Supplementary Information

Conformationally Defined Planar-Chiral [n]Paracyclophanes Stabilized by Chiral Ansa Chains

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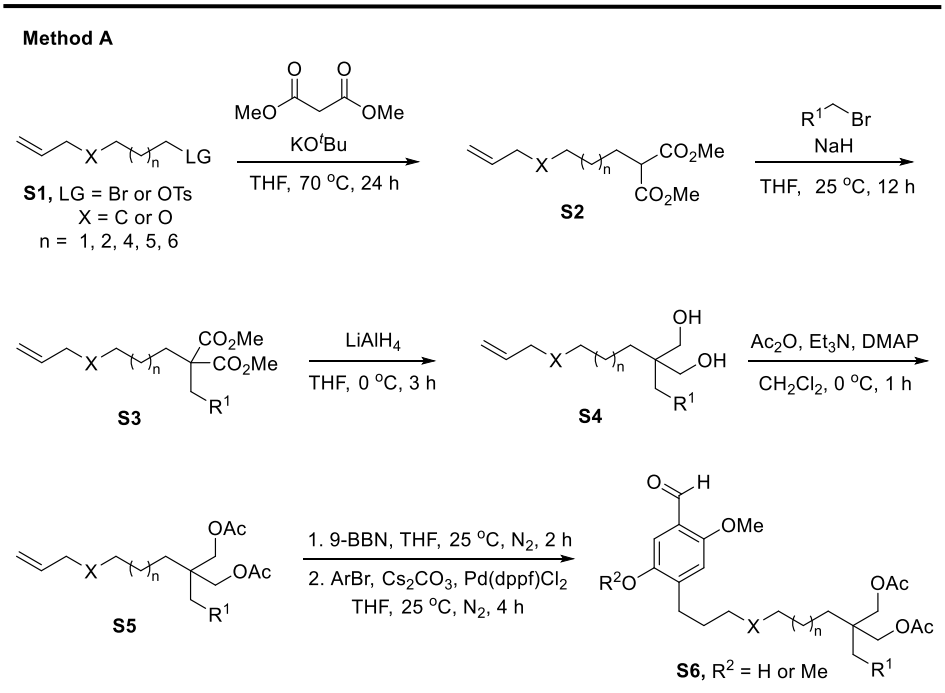
1. General information

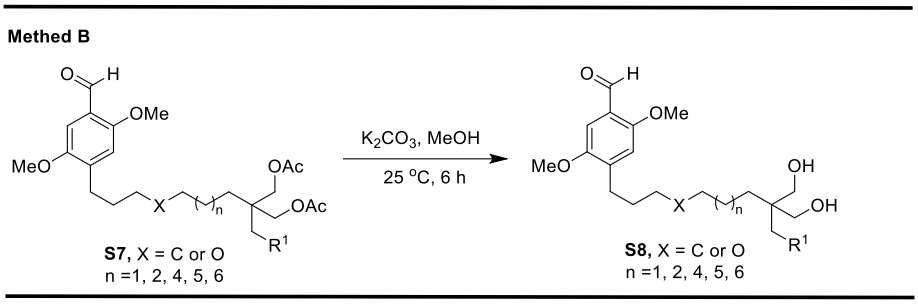
All reactions in non-aqueous media were conducted under a positive pressure of dry argon in glassware that had been dried in oven prior to use unless noted otherwise. Anhydrous solutions of reaction mixtures were transferred *via* an oven dried syringe or cannula. Chemicals were purchased from commercial sources including dichloromethane (DCM), *n*-hexane, ethyl acetate (EA), methanol (MeOH), tetrahydrofuran (THF), acetone and petroleum ether (PE) were purchased from Beijing Chemical Factory (Beijing, China). Column chromatography was performed using silica gal (normal phase, 200 – 300 mesh) from Yantai Xinnuo Chemical Co., Ltd., usually with petroleum Dether (PE, bp 60 – 90 °C) and ethyl acetate (EA) as eluent. Reactions were monitored by thin-layer chromatography (TLC) on G254 silica gal plates (0.2 mm) from Yantai Xinnuo Chemical Co., Ltd. The plates were visualized by UV light. ^{1}H, ^{13}C and ^{19}F NMR spectra were recorded on a JEOL Delta (400 MHz or 600 MHz) spectrometer with $CDCl_3$, DMSO-d_6, Acetone-d_6 as solvents and deuterated solvent residual peak or tetramethylsilane (TMS) as internal standard. Coupling constants (J) are reported in Hertz (Hz), and the chemical shifts (δ) were reported in parts per million (ppm). Multiplicities are indicated as singlet (s), doublet (d), triplet (t), quartet (q), quintet (quint), double doublet (dd), triple doublet (td), triple triplet (tt), multiplet (m), and broad (br). HPLC analysis was conducted on SHIMADZU LC-20ADXR instrument with chiral columns (Chiralpak IB N-5, IC, IF, AD-H and OD-H, column 4.6 × 250 mm, (Daicel Chemical Ind., Ltd.)). High resolution mass spectra (HRMS) were recorded on a Waters LCT Premier XE mass spectrometer with TOF. Crystallographic data were collected using a Rigaku Oxford Diffraction XtaLAB Synergy diffractometer equipped with a HyPix-6000E area detector at 100 K using Cu Kα (λ = 1.54184 Å) from a PhotonJet micro-focus X-ray source.

2. General route for the synthesis of substrates

Supplementary Figure 1. Route for the synthesis of S6

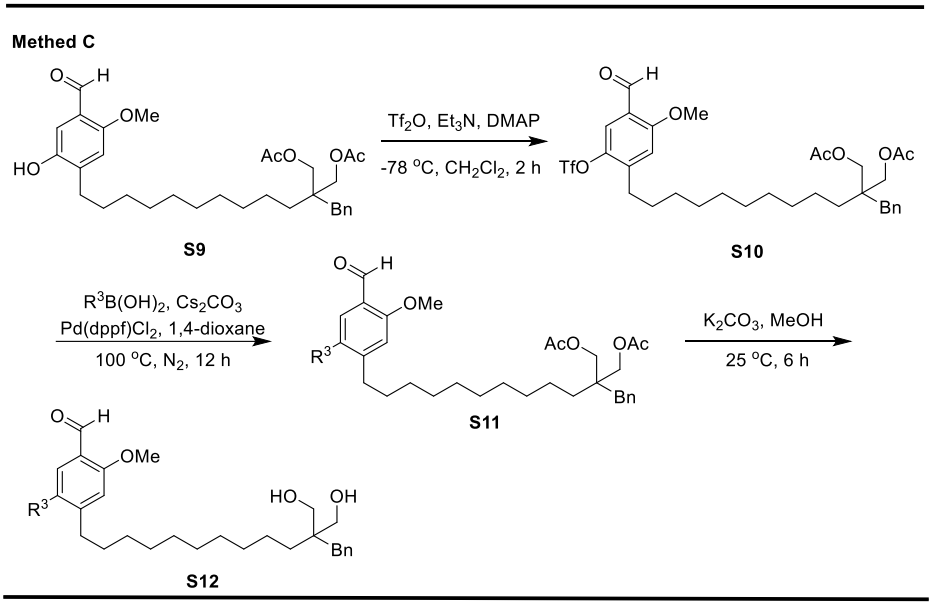


Supplementary Figure 2. Route for the synthesis of S8



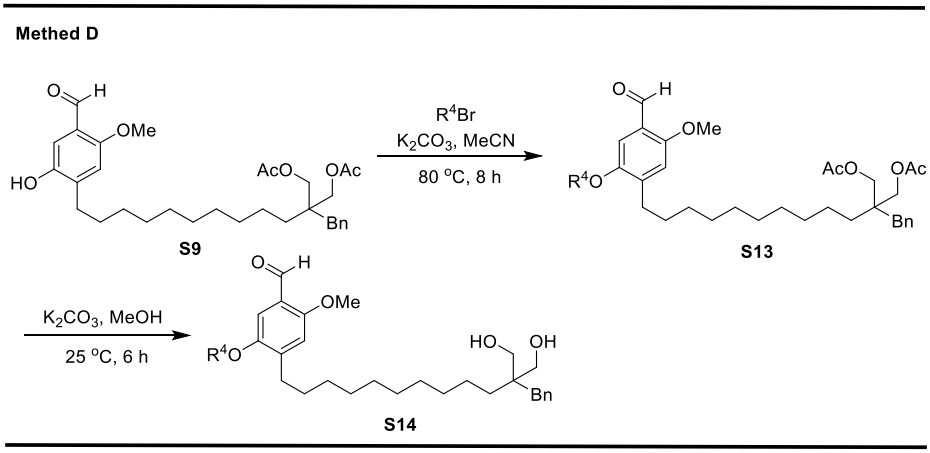
Substrates **1, 3-1**–**12-1**, **22-1**–**31-1** synthesized by **Method A**, **B**.

Supplementary Figure 3. Route for the synthesis of S12



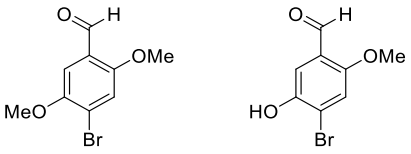
Substrates **13-1**–**19-1** synthesized by **Method C**.

Supplementary Figure 4. Route for the synthesis of S14



Substrates **20-1**, **21-1** synthesized by **Method D**.

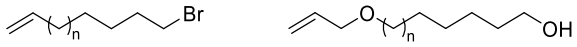
3. General procedure for the synthesis of substrates



S15 **S16**

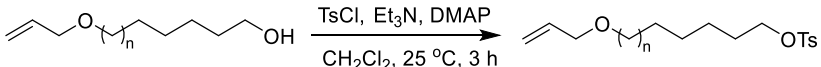
Benzaldehyde derivatives **S15** was obtained from commercial sources and used without further purification. Known benzaldehyde derivative **S16** was prepared according to literature procedure from commercially available materials.[1]

a) General procedures for the synthesis of alkyl chains



n = 1,2,4,5,6 **S17-S21** n = 1,2 **S22-S23**

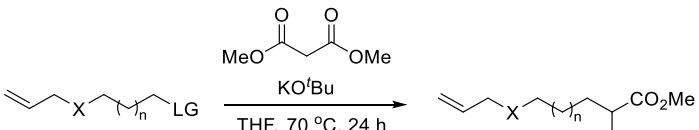
Known alkyl chains **S17-S21**, were obtained from commercial sources and used without further purification. Known alkyl chains **S22**, **S23** were prepared according to literature procedure from commercially available materials.[1]



n = 1,2 **S22-S23** n = 1,2 **S24-S25**

To a solution of **S22-S23** (5.0 mmol, 1.0 equiv.) in dry CH_2Cl_2 (50 mL) was added TsCl (1.15 g, 6.0 mmol, 1.2 equiv.), Et_3N (0.9 mL, 6.5 mmol, 1.3 equiv.) and DMAP (61 mg, 0.5 mmol, 0.1 equiv.) at 0 °C. The reaction mixture was warmed to 25 °C and stirred for 3 h. Then water (30 mL) was added and the organic phase was separated. The aqueous phase was extracted with CH_2Cl_2 (3 × 30 mL), the combined organic phases were washed by brine and dried over anhydrous Na_2SO_4. After filtration and removing the solvent *in vacuum*, the residue was purified by flash column chromatography on silica gel (PE/EA = 10:1, *v/v*) to afford the products **S24-S25**.

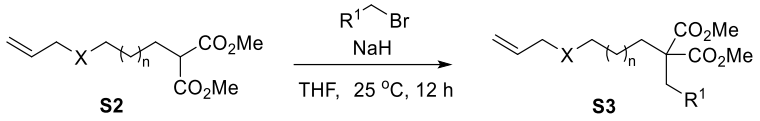
b) General procedures for the synthesis of S6



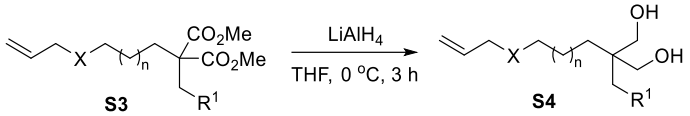
S1, LG = Br or OTs
X = C or O
n = 1, 2, 4, 5, 6

S2

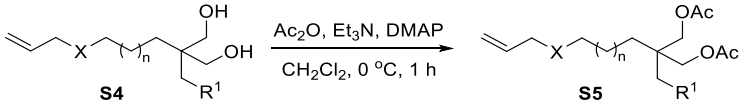
To a solution of **S1** (10.0 mmol, 1.0 equiv.) in dry THF (50 mL) was added dimethyl malonate (2.64 g, 20.0 mmol, 2.0 equiv.), KO^tBu (1.68 g, 15 mmol, 1.5 equiv.). The reaction mixture was warmed to 70 °C and stirred for 24 h. Then water (30 mL) was added and extracted with EtOAc (3 × 30 mL), the combined organic phases were washed by brine and dried over anhydrous Na_2SO_4. After filtration and removing the solvent *in vacuum*, the residue was purified by flash column chromatography on silica gel (PE/EA = 15:1, *v/v*) to afford the products **S2**.



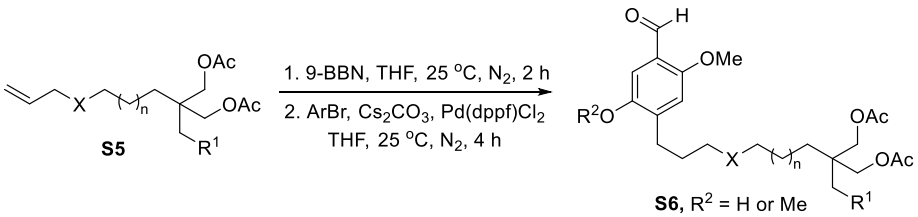
To a solution of NaH (480 mg, 60% in mineral oil, 12.0 mmol, 1.2 equiv.) in dry THF (50 mL) was added **S2** (10.0 mmol, 1.0 equiv.) at 0 °C. The reaction mixture was stirred for 1 h. Then R^1Br (12.0 mmol, 1.2 equiv.) was added. The reaction was stirred at 25 °C for 12 h. Then saturated NH_4Cl (10 mL) was added and the organic phase was separated. The aqueous phase was extracted with EtOAc (3 × 30 mL), the combined organic phases were washed by brine and dried over anhydrous Na_2SO_4. After filtration and removing the solvent *in vacuum*, the residue was purified by flash column chromatography on silica gel (PE/EA = 15:1, *v*/*v*) to afford the products **S3**.



To a solution of $LiAlH_4$ (912 mg, 24.0 mmol, 2.4 equiv.) in dry THF (50 mL) was added **S3** (10.0 mmol, 1.0 equiv.) slowly at 0 °C. The reaction mixture was stirred for 3 h. Upon on completion, Et_2O (30 mL), NaOH (15% aq. 0.95 mL), and H_2O (3.0 mL) were added sequentially to quench the reaction at 0 °C. The mixture was stirred at 25 °C for 20 min before being filtered. The filtrate was concentrated under reduced pressure and the residue was purified by flash column chromatography on silica gel (PE/EA = 2:1, *v*/*v*) to afford the products **S4**.



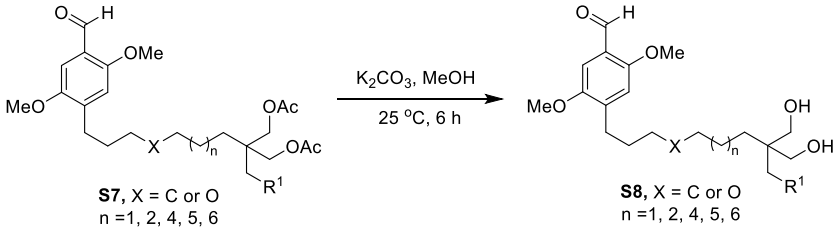
To a solution of **S4** (5.0 mmol, 1.0 equiv.) in dry CH_2Cl_2 (25 mL) was added DMAP (61 mg, 0.5 mmol, 0.1 equiv.), Et_3N (0.9 mL, 6.5 mmol, 1.3 equiv.) and Ac_2O (663 mg, 6.5 mmol, 1.3 equiv.) at 0 °C. The reaction mixture was stirred for 1 h. Then saturated NH_4Cl (30 mL) was added and the organic phase was separated. The aqueous phase was extracted with CH_2Cl_2 (3 × 30 mL), the combined organic phases were washed by brine and dried over anhydrous Na_2SO_4. After filtration and removing the solvent *in vacuum*, the residue was purified by flash column chromatography on silica gel (PE/EA = 10:1, *v*/*v*) to afford the products **S5**.



To a solution of **S5** (5.0 mmol, 1.0 equiv.) in dry THF (5.0 mL) was added 9-BBN (12.0 mL, 6.0 mmol, 0.5 M in THF, 1.2 equiv.) under N_2 atmosphere. The reaction mixture was stirred at 25 °C for 2 h and used directly for next step. In another flask, bromobenzene derivatives (5.0 mmol, 1.0 equiv.), Pd(dppf)Cl_2 (91.3 mg, 0.125 mmol, 0.025 equiv.) and Cs_2CO_3 (4.9 g, 15.0 mmol, 3.0 equiv.) were added under N_2 atmosphere. Then, the above solution was added via syringe. The reaction mixture was stirred at 25 °C for 4 h. Then 1 N HCl (10 mL) was slowly added and the

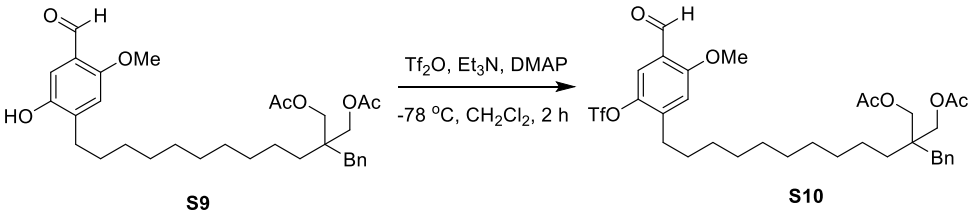
organic phase was separated. The aqueous phase was extracted with EtOAc (3 × 30 mL), the combined organic phases were washed by brine and dried over anhydrous Na_2SO_4. After filtration and removing the solvent *in vacuum*, the residue was purified by flash column chromatography on silica gel (PE/EA = 5:1, *v*/*v*) to afford the products **S6**.

c) General procedures for the synthesis of S8

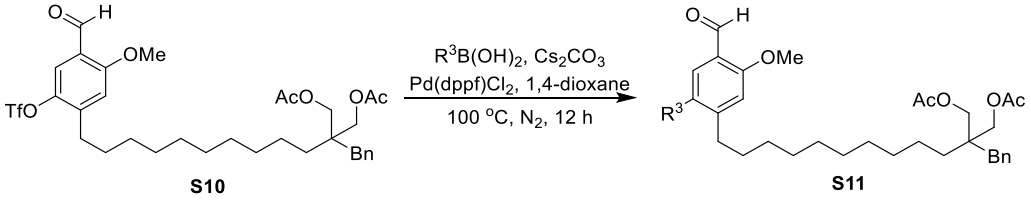


To a solution of **S7** (1.0 mmol, 1.0 equiv.) in MeOH (10 mL) was added K_2CO_3 (276 mg, 2.0 mmol, 2.0 equiv.). The reaction mixture was stirred at 25 °C for 6 h. The reaction mixture was filtered, and the solid was washed by EtOAc. Then, the solvent was removed *in vacuum*, the residue was purified by flash column chromatography on silica gel (PE/EA = 2:1, *v*/*v*) to afford the products **S8**.

d) General procedures for the synthesis of S12

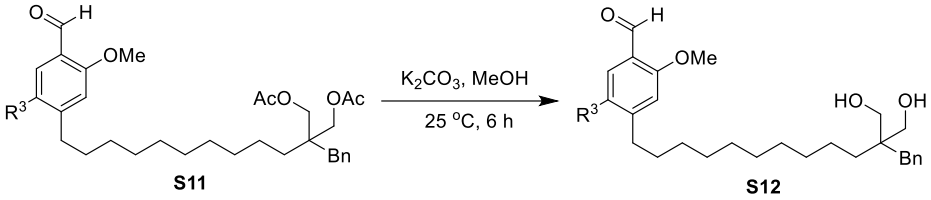


To a solution of **S9** (10.0 mmol, 1.0 equiv.) in dry CH_2Cl_2 (50 mL) was added DMAP (122 mg, 1.0 mmol, 0.1 equiv.), Et_3N (2.77 mL, 20.0 mmol, 2.0 equiv.) and Tf_2O (4.23 g, 15.0 mmol, 1.5 equiv.) at -78 °C. The reaction mixture was stirred at -78 °C for 2 h. Then saturated $NaHCO_3$ (15 mL) was added and the organic phase was separated. The aqueous phase was extracted with CH_2Cl_2 (3 × 30 mL), the combined organic phases were washed by brine and dried over anhydrous Na_2SO_4. After filtration and removing the solvent *in vacuum*, the residue was purified by flash column chromatography on silica gel (PE/EA = 5:1, *v*/*v*) to afford the product **S10**.



S10 (1.0 mmol, 1.0 equiv.), boronic acid (3.0 mmol, 3.0 equiv.), $Pd(dppf)Cl_2$ (73.1 mg, 0.1 mmol, 0.1 equiv.) and Cs_2CO_3 (978 mg, 3.0 mmol, 3.0 equiv.) were added to a dried flask. The flask was evacuated and backfilled with N_2 three times. Then the degassed 1,4-dioxane (10.0 mL) was added to the reaction. The reaction mixtures were stirred for 12 h at 100 °C in a heating mantle. After cooling to 25 °C, the reaction mixtures were diluted with water (30 mL) and extracted with

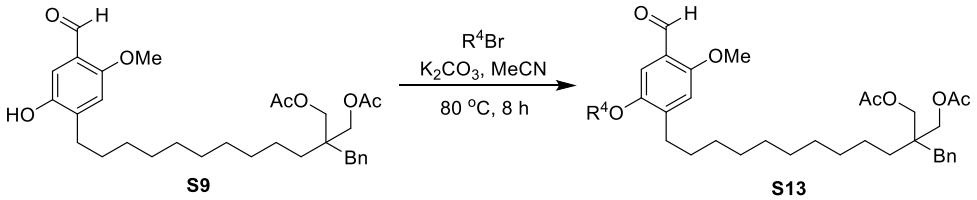
EtOAc (3 × 30 mL). The combined organic layers were dried over anhydrous Na_2SO_4. After filtration and removing the solvent *in vacuum*, the residue was purified by flash column chromatography on silica gel (PE/EA = 5:1, *v*/*v*) affording the product **S11**.



S11 **S12**

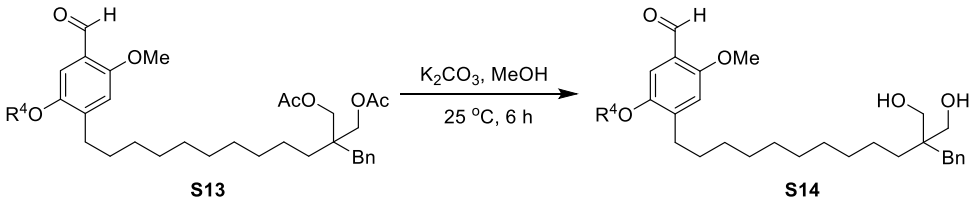
To a solution of **S11** (1.0 mmol, 1.0 equiv.) in MeOH (10 mL) was added K_2CO_3 (276 mg, 2.0 mmol, 2.0 equiv.). The reaction mixture was stirred at 25 °C for 6 h. The reaction mixture was filtered, and the solid was washed by EtOAc. Then, the solvent was removed *in vacuum*, the residue was purified by flash column chromatography on silica gel (PE/EA = 2:1, *v*/*v*) to afford the products **S12**.

e) General procedures for the synthesis of S14



S9 **S13**

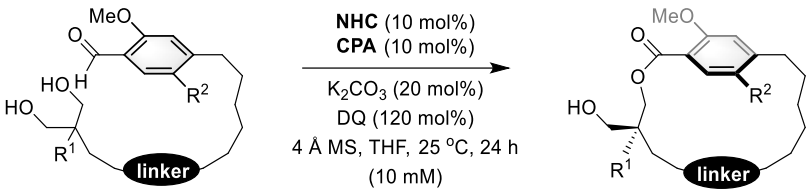
To a solution of **S9** (1.0 mmol, 1.0 equiv.) in dry MeCN (10 mL) was added K_2CO_3 (207 mg, 1.5 mmol, 1.5 equiv.) and R^4Br (1.2 mmol, 1.2 equiv.). The reaction mixture was stirred at 80 °C in a heating mantle for 8 h. After cooling to 25 °C, the reaction mixtures were diluted with water (30 mL) and extracted with EtOAc (3 × 30 mL). The combined organic layers were dried over anhydrous Na_2SO_4. After filtration and removing the solvent *in vacuum*, the residue was purified by flash column chromatography on silica gel (PE/EA = 5:1, *v*/*v*) affording the product **S13**.



S13 **S14**

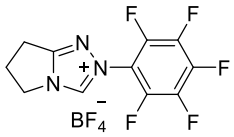
To a solution of **S13** (1.0 mmol, 1.0 equiv.) in MeOH (10 mL) was added K_2CO_3 (276 mg, 2.0 mmol, 2.0 equiv.). The reaction mixture was stirred at 25 °C for 6 h. The reaction mixture was filtered, and the solid was washed by EtOAc. Then, the solvent was removed *in vacuum*, the residue was purified by flash column chromatography on silica gel (PE/EA = 2:1, *v*/*v*) to afford the products **S14**.

f) General procedure for the macrocyclization reaction



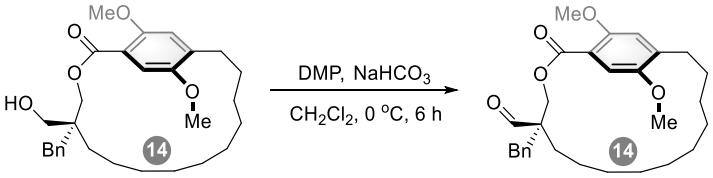
To a 15 mL Schlenk tube equipped with a magnetic stirring bar was added substrate (0.10 mmol, 1.0 equiv.), NHC **IX** (4.3 mg, 0.01 mmol, 0.1 equiv.), **CPA** (3.2 mg, 0.01 mmol, 0.1 equiv.), K_2CO_3 (2.76 mg, 0.02 mmol, 0.2 equiv.), DQ (49.0 mg, 0.12 mmol, 1.2 equiv.) and 4 Å MS (50 mg). The tube was closed with a septum, evacuated, and refilled with nitrogen (3 cycles). After that, dry THF (10.0 mL) was added to the reaction mixture at 25 °C and stirred for 24 h. Upon the reaction completion (monitored by TLC), the solvent was evaporated and the residue was purified by silica gel column chromatography affording products.

Note: K_2CO_3 (0.5 eq) was used for **4**, **22**, **23**, **27**, **28**. Racemic samples for the standard of chiral HPLC spectra were prepared using racemic NHC **S26** as catalyst.



S26

g) General procedure for the synthetic transformations



2 **32**

To a solution of **2** (46.8 mg, 0.1 mmol, 1.0 equiv.) in CH_2Cl_2 (1 mL) was added Dess-Martin oxidation (63.6 mg, 0.15 mmol, 1.5 equiv.), $NaHCO_3$ (25.2 mg, 0.30 mmol, 3.0 equiv.) at 0 °C. The reaction mixture was stirred at 0 °C for 6 h. Then saturated $Na_2S_2O_3$ (1 mL) was added and the organic phase was separated. The aqueous phase was extracted with CH_2Cl_2 (3 × 3 mL), the combined organic phases were washed by brine and dried over anhydrous Na_2SO_4. After filtration and removing the solvent *in vacuum*, the residue was purified by flash column chromatography on silica gel (PE/EA = 10:1, *v/v*) to afford the product **32**.

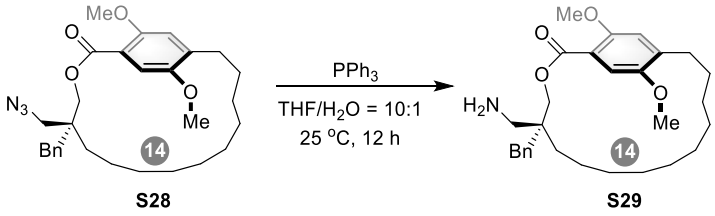
2 **S27**

To a solution of **2** (46.8 mg, 0.1 mmol, 1.0 equiv.) in dry CH_2Cl_2 (2 mL) was added MsCl (13.8 mg, 0.12 mmol, 1.2 equiv.), Et_3N (10.5 mg, 0.15 mmol, 1.5 equiv.) and DMAP (1.2 mg, 0.01 mmol,

0.1 equiv.) at 0 °C. The reaction mixture was stirred for 3 h. Then water (3 mL) was added and the organic phase was separated. The aqueous phase was extracted with CH_2Cl_2 (3 × 3 mL), the combined organic phases were washed by brine and dried over anhydrous Na_2SO_4. After filtration and removing the solvent *in vacuum*, the residue was purified by flash column chromatography on silica gel (PE/EA = 10:1, *v/v*) to afford the product **S27**.

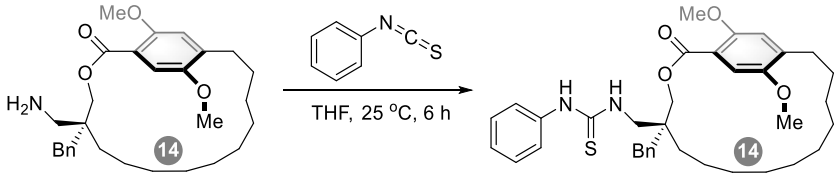
S27 **S28**

To the solution of **S27** (54.6 mg, 0.1 mmol, 1.0 equiv.) in DMSO (1.0 mL) was added NaN_3 (7.2 mg, 0.11 mmol, 1.1 equiv.), the mixture was warmed to 100 °C with stirring for 8 h. After cooling to 25 °C, the reaction mixtures were diluted with water (3 mL) and extracted with EtOAc (3 × 30 mL), the combined organic phases were washed by brine and dried over anhydrous Na_2SO_4. After filtration and removing the solvent *in vacuum*, the residue was purified by flash column chromatography on silica gel (PE/EA = 5:1, *v/v*) to afford the product **S28**.



S28 **S29**

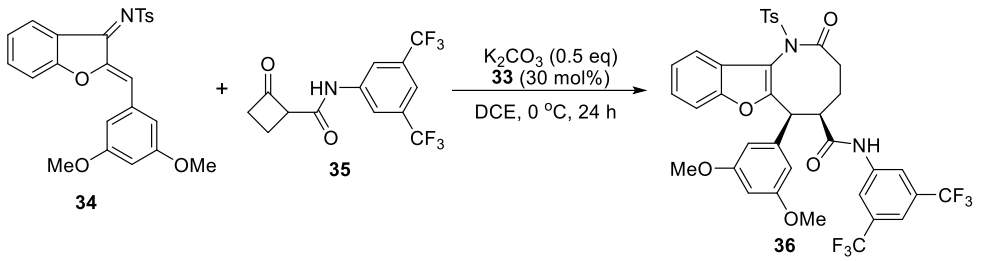
To a solution of the **S28** (49.3 mg, 0.10 mmol, 1.0 equiv.) in THF/water (0.5:0.05 mL) was added triphenylphosphine (26.2 mg, 0.10 mmol, 1.0 equiv.) at 25 °C. The reaction mixture was stirred at 25 °C for 12 h. The mixture was concentrated, and the residue was purified by chromatography on silica gel (PE/EA = 5:1, *v/v*) to afford the product **S29**.



S29 **33**

To a solution of **S29** (46.7 mg, 0.1 mmol, 1.0 equiv.) in THF (1 mL) was added Phenyl isothiocyanate (13.5 mg, 0.1 mmol, 1.0 equiv.). The reaction mixture was stirred at 25 °C for 6 h. Then, the solvent was removed *in vacuum*, the residue was purified by flash column chromatography on silica gel (PE/EA = 2:1, *v/v*) to afford the product **33**.

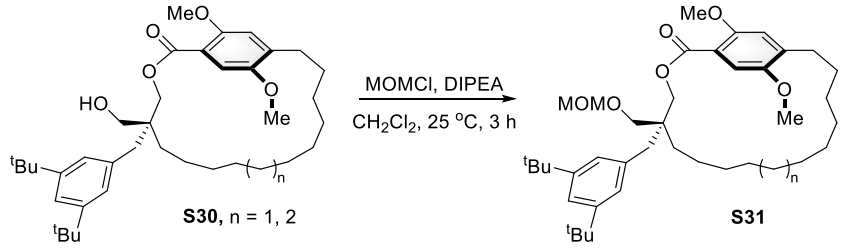
h) Procedure for the synthesis of 36



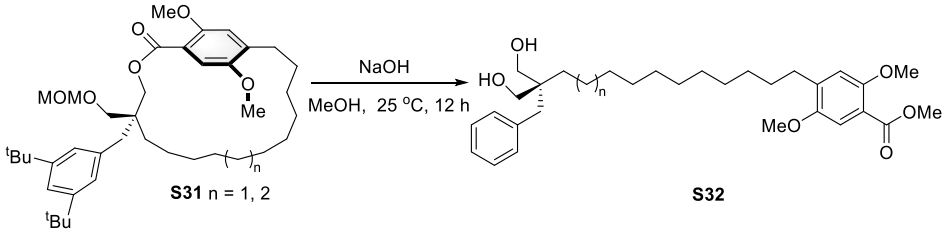
To an over dried flask was added **34** (43.5 mg, 0.1 mmol, 1.0 equiv.), **35** (35.8 mg, 0.11 mmol, 1.1 equiv.), K_2CO_3 (13.8 mg, 0.05 mmol, 0.5 equiv.), **33** (18.1 mg, 0.03 mmol 0.3 equiv.) and dry DCE (1.5 mL) under Ar. The reaction mixture was stirred at 0 °C and monitored by TLC. After completion (~24 h), the reaction mixture was purified by flash column chromatography to yield the final product **36**.

Known products **34**, **35** were prepared according to literature procedure from commercially available materials. The spectra are in accordance with literatures.[2]

i) General procedure for the synthesis of S32



To a solution of **S30** (0.1 mmol, 1.0 equiv.) in CH_2Cl_2 (1 mL) was added MOMCl (16.1 mg, 0.2 mmol, 2.,0 equiv.), DIPEA (25.8 mg, 0.2 mmol, 2.0 equiv.). The reaction mixture was stirred at 25 °C for 3 h. Then, the solvent was removed *in vacuum*, the residue was purified by flash column chromatography on silica gel (PE/EA = 10:1, *v/v*) to afford the products **S31**.

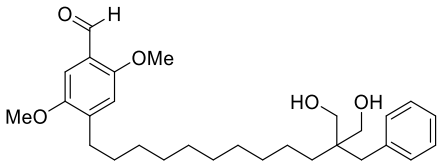


To a solution of **S31** (0.1 mmol, 1.0 equiv.) in MeOH (2 mL) was added NaOH (8.0 mg, 0.2 mmol, 2.,0 equiv.), The reaction mixture was stirred at 25 °C for 12 h. Then, the reaction mixtures were diluted with water (3 mL) and extracted with EtOAc (3 × 5 mL). The combined organic layers were dried over anhydrous Na_2SO_4. After filtration and removing the solvent *in vacuum*, the residue was purified by flash column chromatography on silica gel (PE/EA = 5:1, *v/v*) affording the product **S32.**

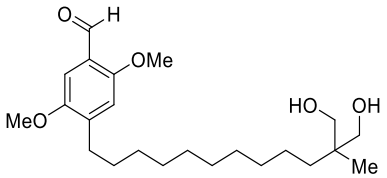
38, 39 were obtained as the above procedures.

4. Characterization data

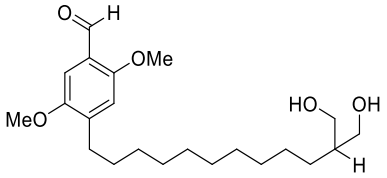
a) Characterization data of unknown substrates



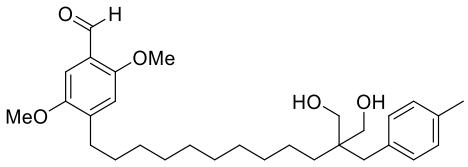
1, colorless oil. 68% yield, 319 mg. **^{1}H NMR** (600 MHz, $CDCl_3$). δ 10.39 (s, 1H), 7.29 – 7.24 (m, 3H), 7.23 – 7.18 (m, 3H), 6.79 (s, 1H), 3.89 (s, 3H), 3.81 (s, 3H), 3.62 – 3.52 (m, 4H), 2.68 (s, 2H), 2.64 (dd, J = 8.83, 6.72 Hz, 2H), 2.47 (s, 2H), 1.62 – 1.54 (m, 2H), 1.39 – 1.31 (m, 6H), 1.31 – 1.25 (m, 10H). **^{13}C NMR** (151 MHz, $CDCl_3$). δ 189.4, 156.9, 151.8, 141.4, 138.0, 130.5, 128.2, 113.9, 108.2, 68.6, 56.3, 55.9, 42.6, 37.3, 31.3, 31.2, 30.6, 29.72, 29.69, 29.6, 29.5, 23.1, 14.3. **HRMS** (ESI): m/z calculated for $C_{29}H_{42}NaO_5^+$ $[M + Na]^+$ 493.2924, found 493.2926.



3-1, colorless oil. 78% yield, 307 mg. **^{1}H NMR** (600 MHz, $CDCl_3$). δ 10.37 (s, 1H), 7.24 (s, 1H), 6.78 (s, 1H), 3.88 (s, 3H), 3.80 (s, 3H), 3.6 – 3.4 (m, 4H), 2.70 – 2.44 (m, 4H), 1.7 – 1.5 (m, 2H), 1.38 – 1.30 (m, 4H), 1.29 – 1.22 (m, 12H), 0.81 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$). δ 189.5, 156.8, 151.8, 141.4, 122.8, 113.9, 108.1, 70.7, 56.2, 55.9, 38.9, 34.1, 31.1, 30.7, 29.7, 29.64, 29.62, 29.5, 23.3, 18.6. **HRMS** (ESI): m/z calculated for $C_{23}H_{38}NaO_5^+$ $[M + Na]^+$ 417.2611, found 417.2615.

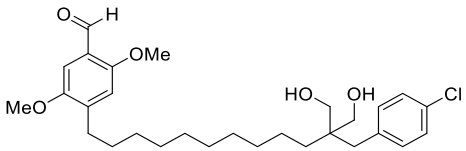


4-1, white solid. 89% yield, 320 mg. **^{1}H NMR** (400 MHz, Acetone-d_6). δ 10.33 (s, 1H), 7.18 (s, 1H), 7.03 (s, 1H), 3.90 (s, 3H), 3.81 (s, 3H), 3.59 – 3.43 (m, 5H), 2.73 – 2.55 (m, 2H), 1.69 – 1.43 (m, 2H), 1.40 – 1.16 (m, 18H). **^{13}C NMR** (101 MHz, Acetone-d_6). δ 187.8, 156.8, 151.8, 140.8, 122.9, 114.5, 107.5, 63.8, 63.7, 55.9, 55.3, 43.1, 30.7, 30.0, 29.6, 29.5, 29.3, 27.9, 27.2. **HRMS** (ESI): m/z calculated for $C_{22}H_{36}NaO_5^+$ $[M + Na]^+$ 403.2455, found 403.2460.

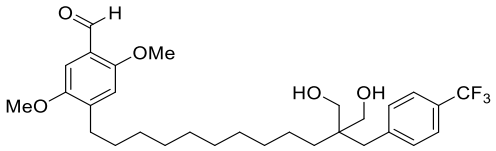


5-1, yellow oil. 83% yield, 402 mg. **^{1}H NMR** (400 MHz, $CDCl_3$). δ 10.39 (s, 1H), 7.26 (s, 1H), 7.17 – 6.98 (m, 4H), 6.79 (s, 1H), 3.89 (s, 3H), 3.82 (s, 3H), 3.58 – 3.48 (m, 4H), 2.67 – 2.62 (m, 2H), 2.32 (s, 3H), 1.61 – 1.55 (m, 2H), 1.38 – 1.31 (m, 4H), 1.31 – 1.22 (m,16H). **^{13}C NMR** (151 MHz,

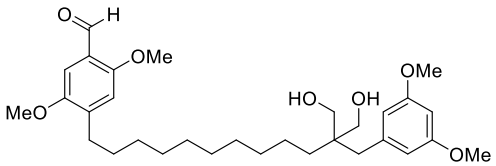
$CDCl_3$). δ 189.4, 156.8, 151.8, 141.4, 134.8, 130.3, 130.3, 122.9, 113.9, 113.7, 108.2, 68.6, 56.3, 55.9, 42.5, 36.9, 32.1, 31.2, 29.6, 29.5, 26.4, 23.1, 22.2, 21.1. **HRMS** (ESI): m/z calculated for $C_{30}H_{44}NaO_5^+$ $[M + Na]^+$ 507.3081, found 507.3077.



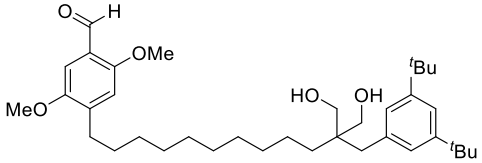
6-1, white solid. 77% yield, 415 mg. **^{1}H NMR** (600 MHz, $CDCl_3$). δ 10.37 (s, 1H), 7.31 – 7.20 (m, 3H), 7.18 – 7.08 (m, 2H), 6.77 (s, 1H), 3.87 (s, 3H), 3.79 (s, 3H), 3.60 – 3.46 (m, 4H), 2.66 (s, 2H), 2.62 (t, J = 7.24 Hz, 2H), 2.56 (s, 2H), 1.60 – 1.54 (m, 2H), 1.37 – 1.28 (m, 4H), 1.29 – 1.18 (m, 10H), 1.11 – 1.05 (m, 2H). **^{13}C NMR** (151 MHz, $CDCl_3$). δ 189.5, 156.9, 151.8, 141.4, 136.5, 131.9, 130.5, 128.2, 122.8, 113.9, 108.2, 68.4, 56.3, 55.9, 42.5, 36.4, 31.24, 31.15, 30.54, 30.53, 29.7, 29.5, 23.1. **HRMS** (ESI): m/z calculated for $C_{29}H_{41}ClNaO_5^+$ $[M + Na]^+$ 527.2535, found 527.2539.



7-1, yellow solid. 65% yield, 349 mg.**^{1}H NMR** (400 MHz, DMSO-d_6). δ 10.25 (s, 1H), 7.88 – 7.50 (m, 2H), 7.44 – 7.29 (m, 2H), 7.11 (s, 1H), 7.01 (s, 1H), 4.51 – 4.33 (m, 2H), 3.83 (s, 3H), 3.73 (s, 3H), 3.18 – 3.02 (m, 4H), 2.67 – 2.50 (m, 4H), 1.51 – 1.45 (m, 2H), 1.26 – 1.09 (m, 14H), 1.02 – 0.89 (m, 2H). **^{13}C NMR** (151 MHz, DMSO-d_6). δ 188.7, 156.8, 151.7, 144.3, 141.0, 131.6, 126.97 (q, $J_{C\text{-}F}$ = 31.97 Hz), 125.1 (q, $J_{C\text{-}F}$ = 277.71 Hz), 124.9, 122.7, 115.1, 108.0, 62.9, 56.8, 56.1, 43.6, 36.9, 31.4, 30.8, 30.6, 29.6, 29.54, 29.49, 29.4, 22.9. **^{19}F NMR** (565 MHz, Acetone-d_6) δ –62.6. **HRMS** (ESI): m/z calculated for $C_{30}H_{41}F_3NaO_5^+$ $[M + Na]^+$ 561.2798, found 561.2794.

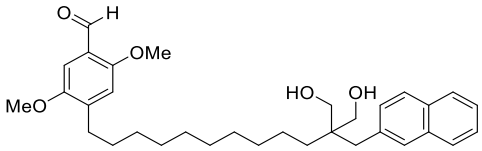


8-1, white solid. 71% yield, 376 mg. **^{1}H NMR** (600 MHz, Acetone-d_6). δ 10.33 (s, 1H), 7.19 (s, 1H), 7.02 (s, 1H), 6.44 (s, 2H), 6.29 (s, 1H), 3.89 (s, 3H), 3.80 (s, 3H), 3.71 (s, 6H), 3.53 – 3.30 (m, 4H), 2.67 – 2.61 (m, 2H), 2.56 (s, 2H), 1.60 – 1.51 (m, 2H), 1.40 – 1.21 (m, 16H), 1.18 – 1.12 (m, 2H). **^{13}C NMR** (151 MHz, Acetone-d_6). δ 187.8, 160.6, 156.8, 151.8, 140.9, 123.0, 114.4, 108.6, 107.5, 97.8, 65.3, 65.2, 55.9, 55.3, 54.6, 42.8, 37.0, 31.2, 30.7, 30.6, 29.61, 29.58, 29.5, 29.4, 22.9. **HRMS** (ESI): m/z calculated for $C_{31}H_{46}NaO_7^+$ $[M + Na]^+$ 553.3136, found 553.3142.

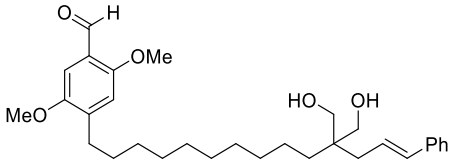


9-1, colorless oil. 57% yield, 331 mg. **^{1}H NMR** (400 MHz, DMSO-d_6). δ 10.24 (s, 1H), 7.11 (s, 2H), 7.00 (s, 1H), 6.98 (s, 2H), 4.34 – 4.28 (m, 2H), 3.81 (s, 3H), 3.72 (s, 3H), 3.20 – 3.07 (m, 4H), 2.55

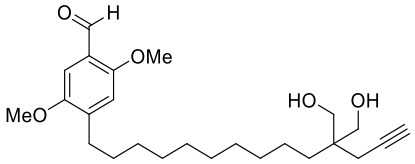
(t, J = 7.67 Hz, 2H), 2.38 (s, 2H), 1.55 – 1.43 (m, 2H), 1.29 – 1.16 (m, 32H), 0.89 – 0.83 (m, 2H). **^{13}C NMR** (101 MHz, DMSO-d_6). δ 188.7, 156.8, 151.7, 149.6, 141.0, 137.8, 125.0, 122.7, 119.2, 115.1, 108.0, 63.5, 56.8, 56.1, 43.2, 36.8, 34.8, 31.8, 30.8, 29.8, 29.7, 29.6, 29.5, 29.3, 23.0. **HRMS** (ESI): m/z calculated for $C_{37}H_{58}NaO_5^+$ $[M + Na]^+$ 605.4176, found 605.4170.



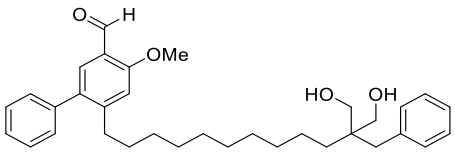
10-1, white solid. 64% yield, 332 mg. **^{1}H NMR** (600 MHz, $CDCl_3$). δ 10.39 (s, 1H), 7.79 (ddd, J = 17.68, 7.36, 2.04 Hz, 3H), 7.64 (s, 1H), 7.48 – 7.41 (m, 2H), 7.36 (dd, J = 8.36, 1.74 Hz, 1H), 7.26 (s, 1H), 6.79 (s, 1H), 3.88 (s, 3H), 3.81 (s, 3H), 3.62 (q, J = 10.30, 9.90 Hz, 4H), 2.86 (s, 2H), 2.71 – 2.60 (m, 2H), 2.52 (s, 2H), 1.62 – 1.56 (m, 2H), 1.43 – 1.33 (m, 4H), 1.32 – 1.24 (m, 10H), 1.22 – 1.16 (m, 2H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 189.5, 156.9, 151.8, 141.4, 135.7, 133.4, 132.1, 129.2, 128.9, 127.62, 127.61, 127.5, 126.0, 125.4, 122.9, 113.9, 108.2, 68.6, 56.3, 55.9, 42.9, 37.4, 31.4, 31.2, 30.6, 29.74, 29.69, 29.65, 29.5, 23.2, 14.3. **HRMS** (ESI): m/z calculated for $C_{33}H_{44}NaO_5^+$ $[M + Na]^+$ 543.3081, found 543.3085.



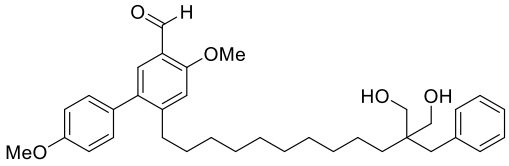
11-1, white solid. 77% yield, 382 mg. **^{1}H NMR** (400 MHz, Acetone-d_6). δ 10.36 (s, 1H), 7.42 – 7.36 (m, 2H), 7.28 (td, J = 7.67, 1.98 Hz, 2H), 7.24 – 7.16 (m, 2H), 7.06 (s, 1H), 6.46 (dd, J = 15.88, 1.98 Hz, 1H), 6.41 – 6.28 (m, 1H), 3.93 (s, 3H), 3.83 (s, 3H), 3.71 (ddd, J = 5.20, 3.17, 2.23 Hz, 1H), 3.54 – 3.50 (m, 4H), 2.75 – 2.59 (m, 2H), 2.24 – 2.19 (m, 2H), 1.63 – 1.54 (m, 2H), 1.40 – 1.20 (m, 17H). **^{13}C NMR** (101 MHz, Acetone-d_6). δ 187.8, 156.8, 151.7, 140.8, 138.1, 132.2, 128.5, 127.0, 126.8, 126.0, 122.9, 114.5, 107.5, 66.0, 65.8, 55.9, 55.3, 42.5, 34.8, 31.3, 30.7, 30.6, 29.61, 29.56, 29.4, 22.6. **HRMS** (ESI): m/z calculated for $C_{31}H_{44}NaO_5^+$ $[M + Na]^+$ 519.3081, found 519.3084.



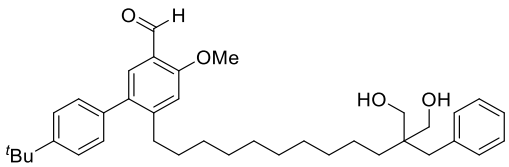
12-1, colorless oil. 54% yield, 226 mg. **^{1}H NMR** (600 MHz, Acetone-d_6). δ 10.36 (s, 1H), 7.21 (s, 1H), 7.05 (s, 1H), 3.93 (s, 3H), 3.84 (s, 3H), 3.54 – 3.48 (m, 4H), 2.69 – 2.63 (m, 2H), 2.31 (t, J = 2.68 Hz, 1H), 2.21 (d, J = 2.75 Hz, 2H), 1.60 (p, J = 7.32 Hz, 2H), 1.40 – 1.33 (m, 6H), 1.33 – 1.26 (m, 12H). **^{13}C NMR** (151 MHz, Acetone-d_6). δ 187.9, 156.8, 151.8, 140.8, 122.9, 114.4, 107.5, 81.6, 70.5, 65.1, 65.0, 55.9, 55.3, 41.8, 31.2, 30.7, 30.6, 29.6, 29.5, 29.43, 29.36, 22.8, 21.0. **HRMS** (ESI): m/z calculated for $C_{25}H_{38}NaO_5^+$ $[M + Na]^+$ 441.2611, found 441.2617.



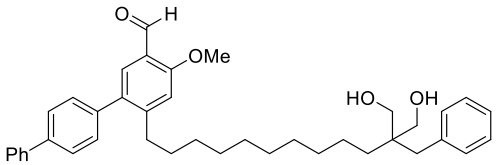
13-1, white solid. 81% yield, 418 mg. **^{1}H NMR** (600 MHz, $CDCl_3$). δ 10.42 (s, 1H), 7.66 (s, 1H), 7.41 – 7.36 (m, 2H), 7.34 – 7.30 (m, 1H), 7.29 – 7.24 (m, 4H), 7.21 – 7.17 (m, 3H), 6.87 (s, 1H), 3.96 (s, 3H), 3.56 (q, J = 10.71 Hz, 4H), 2.67 (s, 2H), 2.63 – 2.58 (m, 2H), 1.49 – 1.42 (m, 2H), 1.34 – 1.29 (m, 2H), 1.26 – 1.22 (m, 4H), 1.20 – 1.12 (m, 10H). **^{13}C NMR** (151 MHz, $CDCl_3$). δ 189.6, 161.0, 149.8, 140.5, 138.0, 134.9, 130.5, 130.3, 129.5, 128.23, 128.18, 127.1, 126.3, 122.7, 112.3, 68.6, 55.8, 42.6, 37.4, 34.1, 31.3, 31.1, 30.5, 29.6, 29.5, 29.4, 29.3, 23.1. **HRMS** (ESI): m/z calculated for $C_{34}H_{44}NaO_4^+$ $[M + Na]^+$ 539.3132, found 539.3128.



14-1, colorless oil. 37% yield, 169 mg. **^{1}H NMR** (400 MHz, $CDCl_3$). δ 10.41 (s, 1H), 7.64 (s, 1H), 7.31 – 7.23 (m, 2H), 7.22 – 7.13 (m, 5H), 6.91 (d, J = 8.65 Hz, 2H), 6.86 (s, 1H), 3.95 (s, 3H), 3.83 (s, 3H), 3.64 – 3.47 (m, 4H), 2.67 (s, 2H), 2.64 – 2.55 (m, 2H), 2.36 (s, 2H), 1.52 – 1.41 (m, 2H), 1.37 – 1.27 (m, 2H), 1.28 – 1.11 (m, 14H). **^{13}C NMR** (101 MHz, $CDCl_3$). δ 189.7, 160.9, 158.7, 150.1, 138.0, 134.5, 132.8, 130.5, 130.4, 128.2, 126.2, 122.6, 113.6, 112.2, 68.6, 55.8, 55.4, 42.6, 37.3, 34.1, 31.3, 31.1, 30.6, 29.7, 29.51, 29.50, 29.3, 23.1. **HRMS** (ESI): m/z calculated for $C_{35}H_{46}NaO_5^+$ $[M + Na]^+$ 569.3237, found 569.3235.

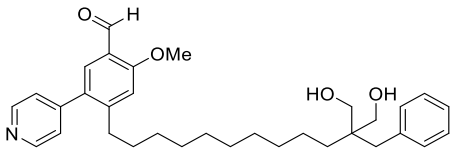


15-1, white solid. 65% yield, 372 mg. **^{1}H NMR** (600 MHz, $CDCl_3$). δ 10.40 (s, 1H), 7.67 (s, 1H), 7.41 – 7.36 (m, 2H), 7.28 – 7.24 (m, 2H), 7.21 – 7.16 (m, 5H), 6.87 (s, 1H), 3.95 (s, 3H), 3.63 – 3.50 (m, 4H), 2.67 (s, 2H), 2.65 – 2.59 (m, 2H), 1.56 – 1.45 (m, 2H), 1.35 (s, 9H), 1.33 – 1.29 (m, 2H), 1.26 – 1.13 (m, 14H). **^{13}C NMR** (151 MHz, $CDCl_3$). δ 189.7, 160.9, 150.0, 149.9, 138.0, 137.4, 134.8, 130.5, 129.1, 128.2, 126.2, 125.1, 122.7, 112.2, 68.6, 55.8, 42.6, 37.3, 34.6, 34.0, 31.5, 31.3, 31.2, 30.6, 29.7, 29.5, 29.4, 29.3, 23.1. **HRMS** (ESI): m/z calculated for $C_{38}H_{52}NaO_4^+$ $[M + Na]^+$ 595.3758, found 595.3754.

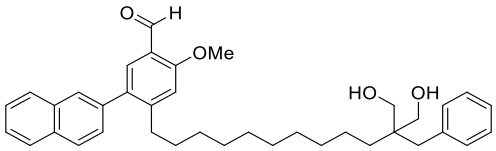


16-1, colorless oil. 69% yield, 408 mg. **^{1}H NMR** (400 MHz, $CDCl_3$). δ 10.44 (s, 1H), 7.72 (s, 1H), 7.67 – 7.59 (m, 4H), 7.49 – 7.41 (m, 2H), 7.37 – 7.32 (m, 3H), 7.28 – 7.24 (m, 2H), 7.22 – 7.16 (m, 3H), 6.90 (s, 1H), 3.97 (s, 3H), 3.60 – 3.51 (m, 4H), 2.69 – 2.63 (m, 4H), 1.58 – 1.48 (m, 2H), 1.24 – 1.12 (m, 16H). **^{13}C NMR** (101 MHz, $CDCl_3$). δ 189.7, 161.1, 150.0, 140.8, 139.9, 139.5, 134.5,

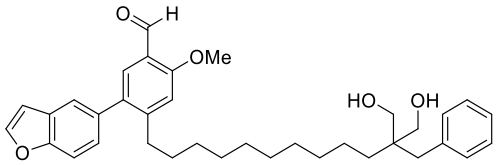
130.5, 130.4, 129.9, 128.9, 128.2, 127.5, 127.2, 127.0, 126.2, 122.7, 112.4, 68.6, 55.9, 42.5, 37.3, 34.1, 31.3, 31.2, 30.6, 29.73, 29.70, 29.6, 29.5, 29.3, 23.1. **HRMS** (ESI): m/z calculated for $C_{40}H_{48}NaO_4^+$ $[M + Na]^+$ 615.3445, found 615.3440.



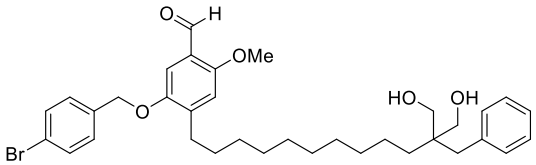
17-1, colorless oil. 87% yield, 450 mg. **^{1}H NMR** (400 MHz, $CDCl_3$). δ 10.41 (s, 1H), 8.60 (d, J = 5.05 Hz, 2H), 7.63 (s, 1H), 7.37 – 7.15 (m, 7H), 6.89 (s, 1H), 3.96 (s, 3H), 3.72 – 3.47 (m, 4H), 2.66 (s, 2H), 2.65 – 2.55 (m, 4H), 1.51 – 1.40 (m, 2H), 1.36 – 1.28 (m, 2H), 1.26 – 1.14 (m, 12H). **^{13}C NMR** (101 MHz, $CDCl_3$). δ 189.3, 161.7, 149.5, 149.4, 148.9, 138.1, 131.8, 130.5, 129.8, 128.1, 126.2, 124.7, 122.9, 112.7, 68.5, 55.9, 42.5, 37.4, 33.9, 31.2, 30.5, 29.6, 29.5, 29.3, 29.1, 23.1. **HRMS** (ESI): m/z calculated for $C_{33}H_{43}NaO_4^+$ $[M + Na]^+$ 540.3084, found 540.3089.



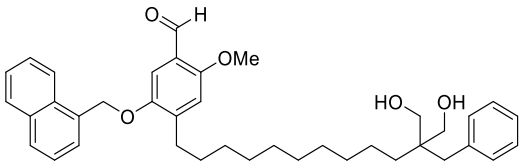
18-1, colorless oil. 61% yield, 339 mg. **^{1}H NMR** (600 MHz, Acetone-d_6). δ 10.42 (s, 1H), 7.95 – 7.91 (m, 3H), 7.81 (s, 1H), 7.63 (s, 1H), 7.55 – 7.48 (m, 2H), 7.47 – 7.42 (m, 1H), 7.27 – 7.19 (m, 5H), 7.17 – 7.11 (m, 1H), 4.02 (s, 3H), 3.43 – 3.33 (m, 4H), 2.73 – 2.67 (m, 2H), 2.61 (s, 2H), 1.55 – 1.46 (m, 2H), 1.38 – 1.29 (m, 2H), 1.16 – 1.07 (m, 16H). **^{13}C NMR** (151 MHz, $CDCl_3$). δ 188.1, 161.3, 149.9, 138.8, 138.2, 134.5, 133.6, 132.6, 130.6, 129.2, 128.03, 128.01, 127.81, 127.75, 127.73, 127.71, 126.4, 126.1, 125.7, 122.8, 113.2, 65.2, 65.1, 55.6, 42.8, 36.7, 33.7, 31.0, 30.8, 30.5, 29.4, 28.9, 22.8. **HRMS** (ESI): m/z calculated for $C_{38}H_{46}NaO_4^+$ $[M + Na]^+$ 589.3288, found 589.3282.



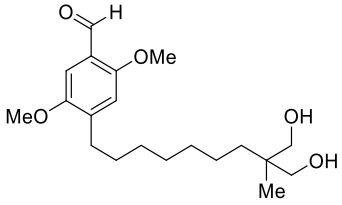
19-1, colorless oil. 45% yield, 250 mg. **^{1}H NMR** (400 MHz, $CDCl_3$). δ 10.44 (s, 1H), 7.78 (s, 1H), 7.62 – 7.55 (m, 2H), 7.31 – 7.22 (m, 3H), 7.26 – 7.12 (m, 4H), 6.96 (s, 1H), 6.80 (d, J = 2.17 Hz, 1H), 3.98 (s, 3H), 3.65 – 3.49 (m, 4H), 2.66 (s, 2H), 2.60 – 2.46 (m, 2H), 1.47 – 1.37 (m, 2H), 1.34 – 1.26 (m, 2H), 1.24 – 1.02 (m, 14H). **^{13}C NMR** (151 MHz, $CDCl_3$). δ 189.7, 161.5, 152.7, 151.2, 145.1, 138.0, 131.0, 130.5, 129.2, 128.2, 127.5, 126.2, 125.8, 124.4, 123.0, 122.8, 120.7, 112.3, 106.9, 68.5, 55.9, 42.5, 37.2, 34.3, 31.2, 30.7, 30.6, 29.6, 29.4, 29.3, 29.2, 23.1. **HRMS** (ESI): m/z calculated for $C_{36}H_{44}NaO_5^+$ $[M + Na]^+$ 579.3081, found 579.3085.



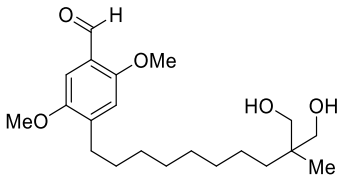
20-1, white solid. 73% yield, 456 mg. **^{1}H NMR** (600 MHz, DMSO-d_6). δ 10.23 (s, 1H), 7.55 – 7.50 (m, 2H), 7.37 – 7.33 (m, 2H), 7.23 – 7.08 (m, 6H), 7.03 (s, 1H), 5.04 (s, 2H), 4.33 (t, J = 4.78 Hz, 2H), 3.82 (s, 3H), 3.11 (qd, J = 10.46, 4.34 Hz, 4H), 2.64 – 2.59 (m, 2H), 2.44 (s, 2H), 1.51 (p, J = 7.41 Hz, 2H), 1.29 – 1.19 (m, 6H), 1.17 – 1.09 (m, 8H), 0.99 – 0.93 (m, 2H). **^{13}C NMR** (151 MHz, DMSO-d_6). δ 188.7, 157.0, 150.5, 141.5, 139.1, 137.2, 131.9, 130.9, 129.9, 128.1, 126.1, 122.7, 121.4, 115.3, 109.7, 69.5, 63.3, 56.8, 43.3, 37.0, 31.3, 31.0, 30.7, 29.7, 29.6, 29.50, 29.48, 29.3, 22.9. **HRMS** (ESI): m/z calculated for $C_{35}H_{45}BrNaO_5^+$ $[M + Na]^+$ 647.2343, found 647.2347.



21-1, white solid. 72% yield, 429 mg. **^{1}H NMR** (600 MHz, DMSO-d_6). δ 10.27 (s, 1H), 8.08 – 8.03 (m, 1H), 7.94 – 7.89 (m, 1H), 7.87 (d, J = 8.22 Hz, 1H), 7.60 (dd, J = 6.98, 1.21 Hz, 1H), 7.54 – 7.48 (m, 2H), 7.45 (dd, J = 8.26, 6.97 Hz, 1H), 7.43 (s, 1H), 7.22 – 7.14 (m, 4H), 7.13 – 7.09 (m, 1H), 7.03 (s, 1H), 5.50 (s, 2H), 4.35 (t, J = 4.87 Hz, 2H), 3.83 (s, 3H), 3.12 (qd, J = 10.49, 4.90 Hz, 4H), 2.55 – 2.49 (m, 2H), 2.44 (s, 2H), 1.46 – 1.38 (m, 2H), 1.30 – 1.20 (m, 2H), 1.15 – 1.03 (m, 12H), 0.99 – 0.93 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$). δ 188.8, 157.0, 150.8, 141.6, 139.1, 133.8, 133.1, 129.2, 129.0, 128.1, 126.9, 126.8, 126.5, 126.1, 125.8, 124.5, 122.8, 115.3, 110.0, 69.0, 63.3, 56.8, 43.3, 37.0, 31.3, 31.0, 30.7, 29.8, 29.6, 29.43, 29.41, 29.2, 22.9. **HRMS** (ESI): m/z calculated for $C_{39}H_{48}NaO_5^+$ $[M + Na]^+$ 619.3394, found 619.3399.

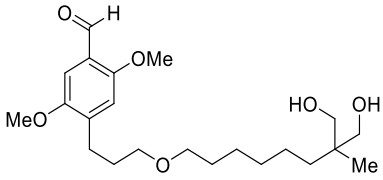


22-1, yellow oil. 44% yield, 155 mg. **^{1}H NMR** (400 MHz, DMSO-d_6). δ 10.24 (s, 1H), 7.11 (s, 1H), 7.01 (s, 1H), 4.28 – 4.14 (m, 2H), 3.82 (s, 3H), 3.73 (s, 3H), 3.14 – 3.07 (m, 4H), 2.60 – 2.52 (m, 2H), 1.56 – 1.44 (m, 2H), 1.30 – 1.23 (m, 4H), 1.17 – 1.07 (m, 6H), 0.64 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$). δ 188.7, 156.8, 151.7, 141.1, 122.7, 115.1, 108.0, 66.3, 56.8, 56.1, 34.2, 30.8, 30.7, 29.6, 29.54, 29.45, 23.3, 19.4. **HRMS** (ESI): m/z calculated for $C_{20}H_{32}NaO_5^+$ $[M + Na]^+$ 375.2142, found 375.2140.

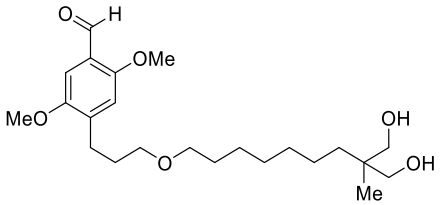


23-1, yellow oil. 54% yield, 198 mg. **^{1}H NMR** (400 MHz, DMSO-d_6). δ 10.24 (s, 1H), 7.11 (s, 1H), 7.01 (s, 1H), 4.28 – 4.11 (m, 2H), 3.83 (s, 3H), 3.73 (s, 3H), 3.12 (dt, J = 5.06, 2.44 Hz, 4H), 2.60 – 2.51 (m, 2H), 1.60 – 1.34 (m, 2H), 1.31 – 0.99 (m, 12H), 0.65 (s, 3H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 188.7, 156.8, 151.7, 141.0, 122.7, 115.1, 108.0, 66.3, 56.8, 56.1, 34.2, 30.8, 29.7, 29.62, 29.58, 29.5, 29.4, 23.3, 19.4. **HRMS** (ESI): m/z calculated for $C_{21}H_{34}NaO_5^+$ $[M + Na]^+$ 389.2298, found

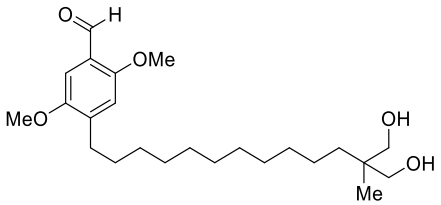
389.2295.



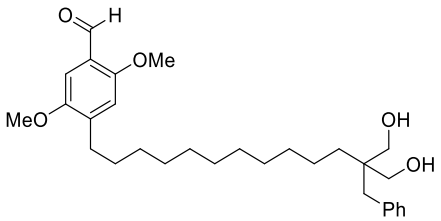
24-1, colorless oil. 54% yield, 198 mg. **^{1}H NMR** (600 MHz, Acetone-d_6). δ 10.33 (s, 1H), 7.18 (s, 1H), 7.01 (s, 1H), 3.90 (s, 3H), 3.81 (s, 3H), 3.69 – 3.57 (m, 2H), 3.49 – 3.22 (m, 8H), 2.78 – 2.57 (m, 2H), 1.83 – 1.77 (m, 2H), 1.55 – 1.49 (m, 2H), 1.40 – 1.32 (m, 2H), 1.26 – 1.18 (m, 6H), 0.76 (s, 3H). **^{13}C NMR** (151 MHz, Acetone-d_6). δ 187.9, 156.7, 151.8, 140.2, 123.0, 114.6, 107.5, 70.6, 69.8, 68.0, 67.9, 55.9, 55.3, 39.0, 34.0, 30.6, 29.8, 29.4, 27.6, 26.3, 23.2, 18.3. **HRMS** (ESI): m/z calculated for $C_{22}H_{36}NaO_6^+$ $[M + Na]^+$ 419.2404, found 419.2400.



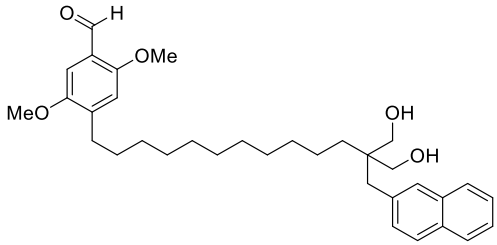
25-1, colorless oil. 47% yield, 193 mg. **^{1}H NMR** (600 MHz, $CDCl_3$). δ 10.33 (s, 1H), 7.19 (s, 1H), 7.02 (s, 1H), 3.90 (s, 3H), 3.81 (s, 3H), 3.43 – 3.29 (m, 8H), 2.76 – 2.63 (m, 2H), 1.89 – 1.74 (m, 2H), 1.61 – 1.48 (m, 2H), 1.35 – 1.14 (m, 12H), 0.76 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$). δ 192.4, 157.3, 139.4, 138.8, 137.9, 132.4, 132.2, 130.4, 128.4, 127.8, 107.5, 63.2, 55.8, 32.9, 30.6, 29.71, 29.69, 29.66, 29.6, 29.5, 25.9. **HRMS** (ESI): m/z calculated for $C_{23}H_{38}NaO_6^+$ $[M + Na]^+$ 433.2561, found 433.2565.



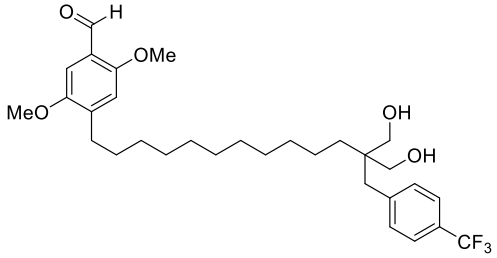
26-1, colorless oil. 63% yield, 257 mg. **^{1}H NMR** (600 MHz, Acetone-d_6). δ 10.33 (s, 1H), 7.18 (s, 1H), 7.01 (s, 1H), 3.89 (s, 3H), 3.80 (s, 3H), 3.67 – 3.59 (m, 2H), 3.47 – 3.29 (m, 4H), 2.70 – 2.60 (m, 2H), 1.67 – 1.51 (m, 2H), 1.38 – 1.21 (m, 18H), 0.76 (s, 3H). **^{13}C NMR** (151 MHz, Acetone-d_6). δ 187.8, 156.8, 151.8, 140.8, 123.0, 114.4, 107.5, 68.1, 55.9, 55.3, 39.0, 34.1, 30.7, 29.63, 29.56, 29.59, 29.5, 29.43, 29.36, 23.2, 18.3. **HRMS** (ESI): m/z calculated for $C_{24}H_{40}NaO_5^+$ $[M + Na]^+$ 431.2768, found 431.2764.



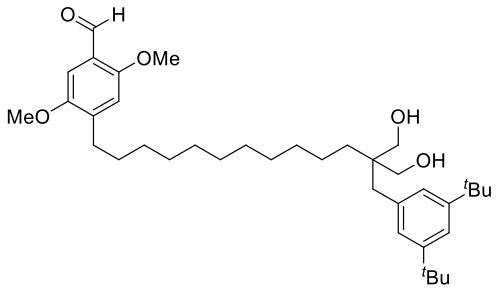
27-1, colorless oil. 67% yield, 324 mg. **^{1}H NMR** (600 MHz, DMSO-d_6). δ 10.24 (s, 1H), 7.22 – 7.17 (m, 2H), 7.16 – 7.12 (m, 2H), 7.13 – 7.09 (m, 2H), 7.00 (s, 1H), 4.34 (t, J = 4.87 Hz, 2H), 3.82 (s, 3H), 3.72 (s, 3H), 3.13 – 3.07 (m, 4H), 2.59 – 2.50 (m, 2H), 2.44 (s, 2H), 1.52 – 1.43 (m, 2H), 1.29 – 1.14 (m, 14H), 1.14 – 1.08 (m, 2H), 1.01 – 0.89 (m, 2H). **^{13}C NMR** (151 MHz, DMSO-d_6). δ 188.7, 156.8, 151.7, 141.0, 139.1, 130.9, 128.1, 126.1, 122.7, 115.1, 108.0, 63.2, 56.8, 56.2, 43.3, 37.0, 31.3, 30.8, 30.7, 29.6, 29.51, 29.47, 29.4, 22.9. **HRMS** (ESI): m/z calculated for $C_{30}H_{44}NaO_5^+$ $[M + Na]^+$ 507.3081, found 507.3084.



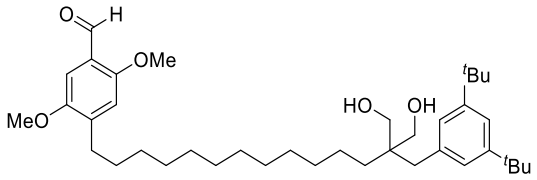
28-1, colorless oil. 81% yield, 433 mg. **^{1}H NMR** (600 MHz, Acetone-d_6). δ 10.34 (s, 1H), 7.81 – 7.65 (m, 4H), 7.53 – 7.33 (m, 3H), 7.19 (s, 1H), 6.99 (s, 1H), 3.94 – 3.83 (m, 5H), 3.79 (s, 3H), 3.49 – 3.41 (m, 4H), 2.82 (s, 2H), 2.69 – 2.62 (m, 2H), 1.64 – 1.53 (m, 2H), 1.50 – 1.40 (m, 2H), 1.37 – 1.15 (m, 16H). **^{13}C NMR** (151 MHz, Acetone-d_6). δ 187.9, 156.8, 151.8, 140.9, 136.6, 133.6, 132.2, 129.5, 128.9, 127.5, 127.0, 125.8, 123.0, 114.4, 107.6, 65.3, 55.9, 55.3, 43.2, 36.9, 31.2, 30.72, 30.67, 30.6, 30.5, 29.6, 29.54, 29.53, 29.49, 22.9. **HRMS** (ESI): m/z calculated for $C_{34}H_{46}NaO_5^+$ $[M + Na]^+$ 557.3247, found 557.3230.



