

Supporting Information for

Dinickel-catalyzed regio- and enantioselective α -alkylation of cyclic ketones with unactivated alkyl halides

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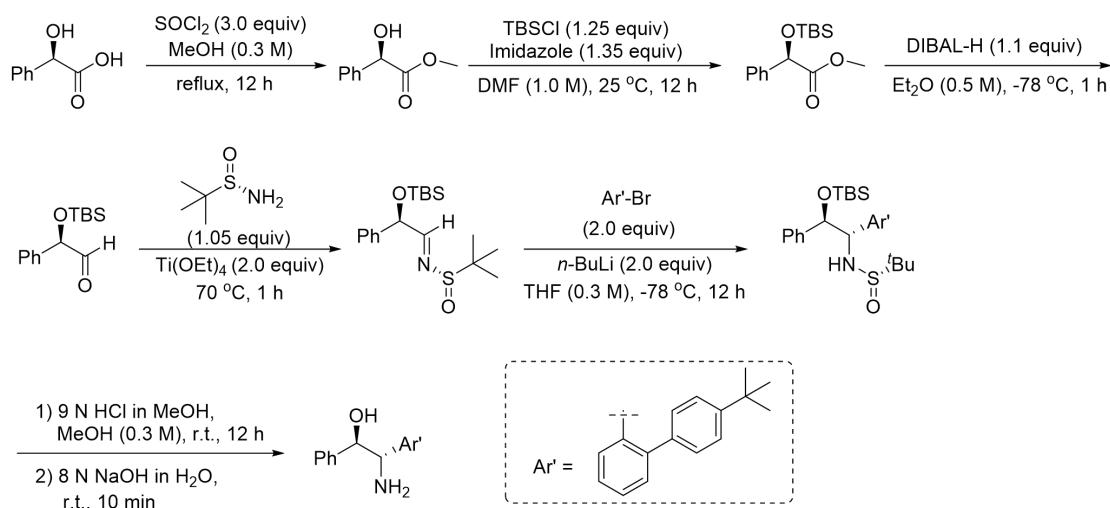
1. General Information

Unless otherwise noted, all reactions were conducted in oven-dried Schlenk tube with a magnetic stirrer under nitrogen atmosphere. Starting materials were purchased from commercial suppliers (Energy Chemical, Adamas, Bide Pharmatech Co., Ltd., etc.) and used as supplied unless otherwise stated. Ni(cod)₂ and NiCl₂:glyme were purchased from Bide Pharmatech Co., Ltd.. Solvents were purified under nitrogen using a solvent purification system. Analytical thin layer chromatography (TLC) was performed using silica gel plates. Visualization was accomplished by ultraviolet fluorescence, and/or phosphomolybdic acid, and/or KMnO₄. Flash column chromatography was performed using EM Science (200-300 mesh) silica gel.

¹H Nuclear Magnetic Resonance (¹H NMR), ¹³C Nuclear Magnetic Resonance (¹³C NMR), and ¹⁹F Nuclear Magnetic Resonance (¹⁹F NMR) spectra were recorded on Bruker 400 MHz at 20 °C with CDCl₃ or DMSO-*d*₆ as solvent. All ¹H NMR spectra are reported in parts per million (ppm) downfield of TMS and were measured relative to the signals for tetramethylsilane (δ = 0 ppm). All ¹³C NMR spectra were reported in ppm relative to CDCl₃ (77.16 ppm) or DMSO-*d*₆ (39.52 ppm). ¹⁹F NMR spectra were reported in ppm relative to CFCl₃ (δ 0.0 ppm). The data are reported as follows: chemical shift (ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad), coupling constant *J* (Hz), and integration. High resolution mass spectra were recorded on a Thermo Scientific Orbitrap Exploris 120. Chiral HPLC (High Pressure Liquid Chromatography) was performed on an SHIMADZU HPLC apparatus with columns (Chiraldak AD-H, IC-H, IBN5, IF, AS-H, Chiralcel OD-H, OJ-H, Chirobiotic ® T Astec, 250 mm × 4.6 mm). Optical rotations were recorded on an Anton Paar MCP-4100 polarimeter. X-ray analysis was recorded on a Bruker D8 Venture diffractometer.

2. Synthesis of Bimetallic Ligands

General procedure A¹



A 500 mL, one-necked Schlenk flask containing an egg-shaped stir bar was charged with (*R*)-2-hydroxy-2-phenylacetic acid (100 mmol) and MeOH (distilled, 240 mL) under nitrogen.

The solution was cooled in an ice bath for 10 min, and SOCl_2 (300 mmol, 3.0 equiv) was added dropwise by syringe over 10 min at 0 °C. The mixture was heated to reflux using a condenser in 75 °C oil bath for 12 h. After the solution was cooled to 25 °C, the volatile components are removed by rotary evaporation. The resulting residue was diluted with ethyl acetate, and saturated NaHCO_3 (aq.) solution was added slowly because of the evolution of gas. The mixture was transferred to a 1000 mL separatory funnel, and the organic layer was removed. The aqueous layer was extracted with ethyl acetate, and the organic layers were combined, washed brine, dried over anhydrous Na_2SO_4 , decanted, and concentrated by rotary evaporation to afford the crude product. The crude product was purified by column chromatography eluting with hexanes/EtOAc, 7:3 to afford methyl (*R*)-2-hydroxy-2-phenylacetate as a white solid.

A 500 mL, one-necked Schlenk flask containing an egg-shaped stir bar was charged with (*R*)-2-hydroxy-2-phenylacetate, TBSCl (1.25 equiv), imidazole (1.35 equiv), and DMF (SDS, 1.0 M) under nitrogen. The mixture was stirred at 25 °C for 12 h. The resulting mixture was diluted in Et_2O , transferred to 1000 mL separatory funnel, washed with water and brine, dried over anhydrous Na_2SO_4 , decanted, and concentrated by rotary evaporation. The crude product was purified by column chromatography eluting with hexanes/ Et_2O , 9:1 to afford methyl (*R*)-2-((*tert*-butyldimethylsilyl)oxy)-2-phenylacetate as a colorless oil.

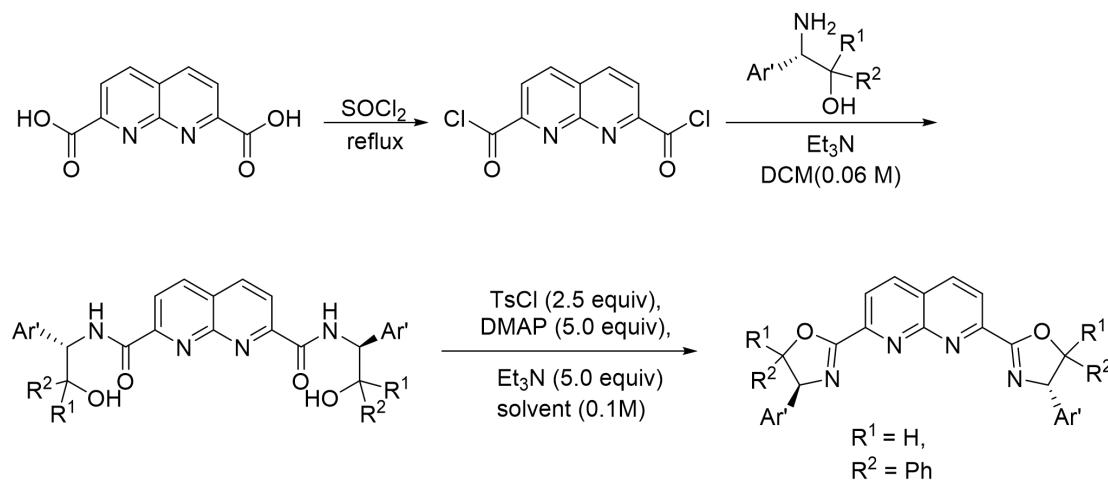
A 500 mL, three-necked round-bottomed flask equipped with nitrogen inlet, an egg-shaped stir bar, an internal temperature probe, and two rubber septa was charged with methyl (*R*)-2-((*tert*-butyldimethylsilyl)oxy)-2-phenylacetate and Et_2O (0.5 M, SDS) under nitrogen. The solution was cooled to -78 °C using a cryocooler in an EtOH bath, and DIBAL-H (1.0 M in hexane, 1.1 equiv) was added dropwise by syringe to maintain the internal temperature below -70 °C. The solution was stirred at -78 °C for 1 h and then reaction was quenched with H_2O . The mixture was slowly warmed to 25 °C. The mixture was stirred for additional 1 h. Then the mixture was filtered through a fritted glass funnel (7.5 mm diameter) containing Celite into a 500 mL filter flask. The Celite cake was washed with Et_2O . The combined filtrates were transferred to a 500 mL separatory funnel, washed with water and brine, dried over Na_2SO_4 , decanted, and concentrated by rotary evaporation. The crude product was purified by column chromatography eluting with hexanes/ Et_2O , 9:1 to afford (*R*)-2-((*tert*-butyldimethylsilyl)oxy)-2-phenylacetaldehyde as a yellow oil.

A 250 mL, one-necked Schlenk flask with an egg-shaped stir bar was charged with (*R*)-2-((*tert*-butyldimethylsilyl)oxy)-2-phenylacetaldehyde, (*S*)-2-methylpropane-2-sulfinamide (1.05 equiv), and titanium(IV) ethoxide (2.0 equiv) under nitrogen. The mixture was stirred in a 70 °C oil bath for 1 h and then was diluted with ethyl acetate. The resulting solution was poured into a 500 mL Erlenmeyer flask with a stir bar and brine, and the vial was rinsed with ethyl acetate to help the transfer. The suspension was stirred at 25 °C for 10 min and then filtered through a fritted glass funnel containing Celite. The Celite cake was washed with ethyl acetate. The combined filtrates were transferred to a 500 mL separatory funnel, washed with water and brine, dried over Na_2SO_4 , decanted, and concentrated by rotary evaporation. The crude product was purified by column chromatography eluting with hexanes/ Et_2O , 8:2 to afford (*S*)-*N*-((*R,E*)-2-((*tert*-butyldimethylsilyl)oxy)-2-phenylethyldene)-2-methylpropane-2-sulfinamide as a yellow oil.

A 250 mL, one-necked Schlenk flask containing an egg-shaped stir bar was charged with aryl bromide (40.0 mmol, 2.0 equiv) and THF (40 mL) under nitrogen. The solution was cooled to -78 °C using a cryocooler in an EtOH bath, and *n*-butyllithium (2.5 M in hexane, 40.0 mmol, 2.0 equiv) was added dropwise by syringe. The resulting solution was stirred at -78 °C using a cryocooler in an EtOH bath for 1 h. Then (*S*)-*N*-((*R,E*)-2-((*tert*-butyldimethylsilyl)oxy)-2-phenylethylidene)-2-methylpropane-2-sulfonamide (20.0 mmol) dissolved in dry THF (20 mL) was added dropwise to resulting solution over 30 min under nitrogen at -78 °C by syringe. The reaction mixture was stirred at -78 °C for 12 h and then quenched by the addition of saturated NH₄Cl (aq.) solution at -78 °C and slowly warmed to 25 °C. The mixture was transferred to a 250 mL separation funnel. The aqueous layer was extracted with ethyl acetate three times, and the organic layers were combined, washed with brine, dried over anhydrous Na₂SO₄ and concentrated under reduced pressure. The crude product was purified by column chromatography eluting with petroleum ether/EtOAc to afford chiral amino alcohol precursor.

A 250 mL, one-necked flask with magnetic stirring bar was charged with chiral amino alcohol precursor and dry methanol (0.3 M) under nitrogen. HCl in MeOH (9 N, 60 equiv) was added dropwise by syringe. The reaction was stirred for 12 h at 25 °C, and then the solvent was removed under reduced pressure. The crude solid was suspended in ethyl acetate with an ice bath, and NaOH in H₂O (8 N, 120 equiv) was added while the solution was stirred vigorously. The solution was stirred for 10 min and then was transferred to a 500 mL separation funnel. The organic layer was separated, and the aqueous layer was extracted with ethyl acetate. pH paper was used to check the neutralization of the solution (pH = 7). The organic layers were combined, dried over anhydrous Na₂SO₄ and concentrated under reduced pressure. The crude product was purified by column chromatography eluting to afford desired amino alcohol.

General procedure B^{2,3}



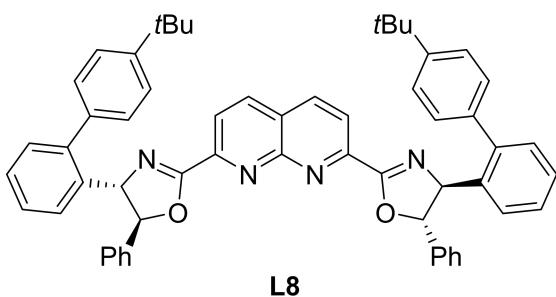
1,8-Naphthyridine-2,7-dicarboxylic acid (5.0 mmol, 1.0 equiv) was placed in a round-bottom flask equipped with a magnetic stir bar and suspended in excess SOCl₂ (10 mL). The flask was fitted

with a reflux condenser under nitrogen. The reaction was refluxed with stirring for 18 h (note: when completed, the reaction should be a homogeneous orange solution; if the flask contains yellow solid, the reaction is not finished). SOCl_2 was removed on the rotary evaporator, giving pure 1,8-naphthyridine-2,7-dicarbonyl dichloride as a yellow solid. This product was immediately carried forward.

A round-bottom flask was charged with the naphthyridine-2,7-dicarbonyl dichloride and equipped with a dry stir bar and a septum. The flask was evacuated and backfilled with nitrogen three times. Dry CH_2Cl_2 (80 mL) was added with a syringe, giving a clear yellow solution. (*S*)-amino alcohol (10.5 mmol, 2.1 equiv) was added quickly under N_2 . Then the reaction mixture was cooled to 0 °C and triethylamine (12.5 mmol, 2.5 equiv) was added dropwise over 15 min with stirring. After 12 h, the reaction mixture was poured into a separation funnel, and the organic phase was washed with saturated NaHCO_3 (aq.) solution (50 mL). The aqueous phase was again further extracted with additional portions of CH_2Cl_2 until there was no white solid in the aqueous phase remaining. The combined organic phases were washed with an additional portion of saturated NaHCO_3 (aq.) solution and brine, dried over anhydrous Na_2SO_4 , filtered, and concentrated under reduced pressure. The resultant *bis*-amide residue was directly used for the final step without further purification.

To an oven-dried, 100 -mL round-bottom flask containing a solution of the *bis*-amide (1.0 equiv) in DCM (or DCE) (0.1 M) was added 4-(dimethylamino)pyridine (DMAP, 5.0 equiv) and triethylamine (5 equiv). Then, a solution of *p*-toluenesulfonyl chloride (2.5 equiv) in DCM (or DCE) was added at room temperature. The resulting mixture was stirred at room temperature for three days (or at room temperature for 3 h, then heated to 90 °C for 36 hours). Upon completion, the reaction mixture was cooled to room temperature and quenched with saturated NaHCO_3 (aq.) solution. The resulting mixture was extracted with CH_2Cl_2 . The combined organic layer was dried over anhydrous Na_2SO_4 , filtered, and concentrated under reduced pressure. The residue was purified by silica gel column chromatography to afford pure ligand.

2,7-bis((4*S*,5*S*)-4-(4'-(*tert*-butyl)-[1,1'-biphenyl]-2-yl)-5-phenyl-4,5-dihydrooxazol-2-yl)-1,8-naphthyridine (L8)



White solid, $R_f = 0.5$ (petroleum ether/ethyl acetate = 2/1), 41% yield.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.49 (d, $J = 8.4$ Hz, 2H), 8.35 (d, $J = 8.4$ Hz, 2H), 7.49 – 7.27 (m, 8H), 7.26 – 7.15 (m, 10H), 7.09 (dt, $J = 9.5, 4.5$ Hz, 8H), 5.62 (q, $J = 7.4$ Hz, 4H), 1.28 (s, 18H).

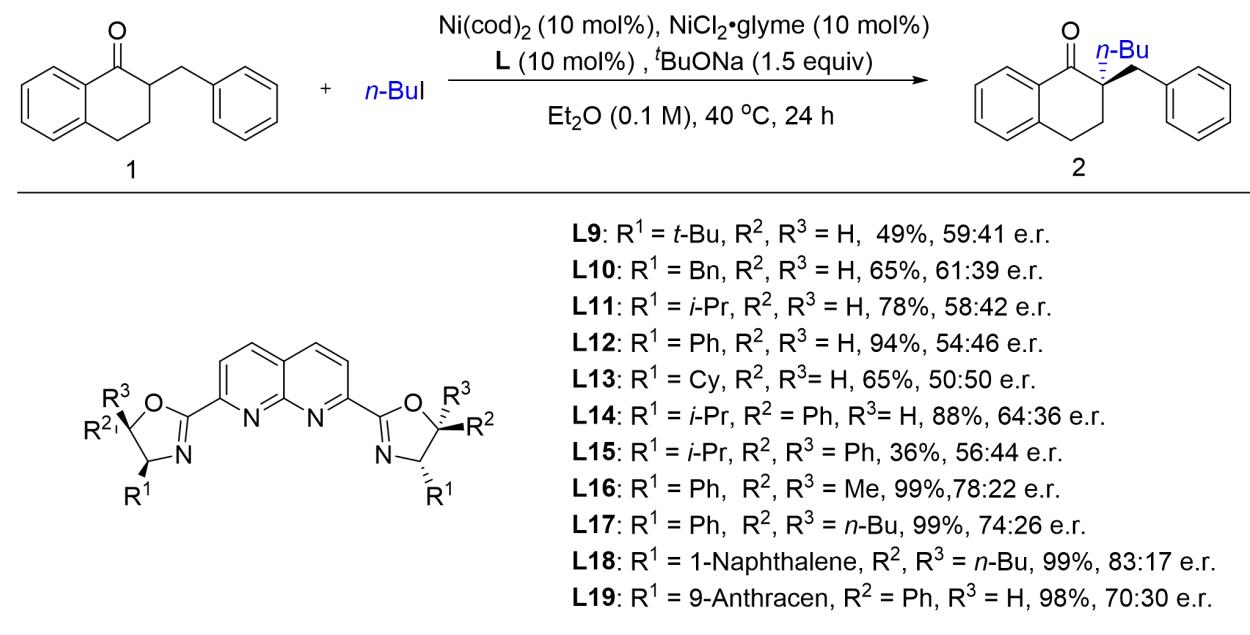
$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 163.4, 154.8, 150.8, 149.9, 141.6, 139.2, 138.9, 137.5, 137.3, 130.2, 129.2, 128.4, 128.2, 128.2, 127.6, 127.2, 126.2, 124.9, 124.5, 123.3, 90.2, 77.2, 74.9, 34.4, 31.3.

HRMS (ESI) m/z calcd. for $\text{C}_{58}\text{H}_{53}\text{N}_4\text{O}_2$ [M + H]⁺ 837.4163, found 837.4163.

