

Supporting Information

Late-stage Cyclization of Natural Products Enabled by C–C bond

Cleavage of Aryl Ketones

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Content

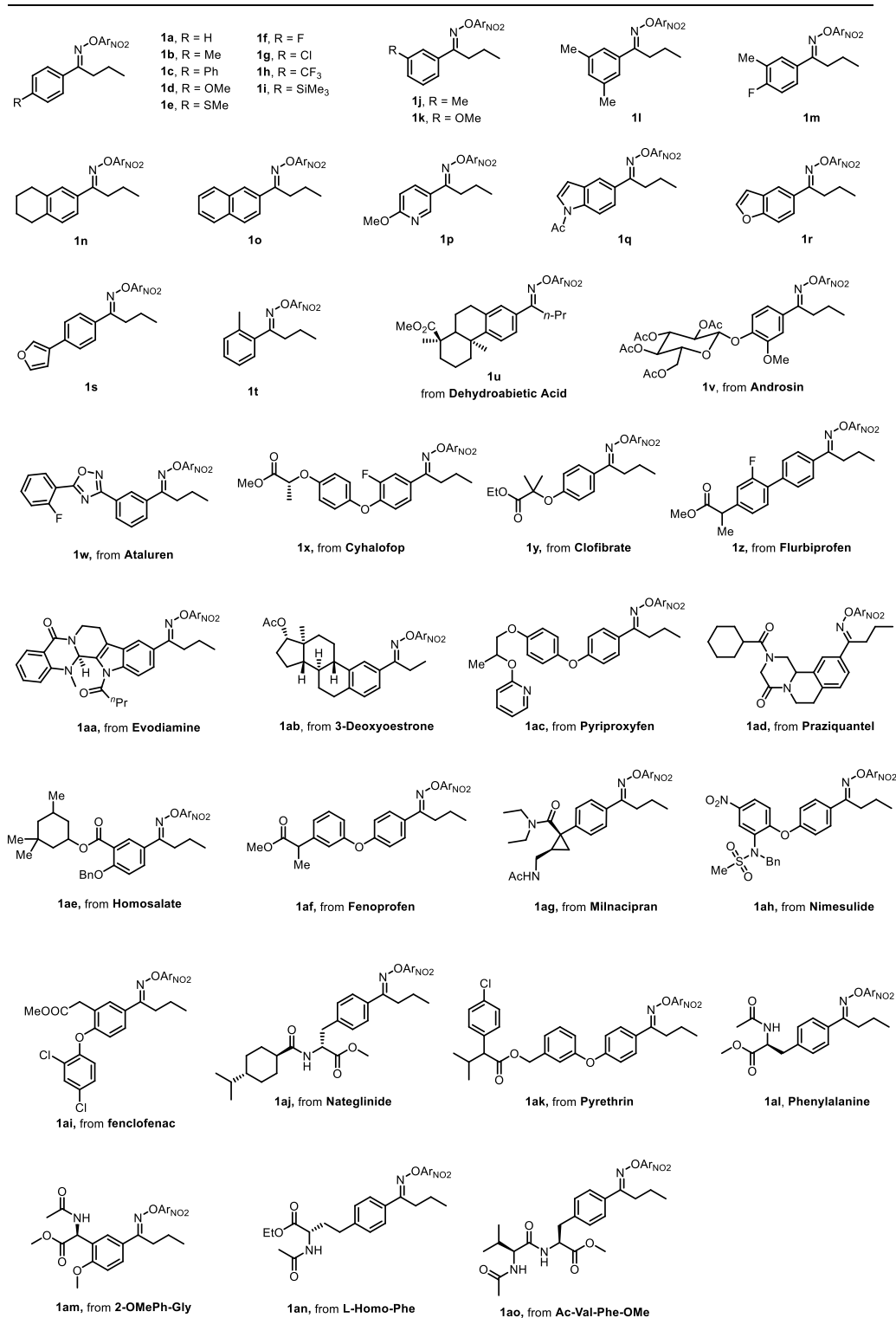
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1. General Information

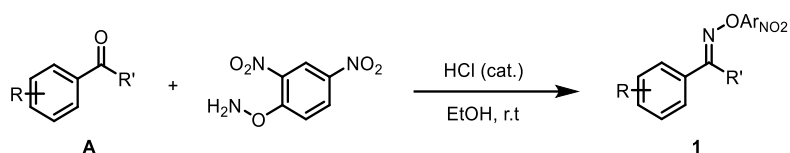
All reagents were purchased from TCI, J&K, STREM, Sigma-Aldrich, Adamas-beta, and Energy Chemical of the highest purity grade, and used directly without further purification. ^1H and ^{13}C NMR spectra were recorded on Bruker AVANCE III 400, 500, 600 and 800 instruments. ^{19}F NMR spectra were recorded on Bruker AVANCE III 500 instrument and are reported relative to the CFCl_3 as the internal standard. Chemical shifts are reported in parts per million (ppm, δ scale) downfield from TMS at 0.00 ppm and referenced to the CDCl_3 at 7.26 ppm (for ^1H NMR) or 77.0 ppm (for ^{13}C NMR). The following abbreviations were used to explain multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, p = quintet, h = sextet, m = multiplet, dd = double of doublets, td = triple doublet, dt = double triplet, tt = triple triplet, ddd = double double doublet, ddt = double double triplet. EI-double focus magnetic-sector high resolution MS(EI-DFS-HRMS) was recorded on a DFS-Thermofischer instrument employing an ultra-high precision toroidal electrostatic analyzer (ESA) and a carefully refined magnetic analyzer at the Center for Mass Spectrometry, Shanghai Institute of Material Medica. ESI with TOF analyzer was carried out at the Center for Mass Spectrometry, Shanghai Institute of Material Medica. Solvents were purified prior to use according to conventional procedures. Column chromatography was performed on silica gel (200–300 mesh) using a mixture of petroleum ether-ethyl acetate as the eluent. Solvents were purified prior to use according to conventional procedures. The aryl ketones were commercially available or readily prepared according to the known method¹⁻⁶.

2. Experimental Procedures

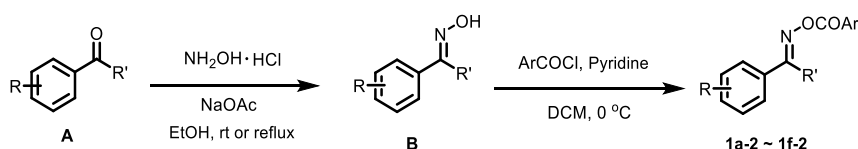
Scheme S1. Ketoxime ethers/esters used in this work



2.1 Preparation of Ketoxime Ethers and Ketoxime Esters³



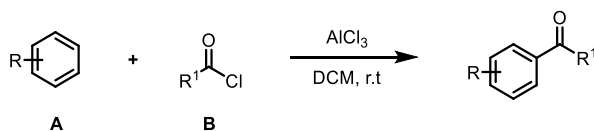
To a mixture of ketone **A** (2.0 mmol), *O*-(2,4-dinitrophenyl)hydroxylamine (2.0 mmol), and EtOH (20 mL) was added conc. HCl (3 drops), and the mixture was stirred at r.t. for overnight. The reaction mixture was filtered and washed with EtOH and hexane to give oxime ethers **1** without further purification or purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate).



A mixture of hydroxylamine hydrochloride (4 mmol), NaOAc (8 mmol), and aryl ketone **A** (2 mmol) in EtOH (10 mL) was stirred at r.t. for overnight or at 90 °C for 2 h. After the reaction completion, the solvent was removed under reduced pressure. The resulting mixture was extracted with EtOAc. The organic layer was then washed with brine and dried over Na₂SO₄. The solvent was removed under vacuum to give oxime **B** without further purification.

To a solution of oxime **B** (2 mmol), pyridine (2.8 mmol) in CH₂Cl₂ (10 mL) was slowly added 4-methylbenzoyl chloride (2.4 mmol) at 0 °C. After completion, aq. HCl (1.0 M) was added, and the organic portion was washed with brine and dried over Na₂SO₄. The solvent was removed under reduced pressure to give the crude product, which was further purified by column chromatography to give desired products.

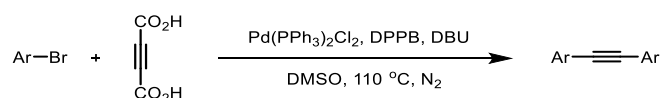
2.2 General Procedure for Acylation of Drug Molecules and Natural Products.



To a solution of the AlCl₃ (5.0 eq, 25.0 mmol) in dry DCM (30.0 mL) was added acyl chloride **B** (25.0 eq, 25.0 mmol). After stirring for 5 minutes, drug molecules and natural products **A** (1.0 eq, 5.0 mmol) was added in one portion. The reaction was monitored by TLC. After completion, the reaction was diluent quenched with HCl. The resulting mixture was washed with diluent HCl (30 mL × 2). The organic layers were washed with brine, dried over Na₂SO₄, filtered and evaporated to give the crude product. Subsequent purification by flash column chromatography afforded the acylation product.

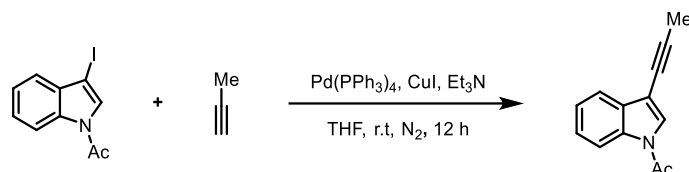
2.3 Preparation of Alkynes **2**

2a and **2m-2p** were commercially available, **2b-2l** were known products and were prepared by the following method.^[7]



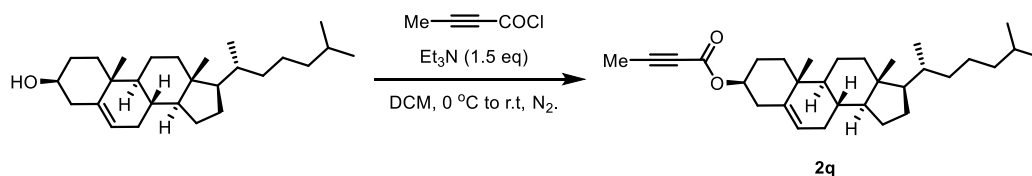
$\text{Pd(PPh}_3)_2\text{Cl}_2$ (0.5 mmol, 350 mg), 1,4-bis(diphenylphosphino)butane (DPPB, 1.0 mmol, 0.43 g), aryl bromide (20.0 mmol), 2-butyne-1-carboxylic acid (10.5 mmol, 1.20 g), and DBU (21.0 mmol, 3.20 g) were successively added into DMSO (30.0 mL) in a flame-dried round bottom flask. The mixture was stirred at 110 °C in a preheated oil bath for 3 h under N_2 , and cooled down to room temperature. The reaction mixture was diluted with EtOAc, and washed with saturated NH_4Cl solution for several times. The organic layer was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate) to afford pure alkynes.

2q was prepared by the following method.



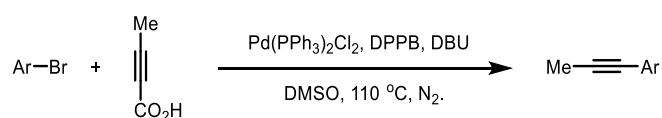
To a mixture of 3-iodo-1-acetylinole (5.0 mmol, 1.42 g), $\text{Pd(PPh}_3)_4$ (0.2 mmol, 231 mg), CuI (0.2 mmol, 38 mg) and THF (10 mL) under N_2 atmosphere, then triethylamine (7.5 mmol, 1.0 mL) was added and stirred for 15 min. Then, propyne (ca. 1 mol/L in THF, 7.5 mmol, 7.5 mL) was added to the reaction mixture via a syringe and stirred at room temperature for 12 h. After completion of the reaction as indicated by TLC, the reaction mixture was diluted with EtOAc, and washed with saturated NH_4Cl solution for several times. The organic layer was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 10:1) to afford **2q** (0.73 g, 74% yield) as a yellowish solid.

2s was prepared according to literature method.



To a solution of Cholesterol (2 mmol, 0.77 g) in 15 mL dichloromethane was added Et_3N (3 mmol, 0.42 mL). The reaction mixture was cooled down to 0 °C and then 2-butyne-1-carboxylic acid (2.5 mmol, 0.22 mL) was added dropwise. After addition, the mixture was warmed to room temperature and stirred for 2 h. Then the mixture was diluted with DCM, and washed with saturated NaHCO_3 solution (30 mL), water (30 mL) and brine (30 mL). The organic layer was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 40:1) to afford **2r** as a white solid (0.78 g, 86%).

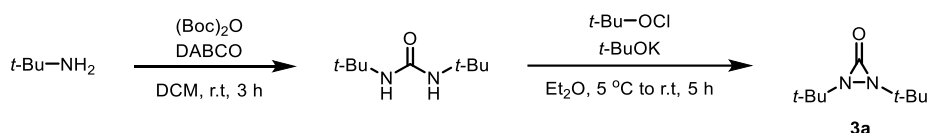
2r, **2t** were prepared by the following method^[8]



$\text{Pd(PPh}_3)_2\text{Cl}_2$ (0.2 mmol, 140 mg), 1,4-bis(diphenylphosphino)butane (DPPB, 0.2 mmol, 86 mg),

aryl bromide (5.0 mmol), 2-butyric acid (7.5 mmol, 0.63 g), and DBU (12.5 mmol, 1.9 g) were successively added into DMSO (12 mL) in a 50 mL sealed tube. The mixture was stirred at 110 °C in a preheated oil bath for 6 h under N₂, and cooled down to room temperature. The reaction mixture was diluted with EtOAc, and washed with saturated NH₄Cl solution for several times. The organic layer was dried over anhydrous Na₂SO₄ and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate) to afford pure alkynes.

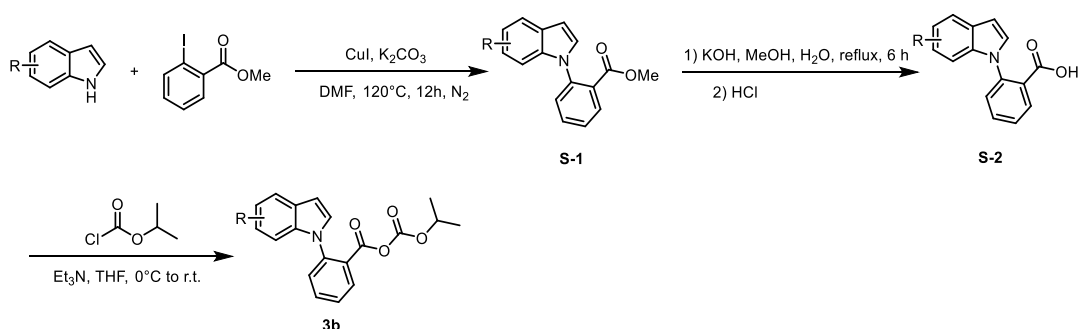
2.4 Preparation of Diaziridinone **3a**^[9,10]



To a solution of *tert*-butylamine (14.6 g, 0.2 mol, 1.0 equiv.) in 300 mL CH₂Cl₂ was added successively DABCO (2.24 g, 20 mmol, 0.1 equiv.) and a solution of (Boc)₂O (23 mL, 0.1 mol, 0.5 equiv.). The mixture was stirred at room temperature for 3 h and then cooled down to 0 °C, 200 mL *n*-hexane was added, the resulting solid was collected and further washed with cold water and diethyl ether to afford 1,3-di-*t*-butylurea (14.6 g, 85% yield).

t-Butyl hypochlorite (6.2 mL, 55 mmol) was added dropwise by syringe to a viscous suspension of 1,3-di-*t*-butylurea (8.6.0 g, 50 mmol) in dry ether (100 mL) with stirring at room temperature. To the resulting clear pale yellow-green solution was cooled to 5 °C and then added potassium *t*-butoxide (7.3.1 g, 65 mmol) in small portions. The resulting mixture was stirred at room temperature for 5 h under strictly exclusion of light, diluted with pentane (100 mL), washed with water (100 mL × 3) and brine (100 mL), dried over Na₂SO₄, filtered, concentrated, and distilled under reduced pressure (56 °C/ 4 mmHg) to give di-*t*-butyldiaziridinone **3a** as a colorless liquid (6.1 g, 72% yield).

2.5 General Procedure for the Preparation of Anhydride **3b** and **3c**

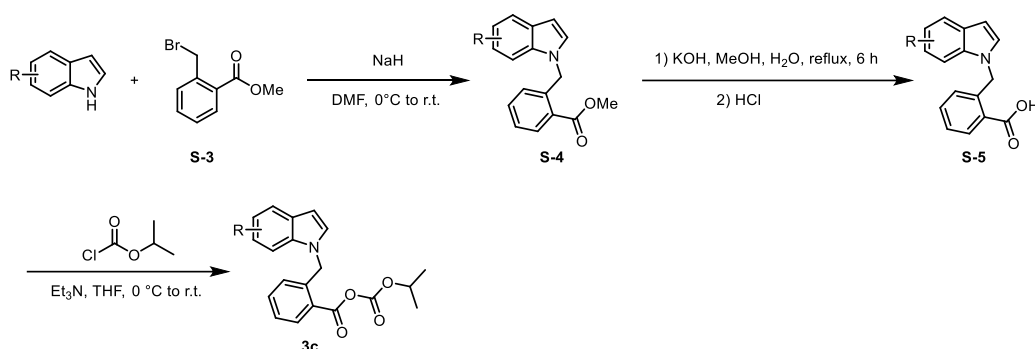


An oven-dried vial was charged with 1H-indole (10 mmol), methyl 2-iodobenzoate (2.62 g, 1.0 eq, 10 mmol), CuI (190.5 mg, 0.1 eq, 1 mmol), K₂CO₃ (2.8 g, 2.0 eq, 20 mmol), and DMF (20 mL) under N₂ atmosphere. The mixture was heated to 120 °C in oil bath for 24 h. After cooling to room temperature, the reaction mixture was filtered through celite. The filtrate was extracted with EtOAc, washed with water, brine, and dried over Na₂SO₄. The solution was concentrated under reduced pressure, and purified by column chromatography over silica gel to give the desired 2-indolyl ester **S-1**.

In a round-bottom flask, 20% KOH aqueous solution (20 mL) was added to 2-indolyl ester **S-1** (10

mmol) in MeOH (50 mL) and heated under reflux for 4 h. The solvents were removed under vacuum and residue was dissolved in water (50 mL) and extracted with EtOAc. The aqueous layer was acidified with 2N HCl and extracted with EtOAc (40 mL×2). The combined extracts were dried over anhydrous Na₂SO₄ and concentrated in vacuo. The residue was purified by column chromatography on silica gel to give the carboxylic acid **S-2** as white solid.

In a round-bottom flask, carboxylic acid **S-2** (10 mmol) and trimethylamine (1.01 g, 1.0 eq, 10 mmol) were dissolved in 50 mL anhydrous THF. The mixture was stirred for 10 min at room temperature. In another round-bottom flask, isopropyl chloroformate (1.47 g, 1.2 eq, 12 mmol) was diluted with 50 mL anhydrous THF. The mixture of carboxylic acid and triethylamine was added dropwise to the isopropyl chloroformate solution at 0°C. Then the reaction mixture was stirred at room temperature for additional 1 hour. When TLC shows full conversion, 10% citric acid aqueous solution (30 mL) was added to the reaction mixture until the system became clear. After extraction with ethyl ether (40 mL×2), the organic layer was washed with saturated sodium bicarbonate solution (40 mL) and brine (40 mL), dried over Na₂SO₄. The solvent was evaporated under vacuum, isopropyl carbonate anhydride **3b** was obtained as a light yellow to brown oil.



1H-indole (10 mmol) in THF (20 mL) was added dropwise to a stirred suspension of sodium hydride (0.86 g, 1.0 eq, 10 mmol, 60% suspension in mineral oil) in THF (70 mL) at 0 °C. The mixture was then stirred at room temperature for 1 h. Then the mixture was added to a stirred suspension of **S-3** (1.0 eq, 10 mmol, 2.29 g). The mixture was then stirred at room temperature for 3 h. Then the reaction mixture was extracted with EtOAc, washed with water, brine, and dried over Na₂SO₄. The solution was concentrated under reduced pressure, and purified by column chromatography over silica gel to give **S-4**.

In a round-bottom flask, 20% KOH aqueous solution (20 mL) was added to 2-indolyl ester **S-4** (10 mmol) in MeOH (50 mL) and heated under reflux for 4 h. The solvents were removed under vacuo and residue was dissolved in water (50 mL) and extracted with EtOAc. The aqueous layer was acidified with 2N HCl and extracted with EtOAc (40 mL×2). The combined extracts were dried over anhydrous Na₂SO₄ and concentrated in vacuo. The crude product was purified by column chromatography over silica gel to give **S-5**.

In a round-bottom flask, carboxylic acid **S-5** (10 mmol) and NEt₃ (1.01 g, 1.0 eq, 10 mmol) were dissolved in 50 mL anhydrous THF. The mixture was stirred for 10 min at room temperature. In another round-bottom flask, isopropyl chloroformate (1.47 g, 1.2 eq, 12 mmol) was diluted with 50

mL anhydrous THF. At 0 °C, the mixture of carboxylic acid and triethylamine was added dropwise to the isopropyl chloroformate solution. Then the reaction mixture was stirred at room temperature for additional 1 hour. When TLC shows full conversion, 10% citric acid aqueous solution (30 mL) was added to the reaction mixture until the system became clear. The mixture was extracted with ethyl ether (40 mL×2), and the organic layer was washed with saturated sodium bicarbonate solution (40 mL) and brine (40 mL), dried over Na₂SO₄. The solvent were evaporated under vacuum, and the isopropyl carbonate anhydride **3c** was obtained as a light yellow oil. The crude products can be directly used without further purification.

2.6 Reaction Optimization

Table S1. Screening of additive^a

Entry	Additive	Yield (%) ^b
1	w/o	61
2	AgTFA	28
3	AgNTf ₂	9
4	AgOTf	19
5	AgSbF ₆	13
6	NaBAR _F	<5

^a Conditions: **1a** (0.1 mmol), **2a** (0.1 mmol), **3a** (0.1 mmol), PdCl₂ (10 mol%), ligand **N1** (20 mol%), Additive (20 mol%), K₃PO₄ (0.2 mmol), DCE (3.0 mL), N₂, 130 °C, 12 h. ^b GC-MS yield using *n*-Icosane as internal standard.

Table S2. Screening of the palladium catalyst^a

Reaction scheme showing the synthesis of compound **4a** from starting materials **1a**, **2a**, and **3a**. The reaction conditions are: 10 mol% [Pd], 20 mol% **N1**, 2.0 eq K_3PO_4 , DCE, 130 °C, N_2 , 12 h. The structure of **N1** is shown as a ligand.

Entry	[Pd]	Yield (%) ^b	Entry	[Pd]	Yield (%) ^b
1	$Pd(OAc)_2$	13	5	$Pd(PPh_3)_2Cl_2$	61
2	$Pd(TFA)_2$	11	6	$Pd(cod)Cl_2$	14
3	$Pd(acac)_2$	6	7	Pd_2dba_3	9
4	$PdCl_2$	17	8	$Pd(PPh_3)_4$	58

^a Conditions: **1a** (0.1 mmol), **2a** (0.1 mmol), **3a** (0.1 mmol), [Pd] (10 mol%), ligand **N1** (20 mol%), additive (20 mol%), K₃PO₄ (0.2 mmol), DCE (3.0 mL), N₂, 130 °C, 12 h. ^b GC-MS yield using *n*-Icosane as internal standard.

Table S3. Screening of the solvent^a

Entry	Solvent (3 ml)	Yield (%) ^b	Entry	Solvent (3 ml)	Yield (%) ^b
1	DMSO	n.d	7	HFIP	n.d
2	DMF	n.d	8	MeOH	n.d
3	THF	n.d	9	CH ₃ CN	n.d
4	Dioxane	n.d	10	<i>n</i> -PrCN	n.d
5	PhMe	5	11	EtOAc	n.d
6	<i>n</i> -Hexane	n.d	12	DCE	61

^a Conditions: **1a** (0.1 mmol), **2a** (0.1 mmol), **3a** (0.1 mmol), Pd(PPh₃)₂Cl₂ (10 mol%), ligand **N1** (20 mol%), K₃PO₄ (0.2 mmol), **Solvent** (3.0 mL), N₂, 130 °C, 12 h. ^b GC-MS yield using *n*-Icosane as internal standard.

Table S4. Screening of the base^a

Entry	Base (2 equiv)	Yield (%) ^b	Entry	Base (2 equiv)	Yield (%) ^b
1	---	n.d	9	K₃PO₄	61
2	Li ₂ CO ₃	n.d	10	K ₂ HPO ₄	< 5
3	Na ₂ CO ₃	< 5	11	KH ₂ PO ₄	< 5
4	NaHCO ₃	< 5	12	KOPiv	< 5
5	K ₂ CO ₃	58	13	KO ^{<i>t</i>} Bu	n.d
6	KHCO ₃	< 5	14	NaOAc	< 5
7	Rb ₂ CO ₃	38	15	KOAc	< 5
8	Cs ₂ CO ₃	45	16	DIPEA	< 5

^a Conditions: **1a** (0.1 mmol), **2a** (0.1 mmol), **3a** (0.1 mmol), Pd(PPh₃)₂Cl₂ (10 mol%), ligand **N1** (20 mol%), **Base** (0.2 mmol), DCE (3.0 mL), N₂, 130 °C, 12 h. ^b GC-MS yield using *n*-Icosane as internal standard.

Table S5. Screening of the PyrOx ligands^a

no ligand n.d.		R = H, N1, 61% R = 3-CF₃, N2, 8% R = 3-OMe, N3, 60% R = 4-CF₃, N4, 6%	R = 4-OMe, N5, 60% R = 5-OMe, N6, 60% R = 5-CF₃, N7, 6% R = 6-OMe, N8, 4%	
	R = H, N9, 15% R = Me, N10, 34% R = <i>i</i>-Pr, N11, 35%	R = <i>t</i>-Bu, N12, 31% R = Ph, N13, 25% R = Bn, N14, 31%		

^a Conditions: **1a** (0.1 mmol), **2a** (0.1 mmol), **3a** (0.1 mmol), Pd(PPh₃)₂Cl₂ (10 mol%), **ligand N** (20 mol%), K₃PO₄ (0.2 mmol), DCE (3.0 mL), N₂, 130 °C, 12 h. ^b GC-MS yield using *n*-Icosane as internal standard.

Table S6. Screening of the phosphine ligands^a

PPh_3 P1, 65% TFP P2, 33% PCy_3 P3, 38% dppe P4, 49% dppf P5, 48% Xphos P6, 28% Bn_3P P13, 32% dppm P14, 26% dppp P15, 46% dppb P16, 59% dpppe P17, 51% dpph P18, 45%	 P7, 43% P11, 19% P23, 50%	 P8, 18% P12, n.d. P24, 45%	 P9, 52% P19, 68% P25, 35%	 P10, 70% (82%)^c P20, n.d. P26, 56%	

^a Conditions: **1a** (0.1 mmol), **2a** (0.1 mmol), **3a** (0.1 mmol), PdCl_2 (10 mol%), ligand **N1** (20 mol%), **Ligand P** (20 mol%), K_3PO_4 (0.2 mmol), DCE (3.0 mL), N_2 , 130 °C, 12 h. ^b GC-MS yield using *n*-Icosane as internal standard.

Table S7. Screening of the ratios of substrates^a

Entry	1a:2a:3a	Yield (%) ^b	Entry	1a:2a:3a	Yield (%) ^b
1	1 : 1 : 1	70	10	1 : 1 : 1.4	76
2	1 : 1.1 : 1	71	11	1 : 1 : 1.5	74
3	1 : 1.2 : 1	74	12	1 : 1.1 : 1.1	78
4	1 : 1.3 : 1	73	13	1 : 1.2 : 1.2	81
5	1 : 1.4 : 1	74	14	1 : 1.3 : 1.3	81
6	1 : 1.5 : 1	74	15	1 : 1.4 : 1.4	80
7	1 : 1 : 1.1	76	16	1 : 1.5 : 1.5	68
8	1 : 1 : 1.2	78	17	1 : 1.2 : 1.3	80
9	1 : 1 : 1.3	78	18	1 : 1.3 : 1.2	81

^a Conditions: **1a** (0.1 mmol), **2a** (x mmol), **3a** (y mmol), PdCl_2 (10 mol%), ligand **N1** (20 mol%), P(o-tol)_3 (20 mol%), K_3PO_4 (0.2 mmol), DCE (3.0 mL), N_2 , 130 °C, 12 h. ^b GC-MS yield using *n*-Icosane as internal standard.

Table S8. Screening of the loadings of ligands^a

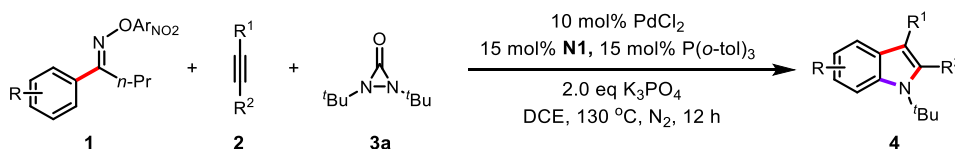
Entry	P(o-tol) ₃ (x mol%)	Ligand N1 (x mol%)	Yield (%) ^b
1	10	10	62
2	10	20	64
3	20	10	64
4	15	15	81 (82)^c
5	20	20	81

^a Conditions: **1a** (0.1 mmol), **2a** (0.12 mmol), **3a** (0.12 mmol), PdCl₂ (10 mol%), ligand **N1** (x mol%), P(o-tol)₃ (y mol%), K₃PO₄ (0.2 mmol), DCE (3.0 mL), N₂, 130 °C, 12 h. ^b GC-MS yield using *n*-Icosane as internal standard.

^c Isolated yield.

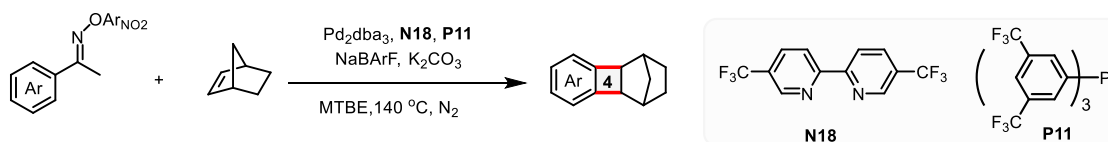
2.7 Experimental Procedures for the Preparation of 4-8 membered ring

2.7.1 Typical Procedure for the Preparation of **4**



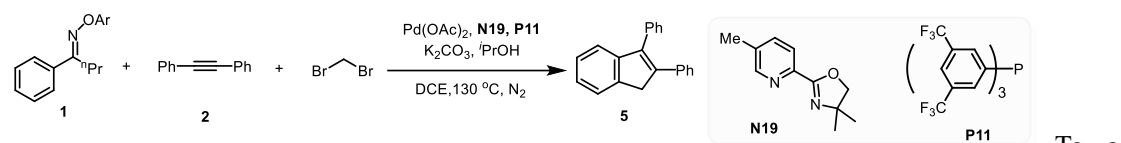
To a 25 mL sealed tube was added oxime ether substrates **1** (0.1 mmol), **2** (0.12 mmol), PdCl₂ (10 mol%, 1.8 mg), K₃PO₄ (2.0 eq, 42.4 mg), **N1** (15 mol%, 2.6 mg), P(o-tol)₃ (15 mol%, 4.5 mg) and DCE (3.0 mL). Then **3a** (0.12 mmol, 25 μ L) was added to the tube via a syringe, and the reaction mixture was stirred in a pre-warmed oil bath maintained at 130 °C for 12 h under N₂ atmosphere. After completion, the mixture was then filtered through Celite. The filtrate was evaporated to give the crude product which was then purified by flash column chromatography on silica gel with a gradient eluent of hexane/ethyl acetate to give the product **4**.

2.7.2 Typical Procedure for the Preparation of **5a-5f**, **6q**, **6ae**



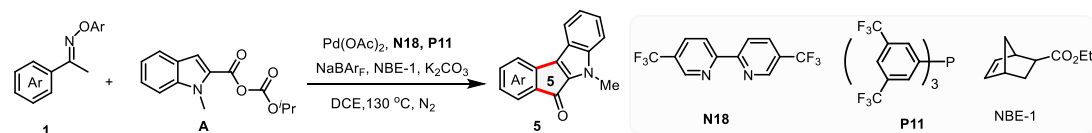
To a 25 mL sealed tube was added oxime ether substrates **1** (0.1 mmol), NBE (18.8 mg, 0.2 mmol), Pd₂dba₃ (4.6 mg, 5 mol%), K₂CO₃ (41.5 mg, 3.0 eq), **N18** (2.9 mg, 10 mol%), **P11** (6.7 mg, 10 mol%), NaBAR_F (8.8 mg, 10 mol%), and MTBE (2.0 mL). Then the reaction mixture was stirred in a pre-warmed oil bath maintained at 140 °C for 12 h under N₂ atmosphere. After completion, the mixture was filtered through Celite. The filtrate was evaporated to give the crude product which was purified by flash column chromatography on silica gel with a gradient eluent of hexane/ethyl acetate to give the product **5a-5f**, **6q**, **6ae**.

2.7.3 Typical Procedure for the Preparation of 5k, 5l, 6r



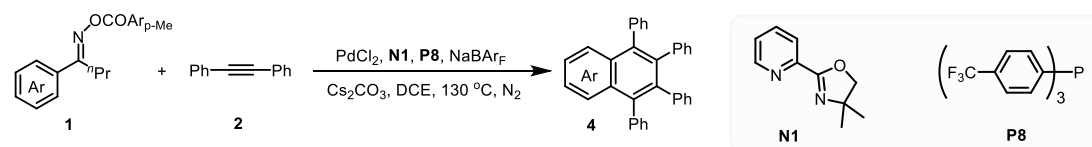
To a 25 mL sealed tube was added oxime ether substrates **1** (0.1 mmol), **2** (0.1 mmol), Pd(OAc)₂ (2.3 mg, 10 mol%), K₂CO₃ (27.6 mg, 2.0 eq), **N19** (2.9 mg, 15 mol%), **P11** (10.1 mg, 15 mol%), and DCE (2 mL). Then CH₂Br₂ (0.5 mmol, 35 μ L) and *i*PrOH (0.1 mmol, 8 μ L) were added to the tube via a syringe, and the reaction mixture was stirred in a pre-warmed oil bath maintained at 130 °C for 12 h under N₂ atmosphere. After completion, the mixture was filtered through Celite. The filtrate was evaporated to give the crude product which was then purified by flash column chromatography on silica gel with a gradient eluent of hexane/ethyl acetate to give the product **5k**, **5l**, **6r**.

2.7.4 Typical Procedure for the Preparation of 5g-5j



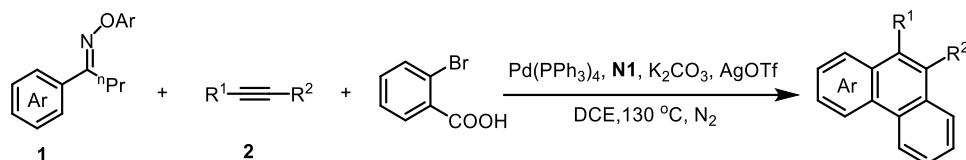
To a 25 mL sealed tube was added oxime ether substrates **1** (0.1 mmol), **A** (0.3 mmol), Pd(OAc)₂ (2.1 mg, 5 mol%), NBE-1 (3.3 mg, 2.0 eq), K₂CO₃ (55.3 mg, 2.0 eq), NaBAR_F (8.9 mg, 10 mol%), **N18** (2.9 mg, 10 mol%), **P11** (6.7 mg, 10 mol%), and DCE (2.0 mL). The reaction mixture was stirred in a pre-warmed oil bath maintained at 130 °C for 12 h under N₂ atmosphere. After completion, the mixture was filtered through Celite. The filtrate was evaporated to give the crude product which was then purified by flash column chromatography on silica gel with a gradient eluent of hexane/ethyl acetate to give the product **5g-5j**.

2.7.5 Typical Procedure for the Preparation of 5m-5p, 6s, 6ag



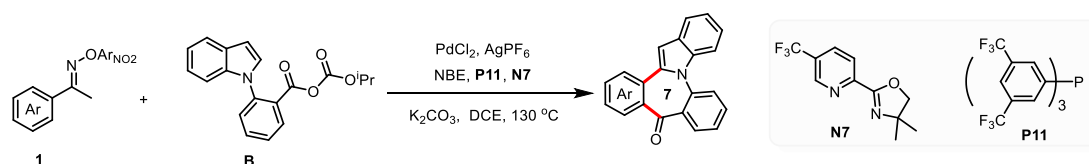
To a 25 mL sealed tube was added oxime ester substrates **1** (0.05 mmol), **2** (0.15 mmol), PdCl₂ (1.3 mg, 15 mol%), Cs₂CO₃ (32.5 mg, 2.0 eq), **N1** (3.5 mg, 20 mol%), **P8** (4.7 mg, 20 mol%), NaBAR_F (8.8 mg, 20 mol%), and DCE (1 mL). Then the reaction mixture was stirred in a pre-warmed oil bath maintained at 130 °C for 12 h under N₂ atmosphere. After completion, the mixture was filtered through Celite. The filtrate was evaporated to give the crude product which was then purified by flash column chromatography on silica gel with a gradient eluent of hexane/ethyl acetate to give the product **5m-5p**, **6s**, **6ag**.

2.7.6 Typical Procedure for the Preparation of 5q-5u, 6t, 6ah



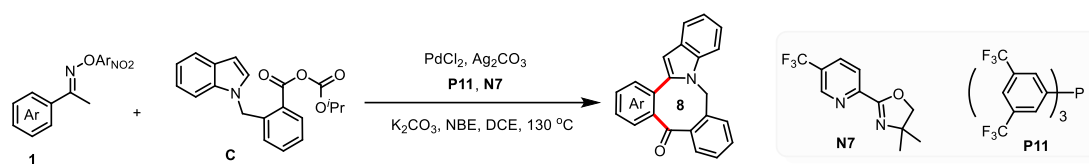
To a 25 mL sealed tube was added oxime ether substrates **1** (0.1 mmol), alkyne **2** (0.12 mmol), 2-bromobenzoic acid (24.1 mg, 0.12 mmol), Pd(PPh₃)₄ (11.6 mg, 10 mol%), K₂CO₃ (41.4 mg, 3.0 eq), **N1** (2.6 mg, 15 mol%), AgOTf (7.7 mg, 30 mol%), and DCE (1.5 mL). Then the reaction mixture was stirred in a pre-warmed oil bath maintained at 130 °C for 12 h under N₂ atmosphere. After completion, the mixture was filtered through Celite. The filtrate was evaporated to give the crude product which was then purified by flash column chromatography on silica gel with a gradient eluent of hexane/ethyl acetate to give the product **5q-5u**, **6t**, **6ah**.

2.7.7 Typical Procedure for the Preparation of **5v-5ab**, **6u**, **6ai**



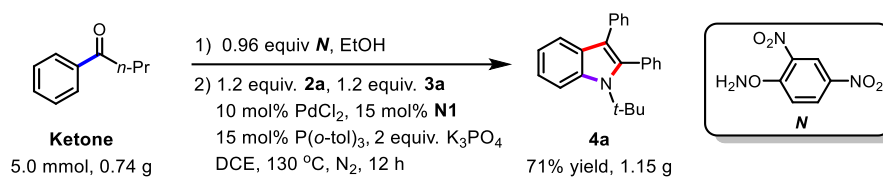
To a 25 mL sealed tube was added oxime ether substrates **1** (0.1 mmol), anhydride **B** (64.6 mg, 0.2 mmol), PdCl₂ (0.9 mg, 5 mol%), K₂CO₃ (41.5 mg, 3.0 eq), NBE (18.8 mg, 2.0 eq), **N7** (2.4 mg, 10 mol%), **P11** (6.7 mg, 10 mol%), AgPF₆ (2.5 mg, 10 mol%), and DCE (2.0 mL). Then the reaction mixture was stirred in a pre-warmed oil bath maintained at 130 °C for 12 h under N₂ atmosphere. After completion, the mixture was filtered through Celite. The filtrate was evaporated to give the crude product which was purified by flash column chromatography on silica gel with a gradient eluent of hexane/ethyl acetate to give the product **5v-5ab**, **6u**, **6ai**.

2.7.8 Typical Procedure for the Preparation of **5ac-5ad**, **6v**, **6aj**



To a 25 mL sealed tube was added oxime ether substrates **1** (0.1 mmol), anhydride **C** (67.4 mg, 0.2 mmol), PdCl₂ (0.9 mg, 5 mol%), K₂CO₃ (41.5 mg, 3.0 eq), NBE (18.8 mg, 2.0 eq), **N1** (2.4 mg, 10 mol%), **P11** (6.7 mg, 10 mol%), Ag₂CO₃ (2.7 mg, 10 mol%), and DCE (2.0 mL). Then the reaction mixture was stirred in a pre-warmed oil bath maintained at 130 °C for 12 h under N₂ atmosphere. After completion, the mixture was filtered through Celite. The filtrate was evaporated to give the crude product which was purified by flash column chromatography on silica gel with a gradient eluent of hexane/ethyl acetate to give the product **5ac-5ad**, **6v**, **6aj**.

2.8. Gram-Scale One-pot Synthesis



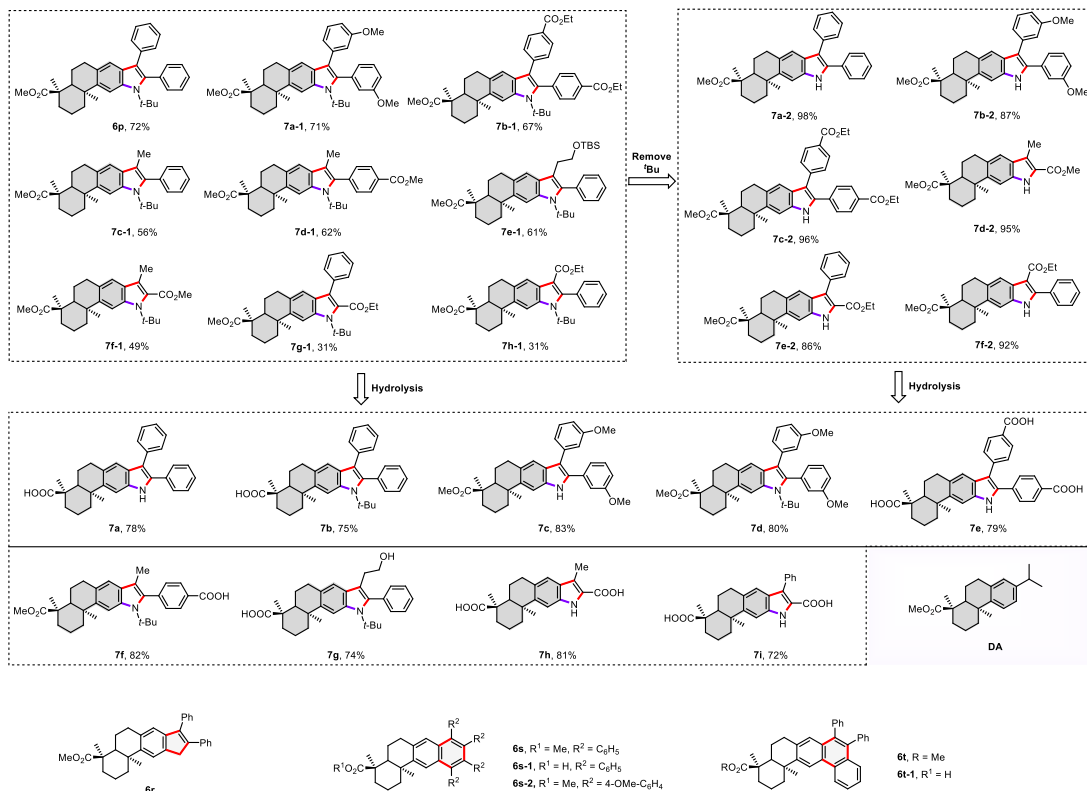
1-phenylbutan-1-one (5.0 mmol, 0.74 g) was added to the solution of *O*-(2,4-dinitrophenyl)hydroxylamine (4.8 mmol, 0.96 g) in EtOH (30.0 mL). Then conc. HCl (5 drops) was added and the solution was stirred for 6 h at room temperature. After completion, solvent was removed to give oxime ether. To a 250 mL sealed tube was added the oxime ether, **2a** (6 mmol, 1.07 g), PdCl₂ (0.5 mmol, 90 mg), K₃PO₄ (10 mmol, 2.12 g), **N1** (0.75 mmol, 132 mg), P(*o*-tol)₃ (0.75 mmol, 228 mg), DCE (100 mL). Then **3a** (6 mmol, 1.25 mL) was added to the tube via a syringe, and the reaction mixture was stirred in a pre-warmed oil bath maintained at 130 °C for 12 h under N₂ atmosphere. After completion, the mixture was filtered through Celite. The filtrate was evaporated to give the crude product which was then purified by flash column chromatography on silica gel with a gradient eluent of hexane/ethyl acetate to give the product **4a** (1.15 g) in 71% yield.

2.9. Screening of Antibacterial Activity of DA-Based Derivatives

2.9.1 Minimum inhibitory concentration (MIC) determination

MIC values for all compounds were measured by broth microdilution, using Mueller-Hinton II broth (cation-adjusted, BD 212322). Generally, *S. pyogenes* was grown to exponential phase in TSB (Tryptone Soya Broth) at 37 °C with shaking at 250 rpm. Then cultures were diluted with MHB to 5*10⁵ CFU/mL and each 100 L dilution was distributed into 96-well microfilter plates (Thermo scientific 167008). All compounds were dissolved in DMSO to 5.12 mg/mL as stock solutions and serially diluted twofold with bacterial culture broth to reach concentrations ranging from 256 to 0.125 mg/mL. The positive control containing diluted cultures plus vancomycin and a negative control containing culture plus DMSO were set up at the same time. 96-well microfilter plates were incubated at 37 °C for 24 h and observed to record the lowest compound concentration to inhibit bacterial growth completely.

2.9.2 Antimicrobial Evaluation of the DA-Based Derivatives

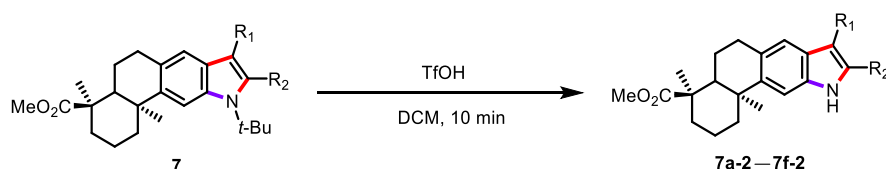


Compounds	MIC ($\mu\text{g/mL}$)				
	PAO1	AB1157	USA300	VB	S.P
6p	>256	>256	>256	>256	>256
7a-1	>256	>256	>256	>256	>256
7b-1	>256	>256	>256	>256	>256
7c-1	>256	>256	>256	>256	>256
7d-1	>256	>256	>256	>256	>256
7e-1	>256	>256	>256	>256	>256
7f-1	>256	>256	>256	>256	>256
7g-1	>256	>256	>256	>256	>256
7h-1	>256	>256	>256	>256	>256
7a-2	>256	>256	>256	>256	>256
7b-2	>256	>256	>256	>256	>256
7c-2	>256	>256	>256	>256	>256
7d-2	>256	>256	>256	>256	>256
7e-2	>256	>256	>256	>256	>256
7f-2	>256	>256	>256	>256	>256
7a	>256	>256	4	1	2
7b	>256	>256	16	2	4
7c	>256	>256	64	2	2
7d	>256	>256	>256	>256	>256
7e	>256	>256	>256	256	256
7f	>256	>256	64	64	32
7g	>256	>256	32	32	16
7h	>256	>256	>256	256	256
7i	>256	>256	>256	256	256
6r	>256	>256	>256	256	4
6s	>256	>256	>256	128	16
6s-1	>256	>256	>256	256	32
6s-2	>256	>256	>256	128	32

6t	>256	>256	>256	256	16
6t-1	>256	>256	>256	256	16
DA	>256	>256	128	128	64
Vancomycin	—	—	1	16	0.25
Polymyxin	4	2	—	—	—

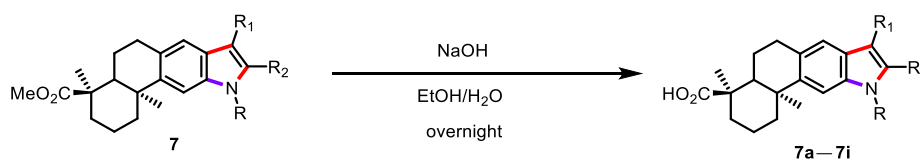
2.9.3 Typical Procedure for the Preparation of DA-Based Derivatives

2.9.3.1 Typical Procedure for the Preparation of 7a-2—7f-2



To a 15 mL sealed tube was added **7** (0.1 mmol), DCM (5 mL), and HOTf (10 drops). Then the mixture was stirred at r.t. for 10 min. Upon completion, the mixture was neutralized by the addition of a saturated sodium bicarbonate and extracted with DCM. The organic layer was dried over anhydrous Na₂SO₄ and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel to afford product **7a-2—7f-2**.

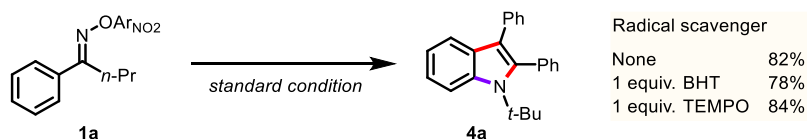
2.9.3.2 Typical Procedure for the Preparation of 7a—7i



To a 15 mL sealed tube was added **8** (0.06 mmol), 2 N NaOH(aq)/EtOH (1:1) (4.0 mL). The reaction mixture was stirred at reflux for 6-18 hours. Upon completion, the mixture was added diluted hydrochloric acid and extracted with EtOAc (10 mL × 3). Then combined organic layers were dried over anhydrous Na₂SO₄, filtered and evaporated. The residue was purified by column chromatography on silica gel to afford product **7a—7i**.

2.10. Mechanistic Studies and Possible Mechanism

2.10.1 Radical Scavenger



To a 25 mL sealed tube was added substrate **1a** (32.9 mg, 0.1 mmol), **2a** (21.0 mg, 0.12 mmol), PdCl₂ (10 mol%, 1.8 mg), K₃PO₄ (2.0 eq, 42.4 mg), **N1** (15 mol%, 2.6 mg), P(*o*-tol)₃ (15 mol%, 4.5 mg), BHT or TEMPO (0.1 mmol), and DCE (3.0 mL). Then **3a** (1.2 eq, 25 μL) was added to the tube via a syringe, and the reaction mixture was stirred in a pre-warmed oil bath maintained at 130 °C for 12 h under N₂ atmosphere. After completion, the mixture was filtered through Celite. The filtrate was evaporated to give the crude product which was then purified by flash column

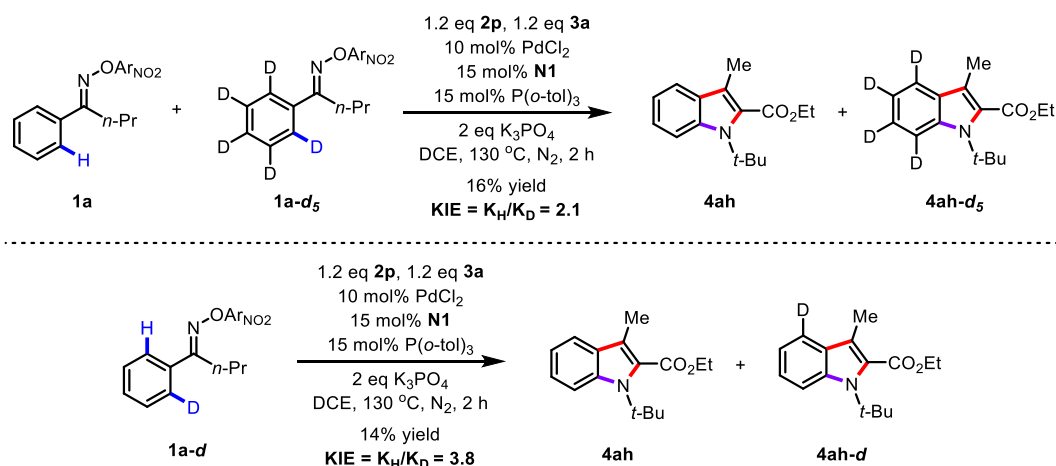
chromatography on silica gel with a gradient eluent of hexane/ethyl acetate to give the product **4a**.

2.10.2 β -C Elimination Pathway



To a 25 mL sealed tube was added **s6** (39.1 mg, 0.1 mmol), **2a** (21.0 mg, 0.12 mmol), PdCl₂ (10 mol%, 1.8 mg), K₃PO₄ (2.0 eq, 42.4 mg), **N1** (15 mol%, 2.6 mg), P(*o*-tol)₃ (15 mol%, 4.5 mg) and DCE (3.0 mL). Then **3a** (1.2 eq, 25 μ L) was added to the tube via a syringe, and the reaction mixture was stirred in a pre-warmed oil bath maintained at 130 °C for 12 h under N₂ atmosphere. After completion, the mixture was filtered through Celite. The filtrate was evaporated to give the crude product which was then purified by flash column chromatography on silica gel with a gradient eluent of hexane/ethyl acetate to give the product **4a** (23.1 mg, 71%) and 3-phenylpropanenitrile (10.7 mg, 82%).

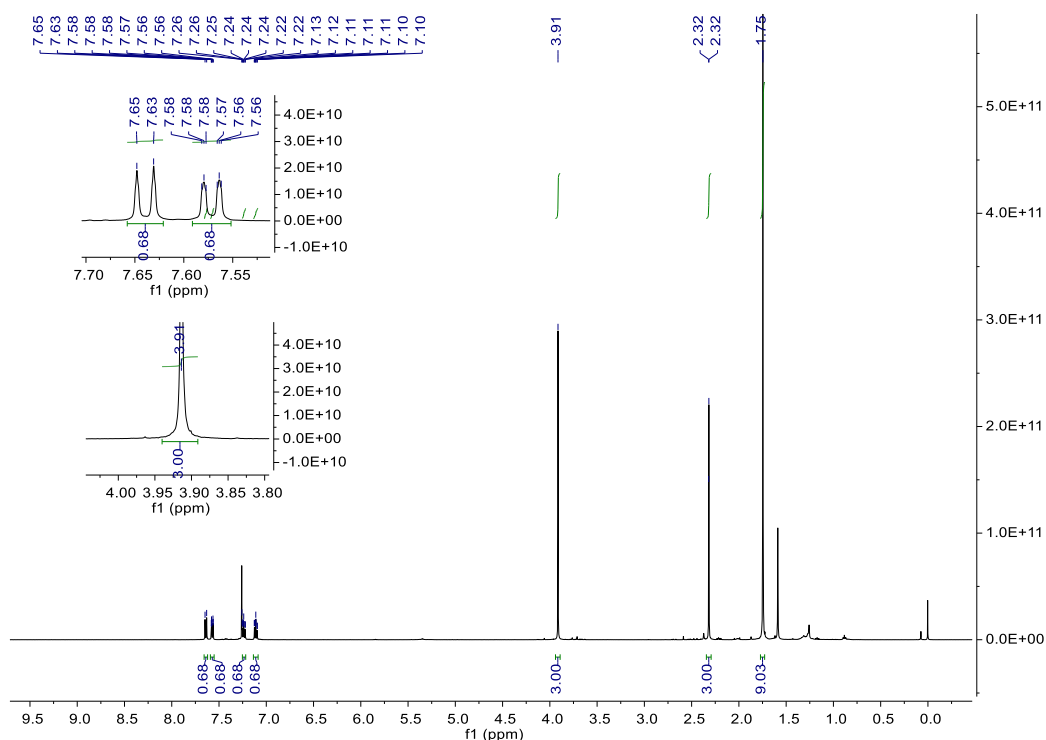
2.10.3 Kinetic Isotope Effect Experiments



A. Intermolecular competition experiment between **1a** and **1a-d₅**:

To a 25 mL sealed tube was added substrates **1a** (16.5 mg, 0.05 mmol), **1a-d₅** (16.7 mg, 0.05 mmol), PdCl₂ (10 mol%, 1.8 mg), K₃PO₄ (2.0 eq, 42.4 mg), **N1** (15 mol%, 2.6 mg), P(*o*-tol)₃ (15 mol%, 4.5 mg), DCE (3.0 mL). Then **2p** (1.2 eq, 10.7 μ L), **3a** (1.2 eq, 25 μ L) was added to the tube via a syringe, and the reaction mixture was stirred in a pre-warmed oil bath maintained at 130 °C for 12 h under N₂ atmosphere. After completion, the mixture was filtered through Celite. The filtrate was evaporated to give a mixture of product **4af** and **4af-d₅** which was purified by flash column chromatography on silica gel with a gradient eluent of hexane and ethyl acetate. The distribution of **4af** and **4af-d₅** was calculated from the integrals of their respective ¹H NMR signals at 3.91 ppm (**4af** and **4af-d₅**) and 7.64 ppm (**4af**) (see Figure S1).

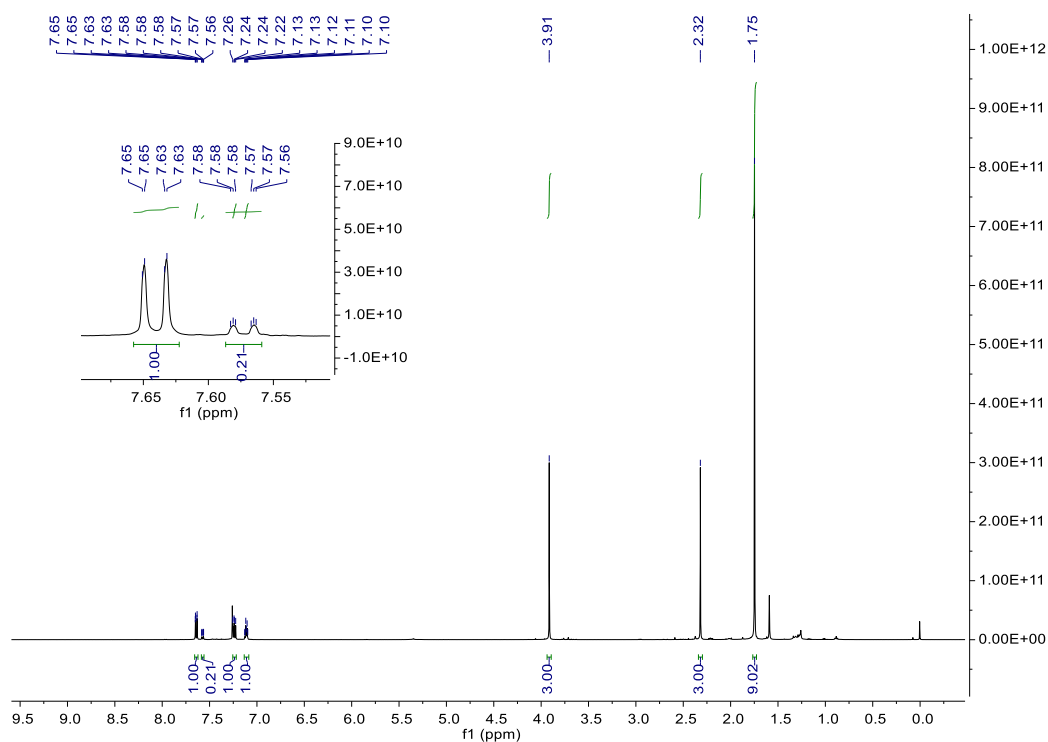
Figure S1. Detail of the ¹H NMR spectrum of the product mixture obtained in the intermolecular KIE experiment



B. Intramolecular competition experiment between **1a** and **1a-d**:

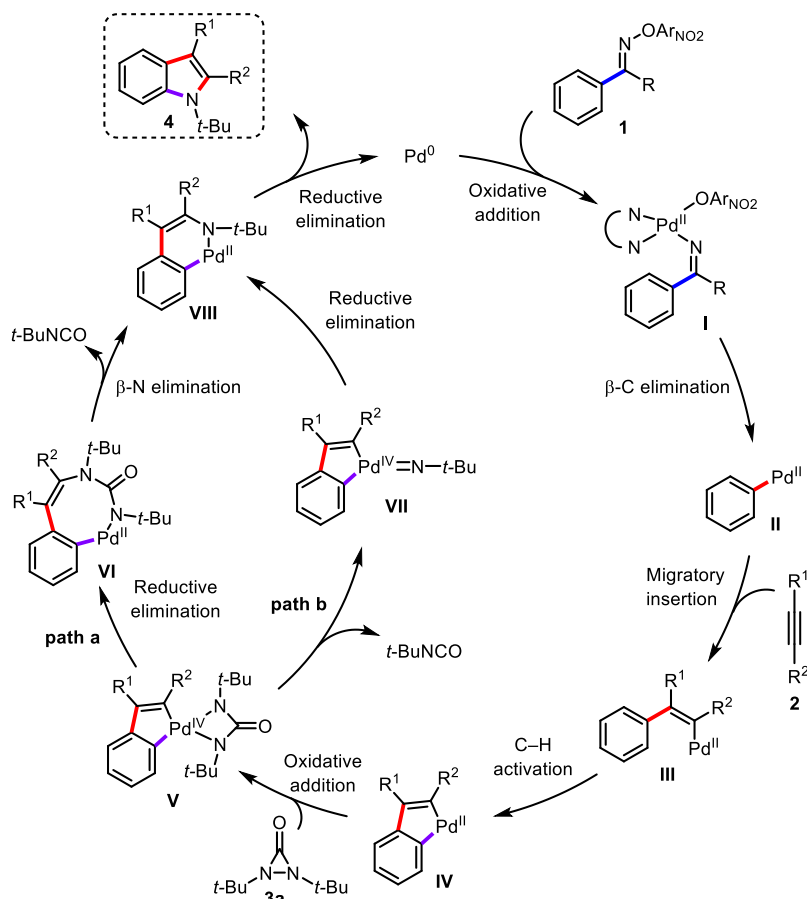
To a 25 mL sealed tube was added substrates **1a-d** (33.0 mg, 0.1 mmol), PdCl₂ (10 mol%, 1.8 mg), K₃PO₄ (2.0 eq, 42.4 mg), **N1** (15 mol%, 2.6 mg), P(*o*-tol)₃ (15 mol%, 4.5 mg), DCE (3.0 mL). Then **2p** (1.2 eq, 10.7 μ L), **3a** (1.2 eq, 25 μ L) was added to the tube via a syringe, and the reaction mixture was stirred in a pre-warmed oil bath maintained at 130 $^{\circ}$ C for 12 h under N₂ atmosphere. After completion, the mixture was filtered through Celite. The filtrate was evaporated to give a mixture of product **4ah** and **4ah-d** which was purified by flash column chromatography on silica gel with a gradient eluent of hexane and ethyl acetate. The distribution of **4ah** and **4ah-d** was calculated from the integrals of their respective ¹H NMR signals at 7.57 ppm (**4ah** and **4ah-d**) and 7.64 ppm (**4ah**) (see Figure S2).

Figure S2. Detail of the ¹H NMR spectrum of the product mixture obtained in the intramolecular KIE experiment



2.10.4 Possible Mechanism of Indole Cyclization Reaction

Initially, the N–O bond of oxime derivatives **1** undergoes oxidative addition to the Pd(0) catalyst to generate the intermediate **I**. Ligand-promoted β -aryl elimination of **I** affords the aryl Pd(II) species **II**. Migratory insertion of **II** into the alkyne **2**, followed by subsequent intramolecular C–H activation to generate C,C-palladacycle **IV**, which is followed by oxidative addition of N–N bond of diaziridinone to C,C-palladacycle **IV**, resulting in Pd(IV) species **V**. Then, two pathways are possible. In path a, reductive elimination of intermediate **V** generates eight-membered Pd(II) species **VI**. Finally, product **4** is formed through β -N elimination and subsequent reductive elimination. In an alternative mechanism (path b), Pd(IV)-nitrene intermediate is formed through the elimination of *tert*-butyl isocyanate. Subsequent two steps of reductive elimination yield the product and regenerate the Pd(0) catalyst.

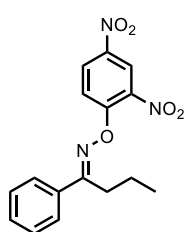


3 Analytical Data

3.1 Characterization of Starting Material

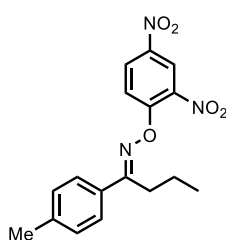
1t, 1w, 1af, 1ap, 1a-1, 1b-1, 1c-1, 1d-1, 1e-1 and 1g-1 are known product and synthesized according to the literature.^{3, 6b}

(E)-1-phenylbutan-1-one O-(2,4-dinitrophenyl) oxime (1a)



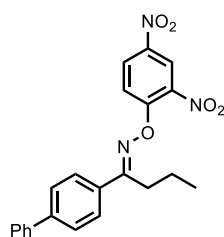
0.54 g, 82% yield; white solid. Mp = 118-120 °C; ¹H NMR (500 MHz, CDCl₃) δ 8.92 (d, *J* = 2.7 Hz, 1H), 8.44 (dd, *J* = 9.4, 2.7 Hz, 1H), 8.07 (d, *J* = 9.4 Hz, 1H), 7.76 (dd, *J* = 8.2, 1.4 Hz, 2H), 7.54–7.45 (m, 3H), 3.06–3.01 (m, 2H), 1.71 (h, *J* = 7.4 Hz, 2H), 1.06 (t, *J* = 7.4 Hz, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 167.4, 157.5, 140.7, 136.0, 133.4, 131.0, 129.4, 128.9, 127.1, 122.1, 117.3, 30.5, 20.4, 14.1; HRMS-EI calcd for C₁₆H₁₅N₃O₅ [M]⁺ 329.1006, found 329.1022.

(E)-1-(p-tolyl)butan-1-one O-(2,4-dinitrophenyl) oxime (1b)



0.58 g, 84% yield; white solid. Mp = 133-135 °C; ¹H NMR (500 MHz, CDCl₃) δ 8.92 (d, *J* = 2.8 Hz, 1H), 8.44 (dd, *J* = 9.4, 2.8 Hz, 1H), 8.07 (d, *J* = 9.4 Hz, 1H), 7.65 (d, *J* = 8.2 Hz, 2H), 7.27 (d, *J* = 8.1 Hz, 2H), 3.04–2.97 (m, 2H), 2.42 (s, 3H), 1.70 (h, *J* = 7.4 Hz, 2H), 1.04 (t, *J* = 7.4 Hz, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 167.2, 157.6, 141.5, 140.6, 135.9, 130.4, 129.6, 129.4, 127.0, 122.1, 117.3, 30.4, 21.4, 20.5, 14.1; HRMS-EI calcd for C₁₇H₁₇N₃O₅ [M]⁺ 343.1163, found 343.1159.

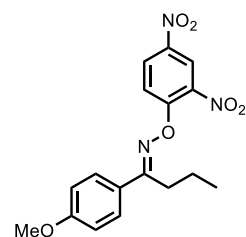
(*E*)-1-([1,1'-biphenyl]-4-yl)butan-1-one *O*-(2,4-dinitrophenyl) oxime (1c)



found 405.1322.

0.70 g, 87% yield; white solid. Mp = 142–144 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.91 (d, J = 2.7 Hz, 1H), 8.45 (dd, J = 9.3, 2.7 Hz, 1H), 8.09 (d, J = 9.4 Hz, 1H), 7.88–7.83 (m, 2H), 7.73–7.68 (m, 2H), 7.66–7.63 (m, 2H), 7.49 (t, J = 7.6 Hz, 2H), 7.44–7.39 (m, 1H), 3.10–3.03 (m, 2H), 1.76 (h, J = 7.4 Hz, 2H), 1.10 (t, J = 7.3 Hz, 3H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 166.9, 157.5, 143.7, 140.6, 139.8, 135.9, 131.9, 129.4, 128.9, 128.0, 127.5, 127.4, 127.0, 122.1, 117.2, 30.3, 20.5, 14.1; **HRMS-EI** calcd for $\text{C}_{22}\text{H}_{19}\text{N}_3\text{O}_5$ $[\text{M}]^+$ 405.1319,

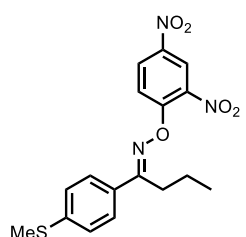
(*E*)-1-(4-methoxyphenyl)butan-1-one *O*-(2,4-dinitrophenyl) oxime (1d)



$\text{C}_{17}\text{H}_{17}\text{N}_3\text{O}_6$ $[\text{M}]^+$ 359.1112, found 359.1113.

0.58 g, 79% yield; white solid. Mp = 107–109 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.90 (d, J = 2.7 Hz, 1H), 8.43 (dd, J = 9.4, 2.7 Hz, 1H), 8.06 (d, J = 9.4 Hz, 1H), 7.75–7.70 (m, 2H), 7.00–6.95 (m, 2H), 3.87 (s, 3H), 3.02–2.96 (m, 2H), 1.69 (h, J = 7.4 Hz, 2H), 1.04 (t, J = 7.4 Hz, 3H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 166.6, 161.8, 157.7, 140.5, 135.9, 129.4, 128.6, 125.3, 122.1, 117.2, 114.2, 55.4, 30.2, 20.5, 14.1; **HRMS-EI** calcd for

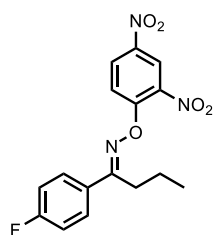
(*E*)-1-(4-(methylthio)phenyl)butan-1-one *O*-(2,4-dinitrophenyl) oxime (1e)



calcd for $\text{C}_{17}\text{H}_{17}\text{N}_3\text{O}_5\text{S}$ $[\text{M}]^+$ 375.0883, found 375.0875.

0.57 g, 76% yield; yellowish solid. Mp = 118–120 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.91 (d, J = 2.8 Hz, 1H), 8.44 (dd, J = 9.4, 2.8 Hz, 1H), 8.06 (d, J = 9.4 Hz, 1H), 7.68 (d, J = 8.5 Hz, 2H), 7.29 (d, J = 8.5 Hz, 2H), 2.99 (t, J = 7.8 Hz, 2H), 2.53 (s, 3H), 1.69 (h, J = 7.4 Hz, 2H), 1.04 (t, J = 7.3 Hz, 3H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 166.7, 157.5, 143.0, 140.6, 135.9, 129.4, 129.3, 127.3, 125.8, 122.1, 117.2, 30.2, 20.5, 15.0, 14.1; **HRMS-EI**

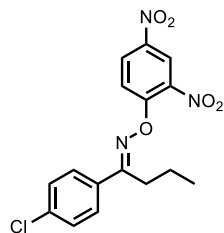
(*E*)-1-(4-fluorophenyl)butan-1-one *O*-(2,4-dinitrophenyl) oxime (1f)



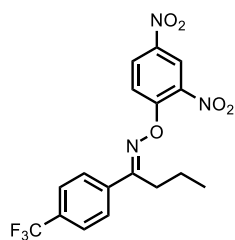
$\text{C}_{16}\text{H}_{14}\text{FN}_3\text{O}_5$ $[\text{M}]^+$ 347.0917, found 347.0939.

0.58 g, 83% yield; white solid. Mp = 100–102 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.91 (d, J = 2.7 Hz, 1H), 8.45 (dd, J = 9.3, 2.7 Hz, 1H), 8.05 (d, J = 9.4 Hz, 1H), 7.80–7.74 (m, 2H), 7.20–7.12 (m, 2H), 3.05–2.96 (m, 2H), 1.70 (h, J = 7.4 Hz, 2H), 1.05 (t, J = 7.4 Hz, 3H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 166.3, 164.4 (d, J = 252.3 Hz), 157.4, 140.8, 136.0, 129.4, 129.2 (d, J = 8.6 Hz), 122.1, 117.2, 116.0 (d, J = 21.9 Hz), 30.4, 20.4, 14.1; **HRMS-EI** calcd for

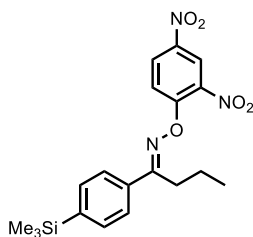
(*E*)-1-(4-chlorophenyl)butan-1-one *O*-(2,4-dinitrophenyl) oxime (1g)



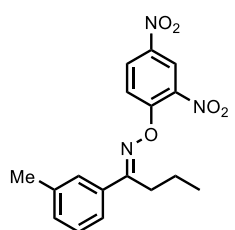
0.59 g, 81% yield; white solid. Mp = 127–129 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.93 (d, J = 2.7 Hz, 1H), 8.45 (dd, J = 9.3, 2.7 Hz, 1H), 8.04 (d, J = 9.3 Hz, 1H), 7.71 (d, J = 8.7 Hz, 2H), 7.45 (d, J = 8.6 Hz, 2H), 3.03–2.98 (m, 2H), 1.70 (h, J = 7.4 Hz, 2H), 1.05 (t, J = 7.4 Hz, 3H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 166.3, 157.3, 140.9, 137.3, 136.1, 131.7, 129.4, 129.2, 128.4, 122.2, 117.2, 30.4, 20.4, 14.1; **HRMS-EI** calcd for $\text{C}_{16}\text{H}_{14}\text{ClN}_3\text{O}_5$ $[\text{M}]^+$ 363.0617, found

(E)-1-(4-(trifluoromethyl)phenyl)butan-1-one O-(2,4-dinitrophenyl) oxime (1h)

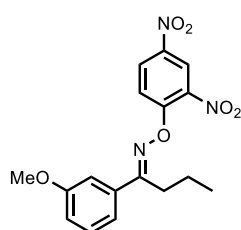
0.67 g, 85% yield; white solid. Mp = 101-103 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.89 (d, J = 2.7 Hz, 1H), 8.45 (dd, J = 9.4, 2.8 Hz, 1H), 8.06 (d, J = 9.4 Hz, 1H), 7.90 (d, J = 8.1 Hz, 2H), 7.73 (d, J = 8.1 Hz, 2H), 3.13–3.06 (m, 2H), 1.72 (h, J = 7.4 Hz, 2H), 1.06 (t, J = 7.4 Hz, 3H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 166.2, 157.1, 141.0, 136.8, 136.0, 132.5 (q, J = 33.1 Hz), 129.4, 127.5, 125.8 (q, J = 4.0 Hz), 123.7 (q, J = 272.3 Hz), 122.0, 117.2, 30.4, 20.2, 14.0; **HRMS-EI** calcd for $\text{C}_{17}\text{H}_{14}\text{F}_3\text{N}_3\text{O}_5$ $[\text{M}]^+$ 397.0880, found 397.0887.

(E)-1-(4-(trimethylsilyl)phenyl)butan-1-one O-(2,4-dinitrophenyl) oxime (1i)

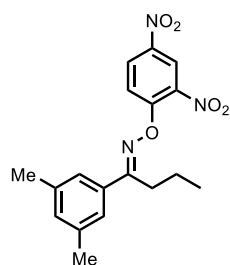
0.61 g, 76% yield; white solid. Mp = 91-93 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.92 (d, J = 2.6 Hz, 1H), 8.44 (dd, J = 9.5, 2.7 Hz, 1H), 8.07 (d, J = 9.2 Hz, 1H), 7.72 (d, J = 7.6 Hz, 2H), 7.63 (d, J = 7.6 Hz, 2H), 3.03 (t, J = 7.8 Hz, 2H), 1.71 (h, J = 7.3 Hz, 2H), 1.05 (t, J = 7.3 Hz, 3H), 0.31 (s, 9H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 167.4, 157.5, 144.4, 140.6, 135.9, 133.8, 133.5, 129.4, 126.2, 122.1, 117.2, 30.4, 20.4, 14.1, -1.3; **HRMS-EI** calcd for $\text{C}_{19}\text{H}_{23}\text{N}_3\text{O}_5\text{Si}$ $[\text{M}]^+$ 401.1402, found 401.1397.

(E)-1-(*m*-tolyl)butan-1-one O-(2,4-dinitrophenyl) oxime (1j)

0.55 g, 80% yield; white solid. Mp = 96-98 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.92 (d, J = 2.8 Hz, 1H), 8.45 (dd, J = 9.4, 2.7 Hz, 1H), 8.08 (d, J = 9.4 Hz, 1H), 7.57–7.51 (m, 2H), 7.38–7.31 (m, 2H), 3.04–2.98 (m, 2H), 2.44 (s, 3H), 1.70 (h, J = 7.4 Hz, 2H), 1.05 (t, J = 7.4 Hz, 3H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 167.6, 157.6, 140.7, 138.7, 136.0, 133.3, 131.8, 129.4, 128.8, 127.7, 124.3, 122.1, 117.3, 30.6, 21.5, 20.4, 14.1; **HRMS-EI** calcd for $\text{C}_{17}\text{H}_{17}\text{N}_3\text{O}_5$ $[\text{M}]^+$ 343.1163, found 343.1171.

(E)-1-(3-methoxyphenyl)butan-1-one O-(2,4-dinitrophenyl) oxime (1k)

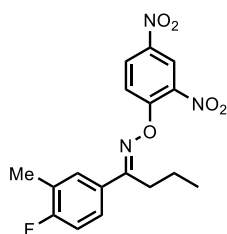
0.59 g, 82% yield; white solid. Mp = 106-108 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.92 (d, J = 2.7 Hz, 1H), 8.44 (dd, J = 9.4, 2.8 Hz, 1H), 8.06 (d, J = 9.4 Hz, 1H), 7.39 (t, J = 8.0 Hz, 1H), 7.32 (d, J = 7.9 Hz, 1H), 7.29–7.27 (m, 1H), 7.05 (dd, J = 8.2, 1.9 Hz, 1H), 3.88 (s, 3H), 3.04–2.98 (m, 2H), 1.70 (h, J = 7.4 Hz, 2H), 1.05 (t, J = 7.4 Hz, 3H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 167.3, 159.8, 157.5, 140.7, 136.0, 134.6, 129.9, 129.4, 122.1, 119.6, 117.3, 116.1, 113.0, 55.4, 30.6, 20.4, 14.2; **HRMS-EI** calcd for $\text{C}_{17}\text{H}_{17}\text{N}_3\text{O}_6$ $[\text{M}]^+$ 359.1112, found 359.1108.

**(E)-1-(3,5-dimethylphenyl)butan-1-one O-(2,4-dinitrophenyl) oxime (1l)**

0.58 g, 81% yield; white solid. Mp = 115-117 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.91 (d, J = 2.7 Hz, 1H), 8.44 (dd, J = 9.4, 2.7 Hz, 1H), 8.08 (d, J = 9.4 Hz, 1H), 7.33 (s, 2H), 7.15 (s, 1H), 3.02–2.97 (m, 2H), 2.40 (s, 6H), 1.69 (h, J = 7.4 Hz, 2H), 1.05 (t, J = 7.3 Hz, 3H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 167.8, 157.6, 140.6, 138.5, 135.9, 133.2, 132.6, 129.4, 124.9,

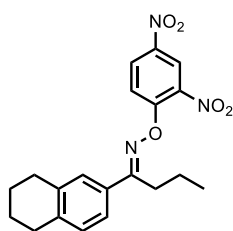
122.1, 117.3, 30.7, 21.3, 20.4, 14.1; **HRMS-EI** calcd for C₁₈H₁₉N₃O₅ [M]⁺ 357.1319, found 357.1327.

(E)-1-(4-fluoro-3-methylphenyl)butan-1-one O-(2,4-dinitrophenyl) oxime (1m)



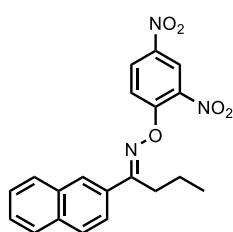
0.56 g, 78% yield; white solid. Mp = 99-101 °C; ¹H NMR (500 MHz, CDCl₃) δ 8.91 (d, *J* = 2.7 Hz, 1H), 8.45 (dd, *J* = 9.4, 2.7 Hz, 1H), 8.05 (d, *J* = 9.4 Hz, 1H), 7.60 (dd, *J* = 7.3, 2.3 Hz, 1H), 7.56 (ddd, *J* = 7.7, 4.8, 2.4 Hz, 1H), 7.09 (t, *J* = 8.8 Hz, 1H), 3.03–2.96 (m, 2H), 2.35 (d, *J* = 2.0 Hz, 3H), 1.69 (h, *J* = 7.5 Hz, 2H), 1.04 (t, *J* = 7.4 Hz, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 166.6, 163.0 (d, *J* = 250.8 Hz), 157.4, 140.7, 135.9, 130.4 (d, *J* = 6.0 Hz), 129.4, 129.0 (d, *J* = 3.8 Hz), 126.5 (d, *J* = 8.6 Hz), 125.7 (d, *J* = 18.0 Hz), 122.1, 117.2, 115.6 (d, *J* = 23.3 Hz), 30.5, 20.4, 14.7 (d, *J* = 3.0 Hz), 14.1; **HRMS-EI** calcd for C₁₇H₁₆FN₃O₅ [M]⁺ 361.1069, found 361.1090.

(E)-1-(5,6,7,8-tetrahydronaphthalen-2-yl)butan-1-one O-(2,4-dinitrophenyl) oxime (1n)



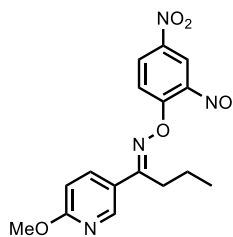
0.68 g, 89% yield; white solid. Mp = 118-120 °C; (Major) ¹H NMR (500 MHz, CDCl₃) δ 8.91 (d, *J* = 2.8 Hz, 1H), 8.44 (dd, *J* = 9.4, 2.8 Hz, 1H), 8.07 (d, *J* = 9.4 Hz, 1H), 7.46 (dd, *J* = 7.9, 2.0 Hz, 1H), 7.44 (s, 1H), 7.15 (d, *J* = 7.9 Hz, 1H), 3.03–2.96 (m, 2H), 2.83 (q, *J* = 7.5 Hz, 4H), 1.84 (p, *J* = 3.2 Hz, 4H), 1.70 (h, *J* = 7.4 Hz, 2H), 1.05 (t, *J* = 7.4 Hz, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 167.5, 157.7, 140.8, 140.5, 137.8, 135.9, 130.3, 129.6, 129.4, 127.8, 124.1, 122.1, 117.3, 30.4, 29.5, 29.4, 22.94, 22.87, 20.5, 14.1; **HRMS-EI** calcd for C₂₀H₂₁N₃O₅ [M]⁺ 383.1476, found 383.1481.

(E)-1-(naphthalen-2-yl)butan-1-one O-(2,4-dinitrophenyl) oxime (1o)



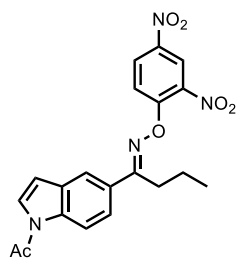
0.63 g, 83% yield; white solid. Mp = 151-153 °C; (Major) ¹H NMR (500 MHz, CDCl₃) δ 8.93 (d, *J* = 2.7 Hz, 1H), 8.46 (dd, *J* = 9.4, 2.7 Hz, 1H), 8.18 (d, *J* = 1.5 Hz, 1H), 8.12 (d, *J* = 9.4 Hz, 1H), 7.97–7.87 (m, 4H), 7.63–7.55 (m, 2H), 3.18–3.12 (m, 2H), 1.78 (h, *J* = 7.4 Hz, 2H), 1.10 (t, *J* = 7.4 Hz, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 167.1, 157.5, 140.7, 136.0, 134.4, 132.9, 130.6, 129.4, 128.8, 128.7, 127.76, 127.75, 127.7, 126.9, 123.6, 122.1, 117.3, 30.3, 20.6, 14.2; **HRMS-EI** calcd for C₂₀H₁₇N₃O₅ [M]⁺ 379.1163, found 379.1160.

(E)-1-(6-methoxypyridin-3-yl)butan-1-one O-(2,4-dinitrophenyl) oxime (1p)



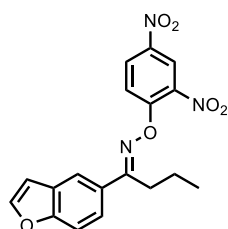
0.57 g, 79% yield; white solid. Mp = 113-115 °C; ¹H NMR (500 MHz, CDCl₃) δ 8.89 (d, *J* = 2.7 Hz, 1H), 8.53 (d, *J* = 2.5 Hz, 1H), 8.43 (dd, *J* = 9.3, 2.7 Hz, 1H), 8.05–7.98 (m, 2H), 6.82 (d, *J* = 8.7 Hz, 1H), 3.98 (s, 3H), 3.01–2.95 (m, 2H), 1.70 (h, *J* = 7.4 Hz, 2H), 1.04 (t, *J* = 7.3 Hz, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 165.7, 164.9, 157.3, 146.3, 140.7, 136.8, 135.9, 129.9, 122.3, 122.1, 117.1, 111.3, 53.8, 29.9, 20.4, 14.1; **HRMS-EI** calcd for C₁₆H₁₆N₄O₆ [M]⁺ 360.1067, found 360.1054.

(E)-1-(5-(1-((2,4-dinitrophenoxy)imino)butyl)-1H-indol-1-yl)ethan-1-one (1q)



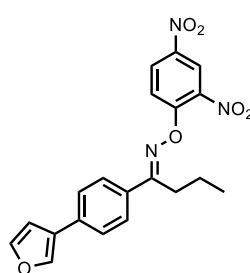
0.68 g, 83% yield; white solid. Mp = 171-173 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.92 (d, J = 2.7 Hz, 1H), 8.52 (d, J = 8.7 Hz, 1H), 8.45 (dd, J = 9.4, 2.7 Hz, 1H), 8.10 (d, J = 9.3 Hz, 1H), 7.95 (d, J = 1.7 Hz, 1H), 7.77 (dd, J = 8.7, 1.7 Hz, 1H), 7.51 (d, J = 3.8 Hz, 1H), 6.73 (d, J = 3.7 Hz, 1H), 3.12–3.06 (m, 2H), 2.68 (s, 3H), 1.73 (h, J = 7.5 Hz, 2H), 1.06 (t, J = 7.3 Hz, 3H); ^{13}C NMR (126 MHz, CDCl_3) δ 168.7, 167.5, 157.6, 140.6, 136.9, 135.9, 130.7, 129.4, 128.7, 126.5, 124.0, 122.1, 120.1, 117.3, 116.9, 109.3, 30.7, 23.9, 20.6, 14.2; HRMS-EI calcd for $\text{C}_{20}\text{H}_{18}\text{N}_4\text{O}_6$ $[\text{M}]^+$ 410.1221, found 410.1218.

(E)-1-(benzofuran-5-yl)butan-1-one O-(2,4-dinitrophenyl) oxime (1r)



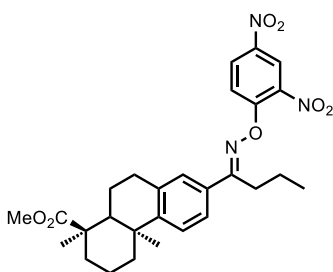
0.62 g, 84% yield; white solid. Mp = 154-156 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.93 (d, J = 2.7 Hz, 1H), 8.45 (dd, J = 9.4, 2.8 Hz, 1H), 8.10 (d, J = 9.3 Hz, 1H), 7.99 (d, J = 1.8 Hz, 1H), 7.74 (dd, J = 8.6, 1.8 Hz, 1H), 7.71 (d, J = 2.2 Hz, 1H), 7.58 (d, J = 8.7 Hz, 1H), 6.86 (dd, J = 2.2, 1.0 Hz, 1H), 3.12–3.06 (m, 2H), 1.74 (h, J = 7.5 Hz, 2H), 1.07 (t, J = 7.4 Hz, 3H); ^{13}C NMR (126 MHz, CDCl_3) δ 167.6, 157.6, 156.3, 146.3, 140.6, 136.0, 129.4, 128.2, 127.9, 123.4, 122.1, 120.6, 117.3, 111.9, 106.9, 30.9, 20.6, 14.2; HRMS-EI calcd for $\text{C}_{18}\text{H}_{15}\text{N}_3\text{O}_6$ $[\text{M}]^+$ 369.0955, found 369.0939.

(E)-1-(4-(furan-3-yl)phenyl)butan-1-one O-(2,4-dinitrophenyl) oxime (1s)



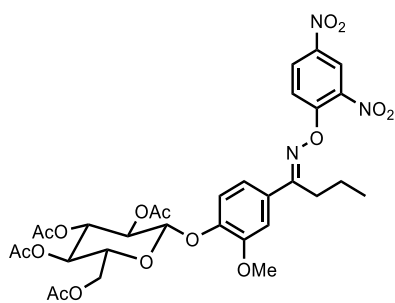
0.64 g, 81% yield; white solid. Mp = 153-155 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.91 (d, J = 2.8 Hz, 1H), 8.45 (dd, J = 9.4, 2.8 Hz, 1H), 8.08 (d, J = 9.4 Hz, 1H), 7.82 (t, J = 1.1 Hz, 1H), 7.77 (d, J = 8.4 Hz, 2H), 7.58 (d, J = 8.3 Hz, 2H), 7.52 (t, J = 1.8 Hz, 1H), 6.75 (dd, J = 1.9, 0.9 Hz, 1H), 3.05–3.00 (m, 2H), 1.72 (h, J = 7.4 Hz, 2H), 1.06 (t, J = 7.4 Hz, 3H); ^{13}C NMR (126 MHz, CDCl_3) δ 166.8, 157.5, 144.1, 140.6, 139.2, 135.9, 135.2, 131.6, 129.4, 127.6, 126.1, 125.5, 122.1, 117.2, 108.6, 30.3, 20.5, 14.1; HRMS-EI calcd for $\text{C}_{20}\text{H}_{17}\text{N}_3\text{O}_6$ $[\text{M}]^+$ 395.1112, found 395.1121.

methyl (1R,4aS)-7-((E)-1-((2,4-dinitrophenoxy)imino)butyl)-1,4a-dimethyl-1,2,3,4,4a,9,10,10a-octahydrophenanthrene-1-carboxylate (1u)



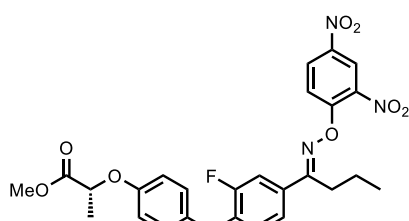
0.84 g, 80% yield; yellowish solid. Mp = 110-112 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.90 (d, J = 2.7 Hz, 1H), 8.43 (dd, J = 9.4, 2.7 Hz, 1H), 8.06 (d, J = 9.4 Hz, 1H), 7.51 (dd, J = 8.3, 2.1 Hz, 1H), 7.40 (d, J = 2.0 Hz, 1H), 7.34 (d, J = 8.3 Hz, 1H), 3.69 (s, 3H), 3.02 – 2.94 (m, 4H), 2.34 (d, J = 12.3 Hz, 1H), 2.24 (dd, J = 12.6, 2.3 Hz, 1H), 1.92 – 1.84 (m, 1H), 1.83 – 1.73 (m, 3H), 1.72 – 1.63 (m, 3H), 1.56 – 1.46 (m, 2H), 1.30 (s, 3H), 1.24 (s, 3H), 1.04 (t, J = 7.4 Hz, 3H); ^{13}C NMR (126 MHz, CDCl_3) δ 178.8, 167.3, 157.6, 152.7, 140.5, 135.9, 135.7, 130.3, 129.4, 127.8, 124.8, 124.5, 122.0, 117.3, 52.0, 47.5, 44.5, 37.7, 37.4, 36.5, 30.4, 29.9, 24.8, 21.4, 20.5, 18.4, 16.5, 14.1; HRMS (ESI-TOF) calcd for $\text{C}_{28}\text{H}_{34}\text{N}_3\text{O}_7$ $[\text{M}+\text{H}]^+$ 524.2391, found 524.2393.

(2R,3R,4S,5R,6S)-2-(acetoxymethyl)-6-(4-((E)-1-((2,4-dinitrophenoxy)imino)butyl)-2-methoxyphenoxy)tetrahydro-2H-pyran-3,4,5-triyl triacetate (1v)



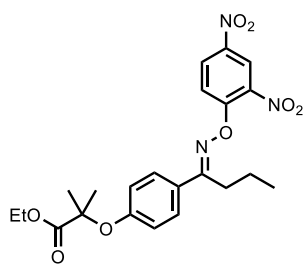
0.96 g, 68% yield; white solid. Mp = 187–189 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.90 (d, J = 2.8 Hz, 1H), 8.44 (dd, J = 9.4, 2.8 Hz, 1H), 8.00 (d, J = 9.4 Hz, 1H), 7.31 (d, J = 2.1 Hz, 1H), 7.26–7.21 (m, 1H), 7.16 (d, J = 8.4 Hz, 1H), 5.34–5.27 (m, 2H), 5.22–5.14 (m, 1H), 5.09–5.01 (m, 1H), 4.28 (dd, J = 12.4, 4.9 Hz, 1H), 4.19 (dd, J = 12.3, 2.6 Hz, 1H), 3.89 (s, 3H), 3.85–3.78 (m, 1H), 2.98 (t, J = 7.7 Hz, 2H), 2.11–2.06 (m, 6H), 2.04 (s, 6H), 1.68 (h, J = 7.5 Hz, 2H), 1.03 (t, J = 7.4 Hz, 3H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 170.5, 170.2, 169.4, 169.3, 166.7, 157.4, 150.7, 148.4, 140.7, 136.1, 129.4, 129.3, 122.1, 120.3, 119.3, 117.2, 111.2, 100.2, 72.4, 72.1, 71.0, 68.2, 61.8, 56.3, 30.4, 20.7, 20.6, 20.59, 20.55, 14.1; **HRMS (ESI-TOF)** calcd for $\text{C}_{31}\text{H}_{35}\text{N}_3\text{NaO}_{16}$ $[\text{M}+\text{Na}]^+$ 728.1910, found 728.1910.

methyl (R,E)-2-(4-(4-(1-((2,4-dinitrophenoxy)imino)butyl)-2-fluorophenoxy)phenoxy)propanoate (1x)



0.82 g, 76% yield; sticky foam; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.85 (d, J = 2.7 Hz, 1H), 8.41 (dd, J = 9.4, 2.7 Hz, 1H), 8.02 (d, J = 9.4 Hz, 1H), 7.61 (dd, J = 11.6, 2.2 Hz, 1H), 7.45–7.41 (m, 1H), 6.99–6.95 (m, 2H), 6.93 (t, J = 8.6 Hz, 1H), 6.89–6.84 (m, 2H), 4.72 (q, J = 6.7 Hz, 1H), 3.76 (s, 3H), 2.99–2.92 (m, 2H), 1.72–1.64 (m, 2H), 1.61 (d, J = 6.8 Hz, 3H), 1.03 (t, J = 7.4 Hz, 3H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 172.3, 165.5, 157.1, 154.2, 153.0 (d, J = 249.1 Hz), 149.7, 147.8 (d, J = 11.3 Hz), 140.7, 135.8, 129.3, 128.3 (d, J = 6.5 Hz), 123.5 (d, J = 3.4 Hz), 121.9, 120.1, 119.1, 117.1, 116.3, 115.4 (d, J = 20.1 Hz), 73.0, 52.2, 30.0, 20.3, 18.4, 14.0; **HRMS (ESI-TOF)** calcd for $\text{C}_{26}\text{H}_{25}\text{FN}_3\text{O}_9$ $[\text{M}+\text{H}]^+$ 542.1569, found 542.1570.

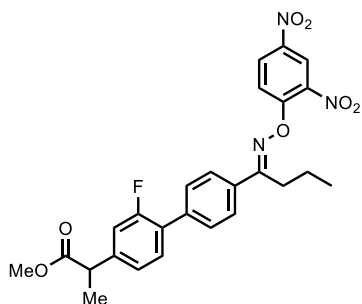
ethyl (E)-2-(4-(1-((2,4-dinitrophenoxy)imino)butyl)phenoxy)-2-methylpropanoate (1y)



0.75 g, 82% yield; yellow solid. Mp = 73–75 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.85 (d, J = 2.8 Hz, 1H), 8.40 (dd, J = 9.4, 2.8 Hz, 1H), 8.03 (d, J = 9.4 Hz, 1H), 7.69–7.63 (m, 2H), 6.88–6.83 (m, 2H), 4.23 (q, J = 7.1 Hz, 2H), 2.97–2.91 (m, 2H), 1.71–1.61 (m, 8H), 1.24 (t, J = 7.1 Hz, 3H), 1.01 (t, J = 7.3 Hz, 3H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 173.6, 166.4, 157.9, 157.5, 140.4, 135.8, 129.3, 128.2, 126.1, 121.9, 118.3, 117.1, 79.2, 61.5, 30.1, 25.2, 20.4, 14.0, 13.9; **HRMS (ESI-TOF)** calcd for $\text{C}_{22}\text{H}_{26}\text{N}_3\text{O}_8$ $[\text{M}+\text{H}]^+$ 460.1714, found 460.1716.

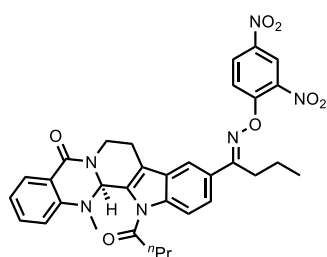
Methyl (E)-2-(4'-(1-((2,4-dinitrophenoxy)imino)butyl)-2-fluoro-[1,1'-biphenyl]-4-yl)propanoate (1z)

0.83 g, 82% yield; white solid. Mp = 89–91 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.91 (d, J = 2.8 Hz,



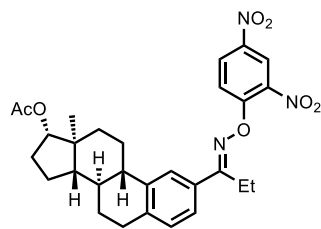
1H), 8.44 (dd, $J = 9.4, 2.8$ Hz, 1H), 8.09 (d, $J = 9.4$ Hz, 1H), 7.84 (d, $J = 8.5$ Hz, 2H), 7.68–7.62 (m, 2H), 7.43 (t, $J = 8.0$ Hz, 1H), 7.22–7.14 (m, 2H), 3.79 (q, $J = 7.2$ Hz, 1H), 3.71 (s, 3H), 3.09–3.01 (m, 2H), 1.80–1.68 (m, 2H), 1.55 (d, $J = 7.2$ Hz, 3H), 1.07 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (126 MHz, CDCl_3) δ 174.2, 166.8, 159.6 (d, $J = 248.9$ Hz), 157.4, 142.6 (d, $J = 7.9$ Hz), 140.7, 138.1, 135.9, 132.3, 130.5 (d, $J = 3.5$ Hz), 129.4, 129.3 (d, $J = 3.0$ Hz), 127.2, 126.5 (d, $J = 13.3$ Hz), 123.7 (d, $J = 3.2$ Hz), 122.1, 117.2, 115.4 (d, $J = 23.7$ Hz), 52.2, 44.8, 30.3, 20.4, 18.3, 14.1; **HRMS-EI** calcd for $\text{C}_{26}\text{H}_{24}\text{FN}_3\text{O}_7$ $[\text{M}]^+$ 509.1593, found 509.1600.

(*S,E*)-13-butyryl-10-(1-((2,4-dinitrophenoxy)imino)butyl)-14-methyl-8,13,13b,14-tetrahydroindolo[2',3':3,4]pyrido[2,1-b]quinazolin-5(7H)-one (1aa)



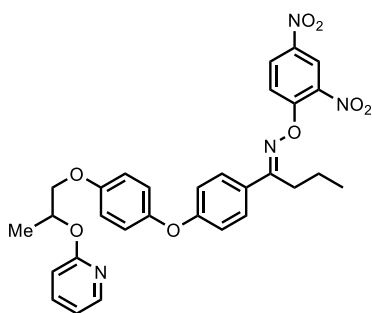
0.76 g, 61% yield; white solid. Mp = 194–196 °C; ^1H NMR (600 MHz, CDCl_3) δ 8.94 (d, $J = 2.9$ Hz, 1H), 8.47 (dd, $J = 9.3, 2.7$ Hz, 1H), 8.29 (d, $J = 8.8$ Hz, 1H), 8.15 – 8.09 (m, 2H), 7.92 (s, 1H), 7.83 (d, $J = 8.8$ Hz, 1H), 7.51 (t, $J = 7.5$ Hz, 1H), 7.26 – 7.22 (m, 1H), 7.13 (d, $J = 8.0$ Hz, 1H), 6.27 (s, 1H), 5.05 – 4.96 (m, 1H), 3.35 – 3.23 (m, 2H), 3.16 – 3.07 (m, 3H), 2.98 – 2.88 (m, 2H), 2.36 (s, 3H), 1.88 (h, $J = 7.2$ Hz, 2H), 1.75 (h, $J = 7.5$ Hz, 2H), 1.08 (t, $J = 7.3$ Hz, 3H), 1.02 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (151 MHz, CDCl_3) δ 173.0, 167.4, 164.3, 157.5, 150.2, 140.7, 138.4, 136.0, 133.4, 129.4, 129.1, 128.6, 127.8, 124.9, 124.4, 123.7, 122.8, 122.3, 122.2, 118.1, 117.3, 116.4, 68.8, 39.7, 37.7, 36.4, 30.7, 20.7, 20.5, 18.3, 14.2, 13.7; **HRMS (ESI-TOF)** calcd for $\text{C}_{33}\text{H}_{33}\text{N}_6\text{O}_7$ $[\text{M}+\text{H}]^+$ 625.2405, found 625.2404.

(*8R,9S,13S,14S,17S*)-2-((*E*)-1-((2,4-dinitrophenoxy)imino)propyl)-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6*H*-cyclopenta[*a*]phenanthren-17-yl acetate (1ab)



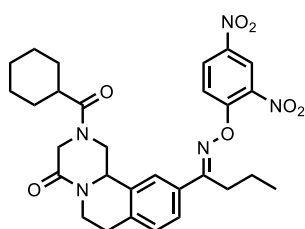
0.78 g, 73% yield; white solid. Mp = 121–123 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.90 (s, 1H), 8.44 (d, $J = 9.5$ Hz, 1H), 8.05 (d, $J = 9.4$ Hz, 1H), 7.66 (s, 1H), 7.48 (d, $J = 8.0$ Hz, 1H), 7.17 (d, $J = 8.0$ Hz, 1H), 4.71 (t, $J = 8.5$ Hz, 1H), 3.10–2.88 (m, 4H), 2.46–2.18 (m, 3H), 2.07 (s, 3H), 1.94 (d, $J = 12.3$ Hz, 2H), 1.82–1.73 (m, 1H), 1.65–1.36 (m, 6H), 1.36–1.22 (m, 4H), 0.86 (s, 3H); ^{13}C NMR (126 MHz, CDCl_3) δ 171.2, 168.7, 157.6, 140.9, 140.5, 140.3, 135.9, 130.2, 129.5, 129.4, 124.3, 124.1, 122.0, 117.3, 82.5, 49.8, 44.1, 42.8, 38.1, 36.7, 29.4, 27.5, 26.9, 25.9, 23.2, 22.3, 21.2, 12.0, 11.4; **HRMS-EI** calcd for $\text{C}_{29}\text{H}_{33}\text{N}_3\text{O}_7$ $[\text{M}]^+$ 535.2313, found 535.2286.

(E)-1-(4-(4-(2-(pyridin-2-yloxy)propoxy)phenoxy)phenyl)butan-1-one O-(2,4-dinitrophenyl) oxime (1ac)



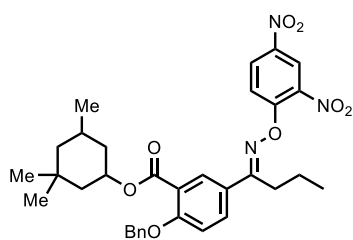
0.83 g, 73% yield; yellow colloid, (Major); $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.92 (d, $J = 2.7$ Hz, 1H), 8.44 (dd, $J = 9.4$, 2.7 Hz, 1H), 8.16 (dd, $J = 5.1$, 2.0 Hz, 1H), 8.05 (d, $J = 9.4$ Hz, 1H), 7.70 (d, $J = 8.8$ Hz, 2H), 7.61–7.55 (m, 1H), 7.03–6.95 (m, 6H), 6.90–6.84 (m, 1H), 6.75 (d, $J = 8.3$ Hz, 1H), 5.59 (dq, $J = 6.4$, 5.2 Hz, 1H), 4.21 (dd, $J = 9.8$, 5.3 Hz, 1H), 4.10 (dd, $J = 9.9$, 4.8 Hz, 1H), 3.04–2.96 (m, 2H), 1.70 (h, $J = 7.4$ Hz, 2H), 1.49 (d, $J = 6.4$ Hz, 3H), 1.04 (t, $J = 7.3$ Hz, 3H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 166.6, 163.1, 161.2, 157.6, 155.9, 148.9, 146.7, 140.6, 138.7, 136.0, 129.4, 128.7, 126.9, 122.1, 121.4, 117.2, 117.1, 116.8, 115.9, 111.7, 71.0, 69.2, 30.3, 20.5, 17.0, 14.1; **HRMS (ESI-TOF)** calcd for $\text{C}_{30}\text{H}_{29}\text{N}_4\text{O}_8$ $[\text{M}+\text{H}]^+$ 573.1980, found 573.1982.

(E)-2-(cyclohexanecarbonyl)-10-(1-((2,4-dinitrophenoxy)imino)butyl)-1,2,3,6,7,11b-hexahydro-4H-pyrazino[2,1-a]isoquinolin-4-one (1ad)



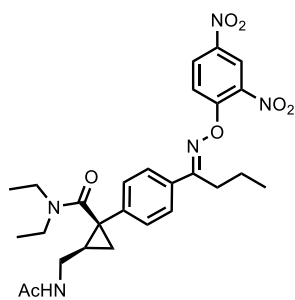
0.89 g, 79% yield; white solid. Mp = 164–166 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.92 (d, $J = 2.8$ Hz, 1H), 8.47 (dd, $J = 9.4$, 2.8 Hz, 1H), 8.07 (d, $J = 9.4$ Hz, 1H), 7.67 (s, 1H), 7.61 (d, $J = 8.0$ Hz, 1H), 7.30 (d, $J = 8.0$ Hz, 1H), 5.20 – 5.11 (m, 1H), 4.91 – 4.81 (m, 2H), 4.48 (d, $J = 17.5$ Hz, 1H), 4.11 (d, $J = 17.4$ Hz, 1H), 3.07 – 2.98 (m, 4H), 2.94 – 2.83 (m, 2H), 2.53 – 2.43 (m, 1H), 1.86 – 1.78 (m, 3H), 1.76 – 1.64 (m, 4H), 1.61 – 1.47 (m, 2H), 1.33 – 1.23 (m, 3H), 1.04 (t, $J = 7.3$ Hz, 3H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 174.8, 166.7, 164.2, 157.2, 140.7, 138.0, 135.9, 133.7, 132.1, 129.9, 129.4, 126.2, 124.0, 122.0, 117.3, 54.8, 48.9, 44.6, 40.7, 38.9, 30.3, 29.1, 29.0, 28.6, 25.6, 20.3, 14.0; **HRMS (ESI-TOF)** calcd for $\text{C}_{29}\text{H}_{34}\text{N}_5\text{O}_7$ $[\text{M}+\text{H}]^+$ 564.2453, found 564.2451.

3,3,5-trimethylcyclohexyl (E)-2-(benzyloxy)-5-(1-((2,4-dinitrophenoxy)imino)butyl)benzoate (1ae)



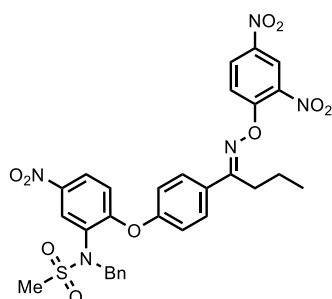
0.87 g, 72% yield; white solid. Mp = 115–117 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.91 (d, $J = 2.7$ Hz, 1H), 8.44 (dd, $J = 9.4$, 2.8 Hz, 1H), 8.16 (d, $J = 2.4$ Hz, 1H), 8.06 (d, $J = 9.4$ Hz, 1H), 7.84 (dd, $J = 8.8$, 2.5 Hz, 1H), 7.51 – 7.48 (m, 2H), 7.43 – 7.38 (m, 2H), 7.37 – 7.33 (m, 1H), 7.09 (d, $J = 8.8$ Hz, 1H), 5.20 (s, 2H), 5.19 – 5.12 (m, 1H), 3.00 (t, $J = 7.8$ Hz, 2H), 2.11 – 2.04 (m, 1H), 1.78 – 1.67 (m, 4H), 1.39 – 1.33 (m, 1H), 1.16 (t, $J = 11.9$ Hz, 1H), 1.05 (t, $J = 7.3$ Hz, 3H), 0.98 (s, 3H), 0.95 (s, 3H), 0.93 – 0.88 (m, 4H), 0.79 (t, $J = 12.7$ Hz, 1H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 166.0, 165.9, 159.7, 157.5, 140.7, 135.9, 131.6, 130.5, 129.4, 128.5, 128.2, 127.4, 125.3, 122.3, 122.1, 117.3, 113.5, 72.4, 70.7, 47.5, 43.9, 40.3, 33.0, 32.3, 30.1, 27.1, 25.5, 22.3, 20.4, 14.1; **HRMS (ESI-TOF)** calcd for $\text{C}_{33}\text{H}_{38}\text{N}_3\text{O}_8$ $[\text{M}+\text{H}]^+$ 604.2653, found 604.2657.

(1S,2R)-2-(acetamidomethyl)-1-(4-((E)-1-((2,4-dinitrophenoxy)imino)butyl)phenyl)-N,N-diethylcyclopropane-1-carboxamide (1ag)



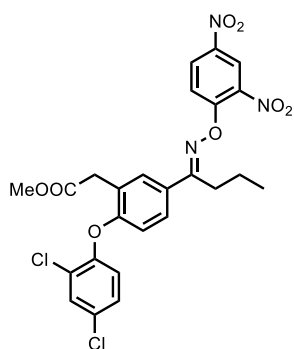
0.83 g, 77% yield; yellow sticky foam; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.91 (d, $J = 2.8$ Hz, 1H), 8.43 (dd, $J = 9.3, 2.8$ Hz, 1H), 8.03 (d, $J = 9.4$ Hz, 1H), 7.69 (d, $J = 8.2$ Hz, 2H), 7.24 (d, $J = 8.3$ Hz, 2H), 7.06 (dd, $J = 8.9, 3.4$ Hz, 1H), 4.22 – 4.14 (m, 1H), 3.56 – 3.42 (m, 2H), 3.39 – 3.24 (m, 2H), 3.03 – 2.95 (m, 2H), 2.58 – 2.51 (m, 1H), 1.97 (s, 3H), 1.68 (h, $J = 7.5$ Hz, 2H), 1.63 – 1.59 (m, 1H), 1.53 (tt, $J = 9.0, 4.3$ Hz, 1H), 1.22 – 1.15 (m, 4H), 1.03 (t, $J = 7.3$ Hz, 3H), 0.94 (t, $J = 7.1$ Hz, 3H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 170.0, 169.9, 166.7, 157.4, 143.8, 140.7, 136.0, 131.5, 129.4, 127.5, 125.7, 122.1, 117.2, 42.0, 41.1, 39.5, 33.7, 30.3, 30.2, 23.5, 20.4, 18.3, 14.1, 13.2, 12.4; **HRMS (ESI-TOF)** calcd for $\text{C}_{27}\text{H}_{34}\text{N}_5\text{O}_7$ $[\text{M}+\text{H}]^+$ 540.2453, found 540.2455.

(E)-N-benzyl-N-(2-(4-(1-((2,4-dinitrophenoxy)imino)butyl)phenoxy)-5-nitrophenyl)methanesulfonamide (1ah)



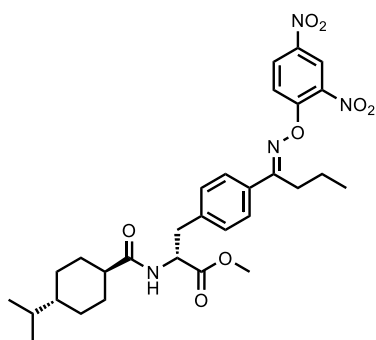
0.95 g, 73% yield; yellow solid. Mp = 65-67 °C; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.92 (d, $J = 2.7$ Hz, 1H), 8.46 (dd, $J = 9.4, 2.8$ Hz, 1H), 8.07 (d, $J = 9.4$ Hz, 1H), 7.90 – 7.83 (m, 3H), 7.68 (d, $J = 2.5$ Hz, 1H), 7.40 (d, $J = 8.7$ Hz, 1H), 7.32 – 7.27 (m, 5H), 7.16 (d, $J = 8.8$ Hz, 2H), 4.91 (s, 2H), 3.09 (s, 3H), 3.08 – 3.02 (m, 2H), 1.75 (h, $J = 7.5$ Hz, 2H), 1.09 (t, $J = 7.3$ Hz, 3H); $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 166.1, 157.3, 156.7, 154.6, 147.8, 140.8, 136.0, 135.1, 135.0, 133.9, 130.6, 129.6, 129.4, 128.7, 128.3, 122.1, 119.8, 118.4, 117.2, 113.0, 54.2, 40.5, 30.4, 20.4, 14.1; **HRMS (ESI-TOF)** calcd for $\text{C}_{30}\text{H}_{28}\text{N}_5\text{O}_{10}\text{S}$ $[\text{M}+\text{H}]^+$ 650.1551, found 650.1550.

methyl (E)-2-(2-(2,4-dichlorophenoxy)-5-(1-((2,4-dinitrophenoxy)imino)butyl)phenyl)acetate (1ai)



0.88 g, 78% yield; white solid. Mp = 113-115 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.90 (d, $J = 2.7$ Hz, 1H), 8.43 (dd, $J = 9.4, 2.7$ Hz, 1H), 8.04 (d, $J = 9.4$ Hz, 1H), 7.75 (d, $J = 2.3$ Hz, 1H), 7.61 (dd, $J = 8.6, 2.3$ Hz, 1H), 7.49 (d, $J = 2.5$ Hz, 1H), 7.25 (dd, $J = 8.7, 2.5$ Hz, 1H), 7.02 (d, $J = 8.7$ Hz, 1H), 6.70 (d, $J = 8.6$ Hz, 1H), 3.84 (s, 2H), 3.70 (s, 3H), 3.03 – 2.94 (m, 2H), 1.70 (h, $J = 7.4$ Hz, 2H), 1.05 (t, $J = 7.3$ Hz, 3H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 171.1, 166.2, 157.4, 157.3, 150.0, 140.6, 135.9, 130.5, 130.3, 129.4, 128.3, 128.2, 127.8, 127.1, 125.1, 122.3, 122.1, 117.2, 116.0, 52.1, 35.7, 30.3, 20.4, 14.1; **HRMS (ESI-TOF)** calcd for $\text{C}_{25}\text{H}_{22}\text{Cl}_2\text{N}_3\text{O}_8$ $[\text{M}+\text{H}]^+$ 562.0778, found 562.0777.

methyl (R)-3-(4-((E)-1-((2,4-dinitrophenoxy)imino)butyl)phenyl)-2-((1r,4R)-4-isopropylcyclohexane-1-carboxamido)propanoate (1aj)

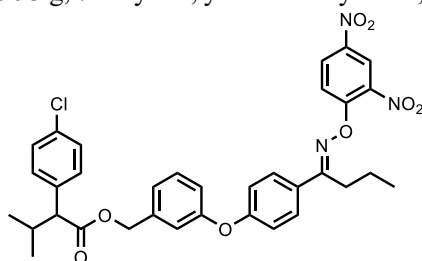


0.88 g, 76% yield; white solid. Mp = 131-133 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.93 (d, J = 2.8 Hz, 1H), 8.45 (dd, J = 9.4, 2.8 Hz, 1H), 8.06 (d, J = 9.4 Hz, 1H), 7.68 (d, J = 7.8 Hz, 2H), 7.19 (d, J = 7.9 Hz, 2H), 5.94 (d, J = 7.6 Hz, 1H), 4.94 (q, J = 6.3 Hz, 1H), 3.77 (s, 3H), 3.26 (dd, J = 13.8, 5.9 Hz, 1H), 3.13 (dd, J = 13.9, 5.6 Hz, 1H), 3.05 – 2.96 (m, 2H), 2.06 – 1.98 (m, 1H), 1.92 – 1.83 (m, 2H), 1.81 – 1.75 (m, 2H), 1.69 (h, J = 7.5 Hz, 2H), 1.46 – 1.35 (m, 3H), 1.09 – 0.94 (m, 6H), 0.85 (d, J = 6.8 Hz, 6H); ^{13}C NMR (126 MHz, CDCl_3) δ 175.6, 172.0, 166.9, 157.4, 140.7, 139.4, 135.9, 132.0, 129.9, 129.4, 127.2, 122.1, 117.2, 52.5, 52.4, 45.4, 43.1, 37.7, 32.7, 30.3, 29.8, 29.4, 28.9, 28.8, 20.4, 19.7, 14.1; HRMS (ESI-TOF) calcd for $\text{C}_{30}\text{H}_{39}\text{N}_4\text{O}_8$ $[\text{M}+\text{H}]^+$ 583.2762, found 583.2763.

(E)-3-(4-(1-((2,4-dinitrophenoxy)imino)butyl)phenoxy)benzyl methylbutanoate (1ak)

2-(4-chlorophenyl)-3-

0.93 g, 72% yield; yellow sticky foam; ^1H NMR (500 MHz, CDCl_3) δ 8.92 (d, J = 2.7 Hz, 1H), 8.44

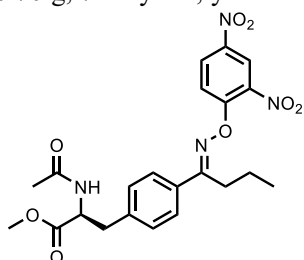


(dd, J = 9.4, 2.8 Hz, 1H), 8.06 (d, J = 9.4 Hz, 1H), 7.75 (d, J = 8.9 Hz, 2H), 7.34 (t, J = 7.9 Hz, 1H), 7.27 – 7.23 (m, 4H), 7.09 – 7.05 (m, 1H), 7.04 – 6.99 (m, 3H), 6.96 – 6.94 (m, 1H), 5.13 (d, J = 12.7 Hz, 1H), 5.06 (d, J = 12.7 Hz, 1H), 3.19 (d, J = 10.6 Hz, 1H), 3.05 – 2.98 (m, 2H), 2.37 – 2.27 (m, 1H), 1.78 – 1.67 (m, 2H), 1.07 (t, J = 7.4 Hz, 3H), 1.01 (d, J = 6.6 Hz, 3H), 0.70 (d, J = 6.7 Hz, 3H); ^{13}C

NMR (126 MHz, CDCl_3) δ 173.2, 166.5, 159.8, 157.5, 156.1, 140.6, 138.2, 136.5, 136.0, 133.1, 130.1, 129.8, 129.4, 128.8, 128.6, 127.8, 123.6, 122.1, 119.3, 119.0, 118.3, 117.2, 65.7, 59.3, 31.8, 30.3, 21.3, 20.5, 20.1, 14.1; HRMS (ESI-TOF) calcd for $\text{C}_{34}\text{H}_{33}\text{ClN}_3\text{O}_8$ $[\text{M}+\text{H}]^+$ 646.1951, found 646.1953.

methyl (S,E)-2-acetamido-3-(4-(1-((2,4-dinitrophenoxy)imino)butyl)phenyl)propanoate (1al)

0.70 g, 74% yield; yellowish solid. Mp = 144-146 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.91 (d, J =

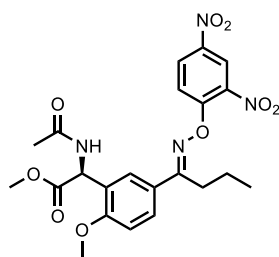


2.9 Hz, 1H), 8.43 (dd, J = 9.5, 2.8 Hz, 1H), 8.05 (d, J = 9.4 Hz, 1H), 7.68 (d, J = 7.8 Hz, 2H), 7.20 (d, J = 7.8 Hz, 2H), 6.03 (d, J = 7.7 Hz, 1H), 4.93 (q, J = 6.4 Hz, 1H), 3.76 (s, 3H), 3.24 (dd, J = 13.9, 5.9 Hz, 1H), 3.14 (dd, J = 13.9, 5.7 Hz, 1H), 3.03 – 2.95 (m, 2H), 2.01 (s, 3H), 1.69 (h, J = 7.5 Hz, 2H), 1.04 (t, J = 7.3 Hz, 3H); ^{13}C NMR (126 MHz, CDCl_3) δ 171.8, 169.6, 166.8, 157.4, 140.7, 139.2, 135.9, 132.1, 129.8, 129.4, 127.2, 122.1, 117.2, 52.9, 52.5, 37.6, 30.4, 23.1, 20.4,

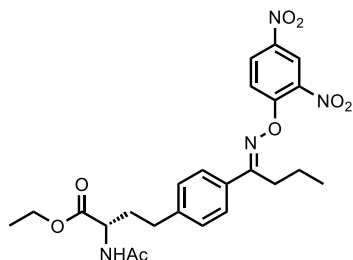
14.1; HRMS (ESI-TOF) calcd for $\text{C}_{22}\text{H}_{25}\text{N}_4\text{O}_8$ $[\text{M}+\text{H}]^+$ 473.1667, found 473.1665.

methyl (S,E)-2-acetamido-2-(5-(1-((2,4-dinitrophenoxy)imino)butyl)-2-methoxyphenyl)acetate (1am)

(S,E)-2-acetamido-2-(5-(1-((2,4-dinitrophenoxy)imino)butyl)-2-

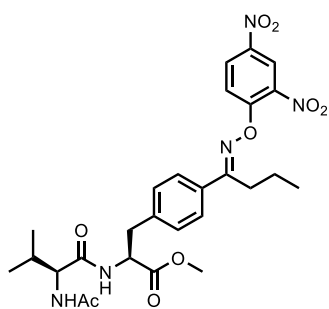


0.77 g, 79% yield; yellowish solid. Mp = 146-148 °C; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.91 (d, J = 2.8 Hz, 1H), 8.45 (dd, J = 9.4, 2.7 Hz, 1H), 8.07 (d, J = 9.4 Hz, 1H), 7.83 (d, J = 2.3 Hz, 1H), 7.72 (dd, J = 8.6, 2.3 Hz, 1H), 6.97 (d, J = 8.7 Hz, 1H), 6.65 (d, J = 8.4 Hz, 1H), 5.82 (d, J = 8.4 Hz, 1H), 3.91 (s, 3H), 3.71 (s, 3H), 3.03 – 2.92 (m, 2H), 2.04 (s, 3H), 1.70 (h, J = 7.5 Hz, 2H), 1.05 (t, J = 7.4 Hz, 3H); $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 171.1, 169.4, 166.1, 159.1, 157.5, 140.7, 136.0, 129.7, 129.4, 129.0, 126.4, 125.9, 122.1, 117.3, 111.2, 55.9, 53.4, 52.8, 30.2, 23.2, 20.5, 14.2; **HRMS (ESI-TOF)** calcd for $\text{C}_{22}\text{H}_{25}\text{N}_4\text{O}_9$ $[\text{M}+\text{H}]^+$ 489.1616, found 489.1619.



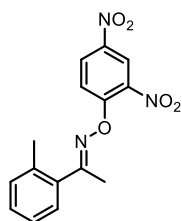
ethyl (S,E)-2-acetamido-4-(4-(1-((2,4-dinitrophenoxy)imino)butyl)phenyl)butanoate (1an)
0.72 g, 72% yield; yellowish solid. Mp = 96-98 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.93 (d, J = 2.8 Hz, 1H), 8.46 (dd, J = 9.4, 2.8 Hz, 1H), 8.07 (d, J = 9.4 Hz, 1H), 7.70 (d, J = 7.9 Hz, 2H), 7.30 (d, J = 8.0 Hz, 2H), 6.14 (d, J = 8.0 Hz, 1H), 4.75 – 4.65 (m, 1H), 4.23 (q, J = 7.1 Hz, 2H), 3.02 (t, J = 7.8 Hz, 2H), 2.82 – 2.68 (m, 2H), 2.32 – 2.21 (m, 1H), 2.11 – 2.00 (m, 4H), 1.71 (h, J = 7.6 Hz, 2H), 1.32 (t, J = 7.1 Hz, 3H), 1.06 (t, J = 7.3 Hz, 3H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 172.3, 169.8, 167.1, 157.5, 144.1, 140.6, 136.0, 131.2, 129.4, 128.9, 127.3, 122.1, 117.2, 61.6, 51.9, 33.8, 31.4, 30.4, 23.2, 20.4, 14.2, 14.1; **HRMS (ESI-TOF)** calcd for $\text{C}_{24}\text{H}_{29}\text{N}_4\text{O}_8$ $[\text{M}+\text{H}]^+$ 501.1980, found 501.1981.

methyl (S)-2-((S)-2-acetamido-3-methylbutanamido)-3-(4-((E)-1-((2,4-dinitrophenoxy)imino)butyl)phenyl)propanoate (1ao)



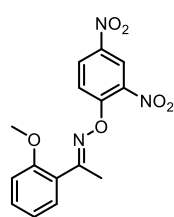
0.72 g, 63% yield; yellowish solid. Mp = 193-195 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.93 (d, J = 2.7 Hz, 1H), 8.45 (dd, J = 9.4, 2.7 Hz, 1H), 8.07 (d, J = 9.4 Hz, 1H), 7.69 (d, J = 8.2 Hz, 2H), 7.23 (d, J = 8.0 Hz, 2H), 6.28 (d, J = 7.9 Hz, 1H), 6.01 (d, J = 8.7 Hz, 1H), 4.97 – 4.89 (m, 1H), 4.21 (dd, J = 8.7, 6.8 Hz, 1H), 3.76 (s, 3H), 3.22 (dd, J = 13.9, 5.6 Hz, 1H), 3.14 (dd, J = 14.0, 6.1 Hz, 1H), 3.03 – 2.96 (m, 2H), 2.08 – 2.01 (m, 4H), 1.70 (h, J = 7.4 Hz, 2H), 1.05 (t, J = 7.3 Hz, 3H), 0.94 (d, J = 3.5 Hz, 3H), 0.93 (d, J = 3.5 Hz, 3H); $^{13}\text{C NMR}$ (101 MHz, $\text{DMSO}-d_6$) δ 172.1, 171.9, 169.7, 167.3, 156.8, 141.1, 136.4, 131.4, 130.5, 130.2, 127.6, 122.4, 117.8, 57.8, 53.6, 52.3, 36.7, 30.9, 29.8, 22.9, 20.4, 19.5, 18.5, 14.3; **HRMS (ESI-TOF)** calcd for $\text{C}_{27}\text{H}_{34}\text{N}_5\text{O}_9$ $[\text{M}+\text{H}]^+$ 572.2351, found 572.2350.

(E)-1-(o-tolyl)ethan-1-one O-(2,4-dinitrophenyl) oxime (1a-1)



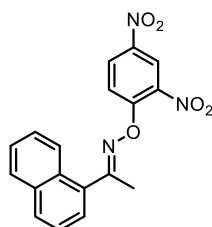
1.18 g, 75% yield; yellow solid. $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.92 (d, J = 2.7 Hz, 1H), 8.41 (dd, J = 9.3, 2.7 Hz, 1H), 7.96 (d, J = 9.4 Hz, 1H), 7.39 – 7.35 (m, 1H), 7.33 – 7.27 (m, 3H), 2.54 (s, 3H), 2.45 (s, 3H)

(E)-1-(2-methoxyphenyl)ethan-1-one O-(2,4-dinitrophenyl) oxime (1b-1)



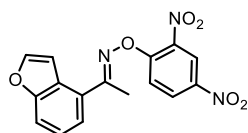
1.27 g, 77% yield; light-yellow solid. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.89 (d, J = 2.8 Hz, 1H), 8.39 (dd, J = 9.4, 2.8 Hz, 1H), 8.00 (d, J = 9.4 Hz, 1H), 7.46 (ddd, J = 8.3, 7.4, 1.8 Hz, 1H), 7.38 (dd, J = 7.5, 1.8 Hz, 1H), 7.05 – 6.97 (m, 2H), 3.89 (s, 3H), 2.53 (s, 3H).

(E)-1-(naphthalen-1-yl)ethan-1-one O-(2,4-dinitrophenyl) oxime (1c-1)



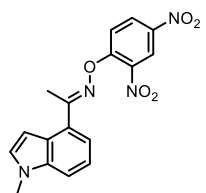
1.44 g, 82% yield; yellow solid. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.92 (d, J = 2.7 Hz, 1H), 8.38 (dd, J = 9.4, 2.8 Hz, 1H), 8.07 – 8.01 (m, 1H), 8.00 – 7.91 (m, 3H), 7.62 – 7.52 (m, 4H), 2.72 (s, 3H).

(E)-1-(benzofuran-4-yl)ethan-1-one O-(2,4-dinitrophenyl) oxime (1d-1)



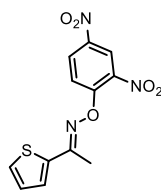
1.10 g, 70% yield; yellow solid. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.96 (d, J = 2.7 Hz, 1H), 8.49 (dd, J = 9.4, 2.8 Hz, 1H), 8.06 (d, J = 9.4 Hz, 1H), 7.78 (d, J = 2.2 Hz, 1H), 7.69 – 7.65 (m, 1H), 7.56 (dd, J = 7.7, 0.9 Hz, 1H), 7.41 (t, J = 7.9 Hz, 1H), 7.25 – 7.24 (m, 1H), 2.72 (s, 3H).

(E)-1-(1-methyl-1H-indol-4-yl)ethan-1-one O-(2,4-dinitrophenyl) oxime (1e-1)



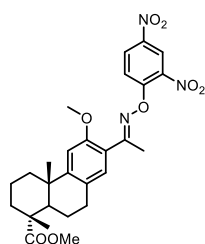
1.15 g, 65% yield; yellow solid. Mp = 78–80 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.93 (s, 1H), 8.46 (d, J = 9.4 Hz, 1H), 8.12 (d, J = 9.4 Hz, 1H), 7.47 (d, J = 7.8 Hz, 1H), 7.47 (d, J = 7.8 Hz, 1H), 7.35 – 7.19 (m, 2H), 6.95 (s, 1H), 3.88 (s, 3H), 2.73 (s, 3H). $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 164.9, 157.9, 140.6, 137.3, 136.0, 130.7, 129.7, 126.1, 125.6, 122.3, 121.4, 120.7, 117.5, 112.3, 102.3, 33.3, 15.8. **HRMS-ESI** calcd for $\text{C}_{17}\text{H}_{15}\text{N}_4\text{O}_5$ $[\text{M}+\text{H}]^+$ 355.1037; found 355.1039.

(E)-1-(thiophen-2-yl)ethan-1-one O-(2,4-dinitrophenyl) oxime (1f-1)



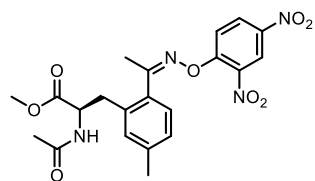
0.95 g, 62% yield; yellow solid. Mp = 88–90 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.81 (d, J = 2.2 Hz, 1H), 8.44 (dd, J = 9.4, 2.6 Hz, 1H), 8.05 (d, J = 9.4 Hz, 1H), 7.84 (d, J = 3.9 Hz, 1H), 7.71 (d, J = 5.1 Hz, 1H), 7.20 (t, J = 4.4 Hz, 1H), 2.55 (s, 3H). $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 158.9, 157.3, 141.0, 137.0, 136.2, 130.1, 129.9, 129.7, 127.8, 122.3, 117.5, 14.9. **HRMS-EI** calcd for $\text{C}_{12}\text{H}_9\text{N}_3\text{O}_5\text{S}$ $[\text{M}]^+$ 307.0257; found 307.0253.

methyl (1R,4aS)-7-((E)-1-((2,4-dinitrophenoxy)imino)ethyl)-6-methoxy-1,4a-dimethyl-1,2,3,4,4a,9,10,10a-octahydrophenanthrene-1-carboxylate (1h-1)



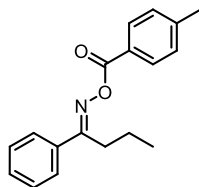
2.15 g, 82% yield; light-yellow solid. Mp = 92-94 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.90 (d, J = 2.8 Hz, 1H), 8.39 (dd, J = 9.4, 2.8 Hz, 1H), 8.00 (d, J = 9.4 Hz, 1H), 7.04 (s, 1H), 6.85 (s, 1H), 3.84 (s, 3H), 3.68 (s, 3H), 2.87 (dd, J = 9.2, 4.6 Hz, 2H), 2.50 (s, 3H), 2.31 (d, J = 12.6 Hz, 1H), 2.23 (dd, J = 12.5, 2.2 Hz, 1H), 1.84 – 1.73 (m, 4H), 1.71 – 1.65 (m, 1H), 1.57 – 1.50 (m, 1H), 1.48 – 1.41 (m, 1H), 1.29 (s, 3H), 1.26 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 179.0, 166.1, 157.7, 155.9, 153.4, 140.7, 136.1, 130.2, 129.4, 127.5, 122.2, 122.0, 117.7, 107.4, 55.7, 52.2, 47.8, 44.8, 38.1, 37.9, 36.7, 29.1, 25.0, 21.7, 18.7, 18.1, 16.7. HRMS-ESI calcd for $\text{C}_{27}\text{H}_{32}\text{N}_3\text{O}_8$ $[\text{M}+\text{H}]^+$ 526.2184; found 526.2184.

Methyl (R,Z)--2-acetamido-3-(2-(1-((2,4-dinitrophenoxy)imino)ethyl)-5-methylphenyl) propanoate (1i-1)



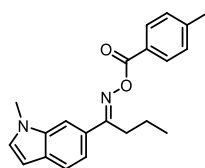
1.74 g, 76% yield; light-yellow solid. Mp = 90-91 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.89 (d, J = 2.7 Hz, 1H), 8.39 (dd, J = 9.4, 2.8 Hz, 1H), 7.93 (d, J = 9.4 Hz, 1H), 7.24 (d, J = 7.7 Hz, 1H), 7.05 – 6.98 (m, 2H), 6.04 (d, J = 7.8 Hz, 1H), 4.94 – 4.86 (m, 1H), 3.76 (s, 3H), 3.18 (dd, J = 13.9, 5.8 Hz, 1H), 3.08 (dd, J = 13.8, 5.8 Hz, 1H), 2.51 (s, 3H), 2.41 (s, 3H), 2.00 (s, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 171.9, 169.7, 165.8, 157.3, 140.8, 137.9, 136.1, 136.0, 133.6, 132.2, 129.4, 128.6, 127.0, 122.1, 117.3, 53.0, 52.5, 37.5, 23.2, 20.6, 18.3. HRMS-ESI calcd for $\text{C}_{21}\text{H}_{23}\text{N}_4\text{O}_8$ $[\text{M}+\text{H}]^+$ 459.1510; found 459.1512.

(E)-1-phenylbutan-1-one O-(4-methylbenzoyl) oxime (1a-2)



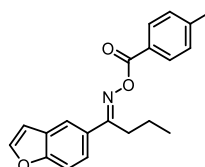
0.85 g, 82% yield; white solid. Mp = 72-74 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.01 (d, J = 8.2 Hz, 2H), 7.79 (dd, J = 7.9, 1.5 Hz, 2H), 7.49–7.39 (m, 3H), 7.30 (d, J = 8.0 Hz, 2H), 2.96 (t, J = 10.0 Hz, 2H), 2.45 (s, 3H), 1.71 (h, J = 7.4 Hz, 2H), 1.04 (t, J = 7.4 Hz, 3H); ^{13}C NMR (126 MHz, CDCl_3) δ 167.2, 164.0, 144.1, 134.2, 130.5, 129.7, 129.4, 128.6, 127.4, 126.5, 30.5, 21.8, 20.4, 14.3; HRMS-EI calcd for $\text{C}_{18}\text{H}_{19}\text{O}_2\text{N}$ $[\text{M}]^+$ 281.1410, found 281.1414.

(E)-1-(1-methyl-1H-indol-6-yl)butan-1-one O-(4-methylbenzoyl) oxime (1b-2)



0.67 g, 70% yield; yellow solid. Mp = 87-90 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.04 (d, J = 8.0 Hz, 2H), 7.87 (s, 1H), 7.65 (d, J = 8.3 Hz, 1H), 7.53–7.45 (m, 1H), 7.31 (d, J = 8.0 Hz, 2H), 7.15 (d, J = 3.1 Hz, 1H), 6.50 (d, J = 3.1 Hz, 1H), 3.86 (s, 3H), 3.09–3.01 (m, 2H), 2.45 (s, 3H), 1.76 (q, J = 7.5 Hz, 2H), 1.06 (t, J = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 168.5, 164.2, 143.9, 136.6, 131.0, 130.4, 129.6, 129.3, 127.3, 126.8, 120.8, 118.6, 108.8, 101.1, 33.1, 30.9, 21.8, 20.7, 14.4. HRMS-EI calcd for $\text{C}_{21}\text{H}_{22}\text{O}_2\text{N}_2$ $[\text{M}]^+$ 334.1676, found 334.1676.

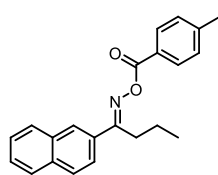
(E)-1-(benzofuran-5-yl)butan-1-one O-(4-methylbenzoyl) oxime (1c-2)



0.65 g, 68% yield; white solid. Mp = 81-83 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.05 (d, J = 1.9 Hz, 1H), 8.02 (d, J = 8.2 Hz, 2H), 7.78 (dd, J = 8.7, 1.9 Hz, 1H), 7.66 (d, J = 2.2 Hz, 1H), 7.54 (d, J = 8.7 Hz, 1H), 7.31 (d, J = 8.0 Hz, 2H), 6.82 (d, J = 1.9 Hz, 1H), 3.08–2.96 (m, 2H), 2.45 (s, 3H), 1.74 (h, J = 7.5 Hz, 2H), 1.05 (t, J = 7.4 Hz, 3H); ^{13}C NMR (126 MHz, CDCl_3) δ 167.4, 164.0, 156.2, 145.9, 144.0, 129.6, 129.4, 129.1, 127.7, 126.6, 123.9, 120.9, 111.6, 106.9, 77.3, 77.1, 76.8,

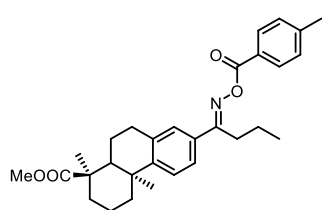
30.8, 21.8, 20.5, 14.3; **HRMS-EI** calcd for C₂₀H₁₉O₃N [M]⁺ 321.1359, found 321.1355.

(E)-1-(naphthalen-2-yl)butan-1-one O-(4-methylbenzoyl) oxime (1d-2)



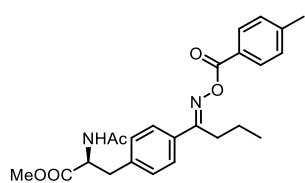
0.66 g, 65% yield; white solid. Mp = 83-85 °C; ¹H NMR (500 MHz, CDCl₃) δ 8.23 (s, 1H), 8.05 (d, *J* = 8.2 Hz, 2H), 8.02 (dd, *J* = 8.6, 1.8 Hz, 1H), 7.94–7.85 (m, 3H), 7.56–7.50 (m, 2H), 7.32 (d, *J* = 8.0 Hz, 2H), 3.12–3.05 (m, 2H), 2.45 (s, 3H), 1.84–1.72 (m, 2H), 1.09 (t, *J* = 7.4 Hz, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 167.0, 164.0, 144.1, 134.4, 133.0, 131.6, 129.7, 129.4, 128.8, 128.4, 127.7, 127.7, 127.3, 126.6, 126.5, 124.3, 30.3, 21.8, 20.6, 14.4; **HRMS-EI** calcd for C₂₂H₂₁O₂N [M]⁺ 331.1567, found 331.1566.

methyl (1R,4aS)-1,4a-dimethyl-7-((E)-1-(((4-methylbenzoyl)oxy)imino)butyl)-1,2,3,4,4a,9,10,10a-octahydrophenanthrene-1-carboxylate (1e-2)



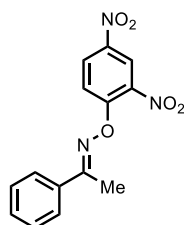
0.75 g, 45% yield; white solid. Mp = 79-81 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.00 (d, *J* = 8.2 Hz, 2H), 7.52 (dd, *J* = 8.3, 2.1 Hz, 1H), 7.49 (s, 1H), 7.33–7.25 (m, 3H), 3.68 (s, 3H), 2.97–2.88 (m, 4H), 2.44 (s, 3H), 2.36–2.28 (m, 1H), 2.25–2.19 (m, 1H), 1.84–1.64 (m, 7H), 1.57–1.48 (m, 1H), 1.49–1.41 (m, 1H), 1.29 (s, 3H), 1.21 (s, 3H), 1.03 (t, *J* = 7.4 Hz, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 179.0, 167.2, 164.0, 152.2, 144.0, 135.5, 131.2, 129.6, 129.3, 128.0, 126.6, 124.8, 124.6, 52.0, 47.6, 44.6, 37.8, 37.4, 36.6, 30.4, 29.9, 24.9, 21.7, 21.5, 20.5, 18.5, 16.6, 14.3; **HRMS (ESI-TOF)** calcd for C₃₀H₃₇NNaO₄ [M+Na]⁺ 498.2615, found 498.2615.

Methyl (S,E)-2-acetamido-3-(4-(1-(((4-methylbenzoyl)oxy)imino)butyl)phenyl)propanoate (1f-2)



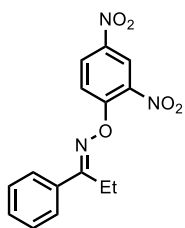
0.75 g, 45% yield; yellow solid. Mp = 111-113 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.99 (d, *J* = 8.2 Hz, 2H), 7.71 (d, *J* = 8.2 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 7.15 (d, *J* = 8.0 Hz, 2H), 6.07 (d, *J* = 7.8 Hz, 1H), 4.96–4.83 (m, 1H), 3.72 (s, 3H), 3.24–3.09 (m, 2H), 2.92 (t, *J* = 7.7 Hz, 2H), 2.43 (s, 3H), 1.98 (s, 3H), 1.69 (h, *J* = 7.6 Hz, 2H), 1.03 (t, *J* = 7.4 Hz, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 171.8, 169.8, 166.9, 163.9, 144.2, 138.7, 133.1, 129.6, 129.5, 129.4, 127.56, 126.34, 53.0, 52.4, 37.57, 30.4, 23.1, 21.8, 20.4, 14.3; **HRMS-EI** calcd for C₂₄H₂₈O₅N₂ [M]⁺ 424.1993, found 424.1990.

(E)-1-phenylethan-1-one O-(2,4-dinitrophenyl) oxime (s1)^[11]



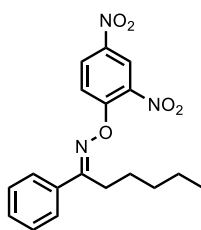
0.49 g, 82% yield; yellowish solid. ¹H NMR (500 MHz, CDCl₃) δ 8.93 (d, *J* = 2.7 Hz, 1H), 8.46 (dd, *J* = 9.3, 2.7 Hz, 1H), 8.08 (d, *J* = 9.4 Hz, 1H), 7.78 (dd, *J* = 7.2, 1.8 Hz, 2H), 7.55–7.45 (m, 4H), 2.60 (s, 3H).

(E)-1-phenylpropan-1-one O-(2,4-dinitrophenyl) oxime (s2)



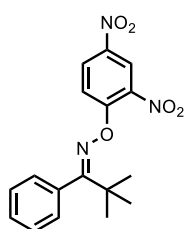
0.50 g, 80% yield; white solid. Mp = 118-120 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.91 (d, J = 2.8 Hz, 1H), 8.44 (dd, J = 9.3, 2.7 Hz, 1H), 8.07 (d, J = 9.4 Hz, 1H), 7.81–7.70 (m, 2H), 7.54–7.46 (m, 3H), 3.05 (q, J = 7.6 Hz, 2H), 1.30 (t, J = 7.6 Hz, 3H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 168.4, 157.5, 140.7, 136.0, 133.0, 131.0, 129.4, 128.9, 127.1, 122.1, 117.3, 22.2, 11.3; **HRMS-EI** calcd for $\text{C}_{15}\text{H}_{13}\text{N}_3\text{O}_5$ $[\text{M}]^+$ 315.0850, found 315.0850.

(E)-1-phenylhexan-1-one O-(2,4-dinitrophenyl) oxime (s3)



0.54 g, 76% yield; white solid. Mp = 88-90 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.91 (d, J = 2.7 Hz, 1H), 8.44 (dd, J = 9.3, 2.8 Hz, 1H), 8.07 (d, J = 9.4 Hz, 1H), 7.75 (dd, J = 7.1, 1.7 Hz, 2H), 7.54–7.45 (m, 3H), 3.07–2.99 (m, 2H), 1.66 (p, J = 7.7 Hz, 2H), 1.47–1.40 (m, 2H), 1.35 (h, J = 7.1 Hz, 2H), 0.89 (t, J = 7.2 Hz, 3H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 167.5, 157.5, 140.7, 136.0, 133.3, 131.0, 129.4, 128.9, 127.1, 122.1, 117.3, 31.8, 28.7, 26.5, 22.2, 13.9; **HRMS-EI** calcd for $\text{C}_{18}\text{H}_{19}\text{N}_3\text{O}_5$ $[\text{M}]^+$ 357.1319, found 357.1329.

EI calcd for $\text{C}_{18}\text{H}_{19}\text{N}_3\text{O}_5$ $[\text{M}]^+$ 357.1319, found 357.1329.

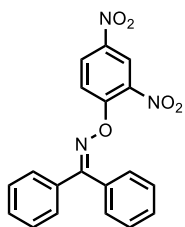


(E)-2,2-dimethyl-1-phenylpropan-1-one O-(2,4-dinitrophenyl) oxime (s4)

0.54 g, 79% yield; white solid. Mp = 117-119 °C; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.72 (d, J = 2.8 Hz, 1H), 8.39 (dd, J = 9.4, 2.8 Hz, 1H), 7.91 (d, J = 9.4 Hz, 1H), 7.49–7.42 (m, 3H), 7.15–7.09 (m, 2H), 1.31 (s, 9H); $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 174.8, 157.3, 140.5, 136.2, 132.2, 128.9, 128.7, 128.0, 126.7, 121.7, 117.3, 38.7, 28.0; **HRMS-EI** calcd for $\text{C}_{17}\text{H}_{17}\text{N}_3\text{O}_5$ $[\text{M}]^+$ 343.1163, found 343.1167.

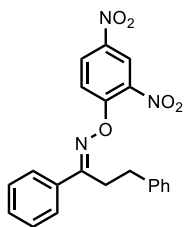
343.1167.

diphenylmethanone O-(2,4-dinitrophenyl) oxime (s5)^[12]



0.61 g, 84% yield; white solid $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.82 (d, J = 2.7 Hz, 1H), 8.46 (dd, J = 9.4, 2.8 Hz, 1H), 8.15 (d, J = 9.4 Hz, 1H), 7.64–7.60 (m, 2H), 7.56–7.47 (m, 6H), 7.45 (t, J = 7.6 Hz, 2H).

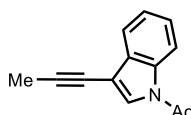
(E)-1,3-diphenylpropan-1-one O-(2,4-dinitrophenyl) oxime (s6)



0.63 g, 81% yield; white solid. Mp = 126-128 °C; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.91 (d, J = 2.7 Hz, 1H), 8.42 (dd, J = 9.4, 2.8 Hz, 1H), 8.00 (d, J = 9.4 Hz, 1H), 8.00–7.74 (m, 2H), 7.57–7.47 (m, 3H), 7.27–7.23 (m, 4H), 7.18–7.12 (m, 1H), 3.38–3.32 (m, 2H), 3.01–2.94 (m, 2H); $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 166.2, 157.3, 140.7, 140.0, 135.9, 133.0, 131.1, 129.3, 128.9, 128.5, 127.1, 126.4, 122.0, 117.2, 32.8, 30.9; **HRMS-EI** calcd for $\text{C}_{21}\text{H}_{17}\text{N}_3\text{O}_5$ $[\text{M}]^+$ 391.1162, found 391.1158.

391.1158.

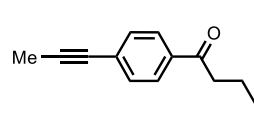
1-(3-(prop-1-yn-1-yl)-1H-indol-1-yl)ethan-1-one (2q)



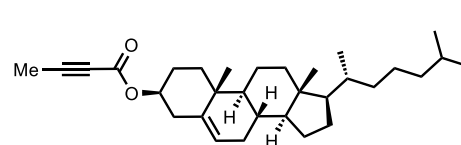
0.73 g, 74% yield; yellowish solid. Mp = 110-112 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.40 (d, J = 8.2 Hz, 1H), 7.66 (d, J = 7.7 Hz, 1H), 7.51 (s, 1H), 7.38 (dd, J = 8.4, 1.4 Hz, 1H), 7.33 (td, J = 7.5, 1.1 Hz, 1H), 2.61 (s, 3H), 2.14 (s,

3H); ^{13}C NMR (126 MHz, CDCl_3) δ 168.1, 134.9, 130.7, 127.2, 125.8, 124.0, 119.9, 116.5, 106.0, 90.0, 70.8, 23.8, 4.6; **HRMS (ESI-TOF)** calcd for $\text{C}_{13}\text{H}_{12}\text{NO}$ $[\text{M}+\text{H}]^+$ 198.0913, found 198.0913.

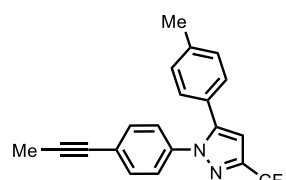
1-(4-(prop-1-yn-1-yl)phenyl)butan-1-one (2r)

 0.83 g, 89% yield; white solid. $\text{Mp} = 34\text{--}36\text{ }^\circ\text{C}$; ^1H NMR (500 MHz, CDCl_3) δ 7.87 (d, $J = 8.4$ Hz, 2H), 7.45 (d, $J = 8.4$ Hz, 2H), 2.92 (t, $J = 7.3$ Hz, 2H), 2.08 (s, 3H), 1.76 (h, $J = 7.4$ Hz, 2H), 1.00 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (126 MHz, CDCl_3) δ 199.7, 135.6, 131.6, 128.8, 127.9, 89.6, 79.3, 40.5, 17.7, 13.9, 4.5; **HRMS (ESI-TOF)** calcd for $\text{C}_{13}\text{H}_{15}\text{O}$ $[\text{M}+\text{H}]^+$ 187.1117, found 187.1116.

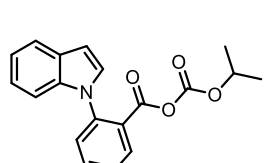
(3S,8S,9S,10R,13R,14S,17R)-10,13-dimethyl-17-((R)-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-yl but-2-ynoate (2s)

 0.78 g, 86% yield; white solid. $\text{Mp} = 128\text{--}130\text{ }^\circ\text{C}$; ^1H NMR (500 MHz, CDCl_3) δ 5.41–5.35 (m, 1H), 4.73–4.65 (m, 1H), 2.41–2.33 (m, 2H), 2.03–1.93 (m, 5H), 1.92–1.78 (m, 3H), 1.69–1.62 (m, 1H), 1.61–1.39 (m, 7H), 1.38–1.29 (m, 3H), 1.27–1.21 (m, 1H), 1.19–1.07 (m, 6H), 1.03–0.94 (m, 6H), 0.94–0.89 (m, 3H), 0.88–0.84 (m, 6H), 0.67 (s, 3H); ^{13}C NMR (126 MHz, CDCl_3) δ 153.1, 139.2, 123.0, 85.0, 75.7, 72.7, 56.6, 56.1, 50.0, 42.3, 39.7, 39.5, 37.8, 36.9, 36.5, 36.2, 35.8, 31.9, 31.8, 28.2, 28.0, 27.5, 24.2, 23.8, 22.8, 22.5, 21.0, 19.2, 18.7, 11.8, 3.8; **HRMS (ESI-TOF)** calcd for $\text{C}_{31}\text{H}_{48}\text{NaO}_2$ $[\text{M}+\text{Na}]^+$ 475.3547, found 475.3547.

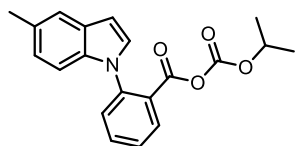
1-(4-(prop-1-yn-1-yl)phenyl)-5-(p-tolyl)-3-(trifluoromethyl)-1H-pyrazole (2t)

 1.1 g, 65% yield; white solid. $\text{Mp} = 80\text{--}82\text{ }^\circ\text{C}$; ^1H NMR (500 MHz, CDCl_3) δ 7.36 (d, $J = 8.6$ Hz, 2H), 7.23 (d, $J = 8.6$ Hz, 2H), 7.13 (d, $J = 8.0$ Hz, 2H), 7.09 (d, $J = 8.2$ Hz, 2H), 6.71 (s, 1H), 2.35 (s, 3H), 2.05 (s, 3H); ^{13}C NMR (126 MHz, CDCl_3) δ 144.7, 143.2 (q, $J = 38.3$ Hz), 139.2, 138.2, 132.1, 129.4, 128.6, 126.0, 125.1, 124.2, 121.2 (q, $J = 268.9$ Hz), 105.4, 87.6, 21.2, 4.2; **HRMS-EI** calcd for $\text{C}_{20}\text{H}_{15}\text{F}_3\text{N}_2$ $[\text{M}]^+$ 340.1182, found 340.1177.

2-(1H-indol-1-yl)benzoic (isopropyl carbonic) anhydride (3c-1)

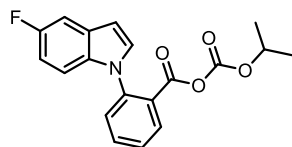
 2.84 g, 88% yield; light-yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 8.14 (dd, $J = 8.1, 1.6$ Hz, 1H), 7.76–7.69 (m, 2H), 7.57–7.52 (m, 2H), 7.28 (d, $J = 3.3$ Hz, 1H), 7.26–7.19 (m, 3H), 6.76 (d, $J = 3.3$ Hz, 1H), 4.85 (hept, $J = 6.3$ Hz, 1H), 1.25 (d, $J = 6.4$ Hz, 6H). ^{13}C NMR (126 MHz, CDCl_3) δ 160.2, 147.9, 139.7, 137.1, 134.5, 132.3, 129.1, 128.9, 128.8, 127.8, 125.9, 122.5, 120.9, 120.4, 109.8, 103.8, 74.4, 21.1. **HRMS-EI** calcd for $\text{C}_{19}\text{H}_{17}\text{NO}_4$ $[\text{M}]^+$ 323.1152; found 323.1146.

