λ= 254 nm, *n*-hexane/2-propanol= 9/1, Flow rate = 1.0 mL/min), $t_R$ = 6.570 min(major), 8.019 min.

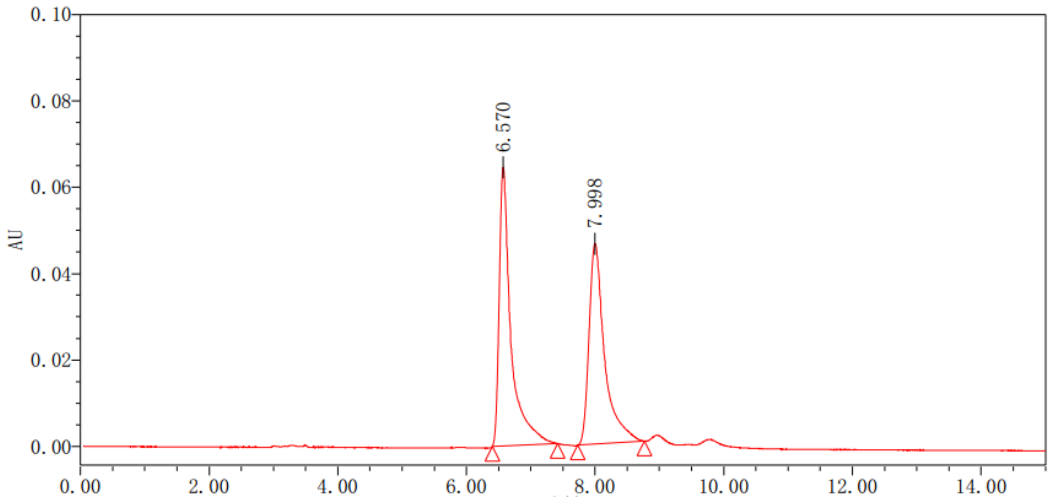
**HPLC chromatogram of racemic 94**

Condition: n-hexane/2-propanol =9:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 6.570 | 814480 | 64518 | 51.01 |
| 2 | 7.998 | 782255 | 46420 | 48.99 |

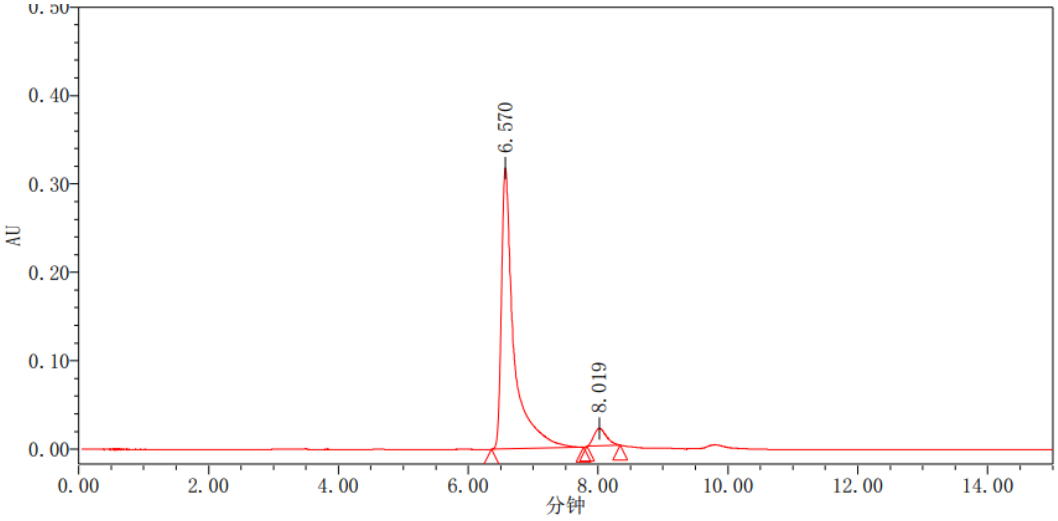
**HPLC chromatogram of chiral 94**

Condition: n-hexane/2-propanol =9:1

Flow rate =1.0 mL/min

λ= 254 nm

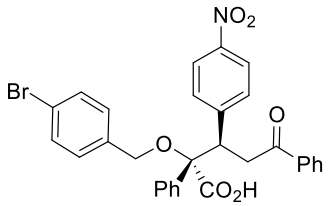
Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| 1 | 6.570 | 4250038 | 317623 | 94.05 |
| 2 | 8.019 | 268945 | 19813 | 5.95 |

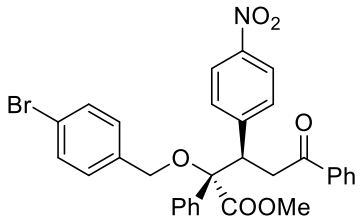
**(2S,3R)-2-((4-Bromobenzyl)oxy)-3-(4-nitrophenyl)-5-oxo-2,5-diphenylpentanoic acid (95)**




**95**

Colorless oil; 43.1 mg, 75% yield. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, *J* = 8.8 Hz, 2H), 7.76 – 7.70 (m, 2H), 7.54 – 7.51 (m, 2H), 7.51 – 7.48 (m, 2H), 7.39 – 7.37 (m, 5H), 7.35 – 7.33 (m, 3H), 7.21 (d, *J* = 8.4 Hz, 2H), 6.19 (s, 1H), 4.74 (d, *J* = 12.0 Hz, 1H), 4.47 (d, *J* = 12.0 Hz, 1H), 4.34 (dd, *J* = 8.6, 5.2 Hz, 1H), 3.65 – 3.49 (m, 2H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 197.3, 147.0, 146.7, 137.1, 136.5, 135.1, 133.4, 131.7, 131.6, 131.2, 129.0, 128.9, 128.8, 128.7, 128.6, 128.0, 128.0, 127.8, 122.6, 121.6, 87.8, 67.9, 51.2, 39.2, 29.7. HRMS (ESI) $[M+Na]^+$ calcd for $C_{30}H_{24}NO_6BrNa^+$, 596.0679, found 596.0675.

**Methyl (2S,3R)-2-((4-bromobenzyl)oxy)-3-(4-nitrophenyl)-5-oxo-2,5-diphenylpentanoate (95-b)**




**95-b**

Colorless oil; 52.4 mg, 70% yield, 89% ee. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 8.8 Hz, 2H), 7.75 (d, *J* = 7.3 Hz, 2H), 7.53 – 7.47 (m, 5H), 7.42 – 7.29 (m, 8H), 7.22

(s, 1H), 4.74 (d, $J$ = 12.2 Hz, 1H), 4.49 (d, $J$ = 12.2 Hz, 1H), 4.33 (dd, $J$ = 9.7, 4.2 Hz, 1H), 3.69 (s, 3H), 3.60 (dd, $J$ = 17.3, 9.7 Hz, 1H), 3.53 (dd, $J$ = 17.4, 4.2 Hz, 1H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 196.1, 170.0, 146.1, 145.9, 136.4, 135.5, 134.8, 132.2, 130.6, 130.0, 127.7, 127.6, 127.4, 126.9, 126.7, 121.5, 120.4, 87.1, 66.9, 51.2, 50.3, 38.1. HRMS (ESI) $[M+Na]^+$ calcd for $C_{31}H_{26}NO_6BrNa^+$, 610.0836, found 610.0840. (Chiral IA, λ= 254 nm, *n*-hexane/2-propanol= 9/1, Flow rate = 1.0 mL/min), $t_R$ = 13.333 min, 21.811 min (major).

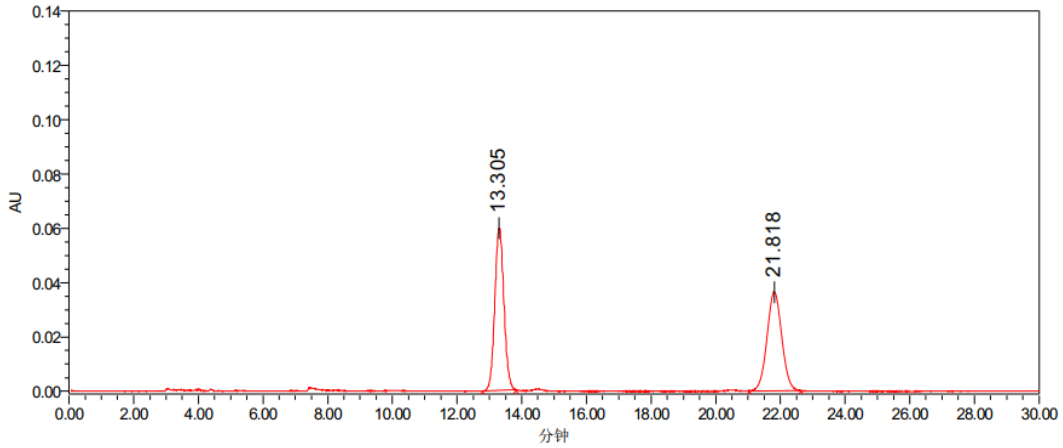
**HPLC chromatogram of racemic 95-b**

Condition: n-hexane/2-propanol =9:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 13.305 | 1157118 | 59812 | 50.05 |
| 2 | 21.818 | 1154629 | 36356 | 49.95 |

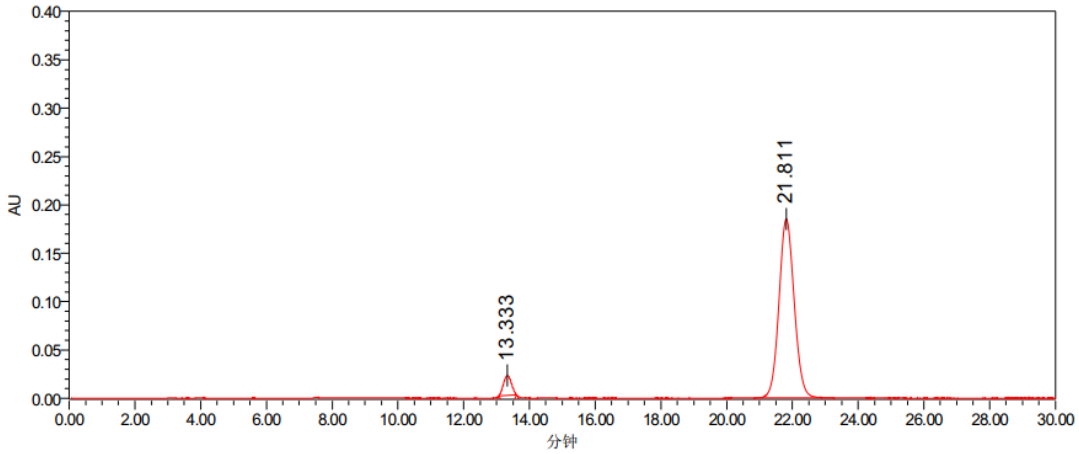
**HPLC chromatogram of chiral 96-b**

Condition: n-hexane/2-propanol =9:1

Flow rate =1.0 mL/min

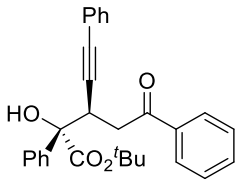
λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 13.333 | 342502 | 20612 | 5.43 |
| 2 | 21.811 | 5965331 | 18497 | 94.57 |

**Tert-butyl (2S,3R)-2-hydroxy-3-(2-oxo-2-phenylethyl)-2,5-diphenylpent-4-ynoate (96)**




**96**

Colorless oil; 26.4 mg, 60% yield, >20:1 d.r., 95% *ee*; $^{1}$H NMR (500 MHz, $CDCl_3$) δ 7.90 (d, *J* = 7.7 Hz, 2H), 7.74 (d, *J* = 7.8 Hz, 2H), 7.52 (t, *J* = 7.4 Hz, 1H), 7.41 (t, *J* = 7.7 Hz, 2H), 7.36 (t, *J* = 7.6 Hz, 2H), 7.29 (d, *J* = 6.9 Hz, 3H), 7.23 (d, *J* = 6.6 Hz, 3H), 4.29 – 4.27 (m, 1H), 4.26 (s, 1H), 3.54 (dd, *J* = 17.1, 10.6 Hz, 1H), 2.65 (dd, *J* = 17.1, 2.8 Hz, 1H), 1.49 (s, 9H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 198.0, 172.9, 138.5, 136.9, 133.1, 131.7, 128.5, 128.4, 128.3, 128.09, 128.1, 127.9, 126.3, 123.1, 88.3, 84.1, 83.3,

79.9, 38.4, 37.5, 27.8. HRMS (ESI) $[M+Na]^+$ calcd for $C_{29}H_{28}O_4Na^+$, 463.1880, found 463.1883. (Chiral IE-3, λ= 254 nm, *n*-hexane/2-propanol= 49/1, Flow rate = 1.0 mL/min), $t_R$ = 10.371 min(major), 15.249 min.

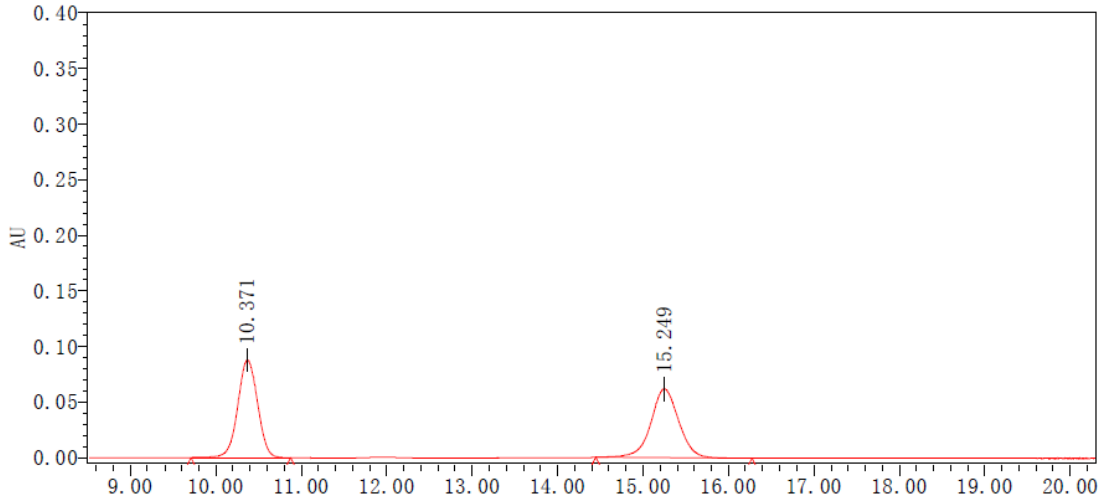
**HPLC chromatogram of racemic 96**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 10.371 | 1415136 | 87699 | 50.21 |
| 2 | 15.249 | 1403227 | 61924 | 49.79 |

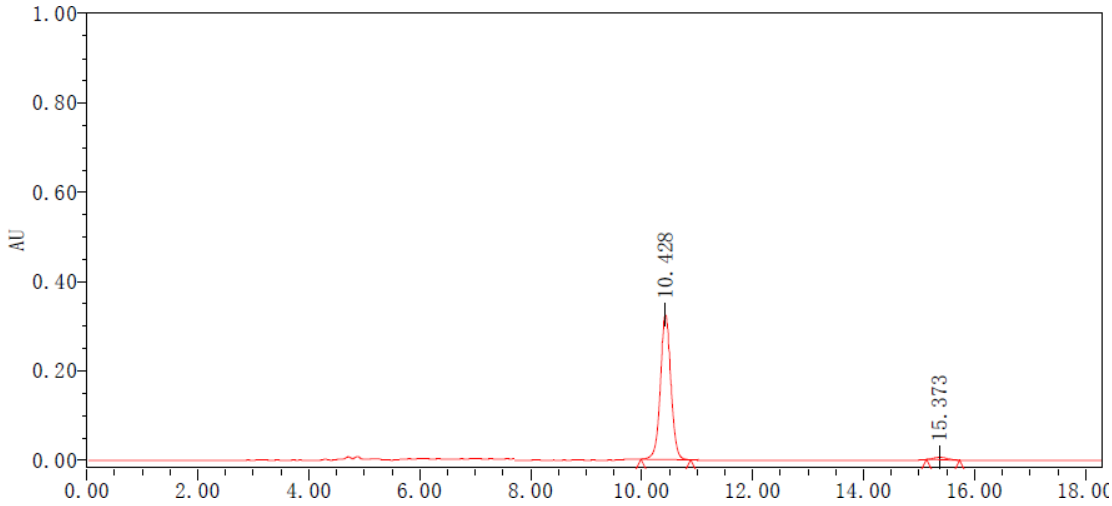
**HPLC chromatogram of chiral 96**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

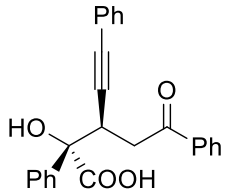
λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 10.428 | 4300933 | 325068 | 97.95 |
| 2 | 15.373 | 90142 | 5299 | 2.05 |

**(2S,3R)-2-hydroxy-3-(2-oxo-2-phenylethyl)-2,5-diphenylpent-4-ynoic acid (97)**

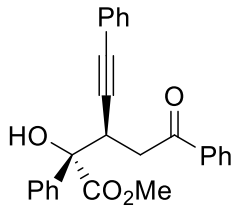



**69**

Colorless oil, 25.0 mg, 65% yield, >20:1 d.r.; $^{1}$H NMR (500 MHz, Acetone) δ 7.89 (dd, *J* = 19.3, 7.6 Hz, 4H), 7.57 (t, *J* = 7.3 Hz, 1H), 7.46 (t, *J* = 7.5 Hz, 2H), 7.25 (t, *J* = 7.4 Hz, 2H), 7.21 – 7.11 (m, 6H), 4.16 (d, *J* = 10.5 Hz, 1H), 3.37 (dd, *J* = 15.6, 11.2 Hz, 1H), 2.58 (d, *J* = 15.7 Hz, 1H). $^{13}$C NMR (126 MHz, Acetone) δ 198.4, 177.6, 143.6, 137.6, 132.7, 131.5, 128.5, 128.0, 127.3, 127.2, 126.6, 126.3, 124.4, 91.8, 81.9, 79.8, 39.1, 39.0. HRMS (ESI) $[M+Na]^+$ calcd for $C_{25}H_{20}O_4Na^+$, 407.1254, found 407.1254.

**Methyl (2S,3R)-2-hydroxy-3-(2-oxo-2-phenylethyl)-2,5-diphenylpent-4-ynoate**

**(97-b)**




**97-b**

Colorless oil; 26.4 mg, 27.9 mg, 70% yield, >20:1 d.r., 95% ee; $^{1}$H NMR (500 MHz, $CDCl_3$) δ 7.89 (d, *J* = 7.8 Hz, 2H), 7.75 (d, *J* = 7.8 Hz, 2H), 7.52 (t, *J* = 7.2 Hz, 1H), 7.44 – 7.35 (m, 5H), 7.31 (d, *J* = 6.4 Hz, 3H), 7.24 (d, *J* = 6.7 Hz, 2H), 4.37 (d, *J* = 10.0 Hz, 1H), 4.18 (s, 1H), 3.87 (s, 3H), 3.52 (dd, *J* = 17.2, 10.5 Hz, 1H), 2.70 (d, *J* = 17.3 Hz, 1H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 197.7, 174.4, 137.7, 136.8, 133.2, 131.8, 128.6, 128.5, 128.4, 128.2, 128.1, 128.1, 126.3, 122.9, 87.9, 83.7, 80.4, 53.8, 38.2, 37.6. HRMS (ESI) $[M+Na]^+$ calcd for $C_{25}H_{22}O_4Na^+$, 421.1410, found 421.1413. (Chiral IE-3, λ= 254 nm, *n*-hexane/2-propanol= 9/1, Flow rate = 1.0 mL/min), $t_R$ = 16.330 min(major), 26.039 min.

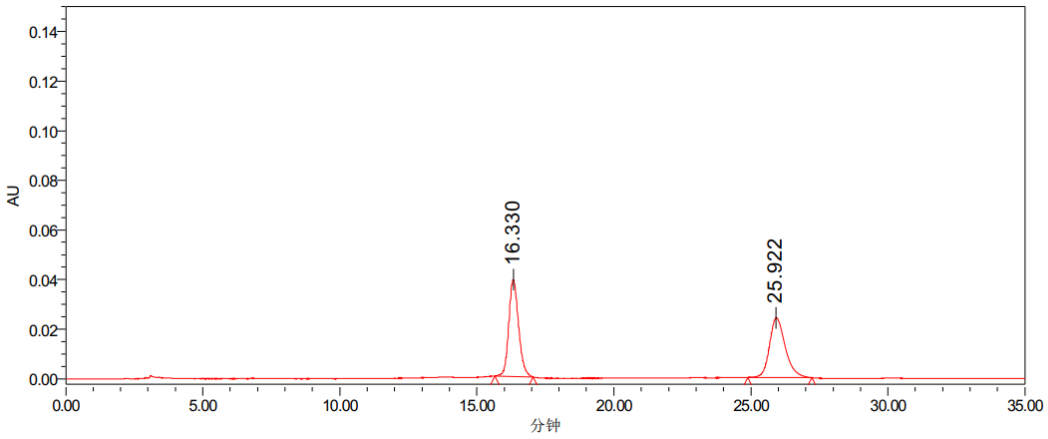
**HPLC chromatogram of racemic 97-b**

Condition: n-hexane/2-propanol =9:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 16.330 | 959906 | 39092 | 50.04 |
| 2 | 25.922 | 958252 | 24055 | 49.96 |

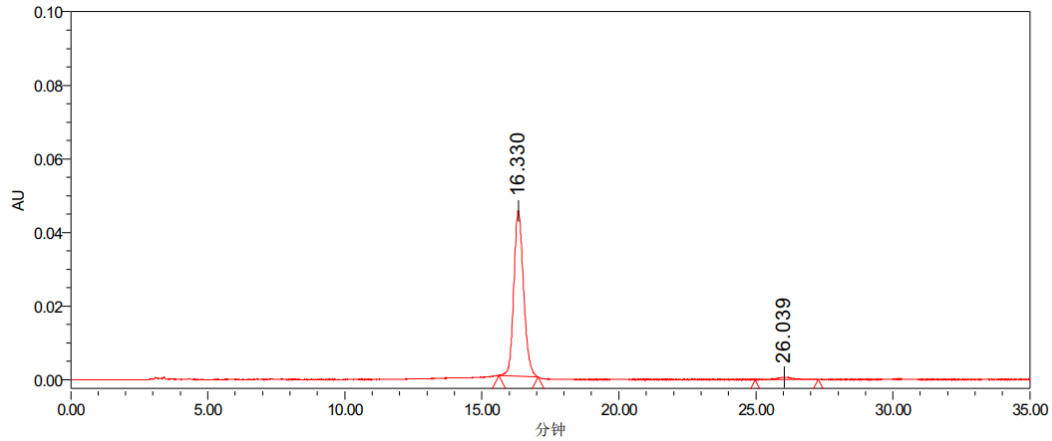
**HPLC chromatogram of chiral 97-b**

Condition: n-hexane/2-propanol =9:1

Flow rate =1.0 mL/min

λ= 254 nm

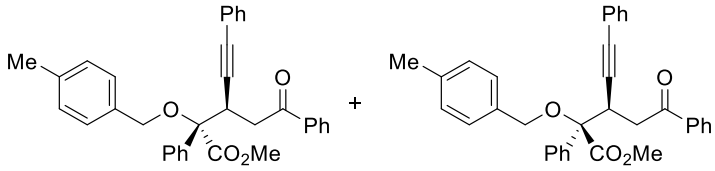
Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 16.330 | 1100042 | 44912 | 97.76 |

| | | | | |
|---|---|---|---|---|
| 2 | 26.039 | 25198 | 594 | 2.24 |

**Methyl (2S,3R)-2-((4-methylbenzyl)oxy)-3-(2-oxo-2-phenylethyl)-2,5-diphenylpent-4-ynoate (*syn*-98)**




*syn*-**98**(major) *anti*-**98**(minor)

Colorless oil; Combined in 53% yield (39.9mg), 83:17 d.r, 21% ee. Composite NMR signals of *syn*-**98**(major) and *anti*-**98** (minor) (The ratio of two diasteroisomers in $^1$H NMR is *syn*-**98** : *anti*-**98** (minor) = 3.00 : 0.72). $^1$H NMR (400 MHz, $CDCl_3$) δ 7.87 – 7.81 (comp, 2.80H), 7.70 – 7.62 (comp, 2.93H), 7.55 – 7.47 (comp, 1.72H), 7.43 – 7.29 (comp, 9.95H), 7.27 – 7.13 (comp, 11.35H), 5.06 (d, *J* = 11.1 Hz, 1.06H), 4.84 (d, *J* = 11.1 Hz, 1.09H), 4.54 (d, *J* = 2.9 Hz, 0.39H), 4.46 (comp, 1.30H), 3.85 (s, 3.02H), 3.83 (s, 0.72H), 3.32 (dd, *J* = 16.7, 10.2 Hz, 1.13H), 3.22 (dd, *J* = 16.5, 3.2 Hz, 0.33H), 3.14 (dd, *J* = 16.7, 3.1 Hz, 1.12H), 3.03 (dd, *J* = 16.5, 10.2 Hz, 0.36H), 2.36 (s, 2.98H), 2.34 (s, 0.79H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 197.3, 171.4, 138.1, 137.2, 136.9, 135.6, 1345.0, 133.1, 131.5, 131.5, 129.0, 128.5, 128.4, 128.3, 128.2, 128.1, 127.9, 127.8, 127.7, 127.3, 126.8, 123.4, 89.2, 88.7, 86.7, 86.0, 84.4, 68.7, 68.0, 52.5, 39.3, 37.1, 36.6, 29.7, 21.2. HRMS (ESI) $[M+Na]^+$ calcd for $C_{34}H_{30}O_4Na^+$, 525.2036, found 525.2039. (Chiral IA, λ= 254 nm, *n*-hexane/2-propanol= 19/1, Flow rate = 1.0 mL/min), $t_R$ = 11.159 min (major), 15.918 min.

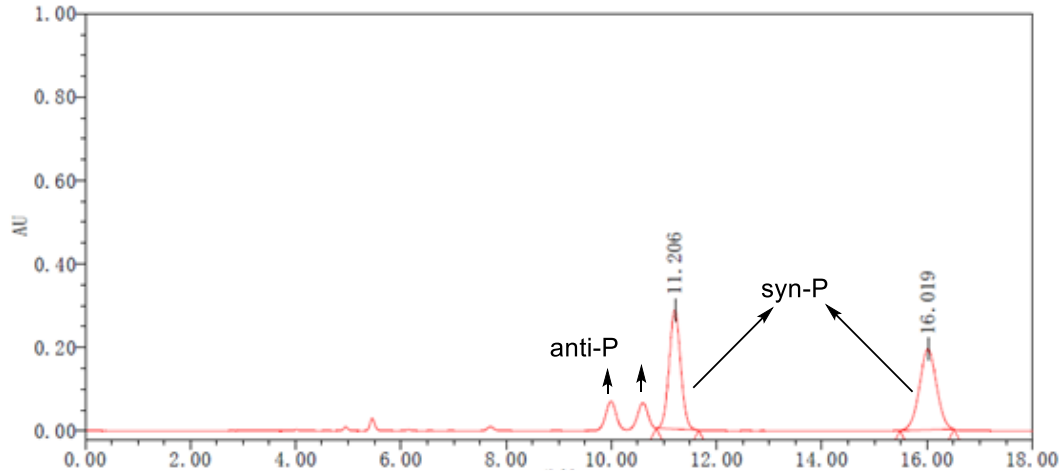
**HPLC chromatogram of racemic 98**

Condition: n-hexane/2-propanol = 19:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 11.206 | 4409358 | 285693 | 50.09 |
| 2 | 16.019 | 4392774 | 193748 | 49.91 |

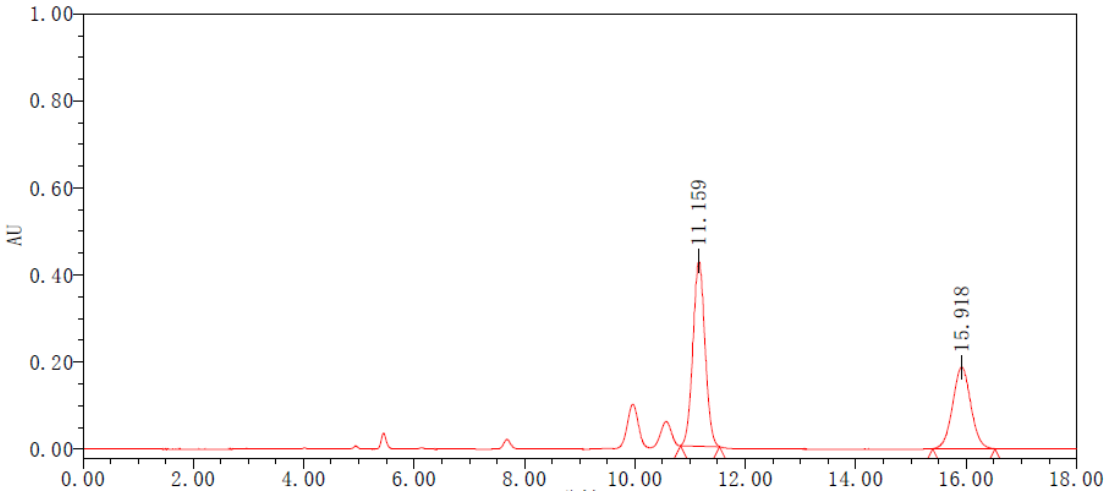
**HPLC chromatogram of chiral 98**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

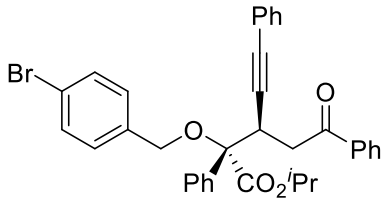
λ= 254 nm

Chiral IA



| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 11.159 | 6535501 | 425356 | 60.47 |
| 2 | 15.918 | 4272173 | 187338 | 39.53 |

**Isopropyl (2S,3R)-2-((4-bromobenzyl)oxy)-3-(2-oxo-2-phenylethyl)-2,5-diphenylpent-4-ynoate (S1)**




**S1**

Colorless oil; 55.3 mg, 62% yield, 96:4 d.r., 80% *ee*; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.86 – 7.81 (m, 2H), 7.69 (d, *J* = 7.2 Hz, 2H), 7.53 (t, *J* = 7.4 Hz, 1H), 7.47 (t, *J* = 6.8 Hz, 2H), 7.44 – 7.40 (m, 2H), 7.41 – 7.36 (m, 3H), 7.33 (dd, *J* = 9.3, 4.7 Hz, 2H), 7.26 – 7.21 (m, 5H), 5.20 (dt, *J* = 12.5, 6.2 Hz, 1H), 5.06 (d, *J* = 11.7 Hz, 1H), 4.90 (d, *J* = 11.7 Hz, 1H), 4.46 (dd, *J* = 10.2, 3.1 Hz, 1H), 3.31 (dd, *J* = 16.6, 10.2 Hz, 1H), 3.10 (dd, *J* = 16.6, 3.1 Hz, 1H), 1.29 (dd, *J* = 14.0, 6.3 Hz, 6H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 197.3, 167.0, 138.0, 137.9, 136.9, 133.1, 131.4, 131.4, 129.3, 128.6, 128.5, 128.4, 128.3, 128.2, 127.9, 126.7, 123.3, 121.3, 89.4, 85.8, 84.3, 69.7, 68.1, 45.7, 39.2, 36.5, 21.8, 21.7. 89.4, 85.8, 84.3, 69.7, 68.1, 45.7, 39.2, 36.5, 21.8, 21.7. HRMS (ESI) $[M+Na]^+$ calcd for $C_{35}H_{31}O_4BrNa^+$, 617.1298, found 617.1302. (Chiral IA-3, λ= 254 nm, *n*-hexane/2-propanol= 49/1, Flow rate = 1.0 mL/min), $t_R$ = 19.432 min(major), 32.117 min.

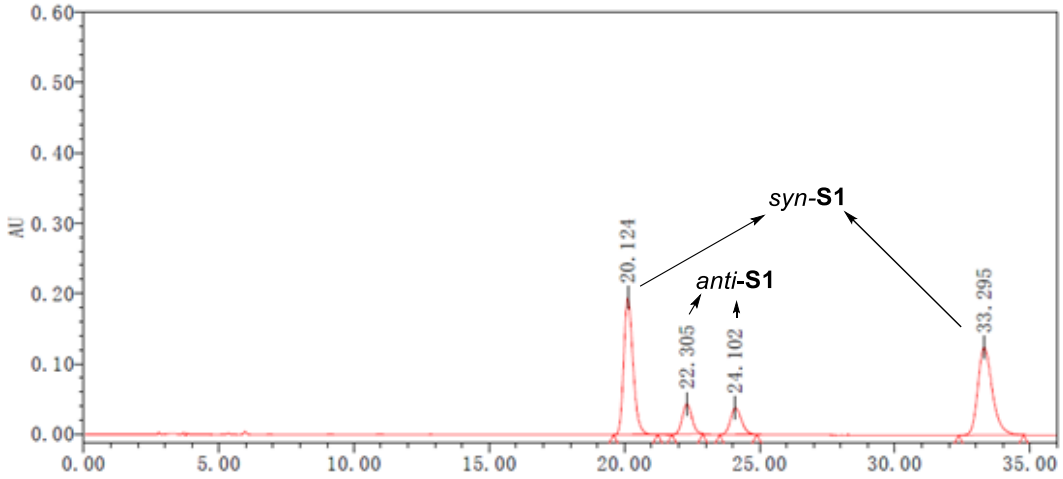
**HPLC chromatogram of racemic S1**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 20.124 | 4594035 | 195267 | 40.42 |
| 2 | 22.305 | 1066902 | 43195 | 9.39 |
| 3 | 24.102 | 1059536 | 37963 | 9.32 |
| 4 | 33.295 | 4645914 | 124850 | 40.87 |

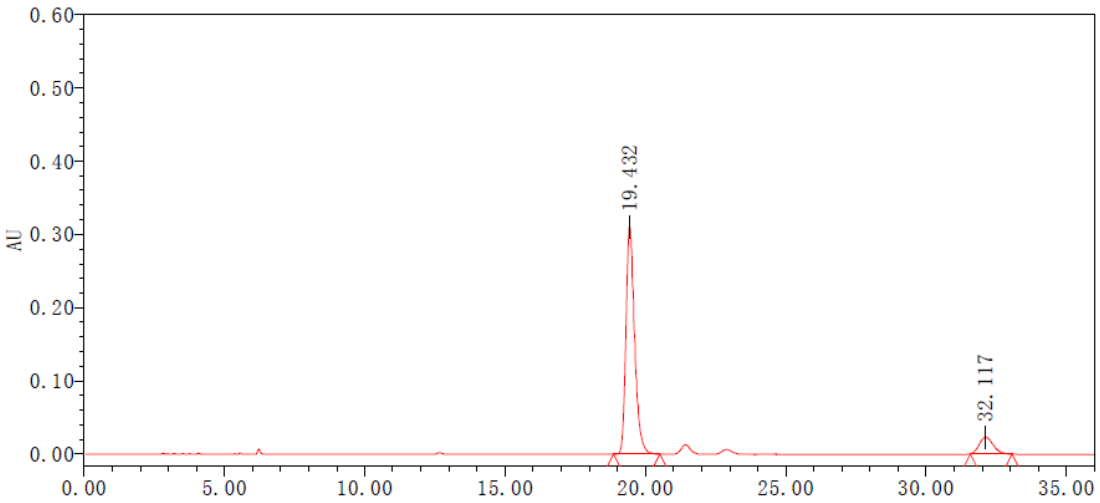
**HPLC chromatogram of chiral S1**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

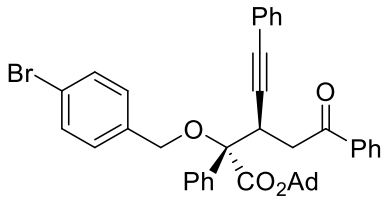
λ= 254 nm

Chiral IA-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 19.432 | 6748195 | 310324 | 89.53 |
| 2 | 32.117 | 789232 | 23019 | 10.47 |

**(3S')-adamantan-1-yl (2S,3R)-2-((4-bromobenzyl)oxy)-3-(2-oxo-2-phenylethyl)-2,5-diphenylpent-4-ynoate(10)**




**S2**

Colorless oil; 57.8 mg, 55% yield, 94:6 d.r., 94% *ee*; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 7.2 Hz, 3H), 7.72 (d, *J* = 7.3 Hz, 2H), 7.56 (t, *J* = 7.4 Hz, 1H), 7.50 (d, *J* = 8.4 Hz, 2H), 7.47 – 7.43 (m, 2H), 7.42 – 7.37 (m, 6H), 7.38 – 7.33 (m, 2H), 7.29 (d, *J* = 9.0 Hz, 1H), 5.05 (d, *J* = 11.7 Hz, 1H), 4.88 (d, *J* = 11.7 Hz, 1H), 4.42 (dd, *J* = 10.1, 3.1 Hz, 1H), 3.77 (s, 1H), 3.34 (dd, *J* = 16.5, 10.1 Hz, 1H), 3.16 (dd, *J* = 16.5, 3.0 Hz, 1H), 2.29 (s, 1H), 2.20 (d, *J* = 9.7 Hz, 7H), 1.74 (s, 1H), 1.68 (s, 5H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 197.5, 169.1, 138.3, 138.1, 137.0, 133.1, 131.6, 131.4, 131.4, 129.2, 128.6, 128.2, 128.2, 128.2, 127.8, 126.8, 123.5, 121.2, 89.7, 85.9, 84.1, 83.11, 67.9,

67.5, 67.3, 66.8, 66.2, 41.8, 41.3, 39.4, 36.8, 36.2, 36.1, 30.9. HRMS (ESI) $[M+Na]^+$ calcd for $C_{42}H_{39}O_4BrNa^+$, 709.1924, found 709.1920. (Chiral IE-3, λ= 254 nm, *n*-hexane/2-propanol= 19/1, Flow rate = 1.0 mL/min), $t_R$ = 11.866 min(major), 23.080 min.

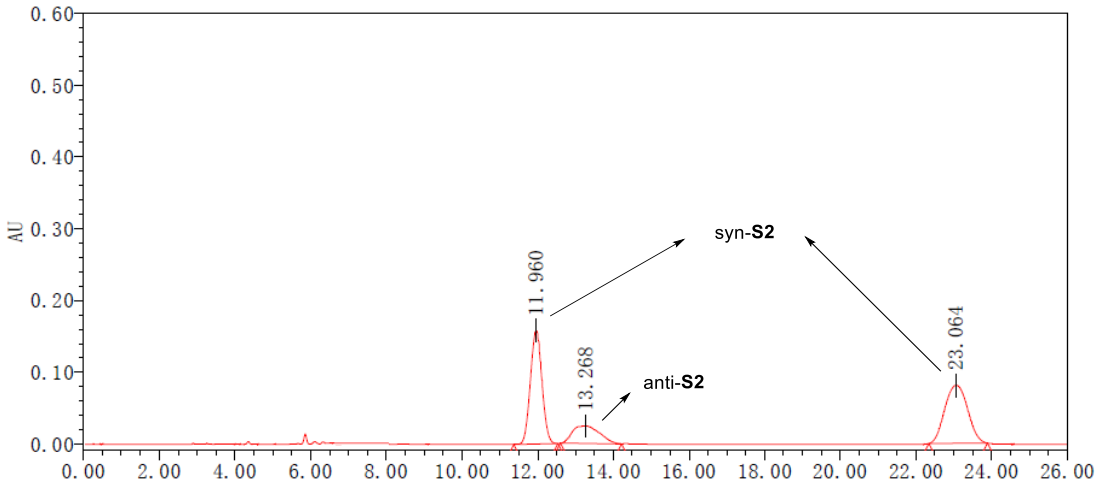
**HPLC chromatogram of racemic S2**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 11.960 | 3399610 | 158056 | 42.40 |
| 2 | 13.268 | 1224706 | 24329 | 15.27 |
| 3 | 23.064 | 3394051 | 81034 | 42.33 |

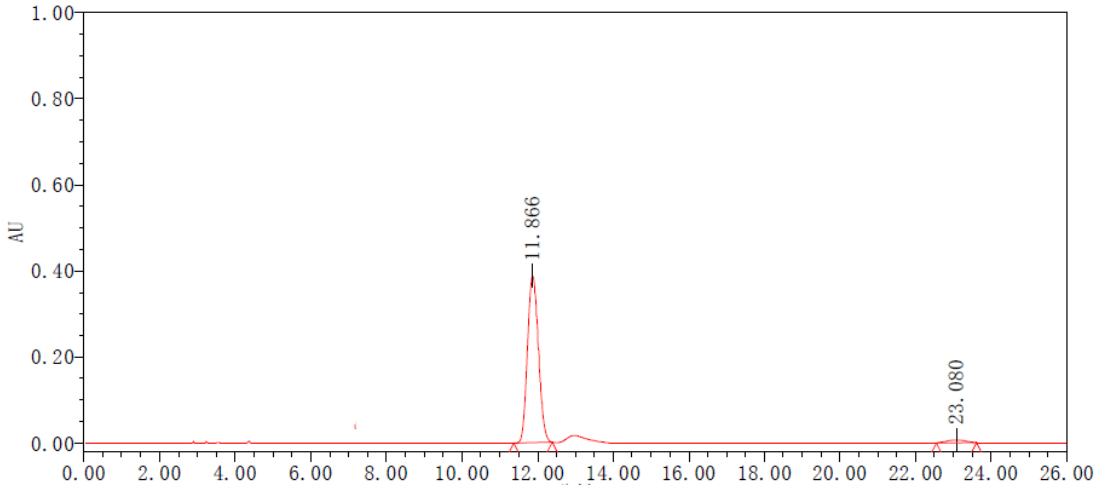
**HPLC chromatogram of chiral S2**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

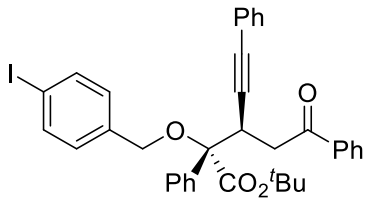
λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 11.866 | 7844491 | 387110 | 97.22 |
| 2 | 23.080 | 224168 | 6254 | 2.78 |

**Tert-butyl (2S,3R)-2-((4-iodobenzyl)oxy)-3-(2-oxo-2-phenylethyl)-2,5-diphenylpent-4-ynoate (S3)**




**S3**

Colorless oil; 52.8 mg, 53% yield, >20:1 d.r., 98% *ee*; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.87 – 7.82 (m, 2H), 7.68 (dd, *J* = 8.1, 1.6 Hz, 4H), 7.53 (t, *J* = 7.4 Hz, 1H), 7.41 (t, *J* = 7.8 Hz, 2H), 7.37 (t, *J* = 7.4 Hz, 2H), 7.32 (d, *J* = 7.1 Hz, 1H), 7.26 (d, *J* = 6.0 Hz, 2H), 7.24 (d, *J* = 5.7 Hz, 5H), 5.04 (d, *J* = 11.8 Hz, 1H), 4.90 (d, *J* = 11.8 Hz, 1H), 4.41 (dd, *J* = 10.2, 3.1 Hz, 1H), 3.32 (dd, *J* = 16.7, 10.2 Hz, 1H), 3.08 (dd, *J* = 16.6, 3.0 Hz,

1H), 1.51 (s, 9H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 197.4, 169.4, 138.7, 138.3, 137.4, 136.9, 133.1, 131.4, 129.5, 128.6, 128.3, 128.3, 128.2, 128.2, 128.2, 127.9, 126.7, 123.4, 92.8, 89.7, 85.9, 84.1, 83.0, 68.1, 39.2, 36.6, 28.1. HRMS (ESI) $[M+Na]^+$ calcd for $C_{36}H_{33}O_4INa^+$, 679.1316, found 679.1312. (Chiral IE-3, λ= 254 nm, *n*-hexane/2-propanol= 9/1, Flow rate = 1.0 mL/min), $t_R$ = 7.571 min(major), 13.849 min.

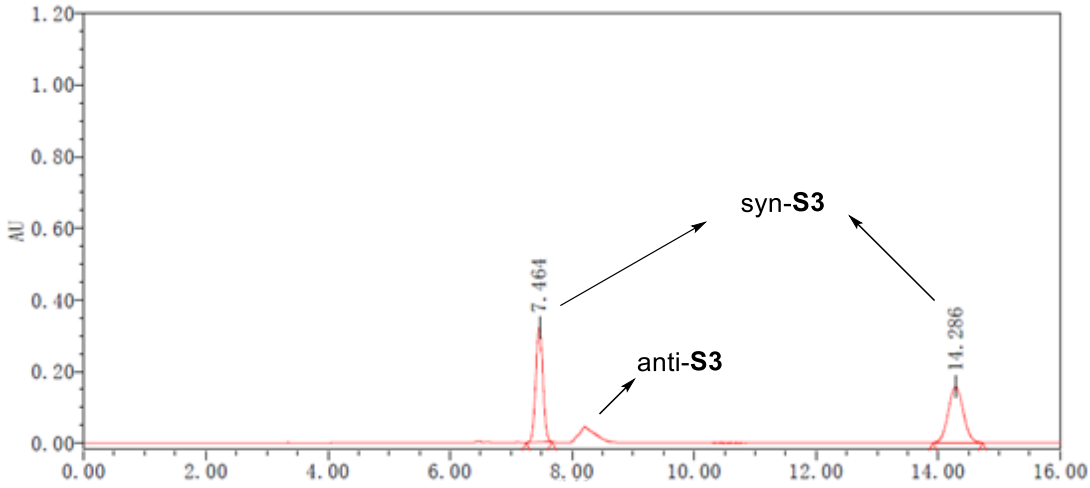
**HPLC chromatogram of racemic S3**

Condition: n-hexane/2-propanol =9:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 7.464 | 2651099 | 320271 | 50.20 |
| 2 | 14.286 | 2630463 | 155712 | 49.80 |

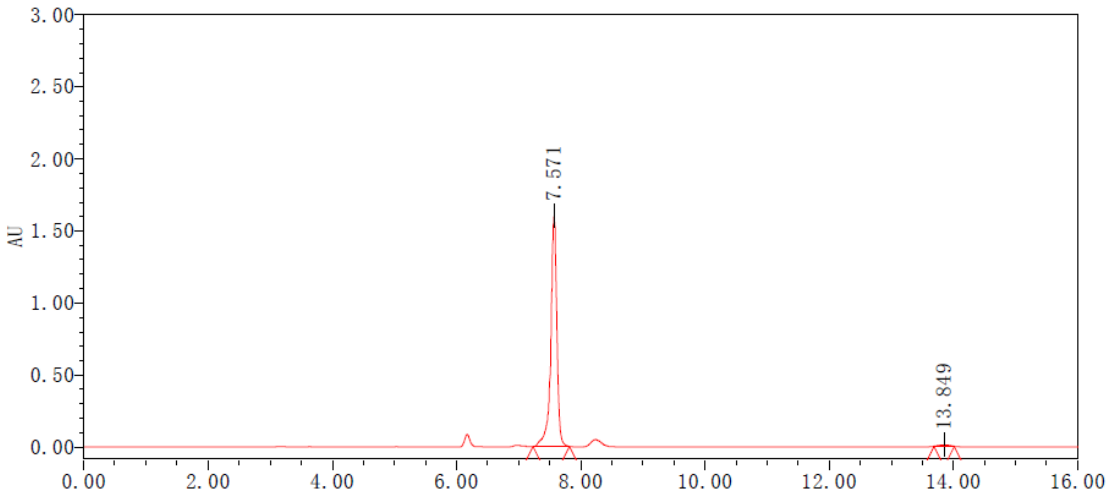
**HPLC chromatogram of chiral S3**

Condition: n-hexane/2-propanol =9:1

Flow rate =1.0 mL/min

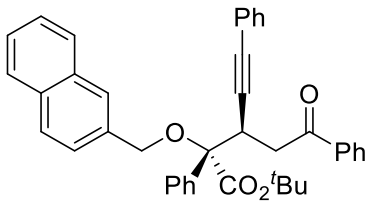
λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 7.571 | 11058138 | 11058138 | 99.02 |
| 2 | 13.849 | 109255 | 109255 | 0.98 |

**Tert-butyl (2S,3R)-2-(naphthalen-2-ylmethoxy)-3-(2-oxo-2-phenylethyl)-2,5-diphenylpent-4-ynoate (S4)**




**S4**

Colorless oil; 55.7 mg, 64% yield, >20:1 d.r., 98% *ee*; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.93 (s, 1H), 7.86 – 7.80 (m, 4H), 7.78 (d, *J* = 3.4 Hz, 1H), 7.75 (d, *J* = 7.3 Hz, 2H), 7.67 (dd, *J* = 8.5, 1.4 Hz, 1H), 7.51 – 7.43 (m, 3H), 7.39 – 7.30 (m, 5H), 7.27 – 7.21 (m, 5H), 5.29 (d, *J* = 11.7 Hz, 1H), 5.13 (d, *J* = 11.6 Hz, 1H), 4.45 (dd, *J* = 10.2, 3.0 Hz, 1H), 3.39 (dd, *J* = 16.6, 10.3 Hz, 1H), 3.11 (dd, *J* = 16.6, 3.0 Hz, 1H), 1.53 (s, 9H).

$^{13}C$ NMR (126 MHz, $CDCl_3$) δ 197.6, 169.6, 138.6, 136.9, 136.5, 133.3, 133.1, 133.0, 131.5, 128.5, 128.3, 128.2, 128.2, 128.2, 128.0, 128.0, 127.9, 127.7, 126.8, 126.1, 126.0, 125.9, 125.8, 123.5, 89.8, 85.9, 84.1, 82.9, 68.8, 39.2, 36.7, 28.1. HRMS (ESI) $[M+Na]^+$ calcd for $C_{40}H_{36}O_4Na^+$, 603.2506, found 603.2503. (Chiral IE-3, λ= 254 nm, *n*-hexane/2-propanol= 9/1, Flow rate = 1.0 mL/min), $t_R$ = 9.133 min(major), 16.891 min.

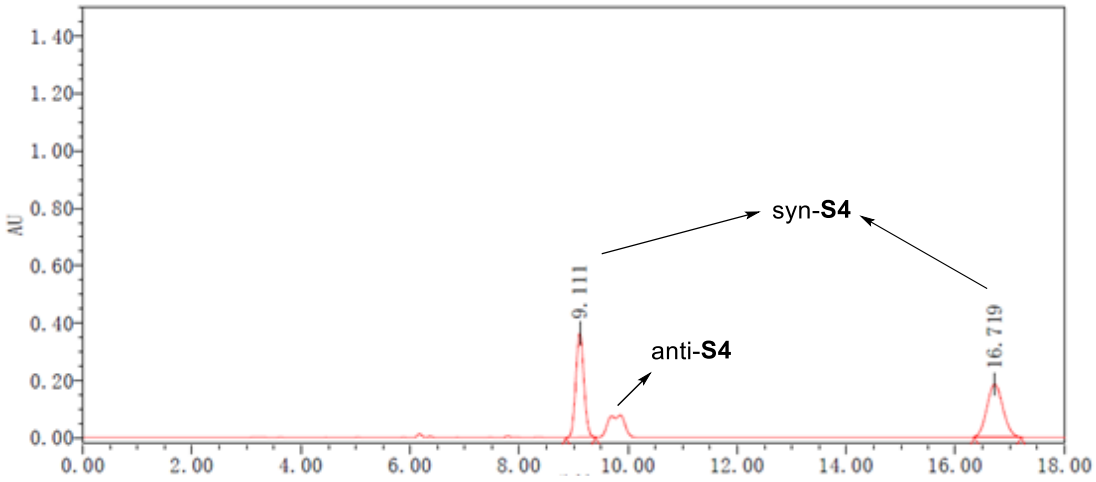
**HPLC chromatogram of racemic S4**

Condition: n-hexane/2-propanol =9:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 9.111 | 3709717 | 363477 | 49.66 |
| 2 | 16.719 | 3759995 | 184301 | 50.34 |

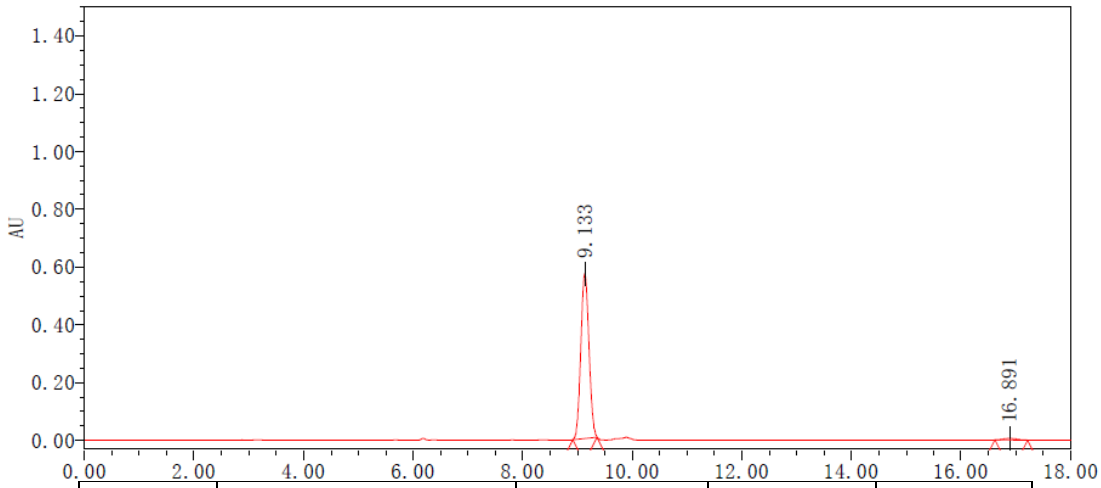
**HPLC chromatogram of chiral S4**

Condition: n-hexane/2-propanol =9:1

Flow rate =1.0 mL/min

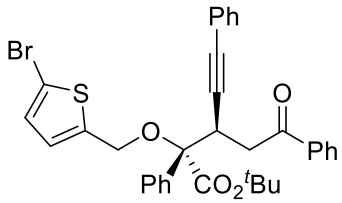
λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 9.133 | 5809594 | 570886 | 98.29 |
| 2 | 16.891 | 100823 | 5493 | 1.71 |

**Tert-butyl (2S,3R)-2-((5-bromothiophen-2-yl)methoxy)-3-(2-oxo-2-phenylethyl)-2,5-diphenylpent-4-ynoate(S5)**




**S5**

Colorless oil; 54.8 mg, 59% yield, >20:1 d.r., 98% *ee*; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.90 – 7.86 (m, 2H), 7.70 – 7.65 (m, 2H), 7.55 – 7.50 (m, 1H), 7.42 (t, *J* = 7.6 Hz, 2H), 7.37 (t, *J* = 7.4 Hz, 2H), 7.31 (d, *J* = 7.1 Hz, 1H), 7.26 – 7.20 (m, 5H), 6.92 (d, *J* = 3.7 Hz, 1H), 6.78 (d, *J* = 3.7 Hz, 1H), 5.25 (d, *J* = 11.9 Hz, 1H), 5.05 (d, *J* = 11.9 Hz, 1H), 4.40 (dd, *J* = 10.3, 2.9 Hz, 1H), 3.37 (dd, *J* = 16.7, 10.3 Hz, 1H), 3.06 (dd, *J* = 16.7, 2.9 Hz, 1H), 1.53 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 197.4, 169.2, 143.8, 138.1, 136.9,

133.2, 131.4, 129.2, 128.6, 128.4, 128.3, 128.2, 128.2, 127.9, 126.6, 125.6, 123.3, 112.3, 89.5, 86.0, 84.2, 83.1, 64.4, 39.1, 36.4, 28.1. HRMS (ESI) $[M+Na]^+$ calcd for $C_{34}H_{31}O_4SNa^+$, 637.1022, found 637.1019. (Chiral IE-3, λ= 254 nm, *n*-hexane/2-propanol= 49/1, Flow rate = 1.0 mL/min), $t_R$ = 11.816 min(major), 26.455 min.

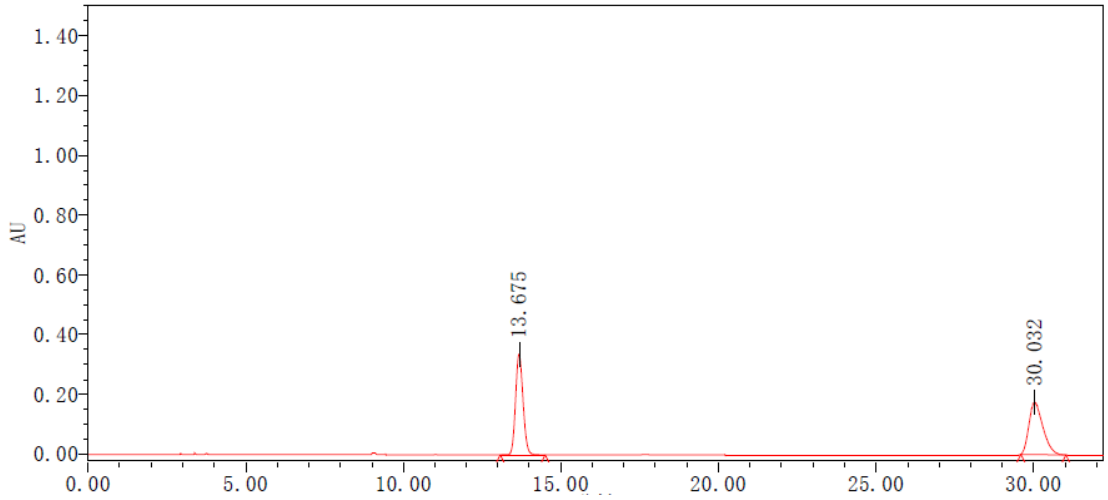
**HPLC chromatogram of racemic S5**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 13.675 | 5450368 | 336283 | 50.13 |
| 2 | 30.032 | 5422602 | 175098 | 49.87 |

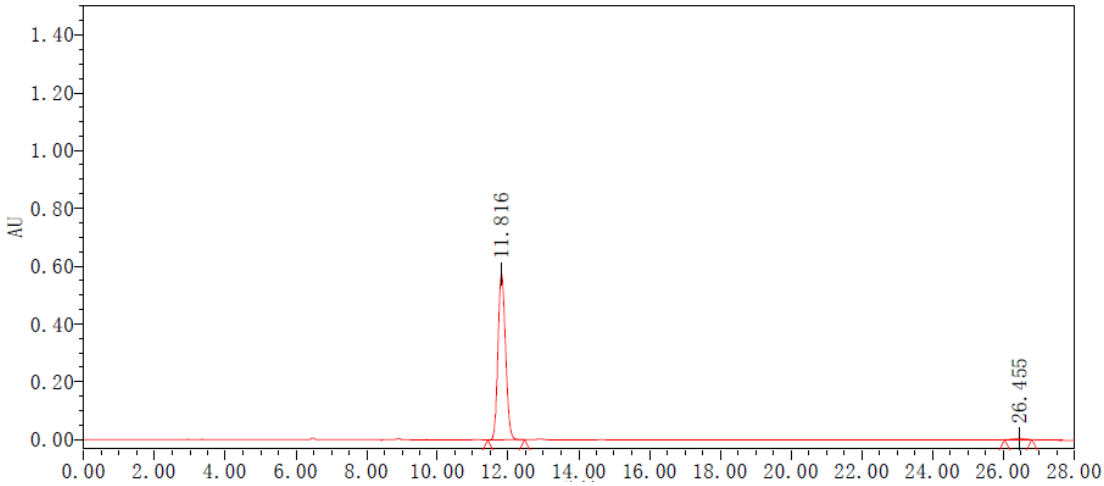
**HPLC chromatogram of chiral S5**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

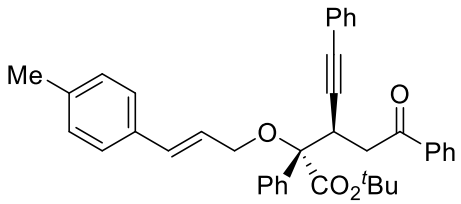
λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 11.816 | 8420273 | 574023 | 98.91 |
| 2 | 26.455 | 92707 | 3488 | 1.09 |

**Tert-butyl (2S,3R)-3-(2-oxo-2-phenylethyl)-2,5-diphenyl-2-(((E)-3-(p-tolyl)allyl)oxy)pent-4-ynoate (S6)**




**S6**

Colorless oil; 57.3 mg, 67% yield, >20:1 d.r., 95% *ee*; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 7.7 Hz, 2H), 7.75 (d, *J* = 7.7 Hz, 2H), 7.55 (t, *J* = 7.3 Hz, 1H), 7.42 (dd, *J* = 17.1, 7.9 Hz, 4H), 7.37 – 7.31 (m, 3H), 7.28 (dd, *J* = 7.9, 3.6 Hz, 5H), 7.16 (d, *J* = 7.8 Hz, 2H), 6.71 (d, *J* = 15.9 Hz, 1H), 6.42 (dt, *J* = 15.9, 5.7 Hz, 1H), 4.72 (dd, *J* = 12.5, 6.1 Hz, 1H), 4.58 (dd, *J* = 12.4, 5.1 Hz, 1H), 4.40 (dd, *J* = 10.1, 2.8 Hz, 1H), 3.42 (dd, *J* = 16.6, 10.2 Hz, 1H), 3.19 (dd, *J* = 16.6, 2.7 Hz, 1H), 2.37 (s, 3H), 1.57 (s, 9H). $^{13}$C

NMR (126 MHz, $CDCl_3$) δ 197.7, 169.6, 138.6, 137.4, 137.0, 134.2, 133.1, 131.5, 131.4, 129.3, 128.5, 128.3, 128.2, 128.1, 127.8, 126.8, 126.5, 125.6, 123.5, 89.8, 85.7, 84.0, 82.7, 67.8, 39.3, 36.7, 28.1, 21.3. HRMS (ESI) $[M+Na]^+$ calcd for $C_{39}H_{38}O_4Na^+$, 593.2662, found 593.2660. (Chiral IE-3, λ= 254 nm, *n*-hexane/2-propanol= 19/1, Flow rate = 1.0 mL/min), $t_R$ = 11.699 min(major), 22.829 min.

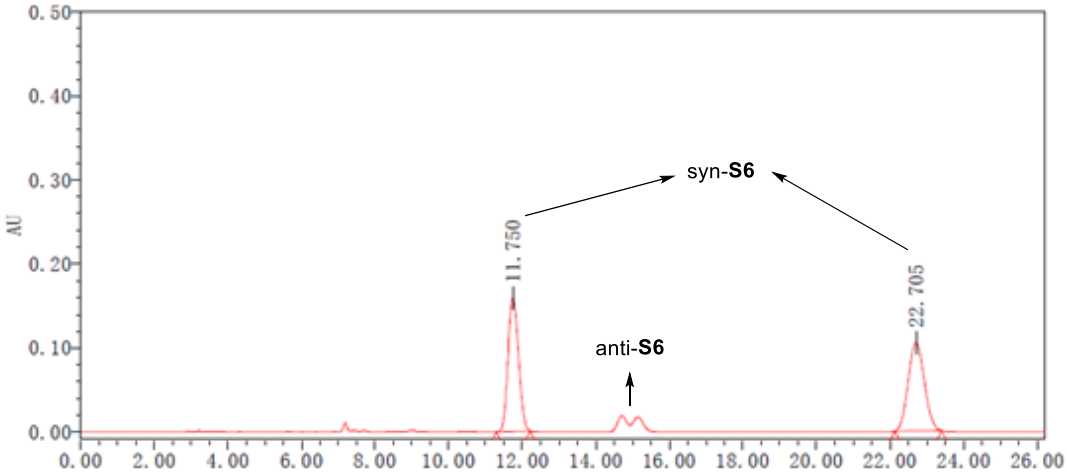
**HPLC chromatogram of racemic S6**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 11.750 | 3169783 | 159177 | 49.73 |
| 2 | 22.705 | 3203819 | 104988 | 50.27 |

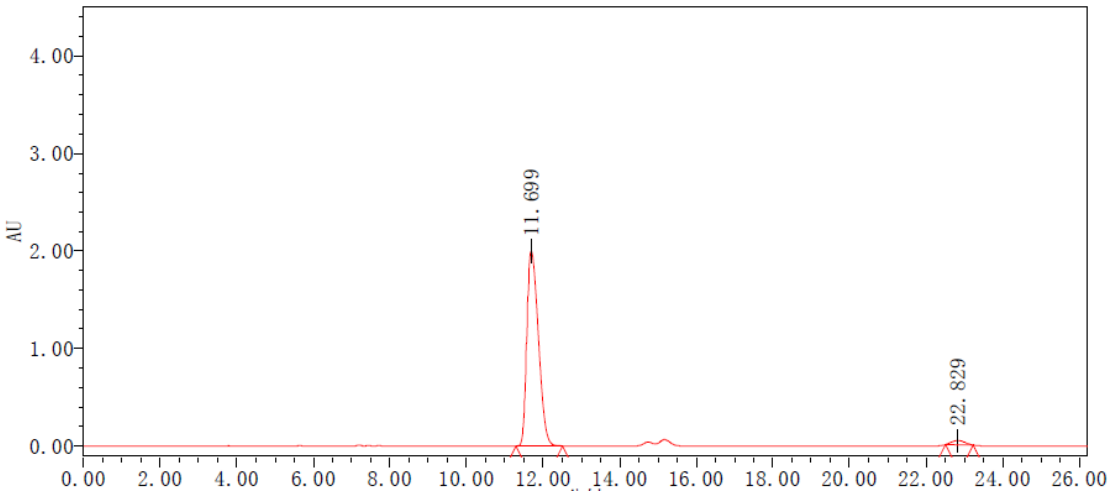
**HPLC chromatogram of chiral S6**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

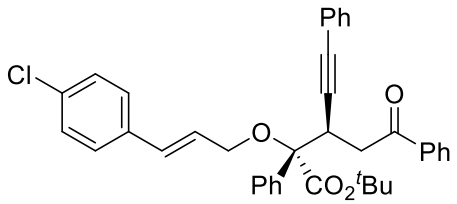
λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 11.699 | 42219463 | 1996671 | 1996671 |
| 2 | 22.829 | 1071593 | 43996 | 43996 |

**Tert-butyl (2S,3R)-2-(((E)-3-(4-chlorophenyl)allyl)oxy)-3-(2-oxo-2-phenylethyl)-2,5-diphenylpent-4-ynoate (S7)**




**S7**

Colorless oil; 48.7 mg, 55% yield, >20:1 d.r., 96% *ee*; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 7.8 Hz, 2H), 7.70 (d, *J* = 7.8 Hz, 2H), 7.52 (t, *J* = 7.3 Hz, 1H), 7.39 (dd, *J* = 16.5, 8.0 Hz, 4H), 7.30 (dd, *J* = 15.9, 6.2 Hz, 4H), 7.24 (d, *J* = 8.7 Hz, 5H), 6.66 (d, *J* = 16.0 Hz, 1H), 6.39 (dt, *J* = 15.9, 5.5 Hz, 1H), 4.67 (dd, *J* = 12.9, 5.8 Hz, 1H), 4.53 (dd, *J* = 12.9, 5.1 Hz, 1H), 4.37 (dd, *J* = 10.0, 2.9 Hz, 1H), 3.36 (dd, *J* = 16.6, 10.1 Hz, 1H), 3.16 (dd, *J* = 16.6, 2.9 Hz, 1H), 1.53 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 197.5, 169.5, 138.4, 137.0, 135.5, 133.1, 131.4, 130.2, 128.7, 128.6, 128.2, 128.2, 127.8, 127.7,

127.4, 126.8, 123.5, 89.7, 85.8, 84.0, 82.8, 67.4, 39.3, 36.7, 28.1. Peak overlapping was observed. HRMS (ESI) $[M+Na]^+$ calcd for $C_{38}H_{35}O_4ClNa^+$, 613.2116 found 613.2117. (Chiral IA, λ= 254 nm, *n*-hexane/2-propanol= 49/1, Flow rate = 1.0 mL/min), $t_R$ = 14.402 min(major), 26.664 min.

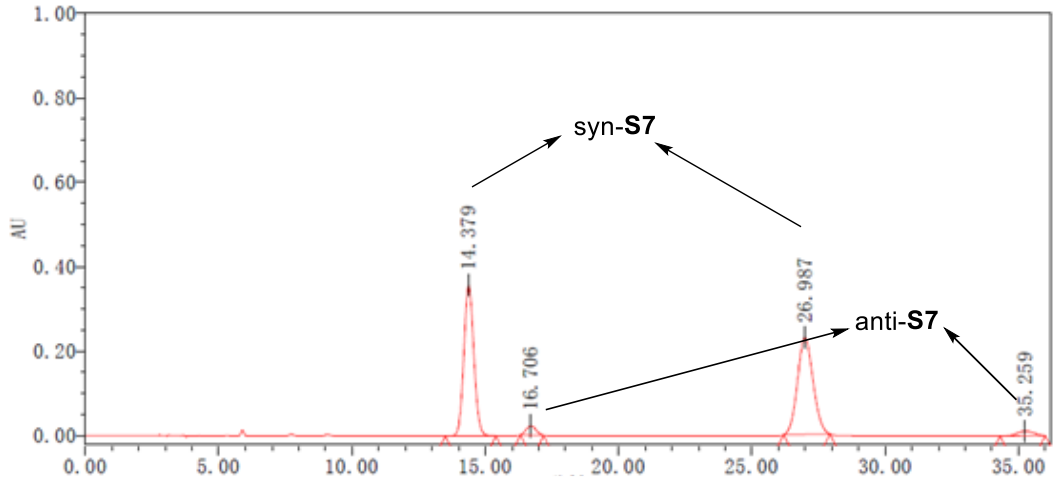
**HPLC chromatogram of racemic S7**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 14.379 | 9188676 | 357265 | 46.81 |
| 2 | 16.706 | 561913 | 21788 | 2.86 |
| 3 | 26.987 | 9386302 | 230325 | 47.81 |
| 4 | 35.259 | 493876 | 11178 | 2.52 |

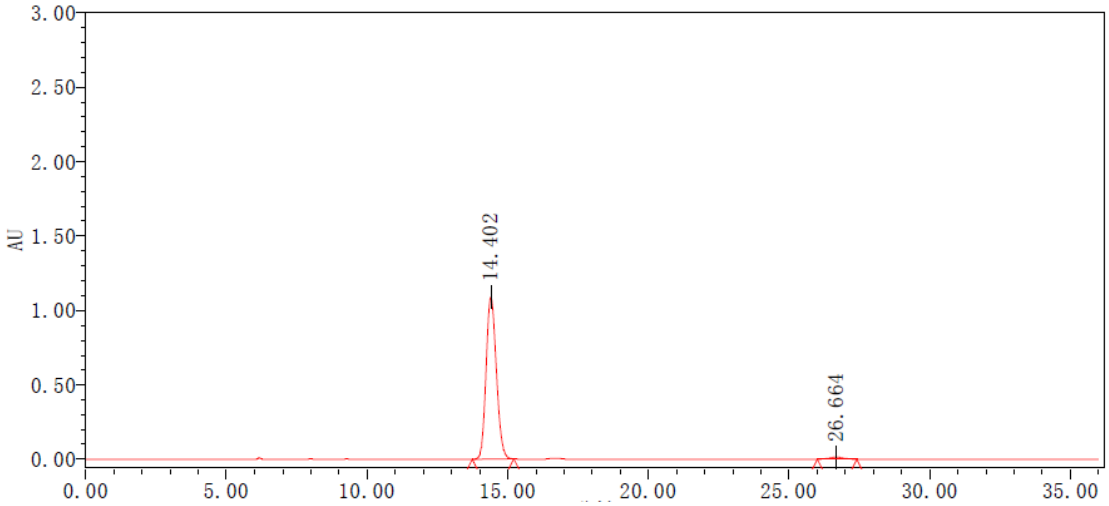
**HPLC chromatogram of chiral S7**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

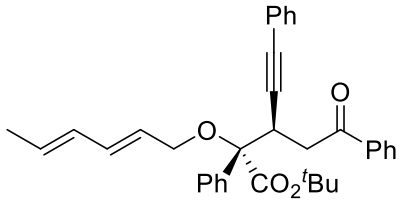
λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 14.402 | 27235904 | 1088645 | 98.15 |
| 2 | 26.664 | 514553 | 13291 | 1.85 |

**Tert-butyl (2S,3R)-2-(((2E,5E)-hepta-2,5-dien-1-yl)oxy)-3-(2-oxo-2-phenylethyl)-2,5-diphenylpent-4-ynoate (S8)**




**S8**

Colorless oil; 47.6 mg, 61% yield, >20:1 d.r., 96% *ee*; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.92 – 7.86 (m, 2H), 7.70 – 7.66 (m, 2H), 7.53 (dd, *J* = 8.3, 6.4 Hz, 1H), 7.42 (t, *J* = 7.6 Hz, 2H), 7.35 (t, *J* = 7.4 Hz, 2H), 7.30 (d, *J* = 7.2 Hz, 1H), 7.23 (d, *J* = 13.3 Hz, 5H), 6.31 (dd, *J* = 15.2, 10.5 Hz, 1H), 6.10 (ddd, *J* = 14.7, 10.5, 1.3 Hz, 1H), 5.82 – 5.74 (m,

1H), 5.68 (dt, *J* = 13.6, 6.8 Hz, 1H), 4.54 (dd, *J* = 12.4, 6.3 Hz, 1H), 4.40 (dd, *J* = 12.4, 5.5 Hz, 1H), 4.31 (dd, *J* = 10.3, 3.0 Hz, 1H), 3.34 (dd, *J* = 16.6, 10.3 Hz, 1H), 3.11 (dd, *J* = 16.6, 3.0 Hz, 1H), 1.76 (d, *J* = 6.6 Hz, 3H), 1.51 (s, 9H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 197.7, 169.6, 138.7, 137.0, 133.0, 132.3, 131.4, 131.1, 129.7, 128.5, 128.3, 128.1, 128.1, 128.1, 127.8, 127.3, 126.8, 123.5, 89.8, 85.6, 83.9, 82.6, 67.4, 39.3, 36.7, 28.1, 18.2. HRMS (ESI) $[M+Na]^+$ calcd for $C_{35}H_{36}O_4Na^+$, 543.2506, found 543.2511. (Chiral IE-3, λ= 254 nm, *n*-hexane/2-propanol= 19/1, Flow rate = 1.0 mL/min), $t_R$ = 12.180 min(major), 29.777 min.

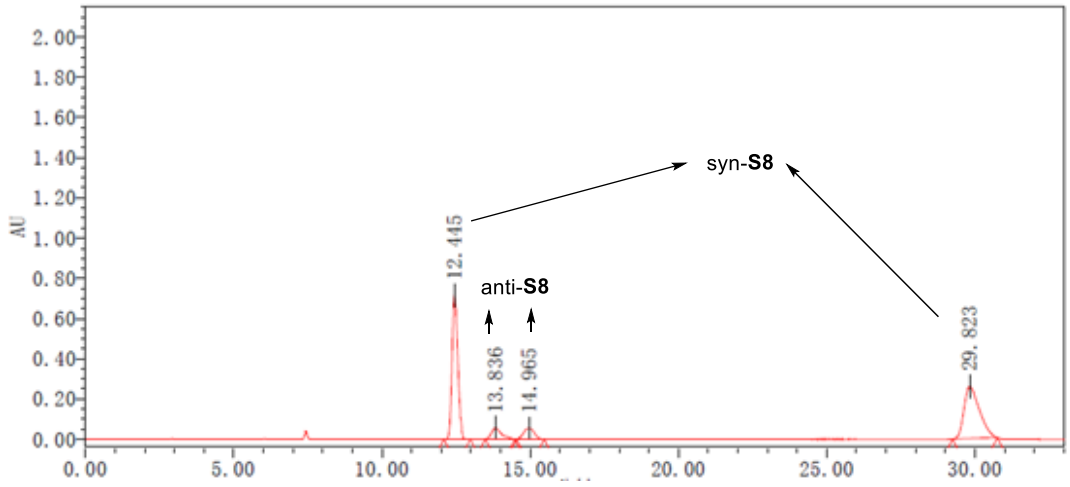
**HPLC chromatogram of racemic S8**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 12.445 | 9526285 | 714973 | 44.16 |
| 2 | 13.836 | 1264612 | 54689 | 5.86 |
| 3 | 14.965 | 1295139 | 53772 | 6.00 |

| | | | | |
|---|---|---|---|---|
| 4 | 29.823 | 9488227 | 258792 | 43.98 |

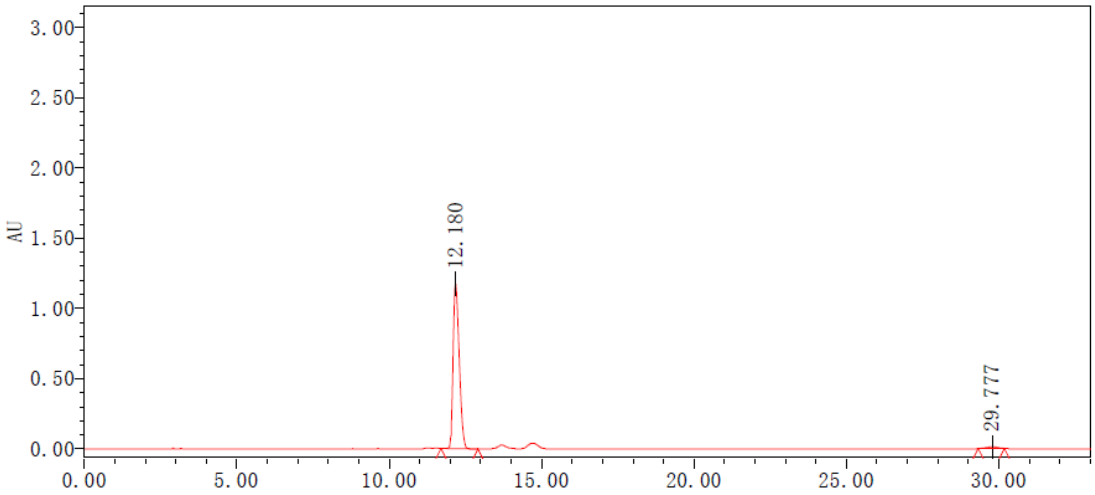
**HPLC chromatogram of chiral S8**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

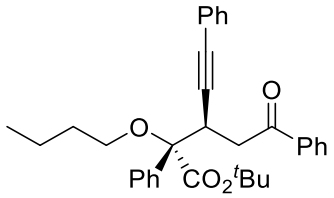
λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 12.180 | 16129059 | 1172400 | 98.07 |
| 2 | 29.777 | 316675 | 11032 | 1.93 |

**Tert-butyl (2S,3R)-2-butoxy-3-(2-oxo-2-phenylethyl)-2,5-diphenylpent-4-ynoate (S9)**




**S9**

Colorless oil; 44.6 mg, 60% yield, >20:1 d.r., 91% *ee*; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.92 – 7.87 (m, 2H), 7.68 – 7.65 (m, 2H), 7.56 – 7.51 (m, 1H), 7.42 (dd, *J* = 10.4, 4.8 Hz, 2H), 7.38 – 7.32 (m, 2H), 7.30 (dt, *J* = 4.8, 1.9 Hz, 1H), 7.27 – 7.21 (m, 5H), 4.30 (dt, *J* = 5.7, 3.1 Hz, 1H), 3.96 (dt, *J* = 8.8, 6.5 Hz, 1H), 3.77 (dt, *J* = 8.8, 6.4 Hz, 1H), 3.27 (dd, *J* = 16.6, 9.9 Hz, 1H), 3.16 (dd, *J* = 16.6, 3.3 Hz, 1H), 1.73 – 1.64 (m, 2H), 1.56 (d, *J* = 12.4 Hz, 2H), 1.51 (s, 9H), 0.95 (t, *J* = 7.4 Hz, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 197.7, 169.7, 139.0, 137.1, 133.0, 131.4, 128.5, 128.2, 128.1, 128.0, 127.9, 127.7, 126.8, 123.6, 89.8, 85.2, 83.8, 82.4, 66.1, 39.4, 36.4, 32.6, 28.1, 19.5, 14.1. HRMS (ESI) $[M+Na]^+$ calcd for $C_{33}H_{36}O_4Na^+$, 519.2506, found 519.2506. (Chiral IC, λ= 254 nm, *n*-hexane/2-propanol= 49/1, Flow rate = 1.0 mL/min), $t_R$ = 6.216 min(major), 10.255 min.

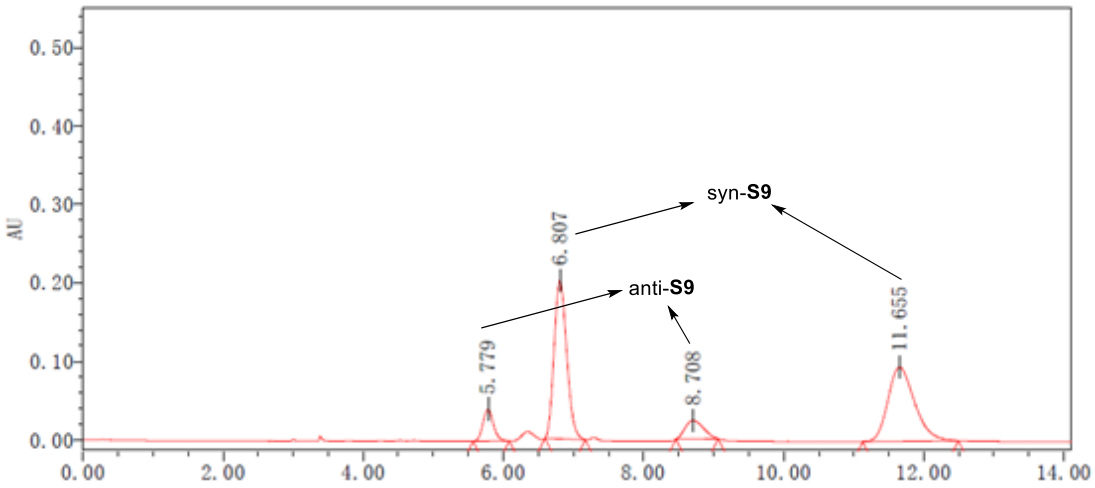
**HPLC chromatogram of racemic S9**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IC




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 5.779 | 424595 | 40448 | 7.25 |
| 2 | 6.807 | 2499194 | 201354 | 42.69 |
| 3 | 8.708 | 437991 | 23845 | 7.48 |
| 4 | 11.655 | 2492428 | 94442 | 42.57 |

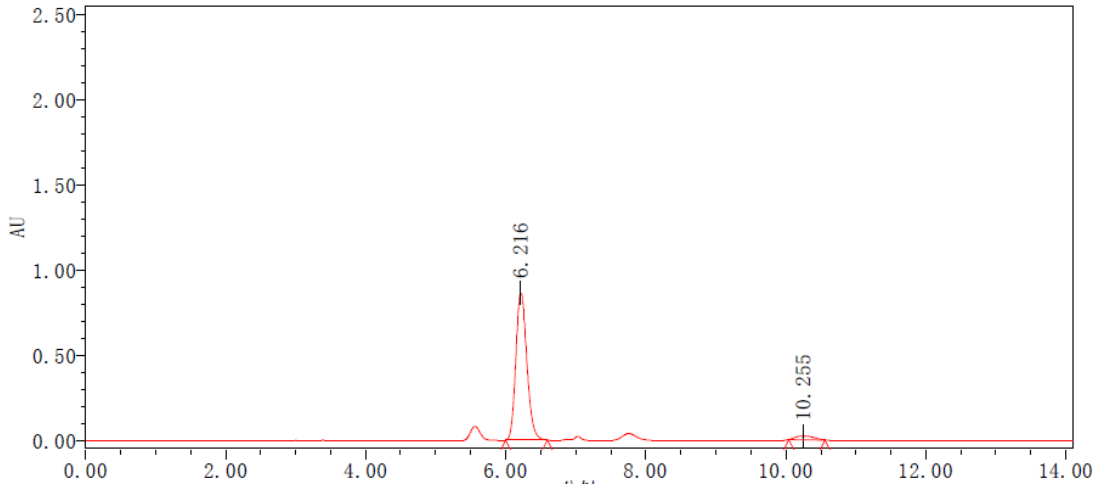
**HPLC chromatogram of chiral S9**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

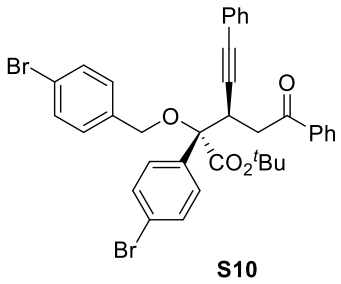
λ= 254 nm

Chiral IC




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 6.216 | 9553422 | 865316 | 95.99 |
| 2 | 10.255 | 398966 | 22998 | 4.01 |

**Tert-butyl (2S,3R)-2-((4-bromobenzyl)oxy)-2-(4-bromophenyl)-3-(2-oxo-2-phenylethyl)-5-phenylpent-4-ynoate (S10)**




**S10**

Colorless oil; 66.9 mg, 65% yield, >20:1 d.r., 98% *ee*; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 7.7 Hz, 2H), 7.60 (d, *J* = 8.5 Hz, 2H), 7.56 (d, *J* = 6.4 Hz, 1H), 7.53 – 7.49 (m, 3H), 7.45 (t, *J* = 7.5 Hz, 3H), 7.38 (d, *J* = 8.0 Hz, 2H), 7.29 (d, *J* = 12.4 Hz, 5H), 5.04 (d, *J* = 11.6 Hz, 1H), 4.91 (d, *J* = 11.6 Hz, 1H), 4.42 (dd, *J* = 9.7, 2.4 Hz, 1H), 3.34 (dd, *J* = 16.6, 9.9 Hz, 1H), 3.11 (dd, *J* = 16.6, 2.3 Hz, 1H), 1.54 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 197.2, 169.0, 137.7, 137.5, 136.8, 133.3, 131.5, 131.4, 131.4, 129.2, 128.6, 128.6, 128.3, 128.2, 128.1, 123.2, 122.6, 121.4, 89.2, 85.5, 84.4, 83.3, 68.0, 39.2, 36.4, 28.1. HRMS (ESI) $[M+Na]^+$ calcd for $C_{36}H_{32}O_4Br_2Na^+$, 709.0560, found

709.0556. (Chiral IB-3, λ= 254 nm, *n*-hexane/2-propanol= 19/1, Flow rate = 1.0 mL/min), $t_R$ = 7.844 min(major), 19.889 min.

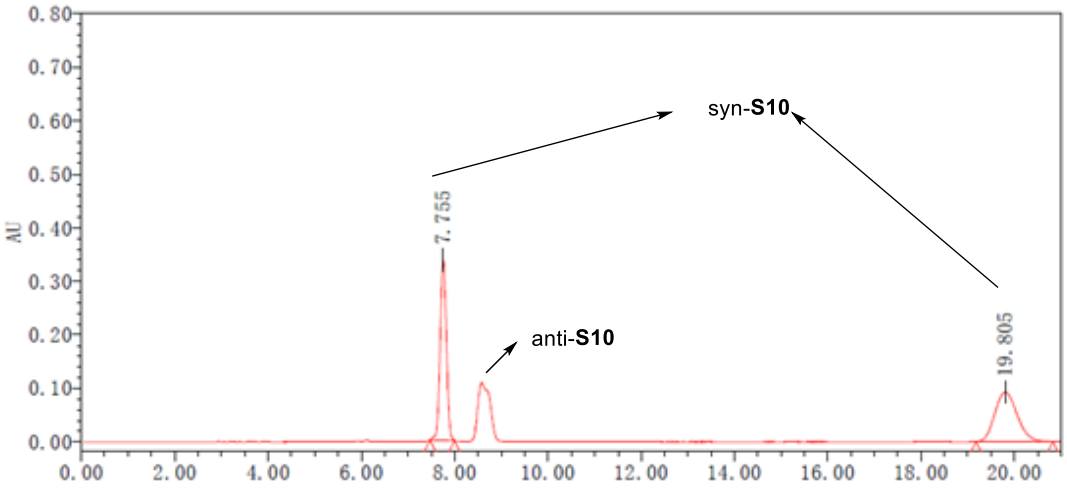
**HPLC chromatogram of racemic S10**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IB-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 7.755 | 3102464 | 336655 | 50.22 |
| 2 | 19.805 | 3074689 | 92541 | 49.78 |

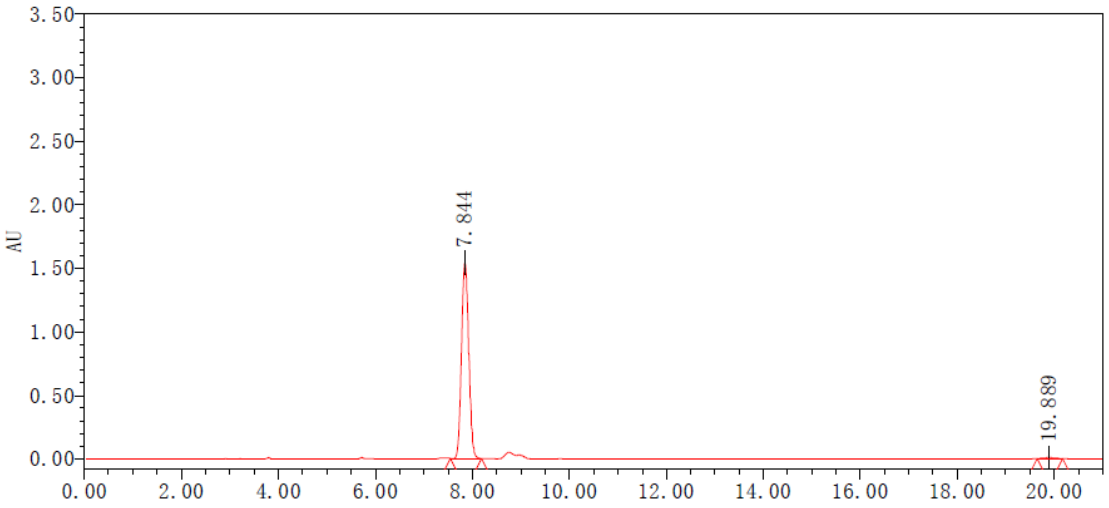
**HPLC chromatogram of chiral S10**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

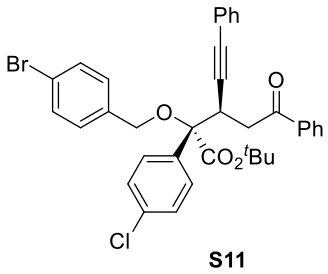
λ= 254 nm

Chiral IB-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 7.844 | 7.844 | 1540462 | 99.26 |
| 2 | 19.889 | 19.889 | 6348 | 0.74 |

**Tert-butyl (2S,3R)-2-((4-bromobenzyl)oxy)-2-(4-chlorophenyl)-3-(2-oxo-2-phenylethyl)-5-phenylpent-4-ynoate (S11)**




**S11**

Colorless oil; 59.7 mg, 62% yield, >20:1 d.r., 99% *ee*; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.94 – 7.90 (m, 2H), 7.55 (dd, *J* = 10.5, 4.3 Hz, 1H), 7.46 – 7.40 (m, 3H), 7.30 (dd, *J* = 7.2, 3.7 Hz, 2H), 7.28 – 7.24 (m, 8H), 7.20 (d, *J* = 8.4 Hz, 2H), 4.93 (d, *J* = 11.4 Hz, 1H), 4.72 (d, *J* = 11.4 Hz, 1H), 3.91 (dd, *J* = 8.6, 4.0 Hz, 1H), 3.65 (dd, *J* = 17.1, 4.0 Hz, 1H), 3.35 (t, *J* = 4.2 Hz, 1H), 1.48 (s, 9H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 197.5, 169.7, 137.2, 136.9, 134.2, 133.2, 132.3, 132.0, 131.5, 131.4, 131.4, 129.1, 128.6, 128.3, 128.2, 128.1, 121.4, 121.3, 89.0, 84.4, 82.8, 66.8, 39.1, 34.0, 28.2. HRMS (ESI)

$[M+Na]^+$ calcd for $C_{36}H_{32}O_4ClBrNa^+$, 665.1065, found 665.1063. (Chiral IE-3, λ= 254 nm, *n*-hexane/2-propanol= 19/1, Flow rate = 1.0 mL/min), $t_R$ = 7.627 min(major), 18.483 min.

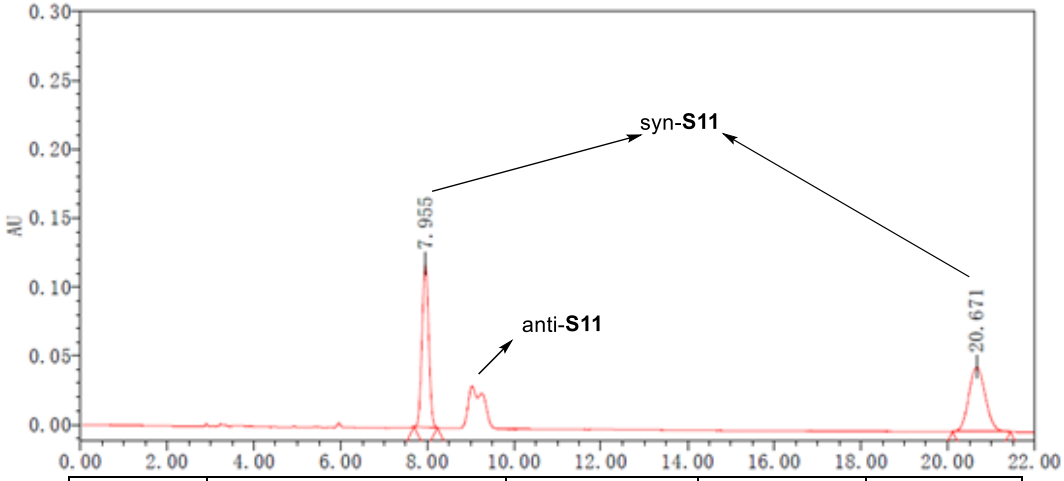
**HPLC chromatogram of racemic S11**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 7.955 | 1251355 | 118414 | 50.23 |
| 2 | 20.671 | 1239917 | 46930 | 49.77 |

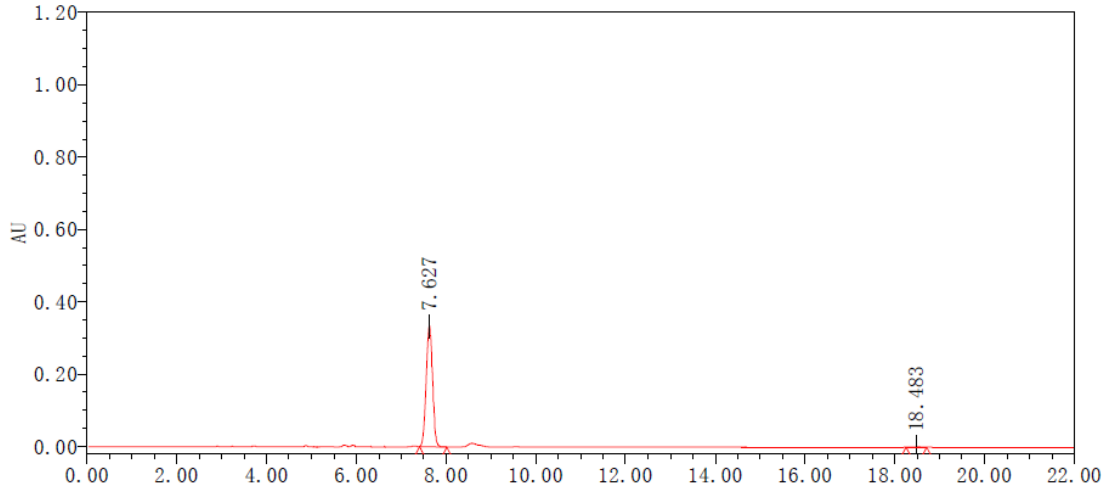
**HPLC chromatogram of chiral S11**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

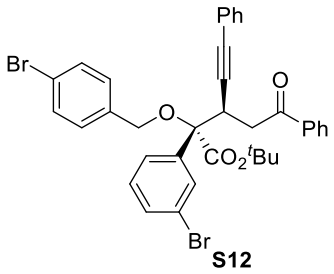
λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 7.627 | 3295096 | 332931 | 99.54 |
| 2 | 18.483 | 15133 | 888 | 0.46 |

**Tert-butyl (2S,3R)-2-((4-bromobenzyl)oxy)-2-(3-bromophenyl)-3-(2-oxo-2-phenylethyl)-5-phenylpent-4-ynoate (S12)**



**S12**

Colorless oil; 64.8 mg, 63% yield, >20:1 d.r., 98% *ee*; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.94 – 7.85 (m, 3H), 7.63 (d, *J* = 7.9 Hz, 1H), 7.56 (d, *J* = 7.3 Hz, 1H), 7.53 – 7.43 (m, 5H), 7.39 (d, *J* = 8.1 Hz, 2H), 7.26 (d, *J* = 9.1 Hz, 6H), 5.05 (d, *J* = 11.6 Hz, 1H), 4.90 (d, *J* = 11.6 Hz, 1H), 4.38 (dd, *J* = 9.9, 2.9 Hz, 1H), 3.34 (dd, *J* = 16.6, 10.0 Hz, 1H), 3.12 (dd, *J* = 16.6, 2.9 Hz, 1H), 1.55 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 197.1, 168.8, 140.7, 137.6, 136.8, 133.2, 131.5, 131.4, 131.4, 130.2, 129.8, 129.3, 128.6, 128.2, 128.2, 128.1, 125.3, 123.1, 122.6, 121.5, 89.0, 85.4, 84.5, 83.4, 68.1, 39.1, 36.8, 28.1.

HRMS (ESI) $[M+Na]^+$ calcd for $C_{36}H_{32}O_4Br_2Na^+$, 709.0560, found 709.0556. (Chiral IB-3, λ= 254 nm, *n*-hexane/2-propanol= 19/1, Flow rate = 1.0 mL/min), $t_R$ = 8.016 min(major), 13.851 min.

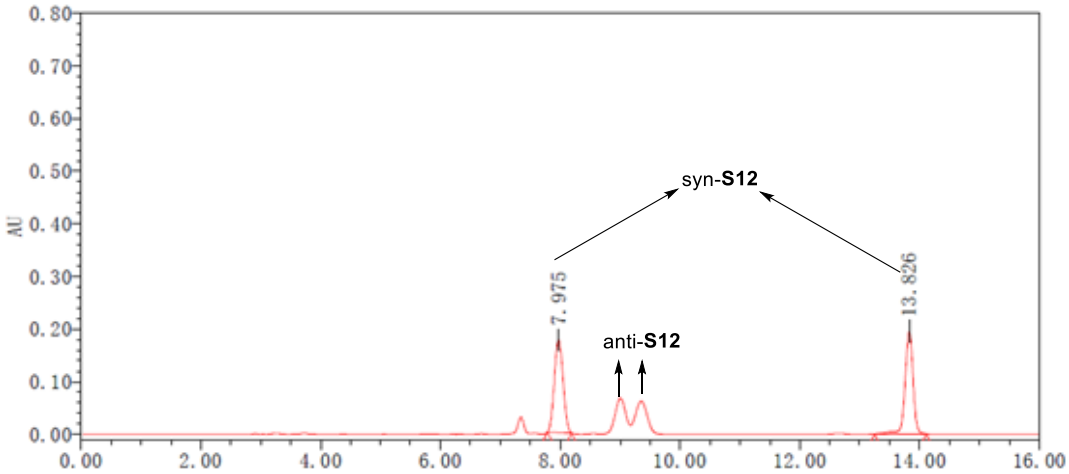
**HPLC chromatogram of racemic S12**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IB-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 7.975 | 1794228 | 176673 | 50.07 |
| 2 | 13.826 | 1789114 | 194895 | 49.93 |

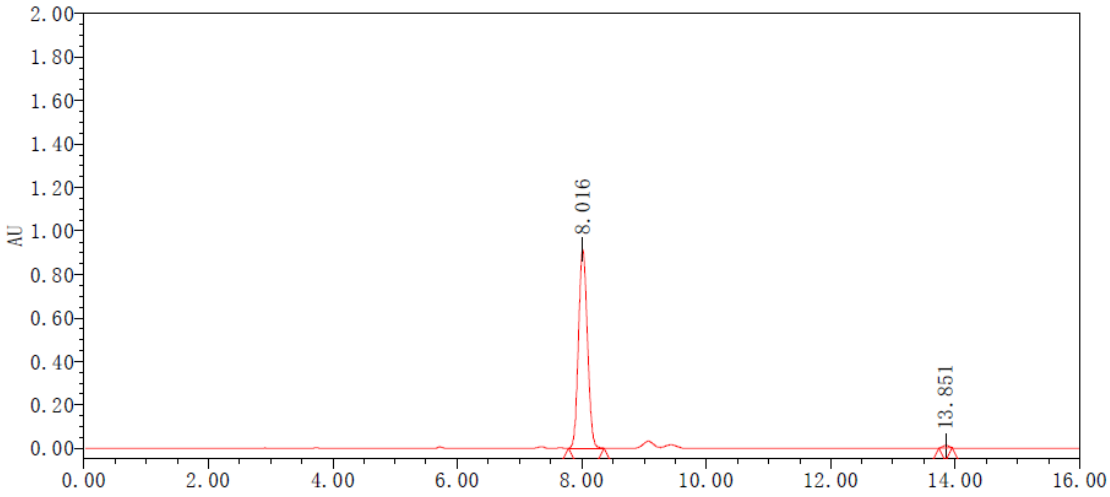
**HPLC chromatogram of chiral S12**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

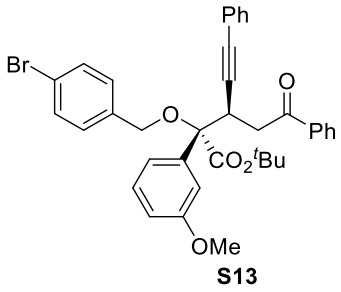
λ= 254 nm

Chiral IB-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 8.016 | 8985138 | 912719 | 99.13 |
| 2 | 13.851 | 79285 | 11462 | 0.87 |

**Tert-butyl (2S,3R)-2-((4-bromobenzyl)oxy)-2-(3-methoxyphenyl)-3-(2-oxo-2-phenylethyl)-5-phenylpent-4-ynoate (S13)**




**S13**

Colorless oil; 53.6 mg, 56% yield, >20:1 d.r., 98% *ee*; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, *J* = 7.8 Hz, 2H), 7.53 (t, *J* = 7.3 Hz, 1H), 7.47 (d, *J* = 8.2 Hz, 2H), 7.40 (dd, *J* = 14.9, 7.8 Hz, 5H), 7.28 – 7.21 (m, 7H), 6.85 (d, *J* = 7.4 Hz, 1H), 5.06 (d, *J* = 11.8 Hz, 1H), 4.91 (d, *J* = 11.8 Hz, 1H), 4.38 (dd, *J* = 10.1, 2.8 Hz, 1H), 3.76 (s, 3H), 3.31 (dd, *J* = 16.5, 10.2 Hz, 1H), 3.10 (dd, *J* = 16.6, 2.7 Hz, 1H), 1.52 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 197.4, 169.3, 159.5, 139.9, 138.1, 136.9, 133.1, 131.4, 129.3, 129.2, 128.6, 128.2, 127.9, 123.4, 121.2, 119.0, 113.8, 112.6, 89.7, 85.8, 84.1, 83.0, 68.0, 55.2,

39.2, 36.7, 28.1. Peak overlapping was observed. HRMS (ESI) $[M+Na]^+$ calcd for $C_{37}H_{35}O_5BrNa^+$, 661.1560, found 661.1562. (Chiral IA, λ= 254 nm, *n*-hexane/2-propanol= 49/1, Flow rate = 1.0 mL/min), $t_R$ = 13.274 min(major), 20.423 min.

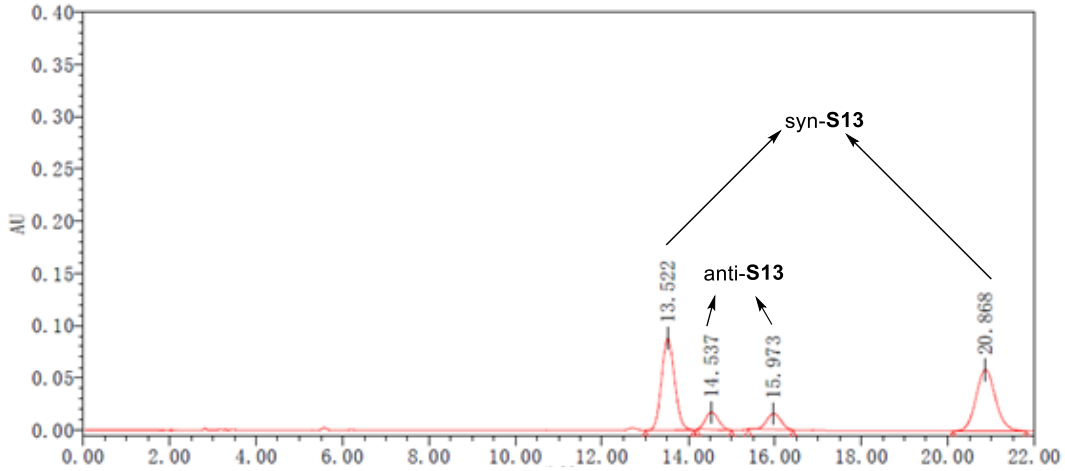
**HPLC chromatogram of racemic S13**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 13.522 | 1839535 | 88180 | 42.01 |
| 2 | 14.537 | 347844 | 16736 | 7.94 |
| 3 | 15.973 | 352199 | 15306 | 8.04 |
| 4 | 20.868 | 1838956 | 58725 | 42.00 |

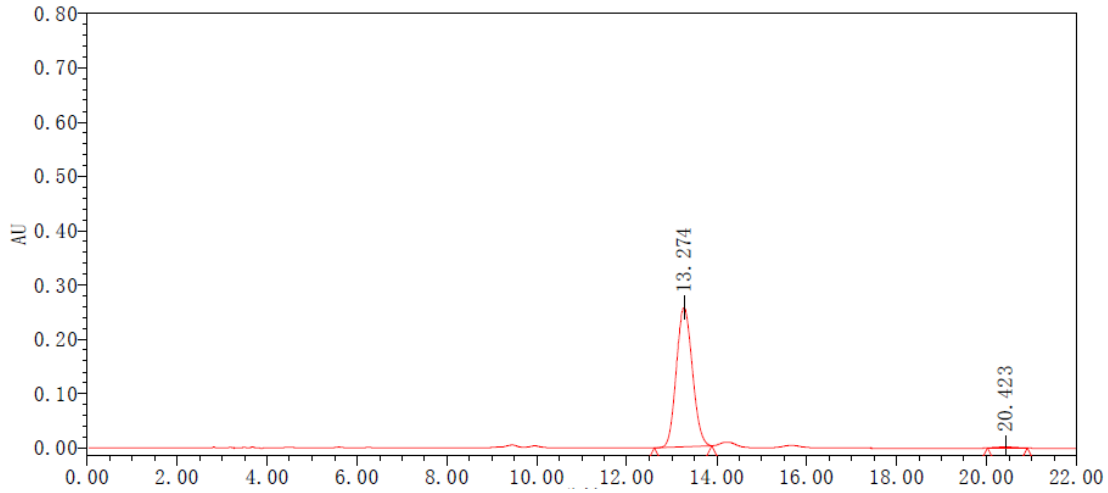
**HPLC chromatogram of chiral S13**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

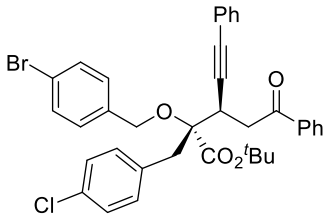
λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 13.274 | 6383182 | 255928 | 99.19 |
| 2 | 20.423 | 51804 | 1808 | 0.81 |

**Tert-butyl (2R,3R)-2-((4-bromobenzyl)oxy)-2-(4-chlorobenzyl)-3-(2-oxo-2-phenylethyl)-5-phenylpent-4-ynoate (S14)**




**S14**

Colorless oil; 39.4 mg, 40% yield, >20:1 d.r., 92% *ee*; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.93 – 7.89 (m, 2H), 7.58 – 7.53 (m, 1H), 7.46 – 7.41 (m, 4H), 7.30 (d, *J* = 3.5 Hz, 2H), 7.27 – 7.24 (m, 7H), 7.20 (d, *J* = 8.4 Hz, 2H), 4.93 (d, *J* = 11.4 Hz, 1H), 4.72 (d, *J* = 11.4 Hz, 1H), 3.91 (dd, *J* = 8.6, 4.0 Hz, 1H), 3.65 (dd, *J* = 17.1, 4.0 Hz, 1H), 3.39 – 3.35 (m, 1H), 3.30 (dd, *J* = 31.9, 9.3 Hz, 2H), 1.48 (s, 9H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 197.5, 169.6, 137.2, 136.9, 134.2, 133.1, 132.8, 132.0, 131.5, 131.4, 129.0, 128.6, 128.2, 128.2, 128.1, 123.1, 123.0, 121.3, 88.9, 84.4, 82.8, 66.8, 39.1, 34.1, 28.2. HRMS

(ESI) $[M+Na]^+$ calcd for $C_{37}H_{34}O_4ClBrNa^+$, 679.1220, found 679.1220. (Chiral IA-3, λ= 254 nm, *n*-hexane/2-propanol= 49/1, Flow rate = 1.0 mL/min), $t_R$ = 12.288 min(major), 15.866 min.

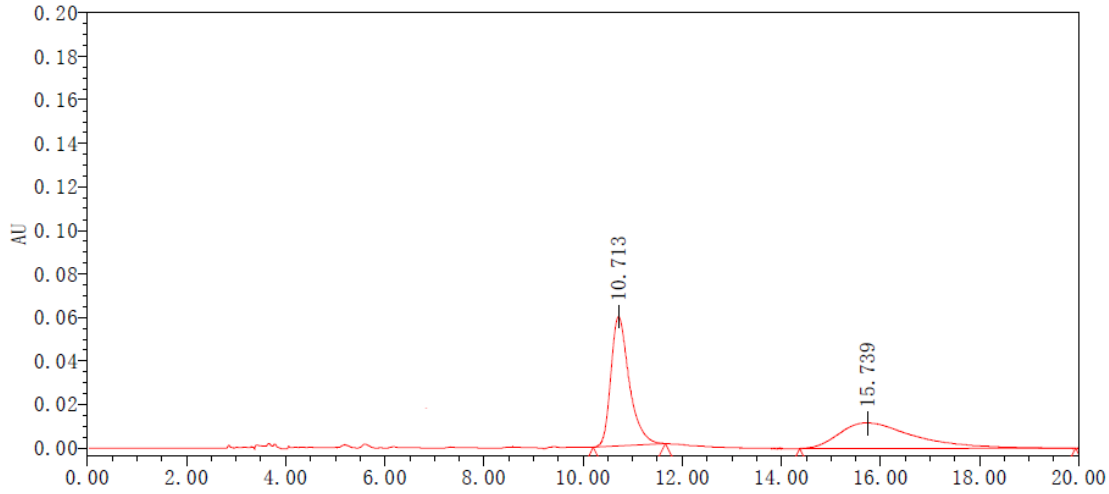
**HPLC chromatogram of racemic S14**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 10.713 | 1376091 | 59478 | 49.57 |
| 2 | 15.739 | 1393337 | 11704 | 50.43 |

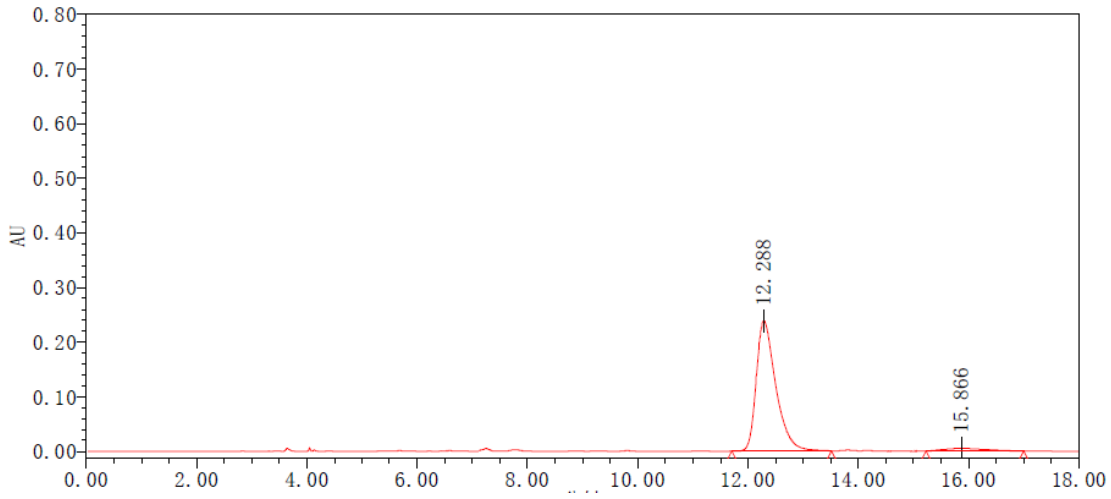
**HPLC chromatogram of chiral S14**

Condition: n-hexane/2-propanol =49:1

Flow rate =1.0 mL/min

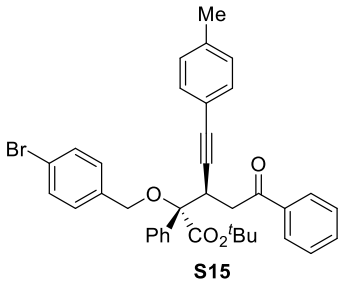
λ= 254 nm

Chiral IA-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 12.288 | 5870048 | 5870048 | 96.00 |
| 2 | 15.866 | 244783 | 244783 | 4.00 |

**Tert-butyl (2S,3R)-2-((4-bromobenzyl)oxy)-3-(2-oxo-2-phenylethyl)-2-phenyl-5-(p-tolyl)pent-4-ynoate (S15)**




**S15**

Colorless oil; 51.3 mg, 55% yield, >20:1 d.r., 99% *ee*; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.86 – 7.80 (m, 2H), 7.71 – 7.67 (m, 2H), 7.52 (t, *J* = 7.4 Hz, 1H), 7.49 – 7.46 (m, 2H), 7.40 (dd, *J* = 7.3, 3.3 Hz, 3H), 7.38 – 7.33 (m, 3H), 7.32 – 7.29 (m, 1H), 7.13 (d, *J* = 8.1 Hz, 2H), 7.03 (d, *J* = 7.9 Hz, 2H), 5.06 (d, *J* = 11.8 Hz, 1H), 4.91 (d, *J* = 11.8 Hz, 1H), 4.40 (dd, *J* = 10.1, 3.0 Hz, 1H), 3.31 (dd, *J* = 16.6, 10.2 Hz, 1H), 3.07 (dd, *J* = 16.6, 3.1 Hz, 1H), 2.30 (s, 3H), 1.51 (s, 9H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 197.5, 169.4, 138.4, 138.1, 137.9, 137.0, 133.1, 131.4, 131.3, 129.2, 129.0, 128.5, 128.3, 128.2,

128.2, 126.7, 121.2, 120.3, 88.9, 85.9, 84.2, 82.9, 68.0, 39.2, 36.6, 28.1, 21.4. HRMS (ESI) $[M+Na]^+$ calcd for $C_{37}H_{35}O_4BrNa^+$, 645.1611, found 645.1608. (Chiral IA-3, λ= 254 nm, *n*-hexane/2-propanol= 19/1, Flow rate = 1.0 mL/min), $t_R$ = 8.054 min(major), 9.316 min.

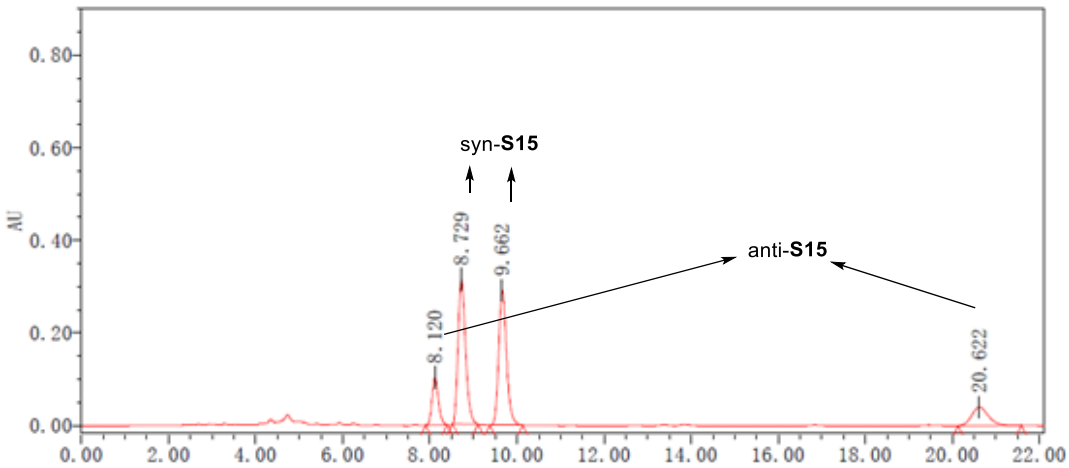
**HPLC chromatogram of racemic S15**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 8.120 | 1046835 | 102902 | 11.07 |
| 2 | 8.729 | 3697670 | 312862 | 39.12 |
| 3 | 9.662 | 3661343 | 291250 | 38.73 |
| 4 | 20.622 | 1047061 | 39932 | 11.08 |

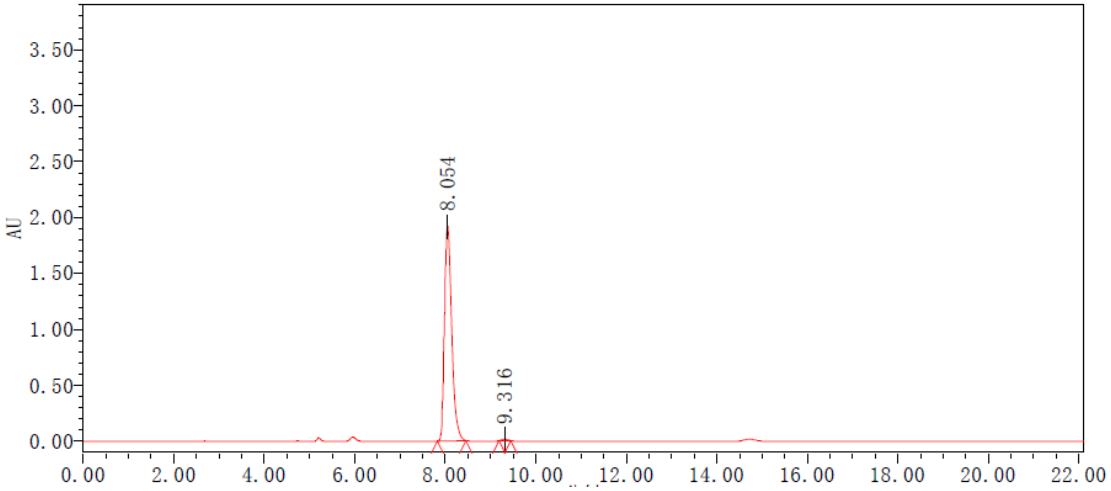
**HPLC chromatogram of chiral S15**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

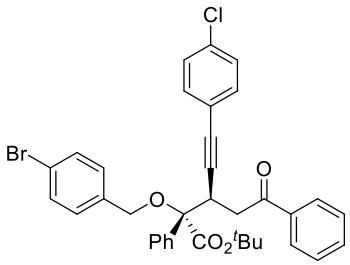
λ= 254 nm

Chiral IA-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 8.054 | 21441076 | 1915487 | 99.47 |
| 2 | 9.316 | 114358 | 12481 | 0.53 |

**Tert-butyl (2S,3R)-2-((4-bromobenzyl)oxy)-5-(4-chlorophenyl)-3-(2-oxo-2-phenylethyl)-2-phenylpent-4-ynoate (S16)**




**S16**

Colorless oil; 57.8 mg, 60% yield, >20:1 d.r., 99% *ee*; $^{1}$H NMR (500 MHz, $CDCl_3$) δ 7.85 (d, *J* = 7.3 Hz, 2H), 7.67 (d, *J* = 7.5 Hz, 2H), 7.53 (t, *J* = 7.4 Hz, 1H), 7.47 (d, *J* = 8.3 Hz, 2H), 7.41 (t, *J* = 7.7 Hz, 2H), 7.39 – 7.34 (m, 4H), 7.32 (t, *J* = 7.2 Hz, 1H), 7.20 (d, *J* = 8.4 Hz, 2H), 7.14 (d, *J* = 8.5 Hz, 2H), 5.00 (d, *J* = 11.7 Hz, 1H), 4.83 (d, *J* = 11.7 Hz, 1H), 4.39 (dd, *J* = 10.2, 3.0 Hz, 1H), 3.31 (dd, *J* = 16.7, 10.2 Hz, 1H), 3.13 (dd, *J* = 16.6, 2.9 Hz, 1H), 1.51 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 197.3, 169.4, 138.1,

137.9, 136.8, 133.9, 133.2, 132.6, 131.42, 129.2, 128.6, 128.5, 128.4, 128.3, 128.2, 126.8, 121.8, 121.3, 90.7, 85.9, 83.0, 67.9, 39.2, 36.8, 28.1. HRMS (ESI) $[M+Na]^+$ calcd for $C_{36}H_{32}O_4ClBrNa^+$, 665.1065, found 665.1065. (Chiral IA, λ= 254 nm, *n*-hexane/2-propanol= 19/1, Flow rate = 1.0 mL/min), $t_R$ = 7.723 min(major), 12.895 min.

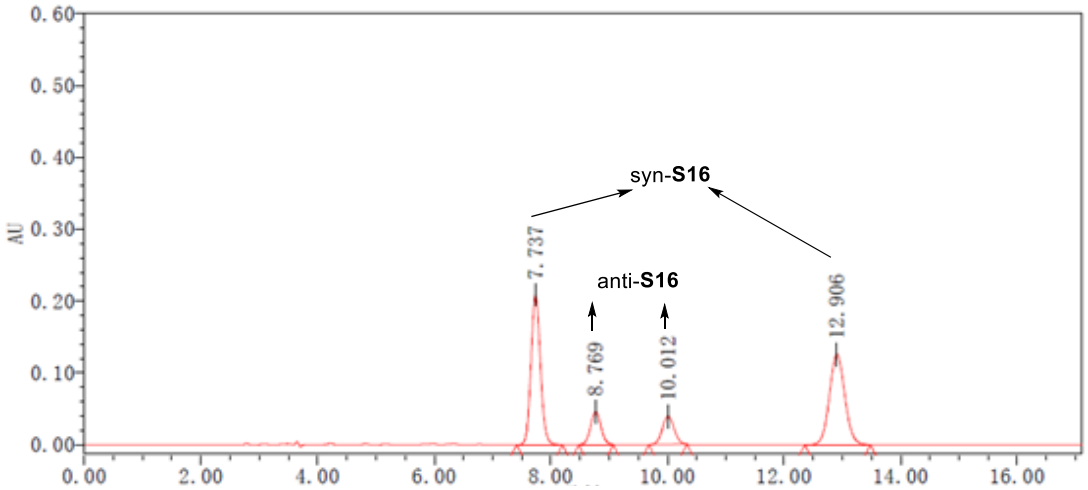
**HPLC chromatogram of racemic S16**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 7.737 | 2307827 | 208651 | 40.28 |
| 2 | 8.769 | 563285 | 45762 | 9.83 |
| 3 | 10.012 | 556478 | 39555 | 9.71 |
| 4 | 12.906 | 2301769 | 125734 | 40.17 |

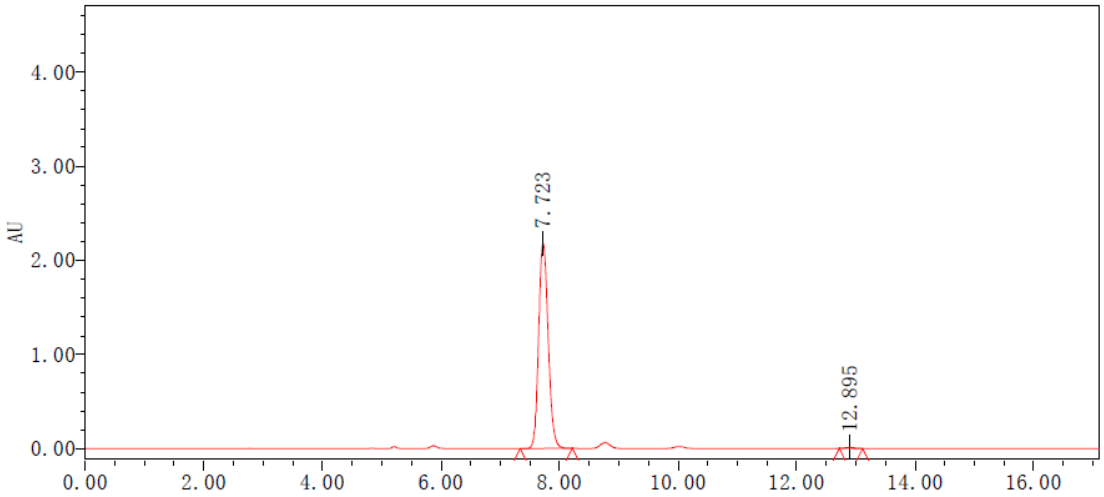
**HPLC chromatogram of chiral S16**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

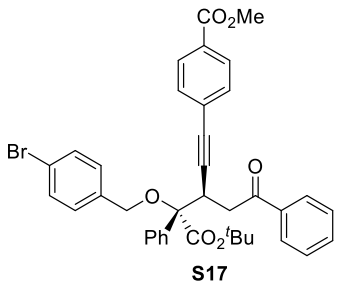
λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 7.723 | 24139359 | 2179871 | 99.53 |
| 2 | 12.895 | 113041 | 8470 | 0.47 |

**Methyl 4-((3R,4S)-4-((4-bromobenzyl)oxy)-5-(tert-butoxy)-5-oxo-3-(2-oxo-2-phenylethyl)-4-phenylpent-1-yn-1-yl)benzoate (S17)**




**S17**

Colorless oil; 56.6 mg, 57% yield, >20:1 d.r., 99% *ee*; $^1$H NMR (500 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.4 Hz, 2H), 7.87 – 7.82 (m, 2H), 7.67 (d, *J* = 7.5 Hz, 2H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.47 (d, *J* = 8.3 Hz, 2H), 7.43 (d, *J* = 7.9 Hz, 2H), 7.40 (d, *J* = 4.0 Hz, 1H), 7.36 (dd, *J* = 17.6, 8.8 Hz, 4H), 7.28 – 7.25 (m, 2H), 5.00 (d, *J* = 11.7 Hz, 1H), 4.83 (d,

*J* = 11.7 Hz, 1H), 4.42 (dd, *J* = 10.2, 3.0 Hz, 1H), 3.89 (s, 3H), 3.33 (dd, *J* = 16.7, 10.2 Hz, 1H), 3.16 (dd, *J* = 16.7, 2.9 Hz, 1H), 1.51 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 197.2, 169.3, 166.6, 138.0, 137.9, 136.8, 133.2, 131.4, 131.3, 129.4, 129.2, 129.1, 128.6, 128.4, 128.4, 128.2, 128.1, 126.8, 121.3, 93.1, 85.9, 83.5, 83.1, 68.0, 52.2, 39.1, 36.9, 28.1. HRMS (ESI) $[M+Na]^+$ calcd for $C_{38}H_{35}O_6BrNa^+$, 689.1509, found 689.1510. (Chiral IA-3, λ= 254 nm, *n*-hexane/2-propanol= 19/1, Flow rate = 1.0 mL/min), $t_R$ = 10.543 min(major), 18.419 min.

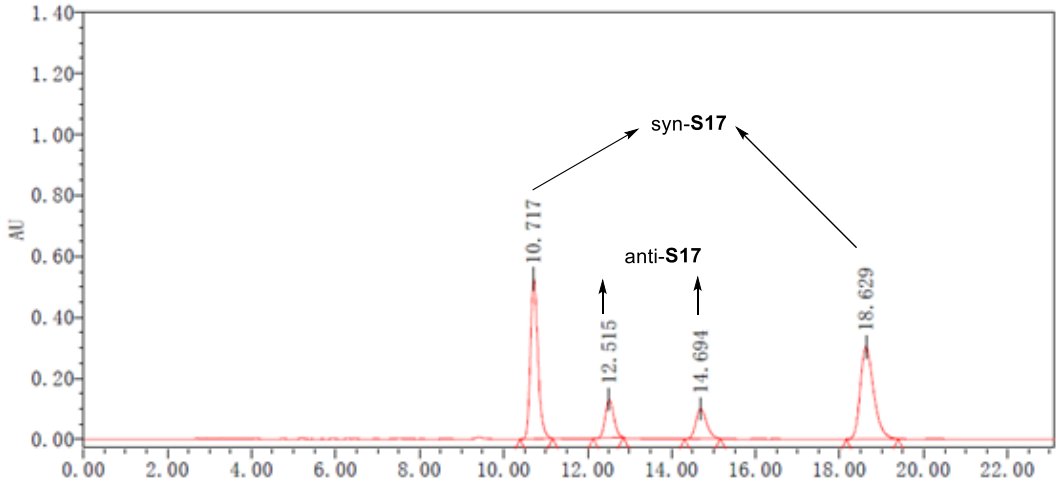
**HPLC chromatogram of racemic S17**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 10.717 | 6550783 | 524511 | 39.14 |
| 2 | 12.515 | 1784250 | 126250 | 10.66 |
| 3 | 14.694 | 1757376 | 98365 | 10.50 |
| 4 | 18.629 | 6642978 | 303082 | 39.69 |

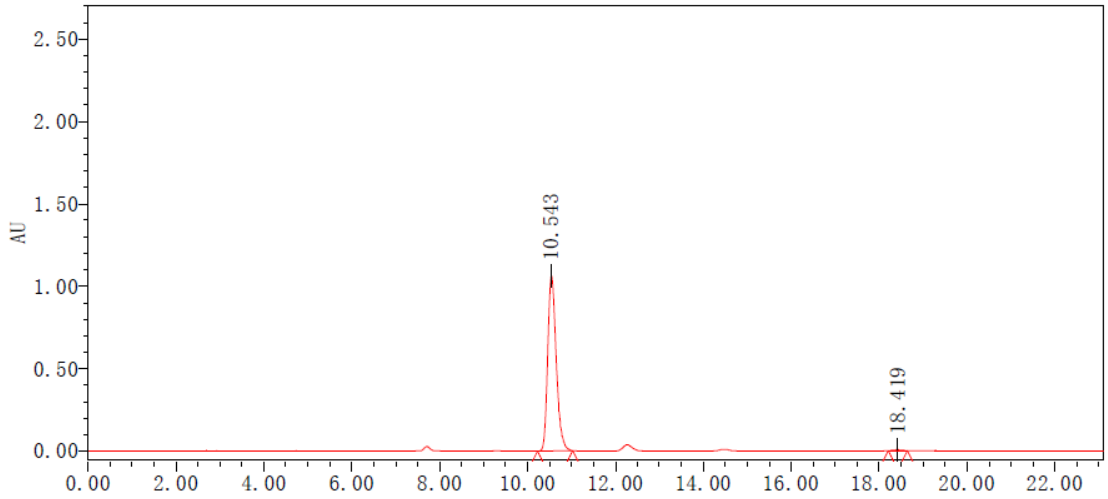
**HPLC chromatogram of chiral S17**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

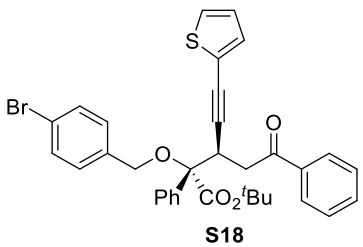
λ= 254 nm

Chiral IA-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 10.543 | 14064028 | 1061555 | 99.50 |
| 2 | 18.419 | 71343 | 4690 | 0.50 |

**Tert-butyl (2S,3R)-2-((4-bromobenzyl)oxy)-3-(2-oxo-2-phenylethyl)-2-phenyl-5-(thiophen-2-yl)pent-4-ynoate (S18)**




**S18**

Colorless oil; 38.7 mg, 42% yield, >20:1 d.r., 98% *ee*; $^{1}$H NMR (500 MHz, $CDCl_3$) δ 7.83 (d, *J* = 7.3 Hz, 2H), 7.67 (d, *J* = 7.6 Hz, 2H), 7.53 (t, *J* = 7.4 Hz, 1H), 7.49 (d, *J* =

8.3 Hz, 2H), 7.39 (dt, *J* = 14.9, 7.8 Hz, 6H), 7.31 (t, *J* = 7.3 Hz, 1H), 7.16 (d, *J* = 5.1 Hz, 1H), 7.01 (d, *J* = 3.2 Hz, 1H), 6.90 (dd, *J* = 5.0, 3.7 Hz, 1H), 5.01 (d, *J* = 11.8 Hz, 1H), 4.88 (d, *J* = 11.8 Hz, 1H), 4.43 (dd, *J* = 10.1, 2.9 Hz, 1H), 3.31 (dd, *J* = 16.9, 10.1 Hz, 1H), 3.08 (dd, *J* = 16.8, 2.8 Hz, 1H), 1.52 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 197.2, 169.3, 138.2, 138.0, 136.8, 133.2, 131.4, 131.3, 129.2, 128.6, 128.3, 128.3, 128.2, 126.8, 126.6, 126.5, 123.4, 121.2, 93.8, 85.9, 83.1, 68.0, 39.0, 36.7, 28.1. HRMS (ESI) $[M+Na]^+$ calcd for $C_{34}H_{31}O_4SBrNa^+$, 637.1019, found 637.1016. (Chiral IE-3, λ= 254 nm, *n*-hexane/2-propanol= 19/1, Flow rate = 1.0 mL/min), $t_R$ = 11.160 min(major), 25.553 min.

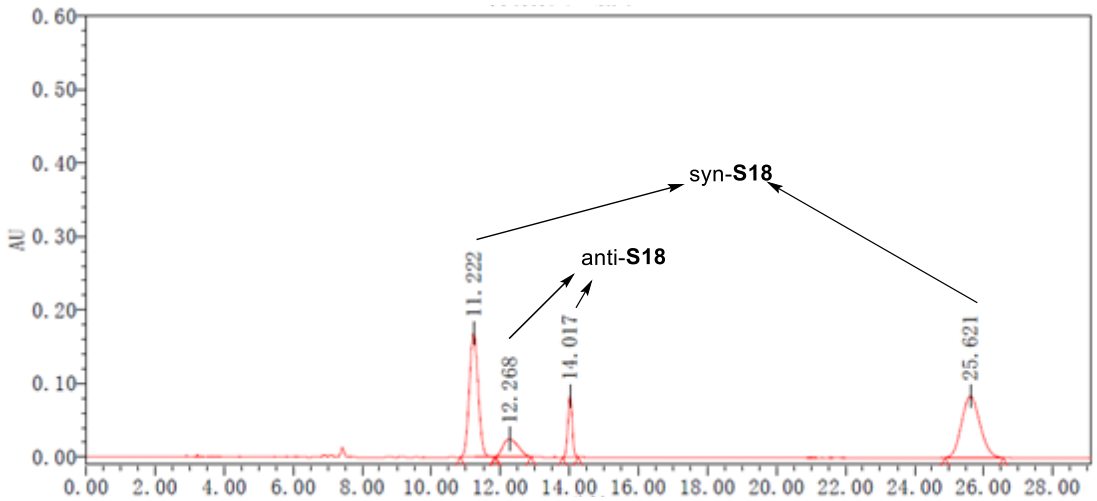
**HPLC chromatogram of racemic S18**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 11.222 | 3070845 | 168973 | 40.51 |
| 2 | 12.268 | 704675 | 23572 | 9.30 |

| | | | | |
|---|---|---|---|---|
| 3 | 14.017 | 710375 | 83303 | 9.37 |
| 4 | 25.621 | 3093886 | 83510 | 40.82 |

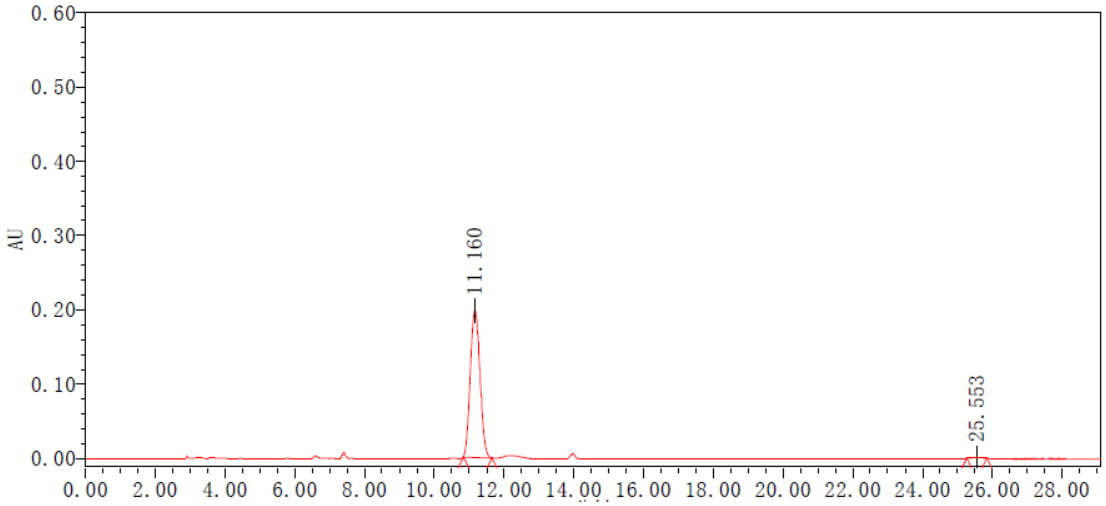
**HPLC chromatogram of chiral S18**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

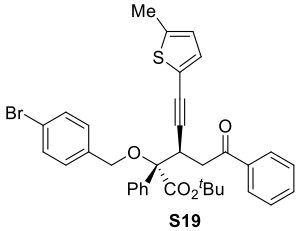
λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 11.160 | 3883914 | 197424 | 99.50 |
| 2 | 25.553 | 19604 | 902 | 0.50 |

**Tert-butyl (2S,3R)-2-((4-bromobenzyl)oxy)-5-(5-methylthiophen-2-yl)-3-(2-oxo-2-phenylethyl)-2-phenylpent-4-ynoate (S19)**




**S19**

Colorless oil; 43.4 mg, 46% yield, >20:1 d.r., 97% *ee*; $^{1}$H NMR (500 MHz, $CDCl_3$) δ 7.85 – 7.79 (m, 2H), 7.69 – 7.64 (m, 2H), 7.53 (t, *J* = 7.4 Hz, 1H), 7.49 (d, *J* = 8.4 Hz, 2H), 7.43 – 7.38 (m, 4H), 7.36 (t, *J* = 7.5 Hz, 2H), 7.31 (d, *J* = 7.2 Hz, 1H), 6.81 (d, *J* = 3.5 Hz, 1H), 6.54 (dd, *J* = 3.5, 1.0 Hz, 1H), 5.02 (d, *J* = 11.8 Hz, 1H), 4.90 (d, *J* = 11.8 Hz, 1H), 4.41 (dd, *J* = 10.1, 2.9 Hz, 1H), 3.30 (dd, *J* = 16.8, 10.1 Hz, 1H), 3.05 (dd, *J* = 16.8, 2.9 Hz, 1H), 2.41 (s, 3H), 1.52 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 197.3, 169.3, 141.2, 138.3, 138.1, 136.8, 133.1, 131.5, 131.4, 129.2, 128.5, 128.3, 128.3, 128.2, 126.6, 125.3, 121.2, 120.9, 92.8, 85.9, 83.0, 77.8, 77.3, 68.0, 39.0, 36.7, 28.1, 15.4. HRMS (ESI) $[M+Na]^+$ calcd for $C_{35}H_{33}O_4SBrNa^+$, 651.1175, found 651.1175. (Chiral IE-3, λ= 254 nm, *n*-hexane/2-propanol= 19/1, Flow rate = 1.0 mL/min), $t_R$ = 11.793 min(major), 31.109 min.

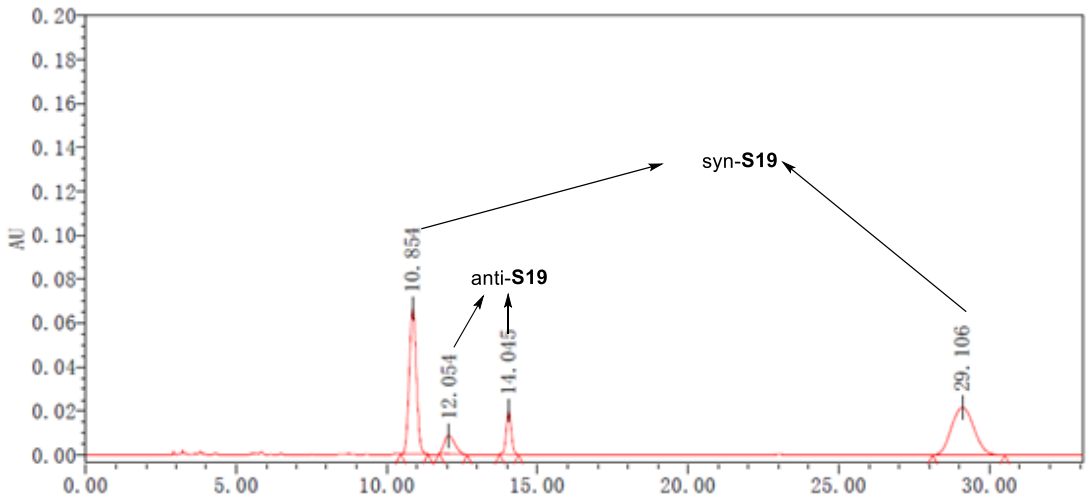
**HPLC chromatogram of racemic S19**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| 1 | 10.854 | 1114806 | 66456 | 41.90 |
| 2 | 12.054 | 204793 | 8366 | 7.70 |
| 3 | 14.045 | 226990 | 19828 | 8.53 |
| 4 | 29.106 | 1113738 | 21527 | 41.86 |

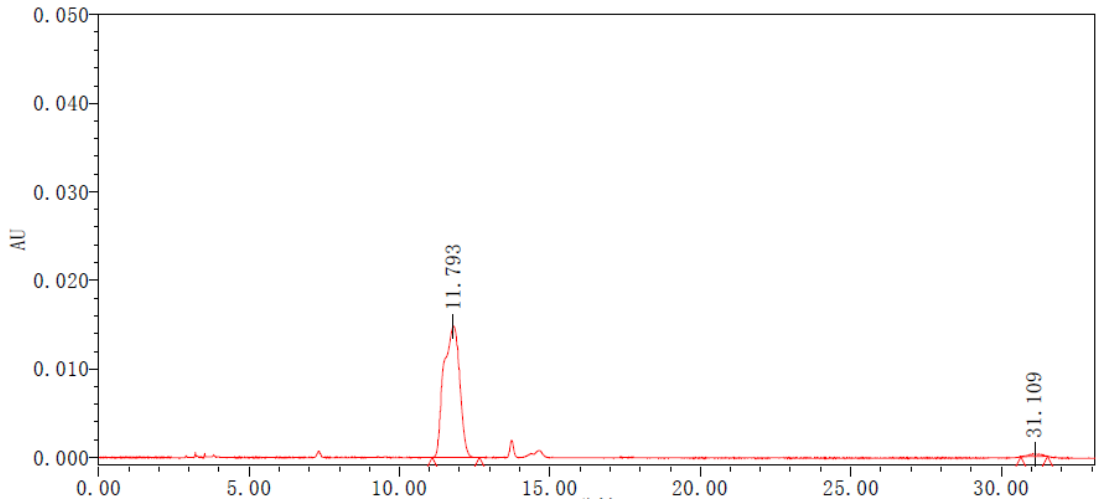
**HPLC chromatogram of chiral S19**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

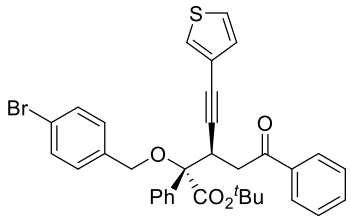
λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 11.793 | 540927 | 14788 | 98.52 |
| 2 | 31.109 | 8101 | 259 | 1.48 |

**Tert-butyl (2S,3R)-2-((4-bromobenzyl)oxy)-3-(2-oxo-2-phenylethyl)-2-phenyl-5-(thiophen-3-yl)pent-4-ynoate (S20)**




**S20**

Colorless oil; 43.3 mg, 47% yield, >20:1 d.r., 99% *ee*; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.87 – 7.80 (m, 2H), 7.70 – 7.64 (m, 2H), 7.55 – 7.50 (m, 1H), 7.47 (d, *J* = 1.8 Hz, 2H), 7.41 (d, *J* = 7.9 Hz, 2H), 7.37 (d, *J* = 8.6 Hz, 4H), 7.34 – 7.30 (m, 1H), 7.21 (dd, *J* = 2.9, 1.1 Hz, 1H), 7.17 (dd, *J* = 5.0, 3.0 Hz, 1H), 6.91 (dd, *J* = 5.0, 1.1 Hz, 1H), 5.03 (d, *J* = 11.8 Hz, 1H), 4.88 (d, *J* = 11.8 Hz, 1H), 4.39 (dd, *J* = 10.1, 3.0 Hz, 1H), 3.31 (dd, *J* = 16.7, 10.2 Hz, 1H), 3.09 (dd, *J* = 16.7, 3.1 Hz, 1H), 1.51 (s, 9H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 197.4, 169.4, 138.3, 138.1, 136.9, 133.1, 131.4, 129.7, 129.2, 128.6, 128.3, 128.3, 128.2, 128.0, 126.7, 125.1, 122.4, 121.3, 89.1, 85.9, 83.0, 79.30, 68.0, 39.2, 36.6, 28.1. HRMS (ESI) $[M+Na]^+$ calcd for $C_{34}H_{31}O_4SBrNa^+$, 637.1019, found 637.1022.( Chiral IA, λ= 254 nm, *n*-hexane/2-propanol= 19/1, Flow rate = 1.0 mL/min), $t_R$ = 8.550 min(major), 14.735 min.

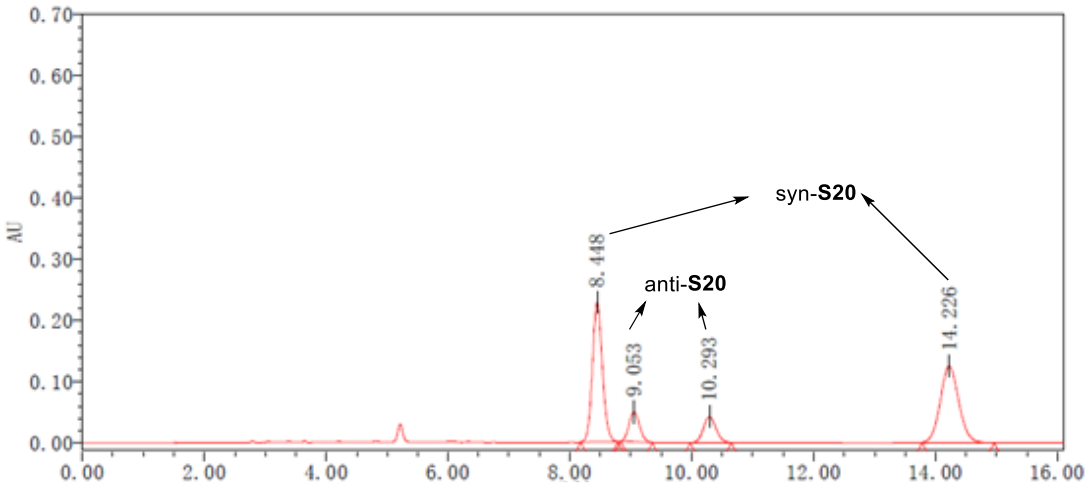
**HPLC chromatogram of racemic S20**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 8.448 | 2620742 | 228355 | 40.67 |
| 2 | 9.053 | 586735 | 48986 | 9.11 |
| 3 | 10.293 | 606430 | 42645 | 9.41 |
| 4 | 14.226 | 2629601 | 124974 | 40.81 |

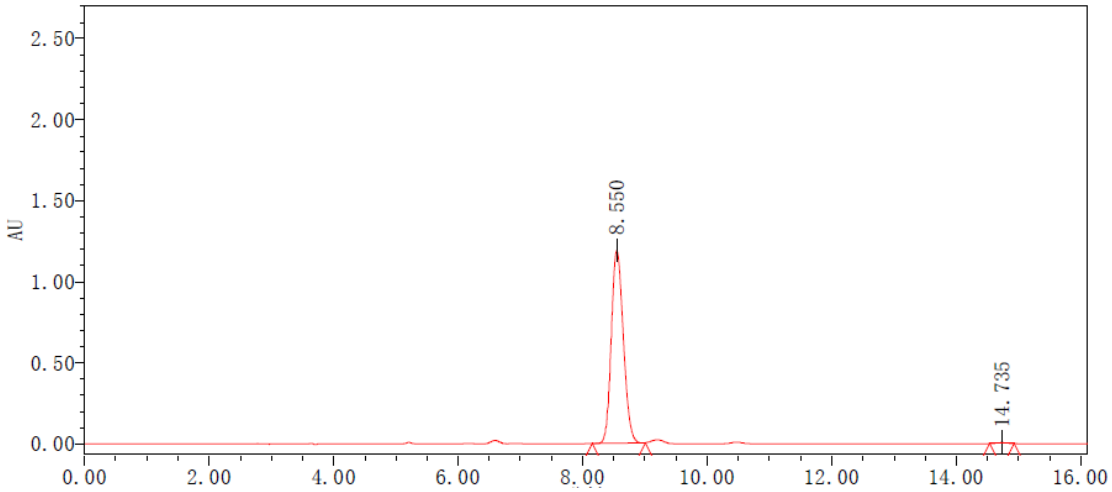
**HPLC chromatogram of chiral S20**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

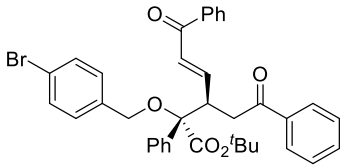
λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 8.550 | 15829834 | 1188323 | 99.48 |
| 2 | 14.735 | 83433 | 5947 | 0.52 |

**Tert-butyl (2S,3R,E)-2-((4-bromobenzyl)oxy)-6-oxo-3-(2-oxo-2-phenylethyl)-2,6-diphenylhex-4-enoate (S21)**




**S21**

Colorless oil; 52.7 mg, 55% yield, >20:1 d.r., 87% *ee*; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.92 – 7.87 (m, 2H), 7.68 – 7.62 (m, 2H), 7.53 (dd, *J* = 7.2, 1.5 Hz, 3H), 7.49 (t, *J* = 7.5 Hz, 1H), 7.44 – 7.39 (m, 6H), 7.38 – 7.34 (m, 3H), 7.19 (d, *J* = 8.3 Hz, 2H), 6.94 (dd, *J* = 15.6, 8.4 Hz, 1H), 6.66 (d, *J* = 15.9 Hz, 1H), 4.71 (d, *J* = 11.8 Hz, 1H), 4.26 (d, *J* = 11.8 Hz, 1H), 4.06 – 3.98 (m, 1H), 3.58 (dd, *J* = 16.7, 2.7 Hz, 1H), 3.13 (dd, *J* = 16.7, 9.7 Hz, 1H), 1.55 (s, 9H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 197.8, 190.7, 169.7, 146.8, 137.8, 137.7, 137.3, 136.8, 133.2, 132.6, 131.3, 128.9, 128.7, 128.6, 128.6, 128.4, 128.1, 127.7, 121.1, 87.1, 83.5, 67.5, 48.3, 38.7, 28.2. HRMS (ESI) $[M+Na]^+$ calcd for $C_{37}H_{35}O_5BrNa^+$, 661.1557, found 661.1560. (Chiral IE-3, λ= 254 nm, *n*-hexane/2-

propanol= 23/2, Flow rate = 1.0 mL/min), $t_R$ = 36.984 min(major), 41.330 min.

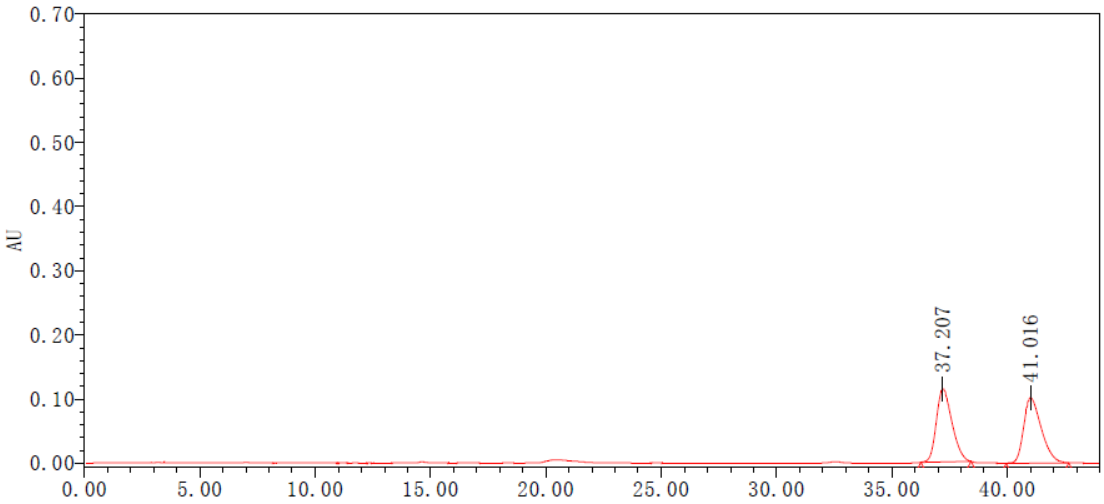
**HPLC chromatogram of racemic S21**

Condition: n-hexane/2-propanol =23:2

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 37.207 | 5419985 | 113974 | 50.04 |
| 2 | 41.016 | 5411834 | 101887 | 49.96 |

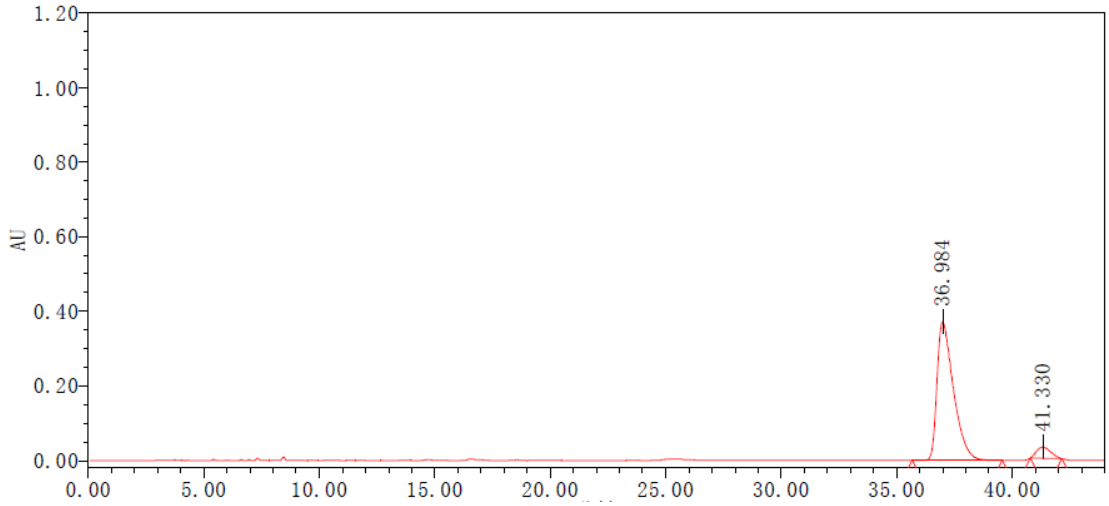
**HPLC chromatogram of chiral S21**

Condition: n-hexane/2-propanol =23:2

Flow rate =1.0 mL/min

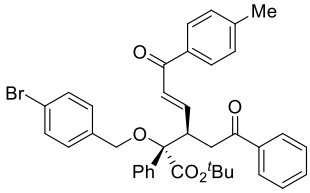
λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 36.984 | 18333034 | 370985 | 93.51 |
| 2 | 41.330 | 1272020 | 29672 | 6.49 |

**Tert-butyl (2S,3R,E)-2-((4-bromobenzyl)oxy)-6-oxo-3-(2-oxo-2-phenylethyl)-2-phenyl-6-(p-tolyl)hex-4-enoate (S22)**




**S22**

Colorless oil; 46.0 mg, 47% yield, >20:1 d.r., 90% *ee*; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.90 – 7.85 (m, 2H), 7.58 – 7.51 (m, 5H), 7.40 (ddd, *J* = 6.7, 6.0, 3.4 Hz, 5H), 7.36 – 7.30 (m, 2H), 7.20 – 7.14 (m, 4H), 6.93 (dd, *J* = 15.6, 8.4 Hz, 1H), 6.66 (d, *J* = 15.4 Hz, 1H), 4.71 (d, *J* = 11.8 Hz, 1H), 4.27 (d, *J* = 11.8 Hz, 1H), 4.01 (dd, *J* = 12.8, 4.8 Hz, 1H), 3.55 (dd, *J* = 16.7, 2.7 Hz, 1H), 3.12 (dd, *J* = 16.7, 9.6 Hz, 1H), 2.37 (s, 3H), 1.55 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 197.8, 190.2, 169.7, 146.2, 143.4, 140.9, 137.8, 137.30, 136.9, 135.1, 133.2, 131.3, 129.5, 129.1, 128.9, 128.7, 128.6, 128.5, 128.1, 127.7, 121.1, 87.1, 83.4, 67.5, 48.2, 38.7, 28.2, 21.6. HRMS (ESI) $[M+Na]^+$ calcd for

$C_{38}H_{37}O_5BrNa^+$,675.1717, found 675.1718. (Chiral IC, λ= 254 nm, *n*-hexane/2-propanol= 9/1, Flow rate = 1.0 mL/min), $t_R$ = 13.163 min(major), 17.953 min.

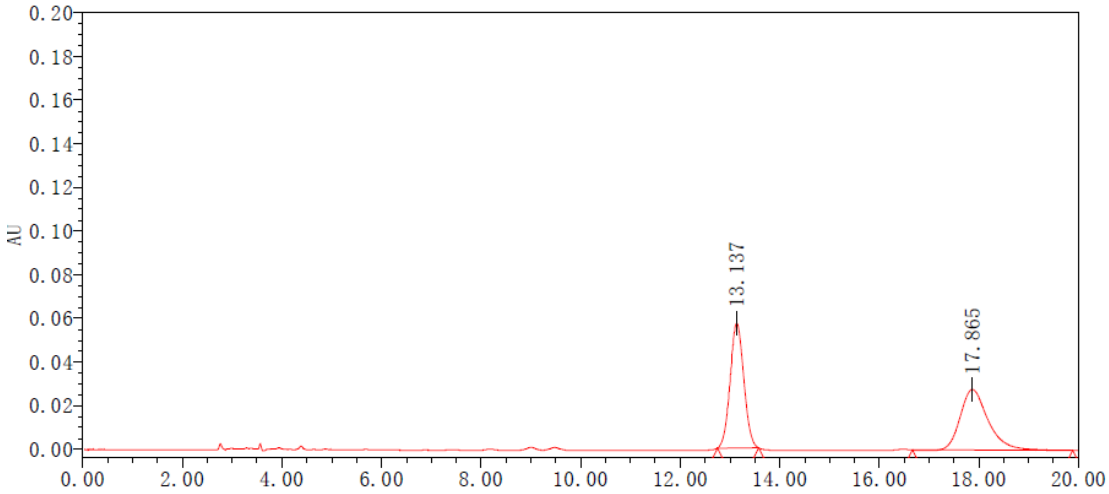
**HPLC chromatogram of racemic S22**

Condition: n-hexane/2-propanol =9:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IC




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 13.137 | 1097650 | 57261 | 50.31 |
| 2 | 17.865 | 1084313 | 27770 | 49.69 |

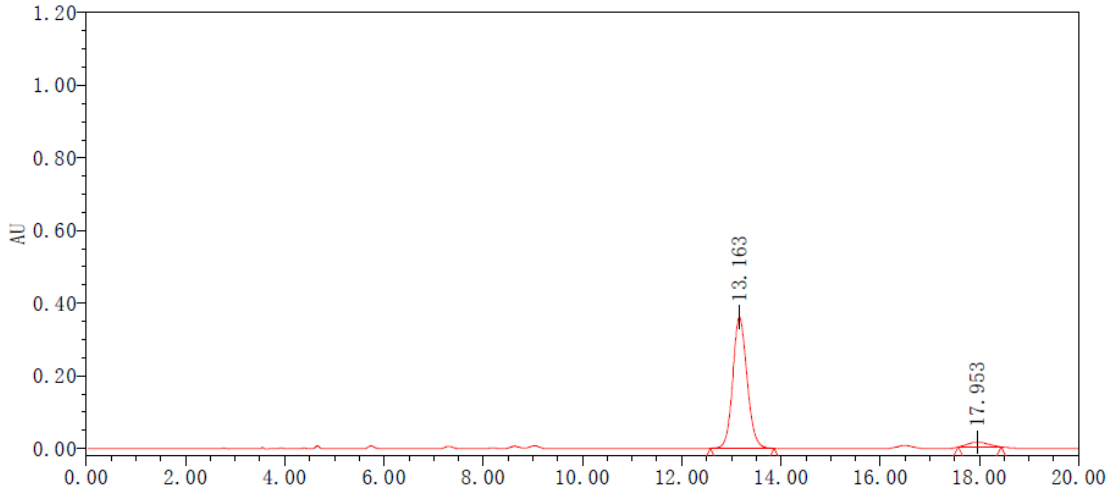
**HPLC chromatogram of chiral S22**

Condition: n-hexane/2-propanol =9:1

Flow rate =1.0 mL/min

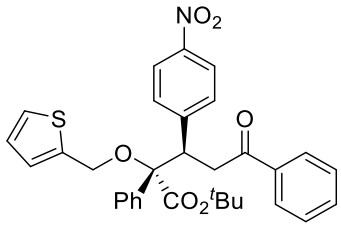
λ= 254 nm

Chiral IC




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 13.163 | 7224693 | 360847 | 94.93 |
| 2 | 17.953 | 385972 | 13380 | 5.07 |

**Tert-butyl (2S,3R)-3-(4-nitrophenyl)-5-oxo-2,5-diphenyl-2-(thiophen-2-ylmethoxy)pentanoate (S23)**




**S23**

Colorless oil; 56.0 mg, 67% yield, >20:1 d.r., 90% *ee*; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.8 Hz, 2H), 7.71 (d, *J* = 7.3 Hz, 2H), 7.62 (d, *J* = 6.8 Hz, 2H), 7.55 (d, *J* = 8.8 Hz, 2H), 7.49 (t, *J* = 7.4 Hz, 1H), 7.37 (dt, *J* = 11.1, 6.9 Hz, 6H), 7.05 (dd, *J* = 5.0, 3.5 Hz, 1H), 6.99 (d, *J* = 2.6 Hz, 1H), 5.16 (d, *J* = 12.2 Hz, 1H), 4.80 (d, *J* = 12.3 Hz, 1H), 4.19 (dd, *J* = 10.7, 3.0 Hz, 1H), 3.63 (dd, *J* = 17.3, 10.7 Hz, 1H), 3.43 (dd, *J* = 17.3, 3.1 Hz, 1H), 1.35 (s, 9H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 197.6, 169.5, 148.1, 146.8, 142.0, 136.7, 136.4, 133.2 131.5, 128.6, 128.5, 127.9, 127.6, 126.7, 125.2, 124.7,

122.6, 87.8, 83.5, 64.1, 51.4, 39.5, 27.9. Peak overlapping was observed. HRMS (ESI) $[M+Na]^+$ calcd for $C_{32}H_{31}NO_6SNa^+$, 580.1764, found 580.1770. (Chiral IA-3, λ= 254 nm, *n*-hexane/2-propanol= 9/1, Flow rate = 1.0 mL/min), $t_R$ = 8.691 min, 10.772 min(major)

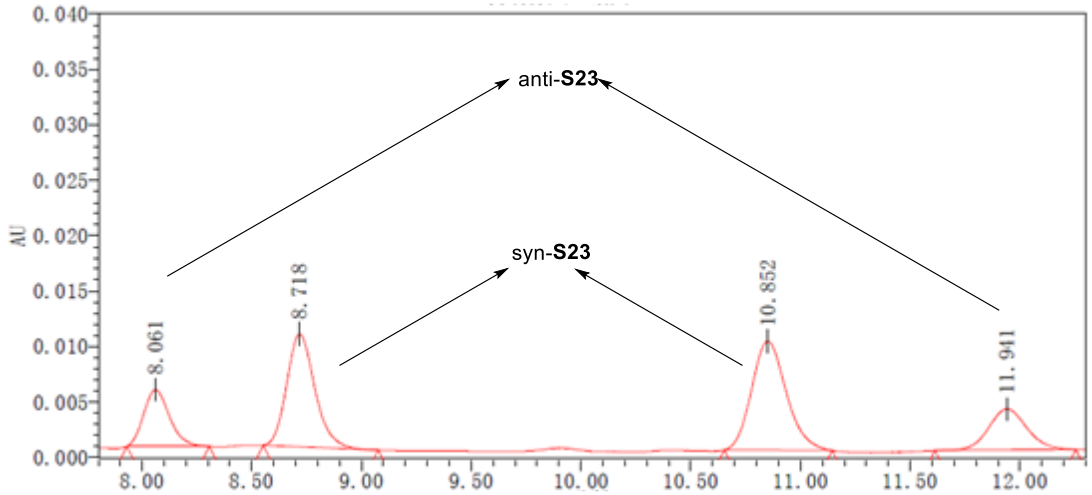
**HPLC chromatogram of racemic S23**

Condition: n-hexane/2-propanol =9:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 8.061 | 41857 | 5104 | 14.66 |
| 2 | 8.718 | 90696 | 10183 | 31.76 |
| 3 | 10.852 | 108117 | 9840 | 37.86 |
| 4 | 11.941 | 44866 | 3695 | 15.71 |

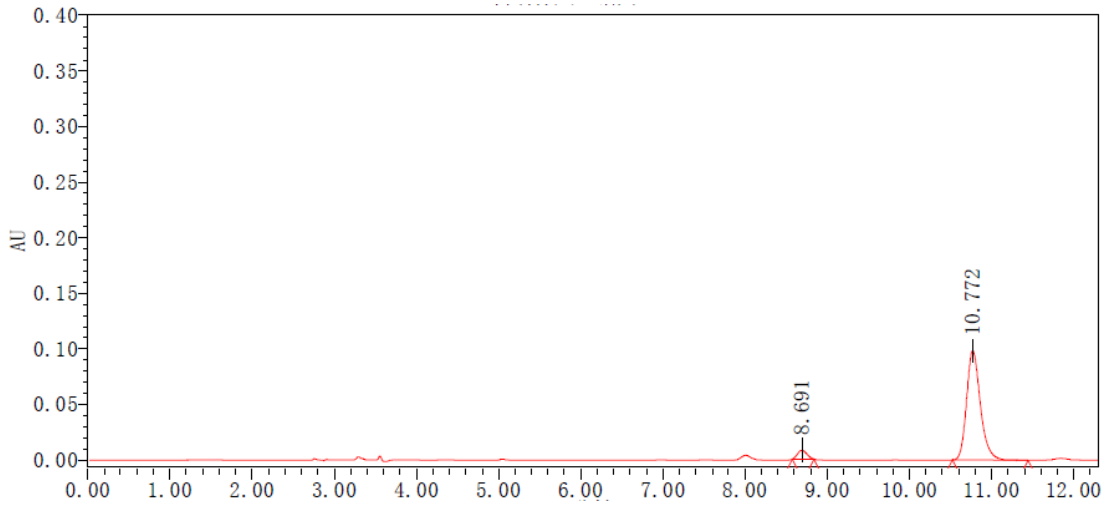
**HPLC chromatogram of chiral S23**

Condition: n-hexane/2-propanol =9:1

Flow rate =1.0 mL/min

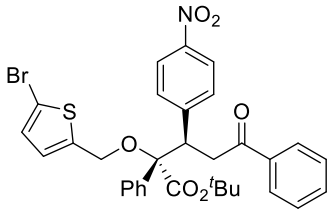
λ= 254 nm

Chiral IA-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 8.691 | 63031 | 7901 | 5.18 |
| 2 | 10.772 | 1153540 | 98382 | 94.82 |

**Tert-butyl (2S,3R)-2-((5-bromothiophen-2-yl)methoxy)-3-(4-nitrophenyl)-5-oxo-2,5-diphenylpentanoate (S24)**




**S24**

Colorless oil; 52.4 mg, 55% yield, >20:1 d.r., 90% *ee*; $^1$H NMR (500 MHz, $CDCl_3$) δ 8.04 (d, *J* = 8.7 Hz, 2H), 7.72 (d, *J* = 7.6 Hz, 2H), 7.59 (d, *J* = 7.4 Hz, 2H), 7.53 (d, *J* = 8.7 Hz, 2H), 7.50 (t, *J* = 7.6 Hz, 3H), 7.42 – 7.34 (m, 5H), 6.98 (d, *J* = 3.7 Hz, 1H), 6.73 (d, *J* = 3.6 Hz, 1H), 5.07 (d, *J* = 12.4 Hz, 1H), 4.70 (d, *J* = 12.4 Hz, 1H), 4.18 (dd, *J* =

10.6, 3.0 Hz, 1H), 3.61 (dd, *J* = 17.3, 10.7 Hz, 1H), 3.42 (dd, *J* = 17.3, 3.0 Hz, 1H), 1.35 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 197.5, 169.4, 148.0, 146.8, 143.6, 136.6, 136.3, 133.2, 131.4, 129.5, 128.6, 128.6, 127.9, 127.5, 125.2, 122.7, 111.9, 87.9, 83.6, 64.3, 51.3, 39.4, 28.0. Peak overlapping was observed. HRMS (ESI) $[M+Na]^+$ calcd for $C_{32}H_{30}NO_6SBrNa^+$, 658.0869, found 658.0867. (Chiral IA-3, λ= 254 nm, *n*-hexane/2-propanol= 19/1, Flow rate = 1.0 mL/min), $t_R$ = 10.980 min, 14.730 min(major)

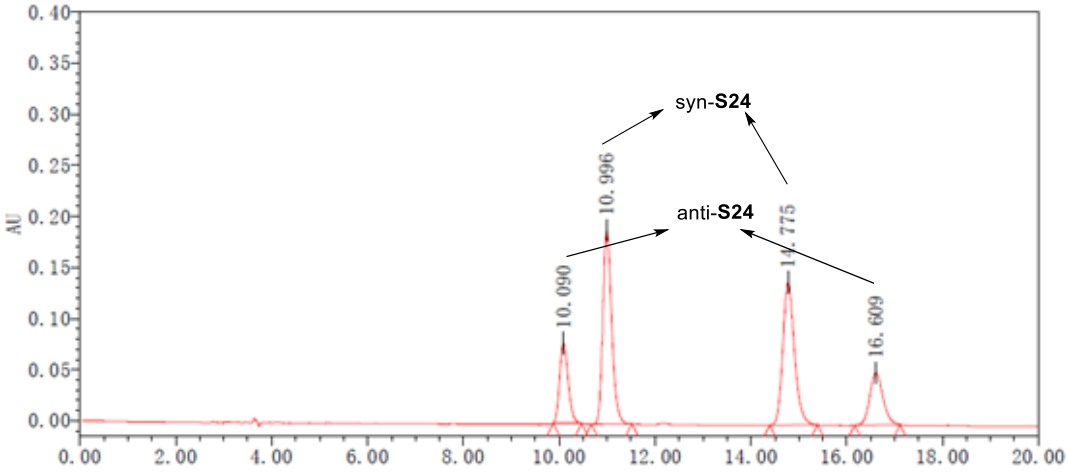
**HPLC chromatogram of racemic S24**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 10.090 | 970254 | 970254 | 14.27 |
| 2 | 10.996 | 2461486 | 2461486 | 36.21 |
| 3 | 14.775 | 2391001 | 2391001 | 35.17 |
| 4 | 16.609 | 975821 | 975821 | 14.35 |

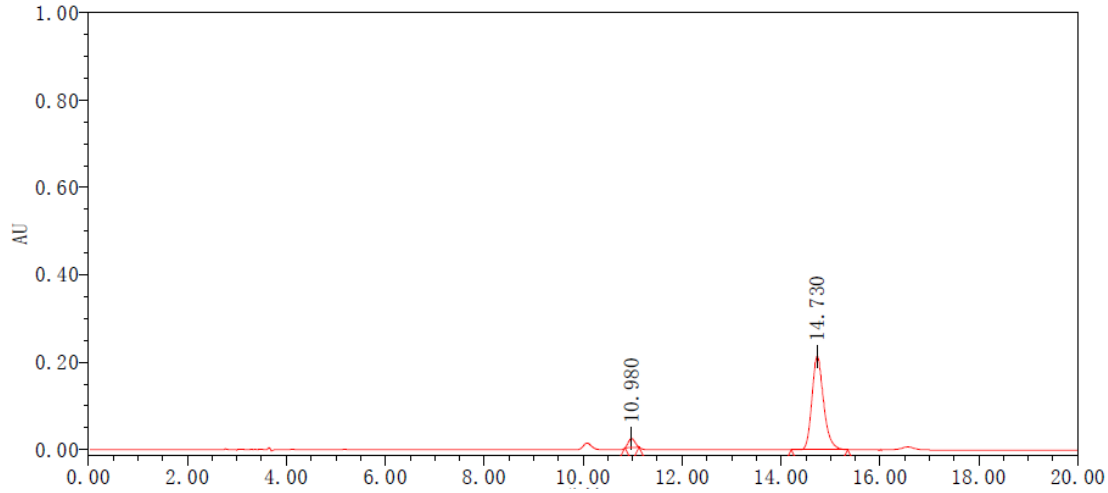
**HPLC chromatogram of chiral S24**

Condition: n-hexane/2-propanol =19:1

Flow rate =1.0 mL/min

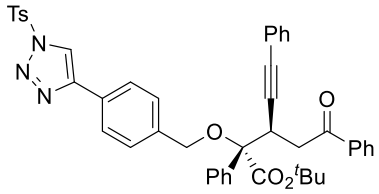
λ= 254 nm

Chiral IA-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 10.980 | 188538 | 20336 | 5.03 |
| 2 | 14.730 | 3557986 | 213954 | 94.97 |

**Tert-butyl (2S,3R)-3-(2-oxo-2-phenylethyl)-2,5-diphenyl-2-((4-(1-tosyl-1H-1,2,3-triazol-4-yl)benzyl)oxy)pent-4-ynoate (S25)**




**S25**

Colorless oil; 64.6mg, 86% yield, >20:1 d.r., 94% ee. $^1$H NMR (400 MHz, $CDCl_3$) δ 8.31 (s, 1H), 8.03 (d, *J* = 8.4 Hz, 2H), 7.89 – 7.79 (m, 4H), 7.71 (d, *J* = 7.4 Hz, 2H), 7.57 (d, *J* = 8.1 Hz, 2H), 7.51 (t, *J* = 7.4 Hz, 1H), 7.43 – 7.39 (m, 3H), 7.38 – 7.29 (m,

4H), 7.27 – 7.21 (m, 5H), 5.13 (d, *J* = 11.9 Hz, 1H), 4.98 (d, *J* = 11.9 Hz, 1H), 4.43 (dd, *J* = 10.2, 2.9 Hz, 1H), 3.35 (dd, *J* = 16.6, 10.2 Hz, 1H), 3.12 (dd, *J* = 16.6, 2.9 Hz, 1H), 2.44 (s, 3H), 1.51 (s, 9H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 197.5, 169.5, 147.4, 147.3, 140.1, 138.4, 136.9, 133.1, 131.4, 130.5, 128.7, 128.6, 128.3, 128.3, 128.2, 128.1, 128.0, 127.9, 126.8, 126.1, 123.4, 118.9, 89.7, 85.9, 84.2, 82.9, 68.3, 39.3, 36.6, 29.7, 28.1, 21.9. HRMS (ESI) $[M+Na]^+$ calcd for $C_{45}H_{41}N_3O_6SNa^+$, 774.2608, found 774.2606. (Chiral IA, λ= 254 nm, *n*-hexane/2-propanol= 17/3, Flow rate = 1.0 mL/min), $t_R$ = 35.095 min(major), 67.281 min.

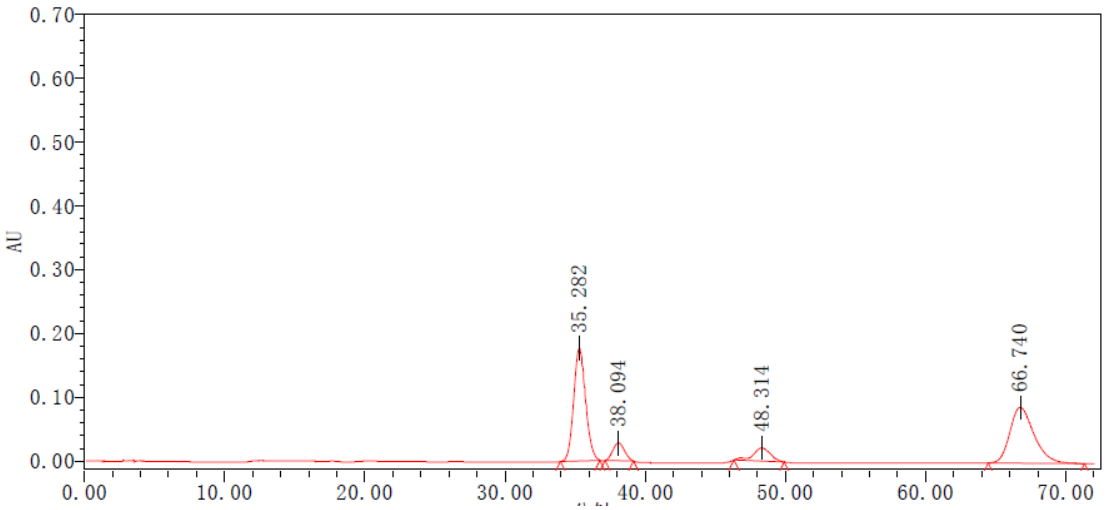
**HPLC chromatogram of racemic S25**

Condition: n-hexane/2-propanol = 17:3

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 35.282 | 10540918 | 177043 | 43.35 |
| 2 | 38.094 | 1613880 | 28161 | 6.64 |
| 3 | 48.314 | 1742795 | 20630 | 7.17 |

| | | | | |
|---|---|---|---|---|
| 4 | 66.740 | 10416644 | 87076 | 42.84 |

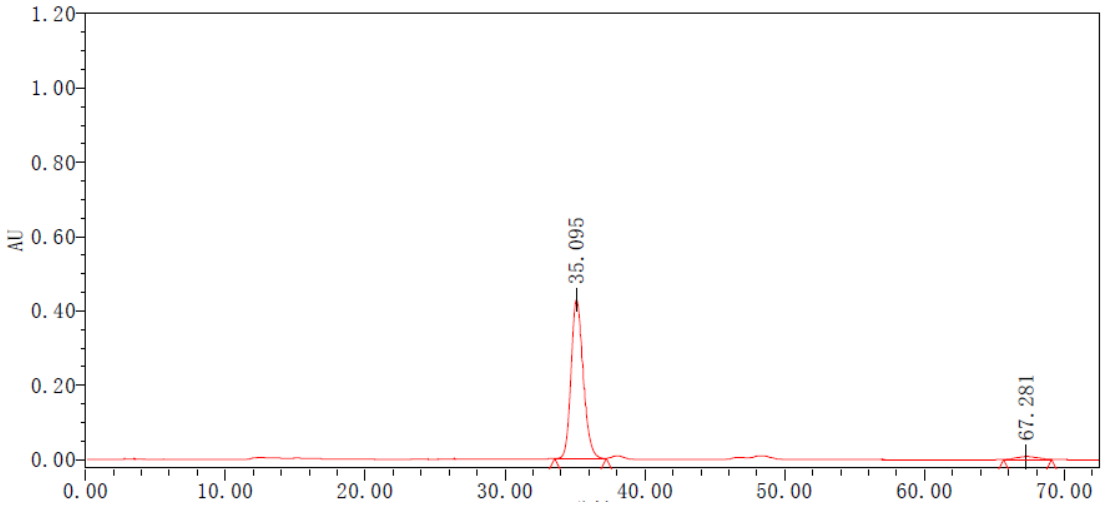
**HPLC chromatogram of chiral S25**

Condition: n-hexane/2-propanol =17:3

Flow rate =1.0 mL/min

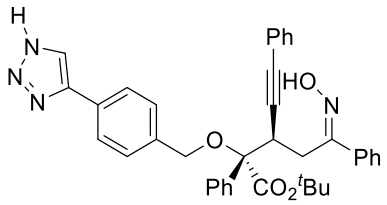
λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 35.095 | 25922700 | 427421 | 96.96 |
| 2 | 67.281 | 811921 | 7766 | 3.04 |

**Tert-butyl (2S,3R)-2-((4-(1H-1,2,3-triazol-4-yl)benzyl)oxy)-3-((E)-2-(hydroxyimino)-2-phenylethyl)-2,5-diphenylpent-4-ynoate (S26)**




**S26**

White solid, 23.0 mg, 75% yield, >20:1 d.r., 92% ee. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.71 (s, 1H), 7.80 (d, *J* = 8.1 Hz, 2H), 7.70 (d, *J* = 7.0 Hz, 2H), 7.65 (d, *J* = 6.0 Hz, 1H), 7.57 – 7.50 (m, 4H), 7.37 (t, *J* = 5.6 Hz, 4H), 7.34 – 7.31 (m, 3H), 7.28 (d, *J* = 7.8 Hz, 4H), 7.19 – 7.12 (m, 3H), 7.04 – 7.00 (m, 2H), 5.57 (s, 2H), 5.16 (d, *J* = 11.8 Hz, 1H), 4.95 (d, *J* = 11.7 Hz, 1H), 4.19 (dd, *J* = 11.7, 4.1 Hz, 1H), 3.21 (t, *J* = 12.4 Hz, 1H), 2.90 (dd, *J* = 13.0, 4.1 Hz, 1H), 1.48 (s, 9H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 169.6, 157.6, 148.2, 139.3, 138.5, 136.1, 134.7, 131.3, 131.3, 129.6, 129.2, 129.0, 128.8, 128.4, 128.3, 128.2, 128.1, 128.1, 128.1, 128.0, 127.8, 127.7, 127.4, 126.8, 126.7, 125.6, 123.5, 119.5, 89.4, 85.96, 84.8, 82.7, 68.4, 54.3, 37.5, 29.7, 28.0, 26.1. HRMS (ESI) $[M+Na]^+$ calcd for $C_{38}H_{36}N_4O_4Na^+$, 635.2629, found 635.2625. (Chiral IA, λ= 254 nm, *n*-hexane/2-propanol= 39/11, Flow rate = 1.0 mL/min), $t_R$ = 13.353 min, 34.548 min (major).

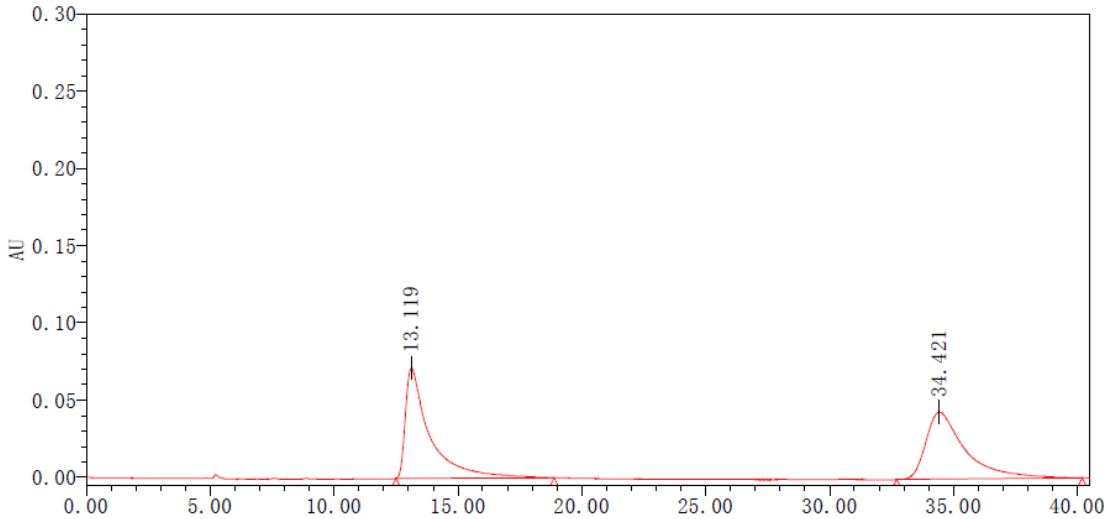
**HPLC chromatogram of racemic S26**

Condition: n-hexane/2-propanol = 39:11

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| 1 | 13.119 | 4815388 | 71330 | 50.28 |
| 2 | 34.421 | 4815388 | 43480 | 49.72 |

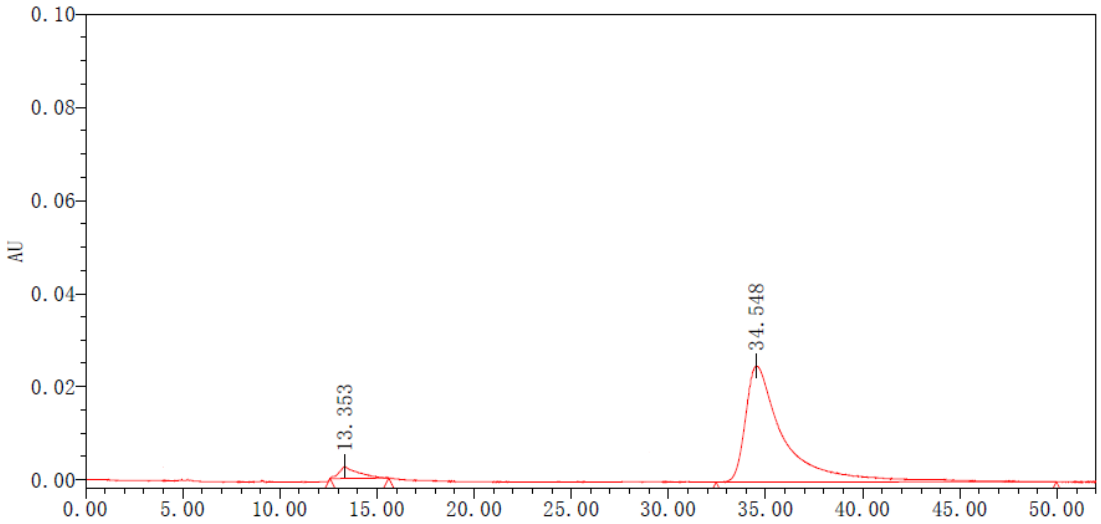
**HPLC chromatogram of chiral S26**

Condition: n-hexane/2-propanol =39:11

Flow rate =1.0 mL/min

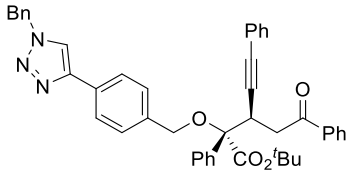
λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 13.353 | 149153 | 2539 | 4.11 |
| 2 | 34.548 | 3479877 | 24976 | 95.89 |

**Tert-butyl (2S,3R)-2-((4-(1-benzyl-1H-1,2,3-triazol-4-yl)benzyl)oxy)-3-(2-oxo-2-phenylethyl)-2,5-diphenylpent-4-ynoate (S27)**




**S27**

Colorless oil; 60.4 mg, 88% yield, >20:1 d.r., 94% *ee*; $^{1}$H NMR (500 MHz, $CDCl_3$) δ 7.84 (d, *J* = 7.4 Hz, 2H), 7.80 (d, *J* = 8.1 Hz, 2H), 7.71 (d, *J* = 7.5 Hz, 2H), 7.66 (s, 1H), 7.54 (d, *J* = 8.1 Hz, 2H), 7.50 (t, *J* = 7.4 Hz, 1H), 7.39 (t, *J* = 5.4 Hz, 4H), 7.37 – 7.34 (m, 3H), 7.33 – 7.28 (m, 3H), 7.26 – 7.20 (m, 5H), 5.58 (s, 2H), 5.13 (d, *J* = 11.7 Hz, 1H), 4.97 (d, *J* = 11.7 Hz, 1H), 4.41 (dd, *J* = 10.3, 2.9 Hz, 1H), 3.35 (dd, *J* = 16.6, 10.3 Hz, 1H), 3.10 (dd, *J* = 16.6, 2.9 Hz, 1H), 1.51 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 197.5, 169.5, 148.2, 139.1, 138.5, 137.0, 134.7, 133.1, 131.4, 129.7, 129.2, 128.8, 128.5, 128.2, 128.2, 128.2, 128.2, 128.1, 128.0, 127.8, 126.8, 125.7, 123.5, 119.4, 89.8, 85.9, 84.1, 82.8, 68.4, 54.3, 39.2, 36.7, 28.1. HRMS (ESI) $[M+Na]^+$ calcd for $C_{45}H_{41}N_3O_4Na^+$, 710.2989, found 710.2987. (Chiral IA-3, λ= 254 nm, *n*-hexane/2-propanol= 17/1, Flow rate = 1.0 mL/min), $t_R$ = 35.411 min(major), 60.438 min.