3. Optimization of Reaction Conditions

Supplementary Table S1

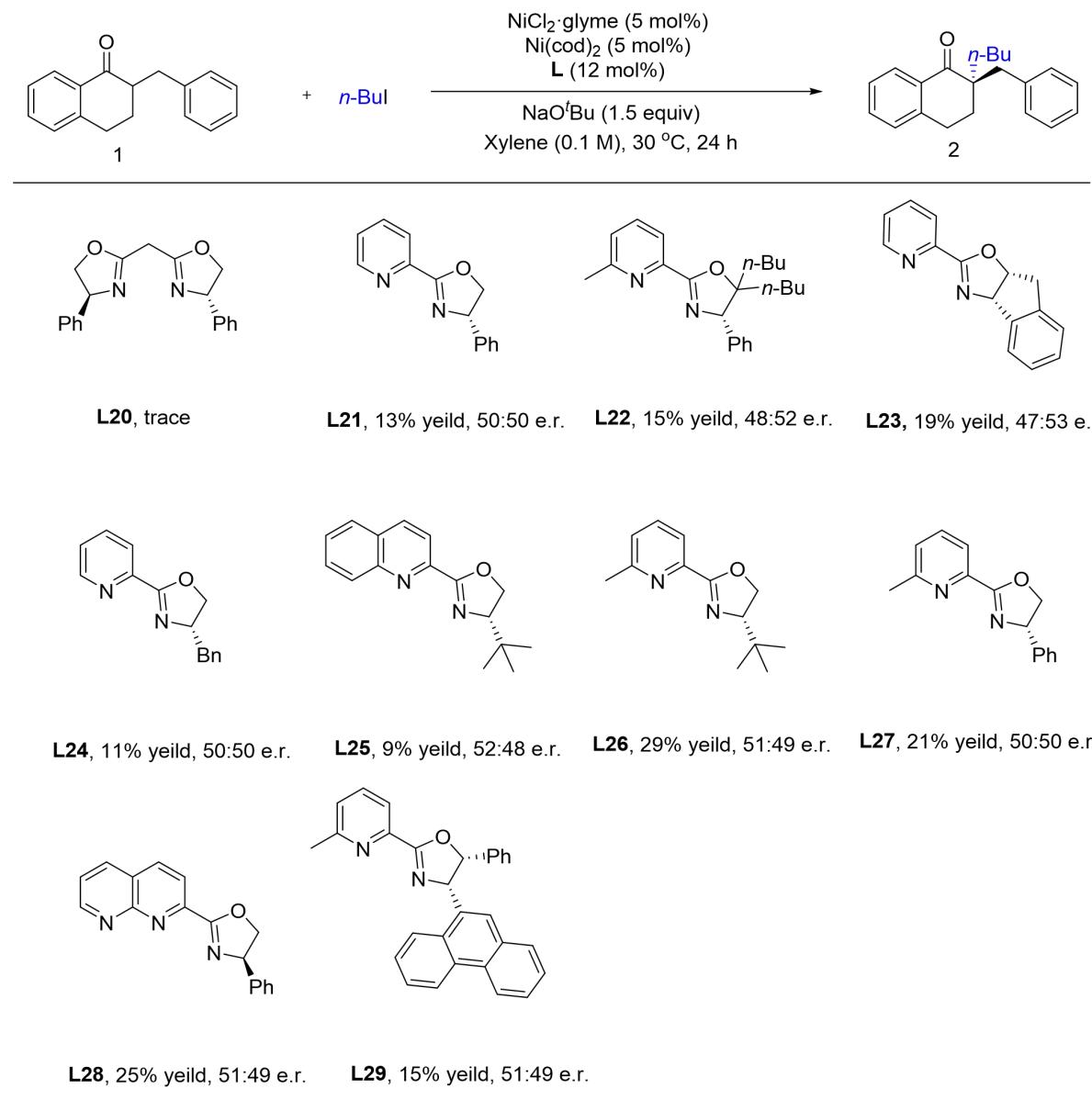
Evaluation of different ligands for cyclic ketone^a



^aStandard conditions: ketone (0.1 mmol, 1.0 equiv), *n*-BuI (1.5 equiv), NiCl₂•glyme (10 mol %), Ni(cod)₂ (10 mol %), **L** (10 mol %), *t*BuONa (1.5 equiv) in Et₂O (1.0 mL) under nitrogen at 40 °C for 24 h.

Supplementary Table S2

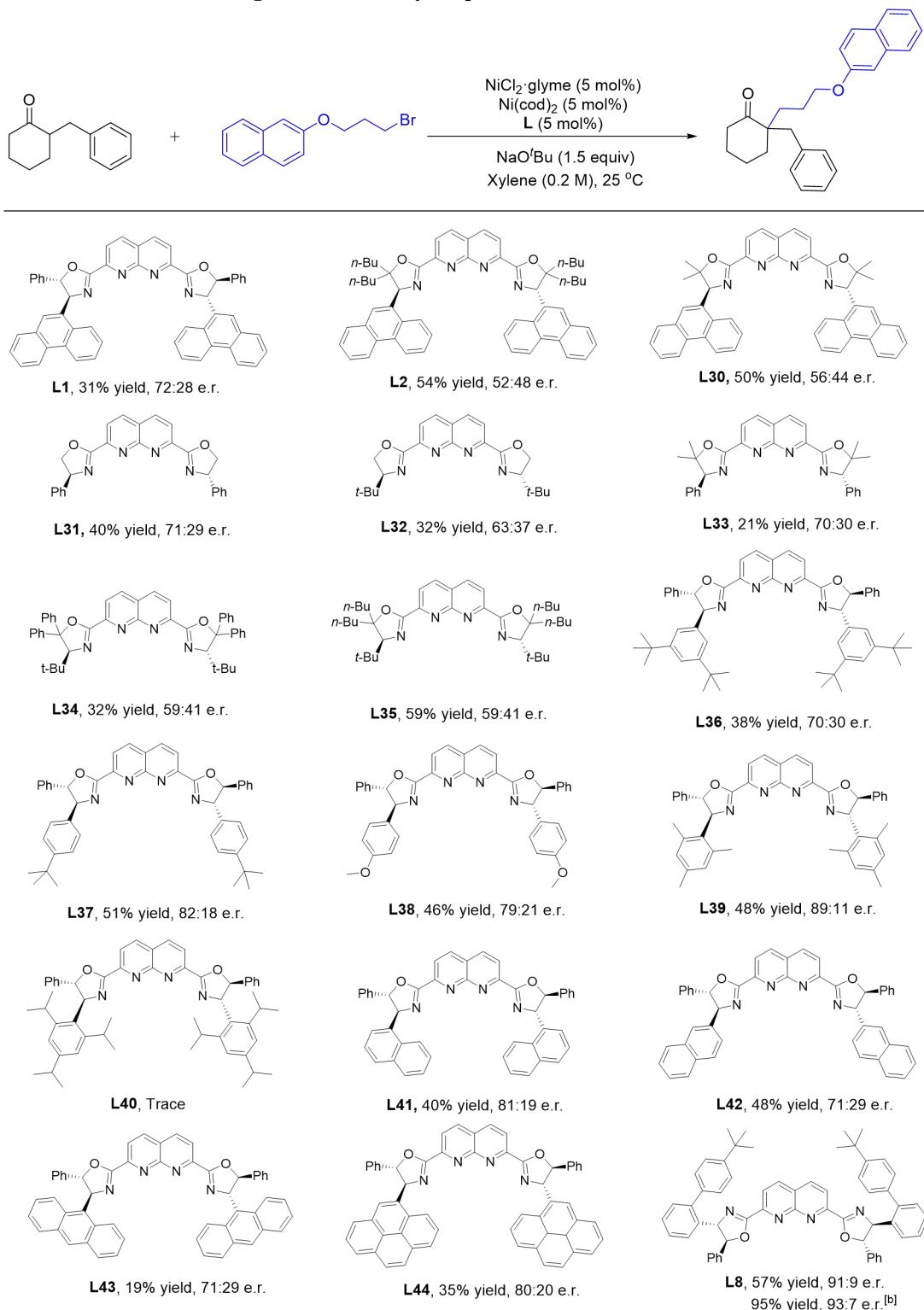
Evaluation of different types of ligands for cyclic ketone^a



^aStandard conditions: ketone (0.1 mmol, 1.0 equiv), *n*-BuI (1.5 equiv), NiCl₂•glyme (5 mol %), Ni(cod)₂ (5 mol %), **L** (12 mol %), ^tBuONa (1.5 equiv) in Xylene (1.0 mL) under nitrogen at 30 °C for 24 h.

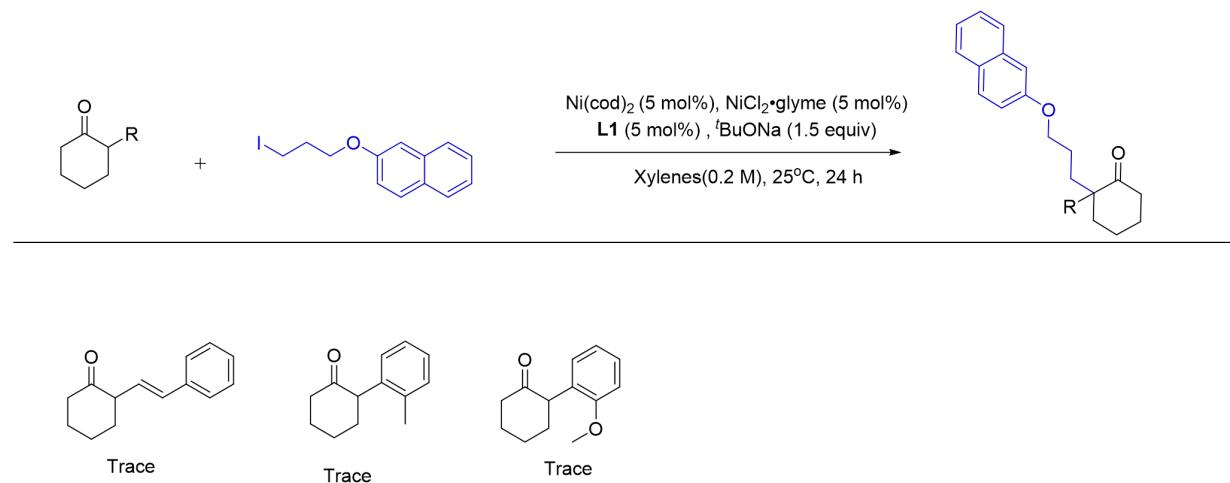
Supplementary Table S3

Evaluation of different ligands for α -Alkyl aliphatic ketones^a



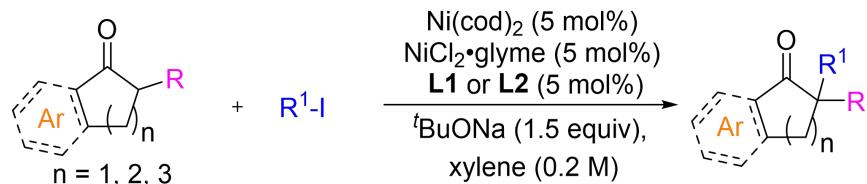
^aStandard conditions: ketone (0.2 mmol, 1.0 equiv), *n*-BuI (1.5 equiv), $\text{NiCl}_2 \cdot \text{glyme}$ (10 mol %), $\text{Ni}(\text{cod})_2$ (10 mol %), **L** (10 mol %), $\text{NaO}^{\prime}\text{Bu}$ (1.5 equiv) in Xylene (1.0 mL) under nitrogen at 25 °C for 24 h; [b] ketone (1.5 equiv), *n*-BuI (0.2 mmol, 1.0 equiv), 0 °C for 48 h.

4. Products with Poor Results



5. General Procedure for Synthesis of Chiral Product

General procedure C



The Ni(cod)₂ (2.8 mg, 0.01 mmol, 5 mol %), NiCl₂•glyme (2.2 mg, 0.01 mmol, 5 mol %), L (0.01 mmol, 5 mol %) and tBuONa (29.0 mg, 0.3 mmol, 1.5 equiv) were introduced into a flame-dried Schlenk tube in an N₂-filled glove box. After taking out from the glove box, Schlenk tube was connected to Schlenk line under N₂. 1 mL dry Xylene was injected into the Schlenk tube, the mixture was stirred at r.t. for 30 min. The ketone (0.2 mmol, 1.0 equiv) was then added rapidly under nitrogen. After 30 min, alkyl iodide (0.3 mmol, 1.5 equiv) was introduced into the system by a microsyringe (solid iodide was added rapidly) under N₂. The resulting mixture was stirred under particular temperature for 24 or 48 hours. The reaction mixture was cooled to room temperature, quenched with saturated NH₄Cl (aq.) solution and extracted with EtOAc (3x). The organic phase was washed with brine, dried over anhydrous Na₂SO₄, filtered, and concentrated under reduced pressure. The crude material was purified using column chromatography to give the enantioenriched product **2-37** and **49-62**.

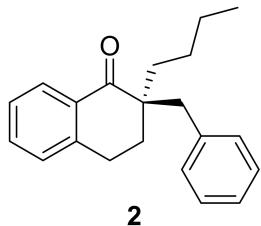
General procedure D



The Ni(cod)₂ (2.8 mg, 0.01 mmol, 5 mol %), NiCl₂•glyme (2.2 mg, 0.01 mmol, 5 mol %), **L8** (0.01 mmol, 5 mol %) and ^tBuONa (29.0 mg, 0.3 mmol, 1.5 equiv) were introduced into a flame-dried Schlenk tube in an N₂-filled glove box. After taking out from the glove box, Schlenk tube was connected to Schlenk line under N₂. 1 mL dry Xylene was injected into the Schlenk tube, the mixture was stirred at r.t. for 30 min. The ketone (0.3 mmol, 1.5 equiv) was then added rapidly under nitrogen. After 30 min, alkyl bromide (0.2 mmol, 1.0 equiv) was introduced into the system by a microsyringe (solid iodide was added rapidly) under N₂. The resulting mixture was stirred under 0 °C for 48 hours. The reaction mixture quenched with saturated NH₄Cl (aq.) solution and extracted with EtOAc (3x). The organic phase was washed with brine, dried over anhydrous Na₂SO₄, filtered, and concentrated under reduced pressure. The crude material was purified using column chromatography to give the enantioenriched product **38-48**.

6. Analytical Data of Product 2-62

(R)-2-benzyl-2-butyl-3,4-dihydronaphthalen-1(2H)-one (2)



Colorless oil, $[\alpha]_D^{20} = 26$ (c=0.5, CH₂Cl₂), $R_f = 0.8$ (petroleum ether/ethyl acetate = 10/1), 99 % yield, 92:8 e.r.

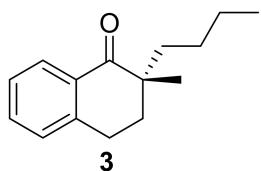
¹H NMR (400 MHz, CDCl₃) δ 8.09 (d, $J = 7.8$ Hz, 1H), 7.44 (t, $J = 7.4$ Hz, 1H), 7.30 (t, $J = 7.6$ Hz, 1H), 7.23 (d, $J = 7.1$ Hz, 2H), 7.18 (t, $J = 8.3$ Hz, 4H), 3.29 (d, $J = 13.5$ Hz, 1H), 3.07 – 2.97 (m, 1H), 2.92 (dt, $J = 17.2, 5.4$ Hz, 1H), 2.78 (d, $J = 13.5$ Hz, 1H), 2.04 – 1.86 (m, 2H), 1.70 (dd, $J = 17.1, 8.0$ Hz, 1H), 1.52 (dd, $J = 19.9, 8.5$ Hz, 1H), 1.39 (t, $J = 13.1$ Hz, 2H), 1.30 (s, 2H), 0.89 (t, $J = 6.8$ Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 201.3, 143.1, 138.1, 133.0, 132.2, 130.7, 128.6, 128.0, 127.9, 126.6, 126.2, 49.2, 40.5, 34.6, 30.4, 26.2, 25.3, 23.4, 14.0.

HRMS(ESI) *m/z* calcd. for C₂₁H₂₅O [M + H]⁺ 293.1900, found 293.1898.

HPLC (ChiralPak OJ-H column), hexanes/*i*-PrOH = 95:5, flow rate = 0.5 mL/min, $\lambda = 254$ nm, $t_R = 14.455$ min (major), $t_R = 10.596$ min (minor);

(R)-2-butyl-2-methyl-3,4-dihydronaphthalen-1(2H)-one (3)



Colorless oil, ; $[\alpha]_D^{20} = -4.1$ (c=0.8, CH₂Cl₂), $R_f = 0.8$ (petroleum ether/ethyl acetate = 10/1), 91 % yield, 84:16 e.r..

¹H NMR (400 MHz, CDCl₃) δ 8.04 (d, $J = 7.8$ Hz, 1H), 7.44 (dd, $J = 10.8, 4.0$ Hz, 1H), 7.29 (t, $J = 7.6$ Hz, 1H), 7.21 (d, $J = 7.6$ Hz, 1H), 3.06 – 2.88 (m, 2H), 2.13 – 2.03 (m, 1H), 1.92 (ddd, $J =$

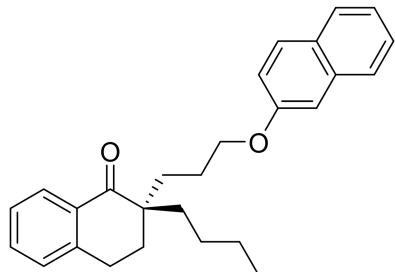
13.6, 8.3, 5.3 Hz, 1H), 1.71 – 1.61 (m, 1H), 1.56 – 1.45 (m, 1H), 1.37 – 1.21 (m, 4H), 1.18 (s, 3H), 0.88 (t, J = 6.8 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 202.7, 143.3, 132.9, 131.8, 128.6, 128.0, 126.6, 44.6, 36.1, 33.7, 26.2, 25.4, 23.3, 22.2, 14.0.

HRMS(ESI) m/z calcd. for $\text{C}_{15}\text{H}_{21}\text{O}$ [$\text{M} + \text{H}]^+$ 217.1587, found 217.1586.

HPLC (ChiralPak OJ-H column), hexanes/*i*-PrOH = 98:2, flow rate = 0.3 mL/min, λ = 254 nm, t_R = 14.250 min (major), t_R = 13.587 min (minor);

(*S*)-2-butyl-2-(3-(naphthalen-2-yloxy)propyl)-3,4-dihydronaphthalen-1(2*H*)-one (4)



4

Colorless oil, $[\alpha]_D^{20} = 5$ ($c=1.44$, CH_2Cl_2), $R_f = 0.8$ (petroleum ether/ethyl acetate = 10/1), 99 % yield, 86:14 e.r.

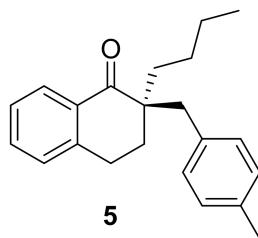
^1H NMR (400 MHz, CDCl_3) δ 8.09 (d, J = 7.7 Hz, 1H), 7.75 (dd, J = 15.0, 8.3 Hz, 3H), 7.52 – 7.39 (m, 2H), 7.33 (dd, J = 13.1, 6.7 Hz, 2H), 7.23 (d, J = 7.5 Hz, 1H), 7.13 (d, J = 8.1 Hz, 2H), 4.08 (t, J = 5.6 Hz, 2H), 3.01 (s, 2H), 2.10 (d, J = 4.9 Hz, 2H), 1.85 (ddd, J = 27.5, 22.7, 9.9 Hz, 4H), 1.72 (d, J = 9.6 Hz, 1H), 1.63 (d, J = 10.1 Hz, 1H), 1.31 (s, 4H), 0.92 (s, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 201.8, 157.0, 143.1, 134.7, 133.0, 132.0, 129.3, 129.0, 128.7, 128.0, 127.6, 126.8, 126.6, 126.3, 123.5, 119.0, 106.7, 68.4, 47.5, 34.1, 31.1, 31.0, 26.0, 25.2, 24.0, 23.4, 14.1.

HRMS(ESI) m/z calcd. for $\text{C}_{27}\text{H}_{31}\text{O}_2$ [$\text{M} + \text{H}]^+$ 387.2319, found 387.2320.

HPLC (ChiralPak AD-H column), hexanes/*i*-PrOH = 98:2, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 17.220 min (major), t_R = 18.657 min (minor);

(*R*)-2-butyl-2-(4-methylbenzyl)-3,4-dihydronaphthalen-1(2*H*)-one (5)



5

Colorless oil, $[\alpha]_D^{20} = 19.6$ ($c=1$, CH_2Cl_2), $R_f = 0.8$ (petroleum ether/ethyl acetate = 10/1), 99 % yield, 93:7 e.r.

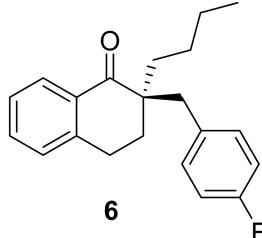
^1H NMR (400 MHz, CDCl_3) δ 8.10 (d, J = 7.8 Hz, 1H), 7.45 (t, J = 7.4 Hz, 1H), 7.31 (t, J = 7.5 Hz, 1H), 7.20 (d, J = 7.6 Hz, 1H), 7.06 (s, 4H), 3.24 (d, J = 13.5 Hz, 1H), 3.08 – 2.89 (m, 2H), 2.76 (d, J = 13.5 Hz, 1H), 2.31 (s, 3H), 2.05 – 1.87 (m, 2H), 1.70 (dd, J = 17.1, 8.1 Hz, 1H), 1.52 (dd, J = 19.4, 8.1 Hz, 1H), 1.40 (dd, J = 11.1, 6.7 Hz, 1H), 1.30 (t, J = 10.0 Hz, 3H), 0.90 (t, J = 6.9 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 201.4, 143.1, 135.6, 134.9, 133.0, 132.2, 130.6, 128.7, 128.6, 128.0, 126.6, 49.2, 40.1, 34.6, 30.4, 26.2, 25.3, 23.4, 21.0, 14.1.

HRMS(ESI) m/z calcd. for C₂₂H₂₇O [M + H]⁺307.2056, found 307.2057.