29-1, colorless oil. 82% yield, 453 mg. **^{1}H NMR** (600 MHz, $CDCl_3$). δ 10.38 (s, 1H), 7.51 (d, J = 7.90 Hz, 2H), 7.33 (d, J = 7.89 Hz, 2H), 7.25 (s, 1H), 6.77 (s, 1H), 3.88 (s, 3H), 3.80 (s, 3H), 3.60 (dd, J = 10.65, 3.50 Hz, 2H), 3.50 (dd, J = 10.68, 4.80 Hz, 2H), 2.77 (s, 2H), 2.62 (dd, J = 8.68, 6.88 Hz, 2H), 2.36 (s, 2H), 1.65 (s, 2H), 1.61 – 1.53 (m, 2H), 1.37 – 1.24 (m, 14H), 1.12 – 1.07 (m, 2H). **^{13}C NMR** (151 MHz, $CDCl_3$). δ 187.8, 156.8, 151.8, 143.9, 140.8, 131.3, 127.5 (q, $J_{C\text{-}F}$ = 31.98 Hz), 124.8 (q, $J_{C\text{-}F}$ = 270.70 Hz), 124.5 (q, $J_{C\text{-}F}$ = 3.90 Hz), 123.0, 114.5, 107.6, 64.6, 64.5, 55.9, 55.3, 43.1, 36.6, 31.2, 30.7, 30.5, 29.5, 29.5, 29.3, 22.8. **^{19}F NMR** (565 MHz, Acetone-d_6) δ –62.6. **HRMS** (ESI): m/z calculated for $C_{31}H_{43}F_3NaO_5^+$ $[M + Na]^+$ 575.2955, found 575.2960.

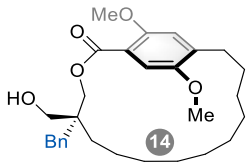


30-1, colorless oil. 57% yield, 340 mg. **^{1}H NMR** (600 MHz, $CDCl_3$). δ 10.40 (s, 1H), 7.25 (s, 2H), 7.01 (s, 2H), 6.78 (s, 1H), 3.88 (s, 3H), 3.80 (s, 3H), 3.60 – 3.53 (m, 4H), 2.67 – 2.58 (m, 4H), 2.14 (t, J = 5.22 Hz, 2H), 1.63 – 1.53 (m, 4H), 1.36 – 1.25 (m, 32H). **^{13}C NMR** (151 MHz, $CDCl_3$). δ 189.4, 156.8, 151.8, 150.5, 141.4, 136.8, 124.6, 122.9, 120.0, 113.9, 108.2, 68.9, 56.3, 55.9, 42.6, 38.0, 34.8, 31.6, 31.3, 31.1, 30.7, 29.84, 29.78, 29.7, 29.6, 29.5, 23.3. **HRMS** (ESI): m/z calculated for $C_{38}H_{60}NaO_5^+$ $[M + Na]^+$ 619.4333, found 619.4337.

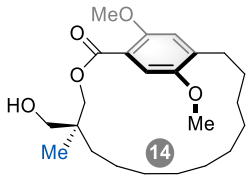


31-1, colorless oil. 67% yield, 409 mg. **^{1}H NMR** (600 MHz, $CDCl_3$). δ 10.33 (s, 1H), 7.25 (s, 1H), 7.19 (s, 1H), 7.11 (s, 2H), 7.02 (s, 1H), 3.89 (s, 3H), 3.80 (s, 3H), 3.73 (t, J = 4.95 Hz, 1H), 3.48 – 3.35 (m, 4H), 2.68 – 2.61 (m, 2H), 2.60 (s, 2H), 1.62 – 1.54 (m, 2H), 1.44 – 1.35 (m, 2H), 1.34 – 1.26 (m, 37H). **^{13}C NMR** (151 MHz, $CDCl_3$). δ 187.8, 170.1, 156.8, 151.8, 149.7, 140.8, 137.5, 124.9, 123.0, 119.3, 114.4, 107.5, 65.7, 65.6, 59.7, 55.9, 55.3, 42.7, 36.9, 34.4, 31.1, 30.9, 30.8, 30.7, 29.8, 29.7, 29.59, 29.56, 29.5, 29.44, 29.36, 23.0, 20.0, 13.7. **HRMS** (ESI): m/z calculated for $C_{39}H_{62}NaO_5^+$ $[M + Na]^+$ 633.4489, found 633.4495.

b) Characterization data of cyclophanes

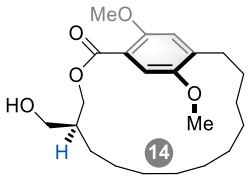


2, colorless oil. 73% yield, 19:1 dr, 98% *ee*. **^{1}H NMR** (600 MHz, $CDCl_3$). δ 7.31 – 7.27 (m, 5H), 7.24 – 7.21 (m, 1H), 6.81 (s, 1H), 4.25 (d, J = 11.28 Hz, 1H), 4.08 (d, J = 11.27 Hz, 1H), 3.90 (s, 3H), 3.81 (s, 3H), 3.44 (dd, J = 11.12, 4.18 Hz, 1H), 3.37 (dd, J = 11.22, 3.95 Hz, 1H), 3.16 (ddd, J = 12.94, 7.17, 3.84 Hz, 1H), 2.88 (d, J = 13.26 Hz, 1H), 2.69 (d, J = 13.21 Hz, 1H), 2.30 (ddd, J = 13.24, 9.49, 4.05 Hz, 1H), 1.79 – 1.69 (m, 2H), 1.66 – 1.59 (m, 2H), 1.35 – 1.25 (m, 4H), 1.22 – 1.10 (m, 3H), 1.03 – 0.93 (m, 2H), 0.90 – 0.80 (m, 4H), 0.72 – 0.62 (m, 1H), 0.58 – 0.47 (m, 1H). **^{13}C NMR** (151 MHz, $CDCl_3$). δ 167.0, 153.7, 151.6, 138.1, 137.8, 130.6, 128.3, 126.4, 117.9, 115.6, 113.3, 66.7, 64.6, 56.7, 56.0, 42.8, 38.7, 35.5, 32.6, 31.4, 29.9, 29.6, 28.9, 28.7, 28.6, 28.0, 26.9, 22.7. **HRMS** (ESI): m/z calculated for $C_{29}H_{40}NaO_5^+$ $[M + Na]^+$ 491.2768, found 491.2772. $[\alpha]_D^{25}$ = +37.5 (c = 0.34, CH_2Cl_2). **HPLC**: Chiralpak IF column, 80:20 hexanes/isopropanol, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 8.02 min (major), 14.50 min (minor).

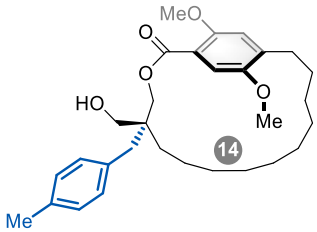


3, colorless oil. 60% yield, >20:1 dr, 97% *ee*. **^{1}H NMR** (400 MHz, $CDCl_3$). δ 7.29 (s, 1H), 6.80 (s, 1H), 4.22 (d, J = 11.32 Hz, 1H), 4.12 (d, J = 11.25 Hz, 1H), 3.88 (s, 3H), 3.82 (s, 3H), 3.57 (dd, J =

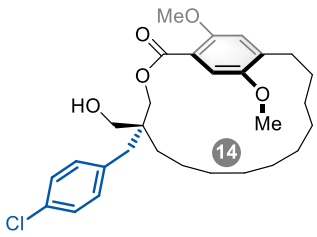
10.96, 6.17 Hz, 1H), 3.45 (dd, *J* = 10.98, 5.94 Hz, 1H), 3.15 (ddd, *J* = 12.95, 7.24, 3.79 Hz, 1H), 2.29 (ddd, *J* = 13.19, 9.37, 4.08 Hz, 1H), 1.85 – 1.71 (m, 2H), 1.64 – 1.59 (m, 1H), 1.33 – 1.24 (m, 3H), 1.21 – 1.07 (m, 5H), 0.99 (s, 3H), 0.96 – 0.78 (m, 6H), 0.66 – 0.51 (m, 1H). **^{13}C NMR** (151 MHz, $CDCl_3$). δ 166.4, 153.8, 151.4, 138.2, 117.4, 115.6, 113.1, 69.2, 68.0, 56.8, 55.9, 39.2, 34.5, 31.4, 29.9, 29.6, 29.0, 28.7, 28.5, 28.0, 26.8, 22.7, 20.0. **HRMS** (ESI): m/z calculated for $C_{23}H_{36}NaO_5^+$ $[M + Na]^+$ 415.2455, found 415.2459. $[\alpha]_D^{25}$ = +80.6 (c = 0.57, CH_2Cl_2). **HPLC**: Chiralpak IF column, 80:20 hexanes/isopropanol, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 9.65 min (major), 13.86 min (minor).



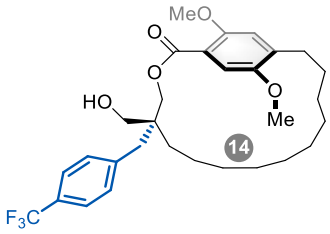
4, colorless oil. 77% yield, 10:1 dr, 97% *ee*. **^{1}H NMR** (600 MHz, $CDCl_3$). δ 7.30 (s, 1H), 6.79 (s, 1H), 4.70 (ddd, *J* = 11.14, 3.56, 1.61 Hz, 1H), 4.13 (ddd, *J* = 11.23, 7.59, 1.69 Hz, 1H), 3.88 (s, 3H), 3.82 (s, 3H), 3.69 – 3.63 (m, 1H), 3.58 (t, *J* = 9.33 Hz, 1H), 3.14 (dddd, *J* = 12.75, 7.06, 3.82, 1.53 Hz, 1H), 2.28 (ddd, *J* = 13.34, 9.19, 4.08 Hz, 1H), 2.06 – 1.97 (m, 1H), 1.79 – 1.71 (m, 1H), 1.60 – 1.52 (m, 1H), 1.45 – 1.33 (m, 2H), 1.30 – 1.18 (m, 4H), 1.18 – 1.01 (m, 3H), 1.00 – 0.91 (m, 3H), 0.83 – 0.73 (m, 3H), 0.70 – 0.62 (m, 1H). **^{13}C NMR** (151 MHz, $CDCl_3$). δ 166.1, 153.8, 151.4, 138.0, 116.0, 113.0, 65.8, 64.8, 56.9, 55.9, 40.3, 31.0, 29.6, 29.4, 29.3, 28.7, 28.6, 28.1, 26.6, 26.51, 26.47. **HRMS** (ESI): m/z calculated for $C_{22}H_{34}NaO_5^+$ $[M + Na]^+$ 401.2298, found 401.2294. $[\alpha]_D^{25}$ = +31.2 (c = 0.32, CH_2Cl_2). **HPLC**: Chiralpak IB N-5 column, 90:10 hexanes/isopropanol, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 18.72 min (major), 11.88 min (minor).



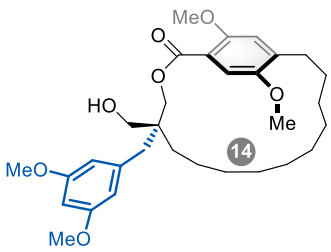
5, colorless oil, 71% yield, 17:1 dr, 99% *ee*, **^{1}H NMR** (400 MHz, $CDCl_3$). δ 7.29 (s, 1H), 7.19 – 7.02 (m, 4H), 6.81 (s, 1H), 4.24 (d, *J* = 11.29 Hz, 1H), 4.08 (d, *J* = 11.29 Hz, 1H), 3.90 (s, 3H), 3.81 (s, 3H), 3.47 – 3.34 (m, 2H), 3.15 (ddd, *J* = 12.94, 7.05, 3.78 Hz, 1H), 2.83 (d, *J* = 13.32 Hz, 1H), 2.64 (d, *J* = 13.33 Hz, 1H), 2.33 (s, 3H), 2.30 – 2.26 (m, 1H), 1.79 – 1.67 (m, 1H), 1.37 – 1.23 (m, 6H), 1.20 – 1.10 (m, 4H), 1.04 – 0.82 (m, 5H), 0.74 – 0.61 (m, 1H), 0.59 – 0.47 (m, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$). δ 166.9, 153.7, 151.5, 138.1, 135.9, 134.5, 130.4, 129.1, 117.7, 115.5, 113.2, 66.7, 64.7, 56.7, 56.0, 42.7, 38.3, 32.5, 31.4, 29.9, 29.6, 28.9, 28.7, 28.5, 28.0, 26.9, 22.6, 21.1. **HRMS** (ESI): m/z calculated for $C_{30}H_{42}NaO_5^+$ $[M + Na]^+$ 505.2924, found 505.2926. $[\alpha]_D^{25}$ = +77.1 (c = 0.28, CH_2Cl_2). **HPLC**: Chiralpak IB N-5 column, 90:10 hexanes/isopropanol, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 7.98 min (major), 12.36 min (minor).



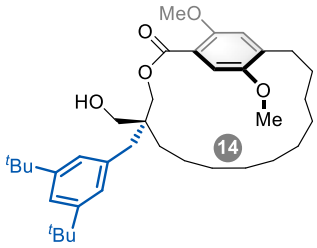
6, colorless oil. 63% yield, 13:1 dr, 97% *ee*. **^{1}H NMR** (600 MHz, $CDCl_3$). δ 7.32 – 7.16 (m, 5H), 6.80 (s, 1H), 4.22 (d, J = 11.26 Hz, 1H), 3.99 (d, J = 11.24 Hz, 1H), 3.88 (s, 3H), 3.79 (s, 3H), 3.38 (dd, J = 11.06, 5.16 Hz, 1H), 3.29 (dd, J = 11.03, 5.11 Hz, 1H), 3.14 (ddd, J = 12.94, 7.09, 3.82 Hz, 1H), 2.84 (d, J = 13.22 Hz, 1H), 2.63 (d, J = 13.25 Hz, 1H), 2.28 (ddd, J = 13.22, 9.53, 4.04 Hz, 1H), 1.87 – 1.78 (m, 1H), 1.76 – 1.66 (m, 1H), 1.62 – 1.55 (m, 1H), 1.36 – 1.22 (m, 3H), 1.19 – 1.05 (m, 4H), 1.03 – 0.88 (m, 2H), 0.89 – 0.76 (m, 4H), 0.70 – 0.62 (m, 1H), 0.55 – 0.47 (m, 1H). **^{13}C NMR** (151 MHz, $CDCl_3$). δ 167.0, 153.6, 151.5, 138.2, 136.2, 132.0, 128.4, 117.6, 115.4, 113.2, 66.4, 64.0, 56.6, 56.0, 42.8, 37.7, 32.3, 31.4, 29.8, 29.6, 28.9, 28.7, 28.5, 28.0, 26.9, 22.6. **HRMS** (ESI): m/z calculated for $C_{29}H_{39}ClNaO_5^+$ $[M + Na]^+$ 525.2378, found 525.2374. $[\alpha]_D^{25}$ = +9.5 (c = 0.13, CH_2Cl_2). **HPLC**: Chiralpak IB N-5 column, 90:10 hexanes/isopropanol, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 14.16 min (major), 23.47 min (minor).



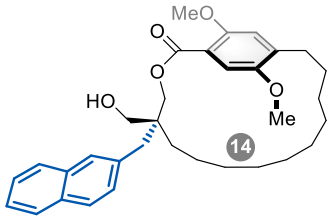
7, colorless oil. 56% yield, 16:1 dr, 98% *ee*. **^{1}H NMR** (600 MHz, $CDCl_3$). δ 7.56 (dd, J = 8.37, 3.22 Hz, 2H), 7.42 (dd, J = 8.95, 2.93 Hz, 2H), 7.28 (s, 1H), 6.82 (s, 1H), 4.35 – 4.21 (m, 1H), 4.01 (dd, J = 11.17, 3.58 Hz, 1H), 3.91 (s, 3H), 3.81 (s, 3H), 3.40 (dd, J = 10.57, 4.68 Hz, 1H), 3.31 (dd, J = 10.99, 4.70 Hz, 1H), 3.16 (ddt, J = 12.78, 7.02, 3.05 Hz, 1H), 2.96 (dd, J = 13.03, 3.30 Hz, 1H), 2.30 (ddd, J = 13.20, 9.47, 4.07 Hz, 1H), 1.86 – 1.82 (m, 1H), 1.77 – 1.69 (m, 1H), 1.66 – 1.57 (m, 1H), 1.39 – 1.24 (m, 1H), 1.20 – 1.10 (m, 4H), 1.03 – 0.98 (m, 3H), 0.98 – 0.91 (m, 2H), 0.90 – 0.80 (m, 4H), 0.72 – 0.64 (m, 1H), 0.56 – 0.49 (m, 1H). **^{13}C NMR** (151 MHz, $CDCl_3$). δ 167.0, 153.6, 151.5, 142.0, 138.3, 131.0, 128.7 (q, $J_{C\text{-}F}$ = 32.29 Hz), 125.1 (q, $J_{C\text{-}F}$ = 3.93 Hz), 124.4 (q, $J_{C\text{-}F}$ = 272.06 Hz), 117.5, 115.4, 113.2, 66.3, 63.8, 56.6, 56.0, 42.9, 38.1, 32.3, 31.4, 29.8, 29.6, 28.9, 28.7, 28.5, 28.0, 26.9, 22.6. **^{19}F NMR** (565 MHz, $CDCl_3$) δ –62.2. **HRMS** (ESI): m/z calculated for $C_{30}H_{39}F_3NaO_5^+$ $[M + Na]^+$ 559.2642, found 559.2648. $[\alpha]_D^{25}$ = +47.1 (c = 0.26, CH_2Cl_2). **HPLC**: Chiralpak IB N-5 column, 90:10 hexanes/isopropanol, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 10.12 min (major), 14.65 min (minor).



8, colorless oil. 46% yield, >20:1 dr, 95% *ee*. **^{1}H NMR** (400 MHz, $CDCl_3$). δ 7.28 (s, 1H), 6.81 (s, 1H), 6.47 (d, J = 2.33 Hz, 2H), 6.35 (t, J = 2.46 Hz, 1H), 4.20 (d, J = 11.23 Hz, 1H), 4.11 (d, J = 11.27 Hz, 1H), 3.90 (s, 3H), 3.81 (s, 3H), 3.77 (s, 6H), 3.43 (qd, J = 11.05, 4.83 Hz, 2H), 3.15 (ddd, J = 12.93, 7.00, 3.78 Hz, 1H), 2.83 (d, J = 13.10 Hz, 1H), 2.63 (d, J = 13.13 Hz, 1H), 2.30 (ddd, J = 13.21, 9.46, 4.09 Hz, 1H), 1.72 (td, J = 8.84, 4.34 Hz, 1H), 1.38 – 1.23 (m, 5H), 1.20 – 1.07 (m, 4H), 1.06 – 0.92 (m, 2H), 0.90 – 0.76 (m, 4H), 0.74 – 0.63 (m, 1H), 0.59 – 0.47 (m, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$). δ 167.0, 160.7, 153.6, 151.5, 140.2, 138.0, 117.8, 115.4, 113.2, 108.6, 98.4, 66.7, 64.9, 56.6, 56.0, 55.4, 42.8, 39.1, 32.9, 31.4, 29.9, 29.7, 28.9, 28.7, 28.6, 27.9, 26.9, 22.6. **HRMS** (ESI): m/z calculated for $C_{31}H_{44}NaO_7^+$ $[M + Na]^+$ 551.2979, found 551.2974. $[\alpha]_D^{25}$ = +24.0 (c = 0.44, CH_2Cl_2). **HPLC**: Chiralpak IB N-5 column, 90:10 hexanes/isopropanol, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 11.12 min (major), 19.63 min (minor).

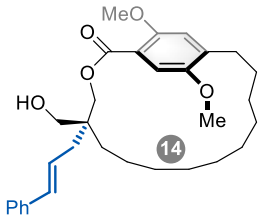


9, colorless oil. 47% yield, 16:1 dr, 96% *ee*. **^{1}H NMR** (400 MHz, $CDCl_3$). δ 7.29 (s, 1H), 7.28 (s, 1H), 7.14 (s, 1H), 7.13 (s, 1H), 6.82 (s, 1H), 4.22 – 4.07 (m, 2H), 3.91 (s, 3H), 3.80 (s, 3H), 3.48 – 3.34 (m, 2H), 3.16 (ddd, J = 12.83, 7.19, 3.83 Hz, 1H), 2.87 (d, J = 13.19 Hz, 1H), 2.68 (d, J = 13.24 Hz, 1H), 2.30 (ddd, J = 13.06, 9.25, 3.95 Hz, 1H), 1.77 – 1.69 (m, 2H), 1.66 – 1.50 (m, 4H), 1.31 (s, 18H), 1.19 – 1.08 (m, 4H), 1.04 – 0.93 (m, 2H), 0.92 – 0.78 (m, 4H), 0.75 – 0.63 (m, 1H), 0.58 – 0.48 (m, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$). δ 166.9, 153.7, 151.4, 150.7, 138.0, 136.7, 124.7, 120.1, 117.8, 115.3, 113.2, 66.7, 65.2, 56.5, 55.9, 42.7, 39.1, 34.8, 32.7, 31.6, 29.9, 29.7, 28.9, 28.7, 28.6, 28.0, 26.9, 22.6. **HRMS** (ESI): m/z calculated for $C_{37}H_{56}NaO_5^+$ $[M + Na]^+$ 603.4020, found 603.4025. $[\alpha]_D^{25}$ = +10.1 (c = 0.17, CH_2Cl_2). **HPLC**: Chiralpak IF column, 90:10 hexanes/isopropanol, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 8.01 min (major), 13.33 min (minor).

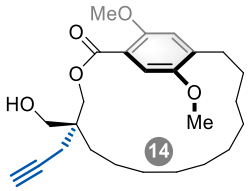


10, colorless oil. 63% yield, >20:1 dr, 96% *ee*. **^{1}H NMR** (600 MHz, $CDCl_3$). δ 7.84 – 7.76 (m, 3H), 7.72 (s, 1H), 7.49 – 7.40 (m, 3H), 7.30 (s, 1H), 6.83 (s, 1H), 4.38 – 4.09 (m, 2H), 3.92 (s, 3H), 3.81 (s, 3H), 3.53 – 3.37 (m, 2H), 3.16 (ddd, J = 12.87, 7.14, 3.78 Hz, 1H), 3.09 – 2.82 (m, 2H), 2.30 (ddd, J = 13.26, 9.49, 4.05 Hz, 1H), 1.78 – 1.68 (m, 2H), 1.65 – 1.56 (m, 1H), 1.53 – 1.33 (m, 2H), 1.32 – 1.24 (m, 1H), 1.23 – 1.09 (m, 4H), 1.05 – 0.93 (m, 2H), 0.91 – 0.82 (m, 4H), 0.75 – 0.64 (m, 1H), 0.60 – 0.49 (m, 1H). **^{13}C NMR** (151 MHz, $CDCl_3$). δ 167.0, 153.7, 151.5, 138.2, 135.4, 133.6, 132.3, 129.2, 129.0, 127.8, 127.7, 126.1, 125.6, 117.7, 115.5, 113.2, 66.7, 64.6, 56.7, 56.1, 43.2, 38.7, 32.6, 31.5, 29.9, 29.7, 29.0, 28.8, 28.6, 28.0, 26.9, 22.7. **HRMS** (ESI): m/z calculated for $C_{33}H_{42}NaO_5^+$ $[M + Na]^+$ 541.2924, found 541.2928. $[\alpha]_D^{25}$ = +2.6 (c = 0.08, CH_2Cl_2). **HPLC**:

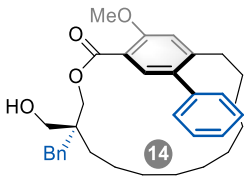
Chiralpak IF column, 80:20 hexanes/isopropanol, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 10.68 min (major), 15.15 min (minor).



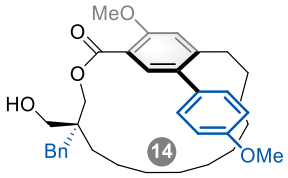
11, colorless oil. 47% yield, 19:1 dr, 97% *ee*. **^{1}H NMR** (600 MHz, $CDCl_3$). δ 7.37 (d, J = 8.18 Hz, 2H), 7.33 – 7.28 (m, 3H), 7.23 (d, J = 7.90 Hz, 1H), 6.80 (s, 1H), 6.50 (d, J = 15.59 Hz, 1H), 6.29 (dt, J = 16.33, 7.98 Hz, 1H), 4.28 (dd, J = 11.35, 3.45 Hz, 1H), 4.21 (dd, J = 11.40, 3.40 Hz, 1H), 3.88 (s, 3H), 3.81 (s, 3H), 3.59 (d, J = 11.53 Hz, 1H), 3.54 (d, J = 10.84 Hz, 1H), 3.14 (dt, J = 11.61, 5.27 Hz, 1H), 2.41 (dd, J = 14.30, 7.70 Hz, 1H), 2.34 – 2.24 (m, 2H), 1.87 – 1.68 (m, 2H), 1.38 – 1.22 (m, 4H), 1.19 – 1.06 (m, 4H), 1.04 – 0.97 (m, 1H), 0.95 – 0.78 (m, 5H), 0.68 – 0.61 (m, 1H), 0.58 – 0.47 (m, 1H). **^{13}C NMR** (151 MHz, $CDCl_3$). δ 166.6, 153.7, 151.4, 138.2, 137.4, 133.3, 128.6, 127.3, 126.2, 125.7, 117.5, 115.5, 113.1, 67.1, 66.0, 56.7, 56.0, 42.6, 36.5, 32.2, 31.5, 30.0, 29.6, 29.0, 28.7, 28.5, 27.9, 26.8, 22.6. **HRMS** (ESI): m/z calculated for $C_{31}H_{42}NaO_5^+$ $[M + Na]^+$ 517.2924, found 517.2920. $[\alpha]_D^{25}$ = +45.9 (c = 0.37, CH_2Cl_2). **HPLC**: Chiralpak IB N-5 column, 80:20 hexanes/isopropanol, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 10.21 min (major), 17.75 min (minor).



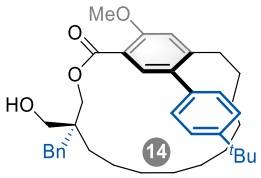
12, colorless oil. 69% yield, 19:1 dr, 97% *ee*. **^{1}H NMR** (600 MHz, $CDCl_3$). δ 7.29 (s, 1H), 6.79 (s, 1H), 4.28 (d, J = 11.32 Hz, 1H), 4.21 (d, J = 11.27 Hz, 1H), 3.87 (s, 3H), 3.81 (s, 3H), 3.65 (s, 2H), 3.15 (ddd, J = 12.92, 6.98, 3.82 Hz, 1H), 2.44 (dd, J = 16.82, 2.68 Hz, 1H), 2.35 (dd, J = 16.82, 2.70 Hz, 1H), 2.28 (ddd, J = 13.35, 9.57, 4.13 Hz, 1H), 2.04 (t, J = 2.70 Hz, 1H), 1.89 (s, 1H), 1.71 (tdd, J = 13.71, 7.08, 3.97 Hz, 1H), 1.64 – 1.54 (m, 1H), 1.45 – 1.39 (m, 1H), 1.35 (ddd, J = 13.71, 11.11, 4.67 Hz, 1H), 1.31 – 1.24 (m, 1H), 1.21 – 1.07 (m, 4H), 1.02 (ddd, J = 13.15, 6.51, 3.73 Hz, 1H), 0.95 – 0.88 (m, 1H), 0.87 – 0.77 (m, 4H), 0.72 – 0.63 (m, 1H), 0.55 – 0.45 (m, 1H).**^{13}C NMR** (101 MHz, $CDCl_3$). δ 166.6, 153.7, 151.5, 138.2, 117.4, 115.5, 113.2, 81.0, 70.9, 66.5, 65.4, 56.7, 56.0, 41.9, 32.0, 31.4, 29.8, 29.6, 28.9, 28.7, 28.5, 27.9, 26.8, 23.0, 22.6. **HRMS** (ESI): m/z calculated for $C_{25}H_{36}NaO_5^+$ $[M + Na]^+$ 439.2455, found 439.2459. $[\alpha]_D^{25}$ = +50.4 (c = 0.38, CH_2Cl_2). **HPLC**: Chiralpak IF column, 80:20 hexanes/isopropanol, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 10.91 min (major), 26.60 min (minor).



13, colorless oil. 63% yield, >20:1 dr, 98% *ee*. **^{1}H NMR** (600 MHz, $CDCl_3$). δ 7.70 (s, 1H), 7.41 – 7.36 (m, 2H), 7.34 – 7.29 (m, 3H), 7.29 – 7.25 (m, 4H), 7.24 – 7.19 (m, 1H), 6.91 (s, 1H), 4.23 – 4.11 (m, 2H), 3.97 (s, 3H), 3.44 (d, J = 11.04 Hz, 2H), 3.35 (d, J = 11.03 Hz, 1H), 3.08 – 2.97 (m, 1H), 2.87 (d, J = 13.26 Hz, 1H), 2.68 (d, J = 13.28 Hz, 1H), 2.52 (ddd, J = 13.08, 8.42, 3.98 Hz, 1H), 1.67 (s, 2H), 1.50 – 1.29 (m, 5H), 1.24 – 1.11 (m, 2H), 1.05 – 0.93 (m, 5H), 0.90 – 0.82 (m, 2H), 0.73 – 0.59 (m, 1H), 0.59 – 0.45 (m, 1H). **^{13}C NMR** (151 MHz, $CDCl_3$). δ 166.8, 158.3, 146.9, 140.8, 137.7, 134.7, 133.4, 130.6, 129.7, 128.3, 126.9, 126.4, 117.6, 113.8, 66.7, 64.4, 56.1, 42.8, 38.5, 34.0, 32.6, 30.0, 29.5, 28.8, 28.3, 27.7, 27.5, 22.7. **HRMS** (ESI): m/z calculated for $C_{34}H_{42}NaO_4^+$ $[M + Na]^+$ 537.2975, found 537.2971. $[\alpha]_D^{25}$ = +15.1 (c = 0.34, CH_2Cl_2). **HPLC**: Chiralpak AD-H column, 90:10 hexanes/isopropanol, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 9.81 min (major), 18.56 min (minor).

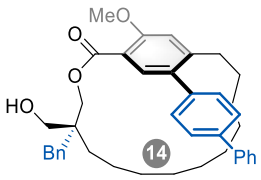


14, white solid. 61% yield, >20:1 dr, 97% *ee*. **^{1}H NMR** (600 MHz, $CDCl_3$). δ 7.68 (s, 1H), 7.32 – 7.27 (m, 4H), 7.24 – 7.19 (m, 3H), 6.93 (d, J = 8.63 Hz, 2H), 6.90 (s, 1H), 4.20 (d, J = 11.23 Hz, 1H), 4.15 (d, J = 11.43 Hz, 1H), 3.97 (s, 3H), 3.85 (s, 3H), 3.45 (dd, J = 11.07, 4.46 Hz, 1H), 3.36 (dd, J = 11.07, 4.32 Hz, 1H), 3.03 (ddd, J = 13.26, 8.25, 3.74 Hz, 1H), 2.87 (d, J = 13.24 Hz, 1H), 2.69 (d, J = 13.26 Hz, 1H), 2.51 (ddd, J = 13.00, 8.32, 3.86 Hz, 1H), 1.64 (s, 1H), 1.60 (s, 1H), 1.45 – 1.30 (m, 5H), 1.27 – 1.16 (m, 2H), 1.07 – 0.95 (m, 5H), 0.89 – 0.84 (m, 2H), 0.71 – 0.61 (m, 1H), 0.57 – 0.48 (m, 1H). **^{13}C NMR** (151 MHz, $CDCl_3$). δ 166.8, 158.7, 158.1, 147.0, 137.7, 134.4, 133.4, 133.2, 130.7, 130.6, 128.3, 126.4, 117.6, 113.8, 66.7, 64.5, 56.1, 55.4, 42.8, 38.6, 34.0, 32.7, 30.0, 29.5, 28.82, 28.78, 28.3, 27.7, 27.5, 22.7. **HRMS** (ESI): m/z calculated for $C_{35}H_{44}NaO_5^+$ $[M + Na]^+$ 567.3081, found 567.3085. $[\alpha]_D^{25}$ = +28.1 (c = 0.63, CH_2Cl_2). **HPLC**: Chiralpak IF column, 80:20 hexanes/isopropanol, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 9.69 min (major), 18.18 min (minor).

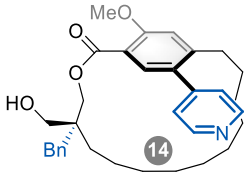


15, colorless oil. 76% yield, >20:1 dr, 97% *ee*. **^{1}H NMR** (400 MHz, $CDCl_3$). δ 7.71 (s, 1H), 7.43 – 7.38 (m, 2H), 7.32 – 7.26 (m, 4H), 7.26 – 7.19 (m, 3H), 6.91 (s, 1H), 4.23 – 4.12 (m, 2H), 3.97 (s, 3H), 3.46 (d, J = 11.13 Hz, 1H), 3.37 (d, J = 10.99 Hz, 1H), 3.11 – 3.01 (m, 1H), 2.87 (d, J = 13.24 Hz, 1H), 2.69 (d, J = 13.25 Hz, 1H), 2.53 (ddd, J = 12.91, 8.05, 3.92 Hz, 1H), 1.68 (s, 1H), 1.49 – 1.40 (m, 2H), 1.36 (s, 9H), 1.36 – 1.29 (m, 2H), 1.27 – 1.14 (m, 3H), 1.06 – 0.94 (m, 6H), 0.95 – 0.83 (m, 2H), 0.75 – 0.61 (m, 1H), 0.59 – 0.48 (m, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$). δ 166.7, 158.2, 149.7, 147.1, 137.8, 137.7, 134.7, 133.5, 130.6, 129.3, 128.3, 126.4, 125.2, 117.5, 113.7, 66.7, 64.5, 56.1, 42.8, 38.5, 34.6, 34.0, 32.6, 31.5, 30.0, 29.5, 28.8, 28.3, 27.8, 27.5, 22.7. **HRMS** (ESI): m/z calculated for $C_{38}H_{50}NaO_4^+$ $[M + Na]^+$ 593.3601, found 593.3601. $[\alpha]_D^{25}$ = +13.6 (c = 0.21, CH_2Cl_2). **HPLC**: Chiralpak IF column, 80:20 hexanes/isopropanol, flow rate = 1.0 mL/min, λ = 254

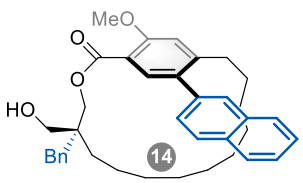
nm, t_R = 6.05 min (major), 12.19 min (minor).



16, colorless oil. 53% yield, 3:1 dr, 97% *ee*. **^{1}H NMR** (600 MHz, $CDCl_3$). δ 7.77 (s, 1H), 7.67 – 7.59 (m, 4H), 7.49 – 7.41 (m, 2H), 7.38 – 7.32 (m, 3H), 7.32 – 7.26 (m, 4H), 7.23 – 7.19 (m, 1H), 6.93 (s, 1H), 4.27 – 4.23 (m, 1H), 4.17 – 4.08 (m, 2H), 3.97 (s, 3H), 3.46 – 3.41 (m, 1H), 3.34 (dd, J = 11.24, 1.75 Hz, 1H), 3.04 (ddd, J = 13.58, 9.01, 3.45 Hz, 1H), 2.86 (dd, J = 13.14, 1.66 Hz, 1H), 2.66 (dd, J = 13.52, 1.96 Hz, 1H), 2.54 (ddd, J = 13.44, 8.67, 3.27 Hz, 1H), 1.67 (s, 2H), 1.47 – 1.34 (m, 3H), 1.31 – 1.23 (m, 2H), 1.22 – 1.17 (m, 1H), 1.15 – 1.09 (m, 1H), 1.06 – 0.98 (m, 2H), 0.98 – 0.92 (m, 4H), 0.92 – 0.85 (m, 2H). **^{13}C NMR** (151 MHz, $CDCl_3$). δ 166.5, 158.5, 147.0, 140.8, 139.9, 139.7, 137.7, 134.3, 133.6, 130.6, 130.0, 128.9, 128.3, 127.4, 127.1, 127.0, 126.4, 66.6, 64.5, 60.5, 56.1, 42.8, 38.3, 33.3, 32.7, 29.9, 29.6, 29.2, 28.7, 28.3, 28.2, 28.0, 26.3, 22.6, 14.3. **HRMS** (ESI): m/z calculated for $C_{40}H_{46}NaO_4^+$ $[M + Na]^+$ 613.3288, found 613.3295. $[\alpha]_D^{25}$ = -8.6 (c = 0.07, CH_2Cl_2). **HPLC**: Chiralpak IF column, 80:20 hexanes/isopropanol, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 14.00 min (major), 10.66 min (minor).

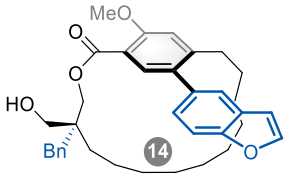


17, colorless oil. 41% yield, 10:1 dr, 96% *ee*. **^{1}H NMR** (600 MHz, $CDCl_3$). δ 8.64 (s, 2H), 7.71 (s, 1H), 7.31 – 7.27 (m, 4H), 7.27 – 7.21 (m, 3H), 6.94 (s, 1H), 4.27 (d, J = 11.17 Hz, 1H), 4.13 (dd, J = 11.34, 1.44 Hz, 1H), 3.99 (s, 3H), 3.43 (dd, J = 10.89, 1.57 Hz, 1H), 3.35 (d, J = 11.34 Hz, 1H), 2.93 (ddd, J = 13.62, 9.24, 3.51 Hz, 1H), 2.88 (d, J = 12.96 Hz, 1H), 2.69 (d, J = 13.18 Hz, 1H), 2.57 (ddd, J = 13.01, 8.67, 3.63 Hz, 1H), 2.10 – 1.77 (m, 2H), 1.42 – 1.29 (m, 4H), 1.26 – 1.17 (m, 2H), 1.15 – 1.07 (m, 2H), 1.01 – 0.92 (m, 5H), 0.91 – 0.81 (m, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$). δ 166.3, 159.1, 149.8, 146.7, 137.7, 133.2, 130.6, 128.3, 126.4, 124.7, 117.8, 114.2, 66.8, 64.4, 56.1, 42.7, 38.4, 33.1, 32.7, 29.9, 29.5, 29.2, 28.7, 28.3, 28.2, 27.9, 26.2, 22.6. **HRMS** (ESI): m/z calculated for $C_{33}H_{41}NNaO_4^+$ $[M + Na]^+$ 538.2928, found 538.2923. $[\alpha]_D^{25}$ = -18.0 (c = 0.07, CH_2Cl_2). **HPLC**: Chiralpak IF column, 80:20 hexanes/isopropanol, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 20.43 min (major), 28.16 min (minor).

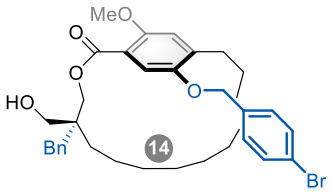


18, colorless oil. 59% yield, >20:1 dr, 95% *ee*. **^{1}H NMR** (600 MHz, $CDCl_3$). δ 7.91 – 7.84 (m, 3H), 7.82 (s, 1H), 7.76 (d, J = 1.66 Hz, 1H), 7.55 – 7.48 (m, 2H), 7.45 (dd, J = 8.36, 1.67 Hz, 1H), 7.34

– 7.29 (m, 4H), 7.26 – 7.22 (m, 1H), 6.96 (s, 1H), 4.23 (d, J = 11.26 Hz, 1H), 4.15 (d, J = 11.25 Hz, 1H), 4.00 (s, 3H), 3.47 – 3.43 (m, 1H), 3.37 (dd, J = 11.09, 4.04 Hz, 1H), 3.09 (ddd, J = 12.66, 8.23, 3.78 Hz, 1H), 2.91 (d, J = 13.21 Hz, 1H), 2.71 (d, J = 13.23 Hz, 1H), 2.58 (ddd, J = 13.00, 8.38, 3.87 Hz, 1H), 1.67 (s, 1H), 1.63 (s, 1H), 1.46 – 1.36 (m, 3H), 1.34 – 1.26 (m, 2H), 1.25 – 1.18 (m, 2H), 1.09 – 0.97 (m, 5H), 0.95 – 0.87 (m, 2H), 0.77 – 0.67 (m, 1H), 0.61 – 0.51 (m, 1H). **^{13}C NMR** (151 MHz, $CDCl_3$). δ 166.8, 158.4, 147.1, 138.4, 137.8, 134.6, 133.6, 133.4, 132.4, 130.6, 128.3, 128.12, 128.08, 127.9, 127.8, 126.4, 126.3, 126.0, 117.8, 113.9, 66.8, 64.4, 56.1, 42.8, 38.6, 34.1, 32.9, 30.1, 29.5, 28.9, 28.8, 28.4, 27.8, 27.4, 22.8. **HRMS** (ESI): m/z calculated for $C_{38}H_{44}NaO_4^+$ $[M + Na]^+$ 587.3132, found 587.3138. $[\alpha]_D^{25}$ = +33.9 (c = 0.33, CH_2Cl_2). **HPLC**: Chiralpak IF column, 80:20 hexanes/isopropanol, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 9.55 min (major), 15.61 min (minor).

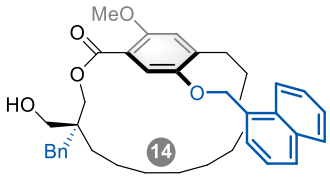


19, colorless oil. 56% yield, >20:1 dr, 98% *ee*. **^{1}H NMR** (600 MHz, $CDCl_3$). δ 7.86 (d, J = 1.08 Hz, 1H), 7.67 – 7.53 (m, 2H), 7.34 – 7.27 (m, 5H), 7.25 – 7.19 (m, 2H), 6.99 (s, 1H), 6.81 (dd, J = 2.25, 1.06 Hz, 1H), 4.26 – 4.13 (m, 2H), 4.01 (d, J = 1.08 Hz, 3H), 3.45 (d, J = 11.03 Hz, 1H), 3.35 (d, J = 11.06 Hz, 1H), 2.88 (d, J = 12.83 Hz, 1H), 2.79 (ddd, J = 12.77, 8.34, 3.66 Hz, 1H), 2.69 (d, J = 12.84 Hz, 1H), 2.60 (ddd, J = 12.97, 8.35, 3.86 Hz, 1H), 1.62 (s, 2H), 1.46 – 1.33 (m, 4H), 1.32 – 1.15 (m, 4H), 1.10 – 1.01 (m, 1H), 1.03 – 0.94 (m, 4H), 0.93 – 0.86 (m, 2H), 0.70 – 0.61 (m, 1H), 0.59 – 0.51 (m, 1H). **^{13}C NMR** (151 MHz, $CDCl_3$). δ 166.6, 158.8, 152.6, 148.3, 145.1, 137.7, 134.1, 130.6, 128.9, 128.3, 127.6, 126.4, 125.9, 124.9, 120.5, 117.8, 113.7, 106.9, 66.7, 64.4, 56.1, 42.8, 38.5, 34.5, 32.6, 30.0, 29.5, 28.80, 28.76, 28.4, 28.1, 27.5, 22.7. **HRMS** (ESI): m/z calculated for $C_{36}H_{42}NaO_5^+$ $[M + Na]^+$ 577.2924, found 577.2921. $[\alpha]_D^{25}$ = +35.9 (c = 0.66, CH_2Cl_2). **HPLC**: Chiralpak IF column, 80:20 hexanes/isopropanol, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 10.47 min (major), 14.97 min (minor).

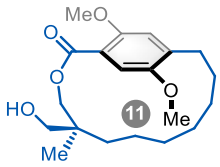


20, colorless oil. 71% yield, >20:1 dr, 97% *ee*. **^{1}H NMR** (400 MHz, $CDCl_3$). δ 7.50 (d, J = 8.36 Hz, 2H), 7.40 – 7.22 (m, 8H), 6.83 (s, 1H), 5.10 – 4.92 (m, 2H), 4.20 (d, J = 11.31 Hz, 1H), 4.08 (d, J = 11.35 Hz, 1H), 3.90 (s, 3H), 3.33 (q, J = 11.09 Hz, 2H), 3.20 (ddd, J = 12.84, 6.99, 3.78 Hz, 1H), 2.84 (d, J = 13.28 Hz, 1H), 2.68 (d, J = 13.17 Hz, 1H), 2.32 (ddd, J = 13.27, 9.45, 4.13 Hz, 1H), 1.91 – 1.56 (m, 4H), 1.34 – 1.25 (m, 3H), 1.20 – 1.06 (m, 4H), 1.04 – 0.89 (m, 2H), 0.89 – 0.77 (m, 4H), 0.73 – 0.63 (m, 1H), 0.59 – 0.48 (m, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$). δ 166.7, 153.9, 150.2, 138.5, 137.7, 136.4, 131.8, 130.6, 128.9, 128.3, 126.4, 121.8, 117.7, 115.5, 114.7, 70.0, 66.6, 64.5, 56.7, 42.7, 38.5, 32.2, 31.6, 29.9, 29.7, 29.0, 28.71, 28.66, 28.1, 27.0, 22.6. **HRMS** (ESI): m/z calculated for $C_{35}H_{43}BrNaO_5^+$ $[M + Na]^+$ 645.2186, found 645.2190. $[\alpha]_D^{25}$ = +106.8 (c = 0.47,

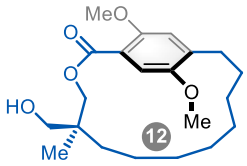
CH_2Cl_2). **HPLC**: Chiralpak IF column, 80:20 hexanes/isopropanol, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 9.83 min (major), 14.66 min (minor).



21, colorless oil. 46% yield, >20:1 dr, 99% *ee*. **^{1}H NMR** (400 MHz, $CDCl_3$). δ 8.18 – 8.01 (m, 1H), 7.97 – 7.79 (m, 2H), 7.61 (d, J = 7.00 Hz, 1H), 7.57 – 7.50 (m, 2H), 7.48 (s, 1H), 7.33 – 7.19 (m, 6H), 6.84 (s, 1H), 5.49 (d, J = 2.99 Hz, 2H), 4.18 (d, J = 11.24 Hz, 1H), 4.09 (d, J = 11.29 Hz, 1H), 3.91 (s, 3H), 3.32 – 3.12 (m, 3H), 2.84 (d, J = 13.20 Hz, 1H), 2.66 (d, J = 13.22 Hz, 1H), 2.28 (ddd, J = 13.25, 9.35, 4.13 Hz, 1H), 1.72 (tt, J = 9.21, 4.77 Hz, 1H), 1.60 – 1.49 (m, 1H), 1.43 – 1.41 (m, 2H), 1.35 – 1.21 (m, 4H), 1.18 – 1.03 (m, 4H), 1.07 – 0.97 (m, 1H), 0.91 – 0.79 (m, 4H), 0.75 – 0.64 (m, 1H), 0.63 – 0.49 (m, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$). δ 166.7, 153.9, 150.6, 138.6, 137.7, 133.8, 132.7, 131.4, 130.6, 128.83, 128.77, 128.3, 126.42, 126.36, 126.1, 126.0, 125.5, 123.8, 69.3, 66.7, 64.4, 56.7, 42.7, 38.6, 32.4, 31.4, 29.9, 29.6, 29.0, 28.8, 28.6, 28.0, 27.01, 26.97, 22.7. **HRMS** (ESI): m/z calculated for $C_{39}H_{46}NaO_5^+$ $[M + Na]^+$ 617.3237, found 617.3233. $[\alpha]_D^{25}$ = +60.3 (c = 0.64, CH_2Cl_2). **HPLC**: Chiralpak IF column, 80:20 hexanes/isopropanol, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 7.51 min (major), 22.76 min (minor).

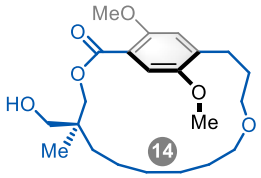


22, colorless oil. 43% yield, 13:1 dr, 90% *ee*. **^{1}H NMR** (600 MHz, $CDCl_3$). δ 7.10 (s, 1H), 6.80 (s, 1H), 4.16 (dd, J = 11.36, 1.14 Hz, 1H), 4.13 – 4.01 (m, 1H), 3.86 (s, 3H), 3.80 (s, 3H), 3.51 – 3.42 (m, 1H), 3.38 (dd, J = 11.03, 1.14 Hz, 1H), 3.18 – 3.11 (m, 1H), 2.37 – 2.29 (m, 1H), 1.72 – 1.63 (m, 1H), 1.55 – 1.46 (m, 1H), 1.29 – 1.25 (m, 1H), 1.11 – 1.03 (m, 2H), 1.02 – 0.96 (m, 1H), 0.92 – 0.86 (m, 1H), 0.85 – 0.75 (m, 2H), 0.73 (s, 3H), 0.71 – 0.62 (m, 1H), 0.42 – 0.28 (m, 2H). **^{13}C NMR** (151 MHz, $CDCl_3$). δ 170.0, 152.5, 152.4, 137.2, 119.5, 115.5, 113.5, 74.2, 69.9, 56.6, 56.2, 39.9, 33.1, 30.3, 29.7, 29.2, 28.3, 26.4, 22.6, 18.7. **HRMS** (ESI): m/z calculated for $C_{20}H_{30}NaO_5^+$ $[M + Na]^+$ 373.1985, found 373.1989. $[\alpha]_D^{25}$ = +7.3 (c = 0.44, CH_2Cl_2). **HPLC**: Chiralpak IB N-5 column, 90:10 hexanes/isopropanol, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 6.52 min (major), 5.93 min (minor).

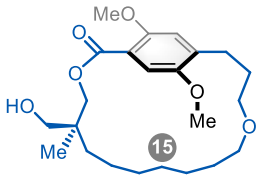


23, colorless oil. 56% yield, 6:1 dr, 93% *ee*. **^{1}H NMR** (600 MHz, $CDCl_3$). δ 7.23 (s, 1H), 6.77 (s, 1H), 4.36 (d, J = 11.15 Hz, 1H), 4.02 (d, J = 11.16 Hz, 1H), 3.87 (s, 3H), 3.81 (s, 3H), 3.50 (dd, J = 10.90, 5.62 Hz, 1H), 3.39 (dd, J = 10.99, 5.92 Hz, 1H), 3.17 – 3.07 (m, 1H), 2.24 (ddd, J = 13.26, 8.32, 5.17 Hz, 1H), 1.81 – 1.77 (m, 1H), 1.70 – 1.50 (m, 2H), 1.27 – 1.01 (m, 5H), 0.97 (s, 3H),

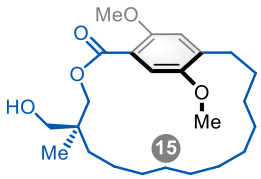
0.93 – 0.85 (m, 2H), 0.83 – 0.66 (m, 4H). **^{13}C NMR** (151 MHz, $CDCl_3$). δ 167.4, 153.3, 151.7, 137.3, 118.4, 116.3, 113.1, 69.7, 69.1, 57.0, 56.1, 39.5, 35.6, 30.3, 29.1, 29.0, 28.0, 27.3, 25.2, 24.0, 20.4. **HRMS** (ESI): m/z calculated for $C_{21}H_{32}NaO_5^+$ $[M + Na]^+$ 387.2142, found 387.2140. $[\alpha]_D^{25}$ = +86.9 (c = 0.52, CH_2Cl_2). **HPLC**: Chiralpak IB N-5 column, 90:10 hexanes/isopropanol, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 11.55 min (major), 9.81 min (minor).



24, colorless oil. 63% yield, 9:1 dr, 90% *ee*. **^{1}H NMR** (600 MHz, $CDCl_3$). δ 7.30 (s, 1H), 6.79 (s, 1H), 4.21 – 4.08 (m, 2H), 3.88 (s, 3H), 3.81 (s, 3H), 3.58 (dd, J = 10.94, 1.14 Hz, 1H), 3.51 – 3.44 (m, 2H), 3.36 (ddt, J = 9.56, 7.87, 1.61 Hz, 1H), 3.17 (ddd, J = 12.34, 7.88, 3.94 Hz, 1H), 3.00 – 2.93 (m, 2H), 2.37 (ddd, J = 13.08, 8.91, 3.92 Hz, 1H), 2.13 – 2.02 (m, 1H), 1.84 – 1.76 (m, 1H), 1.70 – 1.59 (m, 2H), 1.52 – 1.39 (m, 1H), 1.34 – 1.26 (m, 1H), 1.24 – 1.18 (m, 1H), 1.14 – 1.06 (m, 3H), 0.99 (s, 3H), 0.97 – 0.88 (m, 1H), 0.81 – 0.71 (m, 1H). **^{13}C NMR** (151 MHz, $CDCl_3$). δ 166.2, 154.0, 151.4, 138.3, 116.7, 115.2, 112.8, 71.6, 71.2, 69.5, 67.9, 56.7, 55.9, 39.2, 34.1, 30.6, 29.6, 29.5, 28.9, 25.2, 22.2, 19.9. **HRMS** (ESI): m/z calculated for $C_{22}H_{34}NaO_6^+$ $[M + Na]^+$ 417.2248, found 417.2252. $[\alpha]_D^{25}$ = +36.6 (c = 0.43, CH_2Cl_2). **HPLC**: Chiralpak IF column, 80:20 hexanes/isopropanol, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 11.97 min (major), 17.87 min (minor).

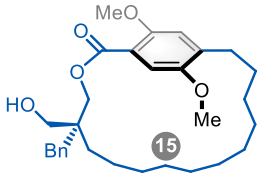


25, colorless oil. 55% yield, 13:1 dr, 92% *ee*. **^{1}H NMR** (600 MHz, $CDCl_3$). δ 7.31 (s, 1H), 6.84 (s, 1H), 4.25 (d, J = 11.39 Hz, 1H), 4.13 (d, J = 11.13 Hz, 1H), 3.87 (s, 3H), 3.82 (d, J = 0.96 Hz, 3H), 3.56 (d, J = 10.98 Hz, 1H), 3.43 (d, J = 10.99 Hz, 1H), 3.38 (t, J = 5.36 Hz, 2H), 3.14 (ddd, J = 13.23, 7.55, 3.97 Hz, 1H), 2.92 – 2.80 (m, 2H), 2.39 (ddd, J = 13.43, 9.37, 3.99 Hz, 1H), 2.11 – 2.03 (m, 1H), 1.92 – 1.80 (m, 1H), 1.41 – 1.35 (m, 1H), 1.33 – 1.24 (m, 2H), 1.24 – 1.17 (m, 3H), 1.15 – 1.06 (m, 4H), 0.99 (s, 3H), 0.91 – 0.80 (m, 2H). **^{13}C NMR** (151 MHz, $CDCl_3$). δ 166.5, 153.7, 151.4, 137.6, 116.9, 115.8, 112.9, 70.7, 70.5, 69.0, 68.4, 56.6, 55.9, 39.2, 35.3, 30.4, 29.63, 29.57, 29.1, 28.1, 25.3, 22.6, 20.3. **HRMS** (ESI): m/z calculated for $C_{23}H_{36}NaO_6^+$ $[M + Na]^+$ 431.2404, found 431.2409. $[\alpha]_D^{25}$ = +26.1 (c = 0.13, CH_2Cl_2). **HPLC**: Chiralpak AD-H column, 90:10 hexanes/isopropanol, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 10.70 min (major), 15.17 min (minor).

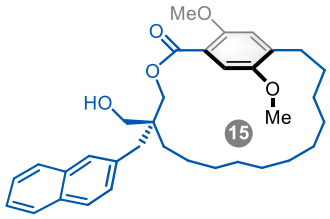


26, colorless oil. 48% yield, 20:1 dr, 96% *ee*. **^{1}H NMR** (600 MHz, $CDCl_3$). δ 7.33 (s, 1H), 6.79 (s,

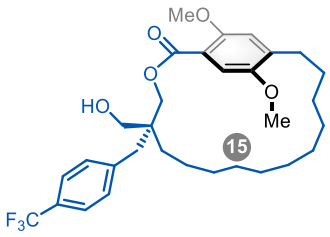
1H), 4.23 (dd, J = 11.24, 1.09 Hz, 1H), 4.12 (dd, J = 11.25, 1.08 Hz, 1H), 3.88 (s, 3H), 3.81 (s, 3H), 3.58 (dd, J = 11.05, 5.79 Hz, 1H), 3.44 (dd, J = 10.97, 5.75 Hz, 1H), 3.14 – 3.08 (m, 1H), 2.26 (ddd, J = 13.09, 9.44, 3.56 Hz, 1H), 1.86 (t, J = 6.09 Hz, 1H), 1.74 – 1.66 (m, 1H), 1.62 – 1.54 (m, 1H), 1.44 – 1.35 (m, 1H), 1.32 – 1.19 (m, 5H), 1.18 – 1.07 (m, 2H), 1.06 – 1.01 (m, 2H), 0.98 (s, 3H), 0.97 – 0.88 (m, 4H), 0.88 – 0.81 (m, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$). δ 166.3, 153.8, 151.3, 138.2, 117.1, 115.9, 113.2, 69.1, 68.1, 56.8, 55.9, 39.2, 35.0, 30.6, 29.9, 29.4, 29.3, 28.8, 28.3, 28.1, 27.3, 26.6, 22.6, 20.0. **HRMS** (ESI): m/z calculated for $C_{24}H_{38}NaO_5^+$ $[M + Na]^+$ 429.2611, found 429.2606. $[\alpha]_D^{25}$ = +43.7 (c = 0.12, CH_2Cl_2). **HPLC**: Chiralpak IF column, 90:10 hexanes/isopropanol, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 20.26 min (major), 30.43 min (minor).



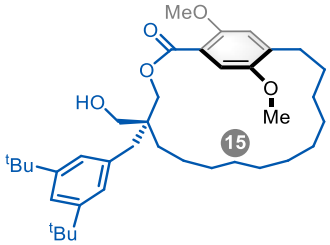
27, colorless oil. 37% yield, 10:1 dr, 96% *ee*. **^{1}H NMR** (400 MHz, $CDCl_3$). δ 7.32 (s, 1H), 7.29 – 7.24 (m, 5H), 6.79 (s, 1H), 4.29 (d, J = 11.29 Hz, 1H), 4.07 (d, J = 11.30 Hz, 1H), 3.88 (s, 3H), 3.80 (s, 3H), 3.44 (dd, J = 11.17, 5.68 Hz, 1H), 3.35 (dd, J = 11.11, 5.78 Hz, 1H), 3.10 (ddd, J = 13.07, 7.63, 3.46 Hz, 1H), 2.86 (d, J = 13.24 Hz, 1H), 2.66 (d, J = 13.25 Hz, 1H), 2.26 (ddd, J = 13.10, 9.20, 3.78 Hz, 1H), 1.81 – 1.76 (m, 1H), 1.73 – 1.63 (m, 1H). 1.40 – 1.32 (m, 2H), 1.27 – 1.11 (m, 6H), 1.04 (d, J = 7.37 Hz, 2H), 0.97 – 0.88 (m, 4H), 0.88 – 0.75 (m, 4H). **^{13}C NMR** (101 MHz, $CDCl_3$). δ 166.8, 153.7, 151.3, 138.2, 137.7, 130.6, 128.3, 126.4, 117.2, 115.7, 113.3, 66.8, 64.6, 56.7, 56.0, 42.8, 38.5, 32.8, 30.7, 29.9, 29.5, 29.4, 28.7, 28.3, 28.2, 27.3, 26.8, 22.5. **HRMS** (ESI): m/z calculated for $C_{30}H_{42}NaO_5^+$ $[M + Na]^+$ 505.2924, found 505.2920. $[\alpha]_D^{25}$ = +85.1 (c = 0.22, CH_2Cl_2). **HPLC**: Chiralpak IF column, 90:10 hexanes/isopropanol, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 16.46 min (major), 38.94 min (minor).



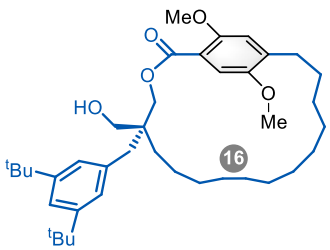
28, colorless oil. 55% yield, 10:1 dr, 92% *ee*. **^{1}H NMR** (400 MHz, $CDCl_3$). δ 7.85 – 7.76 (m, 3H), 7.72 (s, 1H), 7.56 – 7.42 (m, 3H), 7.34 (s, 1H), 6.82 (s, 1H), 4.36 (d, J = 11.36 Hz, 1H), 4.14 (d, J = 11.46 Hz, 1H), 3.91 (s, 3H), 3.81 (s, 3H), 3.48 (dd, J = 11.19, 5.38 Hz, 1H), 3.40 (dd, J = 11.09, 5.61 Hz, 1H), 3.15 – 3.09 (m, 1H), 3.05 (d, J = 13.32 Hz, 1H), 2.84 (d, J = 13.25 Hz, 1H), 2.28 (ddd, J = 13.02, 9.14, 3.71 Hz, 1H), 1.87 – 1.82 (m, 1H), 1.76 – 1.55 (m, 2H), 1.46 – 1.38 (m, 2H), 1.31 – 1.15 (m, 5H), 1.11 – 1.01 (m, 2H), 0.99 – 0.90 (m, 4H), 0.91 – 0.82 (m, 4H). **^{13}C NMR** (101 MHz, $CDCl_3$). δ 166.9, 153.7, 151.4, 138.3, 135.4, 133.5, 132.2, 129.2, 129.0, 127.7, 127.6, 126.0, 125.5, 117.2, 115.7, 113.3, 66.8, 64.6, 56.7, 56.0, 43.1, 38.6, 32.9, 30.7, 29.9, 29.5, 29.4, 28.7, 28.3, 28.2, 27.3, 26.8, 22.5. **HRMS** (ESI): m/z calculated for $C_{34}H_{44}NaO_5^+$ $[M + Na]^+$ 555.3081, found 555.3085. $[\alpha]_D^{25}$ = +49.0 (c = 0.24, CH_2Cl_2). **HPLC**: Chiralpak IF column, 80:20 hexanes/isopropanol, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 9.93 min (major), 14.84 min (minor).



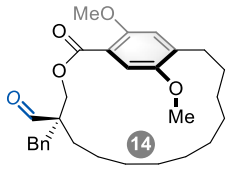
29, colorless oil. 57% yield, 12:1 dr, 97% *ee*. **^{1}H NMR** (600 MHz, $CDCl_3$). δ 7.64 – 7.50 (m, 2H), 7.41 (d, J = 7.88 Hz, 2H), 7.32 (s, 1H), 6.81 (s, 1H), 4.31 (dd, J = 11.32, 1.46 Hz, 1H), 4.01 (dd, J = 11.32, 1.47 Hz, 1H), 3.90 (s, 3H), 3.81 (s, 3H), 3.41 (ddd, J = 11.10, 5.37, 1.47 Hz, 1H), 3.30 (ddd, J = 11.14, 5.68, 1.42 Hz, 1H), 3.12 (dddd, J = 12.86, 7.73, 3.44, 1.39 Hz, 1H), 2.96 (d, J = 13.02 Hz, 1H), 2.73 (d, J = 13.07 Hz, 1H), 2.27 (ddd, J = 13.69, 8.93, 3.63 Hz, 1H), 1.92 – 1.88 (m, 1H), 1.73 – 1.67 (m, 1H), 1.38 – 1.31 (m, 2H), 1.30 – 1.22 (m, 3H), 1.20 – 1.12 (m, 3H), 1.07 – 1.01 (m, 2H), 0.99 – 0.91 (m, 4H), 0.89 – 0.83 (m, 4H). **^{13}C NMR** (151 MHz, $CDCl_3$). δ 166.9, 153.6, 151.4, 142.0, 138.4, 131.0, 128.7 (q, $J_{C\text{-}F}$ = 32.42 Hz), 125.1 (q, $J_{C\text{-}F}$ = 4.23 Hz), 124.4 (q, $J_{C\text{-}F}$ = 272.98 Hz) 117.1, 115.7, 113.4, 66.5, 63.9, 56.6, 56.0, 42.9, 38.0, 32.8, 30.7, 29.8, 29.5, 29.4, 28.6, 28.3, 28.2, 27.3, 26.8, 22.5. **^{19}F NMR** (565 MHz, DMSO-*d6*) δ –60.6. **HRMS** (ESI): m/z calculated for $C_{31}H_{41}F_3NaO_5^+$ $[M + Na]^+$ 573.2798, found 573.2794. $[\alpha]_D^{25}$ = +75.5 (c = 0.21, CH_2Cl_2). **HPLC**: Chiralpak IF column, 90:10 hexanes/isopropanol, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 10.57 min (major), 15.84 min (minor).



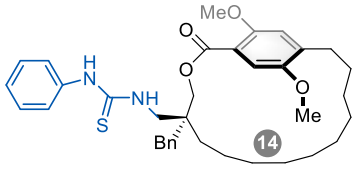
30, colorless oil. 48% yield, 19:1 dr, 96% *ee*. **^{1}H NMR** (600 MHz, $CDCl_3$). δ 7.33 (s, 1H), 7.28 – 7.26 (m, 1H), 7.12 (s, 2H), 6.80 (s, 1H), 4.22 (dd, J = 11.30, 1.18 Hz, 1H), 4.09 (dd, J = 11.34, 1.16 Hz, 1H), 3.89 (s, 3H), 3.79 (s, 3H), 3.47 – 3.42 (m, 1H), 3.39 (dd, J = 11.07, 5.63 Hz, 1H), 3.14 – 3.07 (m, 1H), 2.89 – 2.83 (m, 1H), 2.67 (d, J = 13.25 Hz, 1H), 2.26 (ddd, J = 12.96, 9.24, 3.61 Hz, 1H), 1.75 – 1.67 (m, 1H), 1.66 – 1.63 (m, 1H), 1.62 – 1.58 (m, 1H), 1.40 – 1.33 (m, 3H), 1.30 (s, 18H), 1.26 – 1.18 (m, 2H), 1.18 – 1.11 (m, 2H), 1.07 – 1.03 (m, 2H), 0.98 – 0.89 (m, 4H), 0.89 – 0.82 (m, 4H). **^{13}C NMR** (151 MHz, $CDCl_3$). δ 166.7, 153.7, 151.3, 150.6, 138.1, 136.7, 124.7, 120.1, 117.3, 115.6, 113.4, 66.9, 65.3, 56.6, 42.7, 39.1, 34.8, 33.1, 31.6, 30.7, 29.9, 29.4, 28.7, 28.3, 28.2, 27.4, 26.8, 22.5. **HRMS** (ESI): m/z calculated for $C_{38}H_{58}NaO_5^+$ $[M + Na]^+$ 617.4176, found 617.4179. $[\alpha]_D^{25}$ = +75.5 (c = 0.21, CH_2Cl_2). **HPLC**: Chiralpak IF column, 90:10 hexanes/isopropanol, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 8.30 min (major), 12.01 min (minor).



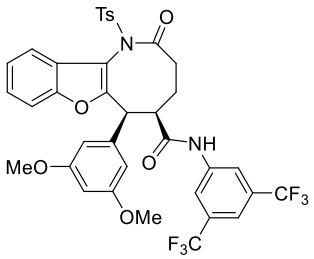
31, colorless oil. 45% yield, 2:1 dr. **^{1}H NMR** (600 MHz, $CDCl_3$). δ 7.42 (s, 1H), 7.27 (s, 1H), 6.993 (s, 1H), 6.991 (s, 1H), 6.76 (s, 1H), 4.36 (dd, J = 11.21, 1.28 Hz, 1H), 4.18 (d, J = 11.14 Hz, 1H), 3.84 (s, 3H), 3.81 (s, 3H), 3.60 (dd, J = 11.16, 2.95 Hz, 1H), 3.54 – 3.47 (m, 1H), 3.12 – 3.04 (m, 2H), 2.67 – 2.56 (m, 2H), 2.31 (ddd, J = 12.95, 9.03, 3.55 Hz, 1H), 1.79 – 1.67 (m, 1H), 1.64 (dd, J = 13.19, 3.19 Hz, 1H), 1.58 – 1.50 (m, 2H), 1.32 (s, 18H), 1.31 – 1.21 (m, 2H), 1.18 – 1.11 (m, 4H), 1.11 – 1.07 (m, 4H), 1.07 – 0.99 (m, 5H), 0.82 – 0.72 (m, 2H).**^{13}C NMR** (151 MHz, $CDCl_3$). δ 166.7, 153.1, 151.5, 150.5, 138.2, 135.8, 124.7, 120.2, 116.4, 115.0, 113.8, 69.8, 68.5, 56.2, 56.0, 41.8, 39.0, 34.8, 31.6, 30.0, 29.9, 29.6, 29.5, 29.3, 27.9, 27.8, 27.7, 27.5, 27.2, 25.5, 21.8. **HRMS** (ESI): m/z calculated for $C_{39}H_{60}NaO_5^+$ $[M + Na]^+$ 631.4333, found 631.4339. $[\alpha]_D^{25}$ = +31.9 (c = 0.16, CH_2Cl_2).



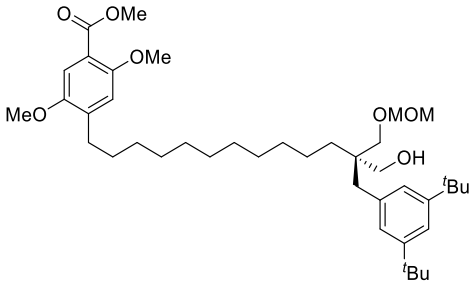
32, colorless oil. 95% yield, 20:1 dr, 98% *ee*. **^{1}H NMR** (600 MHz, $CDCl_3$). δ 9.66 (s, 1H), 7.39 – 7.20 (m, 5H), 7.14 (dd, J = 6.80, 1.44 Hz, 2H), 6.82 (s, 1H), 4.46 (dd, J = 11.71, 1.60 Hz, 1H), 4.25 (dd, J = 11.76, 1.50 Hz, 1H), 3.92 (s, 3H), 3.80 (s, 3H), 3.30 – 3.13 (m, 1H), 3.10 – 2.98 (m, 2H), 2.28 (ddd, J = 13.46, 9.66, 4.10 Hz, 1H), 1.81 – 1.69 (m, 2H), 1.69 – 1.56 (m, 2H), 1.37 – 1.22 (m, 2H), 1.21 – 1.08 (m, 3H), 1.06 – 0.97 (m, 1H), 0.92 – 0.80 (m, 5H), 0.68 – 0.56 (m, 1H), 0.48 – 0.34 (m, 1H). **^{13}C NMR** (151 MHz, $CDCl_3$). δ 204.2, 166.4, 153.7, 151.6, 138.4, 135.9, 130.1, 128.7, 127.0, 117.3, 115.3, 113.4, 63.7, 56.6, 56.0, 54.2, 39.8, 31.7, 31.4, 29.8, 29.4, 28.9, 28.7, 28.33, 28.27, 26.8, 22.9. **HRMS** (ESI): m/z calculated for $C_{29}H_{38}NaO_5^+$ $[M + Na]^+$ 489.2611, found 489.2607. $[\alpha]_D^{25}$ = +87.5 (c = 0.44, CH_2Cl_2). **HPLC**: Chiralpak IB N-5 column, 95:5 hexanes/isopropanol, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 7.62 min (major), 7.14 min (minor).



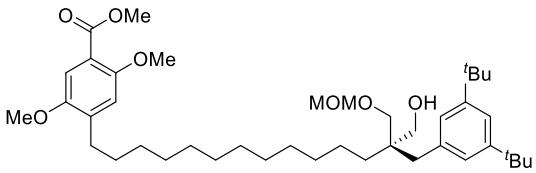
33, colorless oil. 34% yield, 20:1 dr, 98% *ee*. **^{1}H NMR** (600 MHz, $CDCl_3$). δ 7.97 – 7.70 (m, 1H), 7.44 – 7.38 (m, 3H), 7.34 – 7.28 (m, 1H), 7.16 – 7.06 (m, 5H), 6.99 – 6.95 (m, 2H), 6.79 (s, 1H), 5.85 (s, 1H), 4.20 – 4.11 (m, 1H), 4.03 (d, J = 11.39 Hz, 1H), 3.87 (s, 3H), 3.84 (s, 3H), 3.79 – 3.69 (m, 2H), 3.16 (ddd, J = 12.87, 7.08, 3.79 Hz, 1H), 2.67 (d, J = 13.77 Hz, 1H), 2.51 (d, J = 13.73 Hz, 1H), 2.27 (ddd, J = 13.24, 9.51, 4.06 Hz, 1H), 1.79 – 1.70 (m, 1H), 1.65 – 1.53 (m, 1H), 1.41 – 1.35 (m, 1H), 1.33 – 1.25 (m, 3H), 1.23 – 1.17 (m, 1H), 1.14 – 1.05 (m, 3H), 1.05 – 0.97 (m, 1H), 0.95 – 0.86 (m, 3H), 0.85 – 0.77 (m, 2H), 0.68 – 0.58 (m, 1H), 0.56 – 0.47 (m, 1H). **^{13}C NMR** (151 MHz, $CDCl_3$). δ 181.5, 166.2, 153.6, 151.6, 138.2, 136.7, 135.9, 130.4, 129.9, 128.7, 127.7, 126.9, 125.7, 117.3, 115.3, 113.4, 66.7, 56.7, 56.2, 49.6, 42.0, 41.4, 34.2, 31.6, 29.8, 29.6, 29.0, 28.64, 28.58, 28.0, 26.8, 22.8. **HRMS** (ESI): m/z calculated for $C_{36}H_{46}N_2NaO_4S^+$ $[M + Na]^+$ 625.3070, found 625.3074. $[\alpha]_D^{25}$ = +29.0 (c = 0.10, CH_2Cl_2). **HPLC**: Chiralpak IB N-5 column, 80:20 hexanes/isopropanol, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 23.09 min (major), 15.46 min (minor).



36, white solid. 57% yield, >20:1 dr, 19% *ee*. **^{1}H NMR** (600 MHz, $CDCl_3$). δ 7.89 – 7.74 (m, 5H), 7.64 (s, 1H), 7.40 – 7.31 (m, 2H), 7.29 (s, 1H), 7.18 (d, J = 8.05 Hz, 1H), 7.10 (d, J = 7.93 Hz, 2H), 6.52 (d, J = 2.22 Hz, 2H), 6.49 (s, 1H), 3.78 (s, 6H), 3.49 (s, 1H), 2.97 – 2.94 (m, 1H), 2.77 (t, J = 12.70 Hz, 1H), 2.56 – 2.50 (m, 1H), 2.35 (s, 3H), 2.32 – 2.24 (m, 1H), 2.01 – 1.93 (m, 1H).**^{13}C NMR** (151 MHz, $CDCl_3$). δ 174.2, 170.5, 161.6, 154.4, 150.6, 145.5, 140.1, 139.0, 134.2, 132.51 (q, $J_{C\text{-}F}$ = 33.46 Hz), 129.6, 129.0, 126.0, 125.0, 123.1 (q, $J_{C\text{-}F}$ = 272.76 Hz), 120.9, 119.6 (q, $J_{C\text{-}F}$ = 3.68 Hz), 119.0, 117.7, 111.6, 107.1, 99.0, 55.4, 47.8, 43.6, 33.0, 28.6, 21.6. **^{19}F NMR** (565 MHz, $CDCl_3$) δ –62.9. **HRMS** (ESI): m/z calculated for $C_{37}H_{30}F_6N_2NaO_7S^+$ $[M + Na]^+$ 783.1570, found 783.1577. $[\alpha]_D^{25}$ = +13.4 (c = 0.20, CH_2Cl_2). **HPLC**: Chiralpak IF column, 90:10 hexanes/isopropanol, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 12.88 min (major), 14.92 min (minor).