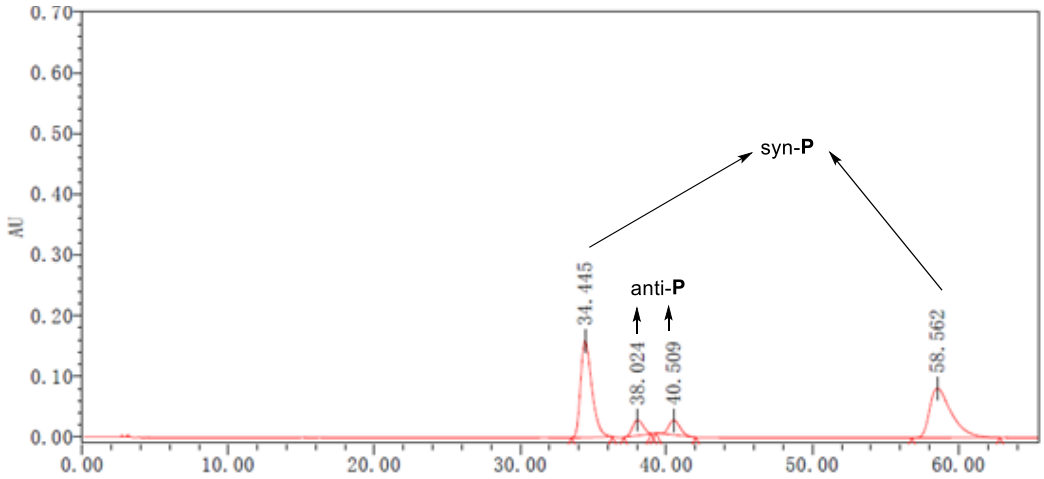
**HPLC chromatogram of racemic S27**

Condition: n-hexane/2-propanol =17:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 34.445 | 8393787 | 159635 | 43.27 |

| | | | | |
|---|---|---|---|---|
| 2 | 38.024 | 1267538 | 25436 | 6.53 |
| 3 | 40.509 | 1267898 | 24111 | 6.54 |
| 4 | 58.562 | 8469407 | 81582 | 43.66 |

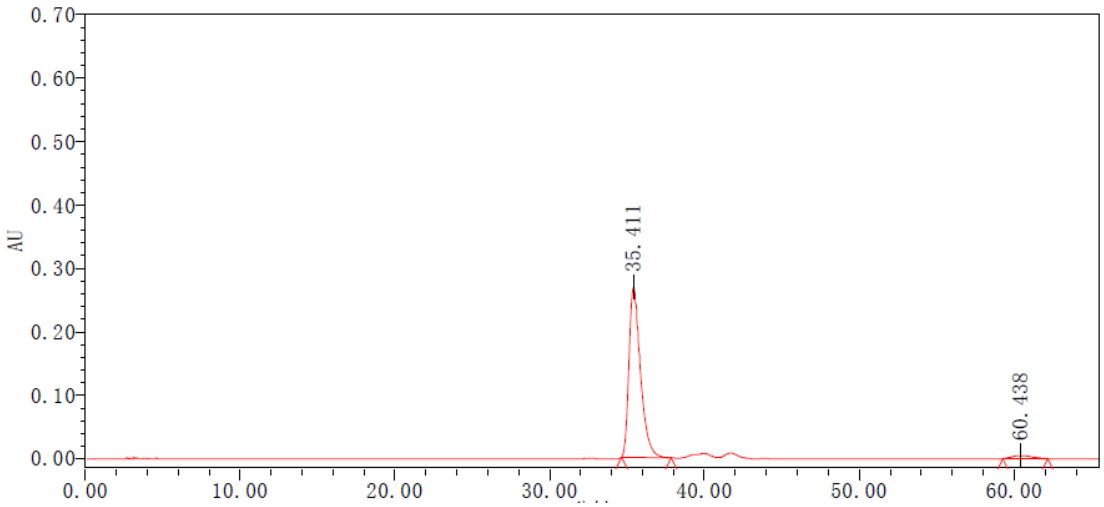
**HPLC chromatogram of chiral S27**

Condition: n-hexane/2-propanol =17:1

Flow rate =1.0 mL/min

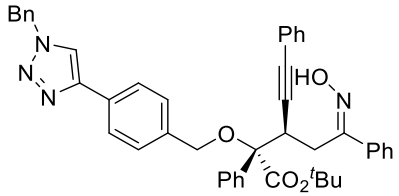
λ= 254 nm

Chiral IE-3




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 35.411 | 13996459 | 268264 | 97.04 |
| 2 | 60.438 | 426965 | 4857 | 2.96 |

**Tert-butyl (2S,3R)-2-((4-(1-benzyl-1H-1,2,3-triazol-4-yl)benzyl)oxy)-3-((E)-2-(hydroxyimino)-2-phenylethyl)-2,5-diphenylpent-4-ynoate (S28)**




**S28**

White solid; 31.6 mg, 75% yield, >20:1 d.r., 94% *ee*; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.71 (s, 1H), 7.80 (d, *J* = 8.1 Hz, 2H), 7.70 (d, *J* = 7.0 Hz, 2H), 7.65 (d, *J* = 6.0 Hz, 1H), 7.57 – 7.50 (m, 4H), 7.37 (t, *J* = 5.6 Hz, 4H), 7.34 – 7.31 (m, 3H), 7.28 (d, *J* = 7.8 Hz, 4H), 7.19 – 7.12 (m, 3H), 7.04 – 7.00 (m, 2H), 5.57 (s, 2H), 5.16 (d, *J* = 11.8 Hz, 1H), 4.95 (d, *J* = 11.7 Hz, 1H), 4.19 (dd, *J* = 11.7, 4.1 Hz, 1H), 3.21 (t, *J* = 12.4 Hz, 1H), 2.90 (dd, *J* = 13.0, 4.1 Hz, 1H), 1.48 (s, 9H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 169.6, 157.6, 148.2, 139.3, 138.5, 136.1, 134.7, 131.3, 129.6, 129.2, 129.0, 128.8, 128.4, 128.3, 128.2, 128.1, 128.1, 128.0, 127.8, 127.7, 127.4, 126.7, 125.6, 123.5, 119.5, 89.4, 86.0, 84.8, 82.7, 68.4, 54.3, 37.5, 29.7, 28.0, 26.1. HRMS (ESI) $[M+Na]^+$ calcd for $C_{45}H_{42}N_4O_4Na^+$, 725.3098, found 725.3096. (Chiral IA, λ= 254 nm, *n*-hexane/2-propanol= 4/1, Flow rate = 1.0 mL/min), $t_R$ = 45.063 min(major), 74.588 min.

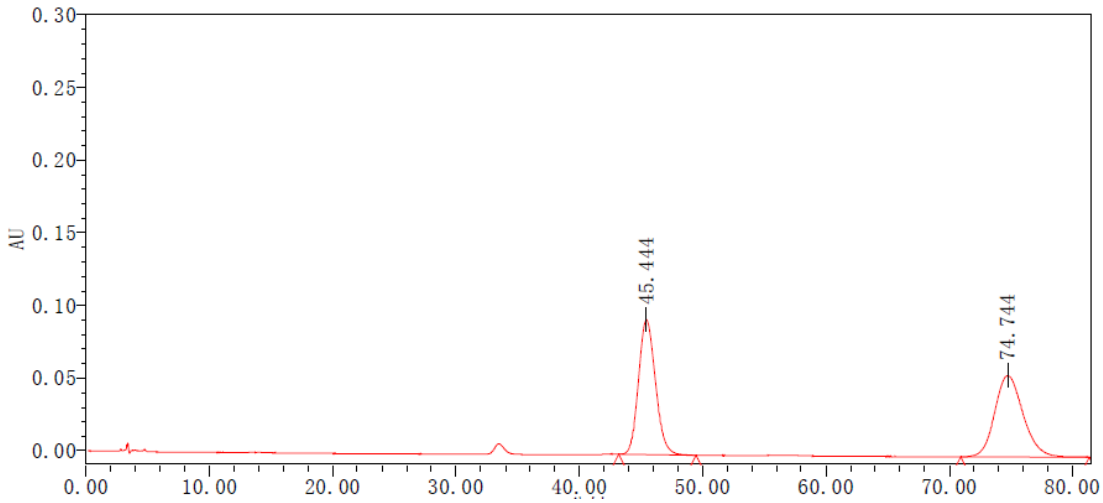
**HPLC chromatogram of racemic S28**

Condition: n-hexane/2-propanol = 4:1

Flow rate =1.0 mL/min

λ= 254 nm

Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|
| 1 | 45.444 | 8793773 | 92761 | 49.71 |
| 2 | 74.744 | 8897465 | 55894 | 50.29 |

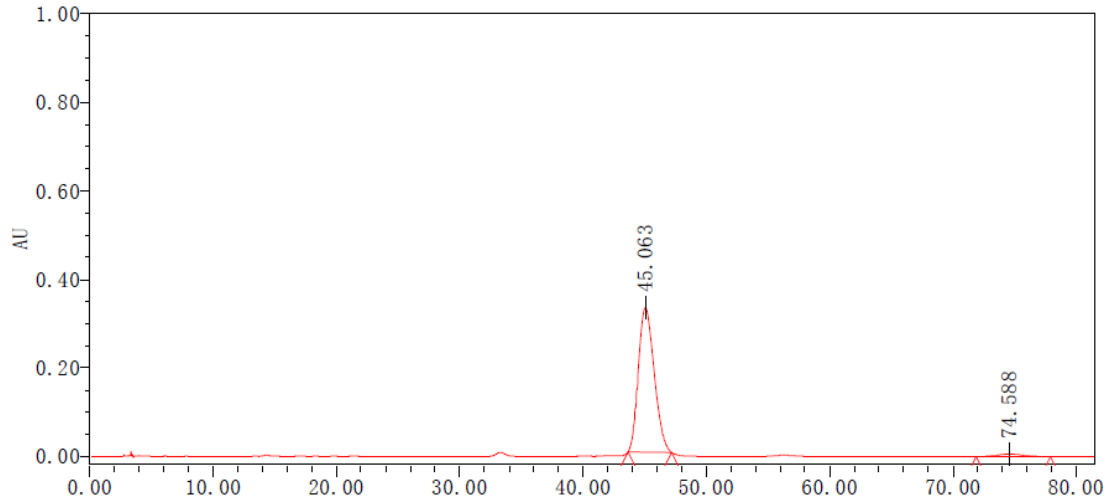
**HPLC chromatogram of chiral S28**

Condition: n-hexane/2-propanol =4:1

Flow rate =1.0 mL/min

λ= 254 nm

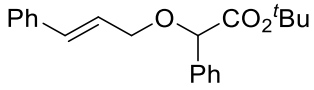
Chiral IA




| Entry | Retention Time/min | Area | Height | Area(%) |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| 1 | 45.063 | 28916180 | 326482 | 97.19 |
| 2 | 74.588 | 835533 | 5543 | 2.81 |

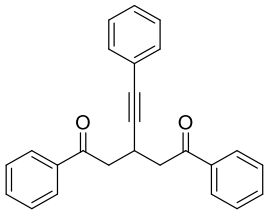
**Tert-butyl 2-(cinnamyloxy)-2-phenylacetate (By-product-1)**



By-product-**1**

Colorless oil; 31.6 mg, 75% yield; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.46 (dd, *J* = 7.9, 1.2 Hz, 2H), 7.39 – 7.35 (m, 3H), 7.34 – 7.26 (m, 4H), 7.26 – 7.22 (m, 1H), 6.59 (d, *J* = 15.9 Hz, 1H), 6.32 (dt, *J* = 15.9, 6.2 Hz, 1H), 4.85 (s, 1H), 4.22 (dd, *J* = 6.2, 1.1 Hz, 2H), 1.38 (s, 9H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 170.0, 137.0, 136.6, 133.2, 128.6, 128.5, 128.4, 127.8, 127.3, 126.6, 125.5, 81.8, 80.2, 77.4, 77.1, 76.8, 70.0, 27.9. HRMS (ESI) $[M+Na]^+$ calcd for $C_{21}H_{24}O_3Na^+$, 347.1620, found 347.1618.

**1,5-diphenyl-3-(phenylethynyl)pentane-1,5-dione (By-product-2)**

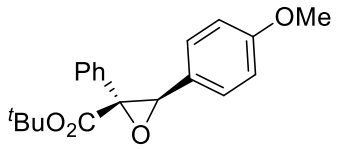


By-product-**2**

$^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.07 – 7.99 (m, 4H), 7.60 – 7.53 (m, 2H), 7.48 (t, *J* = 7.6 Hz, 4H), 7.29 – 7.25 (m, 3H), 7.24 – 7.20 (m, 2H), 3.95 (p, *J* = 6.7 Hz, 1H), 3.47 (dd, *J* = 16.7, 6.7 Hz, 2H), 3.36 (dd, *J* = 16.7, 6.7 Hz, 2H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 197.7, 136.9, 133.3, 131.7, 128.7, 128.3, 128.1, 127.8, 123.3, 100.0, 91.0, 43.1, 29.7, 24.2. HRMS (ESI) $[M+Na]^+$ calcd for $C_{25}H_{20}O_2Na^+$, 375.1356, found 375.1357.

**Tert-butyl (2R,3R)-3-(4-methoxyphenyl)-2-phenyloxirane-2-carboxylate (By-**

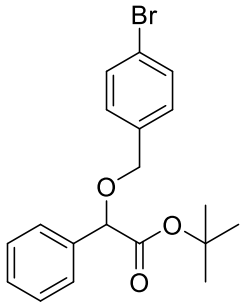
**product-3)**




Byproduct-**3**

$^1$H NMR (500 MHz, $CDCl_3$) δ 7.65 – 7.59 (m, 1H), 7.41 (d, *J* = 1.7 Hz, 1H), 7.39 (d, *J* = 7.6 Hz, 1H), 7.37 (d, *J* = 7.0 Hz, 1H), 7.35 (d, *J* = 8.7 Hz, 2H), 6.89 (d, *J* = 8.7 Hz, 2H), 4.06 (s, 1H), 3.81 (s, 3H), 1.23 (s, 9H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 165.7, 159.8, 135.4, 128.5, 127.6, 126.3, 126.1, 113.6, 82.7, 66.9, 65.6, 55.4, 27.7. HRMS (ESI) $[M+Na]^+$ calcd for $C_{20}H_{22}O_4Na^+$, 349.1410, found 349.1407.

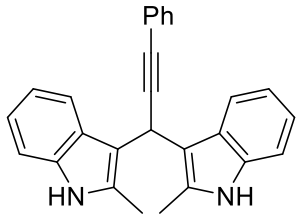
**Tert-Butyl 2-((4-bromobenzyl)oxy)-2-phenylacetate (By-product-4)**




By-product-**4**

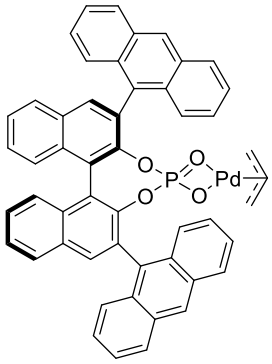
White solid, mp: 87.7 – 88.5 °C; 63.9 mg, 85% yield; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.49 – 7.41 (m, 4H), 7.39 – 7.32 (m, 3H), 7.25 (d, *J* = 8.6 Hz, 2H), 4.78 (s, 1H), 4.56 (d, *J* = 12.0 Hz, 1H), 4.51 (d, *J* = 12.0 Hz, 1H), 1.39 (s, 9H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 169.8, 136.6, 136.6, 131.5, 129.6, 128.54, 128.52, 127.3, 121.7, 82.0, 80.3, 70.3, 27.9. HRMS(ESI) $[M + Na]^+$ calcd for $C_{19}H_{21}BrO_3Na^+$, 399.0566, found 399.0566.

**3,3'-(3-Phenylprop-2-yne-1,1-diyl)bis(2-methyl-1*H*-indole) (By-product-5)**




By-product-**5**

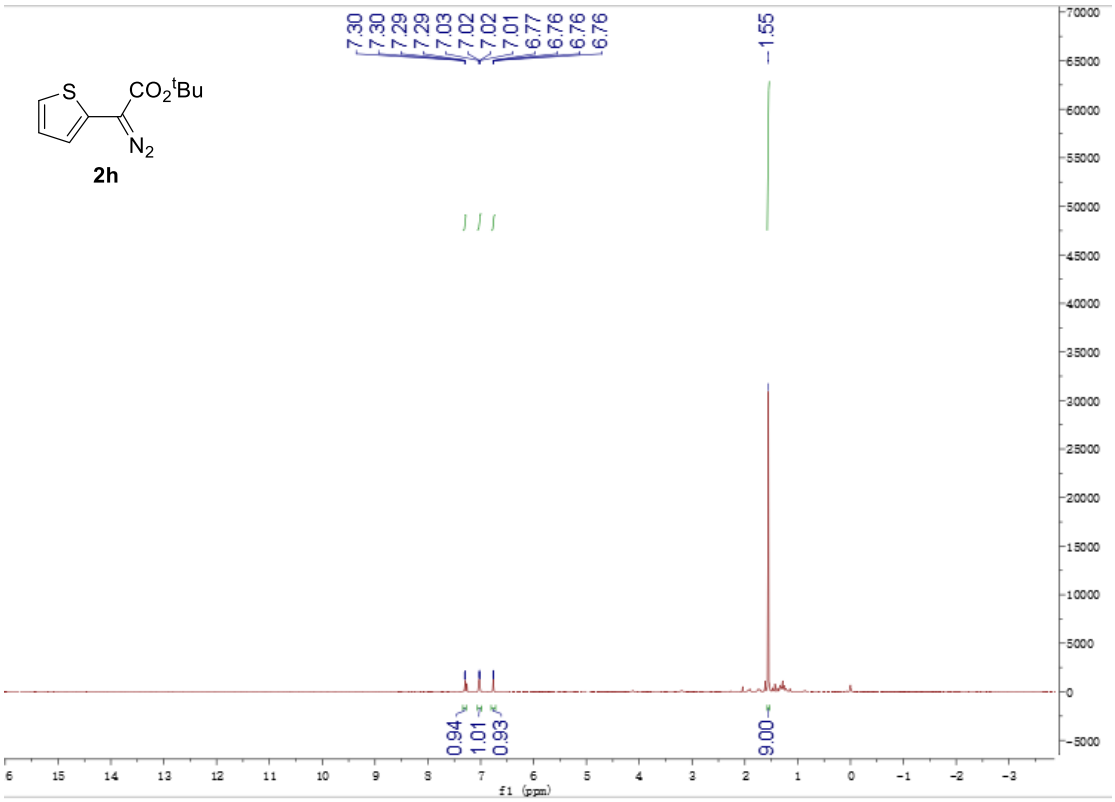
$^{1}$H NMR (400 MHz, Acetone) δ 8.95 (s, 2H), 6.89 (d, *J* = 6.7 Hz, 2H), 6.54 (s, 2H), 6.40 (s, 5H), 6.08 (dd, *J* = 21.4, 6.6 Hz, 4H), 5.00 (s, 1H), 1.60 (s, 6H). $^{13}$C NMR (101 MHz, Acetone) δ 135.5, 131.6, 131.3, 128.5, 128.2, 127.7, 124.3, 120.3, 118.8, 118.6, 110.4, 110.3, 92.1, 81.5, 25.8, 11.7. HRMS(ESI) $[M + Na]^+$ calcd for $C_{27}H_{22}N_2Na^+$, 374.1675, found 374.1665.

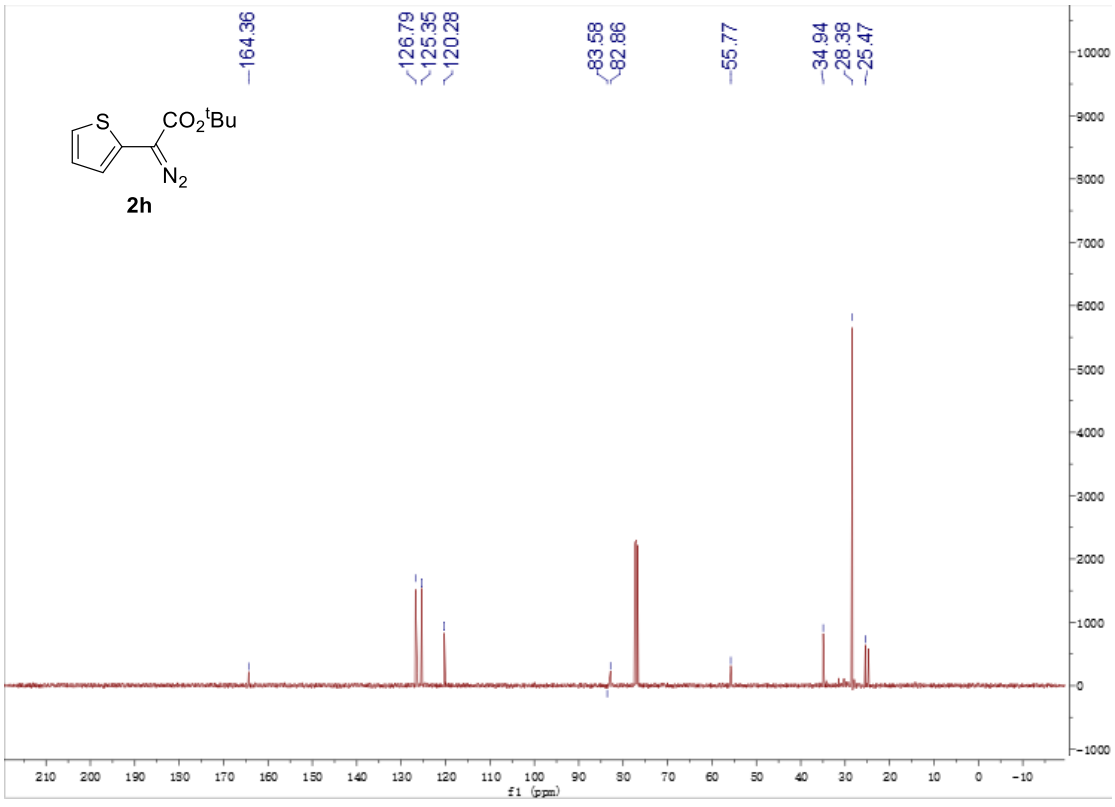


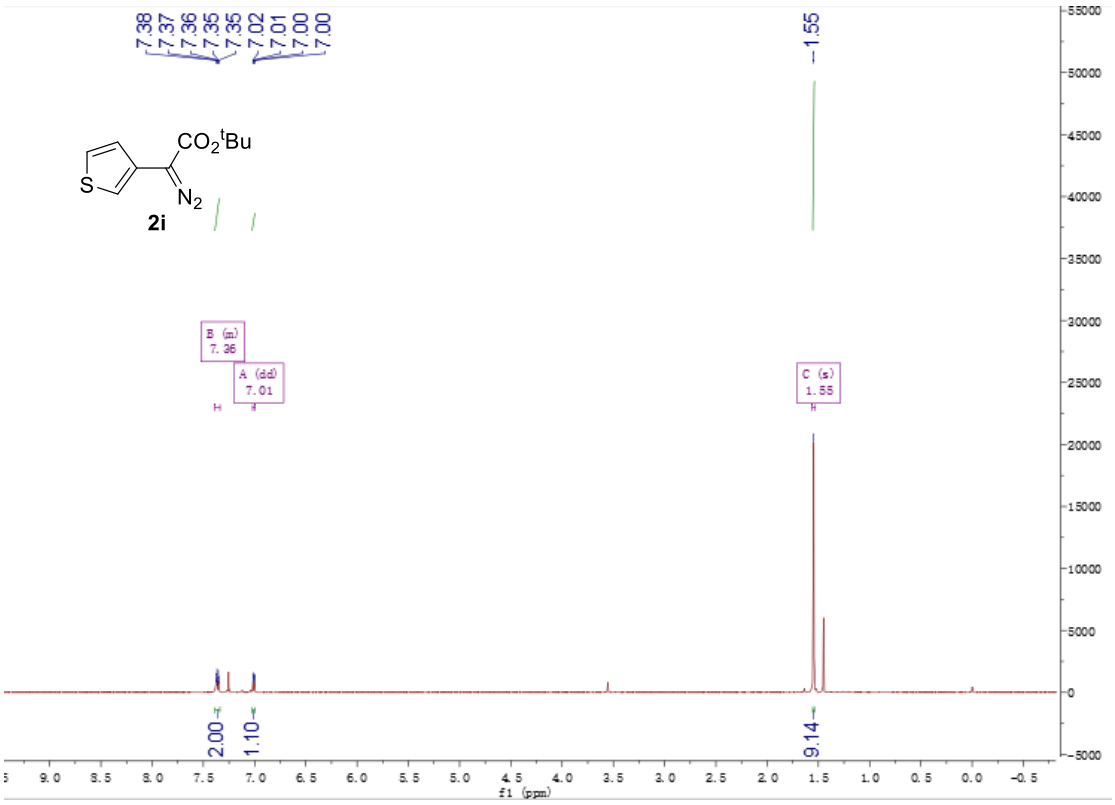

[Pd(allyl)(*R*)-**6b**]

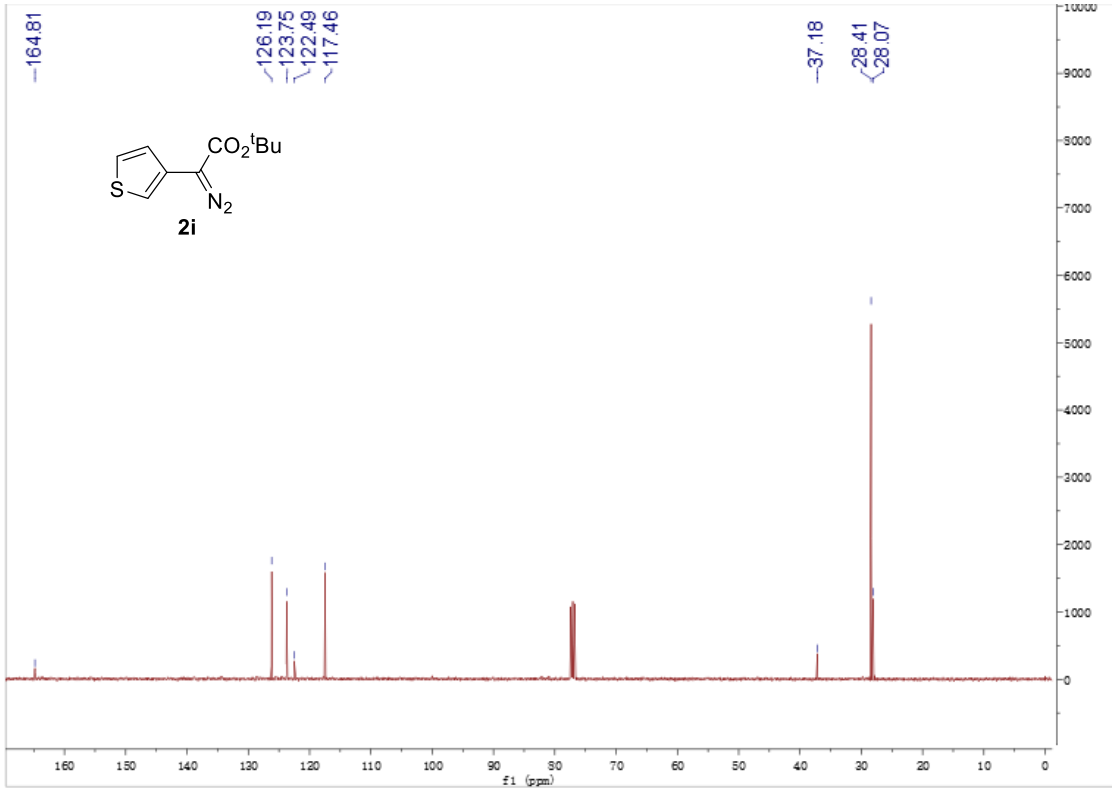
Fluffy yellowish powder (118.47 mg, 70% yield).$^{1}$H NMR (500 MHz, $CDCl_3$) δ 8.48 – 8.14 (m, 2H), 8.00 – 7.76 (m, 9H), 7.60 (d, *J* = 7.7 Hz, 4H), 7.48 – 7.32 (m, 5H), 7.28 (s, 2H), 7.16 (d, *J* = 32.9 Hz, 6H), 4.57 (br, 1H), 3.09 (br, 2H), 1.96 (br, 1H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 148.2, 133.1, 133.0, 131.7, 131.6, 131.5, 131.3, 131.4, 130.7, 129.8, 128.7, 128.7, 128.6, 128.5, 128.4, 128.2, 127.4, 127.3, 127.2, 127.1, 126.6, 126.3, 126.2, 125.9, 125.4, 125.1, 125.0, 124.9, 123.1, 110.3, 44.7, 3.75, 7.4. $^{31}$P NMR (202 MHz, $CDCl_3$) δ 13.59. HRMS (ESI) $[M+Na]^+$ calcd for $C_{51}H_{35}O_4PPdNa^+$, 871.1218, found 871.1238.

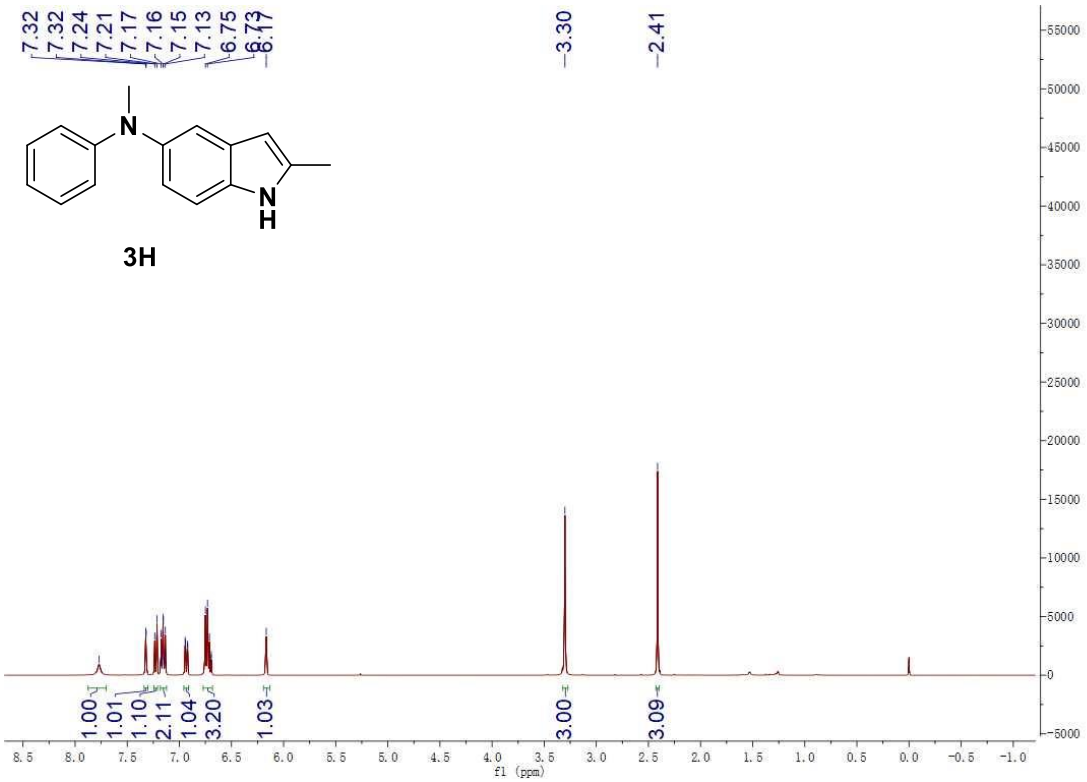
## 11. NMR Spectra for the Products

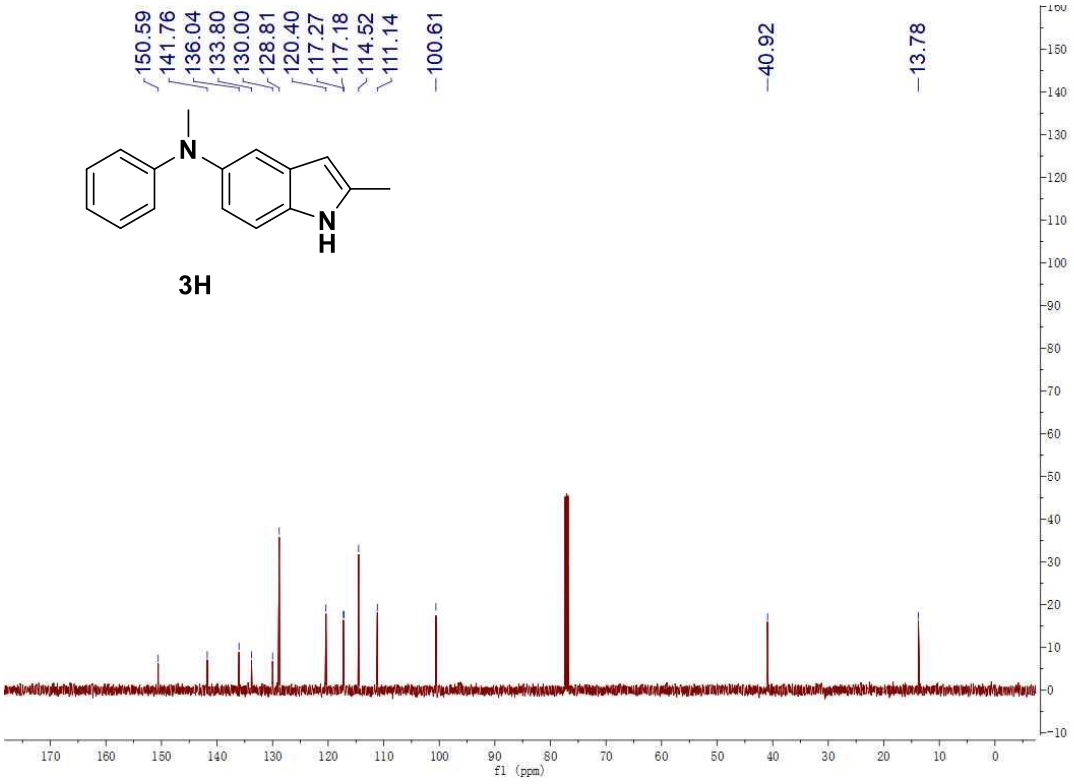


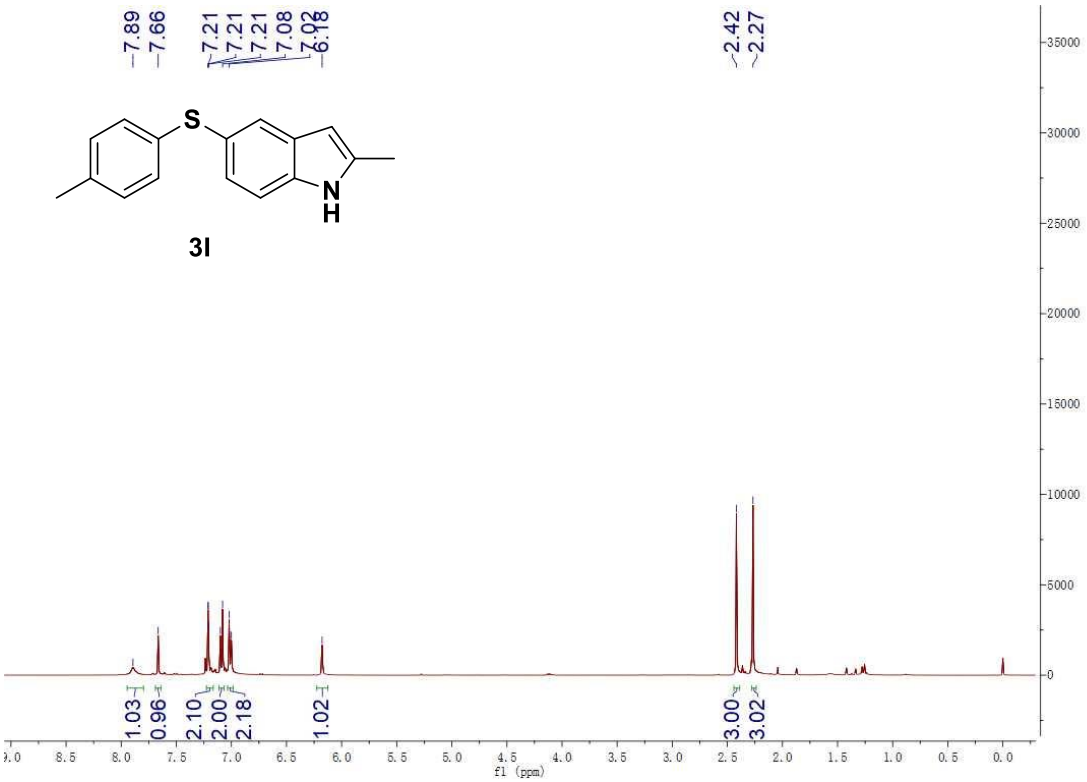



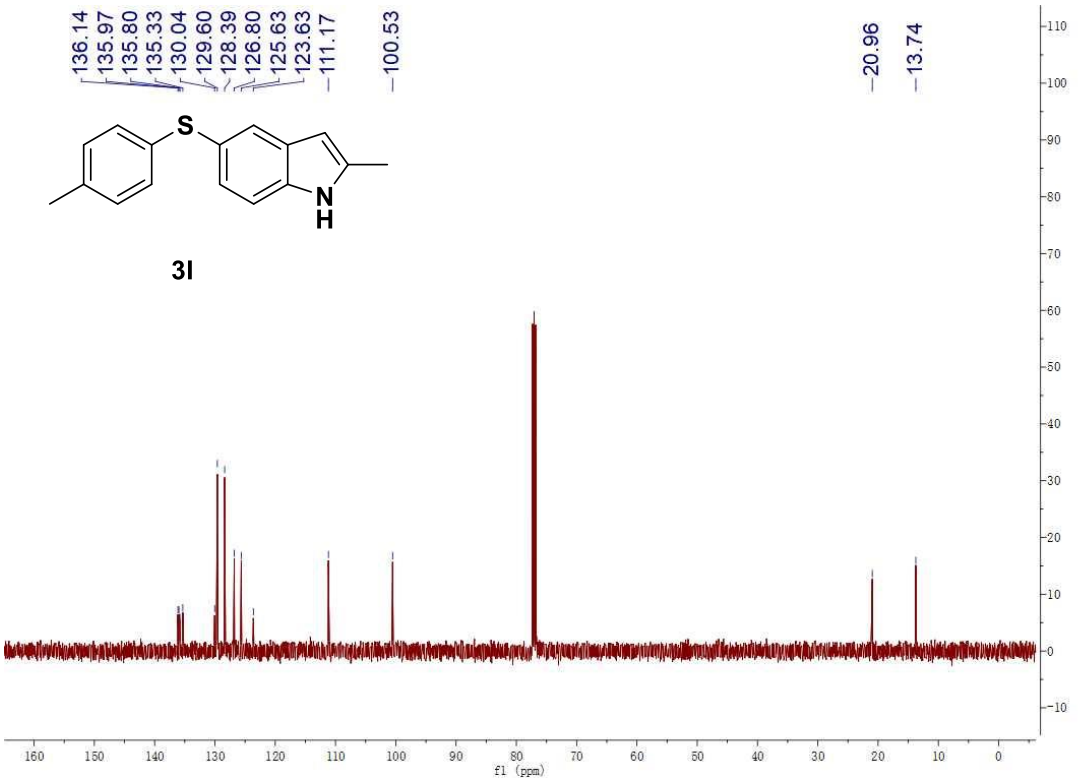

7.38
7.37
7.36
7.35
7.35
7.02
7.01
7.00
7.00
1.55
CO2tBu
S
N2
2i
B (m)
7.36
A (dd)
7.01
C (s)
1.55
2.00
1.10
9.14
f1 (ppm)

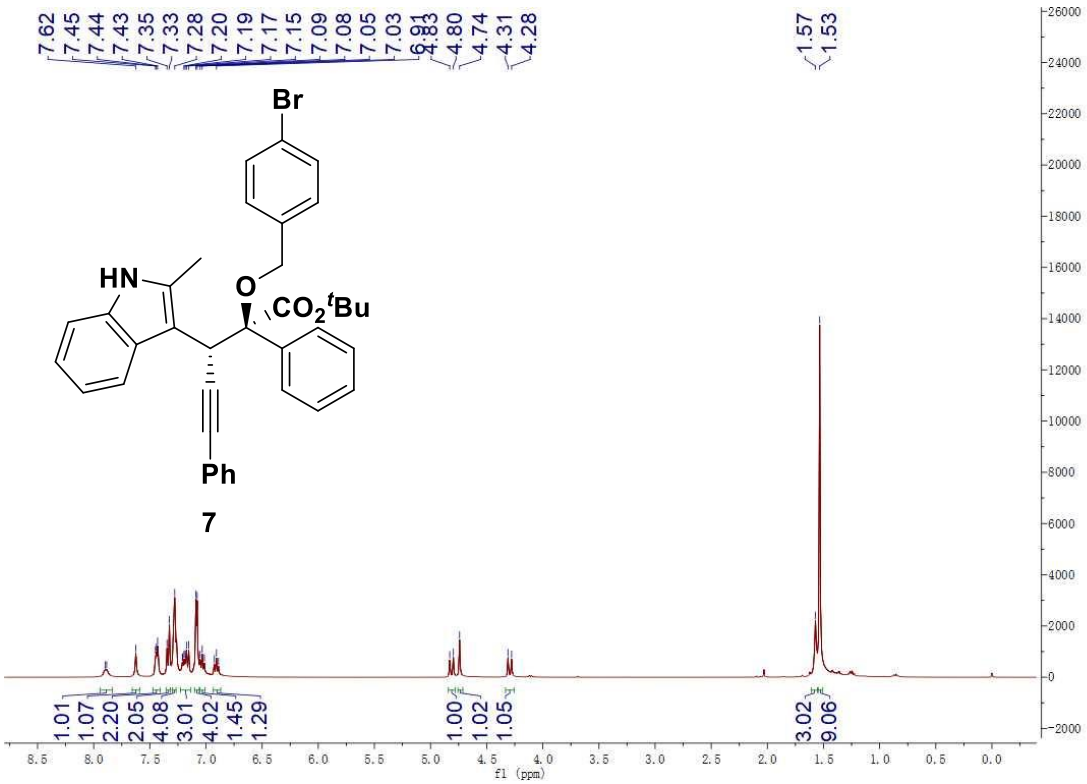

164.81
126.19
123.75
122.49
117.46
37.18
28.41
28.07
CO2tBu
S
N2
2i
f1 (ppm)

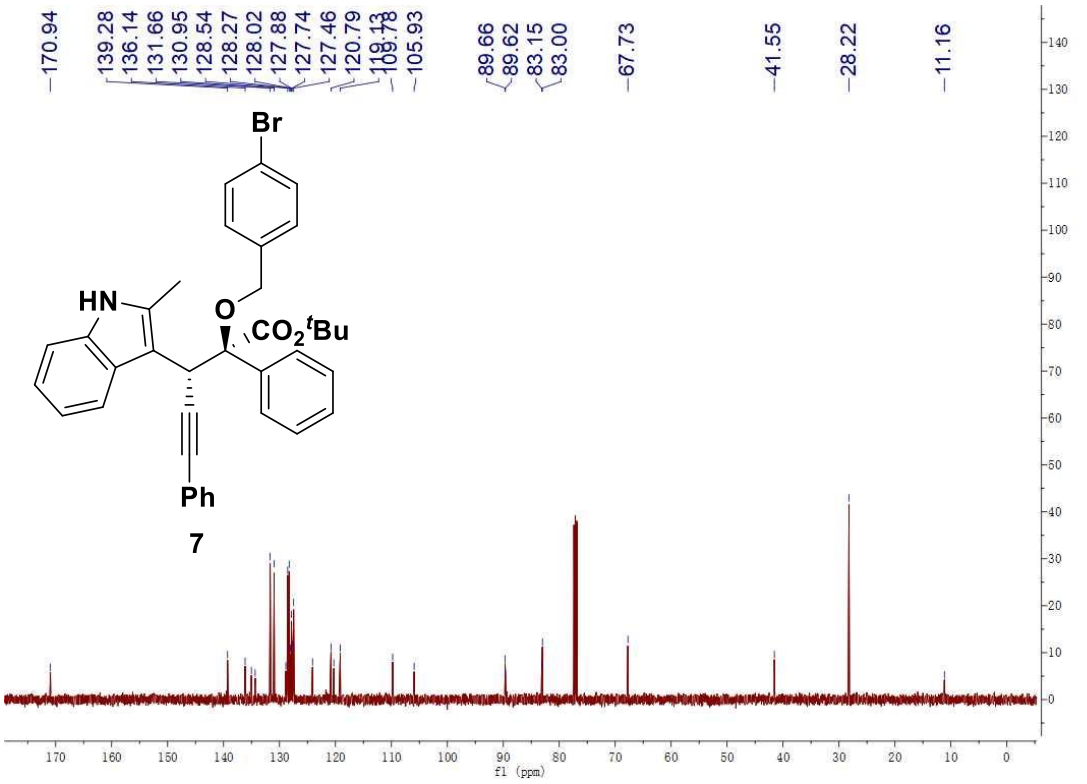

7.32
7.32
7.24
7.21
7.17
7.16
7.15
7.13
6.75
6.73
6.17
3.30
2.41
N
N
H
3H
1.00
1.01
1.10
2.11
1.04
3.20
1.03
3.00
3.09
f1 (ppm)

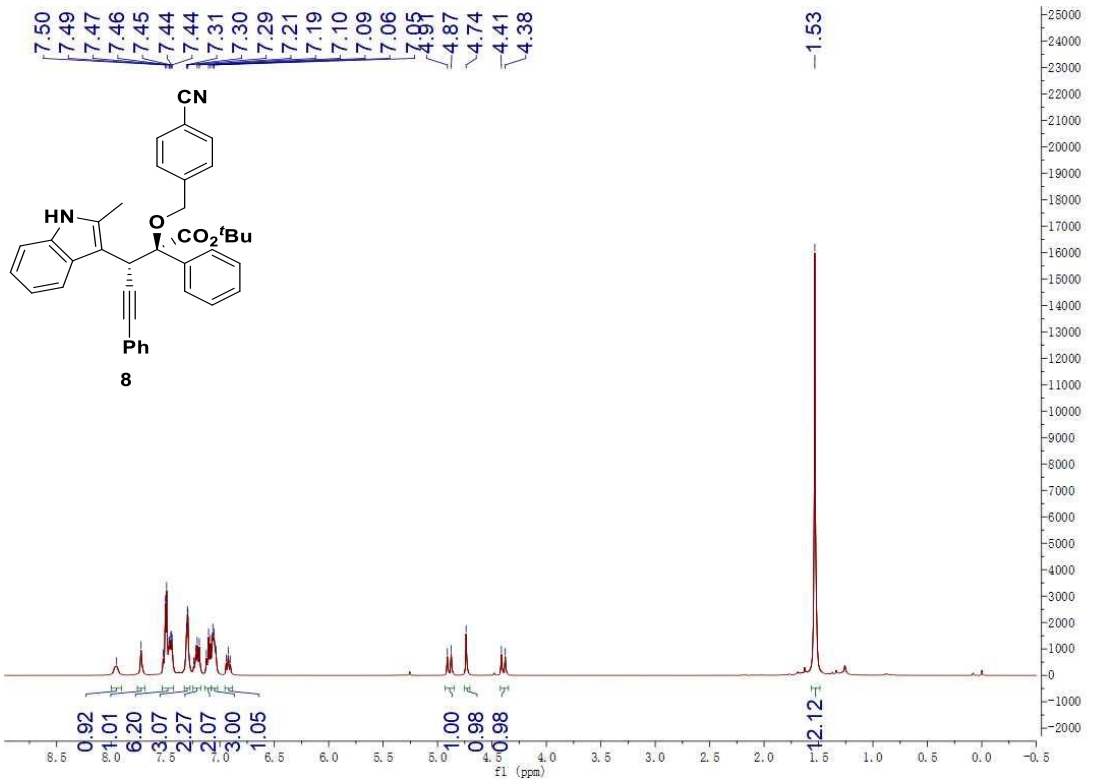

150.59
141.76
136.04
133.80
130.00
128.81
120.40
117.27
117.18
114.52
111.14
100.61
40.92
13.78
N
N
H
3H
f1 (ppm)

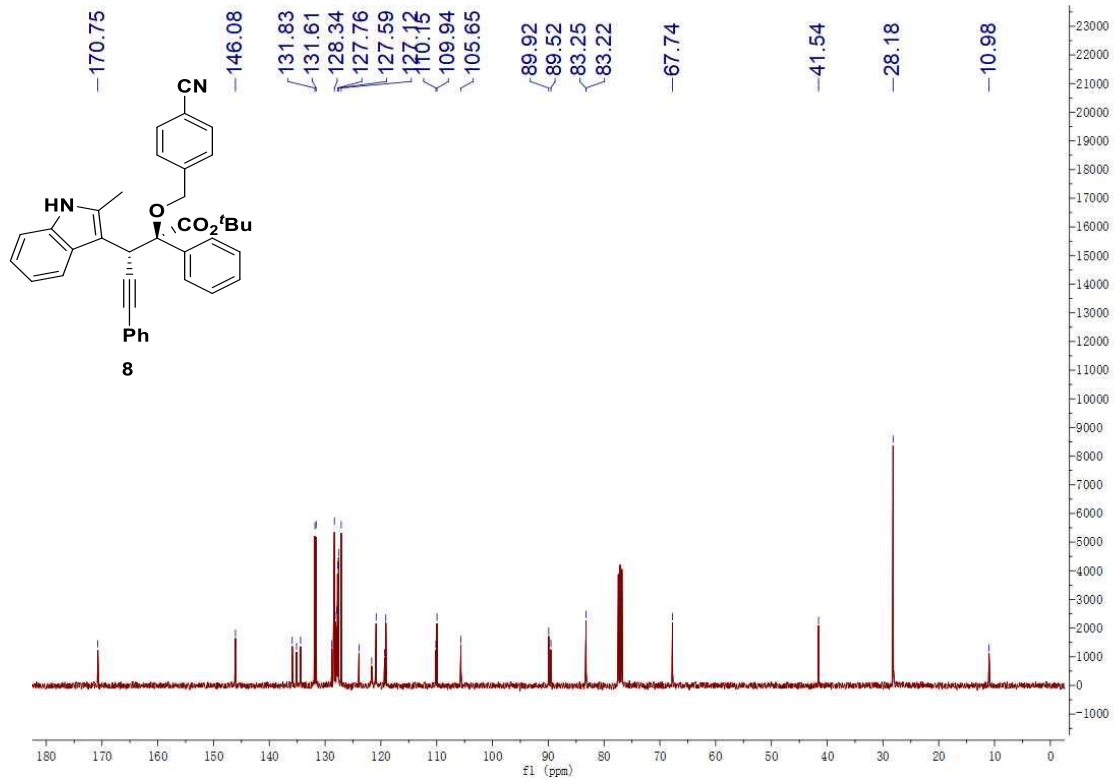

7.89
7.66
7.21
7.21
7.21
7.08
7.02
6.18
2.42
2.27
S
N
H
3l
1.03
0.96
2.10
2.00
2.18
1.02
3.00
3.02
f1 (ppm)

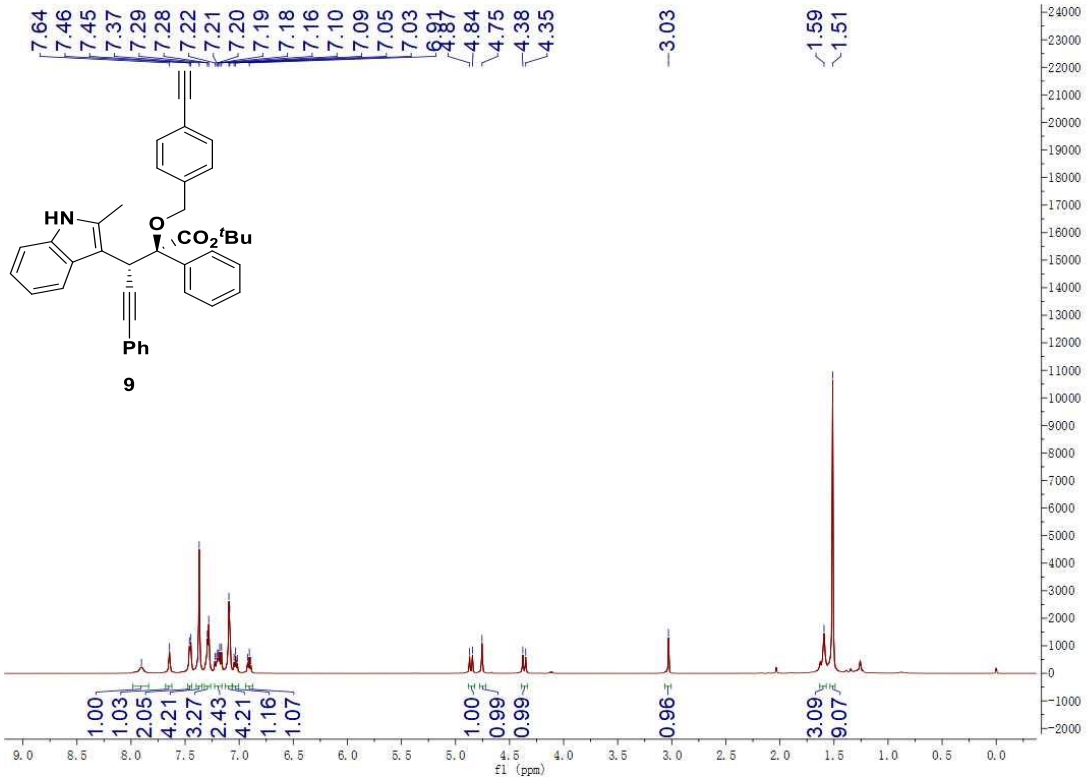

136.14
135.97
135.80
135.33
130.04
129.60
128.39
126.80
125.63
123.63
111.17
100.53
20.96
13.74
S
N
H
3l
f1 (ppm)

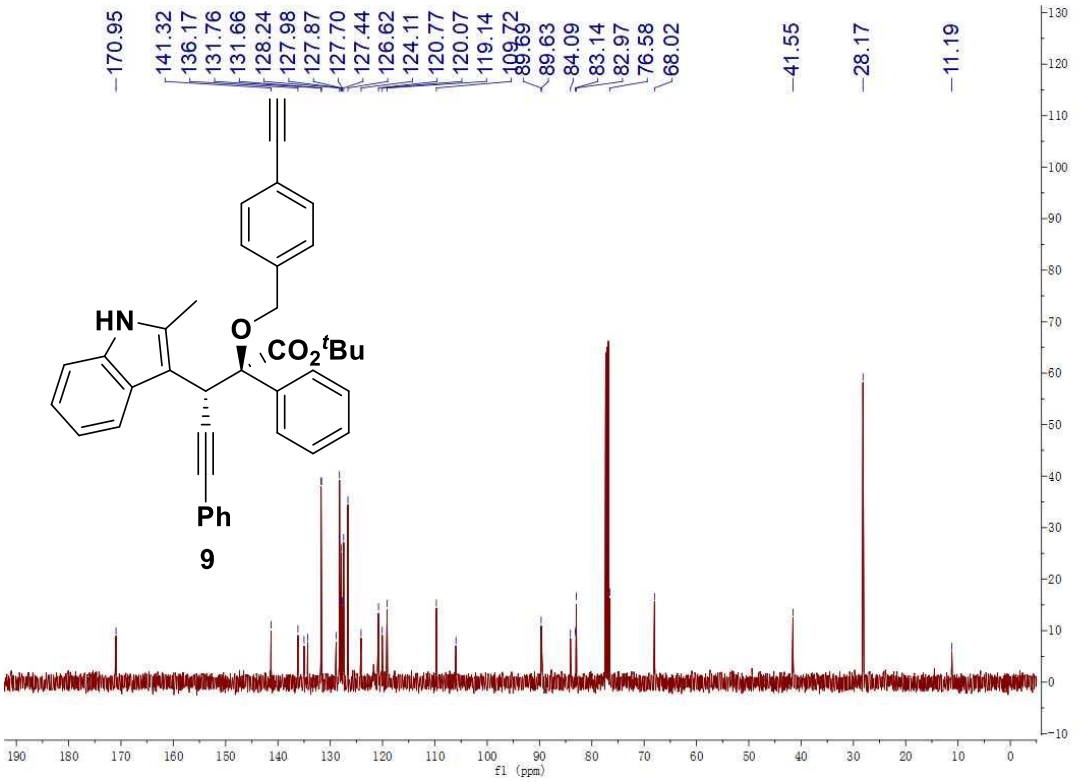

7.62
7.45
7.44
7.43
7.35
7.33
7.28
7.20
7.19
7.17
7.15
7.09
7.08
7.05
7.03
6.81
4.83
4.80
4.74
4.31
4.28
1.57
1.53
Br
HN
O
CO2tBu
Ph
7
1.01
1.07
2.20
2.05
4.08
3.01
4.02
1.45
1.29
1.00
1.02
1.05
3.02
9.06
f1 (ppm)

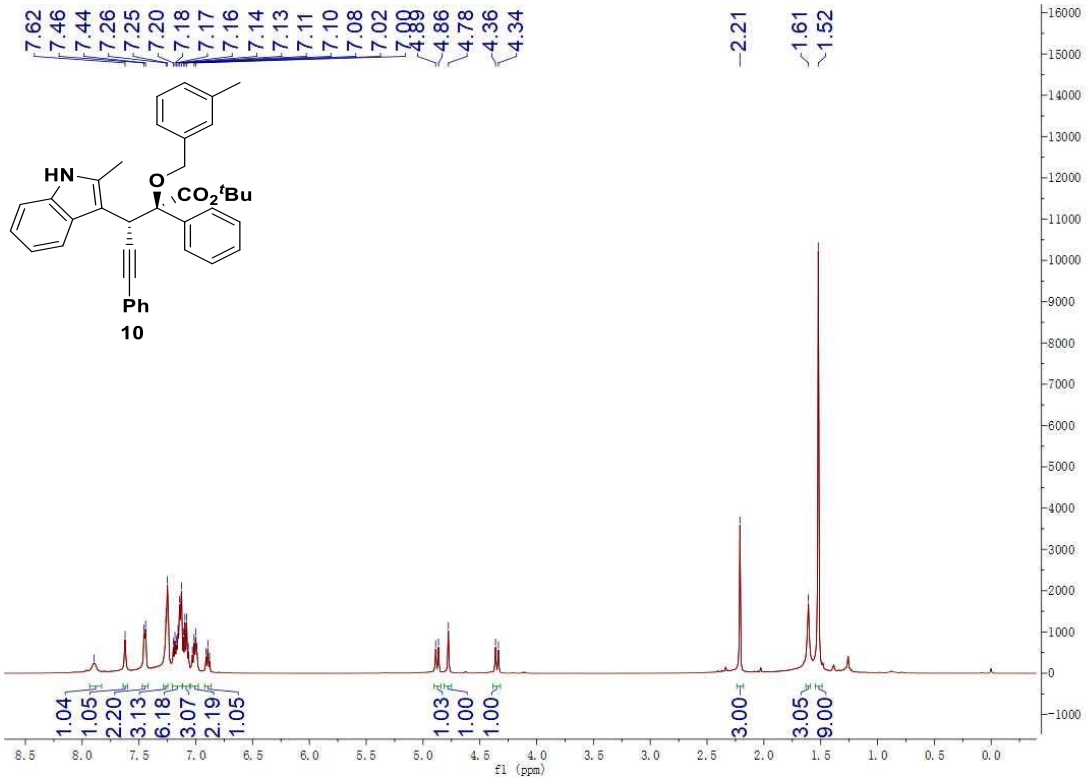

170.94
139.28
136.14
131.66
130.95
128.54
128.27
128.02
127.88
127.74
127.46
120.79
119.13
110.78
105.93
89.66
89.62
83.15
83.00
67.73
41.55
28.22
11.16
Br
HN
O
CO2tBu
Ph
7
f1 (ppm)

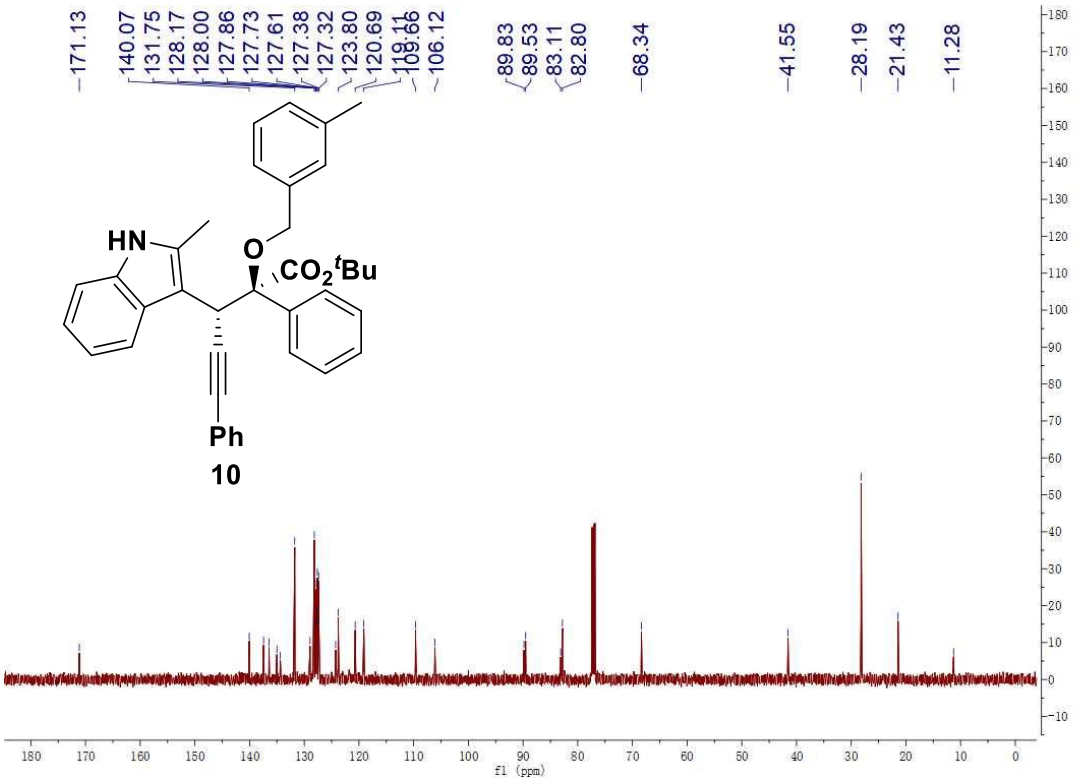

7.50
7.49
7.47
7.46
7.45
7.44
7.44
7.31
7.30
7.29
7.21
7.19
7.10
7.09
7.06
4.91
4.87
4.74
4.41
4.38
1.53
CN
HN
O
CO2tBu
Ph
8
0.92
1.01
6.20
3.07
2.27
2.07
3.00
1.05
1.00
0.98
0.98
12.12
f1 (ppm)

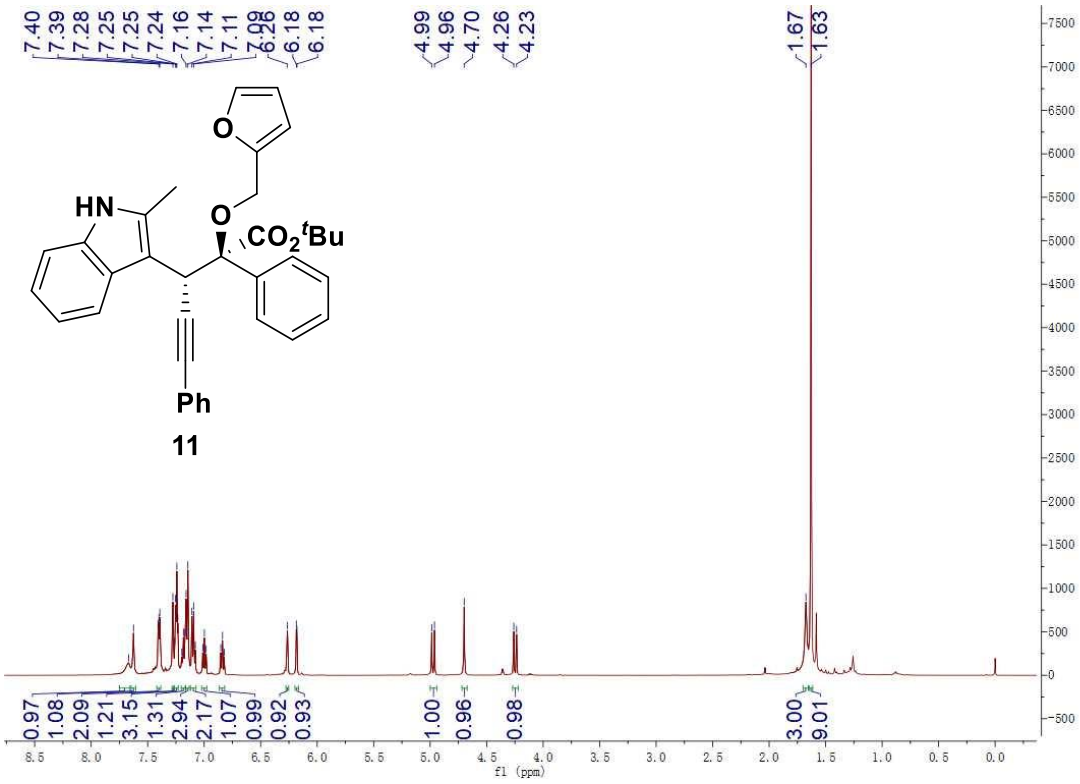

170.75
146.08
131.83
131.61
128.34
127.76
127.59
127.12
110.15
109.94
105.65
89.92
89.52
83.25
83.22
67.74
41.54
28.18
10.98
CN
HN
O
CO2tBu
Ph
8
f1 (ppm)

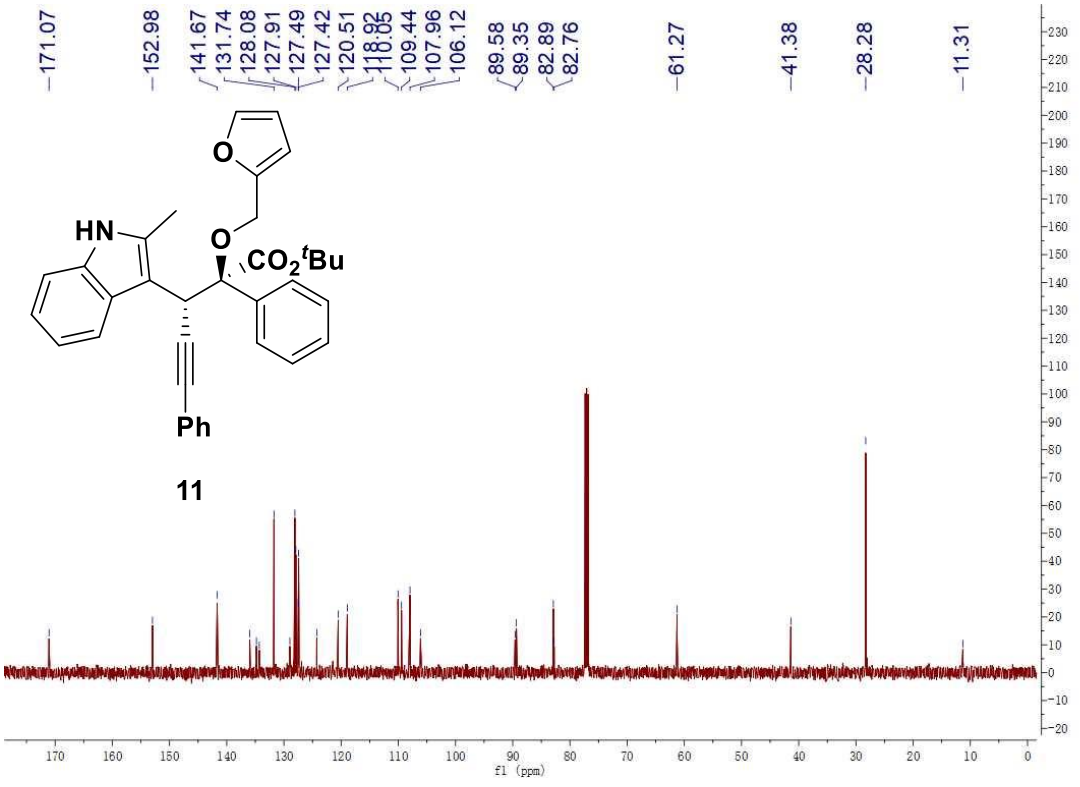

7.64
7.46
7.45
7.37
7.29
7.28
7.22
7.21
7.20
7.19
7.18
7.16
7.10
7.09
7.05
7.03
6.91
4.87
4.84
4.75
4.38
4.35
3.03
1.59
1.51
HN
O
CO2tBu
Ph
9
1.00
1.03
2.05
4.21
3.27
2.43
4.21
1.16
1.07
1.00
0.99
0.99
0.96
3.09
9.07
f1 (ppm)

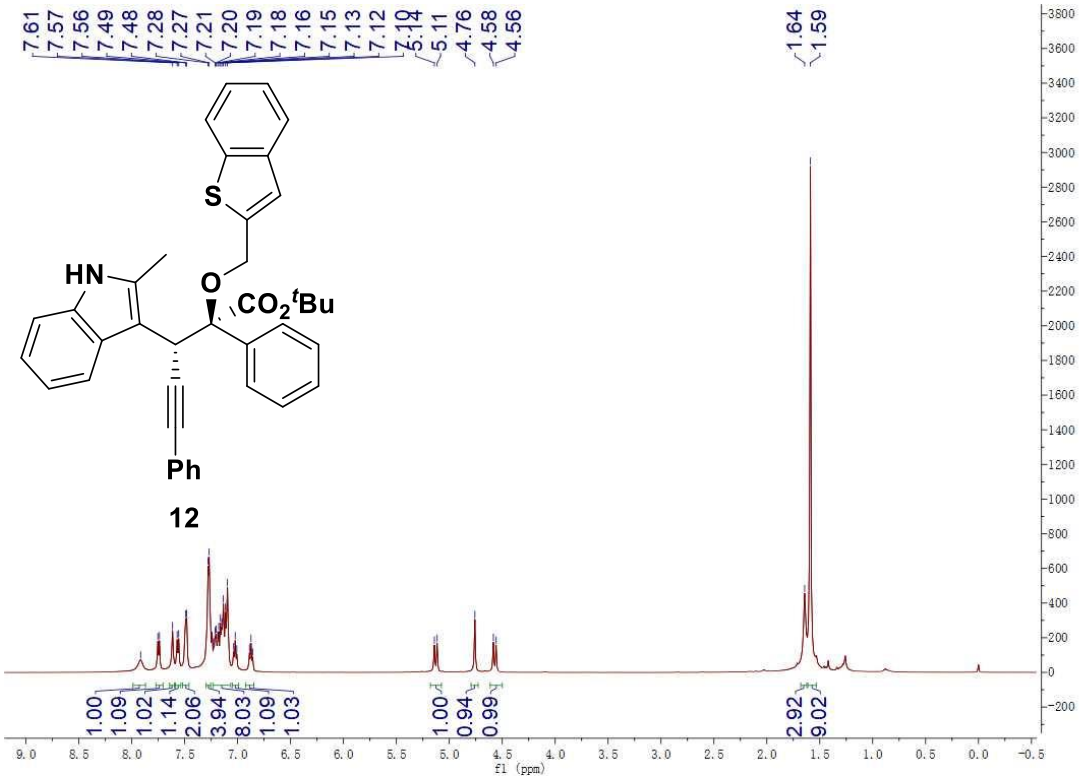

170.95
141.32
136.17
131.76
131.66
128.24
127.98
127.87
127.70
127.44
126.62
124.11
120.77
120.07
119.14
109.72
89.69
89.63
84.09
83.14
82.97
76.58
68.02
41.55
28.17
11.19
HN
O
CO2tBu
Ph
9
f1 (ppm)

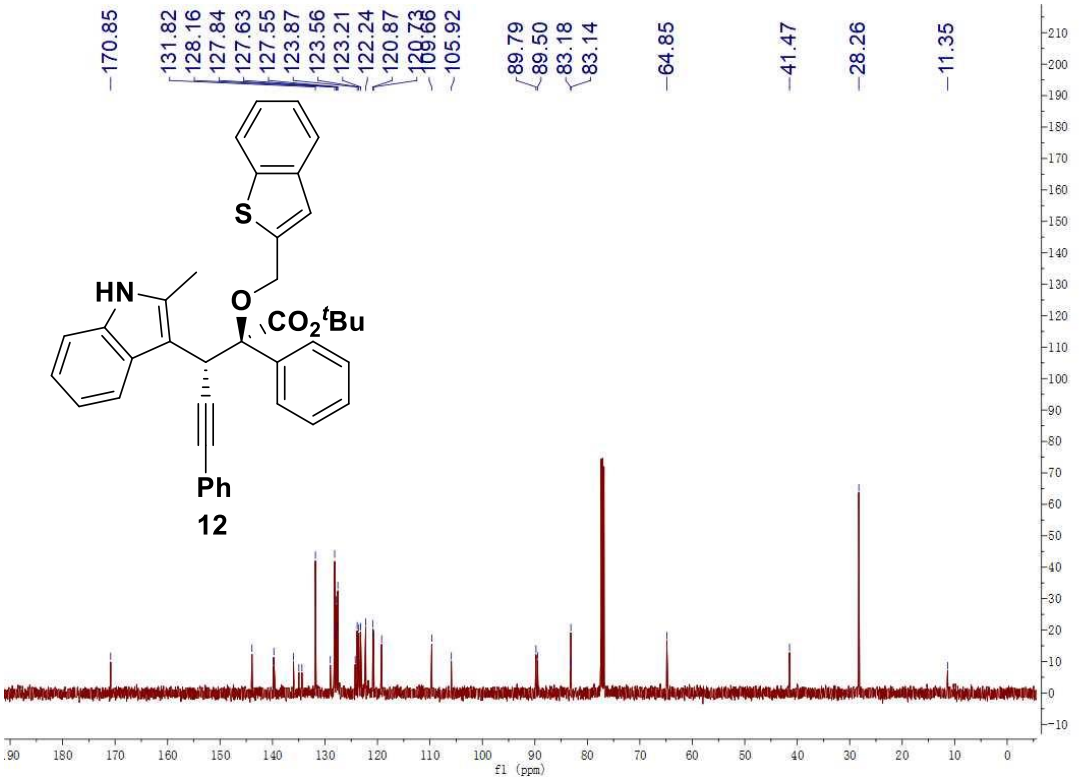

7.62
7.46
7.44
7.26
7.25
7.20
7.18
7.17
7.16
7.14
7.13
7.11
7.10
7.08
7.02
4.89
4.86
4.78
4.36
4.34
2.21
1.61
1.52
HN
O
CO2tBu
Ph
10
1.04
1.05
2.20
3.13
6.18
3.07
2.19
1.05
1.03
1.00
1.00
3.00
3.05
9.00
f1 (ppm)

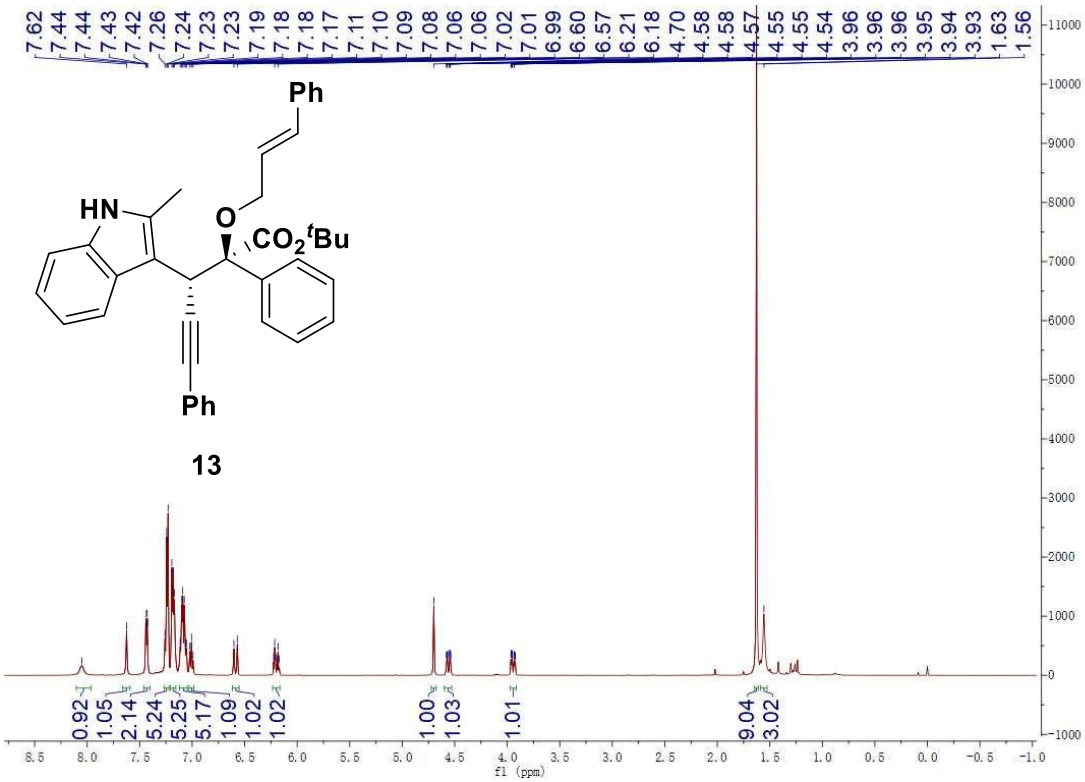

171.13
140.07
131.75
128.17
128.00
127.86
127.73
127.61
127.38
127.32
123.80
120.69
119.11
109.66
106.12
89.83
89.53
83.11
82.80
68.34
41.55
28.19
21.43
11.28
HN
O
CO2tBu
Ph
10
f1 (ppm)


7.40
7.39
7.28
7.25
7.25
7.24
7.16
7.14
7.11
6.18
6.18
4.99
4.96
4.70
4.26
4.23
1.67
1.63
HN
O
O
CO2tBu
Ph
11
0.97
1.08
2.09
1.21
3.15
1.31
2.94
2.17
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0.93
1.00
0.96
0.98
3.00
9.01
f1 (ppm)

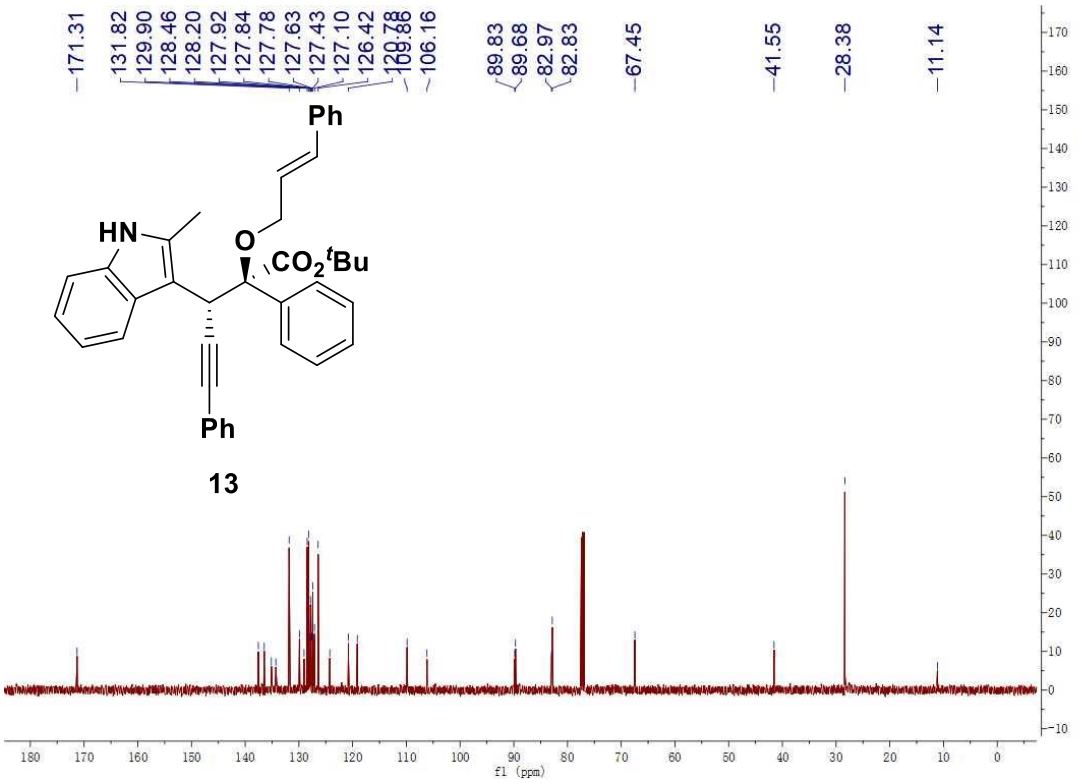

171.07
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141.67
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127.49
127.42
120.51
109.44
107.96
106.12
89.58
89.35
82.89
82.76
61.27
41.38
28.28
11.31
HN
O
O
CO2tBu
Ph
11
f1 (ppm)


7.61
7.57
7.56
7.49
7.48
7.28
7.27
7.21
7.20
7.19
7.18
7.16
7.15
7.13
7.12
5.14
5.11
4.76
4.58
4.56
1.64
1.59
S
HN
O
CO2tBu
Ph
12
1.00
1.09
1.02
1.14
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8.03
1.09
1.03
1.00
0.94
0.99
2.92
9.02
f1 (ppm)

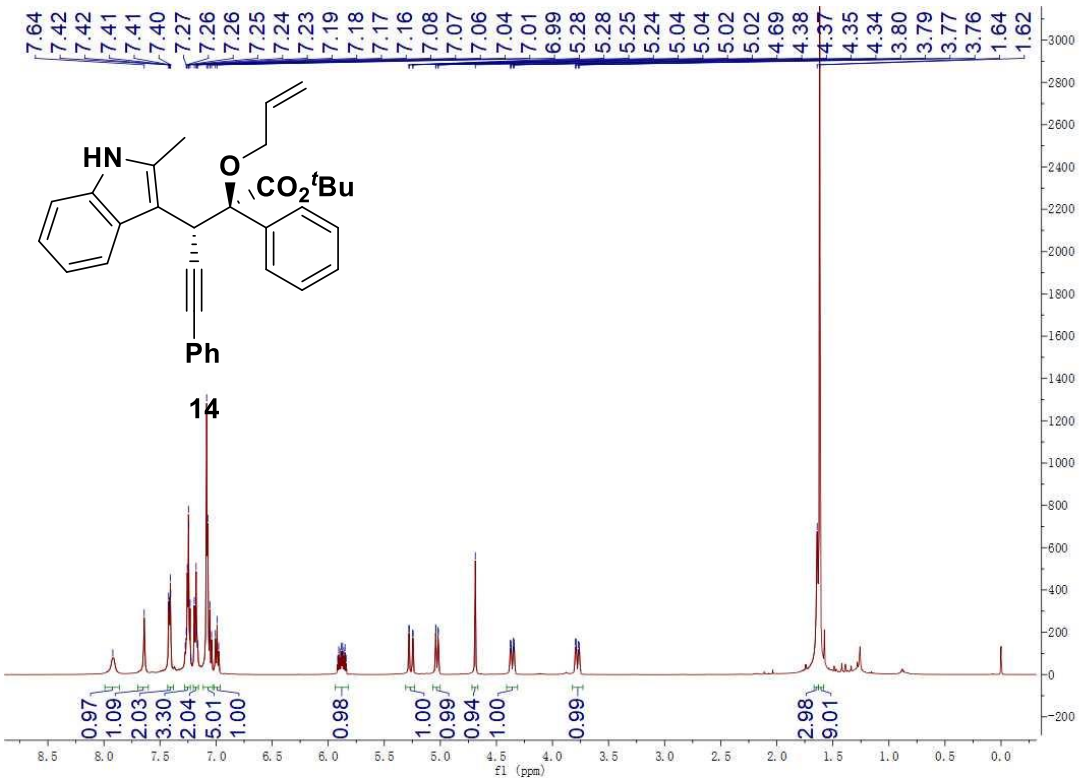

170.85
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128.16
127.84
127.63
127.55
123.87
123.56
123.21
122.24
120.87
105.92
89.79
89.50
83.18
83.14
64.85
41.47
28.26
11.35
S
HN
O
CO2tBu
Ph
12
f1 (ppm)

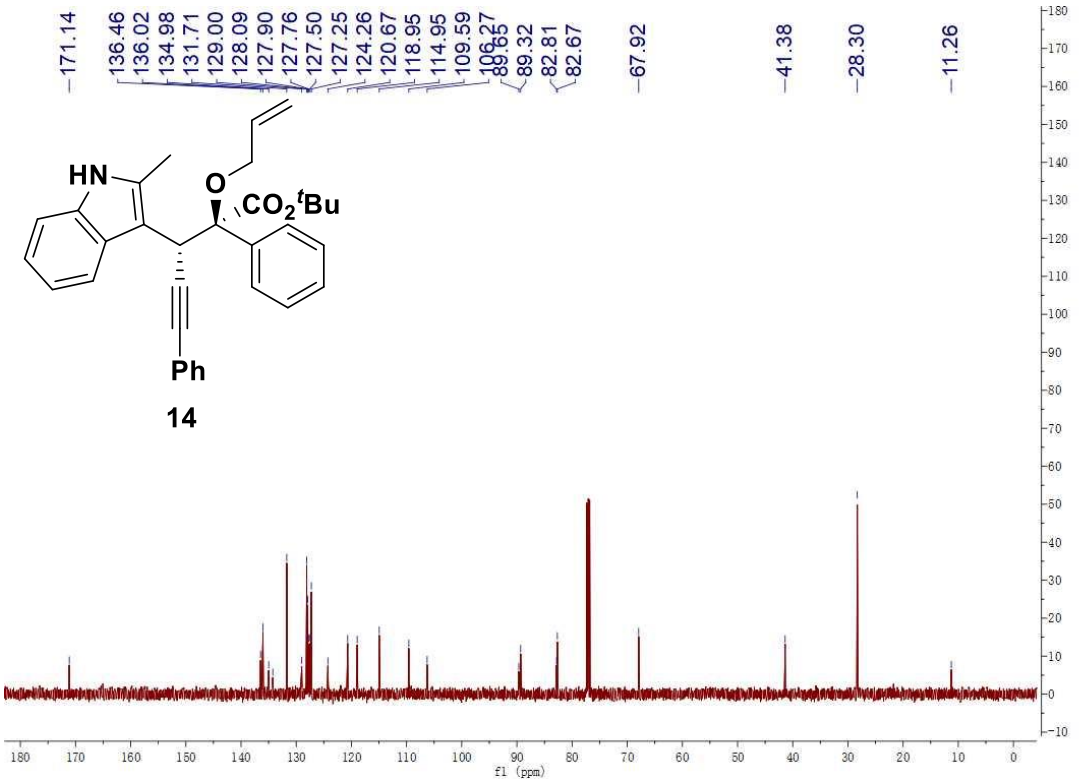

7.62 7.44 7.44 7.43 7.42 7.26 7.24 7.23 7.23 7.19 7.18 7.18 7.17 7.11 7.10 7.09 7.08 7.06 7.06 7.02 7.01 6.99 6.60 6.57 6.21 6.18 4.70 4.58 4.58 4.57 4.55 4.55 4.54 3.96 3.96 3.96 3.95 3.94 3.93 1.63 1.56
Ph
HN
O
CO2tBu
Ph
0.92 1.05 2.14 5.24 5.25 5.17 1.09 1.02 1.02 1.00 1.03 1.01 9.04 3.02
f1 (ppm)

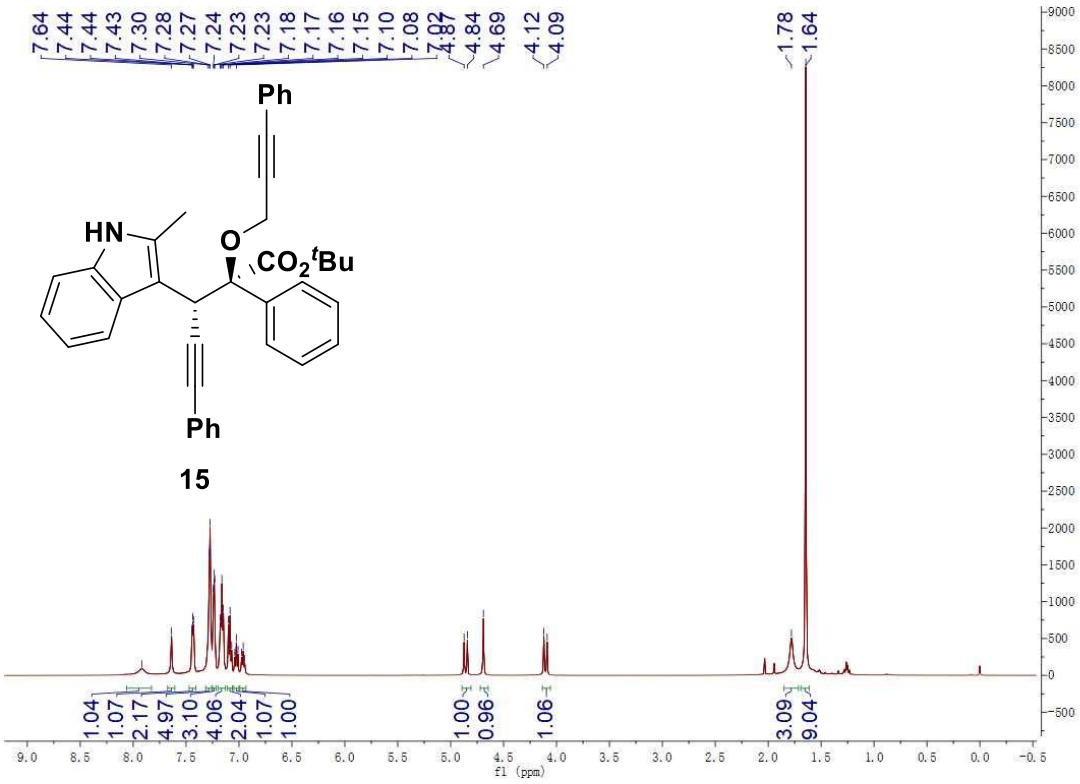
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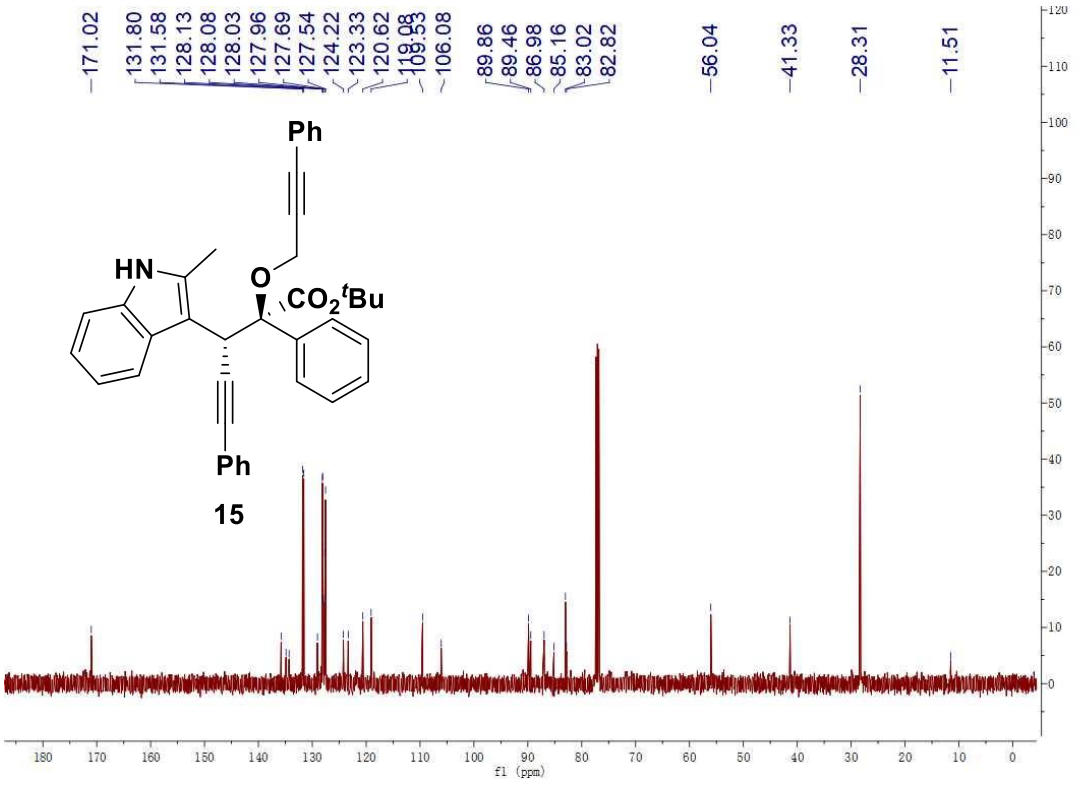

171.31 131.82 129.90 128.46 128.20 127.92 127.84 127.78 127.63 127.43 127.10 126.42 120.78 120.88 106.16 89.83 89.68 82.97 82.83 67.45 41.55 28.38 11.14
Ph
HN
O
CO2tBu
Ph
f1 (ppm)

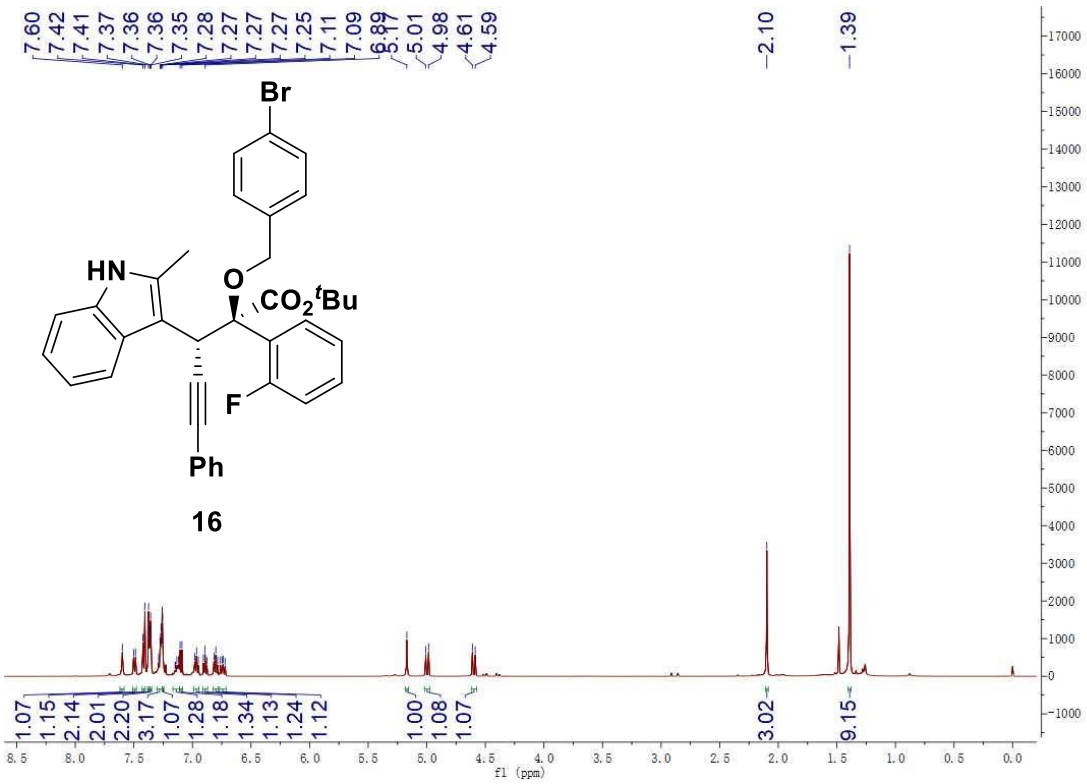
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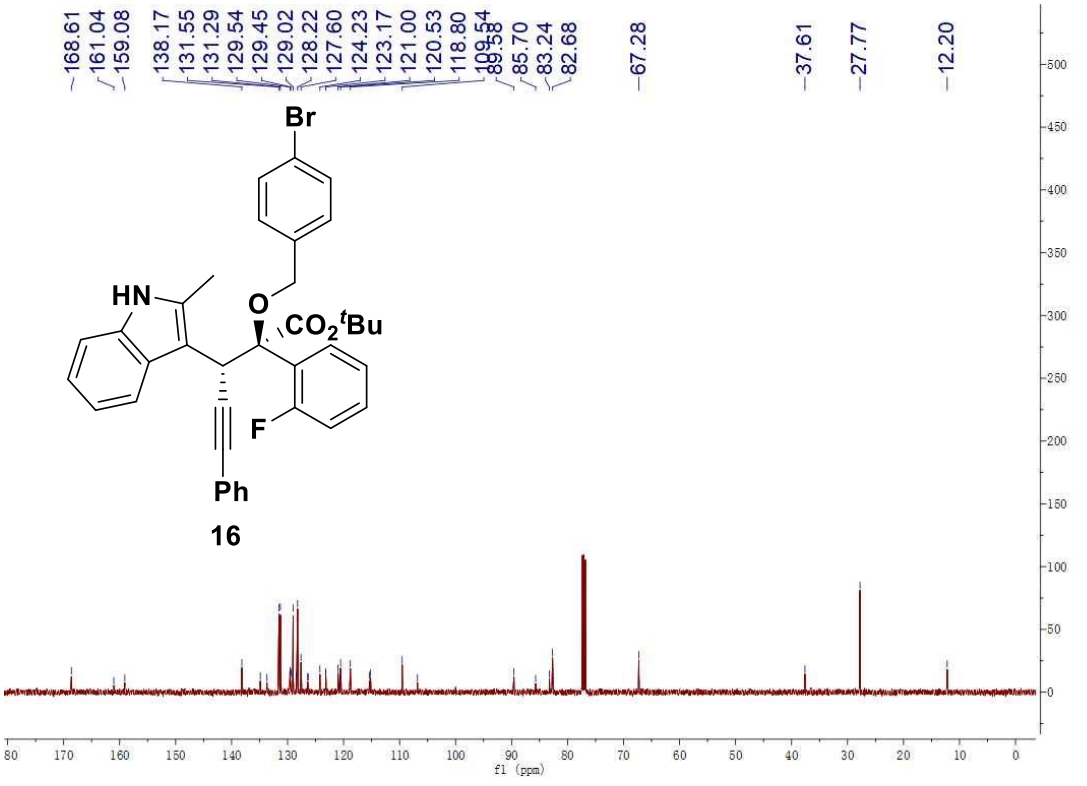

HN
O
CO2tBu
Ph
14

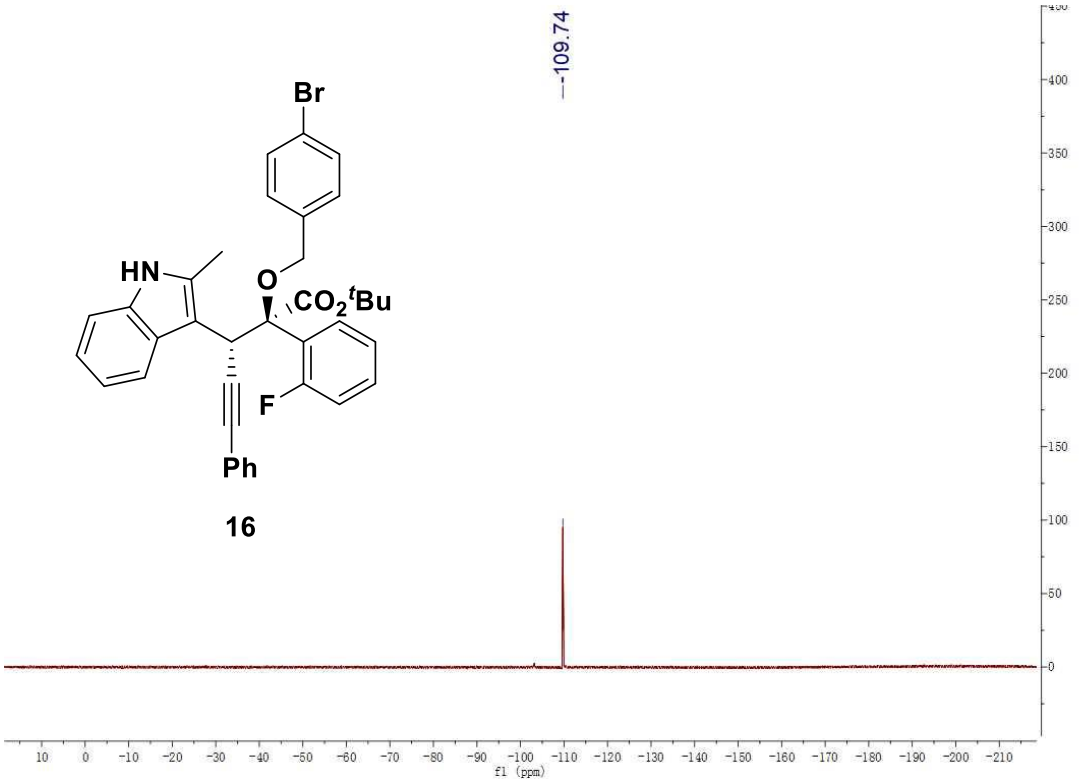

HN
O
CO2tBu
Ph
14

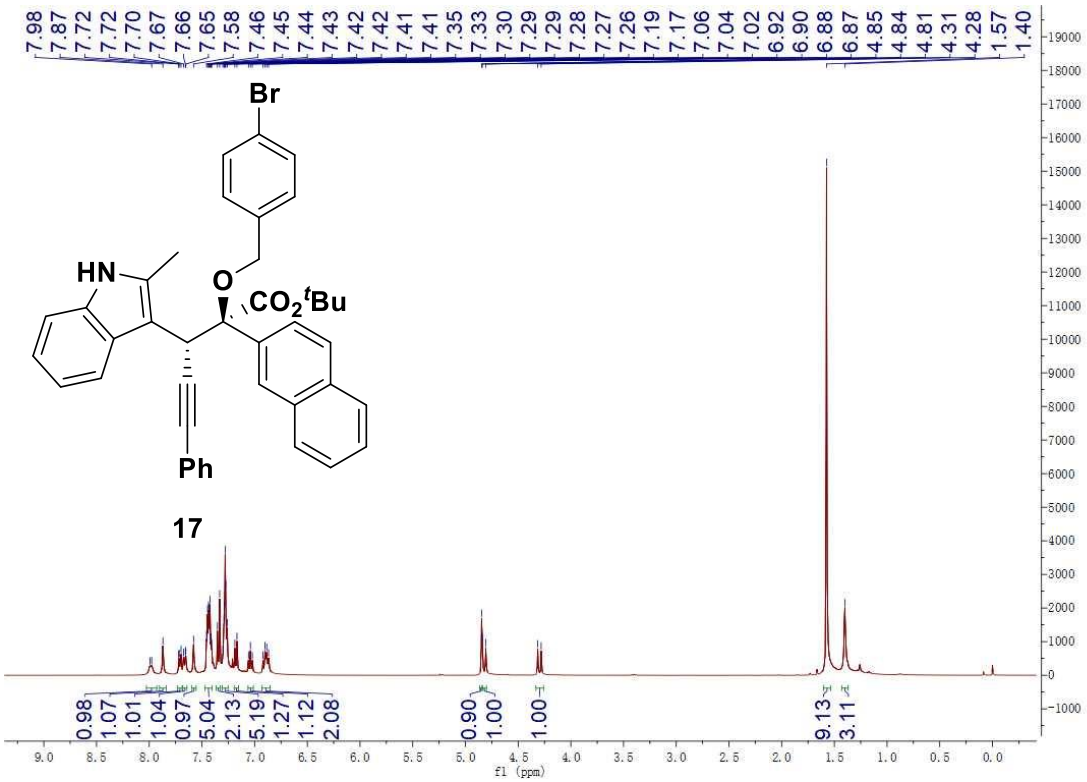

7.64
7.44
7.44
7.43
7.30
7.28
7.27
7.24
7.23
7.23
7.18
7.17
7.16
7.15
7.10
7.08
4.84
4.69
4.12
4.09
1.78
1.64
Ph
HN
O
CO2tBu
Ph
15
1.04
1.07
2.17
4.97
3.10
4.06
2.04
1.07
1.00
1.00
0.96
1.06
3.09
9.04
f1 (ppm)

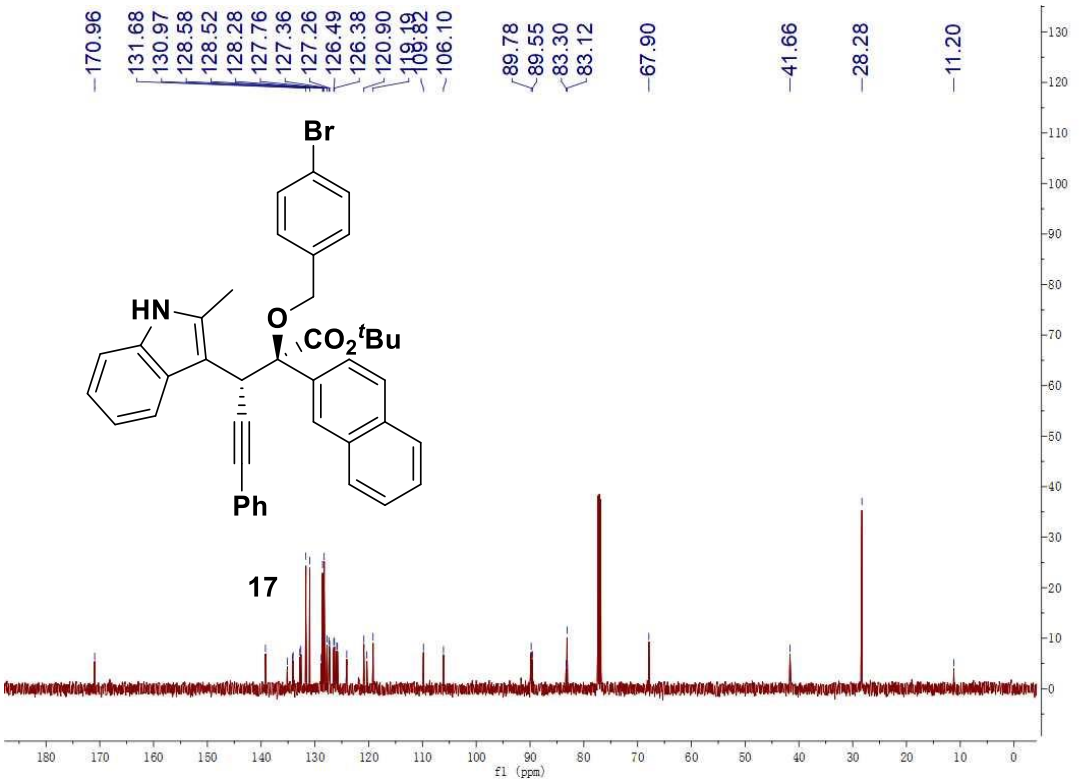

171.02
131.80
131.58
128.13
128.08
128.03
127.96
127.69
127.54
124.22
123.33
120.62
106.08
89.86
89.46
86.98
85.16
83.02
82.82
56.04
41.33
28.31
11.51
Ph
HN
O
CO2tBu
Ph
15
f1 (ppm)

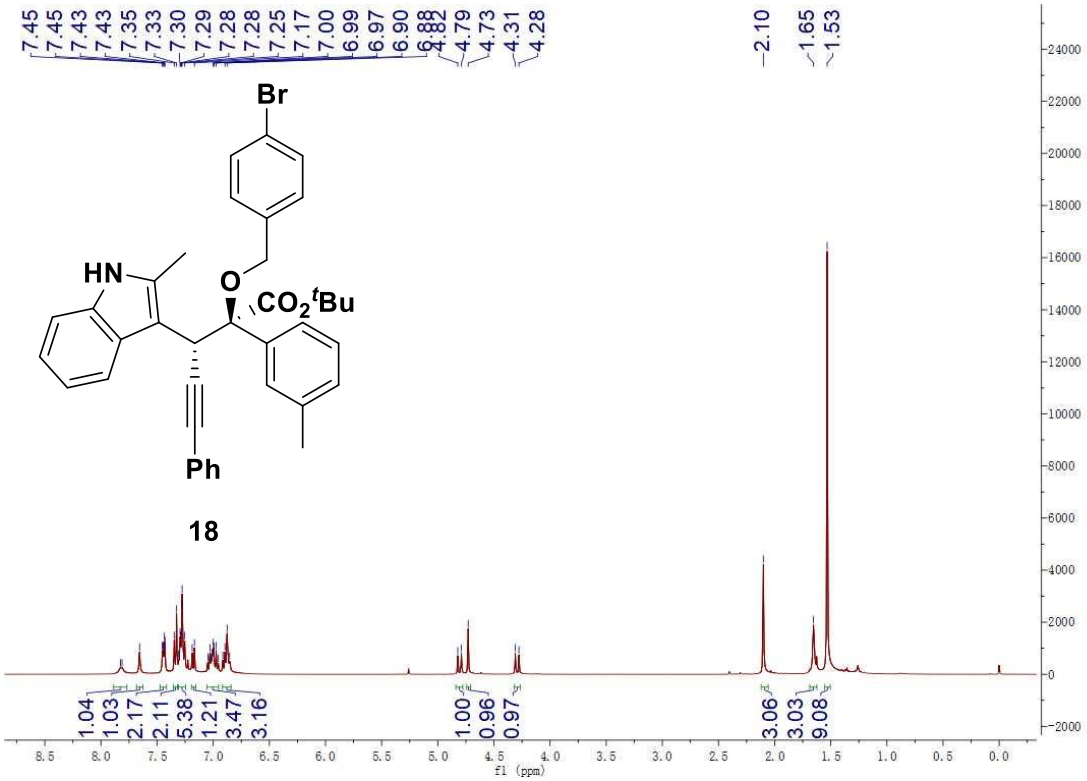

7.60
7.42
7.41
7.37
7.36
7.36
7.35
7.28
7.27
7.27
7.27
7.25
7.11
7.09
6.89
5.17
5.01
4.98
4.61
4.59
2.10
1.39
Br
HN
O
CO2tBu
F
Ph
16
1.07
1.15
2.14
2.01
2.20
3.17
1.07
1.28
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3.02
9.15
f1 (ppm)

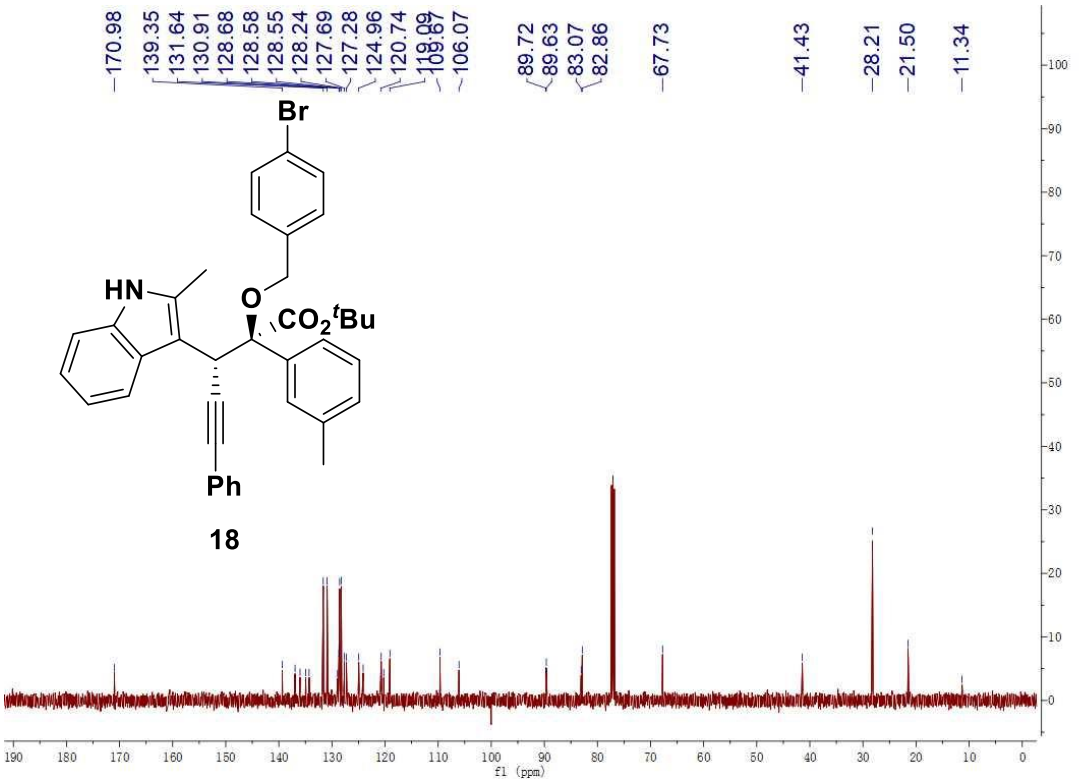

168.61
161.04
159.08
138.17
131.55
131.29
129.54
129.45
129.02
128.22
127.60
124.23
123.17
121.00
120.53
118.80
109.54
89.58
85.70
83.24
82.68
67.28
37.61
27.77
12.20
Br
HN
O
CO2tBu
F
Ph
16
f1 (ppm)

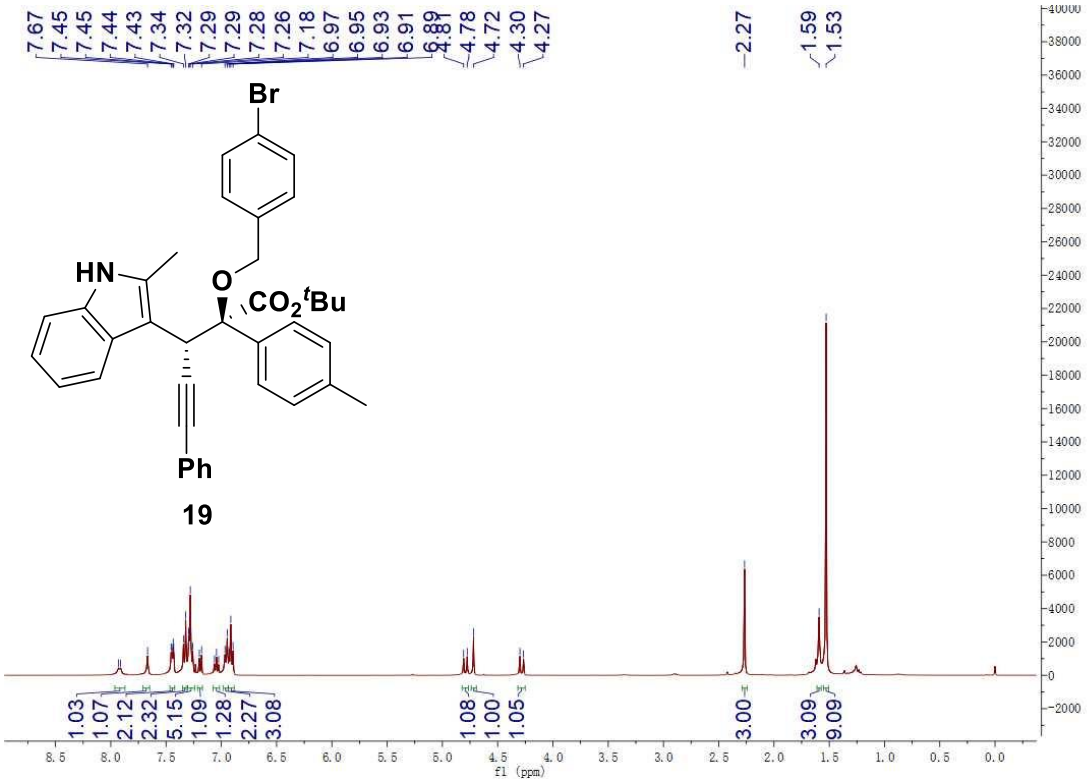

-109.74
Br
HN
O
CO2tBu
F
Ph
16
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

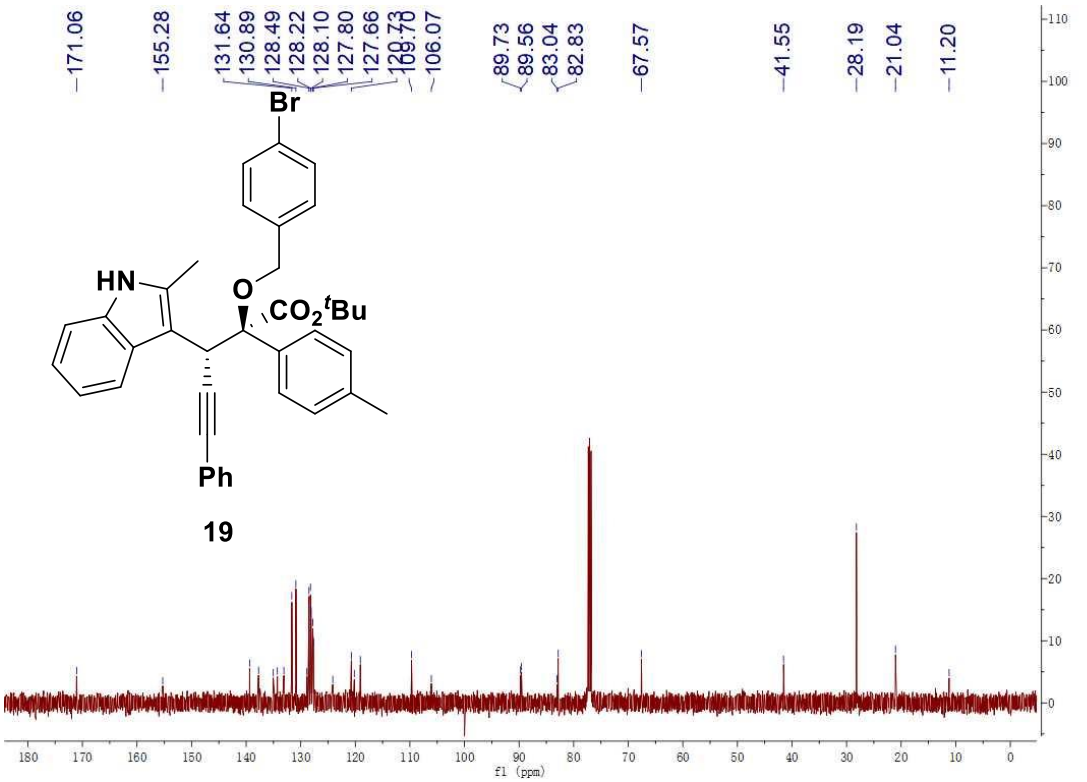

7.98 7.87 7.72 7.72 7.70 7.67 7.66 7.65 7.58 7.46 7.45 7.44 7.43 7.42 7.42 7.41 7.41 7.35 7.33 7.30 7.29 7.29 7.28 7.27 7.26 7.19 7.17 7.06 7.04 7.02 6.92 6.90 6.88 6.87 4.85 4.84 4.81 4.31 4.28 1.57 1.40
Br
HN
O
CO2tBu
Ph
17
0.98 1.07 1.01 1.04 0.97 5.04 2.13 5.19 1.27 1.12 2.08 0.90 1.00 1.00 9.13 3.11
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

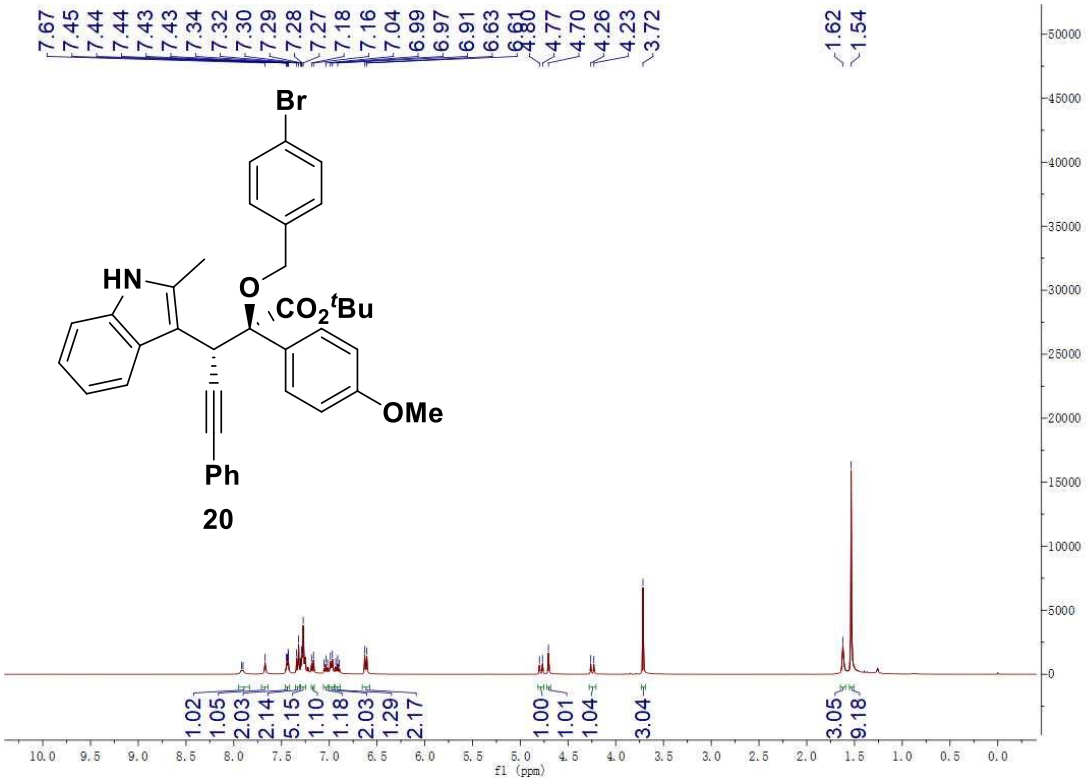

Br
HN
O
CO2tBu
Ph
17
f1 (ppm)

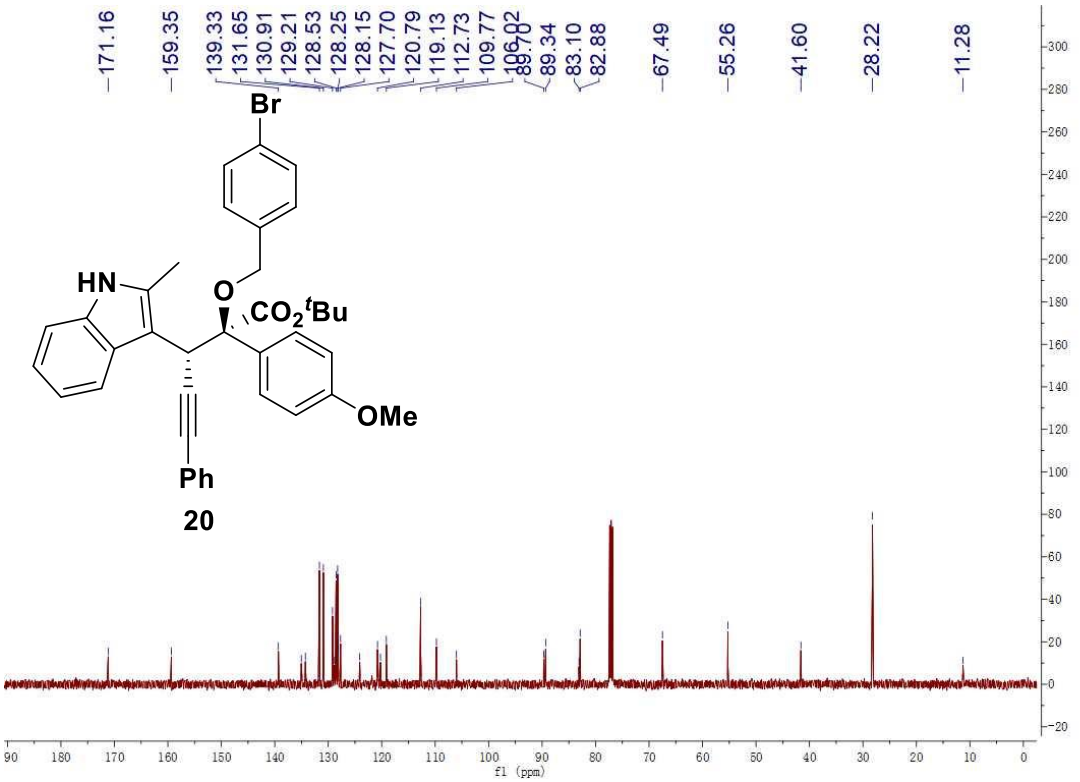

Br
HN
O
CO2tBu
Ph
18
f1 (ppm)

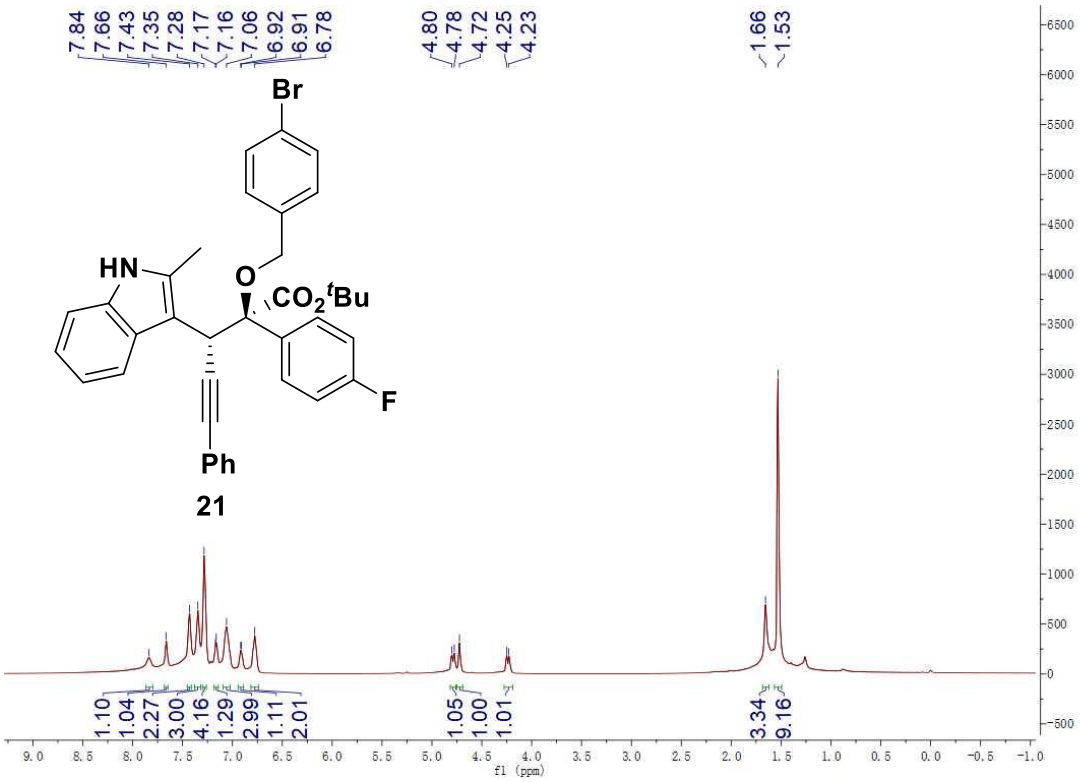

170.98
139.35
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130.91
128.68
128.58
128.55
128.24
127.69
127.28
124.96
120.74
109.07
106.07
89.72
89.63
83.07
82.86
67.73
41.43
28.21
21.50
11.34
Br
HN
O
CO2tBu
Ph
18
f1 (ppm)

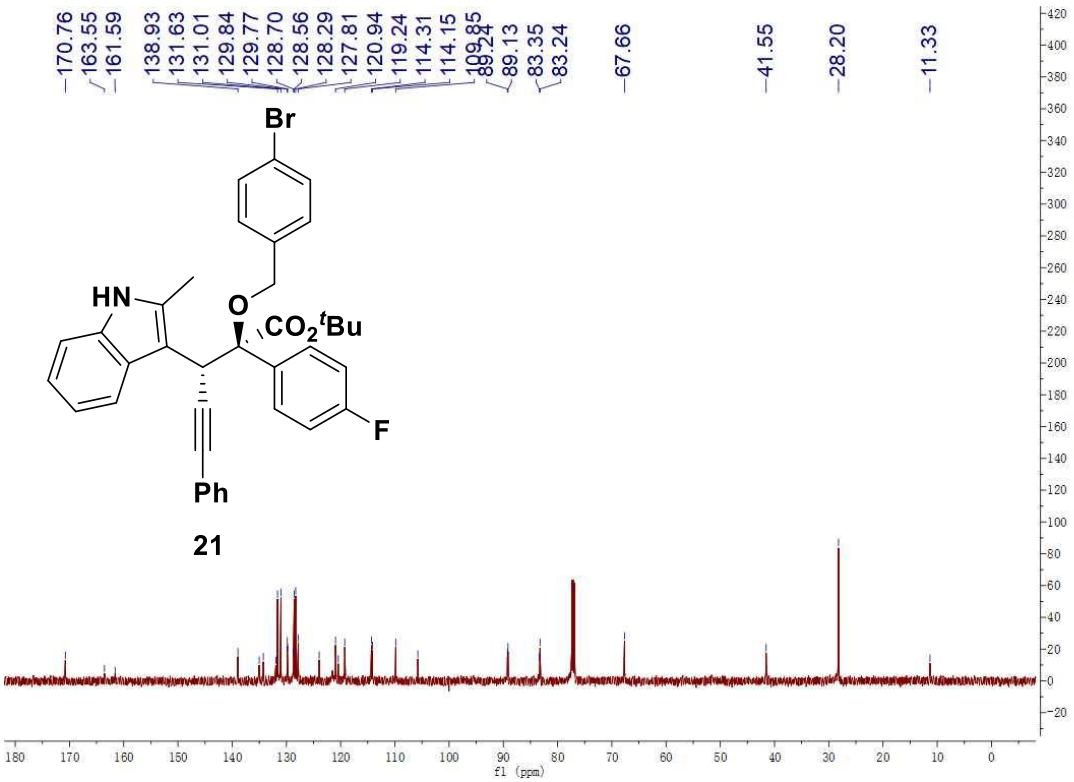

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7.44
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7.29
7.29
7.28
7.26
7.18
6.97
6.95
6.93
6.91
4.78
4.72
4.30
4.27
2.27
1.59
1.53
Br
HN
O
CO2tBu
Ph
19
1.03
1.07
2.12
2.32
5.15
1.09
1.28
2.27
3.08
1.08
1.00
1.05
3.00
3.09
9.09
f1 (ppm)

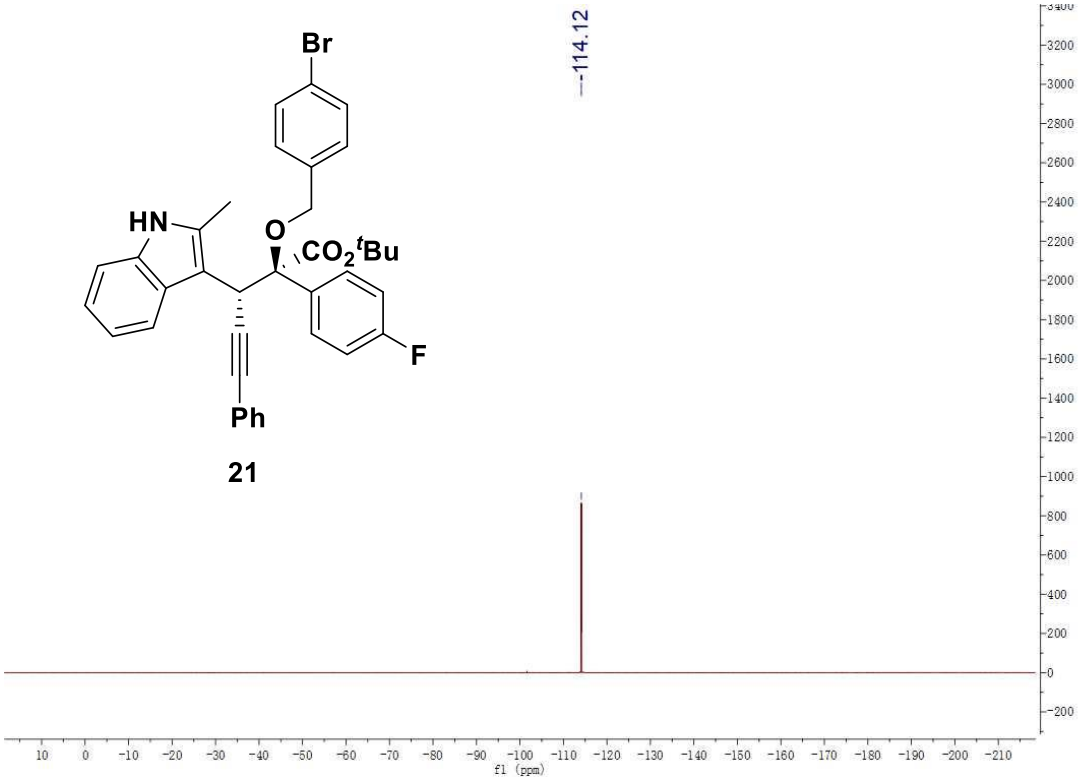

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130.89
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128.22
128.10
127.80
127.66
120.73
109.70
106.07
89.73
89.56
83.04
82.83
67.57
41.55
28.19
21.04
11.20
Br
HN
O
CO2tBu
Ph
19
f1 (ppm)

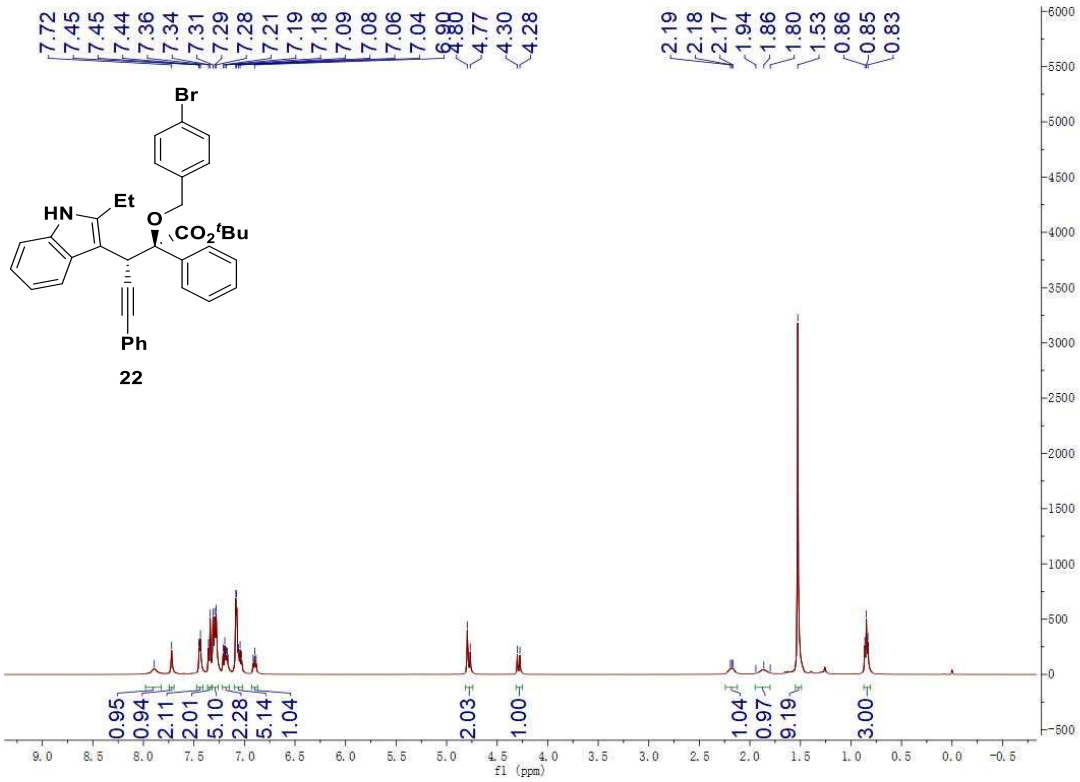

7.67
7.45
7.44
7.44
7.43
7.43
7.34
7.32
7.30
7.29
7.28
7.27
7.18
7.16
7.04
6.99
6.97
6.91
6.63
6.61
4.80
4.77
4.70
4.26
4.23
3.72
1.62
1.54
Br
HN
O
CO2tBu
OMe
Ph
20
1.02
1.05
2.03
2.14
5.15
1.10
1.18
2.03
1.29
2.17
1.00
1.01
1.04
3.04
3.05
9.18
f1 (ppm)

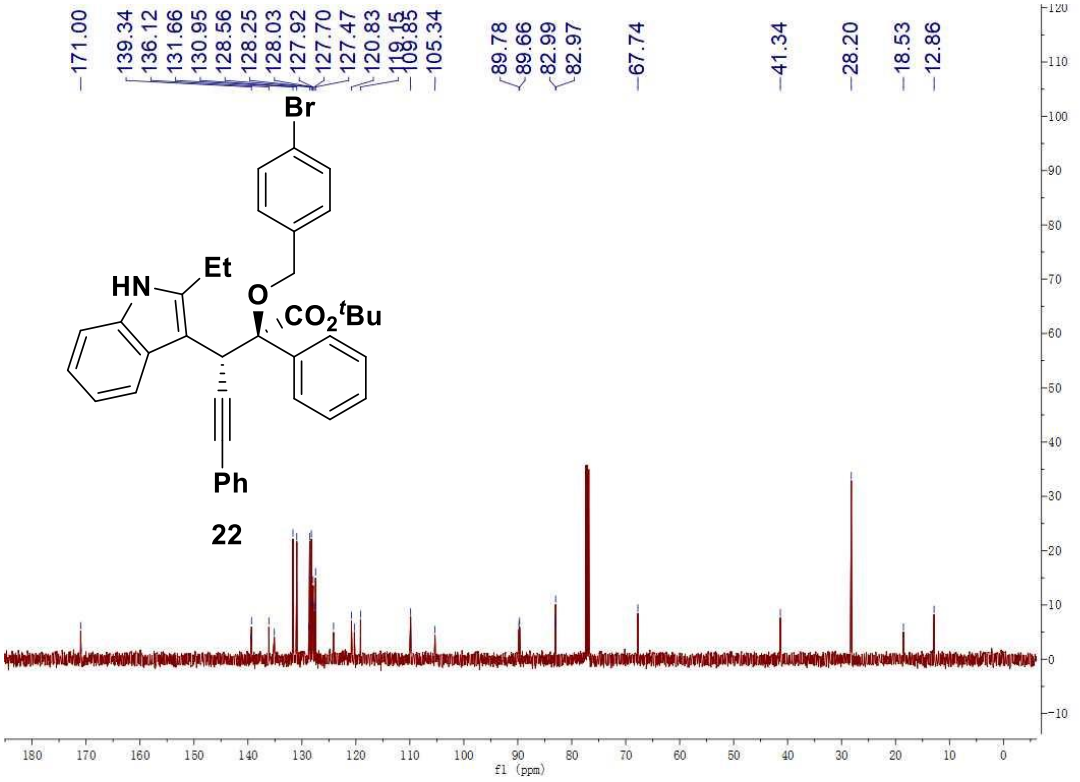

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129.21
128.53
128.25
128.15
127.70
120.79
119.13
112.73
109.77
106.02
89.70
89.34
83.10
82.88
67.49
55.26
41.60
28.22
11.28
Br
HN
O
CO2tBu
OMe
Ph
20
f1 (ppm)

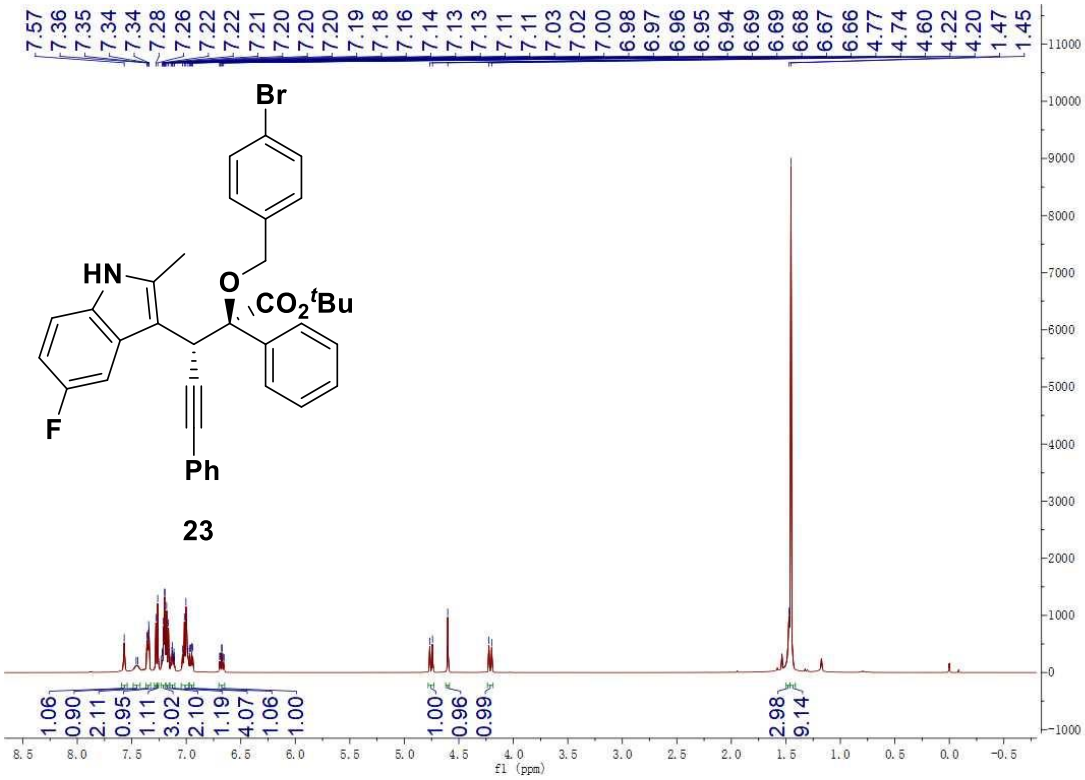

7.84
7.66
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7.17
7.16
7.06
6.92
6.91
6.78
4.80
4.78
4.72
4.25
4.23
1.66
1.53
Br
HN
O
CO2tBu
F
Ph
21
1.10
1.04
2.27
3.00
4.16
1.29
2.99
1.11
2.01
1.05
1.00
1.01
3.34
9.16
f1 (ppm)

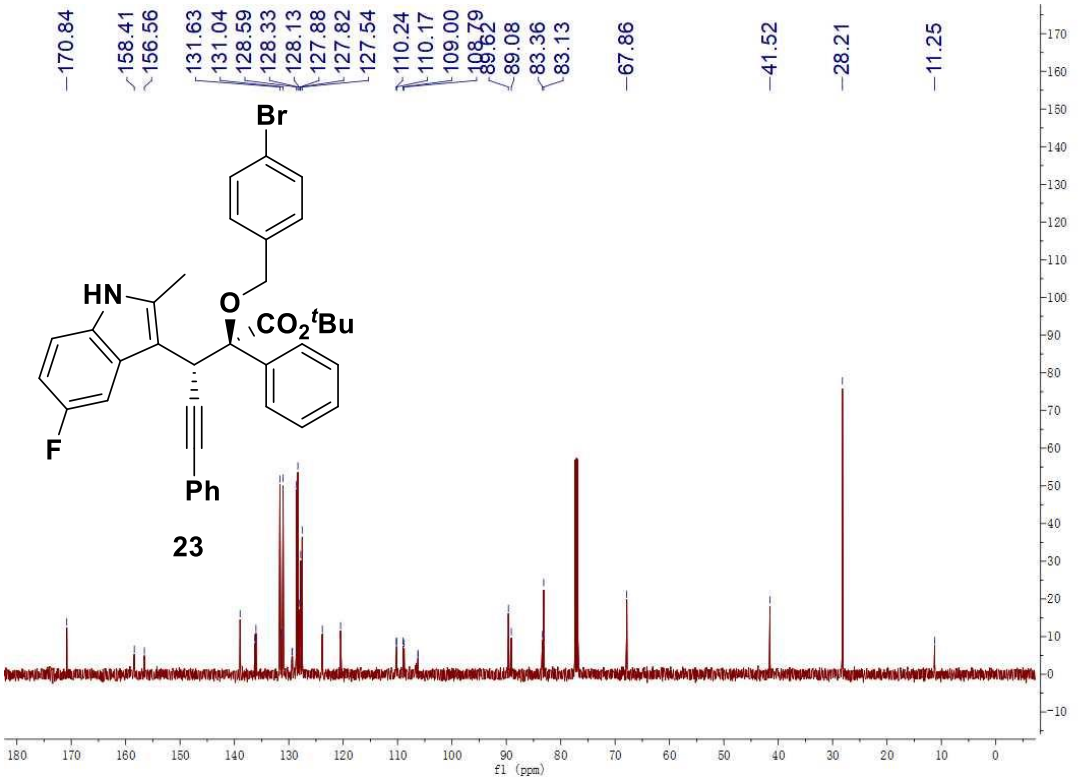

170.76
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131.01
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129.77
128.70
128.56
128.29
127.81
120.94
119.24
114.31
114.15
109.85
89.24
89.13
83.35
83.24
67.66
41.55
28.20
11.33
Br
HN
O
CO2tBu
F
Ph
21
f1 (ppm)

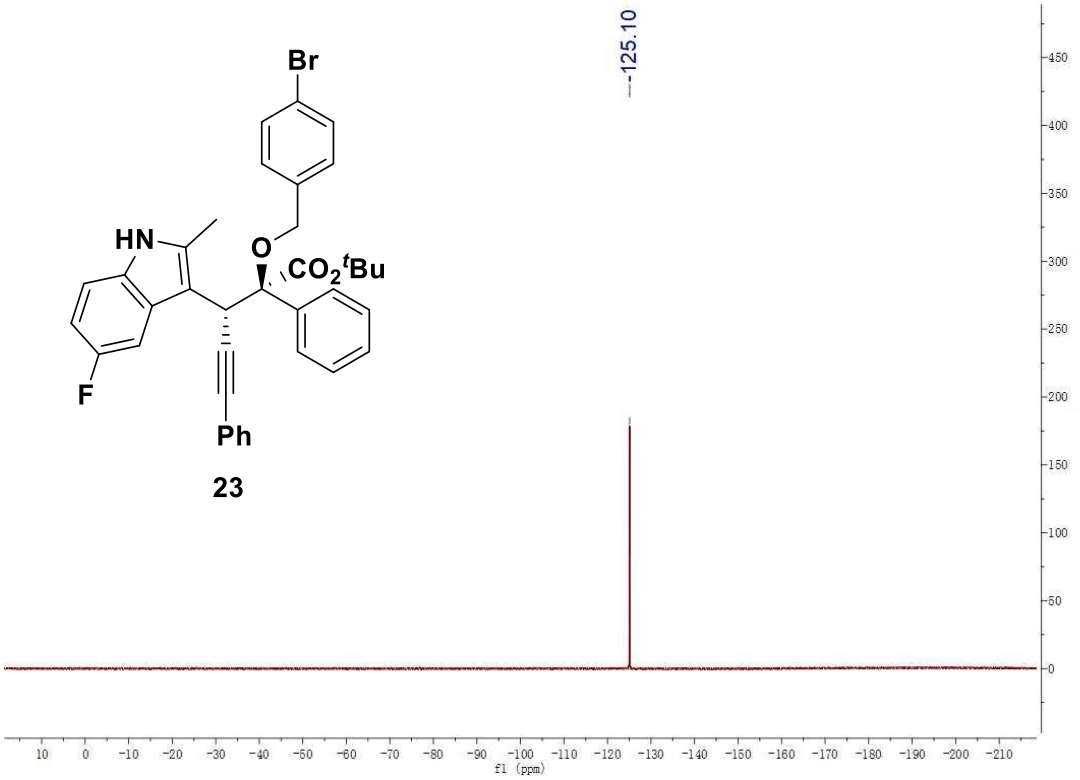

-114.12
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O
CO2tBu
F
Ph
21
f1 (ppm)

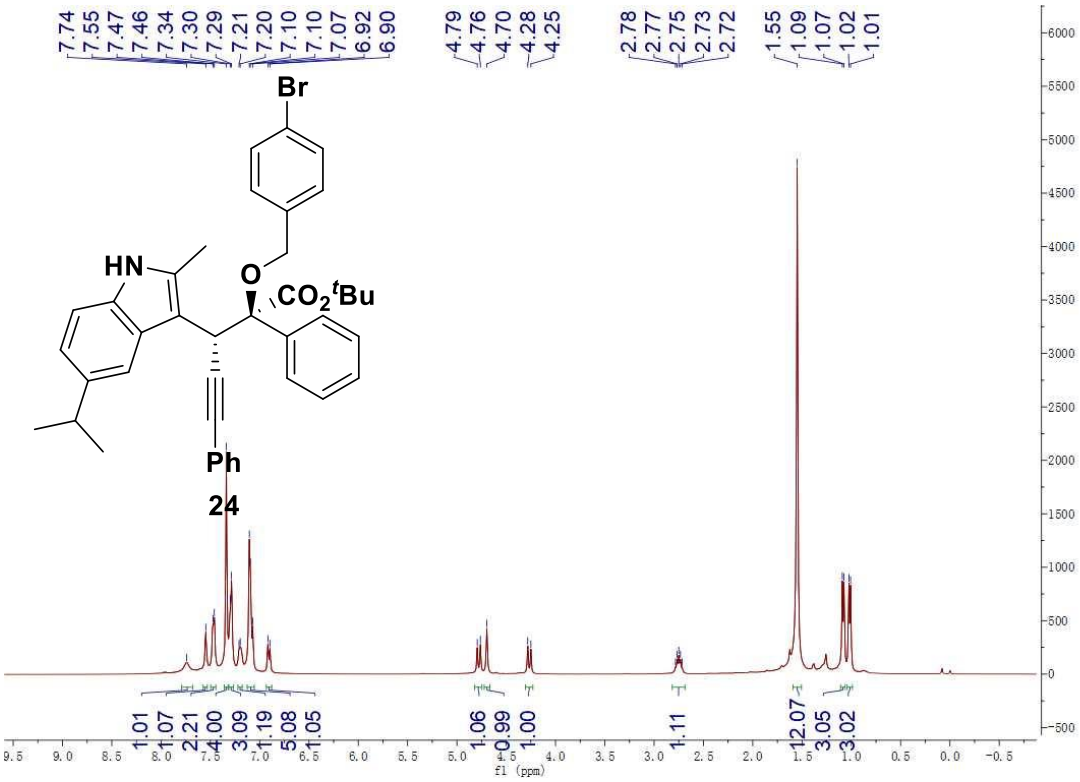

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7.44
7.36
7.34
7.31
7.29
7.28
7.21
7.19
7.18
7.09
7.08
7.06
7.04
6.90
6.88
4.77
4.30
4.28
2.19
2.18
2.17
1.94
1.86
1.80
1.53
0.86
0.85
0.83
Br
HN
Et
O
CO2tBu
Ph
22
0.95
0.94
2.11
2.01
5.10
2.28
5.14
1.04
2.03
1.00
1.04
0.97
9.19
3.00
f1 (ppm)

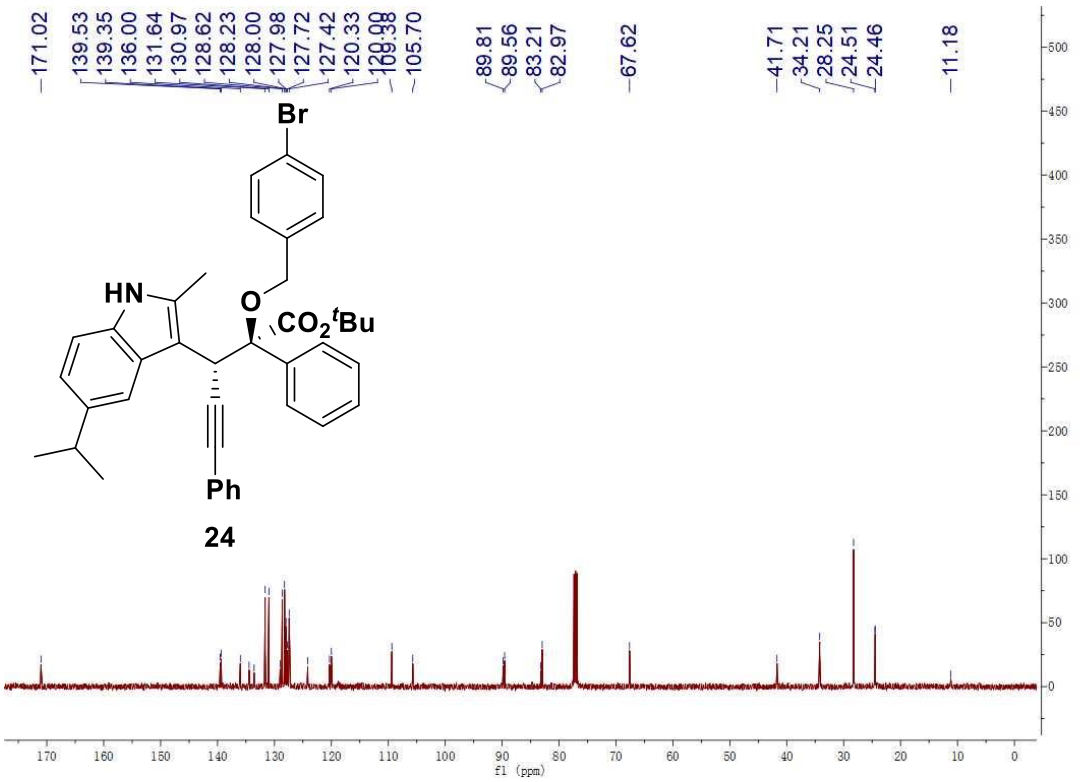

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139.34
136.12
131.66
130.95
128.56
128.25
128.03
127.92
127.70
127.47
120.83
119.15
109.85
105.34
89.78
89.66
82.99
82.97
67.74
41.34
28.20
18.53
12.86
Br
HN
Et
O
CO2tBu
Ph
22
f1 (ppm)

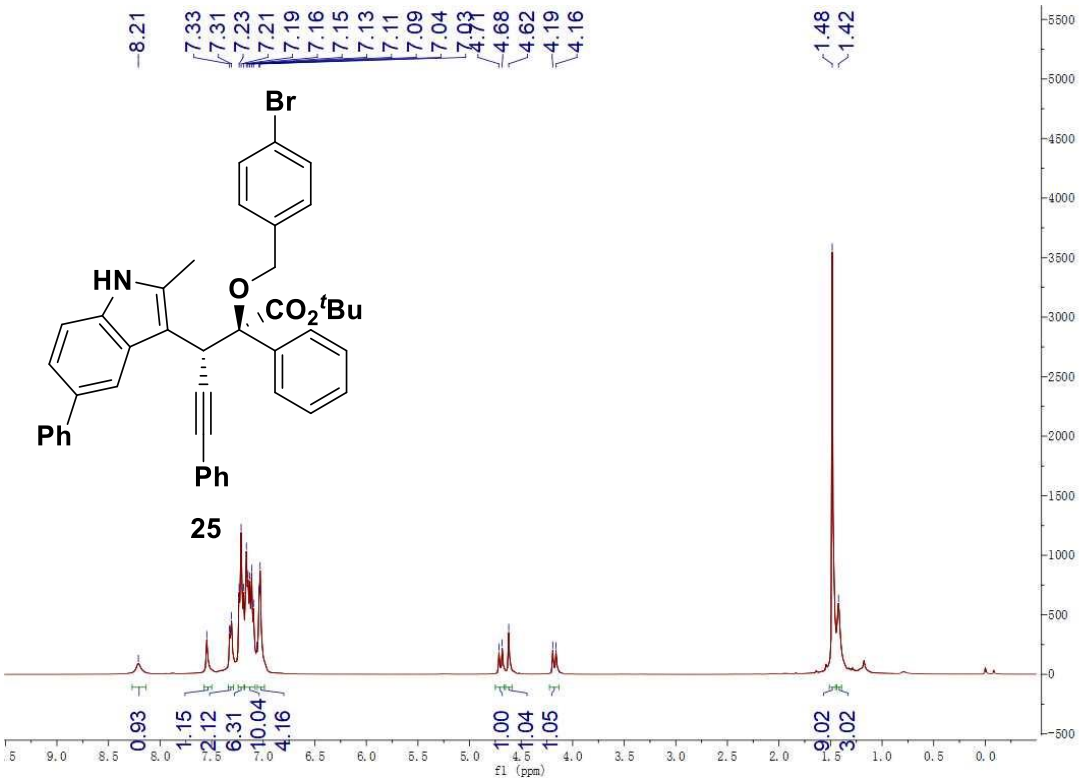

7.57 7.36 7.35 7.34 7.34 7.28 7.26 7.22 7.22 7.21 7.20 7.20 7.20 7.19 7.18 7.16 7.14 7.13 7.13 7.11 7.11 7.03 7.02 7.00 6.98 6.97 6.96 6.95 6.94 6.69 6.69 6.68 6.67 6.66 4.77 4.74 4.60 4.22 4.20 1.47 1.45
Br
HN
O
CO2tBu
F
Ph
23
1.06 0.90 2.11 0.95 1.11 3.02 2.10 1.19 4.07 1.06 1.00 1.00 0.96 0.99 2.98 9.14
f1 (ppm)

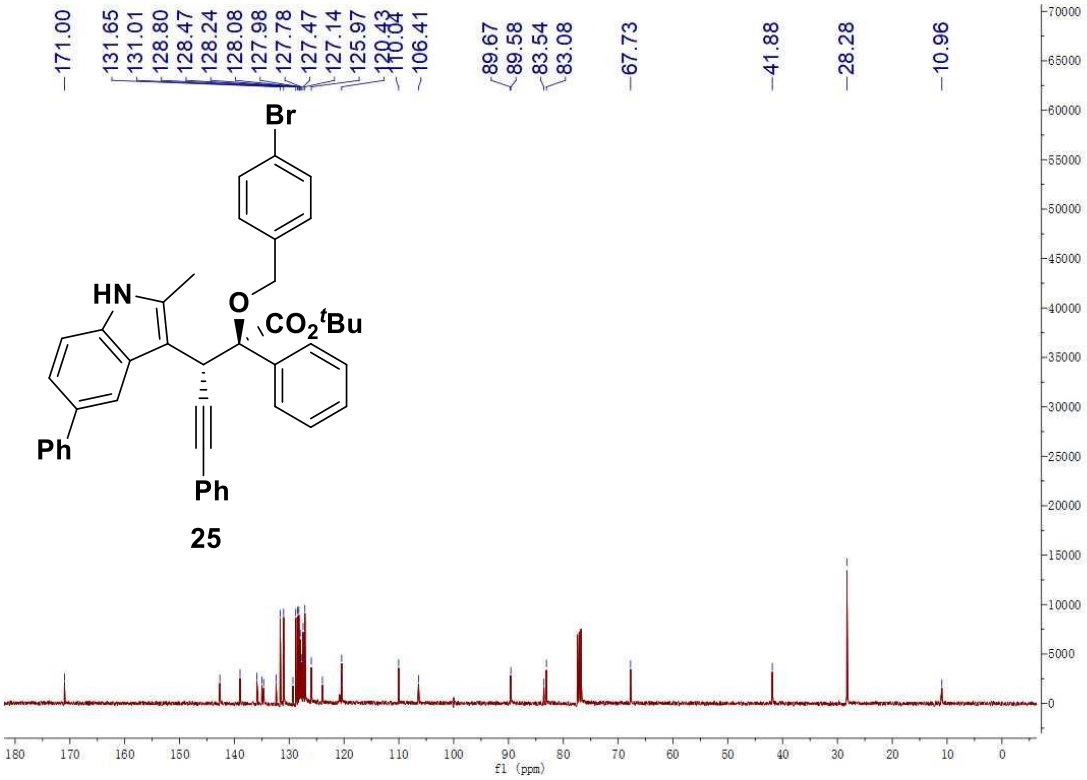

170.84 158.41 156.56 131.63 131.04 128.59 128.33 128.13 127.88 127.82 127.54 110.24 110.17 109.00 89.08 83.36 83.13 67.86 41.52 28.21 11.25
Br
HN
O
CO2tBu
F
Ph
23
f1 (ppm)

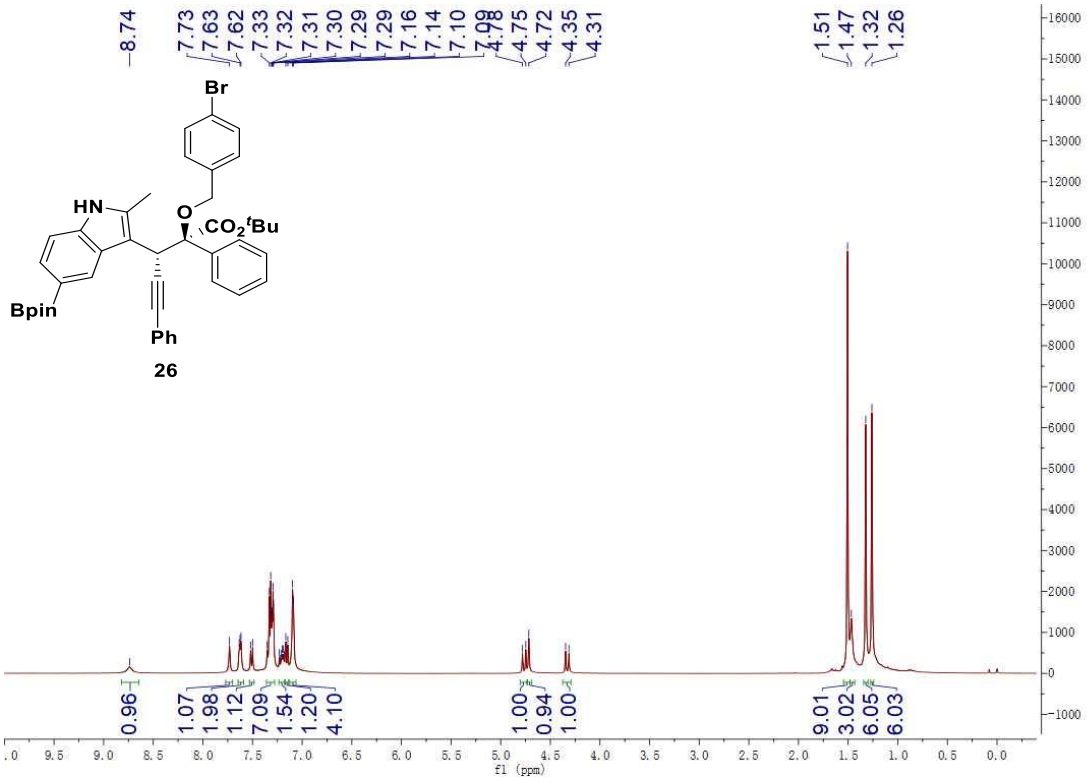

Br
HN
O
CO2tBu
F
Ph
23
-125.10
f1 (ppm)

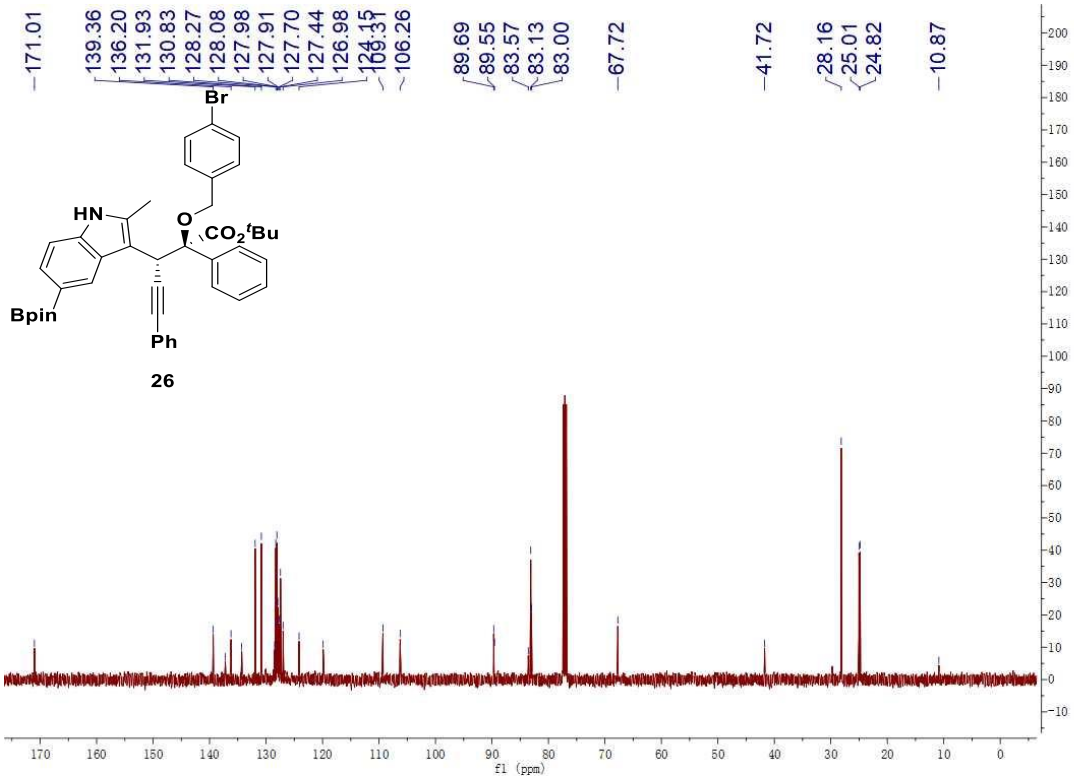

7.74
7.55
7.47
7.46
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7.29
7.21
7.20
7.10
7.10
7.07
6.92
6.90
4.79
4.76
4.70
4.28
4.25
2.78
2.77
2.75
2.73
2.72
1.55
1.09
1.07
1.02
1.01
Br
HN
O
CO2tBu
Ph
24
1.01
1.07
2.21
4.00
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1.06
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1.11
12.07
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3.02
f1 (ppm)

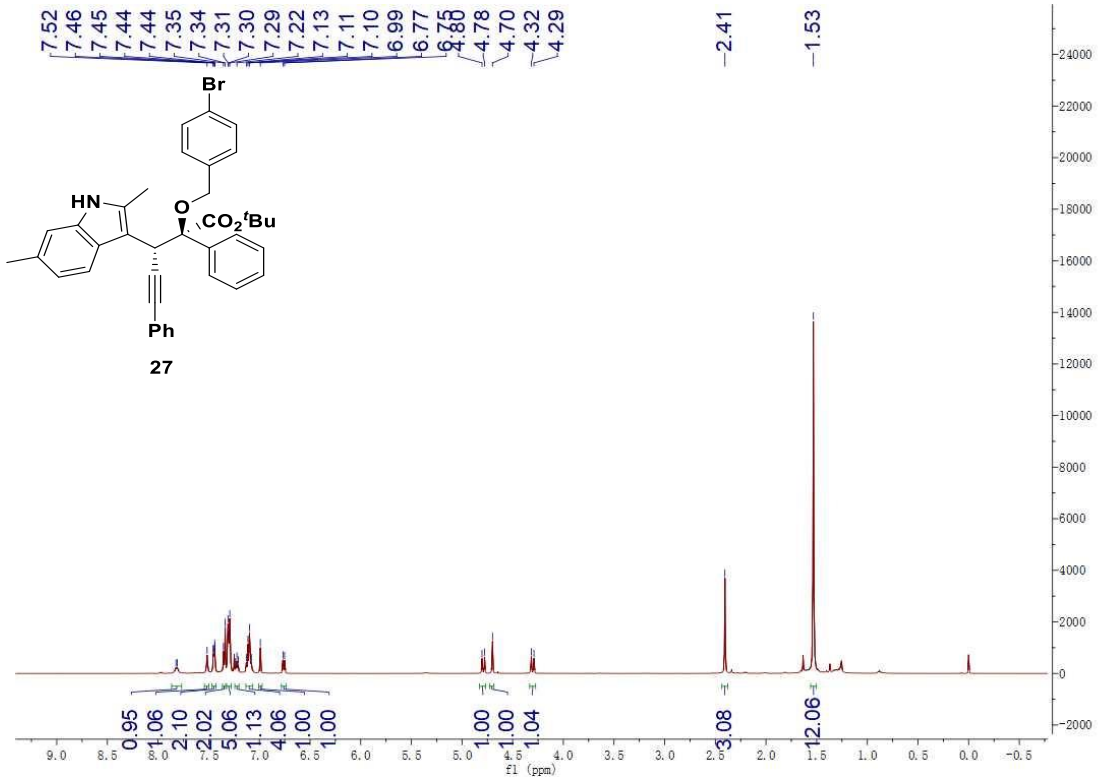

171.02
139.53
139.35
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128.23
128.00
127.98
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127.42
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89.81
89.56
83.21
82.97
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28.25
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24.46
11.18
Br
HN
O
CO2tBu
Ph
24
f1 (ppm)

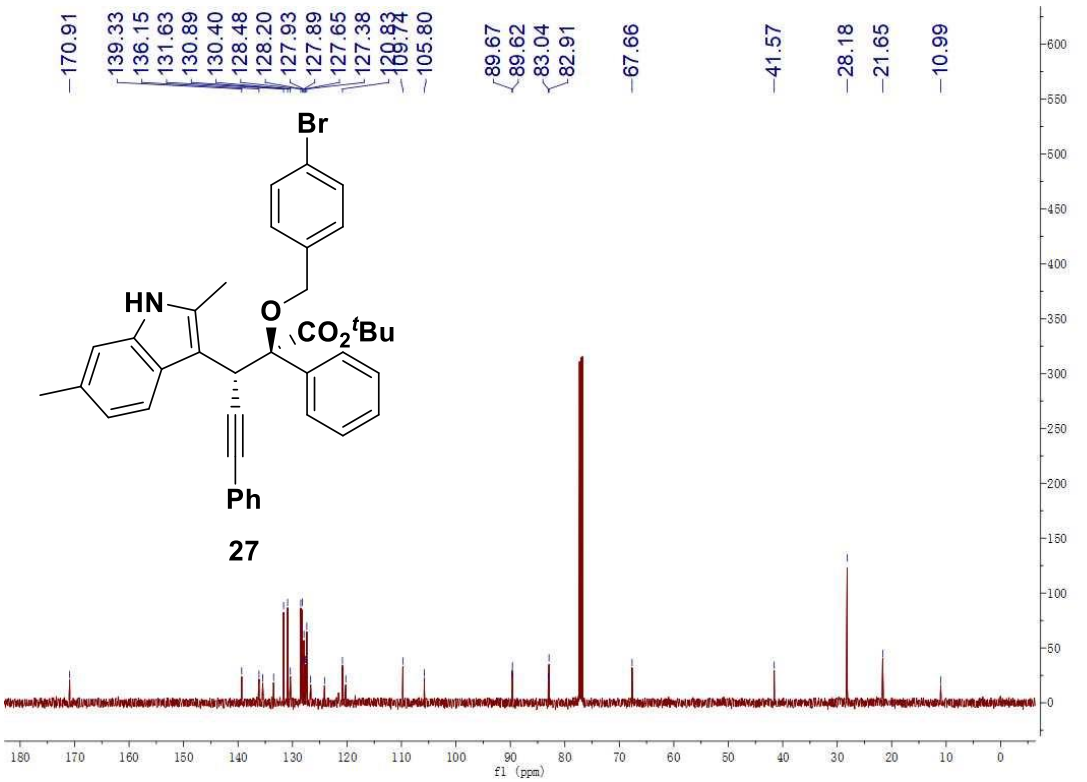

8.21
7.33
7.31
7.23
7.21
7.19
7.16
7.15
7.13
7.11
7.09
7.04
7.03
4.71
4.68
4.62
4.19
4.16
1.48
1.42
Br
HN
O
CO2tBu
Ph
Ph
25
0.93
1.15
2.12
6.31
10.04
4.16
1.00
1.04
1.05
9.02
3.02
f1 (ppm)

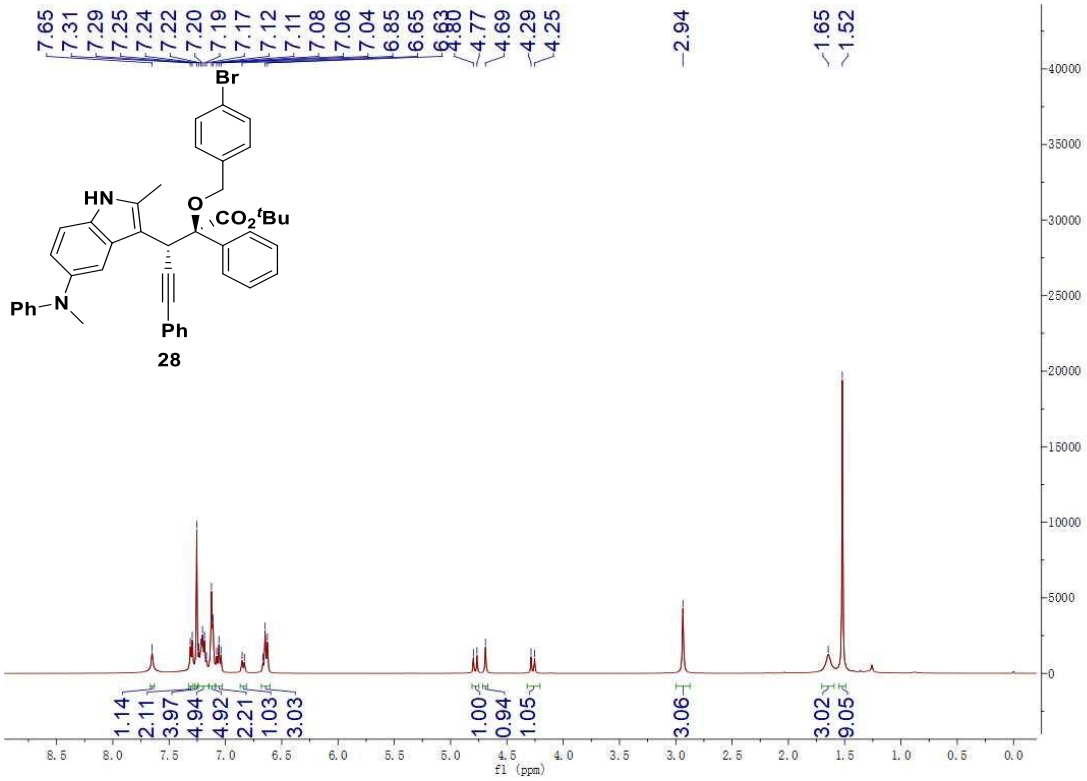

171.00
131.65
131.01
128.80
128.47
128.24
128.08
127.98
127.78
127.47
127.14
125.97
120.43
110.04
106.41
89.67
89.58
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83.08
67.73
41.88
28.28
10.96
Br
HN
O
CO2tBu
Ph
Ph
25
f1 (ppm)

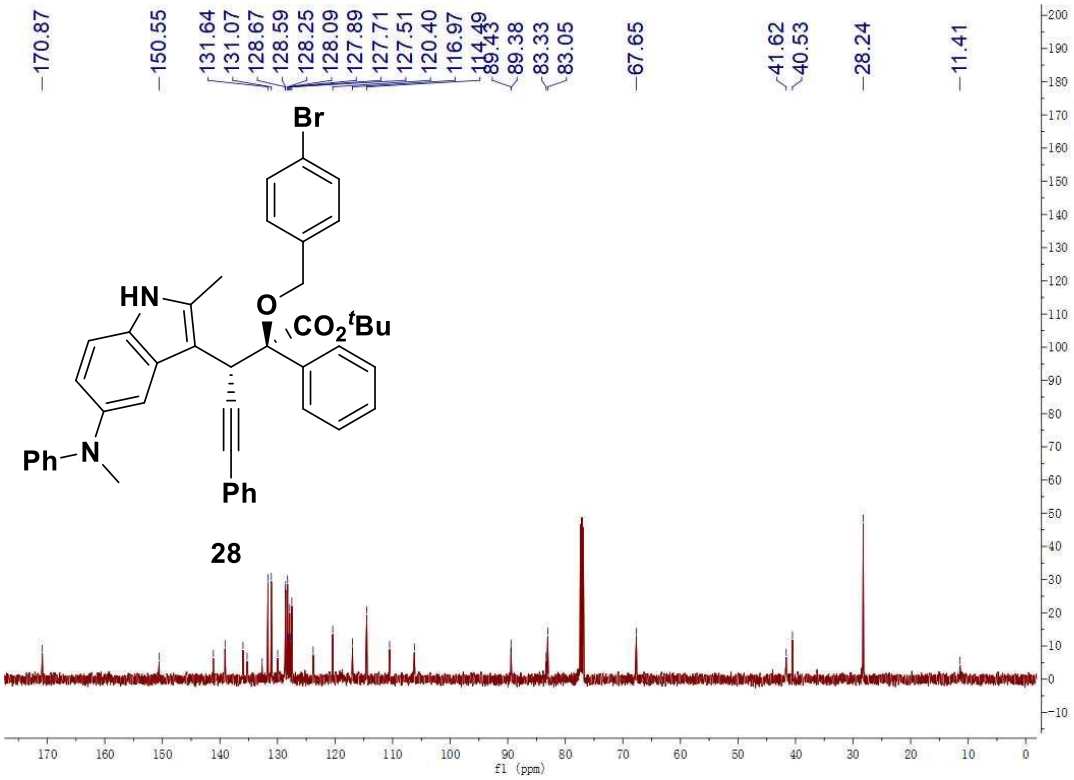

8.74
7.73
7.63
7.62
7.33
7.32
7.31
7.30
7.29
7.29
7.16
7.14
7.10
4.75
4.72
4.35
4.31
1.51
1.47
1.32
1.26
Br
HN
O
CO2tBu
Bpin
Ph
26
0.96
1.07
1.98
1.12
7.09
1.54
1.20
4.10
1.00
0.94
1.00
9.01
3.02
6.05
6.03
f1 (ppm)

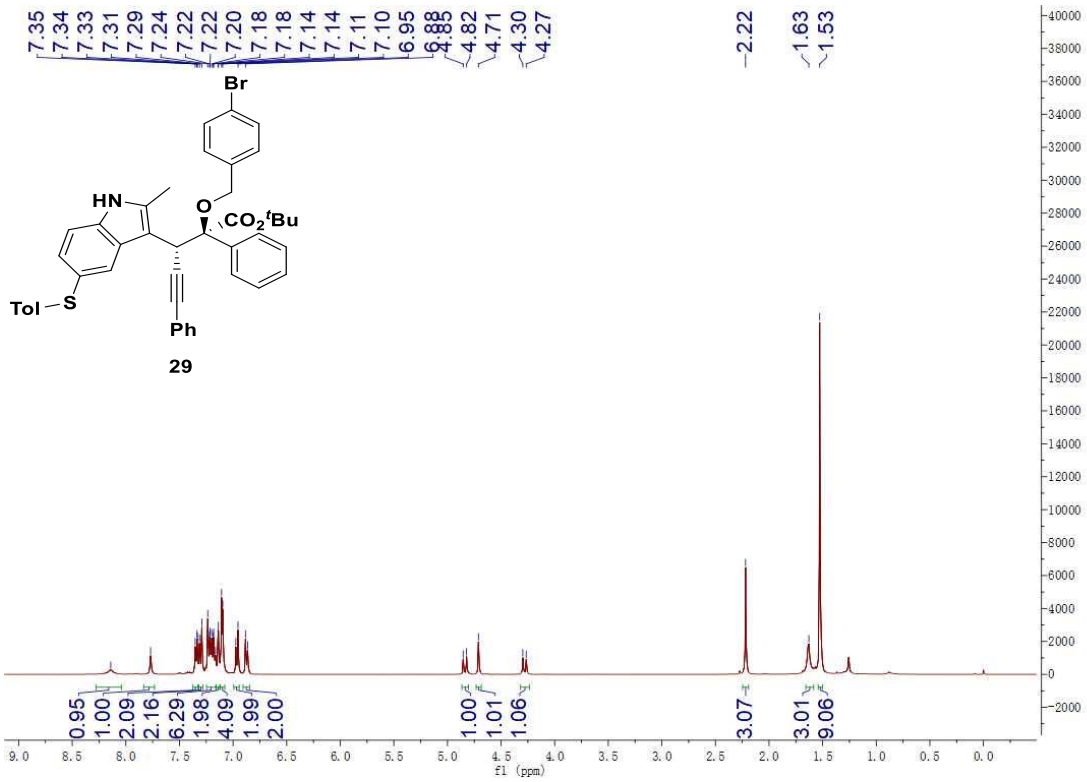

171.01
139.36
136.20
131.93
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128.27
128.08
127.98
127.91
127.70
127.44
126.98
124.15
109.31
106.26
89.69
89.55
83.57
83.13
83.00
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25.01
24.82
10.87
Br
HN
O
CO2tBu
Bpin
Ph
26
f1 (ppm)

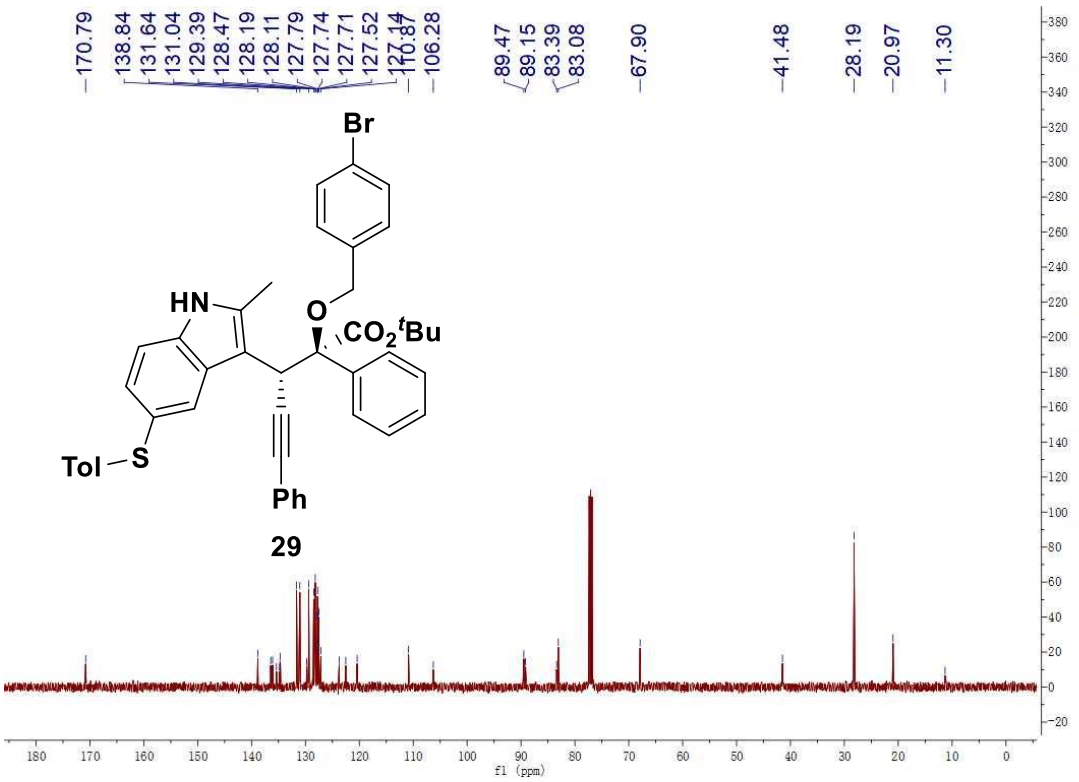

7.52
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7.44
7.44
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7.34
7.31
7.30
7.29
7.22
7.13
7.11
7.10
6.99
6.77
6.75
4.80
4.78
4.70
4.32
4.29
2.41
1.53
Br
HN
O
CO2tBu
Ph
27
0.95
1.06
2.10
2.02
5.06
1.13
4.06
1.00
1.00
1.00
1.00
1.04
3.08
12.06
f1 (ppm)

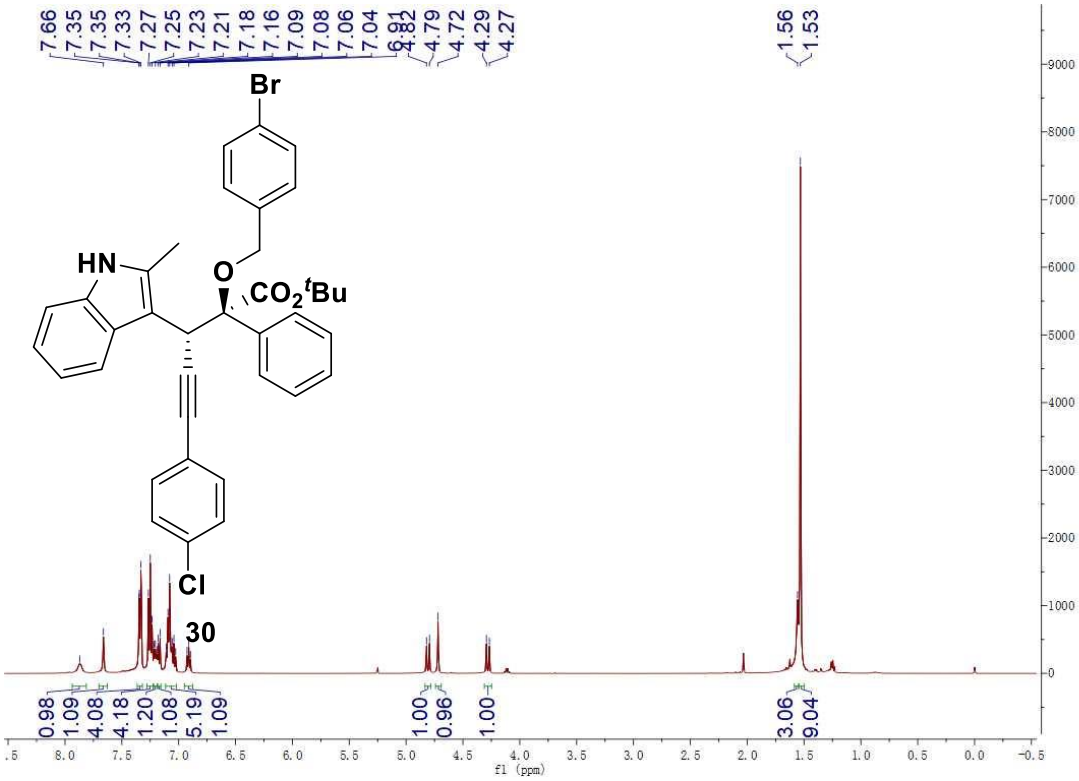

170.91
139.33
136.15
131.63
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130.40
128.48
128.20
127.93
127.89
127.65
127.38
105.80
89.67
89.62
83.04
82.91
67.66
41.57
28.18
21.65
10.99
Br
HN
O
CO2tBu
Ph
27
f1 (ppm)

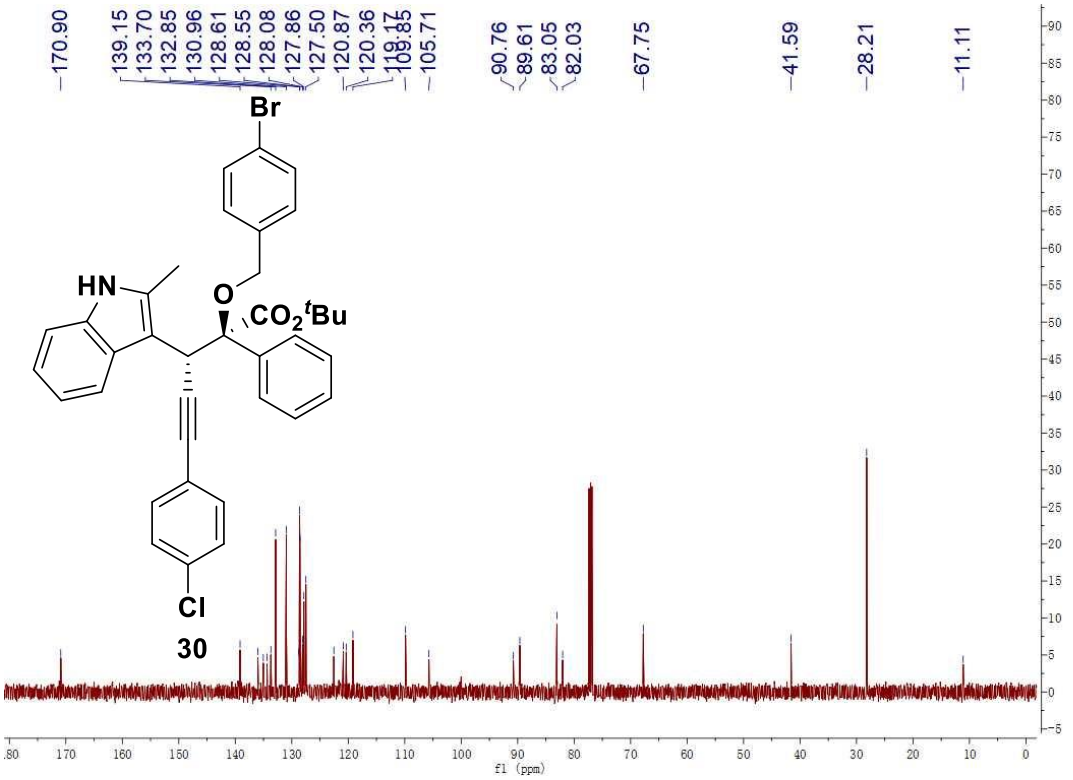

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7.31
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7.25
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7.22
7.20
7.19
7.17
7.12
7.11
7.08
7.06
7.04
6.85
6.65
4.77
4.69
4.29
4.25
2.94
1.65
1.52
Br
HN
O
CO2tBu
Ph–N
Ph
28
1.14
2.11
3.97
4.94
4.92
2.21
1.03
3.03
1.00
0.94
1.05
3.06
3.02
9.05
f1 (ppm)

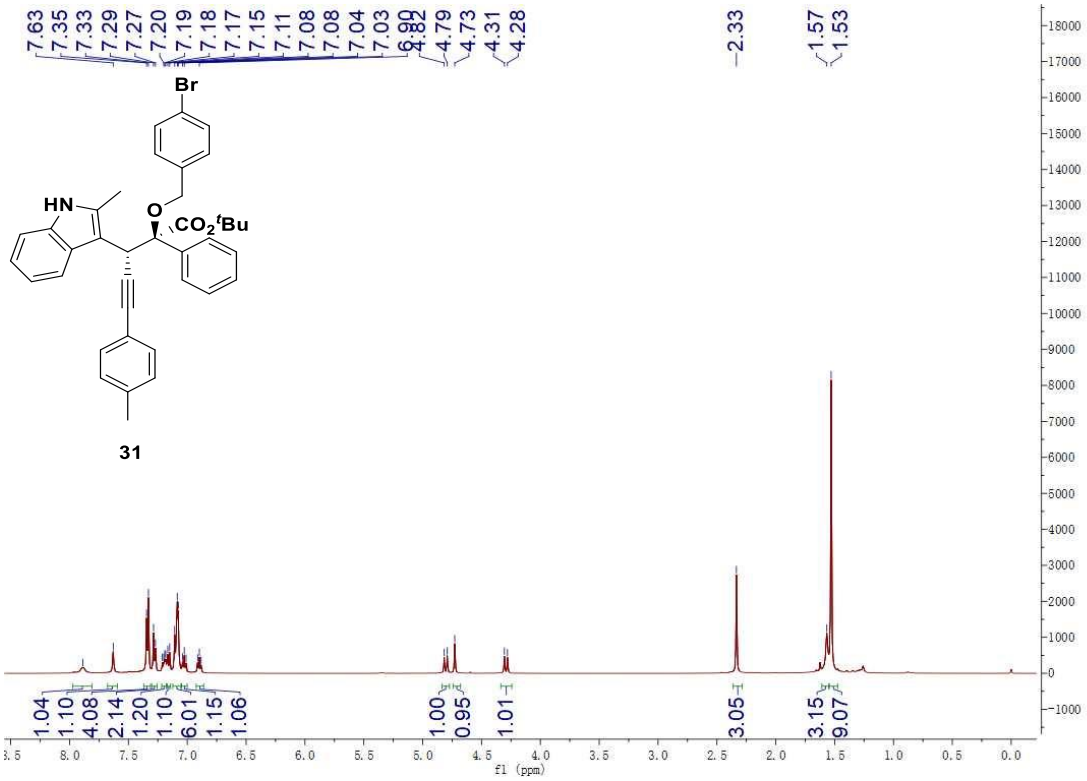

170.87
150.55
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131.07
128.67
128.59
128.25
128.09
127.89
127.71
127.51
120.40
116.97
114.49
89.43
89.38
83.33
83.05
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40.53
28.24
11.41
Br
HN
O
CO2tBu
Ph
N
Ph
28
f1 (ppm)