HPLC (ChiralPak IC-H column), hexanes/i-PrOH = 95:5, flow rate = 1.0 mL/min, λ = 254 nm, *t_R* = 5.598 min (major), *t_R* = 5.931 min (minor);

(R)-2-butyl-2-(4-fluorobenzyl)-3,4-dihydronaphthalen-1(2H)-one (6)



Colorless oil, $[\alpha]_D^{20} = 28.4$ (c=0.88, CH₂Cl₂), *R_f* = 0.8 (petroleum ether/ethyl acetate = 10/1), 74 % yield, 94:6 e.r.

¹H NMR (400 MHz, CDCl₃) δ 8.07 (d, *J* = 7.8 Hz, 1H), 7.44 (t, *J* = 7.4 Hz, 1H), 7.30 (t, *J* = 7.5 Hz, 1H), 7.18 (d, *J* = 7.6 Hz, 1H), 7.11 (dd, *J* = 8.2, 5.7 Hz, 2H), 6.91 (t, *J* = 8.6 Hz, 2H), 3.28 (d, *J* = 13.6 Hz, 1H), 3.10 – 2.97 (m, 1H), 2.90 (dt, *J* = 17.3, 5.3 Hz, 1H), 2.72 (d, *J* = 13.6 Hz, 1H), 2.03 – 1.85 (m, 2H), 1.73 – 1.59 (m, 1H), 1.57 – 1.45 (m, 1H), 1.38 (dd, *J* = 15.1, 10.5 Hz, 1H), 1.34 – 1.22 (m, 3H), 0.89 (t, *J* = 6.9 Hz, 3H).

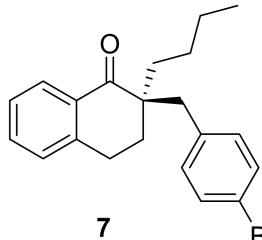
¹³C NMR (101 MHz, CDCl₃) δ 201.1, 161.6 (d, *J* = 244.2 Hz), 143.0, 133.7 (d, *J* = 3.3 Hz), 133.1, 132.1, 132.1(d, *J* = 7.9 Hz), 128.6, 128.0, 126.7, 114.7 (d, *J* = 21.0 Hz), 49.2, 39.7, 34.6, 30.4, 26.1, 25.2, 23.3, 14.0.

¹⁹F NMR (376 MHz, CDCl₃) δ -117.2 (s, 1F).

HRMS(ESI) m/z calcd. for C₂₁H₂₃FOK [M + K]⁺349.1364, found 349.1368.

HPLC (ChiralPak AD-H column), hexanes/i-PrOH = 98:2, flow rate = 0.5 mL/min, λ = 254 nm, *t_R* = 13.466 min (major), *t_R* = 14.277 min (minor);

(R)-2-(4-bromobenzyl)-2-butyl-3,4-dihydronaphthalen-1(2H)-one (7)



Colorless oil, $[\alpha]_D^{20} = 10.8$ (c=1.16, CH₂Cl₂), *R_f* = 0.8 (petroleum ether/ethyl acetate = 10/1), 81 % yield, 95:5 e.r.

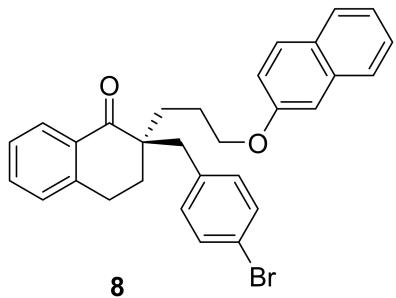
¹H NMR (400 MHz, CDCl₃) δ 8.06 (d, *J* = 7.8 Hz, 1H), 7.44 (t, *J* = 7.4 Hz, 1H), 7.34 (d, *J* = 8.3 Hz, 2H), 7.30 (t, *J* = 7.6 Hz, 1H), 7.18 (d, *J* = 7.6 Hz, 1H), 7.03 (d, *J* = 8.2 Hz, 2H), 3.27 (d, *J* = 13.5 Hz, 1H), 3.09 – 2.96 (m, 1H), 2.88 (dt, *J* = 17.3, 5.2 Hz, 1H), 2.69 (d, *J* = 13.5 Hz, 1H), 2.00 – 1.84 (m, 2H), 1.72 – 1.58 (m, 1H), 1.58 – 1.46 (m, 1H), 1.43 – 1.33 (m, 1H), 1.33 – 1.16 (m, 3H), 0.88 (t, *J* = 6.9 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 200.9, 143.0, 137.1, 133.1, 132.5, 132.0, 131.0, 128.7, 128.0, 126.7, 120.2, 49.1, 39.9, 34.6, 30.4, 26.1, 25.2, 23.3, 14.0.

HRMS(ESI) *m/z* calcd. for C₂₁H₂₄BrO [M + H]⁺ 371.1005, found 371.1005.

HPLC (ChiralPak OJ-H column), hexanes/*i*-PrOH = 95:5, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 6.284 min (major), t_R = 5.678 min (minor);

(S)-2-(4-bromobenzyl)-2-(3-(naphthalen-2-yloxy)propyl)-3,4-dihydronaphthalen-1(2H)-one (8)



White solid, $[\alpha]_D^{20}$ = 15.6 (c=0.8, CH₂Cl₂), R_f = 0.5 (petroleum ether/ethyl acetate = 10/1), 99 % yield, 92:8 e.r.

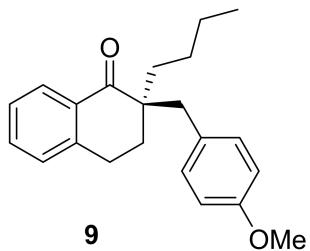
¹H NMR (400 MHz, CDCl₃) δ 8.09 (d, J = 7.8 Hz, 1H), 7.80 – 7.68 (m, 3H), 7.46 (dt, J = 15.3, 7.5 Hz, 2H), 7.40 – 7.29 (m, 4H), 7.22 (d, J = 7.6 Hz, 1H), 7.07 (dd, J = 15.7, 8.5 Hz, 4H), 4.04 (dd, J = 14.4, 6.3 Hz, 2H), 3.26 (d, J = 13.5 Hz, 1H), 3.14 – 3.01 (m, 1H), 2.96 (dt, J = 10.6, 5.1 Hz, 1H), 2.79 (d, J = 13.5 Hz, 1H), 2.08 – 1.92 (m, 3H), 1.91 – 1.78 (m, 2H), 1.73 (t, J = 12.4 Hz, 1H).

¹³C NMR (101 MHz, CDCl₃) δ 200.7, 156.8, 142.9, 136.7, 134.6, 133.4, 132.5, 131.9, 131.1, 129.4, 128.9, 128.8, 128.1, 127.7, 126.8, 126.8, 126.8, 123.6, 120.4, 118.9, 106.6, 68.0, 48.8, 39.9, 31.1, 30.6, 25.1, 24.0.

HRMS(ESI) *m/z* calcd. for C₃₀H₂₈O₂Br [M + H]⁺ 499.1267, found 499.1267.

HPLC (ChiralPak AD-H column), hexanes/*i*-PrOH = 95:5, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 18.967 min (major), t_R = 21.050 min (minor);

(R)-2-butyl-2-(4-methoxybenzyl)-3,4-dihydronaphthalen-1(2H)-one (9)



Colorless oil, $[\alpha]_D^{20}$ = 27.4 (c=0.82, CH₂Cl₂), R_f = 0.8 (petroleum ether/ethyl acetate = 10/1), 77 % yield, 90:10 e.r.

¹H NMR (400 MHz, CDCl₃) δ 8.07 (d, J = 7.8 Hz, 1H), 7.44 (t, J = 7.4 Hz, 1H), 7.30 (t, J = 7.5 Hz, 1H), 7.19 (d, J = 7.6 Hz, 1H), 7.07 (d, J = 8.4 Hz, 2H), 6.78 (d, J = 8.4 Hz, 2H), 3.76 (s, 3H), 3.21 (d, J = 13.7 Hz, 1H), 3.08 – 2.87 (m, 2H), 2.71 (d, J = 13.7 Hz, 1H), 2.03 – 1.83 (m, 2H),

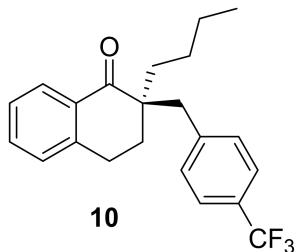
1.74 – 1.58 (m, 1H), 1.50 (dd, J = 19.5, 8.2 Hz, 1H), 1.37 (dd, J = 11.7, 7.3 Hz, 1H), 1.32 – 1.17 (m, 3H), 0.88 (t, J = 6.9 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 201.5, 158.1, 143.1, 133.0, 132.2, 131.6, 130.0, 128.6, 128.0, 126.6, 113.4, 55.2, 49.3, 39.7, 34.6, 30.3, 26.2, 25.3, 23.4, 14.1.

HRMS(ESI) m/z calcd. for $\text{C}_{22}\text{H}_{27}\text{O}_2$ [$\text{M} + \text{H}]^+$ 323.2006, found 323.2007.

HPLC (ChiralPak AD-H column), hexanes/*i*-PrOH = 95:5, flow rate = 0.5 mL/min, λ = 254 nm, t_R = 13.233 min (major), t_R = 14.254 min (minor);

(*R*)-2-butyl-2-(4-(trifluoromethyl)benzyl)-3,4-dihydronaphthalen-1(2*H*)-one (10)



Colorless oil, $[\alpha]_D^{20} = 27.4$ ($c=0.52$, CH_2Cl_2), $R_f = 0.8$ (petroleum ether/ethyl acetate = 10/1), 67 % yield, 93:7 e.r.

^1H NMR (400 MHz, CDCl_3) δ 8.07 (d, J = 7.8 Hz, 1H), 7.46 (dd, J = 18.3, 7.7 Hz, 3H), 7.30 (dd, J = 15.2, 7.8 Hz, 3H), 7.19 (d, J = 7.6 Hz, 1H), 3.40 (d, J = 13.4 Hz, 1H), 3.10 – 2.98 (m, 1H), 2.89 (dt, J = 17.3, 5.1 Hz, 1H), 2.79 (d, J = 13.4 Hz, 1H), 1.97 (dt, J = 13.6, 5.1 Hz, 1H), 1.93 – 1.83 (m, 1H), 1.72 – 1.59 (m, 1H), 1.59 – 1.49 (m, 1H), 1.48 – 1.35 (m, 1H), 1.35 – 1.21 (m, 3H), 0.89 (t, J = 6.9 Hz, 3H).

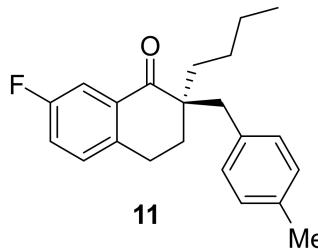
^{13}C NMR (101 MHz, CDCl_3) δ 200.7, 142.9, 142.5, 133.2, 131.9, 131.0, 128.7, 128.1, 127.0 (q, J = 269.1 Hz), 126.7, 124.8 (q, J = 3.7 Hz), 49.3, 40.3, 34.6 30.5 26.1, 25.1, 23.3, 14.0.

^{19}F NMR (376 MHz, CDCl_3) δ -62.4 (s, 3F).

HRMS(ESI) m/z calcd. for $\text{C}_{22}\text{H}_{24}\text{F}_3\text{O}$ [$\text{M} + \text{H}]^+$ 361.1774, found 361.1773.

HPLC (ChiralPak AD-H column), hexanes/*i*-PrOH = 98:2, flow rate = 0.5 mL/min, λ = 254 nm, t_R = 11.633 min (major), t_R = 12.255 min (minor);

(*R*)-2-butyl-7-fluoro-2-(4-methylbenzyl)-3,4-dihydronaphthalen-1(2*H*)-one (11)



Colorless oil, $[\alpha]_D^{20} = 11.54$ ($c=0.52$, CH_2Cl_2), $R_f = 0.8$ (petroleum ether/ethyl acetate = 10/1), 48% yield, 91:9 e.r.

^1H NMR (400 MHz, CDCl_3) δ 7.78 – 7.70 (m, 1H), 7.15 (dd, J = 7.7, 3.2 Hz, 2H), 7.04 (q, J = 8.1 Hz, 4H), 3.21 (d, J = 13.6 Hz, 1H), 3.03 – 2.82 (m, 2H), 2.73 (d, J = 13.6 Hz, 1H), 2.30 (s, 3H), 2.02 – 1.86 (m, 2H), 1.73 – 1.61 (m, 1H), 1.55 – 1.42 (m, 1H), 1.37 (dd, J = 11.0, 6.4 Hz, 1H), 1.33 – 1.18 (m, 3H), 0.89 (t, J = 6.9 Hz, 3H).

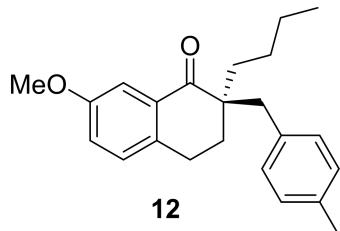
¹³C NMR (101 MHz, CDCl₃) δ 200.4, 161.6 (d, *J* = 245.8 Hz), 138.7 (d, *J* = 3.0 Hz), 135.8, 134.6, 133.8 (d, *J* = 5.8 Hz), 130.6, 130.4 (d, *J* = 7.0 Hz), 128.7, 120.4 (d, *J* = 22.2 Hz), 113.8 (d, *J* = 21.8 Hz), 49.0, 40.0, 34.5, 30.4, 26.2, 24.6, 23.3, 21.0, 14.0.

¹⁹F NMR (376 MHz, CDCl₃) δ -115.4 (s, 1F).

HRMS(ESI) *m/z* calcd. for C₂₂H₂₆FO [M + H]⁺325.1962, found 325.1964.

HPLC (ChiralPak OJ-H column), hexanes/*i*-PrOH = 95:5, flow rate = 1.0 mL/min, λ = 254 nm, *t_R* = 7.027 min (major), *t_R* = 5.523 min (minor);

(R)-2-butyl-7-methoxy-2-(4-methylbenzyl)-3,4-dihydronaphthalen-1(2H)-one (12)



Colorless oil, $[\alpha]_D^{20}$ = 35 (c=1.22, CH₂Cl₂), *R_f* = 0.8 (petroleum ether/ethyl acetate = 10/1), 99 % yield, 95:5 e.r.

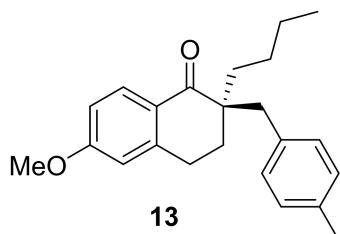
¹H NMR (400 MHz, CDCl₃) δ 7.57 (d, *J* = 2.4 Hz, 1H), 7.10 (d, *J* = 8.4 Hz, 1H), 7.08 – 7.01 (m, 5H), 3.85 (s, 3H), 3.22 (d, *J* = 13.5 Hz, 1H), 3.01 – 2.82 (m, 2H), 2.74 (d, *J* = 13.5 Hz, 1H), 2.30 (s, 3H), 2.00 – 1.86 (m, 2H), 1.69 (dd, *J* = 17.0, 8.1 Hz, 1H), 1.50 (dd, *J* = 19.6, 8.0 Hz, 1H), 1.38 (dd, *J* = 11.0, 7.0 Hz, 1H), 1.27 (dd, *J* = 14.4, 8.8 Hz, 3H), 0.90 (t, *J* = 6.9 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 201.3, 158.4, 135.7, 135.6, 134.9, 133.0, 130.6, 129.8, 128.6, 121.4, 109.9, 55.5, 49.1, 40.1, 34.6, 30.6, 26.3, 24.5, 23.4, 21.0, 14.1.

HRMS(ESI) *m/z* calcd. for C₂₃H₂₉O₂ [M + H]⁺337.2162, found 337.2162.

HPLC (ChiralPak OJ-H column), hexanes/*i*-PrOH = 95:5, flow rate = 1.0 mL/min, λ = 254 nm, *t_R* = 7.722 min (major), *t_R* = 6.751 min (minor);

(R)-2-butyl-6-methoxy-2-(4-methylbenzyl)-3,4-dihydronaphthalen-1(2H)-one (13)



Colorless oil, $[\alpha]_D^{20}$ = 11.4 (c=0.9, CH₂Cl₂), *R_f* = 0.8 (petroleum ether/ethyl acetate = 10/1), 72 % yield, 86:14 e.r.

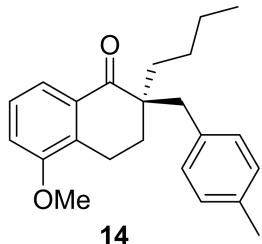
¹H NMR (400 MHz, CDCl₃) δ 8.05 (d, *J* = 8.8 Hz, 1H), 7.05 (s, 4H), 6.82 (dd, *J* = 8.7, 2.3 Hz, 1H), 6.63 (d, *J* = 1.9 Hz, 1H), 3.84 (s, 3H), 3.22 (d, *J* = 13.5 Hz, 1H), 2.93 (dtt, *J* = 22.8, 17.1, 5.6 Hz, 2H), 2.72 (d, *J* = 13.5 Hz, 1H), 2.30 (s, 3H), 2.01 – 1.84 (m, 2H), 1.74 – 1.60 (m, 1H), 1.49 (dd, *J* = 19.5, 7.9 Hz, 1H), 1.37 (dd, *J* = 10.5, 6.1 Hz, 1H), 1.34 – 1.18 (m, 3H), 0.89 (t, *J* = 6.9 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 200.2, 163.3, 145.5, 135.6, 135.0, 130.6, 130.4, 128.6, 126.0, 113.2, 112.5, 55.4, 48.9, 40.2, 34.8, 30.4, 26.3, 25.7, 23.4, 21.0, 14.1.

HRMS(ESI) *m/z* calcd. for C₂₃H₂₉O₂ [M + H]⁺337.2162, found 337.2163.

HPLC (ChiralPak AD-H column), hexanes/*i*-PrOH = 95:5, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 12.115 min (major), t_R = 10.389 min (minor);

(*R*)-2-butyl-5-methoxy-2-(4-methylbenzyl)-3,4-dihydronaphthalen-1(2*H*)-one (14)



Colorless oil, $[\alpha]_D^{20} = -2.2$ ($c=0.94$, CH_2Cl_2), $R_f = 0.8$ (petroleum ether/ethyl acetate = 10/1), 78 % yield, 88:12 e.r.

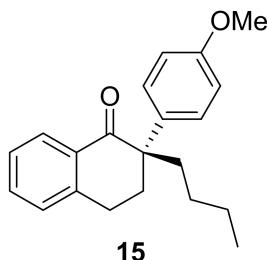
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.70 (d, $J = 7.9$ Hz, 1H), 7.29 (d, $J = 8.0$ Hz, 1H), 7.05 (s, 4H), 6.99 (d, $J = 8.0$ Hz, 1H), 3.86 (s, 3H), 3.17 (d, $J = 13.6$ Hz, 1H), 3.00 – 2.80 (m, 2H), 2.77 (d, $J = 13.6$ Hz, 1H), 2.30 (s, 3H), 1.93 (tdd, $J = 14.0, 11.3, 5.6$ Hz, 2H), 1.66 (dd, $J = 17.1, 8.2$ Hz, 1H), 1.55 – 1.45 (m, 1H), 1.45 – 1.34 (m, 1H), 1.33 – 1.16 (m, 3H), 0.88 (t, $J = 7.0$ Hz, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 201.6, 156.6, 135.6, 134.9, 133.2, 132.1, 130.6, 128.6, 126.8, 119.6, 113.7, 55.6, 48.7, 39.8, 34.2, 29.8, 26.2, 23.4, 21.0, 19.0, 14.1.

HRMS(ESI) m/z calcd. for $\text{C}_{23}\text{H}_{29}\text{O}_2$ $[\text{M} + \text{H}]^+$ 337.2162, found 337.2161.

HPLC (ChiralPak AD-H column), hexanes/*i*-PrOH = 95:5, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 6.889 min (major), t_R = 7.742 min (minor);

(*S*)-2-butyl-2-(4-methoxyphenyl)-3,4-dihydronaphthalen-1(2*H*)-one (15)



Colorless oil, $[\alpha]_D^{20} = -37.7$ ($c=0.30$, CH_2Cl_2), $R_f = 0.8$ (petroleum ether/ethyl acetate = 10/1), 99 % yield, 86:14 e.r.