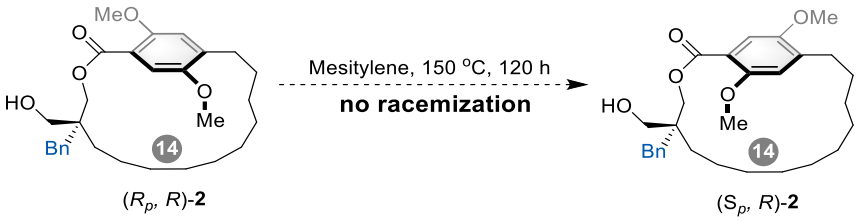
38, colorless oil. 41% yield, 91% *ee*. **^{1}H NMR** (600 MHz, $CDCl_3$). δ 7.30 (s, 1H), 7.26 (s, 1H), 7.02 (s, 2H), 6.79 (s, 1H), 4.68 – 4.61 (m, 2H), 3.89 (s, 3H), 3.87 (s, 3H), 3.81 (s, 3H), 3.55 – 3.48 (m, 2H), 3.46 (dd, J = 9.36, 1.19 Hz, 1H), 3.42 – 3.39 (m, 4H), 2.71 (d, J = 13.40 Hz, 1H), 2.66 – 2.58 (m, 3H), 1.57 (dd, J = 10.95, 4.37 Hz, 2H), 1.41 – 1.30 (m, 25H), 1.29 – 1.21 (m, 11H). **^{13}C NMR** (151 MHz, $CDCl_3$). δ 166.7, 153.7, 151.1, 150.3, 138.1, 136.8, 129.6, 129.2, 124.8, 119.9, 117.2, 114.9, 113.2, 97.0, 73.5, 67.9, 57.0, 56.0, 55.6, 52.0, 42.2, 37.8, 34.7, 31.6, 31.4, 30.7, 29.9, 29.81, 29.75, 29.73, 29.69, 29.63, 29.58, 23.3. **HRMS** (ESI): m/z calculated for $C_{41}H_{66}NaO_7^+$ $[M + Na]^+$ 693.4701, found 693.4706. $[\alpha]_D^{25}$ = +10.7 (c = 0.13, CH_2Cl_2). **HPLC**: Chiralpak IC column, 90:10 hexanes/isopropanol, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 32.79 min (major), 28.46 min (minor).



39, colorless oil. 56% yield, 86% *ee*. **^{1}H NMR** (600 MHz, Acetone-d_6). δ 7.27 (s, 1H), 7.23 (s, 1H), 7.09 (s, 2H), 6.93 (s, 1H), 3.79 (s, 3H), 3.78 (s, 3H), 3.77 (s, 3H), 3.38 – 3.24 (m, 7H), 2.66 – 2.53 (m, 4H), 1.58 – 1.54 (m, 2H), 1.43 – 1.36 (m, 2H), 1.35 – 1.21 (m, 37H), 1.15 – 1.05 (m, 2H).**^{13}C NMR** (151 MHz, Acetone-d_6). δ 167.0, 154.2, 151.9, 1 50.6, 138.1, 138.0, 125.7, 120.3, 119.1,

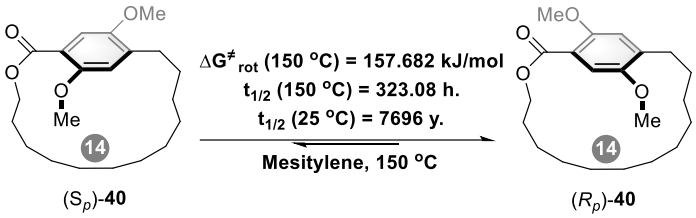
116.2, 113.6, 97.6, 70.8, 64.5, 57.1, 56.3, 55.4, 51.9, 43.3, 38.0, 35.2, 32.0, 31.9, 31.5, 31.1, 30.6, 30.51, 30.46, 30.40, 30.38, 30.3, 23.7. **HRMS** (ESI): m/z calculated for $C_{42}H_{68}NaO_7^+$ $[M + Na]^+$ 707.4857 found 707.4850. $[\alpha]_D^{25}$ = +10.7 (c = 0.13, CH_2Cl_2). **HPLC**: Chiralpak IC column, 90:10 hexanes/isopropanol, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 28.64 min (major), 25.40 min (minor).

5. Racemization experiment



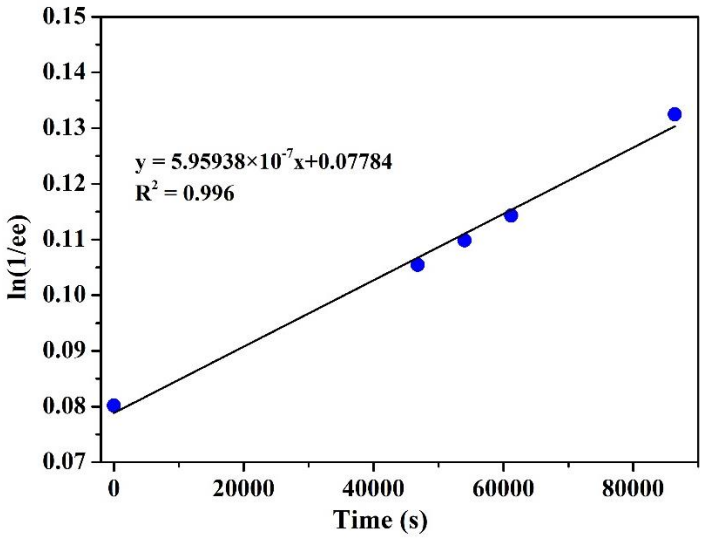
(R_p, R)-**2** (S_p, R)-**2**

15 mg of (**2**) was heated at 150 °C in mesitylene (10 mL). 30 mg of (**26, 27, 30**) was heated at 110 °C in DMSO-*d6* (20 mL). The de of the sample in this solution was determined by ^{1}H NMR spectroscopy at different times to monitor the percentage change in diastereoisomers over time.



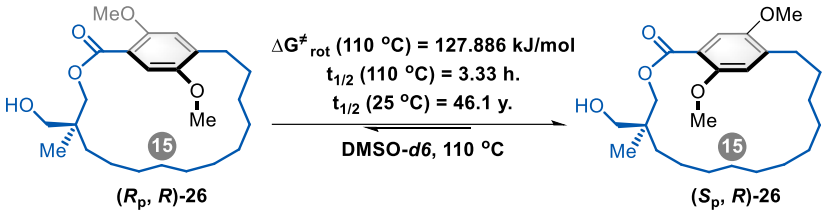
(S_p)-**40** (R_p)-**40**

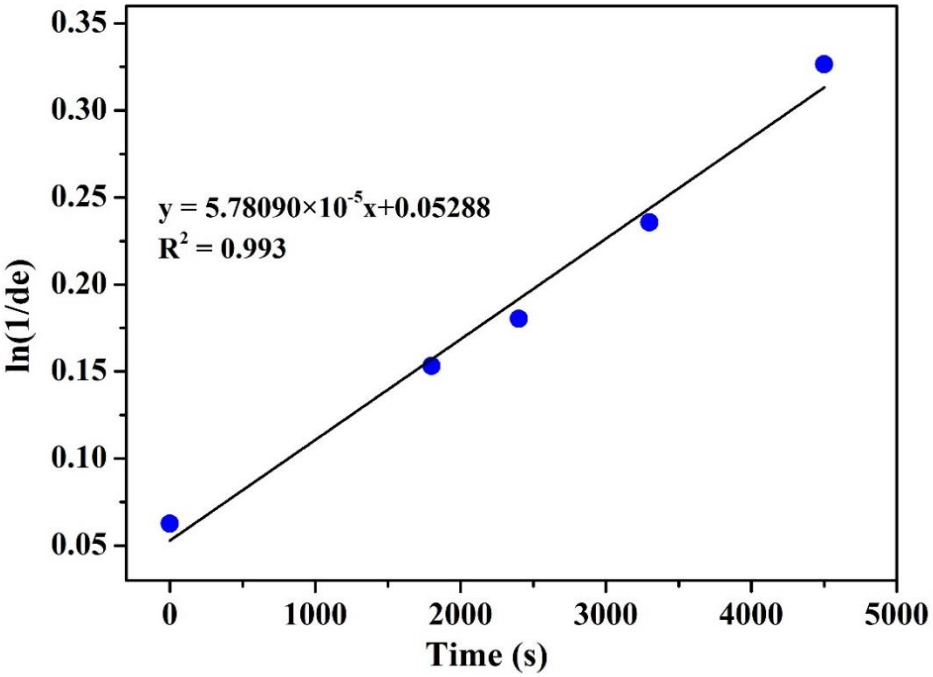
About 3 mg of enantio-enriched (**40**) was heated at 150 °C in mesitylene (15 mL). Samples of 7 µL of this solution were injected on Chiralpak IB N-5 (hexanes/^{i}PrOH 90/10, 1.0 mL/min, UV detection at 254 nm) to monitor the percentage decrease of the second eluted enantiomer over time.



Time (s)	% second eluted enantiomer (%t)	ln(1/ee)
0	92.30	0.0802
46800	89.99	0.1054
54000	89.60	0.1098
61200	89.20	0.1143
86400	87.59	0.1324

k racemization =	5.95938E-07 s^{-1}
k enantiomerisation =	2.97969E-07 s^{-1}
$\Delta G^{\neq}$ enantiomerisation =	157.68 kJ/mol
	37.6 kcal/mol
25°C half-life time $t_{1/2}$ =	7696 y.

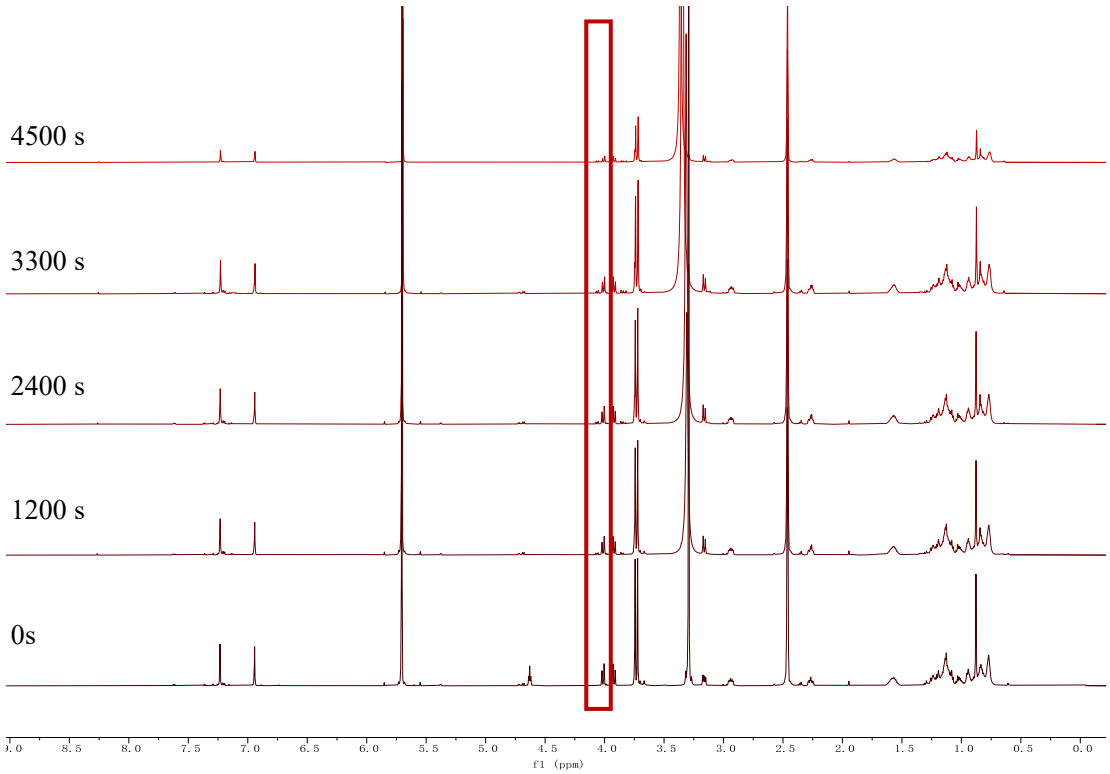




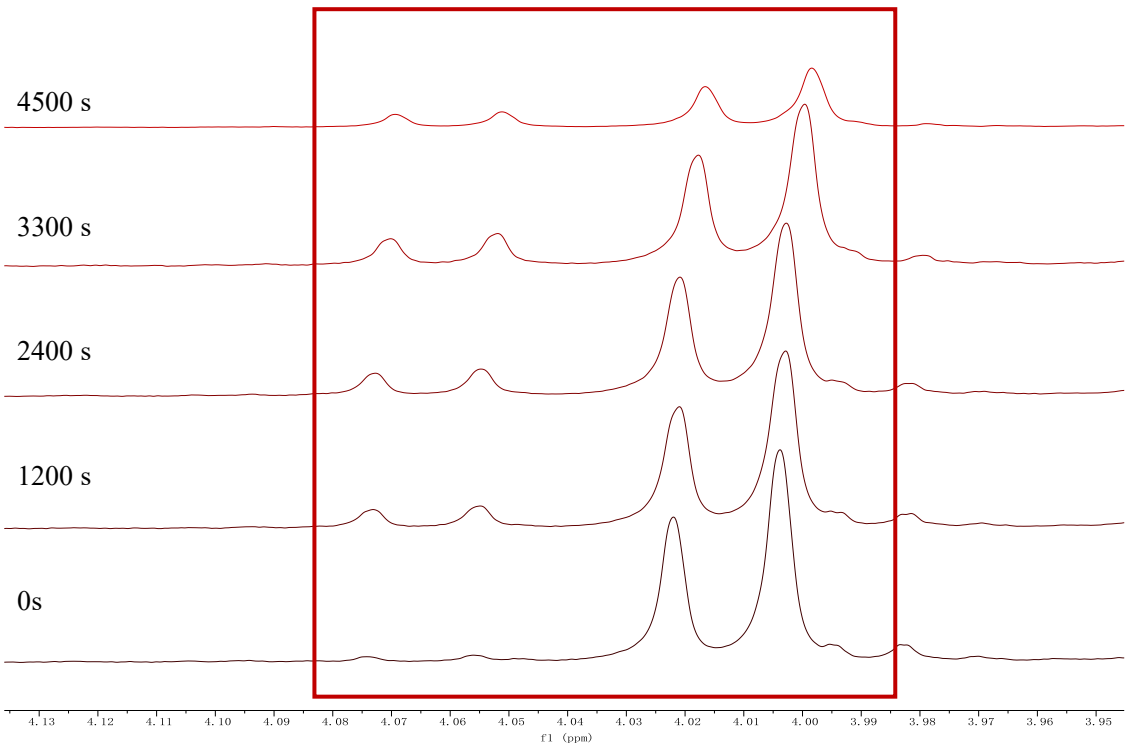
Time (s)	% second eluted diastereoisomer (%t)	ln(1/de)
0	93.94	0.0625
1800	85.79	0.1531
2400	83.01	0.1862
3300	78.99	0.2357
4500	72.15	0.3264

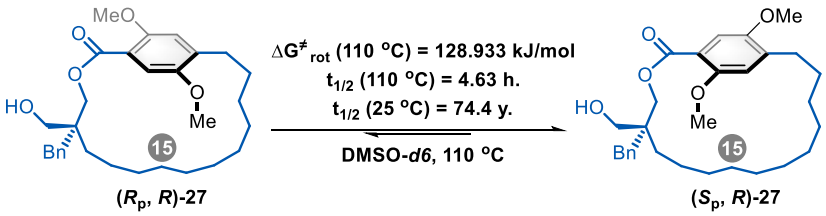
k racemization =	5.78090E-05 s^{-1}
k enantiomerisation =	2.89045E-05 s^{-1}
$\Delta G^{\neq}$ enantiomerisation =	127.89 kJ/mol
	30.5 kcal/mol
25°C half-life time $t_{1/2}$ =	46.1 y.

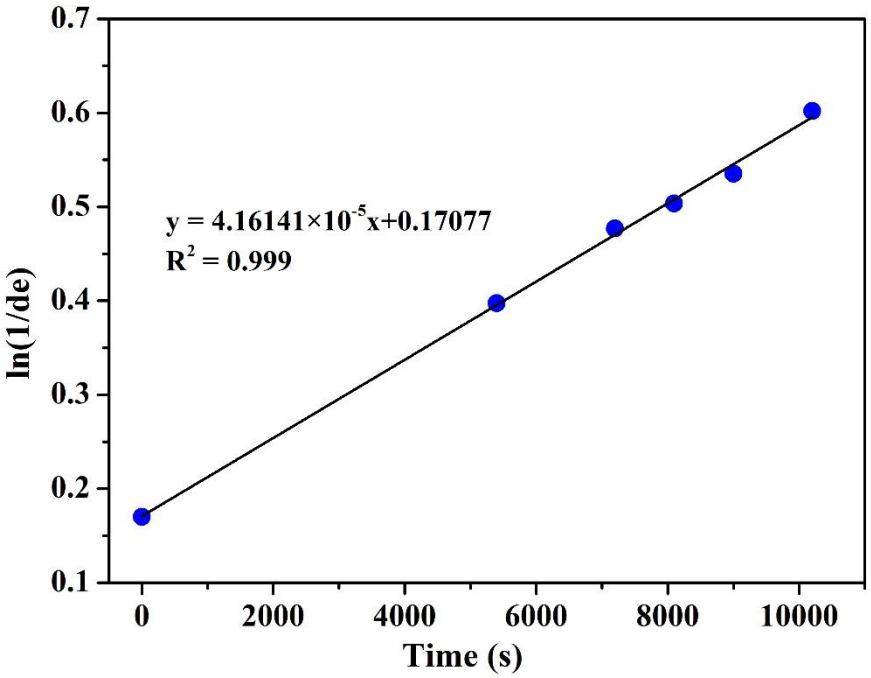
Full ^{1}H NMR spectrum of **26** in DMSO-d_6 was recorded at various times (110°C)



Zoom on the 3.95 – 4.12 ppm



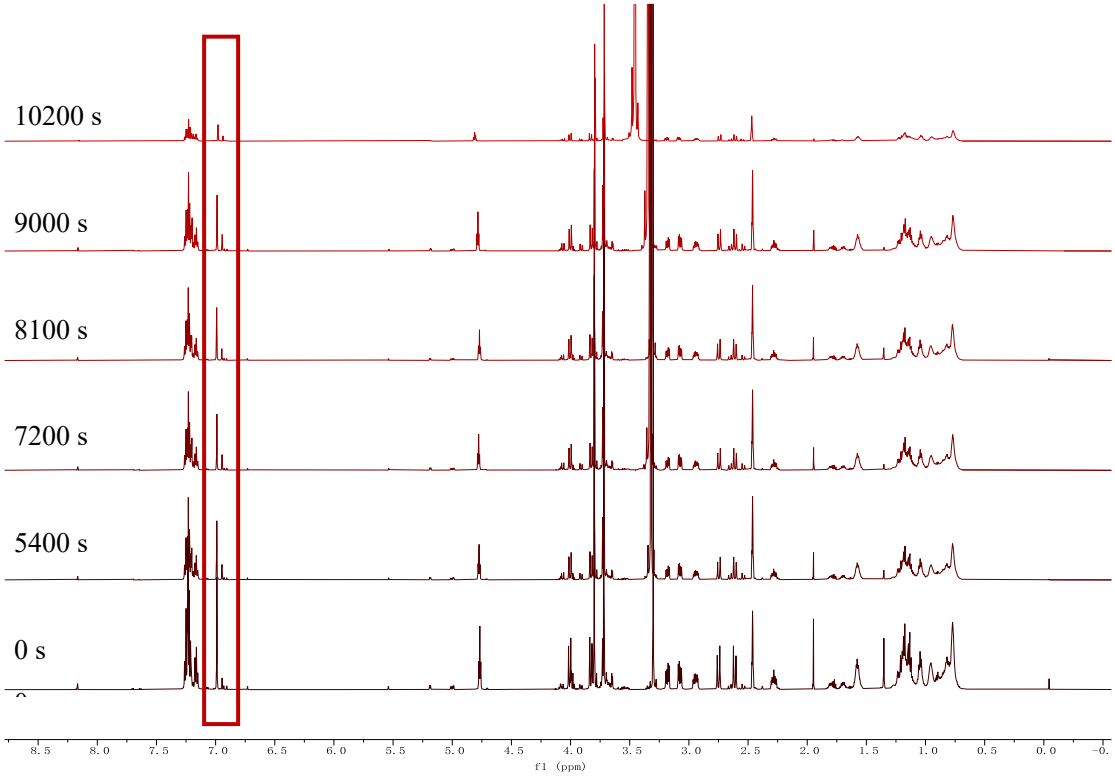




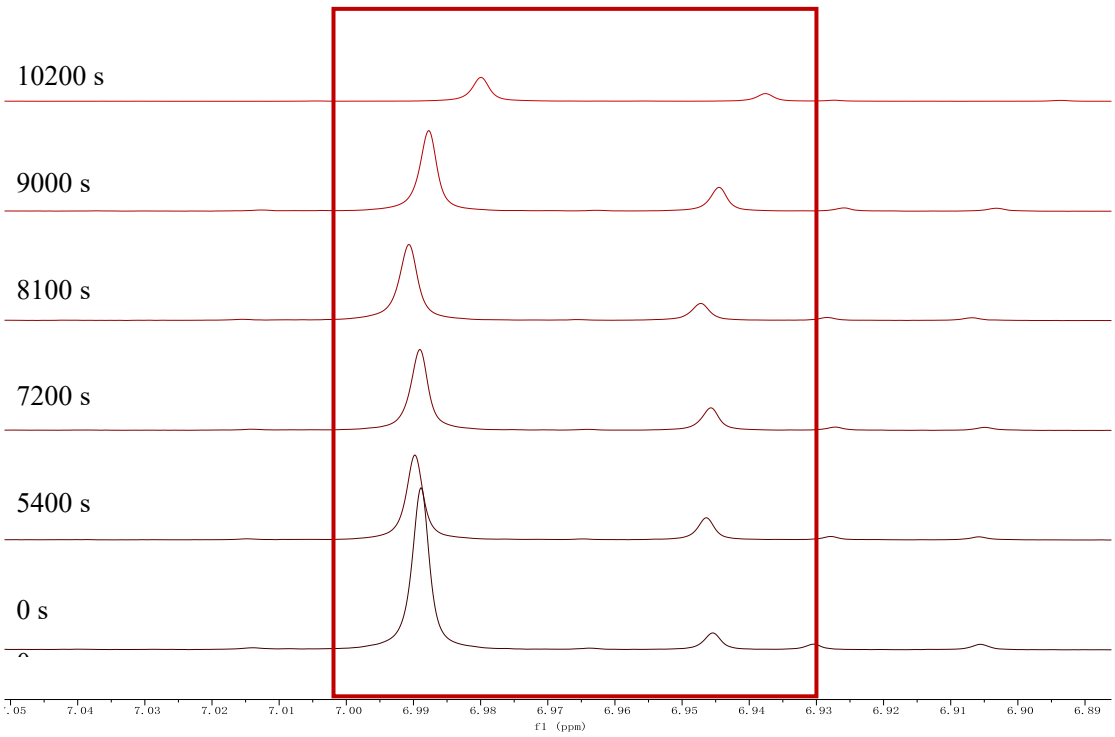
Time (s)	% second eluted diastereoisomer (%t)	ln(1/de)
0	84.32	0.1700
5400	67.20	0.3974
7200	62.07	0.4769
8100	60.42	0.5037
9000	57.98	0.5451
10200	54.78	0.6019

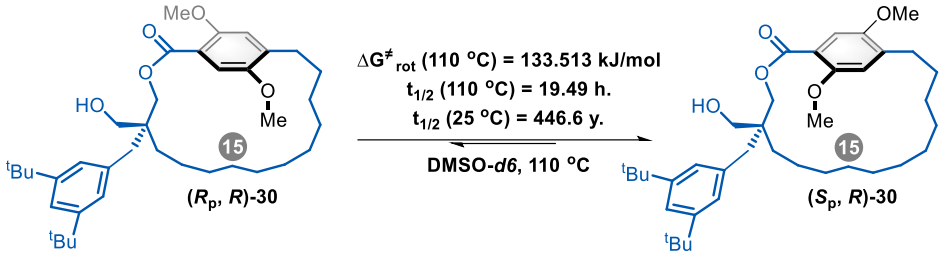
k racemization =	4.16141E-05 s^{-1}
k enantiomerisation =	2.08071E-05 s^{-1}
$\Delta G^{\neq}$ enantiomerisation =	128.93 kJ/mol
	30.8 kcal/mol
25°C half-life time $t_{1/2}$ =	74.4 y.

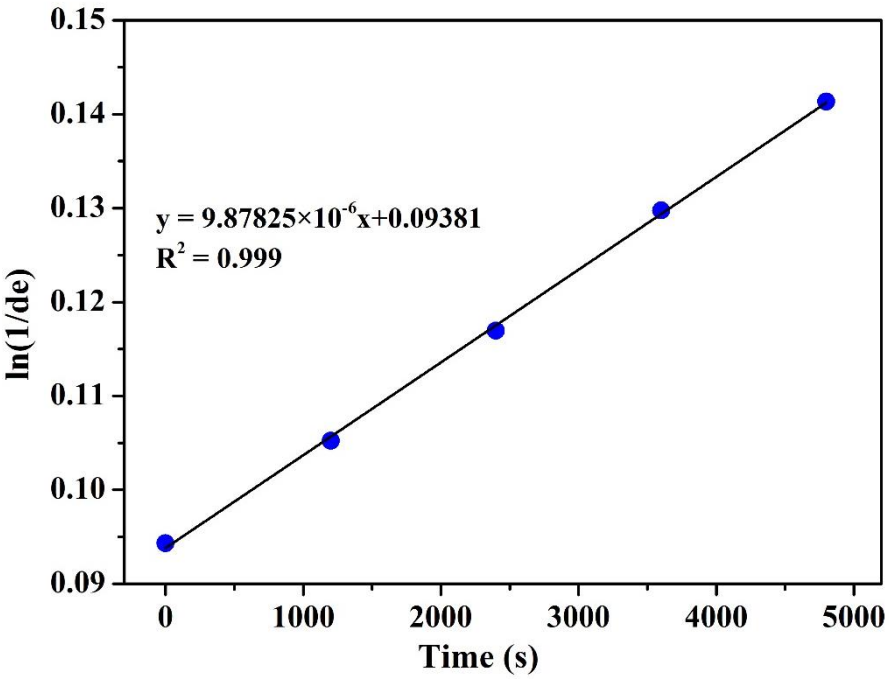
Full ^{1}H NMR spectrum of **27** in DMSO-d_6 was recorded at various times (110°C)



Zoom on the 6.89 – 7.05 ppm



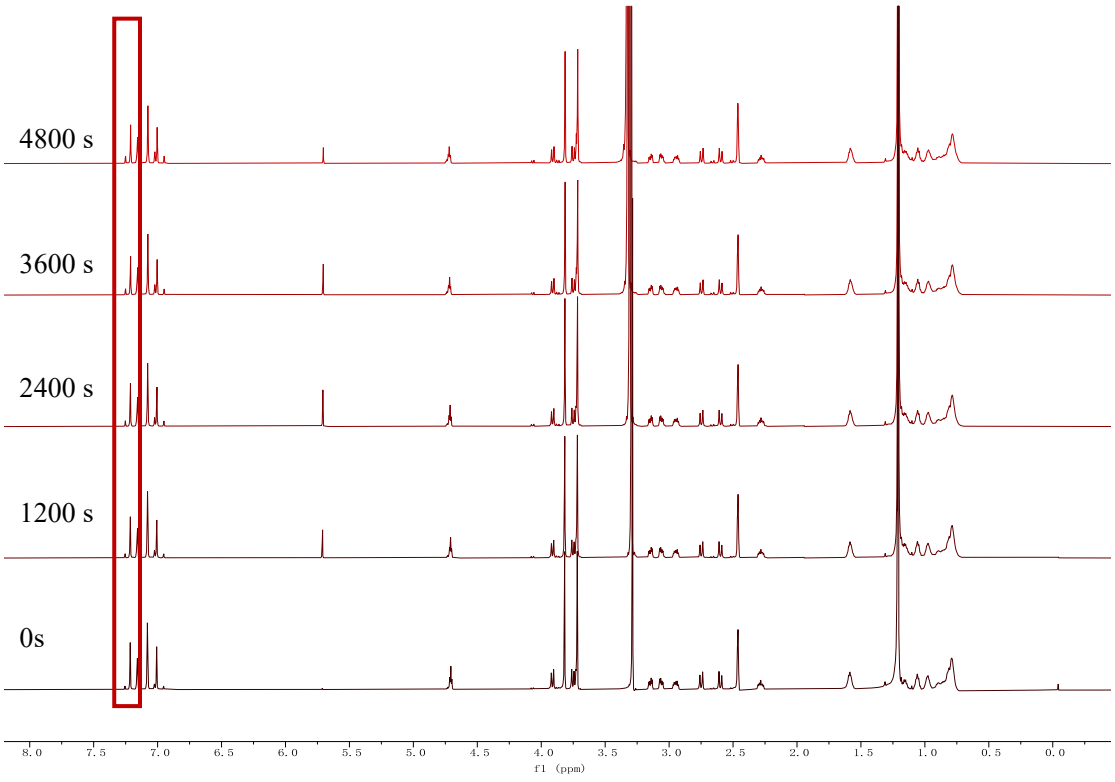




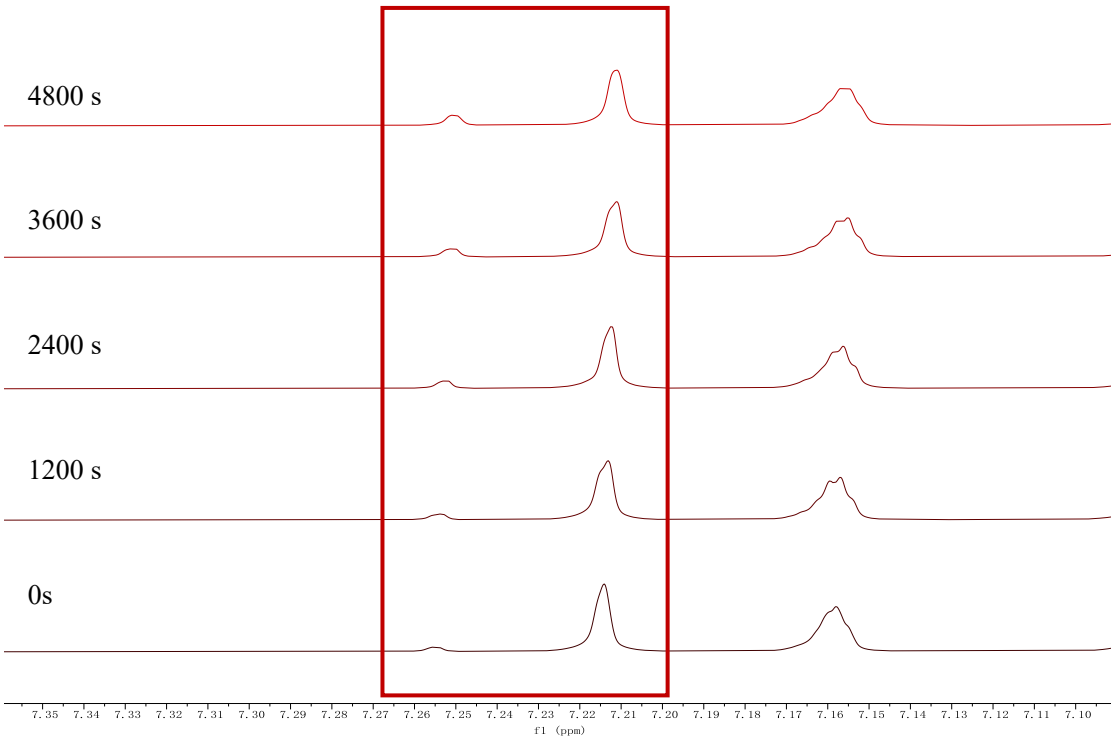
Time (s)	% second eluted diastereoisomer (%t)	ln(1/de)
0	91.00	0.0943
1200	90.01	0.1052
2400	88.96	0.1169
3600	87.83	0.1297
4800	86.82	0.1413

k racemization =	9.87825E-06 s^{-1}
k enantiomerisation =	4.93913E-06 s^{-1}
$\Delta G^{\neq}$ enantiomerisation =	133.51 kJ/mol
	31.9 kcal/mol
25°C half-life time $t_{1/2}$ =	446.6 y.

Full ^{1}H NMR spectrum of **30** in DMSO-d_6 was recorded at various times (110°C)



Zoom on the 7.10 – 7.35 ppm

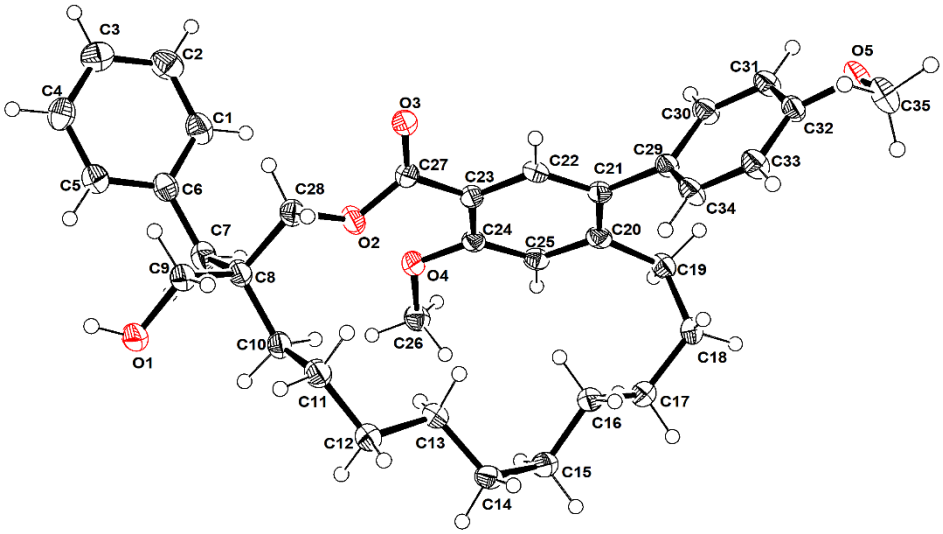


6. References

[1] Wang, J. M., Wang, M., Wen, Y. L., Teng, P., Li, C. Y. & Zhao, C. G. N-heterocyclic carbene-catalyzed highly enantioselective macrolactonization to access planar-chiral macrocycles. *Org. Lett.* **26**, 1040–1045 (2024).

[2] Wang, J. M., Li, J. & Zhao, C. G. A lewis acid-promoted michael addition and ring-expansion cascade for the construction of nitrogen-containing medium-sized rings. *Molecules* **28**, 1650 (2023).

7. X-Ray report



Supplementary Figure 5. Thermal ellipsoid plot for the crystal structure of 14 (at 50% probability level, CCDC No. 2383321)

Experimental

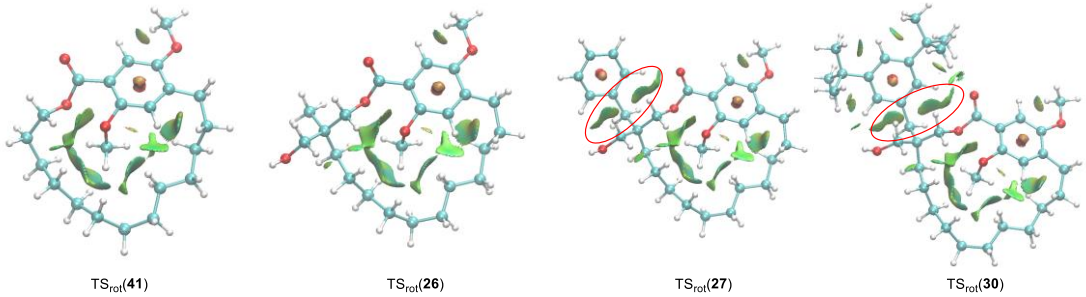
Single crystals of $C_{35}H_{44}O_5$ (**14**) were recrystallised from ethyl acetate (EA), petroleum ether (PE) mounted in inert oil and transferred to the cold gas stream of the diffractometer.

Supplementary Table 1 Crystal data and structure refinement for exp_22172_auto.

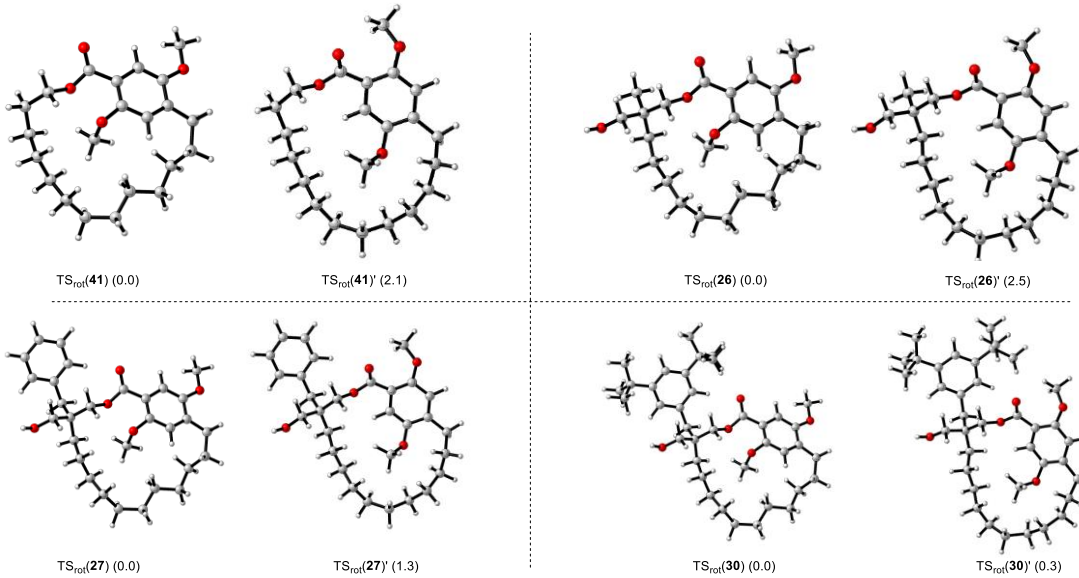
Identification code	exp_22172_auto
Empirical formula	$C_{35}H_{44}O_5$
Formula weight	544.70
Temperature/K	99.9(3)
Crystal system	orthorhombic

Space group	$P2_12_12_1$
a/Å	8.1497(3)
b/Å	12.7732(5)
c/Å	29.0573(10)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	3024.80(19)
Z	4
ρ_{calc}g/cm^3	1.196
μ/mm^{-1}	0.621
F(000)	1176.0
Crystal size/mm^3	0.1 × 0.05 × 0.02
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	7.56 to 133.178
Index ranges	$-9 \leq h \leq 9$, $-15 \leq k \leq 15$, $-34 \leq l \leq 33$
Reflections collected	28838
Independent reflections	5319 [R_{int} = 0.1063, R_{sigma} = 0.0552]
Data/restraints/parameters	5319/0/365
Goodness-of-fit on F^2	1.099
Final R indexes [I>=2σ (I)]	R_1 = 0.0459, wR_2 = 0.1129
Final R indexes [all data]	R_1 = 0.0543, wR_2 = 0.1206
Largest diff. peak/hole / e Å^{-3}	0.19/-0.16
Flack parameter	0.12(18)

8. Computational studies



Supplementary Figure 6. NCI analysis of **TS$_{rot}$(41)**, **TS$_{rot}$(26)**, **TS$_{rot}$(27)** and **TS$_{rot}$(30)** with key steric interaction highlighted by the red circles.



Supplementary Figure 7. Energy comparisons between two rotational transition states of **41**, **26**, **27** and **30**, respectively. The numbers in parenthesis are $\Delta\Delta G^{\neq}$ (in kcal/mol).

Computational methods

The M06-2X[1] density functional method was employed to perform the computational studies. For geometry optimizations, the 6-31G(d,p) basis set was used for all atoms. Subsequently, frequency calculations at the same theoretical level were performed to ensure the optimized stationary points are either local minima (no imaginary frequencies) or transition states (one imaginary frequency). Moreover, intrinsic reaction coordinate (IRC)[2] calculations were carried out to confirm that the optimized transition states connect to their respective reactants and products. The solvation energies were evaluated by a self-consistent reaction field (SCRF) using the SMD[3] implicit solvent model (tetrahydrofuran). A larger basis set (6-311++G(d,p) for all atoms) was utilized for such single-point energy calculations. Solution–phase Gibbs energy was determined by the sum of solvation single-point energy and gas-phase thermal correction to Gibbs energy. Non-covalent interaction was analysed with NCIplot developed by Yang and co-workers.[4] All calculations were executed with the Gaussian 09 suite of programs[5]. The 3D structures of optimized intermediates or transition states were demonstrated using the software of CYLView[6].

References

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Cartesion coordinates and energies:

(S_p)-41

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.180883	-1.410187	2.694517
2	8	0	1.652727	-2.222881	0.834823
3	8	0	0.708349	-3.699320	-0.571328
4	6	0	-0.650310	-1.993223	0.403014
5	6	0	-2.644607	-1.107388	-0.652789
6	6	0	-0.960249	-1.300843	1.573870
7	6	0	0.611251	-2.759860	0.184130
8	6	0	-1.523559	-1.930139	-0.688264
9	1	0	-1.263931	-2.510082	-1.565745
10	6	0	-2.105713	-0.506642	1.606652
11	1	0	-2.325346	0.035620	2.523038
12	6	0	-2.931377	-0.351541	0.500169
13	6	0	3.388604	-2.438625	-0.908782
14	6	0	-1.227480	3.495952	0.104579
15	1	0	-1.593519	4.476782	-0.223027
16	1	0	-1.165866	3.540873	1.200736
17	6	0	2.971888	-1.047563	-1.390401
18	1	0	3.377063	-0.892958	-2.397882
19	1	0	1.879240	-1.017499	-1.497591
20	6	0	0.632035	-0.273271	2.936239
21	1	0	1.353954	-0.138088	2.123323
22	1	0	1.162329	-0.460169	3.870790
23	1	0	0.025321	0.635648	3.038559
24	6	0	-3.327934	2.111381	0.686369
25	1	0	-4.091207	2.895407	0.623999
26	1	0	-2.919271	2.159508	1.704008
27	6	0	2.946698	-2.758049	0.520876
28	1	0	2.939720	-3.838083	0.691189

29	1	0	3.603330	-2.283857	1.253527
30	6	0	3.194027	2.625465	-0.079621
31	1	0	2.727476	2.371498	0.883722
32	1	0	4.267121	2.721927	0.124254
33	6	0	-3.987267	0.729816	0.490288
34	1	0	-4.713741	0.557307	1.292073
35	1	0	-4.531858	0.699429	-0.455331
36	6	0	-2.192146	2.375948	-0.305798
37	1	0	-1.601170	1.457169	-0.398016
38	1	0	-2.602426	2.568275	-1.304958
39	6	0	2.992200	1.464839	-1.057143
40	1	0	1.940177	1.415216	-1.362606
41	1	0	3.560888	1.665430	-1.975154
42	6	0	3.401297	0.106946	-0.487201
43	1	0	4.488252	0.079308	-0.326800
44	1	0	2.937127	-0.019929	0.499664
45	6	0	2.630197	3.970343	-0.575865
46	1	0	2.634357	3.979239	-1.674405
47	1	0	3.291128	4.785803	-0.263554
48	6	0	0.174325	3.232642	-0.446128
49	1	0	0.128775	3.131419	-1.540209
50	1	0	0.494253	2.254555	-0.062219
51	6	0	1.215254	4.282090	-0.070580
52	1	0	1.244014	4.375019	1.024218
53	1	0	0.900509	5.261122	-0.453464
54	1	0	4.481148	-2.533361	-0.938063
55	1	0	2.977653	-3.189395	-1.587275
56	8	0	-3.489193	-0.939386	-1.707951
57	6	0	-3.216080	-1.669987	-2.882845
58	1	0	-4.002257	-1.410704	-3.591486
59	1	0	-2.240997	-1.397929	-3.304910
60	1	0	-3.236571	-2.750080	-2.695508

Zero-point correction= 0.537390 (Hartree/Particle)
Thermal correction to Energy= 0.563450
Thermal correction to Enthalpy= 0.564394
Thermal correction to Gibbs Free Energy= 0.482129
Sum of electronic and zero-point Energies= -1158.691169
Sum of electronic and thermal Energies= -1158.665110
Sum of electronic and thermal Enthalpies= -1158.664166
Sum of electronic and thermal Free Energies= -1158.746430
M06-2X/6-311++G(d,p)/SMD// M06-2X//6-31G(d,p) energy in solvent (THF) = -1159.5492071

(R_p)-41

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.982081	-0.780557	-1.981520
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3	8	0	1.908897	-1.040331	1.997497
4	6	0	0.303011	-1.333075	0.271765
5	6	0	-2.060191	-1.519744	0.759390
6	6	0	0.008968	-1.105951	-1.072368
7	6	0	1.678548	-1.341846	0.847789
8	6	0	-0.741975	-1.520743	1.187103
9	1	0	-0.473360	-1.655652	2.227721
10	6	0	-1.325413	-1.104381	-1.488825
11	1	0	-1.534034	-0.897328	-2.535216
12	6	0	-2.370910	-1.304012	-0.600257
13	6	0	4.625255	-0.583186	-0.589013
14	6	0	-3.141444	2.481129	-0.602116
15	1	0	-3.185406	3.431472	-1.149085
16	1	0	-3.701091	2.644989	0.329373
17	6	0	3.845106	0.731707	-0.646286
18	1	0	4.318572	1.391400	-1.383602
19	1	0	2.841668	0.514060	-1.030556
20	6	0	1.418181	-1.869268	-2.781642
21	1	0	1.857673	-2.653436	-2.158143
22	1	0	2.173891	-1.472105	-3.460932
23	1	0	0.585926	-2.282849	-3.364442
24	6	0	-4.371384	0.202392	-0.592558
25	1	0	-5.463217	0.166307	-0.665815
26	1	0	-4.143270	0.352262	0.468987
27	6	0	3.988526	-1.611206	0.339502
28	1	0	4.449678	-2.594775	0.218360
29	1	0	4.049872	-1.319155	1.388666
30	6	0	1.312168	2.267832	0.645868
31	1	0	1.102801	1.546642	-0.157017
32	1	0	1.075949	1.752057	1.587711
33	6	0	-3.811568	-1.171301	-1.008284
34	1	0	-4.397029	-1.960846	-0.528388
35	1	0	-3.903370	-1.297021	-2.092555
36	6	0	-3.833511	1.386620	-1.424171
37	1	0	-3.126646	1.024652	-2.183113

38	1	0	-4.663478	1.832083	-1.982322
39	6	0	2.793591	2.659049	0.639867
40	1	0	3.003732	3.260834	-0.256242
41	1	0	2.977855	3.317467	1.497884
42	6	0	3.758111	1.471688	0.690340
43	1	0	4.761789	1.818522	0.968277
44	1	0	3.429700	0.794362	1.487578
45	6	0	0.423601	3.499835	0.473588
46	1	0	0.599907	3.917440	-0.527699
47	1	0	0.747967	4.271183	1.184804
48	6	0	-1.671406	2.201499	-0.278927
49	1	0	-1.109414	2.172821	-1.224113
50	1	0	-1.553350	1.205675	0.167877
51	6	0	-1.077000	3.266757	0.650243
52	1	0	-1.289464	2.996493	1.692767
53	1	0	-1.591979	4.220554	0.474112
54	1	0	5.653150	-0.411771	-0.244458
55	1	0	4.692046	-1.009712	-1.596438
56	8	0	-3.128692	-1.699922	1.583343
57	6	0	-2.866002	-1.877390	2.958659
58	1	0	-3.836217	-1.993537	3.440539
59	1	0	-2.260623	-2.774094	3.136207
60	1	0	-2.349295	-1.006970	3.380062

Zero-point correction= 0.539109 (Hartree/Particle)
Thermal correction to Energy= 0.565337
Thermal correction to Enthalpy= 0.566281
Thermal correction to Gibbs Free Energy= 0.484080
Sum of electronic and zero-point Energies= -1158.699098
Sum of electronic and thermal Energies= -1158.672870
Sum of electronic and thermal Enthalpies= -1158.671926
Sum of electronic and thermal Free Energies= -1158.754127
M06-2X/6-311++G(d,p)/SMD// M06-2X//6-31G(d,p) energy in solvent (THF) = -1159.5545543

TS_{rot}(41)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.380468	-0.635226	-1.151066
2	8	0	-0.348043	-2.881451	0.272394
3	8	0	1.411512	-4.033920	-0.553070
4	6	0	1.624314	-1.664825	-0.287520
5	6	0	3.509394	-0.188229	0.124461
6	6	0	0.949209	-0.585442	-0.831021
7	6	0	0.921424	-2.989288	-0.213693
8	6	0	2.952670	-1.468134	0.130291
9	1	0	3.502728	-2.320229	0.512201
10	6	0	1.546994	0.666018	-0.915389
11	1	0	0.934087	1.461805	-1.322423
12	6	0	2.787531	0.922987	-0.376127
13	6	0	-2.678396	-3.664384	0.307540
14	6	0	-0.288635	4.054769	0.060212
15	1	0	-0.549947	4.908549	0.695866
16	1	0	-0.193369	4.454955	-0.957379
17	6	0	-3.359403	-2.426779	0.923975
18	1	0	-4.191586	-2.786498	1.540870
19	1	0	-2.661662	-1.966134	1.632119
20	6	0	-1.107997	-0.150726	-0.025562
21	1	0	-1.361787	-0.974239	0.634458
22	1	0	-1.988342	0.345677	-0.401872
23	1	0	-0.510465	0.568950	0.536862
24	6	0	2.204793	3.417563	-0.515788
25	1	0	2.691605	4.398414	-0.542442
26	1	0	1.792680	3.273764	-1.521721
27	6	0	-1.400236	-3.477640	-0.508494
28	1	0	-1.057536	-4.450049	-0.874433
29	1	0	-1.570401	-2.814295	-1.365101
30	6	0	-4.192704	1.245824	-0.293557
31	1	0	-3.477053	1.154356	-1.120332
32	1	0	-5.176087	1.249468	-0.776291
33	6	0	3.285829	2.349162	-0.249692
34	1	0	4.133462	2.504440	-0.927991
35	1	0	3.695749	2.473824	0.760208
36	6	0	1.065752	3.443286	0.526355
37	1	0	0.883017	2.419073	0.871659
38	1	0	1.427146	3.981534	1.409405
39	6	0	-4.091121	0.014396	0.635662
40	1	0	-3.251122	0.176750	1.324188
41	1	0	-4.979870	-0.021121	1.278255
42	6	0	-3.896405	-1.356090	-0.050995
43	1	0	-4.844692	-1.697880	-0.482894
44	1	0	-3.209415	-1.247861	-0.898664
45	6	0	-3.966058	2.594164	0.448023
46	1	0	-3.735655	2.384114	1.501248

47	1	0	-4.906241	3.155116	0.461464
48	6	0	-1.432009	3.025298	0.109913
49	1	0	-1.385861	2.527296	1.089121
50	1	0	-1.220259	2.254759	-0.637181
51	6	0	-2.865363	3.539482	-0.089632
52	1	0	-3.044577	3.756455	-1.150455
53	1	0	-2.971813	4.495893	0.438851
54	1	0	-3.385928	-4.167305	-0.364905
55	1	0	-2.464046	-4.372463	1.115671
56	8	0	4.748237	0.106773	0.606524
57	6	0	5.508386	-0.954330	1.140191
58	1	0	6.451318	-0.519233	1.470160
59	1	0	5.001564	-1.417682	1.995444
60	1	0	5.706647	-1.722096	0.382854

Zero-point correction= 0.539135 (Hartree/Particle)
Thermal correction to Energy= 0.564119
Thermal correction to Enthalpy= 0.565063
Thermal correction to Gibbs Free Energy= 0.486454
Sum of electronic and zero-point Energies= -1158.646434
Sum of electronic and thermal Energies= -1158.621450
Sum of electronic and thermal Enthalpies= -1158.620506
Sum of electronic and thermal Free Energies= -1158.699115
M06-2X/6-311++G(d,p)/SMD// M06-2X//6-31G(d,p) energy in solvent (THF) = -1159.5083255

(R_p, *R*)-26

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.450325	-1.633212	-1.688353
2	8	0	2.038748	-1.679149	0.508189
3	8	0	1.216353	-0.498333	2.242755
4	6	0	-0.298049	-1.283502	0.595853
5	6	0	-2.681780	-1.239321	1.032370
6	6	0	-0.548240	-1.530701	-0.754442
7	6	0	1.050551	-1.097343	1.203238
8	6	0	-1.376328	-1.126140	1.480179
9	1	0	-1.138030	-0.907056	2.513541
10	6	0	-1.873613	-1.615478	-1.195481
11	1	0	-2.045622	-1.773920	-2.256898
12	6	0	-2.949888	-1.469968	-0.333911
13	6	0	3.996781	-0.435673	-0.196571
14	6	0	-3.721449	2.223003	-1.370488
15	1	0	-3.707388	2.985356	-2.159308
16	1	0	-4.393614	2.607974	-0.591054
17	6	0	3.131115	0.814915	-0.430451
18	1	0	3.556413	1.351493	-1.286220
19	1	0	2.139911	0.468705	-0.749482
20	6	0	0.829243	-2.976209	-1.956551
21	1	0	1.297815	-3.425840	-1.074990
22	1	0	1.547471	-2.943335	-2.776850
23	1	0	-0.040367	-3.572451	-2.258581
24	6	0	5.392040	-0.051803	0.297953
25	1	0	5.317705	0.400775	1.298919
26	6	0	-4.907767	0.007587	-0.829212
27	1	0	-5.995769	-0.022380	-0.948796
28	1	0	-4.722692	0.437689	0.161337
29	6	0	3.382148	-1.343511	0.874686
30	1	0	3.928237	-2.291019	0.930939
31	1	0	3.377261	-0.873274	1.860337
32	6	0	0.532062	2.471383	0.435535
33	1	0	0.394600	1.597675	-0.215551
34	1	0	0.235066	2.147019	1.442696
35	6	0	-4.373452	-1.436821	-0.817907
36	1	0	-4.995194	-2.046768	-0.155521
37	1	0	-4.431897	-1.865947	-1.824061
38	6	0	-4.287003	0.906776	-1.918100
39	1	0	-3.478870	0.371562	-2.434949
40	1	0	-5.042001	1.119572	-2.681864
41	6	0	2.001175	2.908067	0.445126
42	1	0	2.242903	3.358131	-0.528577
43	1	0	2.116302	3.709605	1.185607
44	6	0	3.012317	1.795293	0.736977
45	1	0	3.995642	2.248417	0.913516
46	1	0	2.719546	1.278750	1.659030
47	6	0	4.102925	-1.201649	-1.518405
48	1	0	3.100338	-1.415928	-1.899345
49	1	0	4.641511	-0.601558	-2.255545
50	6	0	-0.363195	3.611035	-0.052366
51	1	0	-0.071361	3.857645	-1.083038
52	1	0	-0.153274	4.508660	0.544314
53	6	0	-2.301391	2.093388	-0.811893
54	1	0	-1.615504	1.920378	-1.653661
55	1	0	-2.219060	1.202655	-0.174722
56	1	0	6.007232	-0.962318	0.389430

57	8	0	5.955881	0.854063	-0.627898
58	1	0	6.834286	1.098343	-0.321452
59	6	0	-1.867269	3.337653	-0.027959
60	1	0	-2.214259	3.247907	1.009913
61	1	0	-2.378350	4.216671	-0.442815
62	8	0	-3.774942	-1.116873	1.834580
63	6	0	-3.549808	-0.790819	3.189164
64	1	0	-4.533388	-0.710065	3.650820
65	1	0	-2.972171	-1.572100	3.697135
66	1	0	-3.020192	0.164762	3.283544
67	1	0	4.639106	-2.148734	-1.386044

Zero-point correction= 0.600445 (Hartree/Particle)
Thermal correction to Energy= 0.630621
Thermal correction to Enthalpy= 0.631565
Thermal correction to Gibbs Free Energy= 0.540908
Sum of electronic and zero-point Energies= -1312.417384
Sum of electronic and thermal Energies= -1312.387208
Sum of electronic and thermal Enthalpies= -1312.386264
Sum of electronic and thermal Free Energies= -1312.476921
M06-2X/6-311++G(d,p)/SMD// M06-2X//6-31G(d,p) energy in solvent (THF) = -1313.3858565

(*S*$_p$, *R*)-26

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.041388	-0.925303	2.834295
2	8	0	2.062099	-1.121875	1.125738
3	8	0	1.833256	-2.862597	-0.277200
4	6	0	-0.127888	-1.835709	0.598157
5	6	0	-2.282956	-2.050658	-0.494169
6	6	0	-0.747831	-1.272612	1.714763
7	6	0	1.343831	-2.025425	0.446531
8	6	0	-0.907349	-2.247922	-0.489958
9	1	0	-0.389672	-2.706667	-1.323561
10	6	0	-2.132191	-1.108897	1.707405
11	1	0	-2.602037	-0.686125	2.592545
12	6	0	-2.916244	-1.467537	0.618843
13	6	0	3.934721	-0.429319	-0.391348
14	6	0	-3.784969	2.330211	-0.920019
15	1	0	-3.996590	2.827616	-1.873855
16	1	0	-4.362371	2.875870	-0.160032
17	6	0	2.815407	0.443299	-0.983490
18	1	0	3.162135	0.811046	-1.955175
19	1	0	1.946649	-0.194284	-1.190682
20	6	0	0.172247	0.472263	2.945352
21	1	0	0.731126	0.843666	2.079766
22	1	0	0.752668	0.632432	3.855031
23	1	0	-0.779406	1.014964	3.020324
24	6	0	5.132007	0.452088	-0.014426
25	1	0	4.838666	1.144435	0.790198
26	6	0	-4.606720	0.357395	0.448941
27	1	0	-5.648270	0.614719	0.673445
28	1	0	-3.993915	0.879576	1.196280
29	6	0	3.480016	-1.135711	0.916393
30	1	0	3.831883	-2.170773	0.934385
31	1	0	3.868071	-0.613327	1.796088
32	6	0	0.625212	3.441630	0.247940
33	1	0	0.320103	3.181156	1.271900
34	1	0	1.528415	4.056450	0.352087
35	6	0	-4.391363	-1.153449	0.627150
36	1	0	-4.817617	-1.473299	1.584083
37	1	0	-4.901181	-1.706145	-0.165603
38	6	0	-4.245780	0.869357	-0.951404
39	1	0	-3.446031	0.252253	-1.380863
40	1	0	-5.110868	0.744350	-1.611528
41	6	0	1.016288	2.173105	-0.519818
42	1	0	0.271761	1.378697	-0.372840
43	1	0	1.021114	2.392359	-1.596974
44	6	0	2.393219	1.638069	-0.126228
45	1	0	3.137814	2.437216	-0.237223
46	1	0	2.388066	1.364686	0.937198
47	6	0	4.389593	-1.452322	-1.439526
48	1	0	3.554576	-2.079090	-1.755646
49	1	0	4.809865	-0.933485	-2.304229
50	6	0	-0.456765	4.305256	-0.416083
51	1	0	-0.257525	4.340070	-1.496021
52	1	0	-0.349853	5.335670	-0.057351
53	6	0	-2.287014	2.468403	-0.624906
54	1	0	-1.727400	2.185656	-1.526930
55	1	0	-1.988244	1.746557	0.150498
56	1	0	5.938459	-0.189914	0.377654
57	8	0	5.548758	1.159521	-1.162669
58	1	0	6.343027	1.657127	-0.946650
59	6	0	-1.912820	3.889275	-0.193955
60	1	0	-2.172177	4.015758	0.865961

61	1	0	-2.547581	4.597874	-0.742890
62	8	0	-3.092727	-2.378228	-1.539548
63	6	0	-2.492617	-2.991679	-2.659471
64	1	0	-3.298389	-3.187180	-3.366334
65	1	0	-1.750952	-2.332269	-3.126096
66	1	0	-2.009547	-3.936865	-2.384996
67	1	0	5.165051	-2.107589	-1.026936

Zero-point correction= 0.600457 (Hartree/Particle)
Thermal correction to Energy= 0.630587
Thermal correction to Enthalpy= 0.631531
Thermal correction to Gibbs Free Energy= 0.540949
Sum of electronic and zero-point Energies= -1312.407943
Sum of electronic and thermal Energies= -1312.377813
Sum of electronic and thermal Enthalpies= -1312.376868
Sum of electronic and thermal Free Energies= -1312.467450
M06-2X/6-311++G(d,p)/SMD// M06-2X//6-31G(d,p) energy in solvent (THF) = -1313.3791137

TS_{rot}(26)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.049601	-0.089712	-1.164486
2	8	0	-1.284878	-2.001378	0.205164
3	8	0	-0.461297	-3.926629	-0.644956
4	6	0	1.034552	-2.082815	-0.341793
5	6	0	3.421409	-1.920631	0.083195
6	6	0	1.079696	-0.798761	-0.857219
7	6	0	-0.286853	-2.791739	-0.288014
8	6	0	2.244835	-2.671087	0.067454
9	1	0	2.224283	-3.693917	0.424838
10	6	0	2.275175	-0.093166	-0.921116
11	1	0	2.213189	0.917872	-1.306406
12	6	0	3.445044	-0.584213	-0.386356
13	6	0	-3.678870	-1.390712	0.229455
14	6	0	2.632453	3.723048	0.126407
15	1	0	2.874185	4.562150	0.788861
16	1	0	2.952263	4.029931	-0.877757
17	6	0	-3.534795	0.019494	0.857852
18	1	0	-4.426168	0.172306	1.475407
19	1	0	-2.692698	-0.012059	1.558571
20	6	0	-0.387867	0.689751	-0.019248
21	1	0	-1.056468	0.130364	0.627529
22	1	0	-0.843943	1.599248	-0.375817
23	1	0	0.508640	0.943349	0.548843
24	6	0	-4.855637	-1.380417	-0.755161
25	1	0	-4.596607	-0.760635	-1.629099
26	6	0	4.353932	1.814254	-0.470974
27	1	0	5.305799	2.355993	-0.477770
28	1	0	3.941796	1.943866	-1.478925
29	6	0	-2.474555	-1.879654	-0.590495
30	1	0	-2.709581	-2.861409	-1.018192
31	1	0	-2.240244	-1.181086	-1.403916
32	6	0	-2.180961	3.553233	-0.281043
33	1	0	-1.634604	3.086974	-1.110804
34	1	0	-2.986958	4.117360	-0.762878
35	6	0	4.652065	0.319361	-0.229585
36	1	0	5.450852	-0.012325	-0.903852
37	1	0	5.048705	0.175728	0.783263
38	6	0	3.413782	2.452588	0.575246
39	1	0	2.688418	1.698463	0.902091
40	1	0	4.007509	2.682291	1.466816
41	6	0	-2.800310	2.463729	0.625045
42	1	0	-2.026430	2.121540	1.324848
43	1	0	-3.570122	2.921497	1.258803
44	6	0	-3.391542	1.227853	-0.090869
45	1	0	-4.376305	1.470359	-0.507473
46	1	0	-2.758306	0.964952	-0.948198
47	6	0	-3.958018	-2.392352	1.354241
48	1	0	-3.148983	-2.374768	2.089258
49	1	0	-4.898616	-2.145461	1.852140
50	6	0	-1.241950	4.529334	0.483664
51	1	0	-1.165919	4.200669	1.529038
52	1	0	-1.712581	5.517238	0.522261
53	6	0	1.110018	3.495549	0.143478
54	1	0	0.856699	3.038271	1.110560
55	1	0	0.875718	2.748552	-0.620777
56	1	0	-5.036457	-2.405728	-1.114225
57	8	0	-5.991474	-0.865757	-0.090658
58	1	0	-6.741556	-0.905637	-0.691634
59	6	0	0.199248	4.717864	-0.047908
60	1	0	0.174585	5.010195	-1.105513
61	1	0	0.635670	5.567872	0.492881
62	8	0	4.612412	-2.379839	0.557442
63	6	0	4.643542	-3.690087	1.078104
64	1	0	5.666834	-3.862951	1.410114

65	1	0	3.960618	-3.796563	1.929712
66	1	0	4.379267	-4.429288	0.312426
67	1	0	-4.030130	-3.411221	0.958770

Zero-point correction= 0.601095 (Hartree/Particle)
Thermal correction to Energy= 0.629907
Thermal correction to Enthalpy= 0.630851
Thermal correction to Gibbs Free Energy= 0.544436
Sum of electronic and zero-point Energies= -1312.364178
Sum of electronic and thermal Energies= -1312.335366
Sum of electronic and thermal Enthalpies= -1312.334422
Sum of electronic and thermal Free Energies= -1312.420837
M06-2X/6-311++G(d,p)/SMD// M06-2X//6-31G(d,p) energy in solvent (THF) = -1313.3392149

(R_p, R)-27

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.038133	-1.355279	-1.279846
2	8	0	1.340407	-0.619133	0.985518
3	8	0	0.031321	0.488747	2.447356
4	6	0	-1.014675	-0.926546	0.861778
5	6	0	-3.345598	-1.528926	1.144872
6	6	0	-1.046268	-1.419475	-0.442737
7	6	0	0.156592	-0.269427	1.511181
8	6	0	-2.179461	-0.972789	1.643487
9	1	0	-2.121483	-0.551948	2.639480
10	6	0	-2.239146	-1.954473	-0.941285
11	1	0	-2.249028	-2.303577	-1.970557
12	6	0	-3.394540	-2.018778	-0.177904
13	6	0	2.923307	1.051925	0.220514
14	6	0	-5.085201	1.075183	-1.872308
15	1	0	-5.206045	1.682024	-2.778257
16	1	0	-5.916099	1.353909	-1.209401
17	6	0	4.565509	-0.708465	-0.722023
18	6	0	1.763216	1.933904	-0.277176
19	1	0	2.111455	2.456324	-1.175628
20	1	0	0.959104	1.263331	-0.606478
21	6	0	0.768358	-2.572064	-1.321042
22	1	0	1.136168	-2.830371	-0.321435
23	1	0	1.612931	-2.416236	-1.994811
24	1	0	0.143826	-3.390273	-1.700692
25	6	0	4.079170	1.906395	0.737914
26	1	0	3.734949	2.506241	1.593209
27	6	0	-5.634620	-1.288338	-1.024147
28	1	0	-6.649469	-1.662823	-1.193489
29	1	0	-5.682692	-0.681312	-0.113256
30	6	0	2.482439	0.154472	1.381615
31	1	0	3.267895	-0.564150	1.632289
32	1	0	2.230580	0.736357	2.270317
33	6	0	5.866539	-0.228125	-0.908728
34	1	0	5.997296	0.796368	-1.249324
35	6	0	-1.293121	2.829277	0.116553
36	1	0	-1.100864	1.871448	-0.385427
37	1	0	-1.599652	2.577093	1.141390
38	6	0	-4.709327	-2.485913	-0.739151
39	1	0	-5.192756	-3.152698	-0.018733
40	1	0	-4.537217	-3.053558	-1.660058
41	6	0	-5.194057	-0.415017	-2.216915
42	1	0	-4.220092	-0.754679	-2.594764
43	1	0	-5.899989	-0.551573	-3.042506
44	6	0	-0.020910	3.682752	0.152704
45	1	0	0.193429	4.041598	-0.864377
46	1	0	-0.226346	4.578656	0.751916
47	6	0	1.225759	2.981094	0.699737
48	1	0	2.004834	3.734301	0.869189
49	1	0	0.988320	2.532563	1.671639
50	6	0	6.969805	-1.036921	-0.654952
51	1	0	7.971614	-0.646957	-0.807449
52	6	0	6.791477	-2.345343	-0.210387
53	1	0	7.651200	-2.978050	-0.013916
54	6	0	3.378981	0.185384	-0.982283
55	1	0	2.511691	-0.409564	-1.289957
56	1	0	3.618047	0.868688	-1.802639
57	6	0	-2.412023	3.570539	-0.616579
58	1	0	-2.088598	3.737948	-1.653685
59	1	0	-2.528258	4.567628	-0.171491
60	6	0	-3.752857	1.456425	-1.220897
61	1	0	-2.962053	1.371442	-1.980126
62	1	0	-3.488710	0.735385	-0.435725
63	6	0	4.401533	-2.022525	-0.274748
64	6	0	5.503009	-2.836182	-0.020211
65	1	0	4.890612	1.252479	1.091548
66	8	0	4.521077	2.736053	-0.321111
67	1	0	5.233414	3.294043	0.006139

68	6	0	-3.773076	2.874991	-0.640186
69	1	0	-4.194058	2.842388	0.373406
70	1	0	-4.459763	3.493511	-1.233312
71	1	0	5.354210	-3.854682	0.325188
72	1	0	3.395199	-2.406410	-0.124710
73	8	0	-4.505257	-1.624923	1.851303
74	6	0	-4.523262	-1.061396	3.145261
75	1	0	-5.531815	-1.211523	3.529061
76	1	0	-3.804070	-1.558287	3.807017
77	1	0	-4.298474	0.011402	3.112901

Zero-point correction= 0.683056 (Hartree/Particle)
Thermal correction to Energy= 0.717545
Thermal correction to Enthalpy= 0.718489
Thermal correction to Gibbs Free Energy= 0.617217
Sum of electronic and zero-point Energies= -1543.296256
Sum of electronic and thermal Energies= -1543.261767
Sum of electronic and thermal Enthalpies= -1543.260823
Sum of electronic and thermal Free Energies= -1543.362096
M06-2X/6-311++G(d,p)/SMD// M06-2X//6-31G(d,p) energy in solvent (THF) = -1544.4064706

(*S*$_p$, *R*)-27

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.038804	-0.631590	2.915325
2	8	0	1.109908	-0.189363	1.302774
3	8	0	1.557069	-2.019159	0.074497
4	6	0	-0.692783	-1.594215	0.729318
5	6	0	-2.597751	-2.490061	-0.473639
6	6	0	-1.530686	-1.211297	1.777400
7	6	0	0.772718	-1.323085	0.680917
8	6	0	-1.230013	-2.259975	-0.379122
9	1	0	-0.540985	-2.566555	-1.156804
10	6	0	-2.895002	-1.480346	1.683105
11	1	0	-3.532175	-1.196479	2.517579
12	6	0	-3.454377	-2.094852	0.570369
13	6	0	2.762081	0.992248	-0.154538
14	6	0	-5.355073	1.226317	-1.150891
15	1	0	-5.648795	1.616882	-2.132256
16	1	0	-6.124141	1.572130	-0.445458
17	6	0	4.812836	-0.483936	-0.729588
18	6	0	1.465210	1.492366	-0.814353
19	1	0	1.731254	1.931351	-1.782069
20	1	0	0.832635	0.622812	-1.035847
21	6	0	-1.279714	0.764547	2.980203
22	1	0	-0.801592	1.274209	2.136850
23	1	0	-0.846609	1.116915	3.917319
24	1	0	-2.355645	0.983420	2.971605
25	6	0	3.656518	2.181066	0.211540
26	1	0	3.115376	2.833249	0.913605
27	6	0	-5.608468	-0.882633	0.236527
28	1	0	-6.691363	-0.956060	0.389473
29	1	0	-5.237826	-0.184845	0.999754
30	6	0	2.468437	0.254867	1.177185
31	1	0	3.144648	-0.592587	1.313600
32	1	0	2.587667	0.935659	2.024964
33	6	0	5.992603	0.257487	-0.862349
34	1	0	5.936022	1.248477	-1.307266
35	6	0	-1.600059	3.684609	0.229992
36	1	0	-1.865847	3.356485	1.245362
37	1	0	-0.940036	4.552037	0.358891
38	6	0	-4.952055	-2.250094	0.480322
39	1	0	-5.322560	-2.671066	1.421218
40	1	0	-5.213586	-2.945482	-0.320771
41	6	0	-5.329021	-0.305856	-1.156913
42	1	0	-4.347193	-0.645281	-1.512081
43	1	0	-6.061974	-0.708925	-1.864032
44	6	0	-0.793772	2.589826	-0.478935
45	1	0	-1.259220	1.604839	-0.337726
46	1	0	-0.803684	2.780265	-1.561538
47	6	0	0.660604	2.517488	-0.012047
48	1	0	1.123567	3.507024	-0.120189
49	1	0	0.688400	2.278230	1.059064
50	6	0	7.211804	-0.258766	-0.434301
51	1	0	8.118225	0.328658	-0.546716
52	6	0	7.271598	-1.530209	0.131912
53	1	0	8.222161	-1.935226	0.464701
54	6	0	3.493413	0.089003	-1.187515
55	1	0	2.819717	-0.725693	-1.464021
56	1	0	3.663770	0.703758	-2.076835
57	6	0	-2.857737	4.158253	-0.512546
58	1	0	-2.615480	4.248104	-1.580443
59	1	0	-3.102108	5.171714	-0.173415
60	6	0	-3.999560	1.835257	-0.773789

61	1	0	-3.323703	1.736268	-1.634021
62	1	0	-3.538610	1.251433	0.037470
63	6	0	4.886289	-1.762190	-0.166941
64	6	0	6.106196	-2.280144	0.262657
65	1	0	4.558625	1.812442	0.723454
66	8	0	3.988691	2.879161	-0.972899
67	1	0	4.568896	3.611597	-0.742768
68	6	0	-4.119506	3.304996	-0.361054
69	1	0	-4.470349	3.351129	0.678830
70	1	0	-4.909933	3.772492	-0.963494
71	1	0	6.146688	-3.275227	0.695169
72	1	0	3.973504	-2.345601	-0.074452
73	8	0	-3.194969	-3.078517	-1.547011
74	6	0	-2.360834	-3.513671	-2.598571
75	1	0	-3.018798	-3.964013	-3.341114
76	1	0	-1.820172	-2.674502	-3.052609
77	1	0	-1.637317	-4.260301	-2.250599

Zero-point correction= 0.683169 (Hartree/Particle)
Thermal correction to Energy= 0.717518
Thermal correction to Enthalpy= 0.718463
Thermal correction to Gibbs Free Energy= 0.618079
Sum of electronic and zero-point Energies= -1543.287757
Sum of electronic and thermal Energies= -1543.253408
Sum of electronic and thermal Enthalpies= -1543.252463
Sum of electronic and thermal Free Energies= -1543.352847
M06-2X/6-311++G(d,p)/SMD// M06-2X//6-31G(d,p) energy in solvent (THF) = -1544.3996992