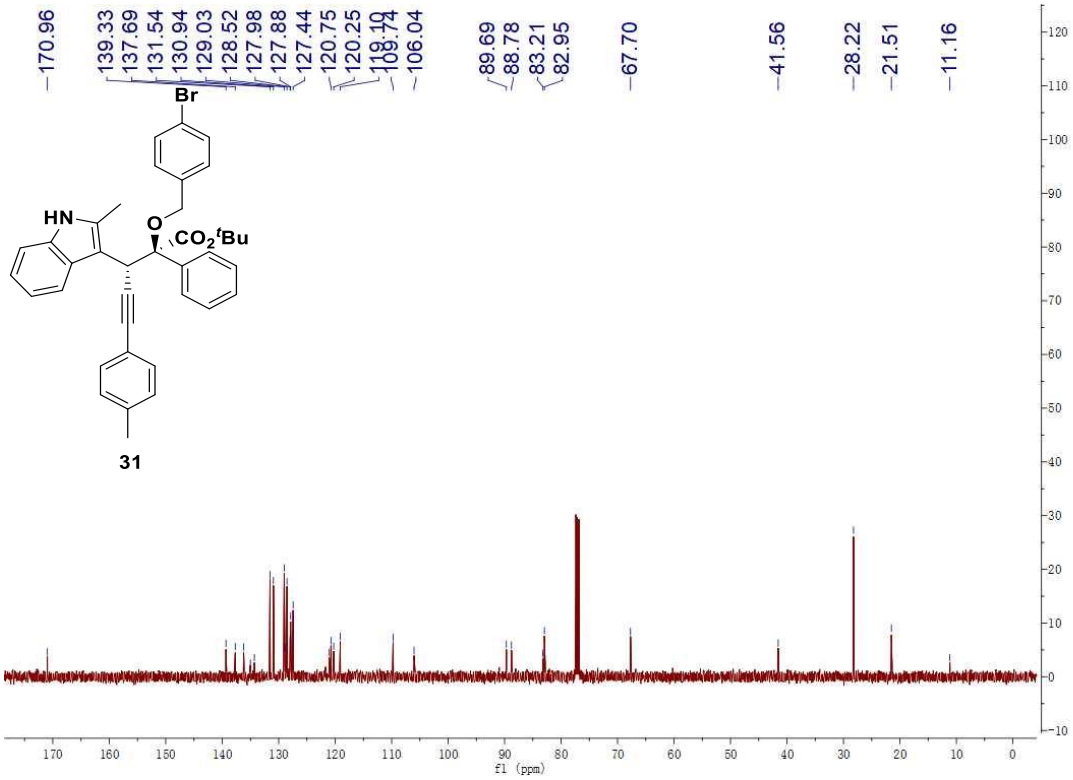

7.35
7.34
7.33
7.31
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7.24
7.22
7.22
7.20
7.18
7.18
7.14
7.14
7.11
7.10
6.95
4.82
4.71
4.30
4.27
2.22
1.63
1.53
Br
HN
O
CO2tBu
Tol
S
Ph
29
0.95
1.00
2.09
2.16
6.29
1.98
4.09
1.99
2.00
1.00
1.01
1.06
3.07
3.01
9.06
f1 (ppm)

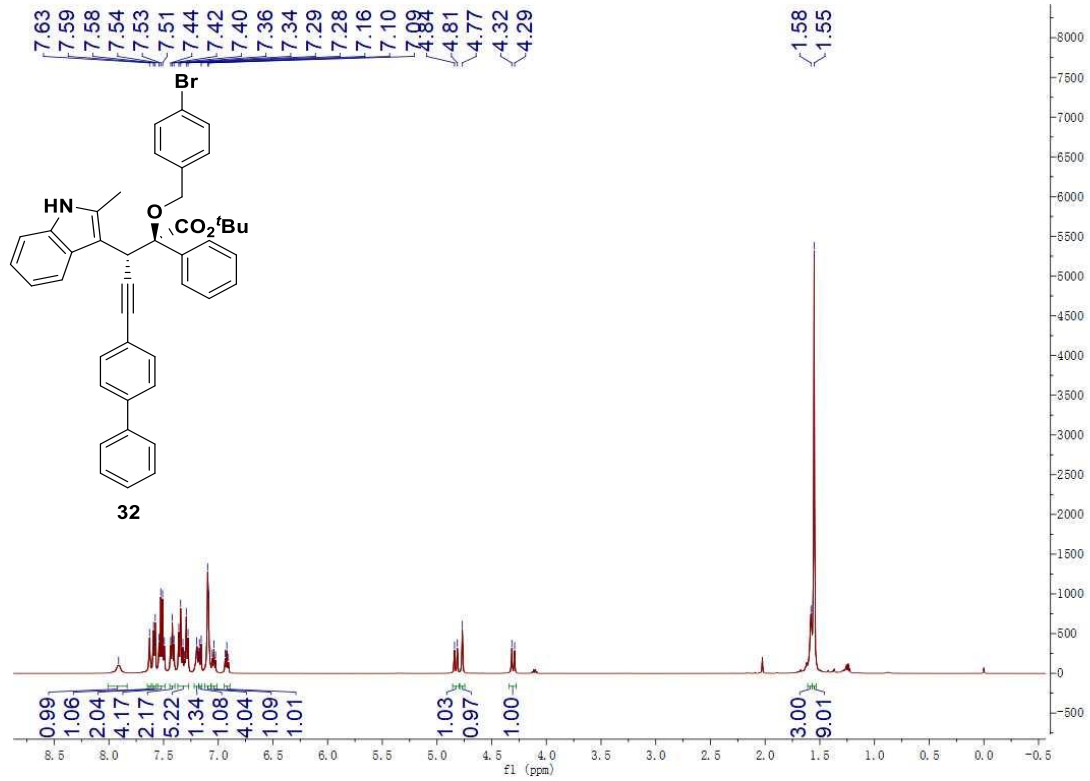

170.79
138.84
131.64
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129.39
128.47
128.19
128.11
127.79
127.74
127.71
127.52
127.14
110.87
106.28
89.47
89.15
83.39
83.08
67.90
41.48
28.19
20.97
11.30
Br
HN
O
CO2tBu
Tol
S
Ph
29
f1 (ppm)

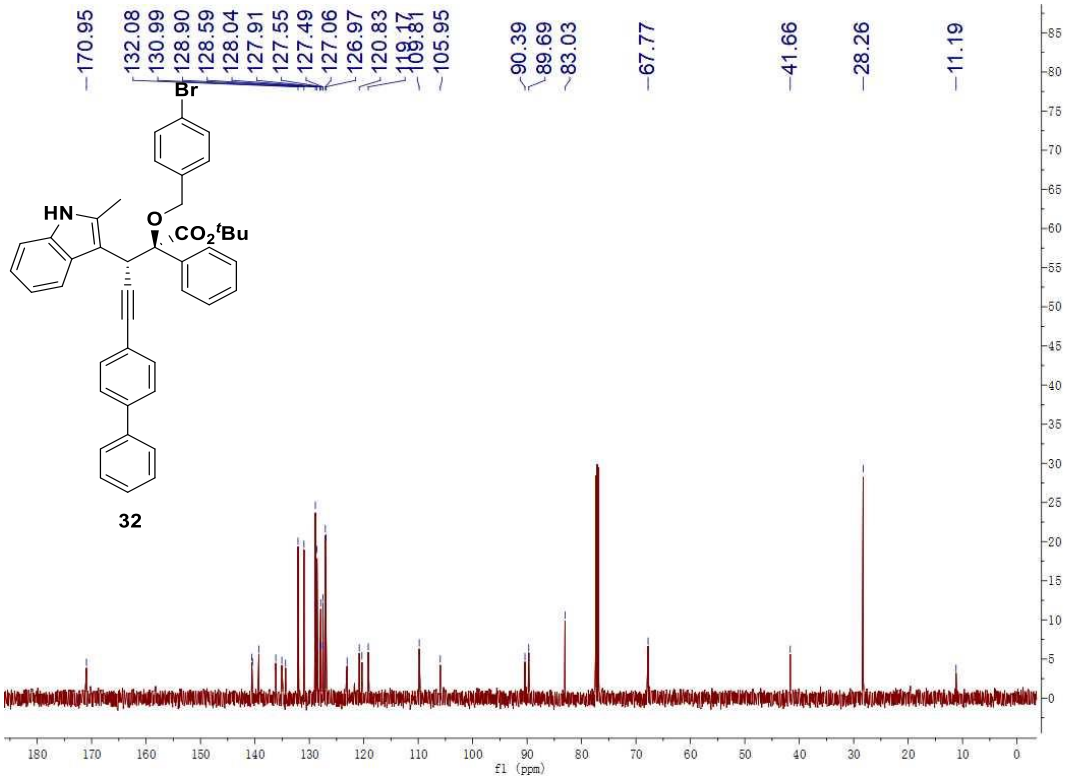

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7.35
7.33
7.27
7.25
7.23
7.21
7.18
7.16
7.09
7.08
7.06
7.04
6.91
4.82
4.79
4.72
4.29
4.27
1.56
1.53
Br
HN
O
CO2tBu
Cl
30
0.98
1.09
4.08
4.18
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1.08
5.19
1.09
1.00
0.96
1.00
3.06
9.04
f1 (ppm)

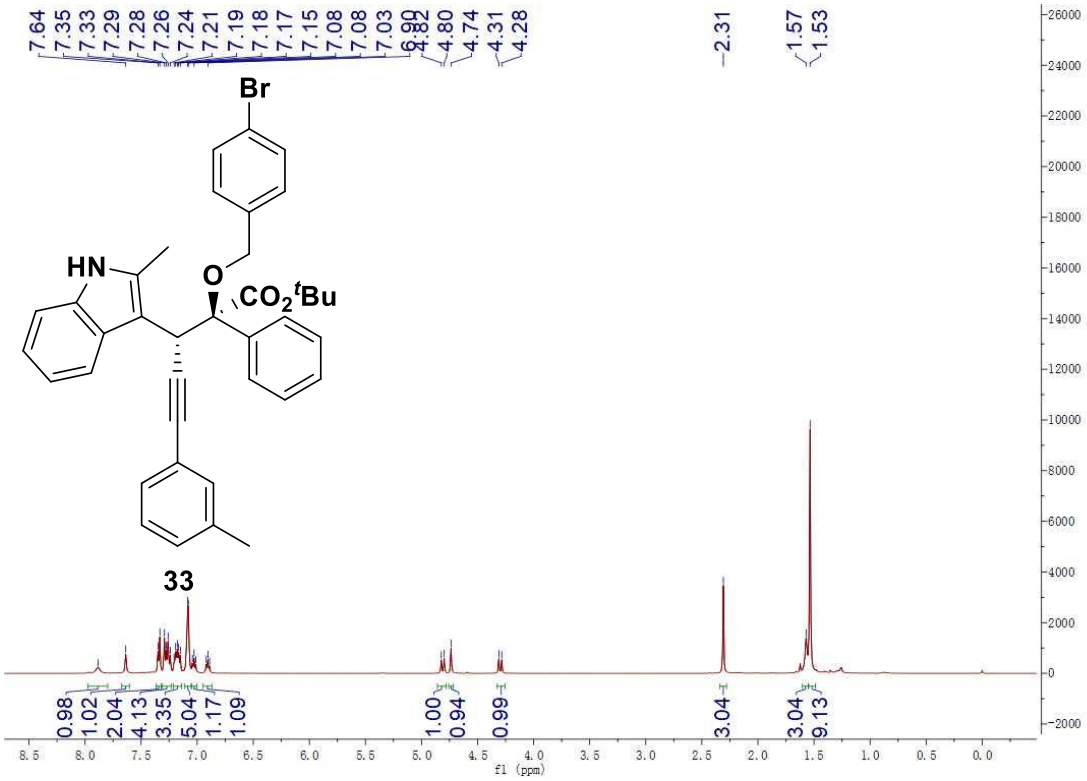

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130.96
128.61
128.55
128.08
127.86
127.50
120.87
120.36
119.17
109.85
105.71
90.76
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67.75
41.59
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11.11
Br
HN
O
CO2tBu
Cl
30
f1 (ppm)

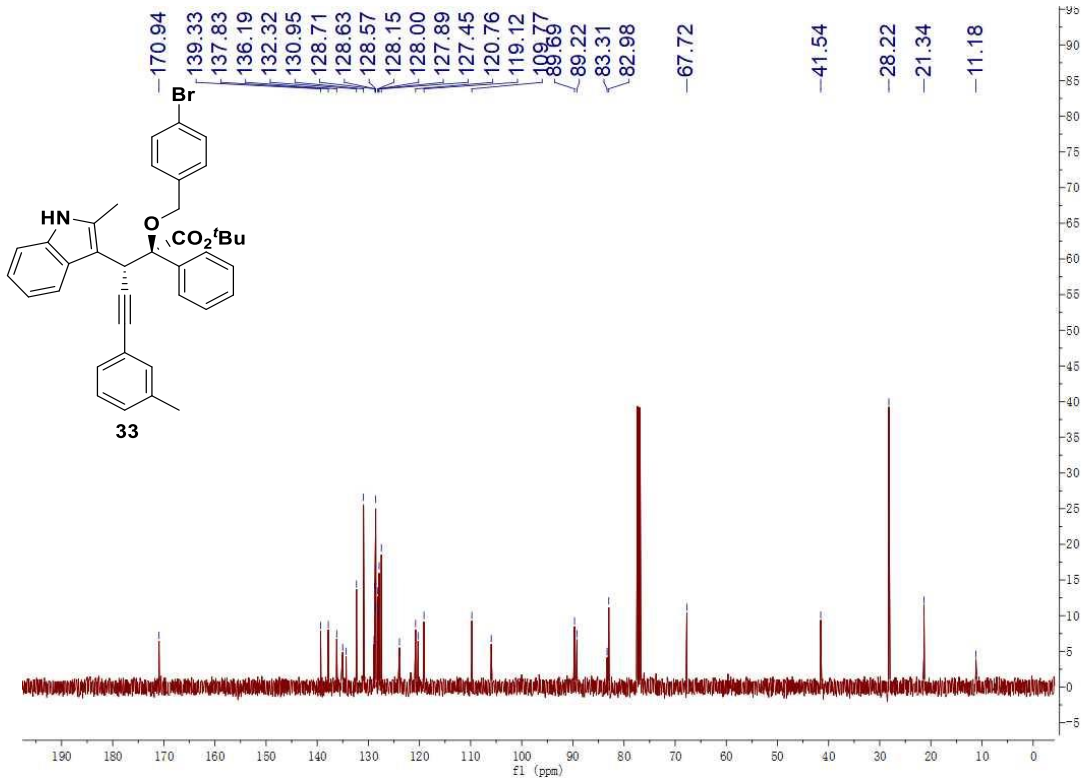

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7.29
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7.20
7.19
7.18
7.17
7.15
7.11
7.08
7.08
7.04
7.03
6.90
4.82
4.79
4.73
4.31
4.28
2.33
1.57
1.53
Br
HN
O
CO2tBu
31
1.04
1.10
4.08
2.14
1.20
1.10
6.01
1.15
1.06
1.00
0.95
1.01
3.05
3.15
9.07
f1 (ppm)

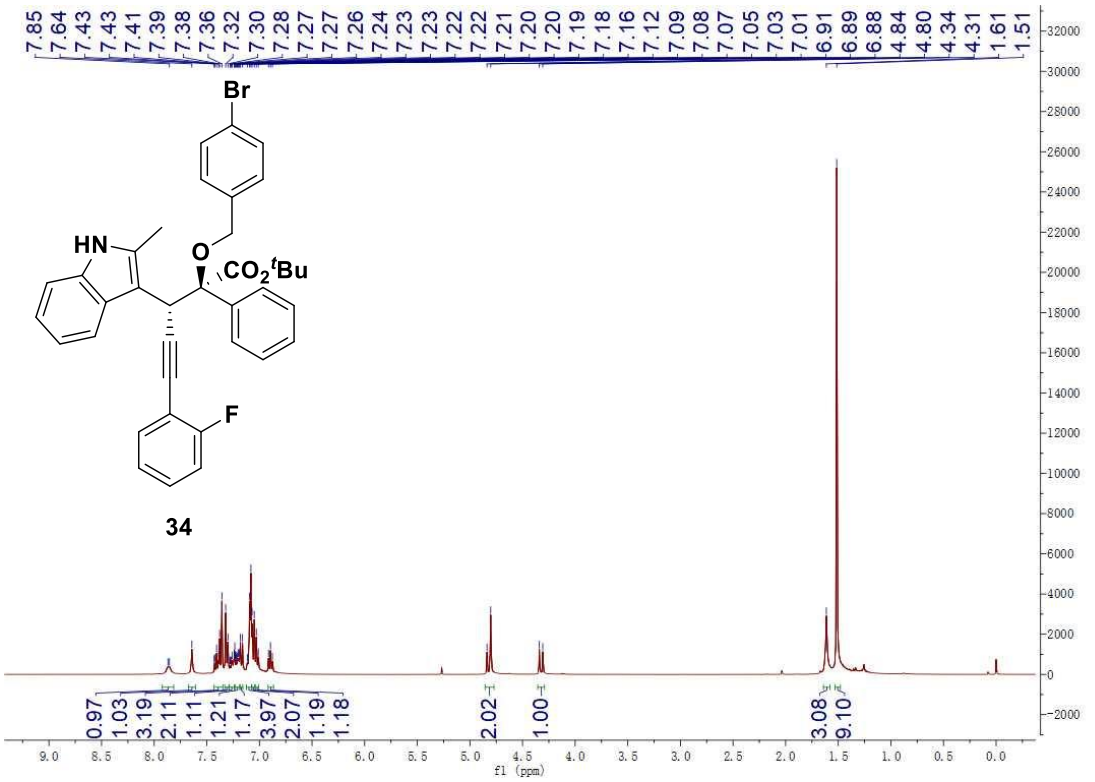

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129.03
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127.88
127.44
120.75
120.25
119.10
109.74
106.04
89.69
88.78
83.21
82.95
67.70
41.56
28.22
21.51
11.16
Br
HN
O
CO2tBu
31
f1 (ppm)

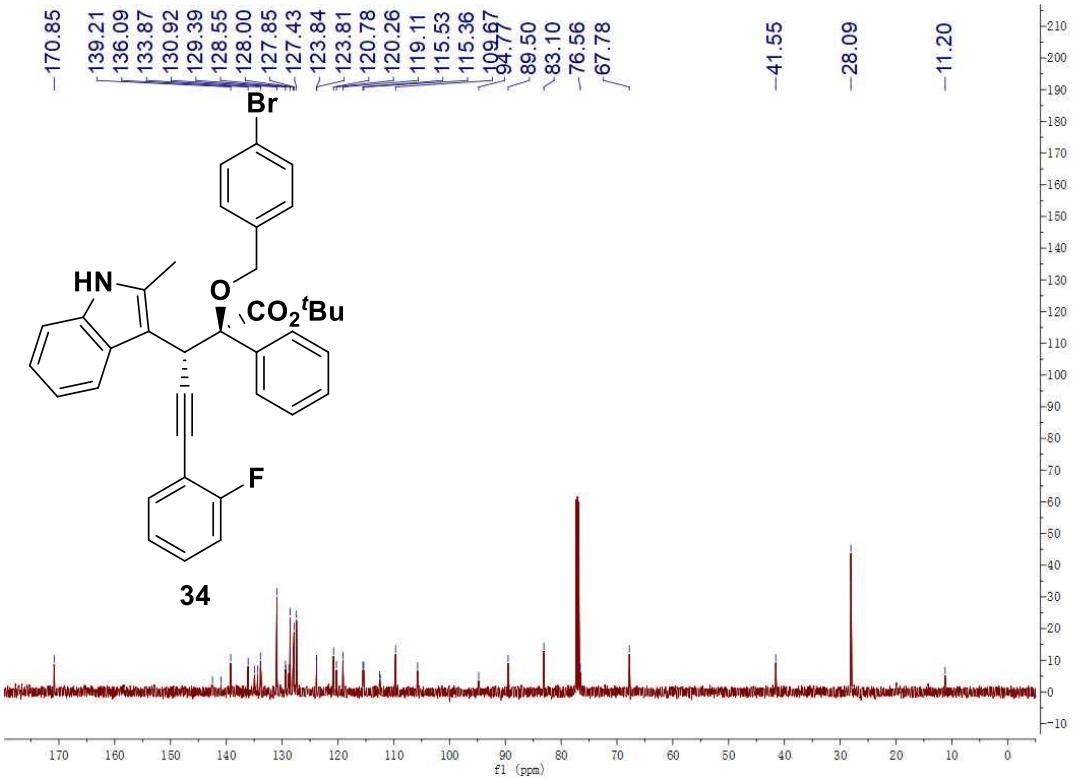

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7.40
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7.29
7.28
7.16
7.10
4.84
4.81
4.77
4.32
4.29
1.58
1.55
Br
HN
O
CO2tBu
32
0.99
1.06
2.04
4.17
2.17
5.22
1.34
1.08
4.04
1.09
1.01
1.03
0.97
1.00
3.00
9.01
f1 (ppm)

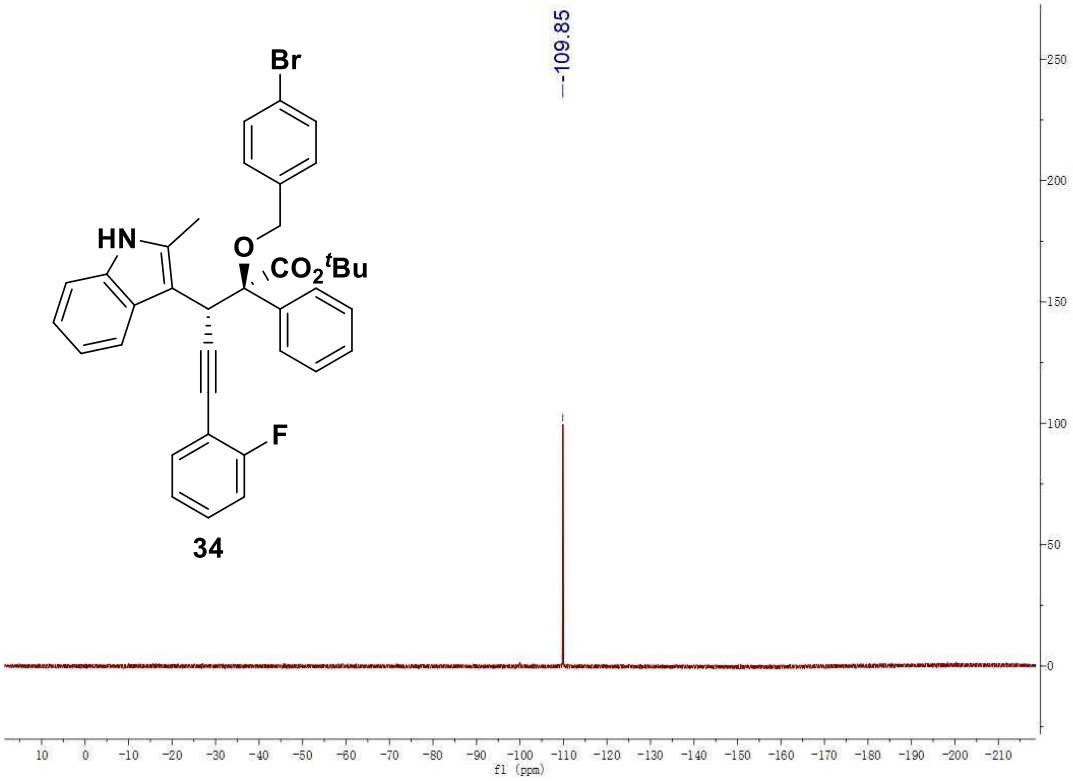

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128.90
128.59
128.04
127.91
127.55
127.49
127.06
126.97
120.83
119.17
111.81
105.95
90.39
89.69
83.03
67.77
41.66
28.26
11.19
Br
HN
O
CO2tBu
32
f1 (ppm)

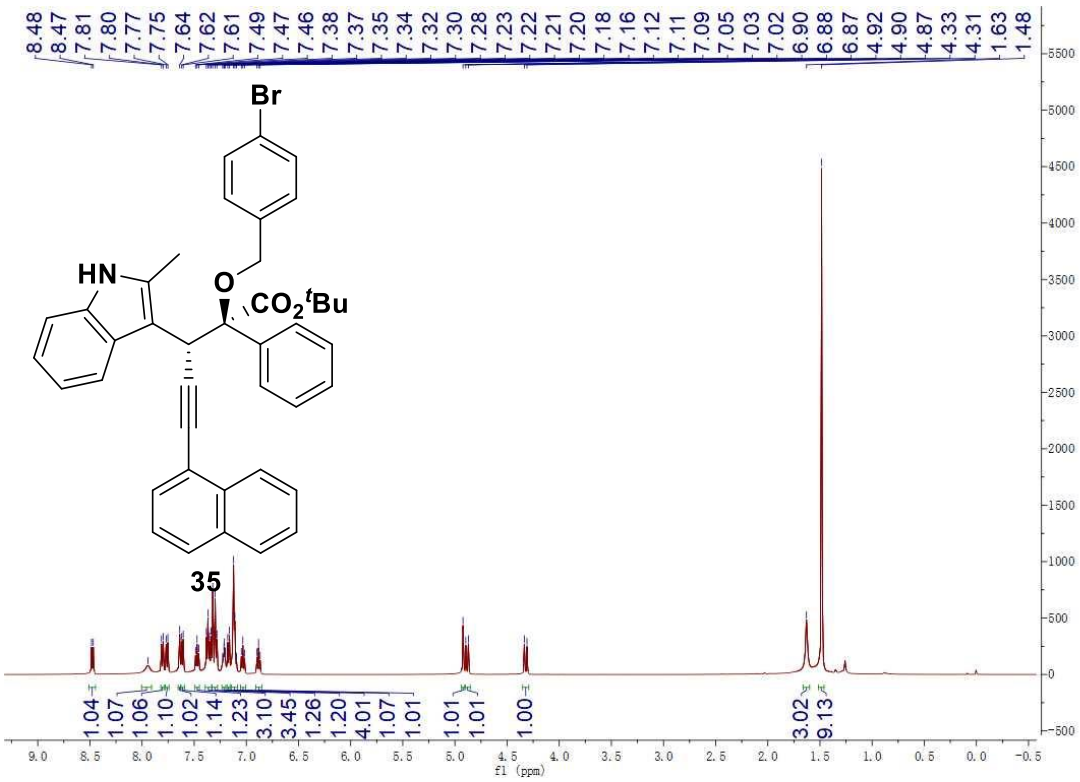

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7.19
7.18
7.17
7.15
7.08
7.03
6.90
6.88
4.82
4.80
4.74
4.31
4.28
2.31
1.57
1.53
Br
HN
O
CO2tBu
33
0.98
1.02
2.04
4.13
3.35
5.04
1.17
1.09
1.00
0.94
0.99
3.04
3.04
9.13
f1 (ppm)

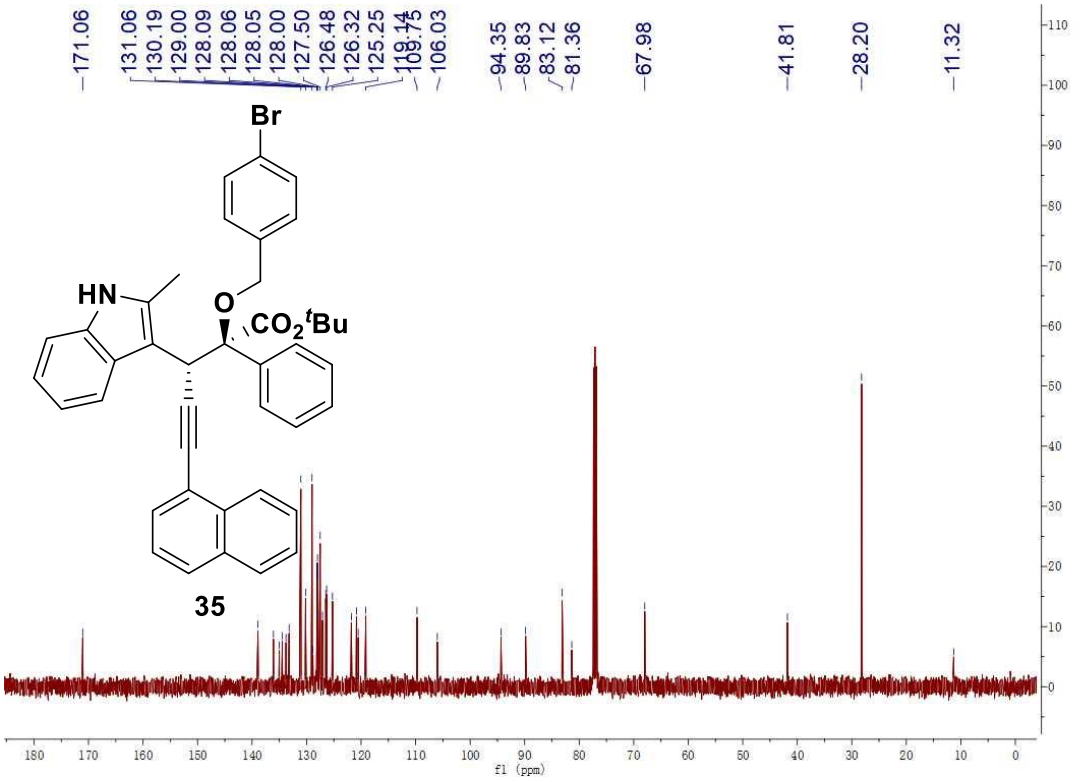

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136.19
132.32
130.95
128.71
128.63
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128.15
128.00
127.89
127.45
120.76
119.12
109.77
89.69
89.22
83.31
82.98
67.72
41.54
28.22
21.34
11.18
Br
HN
O
CO2tBu
33
f1 (ppm)

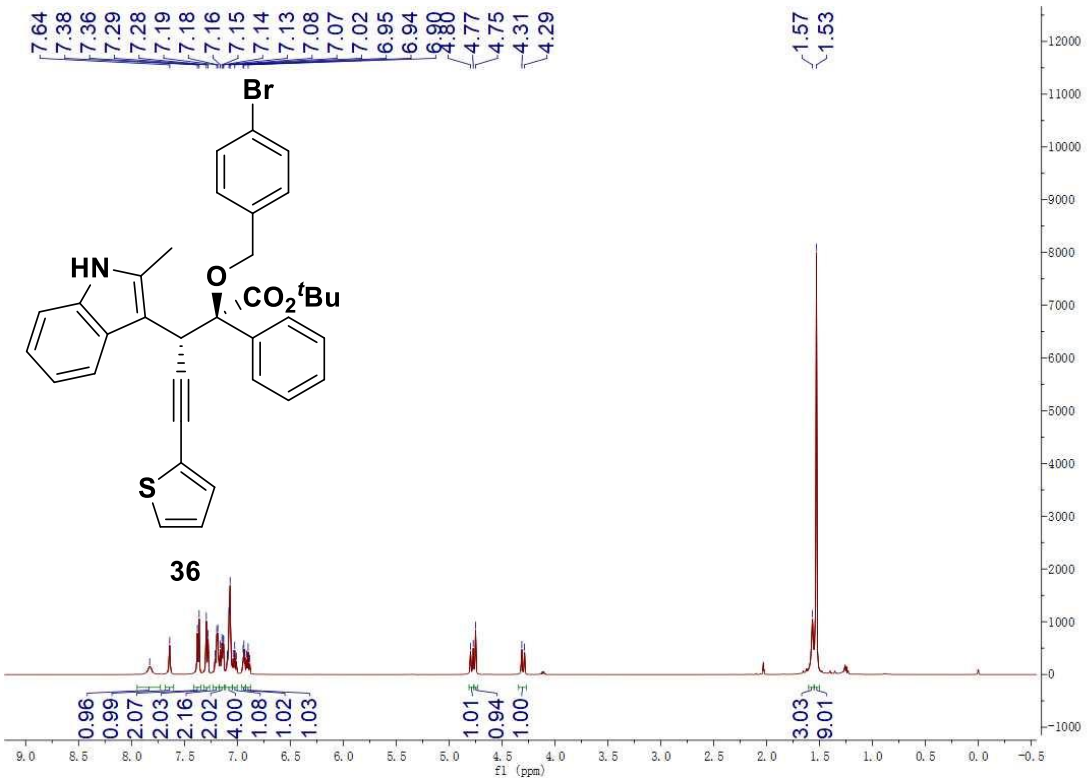

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7.39
7.38
7.36
7.32
7.30
7.28
7.27
7.27
7.26
7.24
7.23
7.23
7.22
7.22
7.21
7.20
7.19
7.18
7.16
7.12
7.09
7.08
7.07
7.05
7.03
7.01
6.91
6.89
6.88
4.84
4.80
4.34
4.31
1.61
1.51
Br
HN
O
CO2tBu
F
34
0.97
1.03
3.19
2.11
1.11
1.21
1.17
3.97
2.07
1.19
1.18
2.02
1.00
3.08
9.10
f1 (ppm)

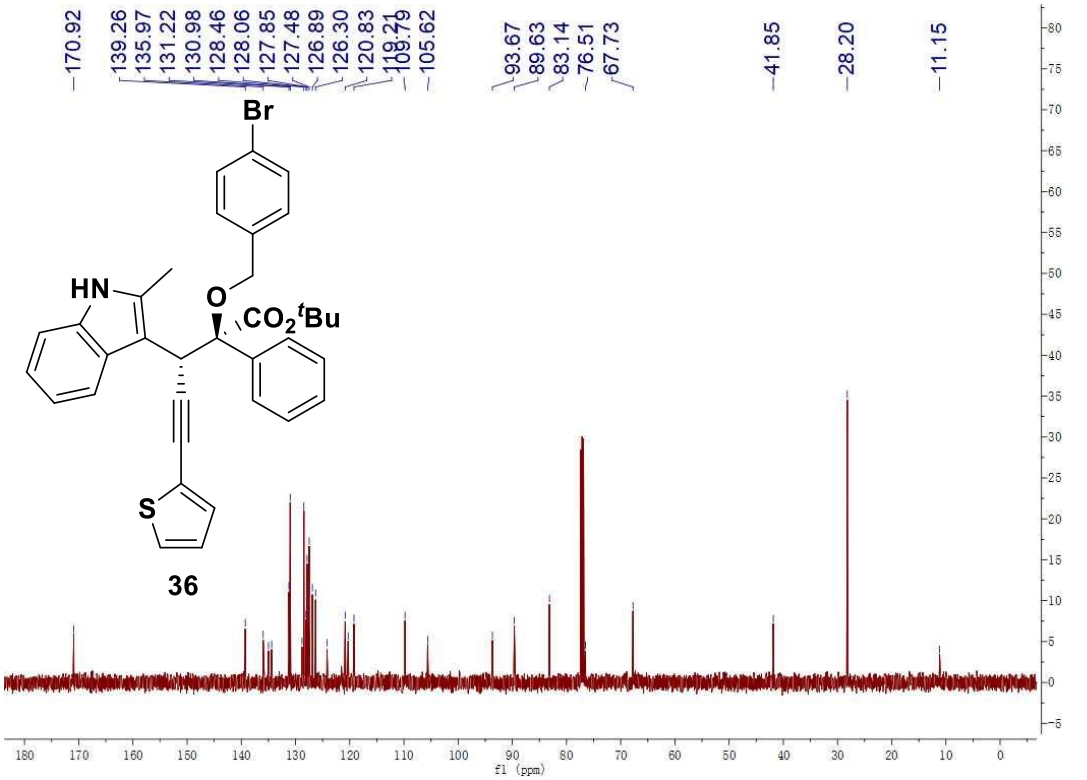

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129.39
128.55
128.00
127.85
127.43
123.84
123.81
120.78
120.26
119.11
115.53
115.36
109.67
94.77
89.50
83.10
76.56
67.78
41.55
28.09
11.20
Br
HN
O
CO2tBu
F
34
f1 (ppm)

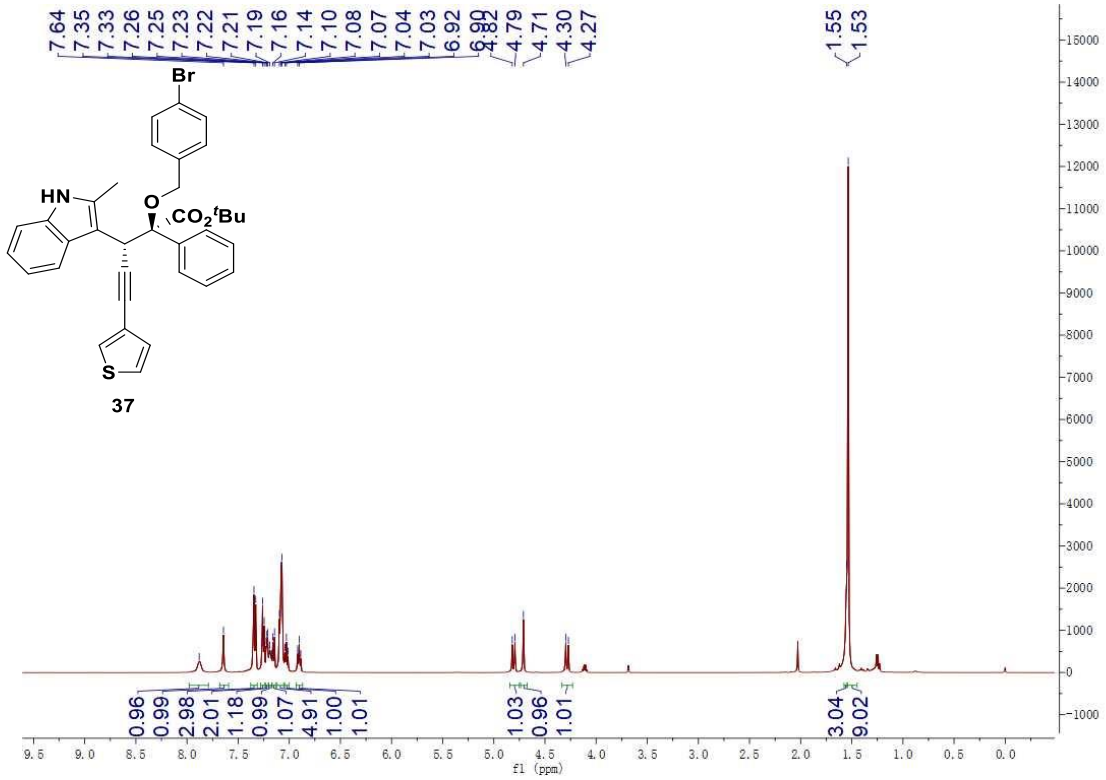

109.85
Br
HN
O
CO2tBu
F
34
f1 (ppm)

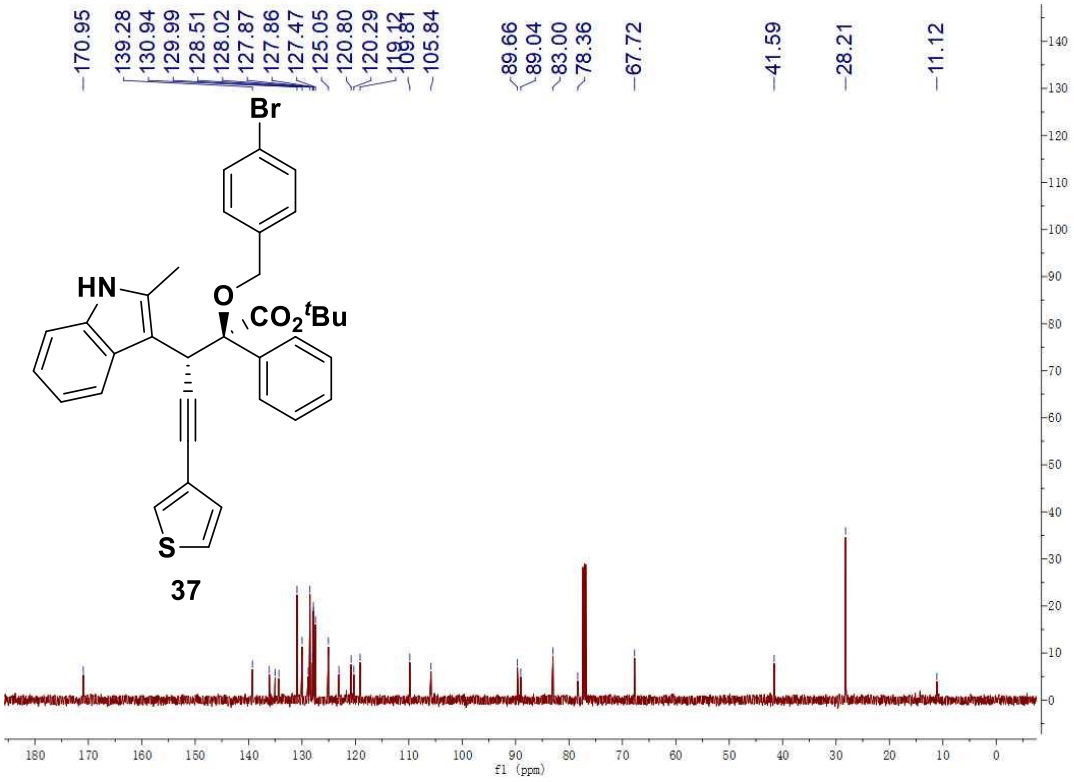

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7.77
7.75
7.64
7.62
7.61
7.49
7.47
7.46
7.38
7.37
7.35
7.34
7.32
7.30
7.28
7.23
7.22
7.21
7.20
7.18
7.16
7.12
7.11
7.09
7.05
7.03
7.02
6.90
6.88
6.87
4.92
4.90
4.87
4.33
4.31
1.63
1.48
Br
HN
O
CO2tBu
35
1.04
1.07
1.06
1.10
1.02
1.14
1.23
3.10
3.45
1.26
1.20
4.01
1.07
1.01
1.01
1.01
1.00
3.02
9.13
f1 (ppm)

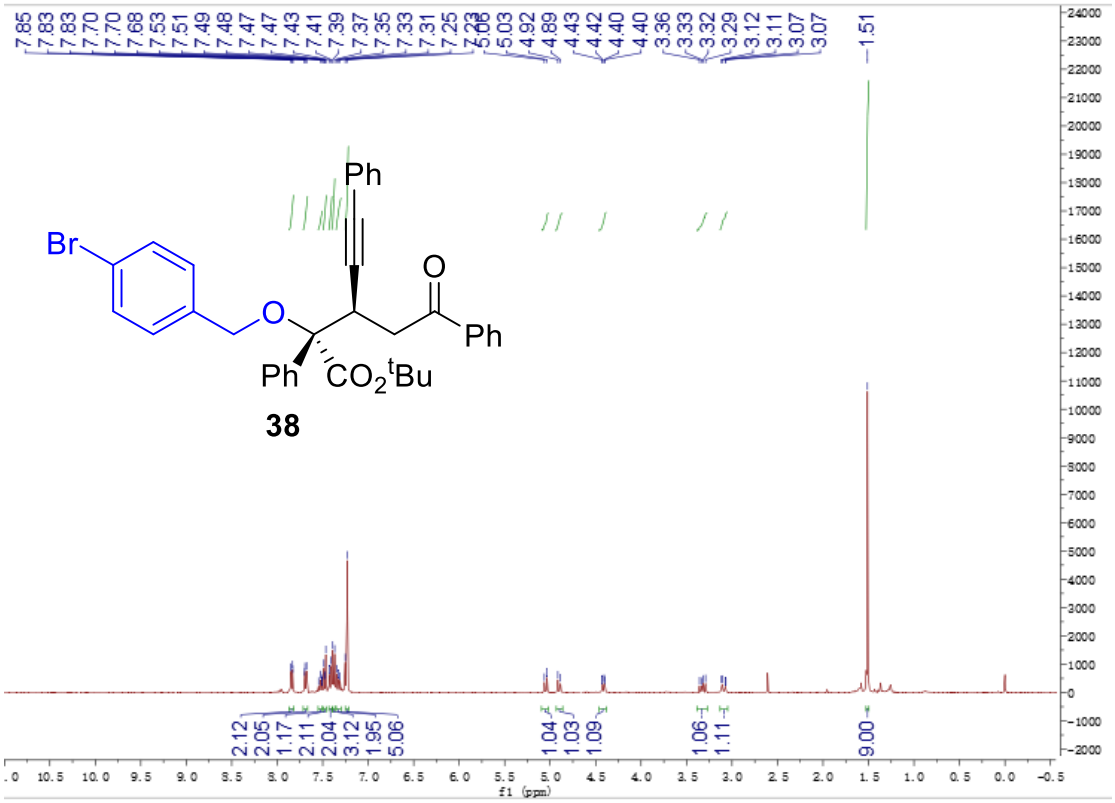

171.06
131.06
130.19
129.00
128.09
128.06
128.05
128.00
127.50
126.48
126.32
125.25
119.14
109.75
106.03
94.35
89.83
83.12
81.36
67.98
41.81
28.20
11.32
Br
HN
O
CO2tBu
35
f1 (ppm)

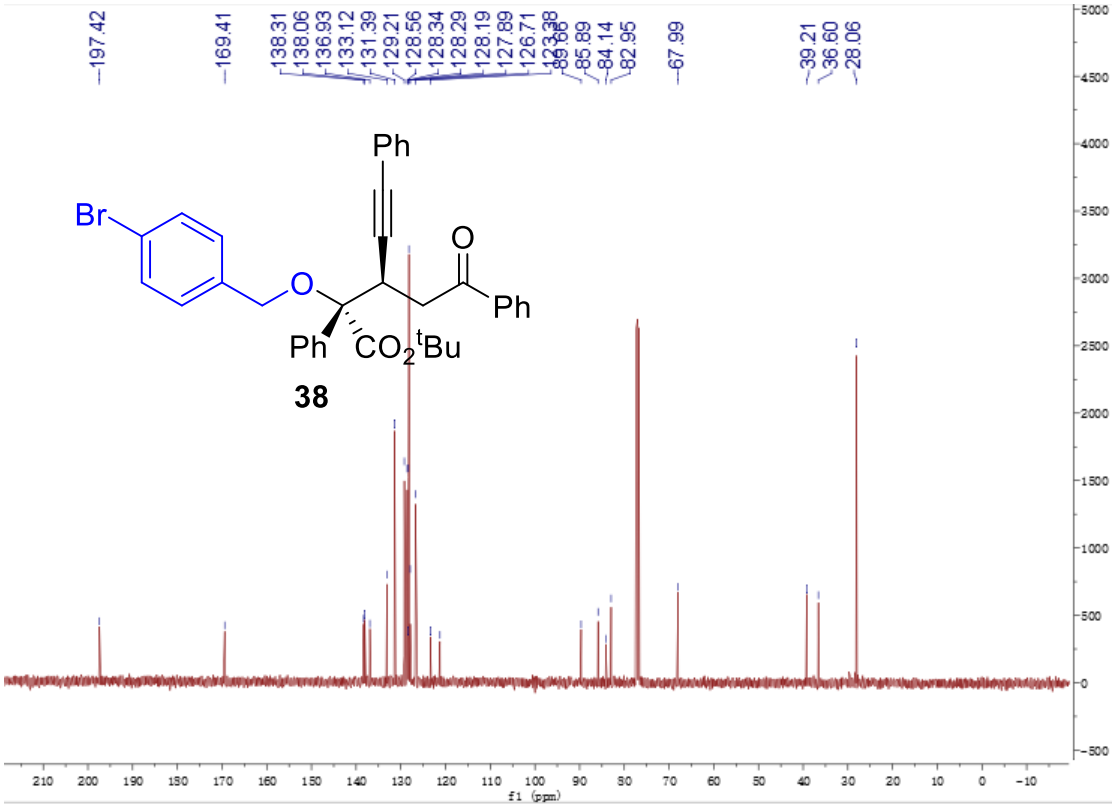

7.64
7.38
7.36
7.29
7.28
7.19
7.18
7.16
7.15
7.14
7.13
7.08
7.07
7.02
6.95
6.94
4.77
4.75
4.31
4.29
1.57
1.53
Br
HN
O
CO2tBu
S
36
0.96
0.99
2.07
2.03
2.16
2.02
4.00
1.08
1.02
1.03
1.01
0.94
1.00
3.03
9.01
f1 (ppm)

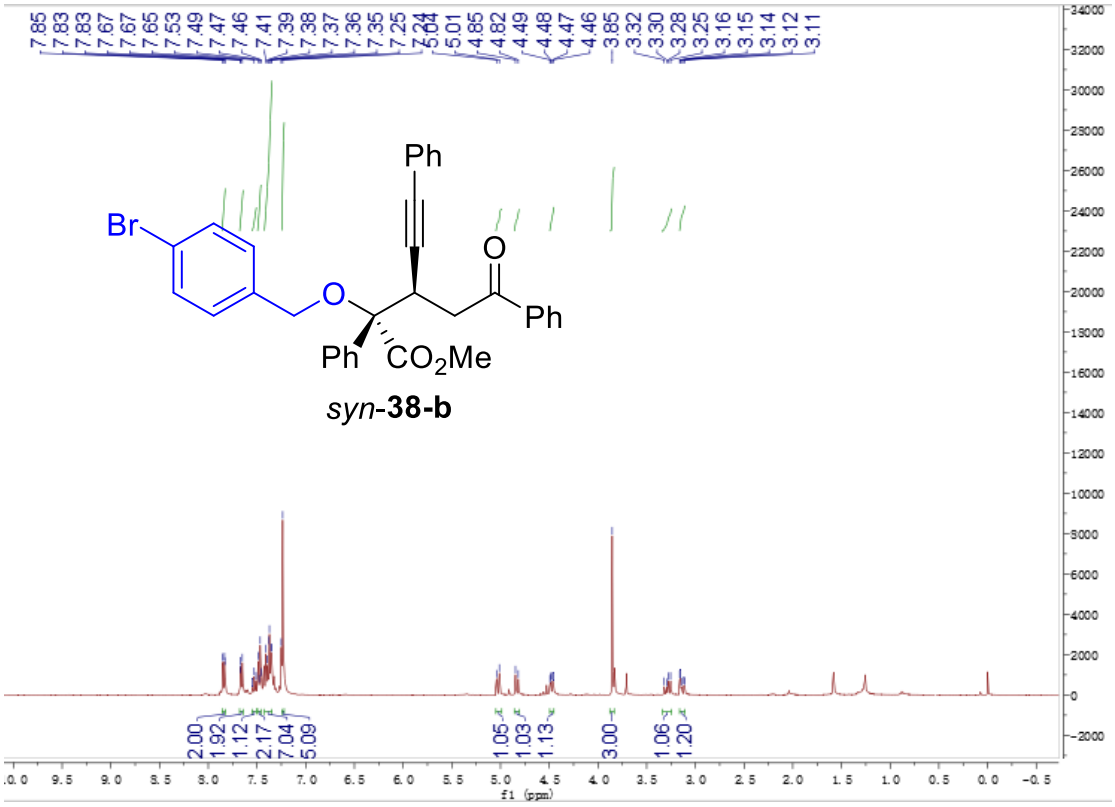

170.92
139.26
135.97
131.22
130.98
128.46
128.06
127.85
127.48
126.89
126.30
120.83
105.62
93.67
89.63
83.14
76.51
67.73
41.85
28.20
11.15
Br
HN
O
CO2tBu
S
36
f1 (ppm)


7.64
7.35
7.33
7.26
7.25
7.23
7.22
7.21
7.19
7.16
7.14
7.10
7.08
7.07
7.04
7.03
6.92
6.90
6.82
4.79
4.71
4.30
4.27
1.55
1.53
Br
HN
O
CO2tBu
S
37
0.96
0.99
2.98
2.01
1.18
0.99
1.07
4.91
1.00
1.01
1.03
0.96
1.01
3.04
9.02
f1 (ppm)

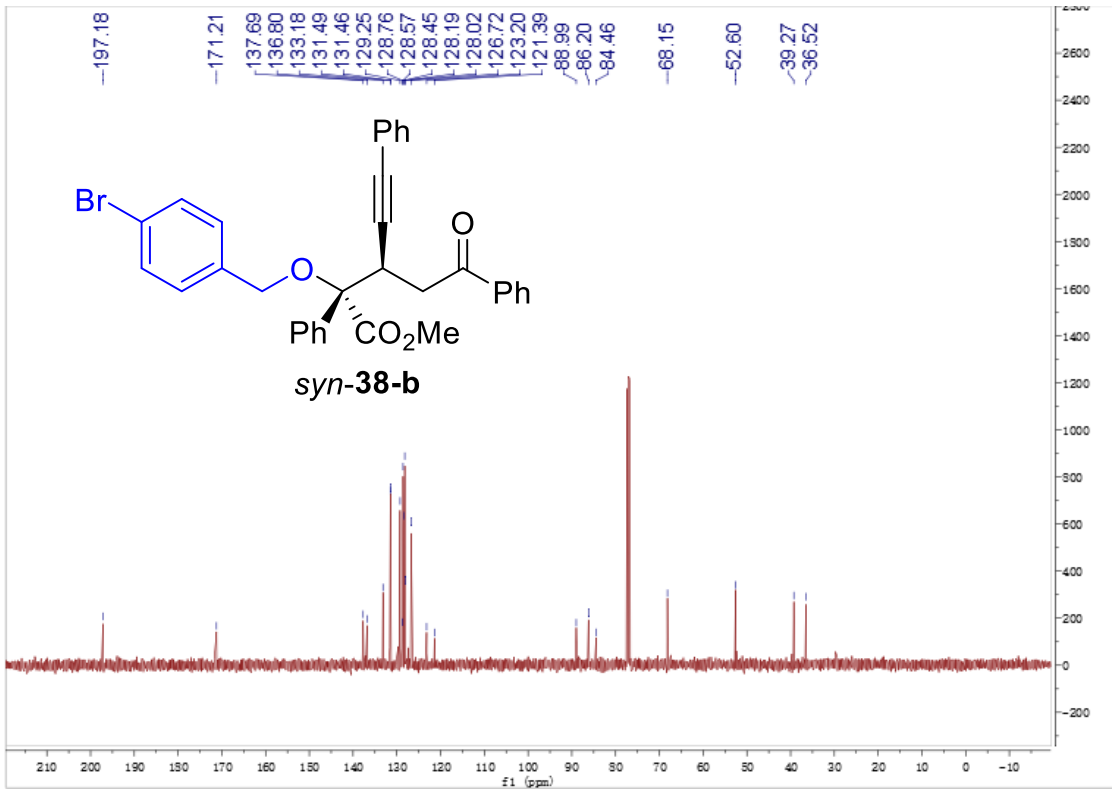

170.95
139.28
130.94
129.99
128.51
128.02
127.87
127.86
127.47
125.05
120.80
120.29
105.84
89.66
89.04
83.00
78.36
67.72
41.59
28.21
11.12
Br
HN
O
CO2tBu
S
37
f1 (ppm)


Br
O
Ph
O
Ph
Ph
CO2tBu
38

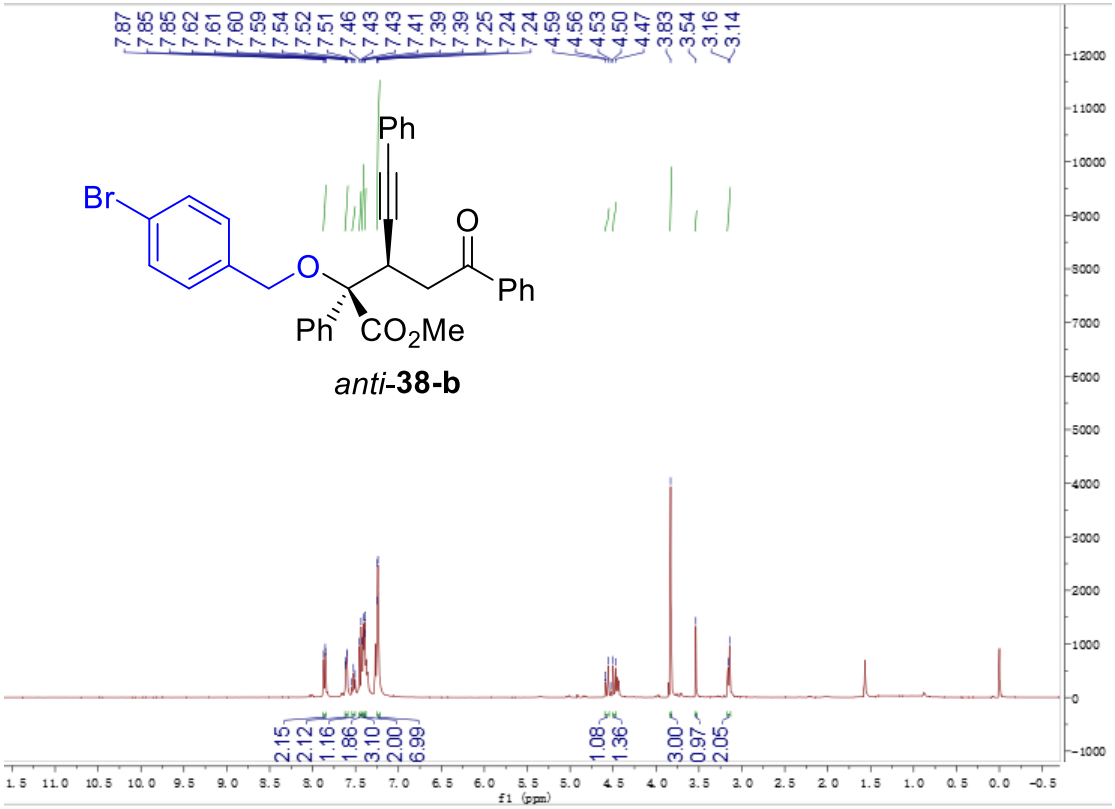

Br
O
Ph
O
Ph
Ph
CO2tBu
38



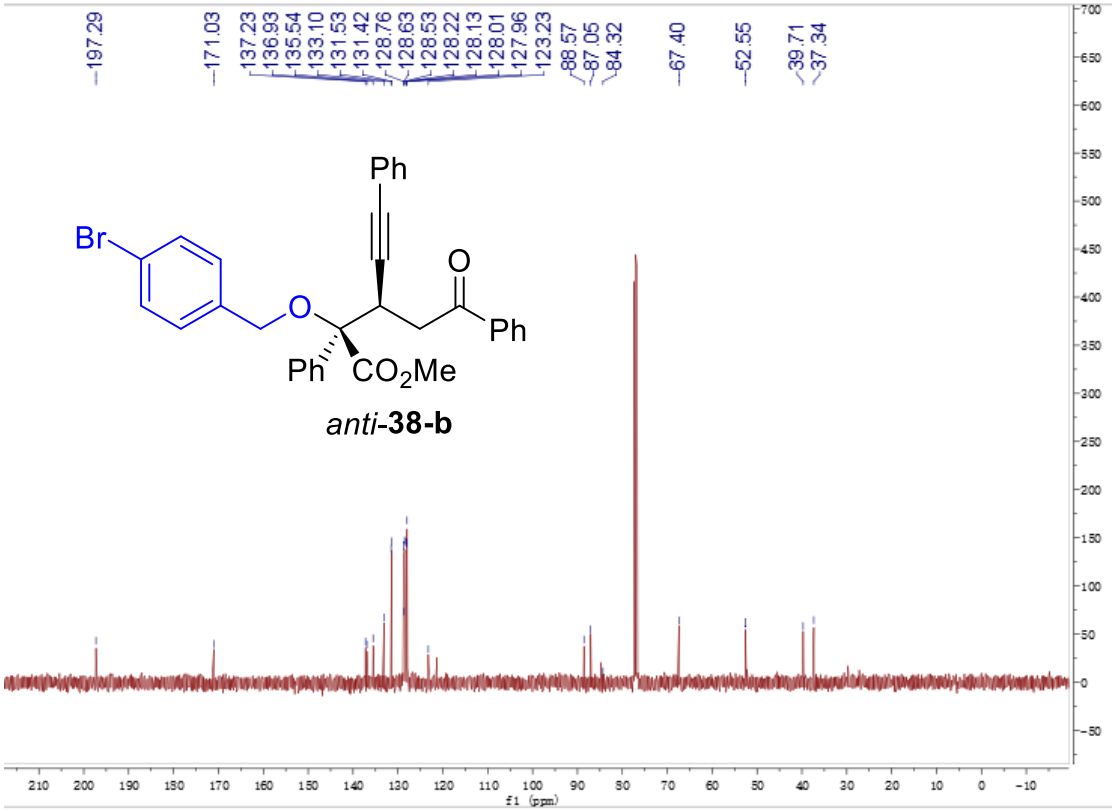

*syn*-**38-b**



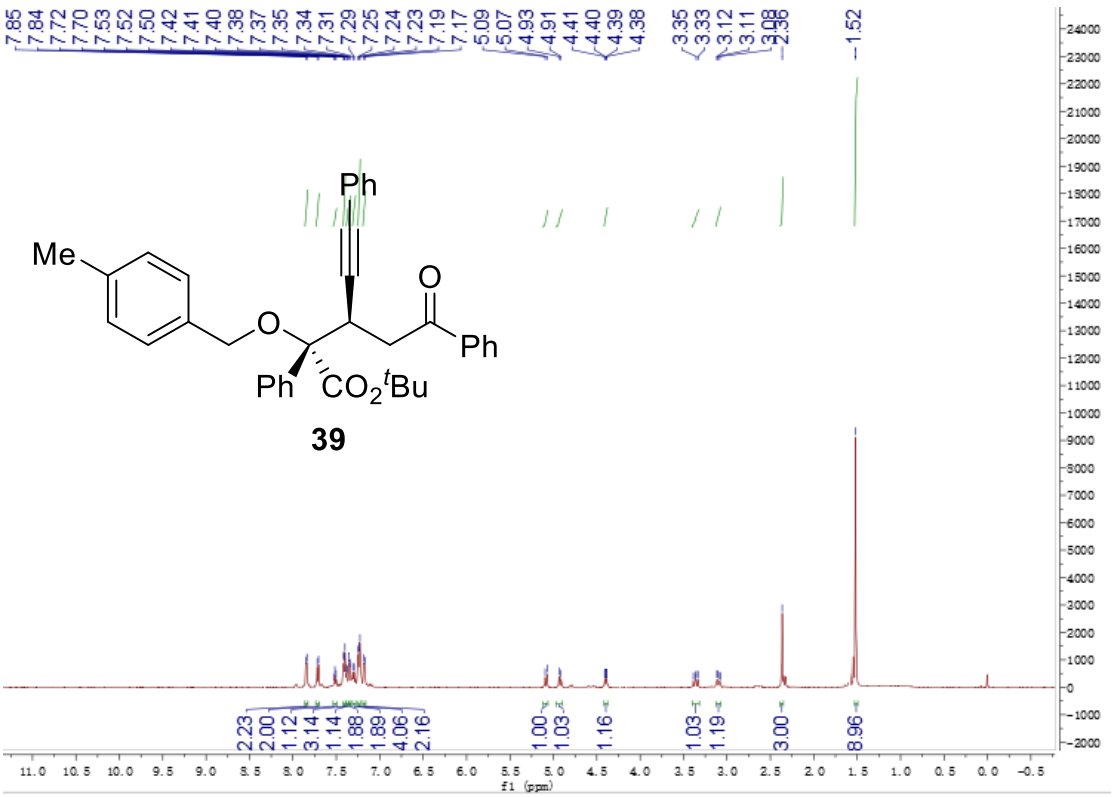

*syn*-**38-b**



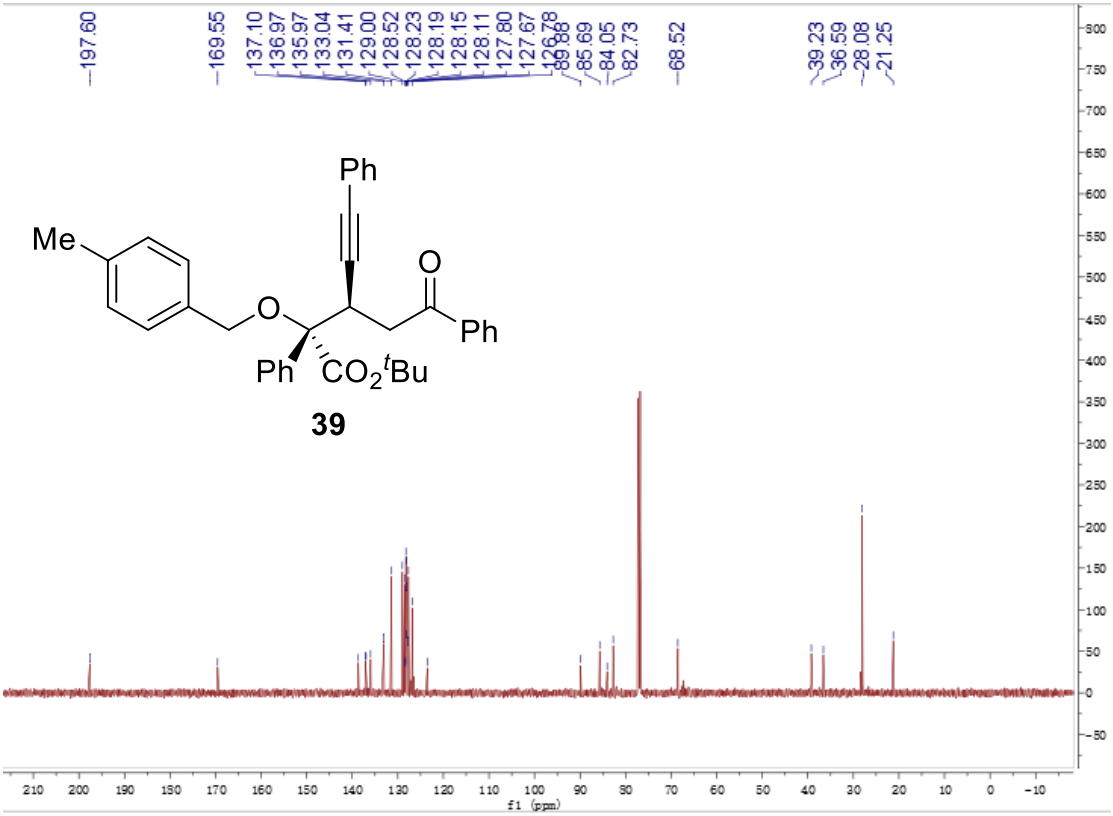

*anti*-**38-b**



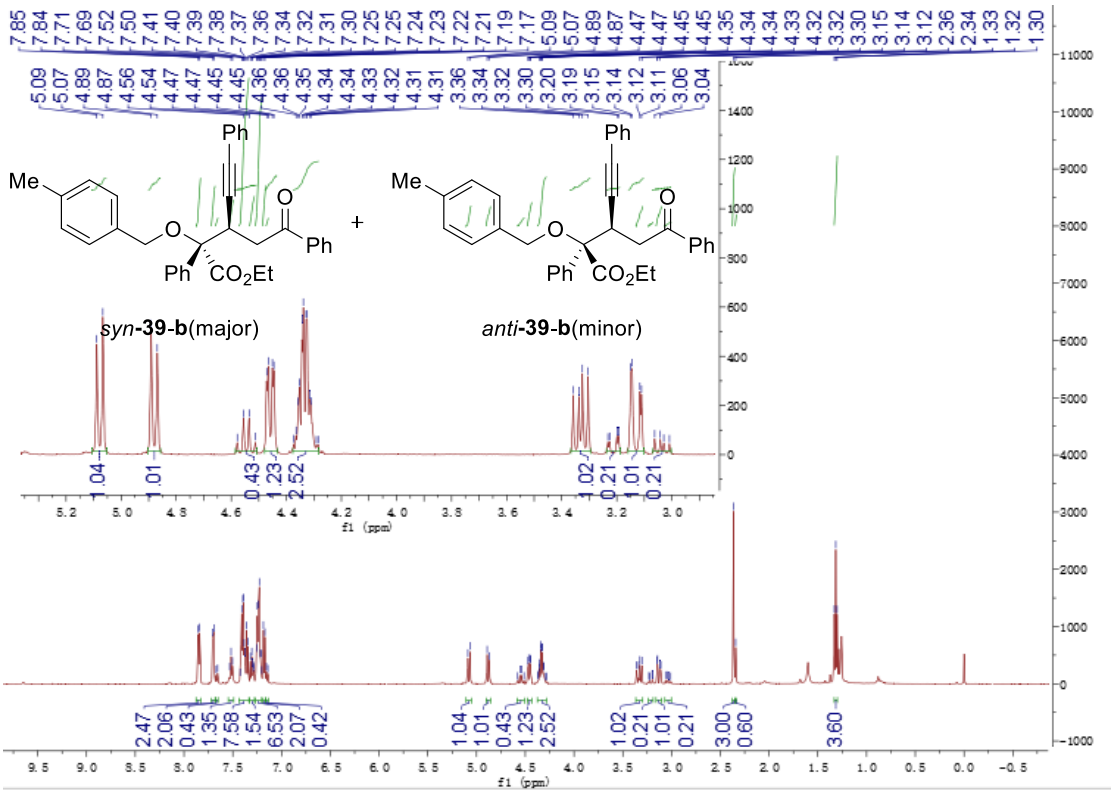

*anti*-**38-b**

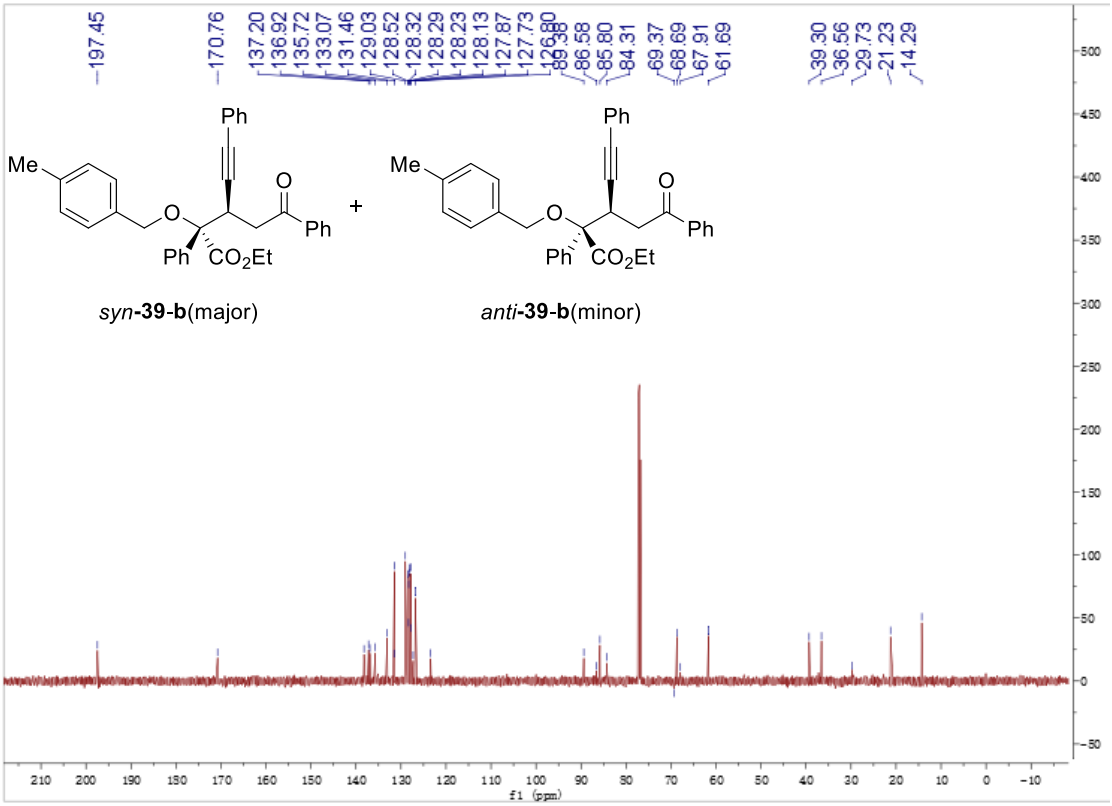


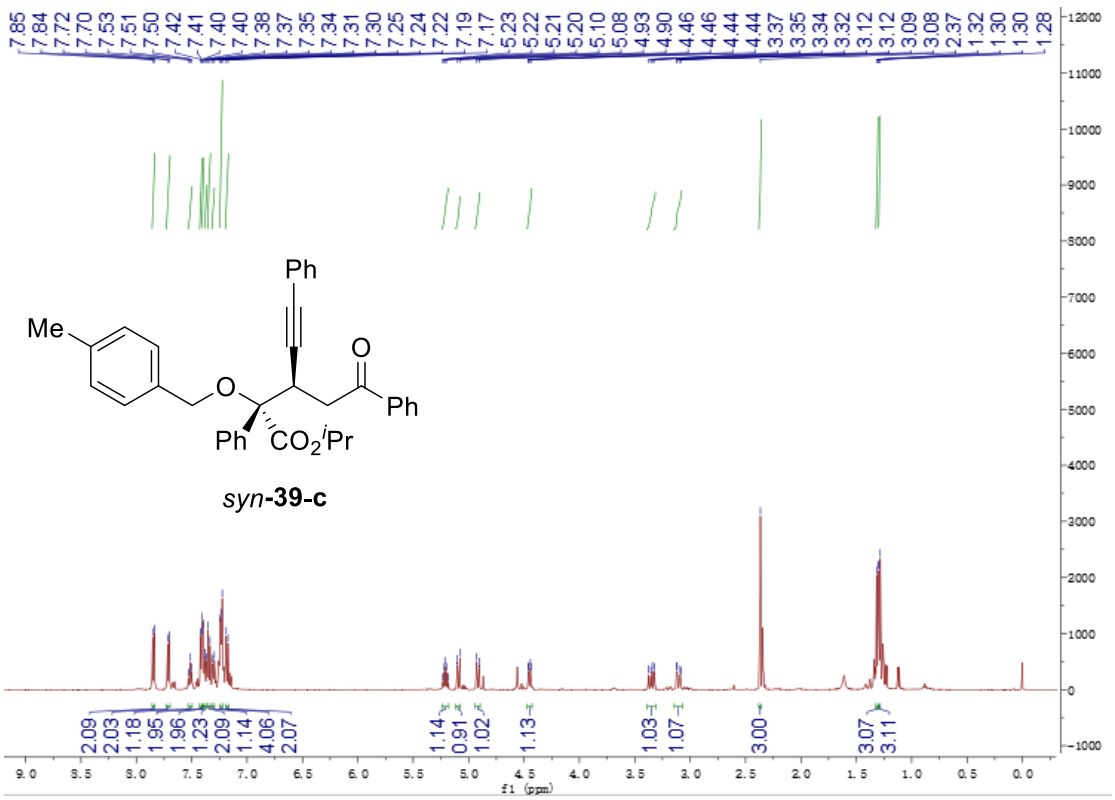

**39**



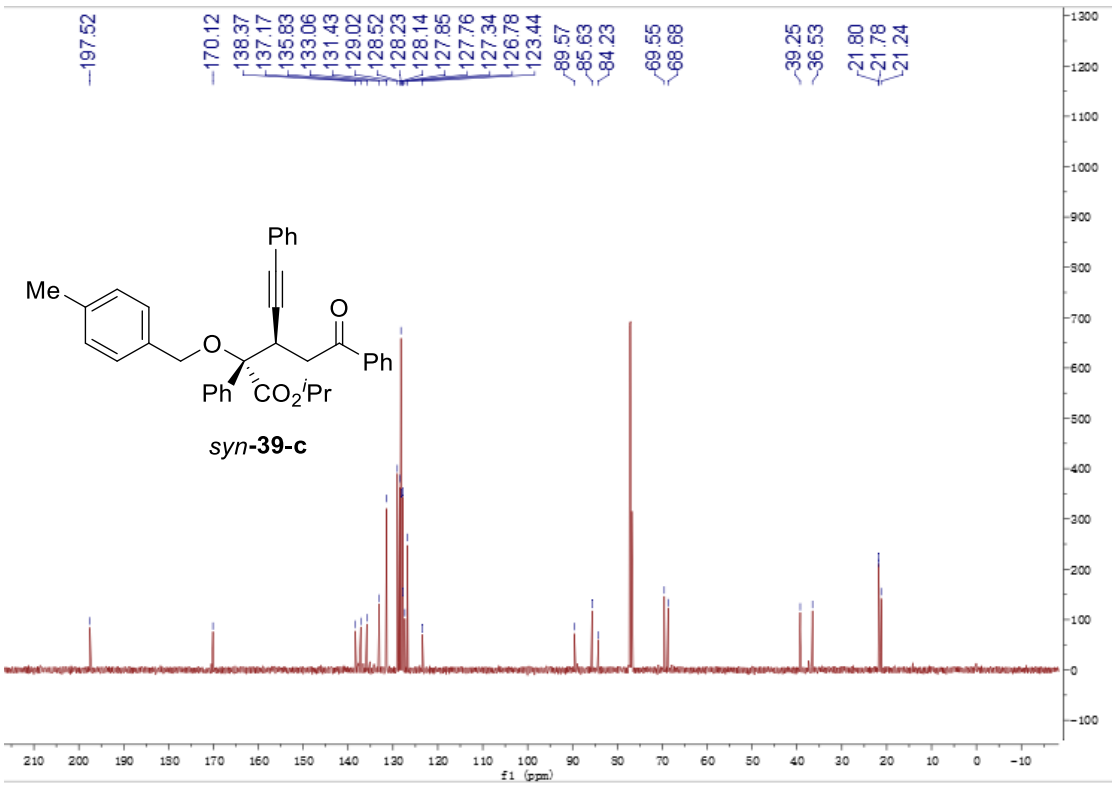

**39**


Me
Ph
O
Ph
Ph
CO2Et
+
syn-39-b(major)
anti-39-b(minor)

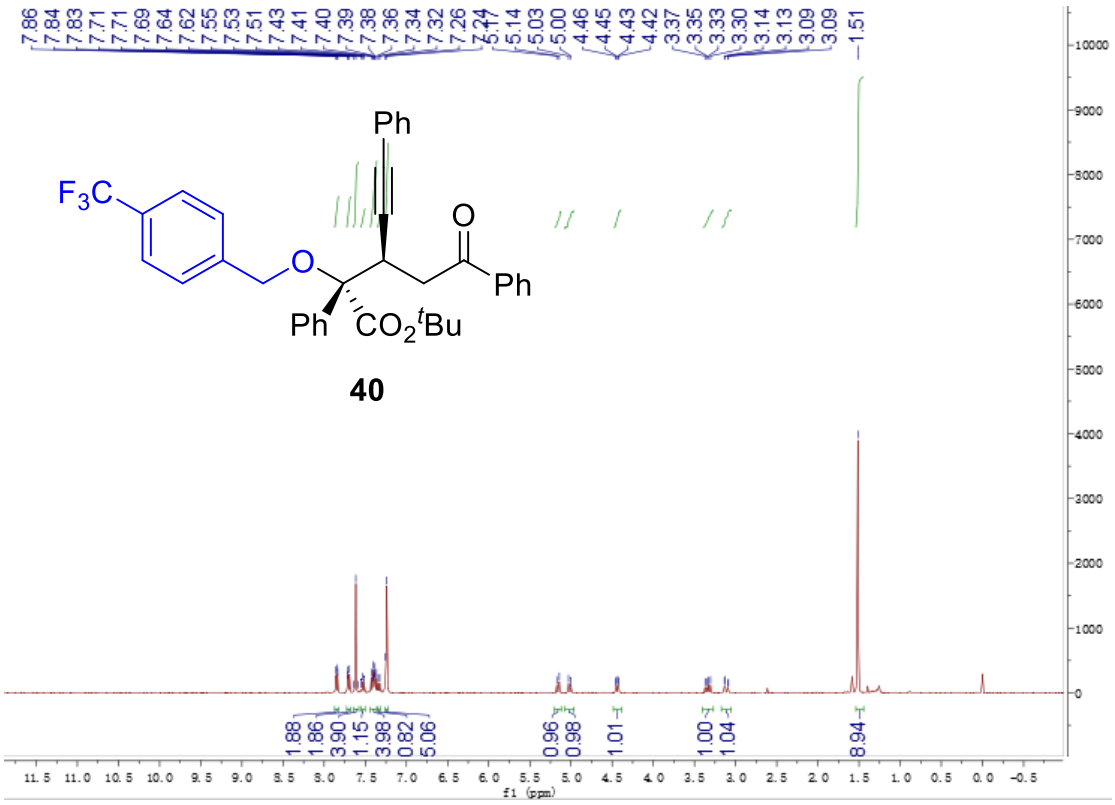

Me
Ph
O
Ph
Ph
CO2Et
+
syn-39-b(major)
anti-39-b(minor)

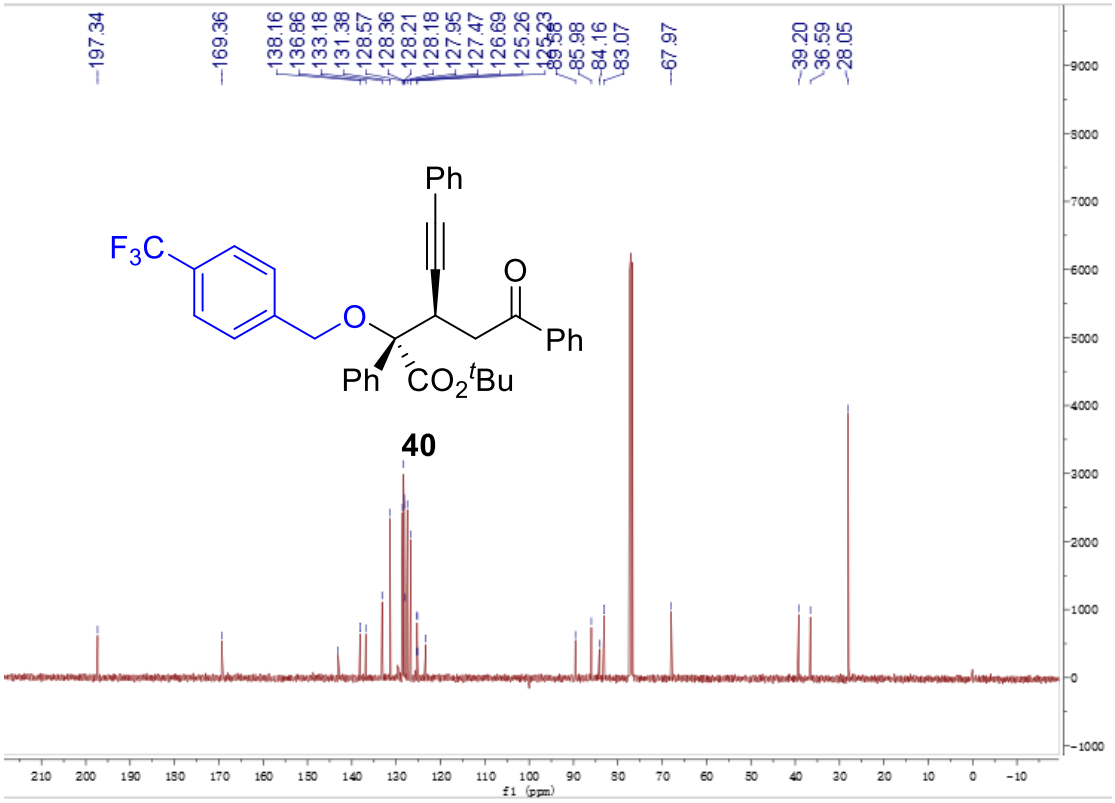


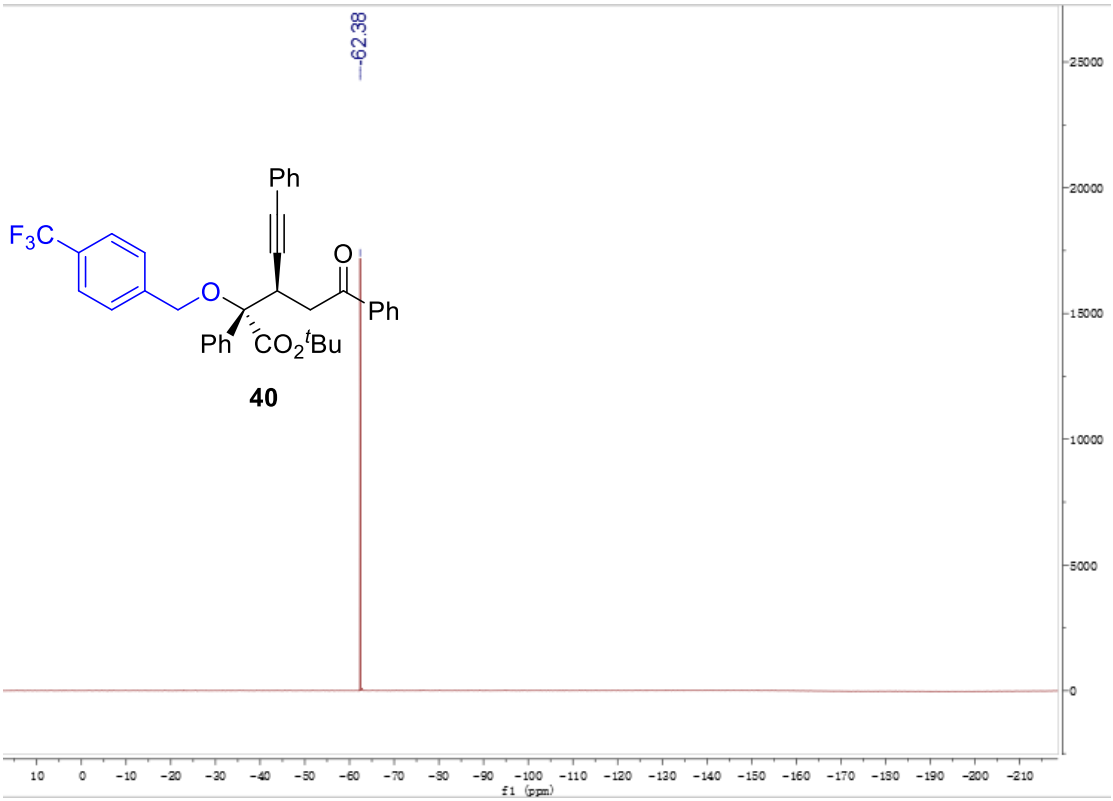

*syn*-**39-c**

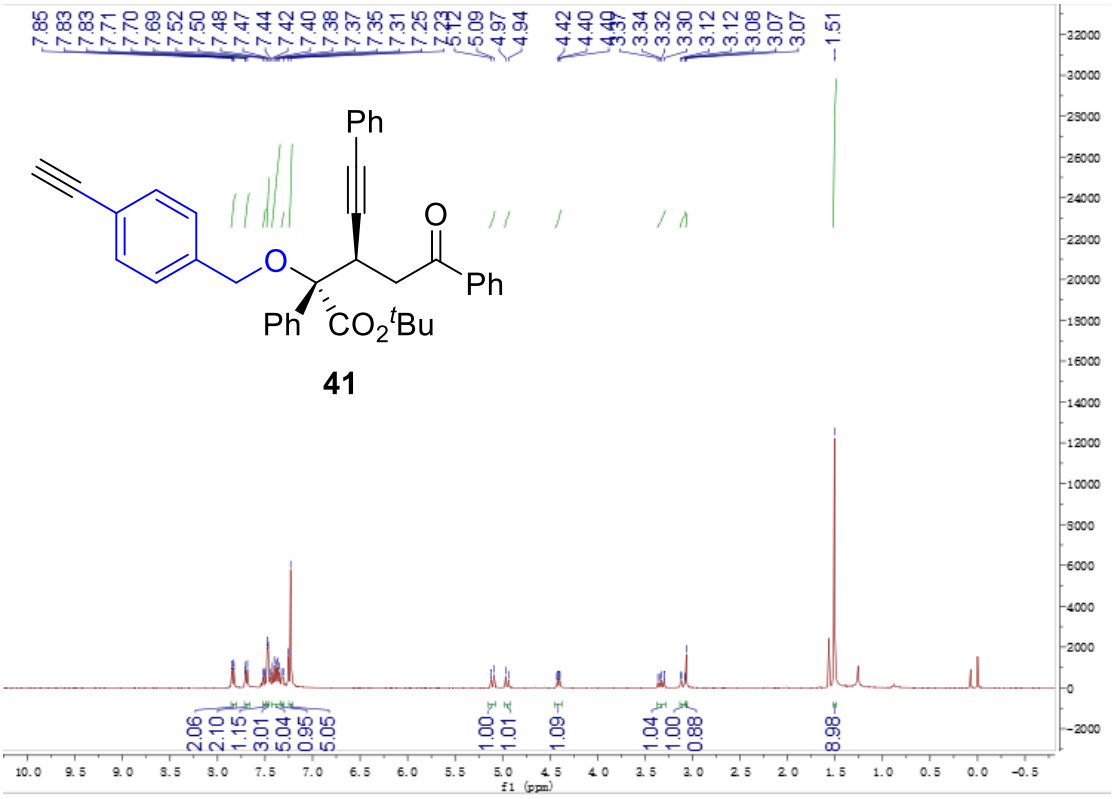


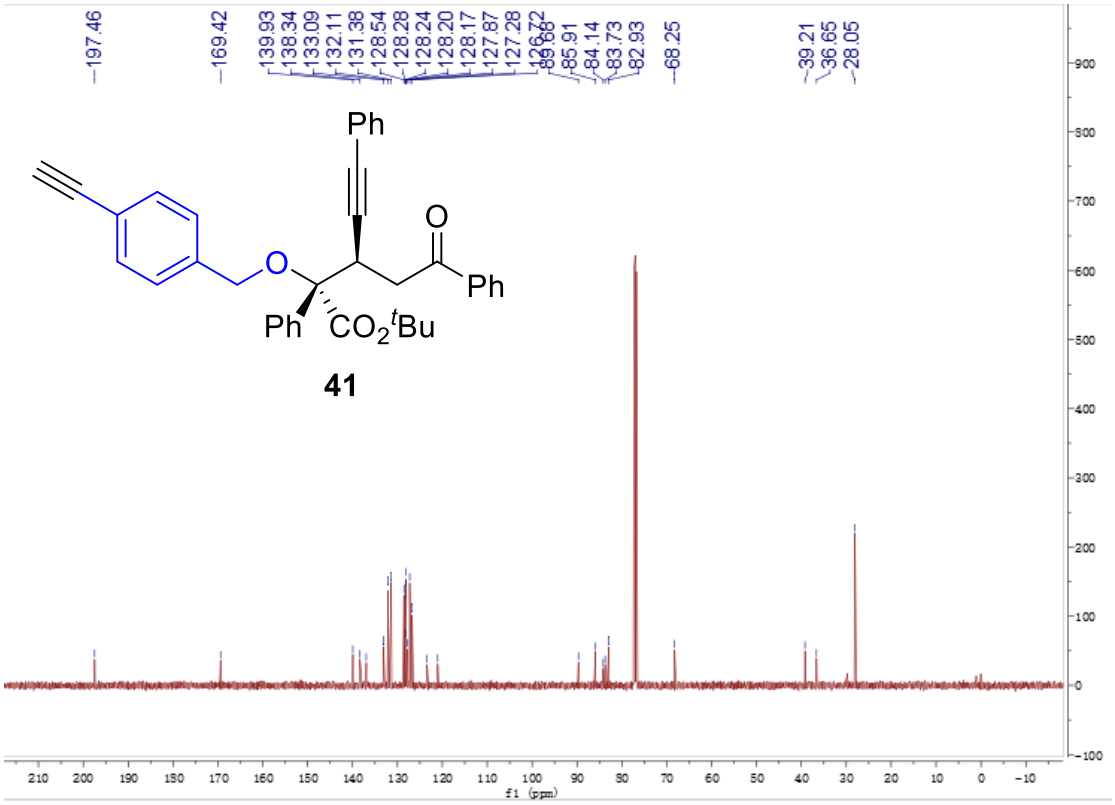

*syn*-**39-c**

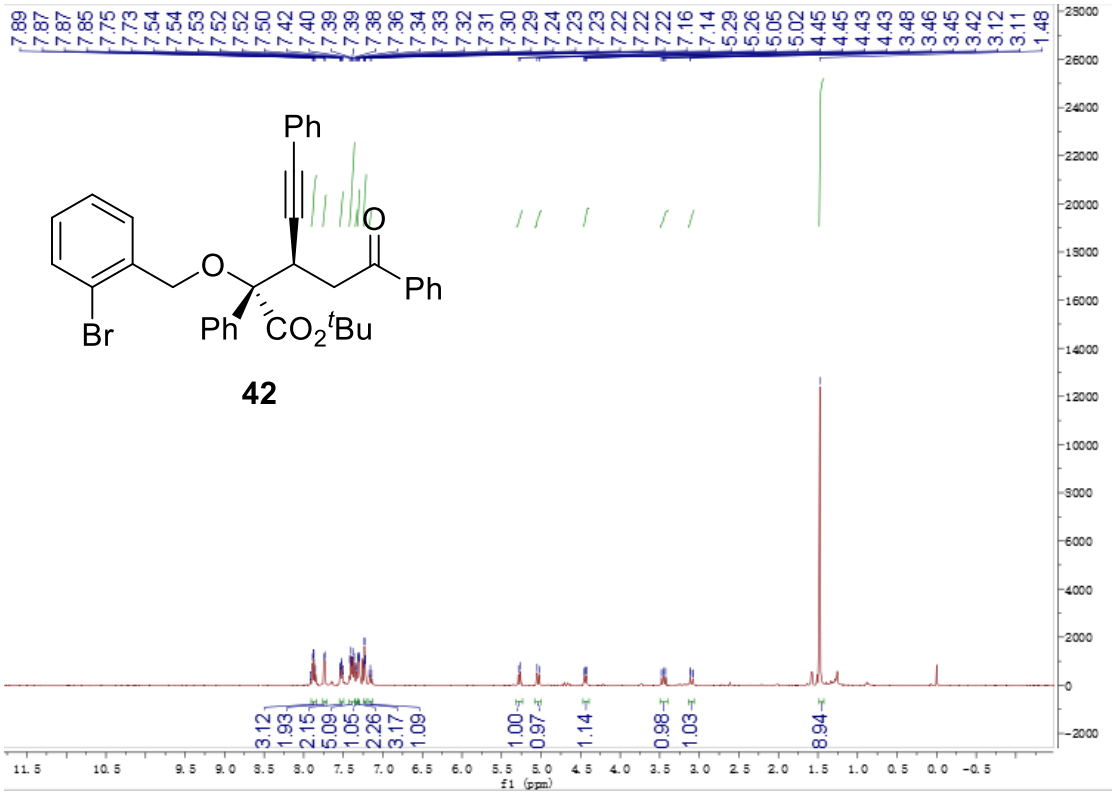

Ph
F3C
O
O
Ph
Ph
CO2tBu
40

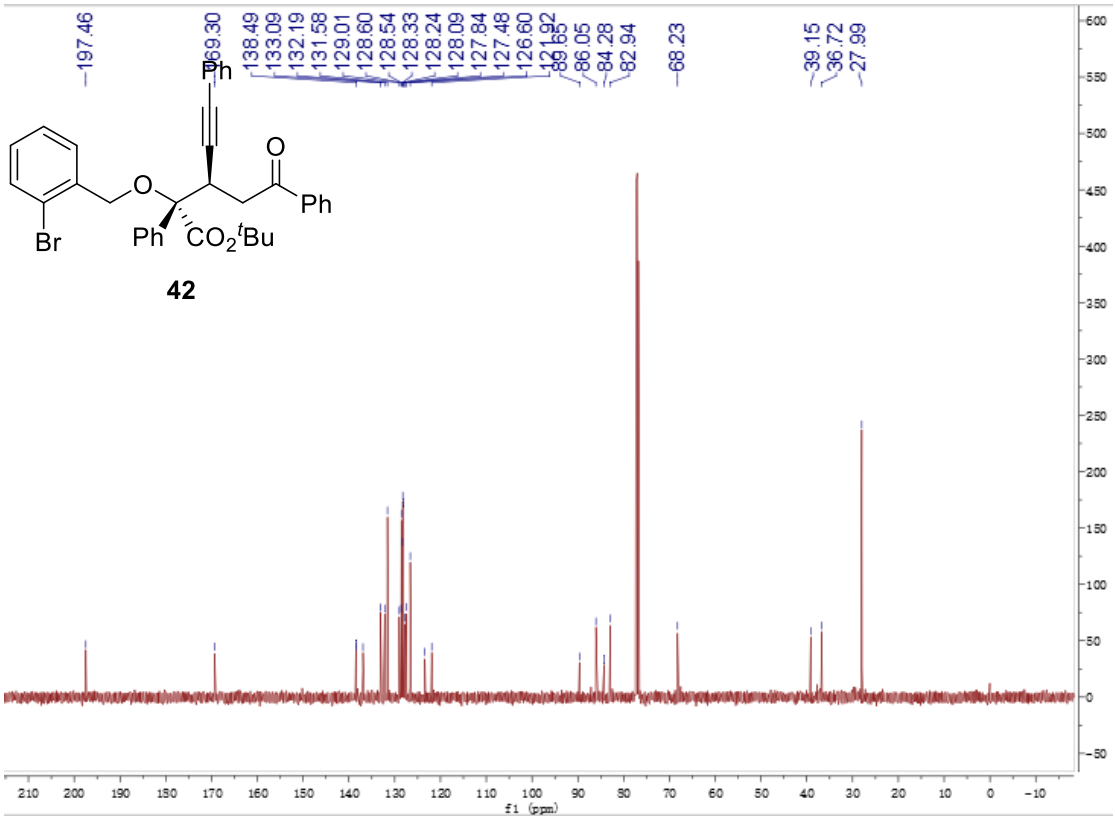

Ph
F3C
O
O
Ph
Ph
CO2tBu
40


-62.38
Ph
F3C
O
O
Ph
Ph
CO2tBu
40

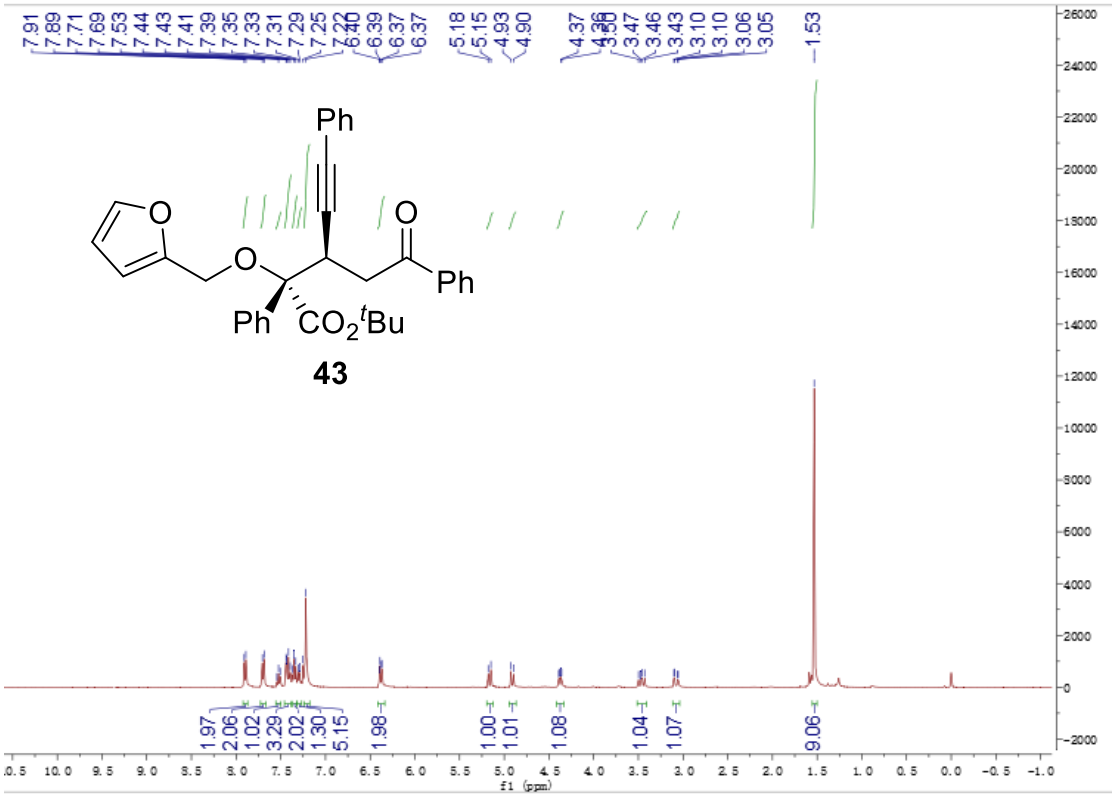

7.85
7.83
7.83
7.71
7.70
7.69
7.52
7.50
7.48
7.47
7.44
7.42
7.40
7.38
7.37
7.35
7.31
7.25
5.12
5.09
4.97
4.94
4.42
4.40
3.37
3.34
3.32
3.30
3.12
3.12
3.08
3.07
3.07
1.51
Ph
O
O
Ph
Ph
CO2tBu
41
2.06
2.10
1.15
3.01
5.04
0.95
5.05
1.00
1.01
1.09
1.04
1.00
0.88
8.98


197.46
169.42
139.93
138.34
133.09
132.11
131.38
128.54
128.28
128.24
128.20
128.17
127.87
127.28
126.72
89.68
85.91
84.14
83.73
82.93
68.25
39.21
36.65
28.05
Ph
O
Ph
O
Ph
CO2tBu
41

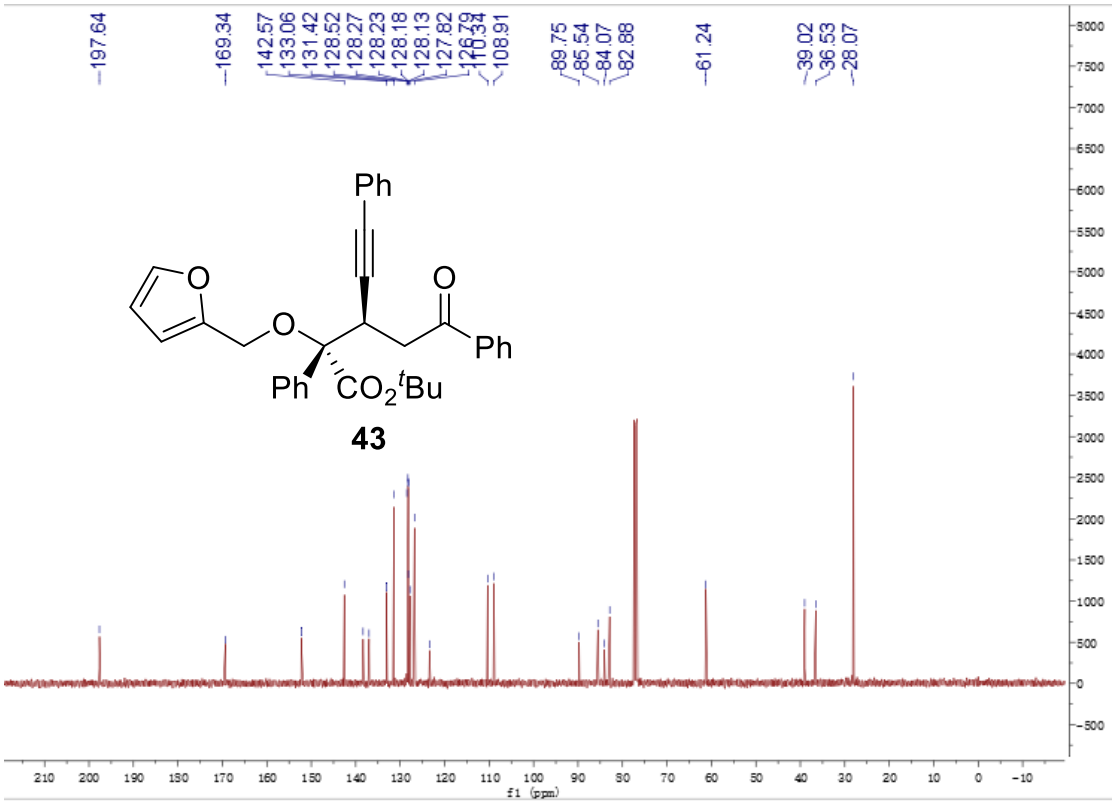

7.89
7.87
7.87
7.85
7.75
7.73
7.54
7.54
7.53
7.52
7.52
7.50
7.42
7.40
7.39
7.39
7.38
7.36
7.34
7.33
7.32
7.31
7.30
7.29
7.24
7.23
7.23
7.22
7.22
7.22
7.16
7.14
5.29
5.26
5.05
5.02
4.45
4.45
4.43
4.43
3.48
3.46
3.45
3.42
3.12
3.11
1.48
Ph
O
O
Ph
Br
Ph
CO2tBu
42

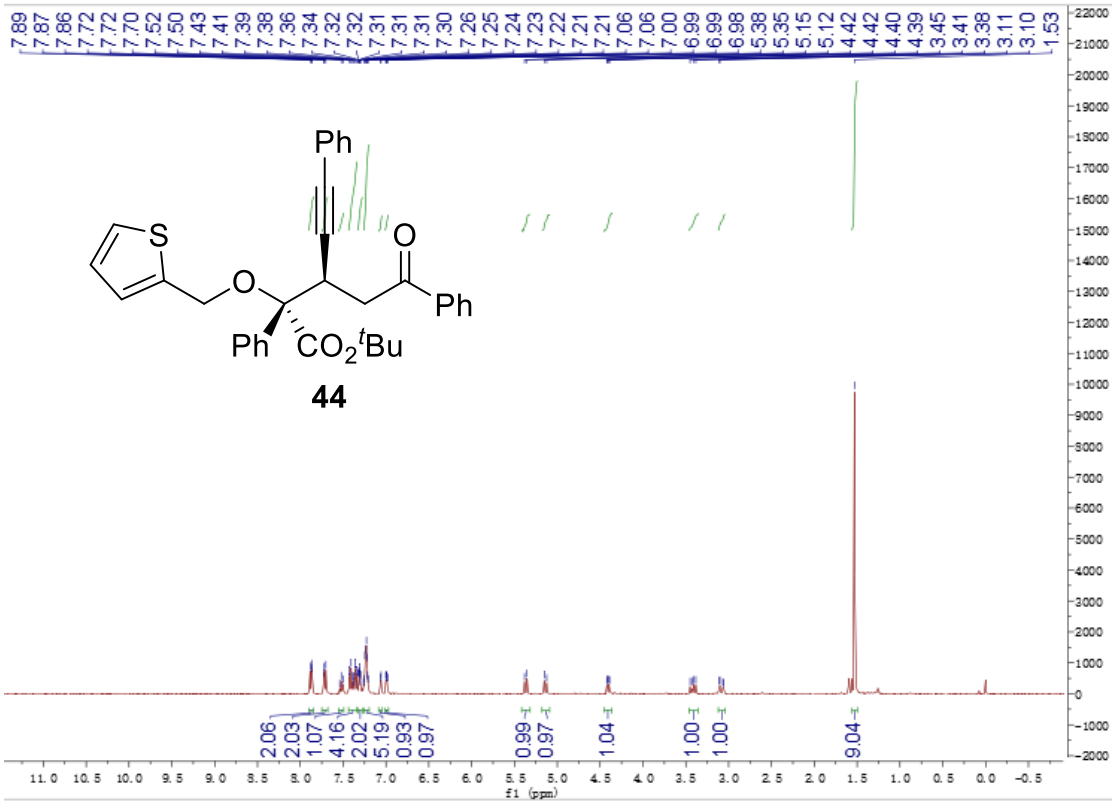

197.46
169.30
138.49
133.09
132.19
131.58
129.01
128.60
128.54
128.33
128.24
128.09
127.84
127.48
126.60
121.92
89.65
86.05
84.28
82.94
68.23
39.15
36.72
27.99
Ph
O
Ph
O
Br
Ph
CO2tBu
f1 (ppm)

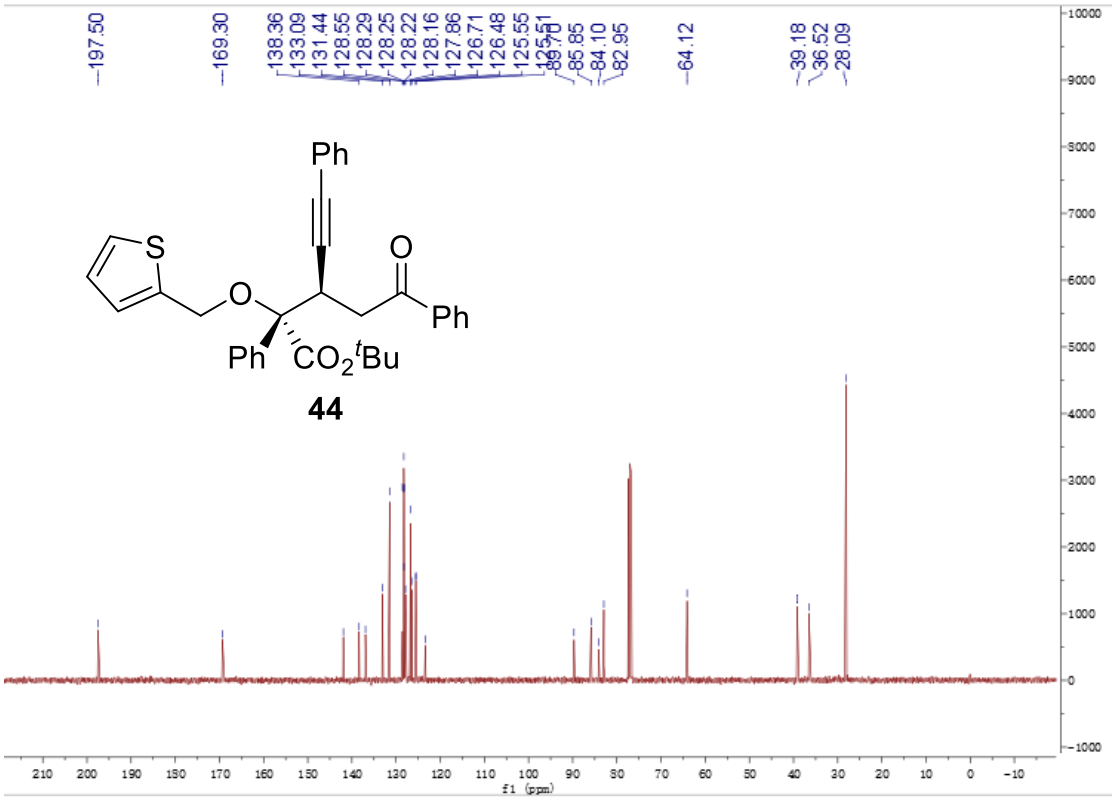
**42**


7.91
7.89
7.71
7.69
7.53
7.44
7.43
7.41
7.39
7.35
7.33
7.31
7.29
7.25
6.39
6.37
6.37
5.18
5.15
4.93
4.90
4.37
3.47
3.46
3.43
3.10
3.06
3.05
1.53
Ph
O
O
Ph
Ph
CO2tBu
1.97
2.06
1.02
3.29
2.02
1.30
5.15
1.98
1.00
1.01
1.08
1.04
1.07
9.06
f1 (ppm)

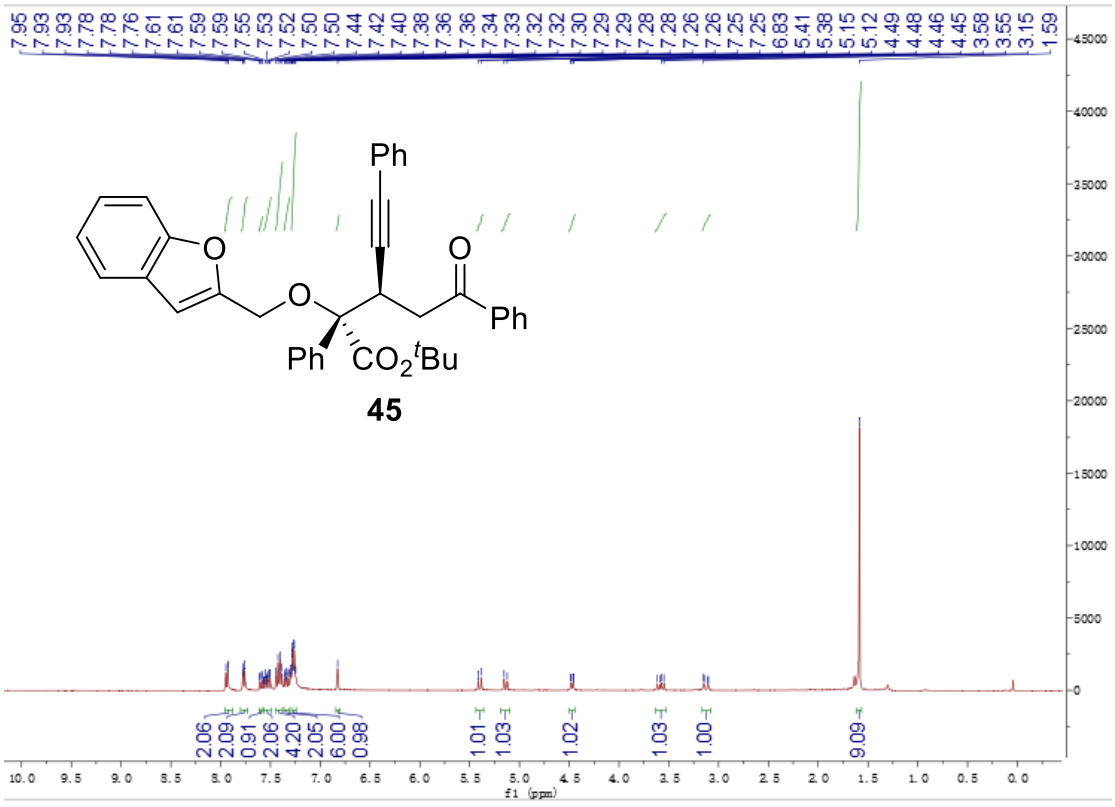
**43**


197.64
169.34
142.57
133.06
131.42
128.52
128.27
128.23
128.18
128.13
127.82
126.79
110.34
108.91
89.75
85.54
84.07
82.88
61.24
39.02
36.53
28.07
Ph
O
O
O
Ph
Ph
CO2tBu
43

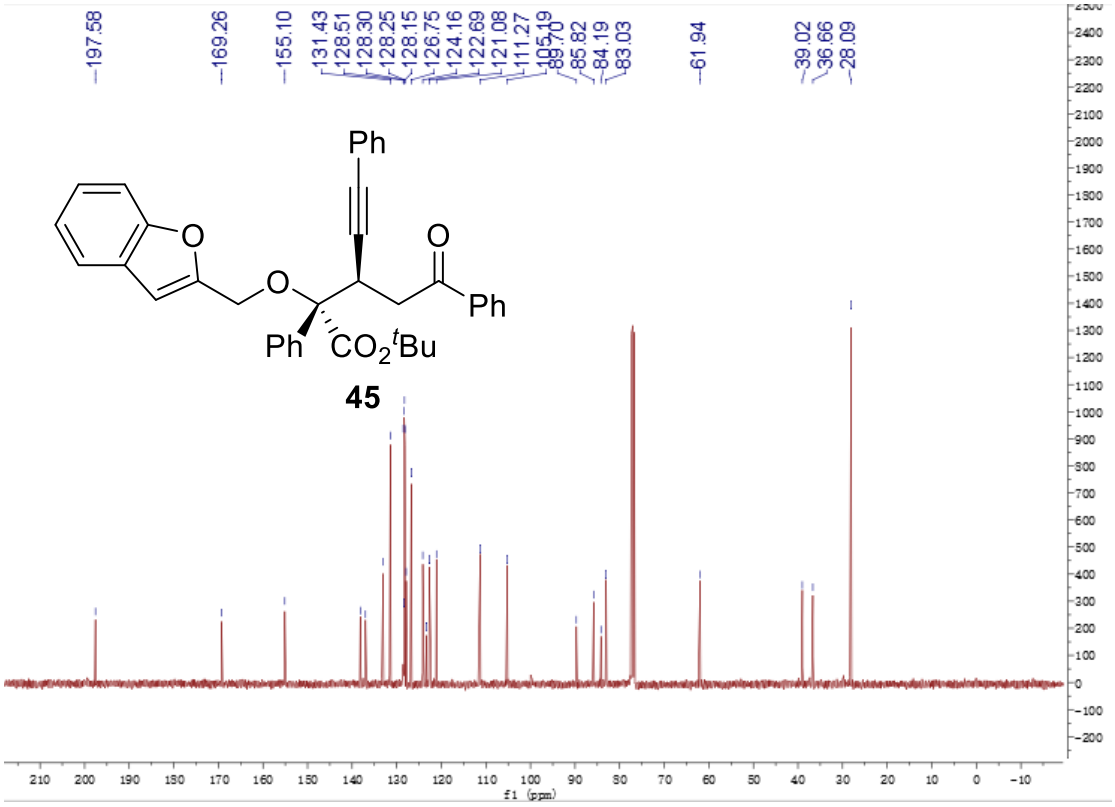

7.89
7.87
7.86
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7.72
7.70
7.52
7.50
7.43
7.41
7.39
7.38
7.36
7.34
7.32
7.32
7.31
7.31
7.31
7.30
7.26
7.25
7.24
7.23
7.22
7.21
7.21
7.06
7.06
7.00
6.99
6.99
6.98
5.38
5.35
5.15
5.12
4.42
4.42
4.40
4.39
3.45
3.41
3.38
3.11
3.10
1.53
Ph
S
O
O
Ph
Ph
CO2tBu
44
2.06
2.03
1.07
4.16
2.02
5.19
0.93
0.97
0.99
0.97
1.04
1.00
1.00
9.04

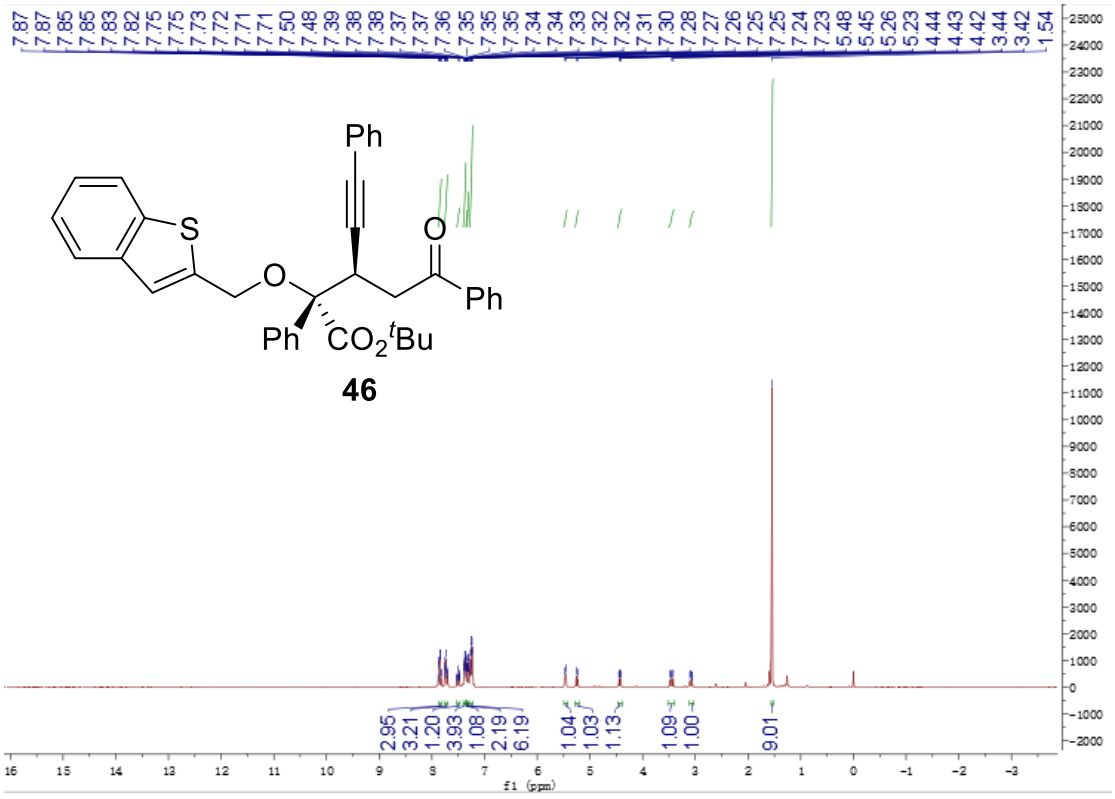

197.50
169.30
138.36
133.09
131.44
128.55
128.29
128.25
128.22
128.16
127.86
126.71
126.48
125.55
125.51
89.70
85.85
84.10
82.95
64.12
39.18
36.52
28.09
Ph
S
O
O
Ph
Ph
CO2tBu
f1 (ppm)

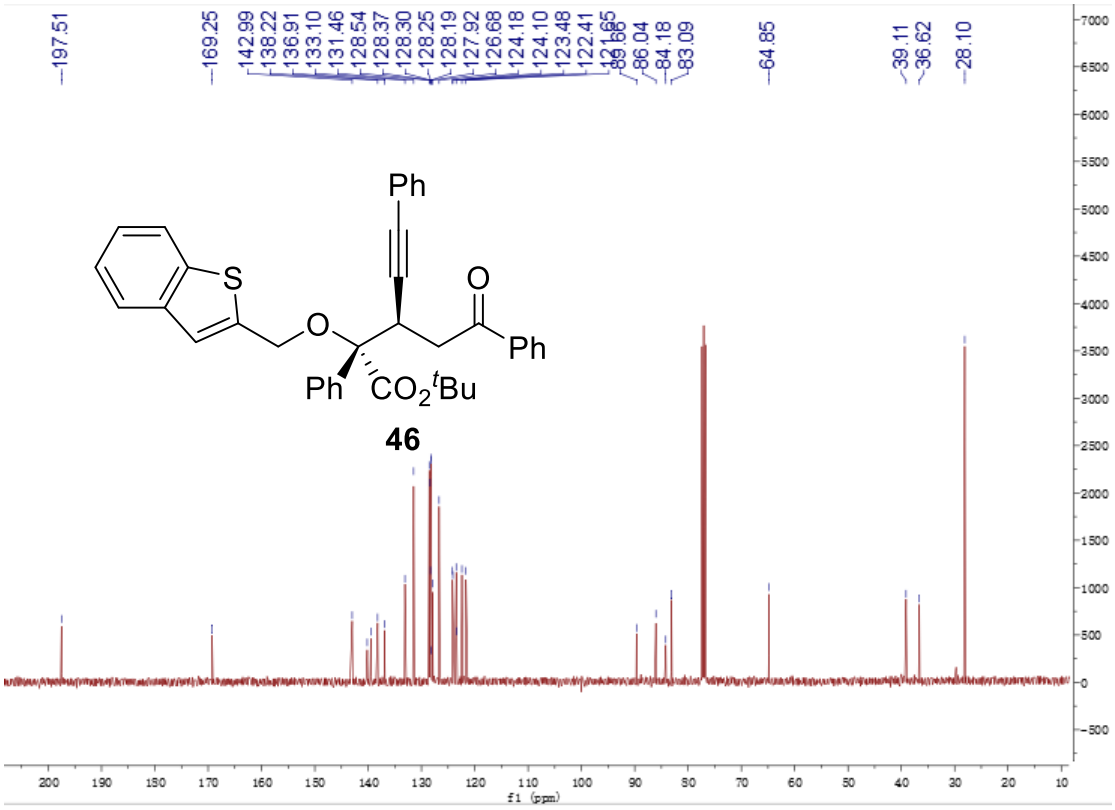
**44**


7.95
7.93
7.93
7.78
7.78
7.76
7.61
7.61
7.59
7.59
7.55
7.53
7.52
7.50
7.50
7.44
7.42
7.40
7.38
7.36
7.36
7.34
7.33
7.32
7.32
7.30
7.29
7.29
7.28
7.28
7.26
7.26
7.25
7.25
6.83
5.41
5.38
5.15
5.12
4.49
4.48
4.46
4.45
3.58
3.55
3.15
1.59
Ph
O
O
O
Ph
Ph
CO2tBu
2.06
2.09
0.91
2.06
4.20
2.05
6.00
0.98
1.01
1.03
1.02
1.03
1.00
9.09
f1 (ppm)

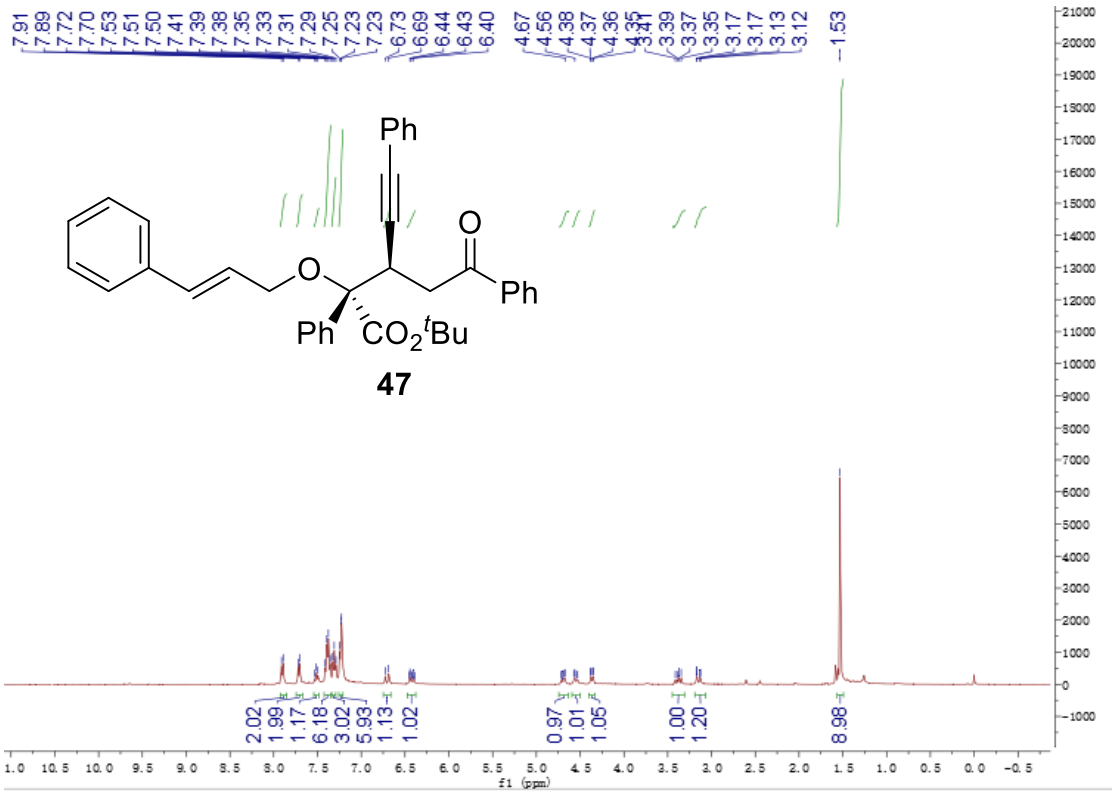
**45**


197.58
169.26
155.10
131.43
128.51
128.30
128.25
128.15
126.75
124.16
122.69
121.08
111.27
105.19
89.70
85.82
84.19
83.03
61.94
39.02
36.66
28.09
Ph
O
O
O
Ph
Ph
CO2tBu
45

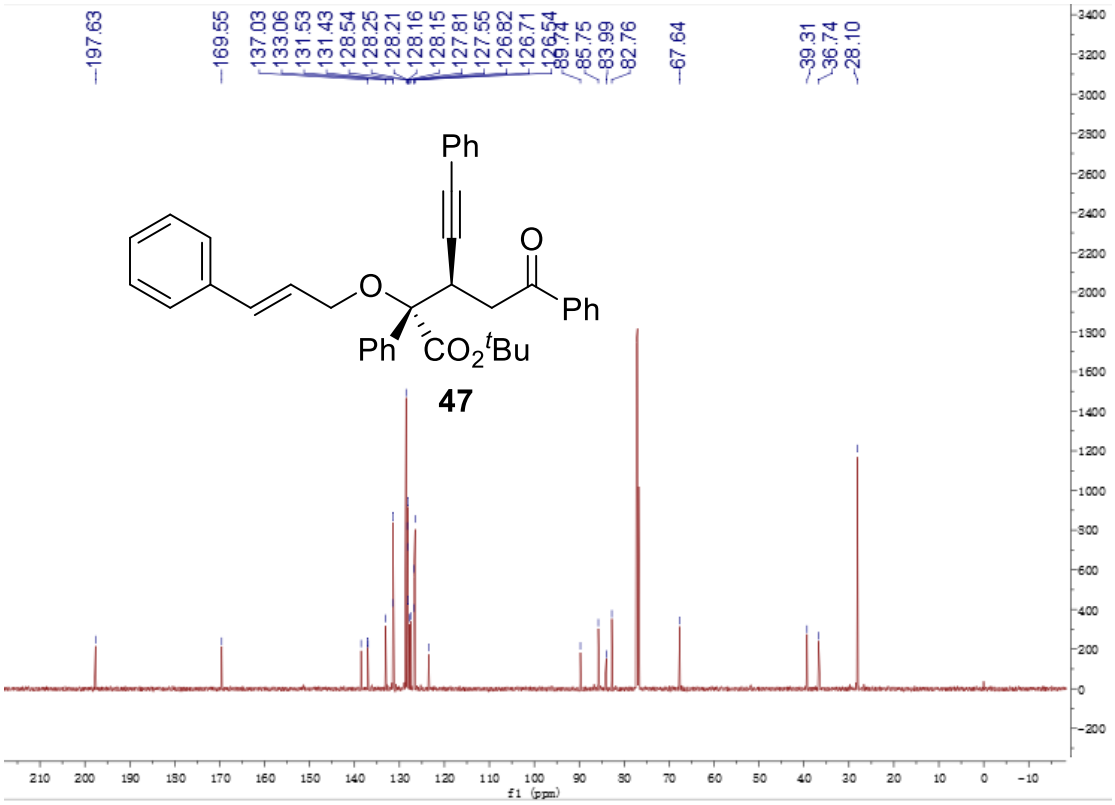

7.87
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7.85
7.85
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7.82
7.75
7.75
7.73
7.72
7.71
7.71
7.50
7.48
7.39
7.38
7.38
7.37
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7.26
7.25
7.25
7.24
7.23
5.48
5.45
5.26
5.23
4.44
4.43
4.42
3.44
3.42
1.54
Ph
S
O
O
Ph
Ph
CO2tBu
46
2.95
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1.08
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6.19
1.04
1.03
1.13
1.09
1.00
9.01

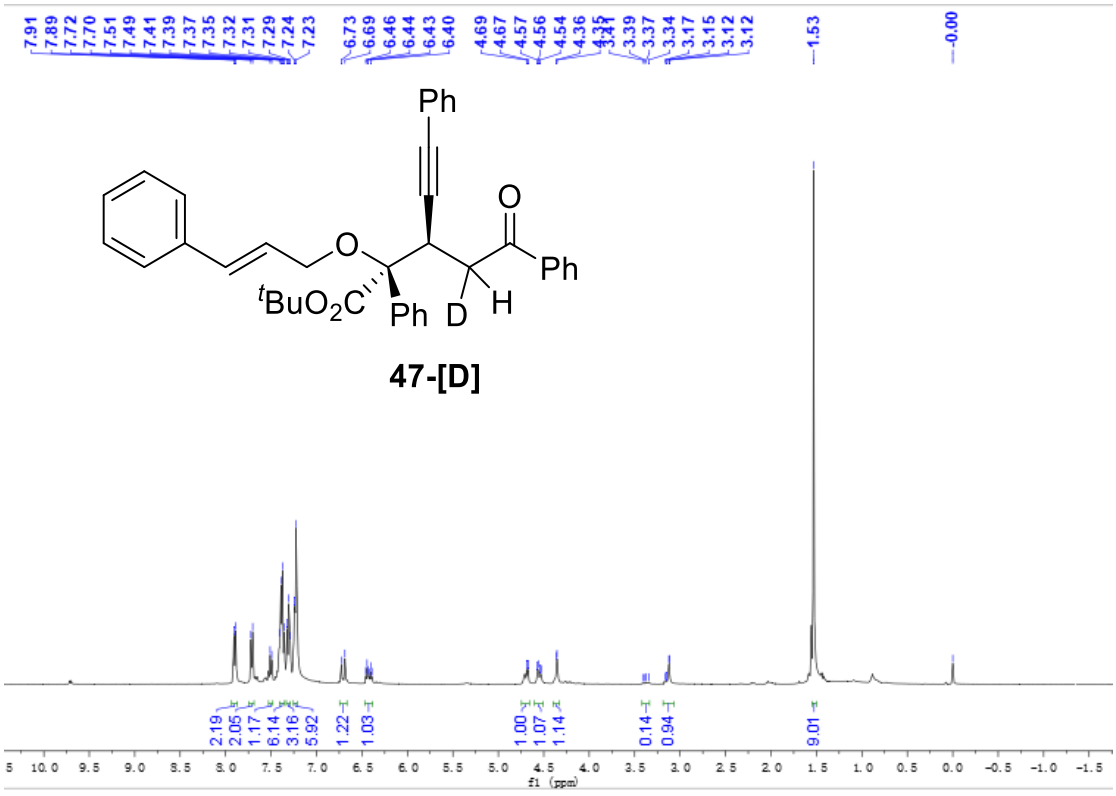

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131.46
128.54
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128.30
128.25
128.19
127.92
126.68
124.18
124.10
123.48
122.41
89.68
86.04
84.18
83.09
64.85
39.11
36.62
28.10
Ph
S
O
O
Ph
Ph
CO2tBu
f1 (ppm)

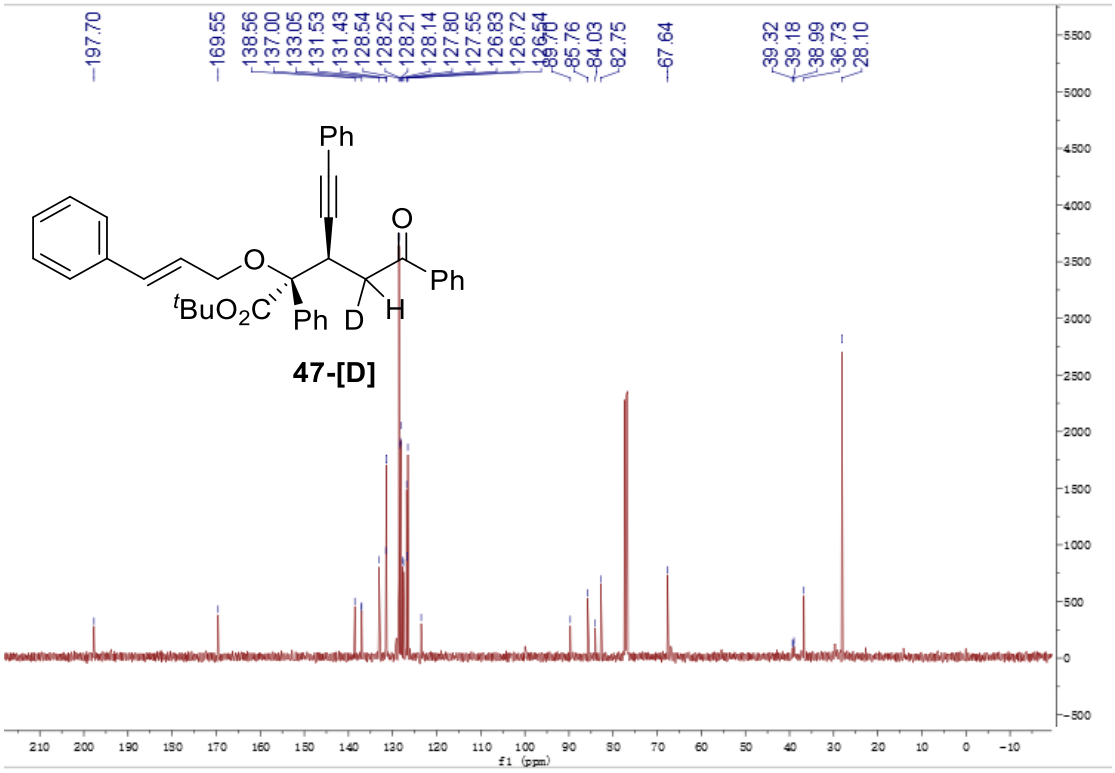
**46**

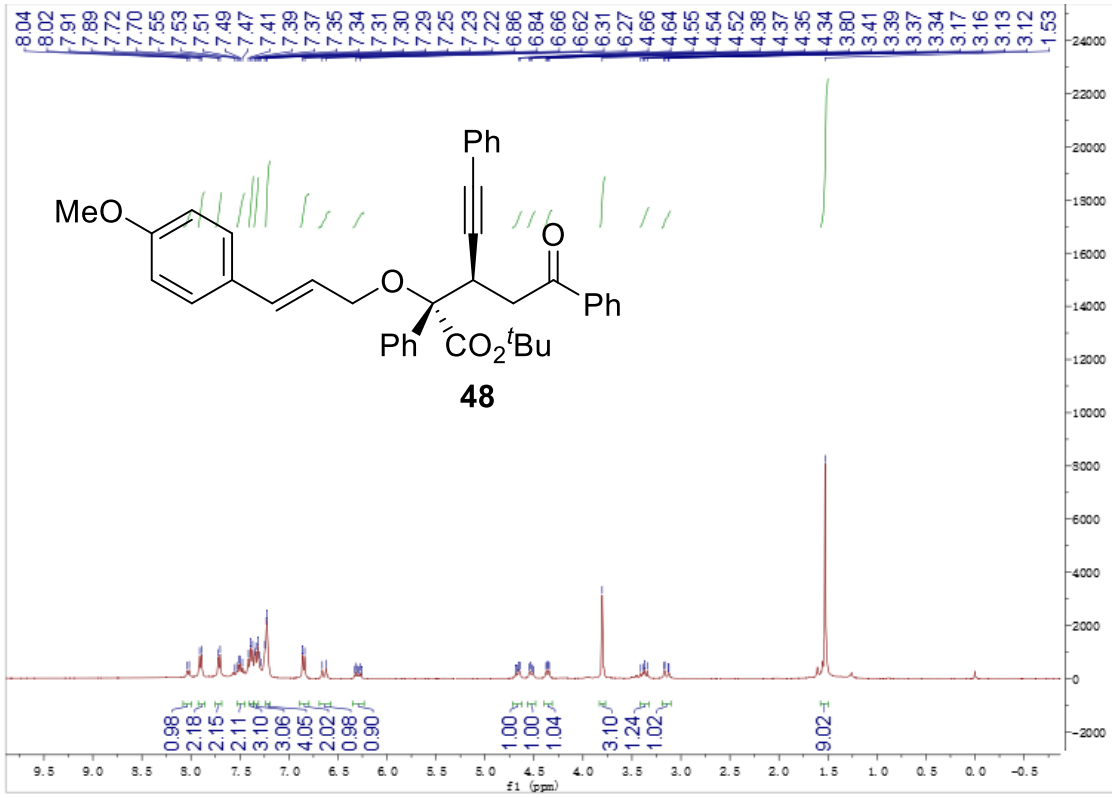

7.91
7.89
7.72
7.70
7.53
7.51
7.50
7.41
7.39
7.38
7.35
7.33
7.31
7.29
7.25
7.23
7.23
6.73
6.69
6.44
6.43
6.40
4.67
4.56
4.38
4.37
4.36
4.35
4.34
3.39
3.37
3.35
3.17
3.17
3.13
3.12
1.53
Ph
O
O
Ph
Ph
CO2tBu
2.02
1.99
1.17
6.18
3.02
5.93
1.13
1.02
0.97
1.01
1.05
1.00
1.20
8.98
f1 (ppm)

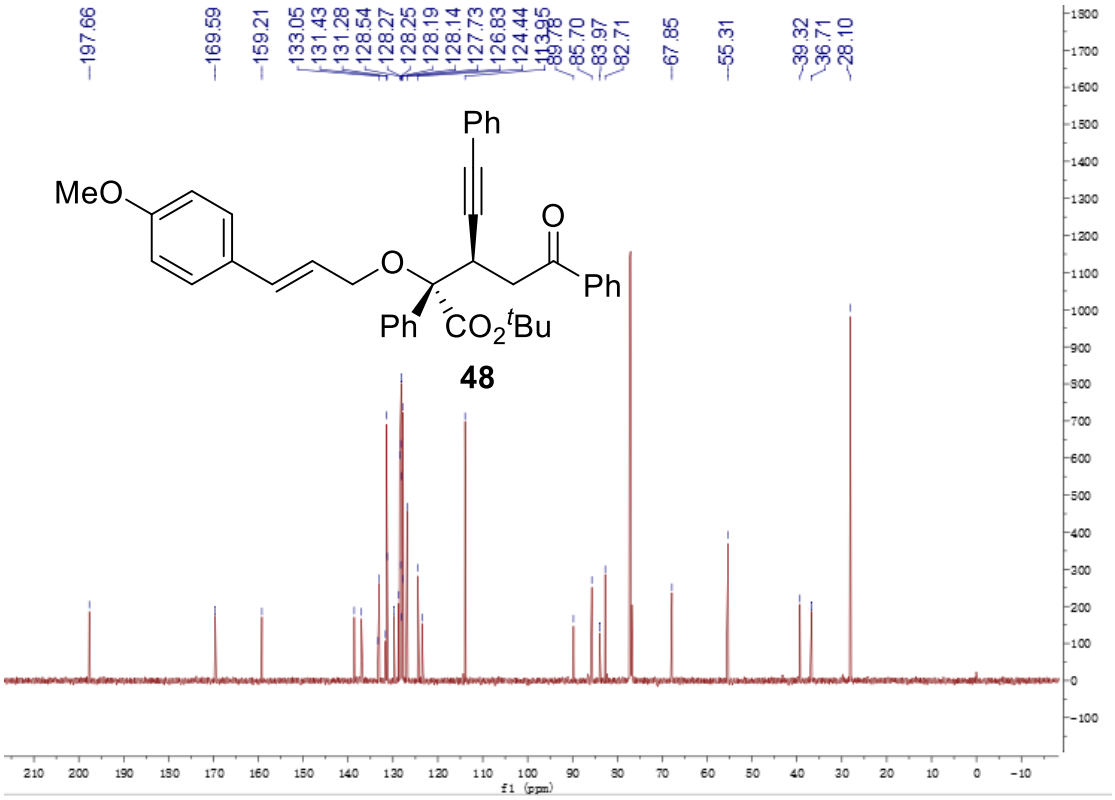
**47**

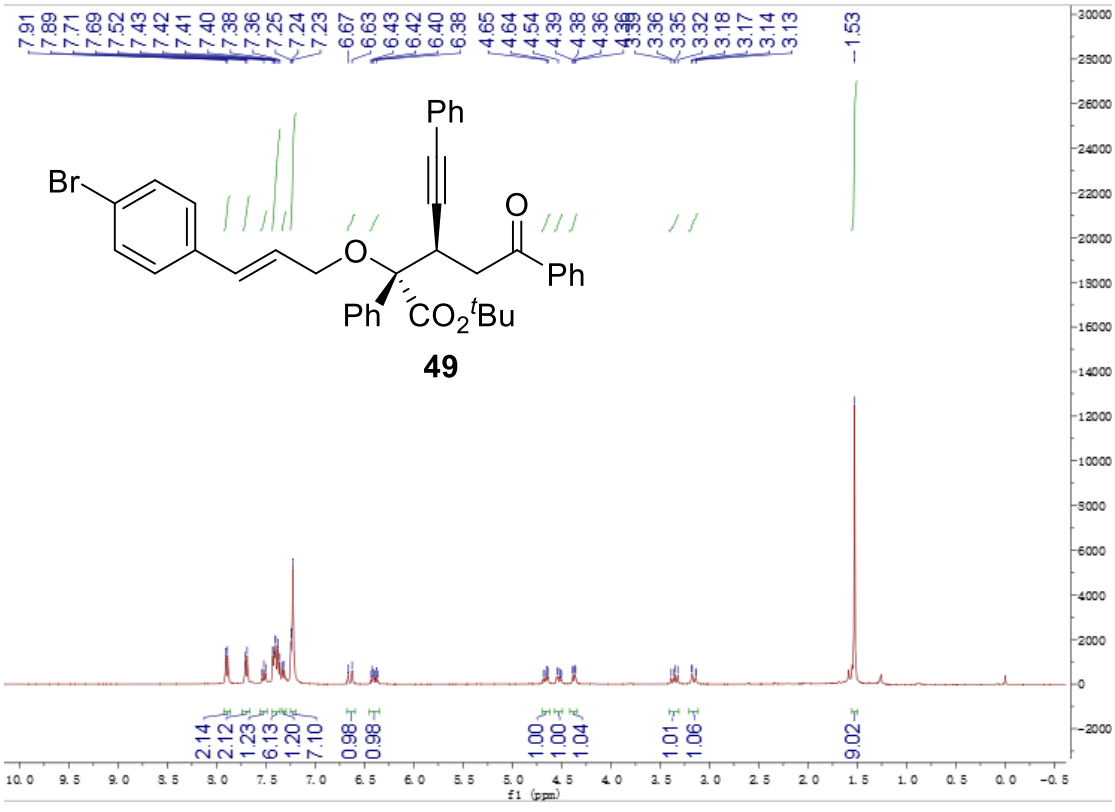

197.63
169.55
137.03
133.06
131.53
131.43
128.54
128.25
128.21
128.16
128.15
127.81
127.55
126.82
126.71
126.54
89.74
85.75
83.99
82.76
67.64
39.31
36.74
28.10
Ph
O
O
Ph
Ph
CO2tBu
47

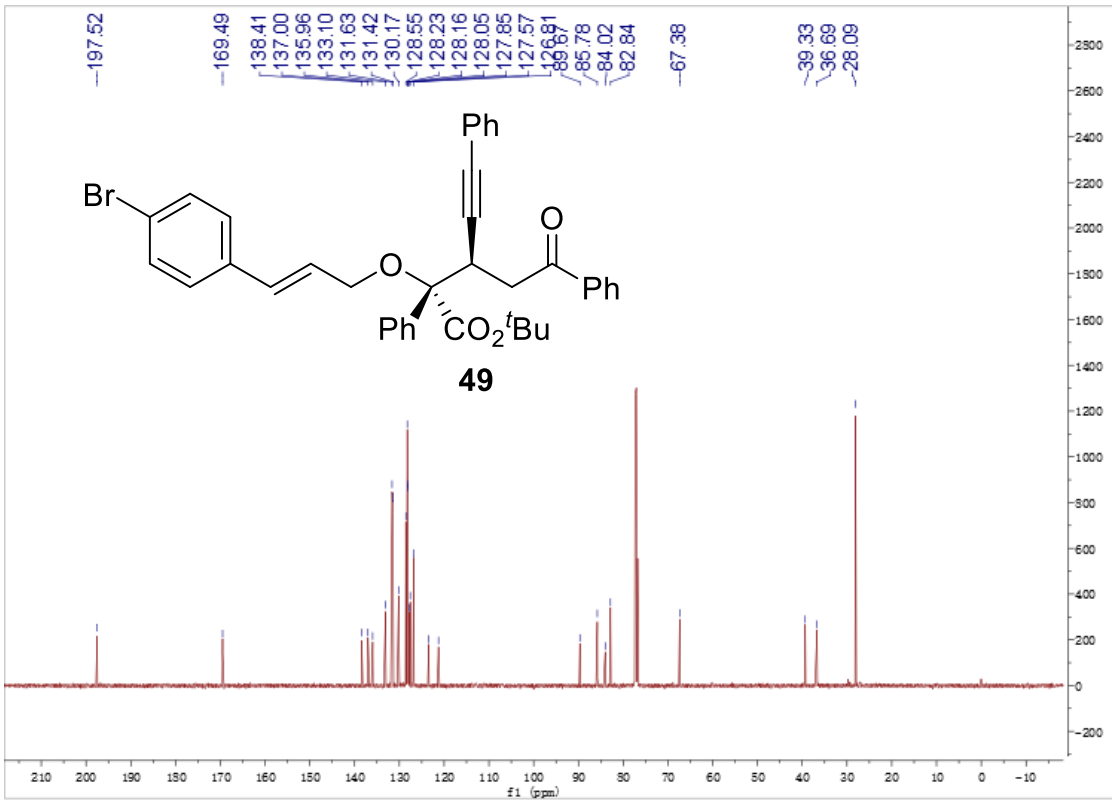

7.91
7.89
7.72
7.70
7.51
7.49
7.41
7.39
7.37
7.35
7.32
7.31
7.29
7.24
7.23
6.73
6.69
6.46
6.44
6.43
6.40
4.69
4.67
4.57
4.56
4.54
4.36
3.41
3.39
3.37
3.34
3.17
3.15
3.12
3.12
1.53
0.00
Ph
O
O
Ph
tBuO2C
Ph
D
H
47-[D]
2.19
2.05
1.17
6.14
3.16
5.92
1.22
1.03
1.00
1.07
1.14
0.14
0.94
9.01


Ph
O
Ph
O
tBuO2C
Ph
D
H
47-[D]
f1 (ppm)

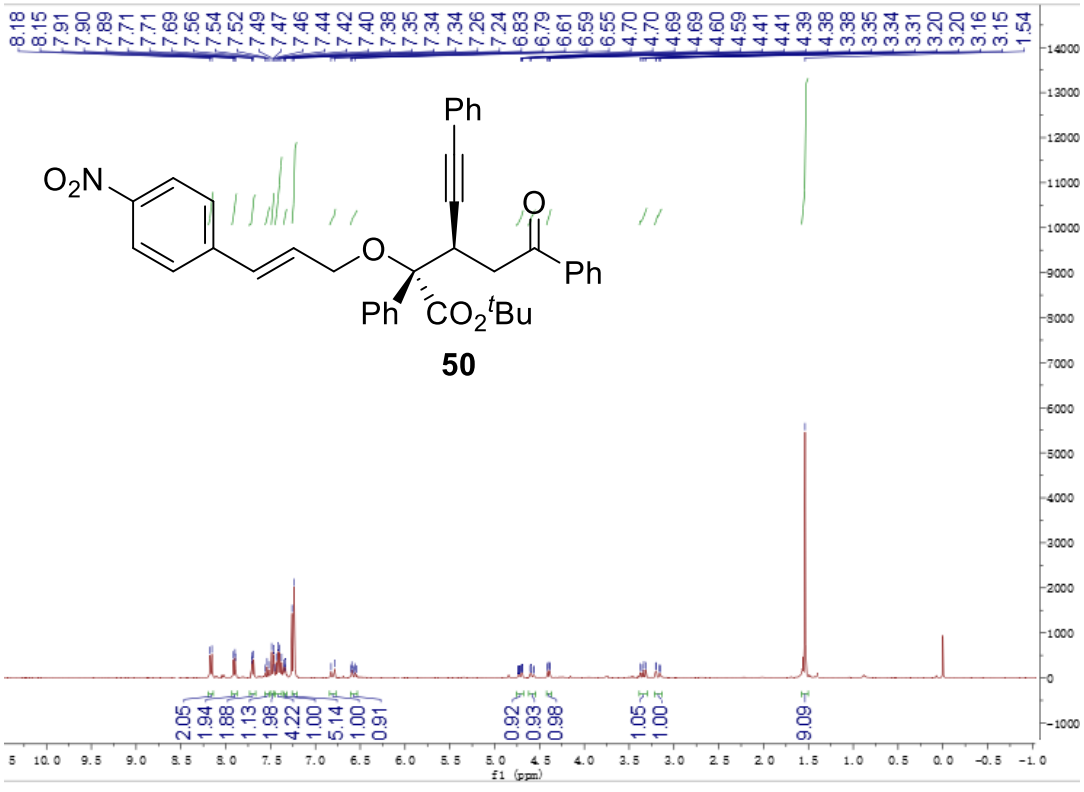

MeO
Ph
O
O
Ph
Ph
CO2tBu
48
f1 (ppm)


197.66
169.59
159.21
133.05
131.43
131.28
128.54
128.27
128.25
128.19
128.14
127.73
126.83
124.44
113.95
89.78
85.70
83.97
82.71
67.85
55.31
39.32
36.71
28.10
MeO
O
Ph
O
Ph
Ph
CO2tBu
48
f1 (ppm)

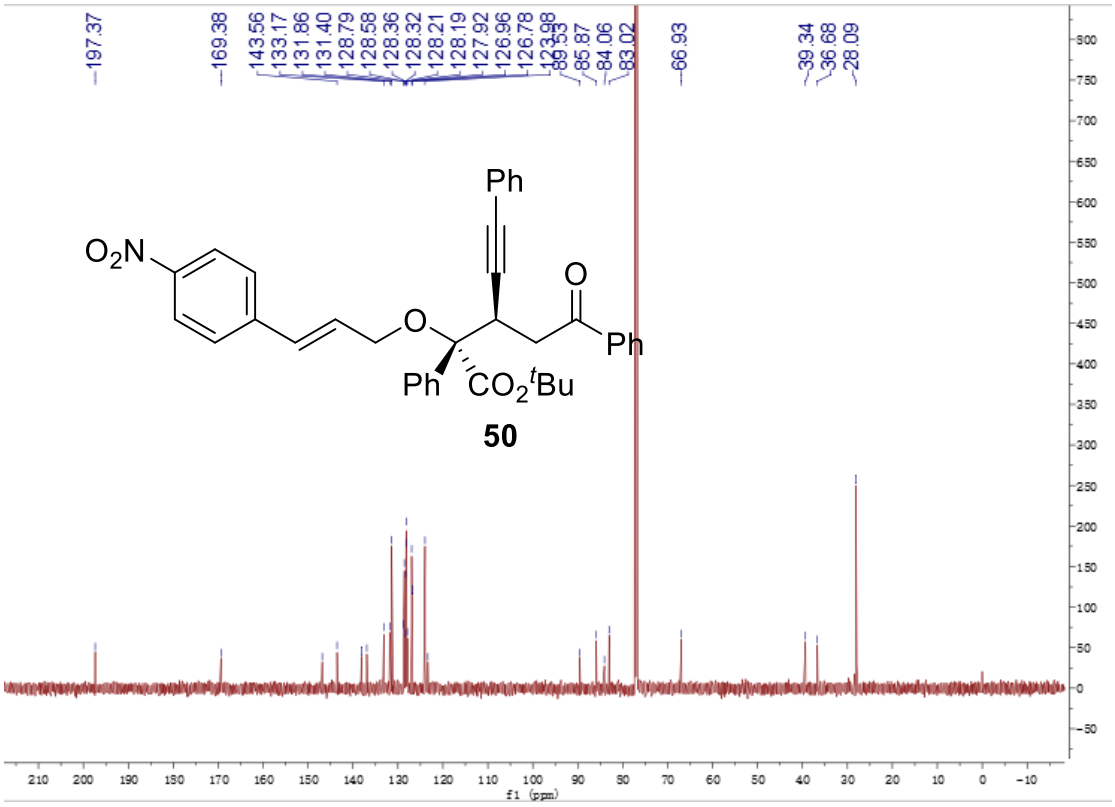

7.91
7.89
7.71
7.69
7.52
7.43
7.42
7.41
7.40
7.38
7.36
7.25
7.24
7.23
6.67
6.63
6.43
6.42
6.40
6.38
4.65
4.64
4.54
4.39
4.38
4.36
3.36
3.35
3.32
3.18
3.17
3.14
3.13
1.53
Br
Ph
O
O
Ph
Ph
CO2tBu
49
2.14
2.12
1.23
6.13
1.20
7.10
0.98
0.98
1.00
1.00
1.04
1.01
1.06
9.02
f1 (ppm)

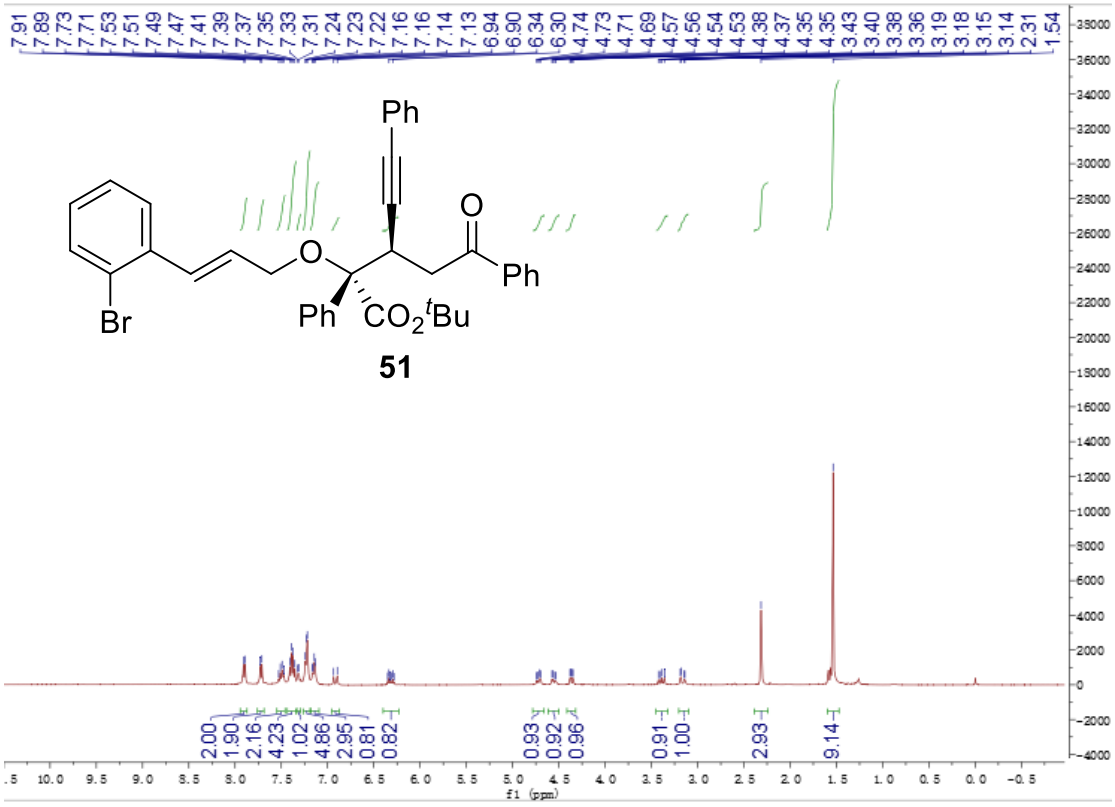


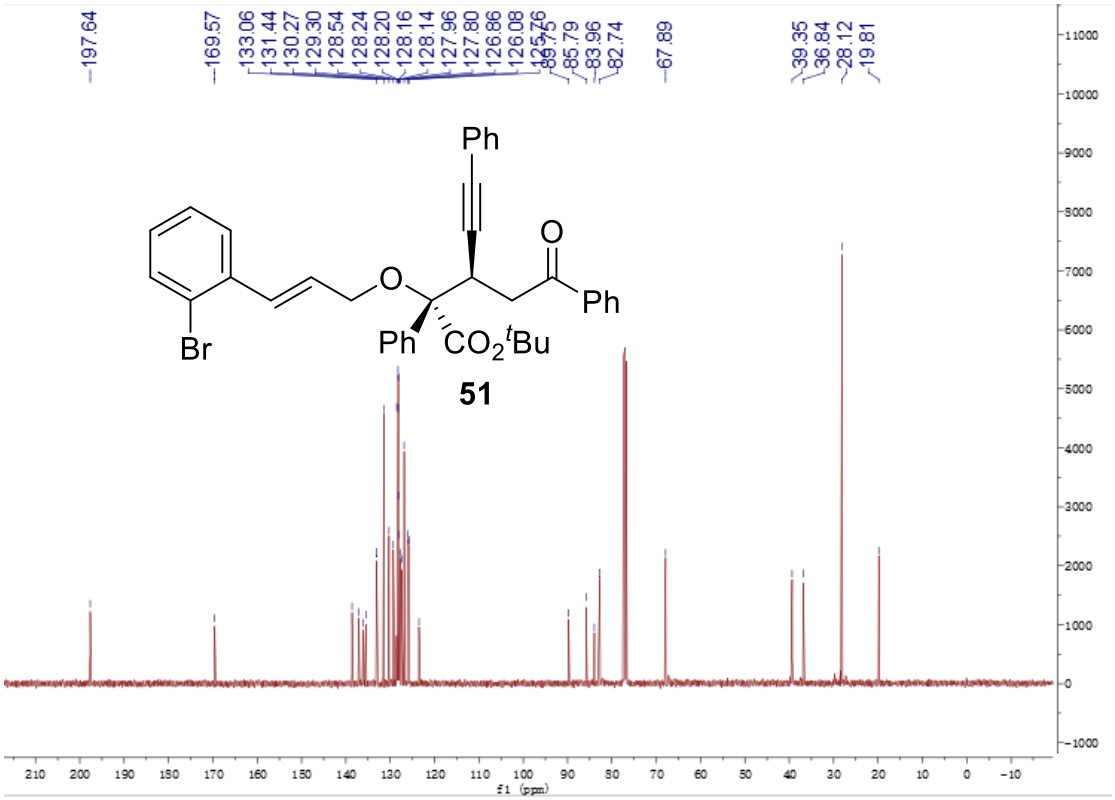

**49**

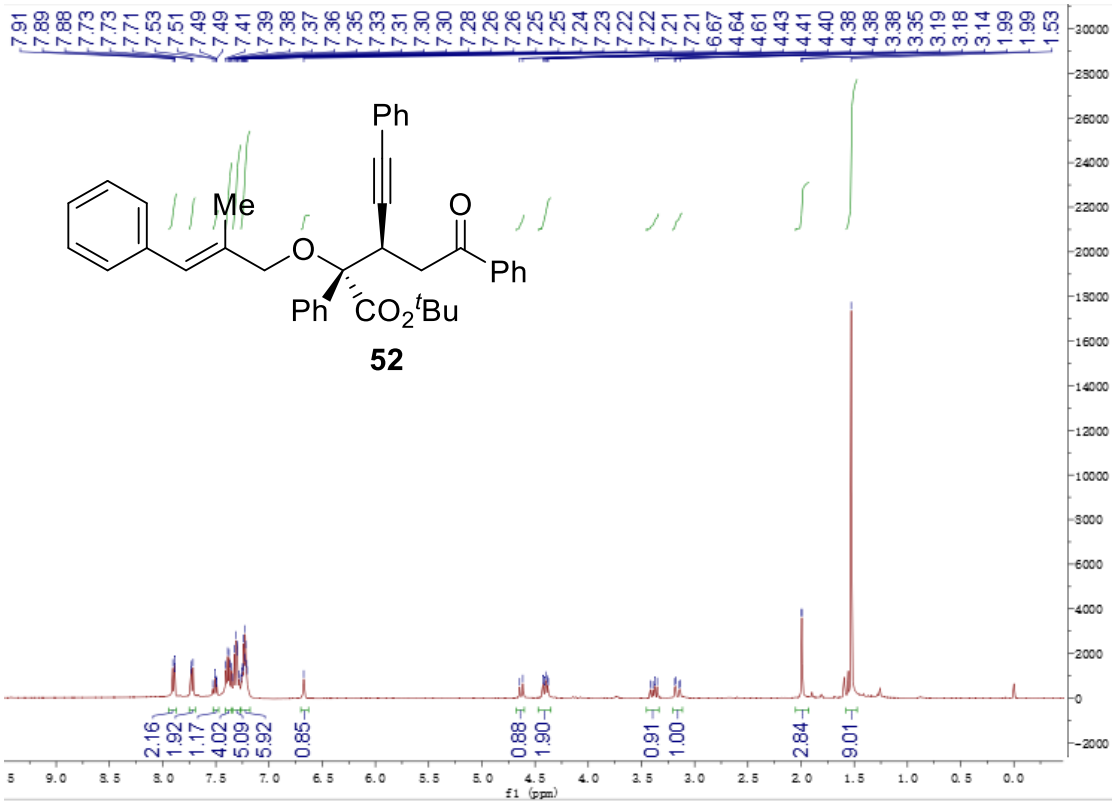


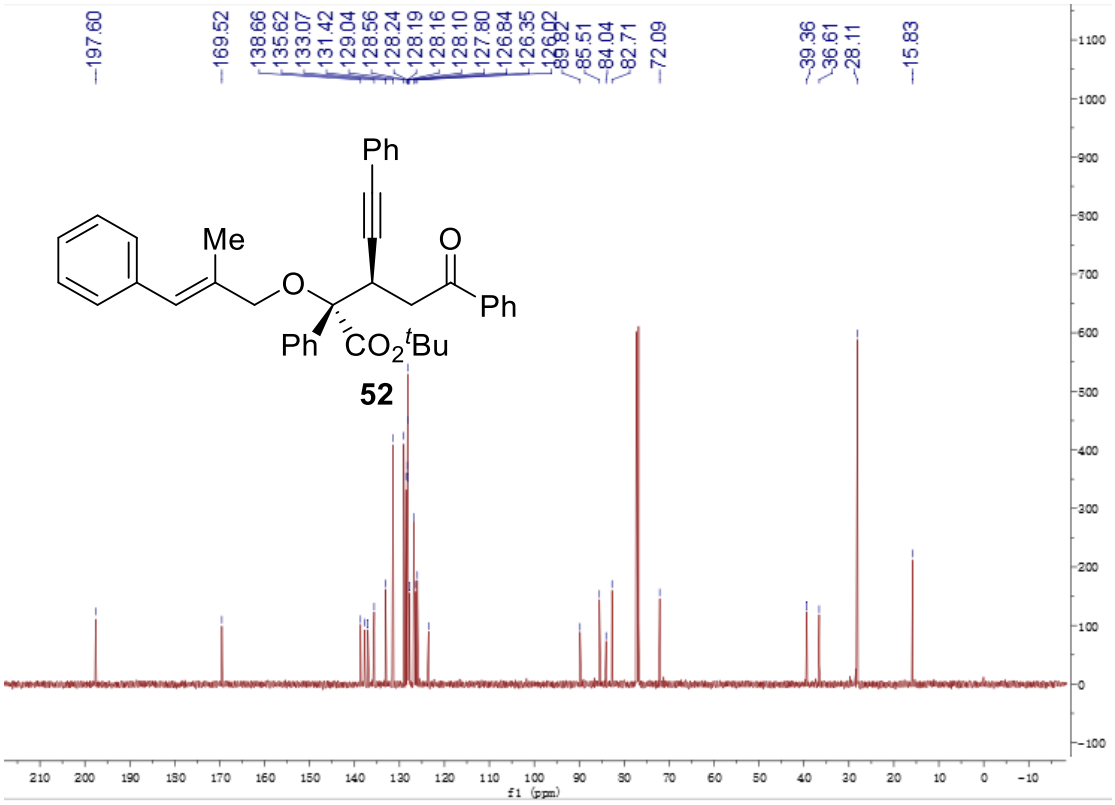

**50**


197.37
169.38
143.56
133.17
131.86
131.40
128.79
128.58
128.36
128.32
128.21
128.19
127.92
126.96
126.78
123.98
88.33
85.87
84.06
83.02
66.93
39.34
36.68
28.09
Ph
$O_2N$
O
O
Ph
Ph
$CO_2{}^tBu$
50

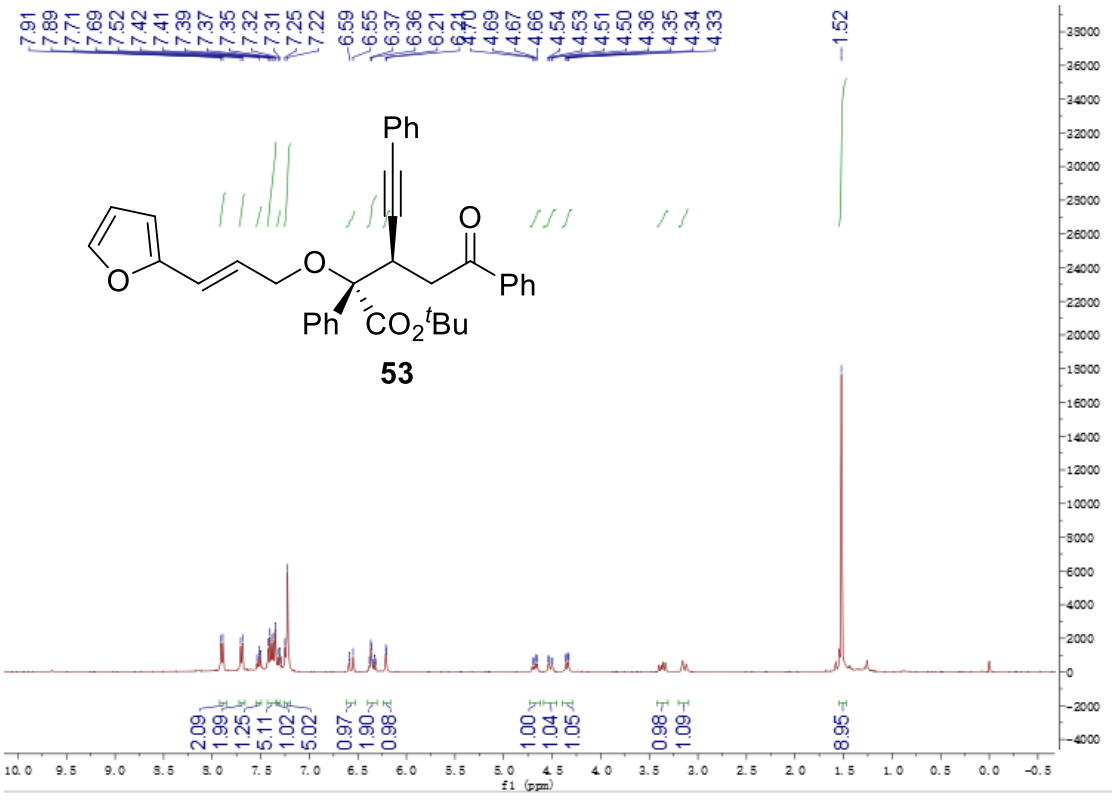

7.91
7.89
7.73
7.71
7.53
7.51
7.49
7.47
7.41
7.39
7.37
7.35
7.33
7.31
7.24
7.23
7.22
7.16
7.16
7.14
7.13
6.94
6.90
6.34
6.30
4.74
4.73
4.71
4.69
4.57
4.56
4.54
4.53
4.38
4.37
4.35
4.35
3.43
3.40
3.38
3.36
3.19
3.18
3.15
3.14
2.31
1.54
Ph
O
O
Ph
Br
Ph
$CO_2{}^tBu$
51
2.00
1.90
2.16
4.23
1.02
4.86
2.95
0.81
0.82
0.93
0.92
0.96
0.91
1.00
2.93
9.14


197.64
169.57
133.06
131.44
130.27
129.30
128.54
128.24
128.20
128.16
128.14
127.96
127.80
126.86
126.08
125.76
89.75
85.79
83.96
82.74
67.89
39.35
36.84
28.12
19.81
Ph
O
O
Ph
Br
Ph
CO2tBu
51
f1 (ppm)

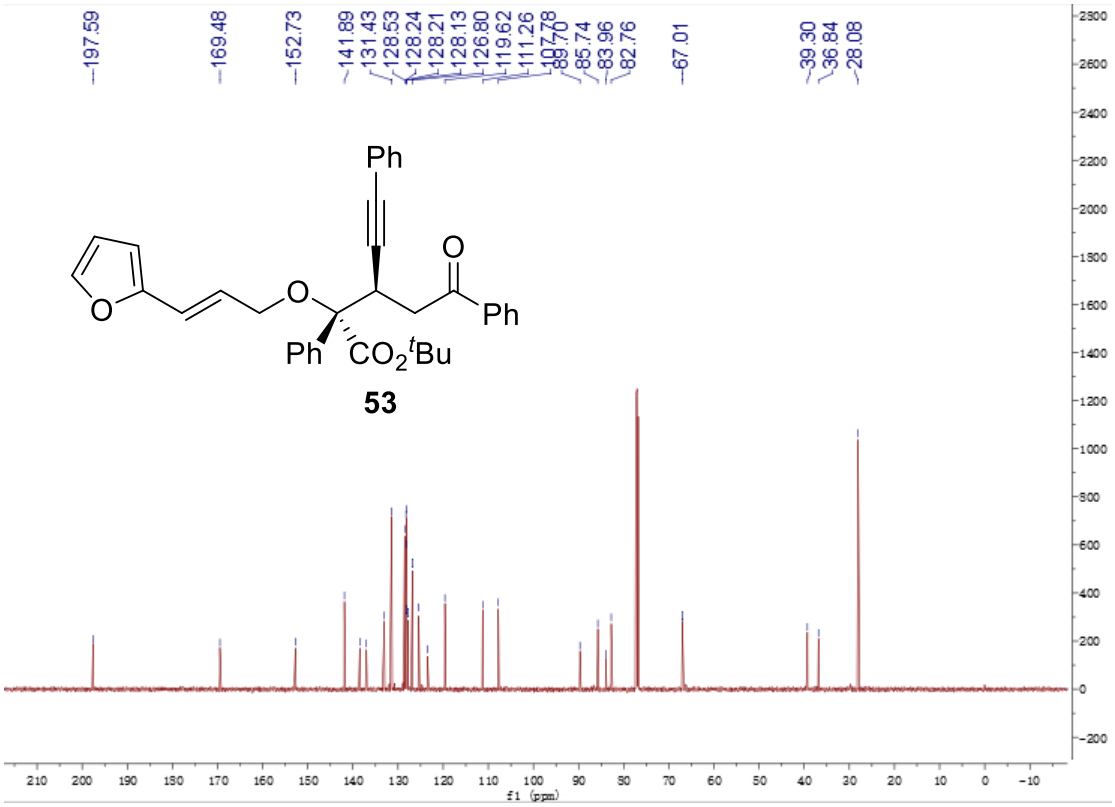

7.91
7.89
7.88
7.73
7.73
7.71
7.53
7.51
7.49
7.49
7.41
7.39
7.38
7.37
7.36
7.35
7.33
7.31
7.30
7.30
7.28
7.26
7.26
7.25
7.25
7.24
7.23
7.22
7.22
7.21
7.21
6.67
4.64
4.61
4.43
4.41
4.40
4.38
4.38
3.38
3.35
3.19
3.18
3.14
1.99
1.99
1.53
Ph
Me
O
O
Ph
Ph
CO2tBu
52
2.16
1.92
1.17
4.02
5.09
5.92
0.85
0.88
1.90
0.91
1.00
2.84
9.01
f1 (ppm)

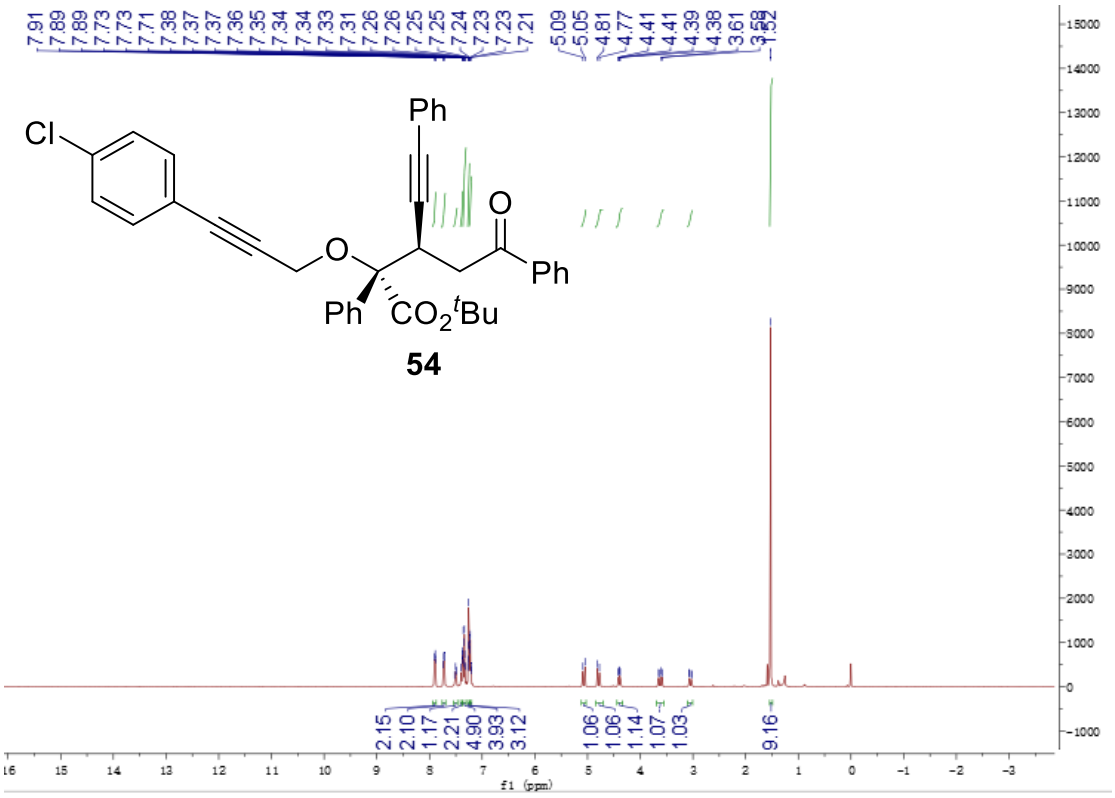

197.60
169.52
138.66
135.62
133.07
131.42
129.04
128.56
128.24
128.19
128.16
128.10
127.80
126.84
126.35
126.02
89.82
85.51
84.04
82.71
72.09
39.36
36.61
28.11
15.83
Ph
Me
O
Ph
Ph
CO2tBu

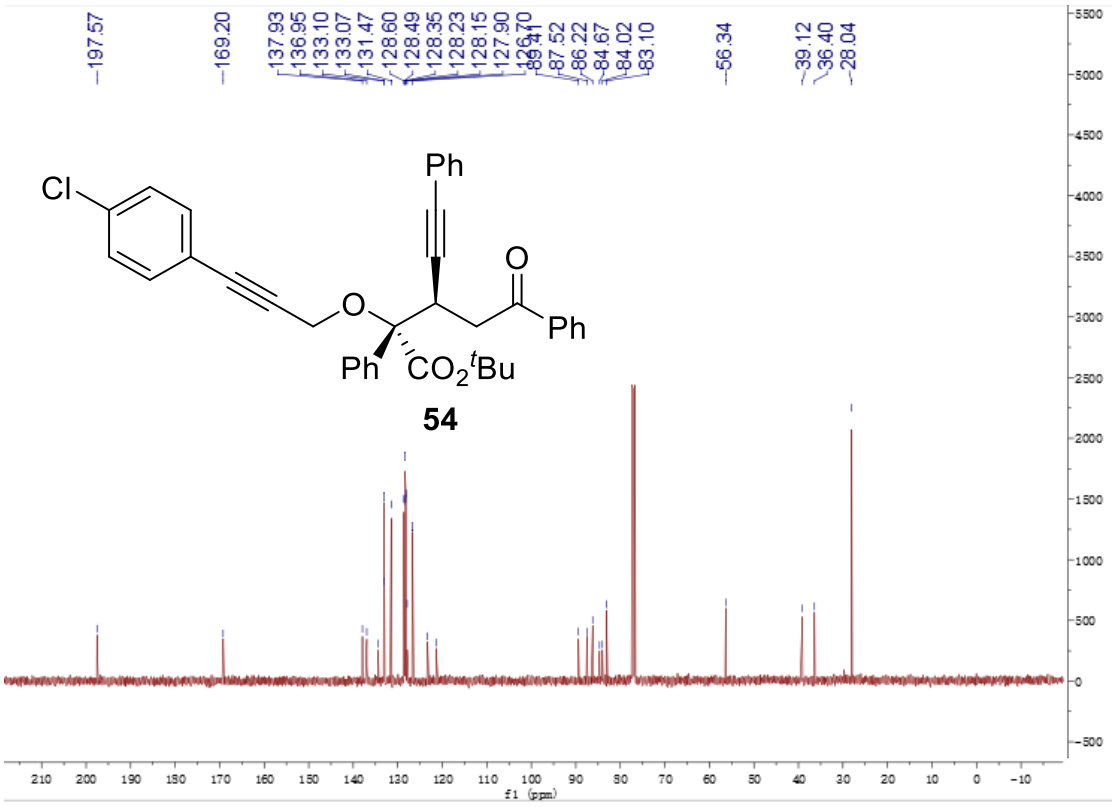
**52**

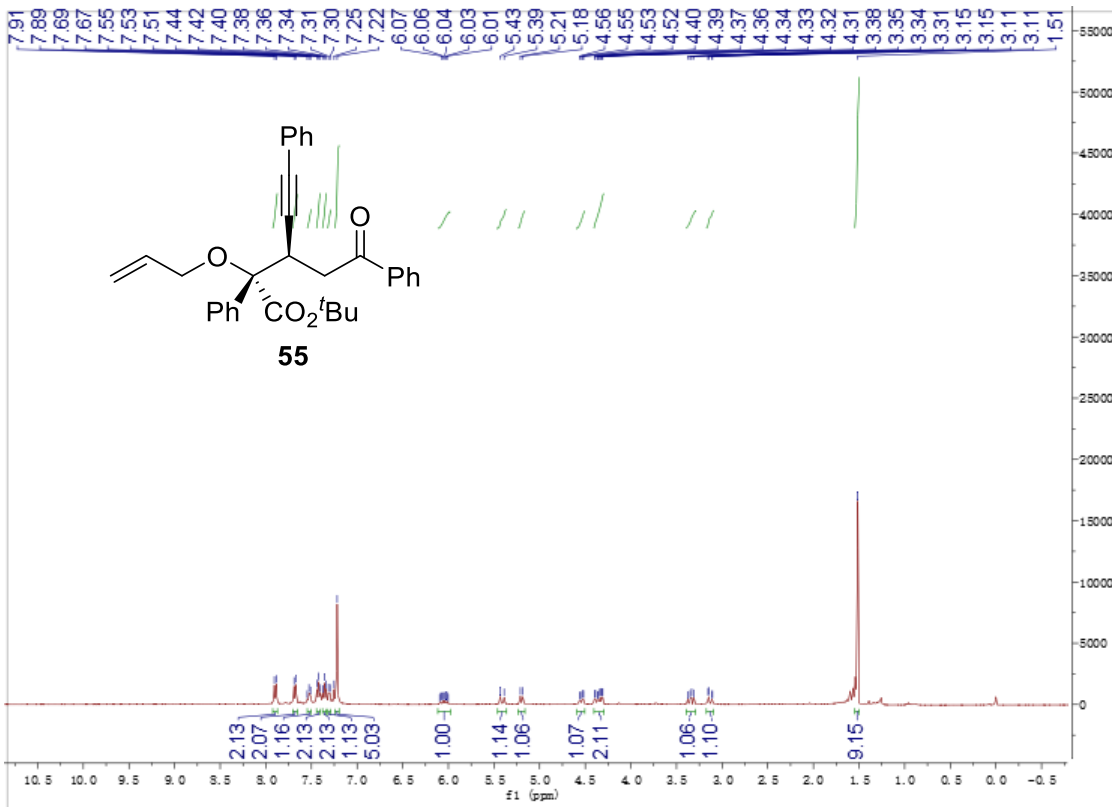

7.91
7.89
7.71
7.69
7.52
7.42
7.41
7.39
7.37
7.35
7.32
7.31
7.25
7.22
6.59
6.55
6.37
6.36
6.21
4.69
4.67
4.66
4.54
4.53
4.51
4.50
4.36
4.35
4.34
4.33
1.52
Ph
O
O
Ph
Ph
CO2tBu
2.09
1.99
1.25
5.11
1.02
5.02
0.97
1.90
0.98
1.00
1.04
1.05
0.98
1.09
8.95

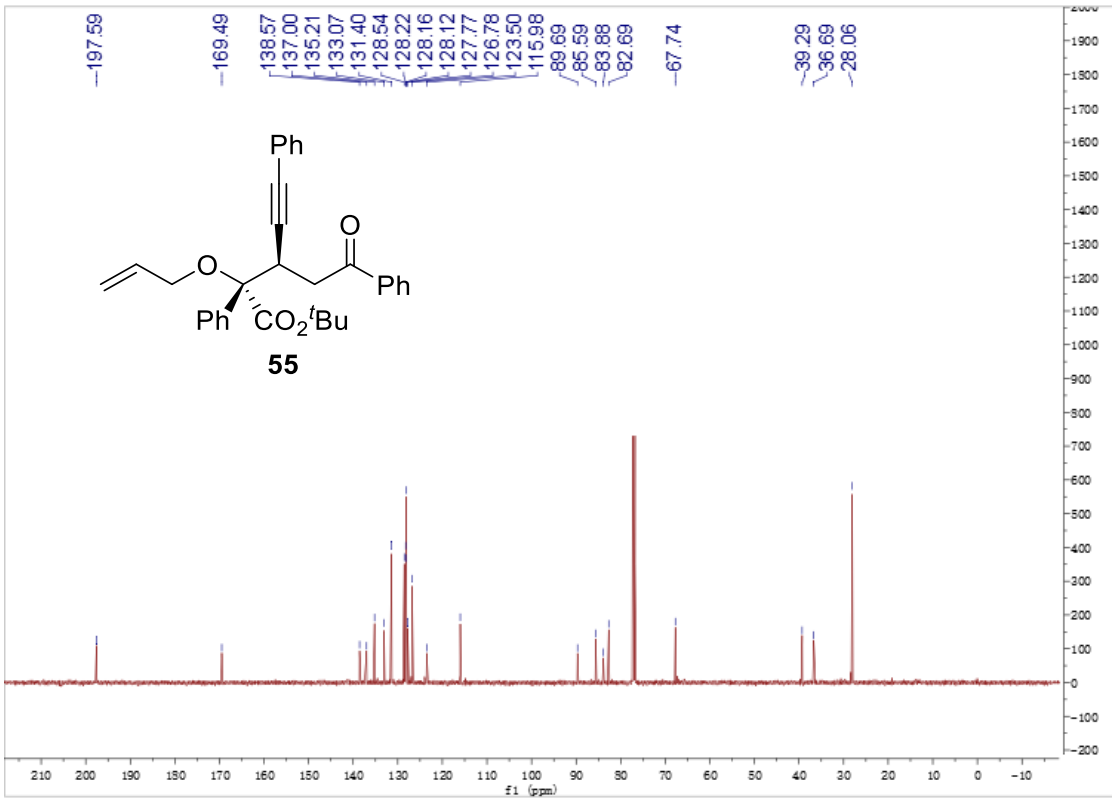
**53**

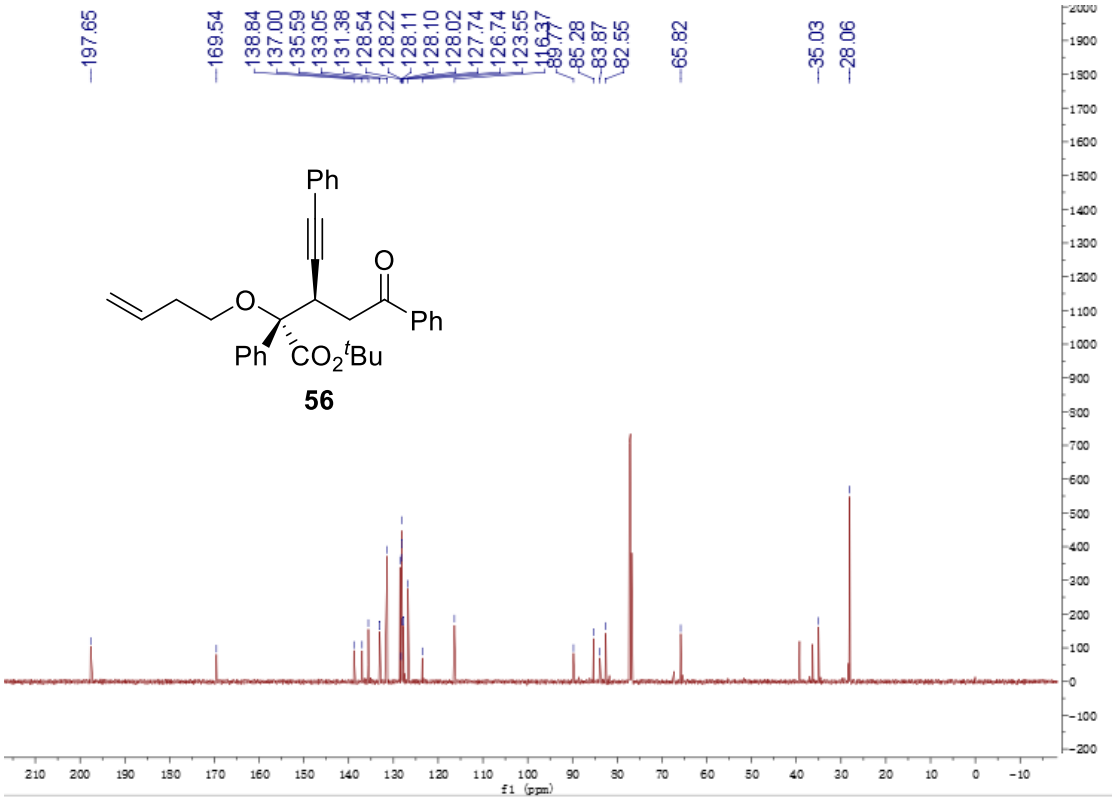

197.59
169.48
152.73
141.89
131.43
128.53
128.24
128.21
128.13
126.80
119.62
111.26
107.78
89.70
85.74
83.96
82.76
67.01
39.30
36.84
28.08
Ph
O
O
Ph
Ph
CO2tBu
53

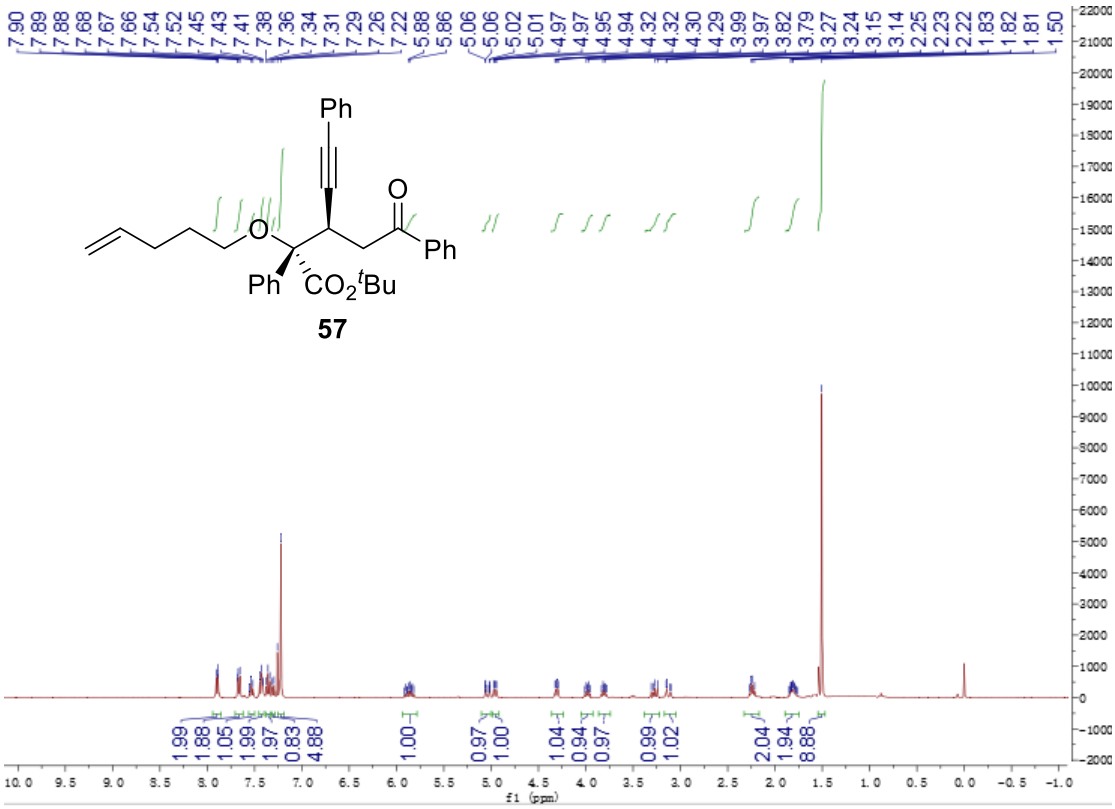

7.91
7.89
7.89
7.73
7.73
7.71
7.38
7.37
7.37
7.36
7.35
7.34
7.34
7.33
7.31
7.26
7.26
7.25
7.25
7.24
7.23
7.23
7.21
5.09
5.05
4.81
4.77
4.41
4.41
4.39
4.38
3.61
3.59
3.52
Cl
Ph
O
O
Ph
Ph
CO2tBu
54
2.15
2.10
1.17
2.21
4.90
3.93
3.12
1.06
1.06
1.14
1.07
1.03
9.16