(isopropyl carbonic) 2-(5-methyl-1H-indol-1-yl)benzoic anhydride (3c-2)



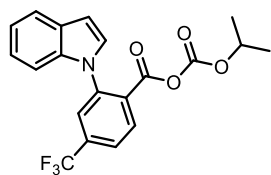
2.76g, 82% yield; light-yellow oil. **¹H NMR** (500 MHz, CDCl₃) δ 8.12–8.08 (m, 1H), 7.75–7.69 (m, 1H), 7.55–7.49 (m, 2H), 7.47–7.45 (m, 1H), 7.19 (d, *J* = 3.2 Hz, 1H), 7.11 (d, *J* = 8.4 Hz, 1H), 7.03 (dd, *J* = 8.4, 1.7 Hz, 1H), 6.63 (dd, *J* = 3.3, 0.8 Hz, 1H), 4.82 (hept, *J* = 6.3 Hz, 1H), 2.47 (s, 3H), 1.22 (d, *J* = 6.3 Hz, 6H). **¹³C NMR** (126 MHz, CDCl₃) δ 160.4, 148.0, 140.1, 135.6, 134.5, 132.4, 129.7, 129.3, 128.9, 128.9, 127.7, 125.9, 124.2, 120.8, 109.7, 103.6, 74.5, 21.4, 21.3. **HRMS-EI** calcd for C₂₀H₁₉NO₄ [M]⁺ 337.1309; found 337.1309.

2-(5-fluoro-1H-indol-1-yl)benzoic (isopropyl carbonic) anhydride (3c-3)



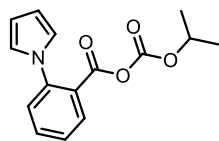
2.55 g, 75% yield; light-yellow oil. **¹H NMR** (500 MHz, CDCl₃) δ 8.09 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.69 (td, *J* = 7.7, 1.6 Hz, 1H), 7.51 (td, *J* = 7.6, 1.2 Hz, 1H), 7.46 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.32 (dd, *J* = 9.4, 2.5 Hz, 1H), 7.26 (d, *J* = 3.3 Hz, 1H), 7.09 (dd, *J* = 9.0, 4.3 Hz, 1H), 6.93 (td, *J* = 9.0, 2.5 Hz, 1H), 6.66 (dd, *J* = 3.2, 0.9 Hz, 1H), 4.83 (hept, *J* = 6.3 Hz, 1H), 1.22 (d, *J* = 6.3 Hz, 6H). **¹³C NMR** (126 MHz, CDCl₃) δ 160.1, 158.2 (d, *J* = 235.0 Hz), 147.8, 139.4, 134.6, 133.8, 132.4, 130.5, 129.2 (d, *J* = 10.3 Hz), 128.9, 128.1, 125.9, 110.7 (d, *J* = 18.7 Hz), 110.6 (d, *J* = 1.8 Hz), 105.7 (d, *J* = 23.6 Hz), 103.7 (d, *J* = 4.4 Hz), 74.5, 21.1. **¹⁹F NMR** (471 MHz, CDCl₃) δ -124.14. **HRMS-EI** calcd for C₁₉H₁₆FN₂O₄ [M]⁺ 341.1058; found 341.1061.

2-(1H-indol-1-yl)-4-(trifluoromethyl)benzoic (isopropyl carbonic) anhydride (3c-4)



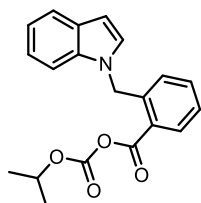
3.2 g, 82% yield; yellow oil. **¹H NMR** (500 MHz, CDCl₃) δ 8.22–8.20 (m, 1H), 7.86 (d, *J* = 1.7 Hz, 1H), 7.80 (ddd, *J* = 8.2, 1.7, 0.8 Hz, 1H), 7.71–7.68 (m, 1H), 7.28–7.19 (m, 4H), 6.76 (dd, *J* = 3.3, 0.7 Hz, 1H), 4.82 (hept, *J* = 6.3 Hz, 1H), 1.21 (d, *J* = 6.3 Hz, 6H). **¹³C NMR** (126 MHz, CDCl₃) δ 159.7, 147.5, 140.3, 137.0, 136.0 (q, *J* = 34.2 Hz), 133.1, 129.4, 129.2, 128.6, 125.9 (q, *J* = 1.3 Hz), 124.4 (q, *J* = 2.5 Hz), 123.2, 122.9 (q, *J* = 273.3 Hz), 121.4, 121.1, 109.6, 105.8, 75.0, 21.6. **¹⁹F NMR** (471 MHz, CDCl₃) δ -63.23. **HRMS-EI** calcd for C₂₀H₁₆F₃NO₄ [M]⁺ 391.1026; found 391.1022.

2-(1H-pyrrol-1-yl)benzoic (isopropyl carbonic) anhydride (3c-5)



1.80 g, 66% yield; brown oil. **¹H NMR** (400 MHz, CDCl₃) δ 7.94 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.65 (td, *J* = 7.7, 1.6 Hz, 1H), 7.48 – 7.40 (m, 2H), 6.87 (t, *J* = 2.2 Hz, 2H), 6.33 (t, *J* = 2.2 Hz, 2H), 4.95 (hept, *J* = 6.3 Hz, 1H), 1.32 (d, *J* = 6.2 Hz, 6H). **¹³C NMR** (101 MHz, CDCl₃) δ 161.0, 148.2, 141.5, 134.1, 131.9, 127.2, 124.9, 122.2, 110.3, 74.6, 21.5. **HRMS-EI** calcd for C₁₅H₁₅NO₄ [M]⁺ 273.0996; found 273.0997.

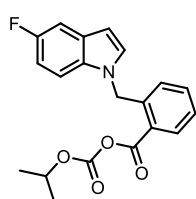
2-((1H-indol-1-yl)methyl)benzoic (isopropyl carbonic) anhydride (3c-6)



2.56 g, 76% yield; light-yellow oil. **¹H NMR** (500 MHz, CDCl₃) δ 8.15 (dd, *J* = 7.5, 1.8 Hz, 1H), 7.72–7.69 (m, 1H), 7.41–7.33 (m, 2H), 7.22–7.13 (m, 4H), 6.64 (d, *J* = 3.1 Hz, 1H), 6.48–6.45 (m, 1H), 5.83 (s, 2H), 5.15 (hept, *J* = 6.3 Hz, 1H), 1.47 (d, *J* = 6.3 Hz, 6H). **¹³C NMR** (126 MHz, CDCl₃) δ 161.5, 148.8, 142.5, 136.5, 134.8, 132.0, 128.8, 127.5, 127.3, 124.8, 122.0, 121.1, 119.8,

109.8, 102.3, 75.0, 48.6, 21.6. **HRMS-EI** calcd for C₂₀H₁₉NO₄ [M]⁺ 337.1309; found 337.1299.

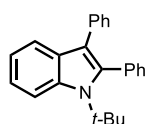
2-((5-fluoro-1*H*-indol-1-yl)methyl)benzoic (isopropyl carbonic) anhydride (**3c-7**)



2.73 g, 77% yield; light-yellow oil. **¹H NMR** (400 MHz, CDCl₃) δ 8.16–8.12 (m, 1H), 7.43–7.30 (m, 3H), 7.18 (d, *J* = 3.2 Hz, 1H), 7.10–7.06 (m, 1H), 6.91 (td, *J* = 9.1, 2.5 Hz, 1H), 6.58 (dd, *J* = 3.1, 0.8 Hz, 1H), 6.46–6.41 (m, 1H), 5.79 (s, 2H), 5.13 (hept, *J* = 6.3 Hz, 1H), 1.45 (d, *J* = 6.3 Hz, 6H). **¹³C NMR** (126 MHz, CDCl₃) δ 161.5, 158.1 (d, *J* = 234.6 Hz), 148.7, 142.1, 134.8, 133.1, 132.1, 130.4, 129.0 (d, *J* = 10.3 Hz), 127.7, 127.2, 124.9, 110.5 (d, *J* = 8.2 Hz), 110.4 (d, *J* = 8.3 Hz), 105.8 (d, *J* = 23.5 Hz), 102.2 (d, *J* = 4.7 Hz), 75.1, 48.9, 21.6. **¹⁹F NMR** (471 MHz, CDCl₃) δ -125.01. **HRMS-EI** calcd for C₂₀H₁₈FO₄ [M]⁺ 355.1214; found 355.1217.

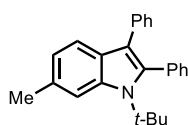
3.2 Characterization of Product

1-(*tert*-butyl)-2,3-diphenyl-1*H*-indole (**4a**)^[13]



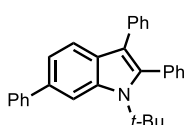
26.6 mg, 82% yield: white solid; **¹H NMR** (500 MHz, CDCl₃) δ 7.81 (dt, *J* = 8.6, 0.9 Hz, 1H), 7.65 (ddd, *J* = 7.9, 1.3, 0.7 Hz, 1H), 7.34 (dd, *J* = 7.8, 1.8 Hz, 2H), 7.31–7.23 (m, 4H), 7.22–7.18 (m, 2H), 7.16–7.10 (m, 4H), 1.66 (s, 9H).

1-(*tert*-butyl)-6-methyl-2,3-diphenyl-1*H*-indole (**4b**)^[13]



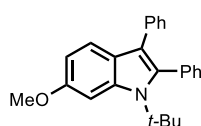
27.5 mg, 81% yield: white solid; **¹H NMR** (500 MHz, CDCl₃) δ 7.60 (s, 1H), 7.54 (d, *J* = 8.1 Hz, 1H), 7.33 (dd, *J* = 7.7, 1.9 Hz, 2H), 7.30–7.24 (m, 3H), 7.21–7.17 (m, 2H), 7.15–7.09 (m, 3H), 6.99 (dd, *J* = 8.1, 1.3 Hz, 1H), 2.57 (s, 3H), 1.65 (s, 9H).

1-(*tert*-butyl)-2,3,6-triphenyl-1*H*-indole (**4c**)^[13]



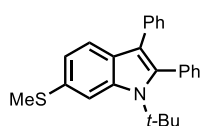
31.6 mg, 79% yield: white solid; **¹H NMR** (500 MHz, CDCl₃) δ 7.98 (d, *J* = 1.5 Hz, 1H), 7.72–7.67 (m, 3H), 7.49 (t, *J* = 7.7 Hz, 2H), 7.40–7.36 (m, 2H), 7.35–7.32 (m, 2H), 7.29 (td, *J* = 7.0, 3.2 Hz, 3H), 7.20 (t, *J* = 7.9 Hz, 2H), 7.17–7.11 (m, 3H), 1.69 (s, 9H).

1-(*tert*-butyl)-6-methoxy-2,3-diphenyl-1*H*-indole (**4d**)^[13]



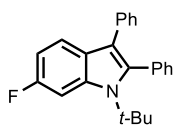
23.1 mg, 65% yield: white solid; **¹H NMR** (500 MHz, CDCl₃) δ 7.53 (dd, *J* = 8.7, 0.9 Hz, 1H), 7.35–7.30 (m, 3H), 7.29–7.24 (m, 3H), 7.19 (dd, *J* = 8.2, 7.0 Hz, 2H), 7.14–7.08 (m, 3H), 6.84 (ddd, *J* = 8.7, 2.2, 0.8 Hz, 1H), 3.94 (s, 3H), 1.64 (s, 9H).

1-(*tert*-butyl)-6-(methylthio)-2,3-diphenyl-1*H*-indole (**4e**)^[13]



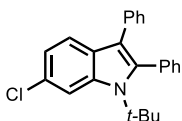
31.9 mg, 86% yield: white solid; **¹H NMR** (500 MHz, CDCl₃) δ 7.82 (d, *J* = 1.4 Hz, 1H), 7.56 (d, *J* = 8.3 Hz, 1H), 7.33–7.24 (m, 5H), 7.21–7.15 (m, 3H), 7.14–7.09 (m, 3H), 2.59 (s, 3H), 1.64 (s, 9H).

1-(*tert*-butyl)-6-fluoro-2,3-diphenyl-1*H*-indole (**4f**)^[13]



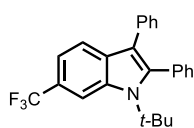
21.2 mg, 62% yield: white solid; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.54 (dd, $J = 8.7$, 6.0 Hz, 1H), 7.48 (dd, $J = 11.8$, 2.2 Hz, 1H), 7.32 (dd, $J = 7.8$, 1.8 Hz, 2H), 7.30–7.24 (m, 3H), 7.21–7.17 (m, 2H), 7.12 (tt, $J = 8.0$, 1.4 Hz, 3H), 6.91 (td, $J = 8.9$, 2.2 Hz, 1H), 1.62 (s, 9H).

1-(*tert*-butyl)-6-chloro-2,3-diphenyl-1*H*-indole (4g)^[13]



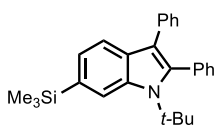
18.3 mg, 51% yield: white solid; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.78 (d, $J = 1.8$ Hz, 1H), 7.52 (d, $J = 8.5$ Hz, 1H), 7.33–7.24 (m, 5H), 7.19 (tt, $J = 8.2$, 1.5 Hz, 2H), 7.14–7.07 (m, 4H), 1.62 (s, 9H).

1-(*tert*-butyl)-2,3-diphenyl-6-(trifluoromethyl)-1*H*-indole (4h)



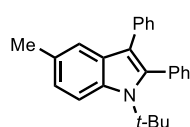
14.9 mg, 38% yield: white solid. Mp = 174–176 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.09 (s, 1H), 7.71 (d, $J = 8.4$ Hz, 1H), 7.38 (dd, $J = 8.4$, 1.4 Hz, 1H), 7.36–7.27 (m, 5H), 7.22 (dd, $J = 8.1$, 6.7 Hz, 2H), 7.18–7.15 (m, 1H), 7.15–7.11 (m, 2H), 1.68 (s, 9H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 140.7, 135.5, 135.2, 134.3, 131.5, 130.9, 130.2, 128.0, 127.8, 127.5, 125.8, 125.4 (q, $J = 271.6$ Hz), 123.0 (q, $J = 31.4$ Hz), 120.0, 118.1, 116.2 (q, $J = 3.1$ Hz), 112.1 (q, $J = 4.5$ Hz), 59.9, 32.2; **HRMS-EI** calcd for $\text{C}_{25}\text{H}_{22}\text{NF}_3$ $[\text{M}]^+$ 393.1699, found 393.1698.

1-(*tert*-butyl)-2,3-diphenyl-6-(trimethylsilyl)-1*H*-indole (4i)



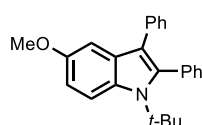
28.2 mg, 71% yield: white solid. Mp = 102–104 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.97 (s, 1H), 7.65 (d, $J = 7.8$ Hz, 1H), 7.33–7.24 (m, 6H), 7.21–7.16 (m, 2H), 7.14–7.09 (m, 3H), 1.66 (s, 9H), 0.37 (s, 9H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 138.5, 136.4, 136.3, 135.1, 131.8, 131.7, 130.3, 129.3, 127.6, 127.3, 125.4, 124.0, 119.9, 119.2, 117.9, 59.3, 32.2, -0.7; **HRMS-EI** calcd for $\text{C}_{27}\text{H}_{31}\text{NSi}$ $[\text{M}]^+$ 397.2220, found 397.2228.

1-(*tert*-butyl)-5-methyl-2,3-diphenyl-1*H*-indole (4j)^[13]



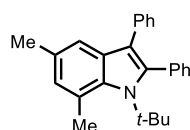
27.1 mg, 80% yield: white solid; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.73 (d, $J = 8.6$ Hz, 1H), 7.49–7.44 (m, 1H), 7.36 (dd, $J = 7.8$, 1.8 Hz, 2H), 7.34–7.26 (m, 3H), 7.27–7.20 (m, 2H), 7.20–7.13 (m, 3H), 7.16–7.08 (m, 1H), 2.47 (s, 3H), 1.66 (s, 9H).

1-(*tert*-butyl)-5-methoxy-2,3-diphenyl-1*H*-indole (4k)^[13]



24.1 mg, 68% yield: white solid; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.69 (d, $J = 9.1$ Hz, 1H), 7.31 (dd, $J = 7.8$, 1.8 Hz, 2H), 7.29–7.23 (m, 3H), 7.21–7.17 (m, 2H), 7.14–7.09 (m, 3H), 7.08 (d, $J = 2.6$ Hz, 1H), 6.90 (dd, $J = 9.1$, 2.7 Hz, 1H), 3.81 (s, 3H), 1.62 (s, 9H).

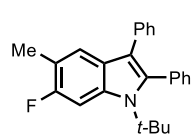
1-(*tert*-butyl)-5,7-dimethyl-2,3-diphenyl-1*H*-indole (4l)



15.9 mg, 45% yield: white sticky foam; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.79 (d, $J = 8.5$ Hz, 1H), 7.69 – 7.65 (m, 1H), 7.33 (dd, $J = 7.5$, 2.0 Hz, 2H), 7.30–7.25 (m, 3H), 7.23 (ddd, $J = 8.5$, 7.1, 1.4 Hz, 1H), 7.16 – 7.11 (m, 1H), 6.81–6.76 (m, 3H), 2.17 (s, 6H), 1.64 (s, 9H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 137.9, 136.8,

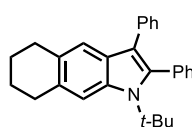
136.5, 136.4, 134.8, 131.8, 128.6, 128.1, 127.5, 127.2, 127.0, 121.0, 119.8, 119.3, 117.8, 114.9, 59.2, 32.1, 21.3; **HRMS-EI** calcd for C₂₆H₂₇N [M]⁺ 353.2138, found 353.2138.

1-(*tert*-butyl)-6-fluoro-5-methyl-2,3-diphenyl-1*H*-indole (4m)^[13]



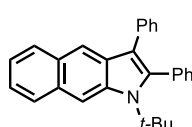
23.9 mg, 67% yield: white solid; **¹H NMR** (500 MHz, CDCl₃) δ 7.44 (d, *J* = 12.5 Hz, 1H), 7.36 (d, *J* = 8.2 Hz, 1H), 7.31 (dd, *J* = 7.5, 1.8 Hz, 2H), 7.29–7.23 (m, 3H), 7.19 (t, *J* = 7.5 Hz, 2H), 7.15–7.08 (m, 3H), 2.36–2.32 (m, 3H), 1.60 (s, 9H).

1-(*tert*-butyl)-2,3-diphenyl-5,6,7,8-tetrahydro-1*H*-benzo[*f*]indole (4n)



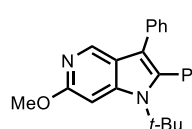
28.8 mg, 76% yield: white solid. Mp = 160–162 °C; **¹H NMR** (500 MHz, CDCl₃) δ 7.50 (s, 1H), 7.33 (s, 1H), 7.30 (dd, *J* = 7.7, 1.9 Hz, 2H), 7.28–7.23 (m, 3H), 7.21–7.17 (m, 2H), 7.12 (d, *J* = 7.5 Hz, 3H), 3.01 (t, *J* = 6.1 Hz, 2H), 2.88 (t, *J* = 6.0 Hz, 2H), 1.93–1.81 (m, 4H), 1.63 (s, 9H); **¹³C NMR** (126 MHz, CDCl₃) δ 137.8, 136.6, 135.5, 135.4, 131.7, 130.7, 130.3, 128.9, 127.6, 127.4, 127.4, 127.3, 125.2, 118.8, 117.2, 114.6, 58.9, 32.0, 30.7, 29.5, 23.9, 23.8; **HRMS-EI** calcd for C₂₈H₂₉N [M]⁺ 379.2295, found 379.2296.

1-(*tert*-butyl)-2,3-diphenyl-1*H*-benzo[*f*]indole (4o)



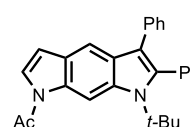
31.5 mg, 84% yield: white solid. Mp = 165–167 °C; **¹H NMR** (500 MHz, CDCl₃) δ 8.20 (s, 1H), 8.12 (s, 1H), 7.99 (d, *J* = 8.3 Hz, 1H), 7.89 (d, *J* = 8.2 Hz, 1H), 7.43–7.38 (m, 3H), 7.37–7.30 (m, 4H), 7.29–7.23 (m, 4H), 7.22–7.17 (m, 1H), 1.74 (s, 9H); **¹³C NMR** (126 MHz, CDCl₃) δ 141.9, 137.3, 136.2, 135.0, 131.4, 130.5, 130.4, 129.6, 128.3, 127.8, 127.8, 127.7, 127.4, 125.6, 123.6, 122.8, 117.2, 116.5, 110.8, 59.4, 31.9; **HRMS-EI** calcd for C₂₈H₂₅N [M]⁺ 375.1982, found 375.1982.

1-(*tert*-butyl)-6-methoxy-2,3-diphenyl-1*H*-pyrrolo[3,2-*c*]pyridine (4p)



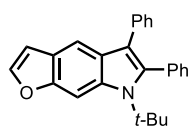
14.6 mg, 41% yield: white solid. Mp = 170–172 °C; **¹H NMR** (500 MHz, CDCl₃) δ 7.81 (d, *J* = 8.5 Hz, 1H), 7.38–7.34 (m, 2H), 7.34–7.26 (m, 3H), 7.20–7.16 (m, 2H), 7.13–7.08 (m, 3H), 6.60 (d, *J* = 8.5 Hz, 1H), 4.03 (s, 3H), 1.71 (s, 9H); **¹³C NMR** (126 MHz, CDCl₃) δ 159.1, 146.5, 135.9, 134.9, 132.1, 130.1, 129.8, 127.8, 127.8, 127.4, 125.4, 115.5, 114.6, 103.6, 60.0, 53.5, 31.4; **HRMS-EI** calcd for C₂₄H₂₄N₂O [M]⁺ 356.1883, found 356.1887.

1-(7-(*tert*-butyl)-5,6-diphenylpyrrolo[3,2-*f*]indol-1(7*H*)-yl)ethan-1-one (4q)



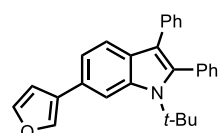
19.5 mg, 48% yield: white solid. Mp = 224–226 °C; **¹H NMR** (500 MHz, CDCl₃) δ 9.12 (s, 1H), 7.71 (s, 1H), 7.36–7.33 (m, 3H), 7.30–7.24 (m, 3H), 7.23–7.19 (m, 2H), 7.18–7.15 (m, 2H), 7.15–7.10 (m, 1H), 6.64 (d, *J* = 3.8 Hz, 1H), 2.67 (s, 3H), 1.70 (s, 9H); **¹³C NMR** (126 MHz, CDCl₃) δ 168.5, 139.0, 136.5, 135.8, 135.3, 132.5, 131.6, 130.4, 127.7, 127.6, 127.3, 126.9, 125.4, 125.0, 124.9, 117.4, 109.9, 109.7, 103.0, 59.4, 32.0, 24.0; **HRMS-EI** calcd for C₂₈H₂₆N₂O [M]⁺ 406.2040, found 406.2034.

7-(*tert*-butyl)-5,6-diphenyl-7*H*-furo[3,2-*f*]indole (4r)



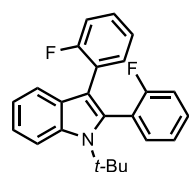
23.7 mg, 65% yield: white solid. Mp = 183–185 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.89 (s, 1H), 7.73 (s, 1H), 7.60 (d, J = 2.3 Hz, 1H), 7.35 (dd, J = 7.5, 1.9 Hz, 2H), 7.30–7.24 (m, 3H), 7.22 (t, J = 7.5 Hz, 2H), 7.19–7.16 (m, 2H), 7.14 (td, J = 6.8, 1.6 Hz, 1H), 6.76 (d, J = 1.9 Hz, 1H), 1.67 (s, 9H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 152.3, 144.5, 138.5, 136.5, 135.3, 131.7, 130.4, 127.7, 127.6, 127.3, 126.6, 125.4, 121.7, 117.4, 109.8, 106.3, 96.7, 59.2, 31.9; **HRMS-EI** calcd for $\text{C}_{26}\text{H}_{23}\text{NO}$ $[\text{M}]^+$ 365.1774, found 365.1770.

1-(*tert*-butyl)-6-(furan-3-yl)-2,3-diphenyl-1H-indole (4s)



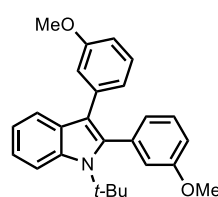
(28.5 mg, 73% yield): white solid. Mp = 156–158 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.89 (d, J = 1.3 Hz, 1H), 7.78 (t, J = 1.1 Hz, 1H), 7.62 (d, J = 8.2 Hz, 1H), 7.52 (t, J = 1.7 Hz, 1H), 7.33 (dd, J = 7.7, 1.9 Hz, 2H), 7.28 (td, J = 6.7, 3.4 Hz, 4H), 7.22–7.18 (m, 2H), 7.16–7.10 (m, 3H), 6.82–6.79 (m, 1H), 1.67 (s, 9H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 143.4, 138.5, 138.0, 136.8, 136.2, 135.0, 131.7, 130.3, 128.0, 127.9, 127.7, 127.7, 127.4, 125.5, 125.4, 119.9, 118.4, 118.0, 112.4, 109.5, 59.4, 32.2; **HRMS-EI** calcd for $\text{C}_{28}\text{H}_{25}\text{NO}$ $[\text{M}]^+$ 391.1931, found 391.1929.

1-(*tert*-butyl)-2,3-bis(2-fluorophenyl)-1H-indole (4t)



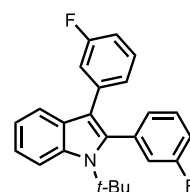
29.6 mg, 82% yield: white solid. Mp = 163–165 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.84 (d, J = 8.5 Hz, 1H), 7.46 (s, 1H), 7.33–7.20 (m, 3H), 7.20–7.15 (m, 2H), 7.09–6.92 (m, 5H), 1.71 (s, 9H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 162.4–161.4 (m), 160.4–159.4 (m), 136.6–136.2 (m), 133.0, 133.0–132.6 (m), 130.2 (d, J = 8.3 Hz), 128.8, 128.2 (d, J = 7.6 Hz), 124.3 (d, J = 16.5 Hz), 123.7–122.9 (m), 122.4 (d, J = 16.4 Hz), 121.3, 120.2–119.6 (m), 119.4, 115.6–114.4 (m), 114.9, 113.0–112.6 (m), 59.3, 31.2; **HRMS-EI** calcd for $\text{C}_{24}\text{H}_{21}\text{NF}_2$ $[\text{M}]^+$ 361.1637, found 361.1632.

1-(*tert*-butyl)-2,3-bis(3-methoxyphenyl)-1H-indole (4u)^[13]



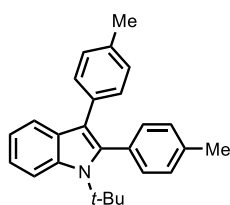
30.8 mg, 80% yield: white solid; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.81 (d, J = 8.4 Hz, 1H), 7.70 (dd, J = 7.9, 1.2 Hz, 1H), 7.25 (ddd, J = 8.4, 6.9, 1.3 Hz, 1H), 7.21 (t, J = 7.9 Hz, 1H), 7.15 (td, J = 7.6, 3.7 Hz, 2H), 6.97 (dt, J = 7.5, 1.1 Hz, 1H), 6.90 (t, J = 2.1 Hz, 1H), 6.86 (dd, J = 8.2, 2.7 Hz, 1H), 6.82 (dd, J = 7.7, 1.2 Hz, 1H), 6.72–6.67 (m, 2H), 3.75 (s, 3H), 3.63 (s, 3H), 1.69 (s, 9H).

1-(*tert*-butyl)-2,3-bis(3-fluorophenyl)-1H-indole (4v)



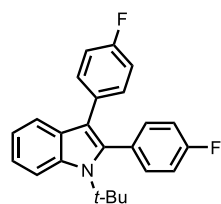
30.6 mg, 85% yield: white solid. Mp = 97–99 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.82 (dd, J = 8.5, 0.9 Hz, 1H), 7.66–7.61 (m, 1H), 7.31–7.24 (m, 2H), 7.21–7.12 (m, 3H), 7.07–7.01 (m, 2H), 6.91 (dt, J = 7.7, 1.2 Hz, 1H), 6.88–6.82 (m, 2H), 1.67 (s, 9H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 162.5 (d, J = 244.5 Hz), 162.0 (d, J = 247.0 Hz), 138.1 (d, J = 8.1 Hz), 137.1 (d, J = 8.4 Hz), 136.5 (d, J = 2.0 Hz), 129.1 (d, J = 8.6 Hz), 129.0 (d, J = 8.6 Hz), 128.3, 127.7 (d, J = 2.9 Hz), 126.0 (d, J = 2.8 Hz), 121.6, 119.9, 119.6, 118.7 (d, J = 21.2 Hz), 117.1 (d, J = 2.2 Hz), 116.9 (d, J = 21.3 Hz), 115.1, 115.0 (d, J = 21.0 Hz), 112.5 (d, J = 21.0 Hz), 59.5, 32.0; **HRMS-EI** calcd for $\text{C}_{24}\text{H}_{21}\text{NF}_2$ $[\text{M}]^+$ 361.1637, found 361.1611.

1-(*tert*-butyl)-2,3-di-*p*-tolyl-1*H*-indole (4w)^[13]



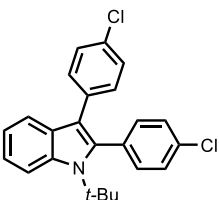
27.8 mg, 79% yield: white solid; ¹H NMR (500 MHz, CDCl₃) δ 7.81 (dt, *J* = 8.5, 1.0 Hz, 1H), 7.66 (dt, *J* = 7.9, 1.2 Hz, 1H), 7.26–7.21 (m, 3H), 7.14 (ddt, *J* = 8.0, 7.0, 1.1 Hz, 1H), 7.12–7.06 (m, 4H), 7.04 (d, *J* = 7.9 Hz, 2H), 2.38 (s, 3H), 2.32 (s, 3H), 1.66 (s, 9H).

1-(*tert*-butyl)-2,3-bis(4-fluorophenyl)-1*H*-indole (4x)^[13]



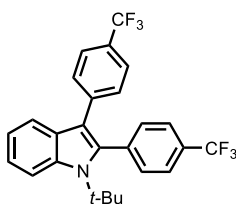
31.0 mg, 86% yield: white solid; ¹H NMR (500 MHz, CDCl₃) δ 7.80 (d, *J* = 8.5 Hz, 1H), 7.57 (d, *J* = 7.9 Hz, 1H), 7.31–7.23 (m, 3H), 7.15 (t, *J* = 7.4 Hz, 1H), 7.10–7.05 (m, 2H), 6.99 (t, *J* = 8.6 Hz, 2H), 6.91 (t, *J* = 8.8 Hz, 2H), 1.65 (s, 9H).

1-(*tert*-butyl)-2,3-bis(4-chlorophenyl)-1*H*-indole (4y)^[13]



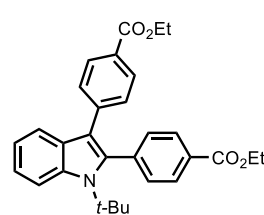
29.5 mg, 75% yield: white solid; ¹H NMR (500 MHz, CDCl₃) δ 7.80 (d, *J* = 8.5 Hz, 1H), 7.57 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.31–7.21 (m, 5H), 7.19 (d, *J* = 8.4 Hz, 2H), 7.15 (t, *J* = 7.4 Hz, 1H), 7.04 (d, *J* = 8.5 Hz, 2H), 1.64 (s, 9H).

1-(*tert*-butyl)-2,3-bis(4-(trifluoromethyl)phenyl)-1*H*-indole (4z)



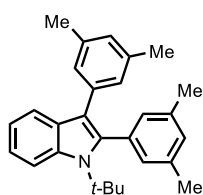
32.7 mg, 71% yield: white solid. Mp = 160–162 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.83 (d, *J* = 8.5 Hz, 1H), 7.63–7.56 (m, 3H), 7.47 (d, *J* = 8.1 Hz, 4H), 7.30 (t, *J* = 7.8 Hz, 1H), 7.22–7.16 (m, 3H), 1.66 (s, 9H); ¹³C NMR (126 MHz, CDCl₃) δ 139.8, 138.6, 136.8, 136.6, 131.9, 130.3, 130.1 (q, *J* = 32.6 Hz), 128.3, 127.7 (q, *J* = 32.4 Hz), 124.9 (q, *J* = 4.1 Hz), 124.6 (q, *J* = 3.8 Hz), 124.3 (q, *J* = 271.8 Hz), 124.0 (q, *J* = 272.5 Hz), 122.0, 120.2, 119.5, 117.3, 115.2, 59.7, 32.2; HRMS-EI calcd for C₂₆H₂₁NF₆ [M]⁺ 461.1573, found 461.1583.

diethyl 4,4'-(1-(*tert*-butyl)-1*H*-indole-2,3-diyl)dibenzoate (4aa)



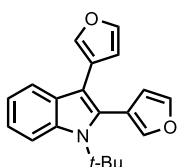
33.7 mg, 72% yield: white solid. Mp = 149–151 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.97 (d, *J* = 8.2 Hz, 2H), 7.87 (d, *J* = 8.3 Hz, 2H), 7.81 (d, *J* = 8.5 Hz, 1H), 7.61 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.41 (d, *J* = 8.2 Hz, 2H), 7.27 (t, *J* = 7.2 Hz, 1H), 7.18–7.13 (m, 3H), 4.40 (q, *J* = 7.1 Hz, 2H), 4.34 (q, *J* = 7.1 Hz, 2H), 1.64 (s, 9H), 1.42 (t, *J* = 7.2 Hz, 3H), 1.37 (t, *J* = 7.1 Hz, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 166.7, 166.2, 140.8, 139.8, 137.2, 136.8, 131.6, 130.0, 129.9, 129.1, 128.7, 128.3, 127.5, 121.8, 120.1, 119.5, 117.4, 115.2, 61.1, 60.7, 59.6, 32.2, 14.32, 14.28; HRMS-EI calcd for C₃₀H₃₁NO₄ [M]⁺ 469.2248, found 469.2256.

1-(*tert*-butyl)-2,3-bis(3,5-dimethylphenyl)-1*H*-indole (4ab)^[13]



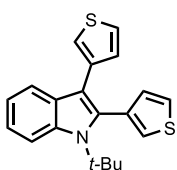
25.9 mg, 68% yield: white solid; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.81 (dt, J = 8.6, 0.9 Hz, 1H), 7.73–7.69 (m, 1H), 7.25 (ddd, J = 8.4, 7.0, 1.4 Hz, 1H), 7.16 (ddd, J = 7.8, 6.9, 0.9 Hz, 1H), 7.00–6.98 (m, 2H), 6.96–6.94 (m, 1H), 6.86–6.84 (m, 2H), 6.81–6.79 (m, 1H), 2.31 (s, 6H), 2.24 (s, 6H), 1.68 (s, 9H).

1-(*tert*-butyl)-2,3-di(furan-3-yl)-1*H*-indole (4ac)^[13]



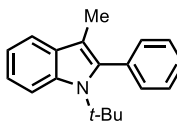
12.8 mg, 42% yield: white solid; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.77 (d, J = 8.5 Hz, 1H), 7.71 (dd, J = 7.9, 1.3 Hz, 1H), 7.50 (t, J = 1.7 Hz, 1H), 7.36–7.33 (m, 3H), 7.22 (ddd, J = 8.5, 6.9, 1.4 Hz, 1H), 7.14 (t, J = 7.5 Hz, 1H), 6.49 (d, J = 1.7 Hz, 1H), 6.26 (t, J = 1.3 Hz, 1H), 1.73 (s, 9H).

1-(*tert*-butyl)-2,3-di(thiophen-3-yl)-1*H*-indole (4ad)



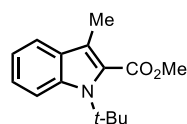
12.1 mg, 36% yield: white solid. Mp = 116–118 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.78 (d, J = 8.5 Hz, 1H), 7.75 (d, J = 8.0 Hz, 1H), 7.31 (dd, J = 4.9, 3.0 Hz, 1H), 7.23 (t, J = 7.8 Hz, 1H), 7.18–7.12 (m, 3H), 7.10 (dd, J = 4.9, 1.2 Hz, 1H), 6.94–6.92 (m, 1H), 6.81 (dd, J = 5.0, 1.2 Hz, 1H), 1.67 (s, 9H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 136.4, 136.0, 135.1, 132.4, 131.2, 128.7, 128.1, 126.0, 124.5, 123.8, 121.3, 121.2, 119.8, 119.5, 114.9, 113.8, 59.2, 31.6; **HRMS-EI** calcd for $\text{C}_{20}\text{H}_{19}\text{NS}_2$ $[\text{M}]^+$ 337.0953, found 337.0952.

1-(*tert*-butyl)-3-methyl-2-phenyl-1*H*-indole (4ae)^[13]



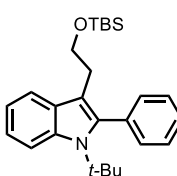
19.7 mg, 75% yield: pale yellow oil; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.73 (d, J = 8.4 Hz, 1H), 7.58 (dt, J = 7.7, 1.1 Hz, 1H), 7.42–7.37 (m, 3H), 7.36–7.32 (m, 2H), 7.21 (ddd, J = 8.4, 7.0, 1.5 Hz, 1H), 7.15 (t, J = 7.3 Hz, 1H), 1.99 (s, 3H), 1.58 (s, 9H).

methyl 1-(*tert*-butyl)-3-methyl-1*H*-indole-2-carboxylate (4af)



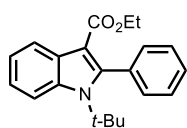
15.4 mg, 63% yield: pale yellow oil $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.65 (d, J = 8.6 Hz, 1H), 7.58 (dd, J = 7.8, 1.2 Hz, 1H), 7.25 (ddd, J = 8.5, 7.0, 1.3 Hz, 1H), 7.12 (t, J = 7.4 Hz, 1H), 3.92 (s, 3H), 2.33 (s, 3H), 1.76 (s, 9H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 166.1, 138.0, 128.8, 128.7, 123.2, 120.2, 119.2, 116.6, 114.9, 58.4, 52.0, 30.4, 9.0; **HRMS-EI** calcd for $\text{C}_{15}\text{H}_{19}\text{NO}_2$ $[\text{M}]^+$ 245.1410, found 245.1414.

1-(*tert*-butyl)-3-(2-((*tert*-butyldimethylsilyl)oxy)ethyl)-2-phenyl-1*H*-indole (4ag)



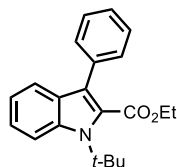
28.9 mg, 71% yield: pale yellow oil $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.72 (d, J = 8.4 Hz, 1H), 7.64 (dt, J = 7.7, 1.0 Hz, 1H), 7.40–7.37 (m, 3H), 7.36–7.33 (m, 2H), 7.20 (ddd, J = 8.5, 7.0, 1.5 Hz, 1H), 7.13 (td, J = 7.5, 0.9 Hz, 1H), 3.63 (t, J = 8.3 Hz, 2H), 2.66 (t, J = 8.3 Hz, 2H), 1.57 (s, 9H), 0.83 (s, 9H), -0.08 (s, 6H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 138.8, 136.7, 136.3, 131.0, 128.9, 127.7, 127.6, 120.7, 118.9, 118.8, 114.8, 111.7, 63.7, 58.7, 32.0, 28.3, 26.0, 18.4, -5.3; **HRMS-EI** calcd for $\text{C}_{26}\text{H}_{37}\text{NOSi}$ $[\text{M}]^+$ 407.2639, found 407.2643.

ethyl 1-(*tert*-butyl)-2-phenyl-1*H*-indole-3-carboxylate (4ah-1)^[13]



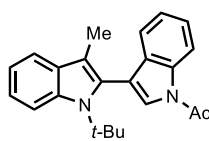
11.9 mg, 37% yield: pale yellow oil; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.34–8.30 (m, 1H), 7.81–7.76 (m, 1H), 7.46–7.35 (m, 5H), 7.31–7.24 (m, 2H), 4.10 (q, J = 7.1 Hz, 2H), 1.60 (s, 9H), 1.09 (t, J = 7.1 Hz, 3H).

ethyl 1-(tert-butyl)-3-phenyl-1H-indole-2-carboxylate (4ah-2)^[13]



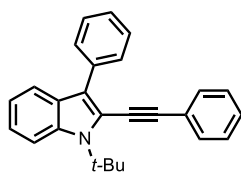
11.9 mg, 37% yield: pale yellow oil; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.74 (d, J = 8.6 Hz, 1H), 7.60 (dd, J = 8.1, 1.2 Hz, 1H), 7.47–7.39 (m, 4H), 7.33 (t, J = 7.2 Hz, 1H), 7.27 (ddd, J = 8.6, 7.0, 1.2 Hz, 1H), 7.12 (t, J = 7.5 Hz, 1H), 4.18 (q, J = 7.2 Hz, 2H), 1.85 (s, 9H), 1.12 (t, J = 7.1 Hz, 3H).

1-(1-(tert-butyl)-3-methyl-1H,1'H-[2,3'-biindol]-1'-yl)ethan-1-one (4ai)



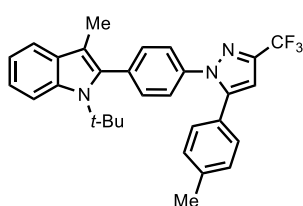
14.1 mg, 41% yield: white solid. Mp = 137–139 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.51 (d, J = 8.4 Hz, 1H), 7.79 (d, J = 8.5 Hz, 1H), 7.62 (d, J = 7.6 Hz, 1H), 7.46–7.40 (m, 2H), 7.33–7.24 (m, 3H), 7.18 (ddd, J = 7.9, 6.9, 0.9 Hz, 1H), 2.72 (s, 3H), 2.04 (s, 3H), 1.67 (s, 9H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 168.6, 136.9, 135.1, 132.3, 129.4, 127.8, 125.5, 124.9, 124.2, 121.1, 120.3, 119.00, 118.97, 118.6, 116.5, 114.6, 113.3, 58.7, 31.1, 24.1, 9.2; **HRMS (ESI-TOF)** calcd for $\text{C}_{23}\text{H}_{25}\text{N}_2\text{O}$ $[\text{M}+\text{H}]^+$ 345.1961, found 345.1962.

1-(tert-butyl)-3-phenyl-2-(phenylethynyl)-1H-indole (4aj)



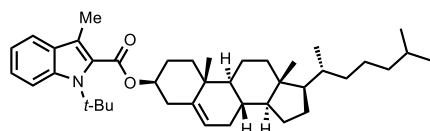
13.2 mg, 38% yield: white solid. Mp = 100–102 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.83 (d, J = 8.7 Hz, 1H), 7.78 (d, J = 7.7 Hz, 2H), 7.75 (d, J = 8.1 Hz, 1H), 7.51 (t, J = 7.6 Hz, 2H), 7.40–7.30 (m, 6H), 7.26–7.22 (m, 1H), 7.13 (t, J = 7.5 Hz, 1H), 2.08 (s, 9H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 136.7, 134.4, 130.5, 130.1, 128.4, 128.1, 127.2, 126.5, 125.5, 123.5, 123.1, 120.1, 119.7, 118.6, 114.2, 97.5, 85.3, 60.2, 31.6; **HRMS (ESI-TOF)** calcd for $\text{C}_{26}\text{H}_{24}\text{N}$ $[\text{M}+\text{H}]^+$ 350.1903, found 350.1905.

1-(tert-butyl)-3-methyl-2-(4-(5-(p-tolyl)-3-(trifluoromethyl)-1H-pyrazol-1-yl)phenyl)-1H-indole (4ak)



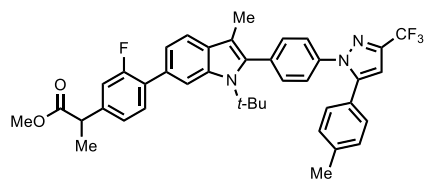
34.6 mg, 71% yield: white solid. Mp = 201–203 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.74 (dt, J = 8.5, 0.9 Hz, 1H), 7.59 (ddd, J = 7.8, 1.4, 0.7 Hz, 1H), 7.40–7.35 (m, 4H), 7.24 (ddd, J = 8.4, 7.0, 1.4 Hz, 1H), 7.19–7.14 (m, 5H), 6.80 (s, 1H), 2.41 (s, 3H), 2.01 (s, 3H), 1.61 (s, 9H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 144.9, 143.2 (q, J = 38.3 Hz), 139.2, 138.4, 137.8, 136.6, 136.3, 131.6, 129.3, 129.3, 128.6, 126.1, 125.0, 121.3 (q, J = 268.9 Hz), 121.1, 118.8, 114.7, 111.6, 105.2, 58.7, 32.0, 21.2, 8.9; **HRMS-EI** calcd for $\text{C}_{30}\text{H}_{28}\text{F}_3\text{N}_3$ $[\text{M}]^+$ 487.2230, found 487.2234.

(3S,8S,9S,10R,13R,14S,17R)-10,13-dimethyl-17-((R)-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-yl 1-(tert-butyl)-3-methyl-1H-indole-2-carboxylate (4al)



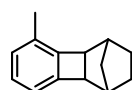
37.7 mg, 63% yield: white solid. Mp = 144-146 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.64 (d, *J* = 8.5 Hz, 1H), 7.57 (d, *J* = 7.8 Hz, 1H), 7.23 (ddd, *J* = 8.4, 6.9, 1.3 Hz, 1H), 7.10 (t, *J* = 7.4 Hz, 1H), 5.46 (d, *J* = 4.2 Hz, 1H), 4.95–4.85 (m, 1H), 2.50 (d, *J* = 8.1 Hz, 2H), 2.33 (s, 3H), 2.10–1.98 (m, 3H), 1.93 (dt, *J* = 13.4, 3.6 Hz, 1H), 1.89–1.82 (m, 1H), 1.81–1.74 (m, 10H), 1.60–1.45 (m, 6H), 1.43–1.30 (m, 3H), 1.30–1.18 (m, 3H), 1.18–1.09 (m, 5H), 1.09–0.96 (m, 6H), 0.93 (d, *J* = 6.5 Hz, 3H), 0.88 (d, *J* = 6.6 Hz, 3H), 0.87 (d, *J* = 6.6 Hz, 3H), 0.69 (s, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 165.1, 139.4, 137.8, 129.4, 128.8, 122.96, 122.98, 120.1, 119.1, 115.7, 114.8, 75.2, 58.5, 56.7, 56.1, 50.0, 42.3, 39.7, 39.5, 38.1, 37.0, 36.6, 36.2, 35.8, 31.9, 31.8, 30.6, 28.2, 28.0, 27.8, 24.3, 23.8, 22.8, 22.6, 21.0, 19.3, 18.7, 11.9, 9.1; HRMS-EI calcd for C₄₁H₆₁NO₂ [M]⁺ 599.4697, found 599.4699.

methyl 2-(4-(1-(*tert*-butyl)-3-methyl-2-(4-(5-(*p*-tolyl)-3-(trifluoromethyl)-1*H*-pyrazol-1-yl)phenyl)-1*H*-indol-6-yl)-3-fluorophenyl)propanoate (4am)



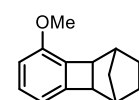
46.7 mg, 70% yield: white solid. Mp = 200-202 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.93 (s, 1H), 7.64 (d, *J* = 8.1 Hz, 1H), 7.52 (t, *J* = 8.0 Hz, 1H), 7.41–7.36 (m, 4H), 7.33 (d, *J* = 8.2 Hz, 1H), 7.23–7.14 (m, 6H), 6.80 (s, 1H), 3.82 (q, *J* = 7.2 Hz, 1H), 3.75 (s, 3H), 2.41 (s, 3H), 2.02 (s, 3H), 1.63 (s, 9H), 1.59 (d, *J* = 7.2 Hz, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 174.5, 159.8 (d, *J* = 247.4 Hz), 144.9, 143.3 (q, *J* = 38.3 Hz), 141.0 (d, *J* = 7.5 Hz), 139.2, 138.5, 137.6, 137.3, 136.6, 131.5, 131.2 (d, *J* = 3.3 Hz), 129.4 (d, *J* = 13.5 Hz), 129.3, 128.8, 128.6, 128.2, 126.1, 125.1, 123.4 (d, *J* = 3.3 Hz), 121.3 (q, *J* = 269.0 Hz), 120.1, 118.7, 115.5 (d, *J* = 3.6 Hz), 115.2 (d, *J* = 23.8 Hz), 111.6, 105.2, 58.9, 52.2, 44.9, 32.1, 21.3, 18.4, 8.9; HRMS-EI calcd for C₄₀H₃₇F₄N₃O₂ [M]⁺ 667.2816, found 667.2809.

5-methyl-1,2,3,4,4a,8b-hexahydro-1,4-methanobiphenylene (5a)^[14]



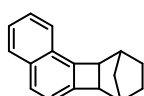
12.0 mg, 65% yield: colorless oil. ¹H NMR (500 MHz, CDCl₃) δ 7.10 (t, *J* = 7.5 Hz, 1H), 6.98 (d, *J* = 7.8 Hz, 1H), 6.81 (d, *J* = 7.2 Hz, 1H), 3.14 (q, *J* = 4.0 Hz, 2H), 2.32–2.23 (m, 2H), 2.18 (s, 3H), 1.63–1.57 (m, 2H), 1.21–1.15 (m, 2H), 0.98–0.93 (m, 1H), 0.87–0.83 (m, 1H).

5-methoxy-1,2,3,4,4a,8b-hexahydro-1,4-methanobiphenylene (5b)^[14]



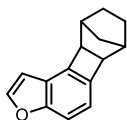
13.4 mg, 67% yield: colorless oil. ¹H NMR (400 MHz, CDCl₃) δ 7.15–7.10 (m, 1H), 6.68 (d, *J* = 8.4, 0.6 Hz, 1H), 6.60 (d, *J* = 7.1 Hz, 1H), 3.88 (s, 3H), 3.30 (d, *J* = 3.9 Hz, 1H), 3.15 (d, *J* = 3.9 Hz, 1H), 2.34–2.30 (m, 1H), 2.26 (dp, *J* = 2.5, 1.4 Hz, 1H), 1.65–1.58 (m, 2H), 1.23–1.16 (m, 2H), 1.03–0.98 (m, 2H).

6b,7,8,9,10a-hexahydro-7,10-methanobenzo[*a*]biphenylene (5c)^[15]



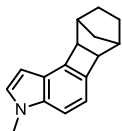
17.0 mg, 77% yield: colorless oil. ¹H NMR (400 MHz, CDCl₃) δ 7.88–7.83 (m, 1H), 7.77–7.72 (m, 2H), 7.50–7.38 (m, 2H), 7.20 (d, *J* = 8.1 Hz, 1H), 3.44 (d, *J* = 3.6 Hz, 1H), 3.31–3.28 (m, 1H), 2.44 (dq, *J* = 2.8, 1.5 Hz, 1H), 2.31 (dq, *J* = 3.1, 1.5 Hz, 1H), 1.70–1.63 (m, 2H), 1.31–1.25 (m, 2H), 0.99–0.93 (m, 1H), 0.79–0.73 (m, 1H).

5b,6,7,8,9a-hexahydro-6,9-methanobiphenyleno[2,1-*b*]furan (5d)



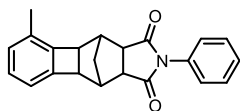
7.1 mg, 34% yield: colorless oil. $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.61 (d, $J = 2.3$ Hz, 1H), 7.39 (d, $J = 8.1$ Hz, 1H), 6.92 (d, $J = 8.2$ Hz, 1H), 6.64 (dd, $J = 2.4, 1.0$ Hz, 1H), 3.27 (dd, $J = 27.2, 3.7$ Hz, 2H), 2.36–2.25 (m, 2H), 1.68–1.58 (m, 2H), 1.25–1.18 (m, 2H), 0.98–0.91 (m, 1H), 0.81–0.75 (m, 1H). $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 155.9, 145.5, 140.3, 138.1, 122.4, 117.7, 110.8, 104.0, 50.5, 49.7, 36.6, 36.2, 32.0, 28.0, 27.9. **HRMS-EI** calcd for $\text{C}_{15}\text{H}_{14}\text{O}$ $[\text{M}]^+$ 210.1039; found 210.1019.

3-methyl-5b,6,7,8,9a-hexahydro-3*H*-6,9-methanobenzo[3,4]cyclobuta[1,2-*e*]indole (5e)



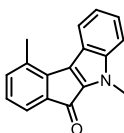
7.8 mg, 35% yield: colorless oil. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.19 (d, $J = 8.1$ Hz, 1H), 7.04 (d, $J = 3.1$ Hz, 1H), 6.88 (d, $J = 8.1$ Hz, 1H), 6.33 (dd, $J = 3.1, 1.0$ Hz, 1H), 3.77 (s, 3H), 3.32 (d, $J = 3.6$ Hz, 1H), 3.23 (d, $J = 3.6$ Hz, 1H), 2.38–2.24 (m, 2H), 1.68–1.52 (m, 2H), 1.29–1.18 (m, 2H), 0.95–0.88 (m, 1H), 0.80–0.75 (m, 1H). $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 137.6, 137.2, 136.9, 129.3, 123.6, 115.3, 108.7, 97.6, 50.4, 49.8, 36.7, 36.1, 33.1, 32.0, 28.2, 28.1. **HRMS-EI** calcd for $\text{C}_{16}\text{H}_{17}\text{N}$ $[\text{M}]^+$ 223.1356; found 223.1354.

5-methyl-2-phenyl-3a,4,4a,8b,9,9a-hexahydro-1*H*-4,9-methanobenzo[3,4]cyclobuta[1,2-*f*]isoindole-1,3(2*H*)-dione (5f)



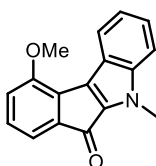
17.7 mg, 54% yield: white solid. Mp = 76–78 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.48 (dd, $J = 8.4, 6.9$ Hz, 2H), 7.43–7.38 (m, 1H), 7.29–7.24 (m, 2H), 7.16 (t, $J = 7.6$ Hz, 1H), 7.03 (d, $J = 7.9$ Hz, 1H), 6.83 (d, $J = 7.2$ Hz, 1H), 3.53–3.48 (m, 2H), 3.41–3.35 (m, 2H), 3.02–2.93 (m, 2H), 2.18 (s, 3H), 1.44 (dt, $J = 11.0, 1.6$ Hz, 1H), 1.38–1.32 (m, 1H). $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 177.0, 143.8, 142.6, 132.7, 131.9, 129.4, 129.2, 128.9, 128.8, 126.9, 119.5, 47.8, 47.7, 44.9, 44.7, 39.5, 38.9, 36.1, 16.7. **HRMS-EI** calcd for $\text{C}_{22}\text{H}_{19}\text{NO}_2$ $[\text{M}]^+$ 329.1410; found 329.1411.

5,10-dimethylindeno[2,1-*b*]indol-6(5*H*)-one (5g)



13.1 mg, 53% yield: red solid; Mp = 132–133 °C. $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.86 (d, $J = 8.3$ Hz, 1H), 7.30–7.24 (m, 2H), 7.17–7.10 (m, 2H), 7.02 (d, $J = 7.8$ Hz, 1H), 6.88 (t, $J = 7.4$ Hz, 1H), 3.86 (s, 3H), 2.60 (s, 3H). $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 185.2, 144.0, 139.8, 137.1, 136.9, 136.6, 133.6, 128.7, 126.7, 125.7, 122.8, 121.9, 121.4, 121.3, 111.5, 30.5, 21.3. **HRMS-ESI** calcd for $\text{C}_{17}\text{H}_{14}\text{NO}$ $[\text{M}+\text{H}]^+$, 248.1070; found 248.1071.

10-methoxy-5-methylindeno[2,1-*b*]indol-6(5*H*)-one (5h)



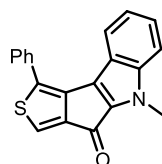
8.7 mg, 33% yield: red solid; Mp = 135–136 °C. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.90 (d, $J = 7.9$ Hz, 1H), 7.25–7.19 (m, 2H), 7.15–7.09 (m, 1H), 6.99–6.95 (m, 2H), 6.92–6.85 (m, 1H), 3.98 (s, 3H), 3.85 (s, 3H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 184.8, 151.0, 144.1, 138.3, 135.5, 133.3, 128.4, 127.2, 126.0, 123.8, 121.7, 121.6, 118.8, 116.8, 111.1, 55.9, 30.6. **HRMS-ESI** calcd for $\text{C}_{17}\text{H}_{14}\text{NO}_2$ $[\text{M}+\text{H}]^+$, 264.1019; found 264.1019.

10-fluoro-5-methylindeno[2,1-*b*]indol-6(5*H*)-one (5i)



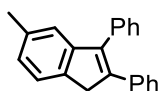
6.3 mg, 25% yield: red solid; Mp = 129-130 °C. $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.84–7.78 (m, 1H), 7.37–7.31 (m, 1H), 7.31–7.28 (m, 1H), 7.23–7.18 (m, 1H), 7.16–7.12 (m, 1H), 7.04–6.96 (m, 2H), 3.90 (s, 3H). $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 183.2, 153.9 (d, $J = 249.0$ Hz), 143.9, 139.3 (d, $J = 5.7$ Hz), 136.0, 130.7, 128.5 (d, $J = 5.9$ Hz), 126.4, 125.2 (d, $J = 18.1$ Hz), 122.8, 122.6, 122.1, 121.2, 119.7, 111.2, 30.6. $^{19}\text{F NMR}$ (471 MHz, CDCl_3) δ -120.14. **HRMS-ESI** calcd for $\text{C}_{16}\text{H}_{11}\text{FNO}$ $[\text{M}+\text{H}]^+$ 252.0819, found 252.0820.

5-methyl-1-phenylthieno[3',4':3,4]cyclopenta[1,2-*b*]indol-4(5*H*)-one (5j)



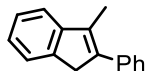
13.5 mg, 43% yield: red solid; Mp = 134-135 °C. $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.69 (d, $J = 7.4$ Hz, 2H), 7.53 (t, $J = 7.4$ Hz, 2H), 7.51–7.45 (m, 2H), 7.34–7.29 (m, 3H), 7.05 (t, $J = 7.5$ Hz, 1H), 3.94 (s, 3H). $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 178.2, 145.4, 143.3, 143.2, 134.3, 133.6, 130.9, 130.1, 128.8, 128.7, 126.2, 126.1, 123.8, 121.6, 120.4, 111.2, 30.4. **HRMS-ESI** calcd for $\text{C}_{20}\text{H}_{14}\text{NOS}$ $[\text{M}+\text{H}]^+$, 316.0791; found 316.0792.

5-methyl-2,3-diphenyl-1*H*-indene (5k)



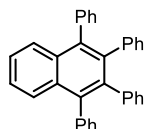
7.8 mg, 28% yield: white solid. Mp = 105-108 °C. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.47–7.38 (m, 3H), 7.41–7.32 (m, 3H), 7.29–7.27 (m, 1H), 7.28–7.23 (m, 1H), 7.24–7.13 (m, 3H), 7.05 (d, $J = 7.5$ Hz, 1H), 7.02 (s, 1H), 3.88 (s, 2H), 2.35 (s, 3H). $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 147.1, 141.3, 139.9, 139.4, 136.6, 136.2, 136.2, 129.4, 128.8, 128.2, 128.1, 127.3, 126.8, 125.9, 123.3, 120.9, 40.8, 21.5. **HRMS-EI** calcd for $\text{C}_{22}\text{H}_{18}$ $[\text{M}]^+$ 282.1403, found 282.1410.

3-methyl-2-phenyl-1*H*-indene (5l)^[16]



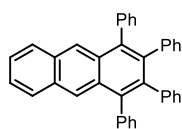
4.9 mg, 24% yield: white solid. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.50–7.46 (m, 3H), 7.44–7.36 (m, 3H), 7.34 (t, $J = 7.3$ Hz, 1H), 7.29 (d, $J = 7.3$ Hz, 1H), 7.23 (dd, $J = 7.3$, 1.4 Hz, 1H), 3.74 (q, $J = 2.2$ Hz, 2H), 2.31 (t, $J = 2.1$ Hz, 3H).

1,2,3,4-tetraphenylnaphthalene (5m)^[17a]



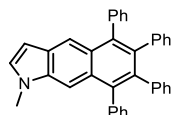
32.4 mg, 75% yield; white solid; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.66 (dd, $J = 6.5$, 3.3 Hz, 2H), 7.40 (dd, $J = 6.5$, 3.3 Hz, 2H), 7.29–7.17 (m, 10H), 6.92–6.79 (m, 10H).

1,2,3,4-tetraphenylanthracene (5n)^[17b]



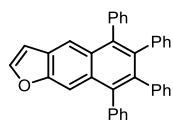
14.5 mg, 30% yield; yellow solid; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.21 (s, 2H), 7.86–7.81 (m, 2H), 7.43–7.34 (m, 2H), 7.34–7.24 (m, 10H), 6.93–6.84 (m, 10H).

1-methyl-5,6,7,8-tetraphenyl-1*H*-benzo[*f*]indole (5o)



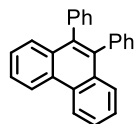
20.4 mg, 42% yield; white solid. Mp = 114-116 °C; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.89 (d, $J = 0.9$ Hz, 1H), 7.46 (s, 1H), 7.33–7.27 (m, 8H), 7.24–7.16 (m, 3H), 6.91–6.79 (m, 10H), 6.48 (d, $J = 3.3$ Hz, 1H), 3.68 (s, 3H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 141.3, 141.2, 140.7, 140.6, 138.1, 137.4, 136.8, 135.7, 133.1, 131.6, 131.5, 131.4, 129.9, 128.9, 127.5, 127.4, 127.3, 126.4, 126.2, 126.1, 125.0, 124.9, 118.0, 104.0, 100.4, 32.9; **HRMS (ESI-TOF)** calcd for $\text{C}_{37}\text{H}_{28}\text{N}$ $[\text{M}+\text{H}]^+$ 486.2216, found 486.2218.

5,6,7,8-tetraphenylnaphtho[2,3-*b*]furan (5p)



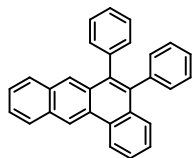
25.2 mg, 53% yield; yellow solid. Mp = 90–92 °C; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.57 (s, 2H), 7.37 (d, $J = 2.3$ Hz, 1H), 7.30–7.22 (m, 11H), 6.91–6.81 (m, 10H); $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 153.4, 142.6, 141.4, 140.6, 140.3, 139.8, 139.3, 137.7, 137.0, 131.4, 131.3, 131.2, 131.0, 129.2, 128.0, 127.5, 126.9, 126.7, 126.5, 126.4, 126.3, 125.3, 125.2, 124.7, 122.4, 112.5, 108.7; **HRMS-EI** calcd for $\text{C}_{36}\text{H}_{24}\text{O}$ $[\text{M}]^+$ 472.1822, found 472.1822.

9,10-diphenylphenanthrene (5q)^[18]



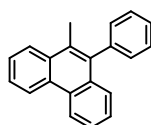
18.1 mg, 55% yield: white solid. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.81 (d, $J = 8.3$ Hz, 2H), 7.69–7.63 (m, 2H), 7.60–7.54 (m, 2H), 7.52–7.45 (m, 2H), 7.26 (t, 1H), 7.25–7.14 (m, 9H).

5,6-diphenyltetraphen (5r)^[18]



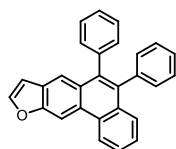
13.3 mg, 35% yield: white solid. $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 9.29 (s, 1H), 8.96 (d, $J = 8.2$ Hz, 1H), 8.14 (d, $J = 8.3$ Hz, 1H), 8.01 (s, 1H), 7.83 (d, $J = 8.3$ Hz, 1H), 7.73–7.64 (m, 1H), 7.59–7.42 (m, 4H), 7.32–7.25 (m, 3H), 7.26–7.16 (m, 7H).

9-methyl-10-phenylphenanthrene (5s)^[18]



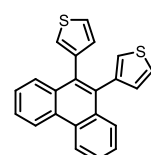
(7.0 mg, 25% yield): white solid. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.85–8.79 (m, 1H), 8.79–8.72 (m, 1H), 8.21–8.15 (m, 1H), 7.76–7.67 (m, 2H), 7.63–7.58 (m, 1H), 7.58–7.53 (m, 2H), 7.52–7.42 (m, 2H), 7.39 (dd, $J = 8.4, 1.5$ Hz, 1H), 7.36–7.32 (m, 2H), 2.49 (s, 3H).

5,6-diphenylphenanthro[3,2-b]furan (5t)



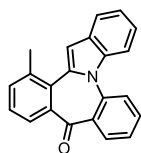
9.6 mg, 26% yield: white solid. Mp = 200–202 °C; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.89 (s, 1H), 8.81 (d, $J = 8.5$ Hz, 1H), 7.74 (d, $J = 2.3$ Hz, 1H), 7.73 (s, 1H), 7.71–7.64 (m, 1H), 7.56–7.52 (m, 1H), 7.51–7.45 (m, 2H), 7.25–7.15 (m, 9H), 6.79 (dd, $J = 2.3, 1.0$ Hz, 1H), $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 153.9, 146.5, 139.7, 139.3, 136.9, 135.2, 131.4, 130.8, 130.7, 130.7, 129.9, 128.4, 127.7, 127.5, 127.3, 127.2, 127.2, 126.1, 126.0, 125.9, 122.2, 119.5, 106.3, 103.1; **HRMS-EI** calcd for $\text{C}_{28}\text{H}_{18}\text{O}$ $[\text{M}]^+$ 370.1355, found 370.1352.

9,10-di(thiophen-2-yl)phenanthrene (5u)^[18]



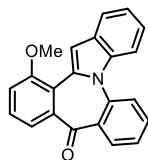
7.9 mg, 23% yield: white solid. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.78 (d, $J = 8.3$ Hz, 2H), 7.73 (d, $J = 8.2$ Hz, 2H), 7.70–7.62 (m, 2H), 7.55–7.49 (m, 2H), 7.28–7.24 (m, 2H), 6.97 (m, 4H).

14-methyl-10H-dibenzo[3,4:6,7]azepino[1,2-a]indol-10-one (5v)



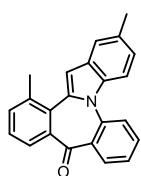
19.8 mg, 64% yield: light-yellow solid. Mp = 162-164 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.82–7.76 (m, 1H), 7.71–7.68 (m, 1H), 7.67–7.63 (m, 3H), 7.52 (d, J = 7.6 Hz, 2H), 7.38 (td, J = 7.5, 1.1 Hz, 1H), 7.32 (t, J = 7.6 Hz, 1H), 7.28–7.22 (m, 2H), 6.85 (s, 1H), 2.70 (s, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 197.7, 143.7, 139.4, 137.5, 136.3, 135.7, 135.3, 135.2, 132.1, 129.1, 128.4, 128.0, 127.9, 126.7, 125.3, 125.2, 123.3, 121.8, 120.9, 111.2, 108.2, 22.5. HRMS-EI calcd for $\text{C}_{22}\text{H}_{15}\text{NO}$ $[\text{M}]^+$ 309.1148; found 309.1148.

14-methoxy-10H-dibenzo[3,4:6,7]azepino[1,2-a]indol-10-one (5w)



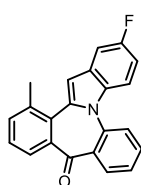
17.6 mg, 54% yield: light-yellow solid. Mp = 160-162 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.74 (d, J = 8.1 Hz, 1H), 7.71–7.67 (m, 1H), 7.62 (q, J = 7.4 Hz, 3H), 7.38–7.34 (m, 2H), 7.32–7.26 (m, 2H), 7.22 (m, 2H), 7.18 (s, 1H), 3.97 (s, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 197.7, 157.4, 143.7, 139.0, 136.9, 136.4, 133.1, 132.5, 129.1, 128.7, 128.6, 128.2, 126.8, 125.6, 123.4, 121.9, 121.4, 120.3, 119.4, 115.3, 111.7, 108.5, 56.6. HRMS-EI calcd for $\text{C}_{22}\text{H}_{15}\text{NO}_2$ $[\text{M}]^+$ 325.1100; found 325.1097.

2,14-dimethyl-10H-dibenzo[3,4:6,7]azepino[1,2-a]indol-10-one (5x)



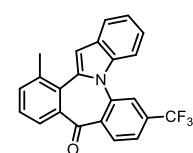
22.4 mg, 69% yield: light-yellow solid. Mp = 168-169 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.79–7.74 (m, 1H), 7.66–7.59 (m, 2H), 7.54–7.45 (m, 4H), 7.38–7.28 (m, 2H), 7.08 (dd, J = 8.6, 1.7 Hz, 1H), 6.75 (s, 1H), 2.68 (s, 3H), 2.48 (s, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 197.9, 143.6, 139.3, 137.4, 135.9, 135.3, 135.2, 134.7, 132.2, 131.2, 129.3, 128.4, 128.2, 127.8, 126.5, 125.2, 125.1, 124.9, 120.5, 110.9, 107.8, 22.5, 21.5. HRMS-EI calcd for $\text{C}_{23}\text{H}_{17}\text{NO}$ $[\text{M}]^+$ 323.1463; found 323.1461.

2-fluoro-14-methyl-10H-dibenzo[3,4:6,7]azepino[1,2-a]indol-10-one (5y)



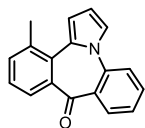
24.4 mg, 74% yield: light-yellow solid. Mp = 157-159 °C; ^1H NMR (500 MHz, CDCl_3) δ 7.74 (d, J = 8.0 Hz, 1H), 7.64 (t, J = 8.1 Hz, 2H), 7.57–7.48 (m, 3H), 7.39 (t, J = 7.6 Hz, 1H), 7.35–7.28 (m, 2H), 7.02–6.95 (m, 1H), 6.79 (s, 1H), 2.68 (s, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 197.5, 158.9 (d, J = 237.4 Hz), 143.6, 139.4, 137.5, 136.8, 135.5, 135.3, 132.9, 132.3, 128.8, 128.5, 128.4 (d, J = 10.7 Hz), 128.2, 126.9, 125.3, 125.1, 112.2 (d, J = 9.3 Hz), 111.6 (d, J = 26.2 Hz), 107.9 (d, J = 4.2 Hz), 105.6 (d, J = 23.4 Hz), 22.5. ^{19}F NMR (471 MHz, CDCl_3) δ -122.31. HRMS-EI calcd for $\text{C}_{22}\text{H}_{14}\text{FNO}$ $[\text{M}]^+$ 327.1210; found 327.1215.

14-methyl-7-(trifluoromethyl)-10H-dibenzo[3,4:6,7]azepino[1,2-a]indol-10-one (5z)



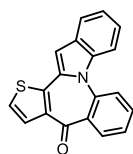
26.3 mg, 70% yield: light-yellow solid. Mp = 157-159 °C. ^1H NMR (400 MHz, CDCl_3) δ 8.07 (d, J = 1.6 Hz, 1H), 7.79 – 7.69 (m, 2H), 7.65 – 7.58 (m, 2H), 7.57 – 7.49 (m, 2H), 7.37 – 7.26 (m, 3H), 6.88 (s, 1H), 2.70 (s, 3H). ^{13}C NMR (201 MHz, CDCl_3) δ 196.6, 143.0, 141.9, 137.8, 136.22, 136.21, 135.7, 135.2, 134.1 (q, J = 33.2 Hz), 129.2, 129.0, 128.1, 125.4, 123.9, 123.4 (q, J = 272.9 Hz), 123.2 (q, J = 3.7 Hz), 122.4 (q, J = 3.8 Hz), 122.3, 121.2, 110.7, 109.0, 22.5. ^{19}F NMR (471 MHz, CDCl_3) δ -62.94. HRMS-EI calcd for $\text{C}_{23}\text{H}_{14}\text{F}_3\text{NO}$ $[\text{M}]^+$ 377.1022; found 377.1024.

13-methyl-9H-dibenzo[*c,f*]pyrrolo[1,2-*a*]azepin-9-one (5aa)



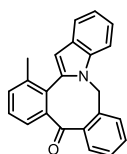
13.0 mg, 50% yield: light-yellow solid. Mp = 160-162 °C. **¹H NMR** (500 MHz, CDCl₃) δ 7.63 (d, *J* = 7.7, 1.4 Hz, 1H), 7.60 – 7.55 (m, 1H), 7.54 – 7.43 (m, 3H), 7.34 (t, *J* = 7.5 Hz, 1H), 7.25 – 7.22 (m, 1H), 7.09 – 7.06 (m, 1H), 6.58 – 6.55 (m, 1H), 6.45 (t, *J* = 3.4 Hz, 1H), 2.59 (s, 3H). **¹³C NMR** (126 MHz, CDCl₃) δ 197.4, 142.2, 137.6, 137.0, 136.6, 135.2, 133.1, 129.5, 129.2, 128.6, 126.8, 126.6, 125.6, 122.9, 122.4, 115.3, 110.0, 22.7. **HRMS-EI** calcd for C₁₈H₁₃NO [M]⁺ 259.0992; found 259.0994.

10H-benzo[6,7]thieno[2',3':3,4]azepino[1,2-a]indol-10-one (5ab)



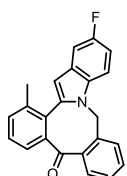
8.2 mg, 27% yield: yellow solid. Mp = 165-167 °C. **¹H NMR** (400 MHz, CDCl₃) δ 8.02 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.91 (d, *J* = 8.2 Hz, 1H), 7.77 (d, *J* = 8.0 Hz, 1H), 7.70 (dd, *J* = 7.3, 1.7 Hz, 1H), 7.64 (td, *J* = 7.8, 1.7 Hz, 1H), 7.48 – 7.40 (m, 2H), 7.34 – 7.26 (m, 2H), 7.23 (d, *J* = 5.3 Hz, 1H), 6.98 (s, 1H). **¹³C NMR** (101 MHz, CDCl₃) δ 186.9, 140.4, 139.7, 138.3, 136.7, 135.2, 133.4, 132.7, 130.9, 129.3, 128.6, 126.4, 125.2, 124.5, 123.9, 122.5, 121.5, 113.3, 105.2. **HRMS-EI** calcd for C₁₉H₁₁NOS [M]⁺ 301.0712; found 301.0688.

1-methyldibenzo[3,4:6,7]azocino[1,2-a]indol-5(10H)-one (5ac)



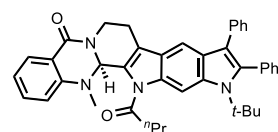
13.6 mg, 42% yield: white solid. Mp = 158-159 °C. **¹H NMR** (400 MHz, CDCl₃) δ 7.84 (d, *J* = 7.7 Hz, 1H), 7.62 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.55 – 7.52 (m, 2H), 7.45 – 7.39 (m, 2H), 7.36 (t, *J* = 7.6 Hz, 1H), 7.25 (dd, *J* = 7.2, 1.0 Hz, 1H), 7.18 – 7.08 (m, 3H), 6.65 (s, 1H), 5.29 (d, *J* = 16.1 Hz, 1H), 5.06 (d, *J* = 16.1 Hz, 1H), 2.49 (s, 3H). **¹³C NMR** (101 MHz, CDCl₃) δ 200.9, 144.5, 139.1, 138.3, 137.3, 136.3, 135.9, 132.5, 131.2, 130.3, 128.7, 128.6, 128.6, 128.5, 128.1, 123.4, 122.0, 121.1, 120.5, 109.5, 102.9, 47.6, 20.4. **HRMS-EI** calcd for C₂₃H₁₇NO [M]⁺ 323.1305; found 323.1313.

14-fluoro-1-methyldibenzo[3,4:6,7]azocino[1,2-a]indol-5(10H)-one (5ad)



15.0 mg, 44% yield: white solid. Mp = 160-162 °C. **¹H NMR** (500 MHz, CDCl₃) δ 7.84 (dd, *J* = 7.7, 1.4 Hz, 1H), 7.57 – 7.50 (m, 2H), 7.45 – 7.40 (m, 2H), 7.37 (t, *J* = 7.6 Hz, 1H), 7.24 (dd, *J* = 9.5, 2.5 Hz, 1H), 7.15 – 7.08 (m, 2H), 6.88 (td, *J* = 9.1, 2.5 Hz, 1H), 6.59 (s, 1H), 5.28 (d, *J* = 16.1 Hz, 1H), 5.01 (d, *J* = 16.1 Hz, 1H), 2.48 (s, 3H). **¹³C NMR** (126 MHz, CDCl₃) δ 200.2, 157.8 (d, *J* = 235.2 Hz), 143.7, 138.2, 137.6, 136.9, 136.6, 132.3, 131.9, 130.7, 129.8, 128.3, 128.2, 128.1, 128.0, 127.2, 122.8, 109.7 (d, *J* = 26.3 Hz), 109.5 (d, *J* = 9.8 Hz), 105.3 (d, *J* = 23.5 Hz), 102.3 (d, *J* = 4.6 Hz), 47.1, 19.7. **¹⁹F NMR** (471 MHz, CDCl₃) δ -123.96. **HRMS-EI** calcd for C₂₃H₁₆FNO [M]⁺ 341.1210; found 341.1211.

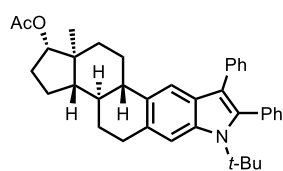
(S)-12-(tert-butyl)-14-butyryl-15-methyl-10,11-diphenyl-7,8,12,14,14b,15-hexahydro-5H-pyrrolo[3'',2'':5',6']indolo[2',3':3,4]pyrido[2,1-b]quinazolin-5-one (6a)



26.7 mg, 43% yield: white solid. Mp > 200 °C; **¹H NMR** (400 MHz, CDCl₃) δ 9.03 (d, *J* = 2.4 Hz, 1H), 8.19 – 8.12 (m, 1H), 7.67 (s, 1H), 7.55 – 7.47 (m, 1H), 7.38 – 7.33 (m, 2H), 7.32 – 7.21 (m, 6H), 7.20 – 7.13 (m, 4H), 6.24 (s, 1H), 4.96 (dd, *J* = 12.9, 5.1 Hz, 1H), 3.43 – 3.32 (m, 1H), 3.31 – 3.21 (m, 1H), 3.09 – 3.00 (m, 1H), 2.98 – 2.79 (m, 2H), 2.38 (s, 3H), 1.91 (h, *J* = 7.4 Hz, 2H), 1.73 (s, 9H), 1.02 (t, *J* = 7.4 Hz, 3H); **¹³C NMR** (101 MHz, CDCl₃) δ 173.0, 164.2, 150.3, 139.5, 136.6, 136.2, 135.1, 134.3, 133.2, 131.6, 131.5, 130.3, 129.0, 127.8, 127.7, 127.4,

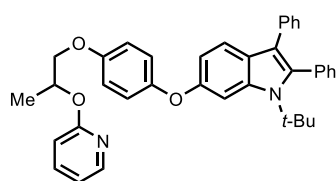
127.3, 126.8, 126.7, 125.6, 124.2, 124.1, 123.7, 122.3, 122.2, 117.5, 107.8, 102.9, 69.1, 59.4, 39.3, 37.5, 36.1, 32.0, 20.9, 18.4, 13.8; **HRMS (ESI-TOF)** calcd for $C_{41}H_{41}N_4O_2$ $[M+H]^+$ 621.3224, found 621.3226.

(1*S*,3*aS*,3*bR*,10*bS*,12*aS*)-7-(*tert*-butyl)-12*a*-methyl-8,9-diphenyl-1,2,3,3*a*,3*b*,4,5,7,10*b*,11,12,12*a*-dodecahydrocyclopenta[5,6]naphtho[1,2-*f*]indol-1-yl acetate (6b)



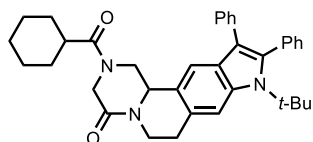
32.1 mg, 59% yield: white solid. Mp = 188–190 °C; **¹H NMR** (500 MHz, $CDCl_3$) δ 7.53 (d, J = 6.4 Hz, 2H), 7.32–7.23 (m, 5H), 7.21–7.16 (m, 2H), 7.14–7.09 (m, 3H), 4.69 (t, J = 8.4 Hz, 1H), 3.16–3.09 (m, 2H), 2.40–2.30 (m, 2H), 2.29–2.20 (m, 1H), 2.07 (s, 3H), 2.00–1.94 (m, 1H), 1.89–1.83 (m, 1H), 1.82–1.73 (m, 1H), 1.62 (s, 9H), 1.59–1.51 (m, 3H), 1.50–1.42 (m, 2H), 1.41–1.28 (m, 2H), 0.83 (s, 3H); **¹³C NMR** (126 MHz, $CDCl_3$) δ 171.3, 137.8, 136.5, 135.4, 135.1, 132.3, 131.8, 131.7, 130.3, 130.2, 127.6, 127.5, 127.3, 127.2, 127.2, 125.2, 117.6, 115.4, 114.5, 82.8, 59.0, 50.0, 44.3, 42.8, 38.9, 36.8, 32.1, 30.6, 27.8, 27.6, 26.3, 23.3, 21.2, 12.0; **HRMS-EI** calcd for $C_{38}H_{43}NO_2$ $[M]^+$ 545.3288, found 545.3285.

1-(*tert*-butyl)-2,3-diphenyl-6-(4-(2-(pyridin-2-yloxy)propoxy)phenoxy)-1*H*-indole (6c)



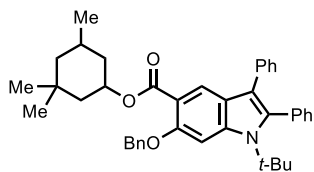
39.2 mg, 69% yield: white solid. Mp = 149–151 °C; **¹H NMR** (500 MHz, $CDCl_3$) δ 8.16 (dd, J = 5.1, 2.0 Hz, 1H), 7.60–7.53 (m, 2H), 7.44 (d, J = 2.0 Hz, 1H), 7.37–7.32 (m, 2H), 7.30–7.25 (m, 3H), 7.21–7.16 (m, 2H), 7.15–7.09 (m, 3H), 7.01 (d, J = 9.0 Hz, 2H), 6.93 (d, J = 9.1 Hz, 2H), 6.88–6.82 (m, 2H), 6.76 (d, J = 8.3 Hz, 1H), 5.65–5.56 (m, 1H), 4.20 (dd, J = 9.9, 5.3 Hz, 1H), 4.09 (dd, J = 9.8, 4.8 Hz, 1H), 1.58 (s, 9H), 1.50 (d, J = 6.4 Hz, 3H); **¹³C NMR** (126 MHz, $CDCl_3$) δ 163.1, 154.4, 152.5, 152.4, 146.7, 138.7, 137.9, 136.8, 136.2, 135.0, 131.8, 130.2, 127.7, 127.6, 127.4, 125.4, 124.9, 120.2, 119.1, 117.7, 116.7, 115.7, 112.2, 111.7, 105.6, 71.1, 69.3, 59.3, 32.0, 17.0; **HRMS-EI** calcd for $C_{38}H_{36}N_2O_3$ $[M]^+$ 568.2720, found 568.2746.

9-(*tert*-butyl)-2-(cyclohexanecarbonyl)-10,11-diphenyl-2,3,6,7,9,12*b*-hexahydropyrazino[2,1-*a*]pyrrolo[2,3-*g*]isoquinolin-4(1*H*)-one (6d)



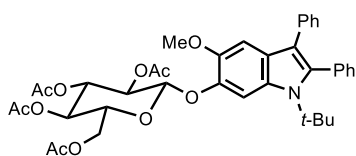
30.2 mg, 54% yield: white solid. Mp > 200 °C; **¹H NMR** (500 MHz, $CDCl_3$) δ 7.58 (s, 1H), 7.47 (s, 1H), 7.33–7.23 (m, 5H), 7.21–7.15 (m, 2H), 7.14–7.03 (m, 3H), 5.22–5.12 (m, 1H), 4.97–4.85 (m, 1H), 4.74–4.65 (m, 1H), 4.46 (d, J = 17.3 Hz, 1H), 4.15–4.03 (m, 1H), 3.22–3.05 (m, 2H), 3.04–2.96 (m, 1H), 2.86 (t, J = 12.0 Hz, 1H), 2.51–2.42 (m, 1H), 1.85–1.68 (m, 5H), 1.62 (s, 9H), 1.59–1.45 (m, 2H), 1.33–1.20 (m, 3H); **¹³C NMR** (126 MHz, $CDCl_3$) δ 174.6, 164.5, 138.9, 135.9, 135.7, 134.4, 131.6, 131.5, 130.1, 128.0, 127.9, 127.7, 127.3, 125.7, 124.5, 117.8, 116.0, 114.6, 59.3, 54.8, 48.9, 45.6, 40.7, 40.1, 32.0, 29.9, 29.2, 28.9, 25.6; **HRMS (ESI-TOF)** calcd for $C_{37}H_{42}N_3O_2$ $[M+H]^+$ 560.3272, found 560.3274.

3,3,5-trimethylcyclohexyl 6-(benzyloxy)-1-(*tert*-butyl)-2,3-diphenyl-1*H*-indole-5-carboxylate (6e)



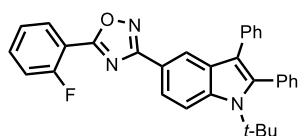
45.5 mg, 76% yield: white solid. Mp = 148-150 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.08 (s, 1H), 7.57 (d, *J* = 7.2 Hz, 2H), 7.41 (t, *J* = 7.4 Hz, 2H), 7.35 – 7.27 (m, 6H), 7.25 (s, 1H), 7.20 (t, *J* = 7.3 Hz, 2H), 7.15 – 7.09 (m, 3H), 5.26 (s, 2H), 5.21 – 5.11 (m, 1H), 2.14 – 2.07 (m, 1H), 1.83 – 1.70 (m, 2H), 1.53 (s, 9H), 1.38 – 1.33 (m, 1H), 1.22 – 1.15 (m, 1H), 0.99 (s, 3H), 0.95-0.90 (m, 7H), 0.79 (t, *J* = 12.7 Hz, 1H); ¹³C NMR (101 MHz, CDCl₃) δ 167.0, 153.3, 138.8, 138.3, 137.5, 135.9, 134.4, 131.7, 130.2, 128.4, 127.8, 127.7, 127.5, 127.4, 125.6, 123.5, 123.0, 118.6, 115.8, 102.1, 72.5, 71.2, 59.3, 47.6, 43.9, 40.4, 33.1, 32.2, 31.8, 27.1, 25.5, 22.3; **HRMS (ESI-TOF)** calcd for C₄₁H₄₆NO₃ [M+H]⁺ 600.3472, found 600.3472.

(2R,3R,4S,5R,6S)-2-(acetoxymethyl)-6-((1-(tert-butyl)-5-methoxy-2,3-diphenyl-1H-indol-6-yl)oxy)tetrahydro-2H-pyran-3,4,5-triyl triacetate (6f)



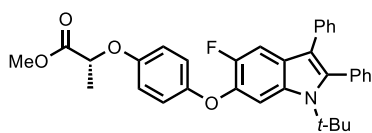
44.8 mg, 64% yield: white solid. Mp = 86-88 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.66 (s, 1H), 7.32–7.29 (m, 1H), 7.28–7.22 (m, 4H), 7.21–7.16 (m, 2H), 7.13–7.08 (m, 3H), 7.05 (s, 1H), 5.37–5.30 (m, 2H), 5.26–5.20 (m, 1H), 5.01–4.95 (m, 1H), 4.28 (dd, *J* = 12.3, 4.3 Hz, 1H), 4.20 (dd, *J* = 12.3, 2.5 Hz, 1H), 3.79 (s, 3H), 3.75–3.70 (m, 1H), 2.14 (s, 3H), 2.08 (s, 3H), 2.06 (s, 3H), 2.04 (s, 3H), 1.59 (s, 9H); ¹³C NMR (126 MHz, CDCl₃) δ 170.6, 170.3, 169.6, 169.4, 146.2, 141.6, 138.4, 136.1, 135.0, 131.7, 130.1, 127.8, 127.6, 127.30, 127.26, 125.4, 125.3, 117.4, 109.7, 102.0, 101.5, 72.6, 71.9, 71.2, 68.4, 61.9, 59.2, 56.4, 32.0, 20.7, 20.61, 20.55; **HRMS-EI** calcd for C₃₉H₄₃NO₁₁ [M]⁺ 701.2831, found 701.2859.

3-(1-(tert-butyl)-2,3-diphenyl-1H-indol-5-yl)-5-(2-fluorophenyl)-1,2,4-oxadiazole (6g)



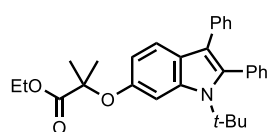
27.8 mg, 57% yield: white solid. Mp > 200 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.46 (s, 1H), 8.24 (t, *J* = 7.1 Hz, 1H), 8.07 (d, *J* = 8.7 Hz, 1H), 7.91 (d, *J* = 8.9 Hz, 1H), 7.62 – 7.53 (m, 1H), 7.38 – 7.15 (m, 12H), 1.68 (s, 9H); ¹³C NMR (101 MHz, CDCl₃) δ 172.3 (d, *J* = 4.0 Hz), 169.5, 160.7 (d, *J* = 260.3 Hz), 139.2, 138.0, 135.8, 134.5, 134.2 (d, *J* = 8.5 Hz), 131.7, 131.0, 130.4, 128.8, 127.9, 127.4, 125.7, 124.5 (d, *J* = 3.7 Hz), 120.4, 119.8, 118.9, 118.0, 117.0 (d, *J* = 21.0 Hz), 115.2, 113.1 (d, *J* = 11.5 Hz), 59.7, 32.1; **HRMS (ESI-TOF)** calcd for C₃₂H₂₇FN₃O [M+H]⁺ 488.2133, found 488.2136.

methyl (R)-2-(4-((1-(tert-butyl)-5-fluoro-2,3-diphenyl-1H-indol-6-yl)oxy)phenoxy)propanoate (6h)



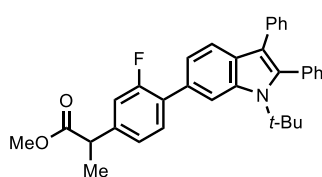
22.6 mg, 42% yield: white solid. Mp = 137-139 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.50 (d, *J* = 6.8 Hz, 1H), 7.37 (d, *J* = 11.0 Hz, 1H), 7.34 – 7.31 (m, 2H), 7.31 – 7.25 (m, 3H), 7.22 – 7.17 (m, 2H), 7.14 – 7.09 (m, 3H), 6.96 (d, *J* = 9.0 Hz, 2H), 6.86 (d, *J* = 9.2 Hz, 2H), 4.72 (q, *J* = 6.8 Hz, 1H), 3.77 (s, 3H), 1.62 (d, *J* = 6.9 Hz, 3H), 1.57 (s, 9H); ¹³C NMR (126 MHz, CDCl₃) δ 172.8, 153.5, 152.8, 150.3 (d, *J* = 240.3 Hz), 139.2, 138.6 (d, *J* = 14.8 Hz), 135.8, 134.5, 132.2, 131.7, 130.0, 127.9, 127.4, 125.7, 125.2 (d, *J* = 8.1 Hz), 117.7 (d, *J* = 3.9 Hz), 117.2, 116.4, 108.5, 105.6 (d, *J* = 20.1 Hz), 73.4, 59.5, 52.3, 32.0, 18.6; **HRMS (ESI-TOF)** calcd for C₃₄H₃₃FO₄ [M+H]⁺ 538.2388, found 538.2387.

ethyl 2-((1-(tert-butyl)-2,3-diphenyl-1H-indol-6-yl)oxy)-2-methylpropanoate (6i)



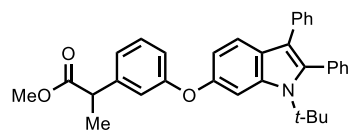
28.2 mg, 62% yield: white solid. Mp = 115–117 °C; ^1H NMR (500 MHz, CDCl_3) δ 7.47 (d, J = 8.6 Hz, 1H), 7.37 – 7.34 (m, 1H), 7.33 – 7.30 (m, 2H), 7.29 – 7.24 (m, 3H), 7.19 – 7.14 (m, 2H), 7.13 – 7.08 (m, 3H), 6.77 (dd, J = 8.6, 2.1 Hz, 1H), 4.29 (q, J = 7.2 Hz, 2H), 1.64 (s, 6H), 1.60 (d, J = 2.1 Hz, 9H), 1.33 (t, J = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, CDCl_3) δ 174.7, 150.2, 137.6, 136.5, 136.4, 135.1, 131.8, 130.2, 127.6, 127.6, 127.3, 125.3, 124.6, 119.4, 117.5, 114.2, 106.9, 79.8, 61.3, 59.1, 32.0, 25.4, 14.2; **HRMS (ESI-TOF)** calcd for $\text{C}_{30}\text{H}_{34}\text{NO}_3$ $[\text{M}+\text{H}]^+$ 456.2533, found 456.2536.

methyl 2-(4-(1-(tert-butyl)-2,3-diphenyl-1H-indol-6-yl)-3-fluorophenyl)propanoate (6j)



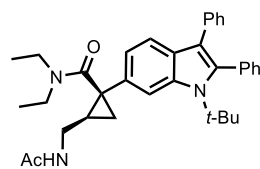
37.8 mg, 75% yield: white solid. Mp = 187–189 °C; ^1H NMR (500 MHz, CDCl_3) δ 7.99 (s, 1H), 7.69 (d, J = 8.2 Hz, 1H), 7.52 (t, J = 8.0 Hz, 1H), 7.36–7.27 (m, 6H), 7.23–7.11 (m, 7H), 3.80 (q, J = 7.2 Hz, 1H), 3.73 (s, 3H), 1.67 (s, 9H), 1.57 (s, 3H); ^{13}C NMR (126 MHz, CDCl_3) δ 174.6, 159.8 (d, J = 247.7 Hz), 141.0 (d, J = 7.5 Hz), 139.0, 136.4, 136.2, 135.0, 131.7, 131.3 (d, J = 3.9 Hz), 130.3, 129.4 (d, J = 13.4 Hz), 128.2, 128.2, 127.7, 127.4, 125.5, 123.5 (d, J = 2.5 Hz), 120.7, 119.5, 117.8, 115.8 (d, J = 3.6 Hz), 115.2 (d, J = 23.8 Hz), 59.4, 52.2, 44.9, 32.2, 18.5; **HRMS-EI** calcd for $\text{C}_{34}\text{H}_{32}\text{FNO}_2$ $[\text{M}]^+$ 505.2412, found 505.2408.

methyl 2-(3-((1-(tert-butyl)-2,3-diphenyl-1H-indol-6-yl)oxy)phenyl)propanoate (6k)



41.2 mg, 82% yield: white solid. Mp = 108–110 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.63 (d, J = 8.6 Hz, 1H), 7.53 (d, J = 2.0 Hz, 1H), 7.41 – 7.37 (m, 2H), 7.34 – 7.28 (m, 4H), 7.26 – 7.21 (m, 2H), 7.20 – 7.13 (m, 3H), 7.09 – 7.07 (m, 1H), 7.06 – 7.02 (m, 1H), 6.96 (dd, J = 8.6, 2.9 Hz, 1H), 6.93 (dd, J = 8.7, 2.1 Hz, 1H), 3.75 (q, J = 7.4 Hz, 1H), 3.71 (s, 3H), 1.64 (s, 9H), 1.54 (d, J = 7.2 Hz, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 174.7, 159.2, 150.8, 142.3, 138.2, 136.7, 136.2, 134.9, 131.8, 130.2, 129.7, 127.72, 127.69, 127.4, 125.5, 121.1, 120.3, 117.8, 116.6, 115.8, 113.0, 106.7, 59.3, 52.0, 45.3, 32.0, 18.5; **HRMS (ESI-TOF)** calcd for $\text{C}_{34}\text{H}_{34}\text{NO}_3$ $[\text{M}+\text{H}]^+$ 504.2533, found 504.2536.

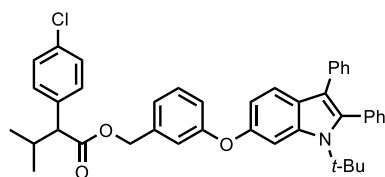
(1S,2R)-2-(acetamidomethyl)-1-(1-(tert-butyl)-2,3-diphenyl-1H-indol-6-yl)-N,N-diethylcyclopropane-1-carboxamide (6l)



39.6 mg, 74% yield: white solid. Mp = 66–68 °C; ^1H NMR (500 MHz, CDCl_3) δ 7.70 (d, J = 1.6 Hz, 1H), 7.54 (d, J = 8.3 Hz, 1H), 7.31 – 7.24 (m, 6H), 7.19 – 7.14 (m, 2H), 7.12 – 7.06 (m, 3H), 6.92 (dd, J = 8.4, 1.6 Hz, 1H), 4.32 – 4.24 (m, 1H), 3.77 – 3.66 (m, 1H), 3.55 – 3.46 (m, 1H), 3.41 – 3.27 (m, 2H), 2.57 – 2.49 (m, 1H), 2.00 (s, 3H), 1.67 (dd, J = 8.8, 5.4 Hz, 1H), 1.61 (s, 9H), 1.57 – 1.49 (m, 1H), 1.21 – 1.14 (m, 4H), 0.99 (t, J = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, CDCl_3) δ 171.3, 169.7, 138.5, 136.6, 136.1, 134.8, 133.3, 131.7, 131.6, 130.2, 127.7, 127.5, 127.4, 125.4, 119.8, 117.6, 116.8, 112.8, 59.3, 42.1, 41.4, 39.5, 34.4, 32.1, 29.5, 23.6, 17.5, 13.3, 12.6; **HRMS (ESI-TOF)** calcd for $\text{C}_{35}\text{H}_{42}\text{N}_3\text{O}_2$ $[\text{M}+\text{H}]^+$ 536.3272, found 536.3275.

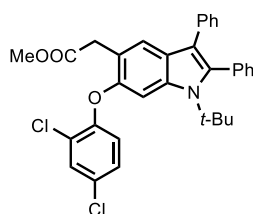
3-((1-(tert-butyl)-2,3-diphenyl-1H-indol-6-yl)oxy)benzyl methylbutanoate (6m)

2-(4-chlorophenyl)-3-



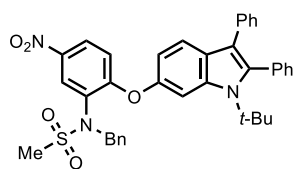
51.3 mg, 80% yield: white solid. Mp = 53-55 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.61 (d, *J* = 8.8 Hz, 1H), 7.53 (d, *J* = 2.0 Hz, 1H), 7.38 – 7.34 (m, 2H), 7.32 – 7.25 (m, 8H), 7.23 – 7.19 (m, 2H), 7.18 – 7.11 (m, 3H), 7.03 – 6.98 (m, 2H), 6.98 – 6.94 (m, 1H), 6.88 (dd, *J* = 8.6, 2.0 Hz, 1H), 5.13 (d, *J* = 12.6 Hz, 1H), 5.02 (d, *J* = 12.6 Hz, 1H), 3.20 (d, *J* = 10.5 Hz, 1H), 2.38 – 2.29 (m, 1H), 1.62 (s, 9H), 1.02 (d, *J* = 6.5 Hz, 3H), 0.72 (d, *J* = 6.8 Hz, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 173.3, 159.4, 150.7, 138.3, 137.5, 136.7, 136.6, 136.1, 134.8, 133.1, 131.8, 130.2, 129.8, 129.7, 128.6, 127.7, 127.4, 125.6, 125.5, 121.4, 120.4, 117.8, 116.9, 116.5, 113.1, 106.9, 66.1, 59.4, 32.0, 31.9, 21.3, 20.1; HRMS (ESI-TOF) calcd for C₄₂H₄₁ClNO₃ [M+H]⁺ 642.2769, found 642.2769.

methyl 2-(1-(tert-butyl)-6-(2,4-dichlorophenoxy)-2,3-diphenyl-1H-indol-5-yl)acetate (6n)



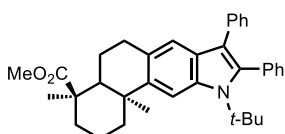
45.1 mg, 81% yield: white solid. Mp = 144-146 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.56 (s, 1H), 7.52 (d, *J* = 2.5 Hz, 1H), 7.36 – 7.33 (m, 3H), 7.33 – 7.28 (m, 3H), 7.25 – 7.21 (m, 2H), 7.18 – 7.13 (m, 4H), 6.84 (d, *J* = 8.9 Hz, 1H), 3.70 (s, 2H), 3.60 (s, 3H), 1.57 (s, 9H); ¹³C NMR (126 MHz, CDCl₃) δ 172.1, 153.1, 148.4, 138.7, 135.9, 135.8, 134.6, 131.7, 130.23, 130.19, 127.8, 127.6, 127.41, 127.35, 126.1, 125.6, 124.4, 122.0, 118.5, 117.9, 117.7, 106.4, 59.4, 51.9, 36.1, 32.0; HRMS (ESI-TOF) calcd for C₃₃H₃₀Cl₂NO₃ [M+H]⁺ 558.1597, found 558.1595.

N-benzyl-N-(2-((1-(tert-butyl)-2,3-diphenyl-1H-indol-6-yl)oxy)-5-nitrophenyl)methanesulfonamide (6o)



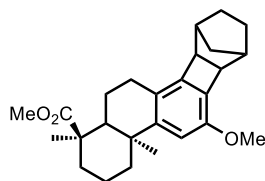
32.9 mg, 51% yield: white solid. Mp = 184-186 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.77 (dd, *J* = 8.7, 2.6 Hz, 1H), 7.72 – 7.67 (m, 2H), 7.53 (d, *J* = 2.1 Hz, 1H), 7.42 – 7.37 (m, 5H), 7.35 – 7.29 (m, 6H), 7.27 – 7.21 (m, 2H), 7.20 – 7.15 (m, 3H), 6.85 (dd, *J* = 8.6, 2.1 Hz, 1H), 5.04 (s, 2H), 3.22 (s, 3H), 1.65 (s, 9H); ¹³C NMR (101 MHz, CDCl₃) δ 156.7, 148.4, 148.0, 139.3, 136.6, 135.7, 135.5, 134.4, 134.2, 133.5, 131.7, 130.2, 128.7, 128.6, 128.2, 127.9, 127.8, 127.5, 126.9, 125.8, 121.4, 118.1, 116.9, 112.3, 111.4, 106.8, 59.6, 53.9, 40.4, 32.0; HRMS (ESI-TOF) calcd for C₃₈H₃₆N₃O₅S [M+H]⁺ 646.2370, found 646.2374.

methyl (4*R*,11*bS*)-10-(tert-butyl)-4,11*b*-dimethyl-8,9-diphenyl-2,3,4,4*a*,5,6,10,11*b*-octahydro-1*H*-naphtho[2,1-*f*]indole-4-carboxylate (6p)



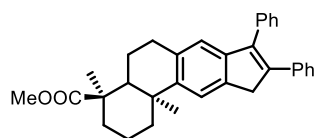
37.4 mg, 72% yield: white solid. Mp = 165-167 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.71 (s, 1H), 7.36 – 7.26 (m, 6H), 7.21 (dd, *J* = 8.4, 6.8 Hz, 2H), 7.15 – 7.10 (m, 3H), 3.71 (s, 3H), 3.08 – 3.01 (m, 2H), 2.52 (d, *J* = 12.1 Hz, 1H), 2.41 (dd, *J* = 12.5, 2.6 Hz, 1H), 1.99 – 1.82 (m, 4H), 1.81 – 1.71 (m, 2H), 1.66 (s, 9H), 1.54 – 1.47 (m, 1H), 1.40 (s, 3H), 1.37 (s, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 179.1, 143.7, 138.3, 136.5, 135.6, 135.4, 131.74, 131.67, 130.3, 127.6, 127.3, 127.2, 126.9, 125.2, 118.7, 116.9, 110.1, 58.9, 51.9, 47.7, 45.2, 38.9, 37.7, 36.7, 32.1, 29.6, 25.7, 22.0, 18.8, 16.6; HRMS (ESI-TOF) calcd for C₃₆H₄₂NO₂ [M+H]⁺ 520.3210, found 520.3213.

methyl (4*aS*)-6-methoxy-1,4*a*-dimethyl-1,2,3,4,4*a*,6*b*,7,8,9,10,10*a*,11,12,12*a*-tetradecahydro-7,10-methanobenzo[3,4]cyclobuta[1,2-*a*]phenanthrene-1-carboxylate (6*q*) (d.r. = 1:1)



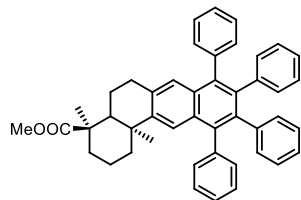
6.7 mg, 17% yield: colorless oil. $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 6.61 (s, 1H), 3.87 (s, 3H), 3.67 (s, 3H), 3.22 (d, $J = 3.8$ Hz, 1H), 3.05 (d, $J = 3.8$ Hz, 1H), 2.71 – 2.65 (m, 2H), 2.32 – 2.28 (m, 2H), 2.28 – 2.24 (m, 3H), 2.24 – 2.20 (m, 2H), 2.06 – 2.01 (m, 2H), 1.85 – 1.73 (m, 2H), 1.71 – 1.60 (m, 4H), 1.36 – 1.34 (m, 2H), 1.28 (s, 3H), 1.21 (s, 3H). $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 179.3, 151.8, 150.8, 146.1, 130.2, 129.9, 110.0, 56.7, 52.0, 49.6, 49.4, 47.9, 45.0, 38.4, 38.0, 36.8, 36.0, 35.4, 32.1, 32.0, 28.0, 27.9, 27.4, 27.3, 25.6, 25.3, 24.7, 22.8, 21.4, 18.8, 16.7, 14.3. **HRMS-EI** calcd for $\text{C}_{26}\text{H}_{34}\text{O}_3$ $[\text{M}]^+$ 394.2502; found 394.2502.

methyl 5*a*,9-dimethyl-2,3-diphenyl-5,5*a*,6,7,8,9,9*a*,10-octahydro-1*H*-cyclopenta[*b*]anthracene-9-carboxylate (6*r*)



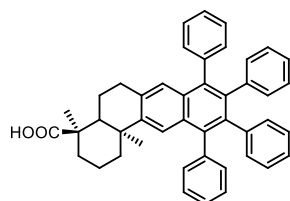
5.5 mg, 12% yield: white sticky foam. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.45 (s, 1H), 7.45–7.35 (m, 2H), 7.38–7.30 (m, 3H), 7.28–7.25 (m, 1H), 7.26–7.22 (m, 1H), 7.23–7.12 (m, 3H), 6.87 (s, 1H), 3.87 (s, 2H), 3.66 (s, 3H), 2.92–2.85 (m, 2H), 2.44–2.36 (m, 1H), 2.30–2.24 (m, 1H), 1.87–1.73 (m, 4H), 1.71–1.61 (m, 2H), 1.46–1.39 (m, 1H), 1.29 (s, 3H), 1.27 (s, 3H). $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 179.1, 146.8, 144.6, 140.8, 139.9, 139.7, 136.8, 136.4, 133.3, 129.3, 128.8, 128.2, 128.1, 127.3, 126.8, 120.6, 119.5, 51.9, 47.7, 45.1, 40.9, 38.4, 37.5, 36.7, 30.2, 25.2, 21.8, 18.7, 16.6; **HRMS (ESI-TOF)** calcd for $\text{C}_{33}\text{H}_{35}\text{O}_2$ $[\text{M}+\text{H}]^+$ 463.2632, found 463.2635.

methyl (4*R*,12*bS*)-4,12*b*-dimethyl-8,9,10,11-tetraphenyl-1,2,3,4,4*a*,5,6,12*b*-octahydrotetraphene-4-carboxylate (6*s*)



21.9 mg, 35% yield; yellowish solid. $\text{Mp} = 106\text{--}108$ °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.57 (s, 1H), 7.35 (d, $J = 1.4$ Hz, 1H), 7.31–7.17 (m, 10H), 6.91–6.80 (m, 10H), 3.67 (s, 3H), 3.07–2.94 (m, 2H), 2.27 (dd, $J = 12.5, 2.7$ Hz, 1H), 2.09–2.01 (m, 1H), 1.94–1.85 (m, 1H), 1.80–1.71 (m, 2H), 1.71–1.65 (m, 2H), 1.52–1.44 (m, 2H), 1.30 (s, 3H), 1.20 (s, 3H). $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 179.0, 148.9, 140.9, 140.8, 139.8, 138.3, 138.1, 137.9, 137.3, 134.4, 131.5, 131.4, 131.3, 130.7, 130.4, 127.5, 127.4, 127.3, 126.6, 126.5, 126.3, 126.2, 126.0, 125.2, 121.7, 52.0, 47.7, 44.7, 38.0, 37.7, 36.8, 29.8, 25.2, 21.7, 18.6, 16.7; **HRMS (ESI-TOF)** calcd for $\text{C}_{46}\text{H}_{43}\text{O}_2$ $[\text{M}+\text{H}]^+$ 627.3258, found 627.3257.

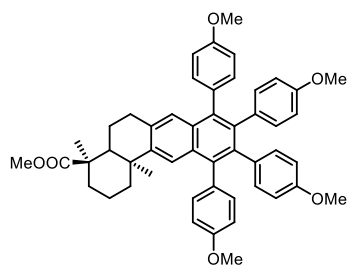
(4*R*,12*bS*)-4,12*b*-dimethyl-8,9,10,11-tetraphenyl-1,2,3,4,4*a*,5,6,12*b*-octahydrotetraphene-4-carboxylic acid (6*s*-1)



8.9 mg, 92% yield; yellowish solid. $\text{Mp} > 200$ °C; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.53 (s, 1H), 7.31 (s, 1H), 7.25–7.16 (m, 10H), 6.88–6.77 (m, 10H), 2.98 (s, 2H), 2.24 (d, $J = 12.4$ Hz, 1H), 2.08–1.98 (m, 1H), 1.95–1.83 (m, 1H), 1.82–1.71 (m, 1H), 1.73–1.61 (m, 3H), 1.62–1.51 (m, 1H), 1.51–1.40 (m, 1H), 1.26 (s, 3H), 1.17 (s, 3H). $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 183.7, 148.3, 140.3, 140.2, 139.3, 137.8, 137.5, 137.4, 136.7, 133.8, 127.0, 126.9, 126.8, 126.1, 126.0, 125.9, 125.8, 125.6, 124.7, 121.2, 44.0, 37.4, 37.1, 36.1,

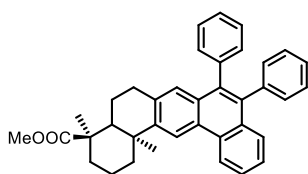
29.2, 24.7, 21.2, 18.0, 15.9, 13.7; **HRMS (ESI-TOF)** calcd for C₄₅H₃₉O₂ [M-H]⁻ 611.2956, found 611.2957.

methyl (4*R*,12*bS*)-8,9,10,11-tetrakis(4-methoxyphenyl)-4,12b-dimethyl-1,2,3,4,4a,5,6,12b-octahydrotetraphene-4-carboxylate (6s-2)



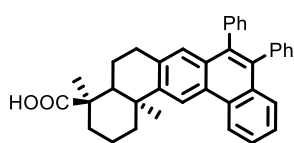
20.9 mg, 28% yield; yellow solid. Mp = 127-130 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.54 (s, 1H), 7.30 (s, 1H), 7.15–7.01 (m, 4H), 6.84–6.74 (m, 4H), 6.71–6.64 (m, 4H), 6.45–6.39 (m, 4H), 3.81 (s, 3H), 3.80 (s, 3H), 3.65 (s, 3H), 3.63 (s, 3H), 3.63 (s, 3H), 2.99–2.93 (m, 2H), 2.23 (dd, *J* = 12.4, 2.6 Hz, 1H), 2.06 (d, *J* = 13.0 Hz, 1H), 1.91–1.81 (m, 1H), 1.78–1.69 (m, 2H), 1.68–1.61 (m, 2H), 1.50–1.40 (m, 2H), 1.27 (s, 3H), 1.17 (s, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 179.1, 157.8, 157.7, 156.8, 148.6, 138.5, 138.1, 137.8, 137.0, 134.0, 133.7, 133.6, 132.3, 132.2, 131.0, 130.7, 126.0, 121.7, 112.9, 112.9, 112.8, 112.7, 112.1, 55.1, 54.9, 53.8, 52.0, 47.7, 44.8, 38.0, 37.6, 36.7, 29.8, 29.3, 25.2, 21.7, 18.6, 16.7; **HRMS (ESI-TOF)** calcd for C₅₀H₅₁O₆ [M+H]⁺ 747.368, found 747.3682.

methyl 8a,12-dimethyl-5,6-diphenyl-8,8a,9,10,11,12,12a,13-octahydrobenzo[*a*]tetracene-12-carboxylate (6t)



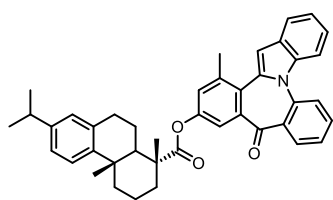
13.1 mg, 25% yield; white solid. Mp = 85-87 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.76 (d, *J* = 8.3 Hz, 1H), 8.70 (s, 1H), 7.65–7.58 (m, 1H), 7.51 (dd, *J* = 8.3, 1.4 Hz, 1H), 7.44 (dd, *J* = 6.9, 1.2 Hz, 1H), 7.25–7.14 (m, 8H), 7.16–7.10 (m, 3H), 3.66 (s, 3H), 2.96 (dd, *J* = 9.0, 4.8 Hz, 2H), 2.71 (d, *J* = 13.3 Hz, 1H), 2.34 (dd, *J* = 12.5, 2.5 Hz, 1H), 1.95–1.79 (m, 4H), 1.78–1.67 (m, 2H), 1.51–1.43 (m, 1H), 1.36 (s, 3H), 1.33 (s, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 179.0, 148.9, 139.7, 139.6, 136.5, 136.5, 134.7, 131.6, 131.1, 131.0, 131.0, 130.1, 129.9, 128.1, 127.8, 127.5, 127.5, 127.4, 126.3, 126.1, 126.0, 122.1, 117.6, 51.9, 47.7, 44.7, 38.5, 37.8, 36.7, 29.7, 25.5, 21.6, 18.7, 16.7; **HRMS (ESI-TOF)** calcd for C₃₈H₃₇O₂ [M+H]⁺ 525.2788, found 525.2788.

(4*R*,14*bS*)-4,14b-dimethyl-8,9-diphenyl-1,2,3,4,4a,5,6,14b-octahydrobenzo[*m*]tetraphene-4-carboxylic acid(6t-1)



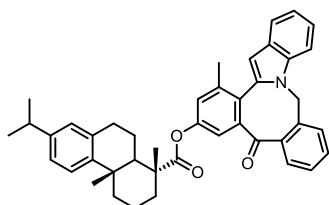
8.2 mg, 65% yield; white solid, Mp = 110-112 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.76 (d, *J* = 8.3 Hz, 1H), 8.69 (s, 1H), 7.62 (ddd, *J* = 8.3, 6.8, 1.5 Hz, 1H), 7.50 (dd, *J* = 8.3, 1.4 Hz, 1H), 7.43 (ddd, *J* = 8.1, 6.7, 1.1 Hz, 1H), 7.24–7.16 (m, 7H), 7.15–7.09 (m, 4H), 3.01–2.93 (m, 2H), 2.72 (d, *J* = 12.3 Hz, 1H), 2.37–2.29 (m, 1H), 2.03–1.94 (m, 1H), 1.94–1.80 (m, 4H), 1.84–1.74 (m, 2H), 1.37 (s, 3H), 1.34 (s, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 183.5, 148.7, 139.7, 139.6, 136.6, 136.5, 134.6, 131.6, 131.1, 131.0, 131.0, 130.1, 129.9, 128.1, 127.9, 127.5, 127.5, 127.4, 126.3, 126.1, 126.0, 122.1, 117.6, 47.4, 44.5, 38.5, 37.7, 36.7, 29.8, 25.5, 21.7, 18.6, 16.4; **HRMS (ESI-TOF)** calcd for C₃₇H₃₅O₂ [M+H]⁺ 511.2632, found 511.2628.

14-methyl-10-oxo-10*H*-dibenzo[3,4:6,7]azepino[1,2-*a*]indol-12-yl (1*R*,4*aS*)-7-isopropyl- 1,4a-dimethyl-1,2,3,4,4a,9,10,10a-octahydrophenanthrene-1-carboxylate (6u) (d.r. = 1:1)



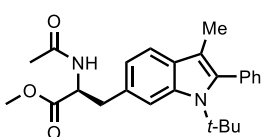
32.9 mg, 54% yield: white solid. ^1H NMR (500 MHz, CDCl_3) δ 7.79 (dd, $J = 8.0, 1.0$ Hz, 1H), 7.72–7.60 (m, 4H), 7.39 (td, $J = 7.6, 1.1$ Hz, 1H), 7.30–7.26 (m, 1H), 7.26–7.24 (m, 1H), 7.23–7.19 (m, 3H), 7.06–7.01 (m, 1H), 6.94 (dd, $J = 5.5, 2.0$ Hz, 1H), 6.83 (s, 1H), 3.09–2.92 (m, 2H), 2.89–2.81 (m, 1H), 2.69 (s, 3H), 2.47–2.41 (m, 1H), 2.37 (d, $J = 13.1$ Hz, 1H), 2.03–1.94 (m, 2H), 1.90–1.79 (m, 3H), 1.66–1.56 (m, 2H), 1.42 (s, 1.5H), 1.41 (s, 1.5H), 1.28–1.22 (m, 9H). ^{13}C NMR (126 MHz, CDCl_3) δ 196.6, 177.1, 177.1, 150.2, 146.8, 146.8, 146.0, 144.6, 139.5, 138.9, 136.3, 135.7, 134.7, 134.7, 134.6, 132.4, 128.7, 127.9, 127.9, 127.8, 127.1, 126.8, 126.7, 125.3, 124.3, 124.2, 124.2, 123.3, 121.8, 120.9, 118.3, 111.2, 108.3, 48.2, 45.0, 44.9, 38.1, 37.1, 36.7, 36.6, 33.6, 30.3, 25.3, 24.1, 22.6, 22.2, 22.1, 18.7, 16.8, 14.3. HRMS-ESI calcd for $\text{C}_{42}\text{H}_{42}\text{NO}_3$ $[\text{M}+\text{H}]^+$ 608.3157; found 608.3159.

1-methyl-5-oxo-5,10-dihydrodibenzo[3,4:6,7]azocino[1,2-a]indol-3-yl (1R,4aS)-7-isopropyl-1,4a-dimethyl-1,2,3,4,4a,9,10,10a-octahydrophenanthrene-1-carboxylate (6v) (d.r. = 1:1)



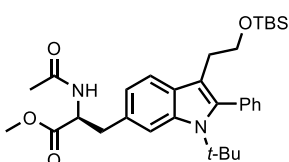
21.8 mg, 35% yield: white solid. ^1H NMR (500 MHz, CDCl_3) δ 7.84 (d, $J = 7.8$ Hz, 1H), 7.63 (d, $J = 7.8$ Hz, 1H), 7.58–7.55 (m, 2H), 7.46–7.40 (m, 1H), 7.28–7.24 (m, 1H), 7.22 (d, $J = 8.1$ Hz, 1H), 7.19–7.11 (m, 3H), 7.04 (d, $J = 8.3$ Hz, 1H), 6.93 (s, 1H), 6.87–6.85 (m, 1H), 6.65 (s, 1H), 5.35 (d, $J = 16.6$ Hz, 1H), 5.08 (d, $J = 16.0$ Hz, 1H), 3.01–2.94 (m, 2H), 2.89–2.83 (m, 1H), 2.50 (s, 3H), 2.46–2.41 (m, 1H), 2.38 (d, $J = 12.9$ Hz, 1H), 2.27–2.21 (m, 1H), 2.01–1.94 (m, 2H), 1.88–1.80 (m, 2H), 1.65 (d, $J = 11.9$ Hz, 2H), 1.39 (s, 1.5H), 1.38 (s, 1.5H), 1.27–1.23 (m, 9H). ^{13}C NMR (126 MHz, CDCl_3) δ 199.4, 177.1, 151.2, 146.8, 146.0, 145.3, 139.1, 137.8, 136.3, 135.0, 134.7, 134.6, 132.8, 130.6, 128.8, 128.7, 128.4, 127.1, 125.7, 124.4, 124.2, 124.2, 124.1, 122.1, 121.1, 120.5, 116.9, 116.8, 109.6, 103.2, 48.2, 47.5, 45.0, 44.9, 38.1, 37.2, 36.8, 36.6, 33.6, 30.3, 25.3, 24.1, 22.2, 22.1, 20.5, 18.7, 16.8, 14.3. HRMS-ESI calcd for $\text{C}_{43}\text{H}_{44}\text{NO}_3$ $[\text{M}+\text{H}]^+$ 622.3316; found 622.3316.

methyl (S)-2-acetamido-3-(1-(tert-butyl)-3-methyl-2-phenyl-1H-indol-6-yl)propanoate (6w)



26.4 mg, 65% yield: white solid. Mp = 168–170 °C; ^1H NMR (500 MHz, CDCl_3) δ 7.47 (d, $J = 8.0$ Hz, 1H), 7.43 (s, 1H), 7.41–7.36 (m, 3H), 7.34–7.29 (m, 2H), 6.85 (dd, $J = 8.0, 1.3$ Hz, 1H), 5.97 (d, $J = 7.8$ Hz, 1H), 4.96 (dt, $J = 7.8, 5.4$ Hz, 1H), 3.78 (s, 3H), 3.36–3.27 (m, 2H), 1.99 (s, 3H), 1.95 (s, 3H), 1.55 (s, 9H); ^{13}C NMR (126 MHz, CDCl_3) δ 172.3, 169.5, 138.2, 137.0, 136.5, 130.9, 128.6, 127.8, 127.6, 127.5, 120.0, 118.8, 115.4, 110.9, 58.6, 53.5, 52.3, 38.3, 31.9, 23.2, 9.0; HRMS (ESI-TOF) calcd for $\text{C}_{25}\text{H}_{31}\text{N}_2\text{O}_3$ $[\text{M}+\text{H}]^+$ 407.2329, found 407.2326.

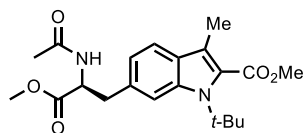
methyl (S)-2-acetamido-3-(1-(tert-butyl)-3-(2-((tert-butyldimethylsilyl)oxy)ethyl)-2-phenyl-1H-indol-6-yl)propanoate (6x)



36.9 mg, 67% yield: white solid. Mp = 116–118 °C; ^1H NMR (500 MHz, CDCl_3) δ 7.54 (d, $J = 8.0$ Hz, 1H), 7.43 (s, 1H), 7.40–7.36 (m, 3H), 7.34–7.30 (m, 2H), 6.84 (dd, $J = 8.1, 1.4$ Hz, 1H), 6.05–5.96 (m, 1H), 4.96 (dt, $J = 7.7, 5.4$ Hz, 1H), 3.78 (s, 3H), 3.64–3.57 (m,

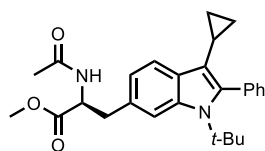
2H), 3.35 – 3.26 (m, 2H), 2.66 – 2.59 (m, 2H), 1.99 (s, 3H), 1.54 (s, 9H), 0.81 (s, 9H), -0.10 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 172.2, 169.5, 139.0, 136.5, 136.4, 130.9, 128.1, 127.8, 127.6, 120.2, 119.0, 115.5, 111.7, 63.6, 58.7, 53.4, 52.3, 38.2, 31.9, 28.2, 25.9, 23.1, 18.3, -5.4; **HRMS (ESI-TOF)** calcd for C₃₂H₄₇N₂O₄Si [M+H]⁺ 551.3300, found 551.3299.

methyl (S)-6-(2-acetamido-3-methoxy-3-oxopropyl)-1-(tert-butyl)-3-methyl-1H-indole-2-carboxylate (6y)



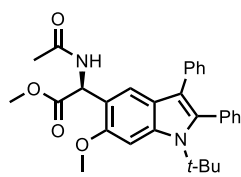
22.5 mg, 58% yield: white solid. Mp = 119-121 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.47 (d, *J* = 8.1 Hz, 1H), 7.35 (d, *J* = 1.4 Hz, 1H), 6.82 (dd, *J* = 8.1, 1.3 Hz, 1H), 6.00 (d, *J* = 7.7 Hz, 1H), 4.92 (dt, *J* = 7.8, 5.6 Hz, 1H), 3.90 (s, 3H), 3.72 (s, 3H), 3.25 (d, *J* = 5.6 Hz, 2H), 2.28 (s, 3H), 1.96 (s, 3H), 1.72 (s, 9H); ¹³C NMR (101 MHz, CDCl₃) δ 172.1, 169.5, 165.8, 138.2, 130.6, 128.9, 127.9, 120.7, 120.3, 116.5, 115.5, 58.4, 53.4, 52.3, 52.0, 38.3, 30.4, 23.0, 9.0; **HRMS (ESI-TOF)** calcd for C₂₁H₂₈N₂NaO₅ [M+Na]⁺ 411.1890, found 411.1890.

methyl (S)-2-acetamido-3-(1-(tert-butyl)-3-cyclopropyl-2-phenyl-1H-indol-6-yl)propanoate (6z)



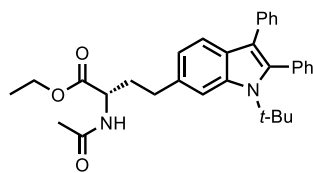
13.4 mg, 31% yield: white solid. Mp = 147-149 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.62 (d, *J* = 8.1 Hz, 1H), 7.42 (s, 1H), 7.39 – 7.33 (m, 5H), 6.81 (dd, *J* = 8.1, 1.3 Hz, 1H), 5.94 (d, *J* = 7.7 Hz, 1H), 4.95 (dt, *J* = 7.8, 5.4 Hz, 1H), 3.78 (s, 3H), 3.34 – 3.24 (m, 2H), 1.98 (s, 3H), 1.57 – 1.50 (m, 10H), 0.57 – 0.52 (m, 2H), 0.48 – 0.44 (m, 2H); ¹³C NMR (126 MHz, CDCl₃) δ 172.3, 169.5, 139.8, 137.2, 136.3, 131.2, 128.1, 127.53, 127.51, 127.4, 120.1, 119.4, 115.6, 115.4, 58.8, 53.4, 52.3, 38.2, 32.0, 23.2, 6.5, 5.3; **HRMS (ESI-TOF)** calcd for C₂₇H₃₃N₂O₃ [M+H]⁺ 433.2486, found 433.2488.

methyl (R)-2-acetamido-2-(1-(tert-butyl)-6-methoxy-2,3-diphenyl-1H-indol-5-yl)acetate (6aa)



31.9 mg, 66% yield: white solid. Mp > 200 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.57 (s, 1H), 7.32 – 7.23 (m, 6H), 7.21 – 7.16 (m, 2H), 7.13 – 7.07 (m, 3H), 6.62 (d, *J* = 8.7 Hz, 1H), 5.86 (d, *J* = 8.7 Hz, 1H), 3.95 (s, 3H), 3.68 (s, 3H), 2.02 (s, 3H), 1.63 (s, 9H); ¹³C NMR (126 MHz, CDCl₃) δ 172.1, 169.2, 152.7, 137.4, 136.6, 136.2, 134.6, 131.9, 131.7, 130.1, 127.8, 127.6, 127.4, 127.3, 125.5, 122.8, 121.3, 119.2, 118.0, 98.1, 59.1, 56.1, 53.6, 52.4, 32.0, 23.3; **HRMS (ESI-TOF)** calcd for C₃₀H₃₃N₂O₄ [M+H]⁺ 485.2435, found 485.2435.

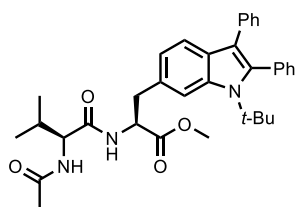
ethyl (S)-2-acetamido-4-(1-(tert-butyl)-2,3-diphenyl-1H-indol-6-yl)butanoate (6ab)



38.2 mg, 77% yield: white solid. Mp = 105-107 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.59 (d, *J* = 1.3 Hz, 1H), 7.55 (d, *J* = 8.1 Hz, 1H), 7.33 – 7.23 (m, 5H), 7.20 – 7.16 (m, 2H), 7.13 – 7.09 (m, 3H), 6.96 (dd, *J* = 8.2, 1.4 Hz, 1H), 6.10 (d, *J* = 8.0 Hz, 1H), 4.75 (td, *J* = 7.7, 5.1 Hz, 1H), 4.29 – 4.18 (m, 2H), 2.90 – 2.78 (m, 2H), 2.34 – 2.26 (m, 1H), 2.14 – 2.06 (m, 1H), 2.03 (s, 3H), 1.64 (s, 9H), 1.31 (t, *J* = 7.2 Hz, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 172.6, 169.8, 137.9, 136.7, 136.3, 135.1, 133.7, 131.7, 130.2, 127.6, 127.6, 127.3, 127.2, 125.3, 120.2, 119.6, 117.7, 114.6, 61.5, 59.2, 52.2, 35.0, 32.5, 32.1, 23.2, 14.2; **HRMS (ESI-**

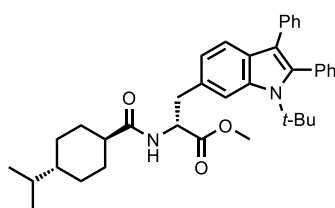
TOF) calcd for $C_{32}H_{37}N_2O_3$ $[M+H]^+$ 497.2799, found 497.2799.

methyl (S)-2-((S)-2-acetamido-3-methylbutanamido)-3-(1-(tert-butyl)-2,3-diphenyl-1H-indol-6-yl)propanoate (6ac)



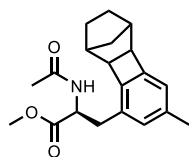
25.5 mg, 45% yield: white solid. Mp = 196-198 °C; 1H NMR (500 MHz, $CDCl_3$) δ 7.54 (d, J = 8.1 Hz, 1H), 7.51 (s, 1H), 7.33 – 7.23 (m, 5H), 7.17 (t, J = 7.6 Hz, 2H), 7.12 – 7.08 (m, 3H), 6.86 (dd, J = 8.1, 1.4 Hz, 1H), 6.35 (d, J = 7.7 Hz, 1H), 6.19 (d, J = 8.6 Hz, 1H), 4.97 – 4.91 (m, 1H), 4.29 (dd, J = 8.6, 6.2 Hz, 1H), 3.75 (s, 3H), 3.36 – 3.24 (m, 2H), 2.09 – 2.01 (m, 1H), 1.98 (s, 3H), 1.61 (s, 9H), 0.95 – 0.90 (m, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.9, 170.8, 169.8, 138.3, 136.6, 136.1, 134.9, 131.74, 131.70, 130.2, 128.0, 127.9, 127.7, 127.4, 125.4, 120.8, 119.9, 117.7, 115.5, 59.3, 58.1, 53.5, 52.3, 38.4, 32.1, 31.5, 23.2, 18.9, 18.0; **HRMS (ESI-TOF)** calcd for $C_{35}H_{42}N_3O_4$ $[M+H]^+$ 568.3170, found 568.3171.

methyl (R)-3-(1-(tert-butyl)-2,3-diphenyl-1H-indol-6-yl)-2-((1*r*,4*R*)-4-isopropylcyclohexane-1-carboxamido)propanoate (6ad)



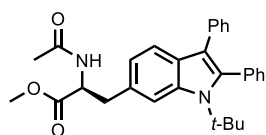
43.4 mg, 75% yield: white solid. Mp = 187-189 °C; 1H NMR (500 MHz, $CDCl_3$) δ 7.56 (d, J = 8.1 Hz, 1H), 7.51 (d, J = 1.4 Hz, 1H), 7.35 – 7.24 (m, 5H), 7.21 – 7.16 (m, 2H), 7.15 – 7.09 (m, 3H), 6.85 (d, J = 8.2 Hz, 1H), 6.02 (d, J = 7.7 Hz, 1H), 5.04 – 4.98 (m, 1H), 3.78 (s, 3H), 3.37 (dd, J = 13.9, 4.9 Hz, 1H), 3.30 (dd, J = 13.9, 5.7 Hz, 1H), 2.07 – 1.99 (m, 1H), 1.96 – 1.90 (m, 2H), 1.83 – 1.75 (m, 2H), 1.63 (d, J = 1.6 Hz, 9H), 1.52 – 1.37 (m, 3H), 1.11 – 1.03 (m, 1H), 1.02 – 0.92 (m, 2H), 0.87 (d, J = 6.8 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 175.6, 172.3, 138.1, 136.5, 136.1, 134.9, 131.7, 131.6, 130.2, 128.4, 127.8, 127.6, 127.3, 125.4, 121.1, 119.6, 117.6, 115.6, 59.2, 53.0, 52.2, 45.5, 43.1, 38.3, 32.7, 32.0, 29.6, 29.5, 28.9, 28.9, 19.7; **HRMS (ESI-TOF)** calcd for $C_{38}H_{47}N_2O_3$ $[M+H]^+$ 579.3581, found 579.3580.

methyl 2-acetamido-3-(7-methyl-1,2,3,4,4a,8b-hexahydro-1,4-methanobiphenylen-5-yl)propanoate (6ae) (d.r. = 1:1)



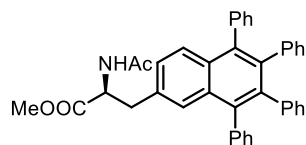
17.3 mg, 53% yield: colorless oil. 1H NMR (500 MHz, $CDCl_3$) δ 6.71 (s, 0.5H), 6.69 (s, 0.5H), 6.55 (s, 0.5H), 6.52 (s, 0.5H), 5.90 – 5.83 (m, 1H), 4.86 – 4.76 (m, 1H), 3.71 (s, 1.5H), 3.70 (s, 1.5H), 3.09 (q, J = 4.5 Hz, 2H), 3.05 – 3.00 (m, 2H), 2.28 – 2.25 (m, 1H), 2.23 – 2.20 (m, 1H), 2.15 (s, 1.5H), 2.14 (s, 1.5H), 1.99 (s, 1.5H), 1.98 (s, 1.5H), 1.61 – 1.54 (m, 2H), 1.18 – 1.15 (m, 2H), 0.96 – 0.94 (m, 0.5H), 0.94 – 0.92 (m, 0.5H), 0.79 – 0.77 (m, 0.5H), 0.77 – 0.75 (m, 0.5H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 172.5, 172.3, 169.7, 169.6, 146.5, 146.4, 143.9, 135.2, 135.2, 132.3, 132.3, 129.3, 129.1, 120.1, 119.9, 53.6, 53.6, 52.3, 52.3, 49.6, 49.6, 49.2, 38.7, 38.6, 36.6, 35.9, 35.9, 32.1, 32.1, 32.0, 27.9, 27.9, 23.3, 23.3, 22.8, 16.7, 14.3. **HRMS-ESI** calcd for $C_{20}H_{26}NO_3$ $[M+H]^+$ 328.1907, found 328.1909.

methyl (S)-2-acetamido-3-(1-(tert-butyl)-3-methyl-2-phenyl-1H-indol-6-yl)propanoate (6af)



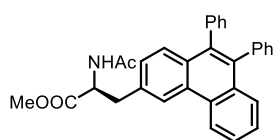
35.6 mg, 76% yield: white solid. Mp = 118–120 °C; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.58 – 7.49 (m, 2H), 7.33 – 7.23 (m, 5H), 7.21 – 7.15 (m, 2H), 7.13 – 7.08 (m, 3H), 6.84 (dd, J = 8.1, 1.4 Hz, 1H), 5.99 (d, J = 7.9 Hz, 1H), 4.98 (dt, J = 7.8, 5.3 Hz, 1H), 3.78 (s, 3H), 3.36 – 3.30 (m, 2H), 2.00 (s, 3H), 1.62 (s, 9H); $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 172.2, 169.5, 138.2, 136.6, 136.1, 134.9, 131.7, 130.2, 128.2, 127.9, 127.7, 127.4, 125.4, 120.9, 119.7, 117.7, 115.7, 59.2, 53.5, 52.3, 38.3, 32.1, 23.2; **HRMS (ESI-TOF)** calcd for $\text{C}_{30}\text{H}_{33}\text{N}_2\text{O}_3$ $[\text{M}+\text{H}]^+$ 469.2486, found 469.2487.

methyl (S)-2-acetamido-3-(5,6,7,8-tetraphenyl-naphthalen-2-yl)propanoate (6ag)



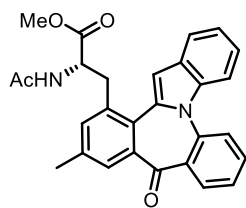
20.8 mg, 36% yield; yellowish solid. Mp = 70–72 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.58 (d, J = 8.7 Hz, 1H), 7.31 (s, 1H), 7.25–7.15 (m, 10H), 7.12 (dd, J = 8.7, 1.9 Hz, 1H), 6.91–6.78 (m, 10H), 5.84 (d, J = 7.7 Hz, 1H), 4.92–4.85 (m, 1H), 3.57 (s, 3H), 3.28–3.13 (m, 2H), 1.89 (s, 3H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 171.8, 169.4, 140.4, 140.3, 139.5, 139.4, 139.3, 138.9, 138.3, 138.0, 133.3, 132.0, 131.3, 131.2, 131.2, 131.1, 127.7, 127.6, 127.5, 127.4, 127.1, 126.6, 126.5, 125.4, 53.0, 52.3, 37.7, 23.1; **HRMS (ESI-TOF)** calcd for $\text{C}_{40}\text{H}_{34}\text{NO}_3$ $[\text{M}+\text{H}]^+$ 576.2533, found 576.253.

methyl 2-acetamido-3-(9,10-diphenylphenanthren-3-yl)propanoate (6ah)



9.9 mg, 21% yield: white solid. Mp = 183–185 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.75 (d, J = 8.3 Hz, 1H), 8.53 (s, 1H), 7.66 (m, 1H), 7.56 (d, J = 8.0 Hz, 1H), 7.52–7.46 (m, 2H), 7.25–7.17 (m, 7H), 7.17–7.12 (m, 4H), 6.00–5.94 (m, 1H), 5.10–4.99 (m, 1H), 3.77 (s, 3H), 3.50–3.34 (m, 2H), 2.01 (s, 3H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 172.1, 169.7, 139.4, 139.4, 137.2, 136.9, 133.9, 132.1, 131.0, 130.9, 130.0, 129.8, 129.7, 128.2, 127.9, 127.7, 127.6, 126.8, 126.5, 123.1, 122.2, 53.3, 52.5, 38.15, 23.3; **HRMS (ESI-TOF)** calcd for $\text{C}_{32}\text{H}_{28}\text{NO}_3$ $[\text{M}+\text{H}]^+$ 474.2064, found 474.2068.

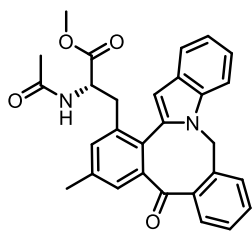
methyl (S)-2-acetamido-3-(12-methyl-10-oxo-10H-dibenzo[3,4:6,7]azepino[1,2-a]indol-14-yl)propanoate (6ai) (d.r. = 1:1)



20.3 mg, 45% yield: yellow solid. $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.78 (d, J = 8.0 Hz, 1H), 7.70 – 7.57 (m, 4H), 7.38 (t, J = 7.5 Hz, 1H), 7.28 – 7.26 (m, 1H), 7.26 – 7.19 (m, 3H), 6.83 (s, 1H), 6.07 – 5.97 (m, 1H), 4.95 – 4.84 (m, 1H), 3.78 (s, 1.5H), 3.77 (s, 1.5H), 3.23 – 3.17 (m, 1H), 3.15 – 3.07 (m, 1H), 2.66 (s, 3H), 2.03 (s, 1.5H), 2.02 (s, 1.5H). $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 197.5, 197.4, 171.9, 171.9, 169.9, 169.8, 143.7, 143.6, 139.3, 137.8, 136.4, 136.0, 135.9, 135.8, 135.7, 135.7, 135.1, 132.3, 128.3, 128.2, 128.1, 128.0, 127.9, 126.8, 126.7, 126.2, 126.1, 125.3, 125.3, 123.3, 121.8, 120.9, 111.2, 108.2, 53.2, 53.1, 52.7, 52.6, 37.4, 37.3, 23.4, 23.3, 22.5, 22.5. **HRMS (ESI-TOF)** calcd for $\text{C}_{28}\text{H}_{25}\text{N}_2\text{O}_4$ $[\text{M}+\text{H}]^+$ 453.1809, found 453.1808.

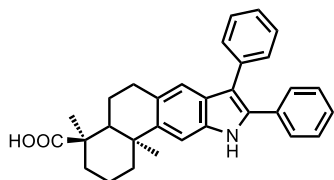
methyl (S)-2-acetamido-3-(3-methyl-5-oxo-5,10-dihydrodibenzo[3,4:6,7]azocino[1,2-a]indol-1-yl)propanoate (6aj) (d.r. = 1:1)

10.7 mg, 23% yield: white solid. $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.83 – 7.79 (m, 1H), 7.62 – 7.58



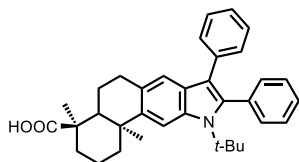
(m, 1H), 7.55 – 7.52 (m, 2H), 7.44 – 7.38 (m, 1H), 7.25 – 7.22 (m, 1H), 7.19 – 7.12 (m, 2H), 7.12 – 7.08 (m, 1H), 6.82 (d, $J = 1.8$ Hz, 0.5H), 6.79 (d, $J = 1.7$ Hz, 0.5H), 6.64 – 6.61 (m, 1H), 6.00 (t, $J = 6.7$ Hz, 1H), 5.28 – 5.19 (m, 1H), 5.06 (d, $J = 3.4$ Hz, 0.5H), 5.03 (d, $J = 3.4$ Hz, 0.5H), 4.91 – 4.83 (m, 1H), 3.70 (s, 1.5H), 3.69 (s, 1.5H), 3.21 – 3.13 (m, 1H), 3.12 – 3.04 (m, 1H), 2.44 (s, 3H), 1.97 (s, 1.5H), 1.95 (s, 1.5H). ^{13}C NMR (151 MHz, CDCl_3) δ 200.6, 200.4, 172.0, 171.9, 169.8, 144.7, 144.6, 139.1, 139.1, 138.1, 137.6, 137.5, 136.8, 136.7, 136.4, 135.6, 135.5, 132.6, 132.0, 131.9, 130.4, 130.3, 128.7, 128.7, 128.7, 128.6, 128.5, 127.1, 124.5, 124.5, 122.1, 121.1, 120.5, 109.6, 103.1, 103.0, 53.3, 52.6, 52.5, 47.6, 47.5, 37.8, 37.8, 23.3, 23.2, 20.4, 20.4. **HRMS-ESI** calcd for $\text{C}_{29}\text{H}_{27}\text{N}_2\text{O}_4$ $[\text{M}+\text{H}]^+$ 467.1965, found 467.1964.

(4R,11bS)-4,11b-dimethyl-8,9-diphenyl-2,3,4,4a,5,6,10,11b-octahydro-1H-naphtho[2,1-f]indole-4-carboxylic acid (7a)



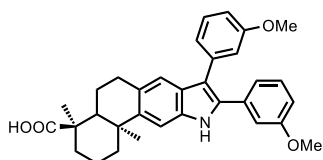
35.0 mg, 78% yield: white solid. Mp = 128–130 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.11 (s, 1H), 7.49 – 7.28 (m, 12H), 3.15 – 3.03 (m, 2H), 2.44 (d, $J = 12.7$ Hz, 1H), 2.40 – 2.34 (m, 1H), 2.03 – 1.92 (m, 1H), 1.93 – 1.76 (m, 4H), 1.76 – 1.61 (m, 2H), 1.37 (s, 3H), 1.34 (s, 3H); ^{13}C NMR (126 MHz, CDCl_3) δ 184.6, 145.5, 135.4, 135.1, 134.3, 133.0, 130.1, 128.6, 128.4, 128.0, 127.7, 127.5, 127.2, 126.0, 118.9, 114.2, 105.8, 47.5, 44.8, 38.6, 37.6, 36.8, 30.0, 25.6, 22.0, 18.7, 16.4; **HRMS (ESI-TOF)** calcd for $\text{C}_{31}\text{H}_{30}\text{NO}_2$ $[\text{M}-\text{H}]^-$ 448.2282, found 448.2285.

(4R,11bS)-10-(tert-butyl)-4,11b-dimethyl-8,9-diphenyl-2,3,4,4a,5,6,10,11b-octahydro-1H-naphtho[2,1-f]indole-4-carboxylic acid (7b)



22.7 mg, 75% yield: white solid. Mp = 133–135 °C; ^1H NMR (500 MHz, CDCl_3) δ 7.67 (s, 1H), 7.33 – 7.23 (m, 6H), 7.18 (t, $J = 7.6$ Hz, 2H), 7.10 (d, $J = 7.3$ Hz, 3H), 3.11 – 2.98 (m, 2H), 2.49 (d, $J = 12.4$ Hz, 1H), 2.38 (d, $J = 12.2$ Hz, 1H), 2.00 – 1.82 (m, 4H), 1.80 – 1.70 (m, 2H), 1.67 – 1.58 (m, 10H), 1.37 (s, 3H), 1.35 (s, 3H); ^{13}C NMR (126 MHz, CDCl_3) δ 185.1, 143.6, 138.3, 136.5, 135.6, 135.4, 131.8, 131.7, 130.3, 127.6, 127.5, 127.3, 127.2, 127.1, 126.9, 125.2, 118.7, 116.9, 110.2, 58.9, 47.5, 44.9, 38.9, 37.7, 36.8, 32.1, 29.7, 25.9, 22.1, 18.8, 16.3; **HRMS (ESI-TOF)** calcd for $\text{C}_{35}\text{H}_{38}\text{NO}_2$ $[\text{M}-\text{H}]^-$ 504.2908, found 504.2908.

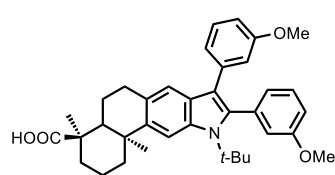
(4R,11bS)-8,9-bis(3-methoxyphenyl)-4,11b-dimethyl-2,3,4,4a,5,6,10,11b-octahydro-1H-naphtho[2,1-f]indole-4-carboxylic acid (7c)



25.3 mg, 83% yield: white solid. Mp = 113–115 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.10 (s, 1H), 7.34 (s, 1H), 7.31 (s, 1H), 7.28 (t, $J = 7.9$ Hz, 1H), 7.23 (t, $J = 8.0$ Hz, 1H), 7.03 – 6.98 (m, 3H), 6.95 (t, $J = 2.0$ Hz, 1H), 6.86 – 6.80 (m, 2H), 3.75 (s, 3H), 3.67 (s, 3H), 3.11 – 3.01 (m, 2H), 2.40 (d, $J = 12.5$ Hz, 1H), 2.33 (dd, $J = 12.4, 2.5$ Hz, 1H), 1.99 – 1.88 (m, 1H), 1.88 – 1.73 (m, 4H), 1.69 – 1.56 (m, 2H), 1.33 (s, 3H), 1.30 (s, 3H); ^{13}C NMR (126 MHz, CDCl_3) δ 184.6, 159.63, 159.56, 145.7, 136.8, 135.0, 134.2, 129.7, 129.4, 127.8, 127.2, 122.8, 120.3, 119.0, 115.4, 114.3, 113.5, 113.3, 112.0, 105.9, 55.2, 55.1, 47.5, 44.8, 38.7,

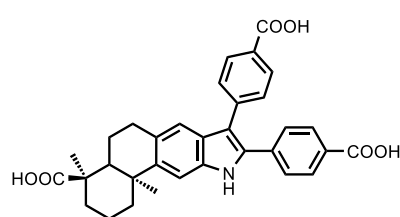
37.6, 36.8, 30.0, 29.7, 25.6, 22.1, 18.7, 16.4; **HRMS (ESI-TOF)** calcd for $C_{33}H_{34}NO_4$ $[M-H]^-$ 508.2493, found 508.2493.

(4R,11bS)-10-(tert-butyl)-8,9-bis(3-methoxyphenyl)-4,11b-dimethyl-2,3,4,4a,5,6,10,11b-octahydro-1H-naphtho[2,1-f]indole-4-carboxylic acid (7d)



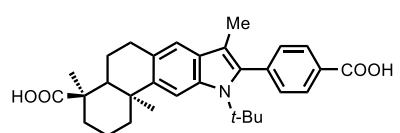
27.1 mg, 83% yield: white solid. Mp = 130-132 °C; **¹H NMR** (500 MHz, $CDCl_3$) δ 7.67 (s, 1H), 7.34 (s, 1H), 7.21 – 7.16 (m, 1H), 7.13 (t, J = 7.9 Hz, 1H), 6.97 – 6.91 (m, 1H), 6.89 – 6.82 (m, 2H), 6.79 (d, J = 7.6 Hz, 1H), 6.68 (dd, J = 8.1, 2.7 Hz, 1H), 6.66 – 6.63 (m, 1H), 3.74 (d, J = 7.5 Hz, 3H), 3.61 (s, 3H), 3.12 – 2.98 (m, 2H), 2.49 (d, J = 12.4 Hz, 1H), 2.39 (dd, J = 12.4, 2.3 Hz, 1H), 1.99 – 1.82 (m, 4H), 1.81 – 1.71 (m, 2H), 1.69 – 1.60 (m, 10H), 1.38 (s, 3H), 1.35 (s, 3H); **¹³C NMR** (126 MHz, $CDCl_3$) δ 184.8, 158.9, 158.7, 158.6, 143.6, 138.0, 137.8, 136.7, 135.6, 128.5, 128.3, 128.2, 127.0, 126.9, 124.6, 124.5, 122.7, 118.8, 117.6, 117.5, 116.6, 114.9, 113.1, 113.0, 111.7, 110.2, 59.0, 55.2, 54.9, 47.5, 44.9, 38.8, 37.7, 36.8, 32.0, 29.7, 25.8, 22.1, 18.8, 16.4; **HRMS (ESI-TOF)** calcd for $C_{37}H_{42}NO_4$ $[M-H]^-$ 564.3119, found 564.3118.

4,4'-((4R,11bS)-4-carboxy-4,11b-dimethyl-2,3,4,4a,5,6,10,11b-octahydro-1H-naphtho[2,1-f]indole-8,9-diyl)dibenzoic acid (7e)



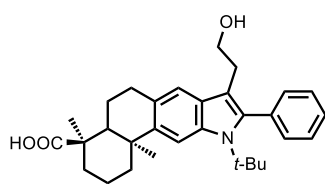
25.4 mg, 79% yield: white solid. Mp > 200 °C; **¹H NMR** 500 MHz, CD_3OD) δ 8.00 (d, J = 7.9 Hz, 2H), 7.94 (d, J = 8.1 Hz, 2H), 7.48 (d, J = 8.1 Hz, 2H), 7.40 (d, J = 8.0 Hz, 2H), 7.35 (s, 1H), 7.21 (s, 1H), 3.01 – 2.93 (m, 2H), 2.46 – 2.40 (m, 1H), 2.25 (dd, J = 12.5, 2.4 Hz, 1H), 1.92 – 1.78 (m, 3H), 1.76 – 1.65 (m, 2H), 1.60 – 1.48 (m, 2H), 1.28 (s, 3H), 1.24 (s, 3H); **¹³C NMR** (126 MHz, CD_3OD) δ 181.4, 168.9, 168.6, 145.9, 141.0, 137.3, 136.2, 133.8, 129.7, 129.60, 129.55, 129.4, 128.0, 127.8, 127.3, 126.4, 118.0, 113.3, 106.1, 45.1, 38.6, 37.4, 36.7, 29.9, 24.7, 21.8, 19.5, 18.4, 15.8; **HRMS (ESI-TOF)** calcd for $C_{33}H_{30}NO_6$ $[M-H]^-$ 536.2079, found 536.2080.

(4R,11bS)-10-(tert-butyl)-9-(4-carboxyphenyl)-4,8,11b-trimethyl-2,3,4,4a,5,6,10,11b-octahydro-1H-naphtho[2,1-f]indole-4-carboxylic acid (7f)



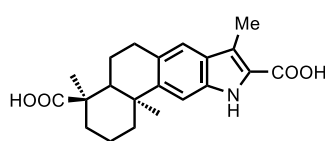
24.0 mg, 82% yield: white solid. Mp = 87-89 °C; **¹H NMR** 500 MHz, $DMSO-d_6$) δ 7.94 (t, J = 7.8 Hz, 2H), 7.45 (s, 1H), 7.40 – 7.33 (m, 2H), 7.07 (s, 1H), 2.99 – 2.81 (m, 2H), 2.37 (d, J = 12.3 Hz, 1H), 2.09 (dd, J = 11.9, 2.3 Hz, 1H), 1.79 (s, 3H), 1.76 – 1.62 (m, 4H), 1.58 – 1.52 (m, 1H), 1.48 – 1.37 (m, 11H), 1.15 (s, 6H); **¹³C NMR** (126 MHz, $DMSO-d_6$) δ 180.2, 167.9, 143.9, 141.9, 137.2, 136.2, 131.2, 131.1, 130.3, 129.14, 129.09, 127.9, 125.9, 118.2, 110.11, 110.05, 58.4, 47.0, 45.5, 37.6, 36.8, 31.9, 29.8, 25.9, 22.0, 18.8, 16.9, 9.3; **HRMS (ESI-TOF)** calcd for $C_{31}H_{36}NO_4$ $[M-H]^-$ 486.2650, found 486.2648.