TS_{rot}(27)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.972396	0.205792	-1.201947
2	8	0	-1.146002	-0.706675	0.133076
3	8	0	-1.487338	-2.812863	-0.611837
4	6	0	0.764290	-2.054462	-0.384942
5	6	0	2.837336	-3.245402	0.051065
6	6	0	1.516603	-1.010659	-0.894872
7	6	0	-0.727411	-1.926555	-0.318444
8	6	0	1.442974	-3.216553	0.026662
9	1	0	0.854553	-4.055487	0.379360
10	6	0	2.903643	-1.085913	-0.947644
11	1	0	3.415365	-0.208596	-1.325746
12	6	0	3.600923	-2.143852	-0.408914
13	6	0	-2.797583	1.134739	0.070809
14	6	0	5.306739	1.880677	0.223718
15	1	0	5.948215	2.426640	0.924952
16	1	0	5.778372	1.986543	-0.761753
17	6	0	-4.740257	-0.447263	0.702831
18	6	0	-1.908629	2.210018	0.750801
19	1	0	-2.582758	2.834178	1.346386
20	1	0	-1.259461	1.702444	1.473973
21	6	0	1.111710	1.035963	-0.051074
22	1	0	0.231455	0.949278	0.578011
23	1	0	1.256018	2.045694	-0.400816
24	1	0	1.983614	0.736795	0.532791
25	6	0	-3.697228	1.819006	-0.963826
26	1	0	-3.069376	2.245222	-1.761922
27	6	0	5.683554	-0.644739	-0.437749
28	1	0	6.776352	-0.718037	-0.432594
29	1	0	5.424317	-0.283636	-1.440244
30	6	0	-2.038072	0.047608	-0.709411
31	1	0	-2.758499	-0.642989	-1.162008
32	1	0	-1.422662	0.496109	-1.499094
33	6	0	-6.024947	0.044978	0.449207
34	1	0	-6.219224	1.102258	0.613189
35	6	0	1.219662	4.414472	-0.245355
36	1	0	1.440889	3.744605	-1.086134
37	1	0	0.872305	5.341453	-0.714462
38	6	0	5.104628	-2.061128	-0.236994
39	1	0	5.593118	-2.761921	-0.924787
40	1	0	5.346777	-2.425123	0.769153
41	6	0	5.238286	0.378824	0.629072
42	1	0	4.209116	0.148595	0.928750
43	1	0	5.841560	0.212251	1.528242
44	6	0	0.076725	3.827065	0.614675
45	1	0	0.511985	3.098624	1.311380
46	1	0	-0.331966	4.618929	1.254822
47	6	0	-1.076037	3.142880	-0.153983
48	1	0	-1.739496	3.902778	-0.583667
49	1	0	-0.667961	2.584530	-1.006322
50	6	0	-7.031418	-0.795887	-0.016509
51	1	0	-8.024471	-0.398127	-0.203350
52	6	0	-6.766807	-2.145932	-0.236895
53	1	0	-7.550735	-2.803900	-0.598586

54	6	0	-3.653592	0.481120	1.187413
55	1	0	-2.969428	-0.060633	1.850124
56	1	0	-4.108123	1.287906	1.769974
57	6	0	2.520040	4.690348	0.561900
58	1	0	2.372990	4.351845	1.596485
59	1	0	2.674001	5.772376	0.628233
60	6	0	3.913127	2.533892	0.210261
61	1	0	3.418593	2.271734	1.156372
62	1	0	3.329282	2.058639	-0.583862
63	6	0	-4.486304	-1.803135	0.478869
64	6	0	-5.491144	-2.645576	0.009301
65	1	0	-4.368601	1.077365	-1.419040
66	8	0	-4.434263	2.832970	-0.304862
67	1	0	-5.039240	3.228594	-0.940147
68	6	0	3.838054	4.060101	0.051739
69	1	0	4.008655	4.341485	-0.995300
70	1	0	4.657334	4.512291	0.625933
71	1	0	-5.272838	-3.694587	-0.164588
72	1	0	-3.489279	-2.198964	0.652780
73	8	0	3.570503	-4.289240	0.526508
74	6	0	2.866383	-5.402341	1.031187
75	1	0	3.620124	-6.116911	1.360535
76	1	0	2.233659	-5.121303	1.881758
77	1	0	2.241627	-5.862586	0.256401

Zero-point correction= 0.684200 (Hartree/Particle)
Thermal correction to Energy= 0.717140
Thermal correction to Enthalpy= 0.718084
Thermal correction to Gibbs Free Energy= 0.621485
Sum of electronic and zero-point Energies= -1543.243275
Sum of electronic and thermal Energies= -1543.210335
Sum of electronic and thermal Enthalpies= -1543.209391
Sum of electronic and thermal Free Energies= -1543.305990

M06-2X/6-311++G(d,p)/SMD// M06-2X//6-31G(d,p) energy in solvent (THF) = -1544.358664

(R_p, R)-30

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.155376	-0.958319	-1.374878
2	8	0	0.003515	-0.219948	0.961358
3	8	0	-1.453717	0.570359	2.487489
4	6	0	-2.289699	-0.822702	0.764163
5	6	0	-4.533771	-1.722891	0.940541
6	6	0	-2.239097	-1.213378	-0.574082
7	6	0	-1.220624	-0.078660	1.491631
8	6	0	-3.452503	-1.071461	1.509843
9	1	0	-3.462369	-0.726339	2.536070
10	6	0	-3.350121	-1.845777	-1.142866
11	1	0	-3.300039	-2.111896	-2.195523
12	6	0	-4.501886	-2.107484	-0.417048
13	6	0	1.352772	1.713275	0.382468
14	6	0	-6.543748	0.890630	-1.896777
15	1	0	-6.721634	1.552123	-2.753703
16	1	0	-7.418977	1.003189	-1.241907
17	6	0	3.189919	0.257810	-0.680206
18	6	0	0.090284	2.483330	-0.046183
19	1	0	0.371032	3.129663	-0.885931
20	1	0	-0.617179	1.747718	-0.450468
21	6	0	-0.277645	-2.069283	-1.475834
22	1	0	0.090823	-2.357955	-0.483819
23	1	0	0.561263	-1.758929	-2.102167
24	1	0	-0.782961	-2.926594	-1.937909
25	6	0	2.390628	2.650331	1.000353
26	1	0	1.963757	3.124770	1.896096
27	6	0	-6.800711	-1.584359	-1.259121
28	1	0	-7.759221	-2.062224	-1.486717
29	1	0	-6.938909	-1.066086	-0.303768
30	6	0	1.028072	0.659936	1.447756
31	1	0	1.900483	0.031387	1.648116
32	1	0	0.692994	1.119133	2.379860
33	6	0	4.426029	0.900102	-0.750731
34	1	0	4.434459	1.959202	-0.999974
35	6	0	-3.058472	2.933805	0.360367
36	1	0	-2.733086	2.057730	-0.216521
37	1	0	-3.348395	2.553234	1.349752
38	6	0	-5.741338	-2.681557	-1.046433
39	1	0	-6.151358	-3.457753	-0.393169
40	1	0	-5.487237	-3.147709	-2.004569
41	6	0	-6.448870	-0.566885	-2.363700
42	1	0	-5.429833	-0.746530	-2.732483
43	1	0	-7.110548	-0.723821	-3.221688
44	6	0	-1.909817	3.937452	0.508457
45	1	0	-1.733426	4.419086	-0.464198
46	1	0	-2.237601	4.736061	1.185735

47	6	0	-0.587242	3.353194	1.014092
48	1	0	0.084834	4.181118	1.270827
49	1	0	-0.772712	2.785750	1.933605
50	6	0	5.616830	0.223475	-0.481002
51	6	0	5.547591	-1.135552	-0.154925
52	6	0	1.915739	1.032677	-0.893411
53	1	0	1.126598	0.376898	-1.278723
54	1	0	2.086001	1.819291	-1.634556
55	6	0	-4.250984	3.587129	-0.339579
56	1	0	-3.932021	3.888852	-1.347268
57	1	0	-4.506859	4.516059	0.187158
58	6	0	-5.287604	1.381207	-1.171128
59	1	0	-4.477116	1.470209	-1.908790
60	1	0	-4.946273	0.631132	-0.445050
61	6	0	3.159545	-1.096189	-0.352617
62	6	0	4.327446	-1.814590	-0.086785
63	1	0	3.270885	2.069296	1.315339
64	8	0	2.746660	3.620622	0.031730
65	1	0	3.361723	4.241171	0.435107
66	6	0	-5.507238	2.725573	-0.468001
67	1	0	-5.940892	2.545671	0.524587
68	1	0	-6.257622	3.301325	-1.026038
69	1	0	2.192321	-1.589103	-0.292049
70	8	0	-5.683851	-2.014176	1.608104
71	6	0	-5.789978	-1.563417	2.941420
72	1	0	-6.778247	-1.864584	3.287276
73	1	0	-5.025341	-2.021933	3.579509
74	1	0	-5.697393	-0.472295	2.998996
75	1	0	6.462722	-1.674397	0.055305
76	6	0	4.218415	-3.297032	0.280885
77	6	0	6.937612	0.997232	-0.531379
78	6	0	5.586900	-3.933808	0.540700
79	1	0	5.458769	-4.990591	0.793880
80	1	0	6.230584	-3.876385	-0.342775
81	1	0	6.102879	-3.449656	1.375787
82	6	0	3.540322	-4.058702	-0.870278
83	1	0	2.533744	-3.675639	-1.063950
84	1	0	4.120679	-3.964463	-1.793028
85	1	0	3.454034	-5.122177	-0.622712
86	6	0	3.365724	-3.440362	1.553322
87	1	0	3.824997	-2.904211	2.389555
88	1	0	2.357332	-3.039334	1.409086
89	1	0	3.272397	-4.495905	1.830763
90	6	0	8.143408	0.119536	-0.183823
91	1	0	9.057352	0.719834	-0.225153
92	1	0	8.061326	-0.297013	0.825142
93	1	0	8.255694	-0.708507	-0.890754
94	6	0	7.143634	1.567672	-1.944036
95	1	0	7.192205	0.761952	-2.682746
96	1	0	6.327119	2.236942	-2.228868
97	1	0	8.079248	2.135296	-1.990935
98	6	0	6.875866	2.154699	0.480601
99	1	0	7.807209	2.730716	0.457773
100	1	0	6.050345	2.837598	0.256501
101	1	0	6.731264	1.771453	1.495724

Zero-point correction= 0.909885 (Hartree/Particle)
Thermal correction to Energy= 0.955375
Thermal correction to Enthalpy= 0.956319
Thermal correction to Gibbs Free Energy= 0.831611
Sum of electronic and zero-point Energies= -1857.439949
Sum of electronic and thermal Energies= -1857.394458
Sum of electronic and thermal Enthalpies= -1857.393514
Sum of electronic and thermal Free Energies= -1857.518223
M06-2X/6-311++G(d,p)/SMD// M06-2X//6-31G(d,p) energy in solvent (THF) = -1858.8502352

(S_p, *R*)-30

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.430033	-0.844217	2.787349
2	8	0	-0.345860	-0.042478	1.219821
3	8	0	0.264573	-1.731266	-0.136151
4	6	0	-2.019400	-1.537714	0.514165
5	6	0	-3.852914	-2.438590	-0.790660
6	6	0	-2.882149	-1.331684	1.591102
7	6	0	-0.579874	-1.148756	0.508338
8	6	0	-2.505347	-2.120742	-0.662095
9	1	0	-1.796449	-2.291198	-1.463298
10	6	0	-4.222710	-1.688815	1.459214
11	1	0	-4.878865	-1.544327	2.314465
12	6	0	-4.735791	-2.219946	0.282942
13	6	0	1.190873	1.434086	-0.080473
14	6	0	-6.906761	1.135294	-1.023905
15	1	0	-7.238478	1.616785	-1.951239

16	1	0	-7.698889	1.324073	-0.285227
17	6	0	3.320722	0.183023	-0.834089
18	6	0	-0.148645	1.916716	-0.663166
19	1	0	0.069126	2.490698	-1.570451
20	1	0	-0.719409	1.035933	-0.985413
21	6	0	-2.786419	0.510037	3.011629
22	1	0	-2.355459	1.151576	2.235647
23	1	0	-2.380520	0.786363	3.985723
24	1	0	-3.876784	0.638741	3.022425
25	6	0	2.009912	2.628842	0.419675
26	1	0	1.430933	3.159712	1.190430
27	6	0	-6.977873	-1.141812	0.091596
28	1	0	-8.051457	-1.316049	0.227722
29	1	0	-6.659373	-0.517186	0.937264
30	6	0	0.969663	0.527069	1.156835
31	1	0	1.717579	-0.269030	1.199433
32	1	0	1.032773	1.115386	2.076896
33	6	0	4.432605	1.026662	-0.852560
34	1	0	4.288887	2.050198	-1.193151
35	6	0	-3.361595	3.707536	0.663365
36	1	0	-3.586691	3.231278	1.628658
37	1	0	-2.772877	4.602746	0.901383
38	6	0	-6.218179	-2.474892	0.167098
39	1	0	-6.551631	-3.036593	1.046442
40	1	0	-6.429921	-3.083287	-0.715294
41	6	0	-6.748891	-0.376937	-1.217697
42	1	0	-5.741150	-0.585202	-1.600667
43	1	0	-7.444309	-0.751492	-1.976542
44	6	0	-2.478719	2.782585	-0.182591
45	1	0	-2.860671	1.752824	-0.166914
46	1	0	-2.519019	3.107542	-1.231980
47	6	0	-1.016487	2.769409	0.265112
48	1	0	-0.633985	3.798382	0.279109
49	1	0	-0.954494	2.402459	1.297967
50	6	0	5.687970	0.588290	-0.428214
51	6	0	5.814202	-0.736289	0.004285
52	6	0	1.959786	0.706770	-1.221341
53	1	0	1.336912	-0.117426	-1.579005
54	1	0	2.069597	1.427761	-2.037511
55	6	0	-4.663329	4.166659	-0.009251
56	1	0	-4.441575	4.415987	-1.056011
57	1	0	-4.987743	5.102497	0.460660
58	6	0	-5.606204	1.806845	-0.567596
59	1	0	-4.930816	1.875455	-1.431049
60	1	0	-5.091545	1.166652	0.164966
61	6	0	3.485807	-1.136341	-0.415330
62	6	0	4.726830	-1.614788	0.013672
63	1	0	2.937670	2.264710	0.887376
64	8	0	2.290719	3.479824	-0.675214
65	1	0	2.812862	4.223024	-0.356691
66	6	0	-5.847267	3.196723	0.028601
67	1	0	-6.192141	3.079764	1.064922
68	1	0	-6.679432	3.668260	-0.511097
69	1	0	2.614873	-1.786664	-0.420428
70	8	0	-4.405702	-2.951030	-1.925050
71	6	0	-3.541549	-3.213833	-3.008937
72	1	0	-4.164406	-3.631617	-3.799229
73	1	0	-3.063081	-2.295432	-3.369933
74	1	0	-2.765785	-3.938031	-2.733584
75	1	0	6.780081	-1.090266	0.341634
76	6	0	6.863098	1.570537	-0.442616
77	6	0	4.835617	-3.068802	0.481312
78	6	0	3.848613	-3.301455	1.638497
79	1	0	2.815669	-3.111432	1.331978
80	1	0	3.911551	-4.337952	1.987211
81	1	0	4.080118	-2.641250	2.480541
82	6	0	4.477028	-4.003664	-0.685781
83	1	0	3.460274	-3.820841	-1.044439
84	1	0	5.164112	-3.856377	-1.524776
85	1	0	4.540979	-5.049587	-0.366434
86	6	0	6.243967	-3.420669	0.969165
87	1	0	6.986007	-3.308496	0.172144
88	1	0	6.546035	-2.792169	1.813139
89	1	0	6.266720	-4.462845	1.302097
90	6	0	6.510590	2.792947	0.422280
91	1	0	7.339054	3.509551	0.426534
92	1	0	5.622064	3.307285	0.042557
93	1	0	6.310976	2.490475	1.455185
94	6	0	7.124324	2.029049	-1.886731
95	1	0	6.244051	2.515237	-2.316330
96	1	0	7.955554	2.742266	-1.915369
97	1	0	7.380567	1.175268	-2.521226
98	6	0	8.150358	0.949478	0.108080
99	1	0	8.025542	0.618348	1.143935
100	1	0	8.471291	0.092239	-0.491795
101	1	0	8.954357	1.691638	0.087016

Zero-point correction= 0.909601 (Hartree/Particle)
Thermal correction to Energy= 0.955178
Thermal correction to Enthalpy= 0.956122
Thermal correction to Gibbs Free Energy= 0.831139
Sum of electronic and zero-point Energies= -1857.431298
Sum of electronic and thermal Energies= -1857.385721
Sum of electronic and thermal Enthalpies= -1857.384777
Sum of electronic and thermal Free Energies= -1857.509760
M06-2X/6-311++G(d,p)/SMD// M06-2X//6-31G(d,p) energy in solvent (THF) = -1858.8427723

TS_{rot}(30)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.410513	-0.269185	-1.182218
2	8	0	-0.228237	0.348081	0.201477
3	8	0	0.358260	2.438596	-0.422622
4	6	0	-1.966462	1.919971	-0.267958
5	6	0	-3.903774	3.308827	0.204785
6	6	0	-2.820743	0.987051	-0.830859
7	6	0	-0.500130	1.624607	-0.189103
8	6	0	-2.520549	3.130102	0.189694
9	1	0	-1.850164	3.883067	0.587403
10	6	0	-4.190348	1.216967	-0.894063
11	1	0	-4.789125	0.418642	-1.316578
12	6	0	-4.776072	2.318408	-0.311709
13	6	0	1.212961	-1.655196	0.120595
14	6	0	-6.913535	-1.525618	0.105518
15	1	0	-7.634698	-2.026934	0.760996
16	1	0	-7.362853	-1.529144	-0.895931
17	6	0	3.329405	-0.377310	0.853207
18	6	0	0.192232	-2.650127	0.735004
19	1	0	0.776005	-3.365102	1.323953
20	1	0	-0.418674	-2.099648	1.460011
21	6	0	-2.659574	-1.121850	-0.065937
22	1	0	-1.790834	-1.146210	0.584011
23	1	0	-2.894602	-2.098706	-0.456513
24	1	0	-3.511457	-0.757009	0.509843
25	6	0	2.076730	-2.400054	-0.903336
26	1	0	1.442197	-2.727887	-1.742088
27	6	0	-7.008771	1.056386	-0.425527
28	1	0	-8.087105	1.248159	-0.420066
29	1	0	-6.782183	0.719620	-1.444317
30	6	0	0.593580	-0.474518	-0.648938
31	1	0	1.393715	0.143743	-1.071944
32	1	0	-0.052661	-0.832077	-1.459838
33	6	0	4.534287	-1.071355	0.743309
34	1	0	4.539352	-2.128385	0.998650
35	6	0	-3.127306	-4.458865	-0.420975
36	1	0	-3.264209	-3.719875	-1.220697
37	1	0	-2.869666	-5.387179	-0.942378
38	6	0	-6.281714	2.389962	-0.152601
39	1	0	-6.684780	3.172002	-0.807374
40	1	0	-6.493933	2.728864	0.868946
41	6	0	-6.686771	-0.062586	0.588717
42	1	0	-5.641825	0.039095	0.904004
43	1	0	-7.276522	0.120946	1.493478
44	6	0	-1.945233	-4.045272	0.486253
45	1	0	-2.312496	-3.309845	1.214049
46	1	0	-1.638845	-4.909406	1.088900
47	6	0	-0.708345	-3.452901	-0.227189
48	1	0	-0.114464	-4.258327	-0.675224
49	1	0	-1.034771	-2.820663	-1.062594
50	6	0	5.697259	-0.447325	0.290173
51	6	0	5.630732	0.909504	-0.040137
52	6	0	2.085492	-1.114341	1.285706
53	1	0	1.450946	-0.463314	1.897325
54	1	0	2.378388	-1.966809	1.905712
55	6	0	-4.462935	-4.644386	0.353697
56	1	0	-4.299173	-4.383935	1.408131
57	1	0	-4.730526	-5.706097	0.353534
58	6	0	-5.603263	-2.333427	0.092515
59	1	0	-5.105849	-2.169557	1.059232
60	1	0	-4.950122	-1.895581	-0.668213
61	6	0	3.295783	0.974976	0.512135
62	6	0	4.440955	1.638397	0.060729
63	1	0	2.844756	-1.722802	-1.302212
64	8	0	2.670094	-3.511831	-0.256500
65	1	0	3.296263	-3.915404	-0.865891
66	6	0	-5.697172	-3.849412	-0.134790
67	1	0	-5.884570	-4.061611	-1.195143
68	1	0	-6.568688	-4.233154	0.411448
69	1	0	2.352179	1.511039	0.583159
70	8	0	-4.525575	4.402676	0.723631
71	6	0	-3.710388	5.413516	1.274700
72	1	0	-4.385771	6.189465	1.633501

73	1	0	-3.114420	5.031871	2.112574
74	1	0	-3.037440	5.836988	0.519553
75	1	0	6.525255	1.410811	-0.386322
76	6	0	6.980458	-1.272440	0.154780
77	6	0	4.343824	3.108387	-0.359163
78	6	0	7.369765	-1.846149	1.527154
79	1	0	6.580938	-2.486135	1.931613
80	1	0	8.283038	-2.445175	1.442944
81	1	0	7.550797	-1.040074	2.244451
82	6	0	6.726832	-2.430252	-0.826443
83	1	0	7.628257	-3.042820	-0.936027
84	1	0	5.917715	-3.077627	-0.474256
85	1	0	6.448976	-2.044806	-1.812609
86	6	0	8.155750	-0.443787	-0.372531
87	1	0	7.943809	-0.027979	-1.362645
88	1	0	8.398634	0.382028	0.303434
89	1	0	9.043565	-1.077926	-0.458119
90	6	0	3.636033	3.927994	0.732446
91	1	0	3.604302	4.983401	0.441420
92	1	0	2.604922	3.596243	0.878351
93	1	0	4.166707	3.849881	1.686525
94	6	0	3.518660	3.189048	-1.655686
95	1	0	3.443894	4.229510	-1.991761
96	1	0	3.993176	2.604631	-2.450690
97	1	0	2.505496	2.809081	-1.496869
98	6	0	5.721393	3.730122	-0.611455
99	1	0	6.361785	3.661637	0.274209
100	1	0	6.237050	3.248917	-1.448405
101	1	0	5.603788	4.788533	-0.863098

Zero-point correction= 0.911316 (Hartree/Particle)
Thermal correction to Energy= 0.955241
Thermal correction to Enthalpy= 0.956185
Thermal correction to Gibbs Free Energy= 0.836351
Sum of electronic and zero-point Energies= -1857.387629
Sum of electronic and thermal Energies= -1857.343704
Sum of electronic and thermal Enthalpies= -1857.342760
Sum of electronic and thermal Free Energies= -1857.462594
M06-2X/6-311++G(d,p)/SMD// M06-2X//6-31G(d,p) energy in solvent (THF) = -1858.8011867

(R_p, *R*)-31

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.869684	-1.205747	-1.263922
2	8	0	0.183754	-0.529187	1.120055
3	8	0	-1.302068	-0.027714	2.737066
4	6	0	-2.070471	-1.241791	0.851775
5	6	0	-4.333720	-2.120373	0.862729
6	6	0	-1.976816	-1.512373	-0.515653
7	6	0	-1.039152	-0.538560	1.670233
8	6	0	-3.260848	-1.549833	1.528971
9	1	0	-3.305273	-1.300753	2.581901
10	6	0	-3.076618	-2.065684	-1.177488
11	1	0	-2.994982	-2.219818	-2.250132
12	6	0	-4.261768	-2.364871	-0.523892
13	6	0	1.378612	1.538338	0.693891
14	6	0	-6.997392	0.746885	-1.929819
15	1	0	-7.859233	0.462154	-2.546360
16	1	0	-7.384548	0.880581	-0.910956
17	6	0	3.251528	0.334159	-0.600693
18	6	0	0.063082	2.288675	0.406305
19	1	0	0.268132	3.027828	-0.377251
20	1	0	-0.634927	1.562546	-0.031132
21	6	0	0.050255	-2.283356	-1.351757
22	1	0	0.387992	-2.586054	-0.353404
23	1	0	0.902978	-1.926977	-1.933124
24	1	0	-0.406176	-3.143919	-1.856919
25	6	0	2.413942	2.455453	1.344755
26	1	0	2.031257	2.812039	2.312329
27	6	0	-6.536068	-1.690314	-1.362924
28	1	0	-7.374034	-2.034444	-1.981115
29	1	0	-6.935116	-1.507399	-0.359030
30	6	0	1.149105	0.378211	1.670911
31	1	0	2.068314	-0.198410	1.808720
32	1	0	0.798658	0.730897	2.643416
33	6	0	4.410176	1.082939	-0.775093
34	1	0	4.302608	2.145771	-0.980262
35	6	0	-2.986241	2.768808	0.653197
36	1	0	-2.691911	2.405374	-0.339035
37	1	0	-3.076924	1.879730	1.294851
38	6	0	-5.486057	-2.814820	-1.276335
39	1	0	-5.929938	-3.685215	-0.782887
40	1	0	-5.187995	-3.118597	-2.285800
41	6	0	-5.974911	-0.385415	-1.922474

42	1	0	-5.112697	-0.085649	-1.315542
43	1	0	-5.589157	-0.546118	-2.940280
44	6	0	-1.902213	3.697132	1.207581
45	1	0	-1.698623	4.483495	0.467717
46	1	0	-2.297449	4.208064	2.095323
47	6	0	-0.590932	3.003579	1.588224
48	1	0	0.097240	3.763846	1.977024
49	1	0	-0.789941	2.296592	2.402000
50	6	0	5.680547	0.506535	-0.654553
51	6	0	5.757080	-0.856077	-0.374083
52	6	0	1.901787	1.002524	-0.665358
53	1	0	1.144029	0.311709	-1.052626
54	1	0	1.955342	1.853540	-1.350623
55	6	0	-4.337072	3.482438	0.564548
56	1	0	-4.196971	4.448575	0.058596
57	1	0	-4.671462	3.719358	1.582350
58	6	0	-5.202237	2.578678	-1.671500
59	1	0	-4.924689	3.564611	-2.066377
60	1	0	-4.344913	1.923753	-1.867027
61	6	0	3.366912	-1.031581	-0.316217
62	6	0	4.610917	-1.647177	-0.202882
63	1	0	3.335323	1.885895	1.538175
64	8	0	2.664208	3.537474	0.465693
65	1	0	3.302495	4.125192	0.882330
66	6	0	-5.433132	2.700448	-0.162869
67	1	0	-5.521918	1.700591	0.285597
68	1	0	-6.398475	3.197987	0.002680
69	1	0	2.453200	-1.599454	-0.175821
70	8	0	-5.512107	-2.452844	1.457975
71	6	0	-5.639515	-2.189716	2.838681
72	1	0	-6.637732	-2.523323	3.120314
73	1	0	-4.891894	-2.742233	3.420086
74	1	0	-5.538406	-1.118724	3.051285
75	1	0	6.730465	-1.326278	-0.280115
76	6	0	4.765248	-3.138022	0.110786
77	6	0	6.915935	1.396821	-0.811909
78	6	0	5.527812	-3.302000	1.436069
79	1	0	5.650539	-4.363821	1.675343
80	1	0	6.522630	-2.850822	1.384362
81	1	0	4.983131	-2.824770	2.256558
82	6	0	5.554054	-3.821653	-1.018329
83	1	0	5.030864	-3.717692	-1.973773
84	1	0	6.551602	-3.388128	-1.131774
85	1	0	5.673018	-4.889150	-0.804072
86	6	0	3.410689	-3.841713	0.244548
87	1	0	2.811150	-3.412770	1.054547
88	1	0	2.832957	-3.776877	-0.683703
89	1	0	3.567775	-4.901117	0.469000
90	6	0	8.222507	0.617109	-0.638296
91	1	0	9.073349	1.295330	-0.754829
92	1	0	8.290569	0.161338	0.354624
93	1	0	8.319437	-0.173764	-1.388841
94	6	0	6.913485	2.034574	-2.210798
95	1	0	6.940078	1.263444	-2.986520
96	1	0	6.020486	2.644307	-2.372362
97	1	0	7.790600	2.678874	-2.334861
98	6	0	6.867528	2.506212	0.253309
99	1	0	7.732774	3.169990	0.151070
100	1	0	5.961260	3.111662	0.154434
101	1	0	6.879490	2.075449	1.259512
102	6	0	-6.429748	2.074086	-2.440496
103	1	0	-6.168437	1.968698	-3.501023
104	1	0	-7.216482	2.837552	-2.390065

Zero-point correction= 0.938225 (Hartree/Particle)
Thermal correction to Energy= 0.985142
Thermal correction to Enthalpy= 0.986086
Thermal correction to Gibbs Free Energy= 0.857097
Sum of electronic and zero-point Energies= -1896.709839
Sum of electronic and thermal Energies= -1896.662921
Sum of electronic and thermal Enthalpies= -1896.661977
Sum of electronic and thermal Free Energies= -1896.790967
M06-2X/6-311++G(d,p)/SMD// M06-2X//6-31G(d,p) energy in solvent (THF) = -1898.1585692

(*S*$_p$, *R*)-31

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.572913	-0.753311	-2.379400
2	8	0	0.296703	-0.101014	-1.071413
3	8	0	-0.615114	-1.981103	-0.222724
4	6	0	1.755339	-1.805849	-0.387565
5	6	0	3.301435	-2.983142	1.053318
6	6	0	2.810699	-1.432118	-1.215707
7	6	0	0.351813	-1.339663	-0.570284

8	6	0	2.002506	-2.620181	0.725201
9	1	0	1.151693	-2.924820	1.322634
10	6	0	4.110627	-1.806468	-0.873603
11	1	0	4.917215	-1.492249	-1.528307
12	6	0	4.387575	-2.546594	0.267686
13	6	0	-1.280569	1.418679	0.082175
14	6	0	7.238221	0.395602	-0.703872
15	1	0	8.268488	0.128700	-0.971998
16	1	0	6.632644	0.209828	-1.604186
17	6	0	-3.457959	0.181435	0.734522
18	6	0	0.014986	1.919451	0.748278
19	1	0	-0.268457	2.466587	1.654057
20	1	0	0.593380	1.045864	1.075400
21	6	0	3.095733	0.562376	-2.404094
22	1	0	2.757689	1.129474	-1.528389
23	1	0	2.718865	1.034173	-3.312927
24	1	0	4.193421	0.561039	-2.430102
25	6	0	-2.108474	2.605230	-0.420912
26	1	0	-1.524479	3.157592	-1.172221
27	6	0	6.874191	-2.016318	0.047403
28	1	0	7.859953	-2.387021	0.347117
29	1	0	6.836554	-2.140019	-1.042324
30	6	0	-0.974474	0.554018	-1.160984
31	1	0	-1.763263	-0.183303	-1.334232
32	1	0	-0.880685	1.186071	-2.049177
33	6	0	-4.545831	1.047156	0.861383
34	1	0	-4.368616	2.026757	1.299711
35	6	0	3.121199	4.106914	-0.154129
36	1	0	3.375139	3.753174	-1.164446
37	1	0	2.501990	5.000105	-0.299071
38	6	0	5.797394	-2.883749	0.700899
39	1	0	5.988323	-3.946345	0.505702
40	1	0	5.846521	-2.775854	1.790695
41	6	0	6.743944	-0.527431	0.407369
42	1	0	5.693946	-0.294075	0.617666
43	1	0	7.293485	-0.320607	1.335037
44	6	0	2.267951	3.055966	0.558441
45	1	0	2.816856	2.104856	0.628391
46	1	0	2.101041	3.383353	1.593904
47	6	0	0.909021	2.822175	-0.102004
48	1	0	0.416349	3.793124	-0.242430
49	1	0	1.050267	2.392331	-1.102743
50	6	0	-5.819687	0.688237	0.418811
51	6	0	-5.990690	-0.579049	-0.150228
52	6	0	-2.078230	0.626783	1.157975
53	1	0	-1.481634	-0.243446	1.450800
54	1	0	-2.166155	1.279871	2.032041
55	6	0	4.405761	4.491939	0.607203
56	1	0	4.305224	4.188284	1.657918
57	1	0	4.508419	5.582262	0.619379
58	6	0	5.775199	2.378301	0.042611
59	1	0	5.514959	2.000039	1.039901
60	1	0	5.022618	1.966368	-0.645974
61	6	0	-3.667545	-1.080774	0.181907
62	6	0	-4.927505	-1.477036	-0.274772
63	1	0	-3.021141	2.233746	-0.910718
64	8	0	-2.421515	3.435563	0.681836
65	1	0	-2.974469	4.159434	0.370427
66	6	0	5.700362	3.904051	0.043478
67	1	0	5.844366	4.265706	-0.984031
68	1	0	6.546467	4.295372	0.623793
69	1	0	-2.818655	-1.753209	0.103643
70	8	0	3.630688	-3.747090	2.130781
71	6	0	2.574785	-4.210912	2.943464
72	1	0	3.035511	-4.804933	3.732185
73	1	0	2.020305	-3.377675	3.391630
74	1	0	1.879451	-4.837534	2.372554
75	1	0	-6.971885	-0.870613	-0.503475
76	6	0	7.168095	1.883410	-0.360238
77	1	0	7.871487	2.106014	0.453477
78	1	0	7.512211	2.462843	-1.226644
79	6	0	-6.965962	1.694134	0.558864
80	6	0	-5.078413	-2.867692	-0.897412
81	6	0	-7.166850	2.036704	2.044362
82	1	0	-6.262788	2.471221	2.479955
83	1	0	-7.981628	2.759696	2.160708
84	1	0	-7.417960	1.138680	2.616680
85	6	0	-6.606610	2.975367	-0.213112
86	1	0	-7.409730	3.714744	-0.121921
87	1	0	-5.686504	3.425966	0.172148
88	1	0	-6.457284	2.756350	-1.275178
89	6	0	-8.287537	1.154168	0.004503
90	1	0	-8.209580	0.915774	-1.060912
91	1	0	-8.607165	0.252837	0.536776
92	1	0	-9.071447	1.908530	0.123590
93	6	0	-6.501137	-3.130102	-1.399258
94	1	0	-7.229916	-3.090015	-0.583344

95	1	0	-6.798420	-2.404561	-2.163350
96	1	0	-6.554826	-4.127801	-1.845629
97	6	0	-4.110430	-2.994236	-2.087055
98	1	0	-4.331517	-2.236784	-2.845921
99	1	0	-3.069720	-2.868914	-1.773239
100	1	0	-4.207644	-3.982388	-2.549783
101	6	0	-4.726931	-3.934359	0.153072
102	1	0	-3.699781	-3.817268	0.509390
103	1	0	-5.396965	-3.863844	1.015428
104	1	0	-4.823956	-4.936398	-0.278883

Zero-point correction= 0.937764 (Hartree/Particle)
Thermal correction to Energy= 0.984920
Thermal correction to Enthalpy= 0.985865
Thermal correction to Gibbs Free Energy= 0.856292
Sum of electronic and zero-point Energies= -1896.698985
Sum of electronic and thermal Energies= -1896.651829
Sum of electronic and thermal Enthalpies= -1896.650885
Sum of electronic and thermal Free Energies= -1896.780457
M06-2X/6-311++G(d,p)/SMD// M06-2X//6-31G(d,p) energy in solvent (THF) = -1898.1485853

TS_{rot}(31)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.442198	-0.226511	-1.030492
2	8	0	-0.124798	0.226804	0.166144
3	8	0	0.571371	2.314626	-0.347701
4	6	0	-1.765886	1.914569	-0.113892
5	6	0	-3.536971	3.492470	0.399248
6	6	0	-2.719558	1.058504	-0.645899
7	6	0	-0.322141	1.534710	-0.118101
8	6	0	-2.182792	3.173443	0.354252
9	1	0	-1.424314	3.855882	0.719503
10	6	0	-4.057738	1.437510	-0.693723
11	1	0	-4.740638	0.722098	-1.136315
12	6	0	-4.511790	2.603724	-0.114641
13	6	0	1.413022	-1.679316	0.151585
14	6	0	-7.193580	-0.698090	-0.924028
15	1	0	-8.192641	-0.517404	-1.340918
16	1	0	-6.498233	-0.594653	-1.770485
17	6	0	3.553466	-0.402612	0.821134
18	6	0	0.356600	-2.594137	0.811423
19	1	0	0.895934	-3.296292	1.456474
20	1	0	-0.247226	-1.966356	1.478181
21	6	0	-2.749619	-1.079166	0.067786
22	1	0	-1.962665	-1.016392	0.823391
23	1	0	-2.832916	-2.083913	-0.321496
24	1	0	-3.704699	-0.792788	0.518308
25	6	0	2.248372	-2.485492	-0.845495
26	1	0	1.596819	-2.844201	-1.657508
27	6	0	-6.900431	1.805249	-0.584873
28	1	0	-7.926903	2.186609	-0.593250
29	1	0	-6.623467	1.690176	-1.640996
30	6	0	0.794413	-0.523792	-0.644392
31	1	0	1.579704	0.143165	-1.015670
32	1	0	0.211878	-0.904855	-1.492746
33	6	0	4.746774	-1.110080	0.677247
34	1	0	4.747885	-2.167026	0.933770
35	6	0	-2.964769	-4.483053	-0.106823
36	1	0	-3.142481	-3.799727	-0.946815
37	1	0	-2.760680	-5.453100	-0.573645
38	6	0	-5.991694	2.880226	0.031698
39	1	0	-6.220231	3.855503	-0.413459
40	1	0	-6.206778	2.995600	1.102493
41	6	0	-6.892746	0.413843	0.093081
42	1	0	-5.928394	0.229127	0.579609
43	1	0	-7.640235	0.389487	0.895227
44	6	0	-1.735251	-4.015349	0.697889
45	1	0	-2.073117	-3.259148	1.417847
46	1	0	-1.360755	-4.844865	1.310525
47	6	0	-0.570849	-3.406638	-0.105853
48	1	0	0.003810	-4.199779	-0.599180
49	1	0	-0.969166	-2.769581	-0.906515
50	6	0	5.902909	-0.498318	0.189499
51	6	0	5.842113	0.858909	-0.142725
52	6	0	2.308302	-1.115592	1.288676
53	1	0	1.688720	-0.439856	1.889634
54	1	0	2.597533	-1.953003	1.930433
55	6	0	-4.237752	-4.575745	0.767563
56	1	0	-4.096215	-3.961474	1.667242
57	1	0	-4.350859	-5.603545	1.129349
58	6	0	-5.694918	-2.612309	-0.068723
59	1	0	-5.375673	-2.121830	0.859956
60	1	0	-5.009122	-2.266444	-0.853627

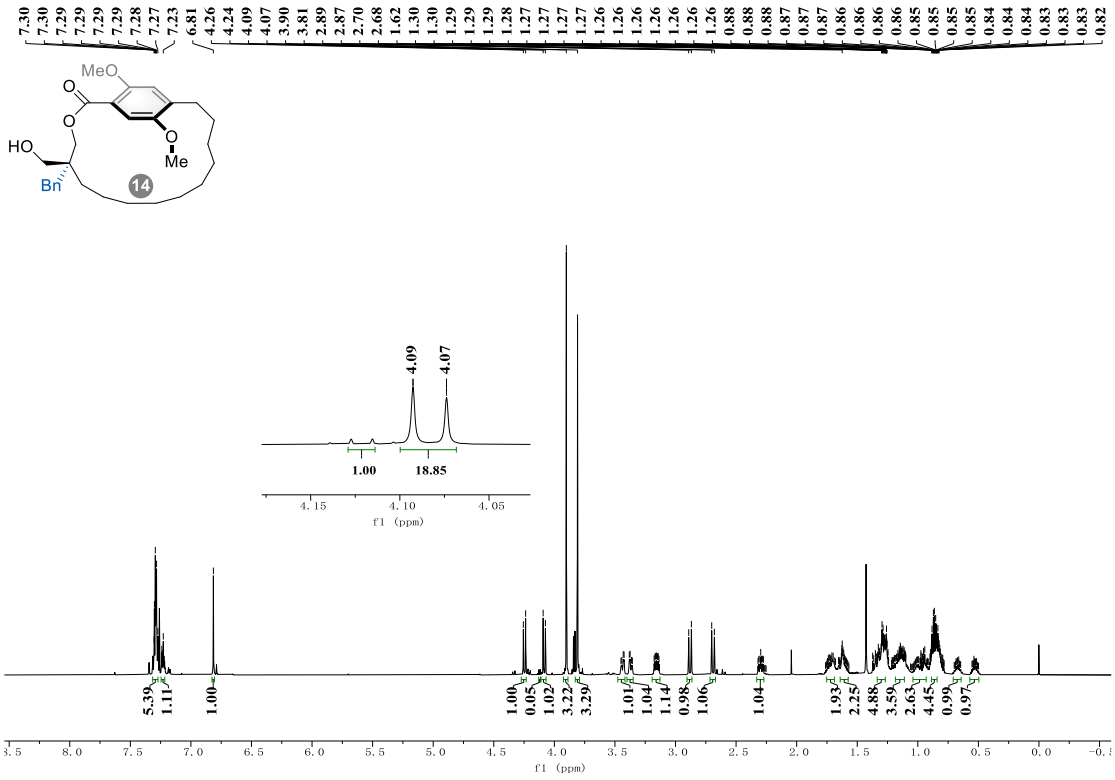
61	6	0	3.527472	0.949728	0.482024
62	6	0	4.664467	1.600373	-0.006416
63	1	0	3.019693	-1.840148	-1.289807
64	8	0	2.832969	-3.572550	-0.150789
65	1	0	3.413008	-4.041964	-0.758522
66	6	0	-5.557459	-4.131064	0.111121
67	1	0	-5.684025	-4.627717	-0.860157
68	1	0	-6.386266	-4.479157	0.741299
69	1	0	2.592380	1.495732	0.579056
70	8	0	-4.035640	4.643204	0.928029
71	6	0	-3.112407	5.560901	1.471764
72	1	0	-3.699854	6.396727	1.850281
73	1	0	-2.543466	5.111795	2.294668
74	1	0	-2.413514	5.922754	0.708413
75	1	0	6.731589	1.348951	-0.518064
76	6	0	-7.112719	-2.148120	-0.422713
77	1	0	-7.770947	-2.284991	0.445450
78	1	0	-7.508366	-2.801248	-1.211259
79	6	0	7.173685	-1.337045	0.025908
80	6	0	4.564634	3.069744	-0.425595
81	6	0	7.599593	-1.892118	1.395005
82	1	0	6.817811	-2.517955	1.834000
83	1	0	8.504908	-2.500621	1.293365
84	1	0	7.809594	-1.076094	2.092947
85	6	0	6.881616	-2.507596	-0.928945
86	1	0	7.773690	-3.131318	-1.052569
87	1	0	6.076063	-3.141560	-0.545598
88	1	0	6.581310	-2.135444	-1.913661
89	6	0	8.338692	-0.526494	-0.549603
90	1	0	8.100507	-0.125973	-1.540058
91	1	0	8.607236	0.308927	0.104429
92	1	0	9.219032	-1.169014	-0.649505
93	6	0	5.935646	3.678497	-0.736980
94	1	0	6.611127	3.609804	0.122152
95	1	0	6.413136	3.188990	-1.591563
96	1	0	5.816124	4.736422	-0.989772
97	6	0	3.686813	3.154583	-1.686647
98	1	0	4.123864	2.563944	-2.498439
99	1	0	2.678424	2.781679	-1.485668
100	1	0	3.606292	4.194485	-2.023087
101	6	0	3.909957	3.897517	0.692823
102	1	0	2.880083	3.580415	0.876550
103	1	0	4.473739	3.808273	1.626749
104	1	0	3.883464	4.954065	0.405560

Zero-point correction= 0.939513 (Hartree/Particle)
Thermal correction to Energy= 0.984923
Thermal correction to Enthalpy= 0.985867
Thermal correction to Gibbs Free Energy= 0.862646
Sum of electronic and zero-point Energies= -1896.675144
Sum of electronic and thermal Energies= -1896.629735
Sum of electronic and thermal Enthalpies= -1896.628791
Sum of electronic and thermal Free Energies= -1896.752011

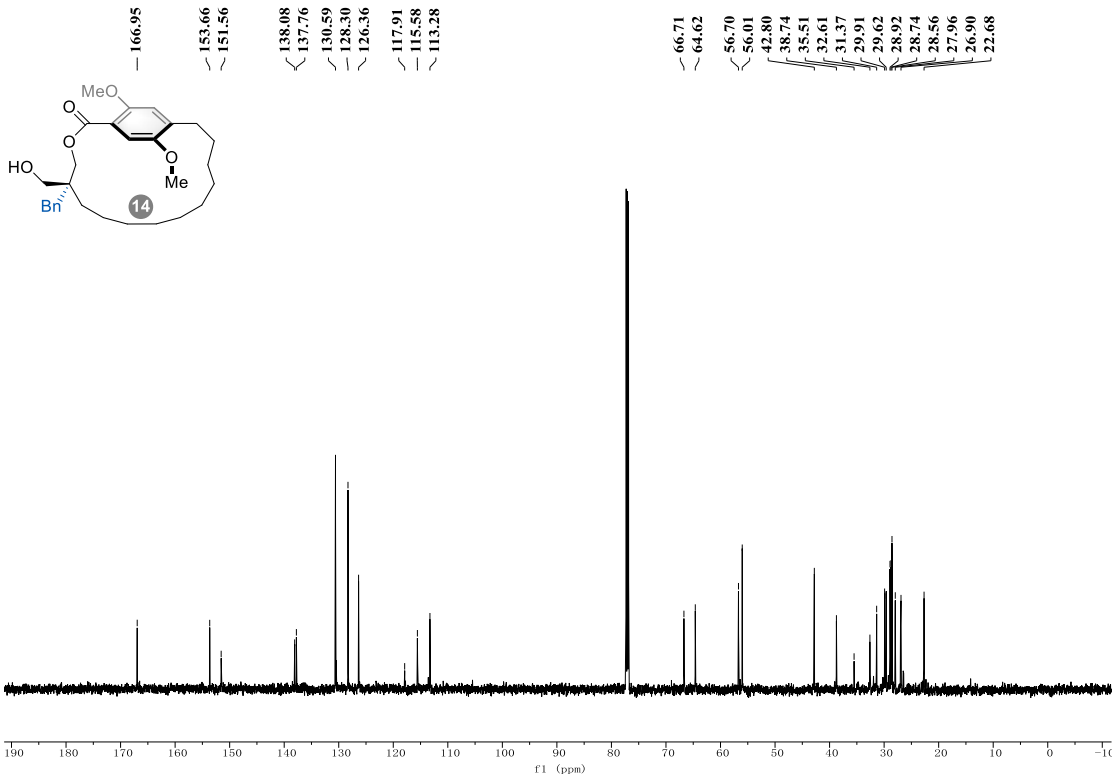
M06-2X/6-311++G(d,p)/SMD// M06-2X//6-31G(d,p) energy in solvent (THF) = -1898.1261225

9. Copies of NMR spectra

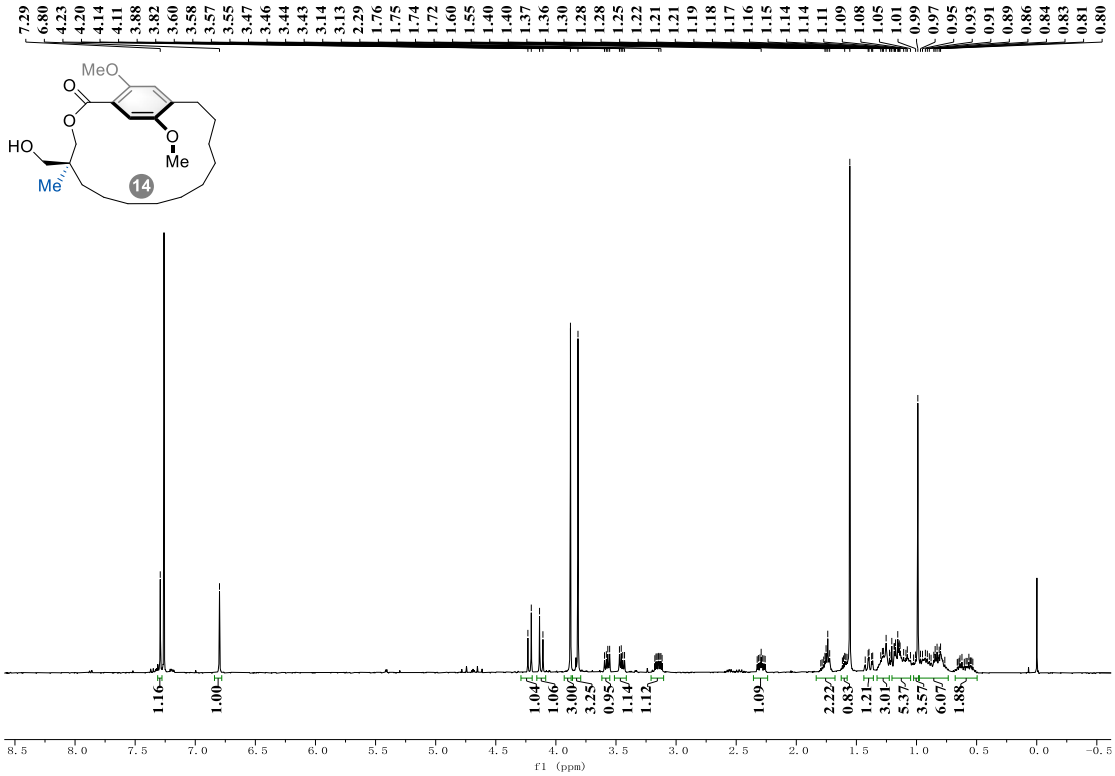
2, **^{1}H NMR** (600 MHz, $CDCl_3$)



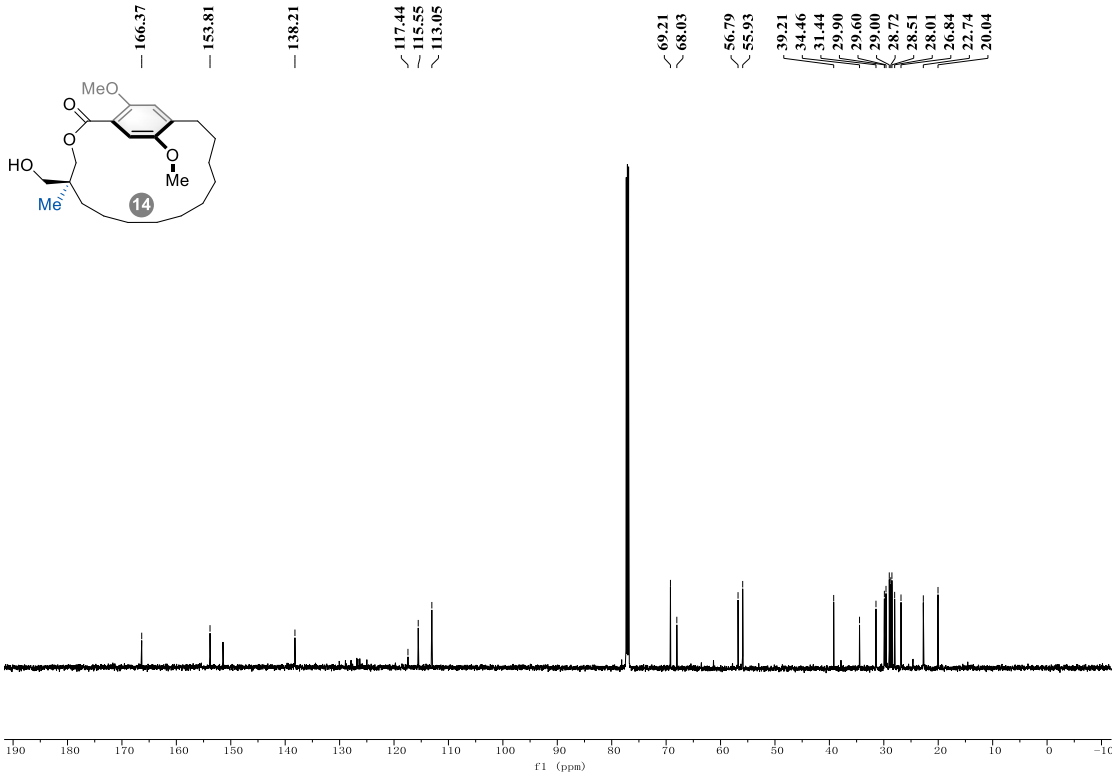
2, **^{13}C NMR** (151 MHz, $CDCl_3$)



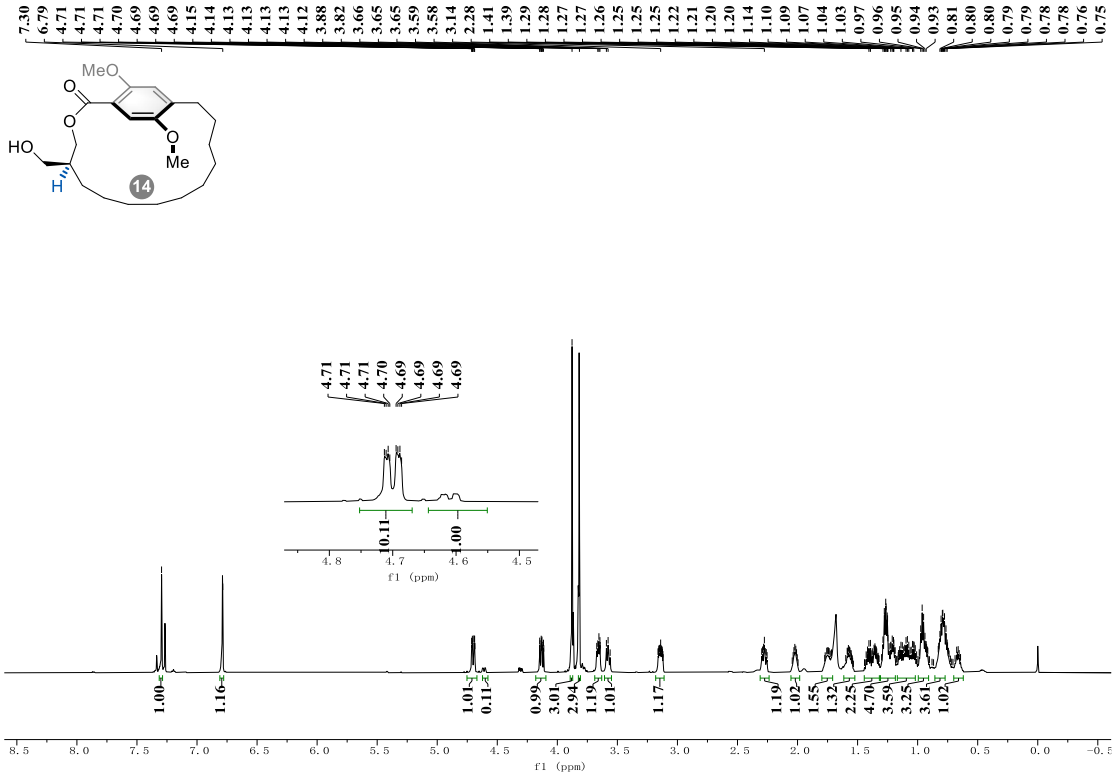
3, **^{1}H NMR** (400 MHz, $CDCl_3$)



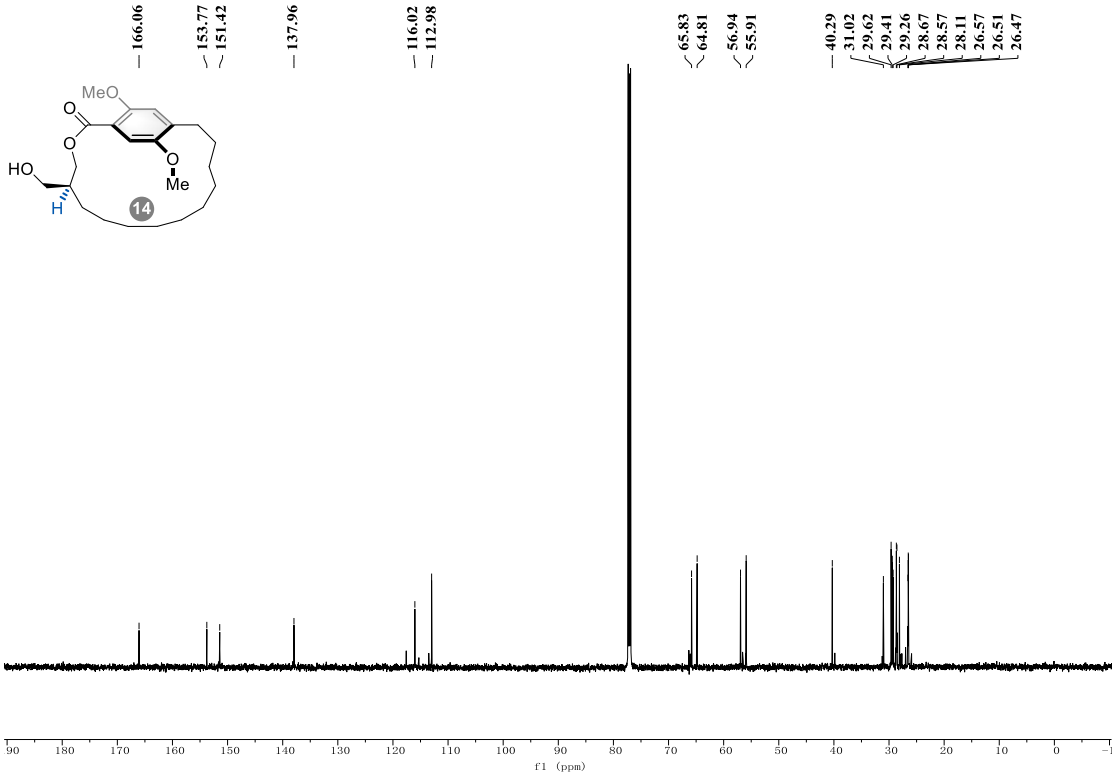
3, **^{13}C NMR** (151 MHz, $CDCl_3$)



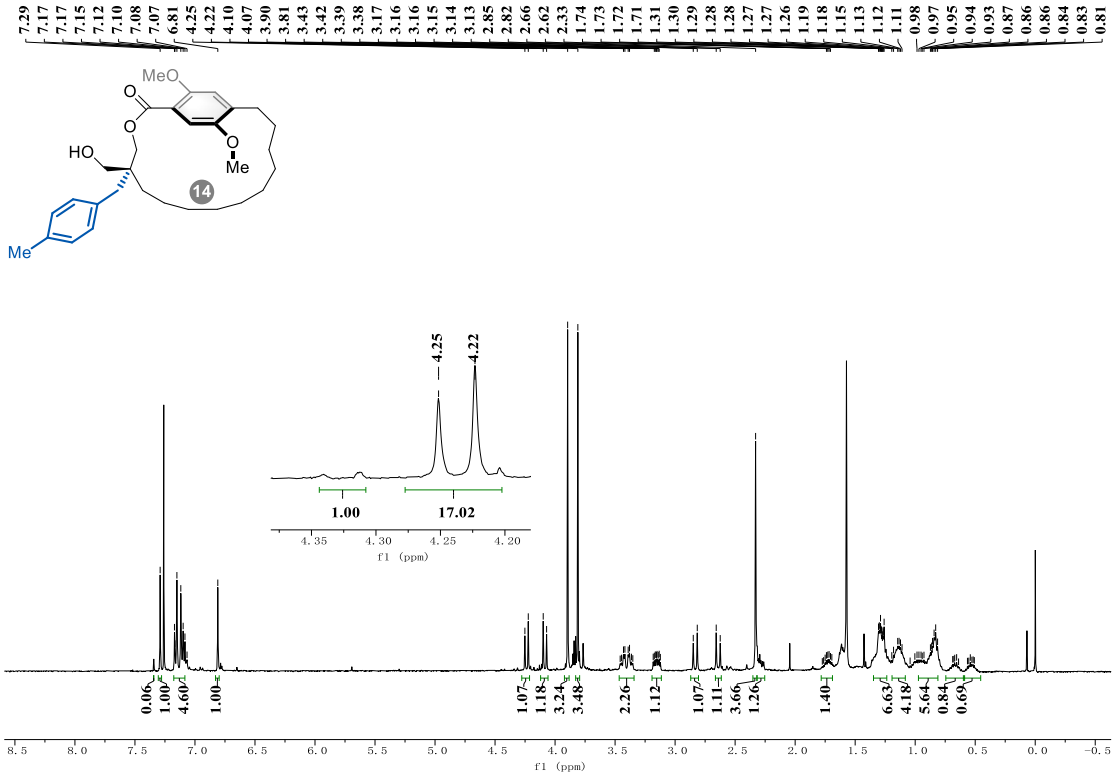
4, **^{1}H NMR** (600 MHz, $CDCl_3$)



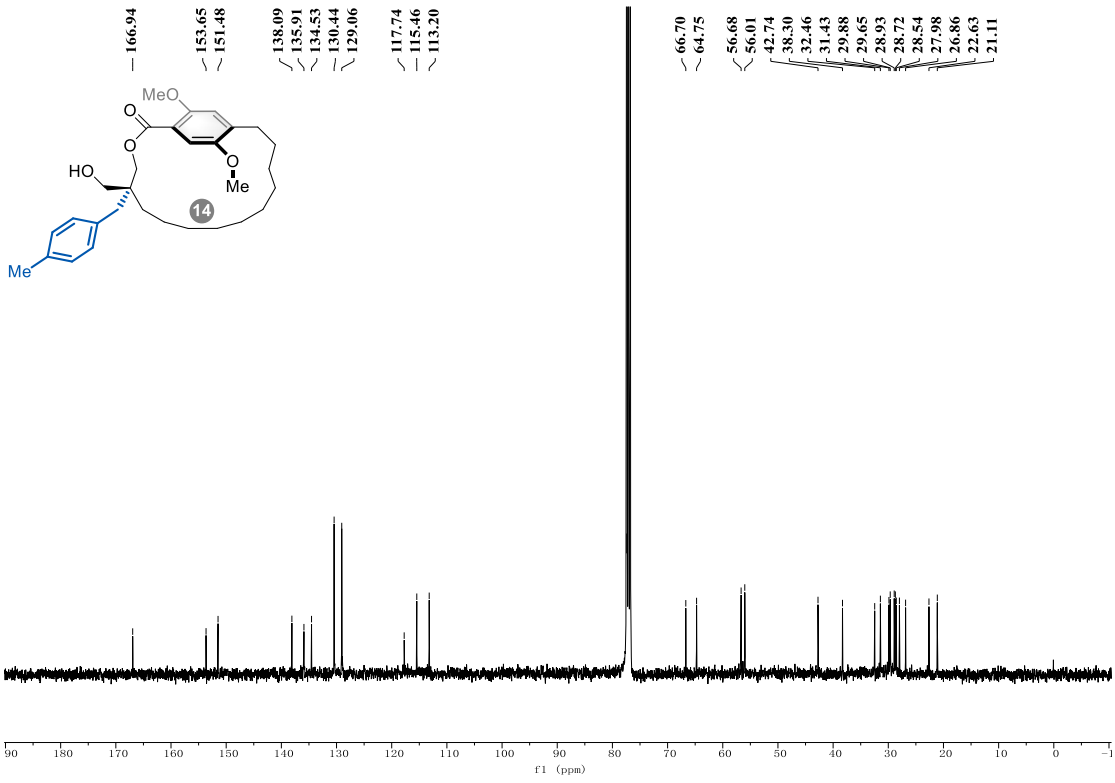
4, **^{13}C NMR** (151 MHz, $CDCl_3$)



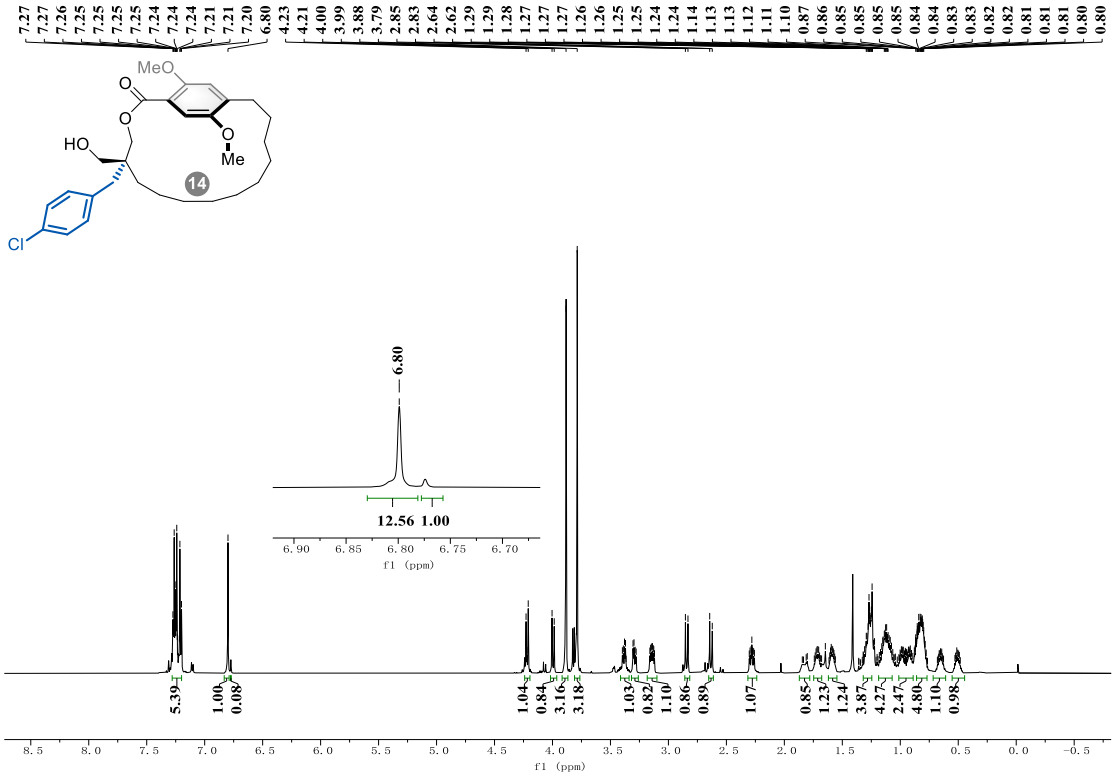
5, **^{1}H NMR** (400 MHz, $CDCl_3$)



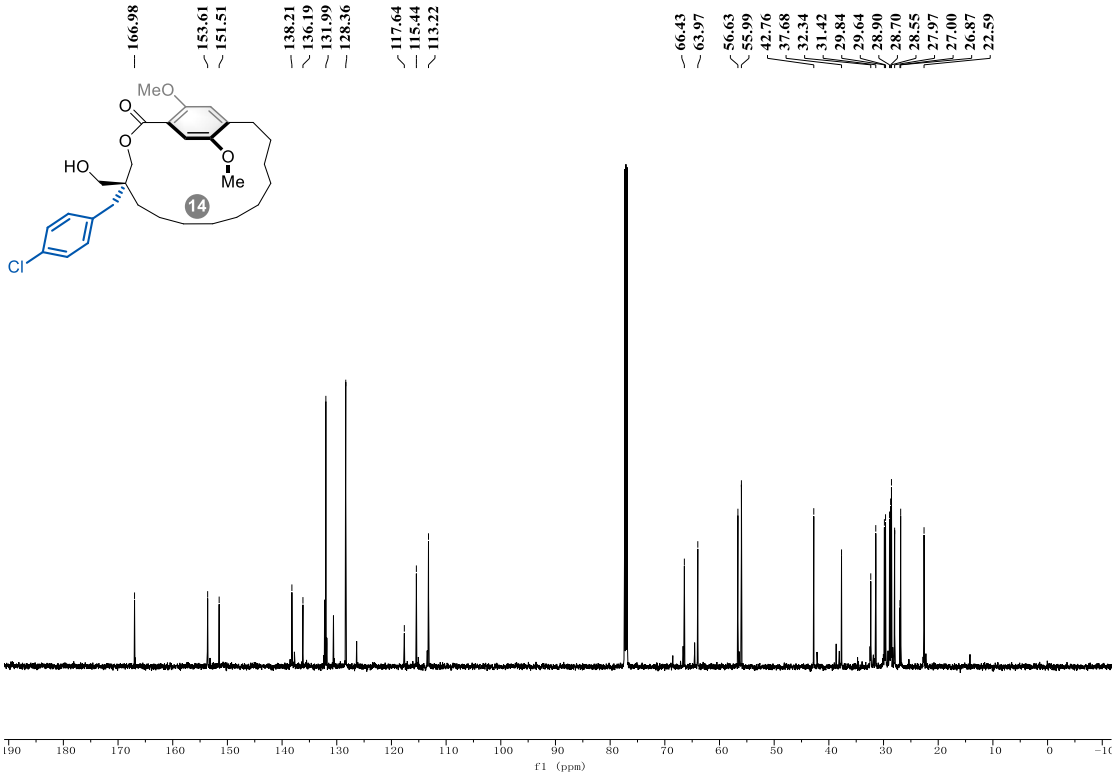
5, **^{13}C NMR** (101 MHz, $CDCl_3$)



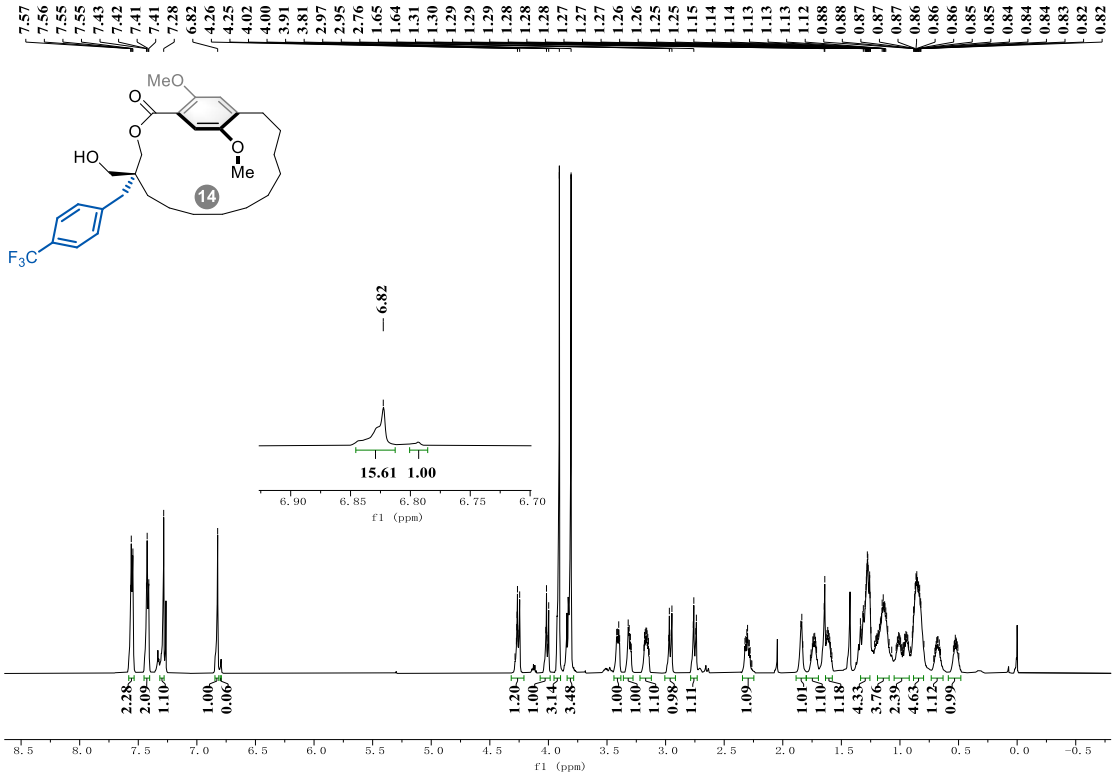
6, **^{1}H NMR** (600 MHz, $CDCl_3$)



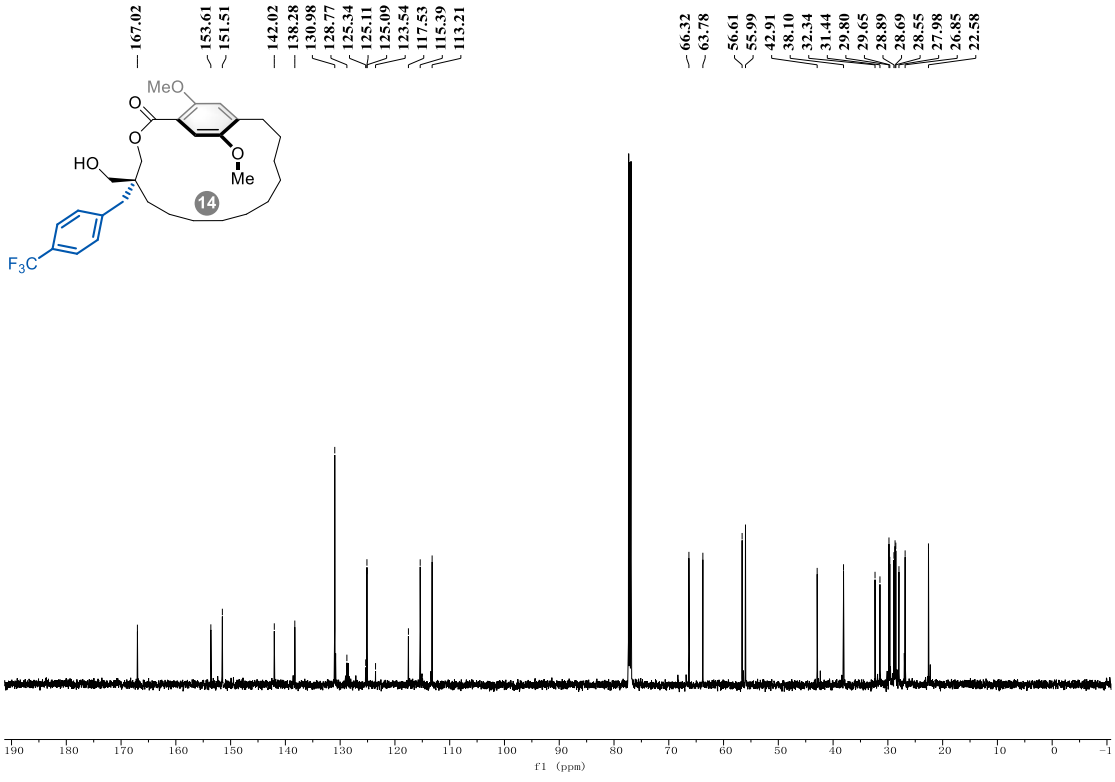
6, **^{13}C NMR** (151 MHz, $CDCl_3$)



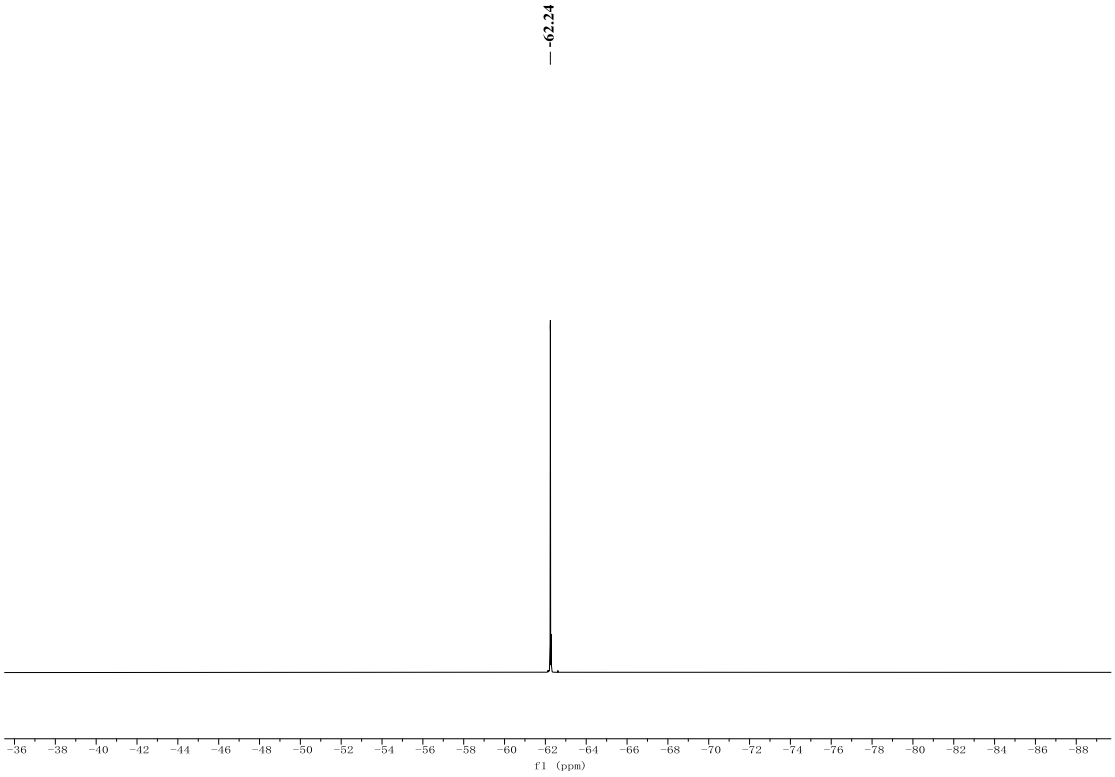
7, **^{1}H NMR** (600 MHz, $CDCl_3$)