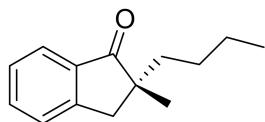
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.13 (d, $J = 7.8$ Hz, 1H), 7.38 (t, $J = 7.4$ Hz, 1H), 7.28 (d, $J = 7.6$ Hz, 1H), 7.16 (d, $J = 8.5$ Hz, 2H), 7.09 (d, $J = 7.6$ Hz, 1H), 6.81 (d, $J = 8.5$ Hz, 2H), 3.75 (s, 3H), 3.01 – 2.76 (m, 2H), 2.57 (dt, $J = 13.9, 3.5$ Hz, 1H), 2.33 (td, $J = 13.1, 4.6$ Hz, 1H), 2.02 – 1.89 (m, 1H), 1.87 – 1.73 (m, 1H), 1.37 – 1.13 (m, 4H), 0.86 (t, $J = 7.0$ Hz, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 200.5, 158.2, 143.3, 133.0, 132.9, 132.0, 128.5, 128.0, 128.0, 126.4, 113.8, 55.2, 53.0, 40.2, 31.9, 26.8, 25.9, 23.4, 14.0.

HRMS(ESI) m/z calcd. for $\text{C}_{21}\text{H}_{25}\text{O}_2$ $[\text{M} + \text{H}]^+$ 309.1849, found 309.1854.

HPLC (ChiralPak AD-H column), hexanes/*i*-PrOH = 70:30, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 4.690 min (major), t_R = 5.330 min (minor);

(*R*)-2-butyl-2-methyl-2,3-dihydro-1*H*-inden-1-one (16)



16

Colorless oil, $[\alpha]_D^{20} = -21$ ($c=0.6$, CH_2Cl_2), $R_f = 0.8$ (petroleum ether/ethyl acetate = 10/1), 99 % yield, 91:9 e.r.

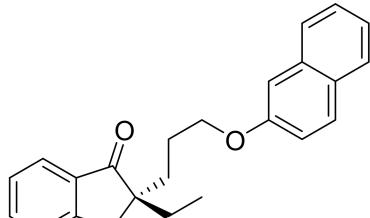
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.75 (d, $J = 7.6$ Hz, 1H), 7.58 (t, $J = 7.4$ Hz, 1H), 7.43 (d, $J = 7.6$ Hz, 1H), 7.36 (t, $J = 7.4$ Hz, 1H), 3.12 (d, $J = 17.2$ Hz, 1H), 2.87 (d, $J = 17.2$ Hz, 1H), 1.67 – 1.51 (m, 2H), 1.30 – 1.22 (m, 3H), 1.20 (s, 3H), 1.08 (dt, $J = 12.6, 5.5$ Hz, 1H), 0.84 (t, $J = 7.1$ Hz, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 211.6, 152.8, 136.2, 134.7, 127.3, 126.5, 124.2, 49.1, 40.2, 38.2, 26.8, 24.0, 23.2, 13.9.

HRMS(ESI) m/z calcd. for $\text{C}_{14}\text{H}_{19}\text{O}$ $[\text{M} + \text{H}]^+$ 203.1430, found 203.1429.

HPLC (ChiralPak IC-H column), hexanes/*i*-PrOH = 95:5, flow rate = 0.5 mL/min, $\lambda = 254$ nm, $t_R = 13.892$ min (major), $t_R = 12.252$ min (minor);

(R)-2-ethyl-2-(3-(naphthalen-2-yloxy)propyl)-2,3-dihydro-1*H*-inden-1-one (17)



17

Colorless oil, $[\alpha]_D^{20} = 25.2$ ($c=0.4$, CH_2Cl_2), $R_f = 0.8$ (petroleum ether/ethyl acetate = 10/1), 92 % yield, 90:10 e.r.

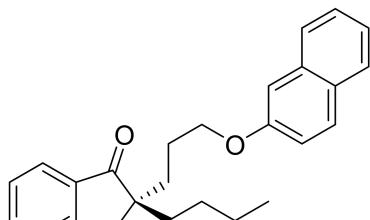
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.76 (t, $J = 8.3$ Hz, 2H), 7.74 – 7.66 (m, 2H), 7.60 (t, $J = 7.3$ Hz, 1H), 7.47 (d, $J = 7.7$ Hz, 1H), 7.45 – 7.41 (m, 1H), 7.38 (t, $J = 7.5$ Hz, 1H), 7.32 (t, $J = 7.4$ Hz, 1H), 7.15 – 7.04 (m, 2H), 4.01 (t, $J = 6.0$ Hz, 2H), 3.07 (s, 2H), 1.94 – 1.82 (m, 2H), 1.77 (dd, $J = 13.4, 7.3$ Hz, 2H), 1.73 – 1.54 (m, 2H), 0.83 (t, $J = 7.4$ Hz, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 211.1, 156.9, 153.2, 137.3, 134.8, 134.6, 129.3, 129.0, 127.6, 127.4, 126.7, 126.5, 126.3, 123.9, 123.5, 118.9, 106.6, 68.1, 52.7, 37.4, 33.6, 30.2, 24.4, 8.7.

HRMS(ESI) m/z calcd. for $\text{C}_{24}\text{H}_{25}\text{O}_2$ $[\text{M} + \text{H}]^+$ 345.1849, found 345.1849.

HPLC (ChiralPak AD-H column), hexanes/*i*-PrOH = 95:5, flow rate = 1.0 mL/min, $\lambda = 254$ nm, $t_R = 14.799$ min (major), $t_R = 19.542$ min (minor);

(R)-2-butyl-2-(3-(naphthalen-2-yloxy)propyl)-2,3-dihydro-1*H*-inden-1-one (18)



18

Colorless oil, $[\alpha]_D^{20} = 13.8$ ($c=1.36$, CH_2Cl_2), $R_f = 0.8$ (petroleum ether/ethyl acetate = 10/1), 97 % yield, 94:6 e.r.

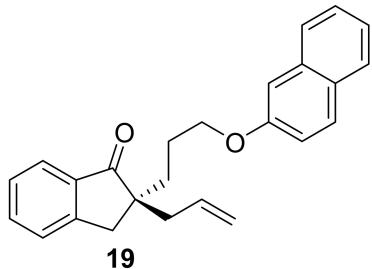
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.77 (t, $J = 8.6$ Hz, 2H), 7.74 – 7.67 (m, 2H), 7.60 (t, $J = 7.3$ Hz, 1H), 7.44 (dd, $J = 17.3, 8.0$ Hz, 2H), 7.38 (t, $J = 7.5$ Hz, 1H), 7.32 (t, $J = 7.4$ Hz, 1H), 7.16 – 7.02 (m, 2H), 4.01 (t, $J = 6.0$ Hz, 2H), 3.08 (s, 2H), 1.97 – 1.82 (m, 2H), 1.82 – 1.75 (m, 1H), 1.68 (qd, $J = 13.6, 8.7$ Hz, 3H), 1.27 (dt, $J = 15.6, 6.3$ Hz, 3H), 1.12 (dt, $J = 12.7, 6.3$ Hz, 1H), 0.86 (t, $J = 7.0$ Hz, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 211.1, 156.9, 153.2, 137.2, 134.8, 134.6, 129.3, 129.0, 127.6, 127.4, 126.7, 126.5, 126.3, 123.9, 123.5, 118.9, 106.6, 68.1, 52.4, 37.9, 37.4, 34.0, 26.5, 24.4, 23.3, 13.9.

HRMS(ESI) m/z calcd. for $\text{C}_{26}\text{H}_{29}\text{O}_2$ $[\text{M} + \text{H}]^+$ 373.2162, found 373.2162.

HPLC (ChiralPak AD-H column), hexanes/*i*-PrOH = 95:5, flow rate = 1.0 mL/min, $\lambda = 254$ nm, $t_R = 15.954$ min (major), $t_R = 18.034$ min (minor);

(*S*)-2-allyl-2-(3-(naphthalen-2-yloxy)propyl)-2,3-dihydro-1*H*-inden-1-one (19)



Colorless oil, $[\alpha]_D^{20} = 18.4$ ($c=1.06$, CH_2Cl_2), $R_f = 0.8$ (petroleum ether/ethyl acetate = 10/1), 94 % yield, 90:10 e.r.

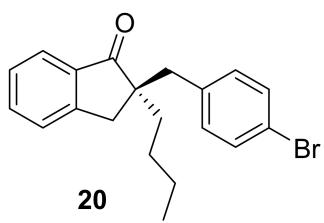
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.76 (t, $J = 8.4$ Hz, 2H), 7.71 (dd, $J = 8.3, 4.1$ Hz, 2H), 7.60 (t, $J = 7.4$ Hz, 1H), 7.52 – 7.40 (m, 2H), 7.40 – 7.35 (m, 1H), 7.32 (t, $J = 7.4$ Hz, 1H), 7.15 – 7.00 (m, 2H), 5.66 (td, $J = 16.9, 7.6$ Hz, 1H), 5.11 (d, $J = 16.9$ Hz, 1H), 5.02 (d, $J = 10.0$ Hz, 1H), 4.00 (t, $J = 6.1$ Hz, 2H), 3.09 (dd, $J = 40.8, 17.4$ Hz, 2H), 2.49 (dd, $J = 13.6, 6.5$ Hz, 1H), 2.39 (dd, $J = 13.5, 8.1$ Hz, 1H), 1.98 – 1.72 (m, 3H), 1.72 – 1.59 (m, 1H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 210.3, 156.9, 153.0, 136.9, 135.0, 134.6, 133.5, 129.3, 129.0, 127.6, 127.5, 126.7, 126.5, 126.3, 124.0, 123.5, 118.9, 118.5, 106.6, 68.0, 52.2, 42.0, 37.0, 33.8, 24.3.

HRMS(ESI) m/z calcd. for $\text{C}_{25}\text{H}_{25}\text{O}_2$ $[\text{M} + \text{H}]^+$ 357.1849, found 357.1848.

HPLC (ChiralPak AD-H column), hexanes/*i*-PrOH = 95:5, flow rate = 1.0 mL/min, $\lambda = 254$ nm, $t_R = 14.985$ min (major), $t_R = 20.209$ min (minor);

(*S*)-2-(4-bromobenzyl)-2-butyl-2,3-dihydro-1*H*-inden-1-one (20)



Colorless oil, $[\alpha]_D^{20} = 145.2$ ($c=0.4$, CH_2Cl_2), $R_f = 0.8$ (petroleum ether/ethyl acetate = 10/1), 98 % yield, 94:6 e.r.

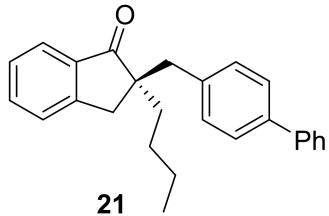
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.69 (d, $J = 7.5$ Hz, 1H), 7.51 (t, $J = 7.1$ Hz, 1H), 7.38 – 7.26 (m, 4H), 6.97 (d, $J = 7.7$ Hz, 2H), 3.06 (d, $J = 15.0$ Hz, 2H), 2.90 (d, $J = 17.3$ Hz, 1H), 2.74 (d, $J = 13.4$ Hz, 1H), 1.84 – 1.68 (m, 1H), 1.60 – 1.48 (m, 1H), 1.24 (d, $J = 8.8$ Hz, 2H), 1.17 – 0.94 (m, 2H), 0.82 (t, $J = 7.0$ Hz, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 210.6, 153.0, 137.0, 136.6, 134.9, 131.9, 131.1, 127.3, 126.3, 123.8, 120.3, 53.8, 42.3, 38.4, 36.1, 26.5, 23.2, 13.9.

HRMS(ESI) m/z calcd. for $\text{C}_{20}\text{H}_{22}\text{BrO}$ $[\text{M} + \text{H}]^+$ 357.0848, found 357.0848.

HPLC (ChiralPak OJ-H column), hexanes/*i*-PrOH = 95:5, flow rate = 1.0 mL/min, $\lambda = 254$ nm, $t_R = 8.689$ min (major), $t_R = 6.131$ min (minor);

(*S*)-2-([1,1'-biphenyl]-4-ylmethyl)-2-butyl-2,3-dihydro-1*H*-inden-1-one (21)



Colorless oil, $[\alpha]_D^{20} = 47.8$ ($c=0.8$, CH_2Cl_2), $R_f = 0.8$ (petroleum ether/ethyl acetate = 10/1), 99 % yield, 94:6 e.r.

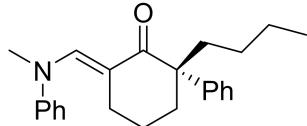
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.73 (d, $J = 7.6$ Hz, 1H), 7.50 (t, $J = 8.6$ Hz, 3H), 7.40 (t, $J = 8.3$ Hz, 4H), 7.36 – 7.27 (m, 3H), 7.19 (d, $J = 8.1$ Hz, 2H), 3.16 (dd, $J = 21.8, 15.4$ Hz, 2H), 2.90 (dd, $J = 28.7, 15.4$ Hz, 2H), 1.87 – 1.77 (m, 1H), 1.64 – 1.55 (m, 1H), 1.36 – 1.19 (m, 3H), 1.19 – 1.03 (m, 2H), 0.84 (t, $J = 7.3$ Hz, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 211.0, 153.2, 140.8, 139.1, 137.1, 136.8, 134.7, 130.6, 128.7, 127.2, 127.1, 126.9, 126.7, 126.3, 123.8, 54.1, 42.6, 38.3, 36.3, 26.5, 23.3, 13.9.

HRMS(ESI) m/z calcd. for $\text{C}_{26}\text{H}_{27}\text{O}$ $[\text{M} + \text{H}]^+$ 355.2056, found 355.2053.

HPLC (ChiralPak AD-H column), hexanes/*i*-PrOH = 95:5, flow rate = 0.5 mL/min, $\lambda = 254$ nm, $t_R = 13.807$ min (major), $t_R = 14.904$ min (minor);

(*S, E*)-2-butyl-6-((methyl(phenyl)amino)methylene)-2-phenylcyclohexan-1-one (22)



Yellow oil, $[\alpha]_D^{20} = -295.3$ ($c=0.42$, CH_2Cl_2), $R_f = 0.4$ (petroleum ether/ethyl acetate = 10/1), 93 % yield, 94:6 e.r..

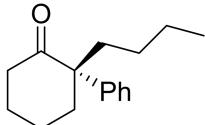
$^1\text{H NMR}$ (400 MHz, $\text{DMSO}-d_6$) δ 7.47 (s, 1H), 7.37 – 7.24 (m, 6H), 7.17 (t, $J = 6.7$ Hz, 1H), 7.10 – 7.04 (m, 3H), 3.39 (s, 3H), 2.26 (d, $J = 14.0$ Hz, 1H), 2.17 – 2.09 (m, 1H), 2.01 – 1.78 (m, 3H), 1.73 – 1.62 (m, 1H), 1.57 – 1.44 (m, 1H), 1.26 – 1.03 (m, 5H), 0.81 (t, $J = 7.0$ Hz, 3H).

$^{13}\text{C NMR}$ (101 MHz, $\text{DMSO}-d_6$) δ 200.3, 146.3, 145.3, 145.0, 129.4, 128.6, 127.2, 126.3, 124.0, 121.0, 113.0, 54.4, 42.0, 41.3, 32.5, 27.3, 27.2, 23.4, 19.4, 14.4.

HRMS(ESI) m/z calcd. for $C_{24}H_{30}NO$ $[M + H]^+$ 348.2322, found 348.2322.

HPLC (ChiralPak AD-H column), hexanes/*i*-PrOH = 70:30, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 4.910 min (major), t_R = 5.806 min (minor);

(S)-2-butyl-2-phenylcyclohexan-1-one (23)



23

Colorless oil, $[\alpha]_D^{20} = -80.5$ ($c=0.64$, CH_2Cl_2), $R_f = 0.8$ (petroleum ether/ethyl acetate = 10/1), 85 % yield, 92:8 e.r..

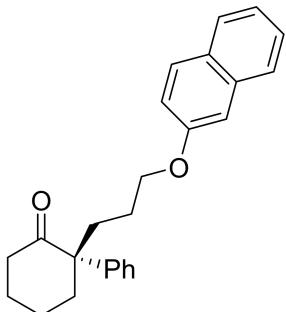
1H NMR (400 MHz, CDCl₃) δ 7.36 (t, $J = 7.6$ Hz, 2H), 7.25 (d, $J = 14.7$ Hz, 1H), 7.17 (d, $J = 7.8$ Hz, 2H), 2.78 – 2.72 (m, 1H), 2.40 – 2.24 (m, 2H), 1.98 – 1.92 (m, 1H), 1.82 – 1.60 (m, 6H), 1.26 – 1.13 (m, 2H), 1.13 – 1.00 (m, 1H), 0.80 (t, $J = 7.3$ Hz, 4H).

^{13}C NMR (101 MHz, CDCl₃) δ 213.9, 141.1, 128.7, 127.0, 126.5, 57.3, 40.2, 39.9, 35.0, 28.4, 25.8, 23.2, 21.7, 14.0.

HRMS(ESI) m/z calcd. for $C_{16}H_{23}O_3$ $[M + H]^+$ 231.1743, found 231.1743.

HPLC (ChiralPak IC-H column), hexanes/*i*-PrOH = 95:5, flow rate = 0.5 mL/min, λ = 220 nm, t_R = 11.106 min (major), t_R = 9.356 min (minor);

(R)-2-(3-(naphthalen-2-yloxy)propyl)-2-phenylcyclohexan-1-one (24)



24

Colorless oil, $[\alpha]_D^{20} = -87.8$ ($c=0.4$, CH_2Cl_2), $R_f = 0.5$ (petroleum ether/ethyl acetate = 10/1), 99 % yield, 94:6 e.r.

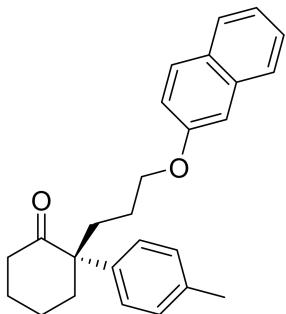
1H NMR (400 MHz, CDCl₃) δ 7.82 – 7.66 (m, 3H), 7.47 – 7.36 (m, 3H), 7.31 (dt, $J = 18.4, 7.5$ Hz, 2H), 7.23 (d, $J = 7.7$ Hz, 2H), 7.10 (dd, $J = 9.0, 2.5$ Hz, 1H), 7.05 (d, $J = 2.4$ Hz, 1H), 3.95 (td, $J = 6.7, 2.3$ Hz, 2H), 2.85 – 2.78 (m, 1H), 2.52 – 2.30 (m, 2H), 2.10 – 1.96 (m, 2H), 1.92 – 1.61 (m, 6H), 1.54 – 1.43 (m, 1H).

^{13}C NMR (101 MHz, CDCl₃) δ 213.6, 157.0, 140.6, 134.6, 129.3, 129.0, 128.9, 127.6, 127.0, 126.8, 126.8, 126.3, 123.5, 119.0, 106.6, 68.4, 57.1, 40.2, 36.7, 35.2, 28.4, 23.8, 21.7.

HRMS(ESI) m/z calcd. for $C_{25}H_{27}O_2$ $[M + H]^+$ 359.2006, found 359.2006.

HPLC (ChiralPak AD-H column), hexanes/*i*-PrOH = 95:5, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 12.934 min (major), t_R = 12.299 min (minor);

(R)-2-(3-(naphthalen-2-yloxy)propyl)-2-(p-tolyl)cyclohexan-1-one (25)



25

White solid, $[\alpha]_D^{20} = -69.2$ ($c=0.18$, CH_2Cl_2), $R_f = 0.6$ (petroleum ether/ethyl acetate = 10/1), 99 % yield, 91:9 e.r.

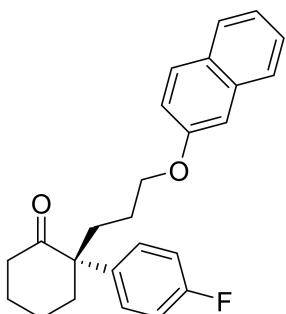
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.76 (d, $J = 8.1$ Hz, 1H), 7.70 (dd, $J = 8.4, 3.8$ Hz, 2H), 7.43 (t, $J = 7.5$ Hz, 1H), 7.33 (t, $J = 7.4$ Hz, 1H), 7.19 (d, $J = 7.8$ Hz, 2H), 7.10 (d, $J = 7.9$ Hz, 3H), 7.04 (s, 1H), 4.01 – 3.86 (m, 2H), 2.77 (d, $J = 12.9$ Hz, 1H), 2.49 – 2.26 (m, 5H), 2.08 – 1.91 (m, 2H), 1.90 – 1.60 (m, 6H), 1.48 (m, $J = 18.0, 11.8, 6.0$ Hz, 1H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 213.7, 157.0, 137.6, 136.4, 134.6, 129.7, 129.3, 128.9, 127.6, 126.9, 126.8, 126.6, 123.5, 119.0, 106.6, 68.4, 56.8, 40.1, 36.6, 35.2, 28.4, 23.8, 21.8, 21.0.