(4R,11bS)-10-(tert-butyl)-9-(4-carboxyphenyl)-4,8,11b-trimethyl-2,3,4,4a,5,6,10,11b-octahydro-1H-naphtho[2,1-f]indole-4-carboxylic acid (7g)



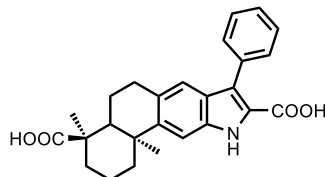
19.4 mg, 74% yield: white solid. Mp = 123-125 °C; $^1\text{H NMR}$ 500 MHz, CDCl_3) δ 7.62 (s, 1H), 7.41 – 7.36 (m, 3H), 7.35 – 7.30 (m, 3H), 3.68 (t, J = 6.9 Hz, 2H), 3.17 – 3.06 (m, 2H), 2.64 (td, J = 6.9, 4.7 Hz, 2H), 2.47 (d, J = 12.4 Hz, 1H), 2.38 (dd, J = 12.5, 2.4 Hz, 1H), 2.02 – 1.92 (m, 1H), 1.91 – 1.68 (m, 5H), 1.63 (dq, J = 9.6, 3.3 Hz, 1H), 1.56 (s, 9H), 1.36 (s, 3H), 1.35 (s, 3H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 184.6, 143.4, 139.5, 136.8, 135.5, 131.1, 131.0, 127.7, 127.60, 127.59, 127.4, 126.4, 118.0, 110.3, 110.0, 63.1, 58.5, 47.5, 45.0, 38.8, 37.7, 36.7, 31.9, 29.8, 27.9, 25.8, 22.1, 18.8, 16.4; **HRMS (ESI-TOF)** calcd for $\text{C}_{31}\text{H}_{38}\text{NO}_3$ $[\text{M}-\text{H}]^-$ 472.2857, found 472.2860.

(4R,11bS)-4,8,11b-trimethyl-2,3,4,4a,5,6,10,11b-octahydro-1H-naphtho[2,1-f]indole-4,9-dicarboxylic acid (7h)



17.3 mg, 81% yield: white solid. Mp = 192-194 °C; $^1\text{H NMR}$ 500 MHz, CD_3OD) δ 7.17 (s, 1H), 7.13 (s, 1H), 2.98 – 2.84 (m, 2H), 2.42 (s, 3H), 2.33 – 2.26 (m, 1H), 2.12 (dd, J = 12.4, 2.5 Hz, 1H), 1.83 – 1.75 (m, 1H), 1.75 – 1.66 (m, 2H), 1.64 – 1.54 (m, 2H), 1.47 – 1.39 (m, 2H), 1.17 (s, 3H), 1.12 (s, 3H); $^{13}\text{C NMR}$ (126 MHz, CD_3OD) δ 181.3, 164.8, 148.3, 135.9, 126.7, 126.5, 123.7, 119.1, 118.3, 106.4, 45.0, 38.6, 37.5, 36.7, 29.7, 24.5, 21.8, 18.4, 15.8, 8.7; **HRMS (ESI-TOF)** calcd for $\text{C}_{21}\text{H}_{24}\text{NO}_4$ $[\text{M}-\text{H}]^-$ 354.1711, found 354.1711.

(4R,11bS)-4,11b-dimethyl-8-phenyl-2,3,4,4a,5,6,10,11b-octahydro-1H-naphtho[2,1-f]indole-4,9-dicarboxylic acid (7i)



18.0 mg, 72% yield: white solid. Mp = 177-179 °C; $^1\text{H NMR}$ 500 MHz, CD_3OD) δ 7.52 – 7.48 (m, 2H), 7.42 – 7.37 (m, 3H), 7.33 – 7.28 (m, 1H), 7.17 (s, 1H), 3.00 – 2.89 (m, 2H), 2.46 – 2.41 (m, 1H), 2.24 (dd, J = 12.4, 2.5 Hz, 1H), 1.92 – 1.79 (m, 3H), 1.76 – 1.70 (m, 1H), 1.70 – 1.65 (m, 1H), 1.60 – 1.49 (m, 2H), 1.28 (s, 3H), 1.24 (s, 3H); $^{13}\text{C NMR}$ (126 MHz, CD_3OD) δ 181.2, 164.0, 148.5, 135.7, 134.5, 130.3, 127.6, 127.3, 126.3, 126.1, 122.9, 122.7, 119.7, 106.6, 47.1, 44.9, 38.6, 37.5, 36.7, 29.7, 24.5, 21.7, 18.4, 15.8; **HRMS (ESI-TOF)** calcd for $\text{C}_{26}\text{H}_{26}\text{NO}_4$ $[\text{M}-\text{H}]^-$ 416.1867, found 416.1868.

4. Supplemental References

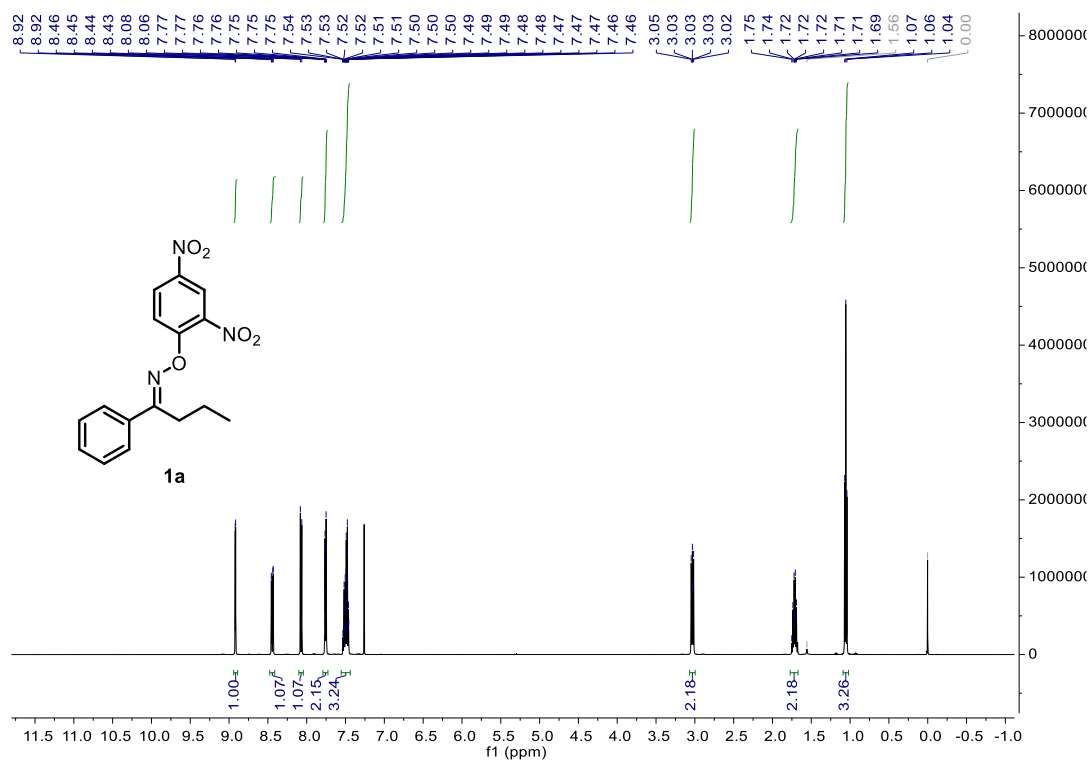
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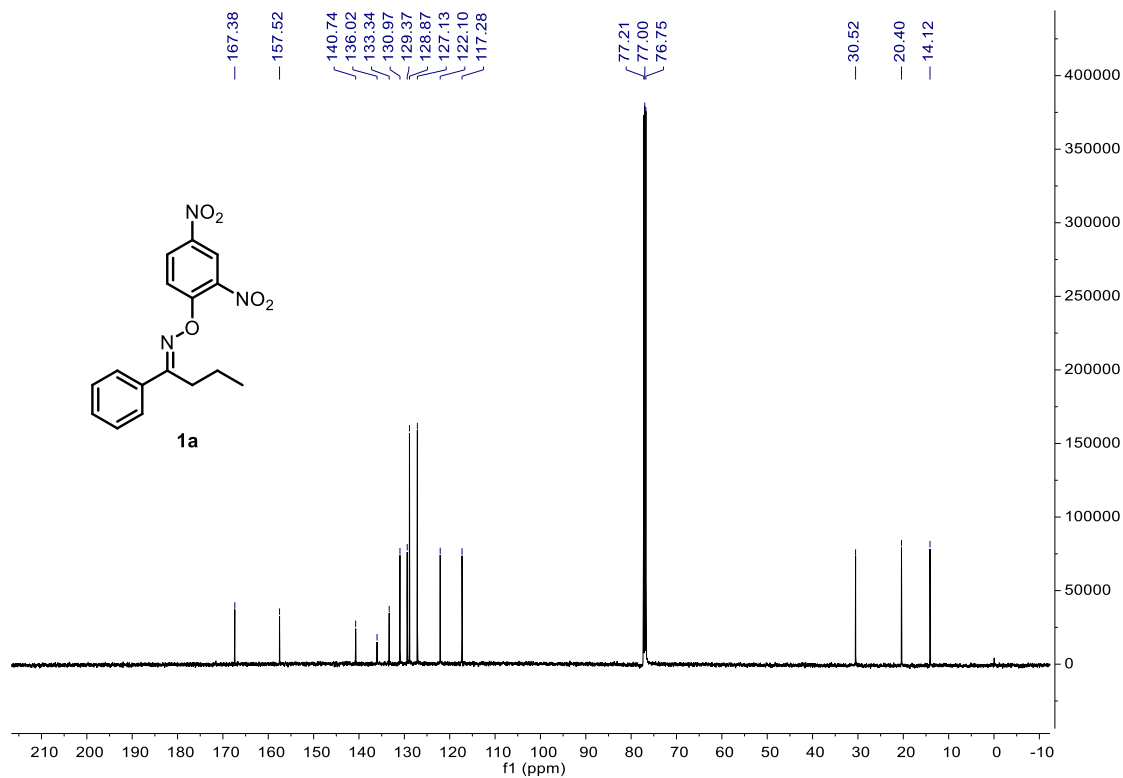
5. NMR Spectra

5.1 NMR Spectra for New Starting Material

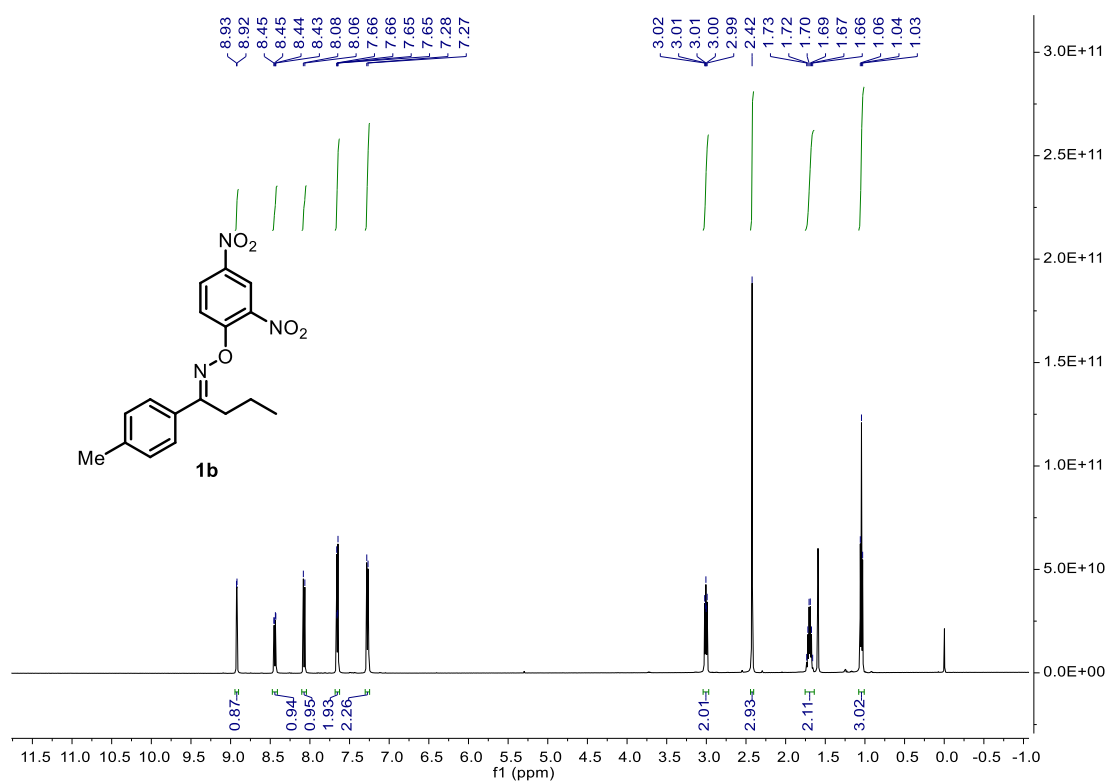
(*E*)-1-phenylbutan-1-one *O*-(2,4-dinitrophenyl) oxime (1a) (^1H NMR 500 MHz, CDCl_3)



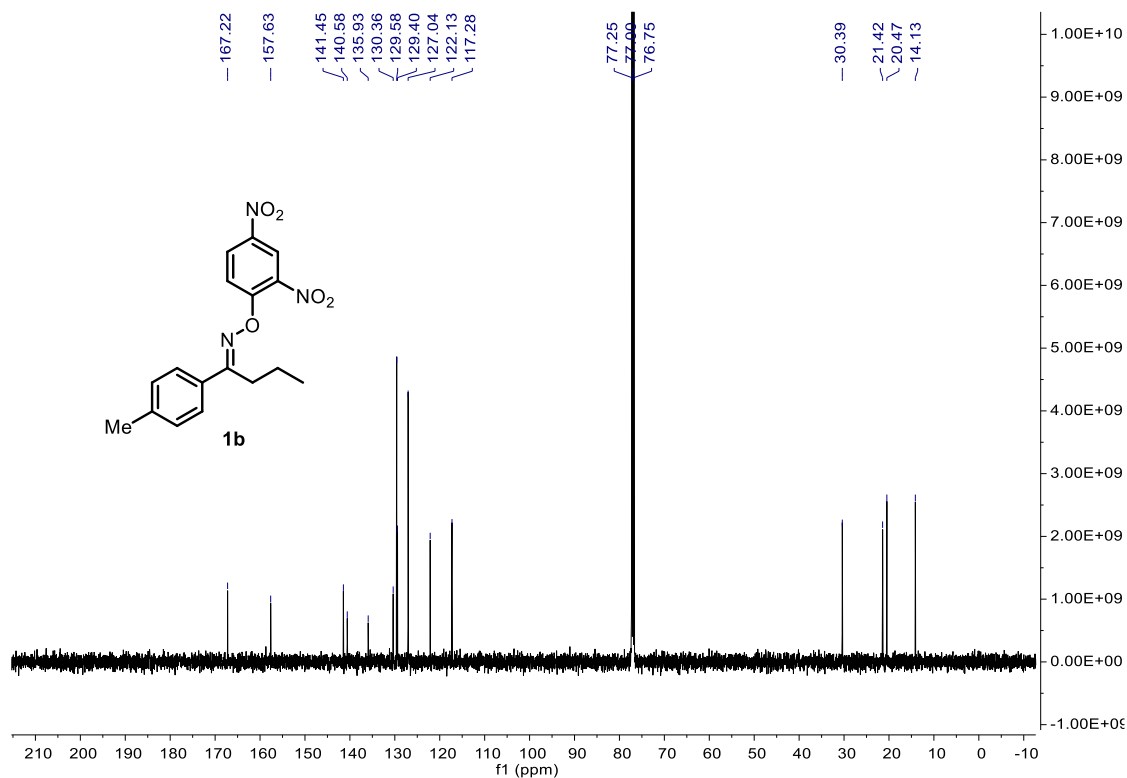
(*E*)-1-phenylbutan-1-one *O*-(2,4-dinitrophenyl) oxime (1a) (^{13}C NMR 126 MHz, CDCl_3)



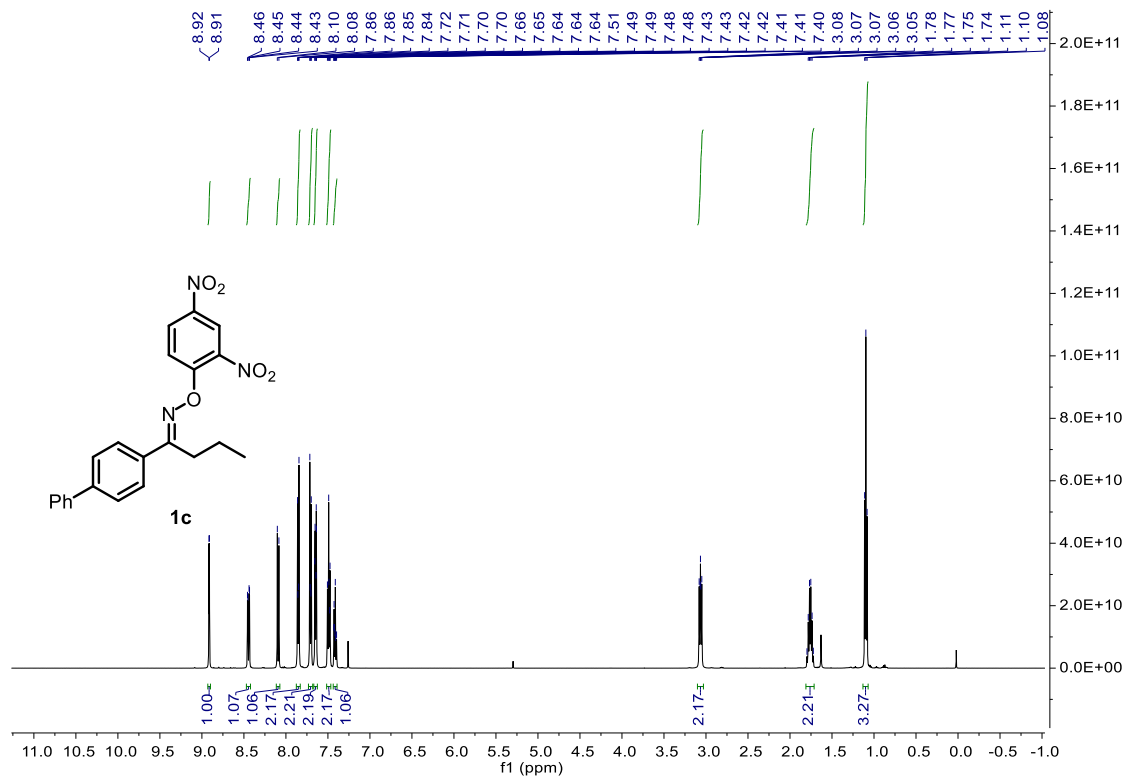
(*E*)-1-(*p*-tolyl)butan-1-one *O*-(2,4-dinitrophenyl) oxime (1b) (¹H NMR 500 MHz, CDCl₃)



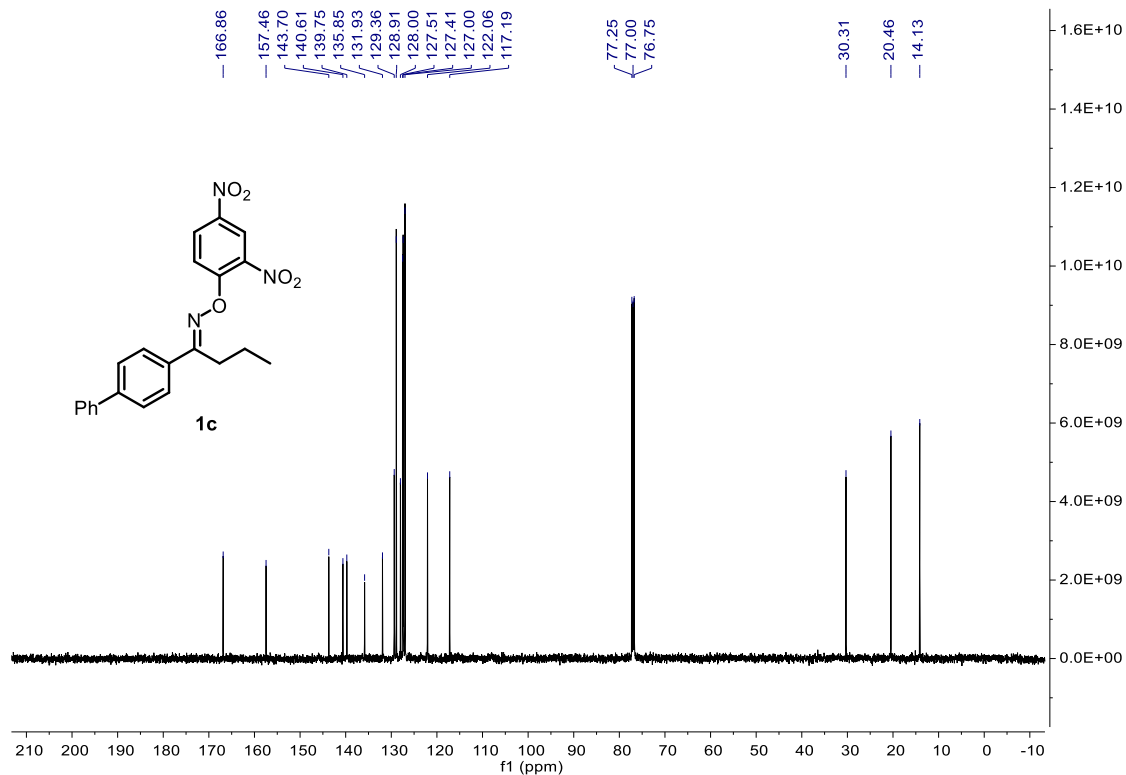
(*E*)-1-(*p*-tolyl)butan-1-one *O*-(2,4-dinitrophenyl) oxime (1b) (¹³C NMR 126 MHz, CDCl₃)



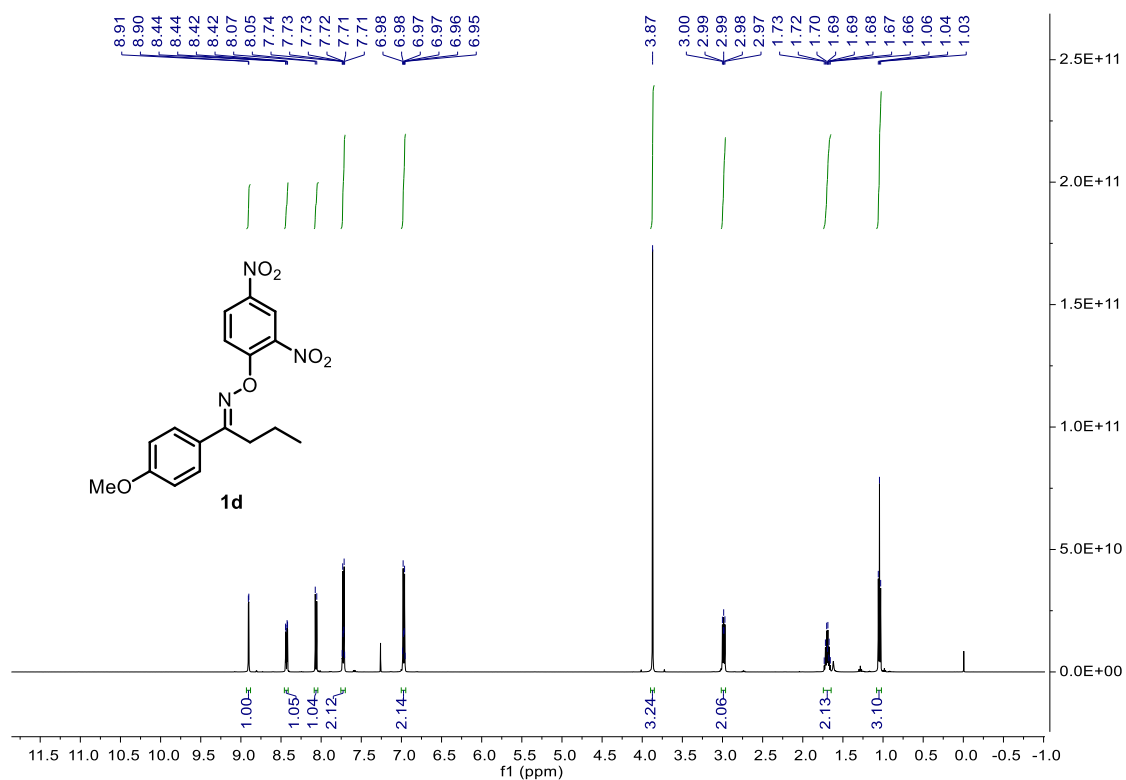
(*E*)-1-([1,1'-biphenyl]-4-yl)butan-1-one *O*-(2,4-dinitrophenyl) oxime (1c) (^1H NMR 500 MHz, CDCl_3)



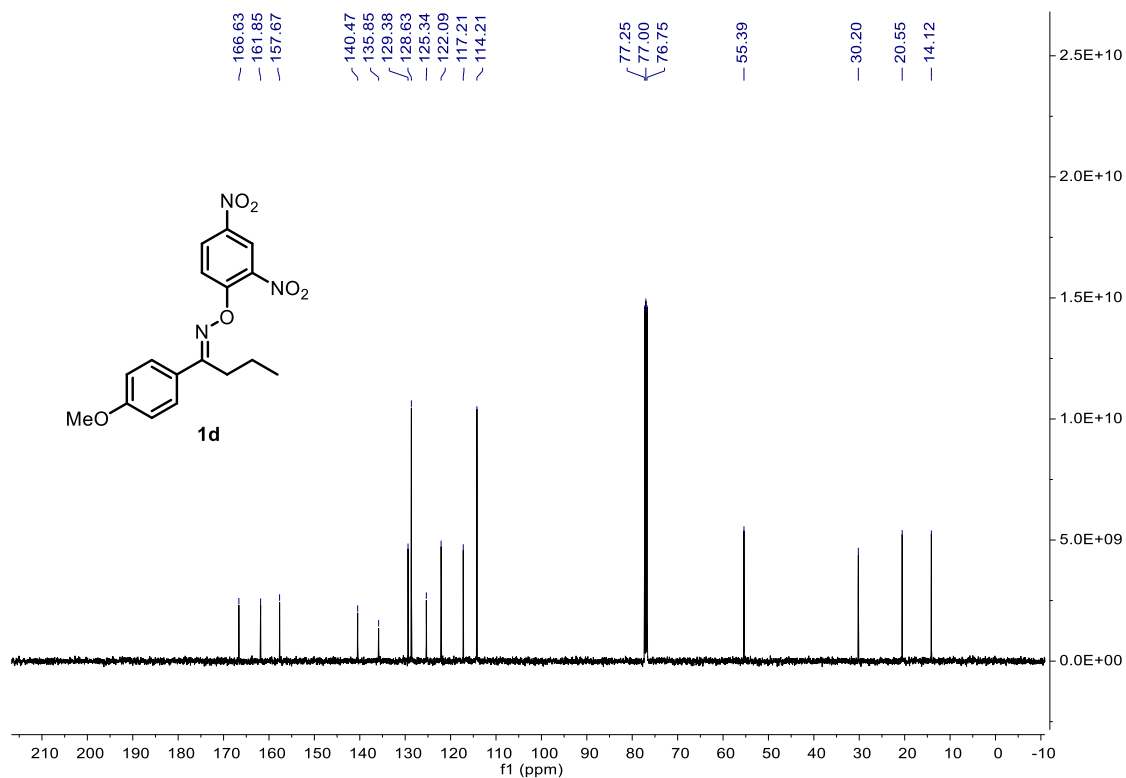
(*E*)-1-([1,1'-biphenyl]-4-yl)butan-1-one *O*-(2,4-dinitrophenyl) oxime (1c) (^{13}C NMR 126 MHz, CDCl_3)



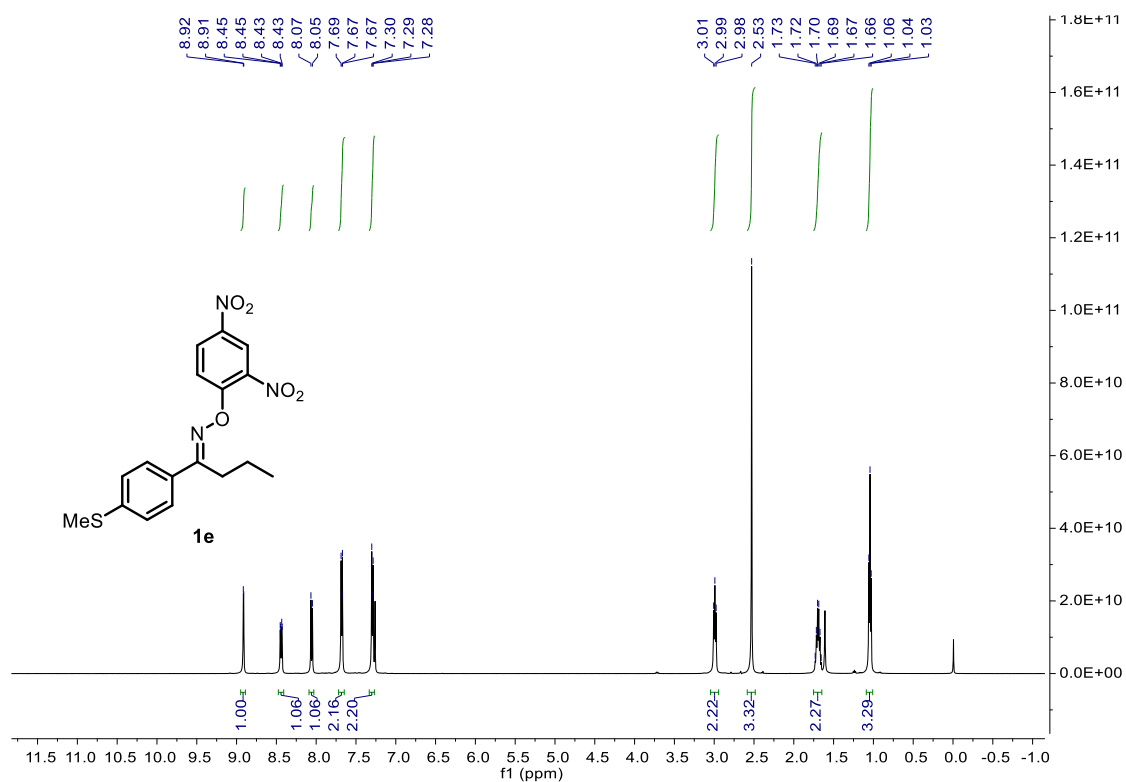
(*E*)-1-(4-methoxyphenyl)butan-1-one *O*-(2,4-dinitrophenyl) oxime (1d) (^1H NMR 500 MHz, CDCl_3)



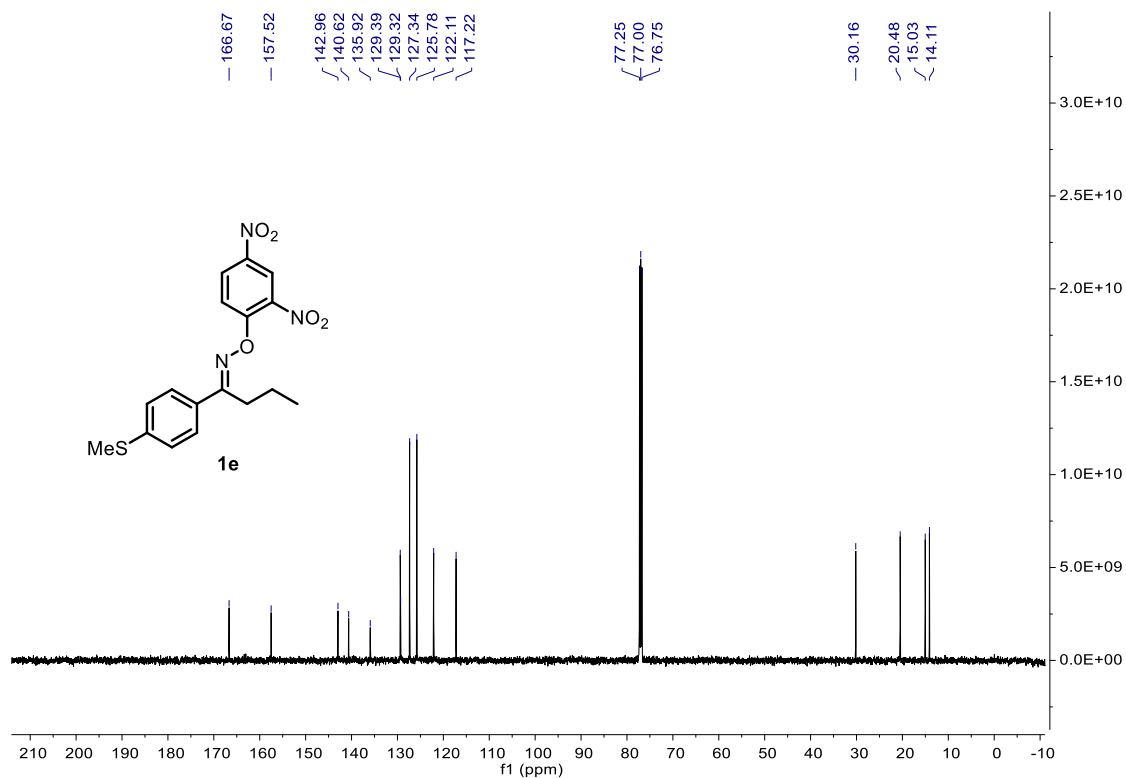
(*E*)-1-(4-methoxyphenyl)butan-1-one *O*-(2,4-dinitrophenyl) oxime (1d) (¹³C NMR 126 MHz, CDCl₃)



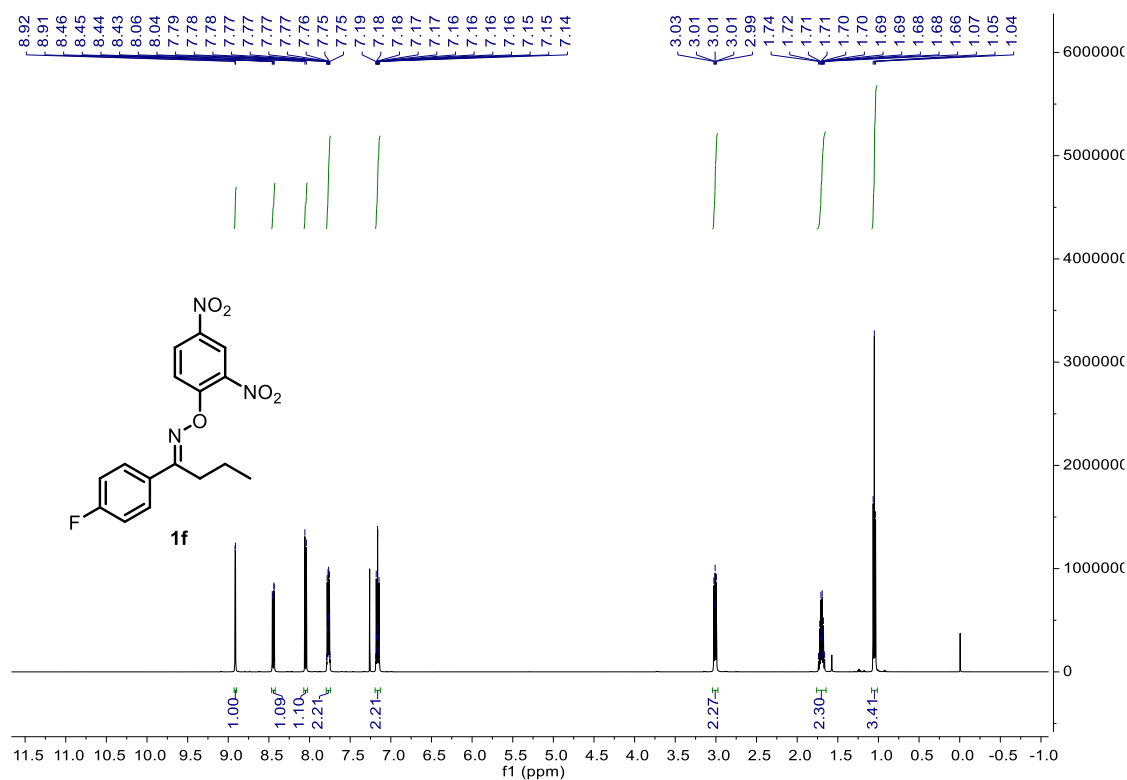
(*E*)-1-(4-(methylthio)phenyl)butan-1-one *O*-(2,4-dinitrophenyl) oxime (1e) (¹H NMR 500 MHz, CDCl₃)



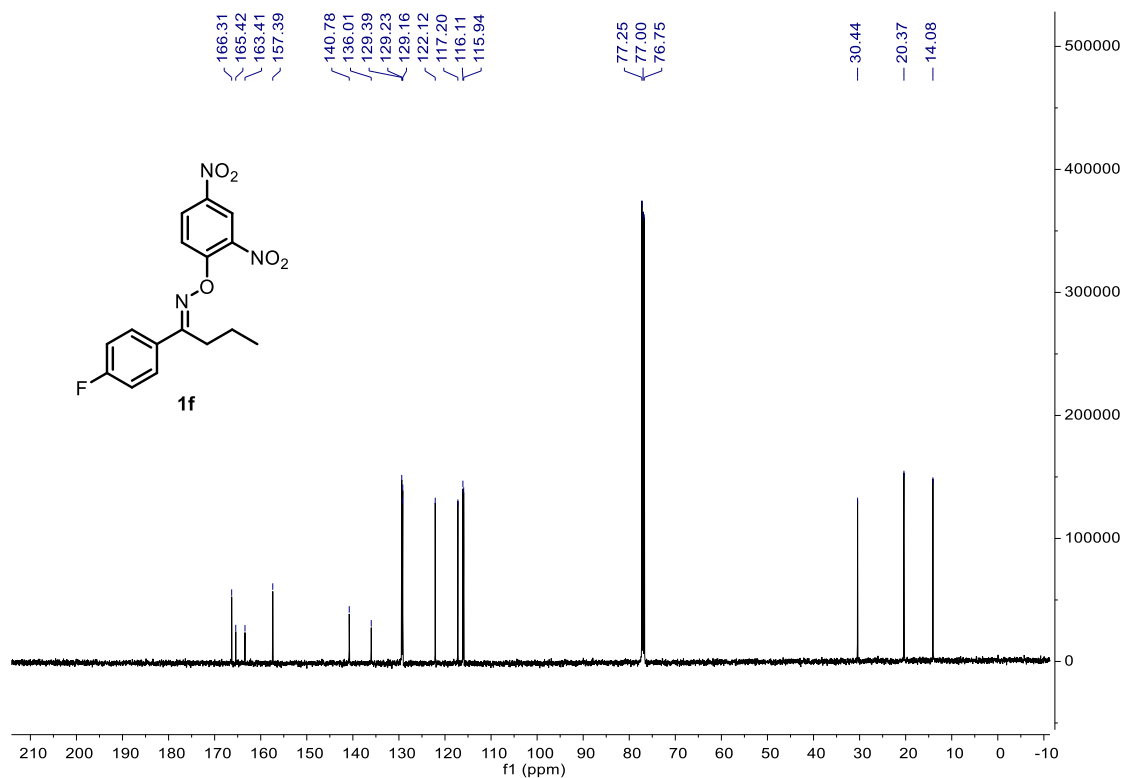
(*E*)-1-(4-(methylthio)phenyl)butan-1-one *O*-(2,4-dinitrophenyl) oxime (1e**)** (¹³C NMR 126 MHz, CDCl₃)



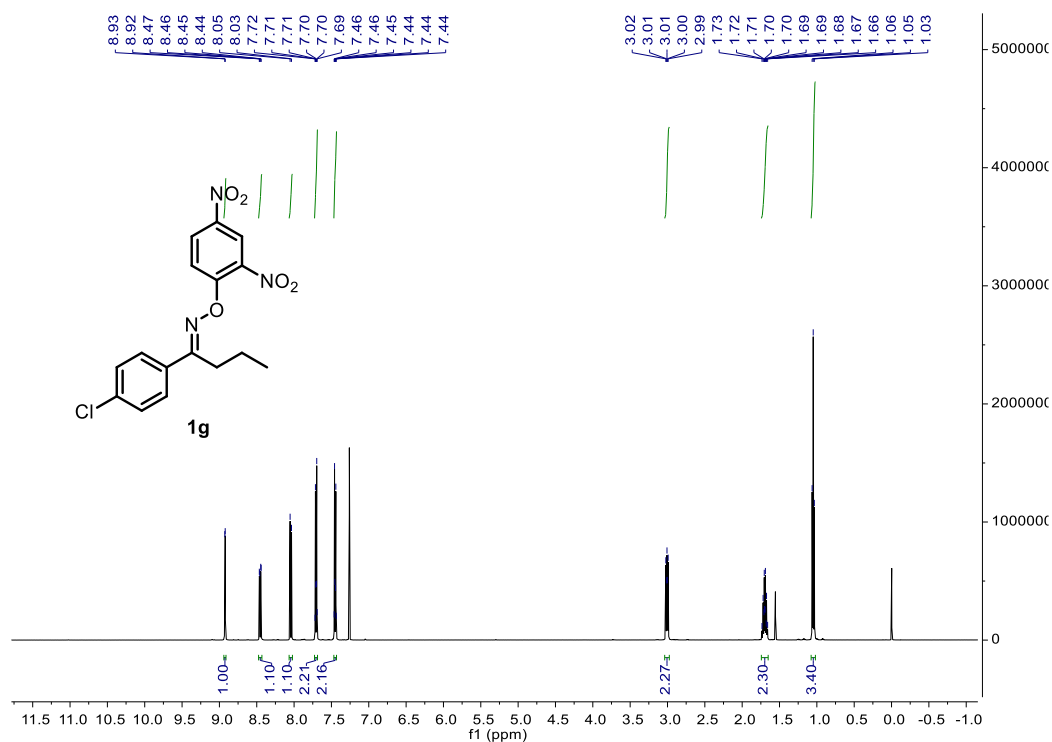
(*E*)-1-(4-fluorophenyl)butan-1-one *O*-(2,4-dinitrophenyl) oxime (1f**)** (¹H NMR 500 MHz, CDCl₃)



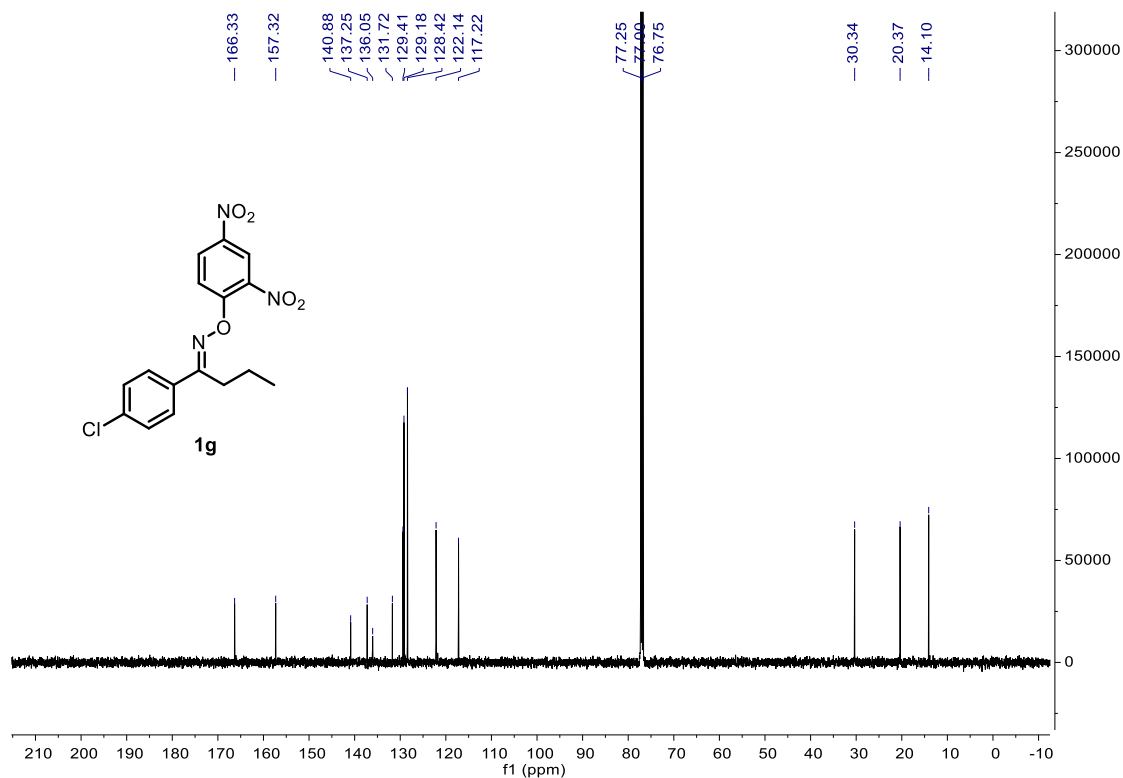
(*E*)-1-(4-fluorophenyl)butan-1-one *O*-(2,4-dinitrophenyl) oxime (1f) (¹³C NMR 126 MHz, CDCl₃)



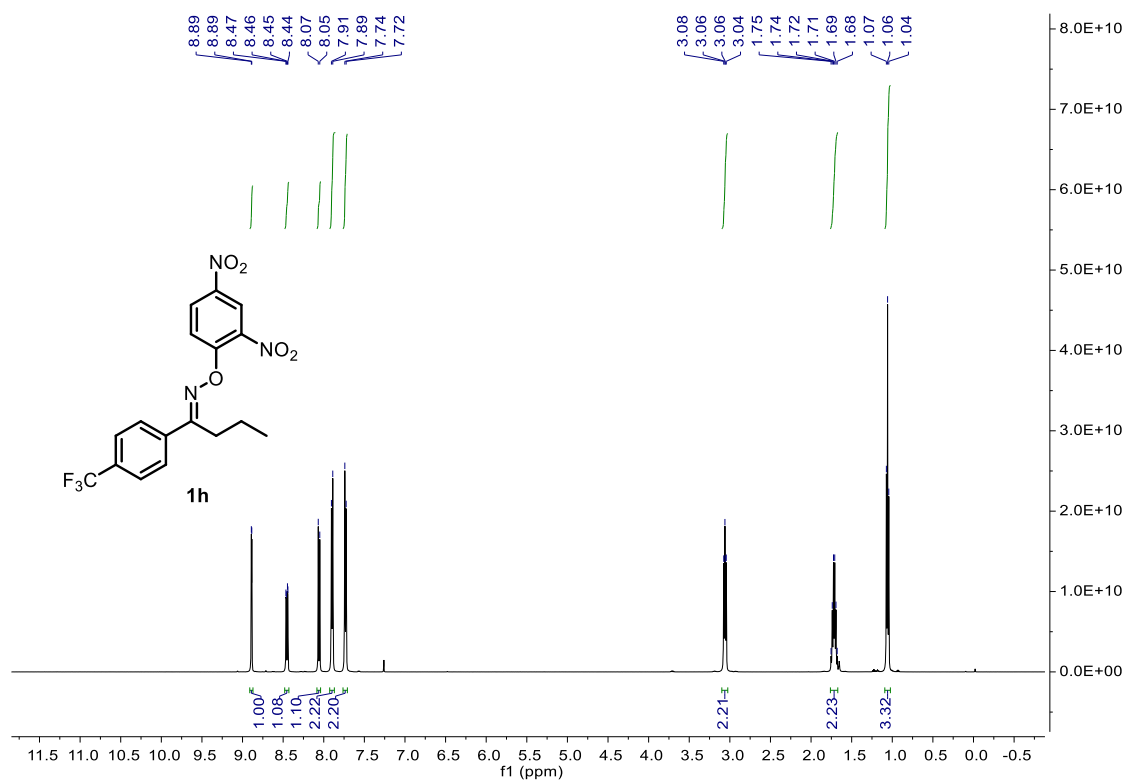
(*E*)-1-(4-chlorophenyl)butan-1-one *O*-(2,4-dinitrophenyl) oxime (1g) (¹H NMR 500 MHz, CDCl₃)



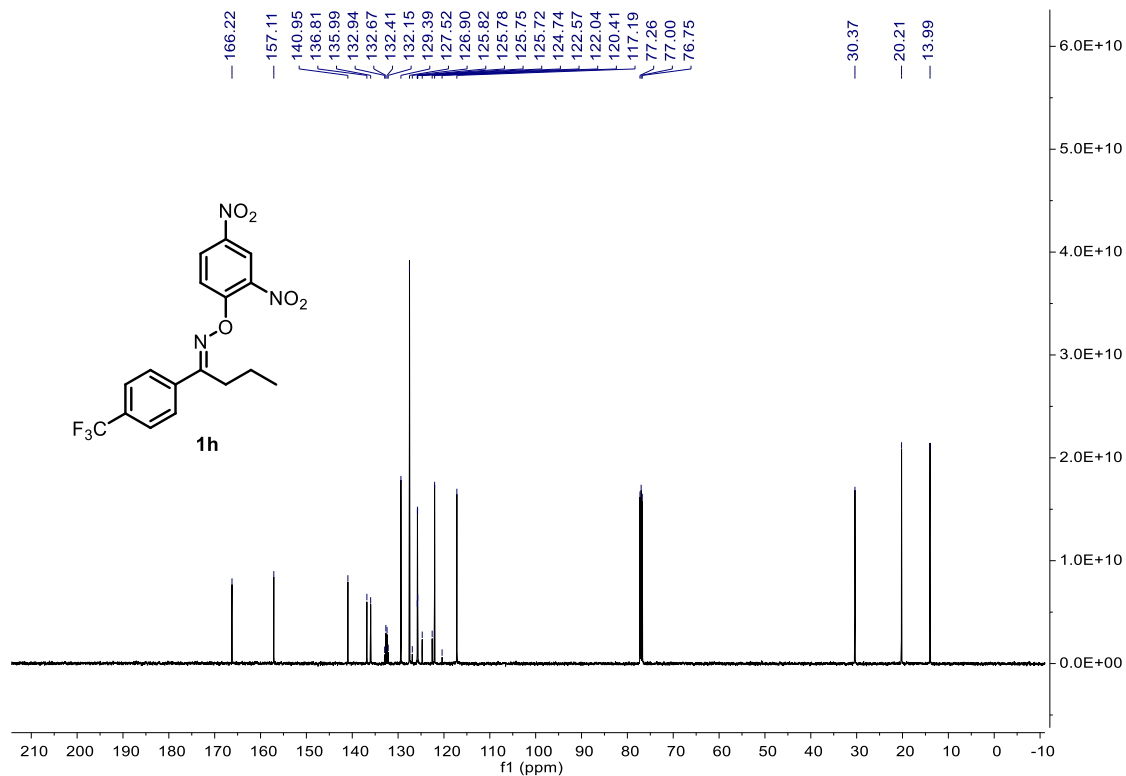
(*E*)-1-(4-chlorophenyl)butan-1-one *O*-(2,4-dinitrophenyl) oxime (1g) (¹³C NMR 126 MHz, CDCl₃)



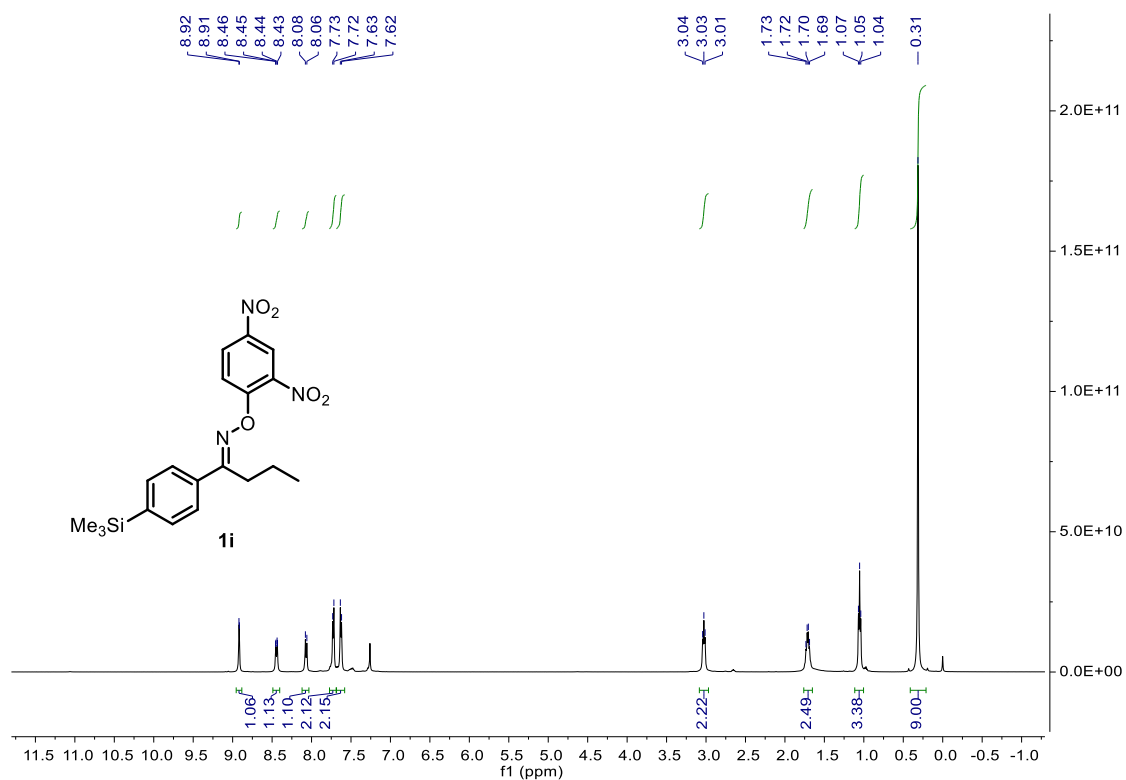
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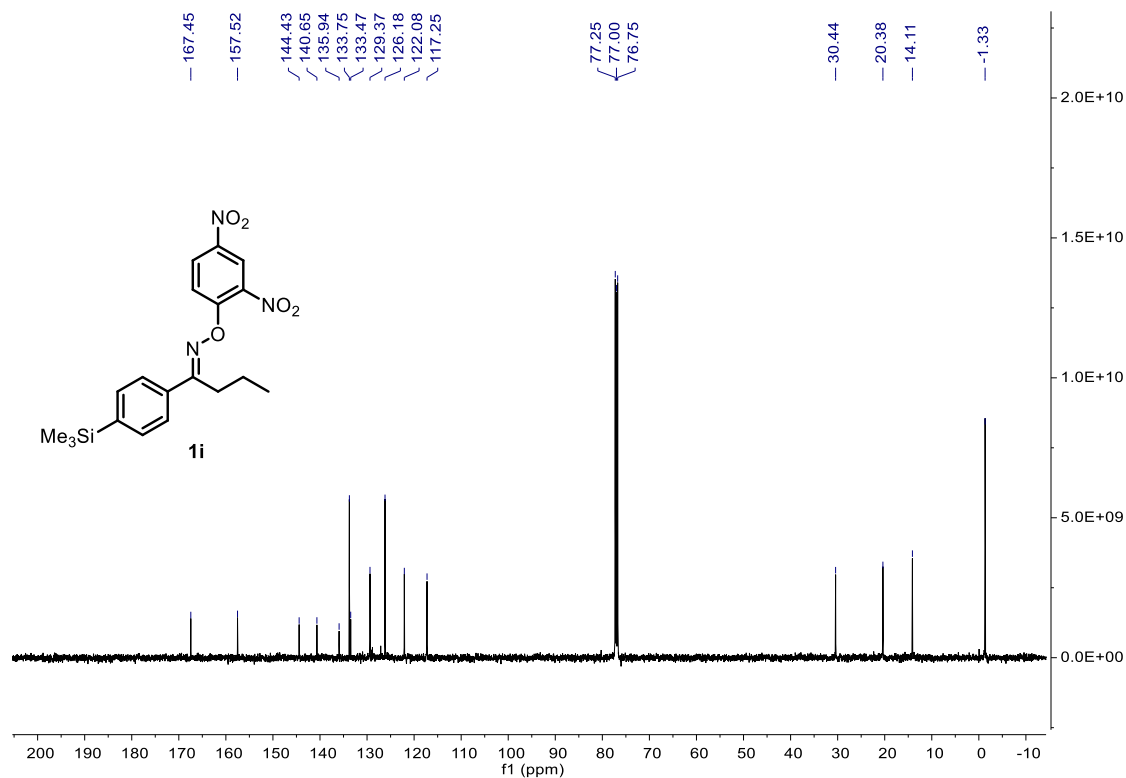
(*E*)-1-(4-(trifluoromethyl)phenyl)butan-1-one *O*-(2,4-dinitrophenyl) oxime (1h) (¹³C NMR 126 MHz, CDCl₃)



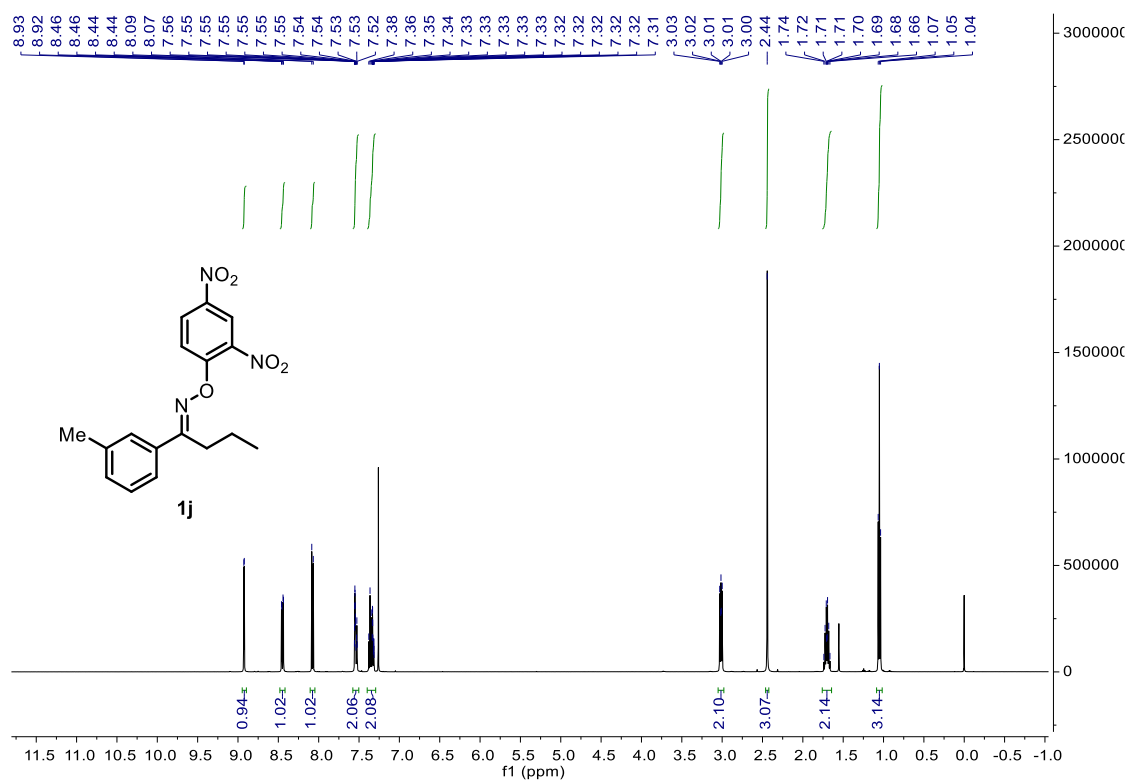
(*E*)-1-(4-(trimethylsilyl)phenyl)butan-1-one *O*-(2,4-dinitrophenyl) oxime (1i) (¹H NMR 500 MHz, CDCl₃)



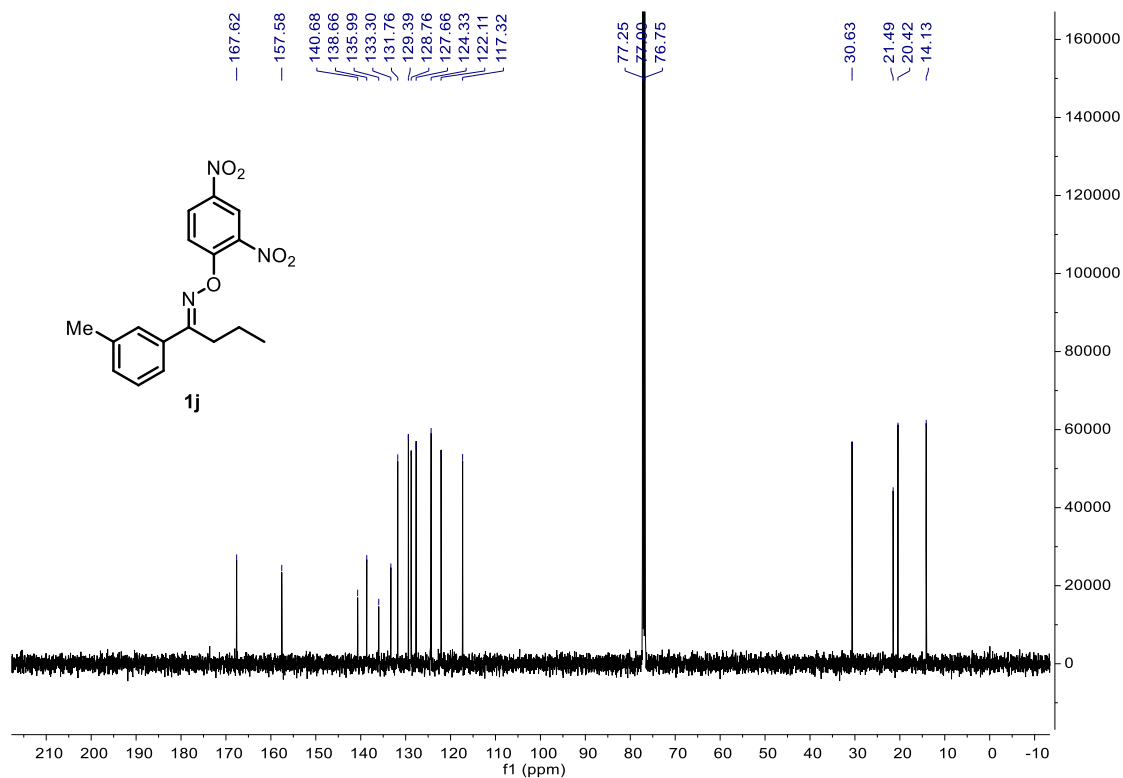
(*E*)-1-(4-(trimethylsilyl)phenyl)butan-1-one *O*-(2,4-dinitrophenyl) oxime (1i**)** (¹³C NMR 126 MHz, CDCl₃)



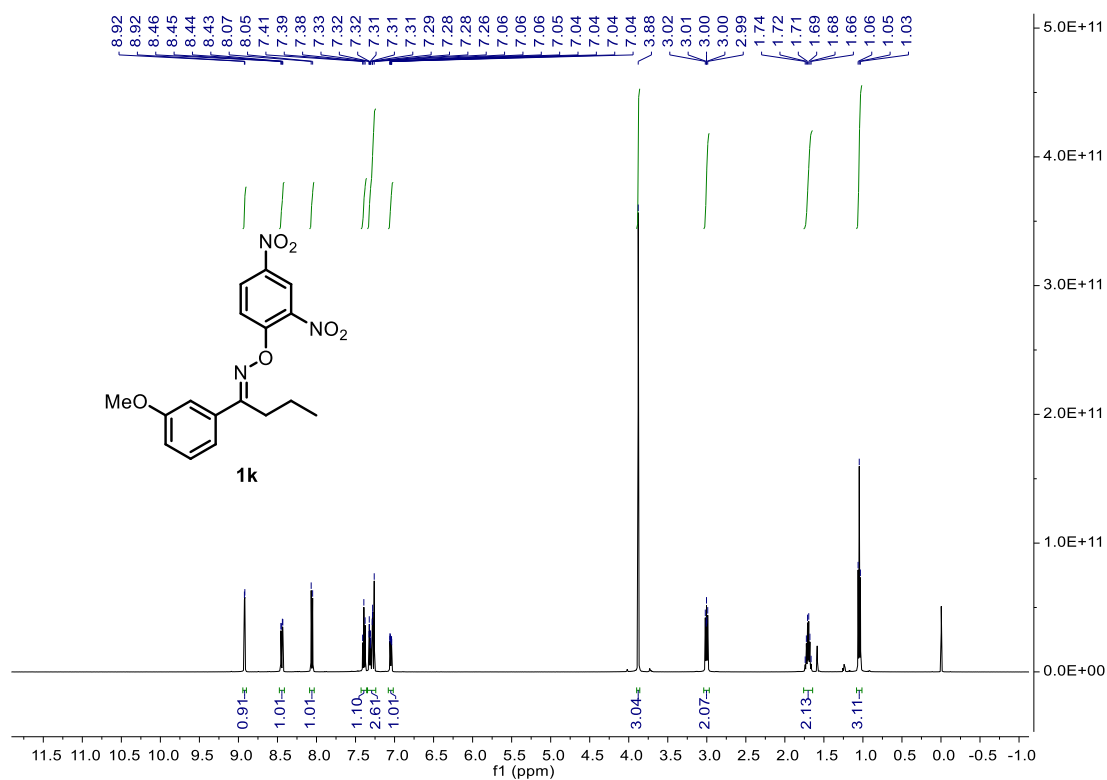
(*E*)-1-(*m*-tolyl)butan-1-one *O*-(2,4-dinitrophenyl) oxime (1j**)** (¹H NMR 500 MHz, CDCl₃)



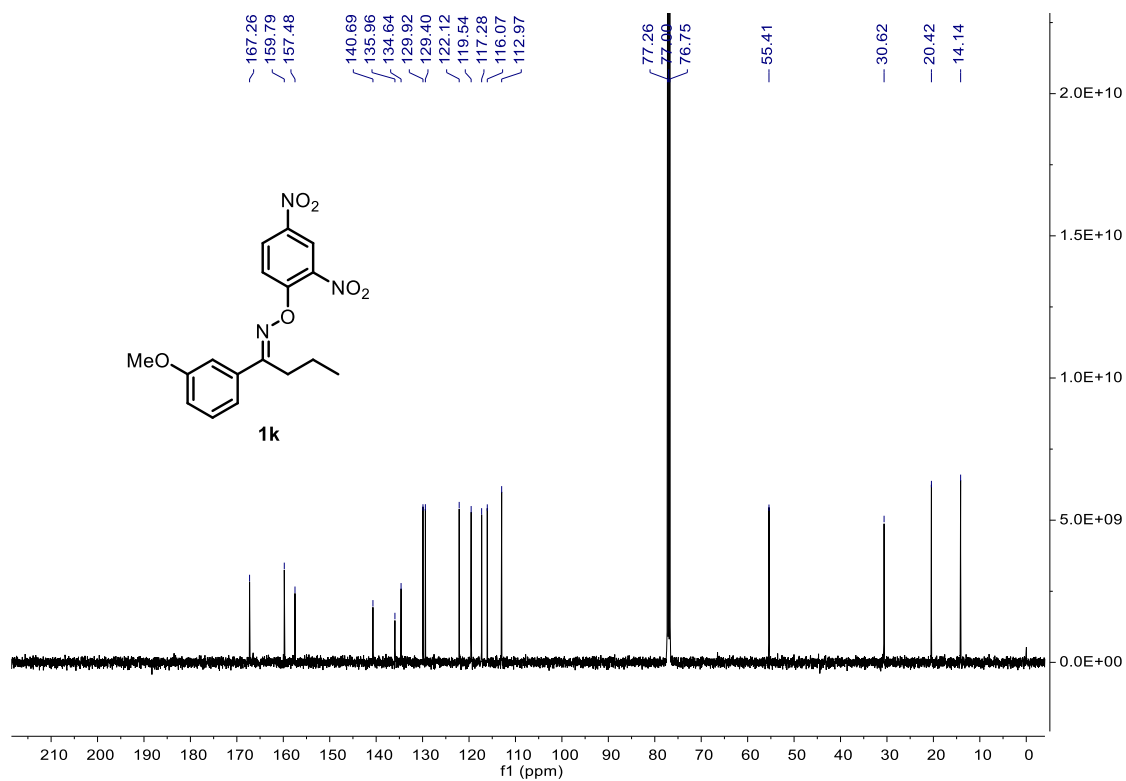
(*E*)-1-(*m*-tolyl)butan-1-one *O*-(2,4-dinitrophenyl) oxime (1j) (¹³C NMR 126 MHz, CDCl₃)



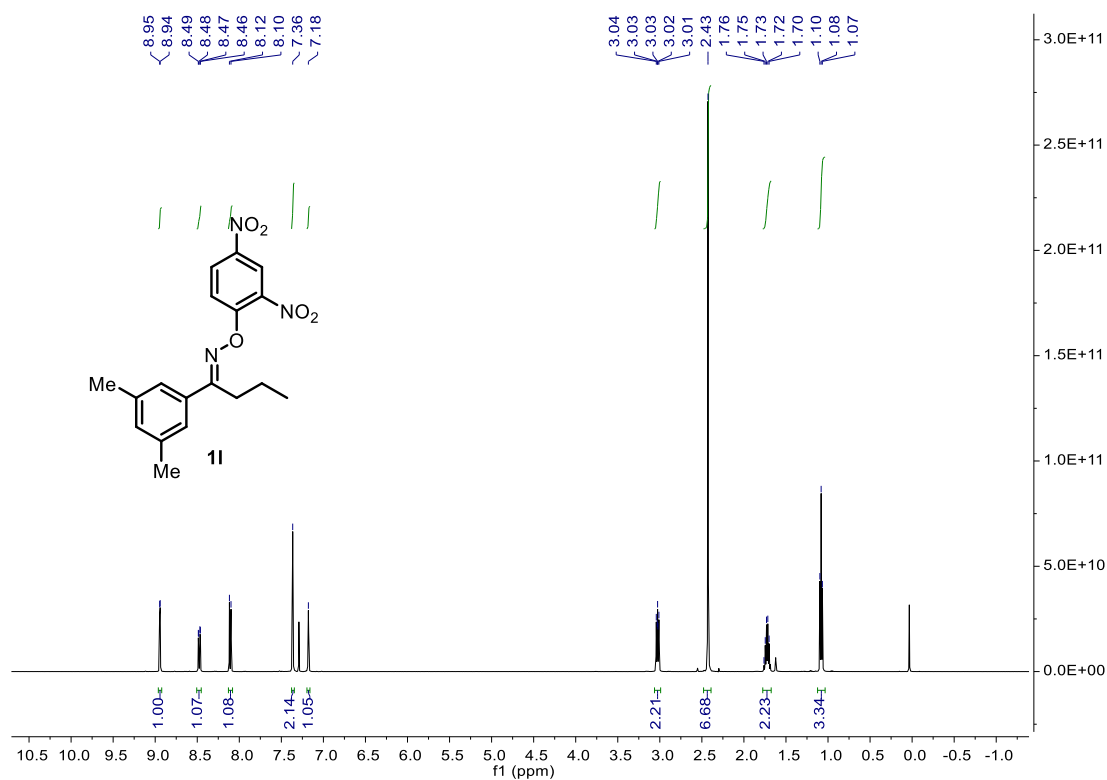
(*E*)-1-(3-methoxyphenyl)butan-1-one *O*-(2,4-dinitrophenyl) oxime (1k) (¹H NMR 500 MHz, CDCl₃)



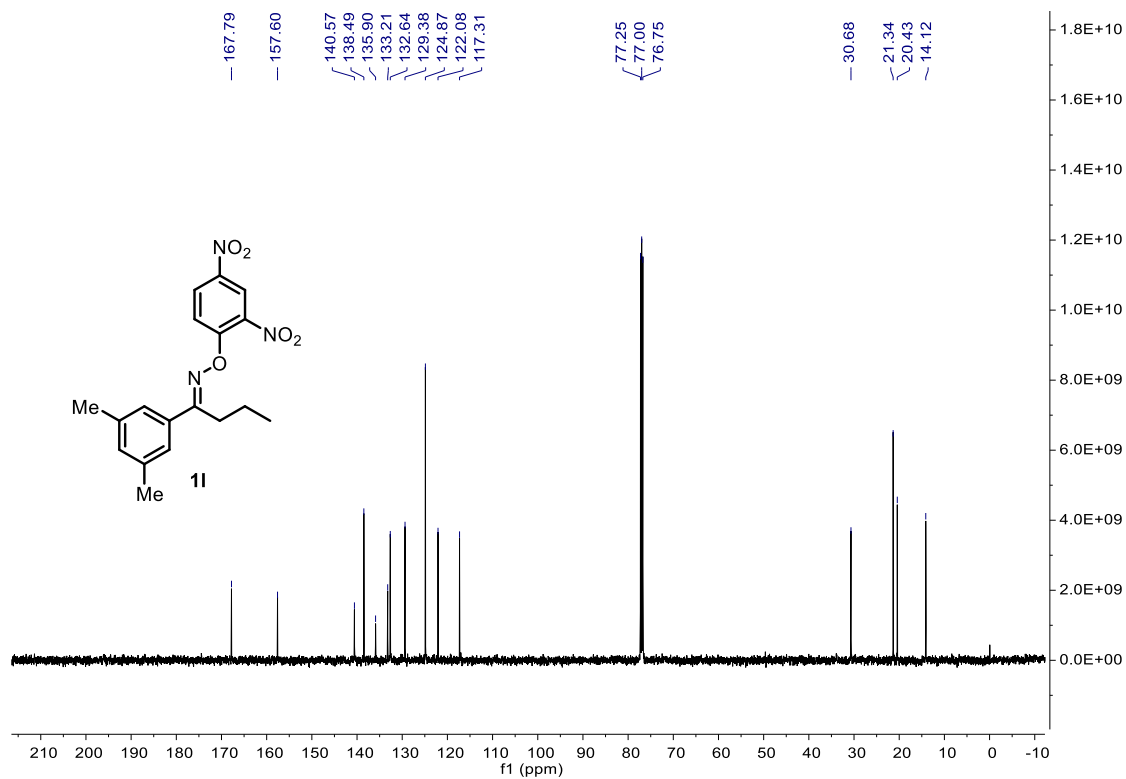
(*E*)-1-(3-methoxyphenyl)butan-1-one *O*-(2,4-dinitrophenyl) oxime (1k) (¹³C NMR 126 MHz, CDCl₃)



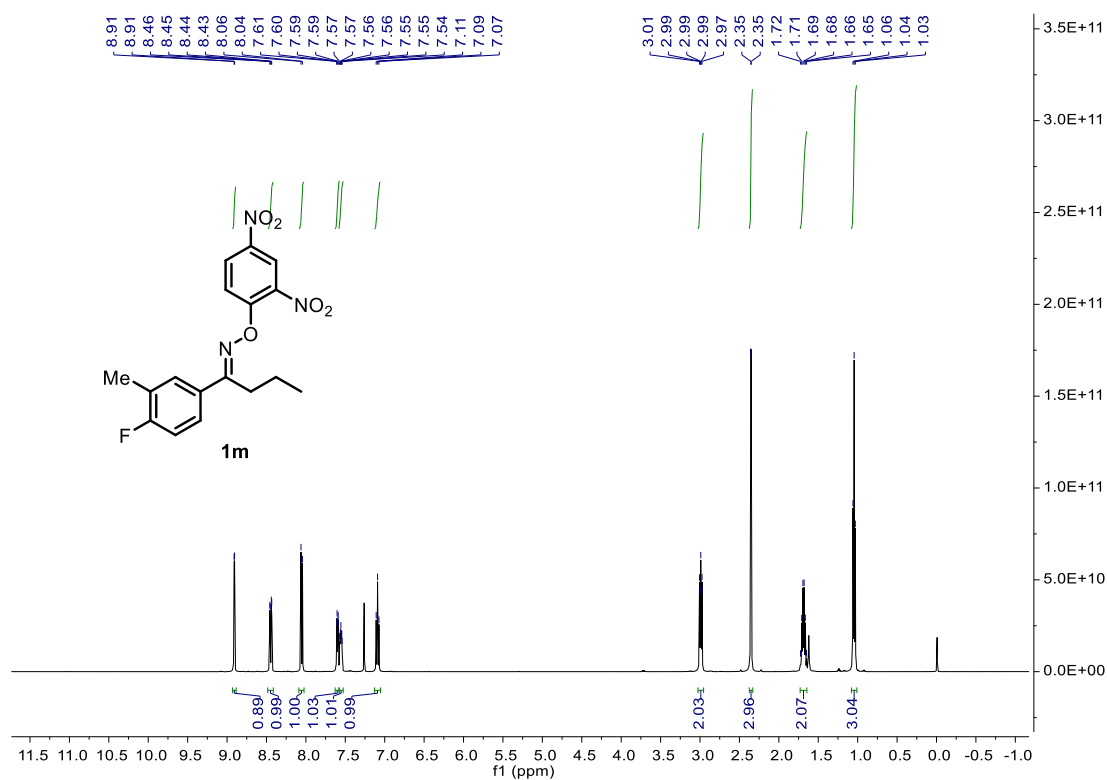
(*E*)-1-(3,5-dimethylphenyl)butan-1-one *O*-(2,4-dinitrophenyl) oxime (1l) (¹H NMR 500 MHz, CDCl₃)



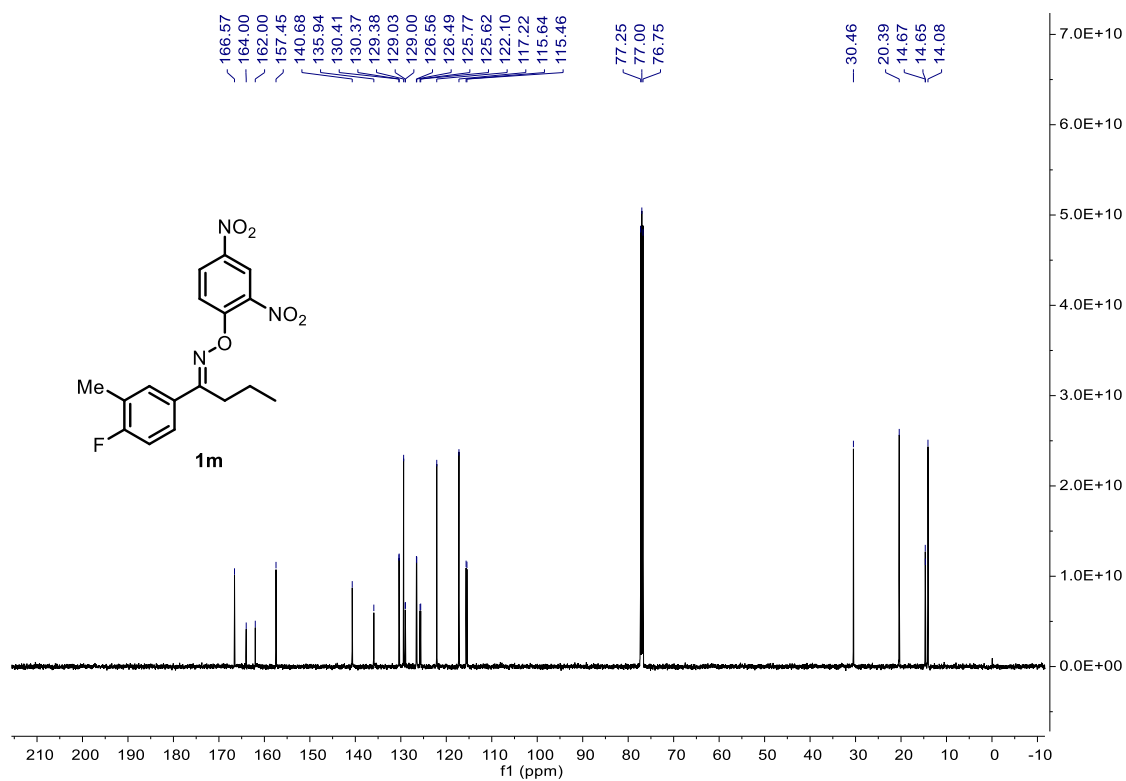
(*E*)-1-(3,5-dimethylphenyl)butan-1-one *O*-(2,4-dinitrophenyl) oxime (1l) (¹³C NMR 125 MHz, CDCl₃)



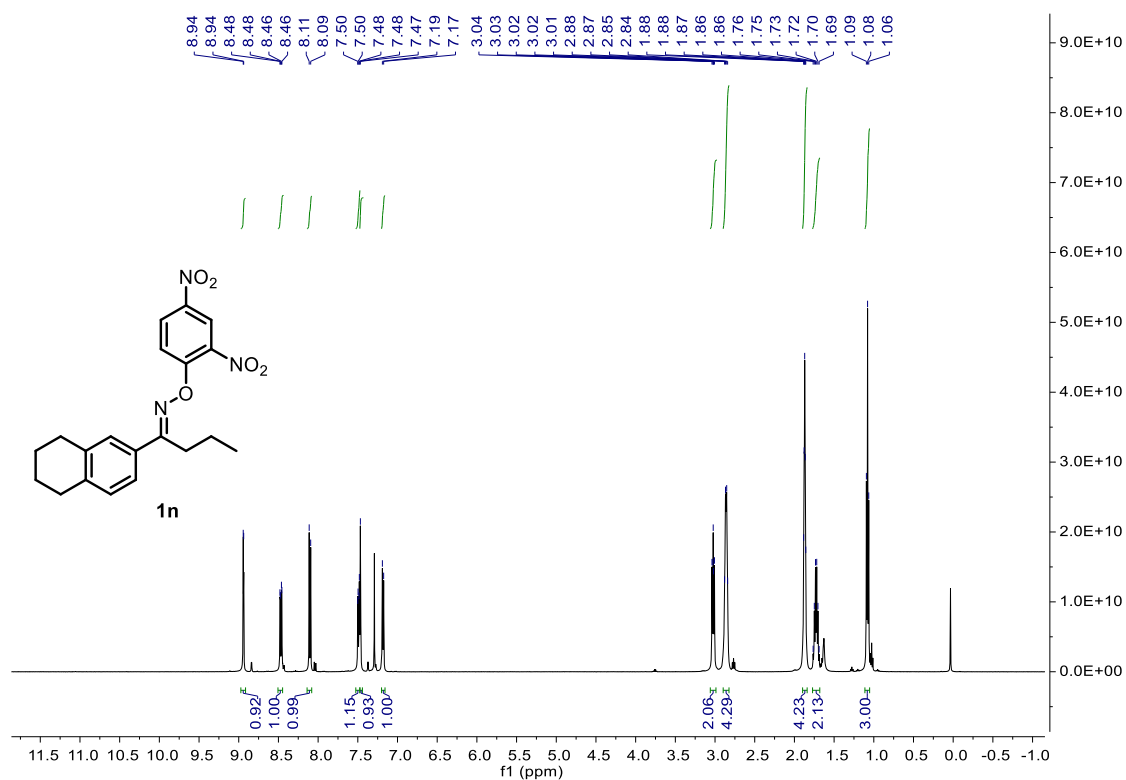
(*E*)-1-(4-fluoro-3-methylphenyl)butan-1-one *O*-(2,4-dinitrophenyl) oxime (1m) (¹H NMR 500 MHz, CDCl₃)



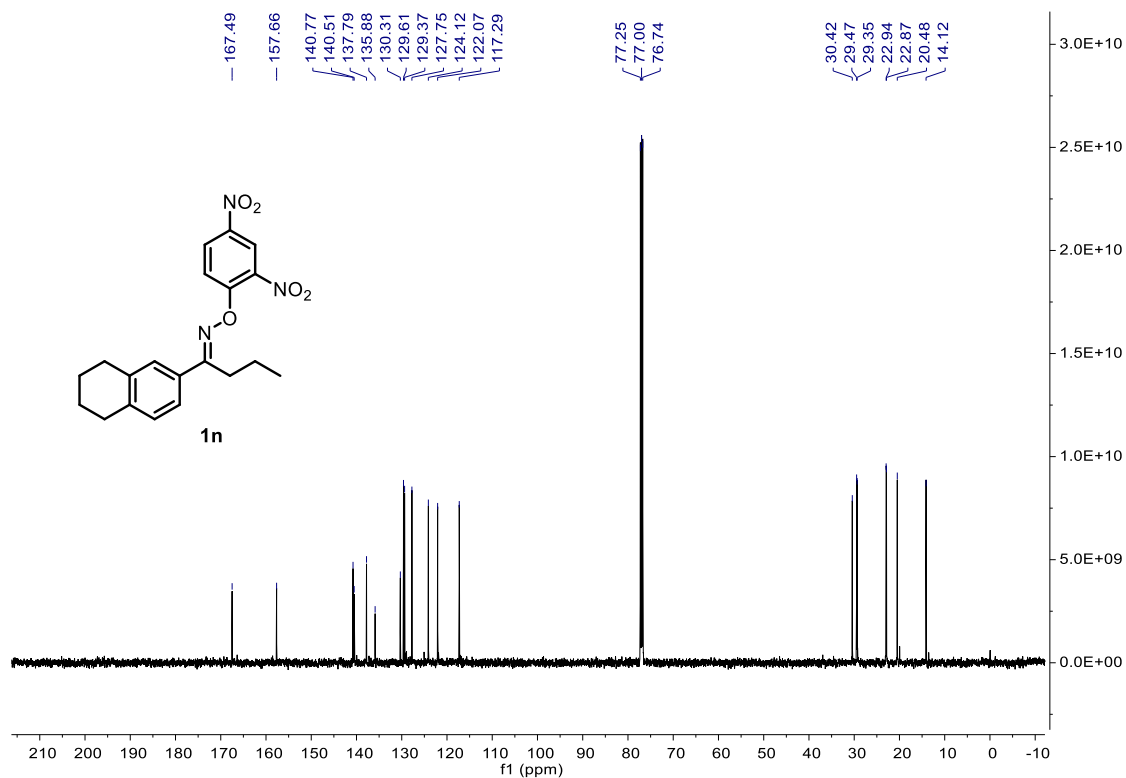
(*E*)-1-(4-fluoro-3-methylphenyl)butan-1-one *O*-(2,4-dinitrophenyl) oxime (1m) (¹³C NMR 126 MHz, CDCl₃)



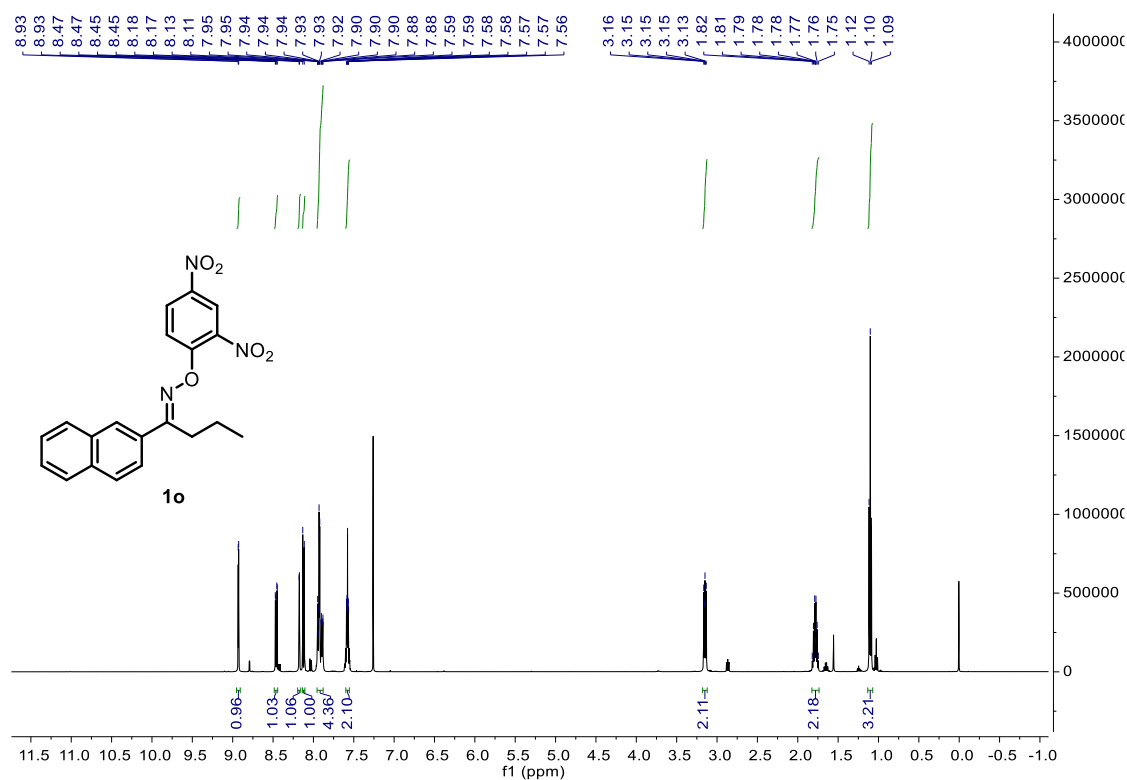
(*E*)-1-(5,6,7,8-tetrahydronaphthalen-2-yl)butan-1-one *O*-(2,4-dinitrophenyl) oxime (1n) (¹H NMR 500 MHz, CDCl₃)



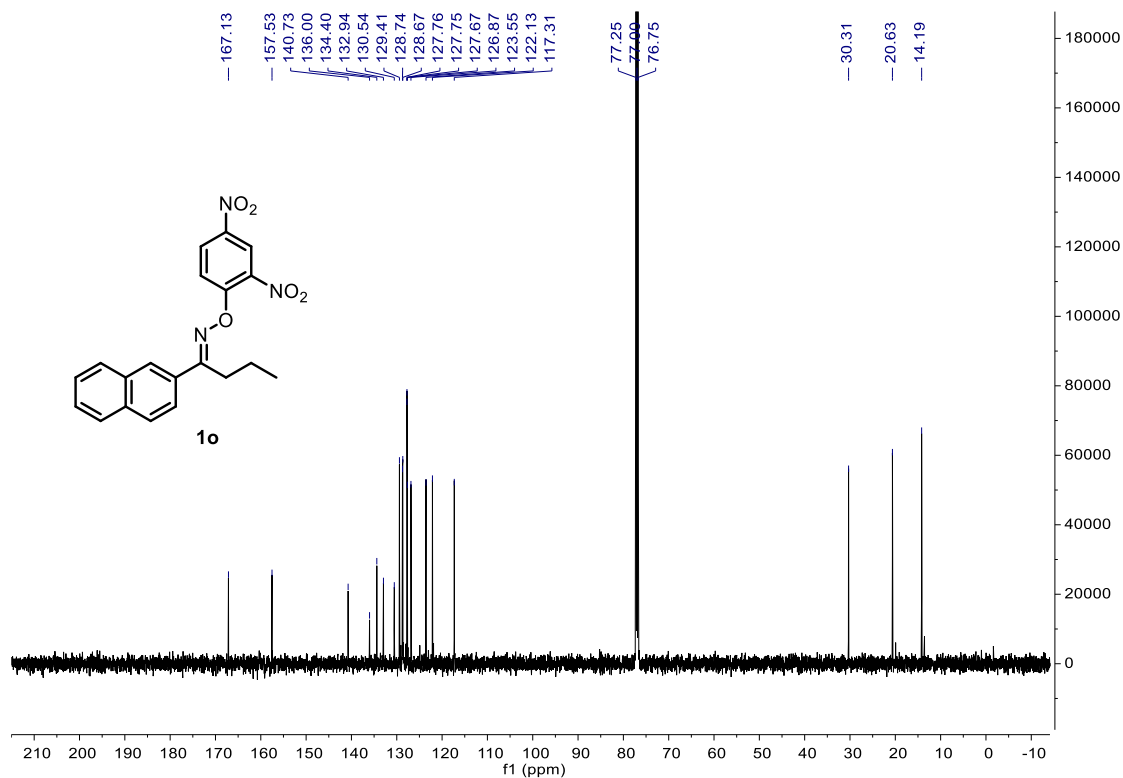
(*E*)-1-(5,6,7,8-tetrahydronaphthalen-2-yl)butan-1-one *O*-(2,4-dinitrophenyl) oxime (1n) (¹³C NMR 126 MHz, CDCl₃)



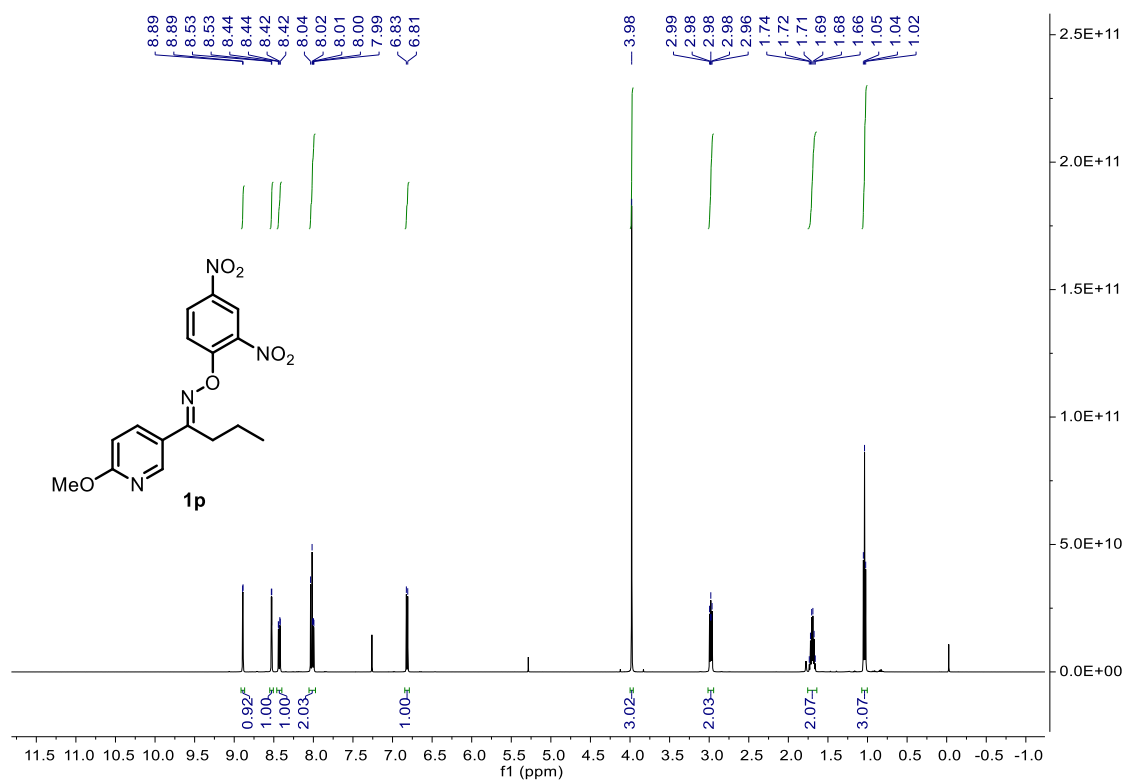
(*E*)-1-(naphthalen-2-yl)butan-1-one *O*-(2,4-dinitrophenyl) oxime (1o) (¹H NMR 500 MHz, CDCl₃)



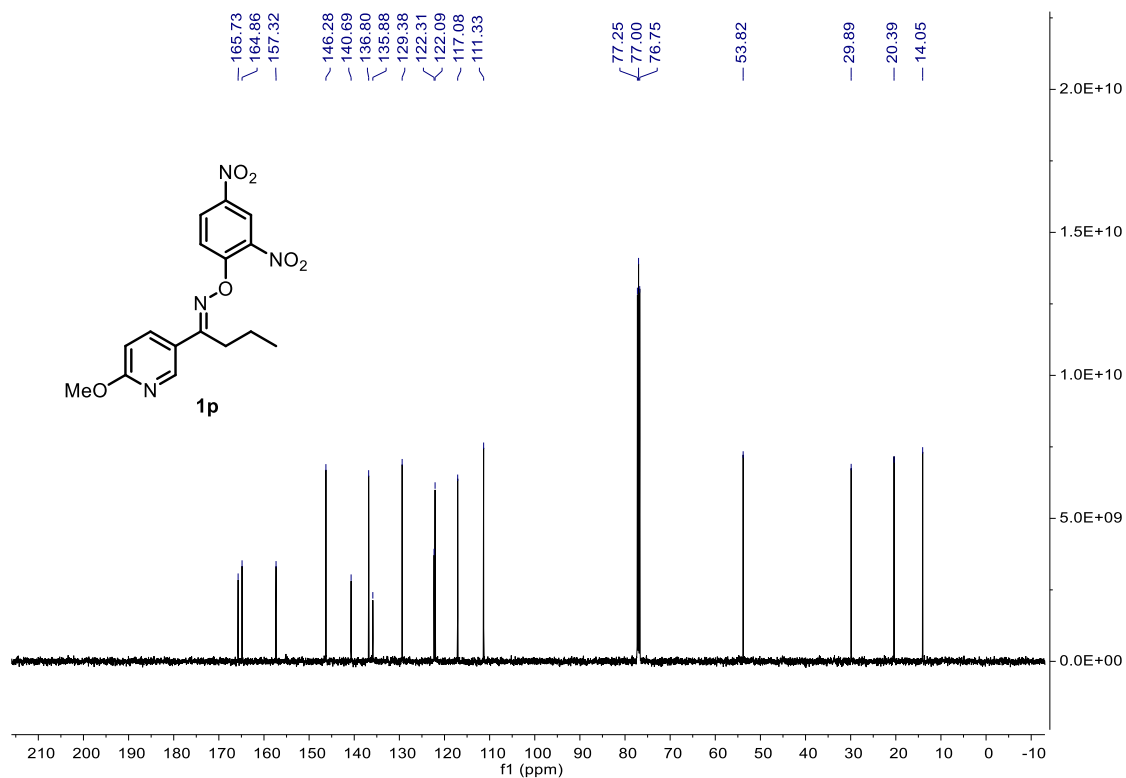
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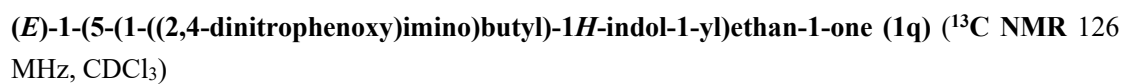
(*E*)-1-(6-methoxypyridin-3-yl)butan-1-one *O*-(2,4-dinitrophenyl) oxime (1p) (¹H NMR 500 MHz, CDCl₃)

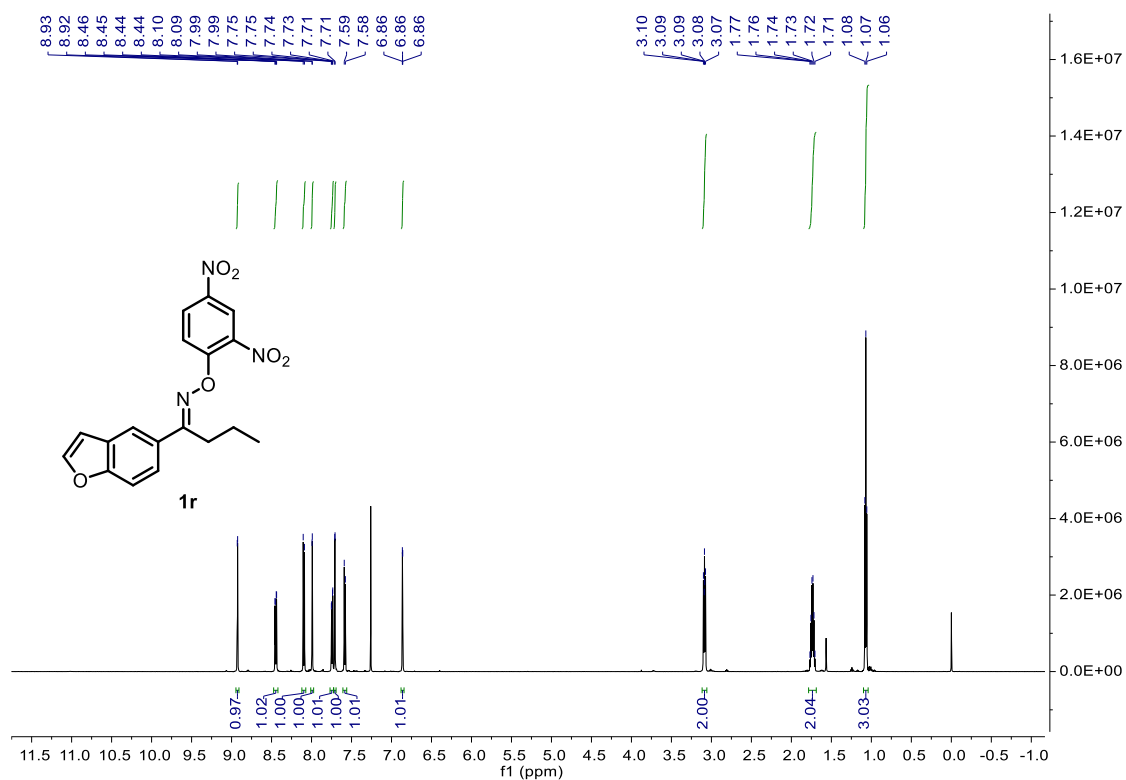


(*E*)-1-(6-methoxypyridin-3-yl)butan-1-one *O*-(2,4-dinitrophenyl) oxime (1p) (¹³C NMR 126 MHz, CDCl₃)

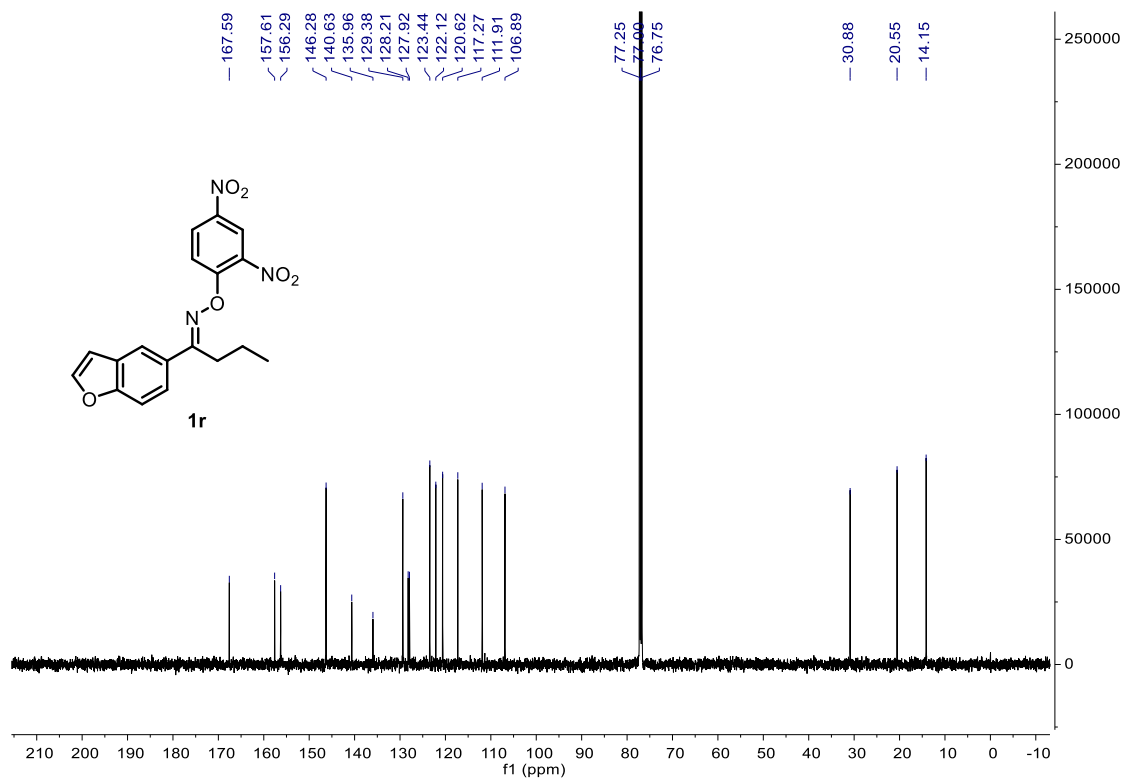


(*E*)-1-(5-(1-((2,4-dinitrophenoxy)imino)butyl)-1*H*-indol-1-yl)ethan-1-one (1q) (¹H NMR 500 MHz, CDCl₃)

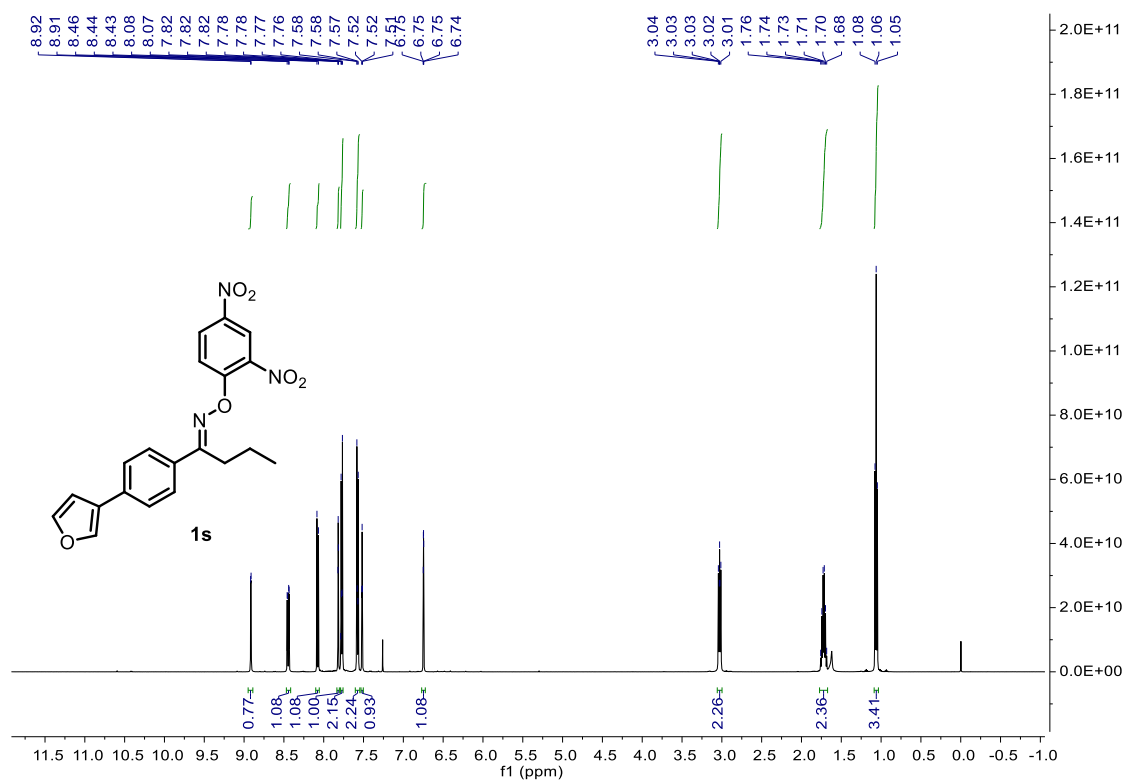




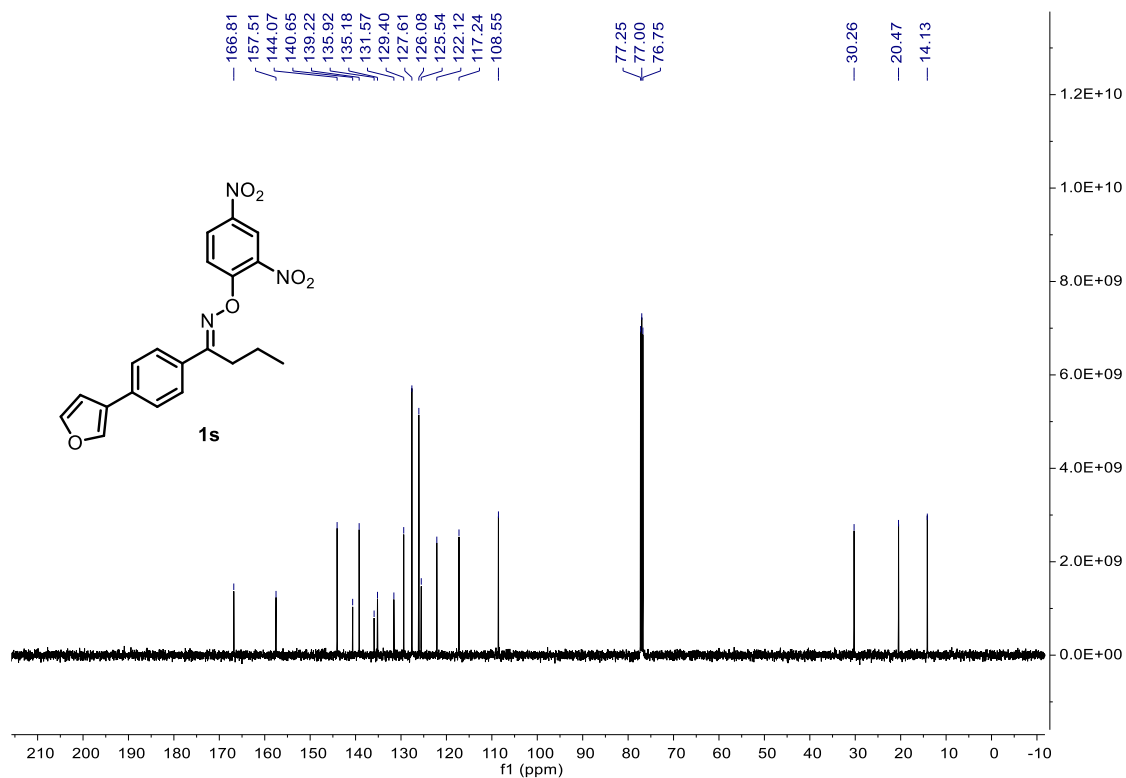
(*E*)-1-(benzofuran-5-yl)butan-1-one *O*-(2,4-dinitrophenyl) oxime (1r) (¹³C NMR 126 MHz, CDCl₃)



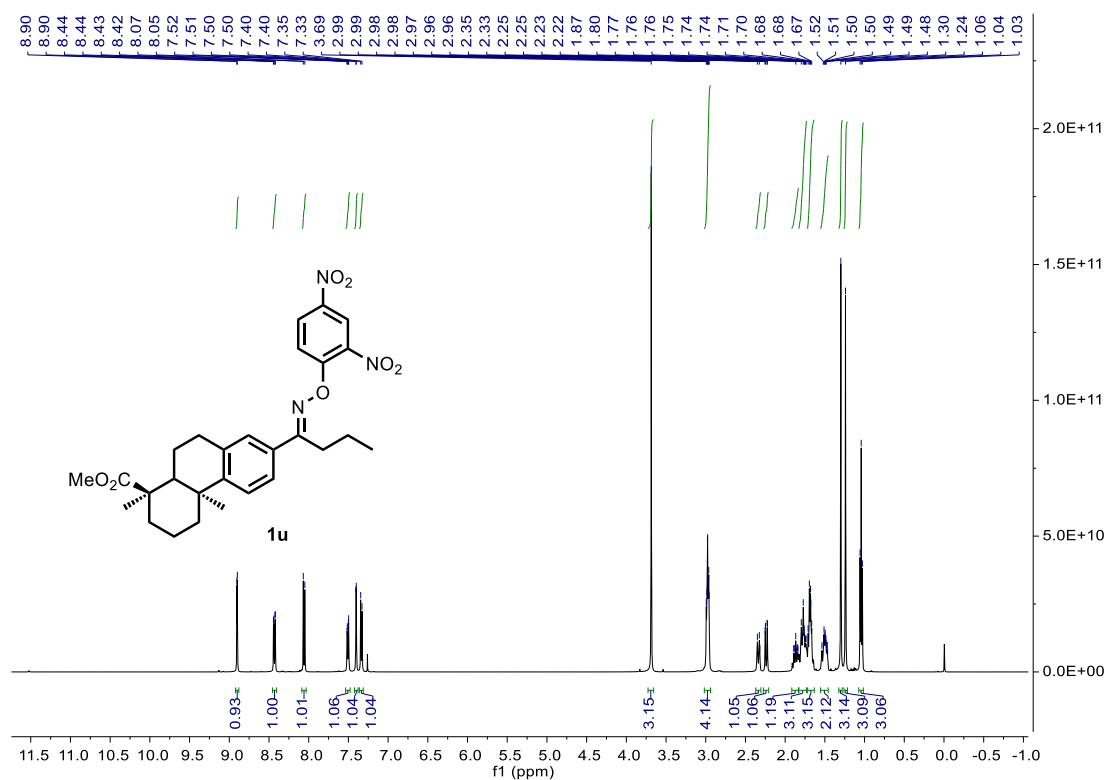
(*E*)-1-(4-(furan-3-yl)phenyl)butan-1-one *O*-(2,4-dinitrophenyl) oxime (1s) (¹H NMR 500 MHz, CDCl₃)



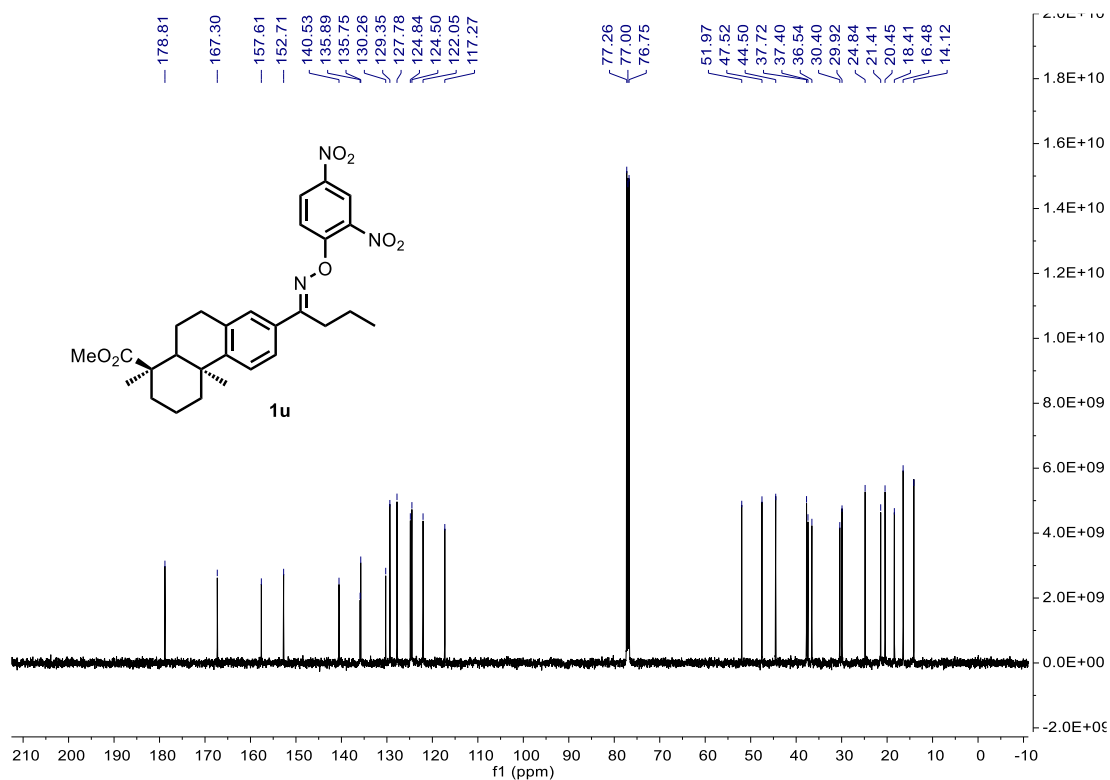
(E)-1-(4-(furan-3-yl)phenyl)butan-1-one O-(2,4-dinitrophenyl) oxime (1s) (¹³C NMR 126 MHz, CDCl₃)



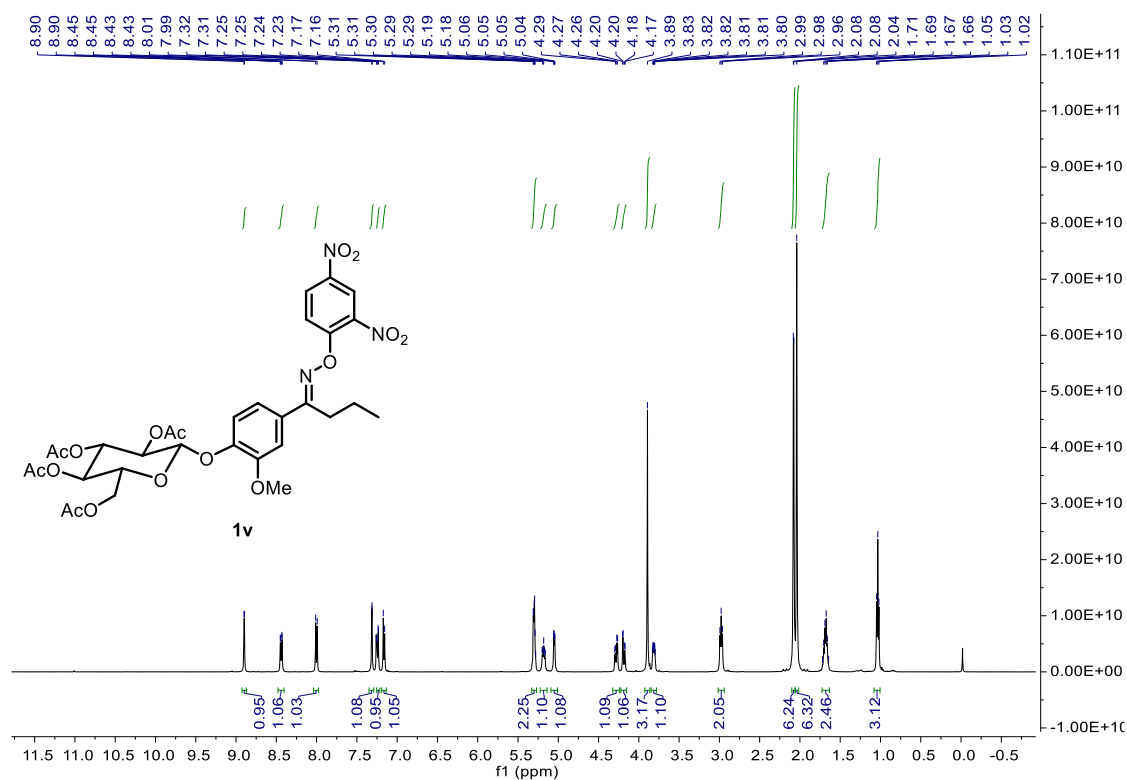
methyl (1R,4aS)-7-((E)-1-((2,4-dinitrophenoxy)imino)butyl)-1,4a-dimethyl-1,2,3,4,4a,9,10,10a-octahydrophenanthrene-1-carboxylate (1u) (¹H NMR 500 MHz, CDCl₃)



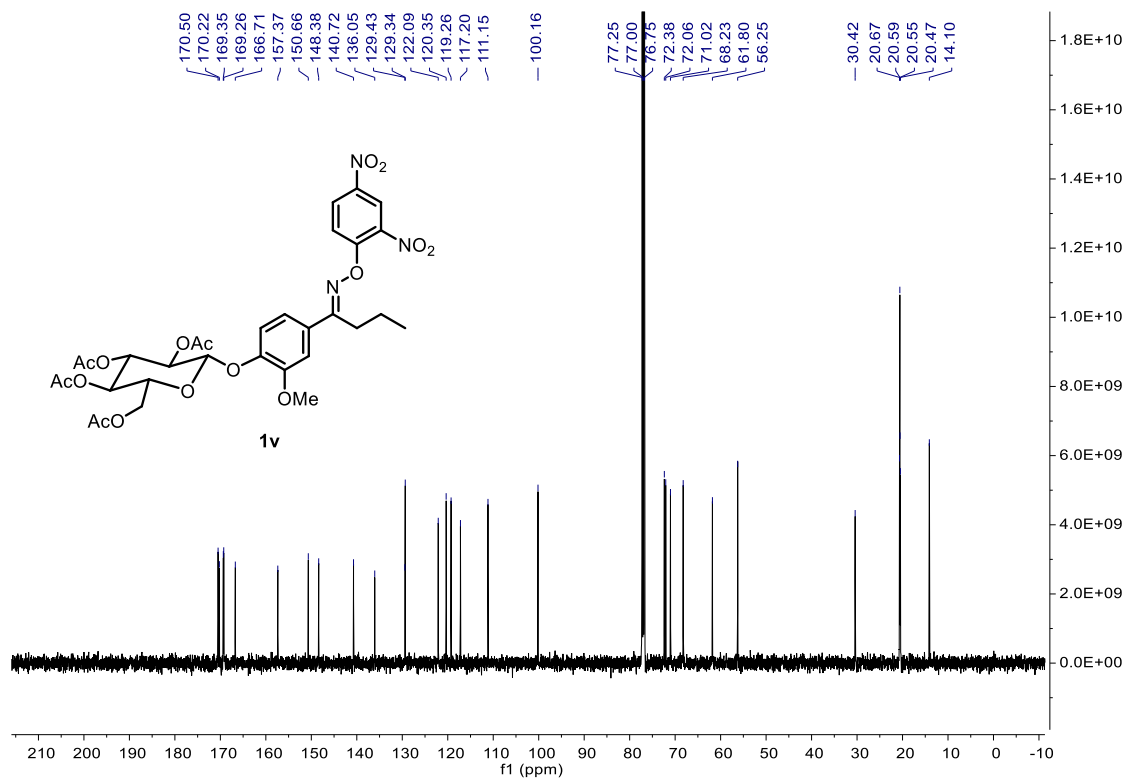
methyl (1*R*,4*aS*)-7-((*E*)-1-((2,4-dinitrophenoxy)imino)butyl)-1,4*a*-dimethyl-1,2,3,4,4*a*,9,10,10*a*-octahydrophenanthrene-1-carboxylate (1u) (¹³C NMR 126 MHz, CDCl₃)



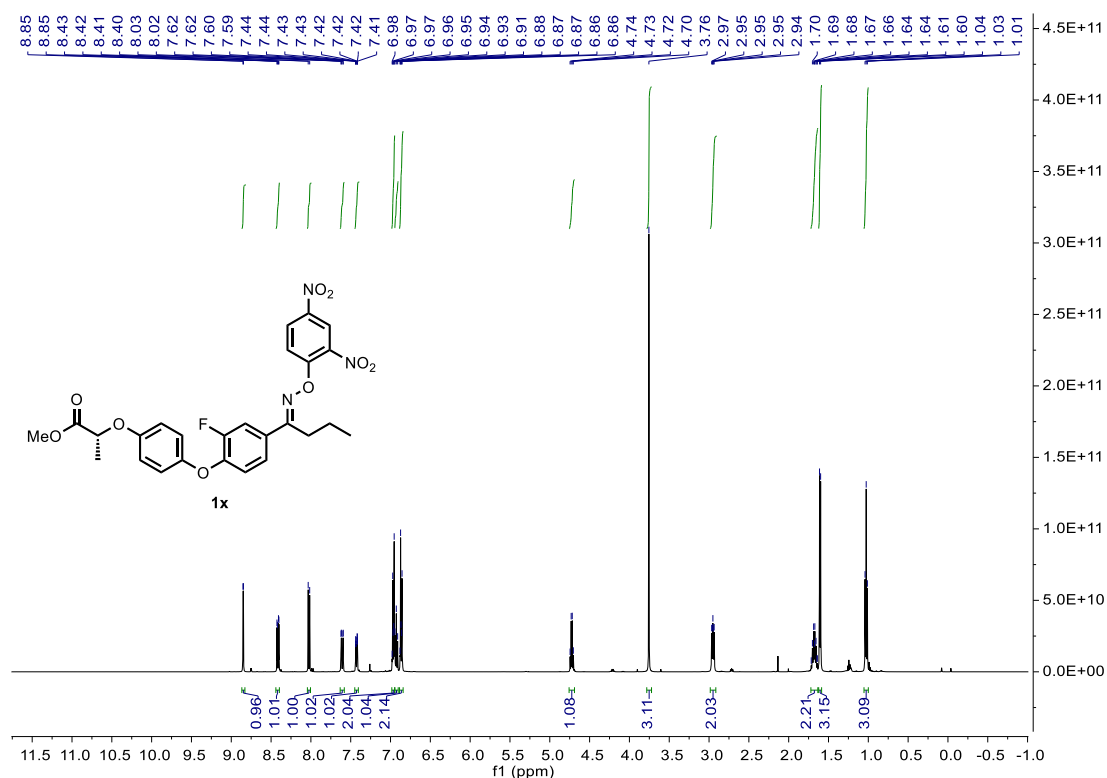
(2*R*,3*R*,4*S*,5*R*,6*S*)-2-(acetoxymethyl)-6-(4-((*E*)-1-((2,4-dinitrophenoxy)imino)butyl)-2-methoxyphenoxy)tetrahydro-2*H*-pyran-3,4,5-triyl triacetate (1v) (¹H NMR 500 MHz, CDCl₃)



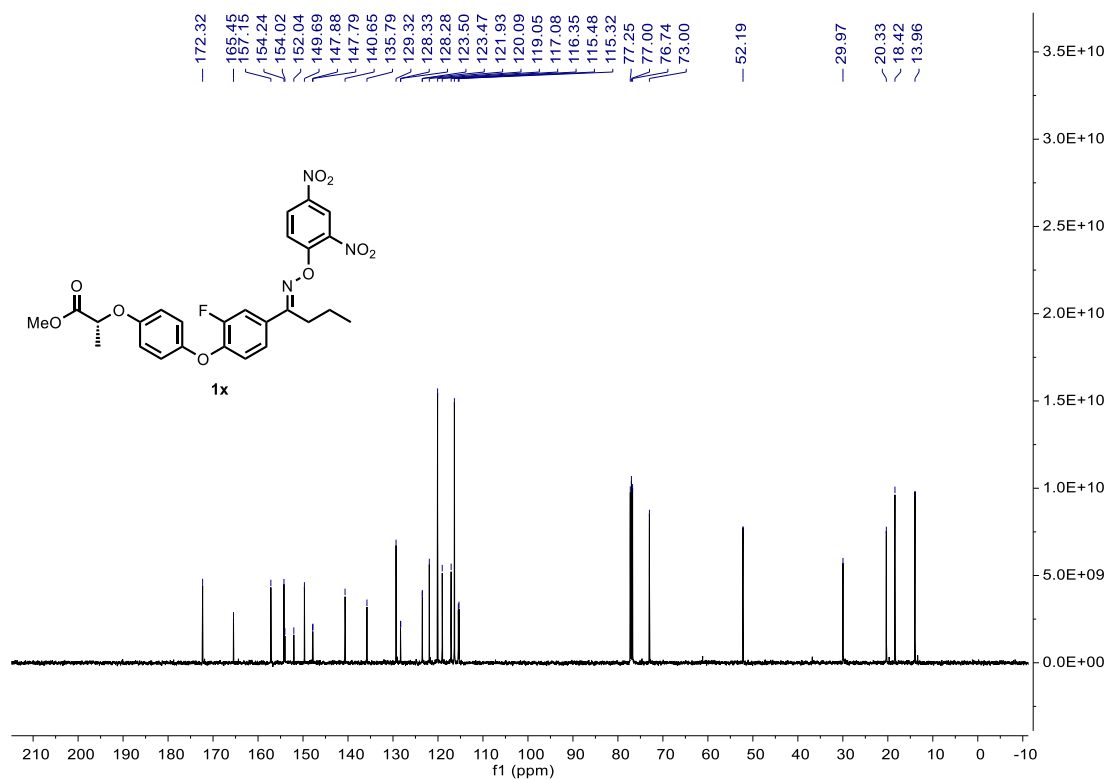
(2*R*,3*R*,4*S*,5*R*,6*S*)-2-(acetoxymethyl)-6-(4-((*E*)-1-((2,4-dinitrophenoxy)imino)butyl)-2-methoxyphenoxy)tetrahydro-2*H*-pyran-3,4,5-tri-*l* triacetate (1v**)** (¹³C NMR 126 MHz, CDCl₃)



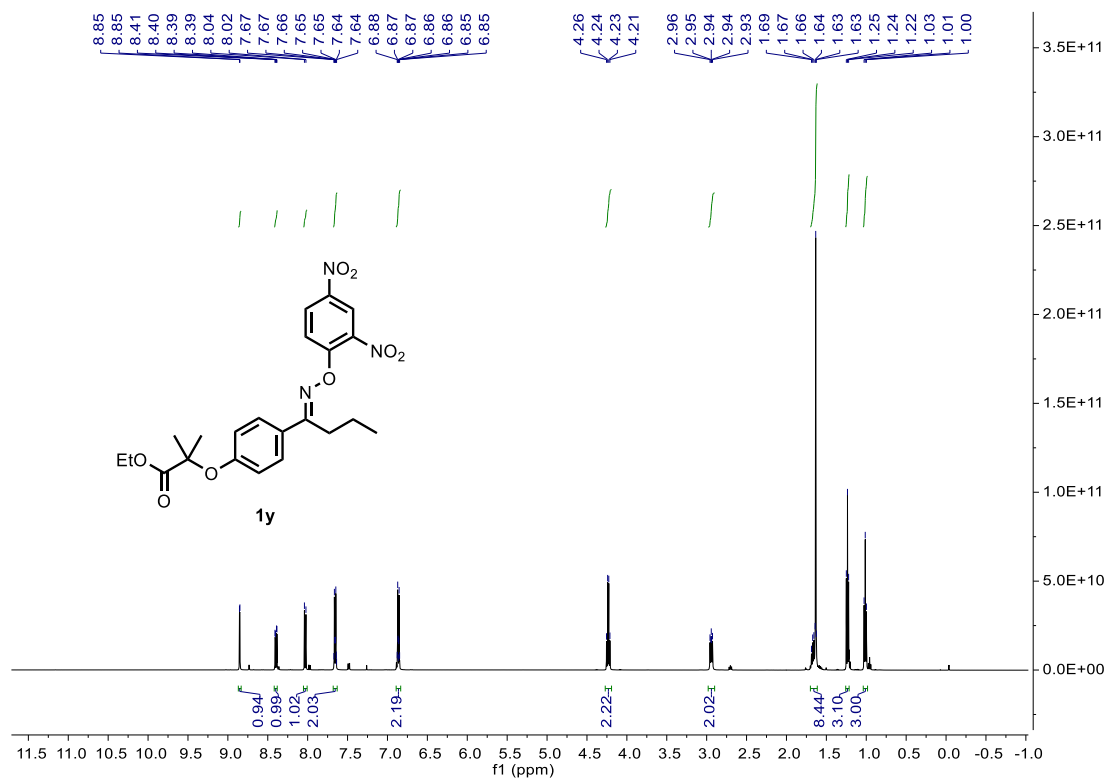
methyl (R,E)-2-(4-(4-(1-((2,4-dinitrophenoxy)imino)butyl)-2-fluorophenoxy)phenoxy)propanoate (1x) (¹H NMR 500 MHz, CDCl₃)



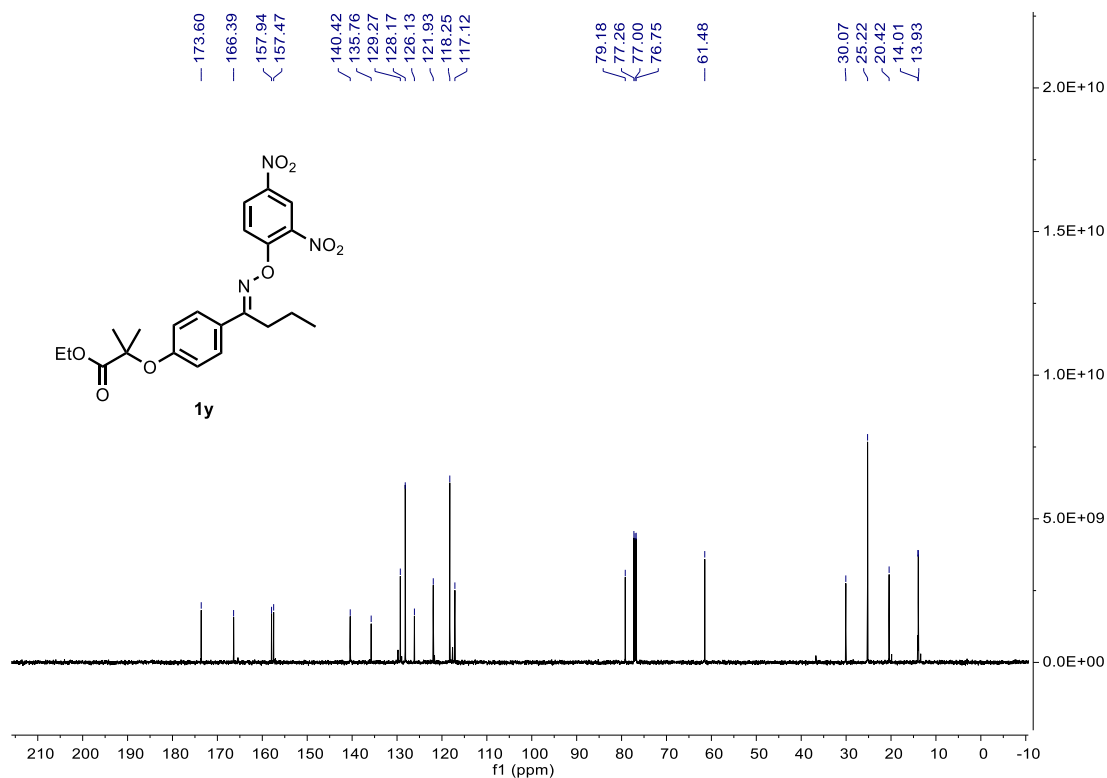
methyl (R,E)-2-(4-(4-(1-((2,4-dinitrophenoxy)imino)butyl)-2-fluorophenoxy)phenoxy)propanoate (1x) (¹³C NMR 126 MHz, CDCl₃)



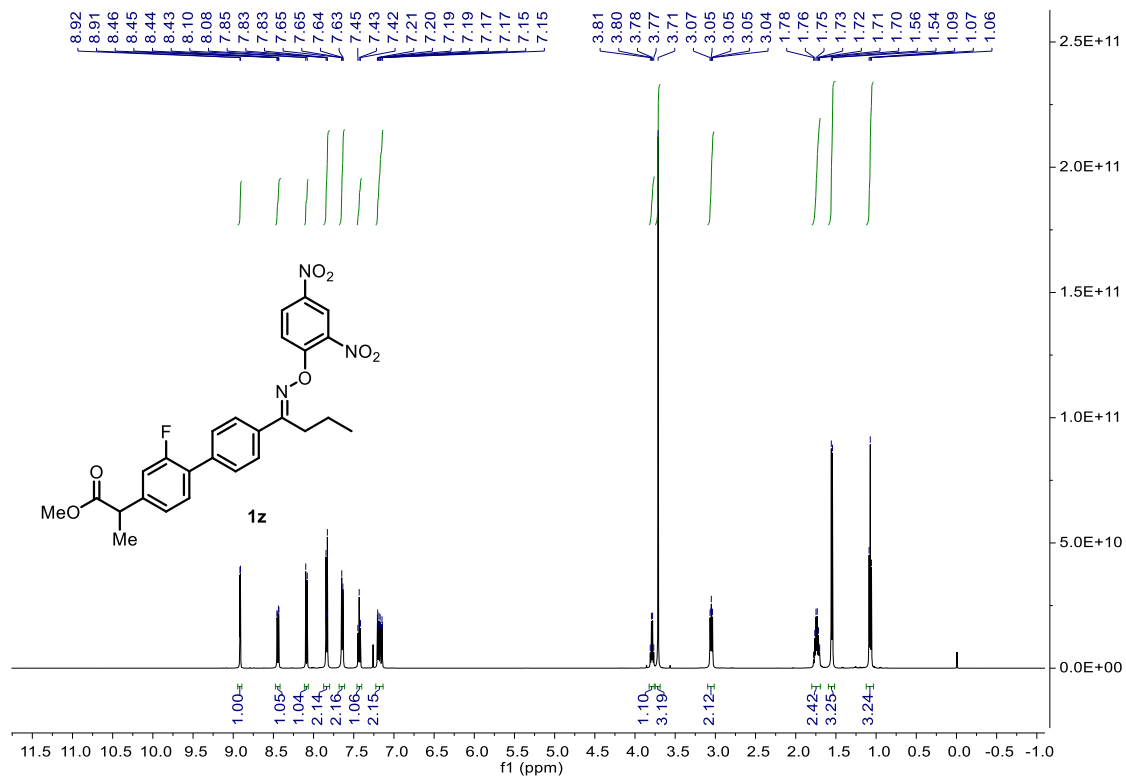
ethyl (E)-2-(4-(1-((2,4-dinitrophenoxy)imino)butyl)phenoxy)-2-methylpropanoate (1y) (¹H NMR 500 MHz, CDCl₃)



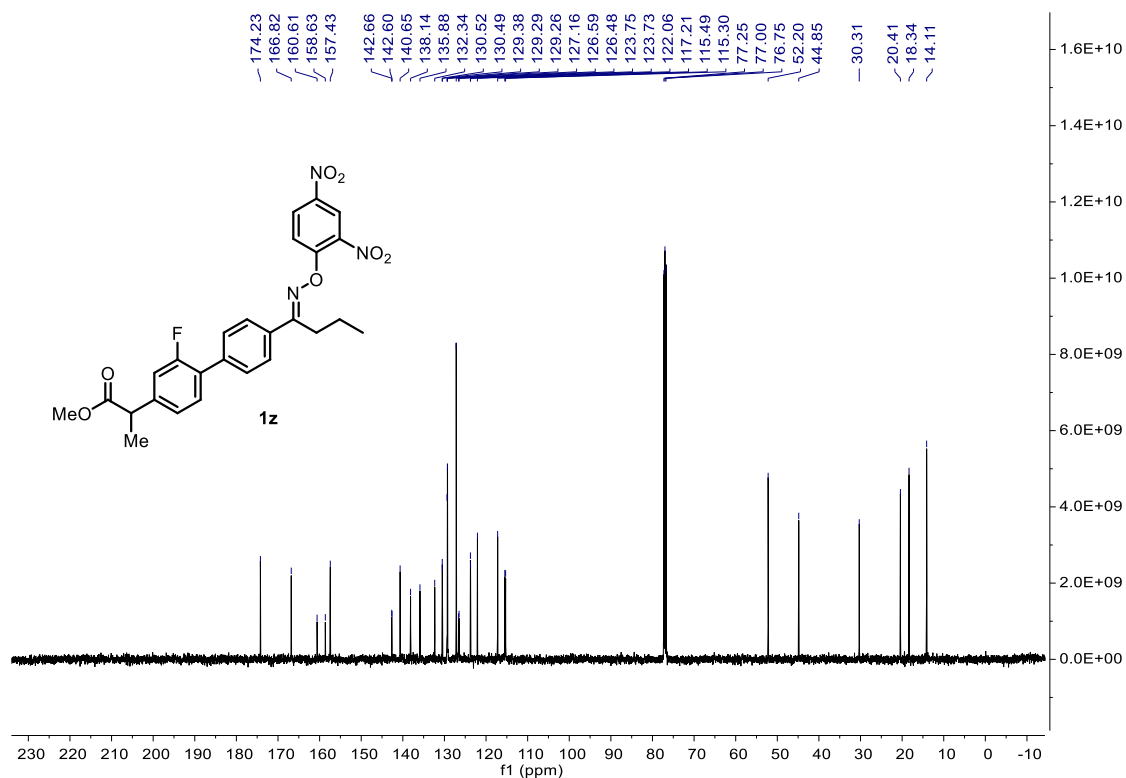
ethyl (E)-2-(4-(1-((2,4-dinitrophenoxy)imino)butyl)phenoxy)-2-methylpropanoate (1y) (¹³C NMR 126 MHz, CDCl₃)



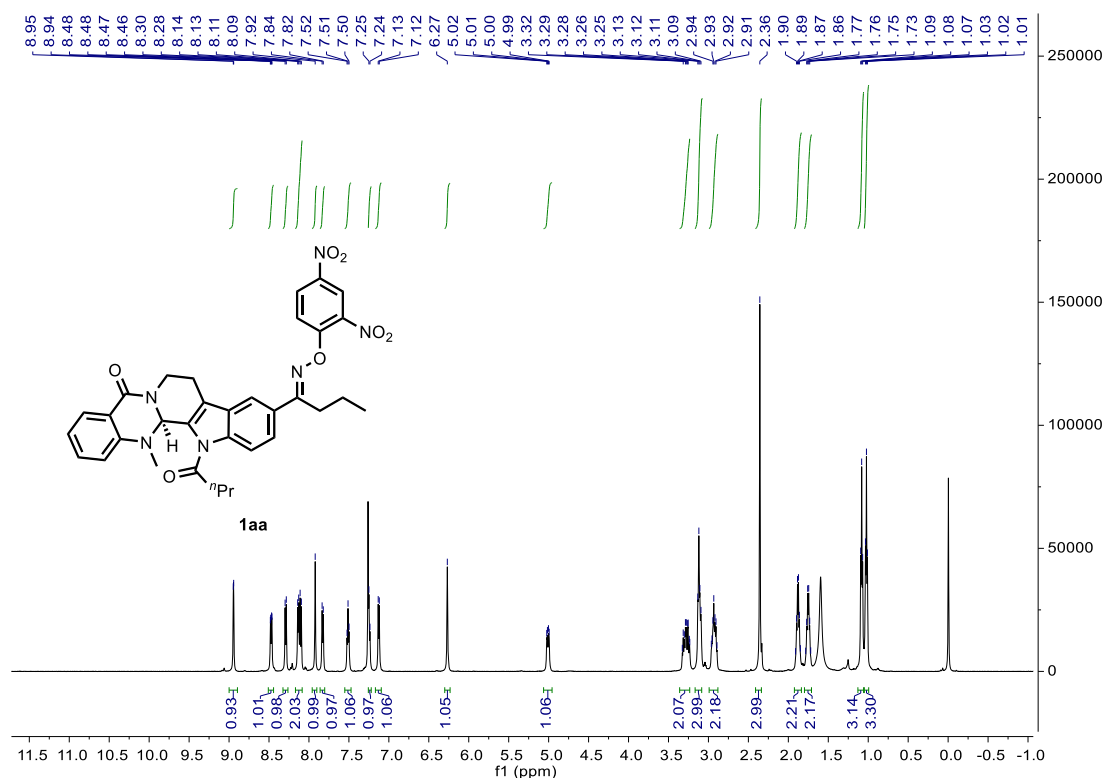
Methyl (E)-2-(4'-(1-((2,4-dinitrophenoxy)imino)butyl)-2-fluoro-[1,1'-biphenyl]-4-yl)propanoate (1z) (¹H NMR 500 MHz, CDCl₃)



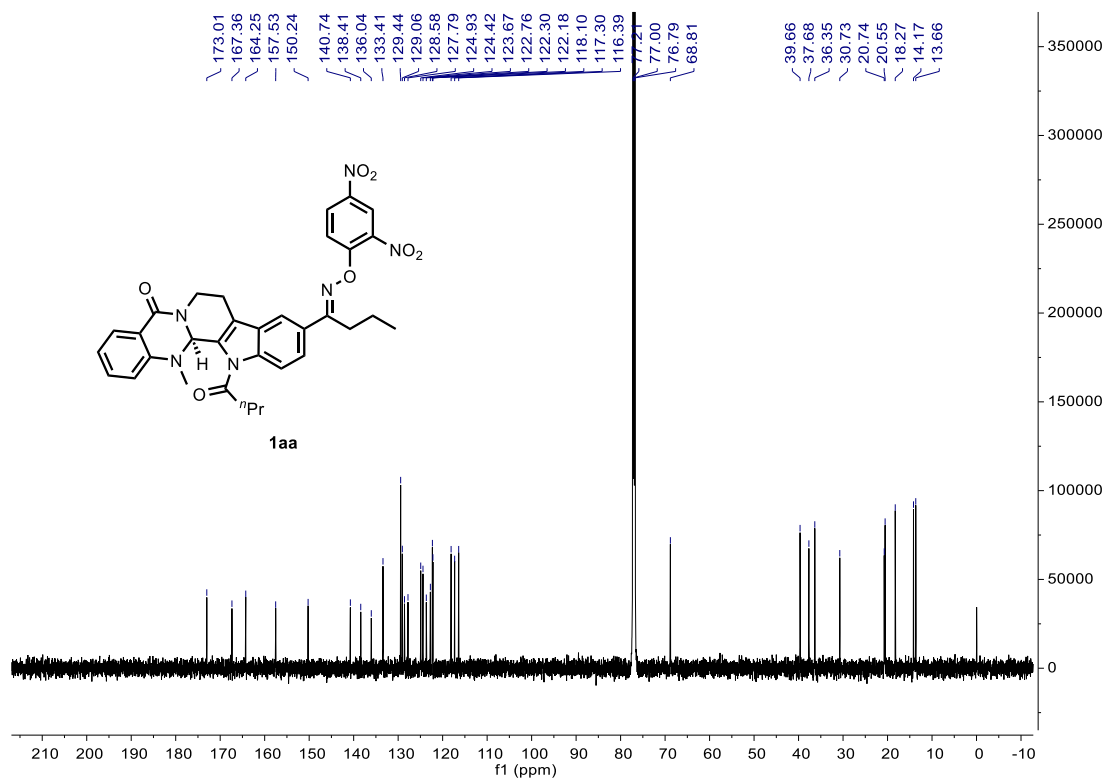
Methyl (E)-2-(4'-(1-((2,4-dinitrophenoxy)imino)butyl)-2-fluoro-[1,1'-biphenyl]-4-yl)propanoate (1z) (¹³C NMR 126 MHz, CDCl₃)



(*S,E*)-13-butryl-10-(1-((2,4-dinitrophenoxy)imino)butyl)-14-methyl-8,13,13b,14-tetrahydroindolo[2',3':3,4]pyrido[2,1-b]quinazolin-5(7H)-one (1aa) (^1H NMR 500 MHz, CDCl_3)



(*S,E*)-13-butryl-10-(1-((2,4-dinitrophenoxy)imino)butyl)-14-methyl-8,13,13b,14-tetrahydroindolo[2',3':3,4]pyrido[2,1-b]quinazolin-5(7H)-one (1aa) (^{13}C NMR 126 MHz, CDCl_3)

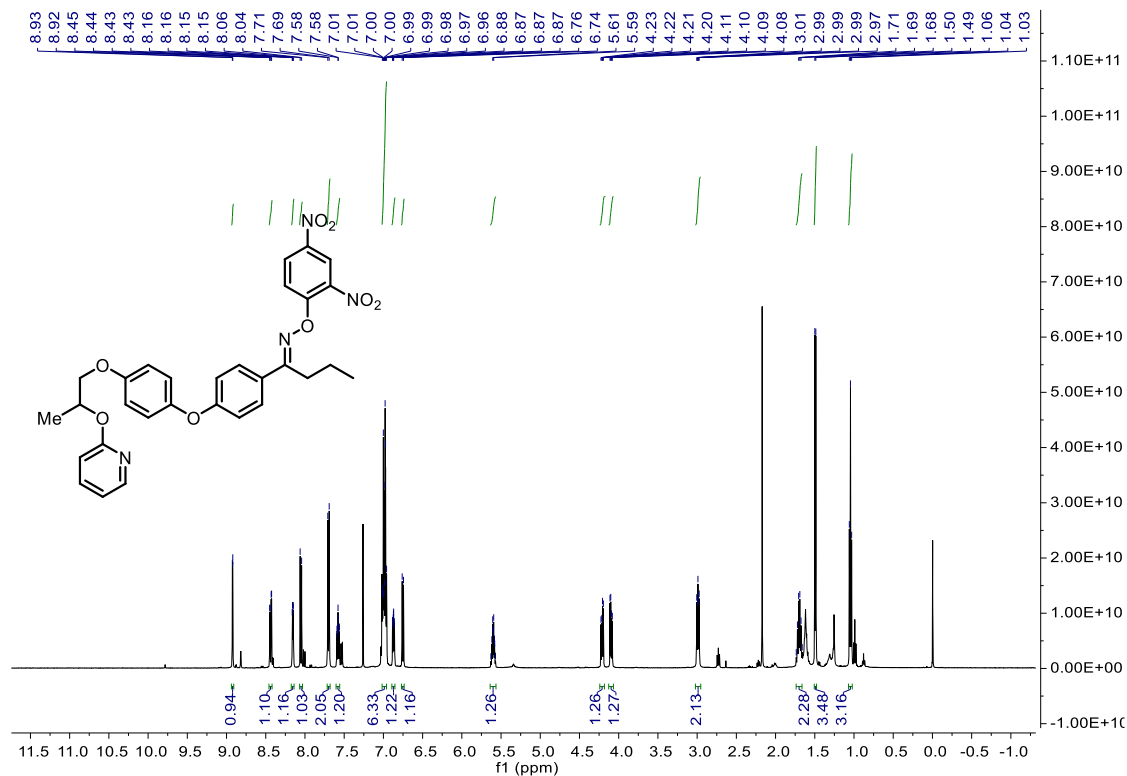


[illegible]

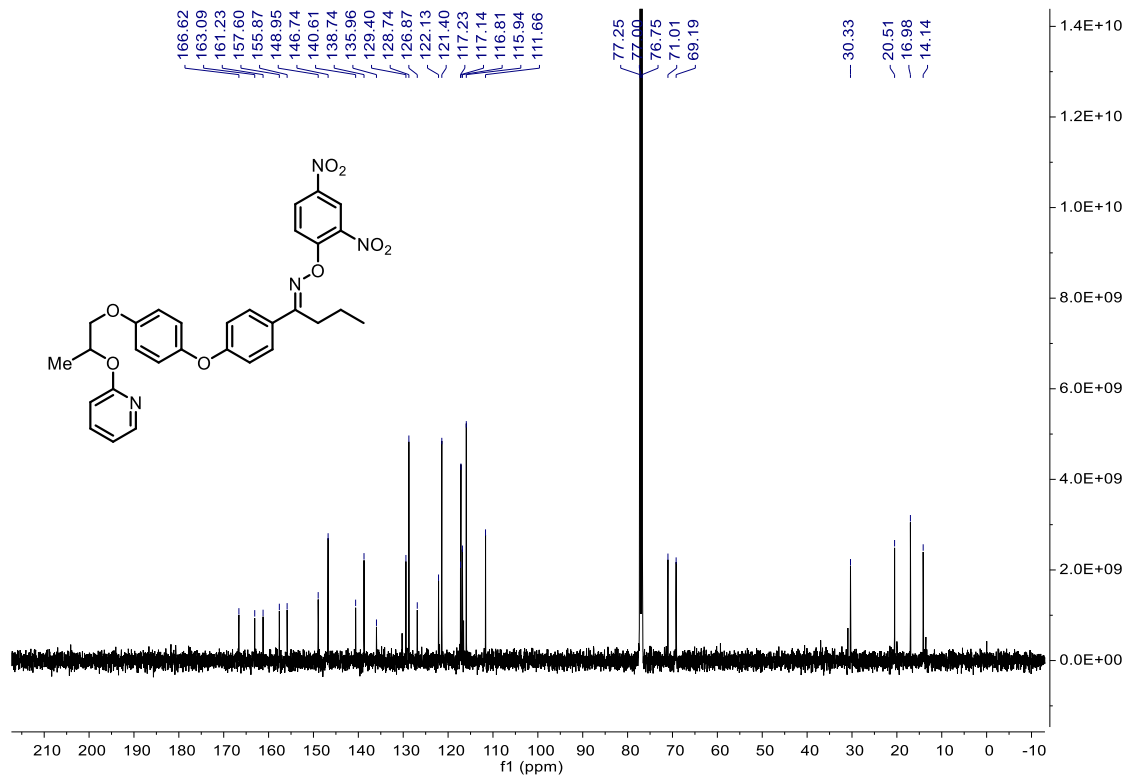
Chemical structure of **1ab** is shown. The ¹³C NMR spectrum (f1 (ppm)) displays peaks corresponding to the structure, with labeled chemical shifts (ppm) as follows:

- 171.20, 168.72, 157.61, 140.90, 140.54, 140.28, 135.94, 130.25, 129.51, 129.38, 124.31, 124.10, 122.05, 117.30, 82.52, 77.25, 77.00, 76.75, 49.83, 44.13, 42.78, 38.09, 36.74, 29.43, 27.49, 26.87, 25.93, 23.20, 22.29, 21.15, 12.01, 11.37.