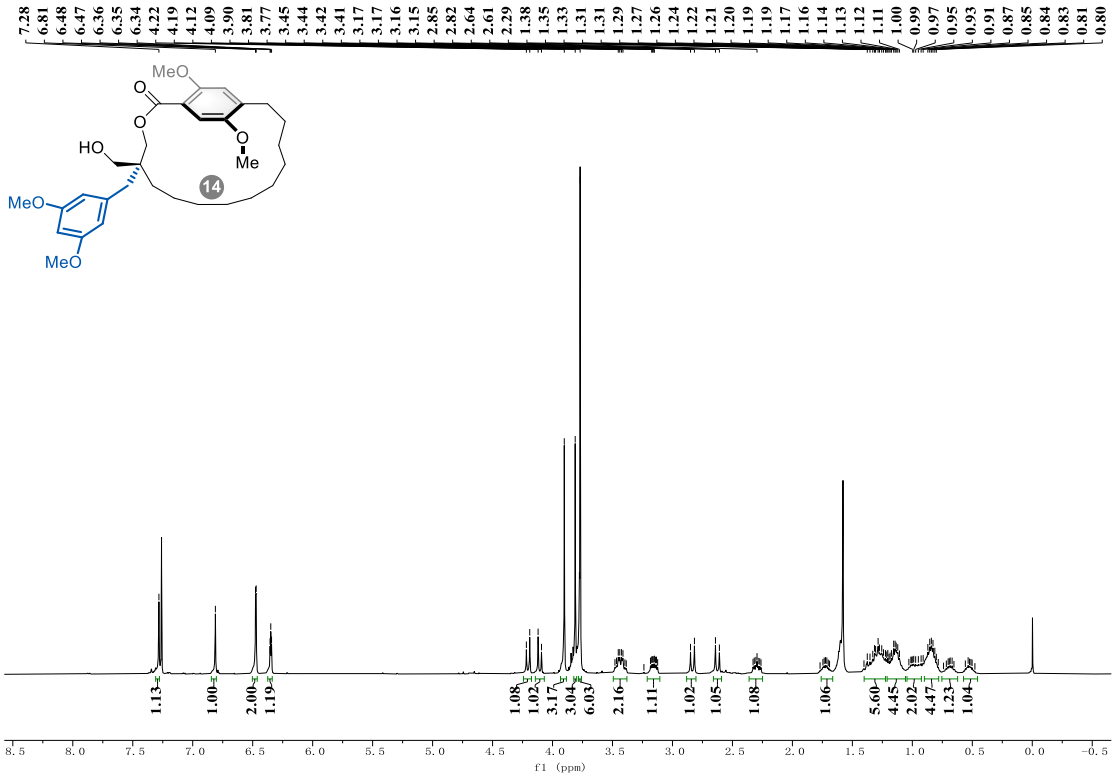
7, **^{13}C NMR** (151 MHz, $CDCl_3$)



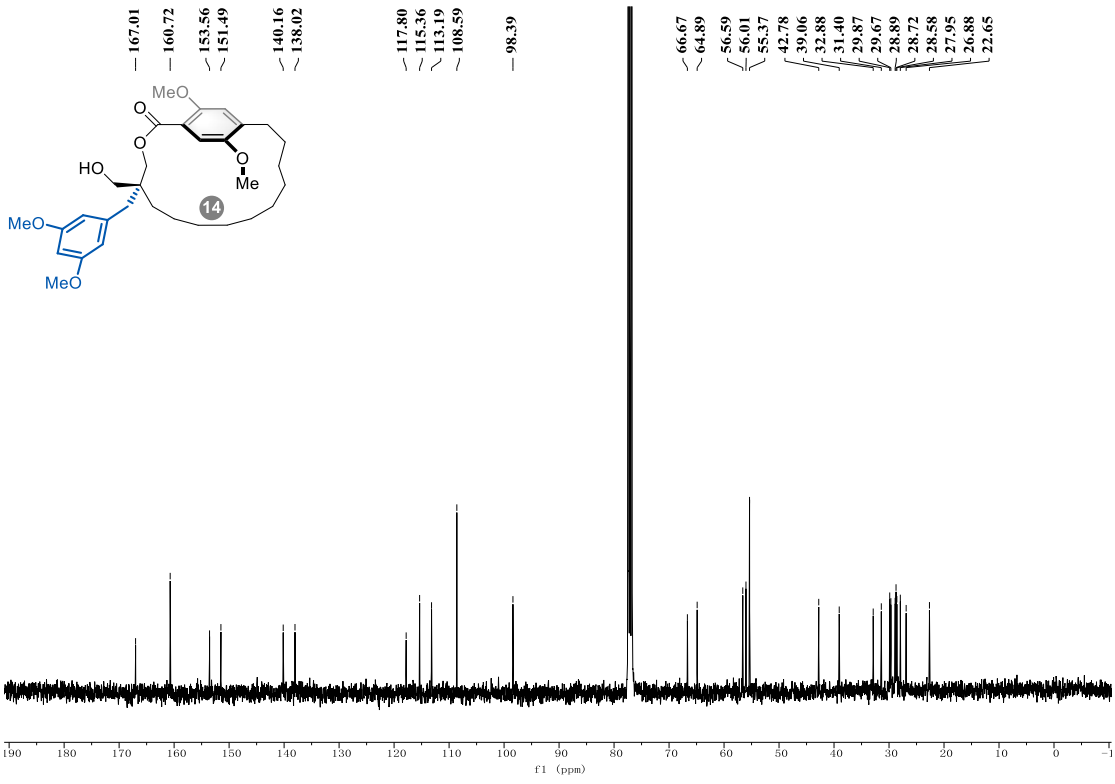
7, **^{19}F NMR** (565 MHz, $CDCl_3$)



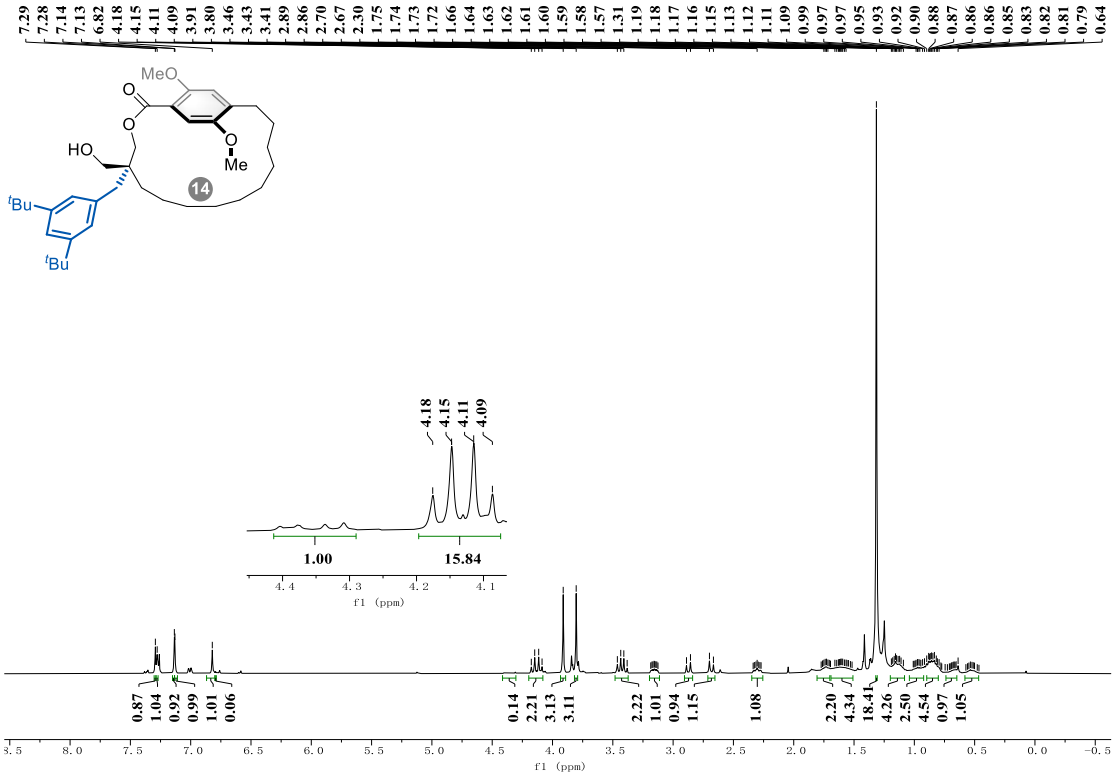
8, **^{1}H NMR** (400 MHz, $CDCl_3$)



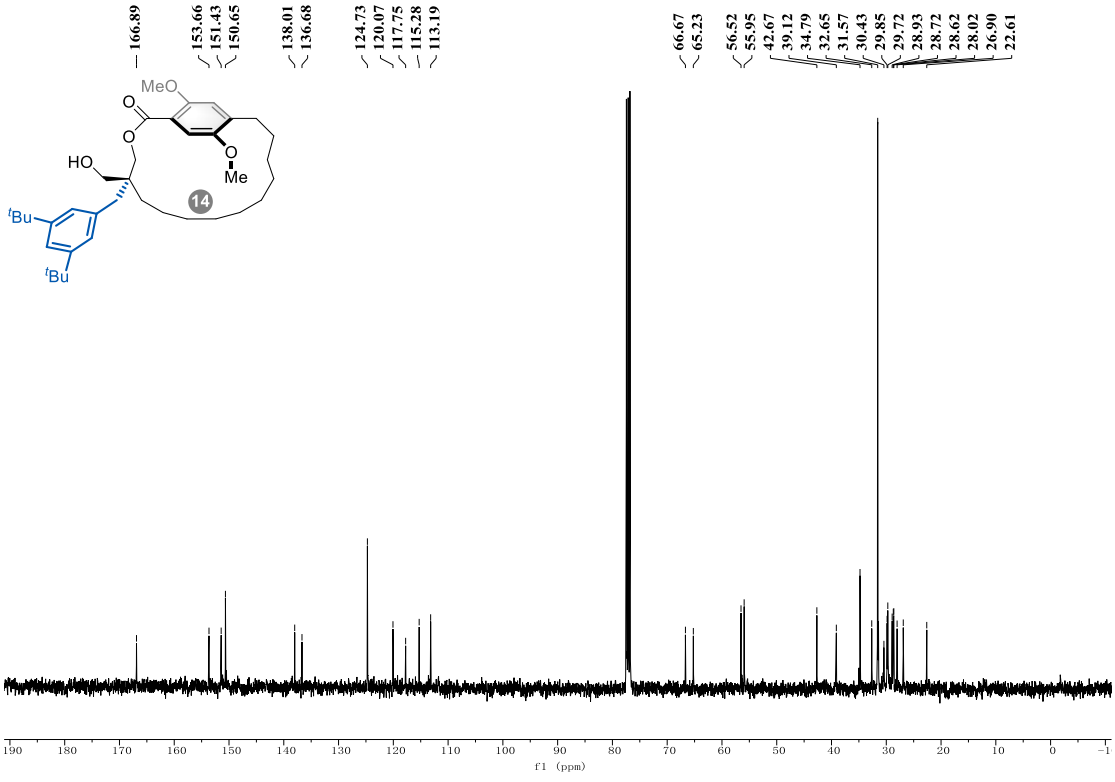
8, **^{13}C NMR** (101 MHz, $CDCl_3$)



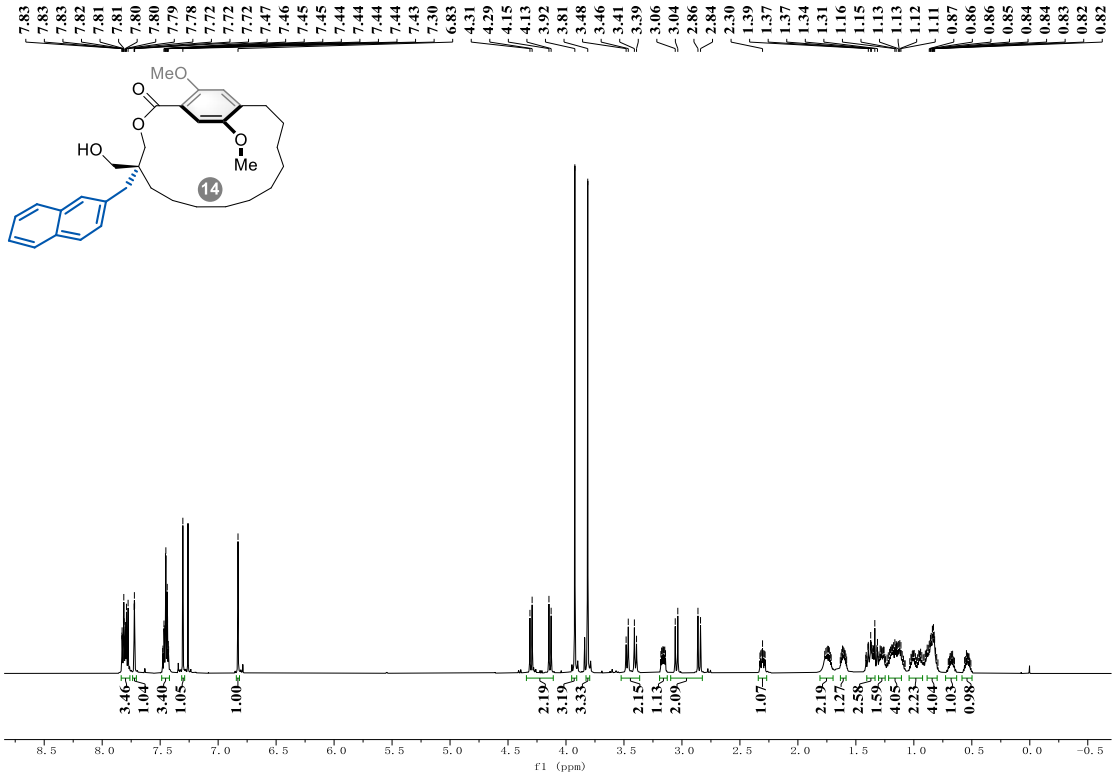
9, **^{1}H NMR** (400 MHz, $CDCl_3$)



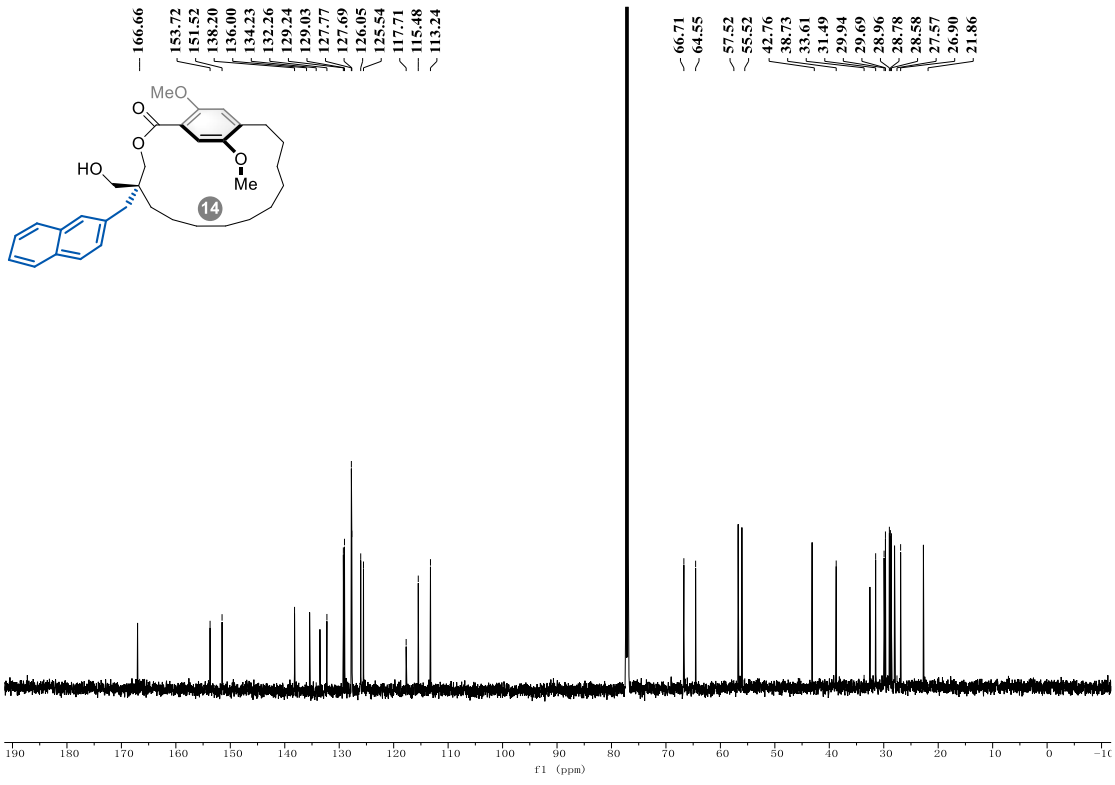
9, **^{13}C NMR** (101 MHz, $CDCl_3$)



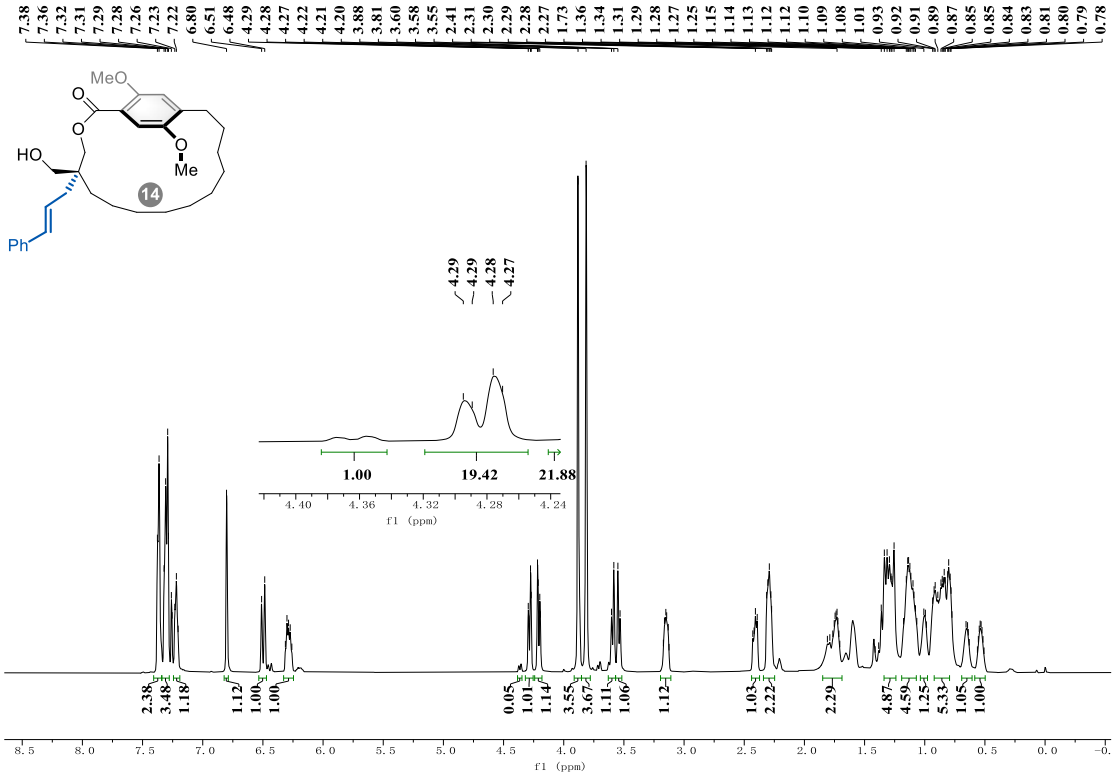
10, **^{1}H NMR** (600 MHz, $CDCl_3$)



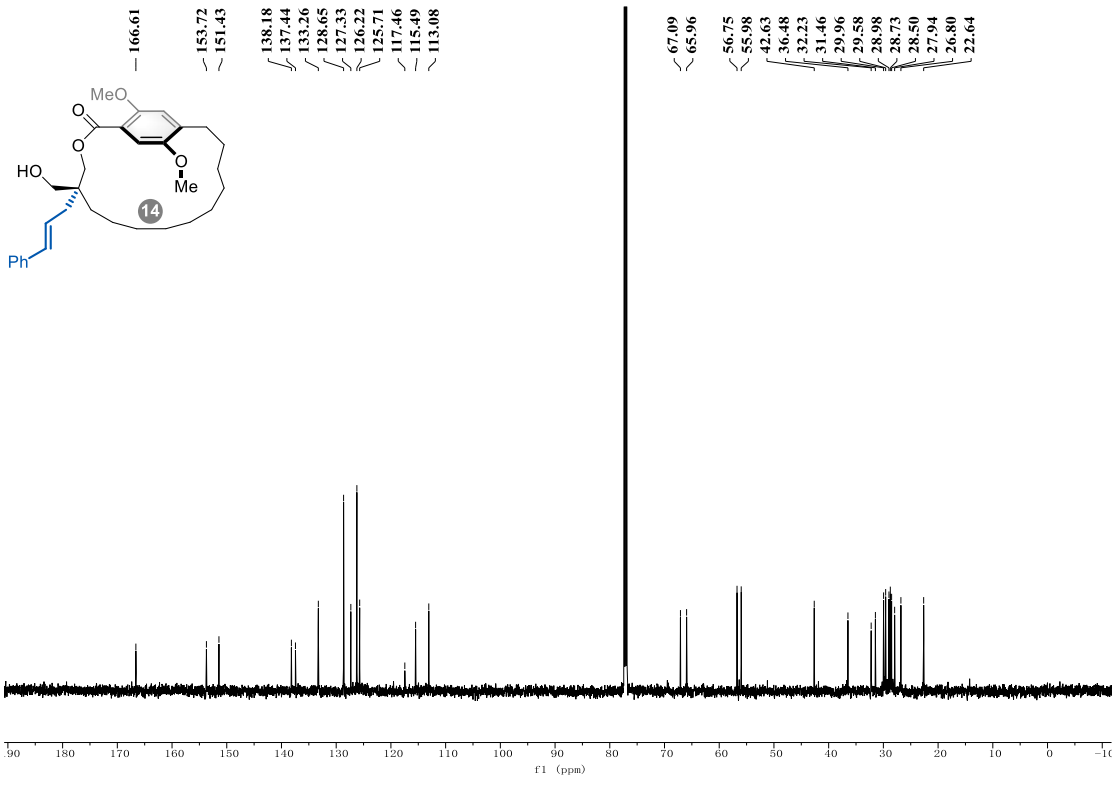
10, **^{13}C NMR** (151 MHz, $CDCl_3$)



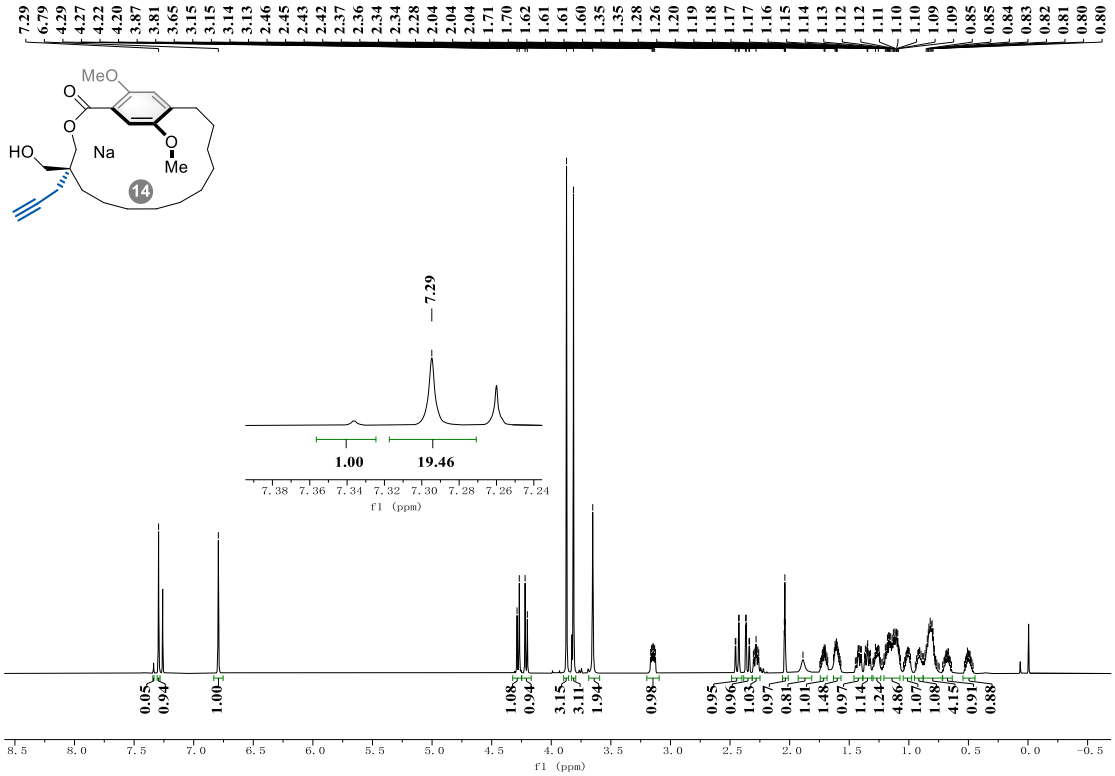
11, **^{1}H NMR** (600 MHz, $CDCl_3$)



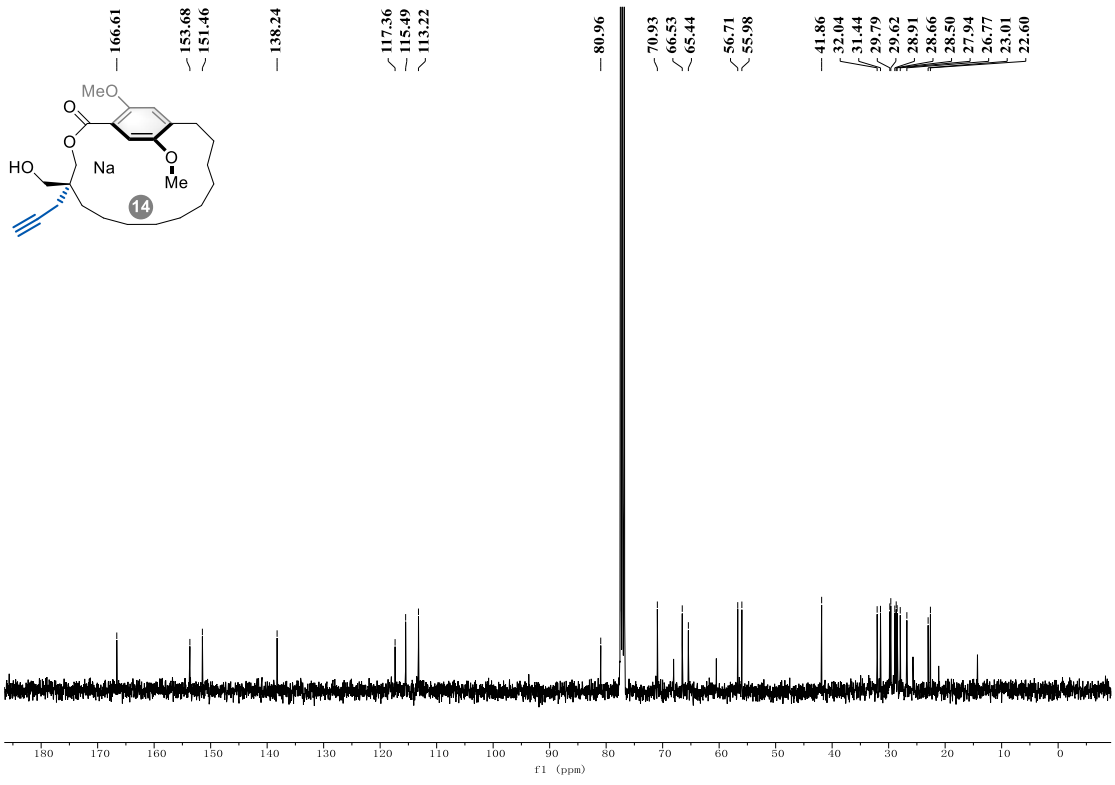
11, **^{13}C NMR** (151 MHz, $CDCl_3$)



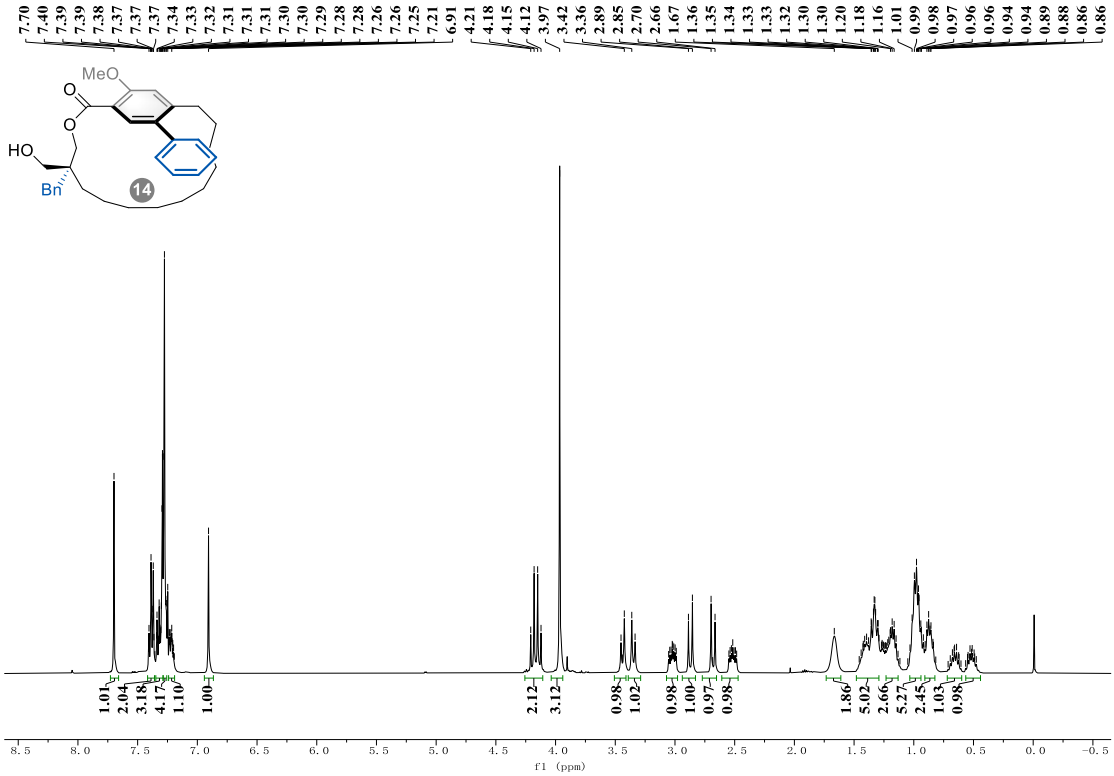
12, **^{1}H NMR** (600 MHz, $CDCl_3$)



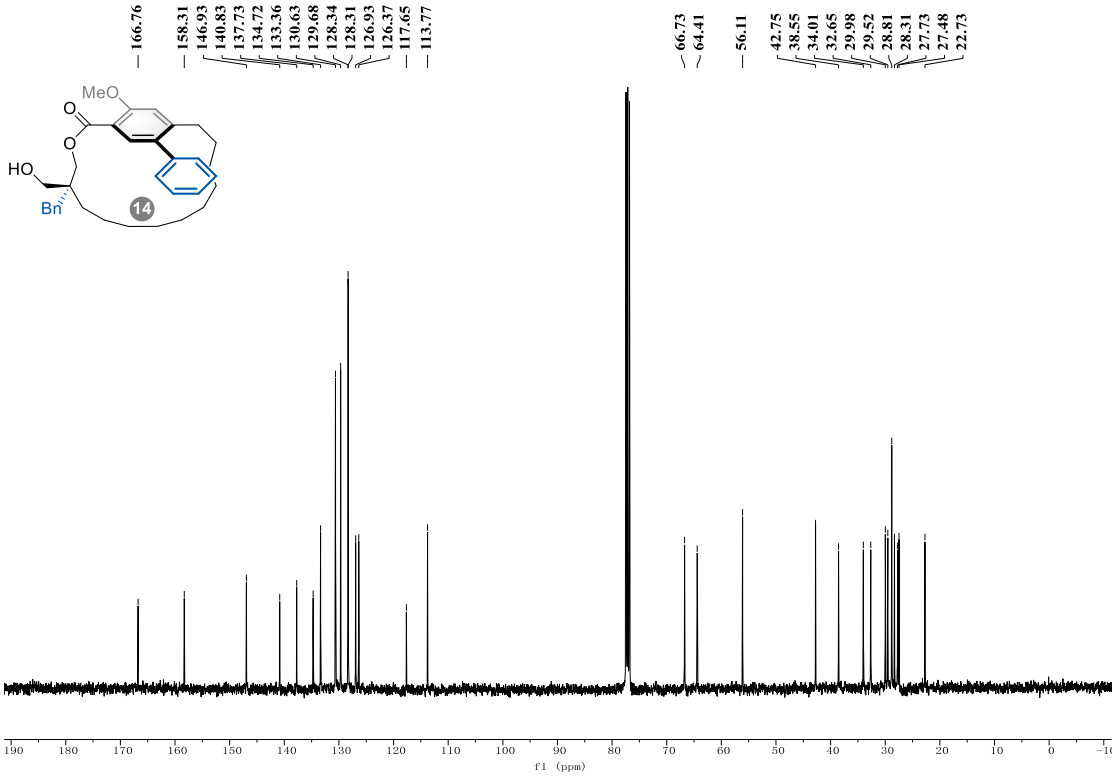
12, **^{13}C NMR** (101 MHz, $CDCl_3$)



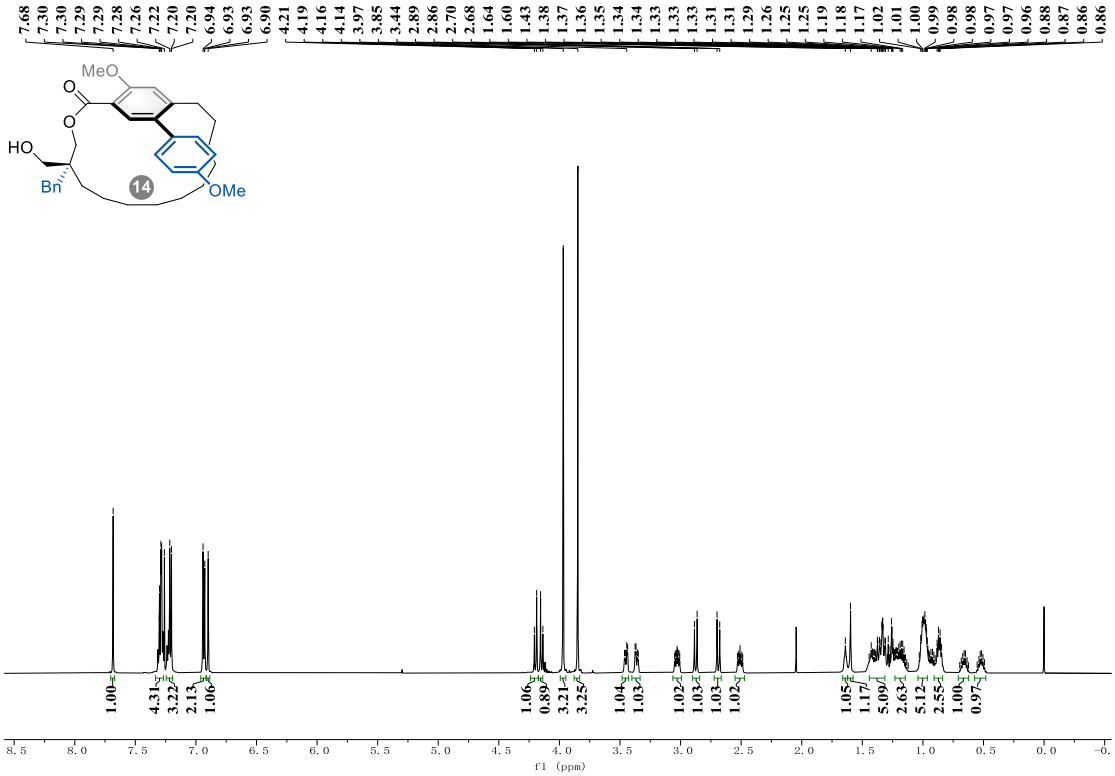
13, **^{1}H NMR** (600 MHz, $CDCl_3$)



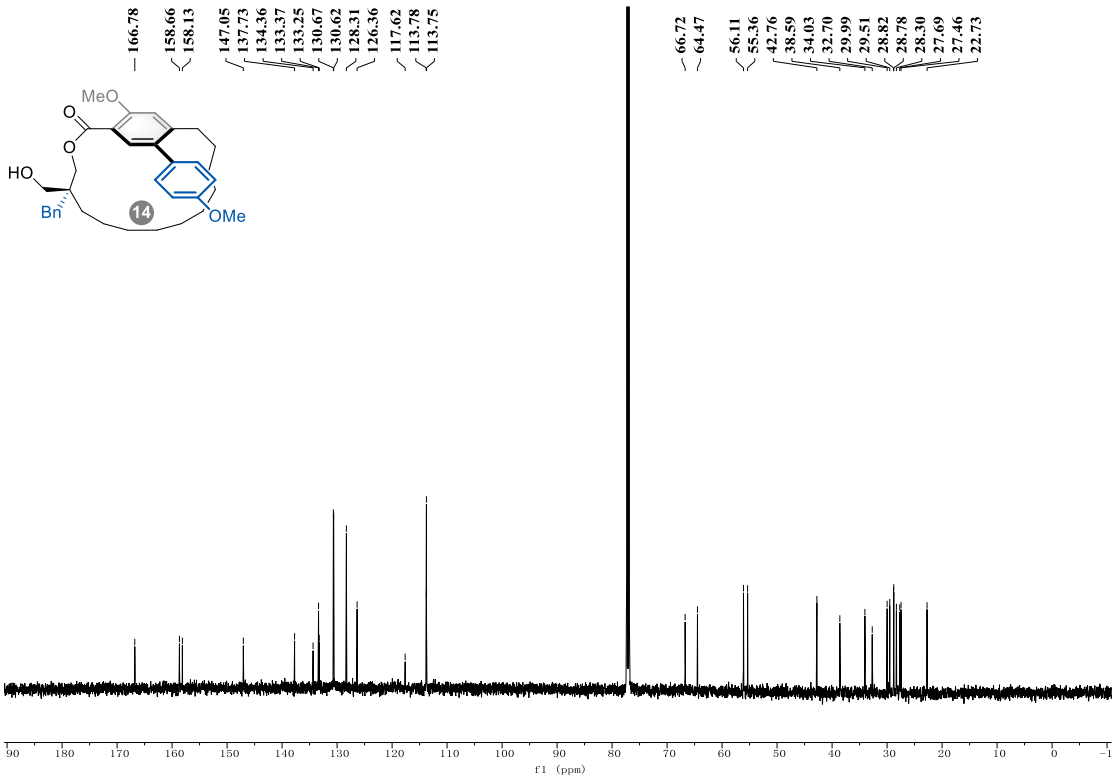
13, **^{13}C NMR** (151 MHz, $CDCl_3$)



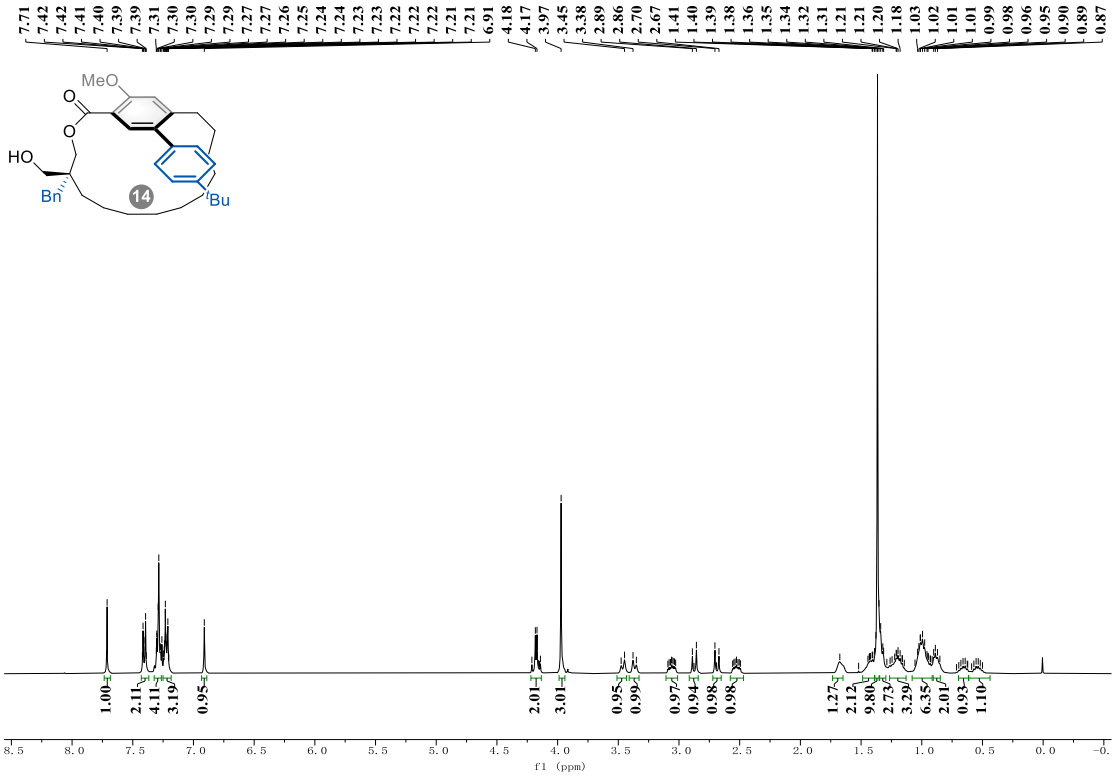
14, **^{1}H NMR** (600 MHz, $CDCl_3$)



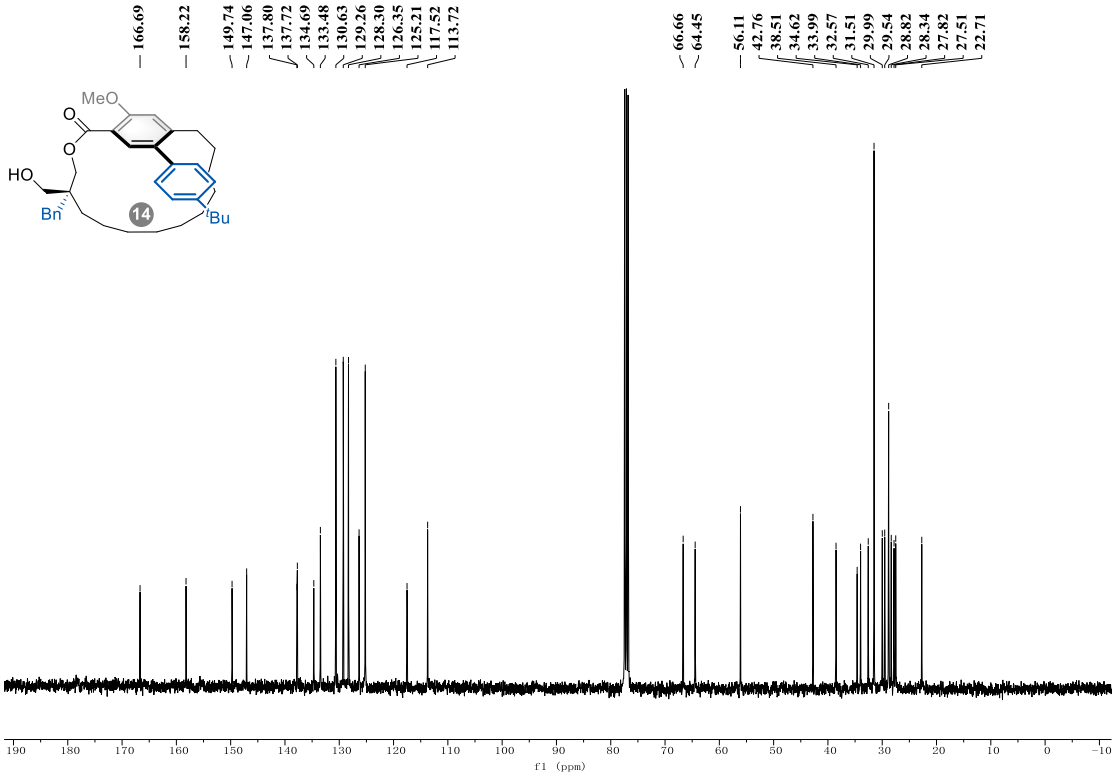
14, **^{13}C NMR** (151 MHz, $CDCl_3$)



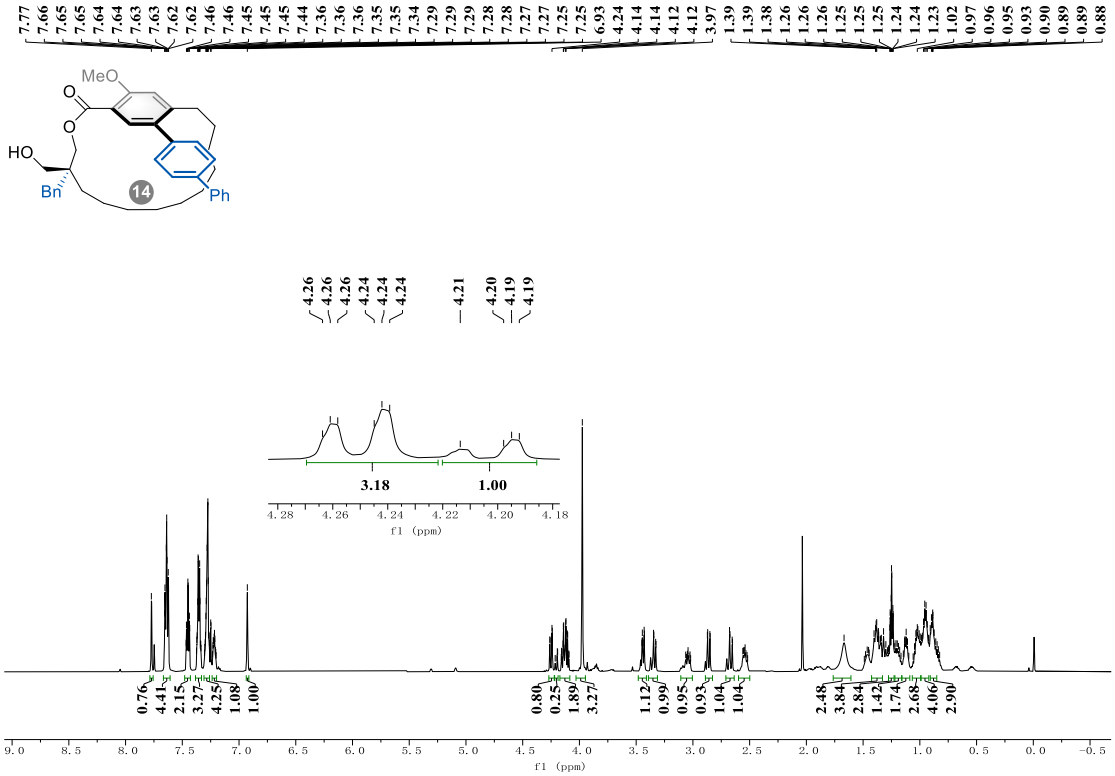
15, **^{1}H NMR** (400 MHz, $CDCl_3$)



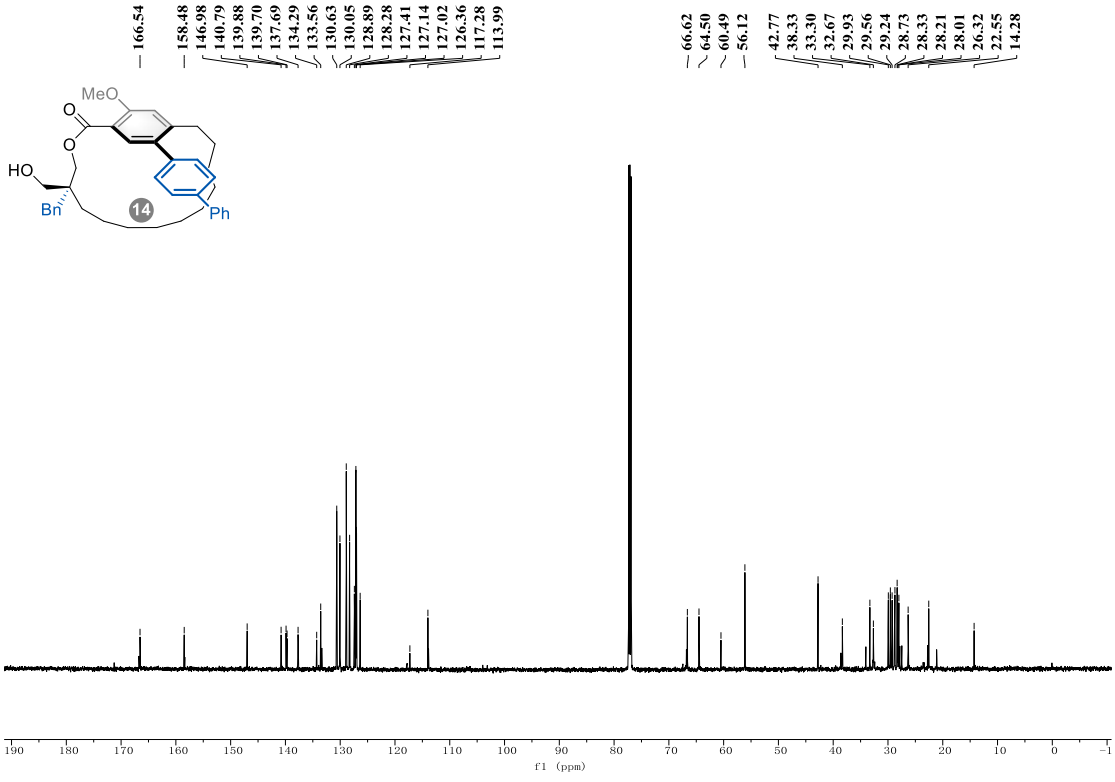
15, **^{13}C NMR** (101 MHz, $CDCl_3$)



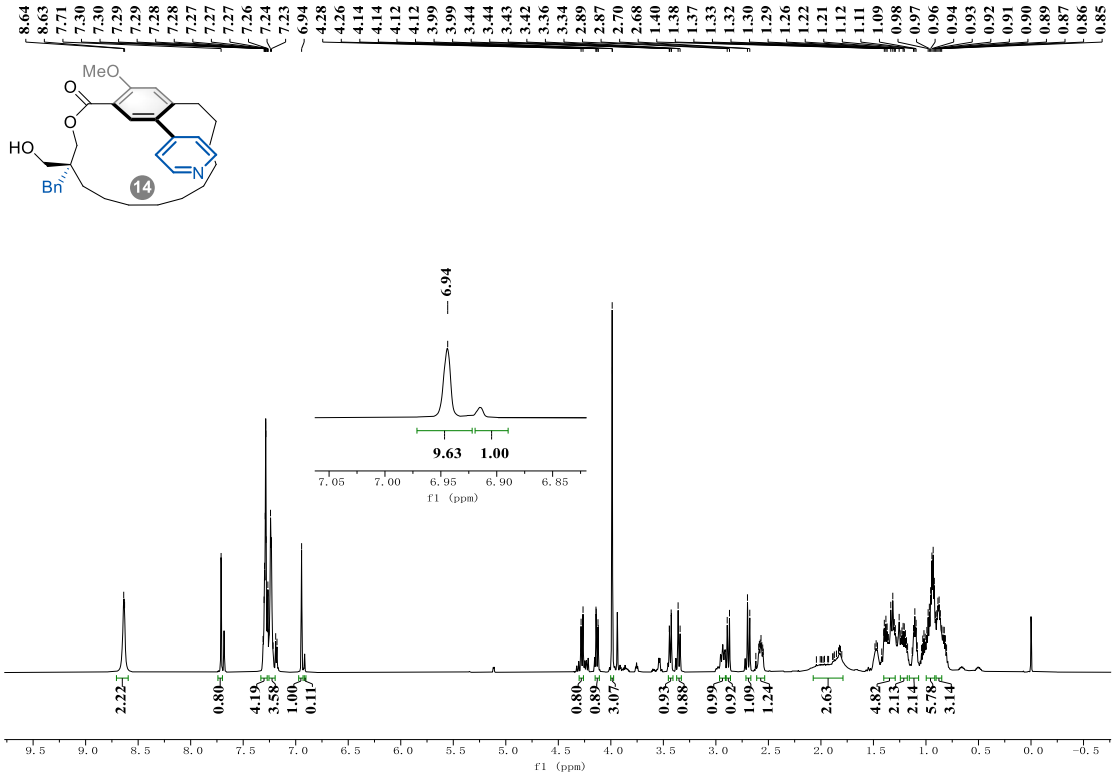
16, **^{1}H NMR** (600 MHz, $CDCl_3$)



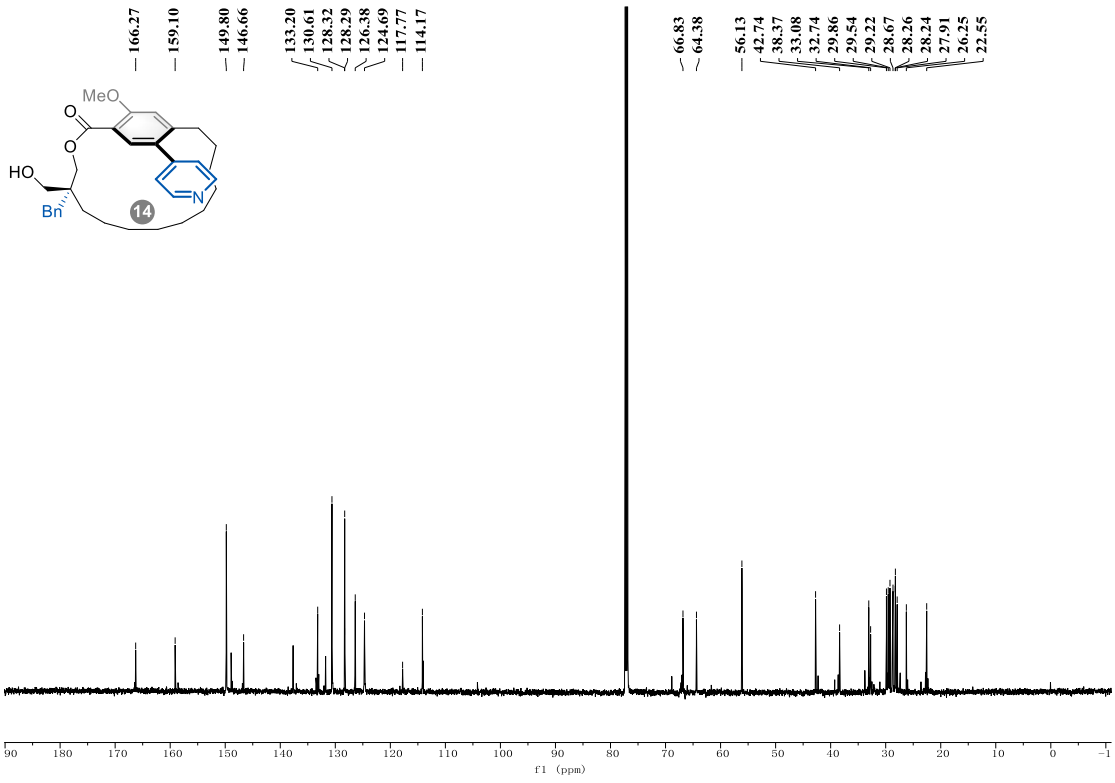
16, **^{13}C NMR** (151 MHz, $CDCl_3$)



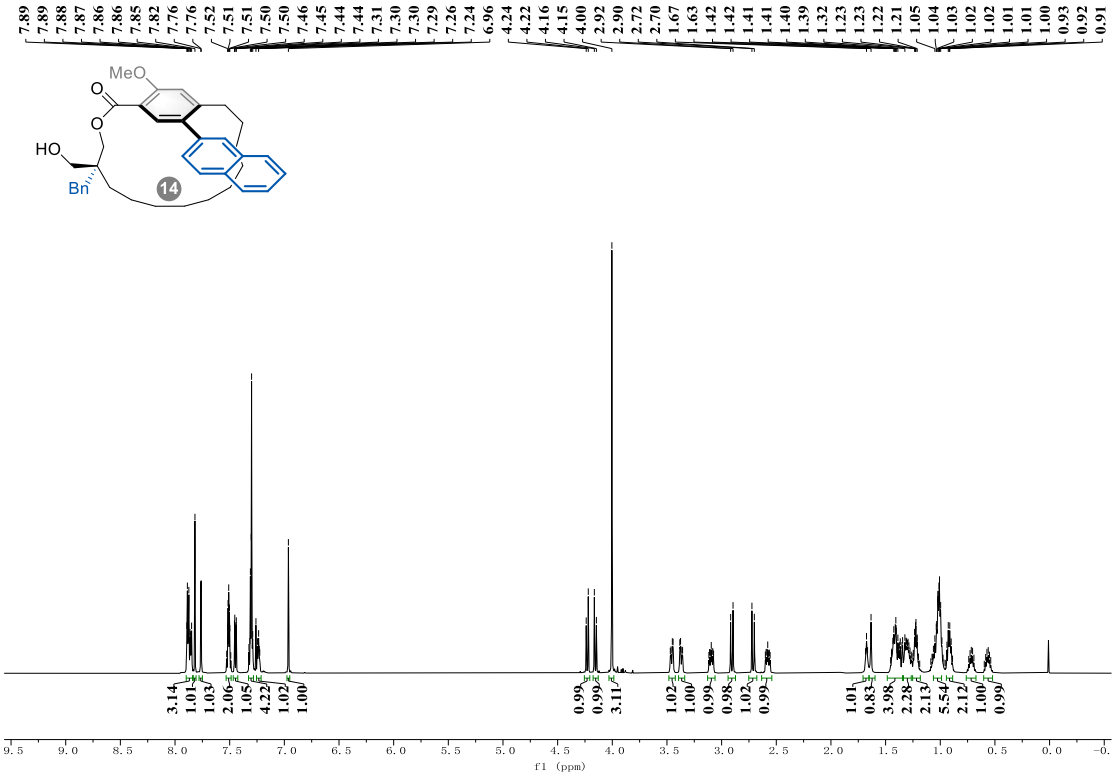
17, **^{1}H NMR** (600 MHz, $CDCl_3$)



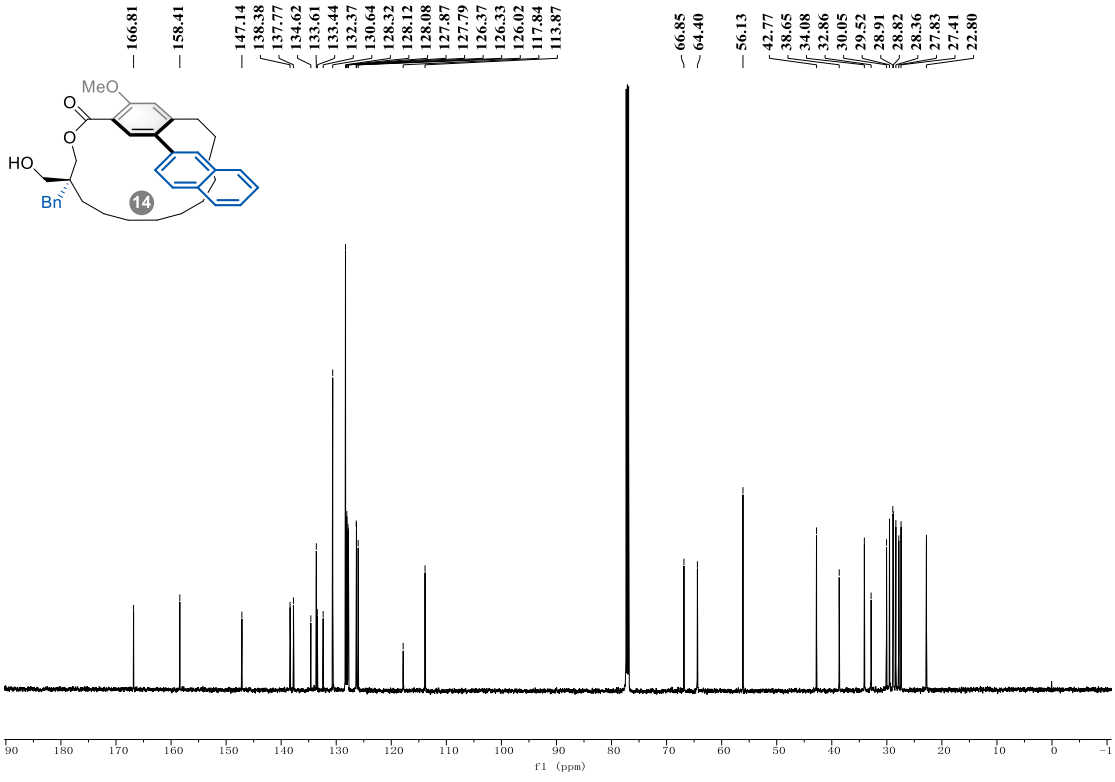
17, **^{13}C NMR** (151 MHz, $CDCl_3$)



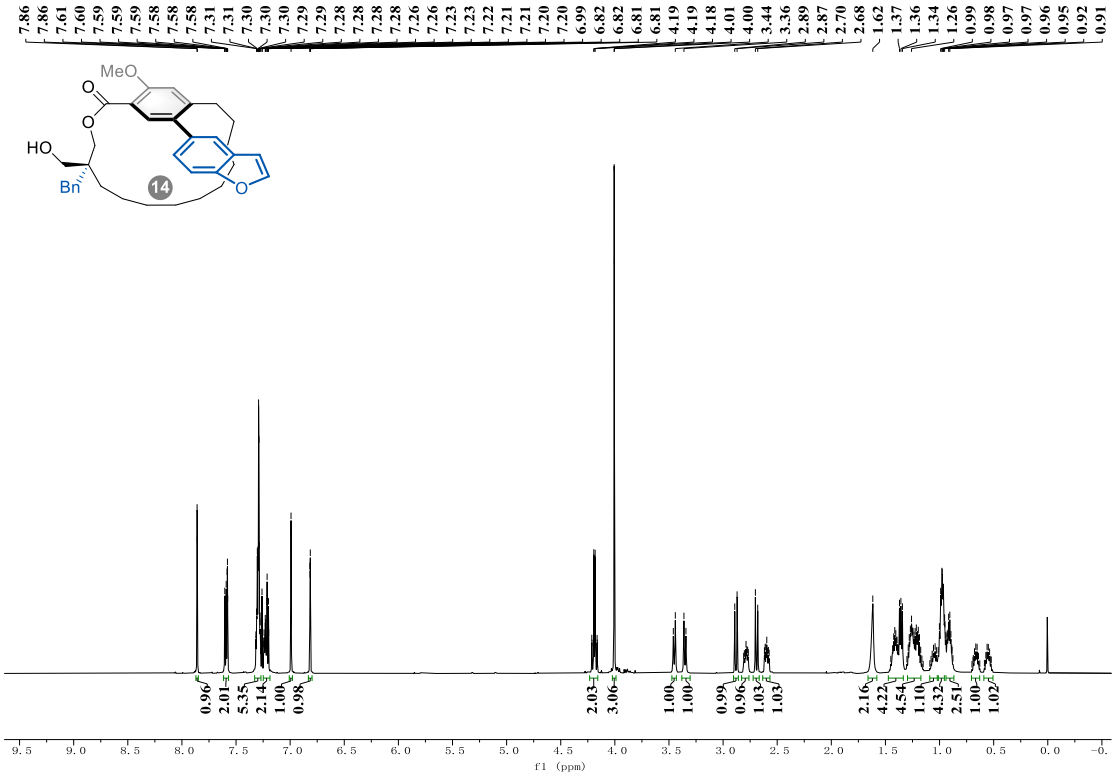
18, **^{1}H NMR** (600 MHz, $CDCl_3$)



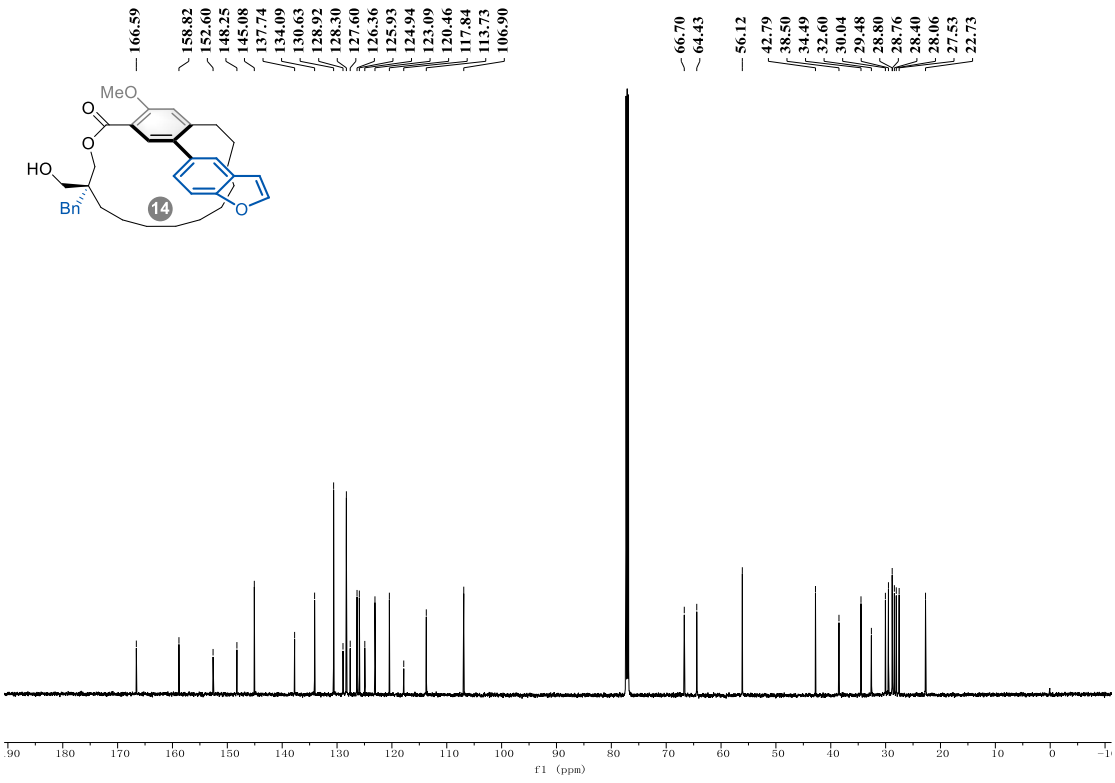
18, **^{13}C NMR** (151 MHz, $CDCl_3$)



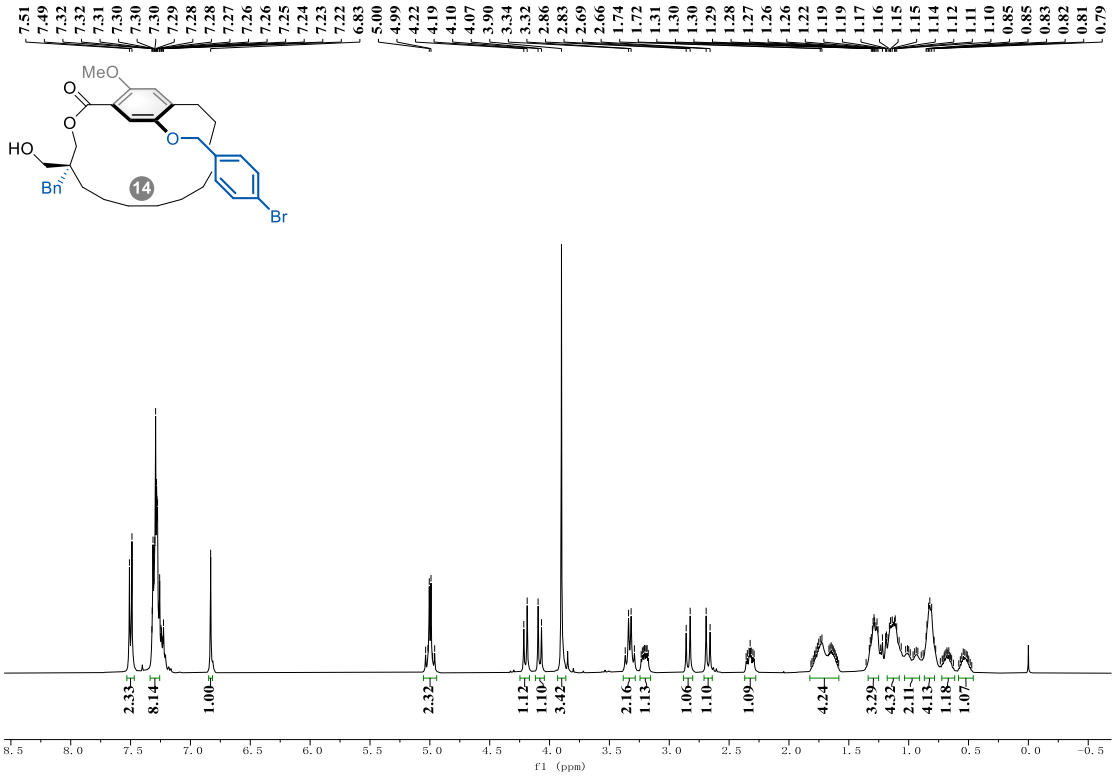
19, **^{1}H NMR** (600 MHz, $CDCl_3$)



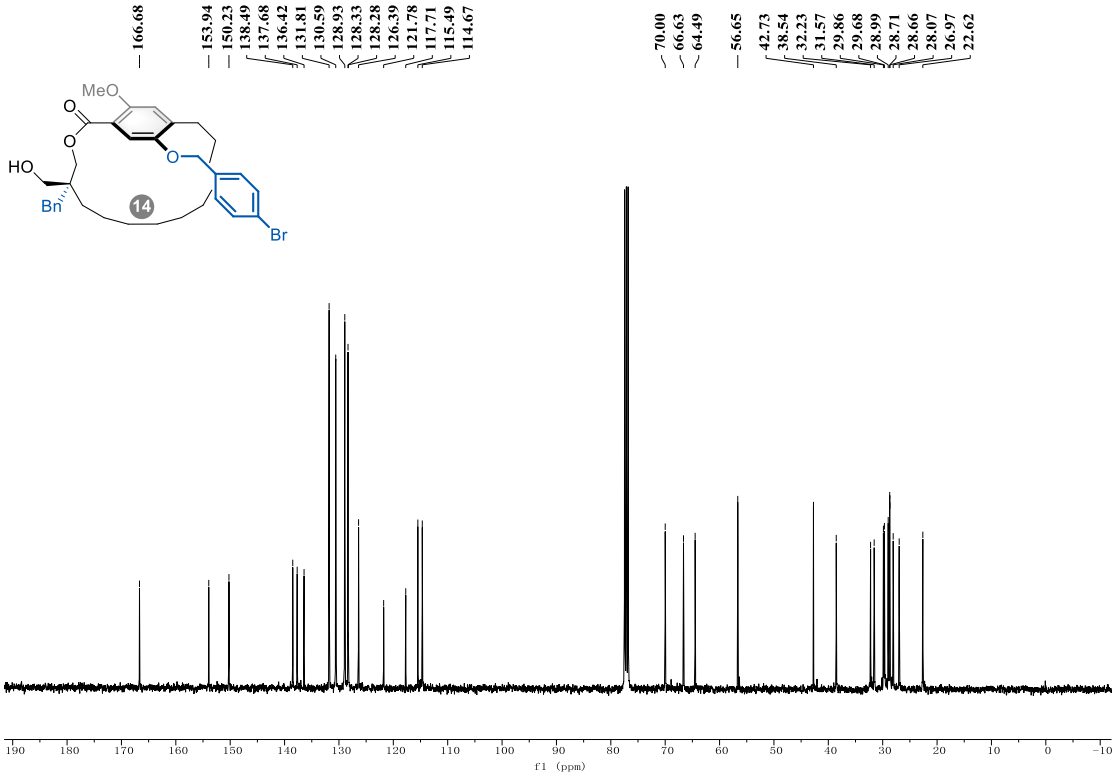
19, **^{13}C NMR** (151 MHz, $CDCl_3$)



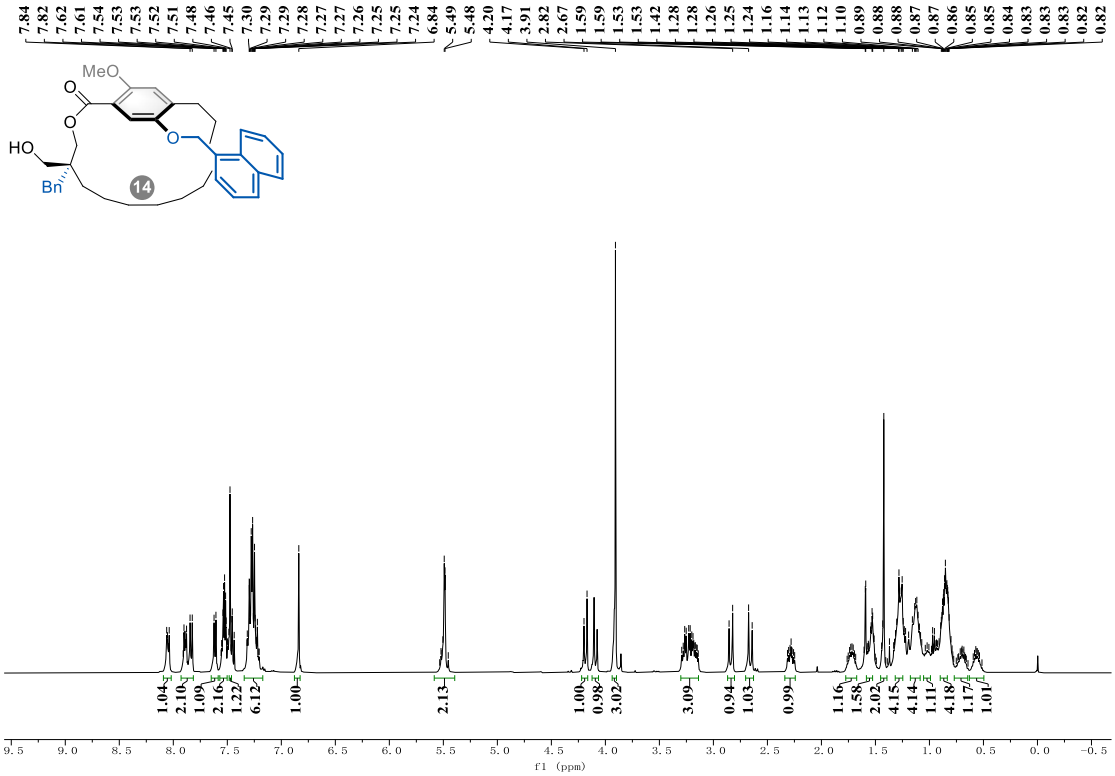
20, **^{1}H NMR** (400 MHz, $CDCl_3$)