HRMS(ESI) m/z calcd. for $\text{C}_{26}\text{H}_{29}\text{O}_2$ [$\text{M} + \text{H}]^+$ 373.2162, found 373.2162.

HPLC (ChiralPak IBN5-H column), hexanes/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, $\lambda = 254$ nm, $t_R = 8.107$ min (major), $t_R = 8.986$ min (minor);

(R)-2-(4-fluorophenyl)-2-(3-(naphthalen-2-yloxy)propyl)cyclohexan-1-one (26)



26

White solid, $[\alpha]_D^{20} = -76.7$ ($c=1.26$, CH_2Cl_2), $R_f = 0.5$ (petroleum ether/ethyl acetate = 10/1), 93 % yield, 90:10 e.r.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.75 (d, $J = 8.1$ Hz, 1H), 7.70 (dd, $J = 7.7, 5.5$ Hz, 2H), 7.43 (t, $J = 7.5$ Hz, 1H), 7.32 (t, $J = 7.5$ Hz, 1H), 7.20 – 7.14 (m, 2H), 7.12 – 7.02 (m, 4H), 3.94 (t, $J = 6.3$ Hz, 2H), 2.72 (d, $J = 8.5$ Hz, 1H), 2.33 (s, 2H), 2.07 – 1.92 (m, 2H), 1.90 – 1.79 (m, 1H), 1.79 – 1.57 (m, 5H), 1.44 (m, $J = 12.2, 5.9$ Hz, 1H).

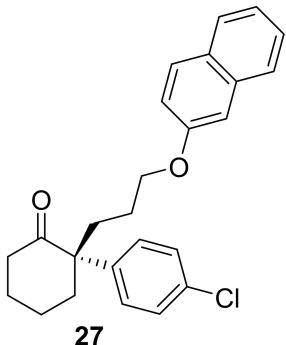
$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 213.2, 161.6 (d, $J = 246.2$ Hz), 156.9, 136.3 (d, $J = 3.3$ Hz), 134.6, 129.3, 128.9, 128.6 (d, $J = 7.8$ Hz), 127.6, 126.7 126.3, 123.5, 118.9, 115.8 (d, $J = 21.2$ Hz), 106.6, 68.2, 56.5, 40.1, 36.6, 35.3, 28.2, 23.7, 21.6.

$^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -115.8 (s, 1F).

HRMS(ESI) m/z calcd. for $\text{C}_{25}\text{H}_{26}\text{O}_2\text{F}$ [$\text{M} + \text{H}]^+$ 377.1911, found 377.1911.

HPLC (ChiralPak IBN5-H column), hexanes/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 10.003 min (major), t_R = 13.104 min (minor);

(*R*)-2-(4-chlorophenyl)-2-(3-(naphthalen-2-yloxy)propyl)cyclohexan-1-one (27)



Colorless oil, $[\alpha]_D^{20} = -71.7$ ($c=1.21$, CH_2Cl_2), $R_f = 0.6$ (petroleum ether/ethyl acetate = 10/1), 99 % yield, 89:11 e.r.

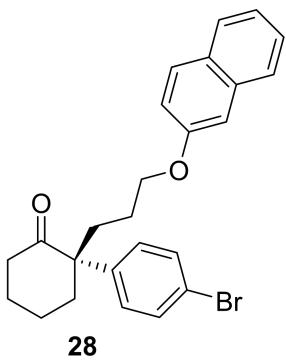
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.75 (d, $J = 8.1$ Hz, 1H), 7.73 – 7.66 (m, 2H), 7.42 (t, $J = 7.5$ Hz, 1H), 7.33 (dd, $J = 15.0, 7.8$ Hz, 3H), 7.13 (d, $J = 8.3$ Hz, 2H), 7.08 (d, $J = 9.0$ Hz, 1H), 7.03 (s, 1H), 3.93 (t, $J = 6.5$ Hz, 2H), 2.72 (d, $J = 8.2$ Hz, 1H), 2.33 (d, $J = 7.1$ Hz, 2H), 1.98 (td, $J = 13.3, 4.2$ Hz, 2H), 1.89 – 1.79 (m, 1H), 1.78 – 1.56 (m, 5H), 1.50 – 1.35 (m, 1H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 213.0, 156.8, 139.2, 134.6, 132.8, 129.3, 129.1, 128.9, 128.5, 127.6, 126.7, 126.3, 123.5, 118.9, 106.5, 68.2, 56.7, 40.1, 36.5, 35.1, 28.3, 23.7, 21.6.

HRMS(ESI) m/z calcd. for $\text{C}_{25}\text{H}_{26}\text{O}_2\text{Cl}$ [$\text{M} + \text{H}]^+$ 393.1616, found 393.1616.

HPLC (ChiralPak IBN5-H column), hexanes/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 11.181 min (major), t_R = 15.207 min (minor);

(*R*)-2-(4-bromophenyl)-2-(3-(naphthalen-2-yloxy)propyl)cyclohexan-1-one (28)



Colorless oil, $[\alpha]_D^{20} = -54.9$ ($c=1.07$, CH_2Cl_2), $R_f = 0.5$ (petroleum ether/ethyl acetate = 10/1), 77 % yield, 87:13 e.r.

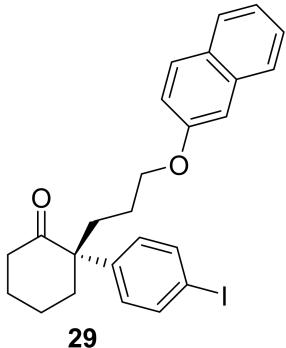
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.75 (d, $J = 8.1$ Hz, 1H), 7.70 (dd, $J = 8.4, 5.1$ Hz, 2H), 7.50 (d, $J = 8.3$ Hz, 2H), 7.42 (t, $J = 7.5$ Hz, 1H), 7.32 (t, $J = 7.4$ Hz, 1H), 7.07 (d, $J = 7.8$ Hz, 3H), 7.03 (s, 1H), 3.93 (t, $J = 6.5$ Hz, 2H), 2.78 – 2.65 (m, 1H), 2.33 (d, $J = 7.5$ Hz, 2H), 1.97 (td, $J = 13.0, 4.4$ Hz, 2H), 1.90 – 1.78 (m, 1H), 1.78 – 1.57 (m, 5H), 1.42 (ddt, $J = 18.5, 12.2, 6.1$ Hz, 1H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 213.0, 156.8, 139.7, 134.6, 132.1, 129.3, 128.9, 128.8, 127.6, 126.7, 126.3, 123.5, 120.9, 118.9, 106.5, 68.1, 56.8, 40.1, 36.4, 35.1, 28.3, 23.7, 21.6.

HRMS(ESI) m/z calcd. for $C_{25}H_{25}O_2K$ [M + K]⁺ 475.0670, found 475.0670.

HPLC (ChiralPak IBN5-H column), hexanes/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 12.785 min (major), t_R = 17.303 min (minor);

(*R*)-2-(4-iodophenyl)-2-(3-(naphthalen-2-yloxy)propyl)cyclohexan-1-one (29)



29

Colorless oil, $[\alpha]_D^{20} = -47.8$ (c=1.6, CH₂Cl₂), $R_f = 0.5$ (petroleum ether/ethyl acetate = 10/1), 99 % yield, 87:13 e.r.

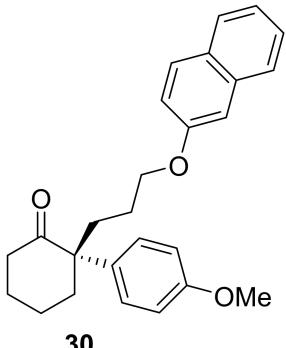
¹H NMR (400 MHz, CDCl₃) δ 7.79 – 7.65 (m, 5H), 7.43 (t, J = 7.5 Hz, 1H), 7.32 (t, J = 7.4 Hz, 1H), 7.08 (dd, J = 8.9, 2.0 Hz, 1H), 7.03 (s, 1H), 6.94 (d, J = 8.3 Hz, 2H), 3.93 (t, J = 6.5 Hz, 2H), 2.70 (d, J = 8.3 Hz, 1H), 2.32 (s, 2H), 1.97 (td, J = 13.1, 4.4 Hz, 2H), 1.89 – 1.77 (m, 1H), 1.76 – 1.56 (m, 5H), 1.42 (ddt, J = 18.6, 12.3, 6.2 Hz, 1H).

¹³C NMR (101 MHz, CDCl₃) δ 213.0, 156.8, 140.5, 138.0, 134.6, 129.3, 129.1, 128.9, 127.7, 126.8, 126.3, 123.5, 119.0, 106.5, 92.5, 68.2, 56.9, 40.2, 36.4, 35.0, 28.3, 23.7, 21.7.

HRMS(ESI) m/z calcd. for $C_{25}H_{26}O_2I$ [M + H]⁺ 485.0972, found 485.0968.

HPLC (ChiralPak IBN5-H column), hexanes/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 14.798 min (major), t_R = 18.983 min (minor);

(*R*)-2-(4-methoxyphenyl)-2-(3-(naphthalen-2-yloxy)propyl)cyclohexan-1-one (30)



30

Colorless oil, $[\alpha]_D^{20} = -85.3$ (c=1.35, CH₂Cl₂), $R_f = 0.4$ (petroleum ether/ethyl acetate = 10/1), 99 % yield, 93:7 e.r.

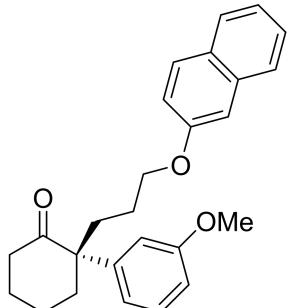
¹H NMR (400 MHz, CDCl₃) δ 7.75 (d, J = 8.0 Hz, 1H), 7.70 (dd, J = 8.0, 4.8 Hz, 2H), 7.42 (t, J = 7.4 Hz, 1H), 7.32 (t, J = 7.4 Hz, 1H), 7.10 (t, J = 9.1 Hz, 3H), 7.03 (s, 1H), 6.90 (d, J = 8.6 Hz, 2H), 3.93 (t, J = 5.8 Hz, 2H), 3.80 (s, 3H), 2.73 (d, J = 12.8 Hz, 1H), 2.40 (td, J = 13.0, 5.7 Hz, 1H), 2.30 (d, J = 13.2 Hz, 1H), 2.05 – 1.92 (m, 2H), 1.89 – 1.58 (m, 6H), 1.47 (dt, J = 12.1, 5.8 Hz, 1H).

^{13}C NMR (101 MHz, CDCl_3) δ 213.7, 158.3, 156.9, 134.6, 132.5, 129.2, 128.9, 128.1, 127.6, 126.7, 126.3, 123.5, 119.0, 114.3, 106.6, 68.4, 56.3, 55.3, 40.0, 36.6, 35.3, 28.4, 23.8, 21.7.

HRMS(ESI) m/z calcd. for $\text{C}_{26}\text{H}_{29}\text{O}_3$ [$\text{M} + \text{H}]^+$ 389.2111, found 389.2111.

HPLC (ChiralPak IBN5-H column), hexanes/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 13.099 min (major), t_R = 14.195 min (minor);

(*R*)-2-(3-methoxyphenyl)-2-(3-(naphthalen-2-yloxy)propyl)cyclohexan-1-one (31)



31

Colorless oil, $[\alpha]_D^{20} = -76.6$ ($c=1.24$, CH_2Cl_2), $R_f = 0.5$ (petroleum ether/ethyl acetate = 10/1), 99 % yield, 90:10 e.r.

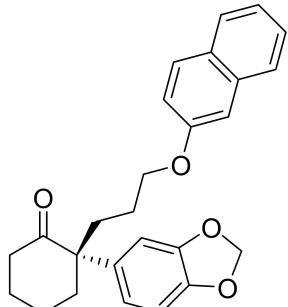
^1H NMR (400 MHz, CDCl_3) δ 7.74 (d, $J = 8.1$ Hz, 1H), 7.72 – 7.66 (m, 2H), 7.42 (t, $J = 7.4$ Hz, 1H), 7.30 (dd, $J = 16.0, 8.0$ Hz, 2H), 7.08 (d, $J = 9.0$ Hz, 1H), 7.03 (s, 1H), 6.86 – 6.73 (m, 3H), 3.93 (t, $J = 6.5$ Hz, 2H), 3.80 (s, 3H), 2.76 (d, $J = 13.0$ Hz, 1H), 2.40 (td, $J = 13.2, 5.8$ Hz, 1H), 2.32 (d, $J = 13.1$ Hz, 1H), 2.09 – 1.91 (m, 2H), 1.83 (t, $J = 13.1$ Hz, 2H), 1.78 – 1.60 (m, 4H), 1.48 (dt, $J = 12.3, 5.8$ Hz, 1H).

^{13}C NMR (101 MHz, CDCl_3) δ 213.4, 160.1, 156.9, 142.3, 134.6, 129.9, 129.3, 128.9, 127.6, 126.7, 126.2, 123.4, 119.4, 119.0, 113.4, 111.5, 106.5, 68.3, 57.1, 55.3, 40.3, 36.5, 35.3, 28.3, 23.8, 21.8.

HRMS(ESI) m/z calcd. for $\text{C}_{26}\text{H}_{29}\text{O}_3$ [$\text{M} + \text{H}]^+$ 389.2111, found 389.2111.

HPLC (ChiralPak AD-H column), hexanes/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 12.851 min (major), t_R = 11.813 min (minor);

(*R*)-2-(benzo[d][1,3]dioxol-5-yl)-2-(3-(naphthalen-2-yloxy)propyl)cyclohexan-1-one (32)



32

Colorless oil, $[\alpha]_D^{20} = -80.6$ ($c=1.40$, CH_2Cl_2), $R_f = 0.5$ (petroleum ether/ethyl acetate = 10/1), 99 % yield, 91:9 e.r.

^1H NMR (400 MHz, CDCl_3) δ 7.84 – 7.60 (m, 3H), 7.43 (t, $J = 7.5$ Hz, 1H), 7.32 (t, $J = 7.4$ Hz, 1H), 7.10 (dd, $J = 8.9, 1.8$ Hz, 1H), 7.04 (s, 1H), 6.81 (d, $J = 8.1$ Hz, 1H), 6.72 (s, 1H), 6.64 (d, $J =$

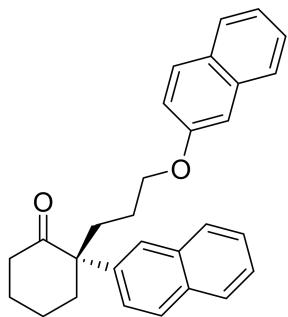
8.1 Hz, 1H), 5.95 (s, 2H), 3.94 (t, J = 6.6 Hz, 2H), 2.71 – 2.63 (m, 1H), 2.48 – 2.35 (m, 1H), 2.30 (d, J = 13.2 Hz, 1H), 2.05 – 1.93 (m, 2H), 1.90 – 1.57 (m, 6H), 1.55 – 1.40 (m, 1H).

^{13}C NMR (101 MHz, CDCl_3) δ 213.5, 156.9, 148.3, 146.3, 134.6, 134.4, 129.3, 128.9, 127.6, 126.8, 126.3, 123.5, 120.3, 119.0, 108.6, 107.4, 106.5, 101.2, 68.3, 56.7, 40.0, 36.6, 35.4, 28.3, 23.7, 21.7.

HRMS(ESI) m/z calcd. for $\text{C}_{26}\text{H}_{27}\text{O}_4$ [$\text{M} + \text{H}$]⁺ 403.1904, found 403.1904.

HPLC (ChiralPak IBN5-H column), hexanes/*i*-PrOH = 98:2, flow rate = 1.0 mL/min, λ = 220 nm, t_R = 33.523 min (major), t_R = 36.183 min (minor);

(*R*)-2-(naphthalen-2-yl)-2-(3-(naphthalen-2-yloxy)propyl)cyclohexan-1-one (33)



33

White solid, $[\alpha]_D^{20} = -76.6$ ($c=1.52$, CH_2Cl_2), $R_f = 0.5$ (petroleum ether/ethyl acetate = 10/1), 99 % yield, 91:9 e.r.

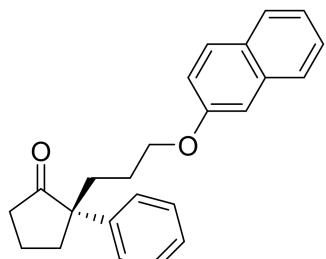
^1H NMR (400 MHz, CDCl_3) δ 7.87 (t, J = 6.7 Hz, 3H), 7.78 – 7.64 (m, 4H), 7.57 – 7.48 (m, 2H), 7.42 (t, J = 7.5 Hz, 1H), 7.32 (t, J = 7.6 Hz, 2H), 7.11 – 7.05 (m, 1H), 7.01 (s, 1H), 4.11 – 3.75 (m, 2H), 2.95 (d, J = 11.8 Hz, 1H), 2.48 – 2.34 (m, 2H), 2.14 (td, J = 13.2, 4.0 Hz, 1H), 1.97 (dd, J = 15.1, 7.0 Hz, 2H), 1.94 – 1.65 (m, 5H), 1.57 – 1.38 (m, 1H).

^{13}C NMR (101 MHz, CDCl_3) δ 213.7, 156.9, 138.1, 134.6, 133.6, 132.3, 129.3, 128.9, 128.8, 128.0, 127.6, 127.6, 126.8, 126.4, 126.3, 126.1, 126.02, 125.0, 123.5, 119.0, 106.5, 68.3, 57.3, 40.4, 36.5, 35.3, 28.5, 23.9, 21.9.

HRMS(ESI) m/z calcd. for $\text{C}_{29}\text{H}_{29}\text{O}_2$ [$\text{M} + \text{H}$]⁺ 409.2162, found 409.2162.

HPLC (ChiralPak AD-H column), hexanes/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 13.955 min (major), t_R = 16.238 min (minor);

(*R*)-2-(3-(naphthalen-2-yloxy)propyl)-2-phenylcyclopentan-1-one (34)



34

Colorless oil, $[\alpha]_D^{20} = -11.3$ ($c=1.27$, CH_2Cl_2), $R_f = 0.4$ (petroleum ether/ethyl acetate = 10/1), 89 % yield, 95:5 e.r.

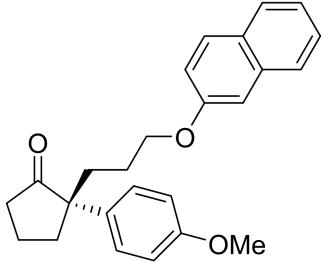
¹H NMR (400 MHz, CDCl₃) δ 7.78 – 7.67 (m, 3H), 7.44 (dd, *J* = 15.1, 7.6 Hz, 3H), 7.39 – 7.30 (m, 3H), 7.26 (t, *J* = 7.2 Hz, 1H), 7.09 (d, *J* = 9.0 Hz, 1H), 7.04 (s, 1H), 3.95 (t, *J* = 6.4 Hz, 2H), 2.69 (dd, *J* = 10.3, 4.6 Hz, 1H), 2.41 – 2.24 (m, 2H), 2.18 – 1.94 (m, 3H), 1.93 – 1.79 (m, 2H), 1.75 – 1.56 (m, 2H).

¹³C NMR (101 MHz, CDCl₃) δ 219.5, 156.9, 139.1, 134.6, 129.3, 128.9, 128.7, 127.6, 126.9, 126.9, 126.7, 126.3, 123.5, 118.9, 106.6, 68.0, 56.5, 37.5, 35.4, 34.0, 24.8, 18.7.

HRMS(ESI) *m/z* calcd. for C₂₄H₂₅O₂ [M + H]⁺345.1849, found 345.1849.

HPLC (ChiralPak AD-H column), hexanes/*i*-PrOH = 95:5, flow rate = 1.0 mL/min, λ = 254 nm, *t_R* = 15.461 min (major), *t_R* = 14.791 min (minor);

(R)-2-(4-methoxyphenyl)-2-(3-(naphthalen-2-yloxy)propyl)cyclopentan-1-one (35)



35

Colorless oil, $[\alpha]_D^{20} = -18.3$ (c=1.26, CH₂Cl₂), *R_f* = 0.4 (petroleum ether/ethyl acetate = 10/1), 96 % yield, 94:6 e.r.