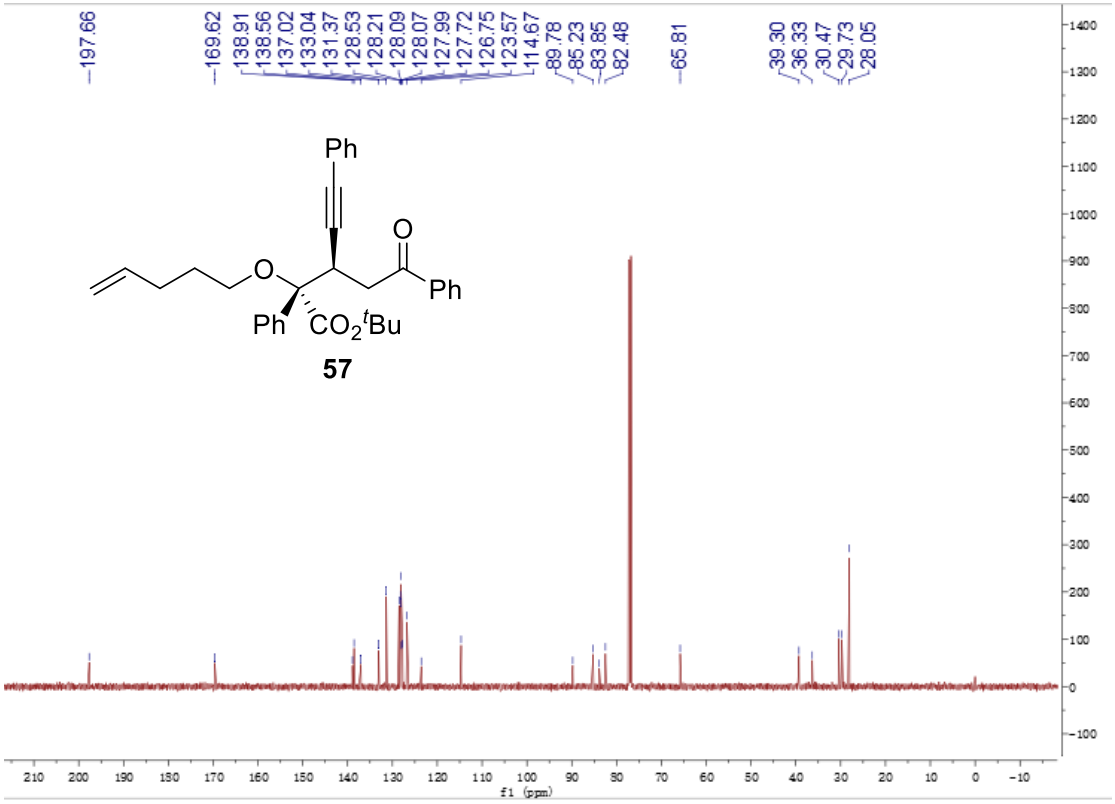

Cl
Ph
O
O
Ph
Ph
CO2tBu
54

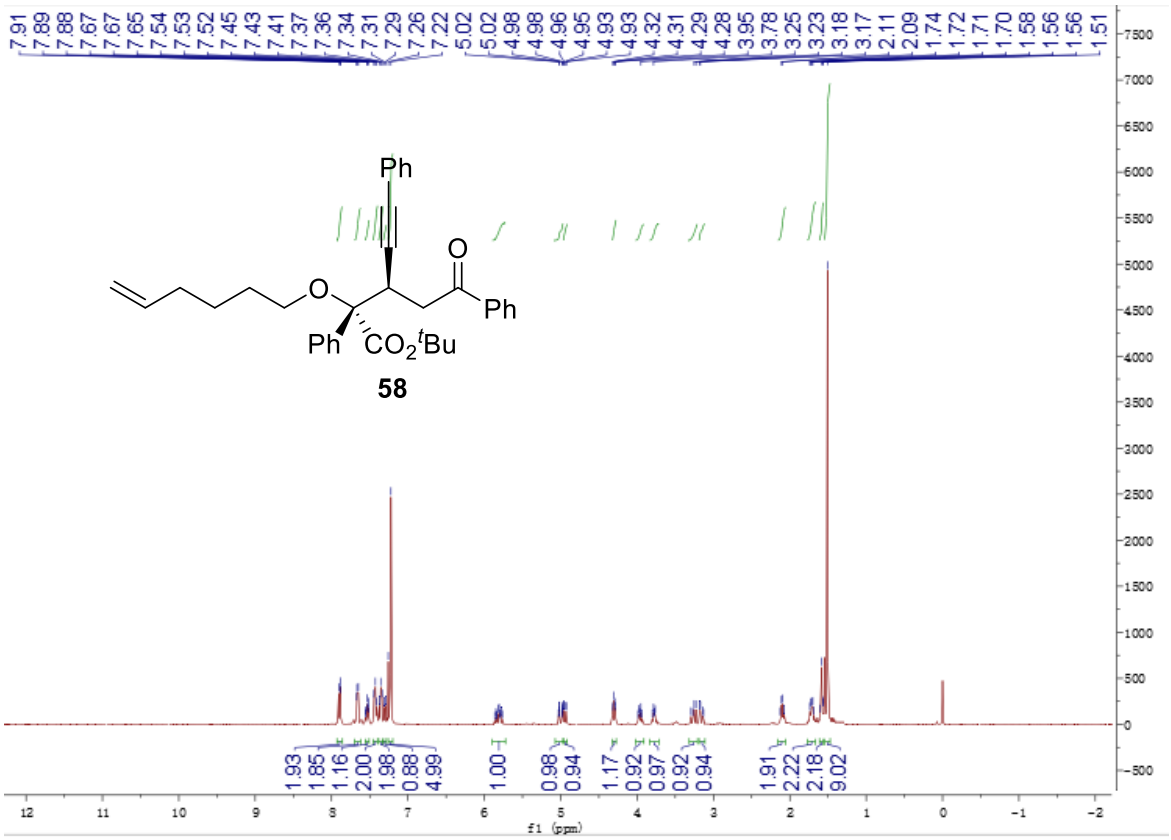

Ph
O
O
Ph
Ph
CO2tBu
55

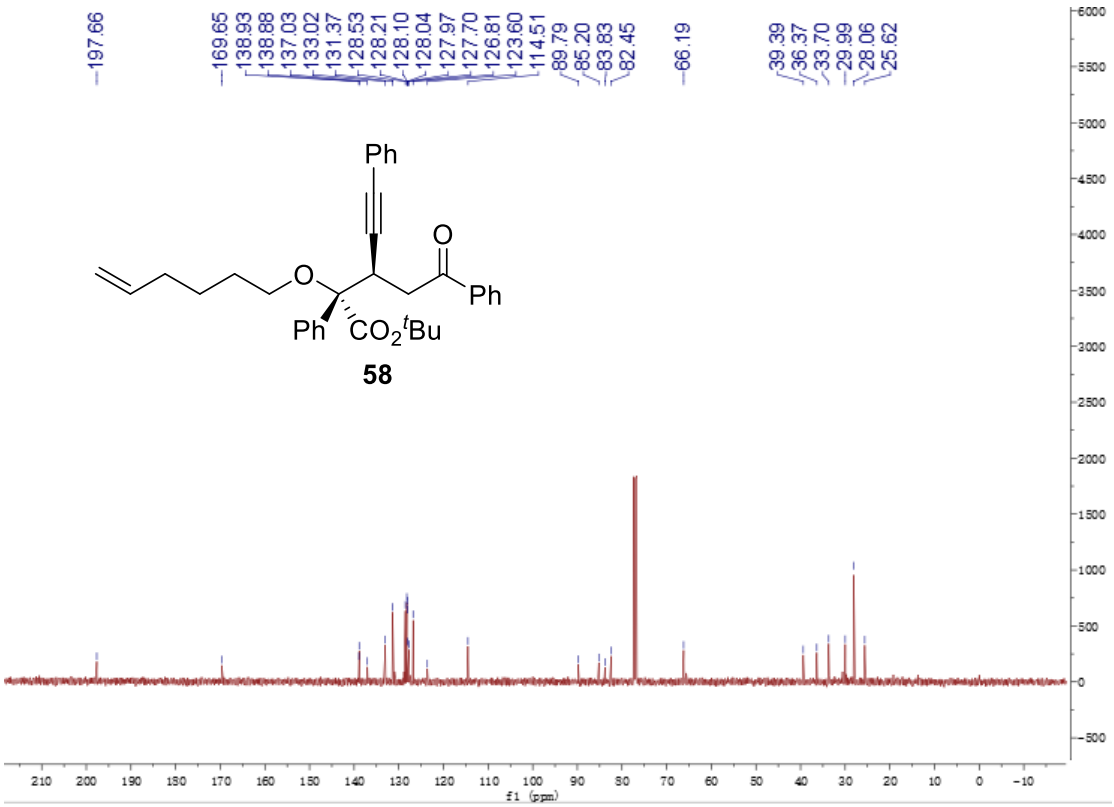

197.59
169.49
138.57
137.00
135.21
133.07
131.40
128.54
128.22
128.16
128.12
127.77
126.78
123.50
115.98
89.69
85.59
83.88
82.69
67.74
39.29
36.69
28.06
Ph
O
O
Ph
Ph
CO2tBu
55
f1 (ppm)

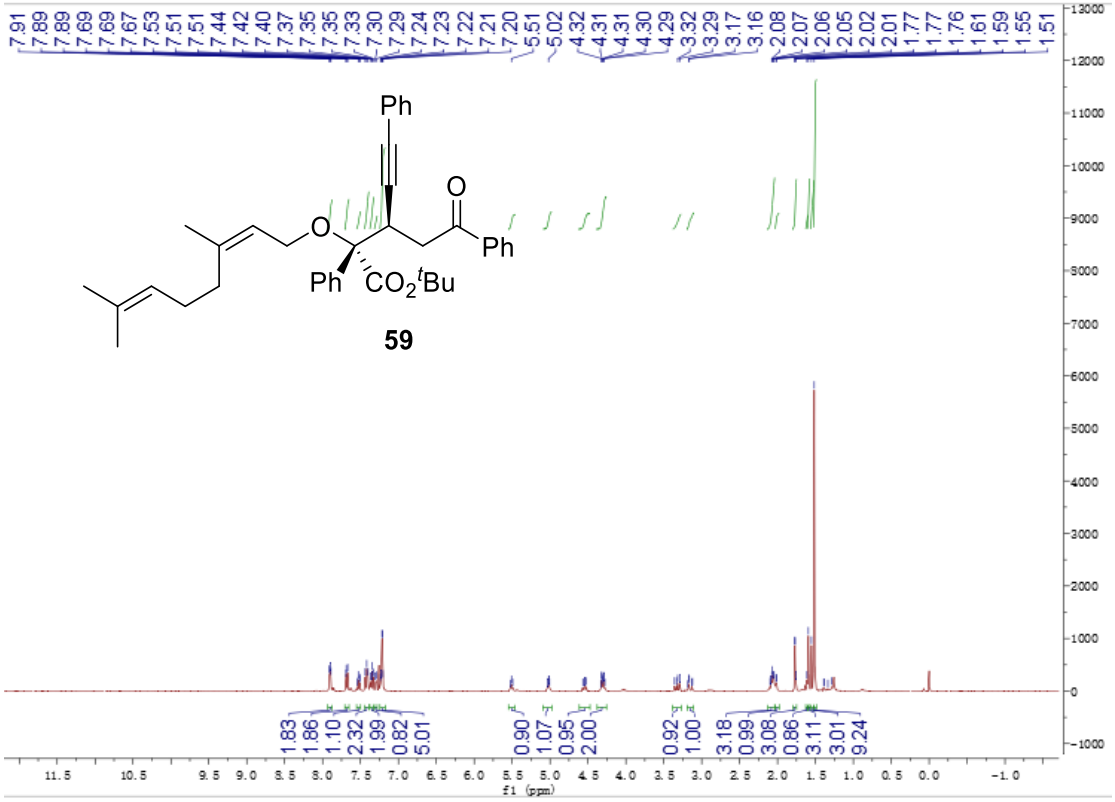

197.65
169.54
138.84
137.00
135.59
133.05
131.38
128.54
128.22
128.11
128.10
128.02
127.74
126.74
123.55
116.37
89.77
85.28
83.87
82.55
65.82
35.03
28.06
Ph
O
O
Ph
Ph
CO2tBu
56
f1 (ppm)


Ph
O
O
Ph
Ph
CO2tBu
57

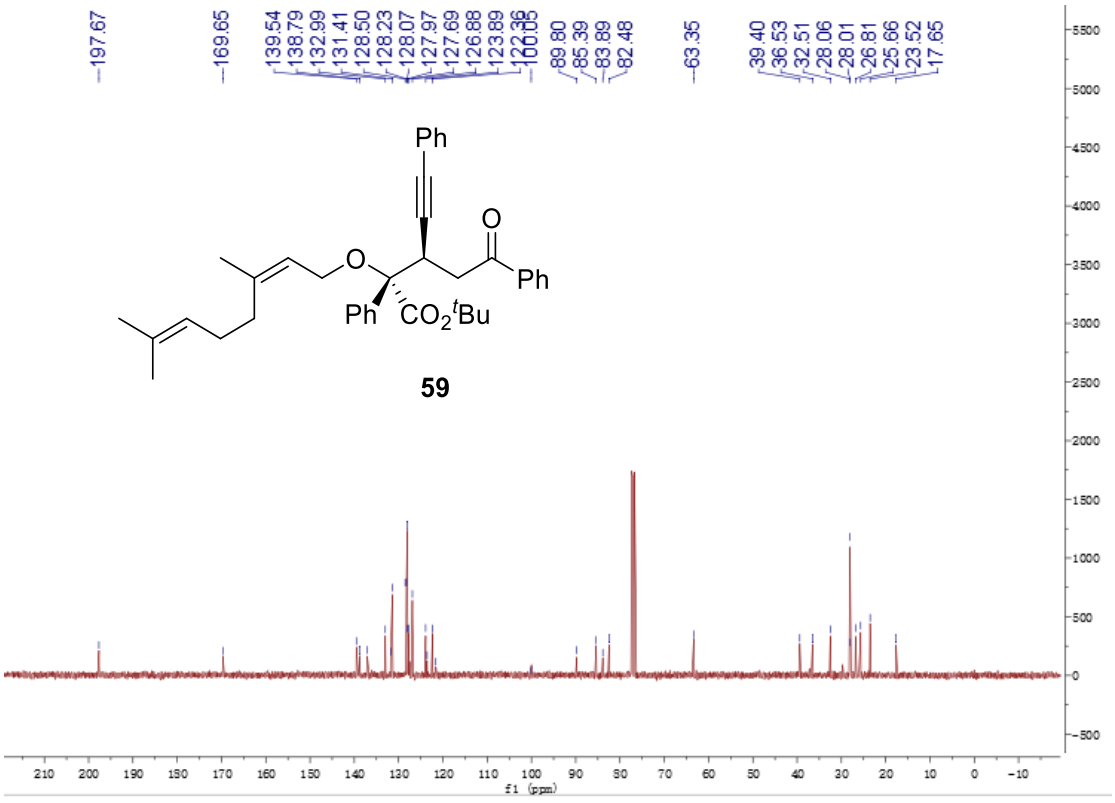

Ph
O
O
Ph
Ph
CO2tBu
57


Ph
O
O
Ph
Ph
CO2tBu
58

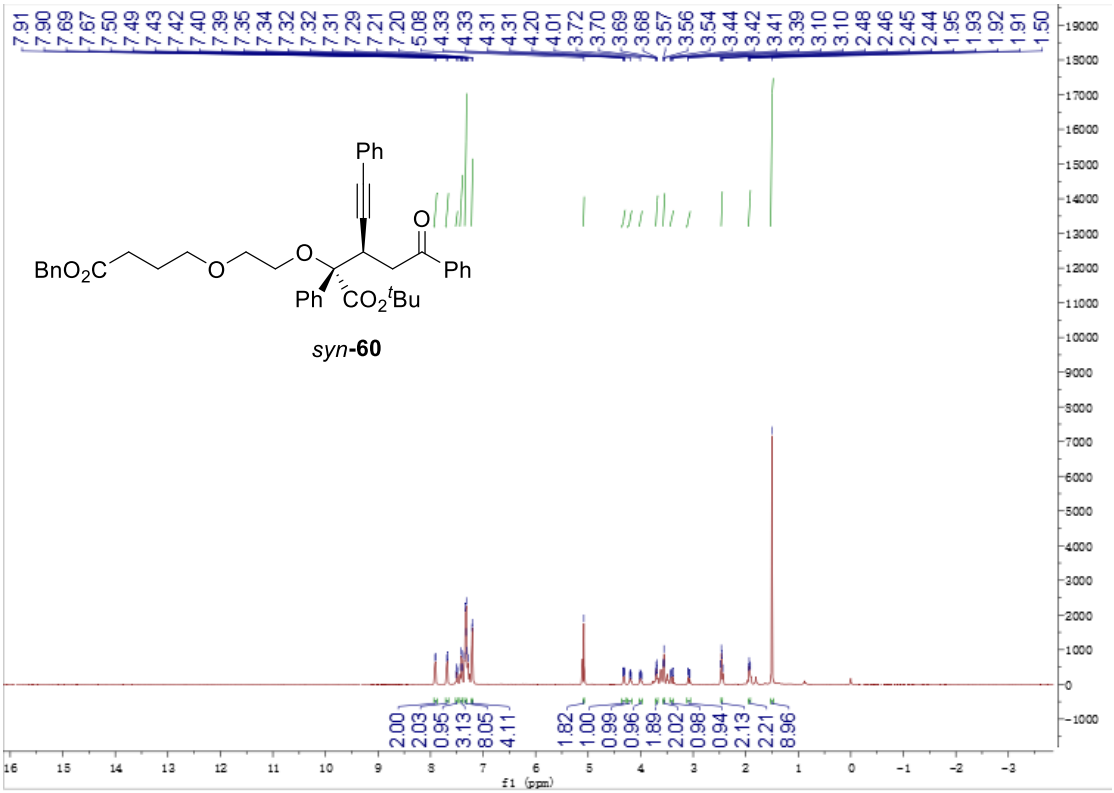

Ph
O
O
Ph
Ph
CO2tBu
58



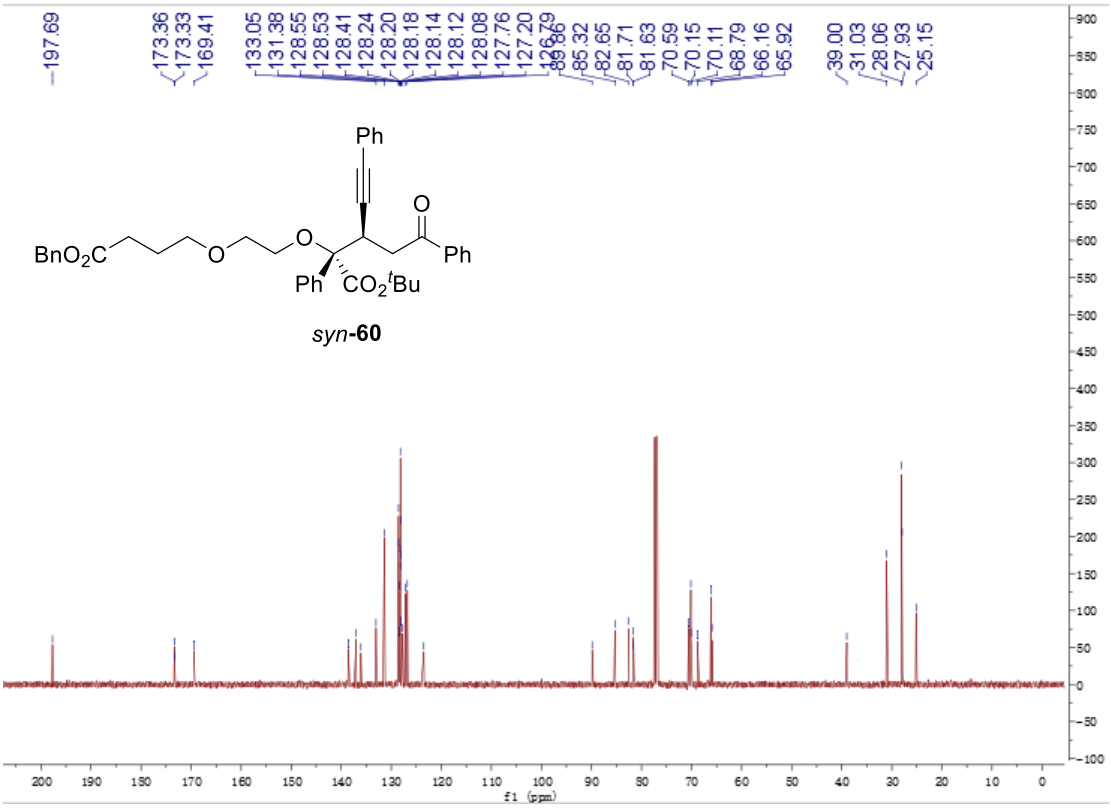

**59**



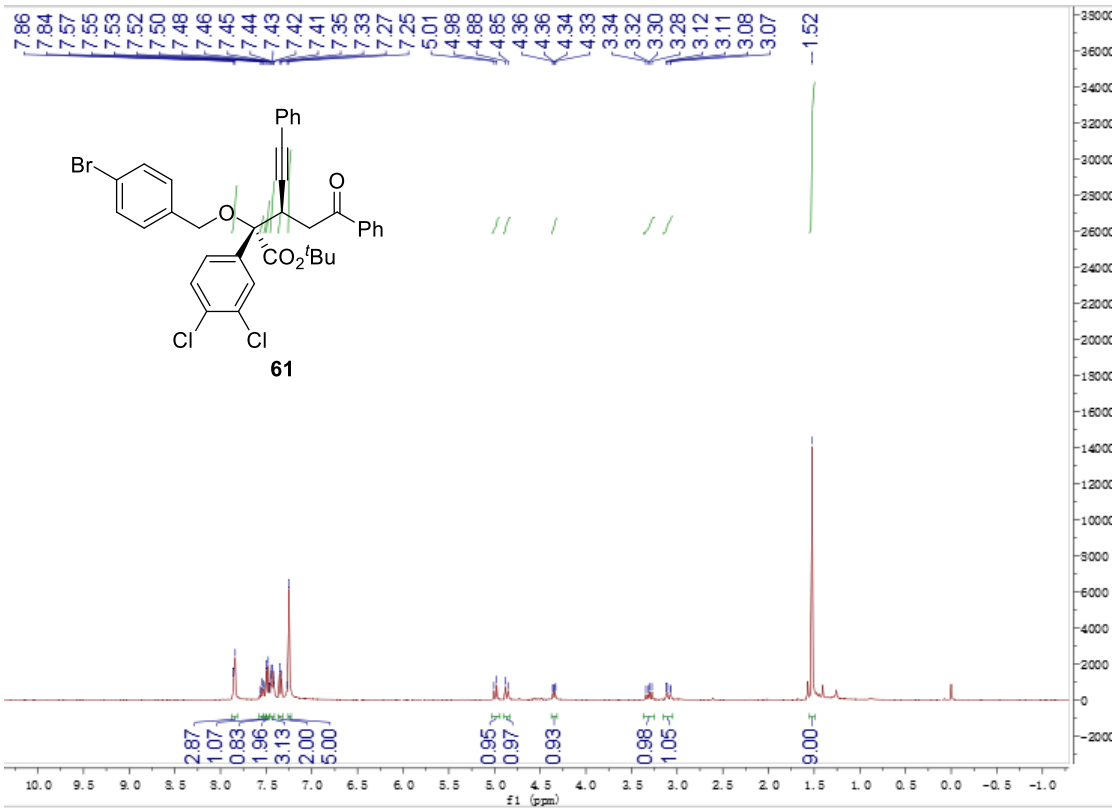

**59**

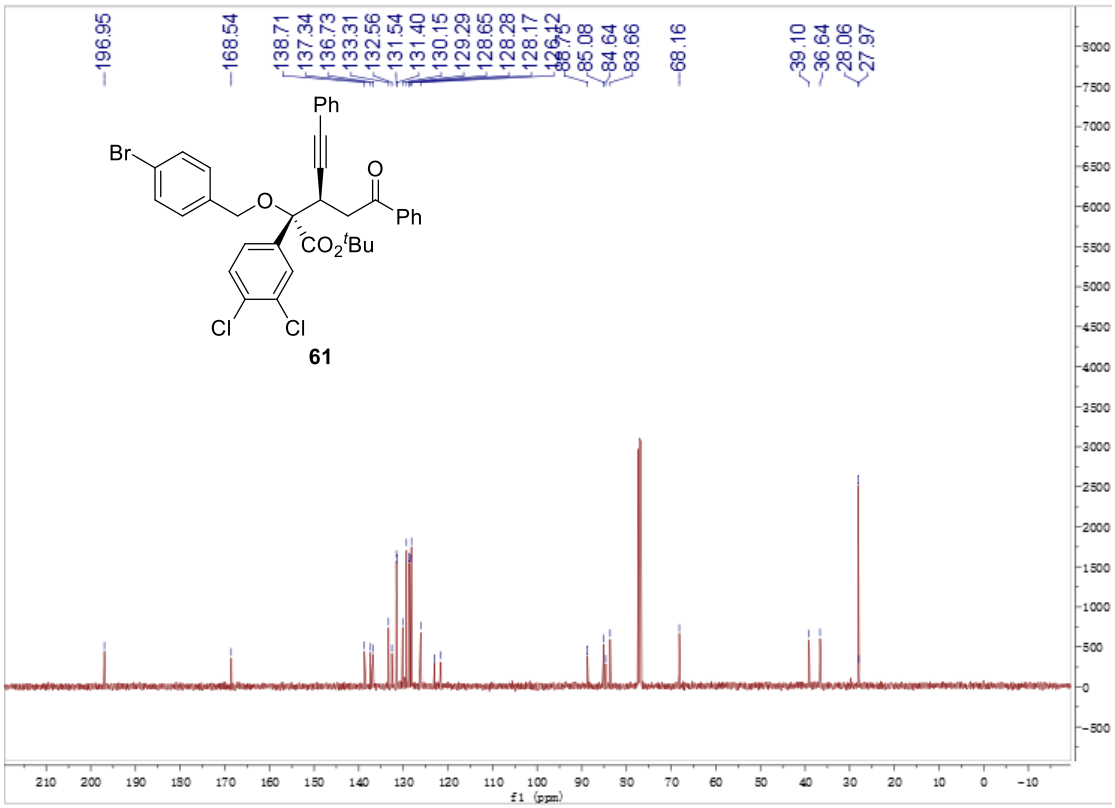


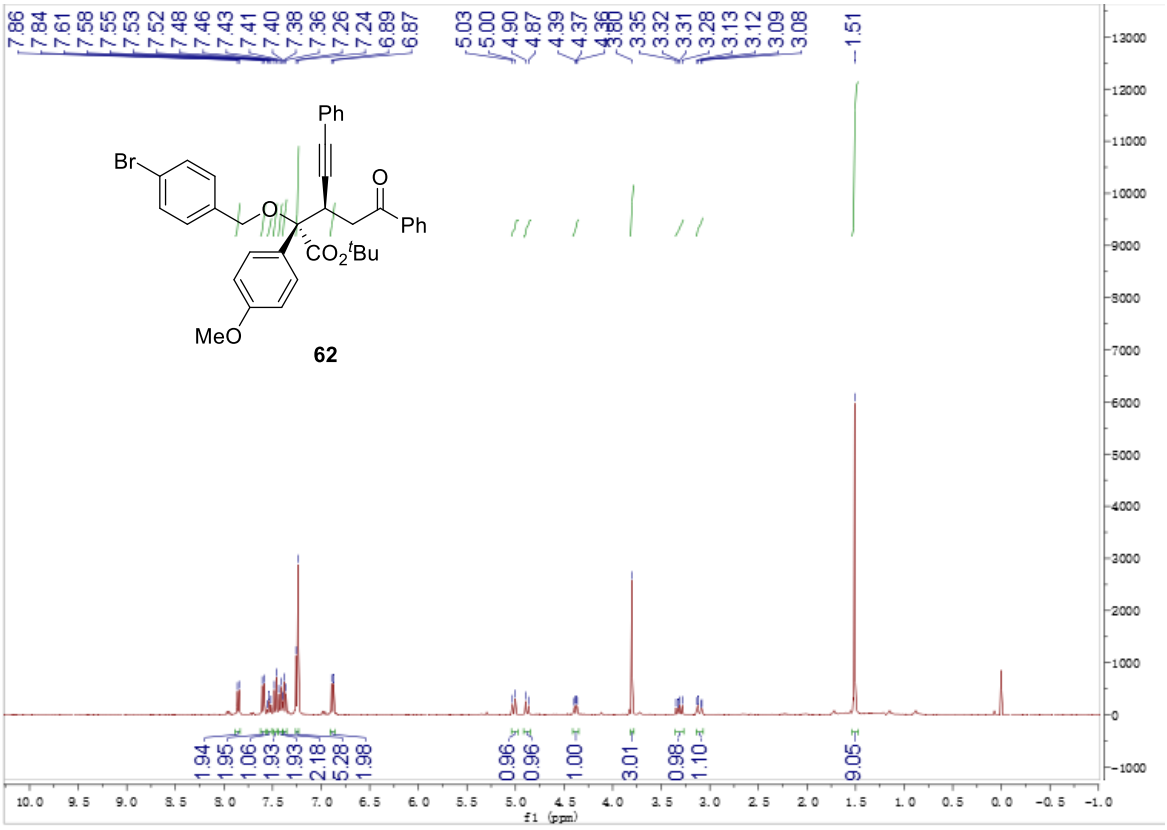

*syn*-**60**

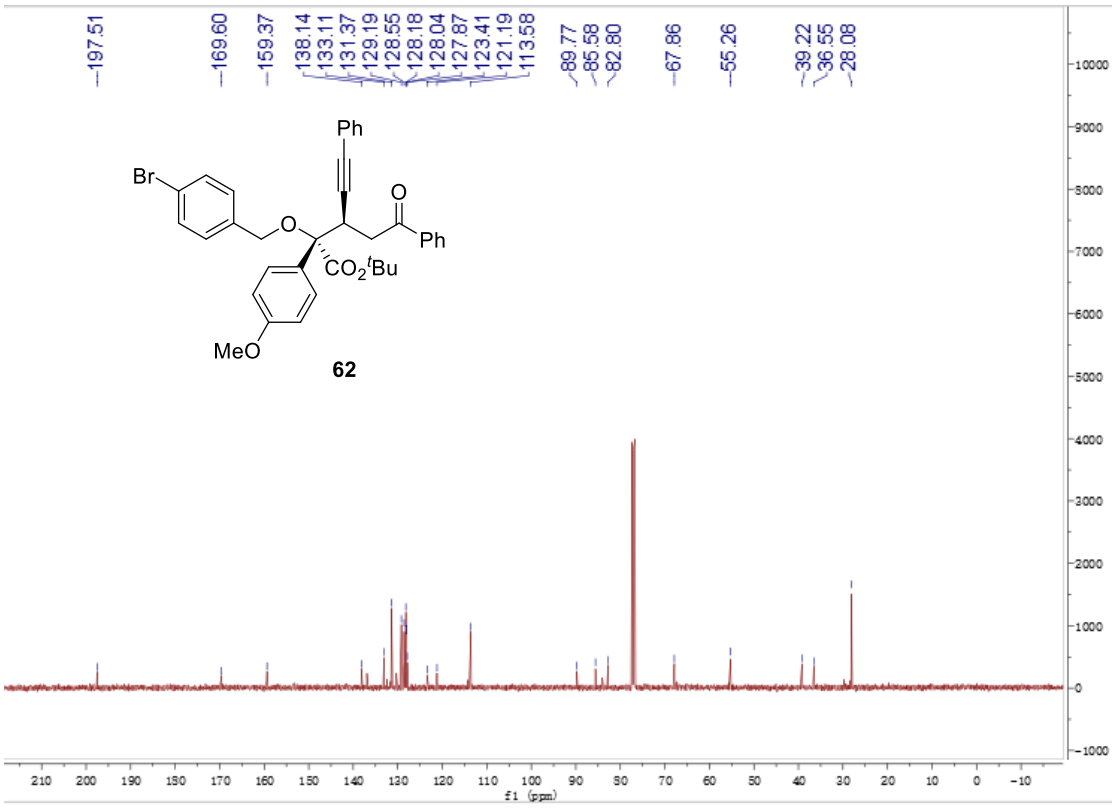


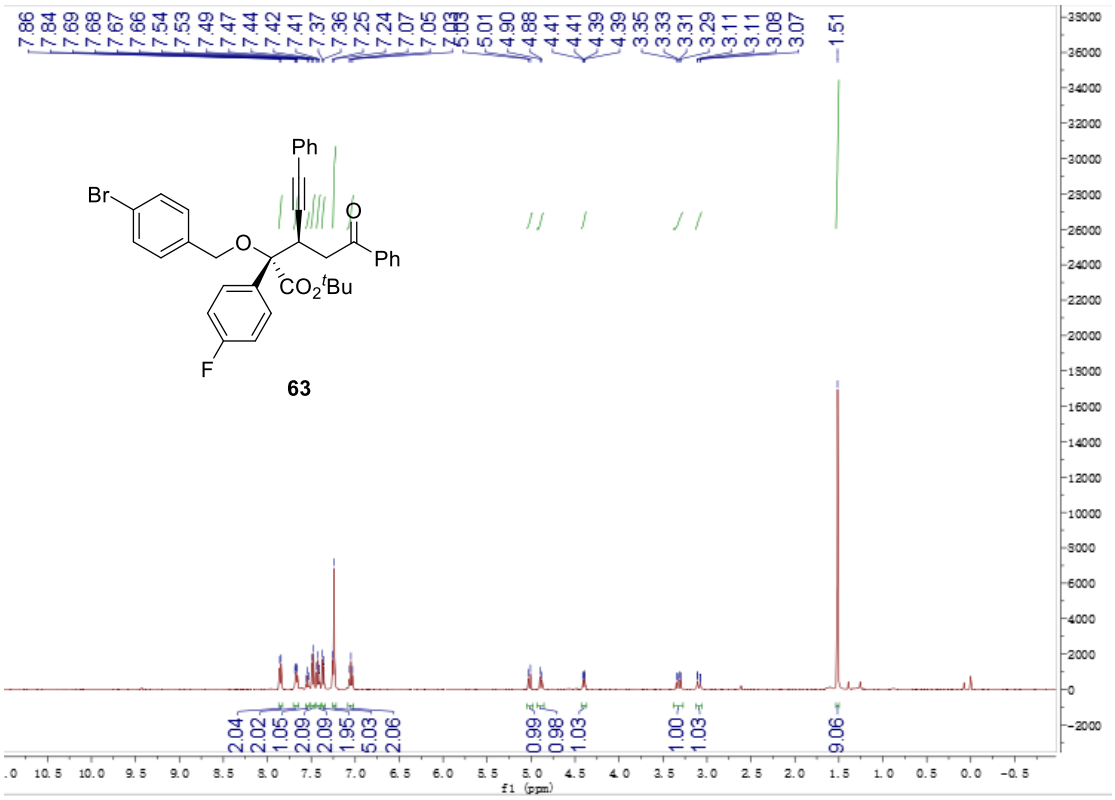

*syn*-**60**

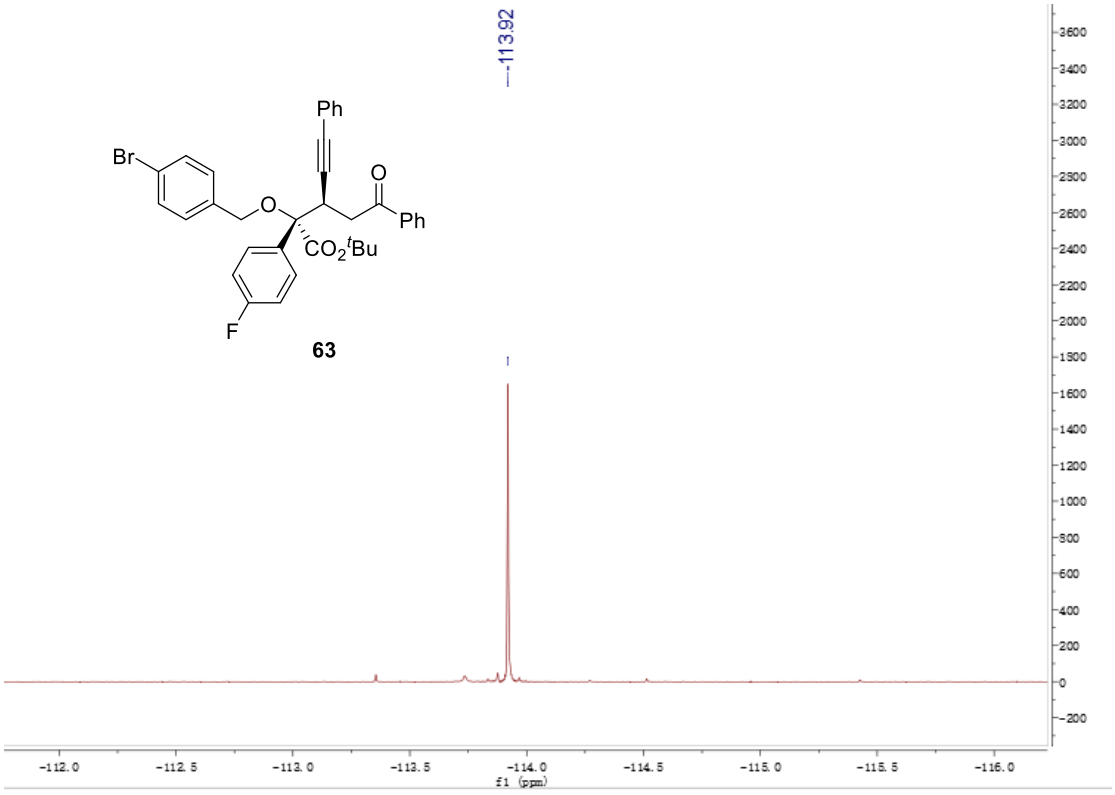

7.86
7.84
7.57
7.55
7.53
7.52
7.50
7.48
7.46
7.45
7.44
7.43
7.42
7.41
7.35
7.33
7.27
7.25
5.01
4.98
4.88
4.85
4.36
4.36
4.34
4.33
3.34
3.32
3.30
3.28
3.12
3.11
3.08
3.07
1.52
Ph
Br
O
O
Ph
CO2tBu
Cl
Cl
61
2.87
1.07
0.83
1.96
3.13
2.00
5.00
0.95
0.97
0.93
0.98
1.05
9.00
f1 (ppm)

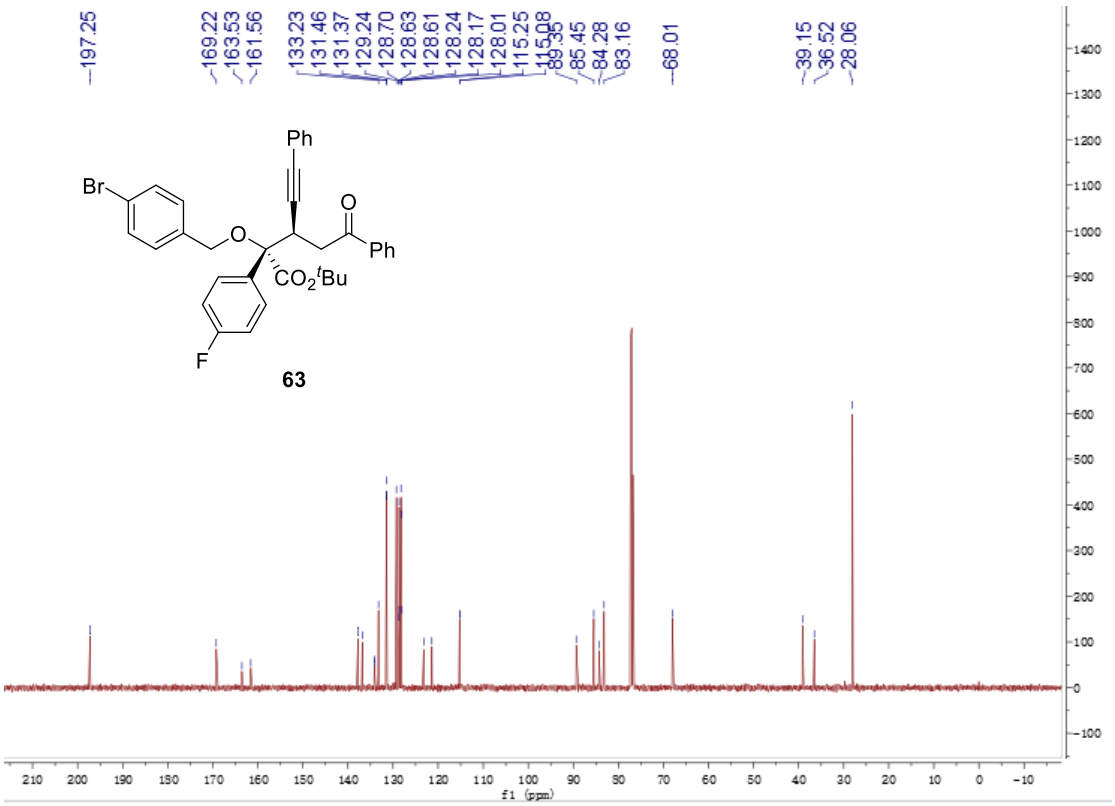

196.95
168.54
138.71
137.34
136.73
133.31
132.56
131.54
131.40
130.15
129.29
128.65
128.28
128.17
88.75
85.08
84.64
83.66
68.16
39.10
36.64
28.06
27.97
Ph
Br
O
O
Ph
CO2tBu
Cl
Cl
61
f1 (ppm)

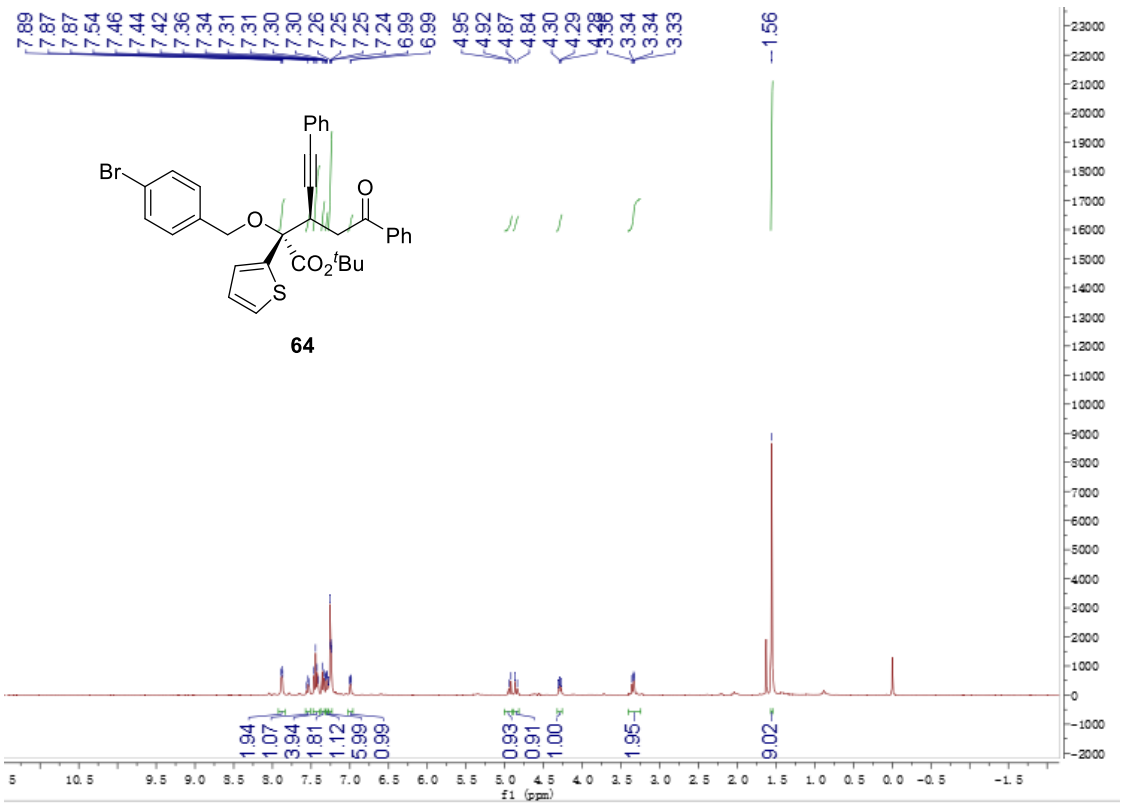

7.86
7.84
7.61
7.58
7.55
7.53
7.52
7.48
7.46
7.43
7.41
7.40
7.38
7.36
7.26
7.24
6.89
6.87
5.03
5.00
4.90
4.87
4.39
4.37
4.35
3.32
3.31
3.28
3.13
3.12
3.09
3.08
1.51
Ph
Br
O
O
Ph
CO2tBu
MeO
62
1.94
1.95
1.06
1.93
1.93
2.18
5.28
1.98
0.96
0.96
1.00
3.01
0.98
1.10
9.05
f1 (ppm)

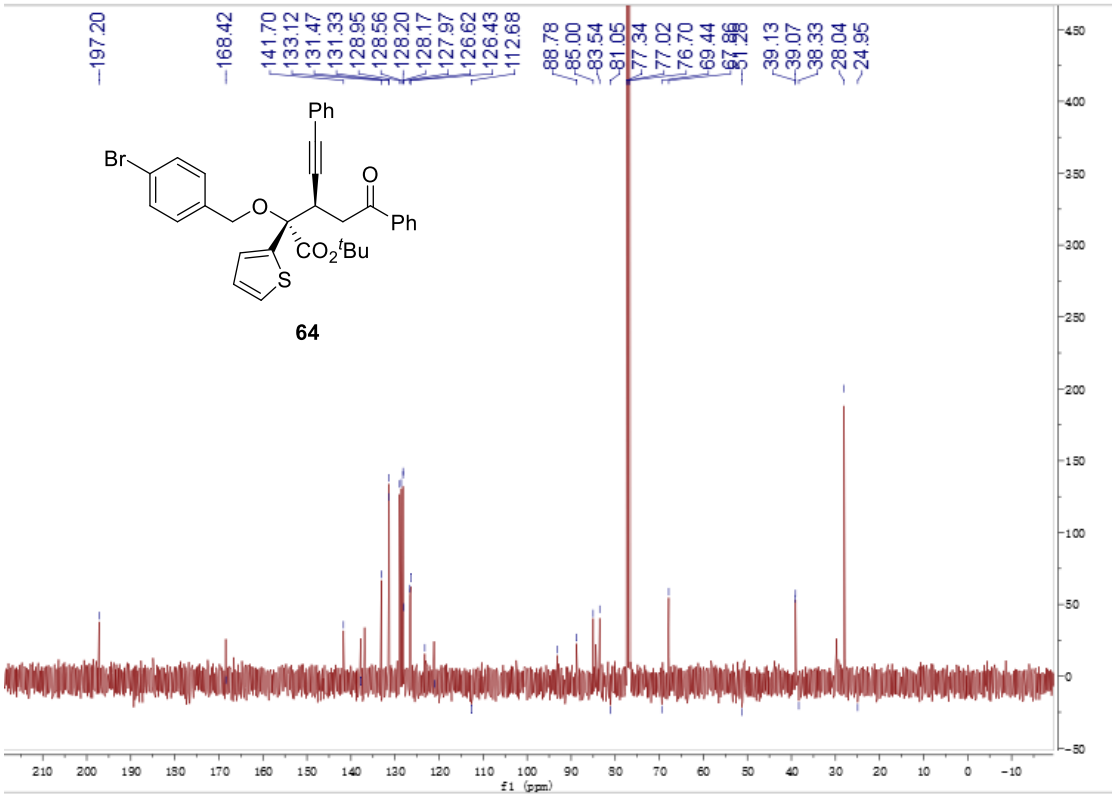

197.51
169.60
159.37
138.14
133.11
131.37
129.19
128.55
128.18
128.04
127.87
123.41
121.19
113.58
89.77
85.58
82.80
67.86
55.26
39.22
36.55
28.08
Ph
Br
O
O
Ph
CO2tBu
MeO
62
f1 (ppm)


7.86
7.84
7.69
7.68
7.67
7.66
7.54
7.53
7.49
7.47
7.44
7.42
7.41
7.37
7.36
7.25
7.24
7.07
7.05
5.01
4.90
4.88
4.41
4.41
4.39
4.39
3.35
3.33
3.31
3.29
3.11
3.11
3.08
3.07
1.51
Ph
Br
O
Ph
CO2tBu
F
63
2.04
2.02
1.05
2.09
2.09
1.95
5.03
2.06
0.99
0.98
1.03
1.00
1.03
9.06
f1 (ppm)

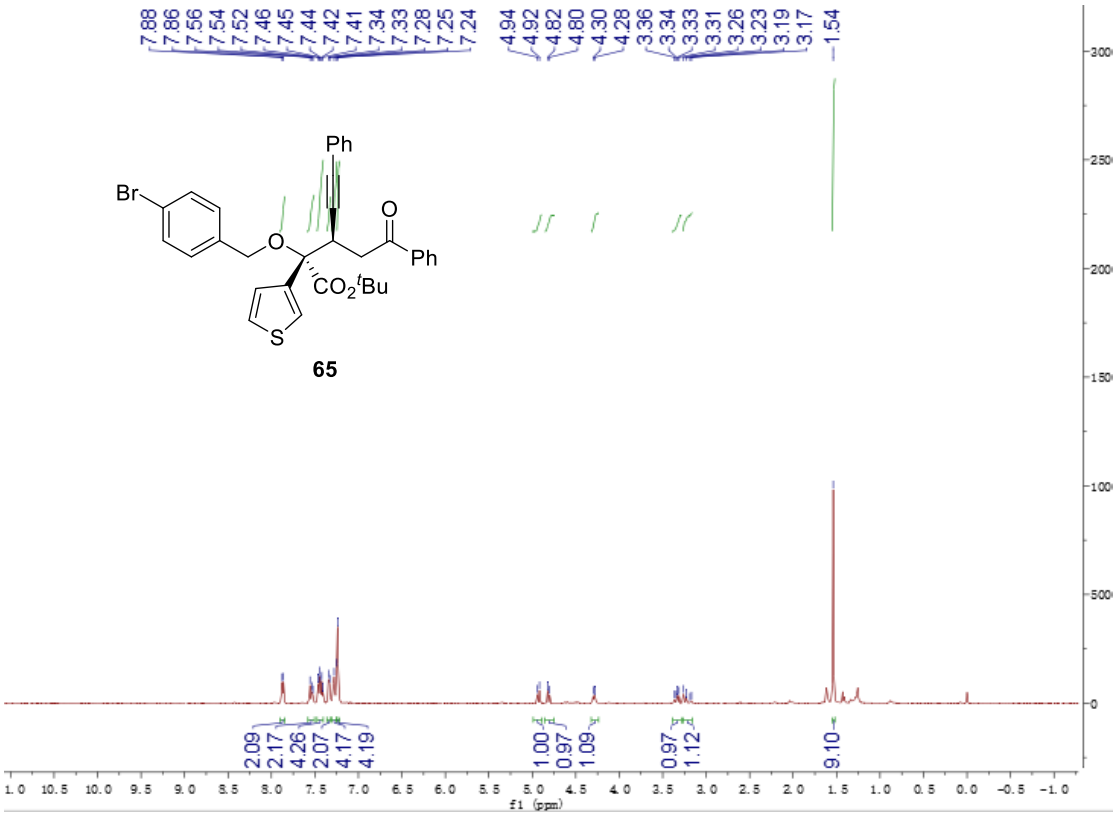

-113.92
Ph
Br
O
Ph
CO2tBu
F
63
f1 (ppm)


197.25
169.22
163.53
161.56
133.23
131.46
131.37
129.24
128.70
128.63
128.61
128.24
128.17
128.01
115.25
115.08
89.35
85.45
84.28
83.16
68.01
39.15
36.52
28.06
Ph
Br
O
O
Ph
CO2tBu
F
63
f1 (ppm)

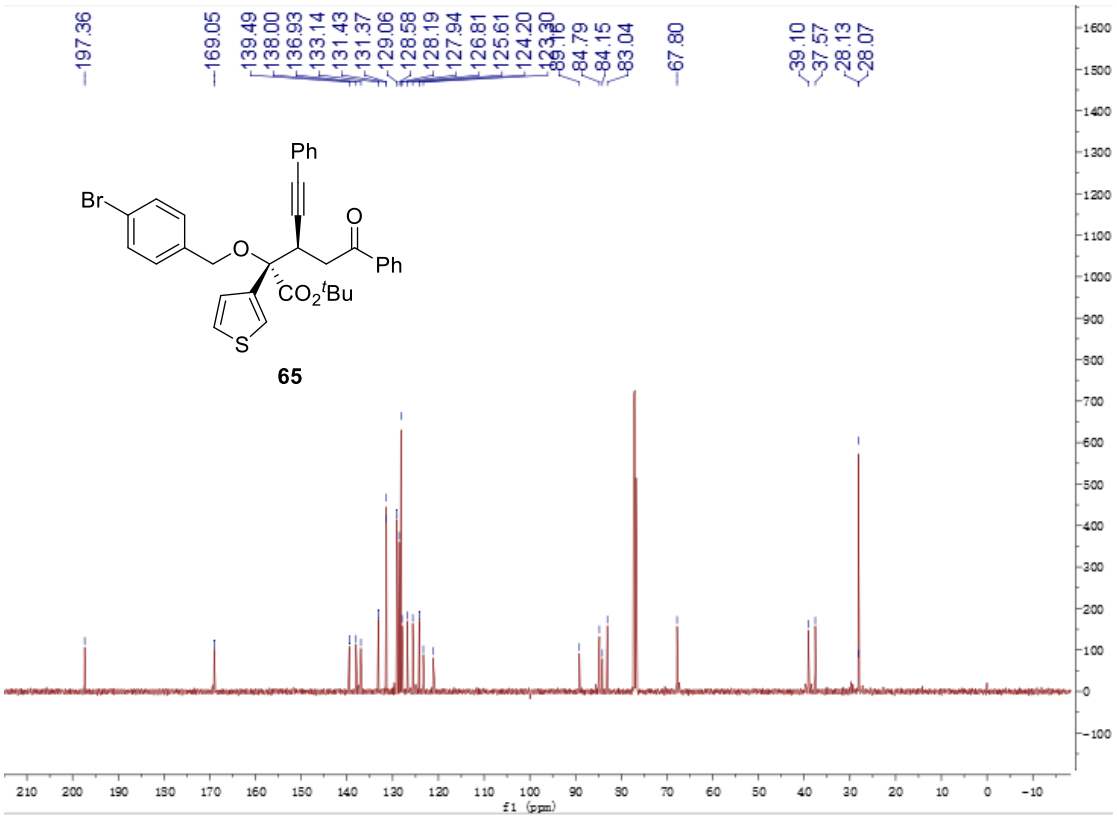

7.89
7.87
7.87
7.54
7.46
7.44
7.42
7.36
7.34
7.31
7.31
7.30
7.30
7.26
7.25
7.25
7.24
6.99
6.99
4.95
4.92
4.87
4.84
4.30
4.29
3.34
3.34
3.33
1.56
Ph
Br
O
O
Ph
CO2tBu
S
64
1.94
1.07
3.94
1.81
1.12
5.99
0.99
0.93
0.91
1.00
1.95
9.02
f1 (ppm)


197.20
168.42
141.70
133.12
131.47
131.33
128.95
128.56
128.20
128.17
127.97
126.62
126.43
112.68
88.78
85.00
83.54
81.05
77.34
77.02
76.70
69.44
39.13
39.07
38.33
28.04
24.95
Ph
Br
O
Ph
CO2tBu
S
f1 (ppm)

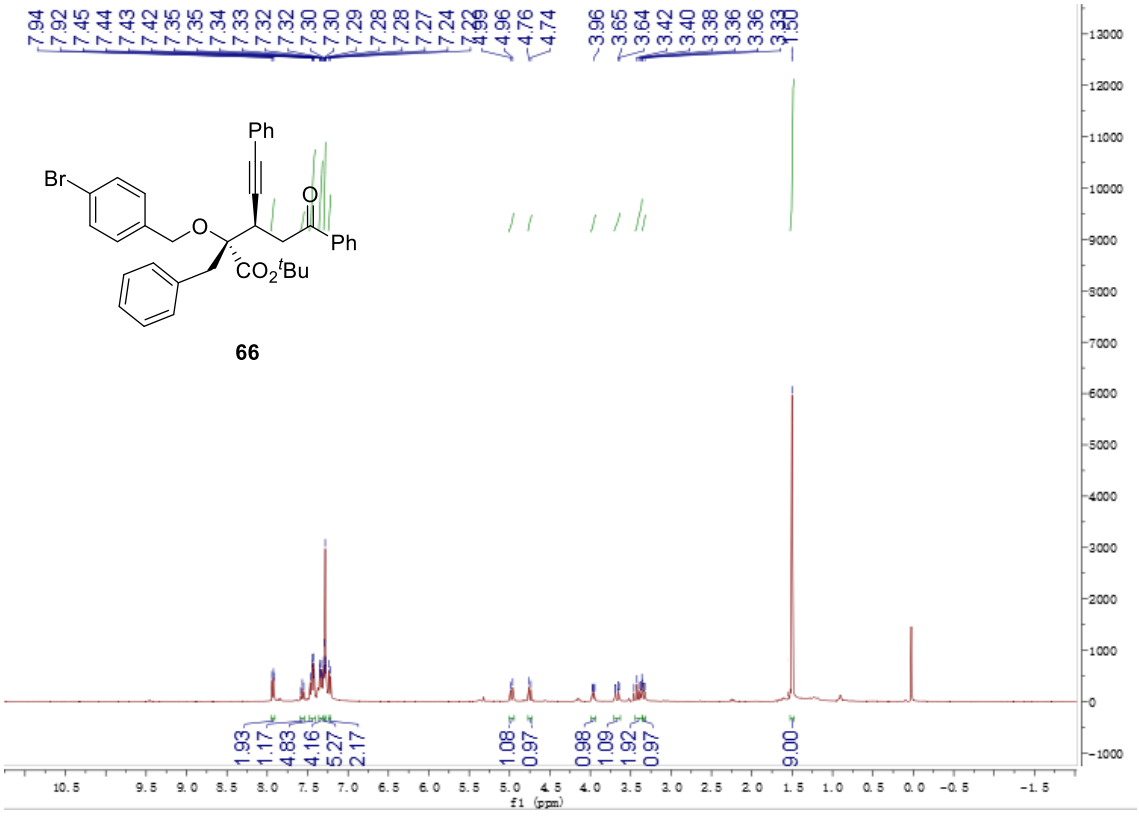
**64**


7.88
7.86
7.56
7.54
7.52
7.46
7.45
7.44
7.42
7.41
7.34
7.33
7.28
7.25
7.24
4.94
4.92
4.82
4.80
4.30
4.28
3.36
3.34
3.33
3.31
3.26
3.23
3.19
3.17
1.54
Ph
Br
O
Ph
CO2tBu
S
2.09
2.17
4.26
2.07
4.17
4.19
1.00
0.97
1.09
0.97
1.12
9.10
f1 (ppm)

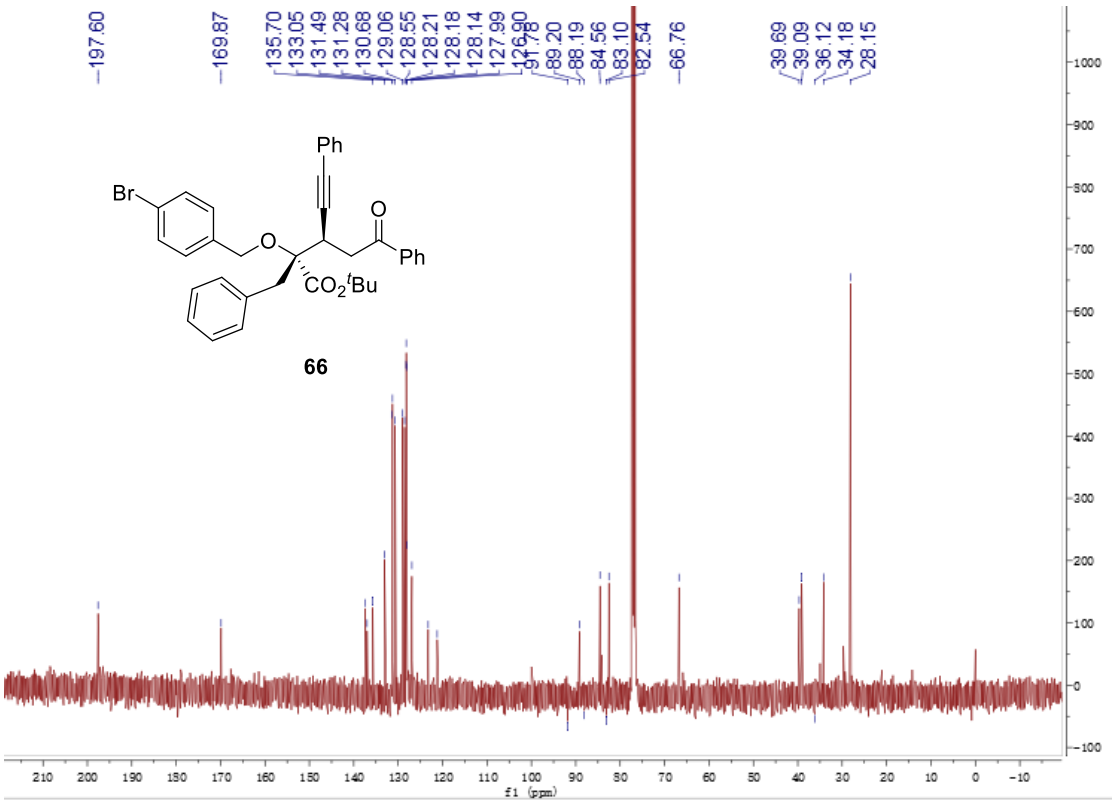
**65**

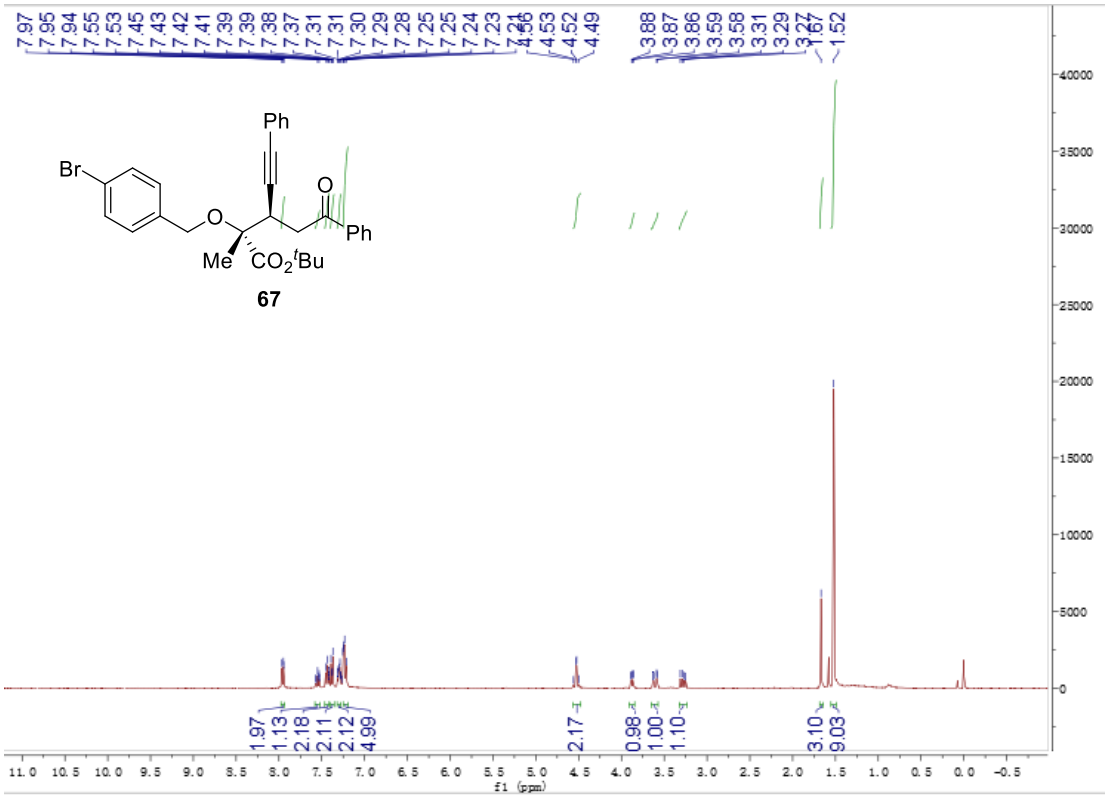

197.36
169.05
139.49
138.00
136.93
133.14
131.43
131.37
129.06
128.58
128.19
127.94
126.81
125.61
124.20
123.30
89.16
84.79
84.15
83.04
67.80
39.10
37.57
28.13
28.07
Ph
Br
O
Ph
CO2tBu
S
f1 (ppm)

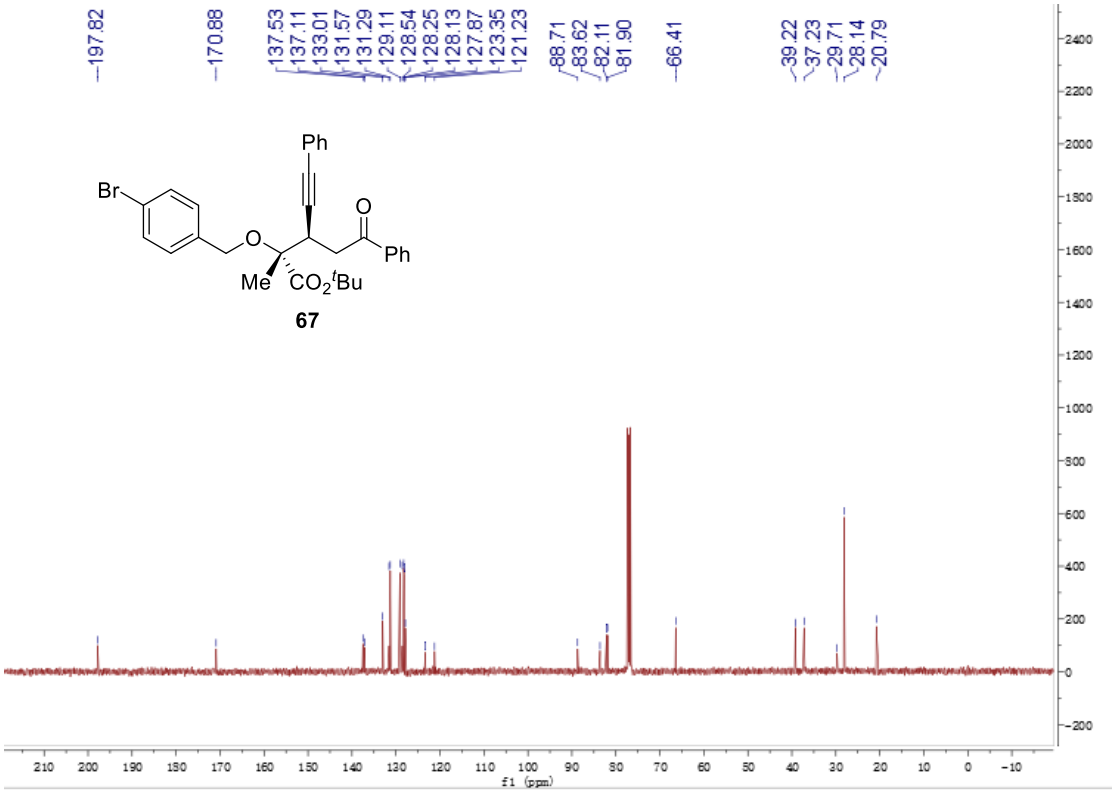
**65**

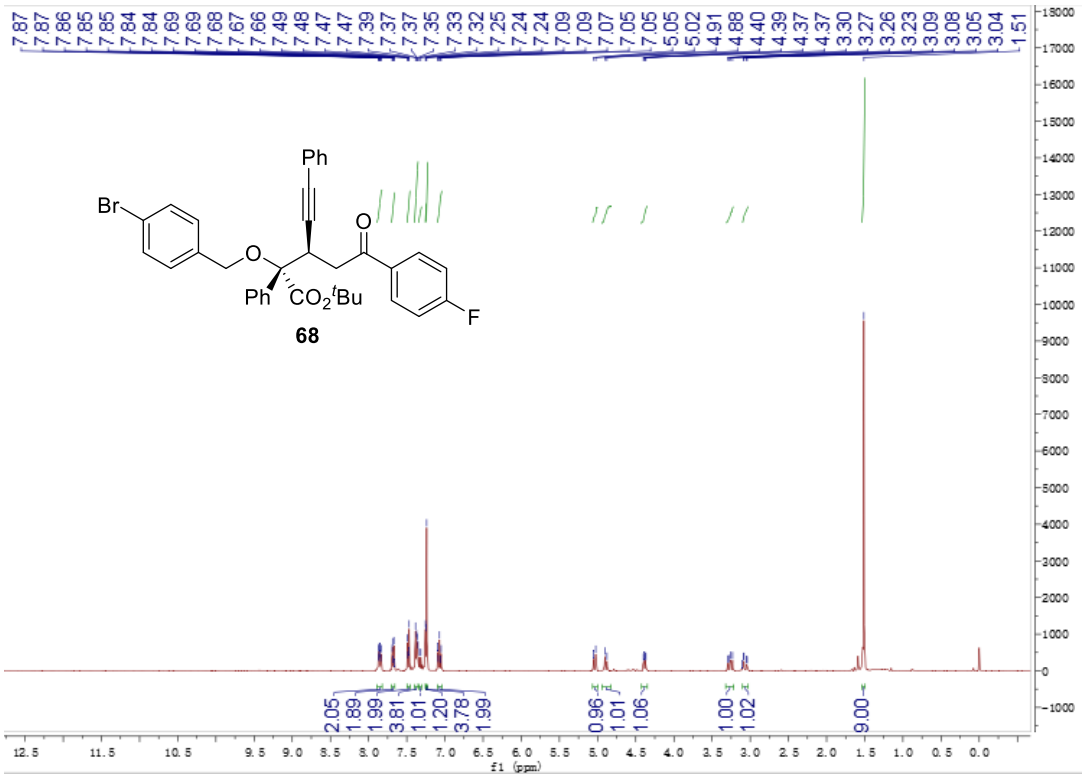

7.94
7.92
7.45
7.44
7.43
7.42
7.35
7.35
7.34
7.33
7.32
7.32
7.30
7.30
7.29
7.28
7.28
7.27
7.24
4.96
4.76
4.74
3.96
3.65
3.64
3.42
3.40
3.38
3.36
3.36
1.50
Ph
Br
O
O
Ph
CO2tBu
1.93
1.17
4.83
4.16
5.27
2.17
1.08
0.97
0.98
1.09
1.92
0.97
9.00
f1 (ppm)

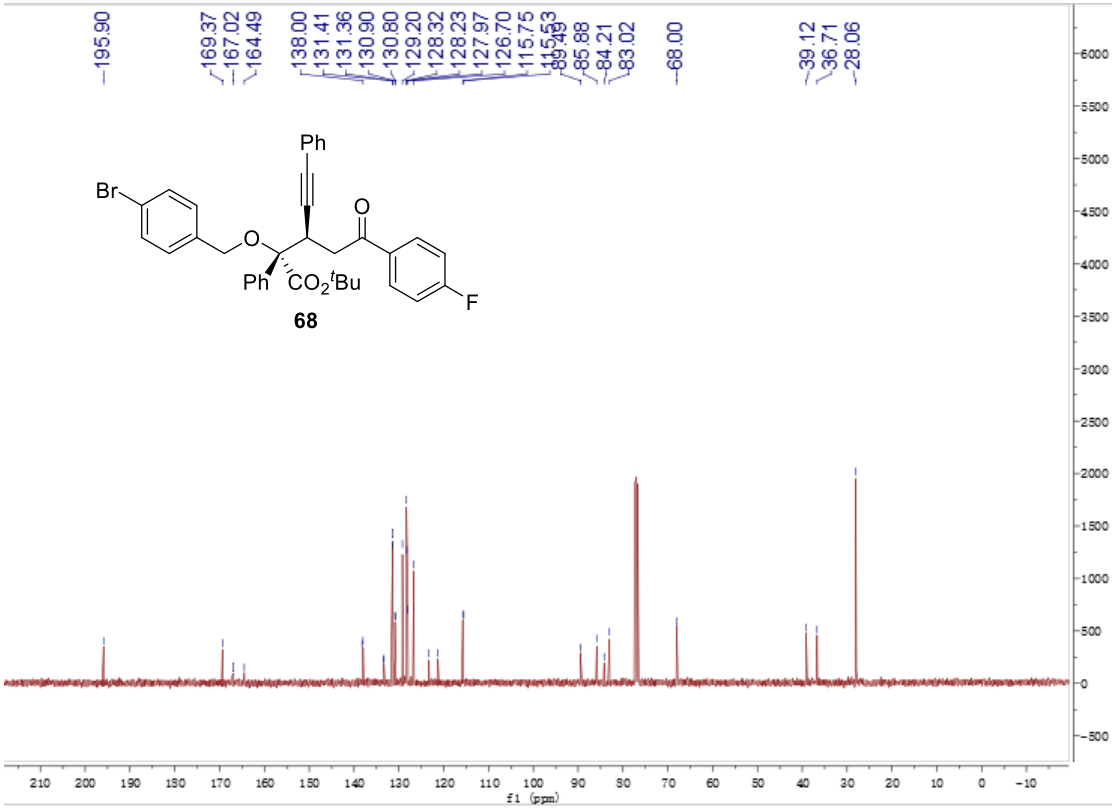
**66**

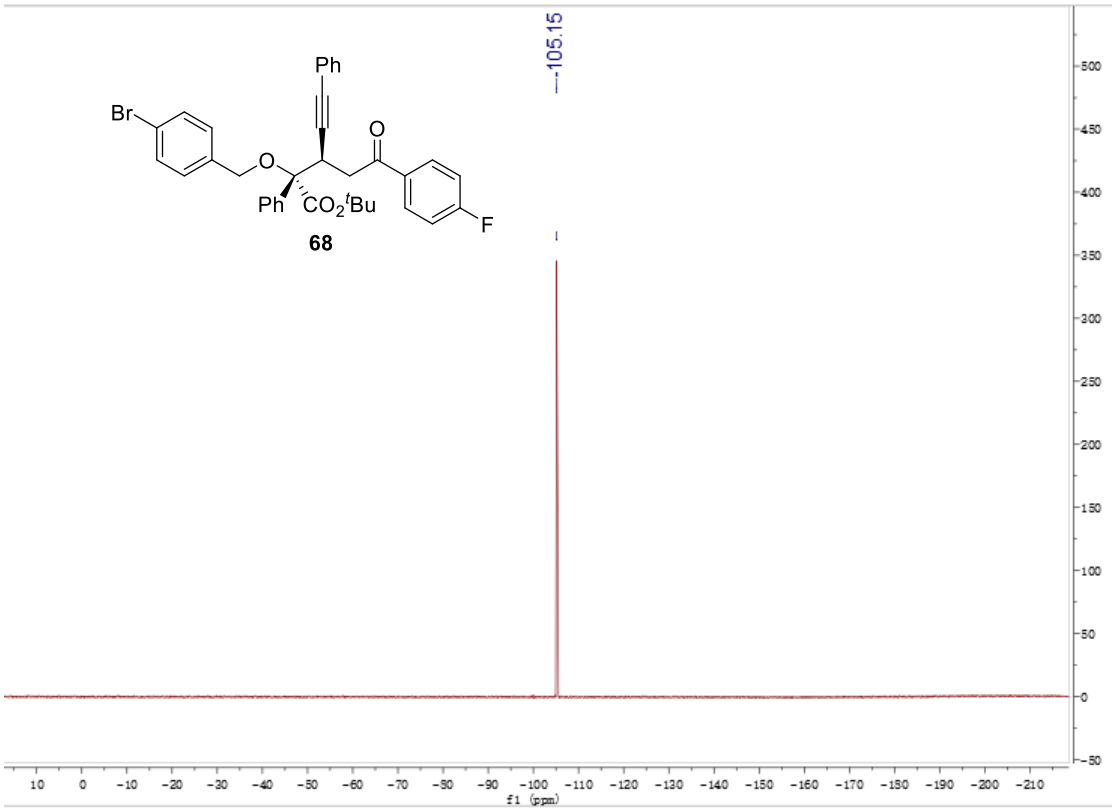

197.60
169.87
135.70
133.05
131.49
131.28
130.68
129.06
128.55
128.21
128.18
128.14
127.99
126.90
91.78
89.20
88.19
84.56
83.10
82.54
66.76
39.69
39.09
36.12
34.18
28.15
Ph
Br
O
Ph
CO2tBu
66

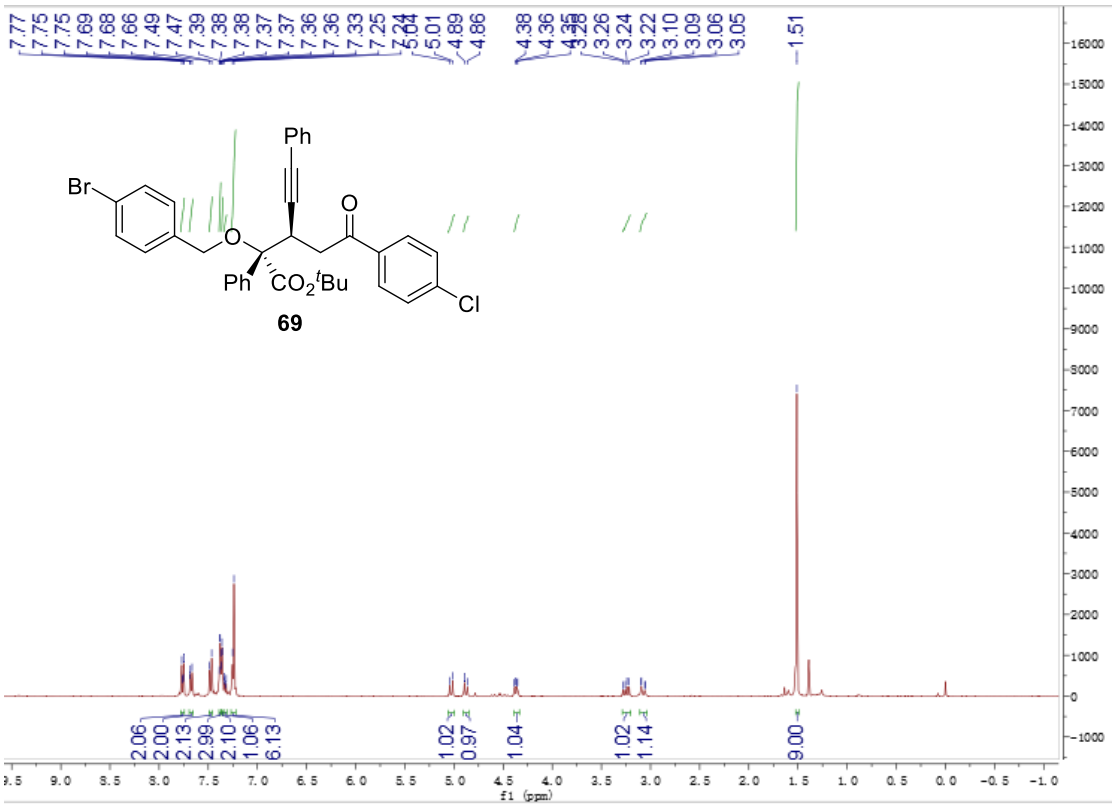

7.97
7.95
7.94
7.55
7.53
7.45
7.43
7.42
7.41
7.39
7.39
7.38
7.37
7.31
7.31
7.30
7.29
7.28
7.25
7.25
7.24
7.23
4.53
4.52
4.49
3.88
3.87
3.86
3.59
3.58
3.31
3.29
1.67
1.52
Ph
Br
O
O
Ph
Me
CO2tBu
67
1.97
1.13
2.18
2.11
2.12
4.99
2.17
0.98
1.00
1.10
3.10
9.03

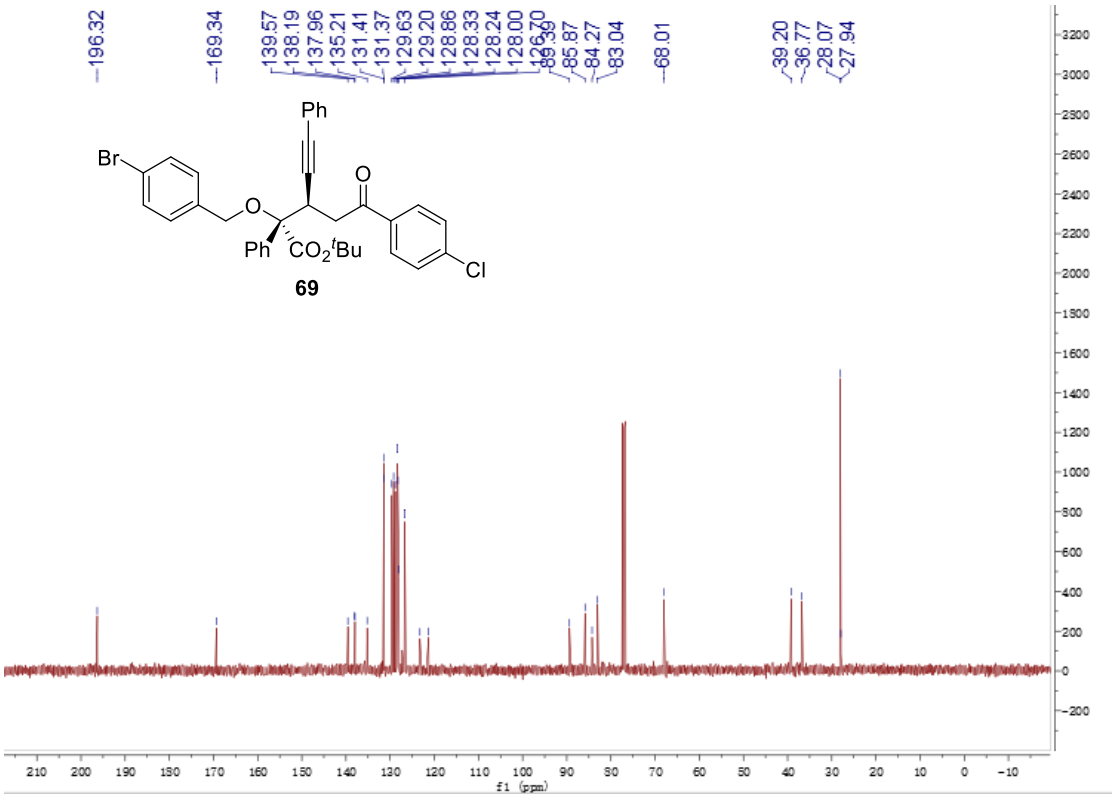

197.82
170.88
137.53
137.11
133.01
131.57
131.29
129.11
128.54
128.25
128.13
127.87
123.35
121.23
88.71
83.62
82.11
81.90
66.41
39.22
37.23
29.71
28.14
20.79
Ph
Br
O
O
Ph
Me
CO2tBu
67

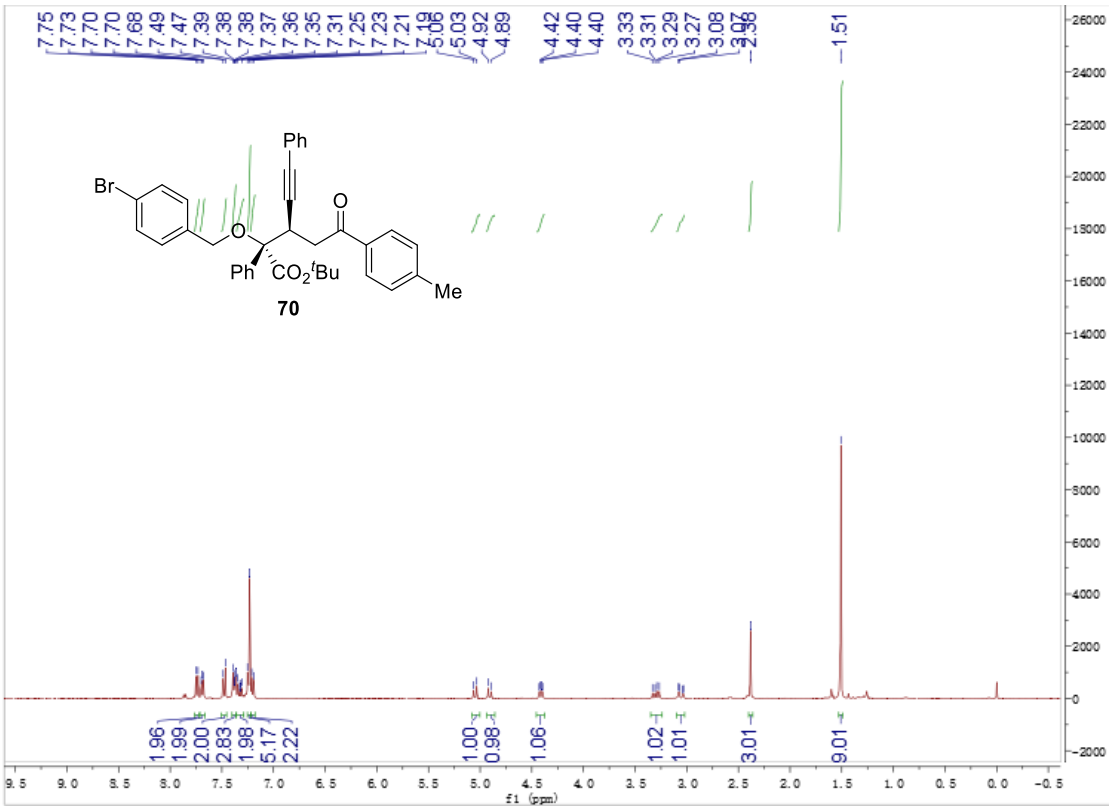

7.87
7.87
7.86
7.85
7.84
7.84
7.69
7.69
7.68
7.67
7.66
7.49
7.48
7.47
7.47
7.39
7.37
7.37
7.35
7.33
7.32
7.25
7.24
7.24
7.09
7.09
7.07
7.05
7.05
5.05
5.02
4.91
4.88
4.40
4.39
4.37
4.37
3.30
3.27
3.26
3.23
3.09
3.08
3.05
3.04
1.51
Ph
Br
O
O
Ph
CO2tBu
F
68
2.05
1.89
1.99
3.81
1.01
1.20
3.78
1.99
0.96
1.01
1.06
1.00
1.02
9.00

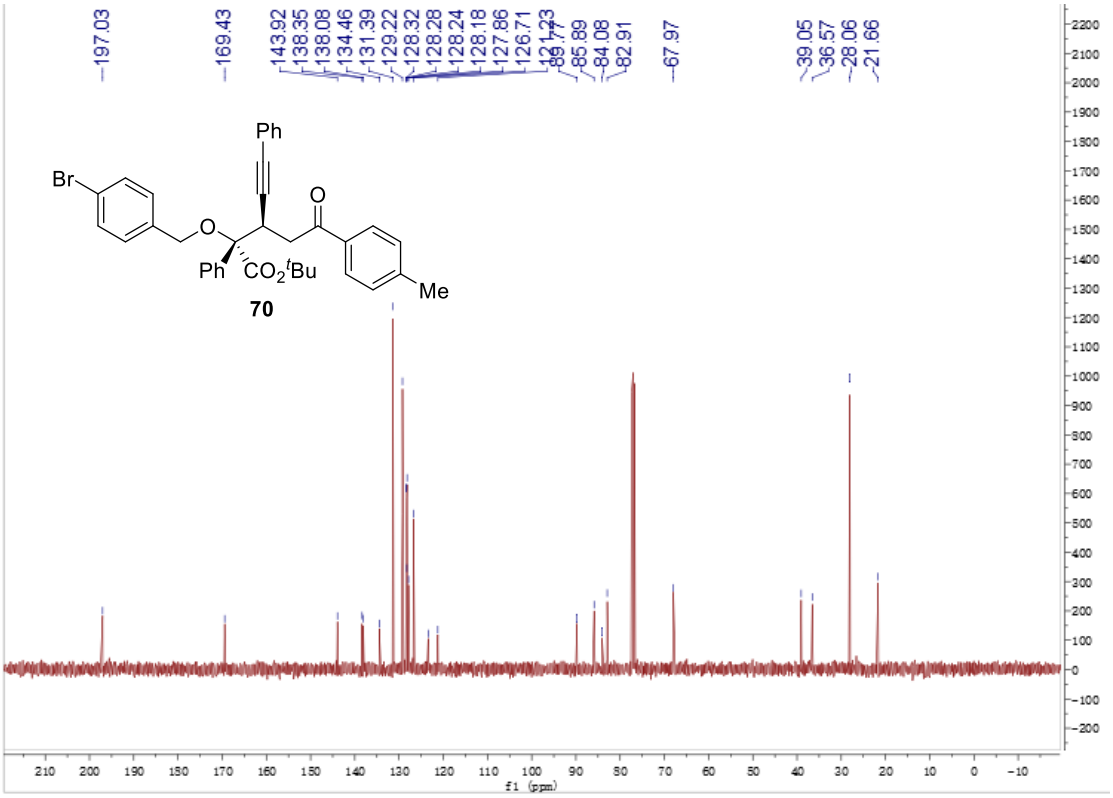

195.90
169.37
167.02
164.49
138.00
131.41
131.36
130.90
130.80
129.20
128.32
128.23
127.97
126.70
115.75
115.53
89.49
85.88
84.21
83.02
68.00
39.12
36.71
28.06
Ph
Br
O
O
Ph
CO2tBu
F
68
f1 (ppm)

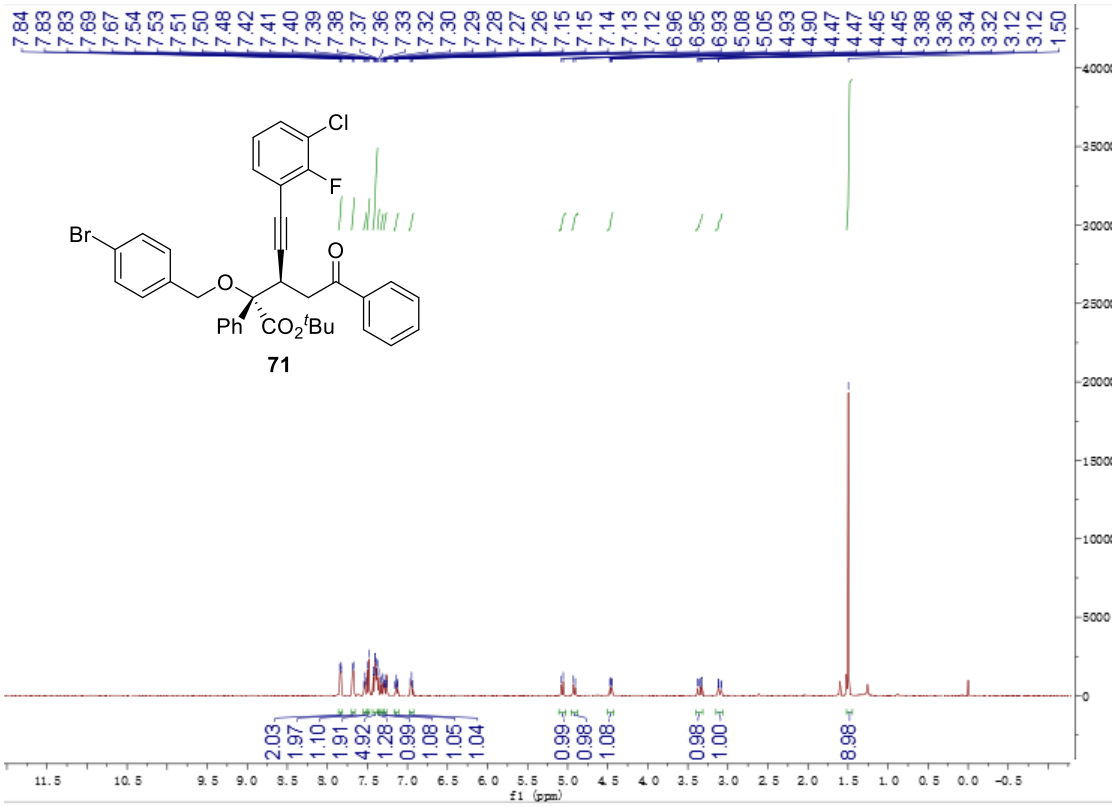

105.15
Ph
Br
O
O
Ph
CO2tBu
F
68
f1 (ppm)

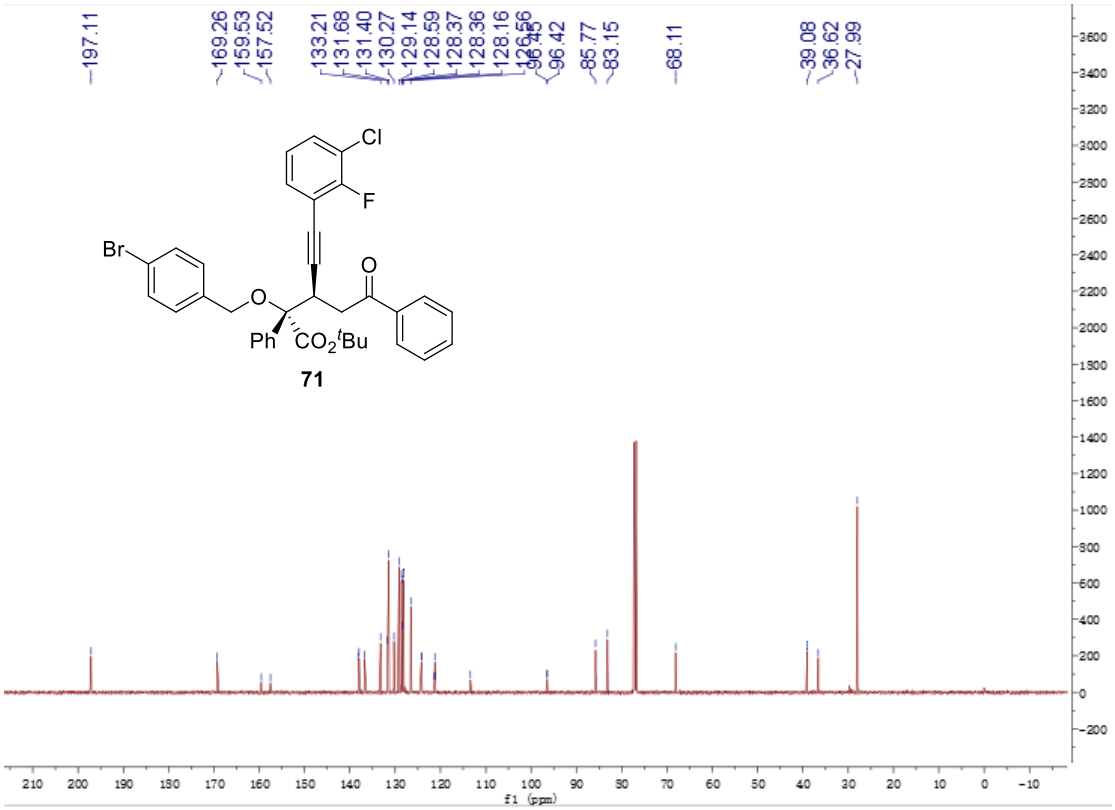

Ph
Br
O
Ph
CO2tBu
Cl
69

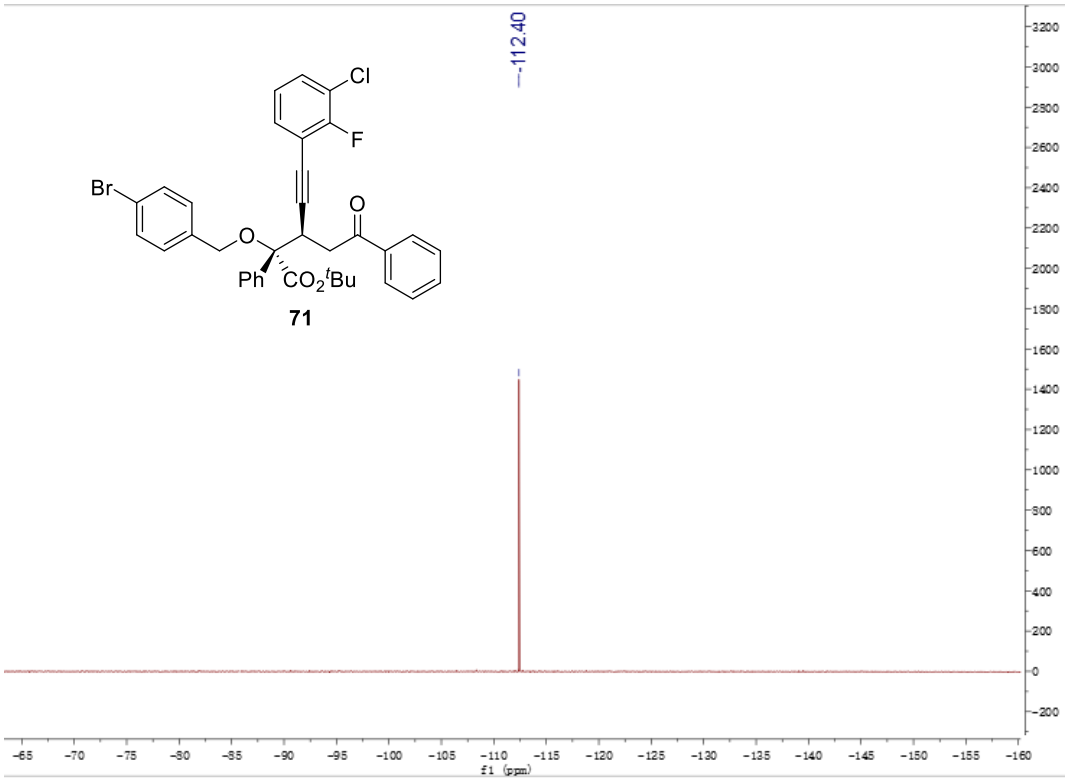

Ph
Br
O
Ph
CO2tBu
Cl
69

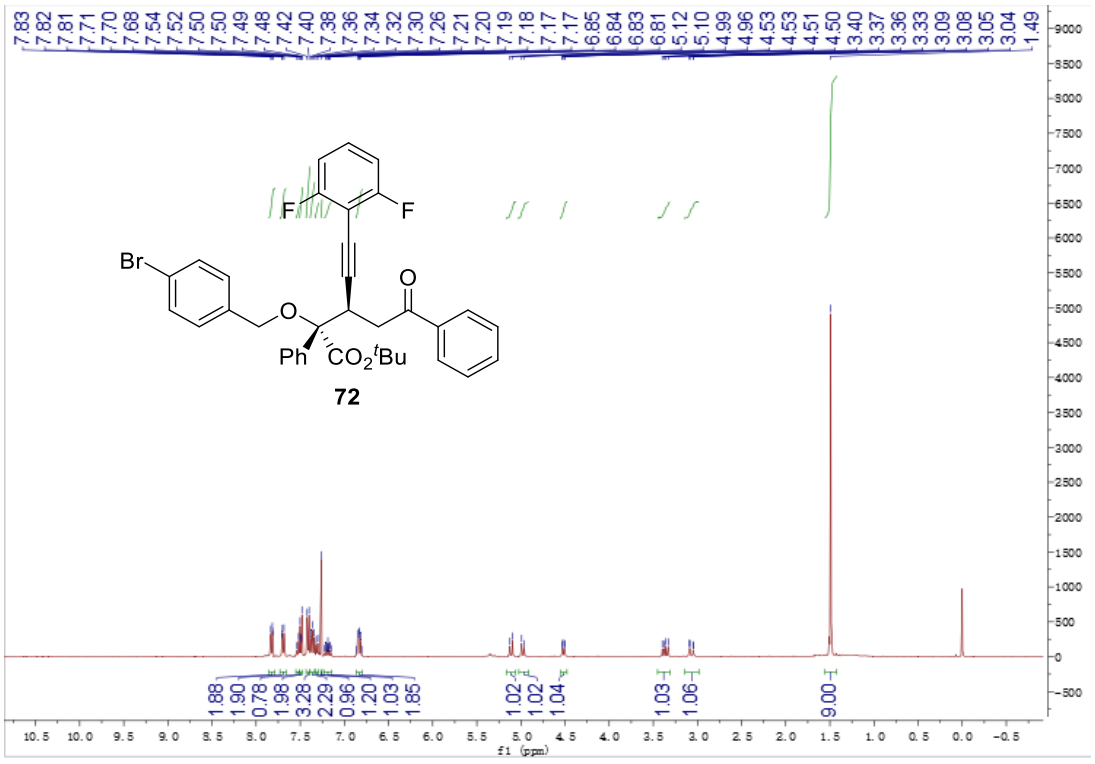

Ph
Br
O
Ph
CO2tBu
Me
70

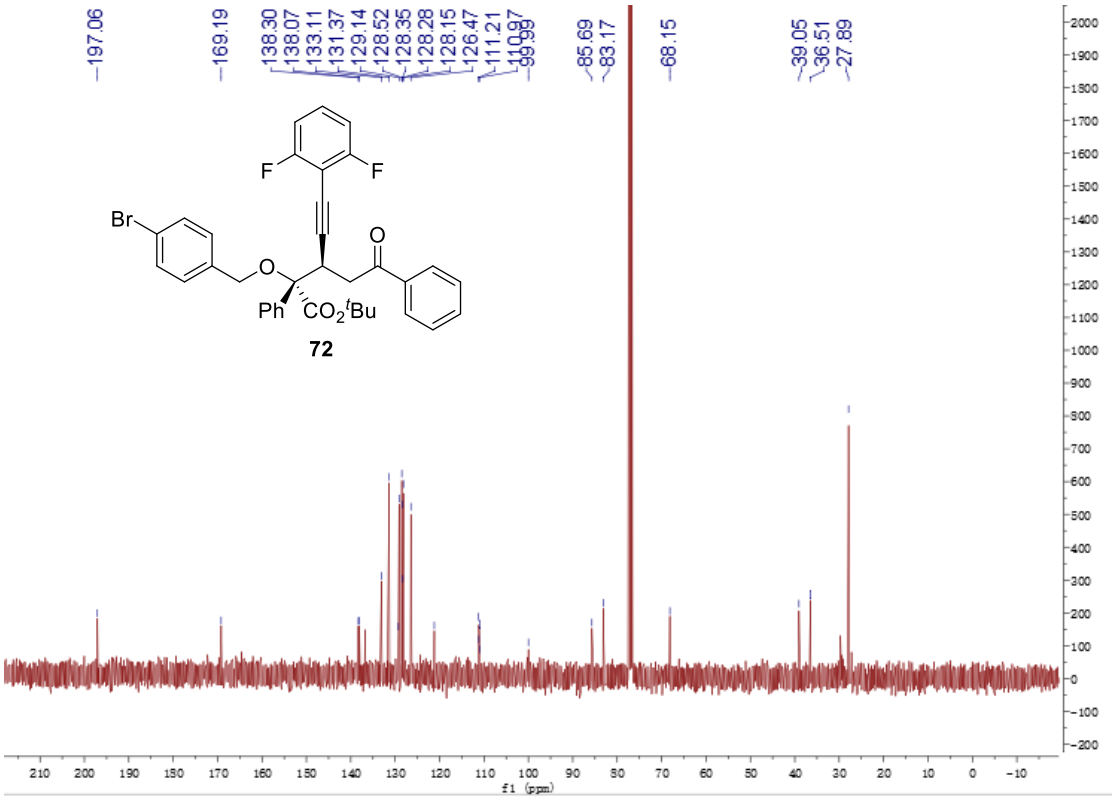

Ph
Br
O
Ph
CO2tBu
Me
70

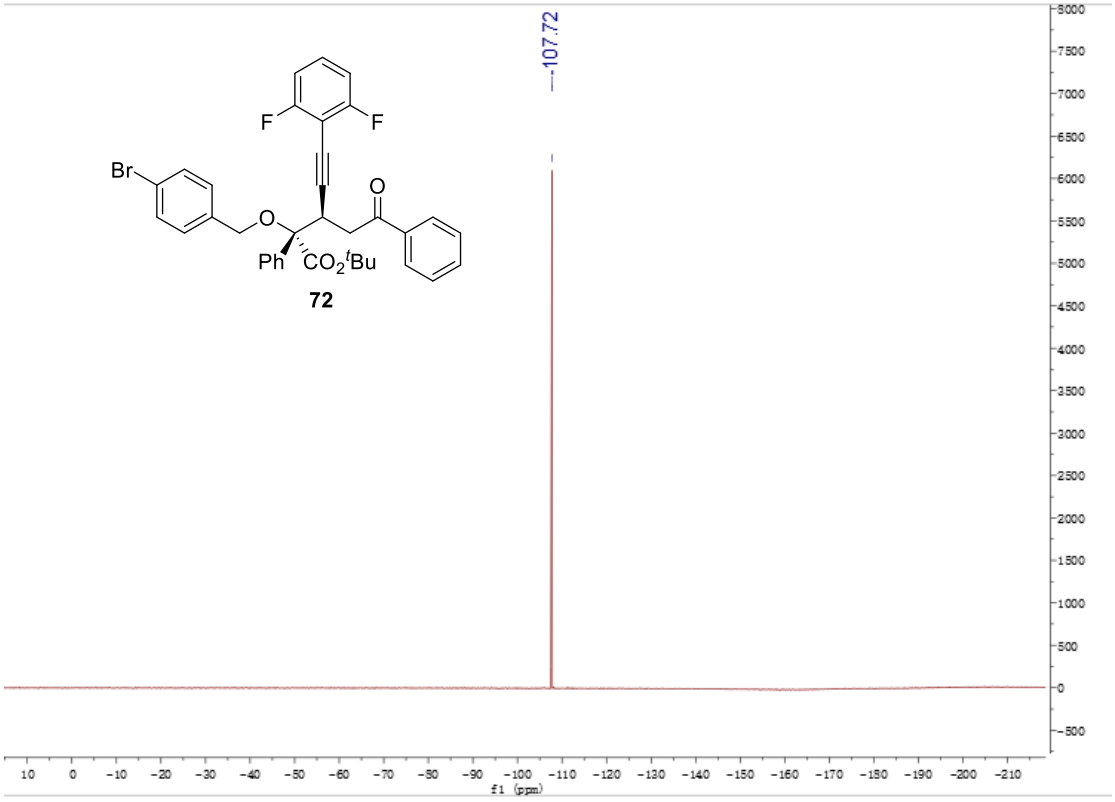

Cl
F
Br
O
O
Ph
CO2tBu
71

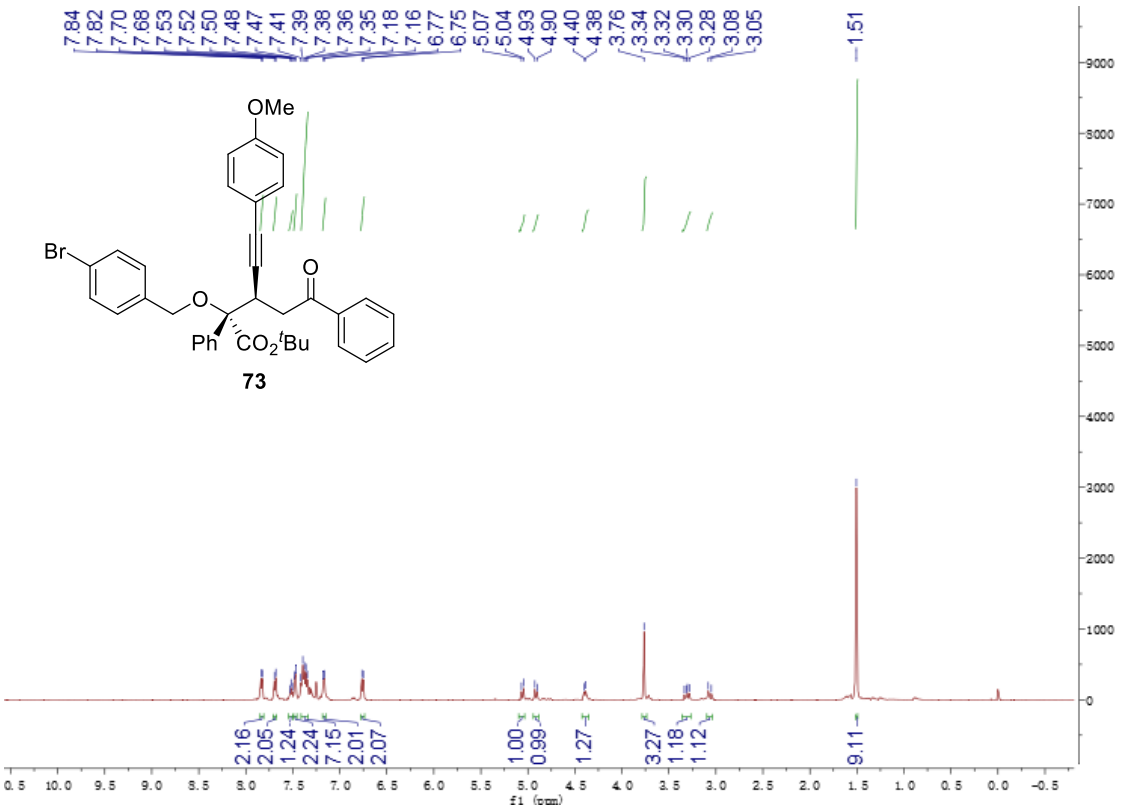

Cl
F
Br
O
O
Ph
CO2tBu
71

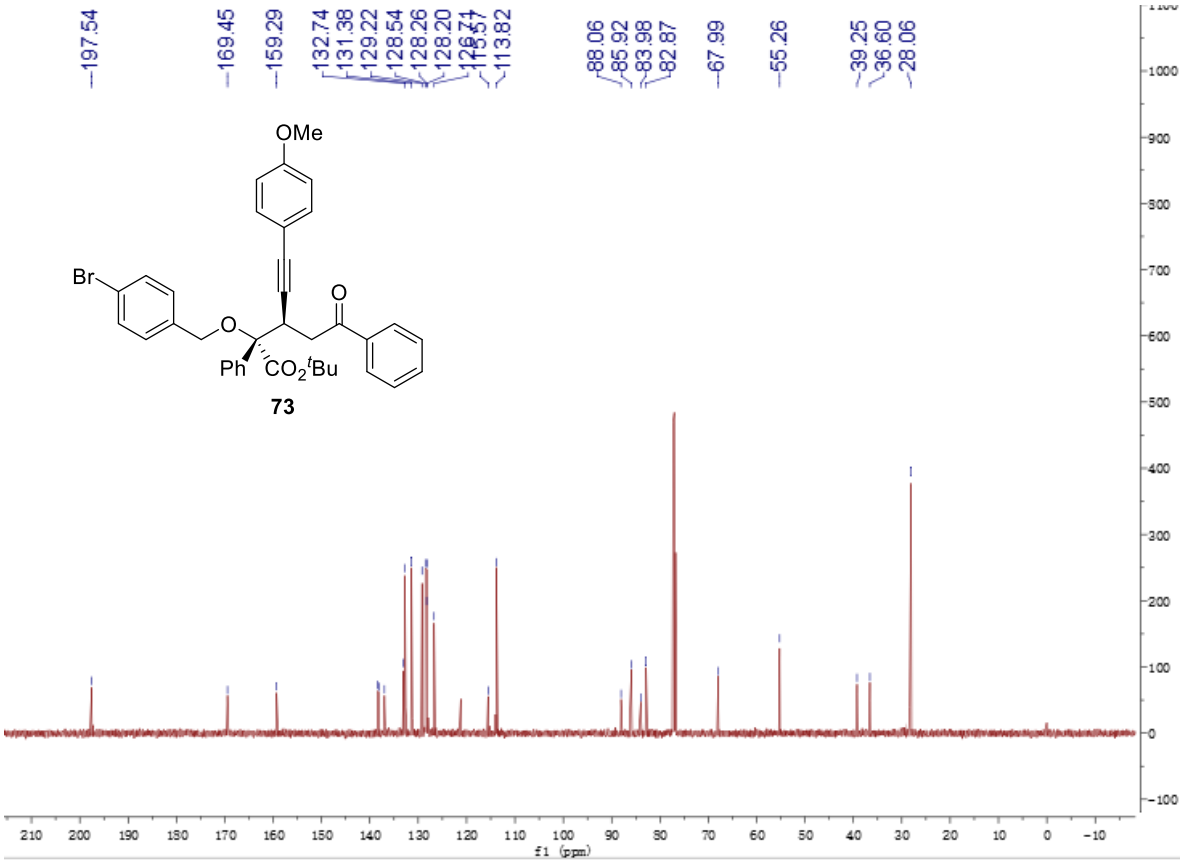

-112.40
Cl
F
Br
O
O
Ph
CO2tBu
71
f1 (ppm)

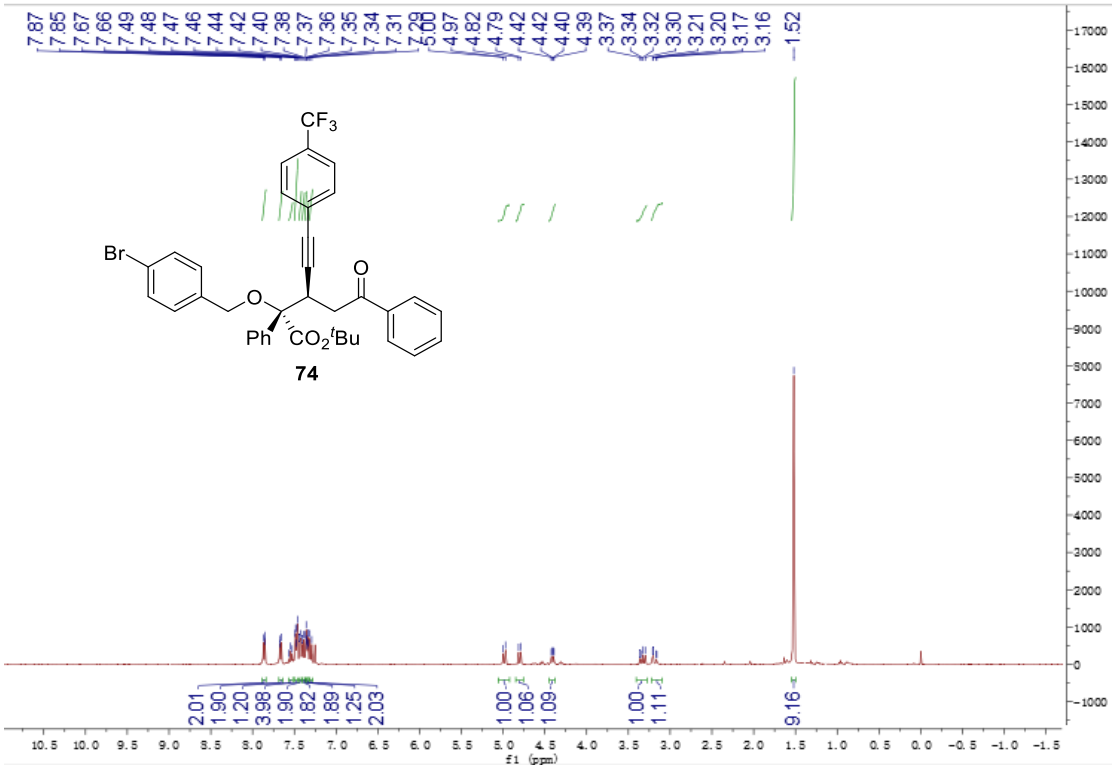

F
F
Br
O
O
Ph
CO2tBu
72
1.88
1.90
0.78
1.98
3.28
2.29
0.96
1.20
1.03
1.85
1.02
1.02
1.04
1.03
1.06
9.00
f1 (ppm)

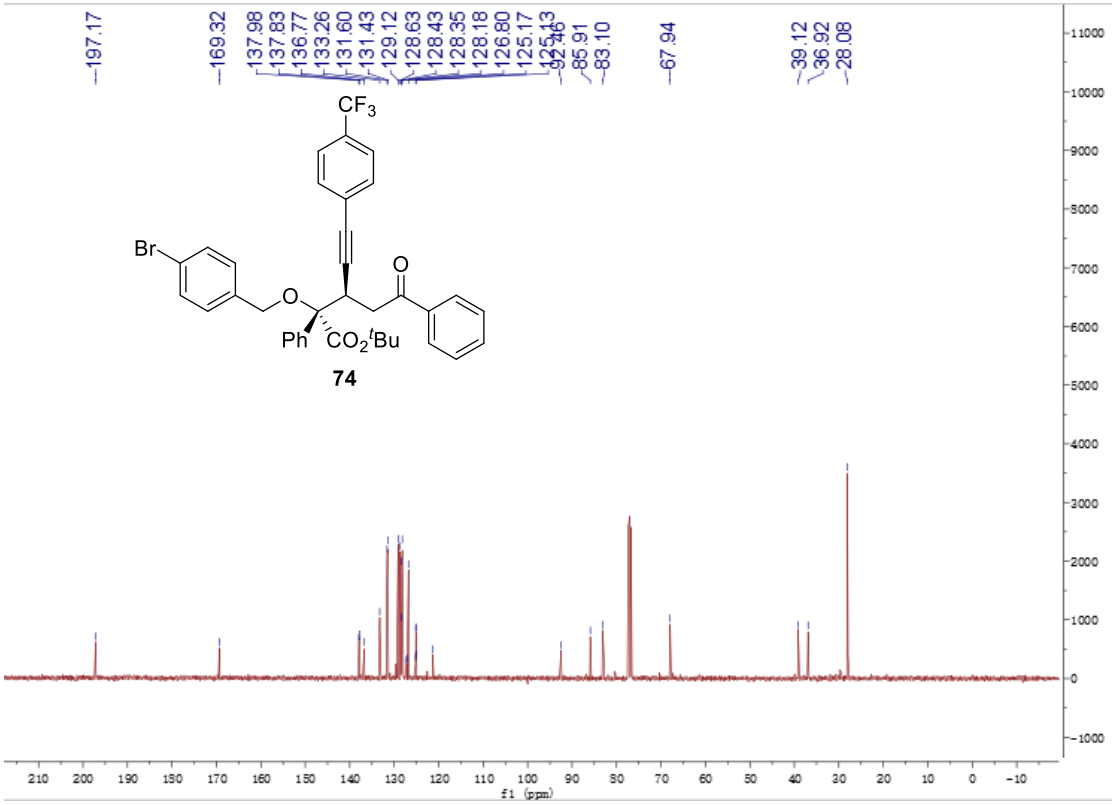

197.06
169.19
138.30
138.07
133.11
131.37
129.14
128.52
128.35
128.28
128.15
126.47
111.21
110.97
99.99
85.69
83.17
68.15
39.05
36.51
27.89
F
F
Br
O
O
Ph
CO2tBu
72
f1 (ppm)

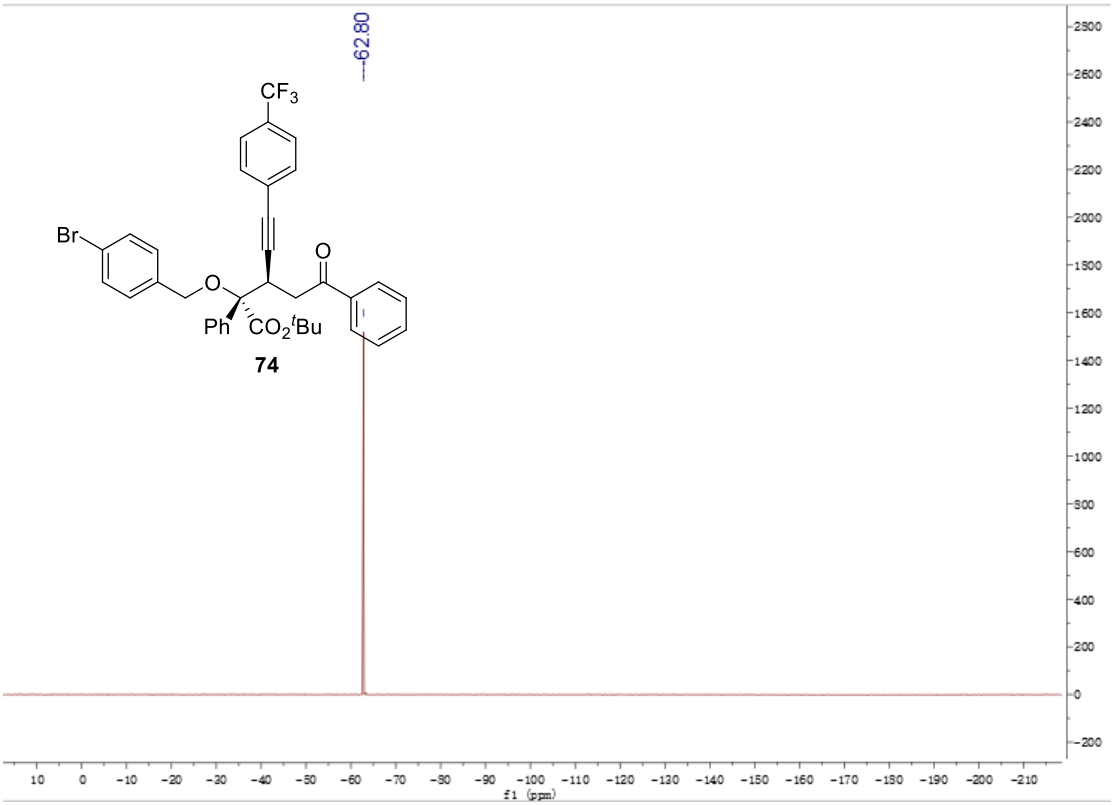

107.72
F
F
Br
O
O
Ph
CO2tBu
72
f1 (ppm)

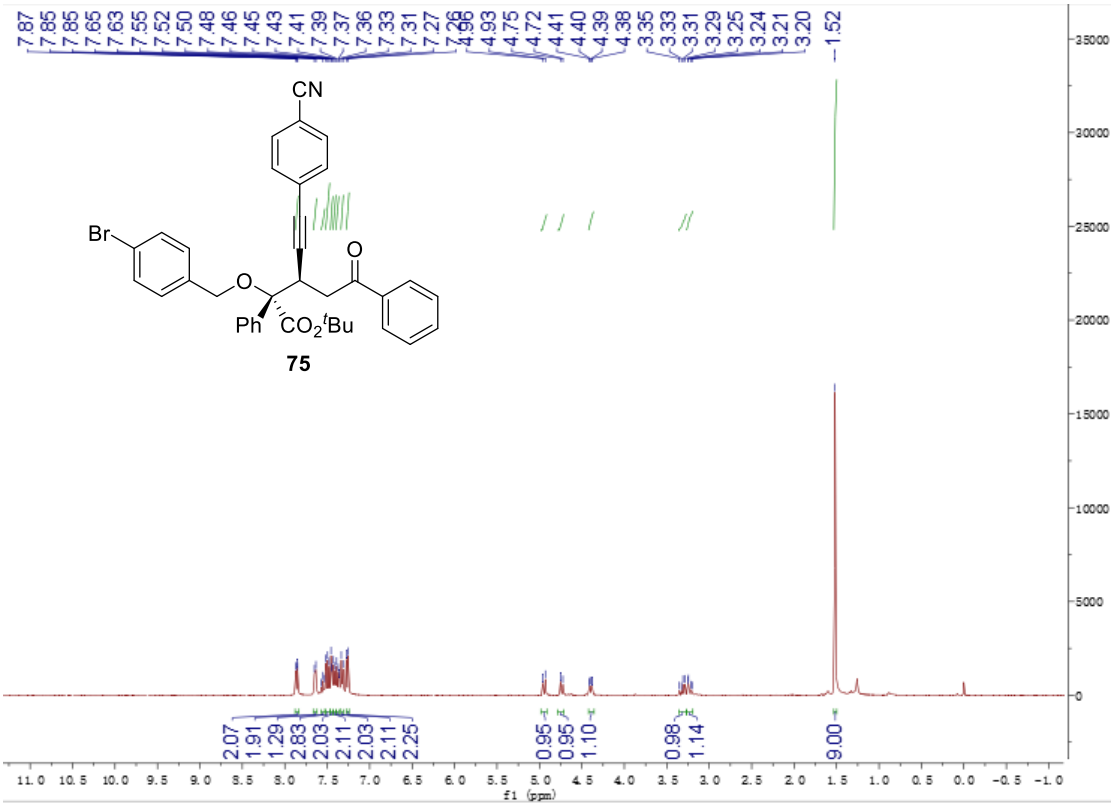

7.84
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7.70
7.68
7.53
7.52
7.50
7.48
7.47
7.41
7.39
7.38
7.36
7.35
7.18
7.16
6.77
6.75
5.07
5.04
4.93
4.90
4.40
4.38
3.76
3.34
3.32
3.30
3.28
3.08
3.05
1.51
OMe
Br
O
O
Ph
CO2tBu
73
2.16
2.05
1.24
2.24
7.15
2.01
2.07
1.00
0.99
1.27
3.27
1.18
1.12
9.11
f1 (ppm)

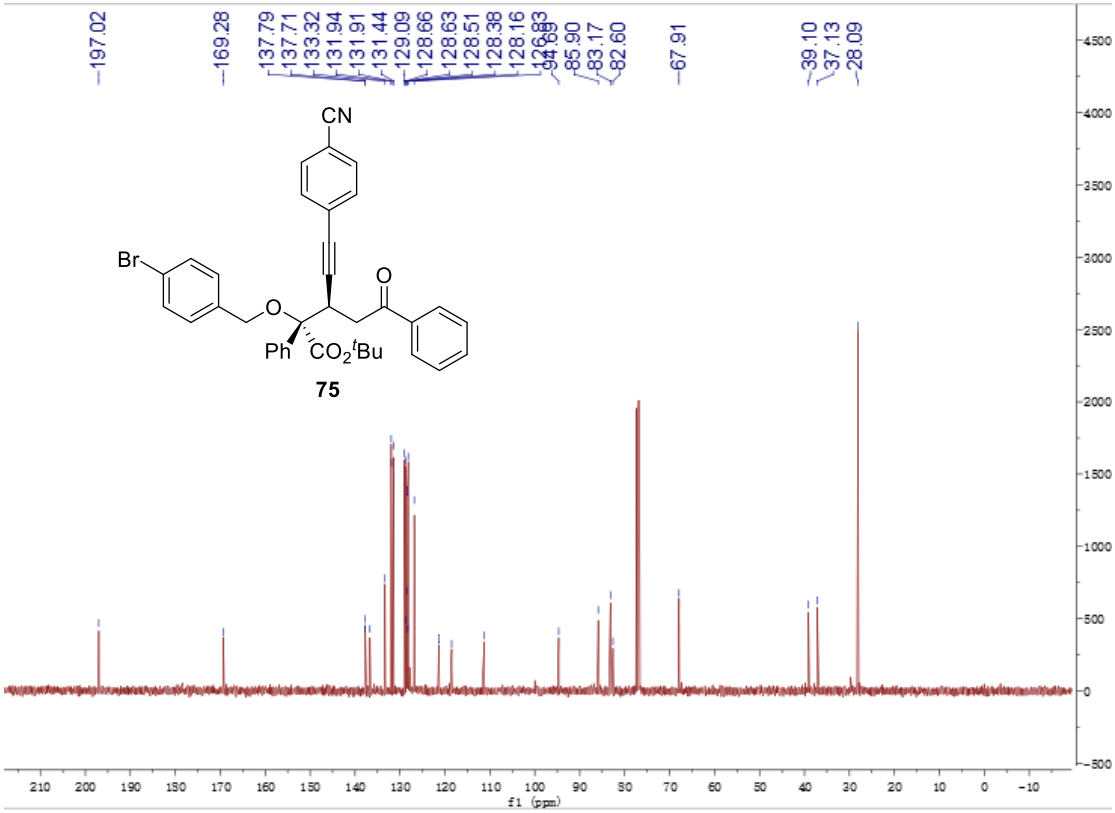

197.54
169.45
159.29
132.74
131.38
129.22
128.54
128.26
128.20
126.71
115.57
113.82
88.06
85.92
83.98
82.87
67.99
55.26
39.25
36.60
28.06
OMe
Br
O
O
Ph
CO2tBu
73
f1 (ppm)

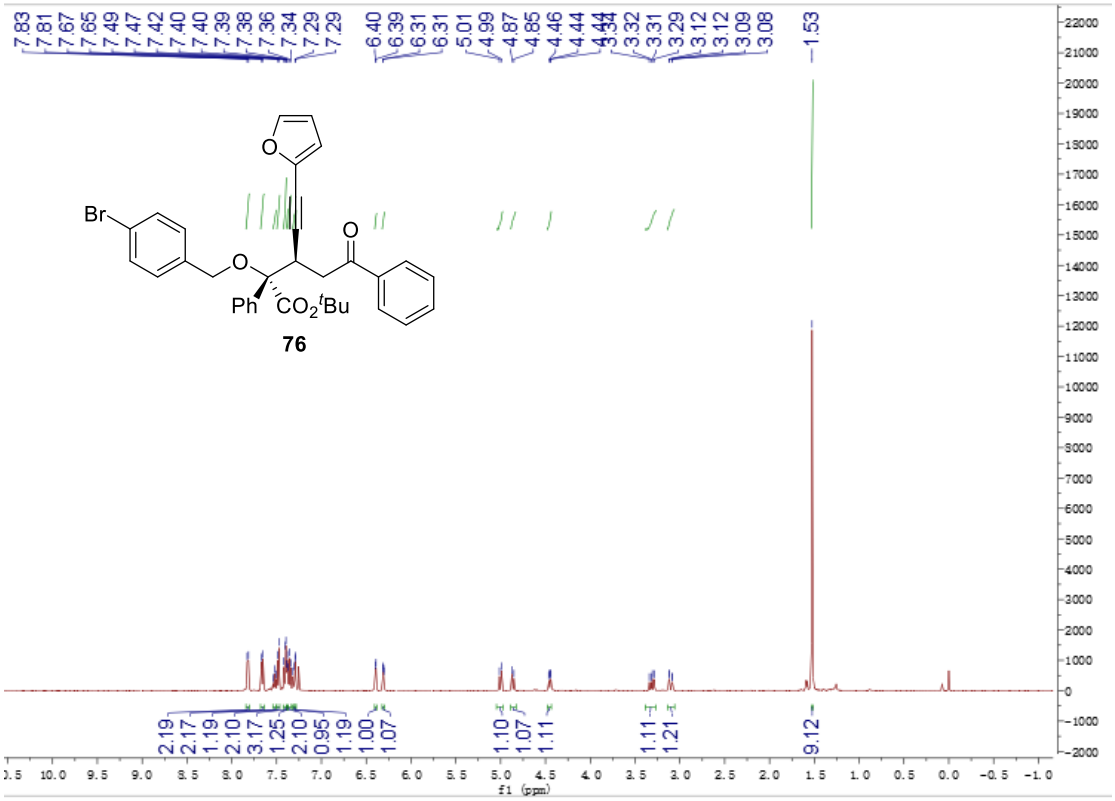

7.87
7.85
7.67
7.66
7.49
7.48
7.47
7.46
7.44
7.42
7.40
7.38
7.37
7.36
7.35
7.34
7.31
7.29
5.00
4.97
4.82
4.79
4.42
4.42
4.40
4.39
3.37
3.34
3.32
3.30
3.21
3.20
3.17
3.16
1.52
CF3
Br
O
O
Ph
CO2tBu
74
2.01
1.90
1.20
3.98
1.90
1.82
1.89
1.25
2.03
1.00
1.06
1.09
1.00
1.11
9.16
f1 (ppm)

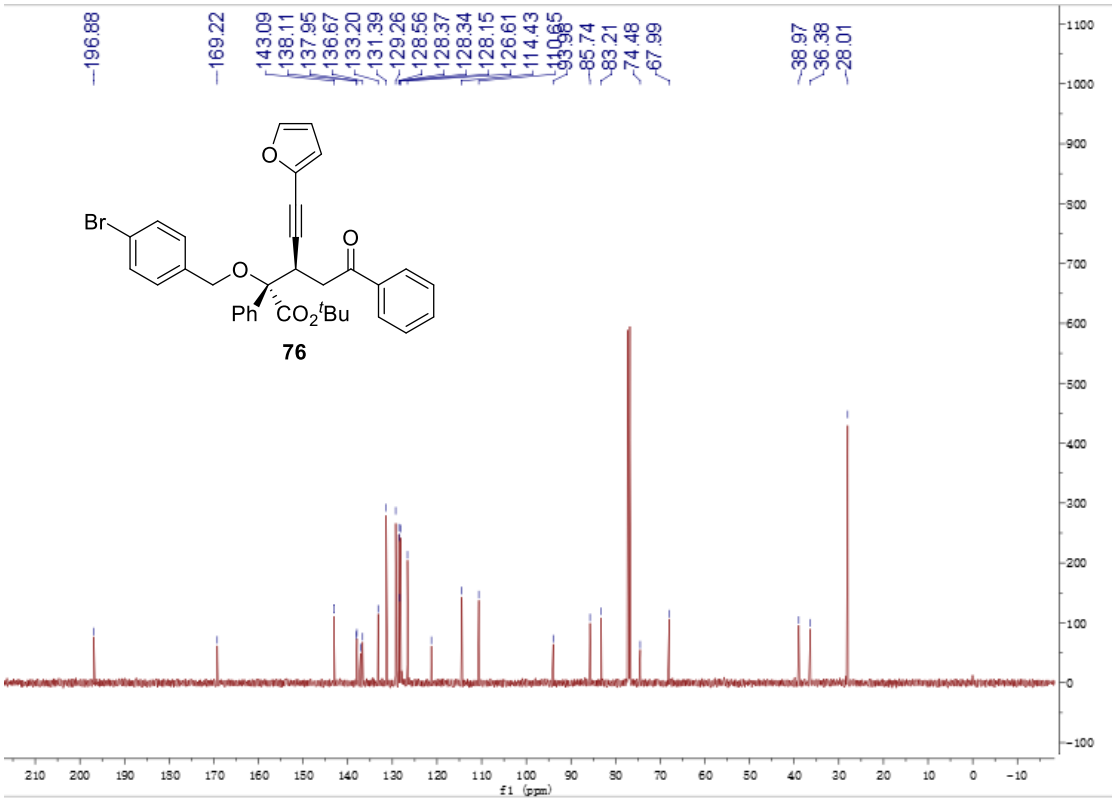

197.17
169.32
137.98
137.83
136.77
133.26
131.60
131.43
129.12
128.63
128.43
128.35
128.18
126.80
125.17
125.13
92.46
85.91
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39.12
36.92
28.08
CF3
Br
O
O
Ph
CO2tBu
74
f1 (ppm)

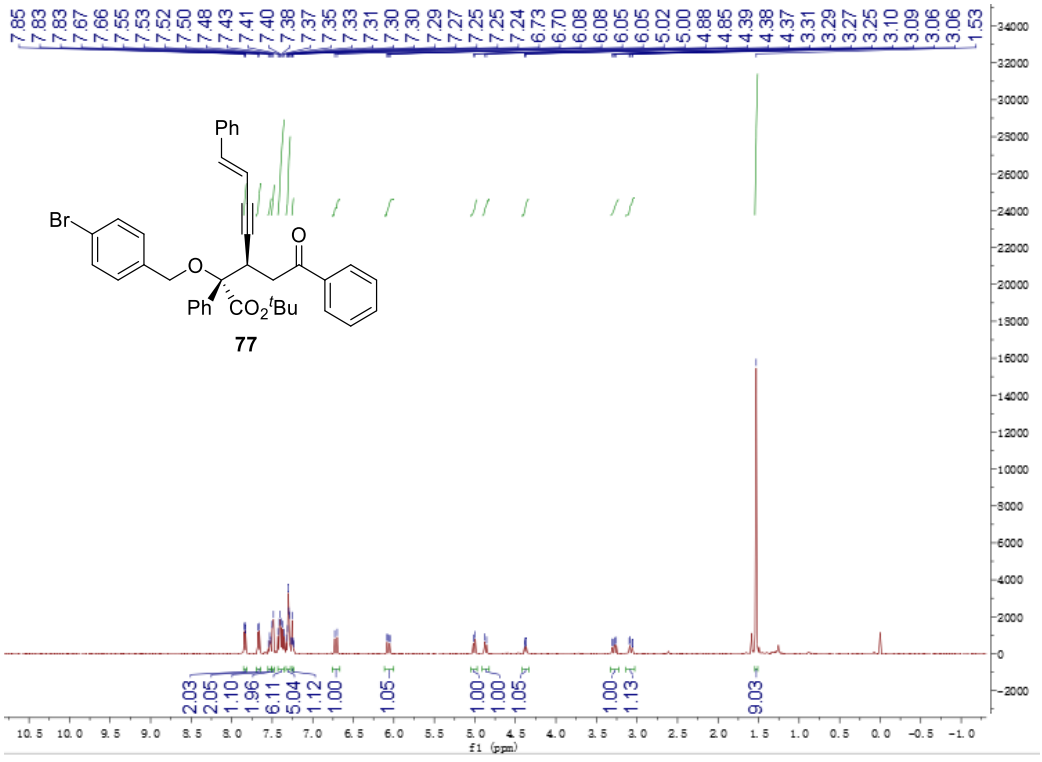

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CF3
Br
O
O
Ph
CO2tBu
74
f1 (ppm)

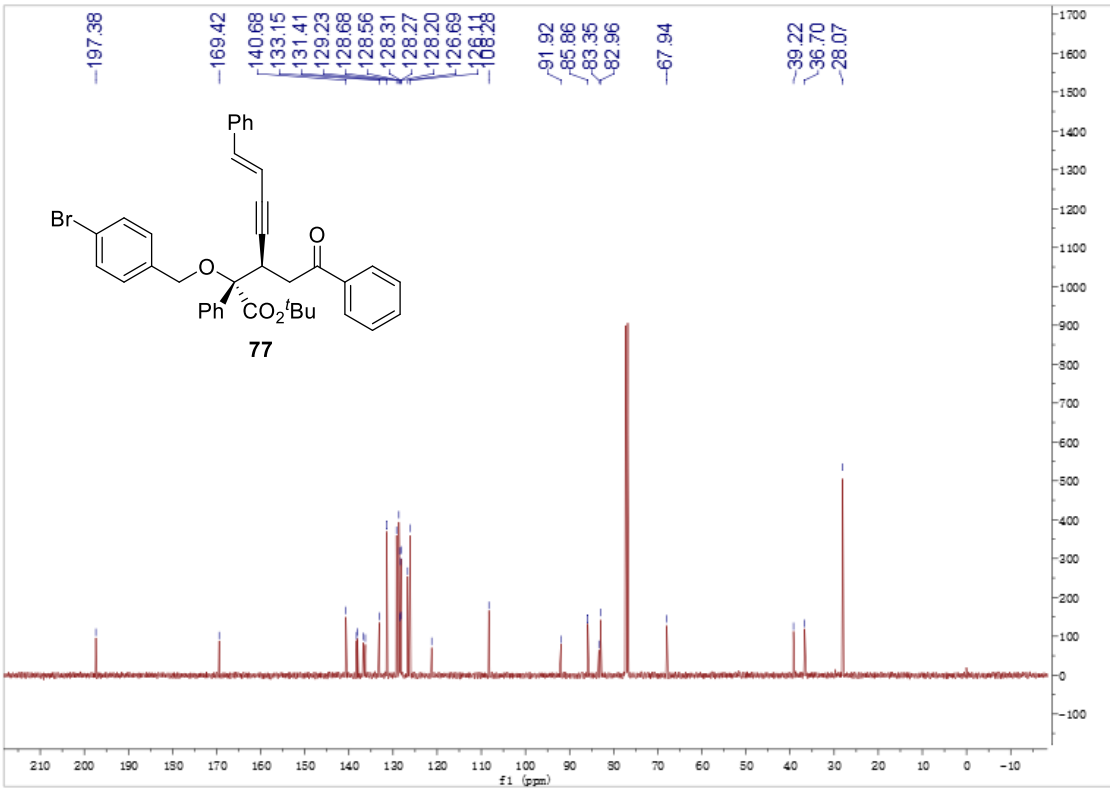

7.87
7.85
7.85
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7.55
7.52
7.50
7.48
7.46
7.45
7.43
7.41
7.39
7.37
7.36
7.33
7.31
7.27
4.96
4.93
4.75
4.72
4.41
4.40
4.39
4.38
3.35
3.33
3.31
3.29
3.25
3.24
3.21
3.20
1.52
CN
Br
O
O
Ph
CO2tBu
75
2.07
1.91
1.29
2.83
2.03
2.11
2.03
2.11
2.25
0.95
0.95
1.10
0.98
1.14
9.00
f1 (ppm)

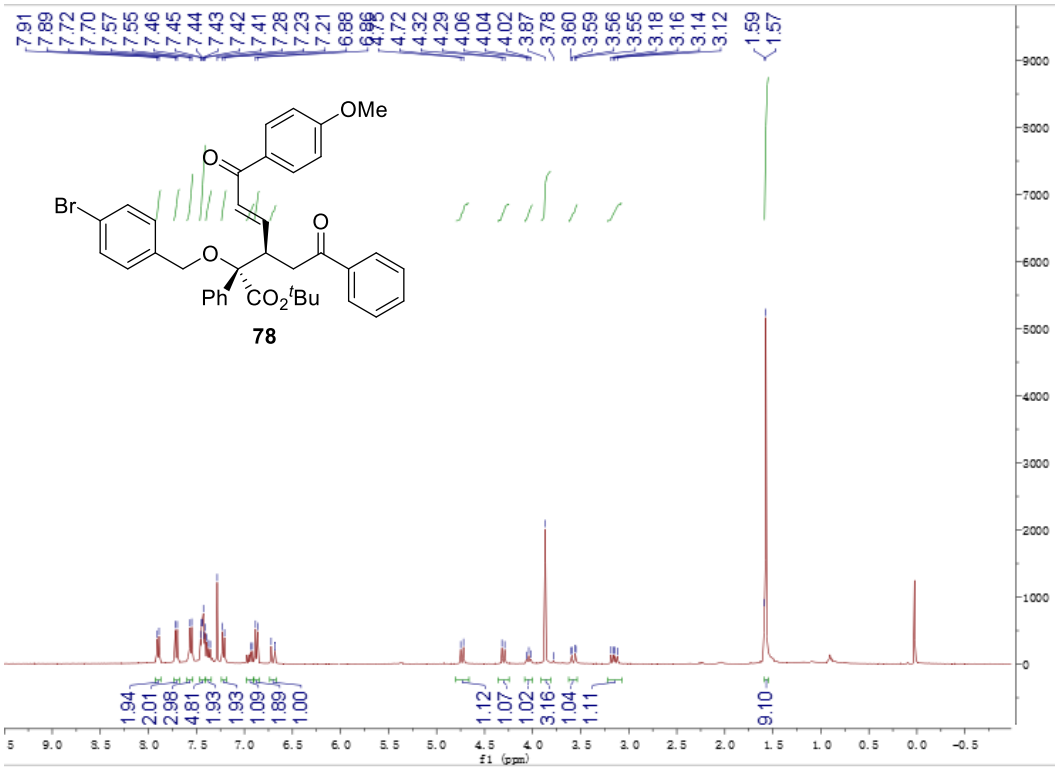

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131.91
131.44
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128.66
128.63
128.51
128.38
128.16
126.83
94.69
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82.60
67.91
39.10
37.13
28.09
CN
Br
O
O
Ph
CO2tBu
75

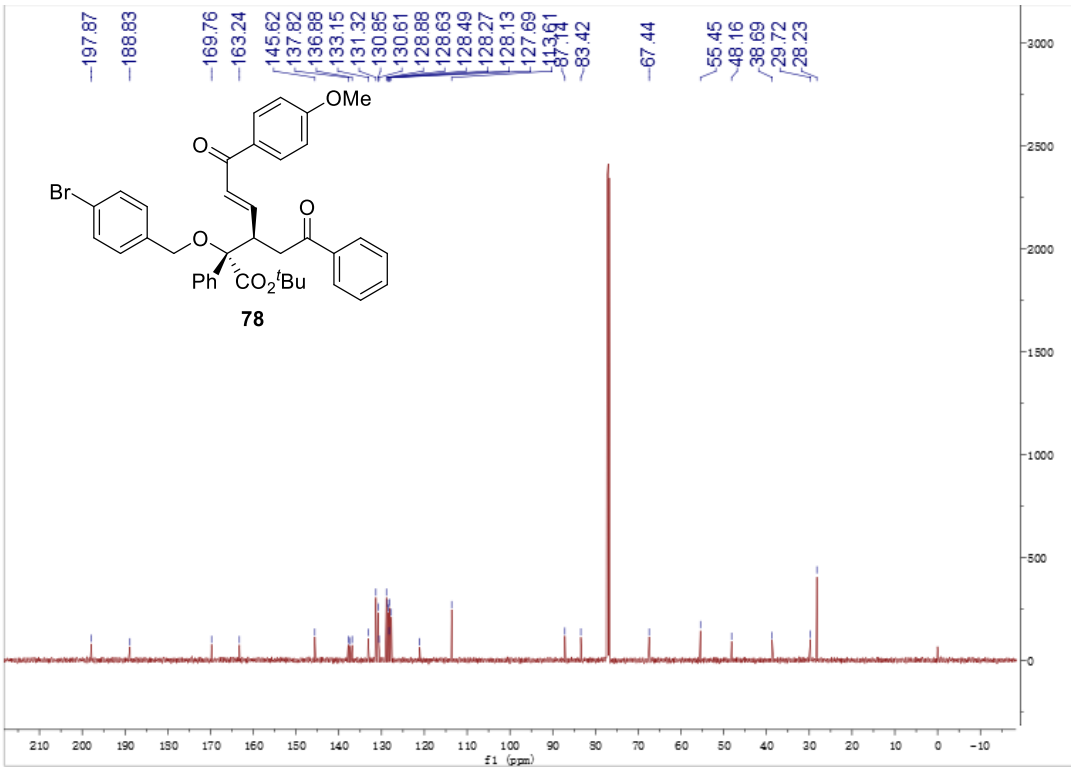

7.83
7.81
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7.47
7.42
7.40
7.40
7.39
7.38
7.36
7.34
7.29
7.29
6.40
6.39
6.31
6.31
5.01
4.99
4.87
4.85
4.46
4.44
4.44
4.34
3.32
3.31
3.29
3.12
3.12
3.09
3.08
1.53
O
Br
O
O
Ph
CO2tBu
76
2.19
2.17
1.19
2.10
3.17
1.25
2.10
0.95
1.19
1.00
1.07
1.10
1.07
1.11
1.11
1.21
9.12
f1 (ppm)

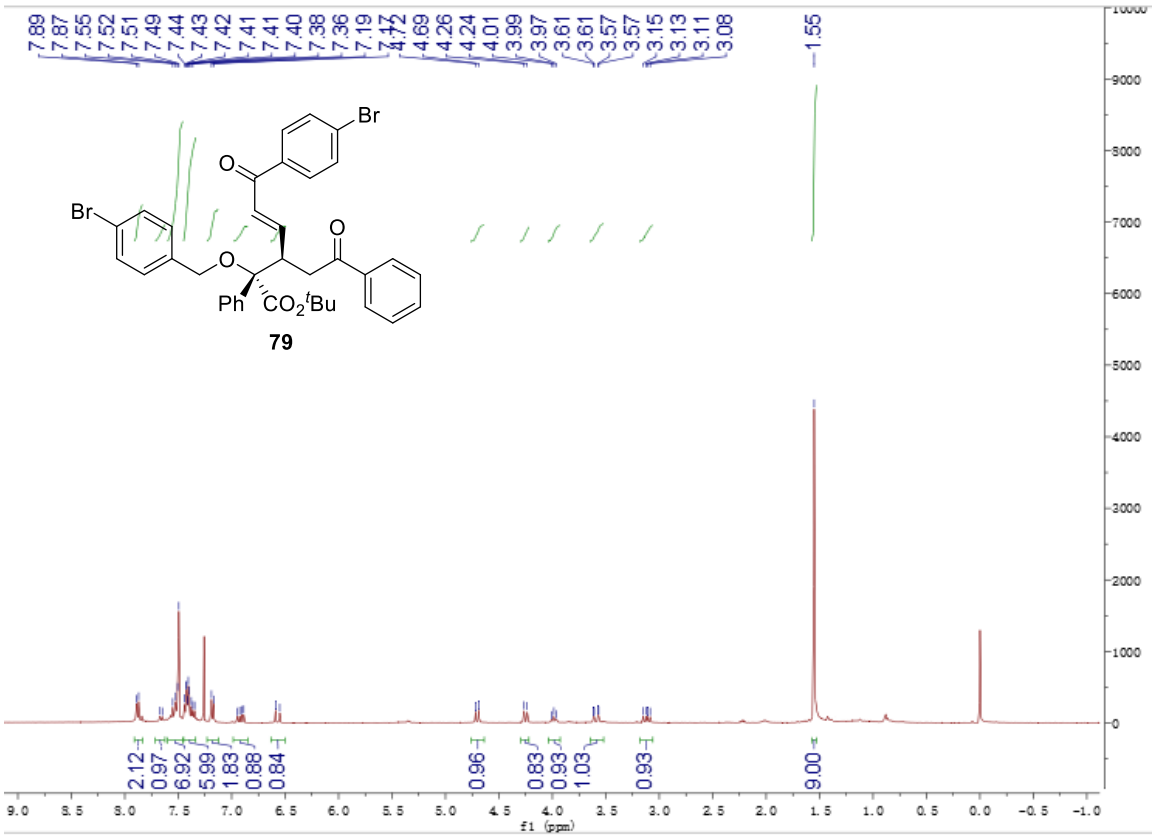

196.88
169.22
143.09
138.11
137.95
136.67
133.20
131.39
129.26
128.56
128.37
128.34
128.15
126.61
114.43
110.65
93.98
85.74
83.21
74.48
67.99
38.97
36.38
28.01
O
Br
O
O
Ph
CO2tBu
76

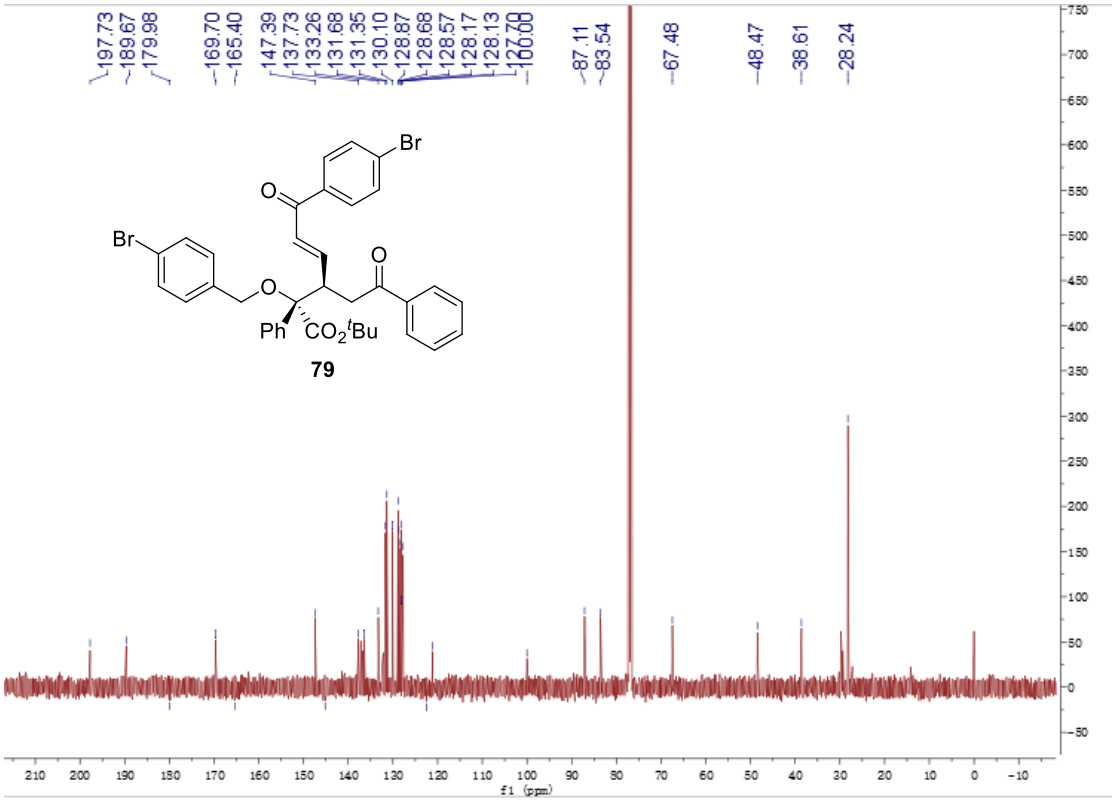

7.85
7.83
7.83
7.67
7.66
7.55
7.53
7.52
7.50
7.48
7.43
7.41
7.40
7.38
7.37
7.35
7.33
7.31
7.30
7.30
7.29
7.27
7.25
7.25
7.24
6.73
6.70
6.08
6.08
6.05
6.05
5.02
5.00
4.88
4.85
4.39
4.38
4.37
3.31
3.29
3.27
3.25
3.10
3.09
3.06
3.06
1.53
Ph
Br
O
O
Ph
CO2tBu
77
2.03
2.05
1.10
1.96
6.11
5.04
1.12
1.00
1.05
1.00
1.00
1.05
1.00
1.13
9.03

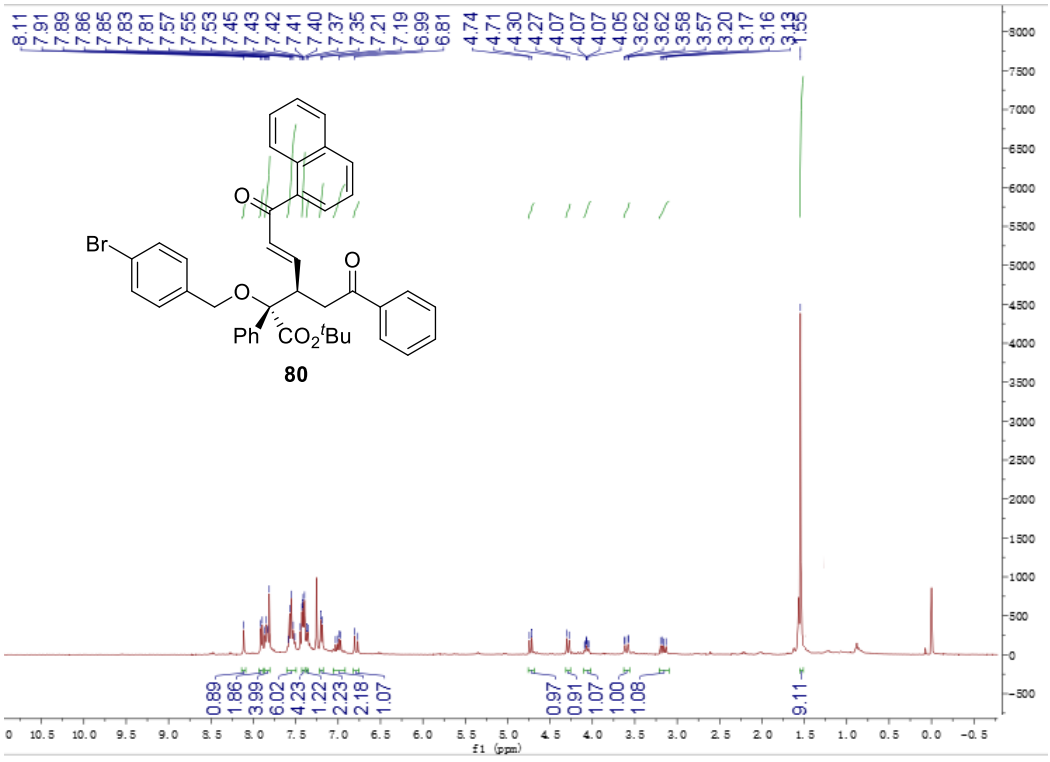

197.38
169.42
140.68
133.15
131.41
129.23
128.68
128.56
128.31
128.27
128.20
126.69
126.11
91.92
85.86
83.35
82.96
67.94
39.22
36.70
28.07
Ph
Br
O
O
Ph
CO2tBu
77
f1 (ppm)

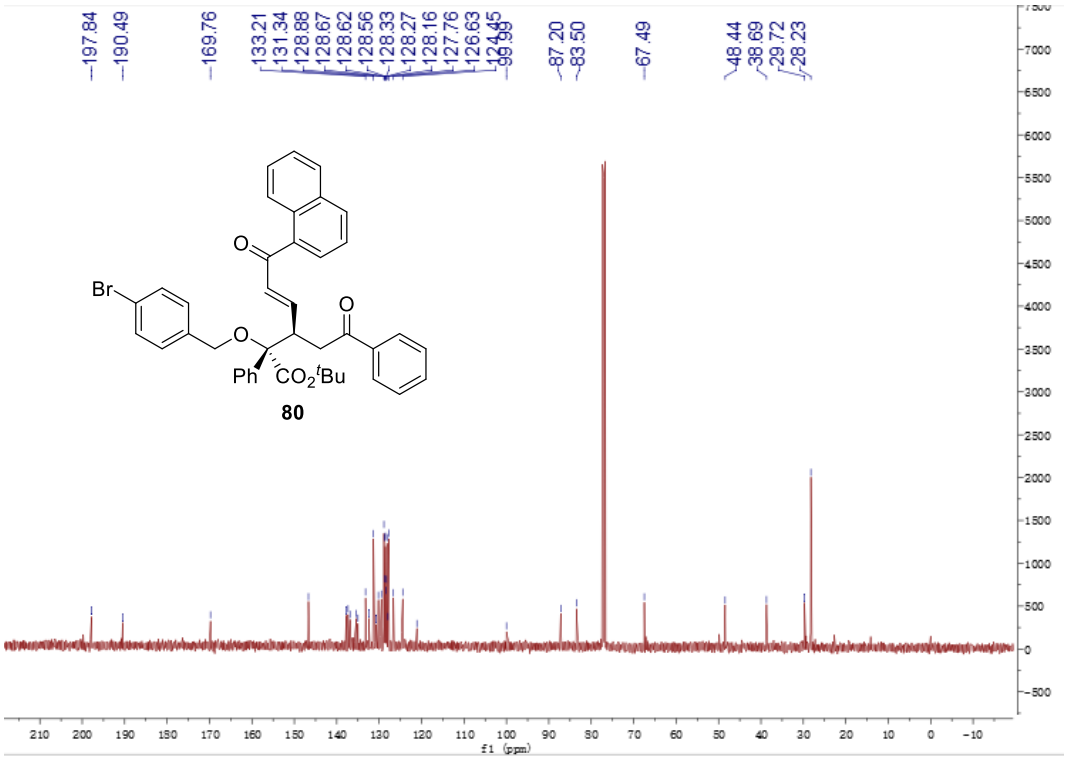

7.91
7.89
7.72
7.70
7.57
7.55
7.46
7.45
7.44
7.43
7.42
7.41
7.28
7.23
7.21
6.88
4.72
4.32
4.29
4.06
4.04
4.02
3.87
3.78
3.60
3.59
3.56
3.55
3.18
3.16
3.14
3.12
1.59
1.57
OMe
O
Br
O
O
Ph
CO2tBu
78
1.94
2.01
2.98
4.81
1.93
1.93
1.09
1.89
1.00
1.12
1.07
1.02
3.16
1.04
1.11
9.10
f1 (ppm)

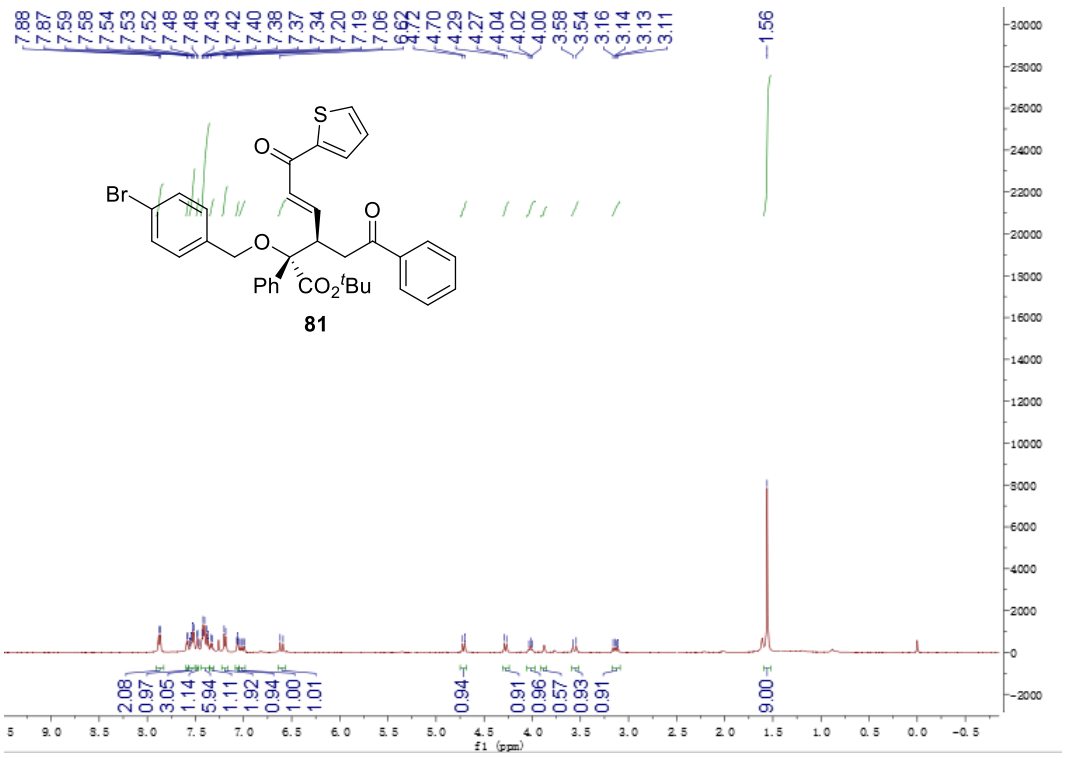

197.87
188.83
169.76
163.24
145.62
137.82
136.88
133.15
131.32
130.85
130.61
128.88
128.63
128.49
128.27
128.13
127.69
113.61
87.14
83.42
67.44
55.45
48.16
38.69
29.72
28.23
OMe
O
Br
O
O
Ph
CO2tBu
78
f1 (ppm)

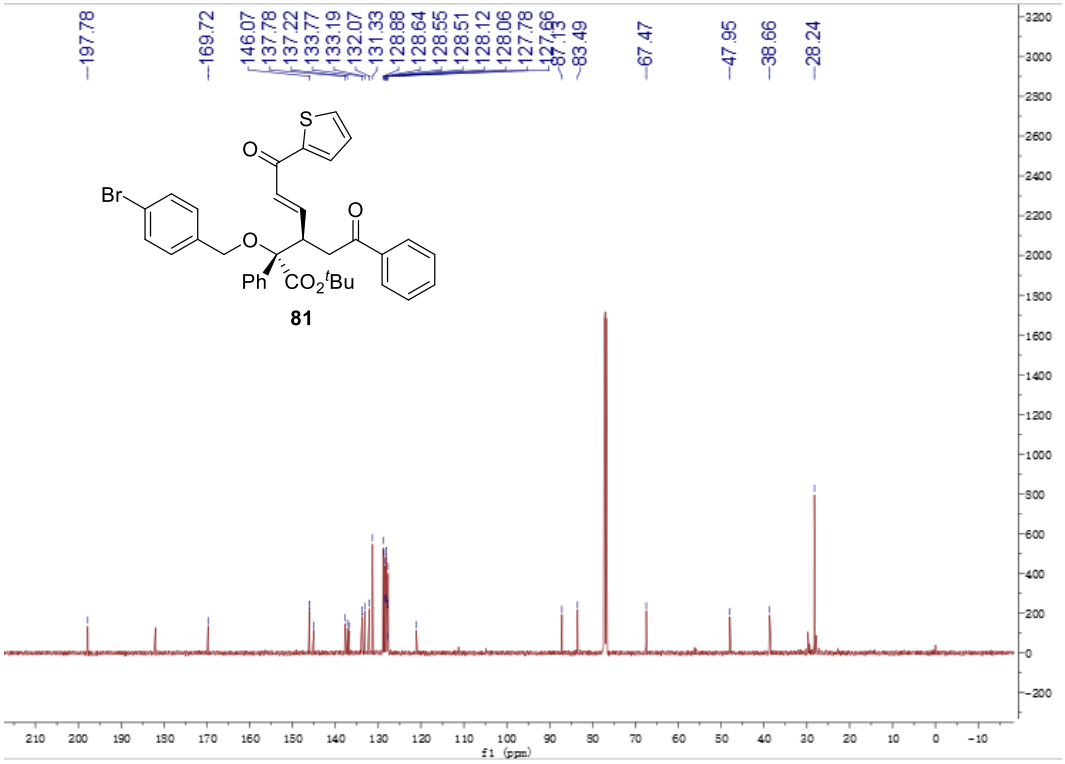

7.89
7.87
7.55
7.52
7.51
7.49
7.44
7.43
7.42
7.41
7.41
7.40
7.38
7.36
7.19
4.69
4.26
4.24
4.01
3.99
3.97
3.61
3.61
3.57
3.57
3.15
3.13
3.11
3.08
1.55
Br
O
Br
O
O
Ph
CO2tBu
79
2.12
0.97
6.92
5.99
1.83
0.88
0.84
0.96
0.83
0.93
1.03
0.93
9.00
f1 (ppm)

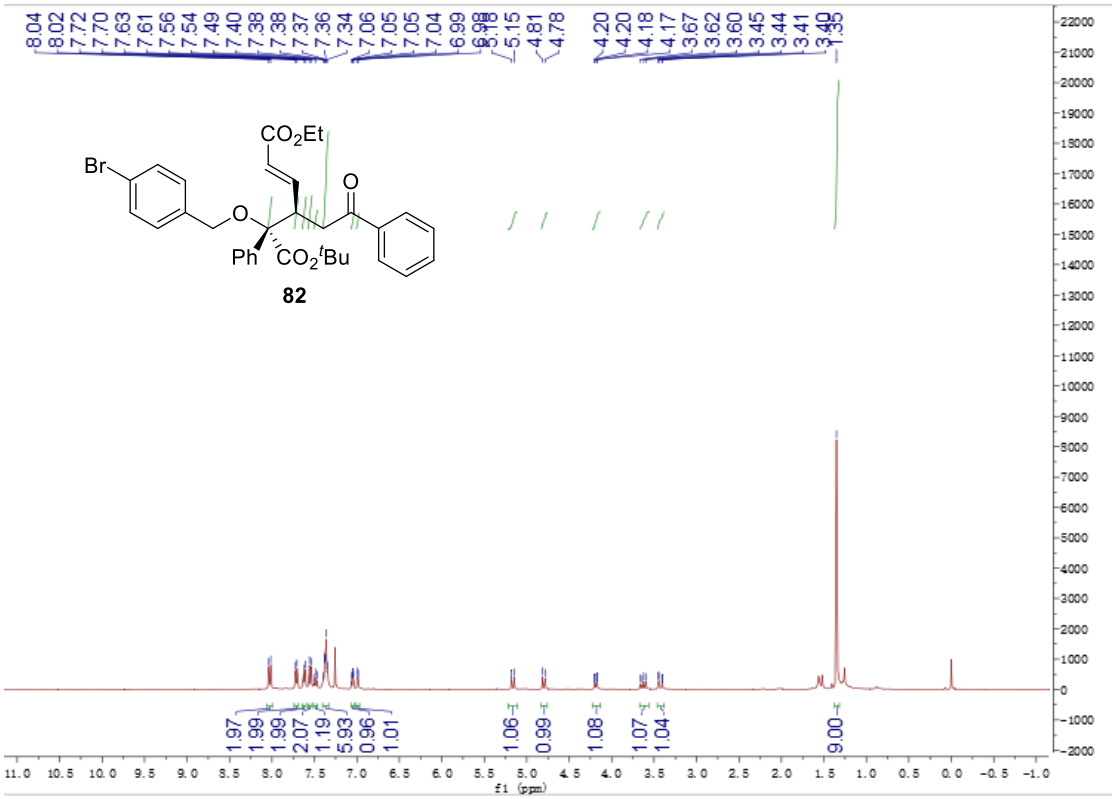

197.73
189.67
179.98
169.70
165.40
147.39
137.73
133.26
131.68
131.35
130.10
128.87
128.68
128.57
128.17
128.13
127.70
100.00
87.11
83.54
67.48
48.47
38.61
28.24
Br
O
Br
O
O
Ph
CO2tBu
79
f1 (ppm)

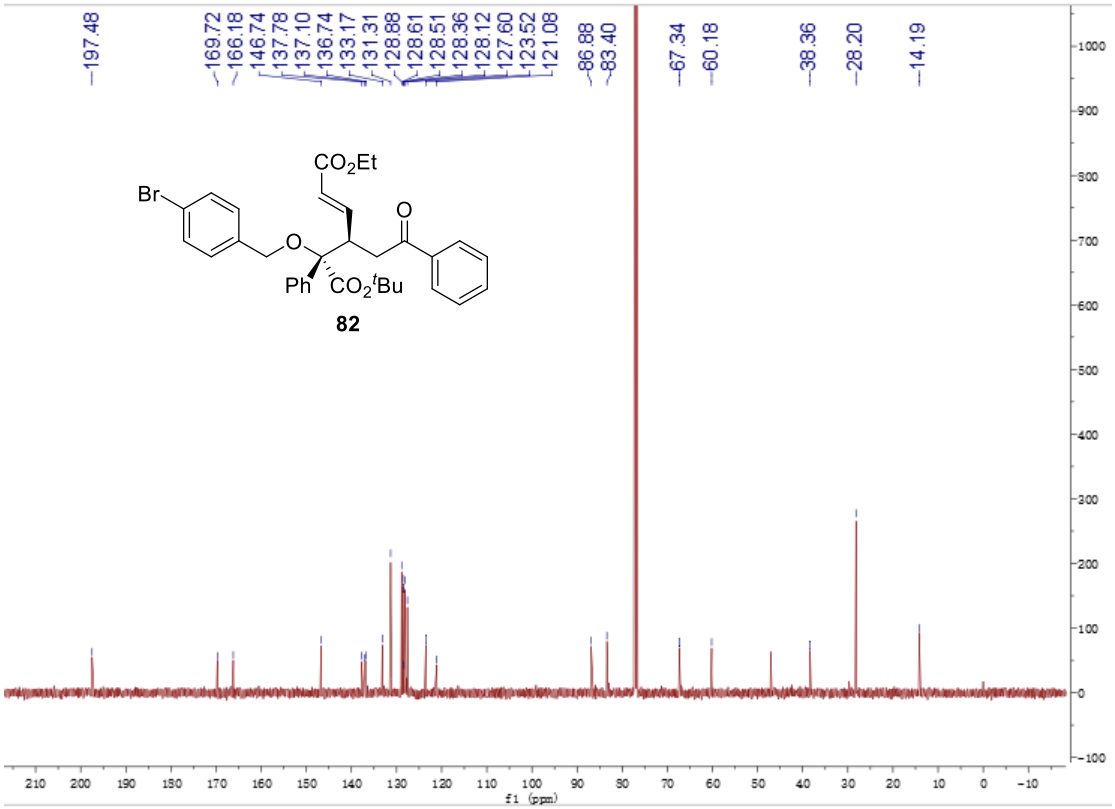

8.11
7.91
7.89
7.86
7.85
7.83
7.81
7.57
7.55
7.53
7.45
7.43
7.42
7.41
7.40
7.37
7.35
7.21
7.19
6.99
6.81
4.74
4.71
4.30
4.27
4.07
4.07
4.07
4.05
3.62
3.62
3.58
3.57
3.20
3.17
3.16
3.13
1.55
Br
O
O
O
Ph
CO2tBu
80
0.89
1.86
3.99
6.02
4.23
1.22
2.23
2.18
1.07
0.97
0.91
1.07
1.00
1.08
9.11
f1 (ppm)

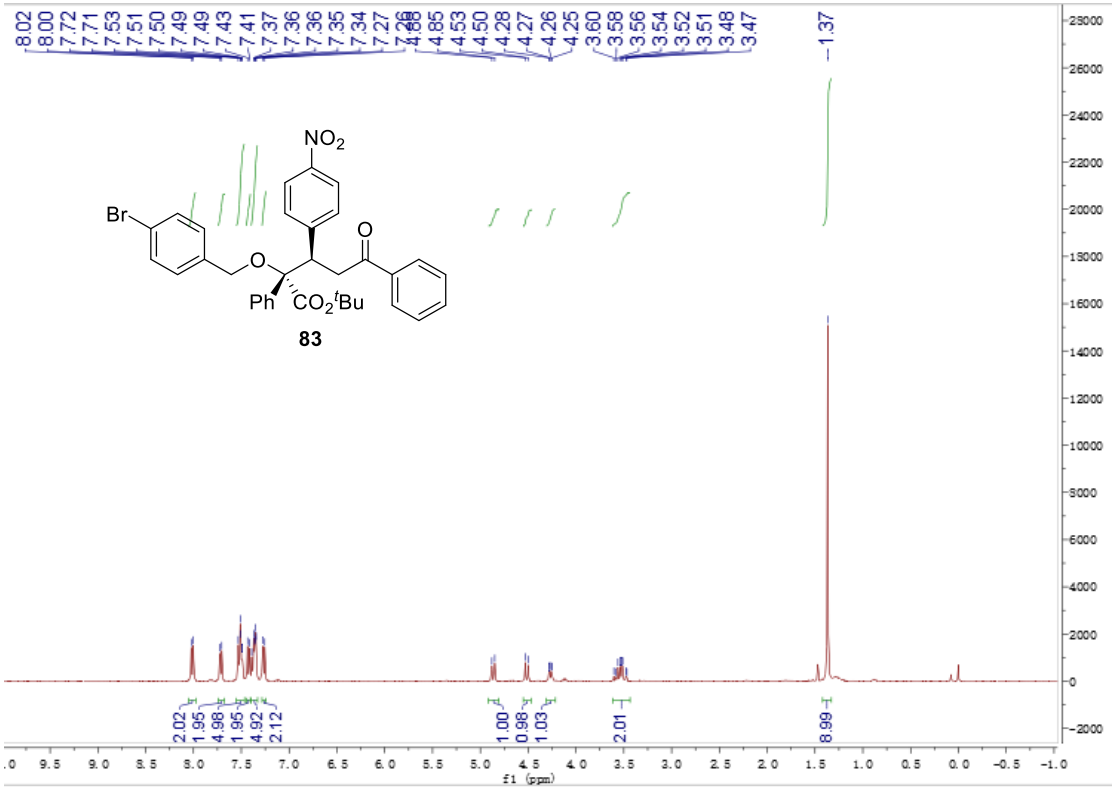

197.84
190.49
169.76
133.21
131.34
128.88
128.67
128.62
128.56
128.33
128.27
128.16
127.76
126.63
124.45
99.99
87.20
83.50
67.49
48.44
38.69
29.72
28.23
Br
O
O
O
Ph
CO2tBu
80
f1 (ppm)

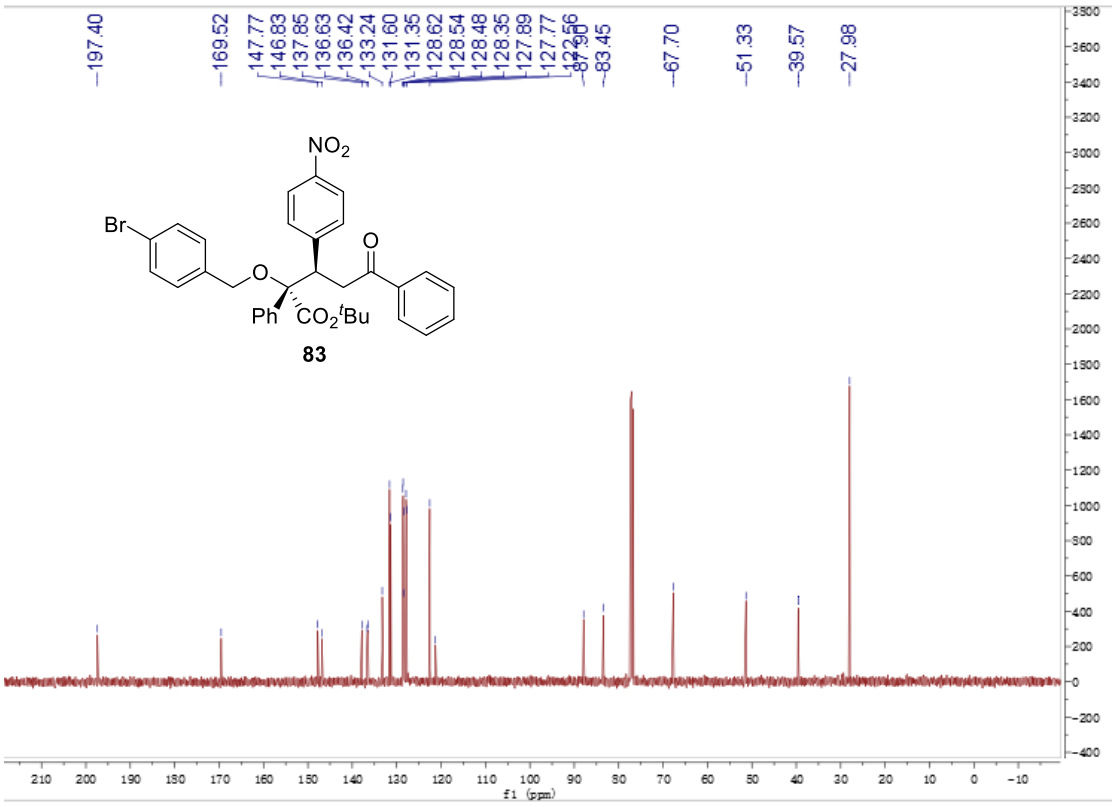

7.88
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7.59
7.58
7.54
7.53
7.52
7.48
7.48
7.43
7.42
7.40
7.38
7.37
7.34
7.20
7.19
7.06
6.62
4.72
4.70
4.29
4.27
4.04
4.02
4.00
3.58
3.54
3.16
3.14
3.13
3.11
1.56
S
O
Br
O
O
Ph
CO2tBu
81
2.08
0.97
3.05
1.14
5.94
1.11
1.92
0.94
1.00
1.01
0.94
0.91
0.96
0.57
0.93
0.91
9.00
f1 (ppm)

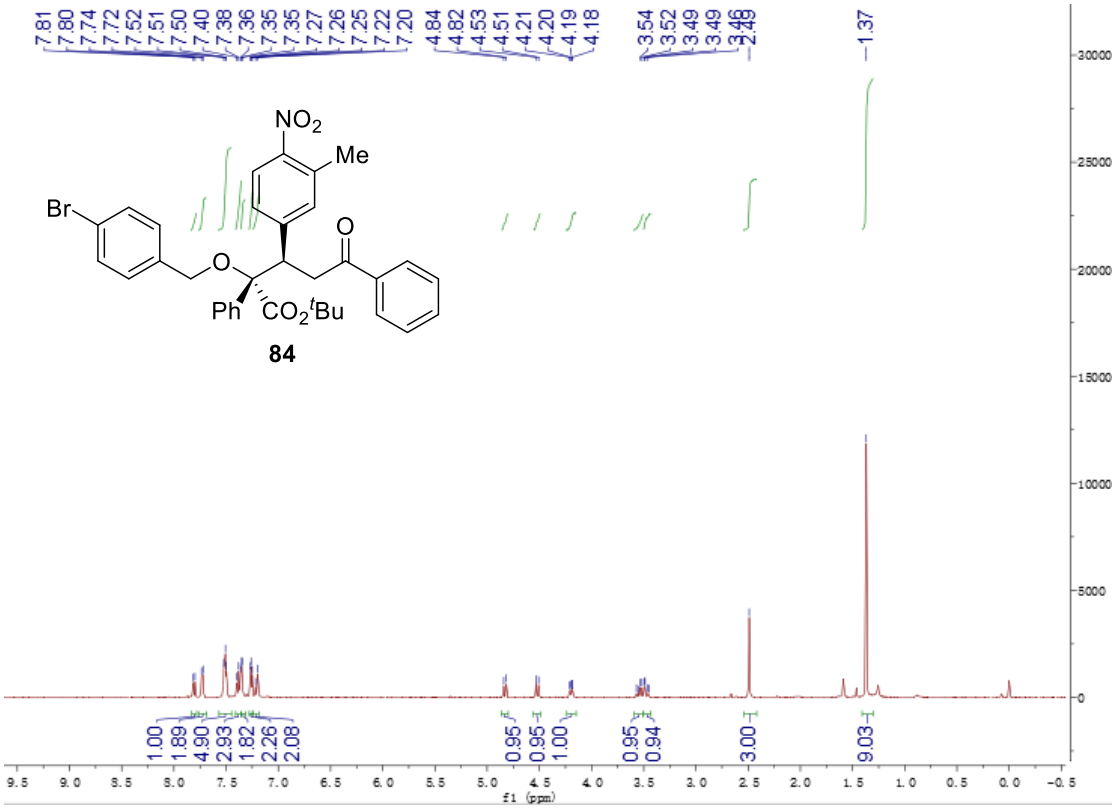

197.78
169.72
146.07
137.78
137.22
133.77
133.19
132.07
131.33
128.88
128.64
128.55
128.51
128.12
128.06
127.78
127.66
87.13
83.49
67.47
47.95
38.66
28.24
S
O
Br
O
O
Ph
CO2tBu
81
f1 (ppm)

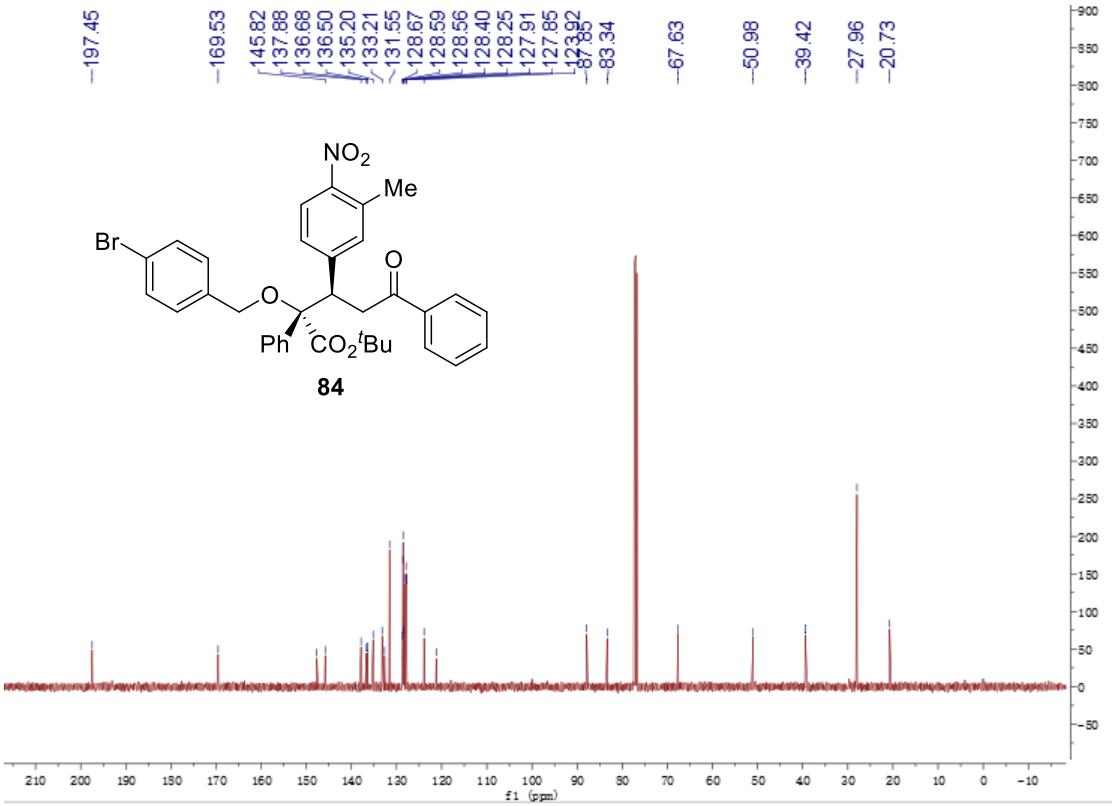

8.04
8.02
7.72
7.70
7.63
7.61
7.56
7.54
7.49
7.40
7.38
7.38
7.37
7.36
7.34
7.06
7.05
7.05
7.04
6.99
5.15
4.81
4.78
4.20
4.20
4.18
4.17
3.67
3.62
3.60
3.45
3.44
3.41
3.40
1.35
CO2Et
Br
O
O
Ph
CO2tBu
82
1.97
1.99
1.99
2.07
1.19
5.93
0.96
1.01
1.06
0.99
1.08
1.07
1.04
9.00
f1 (ppm)

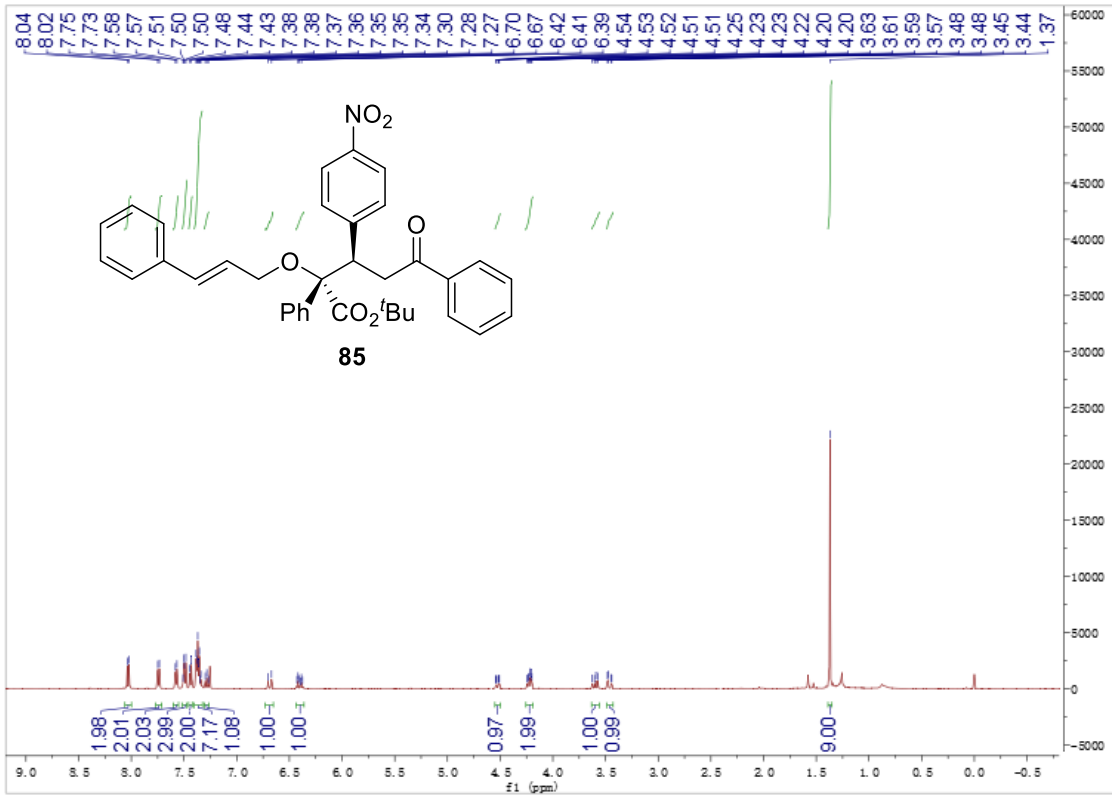

197.48
169.72
166.18
146.74
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137.10
136.74
133.17
131.31
128.88
128.61
128.51
128.36
128.12
127.60
123.52
121.08
86.88
83.40
67.34
60.18
38.36
28.20
14.19
CO2Et
Br
O
O
Ph
CO2tBu
82
f1 (ppm)

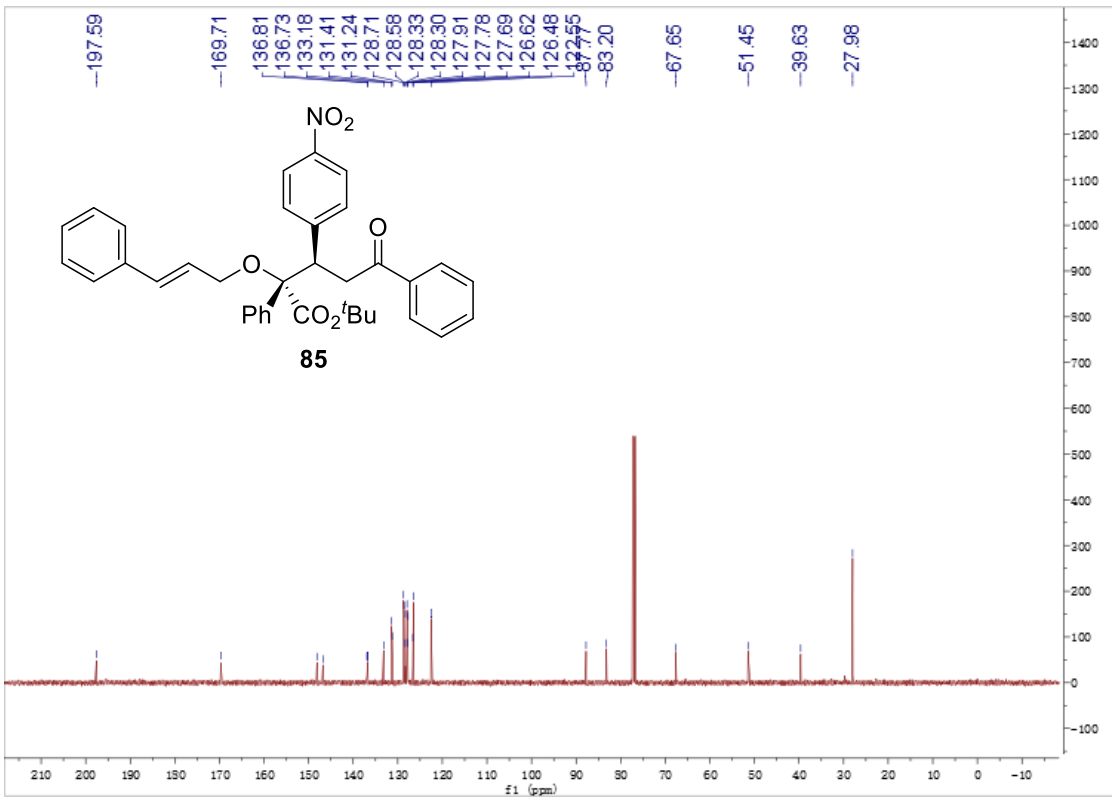

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7.51
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7.49
7.43
7.41
7.37
7.36
7.36
7.35
7.34
7.27
4.88
4.85
4.53
4.50
4.28
4.27
4.26
4.25
3.60
3.58
3.56
3.54
3.52
3.51
3.48
3.47
1.37
NO2
Br
O
O
Ph
CO2tBu
83
2.02
1.95
4.98
1.95
4.92
2.12
1.00
0.98
1.03
2.01
8.99
f1 (ppm)