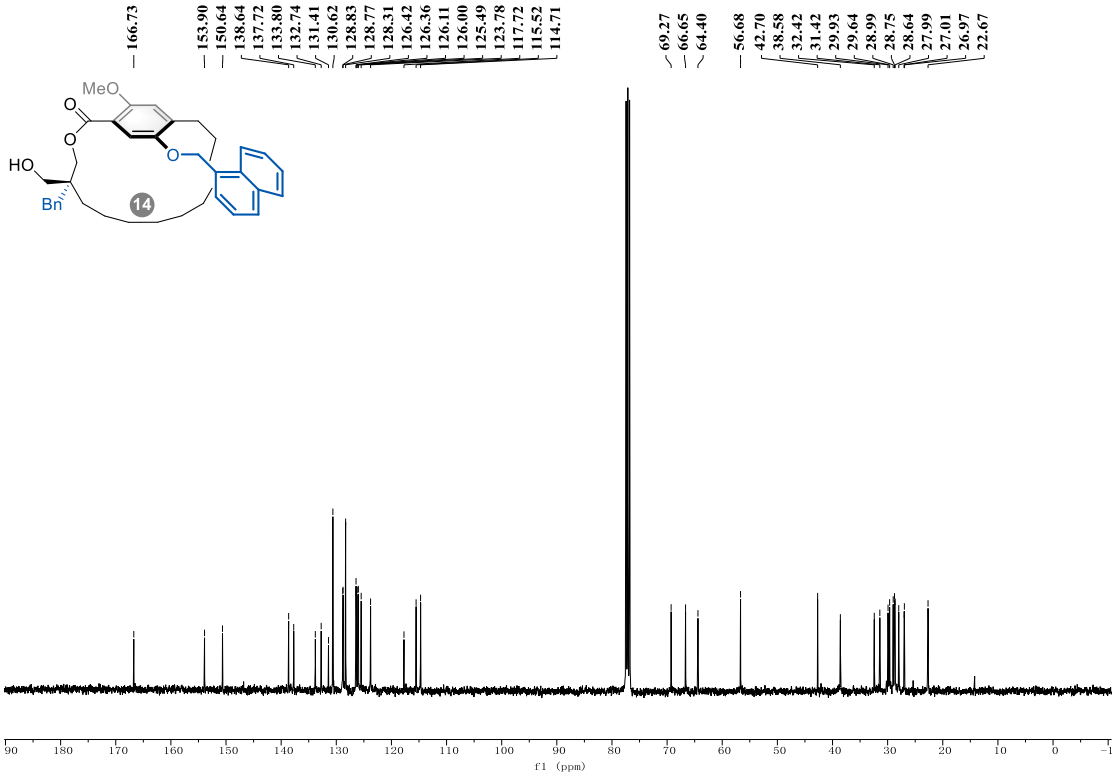
20, **^{13}C NMR** (101 MHz, $CDCl_3$)



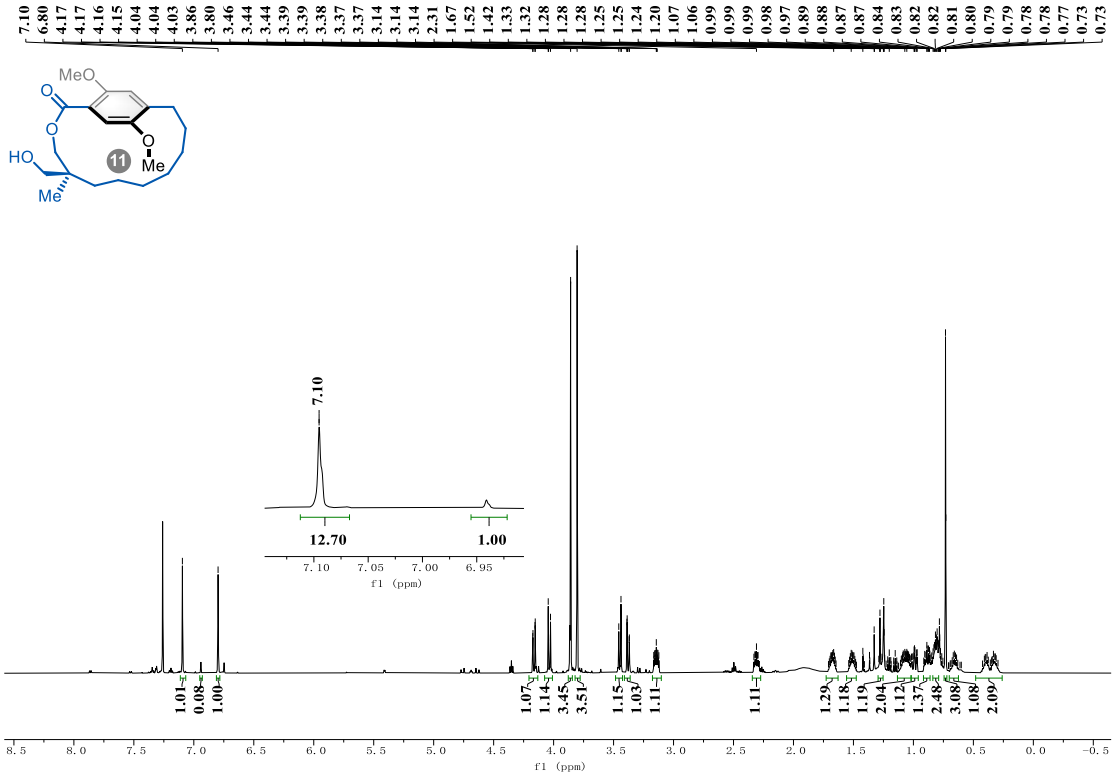
21, **^{1}H NMR** (400 MHz, $CDCl_3$)



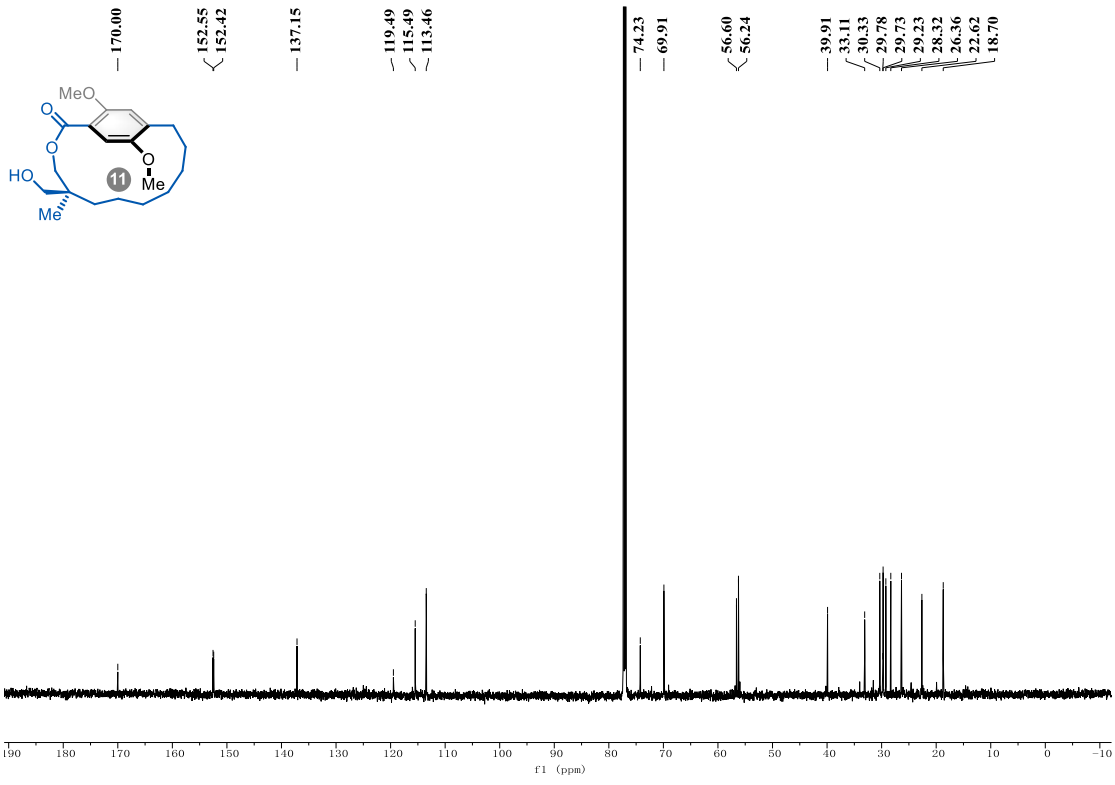
21, **^{13}C NMR** (101 MHz, $CDCl_3$)



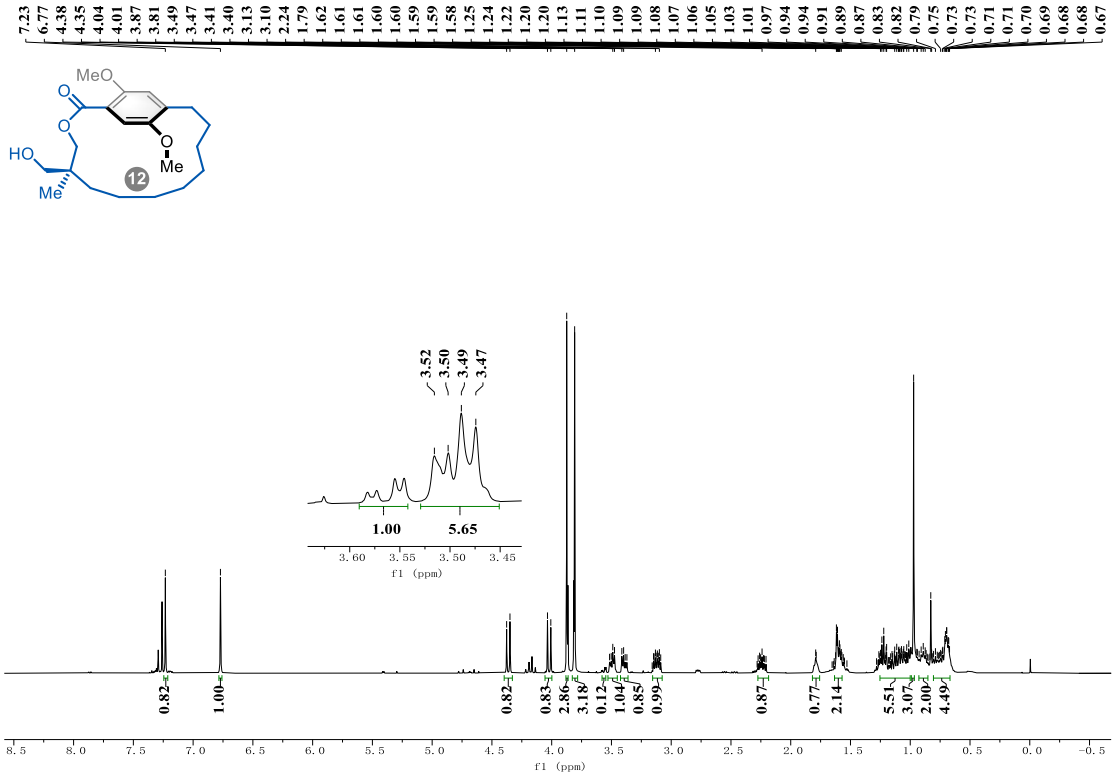
22, **^{1}H NMR** (600 MHz, $CDCl_3$)



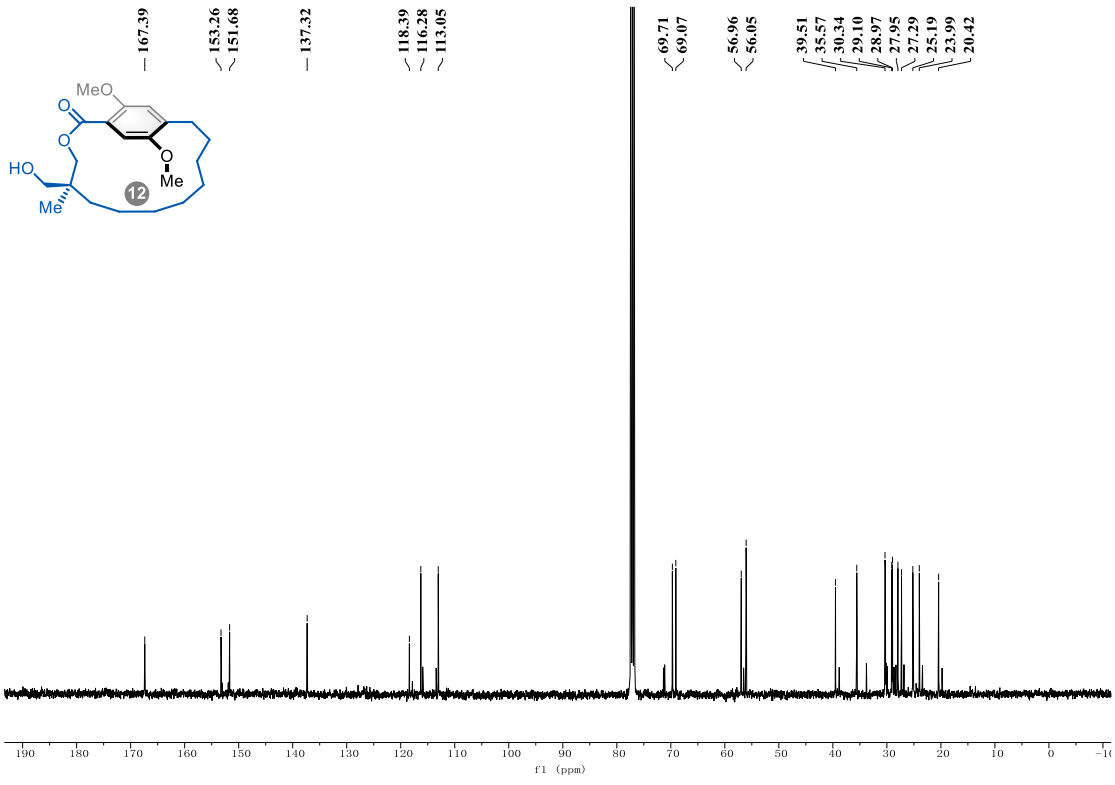
22, **^{13}C NMR** (151 MHz, $CDCl_3$)



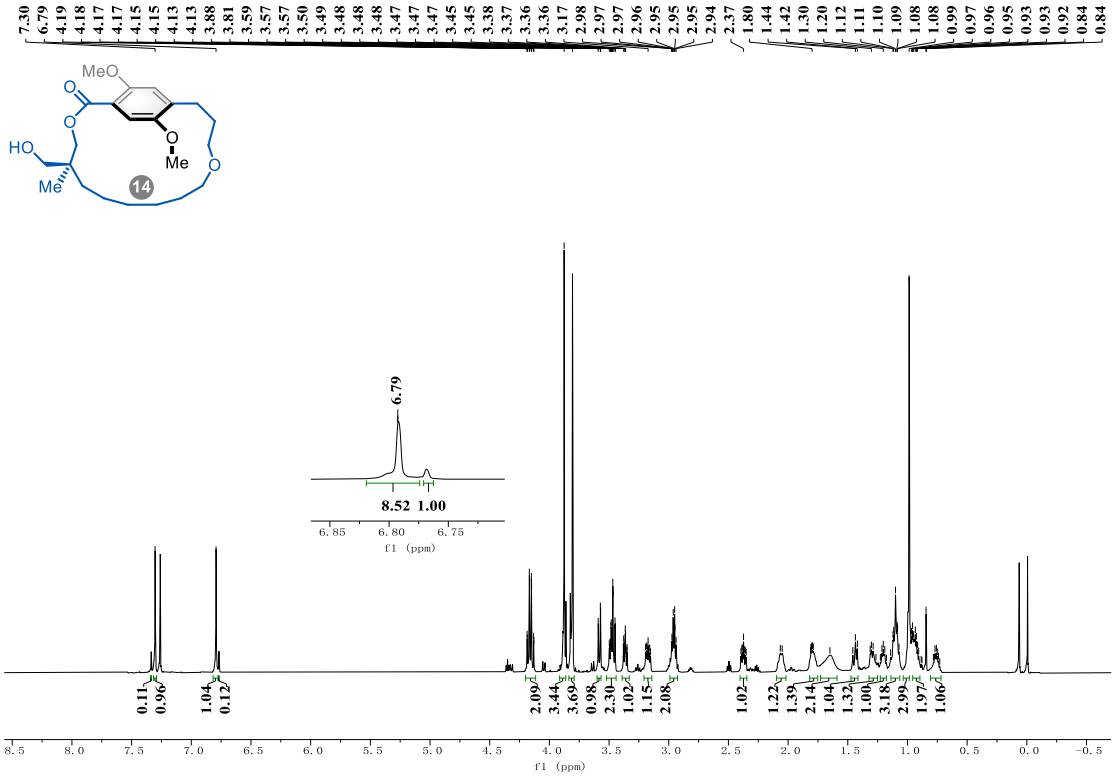
23, **^{1}H NMR** (400 MHz, $CDCl_3$)



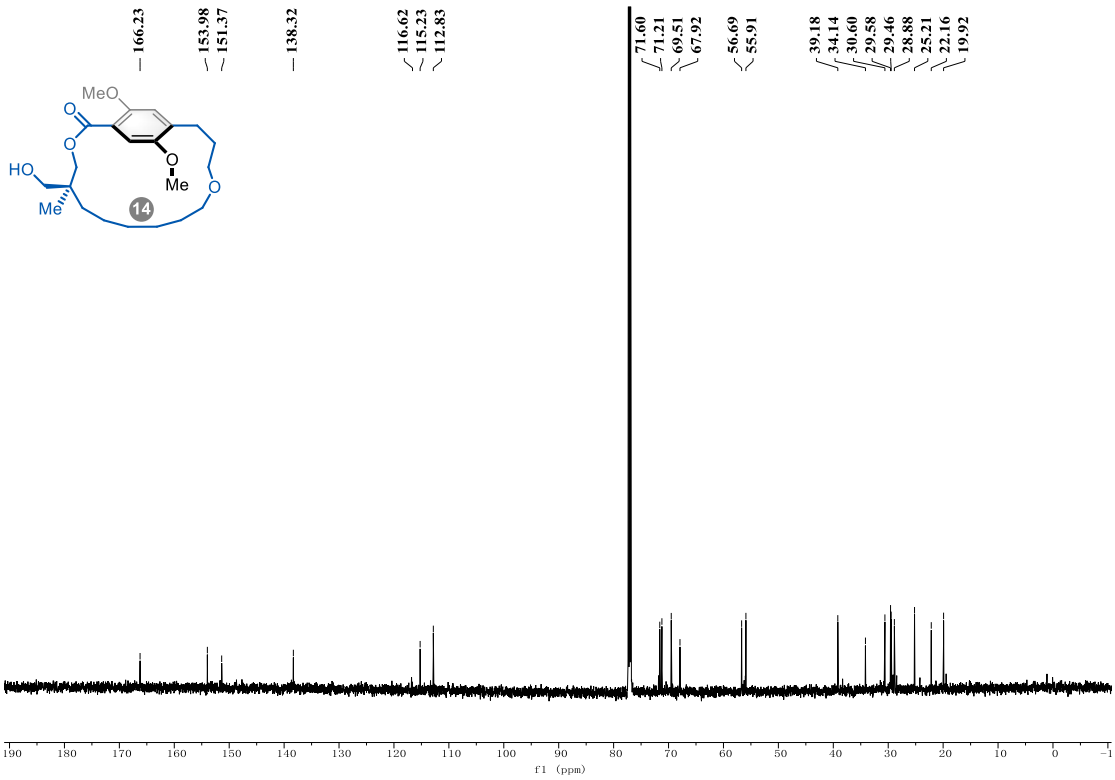
23, **^{13}C NMR** (101 MHz, $CDCl_3$)



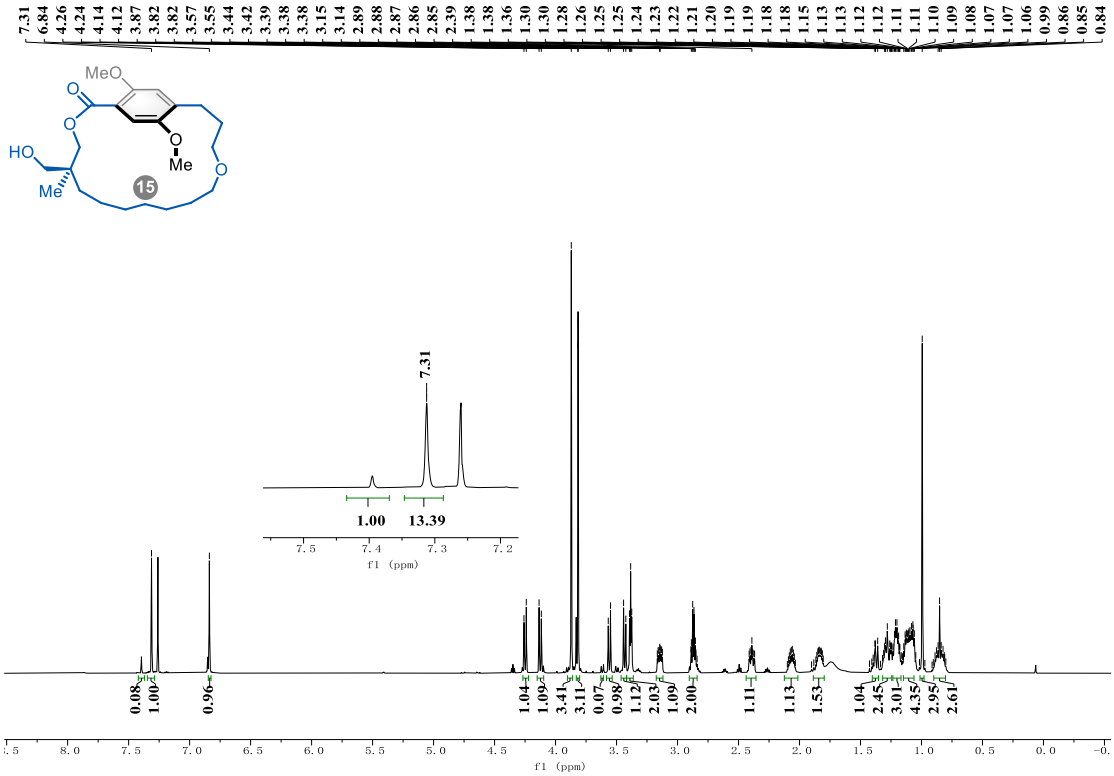
24, **^{1}H NMR** (600 MHz, $CDCl_3$)



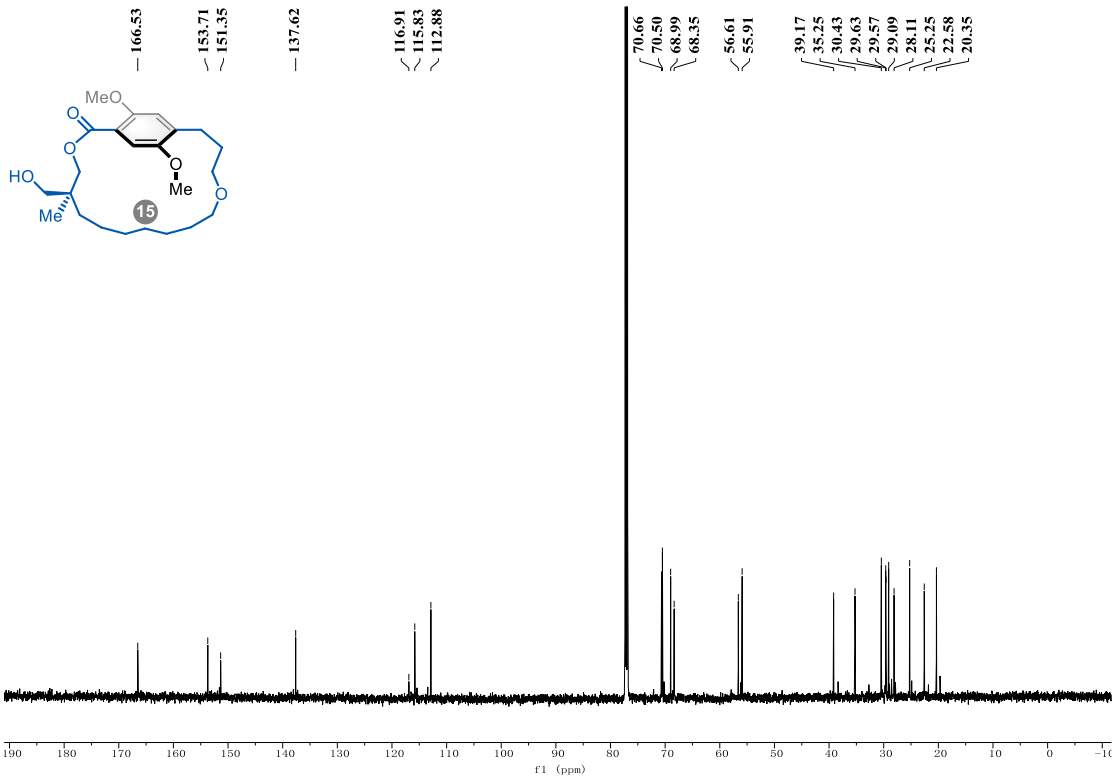
24, **^{13}C NMR** (151 MHz, $CDCl_3$)



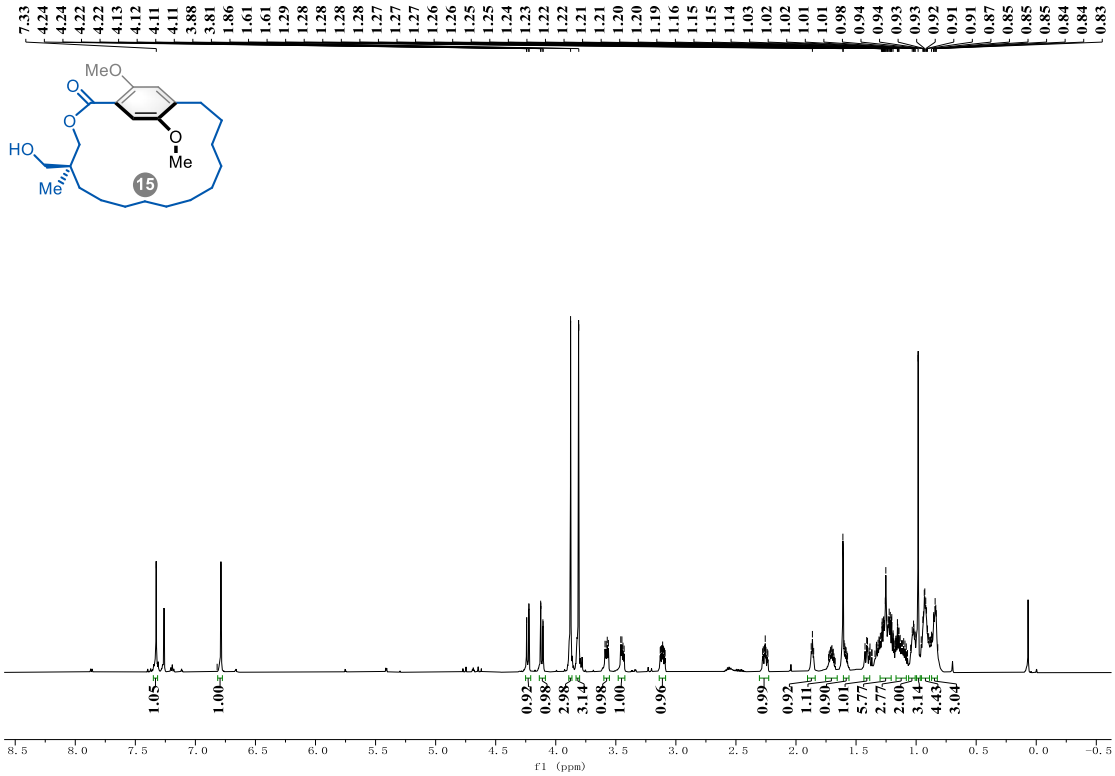
25, **^{1}H NMR** (600 MHz, $CDCl_3$)



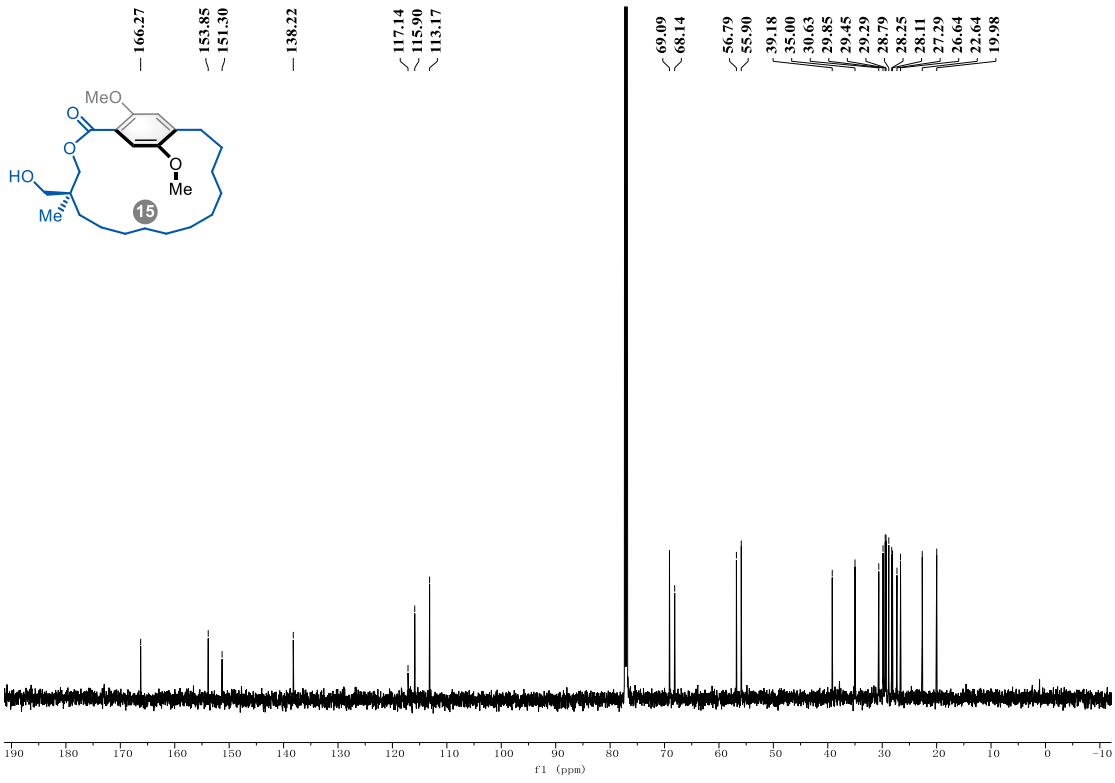
25, **^{13}C NMR** (151 MHz, $CDCl_3$)



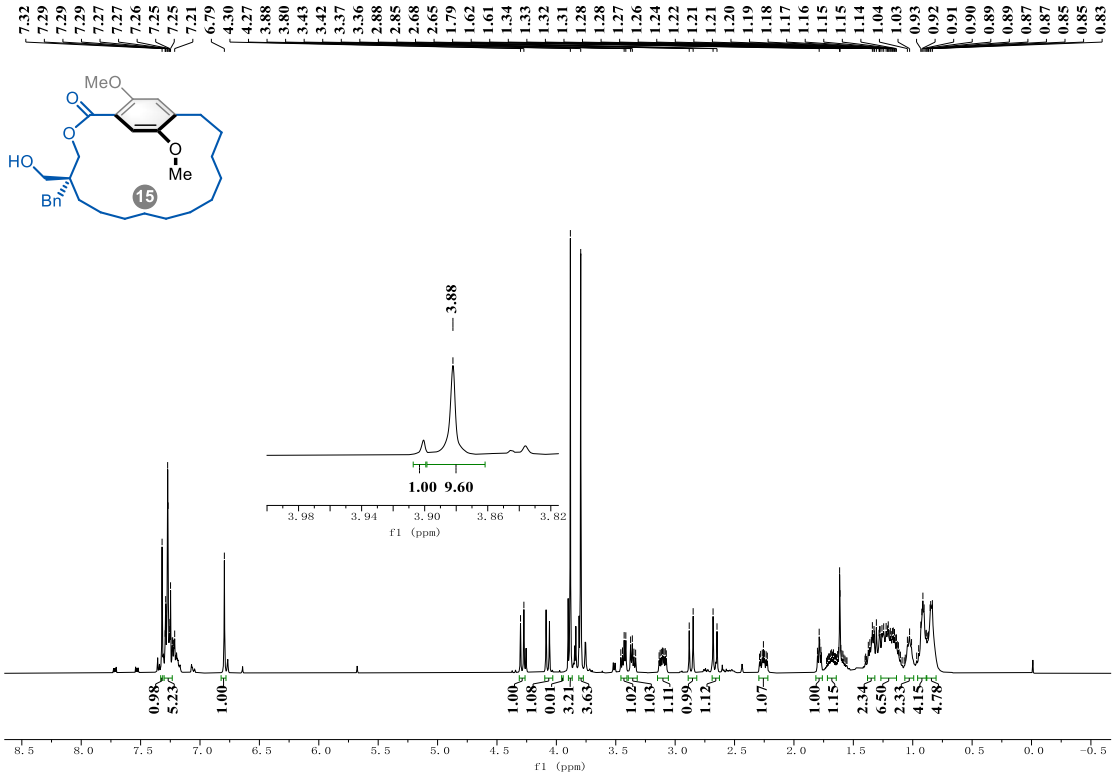
26, **^{1}H NMR** (600 MHz, $CDCl_3$)



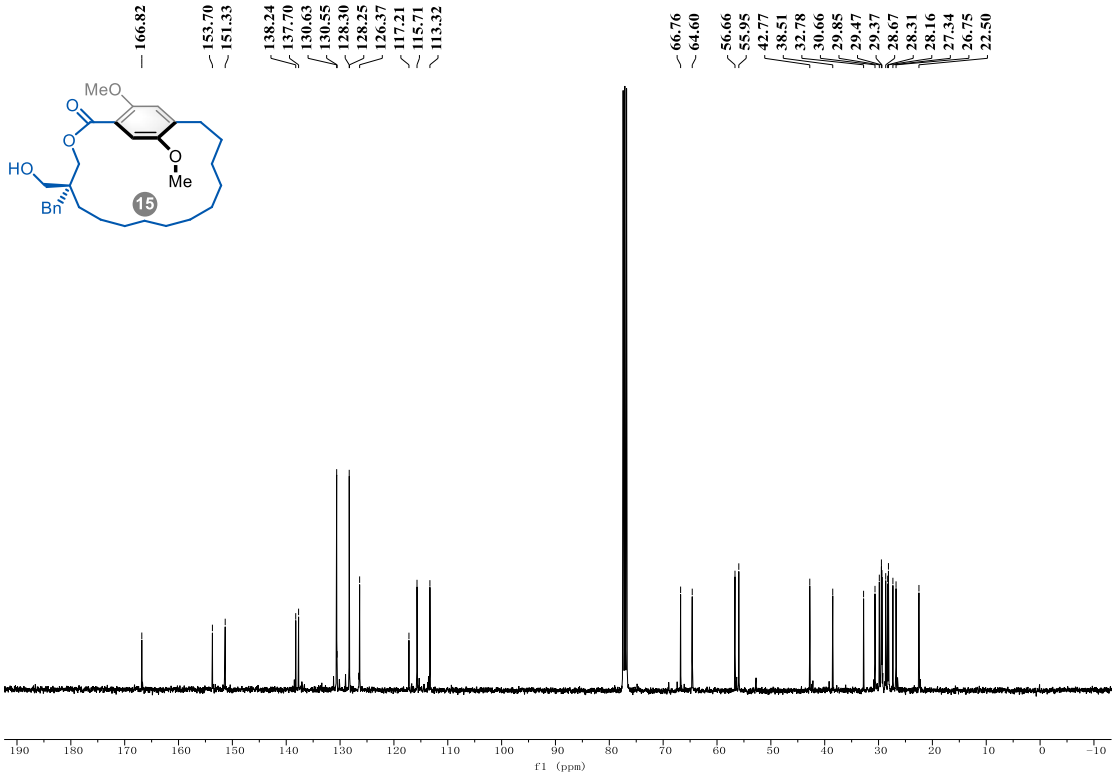
26, **^{13}C NMR** (151 MHz, $CDCl_3$)



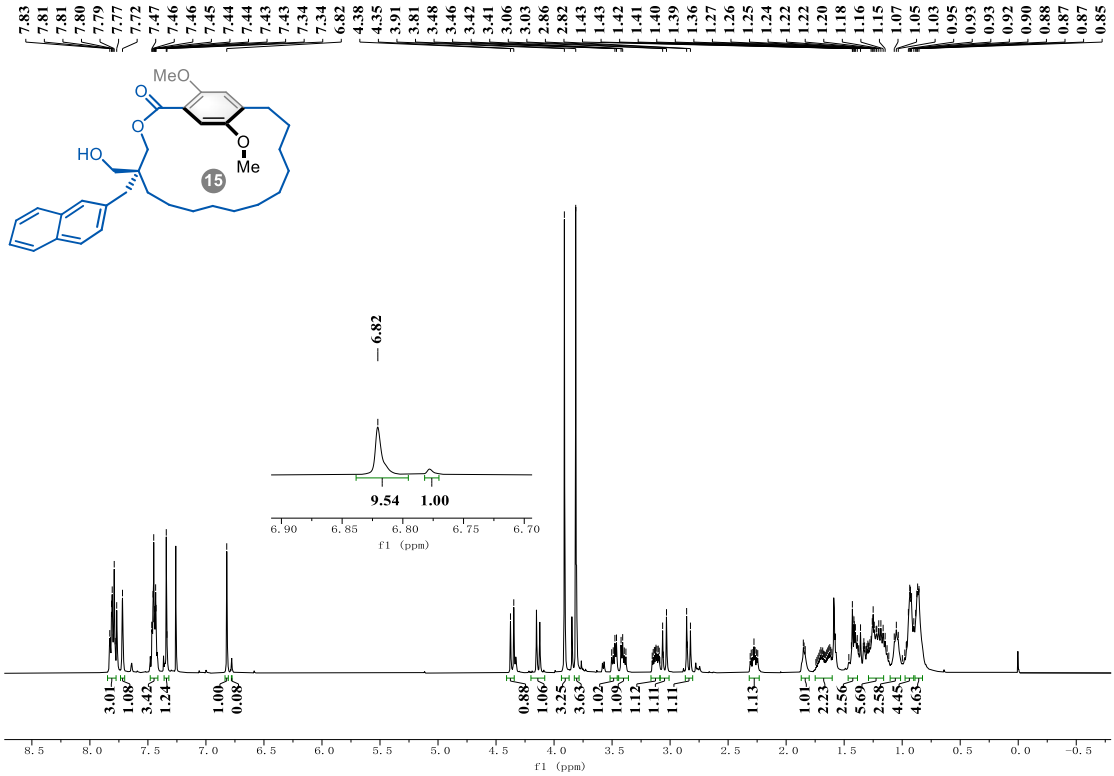
27, **^{1}H NMR** (400 MHz, $CDCl_3$)



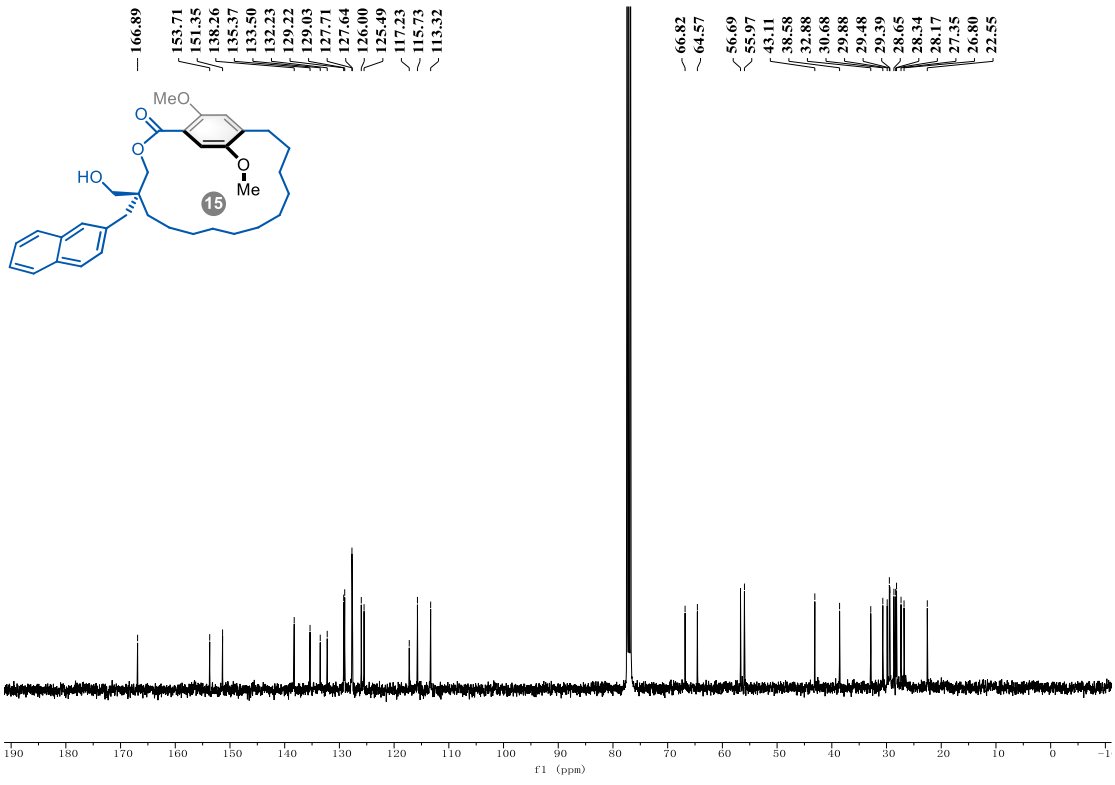
27, **^{13}C NMR** (101 MHz, $CDCl_3$)



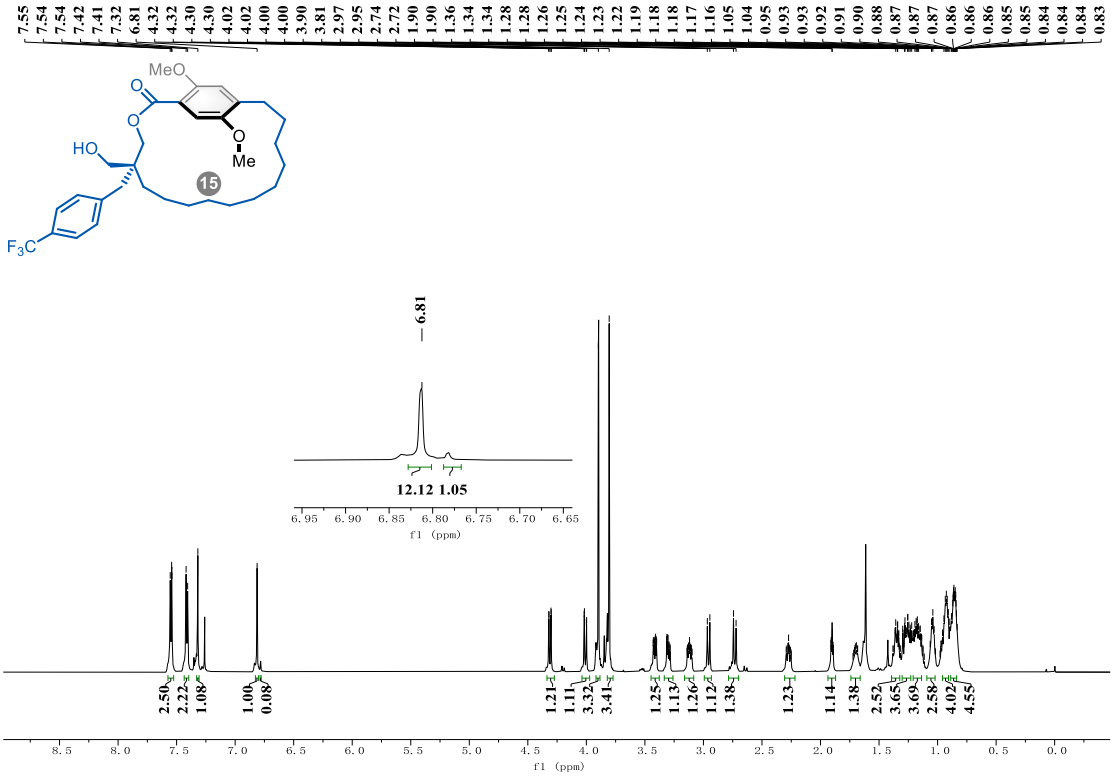
28, **^{1}H NMR** (400 MHz, $CDCl_3$)



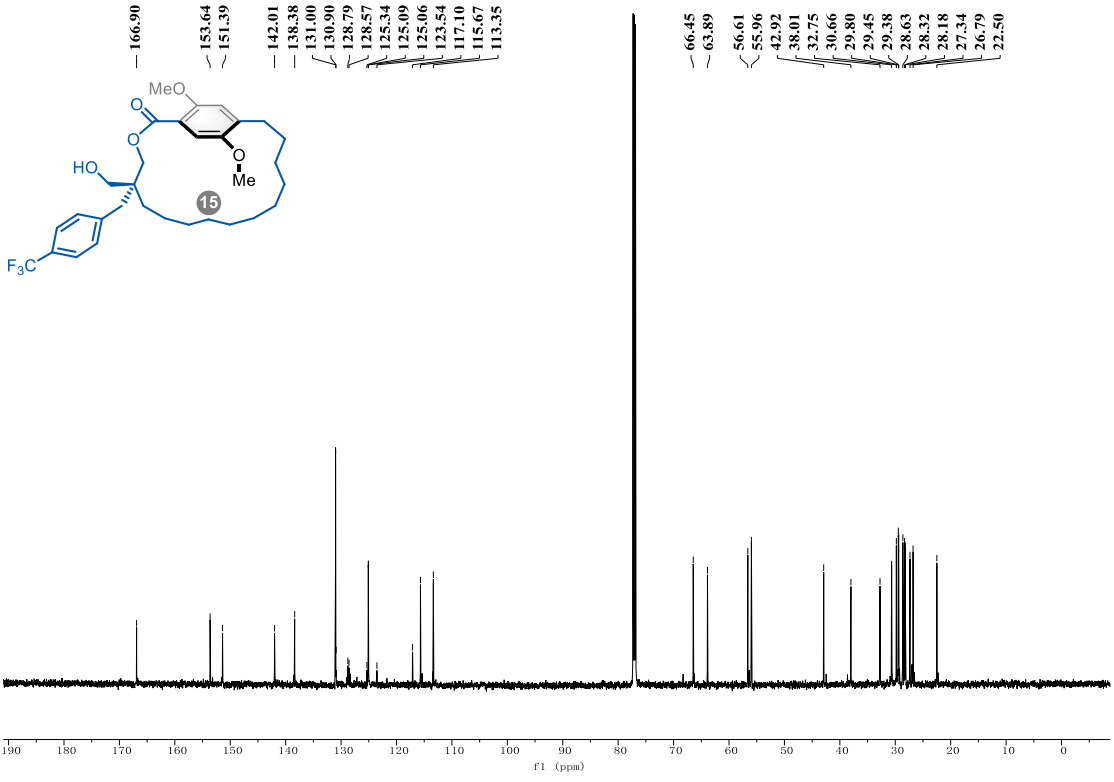
28, **^{13}C NMR** (101 MHz, $CDCl_3$)



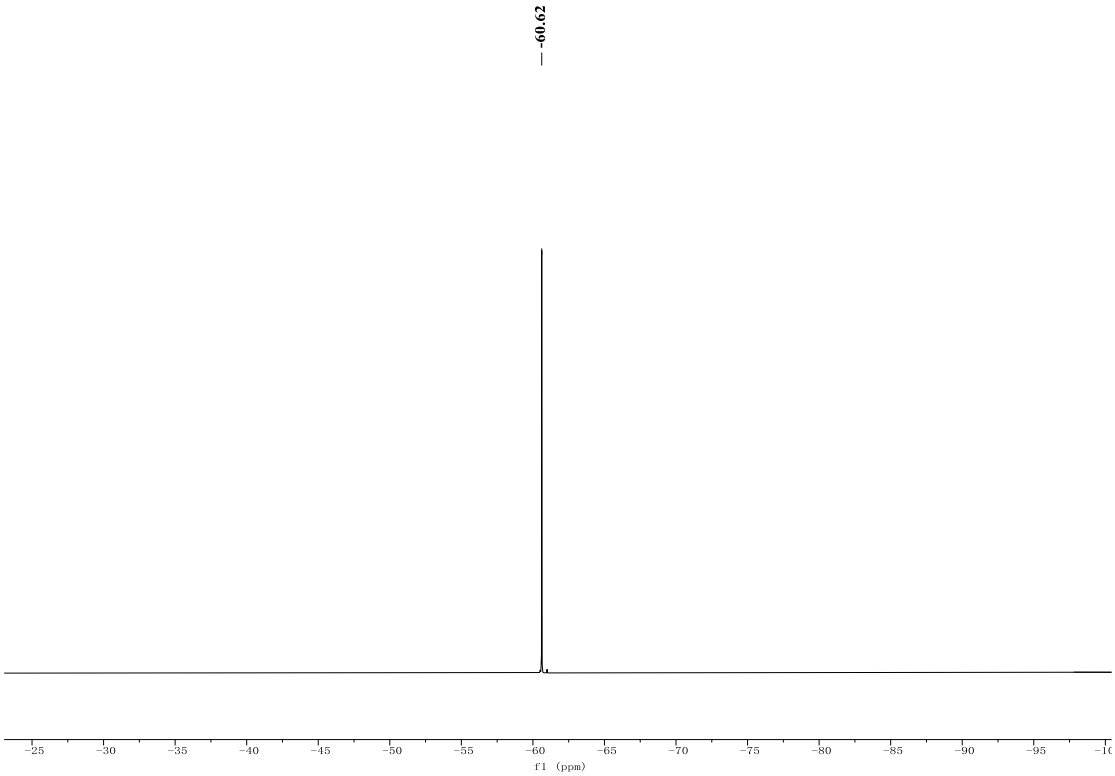
29, **^{1}H NMR** (600 MHz, $CDCl_3$)



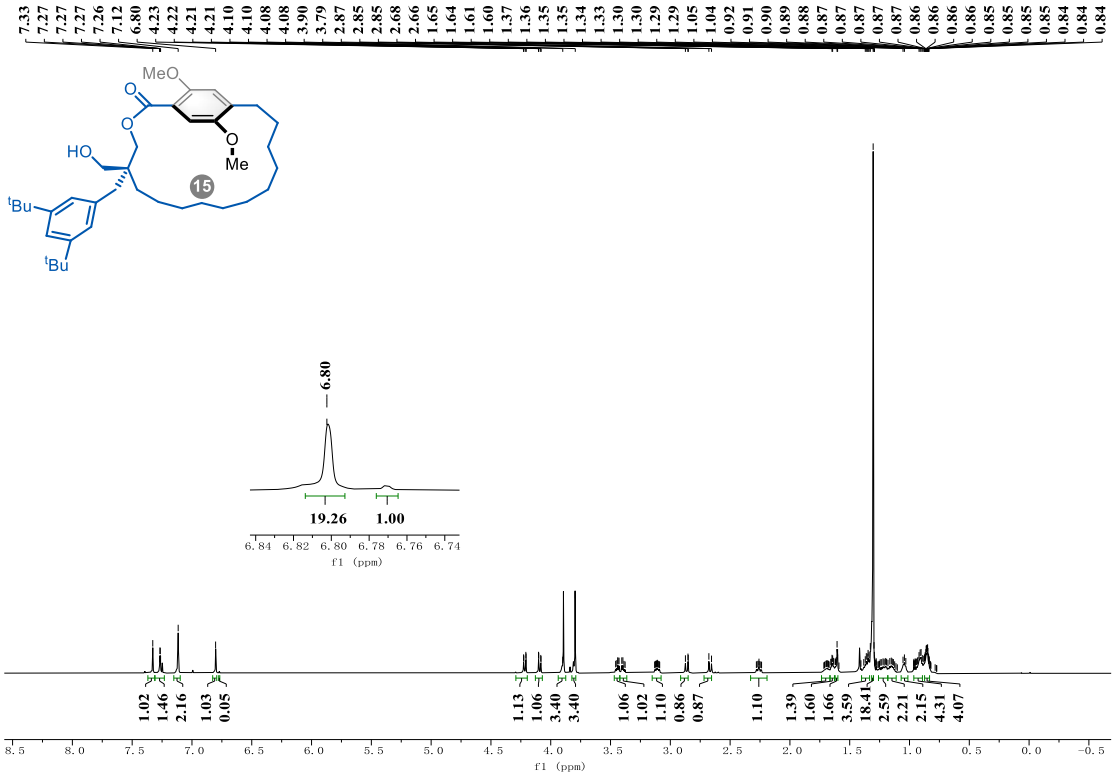
29, **^{13}C NMR** (151 MHz, $CDCl_3$)



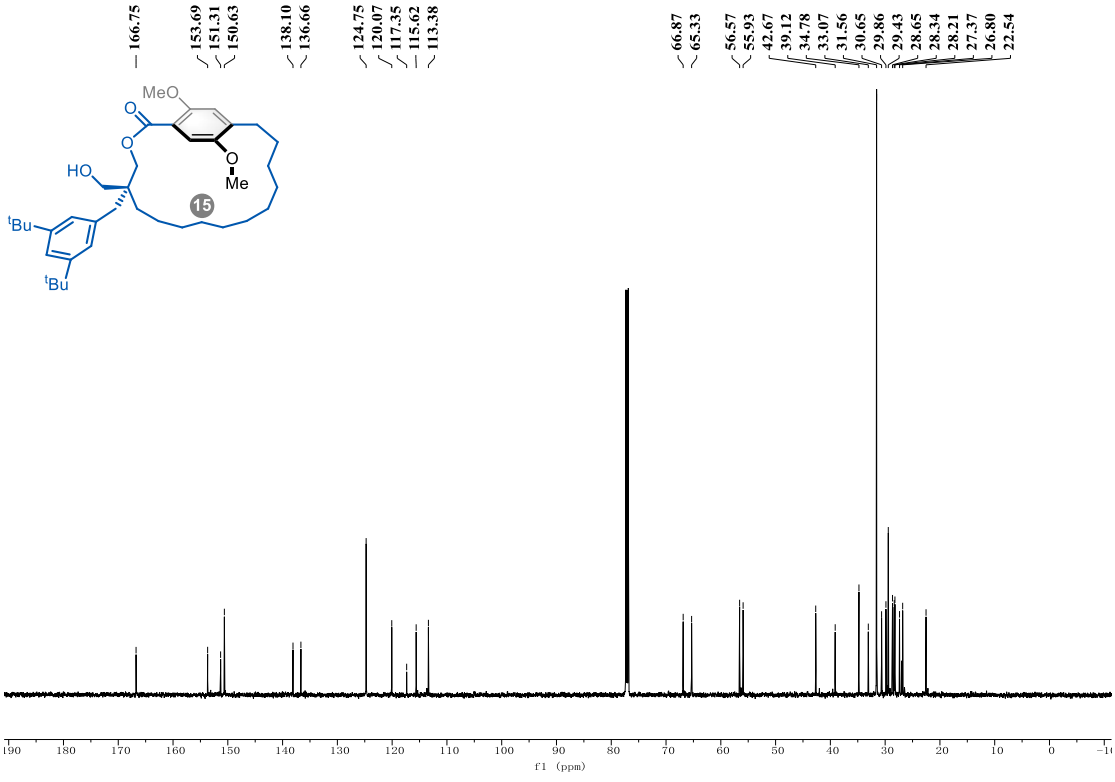
29, **^{19}F NMR** (565 MHz, DMSO-*d6*)



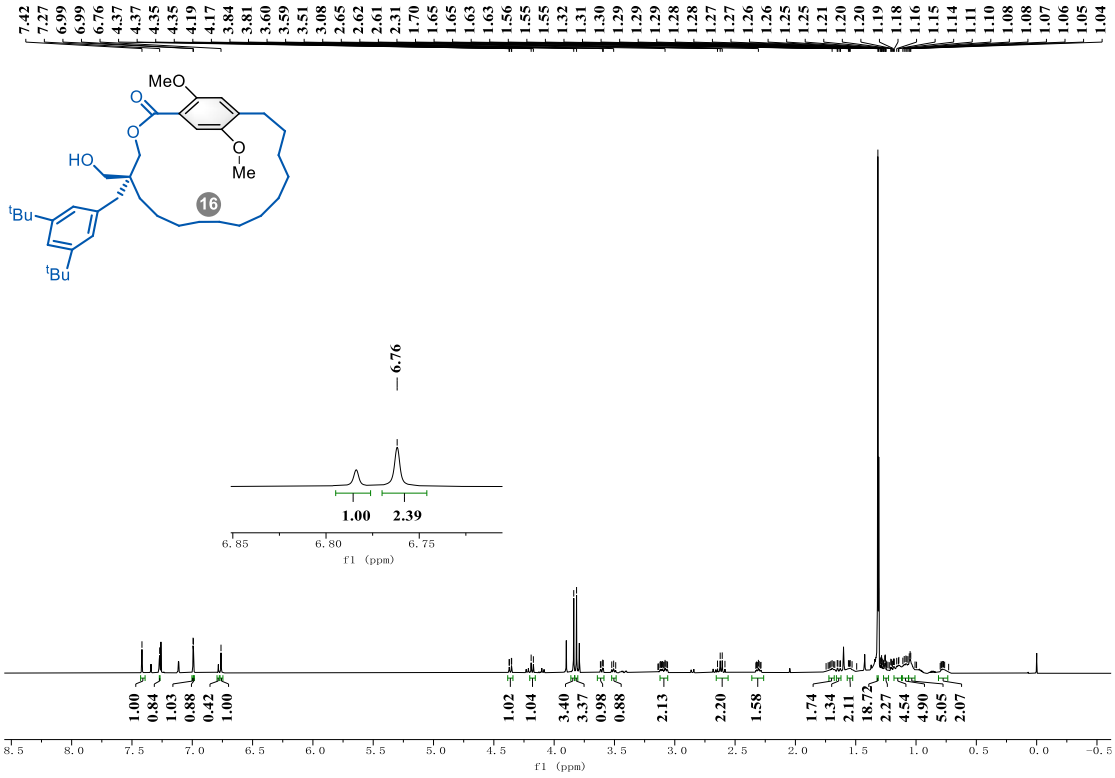
30, **^{1}H NMR** (600 MHz, $CDCl_3$)



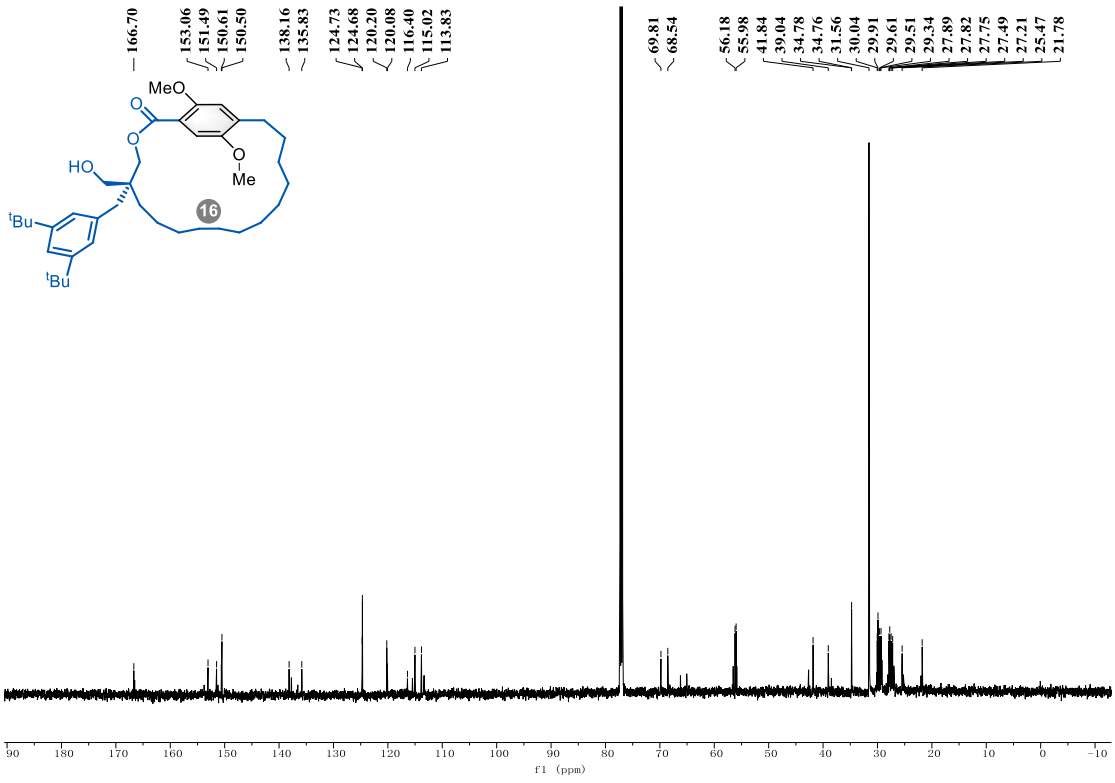
30, **^{13}C NMR** (151 MHz, $CDCl_3$)



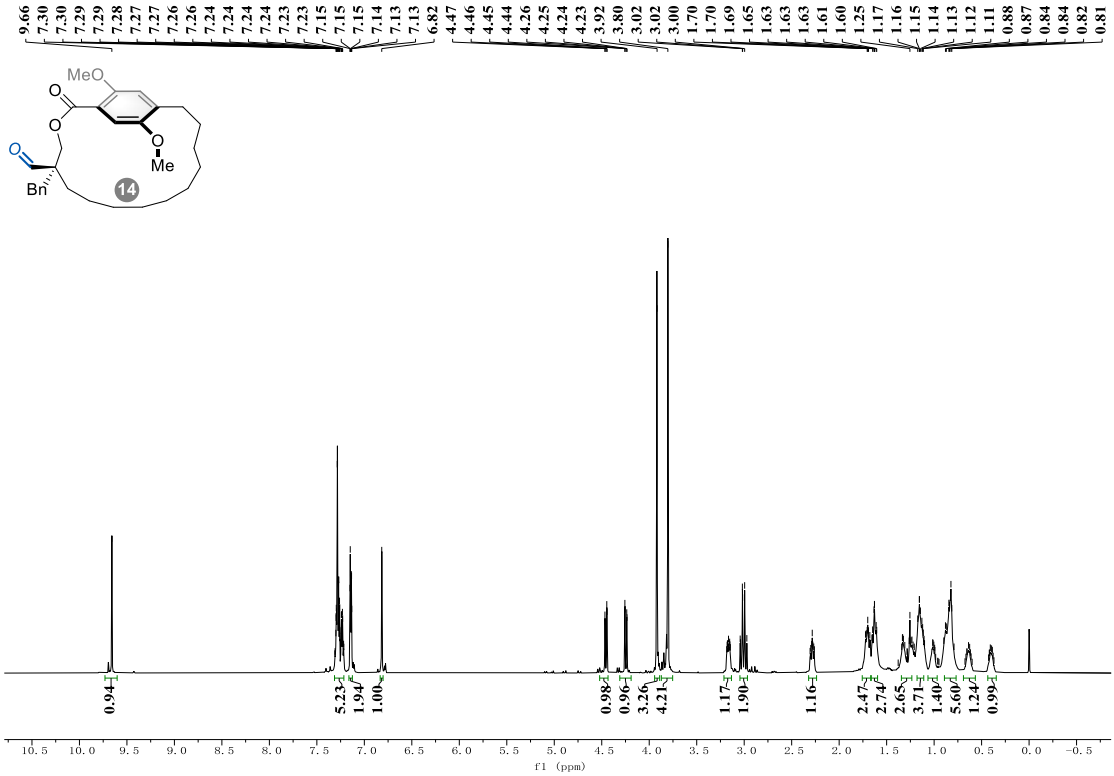
31, **^{1}H NMR** (600 MHz, $CDCl_3$)



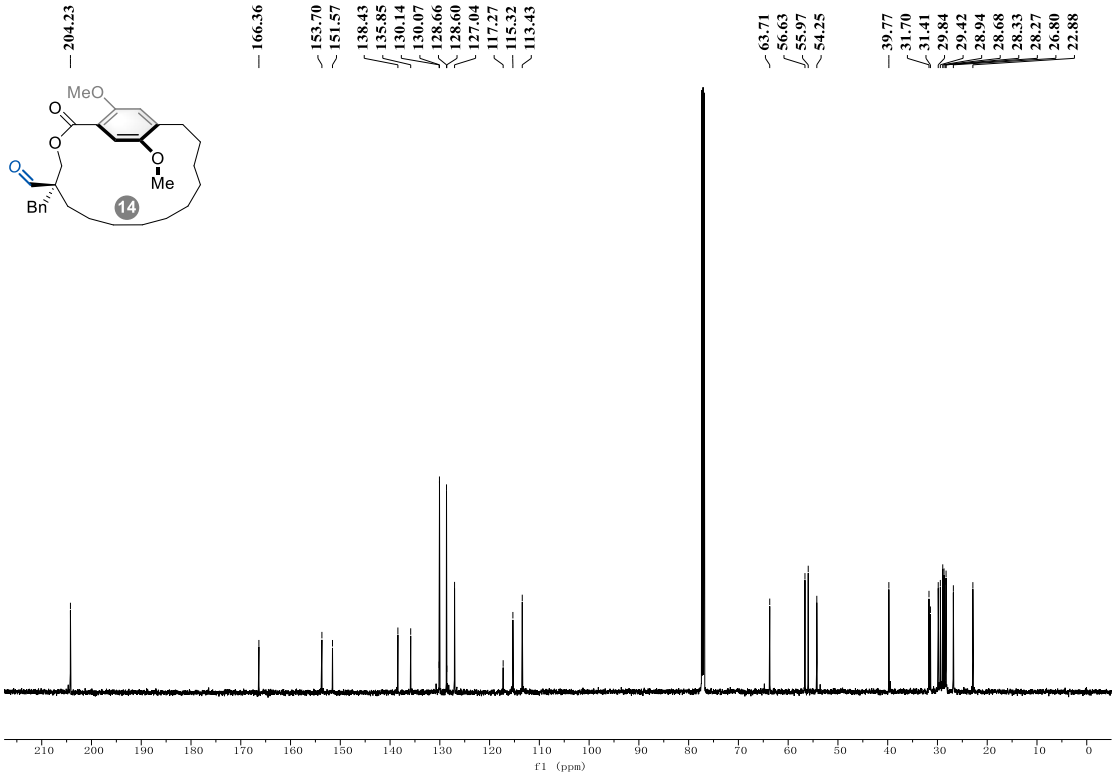
31, **^{13}C NMR** (151 MHz, $CDCl_3$)



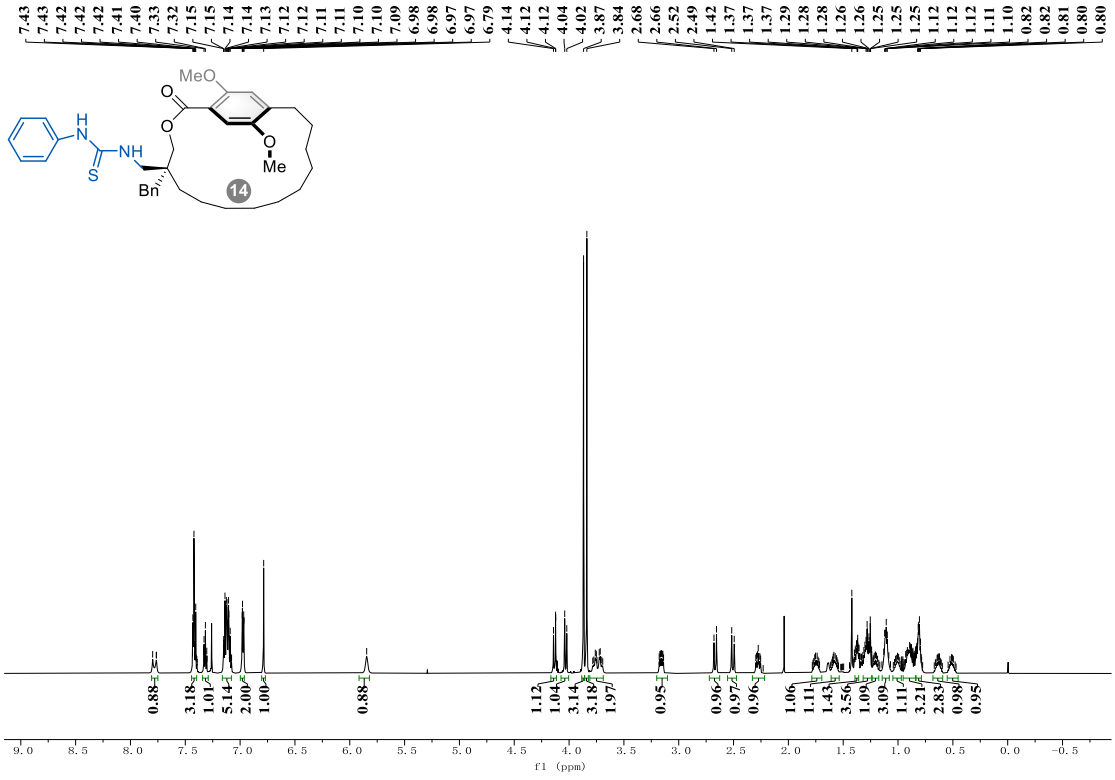
32, **^{1}H NMR** (600 MHz, $CDCl_3$)



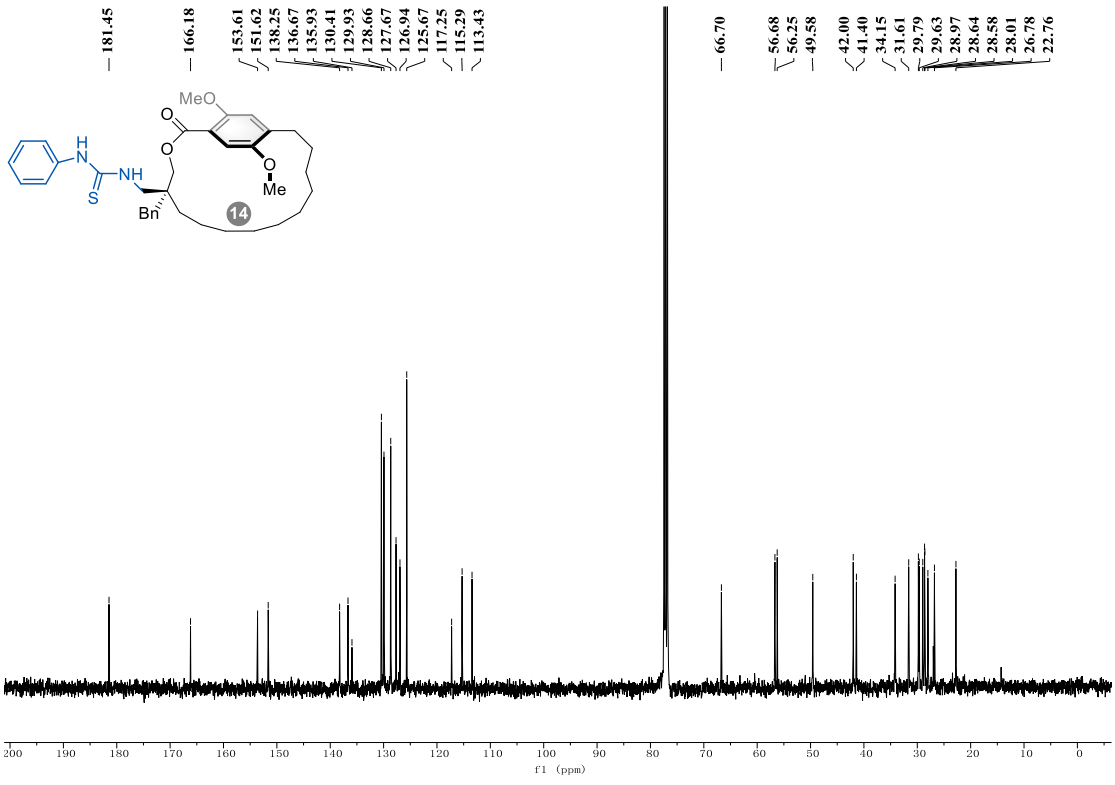
32, **^{13}C NMR** (151 MHz, $CDCl_3$)



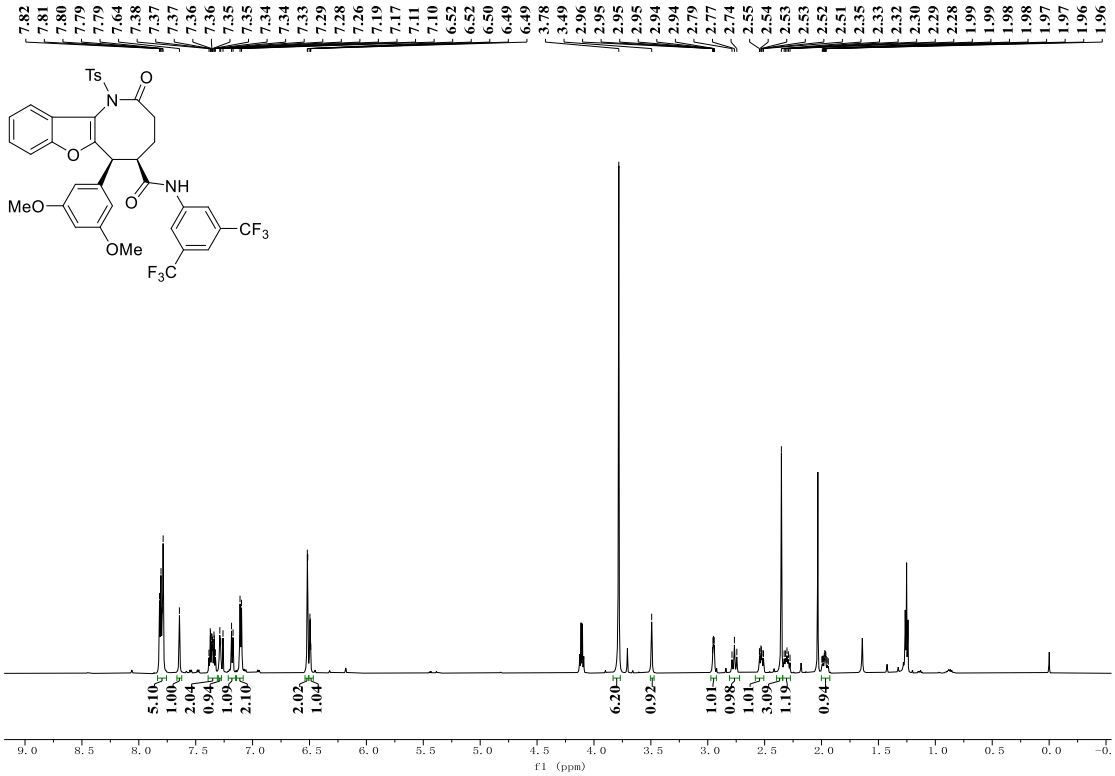
33, **^{1}H NMR** (600 MHz, $CDCl_3$)