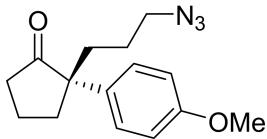
¹H NMR (400 MHz, CDCl₃) δ 7.76 (d, *J* = 8.1 Hz, 1H), 7.72 (t, *J* = 7.8 Hz, 2H), 7.44 (t, *J* = 7.5 Hz, 1H), 7.35 (dd, *J* = 17.8, 8.0 Hz, 3H), 7.11 (d, *J* = 8.9 Hz, 1H), 7.04 (s, 1H), 6.90 (d, *J* = 8.6 Hz, 2H), 3.95 (t, *J* = 6.4 Hz, 2H), 3.79 (s, 3H), 2.65 (dd, *J* = 9.7, 4.6 Hz, 1H), 2.42 – 2.18 (m, 2H), 2.16 – 1.93 (m, 3H), 1.83 (ddd, *J* = 17.7, 14.3, 6.6 Hz, 2H), 1.72 – 1.55 (m, 2H).

¹³C NMR (101 MHz, CDCl₃) δ 219.7, 158.5, 156.9, 134.6, 130.7, 129.3, 128.9, 128.1, 127.7, 126.7, 126.3, 123.5, 119.0, 114.0, 106.5, 68.0, 55.8, 55.3, 37.4, 35.3, 34.0, 24.7, 18.7.

HRMS(ESI) *m/z* calcd. for C₂₅H₂₇O₃ [M + H]⁺375.1955, found 375.1955.

HPLC (ChiralPak IBN5-H column), hexanes/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, λ = 254 nm, *t_R* = 17.799 min (major), *t_R* = 16.184 min (minor);

(R)-2-(3-azidopropyl)-2-(4-methoxyphenyl)cyclopentan-1-one (36)



36

Colorless oil, $[\alpha]_D^{20} = -71.4$ (c=0.44, CH₂Cl₂), *R_f* = 0.35 (petroleum ether/ethyl acetate = 10/1), 63 % yield, 95:5 e.r.

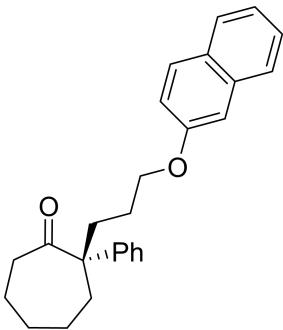
¹H NMR (400 MHz, CDCl₃) δ 7.29 (d, *J* = 8.8 Hz, 2H), 6.87 (d, *J* = 8.9 Hz, 2H), 3.79 (s, 3H), 3.14 (t, *J* = 6.9 Hz, 2H), 2.66 – 2.56 (m, 1H), 2.36 – 2.18 (m, 2H), 2.02 – 1.88 (m, 3H), 1.84 – 1.74 (m, 1H), 1.68 – 1.56 (m, 1H), 1.46 – 1.29 (m, 2H).

^{13}C NMR (101 MHz, CDCl_3) δ 219.3, 158.6, 130.4, 127.9, 114.1, 55.6, 55.2, 51.6, 37.2, 36.0, 34.0, 24.4, 18.6.

HRMS(ESI) m/z calcd. for $\text{C}_{15}\text{H}_{19}\text{N}_3\text{O}_2\text{Na} [\text{M} + \text{Na}]^+$ 296.1370, found 296.1369.

HPLC (ChiralPak IC-H column), hexanes/*i*-PrOH = 95:5, flow rate = 0.5 mL/min, λ = 254 nm, t_R = 19.324 min (major), t_R = 16.081 min (minor);

(*R*)-2-(3-(naphthalen-2-yloxy)propyl)-2-phenylcycloheptan-1-one (37)



37

White solid, $[\alpha]_D^{20} = -62.6$ ($c=1.2$, CH_2Cl_2), $R_f = 0.35$ (petroleum ether/ethyl acetate = 10/1), 91 % yield, 89:11 e.r.

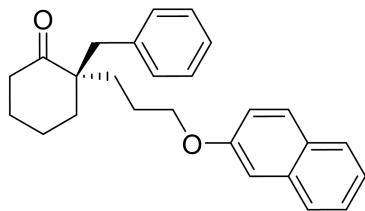
^1H NMR (400 MHz, CDCl_3) δ 7.75 (d, $J = 8.1$ Hz, 1H), 7.73 – 7.67 (m, 2H), 7.42 (t, $J = 7.4$ Hz, 1H), 7.38 – 7.30 (m, 3H), 7.25 (dd, $J = 16.4, 7.7$ Hz, 3H), 7.09 (dd, $J = 8.9, 1.4$ Hz, 1H), 7.03 (s, 1H), 3.92 (t, $J = 6.5$ Hz, 2H), 2.53 (t, $J = 11.6$ Hz, 1H), 2.41 – 2.28 (m, 2H), 2.27 – 2.10 (m, 2H), 1.94 (dd, $J = 13.8, 7.8$ Hz, 1H), 1.84 (t, $J = 10.3$ Hz, 3H), 1.73 – 1.51 (m, 2H), 1.43 (dt, $J = 11.8, 9.4$ Hz, 2H), 1.30 (t, $J = 12.0$ Hz, 1H).

^{13}C NMR (101 MHz, CDCl_3) δ 214.3, 156.9, 142.1, 134.6, 129.3, 128.9, 128.7, 127.6, 126.9, 126.9, 126.7, 126.3, 123.5, 119.0, 106.6, 68.3, 58.8, 40.9, 33.4, 32.5, 30.6, 27.0, 24.4, 24.2.

HRMS(ESI) m/z calcd. for $\text{C}_{26}\text{H}_{29}\text{O}_2 [\text{M} + \text{H}]^+$ 373.2162, found 373.2162.

HPLC (ChiralPak IC-H column), hexanes/*i*-PrOH = 95:5, flow rate = 0.5 mL/min, λ = 254 nm, t_R = 19.324 min (major), t_R = 16.081 min (minor);

(*S*)-2-benzyl-2-(3-(naphthalen-2-yloxy)propyl)cyclohexan-1-one (38)



38

Colorless oil, $[\alpha]_D^{20} = 17.5$ ($c=0.4$, CH_2Cl_2), $R_f = 0.3$ (petroleum ether/ethyl acetate = 20/1), 95 % yield, 93:7 e.r.

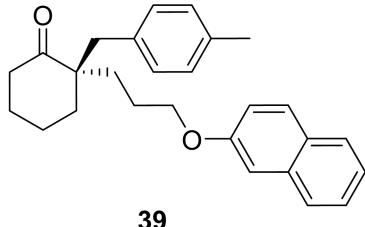
^1H NMR (400 MHz, CDCl_3) δ 7.80 – 7.70 (m, 3H), 7.47–7.43 (m, 1H), 7.36 – 7.32 (m, 1H), 7.30 – 7.27 (m, 2H), 7.25 – 7.21 (m, 1H), 7.17 – 7.12 (m, 4H), 4.06 (t, $J = 5.9$ Hz, 2H), 3.02 (d, $J = 13.8$ Hz, 1H), 2.91 (d, $J = 13.8$ Hz, 1H), 2.51 – 2.47 (m, 2H), 2.04 – 1.60 (m, 10H).

^{13}C NMR (101 MHz, CDCl_3) δ 214.8, 156.9, 137.7, 134.6, 130.7, 129.4, 129.0, 128.0, 127.7, 126.8, 126.4, 126.3, 123.6, 118.9, 106.6, 67.9, 52.3, 40.3, 39.6, 36.4, 30.8, 27.1, 23.9, 20.9.

HRMS(ESI) m/z calcd. for $\text{C}_{26}\text{H}_{29}\text{O}_2$ [$\text{M} + \text{H}]^+$ 373.2162, found 373.2163.

HPLC (ChiralPak IC-H column), hexanes/*i*-PrOH = 95:5, flow rate = 1.0 mL/min, λ = 220 nm, t_R = 13.716 min (minor), t_R = 16.879 min (major);

(*S*)-2-(4-methylbenzyl)-2-(3-(naphthalen-2-yloxy)propyl)cyclohexan-1-one (39)



Colorless oil, $[\alpha]_D^{20} = 20.8$ ($c=0.4$, CH_2Cl_2), $R_f = 0.4$ (petroleum ether/ethyl acetate= 10/1), 83 % yield, 91:9 e.r.

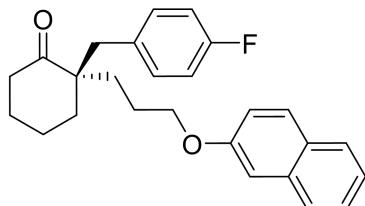
^1H NMR (400 MHz, CDCl_3) δ 7.82 – 7.71 (m, 3H), 7.46 (ddd, $J = 8.1, 6.9, 1.3$ Hz, 1H), 7.35 (ddd, $J = 8.1, 6.9, 1.2$ Hz, 1H), 7.17 (dd, $J = 8.9, 2.5$ Hz, 1H), 7.13 (d, $J = 2.5$ Hz, 1H), 7.10 (d, $J = 7.9$ Hz, 2H), 7.05 (d, $J = 8.1$ Hz, 2H), 4.10 – 4.02 (m, 2H), 2.99 (d, $J = 13.9$ Hz, 1H), 2.87 (d, $J = 13.9$ Hz, 1H), 2.53 – 2.41 (m, 2H), 2.35 (s, 3H), 2.02 – 1.89 (m, 2H), 1.88 – 1.75 (m, 4H), 1.73 – 1.69 (m, 2H), 1.68 – 1.59 (m, 2H).

^{13}C NMR (101 MHz, CDCl_3) δ 214.9, 156.9, 135.8, 134.6, 134.5, 130.5, 129.4, 129.0, 128.8, 127.7, 126.8, 126.4, 123.6, 119.0, 106.6, 68.0, 52.3, 40.0, 39.6, 36.3, 30.8, 27.1, 23.9, 21.1, 20.9.

HRMS(ESI) m/z calcd. for $\text{C}_{27}\text{H}_{31}\text{O}_2$ [$\text{M} + \text{H}]^+$ 387.2319, found 387.2316.

HPLC (Chiralcel OD-H column), hexanes/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, λ = 220 nm, t_R = 13.630 min (minor), t_R = 18.290 min (major);

(*S*)-2-(4-fluorobenzyl)-2-(3-(naphthalen-2-yloxy)propyl)cyclohexan-1-one (40)



Colorless oil, $[\alpha]_D^{20} = 22.8$ ($c=0.4$, CH_2Cl_2), $R_f = 0.3$ (petroleum ether/ethyl acetate= 10/1), 94 % yield, 94:6 e.r.

^1H NMR (400 MHz, CDCl_3) δ 7.76 (q, $J = 8.8$ Hz, 3H), 7.49 – 7.41 (m, 1H), 7.36 – 7.33 (m, 1H), 7.16-7.09 (m, 4H), 7.00 – 6.92 (m, 2H), 4.06 (t, $J = 5.6$ Hz, 2H), 2.98 – 2.85 (m, 2H), 2.53 – 2.42 (m, 2H), 2.03 – 1.54 (m, 10H).

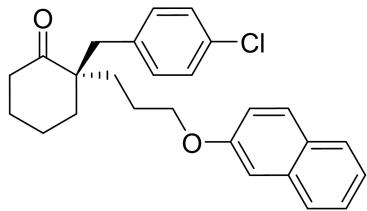
^{13}C NMR (101 MHz, CDCl_3) δ 214.6, 161.6 (d, $J = 244.4$ Hz), 156.8, 134.6, 133.3 (d, $J = 3.3$ Hz), 132.0 (d, $J = 7.7$ Hz), 129.4, 129.0, 127.7, 126.7, 126.4, 123.6, 118.9, 114.8 (d, $J = 21.0$ Hz), 106.5, 77.3, 67.8, 52.2, 39.5, 39.5, 36.3, 31.0, 27.0, 23.8, 20.8.

^{19}F NMR (376 MHz, CDCl_3) δ -116.89 (s, 1F).

HRMS(ESI) m/z calcd. for $\text{C}_{26}\text{H}_{28}\text{FO}_2$ [$\text{M} + \text{H}]^+$ 391.2068, found 391.2068.

HPLC (Chiralcel OD-H column), hexanes/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 15.070 min (minor), t_R = 18.630 min (major);

(S)-2-(4-chlorobenzyl)-2-(3-(naphthalen-2-yloxy)propyl)cyclohexan-1-one (41)



41

Colorless oil, $[\alpha]_D^{20}$ = 20.8 (c=0.4, CH₂Cl₂), R_f = 0.3 (petroleum ether/ethyl acetate= 10/1), 89 % yield, 92:8 e.r.

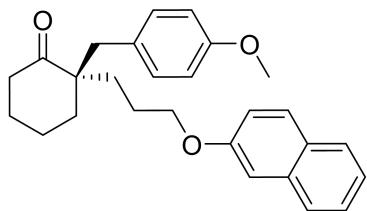
¹H NMR (400 MHz, CDCl₃) δ 7.81 – 7.69 (m, 3H), 7.44 (t, J = 7.5 Hz, 1H), 7.34 (t, J = 7.5 Hz, 1H), 7.23 (d, J = 8.0 Hz, 2H), 7.16 – 7.04 (m, 4H), 4.05 (t, J = 5.3 Hz, 2H), 2.91 (s, 2H), 2.55 – 2.39 (m, 2H), 2.02 – 1.54 (m, 10H).

¹³C NMR (101 MHz, CDCl₃) δ 214.5, 156.8, 136.2, 134.6, 132.2, 132.0, 129.4, 129.0, 128.1, 127.7, 126.7, 126.4, 123.6, 118.9, 106.5, 67.8, 52.2, 39.6, 39.5, 36.3, 31.0, 27.0, 23.8, 20.8.

HRMS(ESI) *m/z* calcd. for C₂₆H₂₈ClO₂ [M + H]⁺ 407.1772, found 407.1772.

HPLC (Chiralcel OD-H column), hexanes/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, λ = 220 nm, t_R = 16.192 min (minor), t_R = 21.095 min (major);

(S)-2-(4-methoxybenzyl)-2-(3-(naphthalen-2-yloxy)propyl)cyclohexan-1-one (42)



42

Colorless oil, $[\alpha]_D^{20}$ = 15.5 (c=0.4, CH₂Cl₂), R_f = 0.3 (petroleum ether/ethyl acetate= 10/1), 80 % yield, 92:8 e.r.

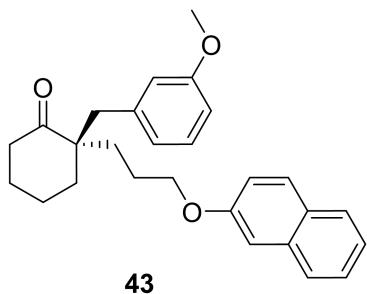
¹H NMR (400 MHz, CDCl₃) δ 7.81 – 7.70 (m, 3H), 7.45 (ddd, J = 8.1, 6.8, 1.3 Hz, 1H), 7.34 (ddd, J = 8.1, 6.9, 1.2 Hz, 1H), 7.19 – 7.10 (m, 2H), 7.10 – 7.03 (m, 2H), 6.85 – 6.79 (m, 2H), 4.06 (t, J = 5.9 Hz, 2H), 3.79 (s, 3H), 2.95 (d, J = 14.0 Hz, 1H), 2.85 (d, J = 14.0 Hz, 1H), 2.55 – 2.45 (m, 2H), 2.04 – 1.58 (m, 10H).

¹³C NMR (101 MHz, CDCl₃) δ 214.9, 158.2, 156.9, 134.6, 131.5, 129.6, 129.0, 127.7, 126.8, 126.4, 123.6, 118.9, 113.4, 106.6, 77.3, 68.0, 55.2, 52.3, 39.6, 39.5, 36.2, 30.9, 27.0, 23.8, 20.9.

HRMS(ESI) *m/z* calcd. for C₂₇H₃₁O₃ [M + H]⁺ 403.2268, found 403.2269.

HPLC (Chiralcel OD-H column), hexanes/*i*-PrOH = 80:20, flow rate = 1.0 mL/min, λ = 220 nm, t_R = 12.598 min (minor), t_R = 18.694 min (major);

(S)-2-(3-methoxybenzyl)-2-(3-(naphthalen-2-yloxy)propyl)cyclohexan-1-one (43)



Colorless oil, $[\alpha]_D^{20} = 16.3$ ($c=0.4$, CH_2Cl_2), $R_f = 0.3$ (petroleum ether/ethyl acetate = 10/1), 75 % yield, 92:8 e.r.

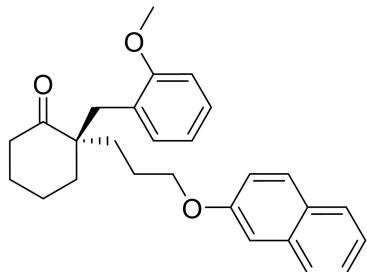
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.81 – 7.70 (m, 3H), 7.44 (ddd, $J = 8.3, 6.8, 1.3$ Hz, 1H), 7.34 (ddd, $J = 8.1, 6.9, 1.2$ Hz, 1H), 7.23 – 7.14 (m, 2H), 7.12 (d, $J = 2.5$ Hz, 1H), 6.82 – 6.71 (m, 3H), 4.06 (t, $J = 5.7$ Hz, 2H), 3.80 (s, 3H), 2.98 (d, $J = 13.8$ Hz, 1H), 2.89 (d, $J = 13.8$ Hz, 1H), 2.51 – 2.46 (m, 2H), 2.04 – 1.53 (m, 10H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 214.8, 159.3, 156.9, 139.3, 134.6, 129.4, 129.0, 128.9, 127.7, 126.8, 126.4, 123.6, 123.1, 119.0, 116.8, 111.3, 106.5, 67.9, 55.1, 52.3, 40.3, 39.5, 36.5, 30.9, 27.1, 23.9, 20.9.

HRMS(ESI) m/z calcd. for $\text{C}_{27}\text{H}_{31}\text{O}_3$ $[\text{M} + \text{H}]^+$ 403.2268, found 403.2263.

HPLC (Chiralcel OD-H column), hexanes/*i*-PrOH = 80:20, flow rate = 1.0 mL/min, $\lambda = 220$ nm, $t_R = 16.423$ min (minor), $t_R = 33.363$ min (major);

(*S*)-2-(2-methoxybenzyl)-2-(3-(naphthalen-2-yloxy)propyl)cyclohexan-1-one (44)



Colorless oil, $[\alpha]_D^{20} = -14.5$ ($c=0.06$, CH_2Cl_2), $R_f = 0.3$ (petroleum ether/ethyl acetate = 10/1), 81 % yield, 90:10 e.r.

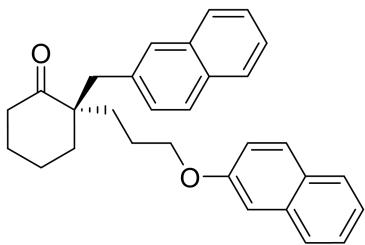
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.80 – 7.69 (m, 3H), 7.45 (m, 1H), 7.38 – 7.30 (m, 1H), 7.24 – 7.19 (m, 1H), 7.17 – 7.04 (m, 3H), 6.93 – 6.79 (m, 2H), 4.11 – 3.96 (m, 2H), 3.75 (s, 3H), 3.27 (d, $J = 13.7$ Hz, 1H), 2.82 (d, $J = 13.7$ Hz, 1H), 2.72 – 2.60 (m, 1H), 2.49 – 2.42 (m, 1H), 2.05 – 1.56 (m, 10H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 214.9, 158.0, 157.0, 134.6, 132.4, 129.4, 128.9, 127.7, 127.7, 126.8, 126.3, 126.2, 123.5, 120.1, 119.0, 110.3, 106.5, 68.3, 54.9, 52.5, 39.5, 36.5, 34.8, 30.8, 27.1, 23.9, 21.1.

HRMS(ESI) m/z calcd. for $\text{C}_{27}\text{H}_{31}\text{O}_3$ $[\text{M} + \text{H}]^+$ 403.2268, found 403.2268.

HPLC (ChiralPak AD-H column), hexanes/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, $\lambda = 254$ nm, $t_R = 9.955$ min (major), $t_R = 11.554$ min (minor);

(*S*)-2-(naphthalen-2-ylmethyl)-2-(3-(naphthalen-2-yloxy)propyl)cyclohexan-1-one (45)



45

Colorless oil, $[\alpha]_D^{20} = 32.8$ ($c=0.4$, CH_2Cl_2), $R_f = 0.4$ (petroleum ether/ethyl acetate = 10/1), 93 % yield, 95:5 e.r.