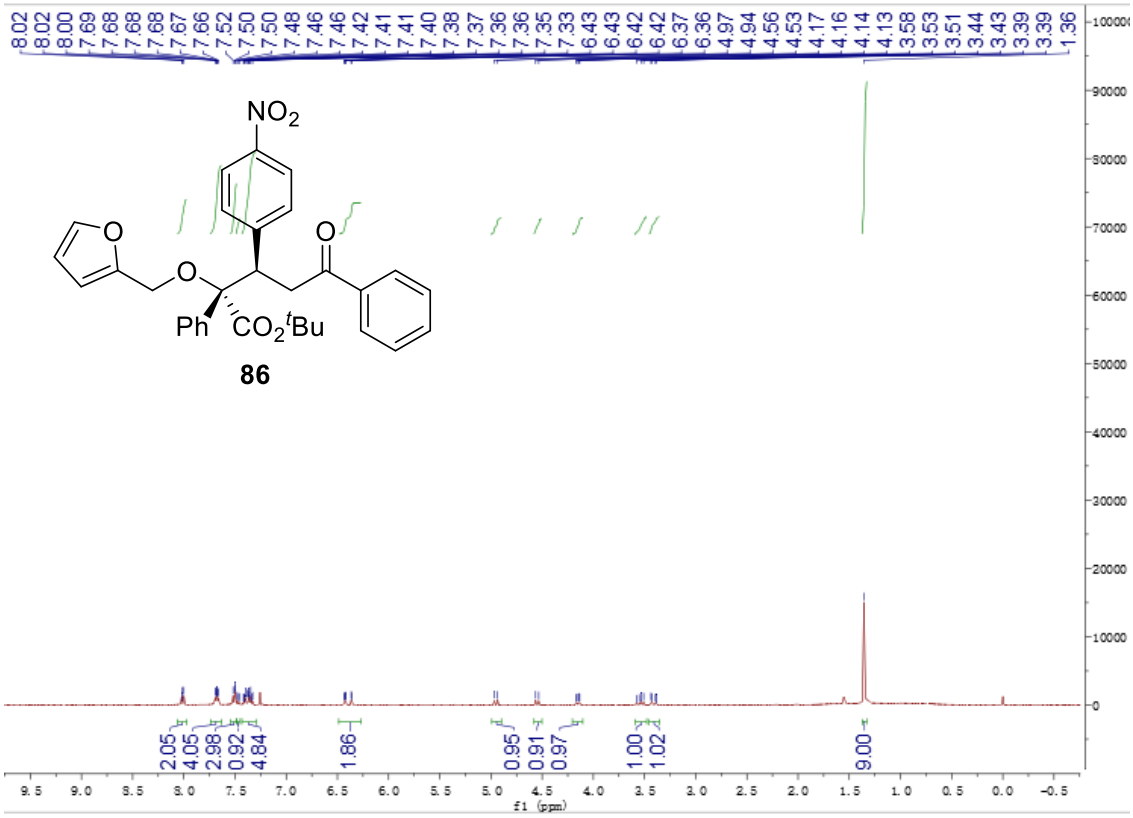

197.40
169.52
147.77
146.83
137.85
136.63
136.42
133.24
131.60
131.35
128.62
128.54
128.48
128.35
127.89
127.77
83.45
67.70
51.33
39.57
27.98
NO2
Br
O
O
Ph
CO2tBu
83
f1 (ppm)

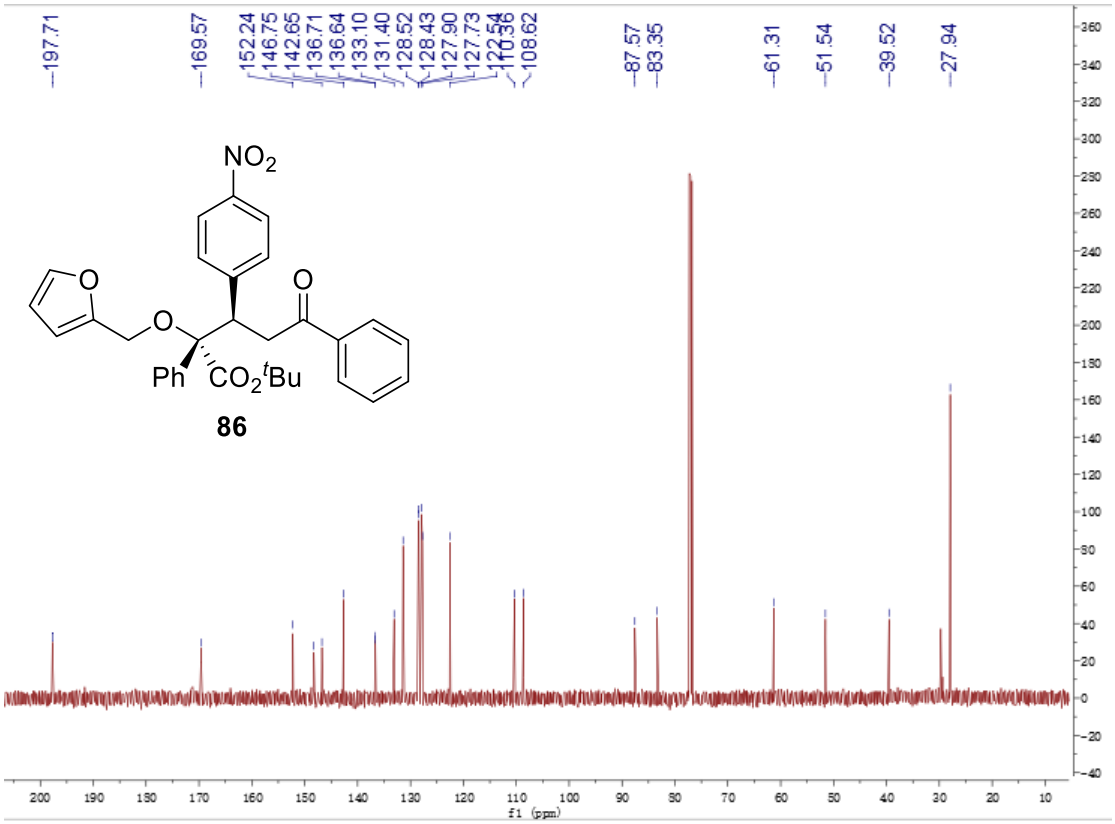

7.81
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7.72
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7.51
7.50
7.40
7.38
7.36
7.35
7.35
7.27
7.26
7.25
7.22
7.20
4.84
4.82
4.53
4.51
4.21
4.20
4.19
4.18
3.54
3.52
3.49
3.49
3.46
2.49
1.37
NO2
Me
Br
O
O
Ph
CO2tBu
84
1.00
1.89
4.90
2.93
1.82
2.26
2.08
0.95
0.95
1.00
0.95
0.94
3.00
9.03
f1 (ppm)

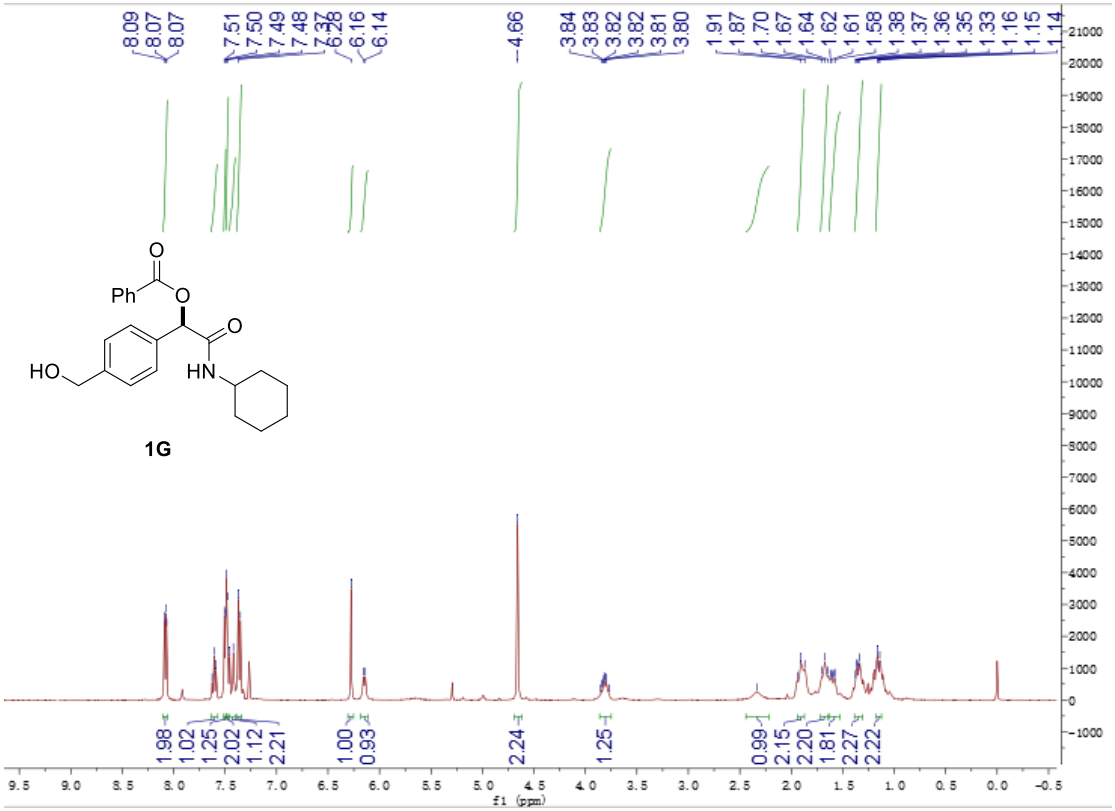

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145.82
137.88
136.68
136.50
135.20
133.21
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128.67
128.59
128.56
128.40
128.25
127.91
127.85
123.92
87.85
83.34
67.63
50.98
39.42
27.96
20.73
NO2
Me
Br
O
O
Ph
CO2tBu
84
f1 (ppm)

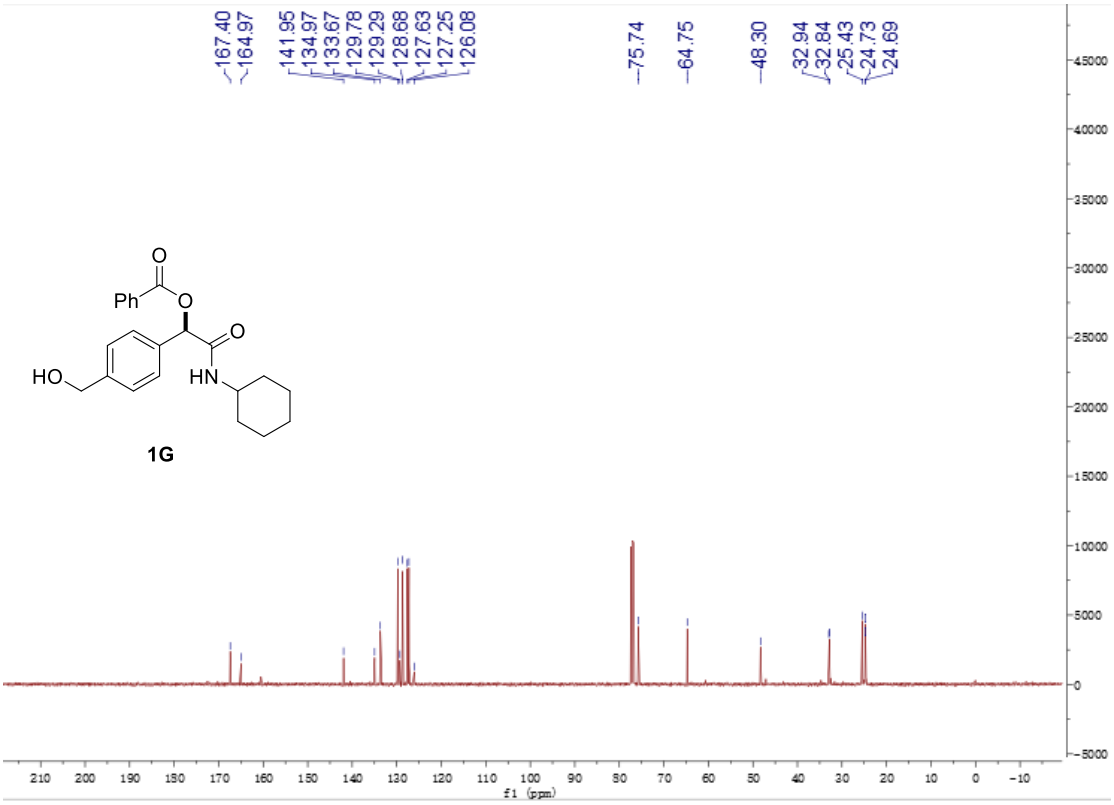

8.04
8.02
7.75
7.73
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7.57
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7.50
7.50
7.48
7.44
7.43
7.38
7.38
7.37
7.36
7.35
7.35
7.34
7.30
7.28
7.27
6.70
6.67
6.42
6.41
6.39
4.54
4.53
4.52
4.51
4.51
4.25
4.23
4.23
4.22
4.20
4.20
3.63
3.61
3.59
3.57
3.48
3.48
3.45
3.44
1.37
NO2
O
O
Ph
CO2tBu
85
1.98
2.01
2.03
2.99
2.00
7.17
1.08
1.00
1.00
0.97
1.99
1.00
0.99
9.00
f1 (ppm)

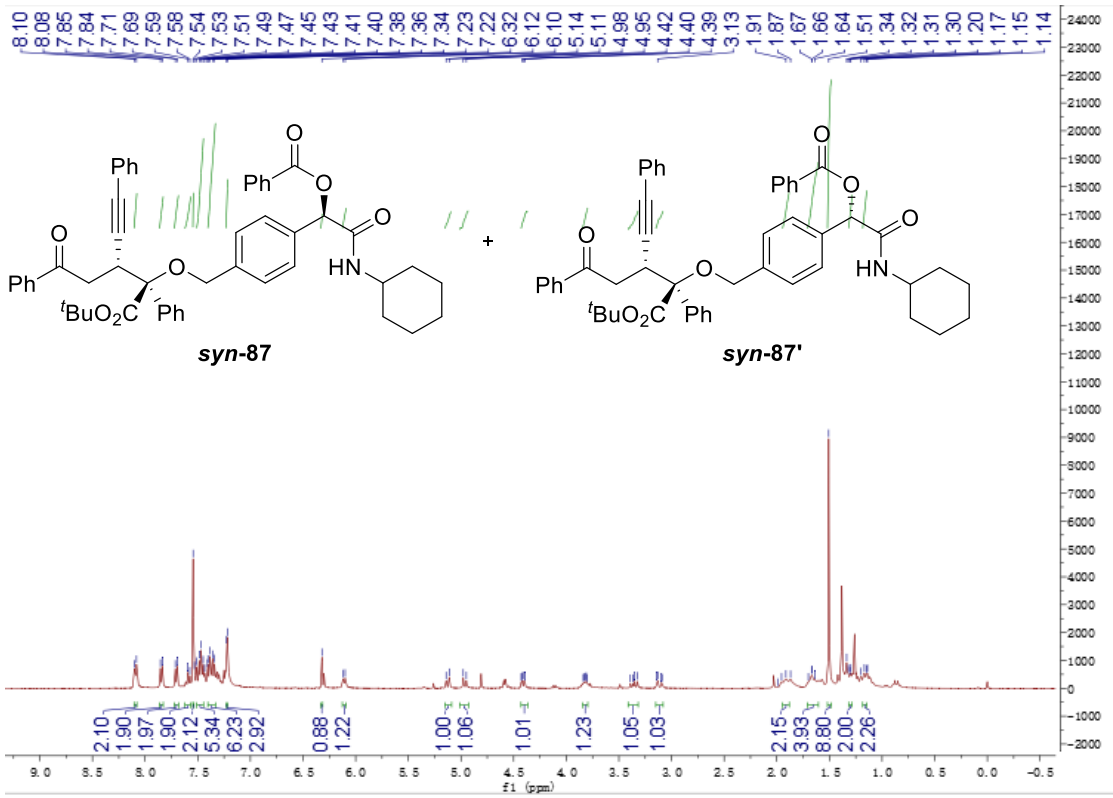

197.59
169.71
136.81
136.73
133.18
131.41
131.24
128.71
128.58
128.33
128.30
127.91
127.78
127.69
126.62
126.48
122.55
83.20
67.65
51.45
39.63
27.98
NO2
O
O
Ph
CO2tBu
85
f1 (ppm)

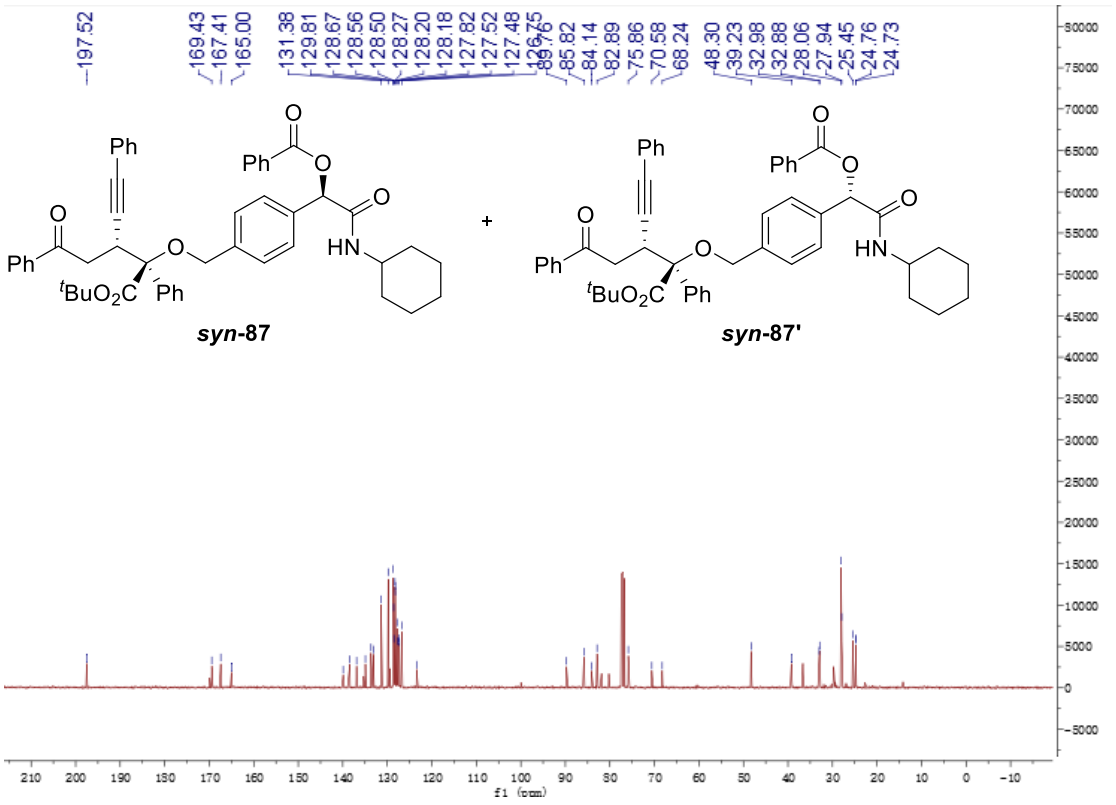

8.02
8.02
8.00
7.69
7.68
7.68
7.67
7.66
7.52
7.50
7.48
7.46
7.46
7.42
7.41
7.41
7.40
7.38
7.37
7.36
7.36
7.35
7.33
6.43
6.42
6.42
6.37
6.36
4.97
4.94
4.56
4.53
4.17
4.16
4.14
4.13
3.58
3.53
3.51
3.44
3.43
3.39
3.39
1.36
NO2
O
O
O
Ph
CO2tBu
86
2.05
4.05
2.98
0.92
4.84
1.86
0.95
0.91
0.97
1.00
1.02
9.00
f1 (ppm)

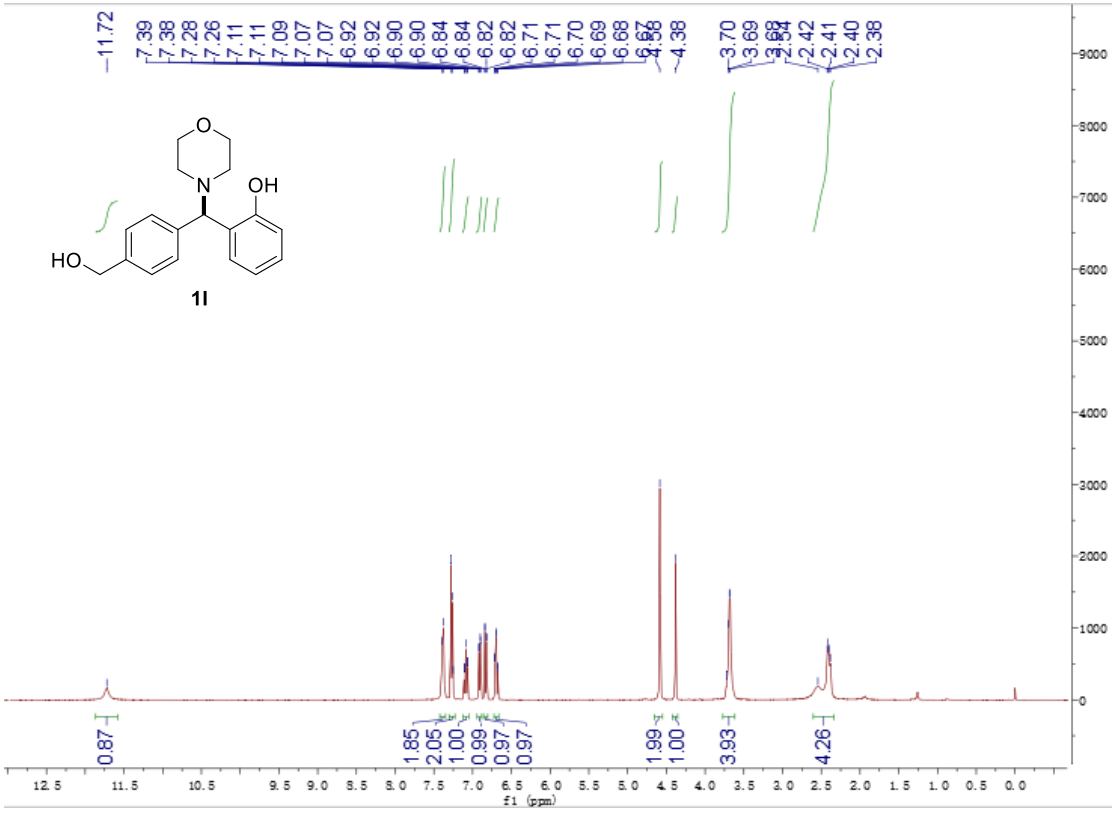

197.71
169.57
152.24
146.75
142.65
136.71
136.64
133.10
131.40
128.52
128.43
127.90
127.73
122.54
110.36
108.62
87.57
83.35
61.31
51.54
39.52
27.94
NO2
O
O
O
Ph
CO2tBu
86
f1 (ppm)

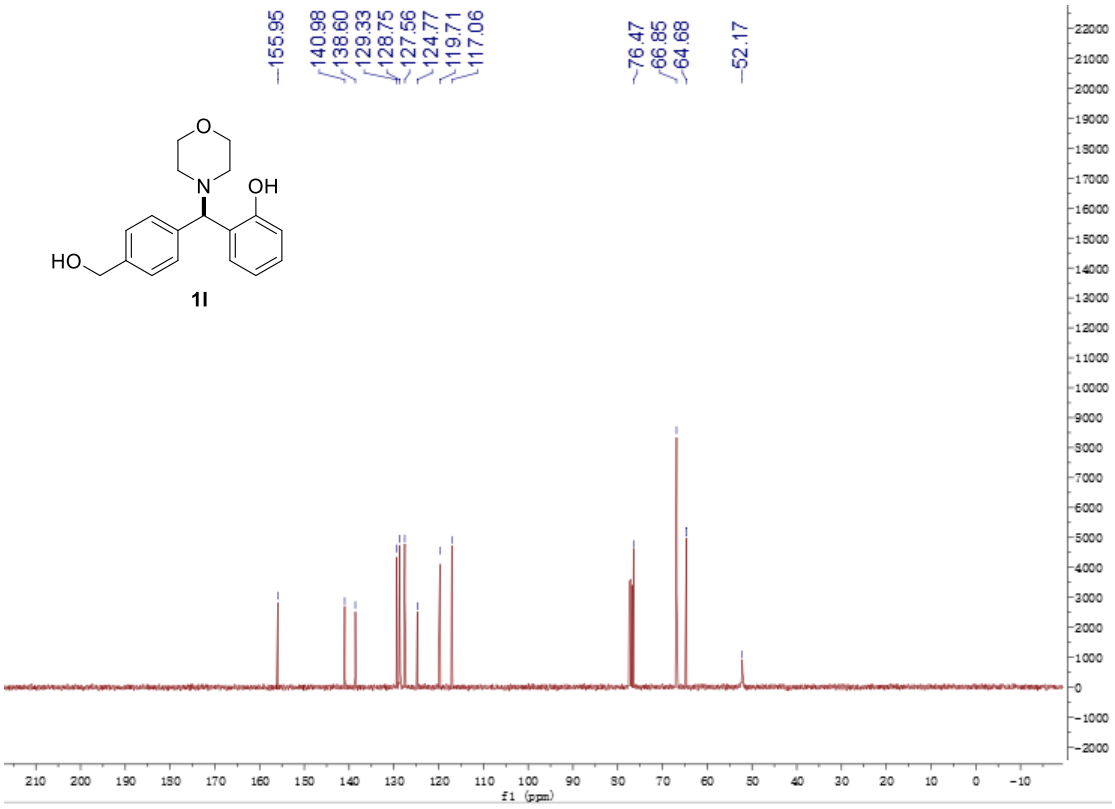

8.09
8.07
8.07
7.51
7.50
7.49
7.48
6.16
6.14
4.66
3.84
3.83
3.82
3.82
3.81
3.80
1.91
1.87
1.70
1.67
1.64
1.62
1.61
1.58
1.38
1.37
1.36
1.35
1.33
1.16
1.15
1.14
O
Ph
O
O
HO
HN
1G
1.98
1.02
1.25
2.02
1.12
2.21
1.00
0.93
2.24
1.25
0.99
2.15
2.20
1.81
2.27
2.22
f1 (ppm)

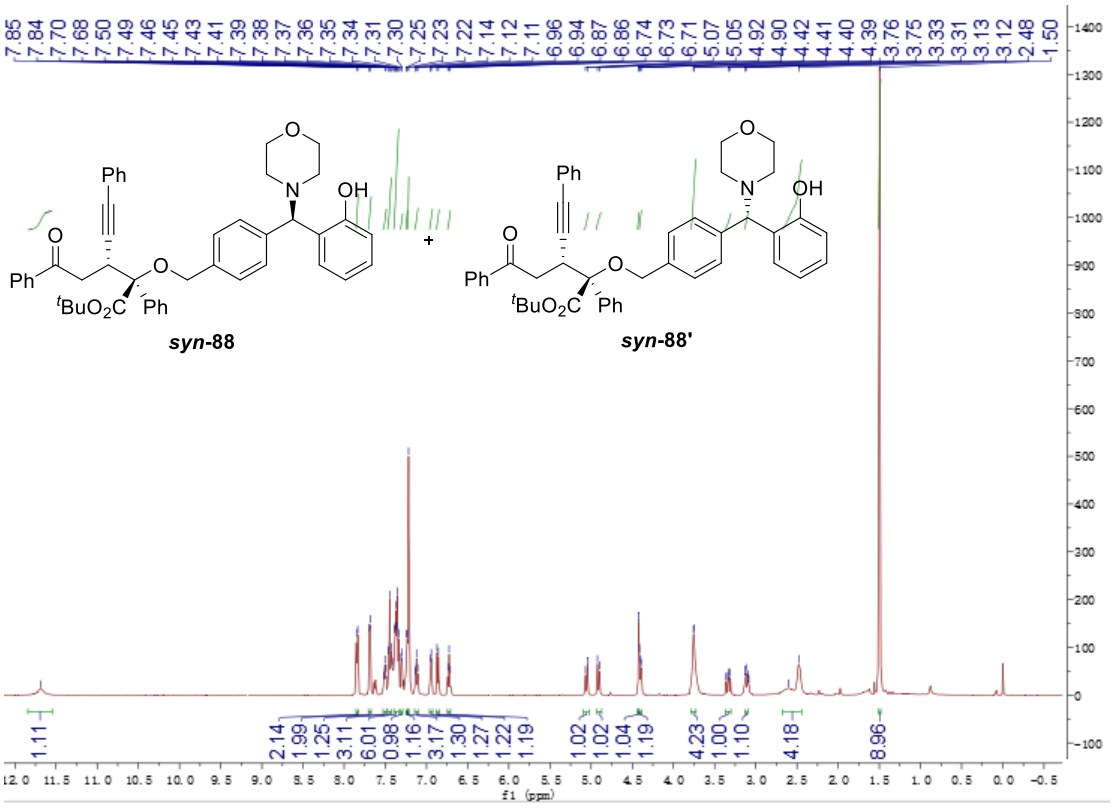

167.40
164.97
141.95
134.97
133.67
129.78
129.29
128.68
127.63
127.25
126.08
75.74
64.75
48.30
32.94
32.84
25.43
24.73
24.69
Ph
O
HO
HN
1G
f1 (ppm)

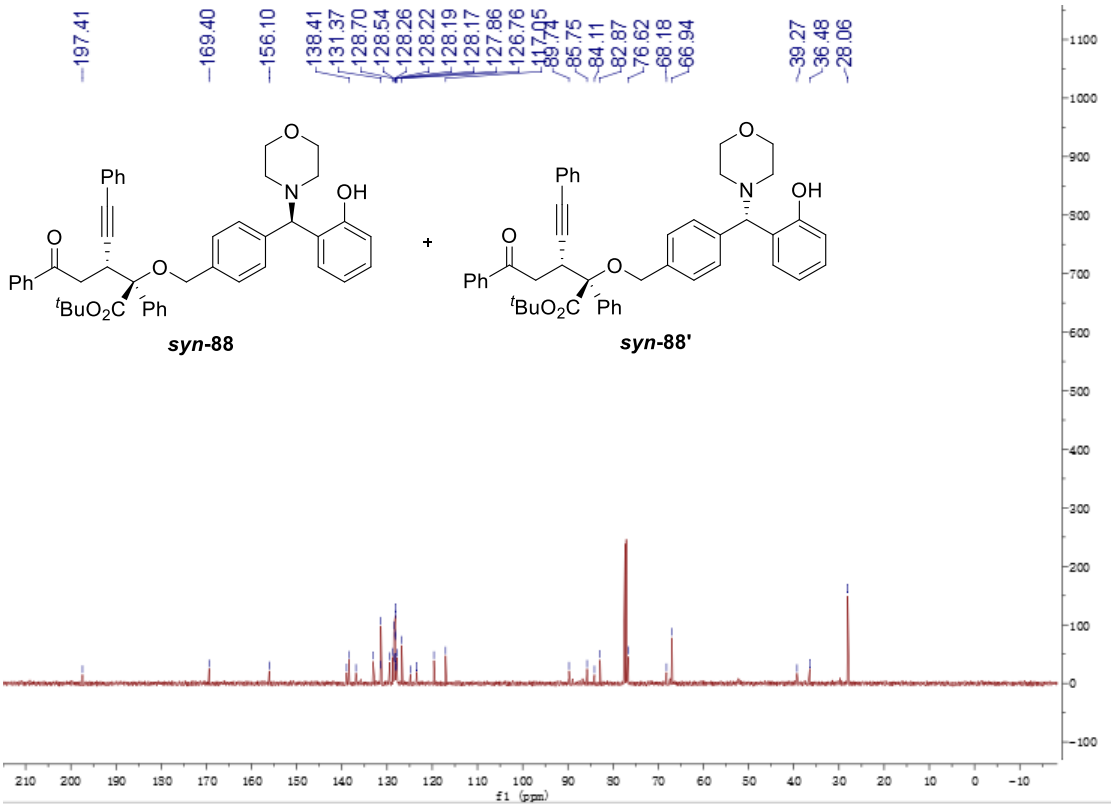

8.10
8.08
7.85
7.84
7.71
7.69
7.59
7.58
7.54
7.53
7.51
7.49
7.47
7.45
7.43
7.41
7.40
7.38
7.36
7.34
7.23
7.22
6.32
6.12
6.10
5.14
5.11
4.98
4.95
4.42
4.40
4.39
3.13
1.91
1.87
1.67
1.66
1.64
1.51
1.34
1.32
1.31
1.30
1.20
1.17
1.15
1.14
Ph
Ph
O
HN
Ph
O
O
tBuO2C
Ph
syn-87
+
Ph
Ph
O
HN
Ph
O
O
tBuO2C
Ph
syn-87'
2.10
1.90
1.97
1.90
2.12
5.34
6.23
2.92
0.88
1.22
1.00
1.06
1.01
1.23
1.05
1.03
2.15
3.93
8.80
2.00
2.26
f1 (ppm)

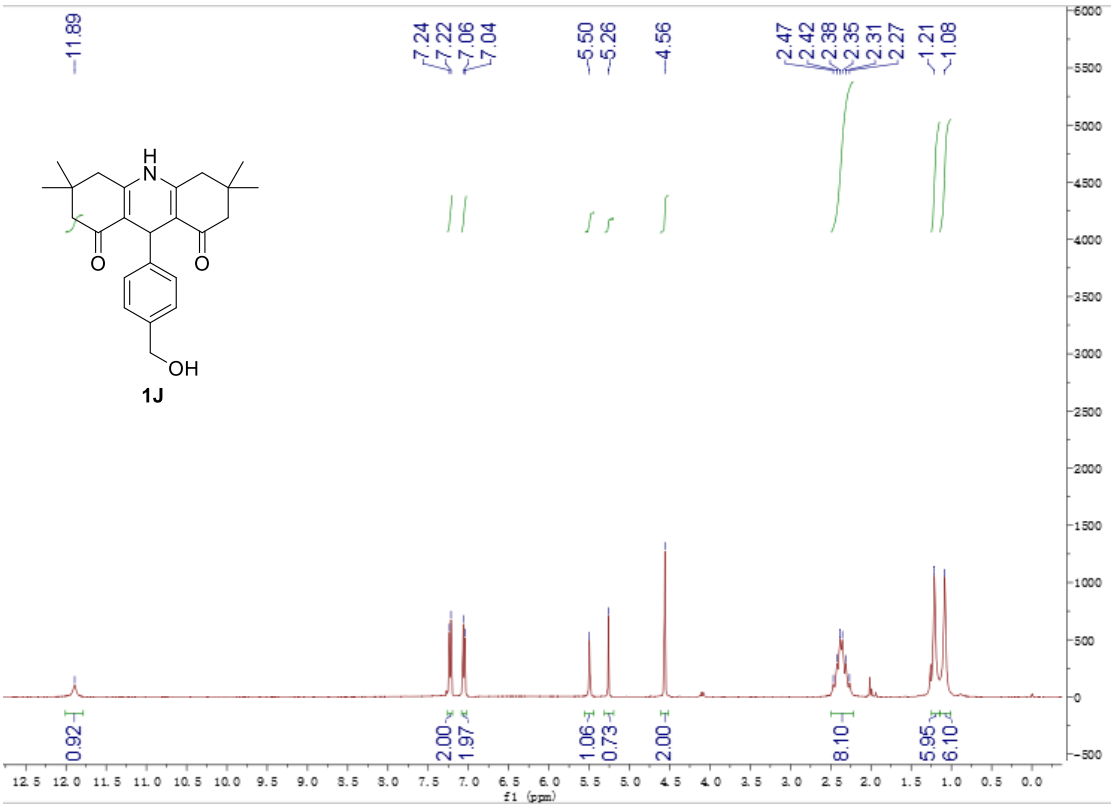

syn-87
syn-87'

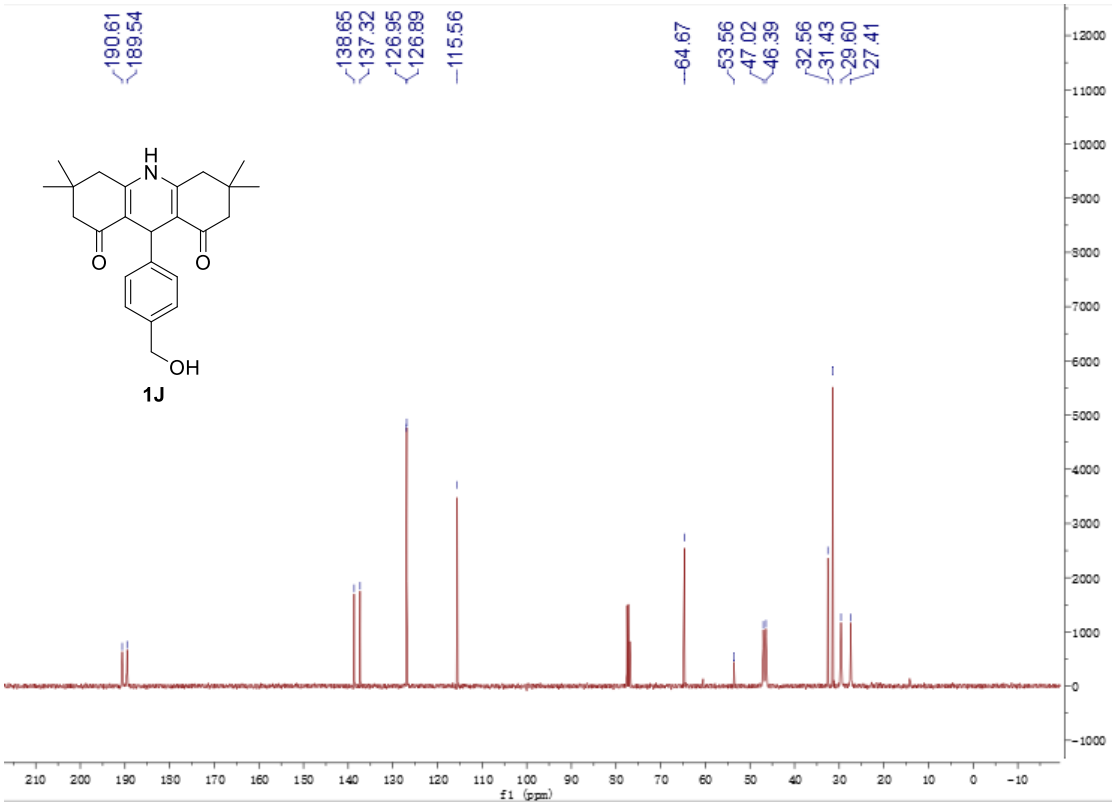

1l

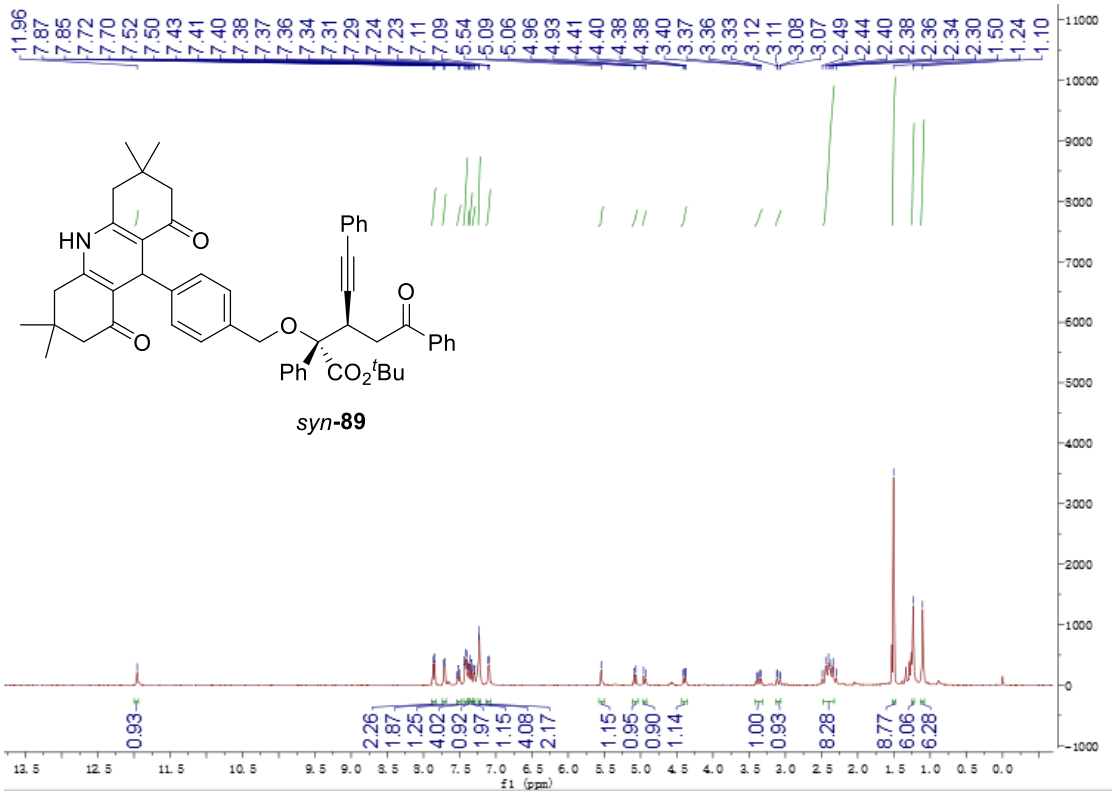

155.95
140.98
138.60
129.33
128.75
127.56
124.77
119.71
117.06
76.47
66.85
64.68
52.17
O
N
OH
HO
1l

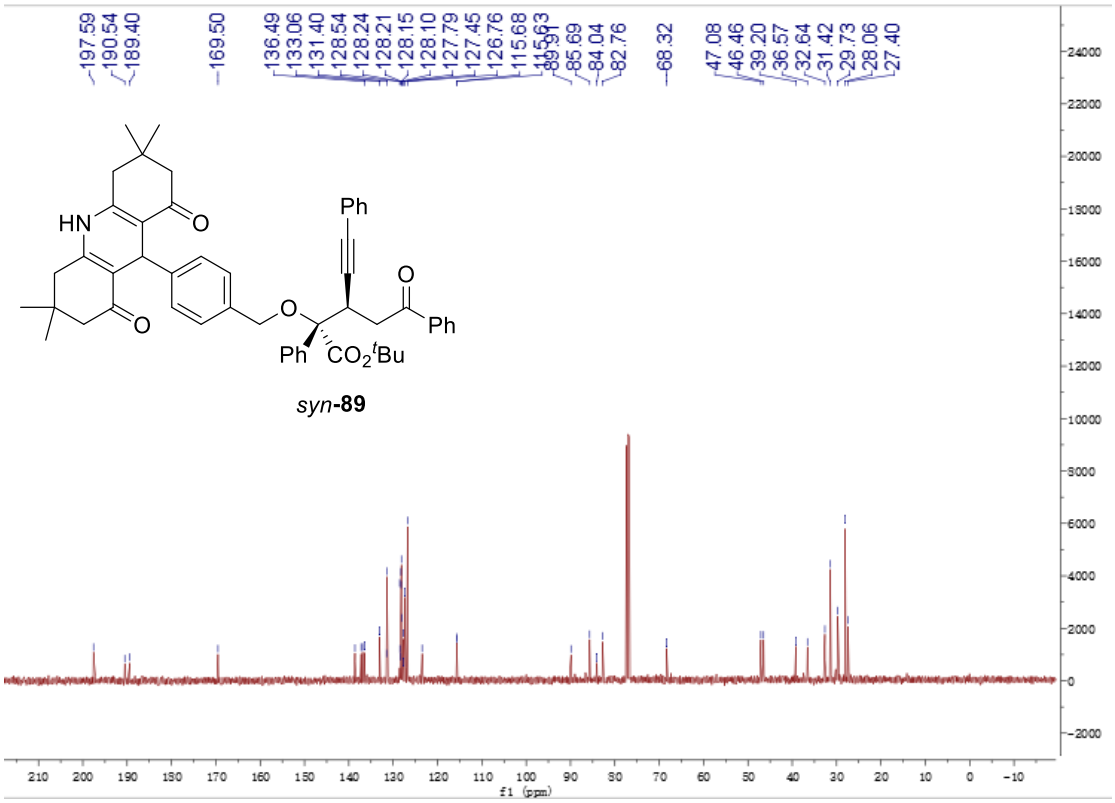

7.85
7.84
7.70
7.68
7.50
7.49
7.46
7.45
7.43
7.41
7.39
7.38
7.37
7.36
7.35
7.34
7.31
7.30
7.25
7.23
7.22
7.14
7.12
7.11
6.96
6.94
6.87
6.86
6.74
6.73
6.71
5.07
5.05
4.92
4.90
4.42
4.41
4.40
4.39
3.76
3.75
3.33
3.31
3.13
3.12
2.48
1.50
Ph
O
N
OH
Ph
O
O
tBuO2C
Ph
syn-88
+
Ph
O
N
OH
Ph
O
O
tBuO2C
Ph
syn-88'
1.11
2.14
1.99
1.25
3.11
6.01
0.98
1.16
3.17
1.30
1.27
1.22
1.19
1.02
1.02
1.04
1.19
4.23
1.00
1.10
4.18
8.96


197.41
169.40
156.10
138.41
131.37
128.70
128.54
128.26
128.22
128.19
128.17
127.86
126.76
117.05
89.74
85.75
84.11
82.87
76.62
68.18
66.94
39.27
36.48
28.06
Ph
O
N
OH
Ph
O
O
tBuO2C
Ph
syn-88
syn-88'
f1 (ppm)

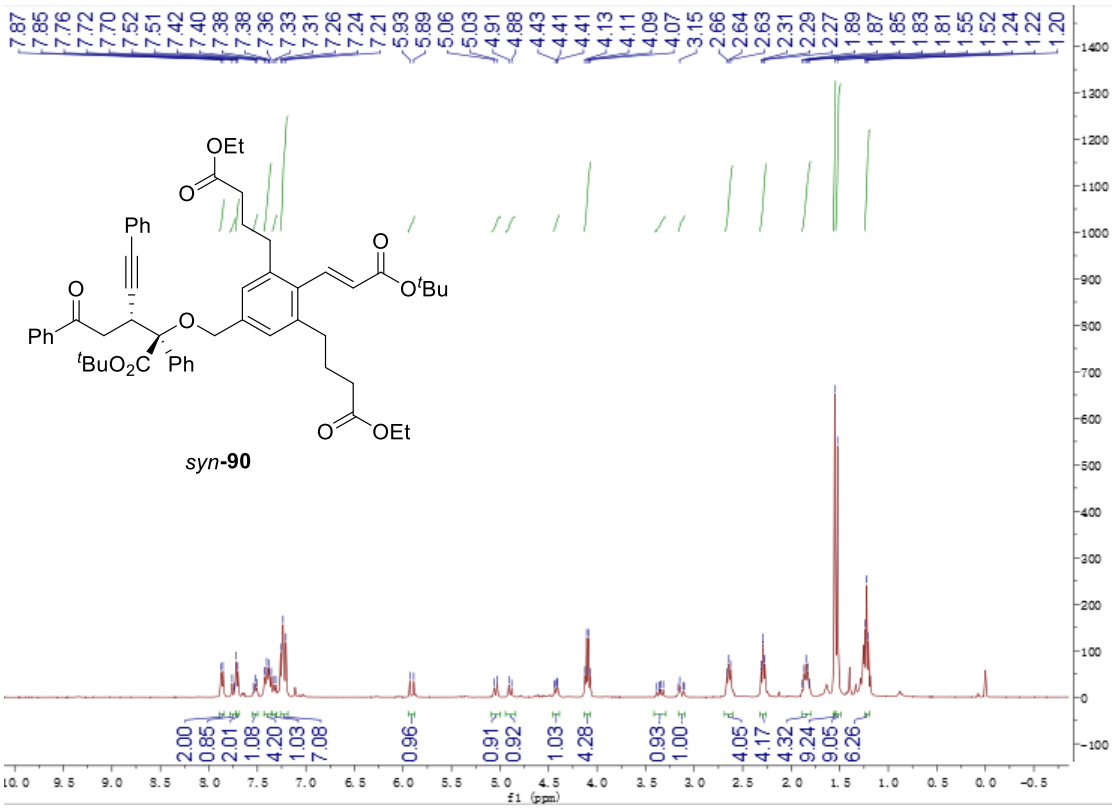

11.89
7.24
7.22
7.06
7.04
5.50
5.26
4.56
2.47
2.42
2.38
2.35
2.31
2.27
1.21
1.08
H
N
O
O
OH
1J
0.92
2.00
1.97
1.06
0.73
2.00
8.10
5.95
6.10
f1 (ppm)


190.61
189.54
138.65
137.32
126.95
126.89
115.56
64.67
53.56
47.02
46.39
32.56
31.43
29.60
27.41
H
N
O
O
OH
1J
f1 (ppm)

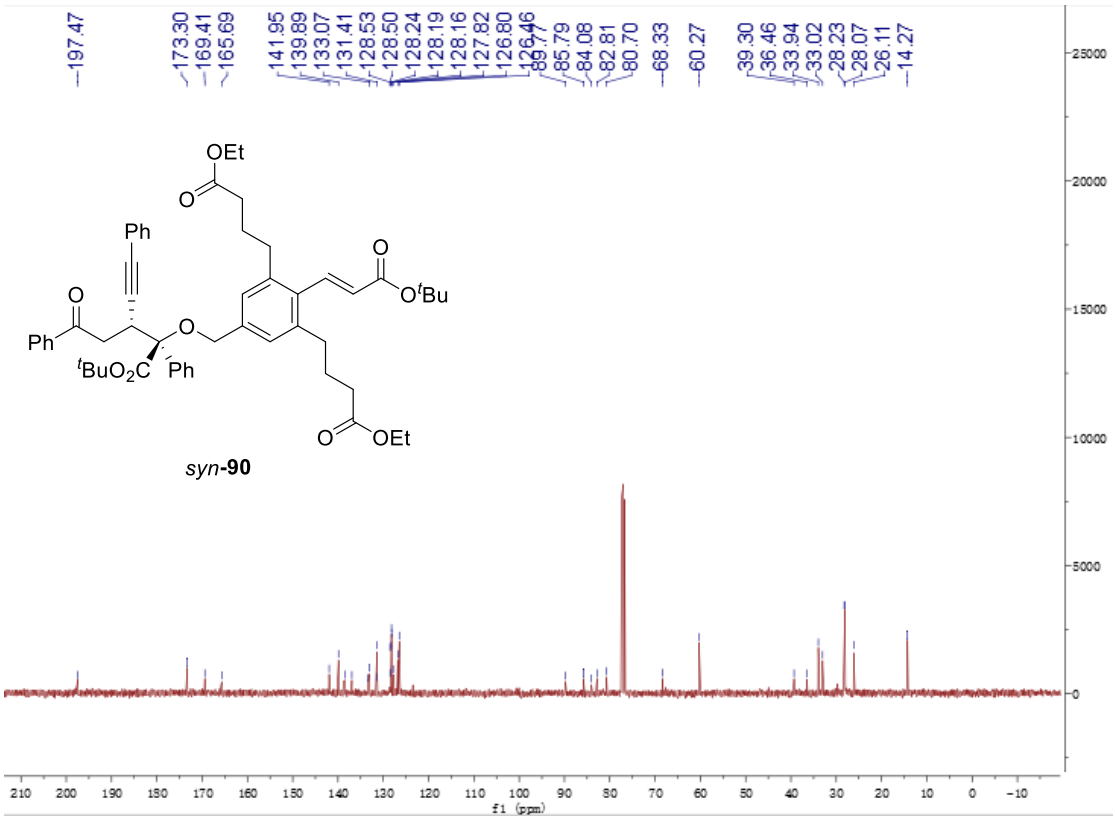

11.96
7.87
7.85
7.72
7.70
7.52
7.50
7.43
7.41
7.40
7.38
7.37
7.36
7.34
7.31
7.29
7.24
7.23
7.11
7.09
5.54
5.09
5.06
4.96
4.93
4.41
4.40
4.38
4.38
4.40
3.37
3.36
3.33
3.12
3.11
3.08
3.07
2.49
2.44
2.40
2.38
2.36
2.34
2.30
1.50
1.24
1.10
HN
O
O
O
O
Ph
Ph
Ph
CO2tBu
syn-89
0.93
2.26
1.87
1.25
4.02
0.92
1.97
1.15
4.08
2.17
1.15
0.95
0.90
1.14
1.00
0.93
8.28
8.77
6.06
6.28
f1 (ppm)

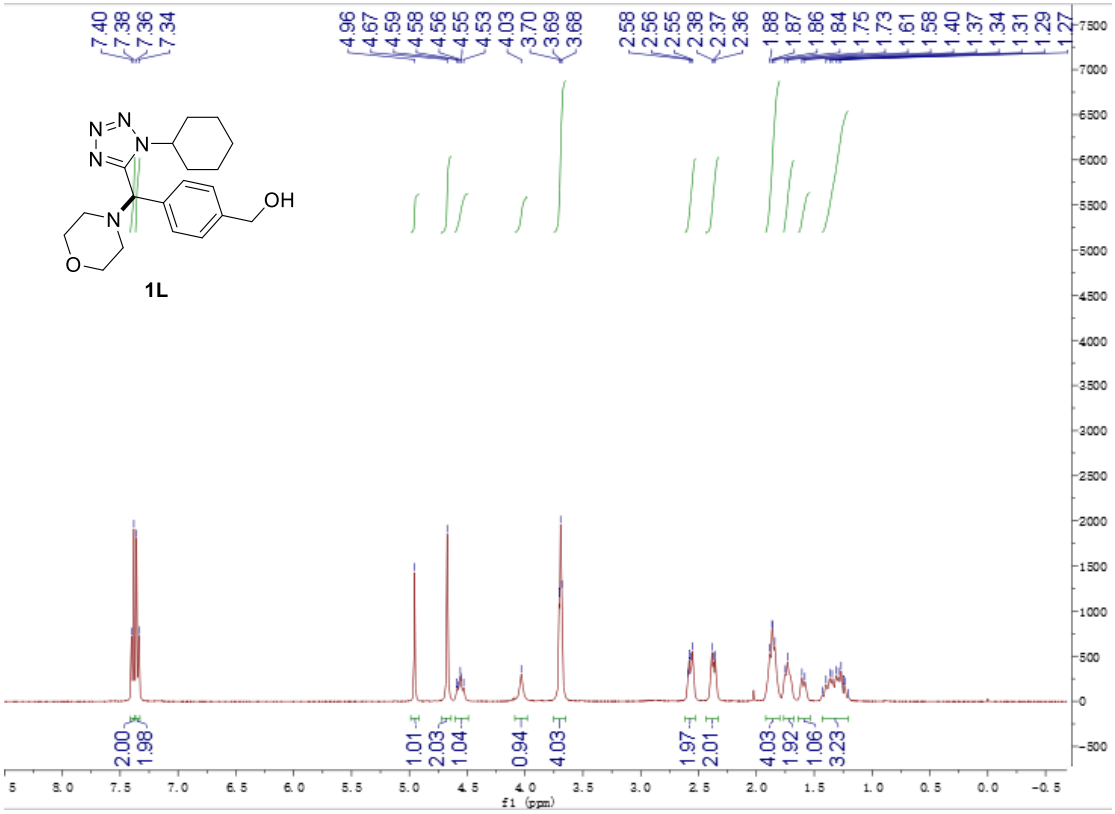

197.59
190.54
189.40
169.50
136.49
133.06
131.40
128.54
128.24
128.21
128.15
128.10
127.79
127.45
126.76
115.68
85.69
84.04
82.76
68.32
47.08
46.46
39.20
36.57
32.64
31.42
29.73
28.06
27.40
HN
O
O
O
O
Ph
Ph
Ph
CO2tBu
f1 (ppm)

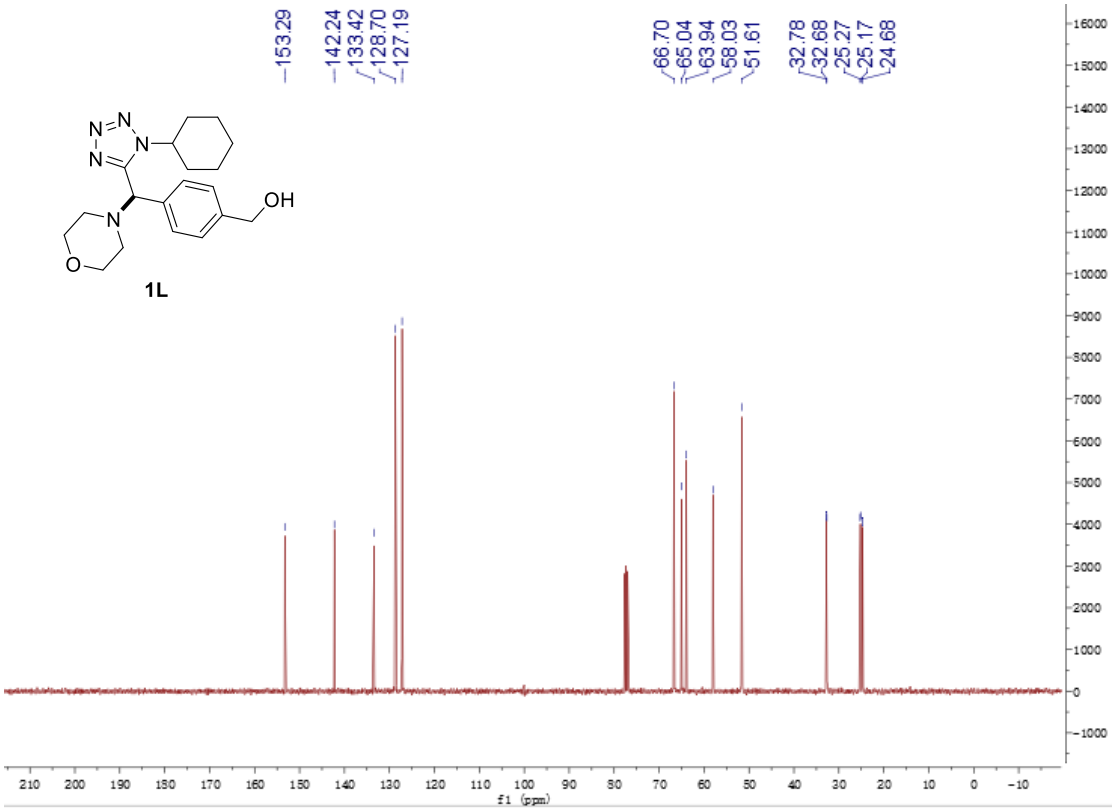
*syn*-**89**

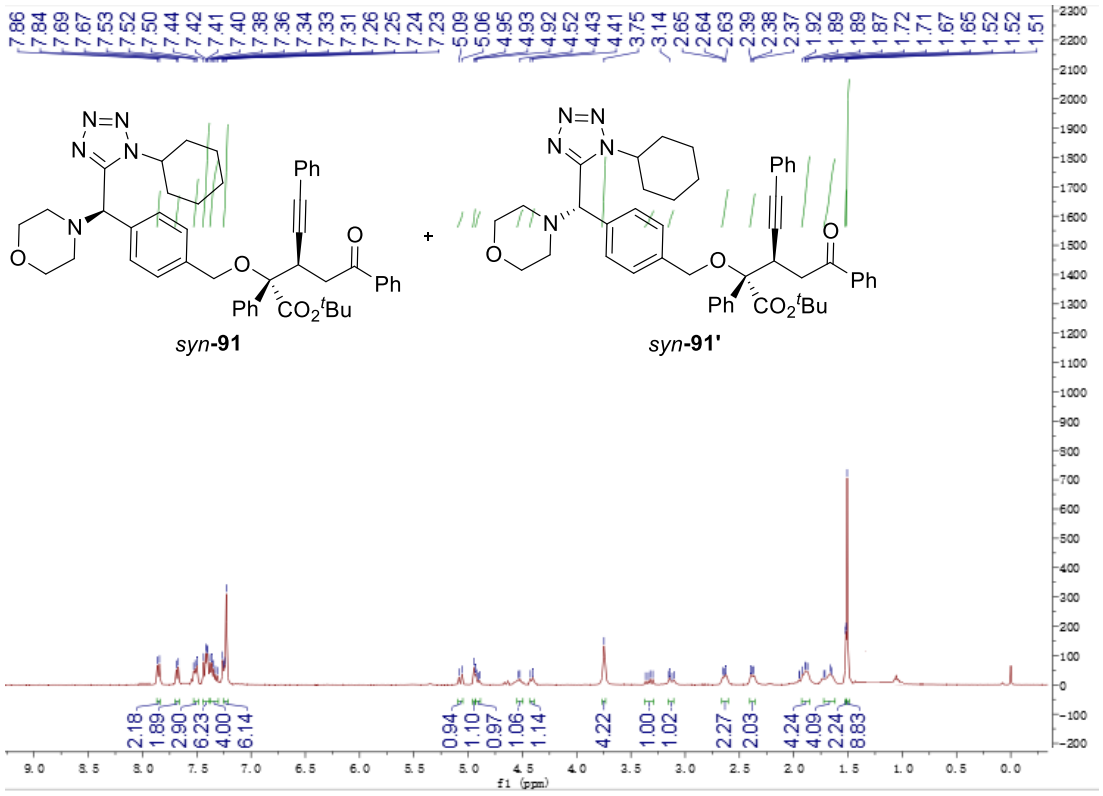

7.87
7.85
7.76
7.72
7.70
7.52
7.51
7.42
7.40
7.38
7.38
7.36
7.33
7.31
7.26
7.24
7.21
5.93
5.89
5.06
5.03
4.91
4.88
4.43
4.41
4.41
4.13
4.11
4.09
4.07
3.15
2.66
2.64
2.63
2.31
2.29
2.27
1.89
1.87
1.85
1.83
1.81
1.55
1.52
1.24
1.22
1.20
OEt
O
Ph
O
O
tBu
Ph
O
tBuO2C
Ph
O
OEt
2.00
0.85
2.01
1.08
4.20
1.03
7.08
0.96
0.91
0.92
1.03
4.28
0.93
1.00
4.05
4.17
4.32
9.24
9.05
6.26
f1 (ppm)

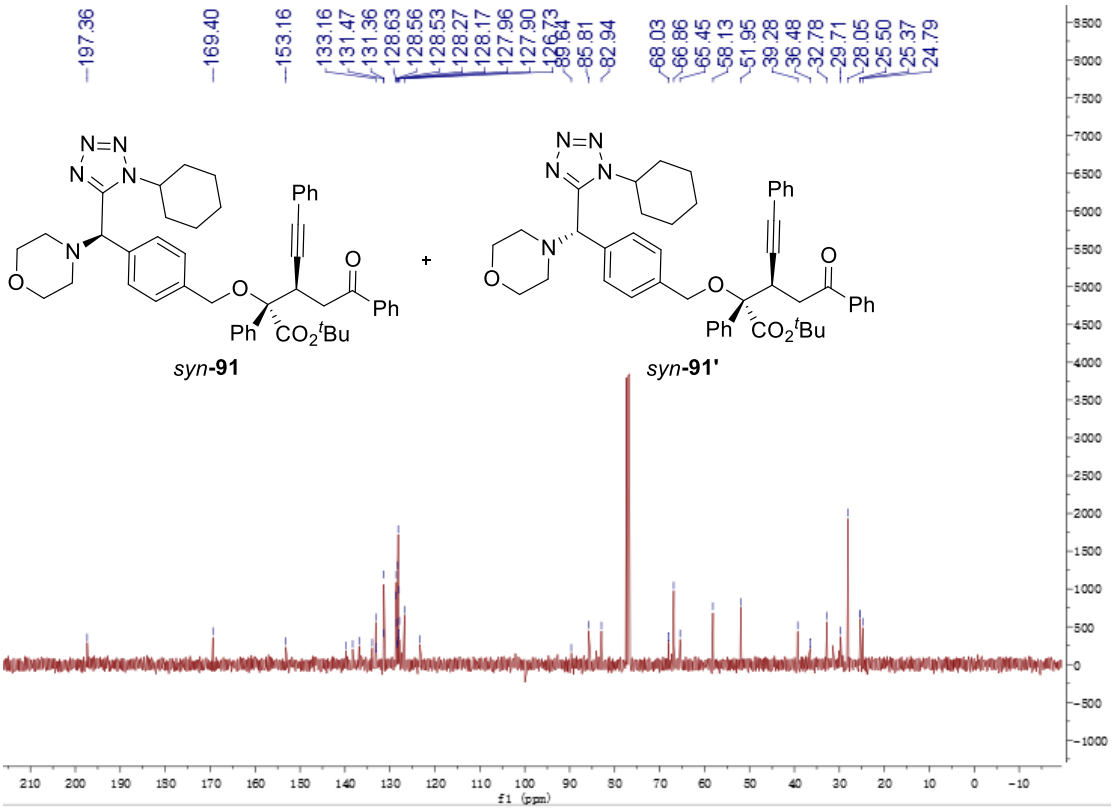
*syn*-**90**

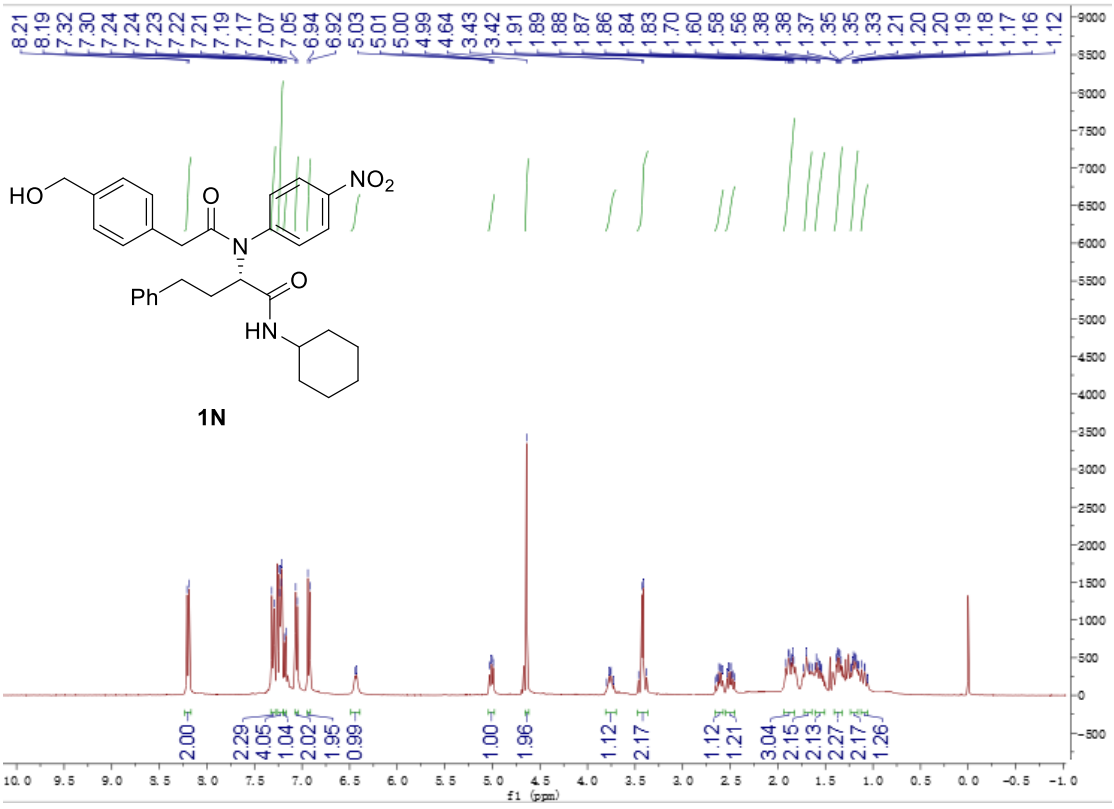

197.47
173.30
169.41
165.69
141.95
139.89
133.07
131.41
128.53
128.50
128.24
128.19
128.16
127.82
126.80
126.46
89.77
85.79
84.08
82.81
80.70
68.33
60.27
39.30
36.46
33.94
33.02
28.23
28.07
26.11
14.27
OEt
O
Ph
O
O
O
tBu
Ph
O
tBuO2C
Ph
O
OEt
syn-90
f1 (ppm)

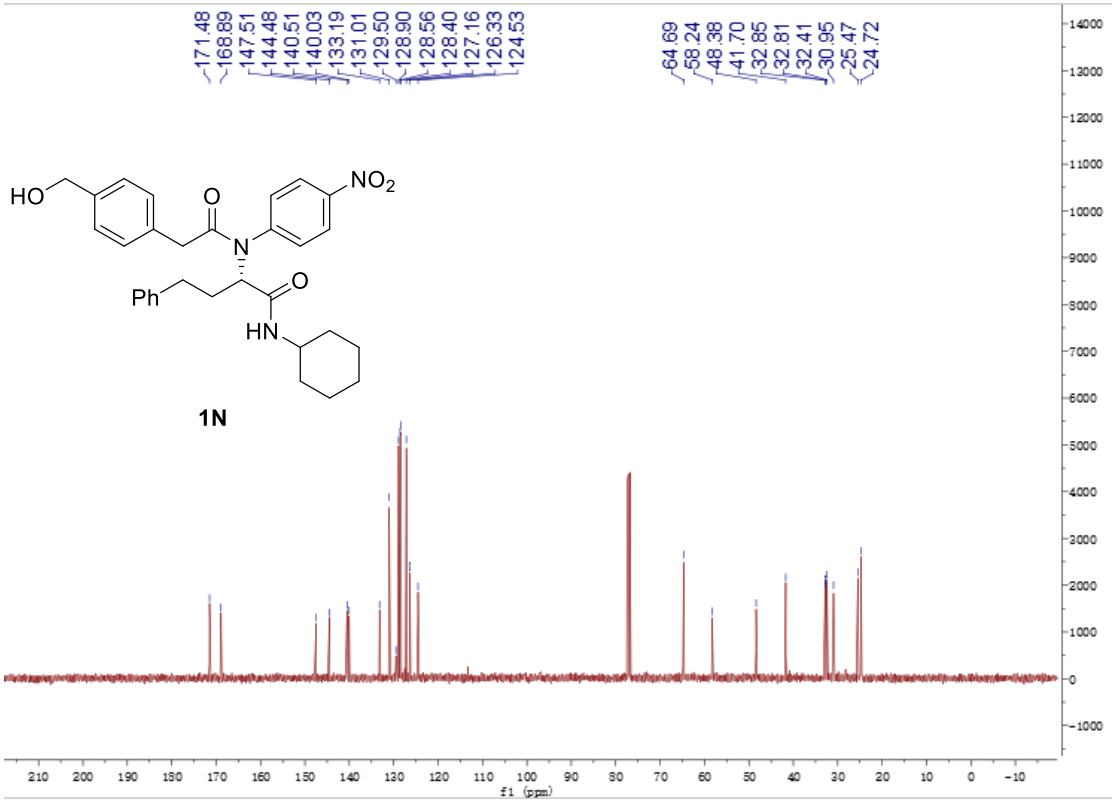

7.40
7.38
7.36
7.34
4.96
4.67
4.59
4.58
4.56
4.55
4.53
4.03
3.70
3.69
3.68
2.58
2.56
2.55
2.38
2.37
2.36
1.88
1.87
1.86
1.84
1.75
1.73
1.61
1.58
1.40
1.37
1.34
1.31
1.29
1.27
N
N
N
N
OH
O
1L
2.00
1.98
1.01
2.03
1.04
0.94
4.03
1.97
2.01
4.03
1.92
1.06
3.23
f1 (ppm)

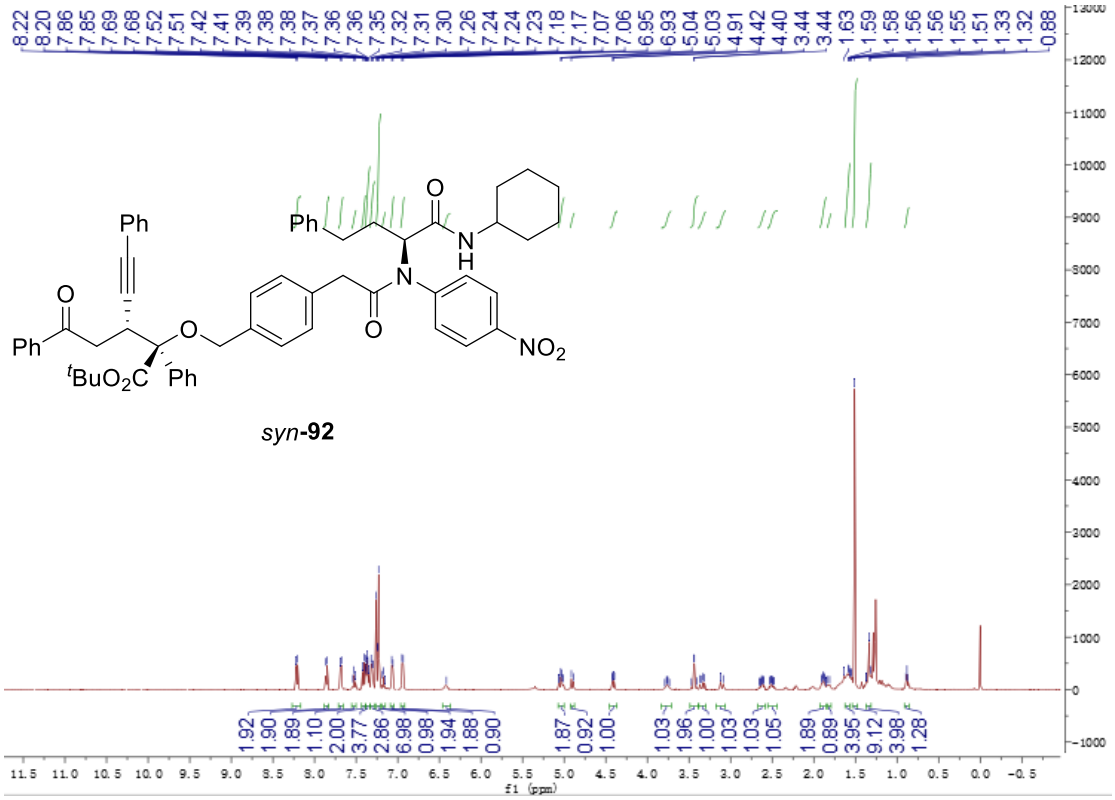

153.29
142.24
133.42
128.70
127.19
66.70
65.04
63.94
58.03
51.61
32.78
32.68
25.27
25.17
24.68
OH
1L

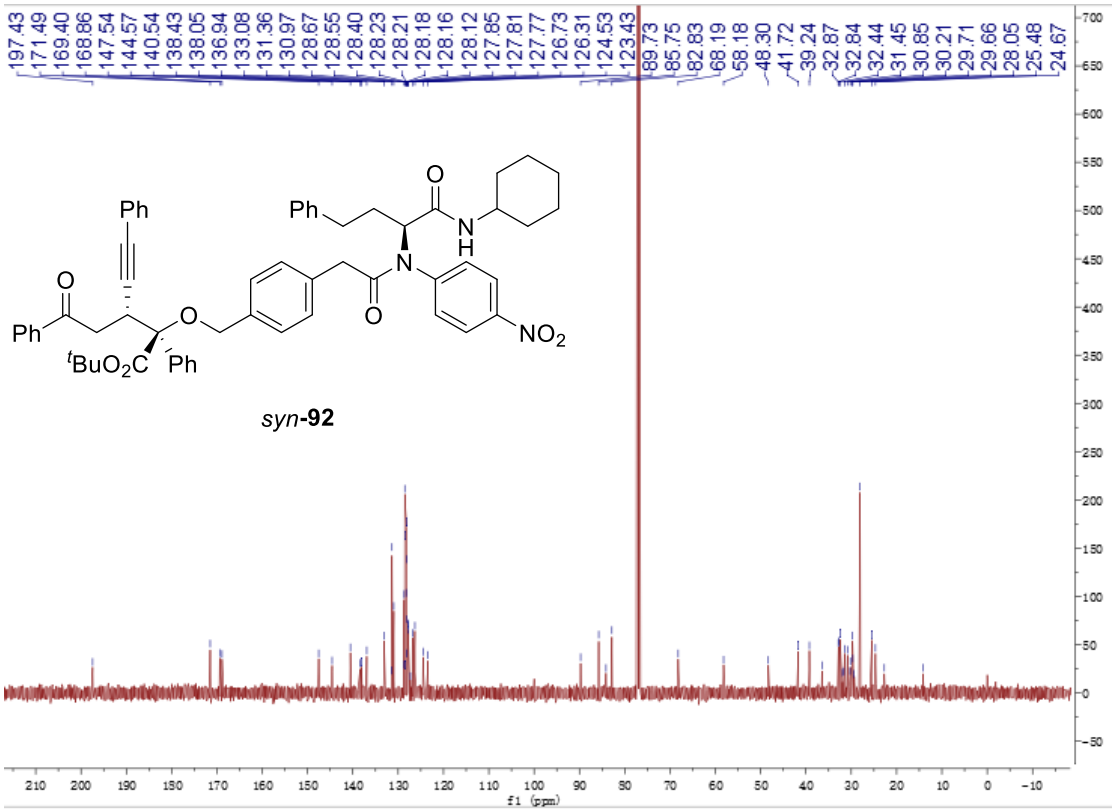

Ph
Ph
CO2tBu
O
Ph
syn-91
syn-91'


197.36
169.40
153.16
133.16
131.47
131.36
128.63
128.56
128.53
128.27
128.17
127.96
127.90
126.73
89.64
85.81
82.94
68.03
66.86
65.45
58.13
51.95
39.28
36.48
32.78
29.71
28.05
25.50
25.37
24.79
N=N
N
N
O
N
O
Ph
O
Ph
Ph
CO2tBu
syn-91
syn-91'
f1 (ppm)

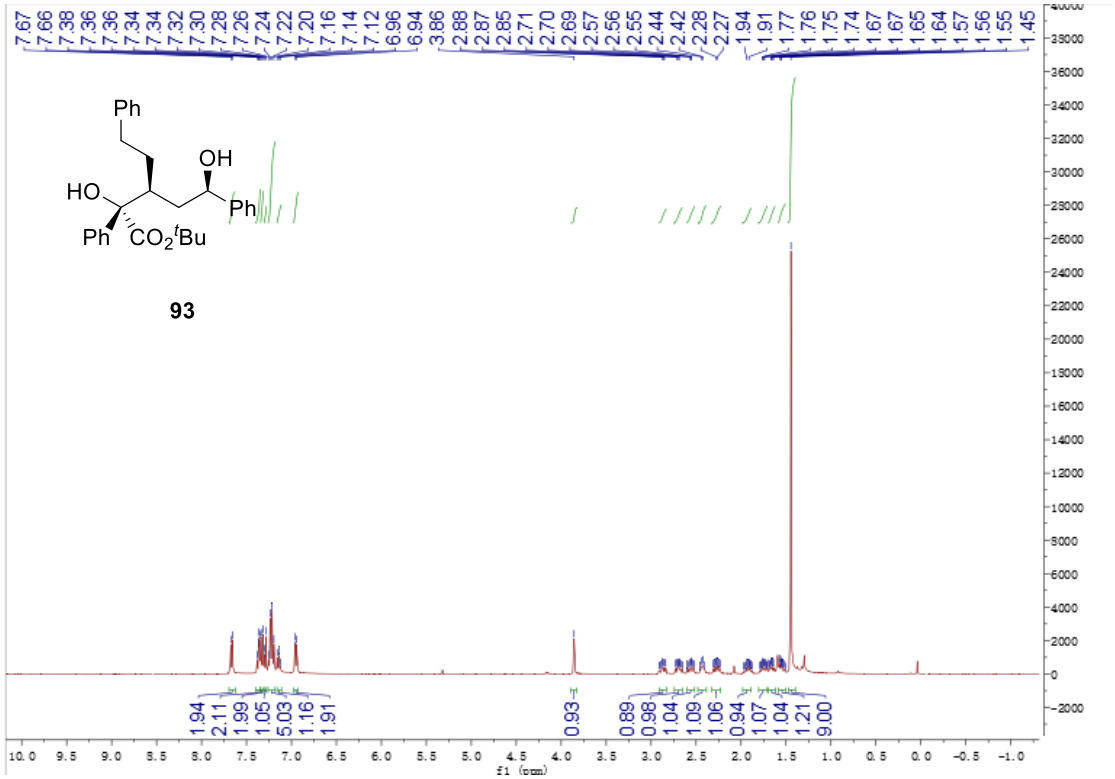

8.21
8.19
7.32
7.30
7.24
7.24
7.23
7.22
7.21
7.19
7.17
7.07
7.05
6.94
6.92
5.03
5.01
5.00
4.99
4.64
3.43
3.42
1.91
1.89
1.88
1.87
1.86
1.84
1.83
1.70
1.60
1.58
1.56
1.38
1.38
1.37
1.35
1.35
1.33
1.21
1.20
1.20
1.19
1.18
1.17
1.16
1.12
HO
O
N
NO2
Ph
O
HN
1N
2.00
2.29
4.05
1.04
2.02
1.95
0.99
1.00
1.96
1.12
2.17
1.12
1.21
3.04
2.15
2.13
2.27
2.17
1.26
f1 (ppm)


171.48
168.89
147.51
144.48
140.51
140.03
133.19
131.01
129.50
128.90
128.56
128.40
127.16
126.33
124.53
64.69
58.24
48.38
41.70
32.85
32.81
32.41
30.95
25.47
24.72
HO
O
N
NO2
Ph
O
HN
1N

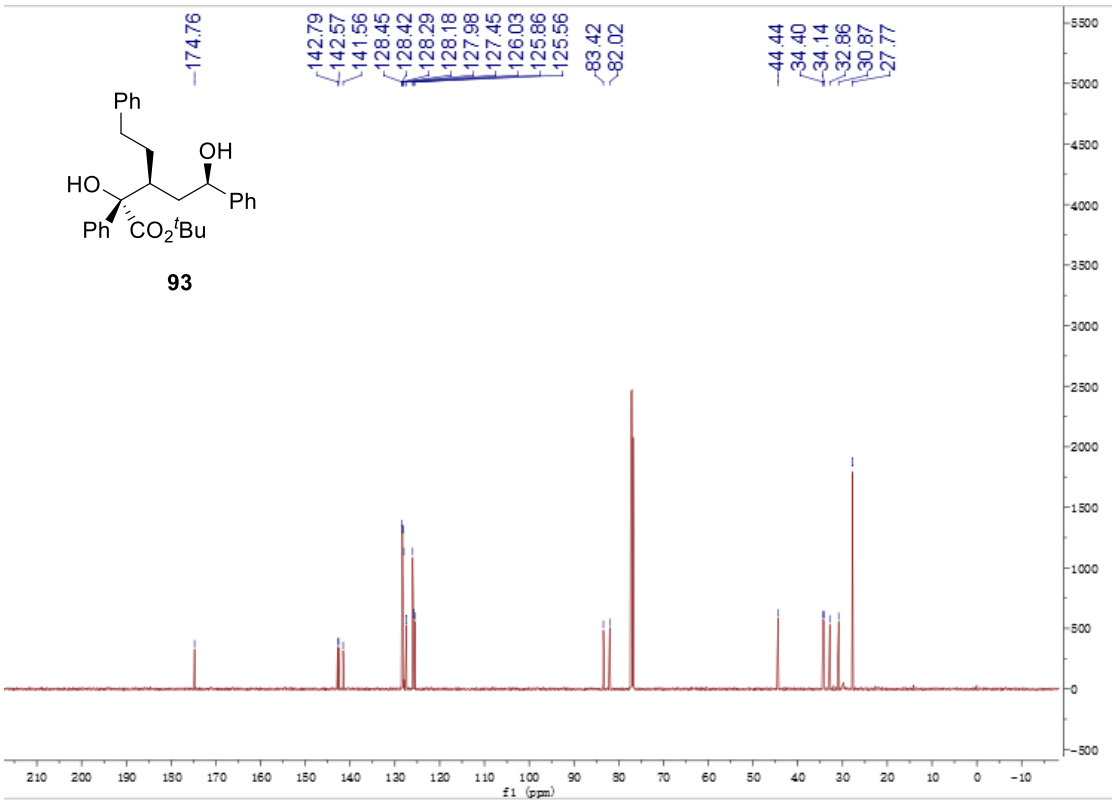

8.22
8.20
7.86
7.85
7.69
7.68
7.52
7.51
7.42
7.41
7.39
7.38
7.38
7.37
7.36
7.36
7.35
7.32
7.31
7.30
7.26
7.24
7.24
7.23
7.18
7.17
7.07
7.06
6.95
6.93
5.04
5.03
4.91
4.42
4.40
3.44
3.44
1.63
1.59
1.58
1.56
1.56
1.55
1.51
1.33
1.32
0.88
Ph
O
N
H
N
O
Ph
O
O
Ph
tBuO2C
Ph
NO2
syn-92


197.43
171.49
169.40
168.86
147.54
144.57
140.54
138.43
138.05
136.94
133.08
131.36
130.97
128.67
128.55
128.40
128.23
128.21
128.18
128.16
128.12
127.85
127.81
127.77
126.73
126.31
124.53
123.43
89.73
85.75
82.83
68.19
58.18
48.30
41.72
39.24
32.87
32.84
32.44
31.45
30.85
30.21
29.71
29.66
28.05
25.48
24.67
Ph
Ph
O
N
H
N
O
O
Ph
O
Ph
$^t$BuO$_2$C
Ph
NO$_2$
f1 (ppm)

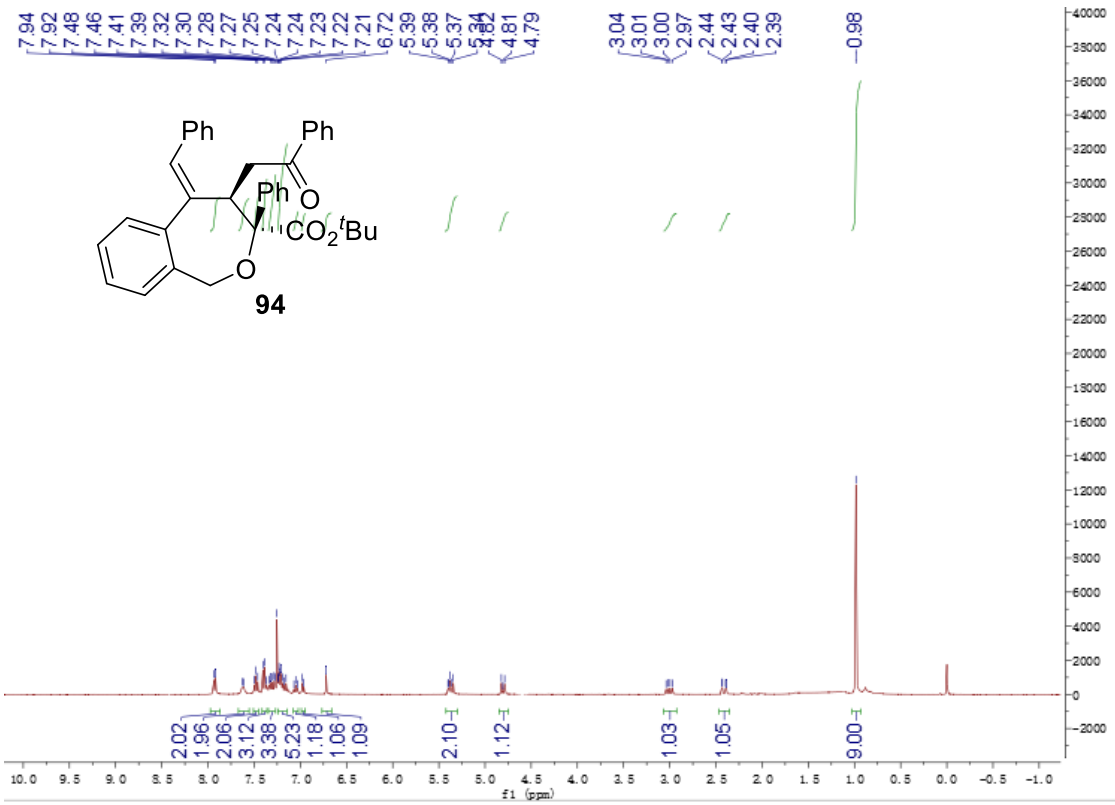
*syn*-**92**


7.67
7.66
7.38
7.36
7.36
7.34
7.34
7.32
7.30
7.28
7.26
7.24
7.22
7.20
7.16
7.14
7.12
6.96
6.94
3.86
2.88
2.87
2.85
2.71
2.70
2.69
2.57
2.56
2.55
2.44
2.42
2.28
2.27
1.94
1.91
1.77
1.76
1.75
1.74
1.67
1.67
1.65
1.64
1.57
1.56
1.55
1.45
Ph
OH
HO
Ph
Ph
CO$_2$$^t$Bu
1.94
2.11
1.99
1.05
5.03
1.16
1.91
0.93
0.89
0.98
1.04
1.09
1.06
0.94
1.07
1.04
1.21
9.00
f1 (ppm)

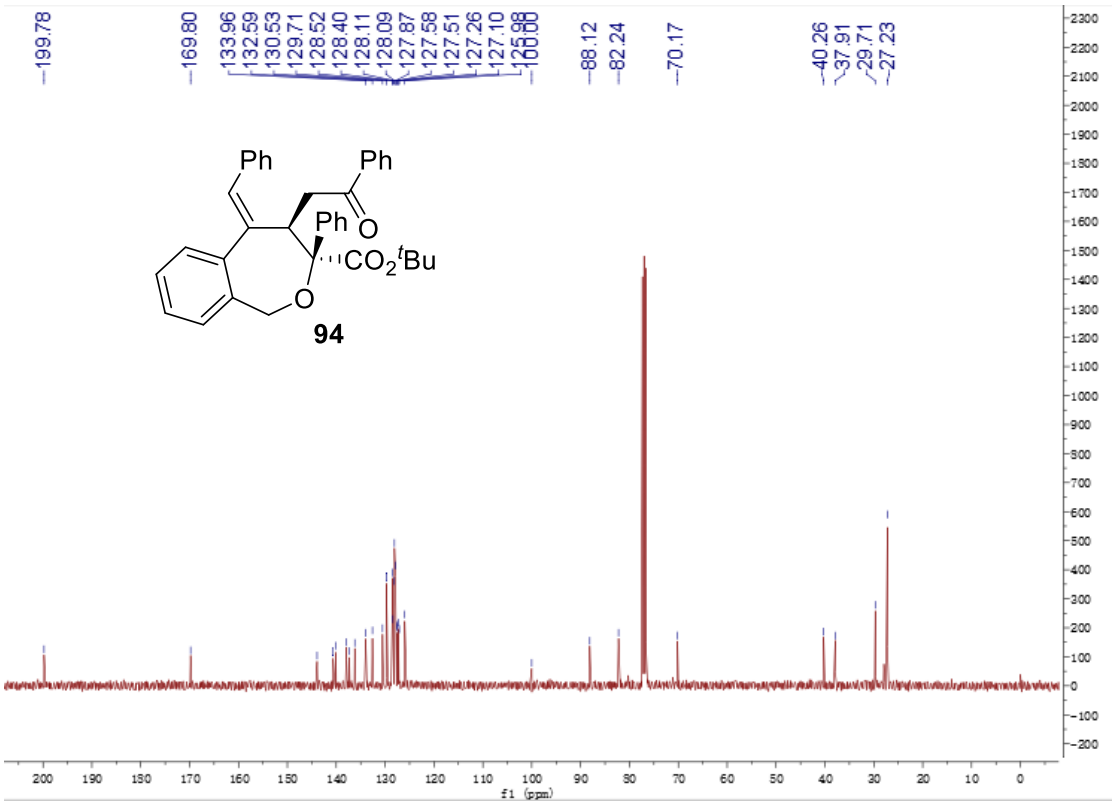
**93**


174.76
142.79
142.57
141.56
128.45
128.42
128.29
128.18
127.98
127.45
126.03
125.86
125.56
83.42
82.02
44.44
34.40
34.14
32.86
30.87
27.77
Ph
OH
HO
Ph
Ph
CO2tBu
f1 (ppm)

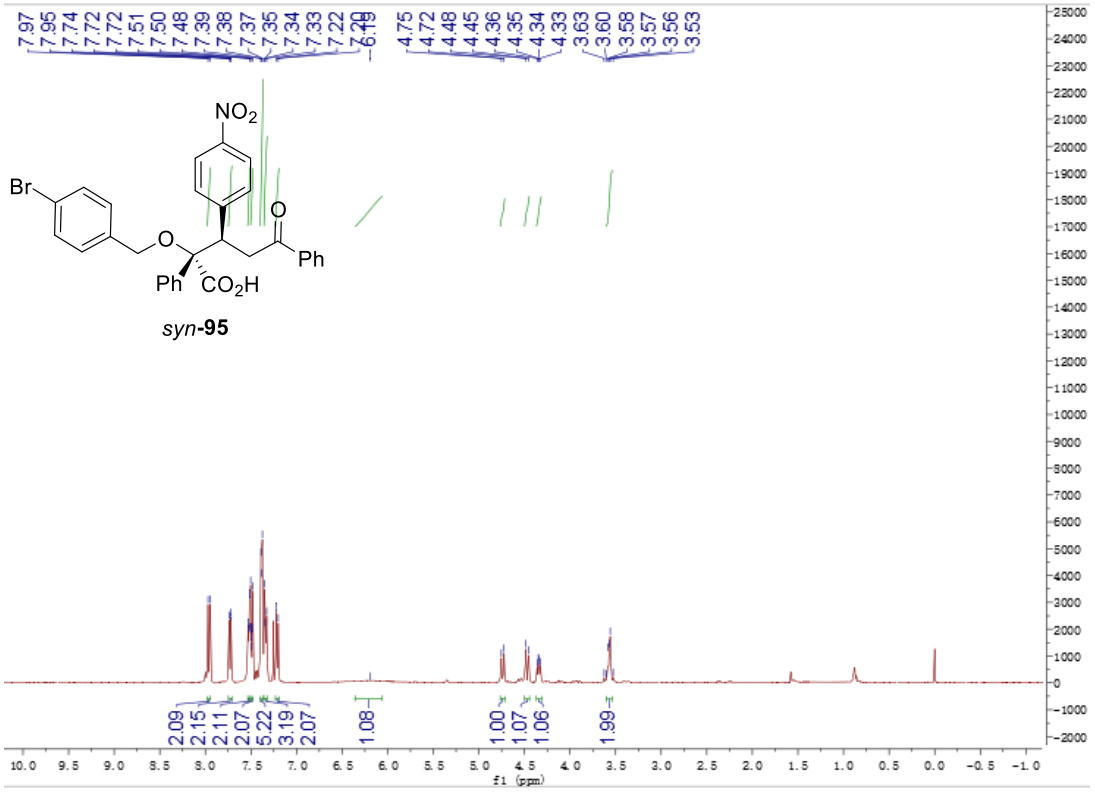
**93**


7.94
7.92
7.48
7.46
7.41
7.39
7.32
7.30
7.28
7.27
7.25
7.24
7.24
7.23
7.22
7.21
6.72
5.39
5.38
5.37
4.81
4.79
3.04
3.01
3.00
2.97
2.44
2.43
2.40
2.39
0.98
Ph
Ph
Ph
O
CO2tBu
O
2.02
1.96
2.06
3.12
3.38
5.23
1.18
1.06
1.09
2.10
1.12
1.03
1.05
9.00
f1 (ppm)

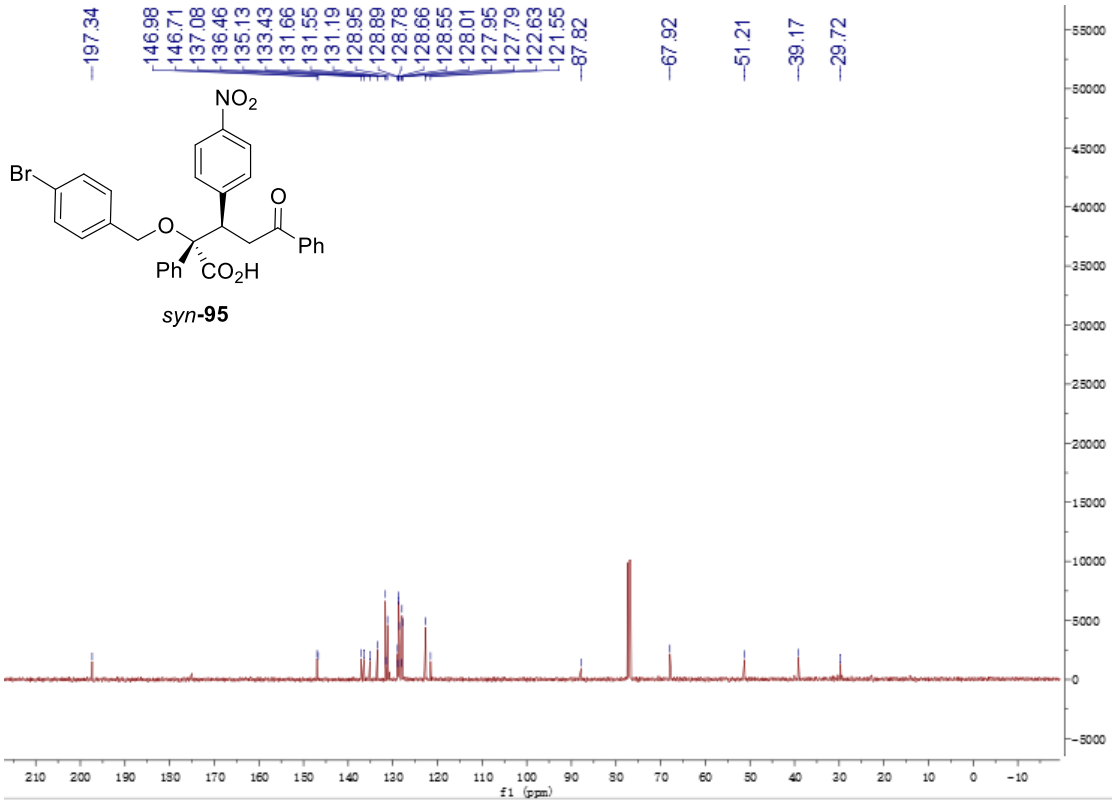
**94**


199.78
169.80
133.96
132.59
130.53
129.71
128.52
128.40
128.11
128.09
127.87
127.58
127.51
127.26
127.10
125.88
88.12
82.24
70.17
40.26
37.91
29.71
27.23
Ph
Ph
Ph
O
CO2tBu
O

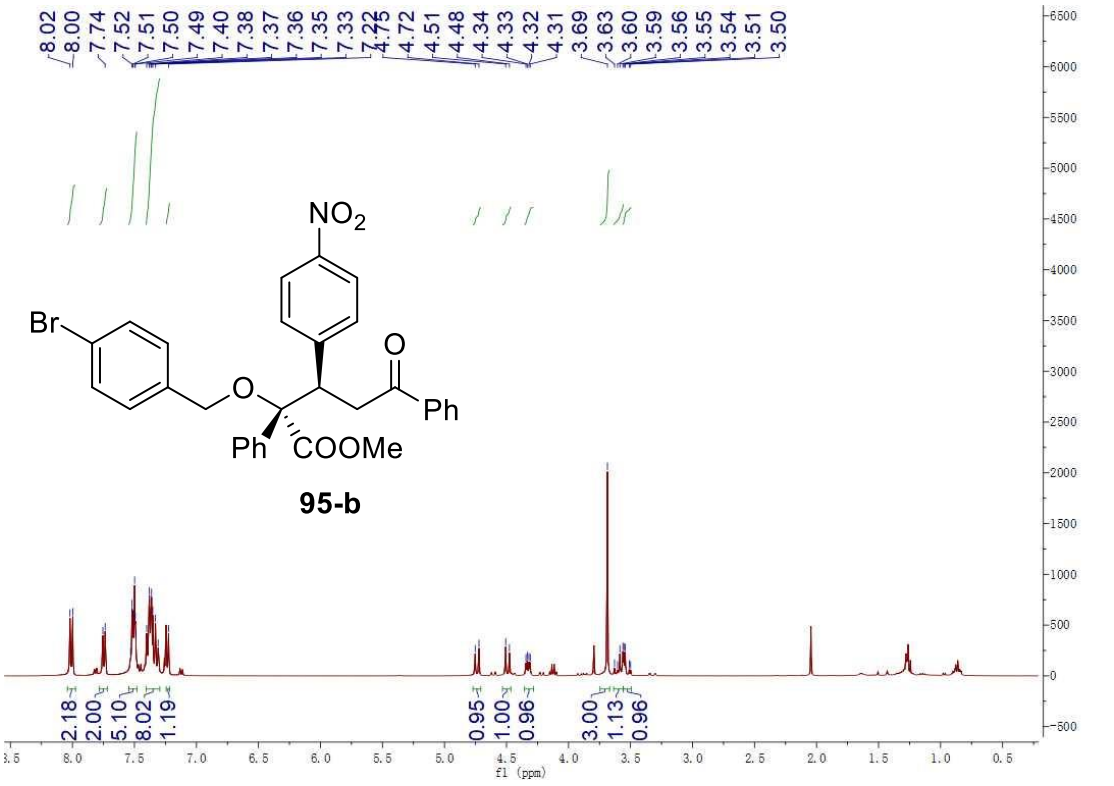
**94**


7.97
7.95
7.74
7.72
7.72
7.51
7.50
7.48
7.39
7.38
7.37
7.35
7.34
7.33
7.22
6.19
4.75
4.72
4.48
4.45
4.36
4.35
4.34
4.33
3.63
3.60
3.58
3.57
3.56
3.53
NO2
Br
O
O
Ph
Ph
CO2H
2.09
2.15
2.11
2.07
5.22
3.19
2.07
1.08
1.00
1.07
1.06
1.99

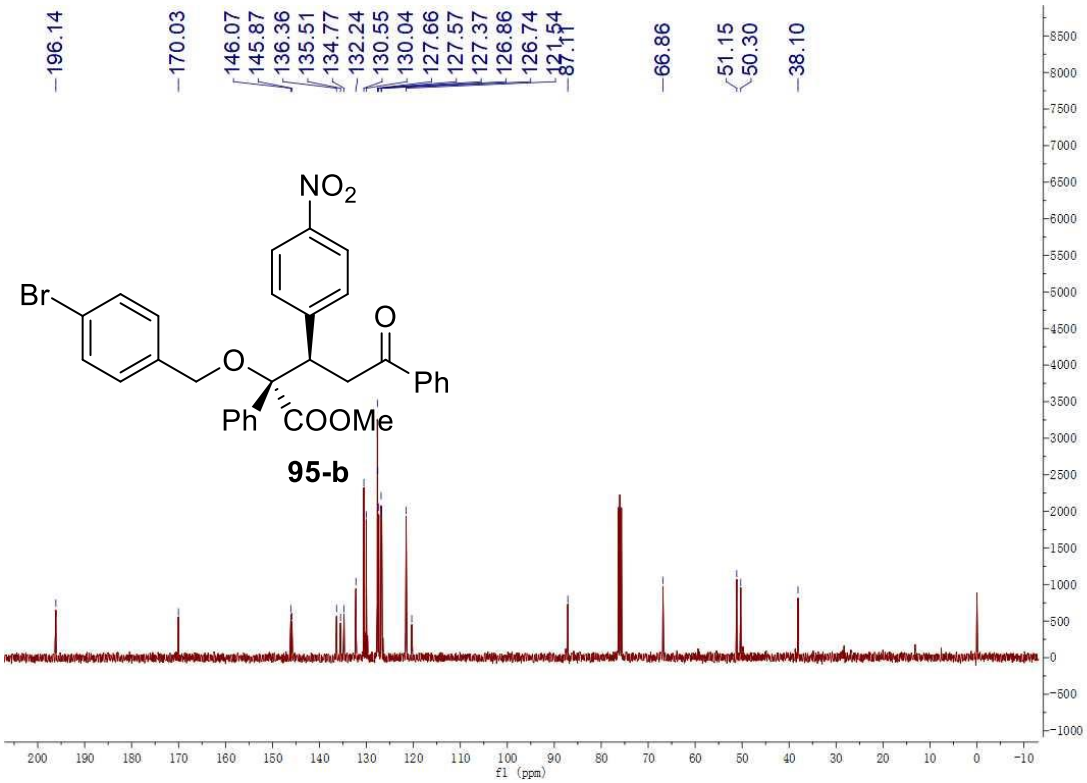
*syn*-**95**

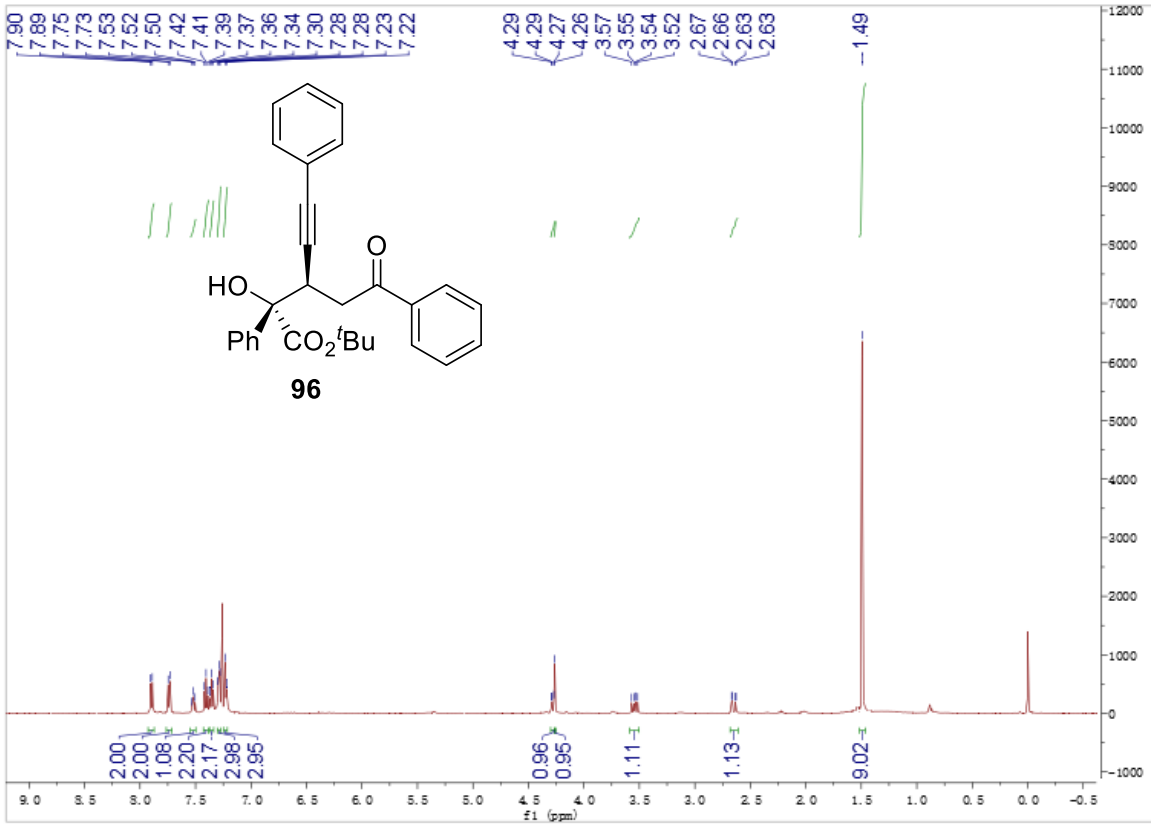

197.34
146.98
146.71
137.08
136.46
135.13
133.43
131.66
131.55
131.19
128.95
128.89
128.78
128.66
128.55
128.01
127.95
127.79
122.63
121.55
87.82
67.92
51.21
39.17
29.72
NO2
Br
O
O
Ph
Ph
CO2H
f1 (ppm)

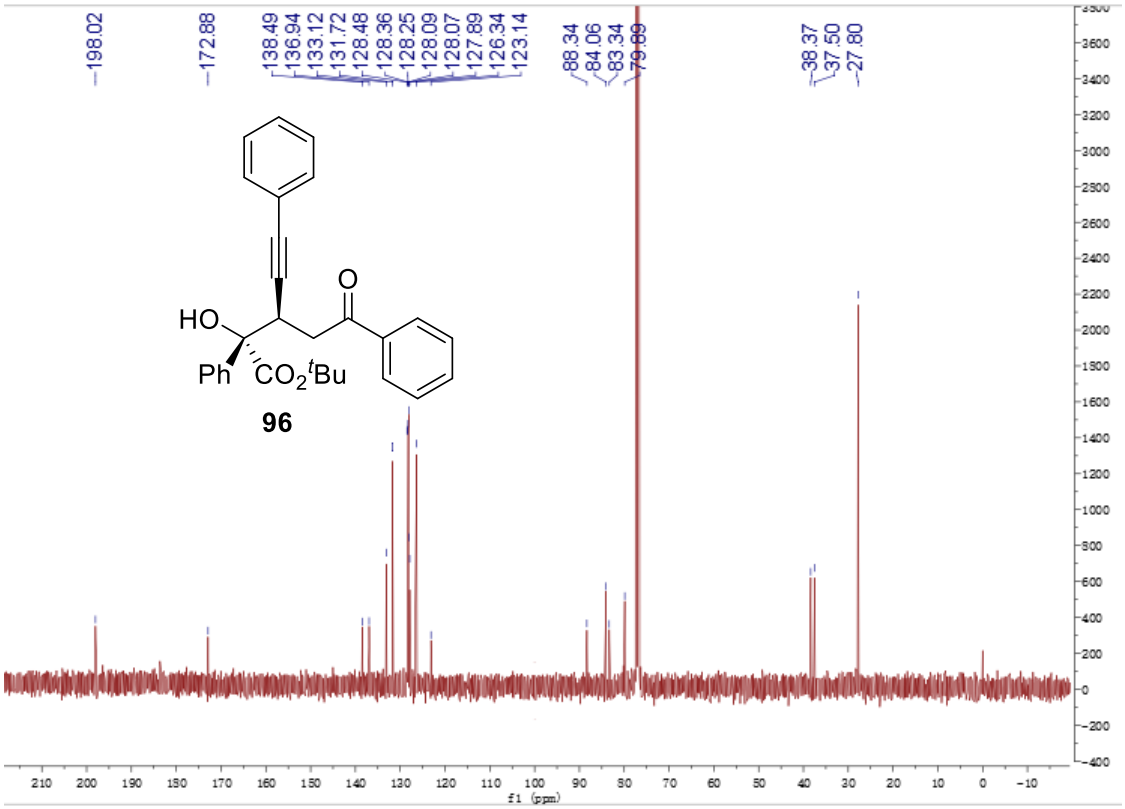
*syn*-**95**

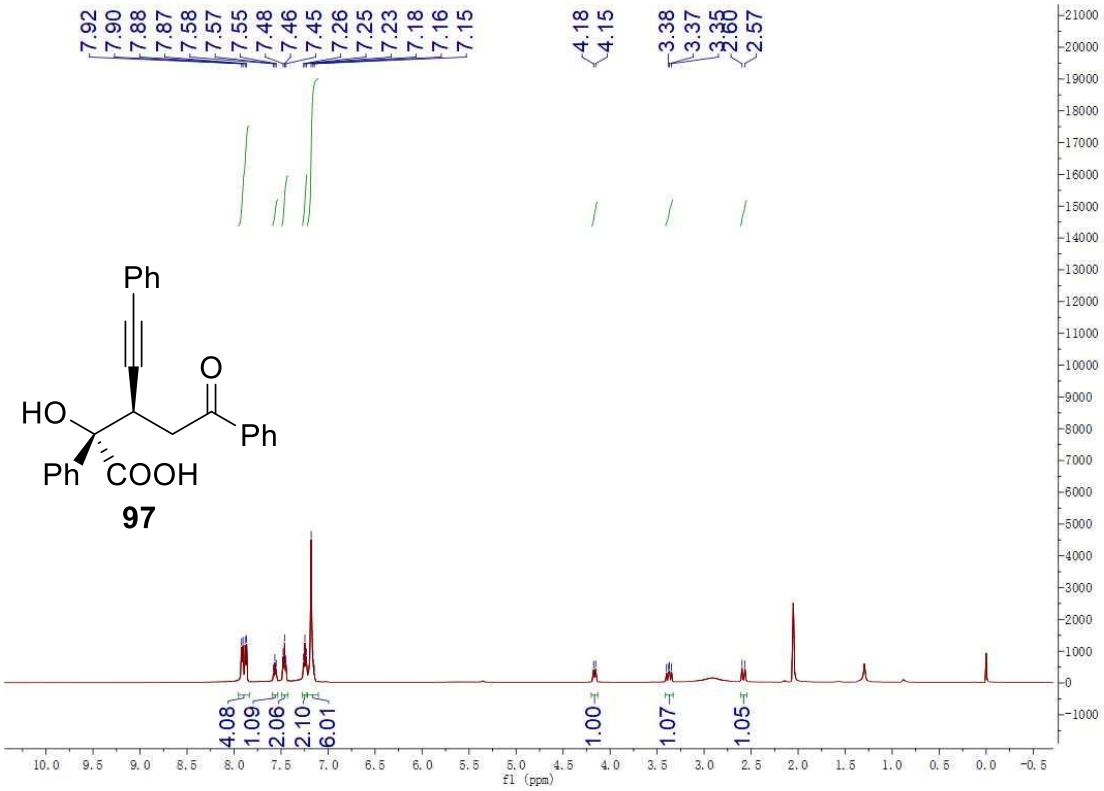

8.02
8.00
7.74
7.52
7.51
7.50
7.49
7.40
7.38
7.37
7.36
7.35
7.33
7.22
4.75
4.72
4.51
4.48
4.34
4.33
4.32
4.31
3.69
3.63
3.60
3.59
3.56
3.55
3.54
3.51
3.50
NO2
Br
O
O
Ph
Ph
COOMe
2.18
2.00
5.10
8.02
1.19
0.95
1.00
0.96
3.00
1.13
0.96
f1 (ppm)

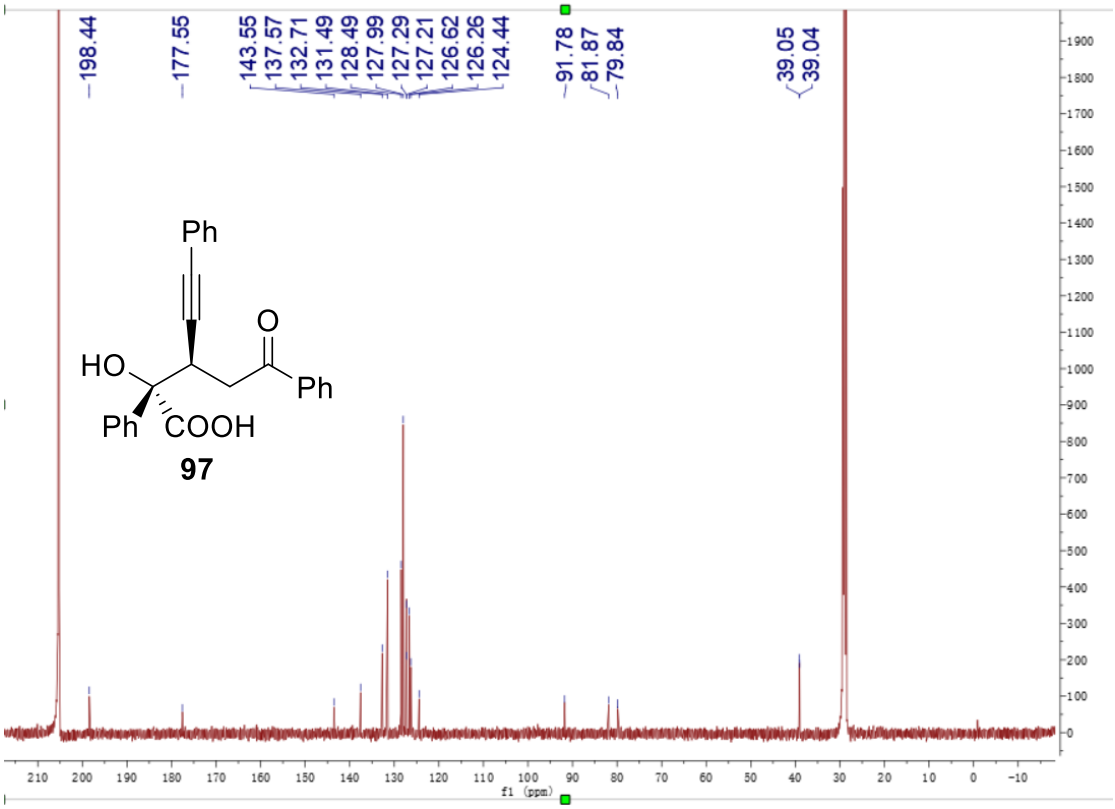
**95-b**

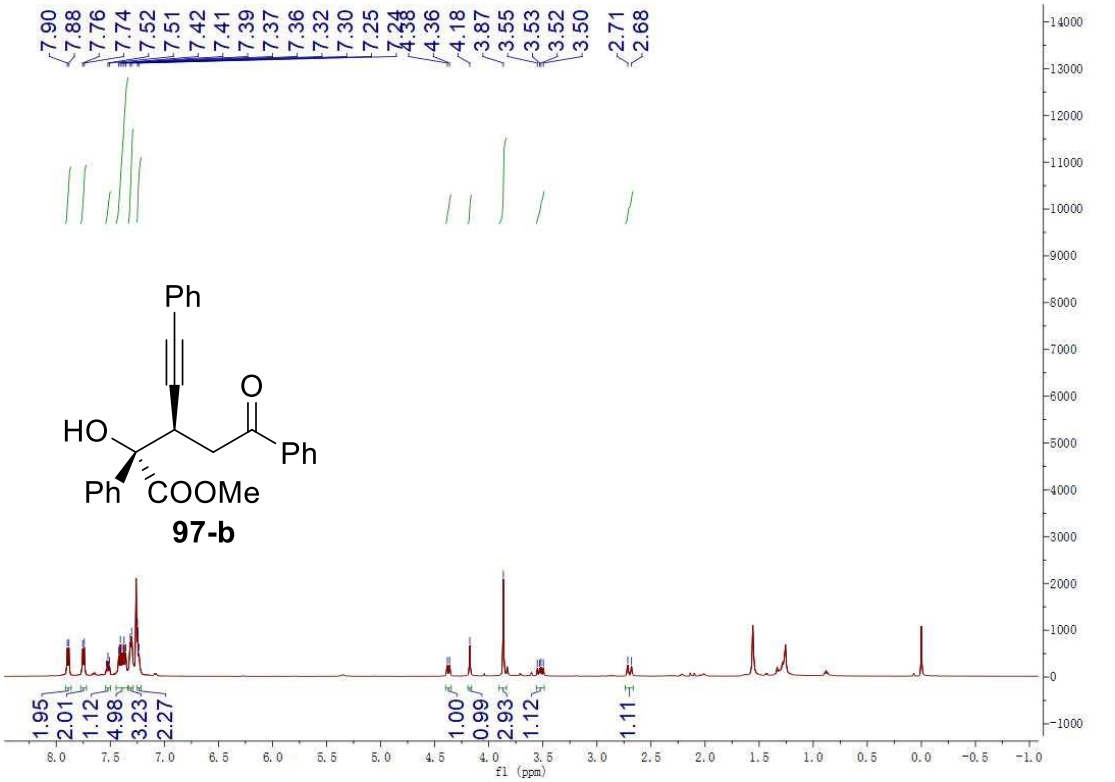

196.14
170.03
146.07
145.87
136.36
135.51
134.77
132.24
130.55
130.04
127.66
127.57
127.37
126.86
126.74
121.54
87.11
66.86
51.15
50.30
38.10
NO2
Br
O
O
Ph
Ph
COOMe
95-b
f1 (ppm)

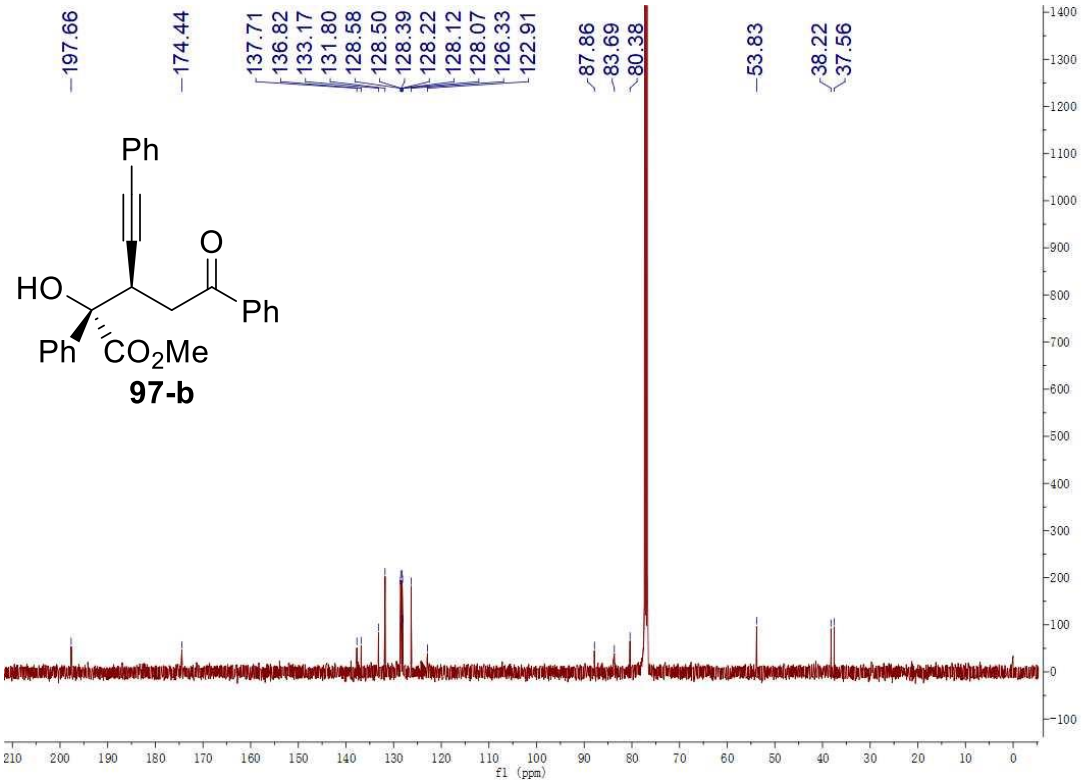

7.90
7.89
7.75
7.73
7.53
7.52
7.50
7.42
7.41
7.39
7.37
7.36
7.34
7.30
7.28
7.28
7.23
7.22
4.29
4.29
4.27
4.26
3.57
3.55
3.54
3.52
2.67
2.66
2.63
2.63
1.49
HO
O
Ph
CO2tBu
96
2.00
2.00
1.08
2.20
2.17
2.98
2.95
0.96
0.95
1.11
1.13
9.02
f1 (ppm)

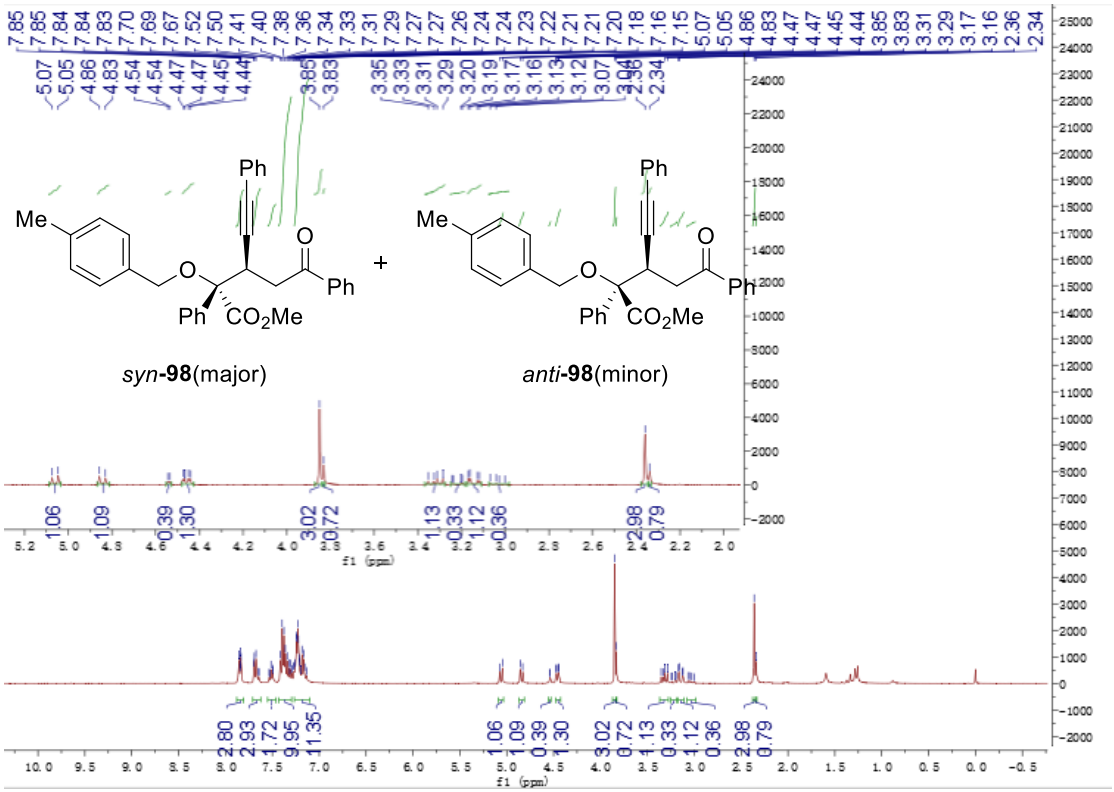

198.02
172.88
138.49
136.94
133.12
131.72
128.48
128.36
128.25
128.09
128.07
127.89
126.34
123.14
88.34
84.06
83.34
79.89
38.37
37.50
27.80
HO
O
Ph
CO2tBu
96
f1 (ppm)

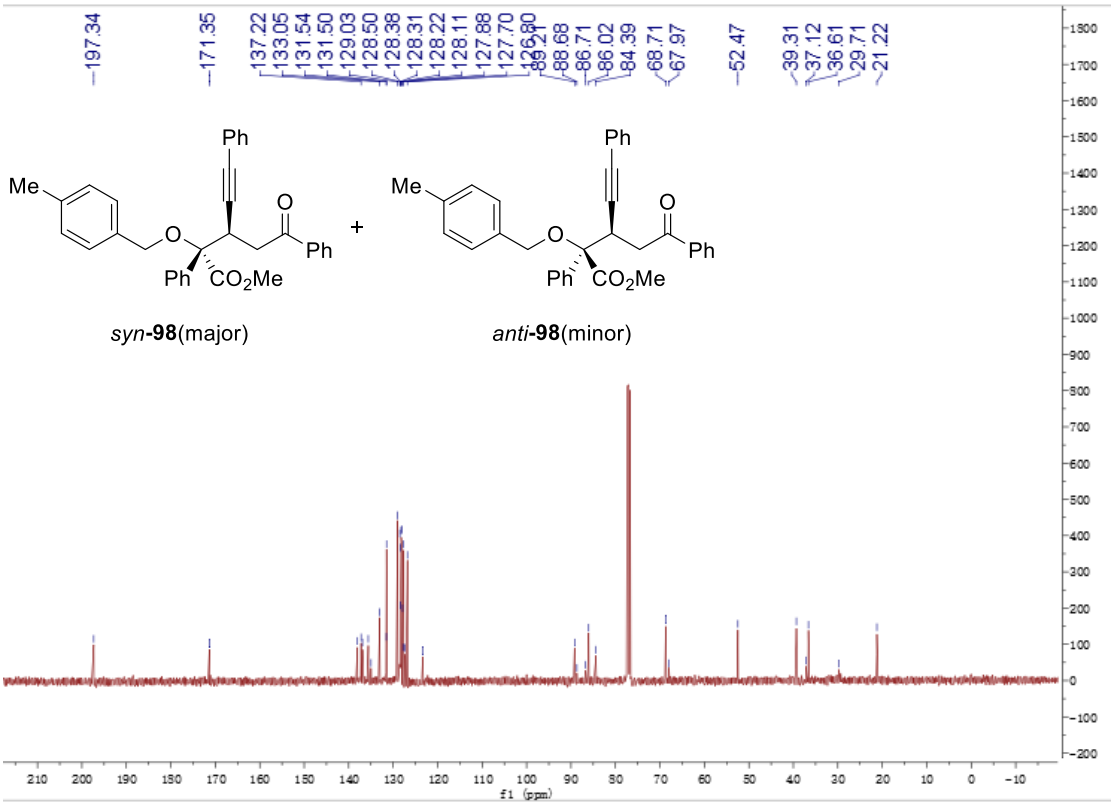

7.92
7.90
7.88
7.87
7.58
7.57
7.55
7.48
7.46
7.45
7.26
7.25
7.23
7.18
7.16
7.15
4.18
4.15
3.38
3.37
2.60
2.57
Ph
HO
O
Ph
Ph
COOH
97
4.08
1.09
2.06
2.10
6.01
1.00
1.07
1.05
f1 (ppm)


198.44
177.55
143.55
137.57
132.71
131.49
128.49
127.99
127.29
127.21
126.62
126.26
124.44
91.78
81.87
79.84
39.05
39.04
Ph
HO
O
Ph
Ph
COOH
97
f1 (ppm)

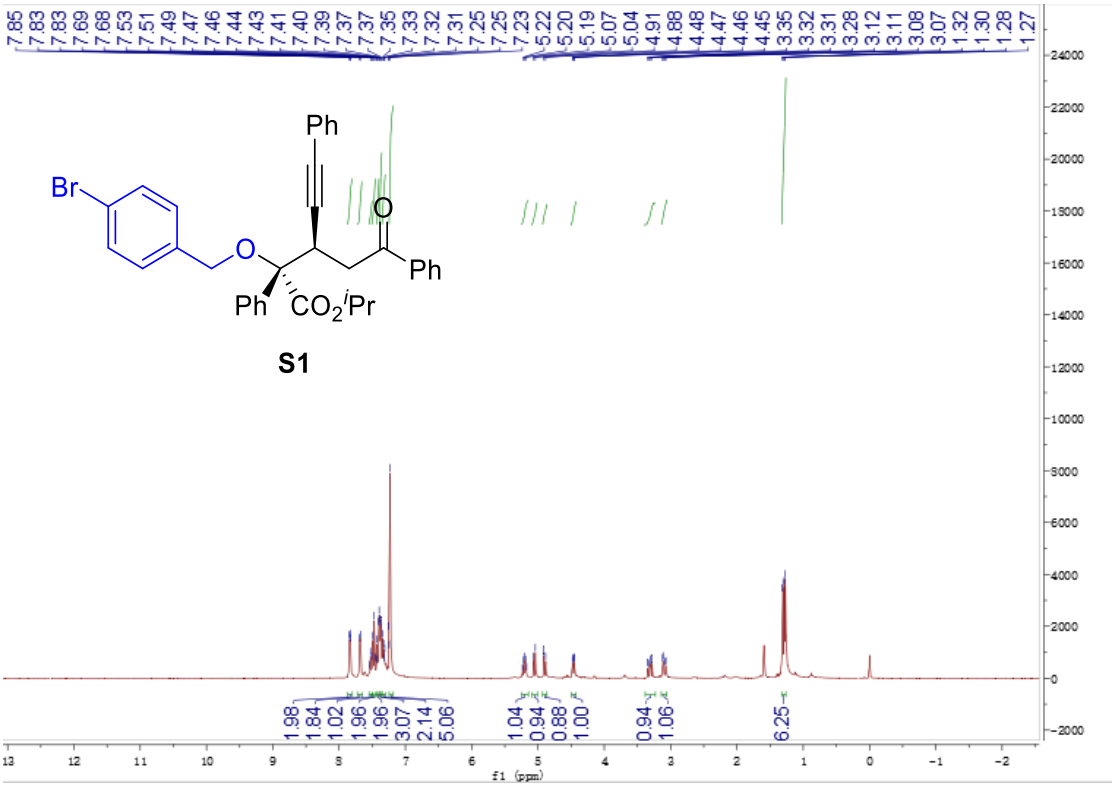

7.90
7.88
7.76
7.74
7.52
7.51
7.42
7.41
7.39
7.37
7.36
7.32
7.30
7.25
4.38
4.36
4.18
3.87
3.55
3.53
3.52
3.50
2.71
2.68
Ph
HO
O
Ph
Ph
COOMe
97-b
1.95
2.01
1.12
4.98
3.23
2.27
1.00
0.99
2.93
1.12
1.11
f1 (ppm)


Ph
HO
O
Ph
Ph
CO2Me
97-b

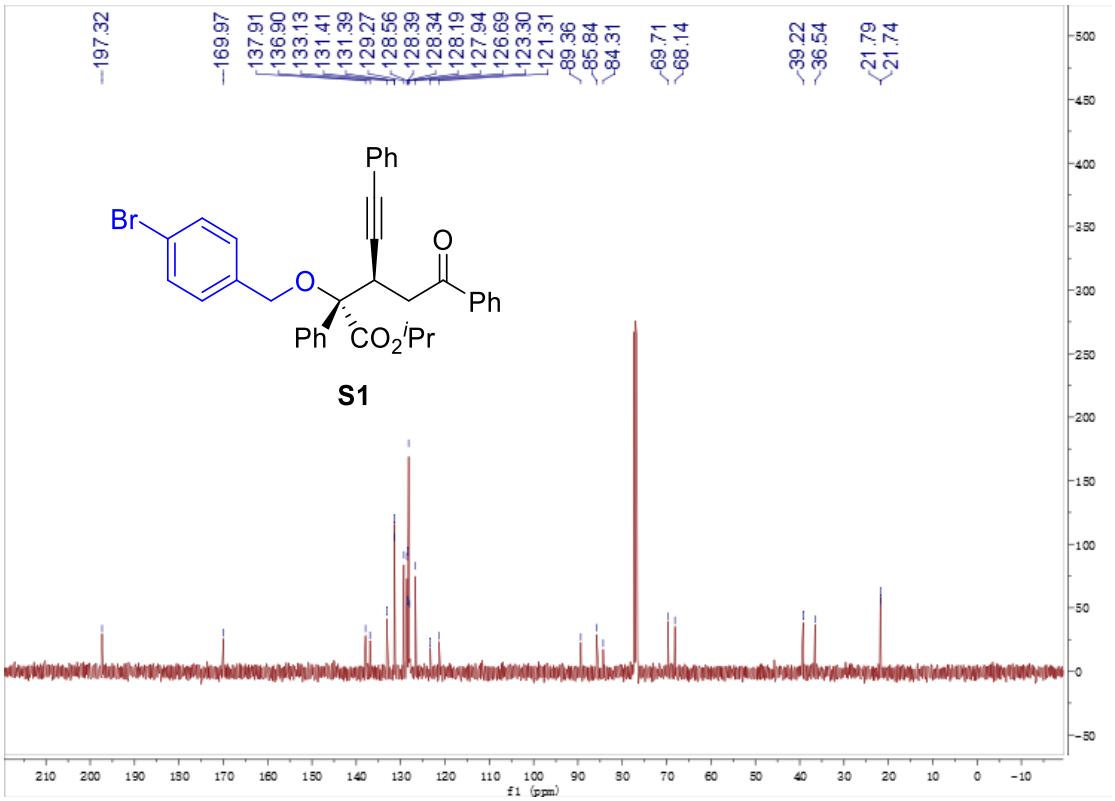

Me
Ph
O
Ph
Ph
CO2Me
+
syn-98(major)
anti-98(minor)

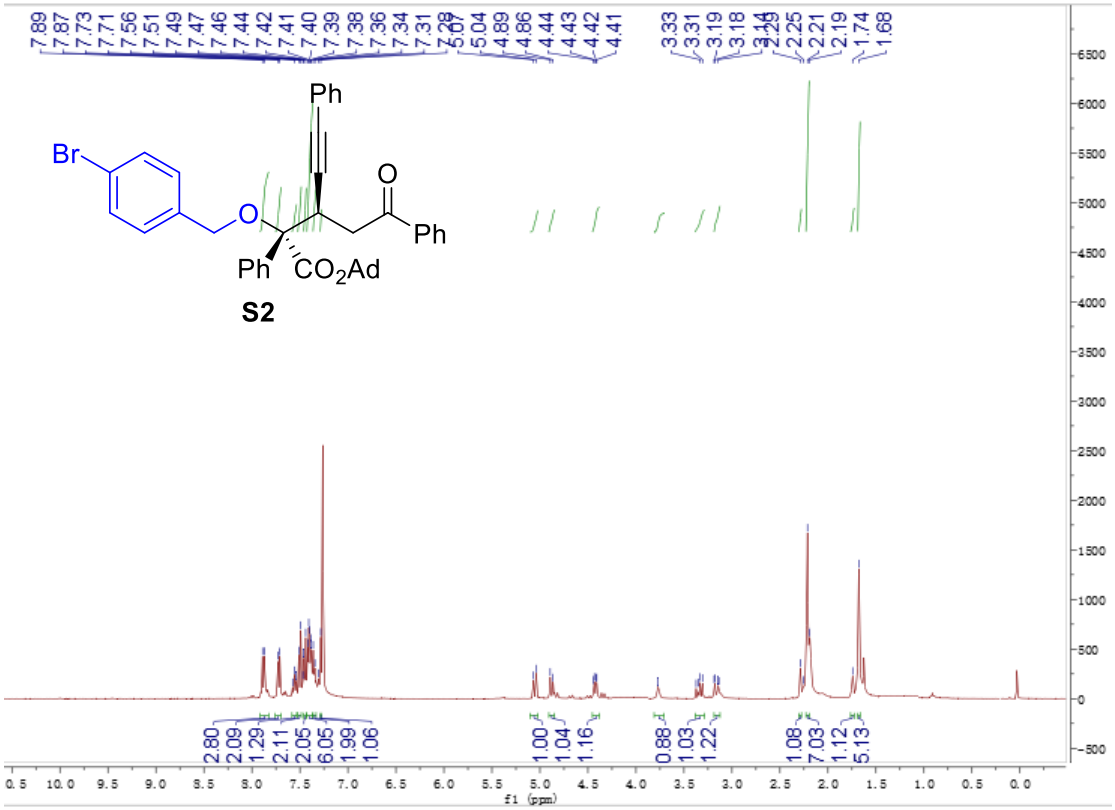


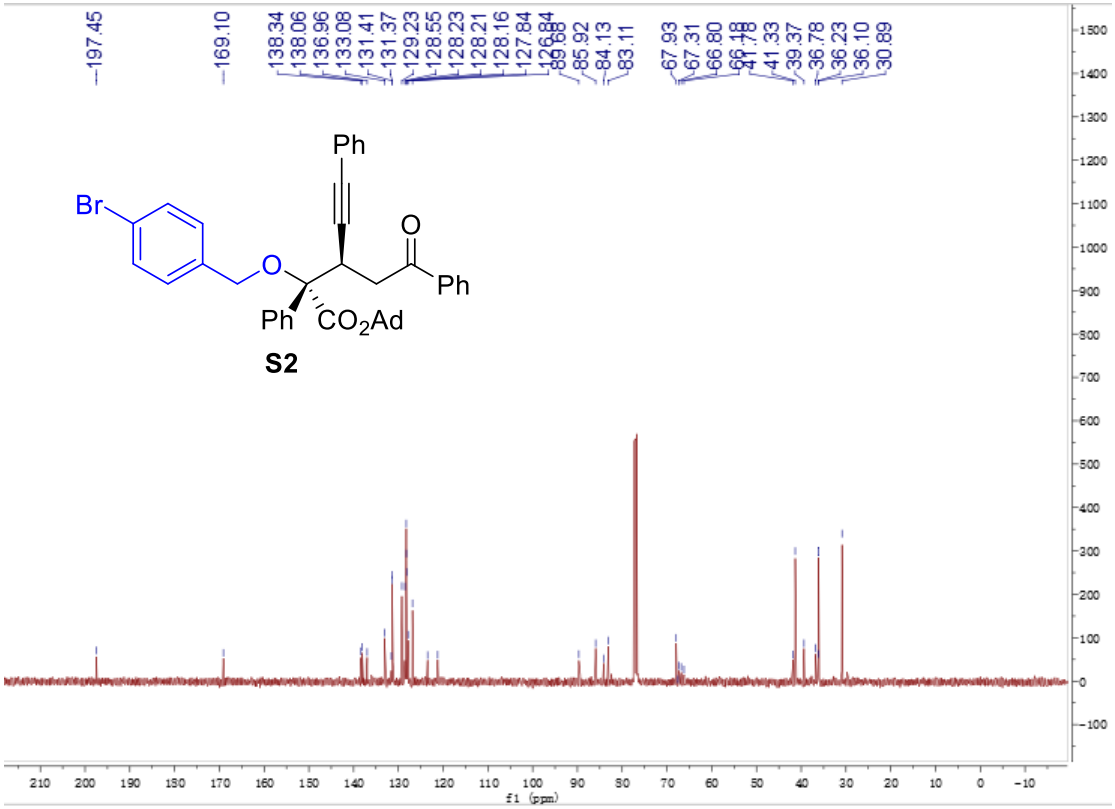

*syn*-**98**(major) *anti*-**98**(minor)



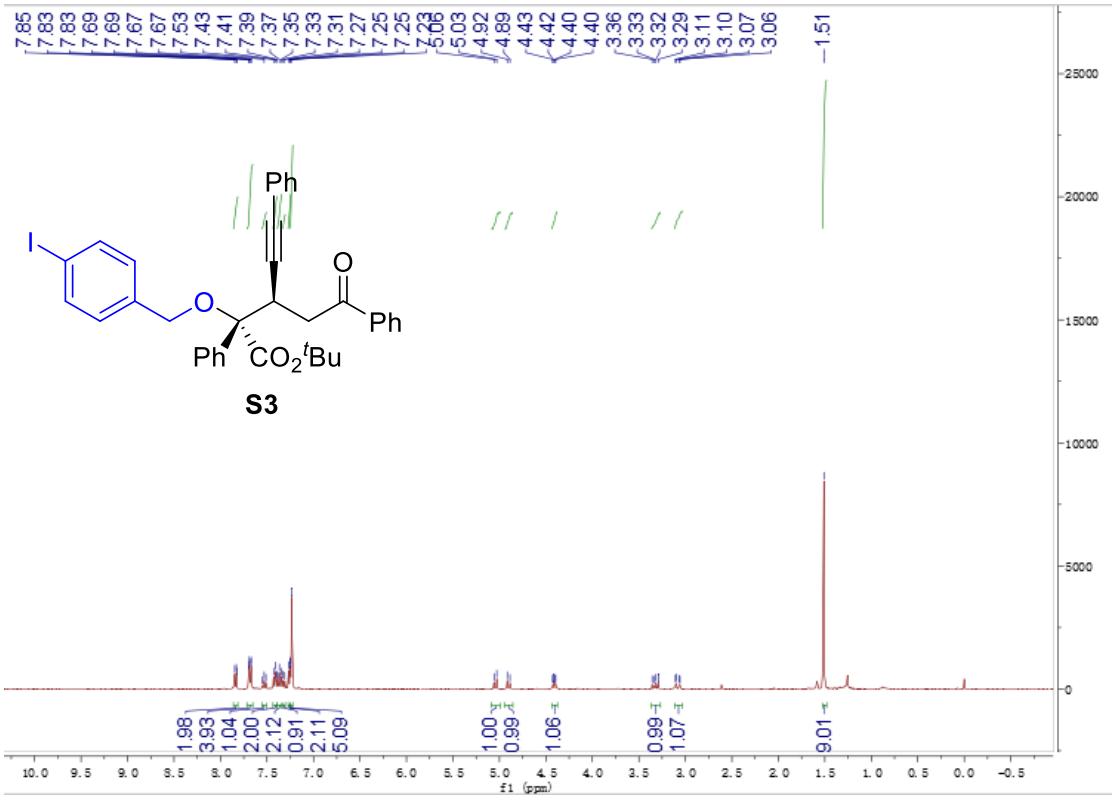

**S1**


197.32
169.97
137.91
136.90
133.13
131.41
131.39
129.27
128.56
128.39
128.34
128.19
127.94
126.69
123.30
121.31
89.36
85.84
84.31
69.71
68.14
39.22
36.54
21.79
21.74
Ph
Br
O
O
Ph
Ph
CO2iPr
S1

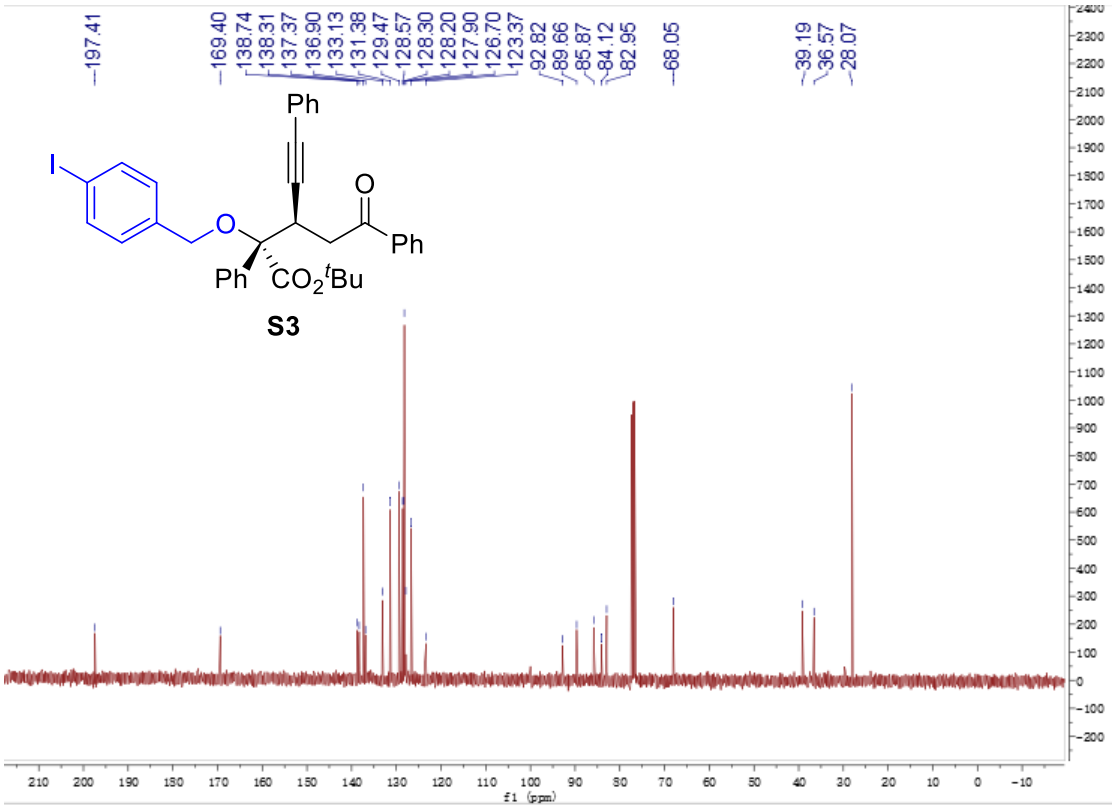

7.89
7.87
7.73
7.71
7.56
7.51
7.49
7.47
7.46
7.44
7.42
7.41
7.40
7.39
7.38
7.36
7.34
7.31
5.04
4.89
4.86
4.44
4.43
4.42
4.41
3.33
3.31
3.19
3.18
2.25
2.21
2.19
1.74
1.68
Ph
Br
O
O
Ph
Ph
CO2Ad
S2
2.80
2.09
1.29
2.11
2.05
6.05
1.99
1.06
1.00
1.04
1.16
0.88
1.03
1.22
1.08
7.03
1.12
5.13

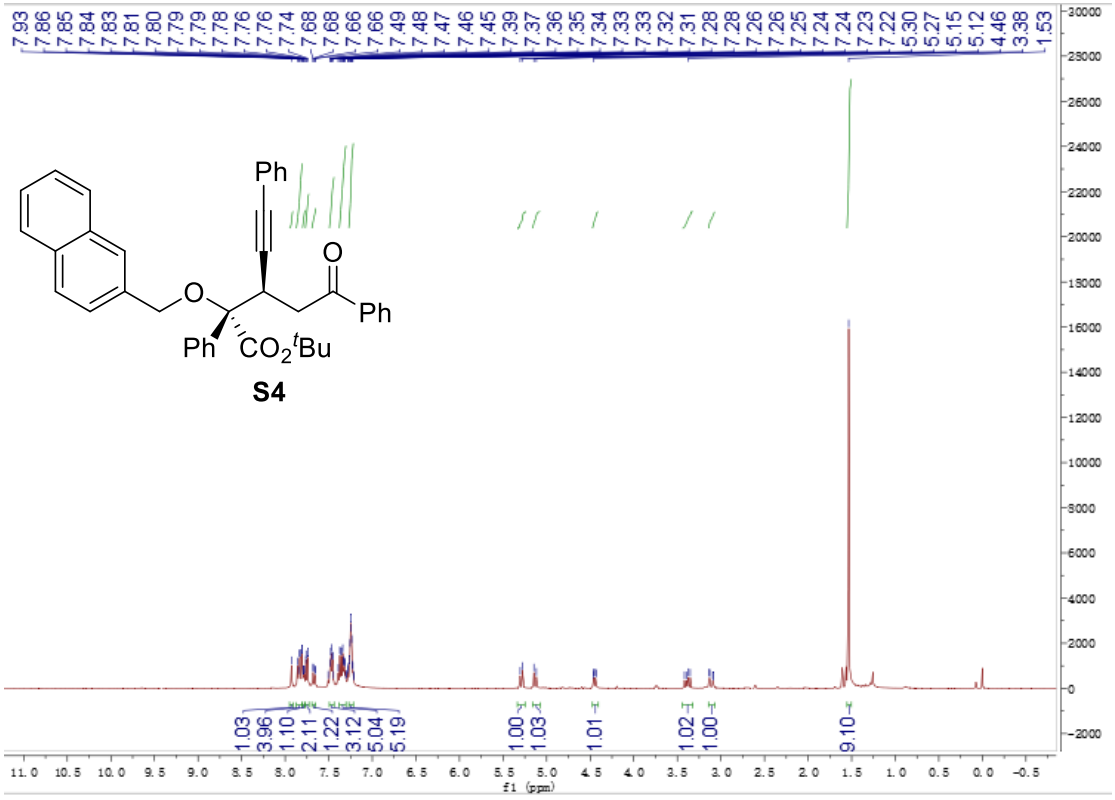


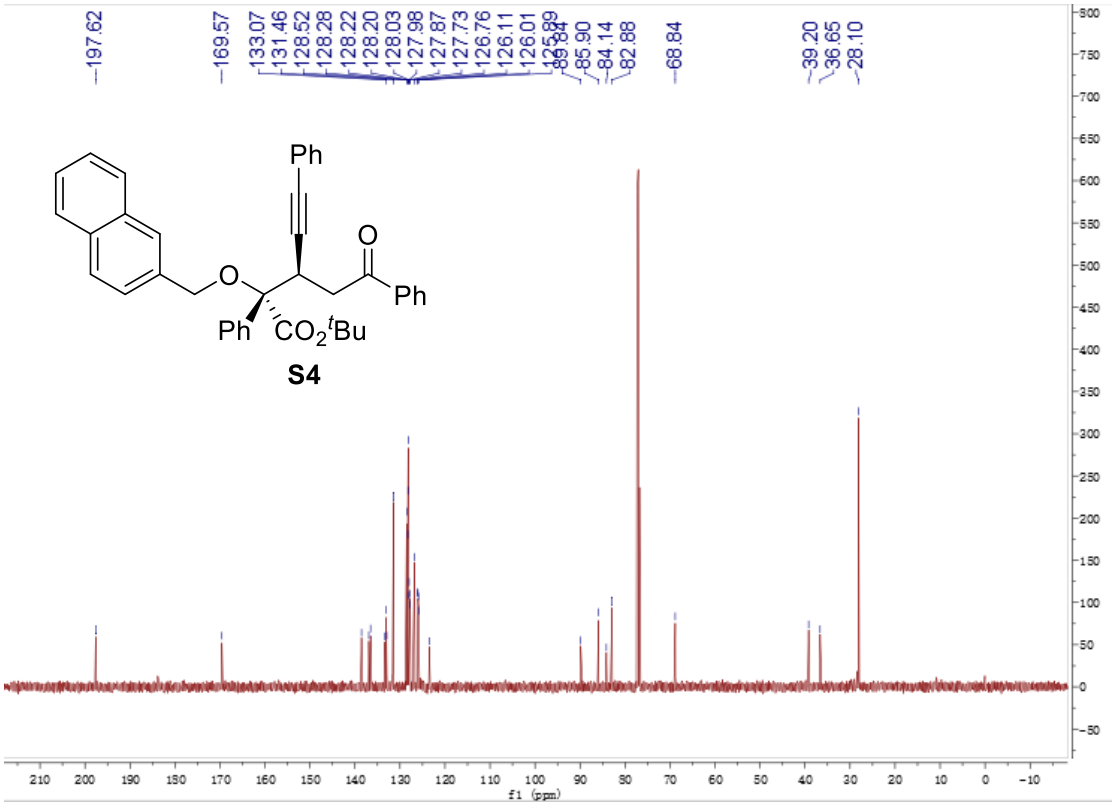

**S2**

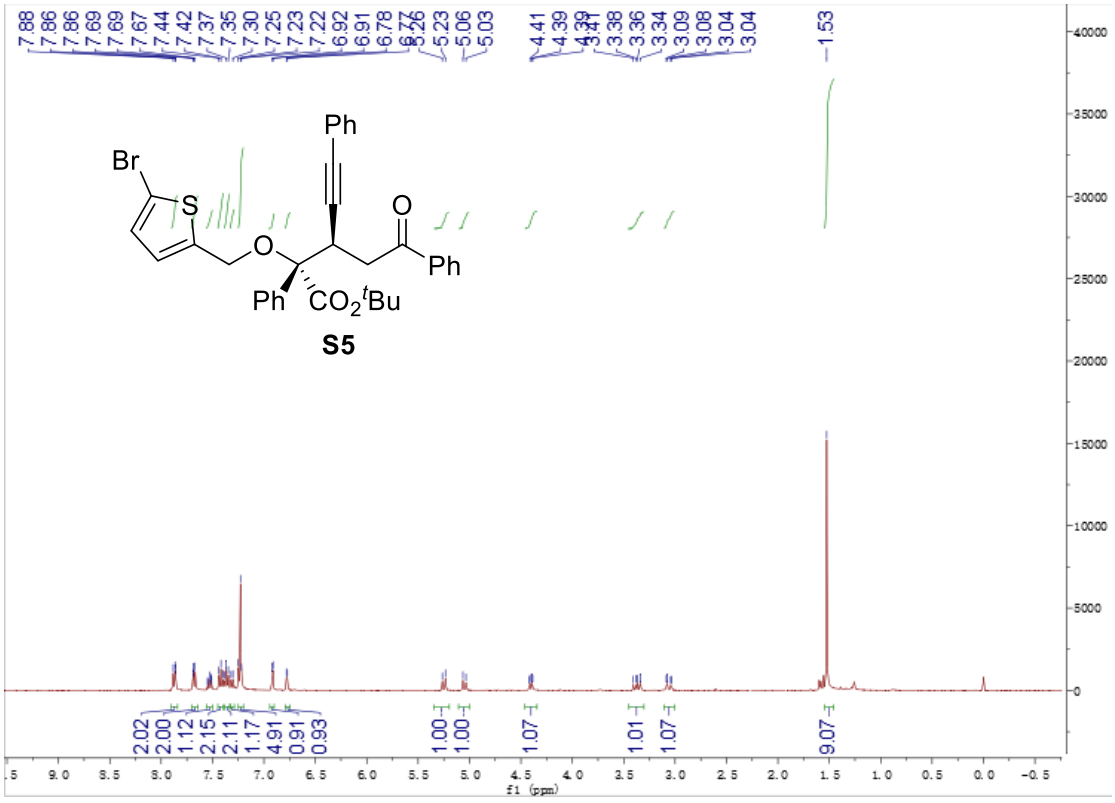


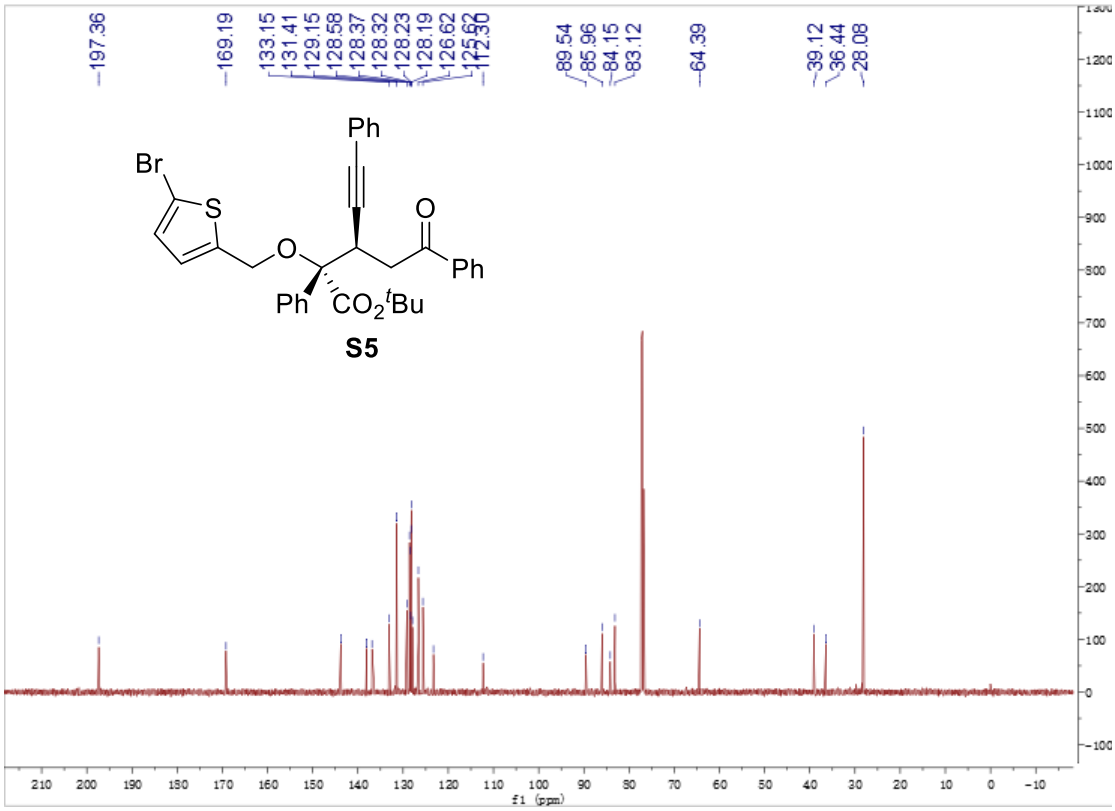

**S3**

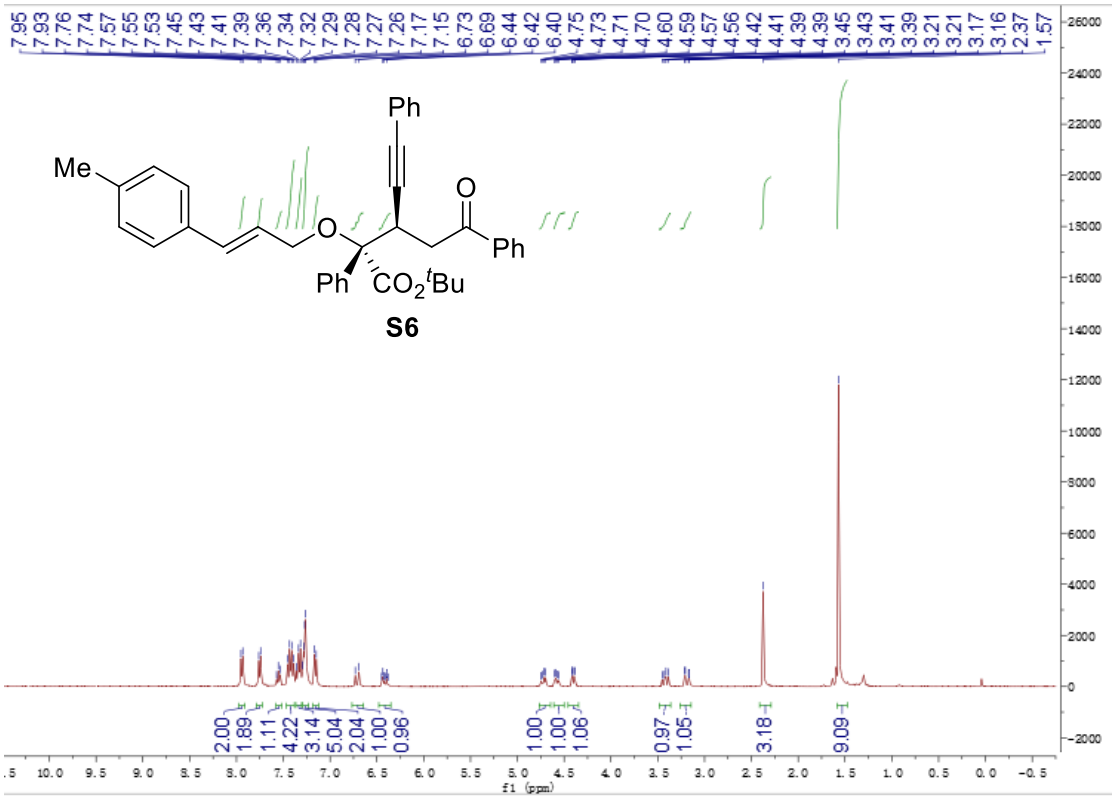

197.41
169.40
138.74
138.31
137.37
136.90
133.13
131.38
129.47
128.57
128.30
128.20
127.90
126.70
123.37
92.82
89.66
85.87
84.12
82.95
68.05
39.19
36.57
28.07
Ph
I
O
O
Ph
Ph
CO2tBu
S3
f1 (ppm)

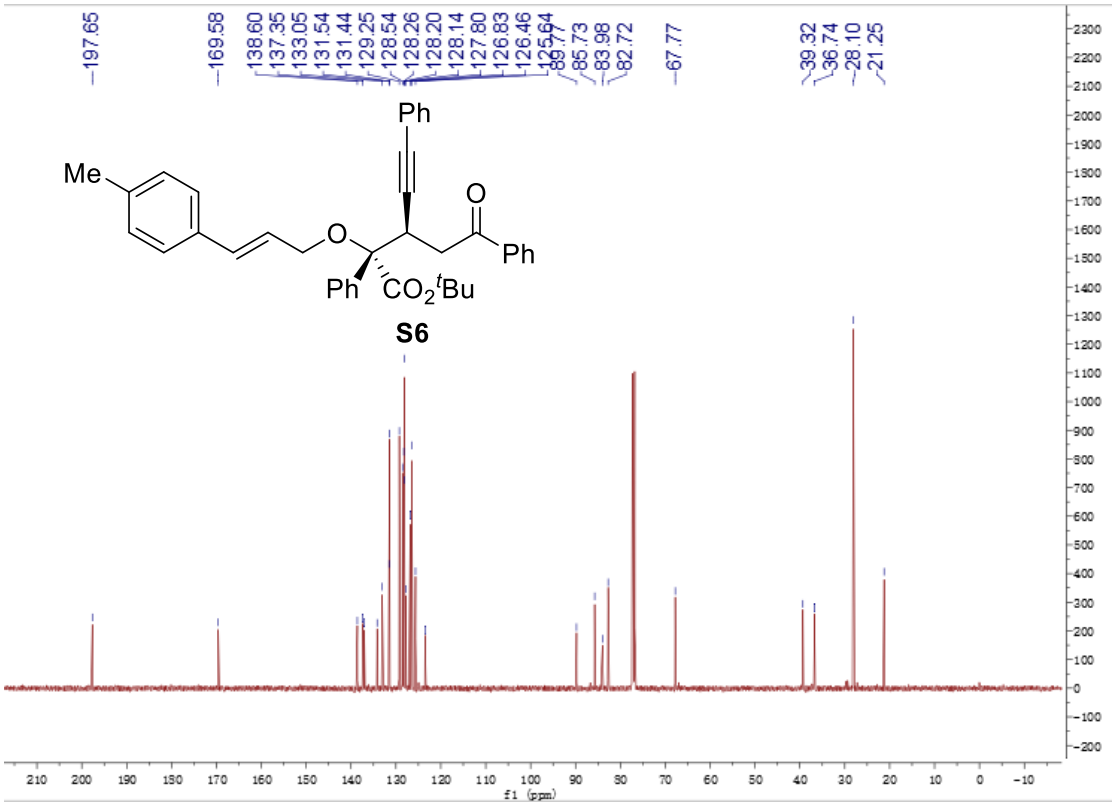

7.93
7.86
7.85
7.84
7.83
7.81
7.80
7.79
7.79
7.78
7.76
7.76
7.74
7.68
7.68
7.66
7.66
7.49
7.48
7.47
7.46
7.45
7.39
7.37
7.36
7.35
7.34
7.33
7.33
7.32
7.31
7.28
7.28
7.26
7.26
7.25
7.24
7.24
7.23
7.22
5.30
5.27
5.15
5.12
4.46
3.38
1.53
Ph
O
O
Ph
Ph
CO2tBu
S4
1.03
3.96
1.10
2.11
1.22
3.12
5.04
5.19
1.00
1.03
1.01
1.02
1.00
9.10
f1 (ppm)


197.62
169.57
133.07
131.46
128.52
128.28
128.22
128.20
128.03
127.98
127.87
127.73
126.76
126.11
126.01
125.89
89.84
85.90
84.14
82.88
68.84
39.20
36.65
28.10
Ph
O
O
Ph
Ph
CO2tBu
S4
f1 (ppm)

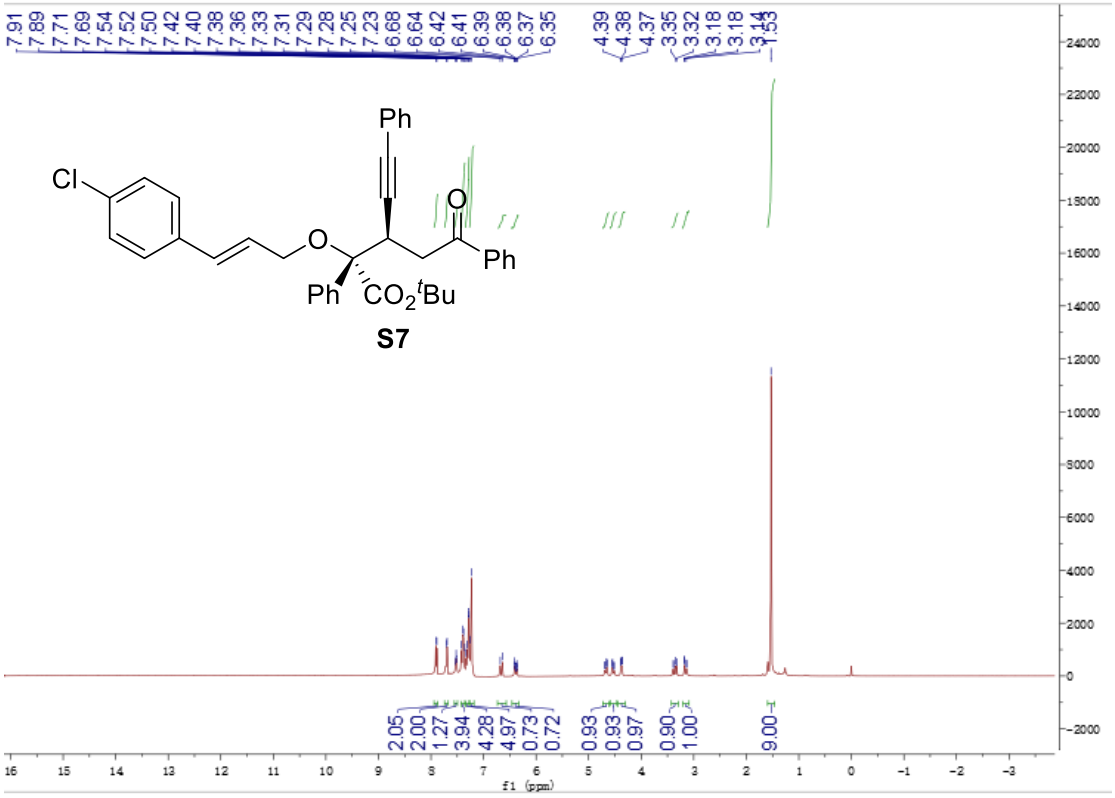

7.88
7.86
7.86
7.69
7.69
7.67
7.44
7.42
7.37
7.35
7.30
7.25
7.23
7.22
6.92
6.91
6.78
6.77
5.26
5.23
5.06
5.03
4.41
4.39
4.39
4.37
3.38
3.36
3.34
3.09
3.08
3.04
3.04
1.53
Br
S
Ph
O
O
Ph
Ph
CO2tBu
S5
2.02
2.00
1.12
2.15
2.11
1.17
4.91
0.91
0.93
1.00
1.00
1.07
1.01
1.07
9.07
f1 (ppm)


197.36
169.19
133.15
131.41
129.15
128.58
128.37
128.32
128.23
128.19
126.62
125.62
112.30
89.54
85.96
84.15
83.12
64.39
39.12
36.44
28.08
Br
S
O
O
Ph
Ph
Ph
CO2tBu
S5

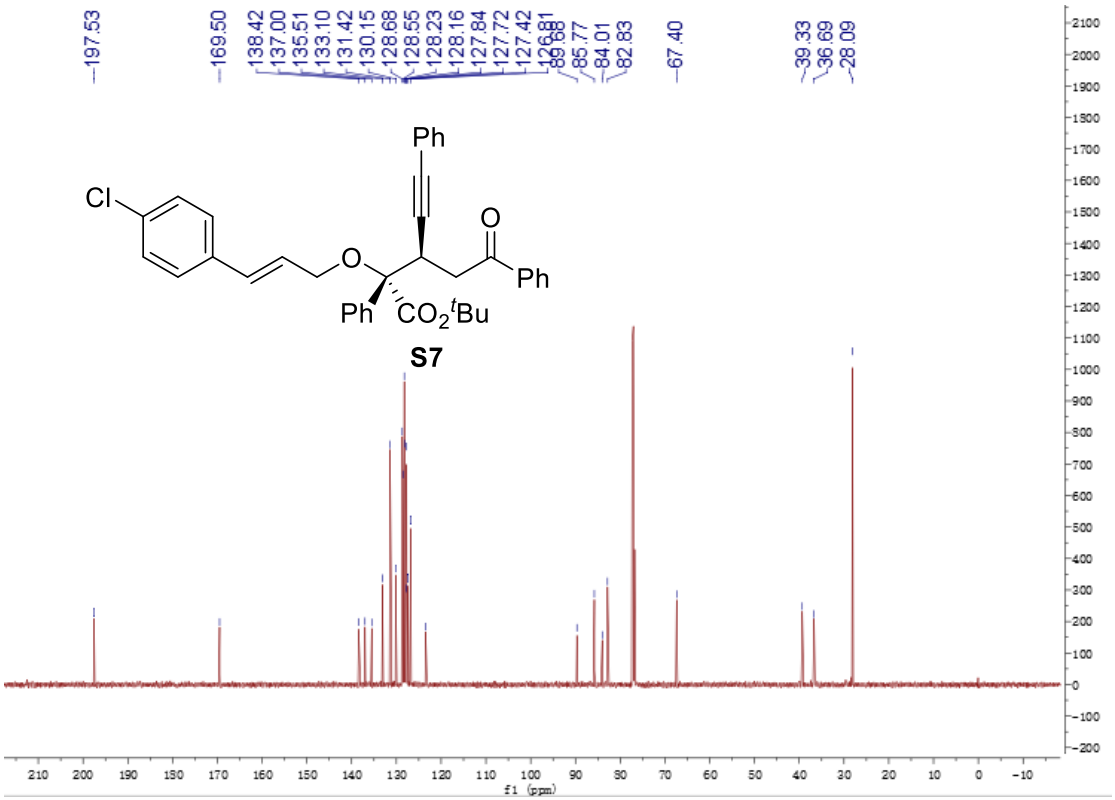

7.95
7.93
7.76
7.74
7.57
7.55
7.53
7.45
7.43
7.41
7.39
7.36
7.34
7.32
7.29
7.28
7.27
7.26
7.17
7.15
6.73
6.69
6.44
6.42
6.40
4.75
4.73
4.71
4.70
4.60
4.59
4.57
4.56
4.42
4.41
4.39
4.39
3.45
3.43
3.41
3.39
3.21
3.21
3.17
3.16
2.37
1.57
Me
O
O
Ph
Ph
Ph
CO2tBu
S6
2.00
1.89
1.11
4.22
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1.00
1.06
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1.05
3.18
9.09



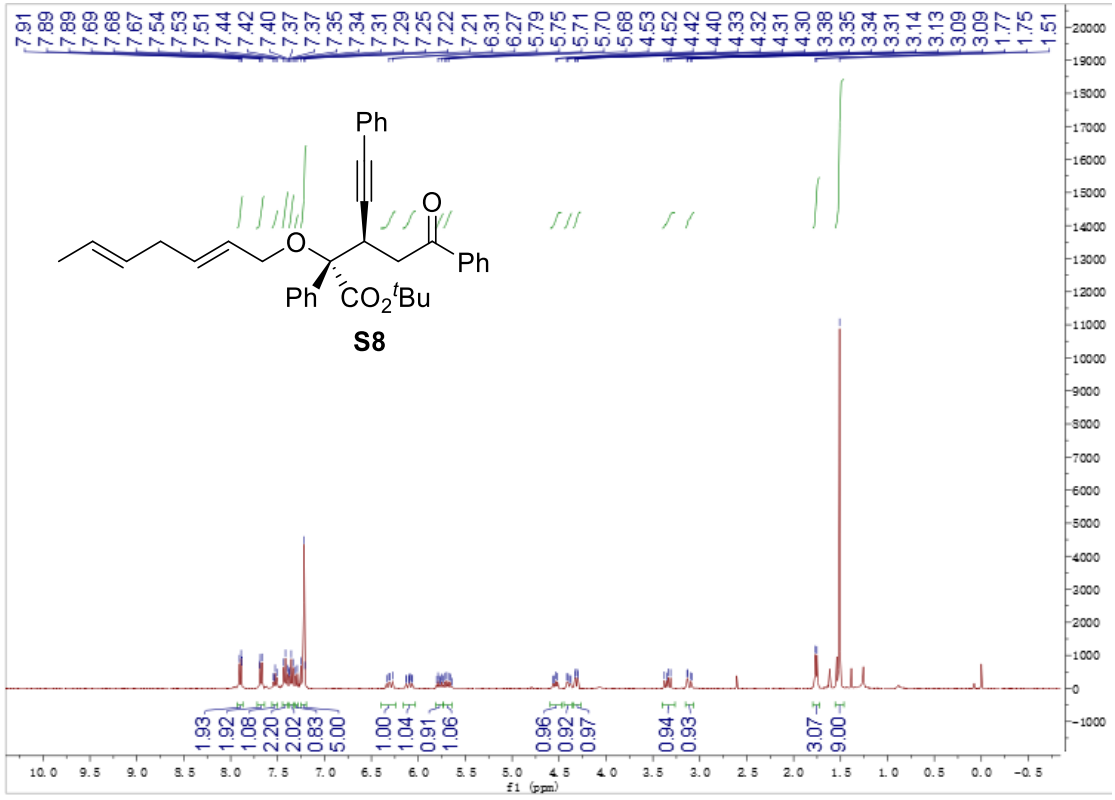

**S6**



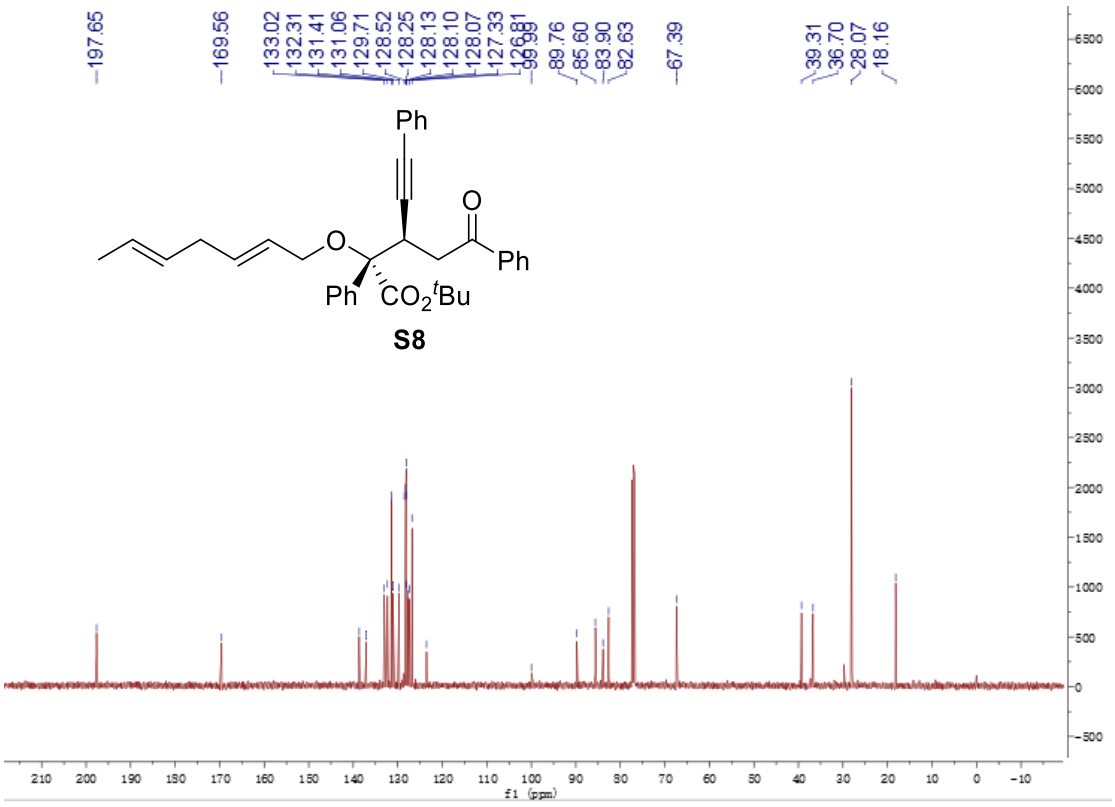

**S7**


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131.42
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128.68
128.55
128.23
128.16
127.84
127.72
127.42
126.81
89.68
85.77
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67.40
39.33
36.69
28.09
Cl
O
Ph
Ph
Ph
CO2tBu
f1 (ppm)

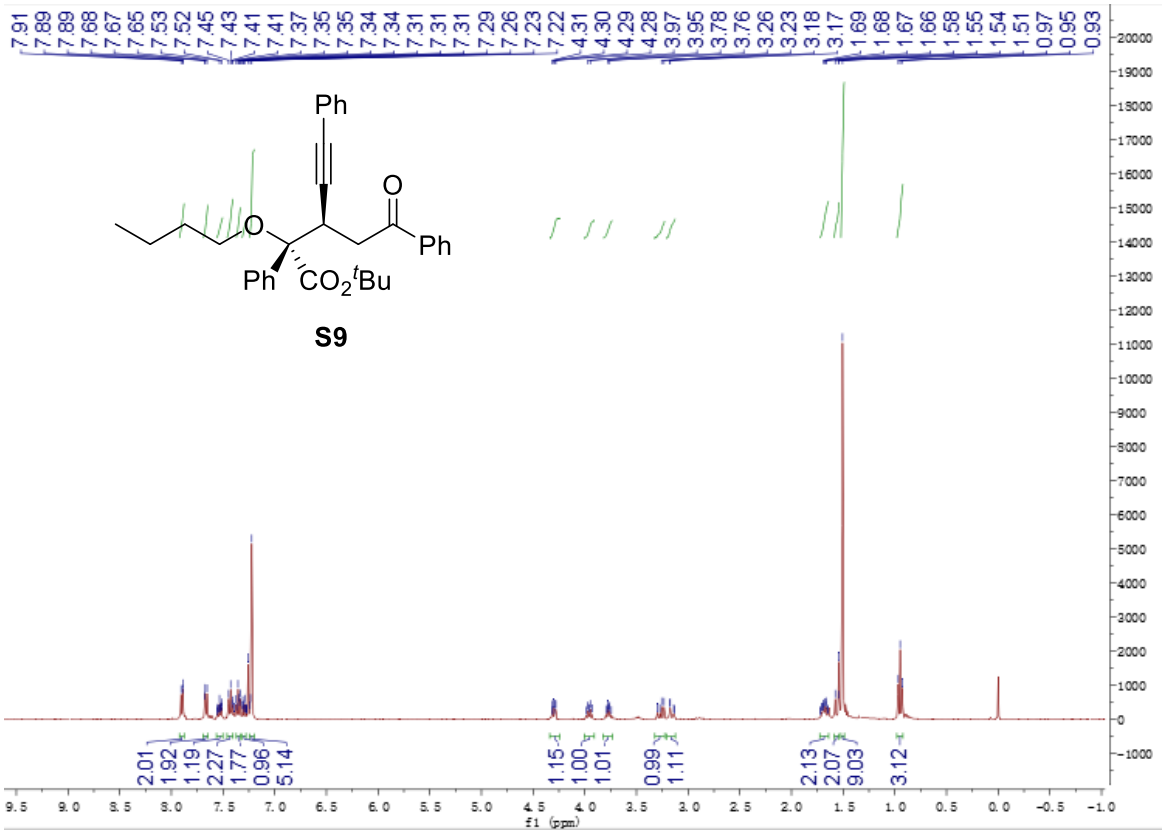
**S7**


7.91
7.89
7.89
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7.68
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7.54
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7.51
7.44
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7.37
7.37
7.35
7.34
7.31
7.29
7.25
7.22
7.21
6.31
6.27
5.79
5.75
5.71
5.70
5.68
4.53
4.52
4.42
4.40
4.33
4.32
4.31
4.30
3.38
3.35
3.34
3.31
3.14
3.13
3.09
3.09
1.77
1.75
1.51
Ph
O
O
Ph
Ph
CO2tBu
1.93
1.92
1.08
2.20
2.02
0.83
5.00
1.00
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1.06
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0.92
0.97
0.94
0.93
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9.00
f1 (ppm)

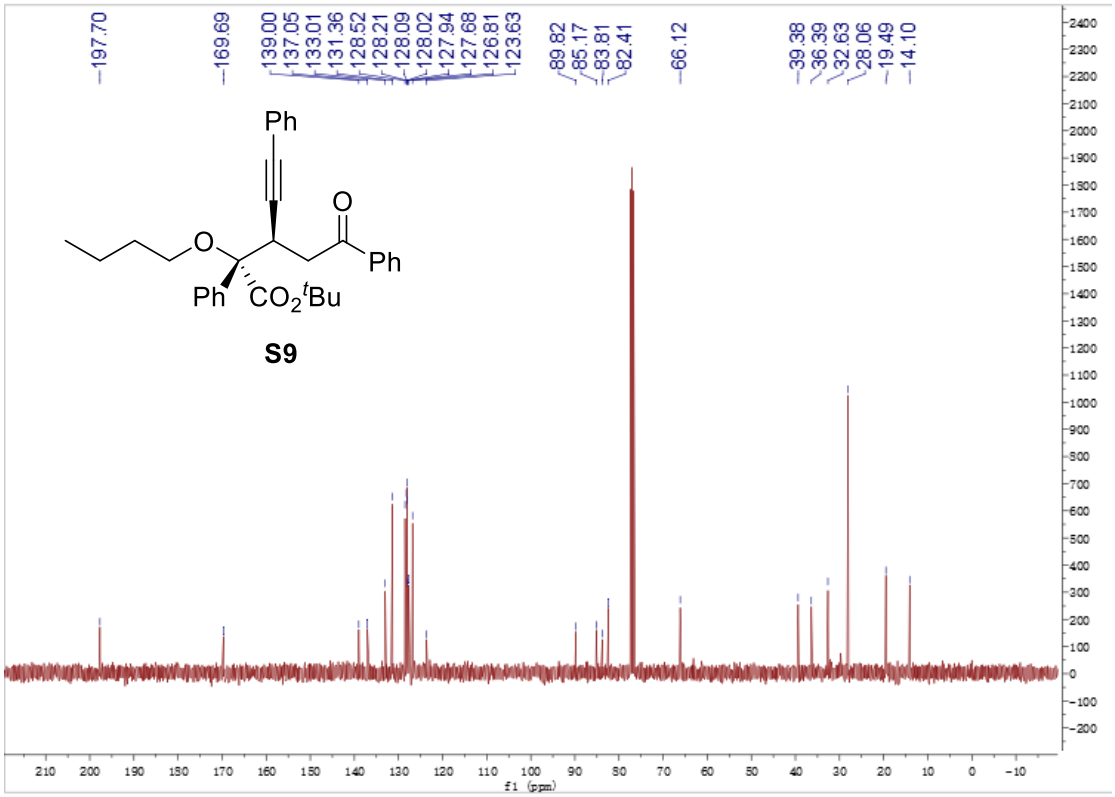
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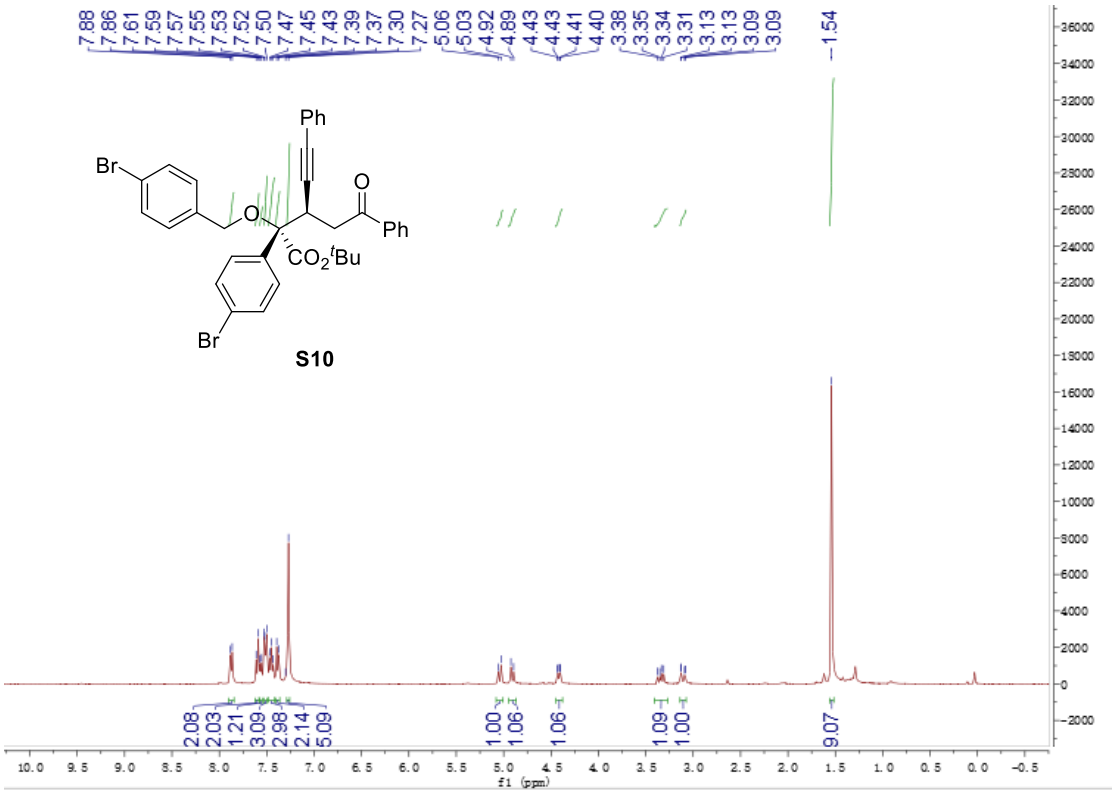

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133.02
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131.06
129.71
128.52
128.25
128.13
128.10
128.07
127.33
126.81
89.76
85.60
83.90
82.63
67.39
39.31
36.70
28.07
18.16
Ph
O
O
Ph
Ph
CO2tBu
f1 (ppm)