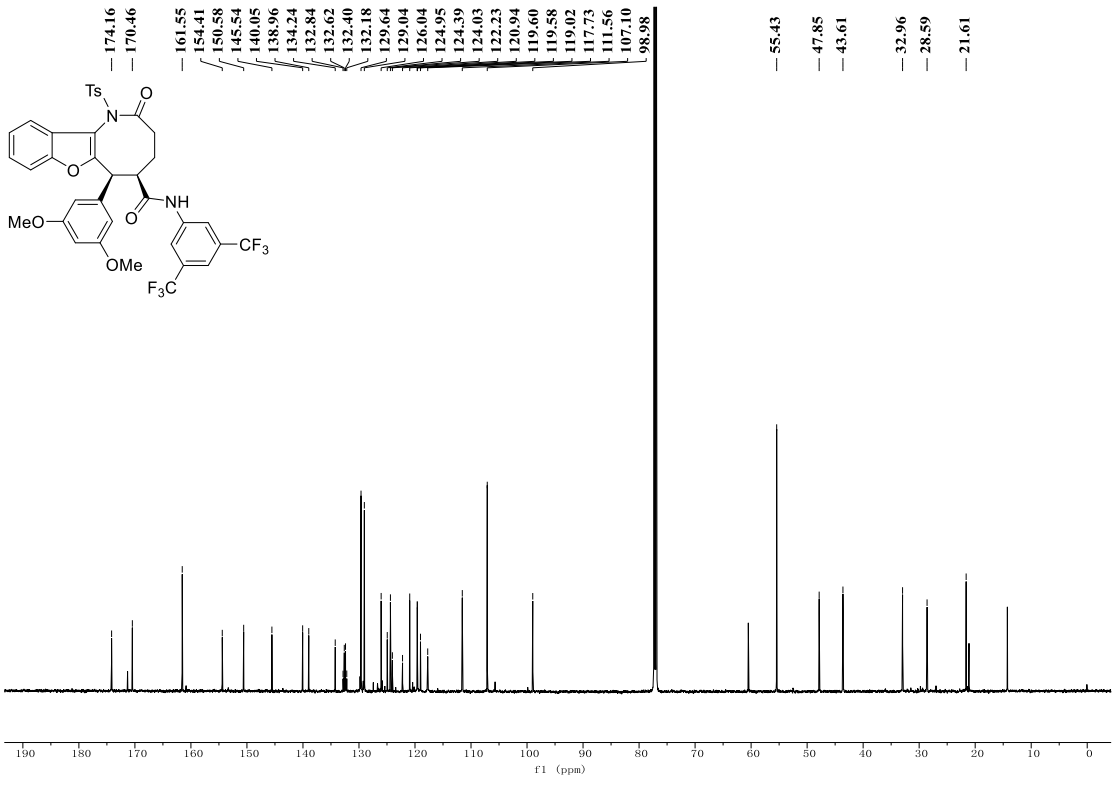
33, **^{13}C NMR** (151 MHz, $CDCl_3$)



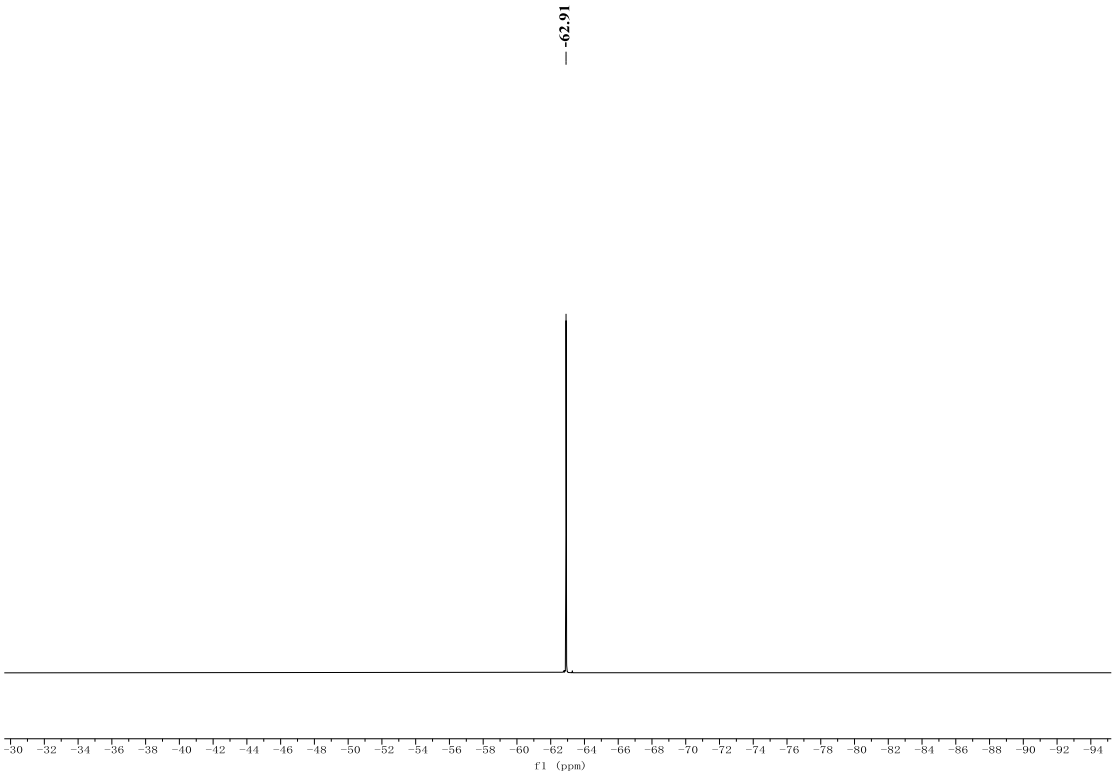
36, **^{1}H NMR** (600 MHz, $CDCl_3$)



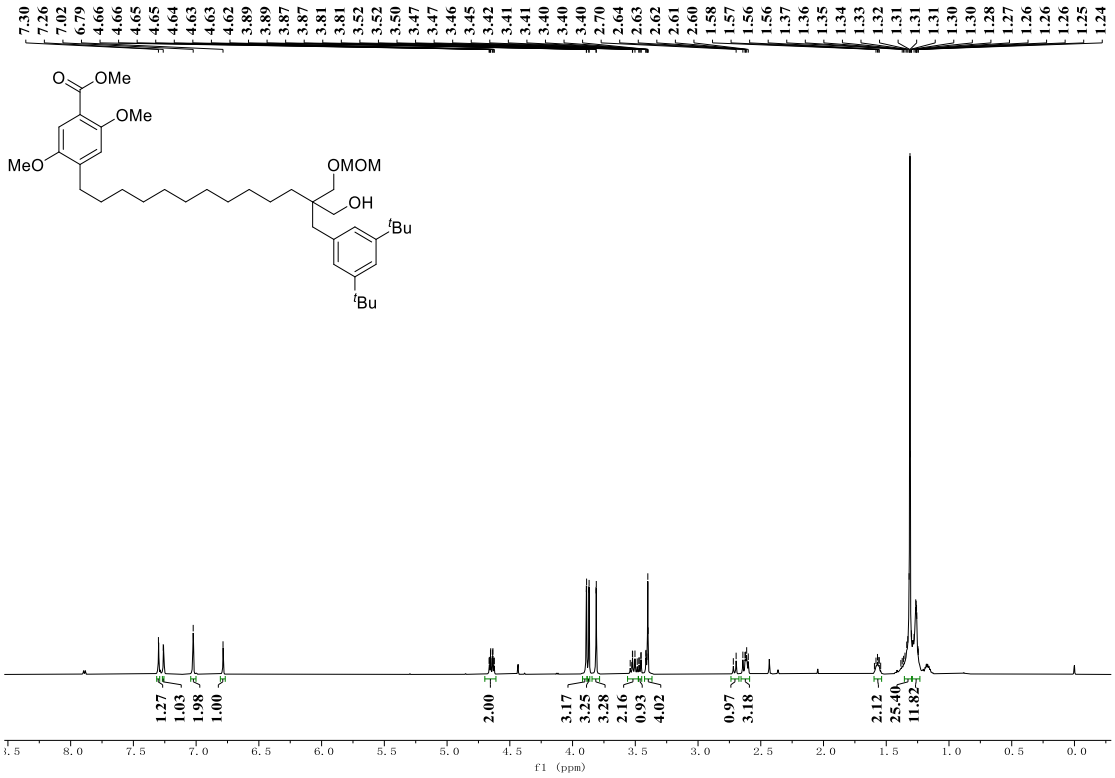
36, **^{13}C NMR** (151 MHz, $CDCl_3$)



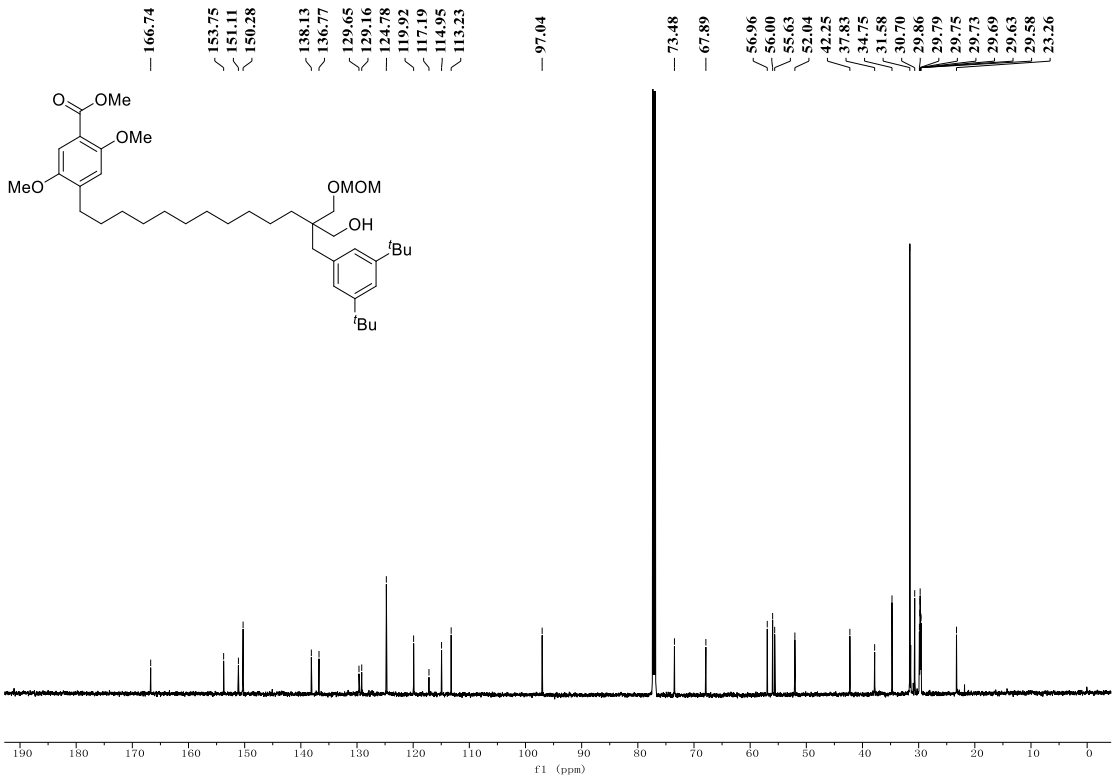
36, ^{19}F NMR (565 MHz, $CDCl_3$)



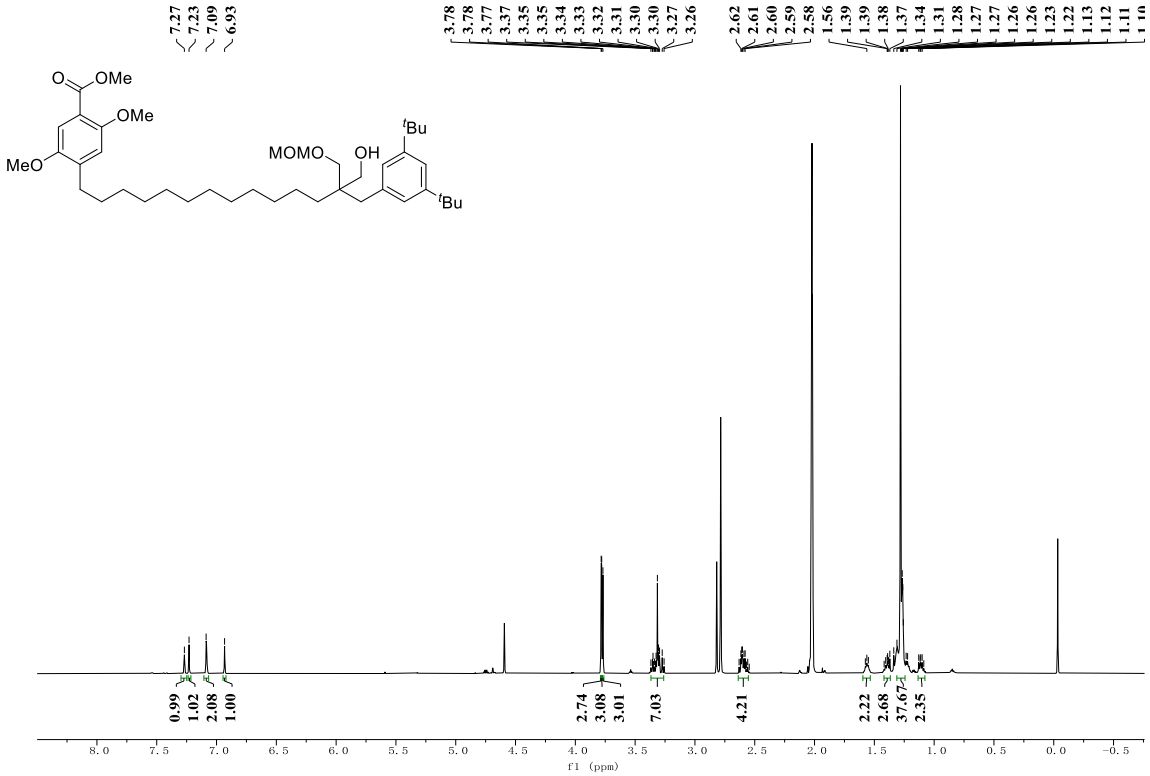
38, **^{1}H NMR** (600 MHz, $CDCl_3$)



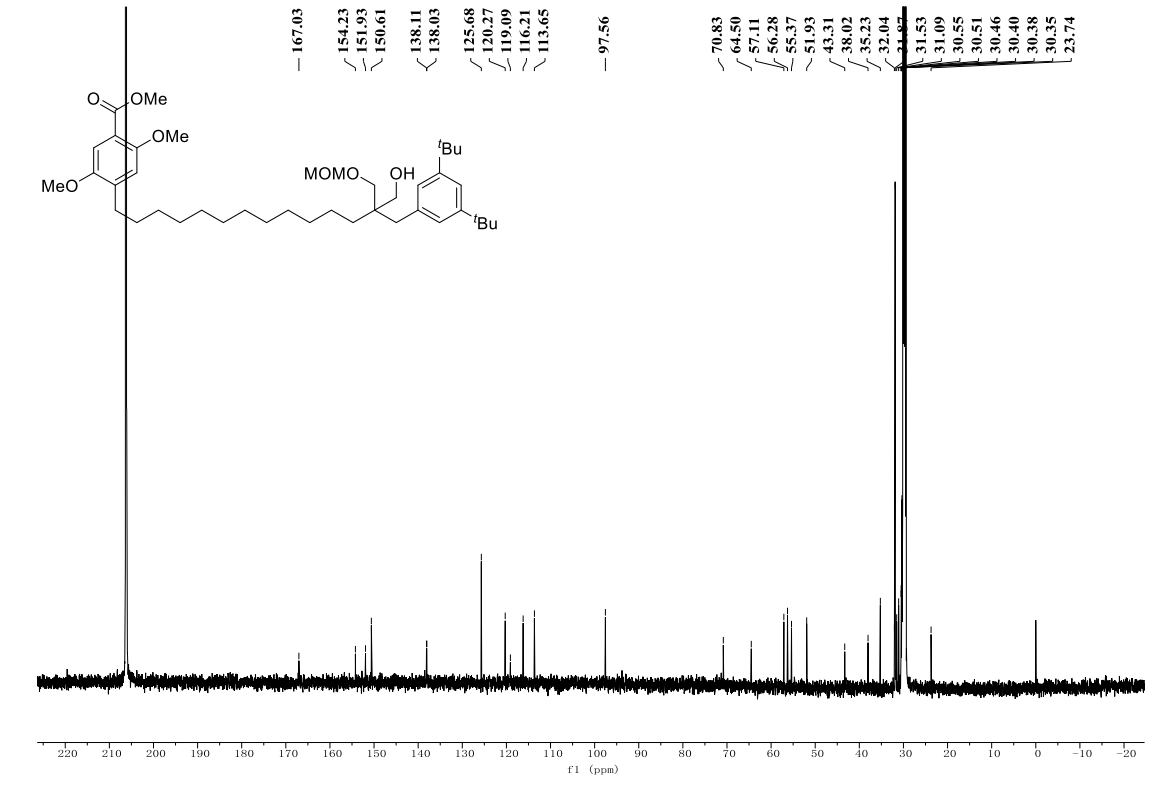
38, **^{13}C NMR** (151 MHz, $CDCl_3$)



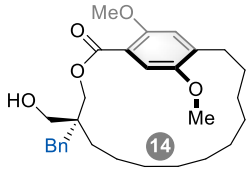
39, **^{1}H NMR** (600 MHz, Acetone-d_6)

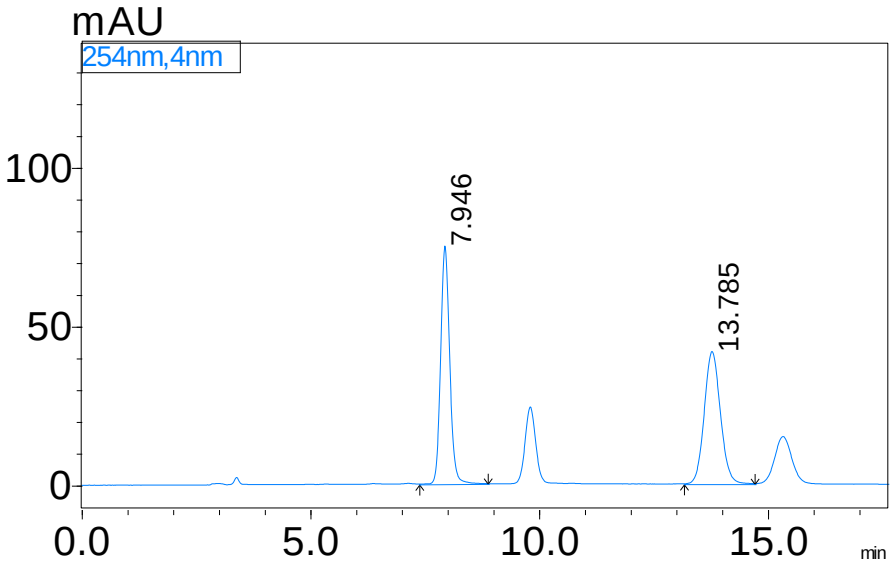


39, **^{13}C NMR** (151 MHz, Acetone-d_6)

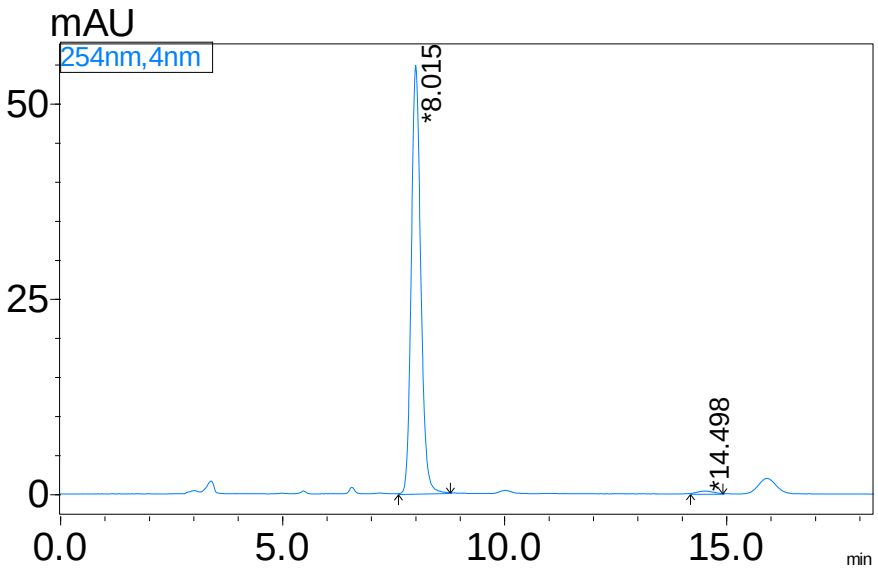


10. Copies of HPLC spectra

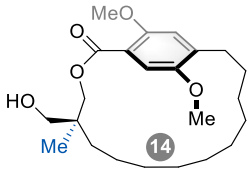


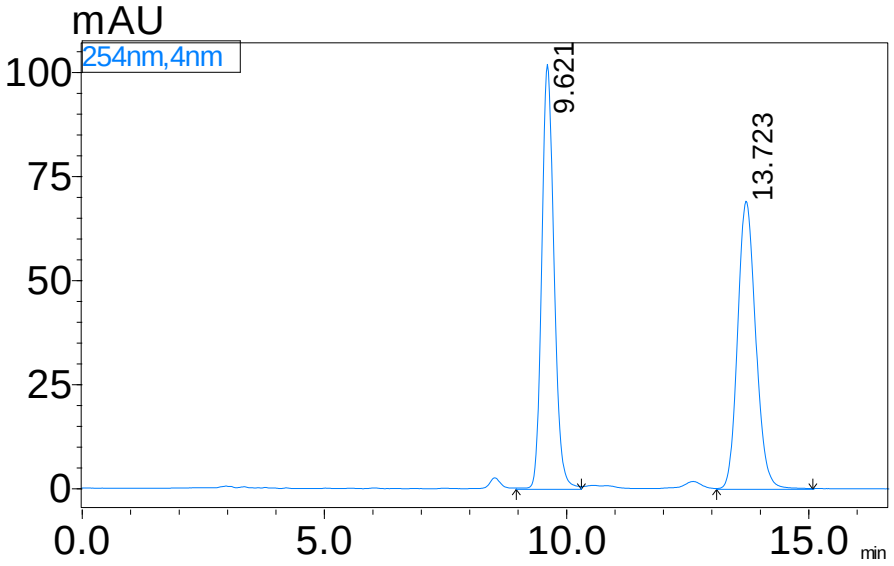


Peak#	Time	Area	Height	Area%
1	7.946	1027880	74839	50.124
2	13.785	1022778	41661	49.876

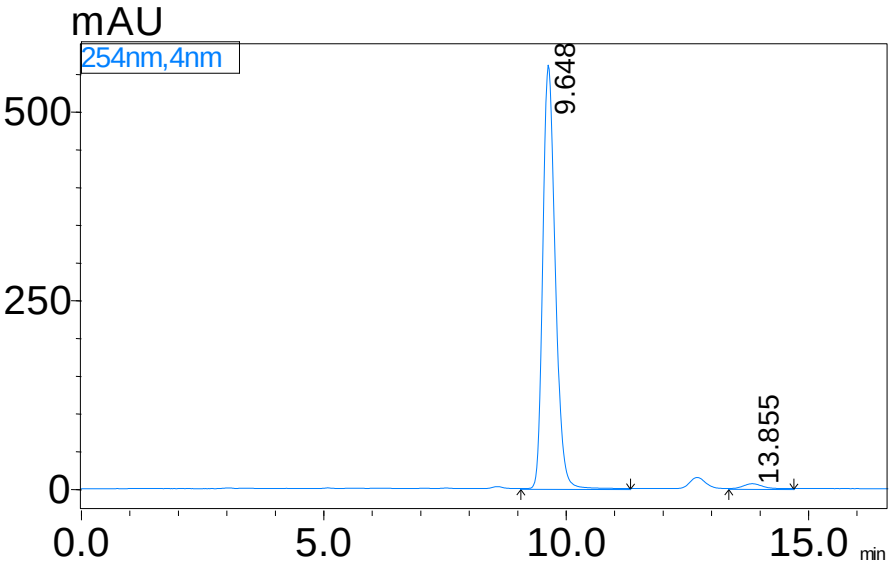


Peak#	Time	Area	Height	Area%
1	8.015	807449	54742	99.112
2	14.498	7237	311	0.888

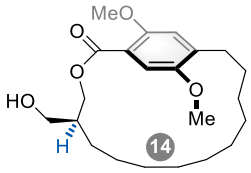


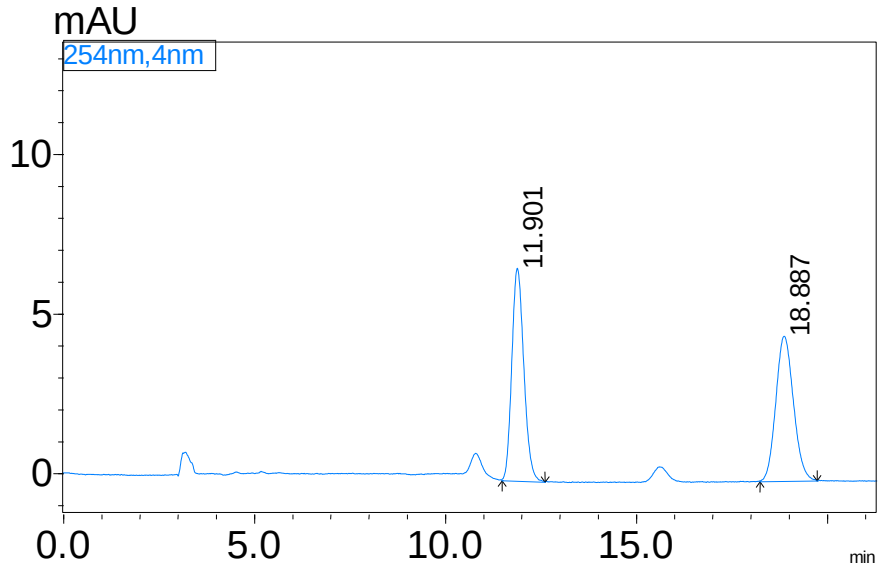


Peak#	Time	Area	Height	Area%
1	9.621	1791924	101899	50.125
2	13.723	1783019	69024	49.875

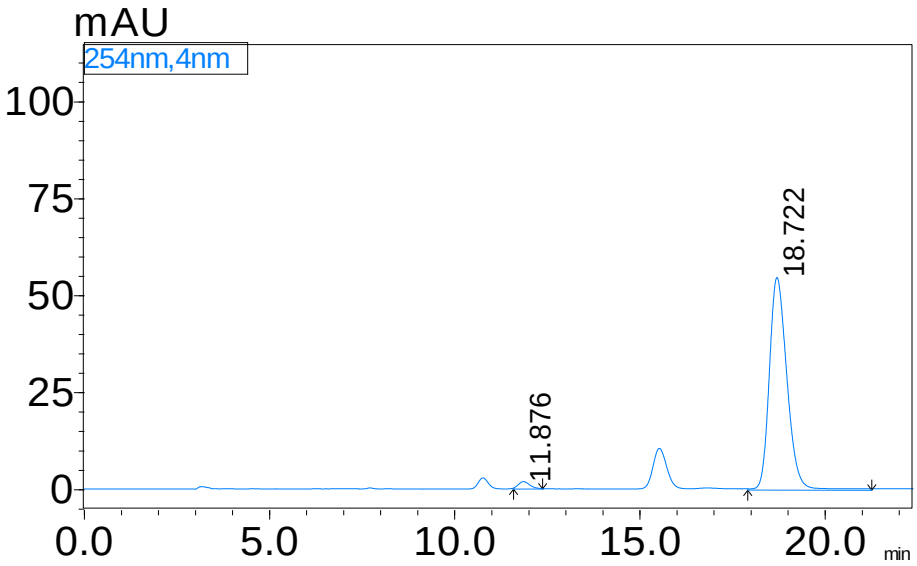


Peak#	Time	Area	Height	Area%
1	9.648	9984012	561044	98.354
2	13.855	167064	6367	1.646

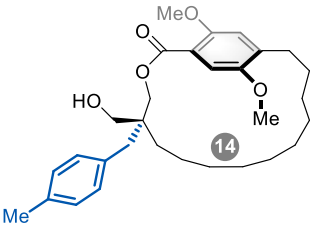


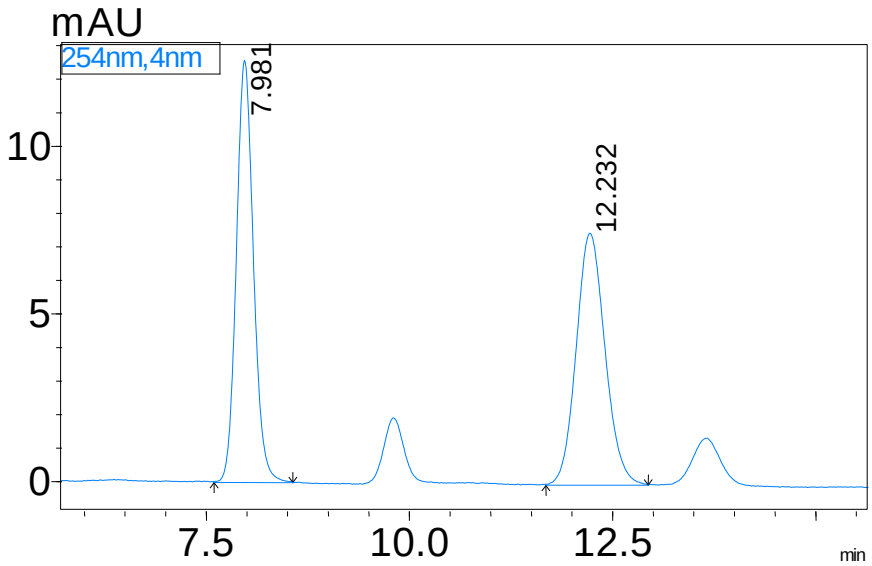


Peak#	Time	Area	Height	Area%
1	11.901	144845	6646	50.028
2	18.887	144680	4529	49.972

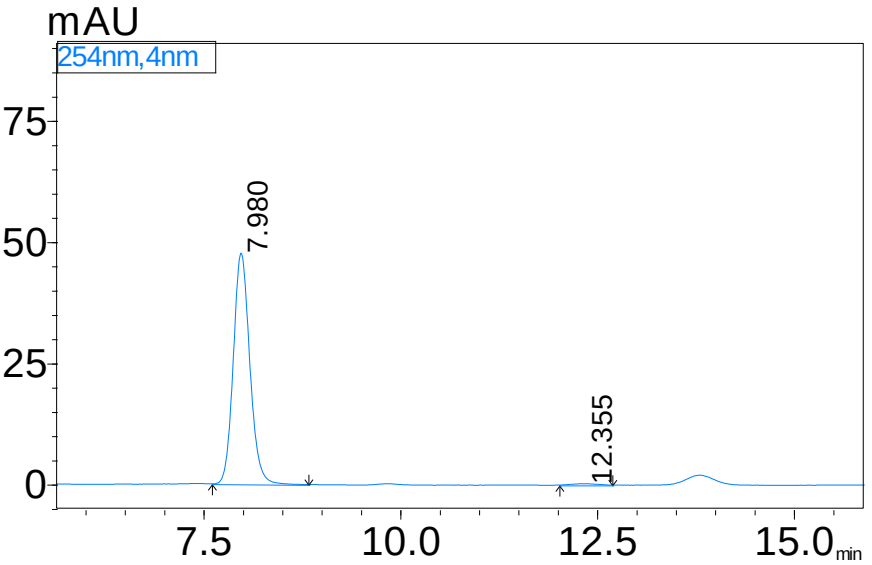


Peak#	Time	Area	Height	Area%
1	11.876	32582	1699	1.781
2	18.722	1797345	54642	98.219

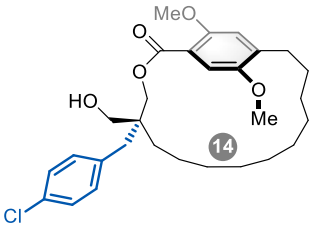


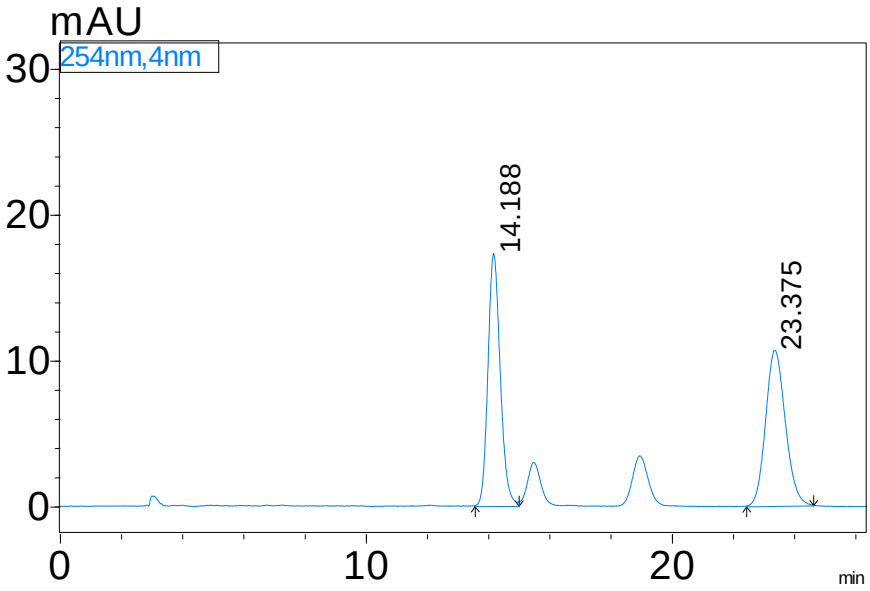


Peak#	Time	Area	Height	Area%
1	7.981	182982	12560	49.899
2	12.232	183721	7491	50.101

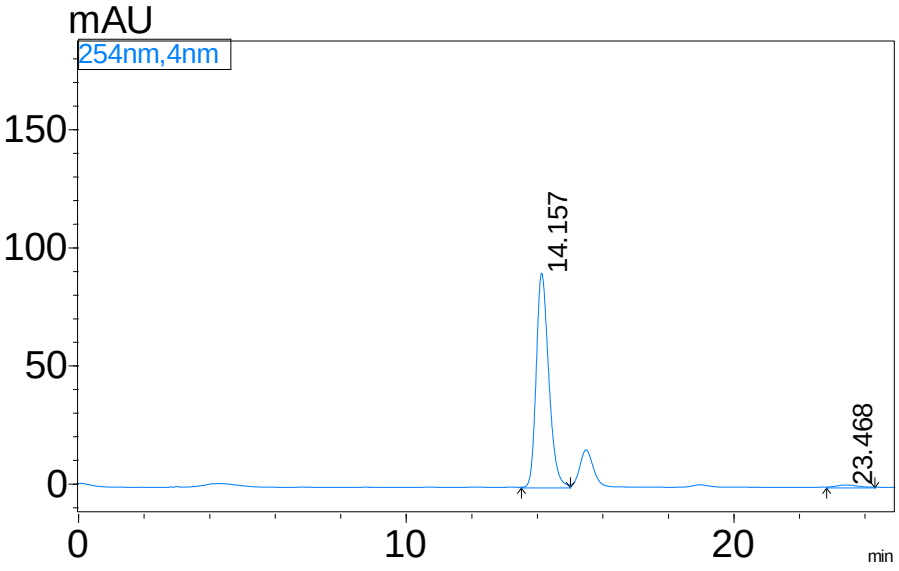


Peak#	Time	Area	Height	Area%
1	7.980	694767	47647	99.225
2	12.355	5428	265	0.775

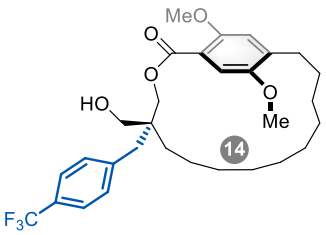


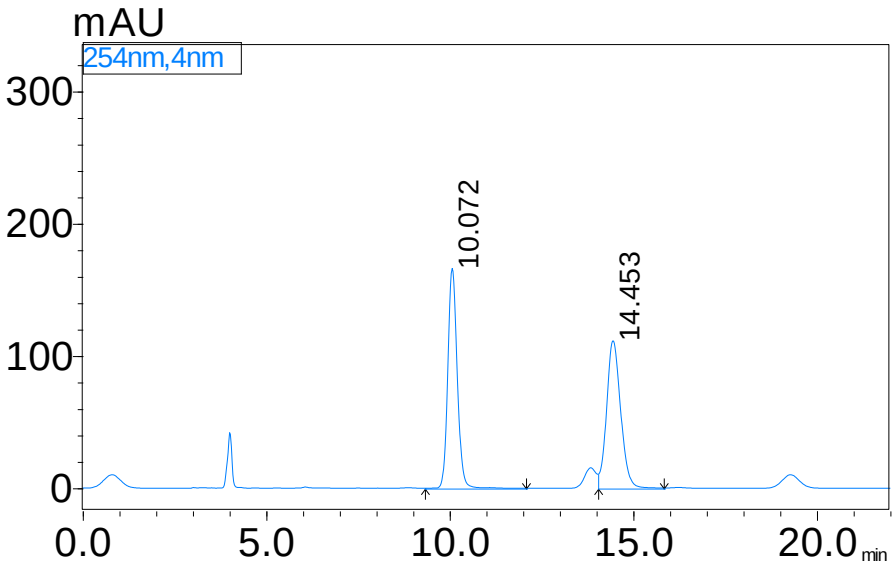


Peak#	Time	Area	Height	Area%
1	14.188	480765	17276	50.228
2	23.375	476393	10653	49.772

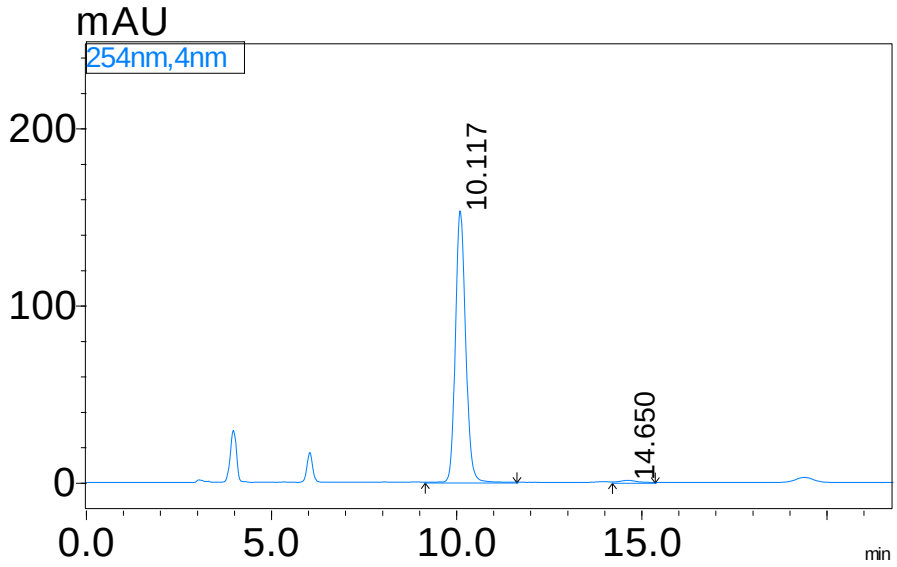


Peak#	Time	Area	Height	Area%
1	14.157	2396973	90611	98.507
2	23.468	36332	895	1.493

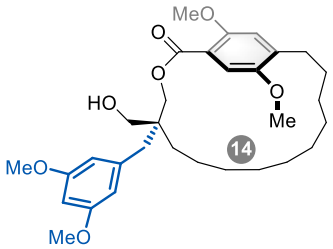


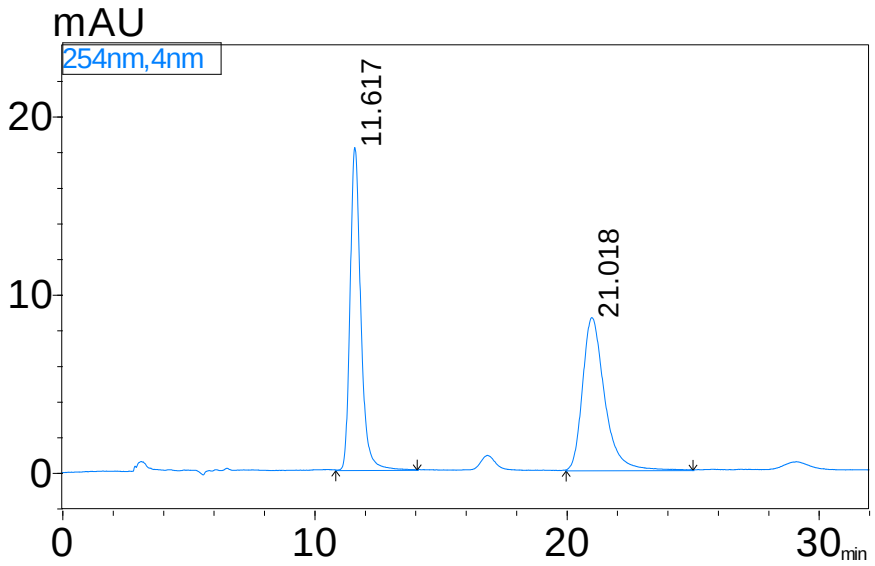


Peak#	Time	Area	Height	Area%
1	10.072	2957671	166222	49.868
2	14.453	2973307	111390	50.132

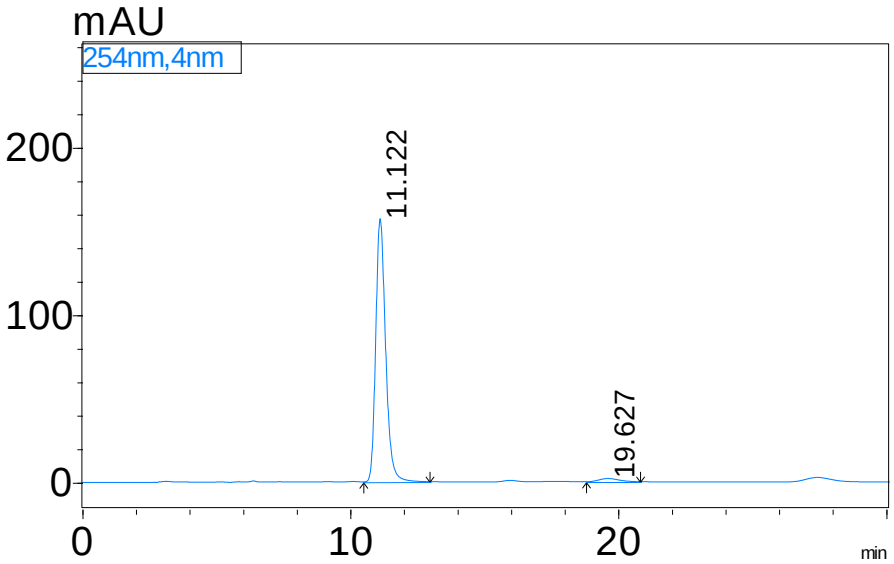


Peak#	Time	Area	Height	Area%
1	10.117	2936324	153235	98.881
2	14.650	33237	1172	1.119

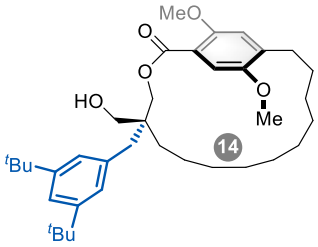


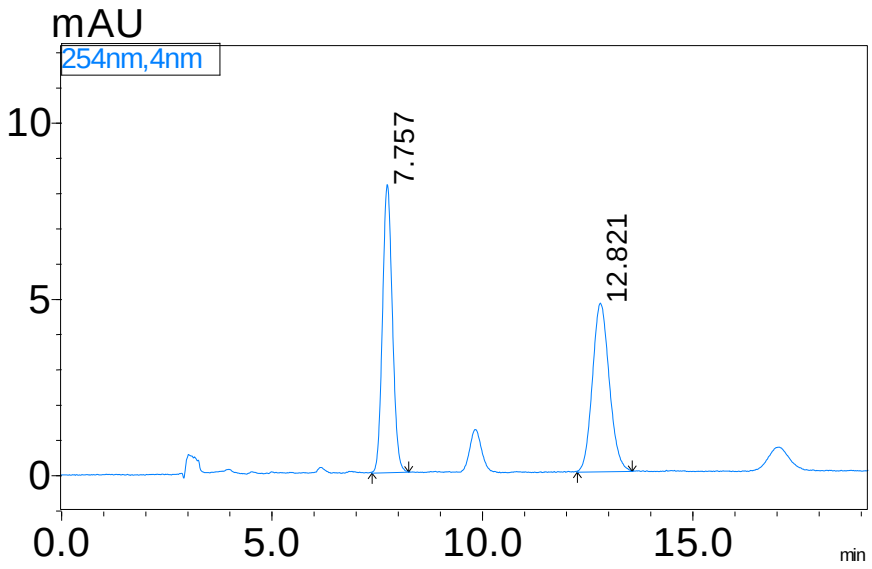


Peak#	Time	Area	Height	Area%
1	11.617	530087	18093	50.768
2	21.018	514039	8555	49.232

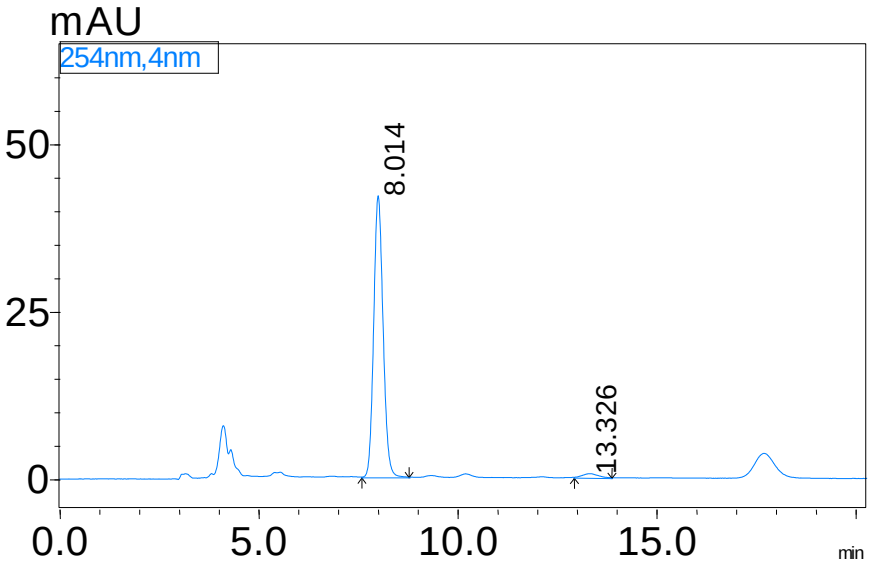


Peak#	Time	Area	Height	Area%
1	11.122	4036610	157129	97.569
2	19.627	100593	1946	2.431

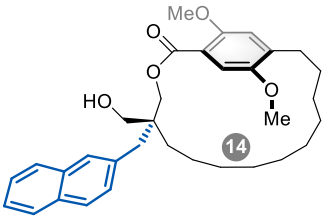


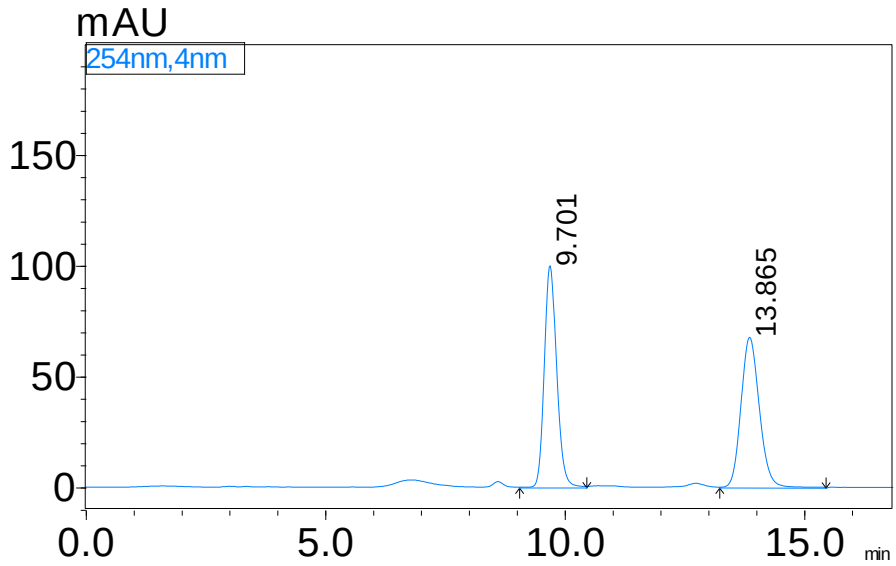


Peak#	Time	Area	Height	Area%
1	7.757	132287	8154	50.097
2	12.821	131772	4764	49.903

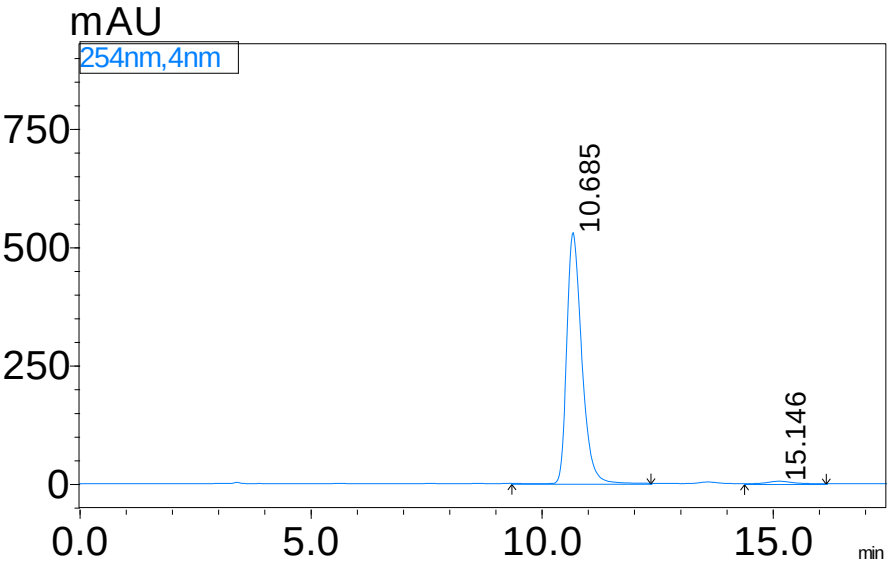


Peak#	Time	Area	Height	Area%
1	8.014	687323	41992	97.880
2	13.326	14889	577	2.120

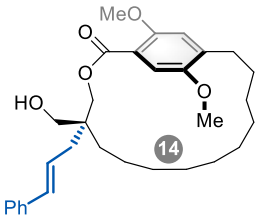


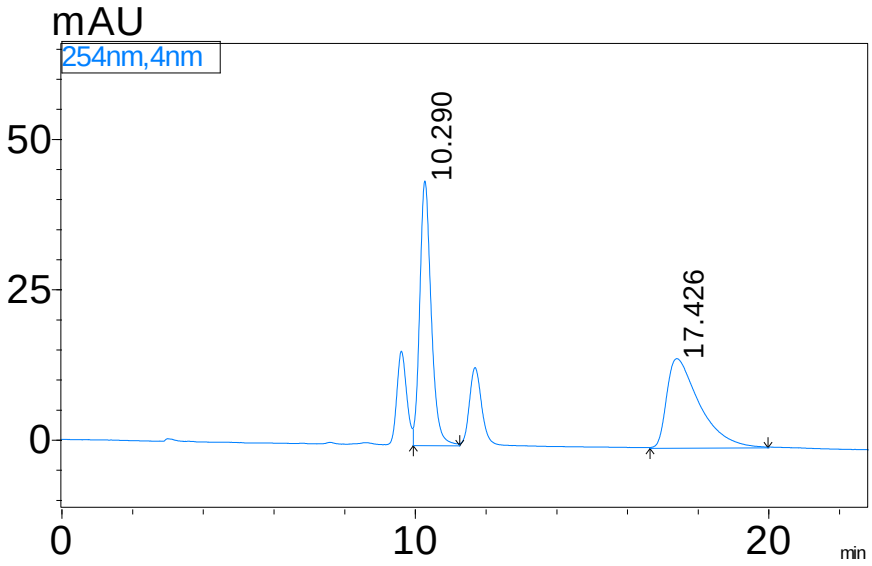


Peak#	Time	Area	Height	Area%
1	9.701	1786076	99871	50.000
2	13.865	1786077	67661	50.000

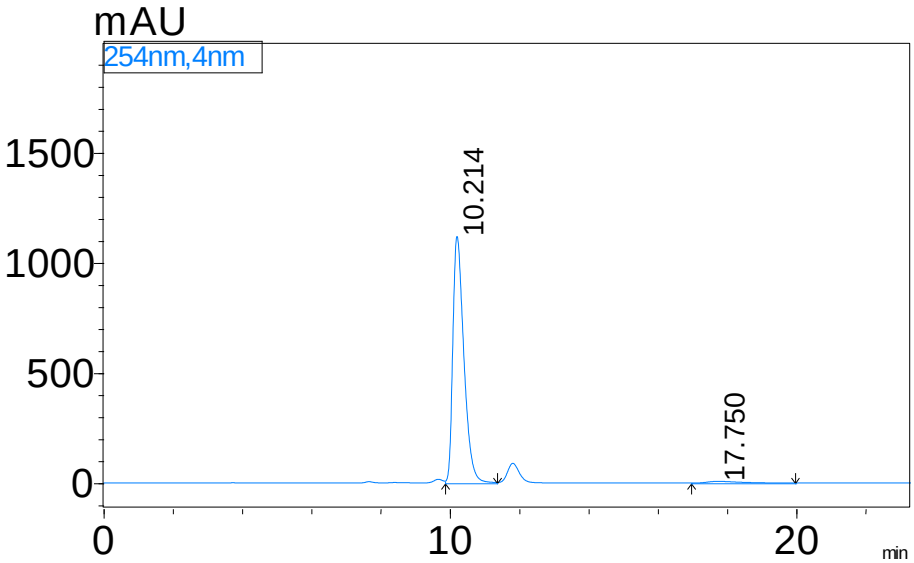


Peak#	Time	Area	Height	Area%
1	10.685	11838689	529877	98.200
2	15.146	217035	5682	1.800

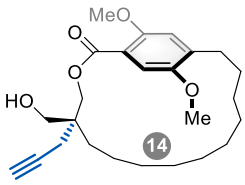


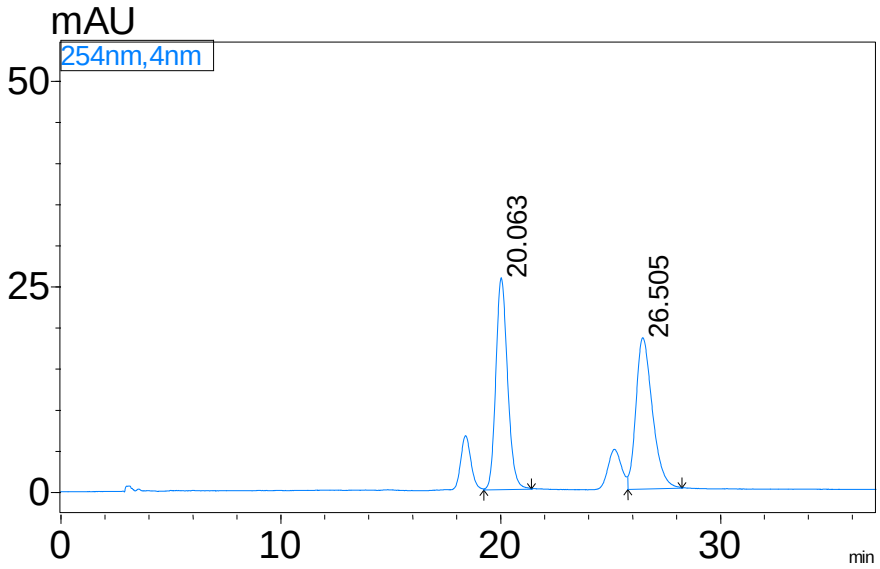


Peak#	Time	Area	Height	Area%
1	10.290	983019	43880	51.176
2	17.426	937851	14759	48.824

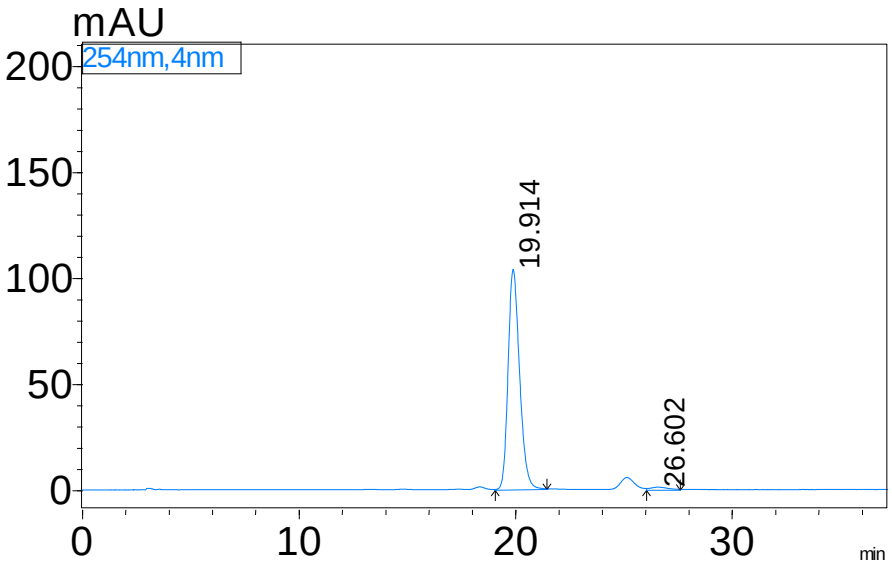


Peak#	Time	Area	Height	Area%
1	10.214	24796782	1119679	98.795
2	17.750	302541	5807	1.205

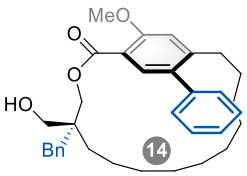


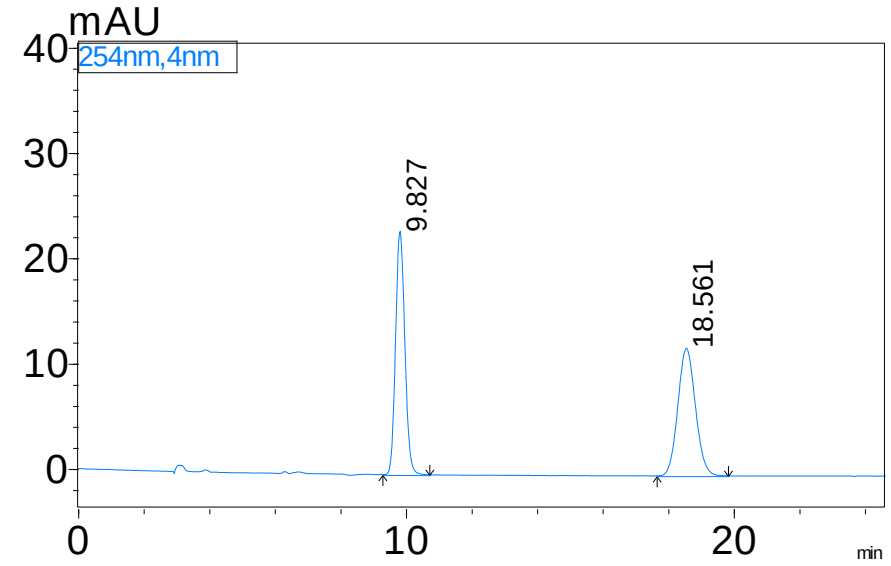


Peak#	Time	Area	Height	Area%
1	20.063	943534	25683	49.836
2	26.505	949750	18323	50.164

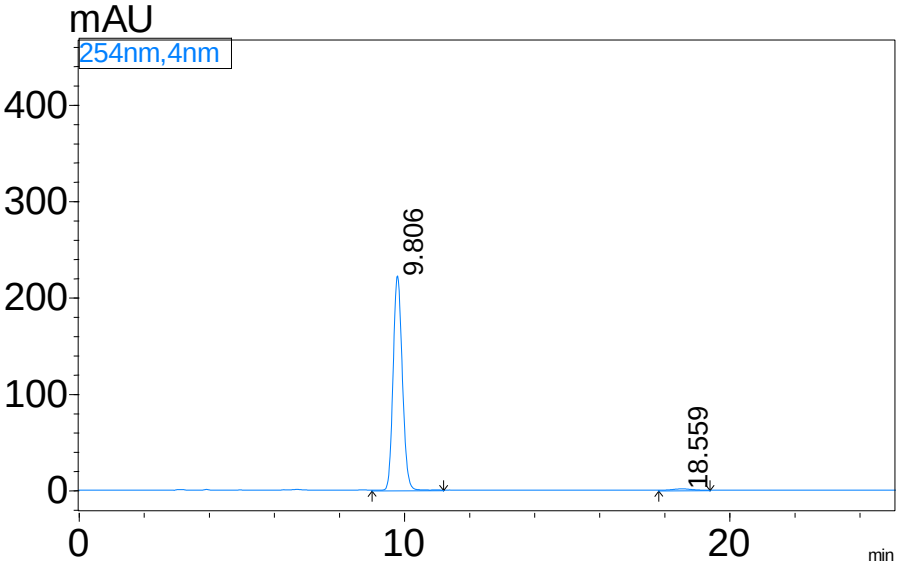


Peak#	Time	Area	Height	Area%
1	19.914	3800069	103672	98.622
2	26.602	53105	1054	1.378

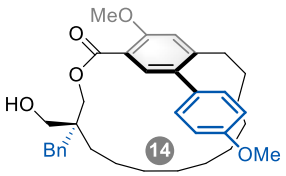


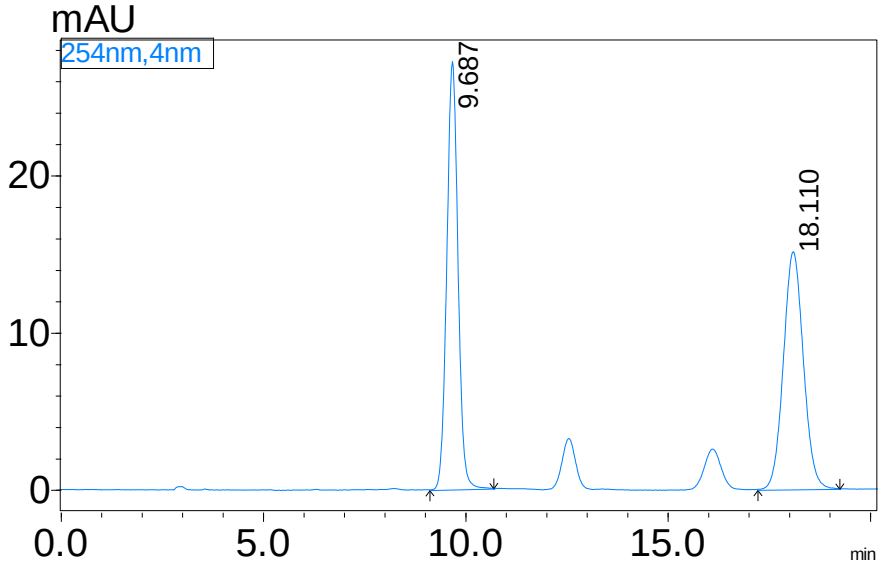


Peak#	Time	Area	Height	Area%
1	9.827	453421	23096	50.100
2	18.561	451612	12113	49.900

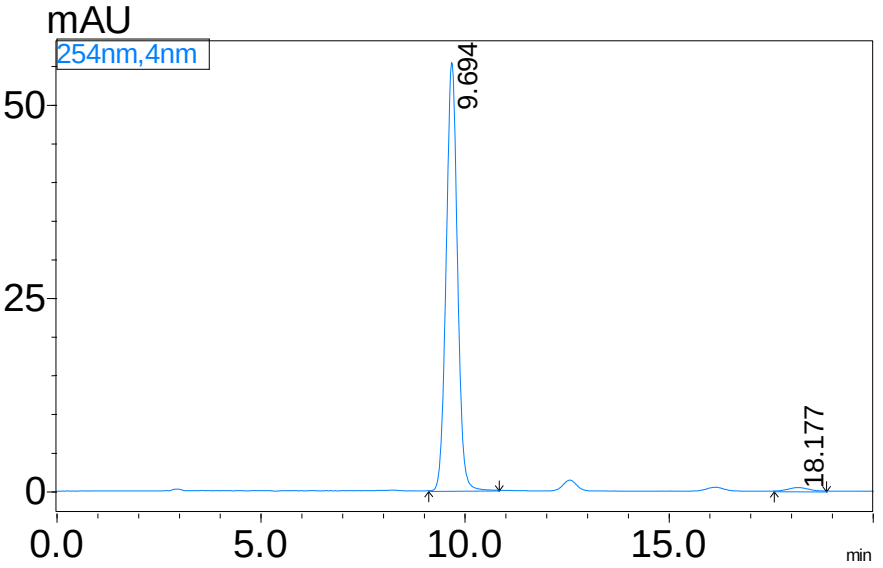


Peak#	Time	Area	Height	Area%
1	9.806	4358220	222204	98.895
2	18.559	48676	1337	1.105

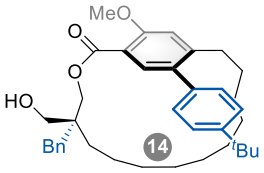


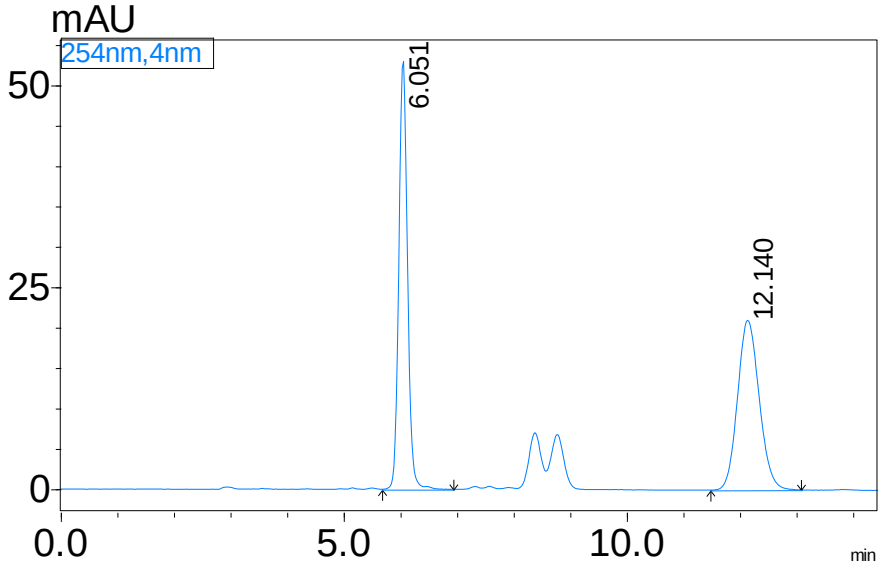


Peak#	Time	Area	Height	Area%
1	9.687	521575	27207	50.142
2	18.110	518623	15120	49.858

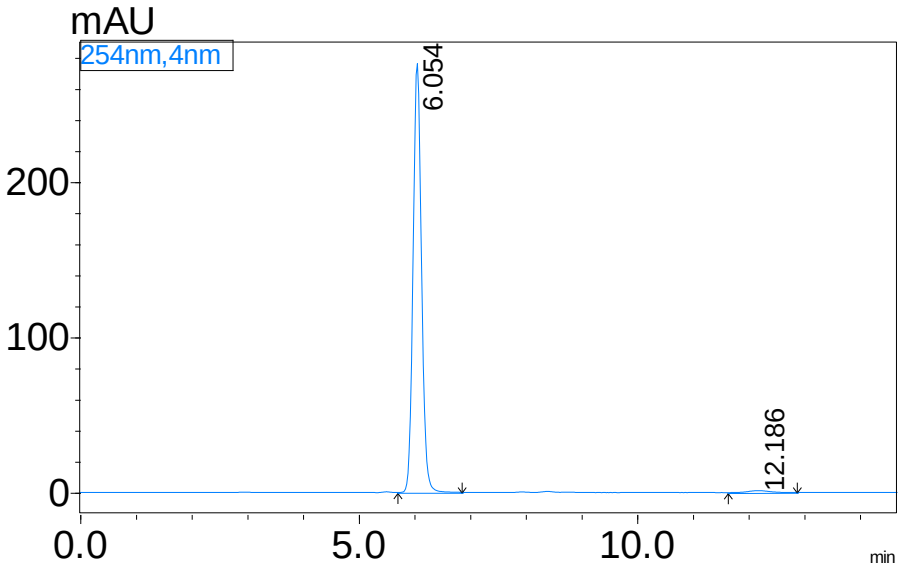


Peak#	Time	Area	Height	Area%
1	9.694	1064056	55367	98.621
2	18.177	14878	450	1.379

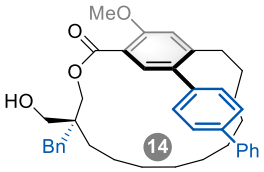


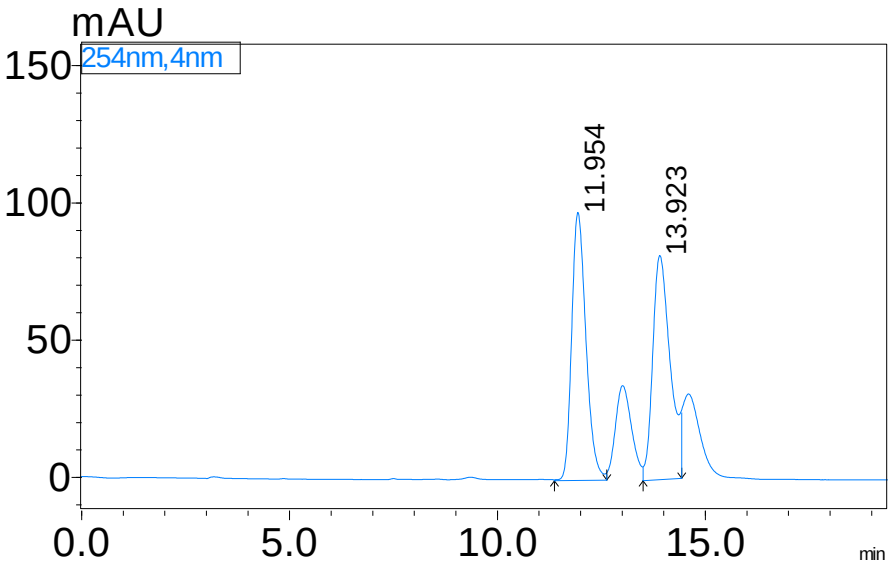


Peak#	Time	Area	Height	Area%
1	6.051	568048	52959	50.447
2	12.140	557987	21031	49.553

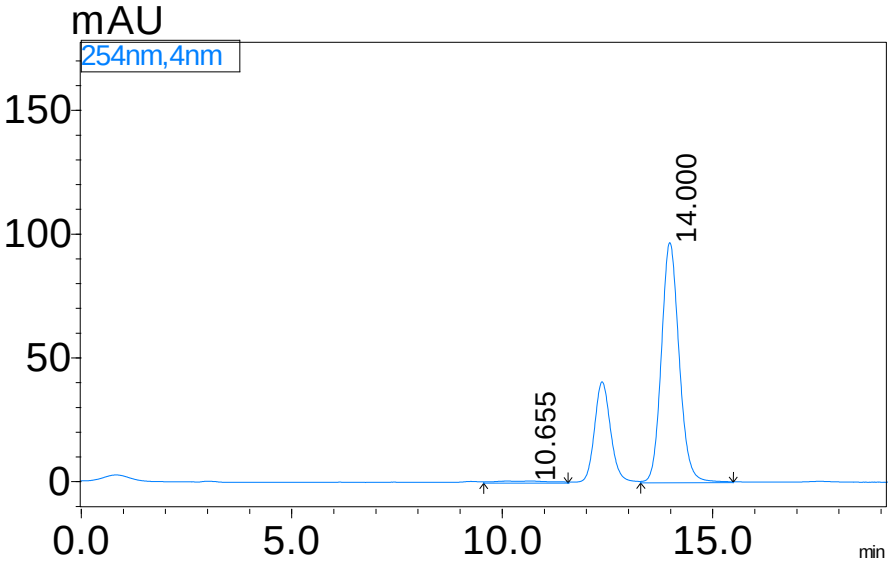


Peak#	Time	Area	Height	Area%
1	6.054	2913416	276088	98.412
2	12.186	47000	1471	1.588

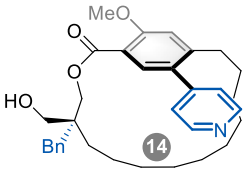


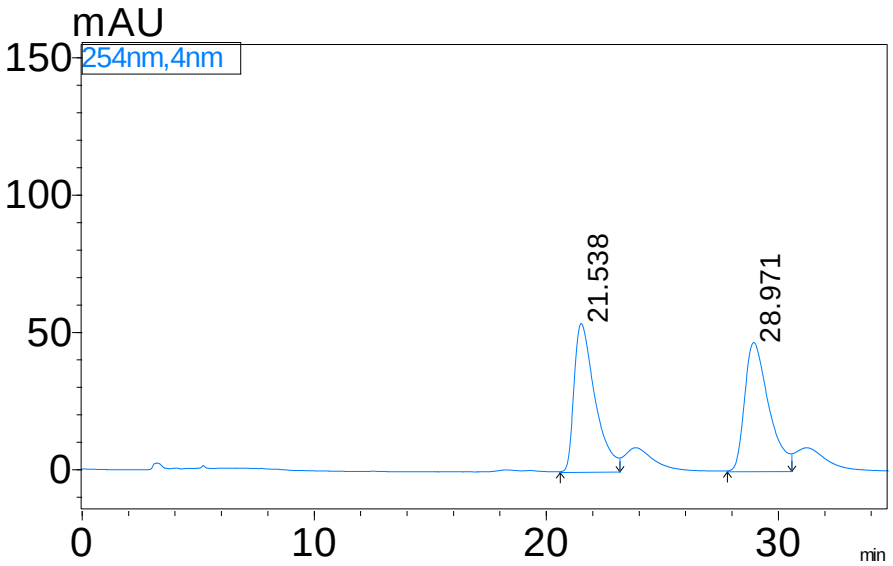


Peak#	Time	Area	Height	Area%
1	11.954	2314041	97352	49.382
2	13.923	2371935	81410	50.618