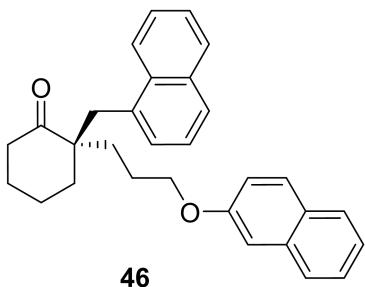
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.89 – 7.71 (m, 6H), 7.63 (s, 1H), 7.54 – 7.40 (m, 3H), 7.40 – 7.26 (m, 2H), 7.21 – 7.11 (m, 2H), 4.08 (t, $J = 5.7$ Hz, 2H), 3.14 (s, 2H), 2.54 – 2.49 (m, 2H), 2.10 – 2.01 (m, 1H), 2.00 – 1.84 (m, 2H), 1.86 – 1.60 (m, 7H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 214.8, 156.9, 135.5, 134.6, 133.3, 132.2, 129.4, 129.2, 129.0, 127.7, 127.7, 127.6, 127.4, 126.8, 126.4, 126.0, 125.5, 123.6, 119.0, 106.7, 77.3, 68.0, 52.6, 40.5, 39.6, 36.4, 31.2, 27.0, 24.0, 20.9.

HRMS(ESI) m/z calcd. for $\text{C}_{30}\text{H}_{30}\text{O}_2\text{Na}$ [$\text{M} + \text{Na}]^+$ 445.2138, found 445.2140.

HPLC (ChiralPak IC-H column), hexanes/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, $\lambda = 220$ nm, $t_R = 12.524$ min (minor), $t_R = 14.345$ min (major);

(*S*)-2-(naphthalen-1-ylmethyl)-2-(3-(naphthalen-2-yloxy)propyl)cyclohexan-1-one (46)



46

Colorless oil, $[\alpha]_D^{20} = 35.2$ ($c=0.4$, CH_2Cl_2), $R_f = 0.4$ (petroleum ether/ethyl acetate= 10/1), 65 % yield, 95:5 e.r.

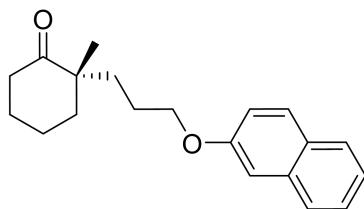
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.12 (d, $J = 8.2$ Hz, 1H), 7.86 (dd, $J = 7.6, 1.9$ Hz, 1H), 7.76 (q, $J = 8.6, 8.1$ Hz, 4H), 7.56 – 7.39 (m, 5H), 7.35 (t, $J = 7.4$ Hz, 1H), 7.19 – 7.10 (m, 2H), 4.06 (tt, $J = 8.8, 4.5$ Hz, 2H), 3.64 (d, $J = 14.4$ Hz, 1H), 3.33 (d, $J = 14.5$ Hz, 1H), 2.56-2.41 (m, 2H), 2.14 – 1.54 (m, 10H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 214.9, 156.9, 134.7, 134.6, 133.9, 133.5, 129.4, 129.0, 128.9, 128.8, 127.7, 127.1, 126.8, 126.4, 125.7, 125.3, 125.3, 124.5, 123.6, 118.9, 106.6, 67.9, 53.4, 39.7, 35.8, 34.9, 31.9, 26.6, 24.1, 20.8.

HRMS(ESI) m/z calcd. for $\text{C}_{30}\text{H}_{30}\text{O}_2\text{Na}$ [$\text{M} + \text{Na}]^+$ 445.2138, found 445.2137.

HPLC (ChiralPak IC-H column), hexanes/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, $\lambda = 220$ nm, $t_R = 10.335$ min (minor), $t_R = 13.483$ min (major);

(*S*)-2-methyl-2-(3-(naphthalen-2-yloxy)propyl)cyclohexan-1-one (47)



47

Colorless oil, $[\alpha]_D^{20} = 15.5$ ($c=0.4$, CH_2Cl_2), $R_f = 0.3$ (petroleum ether/ethyl acetate = 10/1), 59 % yield, 67:33 e.r.

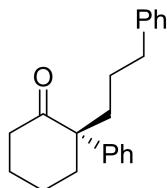
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.80 – 7.71 (m, 3H), 7.48–7.41 (m, 1H), 7.35–7.30 (m, 1H), 7.18 – 7.10 (m, 2H), 4.12 – 4.00 (m, 2H), 2.51 – 2.33 (m, 2H), 1.99 – 1.56 (m, 10H), 1.13 (s, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 215.9, 156.9, 134.6, 129.4, 128.9, 127.7, 126.7, 126.3, 123.6, 119.0, 106.6, 68.1, 48.4, 39.3, 38.8, 34.0, 27.6, 23.9, 22.6, 21.1.

HRMS(ESI) m/z calcd. for $\text{C}_{20}\text{H}_{25}\text{O}_2$ [$\text{M} + \text{H}]^+$ 297.1849, found 297.1852.

HPLC (ChiralPak IC-H column), hexanes/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, $\lambda = 254$ nm, $t_R = 9.599$ min (major), $t_R = 10.765$ min (minor);

(*R*)-2-phenyl-2-(3-phenylpropyl)cyclohexan-1-one (48)



48

Colorless oil, $[\alpha]_D^{20} = -140.1$ ($c=1.0$, CH_2Cl_2), $R_f = 0.4$ (petroleum ether/dichloromethane = 1/1), 99 % yield, 94:6 e.r.

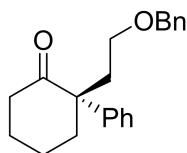
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.40 (t, $J = 7.6$ Hz, 2H), 7.29 (d, $J = 9.1$ Hz, 3H), 7.20 (d, $J = 7.5$ Hz, 3H), 7.12 (d, $J = 7.3$ Hz, 2H), 2.78 (d, $J = 13.7$ Hz, 1H), 2.53 (d, $J = 8.0$ Hz, 2H), 2.44–2.31 (m, 2H), 2.07 – 1.64 (m, 7H), 1.59 – 1.43 (m, 1H), 1.38 – 1.20 (m, 1H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 213.7, 142.5, 140.9, 128.8, 128.4, 128.2, 127.0, 126.6, 125.6, 57.3, 40.2, 40.0, 36.4, 35.0, 28.9, 25.6, 21.7.

HRMS(ESI) m/z calcd. for $\text{C}_{21}\text{H}_{25}\text{O}$ [$\text{M} + \text{H}]^+$ 293.1900, found 293.1899.

HPLC (ChiralPak AD-H column), hexanes/*i*-PrOH = 98:2, flow rate = 0.5 mL/min, $\lambda = 220$ nm, $t_R = 12.317$ min (major), $t_R = 13.442$ min (minor);

(*R*)-2-(2-(benzyloxy)ethyl)-2-phenylcyclohexan-1-one (49)



49

Colorless oil, $[\alpha]_D^{20} = -147.2$ ($c=0.98$, CH_2Cl_2), $R_f = 0.3$ (petroleum ether/dichloromethane = 1/1), 89 % yield, 94:6 e.r.

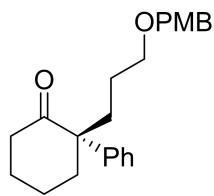
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.37–7.31 (m, 4H), 7.28–7.24 (m, 4H), 7.16 (d, $J = 7.6$ Hz, 2H), 4.35 (q, $J = 11.9$ Hz, 2H), 3.36–3.31 (m, 1H), 3.26–3.20 (m, 1H), 2.84 (d, $J = 10.4$ Hz, 1H), 2.44 – 2.26 (m, 2H), 2.21–2.14 (m, 1H), 2.07–1.99 (m, 1H), 1.97–1.92 (m, 1H), 1.80–1.68 (m, 4H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 213.2, 140.5, 138.5, 128.9, 128.3, 127.5, 127.4, 126.9, 126.8, 72.7, 67.0, 56.8, 40.0, 39.4, 36.0, 28.4, 21.6.

HRMS(ESI) m/z calcd. for $\text{C}_{21}\text{H}_{25}\text{O}_2$ [$\text{M} + \text{H}]^+$ 309.1849, found 309.1849.

HPLC (ChiralPak IF column), hexanes/*i*-PrOH = 98:2, flow rate = 1.0 mL/min, $\lambda = 220$ nm, $t_R = 11.453$ min (minor), $t_R = 13.130$ min (major);

(*R*)-2-(3-((4-methoxybenzyl)oxy)propyl)-2-phenylcyclohexan-1-one (50)



50

Colorless oil, $[\alpha]_D^{20} = -100.8$ ($c=1.18$, CH_2Cl_2), $R_f = 0.3$ (petroleum ether/ethyl acetate = 10/1), 88 % yield, 93:7 e.r.

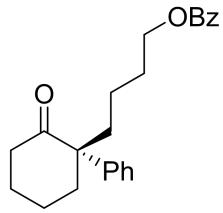
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.33 (t, $J = 7.6$ Hz, 2H), 7.24–7.13 (m, 5H), 6.84 (dd, $J = 8.8, 3.1$ Hz, 2H), 4.32 (s, 2H), 3.78 (s, 3H), 3.34–3.27 (m, 2H), 2.76–2.70 (m, 1H), 2.41 – 2.23 (m, 2H), 1.96–1.90 (m, 1H), 1.88 – 1.60 (m, 6H), 1.46–1.35 (m, 1H), 1.24–1.14 (m, 1H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 213.6, 159.1, 140.7, 130.6, 129.3, 128.8, 127.0, 126.7, 113.7, 72.5, 70.6, 57.1, 55.3, 40.2, 36.6, 35.1, 28.4, 24.1, 21.7.

HRMS(ESI) m/z calcd. for $\text{C}_{23}\text{H}_{29}\text{O}_3$ [$\text{M} + \text{H}]^+$ 353.2111, found 353.2112.

HPLC (ChiralPak AS-H column), hexanes/*i*-PrOH = 95:5, flow rate = 1.0 mL/min, $\lambda = 220$ nm, $t_R = 8.951$ min (minor), $t_R = 12.995$ min (major);

(*R*)-4-(2-oxo-1-phenylcyclohexyl)butyl benzoate (51)



51

Colorless oil, $[\alpha]_D^{20} = -108.5$ ($c=1.08$, CH_2Cl_2), $R_f = 0.3$ (petroleum ether/dichloromethane = 1/1), 87 % yield, 92:8 e.r.

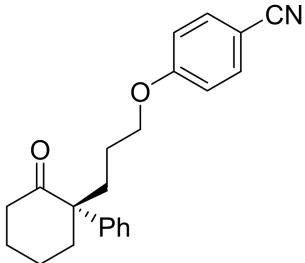
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.97 – 7.90 (m, 2H), 7.58 – 7.49 (m, 1H), 7.41 (dd, $J = 8.4, 7.0$ Hz, 2H), 7.33 (dd, $J = 8.3, 7.0$ Hz, 2H), 7.25 – 7.19 (m, 1H), 7.18 – 7.12 (m, 2H), 4.19 (td, $J = 6.6, 1.5$ Hz, 2H), 2.78 – 2.69 (m, 1H), 2.41 – 2.22 (m, 2H), 2.04 – 1.55 (m, 9H), 1.31 – 1.16 (m, 1H), 1.10 – 0.94 (m, 1H).

^{13}C NMR (101 MHz, CDCl_3) δ 213.6, 166.6, 140.8, 132.7, 130.5, 129.5, 128.8, 128.3, 126.9, 126.7, 64.7, 57.3, 40.2, 39.8, 35.1, 29.1, 28.4, 21.7, 20.1.

HRMS(ESI) m/z calcd. for $\text{C}_{23}\text{H}_{26}\text{O}_3\text{Na} [\text{M} + \text{Na}]^+$ 373.1774, found 373.1775.

HPLC (ChiralPak IBN5-H column), hexanes/*i*-PrOH = 98:2, flow rate = 1.0 mL/min, λ = 220 nm, t_R = 11.605 min (minor), t_R = 15.104 min (major);

(*R*)-4-(3-(2-oxo-1-phenylcyclohexyl)propoxy)benzonitrile (52)



52

Colorless oil, $[\alpha]_D^{20} = -97.7$ ($c=1.27$, CH_2Cl_2), $R_f = 0.25$ (petroleum ether/ethyl acetate = 10/1), 99 % yield, 92:8 e.r.

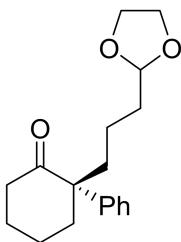
^1H NMR (400 MHz, CDCl_3) δ 7.55 – 7.47 (m, 2H), 7.35 (t, $J = 7.6$ Hz, 2H), 7.29 – 7.21 (m, 1H), 7.19 – 7.13 (m, 2H), 6.84 – 6.78 (m, 2H), 3.86 – 3.78 (m, 2H), 2.80 – 2.71 (m, 1H), 2.43 – 2.24 (m, 2H), 2.08 – 1.87 (m, 2H), 1.82 – 1.64 (m, 5H), 1.64 – 1.52 (m, 1H), 1.49 – 1.35 (m, 1H).

^{13}C NMR (101 MHz, CDCl_3) δ 213.5, 162.2, 140.4, 133.9, 129.0, 126.9, 119.3, 115.1, 103.6, 68.7, 57.0, 40.2, 36.5, 35.2, 28.4, 23.5, 21.7.

HRMS(ESI) m/z calcd. for $\text{C}_{22}\text{H}_{24}\text{NO}_2 [\text{M} + \text{H}]^+$ 334.1802, found 334.1803.

HPLC (ChiralPak AD-H column), hexanes/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, λ = 220 nm, t_R = 20.435 min (minor), t_R = 24.784 min (major);

(*R*)-2-(3-(1,3-dioxolan-2-yl)propyl)-2-phenylcyclohexan-1-one (53)



53

Colorless oil, $[\alpha]_D^{20} = -139.6$ ($c=0.84$, CH_2Cl_2), $R_f = 0.2$ (petroleum ether/ethyl acetate = 10/1), 77 % yield, 90:10 e.r.

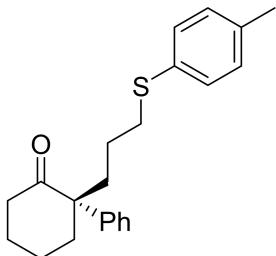
^1H NMR (400 MHz, CDCl_3) δ 7.32 (d, $J = 7.6$ Hz, 2H), 7.22 (t, $J = 7.4$ Hz, 1H), 7.13 (d, $J = 7.6$ Hz, 2H), 4.71 (d, $J = 5.0$ Hz, 1H), 3.92 – 3.72 (m, 4H), 2.74 (d, $J = 13.5$ Hz, 1H), 2.37 – 2.21 (m, 2H), 1.97 – 1.87 (m, 1H), 1.84 – 1.60 (m, 6H), 1.54 – 1.47 (m, 2H), 1.31 – 1.14 (m, 1H), 1.05 – 0.89 (m, 1H).

^{13}C NMR (101 MHz, CDCl_3) δ 213.7, 140.8, 128.8, 126.9, 126.6, 104.5, 64.8, 57.3, 40.1, 40.1, 34.8, 34.4, 28.3, 21.7, 18.3.

HRMS(ESI) m/z calcd. for $C_{18}H_{25}O_3$ [M + H]⁺ 289.1798, found 289.1798.

HPLC (Chiraleel OD-H column), hexanes/*i*-PrOH = 98:2, flow rate = 1.0 mL/min, λ = 220 nm, t_R = 12.859 min (major), t_R = 16.471 min (minor);

(*R*)-2-phenyl-2-(3-(*p*-tolylthio)propyl)cyclohexan-1-one (54)



54

Colorless oil, $[\alpha]_D^{20} = -121.8$ ($c=1.08$, CH₂Cl₂), $R_f = 0.5$ (petroleum ether/dichloromethane = 1/1), 99 % yield, 93:7 e.r.

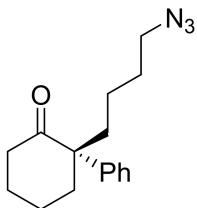
¹H NMR (400 MHz, CDCl₃) δ 7.34 (t, $J = 7.6$ Hz, 2H), 7.27 – 7.19 (m, 1H), 7.16 – 7.07 (m, 4H), 7.03 (d, $J = 7.7$ Hz, 2H), 2.82 – 2.62 (m, 3H), 2.30 (s, 5H), 1.97 – 1.88 (m, 2H), 1.80 – 1.61 (m, 5H), 1.45 – 1.33 (m, 1H), 1.32 – 1.15 (m, 1H).

¹³C NMR (101 MHz, CDCl₃) δ 213.5, 140.6, 135.8, 132.9, 129.8, 129.6, 128.9, 126.9, 126.7, 57.2, 40.1, 39.3, 35.1, 34.9, 28.4, 23.4, 21.7, 21.0.

HRMS(ESI) m/z calcd. for $C_{22}H_{27}OS$ [M + H]⁺ 339.1777, found 339.1777.

HPLC (ChiralPak IC column), hexanes/*i*-PrOH = 99:1, flow rate = 1.0 mL/min, λ = 220 nm, t_R = 19.055 min (minor), t_R = 29.476 min (major);

(*R*)-2-(4-azidobutyl)-2-phenylcyclohexan-1-one (55)



55

Colorless oil, $[\alpha]_D^{20} = -138.9$ ($c=0.79$, CH₂Cl₂), $R_f = 0.5$ (petroleum ether/ethyl acetate = 10/1), 64 % yield, 94:6 e.r.

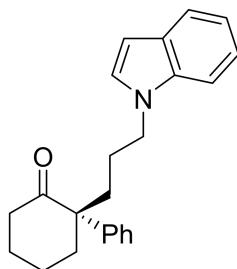
¹H NMR (400 MHz, CDCl₃) δ 7.35 (t, $J = 7.6$ Hz, 2H), 7.25 (d, $J = 7.7$ Hz, 1H), 7.14 (d, $J = 7.6$ Hz, 2H), 3.30 – 2.98 (m, 2H), 2.73 (d, $J = 13.7$ Hz, 1H), 2.46 – 2.14 (m, 2H), 2.03 – 1.88 (m, 1H), 1.83 – 1.56 (m, 6H), 1.52 – 1.36 (m, 2H), 1.22 – 1.07 (m, 1H), 1.02 – 0.82 (m, 1H).

¹³C NMR (101 MHz, CDCl₃) δ 213.7, 140.7, 128.9, 126.9, 126.7, 57.2, 51.23, 40.2, 39.7, 35.0, 29.3, 28.4, 21.7, 20.9.

HRMS(ESI) m/z calcd. for $C_{16}H_{22}N_3ONa$ [M + Na]⁺ 294.1577, found 294.1577.

HPLC (ChiralPak IC column), hexanes/*i*-PrOH = 99:1, flow rate = 1.0 mL/min, λ = 220 nm, t_R = 10.376 min (minor), t_R = 13.302 min (major);

(*R*)-2-(3-(1*H*-indol-1-yl)propyl)-2-phenylcyclohexan-1-one (56)



56

Colorless oil, $[\alpha]_D^{20} = -109.5$ ($c=1.12$, CH_2Cl_2), $R_f = 0.5$ (petroleum ether/dichloromethane = 1/1), 87 % yield, 94:6 e.r.

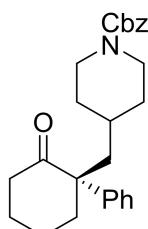
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.61 (dt, $J = 7.8, 1.0$ Hz, 1H), 7.35 (dd, $J = 8.2, 6.8$ Hz, 2H), 7.27 (d, $J = 7.0$ Hz, 1H), 7.22 – 7.10 (m, 4H), 7.10 – 7.05 (m, 1H), 6.99 (d, $J = 3.1$ Hz, 1H), 6.44 (d, $J = 3.1$ Hz, 1H), 4.02 – 3.86 (m, 2H), 2.72 – 2.59 (m, 1H), 2.42 – 2.24 (m, 2H), 1.99 – 1.83 (m, 2H), 1.79 – 1.57 (m, 6H), 1.56 – 1.43 (m, 1H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 213.4, 140.5, 135.9, 129.0, 128.5, 127.7, 126.9, 121.3, 120.9, 119.1, 109.4, 100.8, 57.1, 46.8, 40.2, 37.5, 35.2, 28.3, 24.7, 21.6.

HRMS(ESI) m/z calcd. for $\text{C}_{23}\text{H}_{26}\text{NO}$ [$\text{M} + \text{H}]^+$ 332.2009, found 332.2009.

HPLC (ChiralPak AD-H column), hexanes/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, $\lambda = 220$ nm, $t_R = 6.311$ min (major), $t_R = 7.018$ min (minor);

benzyl (R)-4-((2-oxo-1-phenylcyclohexyl)methyl)piperidine-1-carboxylate (57)



57

White solid, $[\alpha]_D^{20} = -81.8$ ($c=0.85$, CH_2Cl_2), $R_f = 0.5$ (petroleum ether/ethyl acetate = 5/1), 57 % yield, 90:10 e.r.