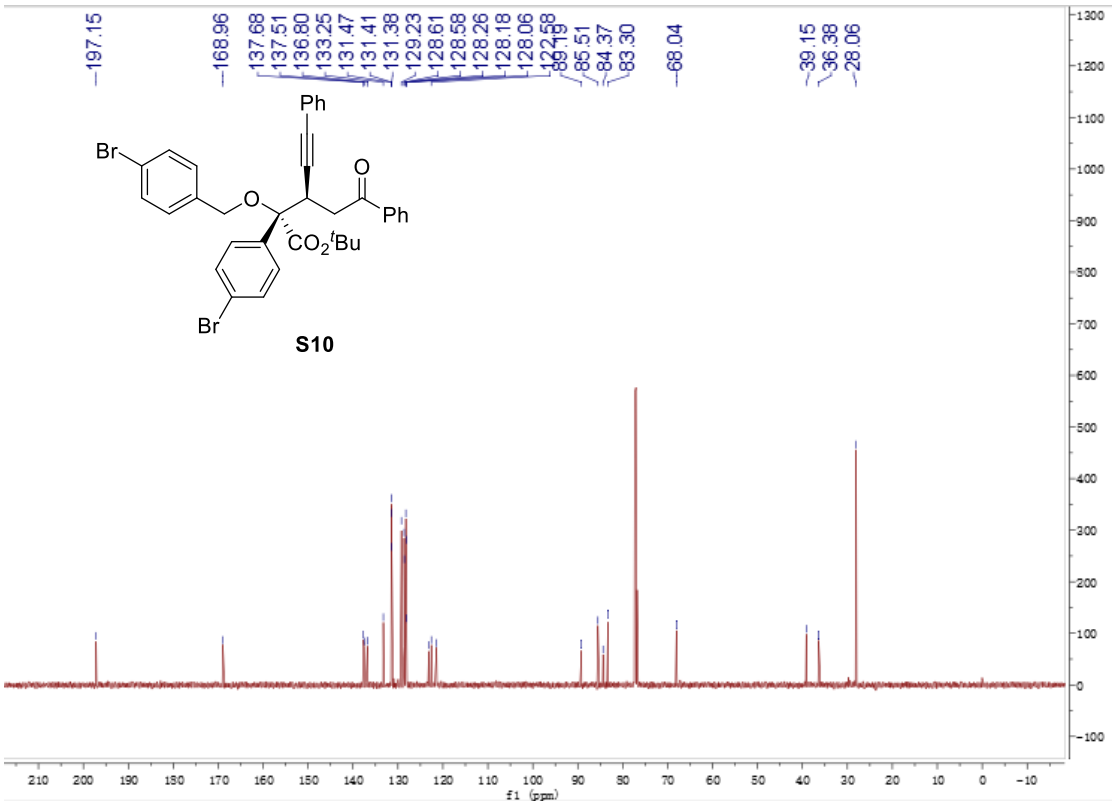
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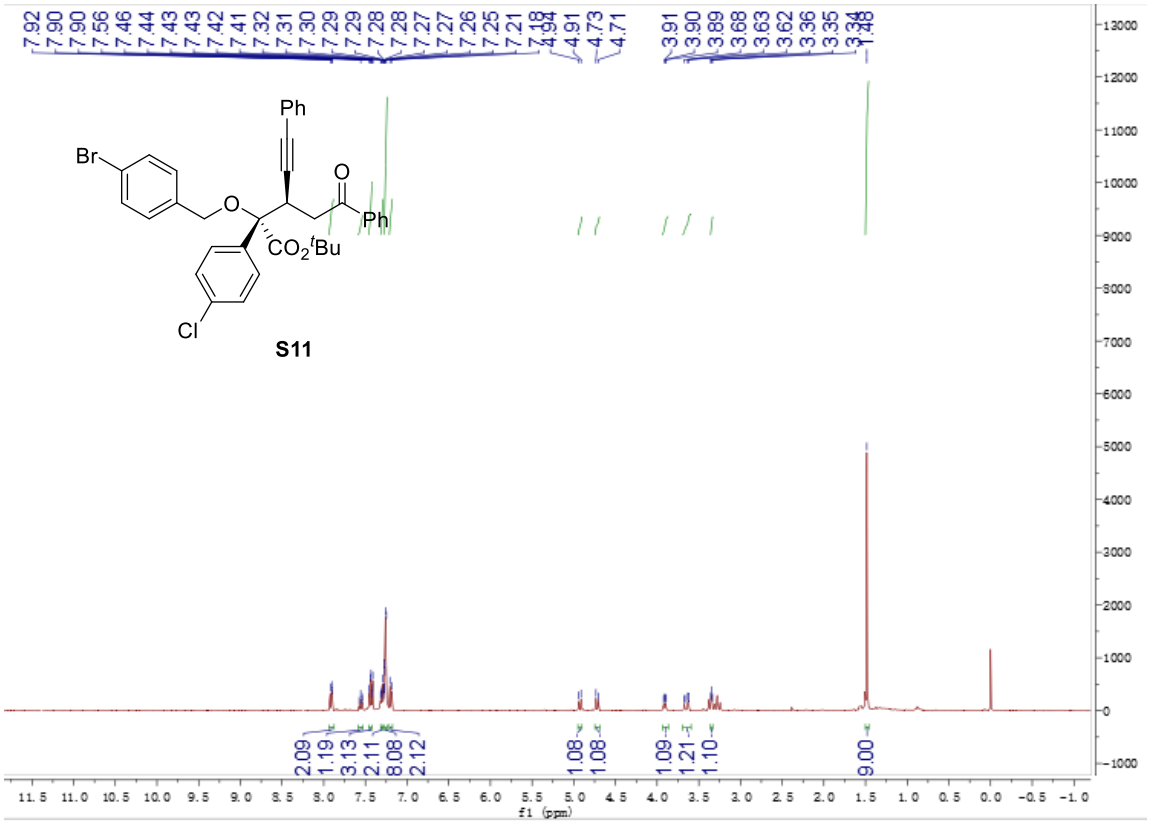

7.91
7.89
7.89
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7.52
7.45
7.43
7.41
7.41
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7.35
7.35
7.34
7.34
7.31
7.31
7.31
7.29
7.26
7.23
7.22
4.31
4.30
4.29
4.28
3.97
3.95
3.78
3.76
3.26
3.23
3.18
3.17
1.69
1.68
1.67
1.66
1.58
1.55
1.54
1.51
0.97
0.95
0.93
Ph
O
O
Ph
Ph
CO2tBu
2.01
1.92
1.19
2.27
1.77
0.96
5.14
1.15
1.00
1.01
0.99
1.11
2.13
2.07
9.03
3.12
f1 (ppm)

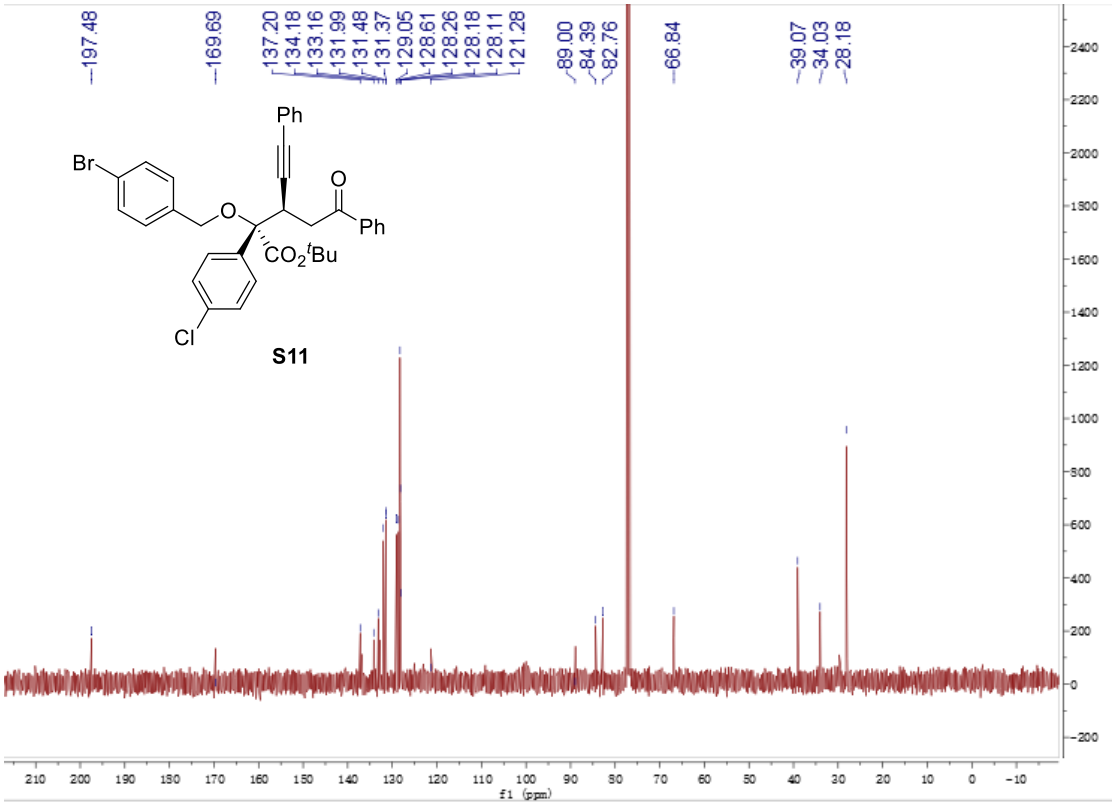
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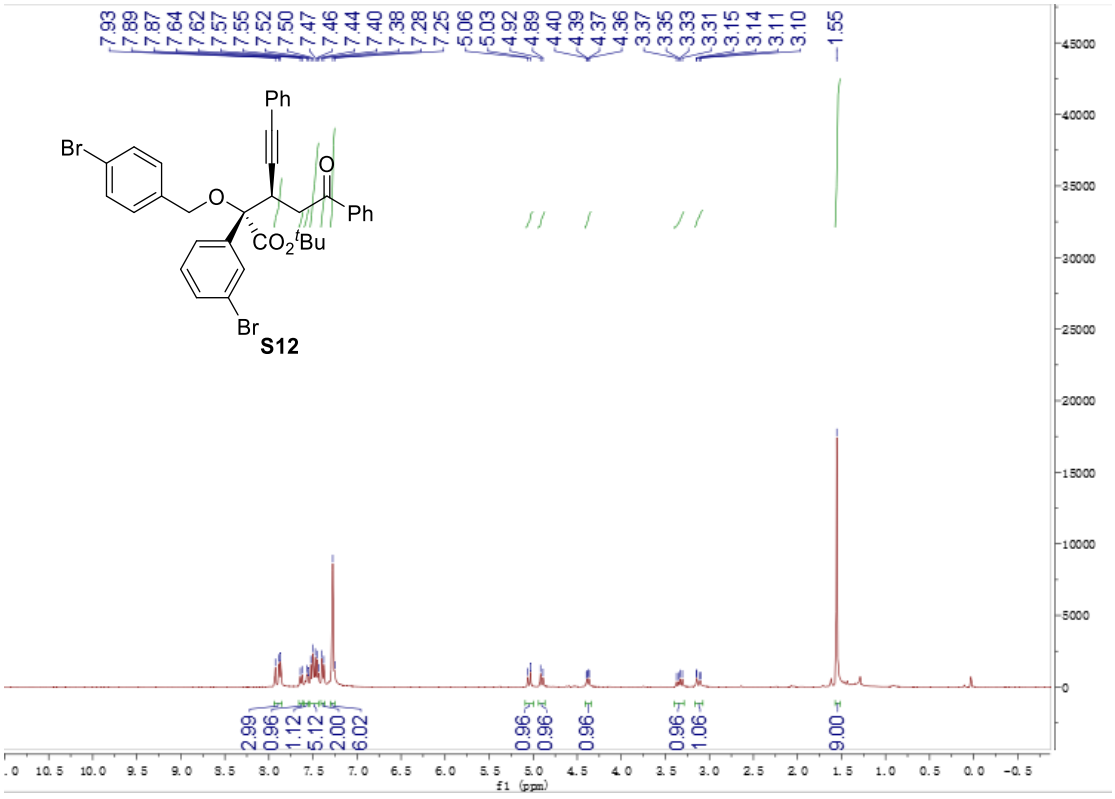

197.70
169.69
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133.01
131.36
128.52
128.21
128.09
128.02
127.94
127.68
126.81
123.63
89.82
85.17
83.81
82.41
66.12
39.38
36.39
32.63
28.06
19.49
14.10
Ph
O
O
Ph
Ph
CO2tBu
S9

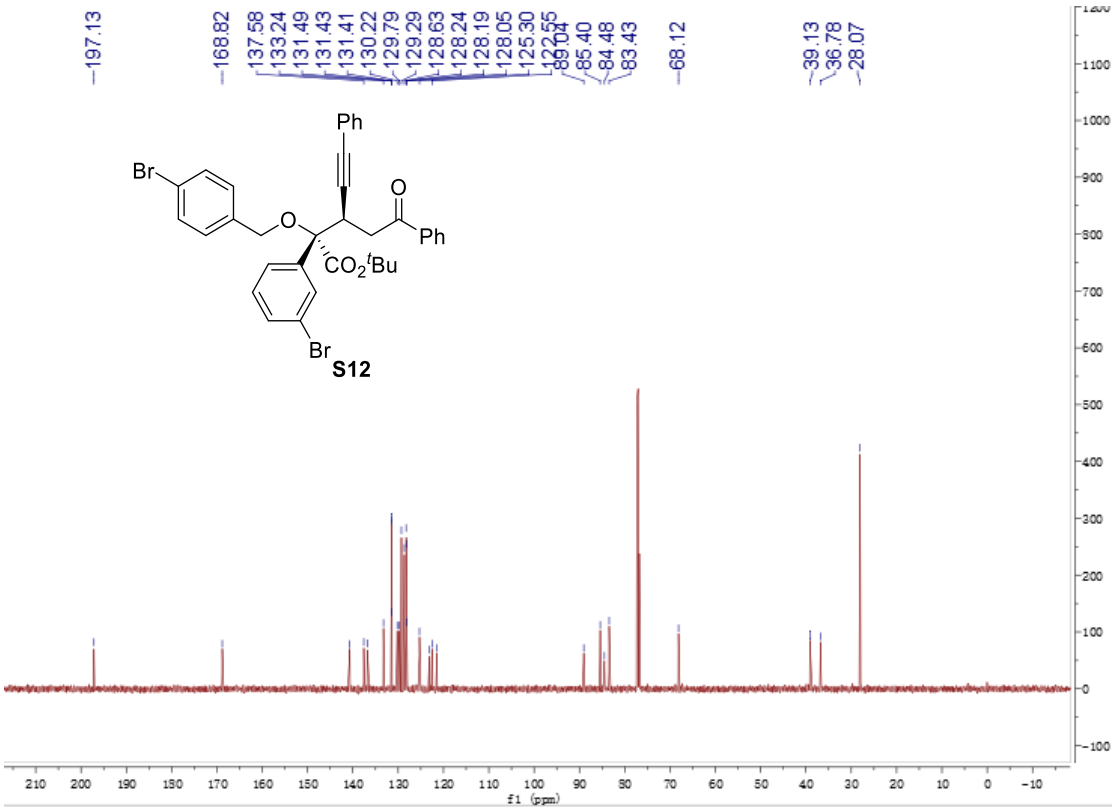

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7.52
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7.47
7.45
7.43
7.39
7.37
7.30
7.27
5.06
5.03
4.92
4.89
4.43
4.43
4.41
4.40
3.38
3.35
3.34
3.31
3.13
3.13
3.09
3.09
1.54
Br
Ph
O
O
Ph
CO2tBu
Br
S10
2.08
2.03
1.21
3.09
2.98
2.14
5.09
1.00
1.06
1.06
1.09
1.00
9.07

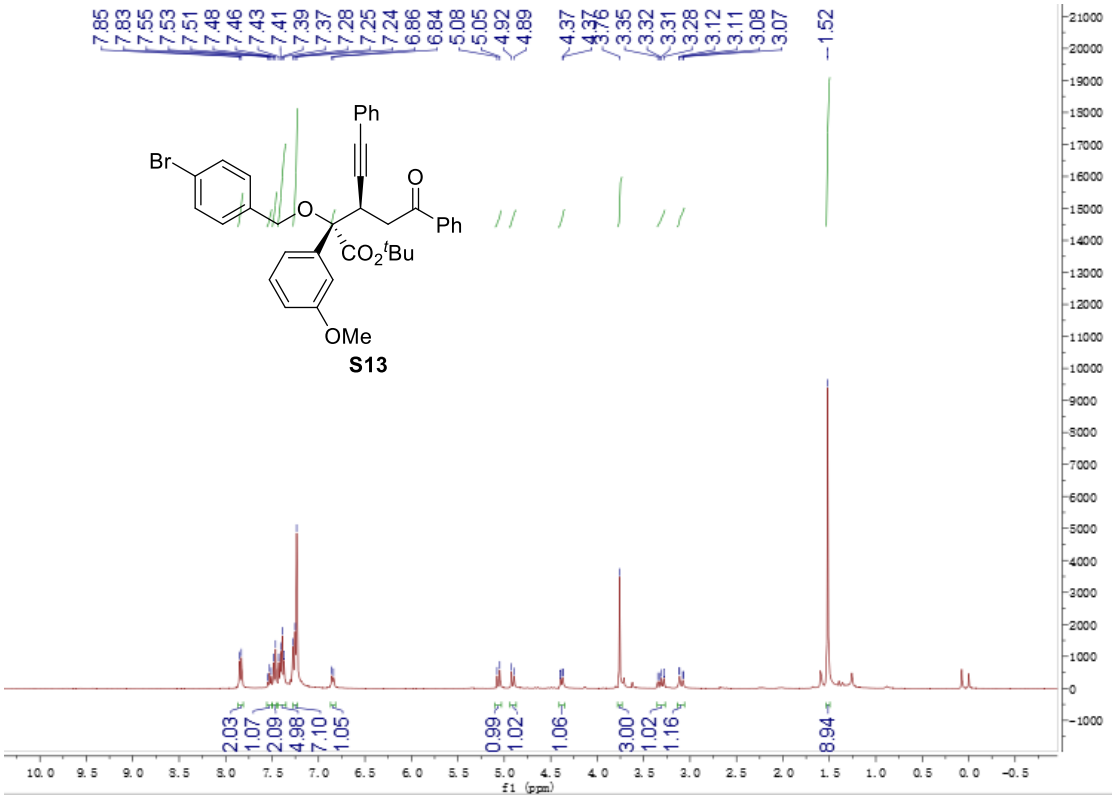

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168.96
137.68
137.51
136.80
133.25
131.47
131.41
131.38
129.23
128.61
128.58
128.26
128.18
128.06
122.58
89.19
85.51
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83.30
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39.15
36.38
28.06
Ph
Br
O
Ph
CO2tBu
Br
S10
f1 (ppm)

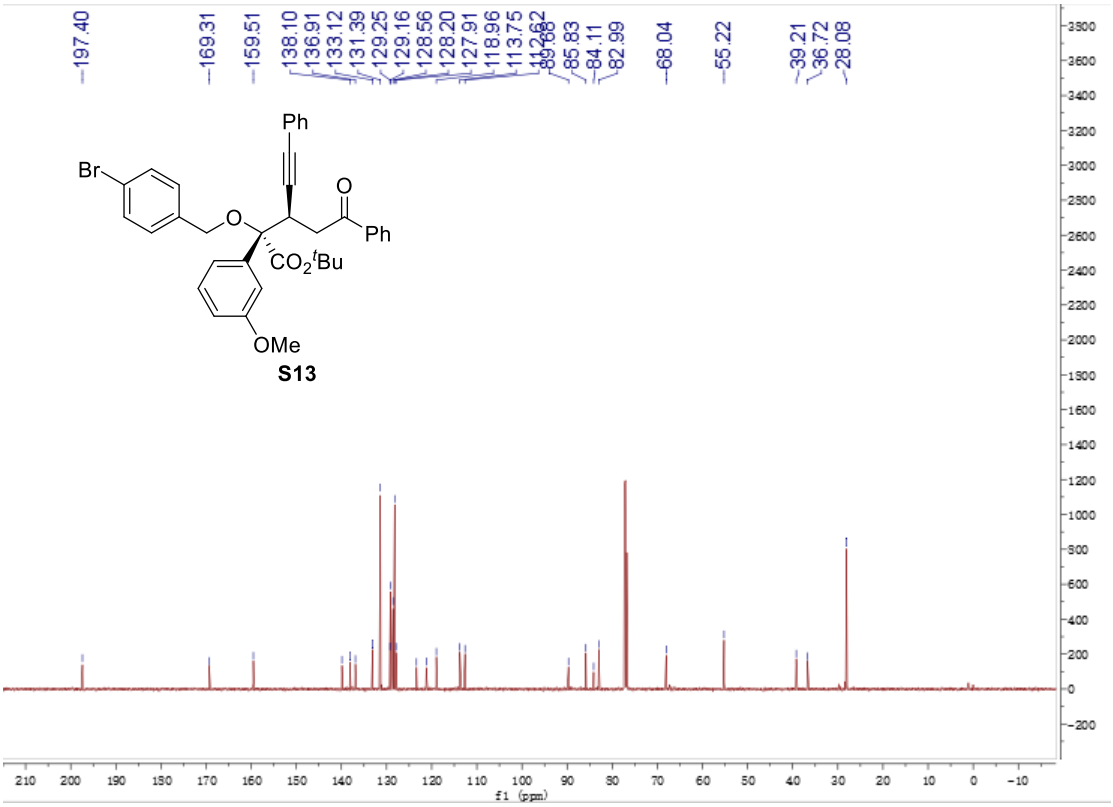

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7.90
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7.43
7.43
7.42
7.41
7.32
7.31
7.30
7.29
7.29
7.28
7.28
7.27
7.27
7.26
7.25
7.21
7.18
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4.91
4.73
4.71
3.91
3.90
3.89
3.68
3.63
3.62
3.36
3.35
3.34
1.48
Ph
Br
O
Ph
CO2tBu
Cl
S11
2.09
1.19
3.13
2.11
8.08
2.12
1.08
1.08
1.09
1.21
1.10
9.00
f1 (ppm)

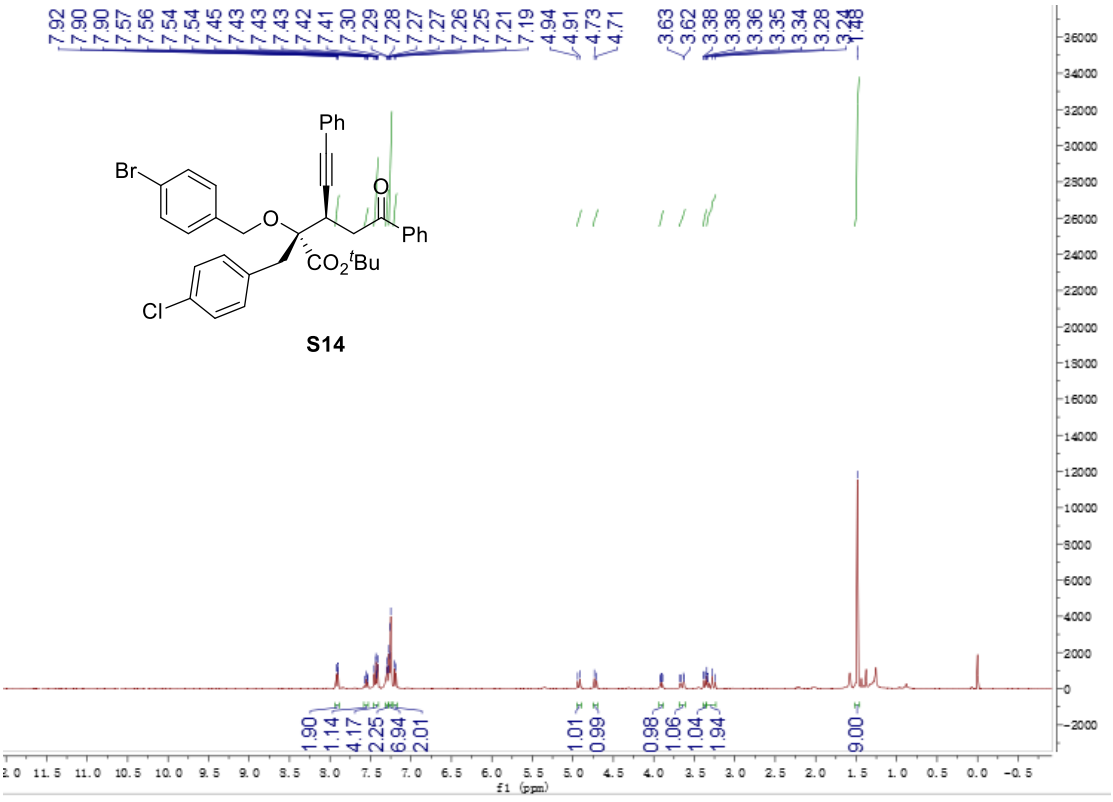

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131.37
129.05
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128.26
128.18
128.11
121.28
89.00
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66.84
39.07
34.03
28.18
Ph
Br
O
Ph
CO2tBu
Cl
S11

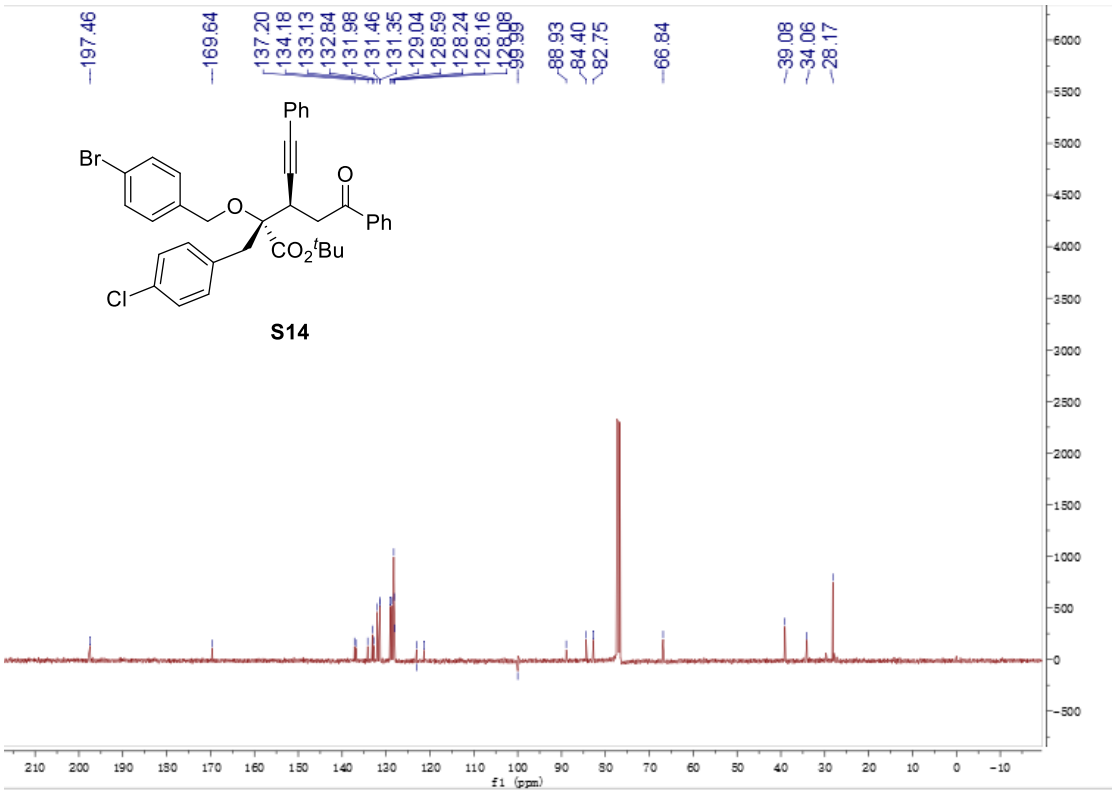

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7.52
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7.40
7.38
7.28
7.25
5.06
5.03
4.92
4.89
4.40
4.39
4.37
4.36
3.37
3.35
3.33
3.31
3.15
3.14
3.11
3.10
1.55
Ph
Br
O
Ph
CO2tBu
Br
S12
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5.12
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6.02
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0.96
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0.96
1.06
9.00

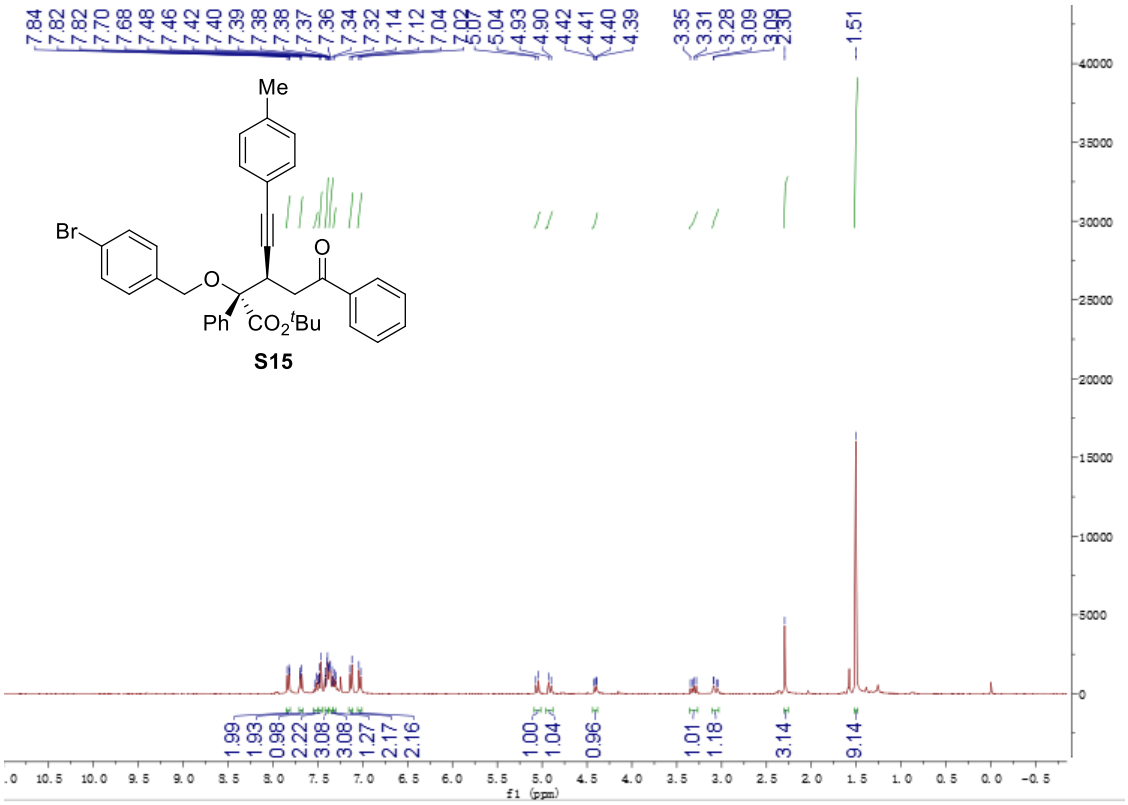

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129.29
128.63
128.24
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128.05
125.30
122.55
89.04
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68.12
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Ph
Br
O
Ph
CO2tBu
Br
S12

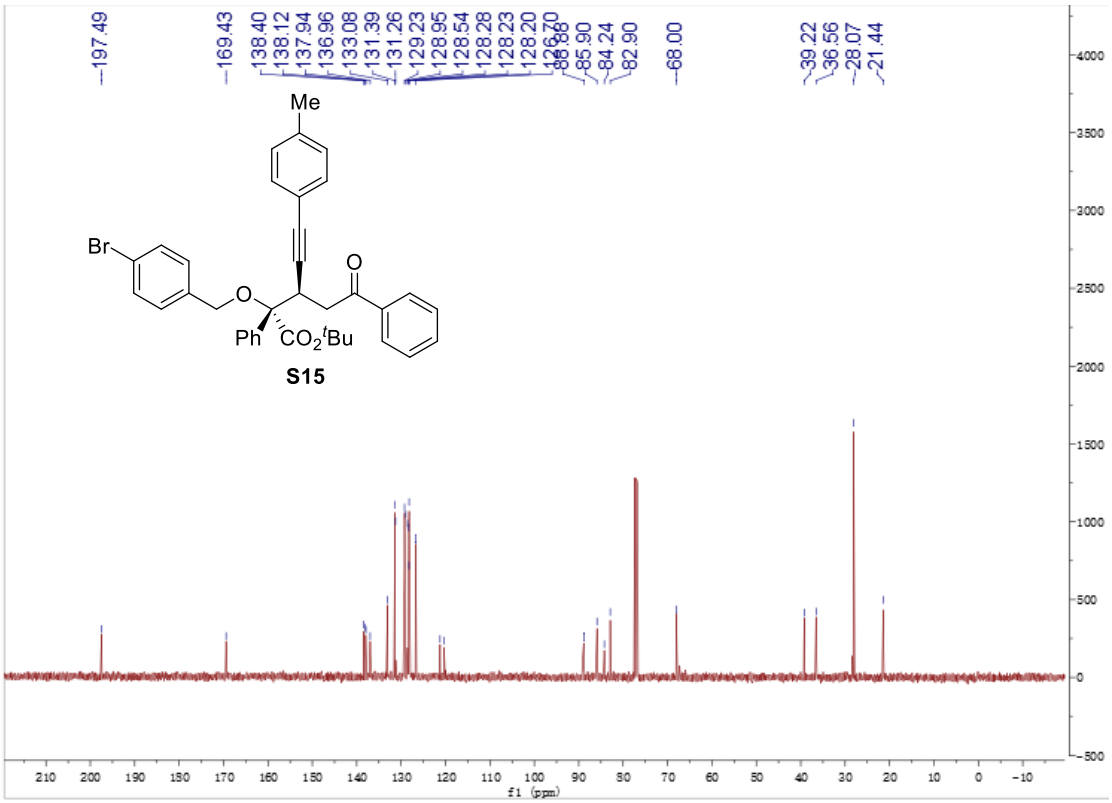

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7.28
7.25
7.24
6.86
6.84
5.08
5.05
4.92
4.89
4.37
4.36
3.76
3.35
3.32
3.31
3.28
3.12
3.11
3.08
3.07
1.52
Ph
Br
O
Ph
CO2tBu
OMe
S13
2.03
1.07
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7.10
1.05
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1.06
3.00
1.02
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8.94

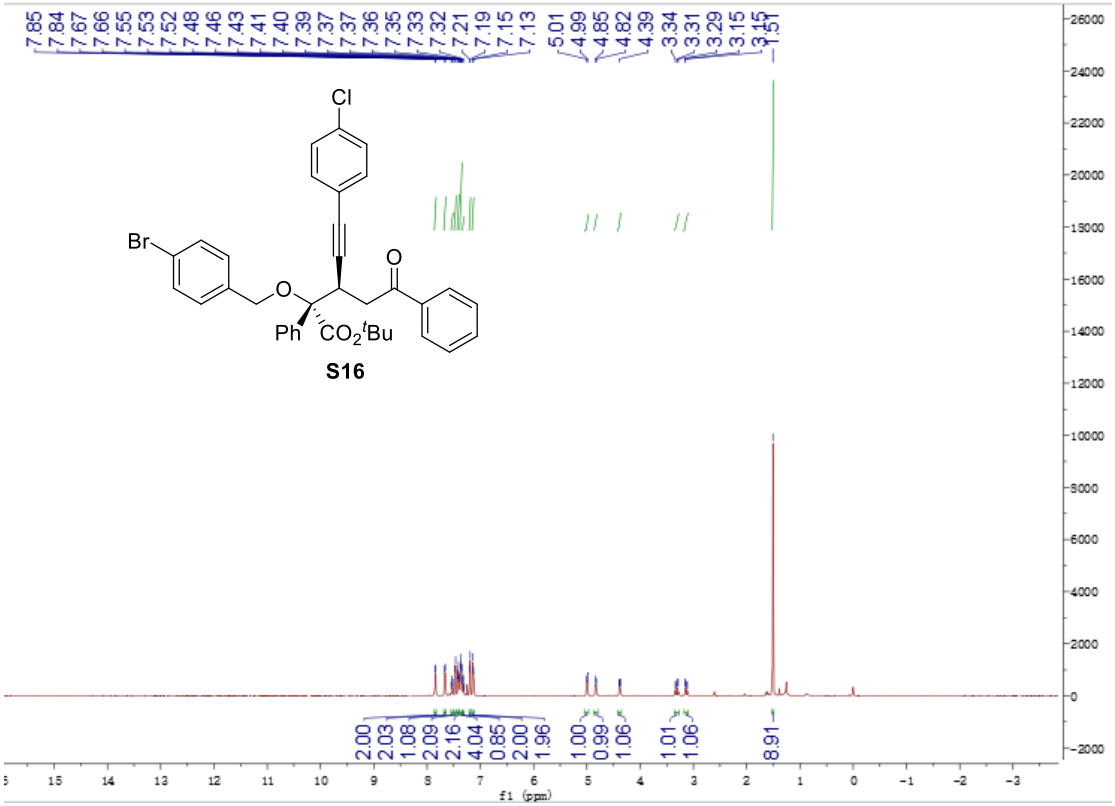

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128.20
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118.96
113.75
112.62
89.68
85.83
84.11
82.99
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36.72
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Ph
Br
O
O
Ph
CO2tBu
OMe
S13
f1 (ppm)

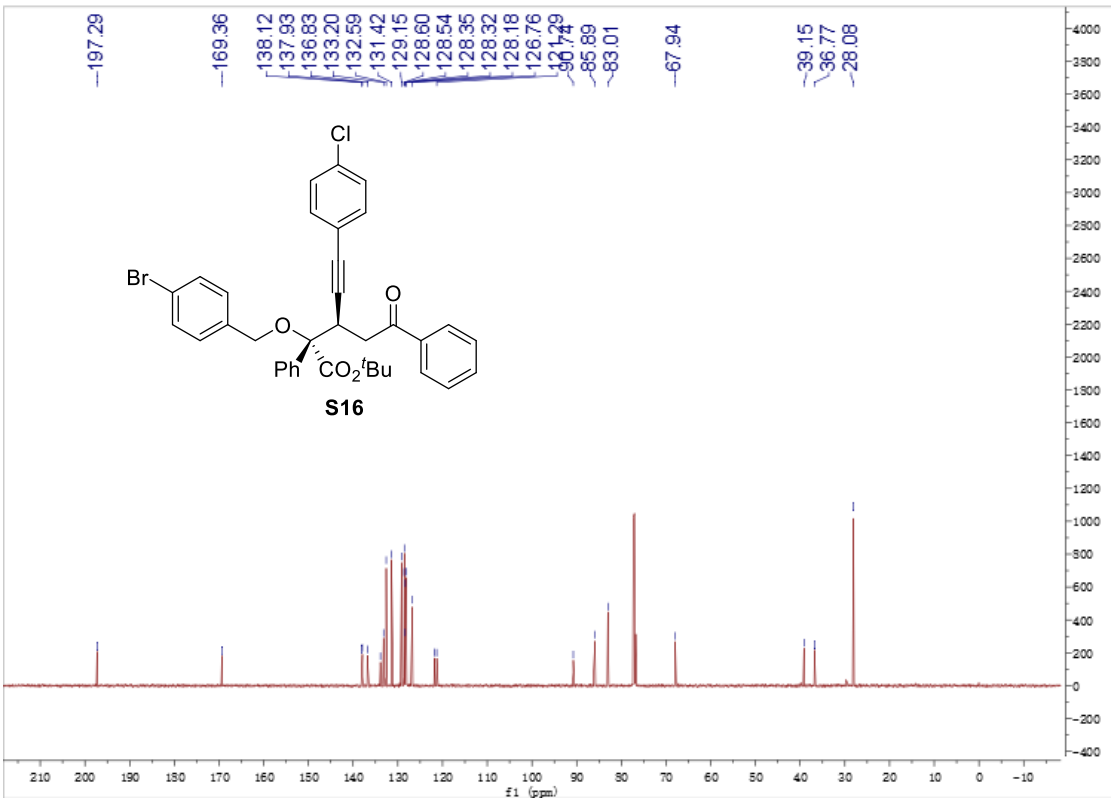

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7.41
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7.29
7.28
7.27
7.27
7.26
7.25
7.21
7.19
4.94
4.91
4.73
4.71
3.63
3.62
3.38
3.38
3.36
3.35
3.34
3.28
3.24
1.48
Ph
Br
O
O
Ph
CO2tBu
Cl
S14
1.90
1.14
4.17
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2.01
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0.99
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1.06
1.04
1.94
9.00
f1 (ppm)

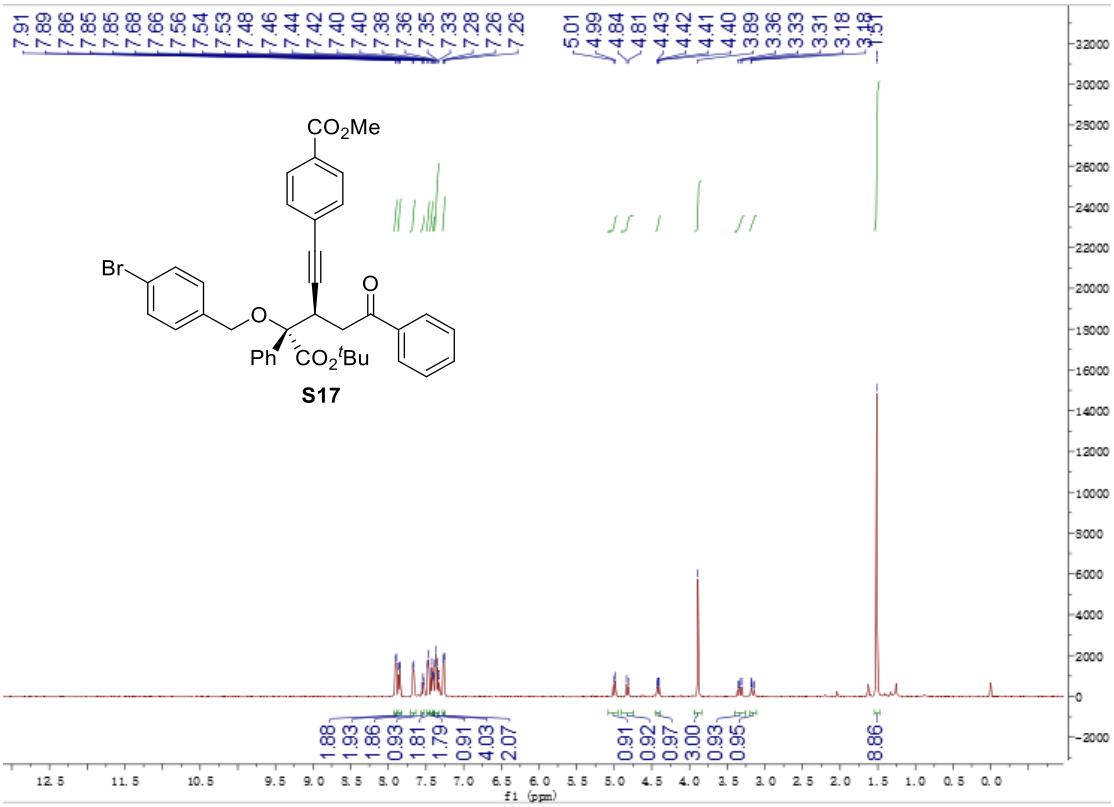

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131.46
131.35
129.04
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128.16
128.08
99.99
88.93
84.40
82.75
66.84
39.08
34.06
28.17
Ph
Br
O
O
Ph
CO2tBu
Cl
S14
f1 (ppm)

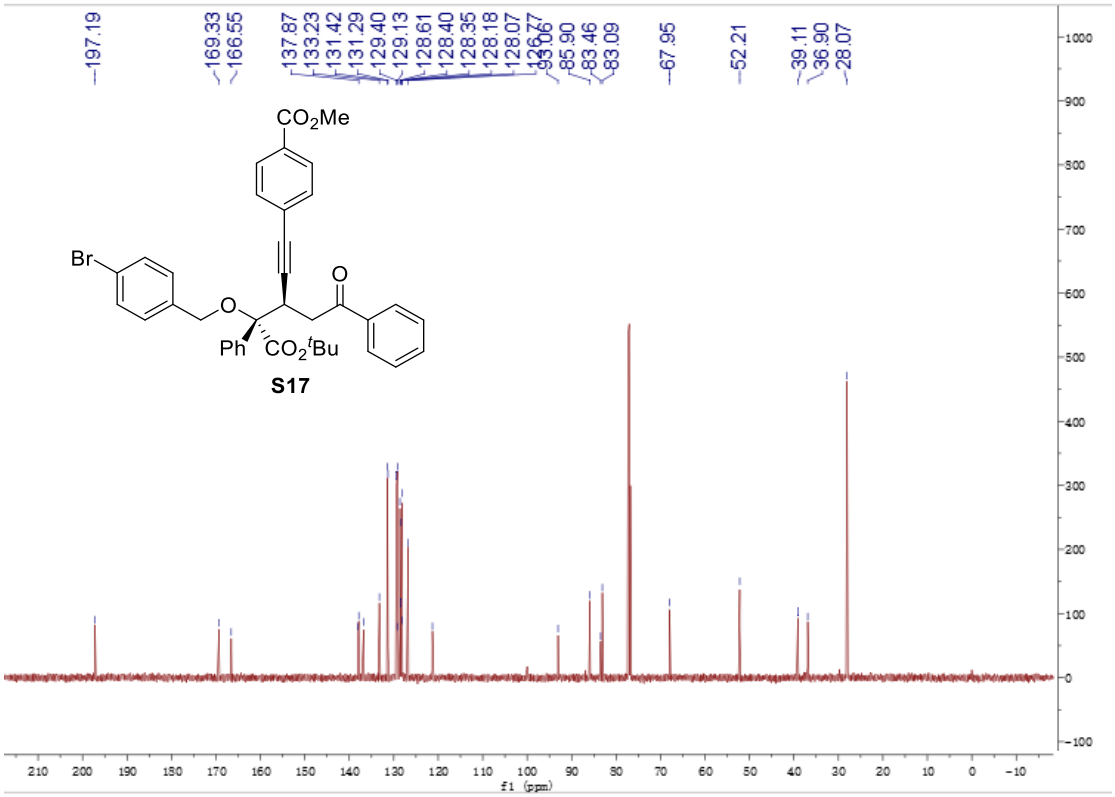

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7.37
7.36
7.34
7.32
7.14
7.12
7.04
5.04
4.93
4.90
4.42
4.41
4.40
4.39
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3.31
3.28
3.09
2.30
1.51
Me
Br
O
O
Ph
CO2tBu
S15
1.99
1.93
0.98
2.22
3.08
3.08
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2.16
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1.04
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9.14
f1 (ppm)

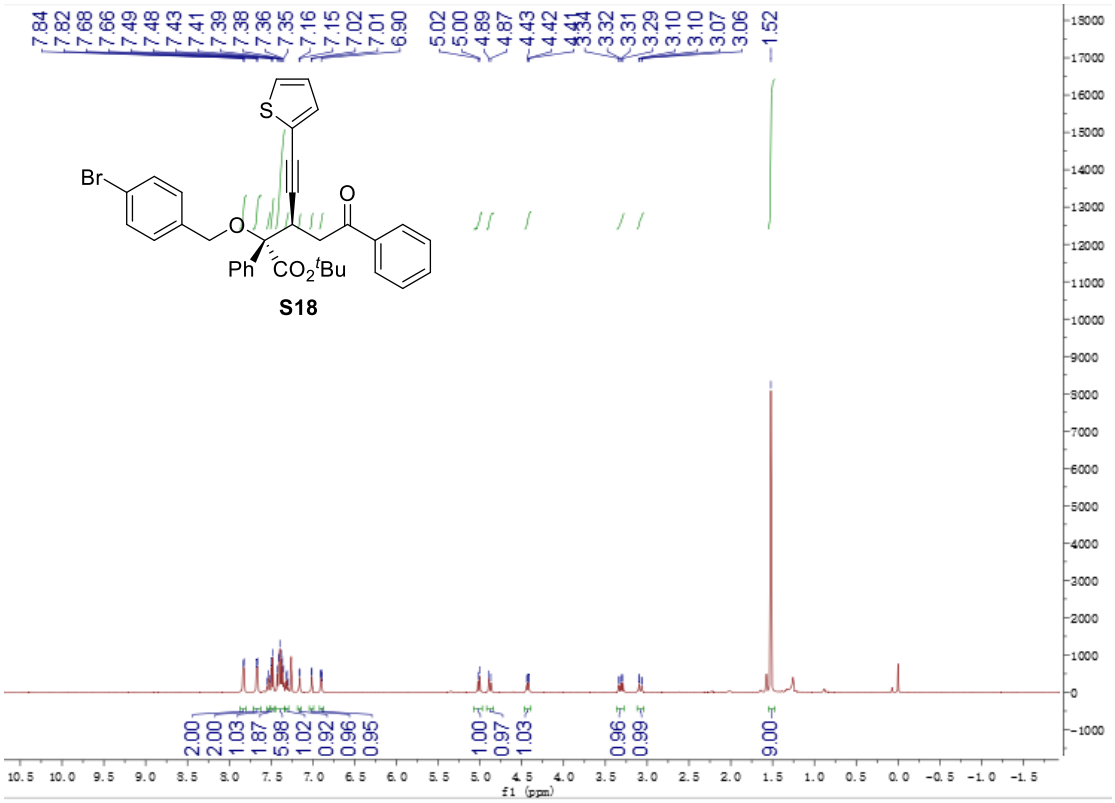

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128.23
128.20
126.70
88.88
85.90
84.24
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28.07
21.44
Me
Br
O
O
Ph
CO2tBu
S15
f1 (ppm)

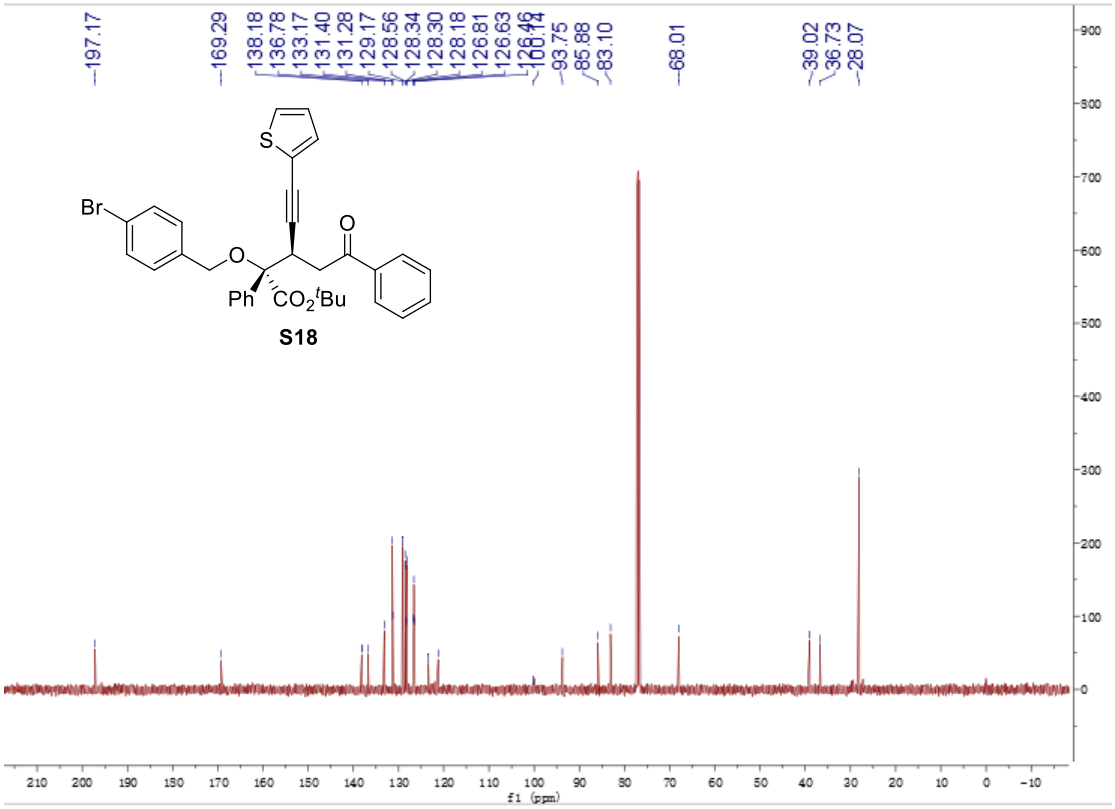

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7.32
7.21
7.19
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7.13
5.01
4.99
4.85
4.82
4.39
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3.15
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1.51
Cl
Br
O
O
Ph
CO2tBu
S16
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2.03
1.08
2.09
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1.00
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1.06
1.01
1.06
8.91
f1 (ppm)

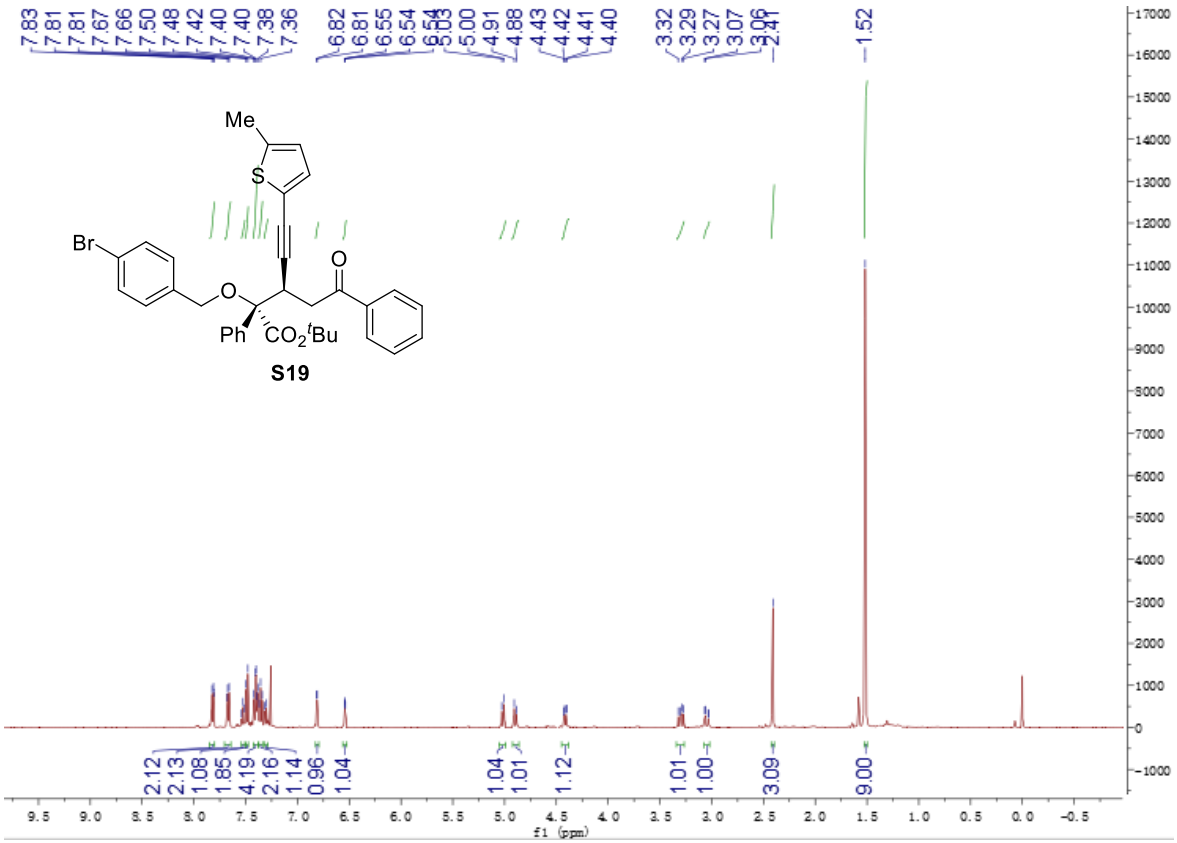

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128.18
126.76
121.29
90.74
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39.15
36.77
28.08
Cl
Br
O
O
Ph
CO2tBu
S16
f1 (ppm)

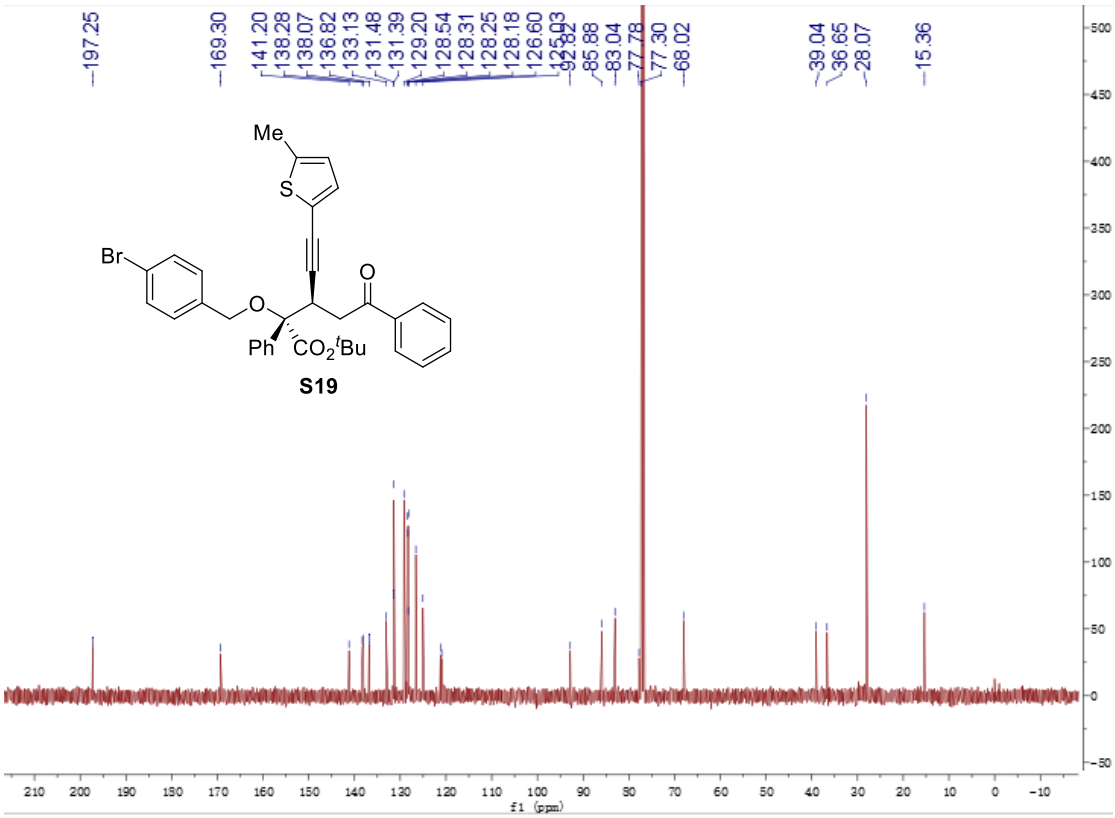

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3.36
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1.51
CO2Me
Br
O
O
Ph
CO2tBu
S17
1.88
1.93
1.86
0.93
1.81
1.79
0.91
4.03
2.07
0.91
0.92
0.97
3.00
0.93
0.95
8.86
f1 (ppm)


197.19
169.33
166.55
137.87
133.23
131.42
131.29
129.40
129.13
128.61
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128.35
128.18
128.07
126.77
85.90
83.46
83.09
67.95
52.21
39.11
36.90
28.07
CO2Me
Br
O
O
Ph
CO2tBu
S17
f1 (ppm)

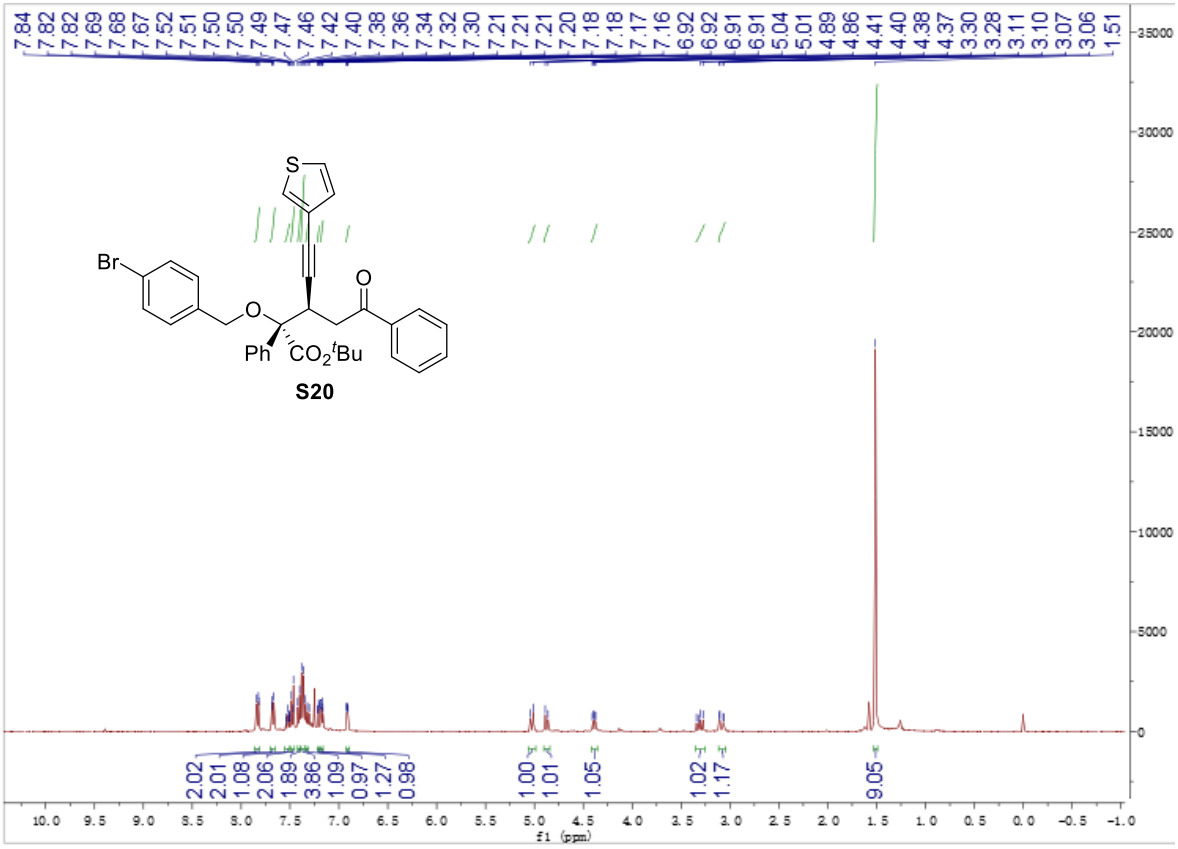

7.84
7.82
7.68
7.66
7.49
7.48
7.43
7.41
7.39
7.38
7.36
7.35
7.16
7.15
7.02
7.01
6.90
5.02
5.00
4.89
4.87
4.43
4.42
4.41
4.34
3.32
3.31
3.29
3.10
3.07
3.06
1.52
S
Br
O
O
Ph
CO2tBu
S18
2.00
2.00
1.03
1.87
5.98
1.02
0.92
0.96
0.95
1.00
0.97
1.03
0.96
0.99
9.00
f1 (ppm)


197.17
169.29
138.18
136.78
133.17
131.40
131.28
129.17
128.56
128.34
128.30
128.18
126.81
126.63
93.75
85.88
83.10
68.01
39.02
36.73
28.07
S
Br
O
O
Ph
CO2tBu
S18
f1 (ppm)

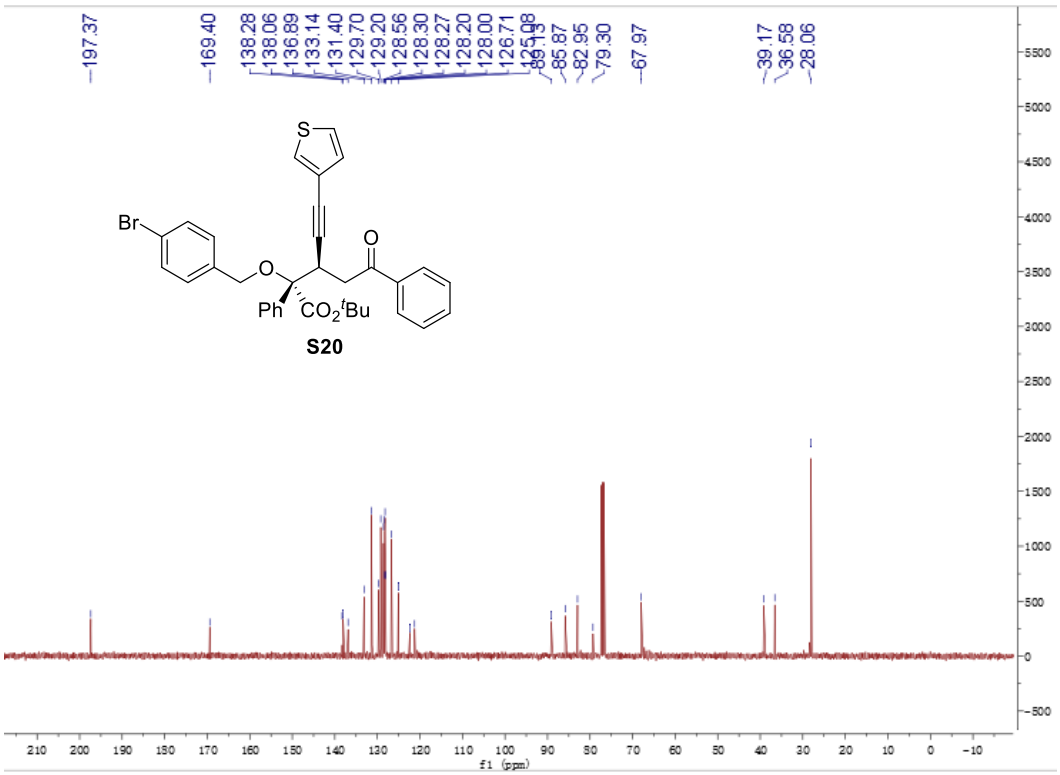

7.83
7.81
7.81
7.67
7.66
7.50
7.48
7.42
7.40
7.40
7.38
7.36
6.82
6.81
6.55
6.54
5.00
4.91
4.88
4.43
4.42
4.41
4.40
3.32
3.29
3.27
3.07
2.41
1.52
Me
S
Br
O
O
Ph
CO2tBu
S19
2.12
2.13
1.08
1.85
4.19
2.16
1.14
0.96
1.04
1.04
1.01
1.12
1.01
1.00
3.09
9.00
f1 (ppm)

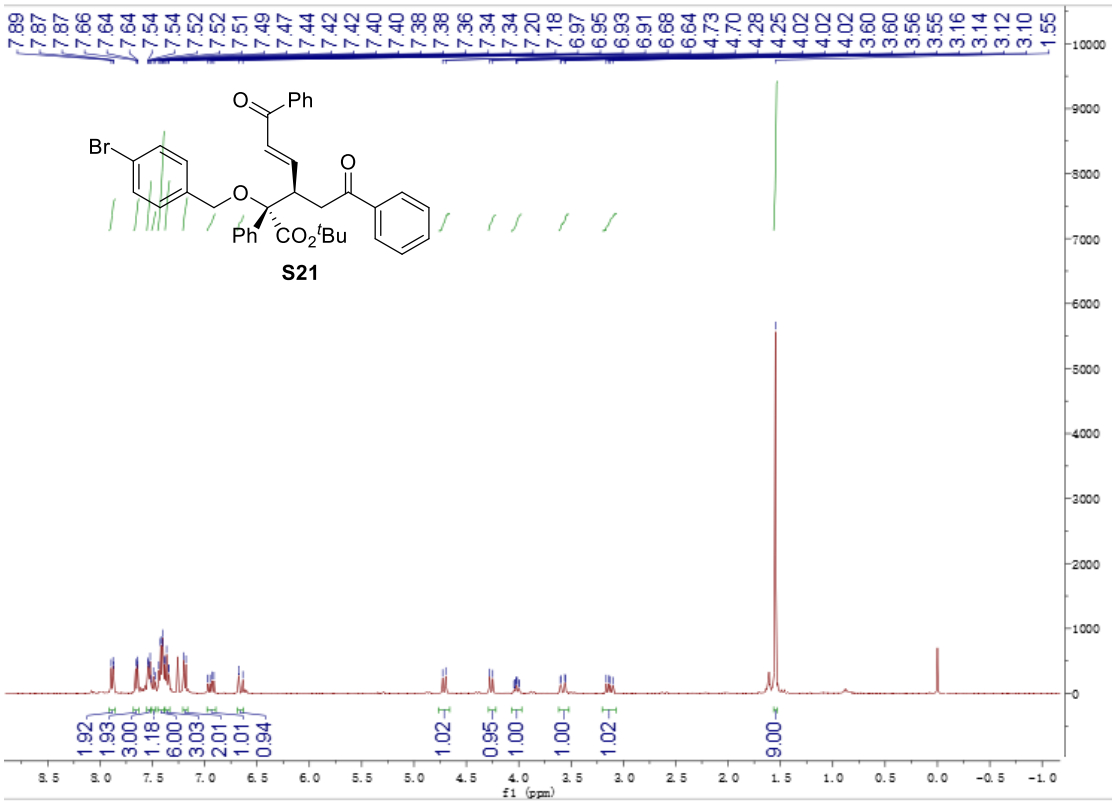

197.25
169.30
141.20
138.28
138.07
136.82
133.13
131.48
131.39
129.20
128.54
128.31
128.25
128.18
126.60
125.03
92.82
85.88
83.04
77.78
77.30
68.02
39.04
36.65
28.07
15.36
Me
S
Br
O
O
Ph
CO2tBu
f1 (ppm)

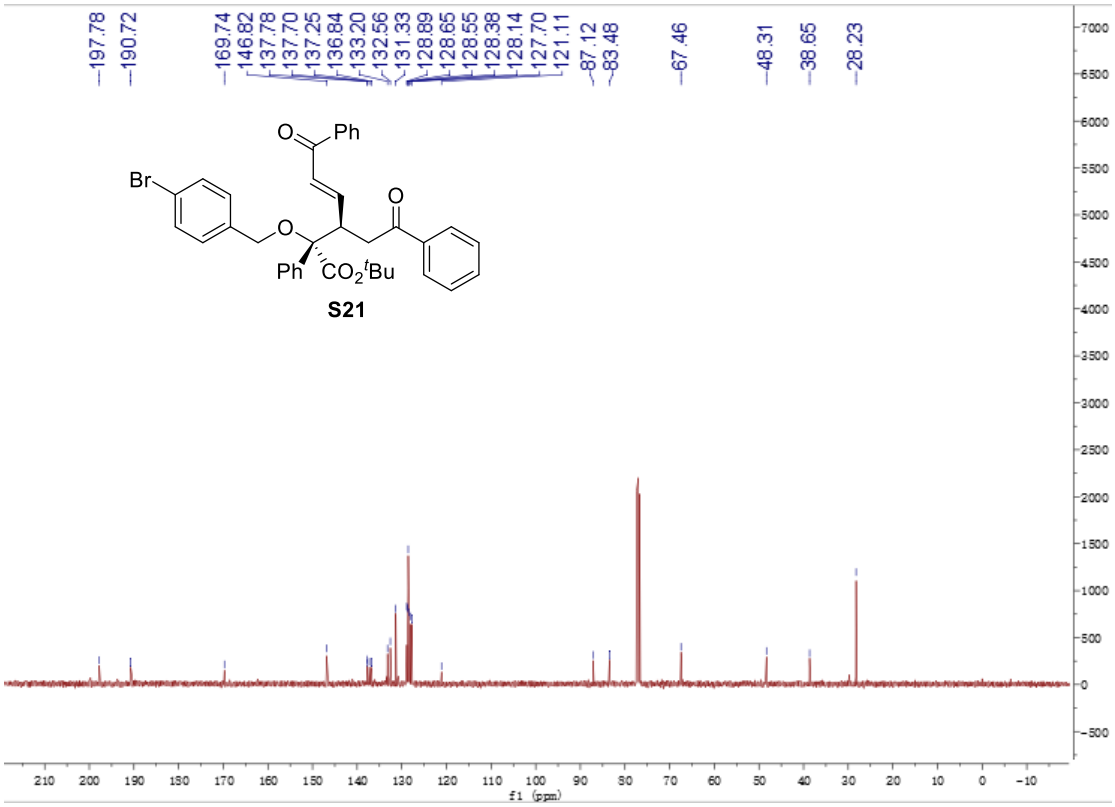
**S19**

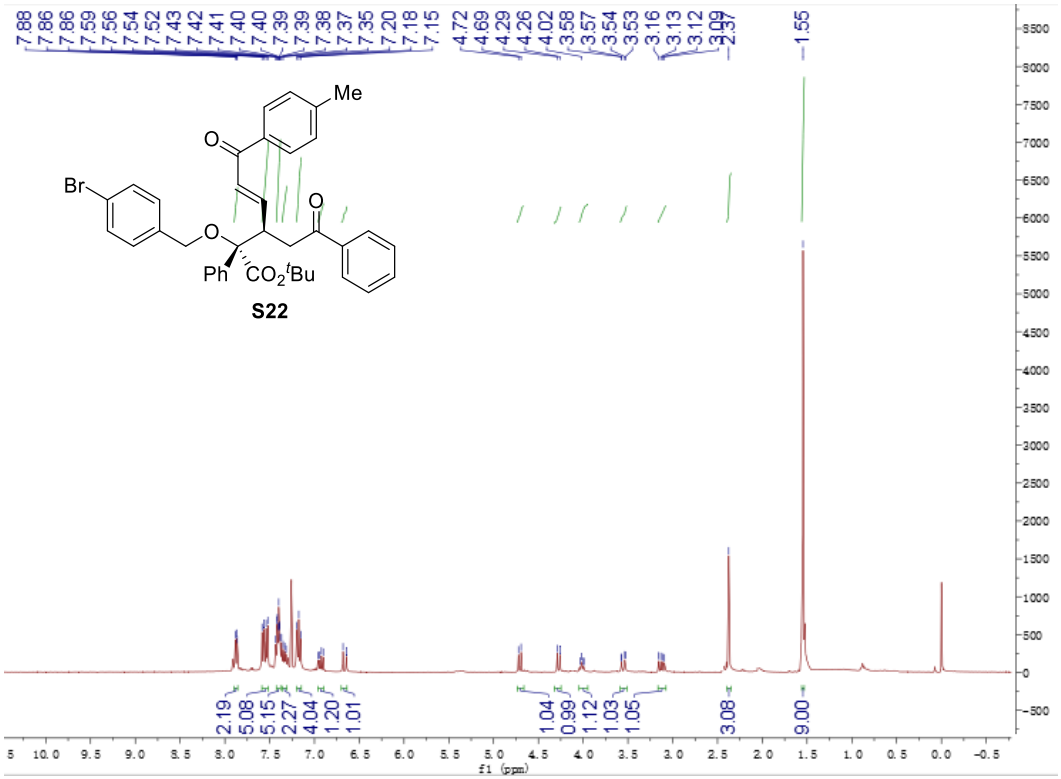

7.84
7.82
7.82
7.69
7.68
7.67
7.52
7.51
7.50
7.50
7.49
7.47
7.46
7.42
7.40
7.38
7.36
7.34
7.32
7.30
7.21
7.21
7.21
7.20
7.18
7.18
7.17
7.16
6.92
6.92
6.91
6.91
5.04
5.01
4.89
4.86
4.41
4.40
4.38
4.37
3.30
3.28
3.11
3.10
3.07
3.06
1.51
S
Br
O
O
Ph
CO2tBu
2.02
2.01
1.08
2.06
1.89
3.86
1.09
0.97
1.27
0.98
1.00
1.01
1.05
1.02
1.17
9.05
f1 (ppm)

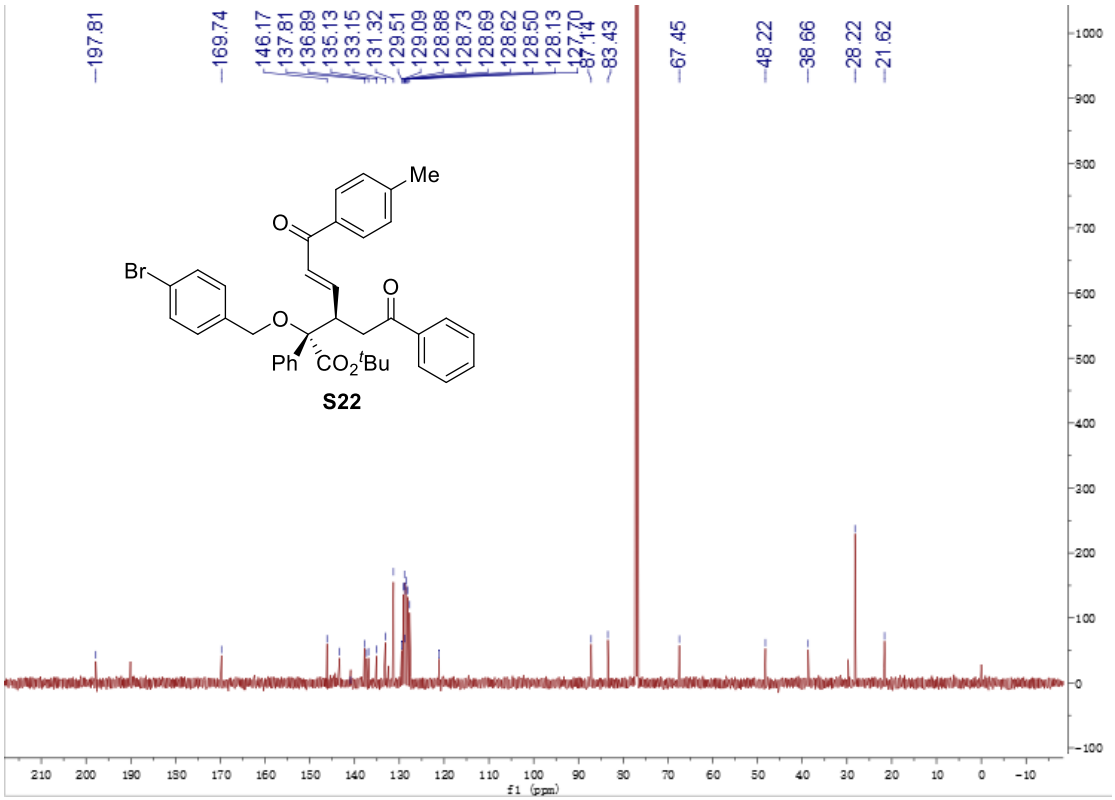
**S20**

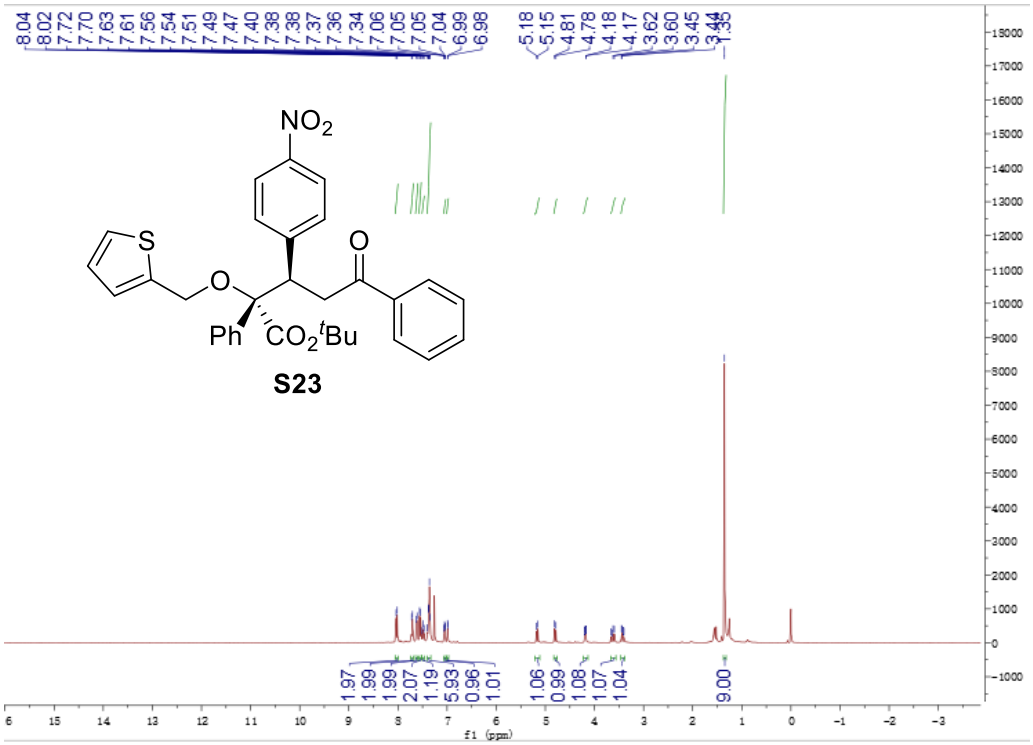

197.37
169.40
138.28
138.06
136.89
133.14
131.40
129.70
129.20
128.56
128.30
128.27
128.20
128.00
126.71
125.08
89.13
85.87
82.95
79.30
67.97
39.17
36.58
28.06
S
Br
O
O
Ph
CO2tBu
S20

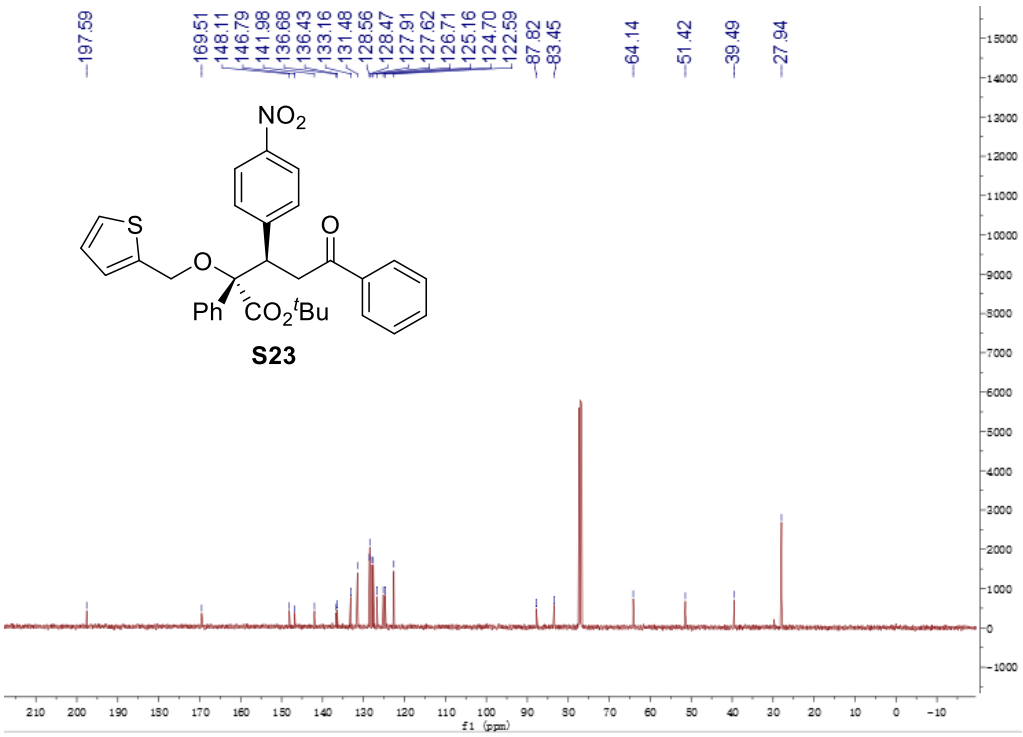

7.89
7.87
7.87
7.66
7.64
7.64
7.54
7.54
7.52
7.52
7.51
7.49
7.47
7.44
7.42
7.42
7.40
7.40
7.38
7.38
7.36
7.34
7.34
7.20
7.18
6.97
6.95
6.93
6.91
6.68
6.64
4.73
4.70
4.28
4.25
4.02
4.02
4.02
3.60
3.60
3.56
3.55
3.16
3.14
3.12
3.10
1.55
O
Ph
Br
O
O
Ph
CO2tBu
S21
1.92
1.93
3.00
1.18
6.00
3.03
2.01
1.01
0.94
1.02
0.95
1.00
1.00
1.02
9.00


197.78
190.72
169.74
146.82
137.78
137.70
137.25
136.84
133.20
132.56
131.33
128.89
128.65
128.55
128.38
128.14
127.70
121.11
87.12
83.48
67.46
48.31
38.65
28.23
O
Ph
Br
O
O
Ph
CO2tBu
S21
f1 (ppm)

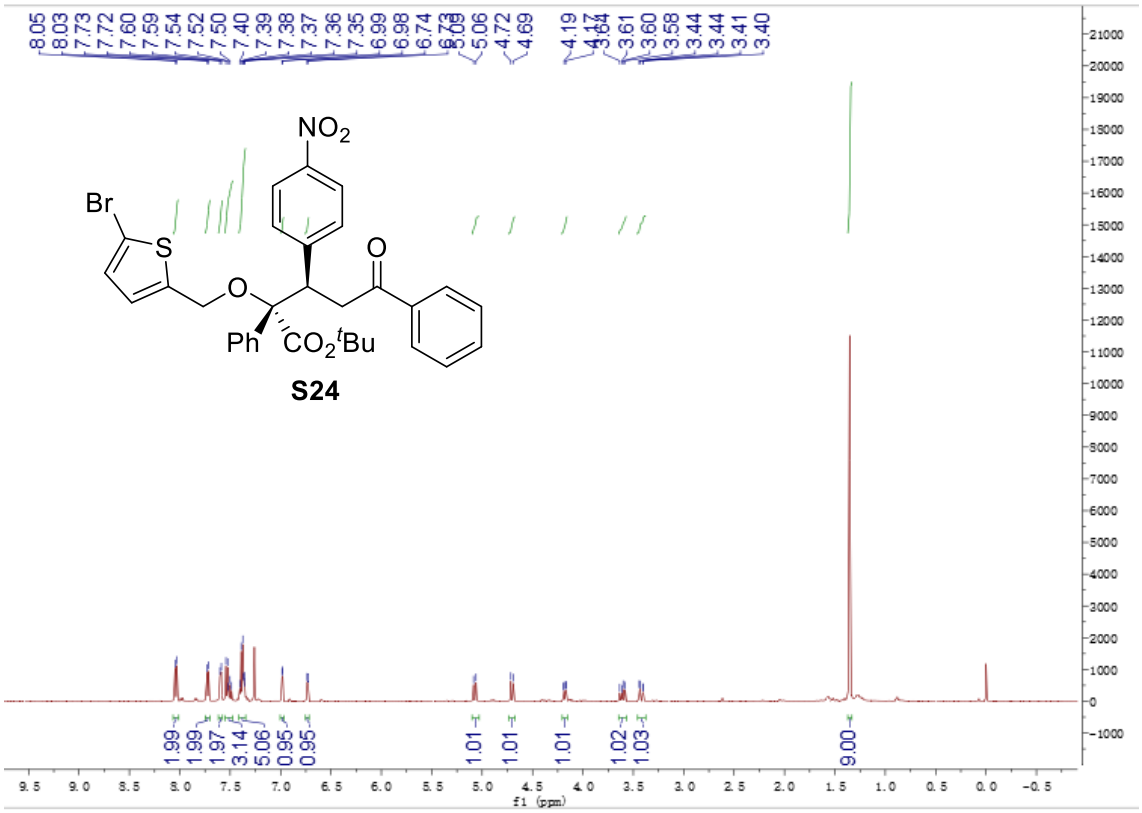

7.88
7.86
7.86
7.59
7.56
7.54
7.52
7.43
7.42
7.41
7.40
7.40
7.39
7.39
7.38
7.37
7.35
7.20
7.18
7.15
4.72
4.69
4.29
4.26
4.02
3.58
3.57
3.54
3.53
3.16
3.13
3.12
3.09
2.97
1.55
Me
O
Br
O
O
Ph
CO2tBu
S22
2.19
5.08
5.15
2.27
4.04
1.20
1.01
1.04
0.99
1.12
1.03
1.05
3.08
9.00
f1 (ppm)


Me
O
Br
O
O
Ph
CO2tBu
S22

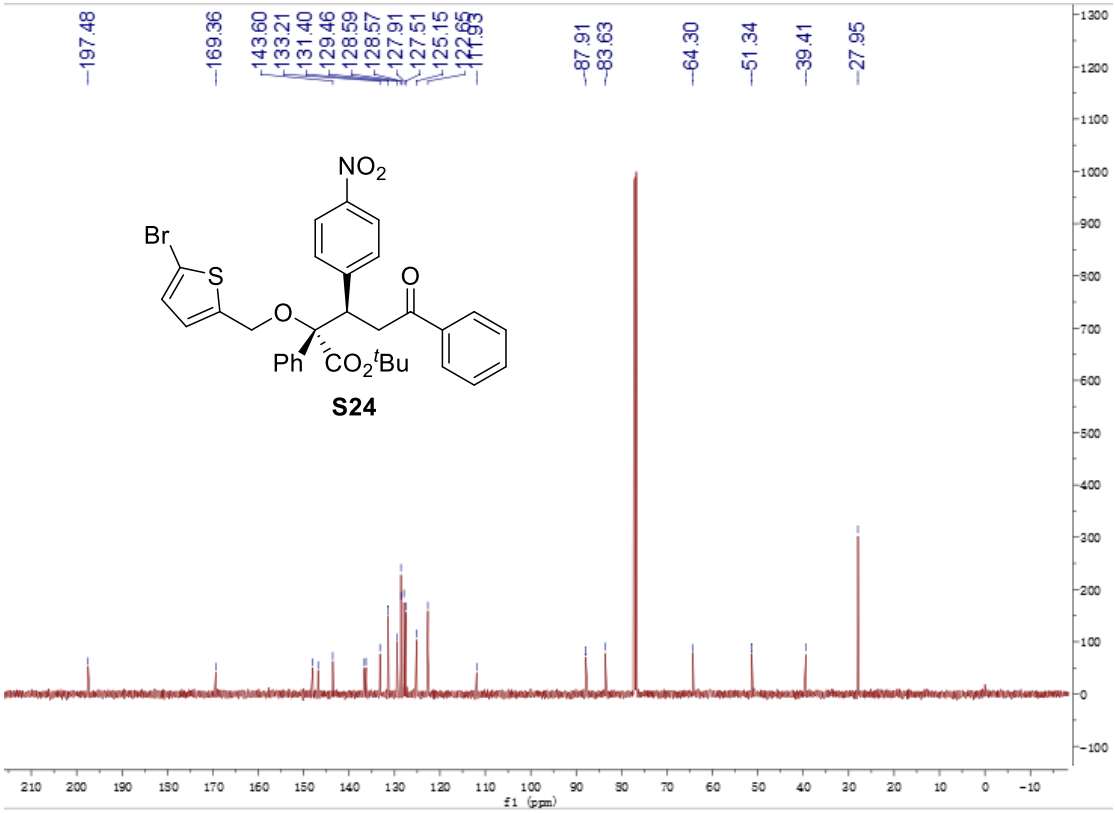

NO2
S
O
O
Ph
CO2tBu
S23

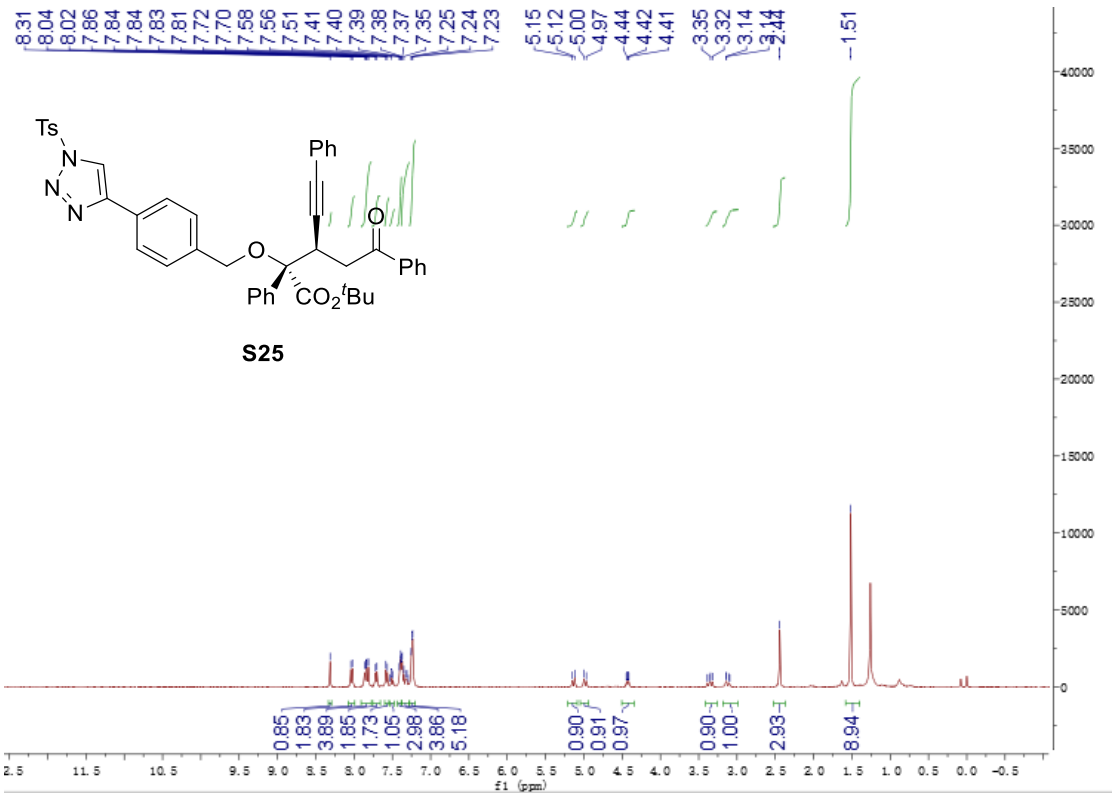

197.59
169.51
148.11
146.79
141.98
136.68
136.43
133.16
131.48
128.56
128.47
127.91
127.62
126.71
125.16
124.70
122.59
87.82
83.45
64.14
51.42
39.49
27.94
NO2
S
O
O
Ph
CO2tBu

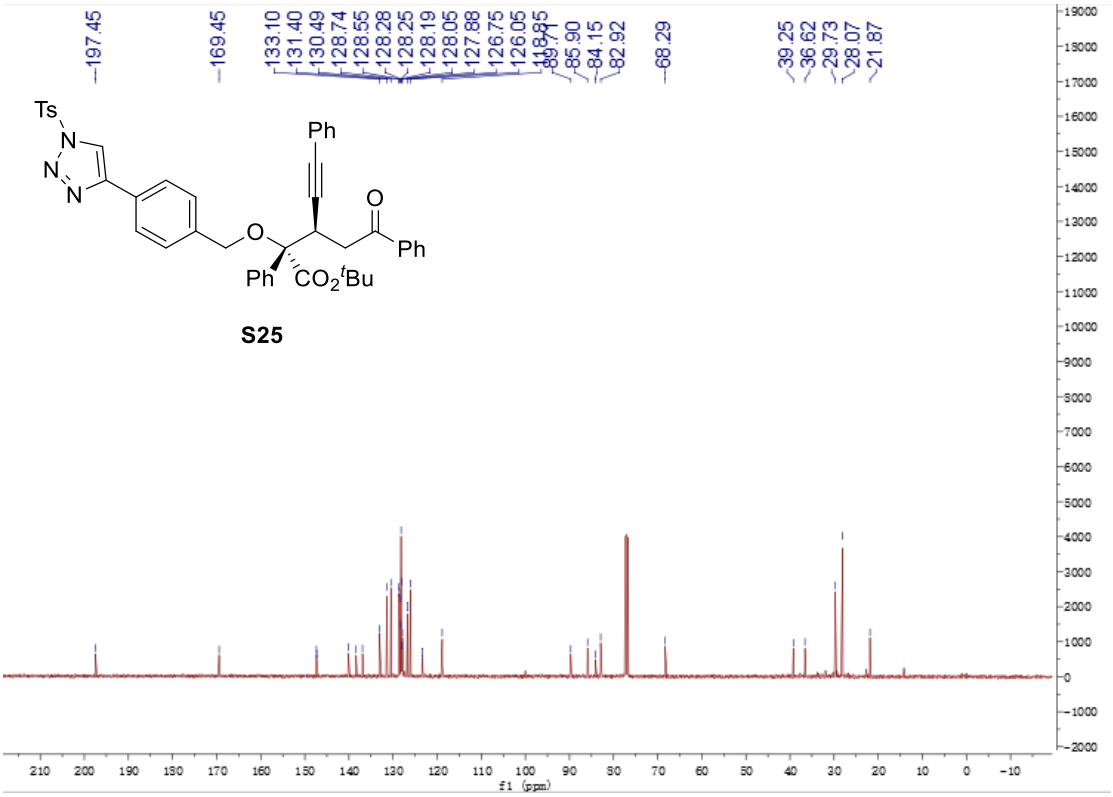
**S23**


8.05
8.03
7.73
7.72
7.60
7.59
7.54
7.52
7.50
7.40
7.39
7.38
7.37
7.36
7.35
6.99
6.98
6.74
6.73
5.06
4.72
4.69
4.19
4.17
3.61
3.60
3.58
3.44
3.44
3.41
3.40
NO2
Br
S
O
O
Ph
CO2tBu
1.99
1.99
1.97
3.14
5.06
0.95
0.95
1.01
1.01
1.01
1.02
1.03
9.00

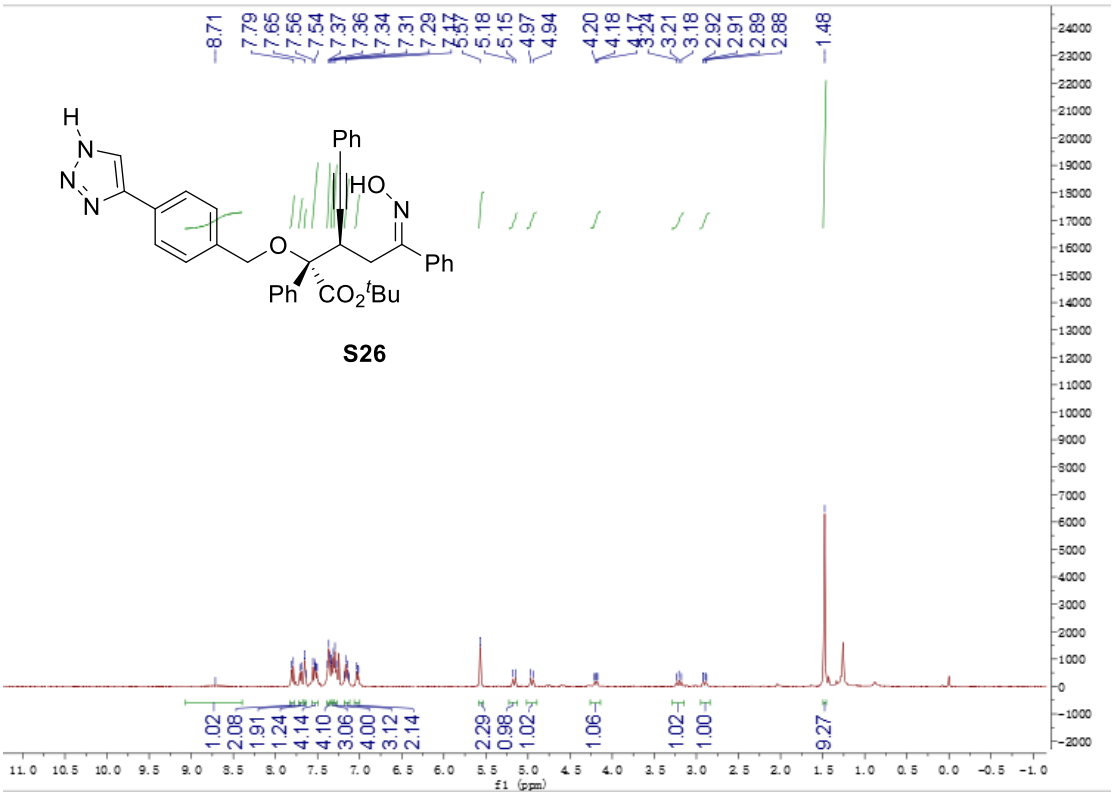
**S24**


197.48
169.36
143.60
133.21
131.40
129.46
128.59
128.57
127.91
127.51
125.15
122.65
87.91
83.63
64.30
51.34
39.41
27.95
NO2
Br
S
O
O
Ph
CO2tBu
S24
f1 (ppm)

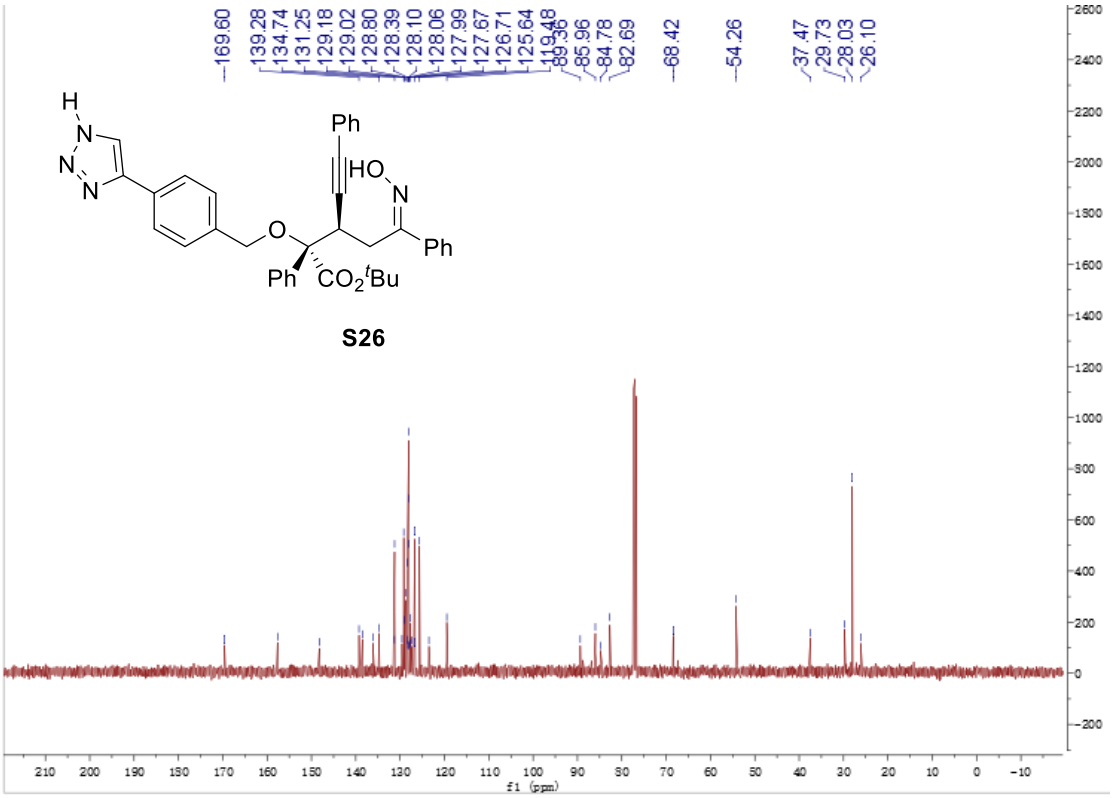

8.31
8.04
8.02
7.86
7.84
7.84
7.83
7.81
7.72
7.70
7.58
7.56
7.51
7.41
7.40
7.39
7.38
7.37
7.35
7.25
7.24
7.23
5.15
5.12
5.00
4.97
4.44
4.42
4.41
3.35
3.32
3.14
2.44
1.51
Ts
N
N
N
Ph
O
O
Ph
Ph
CO2tBu
S25
0.85
1.83
3.89
1.85
1.73
1.05
2.98
3.86
5.18
0.90
0.91
0.97
0.90
1.00
2.93
8.94
f1 (ppm)


197.45
169.45
133.10
131.40
130.49
128.74
128.55
128.28
128.25
128.19
128.05
127.88
126.75
126.05
89.71
85.90
84.15
82.92
68.29
39.25
36.62
29.73
28.07
21.87
Ts
N
N
N
Ph
O
O
Ph
Ph
CO2tBu
f1 (ppm)

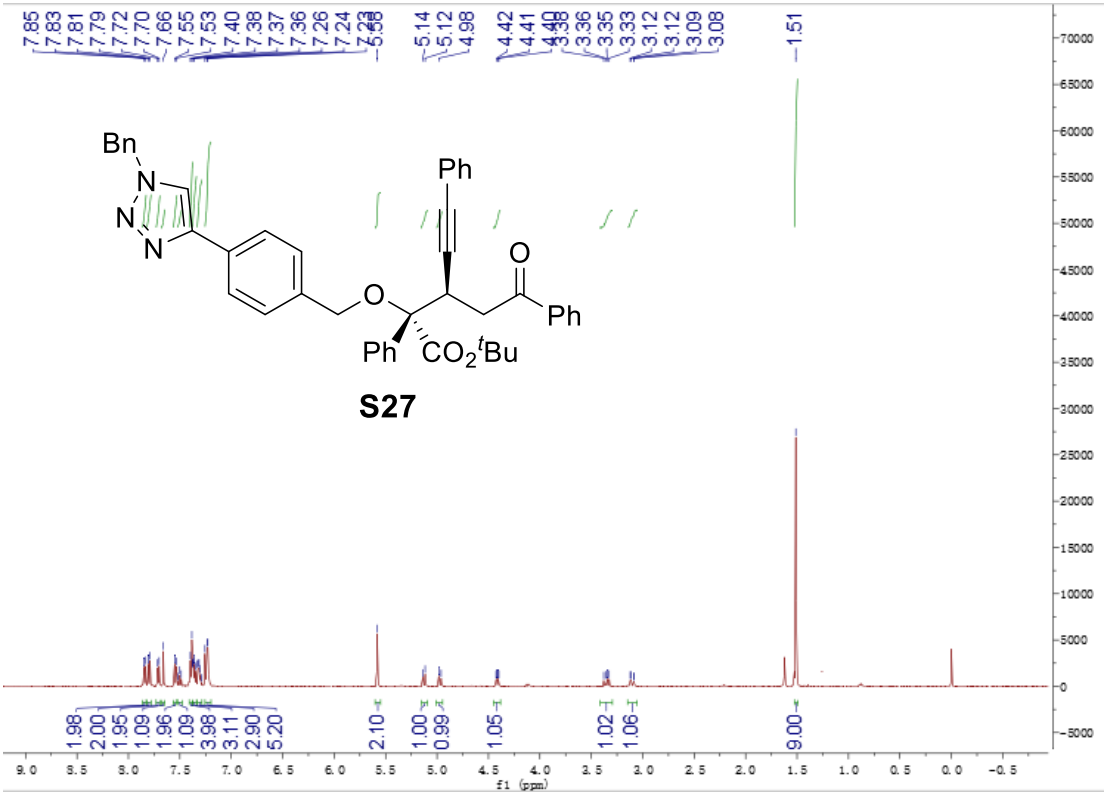
**S25**


8.71
7.79
7.65
7.56
7.54
7.37
7.36
7.34
7.31
7.29
5.18
5.15
4.97
4.94
4.20
4.18
3.24
3.21
3.18
2.92
2.91
2.89
2.88
1.48
H
N
N
N
Ph
HO
N
O
Ph
Ph
CO2tBu
1.02
2.08
1.91
1.24
4.14
4.10
3.06
4.00
3.12
2.14
2.29
0.98
1.02
1.06
1.02
1.00
9.27
f1 (ppm)

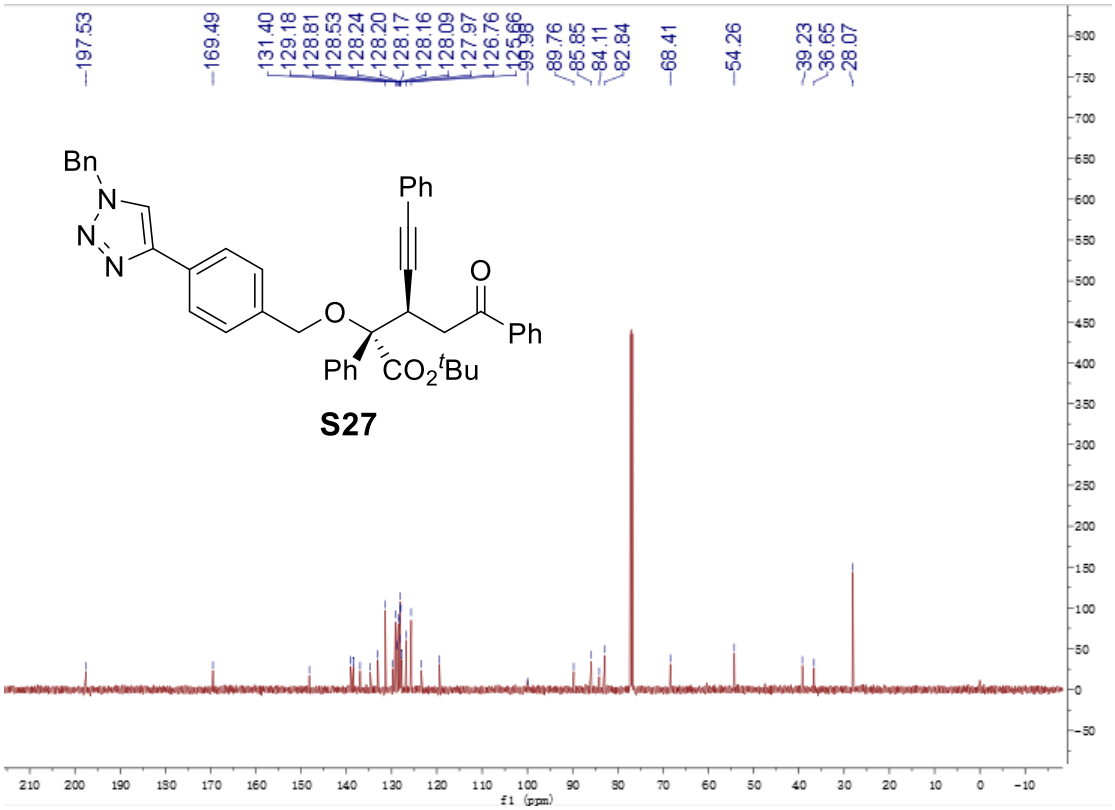
**S26**


169.60
139.28
134.74
131.25
129.18
129.02
128.80
128.39
128.10
128.06
127.99
127.67
126.71
125.64
89.36
85.96
84.78
82.69
68.42
54.26
37.47
29.73
28.03
26.10
H
N
N
N
Ph
HO
N
O
Ph
Ph
CO2tBu
f1 (ppm)

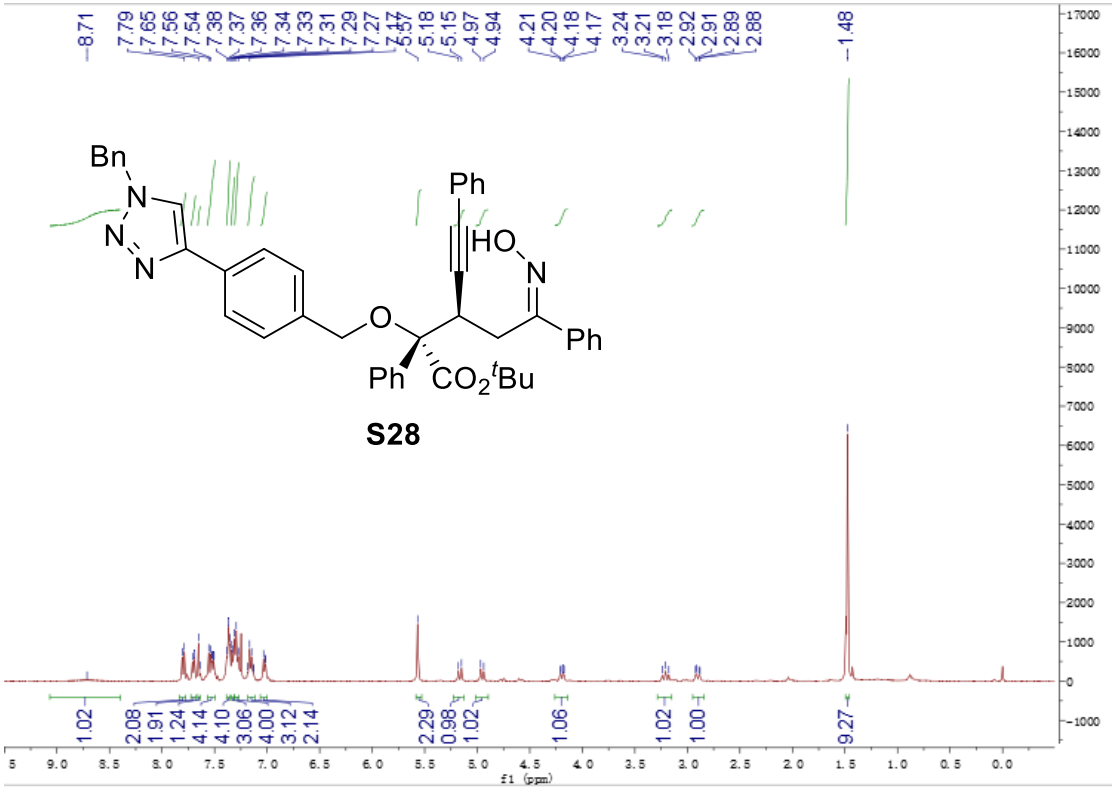
**S26**


7.85
7.83
7.81
7.79
7.72
7.70
7.66
7.55
7.53
7.40
7.38
7.37
7.36
7.26
7.24
5.14
5.12
4.98
4.42
4.41
3.36
3.35
3.33
3.12
3.09
3.08
1.51
Bn
N
N
N
Ph
O
O
Ph
Ph
CO2tBu
1.98
2.00
1.95
1.09
1.96
1.09
3.98
3.11
2.90
5.20
2.10
1.00
0.99
1.05
1.02
1.06
9.00
f1 (ppm)

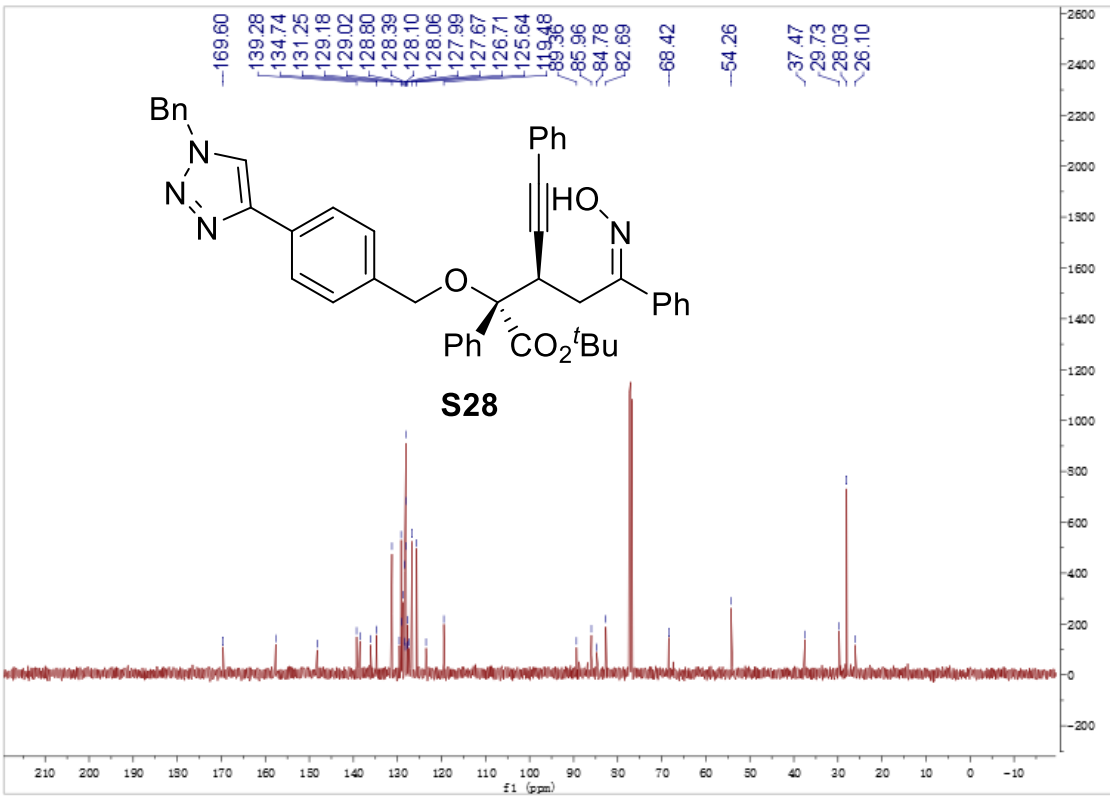
**S27**

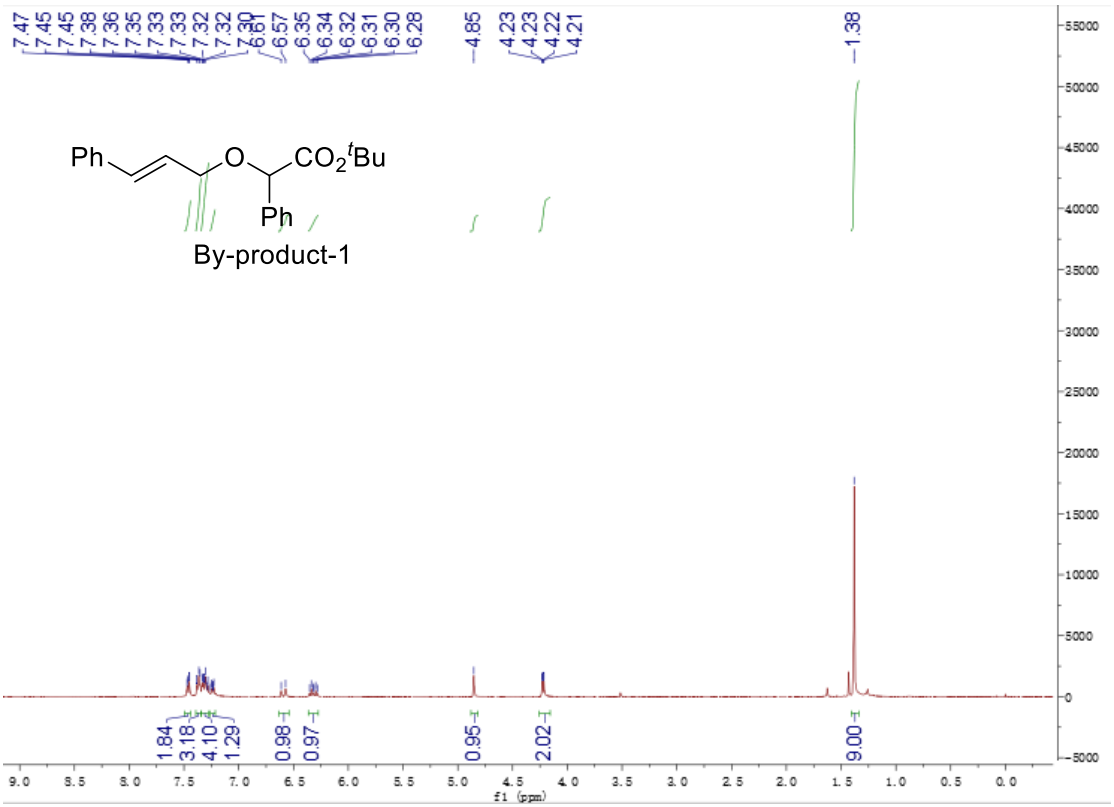

197.53
169.49
131.40
129.18
128.81
128.53
128.24
128.20
128.17
128.16
128.09
127.97
126.76
125.66
89.76
85.85
84.11
82.84
68.41
54.26
39.23
36.65
28.07
Bn
N
N
N
O
Ph
O
Ph
Ph
CO2tBu
f1 (ppm)

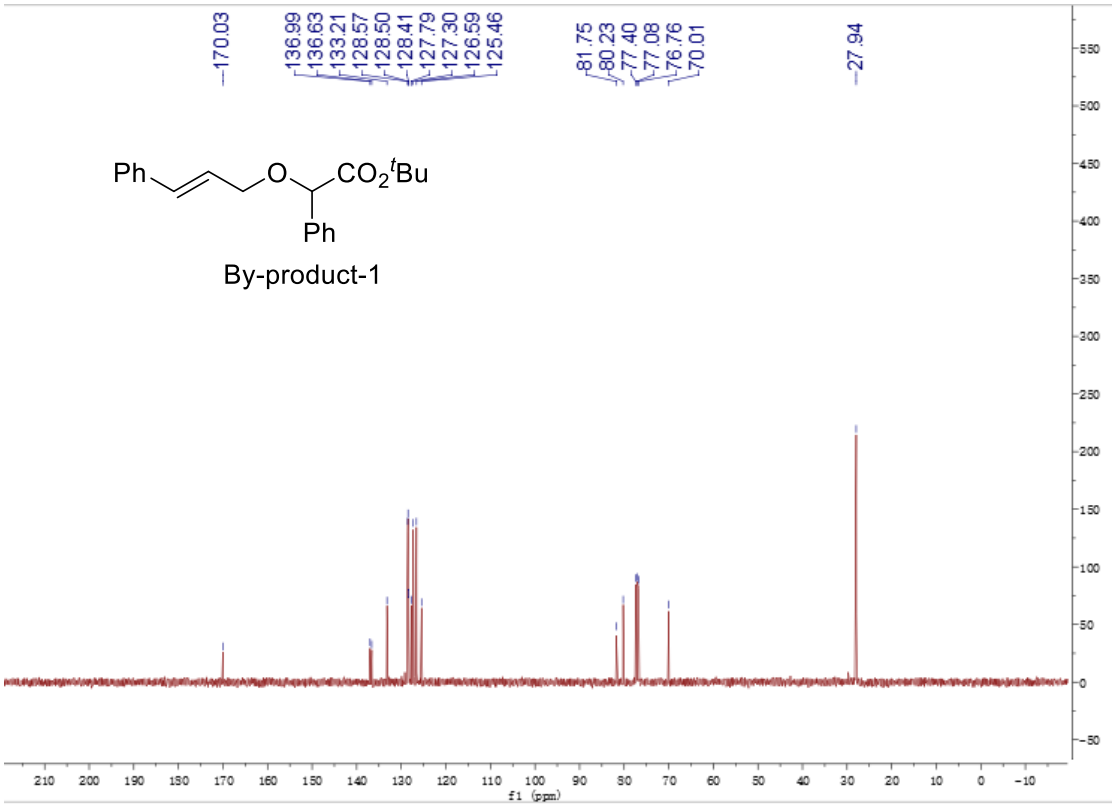
**S27**

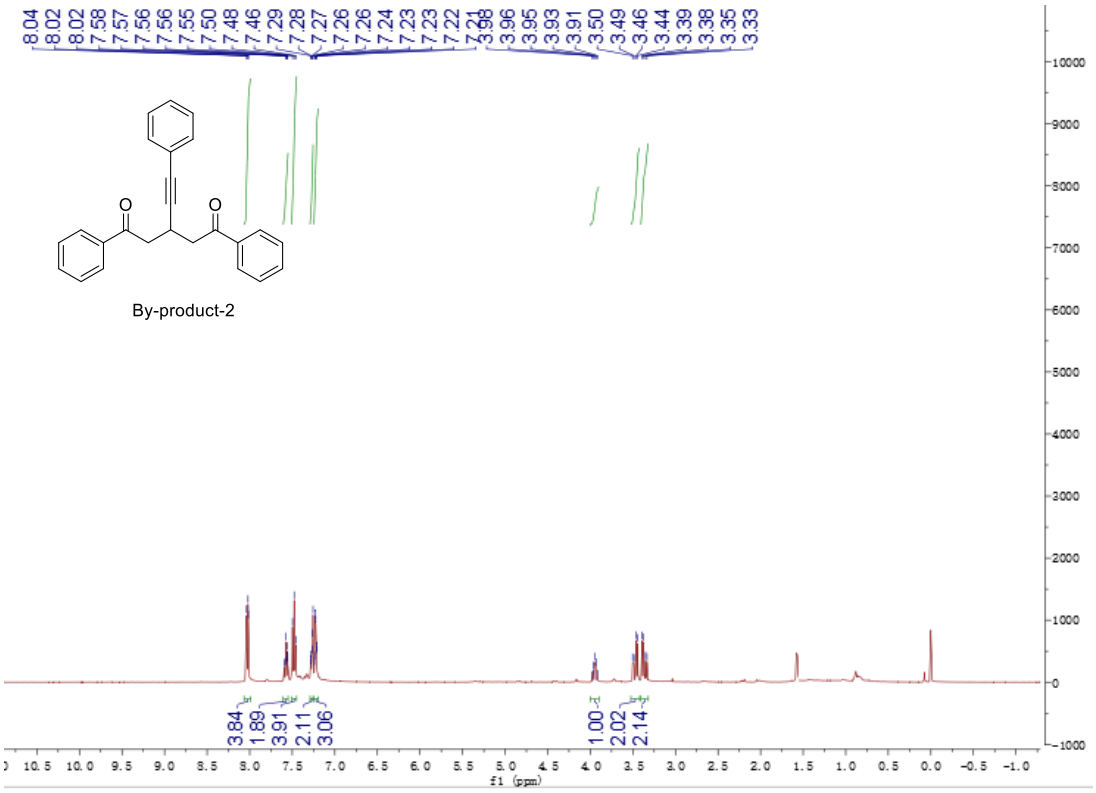

8.71
7.79
7.65
7.56
7.54
7.38
7.37
7.36
7.34
7.33
7.31
7.29
7.27
5.18
5.15
4.97
4.94
4.21
4.20
4.18
4.17
3.24
3.21
3.18
2.92
2.91
2.89
2.88
1.48
Bn
N
N
N
Ph
HO
N
O
Ph
Ph
CO2tBu
1.02
2.08
1.91
1.24
4.14
4.10
3.06
4.00
3.12
2.14
2.29
0.98
1.02
1.06
1.02
1.00
9.27
f1 (ppm)

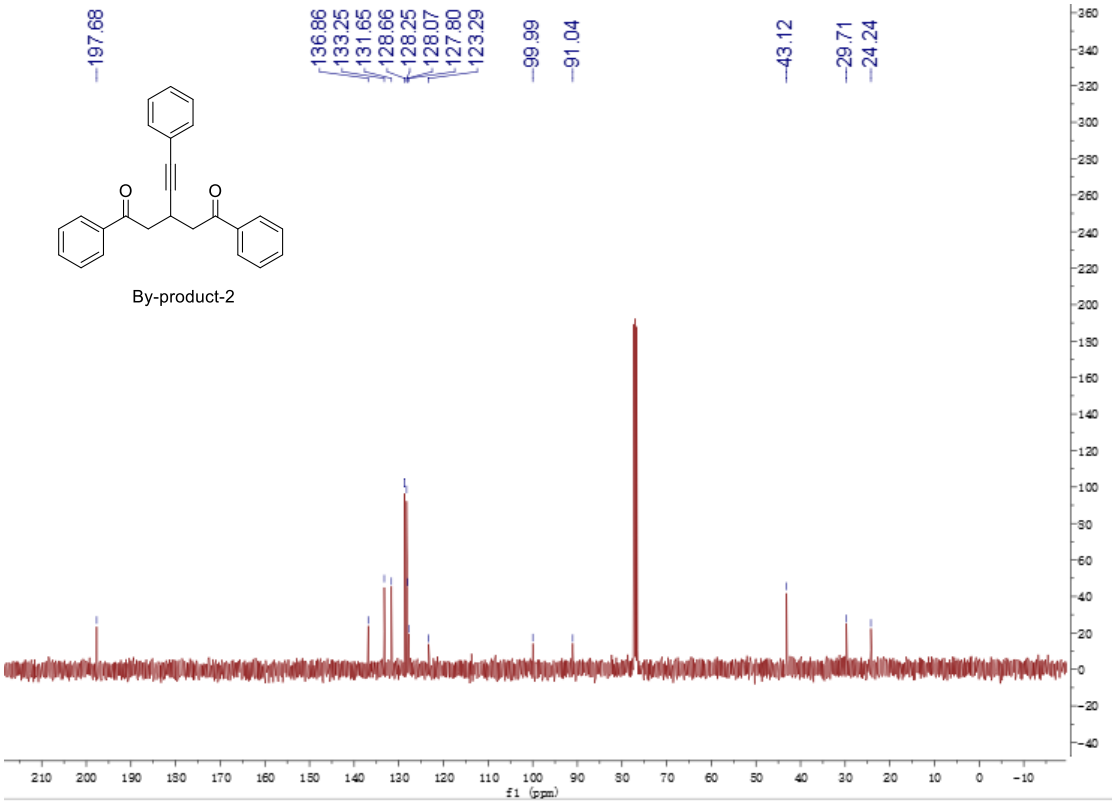
**S28**

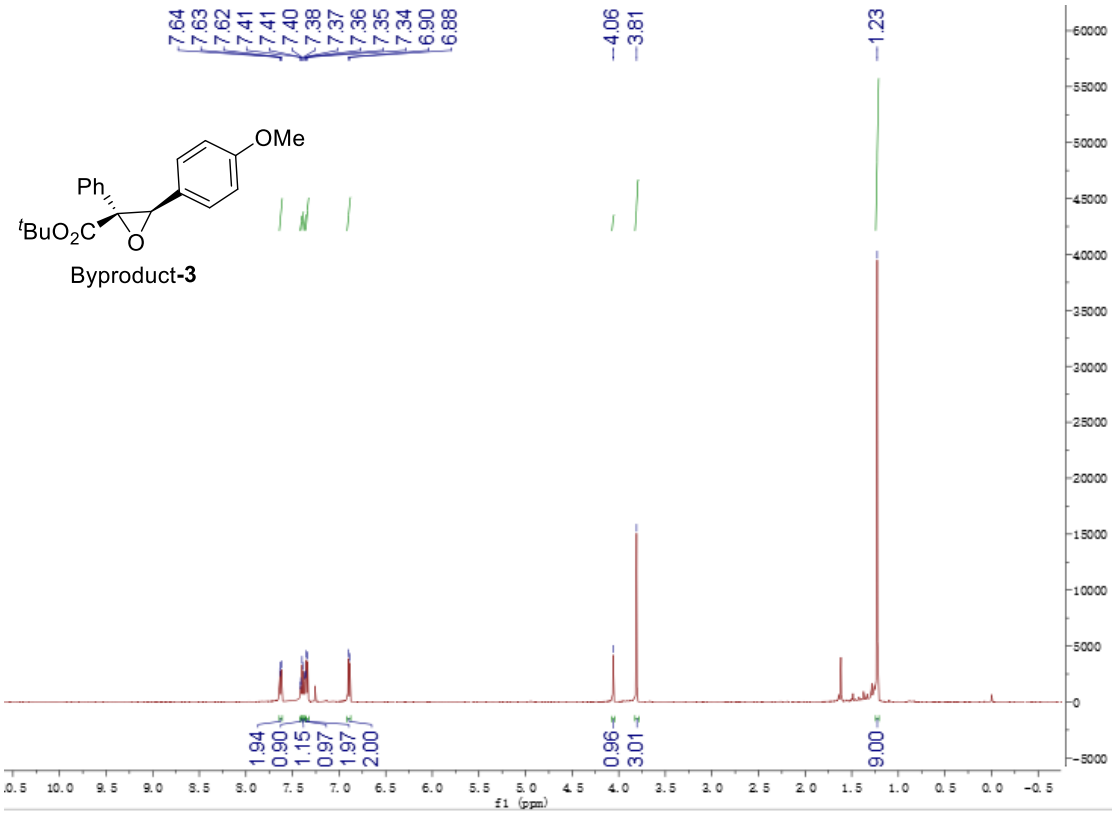

169.60
139.28
134.74
131.25
129.18
129.02
128.80
128.39
128.10
128.06
127.99
127.67
126.71
125.64
119.48
89.36
85.96
84.78
82.69
68.42
54.26
37.47
29.73
28.03
26.10
Bn
N
N
N
Ph
HO
N
O
Ph
Ph
CO2tBu
S28
f1 (ppm)

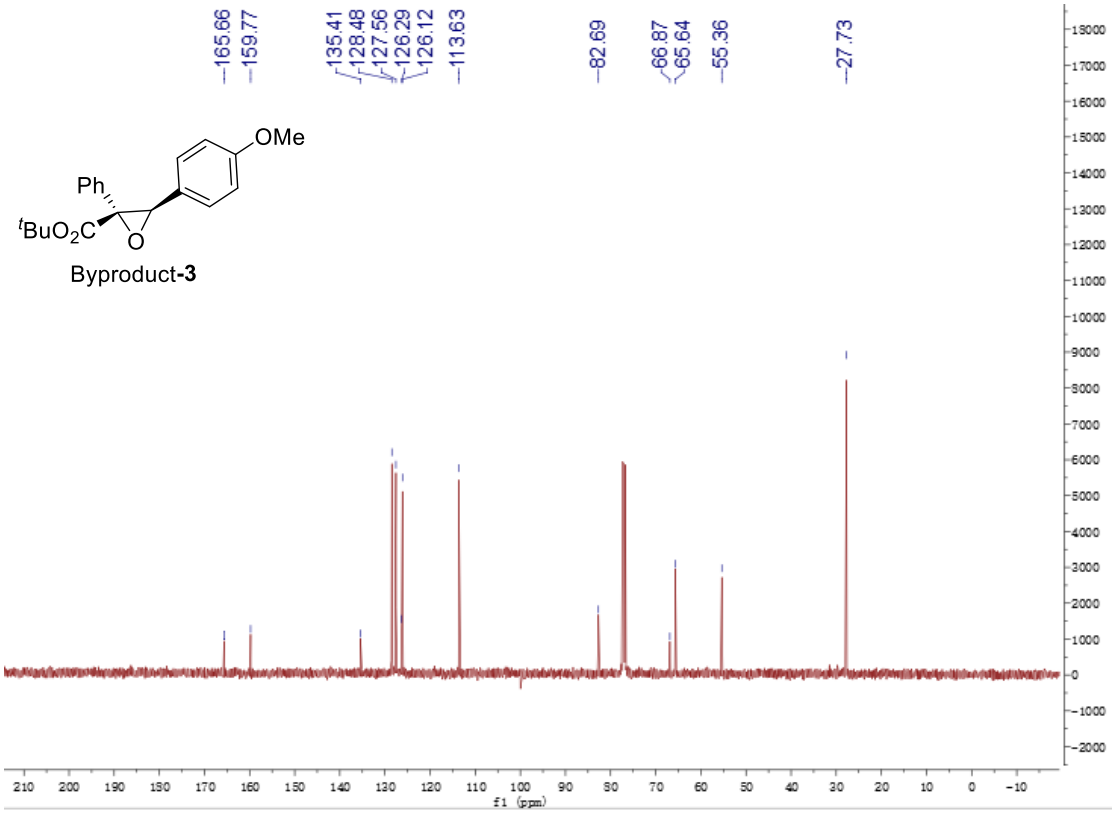

7.47
7.45
7.45
7.38
7.36
7.35
7.33
7.33
7.32
7.32
6.57
6.35
6.34
6.32
6.31
6.30
6.28
4.85
4.23
4.23
4.22
4.21
1.38
Ph
O
CO2tBu
Ph
By-product-1
1.84
3.18
4.10
1.29
0.98
0.97
0.95
2.02
9.00
f1 (ppm)


170.03
136.99
136.63
133.21
128.57
128.50
128.41
127.79
127.30
126.59
125.46
81.75
80.23
77.40
77.08
76.76
70.01
27.94
Ph
O
CO2tBu
Ph
By-product-1
f1 (ppm)

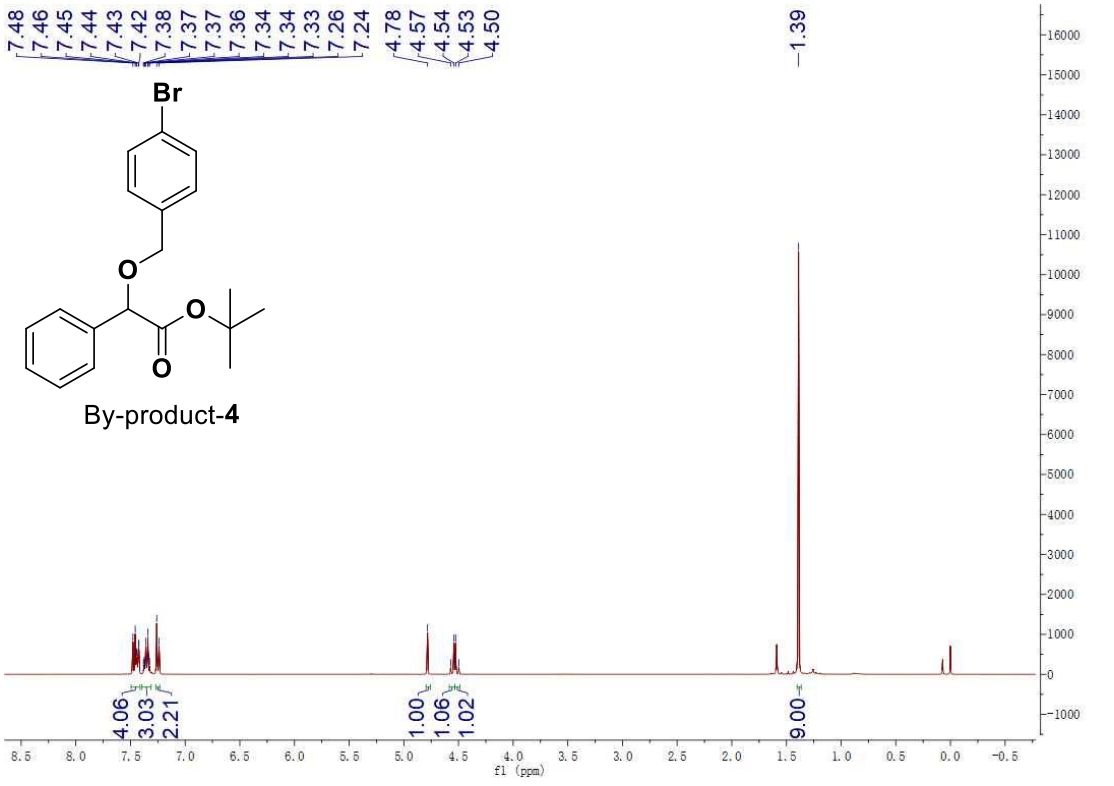

8.04
8.02
8.02
7.58
7.57
7.56
7.56
7.55
7.50
7.48
7.46
7.29
7.28
7.27
7.26
7.26
7.24
7.23
7.23
7.22
7.21
3.98
3.96
3.95
3.93
3.91
3.50
3.49
3.46
3.44
3.39
3.38
3.35
3.33
O
O
By-product-2
3.84
1.89
3.91
2.11
3.06
1.00
2.02
2.14
f1 (ppm)


197.68
136.86
133.25
131.65
128.66
128.25
128.07
127.80
123.29
99.99
91.04
43.12
29.71
24.24
By-product-2

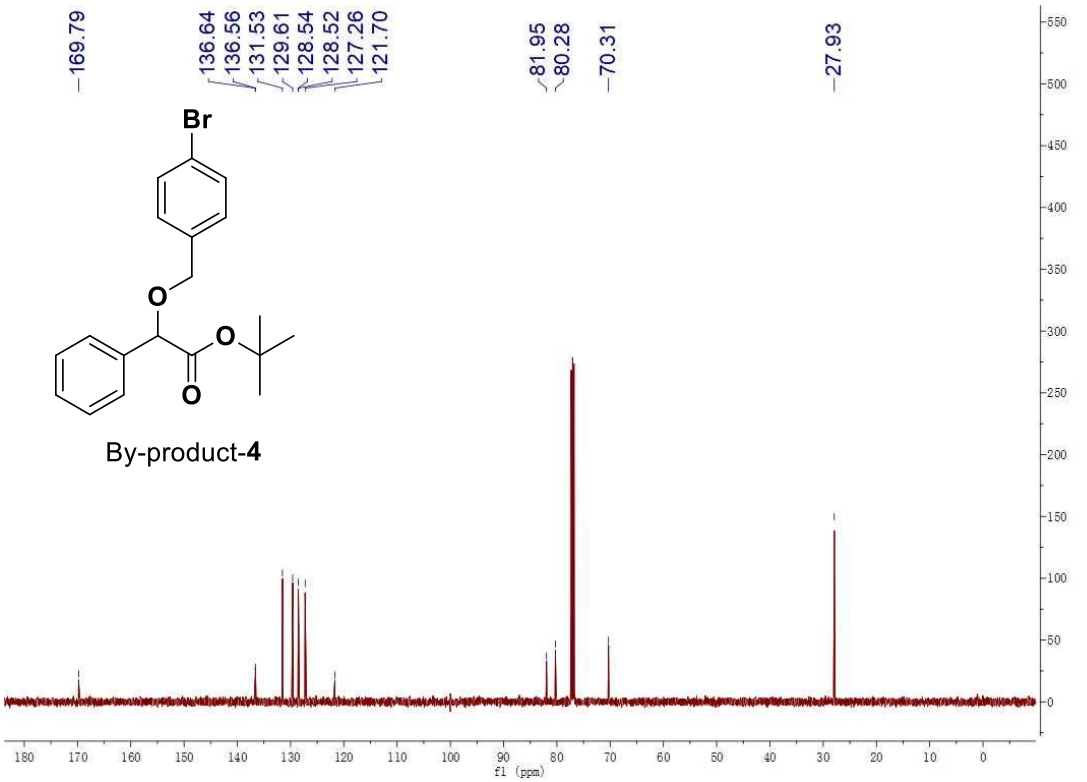

7.64
7.63
7.62
7.41
7.41
7.40
7.38
7.37
7.36
7.35
7.34
6.90
6.88
4.06
3.81
1.23
OMe
Ph
tBuO2C
O
Byproduct-3
1.94
0.90
1.15
0.97
1.97
2.00
0.96
3.01
9.00

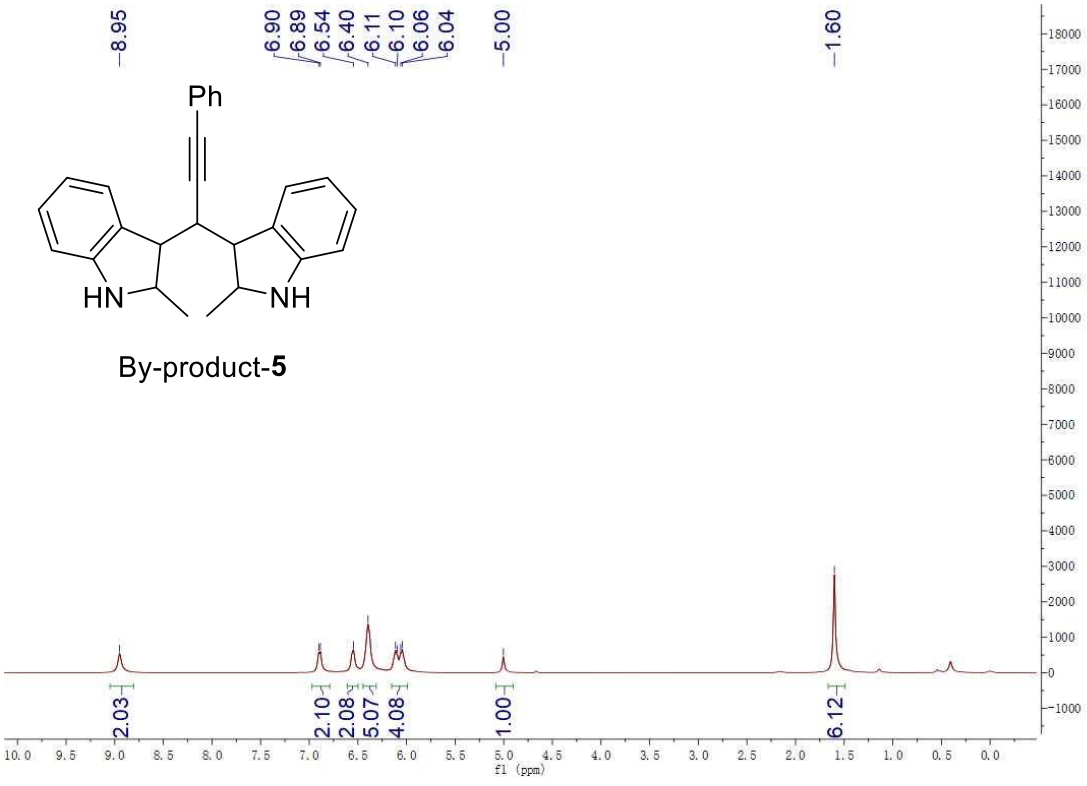


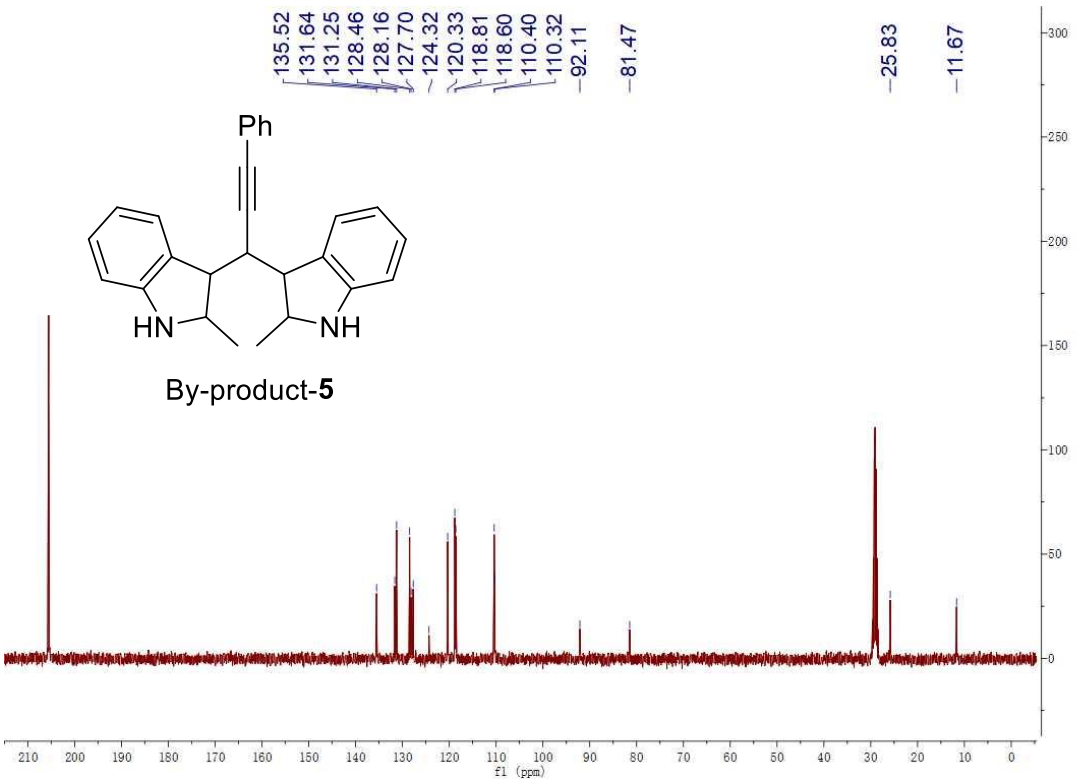

Byproduct-**3**



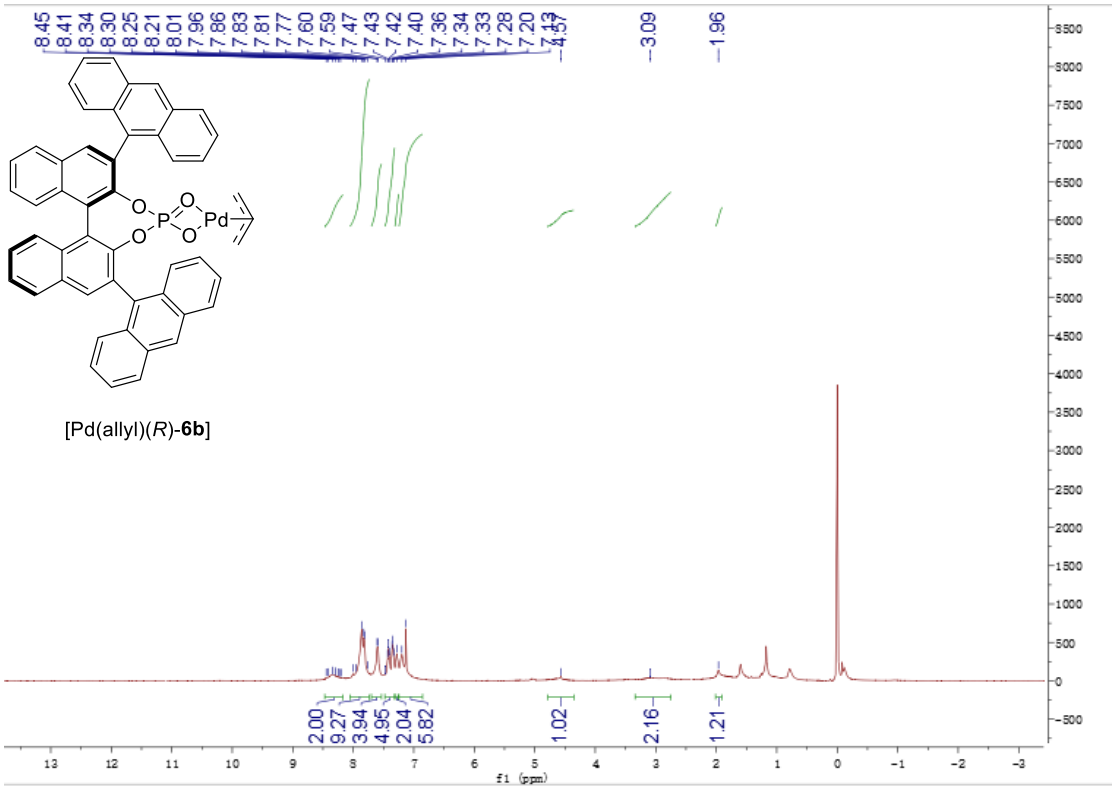

By-product-**4**


169.79
136.64
136.56
131.53
129.61
128.54
128.52
127.26
121.70
81.95
80.28
70.31
27.93
Br
O
O
O
By-product-4
f1 (ppm)

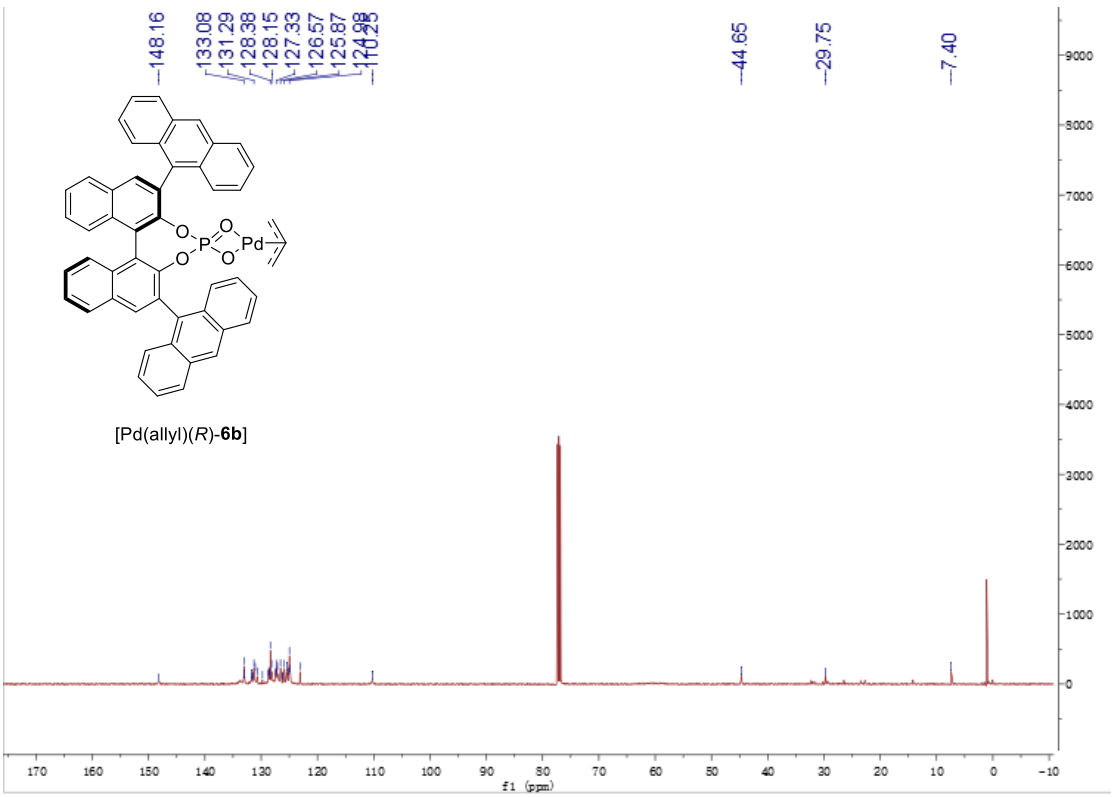

8.95
6.90
6.89
6.54
6.40
6.11
6.10
6.06
6.04
5.00
1.60
Ph
HN
NH
By-product-5
2.03
2.10
2.08
5.07
4.08
1.00
6.12
f1 (ppm)



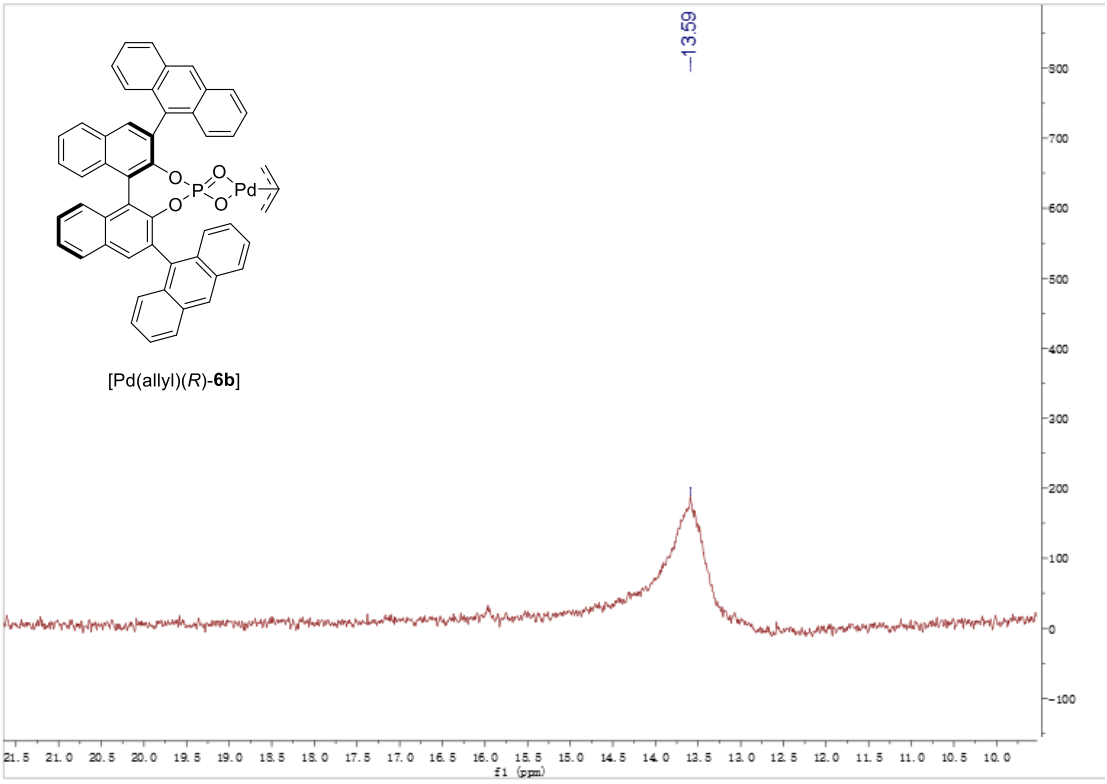

By-product-**5**




[Pd(allyl)(*R*)-**6b**]




[Pd(allyl)(*R*)-**6b**]




[Pd(allyl)(*R*)-**6b**]

**12. Detailed Information of ECD Calculation**

**Cartesian coordinates**

SSS-conf-1

| | | | |
|---|---|---|---|
| C | 0.22632300 | -1.12085000 | -0.84532700 |
| C | -0.09804100 | 0.35022800 | -0.43652200 |
| C | 0.35185600 | 1.33353300 | -1.54442700 |
| C | -1.56921400 | 0.55839100 | 0.02033600 |
| C | -2.71222900 | -0.06091800 | -0.81640300 |
| O | -0.43462300 | -1.42048200 | -2.07512000 |
| O | -2.62754000 | 0.28135600 | -2.20806100 |
| C | 0.37049000 | 2.82746700 | -1.14596300 |
| C | -0.14893000 | -2.17036600 | 0.22056300 |
| C | 0.06769300 | -1.94271300 | 1.58573700 |
| C | -0.24403400 | -2.92203100 | 2.52668800 |
| C | -0.76804500 | -4.14896500 | 2.12053300 |
| C | -0.97595300 | -4.38756500 | 0.76401200 |
| C | -0.66685700 | -3.40681300 | -0.17813400 |
| C | 1.74545000 | -1.30556300 | -1.12252600 |
| O | 2.12518200 | -1.74663900 | -2.19256700 |
| O | 2.50287200 | -0.97776400 | -0.09752400 |
| C | 3.99272700 | -1.21315200 | -0.06486300 |
| C | 4.36217400 | -0.71699600 | 1.32834200 |
| C | 4.66662500 | -0.37636800 | -1.14767400 |
| C | 4.26353200 | -2.70804900 | -0.20803700 |
| C | -4.05759600 | 0.39197800 | -0.28027100 |
| C | -4.65118900 | -0.29384000 | 0.78527400 |
| C | -5.86776400 | 0.13061800 | 1.31731700 |
| C | -6.51292800 | 1.24693400 | 0.78531600 |
| C | -5.93166800 | 1.93287700 | -0.28048300 |
| C | -4.71191400 | 1.50993400 | -0.80825200 |
| C | 1.38088800 | 3.19735300 | -0.08132200 |
| C | 2.72217100 | 3.42203500 | -0.42100800 |
| C | 3.66287900 | 3.76409000 | 0.54931000 |
| C | 3.27895600 | 3.88777600 | 1.88520500 |
| C | 1.94795200 | 3.67027600 | 2.23817200 |
| C | 1.00986800 | 3.33022900 | 1.26268200 |
| H | 0.51744300 | 0.56069600 | 0.44157600 |
| H | 1.36058000 | 1.06565900 | -1.87820700 |
| H | -0.29666000 | 1.23198800 | -2.41533100 |
| H | -1.68149400 | 0.17004700 | 1.03633000 |
| H | -1.74896300 | 1.63442700 | 0.08989300 |
| H | -2.66707400 | -1.15066300 | -0.72394900 |
| H | 0.25231900 | -1.70604700 | -2.70181400 |
| H | -1.88139900 | -0.24026300 | -2.54600200 |
| H | 0.59405400 | 3.39732500 | -2.05362400 |
| H | -0.62591200 | 3.14140800 | -0.82476200 |
| H | 0.48034300 | -1.00108600 | 1.92498400 |
| H | -0.07572300 | -2.72376800 | 3.57976200 |
| H | -1.00976900 | -4.91010300 | 2.85431300 |
| H | -1.37978200 | -5.33846300 | 0.43324500 |
| H | -0.83668700 | -3.59776400 | -1.22962900 |
| H | 3.83713900 | -1.29057800 | 2.09592700 |
| H | 5.43709400 | -0.83417200 | 1.48420300 |
| H | 4.10931600 | 0.33946800 | 1.44415200 |
| H | 4.41023700 | -0.72195000 | -2.14865300 |
| H | 5.75039100 | -0.45230600 | -1.02487200 |
| H | 4.38734800 | 0.67530200 | -1.05008000 |
| H | 3.69835800 | -3.27361800 | 0.53703700 |
| H | 4.00943200 | -3.07621200 | -1.20182700 |
| H | 5.32792000 | -2.88970200 | -0.03744400 |
| H | -4.16068500 | -1.17047500 | 1.19720200 |
| H | -6.31533200 | -0.41515700 | 2.14123400 |
| H | -7.46213300 | 1.57596000 | 1.19435000 |
| H | -6.42857200 | 2.79929900 | -0.70436300 |
| H | -4.27027500 | 2.04437400 | -1.64084600 |
| H | 3.02921300 | 3.34053100 | -1.45933400 |
| H | 4.69397800 | 3.94136700 | 0.26170500 |
| H | 4.00842500 | 4.15799200 | 2.64107400 |
| H | 1.63649000 | 3.77114000 | 3.27265600 |
| H | -0.02609400 | 3.17640300 | 1.54760900 |

SSS-conf-2

| | | | |
|---|---|---|---|
| C | -1.08813200 | -0.06572400 | -0.89963200 |
| C | -0.07541300 | -0.40048100 | 0.25033700 |
| C | -0.29574400 | 0.41006000 | 1.54974900 |
| C | -0.01321100 | -1.90861500 | 0.59159900 |

| | | | |
|---|---|---|---|
| C | 0.70301900 | -2.87258600 | -0.36934700 |
| O | -0.55658200 | -0.68487100 | -2.07444700 |
| O | 0.46743600 | -4.17865200 | 0.20055600 |
| C | 0.98509300 | 0.61994500 | 2.38968300 |
| C | -1.19392000 | 1.45321600 | -1.16133700 |
| C | -2.27601900 | 2.24337300 | -0.75912700 |
| C | -2.30502700 | 3.61058100 | -1.04008700 |
| C | -1.25062500 | 4.21269400 | -1.72057700 |
| C | -0.16544400 | 3.43440200 | -2.12360400 |
| C | -0.14053200 | 2.06942400 | -1.85091800 |
| C | -2.50082400 | -0.67782500 | -0.70052300 |
| O | -3.05469700 | -1.25288500 | -1.61880000 |
| O | -3.00045200 | -0.49162500 | 0.50808300 |
| C | -4.37098800 | -0.97310800 | 0.91355300 |
| C | -4.45613900 | -0.51775000 | 2.36650600 |
| C | -4.42709800 | -2.49511800 | 0.81320800 |
| C | -5.42925100 | -0.28068600 | 0.05889900 |
| C | 2.19297700 | -2.60644800 | -0.51820600 |
| C | 3.08786600 | -2.98435100 | 0.49139800 |
| C | 4.45393800 | -2.74481400 | 0.35832100 |
| C | 4.94914700 | -2.12120500 | -0.78817000 |
| C | 4.06788600 | -1.74464500 | -1.80022500 |
| C | 2.70057300 | -1.98960100 | -1.66633600 |
| C | 1.96469200 | 1.61998000 | 1.81081400 |
| C | 3.18591000 | 1.21251800 | 1.26162700 |
| C | 4.08460900 | 2.14157400 | 0.73405200 |
| C | 3.77666100 | 3.50031500 | 0.74837100 |
| C | 2.56389100 | 3.92233300 | 1.29584100 |
| C | 1.67034200 | 2.99116000 | 1.82045300 |
| H | 0.88793500 | -0.09346900 | -0.17054900 |
| H | -0.71555500 | 1.39126000 | 1.32137800 |
| H | -1.03343200 | -0.10285000 | 2.17162500 |
| H | 0.48021300 | -2.01619000 | 1.56269900 |
| H | -1.02776300 | -2.29645700 | 0.72772700 |
| H | 0.23700500 | -2.82385000 | -1.35416500 |
| H | -1.30812800 | -0.87335300 | -2.65793000 |
| H | 0.86926800 | -4.83216000 | -0.38552000 |
| H | 0.67418400 | 0.96914700 | 3.38036000 |
| H | 1.49435800 | -0.33538600 | 2.54562800 |
| H | -3.10654800 | 1.80693800 | -0.22031800 |
| H | -3.15823100 | 4.20125500 | -0.72406200 |
| H | -1.27342700 | 5.27509300 | -1.93744900 |
| H | 0.66353400 | 3.88939500 | -2.65501600 |
| H | 0.70040400 | 1.47437100 | -2.18384300 |
| H | -4.34833800 | 0.56690100 | 2.44187000 |
| H | -5.42882200 | -0.79683800 | 2.77841900 |
| H | -3.67860200 | -0.99180600 | 2.97003600 |
| H | -4.37214900 | -2.83986000 | -0.21877200 |
| H | -5.37325500 | -2.83860700 | 1.24013900 |
| H | -3.61398500 | -2.94946600 | 1.38461400 |
| H | -5.32848400 | 0.80548200 | 0.12204600 |
| H | -5.37225200 | -0.58229200 | -0.98644200 |
| H | -6.41766900 | -0.55123300 | 0.43992800 |
| H | 2.71227000 | -3.48386300 | 1.37740200 |
| H | 5.13344600 | -3.04824200 | 1.14791500 |
| H | 6.01296600 | -1.93732700 | -0.89344800 |
| H | 4.44375300 | -1.26704600 | -2.69890000 |
| H | 2.02248500 | -1.70165500 | -2.46224500 |
| H | 3.44001500 | 0.15758600 | 1.25195400 |
| H | 5.02555100 | 1.80094600 | 0.31469100 |
| H | 4.47426400 | 4.22444400 | 0.34139500 |
| H | 2.31652300 | 4.97858600 | 1.31806400 |
| H | 0.73339600 | 3.33310100 | 2.24970500 |

SSS-conf-3

| | | | |
|---|---|---|---|
| C | 1.55329800 | -0.78941700 | -1.09975500 |
| C | 0.03778100 | -0.41698800 | -1.21769000 |
| C | -0.13533700 | 0.74420900 | -2.22805300 |
| C | -0.79977600 | -1.63710700 | -1.68226800 |
| C | -1.41446600 | -2.55657500 | -0.61492900 |
| O | 1.98555500 | -1.20622100 | -2.38827000 |
| O | -1.86870700 | -3.71136400 | -1.35492000 |
| C | -1.50135000 | 1.46708900 | -2.18503600 |
| C | 1.84882600 | -1.88595500 | -0.05115400 |
| C | 1.51390100 | -1.71949000 | 1.30003700 |
| C | 1.79628900 | -2.71675500 | 2.23058500 |

| | | | |
|---|---|---|---|
| C | 2.41833400 | -3.89947700 | 1.82975000 |
| C | 2.75811500 | -4.07121300 | 0.49049700 |
| C | 2.47984400 | -3.07024000 | -0.44127700 |
| C | 2.44234400 | 0.42665800 | -0.71666200 |
| O | 3.46808100 | 0.64990400 | -1.33401300 |
| O | 1.99620400 | 1.10693200 | 0.32136300 |
| C | 2.78265800 | 2.21979400 | 0.96875300 |
| C | 1.87499800 | 2.62484300 | 2.12491200 |
| C | 2.95675800 | 3.36785800 | -0.02136800 |
| C | 4.10980800 | 1.66568300 | 1.47935300 |
| C | -2.56402500 | -1.93957900 | 0.16541000 |
| C | -2.42665800 | -1.63414900 | 1.52244600 |
| C | -3.48931300 | -1.08595400 | 2.24336100 |
| C | -4.70850400 | -0.84298400 | 1.61437800 |
| C | -4.85946800 | -1.15287200 | 0.26103300 |
| C | -3.79666500 | -1.69636800 | -0.45592400 |
| C | -1.66151900 | 2.47449500 | -1.06558500 |
| C | -1.12963600 | 3.76569700 | -1.19417500 |
| C | -1.28203100 | 4.71152500 | -0.18191500 |
| C | -1.97209000 | 4.38342500 | 0.98604600 |
| C | -2.50723200 | 3.10428300 | 1.12787100 |
| C | -2.35361600 | 2.16130600 | 0.11014000 |
| H | -0.29672800 | -0.08420200 | -0.23201800 |
| H | 0.64918800 | 1.49436000 | -2.08740900 |
| H | 0.00910700 | 0.34155100 | -3.23460300 |
| H | -1.62137400 | -1.28533600 | -2.31199000 |
| H | -0.18055800 | -2.26917300 | -2.32361800 |
| H | -0.64618200 | -2.87125200 | 0.09486000 |
| H | 2.88148300 | -0.85250300 | -2.50961700 |
| H | -2.27904600 | -4.32011800 | -0.72802000 |
| H | -1.62420900 | 1.99177400 | -3.13790500 |
| H | -2.31055300 | 0.73369100 | -2.13082200 |
| H | 1.02747800 | -0.81115600 | 1.63024100 |
| H | 1.52765900 | -2.56881400 | 3.27113500 |
| H | 2.63630400 | -4.67595500 | 2.55491800 |
| H | 3.24382800 | -4.98471900 | 0.16415200 |
| H | 2.74852800 | -3.21116000 | -1.47959900 |
| H | 1.73115500 | 1.79274200 | 2.81823200 |
| H | 2.33062600 | 3.45349300 | 2.67206200 |
| H | 0.89915000 | 2.94936500 | 1.75678000 |
| H | 3.60146100 | 3.09375800 | -0.85558900 |
| H | 3.41188400 | 4.21387300 | 0.50081600 |
| H | 1.98828300 | 3.69133700 | -0.40963600 |
| H | 3.94281600 | 0.79895600 | 2.12371900 |
| H | 4.77452100 | 1.37967900 | 0.66459100 |
| H | 4.60719500 | 2.43819400 | 2.07180400 |
| H | -1.48522500 | -1.83613300 | 2.02223300 |
| H | -3.36524000 | -0.85796300 | 3.29675700 |
| H | -5.53746500 | -0.42214000 | 2.17317300 |
| H | -5.80801400 | -0.97338100 | -0.23418200 |
| H | -3.92644000 | -1.94939200 | -1.50244300 |
| H | -0.60163700 | 4.03599200 | -2.10380700 |
| H | -0.86906700 | 5.70704800 | -0.30757800 |
| H | -2.09631200 | 5.11954900 | 1.77302100 |
| H | -3.05206100 | 2.83936000 | 2.02806800 |
| H | -2.78721700 | 1.17421300 | 0.22629200 |

SSS-conf-4

| | | | |
|---|---|---|---|
| C | -0.70101200 | -0.84084100 | -0.95881200 |
| C | -0.09761000 | 0.26638700 | -0.00782900 |
| C | -0.73847000 | 0.33256200 | 1.39901800 |
| C | 1.44733500 | 0.22600000 | 0.14144700 |
| C | 2.31438400 | 0.70211200 | -1.03450700 |
| O | -0.32748500 | -0.55807200 | -2.30466800 |
| O | 2.32813500 | -0.34336400 | -2.03242200 |
| C | -0.65085500 | 1.72042100 | 2.07721200 |
| C | -2.24050600 | -0.80289900 | -0.96715500 |
| C | -3.05177200 | -1.78376900 | -0.38858500 |
| C | -4.44337600 | -1.68767900 | -0.44992000 |
| C | -5.04859900 | -0.60873800 | -1.08724000 |
| C | -4.24889500 | 0.37506200 | -1.66894100 |
| C | -2.86158300 | 0.27642100 | -1.61225100 |
| C | -0.17224900 | -2.26696800 | -0.62626900 |
| O | 0.29650900 | -2.99318000 | -1.47712100 |
| O | -0.28322400 | -2.57042100 | 0.66387000 |
| C | 0.14530800 | -3.89470500 | 1.23080700 |

| | | | |
|---|---|---|---|
| C | -0.19766600 | -3.74338200 | 2.70986200 |
| C | 1.64937000 | -4.07486000 | 1.03762100 |
| C | -0.67228800 | -5.01742000 | 0.59548900 |
| C | 3.72771200 | 1.03400500 | -0.58577200 |
| C | 4.06902400 | 2.35310900 | -0.27008300 |
| C | 5.34987900 | 2.66793900 | 0.18173000 |
| C | 6.30907200 | 1.66491500 | 0.31846300 |
| C | 5.97888500 | 0.34787500 | -0.00081700 |
| C | 4.69680800 | 0.03399000 | -0.44940400 |
| C | -1.48495700 | 2.80188500 | 1.42355500 |
| C | -2.87988200 | 2.81032500 | 1.56435100 |
| C | -3.65689800 | 3.79974500 | 0.96541700 |
| C | -3.05258600 | 4.80551600 | 0.20951400 |
| C | -1.66687200 | 4.81229900 | 0.06245800 |
| C | -0.89300200 | 3.81948600 | 0.66572800 |
| H | -0.35616500 | 1.19365200 | -0.53048700 |
| H | -1.79126200 | 0.04857600 | 1.34648700 |
| H | -0.25480100 | -0.39565300 | 2.05455100 |
| H | 1.70015900 | 0.87759500 | 0.98041900 |
| H | 1.78533600 | -0.77478400 | 0.43253200 |
| H | 1.86565500 | 1.60204700 | -1.46964600 |
| H | 0.65216300 | -0.57071200 | -2.35562000 |
| H | 2.79692400 | -0.01704400 | -2.81249800 |
| H | -0.98379800 | 1.59688000 | 3.11337900 |
| H | 0.38984800 | 2.05280700 | 2.12756000 |
| H | -2.61347000 | -2.63156400 | 0.12001700 |
| H | -5.05064000 | -2.46420800 | 0.00282100 |
| H | -6.12965300 | -0.53481600 | -1.13386400 |
| H | -4.70499200 | 1.22130600 | -2.17139600 |
| H | -2.25452300 | 1.04088800 | -2.08031700 |
| H | -1.26467600 | -3.54984100 | 2.84413000 |
| H | 0.05455200 | -4.66524800 | 3.23940600 |
| H | 0.36733600 | -2.92362400 | 3.15988700 |
| H | 1.91611800 | -4.18734200 | -0.01251900 |
| H | 1.96659400 | -4.97482100 | 1.57157400 |
| H | 2.19566500 | -3.22503100 | 1.45442300 |
| H | -1.74253400 | -4.83197600 | 0.71592100 |
| H | -0.45046600 | -5.13501900 | -0.46461800 |
| H | -0.43312500 | -5.95613000 | 1.10254300 |
| H | 3.32873700 | 3.13916000 | -0.38402000 |
| H | 5.60028600 | 3.69644700 | 0.41903100 |
| H | 7.30750900 | 1.90844500 | 0.66524900 |
| H | 6.72105300 | -0.43724500 | 0.09826500 |
| H | 4.44923600 | -0.98954200 | -0.70620100 |
| H | -3.36119000 | 2.03696100 | 2.15526400 |
| H | -4.73444500 | 3.78892800 | 1.09214900 |
| H | -3.65626400 | 5.57742400 | -0.25557500 |
| H | -1.18527900 | 5.59184000 | -0.51871100 |
| H | 0.18643500 | 3.83919700 | 0.55208700 |

SSS-conf-5

| | | | |
|---|---|---|---|
| C | 0.45394200 | -0.88055300 | -0.29318400 |
| C | -0.17986400 | 0.53758900 | -0.21723000 |
| C | 0.27142000 | 1.41481500 | -1.41147300 |
| C | -1.71881900 | 0.54650100 | -0.00864500 |
| C | -2.60619300 | -0.38495600 | -0.86774900 |
| O | 0.07799100 | -1.45636700 | -1.54345700 |
| O | -2.33268800 | -0.27895000 | -2.27307400 |
| C | 0.17698700 | 2.93633200 | -1.15947200 |
| C | 0.05520800 | -1.79419900 | 0.88647400 |
| C | 0.19379400 | -1.35819200 | 2.21115400 |
| C | -0.14890200 | -2.19354400 | 3.27187300 |
| C | -0.62663800 | -3.48120400 | 3.02868800 |
| C | -0.75474200 | -3.92631200 | 1.71514000 |
| C | -0.41336700 | -3.09003100 | 0.65184600 |
| C | 2.00248200 | -0.76602200 | -0.20195100 |
| O | 2.56792600 | -0.01862400 | 0.56739300 |
| O | 2.58662600 | -1.63122900 | -1.02280900 |
| C | 4.07423900 | -1.84574900 | -1.08947500 |
| C | 4.19302200 | -2.93916400 | -2.14547400 |
| C | 4.57205900 | -2.33212600 | 0.26833300 |
| C | 4.74885200 | -0.55709000 | -1.55037600 |
| C | -4.07272300 | -0.07425100 | -0.63038000 |
| C | -4.73806300 | -0.64124000 | 0.46229800 |
| C | -6.07402000 | -0.33797400 | 0.72004000 |
| C | -6.76792400 | 0.53482600 | -0.11788900 |

| | | | |
|---|---|---|---|
| C | -6.11479400 | 1.09976500 | -1.21259400 |
| C | -4.77666500 | 0.79917800 | -1.46617800 |
| C | 1.10379700 | 3.46004400 | -0.08228900 |
| C | 2.48804900 | 3.51805600 | -0.29767700 |
| C | 3.34945100 | 3.99500100 | 0.68794000 |
| C | 2.84244600 | 4.42506500 | 1.91524000 |
| C | 1.46885800 | 4.37541500 | 2.14363000 |
| C | 0.60993900 | 3.89762700 | 1.15220300 |
| H | 0.24000200 | 0.98823200 | 0.68456400 |
| H | 1.30715200 | 1.17867000 | -1.67549900 |
| H | -0.33002800 | 1.18111600 | -2.29065900 |
| H | -1.93669400 | 0.30664500 | 1.03612600 |
| H | -2.06171900 | 1.57461700 | -0.15909600 |
| H | -2.43059100 | -1.41986500 | -0.55867900 |
| H | 0.75351100 | -2.09268200 | -1.81545600 |
| H | -1.47473200 | -0.71439700 | -2.39798900 |
| H | 0.41249800 | 3.43854400 | -2.10422000 |
| H | -0.85229700 | 3.21175200 | -0.91357500 |
| H | 0.57396500 | -0.36615800 | 2.42177700 |
| H | -0.04061200 | -1.83628700 | 4.29028400 |
| H | -0.89309400 | -4.13050400 | 3.85548900 |
| H | -1.12058400 | -4.92708900 | 1.51190500 |
| H | -0.52087400 | -3.44572000 | -0.36468900 |
| H | 3.78479100 | -2.60103600 | -3.10116300 |
| H | 5.24501100 | -3.19537900 | -2.29071400 |
| H | 3.65775200 | -3.83930000 | -1.83332600 |
| H | 4.49835500 | -1.55710000 | 1.03072000 |
| H | 5.62147900 | -2.62378700 | 0.17473700 |
| H | 4.00340500 | -3.20698700 | 0.59387500 |
| H | 4.30103300 | -0.20251700 | -2.48232300 |
| H | 4.67839400 | 0.23023700 | -0.80055900 |
| H | 5.80662000 | -0.76054500 | -1.73746300 |
| H | -4.20842700 | -1.33055900 | 1.11265200 |
| H | -6.57457600 | -0.78990500 | 1.56988100 |
| H | -7.80902900 | 0.76805800 | 0.07765500 |
| H | -6.64760100 | 1.77575700 | -1.87325500 |
| H | -4.27937100 | 1.23761000 | -2.32302600 |
| H | 2.89409600 | 3.19150500 | -1.25014400 |
| H | 4.41691500 | 4.03511400 | 0.49742500 |
| H | 3.51200400 | 4.79786400 | 2.68290700 |
| H | 1.06270000 | 4.71063000 | 3.09235700 |
| H | -0.45928000 | 3.86918500 | 1.33812300 |

SSS-conf-6

| | | | |
|---|---|---|---|
| C | -1.56808500 | 0.75260800 | -1.09871500 |
| C | -0.04320100 | 0.42219800 | -1.21791300 |
| C | 0.16290000 | -0.72915400 | -2.23362600 |
| C | 0.76074700 | 1.66949100 | -1.67459200 |
| C | 1.35417900 | 2.60180300 | -0.59890700 |
| O | -2.01183000 | 1.16517100 | -2.38545400 |
| O | 1.86172400 | 3.79055300 | -1.24629100 |
| C | 1.54580900 | -1.41887300 | -2.18507500 |
| C | -1.89294800 | 1.83640600 | -0.04646600 |
| C | -1.54149900 | 1.67922700 | 1.30162400 |
| C | -1.85152500 | 2.66403500 | 2.23667200 |
| C | -2.51767400 | 3.82509000 | 1.84353800 |
| C | -2.87392800 | 3.98757900 | 0.50737500 |
| C | -2.56821600 | 2.99879200 | -0.42885000 |
| C | -2.42233300 | -0.49029300 | -0.72241800 |
| O | -3.43535300 | -0.74585300 | -1.34854400 |
| O | -1.96446800 | -1.15489400 | 0.32002000 |
| C | -2.72376300 | -2.29051100 | 0.96404500 |
| C | -1.81288600 | -2.66775100 | 2.12682900 |
| C | -2.85796500 | -3.44346500 | -0.02592800 |
| C | -4.06919200 | -1.77227100 | 1.46333500 |
| C | 2.51580400 | 2.00579000 | 0.17295300 |
| C | 3.74901100 | 1.78524800 | -0.45468700 |
| C | 4.82460500 | 1.25928700 | 0.25682000 |
| C | 4.68435800 | 0.94142400 | 1.60912400 |
| C | 3.46301900 | 1.15924500 | 2.24312500 |
| C | 2.38862500 | 1.69253800 | 1.52870100 |
| C | 1.72444100 | -2.42416000 | -1.06658400 |
| C | 2.40397100 | -2.09588800 | 0.11234300 |
| C | 2.57486300 | -3.03583100 | 1.13009300 |
| C | 2.07054600 | -4.32706300 | 0.98466100 |
| C | 1.39398700 | -4.67030500 | -0.18682300 |

| | | | |
|---|---|---|---|
| C | 1.22395700 | -3.72737600 | -1.19903300 |
| H | 0.30102400 | 0.09487700 | -0.23372500 |
| H | -0.60464700 | -1.49847100 | -2.10252200 |
| H | 0.01550700 | -0.32516300 | -3.23924100 |
| H | 1.59116600 | 1.34712900 | -2.30854500 |
| H | 0.11715100 | 2.28061600 | -2.31515100 |
| H | 0.58056200 | 2.89309400 | 0.11455700 |
| H | -2.88761900 | 0.76713000 | -2.51846600 |
| H | 1.13088600 | 4.18553200 | -1.73819100 |
| H | 1.68686400 | -1.93815400 | -3.13837400 |
| H | 2.33637400 | -0.66588100 | -2.12438500 |
| H | -1.02130600 | 0.78760900 | 1.62595800 |
| H | -1.56957500 | 2.52347500 | 3.27469600 |
| H | -2.75712500 | 4.59190700 | 2.57215800 |
| H | -3.39435100 | 4.88399700 | 0.18715700 |
| H | -2.85165000 | 3.13167300 | -1.46431100 |
| H | -1.69858900 | -1.83145500 | 2.82057600 |
| H | -2.24761700 | -3.50933600 | 2.67133300 |
| H | -0.82532400 | -2.96353300 | 1.76577200 |
| H | -3.50288100 | -3.18802100 | -0.86588600 |
| H | -3.29475100 | -4.30071400 | 0.49366000 |
| H | -1.87795400 | -3.74132100 | -0.40553600 |
| H | -3.93110100 | -0.89985200 | 2.10684600 |
| H | -4.73526800 | -1.50634300 | 0.64278800 |
| H | -4.55003300 | -2.55682400 | 2.05363500 |
| H | 3.87066600 | 2.04152500 | -1.50116000 |
| H | 5.77438900 | 1.09945300 | -0.24268400 |
| H | 5.52263600 | 0.53284600 | 2.16312500 |
| H | 3.34625100 | 0.92415100 | 3.29575800 |
| H | 1.44630800 | 1.87677200 | 2.03327700 |
| H | 2.81442000 | -1.09927400 | 0.23114500 |
| H | 3.10938600 | -2.75904400 | 2.03289700 |
| H | 2.20798100 | -5.06069400 | 1.77176600 |
| H | 1.00527300 | -5.67520800 | -0.31518300 |
| H | 0.70672200 | -4.00921800 | -2.11134100 |

SSS-conf-7

| | | | |
|---|---|---|---|
| C | 0.65030900 | -1.07824100 | -0.80499400 |
| C | -0.11373100 | -0.17192100 | 0.21175900 |
| C | 0.45777900 | 1.26130100 | 0.33837000 |
| C | -1.62559600 | -0.21400400 | -0.09316300 |
| C | -2.50544200 | 0.50474700 | 0.93804000 |
| O | 0.35950800 | -0.63715500 | -2.12516500 |
| O | -2.22396200 | -0.08035300 | 2.21902100 |
| C | 0.30062900 | 2.21519600 | -0.86547900 |
| C | 0.28483100 | -2.57450700 | -0.65810600 |
| C | -0.00457700 | -3.33171800 | -1.79734600 |
| C | -0.32204600 | -4.68621400 | -1.69428500 |
| C | -0.35420600 | -5.30788100 | -0.44876300 |
| C | -0.06313500 | -4.56249000 | 0.69349200 |
| C | 0.25663000 | -3.21039100 | 0.59085600 |
| C | 2.18819400 | -0.96740200 | -0.62772900 |
| O | 2.89862700 | -0.68125200 | -1.57494900 |
| O | 2.59133600 | -1.23475400 | 0.59827400 |
| C | 4.04381100 | -1.30468100 | 0.99306900 |
| C | 3.95625800 | -1.66697800 | 2.47152700 |
| C | 4.69544800 | 0.06149900 | 0.79978000 |
| C | 4.72531400 | -2.41095600 | 0.19275300 |
| C | -3.97799400 | 0.39506100 | 0.57117800 |
| C | -4.57926700 | 1.38172100 | -0.21739500 |
| C | -5.91681400 | 1.27443300 | -0.59580300 |
| C | -6.67447700 | 0.17839500 | -0.18344900 |
| C | -6.08509800 | -0.80639300 | 0.60908700 |
| C | -4.74600700 | -0.69943200 | 0.98251400 |
| C | 0.85830800 | 3.58979800 | -0.56623900 |
| C | 0.06245100 | 4.58229300 | 0.02025000 |
| C | 0.58696500 | 5.83849700 | 0.32302100 |
| C | 1.92284900 | 6.12629300 | 0.04402100 |
| C | 2.72712000 | 5.14843800 | -0.54095100 |
| C | 2.19777200 | 3.89395600 | -0.84219400 |
| H | 0.03161300 | -0.62872900 | 1.19218700 |
| H | -0.01967700 | 1.72395800 | 1.20827500 |
| H | 1.51952100 | 1.19755800 | 0.59642000 |
| H | -1.82913700 | 0.22107900 | -1.07393600 |
| H | -1.95402600 | -1.25714600 | -0.13841100 |
| H | -2.24364700 | 1.56823200 | 0.96426600 |

| | | | |
|---|---|---|---|
| H | 1.21108900 | -0.55599200 | -2.58573200 |
| H | -2.71999400 | 0.40999500 | 2.88654700 |
| H | 0.81303600 | 1.79926300 | -1.73401400 |
| H | -0.75655900 | 2.30516700 | -1.13097800 |
| H | 0.00892400 | -2.85595000 | -2.76876800 |
| H | -0.54600400 | -5.25234100 | -2.59222600 |
| H | -0.60314400 | -6.36033700 | -0.36676300 |
| H | -0.08430400 | -5.03320900 | 1.67060100 |
| H | 0.48568100 | -2.65780500 | 1.49274600 |
| H | 3.45297900 | -2.62705000 | 2.60795900 |
| H | 4.96294400 | -1.74252100 | 2.88904800 |
| H | 3.40884200 | -0.90095600 | 3.02620100 |
| H | 4.76331500 | 0.33625200 | -0.25224400 |
| H | 5.70789900 | 0.02705200 | 1.21108200 |
| H | 4.13940800 | 0.83474100 | 1.33556500 |
| H | 4.18129200 | -3.35271200 | 0.30031000 |
| H | 4.79921000 | -2.16238300 | -0.86580100 |
| H | 5.73644900 | -2.55562600 | 0.58224900 |
| H | -3.99738800 | 2.24236800 | -0.53324300 |
| H | -6.36872200 | 2.04949600 | -1.20580500 |
| H | -7.71653600 | 0.09521900 | -0.47279700 |
| H | -6.66860900 | -1.66002800 | 0.93779000 |
| H | -4.29426000 | -1.46325300 | 1.60500600 |
| H | -0.98071700 | 4.37126700 | 0.23554500 |
| H | -0.04911300 | 6.59405600 | 0.77251300 |
| H | 2.33169500 | 7.10383100 | 0.27612700 |
| H | 3.76636000 | 5.36342600 | -0.76722500 |
| H | 2.82984000 | 3.14067000 | -1.30286800 |

SSS-conf-8

| | | | |
|---|---|---|---|
| C | 1.26783100 | -0.74444600 | -0.77730700 |
| C | 0.24302700 | 0.34167100 | -0.33409300 |
| C | 0.19046800 | 1.50990800 | -1.36007000 |
| C | -1.16107300 | -0.22182700 | 0.01933800 |
| C | -1.82426700 | -1.23377300 | -0.94250700 |
| O | 0.88575300 | -1.24064100 | -2.05983100 |
| O | -1.84500700 | -0.77629300 | -2.30462100 |
| C | 0.22179200 | 2.91934600 | -0.72793200 |
| C | 1.42570000 | -1.91006200 | 0.22025900 |
| C | 1.47661000 | -1.69089000 | 1.60329800 |
| C | 1.65311500 | -2.75554100 | 2.48471100 |
| C | 1.79170800 | -4.05603700 | 2.00073200 |
| C | 1.75380900 | -4.28127200 | 0.62664700 |
| C | 1.57455200 | -3.21657700 | -0.25618500 |
| C | 2.68562000 | -0.13337400 | -0.96062400 |
| O | 3.30129500 | -0.31165200 | -1.99629300 |
| O | 3.10901300 | 0.52612700 | 0.09758800 |
| C | 4.50436700 | 1.08808300 | 0.21292300 |
| C | 4.48975000 | 1.69439600 | 1.61161800 |
| C | 4.71233600 | 2.16013500 | -0.85251600 |
| C | 5.51140900 | -0.05452000 | 0.11811900 |
| C | -3.24756400 | -1.52107800 | -0.50283200 |
| C | -3.50686400 | -2.56677200 | 0.38913300 |
| C | -4.80362000 | -2.81892600 | 0.83574400 |
| C | -5.86292900 | -2.02986500 | 0.38908300 |
| C | -5.61482400 | -0.98877000 | -0.50540400 |
| C | -4.31673400 | -0.73427400 | -0.94579300 |
| C | -0.99830600 | 3.29794000 | 0.08469000 |
| C | -0.95142200 | 3.35899700 | 1.48206600 |
| C | -2.08228700 | 3.69958100 | 2.22640600 |
| C | -3.28306400 | 3.99024100 | 1.58218200 |
| C | -3.34279600 | 3.94126400 | 0.18825400 |
| C | -2.21176600 | 3.59995000 | -0.54986100 |
| H | 0.63329900 | 0.75318400 | 0.59911200 |
| H | 1.04074300 | 1.44875200 | -2.04617600 |
| H | -0.69856500 | 1.41279900 | -1.98506500 |
| H | -1.11632900 | -0.70766200 | 0.99844700 |
| H | -1.83183800 | 0.63424300 | 0.13270100 |
| H | -1.26667300 | -2.17473400 | -0.90226400 |
| H | 1.67304500 | -1.19390800 | -2.62871200 |
| H | -0.92043100 | -0.82526700 | -2.59737100 |
| H | 1.11274500 | 3.00629100 | -0.09891300 |
| H | 0.33838300 | 3.64358600 | -1.54189800 |
| H | 1.37773000 | -0.68969600 | 2.00321100 |
| H | 1.68174200 | -2.56598300 | 3.55233800 |
| H | 1.92843300 | -4.88350100 | 2.68835400 |

| | | | |
|---|---|---|---|
| H | 1.86319100 | -5.28729500 | 0.23593900 |
| H | 1.54065400 | -3.40222200 | -1.32171000 |
| H | 4.28802900 | 0.92855600 | 2.36435100 |
| H | 5.46352900 | 2.14092200 | 1.82556500 |
| H | 3.72841100 | 2.47418000 | 1.69013800 |
| H | 4.73159000 | 1.73898100 | -1.85711500 |
| H | 5.66980400 | 2.65505000 | -0.66906400 |
| H | 3.92492900 | 2.91592500 | -0.79812300 |
| H | 5.27481500 | -0.83563100 | 0.84497100 |
| H | 5.53911200 | -0.49347400 | -0.87894700 |
| H | 6.50663400 | 0.33456600 | 0.34863100 |
| H | -2.68822900 | -3.19169800 | 0.73263700 |
| H | -4.98655100 | -3.63591100 | 1.52573800 |
| H | -6.87328000 | -2.22708900 | 0.73094400 |
| H | -6.43365300 | -0.37247900 | -0.86170300 |
| H | -4.13397700 | 0.07394400 | -1.64411900 |
| H | -0.01880900 | 3.14219100 | 1.99360800 |
| H | -2.02213500 | 3.74066600 | 3.30906100 |
| H | -4.16270000 | 4.25738000 | 2.15789700 |
| H | -4.27072900 | 4.17393600 | -0.32385700 |
| H | -2.26882700 | 3.57001600 | -1.63383300 |