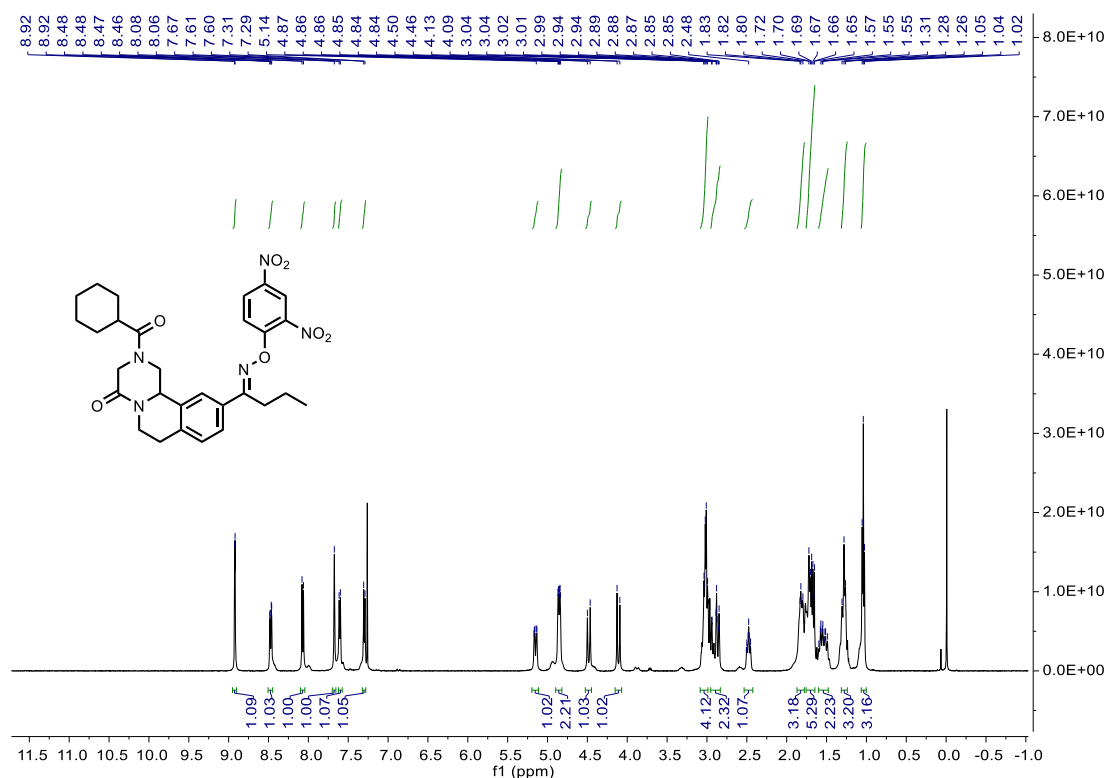
(E)-1-(4-(4-(2-(pyridin-2-yloxy)propoxy)phenoxy)phenyl)butan-1-one O-(2,4-dinitrophenyl) oxime (1ac) (¹H NMR 500 MHz, CDCl₃)



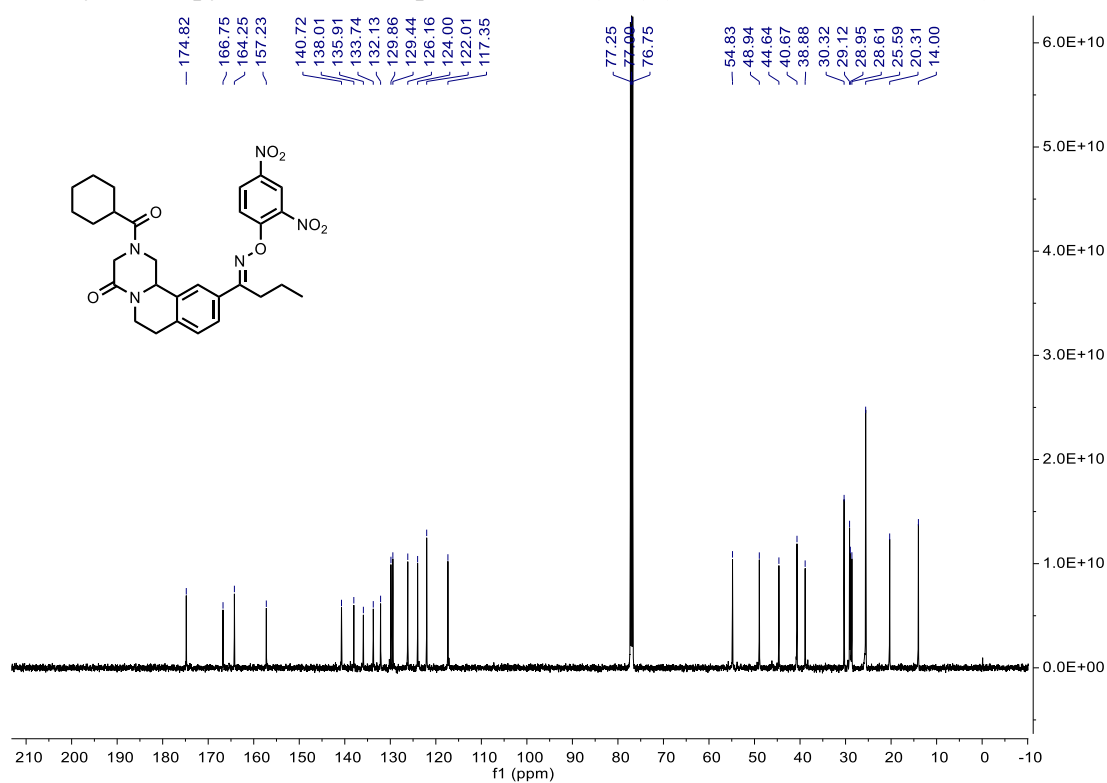
(E)-1-(4-(4-(2-(pyridin-2-yloxy)propoxy)phenoxy)phenyl)butan-1-one O-(2,4-dinitrophenyl) oxime (1ac) (¹³C NMR 126 MHz, CDCl₃)



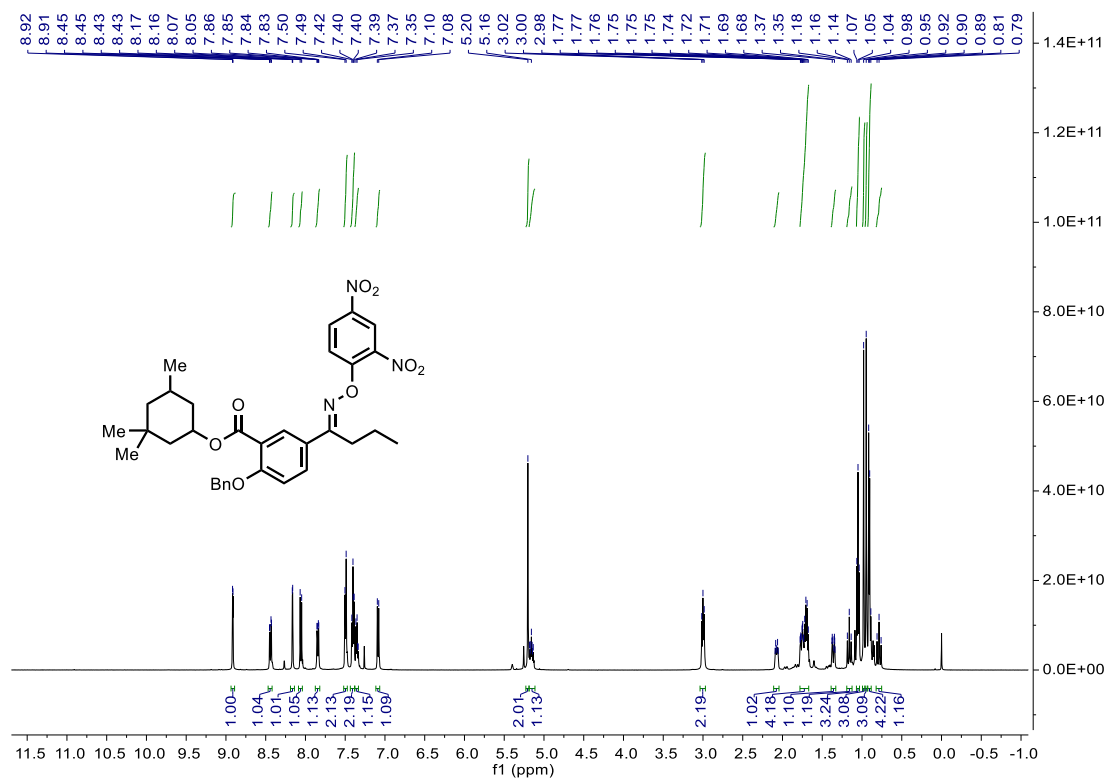
(*E*)-2-(cyclohexanecarbonyl)-10-(1-((2,4-dinitrophenoxy)imino)butyl)-1,2,3,6,7,11b-hexahydro-4H-pyrazino[2,1-a]isoquinolin-4-one (1ad) (¹H NMR 500 MHz, CDCl₃)



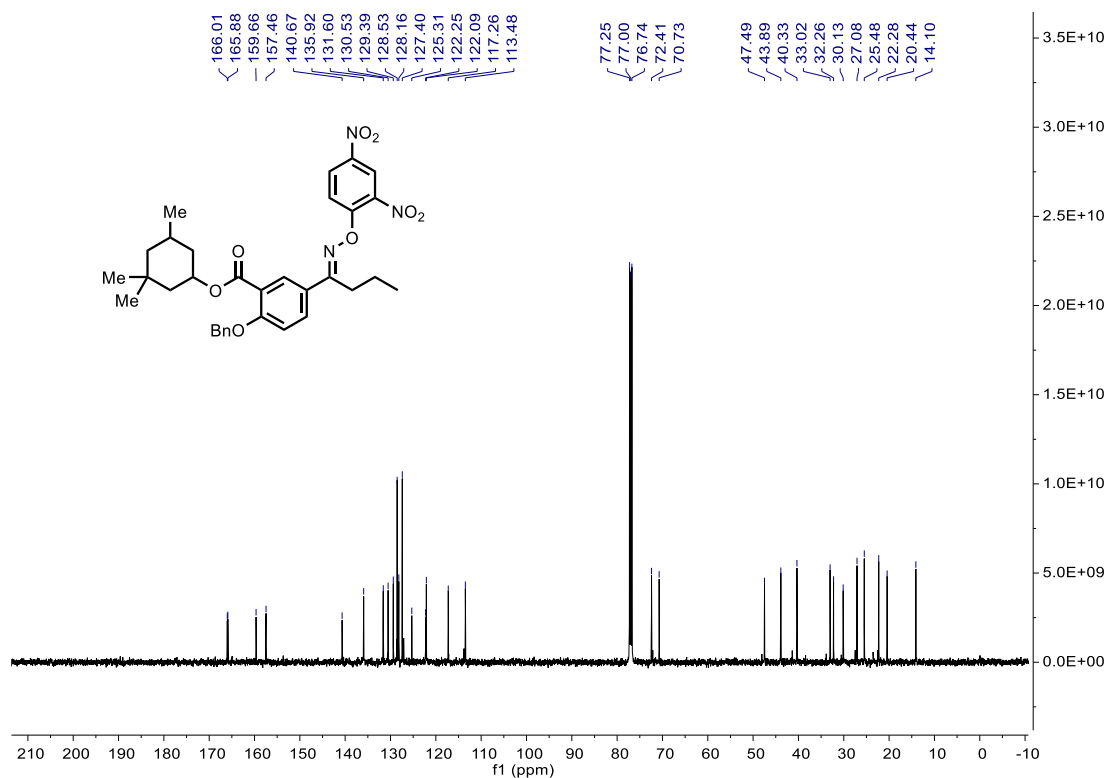
(*E*)-2-(cyclohexanecarbonyl)-10-(1-((2,4-dinitrophenoxy)imino)butyl)-1,2,3,6,7,11b-hexahydro-4H-pyrazino[2,1-a]isoquinolin-4-one (1ad) (¹³C NMR 126 MHz, CDCl₃)



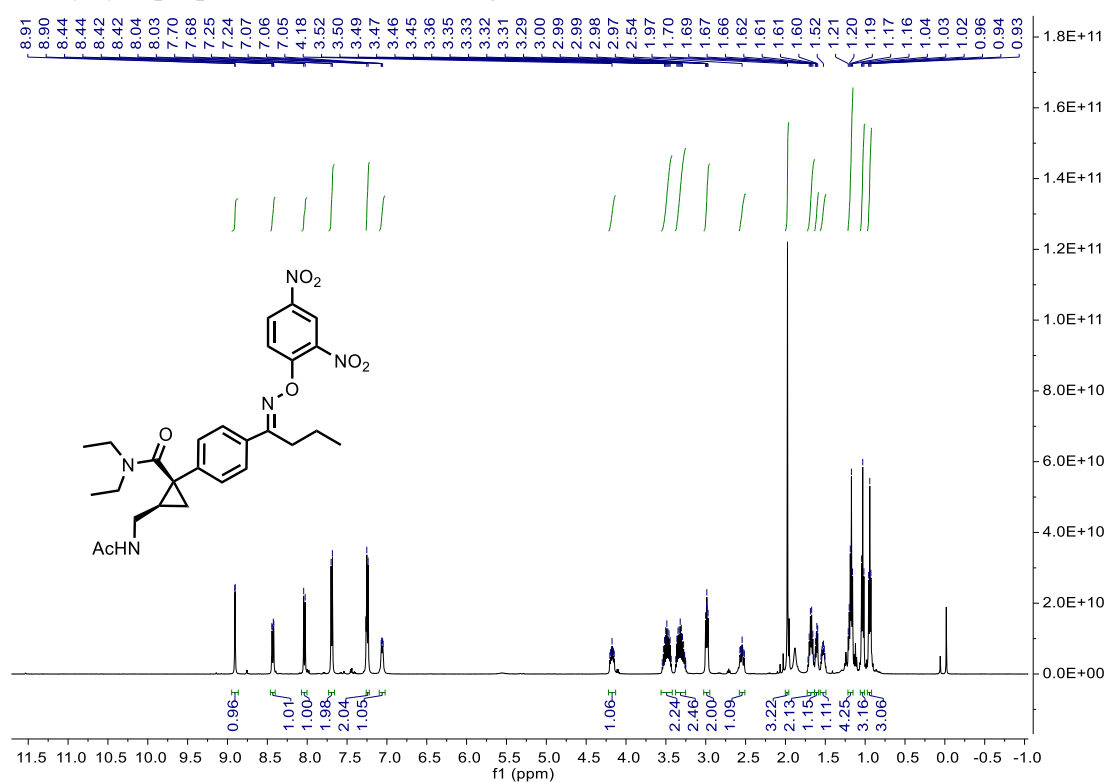
3,3,5-trimethylcyclohexyl (*E*)-2-(benzyloxy)-5-(1-((2,4-dinitrophenoxy)imino)butyl)benzoate (1ae) (¹H NMR 500 MHz, CDCl₃)



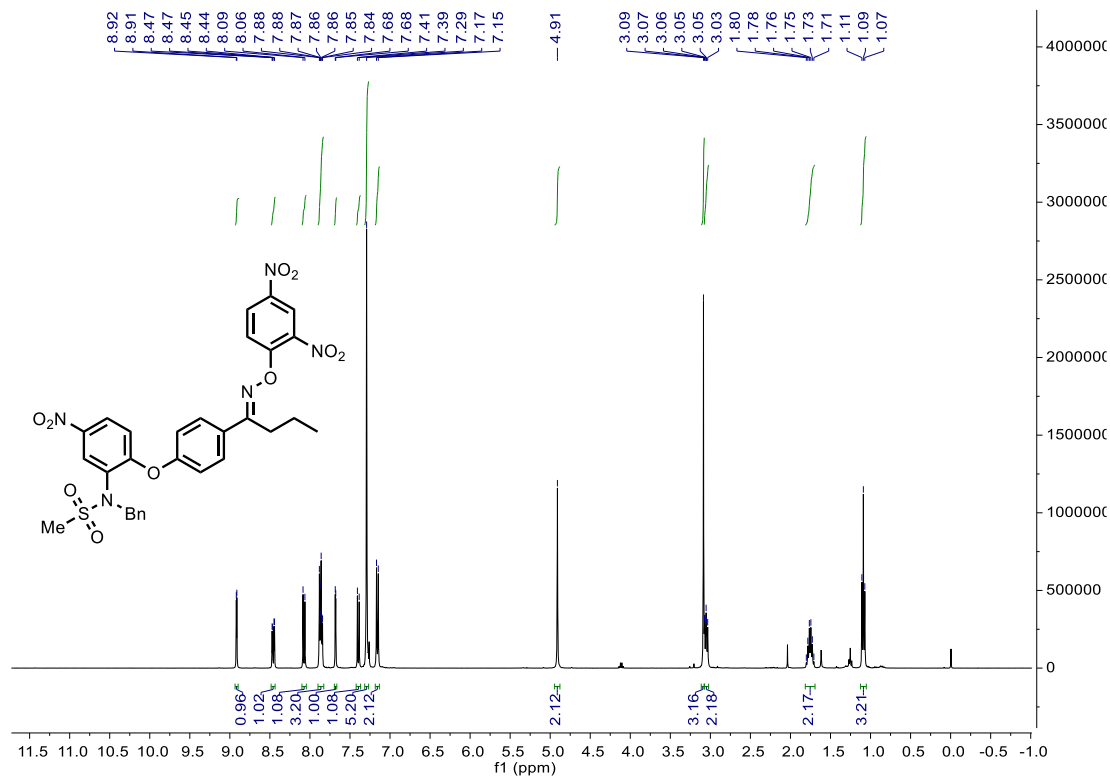
3,3,5-trimethylcyclohexyl (*E*)-2-(benzyloxy)-5-(1-((2,4-dinitrophenoxy)imino)butyl)benzoate (1ae) (¹³C NMR 126 MHz, CDCl₃)



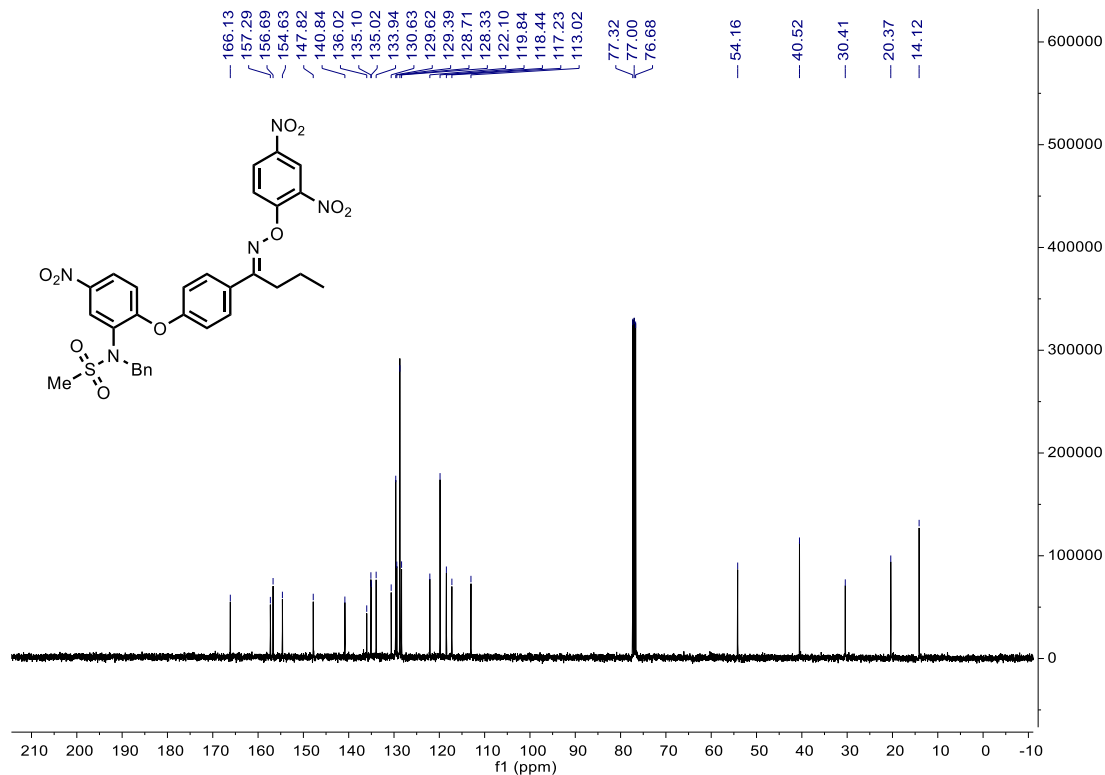
(1*S*,2*R*)-2-(acetamidomethyl)-1-(4-((*E*)-1-((2,4-dinitrophenoxy)imino)butyl)phenyl)-*N,N*-diethylcyclopropane-1-carboxamide (1a_g) (¹H NMR 500 MHz, CDCl₃)



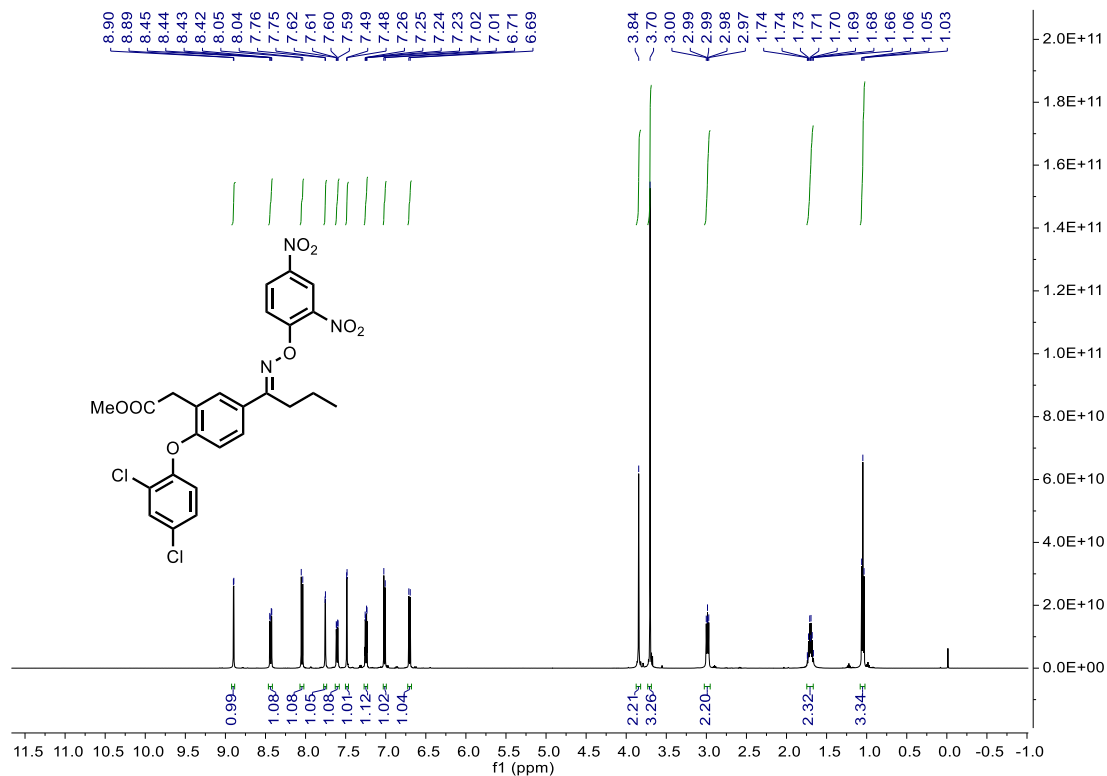
(*E*)-*N*-benzyl-*N*-(2-(4-(1-((2,4-dinitrophenoxy)imino)butyl)phenoxy)-5-nitrophenyl)methanesulfonamide (1ah) (¹H NMR 400 MHz, CDCl₃)



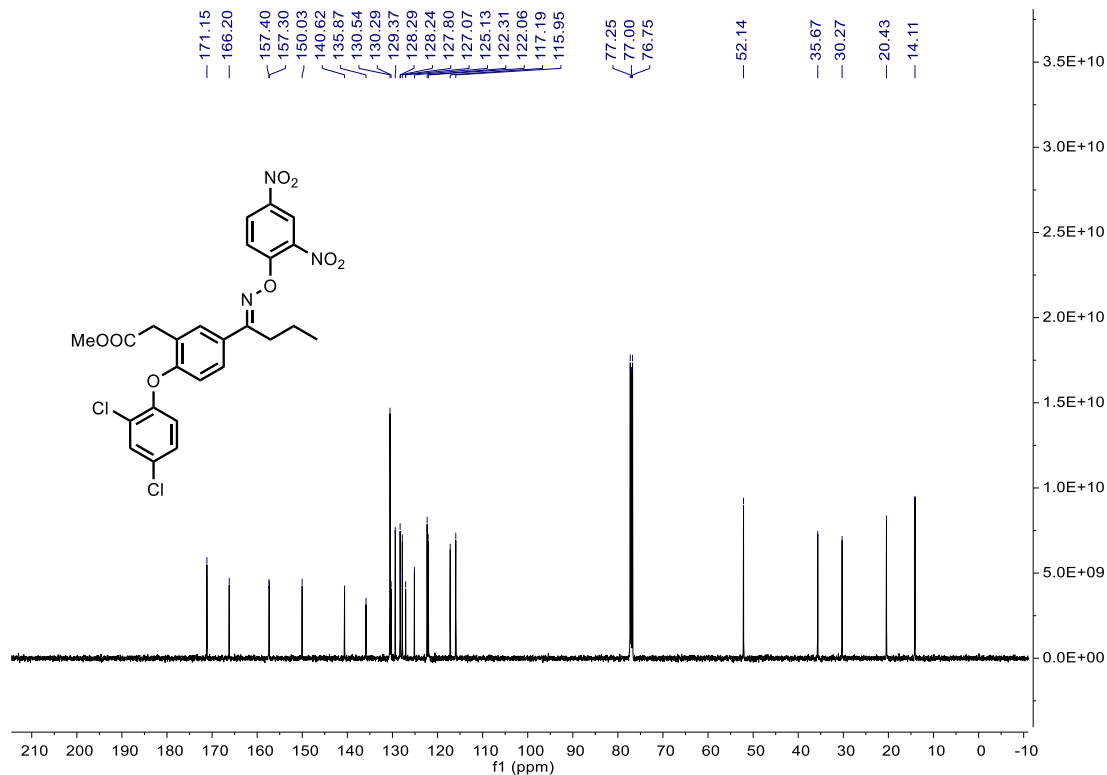
(*E*)-*N*-benzyl-*N*-(2-(4-(1-((2,4-dinitrophenoxy)imino)butyl)phenoxy)-5-nitrophenyl)methanesulfonamide (1ah) (¹³C NMR 101 MHz, CDCl₃)



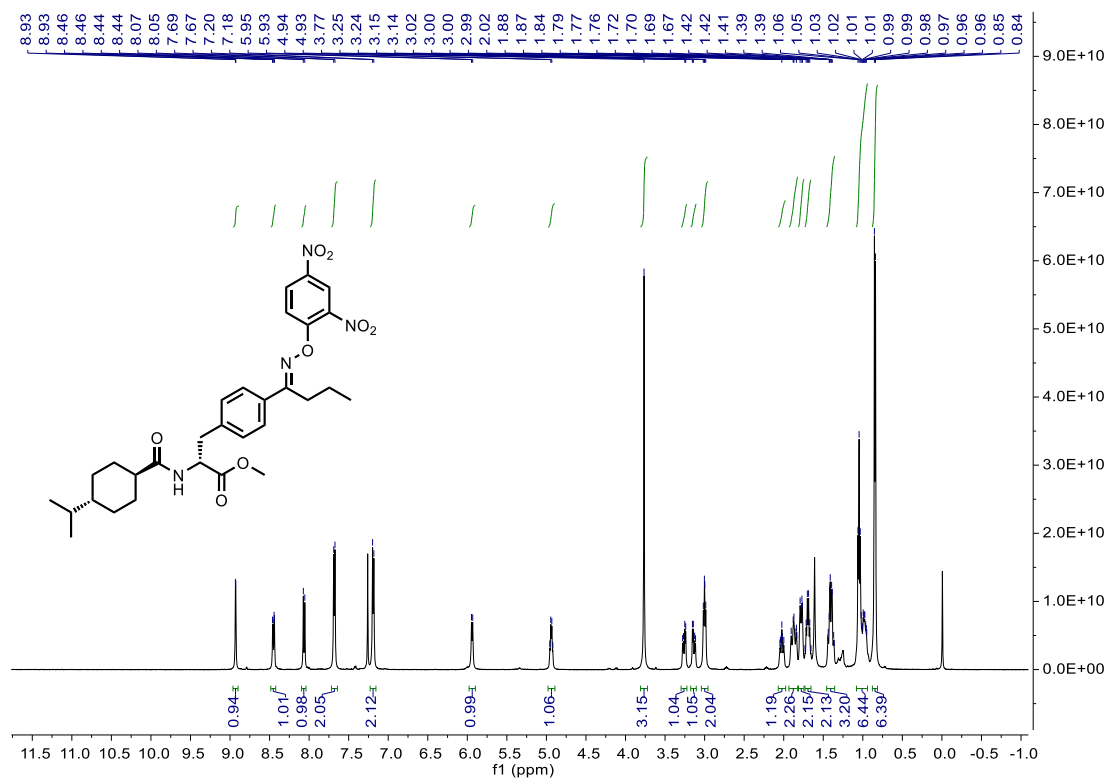
methyl (*E*)-2-(2-(2,4-dichlorophenoxy)-5-(1-((2,4-dinitrophenoxy)imino)butyl)phenyl)acetate (1ai) (¹H NMR 500 MHz, CDCl₃)



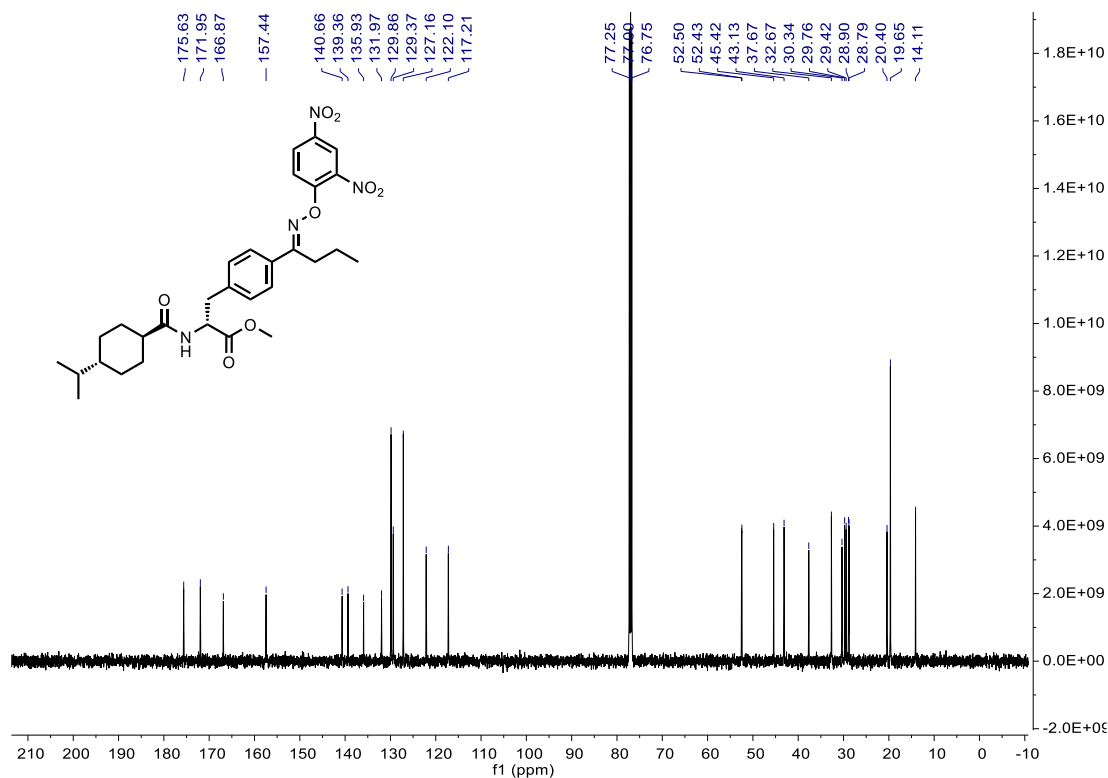
methyl (*E*)-2-(2-(2,4-dichlorophenoxy)-5-(1-((2,4-dinitrophenoxy)imino)butyl)phenyl)acetate (1ai) (¹³C NMR 126 MHz, CDCl₃)



methyl (R)-3-(4-((E)-1-((2,4-dinitrophenoxy)imino)butyl)phenyl)-2-((1*r*,4*R*)-4-isopropylcyclohexane-1-carboxamido)propanoate (1aj) (¹H NMR 500 MHz, CDCl₃)

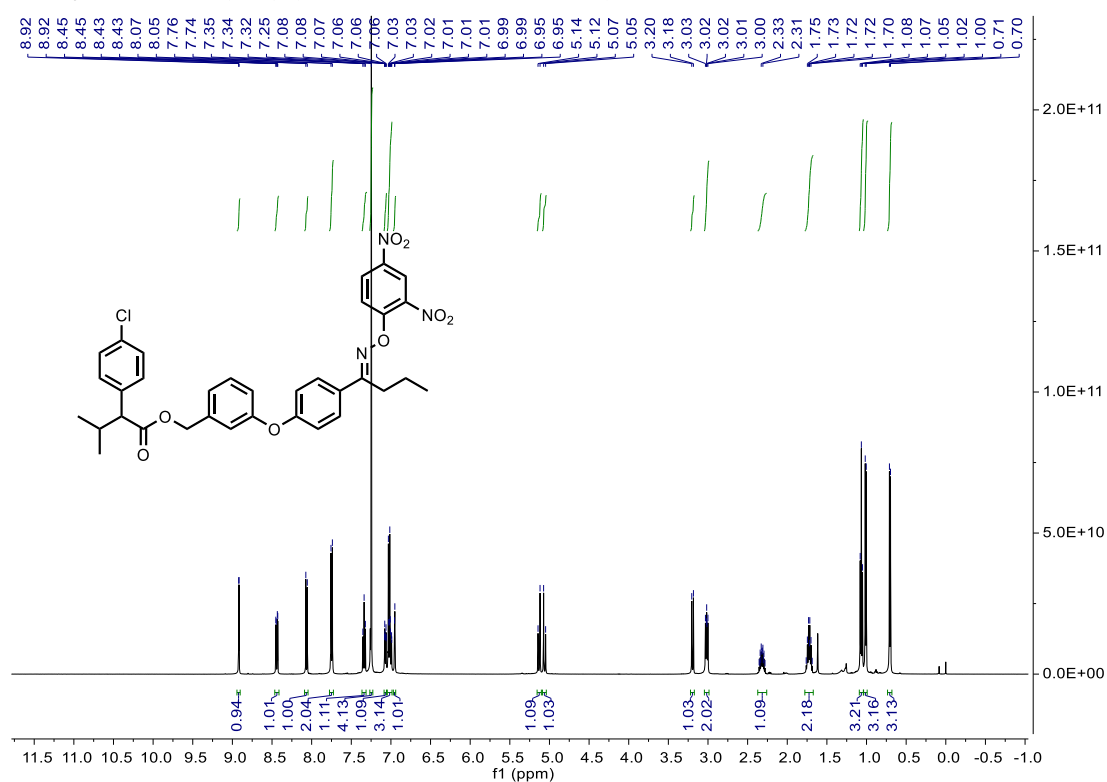


methyl (R)-3-(4-((E)-1-((2,4-dinitrophenoxy)imino)butyl)phenyl)-2-((1*r*,4*R*)-4-isopropylcyclohexane-1-carboxamido)propanoate (1aj) (¹³C NMR 126 MHz, CDCl₃)



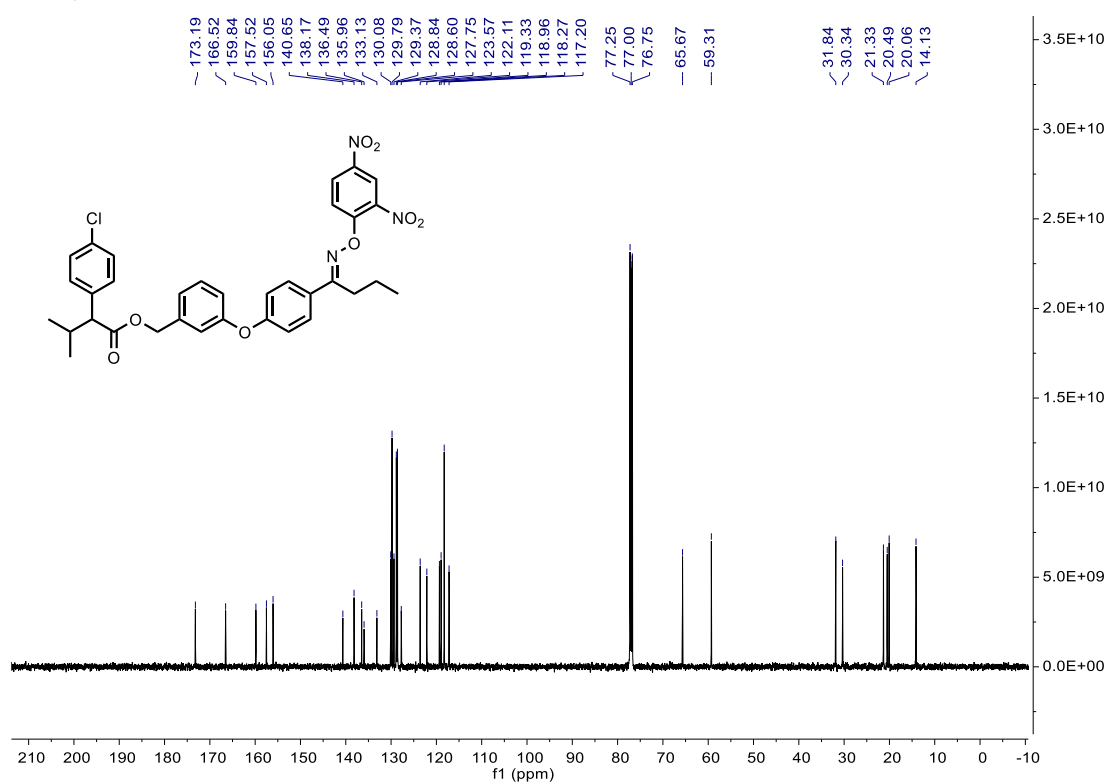
(E)-3-(4-(1-((2,4-dinitrophenoxy)imino)butyl)phenoxy)benzyl methylbutanoate (1ak) (^1H NMR 500 MHz, CDCl_3)

2-(4-chlorophenyl)-3-

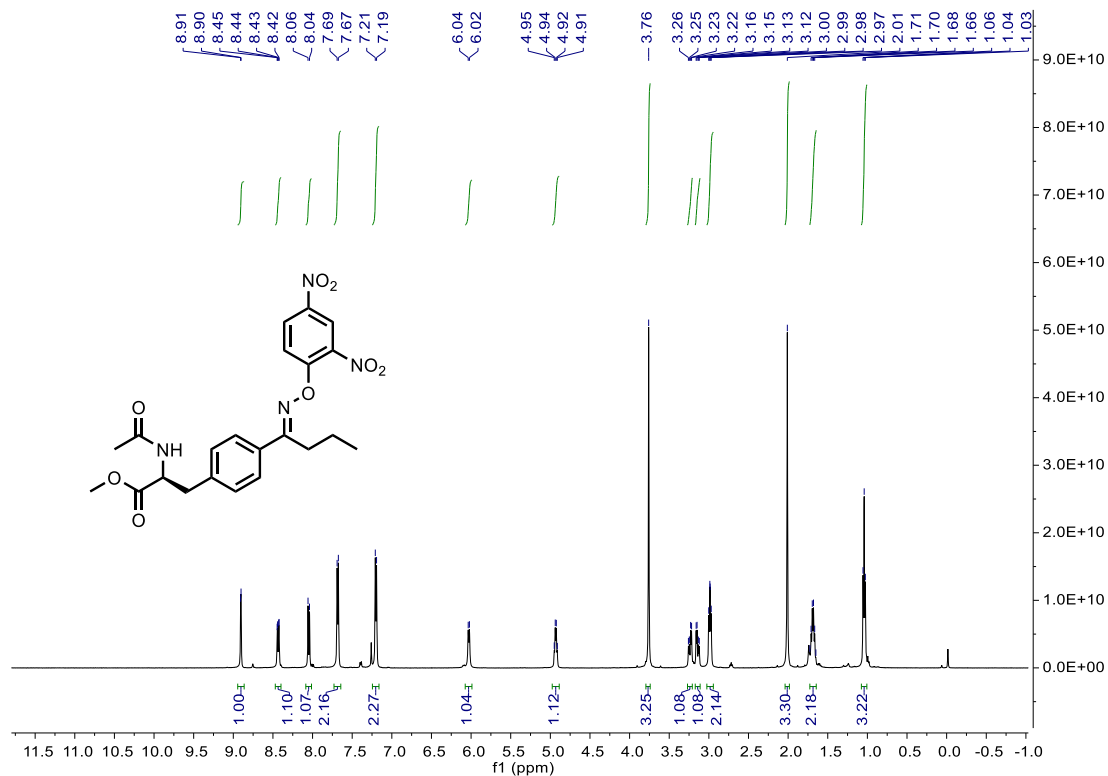


(E)-3-(4-(1-((2,4-dinitrophenoxy)imino)butyl)phenoxy)benzyl methylbutanoate (1ak) (^{13}C NMR 126 MHz, CDCl_3)

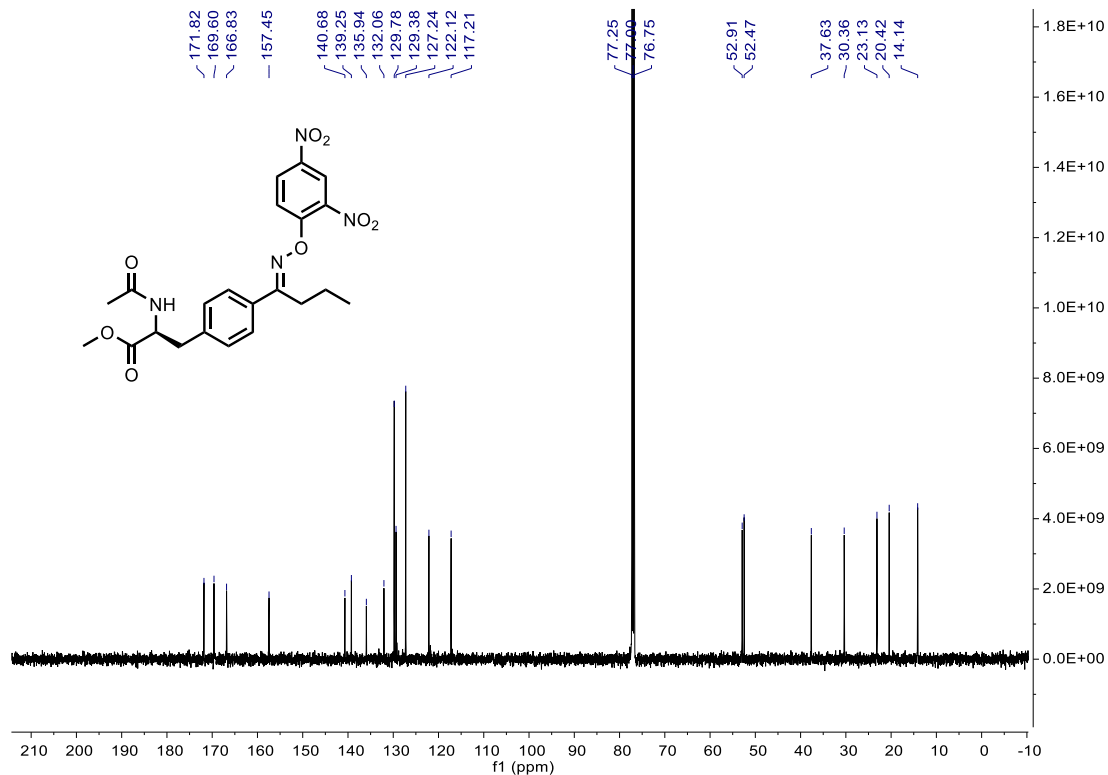
2-(4-chlorophenyl)-3-



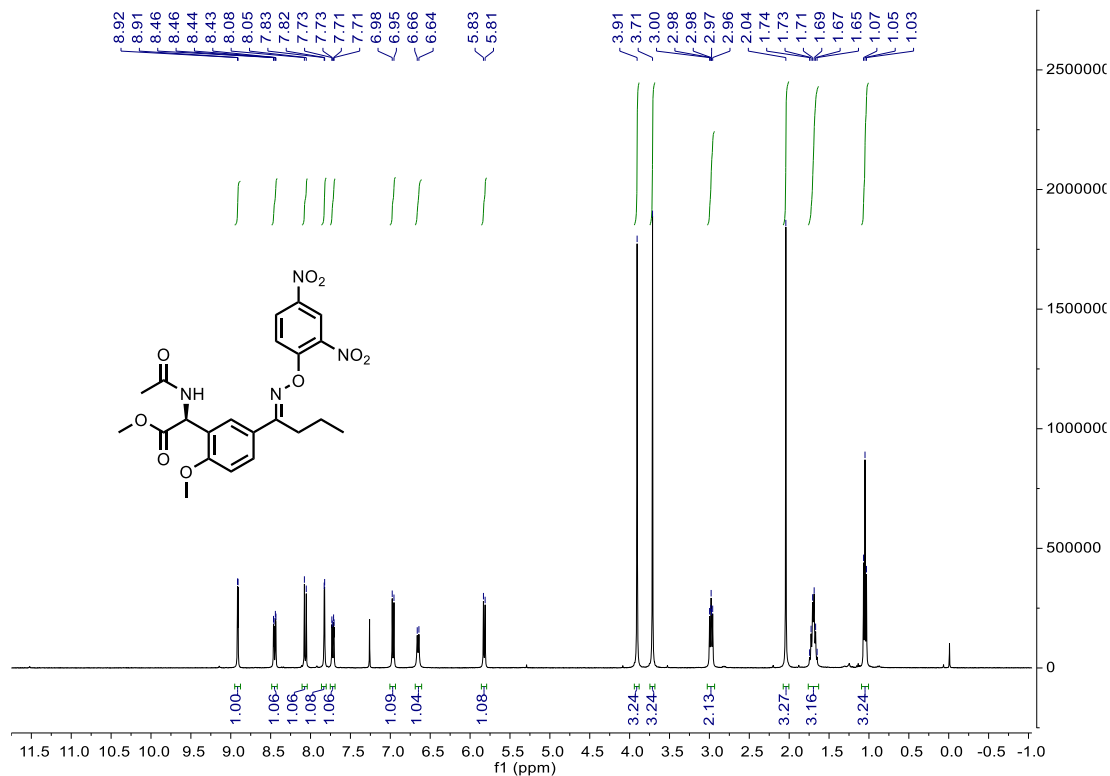
methyl (*S,E*)-2-acetamido-3-(4-(1-((2,4-dinitrophenoxy)imino)butyl)phenyl)propanoate (1a)
(¹H NMR 500 MHz, CDCl₃)



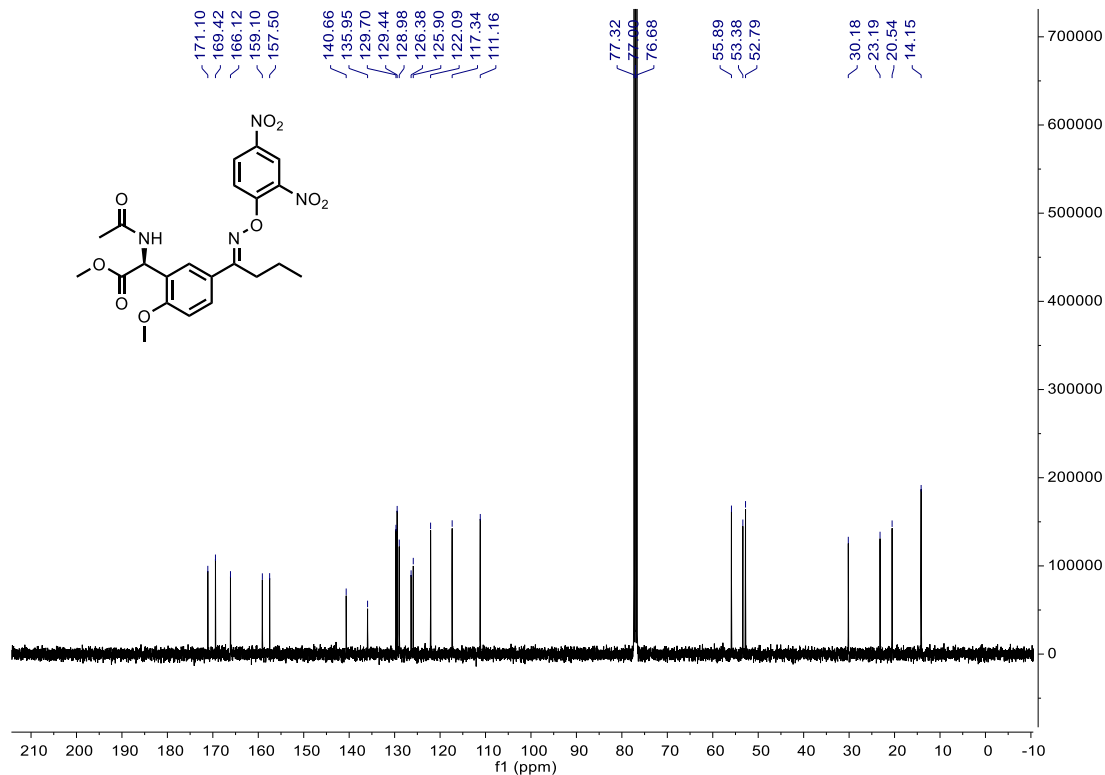
methyl (*S,E*)-2-acetamido-3-(4-(1-((2,4-dinitrophenoxy)imino)butyl)phenyl)propanoate (1a)
(¹³C NMR 126 MHz, CDCl₃)



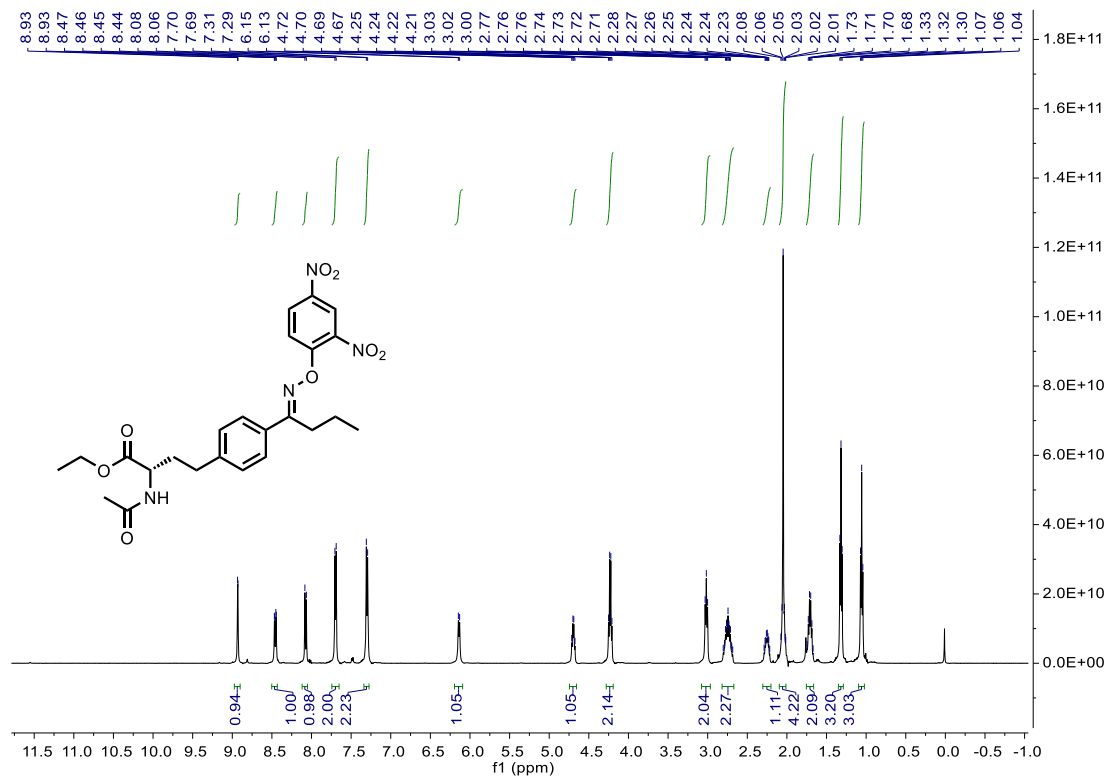
methyl (S,E)-2-acetamido-2-(5-(1-((2,4-dinitrophenoxy)imino)butyl)-2-methoxyphenyl)acetate (1am) (¹H NMR 400 MHz, CDCl₃)



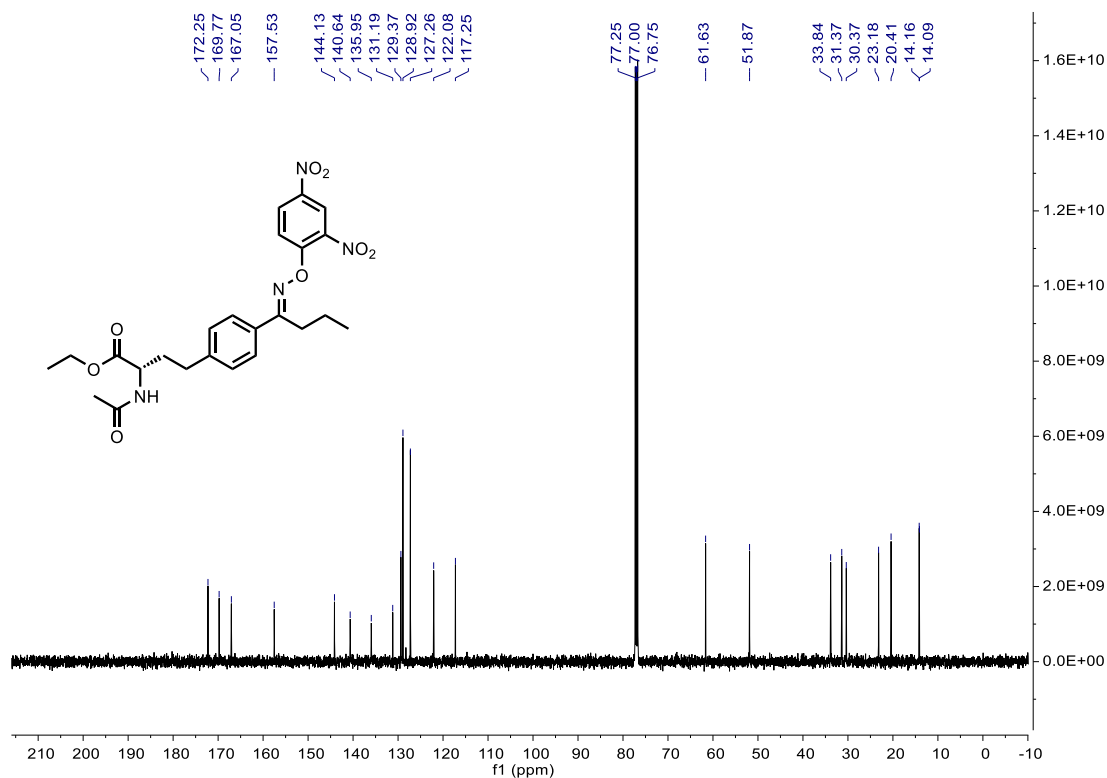
methyl (S,E)-2-acetamido-2-(5-(1-((2,4-dinitrophenoxy)imino)butyl)-2-methoxyphenyl)acetate (1am) (¹³C NMR 101 MHz, CDCl₃)



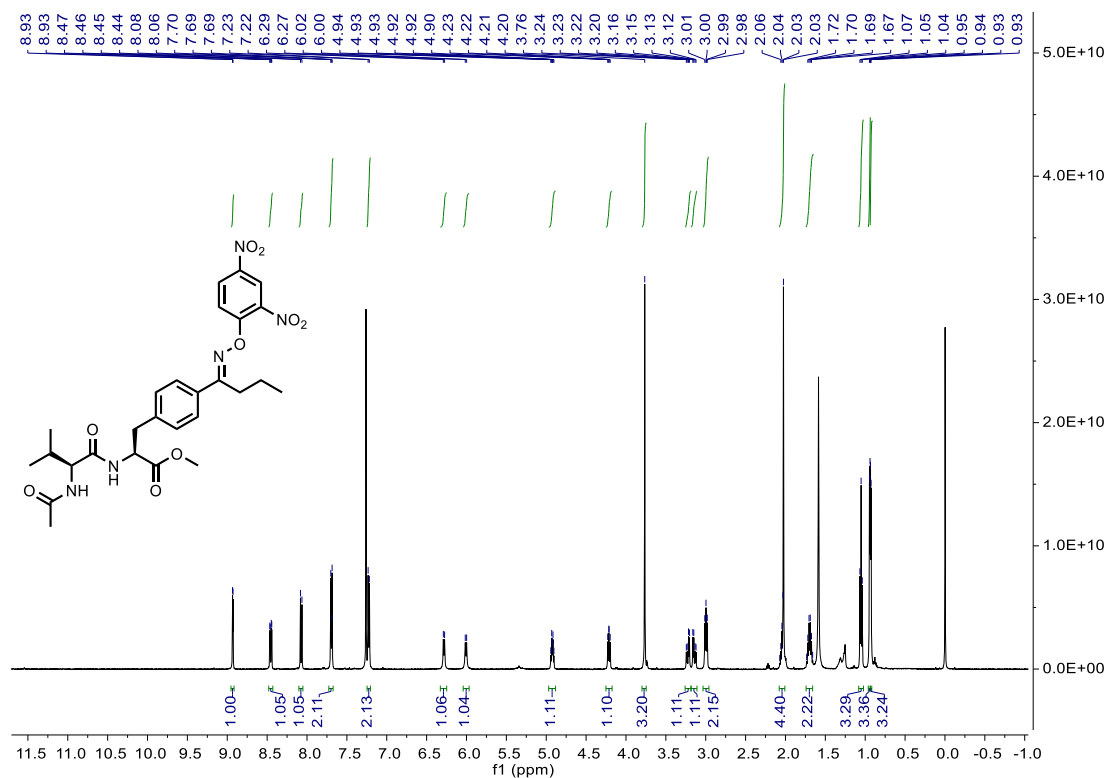
ethyl (*S,E*)-2-acetamido-4-(4-(1-((2,4-dinitrophenoxy)imino)butyl)phenyl)butanoate (1an) (¹H NMR 500 MHz, CDCl₃)



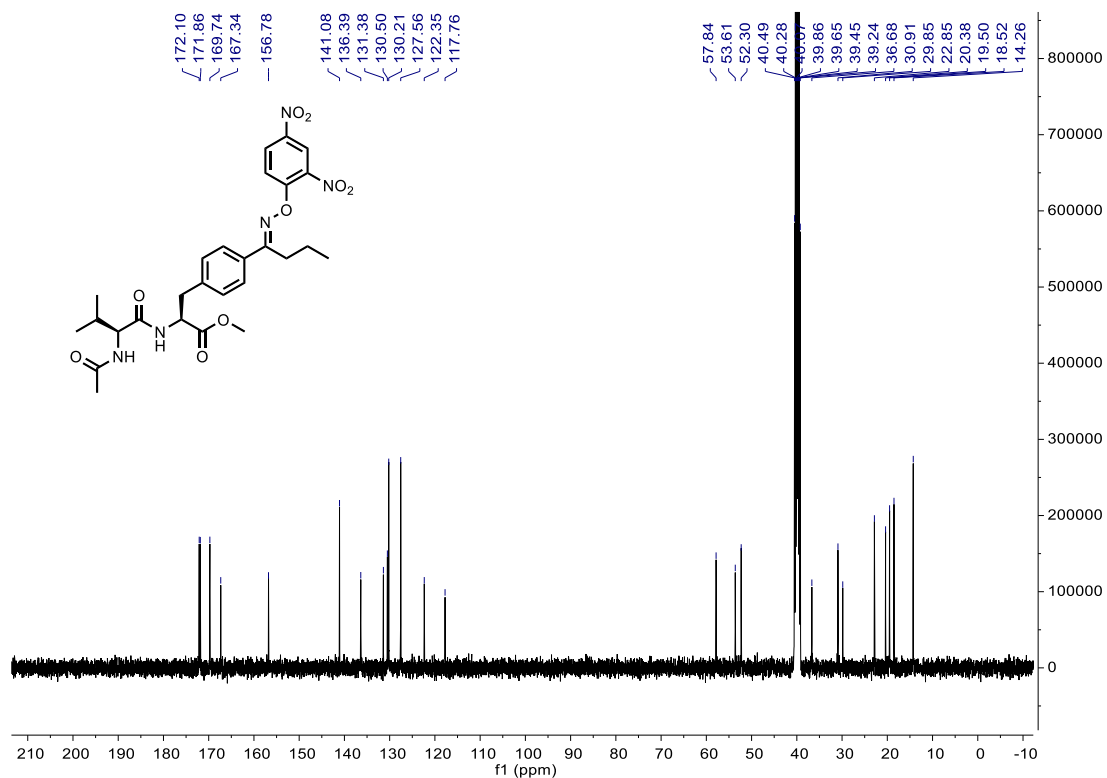
ethyl (*S,E*)-2-acetamido-4-(4-(1-((2,4-dinitrophenoxy)imino)butyl)phenyl)butanoate (1an) (¹³C NMR 126 MHz, CDCl₃)



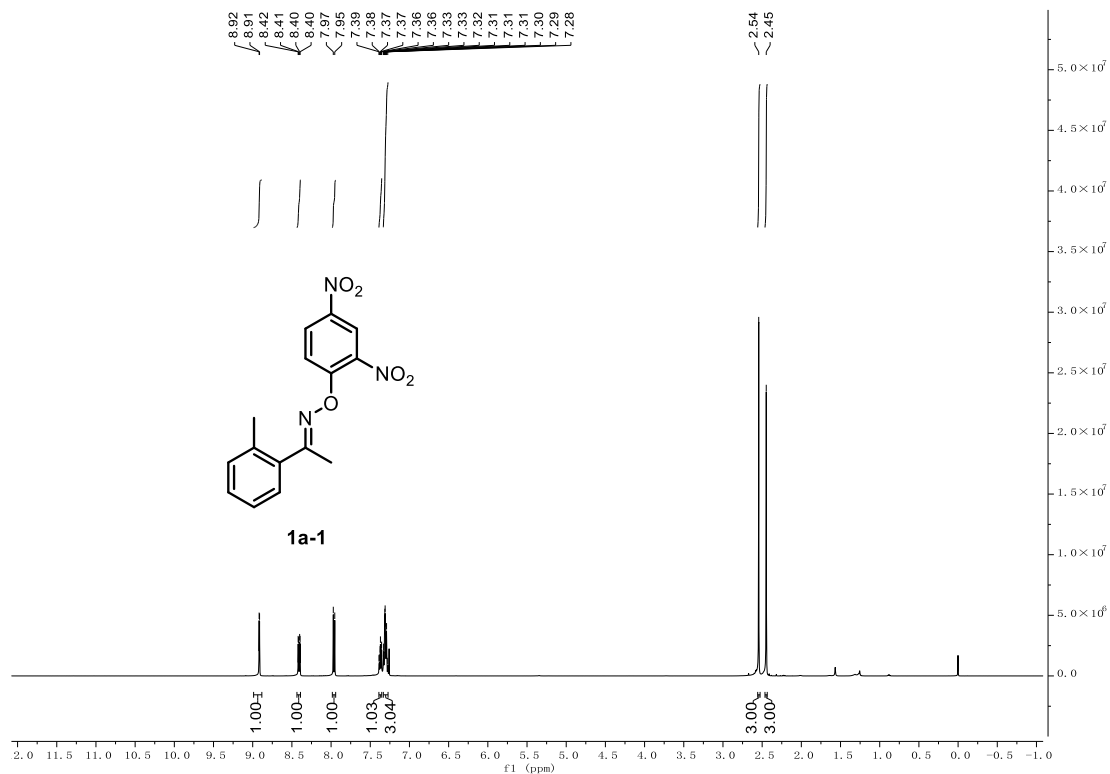
methyl (S)-2-((S)-2-acetamido-3-methylbutanamido)-3-(4-((E)-1-((2,4-dinitrophenoxy)imino)butyl)phenyl)propanoate (1ao) (¹H NMR 500 MHz, CDCl₃)



methyl (S)-2-((S)-2-acetamido-3-methylbutanamido)-3-(4-((E)-1-((2,4-dinitrophenoxy)imino)butyl)phenyl)propanoate (1ao) (¹³C NMR 101 MHz, DMSO-d₆)



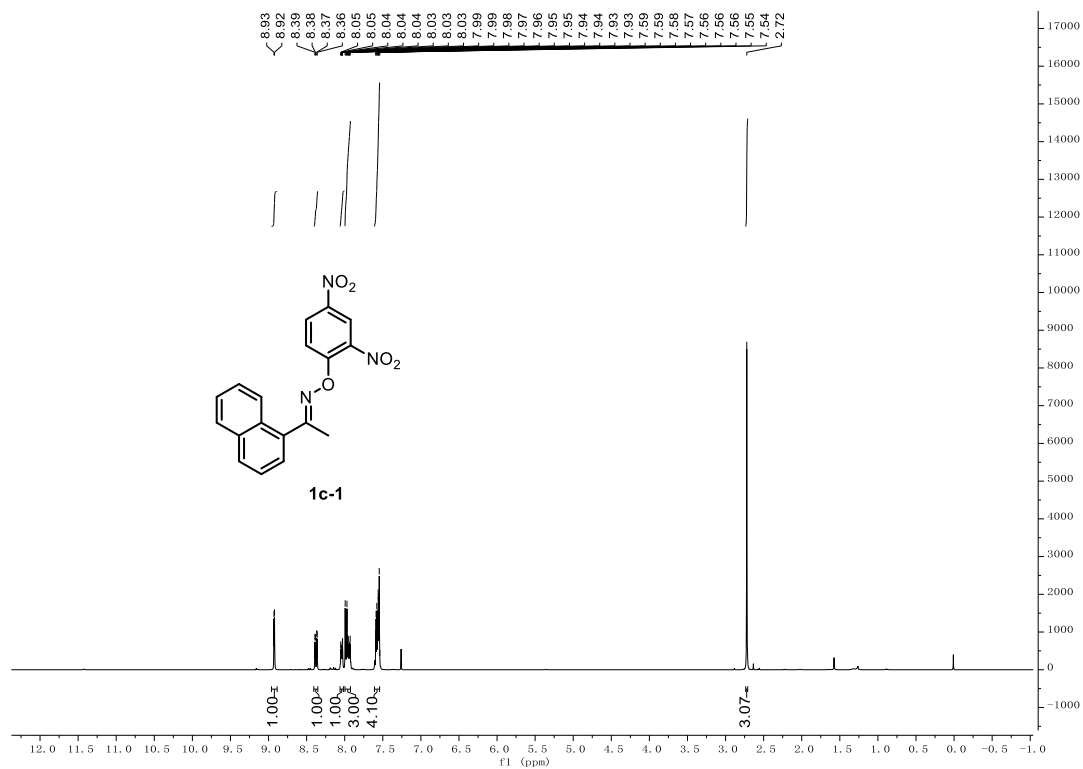
(*E*)-1-(*o*-tolyl)ethan-1-one *O*-(2,4-dinitrophenyl) oxime (1a-1) (¹H NMR 500 MHz, CDCl₃)



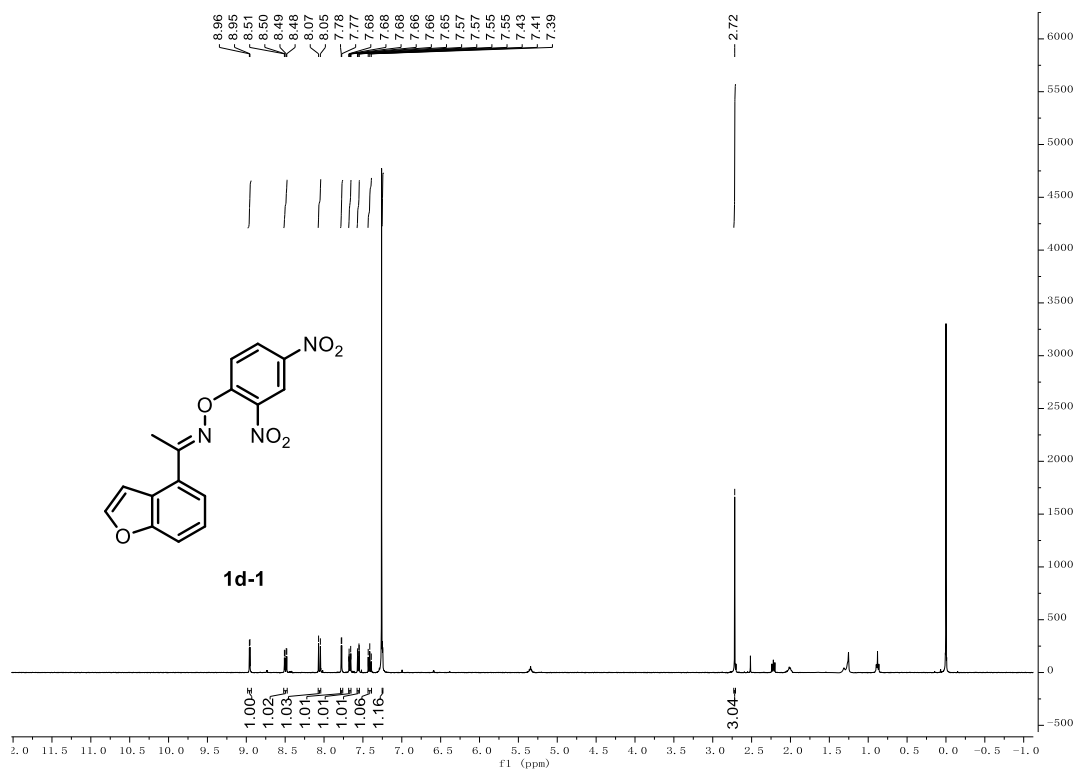
(*E*)-1-(2-methoxyphenyl)ethan-1-one *O*-(2,4-dinitrophenyl) oxime (1b-1) (¹H NMR 400 MHz, CDCl₃)



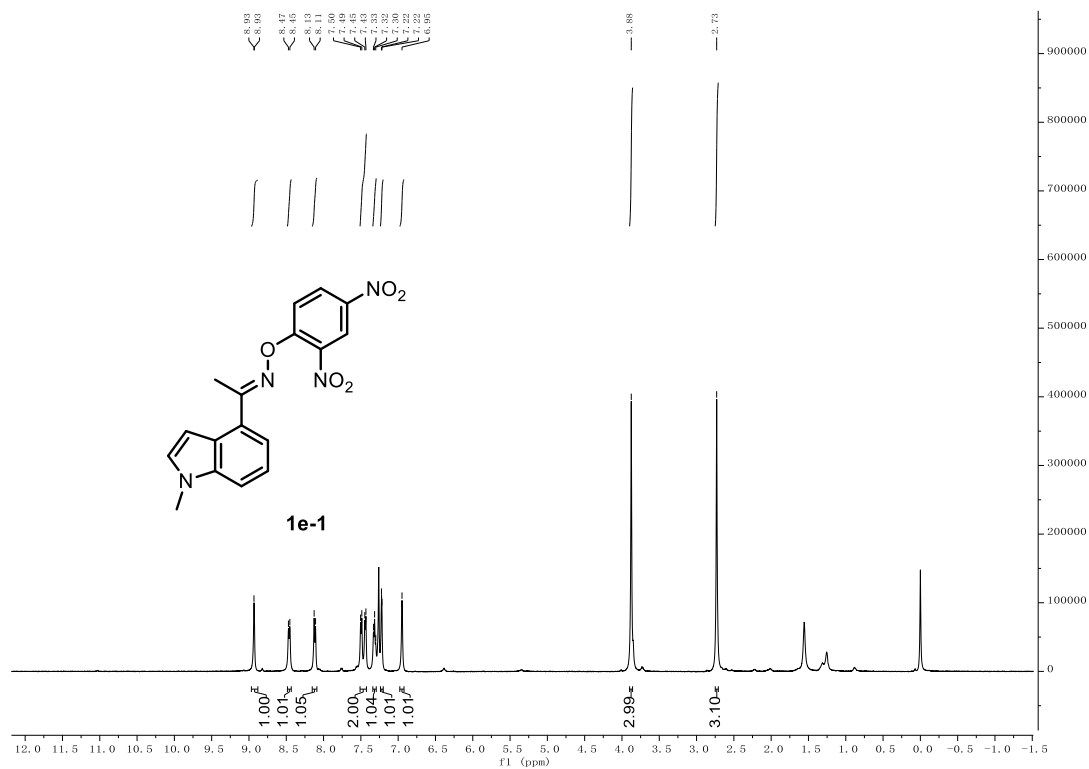
(*E*)-1-(naphthalen-1-yl)ethan-1-one *O*-(2,4-dinitrophenyl) oxime (1c-1) (¹H NMR 400 MHz, CDCl₃)



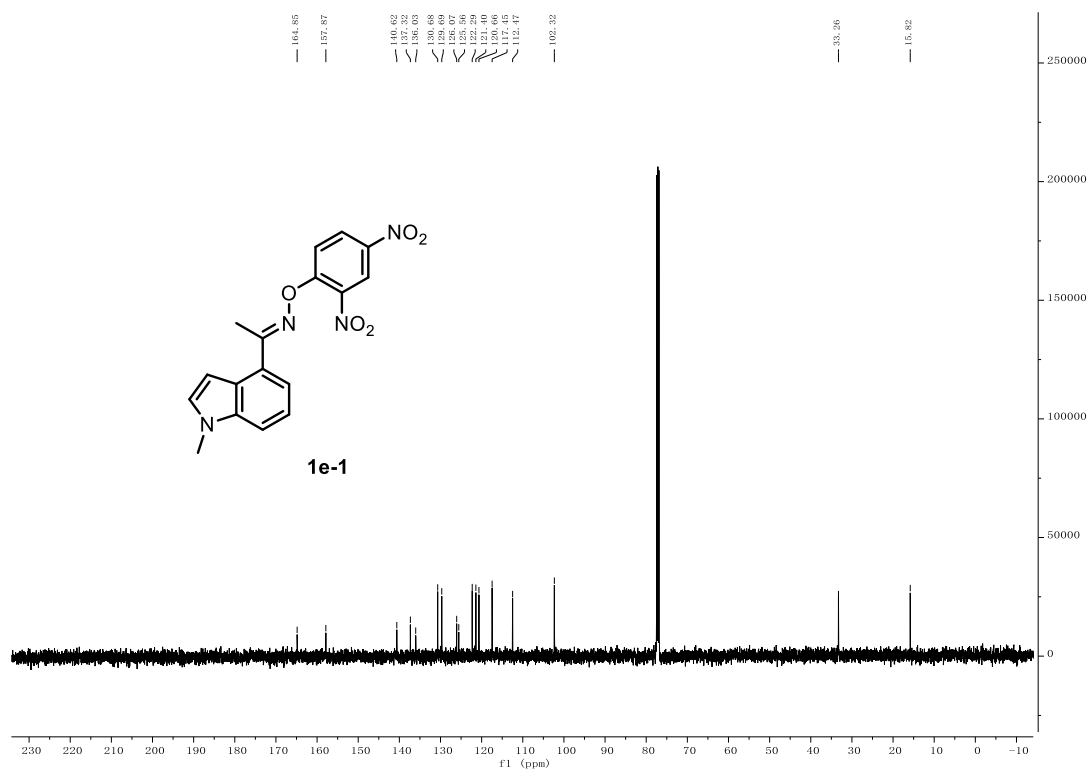
(*E*)-1-(benzofuran-4-yl)ethan-1-one *O*-(2,4-dinitrophenyl) oxime (1d-1) (¹H NMR 400 MHz, CDCl₃)



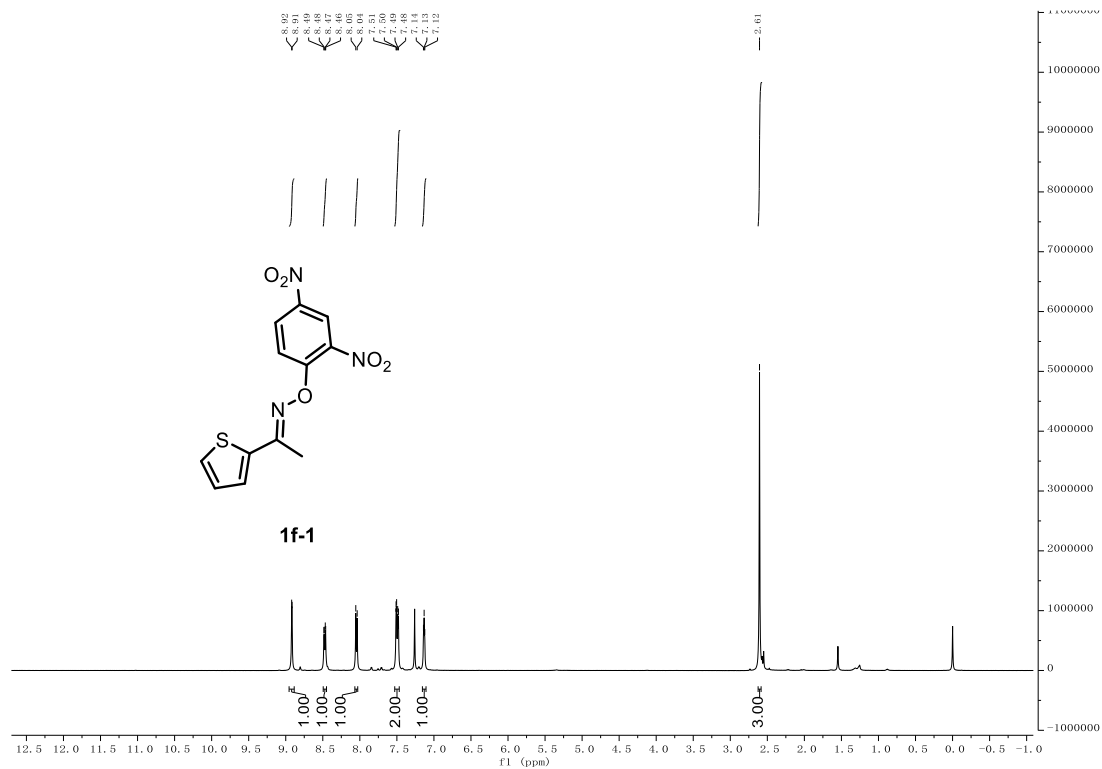
(*E*)-1-(1-methyl-1*H*-indol-4-yl)ethan-1-one *O*-(2,4-dinitrophenyl) oxime (1e-1**) (¹H NMR 400 MHz, CDCl₃)**



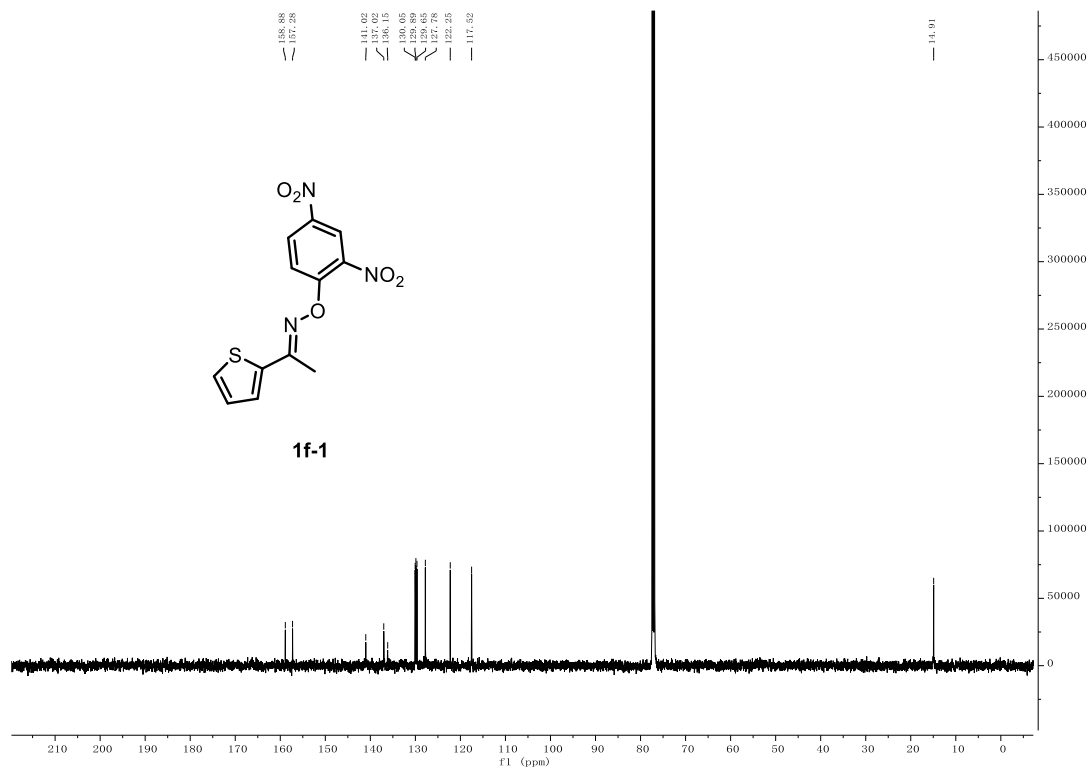
(*E*)-1-(1-methyl-1*H*-indol-4-yl)ethan-1-one *O*-(2,4-dinitrophenyl) oxime (1e-1**) (¹³C NMR 126 MHz, CDCl₃)**



(*E*)-1-(thiophen-2-yl)ethan-1-one *O*-(2,4-dinitrophenyl) oxime (1f-1) (¹H NMR 500 MHz, CDCl₃)



(*E*)-1-(thiophen-2-yl)ethan-1-one *O*-(2,4-dinitrophenyl) oxime (1f-1) (¹³C NMR 126 MHz, CDCl₃)



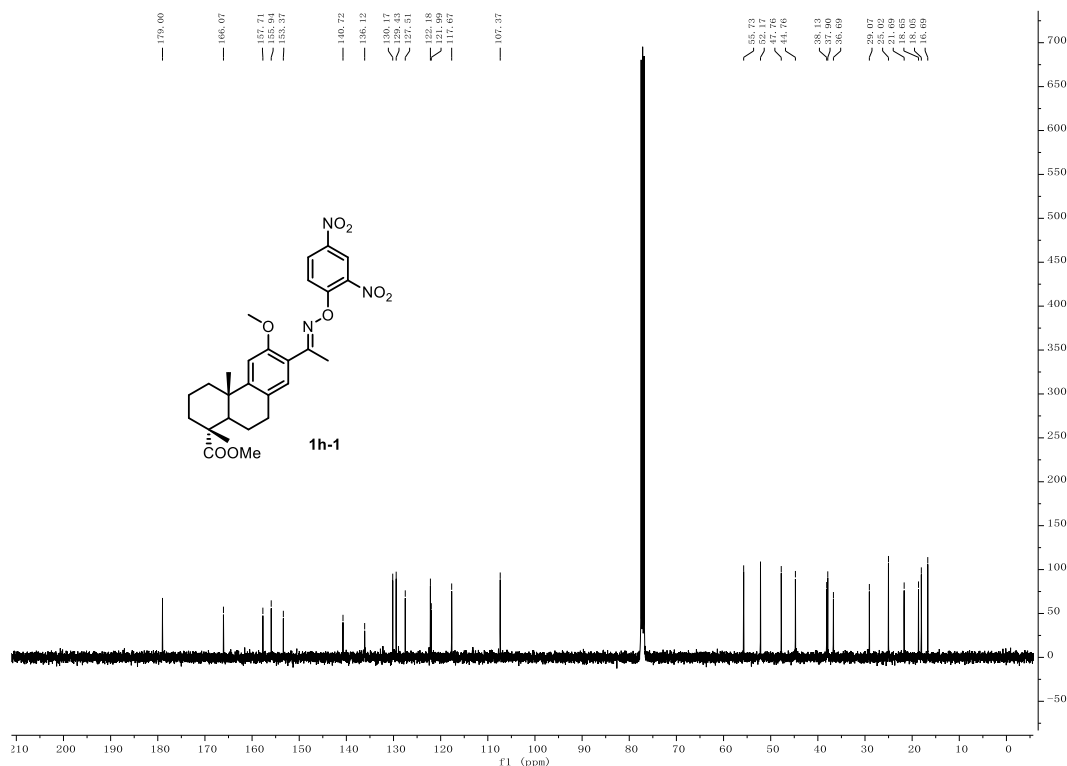
Chemical structure of **19-1** is shown. The ¹H NMR spectrum (CDCl₃) displays peaks from 1.2 to 9.3 ppm. Integration values are provided below the baseline, and a list of peak chemical shifts is on the right.

Chemical structure of 1h-1: COC(=O)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC=C4[C@@]3(CC[C@@H](C4)OC(=O)C5=CC(=C(C=C5)C(=O)N5C(=O)C(=C(C=C5)C)C)C)C

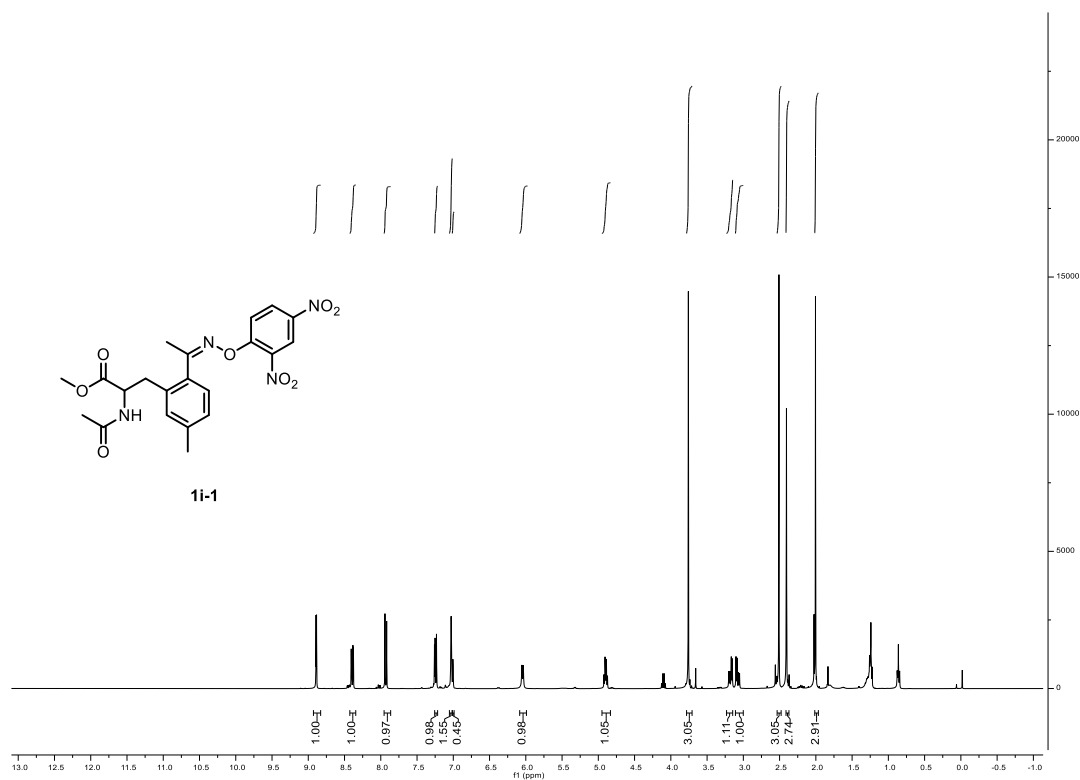
¹H NMR spectrum (CDCl₃):

- Chemical shifts (ppm):** 8.89, 8.86, 8.41, 8.40, 8.38, 8.38, 8.01, 8.01, 7.99, 7.04, 6.98, 3.84, 3.84, 2.89, 2.89, 2.87, 2.87, 2.59, 2.59, 2.55, 2.55, 2.21, 2.21, 2.18, 2.18, 1.80, 1.74, 1.69, 1.69, 1.67, 1.67, 1.54, 1.54, 1.46, 1.46, 1.43, 1.43, 1.29, 1.29, 0.00.
- Integrations:** 1.00, 1.00, 1.00, 1.00, 1.00, 3.00, 3.01, 2.00, 3.00, 1.00, 1.00, 4.01, 1.00, 1.00, 1.00, 3.01.

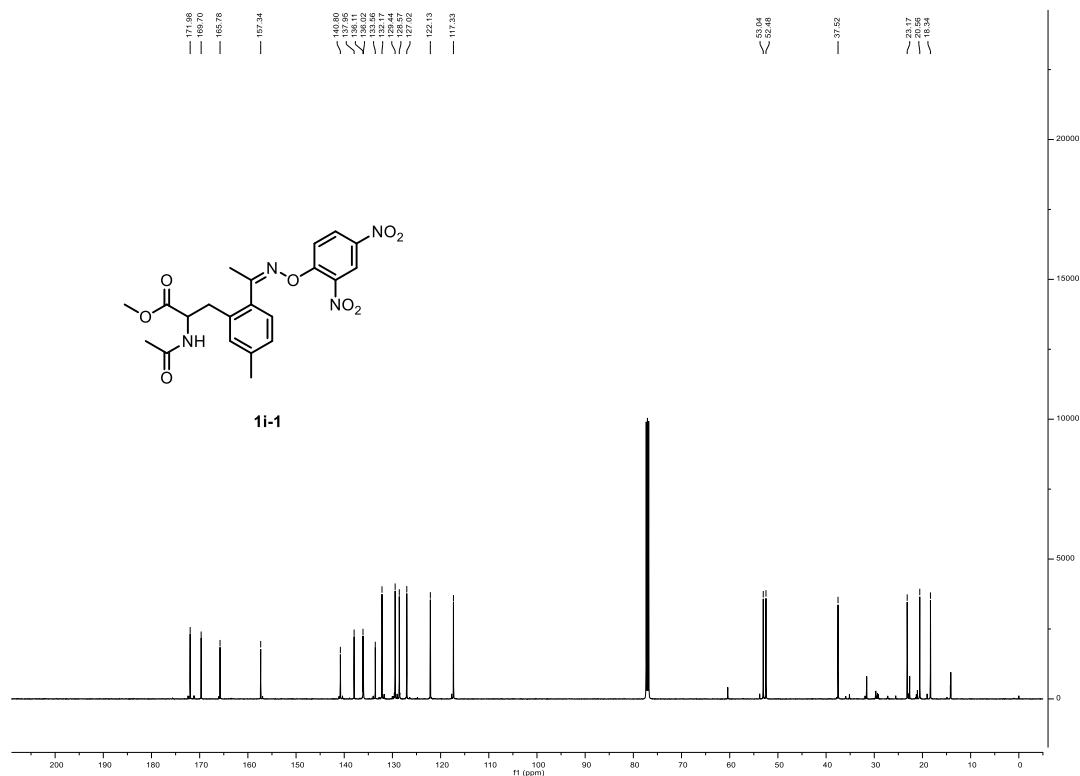
methyl (1*R*,4*aS*)-7-((*E*)-1-((2,4-dinitrophenoxy)imino)ethyl)-6-methoxy-1,4*a*-dimethyl-1,2,3,4,4*a*,9,10,10*a*-octahydrophenanthrene-1-carboxylate (1h-1) (¹³C NMR 101 MHz, CDCl₃)



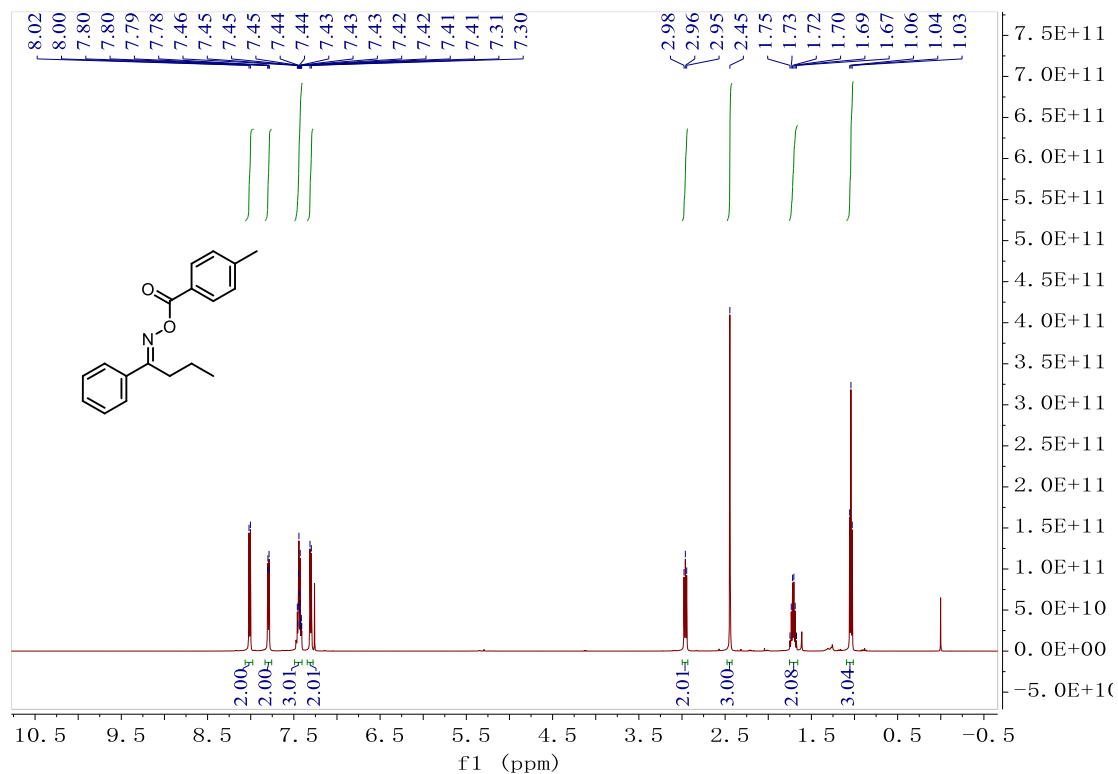
methyl (Z)-2-acetamido-3-(2-(1-((2,4-dinitrophenoxy)imino)ethyl)-5-methylphenyl)propanoate (1i-1) (¹H NMR 400 MHz, CDCl₃)



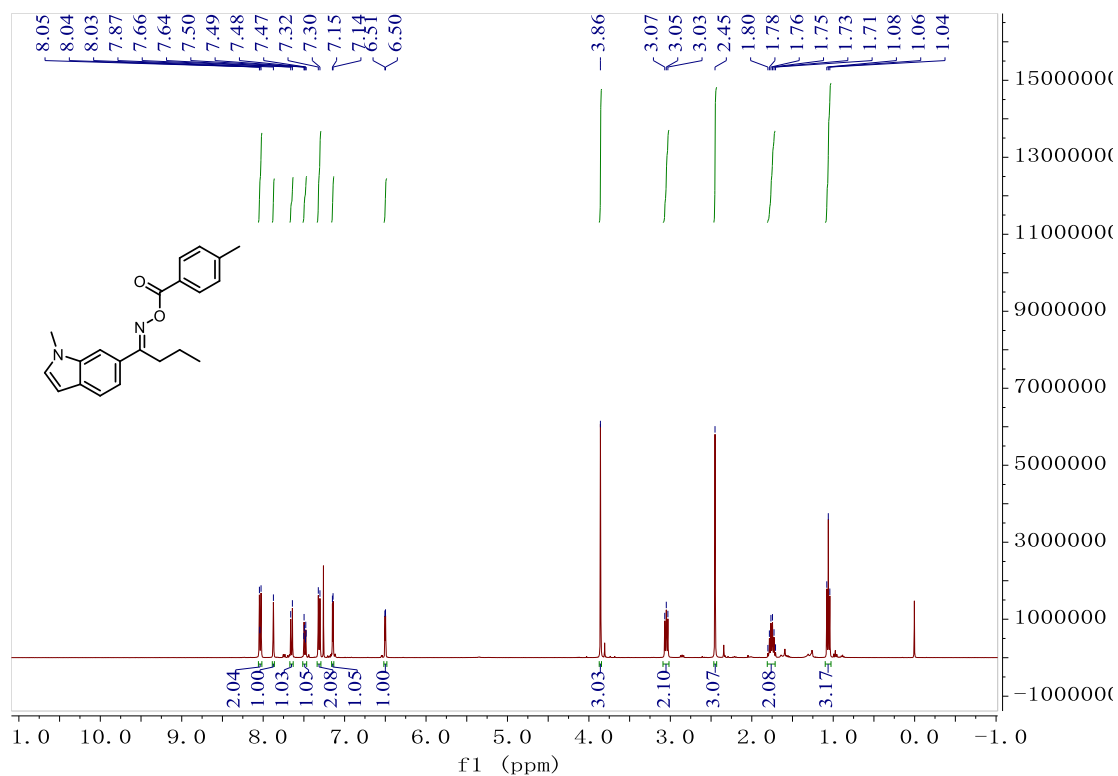
methyl (Z)-2-acetamido-3-(2-(1-((2,4-dinitrophenoxy)imino)ethyl)-5-methylphenyl)propanoate (1i-1) (¹³C NMR 126 MHz, CDCl₃)



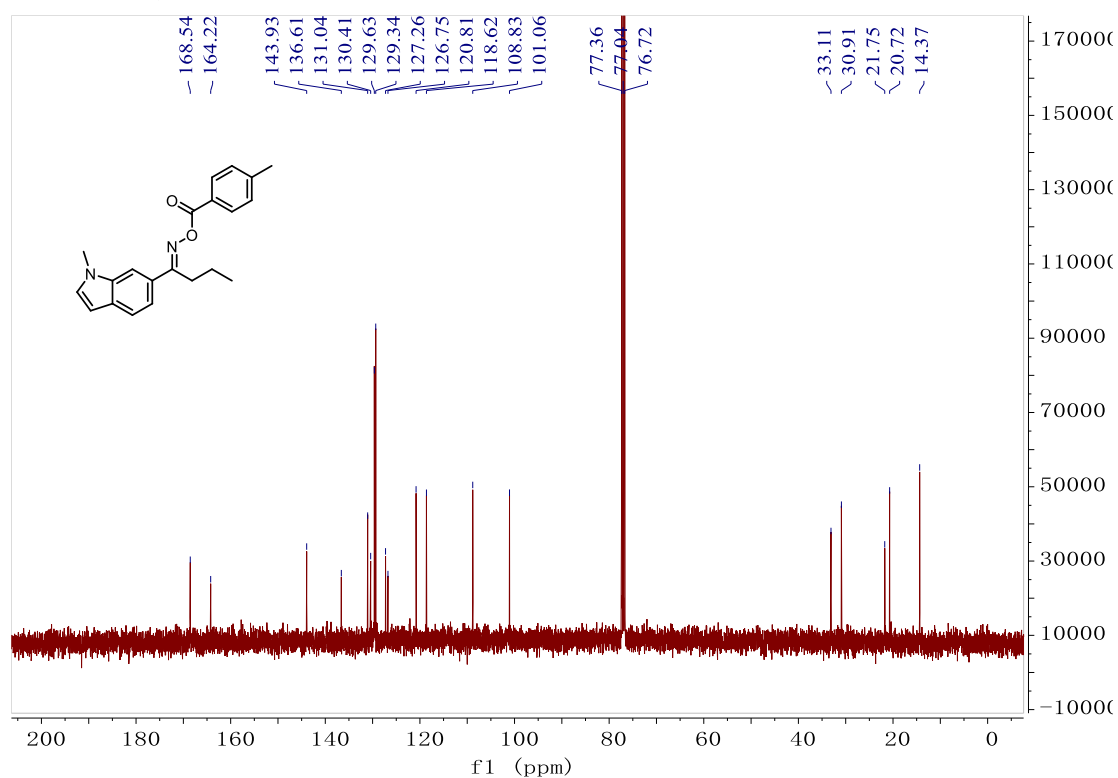
(E)-1-phenylbutan-1-one O-(4-methylbenzoyl) oxime (1a-2) (¹H NMR 500 MHz, CDCl₃)



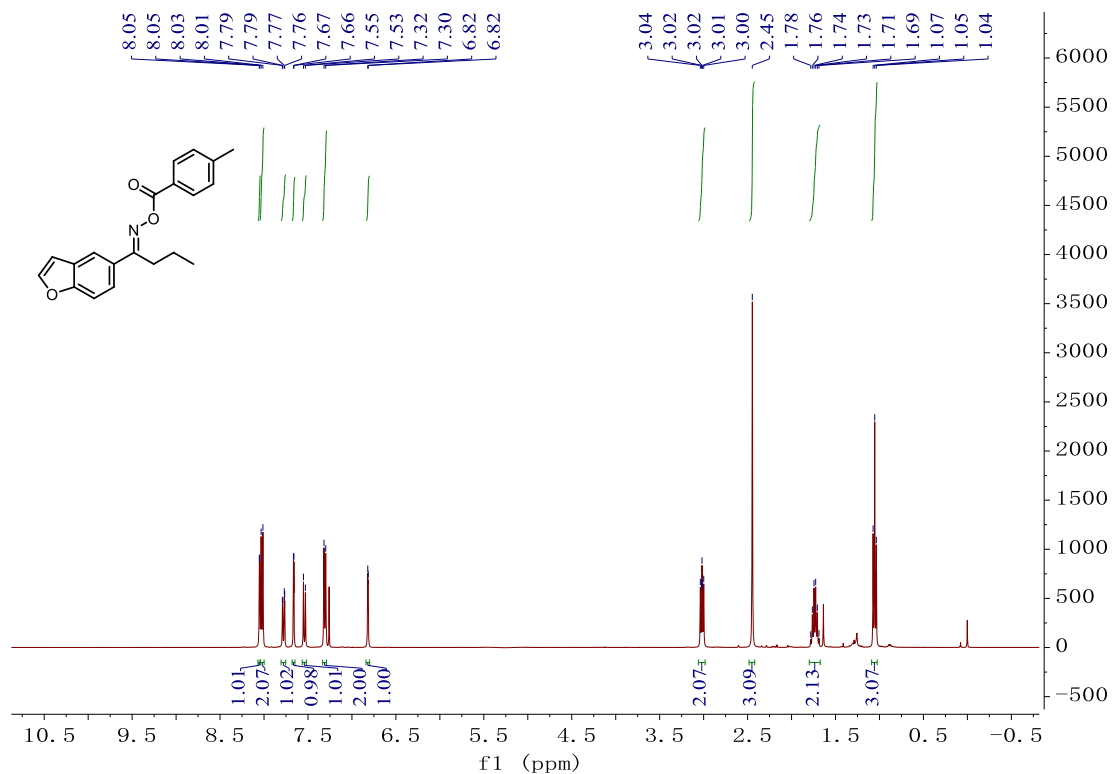
(*E*)-1-(1-methyl-1H-indol-6-yl)butan-1-one *O*-(4-methylbenzoyl) oxime (1b-2) (^1H NMR 400 MHz, CDCl_3)



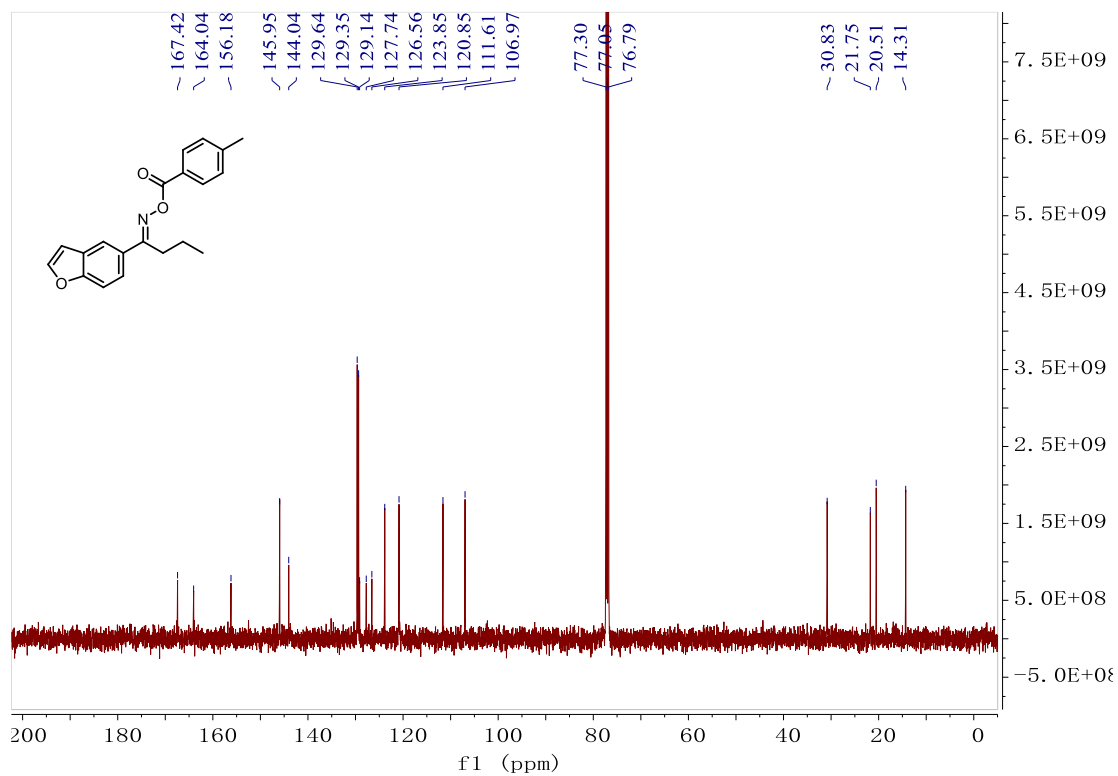
(*E*)-1-(1-methyl-1H-indol-6-yl)butan-1-one *O*-(4-methylbenzoyl) oxime (1b-2) (^{13}C NMR 101 MHz, CDCl_3)



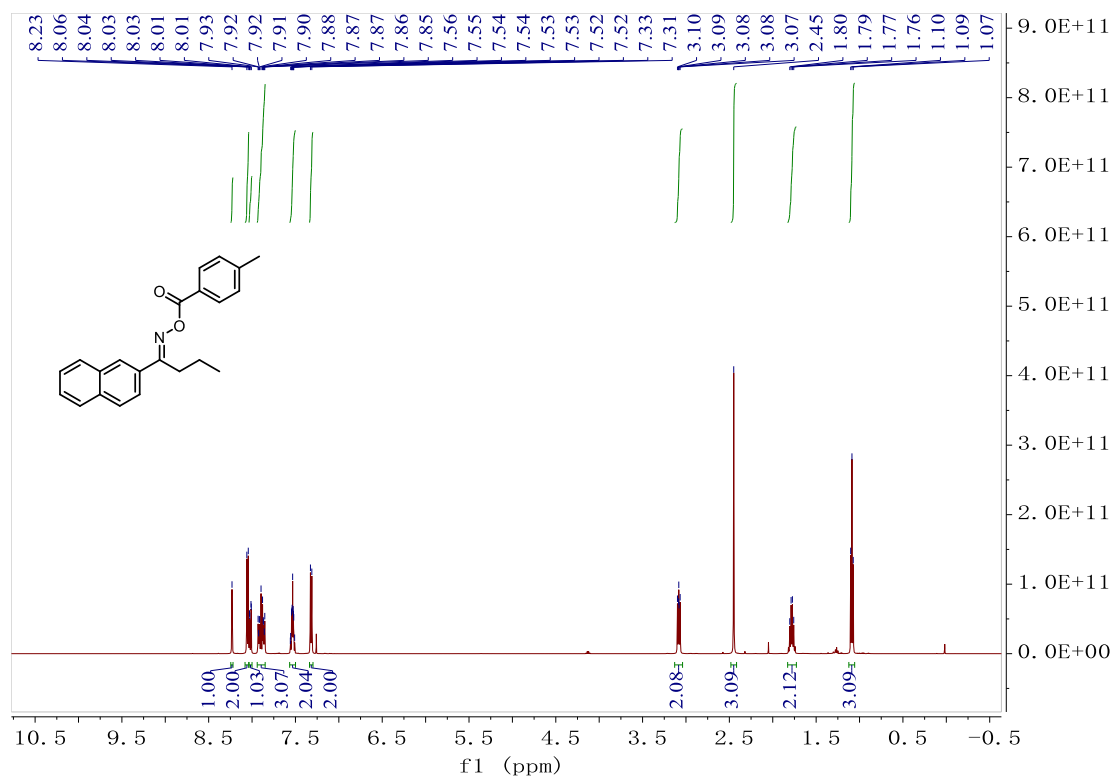
(*E*)-1-(benzofuran-5-yl)butan-1-one *O*-(4-methylbenzoyl) oxime (1c-2) (^1H NMR 400 MHz, CDCl_3)



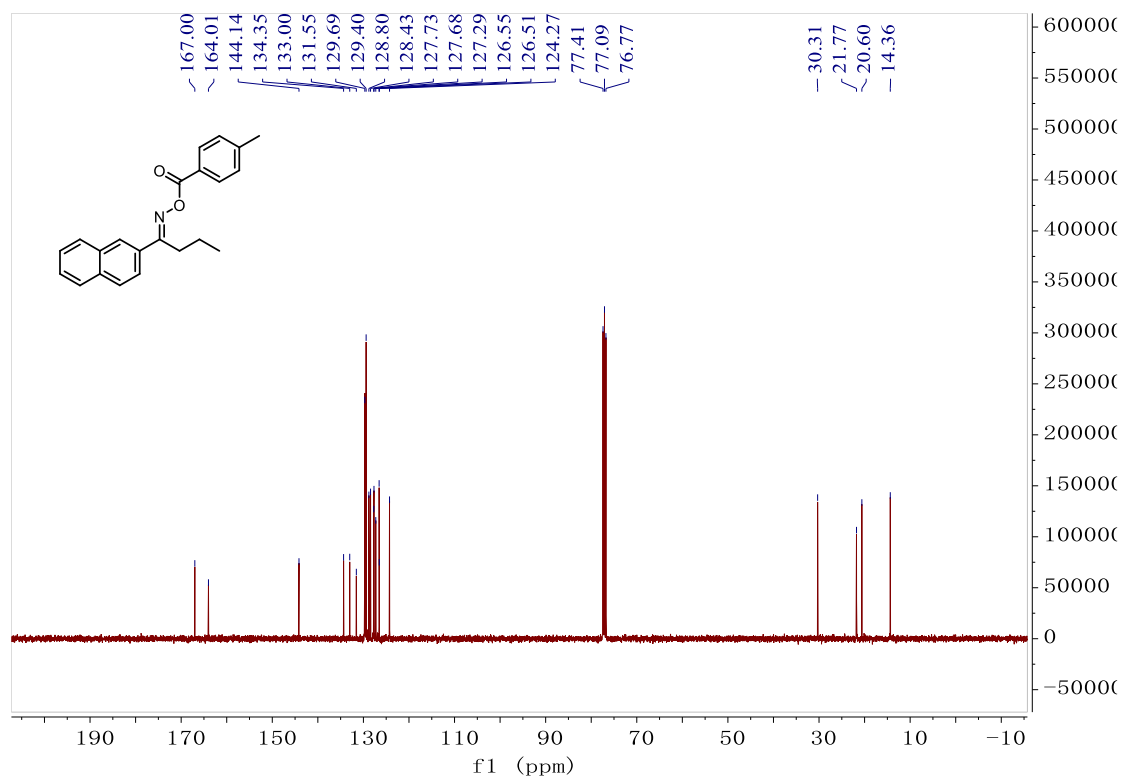
(*E*)-1-(benzofuran-5-yl)butan-1-one *O*-(4-methylbenzoyl) oxime (1c-2) (^{13}C NMR 126 MHz, CDCl_3)



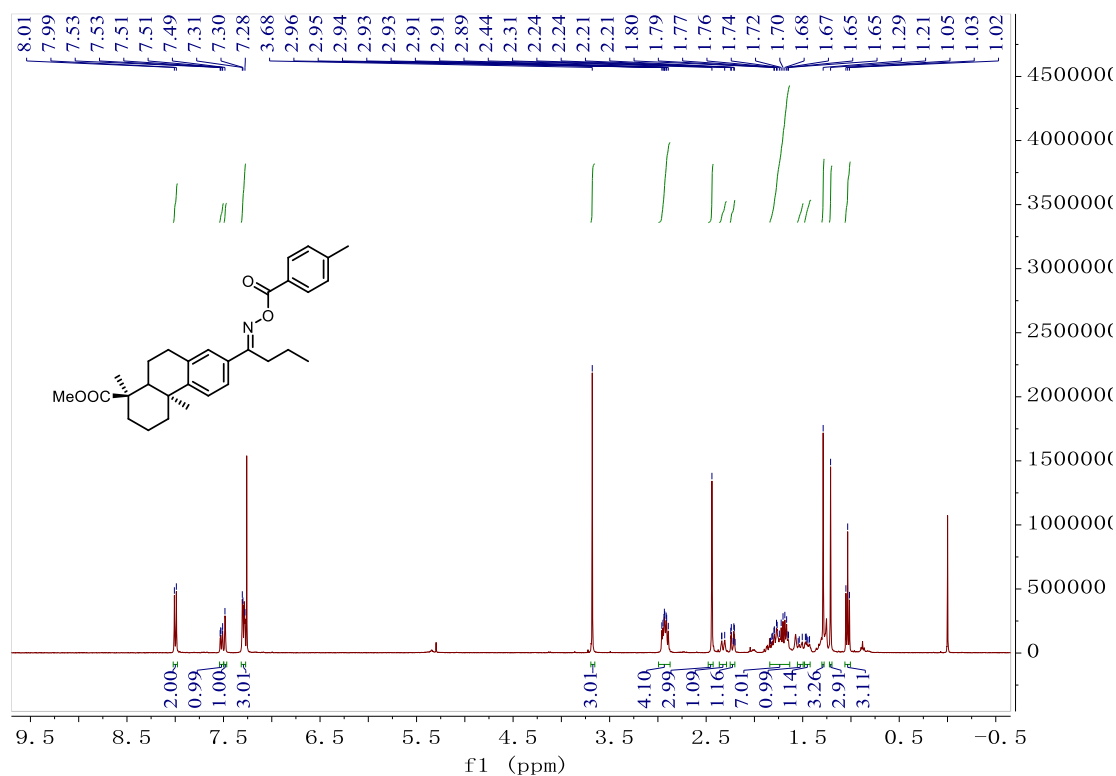
(*E*)-1-(naphthalen-2-yl)butan-1-one *O*-(4-methylbenzoyl) oxime (1d-2) (^1H NMR 500 MHz, CDCl_3)



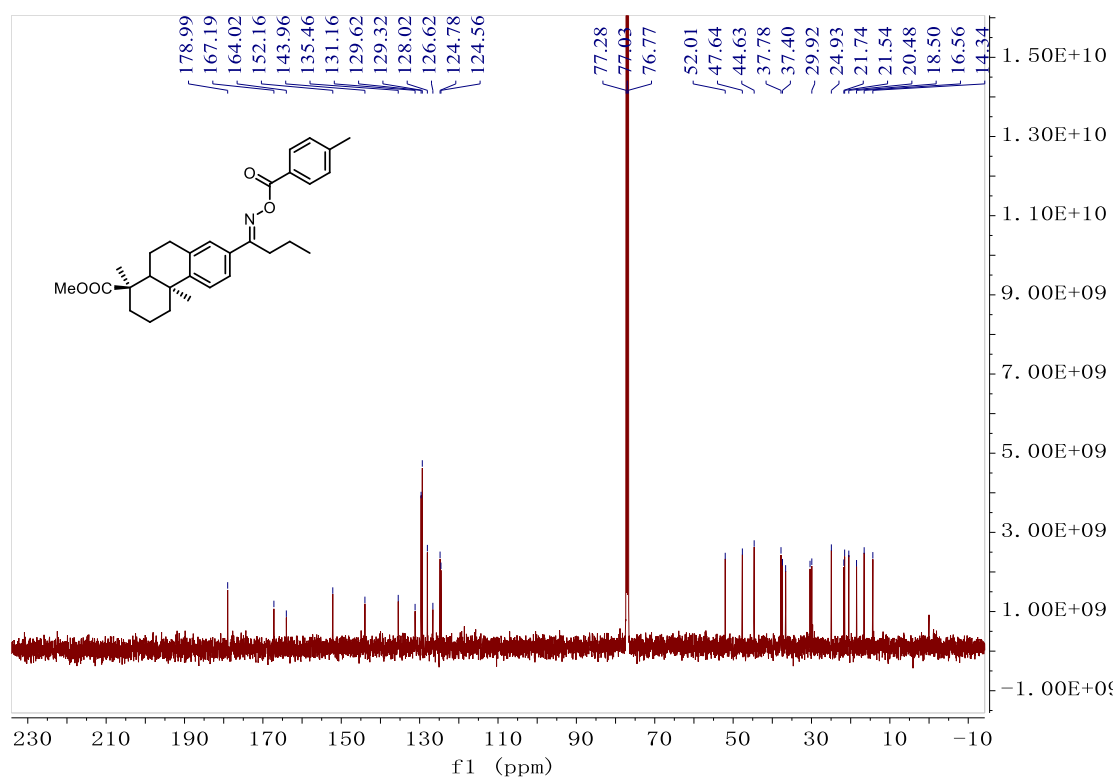
(*E*)-1-(naphthalen-2-yl)butan-1-one *O*-(4-methylbenzoyl) oxime (1d-2) (^{13}C NMR 101 MHz, CDCl_3)



methyl (1R,4aS)-1,4a-dimethyl-7-((E)-1-(((4-methylbenzoyl)oxy)imino)butyl)-1,2,3,4,4a,9,10,10a-octahydrophenanthrene-1-carboxylate (1e-2) (¹H NMR 400 MHz, CDCl₃)

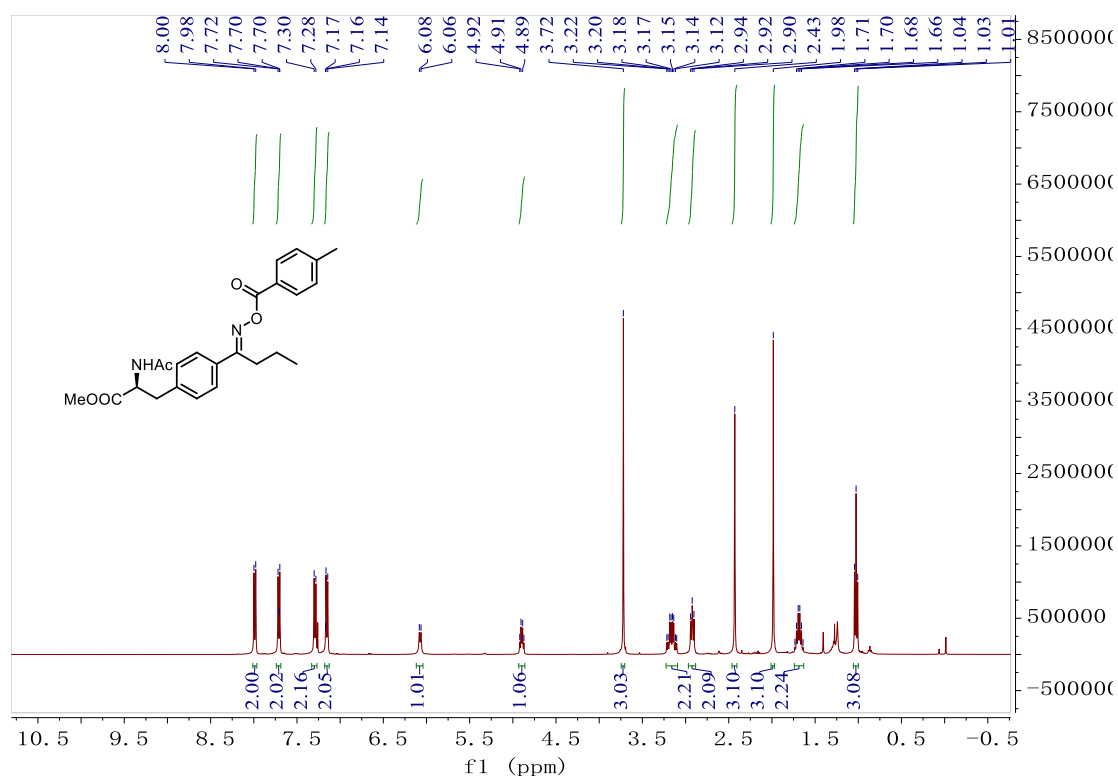


methyl (1R,4aS)-1,4a-dimethyl-7-((E)-1-(((4-methylbenzoyl)oxy)imino)butyl)-1,2,3,4,4a,9,10,10a-octahydrophenanthrene-1-carboxylate (1e-2) (¹³C NMR 126 MHz, CDCl₃)

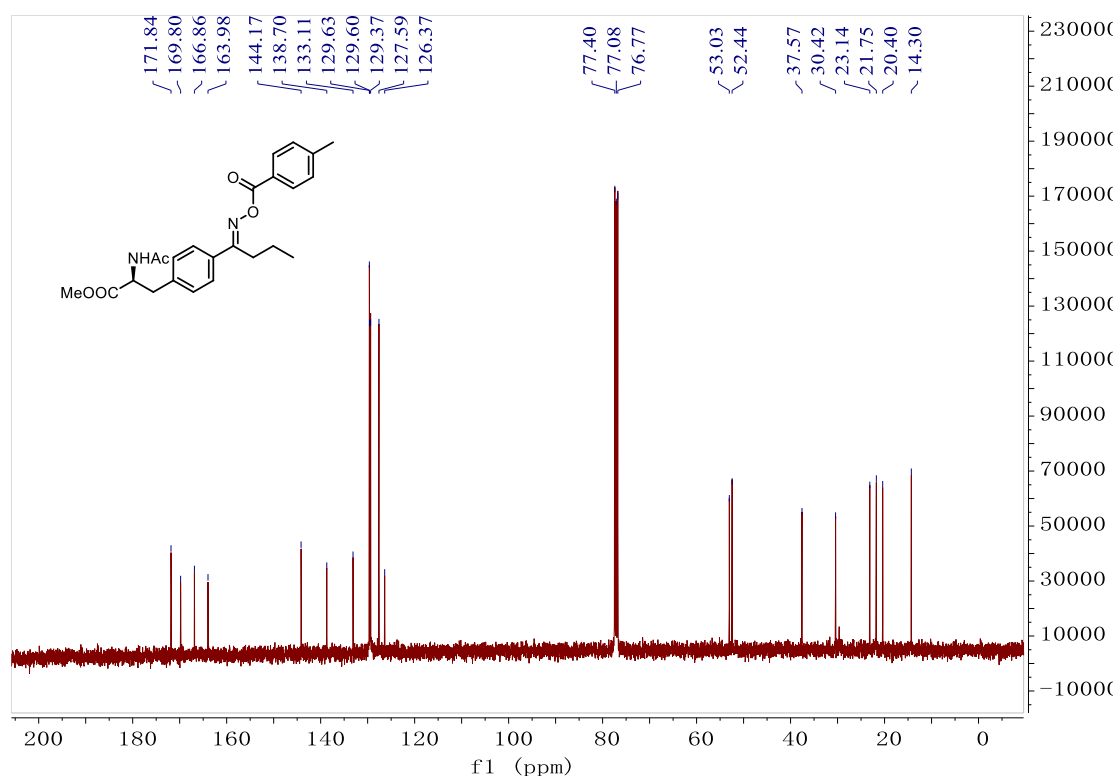


Methyl (S,E)-2-acetamido-3-(4-(1-(((4-methylbenzoyl)oxy)imino)butyl)phenyl)propanoate

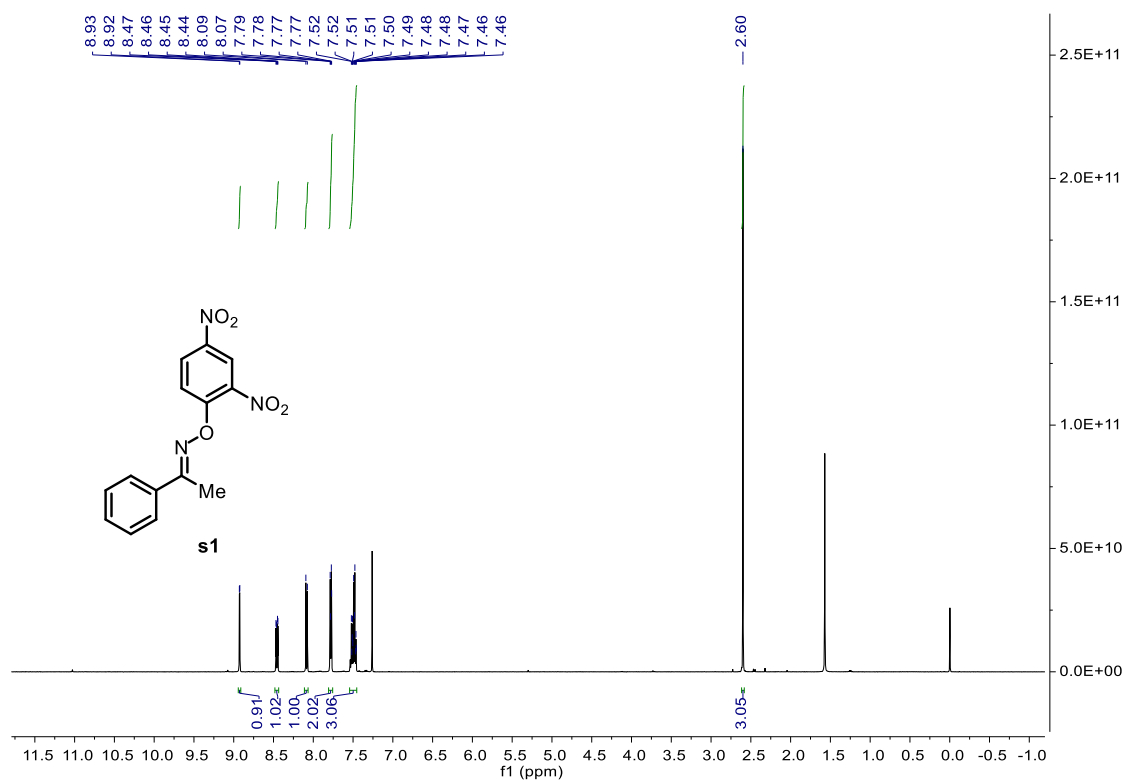
(1f-2) (¹H NMR 400 MHz, CDCl₃)



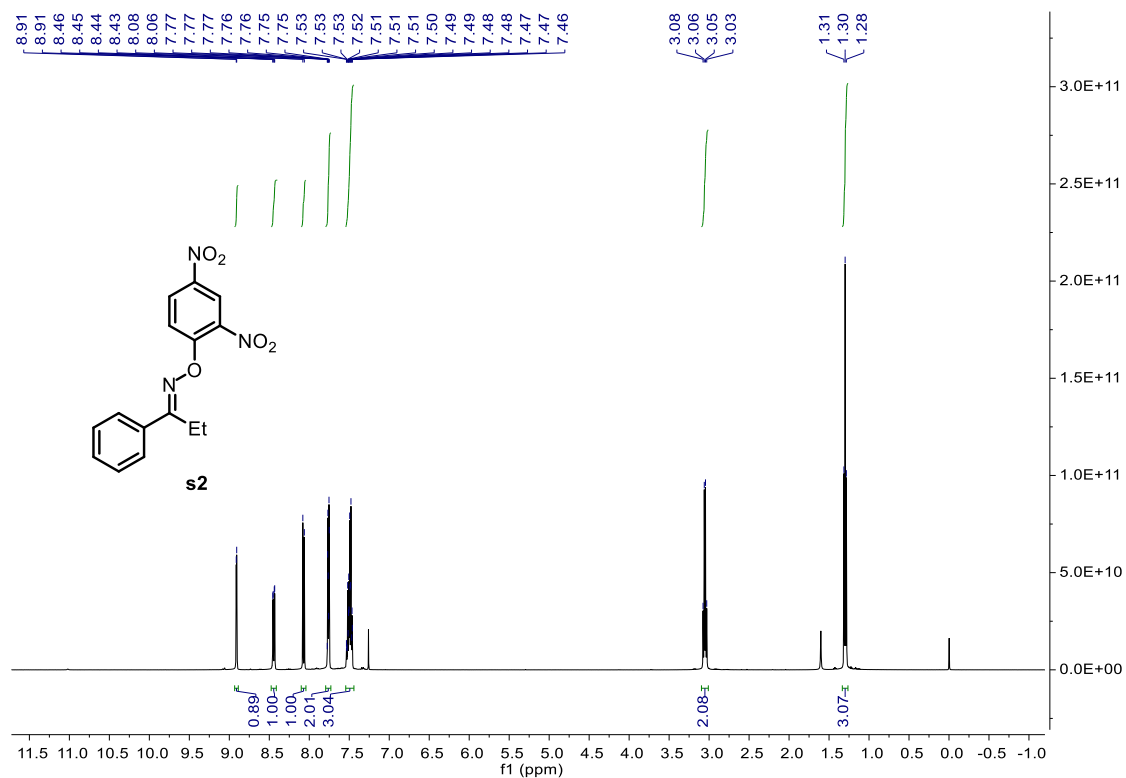
Methyl (S,E)-2-acetamido-3-(4-(1-(((4-methylbenzoyl)oxy)imino)butyl)phenyl)propanoate (1f-2) (¹³C NMR 101 MHz, CDCl₃)



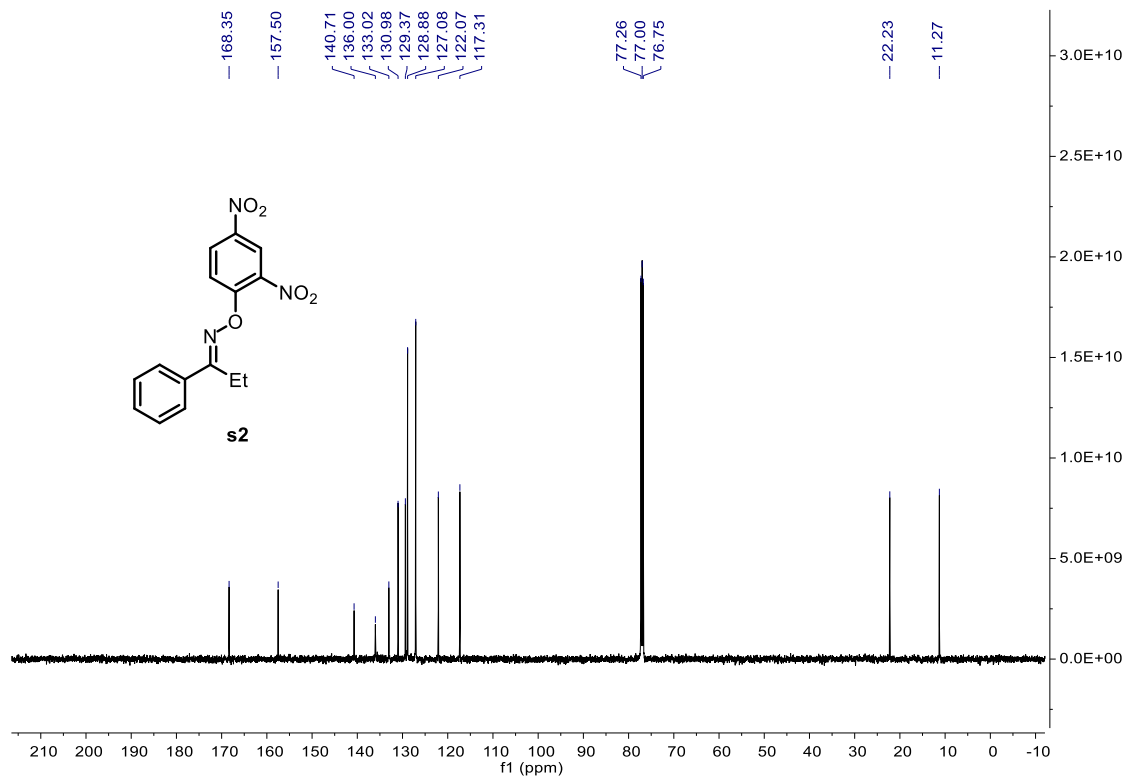
(E)-1-phenylethan-1-one O-(2,4-dinitrophenyl) oxime (s1) (¹H NMR 500 MHz, CDCl₃)



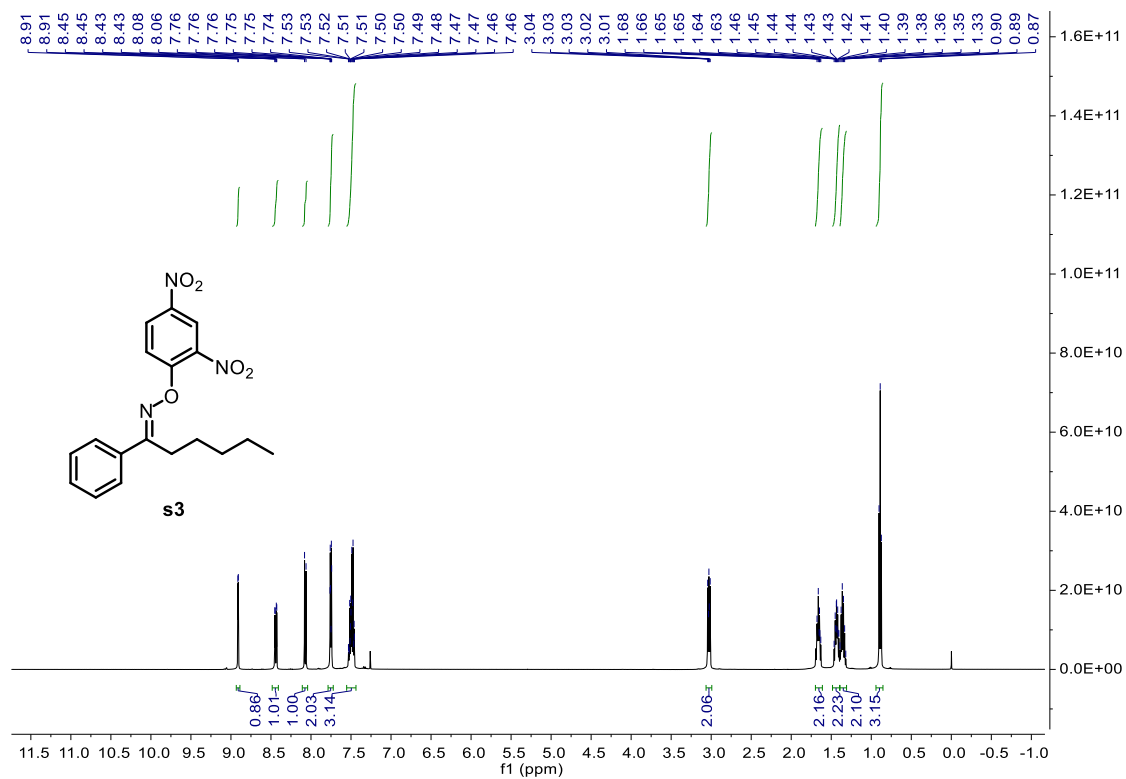
(E)-1-phenylpropan-1-one O-(2,4-dinitrophenyl) oxime (s2) (^1H NMR 500 MHz, CDCl_3)



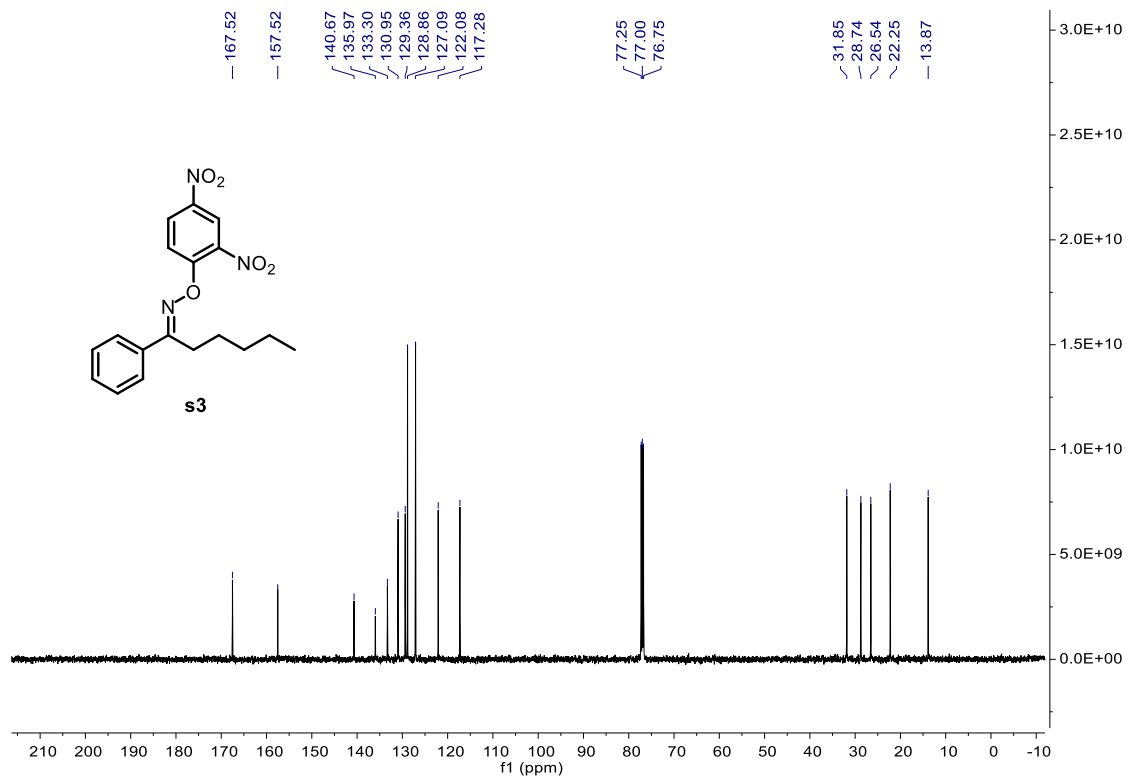
(*E*)-1-phenylpropan-1-one *O*-(2,4-dinitrophenyl) oxime (s2) (¹³C NMR 126 MHz, CDCl₃)



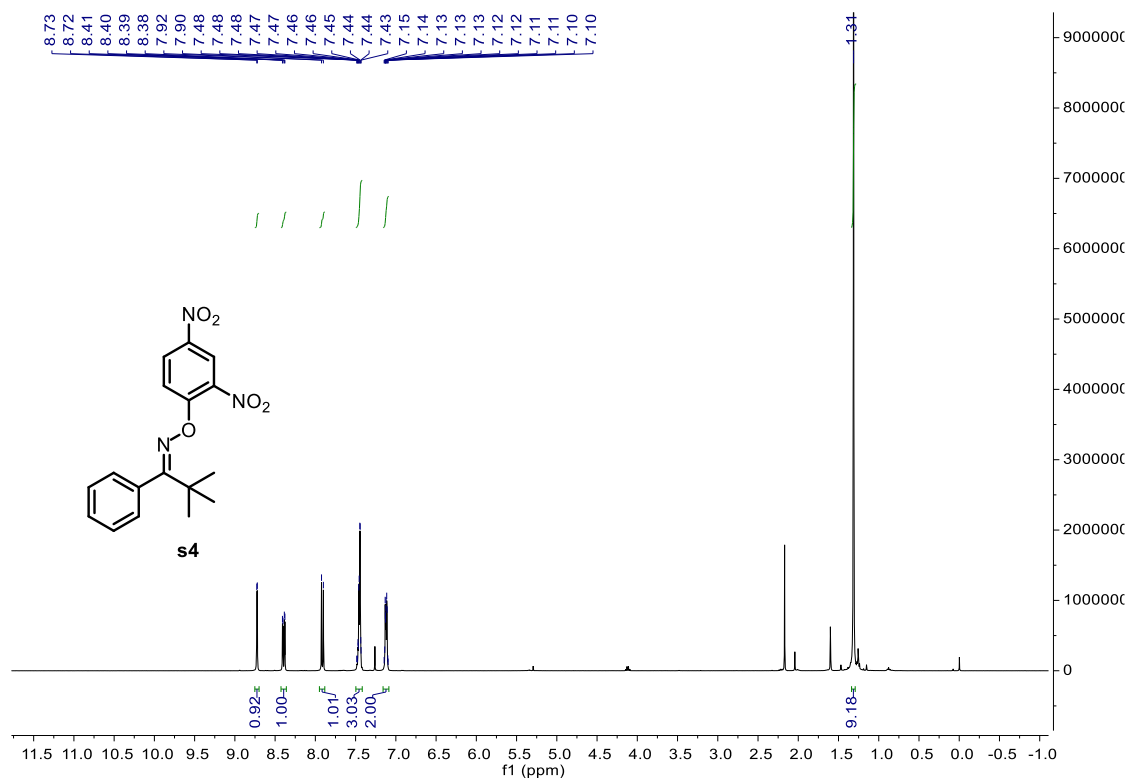
(*E*)-1-phenylhexan-1-one *O*-(2,4-dinitrophenyl) oxime (s3) (¹H NMR 500 MHz, CDCl₃)



(*E*)-1-phenylhexan-1-one *O*-(2,4-dinitrophenyl) oxime (s3) (^{13}C NMR 126 MHz, CDCl_3)

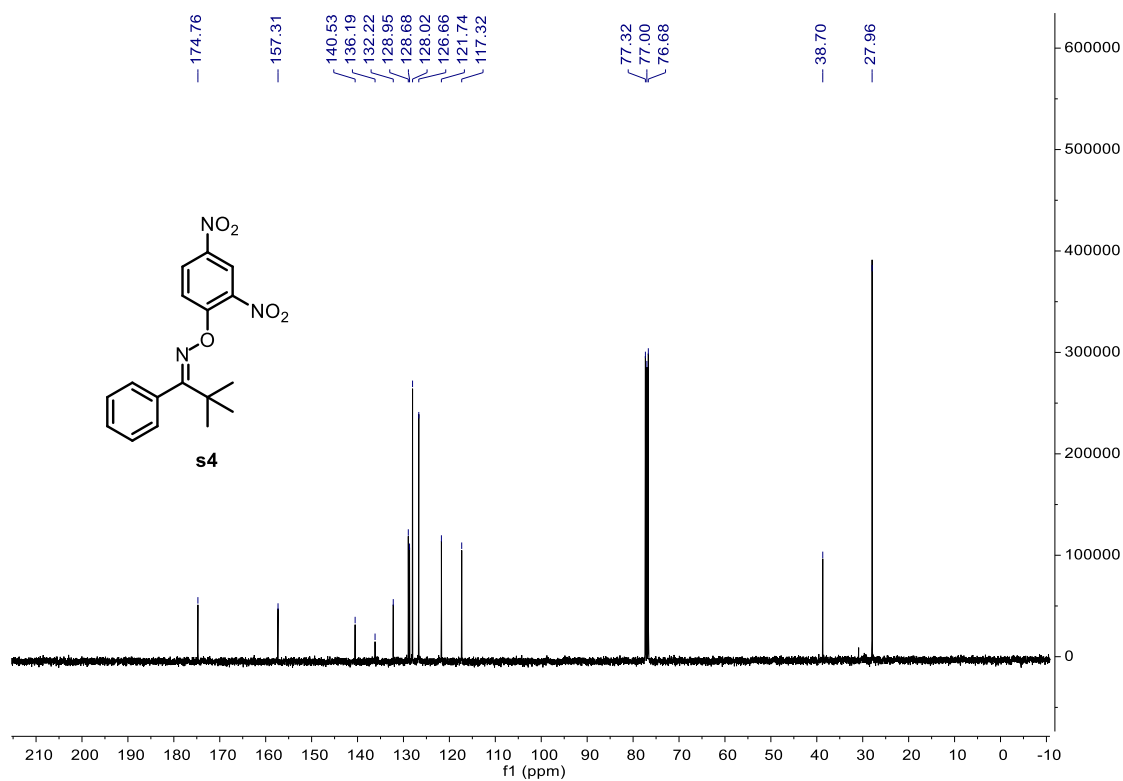


(*E*)-2,2-dimethyl-1-phenylpropan-1-one *O*-(2,4-dinitrophenyl) oxime (s4) (^1H NMR 400 MHz, CDCl_3)

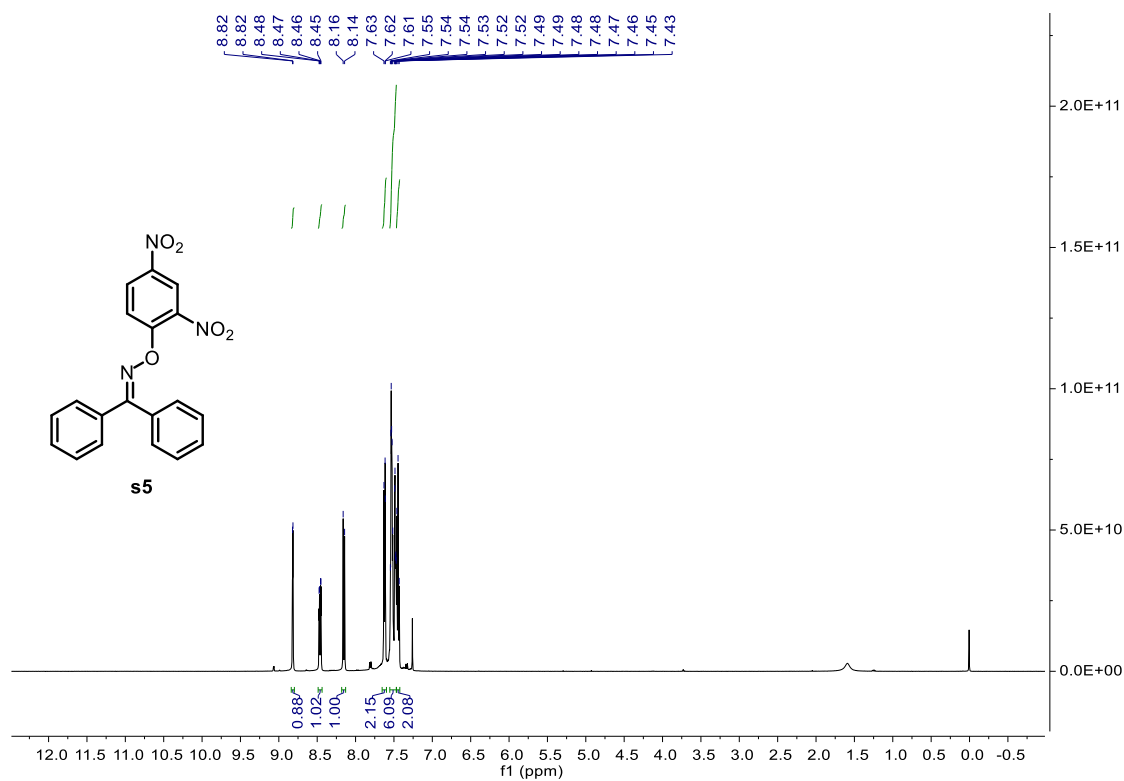


(*E*)-2,2-dimethyl-1-phenylpropan-1-one *O*-(2,4-dinitrophenyl) oxime (s4) (^{13}C NMR 101 MHz, CDCl_3)

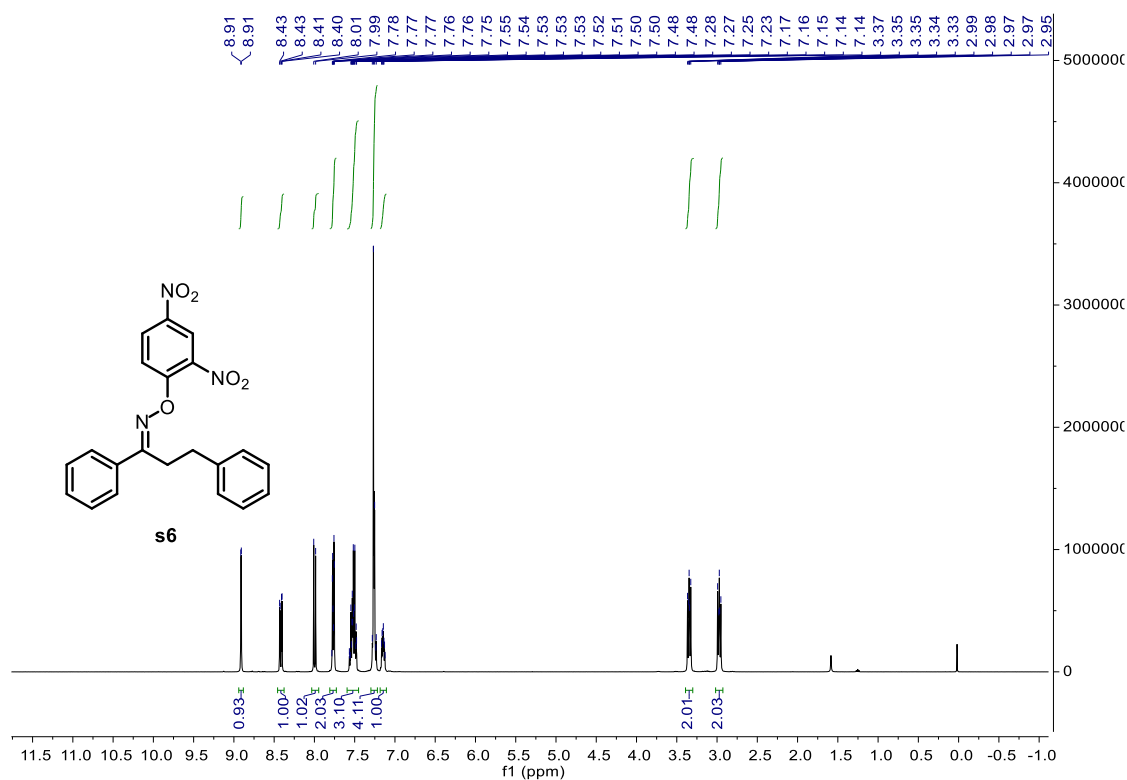
CDCl₃)



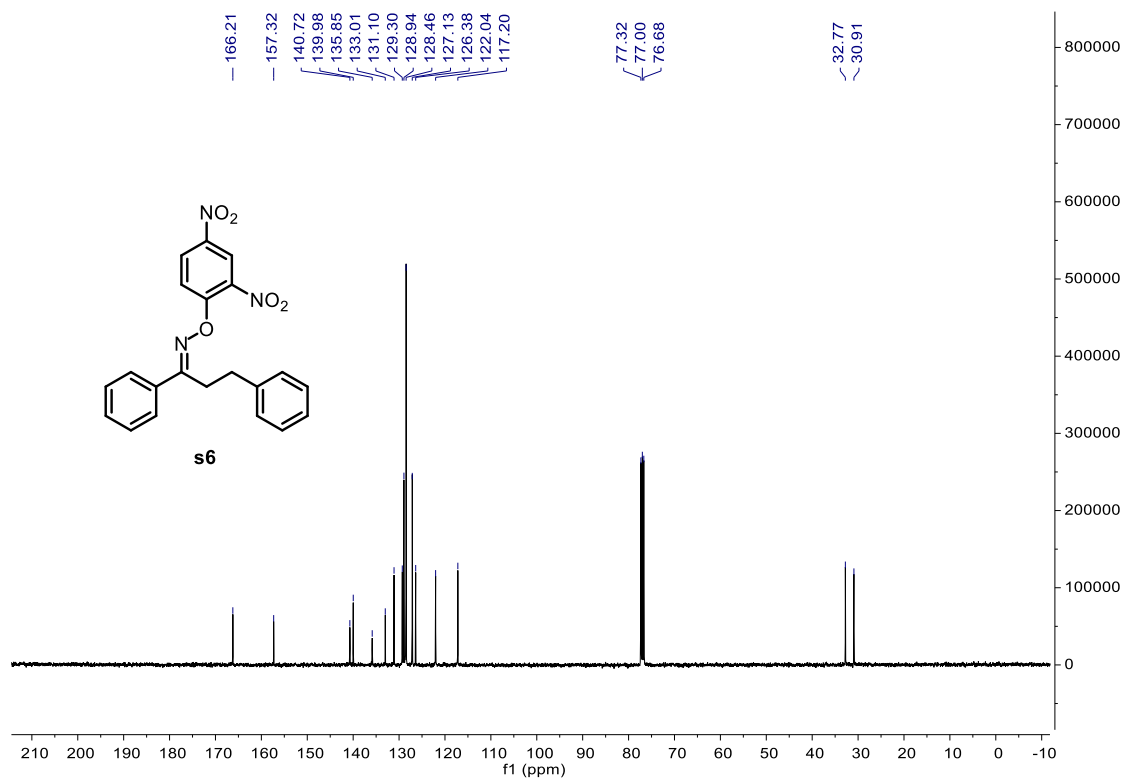
diphenylmethanone *O*-(2,4-dinitrophenyl) oxime (**s5**) (¹H NMR 500 MHz, CDCl₃)



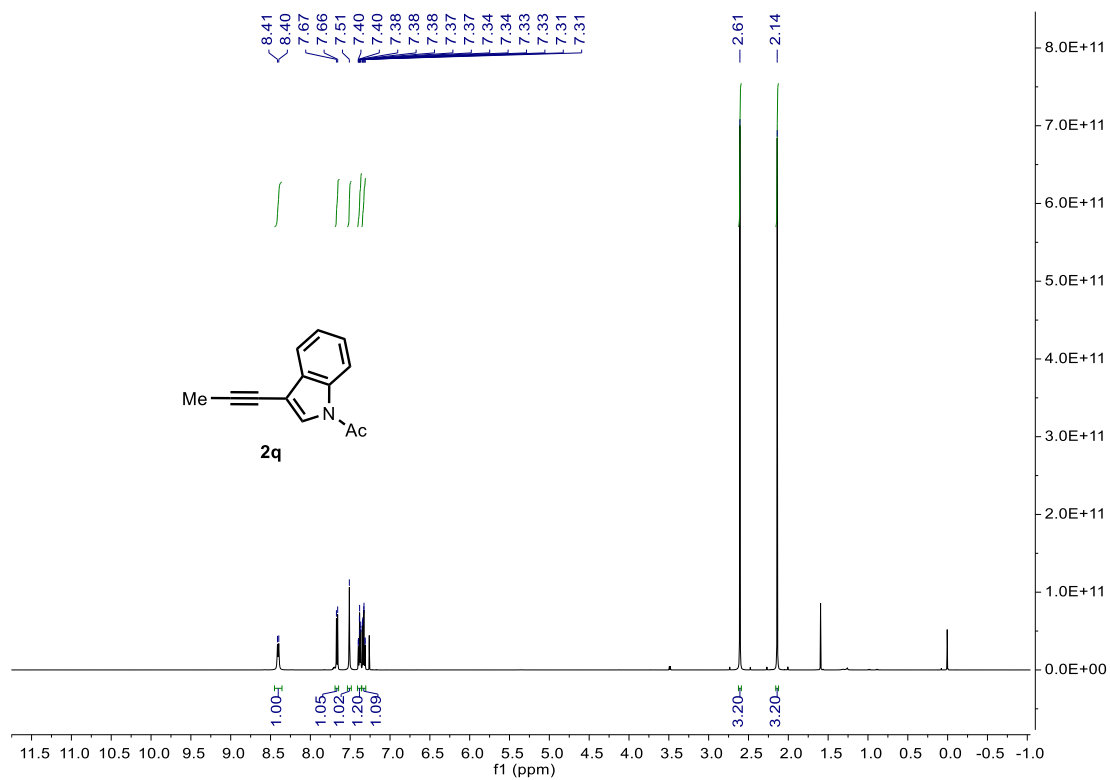
(*E*)-1,3-diphenylpropan-1-one *O*-(2,4-dinitrophenyl) oxime (**s6**) (¹H NMR 400 MHz, CDCl₃)