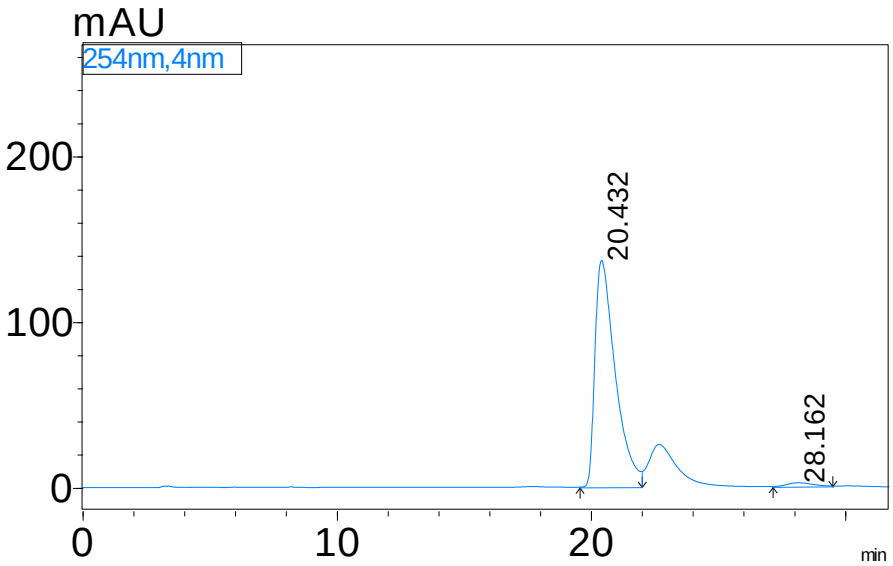


Peak#	Time	Area	Height	Area%
1	10.655	39043	503	1.368
2	14.000	2814842	96719	98.632

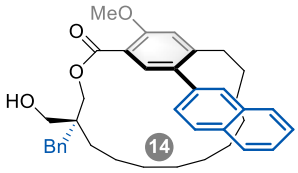


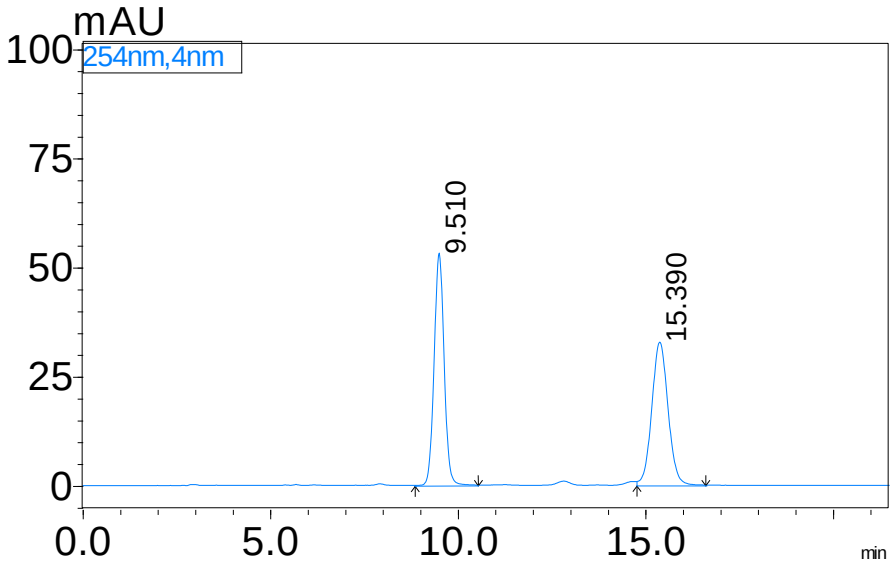


Peak#	Time	Area	Height	Area%
1	21.538	3360117	53906	50.002
2	28.971	3359789	46701	49.998

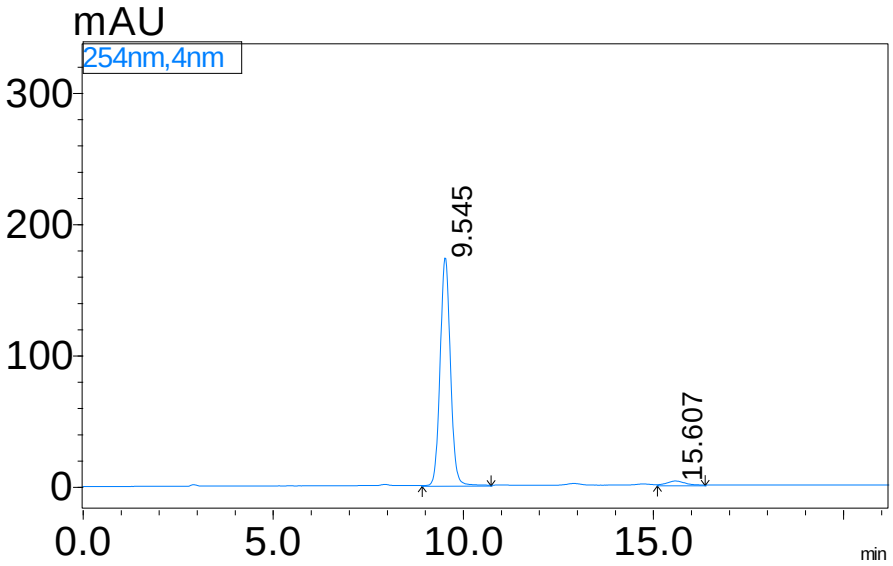


Peak#	Time	Area	Height	Area%
1	20.432	7601087	136832	98.194
2	28.162	139763	2161	1.806

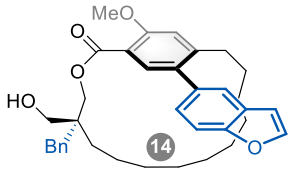


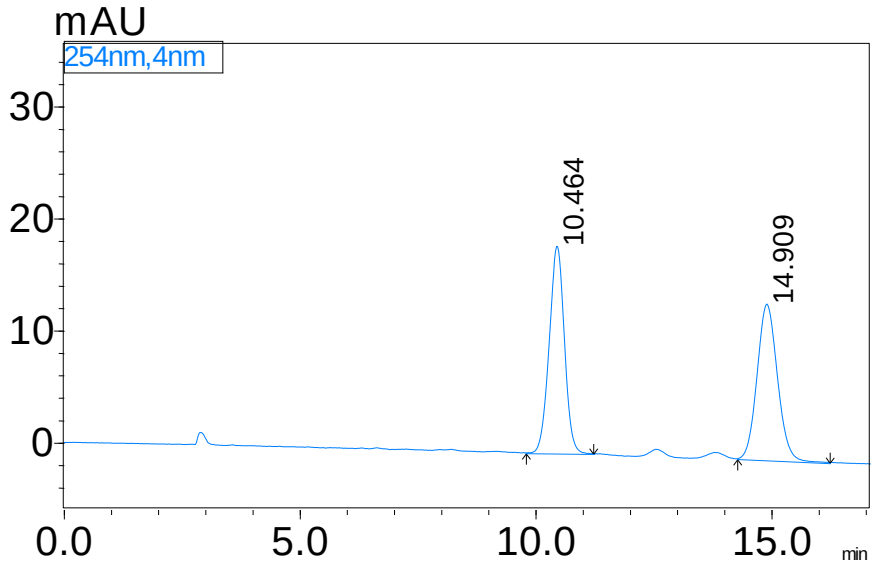


Peak#	Time	Area	Height	Area%
1	9.510	985261	53186	49.990
2	15.390	985639	32756	50.010

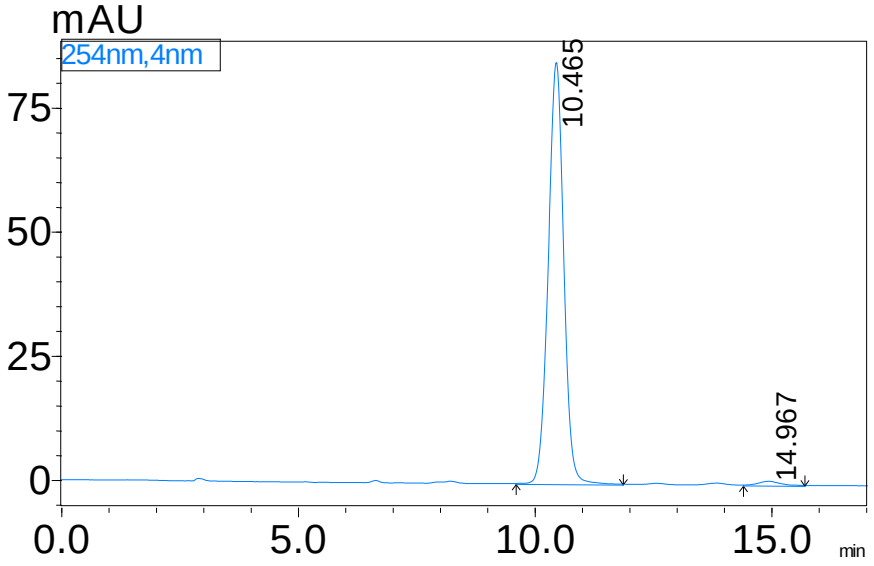


Peak#	Time	Area	Height	Area%
1	9.545	3243523	173256	97.262
2	15.607	91296	3023	2.738

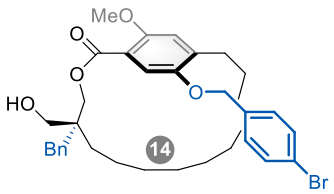


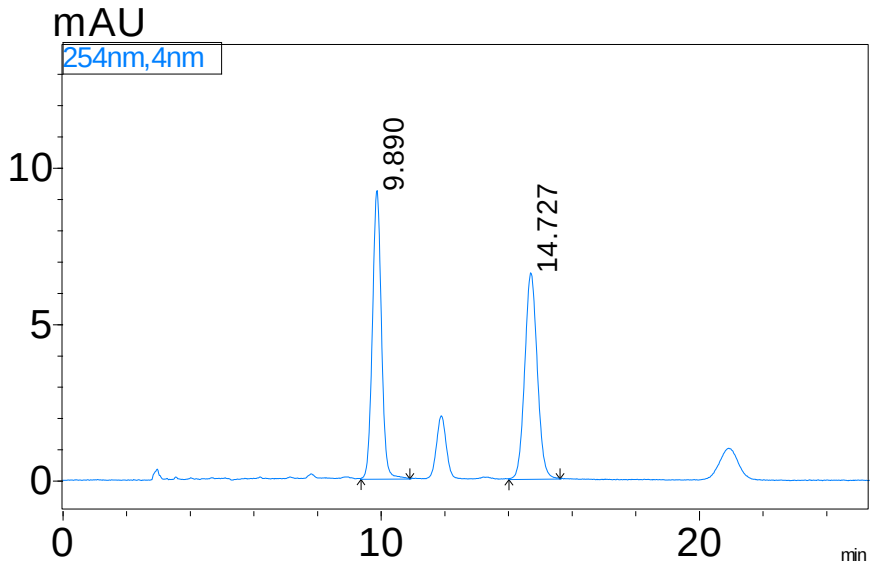


Peak#	Time	Area	Height	Area%
1	10.464	414297	18465	49.983
2	14.909	414584	13913	50.017

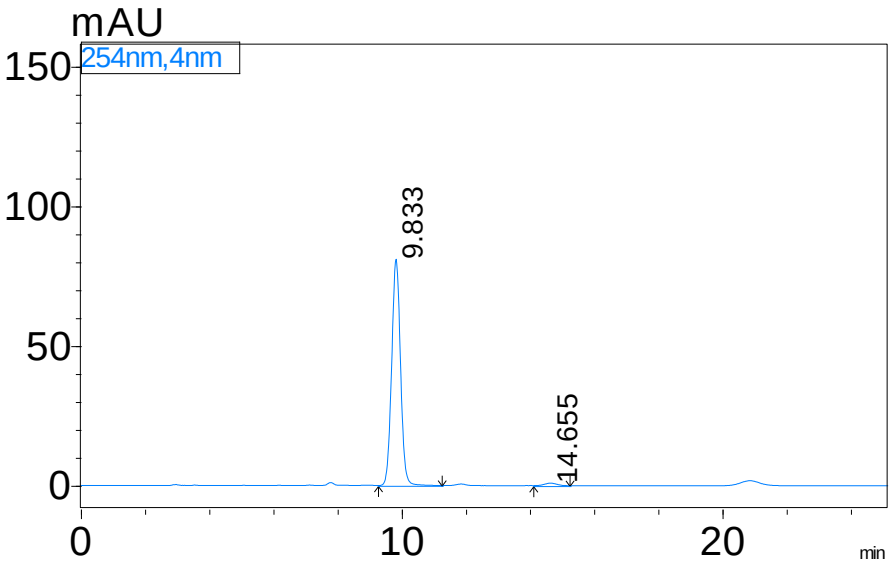


Peak#	Time	Area	Height	Area%
1	10.465	1926462	84832	98.842
2	14.967	22566	769	1.158

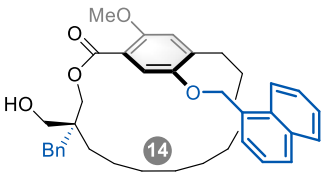


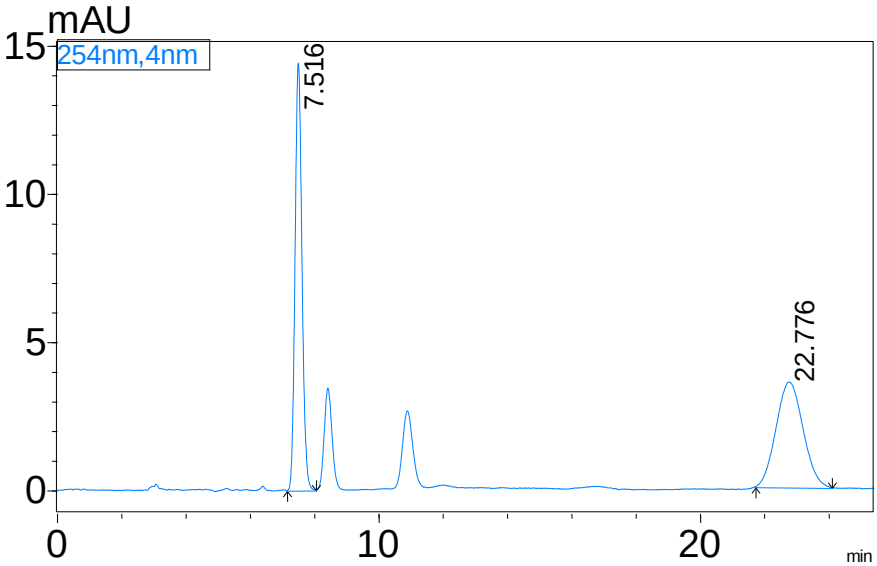


Peak#	Time	Area	Height	Area%
1	9.890	180481	9203	50.289
2	14.727	178407	6572	49.711

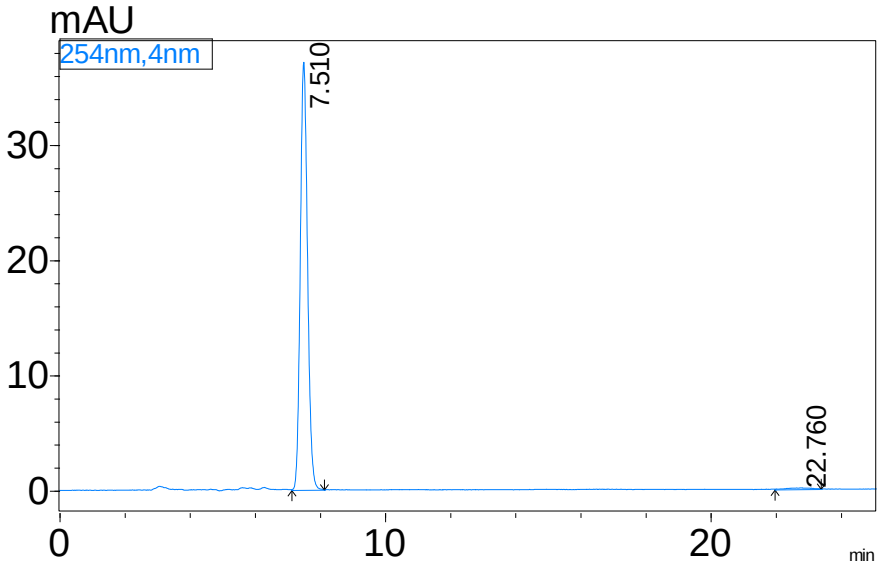


Peak#	Time	Area	Height	Area%
1	9.833	1549416	81059	98.495
2	14.655	23678	905	1.505

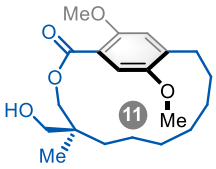


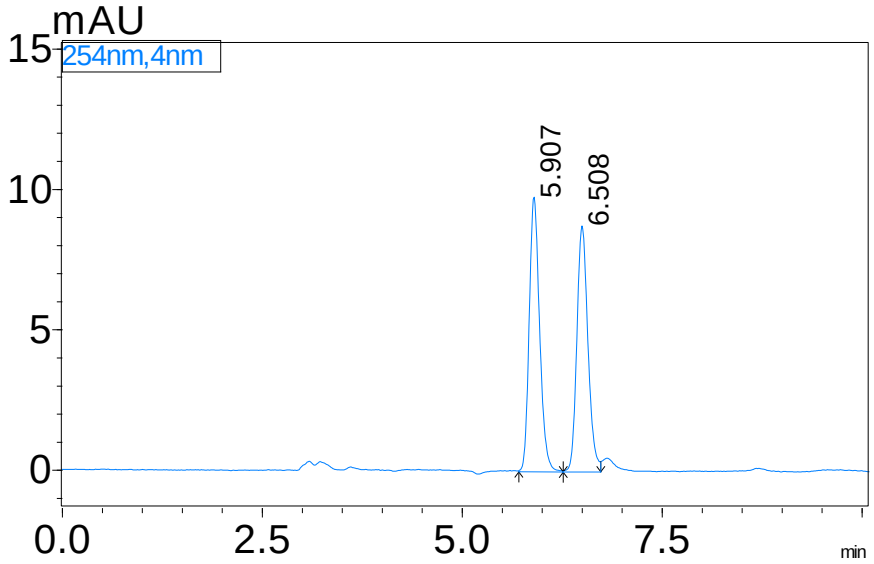


Peak#	Time	Area	Height	Area%
1	7.516	215209	14414	51.003
2	22.776	206747	3549	48.997

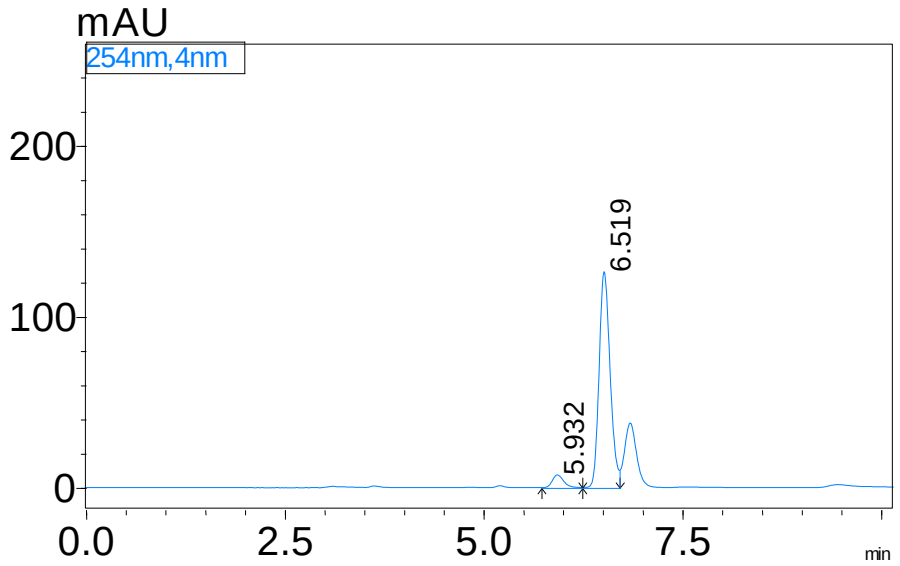


Peak#	Time	Area	Height	Area%
1	7.510	571624	37083	99.369
2	22.760	3629	86	0.631

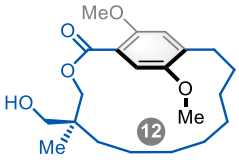


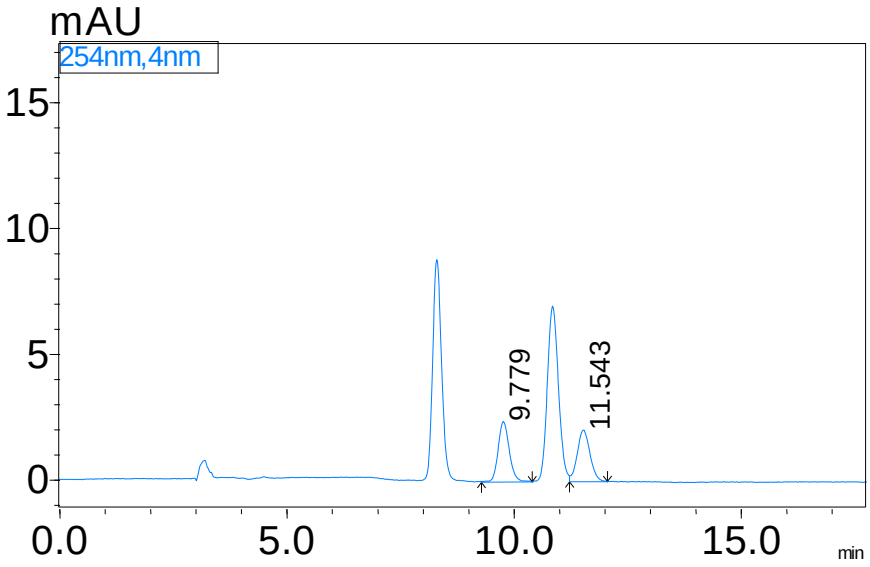


Peak#	Time	Area	Height	Area%
1	5.907	87710	9749	51.203
2	6.508	83587	8734	48.797

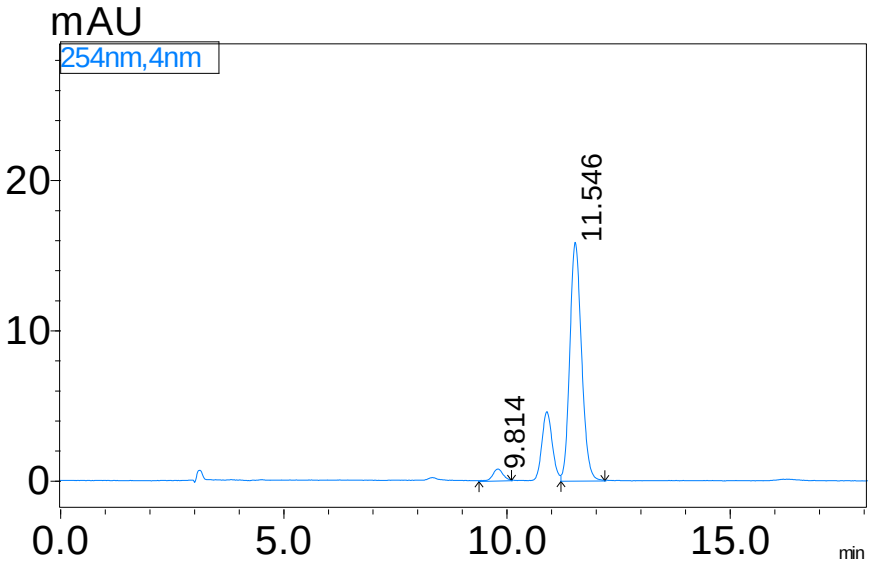


Peak#	Time	Area	Height	Area%
1	5.932	73083	7448	5.667
2	6.519	1216514	126305	94.333

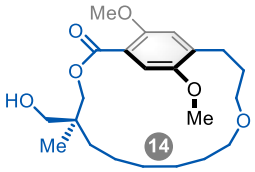


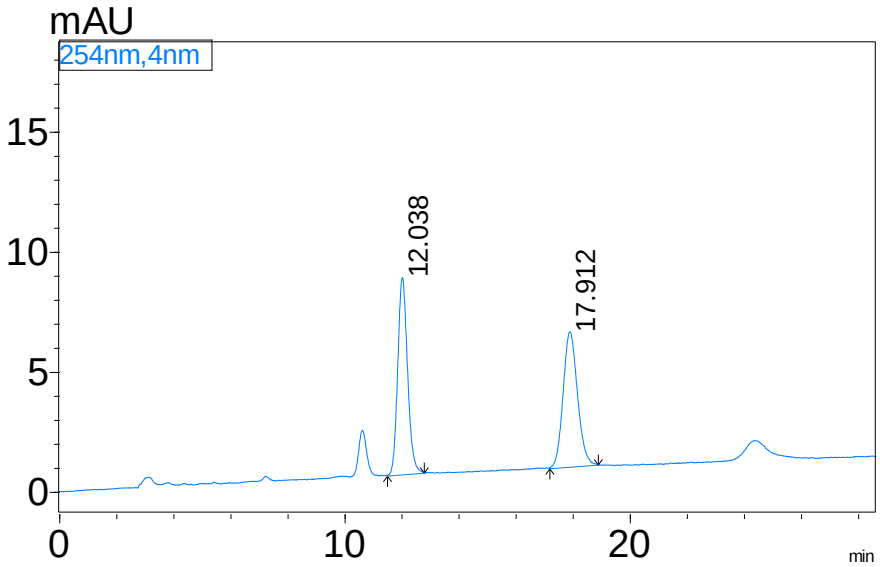


Peak#	Time	Area	Height	Area%
1	9.779	39470	2377	50.455
2	11.543	38758	2022	49.545

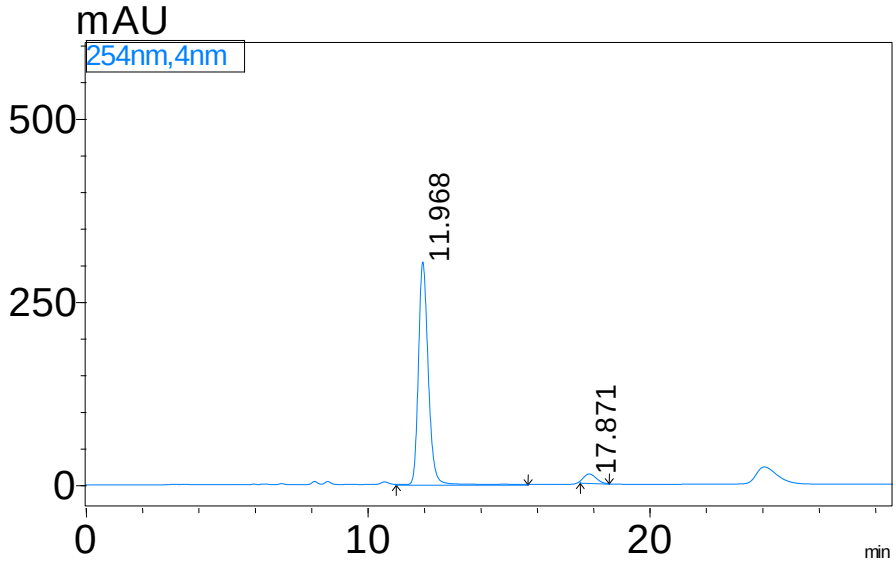


Peak#	Time	Area	Height	Area%
1	9.814	10930	745	3.658
2	11.546	287839	15832	96.342

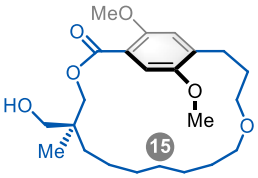


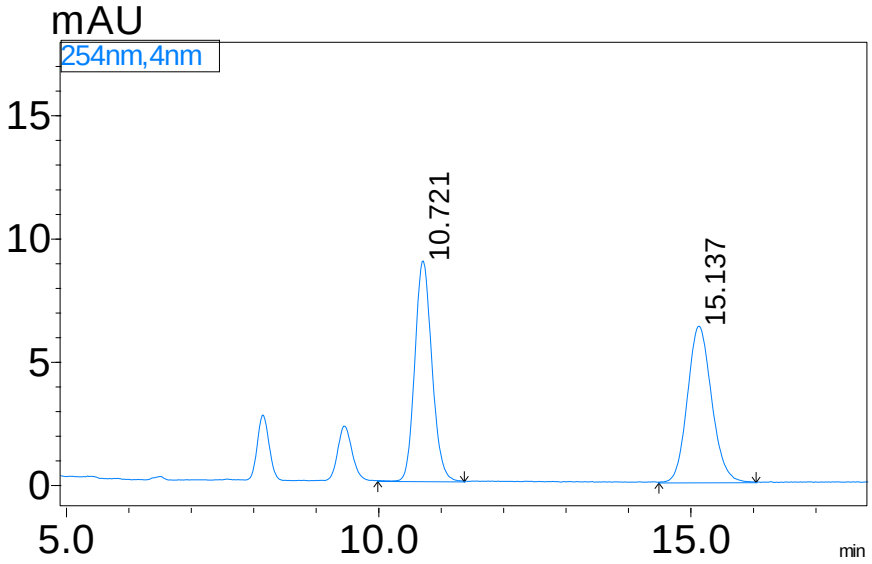


Peak#	Time	Area	Height	Area%
1	12.038	195251	8187	50.041
2	17.912	194930	5607	49.959

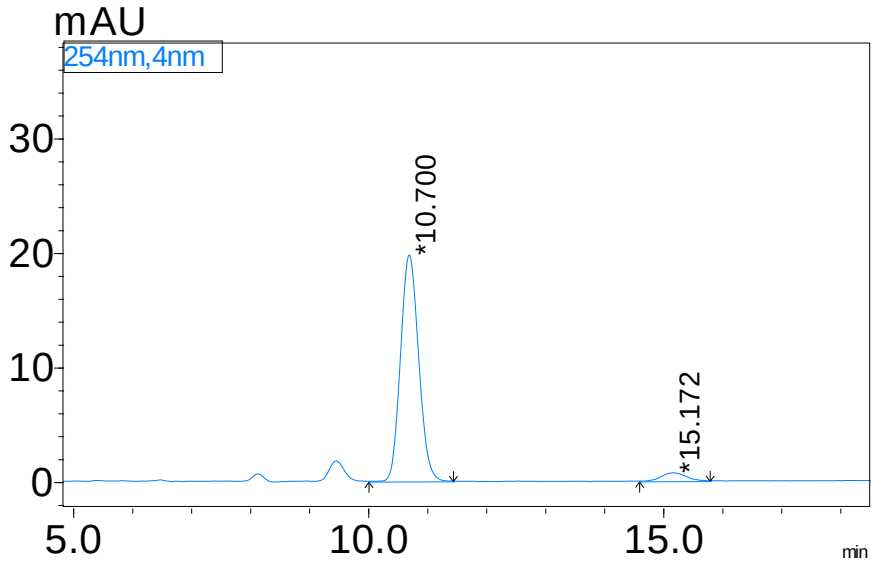


Peak#	Time	Area	Height	Area%
1	11.968	7242056	303605	95.486
2	17.871	342374	11832	4.514

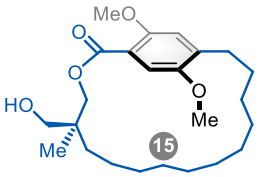


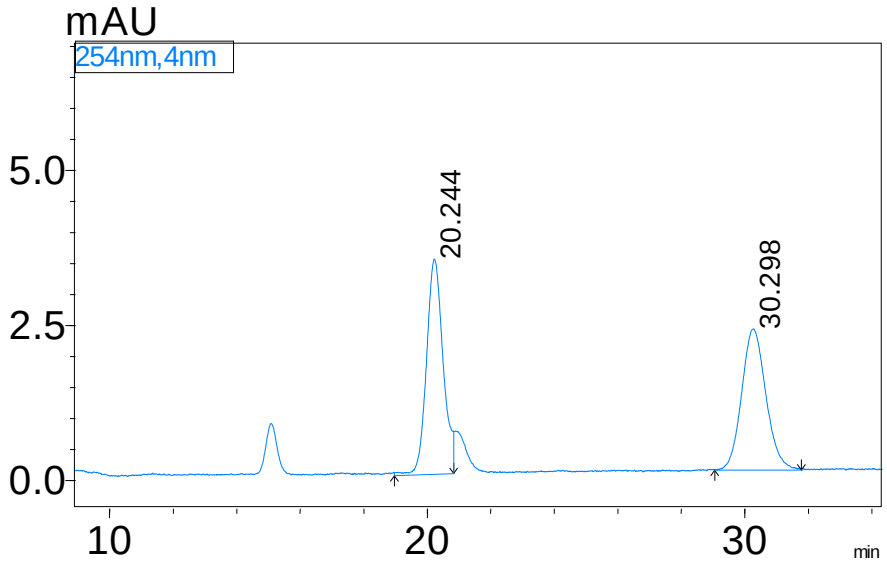


Peak#	Time	Area	Height	Area%
1	10.721	169160	8926	49.911
2	15.137	169762	6323	50.089

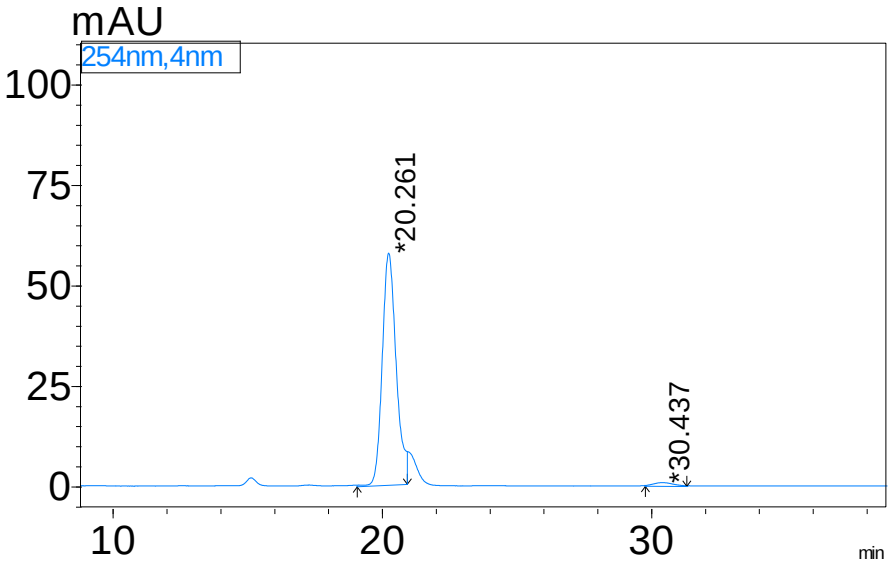


Peak#	Time	Area	Height	Area%
1	10.700	429645	19833	95.970
2	15.172	18043	688	4.030

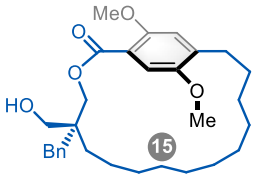


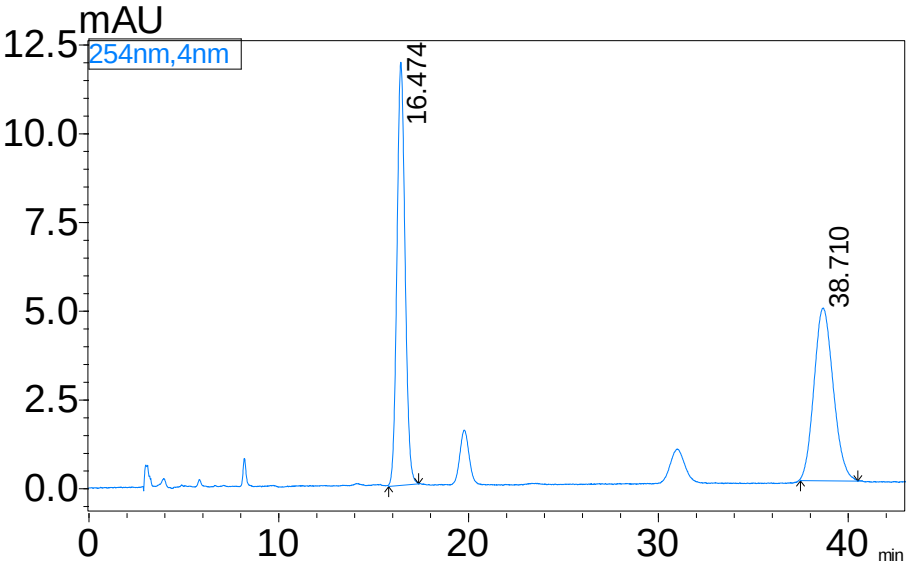


Peak#	Time	Area	Height	Area%
1	20.244	124292	3460	51.117
2	30.298	118861	2263	48.883

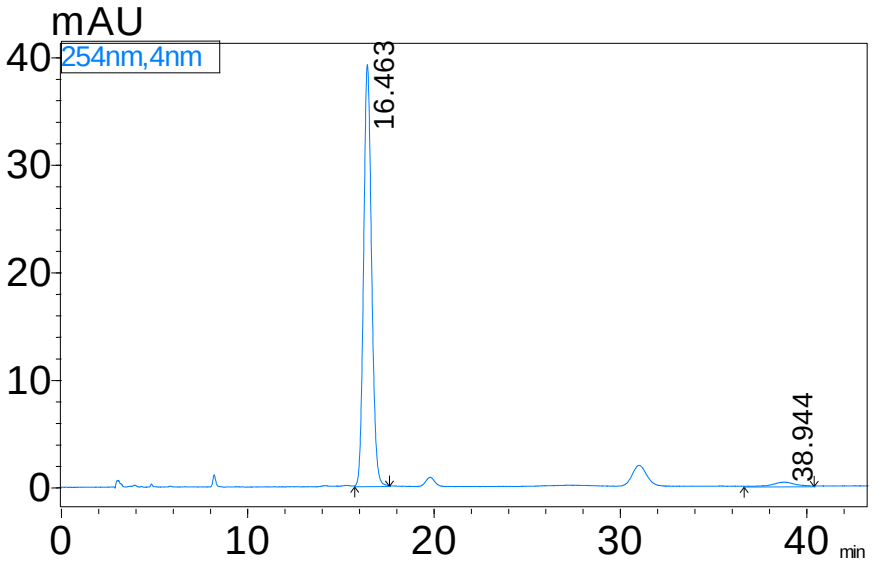


Peak#	Time	Area	Height	Area%
1	20.261	2053048	57614	98.348
2	30.437	34485	760	1.652

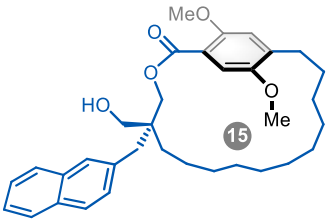


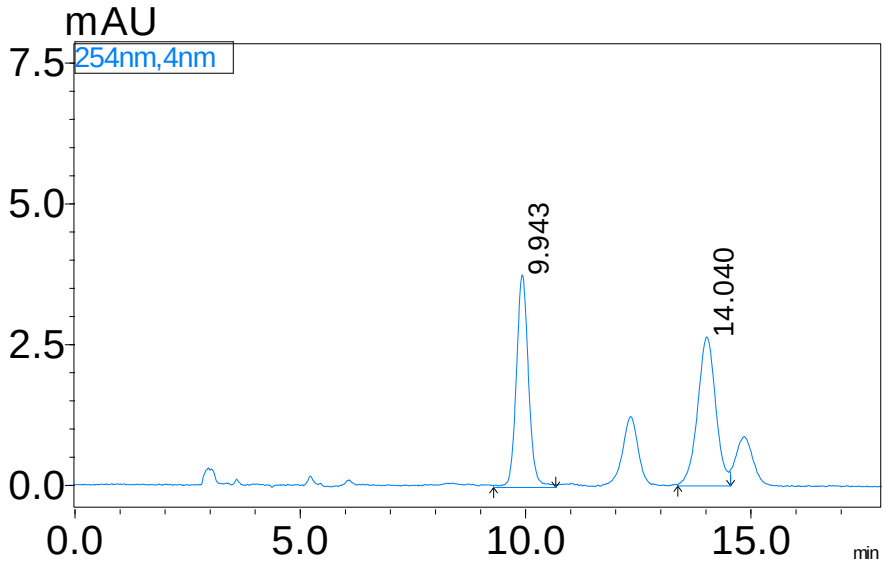


Peak#	Time	Area	Height	Area%
1	16.474	350751	11891	50.809
2	38.710	339579	4839	49.191

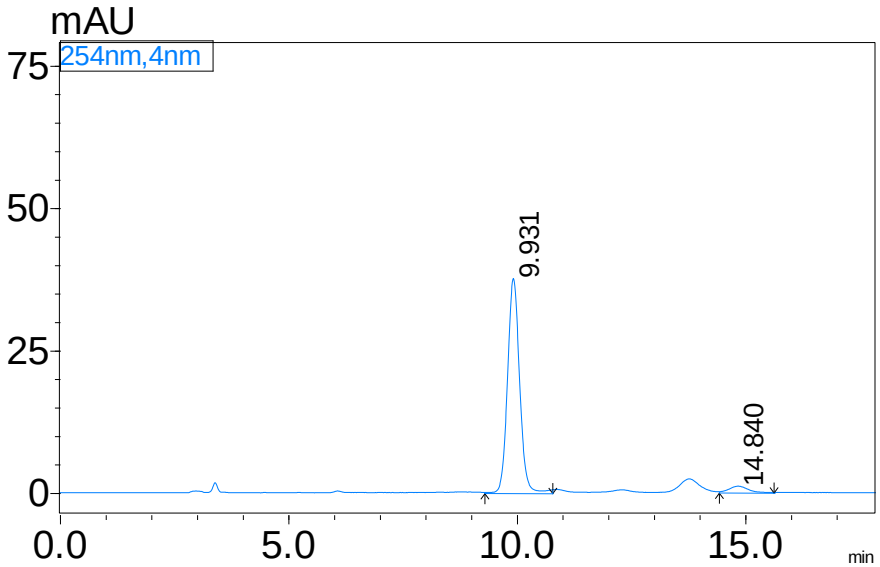


Peak#	Time	Area	Height	Area%
1	16.463	1157328	39149	97.886
2	38.944	24991	356	2.114

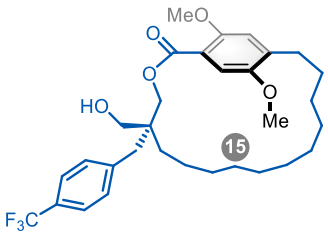


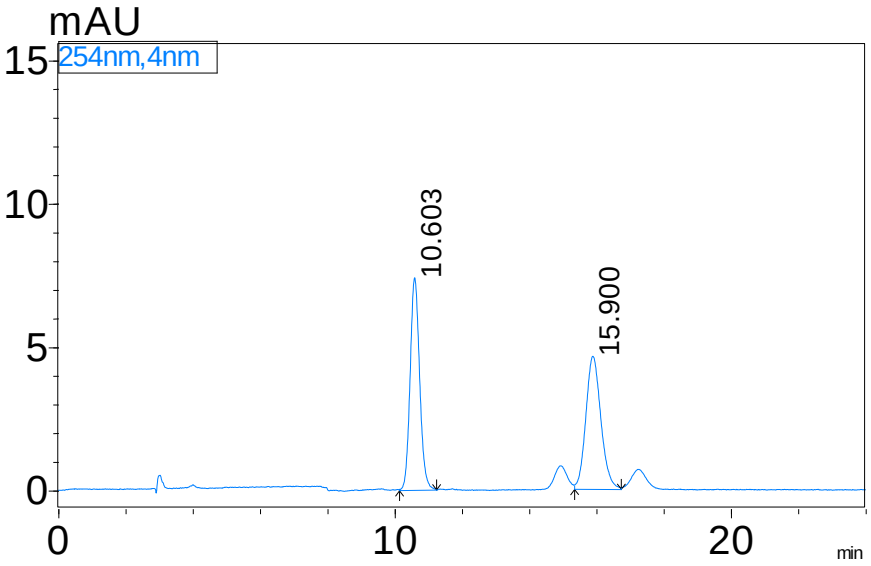


Peak#	Time	Area	Height	Area%
1	9.943	69576	3760	48.653
2	14.040	73429	2632	51.347

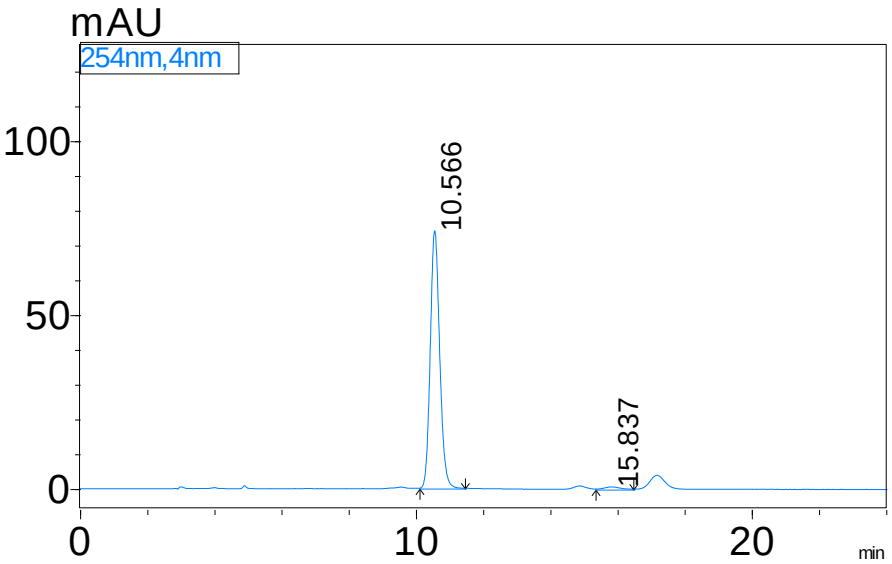


Peak#	Time	Area	Height	Area%
1	9.931	688538	37626	95.942
2	14.840	29125	1087	4.058

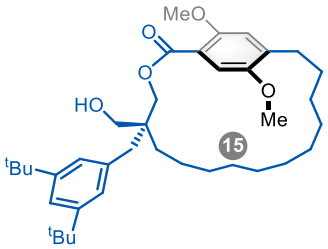


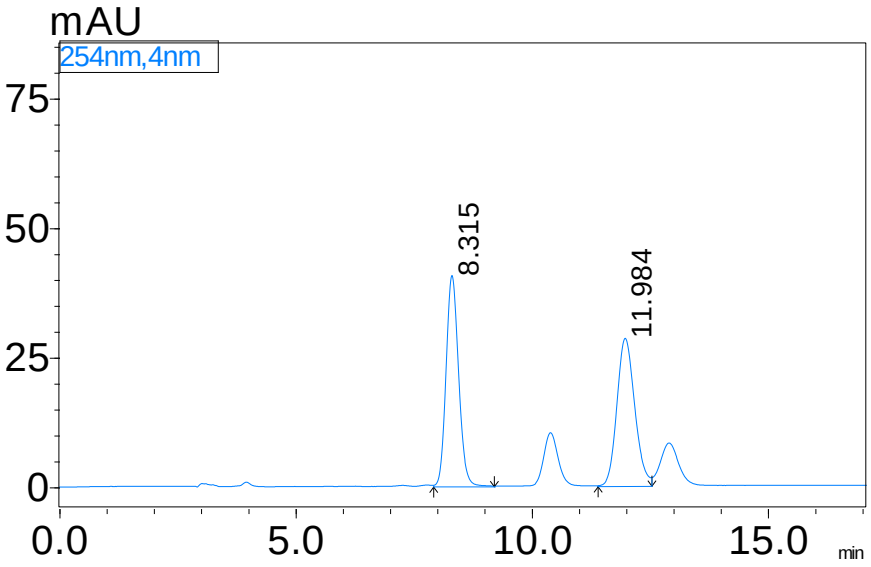


Peak#	Time	Area	Height	Area%
1	10.603	144142	7384	50.215
2	15.900	142907	4619	49.785

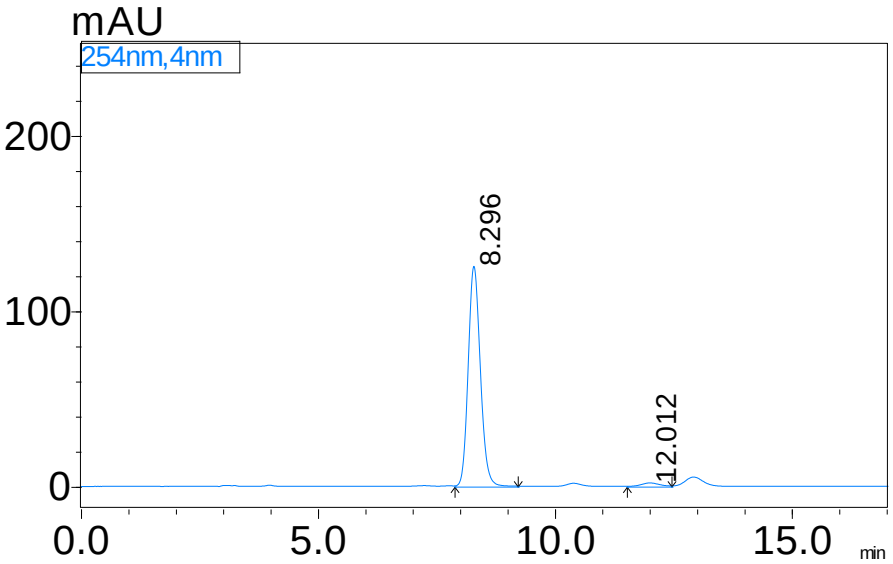


Peak#	Time	Area	Height	Area%
1	10.566	1440065	74003	98.638
2	15.837	19889	671	1.362

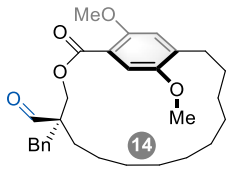


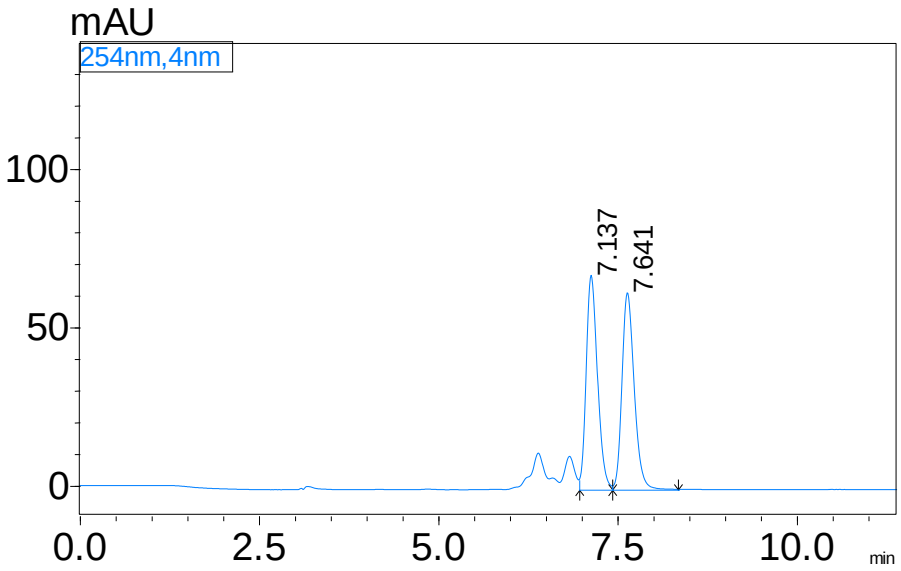


Peak#	Time	Area	Height	Area%
1	8.315	743350	40613	50.118
2	11.984	739846	28424	49.882

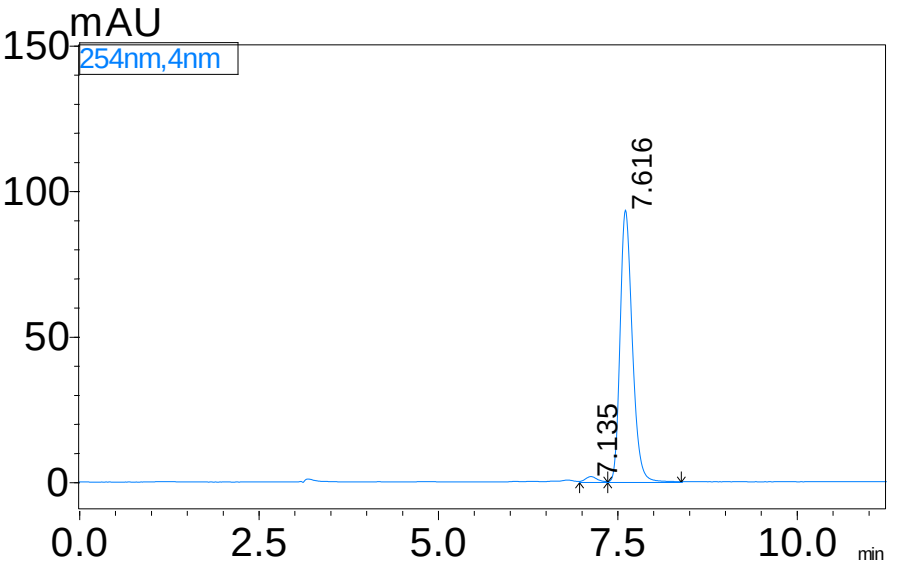


Peak#	Time	Area	Height	Area%
1	8.296	2218442	125399	97.842
2	12.012	48930	1908	2.158

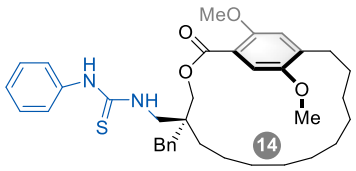


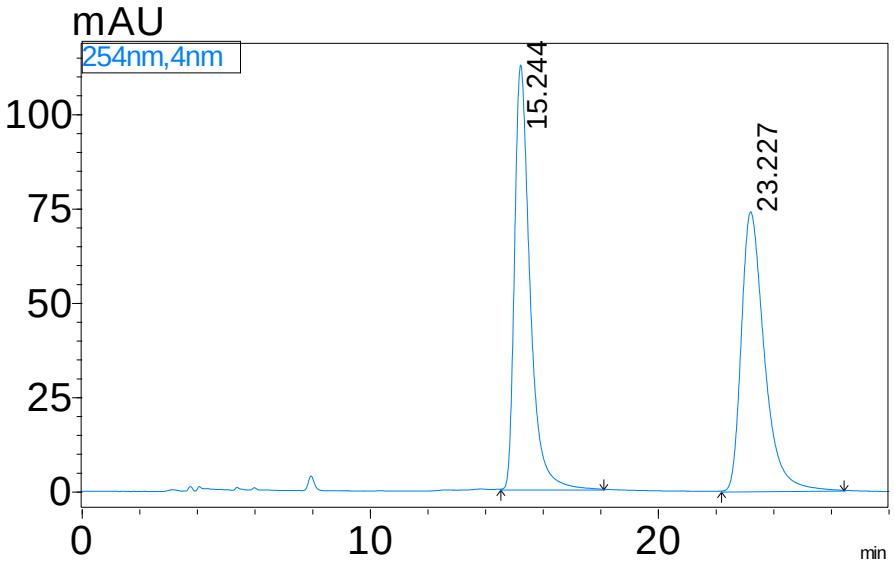


Peak#	Time	Area	Height	Area%
1	7.137	736507	67626	49.911
2	7.641	739135	62076	50.089

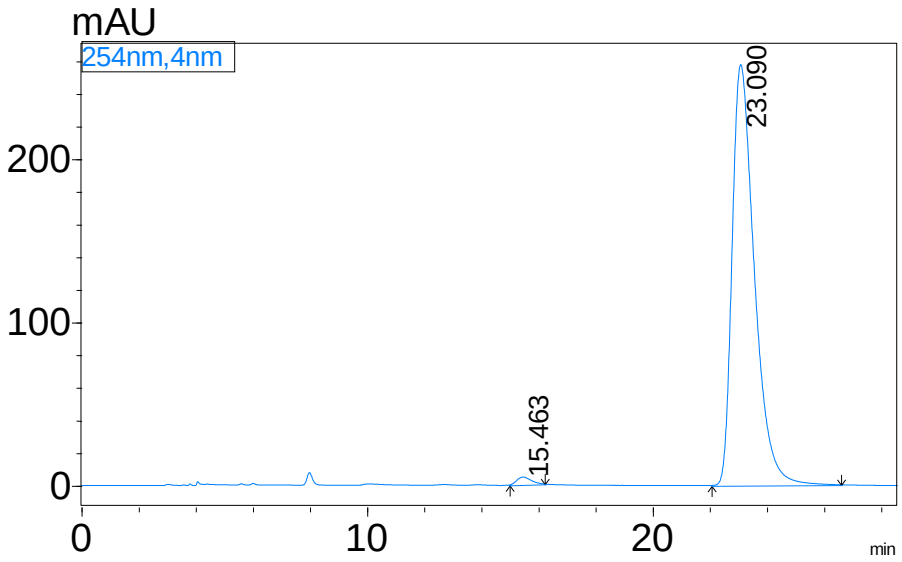


Peak#	Time	Area	Height	Area%
1	7.135	13553	1532	1.218
2	7.616	1099534	93317	98.782

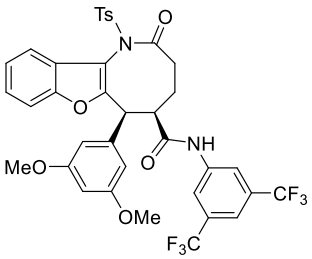


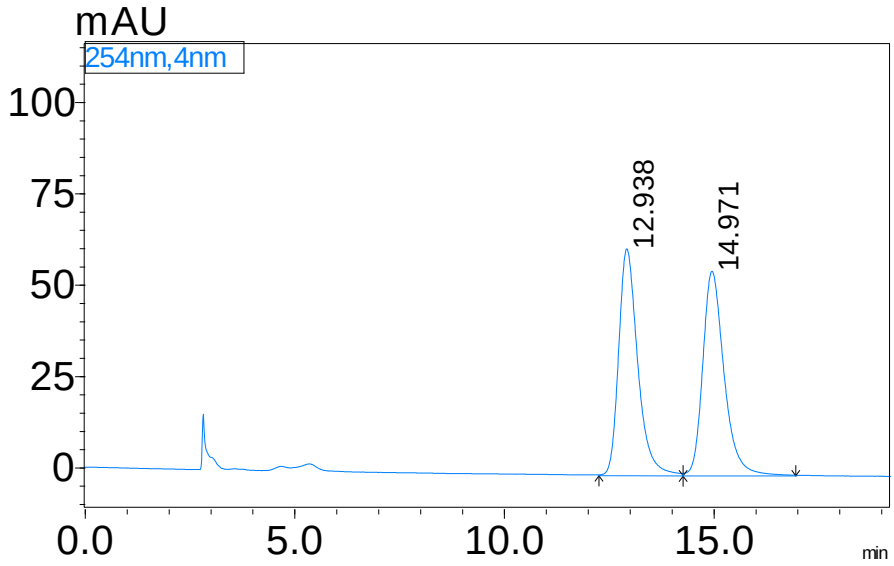


Peak#	Time	Area	Height	Area%
1	15.244	4170266	112430	50.505
2	23.227	4086924	73949	49.495

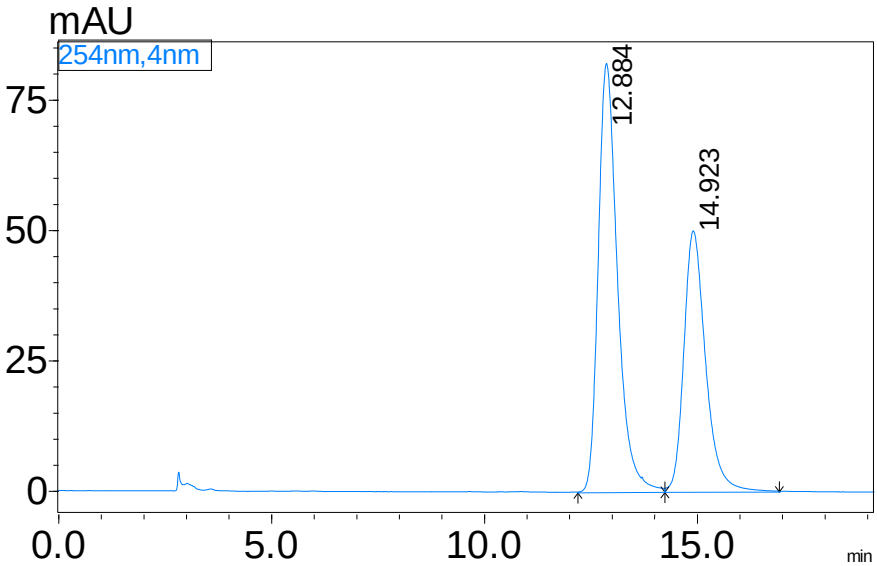


Peak#	Time	Area	Height	Area%
1	15.463	159383	4627	1.131
2	23.090	13932166	257705	98.869

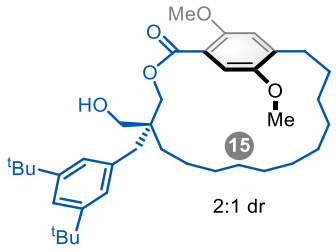


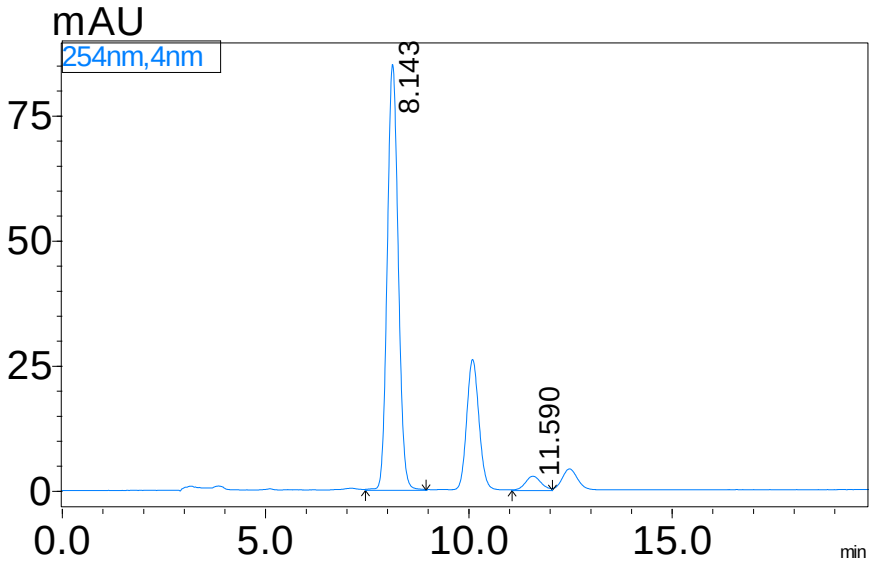


Peak#	Time	Area	Height	Area%
1	12.938	1944600	61861	49.800
2	14.971	1960226	55733	50.200

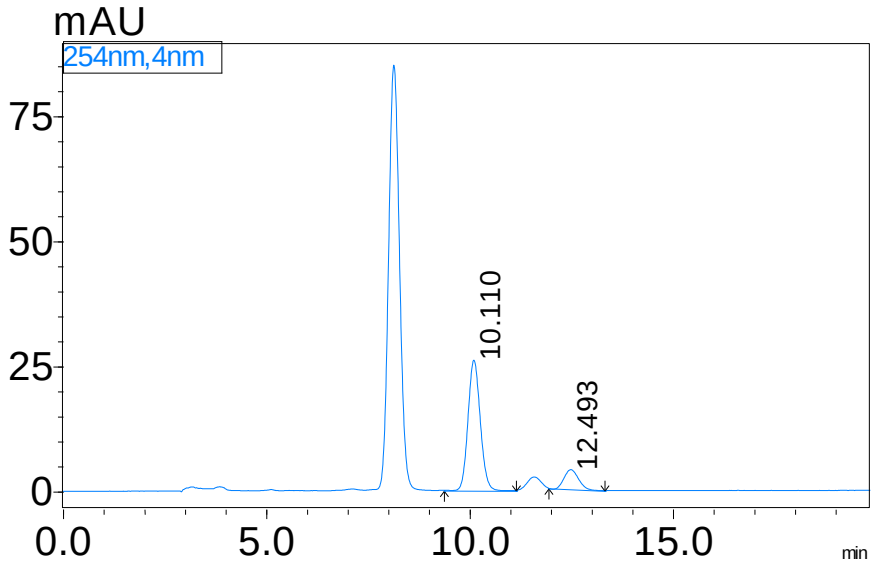


Peak#	Time	Area	Height	Area%
1	12.884	2580285	82118	59.337
2	14.923	1768235	49961	40.663

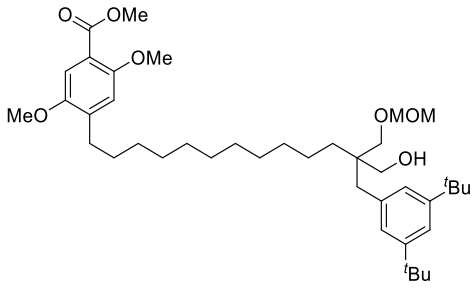


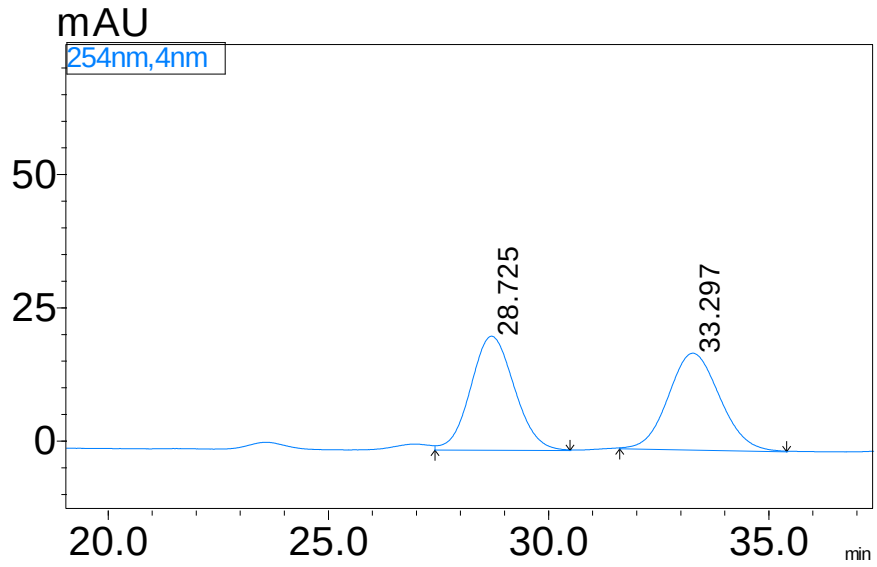


Peak#	Time	Area	Height	Area%
1	8.143	1583604	84950	95.778
2	11.590	69799	2717	4.222

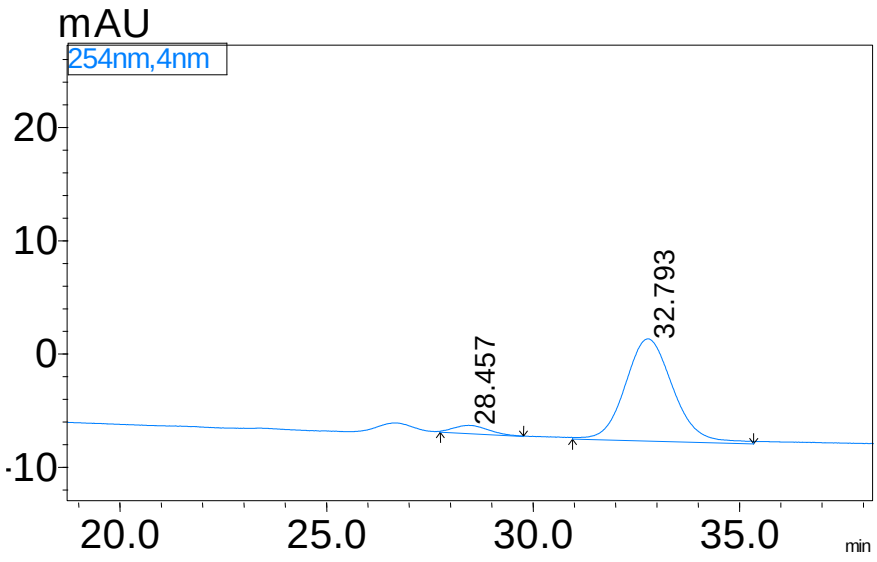


Peak#	Time	Area	Height	Area%
1	10.110	539607	26019	85.630
2	12.493	90557	3882	14.370

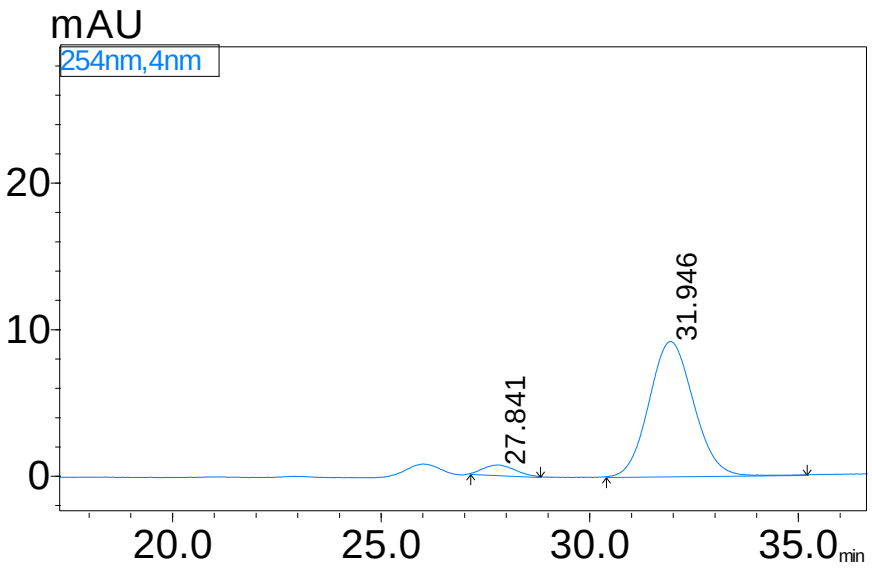




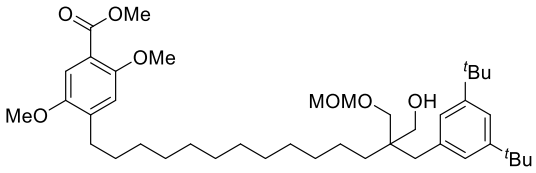
Peak#	Time	Area	Height	Area%
1	28.725	1456032	21267	50.130
2	33.297	1448475	18025	49.870

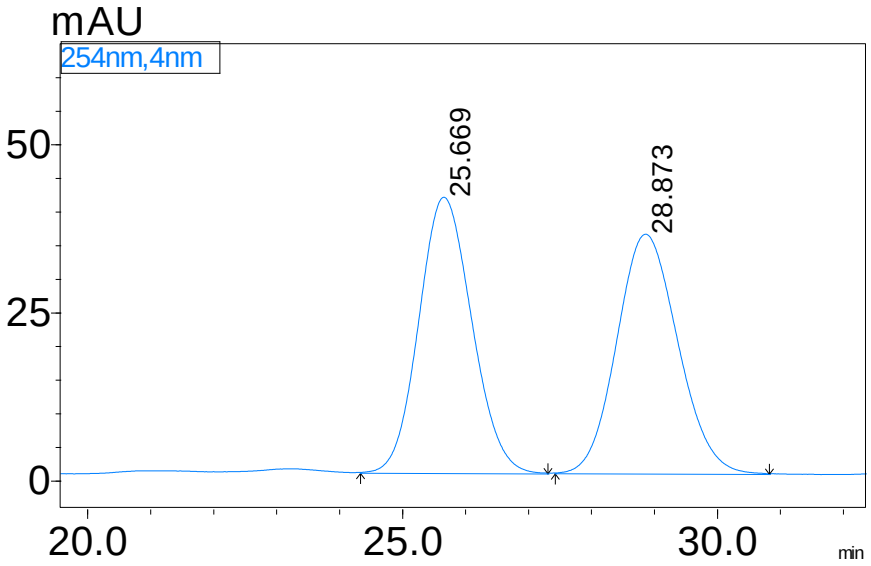


Peak#	Time	Area	Height	Area%
1	28.457	32406	625	4.650
2	32.793	664517	8758	95.350

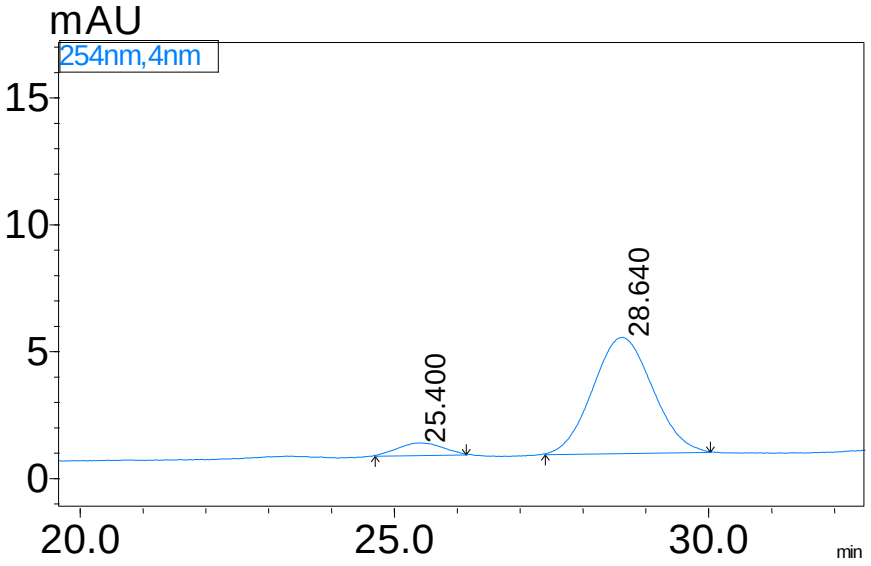


Peak#	Time	Area	Height	Area%
1	27.841	34360	678	4.847
2	31.946	674528	9179	95.153





Peak#	Time	Area	Height	Area%
1	25.669	2390300	40976	50.013
2	28.873	2389079	35556	49.987



Peak#	Time	Area	Height	Area%
1	25.400	22538	469	7.010
2	28.640	298976	4546	92.990