SSS-conf-9

| | | | |
|---|---|---|---|
| C | -1.08870900 | -0.07322300 | -0.90143700 |
| C | -0.07725200 | -0.41205000 | 0.24761200 |
| C | -0.29696600 | 0.39329400 | 1.55024900 |
| C | -0.01313500 | -1.92376000 | 0.57994800 |
| C | 0.71381800 | -2.88681500 | -0.38280900 |
| O | -0.56191700 | -0.70050000 | -2.07396800 |
| O | 0.58280500 | -4.23093800 | 0.13249800 |
| C | 0.98490600 | 0.60100100 | 2.38907200 |
| C | -1.18324100 | 1.44580200 | -1.16678900 |
| C | -2.25560000 | 2.24645600 | -0.75916600 |
| C | -2.27398700 | 3.61331700 | -1.04265900 |
| C | -1.21857400 | 4.20453500 | -1.73113200 |
| C | -0.14311000 | 3.41570100 | -2.13955900 |
| C | -0.12877100 | 2.05106600 | -1.86428500 |
| C | -2.50625200 | -0.67395200 | -0.70048400 |
| O | -3.06585500 | -1.24495900 | -1.61776700 |
| O | -3.00318100 | -0.48365900 | 0.50877900 |
| C | -4.37952800 | -0.94865200 | 0.91394900 |
| C | -4.45996100 | -0.49160400 | 2.36664700 |
| C | -4.45409600 | -2.46993900 | 0.81419700 |
| C | -5.42912600 | -0.24426000 | 0.05843100 |
| C | 2.19853900 | -2.61169000 | -0.52202700 |
| C | 3.09044700 | -2.97927200 | 0.49375600 |
| C | 4.45532100 | -2.72904900 | 0.36670400 |
| C | 4.95113600 | -2.10177300 | -0.77725500 |
| C | 4.07180600 | -1.73239100 | -1.79347700 |
| C | 2.70628200 | -1.99074900 | -1.66732700 |
| C | 1.96144200 | 1.60635400 | 1.81419700 |
| C | 3.18299300 | 1.20472700 | 1.26149500 |
| C | 4.07890600 | 2.13871400 | 0.73791400 |
| C | 3.76779400 | 3.49661800 | 0.75984400 |
| C | 2.55463400 | 3.91283500 | 1.31088300 |
| C | 1.66387500 | 2.97677000 | 1.83150700 |
| H | 0.88635600 | -0.10380400 | -0.17177500 |
| H | -0.71807900 | 1.37500200 | 1.32606100 |
| H | -1.03334400 | -0.12243200 | 2.17126100 |
| H | 0.47295800 | -2.03767400 | 1.55383400 |
| H | -1.03217800 | -2.30739500 | 0.70875000 |
| H | 0.25380100 | -2.83832000 | -1.37015800 |
| H | -1.31265600 | -0.87363000 | -2.66304200 |
| H | -0.36067000 | -4.42100400 | 0.20495400 |
| H | 0.67524600 | 0.94393300 | 3.38233300 |
| H | 1.49620000 | -0.35430700 | 2.53847900 |
| H | -3.08676000 | 1.81864100 | -0.21446400 |
| H | -3.11970800 | 4.21236600 | -0.72231400 |
| H | -1.23317400 | 5.26668500 | -1.94990800 |
| H | 0.68652200 | 3.86209500 | -2.67720400 |
| H | 0.70450400 | 1.44766600 | -2.20139200 |
| H | -4.33935600 | 0.59171300 | 2.44144100 |
| H | -5.43608600 | -0.75891000 | 2.77820800 |
| H | -3.68840400 | -0.97442600 | 2.97092700 |
| H | -4.40324800 | -2.81557500 | -0.21769900 |
| H | -5.40448800 | -2.80174600 | 1.24092700 |

| | | | |
|---|---|---|---|
| H | -3.64709900 | -2.93402000 | 1.38657900 |
| H | -5.31503800 | 0.84061400 | 0.12071100 |
| H | -5.37551400 | -0.54753500 | -0.98660200 |
| H | -6.42082900 | -0.50233400 | 0.43956000 |
| H | 2.71566100 | -3.47771100 | 1.38033200 |
| H | 5.13314200 | -3.02646900 | 1.15998100 |
| H | 6.01383100 | -1.90848000 | -0.87691600 |
| H | 4.44764900 | -1.25079500 | -2.68997200 |
| H | 2.03009400 | -1.70989000 | -2.46720400 |
| H | 3.43954900 | 0.15048800 | 1.24581500 |
| H | 5.02016000 | 1.80253700 | 0.31566800 |
| H | 4.46324100 | 4.22452800 | 0.35593600 |
| H | 2.30479200 | 4.96836600 | 1.33898700 |
| H | 0.72658200 | 3.31420200 | 2.26356900 |

SSS-conf-10

| | | | |
|---|---|---|---|
| C | -0.21353800 | 1.13686300 | -0.88889300 |
| C | -0.01062100 | -0.36569700 | -0.50877300 |
| C | -0.59563000 | -1.27721100 | -1.60943600 |
| C | 1.44379900 | -0.69626100 | -0.08421200 |
| C | 2.58917700 | -0.56271800 | -1.10224500 |
| O | 0.41973300 | 1.38815800 | -2.13724500 |
| O | 2.44062000 | -1.60443500 | -2.08206700 |
| C | -0.63115600 | -2.78685900 | -1.28147000 |
| C | 0.29653100 | 2.12846600 | 0.18036300 |
| C | 0.99500300 | 3.27345700 | -0.21388800 |
| C | 1.43916400 | 4.19976100 | 0.73044900 |
| C | 1.18828400 | 3.99732000 | 2.08515700 |
| C | 0.48516800 | 2.86180700 | 2.48774400 |
| C | 0.03895400 | 1.93843800 | 1.54502400 |
| C | -1.71902500 | 1.47455900 | -1.09207000 |
| O | -2.08895500 | 2.03658600 | -2.10746800 |
| O | -2.47605600 | 1.13568600 | -0.06816000 |
| C | -3.93444500 | 1.50372700 | 0.03285900 |
| C | -4.31396800 | 0.93650300 | 1.39620900 |
| C | -4.71320900 | 0.81872600 | -1.08612300 |
| C | -4.06867600 | 3.02375100 | 0.01246700 |
| C | 3.94014100 | -0.65027500 | -0.40323600 |
| C | 4.57694800 | 0.51520600 | 0.03754800 |
| C | 5.79696100 | 0.45133500 | 0.70887000 |
| C | 6.40192200 | -0.78324400 | 0.94508800 |
| C | 5.77820400 | -1.94981900 | 0.50379600 |
| C | 4.55610000 | -1.88354300 | -0.16486100 |
| C | -1.54499600 | -3.17037300 | -0.13669100 |
| C | -1.03777900 | -3.46427300 | 1.13505800 |
| C | -1.88672400 | -3.81148800 | 2.18691800 |
| C | -3.26418900 | -3.87555300 | 1.98404800 |
| C | -3.78453500 | -3.59233000 | 0.72034100 |
| C | -2.93228800 | -3.24388000 | -0.32622900 |
| H | -0.60812100 | -0.52537900 | 0.39321900 |
| H | -1.62185700 | -0.95838400 | -1.82507300 |
| H | -0.03029100 | -1.14362500 | -2.53213300 |
| H | 1.69814300 | -0.06017000 | 0.76606500 |
| H | 1.46579000 | -1.72155700 | 0.29830200 |
| H | 2.52585500 | 0.40840600 | -1.59873300 |
| H | -0.22241700 | 1.87393200 | -2.68140700 |
| H | 3.12188500 | -1.47787100 | -2.75438200 |
| H | -0.96674600 | -3.30479500 | -2.18628100 |
| H | 0.37940900 | -3.14608900 | -1.07745700 |
| H | 1.19823600 | 3.43602300 | -1.26413800 |
| H | 1.98178400 | 5.07988400 | 0.40210900 |
| H | 1.53535600 | 4.71506400 | 2.82044200 |
| H | 0.28243600 | 2.69180300 | 3.53975000 |
| H | -0.50783500 | 1.06677700 | 1.88173200 |
| H | -3.72387400 | 1.40281600 | 2.18878500 |
| H | -5.37077500 | 1.13260200 | 1.59171500 |
| H | -4.15159800 | -0.14344200 | 1.42590100 |
| H | -4.44523300 | 1.20910800 | -2.06734300 |
| H | -5.78097900 | 0.99181700 | -0.92687000 |
| H | -4.53903000 | -0.25973200 | -1.07129900 |
| H | -3.42992700 | 3.47513600 | 0.77584700 |
| H | -3.81168700 | 3.44421000 | -0.95947800 |
| H | -5.10546200 | 3.28797600 | 0.23679500 |
| H | 4.11526300 | 1.47978800 | -0.15023400 |
| H | 6.27850800 | 1.36517500 | 1.04076700 |
| H | 7.35336700 | -0.83492700 | 1.46338000 |

| | | | |
|---|---|---|---|
| H | 6.24415900 | -2.91403200 | 0.67857900 |
| H | 4.08235600 | -2.79324300 | -0.51541500 |
| H | 0.03410000 | -3.42902200 | 1.30185100 |
| H | -1.46990500 | -4.03694500 | 3.16306200 |
| H | -3.92543600 | -4.14974900 | 2.79897800 |
| H | -4.85424300 | -3.65006800 | 0.54779200 |
| H | -3.34743400 | -3.03781700 | -1.30817200 |

SSR-conf-1

| | | | |
|---|---|---|---|
| C | -0.22025900 | 1.24301600 | -0.54419600 |
| C | 0.34805600 | 0.00368700 | 0.21956900 |
| C | 0.71968000 | -1.11971700 | -0.77260000 |
| C | 1.45816700 | 0.36452600 | 1.23615900 |
| C | 2.73654700 | 1.09273000 | 0.78384100 |
| O | 0.74068500 | 1.67960400 | -1.49639000 |
| O | 3.34309300 | 1.52492400 | 2.02641000 |
| C | 1.01233700 | -2.49849600 | -0.13718400 |
| C | -0.63022600 | 2.41160400 | 0.37921300 |
| C | -0.29250400 | 3.72228800 | 0.02983600 |
| C | -0.67761300 | 4.79703500 | 0.83193200 |
| C | -1.41040400 | 4.57810200 | 1.99545100 |
| C | -1.75785900 | 3.27421600 | 2.34932700 |
| C | -1.37543900 | 2.20105300 | 1.54784000 |
| C | -1.49516200 | 0.87398300 | -1.35666900 |
| O | -1.57077900 | 1.15830200 | -2.53881800 |
| O | -2.43183300 | 0.29546500 | -0.63328200 |
| C | -3.81245300 | 0.00002000 | -1.16356500 |
| C | -4.50158500 | -0.60291000 | 0.05536900 |
| C | -3.71797000 | -1.01241700 | -2.30099500 |
| C | -4.47697400 | 1.30895700 | -1.58066400 |
| C | 3.73638200 | 0.27086200 | -0.01511000 |
| C | 4.39808300 | -0.81448100 | 0.57455300 |
| C | 5.33702700 | -1.55100800 | -0.14350900 |
| C | 5.63505300 | -1.21082700 | -1.46438400 |
| C | 4.99338700 | -0.12457200 | -2.05598200 |
| C | 4.05453100 | 0.61277200 | -1.33300200 |
| C | -0.17915900 | -3.16932100 | 0.51308300 |
| C | -0.38057100 | -3.11911200 | 1.89820600 |
| C | -1.48323100 | -3.73786200 | 2.48869800 |
| C | -2.40625300 | -4.42499000 | 1.70182500 |
| C | -2.21608500 | -4.48907800 | 0.32078500 |
| C | -1.11424300 | -3.86703900 | -0.26422100 |
| H | -0.47775000 | -0.37012000 | 0.83085300 |
| H | -0.09807700 | -1.24973500 | -1.49057400 |
| H | 1.59073100 | -0.82293100 | -1.35850900 |
| H | 1.01789100 | 1.01201600 | 1.99821900 |
| H | 1.75586200 | -0.54891000 | 1.75864000 |
| H | 2.46810300 | 1.97491400 | 0.19907000 |
| H | 0.26694800 | 1.78973500 | -2.33782100 |
| H | 4.15001400 | 2.00672700 | 1.80569200 |
| H | 1.38680000 | -3.14822200 | -0.93490100 |
| H | 1.82064300 | -2.40955600 | 0.59221200 |
| H | 0.28001700 | 3.90048000 | -0.87082000 |
| H | -0.40186000 | 5.80567800 | 0.54299200 |
| H | -1.70874800 | 5.41247000 | 2.62085400 |
| H | -2.32831600 | 3.08921300 | 3.25326100 |
| H | -1.66129100 | 1.19867900 | 1.84056300 |
| H | -4.52900300 | 0.11314600 | 0.88017900 |
| H | -5.52865900 | -0.87171500 | -0.20239500 |
| H | -3.98184000 | -1.50411800 | 0.38870000 |
| H | -3.17092500 | -1.90160900 | -1.97895300 |
| H | -3.23024700 | -0.59349200 | -3.18052000 |
| H | -4.72909100 | -1.31937600 | -2.58191800 |
| H | -5.52379200 | 1.10925400 | -1.82429500 |
| H | -4.45048600 | 2.03085500 | -0.76051900 |
| H | -4.00028600 | 1.74852700 | -2.45654400 |
| H | 4.18422400 | -1.07558500 | 1.60521900 |
| H | 5.83934200 | -2.38940000 | 0.32760700 |
| H | 6.36693000 | -1.78397900 | -2.02338300 |
| H | 5.22640000 | 0.15443800 | -3.07820800 |
| H | 3.56119600 | 1.45941700 | -1.79798300 |
| H | 0.33815800 | -2.59857500 | 2.52307700 |
| H | -1.61671300 | -3.68778800 | 3.56436200 |
| H | -3.26080000 | -4.91162000 | 2.15949200 |
| H | -2.92243800 | -5.03011500 | -0.30026600 |
| H | -0.96979900 | -3.93321100 | -1.33838800 |

SSR-conf-2

| | | | |
|---|---|---|---|
| C | -0.54971900 | -0.98961000 | -1.13021700 |
| C | -0.09645800 | 0.36640200 | -0.49993900 |
| C | 1.40825000 | 0.41842500 | -0.13149900 |
| C | -0.55152700 | 1.53160600 | -1.39931100 |
| C | -0.40679000 | 2.93325300 | -0.78882500 |
| O | -0.02216700 | -1.08363800 | -2.44705500 |
| O | -0.75604900 | 3.83818500 | -1.85504800 |
| C | 2.43807300 | 0.44424700 | -1.28167100 |
| C | -2.08865900 | -1.14446600 | -1.16968100 |
| C | -2.70786200 | -1.60087400 | -2.33738400 |
| C | -4.09178900 | -1.76637500 | -2.39506400 |
| C | -4.88112600 | -1.47920600 | -1.28441300 |
| C | -4.27295500 | -1.02724700 | -0.11364800 |
| C | -2.89044300 | -0.86471700 | -0.05454200 |
| C | 0.00507100 | -2.20404400 | -0.33894200 |
| O | 0.63612700 | -3.07569400 | -0.90943100 |
| O | -0.30558900 | -2.17513900 | 0.94175300 |
| C | 0.02189700 | -3.29402500 | 1.89681900 |
| C | -0.56848900 | -2.78011800 | 3.20530500 |
| C | 1.53578400 | -3.45362700 | 2.00179700 |
| C | -0.68266800 | -4.56649400 | 1.43511500 |
| C | -1.28180900 | 3.16057300 | 0.43310200 |
| C | -2.66804200 | 3.31096200 | 0.29781700 |
| C | -3.47299000 | 3.51024300 | 1.41677600 |
| C | -2.90466900 | 3.56143300 | 2.69103700 |
| C | -1.52613000 | 3.41916100 | 2.83585100 |
| C | -0.72122000 | 3.22441800 | 1.71226800 |
| C | 3.85415200 | 0.56153100 | -0.76113100 |
| C | 4.44426900 | 1.81349200 | -0.54511400 |
| C | 5.73939200 | 1.91978200 | -0.03882300 |
| C | 6.47066500 | 0.77098900 | 0.26252000 |
| C | 5.89642900 | -0.48248600 | 0.05165400 |
| C | 4.60128500 | -0.58349600 | -0.45527100 |
| H | -0.62976700 | 0.44733700 | 0.45030300 |
| H | 1.56195000 | 1.31160600 | 0.48156100 |
| H | 1.64191900 | -0.42419400 | 0.52655700 |
| H | 0.01271700 | 1.52718100 | -2.33491400 |
| H | -1.60402300 | 1.39805300 | -1.66639300 |
| H | 0.63595200 | 3.10795900 | -0.50359100 |
| H | 0.38871500 | -1.96067200 | -2.52118300 |
| H | -0.65598600 | 4.73892800 | -1.52212000 |
| H | 2.34737200 | -0.46447200 | -1.87830700 |
| H | 2.22940600 | 1.28654900 | -1.94728300 |
| H | -2.10414700 | -1.81826300 | -3.20831900 |
| H | -4.54994000 | -2.11943100 | -3.31285900 |
| H | -5.95744000 | -1.60539300 | -1.32857500 |
| H | -4.87476700 | -0.79865600 | 0.75942200 |
| H | -2.44436000 | -0.51949000 | 0.86896700 |
| H | -1.64636700 | -2.62768500 | 3.11252800 |
| H | -0.39014300 | -3.51015300 | 3.99817400 |
| H | -0.10328700 | -1.83474200 | 3.49507100 |
| H | 2.00709000 | -2.50547200 | 2.27197200 |
| H | 1.97341700 | -3.81658100 | 1.07249400 |
| H | 1.75675900 | -4.17748800 | 2.79087300 |
| H | -0.56568100 | -5.33307600 | 2.20565900 |
| H | -1.75127300 | -4.38415200 | 1.29615400 |
| H | -0.26391100 | -4.95007900 | 0.50492100 |
| H | -3.11403800 | 3.28401400 | -0.69014800 |
| H | -4.54471300 | 3.62760700 | 1.29544900 |
| H | -3.53197400 | 3.71772300 | 3.56201000 |
| H | -1.07447000 | 3.46742600 | 3.82104800 |
| H | 0.35343900 | 3.12833500 | 1.83038800 |
| H | 3.88583500 | 2.71394900 | -0.78311900 |
| H | 6.17913200 | 2.89973500 | 0.11548400 |
| H | 7.47936200 | 0.85171200 | 0.65317200 |
| H | 6.45865200 | -1.38269700 | 0.27750300 |
| H | 4.16444500 | -1.56352300 | -0.62216600 |

SSR-conf-3

| | | | |
|---|---|---|---|
| C | -0.19837400 | 1.23976200 | -0.54190900 |
| C | 0.35146500 | -0.00443700 | 0.22701000 |
| C | 0.71239100 | -1.13585100 | -0.75970400 |
| C | 1.46692700 | 0.34804700 | 1.24349500 |
| C | 2.75658000 | 1.06829200 | 0.79326000 |

| | | | |
|---|---|---|---|
| O | 0.77337300 | 1.66196200 | -1.48933100 |
| O | 3.47447300 | 1.48138100 | 1.98271600 |
| C | 0.98164300 | -2.51652300 | -0.11807500 |
| C | -0.59704300 | 2.41463000 | 0.37867500 |
| C | -0.22902300 | 3.71913900 | 0.03690600 |
| C | -0.60134100 | 4.79928000 | 0.83793400 |
| C | -1.35126900 | 4.59199300 | 1.99264800 |
| C | -1.72903300 | 3.29441500 | 2.33878300 |
| C | -1.35935900 | 2.21594800 | 1.53839200 |
| C | -1.47362600 | 0.88660500 | -1.36072200 |
| O | -1.54037200 | 1.17393600 | -2.54260000 |
| O | -2.42034200 | 0.31731800 | -0.64299000 |
| C | -3.80086500 | 0.03703100 | -1.18162500 |
| C | -4.50303500 | -0.56156900 | 0.03199600 |
| C | -3.71011900 | -0.97385500 | -2.32078300 |
| C | -4.44979100 | 1.35344500 | -1.59973800 |
| C | 3.74074500 | 0.24038000 | -0.01213900 |
| C | 4.37857400 | -0.86587600 | 0.56318100 |
| C | 5.30309200 | -1.61193800 | -0.16446400 |
| C | 5.60607900 | -1.26259400 | -1.48134600 |
| C | 4.98506300 | -0.15709600 | -2.05940600 |
| C | 4.06377800 | 0.59152600 | -1.32590400 |
| C | -0.22320400 | -3.16874100 | 0.52648700 |
| C | -0.43319800 | -3.11081300 | 1.91004200 |
| C | -1.54784500 | -3.71281300 | 2.49534500 |
| C | -2.47459000 | -4.39058900 | 1.70475900 |
| C | -2.27605000 | -4.46226300 | 0.32527100 |
| C | -1.16224200 | -3.85691900 | -0.25455900 |
| H | -0.47996300 | -0.36565400 | 0.83823300 |
| H | -0.10295600 | -1.25647000 | -1.48205400 |
| H | 1.59112700 | -0.85336200 | -1.34115000 |
| H | 1.02143400 | 0.99574000 | 2.00461500 |
| H | 1.75779800 | -0.56608700 | 1.76830200 |
| H | 2.49859600 | 1.95681200 | 0.21418400 |
| H | 0.30512900 | 1.78265800 | -2.33237400 |
| H | 2.88127500 | 2.04416700 | 2.49619300 |
| H | 1.35232200 | -3.17393000 | -0.91123400 |
| H | 1.78636400 | -2.43640600 | 0.61628000 |
| H | 0.35669100 | 3.88814400 | -0.85696200 |
| H | -0.30244800 | 5.80296400 | 0.55482700 |
| H | -1.63992800 | 5.43055600 | 2.61698300 |
| H | -2.31350100 | 3.11862300 | 3.23557000 |
| H | -1.66834900 | 1.21859800 | 1.82476500 |
| H | -4.52878500 | 0.15318100 | 0.85800300 |
| H | -5.53101700 | -0.82013700 | -0.23249100 |
| H | -3.99388200 | -1.46829600 | 0.36670500 |
| H | -3.17390100 | -1.86922900 | -1.99765300 |
| H | -3.21322700 | -0.55782400 | -3.19653300 |
| H | -4.72266300 | -1.27003100 | -2.60804900 |
| H | -5.49714700 | 1.16477600 | -1.84976800 |
| H | -4.42076900 | 2.07339400 | -0.77795900 |
| H | -3.96364500 | 1.78991000 | -2.47195200 |
| H | 4.15808800 | -1.13855800 | 1.58927400 |
| H | 5.78900200 | -2.46552800 | 0.29638800 |
| H | 6.32497800 | -1.84416700 | -2.04845400 |
| H | 5.22123000 | 0.12849900 | -3.07905100 |
| H | 3.58789700 | 1.45366700 | -1.78002100 |
| H | 0.28828600 | -2.59769400 | 2.53788400 |
| H | -1.68778700 | -3.65719100 | 3.56992000 |
| H | -3.33846300 | -4.86434600 | 2.15840500 |
| H | -2.98532700 | -4.99620700 | -0.29857500 |
| H | -1.01147200 | -3.92903400 | -1.32746700 |

SSR-conf-4

| | | | |
|---|---|---|---|
| C | -1.51031100 | 0.40325500 | -1.27229600 |
| C | 0.01852700 | 0.05352400 | -1.29098500 |
| C | 0.30736300 | -1.21964600 | -2.12923900 |
| C | 0.78866600 | 1.25757200 | -1.88212200 |
| C | 2.28827500 | 1.29012400 | -1.55267400 |
| O | -1.90312400 | 0.67119500 | -2.61274300 |
| O | 2.87552400 | 2.16890800 | -2.53443300 |
| C | 0.35895100 | -2.57241100 | -1.38533600 |
| C | -1.84963600 | 1.61613200 | -0.37910900 |
| C | -2.76935600 | 2.56793400 | -0.83020300 |
| C | -3.11825500 | 3.65846600 | -0.03333000 |
| C | -2.55368300 | 3.81438900 | 1.23007600 |

| | | | |
|---|---|---|---|
| C | -1.63870700 | 2.86784200 | 1.69067000 |
| C | -1.29214400 | 1.77696100 | 0.89625200 |
| C | -2.40425500 | -0.77032400 | -0.78165400 |
| O | -3.24087900 | -1.25186900 | -1.52486800 |
| O | -2.19066800 | -1.11526400 | 0.47296700 |
| C | -3.11874000 | -2.02784000 | 1.23946400 |
| C | -2.50621300 | -2.01079400 | 2.63526900 |
| C | -3.08931300 | -3.43060200 | 0.64034700 |
| C | -4.51711500 | -1.41565500 | 1.24784500 |
| C | 2.59380900 | 1.77290700 | -0.14394600 |
| C | 2.42783000 | 3.12226500 | 0.19559200 |
| C | 2.70469400 | 3.56930400 | 1.48482000 |
| C | 3.15171900 | 2.67314900 | 2.45824100 |
| C | 3.32578100 | 1.33071300 | 2.12897000 |
| C | 3.05257800 | 0.88637100 | 0.83385400 |
| C | 1.57749600 | -2.77483200 | -0.50832600 |
| C | 2.83900800 | -2.99191900 | -1.08187500 |
| C | 3.96463700 | -3.19871600 | -0.28719500 |
| C | 3.85204200 | -3.19451000 | 1.10434700 |
| C | 2.60550500 | -2.97993300 | 1.68891500 |
| C | 1.48132000 | -2.77076600 | 0.88787400 |
| H | 0.33811700 | -0.10729000 | -0.25883900 |
| H | -0.44441600 | -1.28600400 | -2.92113600 |
| H | 1.26178800 | -1.08815600 | -2.64616400 |
| H | 0.69944600 | 1.22755000 | -2.97186500 |
| H | 0.34815500 | 2.20222300 | -1.55460500 |
| H | 2.71391600 | 0.28767800 | -1.67330300 |
| H | -2.64328800 | 0.07361300 | -2.81004300 |
| H | 3.82089000 | 2.22959200 | -2.34707300 |
| H | -0.53978200 | -2.71709600 | -0.78461600 |
| H | 0.34879300 | -3.35921400 | -2.14789800 |
| H | -3.20700000 | 2.45831600 | -1.81356300 |
| H | -3.83213100 | 4.38573700 | -0.40529900 |
| H | -2.82159100 | 4.66320800 | 1.84983900 |
| H | -1.18982500 | 2.97745400 | 2.67199100 |
| H | -0.58402700 | 1.05412900 | 1.28011900 |
| H | -2.48914900 | -0.99614400 | 3.03992700 |
| H | -3.10249200 | -2.63861300 | 3.30154000 |
| H | -1.48568600 | -2.40011700 | 2.61779000 |
| H | -2.07061800 | -3.82360600 | 0.61792700 |
| H | -3.50183500 | -3.45175300 | -0.36771000 |
| H | -3.69121800 | -4.09024300 | 1.27150600 |
| H | -5.14862500 | -1.99403400 | 1.92720000 |
| H | -4.48284500 | -0.38498900 | 1.60957900 |
| H | -4.97674400 | -1.43082700 | 0.25982600 |
| H | 2.09073700 | 3.82485600 | -0.55851500 |
| H | 2.57283500 | 4.61749700 | 1.73173700 |
| H | 3.36781100 | 3.02191200 | 3.46237500 |
| H | 3.68203100 | 0.62842000 | 2.87514700 |
| H | 3.20382600 | -0.15727300 | 0.58026000 |
| H | 2.93763300 | -3.01060500 | -2.16310900 |
| H | 4.92920400 | -3.37122000 | -0.75342600 |
| H | 4.72652600 | -3.36139700 | 1.72402900 |
| H | 2.50443900 | -2.97734000 | 2.76925700 |
| H | 0.51544700 | -2.60778000 | 1.35425300 |

SSR-conf-5

| | | | |
|---|---|---|---|
| C | -0.18831600 | -1.49163800 | -0.90919400 |
| C | 0.04452200 | 0.05880900 | -0.91707600 |
| C | -1.04525700 | 0.87843900 | -0.18809700 |
| C | 1.44366700 | 0.50350400 | -0.42474600 |
| C | 2.68618000 | -0.09760100 | -1.12077400 |
| O | 0.66162600 | -2.01886600 | -1.94166600 |
| O | 2.55328300 | -0.06273200 | -2.54883300 |
| C | -1.21102900 | 2.30340200 | -0.75809400 |
| C | -1.64063600 | -1.86558100 | -1.27173000 |
| C | -2.04190300 | -1.68048200 | -2.60276700 |
| C | -3.33550900 | -1.99315900 | -3.00944900 |
| C | -4.25506500 | -2.50768200 | -2.09480800 |
| C | -3.86483400 | -2.70348100 | -0.77358600 |
| C | -2.56932800 | -2.38198900 | -0.36332800 |
| C | 0.25456800 | -2.17783600 | 0.40628500 |
| O | 0.97994800 | -3.15495200 | 0.37897700 |
| O | -0.23311100 | -1.60250700 | 1.48892100 |
| C | 0.02541400 | -2.11992500 | 2.88370200 |
| C | -0.75340800 | -1.13053800 | 3.74346000 |

| | | | |
|---|---|---|---|
| C | 1.52016300 | -2.05022600 | 3.18280800 |
| C | -0.54249900 | -3.53010400 | 3.01643400 |
| C | 3.93696800 | 0.66211100 | -0.72346800 |
| C | 4.35962300 | 1.78739500 | -1.44006100 |
| C | 5.49170300 | 2.49729300 | -1.04246300 |
| C | 6.21499900 | 2.09634600 | 0.08087100 |
| C | 5.80140500 | 0.97593400 | 0.80046000 |
| C | 4.67271900 | 0.26309800 | 0.39704000 |
| C | -2.28664100 | 3.08811000 | -0.03995600 |
| C | -3.62031300 | 3.03426700 | -0.46502100 |
| C | -4.61930600 | 3.73092500 | 0.21418000 |
| C | -4.30116800 | 4.49668100 | 1.33562300 |
| C | -2.97721500 | 4.56027800 | 1.76971300 |
| C | -1.98161700 | 3.86228700 | 1.08687600 |
| H | -0.02561200 | 0.30808200 | -1.98178700 |
| H | -2.01009200 | 0.37379800 | -0.26853200 |
| H | -0.81461200 | 0.94054100 | 0.87899600 |
| H | 1.49251600 | 1.58897700 | -0.55273300 |
| H | 1.53309700 | 0.31628700 | 0.65040000 |
| H | 2.80917800 | -1.13747800 | -0.80454100 |
| H | 0.99066700 | -2.87712200 | -1.62783100 |
| H | 1.89678000 | -0.75058200 | -2.74434100 |
| H | -0.26543900 | 2.84860000 | -0.69035100 |
| H | -1.46338300 | 2.22904600 | -1.82102600 |
| H | -1.33325800 | -1.29899300 | -3.32740100 |
| H | -3.62388900 | -1.83886800 | -4.04375700 |
| H | -5.26215100 | -2.75599100 | -2.41152600 |
| H | -4.56647000 | -3.10816300 | -0.05211200 |
| H | -2.30067600 | -2.53548300 | 0.67317400 |
| H | -1.81329700 | -1.13449200 | 3.47855800 |
| H | -0.65972300 | -1.41152700 | 4.79508100 |
| H | -0.36401900 | -0.11700500 | 3.62248500 |
| H | 1.90202900 | -1.04092800 | 3.01130700 |
| H | 2.09129700 | -2.75477100 | 2.57908900 |
| H | 1.67669700 | -2.29567200 | 4.23666000 |
| H | -0.44585200 | -3.84799100 | 4.05800600 |
| H | -1.60322400 | -3.54712100 | 2.75512500 |
| H | -0.01024200 | -4.24573800 | 2.39047900 |
| H | 3.80640000 | 2.10132500 | -2.31747800 |
| H | 5.80955400 | 3.36456500 | -1.61172600 |
| H | 7.09594900 | 2.64906000 | 0.38908500 |
| H | 6.36163300 | 0.65078000 | 1.67077800 |
| H | 4.36462800 | -0.61655800 | 0.95369900 |
| H | -3.87689900 | 2.44419900 | -1.33974800 |
| H | -5.64534200 | 3.67884700 | -0.13500200 |
| H | -5.07652200 | 5.04139800 | 1.86354500 |
| H | -2.71820100 | 5.15719400 | 2.63807000 |
| H | -0.95280200 | 3.92244600 | 1.42916500 |

SSR-conf-6

| | | | |
|---|---|---|---|
| C | 0.64892000 | 1.32684500 | -1.30729600 |
| C | -0.12692400 | -0.03063000 | -1.27363700 |
| C | -1.47631900 | 0.14140900 | -2.01211600 |
| C | 0.74787000 | -1.14136000 | -1.91074200 |
| C | 0.64401400 | -2.53525900 | -1.26719800 |
| O | 0.95517800 | 1.60656000 | -2.66725800 |
| O | 1.14830000 | -3.44683700 | -2.26490500 |
| C | -2.42305500 | -1.07296500 | -2.07182800 |
| C | 1.94028400 | 1.32762300 | -0.45968200 |
| C | 3.13437600 | 1.79558000 | -1.01722700 |
| C | 4.30528300 | 1.84350200 | -0.26060100 |
| C | 4.29975500 | 1.42951900 | 1.06895900 |
| C | 3.11301300 | 0.96402000 | 1.63488800 |
| C | 1.94387000 | 0.91298600 | 0.87874300 |
| C | -0.20623500 | 2.51683000 | -0.79298400 |
| O | -0.31910800 | 3.52640700 | -1.46478900 |
| O | -0.72217000 | 2.31484500 | 0.40421500 |
| C | -1.45613900 | 3.38653600 | 1.17059000 |
| C | -1.77381300 | 2.68233800 | 2.48502400 |
| C | -2.73204600 | 3.76446200 | 0.42399500 |
| C | -0.52212000 | 4.57241100 | 1.39599300 |
| C | 1.41236800 | -2.68235800 | 0.03633900 |
| C | 2.80864300 | -2.79607400 | 0.03052600 |
| C | 3.51417800 | -2.94252000 | 1.22188900 |
| C | 2.83465900 | -2.97681100 | 2.44124200 |
| C | 1.44566200 | -2.86874200 | 2.45776900 |

| | | | |
|---|---|---|---|
| C | 0.74041900 | -2.72662200 | 1.26149200 |
| C | -3.07745700 | -1.49992100 | -0.77011200 |
| C | -3.12630400 | -2.85185000 | -0.40687700 |
| C | -3.77191500 | -3.26630400 | 0.75887900 |
| C | -4.38421600 | -2.33066900 | 1.59038100 |
| C | -4.34999900 | -0.98068200 | 1.23990600 |
| C | -3.70544100 | -0.57231400 | 0.07302800 |
| H | -0.31864900 | -0.26804000 | -0.22468400 |
| H | -2.02542600 | 0.97961300 | -1.57294000 |
| H | -1.25387300 | 0.43340800 | -3.04236900 |
| H | 0.46474600 | -1.25852400 | -2.96086900 |
| H | 1.80156100 | -0.85175600 | -1.90803200 |
| H | -0.40428200 | -2.77188000 | -1.06896200 |
| H | 0.75142000 | 2.54488000 | -2.81223000 |
| H | 1.12748700 | -4.33654700 | -1.89011900 |
| H | -3.22172300 | -0.81099100 | -2.77729200 |
| H | -1.91262400 | -1.93188500 | -2.51532200 |
| H | 3.14756900 | 2.11908200 | -2.04955800 |
| H | 5.22079000 | 2.20749000 | -0.71483500 |
| H | 5.20901400 | 1.46787600 | 1.65901500 |
| H | 3.09503000 | 0.63661100 | 2.66858000 |
| H | 1.03522400 | 0.55093000 | 1.34106300 |
| H | -0.85647100 | 2.39120400 | 3.00218400 |
| H | -2.33553300 | 3.35816900 | 3.13413900 |
| H | -2.37748500 | 1.78859200 | 2.31142600 |
| H | -3.34616000 | 2.88018500 | 0.23699900 |
| H | -2.51791400 | 4.25567000 | -0.52462000 |
| H | -3.31124400 | 4.45357100 | 1.04466200 |
| H | -1.00464300 | 5.27324000 | 2.08242000 |
| H | 0.41483200 | 4.24193800 | 1.85135700 |
| H | -0.29953800 | 5.10078400 | 0.46942400 |
| H | 3.34073500 | -2.78223100 | -0.91423800 |
| H | 4.59524900 | -3.03115400 | 1.20047700 |
| H | 3.38471100 | -3.09324500 | 3.36887900 |
| H | 0.90795600 | -2.90438400 | 3.39939900 |
| H | -0.34241200 | -2.66098500 | 1.28077400 |
| H | -2.65948300 | -3.59176000 | -1.04929300 |
| H | -3.79487500 | -4.32038100 | 1.01534300 |
| H | -4.88615900 | -2.64864700 | 2.49783300 |
| H | -4.83167500 | -0.24325900 | 1.87362700 |
| H | -3.70173700 | 0.48075300 | -0.18638100 |

SSR-conf-7

| | | | |
|---|---|---|---|
| C | 0.10072500 | -0.98783300 | -0.71031100 |
| C | -0.06047600 | 0.15363700 | 0.34717400 |
| C | 1.16844800 | 1.09536200 | 0.44255300 |
| C | -1.35101900 | 0.98207500 | 0.13777400 |
| C | -2.65946400 | 0.37329700 | 0.66275900 |
| O | -0.04221600 | -0.42738800 | -2.00850200 |
| O | -2.47603100 | 0.12742200 | 2.06565300 |
| C | 1.48192100 | 1.99448800 | -0.77292300 |
| C | -0.90259300 | -2.15292100 | -0.52540800 |
| C | -1.61165600 | -2.63509400 | -1.62992900 |
| C | -2.50999100 | -3.69405000 | -1.49638500 |
| C | -2.71004500 | -4.29369100 | -0.25560600 |
| C | -1.99880400 | -3.82759400 | 0.85006600 |
| C | -1.10153400 | -2.77030700 | 0.71724700 |
| C | 1.51654200 | -1.62700700 | -0.65815100 |
| O | 2.19096500 | -1.71098200 | -1.66892500 |
| O | 1.84754900 | -2.06766100 | 0.53938500 |
| C | 3.11695000 | -2.83196400 | 0.81593600 |
| C | 3.00605800 | -3.10647000 | 2.31167200 |
| C | 4.32643200 | -1.95399700 | 0.50761200 |
| C | 3.10023700 | -4.12983100 | 0.01368000 |
| C | -3.83314200 | 1.30486900 | 0.39617000 |
| C | -4.18038300 | 2.31338700 | 1.30115800 |
| C | -5.23613600 | 3.18169000 | 1.02511000 |
| C | -5.95820300 | 3.05517600 | -0.16132900 |
| C | -5.62056200 | 2.05065500 | -1.06837900 |
| C | -4.56735100 | 1.18126200 | -0.78855600 |
| C | 2.63686000 | 2.93132100 | -0.49260700 |
| C | 2.42855600 | 4.16376000 | 0.14049700 |
| C | 3.49607100 | 5.01352400 | 0.42737400 |
| C | 4.79729300 | 4.64502400 | 0.08500200 |
| C | 5.01968600 | 3.42211600 | -0.54713100 |
| C | 3.94832200 | 2.57568900 | -0.83230200 |

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|---|---|---|---|
| H | -0.12843600 | -0.32890800 | 1.32352800 |
| H | 0.99559300 | 1.74160700 | 1.31020100 |
| H | 2.06072200 | 0.51013700 | 0.68353600 |
| H | -1.21953000 | 1.93880500 | 0.65523800 |
| H | -1.48391000 | 1.21710000 | -0.91973100 |
| H | -2.85930800 | -0.57365100 | 0.15447400 |
| H | 0.68686300 | -0.77870300 | -2.54580700 |
| H | -3.25786600 | -0.33469500 | 2.39267900 |
| H | 1.72233800 | 1.37487800 | -1.63819800 |
| H | 0.59736300 | 2.58210600 | -1.03504600 |
| H | -1.46871200 | -2.17048900 | -2.59631500 |
| H | -3.05277300 | -4.04746200 | -2.36670400 |
| H | -3.40929900 | -5.11599600 | -0.14964500 |
| H | -2.14213200 | -4.28713500 | 1.82225400 |
| H | -0.56092800 | -2.43022600 | 1.59049900 |
| H | 2.11710000 | -3.70137500 | 2.53401000 |
| H | 3.88530900 | -3.66156400 | 2.64669900 |
| H | 2.95318600 | -2.17119200 | 2.87431800 |
| H | 4.26388100 | -1.00568400 | 1.04692100 |
| H | 4.42347100 | -1.75143100 | -0.55835000 |
| H | 5.22859600 | -2.47355100 | 0.84166500 |
| H | 3.95072200 | -4.74452500 | 0.32013700 |
| H | 2.18456900 | -4.69217100 | 0.21302400 |
| H | 3.17905700 | -3.94794100 | -1.05802100 |
| H | -3.62856200 | 2.41003000 | 2.22911300 |
| H | -5.49522800 | 3.95729900 | 1.73822600 |
| H | -6.78036600 | 3.72967700 | -0.37492200 |
| H | -6.18141300 | 1.93928400 | -1.99039000 |
| H | -4.31505300 | 0.39514600 | -1.49381300 |
| H | 1.41882200 | 4.46225900 | 0.40644800 |
| H | 3.31147400 | 5.96556700 | 0.91428300 |
| H | 5.62859500 | 5.30615300 | 0.30514500 |
| H | 6.02719100 | 3.12810800 | -0.82277600 |
| H | 4.13009500 | 1.62797300 | -1.33019000 |

SSR-conf-8

| | | | |
|---|---|---|---|
| C | -0.58351100 | -0.99294700 | -1.12124600 |
| C | -0.11123000 | 0.35868400 | -0.49494000 |
| C | 1.39520300 | 0.39326400 | -0.13147100 |
| C | -0.55546500 | 1.52721300 | -1.39695800 |
| C | -0.35875300 | 2.93838800 | -0.81203200 |
| O | -0.06324500 | -1.09362200 | -2.44057700 |
| O | -0.73177900 | 3.91652700 | -1.80492500 |
| C | 2.42094500 | 0.41342700 | -1.28527700 |
| C | -2.12426600 | -1.12929800 | -1.15270000 |
| C | -2.75564900 | -1.57522100 | -2.31792000 |
| C | -4.14186000 | -1.72331600 | -2.36807300 |
| C | -4.92123900 | -1.42907900 | -1.25225000 |
| C | -4.30084400 | -0.98780900 | -0.08381700 |
| C | -2.91612400 | -0.84255100 | -0.03227200 |
| C | -0.03888900 | -2.21404300 | -0.33312600 |
| O | 0.57783800 | -3.09326200 | -0.90778400 |
| O | -0.34128200 | -2.18196000 | 0.94931800 |
| C | -0.02310900 | -3.30656300 | 1.90094100 |
| C | -0.59710400 | -2.78600600 | 3.21402400 |
| C | 1.48900700 | -3.48821200 | 1.99529900 |
| C | -0.74899200 | -4.56813000 | 1.44241300 |
| C | -1.20117800 | 3.20700400 | 0.41942200 |
| C | -2.58611900 | 3.38606200 | 0.31113900 |
| C | -3.36160600 | 3.62060100 | 1.44426600 |
| C | -2.76536600 | 3.67494800 | 2.70527200 |
| C | -1.38796800 | 3.50086500 | 2.82281000 |
| C | -0.61207400 | 3.27376600 | 1.68510800 |
| C | 3.84047000 | 0.51024700 | -0.76981900 |
| C | 4.44649500 | 1.75344400 | -0.54728900 |
| C | 5.74481600 | 1.84045100 | -0.04553600 |
| C | 6.46333000 | 0.68078800 | 0.24461400 |
| C | 5.87316100 | -0.56412700 | 0.02715900 |
| C | 4.57487300 | -0.64589000 | -0.47514900 |
| H | -0.64074800 | 0.44987300 | 0.45650500 |
| H | 1.56006700 | 1.28188900 | 0.48528800 |
| H | 1.62240700 | -0.45474100 | 0.52187100 |
| H | -0.01029500 | 1.48683300 | -2.34490000 |
| H | -1.61633100 | 1.41942800 | -1.64104600 |
| H | 0.69312300 | 3.08869500 | -0.54860800 |
| H | 0.33200800 | -1.97756300 | -2.51804300 |

| | | | |
|---|---|---|---|
| H | -0.22376600 | 3.72721400 | -2.60400300 |
| H | 2.31674100 | -0.49048700 | -1.88706500 |
| H | 2.22008300 | 1.26228900 | -1.94508400 |
| H | -2.15978100 | -1.79839100 | -3.19279300 |
| H | -4.60962500 | -2.06839800 | -3.28405300 |
| H | -5.99927300 | -1.54170600 | -1.29058600 |
| H | -4.89479400 | -0.75413700 | 0.79327800 |
| H | -2.46040000 | -0.50555900 | 0.88957700 |
| H | -1.67324100 | -2.61775900 | 3.12872200 |
| H | -0.42411700 | -3.51976500 | 4.00463800 |
| H | -0.11621600 | -1.84795700 | 3.50200000 |
| H | 1.97606500 | -2.54707000 | 2.26204200 |
| H | 1.91472800 | -3.85754200 | 1.06297700 |
| H | 1.70484600 | -4.21522700 | 2.78288600 |
| H | -0.63649600 | -5.33788600 | 2.21044700 |
| H | -1.81603300 | -4.37072900 | 1.31232000 |
| H | -0.34303400 | -4.95561600 | 0.50815800 |
| H | -3.05592900 | 3.35278000 | -0.66523200 |
| H | -4.43254200 | 3.76213300 | 1.34379000 |
| H | -3.37001900 | 3.85735300 | 3.58713700 |
| H | -0.91396500 | 3.54988800 | 3.79736300 |
| H | 0.46215600 | 3.15402100 | 1.78180900 |
| H | 3.89821300 | 2.66242300 | -0.77626500 |
| H | 6.19691000 | 2.81389300 | 0.11414600 |
| H | 7.47445500 | 0.74655500 | 0.63175800 |
| H | 6.42534900 | -1.47264800 | 0.24431200 |
| H | 4.12546100 | -1.61932600 | -0.64713700 |

SSR-conf-9

| | | | |
|---|---|---|---|
| C | 0.03037600 | -1.21087900 | 0.97822500 |
| C | -0.03965400 | 0.09697500 | 0.13542800 |
| C | -1.31266900 | 0.89800600 | 0.48884800 |
| C | 1.24342000 | 0.95320400 | 0.33169700 |
| C | 2.17141700 | 1.02347600 | -0.88829300 |
| O | 0.09374400 | -0.83318800 | 2.34717300 |
| O | 1.41750800 | 1.61568900 | -1.95774300 |
| C | -1.65651500 | 1.99657000 | -0.53596300 |
| C | 1.22738400 | -2.11552800 | 0.60806600 |
| C | 2.09596400 | -2.56446200 | 1.60691900 |
| C | 3.17323400 | -3.39516600 | 1.29588700 |
| C | 3.39508000 | -3.79571300 | -0.01929700 |
| C | 2.52964100 | -3.35857600 | -1.02230000 |
| C | 1.45499400 | -2.52791900 | -0.71239500 |
| C | -1.24149200 | -2.08736400 | 0.81862700 |
| O | -1.78551200 | -2.56490700 | 1.79738700 |
| O | -1.60187300 | -2.26327100 | -0.43870700 |
| C | -2.73832900 | -3.16262700 | -0.84966800 |
| C | -2.72110000 | -3.02841900 | -2.36847800 |
| C | -4.04569400 | -2.63284600 | -0.26702500 |
| C | -2.42716900 | -4.59314300 | -0.41874900 |
| C | 3.43772000 | 1.80868100 | -0.57880400 |
| C | 3.50767100 | 3.18987200 | -0.78740300 |
| C | 4.66484900 | 3.89888900 | -0.46532200 |
| C | 5.76798600 | 3.23695000 | 0.07212100 |
| C | 5.70808600 | 1.85890400 | 0.28123300 |
| C | 4.55212400 | 1.15169500 | -0.04457000 |
| C | -2.89792900 | 2.77282300 | -0.15470100 |
| C | -4.15873400 | 2.39847600 | -0.63601500 |
| C | -5.30707200 | 3.09706900 | -0.26318500 |
| C | -5.21418700 | 4.18657000 | 0.60204600 |
| C | -3.96466800 | 4.57176200 | 1.08835200 |
| C | -2.81980400 | 3.87044000 | 0.71263300 |
| H | -0.10996000 | -0.19816300 | -0.91312800 |
| H | -2.17322200 | 0.22457400 | 0.55846000 |
| H | -1.19236900 | 1.34699700 | 1.47954500 |
| H | 0.96545500 | 1.97964200 | 0.59047300 |
| H | 1.82387400 | 0.57931500 | 1.17742200 |
| H | 2.46121800 | 0.00745700 | -1.17622200 |
| H | -0.44589600 | -1.47148900 | 2.84046400 |
| H | 1.95005400 | 1.56789600 | -2.76152700 |
| H | -0.81535700 | 2.68766900 | -0.63495300 |
| H | -1.80365000 | 1.53323200 | -1.51680900 |
| H | 1.93198500 | -2.25657700 | 2.63108600 |
| H | 3.83687900 | -3.72855900 | 2.08661900 |
| H | 4.23143900 | -4.44212300 | -0.26211700 |
| H | 2.69041000 | -3.66359000 | -2.05081300 |

| | | | |
|---|---|---|---|
| H | 0.79508900 | -2.20330100 | -1.50666200 |
| H | -1.77030200 | -3.37542300 | -2.78000900 |
| H | -3.52341100 | -3.63304300 | -2.79764100 |
| H | -2.87488800 | -1.98864700 | -2.66729900 |
| H | -4.19803500 | -1.58805700 | -0.54882500 |
| H | -4.07146100 | -2.71499600 | 0.81899400 |
| H | -4.87398100 | -3.21769800 | -0.67595000 |
| H | -3.17988700 | -5.26129100 | -0.84547700 |
| H | -1.44765000 | -4.90201500 | -0.79244700 |
| H | -2.44499400 | -4.70592000 | 0.66501300 |
| H | 2.65723100 | 3.70908400 | -1.21360500 |
| H | 4.70409300 | 4.96965400 | -0.63619800 |
| H | 6.66832900 | 3.78837400 | 0.32088700 |
| H | 6.56392900 | 1.33360700 | 0.69194400 |
| H | 4.51540700 | 0.07809000 | 0.11314700 |
| H | -4.23995800 | 1.55601300 | -1.31628900 |
| H | -6.27335300 | 2.79223500 | -0.65154500 |
| H | -6.10554000 | 4.73294900 | 0.89112700 |
| H | -3.88088300 | 5.42162100 | 1.75781300 |
| H | -1.85110900 | 4.18157700 | 1.09214300 |

SSR-conf-10

| | | | |
|---|---|---|---|
| C | -1.09537800 | -0.83377100 | -0.84988400 |
| C | -0.01543500 | 0.28129500 | -1.12029600 |
| C | -0.06639300 | 1.51510300 | -0.19005300 |
| C | 1.43305500 | -0.24561500 | -1.30397300 |
| C | 2.04778300 | -1.08716200 | -0.17894000 |
| O | -0.86500100 | -1.92192700 | -1.74626500 |
| O | 1.41141500 | -2.38134800 | -0.24759100 |
| C | 0.36888100 | 2.81230000 | -0.90586900 |
| C | -2.49736900 | -0.28814200 | -1.17484700 |
| C | -2.96810100 | -0.36420800 | -2.49165000 |
| C | -4.21804200 | 0.14880200 | -2.83123800 |
| C | -5.02175000 | 0.74694600 | -1.86143800 |
| C | -4.56309400 | 0.82584700 | -0.54888800 |
| C | -3.31102300 | 0.31290600 | -0.20813400 |
| C | -1.11558000 | -1.37114400 | 0.60968400 |
| O | -0.72066300 | -0.74655700 | 1.57297800 |
| O | -1.68233400 | -2.57372600 | 0.65620900 |
| C | -1.88884000 | -3.33881100 | 1.92606900 |
| C | -2.57868100 | -4.60447600 | 1.42439900 |
| C | -2.80553100 | -2.55527400 | 2.86345400 |
| C | -0.53628800 | -3.66717700 | 2.55449700 |
| C | 3.55615800 | -1.20500300 | -0.32396000 |
| C | 4.39468000 | -0.33278700 | 0.37793700 |
| C | 5.77894200 | -0.39880900 | 0.22507600 |
| C | 6.34348700 | -1.34481300 | -0.63010700 |
| C | 5.51485300 | -2.22267800 | -1.32890000 |
| C | 4.13065000 | -2.15264100 | -1.17786500 |
| C | 0.36228000 | 4.01177200 | 0.01550800 |
| C | 1.50069300 | 4.35748200 | 0.75512100 |
| C | 1.48694400 | 5.44325000 | 1.62996800 |
| C | 0.32939400 | 6.20645500 | 1.78146800 |
| C | -0.81131900 | 5.87473000 | 1.05075800 |
| C | -0.79270700 | 4.78778400 | 0.17732700 |
| H | -0.30192700 | 0.63457700 | -2.11754600 |
| H | -1.07861700 | 1.66678800 | 0.18945100 |
| H | 0.56735000 | 1.35597300 | 0.68557400 |
| H | 1.49971100 | -0.83618200 | -2.22310700 |
| H | 2.07360400 | 0.62516000 | -1.46106000 |
| H | 1.82685700 | -0.63427600 | 0.79192000 |
| H | -0.06580700 | -2.37169100 | -1.42106000 |
| H | 1.62118600 | -2.88646600 | 0.54852500 |
| H | 1.37167700 | 2.68833000 | -1.32579000 |
| H | -0.30919500 | 2.99484000 | -1.74618500 |
| H | -2.35707700 | -0.83223300 | -3.25255600 |
| H | -4.56401700 | 0.07781900 | -3.85694100 |
| H | -5.99568700 | 1.14403900 | -2.12602400 |
| H | -5.17836300 | 1.28433600 | 0.21769700 |
| H | -2.97992100 | 0.38488700 | 0.82110400 |
| H | -1.94333500 | -5.13224700 | 0.70878600 |
| H | -2.78411800 | -5.27229100 | 2.26428800 |
| H | -3.52523900 | -4.36020000 | 0.93585100 |
| H | -2.31989600 | -1.66526700 | 3.26189400 |
| H | -3.08537800 | -3.19865400 | 3.70205300 |
| H | -3.72040500 | -2.25906600 | 2.34387200 |

| | | | |
|---|---|---|---|
| H | -0.69559100 | -4.32852000 | 3.41056800 |
| H | 0.10199400 | -4.19042900 | 1.83800000 |
| H | -0.02215700 | -2.77286200 | 2.90545300 |
| H | 3.96058800 | 0.39931800 | 1.05222000 |
| H | 6.41586500 | 0.28252100 | 0.77922200 |
| H | 7.42033300 | -1.40101000 | -0.74720300 |
| H | 5.94663300 | -2.96437100 | -1.99267100 |
| H | 3.49245700 | -2.84426100 | -1.71581800 |
| H | 2.40851900 | 3.77282400 | 0.63955600 |
| H | 2.38144300 | 5.69584100 | 2.18991300 |
| H | 0.31759400 | 7.05335900 | 2.45914200 |
| H | -1.71556100 | 6.46499200 | 1.15745800 |
| H | -1.68444900 | 4.53992700 | -0.39058600 |

**13. Detailed Information of DFT Calculation**

**Energies and Cartesian Coordinates**

$N_2$

*G*sol(DCM) = -109.5346797 Hartree

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| | | | |
|---|---|---|---|
| N | 0.000000 | 0.000000 | 0.552550 |
| N | 0.000000 | 0.000000 | -0.552550 |

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$H_2O$

*G*sol(DCM) = -76.42446535 Hartree

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| | | | |
|---|---|---|---|
| O | 0.000000 | -0.000000 | 0.120375 |
| H | 0.000000 | 0.760308 | -0.481499 |
| H | -0.000000 | -0.760308 | -0.481499 |

---

BnOH

*G*sol(DCM) = -346.6239777 Hartree

---

| | | | |
|---|---|---|---|
| O | 2.777573 | -0.460121 | -0.243476 |
| C | 1.924829 | 0.568235 | 0.249494 |
| H | 2.190431 | 0.671183 | 1.308789 |
| H | 2.146847 | 1.534037 | -0.229428 |
| C | 0.444556 | 0.259681 | 0.112645 |
| C | -0.486828 | 1.297698 | -0.021248 |
| C | -0.016071 | -1.062854 | 0.146441 |
| C | -1.853264 | 1.021806 | -0.107938 |
| H | -0.140192 | 2.328387 | -0.060834 |
| C | -1.381303 | -1.341970 | 0.052251 |
| H | 0.704337 | -1.870243 | 0.239352 |
| C | -2.304708 | -0.300393 | -0.072356 |
| H | -2.563600 | 1.837753 | -0.212847 |
| H | -1.724217 | -2.373175 | 0.077094 |
| H | 2.569535 | -0.583106 | -1.184151 |
| H | -3.366990 | -0.517089 | -0.145900 |

---

**2a**

*G*sol(DCM) = -725.3302168 Hartree

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| | | | |
|---|---|---|---|
| C | 3.719610 | -1.782661 | 0.038489 |
| C | 2.513631 | -2.092208 | -0.595560 |
| C | 1.479981 | -1.157712 | -0.652865 |
| C | 1.631155 | 0.106702 | -0.055832 |
| C | 2.847637 | 0.408744 | 0.583286 |
| C | 3.882432 | -0.524909 | 0.623731 |
| H | 4.522965 | -2.512862 | 0.075582 |
| H | 2.376530 | -3.065109 | -1.059795 |
| H | 0.554343 | -1.405555 | -1.157307 |
| H | 2.984704 | 1.376276 | 1.058830 |
| H | 4.812811 | -0.269946 | 1.123593 |
| C | 0.552888 | 1.120743 | -0.122471 |
| C | -0.915687 | 0.959381 | -0.092115 |
| O | -1.682007 | 1.909148 | -0.183450 |
| O | -1.262181 | -0.326706 | 0.060454 |
| C | -2.680969 | -0.752133 | 0.136782 |
| C | -3.345436 | -0.120286 | 1.363602 |
| H | -3.425714 | 0.962729 | 1.258282 |
| H | -4.351328 | -0.536961 | 1.484430 |
| H | -2.771818 | -0.348708 | 2.268417 |
| C | -2.561918 | -2.268615 | 0.304518 |
| H | -3.559512 | -2.711969 | 0.386453 |
| H | -2.053986 | -2.716915 | -0.555647 |
| H | -1.997769 | -2.515470 | 1.209723 |
| C | -3.400832 | -0.402236 | -1.168768 |
| H | -3.486747 | 0.677762 | -1.298110 |
| H | -2.862722 | -0.821864 | -2.025671 |
| H | -4.406950 | -0.835294 | -1.153928 |
| N | 0.911003 | 2.387919 | -0.177230 |
| N | 1.215247 | 3.482865 | -0.223864 |

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**3a**

*G*sol(DCM) = -595.9426825 Hartree

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| | | | |
|---|---|---|---|
| C | -1.159715 | -1.315169 | 0.004848 |
| C | -2.176685 | -1.227536 | 1.146562 |
| C | -3.355103 | 0.490785 | 0.044216 |
| C | -2.360317 | 0.442930 | -1.120644 |

| | | | |
|---|---|---|---|
| H | -2.338104 | -2.211386 | 1.598401 |
| H | -1.497550 | -2.068006 | -0.719333 |
| H | -0.185907 | -1.625133 | 0.388453 |
| H | -4.360600 | 0.734586 | -0.312597 |
| H | -3.051430 | 1.249221 | 0.782410 |
| H | -2.737828 | -0.272447 | -1.863819 |
| H | -2.267028 | 1.416827 | -1.607730 |
| H | -1.805578 | -0.540206 | 1.924730 |
| O | -3.448343 | -0.787665 | 0.673089 |
| N | -1.038553 | -0.024734 | -0.695144 |
| C | 1.309347 | 0.369322 | -0.102526 |
| C | 1.839869 | -0.536319 | -1.037880 |
| C | 2.126612 | 0.790422 | 0.958838 |
| C | 3.152426 | -0.994328 | -0.922131 |
| H | 1.217147 | -0.868351 | -1.863369 |
| C | 3.440709 | 0.333464 | 1.074383 |
| H | 1.720311 | 1.470869 | 1.701598 |
| C | 3.959104 | -0.560359 | 0.134148 |
| H | 3.547738 | -1.687156 | -1.660348 |
| H | 4.055972 | 0.668713 | 1.905151 |
| H | 4.980477 | -0.919711 | 0.225651 |
| C | -0.078553 | 0.904871 | -0.254900 |
| C | -0.306528 | 2.227148 | -0.084058 |
| H | -1.292235 | 2.672748 | -0.147859 |
| H | 0.524237 | 2.902510 | 0.084815 |

---

**4a**

*G*sol(DCM) = -421.5705362 Hartree

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| | | | |
|---|---|---|---|
| C | -3.594266 | -0.371399 | 0.000038 |
| H | -3.966365 | -1.412955 | 0.000129 |
| C | -2.165272 | -0.244037 | -0.000073 |
| C | -0.949120 | -0.164202 | -0.000032 |
| C | 0.469584 | -0.065221 | -0.000020 |
| C | 1.094258 | 1.199907 | -0.000028 |
| C | 1.263130 | -1.231796 | 0.000005 |
| C | 2.483389 | 1.290171 | -0.000011 |
| H | 0.481906 | 2.095958 | -0.000047 |
| C | 2.651361 | -1.129420 | 0.000020 |
| H | 0.780762 | -2.204030 | 0.000010 |
| C | 3.262894 | 0.128670 | 0.000013 |
| H | 2.959731 | 2.266023 | -0.000017 |
| H | 3.258065 | -2.030024 | 0.000038 |
| H | 4.346484 | 0.203873 | 0.000025 |
| O | -4.369542 | 0.575640 | 0.000048 |

---

**5b**

*G*sol(DCM) = -516.435612 Hartree

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| | | | |
|---|---|---|---|
| C | 0.066349 | 0.737101 | -0.002357 |
| C | -1.318746 | 0.587907 | -0.006998 |
| C | -1.910824 | -0.692123 | -0.008194 |
| C | -1.080719 | -1.815031 | -0.004492 |
| C | 0.313562 | -1.667146 | -0.003375 |
| C | 0.904205 | -0.406842 | -0.001695 |
| H | -1.960425 | 1.462128 | -0.014361 |
| H | -1.513492 | -2.812017 | -0.004759 |
| H | 0.931826 | -2.557695 | 0.001377 |
| N | -3.310946 | -0.816174 | -0.082220 |
| H | -3.810453 | -0.049068 | 0.355573 |
| H | -3.654326 | -1.697960 | 0.283937 |
| O | 2.254472 | -0.160974 | 0.003435 |
| O | 0.712937 | 1.940025 | 0.003186 |
| C | 3.122866 | -1.284132 | 0.006866 |
| H | 2.982828 | -1.906468 | -0.886935 |
| H | 4.137187 | -0.880573 | 0.009772 |
| H | 2.977309 | -1.905299 | 0.900614 |
| C | -0.075116 | 3.123900 | 0.000100 |
| H | -0.712634 | 3.185239 | 0.891165 |
| H | 0.633363 | 3.953998 | 0.004508 |
| H | -0.703297 | 3.186723 | -0.897444 |

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**6b**

*G*sol(DCM) = -2488.123174 Hartree

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| | | | |
|---|---|---|---|
| C | -0.843250 | 4.835041 | -2.389356 |

| | | | |
|---|---|---|---|
| C | -0.338635 | 3.836116 | -1.584677 |
| C | -1.169646 | 2.778112 | -1.121316 |
| C | -2.539423 | 2.761303 | -1.544376 |
| C | -3.033136 | 3.816618 | -2.359629 |
| C | -2.206061 | 4.836208 | -2.772486 |
| H | -0.186529 | 5.627284 | -2.737487 |
| H | 0.709834 | 3.846981 | -1.310627 |
| C | -0.685623 | 1.708106 | -0.289335 |
| C | -3.379404 | 1.684288 | -1.159827 |
| H | -4.077108 | 3.793435 | -2.661317 |
| H | -2.590984 | 5.634197 | -3.400754 |
| C | -2.903638 | 0.611835 | -0.433951 |
| C | -1.537375 | 0.644350 | -0.039561 |
| H | -4.421799 | 1.698975 | -1.466390 |
| C | 0.695341 | 1.706929 | 0.277419 |
| C | 1.173524 | 2.775280 | 1.115173 |
| C | 1.548494 | 0.642071 | 0.033479 |
| C | 0.339812 | 3.833577 | 1.573545 |
| C | 2.539865 | 2.757762 | 1.548582 |
| C | 2.910019 | 0.606821 | 0.442461 |
| C | 0.839297 | 4.832030 | 2.381906 |
| H | -0.706796 | 3.845350 | 1.292893 |
| C | 3.028579 | 3.812490 | 2.367719 |
| C | 3.380464 | 1.678824 | 1.172713 |
| C | 2.199399 | 4.832593 | 2.774662 |
| H | 0.180386 | 5.624315 | 2.725788 |
| H | 4.070231 | 3.788066 | 2.677166 |
| H | 4.419341 | 1.689820 | 1.490957 |
| H | 2.580221 | 5.630196 | 3.405912 |
| O | -1.056530 | -0.453372 | 0.683906 |
| O | 1.078525 | -0.447443 | -0.711315 |
| P | 0.010499 | -1.452107 | -0.024411 |
| O | -0.640547 | -1.983198 | -1.389777 |
| H | -1.155701 | -2.800008 | -1.265552 |
| O | 0.488529 | -2.463109 | 0.939356 |
| C | -3.797549 | -0.526796 | -0.050799 |
| C | -4.169958 | -1.494120 | -1.014617 |
| C | -4.285738 | -0.612593 | 1.275506 |
| C | -5.049496 | -2.578071 | -0.631951 |
| C | -3.704962 | -1.462297 | -2.371171 |
| C | -5.158658 | -1.703967 | 1.645403 |
| C | -3.961795 | 0.352710 | 2.283511 |
| C | -5.423237 | -3.554032 | -1.610172 |
| C | -5.515913 | -2.655217 | 0.684009 |
| C | -4.084422 | -2.420117 | -3.276796 |
| H | -3.037964 | -0.665130 | -2.678461 |
| C | -5.645032 | -1.784873 | 2.988881 |
| C | -4.450474 | 0.240976 | 3.560182 |
| H | -3.322113 | 1.189460 | 2.024323 |
| C | -4.957607 | -3.480675 | -2.895990 |
| H | -6.087370 | -4.358973 | -1.305134 |
| H | -6.174076 | -3.473945 | 0.966677 |
| H | -3.716478 | -2.372379 | -4.298005 |
| H | -6.297862 | -2.613869 | 3.250785 |
| C | -5.301452 | -0.843340 | 3.922574 |
| H | -4.189744 | 0.987268 | 4.305504 |
| H | -5.247595 | -4.227786 | -3.629341 |
| H | -5.677255 | -0.914944 | 4.939303 |
| C | 3.807867 | -0.534994 | 0.080637 |
| C | 4.159330 | -1.494225 | 1.059589 |
| C | 4.324966 | -0.628404 | -1.233549 |
| C | 5.054247 | -2.575184 | 0.706777 |
| C | 3.657561 | -1.455987 | 2.402037 |
| C | 5.210618 | -1.718875 | -1.574970 |
| C | 4.019529 | 0.327785 | -2.255928 |
| C | 5.411222 | -3.539556 | 1.702482 |
| C | 5.551520 | -2.659855 | -0.597520 |
| C | 4.023120 | -2.400965 | 3.325821 |
| H | 2.972917 | -0.663879 | 2.683622 |
| C | 5.726916 | -1.807791 | -2.906768 |
| C | 4.536546 | 0.208219 | -3.520697 |
| H | 3.370788 | 1.163877 | -2.017382 |
| C | 4.914680 | -3.456931 | 2.976163 |
| H | 6.087837 | -4.342754 | 1.421096 |
| H | 6.221250 | -3.476543 | -0.858190 |
| H | 3.626988 | -2.349617 | 4.336234 |

| | | | |
|---|---|---|---|
| H | 6.389114 | -2.635760 | -3.147705 |
| C | 5.400015 | -0.875224 | -3.855422 |
| H | 4.289097 | 0.947415 | -4.277589 |
| H | 5.192708 | -4.194997 | 3.723254 |
| H | 5.798655 | -0.953215 | -4.862979 |

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**Imine**

*G*sol(DCM) = -861.5862063 Hartree

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| | | | |
|---|---|---|---|
| C | 0.624567 | 0.232922 | -0.246062 |
| H | 0.246913 | 1.192989 | -0.619527 |
| C | 2.037092 | 0.118385 | -0.167800 |
| C | 3.254019 | 0.075849 | -0.118390 |
| C | 4.674382 | 0.008382 | -0.050714 |
| C | 5.313109 | -1.163416 | 0.407948 |
| C | 5.462175 | 1.112257 | -0.440566 |
| C | 6.702806 | -1.224102 | 0.472898 |
| H | 4.709723 | -2.014266 | 0.708556 |
| C | 6.851198 | 1.041184 | -0.370920 |
| H | 4.974080 | 2.015189 | -0.794012 |
| C | 7.475152 | -0.124544 | 0.084904 |
| H | 7.185129 | -2.130600 | 0.827175 |
| H | 7.448920 | 1.896478 | -0.672784 |
| H | 8.558919 | -0.175907 | 0.137513 |
| N | -0.153002 | -0.742386 | 0.088627 |
| C | -1.548092 | -0.590102 | 0.048519 |
| C | -2.221413 | 0.652077 | 0.135346 |
| C | -2.305757 | -1.760736 | -0.052880 |
| C | -3.608581 | 0.712559 | 0.091191 |
| H | -1.651002 | 1.562306 | 0.272371 |
| C | -3.701005 | -1.707583 | -0.116882 |
| H | -1.789928 | -2.714193 | -0.102197 |
| C | -4.366656 | -0.484188 | -0.047130 |
| O | -4.342392 | 1.856693 | 0.185674 |
| H | -4.262694 | -2.629404 | -0.211271 |
| O | -5.716436 | -0.322456 | -0.082331 |
| C | -3.644341 | 3.088963 | 0.329813 |
| C | -6.527002 | -1.488511 | -0.196001 |
| H | -2.986592 | 3.279061 | -0.527336 |
| H | -4.412612 | 3.862192 | 0.376340 |
| H | -3.051815 | 3.108196 | 1.252925 |
| H | -6.378866 | -2.162396 | 0.656558 |
| H | -7.558452 | -1.133385 | -0.203892 |
| H | -6.320012 | -2.029826 | -1.127191 |

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**TS-1**

*G*sol(DCM) = -3426.121565 Hartree

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| | | | |
|---|---|---|---|
| H | 1.969999 | -0.700791 | -1.079052 |
| N | 2.977132 | -0.766791 | -0.888042 |
| C | 2.845282 | -0.502953 | 1.350984 |
| H | 2.215926 | -1.396682 | 1.328142 |
| C | -6.523831 | -1.625731 | -2.977548 |
| C | -5.720382 | -1.086300 | -1.995819 |
| C | -4.547199 | -1.760206 | -1.555199 |
| C | -4.205684 | -3.002402 | -2.185256 |
| C | -5.065554 | -3.540489 | -3.181740 |
| C | -6.203627 | -2.870796 | -3.570358 |
| H | -7.409355 | -1.087193 | -3.303350 |
| H | -5.975212 | -0.127082 | -1.560103 |
| C | -3.671884 | -1.229286 | -0.543934 |
| C | -3.009226 | -3.671294 | -1.815783 |
| H | -4.797379 | -4.488707 | -3.640692 |
| H | -6.849906 | -3.287284 | -4.337626 |
| C | -2.122753 | -3.128167 | -0.909356 |
| C | -2.469693 | -1.881301 | -0.316011 |
| H | -2.781663 | -4.628362 | -2.277648 |
| C | -4.010449 | -0.008671 | 0.247527 |
| C | -5.214297 | 0.071053 | 1.033387 |
| C | -3.133849 | 1.066952 | 0.282773 |
| C | -6.102325 | -1.027661 | 1.208541 |
| C | -5.521719 | 1.296650 | 1.710570 |
| C | -3.422416 | 2.293977 | 0.946100 |
| C | -7.242278 | -0.907107 | 1.974187 |
| H | -5.870280 | -1.977883 | 0.742314 |
| C | -6.714783 | 1.394191 | 2.478562 |

| | | | |
|---|---|---|---|
| C | -4.620065 | 2.387899 | 1.624746 |
| C | -7.563049 | 0.318121 | 2.606576 |
| H | -7.898766 | -1.763906 | 2.097925 |
| H | -6.936320 | 2.335916 | 2.974357 |
| H | -4.873858 | 3.316224 | 2.129381 |
| H | -8.468695 | 0.400610 | 3.200575 |
| O | -1.560289 | -1.317795 | 0.576239 |
| O | -1.935102 | 0.994285 | -0.418816 |
| P | -0.730540 | -0.003682 | 0.054249 |
| O | 0.147917 | -0.244397 | -1.127759 |
| O | -0.094670 | 0.524051 | 1.358170 |
| C | -0.860115 | -3.835890 | -0.525853 |
| C | 0.248442 | -3.848170 | -1.405025 |
| C | -0.790484 | -4.502152 | 0.721849 |
| C | 1.461707 | -4.531865 | -1.011308 |
| C | 0.236373 | -3.193396 | -2.680215 |
| C | 0.426894 | -5.182896 | 1.101919 |
| C | -1.890699 | -4.544839 | 1.639006 |
| C | 2.584964 | -4.528951 | -1.900281 |
| C | 1.519505 | -5.176701 | 0.228109 |
| C | 1.331365 | -3.217661 | -3.504861 |
| H | -0.657409 | -2.662387 | -2.985575 |
| C | 0.488475 | -5.852427 | 2.365265 |
| C | -1.792531 | -5.198723 | 2.840697 |
| H | -2.819667 | -4.053863 | 1.369814 |
| C | 2.524511 | -3.893388 | -3.113099 |
| H | 3.487341 | -5.051203 | -1.591524 |
| H | 2.434871 | -5.687852 | 0.518620 |
| H | 1.295626 | -2.712019 | -4.465769 |
| H | 1.412571 | -6.357760 | 2.635246 |
| C | -0.586932 | -5.860763 | 3.213799 |
| H | -2.642792 | -5.216463 | 3.516878 |
| H | 3.381421 | -3.902153 | -3.780921 |
| H | -0.528536 | -6.372982 | 4.170030 |
| C | -2.471912 | 3.449208 | 0.903981 |
| C | -1.748752 | 3.808851 | 2.067224 |
| C | -2.325465 | 4.198056 | -0.288641 |
| C | -0.860493 | 4.950468 | 2.028858 |
| C | -1.840184 | 3.079572 | 3.298434 |
| C | -1.422979 | 5.326937 | -0.317070 |
| C | -3.051292 | 3.896271 | -1.486655 |
| C | -0.139708 | 5.315888 | 3.210481 |
| C | -0.718120 | 5.673789 | 0.840601 |
| C | -1.130298 | 3.461067 | 4.407883 |
| H | -2.481929 | 2.207200 | 3.344380 |
| C | -1.276328 | 6.074571 | -1.529138 |
| C | -2.883966 | 4.637542 | -2.628383 |
| H | -3.749570 | 3.066304 | -1.483570 |
| C | -0.270933 | 4.597673 | 4.369073 |
| H | 0.518361 | 6.180209 | 3.164508 |
| H | -0.045085 | 6.528156 | 0.816692 |
| H | -1.217749 | 2.888990 | 5.327472 |
| H | -0.593050 | 6.920395 | -1.532300 |
| C | -1.981421 | 5.740307 | -2.655401 |
| H | -3.446873 | 4.386194 | -3.523068 |
| H | 0.281390 | 4.884944 | 5.259408 |
| H | -1.862763 | 6.315861 | -3.569102 |
| C | 3.739893 | 0.257254 | -1.485970 |
| C | 5.098732 | 0.085988 | -1.750424 |
| C | 3.129716 | 1.500797 | -1.745581 |
| C | 5.846823 | 1.145651 | -2.279143 |
| H | 5.578924 | -0.867803 | -1.553246 |
| C | 3.872978 | 2.554543 | -2.268768 |
| H | 2.071015 | 1.612418 | -1.546302 |
| C | 5.256094 | 2.380147 | -2.540069 |
| H | 6.899410 | 0.991735 | -2.486007 |
| O | 3.368275 | 3.786626 | -2.560237 |
| O | 5.901317 | 3.469294 | -3.055311 |
| C | 1.985998 | 4.019854 | -2.309538 |
| H | 1.745265 | 3.905377 | -1.245610 |
| H | 1.797219 | 5.050363 | -2.613862 |
| H | 1.351967 | 3.345744 | -2.898368 |
| C | 7.287981 | 3.341480 | -3.342396 |
| H | 7.602299 | 4.309485 | -3.736253 |
| H | 7.866309 | 3.111429 | -2.438403 |
| H | 7.473306 | 2.564933 | -4.095524 |

| | | | |
|---|---|---|---|
| C | 4.228450 | -0.692233 | 1.617992 |
| C | 5.410567 | -0.860491 | 1.854086 |
| C | 6.790994 | -1.053065 | 2.141122 |
| C | 7.355390 | -2.344950 | 2.092459 |
| C | 7.606952 | 0.047920 | 2.475868 |
| C | 8.707185 | -2.525722 | 2.372727 |
| H | 6.726907 | -3.191621 | 1.835177 |
| C | 8.957238 | -0.145016 | 2.754857 |
| H | 7.171732 | 1.041478 | 2.512571 |
| C | 9.509556 | -1.429050 | 2.703954 |
| H | 9.136210 | -3.522597 | 2.333359 |
| H | 9.580416 | 0.706319 | 3.012165 |
| H | 10.563586 | -1.574851 | 2.922078 |
| H | 3.325769 | -1.704507 | -1.072989 |
| H | 1.069479 | 0.593787 | 1.406140 |
| O | 2.312722 | 0.640790 | 1.506455 |

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**INT-1**

*G*sol(DCM) = -3426.134483 Hartree

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| | | | |
|---|---|---|---|
| H | 0.140419 | -2.539242 | -0.290702 |
| N | 0.273004 | -3.548384 | 0.033961 |
| C | 0.431476 | -3.515158 | 1.606006 |
| H | 0.838038 | -4.502684 | 1.842300 |
| C | -0.378073 | 5.210218 | -4.252224 |
| C | -0.209288 | 4.615105 | -3.020330 |
| C | -1.011317 | 3.508382 | -2.622814 |
| C | -1.979219 | 3.009806 | -3.554949 |
| C | -2.140329 | 3.656223 | -4.811308 |
| C | -1.360202 | 4.736756 | -5.155565 |
| H | 0.252910 | 6.048276 | -4.535116 |
| H | 0.554949 | 4.984609 | -2.346362 |
| C | -0.861708 | 2.847565 | -1.354184 |
| C | -2.754672 | 1.872518 | -3.212139 |
| H | -2.887088 | 3.270495 | -5.500867 |
| H | -1.486639 | 5.219731 | -6.120308 |
| C | -2.563356 | 1.186595 | -2.030112 |
| C | -1.573813 | 1.677319 | -1.129349 |
| H | -3.510636 | 1.525942 | -3.911926 |
| C | 0.052411 | 3.369079 | -0.296338 |
| C | -0.099102 | 4.689874 | 0.252265 |
| C | 1.058746 | 2.554454 | 0.204780 |
| C | -1.192108 | 5.543745 | -0.068630 |
| C | 0.867004 | 5.162007 | 1.199836 |
| C | 2.039973 | 3.014552 | 1.130720 |
| C | -1.301645 | 6.799693 | 0.488830 |
| H | -1.956252 | 5.192834 | -0.752579 |
| C | 0.734582 | 6.469071 | 1.744490 |
| C | 1.932500 | 4.311286 | 1.590799 |
| C | -0.324392 | 7.276251 | 1.395784 |
| H | -2.150145 | 7.428595 | 0.233735 |
| H | 1.483377 | 6.813452 | 2.453470 |
| H | 2.674663 | 4.691382 | 2.287955 |
| H | -0.420059 | 8.270804 | 1.822045 |
| O | -1.361668 | 0.977398 | 0.049917 |
| O | 1.162564 | 1.252139 | -0.259253 |
| P | 0.047336 | 0.127411 | 0.217926 |
| O | 0.159606 | -0.981109 | -0.803829 |
| O | 0.151921 | -0.201132 | 1.684909 |
| C | -3.413330 | -0.000112 | -1.696669 |
| C | -3.190214 | -1.242049 | -2.336543 |
| C | -4.481258 | 0.148496 | -0.778666 |
| C | -4.057063 | -2.362622 | -2.041314 |
| C | -2.124492 | -1.452517 | -3.272072 |
| C | -5.340411 | -0.978676 | -0.492794 |
| C | -4.769442 | 1.389047 | -0.121557 |
| C | -3.825053 | -3.615921 | -2.693634 |
| C | -5.104707 | -2.202125 | -1.129196 |
| C | -1.937178 | -2.668723 | -3.876874 |
| H | -1.452408 | -0.631185 | -3.490830 |
| C | -6.424286 | -0.815011 | 0.427147 |
| C | -5.818984 | 1.505650 | 0.753813 |
| H | -4.145213 | 2.251220 | -0.329536 |
| C | -2.798514 | -3.767747 | -3.587674 |
| H | -4.487844 | -4.446357 | -2.462489 |
| H | -5.755362 | -3.046903 | -0.913371 |

| | | | |
|---|---|---|---|
| H | -1.120472 | -2.801691 | -4.581114 |
| H | -7.059798 | -1.673225 | 0.631120 |
| C | -6.660163 | 0.389994 | 1.035003 |
| H | -6.016279 | 2.458671 | 1.236920 |
| H | -2.634092 | -4.723171 | -4.078255 |
| H | -7.488535 | 0.502451 | 1.728853 |
| C | 3.176861 | 2.145727 | 1.570964 |
| C | 3.195986 | 1.610514 | 2.881078 |
| C | 4.258266 | 1.910100 | 0.687735 |
| C | 4.327196 | 0.817037 | 3.311020 |
| C | 2.128968 | 1.810178 | 3.817479 |
| C | 5.380000 | 1.111150 | 1.128128 |
| C | 4.306403 | 2.451431 | -0.638218 |
| C | 4.342686 | 0.284548 | 4.639841 |
| C | 5.383958 | 0.586147 | 2.424950 |
| C | 2.182641 | 1.283059 | 5.082055 |
| H | 1.263824 | 2.385307 | 3.508874 |
| C | 6.472504 | 0.886080 | 0.231022 |
| C | 5.372524 | 2.213891 | -1.468007 |
| H | 3.482744 | 3.066131 | -0.984634 |
| C | 3.304882 | 0.511656 | 5.504022 |
| H | 5.202052 | -0.306558 | 4.946933 |
| H | 6.231813 | -0.011135 | 2.753559 |
| H | 1.359297 | 1.448709 | 5.771443 |
| H | 7.307991 | 0.283431 | 0.578939 |
| C | 6.472560 | 1.419290 | -1.031274 |
| H | 5.384174 | 2.638579 | -2.468044 |
| H | 3.328483 | 0.103160 | 6.510477 |
| H | 7.309965 | 1.245331 | -1.701257 |
| C | 1.410364 | -4.152746 | -0.666029 |
| C | 1.456271 | -5.526406 | -0.844065 |
| C | 2.442526 | -3.317246 | -1.108187 |
| C | 2.565030 | -6.089986 | -1.488136 |
| H | 0.648115 | -6.165200 | -0.500546 |
| C | 3.544637 | -3.877129 | -1.749575 |
| H | 2.356372 | -2.247979 | -0.967388 |
| C | 3.610393 | -5.285647 | -1.939856 |
| H | 2.598290 | -7.162636 | -1.633550 |
| O | 4.598455 | -3.171105 | -2.230627 |
| O | 4.723307 | -5.736694 | -2.573280 |
| C | 4.589408 | -1.754012 | -2.063226 |
| H | 4.567607 | -1.477891 | -1.002859 |
| H | 5.517740 | -1.397215 | -2.509794 |
| H | 3.735672 | -1.298056 | -2.578437 |
| C | 4.849539 | -7.139858 | -2.791768 |
| H | 5.805859 | -7.275381 | -3.298378 |
| H | 4.856036 | -7.691322 | -1.843964 |
| H | 4.041330 | -7.518400 | -3.429085 |
| C | -0.898903 | -3.345723 | 2.188461 |
| C | -1.975492 | -3.213415 | 2.731000 |
| C | -3.237980 | -3.037530 | 3.375392 |
| C | -3.891211 | -4.131040 | 3.977641 |
| C | -3.834369 | -1.762160 | 3.422482 |
| C | -5.115951 | -3.946463 | 4.615429 |
| H | -3.431200 | -5.113627 | 3.941504 |
| C | -5.059647 | -1.588880 | 4.062552 |
| H | -3.330374 | -0.921750 | 2.955708 |
| C | -5.701755 | -2.677556 | 4.660229 |
| H | -5.613872 | -4.793344 | 5.078758 |
| H | -5.514945 | -0.603637 | 4.090877 |
| H | -6.656590 | -2.537990 | 5.159101 |
| H | -0.588865 | -4.056854 | -0.186969 |
| H | 0.925514 | -1.658705 | 1.934334 |
| O | 1.357610 | -2.565457 | 1.949510 |

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**TS-2**

*G*sol(DCM) = -3426.119928 Hartree

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| | | | |
|---|---|---|---|
| H | -0.514459 | -2.556775 | 0.864370 |
| N | -1.221407 | -3.240876 | 0.568530 |
| C | -1.044084 | -3.753083 | -0.688421 |
| H | -1.800282 | -4.476258 | -0.983233 |
| C | 0.685378 | 6.188438 | 2.456684 |
| C | 0.452235 | 5.231032 | 1.492774 |
| C | 1.311127 | 4.104521 | 1.353566 |
| C | 2.406763 | 3.976492 | 2.268738 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 2.630596 | 4.990505 | 3.240417 | C | 4.728912 | -2.428545 | 3.359553 |
| C | 1.791758 | 6.077705 | 3.333313 | C | 5.683293 | -1.595076 | 1.243037 |
| H | 0.009988 | 7.034563 | 2.548047 | C | 2.916761 | -1.211632 | 4.405299 |
| H | -0.406188 | 5.327064 | 0.838035 | H | 2.217750 | 0.548163 | 3.430626 |
| C | 1.101920 | 3.076309 | 0.369650 | C | 6.673209 | -0.789945 | -0.869116 |
| C | 3.242625 | 2.832790 | 2.200254 | C | 5.849334 | 1.258607 | -1.859911 |
| H | 3.473598 | 4.882138 | 3.918218 | H | 4.280122 | 2.282614 | -0.850525 |
| H | 1.967328 | 6.843681 | 4.083222 | C | 3.831812 | -2.304687 | 4.386764 |
| C | 2.999575 | 1.801634 | 1.315675 | H | 5.428166 | -3.260646 | 3.330443 |
| C | 1.892623 | 1.936664 | 0.428959 | H | 6.374620 | -2.435249 | 1.236545 |
| H | 4.087882 | 2.762284 | 2.879742 | H | 2.201022 | -1.128619 | 5.218563 |
| C | 0.049218 | 3.193340 | -0.681814 | H | 7.344093 | -1.645612 | -0.864556 |
| C | 0.022763 | 4.289279 | -1.613551 | C | 6.729910 | 0.138103 | -1.875129 |
| C | -0.915253 | 2.203165 | -0.800368 | H | 5.907144 | 1.994124 | -2.657533 |
| C | 1.052232 | 5.269365 | -1.688800 | H | 3.808989 | -3.038540 | 5.187554 |
| C | -1.064545 | 4.382659 | -2.543062 | H | 7.446622 | 0.028522 | -2.684180 |
| C | -2.007095 | 2.283157 | -1.712348 | C | -3.060822 | 1.221437 | -1.757039 |
| C | 0.989295 | 6.298490 | -2.603722 | C | -3.095025 | 0.303421 | -2.834403 |
| H | 1.904515 | 5.194851 | -1.023489 | C | -4.037013 | 1.158903 | -0.734067 |
| C | -1.108684 | 5.466208 | -3.463150 | C | -4.121626 | -0.718216 | -2.867973 |
| C | -2.069279 | 3.381060 | -2.545818 | C | -2.143904 | 0.324605 | -3.907430 |
| C | -0.106508 | 6.409139 | -3.493335 | C | -5.054495 | 0.132663 | -0.777144 |
| H | 1.792090 | 7.029317 | -2.646326 | C | -4.077744 | 2.091823 | 0.352780 |
| H | -1.946819 | 5.527112 | -4.152817 | C | -4.153457 | -1.642164 | -3.963246 |
| H | -2.897861 | 3.474748 | -3.242882 | C | -5.065387 | -0.781415 | -1.835714 |
| H | -0.146295 | 7.229457 | -4.204244 | C | -2.212612 | -0.575324 | -4.939752 |
| O | 1.643903 | 0.894532 | -0.456879 | H | -1.355570 | 1.067883 | -3.892922 |
| O | -0.852308 | 1.100989 | 0.042512 | C | -6.038600 | 0.079623 | 0.260505 |
| P | 0.310663 | -0.038816 | -0.225266 | C | -5.042125 | 2.010937 | 1.325196 |
| O | 0.371152 | -0.889696 | 1.006047 | H | -3.336232 | 2.882350 | 0.394788 |
| O | 0.109277 | -0.694560 | -1.590800 | C | -3.230983 | -1.572009 | -4.973309 |
| C | 3.900063 | 0.606484 | 1.276092 | H | -4.934233 | -2.398636 | -3.974807 |
| C | 3.855460 | -0.350356 | 2.318213 | H | -5.833139 | -1.551428 | -1.865238 |
| C | 4.831013 | 0.468594 | 0.217942 | H | -1.479005 | -0.534967 | -5.740021 |
| C | 4.771984 | -1.470047 | 2.296911 | H | -6.794080 | -0.700561 | 0.213893 |
| C | 2.926843 | -0.271107 | 3.407619 | C | -6.035228 | 0.989257 | 1.284374 |
| C | 5.734658 | -0.659697 | 0.203519 | H | -5.054174 | 2.734914 | 2.135201 |
| C | 4.935860 | 1.418780 | -0.849492 | H | -3.267647 | -2.275893 | -5.799891 |

| | | | |
|---|---|---|---|
| H | -6.786537 | 0.938038 | 2.066960 |
| C | -2.485780 | -3.101363 | 1.202282 |
| C | -3.544146 | -3.980684 | 0.989529 |
| C | -2.628373 | -2.048760 | 2.126032 |
| C | -4.746552 | -3.802953 | 1.689961 |
| H | -3.457773 | -4.821099 | 0.308834 |
| C | -3.814207 | -1.883732 | 2.834755 |
| H | -1.798793 | -1.366252 | 2.265875 |
| C | -4.899836 | -2.771026 | 2.611416 |
| H | -5.559147 | -4.496852 | 1.509573 |
| O | -4.032535 | -0.902337 | 3.751220 |
| O | -6.026969 | -2.526104 | 3.342205 |
| C | -2.988592 | 0.039715 | 3.982302 |
| H | -2.748982 | 0.597442 | 3.069350 |
| H | -3.371600 | 0.726623 | 4.738583 |
| H | -2.083633 | -0.450939 | 4.360732 |
| C | -7.136490 | -3.396906 | 3.158079 |
| H | -7.918839 | -3.029108 | 3.823939 |
| H | -7.498694 | -3.372313 | 2.122416 |
| H | -6.885305 | -4.430576 | 3.427775 |
| C | 0.301114 | -4.155701 | -1.017173 |
| C | 1.418449 | -4.533598 | -1.299657 |
| C | 2.729707 | -4.987929 | -1.633042 |
| C | 2.906988 | -5.950954 | -2.647028 |
| C | 3.855838 | -4.481311 | -0.954244 |
| C | 4.186390 | -6.396263 | -2.970877 |
| H | 2.039177 | -6.340231 | -3.170121 |
| C | 5.130757 | -4.933142 | -1.287544 |
| H | 3.722449 | -3.738564 | -0.174091 |
| C | 5.299619 | -5.889501 | -2.293351 |
| H | 4.315347 | -7.138796 | -3.752962 |
| H | 5.994652 | -4.537500 | -0.761627 |
| H | 6.295971 | -6.238722 | -2.548907 |
| H | -0.701759 | -1.720077 | -1.744578 |
| O | -1.367213 | -2.611638 | -1.906403 |
| H | -2.292859 | -2.309473 | -1.809249 |

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**INT-2**

*G*sol(DCM) = -3349.717163 Hartree

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| | | | |
|---|---|---|---|
| H | 2.403488 | 0.893977 | 0.968071 |
| N | 3.383495 | 1.138029 | 1.297466 |
| C | 3.958545 | 0.309672 | 2.134695 |
| H | 4.982525 | 0.504808 | 2.439947 |
| C | -2.794266 | -0.361368 | -5.733371 |
| C | -2.811164 | -0.394038 | -4.355287 |
| C | -1.753009 | -0.999591 | -3.620161 |
| C | -0.650287 | -1.544274 | -4.356564 |
| C | -0.671037 | -1.510691 | -5.778167 |
| C | -1.721280 | -0.935502 | -6.457085 |
| H | -3.610518 | 0.114851 | -6.269651 |
| H | -3.635866 | 0.060218 | -3.818383 |
| C | -1.724311 | -1.049758 | -2.182623 |
| C | 0.452144 | -2.094558 | -3.653831 |
| H | 0.169037 | -1.939478 | -6.319071 |
| H | -1.724387 | -0.909189 | -7.543076 |
| C | 0.526783 | -2.067756 | -2.276132 |
| C | -0.569260 | -1.503304 | -1.557544 |
| H | 1.268089 | -2.531794 | -4.223485 |
| C | -2.883850 | -0.599661 | -1.357352 |
| C | -4.191519 | -1.181108 | -1.504741 |
| C | -2.702109 | 0.387847 | -0.397121 |
| C | -4.450399 | -2.311639 | -2.330222 |
| C | -5.284273 | -0.631328 | -0.757174 |
| C | -3.782573 | 0.960221 | 0.338064 |
| C | -5.718385 | -2.842383 | -2.435145 |
| H | -3.631212 | -2.768839 | -2.873119 |
| C | -6.583921 | -1.190677 | -0.900929 |
| C | -5.048397 | 0.452979 | 0.126507 |
| C | -6.802039 | -2.271522 | -1.724932 |
| H | -5.886815 | -3.711239 | -3.065523 |
| H | -7.402240 | -0.752802 | -0.334594 |
| H | -5.890738 | 0.879718 | 0.664807 |
| H | -7.797500 | -2.695360 | -1.822487 |
| O | -0.495208 | -1.481184 | -0.179534 |
| O | -1.436087 | 0.895465 | -0.184273 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| P | -0.307918 | -0.030452 | 0.615782 | C | -2.857984 | 4.922406 | -1.071430 |
| O | 1.002286 | 0.620020 | 0.226225 | H | -3.301919 | 2.856246 | -1.323582 |
| O | -0.674413 | -0.295797 | 2.039034 | C | -3.953982 | 1.540688 | 5.497420 |
| C | 1.712418 | -2.643482 | -1.567174 | H | -3.552411 | 3.635838 | 5.664768 |
| C | 2.964943 | -1.985895 | -1.630624 | H | -3.102264 | 5.101657 | 3.766559 |
| C | 1.587091 | -3.870816 | -0.871293 | H | -4.305282 | -0.552037 | 5.016055 |
| C | 4.115329 | -2.576447 | -0.980808 | H | -2.651489 | 6.603435 | 1.893377 |
| C | 3.153285 | -0.734993 | -2.305511 | C | -2.667475 | 6.001834 | -0.160138 |
| C | 2.741132 | -4.442561 | -0.214466 | H | -2.774897 | 5.103898 | -2.139546 |
| C | 0.353726 | -4.596820 | -0.798984 | H | -4.060871 | 1.388960 | 6.567940 |
| C | 5.380230 | -1.909860 | -1.056720 | H | -2.435474 | 6.992618 | -0.540815 |
| C | 3.972471 | -3.782747 | -0.288557 | C | 3.926446 | 2.317294 | 0.745007 |
| C | 4.382175 | -0.128294 | -2.355446 | C | 5.168417 | 2.837435 | 1.112152 |
| H | 2.299504 | -0.263097 | -2.777568 | C | 3.128521 | 2.974139 | -0.214544 |
| C | 2.602390 | -5.679683 | 0.491836 | C | 5.619987 | 4.012831 | 0.511742 |
| C | 0.261702 | -5.781364 | -0.113982 | H | 5.791247 | 2.360402 | 1.859940 |
| H | -0.520557 | -4.197865 | -1.301534 | C | 3.577451 | 4.144948 | -0.809385 |
| C | 5.515357 | -0.723226 | -1.727466 | H | 2.169758 | 2.542729 | -0.474924 |
| H | 6.234794 | -2.371919 | -0.568179 | C | 4.846594 | 4.677155 | -0.444776 |
| H | 4.839883 | -4.219966 | 0.201429 | H | 6.583683 | 4.411604 | 0.803358 |
| H | 4.495262 | 0.820134 | -2.873105 | O | 2.892656 | 4.853492 | -1.741084 |
| H | 3.479713 | -6.092063 | 0.984253 | O | 5.202573 | 5.819421 | -1.074231 |
| C | 1.398772 | -6.331347 | 0.546287 | C | 1.616943 | 4.363417 | -2.153027 |
| H | -0.686469 | -6.310532 | -0.074736 | H | 0.911955 | 4.329740 | -1.314066 |
| H | 6.481197 | -0.228450 | -1.780237 | H | 1.258123 | 5.070183 | -2.902025 |
| H | 1.305884 | -7.269954 | 1.085428 | H | 1.700822 | 3.366016 | -2.600466 |
| C | -3.564545 | 2.094861 | 1.289257 | C | 6.465468 | 6.406230 | -0.757890 |
| C | -3.694234 | 1.886050 | 2.683699 | H | 6.536965 | 7.300740 | -1.377210 |
| C | -3.269598 | 3.385937 | 0.786603 | H | 6.517701 | 6.687203 | 0.300224 |
| C | -3.529554 | 3.001437 | 3.590902 | H | 7.289717 | 5.725431 | -0.999509 |
| C | -3.969903 | 0.600205 | 3.254951 | C | 3.304247 | -0.802583 | 2.653939 |
| C | -3.091426 | 4.488093 | 1.704998 | C | 2.755555 | -1.773400 | 3.153806 |
| C | -3.150879 | 3.662625 | -0.614361 | C | 2.080109 | -2.883437 | 3.712331 |
| C | -3.673606 | 2.784928 | 4.998733 | C | 2.792592 | -3.854421 | 4.451387 |
| C | -3.229862 | 4.267811 | 3.079486 | C | 0.684542 | -3.017244 | 3.527008 |
| C | -4.097955 | 0.434279 | 4.610018 | C | 2.117633 | -4.944877 | 4.988563 |
| H | -4.069602 | -0.253838 | 2.595349 | H | 3.863092 | -3.741656 | 4.589744 |
| C | -2.785954 | 5.787252 | 1.187599 | C | 0.025981 | -4.114126 | 4.074610 |

| | | | |
|---|---|---|---|
| H | 0.146113 | -2.253879 | 2.970123 |
| C | 0.736599 | -5.076420 | 4.800652 |
| H | 2.664511 | -5.693064 | 5.554313 |
| H | -1.045826 | -4.220570 | 3.936296 |
| H | 0.213870 | -5.929817 | 5.223054 |

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**INT-3**

*G*sol(DCM) = -3945.659243 Hartree

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| | | | |
|---|---|---|---|
| C | 4.262933 | 0.907913 | 1.803199 |
| C | 3.142297 | 0.563492 | 2.472481 |
| H | 1.514736 | -1.297563 | -0.468944 |
| H | 2.169580 | 0.996227 | 2.270914 |
| H | 3.177991 | -0.225863 | 3.215028 |
| N | 2.393435 | -1.881964 | -0.567483 |
| C | 2.632553 | -2.777364 | 0.359216 |
| H | 3.482427 | -3.441501 | 0.230754 |
| C | -5.720781 | 0.701562 | -4.370013 |
| C | -5.095127 | 0.904527 | -3.158365 |
| C | -4.417246 | -0.156141 | -2.493838 |
| C | -4.379545 | -1.436620 | -3.136579 |
| C | -5.049726 | -1.618379 | -4.377597 |
| C | -5.710471 | -0.574116 | -4.984212 |
| H | -6.222925 | 1.530554 | -4.861199 |
| H | -5.104478 | 1.890339 | -2.707685 |
| C | -3.739665 | 0.013529 | -1.236313 |
| C | -3.670658 | -2.501465 | -2.523621 |
| H | -5.019775 | -2.599875 | -4.844365 |
| H | -6.213704 | -0.721528 | -5.935580 |
| C | -2.948102 | -2.324086 | -1.361233 |
| C | -2.955541 | -1.029561 | -0.759597 |
| H | -3.691231 | -3.481145 | -2.993990 |
| C | -3.852614 | 1.275215 | -0.446933 |
| C | -5.128354 | 1.774016 | -0.005934 |
| C | -2.706493 | 1.974045 | -0.090572 |
| C | -6.344468 | 1.051367 | -0.166794 |
| C | -5.184294 | 3.038937 | 0.666006 |
| C | -2.747893 | 3.244318 | 0.558272 |
| C | -7.543527 | 1.564980 | 0.279292 |
| H | -6.322686 | 0.074301 | -0.635317 |
| C | -6.439122 | 3.549297 | 1.098856 |
| C | -3.982998 | 3.754681 | 0.902227 |
| C | -7.598457 | 2.832284 | 0.908120 |
| H | -8.455459 | 0.988110 | 0.151857 |
| H | -6.461841 | 4.515626 | 1.596601 |
| H | -4.041301 | 4.726480 | 1.385560 |
| H | -8.551171 | 3.227909 | 1.248518 |
| O | -2.212918 | -0.846560 | 0.389930 |
| O | -1.472011 | 1.462788 | -0.440672 |
| P | -0.868919 | 0.137486 | 0.364174 |
| O | 0.168855 | -0.400767 | -0.598853 |
| O | -0.551170 | 0.423220 | 1.796105 |
| C | -2.234816 | -3.476887 | -0.727125 |
| C | -1.078528 | -4.024436 | -1.332739 |
| C | -2.757451 | -4.051476 | 0.458252 |
| C | -0.431771 | -5.170872 | -0.731361 |
| C | -0.497315 | -3.484785 | -2.527206 |
| C | -2.095316 | -5.189772 | 1.054497 |
| C | -3.943683 | -3.563844 | 1.097236 |
| C | 0.735401 | -5.720429 | -1.351869 |
| C | -0.953092 | -5.718981 | 0.444367 |
| C | 0.619533 | -4.044146 | -3.093751 |
| H | -0.953277 | -2.613189 | -2.982740 |
| C | -2.627638 | -5.759937 | 2.254616 |
| C | -4.424780 | -4.139709 | 2.245284 |
| H | -4.471336 | -2.724923 | 0.657321 |
| C | 1.246954 | -5.178933 | -2.501842 |
| H | 1.206199 | -6.583737 | -0.887805 |
| H | -0.460642 | -6.578610 | 0.893838 |
| H | 1.039144 | -3.613209 | -3.998253 |
| H | -2.113135 | -6.612447 | 2.691361 |
| C | -3.757172 | -5.250225 | 2.838484 |
| H | -5.326668 | -3.749081 | 2.708495 |
| H | 2.131125 | -5.607608 | -2.965391 |
| H | -4.152317 | -5.691606 | 3.749160 |
| C | -1.504053 | 4.030663 | 0.831515 |

| | | | |
|---|---|---|---|
| C | -1.031201 | 4.173307 | 2.158165 |
| C | -0.836119 | 4.676682 | -0.237040 |
| C | 0.140263 | 4.983285 | 2.415129 |
| C | -1.658085 | 3.536629 | 3.279467 |
| C | 0.339746 | 5.473568 | 0.031525 |
| C | -1.286852 | 4.592251 | -1.594751 |
| C | 0.605784 | 5.132182 | 3.760778 |
| C | 0.795416 | 5.606160 | 1.347840 |
| C | -1.179906 | 3.703834 | 4.553584 |
| H | -2.523019 | 2.907025 | 3.106182 |
| C | 1.009737 | 6.120001 | -1.055776 |
| C | -0.619463 | 5.230084 | -2.609250 |
| H | -2.177303 | 4.014543 | -1.817270 |
| C | -0.034893 | 4.515902 | 4.802491 |
| H | 1.484290 | 5.748570 | 3.935519 |
| H | 1.676472 | 6.212677 | 1.546167 |
| H | -1.673809 | 3.208352 | 5.384993 |
| H | 1.898371 | 6.706489 | -0.836655 |
| C | 0.548155 | 6.002444 | -2.340420 |
| H | -0.983785 | 5.150346 | -3.629823 |
| H | 0.327696 | 4.636925 | 5.819496 |
| H | 1.064594 | 6.498623 | -3.157370 |
| C | 2.995231 | 2.241362 | 0.174448 |
| C | 5.239916 | 2.907790 | 0.775814 |
| C | 3.203474 | 2.929960 | -1.173068 |
| H | 2.498345 | 2.940853 | 0.869144 |
| H | 2.336249 | 1.378299 | 0.038726 |
| C | 5.374538 | 3.573470 | -0.590167 |
| H | 4.897990 | 3.656838 | 1.511564 |
| H | 6.214081 | 2.536162 | 1.101841 |
| H | 2.259358 | 3.343714 | -1.536795 |
| H | 3.577079 | 2.195678 | -1.904975 |
| H | 6.016968 | 4.456410 | -0.520540 |
| H | 5.823711 | 2.864489 | -1.305053 |
| N | 4.284381 | 1.789087 | 0.699987 |
| C | 5.570174 | 0.266381 | 2.137536 |
| C | 5.944792 | 0.046079 | 3.472889 |
| C | 6.438206 | -0.165607 | 1.118994 |
| C | 7.141817 | -0.602119 | 3.782492 |
| H | 5.296074 | 0.398612 | 4.269562 |
| C | 7.635907 | -0.811209 | 1.428066 |
| H | 6.156298 | -0.000688 | 0.083294 |
| C | 7.992355 | -1.033777 | 2.761454 |
| H | 7.414823 | -0.759981 | 4.822570 |
| H | 8.290232 | -1.144792 | 0.626736 |
| H | 8.926626 | -1.533849 | 3.002070 |
| C | 3.161794 | -1.628053 | -1.723782 |
| C | 4.457305 | -2.114604 | -1.900168 |
| C | 2.553392 | -0.828633 | -2.713231 |
| C | 5.140552 | -1.822048 | -3.081684 |
| H | 4.960488 | -2.690281 | -1.131913 |
| C | 3.234268 | -0.536906 | -3.887738 |
| H | 1.549927 | -0.460632 | -2.537733 |
| C | 4.550187 | -1.045790 | -4.082680 |
| H | 6.148398 | -2.197346 | -3.208597 |
| O | 2.740687 | 0.213241 | -4.903744 |
| O | 5.137156 | -0.712747 | -5.254520 |
| C | 1.426284 | 0.751233 | -4.762434 |
| H | 1.363432 | 1.425914 | -3.900709 |
| H | 1.236751 | 1.310856 | -5.678989 |
| H | 0.680588 | -0.045822 | -4.658244 |
| C | 6.458757 | -1.188203 | -5.512201 |
| H | 6.719833 | -0.808905 | -6.500535 |
| H | 7.169251 | -0.803013 | -4.771837 |
| H | 6.491057 | -2.283732 | -5.518622 |
| C | 1.844722 | -2.903274 | 1.498213 |
| C | 1.192733 | -3.029798 | 2.524022 |
| C | 0.413968 | -3.131875 | 3.700264 |
| C | 0.606531 | -4.208777 | 4.594629 |
| C | -0.560599 | -2.145463 | 3.978084 |
| C | -0.169581 | -4.297242 | 5.744920 |
| H | 1.358187 | -4.959703 | 4.373334 |
| C | -1.326383 | -2.250118 | 5.135340 |
| H | -0.689117 | -1.313893 | 3.288898 |
| C | -1.135616 | -3.320741 | 6.015831 |
| H | -0.023892 | -5.125220 | 6.432061 |

| | | | |
|---|---|---|---|
| H | -2.074809 | -1.494182 | 5.353708 |
| H | -1.738967 | -3.394546 | 6.916106 |
| O | 4.114359 | 4.021226 | -1.076577 |

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**TS-3**

*G*sol(DCM) = -3945.641482 Hartree

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| | | | |
|---|---|---|---|
| C | -4.589631 | 0.465287 | -1.567759 |
| C | -3.563297 | -0.300539 | -2.140663 |
| H | -1.532662 | -1.328655 | 0.334705 |
| H | -2.564332 | 0.109685 | -2.234181 |
| H | -3.871754 | -0.954584 | -2.946764 |
| N | -2.512556 | -1.671279 | 0.284815 |
| C | -2.976771 | -2.020551 | -0.933149 |
| H | -3.973366 | -2.445497 | -0.965822 |
| C | 5.759365 | 1.195230 | 4.323924 |
| C | 5.122798 | 1.309717 | 3.106430 |
| C | 4.513154 | 0.182761 | 2.485825 |
| C | 4.554553 | -1.070231 | 3.180613 |
| C | 5.233472 | -1.159448 | 4.426902 |
| C | 5.828197 | -0.052631 | 4.989412 |
| H | 6.208516 | 2.073192 | 4.780171 |
| H | 5.071449 | 2.275449 | 2.616685 |
| C | 3.829298 | 0.257730 | 1.222803 |
| C | 3.913538 | -2.200915 | 2.612318 |
| H | 5.263381 | -2.121231 | 4.933095 |
| H | 6.339049 | -0.129828 | 5.945019 |
| C | 3.185494 | -2.117151 | 1.443089 |
| C | 3.114767 | -0.851424 | 0.786209 |
| H | 3.992600 | -3.157075 | 3.123262 |
| C | 3.859598 | 1.493064 | 0.386136 |
| C | 5.098671 | 2.058551 | -0.077243 |
| C | 2.668249 | 2.100619 | 0.010266 |
| C | 6.359746 | 1.423271 | 0.104919 |
| C | 5.070527 | 3.299013 | -0.794978 |
| C | 2.626535 | 3.348039 | -0.682283 |
| C | 7.521786 | 1.997149 | -0.365003 |
| H | 6.402050 | 0.464785 | 0.609198 |
| C | 6.288412 | 3.873868 | -1.251792 |
| C | 3.824184 | 3.925958 | -1.050469 |
| C | 7.492558 | 3.241363 | -1.040076 |
| H | 8.469825 | 1.486223 | -0.220506 |
| H | 6.246666 | 4.820650 | -1.784721 |
| H | 3.817450 | 4.882064 | -1.567546 |
| H | 8.416754 | 3.685448 | -1.398887 |
| O | 2.371574 | -0.762299 | -0.372260 |
| O | 1.472926 | 1.520243 | 0.380252 |
| P | 0.958778 | 0.129385 | -0.389046 |
| O | -0.050890 | -0.451428 | 0.572792 |
| O | 0.646205 | 0.362652 | -1.831953 |
| C | 2.549733 | -3.339642 | 0.858355 |
| C | 1.411096 | -3.917056 | 1.468744 |
| C | 3.136747 | -3.951854 | -0.276695 |
| C | 0.844256 | -5.130458 | 0.920188 |
| C | 0.773658 | -3.346671 | 2.619307 |
| C | 2.557084 | -5.160264 | -0.818654 |
| C | 4.312683 | -3.436032 | -0.912856 |
| C | -0.302777 | -5.712472 | 1.548624 |
| C | 1.427324 | -5.715106 | -0.208043 |
| C | -0.323748 | -3.936441 | 3.192589 |
| H | 1.169941 | -2.426850 | 3.033886 |
| C | 3.161865 | -5.775049 | -1.960893 |
| C | 4.864764 | -4.056417 | -2.004488 |
| H | 4.776014 | -2.539872 | -0.514990 |
| C | -0.870761 | -5.138051 | 2.654439 |
| H | -0.712710 | -6.626203 | 1.125096 |
| H | 0.997054 | -6.627241 | -0.615977 |
| H | -0.788575 | -3.481786 | 4.062851 |
| H | 2.710512 | -6.681774 | -2.356353 |
| C | 4.282296 | -5.241300 | -2.540894 |
| H | 5.758121 | -3.644171 | -2.465606 |
| H | -1.740052 | -5.590313 | 3.123735 |
| H | 4.733841 | -5.718584 | -3.406118 |
| C | 1.332501 | 4.042354 | -0.971148 |
| C | 0.833006 | 4.095449 | -2.294299 |
| C | 0.639273 | 4.691325 | 0.079445 |

| | | | |
|---|---|---|---|
| C | -0.393046 | 4.814798 | -2.566495 |
| C | 1.485592 | 3.452121 | -3.396790 |
| C | -0.589968 | 5.398077 | -0.203374 |
| C | 1.113383 | 4.695268 | 1.431946 |
| C | -0.885774 | 4.872748 | -3.909590 |
| C | -1.072665 | 5.440886 | -1.516272 |
| C | 0.980074 | 3.530533 | -4.668795 |
| H | 2.391322 | 2.887536 | -3.209330 |
| C | -1.283317 | 6.049715 | 0.865967 |
| C | 0.420520 | 5.333535 | 2.429019 |
| H | 2.042123 | 4.185474 | 1.663961 |
| C | -0.219578 | 4.254043 | -4.933731 |
| H | -1.804800 | 5.422939 | -4.096819 |
| H | -1.993516 | 5.980895 | -1.726180 |
| H | 1.494004 | 3.031800 | -5.485958 |
| H | -2.209355 | 6.570738 | 0.636766 |
| C | -0.797001 | 6.018750 | 2.146295 |
| H | 0.802816 | 5.321242 | 3.446035 |
| H | -0.602711 | 4.306214 | -5.949096 |
| H | -1.332170 | 6.517671 | 2.949399 |
| C | -3.001907 | 1.970012 | -0.411582 |
| C | -5.363750 | 2.595288 | -0.543944 |
| C | -2.994053 | 2.581524 | 0.992348 |
| H | -2.660592 | 2.711753 | -1.146875 |
| H | -2.316685 | 1.123094 | -0.424067 |
| C | -5.251807 | 3.156914 | 0.870641 |
| H | -5.160915 | 3.400626 | -1.264290 |
| H | -6.366319 | 2.215272 | -0.727498 |
| H | -2.009690 | 3.009713 | 1.194211 |
| H | -3.202065 | 1.797565 | 1.735235 |
| H | -5.929706 | 4.007424 | 0.982340 |
| H | -5.525710 | 2.385928 | 1.608246 |
| N | -4.364777 | 1.530797 | -0.762191 |
| C | -5.999322 | 0.041423 | -1.822548 |
| C | -6.450371 | -0.119287 | -3.142203 |
| C | -6.875424 | -0.248302 | -0.761649 |
| C | -7.753491 | -0.550047 | -3.396073 |
| H | -5.784456 | 0.109983 | -3.968624 |
| C | -8.172842 | -0.689653 | -1.019061 |
| H | -6.527821 | -0.150261 | 0.262595 |
| C | -8.616371 | -0.837930 | -2.336501 |
| H | -8.092465 | -0.660027 | -4.422060 |
| H | -8.835460 | -0.922132 | -0.190406 |
| H | -9.628472 | -1.178728 | -2.535021 |
| C | -3.278219 | -1.501051 | 1.453029 |
| C | -4.591196 | -1.953523 | 1.587686 |
| C | -2.640459 | -0.868152 | 2.542026 |
| C | -5.273202 | -1.752112 | 2.794462 |
| H | -5.100396 | -2.473169 | 0.784370 |
| C | -3.315228 | -0.678153 | 3.742143 |
| H | -1.617760 | -0.533476 | 2.415990 |
| C | -4.660494 | -1.119247 | 3.874511 |
| H | -6.292027 | -2.110427 | 2.881125 |
| O | -2.783137 | -0.081164 | 4.841475 |
| O | -5.243503 | -0.884380 | 5.081695 |
| C | -1.436055 | 0.379896 | 4.767850 |
| H | -1.317360 | 1.144614 | 3.991003 |
| H | -1.218738 | 0.815668 | 5.743941 |
| H | -0.741652 | -0.446139 | 4.572891 |
| C | -6.590839 | -1.307521 | 5.265626 |
| H | -6.856057 | -1.020404 | 6.284098 |
| H | -7.265983 | -0.810037 | 4.558389 |
| H | -6.687323 | -2.394732 | 5.156299 |
| C | -2.040192 | -2.513095 | -1.884564 |
| C | -1.253317 | -2.874277 | -2.738437 |
| C | -0.302966 | -3.268734 | -3.724109 |
| C | -0.563098 | -4.356950 | -4.581479 |
| C | 0.906112 | -2.552265 | -3.851226 |
| C | 0.373980 | -4.723614 | -5.544527 |
| H | -1.494952 | -4.905012 | -4.482087 |
| C | 1.832625 | -2.929134 | -4.820957 |
| H | 1.089897 | -1.704333 | -3.196987 |
| C | 1.572128 | -4.012626 | -5.666142 |
| H | 0.169657 | -5.564345 | -6.201323 |
| H | 2.762358 | -2.375795 | -4.917378 |
| H | 2.300072 | -4.301513 | -6.419064 |

| | | | |
|---|---|---|---|
| O | -3.938576 | 3.636094 | 1.121417 |

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**INT-4**

*G*sol(DCM) = -3945.668835 Hartree

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| | | | |
|---|---|---|---|
| C | 4.113801 | 0.606836 | 1.366932 |
| C | 3.000392 | -0.285394 | 1.817622 |
| H | 1.616125 | -1.428232 | -0.321835 |
| H | 2.008243 | 0.151268 | 1.692125 |
| H | 3.159677 | -0.417569 | 2.893002 |
| N | 2.551691 | -1.819992 | -0.167920 |
| C | 2.981340 | -1.754639 | 1.210968 |
| H | 3.991101 | -2.165624 | 1.295586 |
| C | -5.805001 | 1.468155 | -4.224267 |
| C | -5.128452 | 1.536906 | -3.025008 |
| C | -4.535182 | 0.378882 | -2.447266 |
| C | -4.637271 | -0.857257 | -3.165452 |
| C | -5.356399 | -0.898901 | -4.391480 |
| C | -5.932835 | 0.237481 | -4.912618 |
| H | -6.240332 | 2.368969 | -4.648210 |
| H | -5.031891 | 2.490017 | -2.517570 |
| C | -3.809398 | 0.406165 | -1.205853 |
| C | -4.017101 | -2.019272 | -2.638853 |
| H | -5.432283 | -1.848269 | -4.916017 |
| H | -6.474662 | 0.196269 | -5.853276 |
| C | -3.250730 | -1.983042 | -1.491846 |
| C | -3.115626 | -0.732726 | -0.815151 |
| H | -4.145496 | -2.962413 | -3.163730 |
| C | -3.778119 | 1.623755 | -0.343507 |
| C | -4.985898 | 2.210158 | 0.173457 |
| C | -2.559319 | 2.193404 | 0.002908 |
| C | -6.268171 | 1.610249 | 0.021566 |
| C | -4.901928 | 3.433732 | 0.915232 |
| C | -2.463619 | 3.428874 | 0.711296 |
| C | -7.398407 | 2.201627 | 0.544442 |
| H | -6.351743 | 0.665007 | -0.502151 |
| C | -6.088275 | 4.027475 | 1.427449 |
| C | -3.632579 | 4.027043 | 1.135088 |
| C | -7.314449 | 3.429020 | 1.245174 |
| H | -8.363498 | 1.717536 | 0.422150 |
| H | -6.004457 | 4.961315 | 1.978003 |
| H | -3.583912 | 4.973736 | 1.667014 |
| H | -8.214184 | 3.887193 | 1.645982 |
| O | -2.330407 | -0.689190 | 0.317975 |
| O | -1.392266 | 1.588672 | -0.413105 |
| P | -0.893159 | 0.163299 | 0.308078 |
| O | 0.080826 | -0.415057 | -0.687167 |
| O | -0.530799 | 0.357795 | 1.747647 |
| C | -2.646750 | -3.239646 | -0.946728 |
| C | -1.558459 | -3.858833 | -1.606271 |
| C | -3.221751 | -3.843634 | 0.199206 |
| C | -1.024995 | -5.102186 | -1.092091 |
| C | -0.944804 | -3.307765 | -2.779133 |
| C | -2.676562 | -5.083386 | 0.704752 |
| C | -4.355093 | -3.290568 | 0.879712 |
| C | 0.069437 | -5.727928 | -1.770235 |
| C | -1.591652 | -5.675703 | 0.049871 |
| C | 0.097527 | -3.943629 | -3.403721 |
| H | -1.317561 | -2.368737 | -3.172262 |
| C | -3.270807 | -5.691438 | 1.855874 |
| C | -4.899320 | -3.906113 | 1.978040 |
| H | -4.793317 | -2.370205 | 0.509782 |
| C | 0.614679 | -5.171326 | -2.896132 |
| H | 0.455778 | -6.661880 | -1.369329 |
| H | -1.186586 | -6.610299 | 0.431844 |
| H | 0.538887 | -3.509714 | -4.296596 |
| H | -2.844029 | -6.621027 | 2.224484 |
| C | -4.350160 | -5.122162 | 2.478309 |
| H | -5.760773 | -3.465546 | 2.472512 |
| H | 1.442335 | -5.657452 | -3.405001 |
| H | -4.793940 | -5.594310 | 3.350320 |
| C | -1.146139 | 4.096684 | 0.954056 |
| C | -0.591232 | 4.126369 | 2.255774 |
| C | -0.488122 | 4.749800 | -0.116791 |
| C | 0.651827 | 4.830675 | 2.486918 |
| C | -1.204329 | 3.473568 | 3.375353 |

| | | | |
|---|---|---|---|
| C | 0.758323 | 5.442098 | 0.124363 |
| C | -1.015103 | 4.772576 | -1.449435 |
| C | 1.199649 | 4.865761 | 3.809211 |
| C | 1.293450 | 5.465347 | 1.417795 |
| C | -0.645971 | 3.529208 | 4.626258 |
| H | -2.122290 | 2.919705 | 3.217224 |
| C | 1.414988 | 6.098784 | -0.964697 |
| C | -0.356488 | 5.416059 | -2.466205 |
| H | -1.956809 | 4.273540 | -1.650045 |
| C | 0.570183 | 4.238545 | 4.851279 |
| H | 2.130441 | 5.405629 | 3.965967 |
| H | 2.225411 | 5.997431 | 1.597440 |
| H | -1.130359 | 3.023448 | 5.456983 |
| H | 2.353762 | 6.609902 | -0.766608 |
| C | 0.877291 | 6.087814 | -2.224465 |
| H | -0.779030 | 5.418771 | -3.467199 |
| H | 0.994918 | 4.273487 | 5.850707 |
| H | 1.384350 | 6.591592 | -3.042612 |
| C | 2.619024 | 1.967999 | -0.066690 |
| C | 4.892527 | 2.751217 | 0.413508 |
| C | 2.878123 | 2.376857 | -1.523219 |
| H | 2.159746 | 2.794888 | 0.484245 |
| H | 1.956735 | 1.104986 | -0.058004 |
| C | 5.047854 | 3.094711 | -1.067456 |
| H | 4.474348 | 3.616526 | 0.939649 |
| H | 5.843193 | 2.485455 | 0.867020 |
| H | 1.934192 | 2.715669 | -1.956170 |
| H | 3.239849 | 1.508425 | -2.090866 |
| H | 5.707738 | 3.960341 | -1.163482 |
| H | 5.491908 | 2.249230 | -1.614660 |
| N | 3.908342 | 1.653352 | 0.602994 |
| C | 5.472315 | 0.298178 | 1.885462 |
| C | 5.681301 | 0.161649 | 3.269265 |
| C | 6.549129 | 0.090634 | 1.002621 |
| C | 6.948168 | -0.153661 | 3.758836 |
| H | 4.867980 | 0.334412 | 3.966641 |
| C | 7.806557 | -0.246341 | 1.499274 |
| H | 6.390954 | 0.153356 | -0.069138 |
| C | 8.010396 | -0.363294 | 2.876916 |
| H | 7.101580 | -0.237768 | 4.830207 |
| H | 8.625422 | -0.420789 | 0.808165 |
| H | 8.993096 | -0.620379 | 3.260847 |
| C | 3.422952 | -1.684499 | -1.253311 |
| C | 4.775634 | -2.041857 | -1.218746 |
| C | 2.881215 | -1.218094 | -2.476803 |
| C | 5.570477 | -1.922932 | -2.370260 |
| H | 5.230914 | -2.439157 | -0.318579 |
| C | 3.667945 | -1.113478 | -3.619003 |
| H | 1.833105 | -0.942935 | -2.499474 |
| C | 5.043289 | -1.464068 | -3.572051 |
| H | 6.614193 | -2.209856 | -2.309372 |
| O | 3.217458 | -0.675592 | -4.829675 |
| O | 5.739682 | -1.318242 | -4.743063 |
| C | 1.851265 | -0.292056 | -4.939742 |
| H | 1.614692 | 0.548848 | -4.276373 |
| H | 1.710816 | 0.013954 | -5.977706 |
| H | 1.179640 | -1.128373 | -4.711868 |
| C | 7.114125 | -1.675789 | -4.736751 |
| H | 7.477635 | -1.491123 | -5.749250 |
| H | 7.687420 | -1.063433 | -4.028098 |
| H | 7.254475 | -2.735997 | -4.488293 |
| C | 2.078423 | -2.535543 | 2.069695 |
| C | 1.298864 | -3.066628 | 2.831723 |
| C | 0.352390 | -3.629324 | 3.744151 |
| C | 0.575821 | -4.878980 | 4.353296 |
| C | -0.816200 | -2.906373 | 4.060338 |
| C | -0.348362 | -5.389127 | 5.263834 |
| H | 1.474673 | -5.437678 | 4.110603 |
| C | -1.732797 | -3.424846 | 4.972684 |
| H | -0.986803 | -1.945747 | 3.582528 |
| C | -1.501856 | -4.664311 | 5.577882 |
| H | -0.166835 | -6.353268 | 5.730635 |
| H | -2.630503 | -2.861311 | 5.210721 |
| H | -2.218537 | -5.064341 | 6.289689 |
| O | 3.796986 | 3.453395 | -1.627353 |

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**TS-4**

*G*sol(DCM) = -3945.646492 Hartree

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| | | | |
|---|---|---|---|
| C | 1.498781 | 2.122655 | 2.740686 |
| C | 1.833007 | 1.115335 | 1.803010 |
| H | 1.729667 | 0.626126 | -0.812679 |
| H | 0.480177 | 0.920086 | 1.204658 |
| H | 1.886145 | 0.136938 | 2.276653 |
| N | 2.403345 | 1.369443 | -0.623337 |
| C | 2.940287 | 1.309705 | 0.741761 |
| H | 3.434453 | 2.270286 | 0.936348 |
| C | -5.716191 | -4.092446 | -3.042957 |
| C | -5.181771 | -3.127055 | -2.216724 |
| C | -3.935099 | -3.329730 | -1.560934 |
| C | -3.232968 | -4.553648 | -1.813852 |
| C | -3.820274 | -5.537271 | -2.656586 |
| C | -5.038646 | -5.316814 | -3.257543 |
| H | -6.664994 | -3.909009 | -3.539419 |
| H | -5.710732 | -2.191850 | -2.074611 |
| C | -3.332815 | -2.348835 | -0.696850 |
| C | -1.953219 | -4.757959 | -1.237074 |
| H | -3.278339 | -6.463989 | -2.827286 |
| H | -5.475510 | -6.071377 | -3.905307 |
| C | -1.327556 | -3.786545 | -0.482298 |
| C | -2.039114 | -2.574785 | -0.251490 |
| H | -1.442867 | -5.699808 | -1.419756 |
| C | -4.051450 | -1.102960 | -0.296278 |
| C | -5.327909 | -1.152808 | 0.367447 |
| C | -3.484952 | 0.141670 | -0.535610 |
| C | -5.917817 | -2.364959 | 0.824151 |
| C | -6.027930 | 0.071810 | 0.619325 |
| C | -4.168379 | 1.370441 | -0.301764 |
| C | -7.142605 | -2.366096 | 1.456680 |
| H | -5.387272 | -3.299365 | 0.683398 |
| C | -7.298545 | 0.035397 | 1.257514 |
| C | -5.433972 | 1.303607 | 0.245619 |
| C | -7.850046 | -1.157631 | 1.665393 |
| H | -7.566920 | -3.304147 | 1.803555 |
| H | -7.819955 | 0.973778 | 1.428702 |
| H | -5.987365 | 2.222742 | 0.418045 |
| H | -8.817962 | -1.174719 | 2.158029 |
| O | -1.412542 | -1.584976 | 0.504436 |
| O | -2.218763 | 0.218463 | -1.107591 |
| P | -0.881761 | -0.256016 | -0.295613 |
| O | 0.207635 | -0.514819 | -1.278542 |
| O | -0.619218 | 0.762244 | 0.845721 |
| C | 0.040562 | -4.012598 | 0.079488 |
| C | 1.164678 | -4.022001 | -0.781549 |
| C | 0.199828 | -4.251139 | 1.466015 |
| C | 2.480297 | -4.269371 | -0.232358 |
| C | 1.067981 | -3.780969 | -2.191632 |
| C | 1.521384 | -4.486291 | 2.002535 |
| C | -0.905139 | -4.288026 | 2.377670 |
| C | 3.613303 | -4.282094 | -1.107579 |
| C | 2.623801 | -4.489122 | 1.141264 |
| C | 2.177898 | -3.803430 | -2.996485 |
| H | 0.095873 | -3.570033 | -2.621499 |
| C | 1.673494 | -4.721952 | 3.406064 |
| C | -0.718182 | -4.520819 | 3.716382 |
| H | -1.908331 | -4.134504 | 1.994584 |
| C | 3.469724 | -4.060576 | -2.451408 |
| H | 4.594106 | -4.467521 | -0.677418 |
| H | 3.616500 | -4.664896 | 1.549627 |
| H | 2.075409 | -3.618075 | -4.062347 |
| H | 2.674967 | -4.893564 | 3.793176 |
| C | 0.588678 | -4.736861 | 4.242472 |
| H | -1.574097 | -4.544488 | 4.385297 |
| H | 4.336694 | -4.072854 | -3.106024 |
| H | 0.717015 | -4.918370 | 5.305912 |
| C | -3.562148 | 2.692369 | -0.653300 |
| C | -3.202610 | 3.599076 | 0.374497 |
| C | -3.401126 | 3.055756 | -2.013130 |
| C | -2.663621 | 4.895951 | 0.024500 |
| C | -3.344518 | 3.295338 | 1.768975 |
| C | -2.842366 | 4.346535 | -2.347120 |
| C | -3.793170 | 2.202067 | -3.095035 |

| | | | |
|---|---|---|---|
| C | -2.325505 | 5.818888 | 1.066062 |
| C | -2.488965 | 5.229969 | -1.321940 |
| C | -3.016519 | 4.210799 | 2.737070 |
| H | -3.724864 | 2.322544 | 2.058092 |
| C | -2.676953 | 4.703188 | -3.723295 |
| C | -3.623696 | 2.582444 | -4.401692 |
| H | -4.239447 | 1.239374 | -2.871615 |
| C | -2.503219 | 5.493814 | 2.385241 |
| H | -1.931417 | 6.791725 | 0.782615 |
| H | -2.078474 | 6.204187 | -1.578404 |
| H | -3.151883 | 3.959021 | 3.785532 |
| H | -2.249378 | 5.675632 | -3.954826 |
| C | -3.052261 | 3.847427 | -4.724674 |
| H | -3.930777 | 1.915179 | -5.202253 |
| H | -2.257019 | 6.208112 | 3.165956 |
| H | -2.923770 | 4.129464 | -5.765851 |
| C | 1.376599 | 4.000947 | 1.101346 |
| C | 1.365950 | 4.499734 | 3.486222 |
| C | 2.457115 | 5.065571 | 0.911689 |
| H | 0.392418 | 4.477042 | 0.998657 |
| H | 1.456899 | 3.210882 | 0.353652 |
| C | 2.466162 | 5.530141 | 3.209920 |
| H | 0.384759 | 4.986670 | 3.434647 |
| H | 1.497752 | 4.072323 | 4.479063 |
| H | 2.328933 | 5.556748 | -0.056430 |
| H | 3.458437 | 4.607854 | 0.943552 |
| H | 2.373885 | 6.362203 | 3.913336 |
| H | 3.453588 | 5.060594 | 3.343758 |
| N | 1.430805 | 3.438617 | 2.464807 |
| C | 1.062562 | 1.670262 | 4.095242 |
| C | -0.209748 | 2.008528 | 4.585959 |
| C | 1.898999 | 0.845390 | 4.863106 |
| C | -0.633984 | 1.529776 | 5.824651 |
| H | -0.872971 | 2.623314 | 3.984320 |
| C | 1.479416 | 0.386152 | 6.112131 |
| H | 2.880737 | 0.576948 | 4.484165 |
| C | 0.212120 | 0.724518 | 6.592947 |
| H | -1.625714 | 1.782386 | 6.188585 |
| H | 2.139620 | -0.239460 | 6.705670 |
| H | -0.117860 | 0.358113 | 7.560907 |
| C | 3.247558 | 1.612863 | -1.721415 |
| C | 4.476566 | 2.271722 | -1.628836 |
| C | 2.790406 | 1.212380 | -2.998100 |
| C | 5.223495 | 2.540710 | -2.787797 |
| H | 4.879843 | 2.578415 | -0.670344 |
| C | 3.532070 | 1.475637 | -4.143640 |
| H | 1.843771 | 0.688412 | -3.063792 |
| C | 4.773242 | 2.156985 | -4.045560 |
| H | 6.173174 | 3.053462 | -2.683904 |
| O | 3.155787 | 1.115686 | -5.406141 |
| O | 5.434125 | 2.372367 | -5.228580 |
| C | 1.928614 | 0.412595 | -5.559978 |
| H | 1.076393 | 1.010785 | -5.213993 |
| H | 1.826483 | 0.221241 | -6.629607 |
| H | 1.941643 | -0.541528 | -5.018078 |
| C | 6.681270 | 3.047332 | -5.165885 |
| H | 7.036523 | 3.120715 | -6.195533 |
| H | 6.574363 | 4.056572 | -4.746326 |
| H | 7.413986 | 2.488612 | -4.568457 |
| C | 3.959510 | 0.251538 | 0.910423 |
| C | 4.780425 | -0.636092 | 1.026397 |
| C | 5.754991 | -1.675686 | 1.149839 |
| C | 6.618327 | -1.973807 | 0.076199 |
| C | 5.866720 | -2.420147 | 2.341565 |
| C | 7.563930 | -2.991243 | 0.194220 |
| H | 6.536716 | -1.402515 | -0.843368 |
| C | 6.815628 | -3.435612 | 2.451505 |
| H | 5.205771 | -2.193948 | 3.172740 |
| C | 7.665820 | -3.725499 | 1.379857 |
| H | 8.223471 | -3.210692 | -0.640800 |
| H | 6.892261 | -4.001272 | 3.375957 |
| H | 8.404090 | -4.517467 | 1.468781 |
| O | 2.354413 | 6.080523 | 1.904676 |

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**INT-5**

*G*sol(DCM) = -3945.658845 Hartree

| | | | |
|---|---|---|---|
| C | 3.263824 | -1.490486 | 2.333199 |
| C | 3.140250 | -1.107083 | 1.040232 |
| H | 1.557830 | 0.433546 | -0.588785 |
| H | 2.977597 | -1.859125 | 0.274796 |
| N | 2.050078 | 0.991325 | 0.152936 |
| C | 3.363684 | 0.302063 | 0.559931 |
| H | 3.756129 | 0.892551 | 1.392866 |
| C | -6.612345 | -1.381425 | -3.526035 |
| C | -5.841247 | -0.981045 | -2.455779 |
| C | -4.673801 | -1.703350 | -2.079198 |
| C | -4.304206 | -2.841272 | -2.868460 |
| C | -5.130375 | -3.239183 | -3.955433 |
| C | -6.264242 | -2.528878 | -4.278866 |
| H | -7.493643 | -0.807077 | -3.798073 |
| H | -6.117992 | -0.093139 | -1.899071 |
| C | -3.832703 | -1.314987 | -0.978539 |
| C | -3.112620 | -3.545907 | -2.558945 |
| H | -4.839974 | -4.111989 | -4.534972 |
| H | -6.885094 | -2.837161 | -5.115250 |
| C | -2.259000 | -3.132088 | -1.557051 |
| C | -2.626958 | -1.980658 | -0.801027 |
| H | -2.861066 | -4.428103 | -3.141838 |
| C | -4.207477 | -0.204316 | -0.054935 |
| C | -5.433017 | -0.223165 | 0.697715 |
| C | -3.342907 | 0.869264 | 0.113076 |
| C | -6.309248 | -1.344691 | 0.727937 |
| C | -5.778292 | 0.920667 | 1.489619 |
| C | -3.678343 | 2.022009 | 0.883199 |
| C | -7.471745 | -1.320501 | 1.468441 |
| H | -6.048707 | -2.235704 | 0.168472 |
| C | -6.992949 | 0.920863 | 2.229280 |
| C | -4.894652 | 2.029289 | 1.535337 |
| C | -7.827628 | -0.173563 | 2.218581 |
| H | -8.119093 | -2.193053 | 1.480964 |
| H | -7.243177 | 1.801897 | 2.815064 |
| H | -5.181182 | 2.900836 | 2.118106 |
| H | -8.750203 | -0.165925 | 2.792005 |
| O | -1.759177 | -1.553244 | 0.192286 |
| O | -2.128795 | 0.863644 | -0.549330 |
| P | -0.914805 | -0.148602 | -0.045874 |
| O | 0.031988 | -0.239735 | -1.219517 |
| O | -0.366195 | 0.244980 | 1.302716 |
| C | -1.014911 | -3.906073 | -1.250433 |
| C | 0.102563 | -3.834950 | -2.115195 |
| C | -0.987750 | -4.754163 | -0.116702 |
| C | 1.278382 | -4.628359 | -1.828088 |
| C | 0.132443 | -2.995992 | -3.277178 |
| C | 0.193800 | -5.539403 | 0.160518 |
| C | -2.101078 | -4.888738 | 0.775322 |
| C | 2.402476 | -4.556126 | -2.712059 |
| C | 1.294183 | -5.453922 | -0.699252 |
| C | 1.227661 | -2.958218 | -4.101063 |
| H | -0.729476 | -2.376553 | -3.495178 |
| C | 0.208037 | -6.399698 | 1.304189 |
| C | -2.048867 | -5.725847 | 1.860481 |
| H | -3.002512 | -4.318404 | 0.579777 |
| C | 2.379610 | -3.750465 | -3.819912 |
| H | 3.275410 | -5.163208 | -2.484650 |
| H | 2.181036 | -6.046686 | -0.486549 |
| H | 1.223710 | -2.313992 | -4.976046 |
| H | 1.106579 | -6.978620 | 1.501054 |
| C | -0.878567 | -6.491958 | 2.133267 |
| H | -2.908219 | -5.809629 | 2.520119 |
| H | 3.235347 | -3.711537 | -4.488550 |
| H | -0.855686 | -7.149314 | 2.997983 |
| C | -2.761069 | 3.201516 | 0.966378 |
| C | -2.084317 | 3.489098 | 2.176651 |
| C | -2.603393 | 4.049244 | -0.157040 |
| C | -1.232760 | 4.656318 | 2.257965 |
| C | -2.189399 | 2.661098 | 3.342334 |
| C | -1.733979 | 5.200767 | -0.068285 |
| C | -3.285532 | 3.825358 | -1.397152 |
| C | -0.560762 | 4.947381 | 3.487996 |
| C | -1.076693 | 5.475459 | 1.135578 |
| C | -1.528025 | 2.974163 | 4.502356 |

| | | | |
|---|---|---|---|
| H | -2.801290 | 1.767850 | 3.295065 |
| C | -1.568552 | 6.042572 | -1.214048 |
| C | -3.105657 | 4.659180 | -2.471414 |
| H | -3.960358 | 2.980507 | -1.480434 |
| C | -0.705566 | 4.136278 | 4.582190 |
| H | 0.069403 | 5.832368 | 3.532560 |
| H | -0.428920 | 6.347042 | 1.200350 |
| H | -1.627843 | 2.329779 | 5.371568 |
| H | -0.898834 | 6.895174 | -1.133811 |
| C | -2.230594 | 5.781097 | -2.384517 |
| H | -3.636927 | 4.466752 | -3.399515 |
| H | -0.194056 | 4.370492 | 5.511700 |
| H | -2.097315 | 6.427371 | -3.247512 |
| C | 2.106429 | 0.067554 | 3.885093 |
| C | 4.320784 | -0.751914 | 4.447811 |
| C | 2.430340 | 1.362039 | 4.625882 |
| H | 1.613068 | -0.620821 | 4.593007 |
| H | 1.404583 | 0.249382 | 3.067704 |
| C | 4.578849 | 0.573185 | 5.164699 |
| H | 3.955752 | -1.489721 | 5.179703 |
| H | 5.255829 | -1.129579 | 4.022633 |
| H | 1.530553 | 1.769452 | 5.095412 |
| H | 2.829160 | 2.109793 | 3.920970 |
| H | 5.235405 | 0.419915 | 6.026194 |
| H | 5.060514 | 1.281570 | 4.471612 |
| N | 3.356908 | -0.516084 | 3.364890 |
| C | 3.349975 | -2.940120 | 2.674567 |
| C | 2.660011 | -3.473540 | 3.778678 |
| C | 4.142350 | -3.804106 | 1.898885 |
| C | 2.750943 | -4.830115 | 4.087277 |
| H | 2.033538 | -2.829070 | 4.386816 |
| C | 4.235365 | -5.161571 | 2.209355 |
| H | 4.705524 | -3.399532 | 1.063008 |
| C | 3.540807 | -5.678787 | 3.305597 |
| H | 2.203278 | -5.225739 | 4.938069 |
| H | 4.860748 | -5.811208 | 1.603166 |
| H | 3.618709 | -6.733643 | 3.553824 |
| C | 2.166627 | 2.389203 | -0.290020 |
| C | 2.674079 | 3.356765 | 0.561666 |
| C | 1.732113 | 2.707401 | -1.582232 |
| C | 2.766588 | 4.678941 | 0.108170 |
| H | 2.995499 | 3.113341 | 1.568775 |
| C | 1.815716 | 4.023163 | -2.031932 |
| H | 1.312595 | 1.931323 | -2.210128 |
| C | 2.346717 | 5.025725 | -1.175157 |
| H | 3.164873 | 5.433894 | 0.774753 |
| O | 1.418994 | 4.447027 | -3.258309 |
| O | 2.391913 | 6.277723 | -1.699529 |
| C | 0.813832 | 3.496735 | -4.133492 |
| H | -0.099664 | 3.079814 | -3.693280 |
| H | 0.563058 | 4.048592 | -5.040138 |
| H | 1.507156 | 2.684100 | -4.381033 |
| C | 2.928323 | 7.324306 | -0.893328 |
| H | 2.878336 | 8.224920 | -1.506493 |
| H | 2.335995 | 7.469447 | 0.018063 |
| H | 3.971755 | 7.123181 | -0.622556 |
| C | 4.282727 | 0.319971 | -0.575945 |
| C | 5.058229 | 0.268081 | -1.507447 |
| C | 5.966485 | 0.207615 | -2.609262 |
| C | 7.014194 | 1.142556 | -2.725638 |
| C | 5.823210 | -0.792584 | -3.591758 |
| C | 7.897074 | 1.074146 | -3.801421 |
| H | 7.125696 | 1.914128 | -1.970165 |
| C | 6.710676 | -0.852052 | -4.664207 |
| H | 5.015622 | -1.513011 | -3.503663 |
| C | 7.748478 | 0.078752 | -4.772009 |
| H | 8.702133 | 1.798816 | -3.882880 |
| H | 6.592778 | -1.626106 | -5.417120 |
| H | 8.438573 | 0.028878 | -5.609449 |
| O | 3.370350 | 1.132711 | 5.671571 |
| H | 1.348355 | 0.897288 | 0.921233 |

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**TS-5**

*G*sol(DCM) = -3945.638001 Hartree

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| | | | |
|---|---|---|---|
| C | -2.145092 | 0.075385 | 3.569751 |

| | | | |
|---|---|---|---|
| C | -2.822891 | 0.347482 | 2.383564 |
| H | -1.638853 | -0.537699 | 0.036179 |
| H | -2.745772 | 1.384801 | 2.080147 |
| N | -2.356202 | -1.284210 | 0.187103 |
| C | -3.583096 | -0.463495 | 1.473825 |
| H | -3.983240 | -1.414352 | 1.815842 |
| C | 5.347896 | 0.976461 | -4.862062 |
| C | 4.882710 | 0.517346 | -3.648298 |
| C | 4.098107 | 1.347434 | -2.798157 |
| C | 3.776875 | 2.665836 | -3.259917 |
| C | 4.286163 | 3.116006 | -4.509078 |
| C | 5.059606 | 2.293032 | -5.295989 |
| H | 5.937267 | 0.318781 | -5.495143 |
| H | 5.104248 | -0.497594 | -3.339064 |
| C | 3.585267 | 0.908326 | -1.527717 |
| C | 2.944505 | 3.496124 | -2.466970 |
| H | 4.040710 | 4.123541 | -4.835934 |
| H | 5.438343 | 2.644180 | -6.251678 |
| C | 2.380099 | 3.052759 | -1.288289 |
| C | 2.687242 | 1.728021 | -0.853295 |
| H | 2.735147 | 4.505682 | -2.811101 |
| C | 3.967327 | -0.412170 | -0.945324 |
| C | 5.337048 | -0.761483 | -0.679674 |
| C | 2.974494 | -1.329004 | -0.625332 |
| C | 6.413630 | 0.160122 | -0.813482 |
| C | 5.638696 | -2.084524 | -0.216653 |
| C | 3.260280 | -2.658870 | -0.193603 |
| C | 7.711187 | -0.214315 | -0.536667 |
| H | 6.203713 | 1.176596 | -1.125987 |
| C | 6.989518 | -2.444456 | 0.044626 |
| C | 4.582532 | -3.010950 | -0.016588 |
| C | 8.008497 | -1.532465 | -0.113901 |
| H | 8.513498 | 0.511350 | -0.638600 |
| H | 7.200188 | -3.455503 | 0.384592 |
| H | 4.827998 | -4.021216 | 0.300658 |
| H | 9.036229 | -1.815978 | 0.094685 |
| O | 2.126951 | 1.294063 | 0.328844 |
| O | 1.653843 | -0.963888 | -0.783759 |
| P | 0.987242 | 0.075658 | 0.342026 |
| O | -0.300787 | 0.537997 | -0.297074 |
| O | 1.025281 | -0.503736 | 1.720964 |
| C | 1.506172 | 3.960845 | -0.480668 |
| C | 0.215487 | 4.306360 | -0.948880 |
| C | 1.998150 | 4.517618 | 0.725572 |
| C | -0.596391 | 5.232002 | -0.188297 |
| C | -0.341617 | 3.771895 | -2.157475 |
| C | 1.171541 | 5.430606 | 1.482564 |
| C | 3.307444 | 4.230766 | 1.231979 |
| C | -1.892991 | 5.590740 | -0.678014 |
| C | -0.100770 | 5.763753 | 1.006032 |
| C | -1.587593 | 4.142807 | -2.593655 |
| H | 0.240617 | 3.059278 | -2.730227 |
| C | 1.678167 | 5.987496 | 2.699968 |
| C | 3.758153 | 4.786354 | 2.402278 |
| H | 3.952790 | 3.564004 | 0.670911 |
| C | -2.375353 | 5.069754 | -1.849554 |
| H | -2.485294 | 6.293830 | -0.097477 |
| H | -0.716648 | 6.456751 | 1.575200 |
| H | -1.982392 | 3.728561 | -3.517294 |
| H | 1.041752 | 6.670893 | 3.256870 |
| C | 2.933293 | 5.675030 | 3.151866 |
| H | 4.756145 | 4.552051 | 2.762440 |
| H | -3.355810 | 5.359389 | -2.217648 |
| H | 3.308235 | 6.106496 | 4.075799 |
| C | 2.165916 | -3.657460 | 0.020672 |
| C | 1.821518 | -4.071316 | 1.329960 |
| C | 1.503402 | -4.215795 | -1.100091 |
| C | 0.785611 | -5.064965 | 1.515238 |
| C | 2.446379 | -3.535002 | 2.503558 |
| C | 0.462660 | -5.199154 | -0.900689 |
| C | 1.830357 | -3.858573 | -2.448906 |
| C | 0.444611 | -5.480055 | 2.842783 |
| C | 0.132982 | -5.597848 | 0.399152 |
| C | 2.090231 | -3.958230 | 3.758376 |
| H | 3.206068 | -2.771618 | 2.386436 |
| C | -0.203793 | -5.752925 | -2.039951 |

| | | | |
|---|---|---|---|
| C | 1.170873 | -4.414924 | -3.514975 |
| H | 2.620112 | -3.136259 | -2.624255 |
| C | 1.077246 | -4.946650 | 3.934828 |
| H | -0.331195 | -6.232491 | 2.963387 |
| H | -0.646485 | -6.342861 | 0.544882 |
| H | 2.579842 | -3.534180 | 4.630788 |
| H | -0.986221 | -6.488815 | -1.870762 |
| C | 0.135625 | -5.373039 | -3.311503 |
| H | 1.439766 | -4.125845 | -4.527251 |
| H | 0.806206 | -5.266683 | 4.937055 |
| H | -0.376683 | -5.801471 | -4.168423 |
| C | -2.088611 | -2.440011 | 3.614850 |
| C | -1.287940 | -1.200280 | 5.529489 |
| C | -2.863299 | -3.353039 | 4.568272 |
| H | -1.092295 | -2.865972 | 3.435403 |
| H | -2.613707 | -2.386516 | 2.668709 |
| C | -2.093977 | -2.148835 | 6.419872 |
| H | -0.266230 | -1.585824 | 5.413397 |
| H | -1.237028 | -0.216679 | 5.991414 |
| H | -2.898024 | -4.366977 | 4.160924 |
| H | -3.893441 | -2.981349 | 4.686469 |
| H | -1.578243 | -2.286046 | 7.374185 |
| H | -3.089985 | -1.719951 | 6.612967 |
| N | -1.915924 | -1.104627 | 4.199454 |
| C | -1.576401 | 1.302751 | 4.230642 |
| C | -0.205531 | 1.582010 | 4.117088 |
| C | -2.415988 | 2.197379 | 4.907053 |
| C | 0.313205 | 2.748502 | 4.682509 |
| H | 0.433201 | 0.901492 | 3.559103 |
| C | -1.887568 | 3.355639 | 5.482397 |
| H | -3.478668 | 1.984670 | 4.983593 |
| C | -0.523358 | 3.633201 | 5.369396 |
| H | 1.370605 | 2.973414 | 4.575228 |
| H | -2.543267 | 4.041739 | 6.011355 |
| H | -0.113989 | 4.538767 | 5.808576 |
| C | -2.909313 | -1.777354 | -1.031504 |
| C | -3.479506 | -3.045480 | -1.096630 |
| C | -2.917057 | -0.933347 | -2.155897 |
| C | -4.054502 | -3.483619 | -2.294833 |
| H | -3.473296 | -3.700425 | -0.230182 |
| C | -3.493574 | -1.364802 | -3.346267 |
| H | -2.447598 | 0.039745 | -2.083223 |
| C | -4.073693 | -2.660365 | -3.420521 |
| H | -4.486777 | -4.476040 | -2.338470 |
| O | -3.548727 | -0.631432 | -4.490426 |
| O | -4.608800 | -2.994861 | -4.626352 |
| C | -3.003306 | 0.684689 | -4.466570 |
| H | -1.929226 | 0.668562 | -4.245335 |
| H | -3.161964 | 1.089435 | -5.467110 |
| H | -3.517322 | 1.314841 | -3.730430 |
| C | -5.195103 | -4.285493 | -4.762953 |
| H | -5.553986 | -4.341140 | -5.791659 |
| H | -4.458530 | -5.079794 | -4.590104 |
| H | -6.039047 | -4.416543 | -4.074599 |
| C | -4.483562 | 0.241082 | 0.617544 |
| C | -5.240070 | 0.847071 | -0.116559 |
| C | -6.124870 | 1.570084 | -0.969307 |
| C | -7.310988 | 0.972510 | -1.443139 |
| C | -5.819331 | 2.893331 | -1.350694 |
| C | -8.169556 | 1.686388 | -2.275754 |
| H | -7.546800 | -0.046255 | -1.151971 |
| C | -6.683461 | 3.596974 | -2.186444 |
| H | -4.904788 | 3.354190 | -0.990406 |
| C | -7.859128 | 2.997752 | -2.649424 |
| H | -9.081856 | 1.219144 | -2.635117 |
| H | -6.440497 | 4.615264 | -2.476315 |
| H | -8.530884 | 3.550565 | -3.299885 |
| O | -2.220464 | -3.438230 | 5.832232 |
| H | -1.917324 | -2.024819 | 0.733439 |

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**INT-6**

*G*sol(DCM) = -3429.237527 Hartree

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| | | | |
|---|---|---|---|
| C | 6.332562 | -3.641840 | 0.544670 |
| C | 5.015984 | -3.261573 | 0.694931 |
| C | 4.649515 | -1.887768 | 0.773765 |

| | | | |
|---|---|---|---|
| C | 5.690517 | -0.910039 | 0.652995 |
| C | 7.041027 | -1.334196 | 0.515626 |
| C | 7.361282 | -2.672017 | 0.466941 |
| H | 6.582746 | -4.697291 | 0.479497 |
| H | 4.242018 | -4.018870 | 0.741052 |
| C | 3.289818 | -1.443898 | 0.928834 |
| C | 5.353255 | 0.467185 | 0.654488 |
| H | 7.816616 | -0.576128 | 0.437565 |
| H | 8.395391 | -2.985832 | 0.355974 |
| C | 4.043934 | 0.899414 | 0.713709 |
| C | 3.014056 | -0.084792 | 0.822155 |
| H | 6.153851 | 1.199294 | 0.586008 |
| C | 2.175840 | -2.409255 | 1.162758 |
| C | 2.178843 | -3.314041 | 2.281054 |
| C | 1.093612 | -2.432643 | 0.290116 |
| C | 3.142395 | -3.251828 | 3.327407 |
| C | 1.144953 | -4.301989 | 2.379451 |
| C | 0.074785 | -3.431286 | 0.358522 |
| C | 3.103389 | -4.133511 | 4.386480 |
| H | 3.909857 | -2.487027 | 3.294316 |
| C | 1.142677 | -5.208689 | 3.475155 |
| C | 0.133927 | -4.351113 | 1.385515 |
| C | 2.102303 | -5.132174 | 4.459260 |
| H | 3.845604 | -4.057860 | 5.176530 |
| H | 0.356703 | -5.958390 | 3.525797 |
| H | -0.623452 | -5.128234 | 1.449683 |
| H | 2.087557 | -5.825248 | 5.295696 |
| O | 1.711254 | 0.346848 | 0.904163 |
| O | 1.029313 | -1.508289 | -0.727704 |
| P | 0.643913 | 0.085020 | -0.365119 |
| O | 1.058432 | 0.857022 | -1.584605 |
| O | -0.718031 | 0.207451 | 0.243142 |
| C | 3.734230 | 2.363267 | 0.684016 |
| C | 3.935406 | 3.103296 | -0.507153 |
| C | 3.293399 | 3.016523 | 1.861001 |
| C | 3.690368 | 4.529376 | -0.513015 |
| C | 4.362879 | 2.498556 | -1.735378 |
| C | 3.036563 | 4.439221 | 1.837519 |
| C | 3.105079 | 2.327352 | 3.103085 |
| C | 3.908714 | 5.272047 | -1.717359 |
| C | 3.244085 | 5.157049 | 0.654431 |
| C | 4.558207 | 3.245179 | -2.868785 |
| H | 4.524207 | 1.427257 | -1.761061 |
| C | 2.589493 | 5.088574 | 3.032434 |
| C | 2.678499 | 2.986062 | 4.227838 |
| H | 3.310747 | 1.263623 | 3.148563 |
| C | 4.335393 | 4.653324 | -2.862116 |
| H | 3.724842 | 6.343504 | -1.700505 |
| H | 3.061660 | 6.229636 | 0.644761 |
| H | 4.881088 | 2.759932 | -3.785852 |
| H | 2.398500 | 6.158488 | 2.995869 |
| C | 2.411504 | 4.385827 | 4.194707 |
| H | 2.544340 | 2.438443 | 5.156685 |
| H | 4.499025 | 5.228249 | -3.769422 |
| H | 2.073333 | 4.890262 | 5.095622 |
| C | -1.006704 | -3.513623 | -0.673079 |
| C | -2.341062 | -3.183806 | -0.334066 |
| C | -0.696469 | -3.968107 | -1.978616 |
| C | -3.384433 | -3.313708 | -1.328382 |
| C | -2.716100 | -2.704599 | 0.964185 |
| C | -1.746121 | -4.081201 | -2.966103 |
| C | 0.629266 | -4.343378 | -2.372146 |
| C | -4.732309 | -2.983592 | -0.975113 |
| C | -3.060236 | -3.754690 | -2.614759 |
| C | -4.018773 | -2.399247 | 1.263436 |
| H | -1.945345 | -2.575517 | 1.714678 |
| C | -1.420069 | -4.533046 | -4.284732 |
| C | 0.901581 | -4.774284 | -3.645450 |
| H | 1.429162 | -4.285605 | -1.642280 |
| C | -5.045246 | -2.543789 | 0.284062 |
| H | -5.504334 | -3.094532 | -1.732820 |
| H | -3.847910 | -3.846516 | -3.359516 |
| H | -4.274822 | -2.035580 | 2.254637 |
| H | -2.221951 | -4.609294 | -5.015220 |
| C | -0.134252 | -4.866797 | -4.620027 |
| H | 1.916607 | -5.051255 | -3.916767 |

| | | | |
|---|---|---|---|
| H | -6.072187 | -2.299669 | 0.541617 |
| H | 0.100799 | -5.208935 | -5.624073 |
| C | -0.613087 | 3.223745 | -2.967392 |
| C | -0.464226 | 4.746577 | -3.093844 |
| C | -0.623303 | 5.051996 | -0.776347 |
| C | -0.772948 | 3.544286 | -0.566228 |
| H | 0.189093 | 4.969419 | -3.941285 |
| H | 0.355134 | 2.729502 | -2.851251 |
| H | -1.121153 | 2.829493 | -3.844936 |
| H | -0.075017 | 5.481017 | 0.065791 |
| H | -1.613616 | 5.529952 | -0.837718 |
| H | 0.213677 | 3.077827 | -0.489693 |
| H | -1.329309 | 3.308909 | 0.336688 |
| H | -1.450701 | 5.199615 | -3.279614 |
| O | 0.135973 | 5.324225 | -1.945492 |
| N | -1.400686 | 2.924997 | -1.751771 |
| C | -2.852876 | 1.355216 | -2.901809 |
| C | -1.925333 | 0.416553 | -3.391547 |
| C | -4.120035 | 1.463785 | -3.499843 |
| C | -2.273566 | -0.402863 | -4.463759 |
| H | -0.947651 | 0.333573 | -2.924076 |
| C | -4.449732 | 0.654437 | -4.586464 |
| H | -4.833684 | 2.191507 | -3.126917 |
| C | -3.530418 | -0.282431 | -5.064949 |
| H | -1.564667 | -1.140679 | -4.826931 |
| H | -5.424142 | 0.753977 | -5.055115 |
| H | -3.792772 | -0.918819 | -5.905255 |
| C | -2.501508 | 2.193604 | -1.727851 |
| C | -3.377773 | 2.218248 | -0.579101 |
| H | -3.280917 | 3.033150 | 0.127939 |
| C | -4.332939 | 1.272678 | -0.344461 |
| H | -4.429059 | 0.417991 | -1.010572 |
| C | -5.211135 | 1.321956 | 0.747682 |
| C | -5.992792 | 1.345506 | 1.685285 |
| C | -6.893690 | 1.391318 | 2.781200 |
| C | -6.812088 | 2.438611 | 3.725077 |
| C | -7.879694 | 0.392884 | 2.938689 |
| C | -7.697119 | 2.480706 | 4.798140 |
| H | -6.053746 | 3.205525 | 3.603958 |
| C | -8.760002 | 0.446148 | 4.015293 |
| H | -7.942681 | -0.411767 | 2.212953 |
| C | -8.671214 | 1.487360 | 4.945560 |
| H | -7.628910 | 3.288177 | 5.521056 |
| H | -9.516399 | -0.324391 | 4.130987 |
| H | -9.360076 | 1.524432 | 5.784503 |

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**INT-7**

*G*sol(DCM) = -1566.879978 Hartree

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| | | | |
|---|---|---|---|
| Pd | 0.423669 | -1.624314 | 0.260288 |
| Cl | 0.651482 | -2.320171 | -2.088451 |
| C | 0.259421 | -1.560068 | 2.441902 |
| H | -0.726103 | -2.003614 | 2.569855 |
| H | 0.423519 | -0.610649 | 2.943076 |
| C | 1.362495 | -2.361519 | 2.080906 |
| H | 2.373111 | -1.992598 | 2.240224 |
| C | 1.138369 | -3.441176 | 1.196796 |
| H | 1.983445 | -3.947821 | 0.741028 |
| H | 0.214265 | -4.013678 | 1.253138 |
| N | -0.488950 | 0.302596 | -0.204811 |
| C | -1.903285 | 0.409282 | -0.221179 |
| C | -2.567343 | 1.569645 | 0.232978 |
| C | -2.650657 | -0.676099 | -0.680546 |
| C | -3.955016 | 1.646479 | 0.199393 |
| H | -1.994074 | 2.386946 | 0.651707 |
| C | -4.045661 | -0.598950 | -0.726400 |
| H | -2.139414 | -1.563892 | -1.037512 |
| C | -4.712126 | 0.547351 | -0.293478 |
| O | -4.684375 | 2.711159 | 0.627891 |
| H | -4.606668 | -1.445652 | -1.103379 |
| O | -6.059335 | 0.713813 | -0.283405 |
| C | -3.985098 | 3.849761 | 1.122090 |
| C | -6.872060 | -0.362373 | -0.746555 |
| H | -3.322068 | 4.273345 | 0.357847 |
| H | -4.753114 | 4.579340 | 1.382275 |
| H | -3.399732 | 3.602843 | 2.016338 |

| | | | |
|---|---|---|---|
| H | -6.725739 | -1.262513 | -0.137690 |
| H | -7.902470 | -0.018825 | -0.647063 |
| H | -6.663841 | -0.594962 | -1.797693 |
| C | 0.237855 | 1.361481 | -0.402782 |
| H | -0.240665 | 2.312040 | -0.649928 |
| C | 1.644393 | 1.360682 | -0.333977 |
| C | 2.860449 | 1.447236 | -0.296174 |
| C | 4.278541 | 1.524168 | -0.246190 |
| C | 4.933748 | 2.748429 | -0.498786 |
| C | 5.044977 | 0.377882 | 0.055466 |
| C | 6.323081 | 2.818963 | -0.448559 |
| H | 4.344366 | 3.629580 | -0.731728 |
| C | 6.433688 | 0.460676 | 0.102300 |
| H | 4.540632 | -0.563986 | 0.247442 |
| C | 7.075042 | 1.678262 | -0.148617 |
| H | 6.821225 | 3.763960 | -0.644053 |
| H | 7.017854 | -0.425007 | 0.334028 |
| H | 8.158936 | 1.737841 | -0.111226 |

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**INT-8**

*G*sol(DCM) = -1430.606633 Hartree

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| | | | |
|---|---|---|---|
| Pd | -1.613292 | -0.840579 | -0.151109 |
| Cl | -0.153001 | -2.182719 | -1.565792 |
| C | -3.384106 | 0.211788 | 0.657665 |
| H | -3.496093 | 0.980421 | -0.104293 |
| H | -3.364925 | 0.555759 | 1.687852 |
| C | -3.705962 | -1.127710 | 0.375154 |
| H | -3.865400 | -1.834875 | 1.185490 |
| C | -3.468596 | -1.594757 | -0.942228 |
| H | -3.498286 | -2.659324 | -1.151513 |
| H | -3.625156 | -0.935874 | -1.794091 |
| O | 1.518162 | -1.216831 | 1.856426 |
| C | 1.377554 | -0.377954 | 0.984082 |
| C | 0.126564 | 0.480675 | 0.902821 |
| O | 2.239573 | -0.047193 | 0.033808 |
| C | 0.026445 | 1.769195 | 0.132851 |
| N | -0.428478 | 0.510499 | 2.136275 |
| C | 3.593298 | -0.667789 | -0.063730 |
| C | 0.284945 | 1.769779 | -1.249292 |
| C | -0.325164 | 2.974272 | 0.760421 |
| N | -0.871385 | 0.523297 | 3.172790 |
| C | 4.401063 | -0.281678 | 1.177434 |
| C | 4.160599 | -0.005924 | -1.320475 |
| C | 3.478140 | -2.182217 | -0.246086 |
| C | 0.197304 | 2.955029 | -1.977926 |
| H | 0.553822 | 0.842870 | -1.742425 |
| C | -0.424057 | 4.154276 | 0.021167 |
| H | -0.517625 | 3.004920 | 1.829163 |
| H | 3.975586 | -0.724317 | 2.080425 |
| H | 5.429005 | -0.642892 | 1.065345 |
| H | 4.432557 | 0.806942 | 1.293457 |
| H | 5.184753 | -0.353448 | -1.489145 |
| H | 3.558972 | -0.261443 | -2.198582 |
| H | 4.176915 | 1.083319 | -1.212497 |
| H | 3.118124 | -2.669215 | 0.661578 |
| H | 2.792500 | -2.415209 | -1.065744 |
| H | 4.467549 | -2.584387 | -0.490745 |
| C | -0.161926 | 4.151023 | -1.349700 |
| H | 0.403947 | 2.939750 | -3.044389 |
| H | -0.697905 | 5.077039 | 0.524685 |
| H | -0.235349 | 5.070389 | -1.923339 |

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**TS-6**

*G*sol(DCM) = -1430.59058 Hartree

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| | | | |
|---|---|---|---|
| C | 0.251848 | 0.579003 | 0.212234 |
| N | -0.130527 | 0.650254 | 1.949087 |
| C | 3.730857 | 2.070349 | 0.180335 |
| C | 3.467368 | 3.410420 | -0.116717 |
| C | 2.149731 | 3.839162 | -0.306785 |
| C | 1.097302 | 2.933751 | -0.197813 |
| C | 1.348021 | 1.576455 | 0.088049 |
| C | 2.679720 | 1.161531 | 0.280937 |
| H | 4.752441 | 1.733950 | 0.329860 |
| H | 4.285949 | 4.119741 | -0.199871 |

| | | | |
|---|---|---|---|
| H | 1.943136 | 4.880537 | -0.535376 |
| H | 0.079638 | 3.276451 | -0.349833 |
| H | 2.879789 | 0.118665 | 0.508434 |
| C | -1.077558 | 0.921217 | -0.410792 |
| O | -1.119567 | 1.313560 | -1.566642 |
| O | -2.121704 | 0.664002 | 0.378107 |
| N | -0.093810 | 0.314706 | 3.007104 |
| C | -3.529294 | 0.806365 | -0.087573 |
| C | -3.781782 | -0.147123 | -1.257908 |
| H | -4.848338 | -0.135332 | -1.507175 |
| H | -3.214327 | 0.146820 | -2.142510 |
| H | -3.509095 | -1.171548 | -0.982128 |
| C | -4.325608 | 0.382358 | 1.147561 |
| H | -4.097636 | 1.032329 | 1.998444 |
| H | -5.397523 | 0.451068 | 0.937045 |
| H | -4.092167 | -0.650710 | 1.424607 |
| C | -3.805059 | 2.269297 | -0.443864 |
| H | -3.553402 | 2.922406 | 0.398618 |
| H | -3.233760 | 2.582426 | -1.319574 |
| H | -4.871562 | 2.391750 | -0.661561 |
| Pd | 0.641654 | -1.467031 | -0.178567 |
| Cl | 0.560443 | -2.502210 | 2.037592 |
| C | 1.017155 | -1.128264 | -2.286897 |
| H | 2.086046 | -0.921904 | -2.284879 |
| H | 0.390645 | -0.391893 | -2.779712 |
| C | 0.555906 | -2.462748 | -2.145612 |
| H | -0.454731 | -2.715112 | -2.459333 |
| C | 1.250691 | -3.330708 | -1.293278 |
| H | 0.811103 | -4.279109 | -1.002490 |
| H | 2.324923 | -3.231170 | -1.153862 |

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**INT-9**

*G*sol(DCM) = -1321.098245 Hartree

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| | | | |
|---|---|---|---|
| C | -1.412623 | 2.512799 | 0.210177 |
| C | -0.149835 | 1.960071 | -0.141642 |
| C | 0.947178 | 2.847983 | -0.332717 |
| C | 0.784173 | 4.215812 | -0.175972 |
| C | -0.470890 | 4.731738 | 0.176148 |
| C | -1.568080 | 3.881194 | 0.369627 |
| H | -2.249357 | 1.837268 | 0.354620 |
| H | 1.917911 | 2.451355 | -0.611133 |
| H | 1.624846 | 4.885739 | -0.324845 |
| H | -0.594148 | 5.803876 | 0.299240 |
| H | -2.534595 | 4.293349 | 0.641043 |
| C | -0.007359 | 0.544659 | -0.272967 |
| C | 1.314003 | 0.002103 | -0.695217 |
| O | 1.588050 | -0.091848 | -1.882293 |
| O | 2.058274 | -0.366456 | 0.343694 |
| C | 3.368892 | -1.065801 | 0.189067 |
| Pd | -1.399671 | -0.838450 | -0.020341 |
| Cl | -1.359510 | -1.007651 | 2.434735 |
| C | -1.849203 | -1.230395 | -2.082667 |
| H | -1.084915 | -1.959516 | -2.347467 |
| H | -1.929789 | -0.380869 | -2.753937 |
| C | -3.011463 | -1.657307 | -1.366055 |
| H | -3.907016 | -1.040191 | -1.403338 |
| C | -2.901331 | -2.625712 | -0.380623 |
| H | -3.719758 | -2.809913 | 0.307320 |
| H | -2.104846 | -3.365867 | -0.404833 |
| C | 3.152814 | -2.385317 | -0.555093 |
| H | 2.848270 | -2.215580 | -1.589638 |
| H | 4.088235 | -2.955067 | -0.556437 |
| H | 2.388774 | -2.987824 | -0.052166 |
| C | 4.360552 | -0.140877 | -0.520676 |
| H | 4.442109 | 0.813746 | 0.010129 |
| H | 5.349975 | -0.610850 | -0.526183 |
| H | 4.060099 | 0.049693 | -1.552731 |
| C | 3.784791 | -1.311044 | 1.639415 |
| H | 4.750930 | -1.825297 | 1.663571 |
| H | 3.882479 | -0.364509 | 2.180660 |
| H | 3.047025 | -1.933778 | 2.155244 |

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**TS-7**

*G*sol(DCM) = -1667.707288 Hartree

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| | | | |
|---|---|---|---|
| C | 0.642778 | -0.202386 | 0.347110 |
| O | -1.612318 | -0.146783 | 0.096951 |
| C | 0.432472 | -0.249097 | 2.812587 |
| C | 0.518096 | -0.946769 | 1.585198 |
| C | 0.463538 | -2.362119 | 1.612391 |
| C | 0.342440 | -3.044722 | 2.817031 |
| C | 0.267638 | -2.332588 | 4.020091 |
| C | 0.311660 | -0.933774 | 4.016395 |
| H | 0.463074 | 0.835961 | 2.795970 |
| H | 0.523393 | -2.921709 | 0.685015 |
| H | 0.306088 | -4.129875 | 2.823838 |
| H | 0.174607 | -2.868756 | 4.960308 |
| H | 0.250808 | -0.384097 | 4.950739 |
| C | -2.414707 | -1.053964 | -0.679314 |
| H | -2.055147 | -1.090082 | -1.711122 |
| H | -2.249935 | -2.036984 | -0.226064 |
| C | -3.878707 | -0.675389 | -0.624031 |
| C | -4.563471 | -0.665520 | 0.600894 |
| C | -4.570374 | -0.322915 | -1.789031 |
| C | -5.912202 | -0.315917 | 0.657178 |
| H | -4.031859 | -0.931416 | 1.511258 |
| C | -5.923946 | 0.023528 | -1.736890 |
| H | -4.047404 | -0.322268 | -2.742576 |
| C | -6.596843 | 0.028220 | -0.513801 |
| H | -6.431913 | -0.314314 | 1.611661 |
| H | -6.448759 | 0.292082 | -2.649798 |
| C | 0.999789 | -0.923520 | -0.922727 |
| O | 0.341136 | -0.934650 | -1.946754 |
| H | -1.615701 | 0.742212 | -0.330264 |
| O | 2.217511 | -1.471851 | -0.762961 |
| C | 2.982513 | -2.063550 | -1.895457 |
| Pd | 1.105929 | 1.765968 | 0.171914 |
| Cl | -0.954088 | 2.717650 | -0.865672 |
| C | 3.105788 | 1.585667 | 0.908214 |
| H | 3.664976 | 1.291967 | 0.021104 |
| H | 3.267707 | 0.962226 | 1.782606 |
| C | 2.756138 | 2.959736 | 1.094336 |
| H | 2.529758 | 3.315182 | 2.097669 |
| C | 2.372712 | 3.726671 | 0.002271 |
| H | 1.906904 | 4.696179 | 0.145294 |
| H | 2.729321 | 3.497763 | -0.999464 |
| C | 2.241664 | -3.295389 | -2.423384 |
| H | 1.291574 | -3.019830 | -2.883892 |
| H | 2.862892 | -3.796856 | -3.173703 |
| H | 2.051204 | -4.005757 | -1.611587 |
| C | 3.211753 | -1.006693 | -2.978754 |
| H | 3.688161 | -0.116912 | -2.553088 |
| H | 3.880645 | -1.415952 | -3.743583 |
| H | 2.275827 | -0.713391 | -3.457283 |
| C | 4.301298 | -2.460675 | -1.230018 |
| H | 4.962426 | -2.927744 | -1.967017 |
| H | 4.808614 | -1.582415 | -0.817702 |
| H | 4.127160 | -3.175169 | -0.419006 |
| H | -7.648449 | 0.298620 | -0.470545 |

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**TS-7a**

*G*sol(DCM) = -1917.024132 Hartree

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| | | | |
|---|---|---|---|
| C | -1.027713 | -0.382980 | -0.274008 |
| C | 1.293883 | 0.712345 | -1.360945 |
| C | -1.257428 | -1.752070 | -2.324912 |
| C | -0.755290 | -1.600998 | -1.006101 |
| C | -0.014050 | -2.678186 | -0.453006 |
| C | 0.198690 | -3.844735 | -1.177706 |
| C | -0.314236 | -3.970364 | -2.474007 |
| C | -1.042157 | -2.919122 | -3.046173 |
| H | -1.815982 | -0.930325 | -2.762808 |
| H | 0.390251 | -2.593251 | 0.548841 |
| H | 0.766281 | -4.658415 | -0.736201 |
| H | -0.145964 | -4.883586 | -3.037733 |
| H | -1.438150 | -3.015767 | -4.052728 |
| C | -0.703232 | -0.312349 | 1.190027 |
| O | 0.026759 | 0.507641 | 1.718083 |
| H | 0.746046 | 1.635241 | -1.495020 |
| O | -1.428788 | -1.244584 | 1.844068 |
| C | -1.517731 | -1.288147 | 3.327046 |

| | | | |
|---|---|---|---|
| Pd | -2.493006 | 0.942947 | -0.718853 |
| Cl | -1.440438 | 3.102511 | -1.332207 |
| C | -4.052416 | -0.445502 | -0.253906 |
| H | -4.153293 | -0.352141 | 0.826077 |
| H | -3.939947 | -1.461896 | -0.619167 |
| C | -4.666102 | 0.529846 | -1.101672 |
| H | -4.882937 | 0.269366 | -2.135864 |
| C | -4.666917 | 1.865008 | -0.727155 |
| H | -4.932173 | 2.639707 | -1.438822 |
| H | -4.618212 | 2.157110 | 0.319219 |
| C | -0.143617 | -1.620531 | 3.916615 |
| H | 0.569544 | -0.815313 | 3.733347 |
| H | -0.238195 | -1.766259 | 4.998486 |
| H | 0.246407 | -2.548208 | 3.483582 |
| C | -2.076849 | 0.034569 | 3.858451 |
| H | -3.026818 | 0.274268 | 3.368248 |
| H | -2.264689 | -0.059357 | 4.933604 |
| H | -1.378289 | 0.857379 | 3.697831 |
| C | -2.504860 | -2.432519 | 3.566050 |
| H | -2.648819 | -2.581118 | 4.641156 |
| H | -3.477086 | -2.208086 | 3.115159 |
| H | -2.128275 | -3.365667 | 3.134648 |
| C | 2.346752 | 0.574419 | -0.490653 |
| H | 1.104775 | -0.081830 | -2.067177 |
| C | 3.099486 | -0.716391 | -0.482561 |
| C | 3.283798 | -1.430353 | 0.715328 |
| C | 3.584855 | -1.267876 | -1.678296 |
| C | 3.934108 | -2.664386 | 0.713122 |
| H | 2.899499 | -1.017899 | 1.643726 |
| C | 4.239136 | -2.501270 | -1.678914 |
| H | 3.456937 | -0.719344 | -2.606891 |
| C | 4.415501 | -3.203161 | -0.484051 |
| H | 4.061512 | -3.207576 | 1.645551 |
| H | 4.615121 | -2.910460 | -2.612580 |
| H | 4.925634 | -4.162451 | -0.484308 |
| C | 1.932609 | 2.743530 | 0.644973 |
| C | 4.080456 | 1.673498 | 0.932907 |
| C | 2.635748 | 3.923925 | -0.028360 |
| H | 1.880864 | 2.932429 | 1.724994 |
| H | 0.915519 | 2.619484 | 0.278724 |
| C | 4.730622 | 2.894229 | 0.266949 |
| H | 4.056450 | 1.823195 | 2.020064 |
| H | 4.666458 | 0.779455 | 0.722235 |
| H | 2.113021 | 4.859700 | 0.189836 |
| H | 2.658186 | 3.777949 | -1.120054 |
| H | 5.717415 | 3.081525 | 0.701516 |
| H | 4.850511 | 2.701564 | -0.811901 |
| N | 2.702994 | 1.512865 | 0.451256 |
| O | 3.963892 | 4.074405 | 0.472366 |

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**TS-7b**

*G*sol(DCM) = -1742.646463 Hartree

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| | | | |
|---|---|---|---|
| C | -1.232559 | -0.304829 | 0.318286 |
| O | 0.912394 | -0.759365 | 0.255211 |
| C | -1.519606 | -2.566498 | 1.379817 |
| C | -1.388250 | -1.161266 | 1.485204 |
| C | -1.385287 | -0.585167 | 2.775548 |
| C | -1.529289 | -1.374196 | 3.912375 |
| C | -1.668251 | -2.760000 | 3.784032 |
| C | -1.660664 | -3.354340 | 2.516352 |
| H | -1.511784 | -3.036564 | 0.402282 |
| H | -1.271531 | 0.490869 | 2.865175 |
| H | -1.530889 | -0.914356 | 4.896001 |
| H | -1.779913 | -3.378056 | 4.670461 |
| H | -1.763160 | -4.431077 | 2.419740 |
| C | -1.561004 | -0.842418 | -1.048219 |
| O | -0.822219 | -0.820108 | -2.017338 |
| O | -2.840769 | -1.256823 | -1.052405 |
| C | -3.552996 | -1.633008 | -2.305173 |
| Pd | -1.436018 | 1.718524 | 0.344829 |
| Cl | 0.854036 | 2.632273 | 0.141355 |
| C | -3.555555 | 1.672652 | 0.682386 |
| H | -3.624631 | 1.639964 | 1.768586 |
| H | -4.125901 | 0.912987 | 0.157884 |
| C | -3.296670 | 2.919009 | 0.034027 |

| | | | |
|---|---|---|---|
| H | -3.565975 | 3.035389 | -1.013872 |
| C | -2.416748 | 3.825004 | 0.612714 |
| H | -2.046812 | 4.673388 | 0.046635 |
| H | -2.263765 | 3.850904 | 1.689068 |
| C | -3.584371 | -0.439193 | -3.262948 |
| H | -2.585701 | -0.191137 | -3.626646 |
| H | -4.217279 | -0.683563 | -4.123034 |
| H | -4.011451 | 0.439537 | -2.767546 |
| C | -2.890540 | -2.867222 | -2.924629 |
| H | -2.836496 | -3.681098 | -2.193474 |
| H | -3.494120 | -3.212314 | -3.771306 |
| H | -1.884170 | -2.643001 | -3.281283 |
| C | -4.957081 | -1.966791 | -1.797870 |
| H | -5.587479 | -2.285943 | -2.634000 |
| H | -4.920316 | -2.777305 | -1.062893 |
| H | -5.421603 | -1.092779 | -1.329711 |
| C | 1.650085 | -0.238058 | -0.592557 |
| H | 1.222660 | 0.221815 | -1.486566 |
| C | 3.067811 | -0.266682 | -0.485155 |
| C | 4.286200 | -0.295326 | -0.455330 |
| C | 5.705697 | -0.326051 | -0.412234 |
| C | 6.459057 | 0.247620 | -1.458731 |
| C | 6.371960 | -0.929319 | 0.675730 |
| C | 7.849657 | 0.215402 | -1.412571 |
| H | 5.943730 | 0.711477 | -2.293625 |
| C | 7.763045 | -0.955126 | 0.710868 |
| H | 5.789749 | -1.369212 | 1.479007 |
| C | 8.502589 | -0.384493 | -0.330518 |
| H | 8.426012 | 0.658133 | -2.219340 |
| H | 8.272354 | -1.419729 | 1.549797 |
| H | 9.588072 | -0.406904 | -0.298687 |

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**TS-7c**

*G*sol(DCM) = -2182.661235 Hartree

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| | | | |
|---|---|---|---|
| C | -0.194960 | -0.971223 | 0.427145 |
| C | -0.106383 | -0.872776 | 2.921019 |
| C | -0.856860 | -0.837013 | 1.722068 |
| C | -2.261200 | -0.700225 | 1.830312 |
| C | -2.882558 | -0.620223 | 3.073414 |
| C | -2.115863 | -0.648482 | 4.241331 |
| C | -0.722853 | -0.770943 | 4.161536 |
| H | 0.969750 | -0.984415 | 2.858633 |
| H | -2.868446 | -0.669028 | 0.933727 |
| H | -3.962985 | -0.528383 | 3.131609 |
| H | -2.600133 | -0.577872 | 5.211169 |
| H | -0.124944 | -0.795105 | 5.067669 |
| C | -1.078573 | -1.047196 | -0.791771 |
| O | -1.258118 | -0.184322 | -1.626851 |
| O | -1.599616 | -2.294296 | -0.822990 |
| C | -2.370452 | -2.811091 | -1.984062 |
| Pd | 1.534346 | -2.017697 | 0.018493 |
| Cl | 2.259736 | -1.008323 | -2.133847 |
| C | 1.286350 | -3.580748 | 1.496433 |
| H | 0.612983 | -4.260109 | 0.975901 |
| H | 0.984650 | -3.315597 | 2.504214 |
| C | 2.667598 | -3.566431 | 1.155818 |
| H | 3.383306 | -3.152811 | 1.863659 |
| C | 3.046883 | -3.740073 | -0.173948 |
| H | 4.061645 | -3.522752 | -0.490678 |
| H | 2.440740 | -4.330694 | -0.856712 |
| C | -3.672112 | -2.018230 | -2.133966 |
| H | -3.472346 | -0.979234 | -2.401638 |
| H | -4.285488 | -2.471136 | -2.920743 |
| H | -4.246463 | -2.045609 | -1.201170 |
| C | -1.509314 | -2.763454 | -3.248558 |
| H | -0.560086 | -3.284642 | -3.086183 |
| H | -2.039989 | -3.267053 | -4.064115 |
| H | -1.299689 | -1.736241 | -3.550989 |
| C | -2.657734 | -4.256817 | -1.573913 |
| H | -3.246027 | -4.753770 | -2.352187 |
| H | -1.725007 | -4.813755 | -1.436817 |
| H | -3.224598 | -4.289272 | -0.637719 |
| C | -0.473283 | 2.311891 | 0.247572 |
| C | 1.750743 | 1.685453 | 0.274940 |
| C | 2.638310 | 1.095617 | 1.173970 |

| | | | |
|---|---|---|---|
| C | 2.235498 | 2.632372 | -0.652637 |
| C | 3.987516 | 1.463701 | 1.174422 |
| H | 2.278665 | 0.375357 | 1.895952 |
| C | 3.580065 | 2.988324 | -0.669894 |
| H | 1.553765 | 3.047440 | -1.384387 |
| C | 4.475200 | 2.400814 | 0.263406 |
| H | 4.655061 | 1.008235 | 1.896395 |
| N | 0.378246 | 1.340676 | 0.292244 |
| H | -0.103143 | 3.343128 | 0.287637 |
| C | -1.881076 | 2.210328 | 0.166499 |
| C | -3.089780 | 2.349398 | 0.089280 |
| C | -4.501963 | 2.494107 | -0.004313 |
| C | -5.101447 | 3.743792 | 0.262516 |
| C | -5.317890 | 1.402854 | -0.370314 |
| C | -6.482430 | 3.891672 | 0.166740 |
| H | -4.475123 | 4.584897 | 0.542530 |
| C | -6.697880 | 1.562248 | -0.464750 |
| H | -4.859514 | 0.443350 | -0.585721 |
| C | -7.283086 | 2.803812 | -0.196434 |
| H | -6.935742 | 4.856567 | 0.374132 |
| H | -7.318393 | 0.717640 | -0.749582 |
| H | -8.360034 | 2.923748 | -0.271479 |
| O | 5.769480 | 2.811828 | 0.177653 |
| O | 4.137190 | 3.876977 | -1.538197 |
| C | 6.716047 | 2.227652 | 1.067088 |
| H | 7.675864 | 2.684164 | 0.821082 |
| H | 6.467636 | 2.442881 | 2.113604 |
| H | 6.780552 | 1.141903 | 0.924792 |
| C | 3.294218 | 4.472317 | -2.519635 |
| H | 3.936940 | 5.136291 | -3.099507 |
| H | 2.857564 | 3.715829 | -3.183093 |
| H | 2.489998 | 5.056823 | -2.055780 |

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**INT-10**

*G*sol(DCM) = -1667.733868 Hartree

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| | | | |
|---|---|---|---|
| C | -0.618967 | 1.243130 | -2.240057 |
| C | 0.172589 | 1.439222 | -1.088857 |
| C | 0.872138 | 2.652433 | -0.973475 |
| C | 0.797924 | 3.620940 | -1.979325 |
| C | 0.010053 | 3.412875 | -3.110960 |
| C | -0.704869 | 2.216416 | -3.232510 |
| H | -1.168251 | 0.312961 | -2.351160 |
| H | 1.486334 | 2.840238 | -0.101978 |
| H | 1.354336 | 4.547665 | -1.865381 |
| H | -0.048344 | 4.169570 | -3.888341 |
| H | -1.323690 | 2.036002 | -4.107549 |
| C | 0.200207 | 0.355944 | -0.046429 |
| O | -1.247819 | 0.039452 | 0.258391 |
| C | -2.114068 | 0.975354 | 1.057954 |
| H | -1.757157 | 0.933542 | 2.084009 |
| H | -1.901076 | 1.947692 | 0.614203 |
| C | -3.540626 | 0.553921 | 0.897192 |
| C | -4.238266 | 0.842196 | -0.286314 |
| C | -4.191839 | -0.136710 | 1.928232 |
| C | -5.565976 | 0.444581 | -0.434311 |
| H | -3.736413 | 1.377835 | -1.088214 |
| C | -5.523254 | -0.531455 | 1.781433 |
| H | -3.657133 | -0.360157 | 2.847800 |
| C | -6.210156 | -0.242243 | 0.600410 |
| H | -6.100365 | 0.673031 | -1.351999 |
| H | -6.021621 | -1.062538 | 2.587208 |
| C | 0.911829 | 0.523331 | 1.259899 |
| O | 0.420470 | 0.212452 | 2.338876 |
| H | -1.304908 | -0.936758 | 0.550793 |
| O | 2.169070 | 0.975273 | 1.092656 |
| C | 3.119761 | 1.093769 | 2.224226 |
| Pd | 0.970716 | -1.560320 | -0.759547 |
| Cl | -0.822532 | -2.818038 | 0.487078 |
| C | 2.694725 | -0.878926 | -1.823658 |
| H | 3.458502 | -0.872025 | -1.047765 |
| H | 2.599160 | 0.041133 | -2.392551 |
| C | 2.302713 | -2.111283 | -2.420251 |
| H | 1.816531 | -2.101426 | -3.393836 |
| C | 2.218832 | -3.257699 | -1.625019 |
| H | 1.730338 | -4.150722 | -2.002271 |

| | | | |
|---|---|---|---|
| H | 2.868765 | -3.387315 | -0.762283 |
| C | 2.602748 | 2.119298 | 3.238136 |
| H | 1.689715 | 1.771001 | 3.723030 |
| H | 3.366464 | 2.287341 | 4.005536 |
| H | 2.401092 | 3.076913 | 2.745569 |
| C | 3.359065 | -0.282547 | 2.852503 |
| H | 3.662172 | -1.004618 | 2.086290 |
| H | 4.166922 | -0.209110 | 3.588978 |
| H | 2.462913 | -0.652953 | 3.352422 |
| C | 4.389923 | 1.603999 | 1.538926 |
| H | 5.183467 | 1.740407 | 2.280705 |
| H | 4.740148 | 0.889968 | 0.786270 |
| H | 4.207669 | 2.565567 | 1.047894 |
| H | -7.246163 | -0.548559 | 0.485565 |