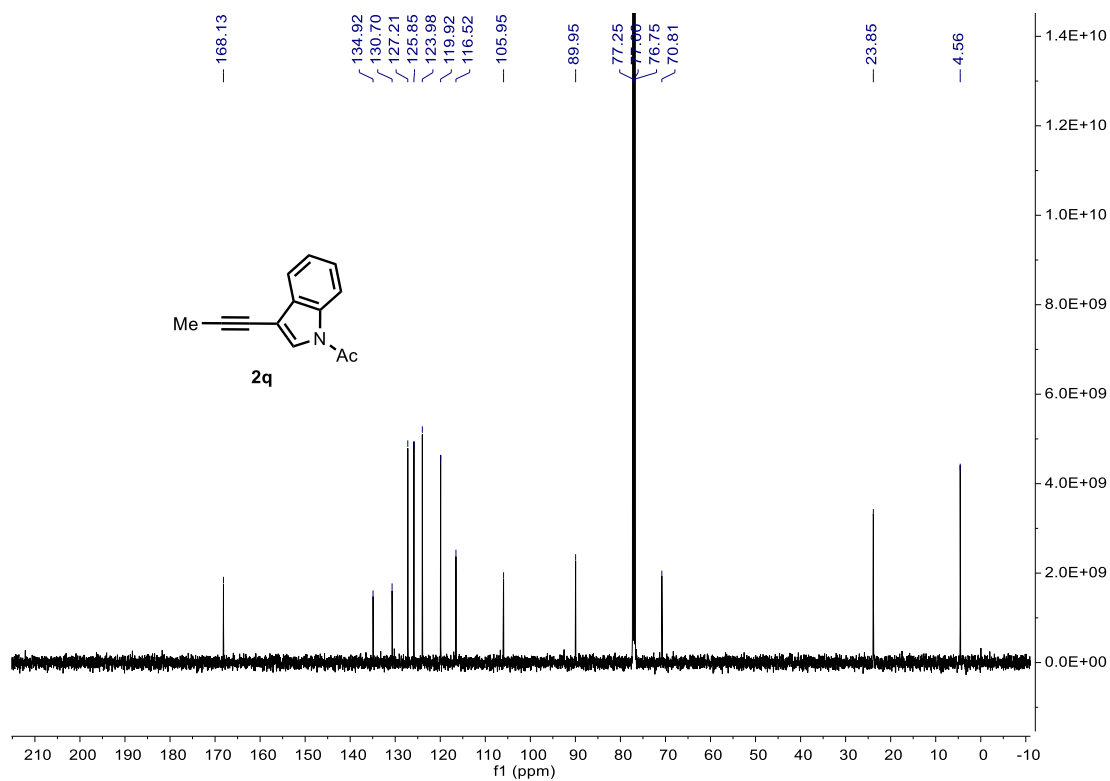
(*E*)-1,3-diphenylpropan-1-one *O*-(2,4-dinitrophenyl) oxime (s6) (¹³C NMR 101 MHz, CDCl₃)



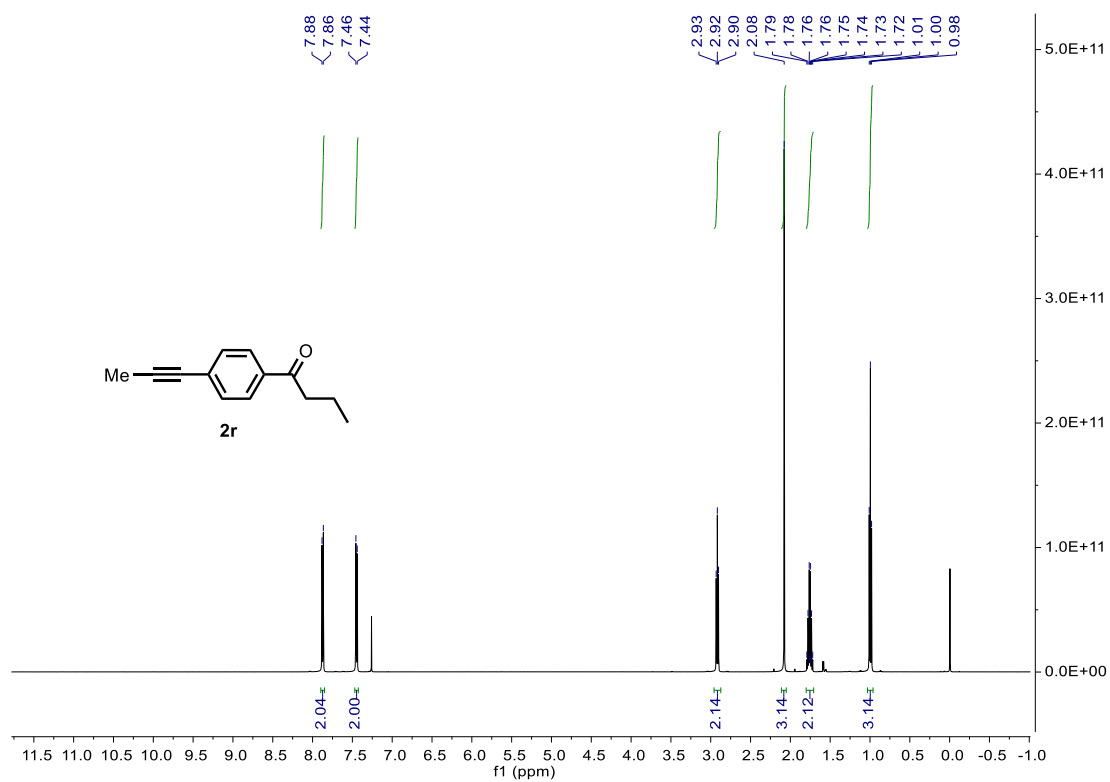
1-(3-(prop-1-yn-1-yl)-1H-indol-1-yl)ethan-1-one (2q) (¹H NMR 500 MHz, CDCl₃)



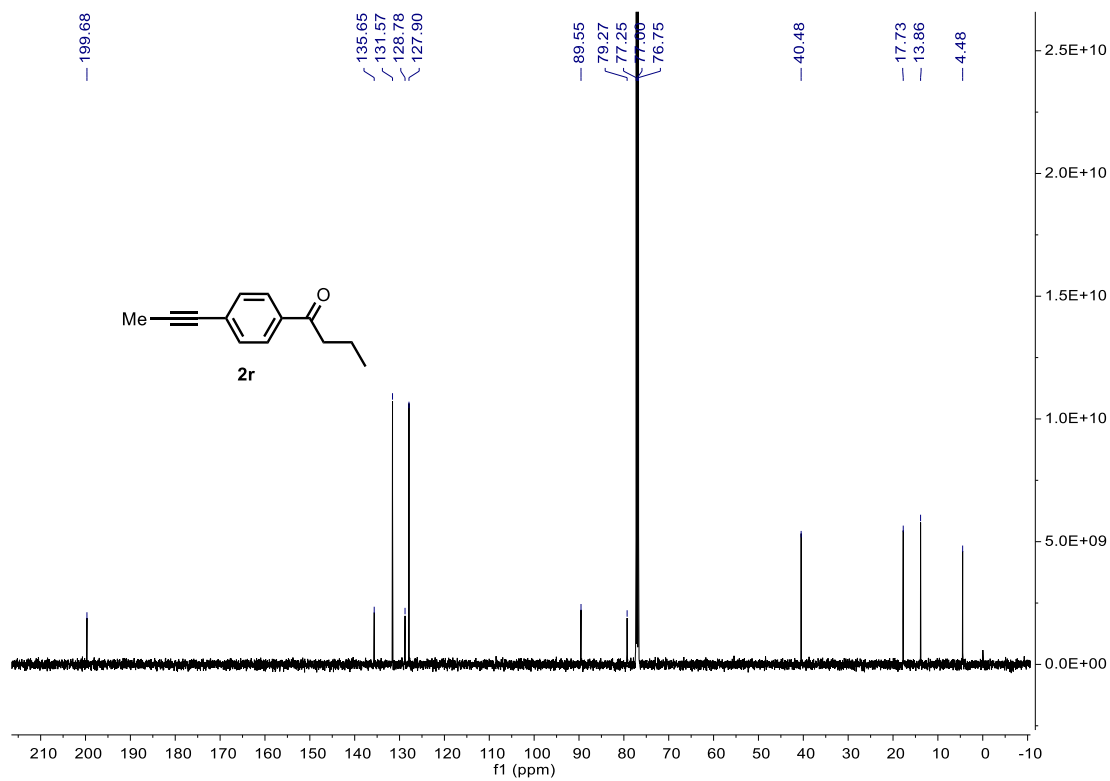
1-(3-(prop-1-yn-1-yl)-1H-indol-1-yl)ethan-1-one (2q) (¹³C NMR 126 MHz, CDCl₃)



1-(4-(prop-1-yn-1-yl)phenyl)butan-1-one (2r) (¹H NMR 500 MHz, CDCl₃)

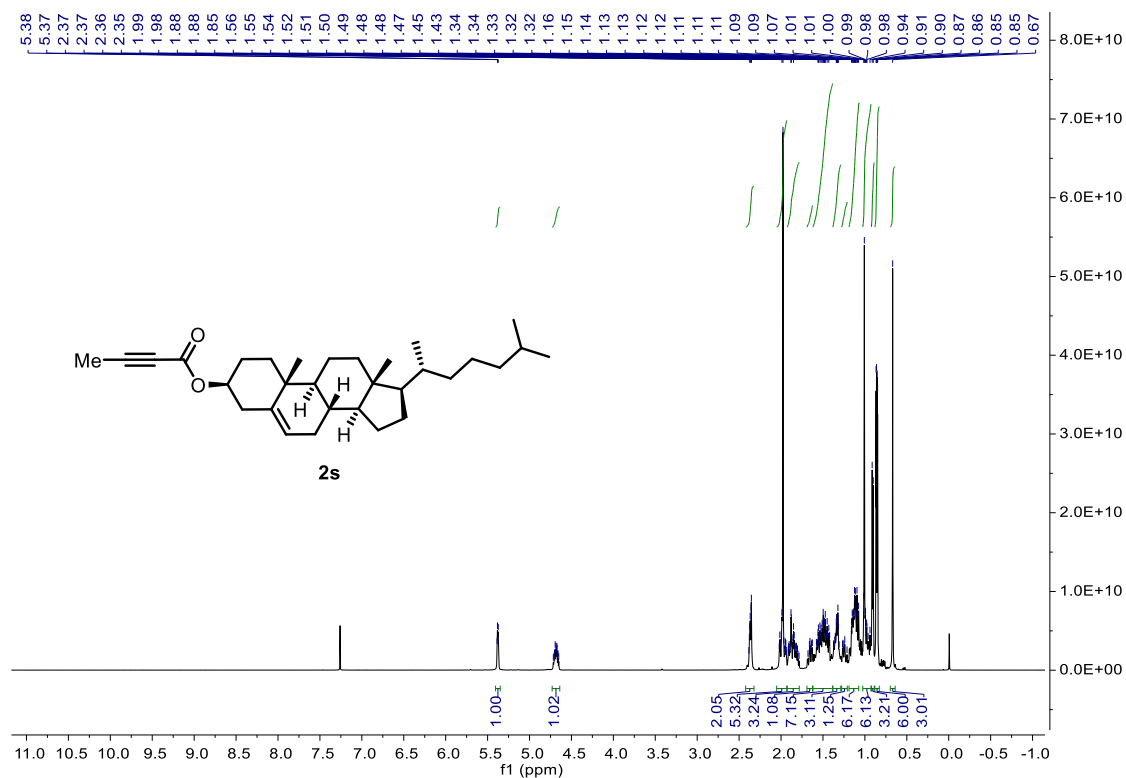


1-(4-(prop-1-yn-1-yl)phenyl)butan-1-one (2r) (¹³C NMR 126 MHz, CDCl₃)

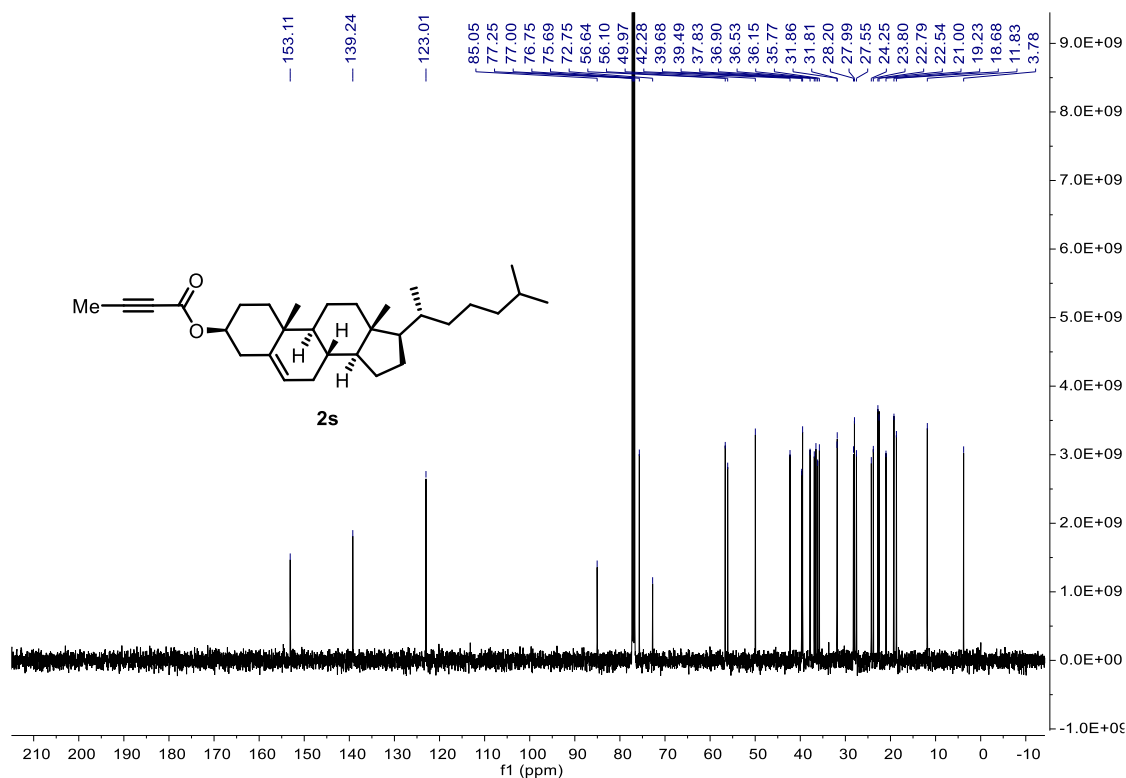


(3*S*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-10,13-dimethyl-17-((*R*)-6-methylheptan-2-yl)-

2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl but-2-ynoate (2s) (¹H NMR 500 MHz, CDCl₃)

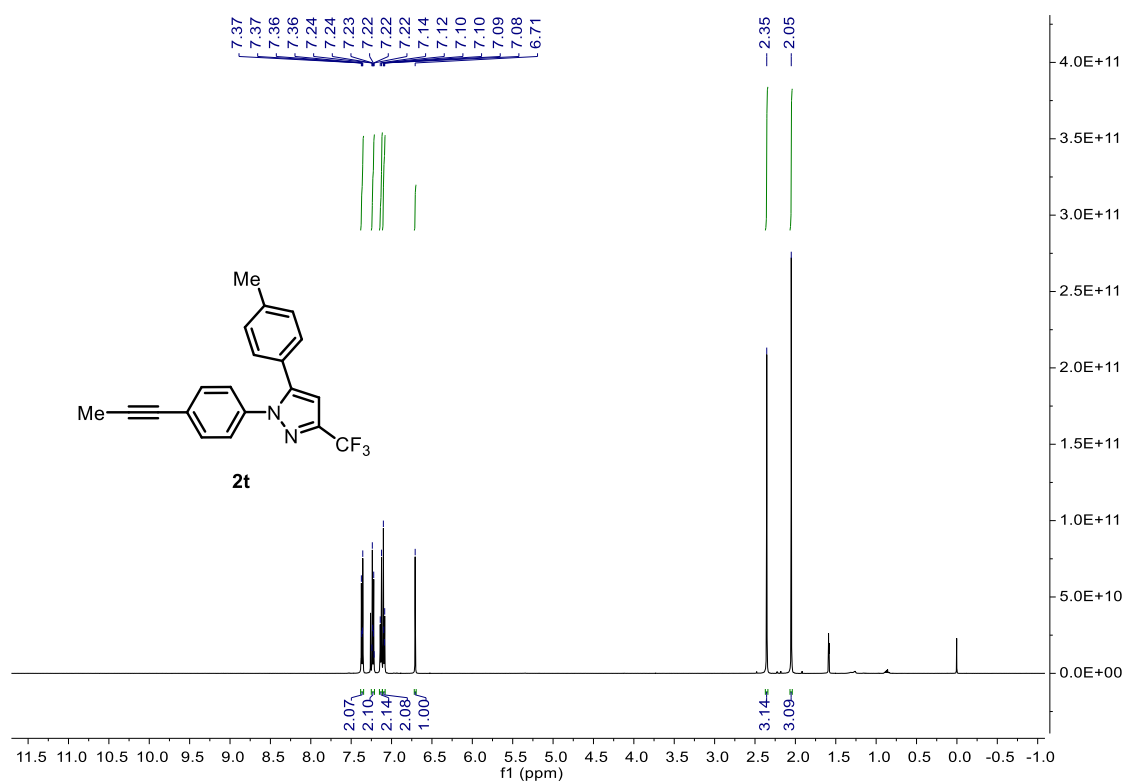


(3*S*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-10,13-dimethyl-17-((*R*)-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl but-2-ynoate (2s) (¹³C NMR 126 MHz, CDCl₃)

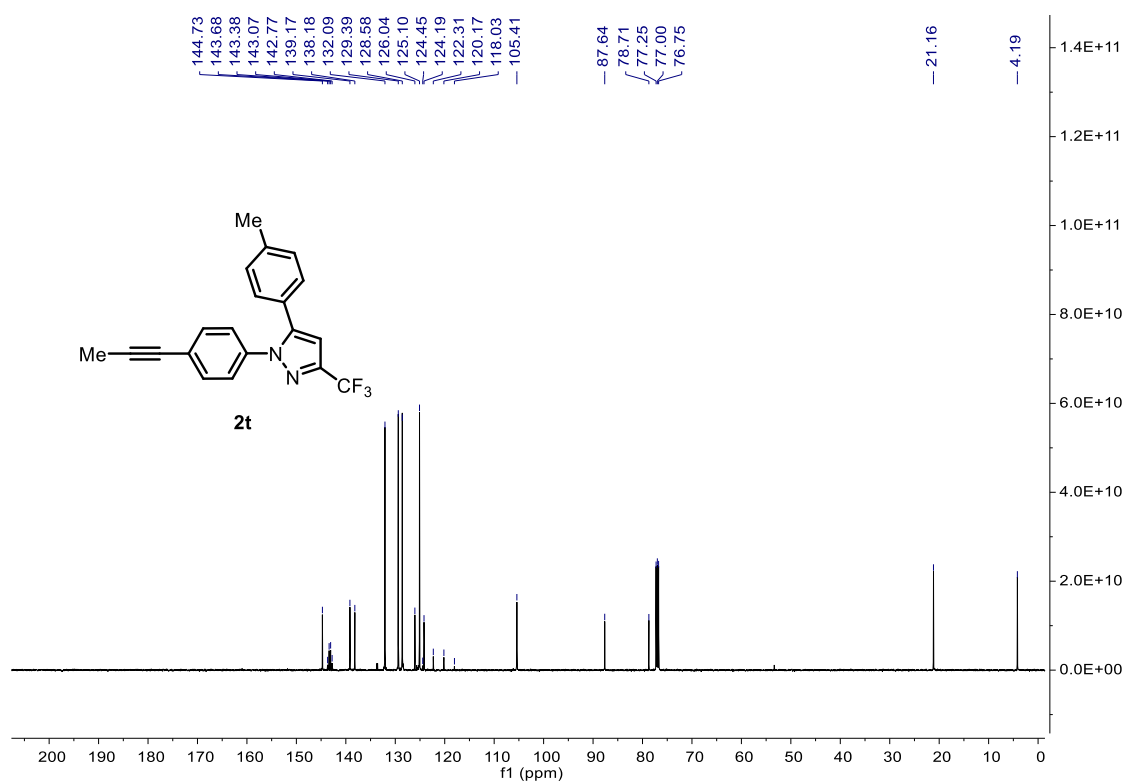


1-(4-(prop-1-yn-1-yl)phenyl)-5-(*p*-tolyl)-3-(trifluoromethyl)-1*H*-pyrazole (2t) (¹H NMR 500

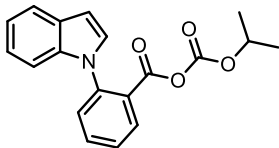
MHz, CDCl₃)



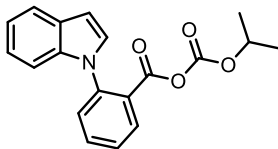
1-(4-(prop-1-yn-1-yl)phenyl)-5-(*p*-tolyl)-3-(trifluoromethyl)-1*H*-pyrazole (2t) (¹³C NMR 126 MHz, CDCl₃)



2-(1*H*-indol-1-yl)benzoic (isopropyl carbonic) anhydride (3c-1) (¹H NMR 400 MHz, CDCl₃)



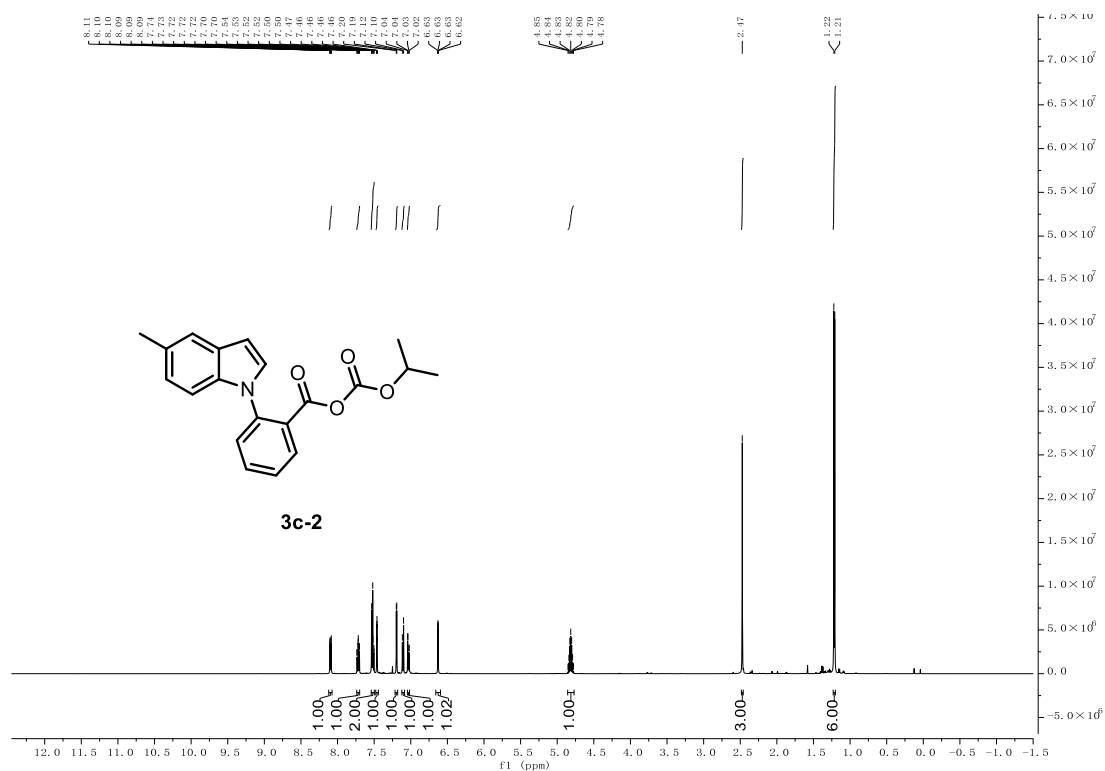
2-(1*H*-indol-1-yl)benzoic (isopropyl carbonic) anhydride (3c-1) (¹³C NMR 126 MHz, CDCl₃)



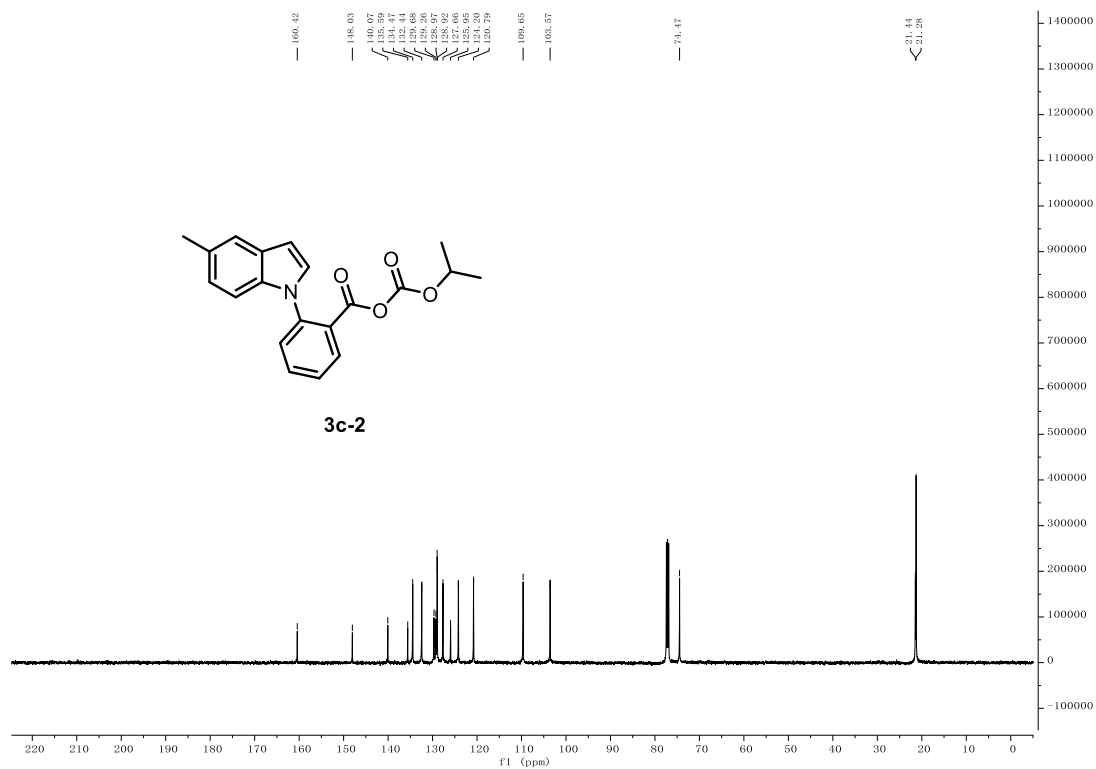
3c-1

S124

CDCl₃)



(isopropyl carbonic) 2-(5-methyl-1H-indol-1-yl)benzoic anhydride (3c-2) (¹³C NMR 126 MHz, CDCl₃)



2-(5-fluoro-1H-indol-1-yl)benzoic (isopropyl carbonic) anhydride (3c-3) (¹H NMR 500 MHz,

Chemical Structure of 3c-3:

CC(C)OC(=O)c1ccccc1C(=O)n2ccc(F)cc2

¹H NMR Spectrum Data (CDCl₃):

Chemical Shift (ppm)	Multiplicity	Integration
~1.2	broad singlet	6.00
~6.5 - 8.0	multiplets	~1.00 each
7.26	singlet (solvent)	-

3c-3

CC(C)OC(=O)C(=O)c1ccccc1C2=Cc3cc(F)ccc3N2

13C NMR spectrum (ppm): 160.12, 159.14, 157.27, 147.84, 138.43, 134.57, 133.85, 132.35, 130.47, 129.17, 128.90, 128.90, 128.92, 118.81, 118.60, 116.60, 116.59, 103.63, 103.69, 103.65, 71.90, 21.12.

S126

Chemical structure of **3c-4** is shown above the spectrum.

¹H NMR spectrum (CDCl₃) of compound **3c-4**. The x-axis represents the chemical shift (δ) in ppm, ranging from -1.0 to 12.0. The y-axis represents the intensity, with a scale from 0.0 to 5.0 × 10⁶.

Integration values are provided below the baseline:

- 1.00
- 1.00
- 1.00
- 1.01
- 4.05
- 0.99
- 0.98
- 6.01

Chemical shifts (δ) are listed at the top of the spectrum:

- 8.22, 8.20, 8.19, 8.18, 8.17, 8.16, 8.15, 8.14, 8.13, 8.12, 8.11, 8.10, 8.09, 8.08, 8.07, 8.06, 8.05, 8.04, 8.03, 8.02, 8.01, 7.99, 7.98, 7.97, 7.96, 7.95, 7.94, 7.93, 7.92, 7.91, 7.90, 7.89, 7.88, 7.87, 7.86, 7.85, 7.84, 7.83, 7.82, 7.81, 7.80, 7.79, 7.78, 7.77, 7.76, 7.75, 7.74, 7.73, 7.72, 7.71, 7.70, 7.69, 7.68, 7.67, 7.66, 7.65, 7.64, 7.63, 7.62, 7.61, 7.60, 7.59, 7.58, 7.57, 7.56, 7.55, 7.54, 7.53, 7.52, 7.51, 7.50, 7.49, 7.48, 7.47, 7.46, 7.45, 7.44, 7.43, 7.42, 7.41, 7.40, 7.39, 7.38, 7.37, 7.36, 7.35, 7.34, 7.33, 7.32, 7.31, 7.30, 7.29, 7.28, 7.27, 7.26, 7.25, 7.24, 7.23, 7.22, 7.21, 7.20, 7.19, 7.18, 7.17, 7.16, 7.15, 7.14, 7.13, 7.12, 7.11, 7.10, 7.09, 7.08, 7.07, 7.06, 7.05, 7.04, 7.03, 7.02, 7.01, 7.00, 6.99, 6.98, 6.97, 6.96, 6.95, 6.94, 6.93, 6.92, 6.91, 6.90, 6.89, 6.88, 6.87, 6.86, 6.85, 6.84, 6.83, 6.82, 6.81, 6.80, 6.79, 6.78, 6.77, 6.76, 6.75, 6.74, 6.73, 6.72, 6.71, 6.70, 6.69, 6.68, 6.67, 6.66, 6.65, 6.64, 6.63, 6.62, 6.61, 6.60, 6.59, 6.58, 6.57, 6.56, 6.55, 6.54, 6.53, 6.52, 6.51, 6.50, 6.49, 6.48, 6.47, 6.46, 6.45, 6.44, 6.43, 6.42, 6.41, 6.40, 6.39, 6.38, 6.37, 6.36, 6.35, 6.34, 6.33, 6.32, 6.31, 6.30, 6.29, 6.28, 6.27, 6.26, 6.25, 6.24, 6.23, 6.22, 6.21, 6.20, 6.19, 6.18, 6.17, 6.16, 6.15, 6.14, 6.13, 6.12, 6.11, 6.10, 6.09, 6.08, 6.07, 6.06, 6.05, 6.04, 6.03, 6.02, 6.01, 6.00, 5.99, 5.98, 5.97, 5.96, 5.95, 5.94, 5.93, 5.92, 5.91, 5.90, 5.89, 5.88, 5.87, 5.86, 5.85, 5.84, 5.83, 5.82, 5.81, 5.80, 5.79, 5.78, 5.77, 5.76, 5.75, 5.74, 5.73, 5.72, 5.71, 5.70, 5.69, 5.68, 5.67, 5.66, 5.65, 5.64, 5.63, 5.62, 5.61, 5.60, 5.59, 5.58, 5.57, 5.56, 5.55, 5.54, 5.53, 5.52, 5.51, 5.50, 5.49, 5.48, 5.47, 5.46, 5.45, 5.44, 5.43, 5.42, 5.41, 5.40, 5.39, 5.38, 5.37, 5.36, 5.35, 5.34, 5.33, 5.32, 5.31, 5.30, 5.29, 5.28, 5.27, 5.26, 5.25, 5.24, 5.23, 5.22, 5.21, 5.20, 5.19, 5.18, 5.17, 5.16, 5.15, 5.14, 5.13, 5.12, 5.11, 5.10, 5.09, 5.08, 5.07, 5.06, 5.05, 5.04, 5.03, 5.02, 5.01, 5.00, 4.99, 4.98, 4.97, 4.96, 4.95, 4.94, 4.93, 4.92, 4.91, 4.90, 4.89, 4.88, 4.87, 4.86, 4.85, 4.84, 4.83, 4.82, 4.81, 4.80, 4.79, 4.78, 4.77, 4.76, 4.75, 4.74, 4.73, 4.72, 4.71, 4.70, 4.69, 4.68, 4.67.

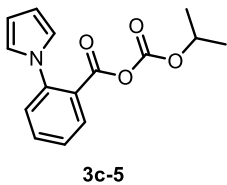
3c-4

Chemical structure of **3c-4** (1-(4-(trifluoromethyl)phenyl)-1H-indole-3-carboxylic acid isopropyl ester) is shown above the spectrum.

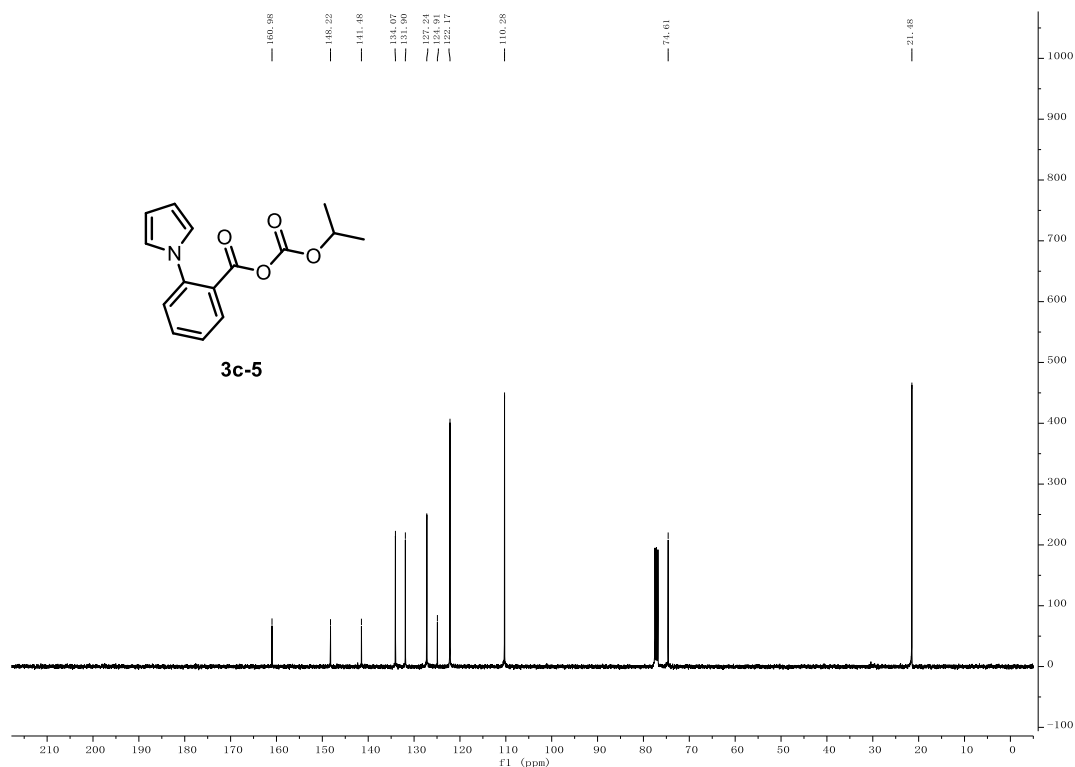
¹H NMR spectrum (CDCl₃) of **3c-4**. The x-axis represents the chemical shift in ppm (f1), ranging from 220 to 0. The y-axis represents intensity, ranging from -50,000 to 750,000. The spectrum shows several peaks, with the following chemical shifts (ppm) labeled above the peaks:

- 159.72
- 147.46
- 146.30
- 145.62
- 138.42
- 138.16
- 138.16
- 138.62
- 138.62
- 138.09
- 129.19
- 128.61
- 128.61
- 128.85
- 128.85
- 125.53
- 125.53
- 124.36
- 124.36
- 124.03
- 124.03
- 121.86
- 121.86
- 121.36
- 121.36
- 118.69
- 109.65
- 108.67
- 75.01
- 21.35

S127

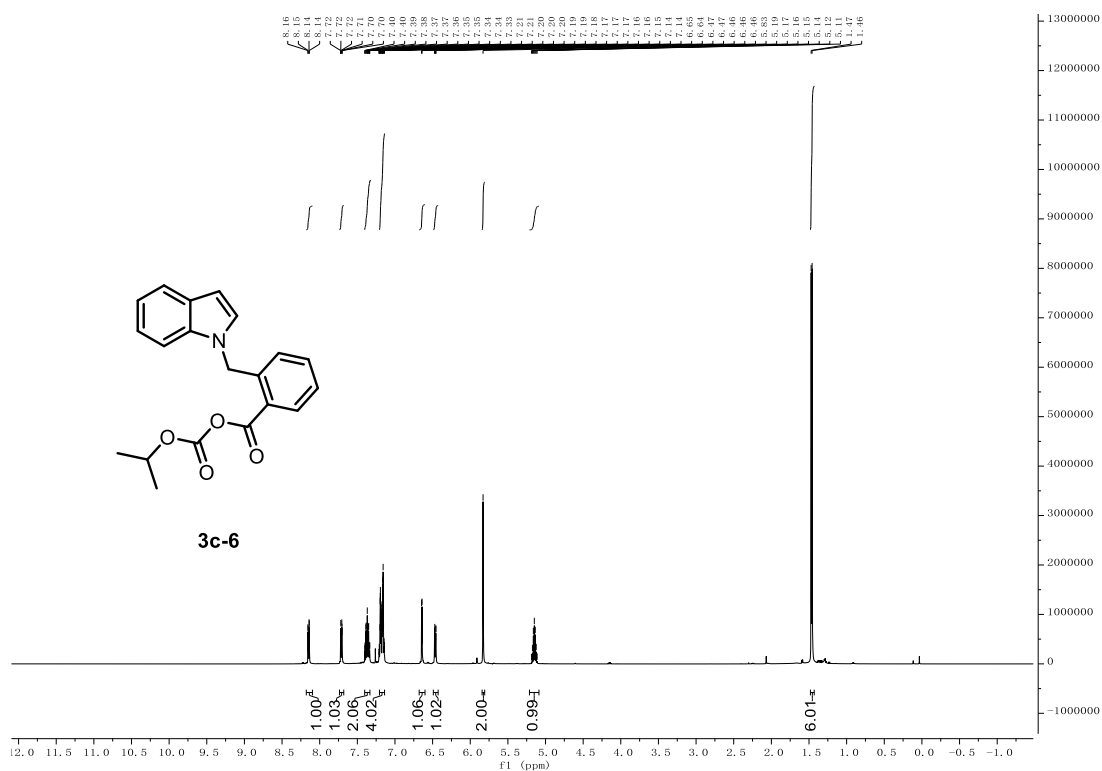


3c-5

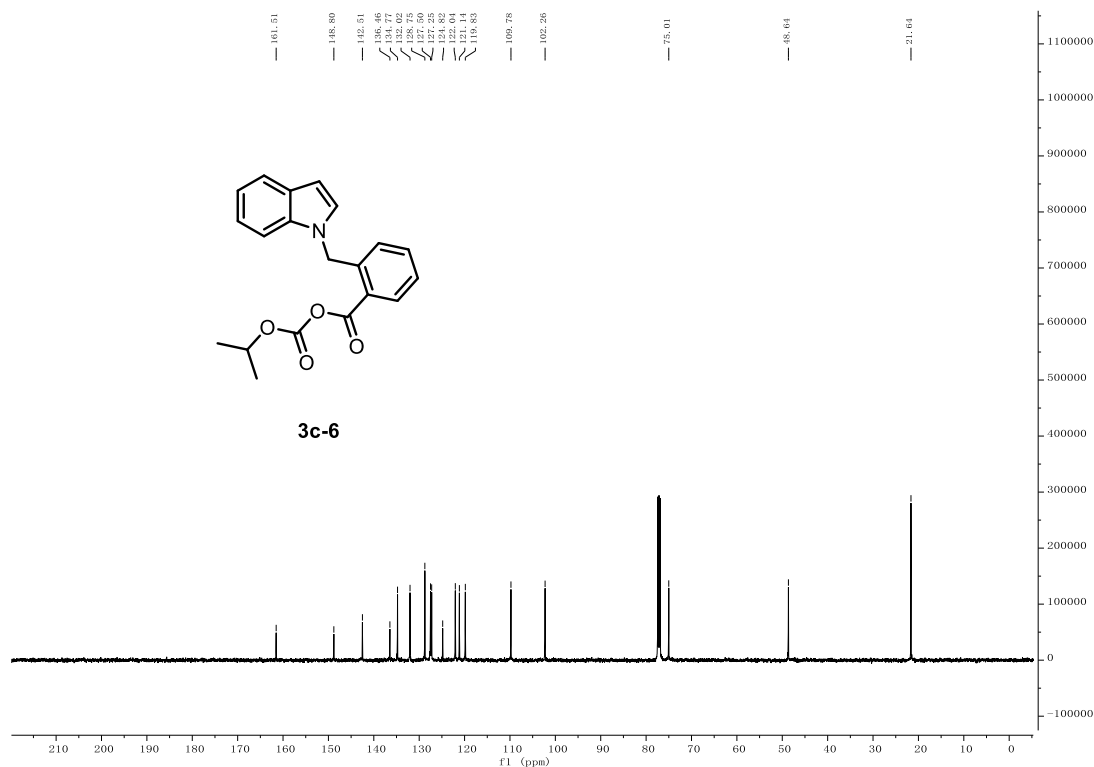


2-((1*H*-indol-1-yl)methyl)benzoic (isopropyl carbonic) anhydride (3c-6) (¹H NMR 500 MHz,

CDCl₃)

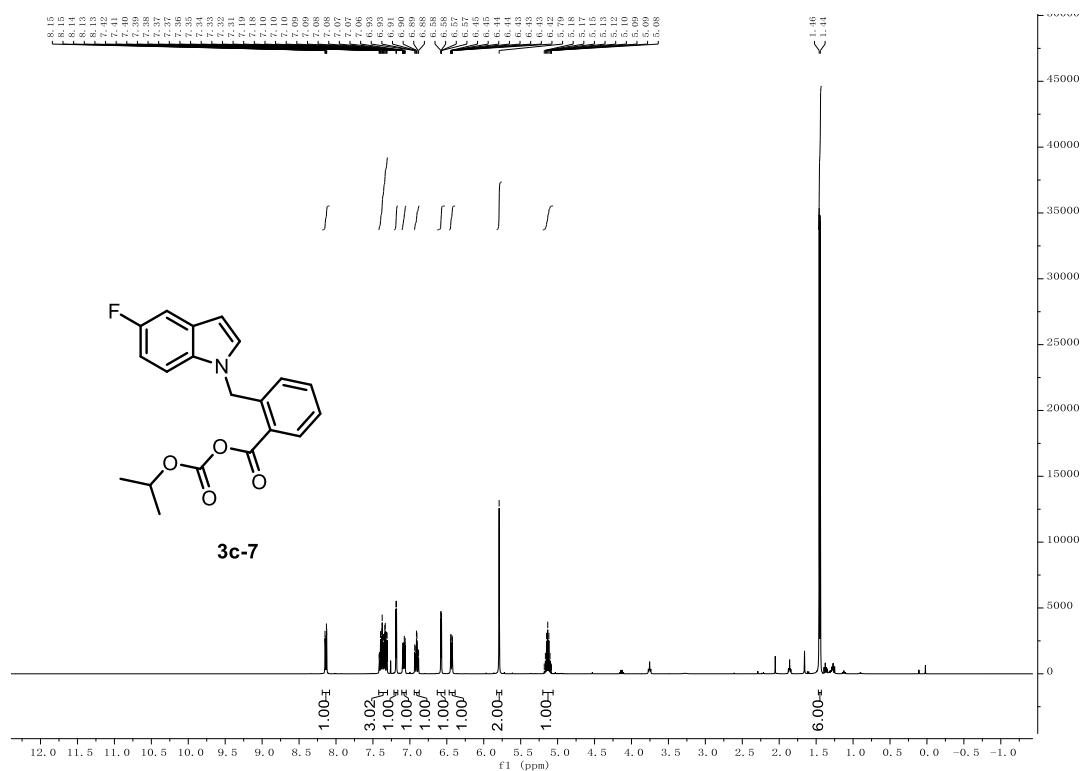


2-((1H-indol-1-yl)methyl)benzoic (isopropyl carbonic) anhydride (3c-6) (¹³C NMR 126 MHz, CDCl₃)

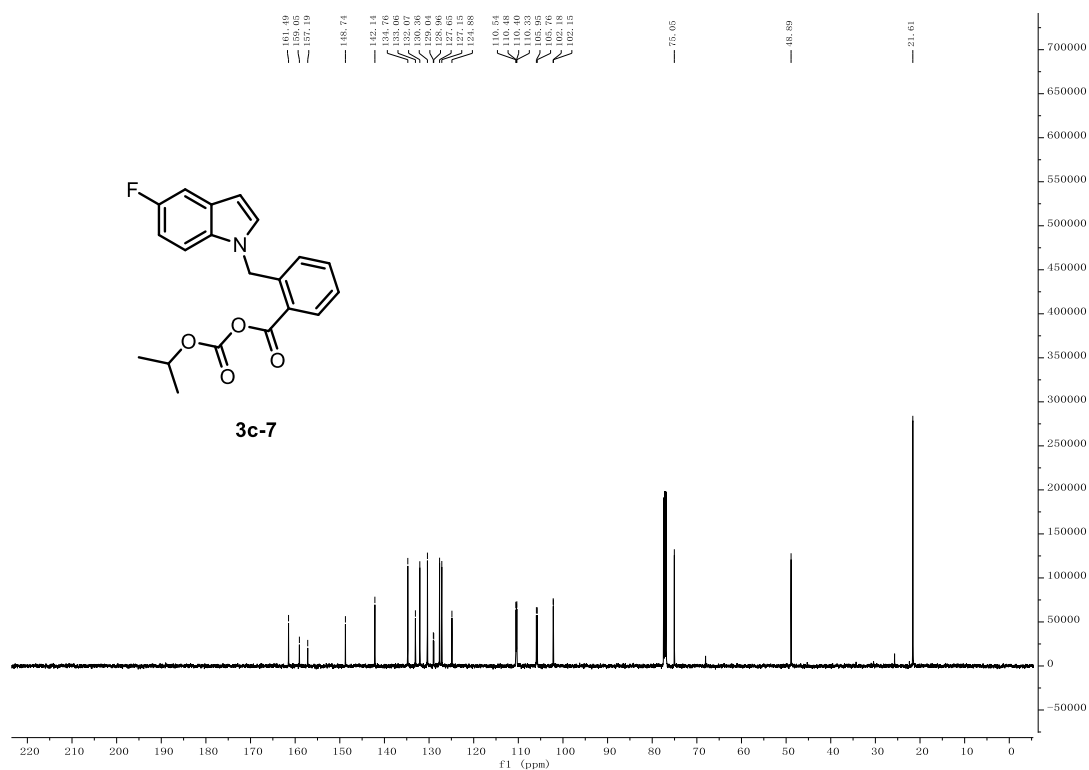


2-((5-fluoro-1H-indol-1-yl)methyl)benzoic (isopropyl carbonic) anhydride (3c-7) (¹H NMR

400 MHz, CDCl₃)

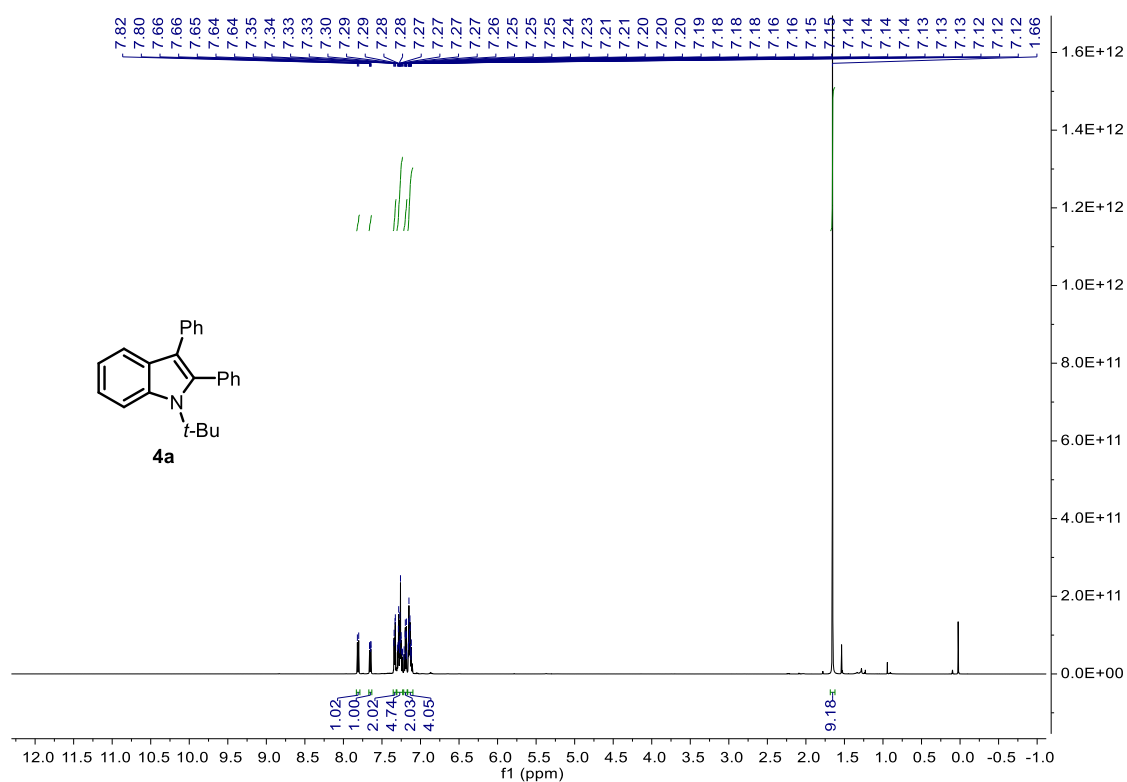


2-((5-fluoro-1H-indol-1-yl)methyl)benzoic (isopropyl carbonic) anhydride (**3c-7**) (¹³C NMR 126 MHz, CDCl₃)

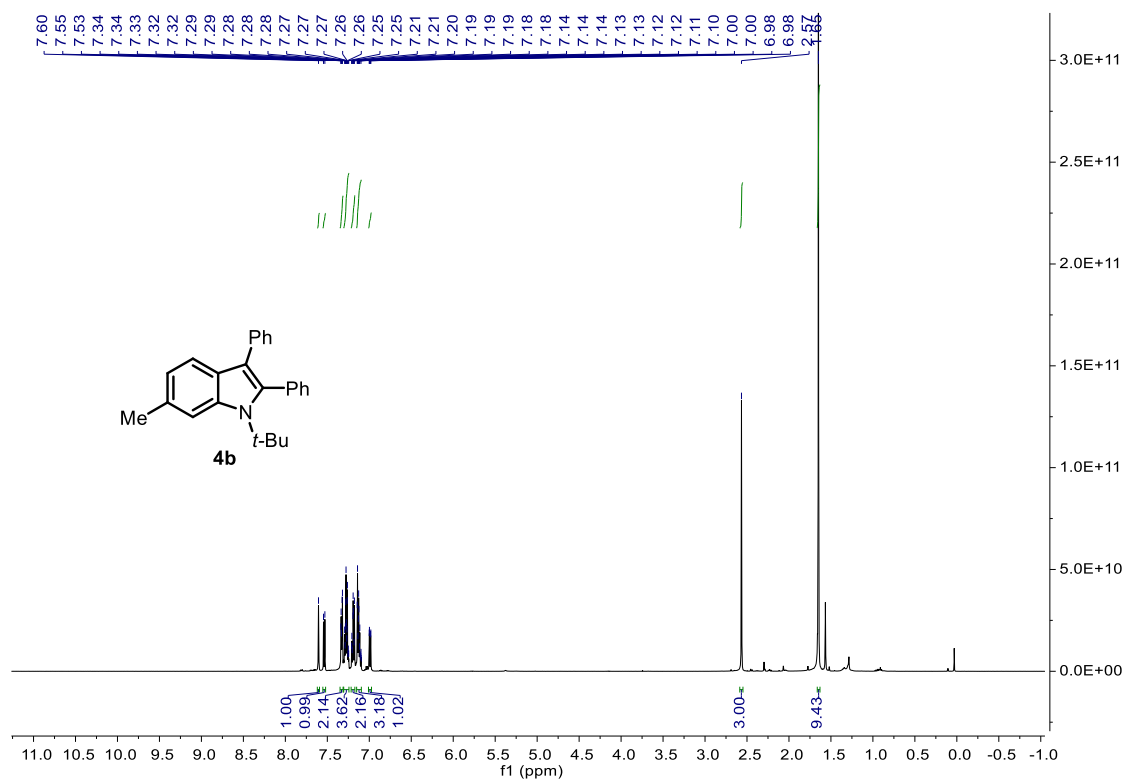


5.2 NMR Spectra for Product

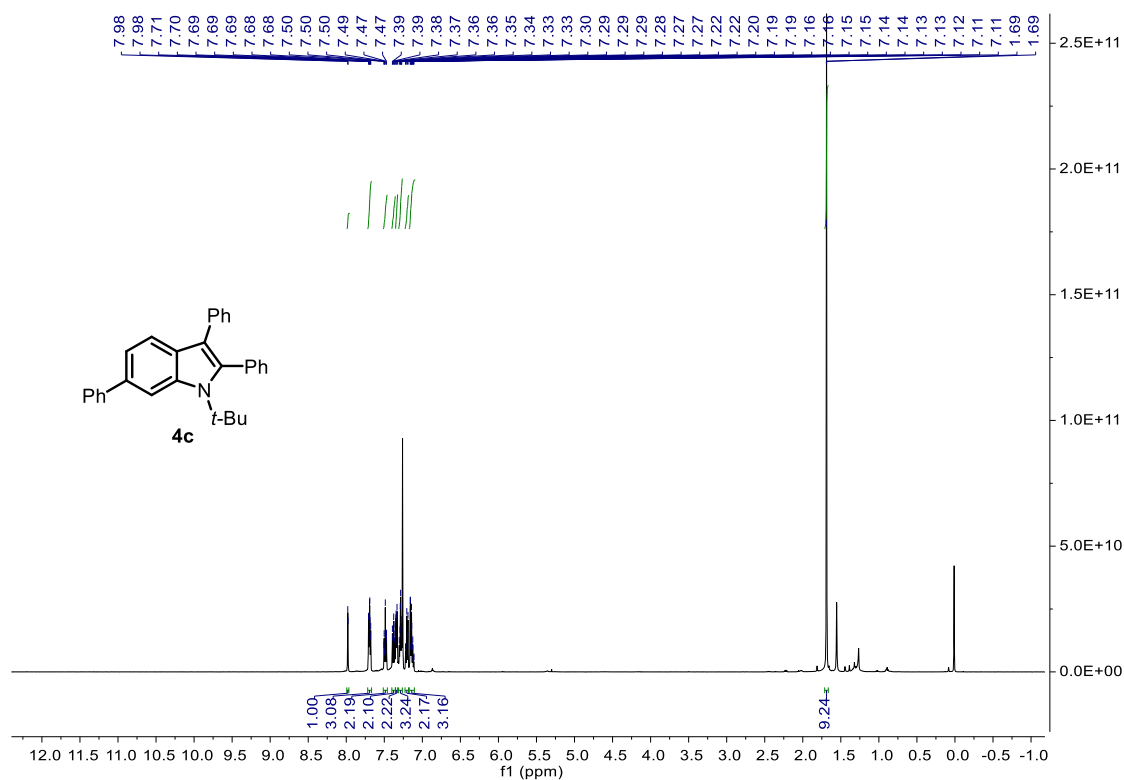
1-(*tert*-butyl)-2,3-diphenyl-1H-indole (**4a**) (¹H NMR 500 MHz, CDCl₃)



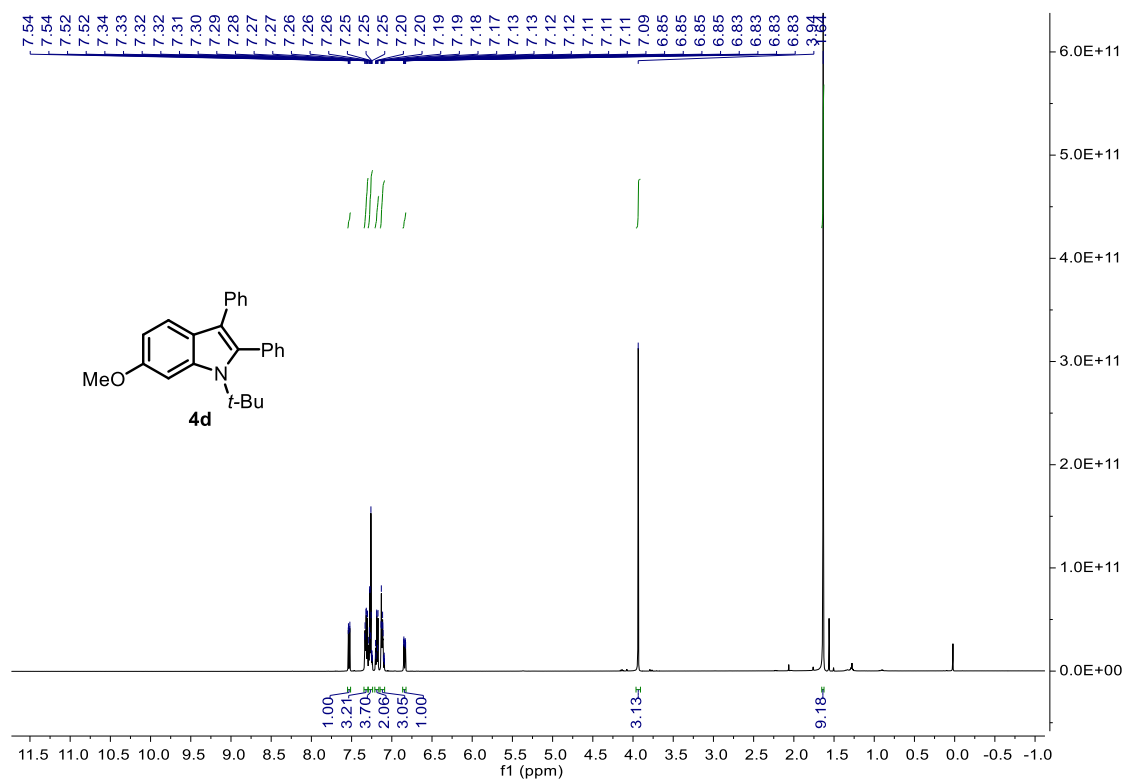
1-(tert-butyl)-6-methyl-2,3-diphenyl-1H-indole (4b) (¹H NMR 500 MHz, CDCl₃)



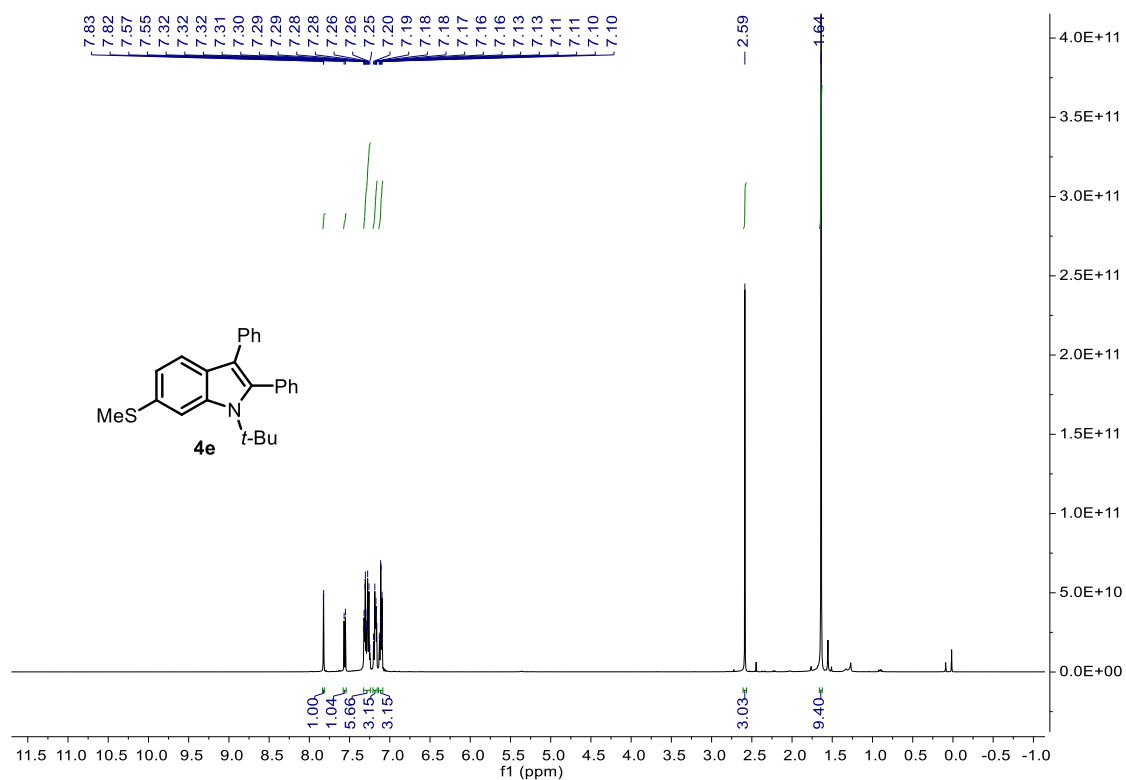
1-(tert-butyl)-2,3,6-triphenyl-1H-indole (4c) (¹H NMR 500 MHz, CDCl₃)



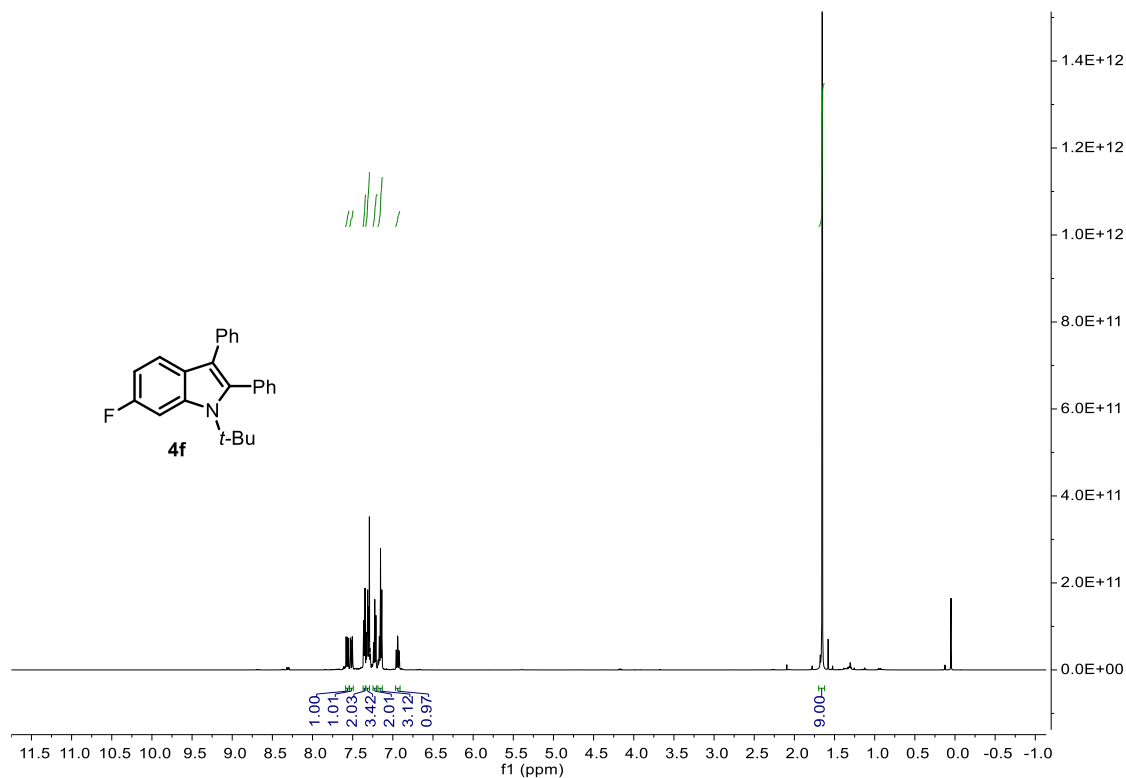
1-(*tert*-butyl)-6-methoxy-2,3-diphenyl-1*H*-indole (4d) (¹H NMR 500 MHz, CDCl₃)



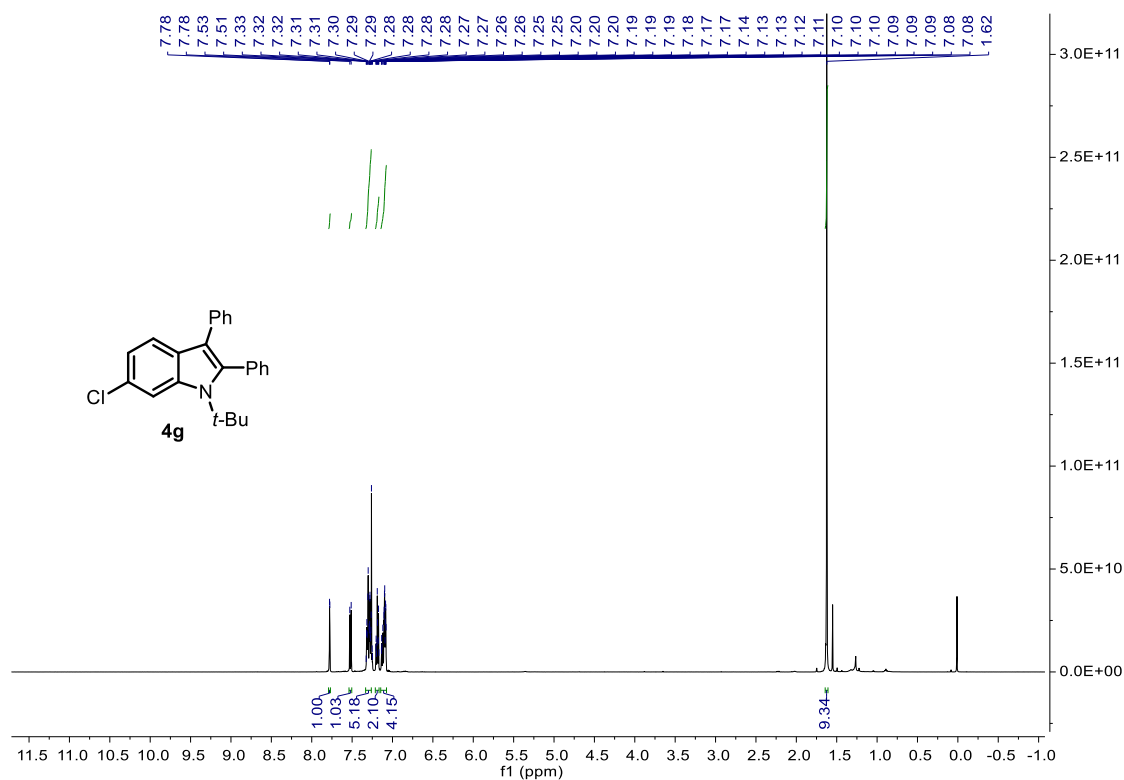
1-(*tert*-butyl)-6-(methylthio)-2,3-diphenyl-1*H*-indole (4e) (¹H NMR 500 MHz, CDCl₃)



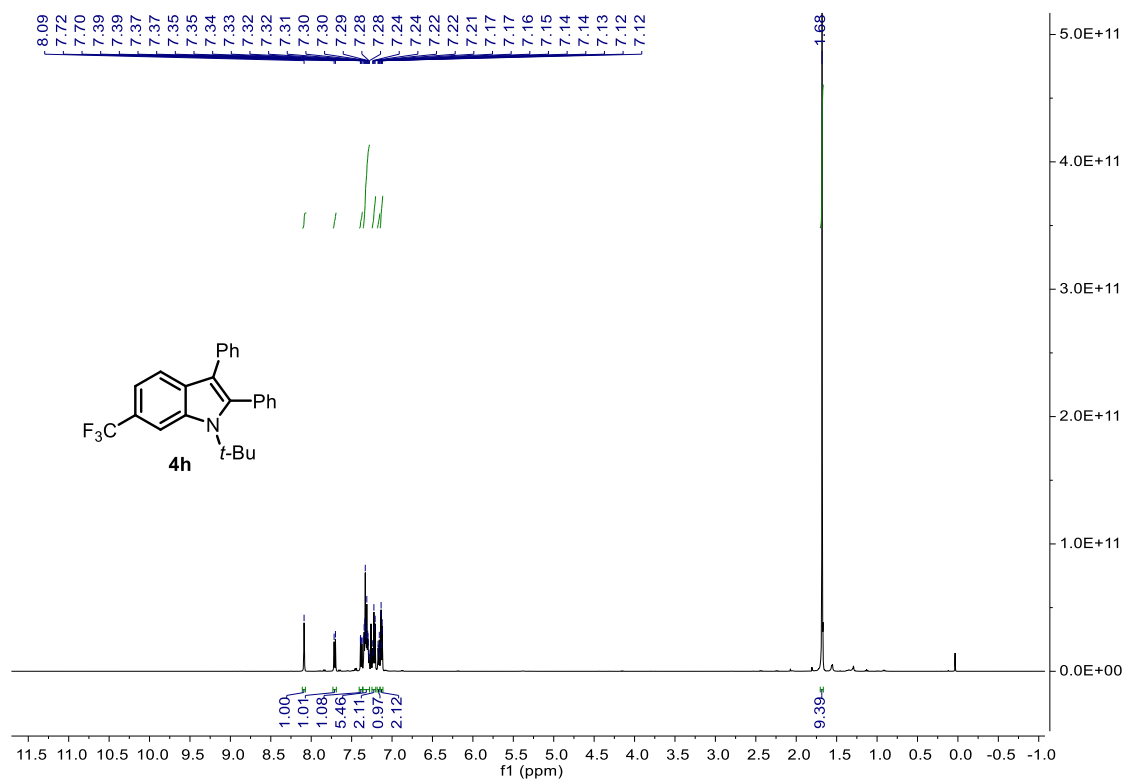
1-(*tert*-butyl)-6-fluoro-2,3-diphenyl-1*H*-indole (4f) (¹H NMR 500 MHz, CDCl₃)



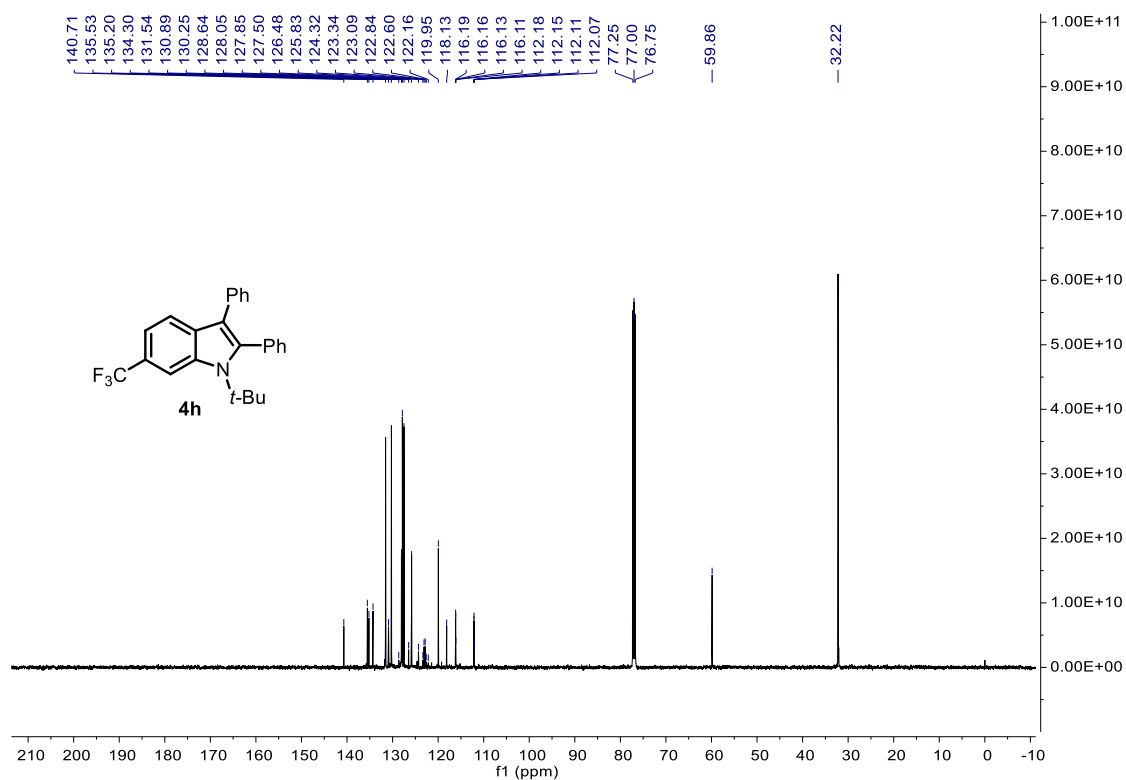
1-(*tert*-butyl)-6-chloro-2,3-diphenyl-1*H*-indole (4g) (¹H NMR 500 MHz, CDCl₃)



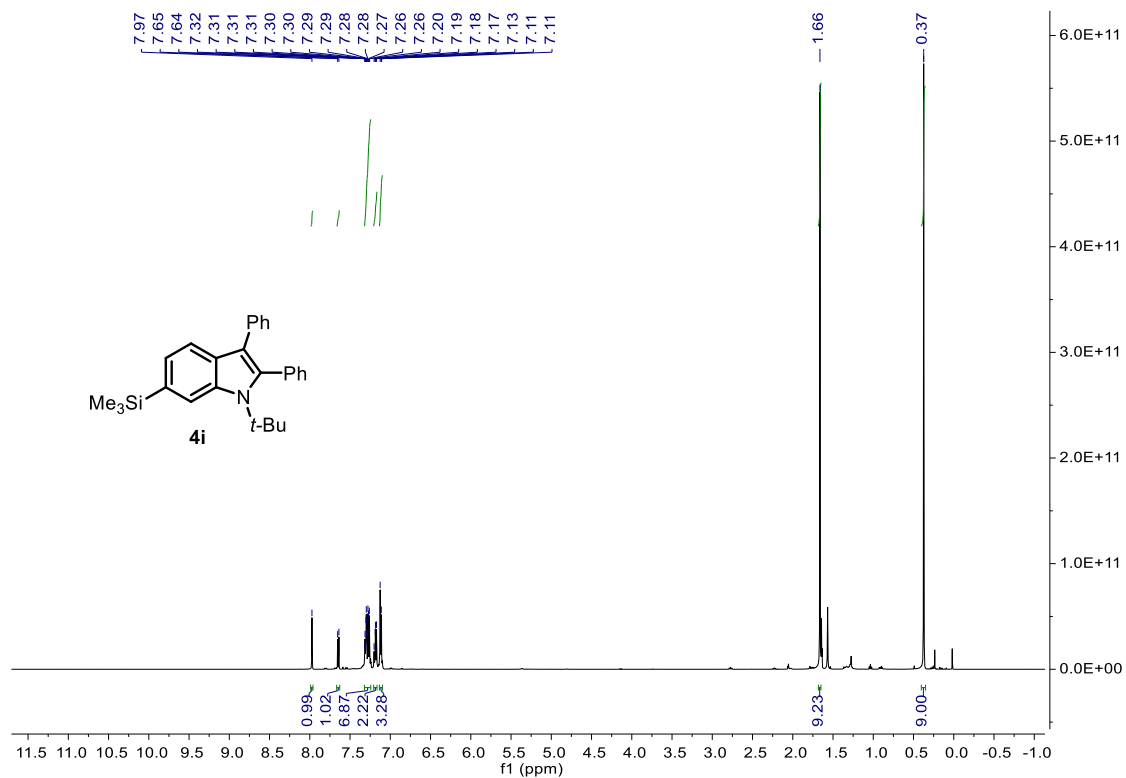
1-(tert-butyl)-2,3-diphenyl-6-(trifluoromethyl)-1H-indole (4h) (¹H NMR 500 MHz, CDCl₃)



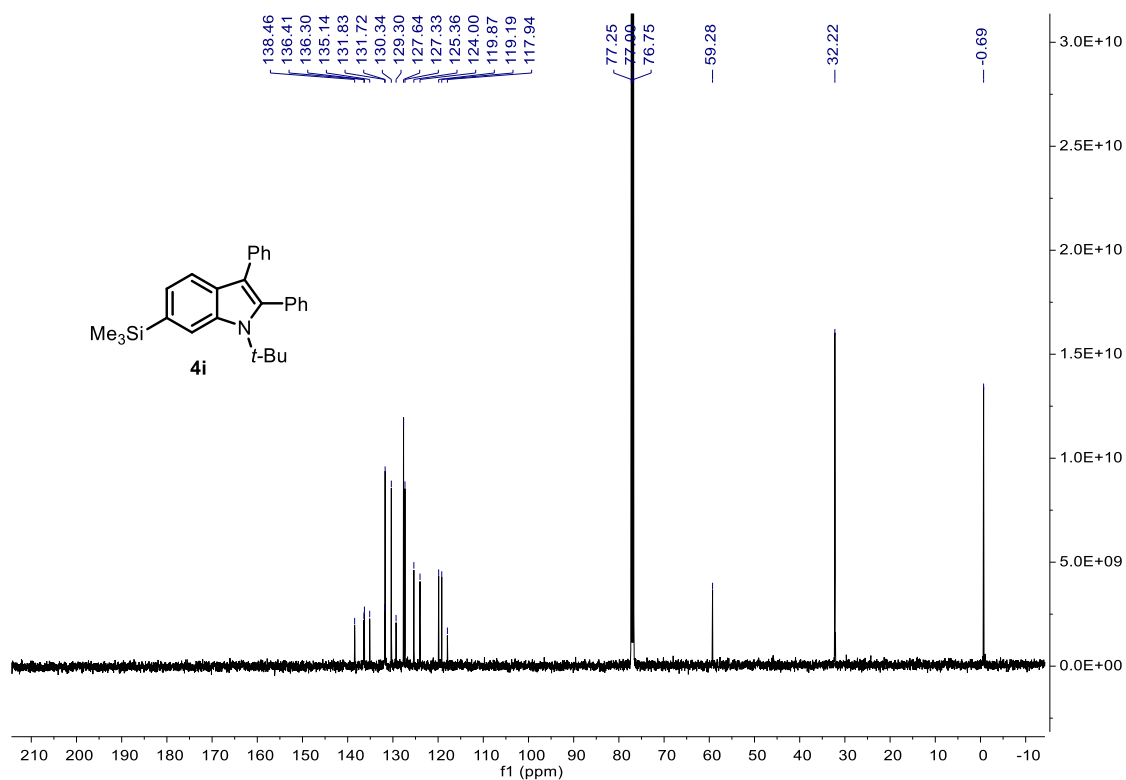
1-(tert-butyl)-2,3-diphenyl-6-(trifluoromethyl)-1H-indole (4i) (¹³C NMR 126 MHz, CDCl₃)



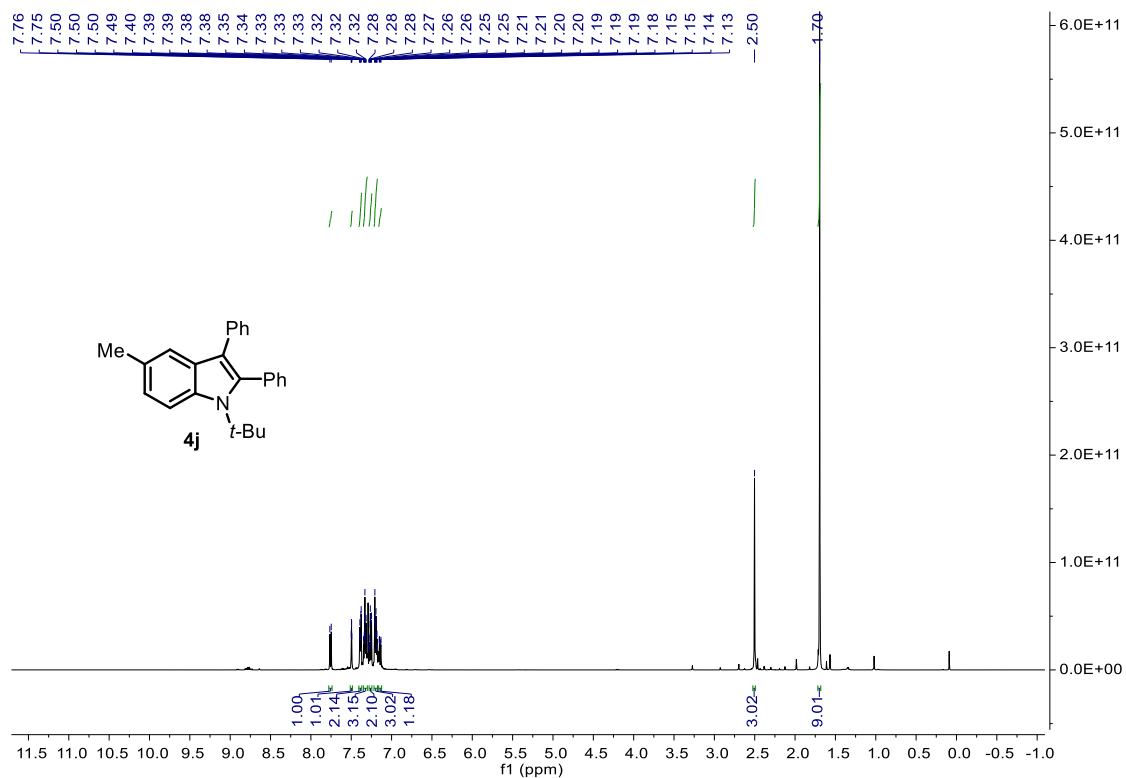
1-(*tert*-butyl)-2,3-diphenyl-6-(trimethylsilyl)-1*H*-indole (4i) (¹H NMR 500 MHz, CDCl₃)



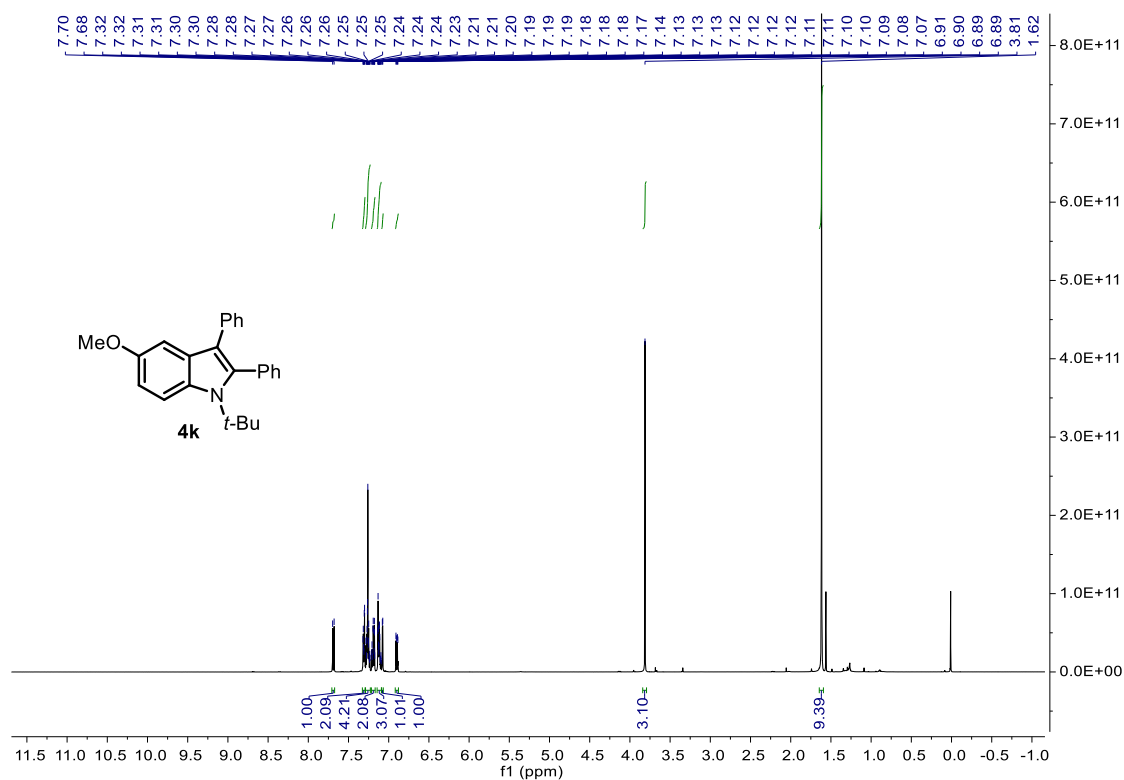
1-(*tert*-butyl)-2,3-diphenyl-6-(trimethylsilyl)-1*H*-indole (4f) (¹³C NMR 126 MHz, CDCl₃)



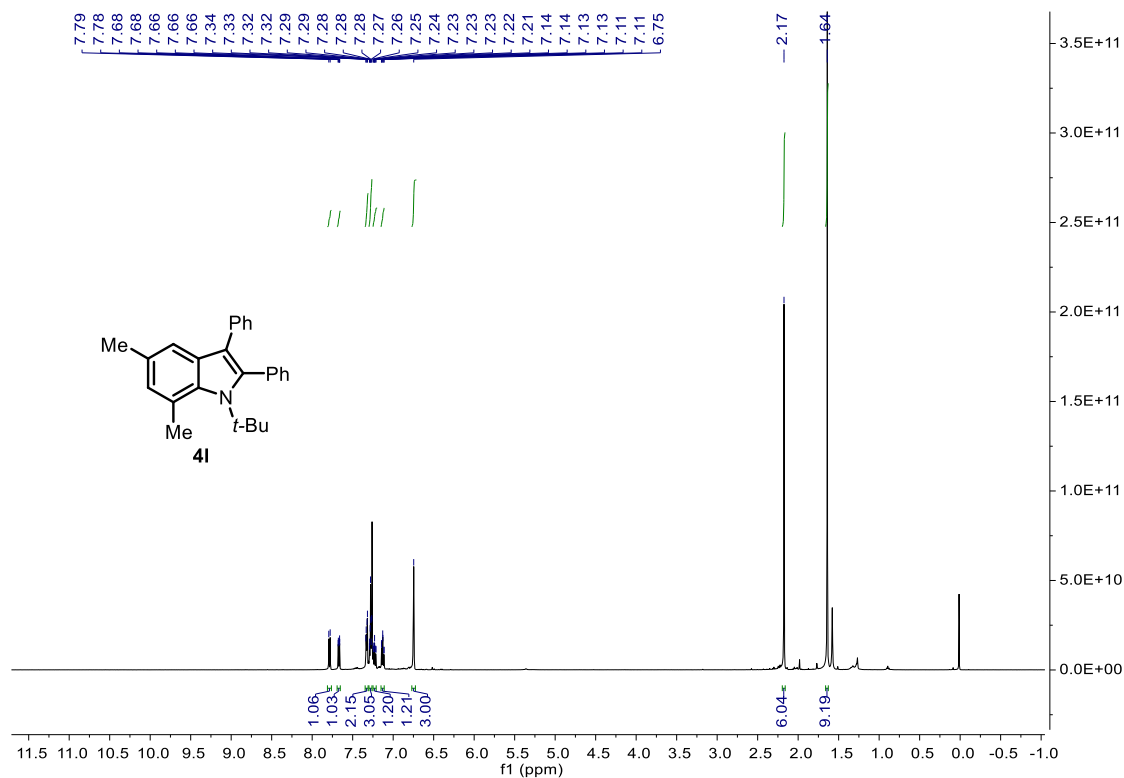
1-(tert-butyl)-5-methyl-2,3-diphenyl-1H-indole (4j) (¹H NMR 500 MHz, CDCl₃)



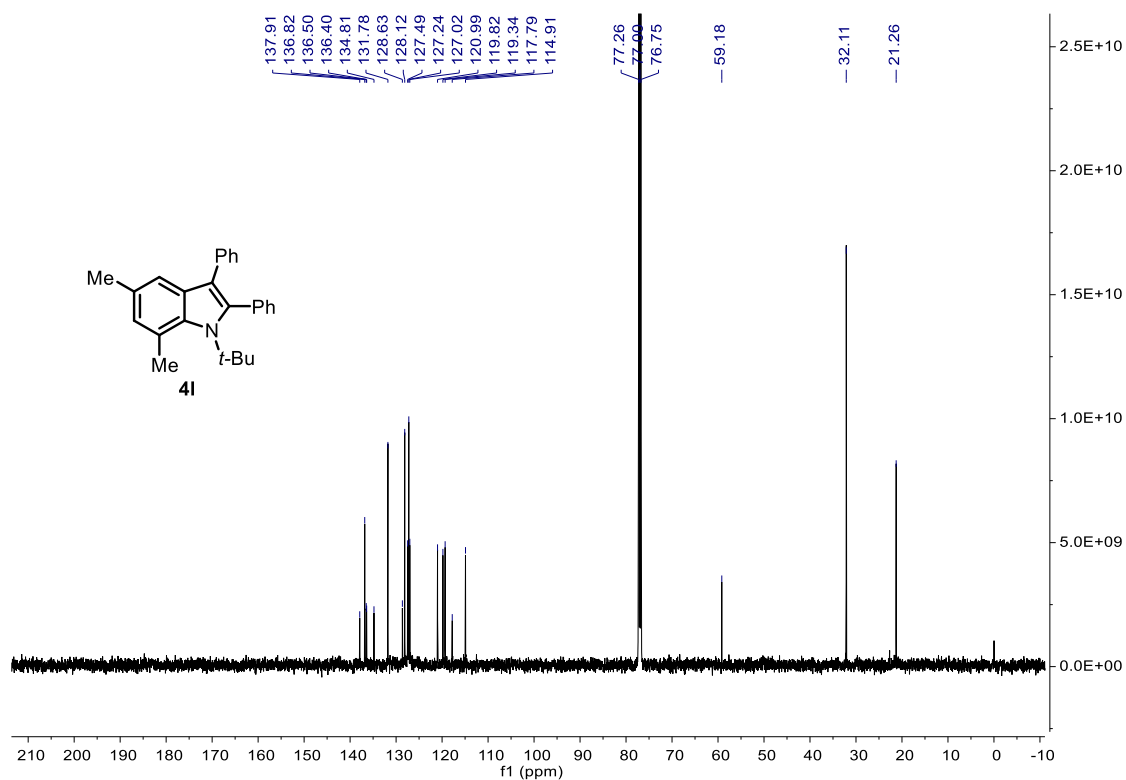
1-(tert-butyl)-5-methoxy-2,3-diphenyl-1H-indole (4k) (¹H NMR 500 MHz, CDCl₃)



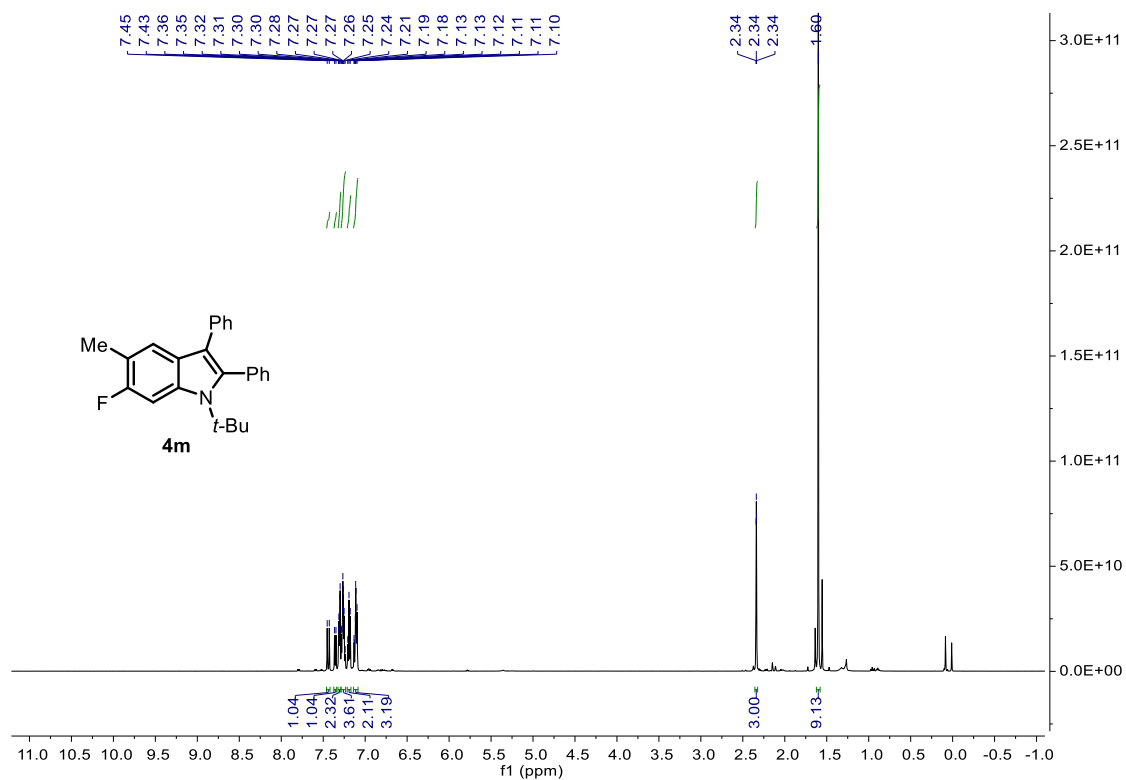
1-(tert-butyl)-5,7-dimethyl-2,3-diphenyl-1H-indole (4l) (¹H NMR 500 MHz, CDCl₃)



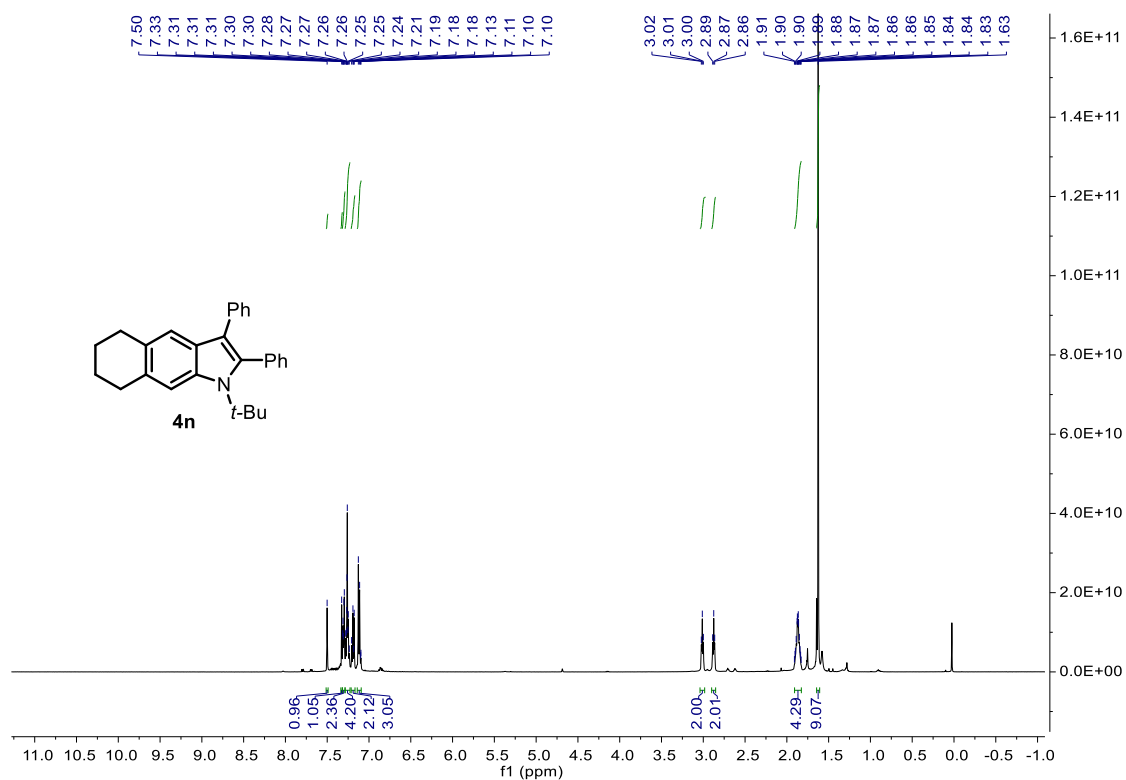
1-(tert-butyl)-5,7-dimethyl-2,3-diphenyl-1H-indole (4l) (¹³C NMR 126 MHz, CDCl₃)



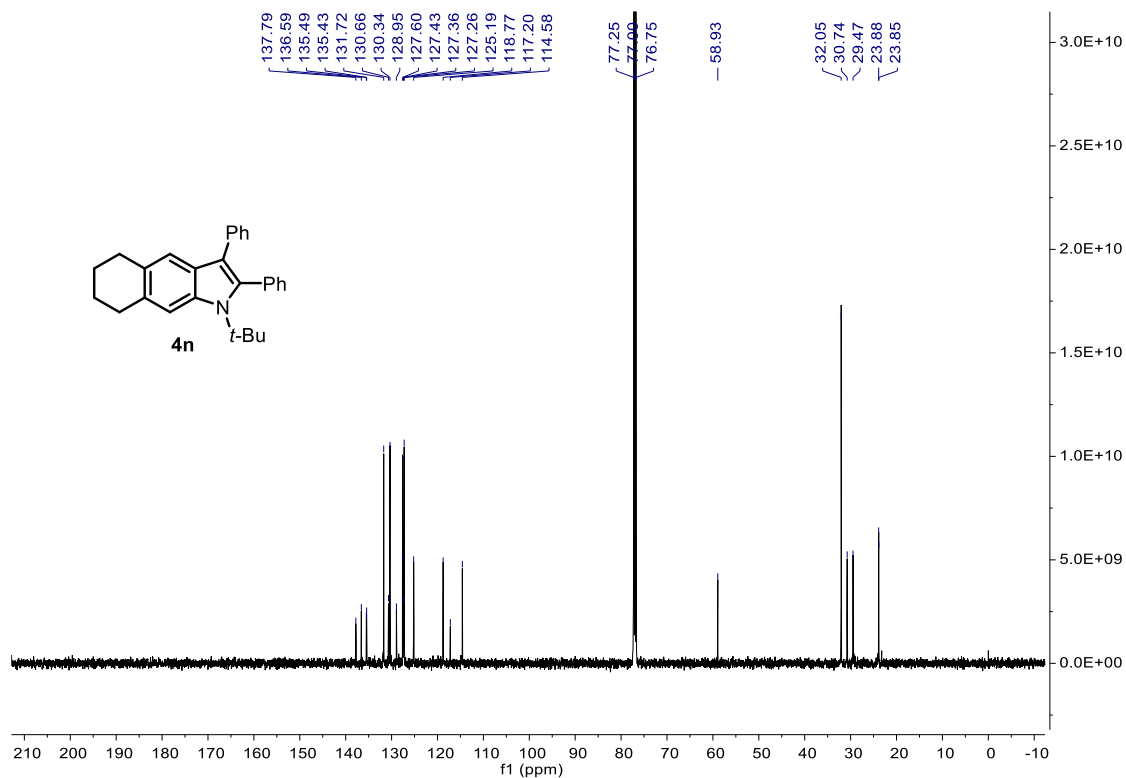
1-(*tert*-butyl)-6-fluoro-5-methyl-2,3-diphenyl-1*H*-indole (4m) (¹H NMR 500 MHz, CDCl₃)



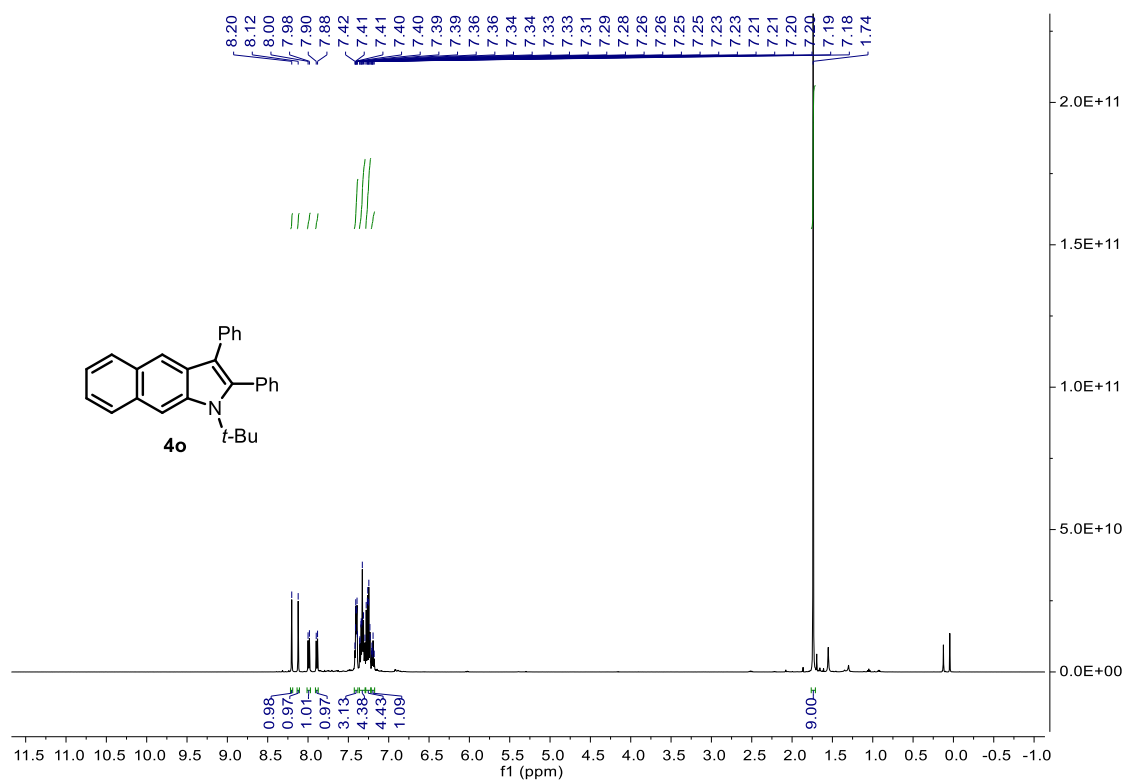
1-(*tert*-butyl)-2,3-diphenyl-5,6,7,8-tetrahydro-1*H*-benzo[*f*]indole (4n) (¹H NMR 500 MHz, CDCl₃)



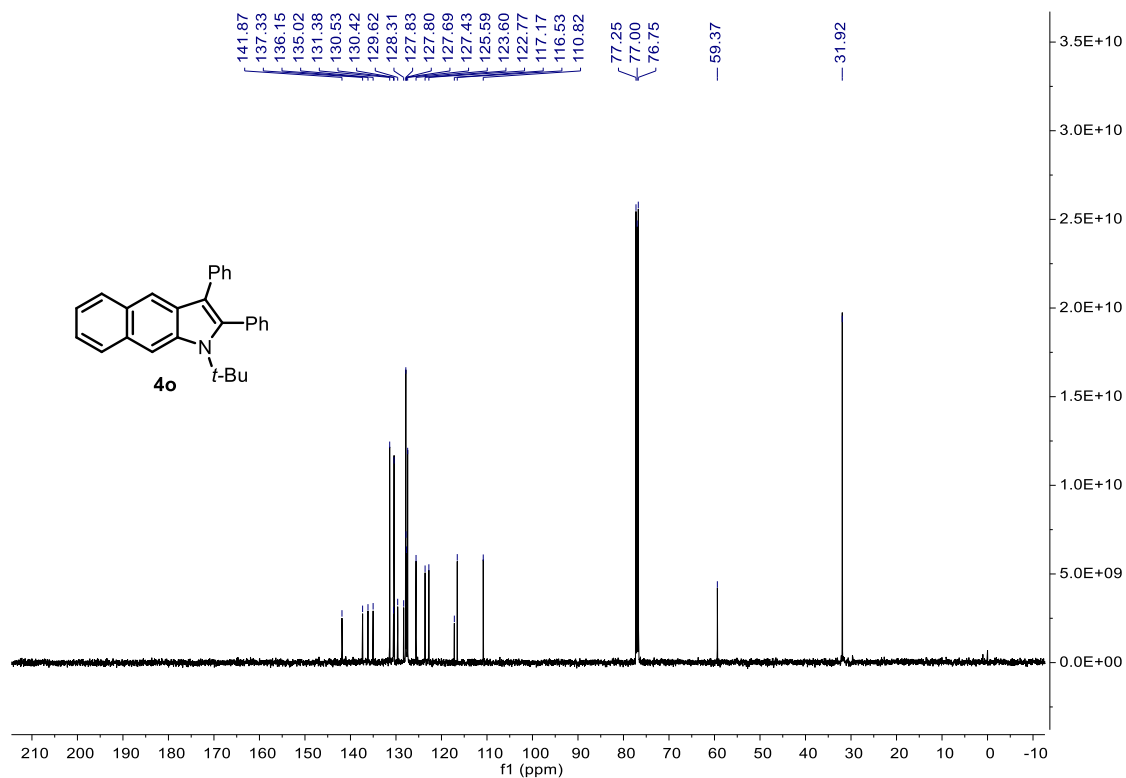
1-(*tert*-butyl)-2,3-diphenyl-5,6,7,8-tetrahydro-1*H*-benzo[*f*]indole (4n) (¹³C NMR 126 MHz, CDCl₃)



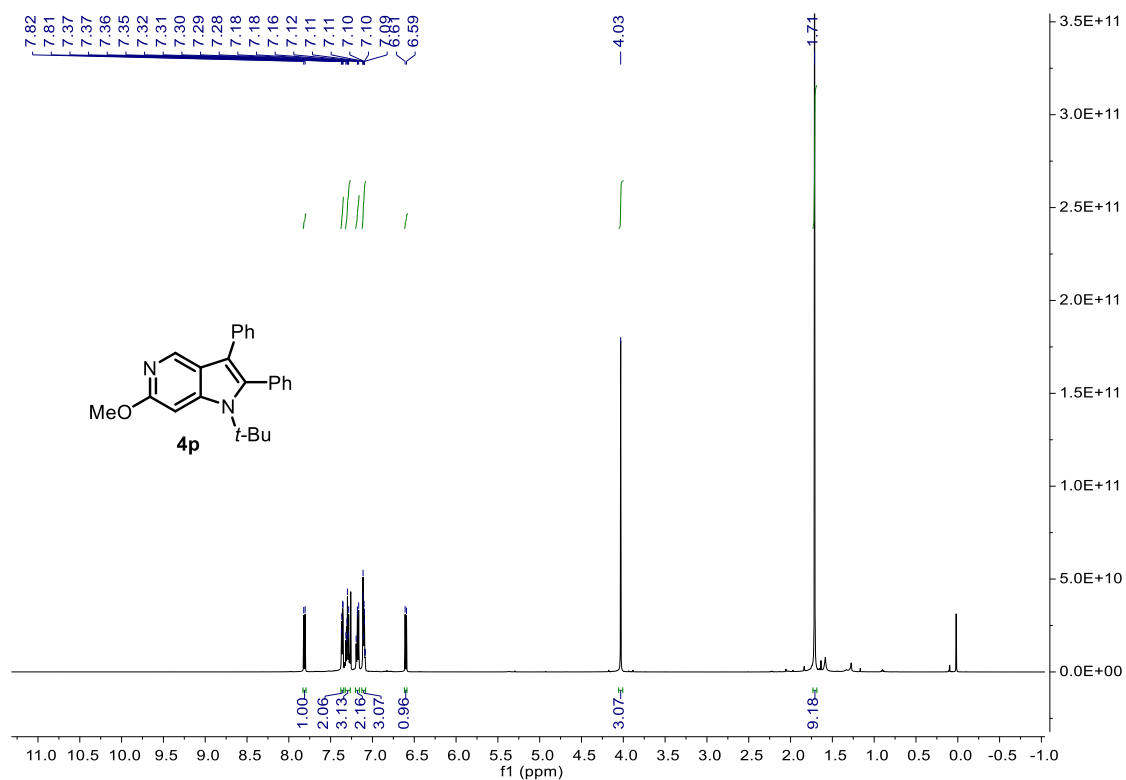
1-(*tert*-butyl)-2,3-diphenyl-1*H*-benzo[*f*]indole (4o) (¹H NMR 500 MHz, CDCl₃)



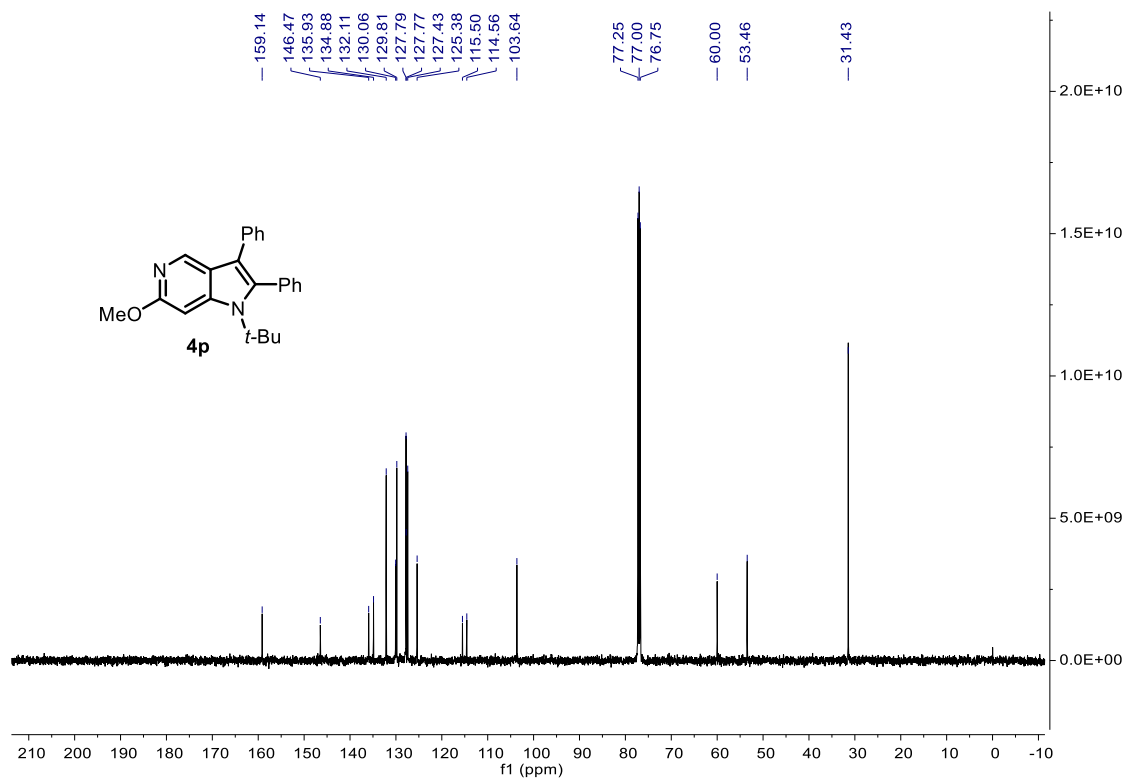
1-(*tert*-butyl)-2,3-diphenyl-1*H*-benzo[*f*]indole (4o) (¹³C NMR 126 MHz, CDCl₃)



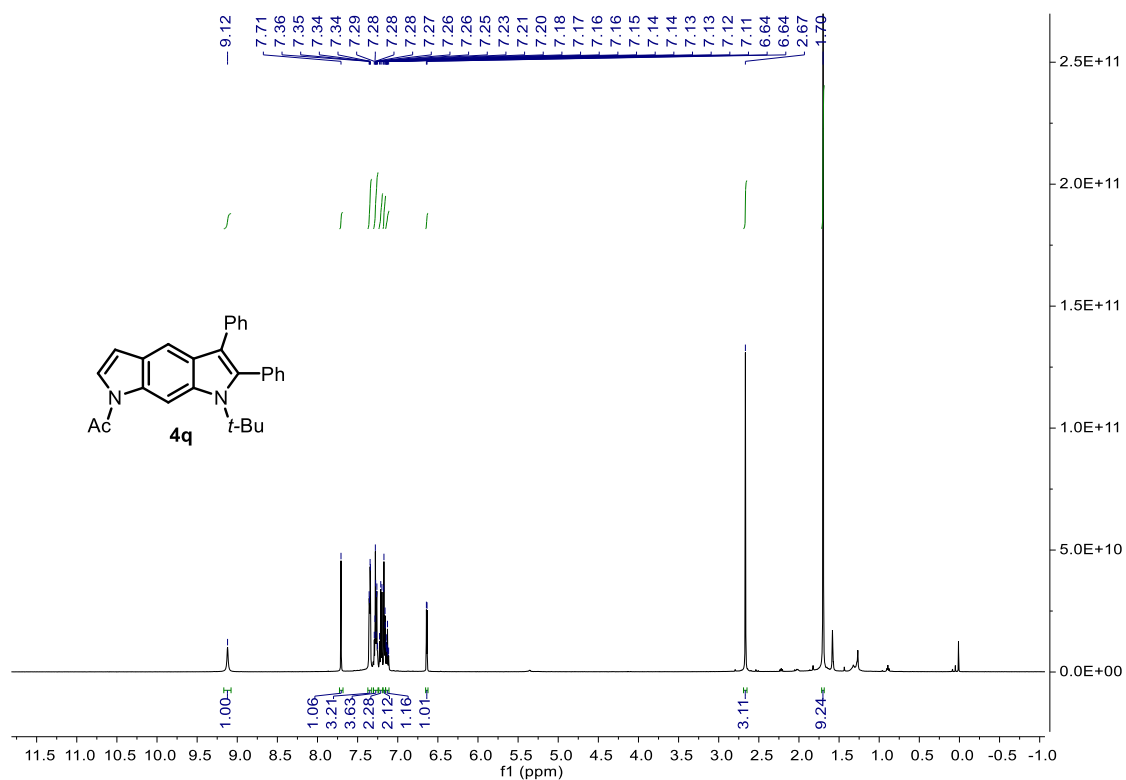
1-(*tert*-butyl)-6-methoxy-2,3-diphenyl-1*H*-pyrrolo[3,2-*c*]pyridine (4p) (¹H NMR 500 MHz, CDCl₃)



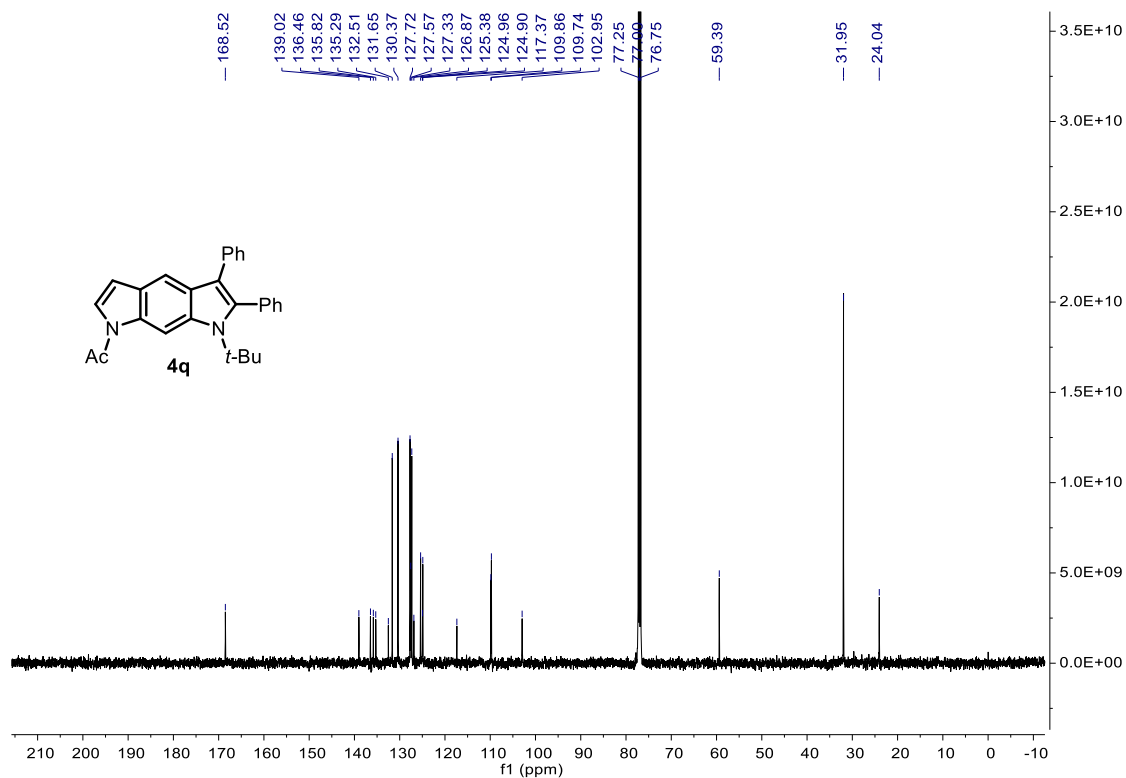
1-(*tert*-butyl)-6-methoxy-2,3-diphenyl-1*H*-pyrrolo[3,2-*c*]pyridine (4p) (¹³C NMR 126 MHz, CDCl₃)



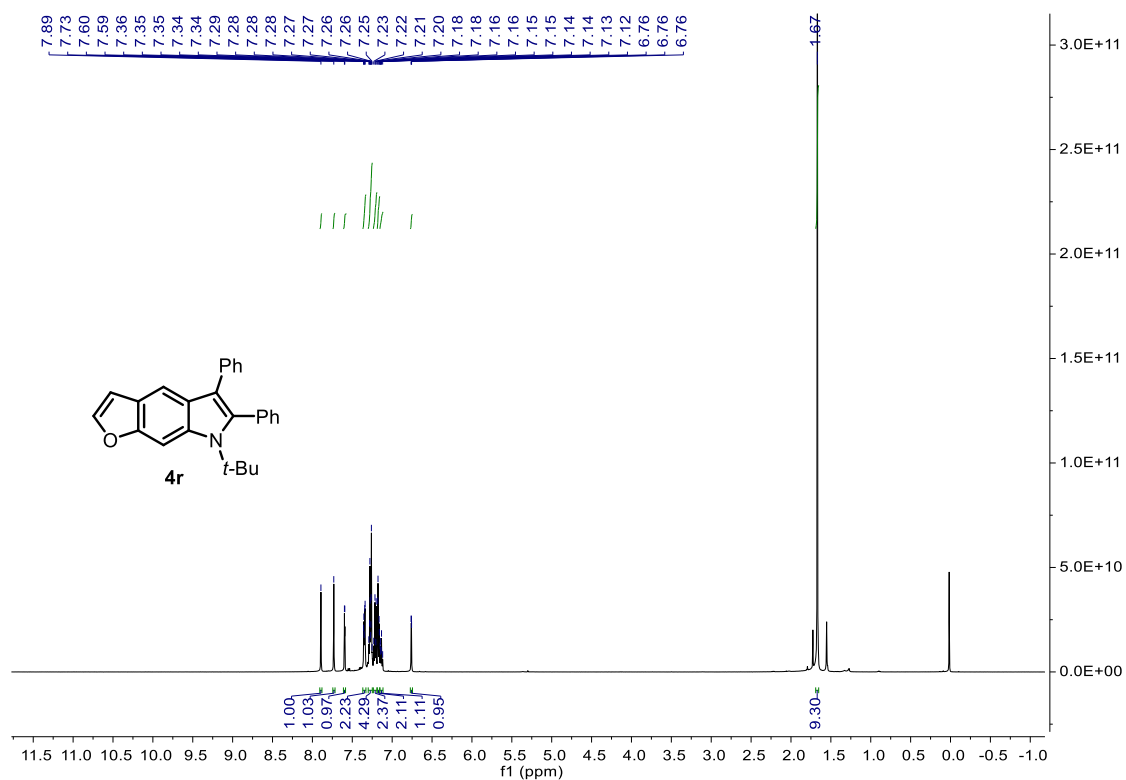
1-(7-(*tert*-butyl)-5,6-diphenylpyrrolo[3,2-*f*]indol-1(7*H*)-yl)ethan-1-one (4q) (¹H NMR 500 MHz, CDCl₃)



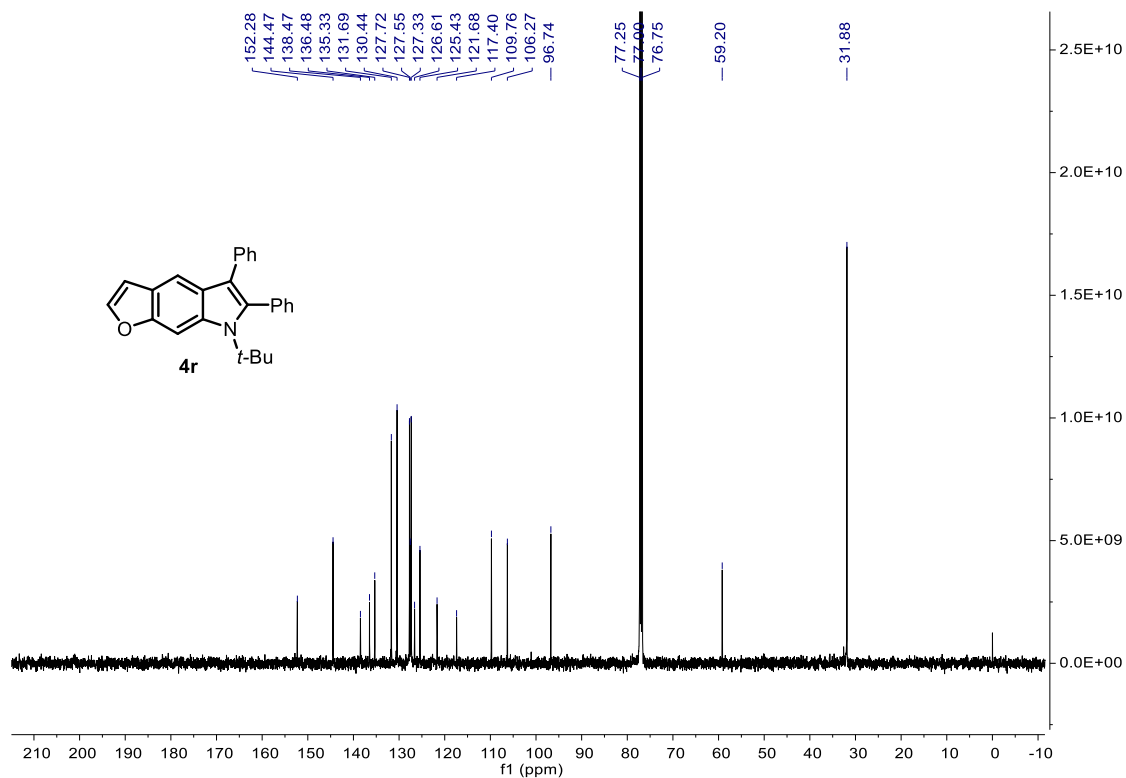
1-(7-(*tert*-butyl)-5,6-diphenylpyrrolo[3,2-*f*]indol-1(7*H*)-yl)ethan-1-one (4q) (¹³C NMR 126 MHz, CDCl₃)



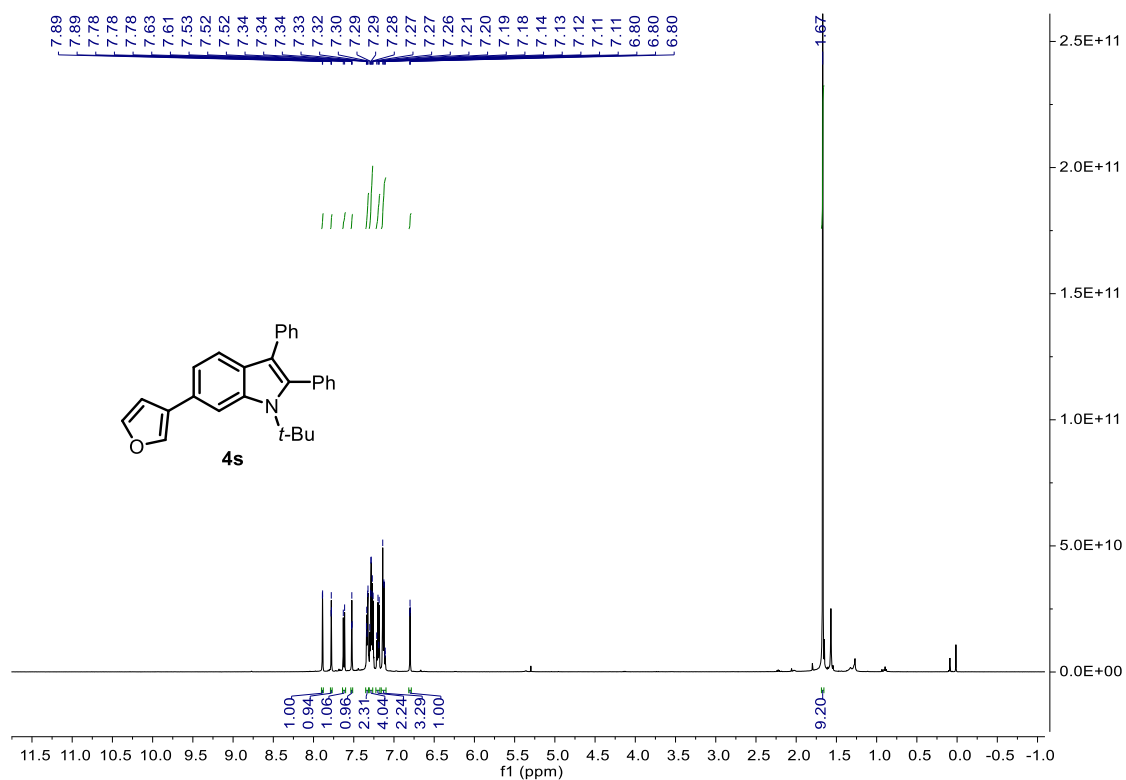
7-(*tert*-butyl)-5,6-diphenyl-7*H*-furo[3,2-*f*]indole (4r) (¹H NMR 500 MHz, CDCl₃)



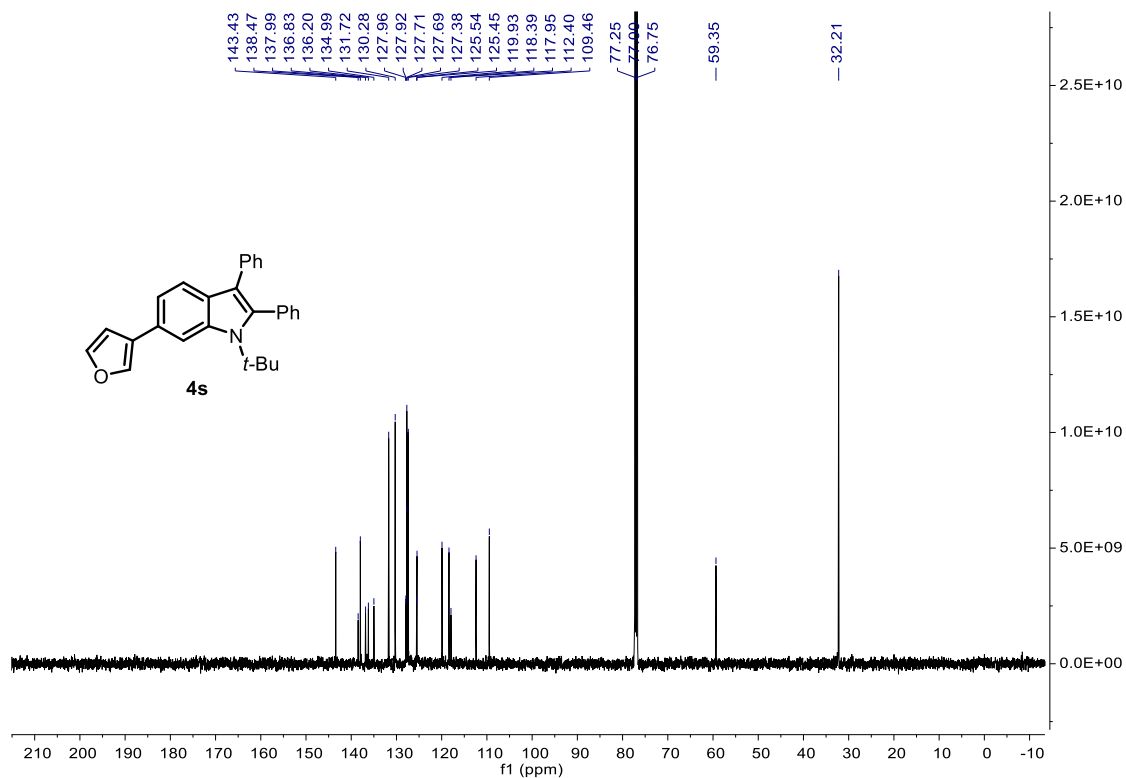
7-(*tert*-butyl)-5,6-diphenyl-7*H*-furo[3,2-*f*]indole (4r) (¹³C NMR 126 MHz, CDCl₃)



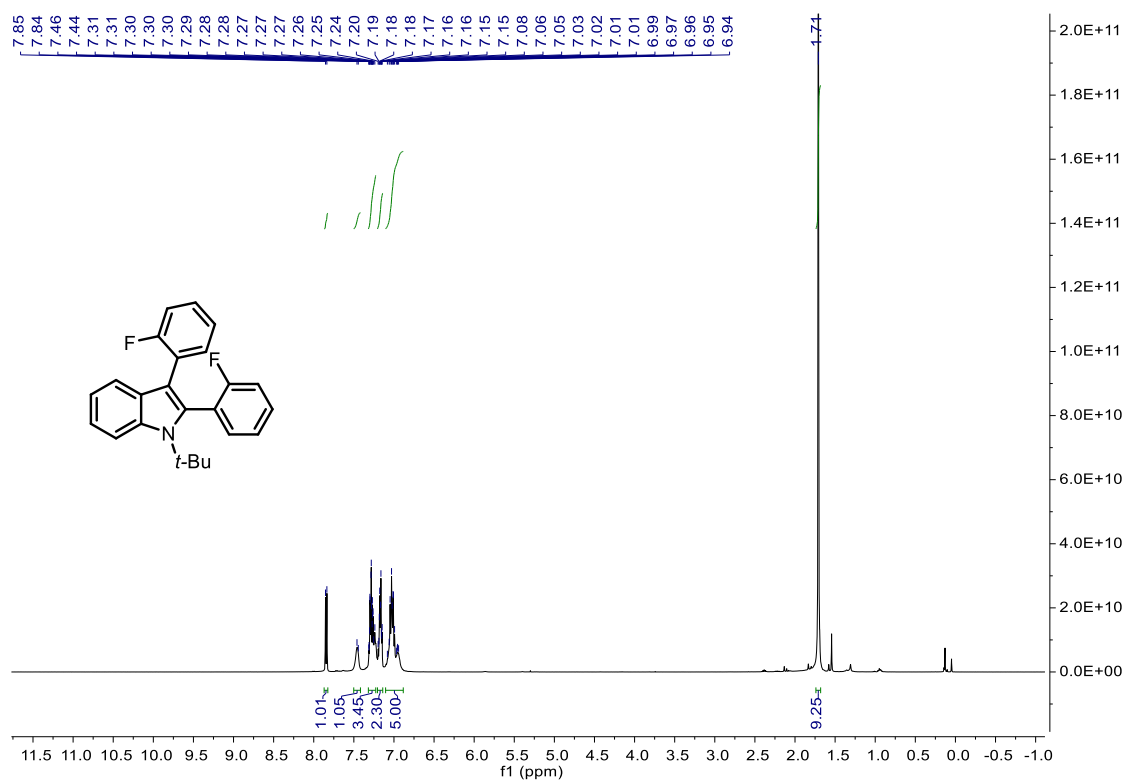
1-(*tert*-butyl)-6-(furan-3-yl)-2,3-diphenyl-1*H*-indole (4s) (¹H NMR 500 MHz, CDCl₃)



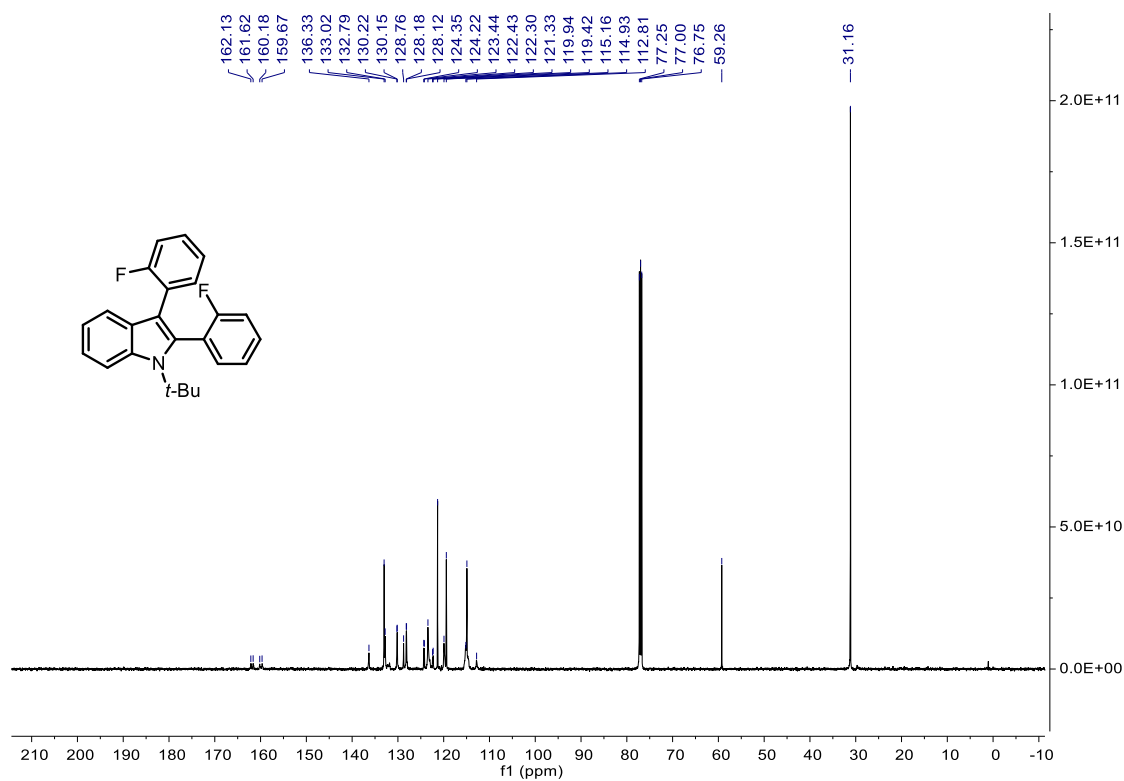
1-(*tert*-butyl)-6-(furan-3-yl)-2,3-diphenyl-1*H*-indole (4s) (¹³C NMR 126 MHz, CDCl₃)



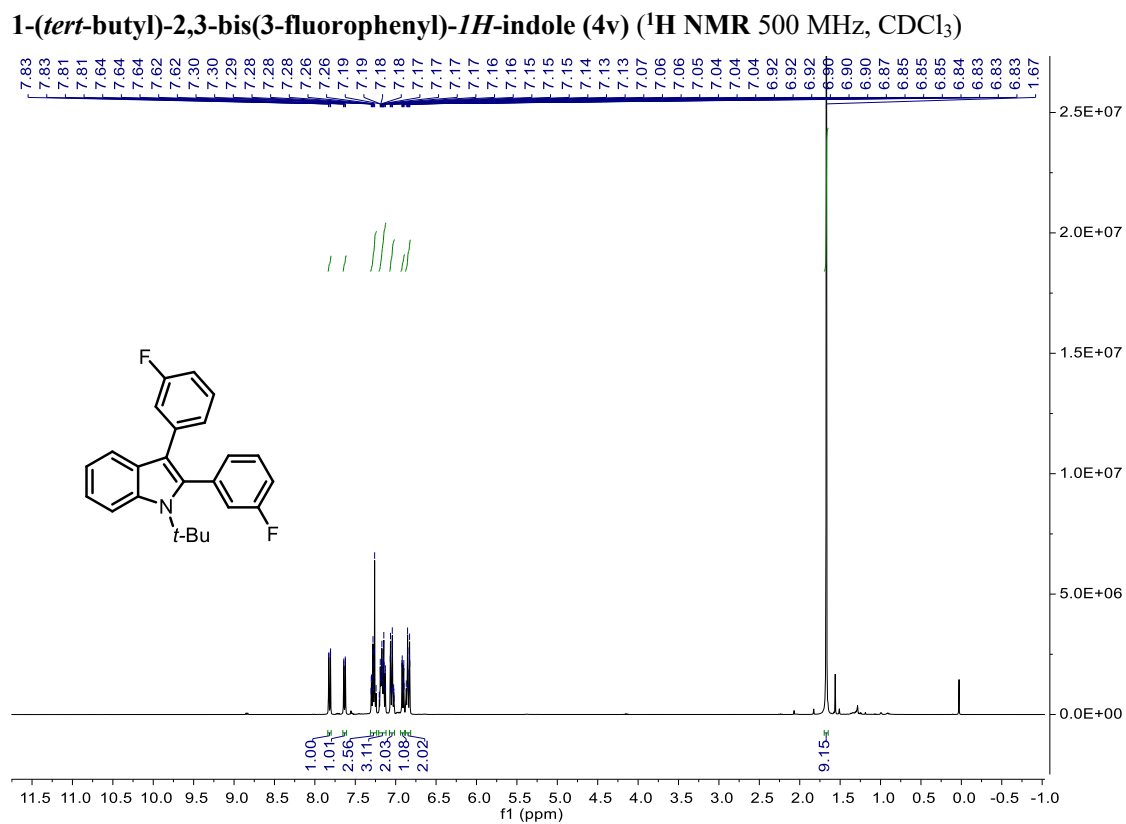
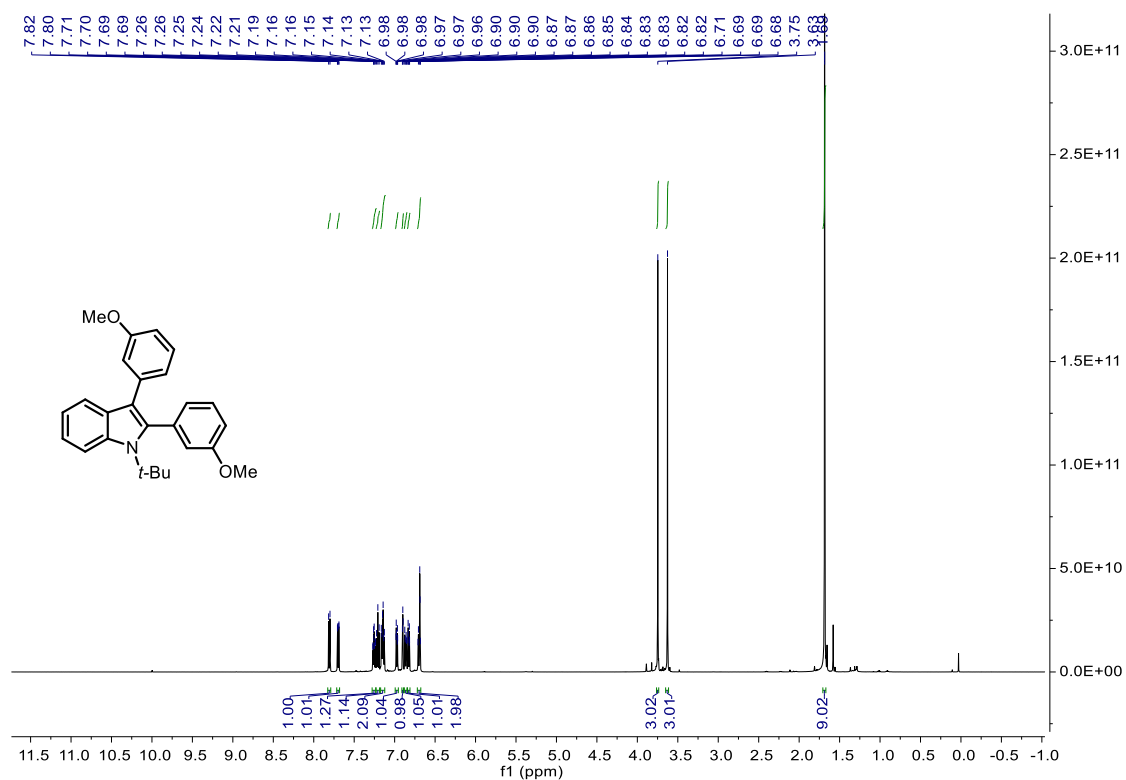
1-(*tert*-butyl)-2,3-bis(2-fluorophenyl)-1*H*-indole (4t) (¹H NMR 500 MHz, CDCl₃)



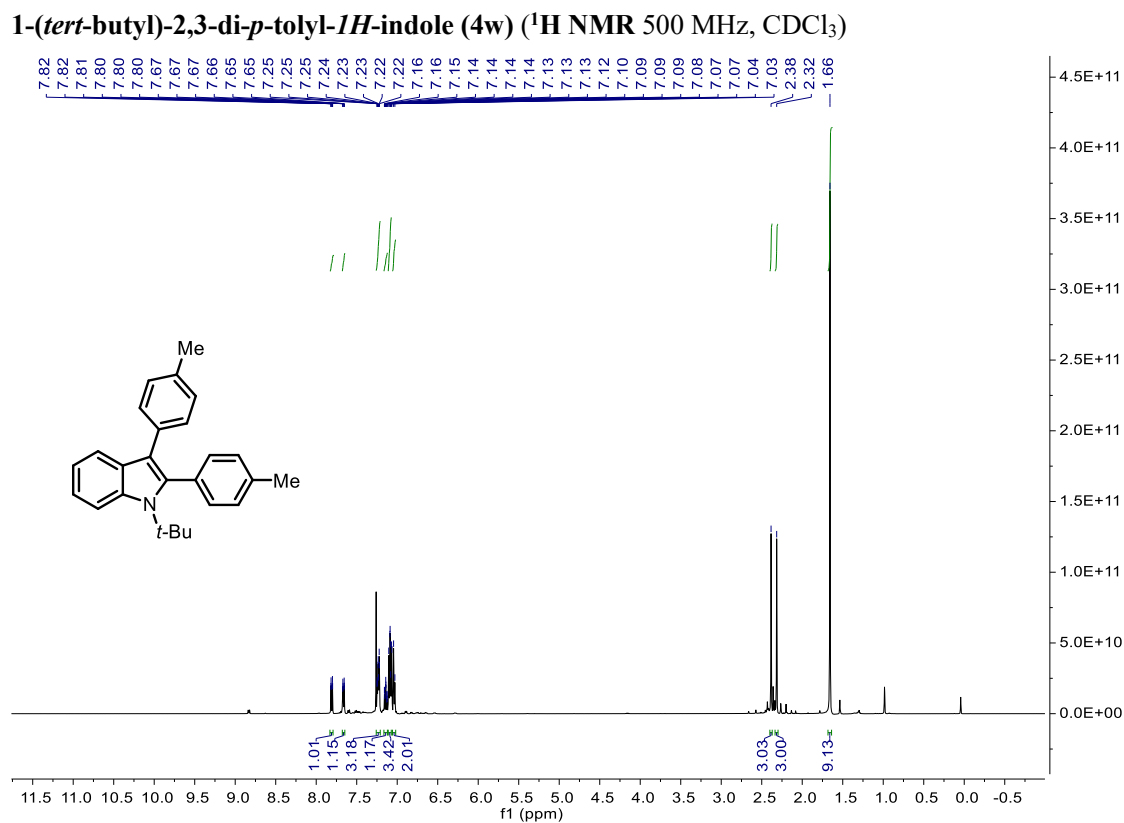
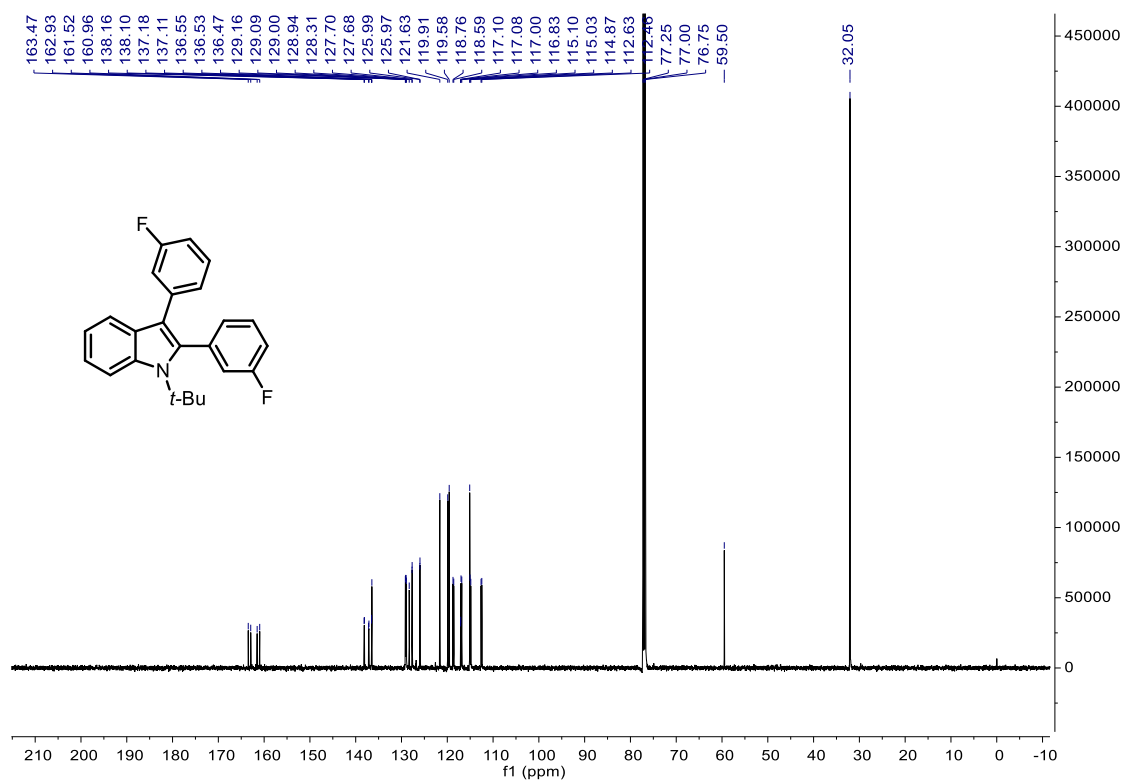
1-(*tert*-butyl)-2,3-bis(2-fluorophenyl)-1*H*-indole (4t) (¹³C NMR 126 MHz, CDCl₃)



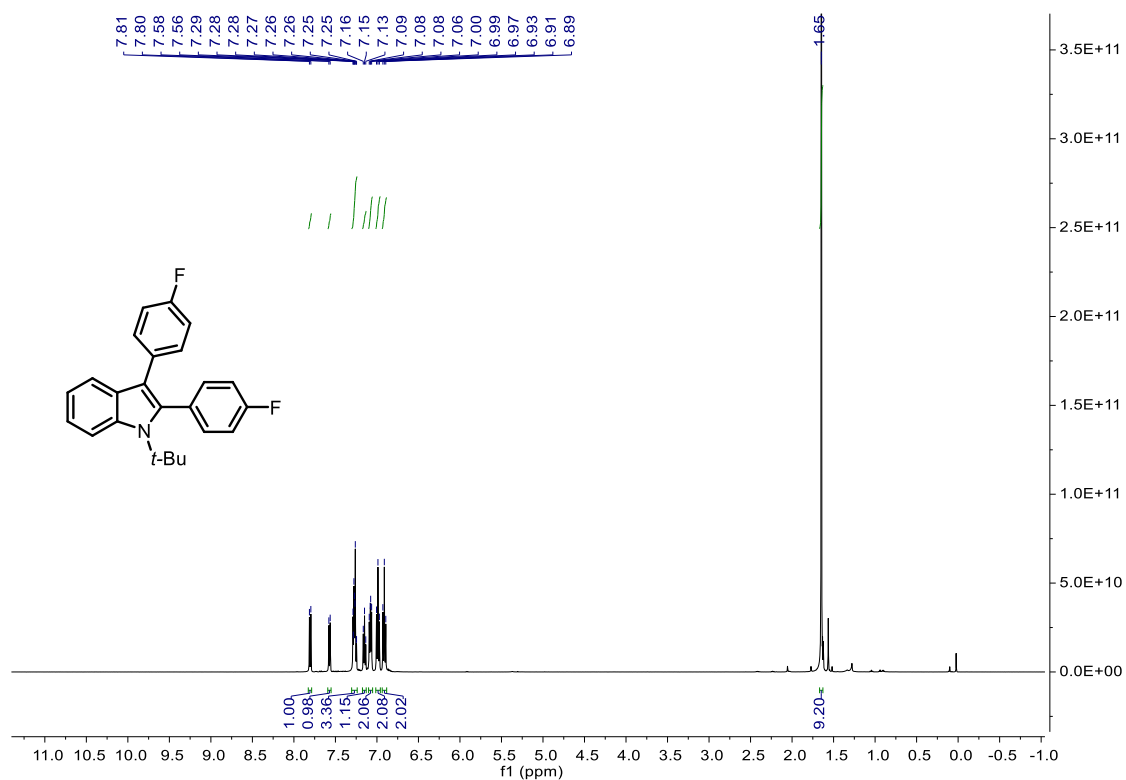
1-(*tert*-butyl)-2,3-bis(3-methoxyphenyl)-1*H*-indole (4u) (¹H NMR 500 MHz, CDCl₃)



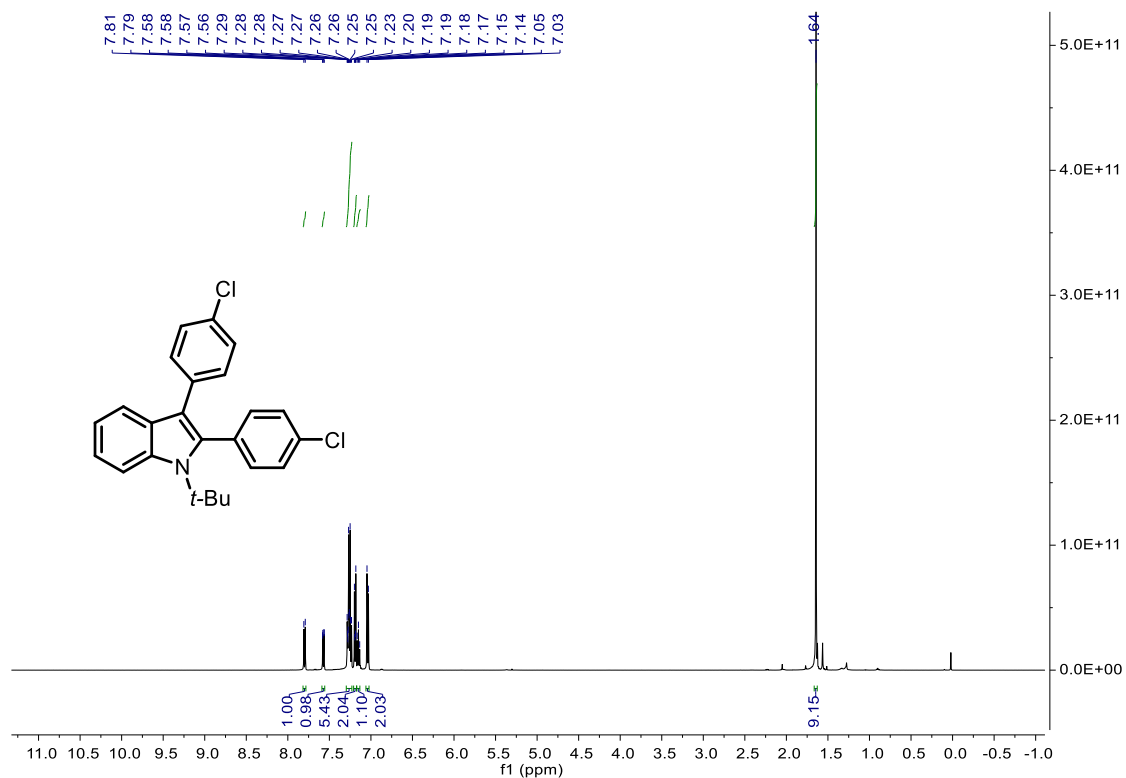
1-(tert-butyl)-2,3-bis(3-fluorophenyl)-1H-indole (4v) (¹³C NMR 126 MHz, CDCl₃)



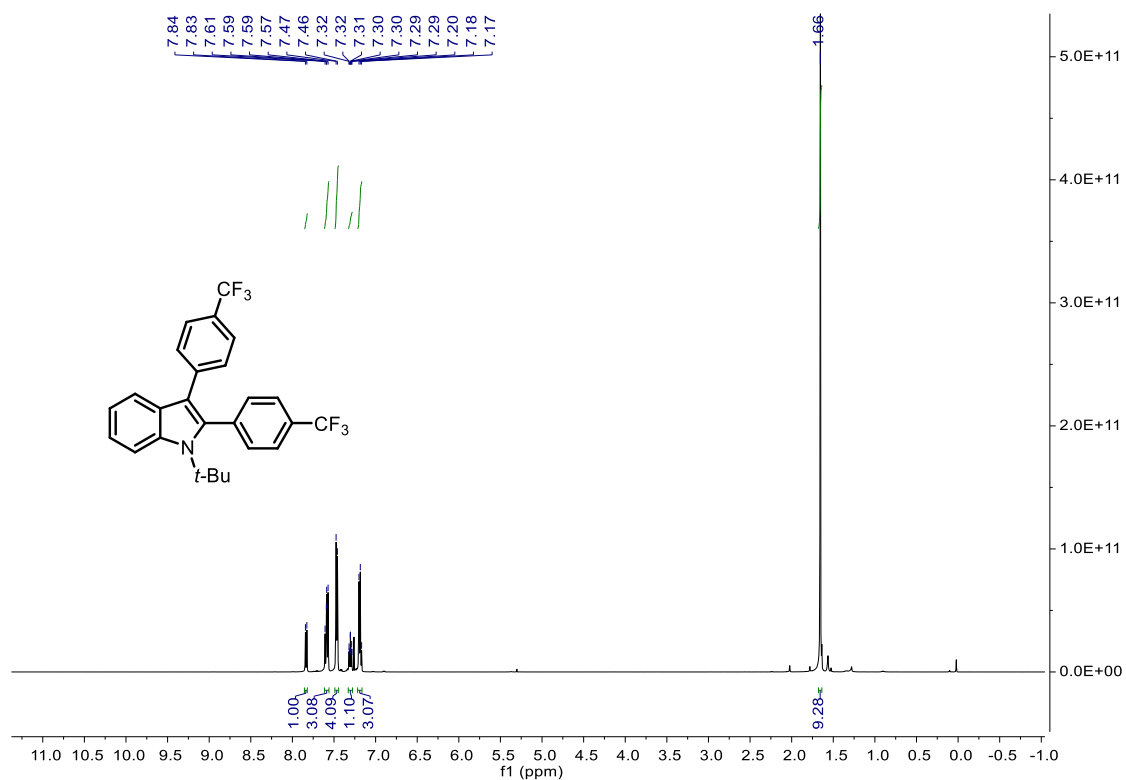
1-(tert-butyl)-2,3-bis(4-fluorophenyl)-1*H*-indole (4x) (¹H NMR 500 MHz, CDCl₃)



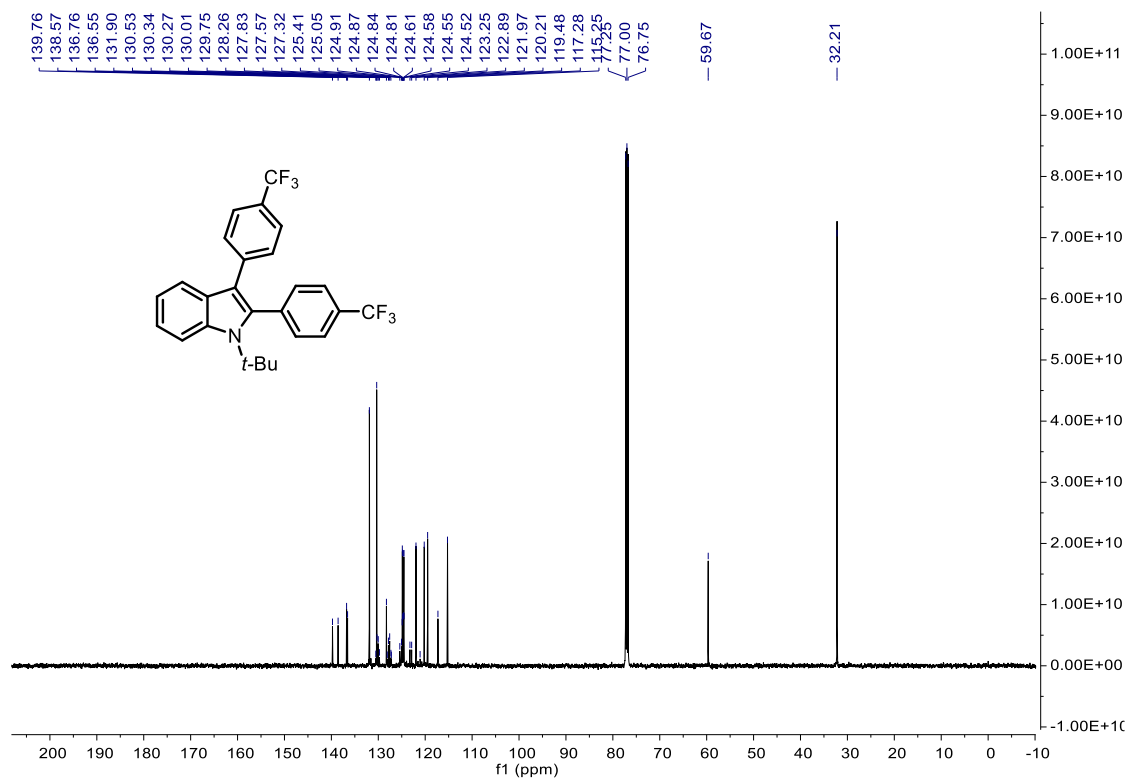
1-(tert-butyl)-2,3-bis(4-chlorophenyl)-1H-indole (4y) (^1H NMR 500 MHz, CDCl_3)



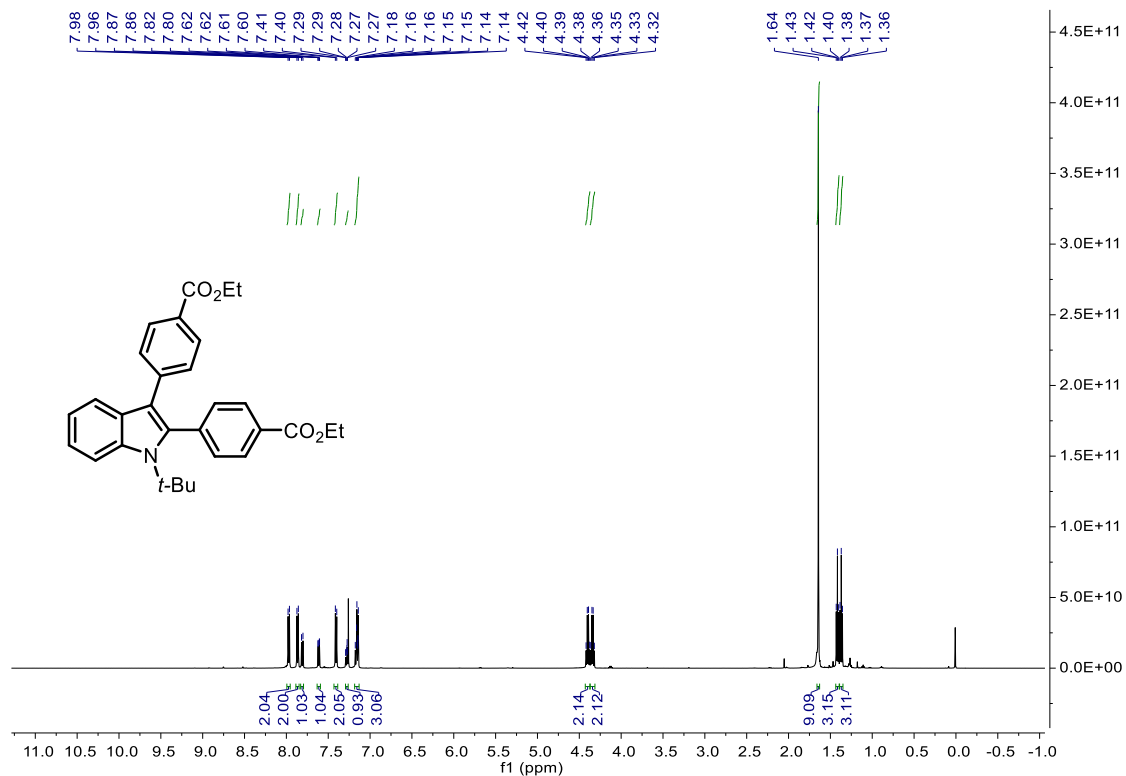
1-(tert-butyl)-2,3-bis(4-(trifluoromethyl)phenyl)-1H-indole (4z) (^1H NMR 500 MHz, CDCl_3)



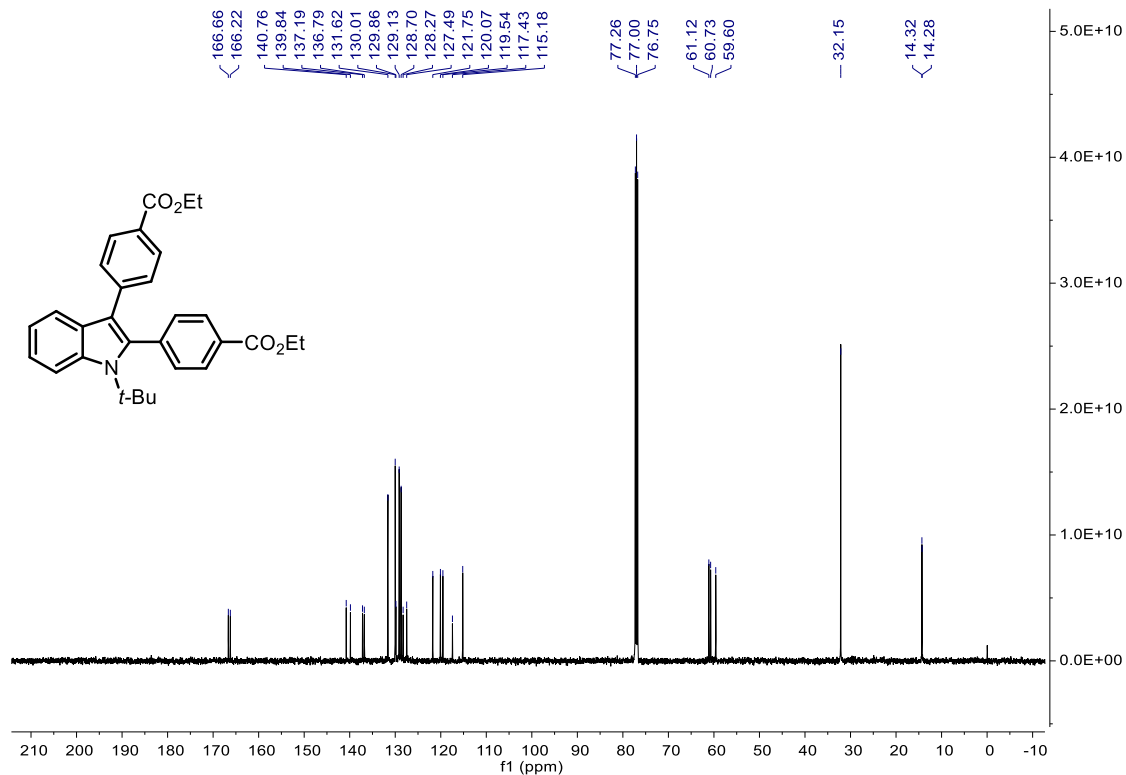
1-(*tert*-butyl)-2,3-bis(4-(trifluoromethyl)phenyl)-1*H*-indole (4z) (¹³C NMR 126 MHz, CDCl₃)



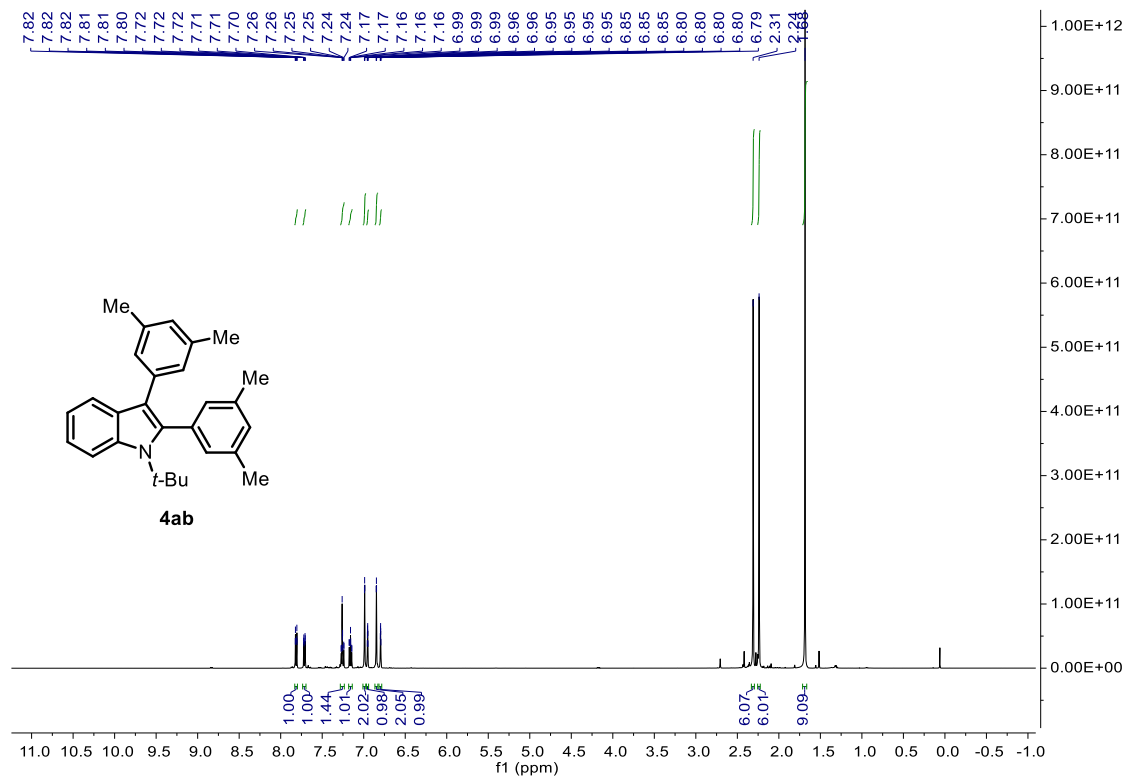
diethyl 4,4'-(1-(*tert*-butyl)-1*H*-indole-2,3-diyl)dibenzoate (4aa) (^1H NMR 500 MHz, CDCl_3)



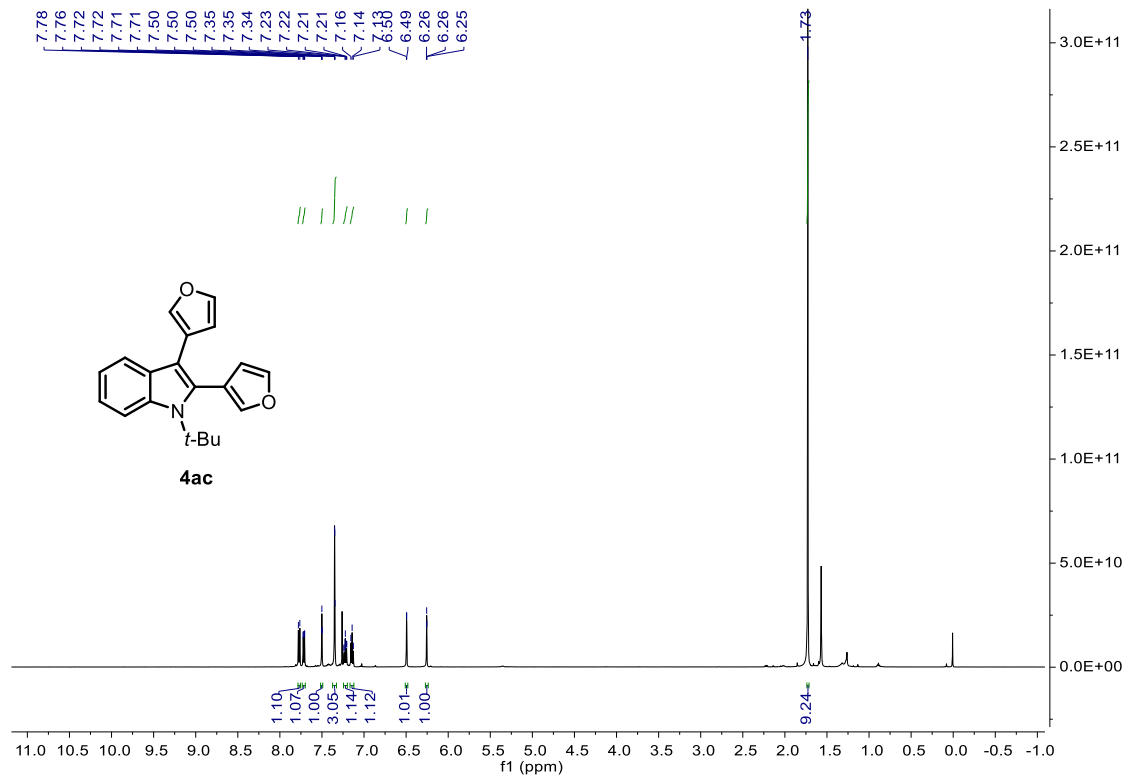
diethyl 4,4'-(1-(*tert*-butyl)-1*H*-indole-2,3-diyl)dibenzoate (4aa) (^{13}C NMR 126 MHz, CDCl_3)



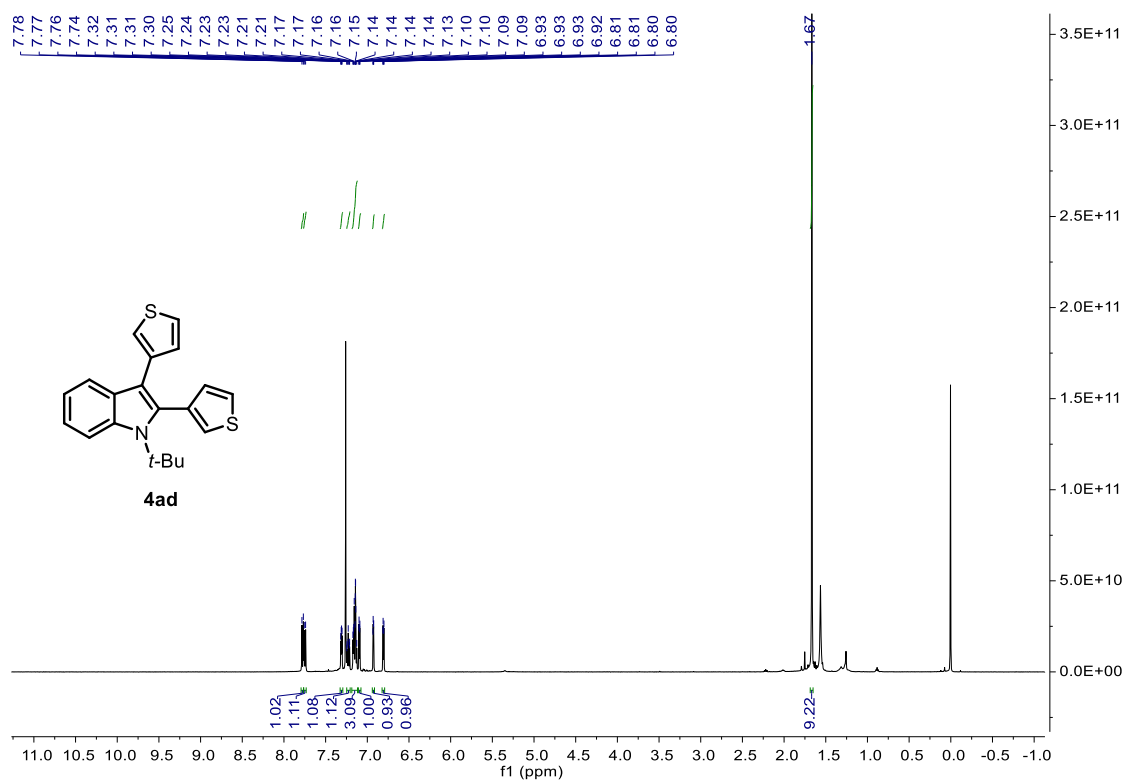
1-(*tert*-butyl)-2,3-bis(3,5-dimethylphenyl)-1*H*-indole (4ab) (¹H NMR 500 MHz, CDCl₃)



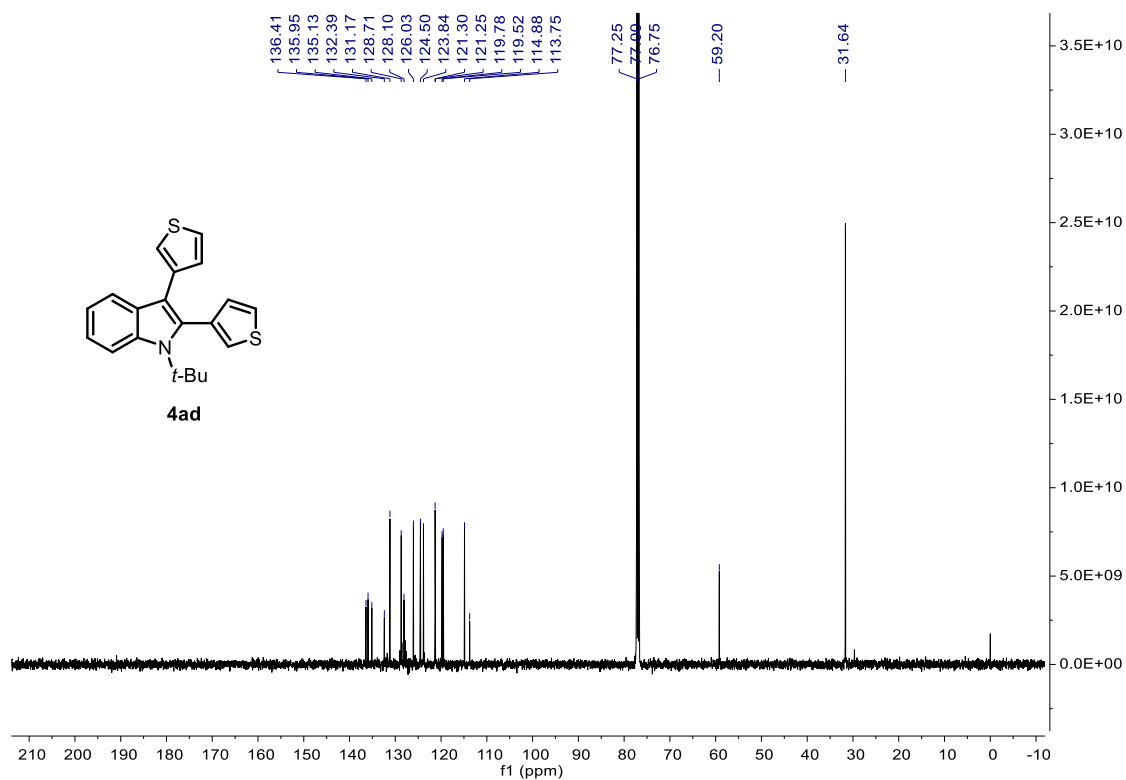
1-(*tert*-butyl)-2,3-di(furan-3-yl)-1*H*-indole (4ac) (¹H NMR 500 MHz, CDCl₃)



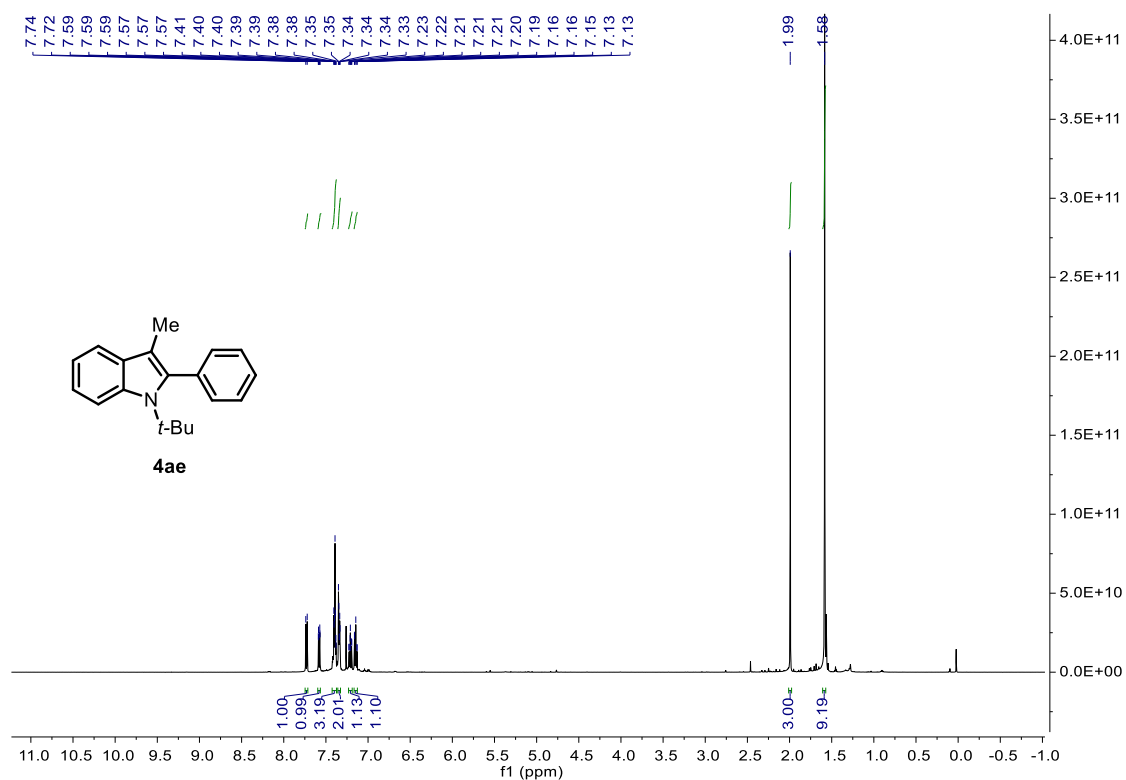
1-(*tert*-butyl)-2,3-di(thiophen-3-yl)-1*H*-indole (4ad) (¹H NMR 500 MHz, CDCl₃)



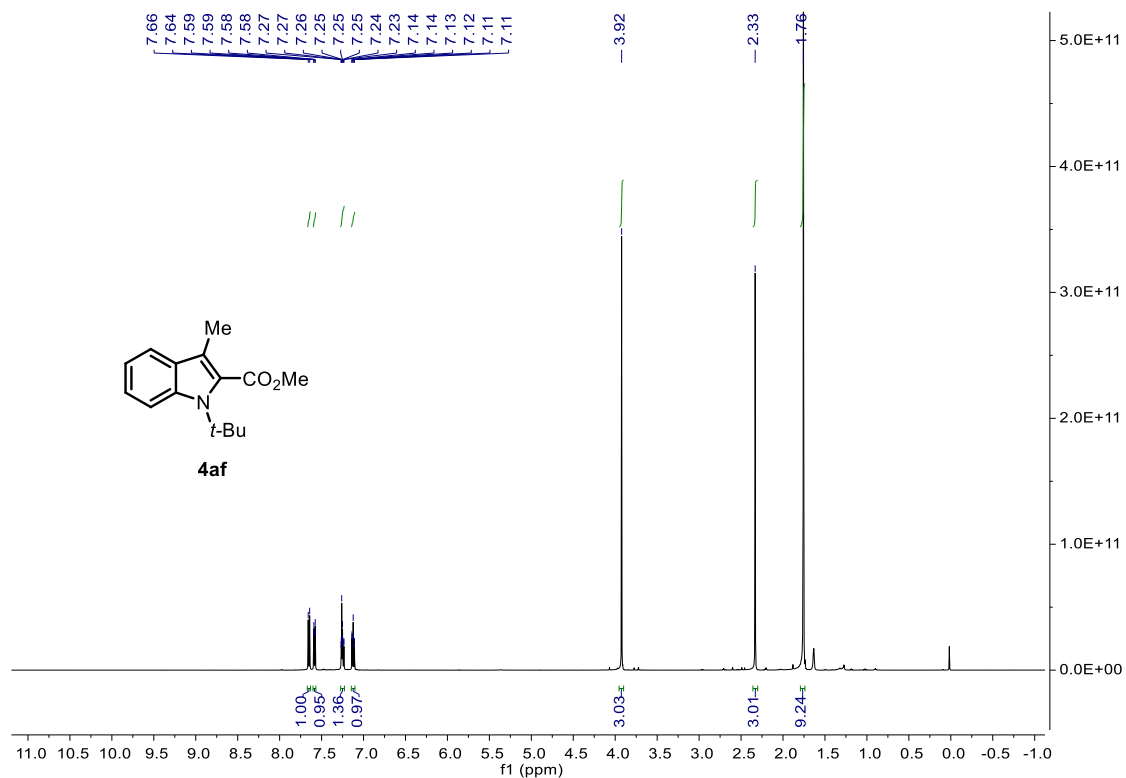
1-(*tert*-butyl)-2,3-di(thiophen-3-yl)-1*H*-indole (4ad) (¹³C NMR 126 MHz, CDCl₃)



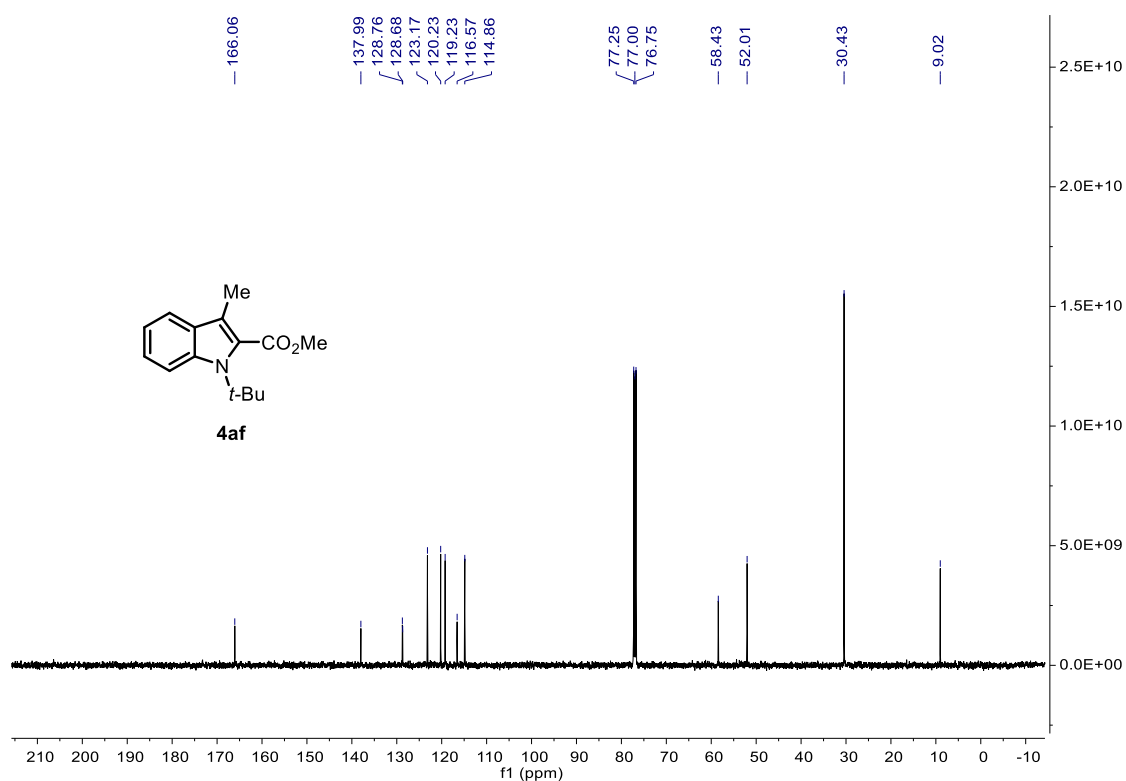
1-(*tert*-butyl)-3-methyl-2-phenyl-1*H*-indole (4ae) (¹H NMR 500 MHz, CDCl₃)



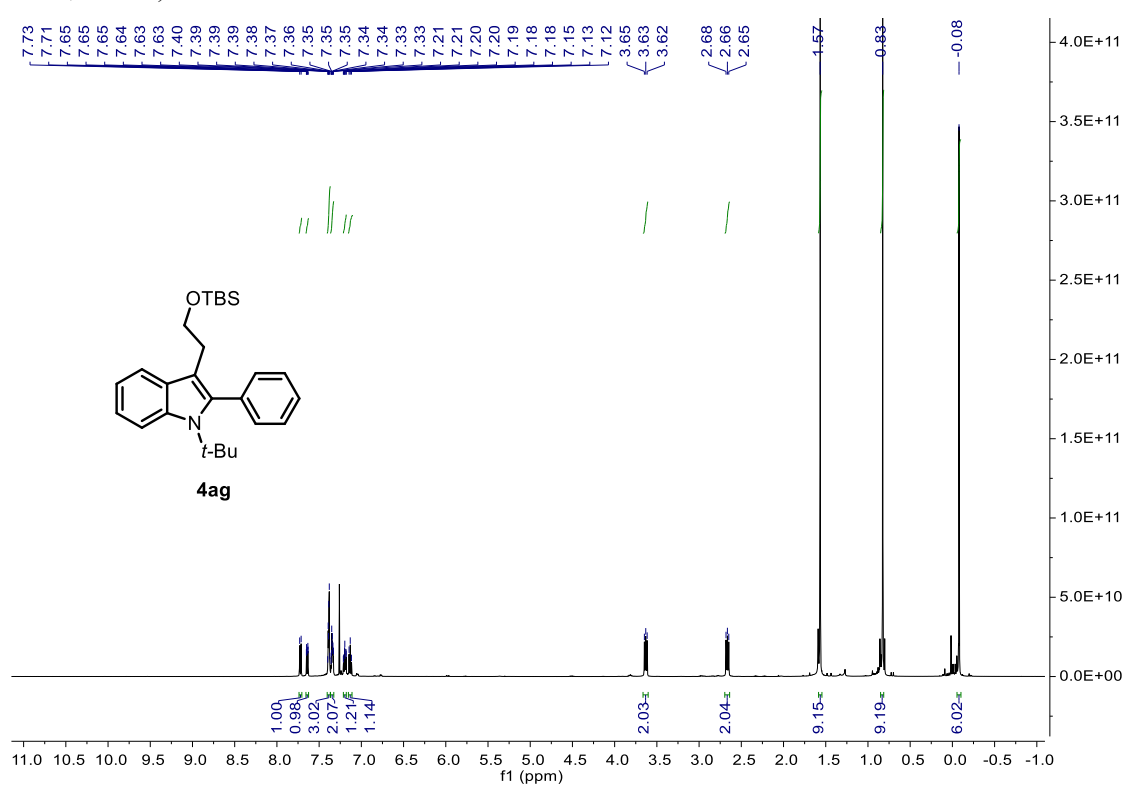
methyl 1-(*tert*-butyl)-3-methyl-1*H*-indole-2-carboxylate (4af) (¹H NMR 500 MHz, CDCl₃)



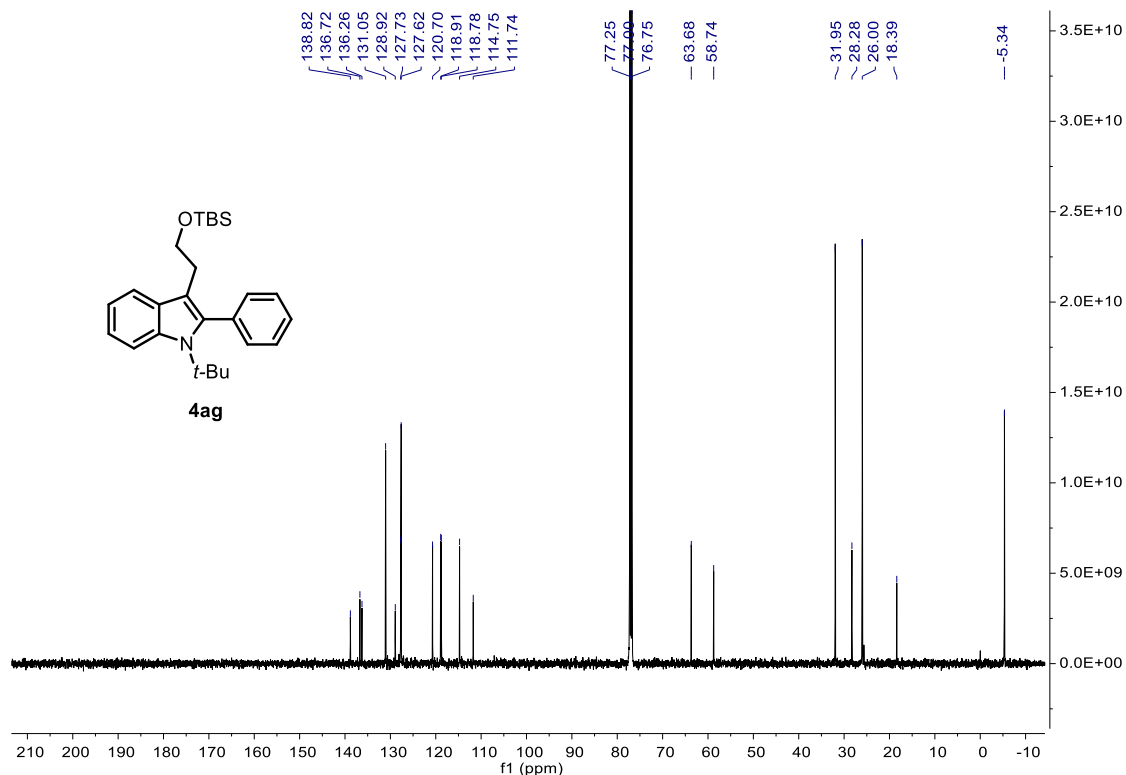
methyl 1-(*tert*-butyl)-3-methyl-1*H*-indole-2-carboxylate (4af) (^{13}C NMR 126 MHz, CDCl_3)



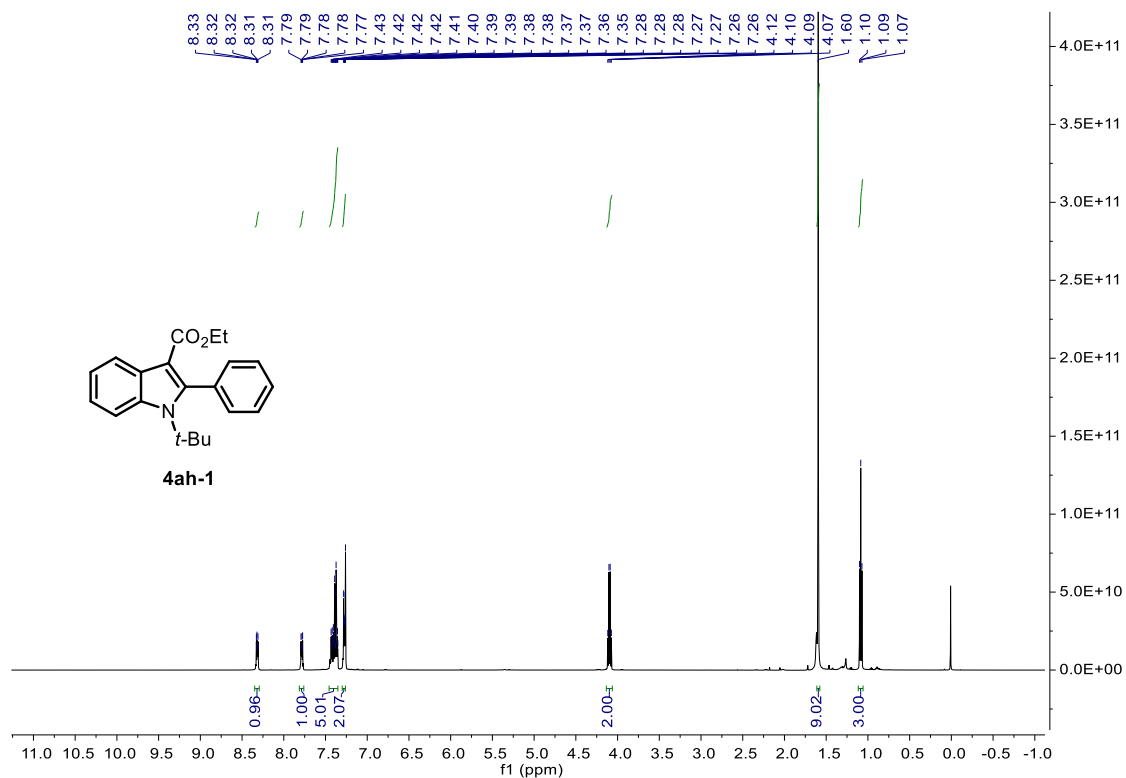
1-(*tert*-butyl)-3-(2-((*tert*-butyldimethylsilyl)oxy)ethyl)-2-phenyl-1*H*-indole (4ag) (^1H NMR 500 MHz, CDCl_3)



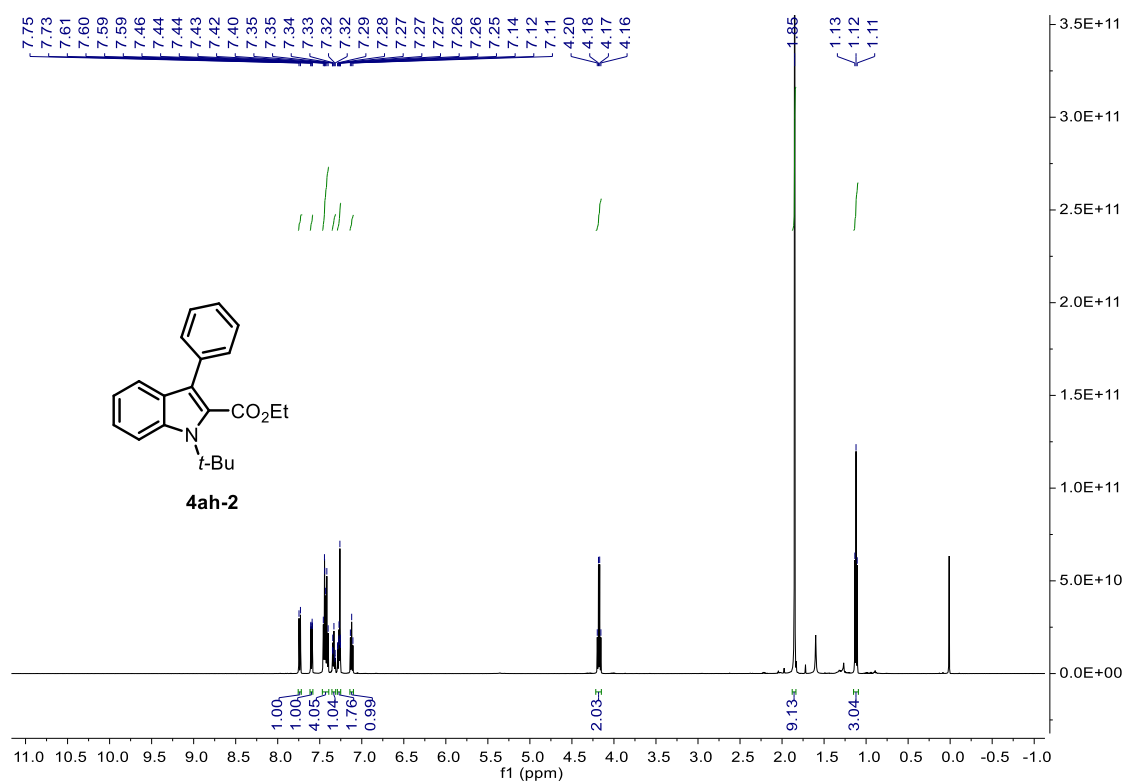
1-(*tert*-butyl)-3-(2-((*tert*-butyldimethylsilyl)oxy)ethyl)-2-phenyl-1*H*-indole (4ag) (¹³C NMR 126 MHz, CDCl₃)



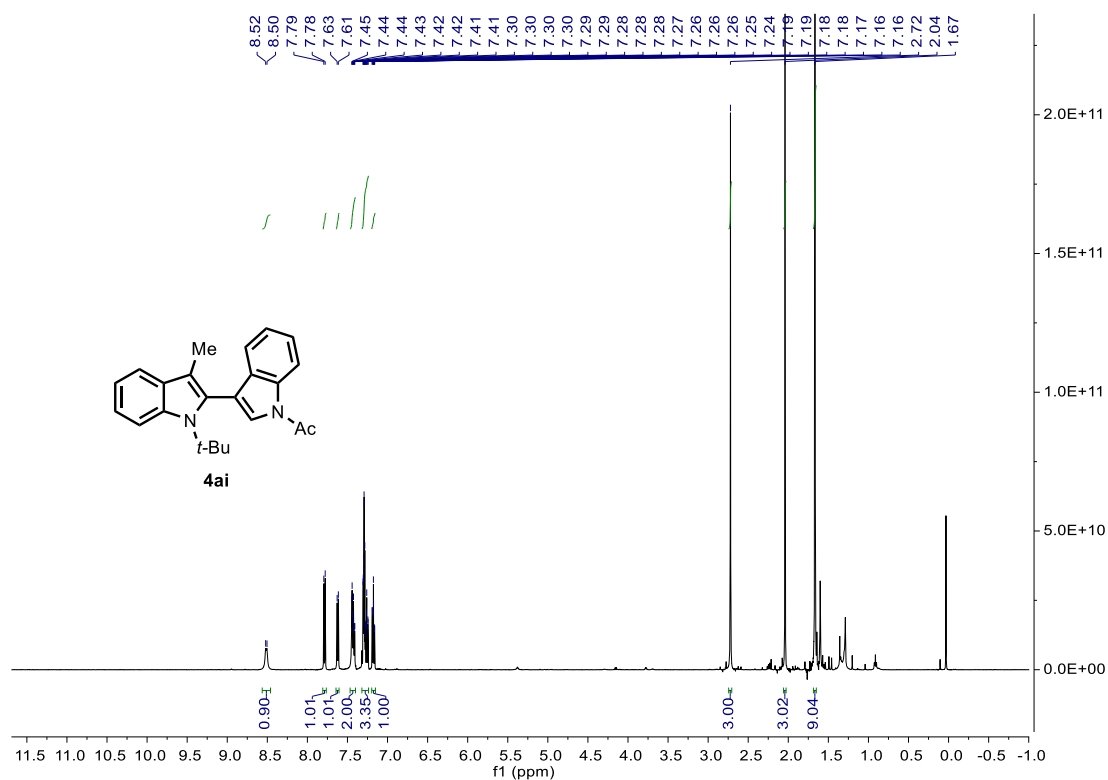
ethyl 1-(*tert*-butyl)-2-phenyl-1*H*-indole-3-carboxylate (4ah-1) (¹H NMR 500 MHz, CDCl₃)



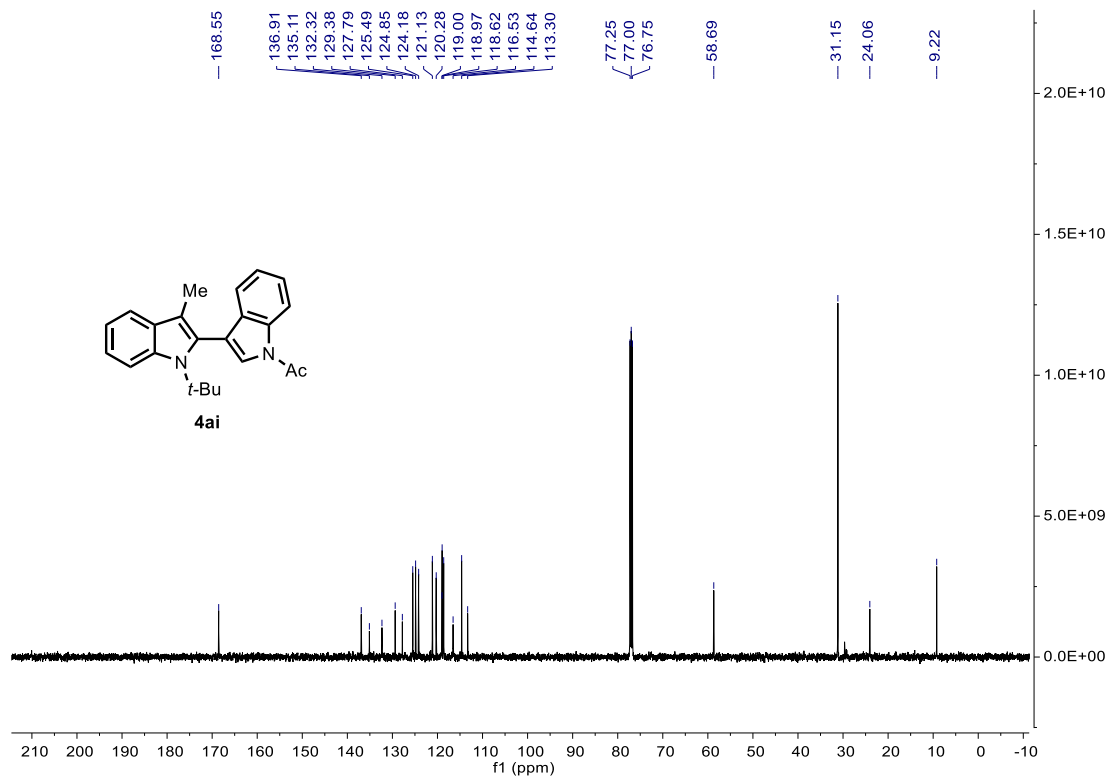
ethyl 1-(*tert*-butyl)-3-phenyl-1*H*-indole-2-carboxylate (4ah-2) (¹H NMR 500 MHz, CDCl₃)



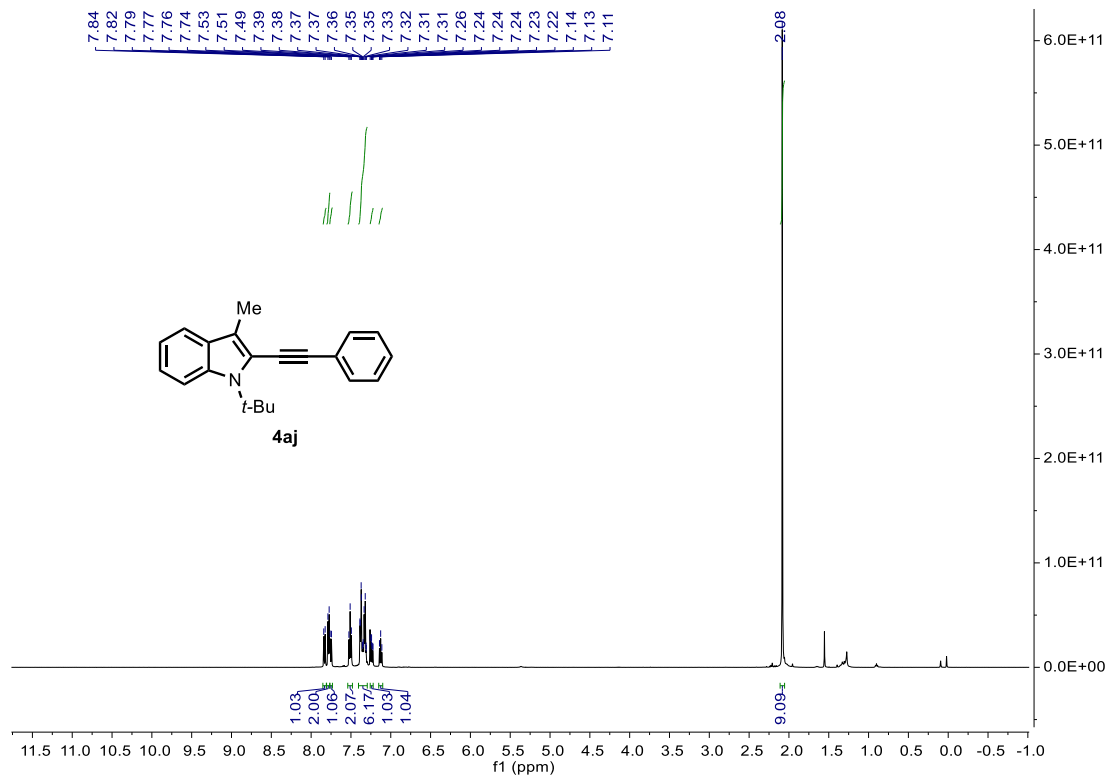
1-(1-(*tert*-butyl)-3-methyl-1*H*,1'*H*-[2,3'-biindol]-1'-yl)ethan-1-one (4ai) (¹H NMR 500 MHz, CDCl₃)



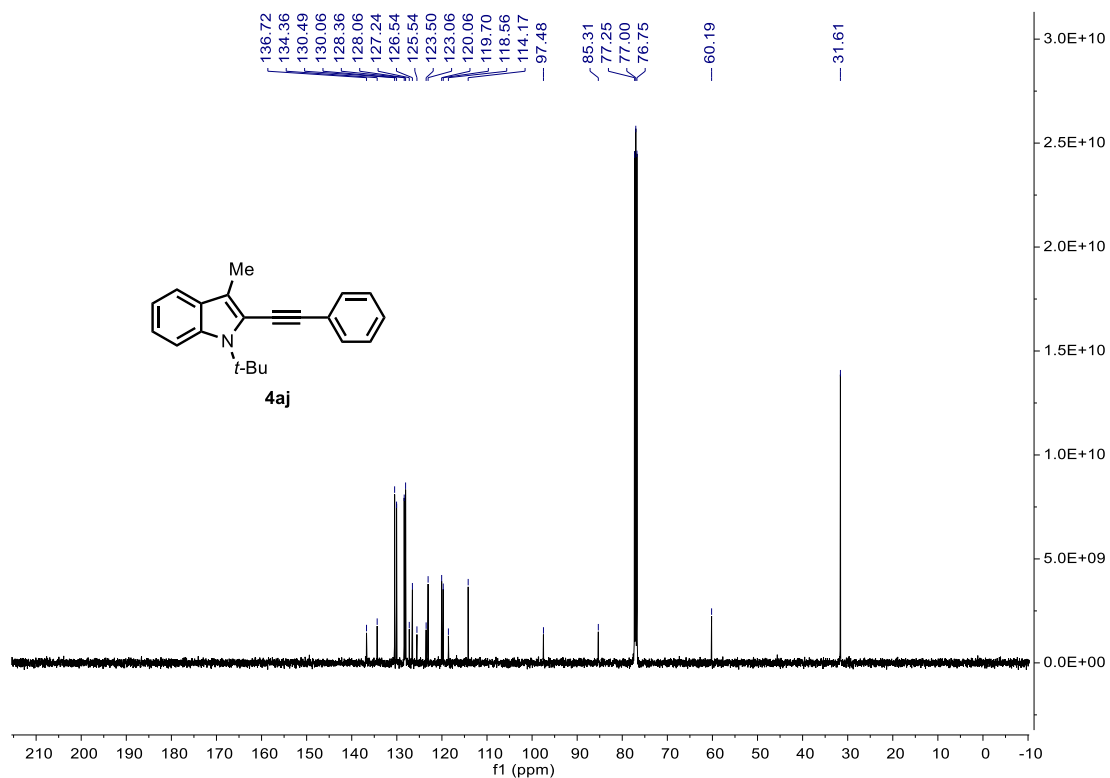
1-(1-(tert-butyl)-3-methyl-1H,1'H-[2,3'-biindol]-1'-yl)ethan-1-one (4ai) (^{13}C NMR 126 MHz, CDCl_3)



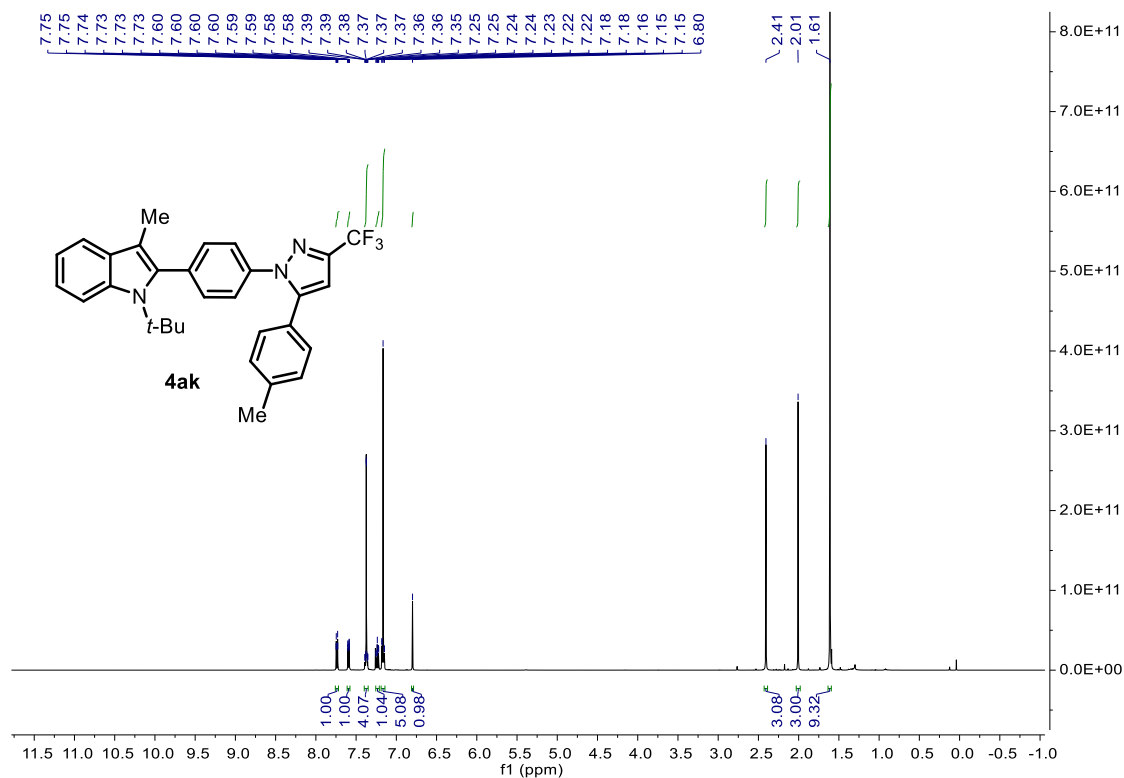
1-(tert-butyl)-3-methyl-2-(phenylethynyl)-1H-indole (4aj) (^1H NMR 500 MHz, CDCl_3)



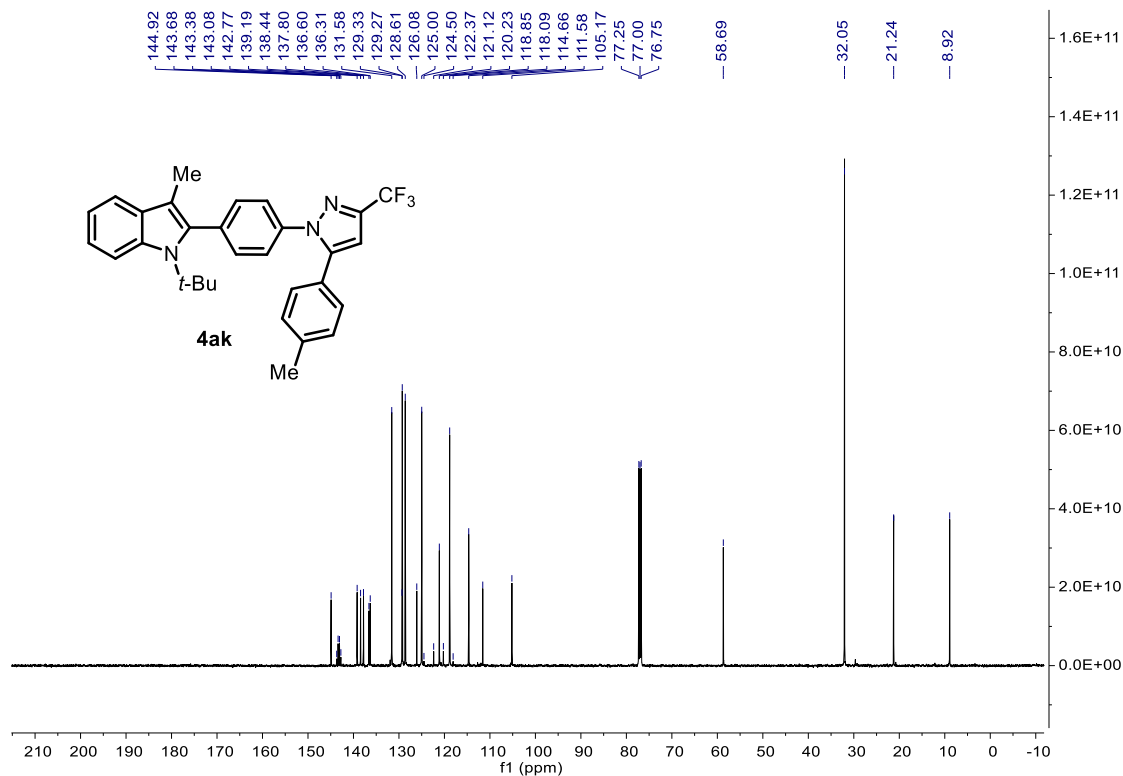
1-(*tert*-butyl)-3-methyl-2-(phenylethynyl)-1H-indole (4aj) (^{13}C NMR 126 MHz, CDCl_3)



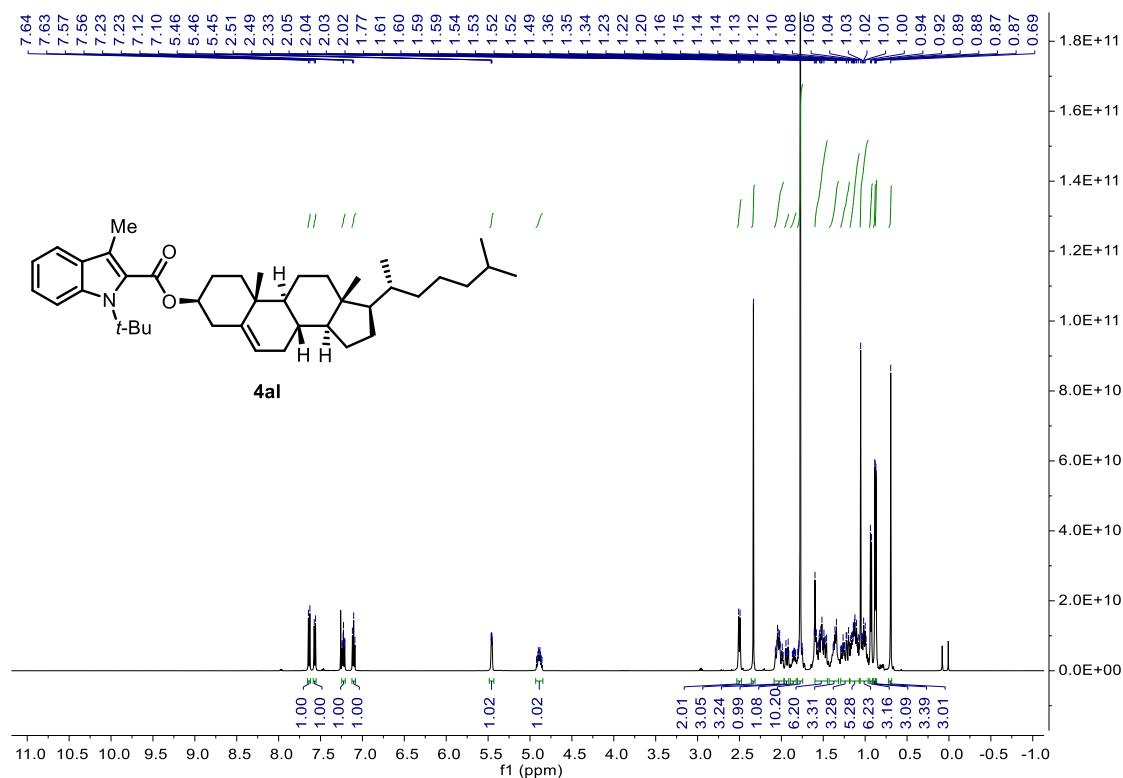
1-(*tert*-butyl)-3-methyl-2-(4-(5-(*p*-tolyl)-3-(trifluoromethyl)-1H-pyrazol-1-yl)phenyl)-1H-indole (4ak) (^1H NMR 500 MHz, CDCl_3)



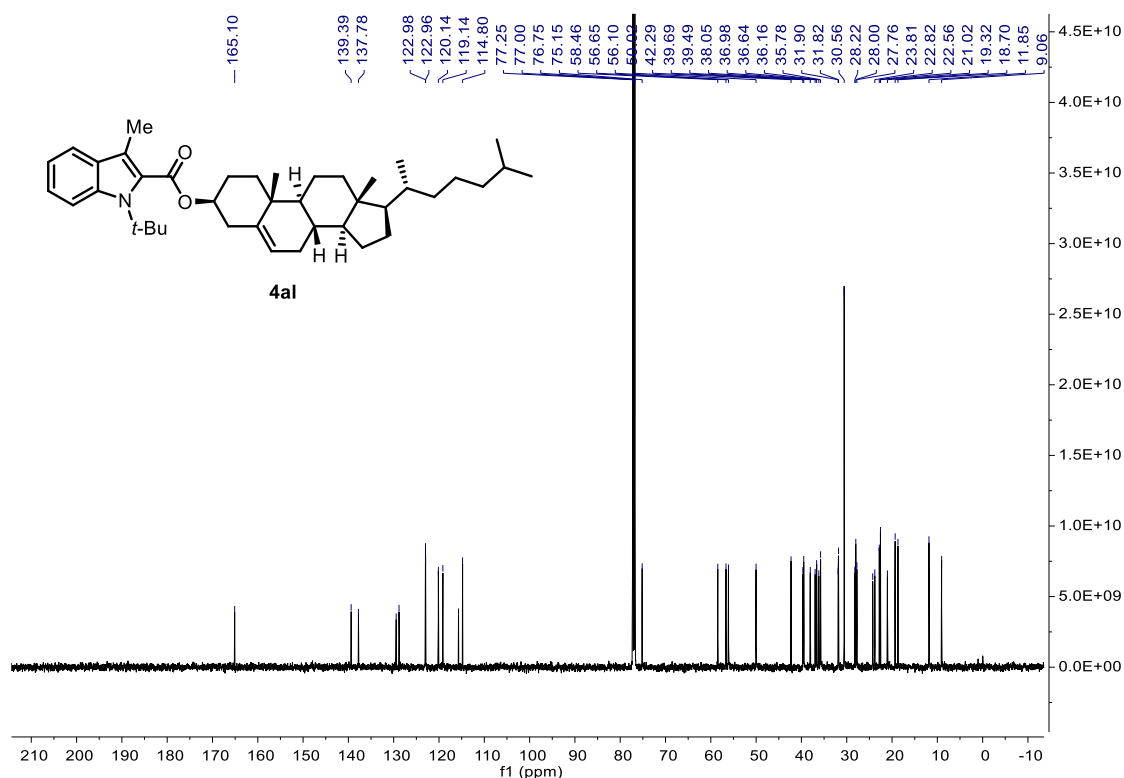
1-(*tert*-butyl)-3-methyl-2-(4-(5-(*p*-tolyl)-3-(trifluoromethyl)-1*H*-pyrazol-1-yl)phenyl)-1*H*-indole (4ak) (¹³C NMR 126 MHz, CDCl₃)



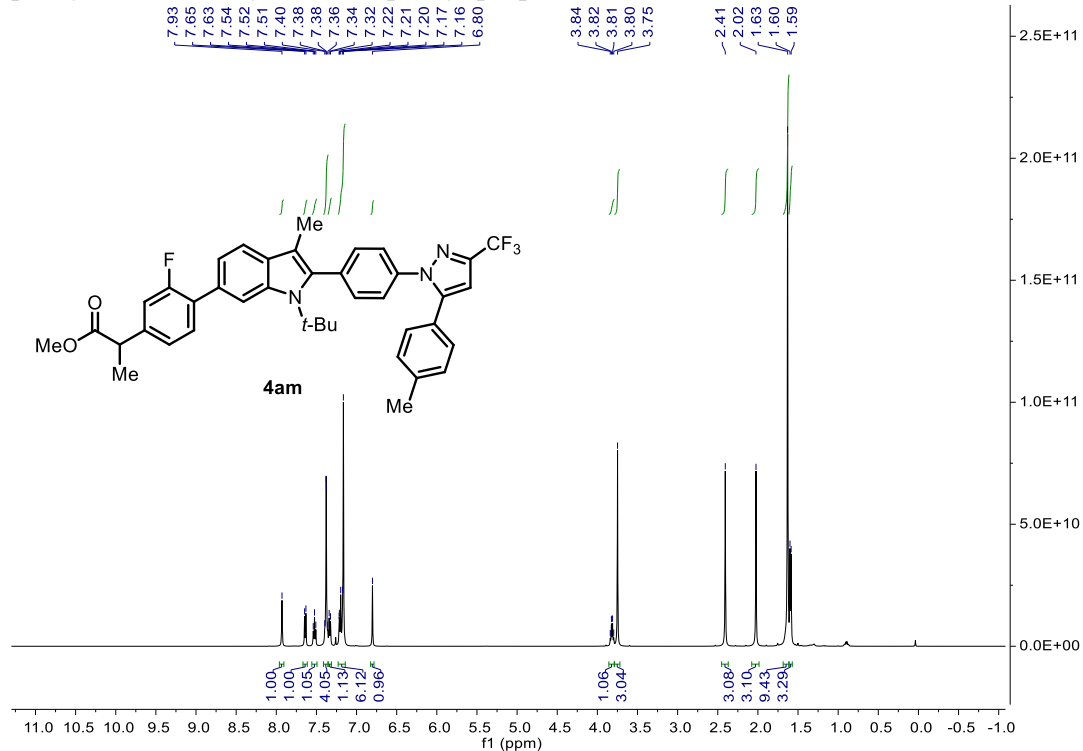
(3*S*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-10,13-dimethyl-17-((*R*)-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl 1-(*tert*-butyl)-3-methyl-1*H*-indole-2-carboxylate (4al) (¹H NMR 500 MHz, CDCl₃)



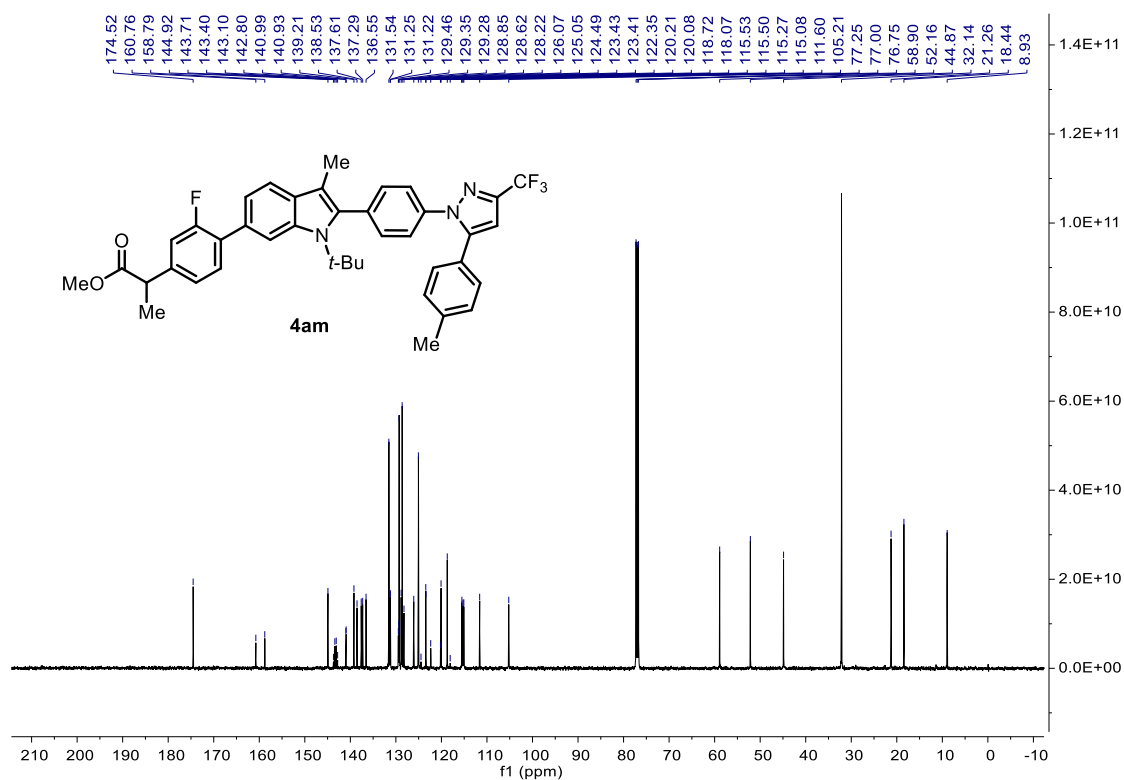
2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl 1-(*tert*-butyl)-3-methyl-1*H*-indole-2-carboxylate (4aI) (¹³C NMR 126 MHz, CDCl₃)



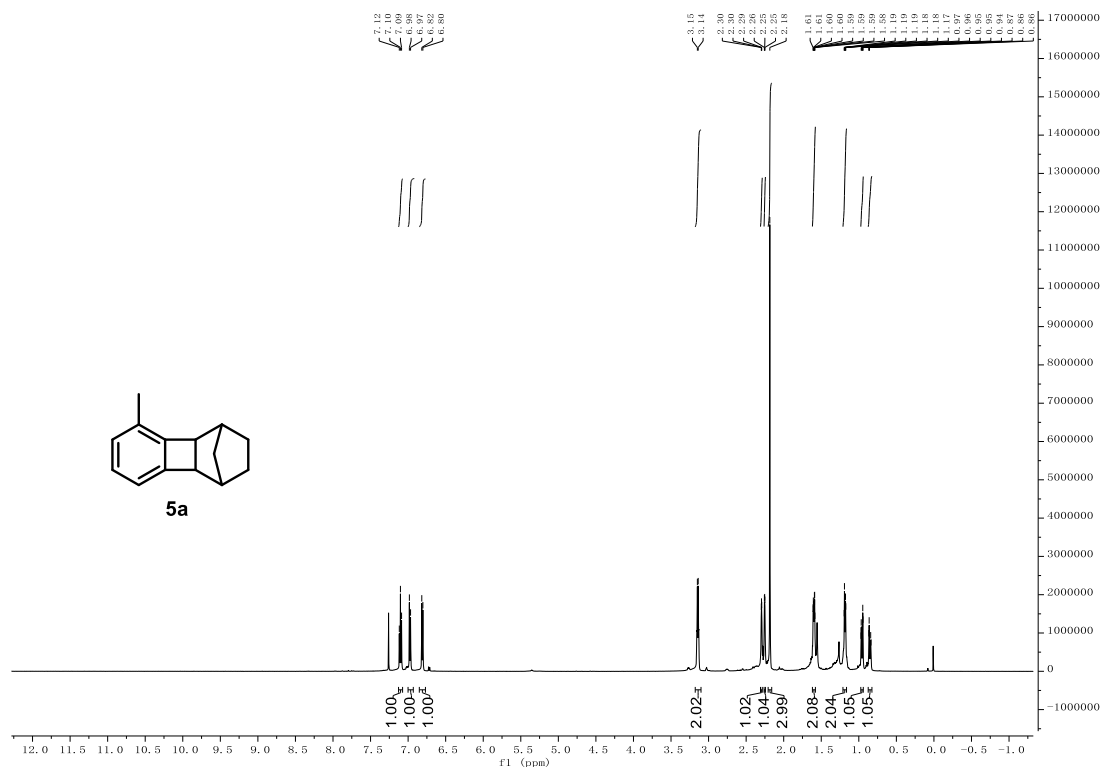
methyl 2-(4-(1-(*tert*-butyl)-3-methyl-2-(4-(5-(*p*-tolyl)-3-(trifluoromethyl)-1*H*-pyrazol-1-yl)phenyl)-1*H*-indol-6-yl)-3-fluorophenyl)propanoate (4am) (¹H NMR 500 MHz, CDCl₃)



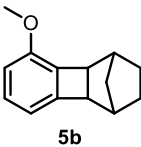
methyl 2-(4-(1-(*tert*-butyl)-3-methyl-2-(4-(5-(*p*-tolyl)-3-(trifluoromethyl)-1*H*-pyrazol-1-yl)phenyl)-1*H*-indol-6-yl)-3-fluorophenyl)propanoate (4am) (¹³C NMR 126 MHz, CDCl₃)



5-methyl-1,2,3,4,4a,8b-hexahydro-1,4-methanobiphenylene (5a) (^1H NMR 500 MHz, CDCl_3)

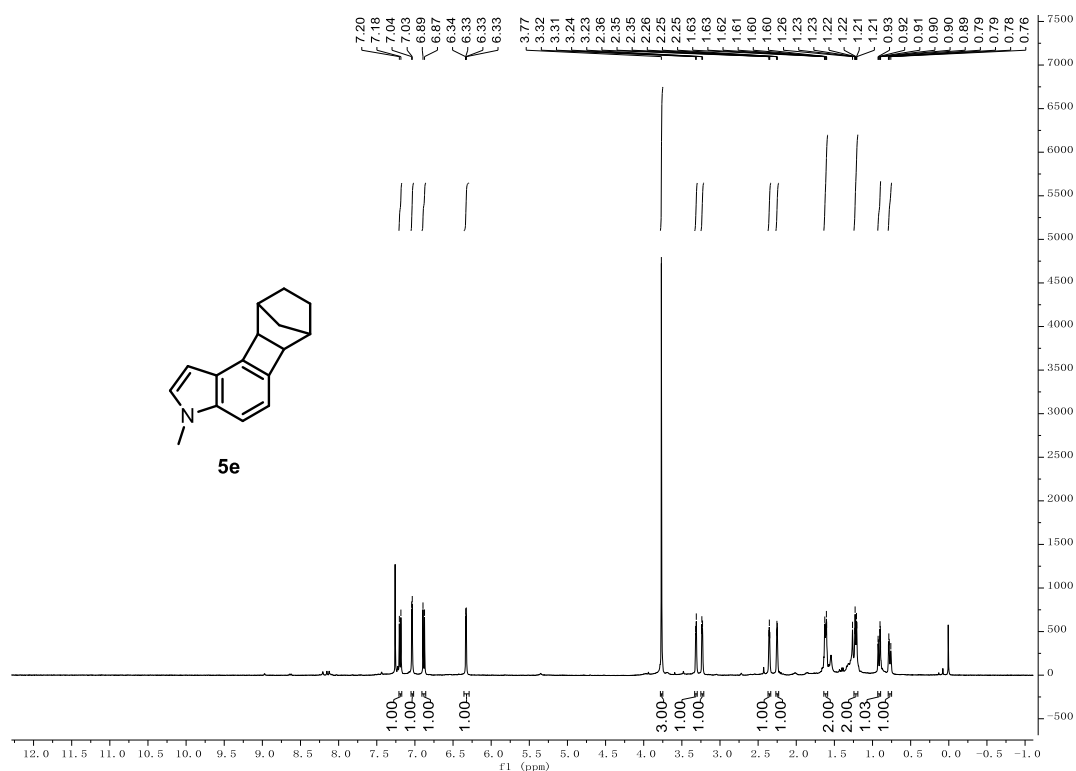


5-methoxy-1,2,3,4,4a,8b-hexahydro-1,4-methanobiphenylene (5b) (^1H NMR 400 MHz, CDCl_3)

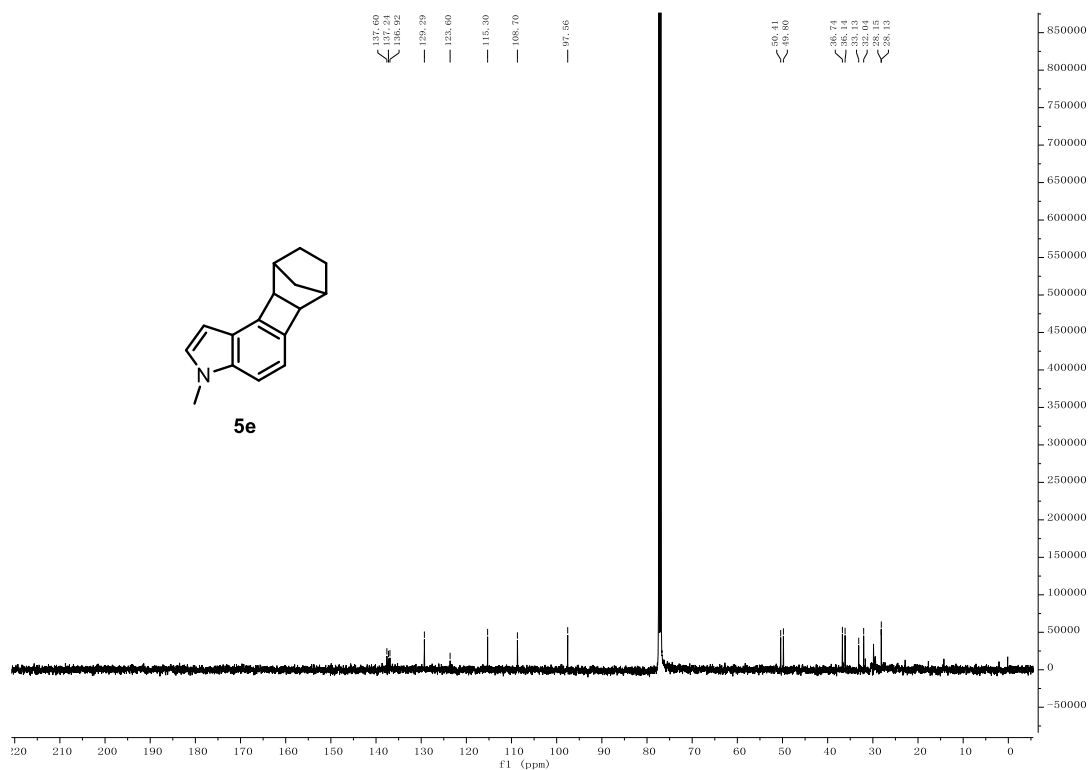


5c

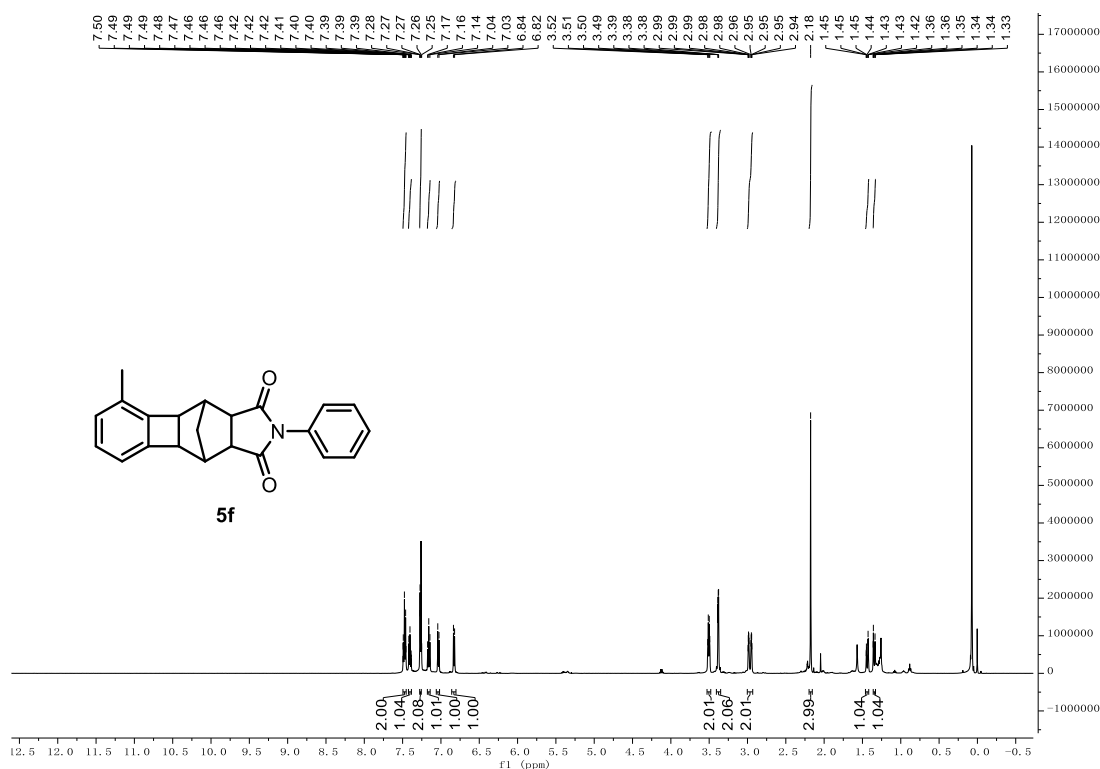
5b,6,7,8,9,9a-hexahydro-6,9-methanobiphenyleno[2,1-*b*]furan (5d) (¹H NMR 500 MHz, CDCl₃)

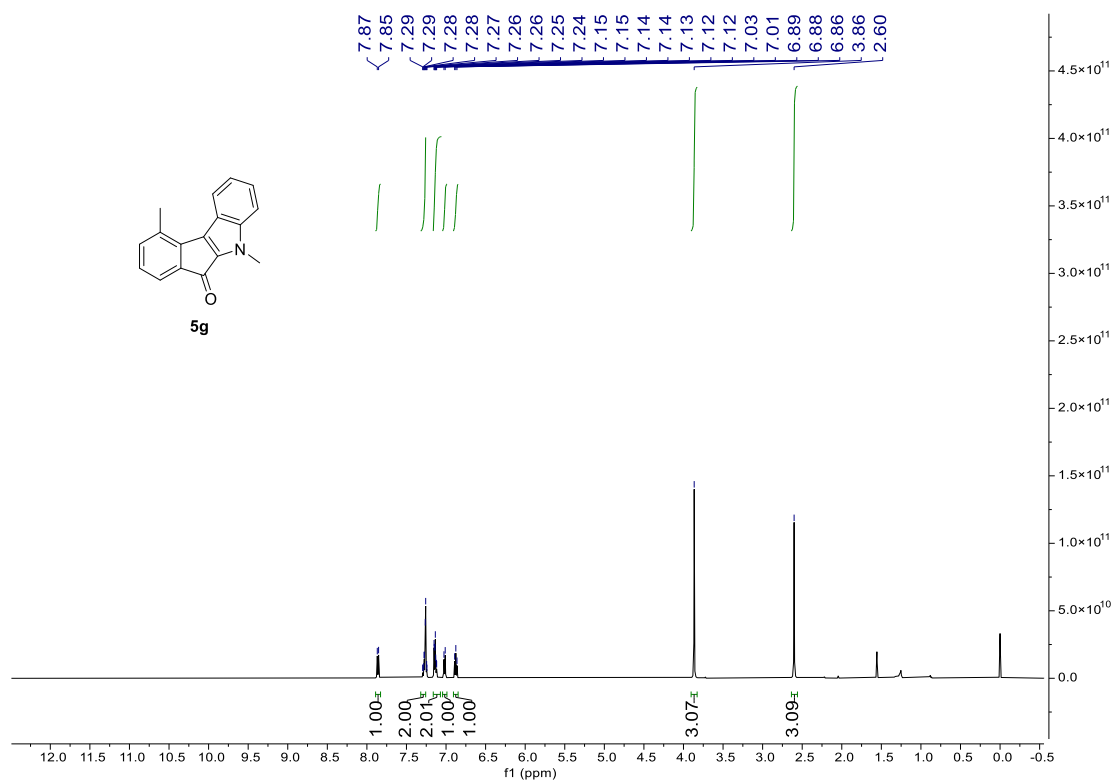


3-methyl-5b,6,7,8,9,9a-hexahydro-3*H*-6,9-methanobenzo[3,4]cyclobuta[1,2-*e*]indole (5e) (¹³C NMR 126 MHz, CDCl₃)

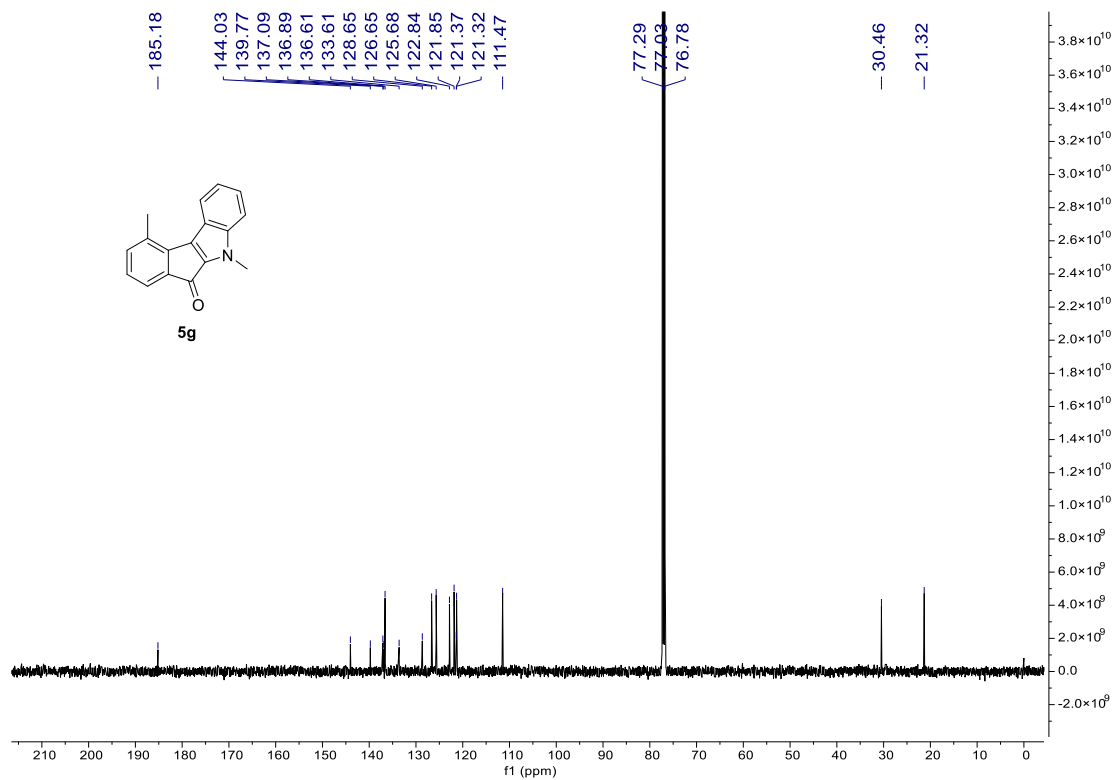


5-methyl-2-phenyl-3a,4,4a,8b,9,9a-hexahydro-1*H*-4,9-methanobenzo[3,4]cyclobuta[1,2-*f*]isoindole-1,3(2*H*)-dione (5f) (¹H NMR 500 MHz, CDCl₃)

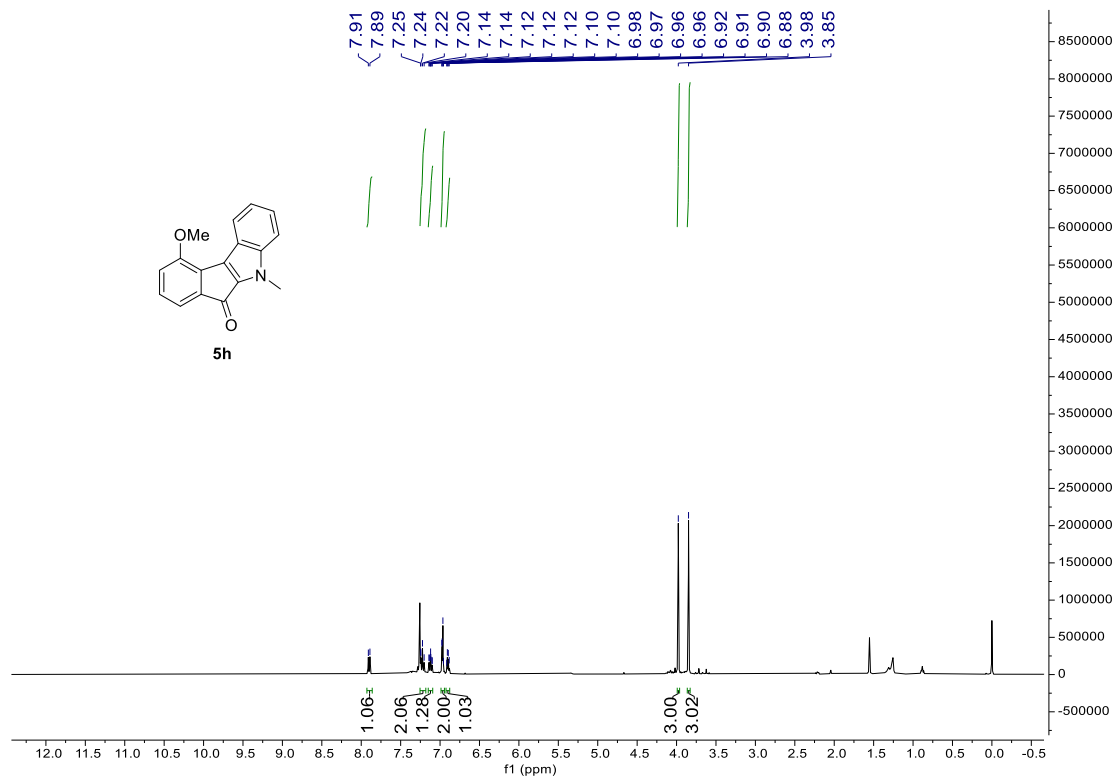




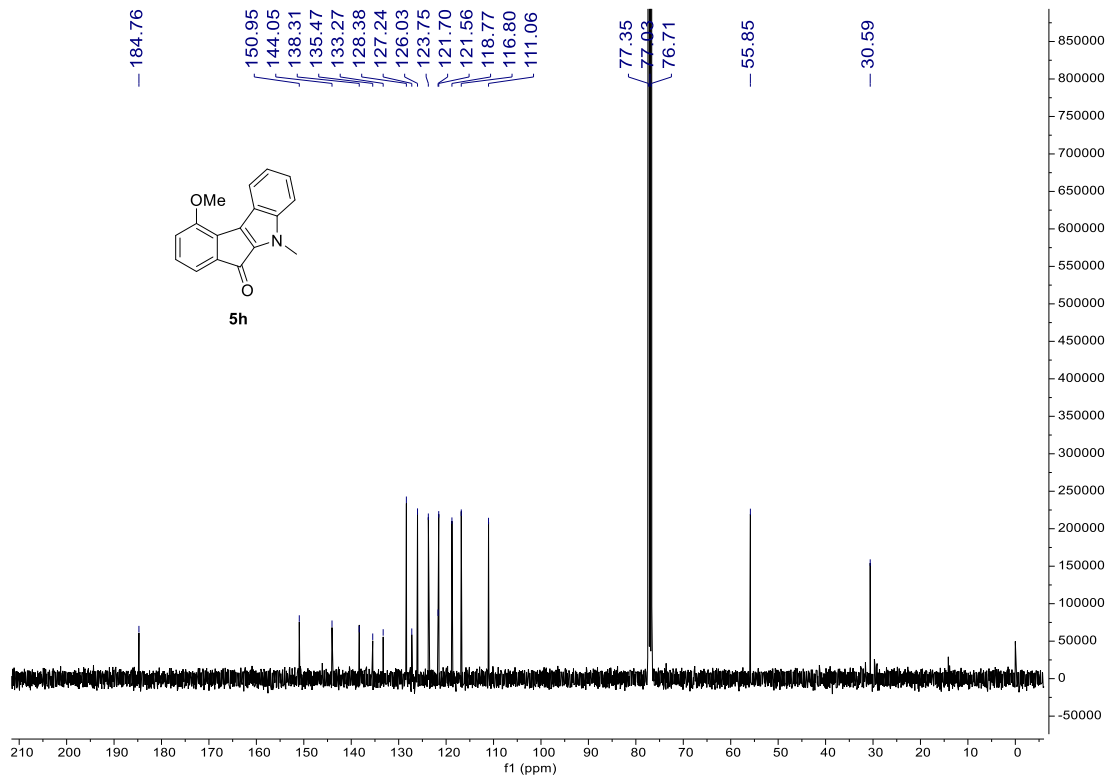
5,10-dimethylindeno[2,1-*b*]indol-6(5H)-one (5g) (¹³C NMR 126 MHz, CDCl₃)



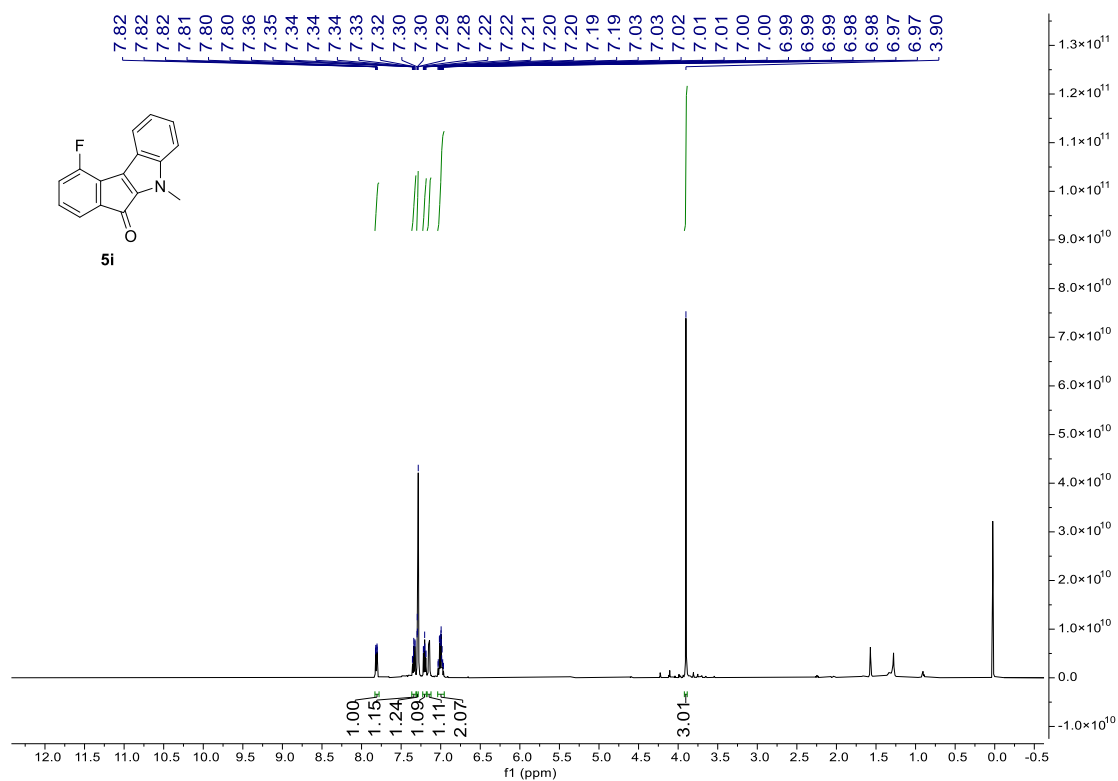
10-methoxy-5-methylindeno[2,1-*b*]indol-6(5*H*)-one (5h) (¹H NMR 400 MHz, CDCl₃)



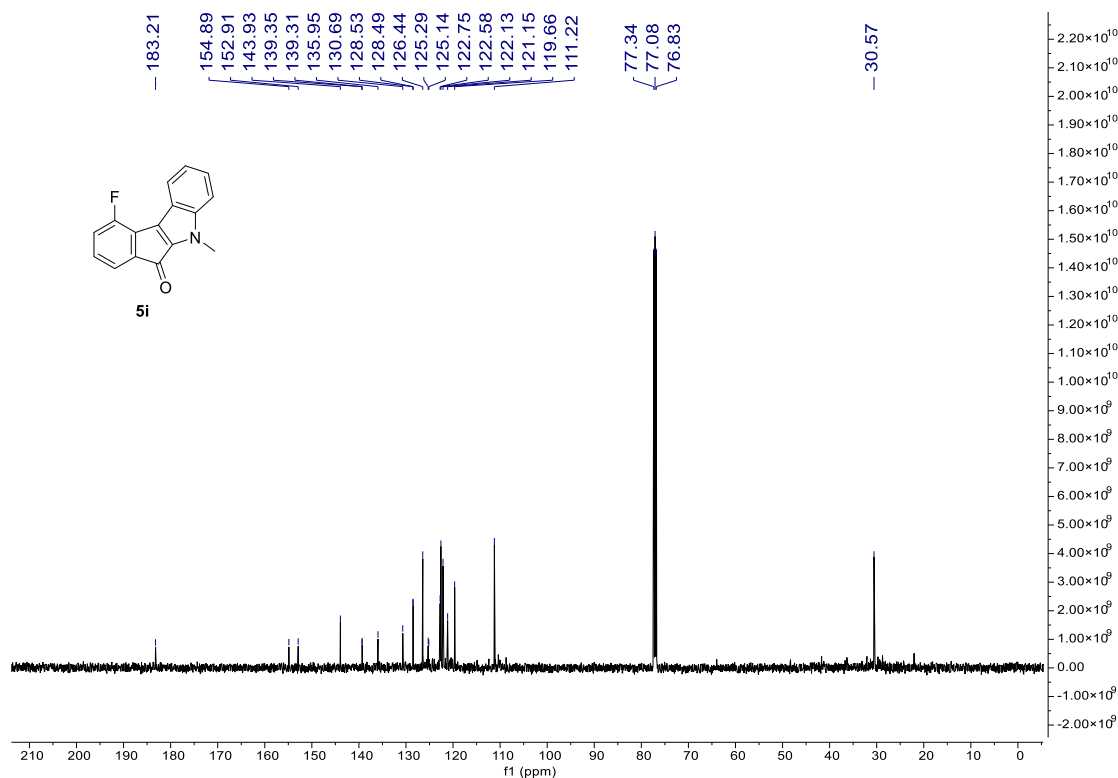
10-methoxy-5-methylindeno[2,1-*b*]indol-6(5*H*)-one (5h) (¹³C NMR (101 MHz, CDCl₃)



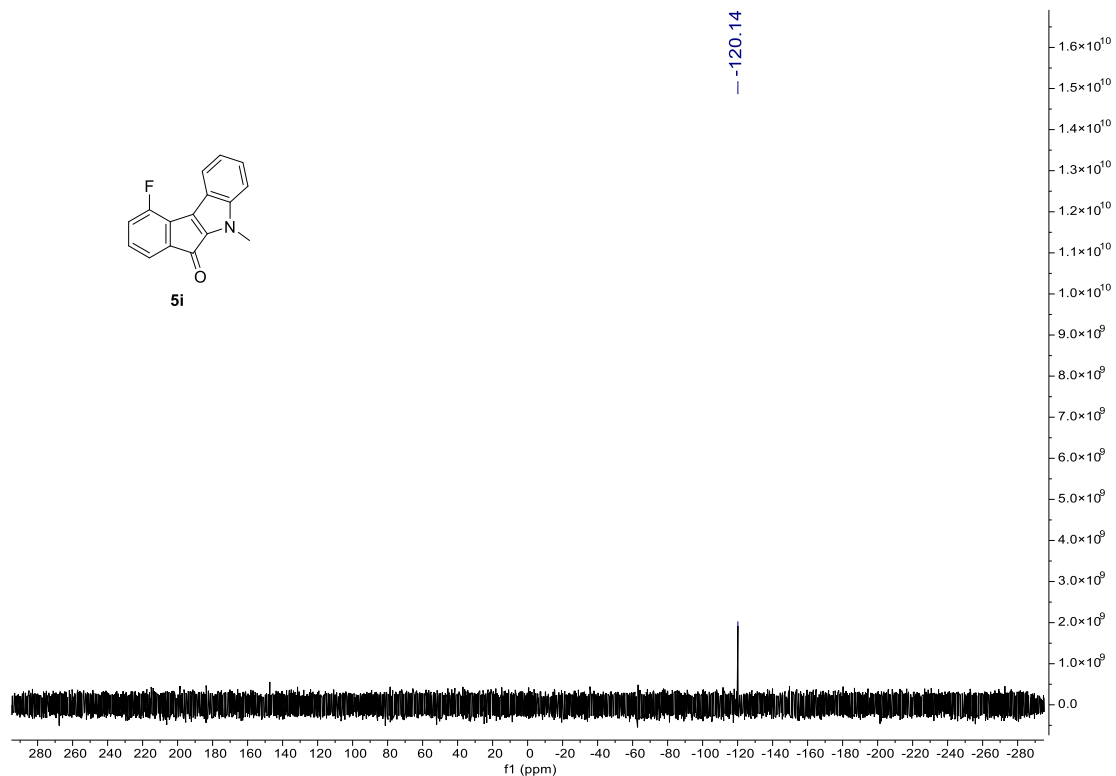
10-fluoro-5-methylindeno[2,1-*b*]indol-6(5*H*)-one (5i) (¹H NMR 500 MHz, CDCl₃)



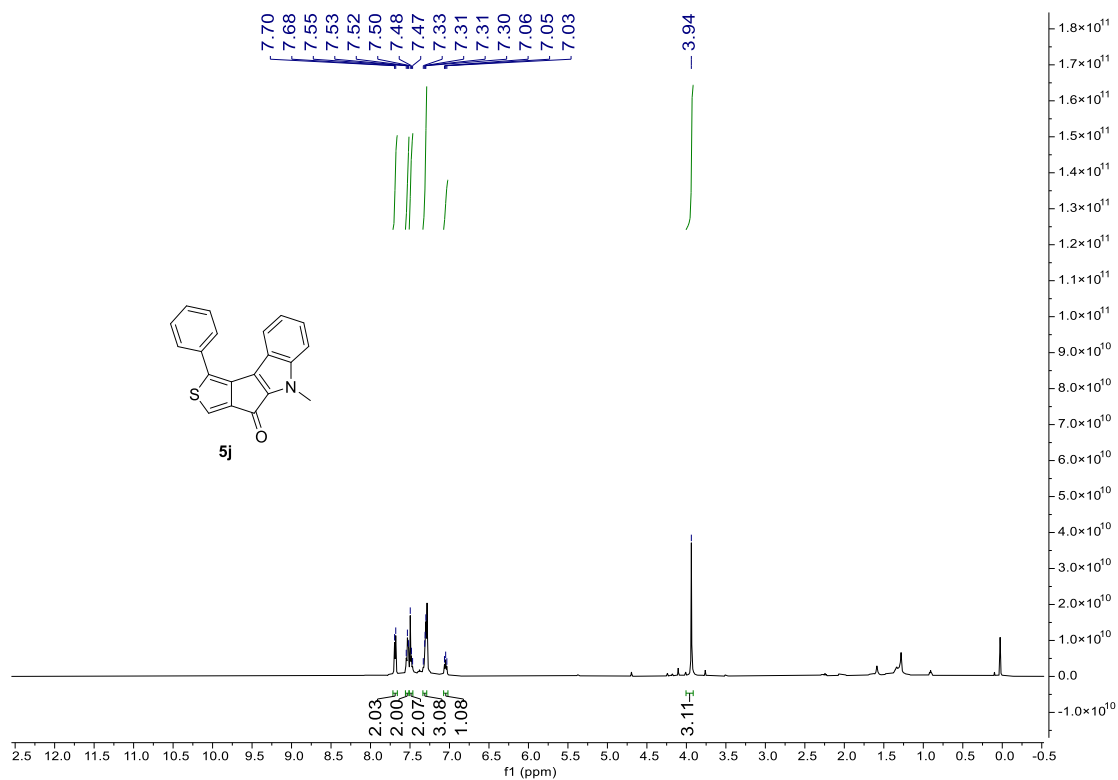
10-fluoro-5-methylindeno[2,1-*b*]indol-6(5*H*)-one (5i) (¹³C NMR 126 MHz, CDCl₃)



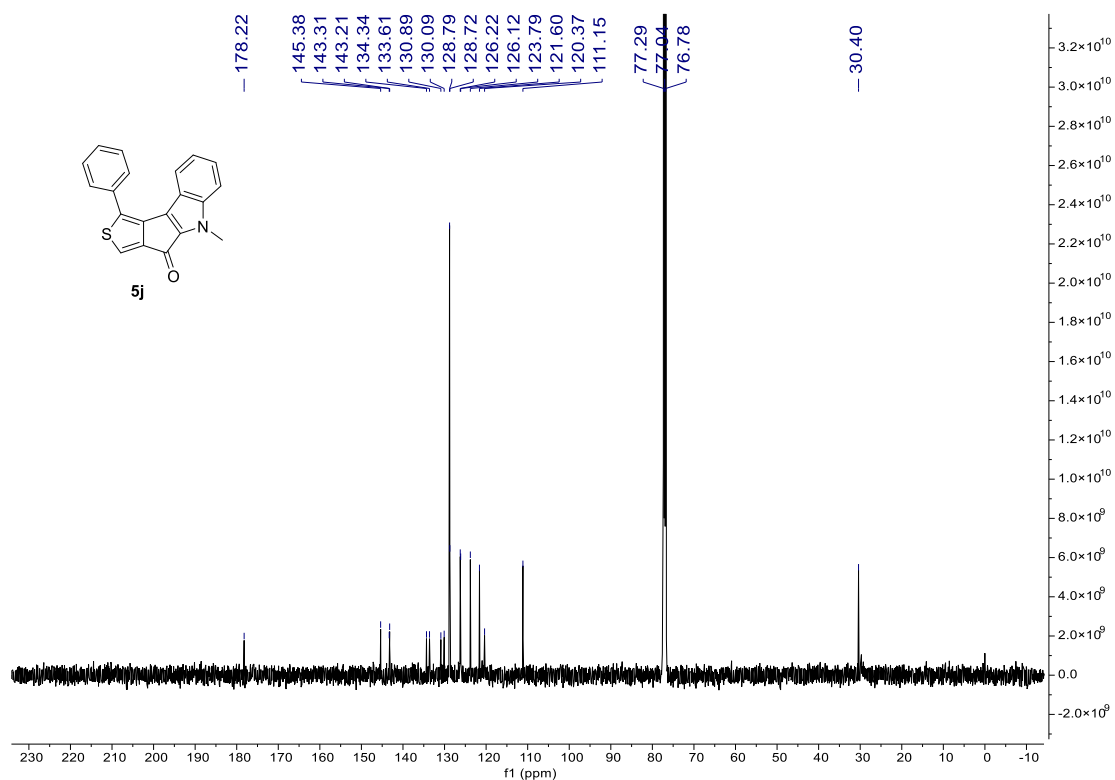
10-fluoro-5-methylindeno[2,1-*b*]indol-6(5*H*)-one (5i) (¹⁹F NMR 471 MHz, CDCl₃)



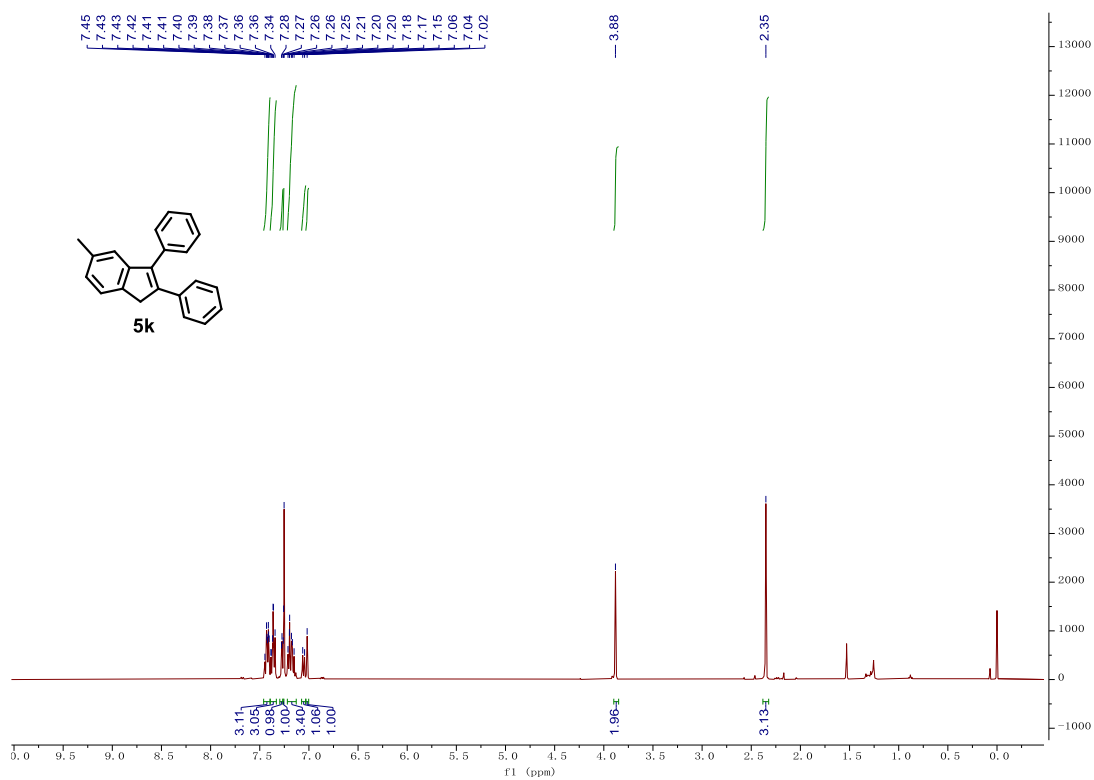
5-methyl-1-phenylthieno[3',4':3,4]cyclopenta[1,2-*b*]indol-4(5*H*)-one (5j) (¹H NMR 500 MHz, CDCl₃)



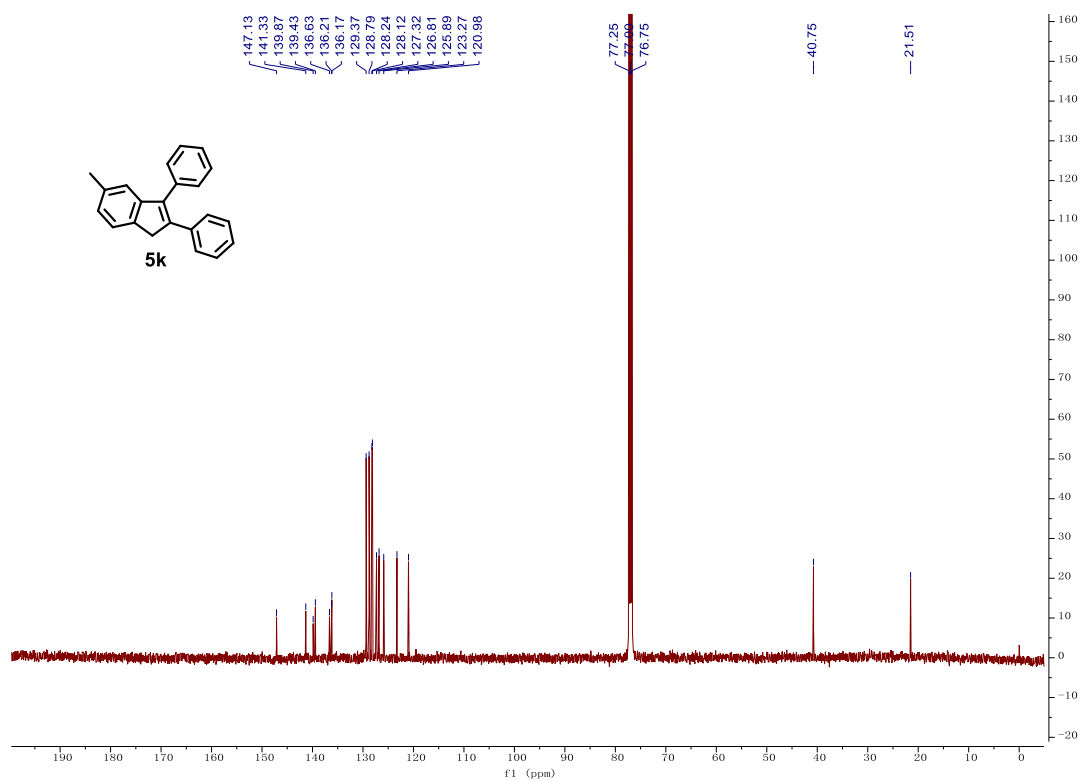
5-methyl-1-phenylthieno[3',4':3,4]cyclopenta[1,2-*b*]indol-4(5*H*)-one (5j) (^{13}C NMR 126 MHz, CDCl_3)



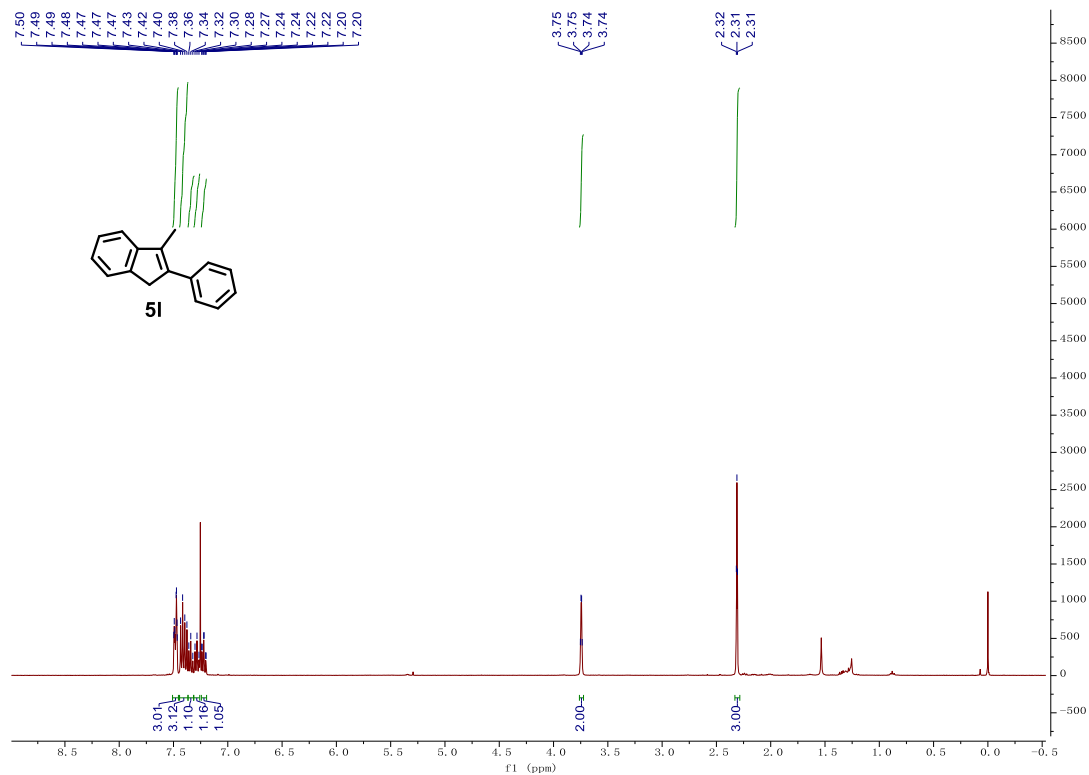
5-methyl-2,3-diphenyl-1H-indene (5k) (^1H NMR 400 MHz, CDCl_3)



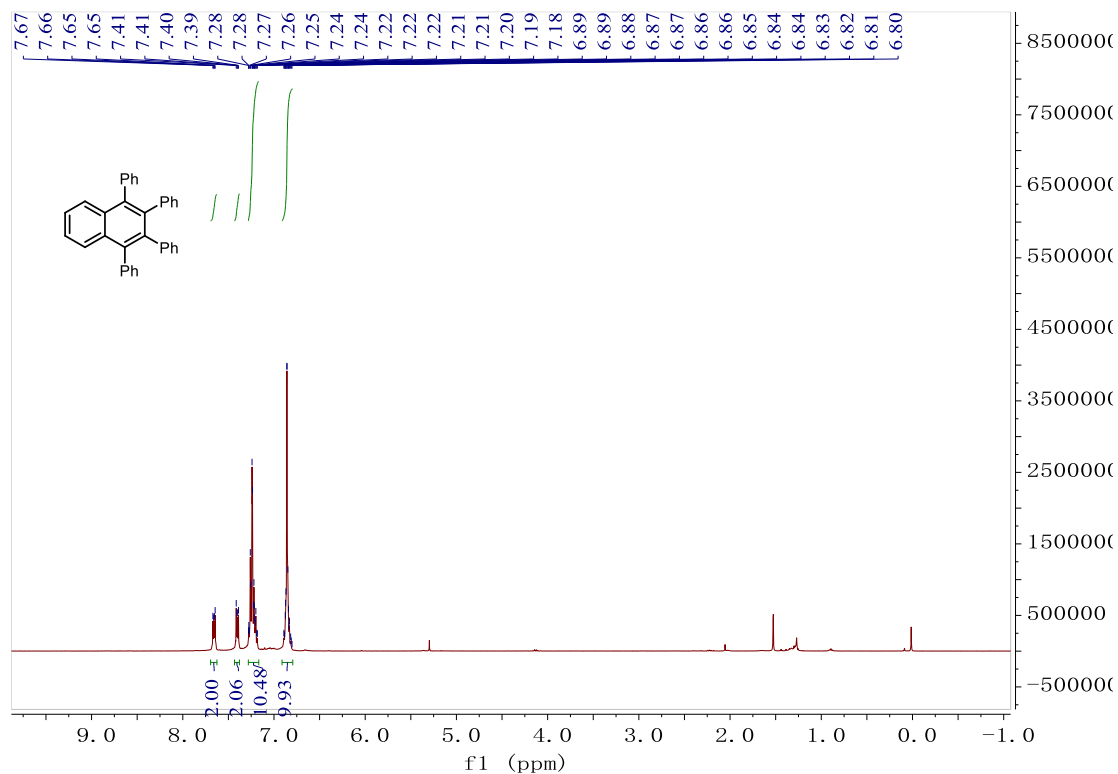
5-methyl-2,3-diphenyl-1H-indene (5k) (^{13}C NMR 126 MHz, CDCl_3)



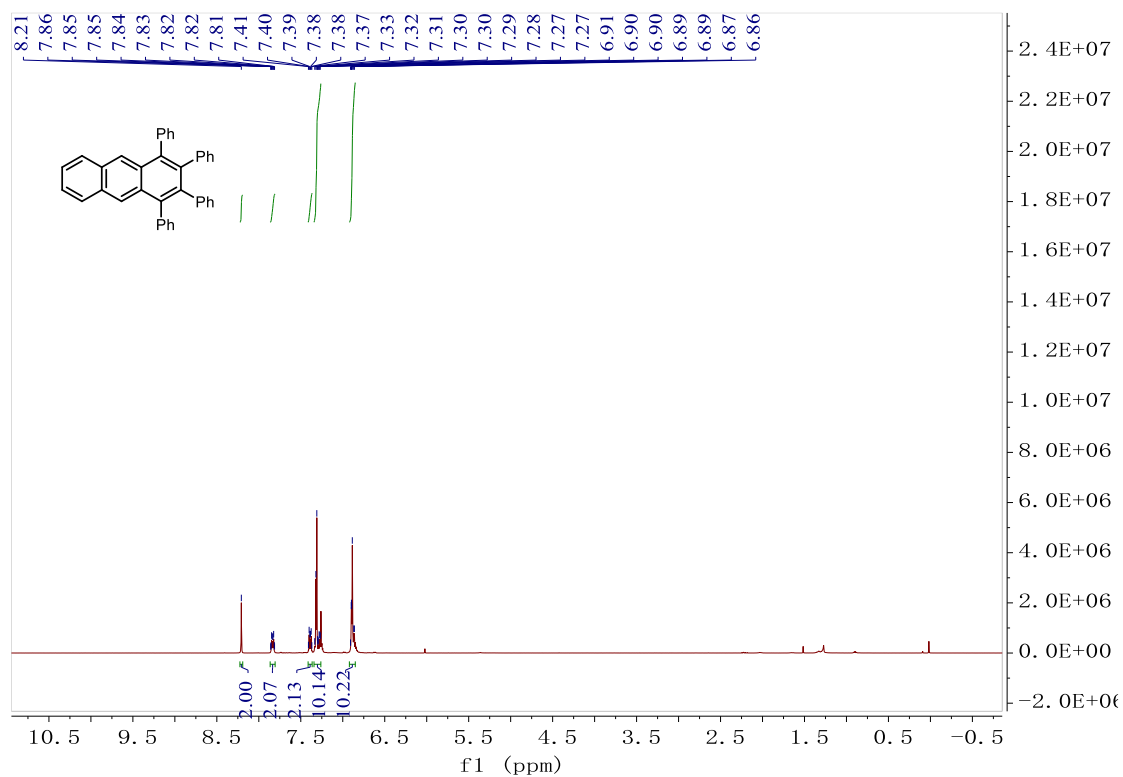
3-methyl-2-phenyl-1H-indene (5l) (^1H NMR 400 MHz, CDCl_3)



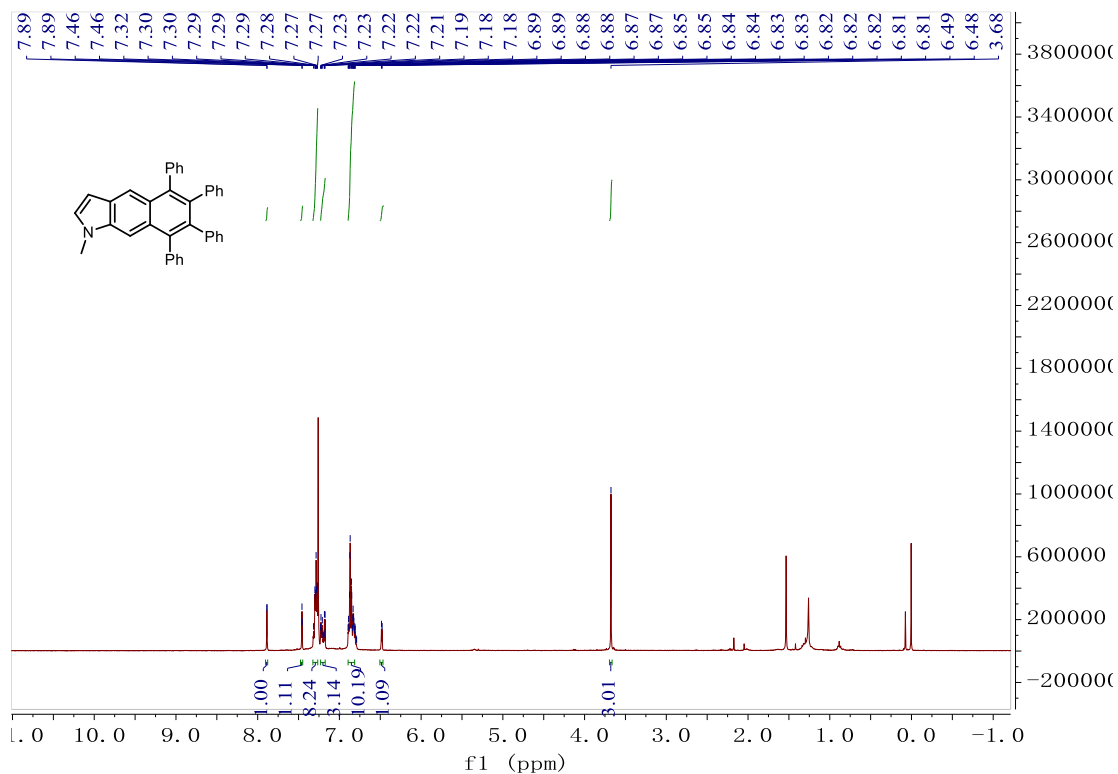
1,2,3,4-tetraphenylanthracene (5m) (^1H NMR 400 MHz, CDCl_3)



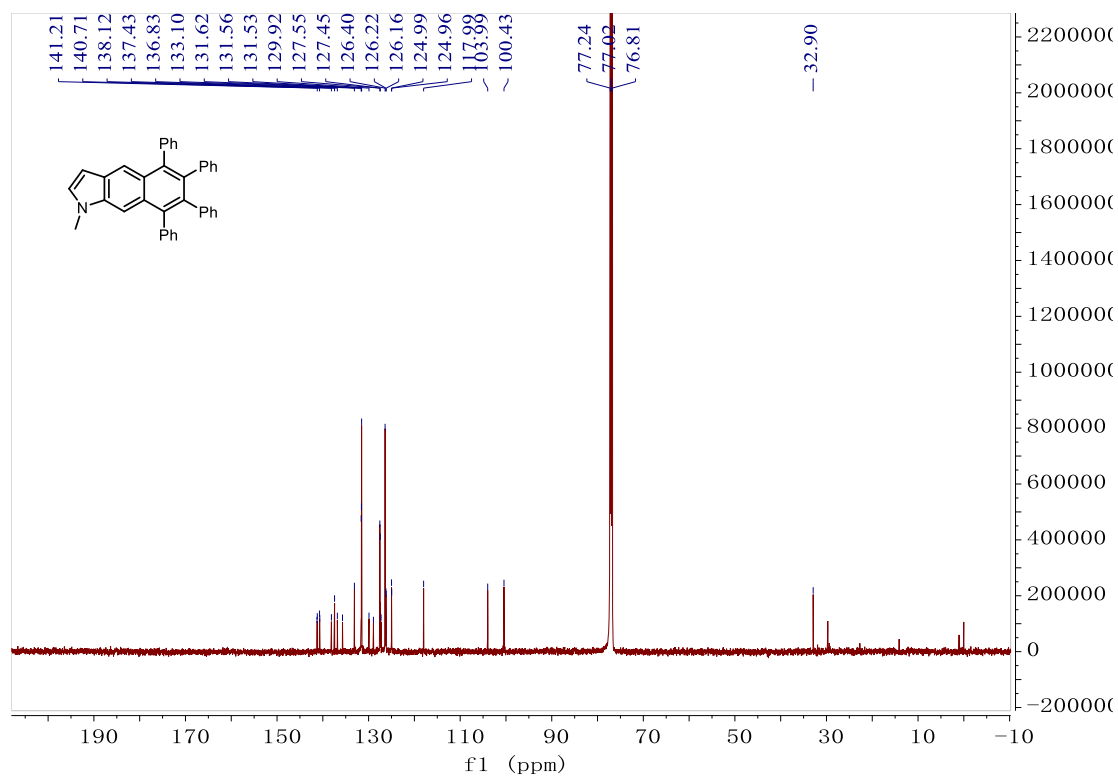
1,2,3,4-tetraphenylanthracene (5n) (^1H NMR 400 MHz, CDCl_3)



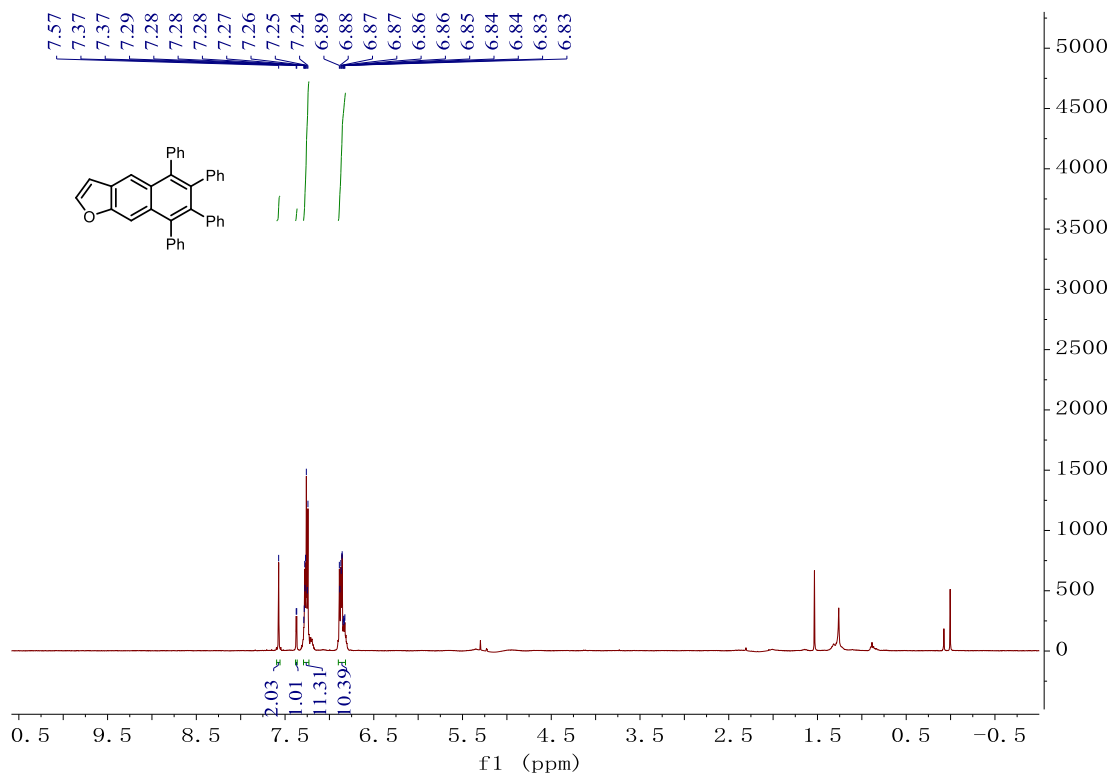
1-methyl-5,6,7,8-tetraphenyl-1*H*-benzo[*f*]indole (5o) (¹H NMR 400 MHz, CDCl₃)



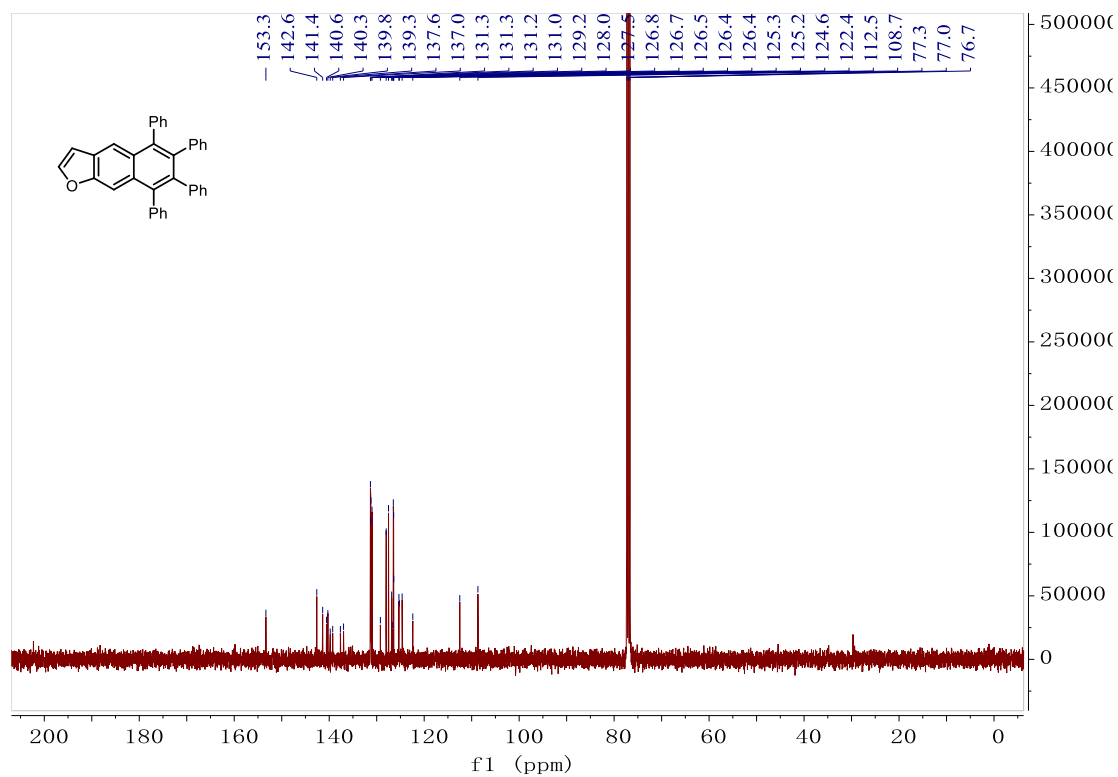
1-methyl-5,6,7,8-tetraphenyl-1*H*-benzo[*f*]indole (5o) (¹³C NMR 151 MHz, CDCl₃)



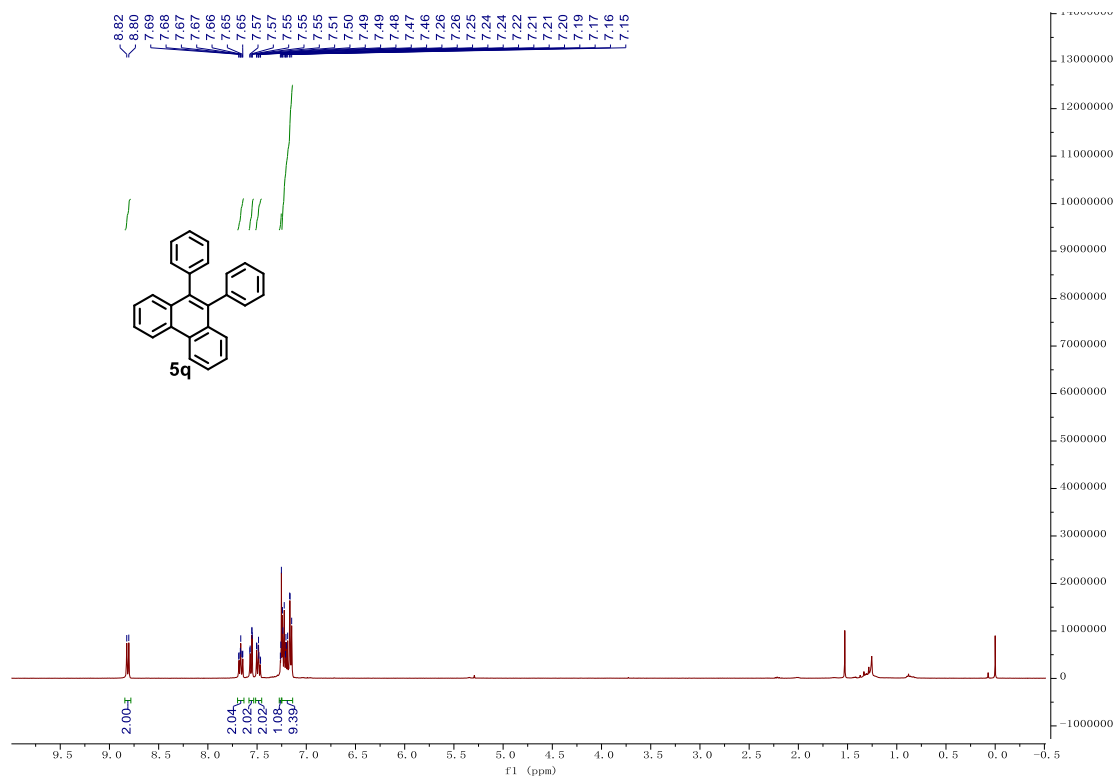
5,6,7,8-tetraphenylnaphtho[2,3-*b*]furan (5p) (¹H NMR 400 MHz, CDCl₃)



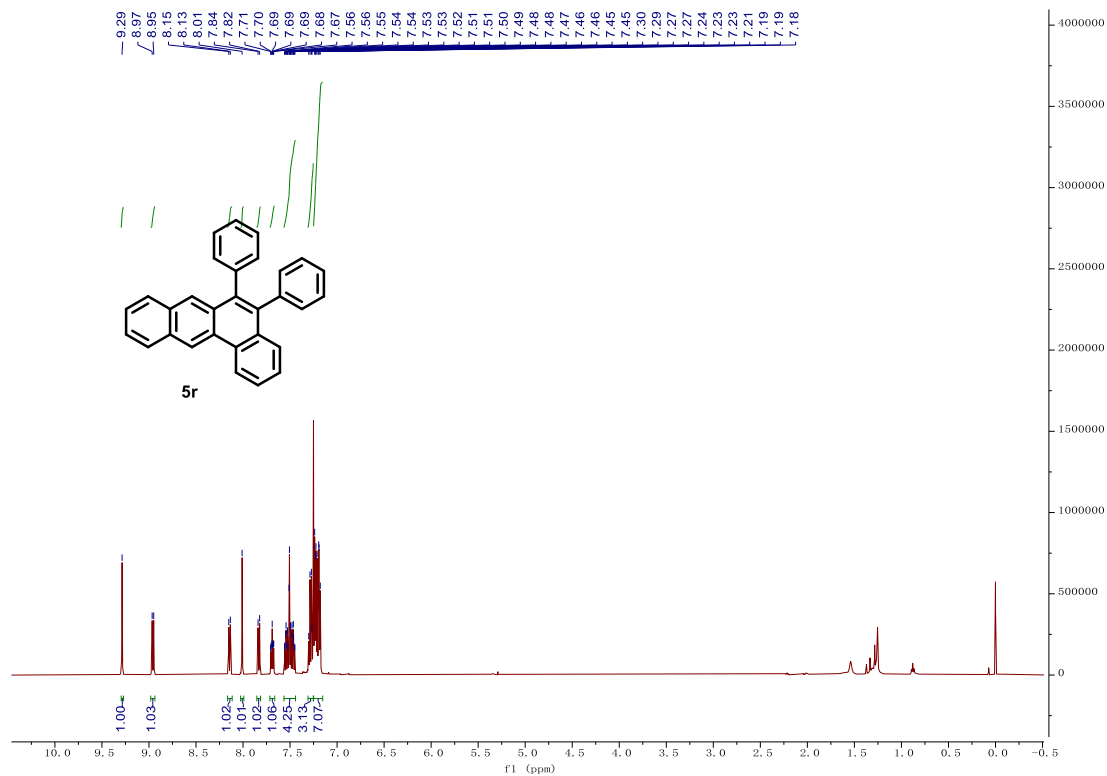
5,6,7,8-tetraphenylnaphtho[2,3-*b*]furan (5p) (¹³C NMR 101 MHz, CDCl₃)



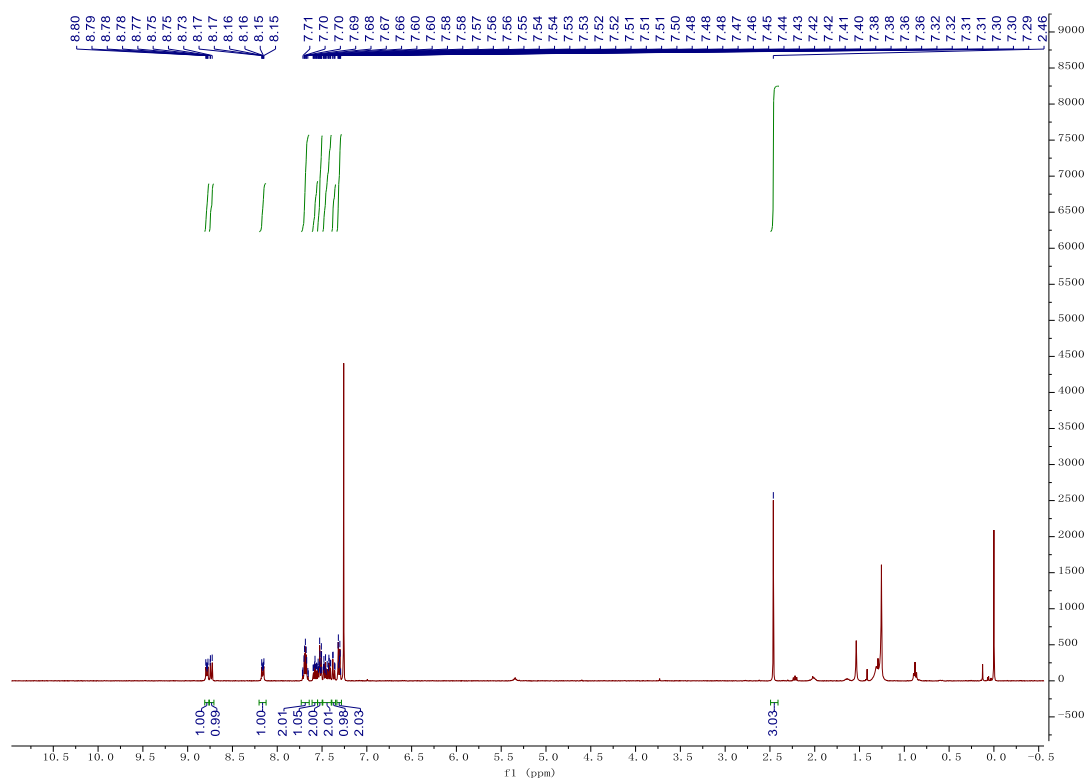
9,10-diphenylphenanthrene (5q) (^1H NMR 400 MHz, CDCl_3)



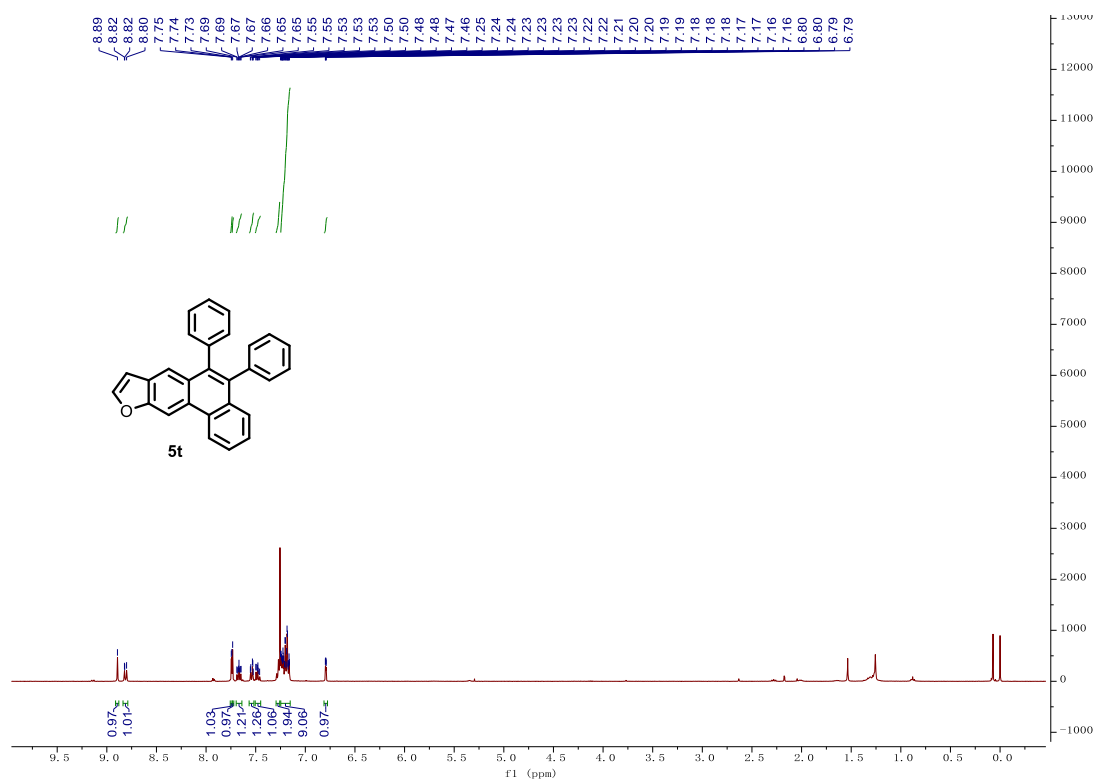
5,6-diphenyltetraphene (5r) (^1H NMR 500 MHz, CDCl_3)



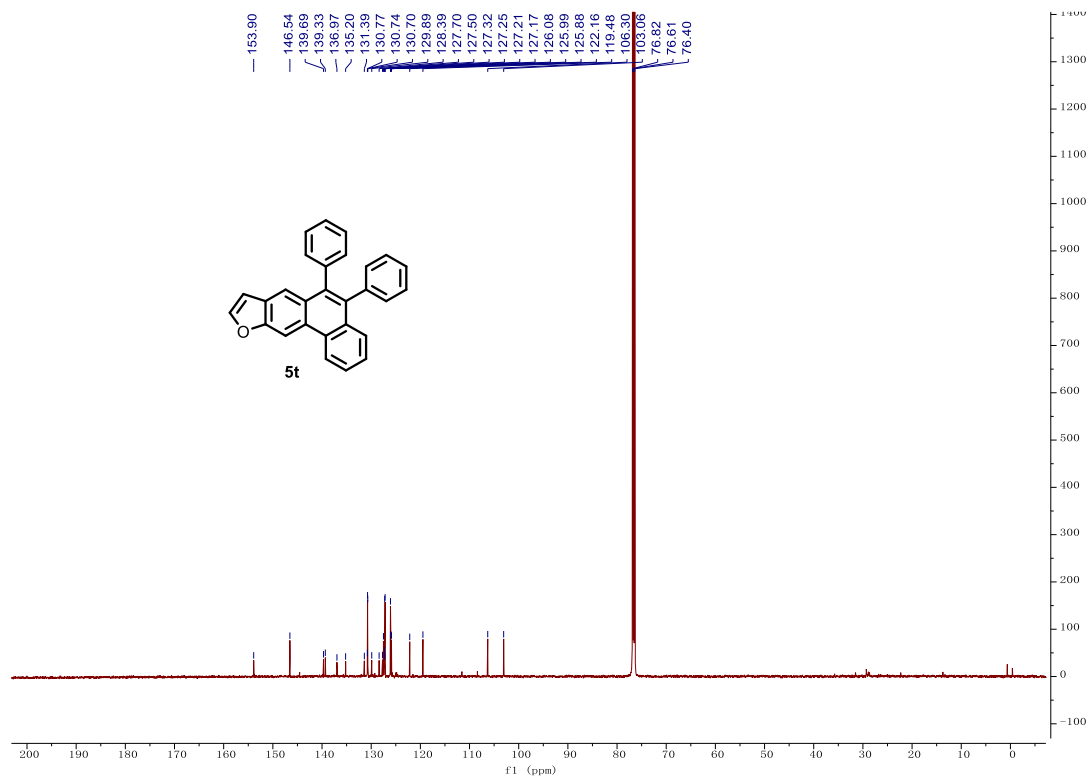
9-methyl-10-phenylphenanthrene (5s) (¹H NMR 400 MHz, CDCl₃)



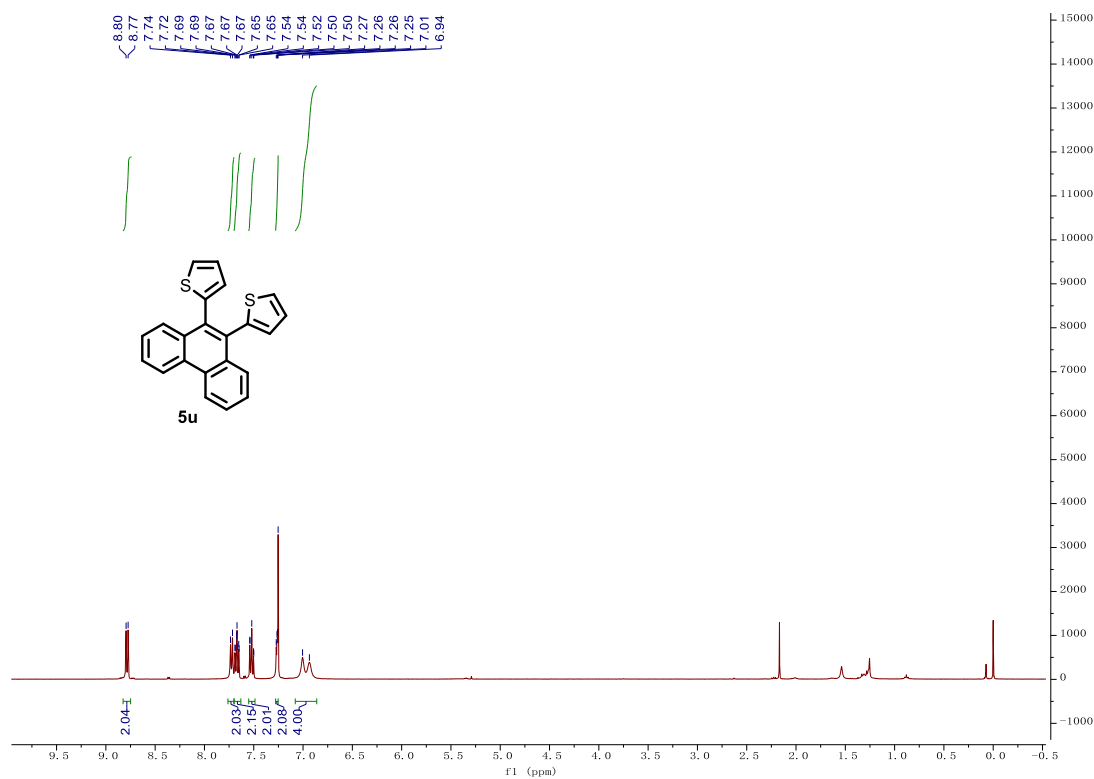
5,6-diphenylphenanthro[3,2-b]furan (5t) (¹H NMR 400 MHz, CDCl₃)



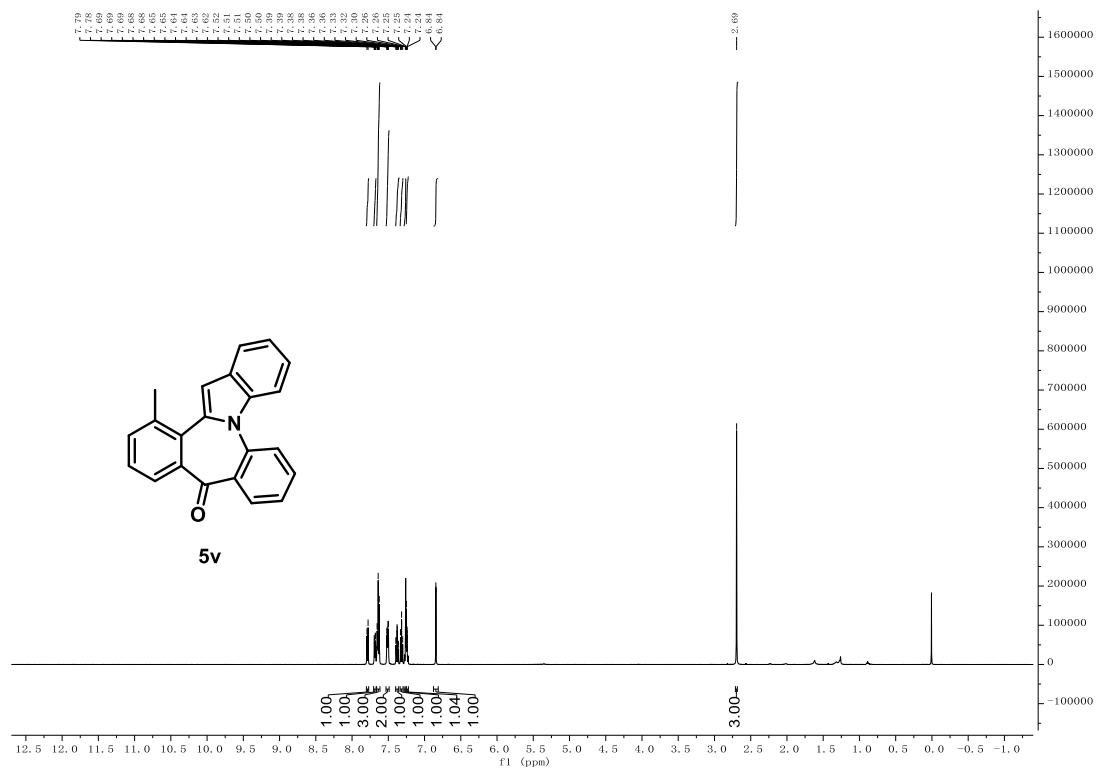
5,6-diphenylphenanthro[3,2-b]furan (5t) (^{13}C NMR 151 MHz, CDCl_3)



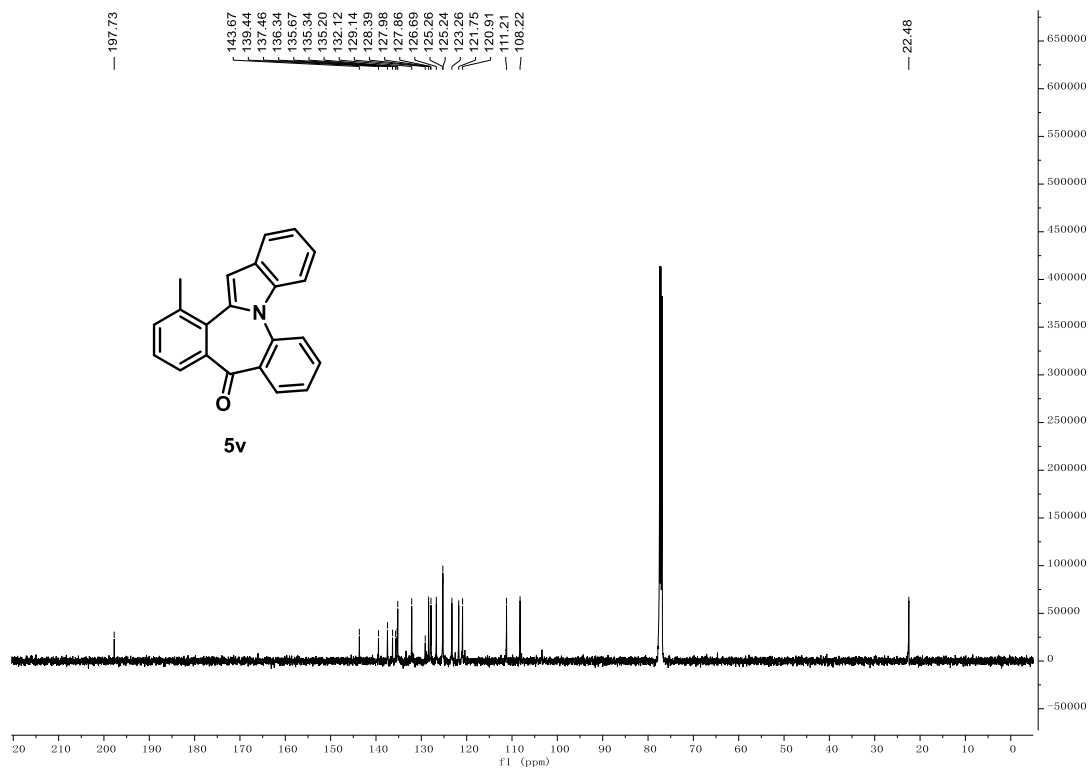
9,10-di(thiophen-2-yl)phenanthrene (5u) (^1H NMR 400 MHz, CDCl_3)



14-methyl-10*H*-dibenzo[3,4:6,7]azepino[1,2-*a*]indol-10-one (5v) (¹H NMR 400 MHz, CDCl₃)



14-methyl-10*H*-dibenzo[3,4:6,7]azepino[1,2-*a*]indol-10-one (5v) (¹³C NMR 126 MHz, CDCl₃)

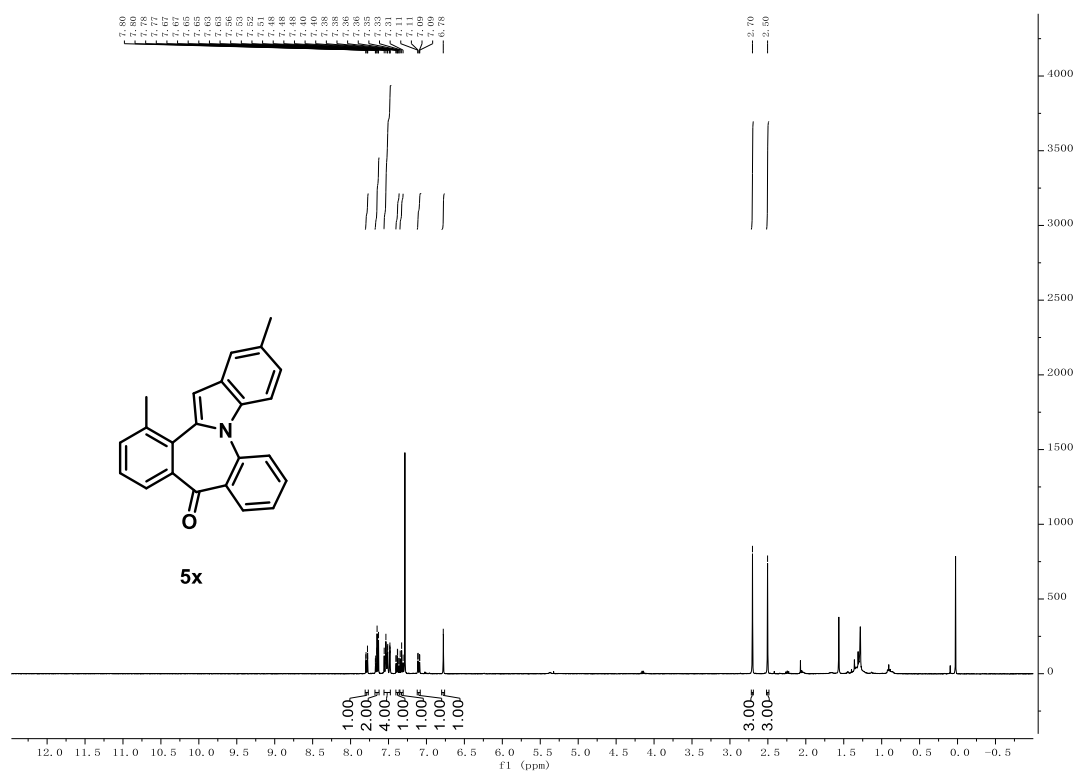


Chemical structure of **5w** is shown as an inset. The ^1H NMR spectrum (CDCl₃) displays peaks from 0 to 8 ppm. Integration values are provided below the baseline: 1.00, 1.00, 3.00, 2.00, 2.00, 1.93, 0.98, and 2.99. A list of chemical shifts (δ) is shown at the top of the spectrum, ranging from 7.75 to 1.18 ppm.