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**TS-8**

*G*sol(DCM) = -1667.721861 Hartree

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| | | | |
|---|---|---|---|
| O | 1.307832 | -0.261040 | -0.007077 |
| H | 1.277067 | 0.881300 | -0.216037 |
| O | 0.543935 | 1.930741 | 0.096834 |
| C | -0.166291 | -2.633304 | 1.182882 |
| C | -0.459129 | -1.279636 | 1.443052 |
| C | -1.026536 | -0.949896 | 2.685246 |
| C | -1.309622 | -1.944280 | 3.625652 |
| C | -1.007508 | -3.280096 | 3.358820 |
| C | -0.425997 | -3.619016 | 2.132462 |
| H | 0.263148 | -2.906684 | 0.222786 |
| H | -1.258780 | 0.083033 | 2.917558 |
| H | -1.756526 | -1.665834 | 4.576311 |
| H | -1.222112 | -4.049496 | 4.095051 |
| H | -0.185199 | -4.654942 | 1.909737 |
| C | -0.150797 | -0.260552 | 0.396512 |
| C | 2.317916 | -0.437388 | 1.081354 |
| H | 2.039042 | 0.218503 | 1.910384 |
| H | 2.237639 | -1.476577 | 1.394076 |
| C | 3.665991 | -0.108093 | 0.514596 |
| C | 4.181951 | 1.191622 | 0.618914 |
| C | 4.415618 | -1.093217 | -0.144302 |
| C | 5.429454 | 1.501267 | 0.074814 |
| H | 3.606565 | 1.960129 | 1.129373 |
| C | 5.661735 | -0.783906 | -0.689721 |
| H | 4.021580 | -2.103057 | -0.225592 |
| C | 6.169952 | 0.513895 | -0.580232 |
| H | 5.823257 | 2.509590 | 0.164466 |
| H | 6.236904 | -1.553850 | -1.195924 |
| C | -0.377837 | 1.185133 | 0.550704 |
| O | -1.497716 | 1.614871 | 1.079464 |
| C | -1.902769 | 3.061009 | 1.088353 |
| Pd | -1.312775 | -0.604539 | -1.450465 |
| Cl | 0.378309 | 0.203329 | -3.060248 |
| C | -3.180621 | -1.191428 | -0.533419 |
| H | -3.692603 | -0.233979 | -0.450384 |
| H | -3.137139 | -1.781977 | 0.376477 |
| C | -3.099488 | -1.842640 | -1.791174 |
| H | -2.889703 | -2.909888 | -1.827232 |
| C | -2.933730 | -1.069624 | -2.948541 |
| H | -2.661865 | -1.541963 | -3.887128 |
| H | -3.358912 | -0.070589 | -3.015348 |
| C | -3.282735 | 2.999586 | 1.742368 |
| H | -3.217341 | 2.584015 | 2.752948 |
| H | -3.700782 | 4.008588 | 1.810253 |
| H | -3.965892 | 2.380912 | 1.151884 |
| C | -0.917924 | 3.857306 | 1.945645 |
| H | -0.831398 | 3.414461 | 2.943404 |
| H | 0.071506 | 3.900152 | 1.487168 |
| H | -1.292654 | 4.880140 | 2.059489 |
| C | -1.992498 | 3.570937 | -0.350185 |
| H | -2.659305 | 2.936163 | -0.942930 |
| H | -2.407018 | 4.584547 | -0.340694 |
| H | -1.012249 | 3.602930 | -0.829101 |
| H | 7.141954 | 0.753963 | -1.001967 |

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**INT-11**

*G*sol(DCM) = -1667.747027 Hartree

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| | | | |
|---|---|---|---|
| C | 0.603828 | 2.720376 | -0.024521 |
| C | -0.272032 | 1.821066 | -0.667307 |
| C | -1.314012 | 2.363913 | -1.443957 |
| C | -1.475181 | 3.746663 | -1.555380 |
| C | -0.604435 | 4.625135 | -0.907453 |
| C | 0.440179 | 4.099520 | -0.142531 |
| H | 1.416647 | 2.322581 | 0.573642 |
| H | -1.999421 | 1.709614 | -1.965121 |
| H | -2.287792 | 4.136151 | -2.163531 |
| H | -0.734630 | 5.699744 | -0.999967 |
| H | 1.132625 | 4.764459 | 0.367312 |
| C | -0.010428 | 0.360504 | -0.485930 |
| O | 1.330018 | 0.033881 | -0.201392 |
| C | 2.214853 | 0.138907 | -1.352120 |
| H | 1.887244 | -0.576930 | -2.115997 |
| H | 2.144908 | 1.150236 | -1.767543 |
| C | 3.617383 | -0.161252 | -0.896066 |
| C | 4.068137 | -1.485682 | -0.807385 |
| C | 4.483058 | 0.876073 | -0.524500 |
| C | 5.358655 | -1.768310 | -0.356728 |
| H | 3.405227 | -2.297565 | -1.097127 |
| C | 5.775379 | 0.597472 | -0.074442 |
| H | 4.142945 | 1.906751 | -0.592589 |
| C | 6.214952 | -0.726146 | 0.010591 |
| H | 5.697091 | -2.799031 | -0.295523 |
| H | 6.438153 | 1.411487 | 0.206376 |
| C | -0.716285 | -0.698548 | -1.100344 |
| O | -0.211202 | -1.930858 | -1.126860 |
| H | 0.379335 | -2.047786 | -0.336582 |
| O | -1.851276 | -0.501441 | -1.737850 |
| C | -2.842500 | -1.574717 | -2.081884 |
| Pd | -0.980408 | -0.230766 | 1.587954 |
| Cl | 0.343067 | -2.313982 | 1.860746 |
| C | -2.537201 | 1.282814 | 1.757428 |
| H | -3.403740 | 0.711847 | 1.428272 |
| H | -2.369974 | 2.227940 | 1.251909 |
| C | -1.987503 | 1.062810 | 3.039668 |
| H | -1.335823 | 1.811566 | 3.484360 |
| C | -1.995722 | -0.250532 | 3.549262 |
| H | -1.396706 | -0.500326 | 4.419355 |
| H | -2.813963 | -0.928744 | 3.316555 |
| C | -3.187089 | -2.399452 | -0.841653 |
| H | -4.019134 | -3.068255 | -1.086307 |
| H | -2.345022 | -3.007703 | -0.507551 |
| H | -3.505104 | -1.749320 | -0.019945 |
| C | -4.045636 | -0.750474 | -2.543066 |
| H | -3.780181 | -0.120352 | -3.397915 |
| H | -4.855345 | -1.421030 | -2.846909 |
| H | -4.410848 | -0.109579 | -1.734413 |
| C | -2.287288 | -2.420786 | -3.229203 |
| H | -1.973639 | -1.779498 | -4.059399 |
| H | -1.439102 | -3.028589 | -2.910079 |
| H | -3.075045 | -3.088658 | -3.594231 |
| H | 7.220954 | -0.944867 | 0.358324 |

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**INT-12**

*G*sol(DCM) = -962.4673818 Hartree

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| | | | |
|---|---|---|---|
| C | 3.216641 | -3.317042 | 0.701684 |
| C | 2.982560 | -2.163974 | 1.456678 |
| C | 2.045394 | -1.218294 | 1.042334 |
| C | 1.322420 | -1.394558 | -0.156881 |
| C | 1.566186 | -2.565496 | -0.905496 |
| C | 2.498607 | -3.511465 | -0.481033 |
| H | 3.943671 | -4.053752 | 1.032260 |
| H | 3.525904 | -2.002592 | 2.384518 |
| H | 1.866365 | -0.337866 | 1.647071 |
| H | 1.024082 | -2.719957 | -1.832912 |
| H | 2.667305 | -4.401987 | -1.081436 |
| C | 0.330710 | -0.426752 | -0.644044 |
| C | 0.259492 | 0.907416 | -0.391323 |
| O | -0.683003 | 1.682329 | -0.991037 |
| O | 1.064025 | 1.549580 | 0.467190 |
| C | 1.840213 | 2.743451 | 0.038366 |
| O | -0.614783 | -0.876998 | -1.580106 |
| C | -1.654827 | -1.746709 | -1.048083 |

| | | | |
|---|---|---|---|
| H | -2.108230 | -2.192827 | -1.937176 |
| H | -1.186078 | -2.541246 | -0.458512 |
| C | -2.683705 | -1.002914 | -0.232637 |
| C | -2.586468 | -0.943540 | 1.164464 |
| C | -3.743023 | -0.335589 | -0.866530 |
| C | -3.523471 | -0.227109 | 1.913155 |
| H | -1.776251 | -1.465551 | 1.667264 |
| C | -4.680950 | 0.380848 | -0.121701 |
| H | -3.834844 | -0.384602 | -1.949527 |
| C | -4.571292 | 0.437291 | 1.271151 |
| H | -3.437158 | -0.190763 | 2.995763 |
| H | -5.499107 | 0.888746 | -0.625133 |
| H | -1.162600 | 1.079744 | -1.594856 |
| C | 2.379349 | 2.543046 | -1.378996 |
| H | 1.569427 | 2.504071 | -2.113225 |
| H | 3.033764 | 3.381097 | -1.640968 |
| H | 2.962812 | 1.618889 | -1.446003 |
| C | 2.978443 | 2.795117 | 1.059717 |
| H | 3.606853 | 3.672807 | 0.876880 |
| H | 2.577360 | 2.864479 | 2.076394 |
| H | 3.602267 | 1.898306 | 0.992563 |
| C | 0.953641 | 3.987459 | 0.151177 |
| H | 0.142770 | 3.964168 | -0.579519 |
| H | 0.519951 | 4.053285 | 1.154687 |
| H | 1.554902 | 4.887326 | -0.021464 |
| H | -5.302601 | 0.991815 | 1.852948 |

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**INT-13**

*G*sol(DCM) = -4391.70692 Hartree

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| | | | |
|---|---|---|---|
| C | -2.403697 | -1.893118 | 2.156521 |
| C | -3.743081 | 1.993488 | 0.239346 |
| C | 7.511154 | -1.957713 | -2.034463 |
| C | 6.471501 | -1.333721 | -1.378508 |
| C | 5.195177 | -1.954079 | -1.265172 |
| C | 5.014634 | -3.235095 | -1.881214 |
| C | 6.111535 | -3.860698 | -2.535265 |
| C | 7.337672 | -3.239753 | -2.610072 |
| H | 8.472507 | -1.457814 | -2.115462 |
| H | 6.620235 | -0.347430 | -0.954151 |
| C | 4.077152 | -1.336926 | -0.603005 |
| C | 3.740385 | -3.854936 | -1.832683 |
| H | 5.957329 | -4.837621 | -2.986863 |
| H | 8.167643 | -3.722606 | -3.118078 |
| C | 2.642948 | -3.232530 | -1.272320 |
| C | 2.828803 | -1.938834 | -0.699247 |
| H | 3.626086 | -4.845428 | -2.265391 |
| C | 4.228235 | -0.068311 | 0.167385 |
| C | 5.151197 | 0.026560 | 1.267668 |
| C | 3.456347 | 1.042781 | -0.155582 |
| C | 5.856237 | -1.095296 | 1.790169 |
| C | 5.353771 | 1.296983 | 1.898594 |
| C | 3.669877 | 2.320828 | 0.446640 |
| C | 6.730796 | -0.959313 | 2.847630 |
| H | 5.690556 | -2.074339 | 1.355793 |
| C | 6.274004 | 1.408334 | 2.977303 |
| C | 4.622054 | 2.421236 | 1.440827 |
| C | 6.954651 | 0.305963 | 3.443381 |
| H | 7.249541 | -1.833525 | 3.231380 |
| H | 6.421296 | 2.383702 | 3.434544 |
| H | 4.809205 | 3.387669 | 1.901459 |
| H | 7.652115 | 0.400151 | 4.270843 |
| O | 1.732444 | -1.283797 | -0.170529 |
| O | 2.520011 | 0.956363 | -1.160092 |
| P | 1.134218 | 0.028126 | -1.028652 |
| O | 0.152785 | 0.666387 | -0.081793 |
| O | 0.767333 | -0.343780 | -2.429456 |
| C | 1.329399 | -3.950665 | -1.233753 |
| C | 0.589567 | -4.143617 | -2.425415 |
| C | 0.877800 | -4.517481 | -0.016475 |
| C | -0.620928 | -4.936555 | -2.395938 |
| C | 0.980424 | -3.571415 | -3.680709 |
| C | -0.339978 | -5.297412 | 0.001763 |
| C | 1.592963 | -4.373607 | 1.217143 |
| C | -1.352974 | -5.139854 | -3.610319 |
| C | -1.052175 | -5.491214 | -1.186673 |

| | | | |
|---|---|---|---|
| C | 0.246990 | -3.783618 | -4.819937 |
| H | 1.862085 | -2.943004 | -3.714002 |
| C | -0.782140 | -5.874078 | 1.235379 |
| C | 1.133762 | -4.938543 | 2.379689 |
| H | 2.517992 | -3.807692 | 1.225003 |
| C | -0.932592 | -4.583736 | -4.789871 |
| H | -2.250918 | -5.752273 | -3.573731 |
| H | -1.959548 | -6.091356 | -1.170721 |
| H | 0.562087 | -3.332815 | -5.756863 |
| H | -1.694397 | -6.466254 | 1.228840 |
| C | -0.071938 | -5.698239 | 2.393601 |
| H | 1.694845 | -4.809649 | 3.300962 |
| H | -1.496152 | -4.745044 | -5.704560 |
| H | -0.417707 | -6.141622 | 3.323156 |
| C | 2.927948 | 3.542569 | 0.004097 |
| C | 1.999819 | 4.159776 | 0.878206 |
| C | 3.216622 | 4.125374 | -1.254804 |
| C | 1.350175 | 5.389393 | 0.476995 |
| C | 1.663360 | 3.619813 | 2.163530 |
| C | 2.550539 | 5.346681 | -1.647711 |
| C | 4.172032 | 3.567639 | -2.165603 |
| C | 0.431106 | 6.020562 | 1.375291 |
| C | 1.638086 | 5.945535 | -0.773004 |
| C | 0.783874 | 4.260441 | 2.998368 |
| H | 2.117372 | 2.686003 | 2.474844 |
| C | 2.850015 | 5.929205 | -2.920215 |
| C | 4.433263 | 4.157301 | -3.376210 |
| H | 4.700026 | 2.663217 | -1.884926 |
| C | 0.159835 | 5.480333 | 2.604533 |
| H | -0.042355 | 6.946976 | 1.059301 |
| H | 1.146332 | 6.869644 | -1.069182 |
| H | 0.553011 | 3.832287 | 3.969695 |
| H | 2.336046 | 6.845551 | -3.200121 |
| C | 3.761877 | 5.353107 | -3.764463 |
| H | 5.162601 | 3.712166 | -4.047430 |
| H | -0.531779 | 5.973907 | 3.281483 |
| H | 3.981607 | 5.804999 | -4.727686 |
| C | -4.323331 | -2.544190 | -2.339621 |
| C | -4.755368 | -1.505315 | -3.376664 |
| C | -2.759566 | -0.330189 | -3.139863 |
| C | -2.234220 | -1.285084 | -2.063852 |
| H | -5.390551 | -1.991003 | -4.121969 |
| H | -3.791826 | -3.357110 | -2.848986 |
| H | -5.179707 | -2.954343 | -1.810385 |
| H | -1.902060 | 0.041942 | -3.703963 |
| H | -3.265008 | 0.518736 | -2.662320 |
| H | -1.604495 | -2.059573 | -2.510997 |
| H | -1.643872 | -0.707842 | -1.359479 |
| H | -5.328134 | -0.698929 | -2.893387 |
| O | -3.629672 | -0.979796 | -4.058451 |
| N | -3.362529 | -1.957610 | -1.377700 |
| C | -4.664413 | -2.732557 | 0.525702 |
| C | -4.631341 | -4.012110 | 1.101474 |
| C | -5.856932 | -1.991193 | 0.537149 |
| C | -5.788905 | -4.551987 | 1.663426 |
| H | -3.707117 | -4.581712 | 1.099429 |
| C | -7.004859 | -2.532253 | 1.115635 |
| H | -5.879213 | -0.990015 | 0.117674 |
| C | -6.974823 | -3.813607 | 1.672684 |
| H | -5.760972 | -5.547118 | 2.097029 |
| H | -7.920348 | -1.948550 | 1.132696 |
| H | -7.872364 | -4.233593 | 2.117284 |
| C | -3.426875 | -2.145397 | -0.067179 |
| C | -2.320617 | -1.820355 | 0.791738 |
| H | -1.374513 | -1.519036 | 0.361038 |
| C | -1.311143 | -1.656430 | 2.995700 |
| C | -0.357499 | -1.463644 | 3.734164 |
| C | 0.775339 | -1.228423 | 4.552494 |
| C | 2.026048 | -0.944551 | 3.958860 |
| C | 0.666530 | -1.273306 | 5.959790 |
| C | 3.138745 | -0.711099 | 4.761670 |
| H | 2.104678 | -0.912583 | 2.876472 |
| C | 1.786030 | -1.036389 | 6.751281 |
| H | -0.295213 | -1.492297 | 6.412652 |
| C | 3.020611 | -0.755847 | 6.155425 |
| H | 4.098825 | -0.496501 | 4.302867 |

| | | | |
|---|---|---|---|
| H | 1.698430 | -1.070497 | 7.833159 |
| H | 3.891859 | -0.572262 | 6.777693 |
| H | -3.336736 | 4.220345 | -0.909969 |
| C | -2.470920 | 3.559430 | -1.031015 |
| O | -2.895760 | 2.181056 | -0.860072 |
| H | -1.741055 | 3.800767 | -0.248214 |
| C | -1.869088 | 3.713994 | -2.403069 |
| C | -0.601692 | 3.181924 | -2.679350 |
| C | -2.572270 | 4.361148 | -3.427297 |
| C | -5.184297 | 2.032157 | -0.056183 |
| C | -3.114700 | 1.741163 | 1.422542 |
| C | -0.052066 | 3.288298 | -3.957705 |
| H | -0.051422 | 2.681943 | -1.888019 |
| C | -2.021316 | 4.475747 | -4.706599 |
| H | -3.554397 | 4.780934 | -3.221605 |
| C | -6.200444 | 1.759021 | 0.889441 |
| C | -5.598355 | 2.339338 | -1.372832 |
| O | -1.775198 | 1.670377 | 1.553519 |
| O | -3.793812 | 1.493157 | 2.563675 |
| C | -0.761039 | 3.936135 | -4.974352 |
| H | 0.929824 | 2.868466 | -4.157458 |
| H | -2.575389 | 4.984478 | -5.490997 |
| C | -7.548082 | 1.809980 | 0.534407 |
| H | -5.926239 | 1.494631 | 1.900839 |
| C | -6.948701 | 2.389755 | -1.719903 |
| H | -4.847314 | 2.533876 | -2.129293 |
| H | -1.309030 | 1.461262 | 0.706913 |
| C | -7.937963 | 2.129062 | -0.769608 |
| H | -8.300893 | 1.595543 | 1.289430 |
| H | -7.225043 | 2.633969 | -2.742791 |
| H | -8.989806 | 2.169412 | -1.038880 |
| C | -2.326121 | 1.901021 | 4.508218 |
| C | -3.590866 | 2.342252 | 3.764059 |
| H | -1.428265 | 2.113074 | 3.925505 |
| H | -2.259785 | 2.431582 | 5.465093 |
| H | -2.360522 | 0.826080 | 4.712069 |
| C | -4.833893 | 2.052611 | 4.608969 |
| C | -3.531782 | 3.816377 | 3.358410 |
| H | -4.767273 | 2.579452 | 5.566519 |
| H | -5.743367 | 2.382115 | 4.096766 |
| H | -4.916344 | 0.979587 | 4.811919 |
| H | -2.648401 | 4.029238 | 2.748704 |
| H | -4.426546 | 4.102061 | 2.795592 |
| H | -3.477893 | 4.440043 | 4.257226 |
| H | -3.347126 | -2.149554 | 2.632527 |
| H | -0.331069 | 4.022662 | -5.968699 |

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**TS-RR**

*G*sol(DCM) = -4391.68811 Hartree

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| | | | |
|---|---|---|---|
| C | -2.807574 | 1.240214 | -0.983207 |
| C | -3.964629 | -0.560661 | 0.503262 |
| C | -6.224697 | 2.464216 | -3.310571 |
| C | -5.951387 | 3.102709 | -2.098205 |
| C | -4.863297 | 2.724096 | -1.312000 |
| C | -3.986832 | 1.685645 | -1.719054 |
| C | -4.306629 | 1.030047 | -2.935888 |
| C | -5.390503 | 1.417622 | -3.717562 |
| H | -7.067822 | 2.772484 | -3.922723 |
| H | -6.588805 | 3.915325 | -1.757294 |
| H | -4.671453 | 3.249940 | -0.388873 |
| H | -3.687691 | 0.200920 | -3.254798 |
| H | -5.588796 | 0.892984 | -4.649181 |
| C | -2.183199 | 1.880284 | 0.145510 |
| O | -1.019799 | 1.624581 | 0.535475 |
| O | -2.953653 | 2.771991 | 0.806538 |
| C | -2.423062 | 3.677793 | 1.845265 |
| O | -1.961765 | 0.365072 | -1.670023 |
| C | -1.035952 | 1.045535 | -2.565646 |
| H | -1.589026 | 1.815179 | -3.116920 |
| H | -0.264040 | 1.537204 | -1.965253 |
| C | -0.417438 | 0.060067 | -3.526042 |
| C | 0.889450 | -0.406567 | -3.330525 |
| C | -1.130537 | -0.386900 | -4.649049 |
| C | 1.469166 | -1.304191 | -4.232335 |
| H | 1.455224 | -0.061852 | -2.470190 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -0.558772 | -1.290029 | -5.546725 | H | -5.657607 | -2.948871 | 0.537880 |
| H | -2.134173 | -0.011578 | -4.830303 | C | -6.570648 | -3.730892 | -2.646470 |
| C | 0.744493 | -1.751915 | -5.339371 | H | -7.368194 | -2.328277 | -4.080700 |
| H | 2.486231 | -1.650569 | -4.070038 | H | -5.770872 | -4.882910 | -1.006611 |
| H | -1.124702 | -1.623950 | -6.412396 | H | -6.619009 | -4.577590 | -3.325289 |
| H | -0.071275 | 0.461168 | 0.261902 | C | -6.416616 | -0.393003 | 0.059841 |
| C | -1.957319 | 2.891622 | 3.074493 | C | -5.258239 | -0.090054 | 0.789760 |
| H | -1.063545 | 2.306349 | 2.860251 | H | -5.357435 | 0.529678 | 1.674410 |
| H | -1.737308 | 3.592623 | 3.887992 | H | -3.783118 | -1.128522 | -0.404046 |
| H | -2.747562 | 2.213332 | 3.412091 | C | -3.018901 | -0.674352 | 1.535702 |
| C | -3.646110 | 4.532254 | 2.195747 | C | -2.257183 | -0.810026 | 2.481490 |
| H | -3.384060 | 5.255362 | 2.974918 | C | -1.431149 | -0.993803 | 3.624175 |
| H | -4.001924 | 5.084027 | 1.319316 | C | -1.886151 | -0.585362 | 4.898150 |
| H | -4.462860 | 3.904819 | 2.568566 | C | -0.159587 | -1.595646 | 3.513479 |
| C | -1.311252 | 4.551978 | 1.255683 | C | -1.087452 | -0.771448 | 6.022810 |
| H | -0.436775 | 3.957850 | 0.986752 | H | -2.865999 | -0.127001 | 4.989351 |
| H | -1.671416 | 5.077456 | 0.364210 | C | 0.630730 | -1.778932 | 4.645762 |
| H | -1.006997 | 5.302127 | 1.993904 | H | 0.196285 | -1.909223 | 2.538558 |
| C | -8.917101 | -0.273924 | 0.050796 | C | 0.172281 | -1.368061 | 5.901209 |
| C | -9.608084 | -0.393866 | 1.415814 | H | -1.447679 | -0.452250 | 6.996797 |
| C | -8.367814 | 1.403188 | 2.290168 | H | 1.607129 | -2.243714 | 4.546370 |
| C | -7.648129 | 1.581438 | 0.950995 | H | 0.793099 | -1.511736 | 6.781051 |
| H | -10.640685 | -0.728277 | 1.281797 | C | 6.245494 | -2.242723 | -3.943562 |
| H | -9.496717 | 0.390480 | -0.600760 | C | 5.832775 | -1.523116 | -2.842649 |
| H | -8.849346 | -1.252935 | -0.420019 | C | 4.907044 | -2.072448 | -1.910721 |
| H | -8.505813 | 2.371496 | 2.778717 | C | 4.390519 | -3.383226 | -2.171218 |
| H | -7.779684 | 0.751017 | 2.954756 | C | 4.850531 | -4.107670 | -3.305495 |
| H | -8.232204 | 2.267693 | 0.325051 | C | 5.762506 | -3.553535 | -4.174482 |
| H | -6.653102 | 2.006419 | 1.073260 | H | 6.945125 | -1.796631 | -4.644840 |
| H | -9.073105 | -1.133273 | 2.032828 | H | 6.205796 | -0.517173 | -2.690704 |
| O | -9.668039 | 0.858028 | 2.087773 | C | 4.440776 | -1.355937 | -0.752156 |
| N | -7.574094 | 0.301103 | 0.235328 | C | 3.414868 | -3.930745 | -1.301234 |
| C | -6.451436 | -1.541360 | -0.890600 | H | 4.455226 | -5.105335 | -3.478630 |
| C | -6.947313 | -1.382637 | -2.196554 | H | 6.102994 | -4.111288 | -5.042108 |
| C | -6.022224 | -2.812697 | -0.475151 | C | 2.893049 | -3.216715 | -0.241795 |
| C | -6.997037 | -2.467862 | -3.069402 | C | 3.403220 | -1.906741 | -0.011703 |
| H | -7.270220 | -0.401431 | -2.528592 | H | 3.051280 | -4.936938 | -1.491304 |
| C | -6.087633 | -3.901190 | -1.347192 | C | 5.030256 | -0.038391 | -0.372893 |

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| C | 6.436615 | 0.119627 | -0.114885 |
| C | 4.212526 | 1.074709 | -0.255893 |
| C | 7.340324 | -0.976932 | -0.038188 |
| C | 6.952206 | 1.436653 | 0.117145 |
| C | 4.703721 | 2.393975 | -0.045470 |
| C | 8.679609 | -0.776846 | 0.219228 |
| H | 6.964164 | -1.984761 | -0.170936 |
| C | 8.342395 | 1.610845 | 0.361864 |
| C | 6.066986 | 2.544773 | 0.113402 |
| C | 9.192181 | 0.529283 | 0.408990 |
| H | 9.348064 | -1.630917 | 0.282319 |
| H | 8.718547 | 2.617717 | 0.524144 |
| H | 6.476888 | 3.540048 | 0.262385 |
| H | 10.251233 | 0.672208 | 0.603419 |
| O | 2.873094 | -1.195693 | 1.063724 |
| O | 2.835680 | 0.899830 | -0.399219 |
| P | 2.048280 | 0.196935 | 0.855871 |
| O | 0.691800 | -0.229207 | 0.188067 |
| O | 2.030466 | 0.979946 | 2.111459 |
| C | 1.851130 | -3.845104 | 0.631312 |
| C | 0.527589 | -3.990362 | 0.150987 |
| C | 2.214398 | -4.367192 | 1.895998 |
| C | -0.452718 | -4.682842 | 0.958822 |
| C | 0.101618 | -3.466741 | -1.112952 |
| C | 1.224450 | -5.055956 | 2.694025 |
| C | 3.541398 | -4.260127 | 2.426375 |
| C | -1.788213 | -4.826234 | 0.463531 |
| C | -0.078301 | -5.197721 | 2.203972 |
| C | -1.188861 | -3.621176 | -1.549229 |
| H | 0.814162 | -2.929461 | -1.726998 |
| C | 1.600911 | -5.584830 | 3.969419 |
| C | 3.861956 | -4.779667 | 3.654915 |
| H | 4.304062 | -3.760786 | 1.838382 |
| C | -2.148453 | -4.314225 | -0.754953 |
| H | -2.512143 | -5.351958 | 1.081457 |
| H | -0.818169 | -5.719683 | 2.806983 |
| H | -1.486644 | -3.205142 | -2.507545 |
| H | 0.843616 | -6.097681 | 4.557321 |
| C | 2.880169 | -5.450794 | 4.441025 |
| H | 4.875631 | -4.683914 | 4.034165 |
| H | -3.165462 | -4.425259 | -1.119304 |
| H | 3.153732 | -5.856340 | 5.411017 |
| C | 3.798719 | 3.585217 | -0.023359 |
| C | 3.576231 | 4.280147 | 1.190275 |
| C | 3.213853 | 4.045259 | -1.228504 |
| C | 2.755385 | 5.471692 | 1.188813 |
| C | 4.119418 | 3.849316 | 2.445277 |
| C | 2.381836 | 5.227511 | -1.211971 |
| C | 3.422717 | 3.397159 | -2.489425 |
| C | 2.544831 | 6.177849 | 2.416294 |
| C | 2.180017 | 5.910552 | -0.007902 |
| C | 3.890006 | 4.551742 | 3.600269 |
| H | 4.713953 | 2.943836 | 2.475457 |
| C | 1.790690 | 5.683776 | -2.432949 |
| C | 2.838040 | 3.865811 | -3.638367 |
| H | 4.061761 | 2.521864 | -2.532431 |
| C | 3.097452 | 5.736448 | 3.589010 |
| H | 1.931355 | 7.075301 | 2.394369 |
| H | 1.561712 | 6.805598 | -0.002720 |
| H | 4.311374 | 4.200363 | 4.538092 |
| H | 1.164856 | 6.572305 | -2.400847 |
| C | 2.006069 | 5.022666 | -3.613115 |
| H | 3.011883 | 3.353226 | -4.580434 |
| H | 2.930069 | 6.280330 | 4.514481 |
| H | 1.551133 | 5.377982 | -4.533441 |
| H | 1.194009 | -2.449719 | -6.040852 |

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**TS-RS**

*G*sol(DCM) = -4391.690605 Hartree

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| C | 3.394110 | 0.892165 | -1.119629 |
| C | 4.879424 | -0.424006 | 0.433217 |
| C | 6.487501 | 2.557715 | -3.623535 |
| C | 5.802080 | 1.413627 | -4.042060 |
| C | 4.794184 | 0.849727 | -3.260726 |
| C | 4.426372 | 1.419350 | -2.016943 |

| | | | |
|---|---|---|---|
| C | 5.137335 | 2.577493 | -1.610149 |
| C | 6.143742 | 3.132587 | -2.396727 |
| H | 7.271521 | 2.990680 | -4.238782 |
| H | 6.050415 | 0.950829 | -4.994622 |
| H | 4.280283 | -0.031928 | -3.614282 |
| H | 4.893018 | 3.030490 | -0.655749 |
| H | 6.663565 | 4.021118 | -2.045912 |
| C | 2.480891 | -0.197485 | -1.336767 |
| O | 1.507901 | -0.428237 | -0.571249 |
| O | 2.779639 | -1.003726 | -2.378395 |
| C | 1.979113 | -2.184926 | -2.753631 |
| O | 3.021953 | 1.722591 | -0.068806 |
| C | 2.034724 | 2.721515 | -0.424216 |
| H | 2.432681 | 3.355384 | -1.225456 |
| H | 1.135677 | 2.219988 | -0.796313 |
| C | 1.717149 | 3.546018 | 0.796368 |
| C | 0.813882 | 3.070006 | 1.757996 |
| C | 2.334356 | 4.786493 | 1.003454 |
| C | 0.538325 | 3.817146 | 2.905366 |
| H | 0.319435 | 2.114214 | 1.604703 |
| C | 2.058958 | 5.538740 | 2.148637 |
| H | 3.031895 | 5.167163 | 0.261026 |
| C | 1.162318 | 5.053108 | 3.104051 |
| H | -0.169316 | 3.439975 | 3.638874 |
| H | 2.541260 | 6.501910 | 2.293031 |
| C | 4.925558 | 1.253920 | 2.912236 |
| C | 6.285015 | 0.904898 | 2.980192 |
| C | 4.553545 | 2.592831 | 3.127846 |
| C | 7.251714 | 1.873236 | 3.254314 |
| H | 6.577878 | -0.129438 | 2.830289 |
| C | 5.522672 | 3.558688 | 3.392706 |
| H | 3.508023 | 2.874874 | 3.063228 |
| C | 6.873517 | 3.202096 | 3.458566 |
| H | 8.298273 | 1.587939 | 3.310878 |
| H | 5.222284 | 4.592095 | 3.540024 |
| H | 7.626322 | 3.956819 | 3.668272 |
| C | 3.899189 | 0.217630 | 2.614235 |
| C | 4.065556 | -0.676648 | 1.540744 |
| H | 3.489028 | -1.594987 | 1.536708 |
| H | 5.421500 | 0.515467 | 0.388839 |
| C | 5.335399 | -1.442957 | -0.424612 |
| C | 5.790043 | -2.305721 | -1.158438 |
| C | 6.342686 | -3.305302 | -2.006964 |
| C | 7.118390 | -2.938532 | -3.128846 |
| C | 6.133891 | -4.675925 | -1.739613 |
| C | 7.666213 | -3.917058 | -3.954393 |
| H | 7.276035 | -1.885545 | -3.341237 |
| C | 6.686816 | -5.646309 | -2.571702 |
| H | 5.541429 | -4.964315 | -0.876801 |
| C | 7.453679 | -5.272108 | -3.679843 |
| H | 8.260152 | -3.622560 | -4.815005 |
| H | 6.519698 | -6.697700 | -2.355294 |
| H | 7.882704 | -6.032256 | -4.326436 |
| H | 0.058533 | 0.110813 | -0.637227 |
| C | -7.107682 | -0.667653 | -3.993887 |
| C | -6.404218 | -0.776129 | -2.813521 |
| C | -5.585906 | 0.290482 | -2.346539 |
| C | -5.487961 | 1.468339 | -3.156193 |
| C | -6.240919 | 1.556783 | -4.359579 |
| C | -7.038416 | 0.513494 | -4.771434 |
| H | -7.717859 | -1.499786 | -4.333691 |
| H | -6.462566 | -1.692819 | -2.238450 |
| C | -4.827030 | 0.220593 | -1.125714 |
| C | -4.633979 | 2.523893 | -2.748808 |
| H | -6.163452 | 2.463055 | -4.954759 |
| H | -7.604453 | 0.587431 | -5.695504 |
| C | -3.834902 | 2.431393 | -1.626420 |
| C | -3.927391 | 1.239354 | -0.852933 |
| H | -4.597318 | 3.427383 | -3.351309 |
| C | -4.979920 | -0.925229 | -0.182961 |
| C | -6.255590 | -1.260913 | 0.390938 |
| C | -3.878121 | -1.690076 | 0.169046 |
| C | -7.412220 | -0.445012 | 0.242769 |
| C | -6.365324 | -2.448217 | 1.185268 |
| C | -3.969216 | -2.891283 | 0.927590 |
| C | -8.611383 | -0.801754 | 0.821133 |

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|---|---|---|---|
| H | -7.343171 | 0.478252 | -0.320725 |
| C | -7.621563 | -2.798348 | 1.752990 |
| C | -5.216612 | -3.250644 | 1.399691 |
| C | -8.724831 | -1.995306 | 1.574403 |
| H | -9.477693 | -0.157052 | 0.702355 |
| H | -7.688895 | -3.708857 | 2.342924 |
| H | -5.321333 | -4.169628 | 1.969881 |
| H | -9.678368 | -2.266736 | 2.018080 |
| O | -3.113845 | 1.141421 | 0.278255 |
| O | -2.619751 | -1.300754 | -0.297569 |
| P | -1.931398 | 0.028635 | 0.361687 |
| O | -0.900649 | 0.446759 | -0.754869 |
| O | -1.443754 | -0.115383 | 1.752952 |
| C | -2.952193 | 3.574228 | -1.235802 |
| C | -1.829873 | 3.905583 | -2.033376 |
| C | -3.290338 | 4.367966 | -0.112058 |
| C | -1.036017 | 5.067761 | -1.698050 |
| C | -1.425787 | 3.131077 | -3.170731 |
| C | -2.474165 | 5.512895 | 0.224001 |
| C | -4.433454 | 4.103272 | 0.710596 |
| C | 0.083752 | 5.411538 | -2.521259 |
| C | -1.375309 | 5.834719 | -0.579277 |
| C | -0.342937 | 3.491754 | -3.931202 |
| H | -1.988852 | 2.240714 | -3.425857 |
| C | -2.817490 | 6.306771 | 1.364431 |
| C | -4.731587 | 4.890538 | 1.793356 |
| H | -5.077465 | 3.265879 | 0.465579 |
| C | 0.420820 | 4.651935 | -3.610179 |
| H | 0.662345 | 6.293993 | -2.259637 |
| H | -0.769869 | 6.702545 | -0.327443 |
| H | -0.059039 | 2.885944 | -4.787324 |
| H | -2.188034 | 7.160014 | 1.604919 |
| C | -3.911416 | 6.005751 | 2.131797 |
| H | -5.604619 | 4.665965 | 2.399911 |
| H | 1.271477 | 4.924053 | -4.228635 |
| H | -4.162771 | 6.616174 | 2.994593 |
| C | -2.791488 | -3.778587 | 1.181954 |
| C | -2.286414 | -3.919571 | 2.497592 |
| C | -2.247243 | -4.544435 | 0.121753 |
| C | -1.223090 | -4.866560 | 2.755524 |
| C | -2.779490 | -3.156391 | 3.607081 |
| C | -1.167101 | -5.467764 | 0.389807 |
| C | -2.739377 | -4.470153 | -1.222095 |
| C | -0.742953 | -5.031820 | 4.094156 |
| C | -0.688971 | -5.607678 | 1.696983 |
| C | -2.287841 | -3.340399 | 4.874281 |
| H | -3.552818 | -2.417081 | 3.432389 |
| C | -0.623970 | -6.240526 | -0.685740 |
| C | -2.193903 | -5.229824 | -2.225437 |
| H | -3.565798 | -3.804333 | -1.444908 |
| C | -1.262577 | -4.298059 | 5.127587 |
| H | 0.047950 | -5.756612 | 4.270720 |
| H | 0.112271 | -6.316002 | 1.896139 |
| H | -2.679589 | -2.747683 | 5.696212 |
| H | 0.188587 | -6.928485 | -0.465503 |
| C | -1.118024 | -6.126047 | -1.958651 |
| H | -2.588558 | -5.154590 | -3.234912 |
| H | -0.890554 | -4.432831 | 6.139203 |
| H | -0.700876 | -6.721284 | -2.765999 |
| C | 2.820951 | 0.541469 | 4.847579 |
| C | 1.597634 | -0.593801 | 3.085250 |
| C | 2.600079 | -0.703536 | 5.719866 |
| H | 2.007650 | 1.258942 | 5.008822 |
| H | 3.765907 | 1.016848 | 5.107234 |
| C | 1.423696 | -1.802979 | 4.002042 |
| H | 0.754148 | 0.088354 | 3.241313 |
| H | 1.606704 | -0.864020 | 2.030184 |
| H | 2.496104 | -0.407914 | 6.767872 |
| H | 3.470924 | -1.372138 | 5.625528 |
| H | 0.465004 | -2.289129 | 3.811644 |
| H | 2.232451 | -2.532098 | 3.834813 |
| N | 2.824412 | 0.136988 | 3.433958 |
| O | 1.408482 | -1.392500 | 5.368371 |
| H | 0.944760 | 5.636972 | 3.994408 |
| C | 1.951281 | -3.211681 | -1.616724 |
| H | 1.411105 | -2.828224 | -0.750534 |

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| H | 1.452988 | -4.123672 | -1.963803 |
| H | 2.970964 | -3.469794 | -1.313477 |
| C | 0.572379 | -1.758242 | -3.188022 |
| H | 0.630743 | -0.971563 | -3.948443 |
| H | 0.052947 | -2.617275 | -3.627392 |
| H | -0.022026 | -1.394470 | -2.350062 |
| C | 2.751740 | -2.741442 | -3.954752 |
| H | 2.255947 | -3.642499 | -4.330627 |
| H | 2.790274 | -2.006525 | -4.766036 |
| H | 3.775761 | -3.001508 | -3.670499 |

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**TS-SR**

*G*sol(DCM) = -4391.694386 Hartree

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| C | -3.350238 | 1.049891 | -0.896440 |
| C | -4.806137 | -1.161770 | 0.312394 |
| C | -6.652320 | 2.886820 | -2.982439 |
| C | -5.833425 | 1.972457 | -3.651859 |
| C | -4.758558 | 1.359131 | -3.010245 |
| C | -4.452034 | 1.642025 | -1.654389 |
| C | -5.300031 | 2.568838 | -0.994163 |
| C | -6.372334 | 3.175523 | -1.643834 |
| H | -7.487432 | 3.360989 | -3.490955 |
| H | -6.029687 | 1.731567 | -4.694538 |
| H | -4.144457 | 0.660249 | -3.558726 |
| H | -5.108987 | 2.793974 | 0.048357 |
| H | -6.995567 | 3.879018 | -1.096044 |
| C | -2.395014 | 0.100018 | -1.296718 |
| O | -1.510844 | -0.326696 | -0.462971 |
| O | -2.525500 | -0.392632 | -2.551286 |
| C | -1.536679 | -1.203103 | -3.273881 |
| O | -3.168691 | 1.557065 | 0.390854 |
| C | -2.167460 | 2.602341 | 0.451369 |
| H | -2.394191 | 3.352342 | -0.317427 |
| H | -1.184630 | 2.169578 | 0.239697 |
| C | -2.184990 | 3.230902 | 1.822286 |
| C | -1.245423 | 2.853969 | 2.792397 |
| C | -3.152762 | 4.191433 | 2.151798 |
| C | -1.283937 | 3.417850 | 4.072027 |
| H | -0.466933 | 2.141608 | 2.530336 |
| C | -3.192700 | 4.756034 | 3.428218 |
| H | -3.874838 | 4.500825 | 1.399788 |
| C | -2.259383 | 4.365364 | 4.393972 |
| H | -0.545263 | 3.124692 | 4.813700 |
| H | -3.944590 | 5.503531 | 3.667484 |
| C | -1.265458 | -2.533079 | -2.560401 |
| H | -0.690278 | -2.409709 | -1.643887 |
| H | -0.697517 | -3.188274 | -3.230654 |
| H | -2.211998 | -3.028405 | -2.320897 |
| C | -2.243120 | -1.469271 | -4.609338 |
| H | -1.596512 | -2.065506 | -5.261383 |
| H | -2.472554 | -0.527942 | -5.119604 |
| H | -3.176910 | -2.017470 | -4.450642 |
| C | -0.267875 | -0.377472 | -3.512385 |
| H | 0.251032 | -0.136571 | -2.583992 |
| H | -0.514539 | 0.554868 | -4.031294 |
| H | 0.424697 | -0.945341 | -4.144050 |
| C | -1.379268 | -1.280097 | 2.755215 |
| C | -0.880060 | -2.491603 | 3.541700 |
| C | -2.075263 | -1.805534 | 5.440816 |
| C | -2.631304 | -0.569873 | 4.717935 |
| H | 0.130770 | -2.753895 | 3.222875 |
| H | -0.688158 | -0.442501 | 2.907023 |
| H | -1.431820 | -1.465290 | 1.684904 |
| H | -1.936187 | -1.572912 | 6.500052 |
| H | -2.795515 | -2.634270 | 5.352324 |
| H | -1.972590 | 0.290594 | 4.877475 |
| H | -3.623159 | -0.331564 | 5.097046 |
| H | -1.540372 | -3.356018 | 3.370482 |
| O | -0.808870 | -2.192983 | 4.932298 |
| N | -2.692881 | -0.850996 | 3.271759 |
| C | -5.004411 | -0.108982 | 3.066822 |
| C | -6.239176 | -0.775886 | 3.142547 |
| C | -4.919826 | 1.232062 | 3.479679 |
| C | -7.365633 | -0.116419 | 3.634802 |
| H | -6.308804 | -1.812575 | 2.829345 |

| | | | |
|---|---|---|---|
| C | -6.052303 | 1.890696 | 3.954122 |
| H | -3.977036 | 1.760990 | 3.398376 |
| C | -7.275374 | 1.217843 | 4.038060 |
| H | -8.312203 | -0.644755 | 3.699986 |
| H | -5.978331 | 2.932365 | 4.251980 |
| H | -8.154823 | 1.733294 | 4.413414 |
| C | -3.809871 | -0.818303 | 2.536056 |
| C | -3.893903 | -1.501755 | 1.286113 |
| H | -3.190804 | -2.298802 | 1.076615 |
| H | -5.456684 | -0.305820 | 0.469235 |
| C | -5.037342 | -1.921152 | -0.843735 |
| C | -5.304438 | -2.572552 | -1.841531 |
| C | -5.632112 | -3.332157 | -2.997042 |
| C | -6.487988 | -2.793011 | -3.982946 |
| C | -5.114824 | -4.634302 | -3.173776 |
| C | -6.814130 | -3.540174 | -5.111408 |
| H | -6.880598 | -1.789512 | -3.851932 |
| C | -5.449059 | -5.372730 | -4.305818 |
| H | -4.459089 | -5.052743 | -2.416642 |
| C | -6.297868 | -4.829939 | -5.276122 |
| H | -7.471766 | -3.116590 | -5.864968 |
| H | -5.047435 | -6.373952 | -4.432439 |
| H | -6.555345 | -5.409532 | -6.157980 |
| H | -0.300255 | -0.574980 | -0.495327 |
| C | 7.084549 | -1.446229 | -3.643301 |
| C | 6.328483 | -0.726685 | -2.742822 |
| C | 5.572937 | -1.381294 | -1.729680 |
| C | 5.596200 | -2.813212 | -1.693394 |
| C | 6.400634 | -3.526205 | -2.624608 |
| C | 7.134202 | -2.859771 | -3.579567 |
| H | 7.644333 | -0.922947 | -4.413494 |
| H | 6.295279 | 0.354209 | -2.814215 |
| C | 4.763521 | -0.672505 | -0.773643 |
| C | 4.812831 | -3.496562 | -0.729753 |
| H | 6.414761 | -4.611989 | -2.573194 |
| H | 7.740528 | -3.413138 | -4.290927 |
| C | 3.964019 | -2.830406 | 0.131778 |
| C | 3.923117 | -1.407246 | 0.051262 |
| H | 4.875763 | -4.580223 | -0.679848 |
| C | 4.813563 | 0.815377 | -0.668962 |
| C | 6.047936 | 1.506610 | -0.405636 |
| C | 3.654052 | 1.564386 | -0.807226 |
| C | 7.258233 | 0.836859 | -0.070323 |
| C | 6.059392 | 2.939022 | -0.440101 |
| C | 3.648726 | 2.988445 | -0.871137 |
| C | 8.415044 | 1.542570 | 0.182659 |
| H | 7.264148 | -0.244487 | 0.000879 |
| C | 7.273529 | 3.637270 | -0.192854 |
| C | 4.855973 | 3.638750 | -0.708179 |
| C | 8.430808 | 2.956433 | 0.109254 |
| H | 9.323444 | 1.008023 | 0.446241 |
| H | 7.264732 | 4.723506 | -0.234821 |
| H | 4.886049 | 4.723390 | -0.766464 |
| H | 9.351683 | 3.498713 | 0.303721 |
| O | 3.056470 | -0.739970 | 0.909128 |
| O | 2.444892 | 0.896874 | -0.964099 |
| P | 1.785741 | 0.121251 | 0.329853 |
| O | 0.814241 | -0.880176 | -0.339735 |
| O | 1.294022 | 1.022092 | 1.405310 |
| C | 3.175341 | -3.597024 | 1.146451 |
| C | 2.135161 | -4.464168 | 0.730514 |
| C | 3.531103 | -3.515185 | 2.516172 |
| C | 1.440818 | -5.268406 | 1.713121 |
| C | 1.722514 | -4.586560 | -0.637268 |
| C | 2.815314 | -4.309929 | 3.489178 |
| C | 4.601841 | -2.690627 | 2.993318 |
| C | 0.403655 | -6.157244 | 1.284597 |
| C | 1.795102 | -5.166945 | 3.062019 |
| C | 0.723801 | -5.451073 | -1.007004 |
| H | 2.211363 | -3.976726 | -1.388291 |
| C | 3.176571 | -4.219070 | 4.871212 |
| C | 4.921512 | -2.635122 | 4.325861 |
| H | 5.173366 | -2.104203 | 2.282629 |
| C | 0.055969 | -6.253241 | -0.036435 |
| H | -0.101817 | -6.757753 | 2.037017 |
| H | 1.268614 | -5.772916 | 3.796265 |

| | | | |
|---|---|---|---|
| H | 0.433393 | -5.524178 | -2.051286 |
| H | 2.621364 | -4.819074 | 5.588007 |
| C | 4.197240 | -3.403765 | 5.282543 |
| H | 5.738493 | -2.000816 | 4.658535 |
| H | -0.730775 | -6.933627 | -0.350056 |
| H | 4.463659 | -3.343818 | 6.334002 |
| C | 2.403773 | 3.772529 | -1.142515 |
| C | 1.863756 | 4.611180 | -0.136309 |
| C | 1.813261 | 3.731291 | -2.429798 |
| C | 0.707001 | 5.428192 | -0.434047 |
| C | 2.408716 | 4.691338 | 1.187826 |
| C | 0.642374 | 4.533451 | -2.704866 |
| C | 2.342354 | 2.940131 | -3.501031 |
| C | 0.183890 | 6.296360 | 0.577019 |
| C | 0.123263 | 5.360463 | -1.703032 |
| C | 1.877124 | 5.535838 | 2.128528 |
| H | 3.256180 | 4.066209 | 1.444448 |
| C | 0.048294 | 4.482022 | -4.006003 |
| C | 1.747934 | 2.922672 | -4.737173 |
| H | 3.235823 | 2.350312 | -3.328386 |
| C | 0.754430 | 6.358209 | 1.820372 |
| H | -0.681129 | 6.907715 | 0.331993 |
| H | -0.748855 | 5.973652 | -1.919691 |
| H | 2.311722 | 5.576561 | 3.123526 |
| H | -0.835743 | 5.087063 | -4.191769 |
| C | 0.580118 | 3.698069 | -4.995549 |
| H | 2.172440 | 2.315396 | -5.531849 |
| H | 0.349293 | 7.021999 | 2.578860 |
| H | 0.122558 | 3.669897 | -5.980460 |
| H | -2.286720 | 4.805153 | 5.387467 |

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**TS-SS**

*G*sol(DCM) = -4391.688349 Hartree

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|---|---|---|---|
| C | 3.362860 | -0.674127 | 0.498218 |
| C | 4.460059 | 1.142358 | -0.650123 |
| C | 6.592759 | -2.564608 | 2.639629 |
| C | 6.098972 | -3.156751 | 1.474533 |
| C | 5.060654 | -2.566496 | 0.753876 |
| C | 4.469894 | -1.357343 | 1.183109 |
| C | 4.985387 | -0.773043 | 2.365015 |
| C | 6.025973 | -1.363625 | 3.077596 |
| H | 7.401367 | -3.029942 | 3.196627 |
| H | 6.523985 | -4.092397 | 1.118929 |
| H | 4.696519 | -3.049822 | -0.142339 |
| H | 4.556618 | 0.159850 | 2.714889 |
| H | 6.395793 | -0.882751 | 3.980047 |
| C | 2.711950 | -1.101214 | -0.729662 |
| O | 1.552506 | -0.775203 | -1.061113 |
| O | 3.507373 | -1.801157 | -1.563194 |
| C | 3.097553 | -2.199615 | -2.926277 |
| O | 2.578556 | 0.151634 | 1.288772 |
| C | 1.785757 | -0.508655 | 2.311999 |
| H | 2.410686 | -1.234957 | 2.841256 |
| H | 0.962518 | -1.046007 | 1.832691 |
| C | 1.270837 | 0.536633 | 3.268742 |
| C | 0.115388 | 1.273629 | 2.971387 |
| C | 1.953158 | 0.801888 | 4.464428 |
| C | -0.342566 | 2.259550 | 3.848370 |
| H | -0.431890 | 1.063196 | 2.056568 |
| C | 1.495186 | 1.783814 | 5.346127 |
| H | 2.845206 | 0.229722 | 4.708635 |
| C | 0.346402 | 2.517356 | 5.037629 |
| H | -1.239738 | 2.821772 | 3.604040 |
| H | 2.031357 | 1.972880 | 6.272376 |
| H | 0.187466 | -0.594778 | -0.353297 |
| C | 2.853956 | -0.954276 | -3.785743 |
| H | 1.999383 | -0.380415 | -3.423627 |
| H | 2.656224 | -1.260196 | -4.819266 |
| H | 3.741356 | -0.311364 | -3.788814 |
| C | 4.328488 | -2.962406 | -3.426423 |
| H | 4.174980 | -3.281093 | -4.462512 |
| H | 4.510411 | -3.852628 | -2.815058 |
| H | 5.218325 | -2.325753 | -3.386530 |
| C | 1.877925 | -3.124892 | -2.879319 |
| H | 0.977618 | -2.588074 | -2.578772 |

| | | | |
|---|---|---|---|
| H | 2.049460 | -3.946602 | -2.176495 |
| H | 1.714009 | -3.556288 | -3.873239 |
| C | 1.898753 | 5.177332 | 0.703741 |
| C | 2.706586 | 6.424570 | 1.084370 |
| C | 3.928641 | 5.229111 | 2.700128 |
| C | 3.148831 | 3.952398 | 2.378811 |
| H | 2.086081 | 7.319069 | 0.978600 |
| H | 0.977990 | 5.137730 | 1.299339 |
| H | 1.628101 | 5.212802 | -0.350474 |
| H | 4.187751 | 5.259582 | 3.762062 |
| H | 4.855886 | 5.265557 | 2.106701 |
| H | 2.255219 | 3.908747 | 3.014263 |
| H | 3.739687 | 3.060291 | 2.576574 |
| H | 3.577049 | 6.515808 | 0.415222 |
| O | 3.131826 | 6.381249 | 2.441418 |
| N | 2.696606 | 3.975594 | 0.983389 |
| C | 2.403668 | 3.124926 | -1.280444 |
| C | 1.076461 | 2.681726 | -1.377075 |
| C | 3.068632 | 3.561837 | -2.436767 |
| C | 0.427979 | 2.666269 | -2.612763 |
| H | 0.566853 | 2.320412 | -0.489035 |
| C | 2.412177 | 3.565095 | -3.668629 |
| H | 4.098232 | 3.900013 | -2.364198 |
| C | 1.092938 | 3.114105 | -3.758270 |
| H | -0.583783 | 2.281307 | -2.680345 |
| H | 2.933429 | 3.912905 | -4.556168 |
| H | 0.582810 | 3.107928 | -4.717394 |
| C | 3.124622 | 3.105447 | 0.030340 |
| C | 4.196990 | 2.233359 | 0.211382 |
| H | 4.847326 | 2.349492 | 1.070993 |
| H | 3.829834 | 1.032901 | -1.526590 |
| C | 5.753713 | 0.589291 | -0.748129 |
| C | 6.874498 | 0.115123 | -0.835429 |
| C | 8.189501 | -0.420490 | -0.934148 |
| C | 9.117745 | -0.234067 | 0.113220 |
| C | 8.588941 | -1.147464 | -2.076426 |
| C | 10.403954 | -0.759758 | 0.015938 |
| H | 8.815208 | 0.320410 | 0.996124 |
| C | 9.877552 | -1.668302 | -2.164459 |
| H | 7.880587 | -1.294781 | -2.886031 |
| C | 10.789144 | -1.477280 | -1.120932 |
| H | 11.108171 | -0.609736 | 0.829545 |
| H | 10.172163 | -2.225450 | -3.049428 |
| H | 11.793259 | -1.885449 | -1.193294 |
| C | -6.269688 | -1.577224 | 4.257189 |
| C | -5.843766 | -1.143674 | 3.019905 |
| C | -4.925370 | -1.911634 | 2.250703 |
| C | -4.432744 | -3.134409 | 2.811060 |
| C | -4.906805 | -3.563941 | 4.081216 |
| C | -5.808668 | -2.804741 | 4.791418 |
| H | -6.962584 | -0.968000 | 4.830758 |
| H | -6.199138 | -0.196067 | 2.631471 |
| C | -4.443575 | -1.494572 | 0.960751 |
| C | -3.478697 | -3.895625 | 2.089919 |
| H | -4.531374 | -4.500317 | 4.486030 |
| H | -6.159048 | -3.137139 | 5.764329 |
| C | -2.940224 | -3.458089 | 0.895657 |
| C | -3.410121 | -2.215206 | 0.381039 |
| H | -3.153313 | -4.847410 | 2.500868 |
| C | -5.035998 | -0.326084 | 0.247601 |
| C | -6.439906 | -0.276358 | -0.066896 |
| C | -4.232423 | 0.726513 | -0.161988 |
| C | -7.324871 | -1.369762 | 0.150138 |
| C | -6.972292 | 0.910453 | -0.667748 |
| C | -4.743743 | 1.923161 | -0.739627 |
| C | -8.661023 | -1.278055 | -0.175703 |
| H | -6.937781 | -2.292939 | 0.564742 |
| C | -8.359038 | 0.980379 | -0.975461 |
| C | -6.104803 | 1.992801 | -0.959948 |
| C | -9.190578 | -0.088719 | -0.732025 |
| H | -9.313851 | -2.130205 | -0.008743 |
| H | -8.746309 | 1.893714 | -1.419764 |
| H | -6.525973 | 2.898137 | -1.388625 |
| H | -10.247178 | -0.028890 | -0.976519 |
| O | -2.850814 | -1.759765 | -0.812813 |
| O | -2.855563 | 0.642925 | 0.058731 |

| | | | |
|---|---|---|---|
| P | -1.977405 | -0.381347 | -0.860170 |
| O | -0.732587 | -0.551853 | 0.092499 |
| O | -1.744694 | 0.005816 | -2.269796 |
| C | -1.952541 | -4.307302 | 0.159411 |
| C | -0.665123 | -4.534132 | 0.705112 |
| C | -2.340417 | -4.946652 | -1.044894 |
| C | 0.252683 | -5.420802 | 0.022641 |
| C | -0.212766 | -3.919545 | 1.918887 |
| C | -1.406295 | -5.816258 | -1.724265 |
| C | -3.643903 | -4.795567 | -1.620937 |
| C | 1.547358 | -5.658426 | 0.585785 |
| C | -0.139207 | -6.031589 | -1.172344 |
| C | 1.034756 | -4.177719 | 2.427917 |
| H | -0.875386 | -3.238088 | 2.439850 |
| C | -1.802648 | -6.456836 | -2.941177 |
| C | -3.987710 | -5.430972 | -2.786796 |
| H | -4.374318 | -4.171347 | -1.118423 |
| C | 1.930545 | -5.059500 | 1.756349 |
| H | 2.220736 | -6.330657 | 0.059642 |
| H | 0.555645 | -6.695928 | -1.681420 |
| H | 1.347550 | -3.702710 | 3.353442 |
| H | -1.083754 | -7.102168 | -3.440018 |
| C | -3.054990 | -6.269493 | -3.463085 |
| H | -4.983807 | -5.298200 | -3.199897 |
| H | 2.916150 | -5.245265 | 2.173187 |
| H | -3.345417 | -6.762108 | -4.386720 |
| C | -3.874186 | 3.095815 | -1.071267 |
| C | -3.586898 | 3.402427 | -2.422916 |
| C | -3.413755 | 3.940716 | -0.032881 |
| C | -2.820864 | 4.588990 | -2.737082 |
| C | -4.016078 | 2.578157 | -3.514773 |
| C | -2.636633 | 5.115262 | -0.360084 |
| C | -3.708046 | 3.700413 | 1.348809 |
| C | -2.544100 | 4.899656 | -4.106735 |
| C | -2.363892 | 5.408566 | -1.700338 |
| C | -3.726123 | 2.908984 | -4.813549 |
| H | -4.573153 | 1.673226 | -3.300616 |
| C | -2.178352 | 5.966499 | 0.695767 |
| C | -3.258386 | 4.546021 | 2.331364 |
| H | -4.308984 | 2.838045 | 1.616424 |
| C | -2.984520 | 4.087812 | -5.118265 |
| H | -1.972648 | 5.798489 | -4.324786 |
| H | -1.786897 | 6.298522 | -1.942171 |
| H | -4.060886 | 2.265085 | -5.622089 |
| H | -1.594180 | 6.844647 | 0.431567 |
| C | -2.476572 | 5.692836 | 2.004851 |
| H | -3.506572 | 4.347008 | 3.370392 |
| H | -2.768952 | 4.334385 | -6.154105 |
| H | -2.129467 | 6.350173 | 2.796962 |
| H | -0.014117 | 3.280133 | 5.722778 |

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**INT-14**

*G*sol(DCM) = -1903.599586 Hartree

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| | | | |
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| C | -0.149724 | 0.982077 | 0.648039 |
| C | -0.301504 | -0.609406 | 0.547895 |
| C | -3.134065 | 2.703794 | 3.321207 |
| C | -2.882291 | 3.306231 | 2.088701 |
| C | -1.945468 | 2.754812 | 1.210043 |
| C | -1.245070 | 1.585451 | 1.539907 |
| C | -1.494765 | 1.002574 | 2.794546 |
| C | -2.430212 | 1.549427 | 3.672671 |
| H | -3.863970 | 3.130970 | 4.003194 |
| H | -3.412467 | 4.210900 | 1.803806 |
| H | -1.772378 | 3.244476 | 0.259716 |
| H | -0.947766 | 0.117652 | 3.103853 |
| H | -2.605481 | 1.073096 | 4.633410 |
| C | -0.112173 | 1.522189 | -0.809113 |
| O | 0.918815 | 1.815108 | -1.379114 |
| O | -1.331412 | 1.512898 | -1.362836 |
| C | -1.564842 | 1.861579 | -2.788735 |
| O | 1.142214 | 1.114335 | 1.239934 |
| C | 1.525784 | 2.329053 | 1.907497 |
| H | 2.312234 | 1.996611 | 2.593340 |
| H | 0.698529 | 2.710005 | 2.513785 |
| C | 2.067062 | 3.427620 | 1.015646 |

| | | | |
|---|---|---|---|
| C | 1.367731 | 4.628706 | 0.851411 |
| C | 3.304692 | 3.274064 | 0.374216 |
| C | 1.885421 | 5.654110 | 0.053404 |
| H | 0.412275 | 4.764840 | 1.352854 |
| C | 3.824590 | 4.291941 | -0.423741 |
| H | 3.858725 | 2.346791 | 0.500097 |
| C | 3.113885 | 5.486512 | -0.587736 |
| H | 1.330358 | 6.581197 | -0.063798 |
| H | 4.785182 | 4.159014 | -0.914683 |
| C | -0.846064 | 0.853743 | -3.689929 |
| H | 0.238198 | 0.937045 | -3.595731 |
| H | -1.120489 | 1.041926 | -4.733699 |
| H | -1.149439 | -0.168230 | -3.438364 |
| C | -3.083280 | 1.724161 | -2.919196 |
| H | -3.389984 | 1.953817 | -3.944861 |
| H | -3.594260 | 2.416203 | -2.241957 |
| H | -3.403899 | 0.705218 | -2.680823 |
| C | -1.124247 | 3.304018 | -3.055702 |
| H | -0.044855 | 3.418658 | -2.946875 |
| H | -1.626436 | 3.993319 | -2.368020 |
| H | -1.405739 | 3.583011 | -4.077162 |
| C | 3.093589 | -3.818838 | -1.070094 |
| C | 4.474017 | -3.974522 | -1.700904 |
| C | 4.298490 | -1.882087 | -2.732023 |
| C | 2.908605 | -1.652590 | -2.139120 |
| H | 4.672180 | -5.026015 | -1.928384 |
| H | 2.340027 | -4.293424 | -1.722536 |
| H | 3.070826 | -4.327042 | -0.103492 |
| H | 4.375134 | -1.402247 | -3.712071 |
| H | 5.059088 | -1.446241 | -2.064198 |
| H | 2.145333 | -1.965744 | -2.873654 |
| H | 2.765963 | -0.586171 | -1.938762 |
| H | 5.243862 | -3.611553 | -1.000665 |
| O | 4.564943 | -3.265914 | -2.932840 |
| N | 2.785063 | -2.392111 | -0.883404 |
| C | 1.864987 | -2.633710 | 1.365246 |
| C | 0.801519 | -3.308434 | 1.986800 |
| C | 3.081570 | -2.511953 | 2.058830 |
| C | 0.942892 | -3.828708 | 3.275461 |
| H | -0.135219 | -3.433358 | 1.450646 |
| C | 3.222610 | -3.030909 | 3.345613 |
| H | 3.912351 | -2.003600 | 1.578687 |
| C | 2.152594 | -3.689602 | 3.959507 |
| H | 0.110213 | -4.350190 | 3.739701 |
| H | 4.167301 | -2.919834 | 3.871291 |
| H | 2.263655 | -4.095654 | 4.961247 |
| C | 1.725899 | -2.065428 | -0.009862 |
| C | 0.719734 | -1.236669 | -0.375943 |
| H | 0.644072 | -0.939808 | -1.416044 |
| H | -0.090216 | -0.943365 | 1.566742 |
| C | -1.657864 | -1.046180 | 0.196798 |
| C | -2.753815 | -1.491414 | -0.078156 |
| C | -4.053955 | -1.990334 | -0.404024 |
| C | -4.339561 | -2.456203 | -1.703797 |
| C | -5.072973 | -2.024367 | 0.569657 |
| C | -5.609162 | -2.938927 | -2.017002 |
| H | -3.558381 | -2.436624 | -2.457787 |
| C | -6.339424 | -2.509198 | 0.248324 |
| H | -4.860042 | -1.667009 | 1.572578 |
| C | -6.612647 | -2.967431 | -1.044066 |
| H | -5.815298 | -3.294433 | -3.022799 |
| H | -7.115401 | -2.529107 | 1.008595 |
| H | -7.601065 | -3.344537 | -1.291120 |
| H | 3.519992 | 6.281896 | -1.207066 |

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**INT-15**

*G*sol(DCM) = -3775.854515 Hartree

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| | | | |
|---|---|---|---|
| C | 3.885523 | -0.214355 | 1.485281 |
| C | 2.488811 | 2.036900 | -1.665013 |
| O | 1.679987 | 2.055202 | -0.499393 |
| H | 1.256911 | 1.162193 | -0.429234 |
| C | 2.742094 | 3.867640 | 1.844119 |
| C | 3.298424 | 4.948100 | 2.774536 |
| C | 1.735672 | 4.408316 | 4.428920 |
| C | 1.115564 | 3.300687 | 3.565135 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 3.654507 | 5.790999 | 2.177336 | C | -4.909497 | -2.718212 | 3.761994 |
| H | 1.934104 | 4.275832 | 1.230558 | C | -4.561955 | -2.092797 | 2.583327 |
| H | 3.499972 | 3.487734 | 1.166646 | C | -3.533782 | -2.615200 | 1.747610 |
| H | 0.953896 | 4.855701 | 5.047815 | C | -2.849412 | -3.796167 | 2.185278 |
| H | 2.504689 | 3.975488 | 5.087089 | C | -3.244583 | -4.428743 | 3.396296 |
| H | 0.294744 | 3.705888 | 2.965334 | C | -4.255366 | -3.905620 | 4.170874 |
| H | 0.736195 | 2.499949 | 4.195591 | H | -5.690883 | -2.292849 | 4.385832 |
| H | 4.140375 | 4.547227 | 3.359547 | H | -5.068158 | -1.180085 | 2.290454 |
| O | 2.286289 | 5.447700 | 3.636947 | C | -3.131060 | -1.991186 | 0.515447 |
| N | 2.145496 | 2.775436 | 2.642561 | C | -1.780986 | -4.307662 | 1.406311 |
| C | 1.668085 | 0.476060 | 3.262310 | H | -2.721793 | -5.330996 | 3.704268 |
| C | 2.232835 | -0.302390 | 4.286189 | H | -4.545128 | -4.392634 | 5.097659 |
| C | 0.333923 | 0.264432 | 2.875463 | C | -1.325485 | -3.662346 | 0.273916 |
| C | 1.459832 | -1.264424 | 4.936545 | C | -1.995463 | -2.466995 | -0.132226 |
| H | 3.265326 | -0.141991 | 4.580732 | H | -1.297773 | -5.227256 | 1.725819 |
| C | -0.425053 | -0.712818 | 3.518813 | C | -3.892838 | -0.846480 | -0.065745 |
| H | -0.095083 | 0.829718 | 2.055289 | C | -5.290444 | -0.957084 | -0.389859 |
| C | 0.131824 | -1.471261 | 4.552728 | C | -3.239289 | 0.349726 | -0.335473 |
| H | 1.895594 | -1.851460 | 5.739391 | C | -6.013607 | -2.181191 | -0.311603 |
| H | -1.450402 | -0.884309 | 3.206475 | C | -5.989187 | 0.204997 | -0.854794 |
| H | -0.467534 | -2.226379 | 5.053005 | C | -3.926938 | 1.519354 | -0.778410 |
| C | 2.495985 | 1.501137 | 2.569533 | C | -7.351506 | -2.241612 | -0.638845 |
| C | 3.672480 | 1.084700 | 1.849376 | H | -5.497403 | -3.082574 | -0.002027 |
| H | 4.411866 | 1.824412 | 1.570753 | C | -7.373196 | 0.113736 | -1.168592 |
| H | 3.136591 | -0.970645 | 1.711656 | C | -5.284060 | 1.426084 | -1.008431 |
| C | 5.017689 | -0.646601 | 0.783513 | C | -8.046158 | -1.082140 | -1.060184 |
| C | 5.983654 | -1.065193 | 0.164575 | H | -7.877018 | -3.190772 | -0.578324 |
| C | 7.101546 | -1.552373 | -0.559920 | H | -7.887549 | 1.009087 | -1.509145 |
| C | 8.182100 | -0.698278 | -0.871375 | H | -5.831111 | 2.306672 | -1.335339 |
| C | 7.138753 | -2.900408 | -0.979407 | H | -9.101999 | -1.142698 | -1.308467 |
| C | 9.272319 | -1.187358 | -1.584527 | O | -1.541841 | -1.826948 | -1.262069 |
| H | 8.151689 | 0.337619 | -0.549019 | O | -1.883394 | 0.437098 | -0.104600 |
| C | 8.233644 | -3.377203 | -1.693426 | P | -0.832959 | -0.313920 | -1.174726 |
| H | 6.303482 | -3.551673 | -0.742180 | O | 0.468432 | -0.384310 | -0.412912 |
| C | 9.300725 | -2.524307 | -1.996259 | O | -0.929938 | 0.258735 | -2.549619 |
| H | 10.101243 | -0.527079 | -1.821415 | C | -0.189507 | -4.239627 | -0.511081 |
| H | 8.256819 | -4.413952 | -2.015645 | C | 1.106078 | -4.304337 | 0.059838 |
| H | 10.153456 | -2.900976 | -2.553668 | C | -0.426416 | -4.788530 | -1.796711 |

| | | | |
|---|---|---|---|
| C | 2.180780 | -4.938157 | -0.673289 |
| C | 1.416921 | -3.761648 | 1.350766 |
| C | 0.663426 | -5.393257 | -2.529144 |
| C | -1.721813 | -4.798338 | -2.409093 |
| C | 3.478345 | -5.032104 | -0.074510 |
| C | 1.934330 | -5.455338 | -1.948068 |
| C | 2.674321 | -3.870516 | 1.889291 |
| H | 0.637527 | -3.255813 | 1.908331 |
| C | 0.417165 | -5.937532 | -3.829790 |
| C | -1.919208 | -5.335310 | -3.655578 |
| H | -2.561883 | -4.375278 | -1.870130 |
| C | 3.721624 | -4.521525 | 1.173044 |
| H | 4.267002 | -5.528759 | -0.634928 |
| H | 2.747337 | -5.924767 | -2.497769 |
| H | 2.874246 | -3.459288 | 2.875163 |
| H | 1.251370 | -6.381096 | -4.367887 |
| C | -0.835562 | -5.907797 | -4.382602 |
| H | -2.912763 | -5.328005 | -4.095264 |
| H | 4.707913 | -4.607001 | 1.620465 |
| H | -1.010931 | -6.324801 | -5.370360 |
| C | -3.217125 | 2.824708 | -0.959112 |
| C | -2.970442 | 3.325847 | -2.259593 |
| C | -2.844871 | 3.581423 | 0.178347 |
| C | -2.328002 | 4.612570 | -2.419656 |
| C | -3.325180 | 2.606665 | -3.447809 |
| C | -2.194216 | 4.860807 | 0.005536 |
| C | -3.108885 | 3.143784 | 1.517171 |
| C | -2.093321 | 5.117607 | -3.738622 |
| C | -1.951984 | 5.341113 | -1.286344 |
| C | -3.084621 | 3.126252 | -4.693401 |
| H | -3.783460 | 1.629968 | -3.348914 |
| C | -1.830247 | 5.621046 | 1.162251 |
| C | -2.751629 | 3.904886 | 2.601229 |
| H | -3.612697 | 2.195269 | 1.668301 |
| C | -2.463860 | 4.400722 | -4.844998 |
| H | -1.612042 | 6.087293 | -3.840195 |
| H | -1.471834 | 6.309393 | -1.411832 |
| H | -3.362379 | 2.559592 | -5.577876 |
| H | -1.342108 | 6.581392 | 1.014866 |
| C | -2.100402 | 5.161353 | 2.425060 |
| H | -2.970901 | 3.552693 | 3.605499 |
| H | -2.281997 | 4.794855 | -5.841011 |
| H | -1.829858 | 5.754028 | 3.294711 |
| C | 2.901050 | 3.443244 | -2.043994 |
| C | 4.186780 | 3.704830 | -2.533924 |
| C | 1.989861 | 4.504934 | -1.944721 |
| C | 4.555767 | 4.994849 | -2.926045 |
| H | 4.906527 | 2.892226 | -2.608067 |
| C | 2.357402 | 5.795823 | -2.328827 |
| H | 0.992988 | 4.311104 | -1.560487 |
| C | 3.641502 | 6.045677 | -2.823513 |
| H | 5.558558 | 5.178730 | -3.303250 |
| H | 1.639722 | 6.608254 | -2.244828 |
| H | 3.926824 | 7.050751 | -3.122981 |
| H | 3.392214 | 1.422373 | -1.517268 |
| H | 1.932576 | 1.584106 | -2.501594 |

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**TS-9**

*G*sol(DCM) = -3775.831712 Hartree

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| | | | |
|---|---|---|---|
| C | -3.195412 | 0.508975 | 0.647314 |
| C | -2.761142 | 0.041958 | -2.055687 |
| O | -2.260901 | -0.056376 | -0.697249 |
| H | -1.269895 | 0.405039 | -0.623820 |
| C | -4.272476 | -3.462801 | 2.002826 |
| C | -5.588784 | -3.653067 | 2.759638 |
| C | -4.495462 | -3.278613 | 4.812591 |
| C | -3.148035 | -3.067019 | 4.111321 |
| H | -6.216667 | -4.394129 | 2.257161 |
| H | -3.767935 | -4.434733 | 1.921224 |
| H | -4.434966 | -3.087324 | 0.992714 |
| H | -4.342742 | -3.746760 | 5.789333 |
| H | -4.989848 | -2.304950 | 4.960063 |
| H | -2.610822 | -4.021871 | 4.051432 |
| H | -2.538241 | -2.359984 | 4.672794 |
| H | -6.138062 | -2.699757 | 2.811846 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| O | -5.340677 | -4.151951 | 4.071410 | C | 3.629489 | 0.573419 | 0.841448 |
| N | -3.377739 | -2.569882 | 2.747206 | C | 3.189068 | 3.091848 | 2.049592 |
| C | -1.929913 | -0.638473 | 3.051817 | H | 4.064122 | 3.278201 | 4.579934 |
| C | -2.141770 | 0.541101 | 3.781913 | H | 5.105483 | 1.469681 | 5.917802 |
| C | -0.636468 | -1.180299 | 2.982002 | C | 2.715706 | 2.871420 | 0.772332 |
| C | -1.077442 | 1.167681 | 4.434422 | C | 2.917949 | 1.580043 | 0.203378 |
| H | -3.142892 | 0.958138 | 3.843295 | H | 3.058199 | 4.070114 | 2.504634 |
| C | 0.427204 | -0.544203 | 3.622784 | C | 3.910033 | -0.703946 | 0.121134 |
| H | -0.463869 | -2.089982 | 2.414160 | C | 5.251204 | -1.189590 | -0.064562 |
| C | 0.209151 | 0.628664 | 4.352476 | C | 2.858925 | -1.437818 | -0.414170 |
| H | -1.254926 | 2.073673 | 5.006940 | C | 6.406113 | -0.439190 | 0.295893 |
| H | 1.428054 | -0.959547 | 3.548434 | C | 5.446908 | -2.470223 | -0.678300 |
| H | 1.039394 | 1.118511 | 4.853218 | C | 3.035048 | -2.723662 | -1.005024 |
| C | -3.067871 | -1.302680 | 2.340820 | C | 7.673697 | -0.940791 | 0.091249 |
| C | -3.731122 | -0.655747 | 1.316542 | H | 6.283522 | 0.548465 | 0.725362 |
| H | -4.640077 | -1.073055 | 0.900710 | C | 6.766989 | -2.966396 | -0.860791 |
| H | -2.351376 | 0.978027 | 1.150176 | C | 4.319560 | -3.216901 | -1.106854 |
| C | -4.127420 | 1.464176 | 0.120575 | C | 7.860924 | -2.221920 | -0.481770 |
| C | -4.907221 | 2.299891 | -0.293387 | H | 8.538681 | -0.343928 | 0.367136 |
| C | -5.817506 | 3.286803 | -0.775363 | H | 6.894571 | -3.944180 | -1.318682 |
| C | -7.165837 | 2.956837 | -1.022236 | H | 4.479500 | -4.198987 | -1.544207 |
| C | -5.374285 | 4.604552 | -1.011576 | H | 8.865551 | -2.607032 | -0.631394 |
| C | -8.047439 | 3.926668 | -1.494045 | O | 2.424005 | 1.349748 | -1.070392 |
| H | -7.507501 | 1.942589 | -0.840777 | O | 1.571500 | -0.940719 | -0.312896 |
| C | -6.264444 | 5.566783 | -1.482352 | P | 1.117522 | 0.355659 | -1.246732 |
| H | -4.335676 | 4.857825 | -0.821856 | O | -0.054585 | 0.956831 | -0.469769 |
| C | -7.600436 | 5.231496 | -1.724492 | O | 0.981917 | 0.025569 | -2.692172 |
| H | -9.084670 | 3.664939 | -1.682081 | C | 2.046705 | 3.970301 | 0.007360 |
| H | -5.915999 | 6.579785 | -1.661640 | C | 0.753581 | 4.410036 | 0.378855 |
| H | -8.291238 | 5.984914 | -2.092062 | C | 2.736621 | 4.602118 | -1.056386 |
| C | 4.994532 | 0.010336 | 4.312394 | C | 0.143266 | 5.512941 | -0.331776 |
| C | 4.628131 | -0.233723 | 3.005612 | C | -0.001242 | 3.799862 | 1.434323 |
| C | 4.045059 | 0.787040 | 2.201976 | C | 2.108364 | 5.691979 | -1.768691 |
| C | 3.822868 | 2.069831 | 2.802025 | C | 4.057860 | 4.219697 | -1.458006 |
| C | 4.228499 | 2.294749 | 4.146597 | C | -1.158215 | 5.963439 | 0.060821 |
| C | 4.804797 | 1.289115 | 4.889731 | C | 0.832373 | 6.119548 | -1.386108 |
| H | 5.429899 | -0.788472 | 4.906416 | C | -1.246475 | 4.259534 | 1.778176 |
| H | 4.774466 | -1.221629 | 2.584286 | H | 0.423727 | 2.952809 | 1.959491 |

| | | | |
|---|---|---|---|
| C | 2.811138 | 6.321252 | -2.844972 |
| C | 4.699749 | 4.849910 | -2.493363 |
| H | 4.557531 | 3.417390 | -0.926245 |
| C | -1.834195 | 5.361200 | 1.088962 |
| H | -1.596079 | 6.801150 | -0.476649 |
| H | 0.367111 | 6.945711 | -1.919572 |
| H | -1.794714 | 3.777611 | 2.582944 |
| H | 2.321236 | 7.136143 | -3.372414 |
| C | 4.069124 | 5.913330 | -3.202156 |
| H | 5.701390 | 4.538893 | -2.777184 |
| H | -2.818197 | 5.716530 | 1.382421 |
| H | 4.592931 | 6.399197 | -4.020586 |
| C | 1.869116 | -3.538327 | -1.473519 |
| C | 1.605814 | -3.671767 | -2.857624 |
| C | 1.062632 | -4.213153 | -0.525911 |
| C | 0.501012 | -4.495904 | -3.297890 |
| C | 2.387565 | -3.013389 | -3.862651 |
| C | -0.045273 | -5.025115 | -0.977597 |
| C | 1.308162 | -4.147531 | 0.884600 |
| C | 0.247049 | -4.632957 | -4.699941 |
| C | -0.296720 | -5.143862 | -2.348995 |
| C | 2.111396 | -3.170917 | -5.196351 |
| H | 3.206716 | -2.375064 | -3.552629 |
| C | -0.852460 | -5.706329 | -0.011099 |
| C | 0.514512 | -4.820266 | 1.779593 |
| H | 2.147715 | -3.562120 | 1.243960 |
| C | 1.029210 | -3.994007 | -5.624907 |
| H | -0.585064 | -5.258682 | -5.013339 |
| H | -1.125816 | -5.762820 | -2.685450 |
| H | 2.718937 | -2.659338 | -5.937740 |
| H | -1.681512 | -6.312202 | -0.368701 |
| C | -0.585208 | -5.608429 | 1.329131 |
| H | 0.728853 | -4.760639 | 2.843149 |
| H | 0.827169 | -4.106296 | -6.686476 |
| H | -1.199731 | -6.137280 | 2.052452 |
| C | -3.741032 | -1.064289 | -2.357738 |
| C | -5.033740 | -0.768255 | -2.805094 |
| C | -3.359944 | -2.407530 | -2.217149 |
| C | -5.932786 | -1.794023 | -3.112385 |
| H | -5.339951 | 0.269279 | -2.911643 |
| C | -4.258185 | -3.432061 | -2.514589 |
| H | -2.357937 | -2.648392 | -1.872250 |
| C | -5.547857 | -3.127486 | -2.964919 |
| H | -6.932552 | -1.549369 | -3.460699 |
| H | -3.950686 | -4.468336 | -2.402827 |
| H | -6.245776 | -3.926462 | -3.200128 |
| H | -3.213118 | 1.025812 | -2.213095 |
| H | -1.864649 | -0.032868 | -2.681049 |

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**INT-16**

*G*sol(DCM) = -3775.844581 Hartree

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| | | | |
|---|---|---|---|
| C | -3.368092 | 0.327752 | 0.347268 |
| C | -3.014597 | 0.653985 | -2.136083 |
| O | -2.500658 | 0.700119 | -0.787597 |
| H | -0.941620 | 0.634391 | -0.388878 |
| C | -2.669518 | -3.974881 | 0.576498 |
| C | -4.044030 | -4.648231 | 0.627241 |
| C | -4.035696 | -4.535538 | 2.982322 |
| C | -2.661543 | -3.857765 | 2.985351 |
| H | -4.152720 | -5.372387 | -0.185808 |
| H | -1.900055 | -4.757594 | 0.608253 |
| H | -2.531512 | -3.407871 | -0.346437 |
| H | -4.152000 | -5.176414 | 3.861955 |
| H | -4.828024 | -3.768802 | 2.998469 |
| H | -1.878776 | -4.623328 | 3.059885 |
| H | -2.570183 | -3.190673 | 3.843989 |
| H | -4.845338 | -3.897849 | 0.538135 |
| O | -4.196342 | -5.379152 | 1.844018 |
| N | -2.453495 | -3.106950 | 1.737088 |
| C | -2.204026 | -0.948009 | 2.835280 |
| C | -3.051972 | -0.110234 | 3.576174 |
| C | -0.850747 | -1.039020 | 3.203330 |
| C | -2.558100 | 0.629836 | 4.653822 |
| H | -4.103614 | -0.048978 | 3.310153 |
| C | -0.357186 | -0.296350 | 4.275687 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -0.187828 | -1.687539 | 2.638325 | C | 5.650883 | 0.055968 | -0.236187 |
| C | -1.209127 | 0.539998 | 5.004720 | C | 3.401832 | -0.837400 | -0.120720 |
| H | -3.229485 | 1.267357 | 5.222604 | C | 6.591430 | 1.123764 | -0.211960 |
| H | 0.693729 | -0.368387 | 4.542211 | C | 6.107957 | -1.235170 | -0.659376 |
| H | -0.823935 | 1.113558 | 5.843293 | C | 3.835345 | -2.131425 | -0.523383 |
| C | -2.727213 | -1.738196 | 1.676599 | C | 7.911164 | 0.916105 | -0.551140 |
| C | -3.348747 | -1.148544 | 0.618533 | H | 6.259187 | 2.117624 | 0.064509 |
| H | -3.807424 | -1.759819 | -0.148489 | C | 7.479803 | -1.420237 | -0.985457 |
| H | -2.895760 | 0.864802 | 1.174036 | C | 5.183081 | -2.305776 | -0.762593 |
| C | -4.727315 | 0.848977 | 0.171297 | C | 8.366984 | -0.369652 | -0.929838 |
| C | -5.865061 | 1.261276 | 0.066949 | H | 8.607807 | 1.749518 | -0.533062 |
| C | -7.206624 | 1.739888 | -0.058317 | H | 7.811022 | -2.408929 | -1.292577 |
| C | -8.230443 | 0.882688 | -0.510053 | H | 5.547963 | -3.285369 | -1.059312 |
| C | -7.524781 | 3.073827 | 0.266962 | H | 9.411464 | -0.519640 | -1.187339 |
| C | -9.536884 | 1.351770 | -0.632109 | O | 2.106441 | 1.567566 | -1.097732 |
| H | -7.989955 | -0.146014 | -0.760513 | O | 2.036636 | -0.665917 | 0.119180 |
| C | -8.834187 | 3.534180 | 0.142988 | P | 1.170080 | 0.247269 | -0.914634 |
| H | -6.738743 | 3.737467 | 0.614270 | O | -0.025786 | 0.626810 | 0.040025 |
| C | -9.842921 | 2.676568 | -0.306419 | O | 0.850969 | -0.327193 | -2.241315 |
| H | -10.317816 | 0.682290 | -0.981556 | C | 1.099658 | 4.118791 | -0.333277 |
| H | -9.067983 | 4.564246 | 0.396893 | C | -0.201241 | 4.209063 | 0.218290 |
| H | -10.862529 | 3.038918 | -0.402361 | C | 1.387248 | 4.708479 | -1.588065 |
| C | 5.686894 | 2.017751 | 3.844898 | C | -1.237110 | 4.907227 | -0.512209 |
| C | 5.217471 | 1.428603 | 2.690562 | C | -0.555788 | 3.624901 | 1.478813 |
| C | 4.261298 | 2.086428 | 1.867096 | C | 0.339793 | 5.392778 | -2.312102 |
| C | 3.770510 | 3.364164 | 2.293726 | C | 2.691933 | 4.673515 | -2.179422 |
| C | 4.288809 | 3.952905 | 3.480083 | C | -2.548993 | 5.002678 | 0.052936 |
| C | 5.230891 | 3.298336 | 4.240435 | C | -0.941029 | 5.474482 | -1.755560 |
| H | 6.410588 | 1.491036 | 4.460595 | C | -1.825359 | 3.738191 | 1.985842 |
| H | 5.569915 | 0.442717 | 2.411003 | H | 0.197643 | 3.078561 | 2.034025 |
| C | 3.736295 | 1.508241 | 0.658114 | C | 0.637810 | 5.981753 | -3.581972 |
| C | 2.760117 | 4.013763 | 1.539093 | C | 2.938106 | 5.252541 | -3.398194 |
| H | 3.914289 | 4.927915 | 3.781287 | H | 3.498851 | 4.183084 | -1.645570 |
| H | 5.615559 | 3.753553 | 5.148513 | C | -2.838042 | 4.439410 | 1.267368 |
| C | 2.188148 | 3.428809 | 0.427839 | H | -3.312927 | 5.535190 | -0.508280 |
| C | 2.686213 | 2.157101 | 0.027243 | H | -1.724970 | 5.994641 | -2.301826 |
| H | 2.412756 | 4.990964 | 1.863458 | H | -2.065654 | 3.283011 | 2.942710 |
| C | 4.262798 | 0.226521 | 0.103127 | H | -0.163026 | 6.489082 | -4.114349 |

| | | | |
|---|---|---|---|
| C | 1.898052 | 5.913227 | -4.114467 |
| H | 3.936935 | 5.211541 | -3.823833 |
| H | -3.836978 | 4.519826 | 1.687026 |
| H | 2.112452 | 6.364414 | -5.079171 |
| C | 2.875920 | -3.272800 | -0.657296 |
| C | 2.490574 | -3.726038 | -1.941404 |
| C | 2.386168 | -3.914783 | 0.505351 |
| C | 1.588426 | -4.851125 | -2.058055 |
| C | 2.945994 | -3.109222 | -3.152722 |
| C | 1.487724 | -5.039742 | 0.374212 |
| C | 2.754655 | -3.507251 | 1.829070 |
| C | 1.198849 | -5.302631 | -3.359696 |
| C | 1.113203 | -5.476379 | -0.901087 |
| C | 2.548917 | -3.571874 | -4.380832 |
| H | 3.612841 | -2.257007 | -3.087935 |
| C | 1.004930 | -5.689797 | 1.554836 |
| C | 2.265766 | -4.153048 | 2.936461 |
| H | 3.440194 | -2.675656 | 1.951943 |
| C | 1.664312 | -4.684502 | -4.490419 |
| H | 0.525083 | -6.153172 | -3.428715 |
| H | 0.437925 | -6.324150 | -0.994745 |
| H | 2.907233 | -3.084152 | -5.283109 |
| H | 0.336841 | -6.539608 | 1.437958 |
| C | 1.377902 | -5.260193 | 2.801520 |
| H | 2.563042 | -3.824731 | 3.928544 |
| H | 1.363446 | -5.037340 | -5.472846 |
| H | 1.007580 | -5.763875 | 3.689927 |
| C | -3.283758 | -0.731565 | -2.685695 |
| C | -4.597346 | -1.159122 | -2.918321 |
| C | -2.221673 | -1.596943 | -2.992329 |
| C | -4.851681 | -2.431611 | -3.438432 |
| H | -5.425572 | -0.493686 | -2.687448 |
| C | -2.474453 | -2.869289 | -3.508455 |
| H | -1.197640 | -1.269585 | -2.829212 |
| C | -3.790233 | -3.290389 | -3.731802 |
| H | -5.875940 | -2.749199 | -3.614828 |
| H | -1.643359 | -3.529448 | -3.743903 |
| H | -3.985083 | -4.279462 | -4.137905 |
| H | -3.920868 | 1.265885 | -2.183335 |
| H | -2.233913 | 1.151758 | -2.718300 |

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**INT-17**

*G*sol(DCM) = -4025.162448 Hartree

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| | | | |
|---|---|---|---|
| C | -3.714207 | -0.429551 | 1.795849 |
| C | -0.181715 | -1.968864 | 3.518758 |
| C | 0.120064 | -2.763974 | 4.790206 |
| C | 0.480124 | -0.797667 | 5.997448 |
| C | 0.189834 | 0.082525 | 4.775955 |
| H | 0.605907 | -3.703936 | 4.518425 |
| H | 0.742036 | -1.770013 | 2.966376 |
| H | -0.859060 | -2.512208 | 2.865056 |
| H | 1.224360 | -0.298561 | 6.623239 |
| H | -0.441626 | -0.932584 | 6.584787 |
| H | 1.100664 | 0.296598 | 4.209870 |
| H | -0.266634 | 1.017023 | 5.094704 |
| H | -0.814120 | -2.987572 | 5.328611 |
| O | 1.020345 | -2.056393 | 5.629979 |
| N | -0.725025 | -0.636088 | 3.861609 |
| C | -2.120294 | 1.326704 | 3.524156 |
| C | -3.333027 | 1.744402 | 4.098855 |
| C | -1.195654 | 2.281479 | 3.062330 |
| C | -3.607976 | 3.104655 | 4.232144 |
| H | -4.046003 | 1.006792 | 4.453379 |
| C | -1.490862 | 3.639036 | 3.181694 |
| H | -0.270457 | 1.948163 | 2.597269 |
| C | -2.690098 | 4.051784 | 3.770731 |
| H | -4.539173 | 3.422982 | 4.690973 |
| H | -0.780930 | 4.373498 | 2.814131 |
| H | -2.910329 | 5.111114 | 3.867277 |
| C | -1.835365 | -0.122053 | 3.360673 |
| C | -2.786702 | -0.949014 | 2.653294 |
| H | -2.760503 | -2.022373 | 2.796612 |
| H | -3.722563 | 0.639292 | 1.590997 |
| C | -4.653341 | -1.209552 | 1.107276 |
| C | -5.486106 | -1.858952 | 0.494403 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -6.447917 | -2.630207 | -0.208382 | H | 7.802048 | 2.736999 | -0.112493 |
| C | -6.500987 | -4.031051 | -0.034856 | H | 5.508310 | 3.563134 | -0.033284 |
| C | -7.360299 | -2.006328 | -1.086923 | H | 9.414579 | 0.887479 | -0.464413 |
| C | -7.445167 | -4.783829 | -0.726920 | O | 2.236986 | -1.419055 | 0.403714 |
| H | -5.799465 | -4.509273 | 0.641157 | O | 1.934461 | 0.859501 | -0.735391 |
| C | -8.300235 | -2.769547 | -1.773115 | P | 1.191381 | -0.104877 | 0.415054 |
| H | -7.319262 | -0.929932 | -1.219819 | O | -0.138534 | -0.456649 | -0.177643 |
| C | -8.345075 | -4.156500 | -1.595453 | O | 1.343054 | 0.473061 | 1.793484 |
| H | -7.481626 | -5.860389 | -0.589397 | C | 1.287170 | -4.037810 | -0.271037 |
| H | -8.999067 | -2.284136 | -2.447809 | C | -0.061727 | -4.255140 | -0.643626 |
| H | -9.080443 | -4.747961 | -2.133136 | C | 1.798937 | -4.617055 | 0.916193 |
| C | 5.086380 | -1.584470 | -5.003053 | C | -0.915022 | -5.066279 | 0.198164 |
| C | 4.761002 | -1.048104 | -3.775547 | C | -0.639686 | -3.695676 | -1.830682 |
| C | 3.960841 | -1.769842 | -2.844699 | C | 0.934278 | -5.420075 | 1.751801 |
| C | 3.475395 | -3.059781 | -3.238171 | C | 3.163366 | -4.462171 | 1.326289 |
| C | 3.843067 | -3.593101 | -4.504265 | C | -2.274604 | -5.289372 | -0.191630 |
| C | 4.635459 | -2.875218 | -5.371158 | C | -0.397530 | -5.621451 | 1.372805 |
| H | 5.690947 | -1.008008 | -5.698000 | C | -1.946394 | -3.935840 | -2.170335 |
| H | 5.107391 | -0.054261 | -3.516904 | H | -0.025108 | -3.066605 | -2.463935 |
| C | 3.589842 | -1.247232 | -1.556742 | C | 1.464225 | -6.006797 | 2.945815 |
| C | 2.623678 | -3.777973 | -2.360739 | C | 3.633896 | -5.040604 | 2.477439 |
| H | 3.473479 | -4.578161 | -4.778718 | H | 3.834123 | -3.878539 | 0.705537 |
| H | 4.905368 | -3.288393 | -6.338935 | C | -2.778285 | -4.746326 | -1.343593 |
| C | 2.193760 | -3.246797 | -1.161754 | H | -2.898647 | -5.906036 | 0.450947 |
| C | 2.664704 | -1.949641 | -0.792223 | H | -1.042124 | -6.232577 | 2.001129 |
| H | 2.287984 | -4.769025 | -2.655192 | H | -2.356325 | -3.501918 | -3.078260 |
| C | 4.152185 | 0.037531 | -1.046066 | H | 0.801509 | -6.611854 | 3.560080 |
| C | 5.569166 | 0.235692 | -0.900140 | C | 2.774396 | -5.822086 | 3.303290 |
| C | 3.293278 | 1.068374 | -0.682242 | H | 4.673361 | -4.907033 | 2.763900 |
| C | 6.522164 | -0.808127 | -1.071727 | H | -3.811781 | -4.922893 | -1.627951 |
| C | 6.053886 | 1.531329 | -0.525218 | H | 3.165424 | -6.275131 | 4.210016 |
| C | 3.762196 | 2.371363 | -0.331689 | C | 2.821676 | 3.500463 | -0.049152 |
| C | 7.871623 | -0.574919 | -0.913039 | C | 2.756673 | 4.055831 | 1.253412 |
| H | 6.175839 | -1.805580 | -1.317216 | C | 2.038712 | 4.050137 | -1.095164 |
| C | 7.453335 | 1.744391 | -0.387049 | C | 1.904126 | 5.198683 | 1.501915 |
| C | 5.126728 | 2.576676 | -0.283668 | C | 3.492032 | 3.525169 | 2.364772 |
| C | 8.348010 | 0.716085 | -0.579317 | C | 1.169718 | 5.173619 | -0.825464 |
| H | 8.576808 | -1.391765 | -1.040422 | C | 2.077842 | 3.550290 | -2.437687 |

| | | | |
|---|---|---|---|
| C | 1.863153 | 5.769801 | 2.814819 |
| C | 1.132506 | 5.723132 | 0.460174 |
| C | 3.417767 | 4.095386 | 3.609863 |
| H | 4.110783 | 2.648956 | 2.210638 |
| C | 0.372560 | 5.713527 | -1.885063 |
| C | 1.297602 | 4.093841 | -3.426231 |
| H | 2.741590 | 2.725745 | -2.671988 |
| C | 2.600165 | 5.239809 | 3.840474 |
| H | 1.228937 | 6.638073 | 2.977564 |
| H | 0.489206 | 6.578941 | 0.653838 |
| H | 3.984793 | 3.669327 | 4.433039 |
| H | -0.275654 | 6.557698 | -1.662198 |
| C | 0.426973 | 5.187566 | -3.148743 |
| H | 1.344012 | 3.690557 | -4.433971 |
| H | 2.560295 | 5.682264 | 4.831969 |
| H | -0.183418 | 5.604533 | -3.944826 |
| C | -4.100245 | 1.428977 | -3.769384 |
| C | -2.673250 | 0.044897 | -2.393460 |
| C | -3.013945 | 1.069381 | -4.814003 |
| H | -5.012049 | 0.849643 | -3.977523 |
| C | -1.417254 | 0.369302 | -3.235142 |
| H | -2.380108 | -0.209700 | -1.374005 |
| H | -3.112997 | 1.704141 | -5.699519 |
| H | -1.005512 | -0.560809 | -3.659942 |
| C | -2.410953 | 2.295924 | -0.607910 |
| H | -1.600232 | 1.577986 | -0.557649 |
| H | -2.423400 | 3.079753 | 0.140645 |
| C | -3.418216 | 2.224110 | -1.510611 |
| N | -3.616541 | 1.159381 | -2.401581 |
| C | -4.485518 | 3.270980 | -1.497940 |
| C | -4.147300 | 4.632412 | -1.437069 |
| C | -5.846453 | 2.918391 | -1.505100 |
| C | -5.139201 | 5.613031 | -1.369371 |
| H | -3.098760 | 4.915956 | -1.455781 |
| C | -6.837721 | 3.897332 | -1.435454 |
| H | -6.120482 | 1.868054 | -1.550810 |
| C | -6.488016 | 5.249559 | -1.367151 |
| H | -4.857253 | 6.661876 | -1.327243 |
| H | -7.884547 | 3.604728 | -1.430894 |
| H | -7.260453 | 6.012288 | -1.317546 |
| O | -1.719986 | 1.298821 | -4.280551 |
| H | -3.195086 | -0.824228 | -2.813108 |
| H | -4.356381 | 2.485614 | -3.851021 |
| H | -3.115245 | 0.022544 | -5.141522 |
| H | -0.642175 | 0.837932 | -2.626508 |

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**TS-10**

*G*sol(DCM) = -4025.149349 Hartree

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| | | | |
|---|---|---|---|
| C | -3.355375 | 0.791569 | 1.247955 |
| C | -0.473686 | -1.837563 | 3.186690 |
| C | 0.097728 | -1.505289 | 4.566075 |
| C | -1.665380 | -2.640131 | 5.623901 |
| C | -2.301874 | -3.000707 | 4.274559 |
| H | 1.189926 | -1.483889 | 4.523530 |
| H | -0.070976 | -2.804271 | 2.858736 |
| H | -0.181450 | -1.083928 | 2.455914 |
| H | -1.853333 | -3.439016 | 6.347067 |
| H | -2.114915 | -1.707744 | 6.001974 |
| H | -1.924836 | -3.972992 | 3.935157 |
| H | -3.384090 | -3.061672 | 4.376980 |
| H | -0.262658 | -0.517938 | 4.895498 |
| O | -0.255256 | -2.502052 | 5.521711 |
| N | -1.935328 | -1.986676 | 3.274106 |
| C | -4.260872 | -1.585596 | 2.692969 |
| C | -5.218085 | -0.844478 | 3.402116 |
| C | -4.663848 | -2.728370 | 1.982884 |
| C | -6.556318 | -1.243038 | 3.404451 |
| H | -4.909596 | 0.037666 | 3.955552 |
| C | -6.003744 | -3.117855 | 1.979669 |
| H | -3.926051 | -3.304451 | 1.431141 |
| C | -6.951528 | -2.378053 | 2.692465 |
| H | -7.288239 | -0.666218 | 3.962521 |
| H | -6.306780 | -3.998554 | 1.420672 |
| H | -7.993563 | -2.684956 | 2.692392 |
| C | -2.824987 | -1.161614 | 2.670091 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -2.453087 | 0.019435 | 2.023493 | H | -8.362933 | 2.130145 | -0.718564 |
| H | -1.420420 | 0.349858 | 2.044543 | H | -9.307312 | -0.011288 | -1.561905 |
| H | -4.409908 | 0.537187 | 1.287607 | O | -2.500079 | 1.927279 | -4.809118 |
| C | -3.083197 | 2.158583 | 0.986268 | H | -1.891638 | 3.193043 | -2.229126 |
| C | -2.898914 | 3.339219 | 0.747076 | H | -5.100389 | 2.051786 | -3.609563 |
| C | -2.664981 | 4.714929 | 0.462618 | H | -2.783443 | 3.925469 | -4.294588 |
| C | -1.361238 | 5.249762 | 0.542186 | H | -1.275994 | 0.647389 | -3.813878 |
| C | -3.730833 | 5.559705 | 0.084129 | C | 6.358204 | -2.354617 | -3.791625 |
| C | -1.136561 | 6.592431 | 0.247575 | C | 5.723792 | -1.810238 | -2.695439 |
| H | -0.537356 | 4.606010 | 0.833978 | C | 4.438816 | -2.266937 | -2.285989 |
| C | -3.494780 | 6.901442 | -0.204988 | C | 3.809469 | -3.288261 | -3.070092 |
| H | -4.736145 | 5.153872 | 0.025538 | C | 4.496885 | -3.841502 | -4.185377 |
| C | -2.198945 | 7.421460 | -0.125588 | C | 5.747652 | -3.389642 | -4.540604 |
| H | -0.128627 | 6.992364 | 0.308058 | H | 7.334934 | -1.981461 | -4.087412 |
| H | -4.322628 | 7.542903 | -0.493396 | H | 6.202638 | -1.011629 | -2.140667 |
| H | -2.018178 | 8.468060 | -0.353437 | C | 3.736460 | -1.724414 | -1.154182 |
| C | -4.246145 | 2.641603 | -3.277065 | C | 2.505190 | -3.723999 | -2.724207 |
| C | -2.026005 | 2.120031 | -2.400281 | H | 4.006972 | -4.623590 | -4.760316 |
| C | -3.358029 | 3.007563 | -4.485950 | H | 6.261981 | -3.814372 | -5.398048 |
| H | -4.624984 | 3.556429 | -2.801629 | C | 1.791782 | -3.149794 | -1.691421 |
| C | -1.513735 | 1.714308 | -3.793297 | C | 2.418590 | -2.111846 | -0.936758 |
| H | -1.457221 | 1.591028 | -1.639409 | H | 2.053121 | -4.525406 | -3.302875 |
| H | -3.992269 | 3.189241 | -5.357485 | C | 4.378352 | -0.744679 | -0.229465 |
| H | -0.598030 | 2.280565 | -4.020266 | C | 5.592033 | -1.056803 | 0.476752 |
| C | -3.229427 | -0.058079 | -0.819460 | C | 3.779976 | 0.491685 | -0.015227 |
| H | -2.147249 | -0.094076 | -0.874305 | C | 6.191060 | -2.348473 | 0.461659 |
| H | -3.723419 | -0.963052 | -0.488789 | C | 6.215221 | -0.038665 | 1.270157 |
| C | -3.980667 | 0.790445 | -1.637336 | C | 4.400079 | 1.520674 | 0.756197 |
| N | -3.464788 | 1.840158 | -2.315338 | C | 7.351908 | -2.604663 | 1.159789 |
| C | -5.463142 | 0.595383 | -1.649725 | H | 5.715720 | -3.145635 | -0.098261 |
| C | -6.001100 | -0.617938 | -2.106144 | C | 7.421421 | -0.329545 | 1.965167 |
| C | -6.327794 | 1.584349 | -1.151980 | C | 5.608259 | 1.239661 | 1.361322 |
| C | -7.380460 | -0.830572 | -2.081739 | C | 7.984455 | -1.584413 | 1.910779 |
| H | -5.335418 | -1.385573 | -2.490453 | H | 7.782968 | -3.601902 | 1.138134 |
| C | -7.704742 | 1.362489 | -1.115520 | H | 7.884441 | 0.459804 | 2.552361 |
| H | -5.917782 | 2.517687 | -0.777215 | H | 6.104865 | 2.011897 | 1.943148 |
| C | -8.234395 | 0.157503 | -1.585445 | H | 8.902665 | -1.798376 | 2.450468 |
| H | -7.786682 | -1.768856 | -2.448735 | O | 1.708433 | -1.533958 | 0.091964 |

| | | | |
|---|---|---|---|
| O | 2.576764 | 0.770550 | -0.624161 |
| P | 1.173719 | 0.049790 | -0.059977 |
| O | 0.192082 | 0.179448 | -1.187919 |
| O | 0.863861 | 0.487879 | 1.341179 |
| C | 0.421207 | -3.652782 | -1.360573 |
| C | -0.657173 | -3.416419 | -2.247758 |
| C | 0.223942 | -4.432998 | -0.194320 |
| C | -1.958253 | -3.980118 | -1.958368 |
| C | -0.525198 | -2.627193 | -3.437914 |
| C | -1.084659 | -4.976882 | 0.091786 |
| C | 1.284448 | -4.737815 | 0.720383 |
| C | -3.036972 | -3.756176 | -2.873365 |
| C | -2.138540 | -4.739306 | -0.797854 |
| C | -1.584393 | -2.433246 | -4.287580 |
| H | 0.434150 | -2.174675 | -3.659622 |
| C | -1.271181 | -5.768713 | 1.270086 |
| C | 1.066787 | -5.502430 | 1.838416 |
| H | 2.279597 | -4.359395 | 0.515357 |
| C | -2.858497 | -3.009606 | -4.008031 |
| H | -4.003731 | -4.199552 | -2.647210 |
| H | -3.117288 | -5.166324 | -0.588899 |
| H | -1.454947 | -1.833629 | -5.184350 |
| H | -2.261601 | -6.171647 | 1.467674 |
| C | -0.229084 | -6.024680 | 2.122649 |
| H | 1.890087 | -5.719837 | 2.513190 |
| H | -3.682902 | -2.852686 | -4.698049 |
| H | -0.381249 | -6.632973 | 3.009873 |
| C | 3.790841 | 2.880730 | 0.893122 |
| C | 3.259304 | 3.294992 | 2.138559 |
| C | 3.804999 | 3.772431 | -0.207278 |
| C | 2.737392 | 4.637006 | 2.282130 |
| C | 3.199878 | 2.433599 | 3.283282 |
| C | 3.267478 | 5.105881 | -0.055015 |
| C | 4.354379 | 3.418700 | -1.482591 |
| C | 2.217368 | 5.053581 | 3.549504 |
| C | 2.753738 | 5.503578 | 1.184299 |
| C | 2.691905 | 2.870338 | 4.479591 |
| H | 3.557543 | 1.415132 | 3.188555 |
| C | 3.286782 | 5.999136 | -1.173255 |
| C | 4.355309 | 4.303925 | -2.530144 |
| H | 4.780319 | 2.430226 | -1.614631 |
| C | 2.198101 | 4.200257 | 4.620398 |
| H | 1.836241 | 6.067858 | 3.640535 |
| H | 2.368458 | 6.514551 | 1.300264 |
| H | 2.658209 | 2.195573 | 5.330606 |
| H | 2.876268 | 6.997399 | -1.041406 |
| C | 3.810752 | 5.612317 | -2.378297 |
| H | 4.777499 | 4.008674 | -3.486810 |
| H | 1.801867 | 4.528462 | 5.577359 |
| H | 3.819645 | 6.299529 | -3.219771 |

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**INT-18**

*G*sol(DCM) = -4025.180008 Hartree

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| | | | |
|---|---|---|---|
| C | 3.443954 | 0.532509 | 0.020885 |
| C | 2.128945 | -0.317806 | 4.048820 |
| C | 2.062394 | -0.428159 | 5.571611 |
| C | 3.349987 | -2.376322 | 5.570303 |
| C | 3.459338 | -2.348532 | 4.049336 |
| H | 1.110290 | -0.030689 | 5.934930 |
| H | 1.227577 | -0.760684 | 3.595777 |
| H | 2.155901 | 0.741335 | 3.772913 |
| H | 3.342975 | -3.409328 | 5.930381 |
| H | 4.211750 | -1.851627 | 6.014771 |
| H | 2.660597 | -2.973747 | 3.616643 |
| H | 4.419815 | -2.768983 | 3.743105 |
| H | 2.882975 | 0.155684 | 6.020012 |
| O | 2.136577 | -1.779384 | 6.013556 |
| N | 3.352073 | -0.962775 | 3.560560 |
| C | 5.114396 | -1.223267 | 1.889320 |
| C | 6.218596 | -0.845809 | 2.671965 |
| C | 5.324939 | -2.078029 | 0.796252 |
| C | 7.501289 | -1.293197 | 2.355303 |
| H | 6.060851 | -0.196258 | 3.528020 |
| C | 6.609414 | -2.527077 | 0.478930 |
| H | 4.473967 | -2.407829 | 0.206267 |

| | | | |
|---|---|---|---|
| C | 7.701282 | -2.133805 | 1.255703 |
| H | 8.345939 | -0.984625 | 2.965536 |
| H | 6.753629 | -3.189633 | -0.370195 |
| H | 8.700407 | -2.483484 | 1.010475 |
| C | 3.747176 | -0.719334 | 2.231262 |
| C | 2.990419 | -0.006081 | 1.362758 |
| H | 1.985461 | 0.294620 | 1.638466 |
| H | 4.452371 | 0.172145 | -0.206816 |
| C | 3.490459 | 2.004226 | 0.041485 |
| C | 3.562206 | 3.216588 | 0.075686 |
| C | 3.675241 | 4.642026 | 0.126430 |
| C | 2.573807 | 5.440132 | 0.494386 |
| C | 4.898583 | 5.269274 | -0.186446 |
| C | 2.698879 | 6.827344 | 0.549517 |
| H | 1.626698 | 4.966928 | 0.733569 |
| C | 5.013745 | 6.656923 | -0.129778 |
| H | 5.750905 | 4.658980 | -0.469557 |
| C | 3.916034 | 7.440539 | 0.238631 |
| H | 1.842688 | 7.430538 | 0.838136 |
| H | 5.962455 | 7.127545 | -0.372484 |
| H | 4.008888 | 8.522003 | 0.283424 |
| C | -6.351395 | -0.354438 | -3.815241 |
| C | -5.530736 | -0.797715 | -2.800040 |
| C | -5.085622 | 0.083737 | -1.774106 |
| C | -5.489743 | 1.456529 | -1.849483 |
| C | -6.352014 | 1.879076 | -2.898568 |
| C | -6.780053 | 0.994280 | -3.862217 |
| H | -6.668485 | -1.046575 | -4.590596 |
| H | -5.204671 | -1.831365 | -2.787447 |
| C | -4.226507 | -0.332827 | -0.697797 |
| C | -5.008030 | 2.374965 | -0.882917 |
| H | -6.656637 | 2.922369 | -2.930306 |
| H | -7.433210 | 1.328210 | -4.663484 |
| C | -4.105992 | 2.004696 | 0.094388 |
| C | -3.696623 | 0.636119 | 0.148380 |
| H | -5.346728 | 3.406670 | -0.931364 |
| C | -3.883750 | -1.769988 | -0.488066 |
| C | -4.903144 | -2.765801 | -0.289225 |
| C | -2.550838 | -2.163702 | -0.457321 |
| C | -6.281843 | -2.447592 | -0.129838 |
| C | -4.520819 | -4.144469 | -0.205463 |
| C | -2.158234 | -3.535228 | -0.397979 |
| C | -7.224296 | -3.434717 | 0.064820 |
| H | -6.591204 | -1.409068 | -0.149069 |
| C | -5.518641 | -5.140956 | -0.021131 |
| C | -3.148785 | -4.490854 | -0.295041 |
| C | -6.845508 | -4.798275 | 0.107833 |
| H | -8.268548 | -3.162658 | 0.192342 |
| H | -5.208506 | -6.181928 | 0.028120 |
| H | -2.873250 | -5.541800 | -0.261843 |
| H | -7.599522 | -5.566381 | 0.254794 |
| O | -2.816324 | 0.263868 | 1.136450 |
| O | -1.565860 | -1.205480 | -0.554509 |
| P | -1.253357 | -0.226234 | 0.775154 |
| O | -0.450618 | 0.912017 | 0.210183 |
| O | -0.811393 | -1.025659 | 1.958645 |
| C | -3.601978 | 3.018594 | 1.072389 |
| C | -2.775067 | 4.079222 | 0.625371 |
| C | -3.997548 | 2.951851 | 2.431492 |
| C | -2.333614 | 5.087478 | 1.564738 |
| C | -2.337046 | 4.206137 | -0.734595 |
| C | -3.532603 | 3.954894 | 3.363066 |
| C | -4.872268 | 1.934429 | 2.934079 |
| C | -1.516582 | 6.167960 | 1.100537 |
| C | -2.715417 | 4.994196 | 2.906184 |
| C | -1.554355 | 5.256607 | -1.140428 |
| H | -2.639442 | 3.452553 | -1.452340 |
| C | -3.932283 | 3.875166 | 4.735120 |
| C | -5.237982 | 1.895565 | 4.255286 |
| H | -5.254614 | 1.185599 | 2.249566 |
| C | -1.141517 | 6.258405 | -0.213959 |
| H | -1.204957 | 6.921436 | 1.819900 |
| H | -2.376023 | 5.751517 | 3.609608 |
| H | -1.245133 | 5.329970 | -2.179658 |
| H | -3.566782 | 4.634522 | 5.422161 |
| C | -4.758008 | 2.874216 | 5.173487 |

| | | | |
|---|---|---|---|
| H | -5.903001 | 1.112360 | 4.608718 |
| H | -0.528001 | 7.087116 | -0.555772 |
| H | -5.056059 | 2.824679 | 6.217056 |
| C | -0.723542 | -3.952845 | -0.479322 |
| C | -0.083169 | -4.512153 | 0.653454 |
| C | -0.030787 | -3.853690 | -1.710765 |
| C | 1.278283 | -4.989584 | 0.542372 |
| C | -0.723122 | -4.621404 | 1.931810 |
| C | 1.334259 | -4.321002 | -1.804213 |
| C | -0.634780 | -3.323617 | -2.897582 |
| C | 1.910898 | -5.572760 | 1.686450 |
| C | 1.950839 | -4.878082 | -0.678697 |
| C | -0.081753 | -5.184339 | 3.004922 |
| H | -1.730635 | -4.239577 | 2.045436 |
| C | 2.021635 | -4.223764 | -3.056733 |
| C | 0.058527 | -3.242082 | -4.078369 |
| H | -1.664919 | -2.987572 | -2.856071 |
| C | 1.251435 | -5.675044 | 2.882868 |
| H | 2.930832 | -5.934579 | 1.581569 |
| H | 2.973463 | -5.241004 | -0.757475 |
| H | -0.590042 | -5.252801 | 3.962708 |
| H | 3.043762 | -4.591393 | -3.112121 |
| C | 1.407133 | -3.696034 | -4.162594 |
| H | -0.424529 | -2.834858 | -4.962223 |
| H | 1.740314 | -6.123609 | 3.743205 |
| H | 1.938401 | -3.631720 | -5.108120 |
| C | 2.199948 | 1.960815 | -4.418307 |
| C | 0.730649 | 1.988556 | -2.455403 |
| C | 0.820055 | 2.142567 | -5.089975 |
| H | 2.749353 | 2.906863 | -4.396437 |
| C | -0.434433 | 1.377525 | -3.255637 |
| H | 0.617330 | 1.756065 | -1.399461 |
| H | 0.931003 | 2.000597 | -6.167212 |
| H | -1.300999 | 2.049455 | -3.182033 |
| C | 2.480618 | 0.008579 | -1.106284 |
| H | 1.446422 | 0.159979 | -0.794902 |
| H | 2.649421 | -1.070245 | -1.194317 |
| C | 2.791152 | 0.617237 | -2.441779 |
| N | 1.998493 | 1.475824 | -3.023419 |
| C | 4.084673 | 0.244994 | -3.065815 |
| C | 4.387068 | -1.106871 | -3.302787 |
| C | 5.044207 | 1.233507 | -3.348406 |
| C | 5.621826 | -1.457062 | -3.847120 |
| H | 3.648624 | -1.876253 | -3.099546 |
| C | 6.286723 | 0.870648 | -3.864783 |
| H | 4.830356 | 2.275293 | -3.131958 |
| C | 6.574122 | -0.472323 | -4.122571 |
| H | 5.840918 | -2.500887 | -4.050083 |
| H | 7.028887 | 1.637384 | -4.064585 |
| H | 7.539941 | -0.751145 | -4.533423 |
| O | -0.079037 | 1.154845 | -4.620960 |
| H | 0.771843 | 3.075606 | -2.567902 |
| H | 2.794921 | 1.217728 | -4.946485 |
| H | 0.424415 | 3.153384 | -4.921015 |
| H | -0.709013 | 0.404817 | -2.840612 |

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**TS-RR-Me**

*G*sol(DCM) = -4273.845167 Hartree

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| | | | |
|---|---|---|---|
| C | 2.817190 | -1.567635 | 0.023704 |
| C | 3.929035 | 0.575540 | 0.524079 |
| C | 6.139957 | -3.928433 | -1.381980 |
| C | 5.882934 | -3.844037 | -0.011102 |
| C | 4.820590 | -3.083443 | 0.476484 |
| C | 3.956069 | -2.382818 | -0.401553 |
| C | 4.255637 | -2.456607 | -1.784157 |
| C | 5.316160 | -3.222077 | -2.263091 |
| H | 6.965123 | -4.528692 | -1.755169 |
| H | 6.515144 | -4.378761 | 0.693762 |
| H | 4.644678 | -3.047386 | 1.541894 |
| H | 3.642045 | -1.901038 | -2.482673 |
| H | 5.500236 | -3.264154 | -3.333968 |
| C | 2.123021 | -1.659901 | 1.286580 |
| O | 0.988283 | -1.191201 | 1.506807 |
| O | 2.792193 | -2.263261 | 2.293198 |
| C | 2.112874 | -2.336695 | 3.559094 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| O | 2.038248 | -1.033224 | -1.001563 | H | 4.762635 | 3.859980 | -3.007226 |
| C | 1.025047 | -1.933709 | -1.535616 | H | 5.276395 | 2.601656 | -5.090466 |
| H | 1.441670 | -2.944378 | -1.604098 | C | 6.287439 | 0.397862 | -0.278221 |
| H | 0.176746 | -1.954670 | -0.844589 | C | 5.309708 | 0.343861 | 0.718209 |
| C | 0.606043 | -1.440124 | -2.896435 | H | 5.621931 | 0.137384 | 1.736008 |
| C | -0.285217 | -0.364089 | -3.019696 | H | 3.557135 | 0.777822 | -0.475149 |
| C | 1.108950 | -2.037629 | -4.060168 | C | 3.147953 | 1.051457 | 1.595491 |
| C | -0.659926 | 0.107006 | -4.279587 | C | 2.485248 | 1.482272 | 2.525987 |
| H | -0.690863 | 0.093640 | -2.122129 | C | 1.735198 | 2.003415 | 3.616475 |
| C | 0.734216 | -1.570527 | -5.322554 | C | 2.258828 | 1.963436 | 4.927581 |
| H | 1.793669 | -2.878282 | -3.976446 | C | 0.460267 | 2.572479 | 3.405551 |
| C | -0.149411 | -0.494584 | -5.434061 | C | 1.524106 | 2.477310 | 5.993328 |
| H | -1.357681 | 0.936102 | -4.362064 | H | 3.239728 | 1.528793 | 5.094198 |
| H | 1.129182 | -2.047849 | -6.215441 | C | -0.263167 | 3.087920 | 4.478096 |
| H | 0.104083 | -0.099521 | 0.828403 | H | 0.052404 | 2.600121 | 2.400933 |
| C | 8.747657 | 0.521216 | -0.710745 | C | 0.263400 | 3.041572 | 5.773141 |
| C | 9.546695 | 1.313132 | 0.332992 | H | 1.936197 | 2.439572 | 6.997840 |
| C | 8.746792 | -0.040053 | 2.085296 | H | -1.240756 | 3.527648 | 4.302618 |
| C | 7.936291 | -0.875164 | 1.090868 | H | -0.305935 | 3.442947 | 6.606734 |
| H | 10.483645 | 1.669165 | -0.104781 | C | -5.259400 | 0.512751 | -4.915579 |
| H | 9.364784 | -0.292355 | -1.109786 | C | -5.053351 | 0.184146 | -3.592820 |
| H | 8.455826 | 1.172959 | -1.532733 | C | -4.411774 | 1.089957 | -2.702102 |
| H | 9.108023 | -0.666988 | 2.905097 | C | -3.954678 | 2.341970 | -3.229790 |
| H | 8.124455 | 0.766586 | 2.503502 | C | -4.197901 | 2.658254 | -4.595151 |
| H | 8.569415 | -1.691132 | 0.721091 | C | -4.840011 | 1.765829 | -5.423423 |
| H | 7.053263 | -1.319732 | 1.547887 | H | -5.743225 | -0.200539 | -5.576891 |
| H | 8.956429 | 2.183128 | 0.662321 | H | -5.369980 | -0.785329 | -3.226637 |
| O | 9.899486 | 0.505948 | 1.450137 | C | -4.165213 | 0.784408 | -1.316793 |
| N | 7.556157 | -0.062634 | -0.071796 | C | -3.256265 | 3.242669 | -2.385419 |
| C | 6.001695 | 1.002712 | -1.612040 | H | -3.855663 | 3.617901 | -4.974043 |
| C | 6.306890 | 0.307879 | -2.795384 | H | -5.015641 | 2.014027 | -6.466177 |
| C | 5.442299 | 2.287688 | -1.703852 | C | -2.940128 | 2.924246 | -1.080735 |
| C | 6.040261 | 0.878232 | -4.038857 | C | -3.377114 | 1.662104 | -0.585978 |
| H | 6.734033 | -0.687726 | -2.732456 | H | -2.948036 | 4.204041 | -2.787333 |
| C | 5.185120 | 2.860790 | -2.950898 | C | -4.707372 | -0.455189 | -0.683999 |
| H | 5.225058 | 2.841614 | -0.795955 | C | -6.115727 | -0.748525 | -0.660634 |
| C | 5.479238 | 2.156629 | -4.120484 | C | -3.843502 | -1.356150 | -0.081138 |
| H | 6.267830 | 0.323879 | -4.944927 | C | -7.108186 | 0.174111 | -1.094993 |

| | | | |
|---|---|---|---|
| C | -6.550798 | -2.010181 | -0.136346 |
| C | -4.248834 | -2.622266 | 0.426482 |
| C | -8.447762 | -0.146994 | -1.044228 |
| H | -6.803916 | 1.149234 | -1.457425 |
| C | -7.939177 | -2.317369 | -0.114475 |
| C | -5.593124 | -2.928520 | 0.366752 |
| C | -8.871218 | -1.408730 | -0.561594 |
| H | -9.186813 | 0.578210 | -1.373129 |
| H | -8.250385 | -3.282991 | 0.275782 |
| H | -5.935831 | -3.891981 | 0.734360 |
| H | -9.929804 | -1.650460 | -0.534255 |
| O | -3.044617 | 1.353078 | 0.732062 |
| O | -2.489991 | -1.026923 | -0.008286 |
| P | -2.058268 | 0.109564 | 1.087975 |
| O | -0.640694 | 0.542186 | 0.546712 |
| O | -2.204596 | -0.272430 | 2.509154 |
| C | -2.203378 | 3.896503 | -0.213245 |
| C | -0.828606 | 4.149549 | -0.437600 |
| C | -2.903382 | 4.596978 | 0.799637 |
| C | -0.142795 | 5.130070 | 0.376503 |
| C | -0.062827 | 3.462733 | -1.436120 |
| C | -2.201903 | 5.563741 | 1.614312 |
| C | -4.300874 | 4.404847 | 1.051572 |
| C | 1.245873 | 5.385932 | 0.141973 |
| C | -0.844364 | 5.806170 | 1.379294 |
| C | 1.267888 | 3.733614 | -1.626508 |
| H | -0.550179 | 2.710785 | -2.045399 |
| C | -2.914586 | 6.262218 | 2.640619 |
| C | -4.948982 | 5.096021 | 2.043244 |
| H | -4.854532 | 3.701153 | 0.439594 |
| C | 1.933623 | 4.711832 | -0.831505 |
| H | 1.742955 | 6.129553 | 0.760036 |
| H | -0.322280 | 6.538843 | 1.990826 |
| H | 1.825999 | 3.193360 | -2.386201 |
| H | -2.370037 | 6.982948 | 3.245720 |
| C | -4.248523 | 6.035222 | 2.854578 |
| H | -6.009253 | 4.930019 | 2.212754 |
| H | 2.987330 | 4.916239 | -0.999226 |
| H | -4.779050 | 6.571820 | 3.636085 |
| C | -3.256605 | -3.597423 | 0.978933 |
| C | -3.194790 | -3.832945 | 2.373184 |
| C | -2.405086 | -4.304004 | 0.095401 |
| C | -2.253016 | -4.802474 | 2.890167 |
| C | -4.020696 | -3.138764 | 3.317092 |
| C | -1.460375 | -5.260794 | 0.626494 |
| C | -2.441641 | -4.123339 | -1.325656 |
| C | -2.200769 | -5.042718 | 4.300553 |
| C | -1.410800 | -5.484831 | 2.006511 |
| C | -3.939201 | -3.397802 | 4.660986 |
| H | -4.714176 | -2.389620 | 2.953441 |
| C | -0.599290 | -5.965982 | -0.273211 |
| C | -1.599648 | -4.819311 | -2.155451 |
| H | -3.154451 | -3.423925 | -1.748907 |
| C | -3.021122 | -4.365823 | 5.163293 |
| H | -1.491034 | -5.778475 | 4.670917 |
| H | -0.702398 | -6.209801 | 2.401618 |
| H | -4.575925 | -2.855742 | 5.354717 |
| H | 0.106633 | -6.680012 | 0.143942 |
| C | -0.661648 | -5.752505 | -1.625151 |
| H | -1.647069 | -4.661092 | -3.229190 |
| H | -2.972768 | -4.557297 | 6.231620 |
| H | -0.003877 | -6.295173 | -2.298248 |
| H | -0.444888 | -0.130607 | -6.414535 |
| H | 1.889102 | -1.336963 | 3.936969 |
| H | 2.806653 | -2.849958 | 4.225479 |
| H | 1.184260 | -2.905622 | 3.466222 |

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**TS-RS-Me**

*G*sol(DCM) = -4273.847564 Hartree

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| | | | |
|---|---|---|---|
| C | -3.709460 | -0.341636 | -1.573258 |
| C | -4.524593 | 1.107992 | 0.256507 |
| C | -6.910765 | 0.193332 | -4.410333 |
| C | -5.766766 | 0.990967 | -4.504341 |
| C | -4.709314 | 0.843846 | -3.607196 |
| C | -4.758923 | -0.123167 | -2.573486 |

| | | | |
|---|---|---|---|
| C | -5.929066 | -0.918900 | -2.493654 |
| C | -6.980519 | -0.763273 | -3.393567 |
| H | -7.729526 | 0.314282 | -5.114322 |
| H | -5.689553 | 1.737700 | -5.291367 |
| H | -3.835402 | 1.470613 | -3.711558 |
| H | -6.001841 | -1.658089 | -1.703760 |
| H | -7.860830 | -1.394527 | -3.297972 |
| C | -2.399161 | 0.240545 | -1.513709 |
| O | -1.522593 | -0.158838 | -0.707121 |
| O | -2.176552 | 1.299613 | -2.325890 |
| C | -0.947596 | 2.020531 | -2.147920 |
| O | -3.839481 | -1.483975 | -0.793325 |
| C | -3.245851 | -2.667562 | -1.381814 |
| H | -3.765767 | -2.901584 | -2.319439 |
| H | -2.193952 | -2.463118 | -1.606098 |
| C | -3.368654 | -3.805932 | -0.403319 |
| C | -2.421578 | -3.961531 | 0.618972 |
| C | -4.439256 | -4.706236 | -0.475991 |
| C | -2.544315 | -4.992429 | 1.552955 |
| H | -1.581257 | -3.274266 | 0.674284 |
| C | -4.566063 | -5.740223 | 0.455468 |
| H | -5.176237 | -4.598395 | -1.268502 |
| C | -3.619763 | -5.883225 | 1.473812 |
| H | -1.798957 | -5.105468 | 2.335637 |
| H | -5.399119 | -6.434408 | 0.384037 |
| C | -5.460654 | -0.856664 | 2.313870 |
| C | -6.545337 | 0.015437 | 2.503583 |
| C | -5.705722 | -2.236598 | 2.201954 |
| C | -7.847668 | -0.480770 | 2.578761 |
| H | -6.361293 | 1.080429 | 2.604783 |
| C | -7.008443 | -2.727659 | 2.267948 |
| H | -4.875277 | -2.916426 | 2.042170 |
| C | -8.082559 | -1.852292 | 2.458545 |
| H | -8.676431 | 0.204169 | 2.733560 |
| H | -7.184788 | -3.794442 | 2.163864 |
| H | -9.096573 | -2.238401 | 2.513229 |
| C | -4.072659 | -0.322153 | 2.231071 |
| C | -3.758339 | 0.741850 | 1.370930 |
| H | -2.833841 | 1.283983 | 1.533657 |
| H | -5.436527 | 0.558775 | 0.044233 |
| C | -4.401403 | 2.375901 | -0.346469 |
| C | -4.322334 | 3.475954 | -0.868250 |
| C | -4.248257 | 4.766527 | -1.463537 |
| C | -4.909553 | 5.031166 | -2.682364 |
| C | -3.521320 | 5.804293 | -0.841155 |
| C | -4.842165 | 6.297927 | -3.257316 |
| H | -5.464640 | 4.233523 | -3.166479 |
| C | -3.462998 | 7.068634 | -1.422910 |
| H | -3.013118 | 5.605914 | 0.097432 |
| C | -4.121026 | 7.319892 | -2.631458 |
| H | -5.353738 | 6.489279 | -4.196410 |
| H | -2.905522 | 7.861240 | -0.931503 |
| H | -4.072515 | 8.306896 | -3.082513 |
| H | -0.000635 | -0.322337 | -0.856239 |
| C | 7.737471 | 0.217688 | -3.220728 |
| C | 6.863763 | 0.392946 | -2.169114 |
| C | 5.917651 | -0.613004 | -1.824239 |
| C | 5.874386 | -1.798438 | -2.628831 |
| C | 6.801709 | -1.956841 | -3.695538 |
| C | 7.719156 | -0.973152 | -3.985987 |
| H | 8.444097 | 1.004890 | -3.468214 |
| H | 6.887864 | 1.316447 | -1.602917 |
| C | 4.981900 | -0.473048 | -0.738843 |
| C | 4.891874 | -2.786431 | -2.365170 |
| H | 6.761073 | -2.868197 | -4.286647 |
| H | 8.418797 | -1.100383 | -4.807024 |
| C | 3.933952 | -2.622098 | -1.385599 |
| C | 3.992907 | -1.435843 | -0.600605 |
| H | 4.881523 | -3.687870 | -2.971876 |
| C | 5.031324 | 0.694045 | 0.190672 |
| C | 6.209706 | 1.016766 | 0.950661 |
| C | 3.912787 | 1.498036 | 0.348992 |
| C | 7.352355 | 0.170653 | 1.005628 |
| C | 6.226531 | 2.223771 | 1.724018 |
| C | 3.910195 | 2.708133 | 1.099075 |
| C | 8.457884 | 0.516745 | 1.752647 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 7.344928 | -0.766679 | 0.461504 | C | 2.297506 | 4.313537 | 0.019773 |
| C | 7.390054 | 2.561276 | 2.469052 | C | 0.809663 | 4.554837 | 2.430725 |
| C | 5.077309 | 3.055203 | 1.749124 | C | 2.316068 | 2.966228 | 3.561564 |
| C | 8.486469 | 1.729475 | 2.482527 | C | 1.125558 | 5.157455 | 0.085203 |
| H | 9.314314 | -0.150829 | 1.785704 | C | 3.017529 | 4.270519 | -1.218366 |
| H | 7.389974 | 3.486238 | 3.039980 | C | 0.081944 | 4.669324 | 3.658283 |
| H | 5.114340 | 3.980302 | 2.318023 | C | 0.417236 | 5.258029 | 1.287582 |
| H | 9.367552 | 1.992925 | 3.060503 | C | 1.592011 | 3.103133 | 4.718169 |
| O | 3.029858 | -1.284480 | 0.397507 | H | 3.166373 | 2.294625 | 3.536070 |
| O | 2.733071 | 1.140783 | -0.305284 | C | 0.718495 | 5.880395 | -1.081359 |
| P | 1.890132 | -0.128350 | 0.284130 | C | 2.599288 | 4.983867 | -2.312572 |
| O | 1.003406 | -0.499806 | -0.961239 | H | 3.914870 | 3.664870 | -1.284915 |
| O | 1.226035 | 0.068640 | 1.593112 | C | 0.461036 | 3.969523 | 4.772954 |
| C | 2.884957 | -3.665177 | -1.159139 | H | -0.782613 | 5.328190 | 3.683722 |
| C | 1.831314 | -3.817407 | -2.092361 | H | -0.457517 | 5.903004 | 1.336281 |
| C | 2.974178 | -4.520540 | -0.034822 | H | 1.878877 | 2.542993 | 5.603836 |
| C | 0.843385 | -4.854530 | -1.887657 | H | -0.173299 | 6.499033 | -1.019327 |
| C | 1.681874 | -2.974521 | -3.242542 | C | 1.429433 | 5.795510 | -2.249347 |
| C | 1.974845 | -5.546401 | 0.162494 | H | 3.164895 | 4.933083 | -3.238844 |
| C | 4.033303 | -4.429168 | 0.926018 | H | -0.097545 | 4.066754 | 5.699622 |
| C | -0.217637 | -5.007036 | -2.836927 | H | 1.110846 | 6.349198 | -3.128047 |
| C | 0.939280 | -5.686430 | -0.767701 | C | -3.425897 | -1.505418 | 4.336574 |
| C | 0.650781 | -3.153195 | -4.128489 | C | -1.690822 | -0.682211 | 2.854393 |
| H | 2.397540 | -2.176801 | -3.403986 | C | -2.784612 | -0.666553 | 5.452605 |
| C | 2.071034 | -6.405331 | 1.303195 | H | -3.002684 | -2.517081 | 4.342200 |
| C | 4.091429 | -5.273180 | 2.005616 | H | -4.501860 | -1.574763 | 4.491692 |
| H | 4.805694 | -3.679817 | 0.788977 | C | -1.108613 | 0.134367 | 4.006822 |
| C | -0.312503 | -4.185137 | -3.928731 | H | -1.230836 | -1.678960 | 2.869703 |
| H | -0.949231 | -5.793435 | -2.668754 | H | -1.483775 | -0.236019 | 1.884174 |
| H | 0.190582 | -6.460745 | -0.616123 | H | -2.909285 | -1.172503 | 6.414484 |
| H | 0.560585 | -2.498714 | -4.991073 | H | -3.284287 | 0.314491 | 5.501258 |
| H | 1.309344 | -7.169479 | 1.437472 | H | -0.023321 | 0.190818 | 3.907140 |
| C | 3.096096 | -6.274194 | 2.202448 | H | -1.520486 | 1.155978 | 4.000957 |
| H | 4.905857 | -5.182318 | 2.719064 | N | -3.135853 | -0.876422 | 3.039660 |
| H | -1.121016 | -4.311678 | -4.643271 | O | -1.387734 | -0.499184 | 5.255029 |
| H | 3.158920 | -6.932594 | 3.064289 | H | -3.714808 | -6.688400 | 2.197375 |
| C | 2.697104 | 3.581068 | 1.164233 | H | -0.092252 | 1.422829 | -2.473226 |
| C | 1.968836 | 3.690512 | 2.373748 | H | -1.039996 | 2.908117 | -2.773896 |

| | | | |
|---|---|---|---|
| H | -0.814188 | 2.311514 | -1.103210 |

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**TS-SR-Me**

*G*sol(DCM) = -4273.847401 Hartree

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| | | | |
|---|---|---|---|
| C | -3.606714 | 0.867394 | -1.225615 |
| C | -4.644294 | -1.067226 | -0.169166 |
| C | -6.795854 | 2.092158 | -3.855795 |
| C | -5.825482 | 1.199448 | -4.319400 |
| C | -4.775545 | 0.786621 | -3.500093 |
| C | -4.656089 | 1.263627 | -2.172047 |
| C | -5.654591 | 2.161210 | -1.718953 |
| C | -6.699913 | 2.567160 | -2.544852 |
| H | -7.609838 | 2.409587 | -4.501794 |
| H | -5.881481 | 0.817596 | -5.336189 |
| H | -4.040198 | 0.097619 | -3.889248 |
| H | -5.601918 | 2.527070 | -0.699839 |
| H | -7.445085 | 3.258958 | -2.159320 |
| C | -2.396861 | 0.135030 | -1.496100 |
| O | -1.495060 | 0.004420 | -0.636004 |
| O | -2.310888 | -0.453917 | -2.708396 |
| C | -1.169444 | -1.287178 | -2.957897 |
| O | -3.560855 | 1.579970 | -0.035521 |
| C | -2.739182 | 2.775500 | -0.091847 |
| H | -3.161380 | 3.460603 | -0.837863 |
| H | -1.727598 | 2.496215 | -0.401693 |
| C | -2.719535 | 3.414419 | 1.271938 |
| C | -1.749028 | 3.044670 | 2.214498 |
| C | -3.684255 | 4.366515 | 1.628545 |
| C | -1.752178 | 3.609563 | 3.492559 |
| H | -0.977469 | 2.328656 | 1.940514 |
| C | -3.688875 | 4.933838 | 2.905013 |
| H | -4.433580 | 4.667628 | 0.899889 |
| C | -2.724031 | 4.552095 | 3.841772 |
| H | -0.990775 | 3.320834 | 4.212336 |
| H | -4.439989 | 5.674585 | 3.166290 |
| C | -1.719122 | -0.860310 | 2.911891 |
| C | -1.307386 | -2.139856 | 3.641153 |
| C | -2.937613 | -1.754159 | 5.295834 |
| C | -3.406981 | -0.465043 | 4.607360 |
| H | -0.233717 | -2.312989 | 3.534895 |
| H | -1.135192 | -0.023392 | 3.315369 |
| H | -1.529036 | -0.910970 | 1.840609 |
| H | -3.040622 | -1.655878 | 6.380366 |
| H | -3.561202 | -2.596610 | 4.955838 |
| H | -2.858854 | 0.393924 | 5.012956 |
| H | -4.471521 | -0.314487 | 4.781680 |
| H | -1.847218 | -3.005959 | 3.226851 |
| O | -1.565211 | -2.021324 | 5.038477 |
| N | -3.135014 | -0.563134 | 3.165817 |
| C | -5.414175 | -0.002109 | 2.516515 |
| C | -6.599931 | -0.740567 | 2.370699 |
| C | -5.489461 | 1.331168 | 2.955078 |
| C | -7.836039 | -0.157819 | 2.655380 |
| H | -6.546719 | -1.774859 | 2.045171 |
| C | -6.725937 | 1.912652 | 3.230164 |
| H | -4.579308 | 1.912673 | 3.055548 |
| C | -7.902046 | 1.169952 | 3.083251 |
| H | -8.744951 | -0.742356 | 2.545011 |
| H | -6.771087 | 2.948827 | 3.553244 |
| H | -8.864150 | 1.624980 | 3.301585 |
| C | -4.097048 | -0.627579 | 2.208583 |
| C | -3.878333 | -1.280893 | 0.989067 |
| H | -3.023936 | -1.941582 | 0.897625 |
| H | -5.494892 | -0.394962 | -0.114722 |
| C | -4.642645 | -1.990604 | -1.234952 |
| C | -4.649923 | -2.782713 | -2.162960 |
| C | -4.662390 | -3.719223 | -3.233960 |
| C | -5.524171 | -3.537533 | -4.337380 |
| C | -3.813592 | -4.847018 | -3.208686 |
| C | -5.533823 | -4.460388 | -5.380348 |
| H | -6.174275 | -2.668446 | -4.363879 |
| C | -3.830386 | -5.763421 | -4.257213 |
| H | -3.149141 | -4.990251 | -2.362005 |
| C | -4.689287 | -5.574885 | -5.344851 |
| H | -6.200969 | -4.309914 | -6.224447 |

| | | | |
|---|---|---|---|
| H | -3.172619 | -6.627499 | -4.226334 |
| H | -4.699829 | -6.291924 | -6.160792 |
| H | -0.058621 | -0.544979 | -0.538366 |
| C | 7.374812 | -1.637376 | -3.174935 |
| C | 6.579682 | -0.879970 | -2.341782 |
| C | 5.699331 | -1.495143 | -1.407750 |
| C | 5.637108 | -2.926686 | -1.385081 |
| C | 6.483568 | -3.679733 | -2.244824 |
| C | 7.339390 | -3.051616 | -3.120465 |
| H | 8.031959 | -1.143206 | -3.885007 |
| H | 6.613907 | 0.201076 | -2.407241 |
| C | 4.845089 | -0.746905 | -0.522780 |
| C | 4.720390 | -3.571826 | -0.517176 |
| H | 6.430814 | -4.764709 | -2.204096 |
| H | 7.977278 | -3.635179 | -3.777981 |
| C | 3.836675 | -2.863799 | 0.272140 |
| C | 3.904941 | -1.442668 | 0.222201 |
| H | 4.702263 | -4.657966 | -0.490844 |
| C | 4.931726 | 0.740204 | -0.429554 |
| C | 6.156277 | 1.408145 | -0.078139 |
| C | 3.809177 | 1.516532 | -0.675565 |
| C | 7.317426 | 0.716086 | 0.366537 |
| C | 6.204565 | 2.839346 | -0.135925 |
| C | 3.838690 | 2.937491 | -0.761830 |
| C | 8.466750 | 1.399332 | 0.701423 |
| H | 7.289971 | -0.363702 | 0.456238 |
| C | 7.411754 | 3.513150 | 0.197954 |
| C | 5.044296 | 3.562807 | -0.511995 |
| C | 8.523003 | 2.810826 | 0.605364 |
| H | 9.337225 | 0.849159 | 1.047597 |
| H | 7.433934 | 4.598208 | 0.137072 |
| H | 5.105253 | 4.645298 | -0.583541 |
| H | 9.438123 | 3.335012 | 0.865306 |
| O | 3.010397 | -0.730933 | 1.023747 |
| O | 2.593154 | 0.874199 | -0.914947 |
| P | 1.834003 | 0.165103 | 0.347568 |
| O | 0.898687 | -0.868260 | -0.385274 |
| O | 1.235833 | 1.081152 | 1.345927 |
| C | 2.874316 | -3.584389 | 1.163280 |
| C | 1.782395 | -4.288542 | 0.600409 |
| C | 3.098451 | -3.611017 | 2.561429 |
| C | 0.901298 | -5.044881 | 1.463831 |
| C | 1.493479 | -4.283611 | -0.803996 |
| C | 2.200574 | -4.357710 | 3.414140 |
| C | 4.201395 | -2.939996 | 3.183024 |
| C | -0.190980 | -5.768941 | 0.887361 |
| C | 1.131726 | -5.057429 | 2.843156 |
| C | 0.435018 | -4.989300 | -1.317088 |
| H | 2.126140 | -3.704340 | -1.466374 |
| C | 2.431897 | -4.377166 | 4.826672 |
| C | 4.389955 | -2.984410 | 4.540787 |
| H | 4.901024 | -2.390468 | 2.562678 |
| C | -0.417396 | -5.749150 | -0.463229 |
| H | -0.837607 | -6.338592 | 1.550301 |
| H | 0.466107 | -5.627680 | 3.487494 |
| H | 0.240582 | -4.970642 | -2.385925 |
| H | 1.743984 | -4.939850 | 5.452909 |
| C | 3.492353 | -3.708310 | 5.378230 |
| H | 5.234254 | -2.465186 | 4.985800 |
| H | -1.244932 | -6.309675 | -0.889409 |
| H | 3.657698 | -3.730127 | 6.451675 |
| C | 2.629362 | 3.733607 | -1.138419 |
| C | 2.018087 | 4.584524 | -0.184865 |
| C | 2.134245 | 3.674277 | -2.464636 |
| C | 0.885337 | 5.395507 | -0.576601 |
| C | 2.462347 | 4.679392 | 1.175331 |
| C | 0.988590 | 4.474141 | -2.835407 |
| C | 2.734908 | 2.863660 | -3.482283 |
| C | 0.284420 | 6.270095 | 0.384306 |
| C | 0.397789 | 5.313060 | -1.884562 |
| C | 1.857653 | 5.528925 | 2.065969 |
| H | 3.290694 | 4.060788 | 1.500910 |
| C | 0.489881 | 4.404309 | -4.175135 |
| C | 2.229571 | 2.826966 | -4.756870 |
| H | 3.611188 | 2.273624 | -3.237086 |
| C | 0.757906 | 6.343219 | 1.667141 |

| | | | |
|---|---|---|---|
| H | -0.561263 | 6.876313 | 0.069122 |
| H | -0.457359 | 5.921244 | -2.171545 |
| H | 2.215878 | 5.580012 | 3.090472 |
| H | -0.376155 | 5.008780 | -4.433424 |
| C | 1.087556 | 3.602391 | -5.110982 |
| H | 2.705816 | 2.203467 | -5.508545 |
| H | 0.293674 | 7.010881 | 2.387361 |
| H | 0.700797 | 3.558317 | -6.125210 |
| H | -2.723912 | 4.993529 | 4.834854 |
| H | -0.247284 | -0.700378 | -2.937885 |
| H | -1.106891 | -2.095584 | -2.224817 |
| H | -1.327126 | -1.699671 | -3.954431 |

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**TS-SS-Me**

*G*sol(DCM) = -4273.843135 Hartree

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| | | | |
|---|---|---|---|
| C | -3.262852 | -0.777337 | 1.286021 |
| C | -4.496835 | 1.031251 | 0.059687 |
| C | -6.341424 | -2.221279 | 3.932807 |
| C | -5.528947 | -1.157116 | 4.335773 |
| C | -4.515857 | -0.669516 | 3.512335 |
| C | -4.270799 | -1.240430 | 2.237101 |
| C | -5.113879 | -2.311689 | 1.845225 |
| C | -6.122901 | -2.793159 | 2.676938 |
| H | -7.125928 | -2.596767 | 4.584169 |
| H | -5.682741 | -0.696589 | 5.308973 |
| H | -3.903876 | 0.150212 | 3.857776 |
| H | -4.960128 | -2.763836 | 0.873551 |
| H | -6.740278 | -3.622514 | 2.339612 |
| C | -2.170431 | 0.127402 | 1.522260 |
| O | -1.296877 | 0.375277 | 0.656354 |
| O | -2.161317 | 0.744446 | 2.725861 |
| C | -1.175897 | 1.767371 | 2.934436 |
| O | -3.127753 | -1.532731 | 0.128792 |
| C | -2.148900 | -2.599173 | 0.230007 |
| H | -2.420177 | -3.243021 | 1.077380 |
| H | -1.162571 | -2.165464 | 0.419028 |
| C | -2.138631 | -3.384282 | -1.057419 |
| C | -1.054290 | -3.285261 | -1.939362 |
| C | -3.216461 | -4.216432 | -1.395789 |
| C | -1.050306 | -4.003492 | -3.139398 |
| H | -0.213083 | -2.646408 | -1.682030 |
| C | -3.217969 | -4.927205 | -2.597217 |
| H | -4.054597 | -4.314865 | -0.710157 |
| C | -2.132628 | -4.820834 | -3.473533 |
| H | -0.200802 | -3.923443 | -3.812742 |
| H | -4.058722 | -5.569414 | -2.846270 |
| H | 0.213556 | 0.655711 | 0.765075 |
| C | -6.379504 | -1.441863 | -3.821424 |
| C | -7.847745 | -1.137543 | -4.146912 |
| C | -8.525153 | -1.650980 | -1.954712 |
| C | -7.082245 | -1.978798 | -1.564982 |
| H | -8.060212 | -1.402599 | -5.186415 |
| H | -6.159031 | -2.491971 | -4.048683 |
| H | -5.725343 | -0.810369 | -4.420207 |
| H | -9.220657 | -2.294676 | -1.409454 |
| H | -8.752806 | -0.600071 | -1.716939 |
| H | -6.894469 | -3.040972 | -1.770512 |
| H | -6.898336 | -1.804623 | -0.505863 |
| H | -8.037560 | -0.061290 | -4.009189 |
| O | -8.736116 | -1.901376 | -3.340581 |
| N | -6.142372 | -1.207166 | -2.388376 |
| C | -4.222442 | 0.234362 | -2.790919 |
| C | -3.295747 | -0.665337 | -3.343463 |
| C | -4.109740 | 1.601942 | -3.089034 |
| C | -2.270050 | -0.201837 | -4.165633 |
| H | -3.366564 | -1.721108 | -3.104939 |
| C | -3.088470 | 2.060451 | -3.922672 |
| H | -4.829816 | 2.300432 | -2.673805 |
| C | -2.163655 | 1.161144 | -4.458545 |
| H | -1.547626 | -0.906226 | -4.567453 |
| H | -3.016192 | 3.119773 | -4.151468 |
| H | -1.360101 | 1.520713 | -5.095033 |
| C | -5.311774 | -0.252601 | -1.896325 |
| C | -5.480100 | 0.290772 | -0.614443 |
| H | -6.410022 | 0.112683 | -0.086145 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -3.546916 | 1.212528 | -0.433098 | C | 5.931075 | -2.919188 | 0.307118 |
| C | -4.819118 | 1.851723 | 1.155121 | C | 8.944194 | -1.845130 | -1.612068 |
| C | -5.095391 | 2.563933 | 2.107652 | H | 9.331979 | 0.141122 | -2.393981 |
| C | -5.411853 | 3.418887 | 3.199368 | H | 8.268626 | -3.693579 | -0.759798 |
| C | -6.664353 | 3.328111 | 3.844794 | H | 6.171052 | -3.969085 | 0.451447 |
| C | -4.476945 | 4.374711 | 3.654056 | H | 9.856933 | -2.269115 | -2.020657 |
| C | -6.967111 | 4.169334 | 4.912435 | O | 2.964456 | 0.818805 | -1.091106 |
| H | -7.385946 | 2.593670 | 3.500622 | O | 3.238016 | -0.552055 | 1.036015 |
| C | -4.790727 | 5.212360 | 4.721276 | P | 2.113601 | -0.121800 | -0.065147 |
| H | -3.513337 | 4.450838 | 3.159632 | O | 1.222876 | 0.824462 | 0.822302 |
| C | -6.034072 | 5.113176 | 5.354200 | O | 1.458508 | -1.214534 | -0.818755 |
| H | -7.933657 | 4.089154 | 5.401891 | C | 2.335024 | 3.576501 | -1.488804 |
| H | -4.063712 | 5.944568 | 5.061192 | C | 1.299529 | 4.211784 | -0.760872 |
| H | -6.274715 | 5.767842 | 6.186957 | C | 2.225733 | 3.413334 | -2.891526 |
| C | 7.913904 | 2.874415 | 1.866727 | C | 0.129491 | 4.695752 | -1.461258 |
| C | 7.093078 | 1.909563 | 1.323364 | C | 1.345813 | 4.395984 | 0.660404 |
| C | 5.949557 | 2.266487 | 0.554988 | C | 1.045355 | 3.890336 | -3.576119 |
| C | 5.655134 | 3.659774 | 0.394037 | C | 3.253867 | 2.806007 | -3.683550 |
| C | 6.532362 | 4.630899 | 0.951191 | C | -0.908979 | 5.347805 | -0.722819 |
| C | 7.642325 | 4.249906 | 1.670047 | C | 0.032953 | 4.520302 | -2.845097 |
| H | 8.775752 | 2.575815 | 2.456932 | C | 0.329659 | 5.027728 | 1.331302 |
| H | 7.311791 | 0.862121 | 1.494400 | H | 2.202471 | 4.023399 | 1.209876 |
| C | 5.059866 | 1.295513 | -0.025839 | C | 0.942316 | 3.719751 | -4.993815 |
| C | 4.483214 | 4.049602 | -0.302606 | C | 3.117341 | 2.659773 | -5.040365 |
| H | 6.299097 | 5.682942 | 0.808056 | H | 4.159065 | 2.460954 | -3.195952 |
| H | 8.302612 | 4.998813 | 2.097806 | C | -0.813920 | 5.515685 | 0.633172 |
| C | 3.575611 | 3.127057 | -0.783007 | H | -1.777862 | 5.709065 | -1.267420 |
| C | 3.881342 | 1.748184 | -0.600464 | H | -0.848749 | 4.886719 | -3.366402 |
| H | 4.286402 | 5.109339 | -0.440332 | H | 0.393623 | 5.158153 | 2.408128 |
| C | 5.365158 | -0.164768 | 0.009501 | H | 0.049082 | 4.087748 | -5.492940 |
| C | 6.578930 | -0.700880 | -0.547090 | C | 1.944587 | 3.117801 | -5.708180 |
| C | 4.457541 | -1.048440 | 0.573082 | H | 3.912415 | 2.194166 | -5.616109 |
| C | 7.500057 | 0.081902 | -1.297867 | H | -1.606701 | 6.016043 | 1.182352 |
| C | 6.861669 | -2.095606 | -0.376453 | H | 1.855525 | 2.994958 | -6.783879 |
| C | 4.723424 | -2.433749 | 0.767006 | C | 3.747920 | -3.332143 | 1.459794 |
| C | 8.648721 | -0.475721 | -1.816997 | C | 3.044538 | -4.313942 | 0.720574 |
| H | 7.285788 | 1.129595 | -1.473686 | C | 3.561168 | -3.220128 | 2.859112 |
| C | 8.064452 | -2.636394 | -0.909203 | C | 2.128201 | -5.199873 | 1.405744 |

| | | | |
|---|---|---|---|
| C | 3.184527 | -4.470628 | -0.697770 |
| C | 2.631455 | -4.102186 | 3.527985 |
| C | 4.272350 | -2.270566 | 3.662691 |
| C | 1.426851 | -6.197114 | 0.655418 |
| C | 1.942286 | -5.066578 | 2.785130 |
| C | 2.493082 | -5.438528 | -1.379963 |
| H | 3.848642 | -3.803869 | -1.235530 |
| C | 2.443069 | -3.977713 | 4.941223 |
| C | 4.066325 | -2.184798 | 5.016009 |
| H | 4.991861 | -1.612500 | 3.187462 |
| C | 1.604278 | -6.319204 | -0.696916 |
| H | 0.746404 | -6.857137 | 1.187927 |
| H | 1.248246 | -5.732215 | 3.293821 |
| H | 2.618343 | -5.534673 | -2.454929 |
| H | 1.736695 | -4.646554 | 5.426878 |
| C | 3.135679 | -3.045404 | 5.667463 |
| H | 4.619692 | -1.455539 | 5.601272 |
| H | 1.066306 | -7.079867 | -1.255520 |
| H | 2.984748 | -2.961004 | 6.739982 |
| H | -2.129757 | -5.377344 | -4.407084 |
| H | -0.175528 | 1.333758 | 3.013176 |
| H | -1.192159 | 2.498217 | 2.122365 |
| H | -1.449279 | 2.242872 | 3.876790 |

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**TS-RR-Ph**

*G*sol(DCM) = -3777.406428 Hartree

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| | | | |
|---|---|---|---|
| C | 2.656755 | -0.752171 | -0.986922 |
| C | 4.259275 | -0.048966 | 1.404509 |
| C | 5.977480 | -1.984296 | -3.445621 |
| C | 5.232280 | -2.945058 | -2.754701 |
| C | 4.154891 | -2.582063 | -1.948831 |
| C | 3.768534 | -1.224638 | -1.803684 |
| C | 4.537161 | -0.267962 | -2.518224 |
| C | 5.615850 | -0.640099 | -3.316953 |
| H | 6.815890 | -2.276682 | -4.072077 |
| H | 5.491347 | -3.997869 | -2.843392 |
| H | 3.597204 | -3.349697 | -1.432294 |
| H | 4.273205 | 0.779191 | -2.430902 |
| H | 6.177206 | 0.128284 | -3.844134 |
| C | 1.818759 | -1.474230 | -0.112795 |
| O | 0.821510 | -0.958081 | 0.504804 |
| O | 2.146408 | -2.777072 | 0.092394 |
| C | 1.429382 | -3.653124 | 1.028486 |
| O | 2.323518 | 0.594216 | -1.136055 |
| C | 1.440065 | 0.860764 | -2.254590 |
| H | 1.836963 | 0.368350 | -3.150554 |
| H | 0.452709 | 0.440784 | -2.037686 |
| C | 1.352218 | 2.350828 | -2.470822 |
| C | 0.407695 | 3.121854 | -1.777300 |
| C | 2.223670 | 2.992434 | -3.362520 |
| C | 0.345349 | 4.505852 | -1.963622 |
| H | -0.288016 | 2.637995 | -1.095030 |
| C | 2.161699 | 4.375311 | -3.554147 |
| H | 2.948132 | 2.401512 | -3.918305 |
| C | 1.222820 | 5.136088 | -2.850920 |
| H | -0.394842 | 5.090114 | -1.423337 |
| H | 2.838184 | 4.856222 | -4.255779 |
| H | -0.337653 | -0.716894 | -0.102891 |
| C | 1.540726 | -3.117052 | 2.461079 |
| H | 0.992798 | -2.180696 | 2.575754 |
| H | 1.131194 | -3.854324 | 3.161267 |
| H | 2.591934 | -2.948433 | 2.720795 |
| C | 2.196159 | -4.974682 | 0.895765 |
| H | 1.772736 | -5.724875 | 1.571794 |
| H | 2.132126 | -5.358229 | -0.128190 |
| H | 3.252604 | -4.837128 | 1.147799 |
| C | -0.027308 | -3.848270 | 0.589748 |
| H | -0.613108 | -2.937548 | 0.714129 |
| H | -0.067872 | -4.152532 | -0.462200 |
| H | -0.485117 | -4.643334 | 1.189536 |
| C | 3.638908 | 4.820325 | 0.795409 |
| C | 4.808169 | 5.798635 | 0.964692 |
| C | 6.144597 | 4.593071 | -0.537384 |
| C | 5.024161 | 3.575238 | -0.765680 |
| H | 4.418849 | 6.804334 | 1.143230 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 2.977378 | 5.159643 | -0.009553 | C | -7.723323 | -3.615502 | -1.083056 |
| H | 3.066105 | 4.753478 | 1.718027 | C | -7.012680 | -2.556005 | -0.560588 |
| H | 6.721218 | 4.719712 | -1.457180 | C | -6.042545 | -1.866938 | -1.340937 |
| H | 6.818102 | 4.239239 | 0.258391 | C | -5.798773 | -2.328746 | -2.675344 |
| H | 4.385853 | 3.910865 | -1.591443 | C | -6.561153 | -3.413430 | -3.190748 |
| H | 5.424168 | 2.598360 | -1.025871 | C | -7.507208 | -4.043943 | -2.415105 |
| H | 5.418738 | 5.495484 | 1.829395 | H | -8.453288 | -4.130095 | -0.464415 |
| O | 5.609560 | 5.867629 | -0.206290 | H | -7.184620 | -2.249179 | 0.464513 |
| N | 4.167859 | 3.492570 | 0.430517 | C | -5.269522 | -0.762753 | -0.838755 |
| C | 2.898727 | 2.405594 | 2.198678 | C | -4.794827 | -1.705297 | -3.456875 |
| C | 1.538999 | 2.521943 | 1.874857 | H | -6.371504 | -3.742708 | -4.209294 |
| C | 3.286461 | 2.291928 | 3.543115 | H | -8.079330 | -4.875761 | -2.816006 |
| C | 0.576841 | 2.520604 | 2.884746 | C | -3.998851 | -0.688350 | -2.963532 |
| H | 1.239664 | 2.576921 | 0.834139 | C | -4.247141 | -0.257368 | -1.626667 |
| C | 2.322075 | 2.317393 | 4.551217 | H | -4.649513 | -2.044062 | -4.478973 |
| H | 4.338350 | 2.192990 | 3.794306 | C | -5.514308 | -0.191985 | 0.519509 |
| C | 0.968192 | 2.428163 | 4.223332 | C | -6.785539 | 0.370131 | 0.886155 |
| H | -0.472575 | 2.566840 | 2.612042 | C | -4.487196 | -0.173793 | 1.451095 |
| H | 2.628929 | 2.240562 | 5.590366 | C | -7.854670 | 0.541729 | -0.036901 |
| H | 0.216953 | 2.426429 | 5.007344 | C | -6.976275 | 0.821053 | 2.232708 |
| C | 3.933640 | 2.371295 | 1.123043 | C | -4.662178 | 0.240877 | 2.805008 |
| C | 4.666178 | 1.174094 | 0.906325 | C | -9.052231 | 1.098232 | 0.358780 |
| H | 5.573579 | 1.198829 | 0.315466 | H | -7.716951 | 0.241370 | -1.069226 |
| H | 3.331748 | -0.116980 | 1.965951 | C | -8.230224 | 1.374271 | 2.613678 |
| C | 5.053142 | -1.199159 | 1.332611 | C | -5.912053 | 0.713730 | 3.161706 |
| C | 5.756131 | -2.197924 | 1.294137 | C | -9.249939 | 1.509477 | 1.699242 |
| C | 6.595357 | -3.343435 | 1.264070 | H | -9.850941 | 1.226809 | -0.366385 |
| C | 7.738070 | -3.368983 | 0.434387 | H | -8.362578 | 1.700062 | 3.642352 |
| C | 6.303529 | -4.468943 | 2.065986 | H | -6.091962 | 1.014493 | 4.190022 |
| C | 8.559997 | -4.492225 | 0.409309 | H | -10.201264 | 1.939984 | 1.998582 |
| H | 7.962200 | -2.507270 | -0.186142 | O | -3.433689 | 0.744999 | -1.099797 |
| C | 7.134454 | -5.585568 | 2.034922 | O | -3.225758 | -0.609524 | 1.048152 |
| H | 5.429497 | -4.450464 | 2.709506 | P | -2.350527 | 0.376693 | 0.067983 |
| C | 8.262722 | -5.601509 | 1.208118 | O | -1.329971 | -0.606770 | -0.575235 |
| H | 9.435244 | -4.503514 | -0.233830 | O | -1.865159 | 1.626963 | 0.706886 |
| H | 6.902810 | -6.445565 | 2.656608 | C | -2.943135 | -0.083619 | -3.819713 |
| H | 8.907885 | -6.475101 | 1.186385 | C | -2.097921 | -0.912184 | -4.577725 |
| H | 1.168628 | 6.210933 | -3.001698 | C | -2.800585 | 1.309749 | -3.943140 |

| | | | |
|---|---|---|---|
| C | -1.141621 | -0.366829 | -5.435996 |
| C | -1.846455 | 1.853847 | -4.802942 |
| C | -1.012993 | 1.019025 | -5.552885 |
| H | -0.268243 | 1.445658 | -6.219033 |
| C | -3.578625 | 0.156842 | 3.821100 |
| C | -3.392170 | 1.208381 | 4.735442 |
| C | -2.770631 | -0.987761 | 3.946265 |
| C | -2.439107 | 1.115136 | 5.751086 |
| C | -1.816435 | -1.078854 | 4.959614 |
| C | -1.647743 | -0.030149 | 5.868010 |
| H | -0.906080 | -0.104846 | 6.658489 |
| H | -3.447384 | 1.967895 | -3.372759 |
| H | -1.755194 | 2.933183 | -4.887787 |
| H | -2.182113 | -1.990977 | -4.480685 |
| H | -0.494802 | -1.026185 | -6.008461 |
| H | -2.901799 | -1.815330 | 3.257777 |
| H | -1.208373 | -1.975542 | 5.043702 |
| H | -3.992756 | 2.108828 | 4.642805 |
| H | -2.315226 | 1.939008 | 6.448944 |

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**TS-RS-Ph**

*G*sol(DCM) = -3777.408566 Hartree

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| | | | |
|---|---|---|---|
| C | 3.066787 | -1.462280 | 0.184130 |
| C | 2.935369 | 0.384448 | 1.263653 |
| C | 7.331150 | -1.806112 | -0.444347 |
| C | 6.797385 | -2.030076 | 0.828210 |
| C | 5.425145 | -1.933271 | 1.051240 |
| C | 4.540191 | -1.617080 | -0.001746 |
| C | 5.096977 | -1.357102 | -1.267960 |
| C | 6.471634 | -1.462295 | -1.487925 |
| H | 8.401051 | -1.888336 | -0.614480 |
| H | 7.453498 | -2.279504 | 1.658042 |
| H | 5.042998 | -2.102027 | 2.049694 |
| H | 4.448101 | -1.071278 | -2.086149 |
| H | 6.867915 | -1.269362 | -2.481486 |
| C | 2.315799 | -2.362566 | 1.038740 |
| O | 1.030808 | -2.420111 | 1.043407 |
| O | 2.975677 | -3.139091 | 1.858046 |
| C | 2.371428 | -4.191535 | 2.749819 |
| O | 2.365368 | -1.102096 | -0.963474 |
| C | 2.009493 | -2.192963 | -1.867437 |
| H | 2.713620 | -3.020623 | -1.735218 |
| H | 1.008649 | -2.542506 | -1.593693 |
| C | 2.032369 | -1.712872 | -3.297600 |
| C | 1.144528 | -0.718279 | -3.736798 |
| C | 2.925934 | -2.278169 | -4.217170 |
| C | 1.160090 | -0.298197 | -5.068045 |
| H | 0.446795 | -0.267627 | -3.036205 |
| C | 2.934984 | -1.864695 | -5.552359 |
| H | 3.616364 | -3.051530 | -3.888688 |
| C | 2.052534 | -0.871098 | -5.980136 |
| H | 0.468538 | 0.473357 | -5.396410 |
| H | 3.631174 | -2.317224 | -6.253403 |
| C | 1.445279 | -3.547512 | 3.779587 |
| H | 0.530590 | -3.165529 | 3.325884 |
| H | 1.175133 | -4.303999 | 4.524316 |
| H | 1.953890 | -2.727842 | 4.295370 |
| C | 3.615972 | -4.776200 | 3.418732 |
| H | 3.320855 | -5.592525 | 4.085193 |
| H | 4.310990 | -5.171425 | 2.671658 |
| H | 4.133131 | -4.015962 | 4.012679 |
| C | 1.672245 | -5.235509 | 1.877716 |
| H | 0.788587 | -4.827692 | 1.383806 |
| H | 2.359057 | -5.625870 | 1.119660 |
| H | 1.357460 | -6.070119 | 2.513078 |
| C | 2.251767 | 2.622436 | -2.343667 |
| C | 1.234036 | 3.759545 | -2.258024 |
| C | 2.934645 | 5.285620 | -1.698974 |
| C | 4.009660 | 4.192460 | -1.769180 |
| H | 0.435219 | 3.608717 | -2.988478 |
| H | 2.632955 | 2.565393 | -3.372303 |
| H | 1.791719 | 1.668859 | -2.094183 |
| H | 3.356231 | 6.245504 | -2.012596 |
| H | 2.575473 | 5.378785 | -0.661261 |
| H | 4.434239 | 4.161847 | -2.780585 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 4.810445 | 4.408243 | -1.062717 | C | -7.731609 | -2.693366 | 1.598155 |
| H | 0.787207 | 3.797392 | -1.254700 | H | -8.390745 | -0.783676 | 2.389799 |
| O | 1.848609 | 5.009876 | -2.573351 | H | -6.640294 | 0.519439 | 1.271132 |
| N | 3.402455 | 2.887678 | -1.470603 | C | -4.659193 | -0.464636 | -0.366184 |
| C | 4.997392 | 2.351458 | 0.288058 | C | -4.763749 | -3.275850 | -0.586088 |
| C | 5.124165 | 2.718708 | 1.637772 | H | -6.822170 | -4.418020 | 0.704350 |
| C | 6.161337 | 2.165331 | -0.477186 | H | -8.514701 | -3.258633 | 2.095524 |
| C | 6.385680 | 2.886694 | 2.211758 | C | -3.712007 | -2.601624 | -1.177641 |
| H | 4.229552 | 2.886325 | 2.229722 | C | -3.673222 | -1.181504 | -1.029698 |
| C | 7.420219 | 2.326213 | 0.099532 | H | -4.834187 | -4.354301 | -0.699802 |
| H | 6.073067 | 1.877329 | -1.520180 | C | -4.572252 | 1.025136 | -0.314853 |
| C | 7.536093 | 2.688533 | 1.445252 | C | -5.623358 | 1.862683 | -0.823607 |
| H | 6.467687 | 3.177381 | 3.255267 | C | -3.430684 | 1.621979 | 0.204460 |
| H | 8.311459 | 2.165078 | -0.500400 | C | -6.760615 | 1.352985 | -1.511152 |
| H | 8.518048 | 2.817540 | 1.891857 | C | -5.507193 | 3.283012 | -0.675068 |
| C | 3.646608 | 2.180895 | -0.325474 | C | -3.307061 | 3.034984 | 0.381275 |
| C | 2.680928 | 1.367745 | 0.253964 | C | -7.738912 | 2.196978 | -1.992154 |
| H | 1.656985 | 1.443819 | -0.092096 | H | -6.849286 | 0.284168 | -1.668997 |
| H | 3.954955 | 0.309755 | 1.632906 | C | -6.542199 | 4.125827 | -1.166896 |
| C | 1.938212 | 0.205797 | 2.269794 | C | -4.357388 | 3.824641 | -0.049533 |
| C | 1.099721 | 0.076823 | 3.143081 | C | -7.638454 | 3.597701 | -1.810243 |
| C | 0.111714 | -0.066444 | 4.163160 | H | -8.593478 | 1.783457 | -2.520668 |
| C | 0.464870 | 0.043801 | 5.523973 | H | -6.442568 | 5.200400 | -1.034747 |
| C | -1.232007 | -0.326196 | 3.819174 | H | -4.305057 | 4.900708 | 0.092080 |
| C | -0.505397 | -0.097915 | 6.514198 | H | -8.419956 | 4.250553 | -2.188609 |
| H | 1.498130 | 0.243252 | 5.791471 | O | -2.613738 | -0.485617 | -1.588991 |
| C | -2.192549 | -0.469345 | 4.819216 | O | -2.380381 | 0.807422 | 0.596318 |
| H | -1.502172 | -0.413318 | 2.771793 | P | -1.434663 | 0.108983 | -0.581192 |
| C | -1.835109 | -0.354784 | 6.166332 | O | -0.769495 | -1.048121 | 0.134550 |
| H | -0.222914 | -0.008612 | 7.559437 | O | -0.665373 | 1.120455 | -1.366821 |
| H | -3.224461 | -0.670750 | 4.545312 | H | 2.057475 | -0.545774 | -7.017031 |
| H | -2.588540 | -0.465789 | 6.941048 | C | -2.675050 | -3.354009 | -1.933766 |
| H | 0.442524 | -1.702165 | 0.531901 | C | -2.135185 | -4.535018 | -1.395037 |
| C | -7.664021 | -1.288201 | 1.758960 | C | -2.250098 | -2.947284 | -3.210562 |
| C | -6.682214 | -0.554115 | 1.128075 | C | -1.200657 | -5.287271 | -2.108786 |
| C | -5.709180 | -1.184307 | 0.302184 | H | -2.439951 | -4.855364 | -0.402586 |
| C | -5.758333 | -2.610831 | 0.173257 | C | -1.318991 | -3.701282 | -3.925126 |
| C | -6.794118 | -3.337591 | 0.823058 | H | -2.657547 | -2.041809 | -3.646968 |

| | | | |
|---|---|---|---|
| C | -0.789085 | -4.873334 | -3.377871 |
| H | -0.792329 | -6.194027 | -1.670416 |
| H | -1.006905 | -3.371498 | -4.912141 |
| H | -0.061396 | -5.456892 | -3.935167 |
| C | -2.115005 | 3.666553 | 1.009426 |
| C | -1.563096 | 4.831948 | 0.448680 |
| C | -1.550836 | 3.166793 | 2.196391 |
| C | -0.484662 | 5.479463 | 1.054745 |
| H | -1.974410 | 5.224840 | -0.476887 |
| C | -0.471973 | 3.812859 | 2.800500 |
| H | -1.964650 | 2.275284 | 2.653929 |
| C | 0.066314 | 4.971478 | 2.233677 |
| H | -0.074068 | 6.377933 | 0.601765 |
| H | -0.054523 | 3.409799 | 3.719210 |
| H | 0.906351 | 5.473344 | 2.706151 |

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**TS-SR-Ph**

*G*sol(DCM) = -3777.408806 Hartree

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| | | | |
|---|---|---|---|
| C | 2.704216 | -1.088379 | 0.473066 |
| C | 4.390083 | 1.146813 | 0.389726 |
| C | 5.704236 | -3.789013 | 1.991218 |
| C | 5.328679 | -3.855667 | 0.645863 |
| C | 4.361512 | -2.997916 | 0.123541 |
| C | 3.724721 | -2.028177 | 0.936737 |
| C | 4.117078 | -1.982375 | 2.299384 |
| C | 5.085898 | -2.841431 | 2.812303 |
| H | 6.459187 | -4.460898 | 2.390263 |
| H | 5.789742 | -4.591204 | -0.009678 |
| H | 4.087620 | -3.077178 | -0.919003 |
| H | 3.656652 | -1.245575 | 2.949218 |
| H | 5.361180 | -2.766781 | 3.861871 |
| C | 2.301147 | -0.797560 | -0.850039 |
| O | 1.348633 | 0.002921 | -1.150868 |
| O | 3.046059 | -1.348976 | -1.836531 |
| C | 2.735626 | -1.202649 | -3.269028 |
| O | 1.958583 | -0.446919 | 1.462120 |
| C | 0.948722 | -1.292224 | 2.073018 |
| H | 1.415756 | -2.224818 | 2.410367 |
| H | 0.192919 | -1.534796 | 1.320457 |
| C | 0.331642 | -0.566734 | 3.242171 |
| C | -0.665840 | 0.399415 | 3.038882 |
| C | 0.752128 | -0.839328 | 4.550545 |
| C | -1.223863 | 1.081155 | 4.122785 |
| H | -1.007657 | 0.603119 | 2.028088 |
| C | 0.193095 | -0.161808 | 5.637452 |
| H | 1.519012 | -1.591891 | 4.719170 |
| C | -0.794609 | 0.803256 | 5.424809 |
| H | -2.000429 | 1.822653 | 3.953507 |
| H | 0.524609 | -0.390131 | 6.647006 |
| C | 2.891624 | 0.257197 | -3.711207 |
| H | 2.122061 | 0.887153 | -3.263376 |
| H | 2.805859 | 0.318537 | -4.802340 |
| H | 3.876262 | 0.638484 | -3.421745 |
| C | 3.810856 | -2.075387 | -3.927657 |
| H | 3.710527 | -2.033073 | -5.017220 |
| H | 3.708545 | -3.119914 | -3.613926 |
| H | 4.812677 | -1.727615 | -3.657682 |
| C | 1.342095 | -1.757504 | -3.585913 |
| H | 0.549943 | -1.112924 | -3.203400 |
| H | 1.224929 | -2.758997 | -3.158173 |
| H | 1.226138 | -1.838853 | -4.673115 |
| C | 0.863266 | 3.338376 | -0.253583 |
| C | 0.883341 | 4.655528 | -1.030582 |
| C | 1.123718 | 5.868244 | 0.975848 |
| C | 1.119316 | 4.583456 | 1.817285 |
| H | 0.228878 | 4.587040 | -1.902396 |
| H | -0.170268 | 3.114096 | 0.037815 |
| H | 1.232305 | 2.495276 | -0.836160 |
| H | 0.654271 | 6.678598 | 1.539808 |
| H | 2.163187 | 6.150646 | 0.747123 |
| H | 0.097462 | 4.340656 | 2.128750 |
| H | 1.737329 | 4.714503 | 2.703554 |
| H | 1.905489 | 4.887527 | -1.366701 |
| O | 0.378692 | 5.718131 | -0.224817 |
| N | 1.636627 | 3.478266 | 0.991810 |

| | | | |
|---|---|---|---|
| C | 3.333266 | 2.815682 | 2.612012 |
| C | 4.674426 | 3.178178 | 2.829073 |
| C | 2.533980 | 2.454771 | 3.711282 |
| C | 5.202732 | 3.187251 | 4.119966 |
| H | 5.293011 | 3.468092 | 1.985950 |
| C | 3.070934 | 2.452583 | 4.997244 |
| H | 1.504496 | 2.151552 | 3.552675 |
| C | 4.403391 | 2.822368 | 5.205661 |
| H | 6.237060 | 3.479457 | 4.275670 |
| H | 2.448019 | 2.153149 | 5.834517 |
| H | 4.816404 | 2.823611 | 6.210397 |
| C | 2.781759 | 2.815418 | 1.231418 |
| C | 3.493442 | 2.178845 | 0.179913 |
| H | 3.310230 | 2.496228 | -0.840148 |
| H | 4.514758 | 0.751465 | 1.393737 |
| C | 5.292776 | 0.685912 | -0.578750 |
| C | 6.133326 | 0.285388 | -1.368954 |
| C | 7.127040 | -0.176208 | -2.274013 |
| C | 7.888328 | -1.326000 | -1.967498 |
| C | 7.374272 | 0.508283 | -3.484316 |
| C | 8.868061 | -1.772623 | -2.849807 |
| H | 7.692956 | -1.859380 | -1.042407 |
| C | 8.357751 | 0.053003 | -4.358489 |
| H | 6.793163 | 1.393729 | -3.722361 |
| C | 9.106757 | -1.085973 | -4.045109 |
| H | 9.447021 | -2.658818 | -2.606226 |
| H | 8.541151 | 0.587087 | -5.286361 |
| H | 9.872727 | -1.437943 | -4.730184 |
| H | 0.114207 | -0.066033 | -0.666329 |
| C | -6.711495 | -1.548580 | 3.297495 |
| C | -6.228896 | -1.116872 | 2.080396 |
| C | -5.153222 | -1.790852 | 1.437531 |
| C | -4.564988 | -2.914171 | 2.104112 |
| C | -5.098424 | -3.346306 | 3.349940 |
| C | -6.151025 | -2.681048 | 3.936493 |
| H | -7.527332 | -1.011712 | 3.773505 |
| H | -6.663409 | -0.242302 | 1.609816 |
| C | -4.605612 | -1.369467 | 0.176760 |
| C | -3.460984 | -3.575376 | 1.511547 |
| H | -4.647896 | -4.207854 | 3.836434 |
| H | -6.546141 | -3.014206 | 4.891939 |
| C | -2.876712 | -3.135192 | 0.337986 |
| C | -3.452078 | -1.986453 | -0.285125 |
| H | -3.065792 | -4.461110 | 2.000985 |
| C | -5.239231 | -0.284516 | -0.629858 |
| C | -6.593622 | -0.394383 | -1.102090 |
| C | -4.501084 | 0.833594 | -0.984880 |
| C | -7.389870 | -1.560132 | -0.922484 |
| C | -7.160818 | 0.703310 | -1.827749 |
| C | -5.045913 | 1.939536 | -1.703235 |
| C | -8.681643 | -1.619586 | -1.400339 |
| H | -6.967844 | -2.418345 | -0.412961 |
| C | -8.502812 | 0.617669 | -2.291922 |
| C | -6.370949 | 1.850082 | -2.088170 |
| C | -9.252265 | -0.517253 | -2.081383 |
| H | -9.266243 | -2.524067 | -1.256963 |
| H | -8.920314 | 1.465120 | -2.829852 |
| H | -6.827106 | 2.683922 | -2.614514 |
| H | -10.273812 | -0.575663 | -2.446041 |
| O | -2.845103 | -1.491597 | -1.436466 |
| O | -3.164505 | 0.890643 | -0.595383 |
| P | -2.077379 | -0.039732 | -1.395995 |
| O | -0.940437 | -0.101485 | -0.333060 |
| O | -1.766402 | 0.374090 | -2.785614 |
| H | -1.233976 | 1.329376 | 6.268176 |
| C | -4.250429 | 3.149386 | -2.044631 |
| C | -3.435488 | 3.795710 | -1.098726 |
| C | -4.345830 | 3.702726 | -3.333647 |
| C | -2.742576 | 4.960396 | -1.431854 |
| H | -3.353967 | 3.390613 | -0.095730 |
| C | -3.653147 | 4.867232 | -3.667333 |
| H | -4.954497 | 3.205159 | -4.083420 |
| C | -2.848160 | 5.499956 | -2.717651 |
| H | -2.106939 | 5.439046 | -0.692500 |
| H | -3.737292 | 5.273630 | -4.671647 |
| H | -2.305227 | 6.405112 | -2.976092 |

| | | | |
|---|---|---|---|
| C | -1.719696 | -3.870673 | -0.241037 |
| C | -0.691166 | -4.335722 | 0.597532 |
| C | -1.655819 | -4.184111 | -1.610582 |
| C | 0.368918 | -5.085983 | 0.086448 |
| H | -0.716646 | -4.095182 | 1.656450 |
| C | -0.599963 | -4.940855 | -2.119565 |
| H | -2.442475 | -3.845986 | -2.276098 |
| C | 0.418263 | -5.393079 | -1.275041 |
| H | 1.157887 | -5.424915 | 0.752167 |
| H | -0.576512 | -5.182620 | -3.178734 |
| H | 1.241143 | -5.979089 | -1.674890 |

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**TS-SS-Ph**

*G*sol(DCM) = -3777.407558 Hartree

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| | | | |
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| C | 2.650303 | -0.846601 | 0.440273 |
| C | 4.226600 | 1.161583 | -0.909503 |
| C | 5.894716 | -2.612865 | 2.659397 |
| C | 5.426840 | -3.238369 | 1.499383 |
| C | 4.384226 | -2.691066 | 0.754215 |
| C | 3.753400 | -1.483344 | 1.148130 |
| C | 4.242753 | -0.868547 | 2.330956 |
| C | 5.289698 | -1.419406 | 3.065527 |
| H | 6.707463 | -3.047376 | 3.235095 |
| H | 5.878142 | -4.170790 | 1.167374 |
| H | 4.040353 | -3.202917 | -0.133389 |
| H | 3.789524 | 0.059979 | 2.658093 |
| H | 5.635191 | -0.911156 | 3.963144 |
| C | 2.116215 | -1.151407 | -0.838070 |
| O | 1.088773 | -0.600296 | -1.345088 |
| O | 2.813884 | -2.059726 | -1.564546 |
| C | 2.469422 | -2.421598 | -2.948357 |
| O | 1.961825 | 0.144206 | 1.137643 |
| C | 1.052277 | -0.366389 | 2.150020 |
| H | 1.571601 | -1.124435 | 2.746643 |
| H | 0.201629 | -0.838597 | 1.650270 |
| C | 0.594638 | 0.768336 | 3.031861 |
| C | -0.500182 | 1.564621 | 2.664508 |
| C | 1.259350 | 1.048101 | 4.234620 |
| C | -0.911961 | 2.625125 | 3.475794 |
| H | -1.034712 | 1.339146 | 1.745682 |
| C | 0.847572 | 2.104974 | 5.050820 |
| H | 2.098180 | 0.425782 | 4.537771 |
| C | -0.238328 | 2.898857 | 4.669963 |
| H | -1.765378 | 3.230580 | 3.181955 |
| H | 1.367091 | 2.302938 | 5.984663 |
| H | -0.100643 | -0.301634 | -0.736099 |
| C | 2.620309 | -1.204008 | -3.868310 |
| H | 1.875980 | -0.440999 | -3.634780 |
| H | 2.489056 | -1.513674 | -4.911513 |
| H | 3.621552 | -0.770559 | -3.765583 |
| C | 3.529574 | -3.477870 | -3.282341 |
| H | 3.415900 | -3.809171 | -4.319746 |
| H | 3.425614 | -4.350652 | -2.628605 |
| H | 4.537468 | -3.069835 | -3.155613 |
| C | 1.068646 | -3.040811 | -3.029692 |
| H | 0.285507 | -2.295886 | -2.885974 |
| H | 0.957052 | -3.822591 | -2.270662 |
| H | 0.936610 | -3.503859 | -4.014697 |
| C | 2.180588 | 4.922446 | 1.567896 |
| C | 2.983469 | 6.146456 | 2.023827 |
| C | 4.580195 | 4.800469 | 3.087970 |
| C | 3.832503 | 3.529147 | 2.678087 |
| H | 2.302094 | 6.978634 | 2.219172 |
| H | 1.418017 | 4.674820 | 2.315709 |
| H | 1.688745 | 5.125822 | 0.618935 |
| H | 5.058948 | 4.650453 | 4.059058 |
| H | 5.355382 | 5.036583 | 2.342485 |
| H | 3.098888 | 3.267315 | 3.449910 |
| H | 4.518757 | 2.693027 | 2.569662 |
| H | 3.686754 | 6.442800 | 1.229919 |
| O | 3.682822 | 5.892826 | 3.234449 |
| N | 3.085302 | 3.766476 | 1.431621 |
| C | 2.275231 | 3.315727 | -0.819094 |
| C | 2.726495 | 4.038288 | -1.934316 |
| C | 0.956904 | 2.841165 | -0.783842 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 1.857636 | 4.301613 | -2.994548 | C | -3.528009 | -1.896004 | 0.585957 |
| H | 3.751741 | 4.395675 | -1.966315 | H | -2.947410 | -3.302023 | 3.616207 |
| C | 0.096676 | 3.098636 | -1.851763 | C | -5.398131 | -0.499868 | -0.285379 |
| H | 0.625238 | 2.247775 | 0.059630 | C | -6.759699 | -0.824057 | -0.618240 |
| C | 0.541936 | 3.832708 | -2.953960 | C | -4.726927 | 0.425630 | -1.068102 |
| H | 2.211087 | 4.867323 | -3.851848 | C | -7.491953 | -1.861426 | 0.024170 |
| H | -0.920245 | 2.719942 | -1.823612 | C | -7.400180 | -0.103900 | -1.678795 |
| H | -0.134727 | 4.031809 | -3.780114 | C | -5.350429 | 1.169288 | -2.112876 |
| C | 3.213997 | 3.037314 | 0.312607 | C | -8.791351 | -2.144289 | -0.339152 |
| C | 4.227428 | 2.065271 | 0.141628 | H | -7.013671 | -2.445657 | 0.801438 |
| H | 5.033990 | 1.991573 | 0.860494 | C | -8.747582 | -0.408475 | -2.018044 |
| H | 3.423924 | 1.191445 | -1.640006 | C | -6.677828 | 0.892443 | -2.380972 |
| C | 5.309182 | 0.314994 | -1.174792 | C | -9.433315 | -1.405233 | -1.361988 |
| C | 6.263457 | -0.409995 | -1.414187 | H | -9.326624 | -2.946457 | 0.161201 |
| C | 7.387498 | -1.232460 | -1.693575 | H | -9.221473 | 0.156052 | -2.817121 |
| C | 8.390688 | -1.425668 | -0.718190 | H | -7.189472 | 1.454725 | -3.157240 |
| C | 7.520222 | -1.867308 | -2.948437 | H | -10.459766 | -1.634944 | -1.633217 |
| C | 9.489932 | -2.234237 | -0.994204 | O | -2.991311 | -1.864129 | -0.698606 |
| H | 8.290117 | -0.942790 | 0.248565 | O | -3.376062 | 0.656648 | -0.807177 |
| C | 8.625078 | -2.671584 | -3.214204 | P | -2.301294 | -0.489580 | -1.272956 |
| H | 6.754963 | -1.716570 | -3.703506 | O | -1.097608 | -0.101758 | -0.354906 |
| C | 9.611507 | -2.858528 | -2.240092 | O | -2.092033 | -0.638597 | -2.732788 |
| H | 10.254638 | -2.378525 | -0.236354 | H | -0.563816 | 3.718541 | 5.304895 |
| H | 8.717964 | -3.154078 | -4.182927 | C | -4.635947 | 2.215480 | -2.893168 |
| H | 10.471518 | -3.487578 | -2.451233 | C | -4.742633 | 2.238488 | -4.294192 |
| C | -6.667619 | -0.212700 | 3.896223 | C | -3.904628 | 3.235043 | -2.259643 |
| C | -6.251091 | -0.266026 | 2.583141 | C | -4.141205 | 3.252248 | -5.041603 |
| C | -5.169637 | -1.103083 | 2.190886 | H | -5.290633 | 1.448084 | -4.799385 |
| C | -4.505833 | -1.869518 | 3.203029 | C | -3.309304 | 4.252112 | -3.007131 |
| C | -4.971439 | -1.806045 | 4.545646 | H | -3.818610 | 3.240751 | -1.177856 |
| C | -6.030885 | -0.996979 | 4.888462 | C | -3.424012 | 4.264797 | -4.400567 |
| H | -7.489844 | 0.441112 | 4.173424 | H | -4.231540 | 3.247920 | -6.124419 |
| H | -6.742537 | 0.348821 | 1.837810 | H | -2.758944 | 5.039110 | -2.498929 |
| C | -4.688494 | -1.179882 | 0.838541 | H | -2.959869 | 5.058135 | -4.980074 |
| C | -3.398462 | -2.679123 | 2.848846 | C | -1.722335 | -3.586306 | 1.249448 |
| H | -4.464114 | -2.402335 | 5.299873 | C | -0.646006 | -3.683996 | 2.149173 |
| H | -6.373827 | -0.949788 | 5.918091 | C | -1.703357 | -4.393025 | 0.097586 |
| C | -2.880498 | -2.707036 | 1.566706 | C | 0.416540 | -4.555775 | 1.906298 |

| | | | |
|---|---|---|---|
| H | -0.636870 | -3.061680 | 3.039366 |
| C | -0.644706 | -5.270028 | -0.140599 |
| H | -2.527356 | -4.344662 | -0.605706 |
| C | 0.420979 | -5.353854 | 0.760250 |
| H | 1.242038 | -4.606884 | 2.610898 |
| H | -0.656756 | -5.894568 | -1.029753 |
| H | 1.245800 | -6.035065 | 0.570508 |

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