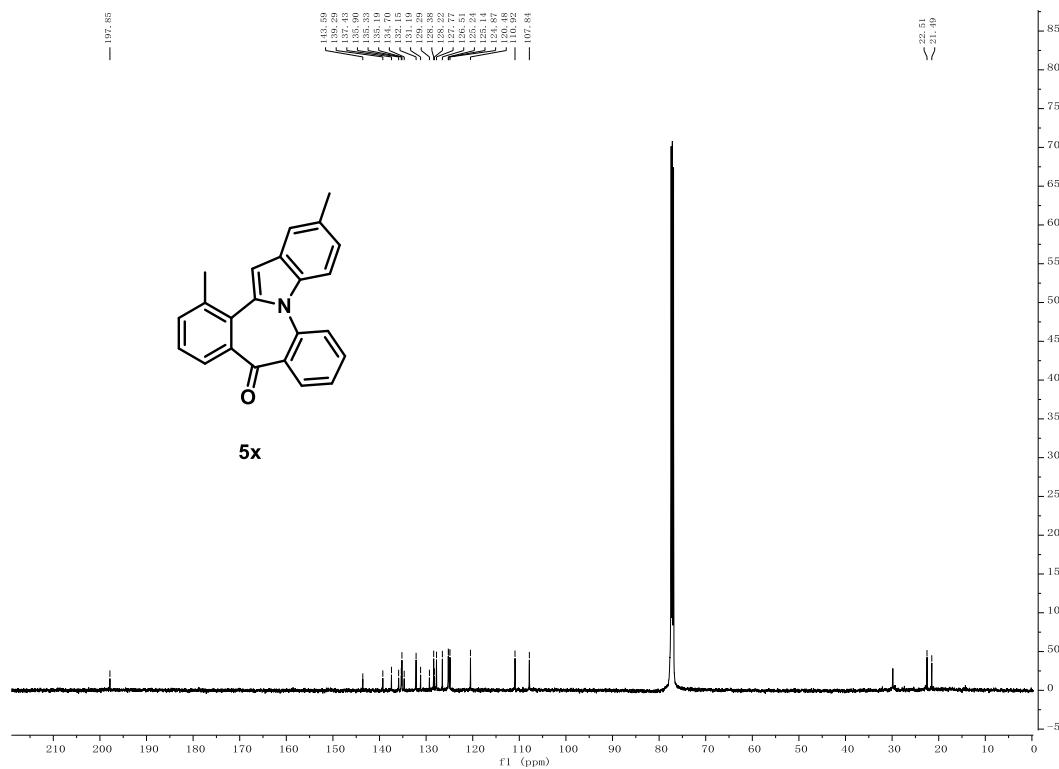
[illegible]

S179

CDCl₃)



2,14-dimethyl-10H-dibenzo[3,4:6,7]azepino[1,2-a]indol-10-one (5x) (¹³C NMR 126 MHz, CDCl₃)



2-fluoro-14-methyl-10H-dibenzo[3,4:6,7]azepino[1,2-a]indol-10-one (5y) (¹H NMR 500 MHz,

Chemical structure of **5y** is shown above the spectrum.

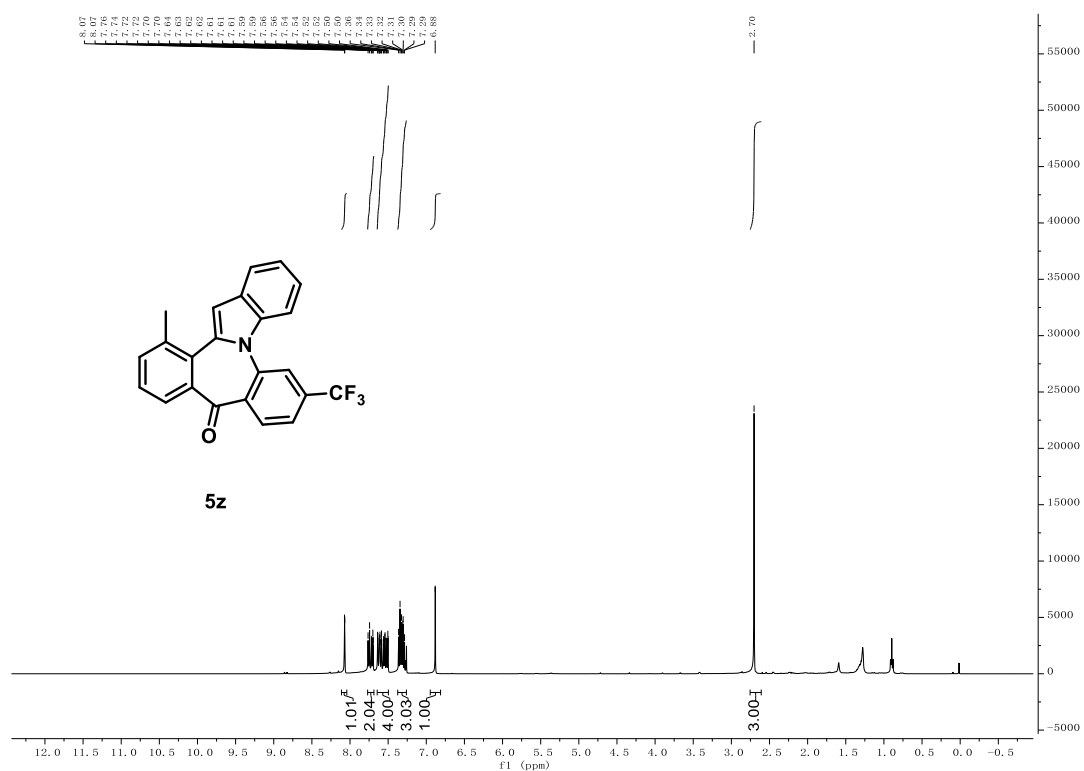
¹H NMR spectrum (CDCl₃) of compound **5y**. The x-axis represents the chemical shift in ppm (δ), ranging from 0 to 10. The y-axis represents the integration value, ranging from 0 to 70. The spectrum shows several peaks corresponding to the protons in the molecule.

Peak list (ppm):

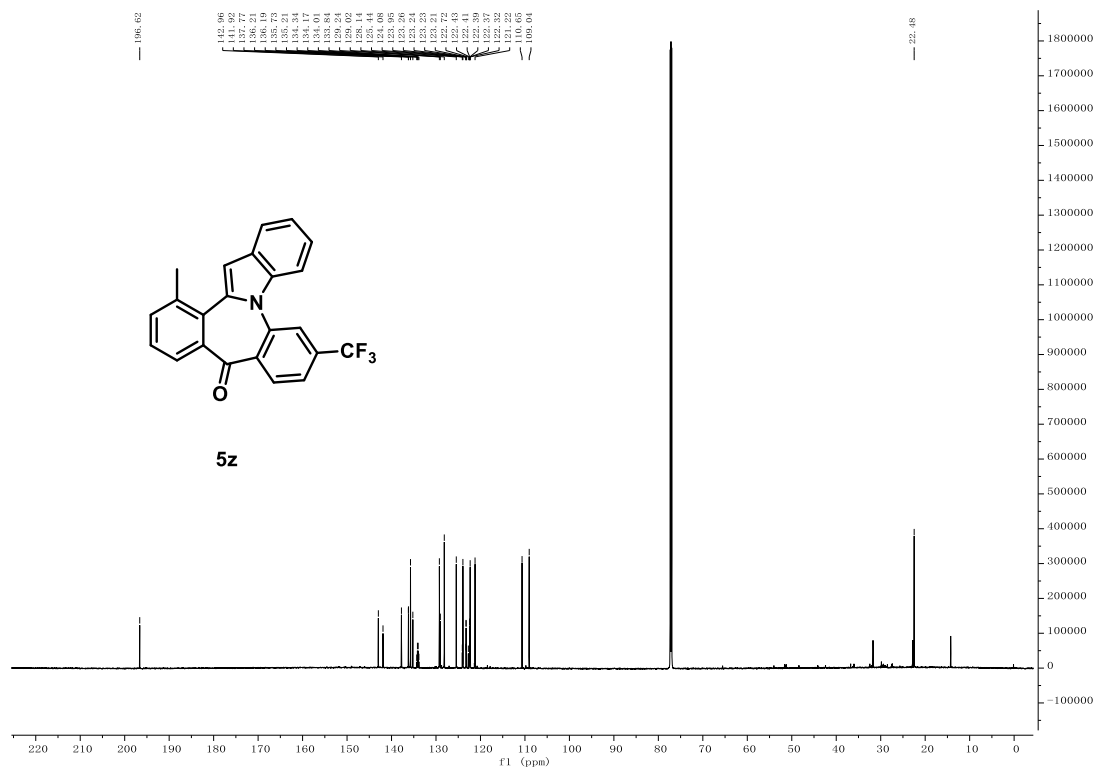
- 8.05, 8.04, 8.03, 8.02, 8.01, 8.00, 7.99, 7.98, 7.97, 7.96, 7.95, 7.94, 7.93, 7.92, 7.91, 7.90, 7.89, 7.88, 7.87, 7.86, 7.85, 7.84, 7.83, 7.82, 7.81, 7.80, 7.79, 7.78, 7.77, 7.76, 7.75, 7.74, 7.73, 7.72, 7.71, 7.70, 7.69, 7.68, 7.67, 7.66, 7.65, 7.64, 7.63, 7.62, 7.61, 7.60, 7.59, 7.58, 7.57, 7.56, 7.55, 7.54, 7.53, 7.52, 7.51, 7.50, 7.49, 7.48, 7.47, 7.46, 7.45, 7.44, 7.43, 7.42, 7.41, 7.40, 7.39, 7.38, 7.37, 7.36, 7.35, 7.34, 7.33, 7.32, 7.31, 7.30, 7.29, 7.28, 7.27, 7.26, 7.25, 7.24, 7.23, 7.22, 7.21, 7.20, 7.19, 7.18, 7.17, 7.16, 7.15, 7.14, 7.13, 7.12, 7.11, 7.10, 7.09, 7.08, 7.07, 7.06, 7.05, 7.04, 7.03, 7.02, 7.01, 7.00, 6.99, 6.98, 6.97, 6.96, 6.95, 6.94, 6.93, 6.92, 6.91, 6.90, 6.89, 6.88, 6.87, 6.86, 6.85, 6.84, 6.83, 6.82, 6.81, 6.80, 6.79, 6.78, 6.77, 6.76, 6.75, 6.74, 6.73, 6.72, 6.71, 6.70, 6.69, 6.68, 6.67, 6.66, 6.65, 6.64, 6.63, 6.62, 6.61, 6.60, 6.59, 6.58, 6.57, 6.56, 6.55, 6.54, 6.53, 6.52, 6.51, 6.50, 6.49, 6.48, 6.47, 6.46, 6.45, 6.44, 6.43, 6.42, 6.41, 6.40, 6.39, 6.38, 6.37, 6.36, 6.35, 6.34, 6.33, 6.32, 6.31, 6.30, 6.29, 6.28, 6.27, 6.26, 6.25, 6.24, 6.23, 6.22, 6.21, 6.20, 6.19, 6.18, 6.17, 6.16, 6.15, 6.14, 6.13, 6.12, 6.11, 6.10, 6.09, 6.08, 6.07, 6.06, 6.05, 6.04, 6.03, 6.02, 6.01, 6.00, 5.99, 5.98, 5.97, 5.96, 5.95, 5.94, 5.93, 5.92, 5.91, 5.90, 5.89, 5.88, 5.87, 5.86, 5.85, 5.84, 5.83, 5.82, 5.81, 5.80, 5.79, 5.78, 5.77, 5.76, 5.75, 5.74, 5.73, 5.72, 5.71, 5.70, 5.69, 5.68, 5.67, 5.66, 5.65, 5.64, 5.63, 5.62, 5.61, 5.60, 5.59, 5.58, 5.57, 5.56, 5.55, 5.54, 5.53, 5.52, 5.51, 5.50, 5.49, 5.48, 5.47, 5.46, 5.45, 5.44, 5.43, 5.42, 5.41, 5.40, 5.39, 5.38, 5.37, 5.36, 5.35, 5.34, 5.33, 5.32, 5.31, 5.30, 5.29, 5.28, 5.27, 5.26, 5.25, 5.24, 5.23, 5.22, 5.21, 5.20, 5.19, 5.18, 5.17, 5.16, 5.15, 5.14, 5.13, 5.12, 5.11, 5.10, 5.09, 5.08, 5.07, 5.06, 5.05, 5.04, 5.03, 5.02, 5.01, 5.00, 4.99, 4.98, 4.97, 4.96, 4.95, 4.94, 4.93, 4.92, 4.91, 4.90, 4.89, 4.88, 4.87, 4.86, 4.85, 4.84, 4.83, 4.82, 4.81, 4.80, 4.79, 4.78, 4.77, 4.76, 4.75, 4.74, 4.73, 4.72, 4.71, 4.70, 4.69, 4.68, 4.67, 4.66, 4.65, 4.64, 4.63, 4.62, 4.61, 4.60, 4.59, 4.58, 4.57, 4.56, 4.55, 4.54, 4.53, 4.52, 4.51, 4.50, 4.49, 4.48, 4.47, 4.46, 4.45, 4.44, 4.43, 4.42, 4.41, 4.40, 4.39, 4.38, 4.37, 4.36, 4.35, 4.34, 4.33, 4.32, 4.31, 4.30, 4.29, 4.28, 4.27, 4.26, 4.25, 4.24, 4.23, 4.22, 4.21, 4.20, 4.19, 4.18, 4.17, 4.16, 4.15, 4.14, 4.13, 4.12, 4.11, 4.10, 4.09, 4.08, 4.07, 4.06, 4.05, 4.04, 4.03, 4.02, 4.01, 4.00, 3.99, 3.98, 3.97, 3.96, 3.95, 3.94, 3.93, 3.92, 3.91, 3.90, 3.89, 3.88, 3.87, 3.86, 3.85, 3.84, 3.83, 3.82, 3.81, 3.80, 3.79, 3.78, 3.77, 3.76, 3.75, 3.74, 3.73, 3.72, 3.71, 3.70, 3.69, 3.68, 3.67, 3.66, 3.65, 3.64, 3.63, 3.62, 3.61, 3.60, 3.59, 3.58, 3.57, 3.56, 3.55, 3.54, 3.53, 3.52, 3.51, 3.50, 3.49, 3.48, 3.47, 3.46, 3.45, 3.44, 3.43, 3.42, 3.41, 3.40, 3.39, 3.38, 3.37, 3.36, 3.35, 3.34, 3.33, 3.32, 3.31, 3.30, 3.29, 3.28, 3.27, 3.26, 3.25, 3.24, 3.23, 3.22, 3.21, 3.20, 3.19, 3.18, 3.17, 3.16, 3.15, 3.14, 3.13, 3.12, 3.11, 3.10, 3.09, 3.08, 3.07, 3.06, 3.05, 3.04, 3.03, 3.02, 3.01, 3.00, 2.99, 2.98, 2.97, 2.96, 2.95, 2.94, 2.93, 2.92, 2.91, 2.90, 2.89, 2.88, 2.87, 2.86, 2.85, 2.84, 2.83, 2.82, 2.81, 2.80, 2.79, 2.78, 2.77, 2.76, 2.75, 2.74, 2.73, 2.72, 2.71, 2.70, 2.69, 2.68, 2.67, 2.66, 2.65, 2.64, 2.63, 2.62, 2.61, 2.60, 2.59, 2.58, 2.57, 2.56, 2.55, 2.54, 2.53, 2.52, 2.51, 2.50, 2.49, 2.48, 2.47, 2.46, 2.45, 2.44, 2.43, 2.42, 2.41, 2.40, 2.39, 2.38, 2.37, 2.36, 2.35, 2.34, 2.33, 2.32, 2.31, 2.30, 2.29, 2.28, 2.27, 2.26, 2.25, 2.24, 2.23, 2.22, 2.21, 2.20, 2.19, 2.18, 2.17, 2.16, 2.15, 2.14, 2.13, 2.12, 2.11, 2.10, 2.09, 2.08, 2.07, 2.06, 2.05, 2.04, 2.03, 2.02, 2.01, 2.00, 1.99, 1.98, 1.97, 1.96, 1.95, 1.94, 1.93, 1.92, 1.91, 1.90, 1.89, 1.88, 1.87, 1.86, 1.85, 1.84, 1.83, 1.82, 1.81, 1.80, 1.79, 1.78, 1.77, 1.76, 1.75, 1.74, 1.73, 1.72, 1.71, 1.70, 1.69, 1.6

S181

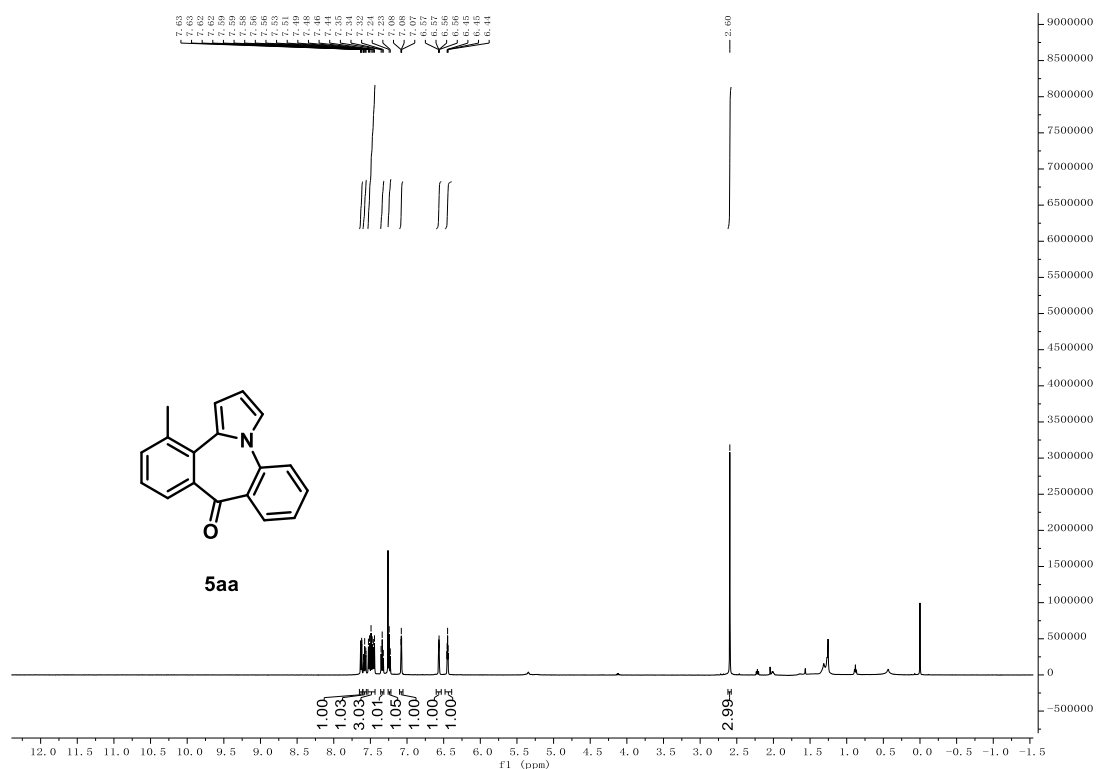
400 MHz, CDCl₃)



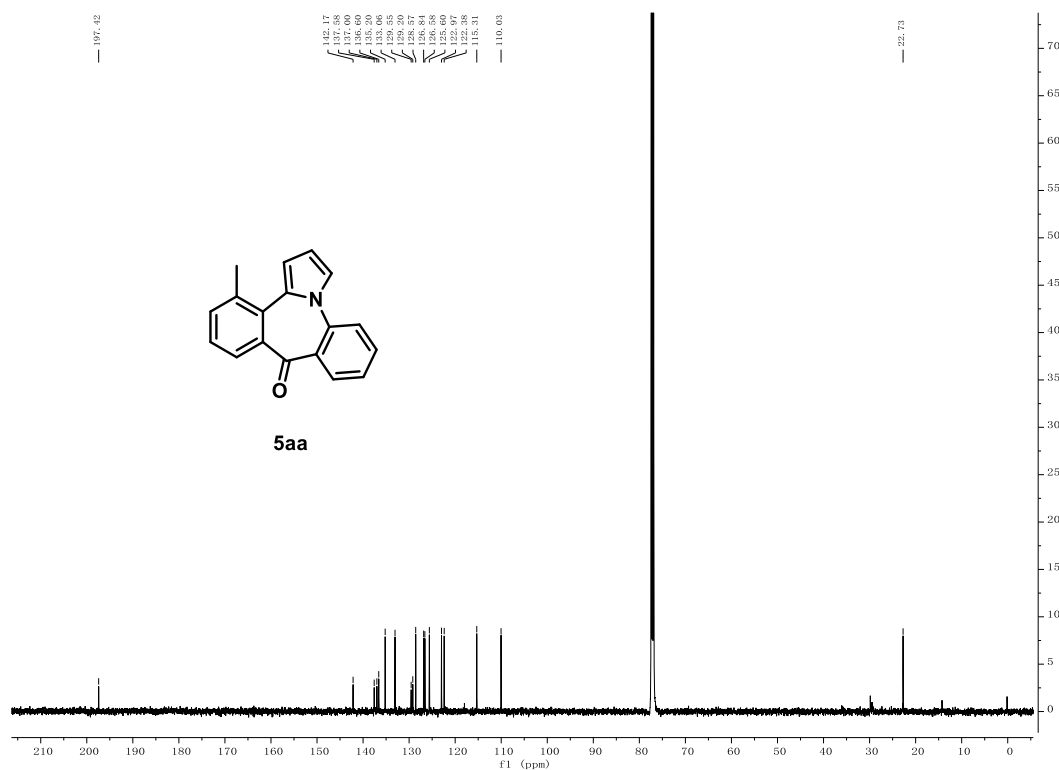
14-methyl-7-(trifluoromethyl)-10H-dibenzo[3,4:6,7]azepino[1,2-a]indol-10-one (5z) (¹³C NMR 201 MHz, CDCl₃)



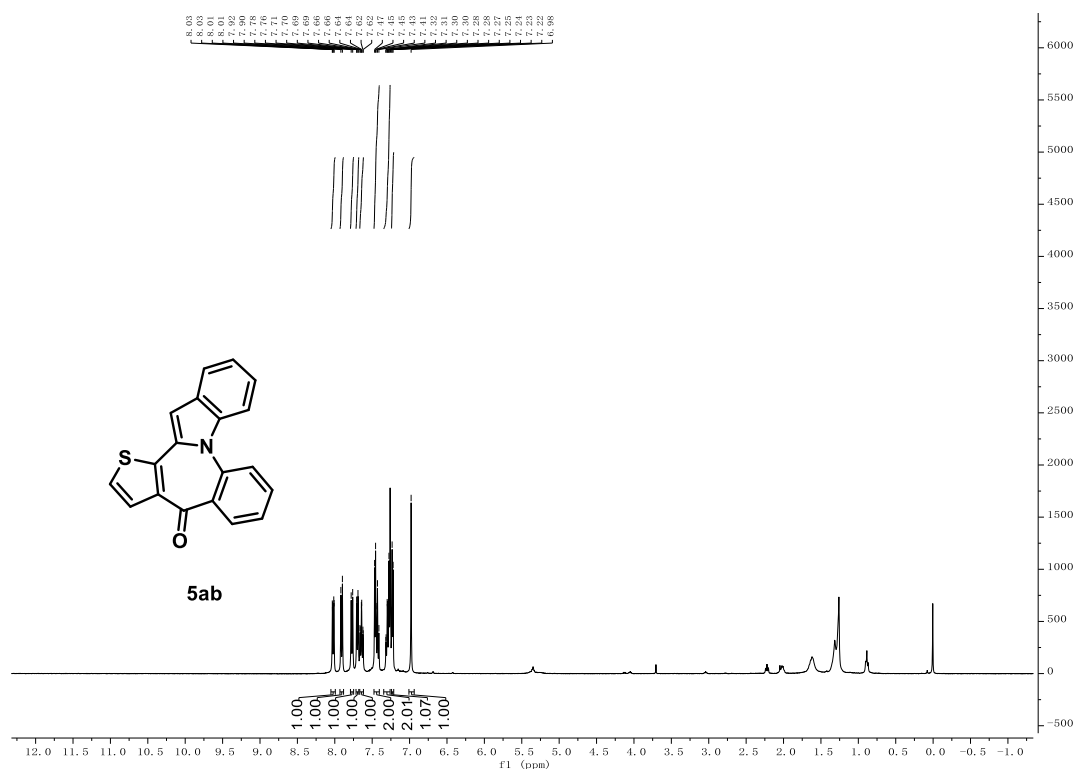
13-methyl-9H-dibenzo[c,f]pyrrolo[1,2-a]azepin-9-one (5aa) (¹H NMR 500 MHz, CDCl₃)



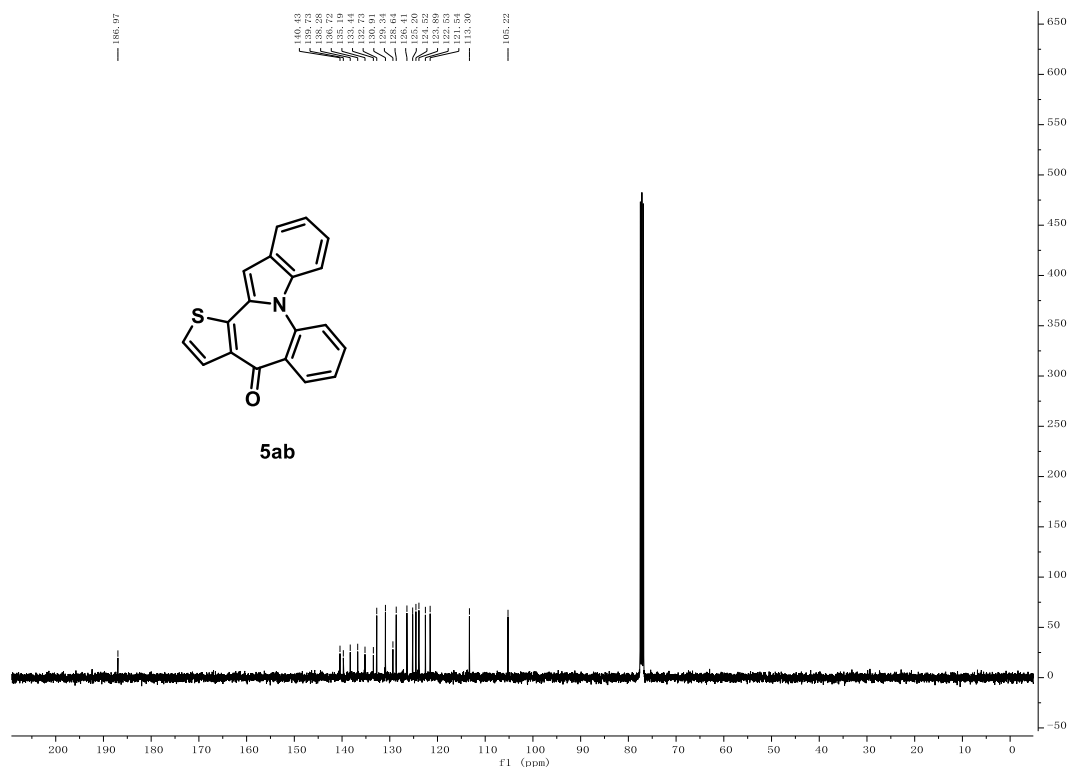
13-methyl-9*H*-dibenzo[*c,f*]pyrrolo[1,2-*a*]azepin-9-one (5aa) (¹³C NMR 126 MHz, CDCl₃)



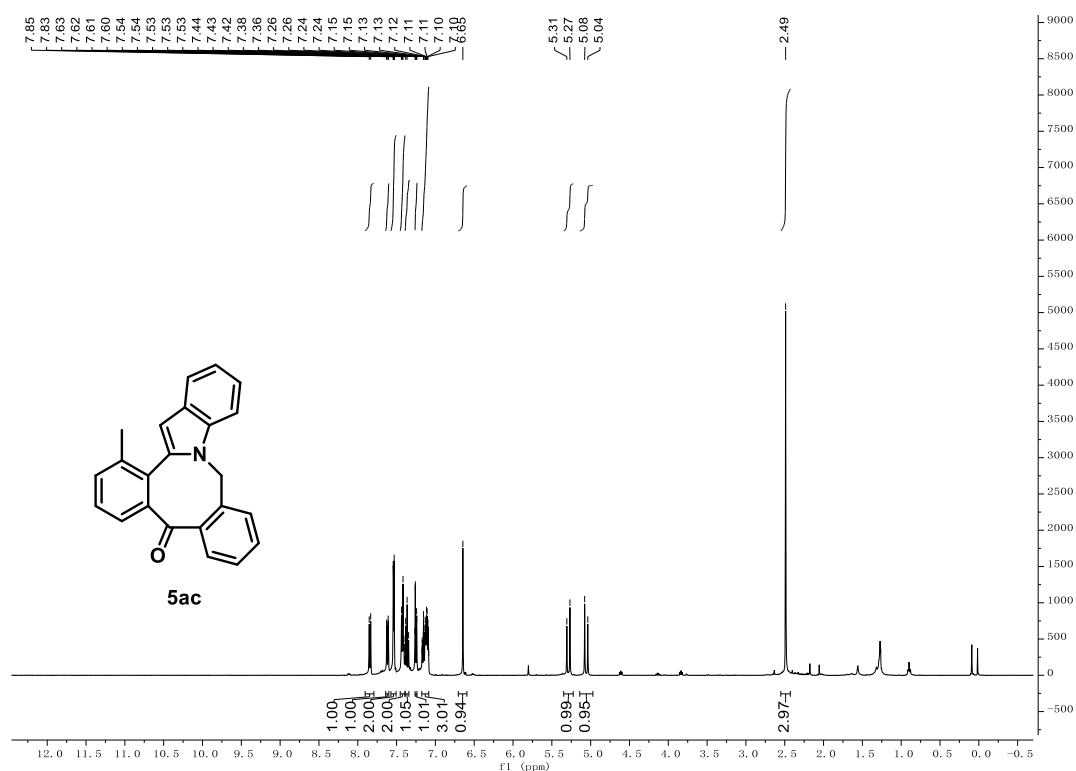
10*H*-benzo[6,7]thieno[2',3':3,4]azepino[1,2-*a*]indol-10-one (5ab) (¹H NMR 400 MHz, CDCl₃)



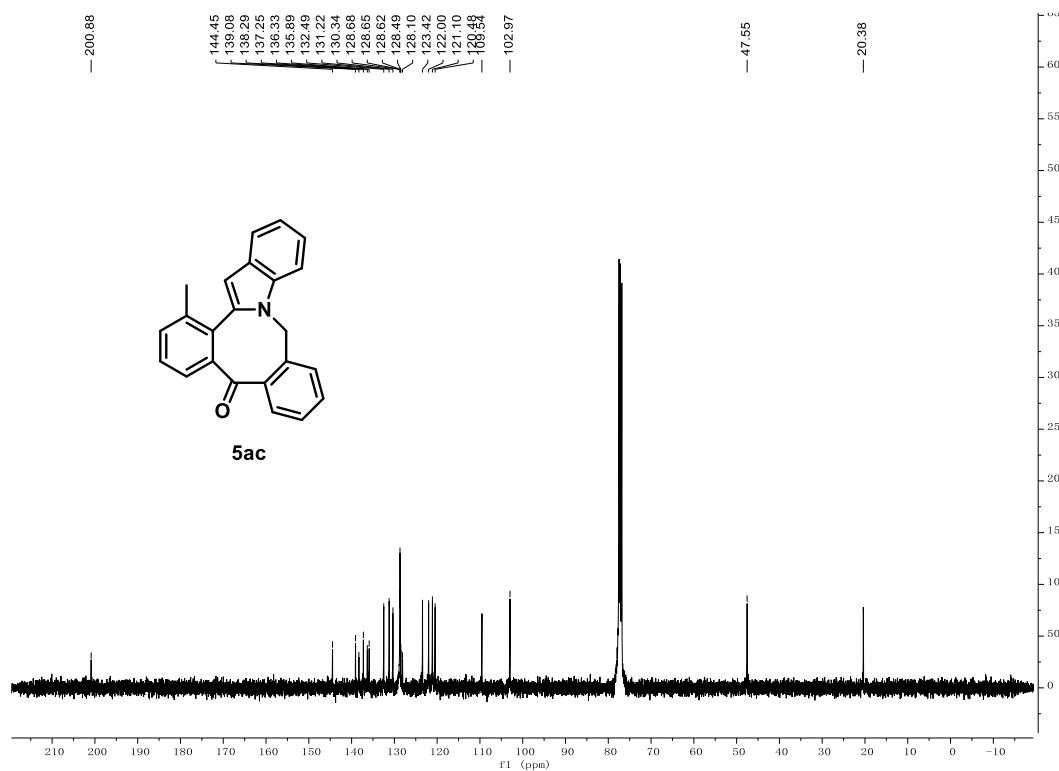
10*H*-benzo[6,7]thieno[2',3':3,4]azepino[1,2-*a*]indol-10-one (5ab) (¹³C NMR 101 MHz, CDCl₃)



1-methyldibenzo[3,4:6,7]azocino[1,2-*a*]indol-5(10*H*)-one (5ac) (¹H NMR 400 MHz, CDCl₃)

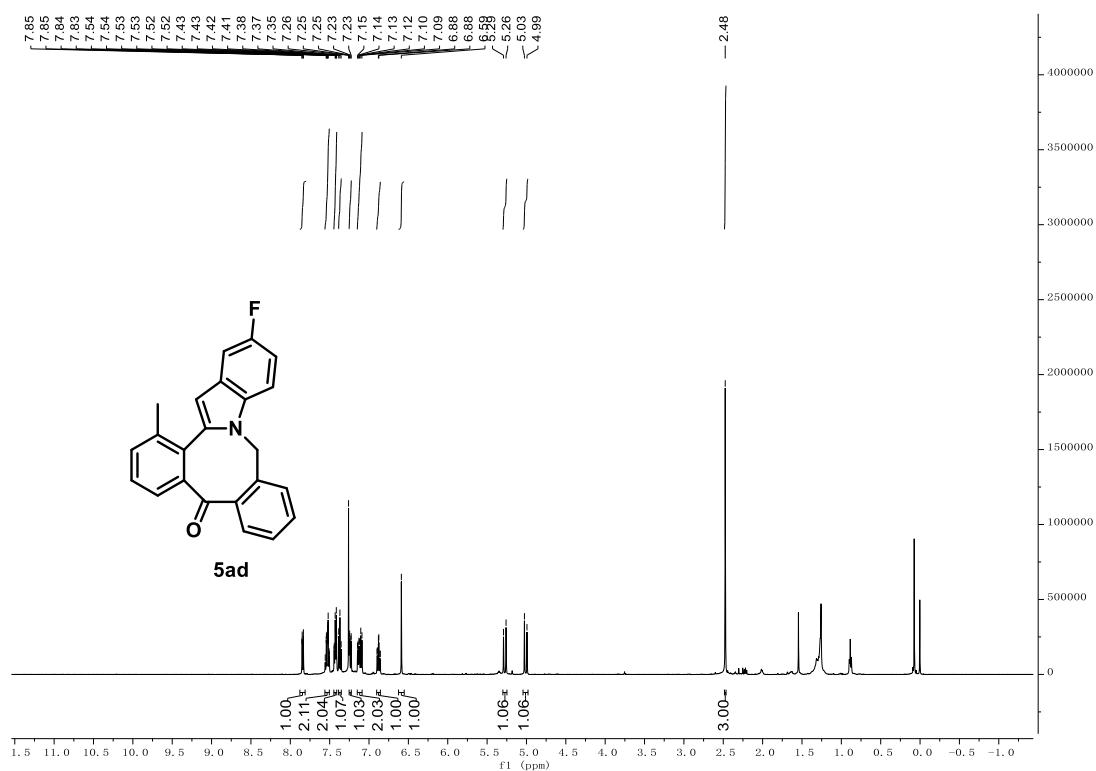


1-methyldibenzo[3,4:6,7]azocino[1,2-*a*]indol-5(10*H*)-one (5ac) (¹³C NMR 101 MHz, CDCl₃)

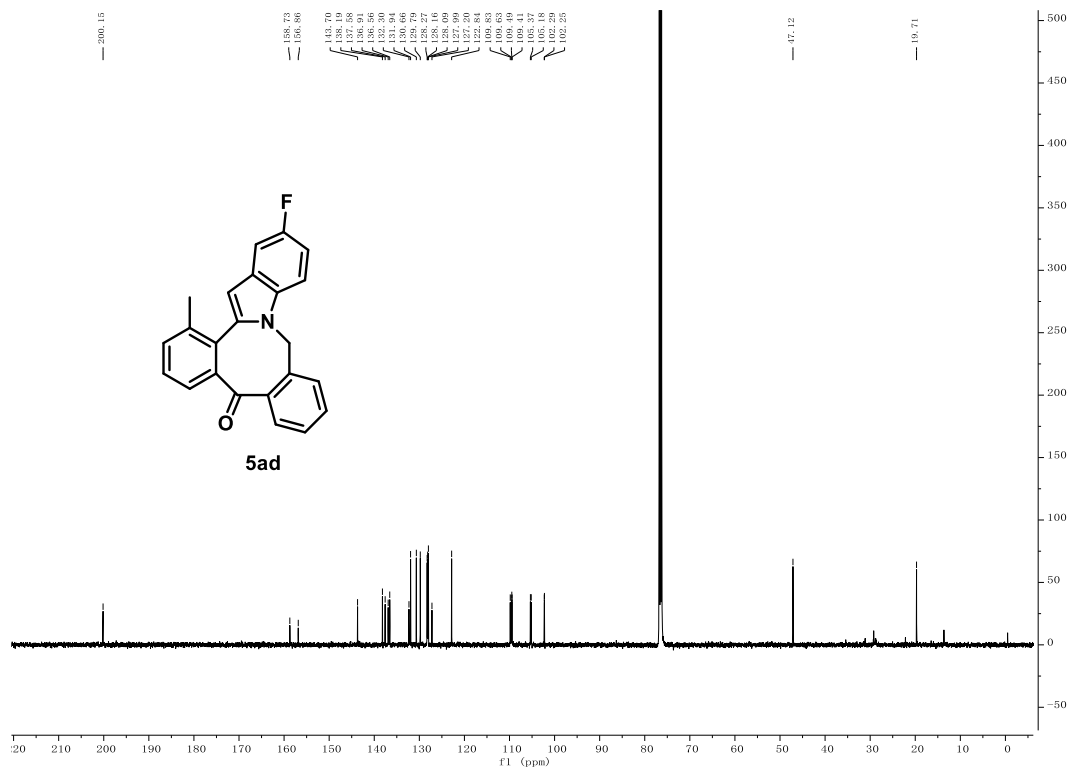


14-fluoro-1-methyldibenzo[3,4:6,7]azocino[1,2-*a*]indol-5(10*H*)-one (5ad) (¹H NMR 500 MHz,

CDCl₃)

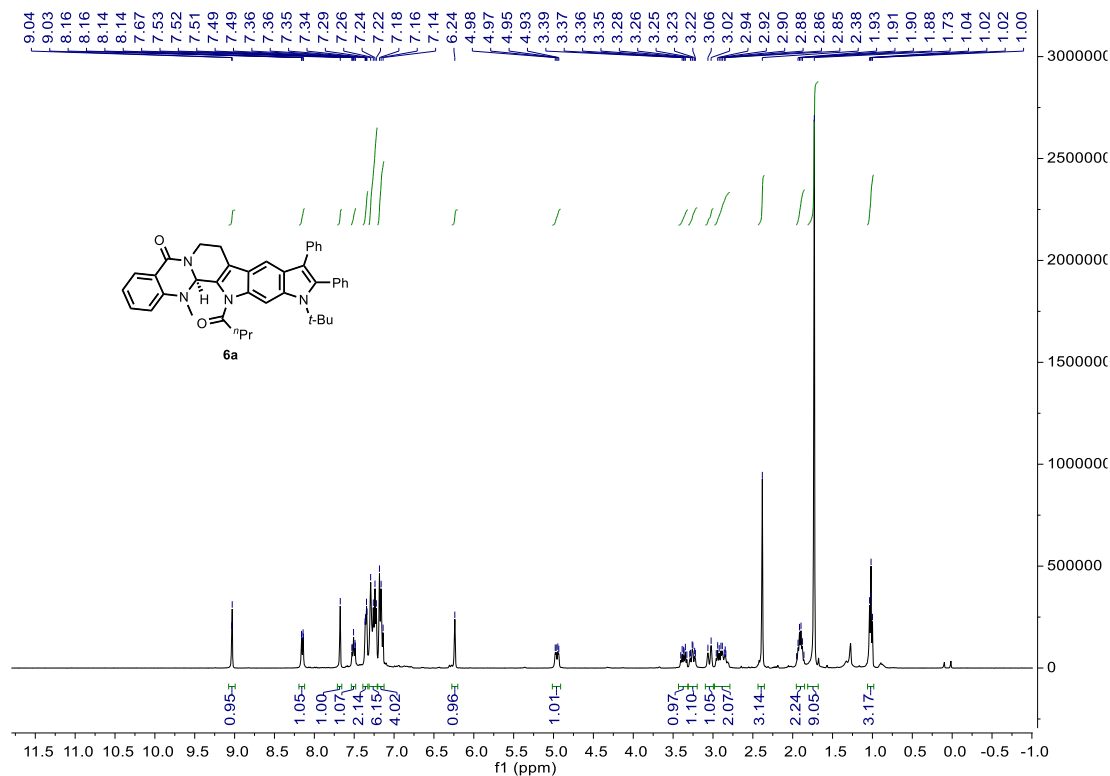


14-fluoro-1-methyldibenzo[3,4:6,7]azocino[1,2-a]indol-5(10H)-one (5ad) (¹³C NMR 126 MHz, CDCl₃)

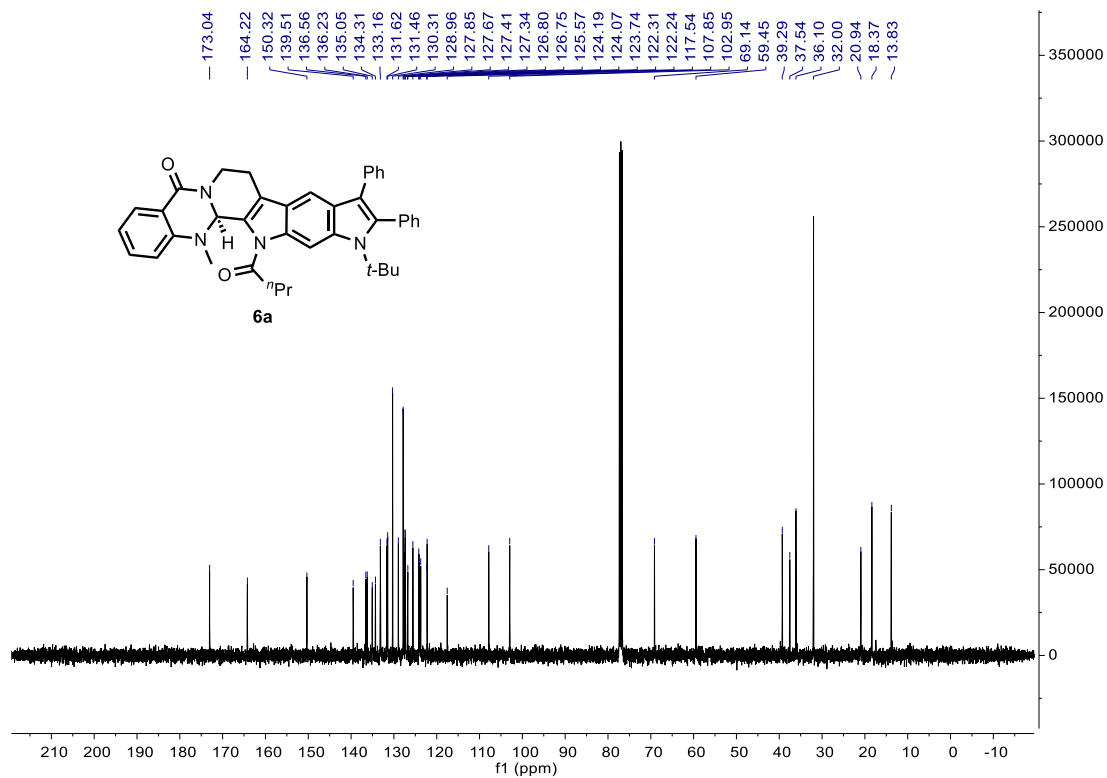


(S)-12-(tert-butyl)-14-butyryl-15-methyl-10,11-diphenyl-7,8,12,14,14b,15-hexahydro-5H-

pyrrolo[3'',2'':5',6']indolo[2',3':3,4]pyrido[2,1-b]quinazolin-5-one (6a) (¹H NMR 400 MHz, CDCl₃)

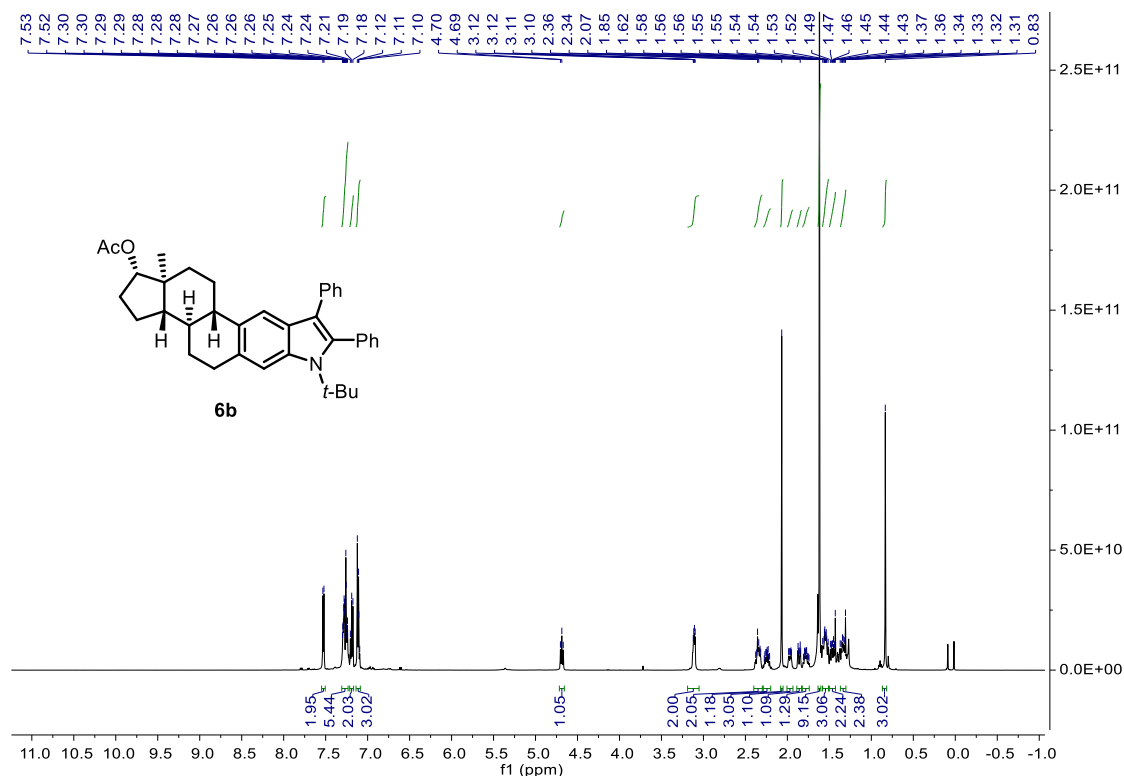


(S)-12-(tert-butyl)-14-butyryl-15-methyl-10,11-diphenyl-7,8,12,14,14b,15-hexahydro-5H-pyrrolo[3'',2'':5',6']indolo[2',3':3,4]pyrido[2,1-b]quinazolin-5-one (6a) (¹³C NMR 101 MHz, CDCl₃)

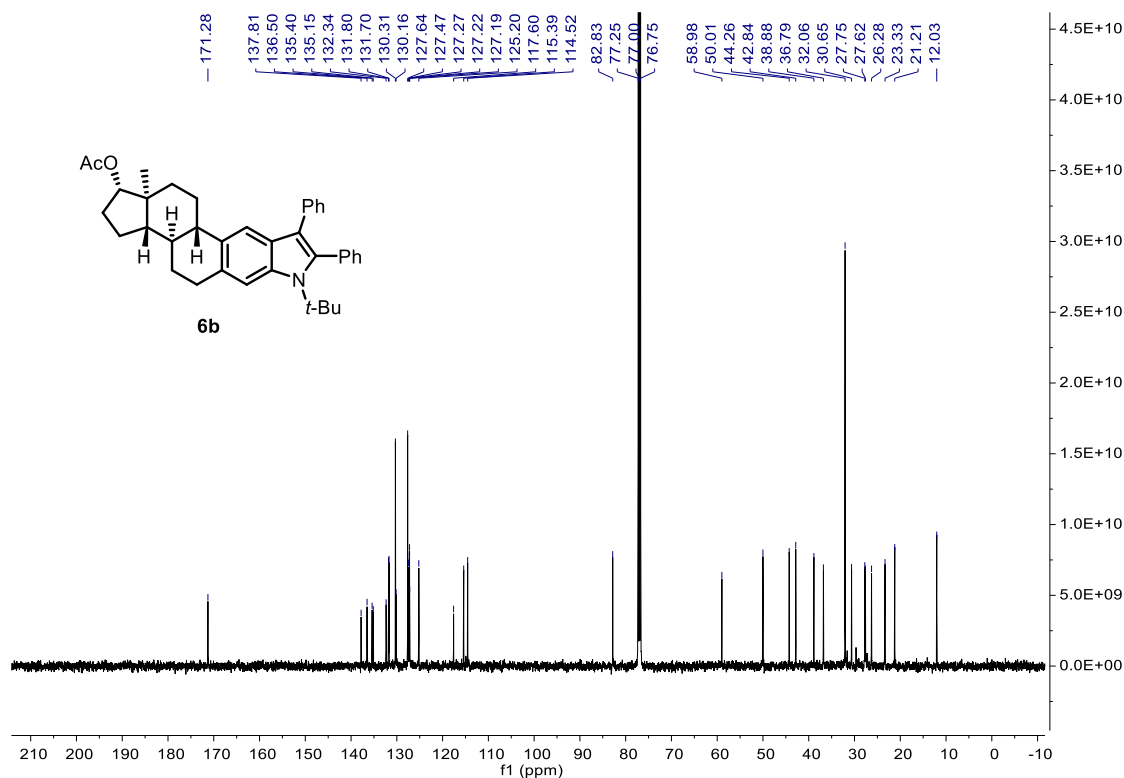


(1S,3aS,3bR,10bS,12aS)-7-(tert-butyl)-12a-methyl-8,9-diphenyl-

1,2,3,3a,3b,4,5,7,10b,11,12,12a-dodecahydrocyclopenta[5,6]naphtho[1,2-f]indol-1-yl acetate (6b) (¹H NMR 500 MHz, CDCl₃)

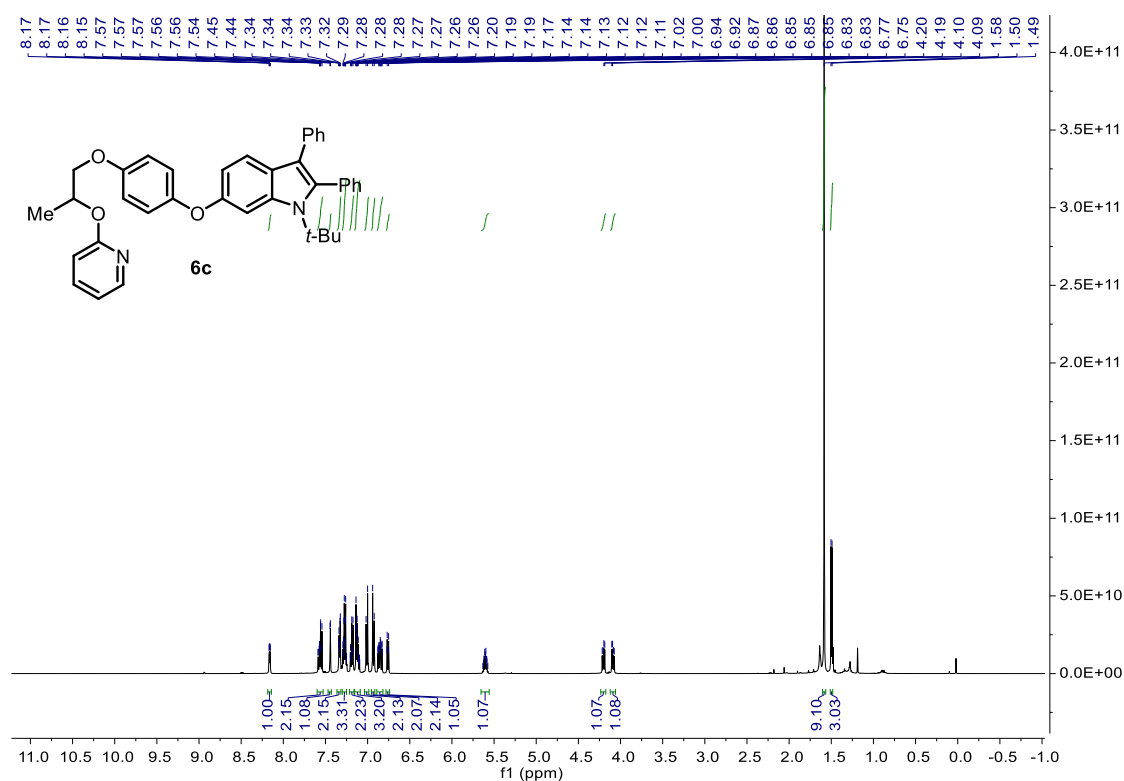


(1S,3aS,3bR,10bS,12aS)-7-(tert-butyl)-12a-methyl-8,9-diphenyl-1,2,3,3a,3b,4,5,7,10b,11,12,12a-dodecahydrocyclopenta[5,6]naphtho[1,2-f]indol-1-yl acetate (6b) (¹³C NMR 126 MHz, CDCl₃)

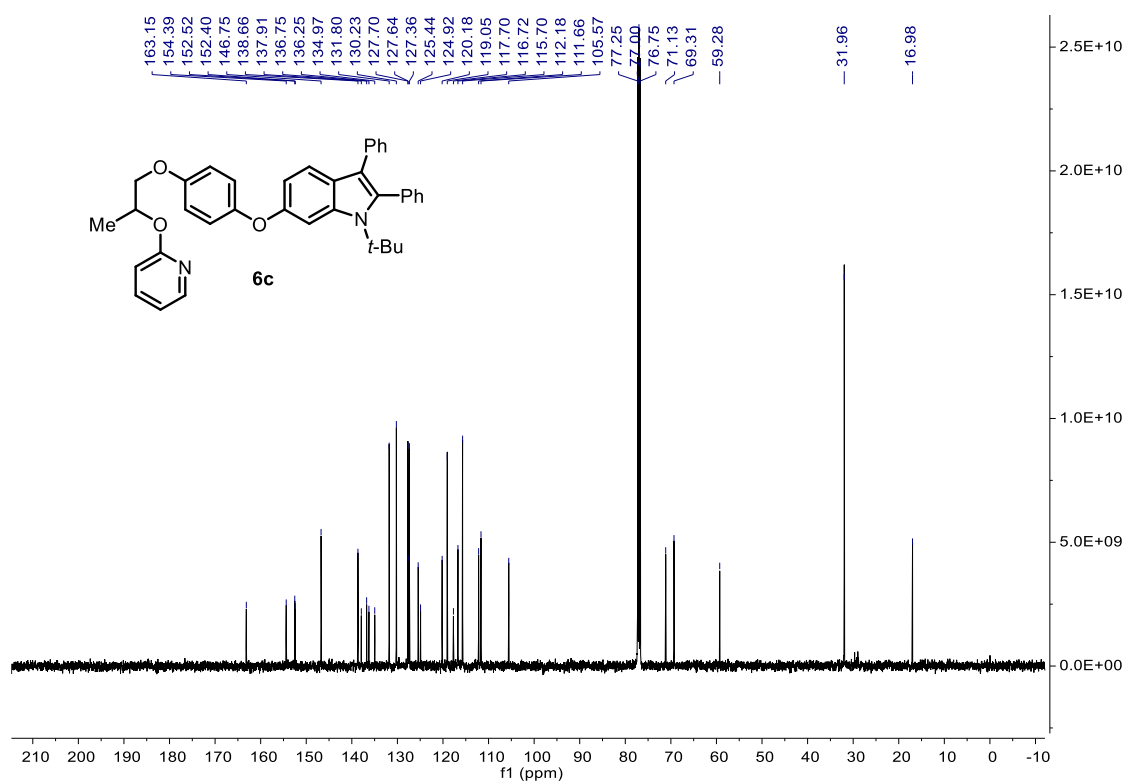


1-(tert-butyl)-2,3-diphenyl-6-(4-(2-(pyridin-2-yloxy)propoxy)phenoxy)-1H-indole (6c) (¹H

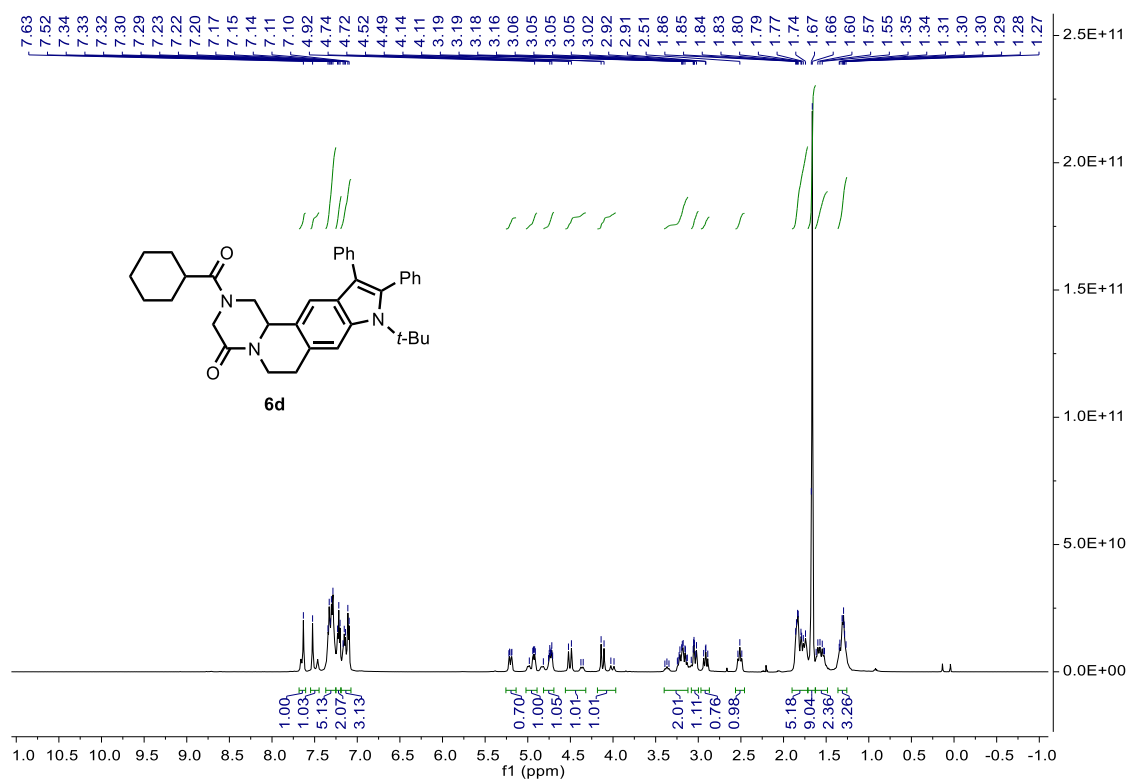
NMR 500 MHz, CDCl₃)



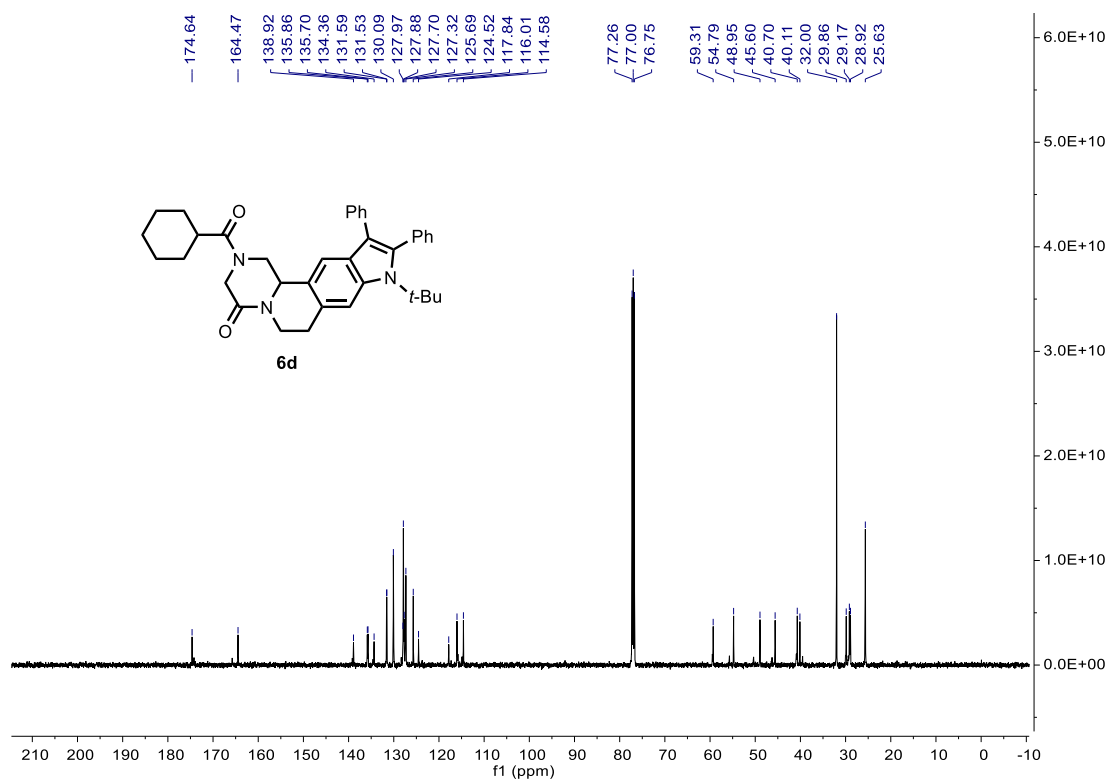
1-(*tert*-butyl)-2,3-diphenyl-6-(4-(2-(pyridin-2-yloxy)propoxy)phenoxy)-1*H*-indole (**6c**) (¹³C NMR 126 MHz, CDCl₃)



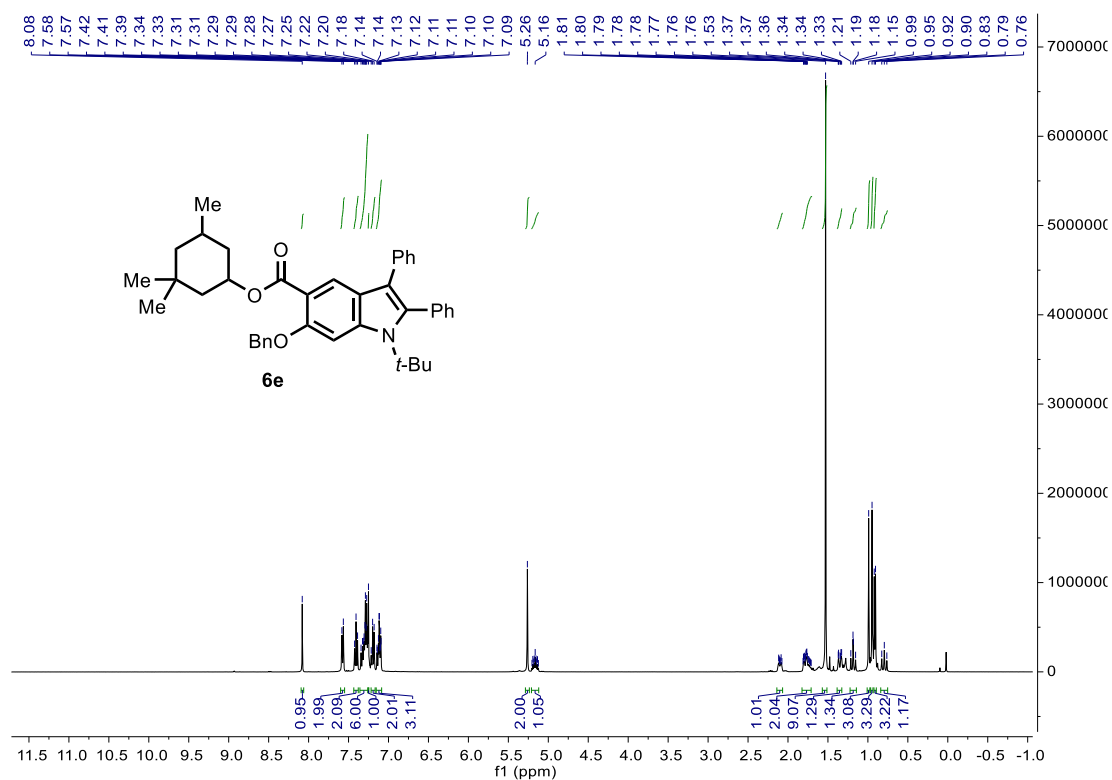
9-(*tert*-butyl)-2-(cyclohexanecarbonyl)-10,11-diphenyl-2,3,6,7,9,12*b*-hexahydropyrazino[2,1-*a*]pyrrolo[2,3-*g*]isoquinolin-4(1*H*)-one (**6d**) (¹H NMR 500 MHz, CDCl₃)



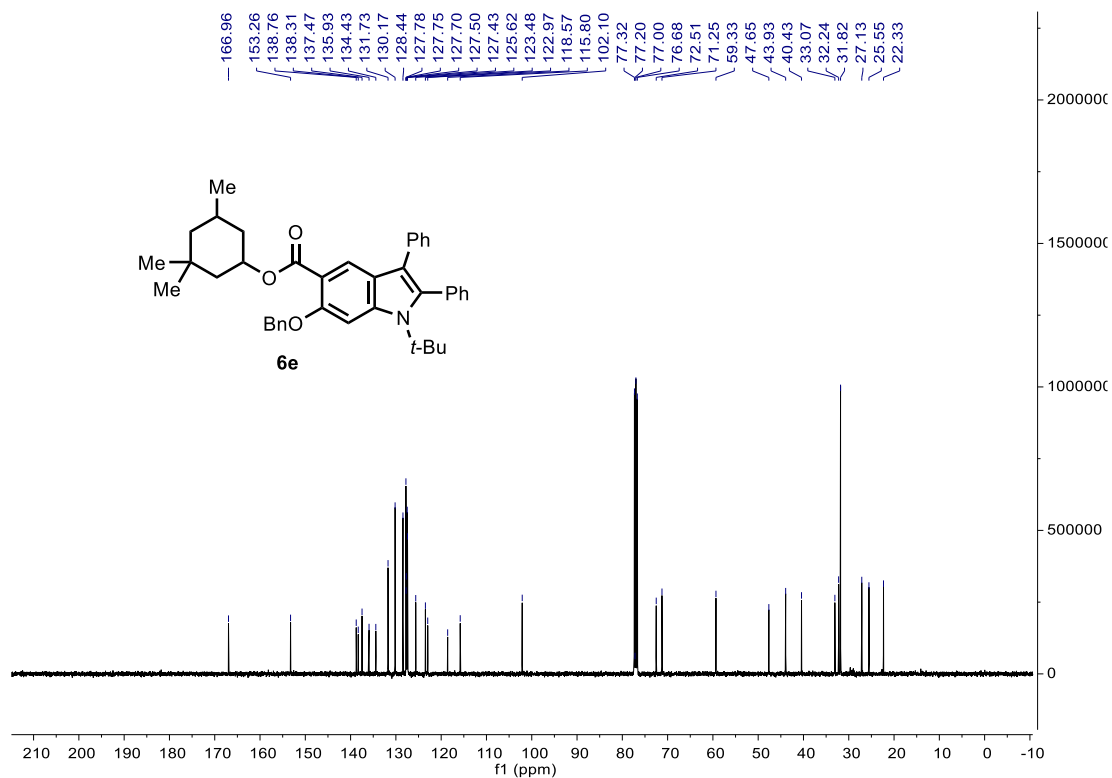
9-(tert-butyl)-2-(cyclohexanecarbonyl)-10,11-diphenyl-2,3,6,7,9,12b-hexahydropyrazino[2,1-a]pyrrolo[2,3-g]isoquinolin-4(1H)-one (6d) (¹³C NMR 126 MHz, CDCl₃)



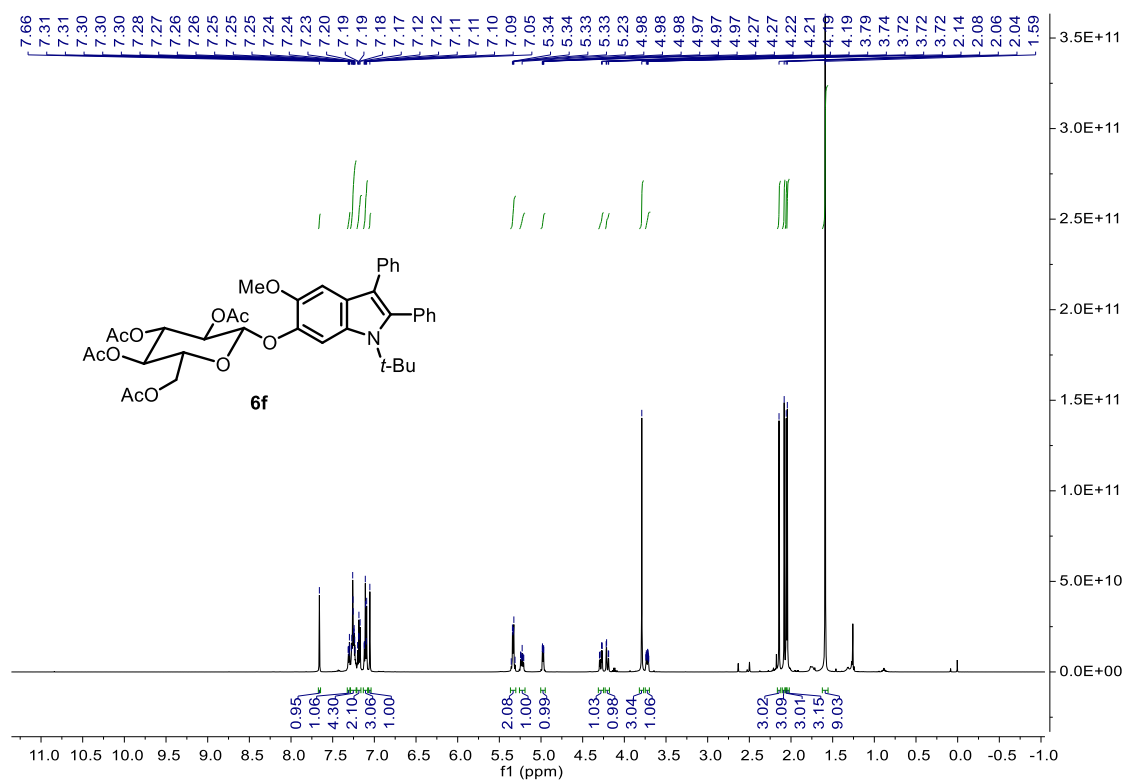
3,3,5-trimethylcyclohexyl 6-(benzyloxy)-1-(tert-butyl)-2,3-diphenyl-1H-indole-5-carboxylate (6e) (¹H NMR 400 MHz, CDCl₃)



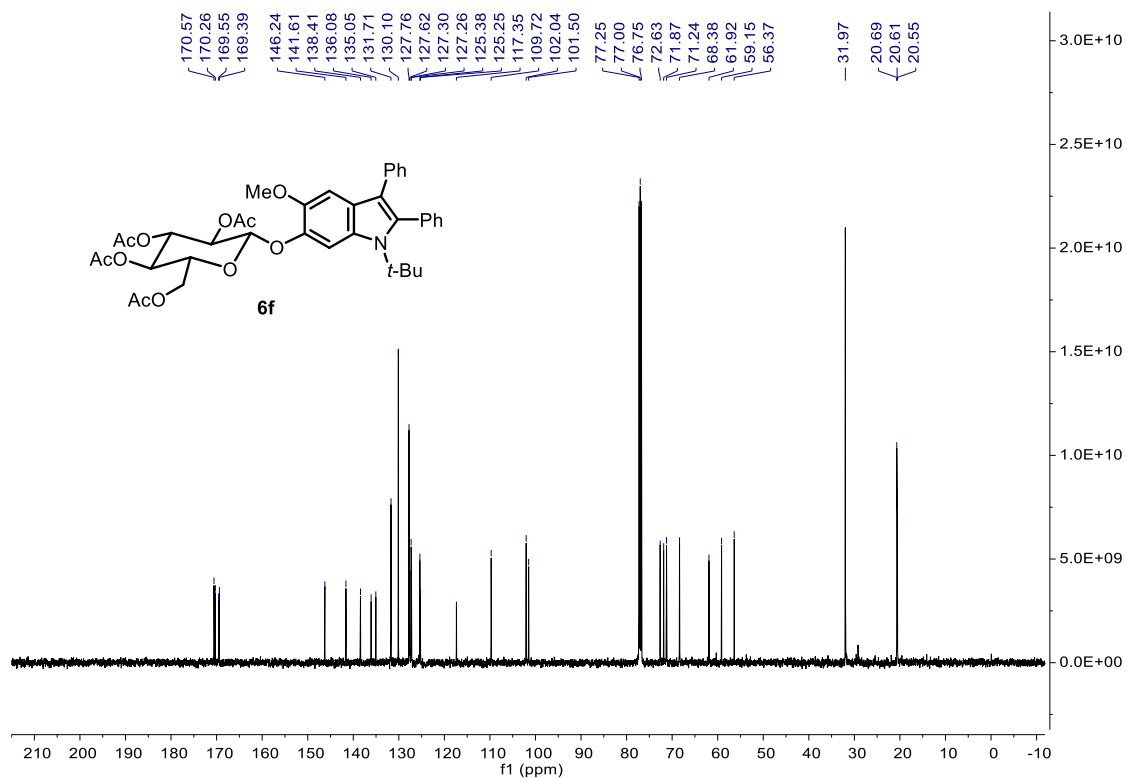
3,3,5-trimethylcyclohexyl 6-(benzyloxy)-1-(tert-butyl)-2,3-diphenyl-1H-indole-5-carboxylate (6e) (¹³C NMR 101 MHz, CDCl₃)



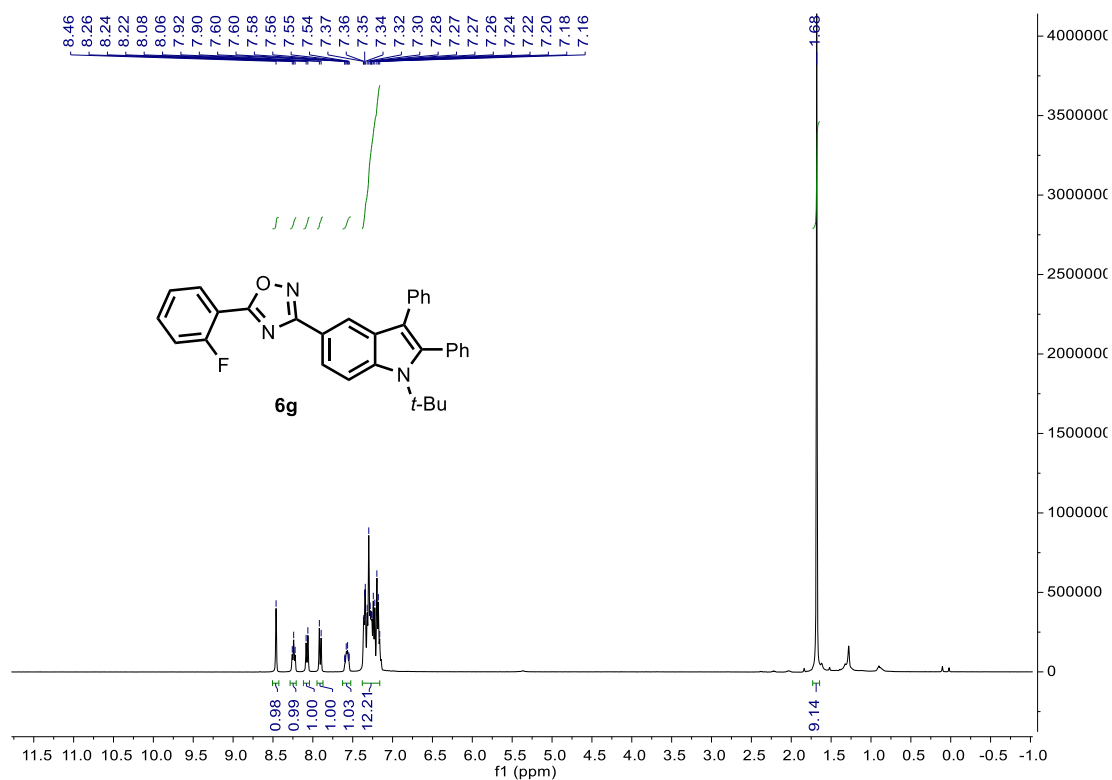
(2R,3R,4S,5R,6S)-2-(acetoxymethyl)-6-((1-(tert-butyl)-5-methoxy-2,3-diphenyl-1H-indol-6-yl)oxy)tetrahydro-2H-pyran-3,4,5-triyl triacetate (6f) (¹H NMR 500 MHz, CDCl₃)



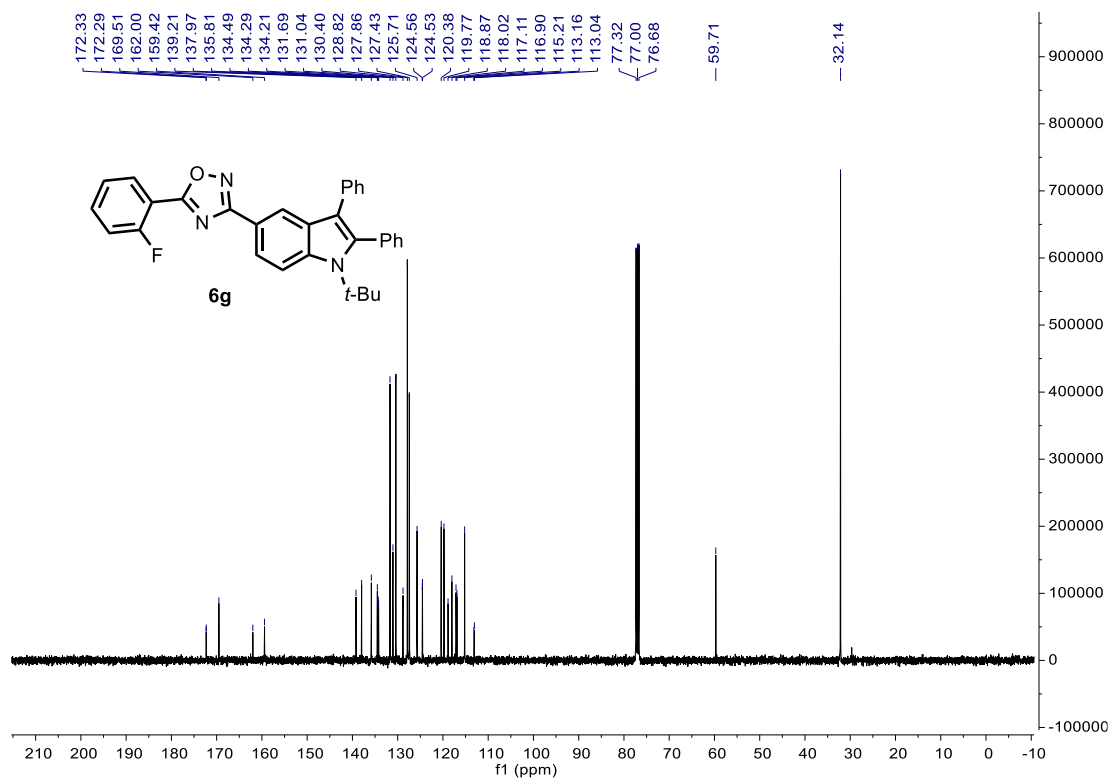
(2*R*,3*R*,4*S*,5*R*,6*S*)-2-(acetoxymethyl)-6-((1-(*tert*-butyl)-5-methoxy-2,3-diphenyl-1*H*-indol-6-yl)oxy)tetrahydro-2*H*-pyran-3,4,5-triyl triacetate (6f) (¹³C NMR 126 MHz, CDCl₃)



3-(1-(*tert*-butyl)-2,3-diphenyl-1*H*-indol-5-yl)-5-(2-fluorophenyl)-1,2,4-oxadiazole (6g) (¹H NMR (400 MHz, CDCl₃))

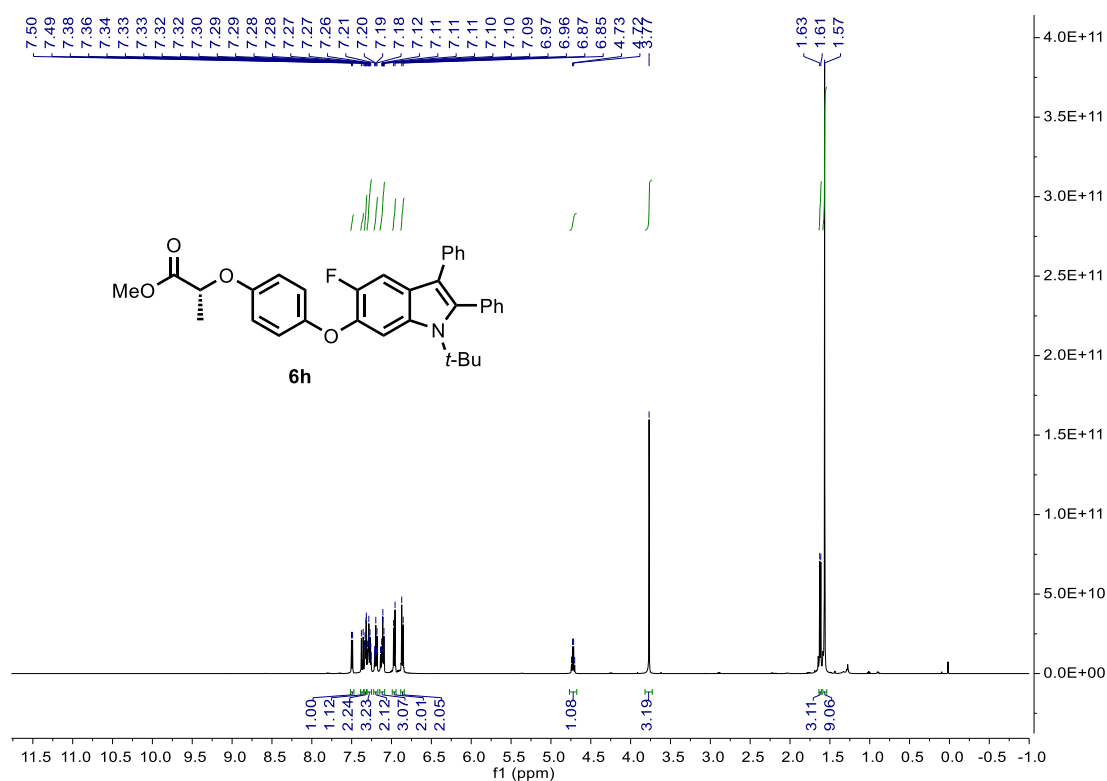


3-(1-(tert-butyl)-2,3-diphenyl-1H-indol-5-yl)-5-(2-fluorophenyl)-1,2,4-oxadiazole (6g) (¹³C NMR 101 MHz, CDCl₃)

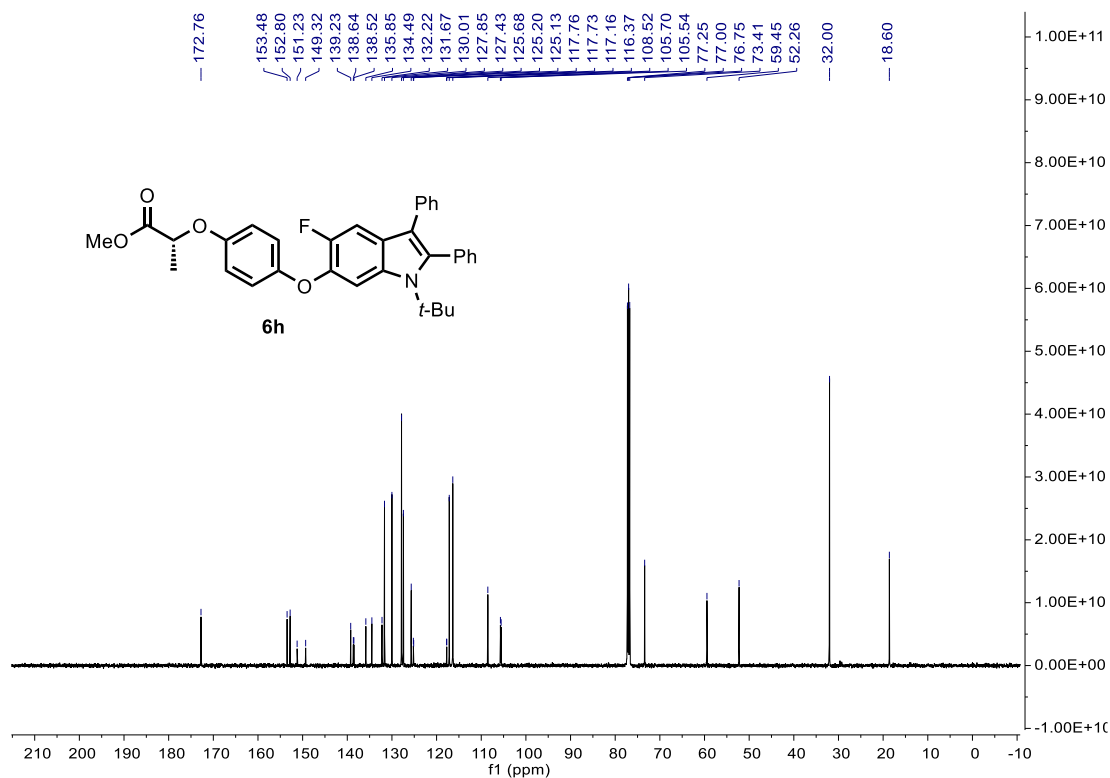


methyl (R)-2-(4-((1-(tert-butyl)-5-fluoro-2,3-diphenyl-1H-indol-6-yl)oxy)phenoxy)

propanoate (6h) (¹H NMR 500 MHz, CDCl₃)

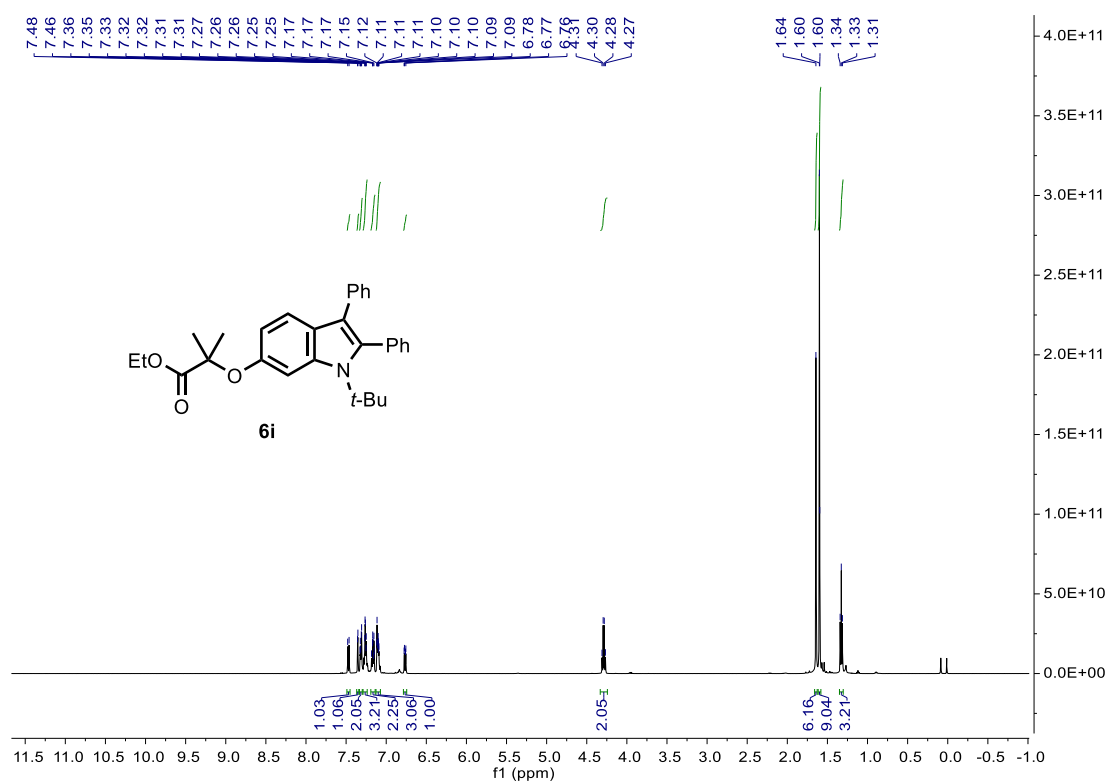


methyl (R)-2-(4-((1-(tert-butyl)-5-fluoro-2,3-diphenyl-1H-indol-6-yl)oxy)phenoxy)propanoate (6h) (¹³C NMR 126 MHz, CDCl₃)

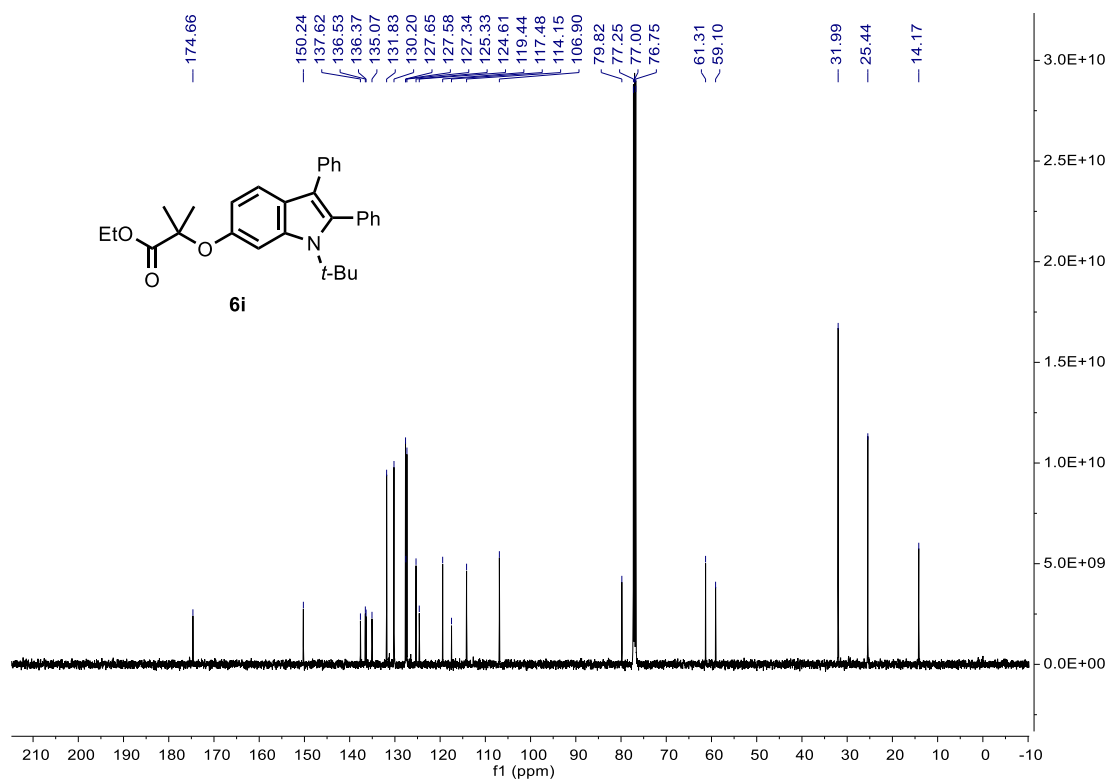


ethyl 2-((1-(tert-butyl)-2,3-diphenyl-1H-indol-6-yl)oxy)-2-methylpropanoate (6i) (¹H NMR

500 MHz, CDCl₃)

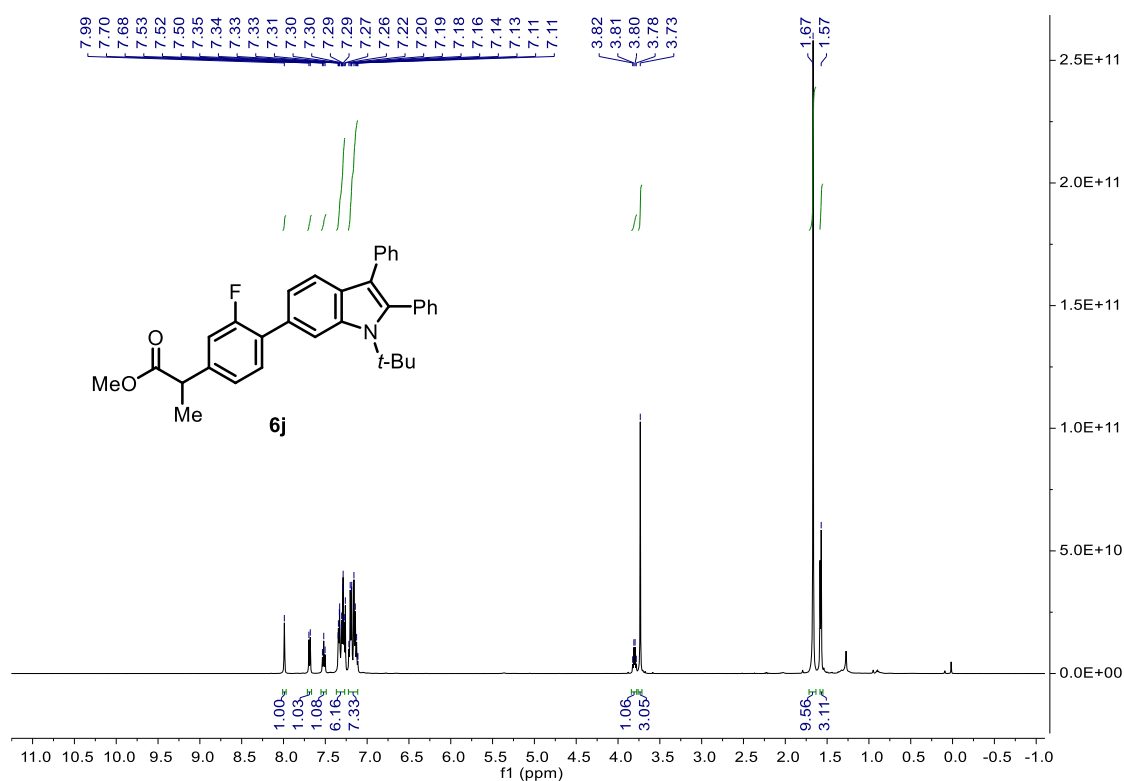


ethyl 2-((1-(tert-butyl)-2,3-diphenyl-1H-indol-6-yl)oxy)-2-methylpropanoate (**6i**) (¹³C NMR 126 MHz, CDCl₃)

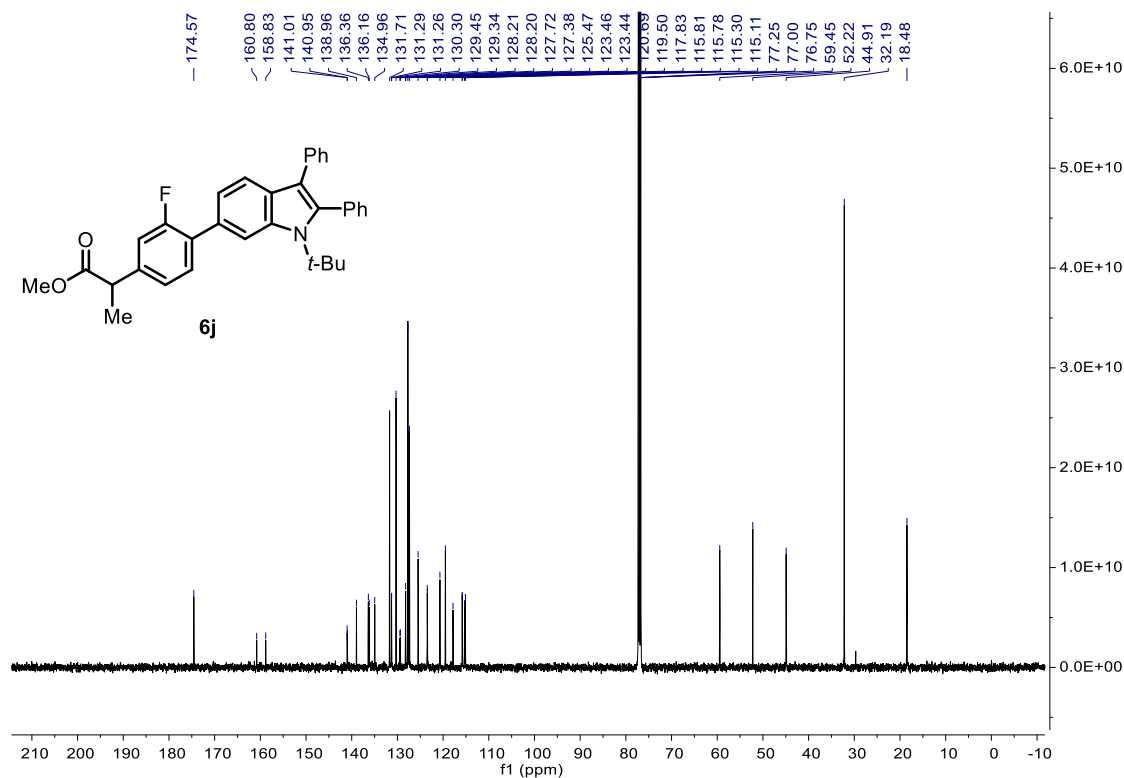


methyl 2-(4-(1-(tert-butyl)-2,3-diphenyl-1H-indol-6-yl)-3-fluorophenyl)propanoate (**6j**) (¹H

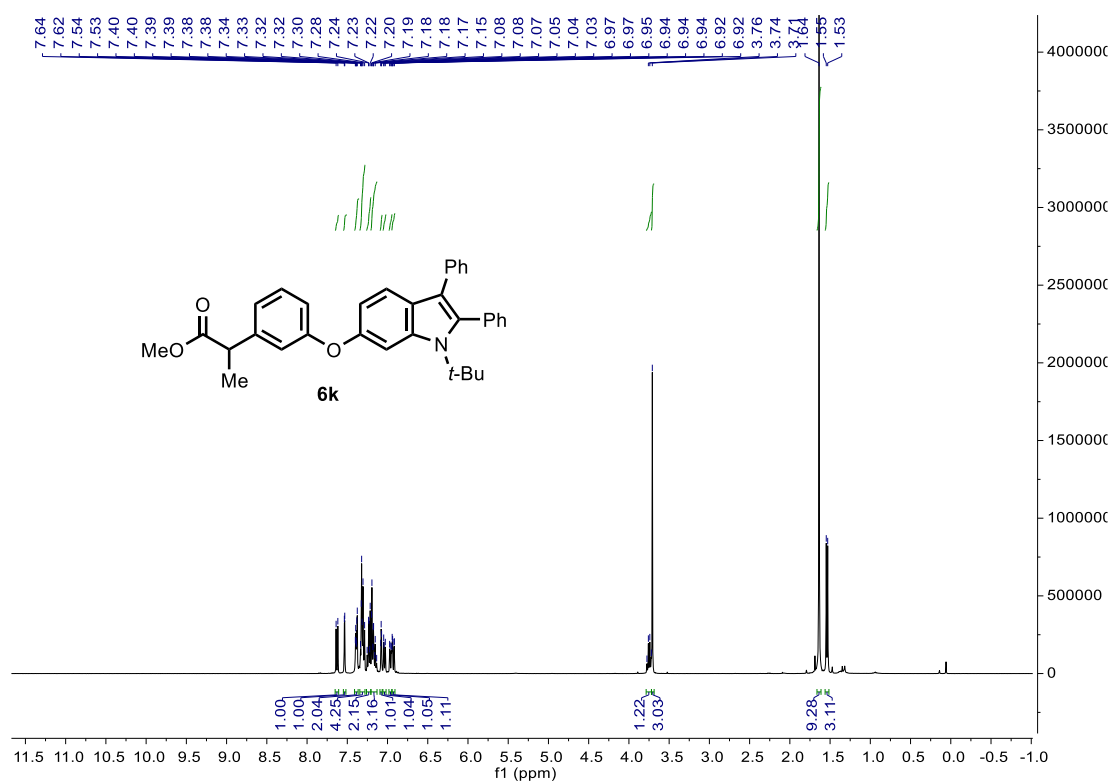
NMR 500 MHz, CDCl₃)



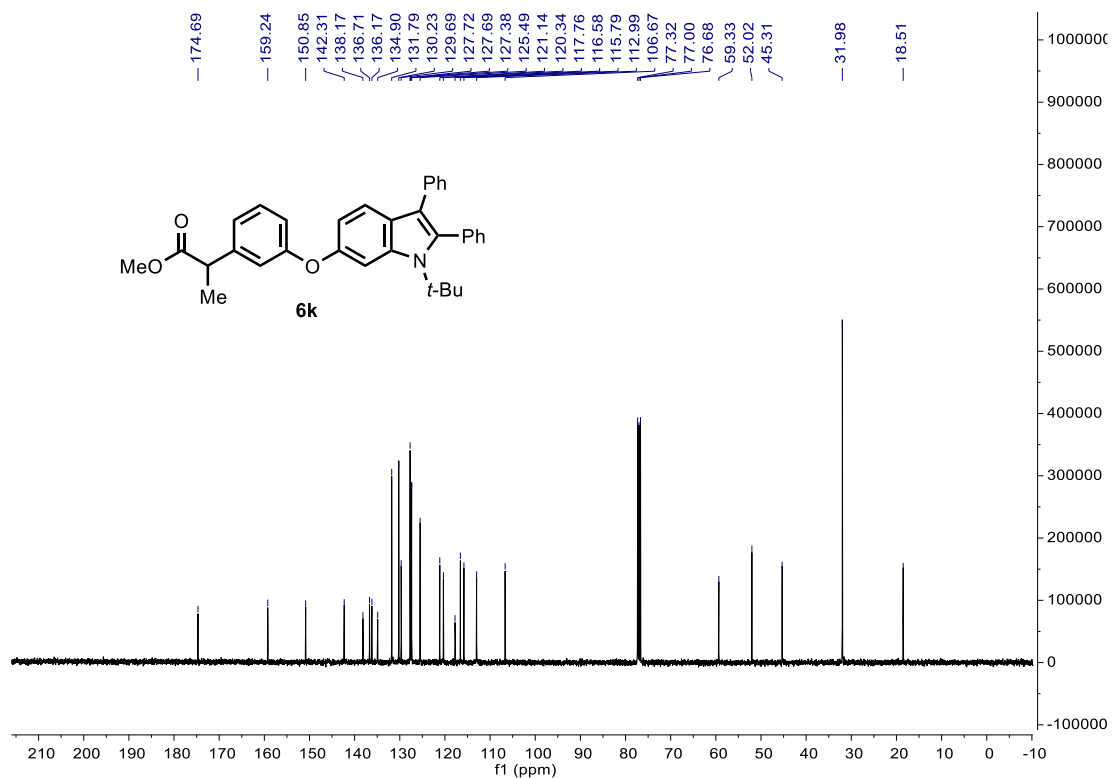
methyl 2-(4-(1-(tert-butyl)-2,3-diphenyl-1H-indol-6-yl)-3-fluorophenyl)propanoate (**6j**) (¹³C NMR 126 MHz, CDCl₃)



methyl 2-(3-((1-(tert-butyl)-2,3-diphenyl-1H-indol-6-yl)oxy)phenyl)propanoate (**6k**) (¹H NMR 400 MHz, CDCl₃)

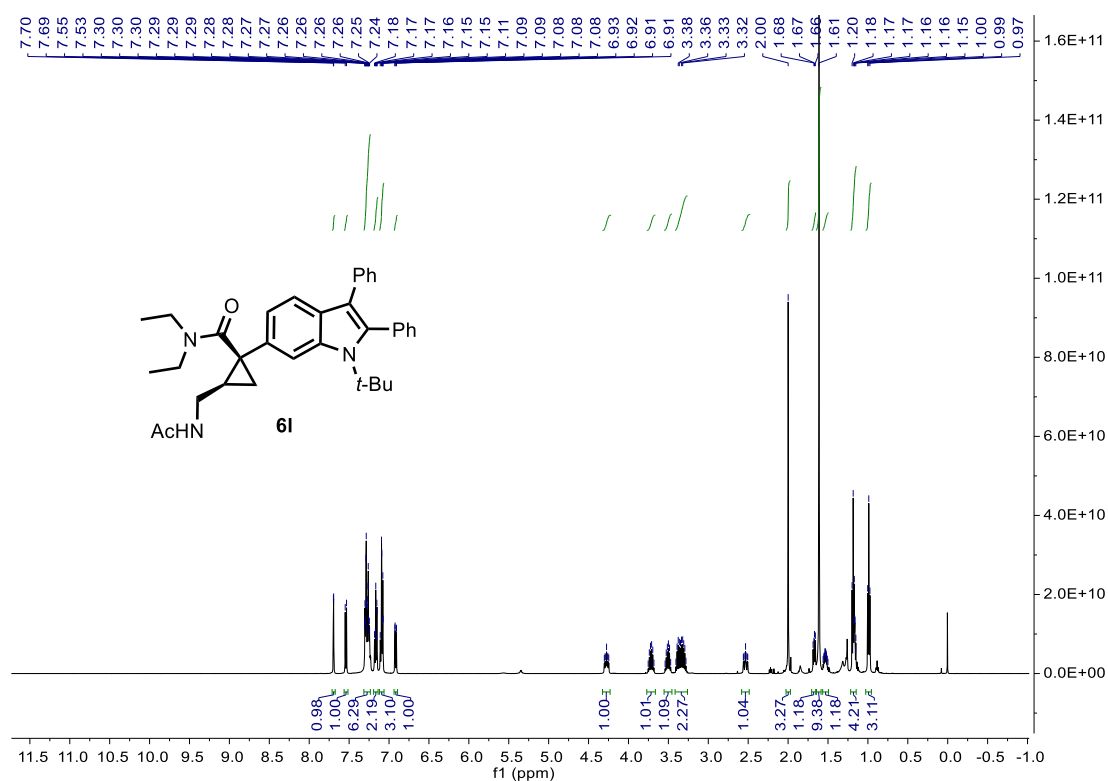


methyl 2-(3-((1-(tert-butyl)-2,3-diphenyl-1H-indol-6-yl)oxy)phenyl)propanoate (6k) (¹³C NMR 101 MHz, CDCl₃)

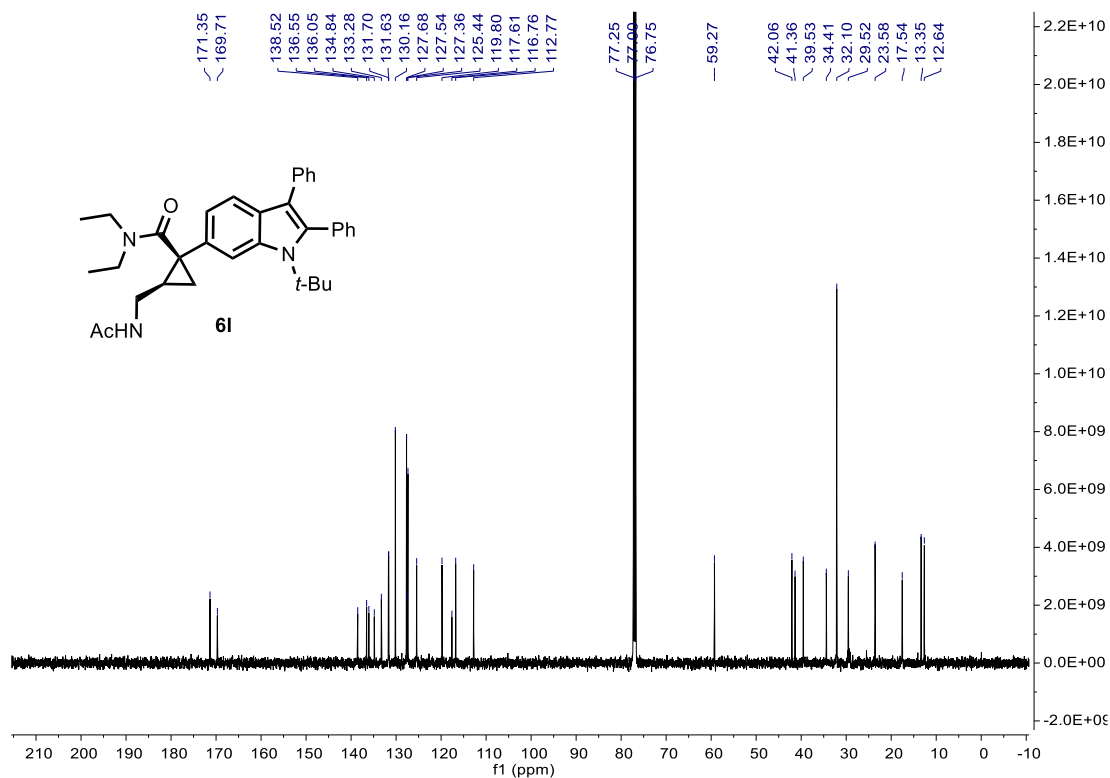


(1*S*,2*R*)-2-(acetamidomethyl)-1-(1-(tert-butyl)-2,3-diphenyl-1H-indol-6-yl)-N,N-

diethylcyclopropane-1-carboxamide (6l) (¹H NMR 500 MHz, CDCl₃)



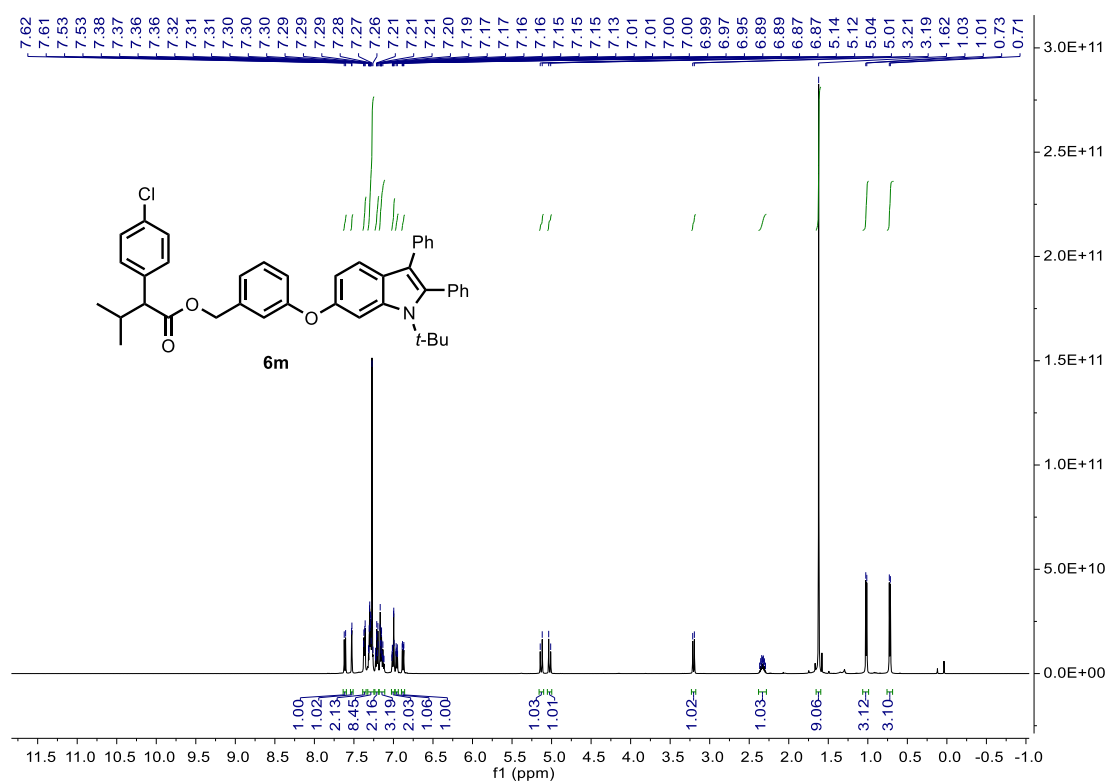
(1*S*,2*R*)-2-(acetamidomethyl)-1-(1-(tert-butyl)-2,3-diphenyl-1*H*-indol-6-yl)-*N,N*-diethylcyclopropane-1-carboxamide (6l) (¹³C NMR 126 MHz, CDCl₃)



3-((1-(tert-butyl)-2,3-diphenyl-1*H*-indol-6-yl)oxy)benzyl

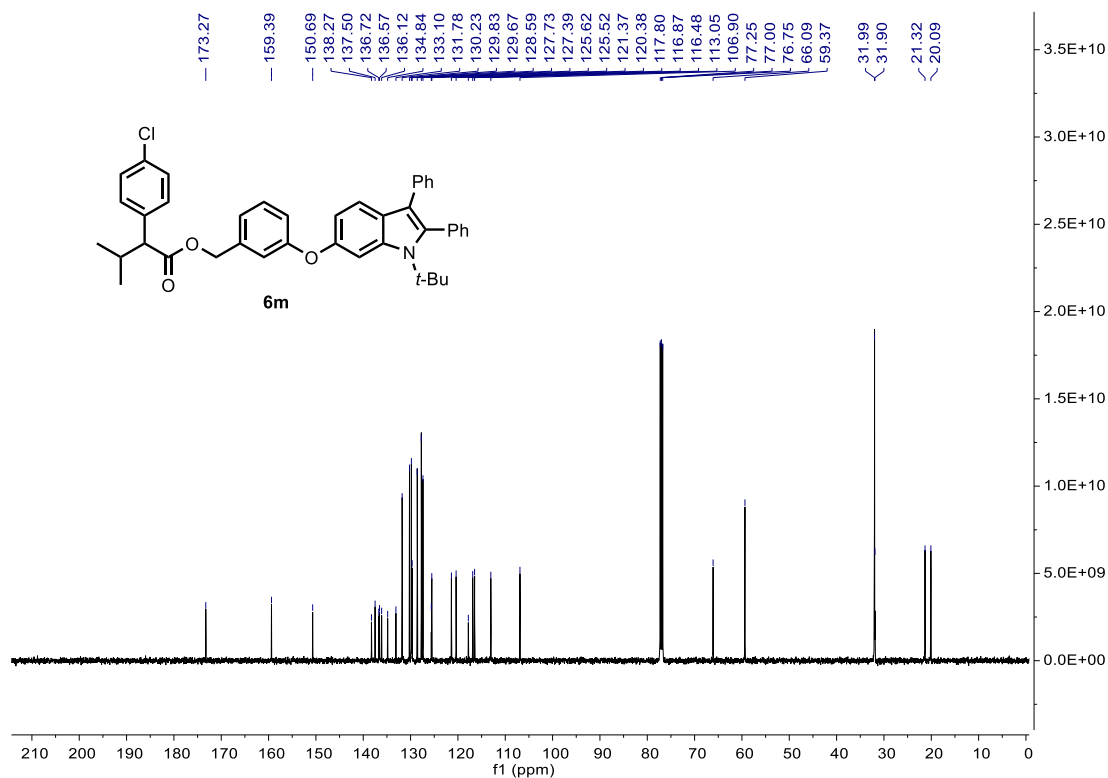
2-(4-chlorophenyl)-3-

methylbutanoate (6m) (¹H NMR 500 MHz, CDCl₃)



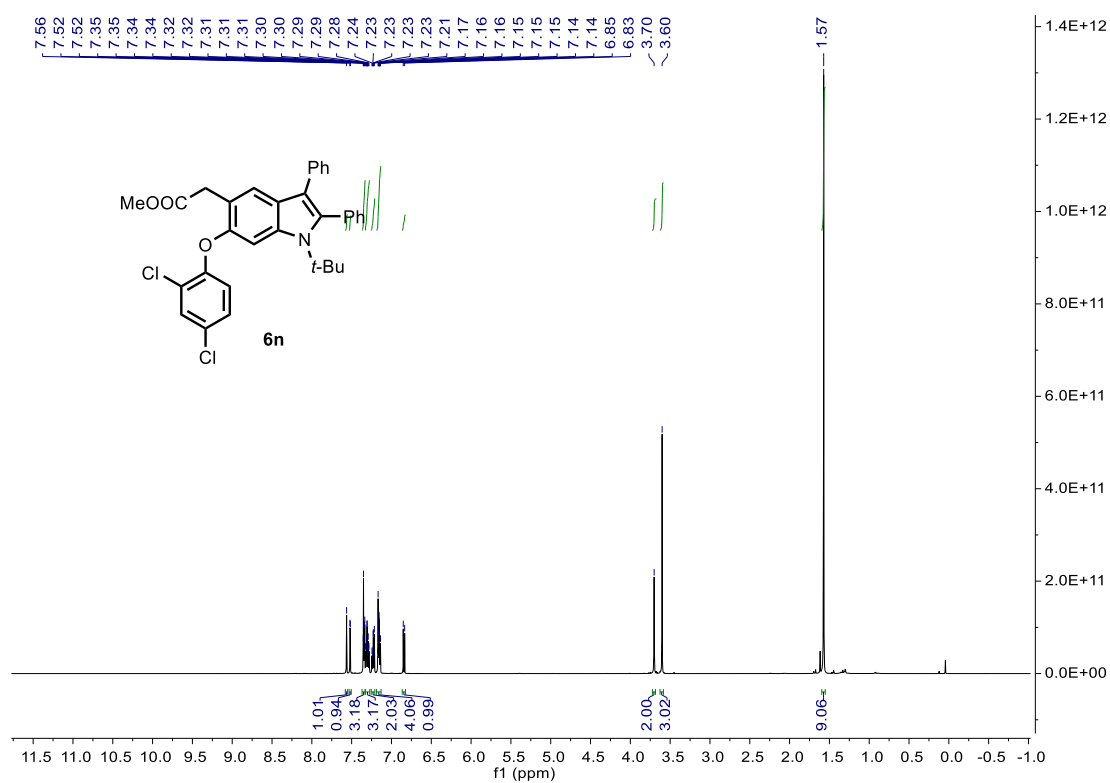
3-((1-(tert-butyl)-2,3-diphenyl-1H-indol-6-yl)oxy)benzyl methylbutanoate (6m) (¹³C NMR 126 MHz, CDCl₃)

2-(4-chlorophenyl)-3-

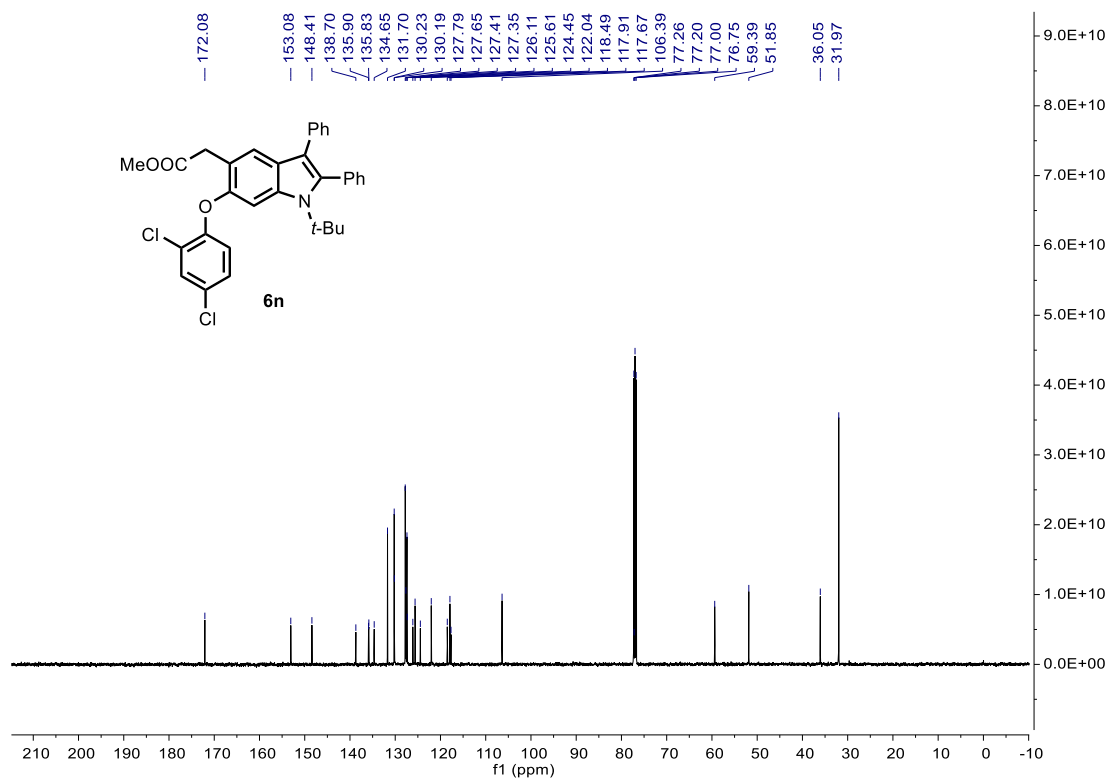


methyl 2-(1-(tert-butyl)-6-(2,4-dichlorophenoxy)-2,3-diphenyl-1H-indol-5-yl)acetate (6n) (¹H

NMR 500 MHz, CDCl₃)

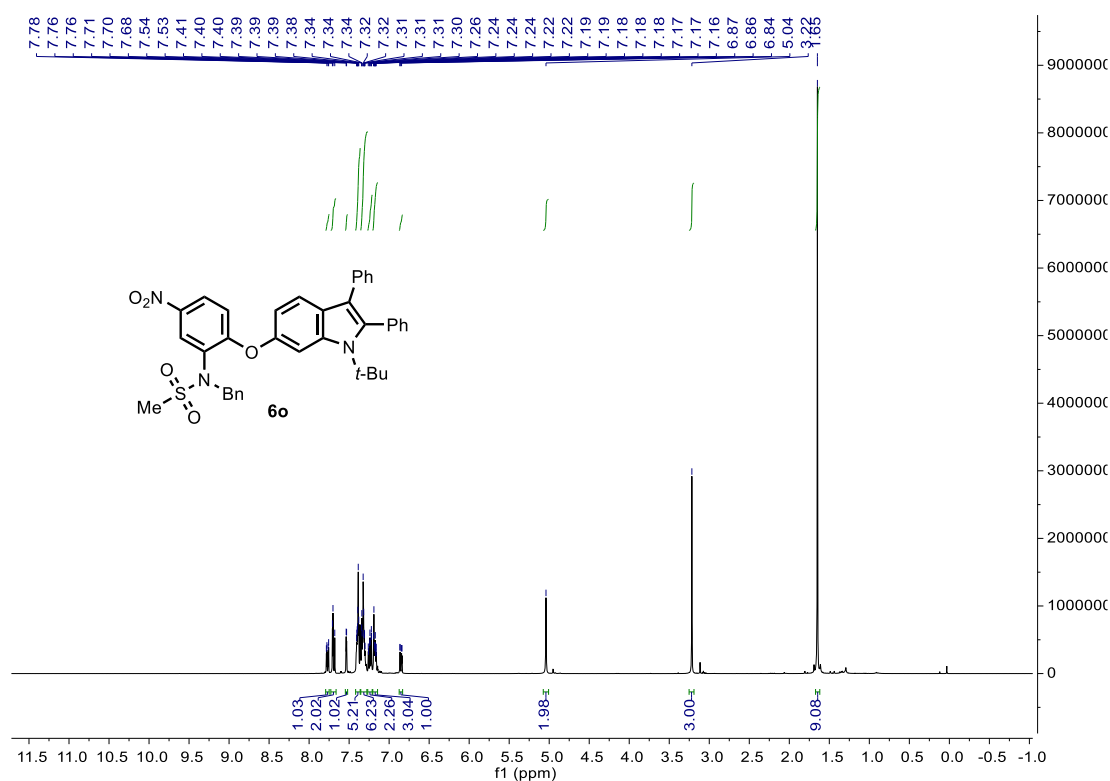


methyl 2-(1-(tert-butyl)-6-(2,4-dichlorophenoxy)-2,3-diphenyl-1H-indol-5-yl)acetate (**6n**) (¹³C NMR 126 MHz, CDCl₃)

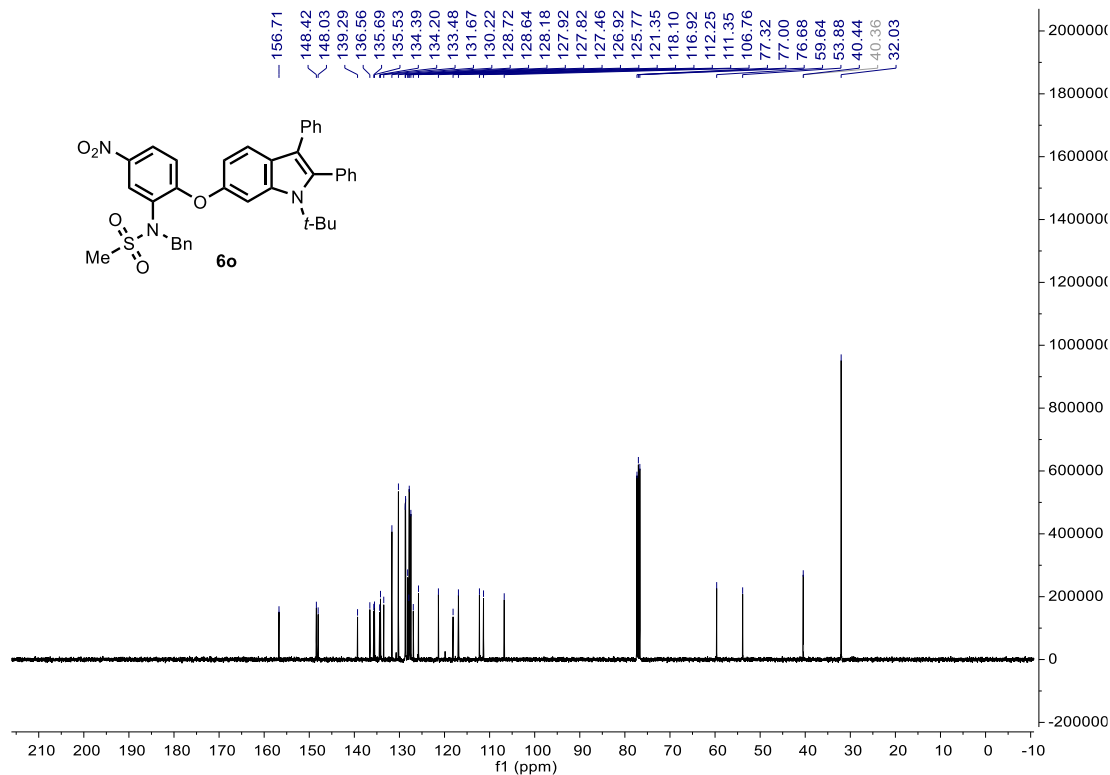


N-benzyl-*N*-(2-((1-(tert-butyl)-2,3-diphenyl-1H-indol-6-yl)oxy)-5-

nitrophenyl)methanesulfonamide (6o) (¹H NMR 400 MHz, CDCl₃)

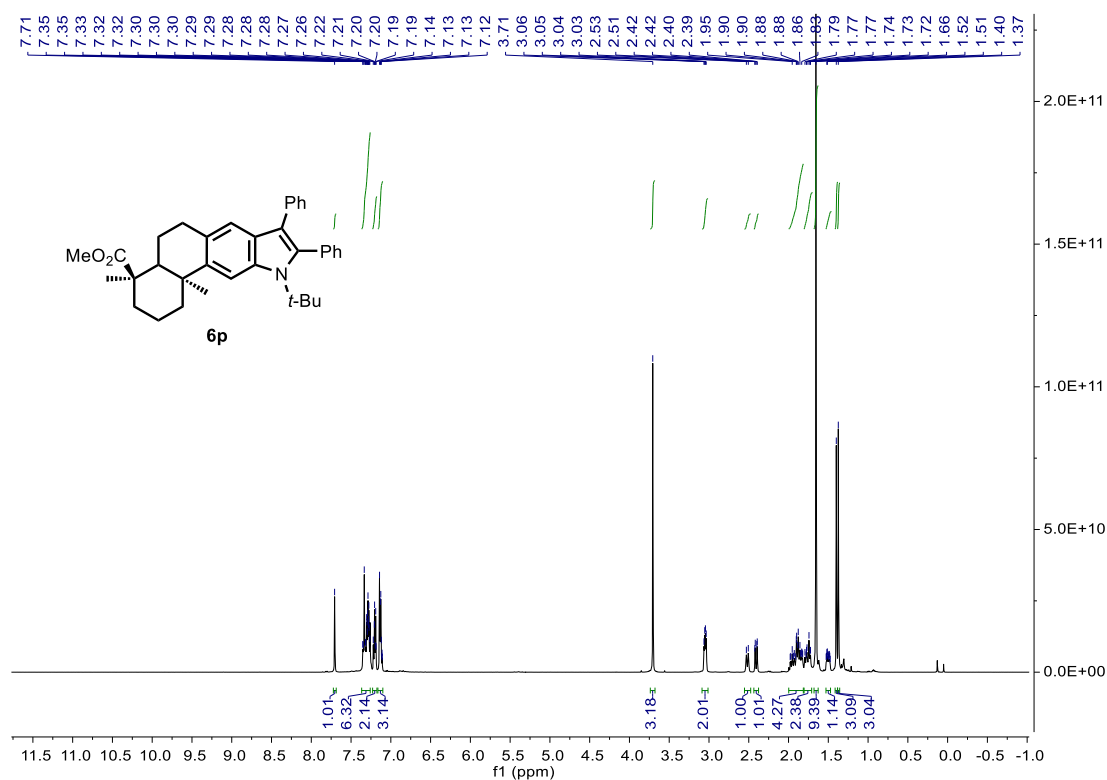


***N*-benzyl-*N*-(2-((1-(*tert*-butyl)-2,3-diphenyl-1H-indol-6-yl)oxy)-5-nitrophenyl)methanesulfonamide (6o) (¹³C NMR 101 MHz, CDCl₃)**

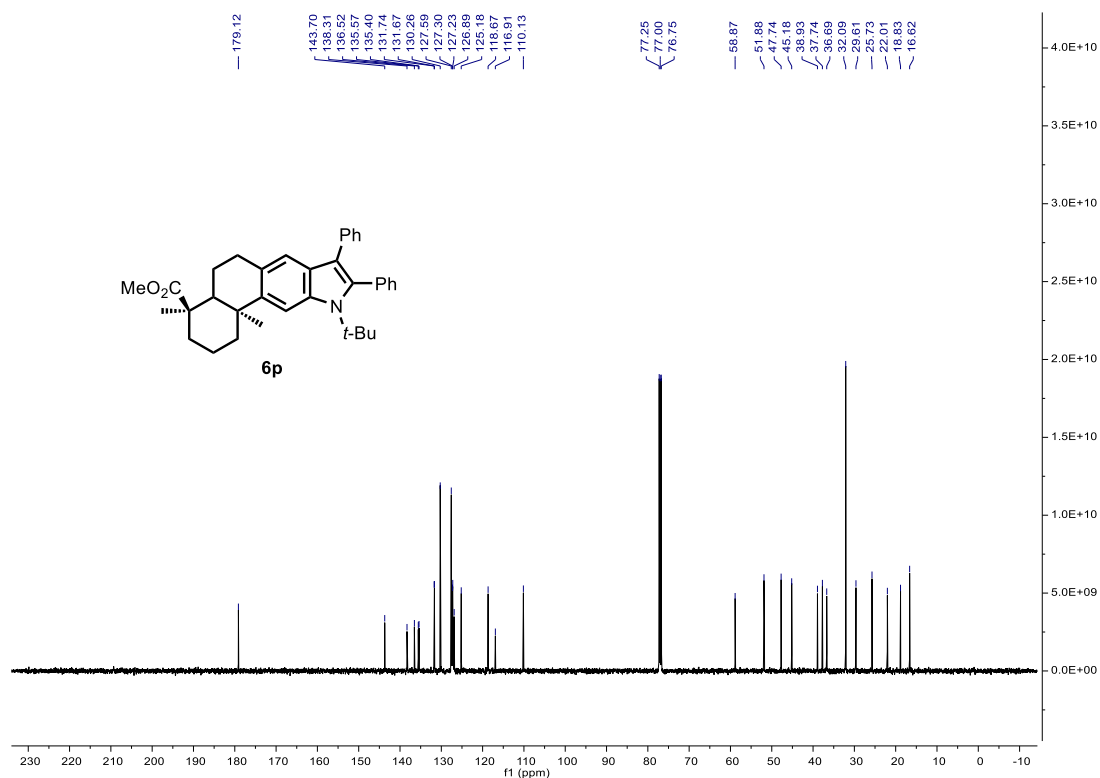


methyl (4*R*,11*bS*)-10-(*tert*-butyl)-4,11*b*-dimethyl-8,9-diphenyl-2,3,4,4*a*,5,6,10,11*b*-octahydro -

1H-naphtho[2,1-f]indole-4-carboxylate (6p) (¹H NMR 500 MHz, CDCl₃)

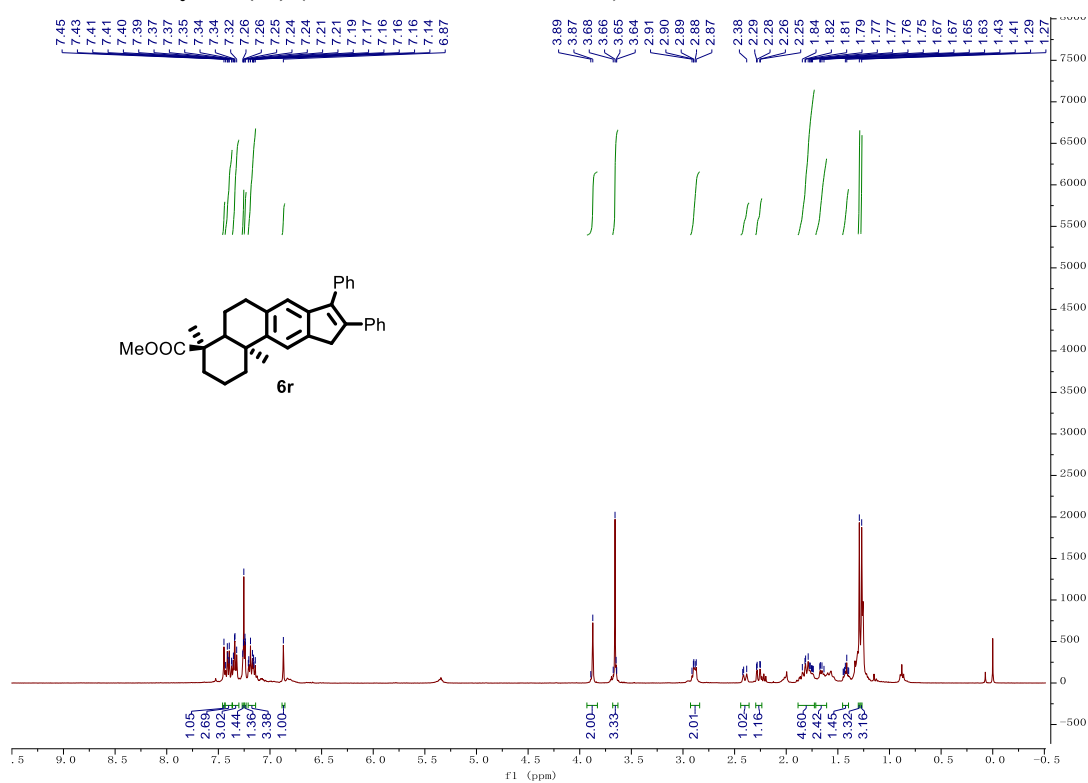


methyl (4R,11bS)-10-(tert-butyl)-4,11b-dimethyl-8,9-diphenyl-2,3,4,4a,5,6,10,11b-octahydro - 1H-naphtho[2,1-f]indole-4-carboxylate (6p) (¹³C NMR 126 MHz, CDCl₃)

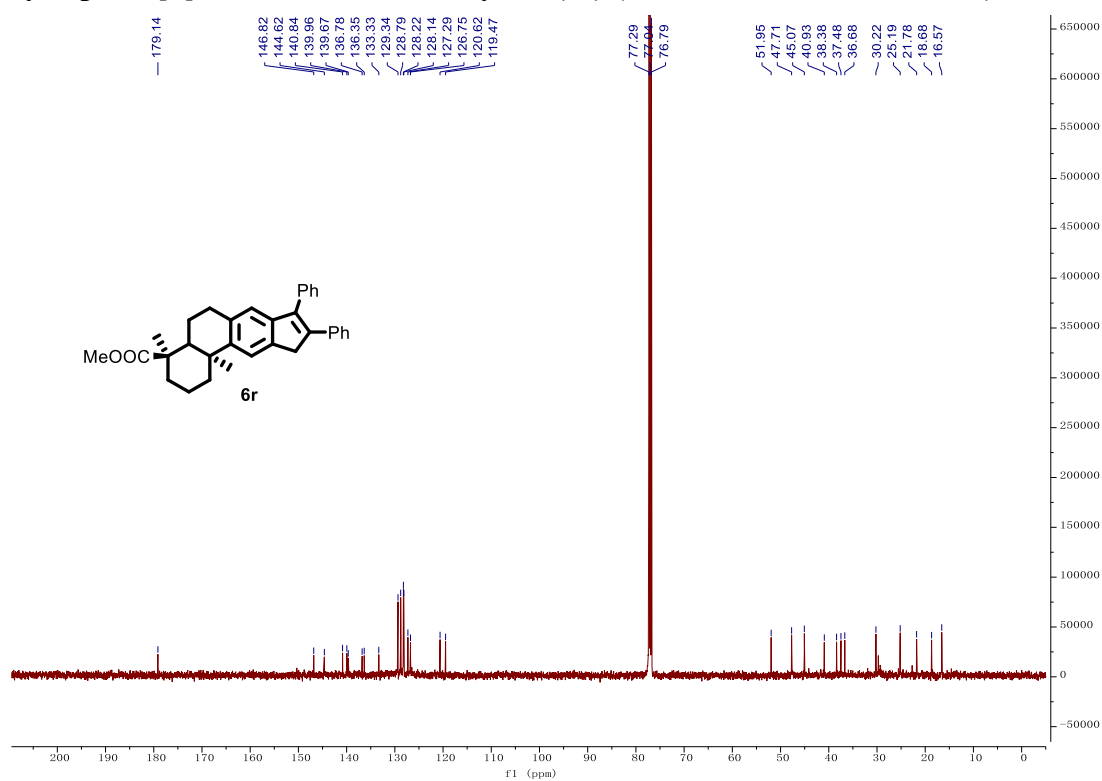


methyl 5a,9-dimethyl-2,3-diphenyl-5,5a,6,7,8,9,9a,10-octahydro-1H-cyclopenta[b]anthra

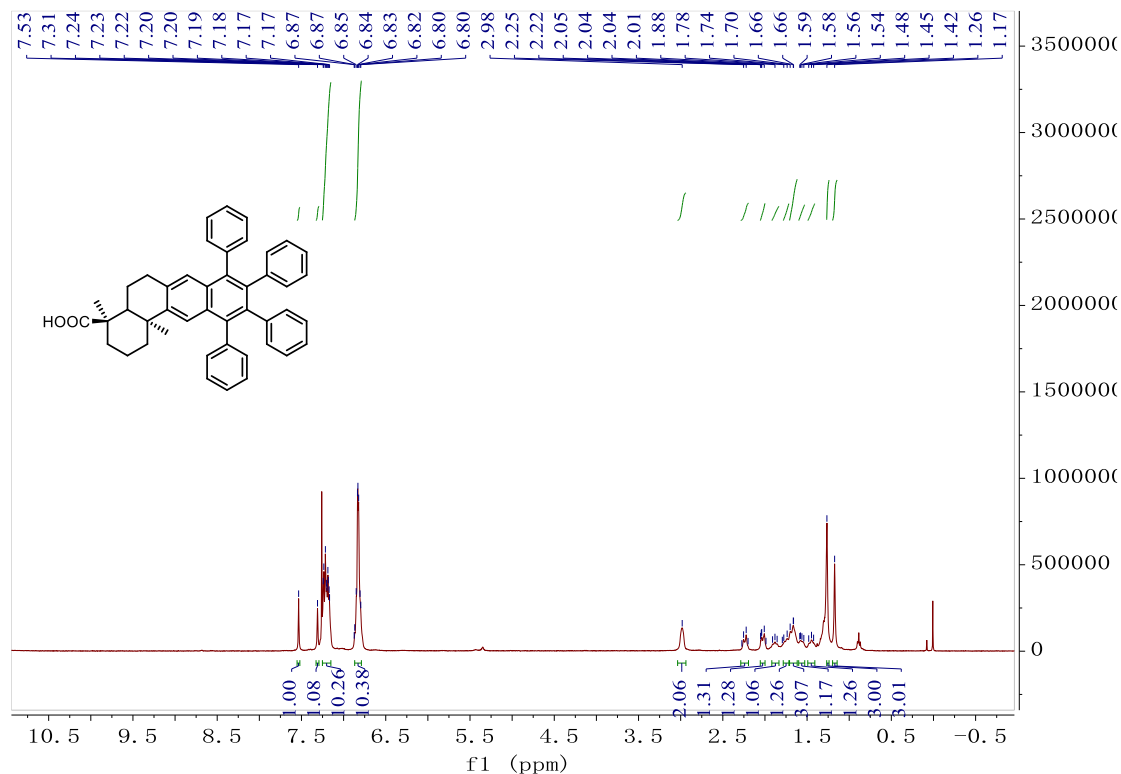
cene-9-carboxylate (6r) (¹H NMR 400 MHz, CDCl₃)



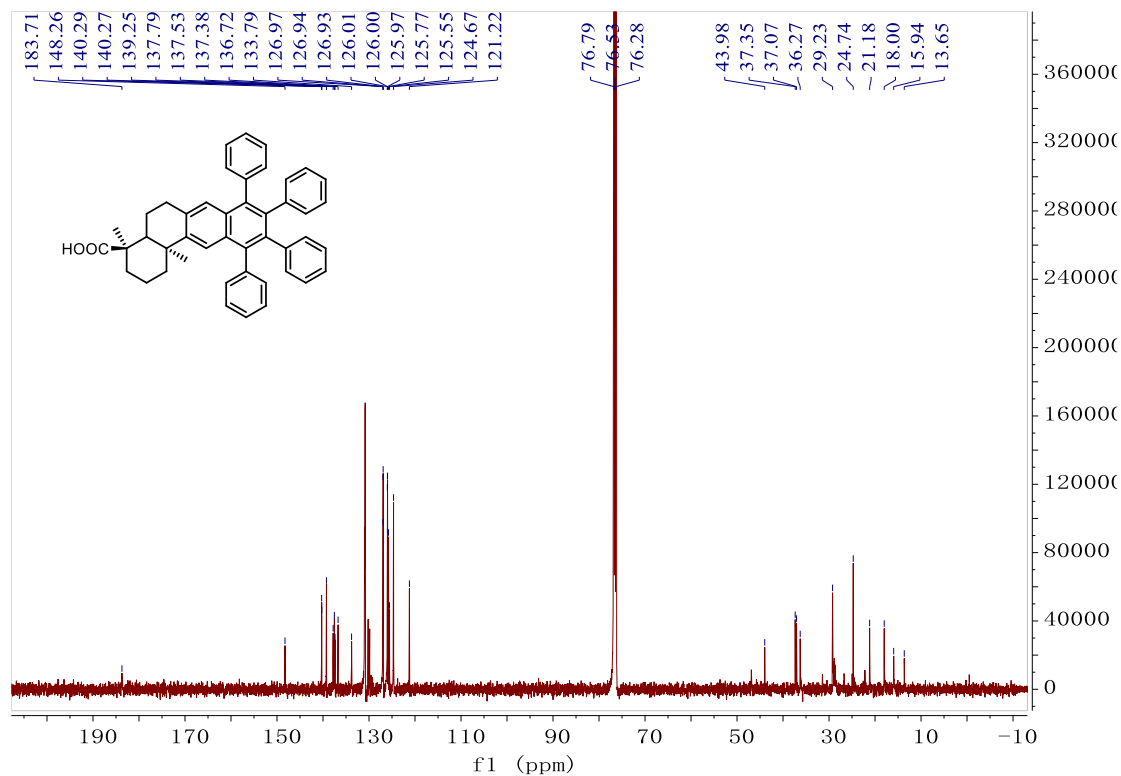
methyl 5a,9-dimethyl-2,3-diphenyl-5,5a,6,7,8,9,9a,10-octahydro-1H-cyclopenta[b]anthracene-9-carboxylate (6r) (¹³C NMR 126 MHz, CDCl₃)



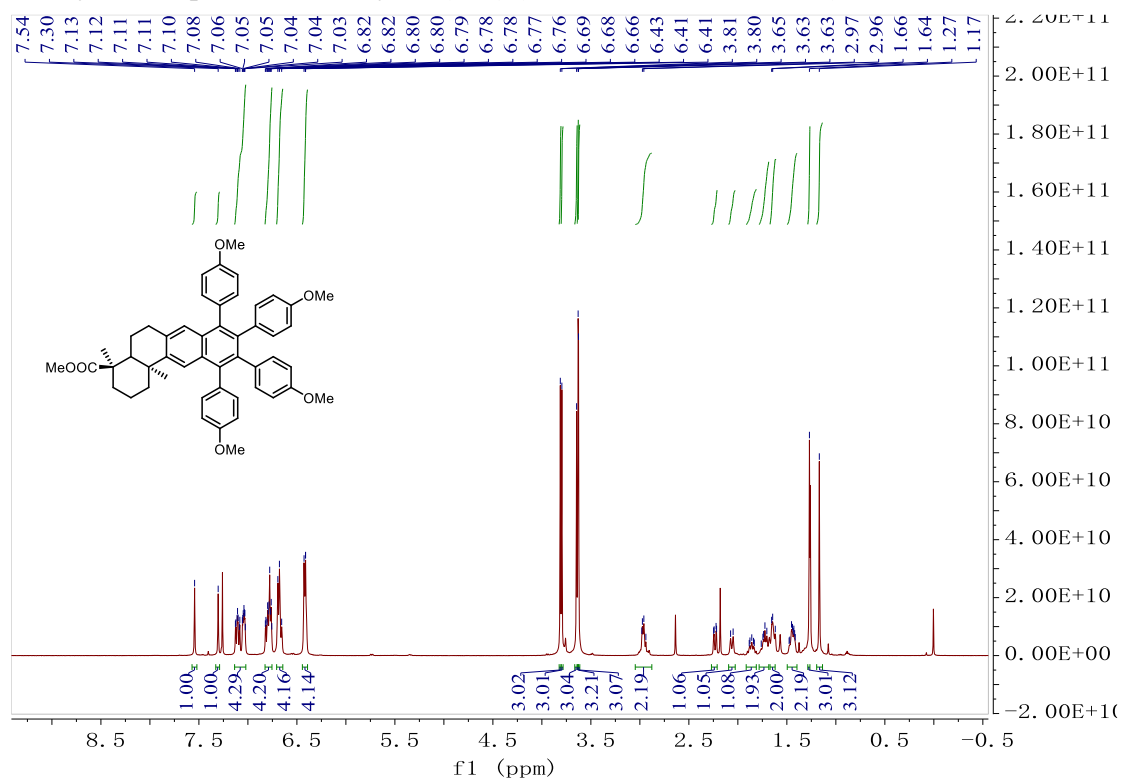
(4*R*,12*bS*)-4,12*b*-dimethyl-8,9,10,11-tetraphenyl-1,2,3,4,4*a*,5,6,12*b*-octahydrotetraphene-4-carboxylic acid (6s-1**) (¹H NMR 400 MHz, CDCl₃)**



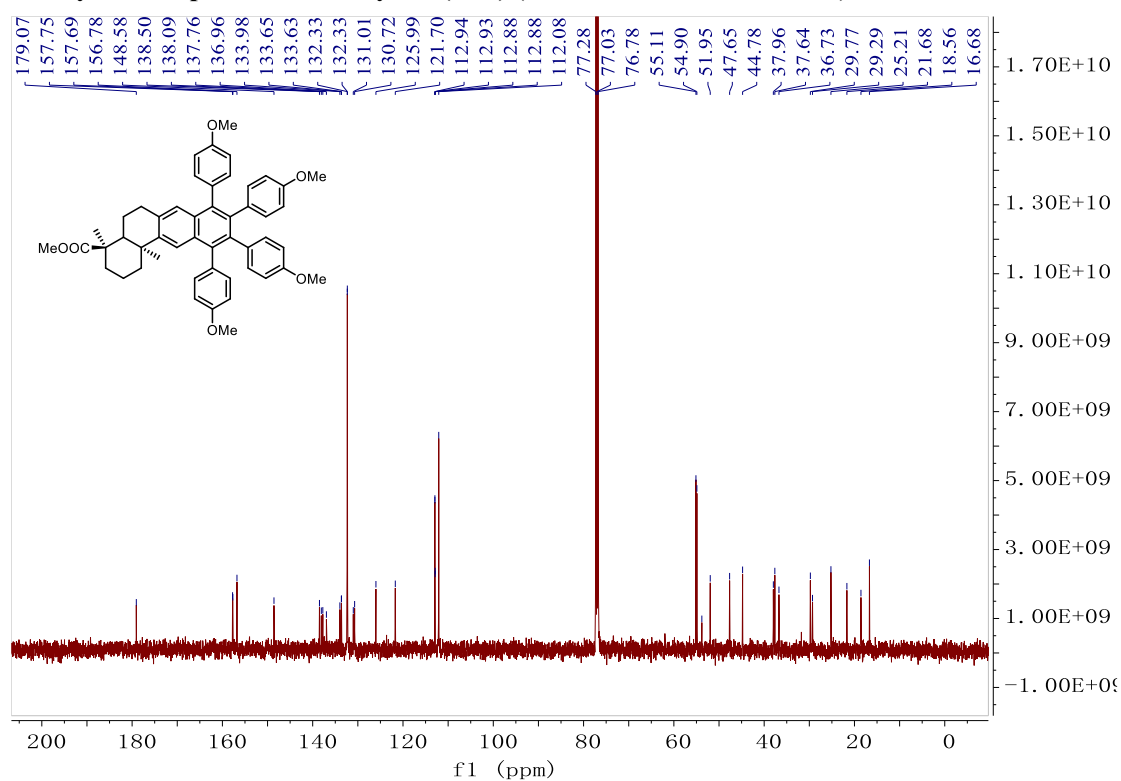
(4*R*,12*bS*)-4,12*b*-dimethyl-8,9,10,11-tetraphenyl-1,2,3,4,4*a*,5,6,12*b*-octahydrotetraphene-4-carboxylic acid (6s-1**) (¹³C NMR 126 MHz, CDCl₃)**



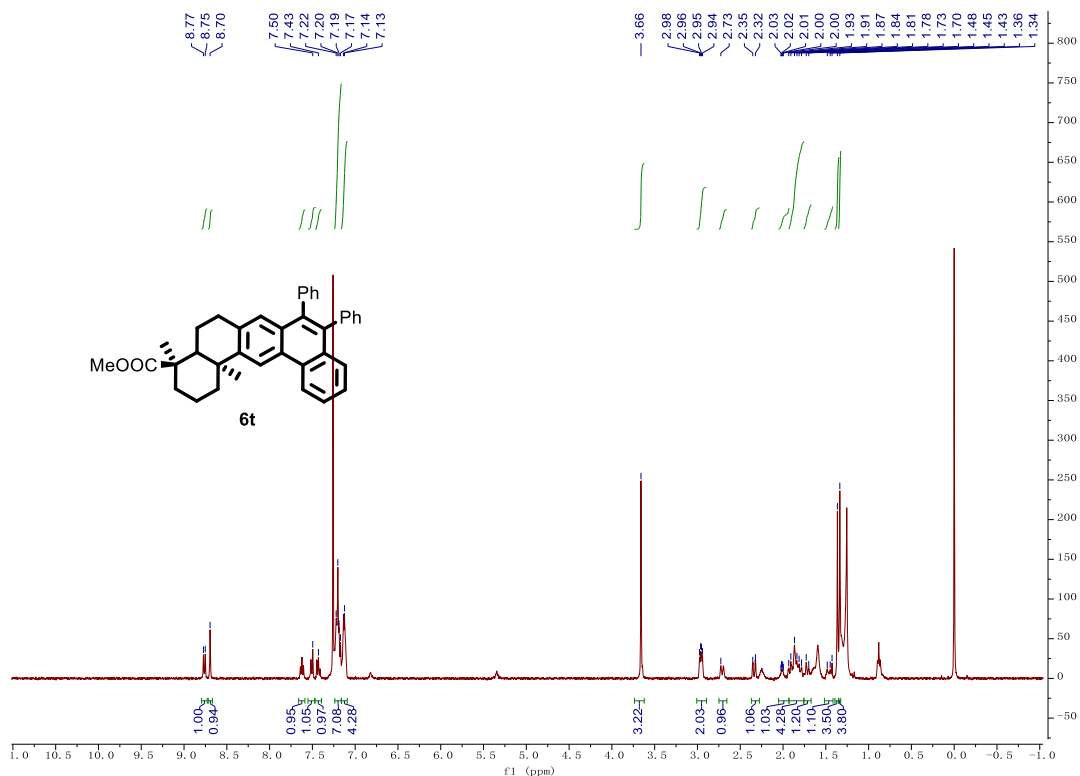
methyl (4*R*,12*bS*)-8,9,10,11-tetrakis(4-methoxyphenyl)-4,12*b*-dimethyl-1,2,3,4,4*a*,5,6,12*b*-octahydrotetraphene-4-carboxylate (6*s*-2) (¹H NMR 500 MHz, CDCl₃)



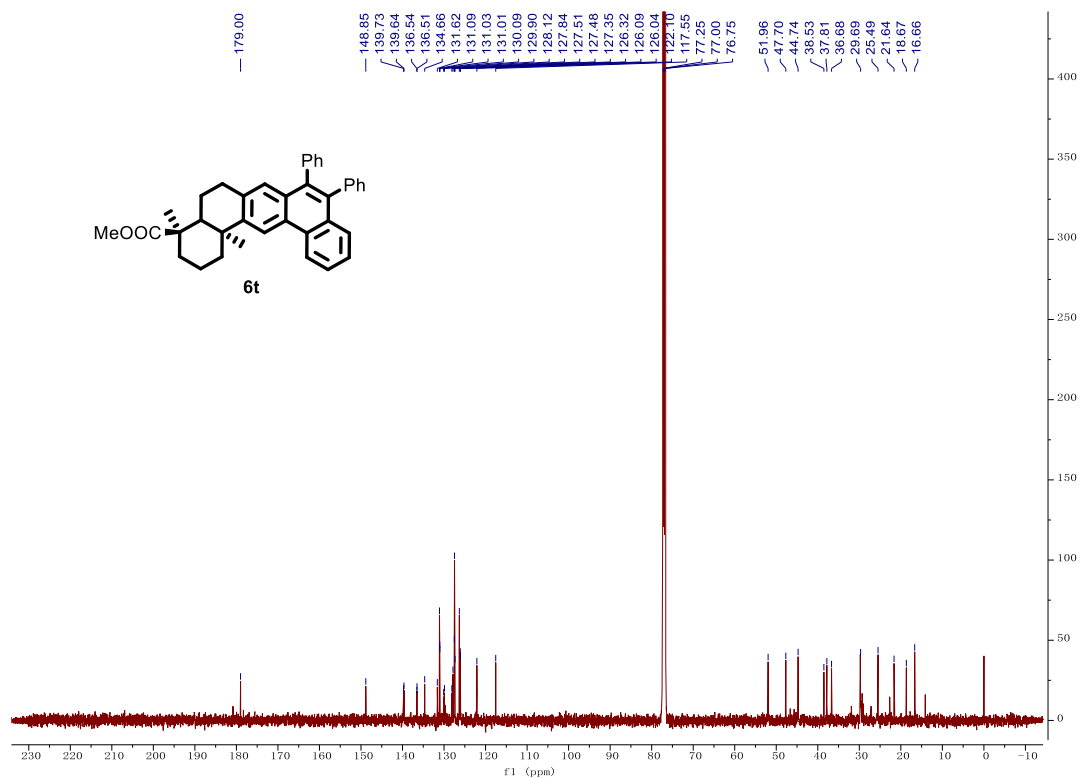
methyl (4*R*,12*bS*)-8,9,10,11-tetrakis(4-methoxyphenyl)-4,12*b*-dimethyl-1,2,3,4,4*a*,5,6,12*b*-octahydrotetraphene-4-carboxylate (6*s*-2) (¹³C NMR 126 MHz, CDCl₃)



methyl 8a,12-dimethyl-5,6-diphenyl-8,8a,9,10,11,12,12a,13-octahydrobenzo[a]tetracene-12-carboxylate (6t) (¹H NMR 400 MHz, CDCl₃)



methyl 8a,12-dimethyl-5,6-diphenyl-8,8a,9,10,11,12,12a,13-octahydrobenzo[a]tetracene-12-carboxylate (6t) (¹³C NMR 126 MHz, CDCl₃)



Chemical structure of compound 10: OC(=O)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC=C4[C@@]3(CC[C@@H](C4)C)C)C

¹H NMR spectrum (CDCl₃):

- Chemical shift range:** 0.5 – 9.5 ppm
- Integration values (from left to right):** 1.00, 1.04, 1.07, 1.06, 1.10, 1.13, 4.33, 2.02, 1.12, 1.40, 1.07, 4.06, 2.35, 3.15, 3.39.

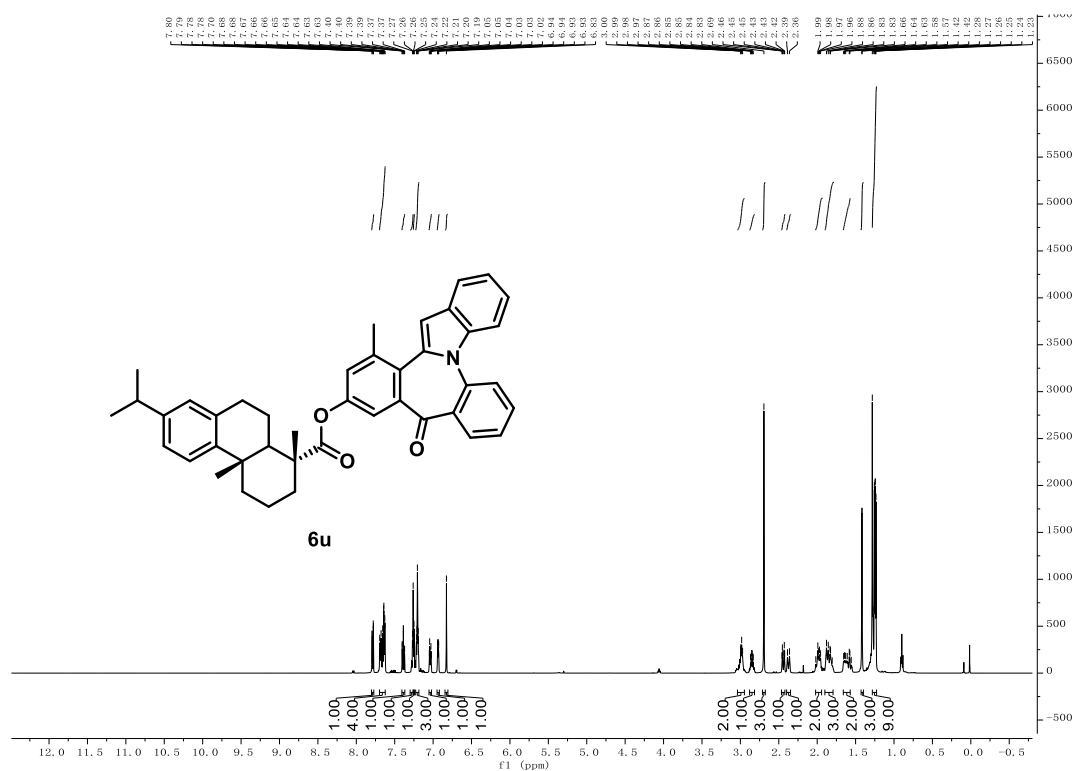
Chemical structure of the compound is shown in the top left corner. The structure is a complex polycyclic molecule with two phenyl groups (Ph) and a carboxylic acid group (HOOC).

The ^{13}C NMR spectrum (f1 (ppm)) is displayed below the structure, showing peaks corresponding to the carbon atoms in the molecule. The x-axis ranges from 0 to 190 ppm, and the y-axis represents intensity from 0 to 1,500,000.

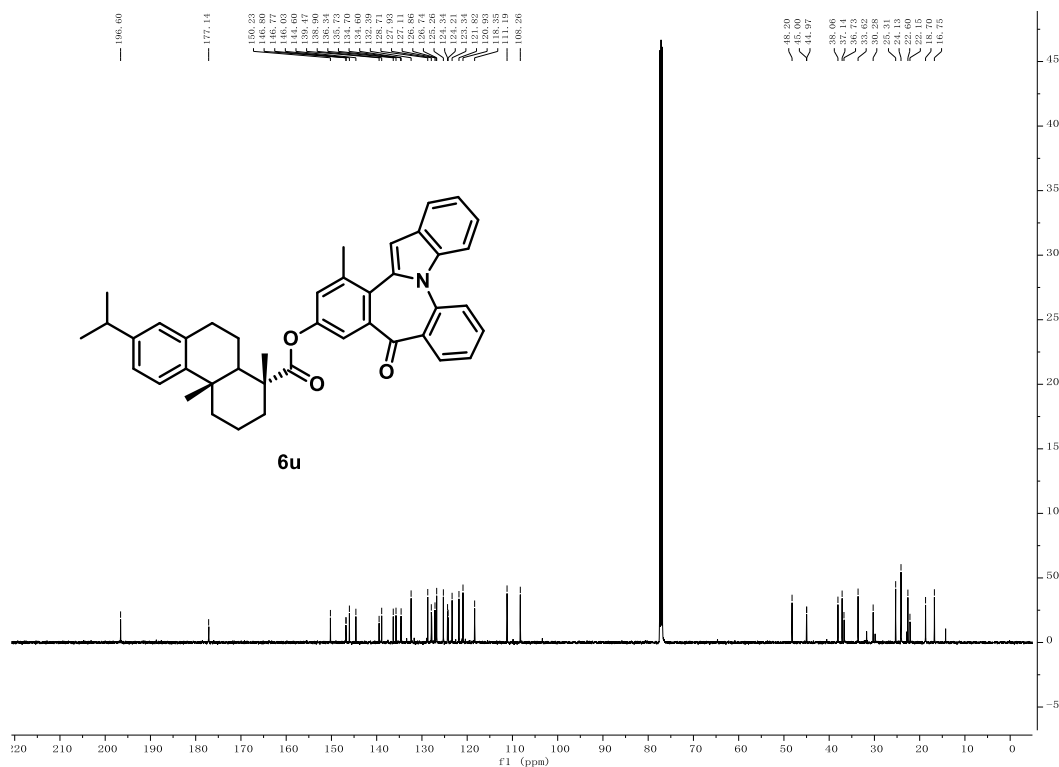
Key peaks are labeled with their chemical shifts (ppm):

- 183.52
- 148.69
- 139.74
- 139.63
- 136.55
- 136.53
- 134.61
- 131.62
- 131.10
- 131.05
- 131.00
- 130.09
- 129.92
- 128.13
- 127.85
- 127.53
- 127.48
- 127.40
- 126.32
- 126.09
- 126.05
- 122.09
- 117.55
- 77.25
- 77.00
- 76.75
- 47.39
- 44.53
- 38.46
- 37.72
- 36.74
- 29.75
- 25.50
- 21.68
- 18.61
- 16.41

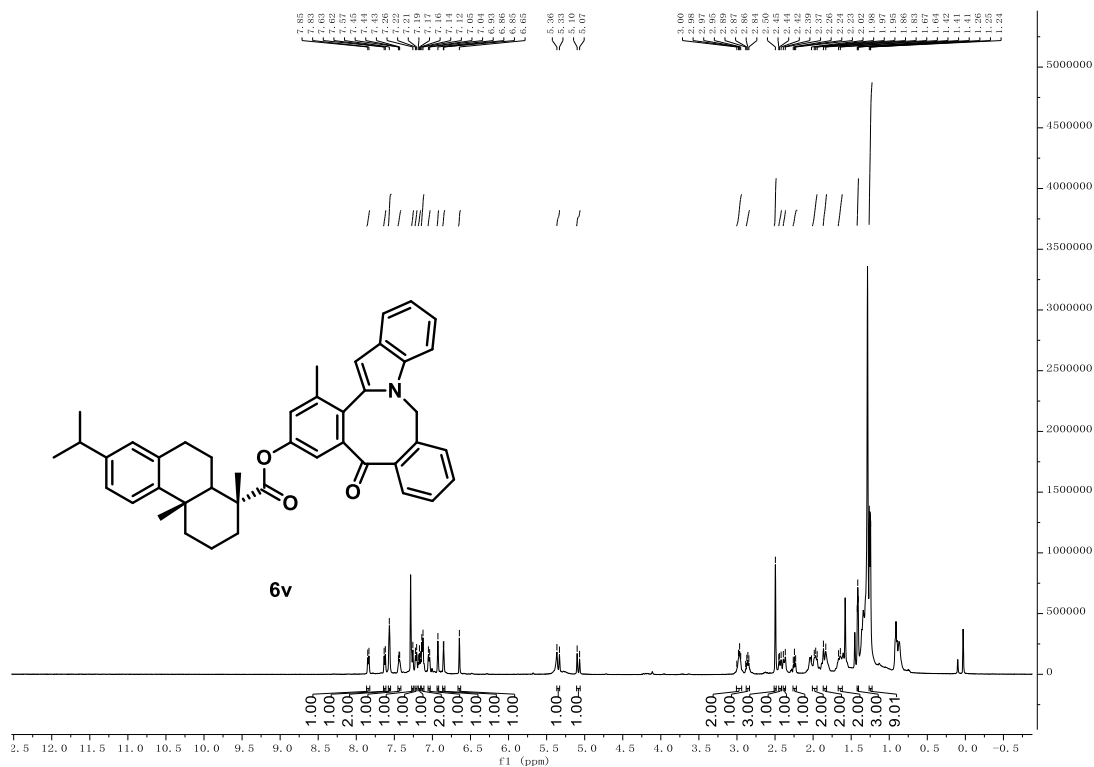
14-methyl-10-oxo-10*H*-dibenzo[3,4:6,7]azepino[1,2-*a*]indol-12-yl (1*R*,4*aS*)-7-isopropyl-1,4a-dimethyl-1,2,3,4,4a,9,10,10a-octahydrophenanthrene-1-carboxylate (6u) (¹H NMR 500 MHz, CDCl₃)



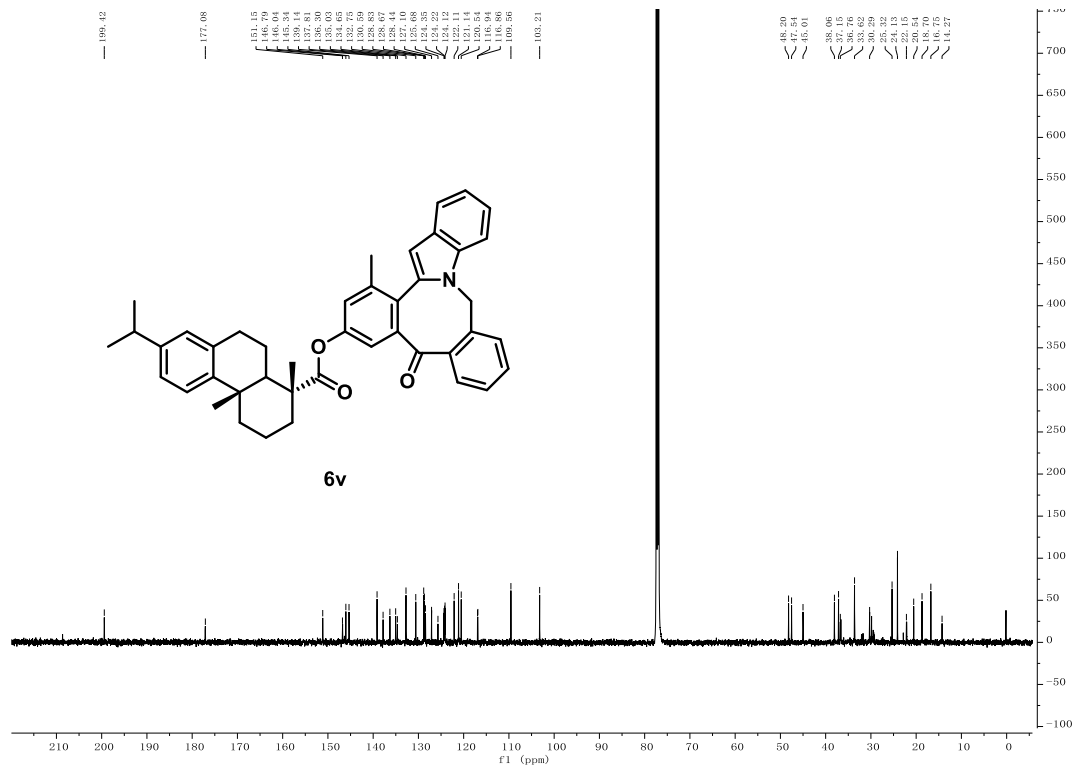
14-methyl-10-oxo-10*H*-dibenzo[3,4:6,7]azepino[1,2-*a*]indol-12-yl (1*R*,4*aS*)-7-isopropyl-1,4a-dimethyl-1,2,3,4,4a,9,10,10a-octahydrophenanthrene-1-carboxylate (6u) (¹³C NMR 126 MHz, CDCl₃)



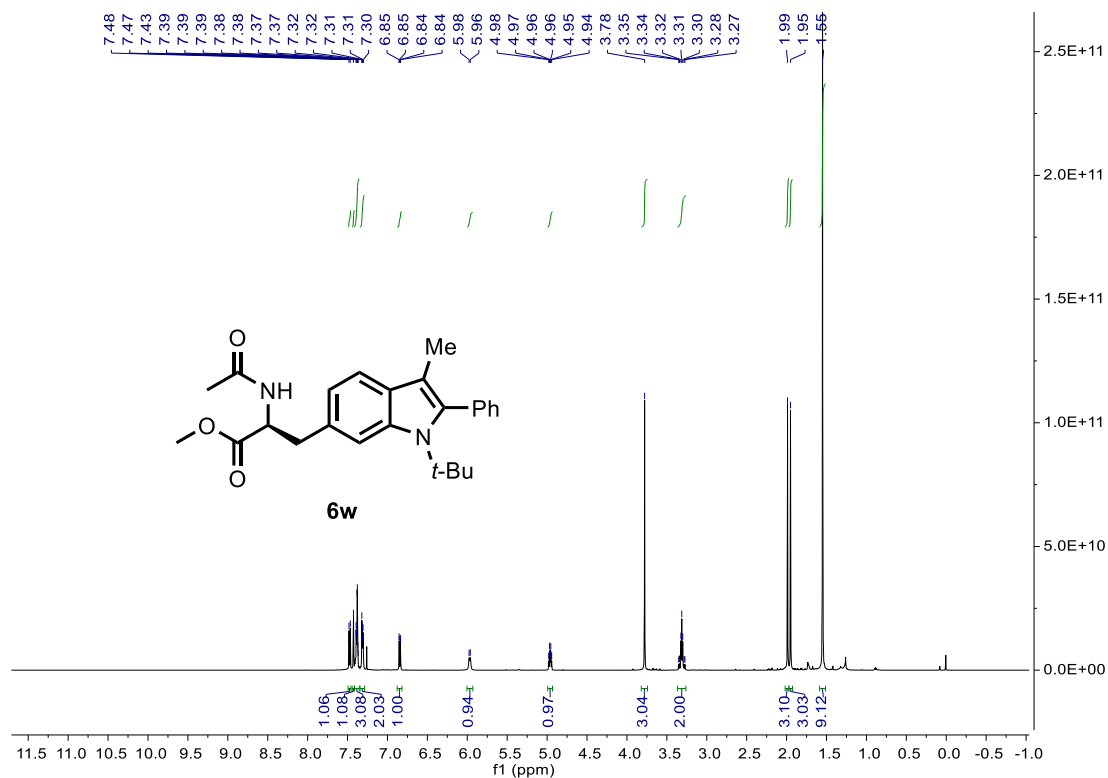
1-methyl-5-oxo-5,10-dihydrodibenzo[3,4:6,7]azocino[1,2-*a*]indol-3-yl (1*R*,4*aS*)-7-isopropyl-1,4*a*-dimethyl-1,2,3,4,4*a*,9,10,10*a*-octahydrophenanthrene-1-carboxylate (6v) (¹H NMR 500 MHz, CDCl₃)



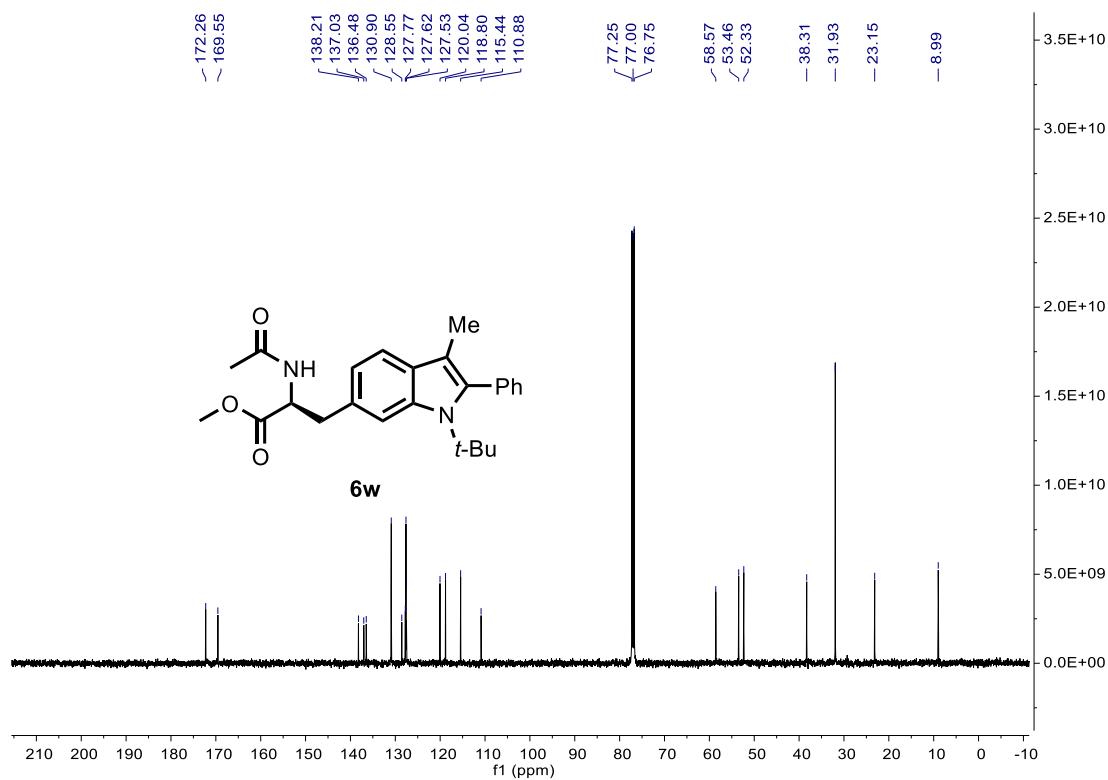
1-methyl-5-oxo-5,10-dihydrodibenzo[3,4:6,7]azocino[1,2-*a*]indol-3-yl (1*R*,4*aS*)-7-isopropyl-1,4*a*-dimethyl-1,2,3,4,4*a*,9,10,10*a*-octahydrophenanthrene-1-carboxylate (6v) (¹³C NMR 126 MHz, CDCl₃)



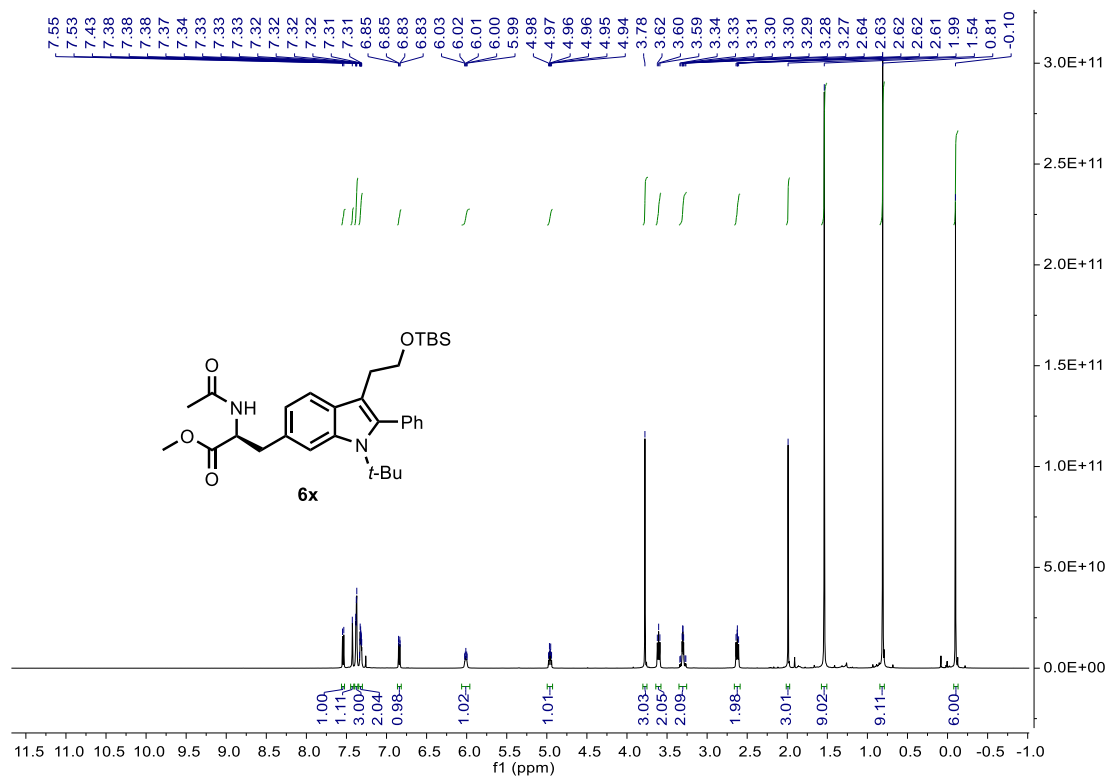
methyl (S)-2-acetamido-3-(1-(tert-butyl)-3-methyl-2-phenyl-1H-indol-6-yl)propanoate (6w)
(¹H NMR 500 MHz, CDCl₃)



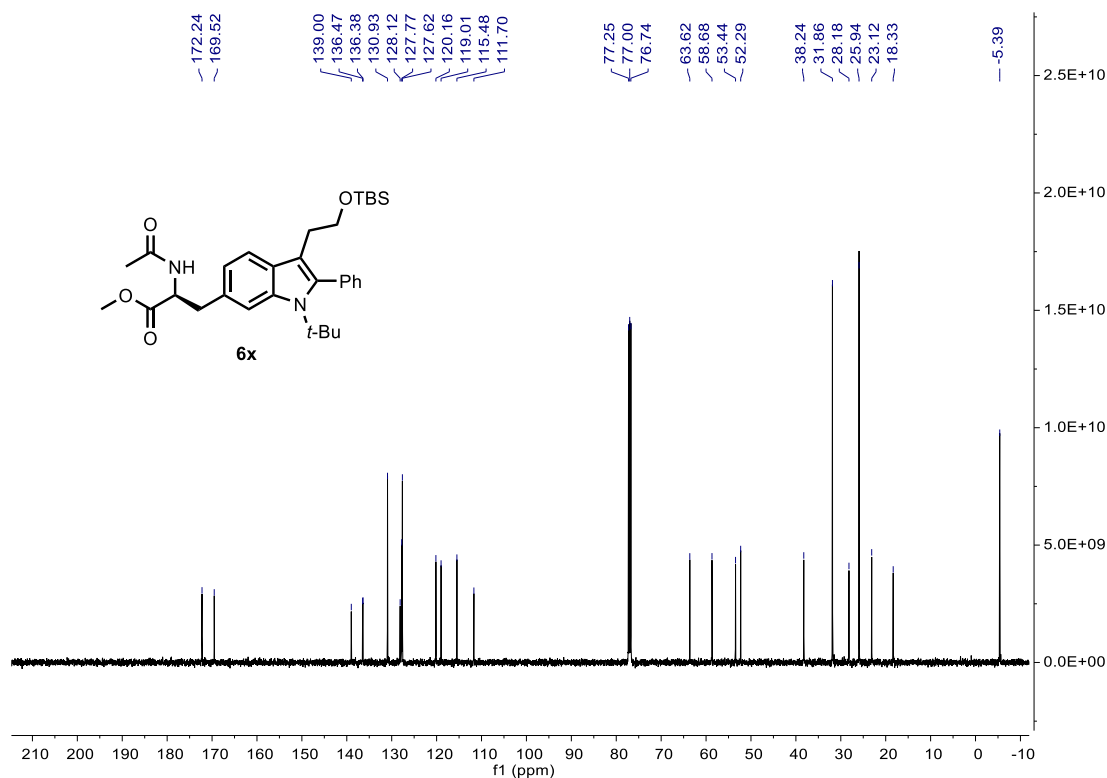
methyl (S)-2-acetamido-3-(1-(tert-butyl)-3-methyl-2-phenyl-1H-indol-6-yl)propanoate (6w)
(¹³C NMR 126 MHz, CDCl₃)



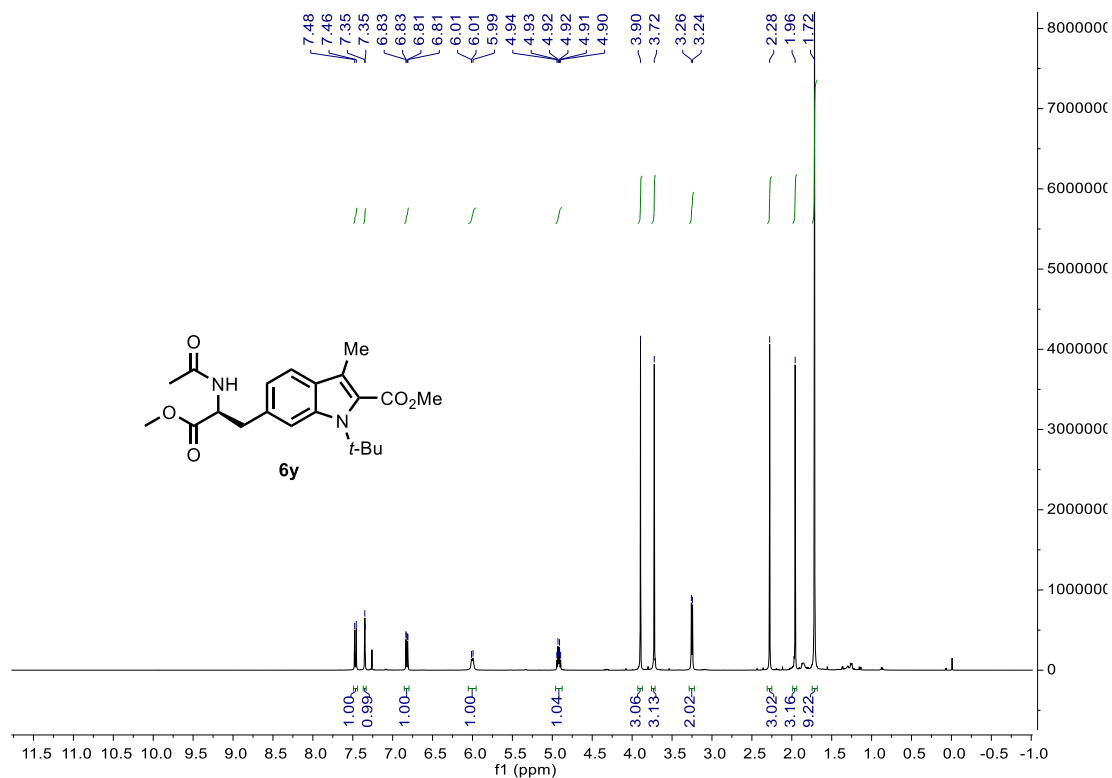
methyl (S)-2-acetamido-3-(1-(tert-butyl)-3-(2-((tert-butyldimethylsilyl)oxy)ethyl)-2-phenyl-1H-indol-6-yl)propanoate (6x) (¹H NMR 500 MHz, CDCl₃)



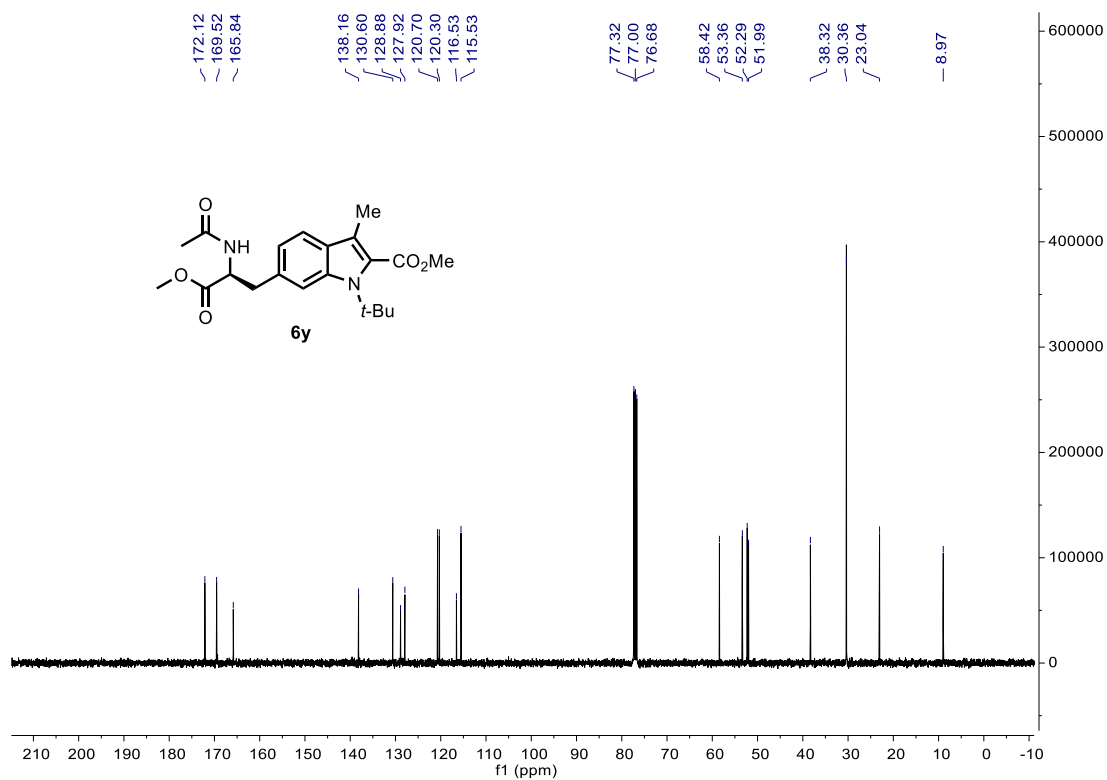
methyl (S)-2-acetamido-3-(1-(tert-butyl)-3-(2-((tert-butyldimethylsilyl)oxy)ethyl)-2-phenyl-1H-indol-6-yl)propanoate (6x) (¹³C NMR 126 MHz, CDCl₃)



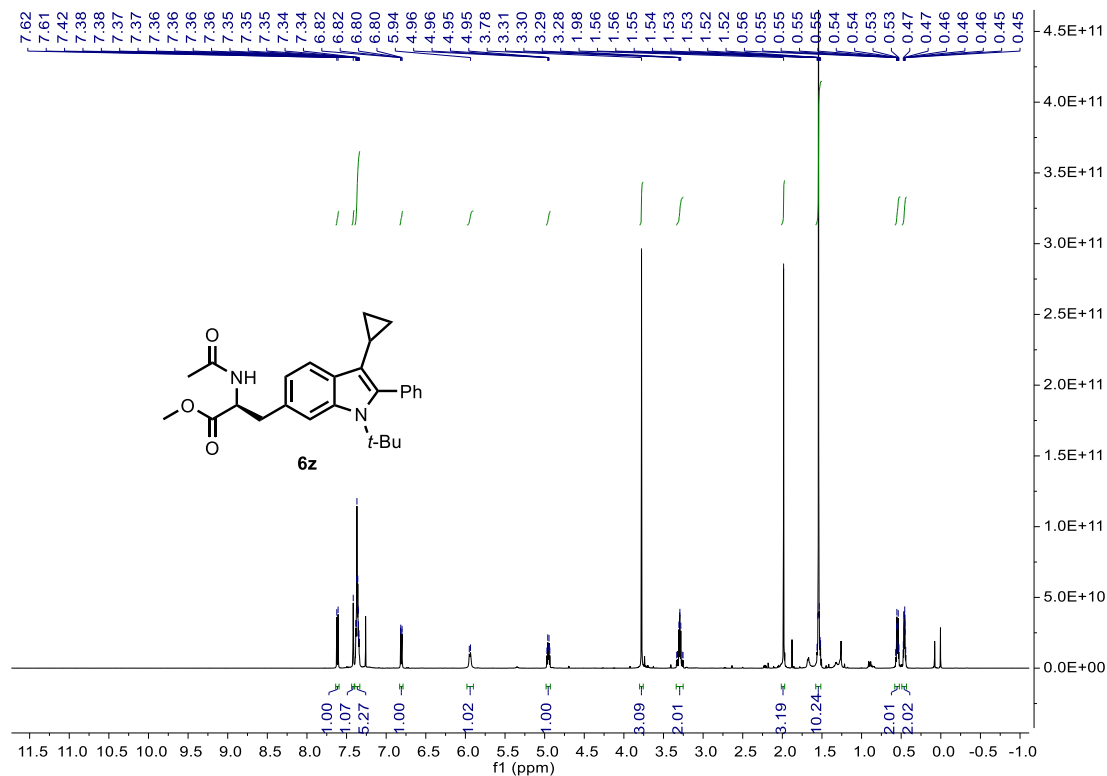
methyl (S)-6-(2-acetamido-3-methoxy-3-oxopropyl)-1-(tert-butyl)-3-methyl-1H-indole-2-carboxylate (6y) (¹H NMR 400 MHz, CDCl₃)



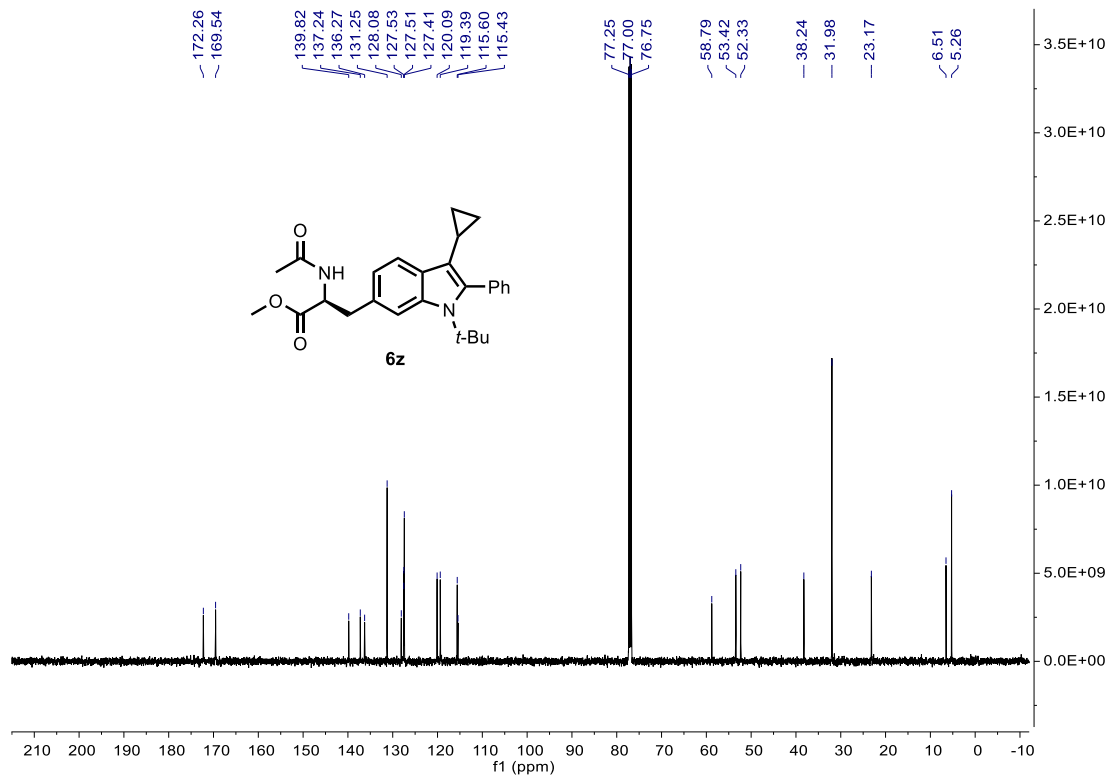
methyl (S)-6-(2-acetamido-3-methoxy-3-oxopropyl)-1-(tert-butyl)-3-methyl-1H-indole-2-carboxylate (6y) (¹³C NMR 126 MHz, CDCl₃)



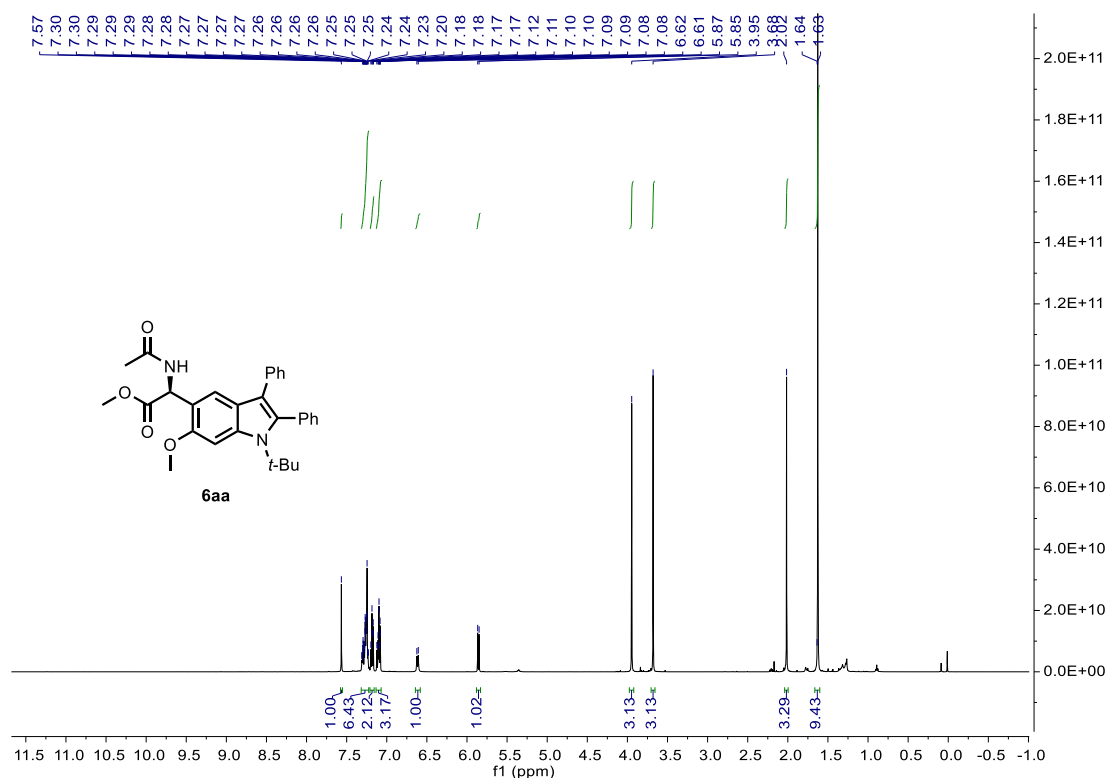
methyl (S)-2-acetamido-3-(1-(tert-butyl)-3-cyclopropyl-2-phenyl-1H-indol-6-yl)propanoate (6z) (¹H NMR 500 MHz, CDCl₃)



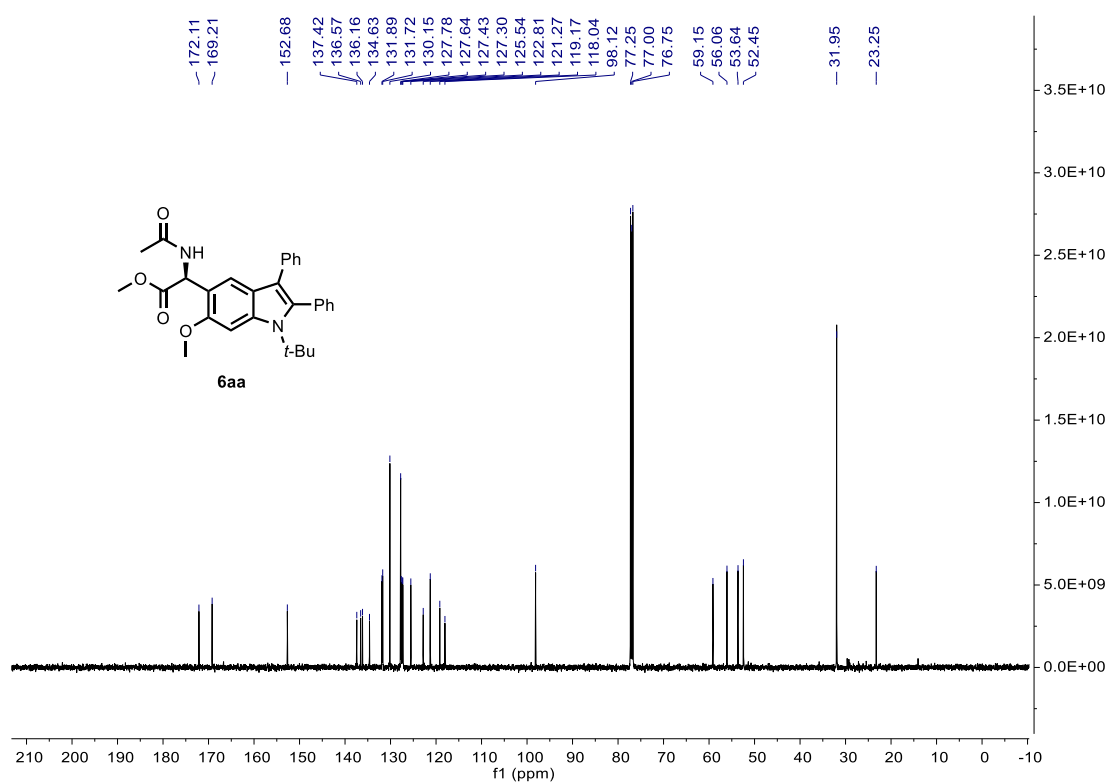
methyl (S)-2-acetamido-3-(1-(tert-butyl)-3-cyclopropyl-2-phenyl-1H-indol-6-yl)propanoate (6z) (¹³C NMR 126 MHz, CDCl₃)



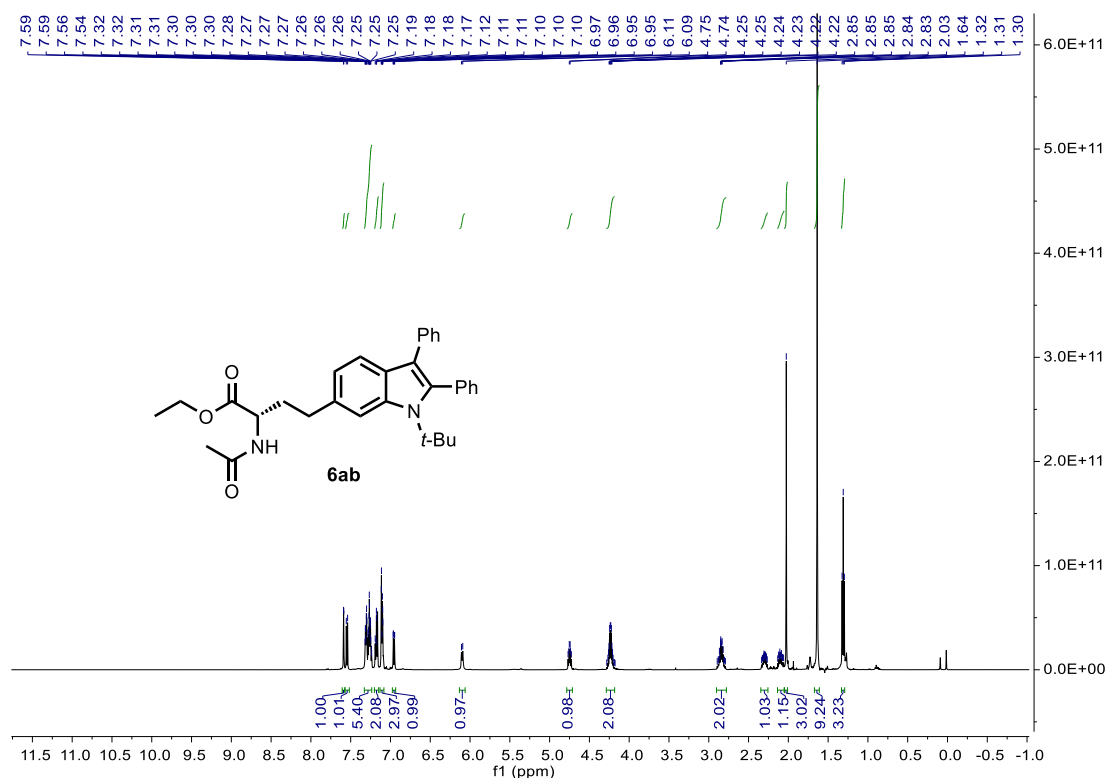
methyl (*R*)-2-acetamido-2-(1-(*tert*-butyl)-6-methoxy-2,3-diphenyl-1*H*-indol-5-yl)acetate (6aa)
(¹H NMR 500 MHz, CDCl₃)



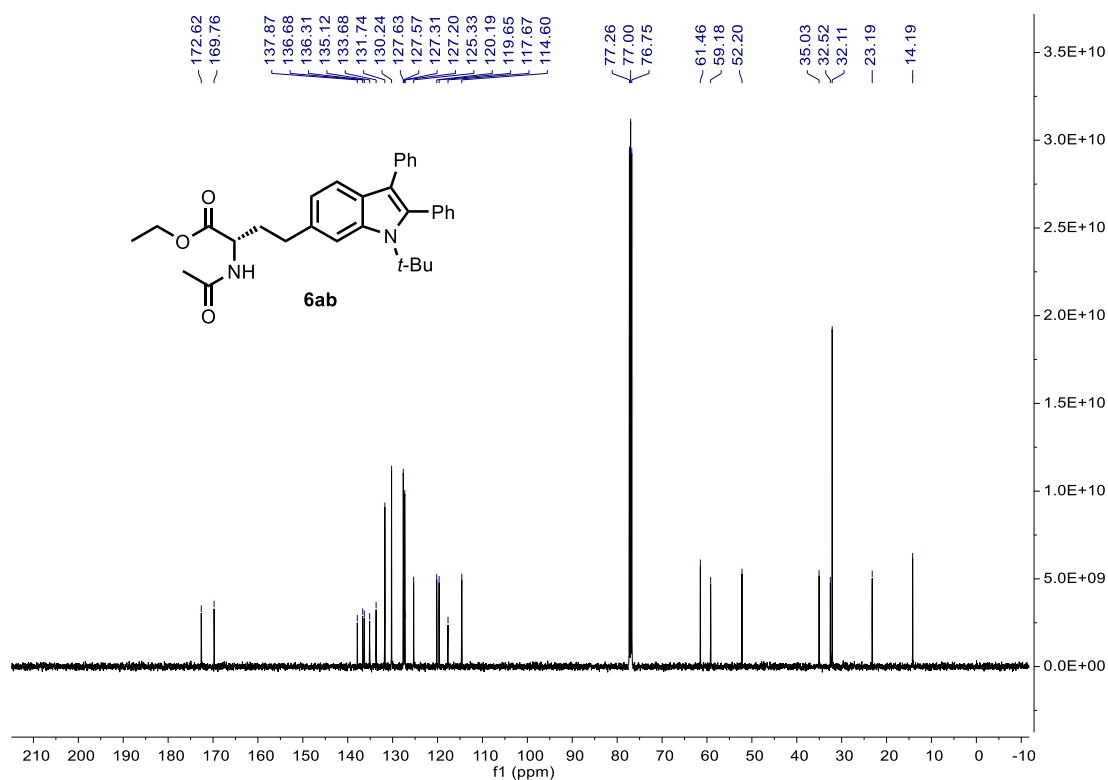
methyl (*R*)-2-acetamido-2-(1-(*tert*-butyl)-6-methoxy-2,3-diphenyl-1*H*-indol-5-yl)acetate (6aa)
(¹³C NMR 126 MHz, CDCl₃)



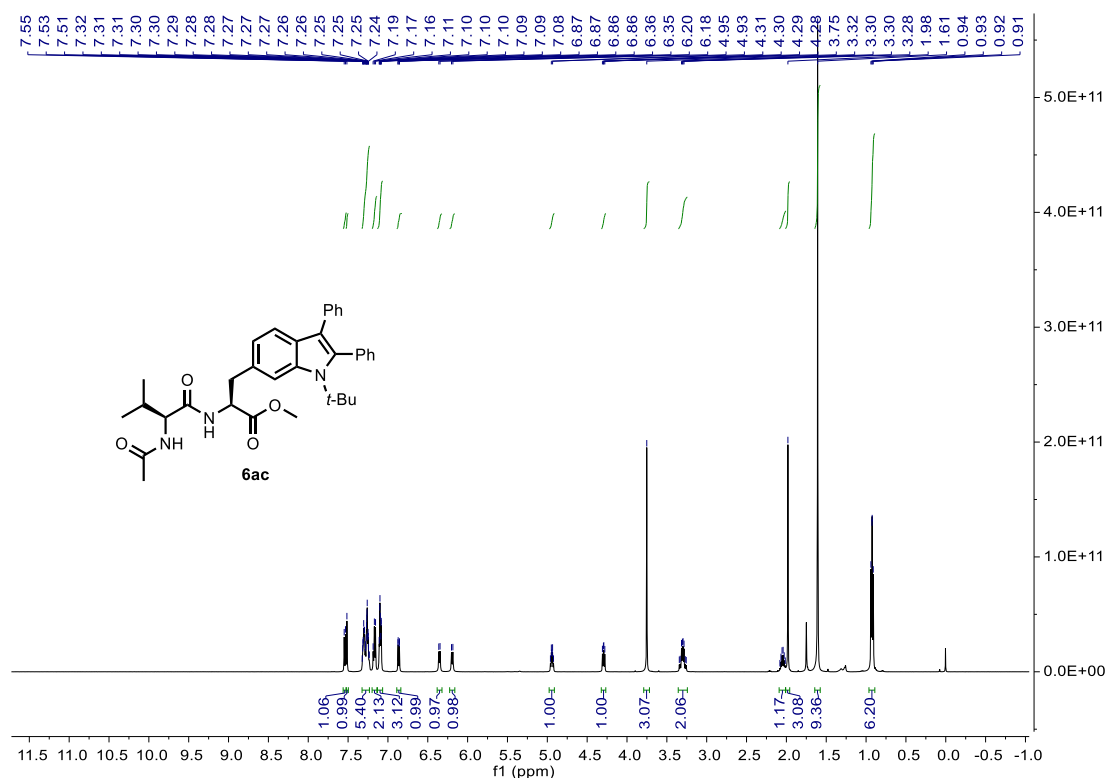
ethyl (*S*)-2-acetamido-4-(1-(*tert*-butyl)-2,3-diphenyl-1H-indol-6-yl)butanoate (**6ab**) (^1H NMR 500 MHz, CDCl_3)



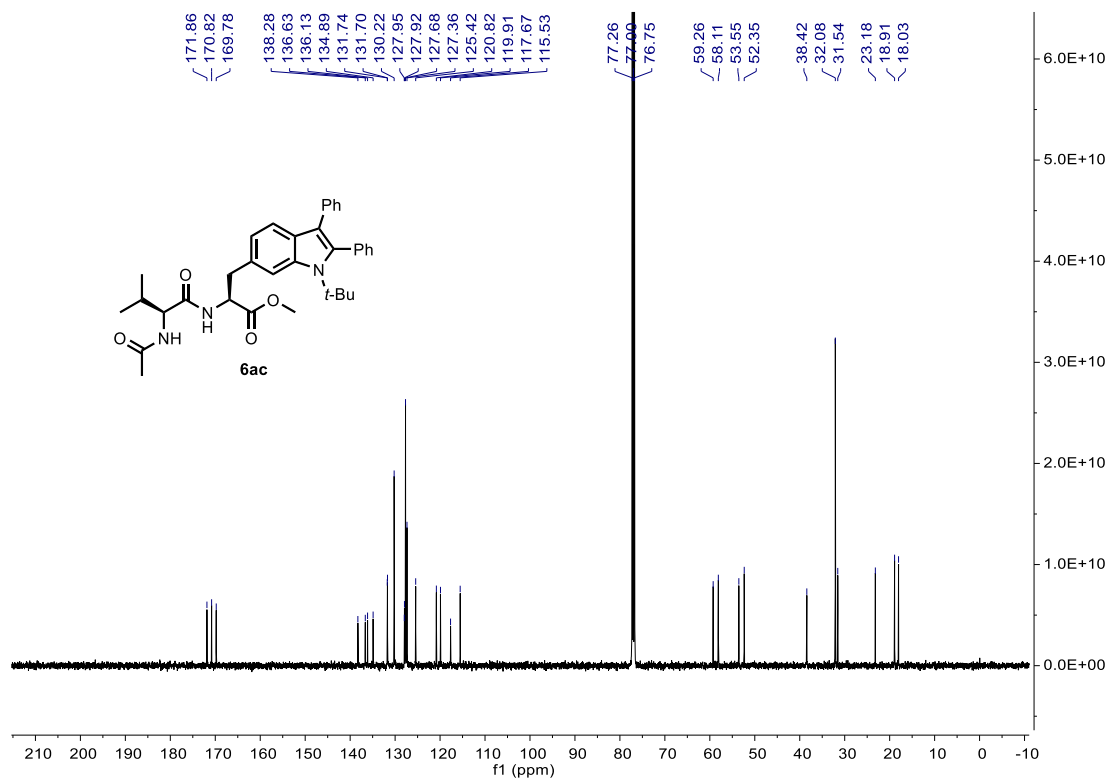
ethyl (*S*)-2-acetamido-4-(1-(*tert*-butyl)-2,3-diphenyl-1H-indol-6-yl)butanoate (**6ab**) (^{13}C NMR 126 MHz, CDCl_3)



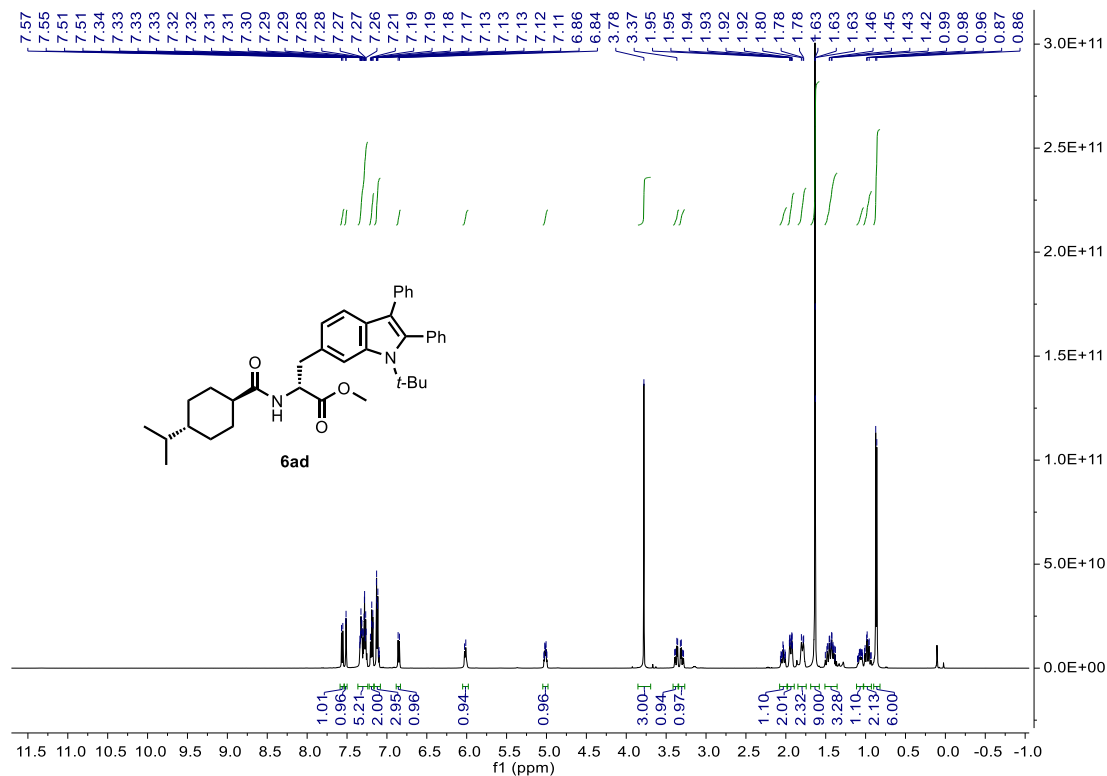
methyl (S)-2-((S)-2-acetamido-3-methylbutanamido)-3-(1-(tert-butyl)-2,3-diphenyl-1H-indol-6-yl)propanoate (6ac) (¹H NMR 500 MHz, CDCl₃)



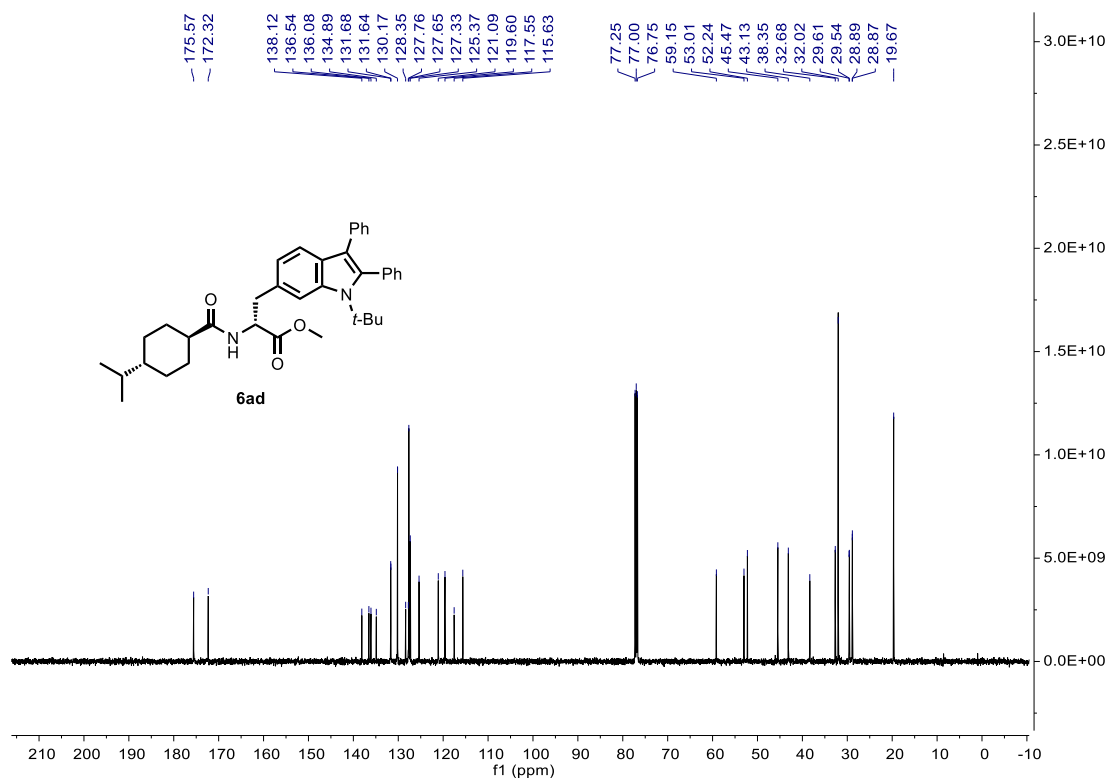
methyl (S)-2-((S)-2-acetamido-3-methylbutanamido)-3-(1-(tert-butyl)-2,3-diphenyl-1H-indol-6-yl)propanoate (6ac) (¹³C NMR 126 MHz, CDCl₃)



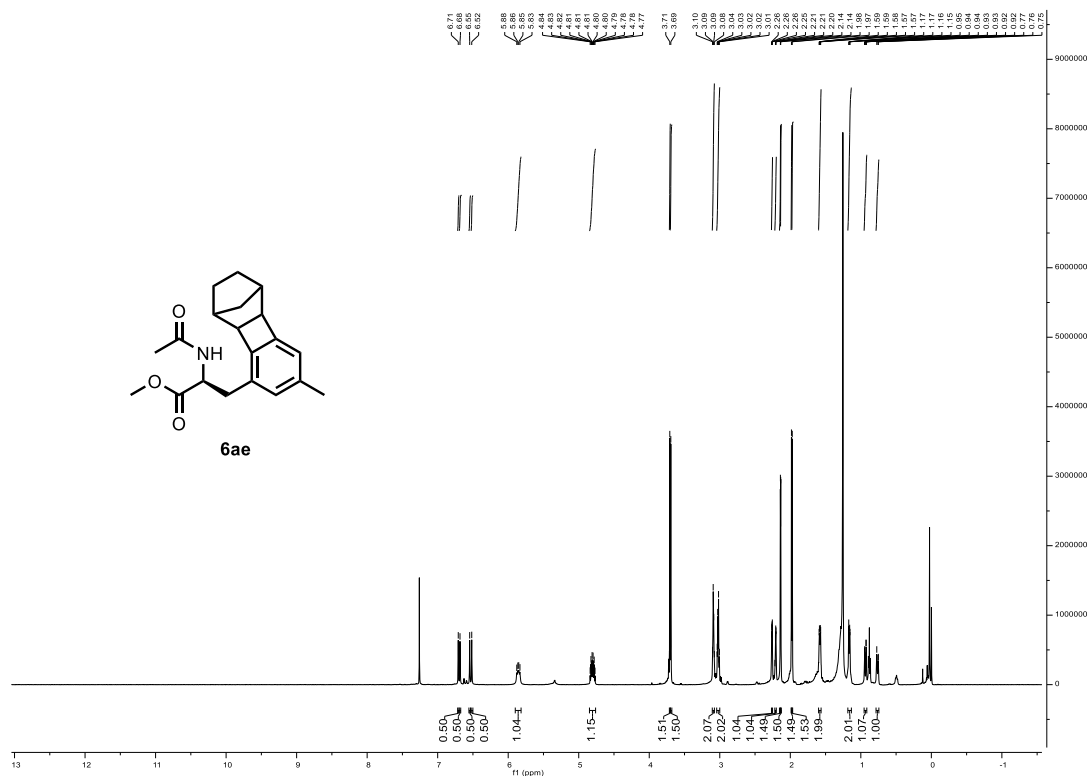
methyl (R)-3-(1-(tert-butyl)-2,3-diphenyl-1H-indol-6-yl)-2-((1*r*,4*R*)-4-isopropylcyclohexane-1-carboxamido)propanoate (6ad) (¹H NMR 500 MHz, CDCl₃)



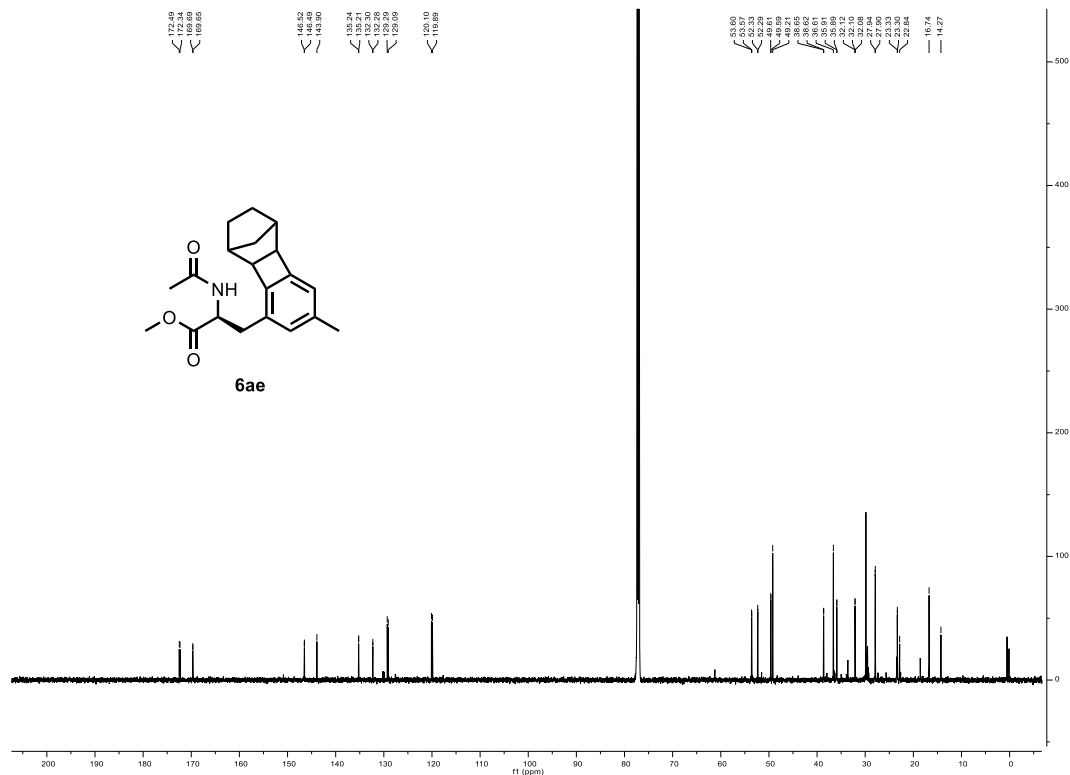
methyl (R)-3-(1-(tert-butyl)-2,3-diphenyl-1H-indol-6-yl)-2-((1*r*,4*R*)-4-isopropylcyclohexane-1-carboxamido)propanoate (6ad) (¹³C NMR 126 MHz, CDCl₃)



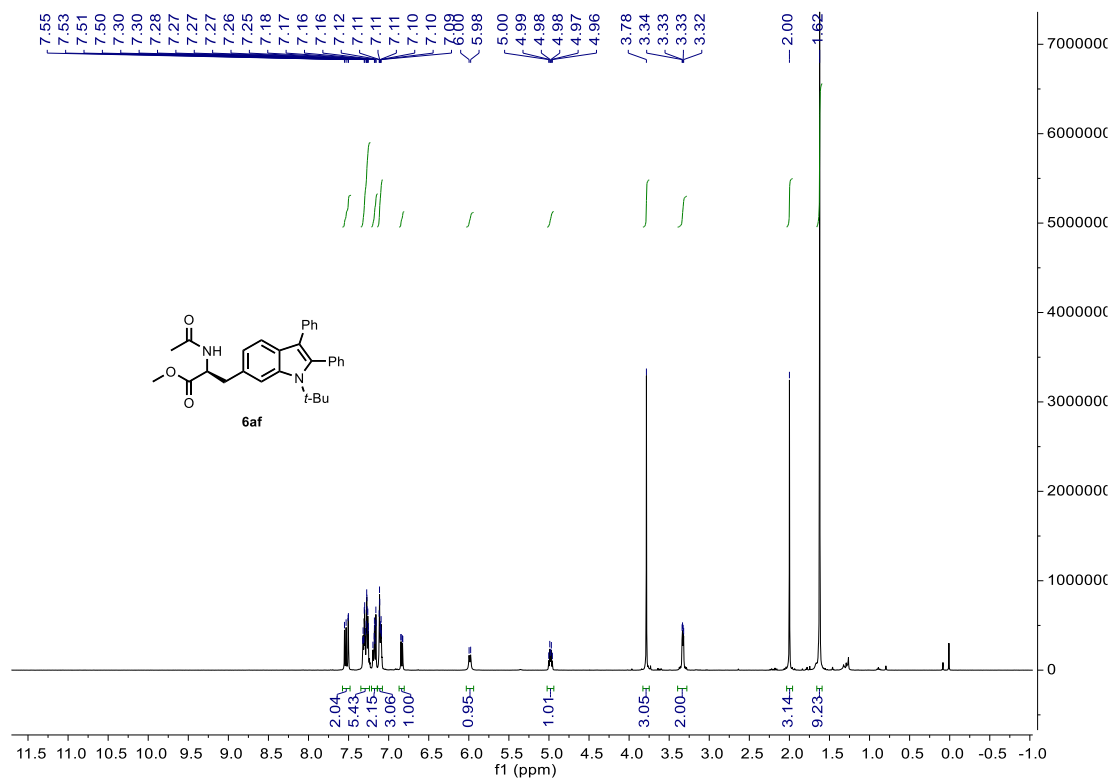
methyl 2-acetamido-3-(7-methyl-1,2,3,4,4a,8b-hexahydro-1,4-methanobiphenylen-5-yl)propanoate (6ae) (d.r. = 1:1) (¹H NMR 500 MHz, CDCl₃)



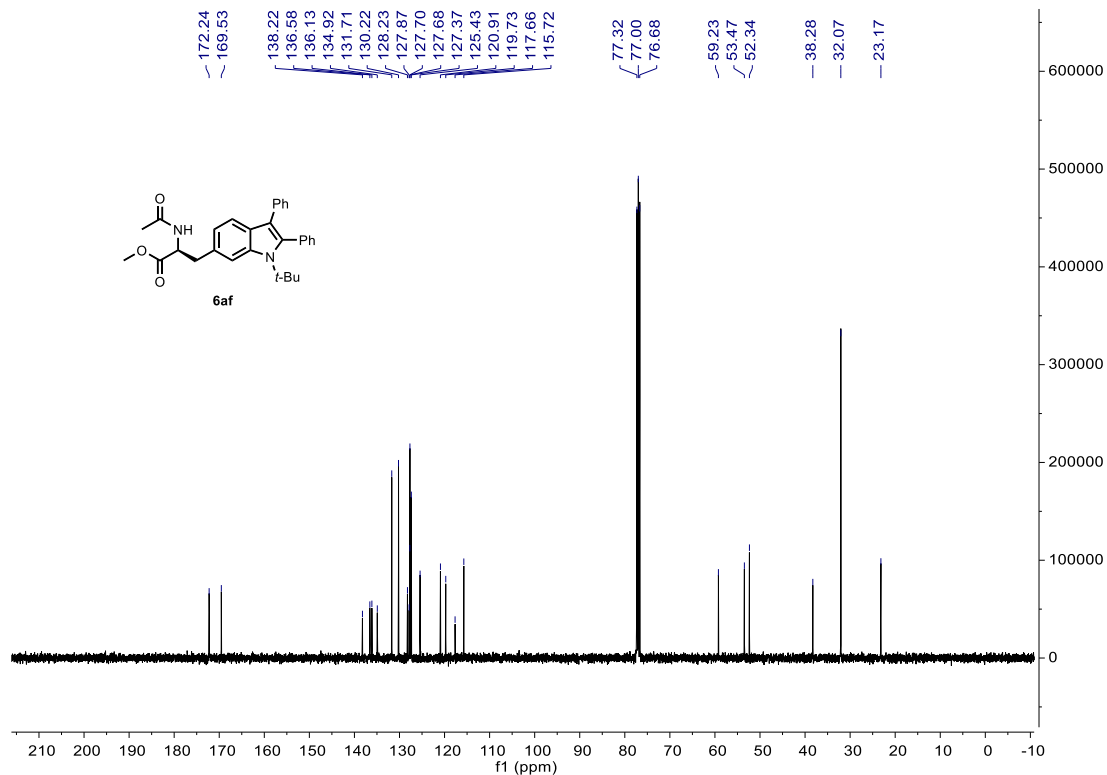
methyl 2-acetamido-3-(7-methyl-1,2,3,4,4a,8b-hexahydro-1,4-methanobiphenylen-5-yl)propanoate (6ae) (d.r. = 1:1) (¹³C NMR 126 MHz, CDCl₃)



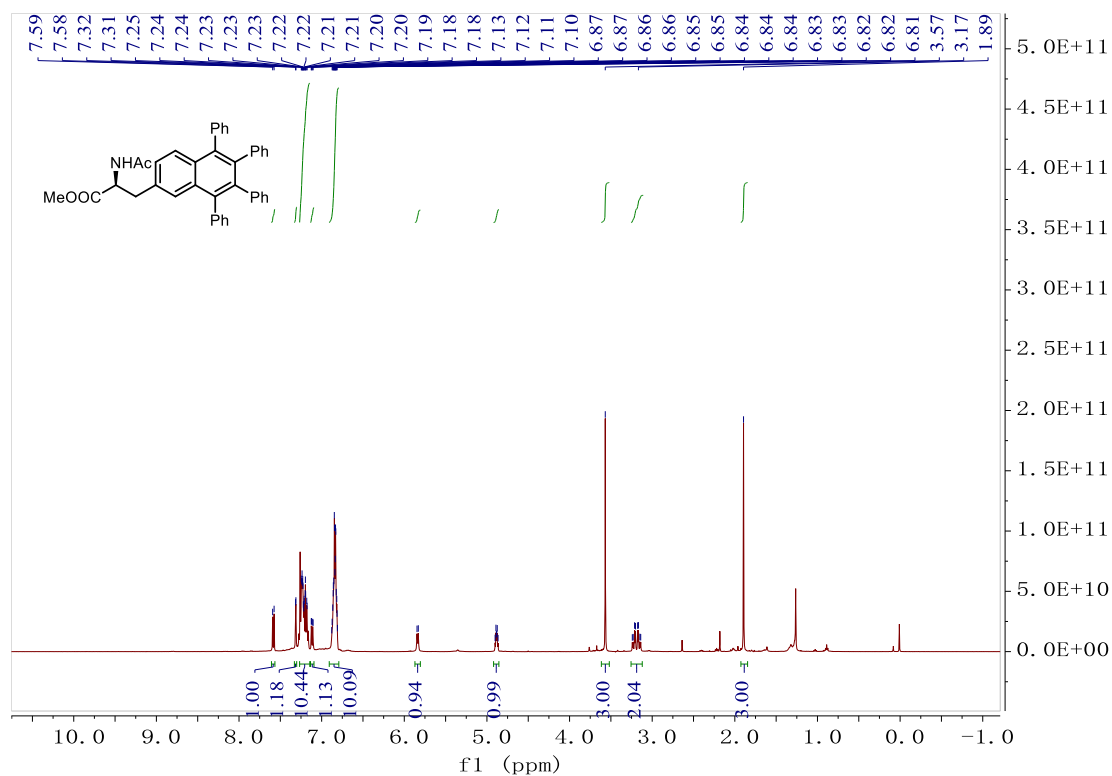
methyl (S)-2-acetamido-3-(1-(tert-butyl)-2,3-diphenyl-1H-indol-6-yl)propanoate (6af) (¹H NMR 400 MHz, CDCl₃)



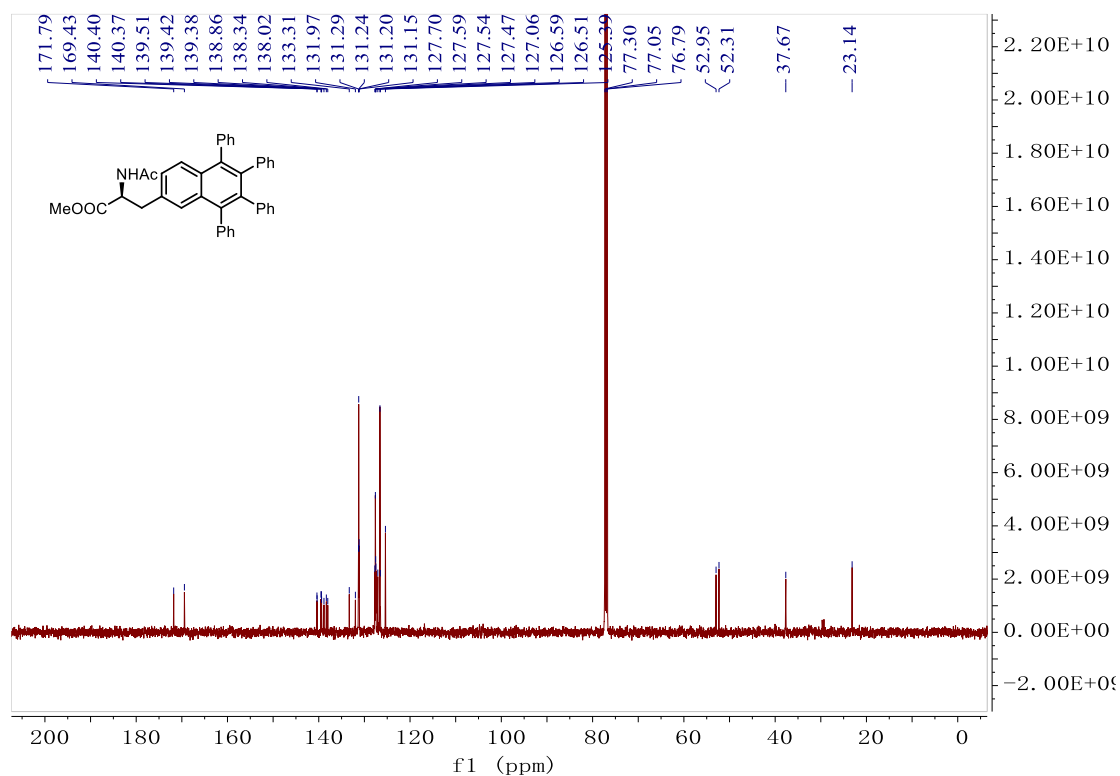
methyl (S)-2-acetamido-3-(1-(tert-butyl)-2,3-diphenyl-1H-indol-6-yl)propanoate (6af) (¹³C NMR 101 MHz, CDCl₃)



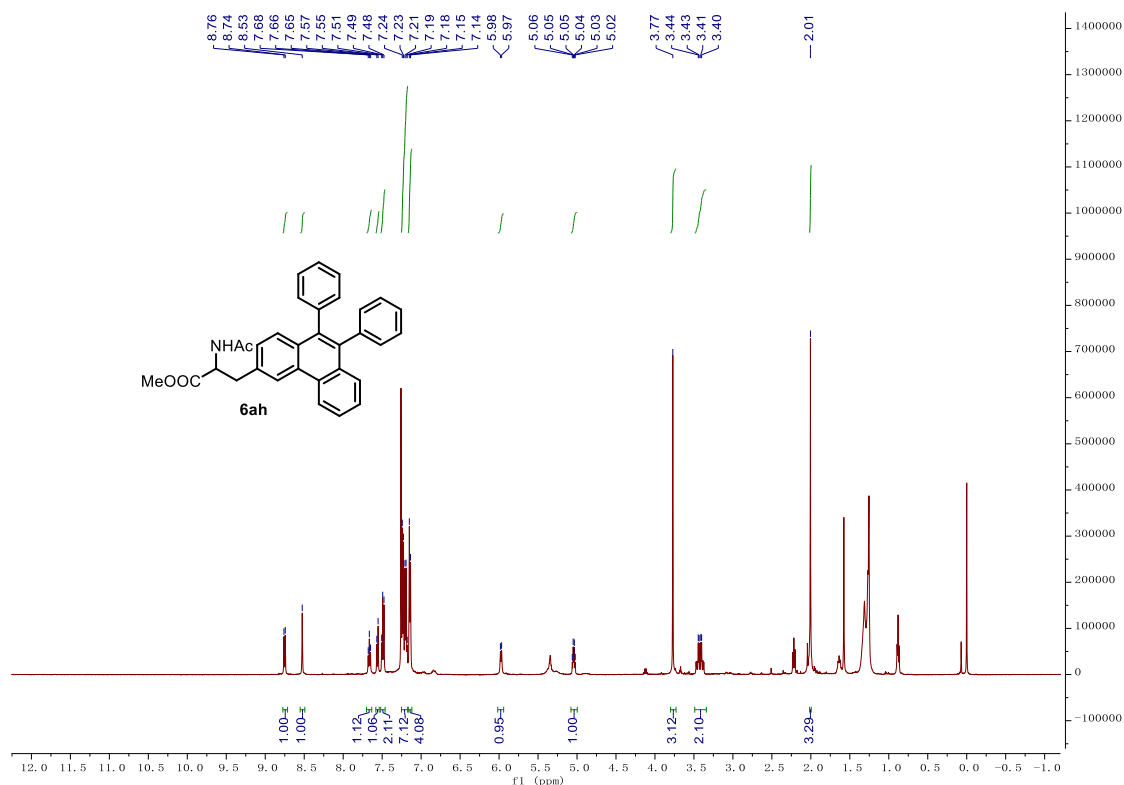
methyl (*S*)-2-acetamido-3-(5,6,7,8-tetraphenylnaphthalen-2-yl)propanoate (6ag) (¹H NMR 500 MHz, CDCl₃)



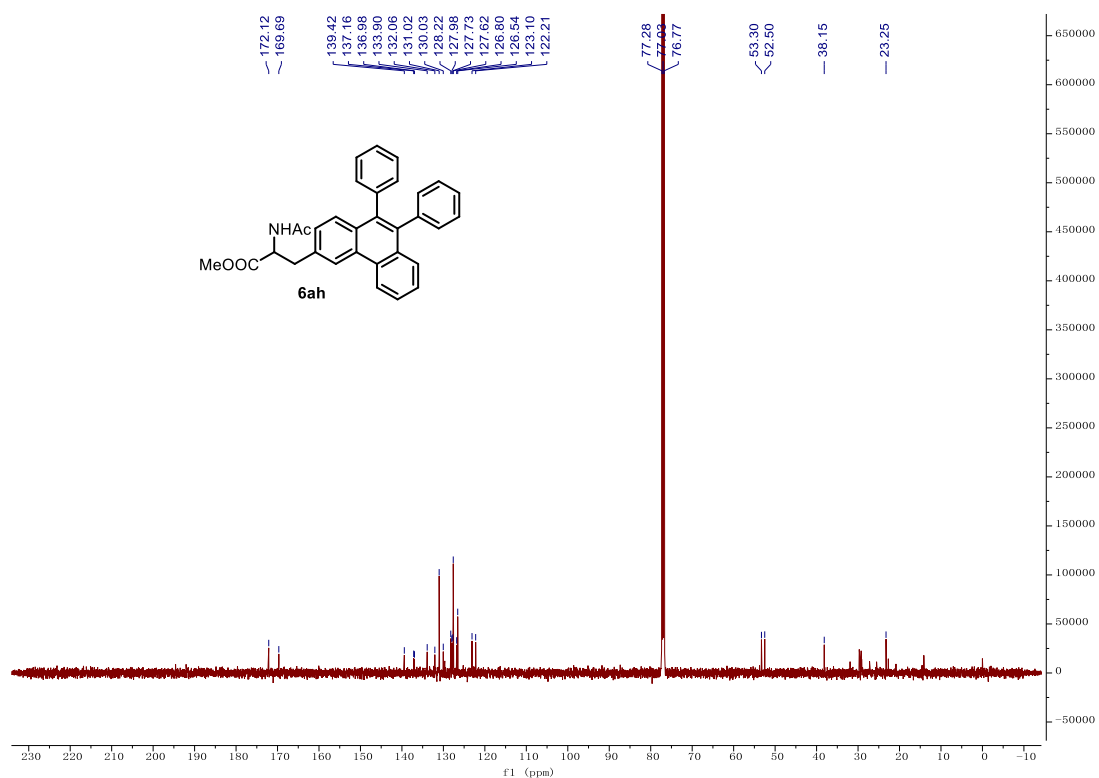
methyl (*S*)-2-acetamido-3-(5,6,7,8-tetraphenylnaphthalen-2-yl)propanoate (6ag) (¹³C NMR 126 MHz, CDCl₃)



methyl 2-acetamido-3-(9,10-diphenylphenanthren-3-yl)propanoate (6ah) (^1H NMR 500 MHz, CDCl_3)



methyl 2-acetamido-3-(9,10-diphenylphenanthren-3-yl)propanoate (6ah) (^{13}C NMR 126 MHz, CDCl_3)



Chemical structure of 6ai: CC1=C(C)C(=O)c2ccccc2N1Cc3ccccc3CC(=O)OC(=O)N(C)C

¹H NMR spectrum (CDCl₃):

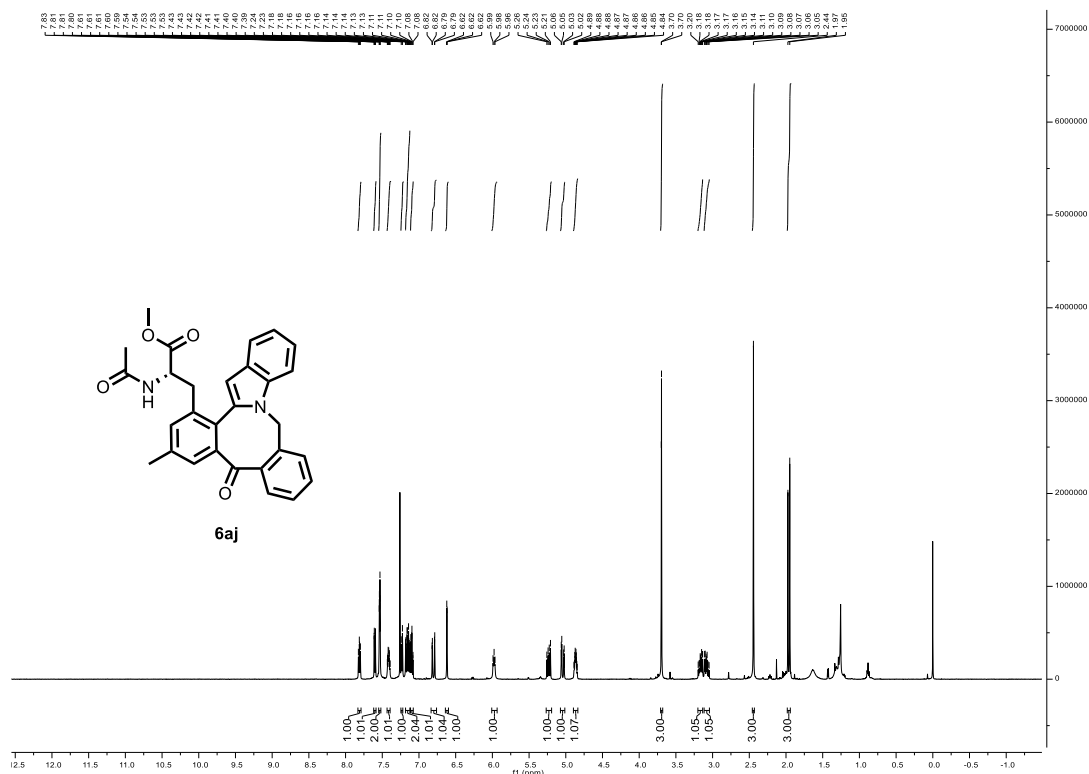
- Chemical shifts (ppm): 7.77, 7.77, 7.69, 7.67, 7.67, 7.66, 7.66, 7.64, 7.64, 7.61, 7.61, 7.58, 7.58, 7.27, 7.27, 7.26, 7.26, 7.24, 7.24, 7.24, 7.24, 7.20, 7.20, 6.01, 6.01, 5.99, 5.99, 4.93, 4.91, 4.91, 4.89, 4.89, 3.77, 3.77, 3.76, 3.76, 3.70, 3.70, 3.70, 3.70, 3.14, 3.14, 3.12, 3.12, 3.11, 3.11, 3.10, 3.10, 2.66, 2.66, 2.61, 2.61, 2.02, 2.02.
- Integrations: 1.00, 4.00, 1.00, 1.00, 3.00, 1.00, 1.00, 1.00, 1.00, 1.00, 3.00, 1.00, 3.00, 3.00, 3.00.

6ai

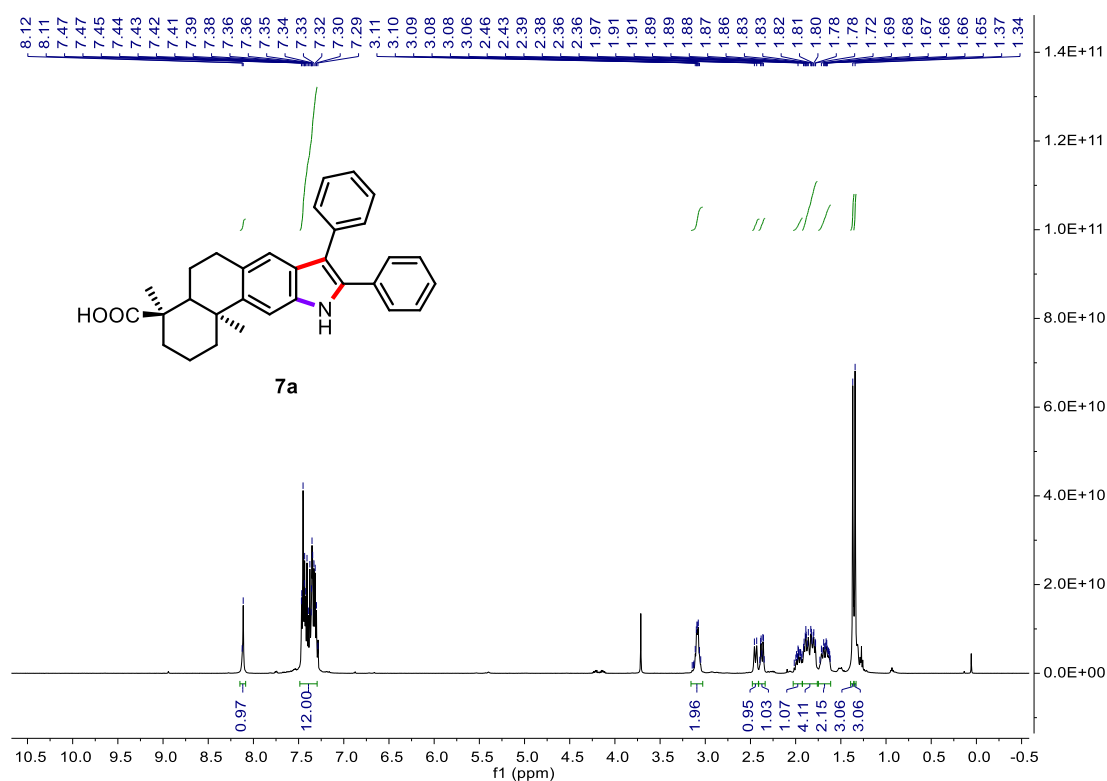
¹H NMR (400 MHz, CDCl₃) peaks (ppm): 7.87, 7.85, 7.83, 7.81, 7.79, 7.77, 7.75, 7.73, 7.71, 7.69, 7.67, 7.65, 7.63, 7.61, 7.59, 7.57, 7.55, 7.53, 7.51, 7.49, 7.47, 7.45, 7.43, 7.41, 7.39, 7.37, 7.35, 7.33, 7.31, 7.29, 7.27, 7.25, 7.23, 7.21, 7.19, 7.17, 7.15, 7.13, 7.11, 7.09, 7.07, 7.05, 7.03, 7.01, 6.99, 6.97, 6.95, 6.93, 6.91, 6.89, 6.87, 6.85, 6.83, 6.81, 6.79, 6.77, 6.75, 6.73, 6.71, 6.69, 6.67, 6.65, 6.63, 6.61, 6.59, 6.57, 6.55, 6.53, 6.51, 6.49, 6.47, 6.45, 6.43, 6.41, 6.39, 6.37, 6.35, 6.33, 6.31, 6.29, 6.27, 6.25, 6.23, 6.21, 6.19, 6.17, 6.15, 6.13, 6.11, 6.09, 6.07, 6.05, 6.03, 6.01, 5.99, 5.97, 5.95, 5.93, 5.91, 5.89, 5.87, 5.85, 5.83, 5.81, 5.79, 5.77, 5.75, 5.73, 5.71, 5.69, 5.67, 5.65, 5.63, 5.61, 5.59, 5.57, 5.55, 5.53, 5.51, 5.49, 5.47, 5.45, 5.43, 5.41, 5.39, 5.37, 5.35, 5.33, 5.31, 5.29, 5.27, 5.25, 5.23, 5.21, 5.19, 5.17, 5.15, 5.13, 5.11, 5.09, 5.07, 5.05, 5.03, 5.01, 4.99, 4.97, 4.95, 4.93, 4.91, 4.89, 4.87, 4.85, 4.83, 4.81, 4.79, 4.77, 4.75, 4.73, 4.71, 4.69, 4.67, 4.65, 4.63, 4.61, 4.59, 4.57, 4.55, 4.53, 4.51, 4.49, 4.47, 4.45, 4.43, 4.41, 4.39, 4.37, 4.35, 4.33, 4.31, 4.29, 4.27, 4.25, 4.23, 4.21, 4.19, 4.17, 4.15, 4.13, 4.11, 4.09, 4.07, 4.05, 4.03, 4.01, 3.99, 3.97, 3.95, 3.93, 3.91, 3.89, 3.87, 3.85, 3.83, 3.81, 3.79, 3.77, 3.75, 3.73, 3.71, 3.69, 3.67, 3.65, 3.63, 3.61, 3.59, 3.57, 3.55, 3.53, 3.51, 3.49, 3.47, 3.45, 3.43, 3.41, 3.39, 3.37, 3.35, 3.33, 3.31, 3.29, 3.27, 3.25, 3.23, 3.21, 3.19, 3.17, 3.15, 3.13, 3.11, 3.09, 3.07, 3.05, 3.03, 3.01, 2.99, 2.97, 2.95, 2.93, 2.91, 2.89, 2.87, 2.85, 2.83, 2.81, 2.79, 2.77, 2.75, 2.73, 2.71, 2.69, 2.67, 2.65, 2.63, 2.61, 2.59, 2.57, 2.55, 2.53, 2.51, 2.49, 2.47, 2.45, 2.43, 2.41, 2.39, 2.37, 2.35, 2.33, 2.31, 2.29, 2.27, 2.25, 2.23, 2.21, 2.19, 2.17, 2.15, 2.13, 2.11, 2.09, 2.07, 2.05, 2.03, 2.01, 1.99, 1.97, 1.95, 1.93, 1.91, 1.89, 1.87, 1.85, 1.83, 1.81, 1.79, 1.77, 1.75, 1.73, 1.71, 1.69, 1.67, 1.65, 1.63, 1.61, 1.59, 1.57, 1.55, 1.53, 1.51, 1.49, 1.47, 1.45, 1.43, 1.41, 1.39, 1.37, 1.35, 1.33, 1.31, 1.29, 1.27, 1.25, 1.23, 1.21, 1.19, 1.17, 1.15, 1.13, 1.11, 1.09, 1.07, 1.05, 1.03, 1.01, 0.99, 0.97, 0.95, 0.93, 0.91, 0.89, 0.87, 0.85, 0.83, 0.81, 0.79, 0.77, 0.75, 0.73, 0.71, 0.69, 0.67, 0.65, 0.63, 0.61, 0.59, 0.57, 0.55, 0.53, 0.51, 0.49, 0.47, 0.45, 0.43, 0.41, 0.39, 0.37, 0.35, 0.33, 0.31, 0.29, 0.27, 0.25, 0.23, 0.21, 0.19, 0.17, 0.15, 0.13, 0.11, 0.09, 0.07, 0.05, 0.03, 0.01, 0.00.

¹³C NMR (100 MHz, CDCl₃) peaks (ppm): 171.96, 171.80, 169.80, 169.60, 167.80, 167.60, 165.80, 165.60, 163.80, 163.60, 161.80, 161.60, 159.80, 159.60, 157.80, 157.60, 155.80, 155.60, 153.80, 153.60, 151.80, 151.60, 149.80, 149.60, 147.80, 147.60, 145.80, 145.60, 143.80, 143.60, 141.80, 141.60, 139.80, 139.60, 137.80, 137.60, 135.80, 135.60, 133.80, 133.60, 131.80, 131.60, 129.80, 129.60, 127.80, 127.60, 125.80, 125.60, 123.80, 123.60, 121.80, 121.60, 119.80, 119.60, 117.80, 117.60, 115.80, 115.60, 113.80, 113.60, 111.80, 111.60, 109.80, 109.60, 107.80, 107.60, 105.80, 105.60, 103.80, 103.60, 101.80, 101.60, 99.80, 99.60, 97.80, 97.60, 95.80, 95.60, 93.80, 93.60, 91.80, 91.60, 89.80, 89.60, 87.80, 87.60, 85.80, 85.60, 83.80, 83.60, 81.80, 81.60, 79.80, 79.60, 77.80, 77.60, 75.80, 75.60, 73.80, 73.60, 71.80, 71.60, 69.80, 69.60, 67.80, 67.60, 65.80, 65.60, 63.80, 63.60, 61.80, 61.60, 59.80, 59.60, 57.80, 57.60, 55.80, 55.60, 53.80, 53.60, 51.80, 51.60, 49.80, 49.60, 47.80, 47.60, 45.80, 45.60, 43.80, 43.60, 41.80, 41.60, 39.80, 39.60, 37.80, 37.60, 35.80, 35.60, 33.80, 33.60, 31.80, 31.60, 29.80, 29.60, 27.80, 27.60, 25.80, 25.60, 23.80, 23.60, 21.80, 21.60, 19.80, 19.60, 17.80, 17.60, 15.80, 15.60, 13.80, 13.60, 11.80, 11.60, 9.80, 9.60, 7.80, 7.60, 5.80, 5.60, 3.80, 3.60, 1.80, 1.60, 0.00.

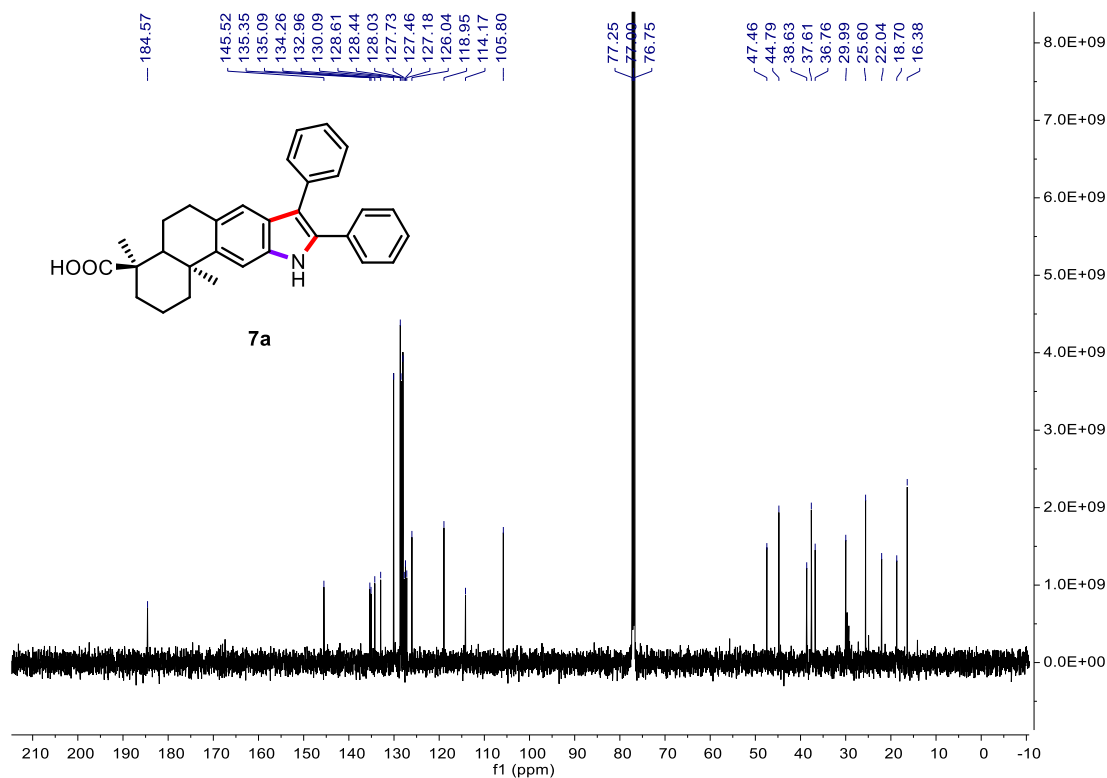
methyl (*S*)-2-acetamido-3-(3-methyl-5-oxo-5,10-dihydrodibenzo[3,4:6,7]azocino[1,2-*a*]indol-1-yl)propanoate (6aj) (d.r. = 1:1) (¹H NMR 500 MHz, CDCl₃)



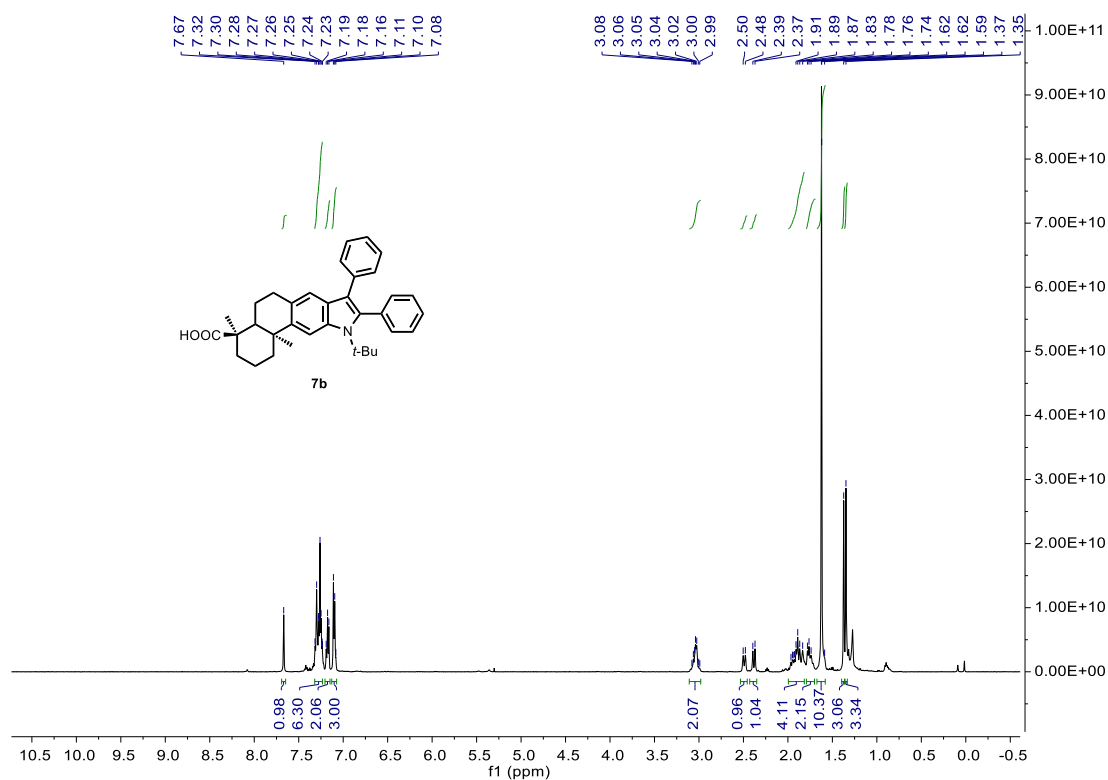
f]indole-4-carboxylic acid (7a) (¹H NMR 500 MHz, CDCl₃)



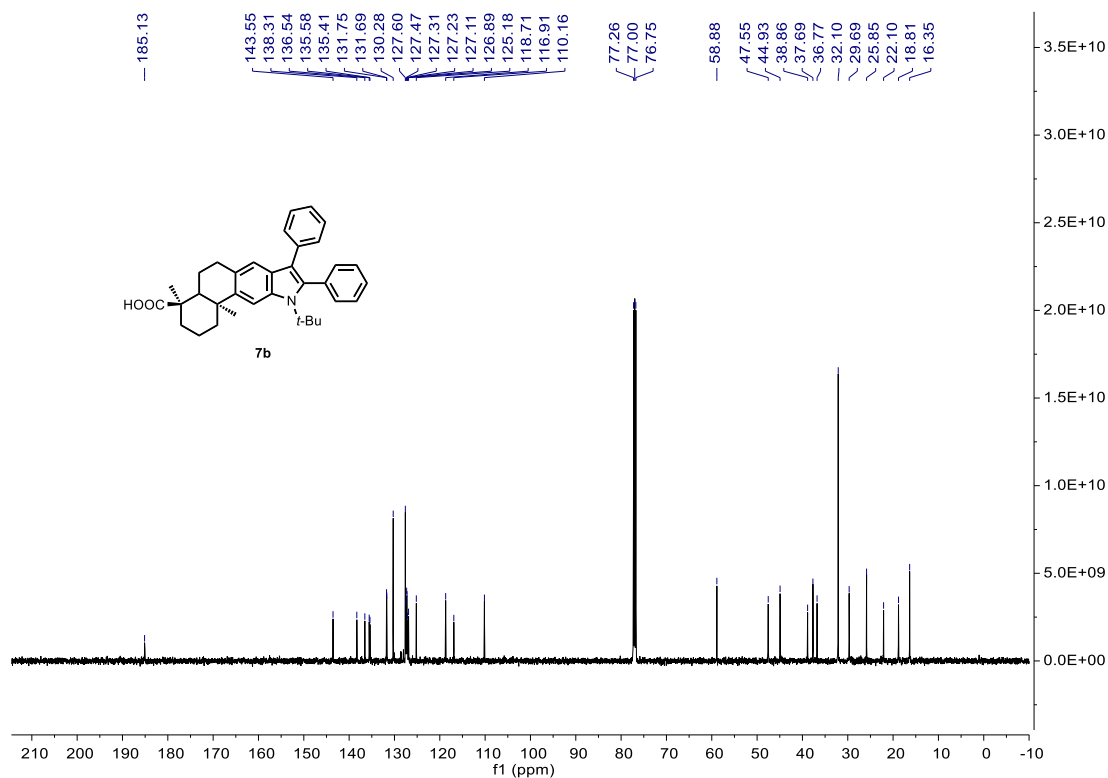
(4R,11bS)-4,11b-dimethyl-8,9-diphenyl-2,3,4,4a,5,6,10,11b-octahydro-1H-naphtho[2,1-f]indole-4-carboxylic acid (7a) (¹³C NMR 126 MHz, CDCl₃)



(4R,11bS)-10-(tert-butyl)-4,11b-dimethyl-8,9-diphenyl-2,3,4,4a,5,6,10,11b-octahydro-1H-naphtho[2,1-f]indole-4-carboxylic acid (7b) (¹H NMR 500 MHz, CDCl₃)

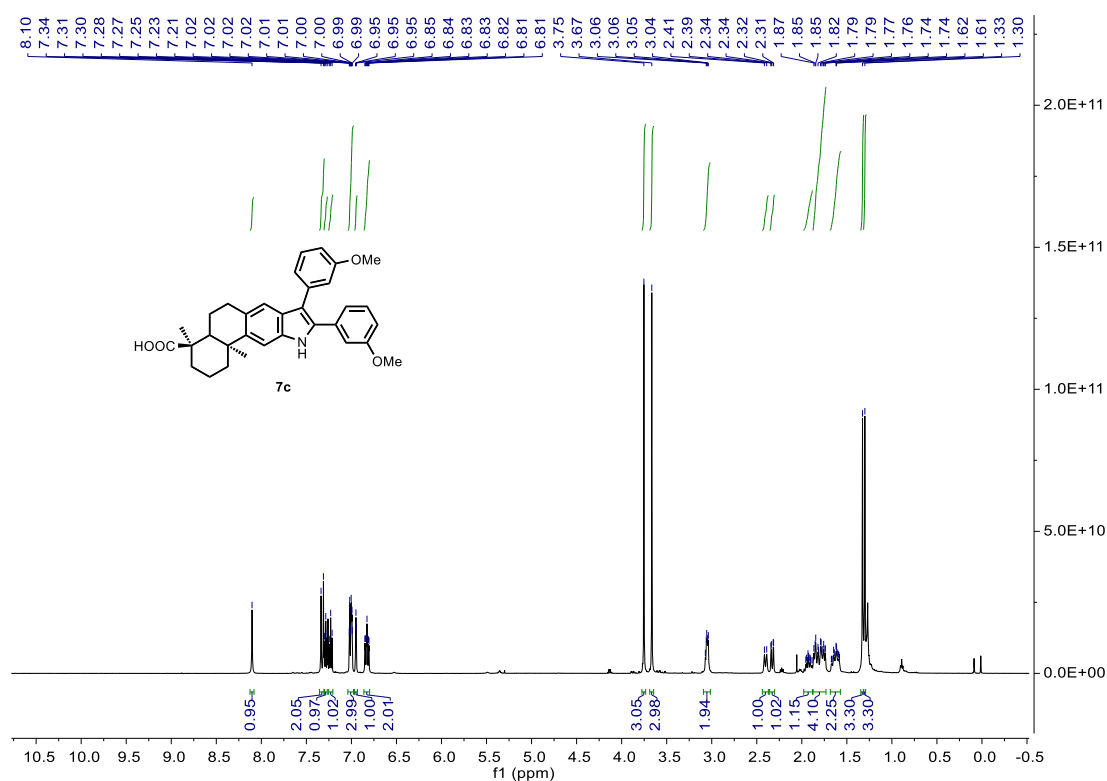


(4R,11bS)-10-(tert-butyl)-4,11b-dimethyl-8,9-diphenyl-2,3,4,4a,5,6,10,11b-octahydro-1H-naphtho[2,1-f]indole-4-carboxylic acid (7b) (¹³C NMR 126 MHz, CDCl₃)

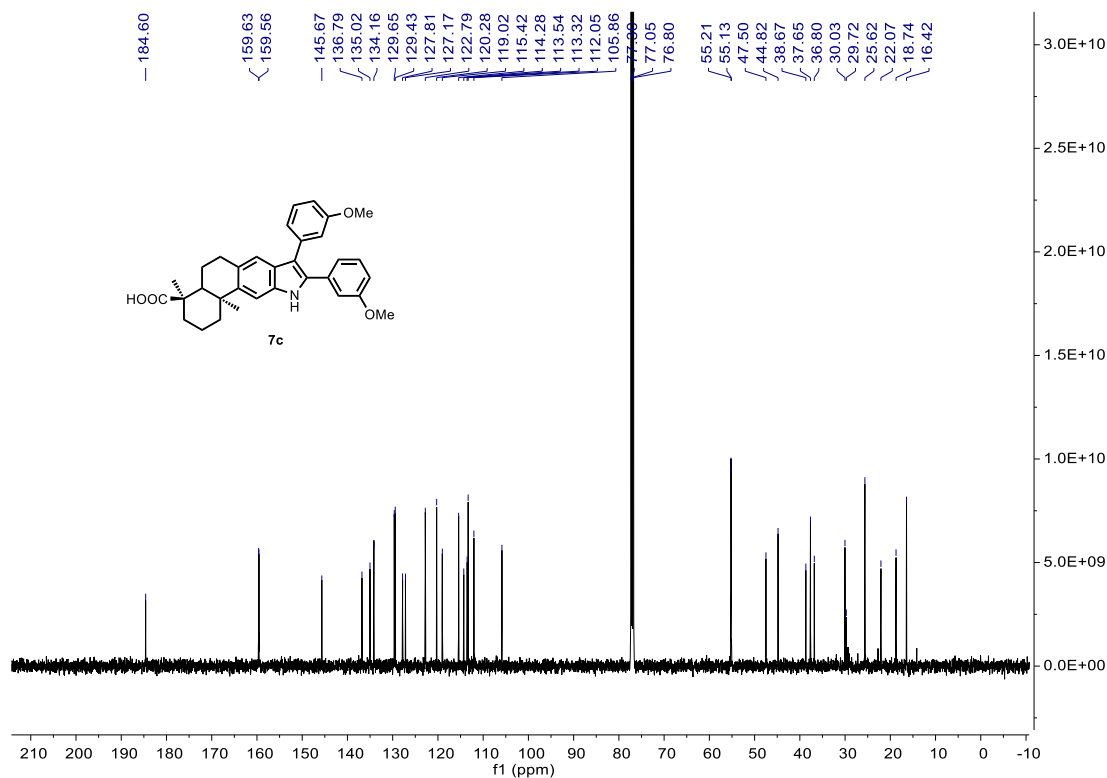


(4R,11bS)-8,9-bis(3-methoxyphenyl)-4,11b-dimethyl-2,3,4,4a,5,6,10,11b-octahydro-1H-

naphtho[2,1-f]indole-4-carboxylic acid (7c) (¹H NMR 500 MHz, CDCl₃)

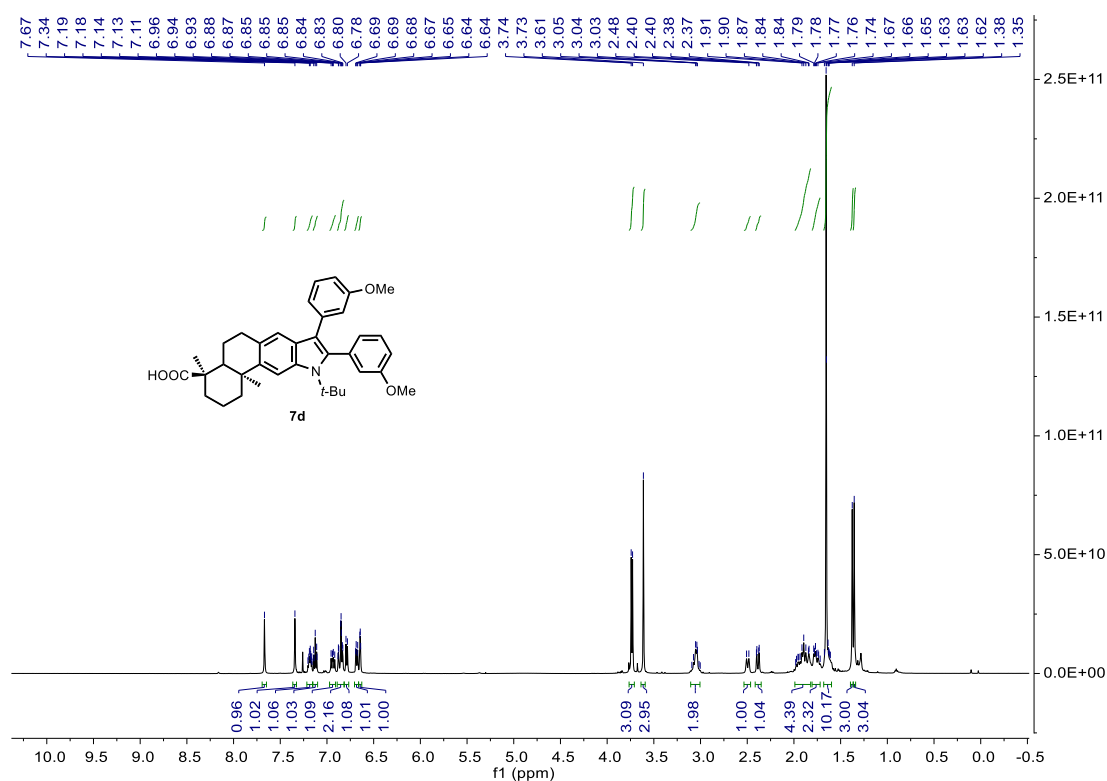


(4R,11bS)-8,9-bis(3-methoxyphenyl)-4,11b-dimethyl-2,3,4,4a,5,6,10,11b-octahydro-1H-naphtho[2,1-f]indole-4-carboxylic acid (7c) (¹³C NMR 126 MHz, CDCl₃)

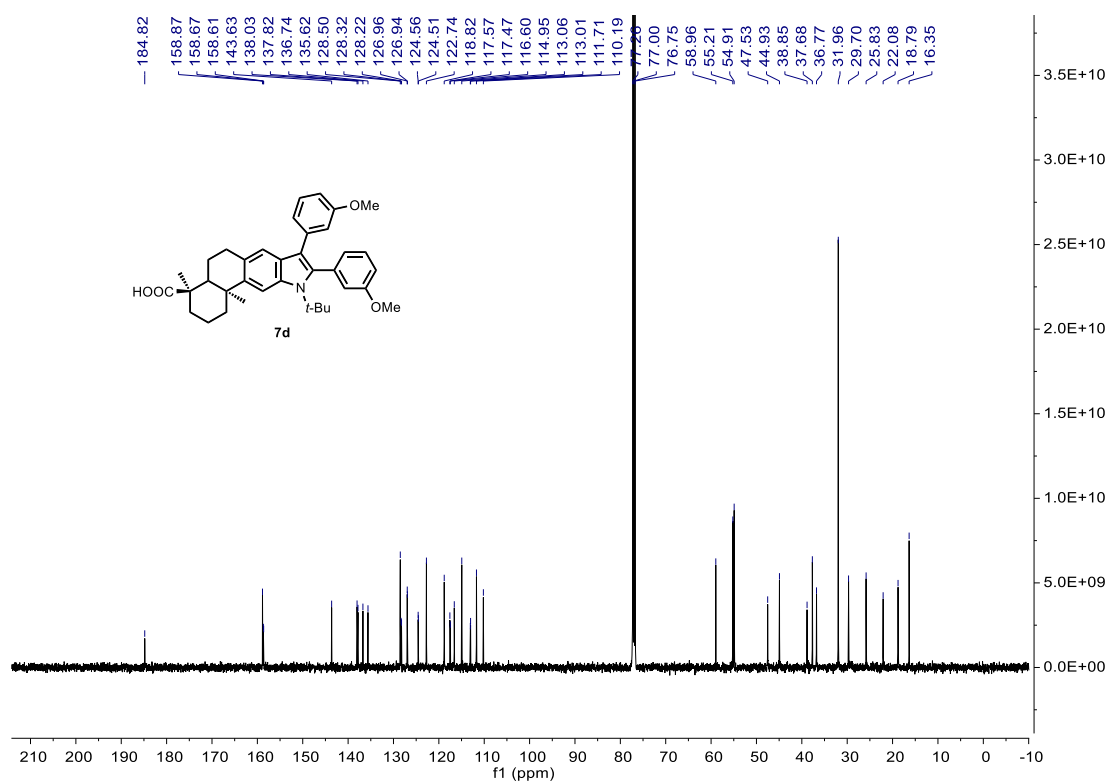


(4R,11bS)-10-(tert-butyl)-8,9-bis(3-methoxyphenyl)-4,11b-dimethyl-2,3,4,4a,5,6,10,11b-

octahydro-1H-naphtho[2,1-f]indole-4-carboxylic acid (7d) (¹H NMR 500 MHz, CDCl₃)

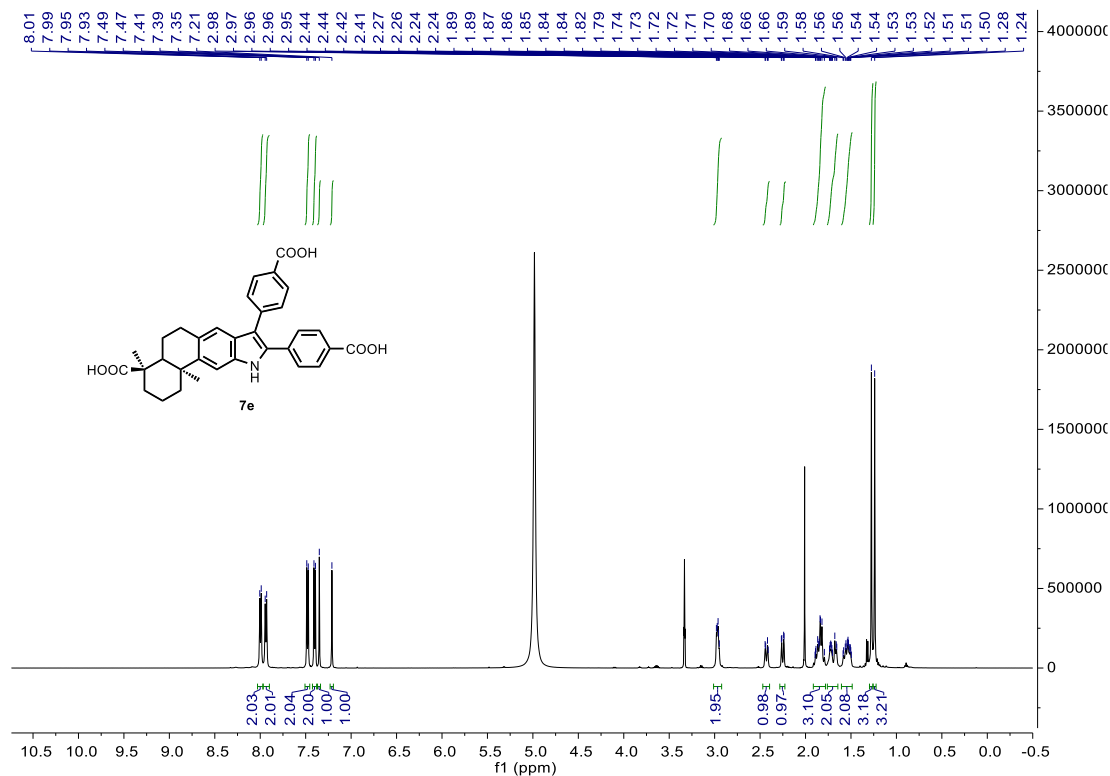


(4R,11bS)-10-(tert-butyl)-8,9-bis(3-methoxyphenyl)-4,11b-dimethyl-2,3,4,4a,5,6,10,11b-octahydro-1H-naphtho[2,1-f]indole-4-carboxylic acid (7d) (¹³C NMR 126 MHz, CDCl₃)

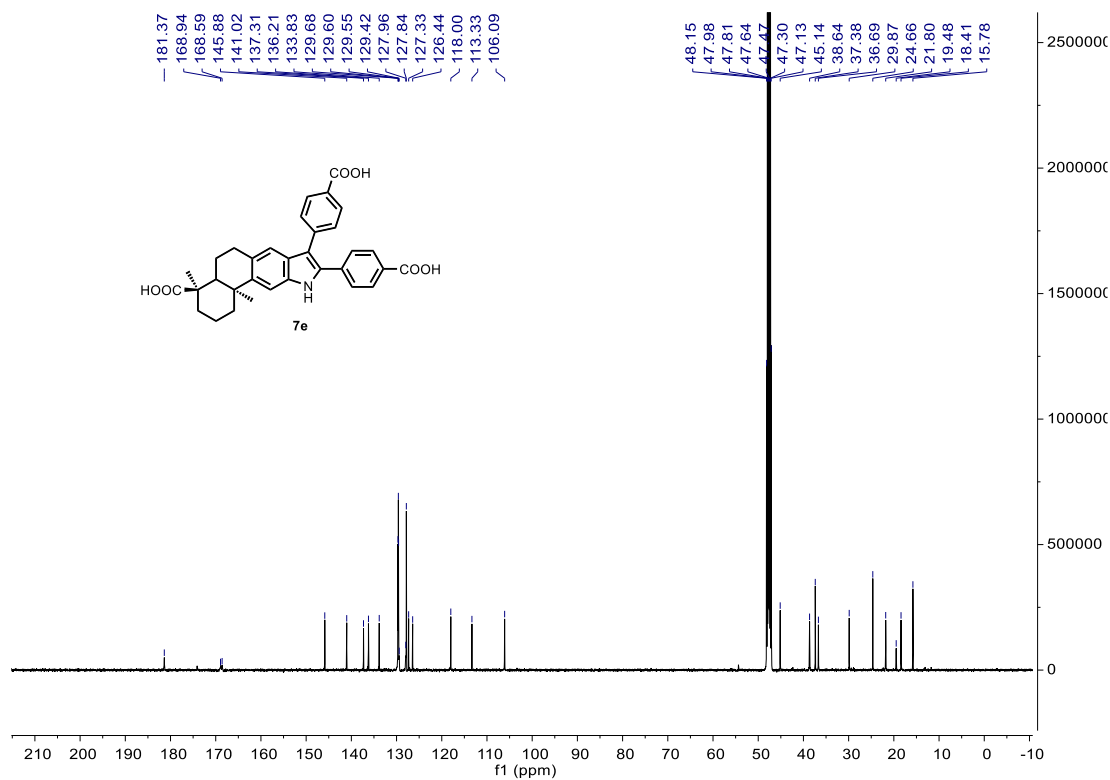


4,4'-((4R,11bS)-4-carboxy-4,11b-dimethyl-2,3,4,4a,5,6,10,11b-octahydro-1H-naphtho[2,1-

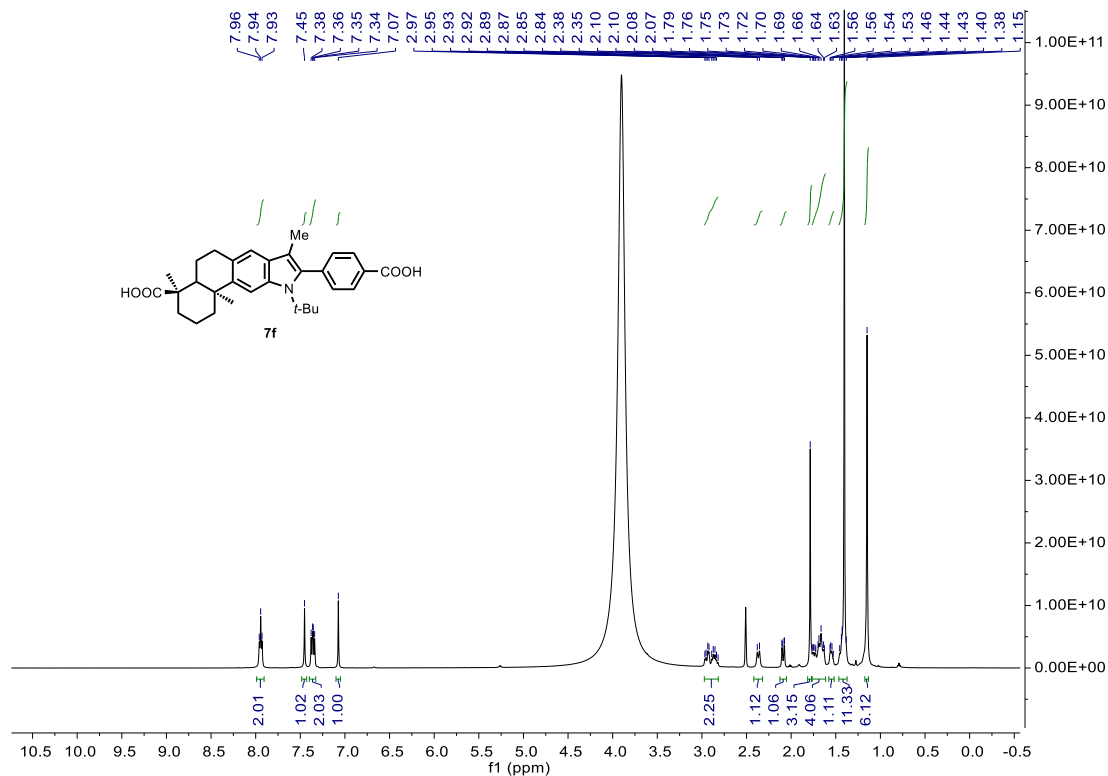
4,4'-((4R,11bS)-4-carboxy-4,11b-dimethyl-2,3,4,4a,5,6,10,11b-octahydro-1H-naphtho[2,1-f]indole-8,9-diyl)dibenzoic acid (7e) (¹H NMR 500 MHz, CD₃OD)



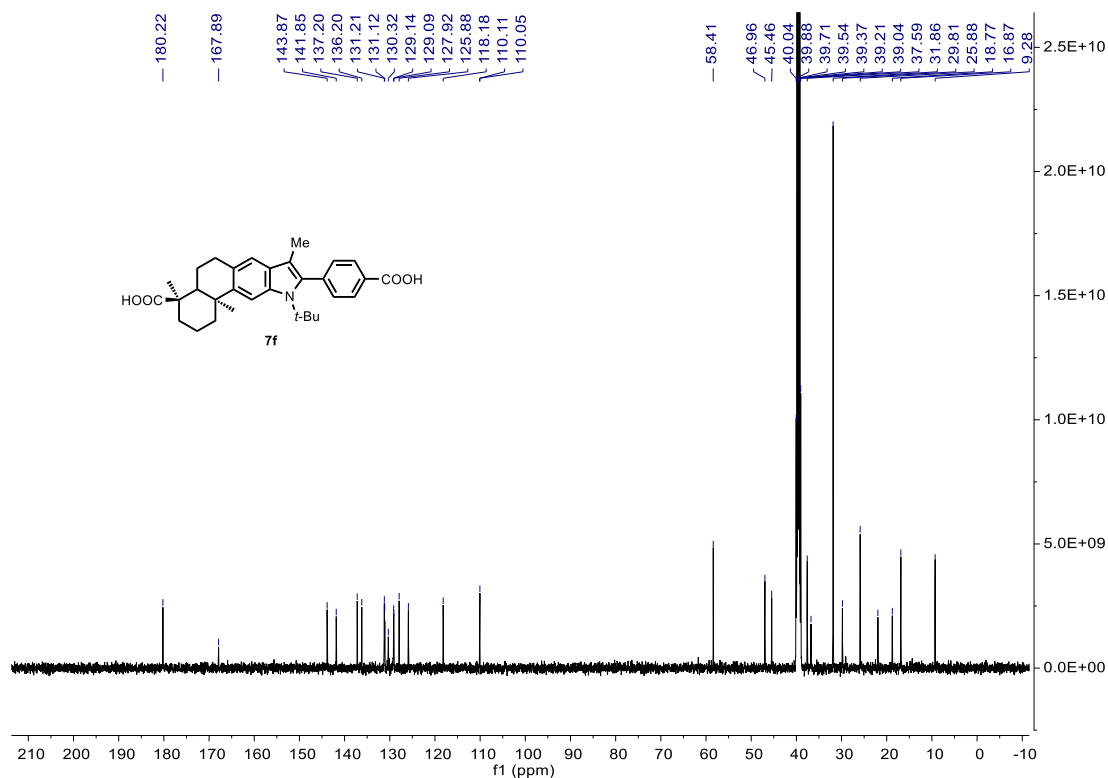
4,4'-((4R,11bS)-4-carboxy-4,11b-dimethyl-2,3,4,4a,5,6,10,11b-octahydro-1H-naphtho[2,1-f]indole-8,9-diyl)dibenzoic acid (7e) (¹³C NMR 126 MHz, CD₃OD)



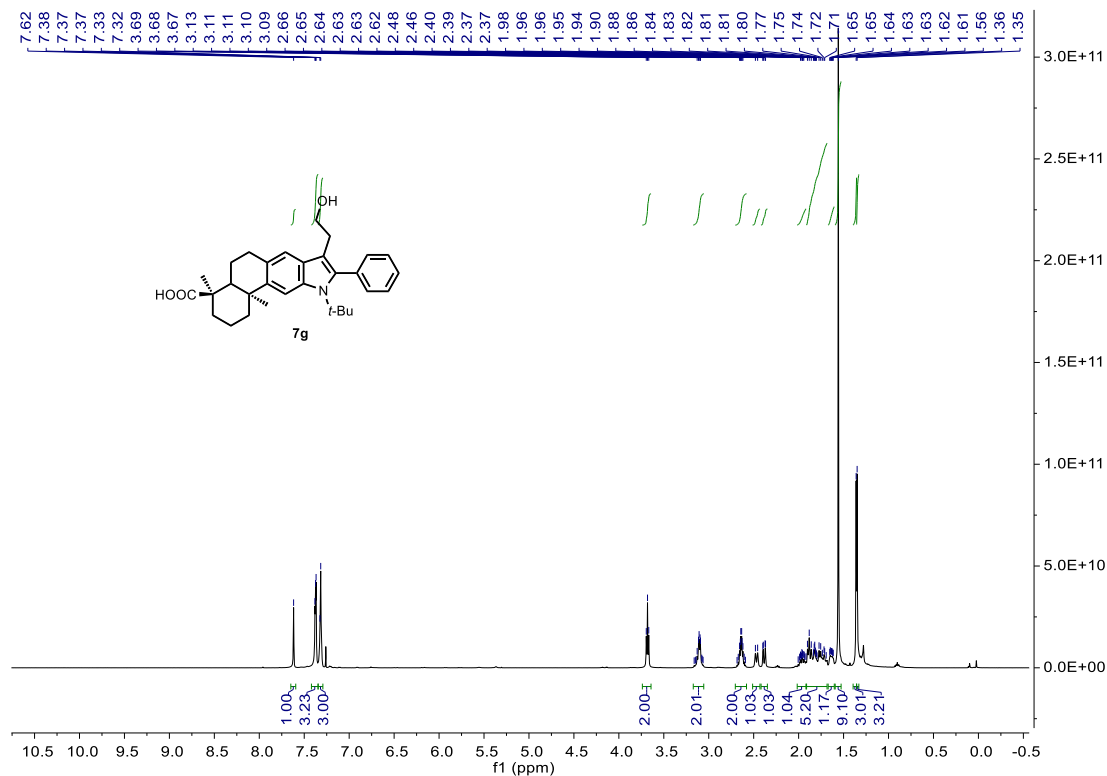
(4R,11bS)-10-(tert-butyl)-9-(4-carboxyphenyl)-4,8,11b-trimethyl-2,3,4,4a,5,6,10,11b-octahydro-1H-naphtho[2,1-f]indole-4-carboxylic acid (7f) (¹H NMR 500 MHz, DMSO-*d*₆)



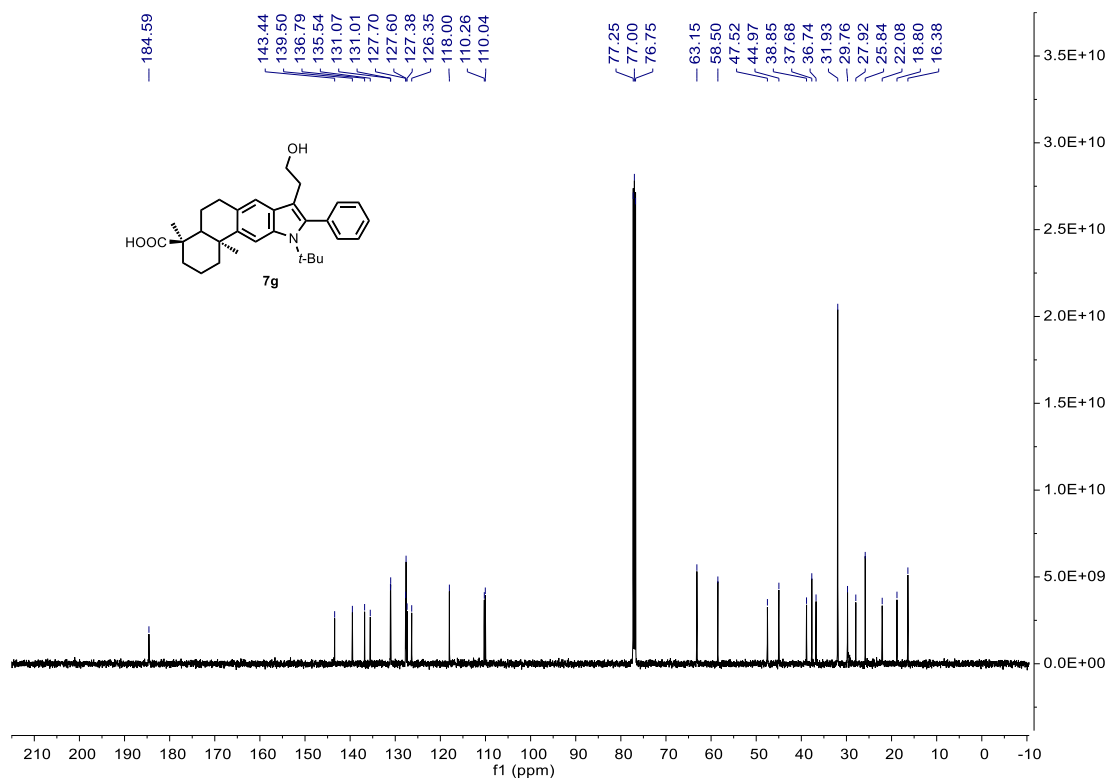
(4R,11bS)-10-(tert-butyl)-9-(4-carboxyphenyl)-4,8,11b-trimethyl-2,3,4,4a,5,6,10,11b-octahydro-1H-naphtho[2,1-f]indole-4-carboxylic acid (7f) (¹³C NMR 126 MHz, DMSO-*d*₆)



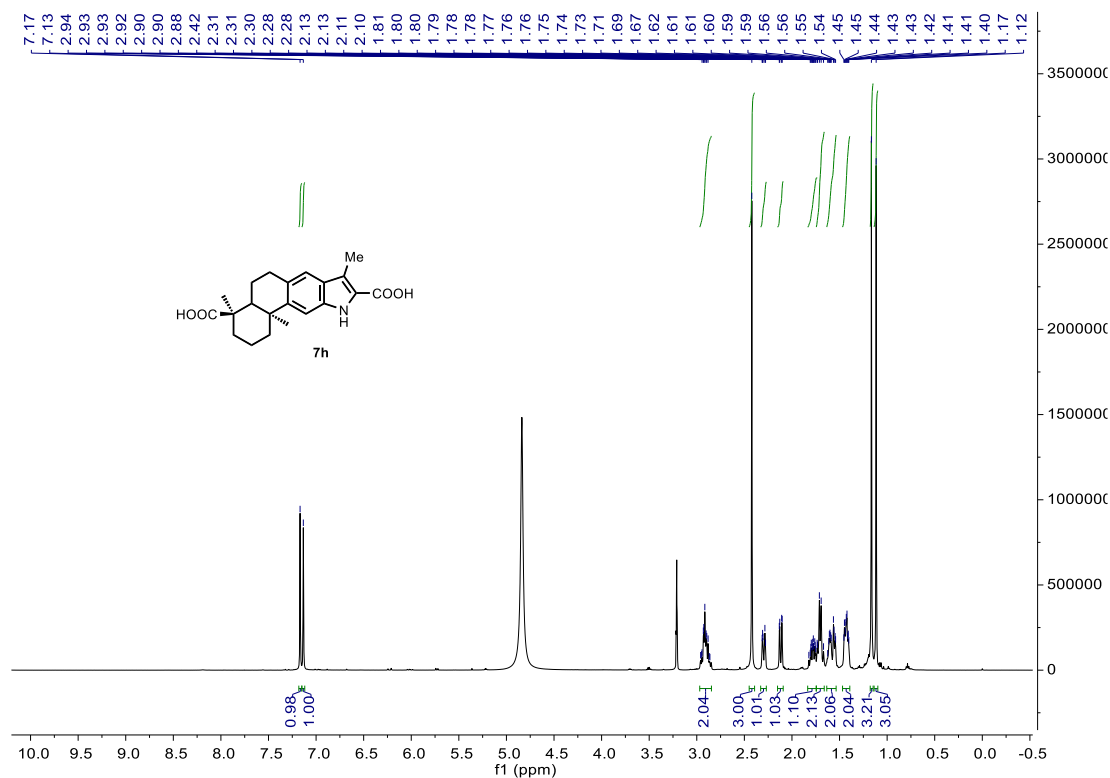
(4R,11bS)-10-(tert-butyl)-9-(4-carboxyphenyl)-4,8,11b-trimethyl-2,3,4,4a,5,6,10,11b-octahydro-1H-naphtho[2,1-f]indole-4-carboxylic acid (7g) (¹H NMR 500 MHz, CDCl₃)



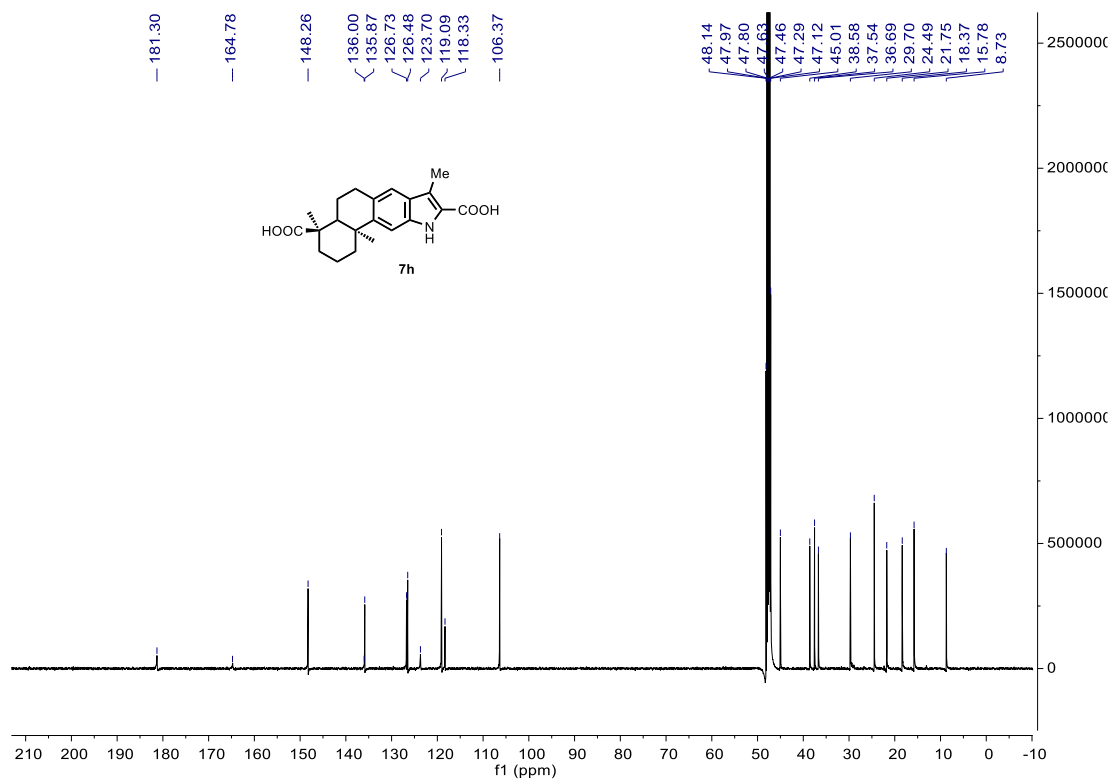
(4R,11bS)-10-(tert-butyl)-9-(4-carboxyphenyl)-4,8,11b-trimethyl-2,3,4,4a,5,6,10,11b-octahydro-1H-naphtho[2,1-f]indole-4-carboxylic acid (7g) (¹³C NMR 126 MHz, CDCl₃)



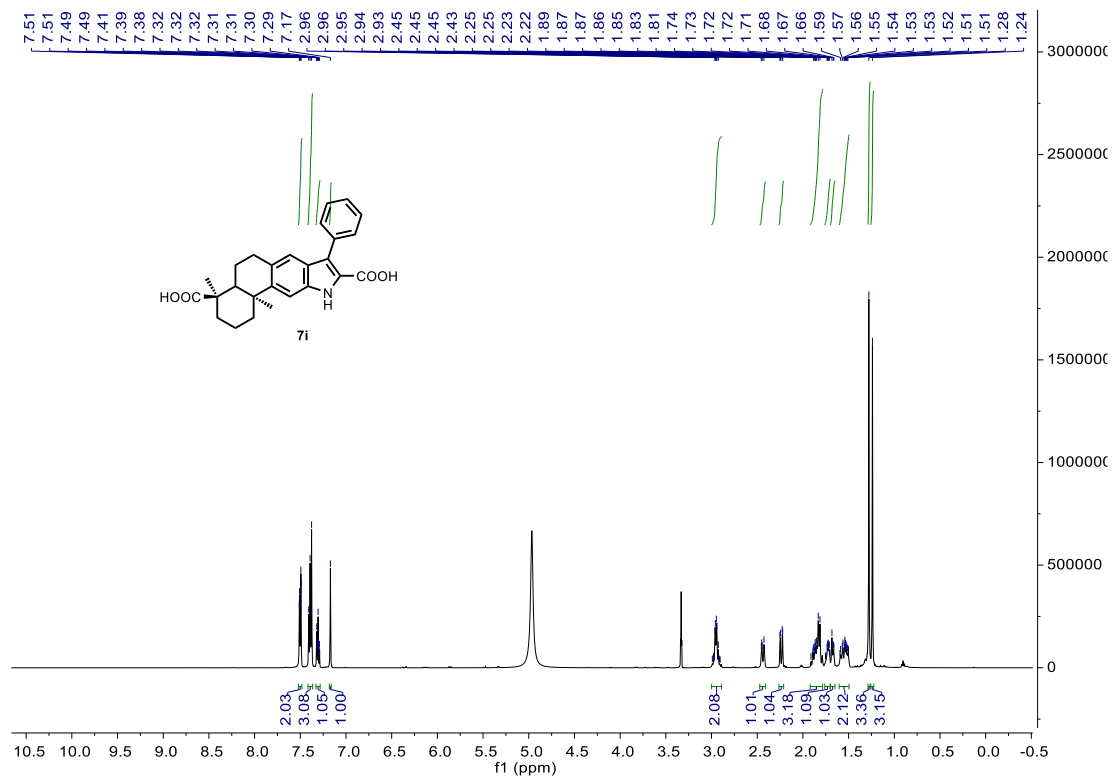
(4R,11bS)-4,8,11b-trimethyl-2,3,4,4a,5,6,10,11b-octahydro-1H-naphtho[2,1-f]indole-4,9-dicarboxylic acid (7h) (¹H NMR 500 MHz, CD₃OD)



(4R,11bS)-4,8,11b-trimethyl-2,3,4,4a,5,6,10,11b-octahydro-1H-naphtho[2,1-f]indole-4,9-dicarboxylic acid (7h) (¹³C NMR 126 MHz, CD₃OD)



(4R,11bS)-4,11b-dimethyl-8-phenyl-2,3,4,4a,5,6,10,11b-octahydro-1H-naphtho[2,1-f]indole-4,9-dicarboxylic acid (7i) (¹H NMR 500 MHz, CD₃OD)



(4R,11bS)-4,11b-dimethyl-8-phenyl-2,3,4,4a,5,6,10,11b-octahydro-1H-naphtho[2,1-f]indole-4,9-dicarboxylic acid (7i) (¹³C NMR 126 MHz, CD₃OD)