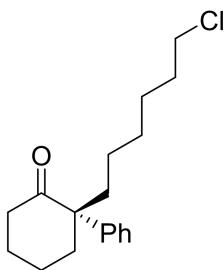
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.37 – 7.21 (m, 8H), 7.16 (d, $J = 7.7$ Hz, 2H), 5.06 (s, 2H), 3.94 (s, 2H), 2.75 (d, $J = 13.2$ Hz, 1H), 2.69 – 2.47 (m, 2H), 2.42 – 2.31 (m, 1H), 2.26 (d, $J = 12.9$ Hz, 1H), 2.04 – 1.90 (m, 1H), 1.87 – 1.58 (m, 5H), 1.50 (dd, $J = 14.5, 4.4$ Hz, 1H), 1.27 (d, $J = 11.0$ Hz, 2H), 1.12 – 0.97 (m, 2H), 0.95 – 0.83 (m, 1H). .

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 213.7, 155.2, 140.9, 137.0, 128.9, 128.4, 127.9, 127.8, 127.0, 126.9, 66.8, 57.6, 46.6, 44.2, 44.1, 40.1, 35.9, 33.9, 33.6, 31.8, 28.3, 21.6.

HRMS(ESI) m/z calcd. for $\text{C}_{26}\text{H}_{32}\text{NO}_3$ [$\text{M} + \text{H}]^+$ 406.2377, found 406.2374.

HPLC (ChiralPak AS column), hexanes/*i*-PrOH = 95:5, flow rate = 1.0 mL/min, $\lambda = 220$ nm, $t_R = 15.815$ min (minor), $t_R = 17.188$ min (major);

(S)-2-(6-chlorohexyl)-2-phenylcyclohexan-1-one (58)



58

Colorless oil, $[\alpha]_D^{20} = -134.3$ ($c=0.94$, CH_2Cl_2), $R_f = 0.7$ (petroleum ether/ethyl acetate = 10/1), 88 % yield, 93:7 e.r.

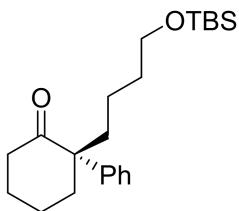
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.33 (t, $J = 7.6$ Hz, 2H), 7.23 (t, $J = 7.5$ Hz, 1H), 7.13 (d, $J = 7.6$ Hz, 2H), 3.44 (t, $J = 6.8$ Hz, 2H), 2.75 – 2.67 (m, 1H), 2.39 – 2.21 (m, 2H), 2.02 – 1.86 (m, 1H), 1.82 – 1.53 (m, 8H), 1.37 – 1.00 (m, 5H), 0.91 – 0.79 (m, 1H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 213.8, 141.0, 128.8, 126.9, 126.6, 57.3, 45.1, 40.2, 40.0, 35.0, 32.5, 29.4, 28.4, 26.7, 23.4, 21.7.

HRMS(ESI) m/z calcd. for $\text{C}_{18}\text{H}_{26}\text{ClO}$ [$\text{M} + \text{H}]^+$ 293.1667, found 293.1667.

HPLC (ChiralPak IC column), hexanes/*i*-PrOH = 95:5, flow rate = 1.0 mL/min, $\lambda = 220$ nm, $t_R = 6.672$ min (minor), $t_R = 8.087$ min (major);

(*R*)-2-(4-((tert-butyldimethylsilyl)oxy)butyl)-2-phenylcyclohexan-1-one (59)



59

Product **59** is difficult to resolve on a chiral column; it can be treated with TBAF in THF to obtain **59-a**.

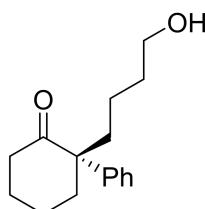
Colorless oil, $R_f = 0.8$ (petroleum ether/ethyl acetate = 10/1), 99 % yield.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.32 (dd, $J = 8.2, 6.9$ Hz, 2H), 7.26 – 7.16 (m, 1H), 7.13 (dd, $J = 8.4, 1.3$ Hz, 2H), 3.48 (td, $J = 6.5, 1.3$ Hz, 2H), 2.74 (dq, $J = 14.0, 2.9$ Hz, 1H), 2.42 – 2.19 (m, 2H), 1.98 – 1.88 (m, 1H), 1.84 – 1.54 (m, 6H), 1.48 – 1.20 (m, 2H), 1.19 – 1.03 (m, 1H), 0.94 – 0.84 (m, 1H), 0.83 (s, 9H), -0.04 (d, $J = 2.6$ Hz, 6H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 213.8, 140.9, 128.7, 127.0, 126.5, 62.9, 57.4, 40.2, 39.9, 35.0, 33.3, 28.4, 25.9, 21.7, 19.8, 18.3.

HRMS(ESI) m/z calcd. for $\text{C}_{22}\text{H}_{37}\text{O}_2\text{Si}$ [$\text{M} + \text{H}]^+$ 361.2557, found 361.2556.

(*R*)-2-(4-((tert-butyldimethylsilyl)oxy)butyl)-2-phenylcyclohexan-1-one (59-a)



59-a

Colorless oil, $[\alpha]_D^{20} = 17.9$ ($c=0.68$, CH_2Cl_2), $R_f = 0.3$ (petroleum ether/ethyl acetate = 10/1), 99 % yield, 94:6 e.r.

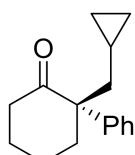
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.33 (dd, $J = 8.3, 7.0$ Hz, 2H), 7.25 – 7.20 (m, 1H), 7.15 – 7.11 (m, 2H), 3.52 (td, $J = 6.5, 3.1$ Hz, 2H), 2.72 (dq, $J = 13.6, 2.4$ Hz, 1H), 2.43 – 2.18 (m, 2H), 1.98 – 1.88 (m, 1H), 1.83 – 1.53 (m, 7H), 1.50 – 1.38 (m, 2H), 1.21 – 1.07 (m, 1H), 1.03 – 0.83 (m, 1H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 214.1, 141.0, 128.8, 126.9, 126.6, 62.5, 57.4, 40.2, 39.7, 35.1, 32.9, 28.4, 21.7, 19.9.

HRMS(ESI) m/z calcd. for $\text{C}_{16}\text{H}_{23}\text{O}_2$ $[\text{M} + \text{H}]^+$ 247.1693, found 247.1693.

HPLC (ChiralPak AD-H column), hexanes/*i*-PrOH = 95:5, flow rate = 1.0 mL/min, $\lambda = 220$ nm, $t_R = 17.576$ min (minor), $t_R = 18.647$ min (major);

(*R*)-2-(cyclopropylmethyl)-2-phenylcyclohexan-1-one (60)



60

Colorless oil, $[\alpha]_D^{20} = -132.7$ ($c=0.4$, CH_2Cl_2), $R_f = 0.4$ (petroleum ether/dichloromethane = 2/1), 87 % yield, 89:11 e.r.

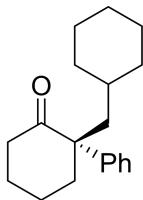
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.33 (dd, $J = 8.2, 6.9$ Hz, 2H), 7.26 – 7.21 (m, 1H), 7.21 – 7.15 (m, 2H), 2.98 – 2.88 (m, 1H), 2.48 – 2.30 (m, 1H), 2.29 – 2.19 (m, 1H), 2.01 – 1.89 (m, 1H), 1.85 – 1.61 (m, 5H), 1.56 (dd, $J = 14.2, 6.9$ Hz, 1H), 0.45 – 0.26 (m, 2H), 0.22 – 0.11 (m, 1H), -0.07 – -0.17 (m, 1H), -0.27 – -0.37 (m, 1H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 214.0, 141.3, 128.7, 127.0, 126.5, 58.3, 45.2, 40.1, 35.1, 28.4, 21.7, 5.9, 4.9, 4.2.

HRMS(ESI) m/z calcd. for $\text{C}_{16}\text{H}_{21}\text{O}$ $[\text{M} + \text{H}]^+$ 229.1587, found 229.1585.

HPLC (ChiralPak IC column), hexanes/*i*-PrOH = 99:1, flow rate = 1.0 mL/min, $\lambda = 220$ nm, $t_R = 6.708$ min (minor), $t_R = 8.814$ min (major);

(*R*)-2-(cyclohexylmethyl)-2-phenylcyclohexan-1-one (61)



61

Colorless oil, $[\alpha]_D^{20} = -118.8$ ($c=0.40$, CH_2Cl_2), $R_f = 0.4$ (petroleum ether/dichloromethane = 2/1), 50 % yield, 91:9 e.r.

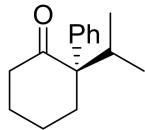
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.32 (dd, $J = 8.3, 6.9$ Hz, 2H), 7.25 – 7.20 (m, 1H), 7.17 (dd, $J = 7.1, 1.8$ Hz, 2H), 2.75 (dq, $J = 13.6, 2.9$ Hz, 1H), 2.39 – 2.20 (m, 2H), 1.99 – 1.88 (m, 1H), 1.84 – 1.63 (m, 5H), 1.60 – 1.38 (m, 5H), 1.17 – 0.82 (m, 6H), 0.74 – 0.58 (m, 1H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 213.8, 141.3, 128.7, 127.0, 126.5, 57.7, 47.5, 40.1, 35.5, 35.3, 35.1, 33.4, 28.2, 26.6, 26.4, 26.2, 21.7.

HRMS(ESI) m/z calcd. for $\text{C}_{19}\text{H}_{27}\text{O}$ [$\text{M} + \text{H}]^+$ 271.2056, found 271.2055.

HPLC (ChiralPak AD-H column), hexanes/*i*-PrOH = 98:2, flow rate = 1.0 mL/min, $\lambda = 220$ nm, $t_R = 4.475$ min (major), $t_R = 5.181$ min (minor);

(*R*)-2-isopropyl-2-phenylcyclohexan-1-one (62)



62

Colorless oil, $[\alpha]_D^{20} = -160.9$ ($c=0.70$, CH_2Cl_2), $R_f = 0.4$ (petroleum ether/dichloromethane = 1/1), 86 % yield, 85:15 e.r.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.36 – 7.30 (m, 2H), 7.25 – 7.20 (m, 1H), 7.19 – 7.14 (m, 2H), 2.63 – 2.52 (m, 1H), 2.43 – 2.29 (m, 1H), 2.29 – 2.18 (m, 2H), 1.92 – 1.85 (m, 1H), 1.83 – 1.72 (m, 3H), 1.74 – 1.56 (m, 1H), 0.90 (d, $J = 6.7$ Hz, 3H), 0.49 (d, $J = 7.0$ Hz, 3H).

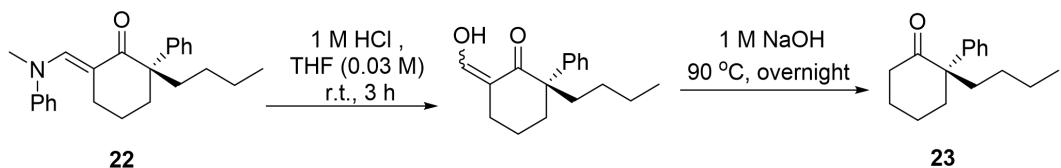
$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 213.0, 140.1, 128.5, 127.5, 126.5, 60.6, 40.6, 34.3, 28.6, 27.6, 21.5, 18.7, 17.5.

HRMS(ESI) m/z calcd. for $\text{C}_{15}\text{H}_{21}\text{O}$ [$\text{M} + \text{H}]^+$ 217.1587, found 217.1588.

HPLC (ChiralPak IC column), hexanes/*i*-PrOH = 99:1, flow rate = 1.0 mL/min, $\lambda = 220$ nm, $t_R = 5.902$ min (minor), $t_R = 6.703$ min (major);

7. Transformations of Chiral Ketone Products

(S)-2-butyl-2-phenylcyclohexan-1-one (23)⁴



(S,E)-2-butyl-6-((methyl(phenyl)amino)methylene)-2-phenylcyclohexan-1-one (69.4 g, 0.2 mmol) was dissolved in THF (6.5 mL). Aqueous 1M HCl (6.5 mL) was added to the reaction mixture, and the resulting mixture was stirred at room temperature for 3 h. The reaction mixture was extracted with EtOAc, and the combined organic layers were concentrated under reduced pressure. To the crude hydroxymethylene ketone was added aqueous 1 M NaOH (6.5 mL) and the reaction mixture was heated at 90 °C overnight, the reaction mixture was cooled to room temperature and neutralized with aqueous 1M HCl. The reaction mixture was extracted with EtOAc. The combined organic layers were washed with brine, dried over anhydrous Na₂SO₄, and concentrated under reduced pressure. The crude product was purified by column chromatography to afford target product.

Colorless oil, $R_f = 0.8$ (petroleum ether/ethyl acetate = 10/1), 84% yield, 94:6 e.r.

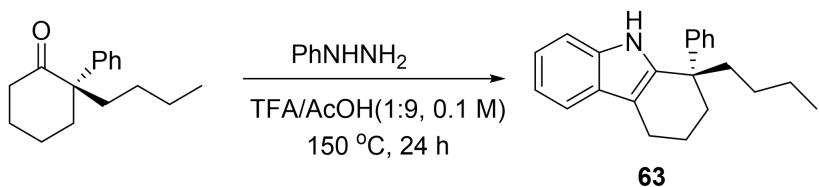
¹H NMR (400 MHz, CDCl₃) δ 7.36 (t, *J* = 7.6 Hz, 2H), 7.25 (d, *J* = 14.7 Hz, 1H), 7.17 (d, *J* = 7.8 Hz, 2H), 2.75 (dq, *J* = 14.1, 2.9 Hz, 1H), 2.40 – 2.24 (m, 2H), 1.98 – 1.92 (m, 1H), 1.82 – 1.60 (m, 6H), 1.26 – 1.13 (m, 2H), 1.13 – 1.00 (m, 1H), 0.90 – 0.78 (m, 4H).

^{13}C NMR (101 MHz, CDCl_3) δ 213.9, 141.1, 128.7, 127.0, 126.5, 57.3, 40.2, 39.9, 35.0, 28.4, 25.8, 23.2, 21.7, 14.0.

HRMS (ESI) m/z calcd. for $C_{16}H_{23}O [M + H]^+$ 231.1743, found 231.1743.

HPLC (ChiralPak IC-H column), hexane/*i*-PrOH = 95:5, flow rate = 0.5 mL/min, λ = 220 nm, t_R = 11.106 min (major), t_R = 9.354 min (minor);

(S)-1-butyl-1-phenyl-2,3,4,9-tetrahydro-1*H*-carbazole (63)⁵



To a 10-mL Schlenk tube were added (*S*)-2-butyl-2-phenylcyclohexan-1-one (23.0 mg, 0.1 mmol), phenylhydrazine (1.2 equiv) and TFA/AcOH (1/9, v/v, 1 mL). The reaction mixture stirred at 150 °C for 24 h. The reaction mixture was cooled to room temperature and quenched by the addition of saturated NaHCO₃ (aq.) solution to neutral. The aqueous layer was extracted with EtOAc, and the organic layers were combined, washed with brine, dried over anhydrous Na₂SO₄ and concentrated under reduced pressure. The crude product was purified by column chromatography to afford target product.

Colorless oil, $R_f = 0.7$ (petroleum ether/dichloromethane = 3/1), 97% yield, 94:6 e.r.

¹H NMR (400 MHz, CDCl₃) δ 7.71 (s, 1H), 7.59 (d, *J* = 7.6 Hz, 1H), 7.35 (d, *J* = 7.1 Hz, 1H), 7.32 – 7.25 (m, 2H), 7.25 – 7.14 (m, 3H), 7.13 – 7.08 (m, 2H), 2.91 – 2.70 (m, 2H), 2.32 – 2.13 (m,

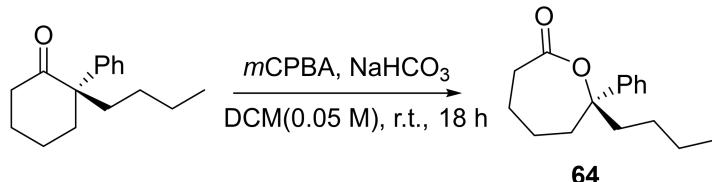
2H), 2.13 – 1.96 (m, 2H), 1.93 – 1.82 (m, 1H), 1.70 – 1.61 (m, 1H), 1.47 – 1.34 (m, 3H), 1.28 – 1.12 (m, 1H), 0.92 (t, J = 7.2 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 148.5, 137.7, 135.9, 128.1, 127.5, 127.2, 126.0, 121.4, 119.1, 118.3, 112.8, 110.7, 44.4, 40.1, 38.4, 27.6, 23.6, 21.2, 19.7, 14.1.

HRMS (ESI) m/z calcd. for $\text{C}_{22}\text{H}_{26}\text{N}$ [$\text{M} + \text{H}]^+$ 304.2060, found 304.2059.

HPLC (ChiralPak OJ-H column), hexane/*i*-PrOH = 95:5, flow rate = 1.0 mL/min, λ = 254 nm, t_R = 7.762 min (major), t_R = 13.037 min (minor).

(*S*)-7-butyl-7-phenyloxepan-2-one (64)⁶



To a 10-mL flame-dried Schlenk tube were added (*S*)-2-butyl-2-phenylcyclohexan-1-one (23.0 mg, 0.1 mmol), *m*-CPBA (85% purity, 5 equiv), NaHCO₃ (5 equiv) and DCM (2 mL) under N₂. The reaction mixture stirred at room temperature for 18 h. The reaction mixture was quenched by the addition of saturated Na₂S₂O₃ (aq.) solution. The aqueous layer was extracted with dichloromethane, and the organic layers were combined, washed with saturated NaHCO₃ (aq.) solution (x3), brine, dried over anhydrous Na₂SO₄ and concentrated under reduced pressure. The crude product was purified by column chromatography to afford target product

Colorless oil, R_f = 0.2 (petroleum ether/ethyl acetate = 10/1), 70% yield, 94:6 e.r.

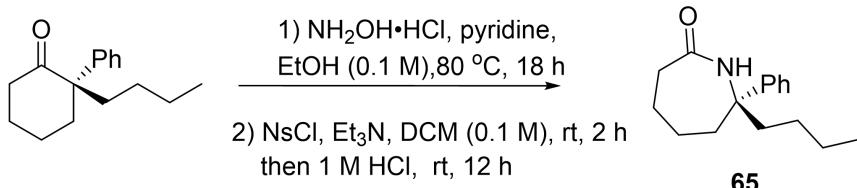
^1H NMR (400 MHz, CDCl_3) δ 7.40 (t, J = 7.7 Hz, 2H), 7.34 – 7.22 (m, 3H), 2.68 – 2.62 (m, 1H), 2.57 – 2.48 (m, 1H), 2.18 – 1.98 (m, 2H), 1.92 – 1.80 (m, 2H), 1.80 – 1.68 (m, 3H), 1.60 – 1.49 (qm, 1H), 1.44 – 1.31 (m, 1H), 1.26 – 1.06 (m, 3H), 0.82 (t, J = 7.2 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 176.0, 142.1, 128.7, 127.1, 125.7, 86.6, 47.7, 37.3, 37.0, 25.6, 24.2, 23.2, 22.7, 13.9.

HRMS (ESI) m/z calcd. for $\text{C}_{16}\text{H}_{23}\text{O}_2$ [$\text{M} + \text{H}]^+$ 247.1693, found 247.1693.

HPLC (ChiralPak OJ-H column), hexane/*i*-PrOH = 95:5, flow rate = 0.5 mL/min, λ = 220 nm, t_R = 11.880 min (major), t_R = 11.211 min (minor).

(*S*)-7-butyl-7-phenylazepan-2-one (65)⁷



To a 10-mL Schlenk tube were added (*S*)-2-butyl-2-phenylcyclohexan-1-one (23.0 mg, 0.1 mmol), NH₂OH•HCl (4 equiv), pyridine (4 equiv) and EtOH (1 mL). The resulting mixture was stirred at 80 °C for 18 h and concentrated under reduced pressure. The crude product was purified by column chromatography to afford intermediate oxime. The intermediate oxime dissolved in DCM (1.0 mL) was introduced to 10-mL Schlenk tube. Then Et₃N (1.5 equiv) was added followed by 4-nitrobenzenesulfonyl chloride (1.3 equiv). The reaction mixture was stirred at room temperature. After 2 h, the reaction mixture was added two drops of 1 M HCl and continuously stirred for 12 h.

The reaction mixture was quenched by the addition of saturated NaHCO₃ (aq.) solution, extracted with dichloromethane. The organic layers were combined, washed with brine, dried over anhydrous Na₂SO₄ and concentrated under reduced pressure. The crude product was purified by column chromatography to afford target product.

Colorless oil, *R*_f = 0.3 (petroleum ether/ethyl acetate = 3/1), 48% yield, 94:6 e.r.

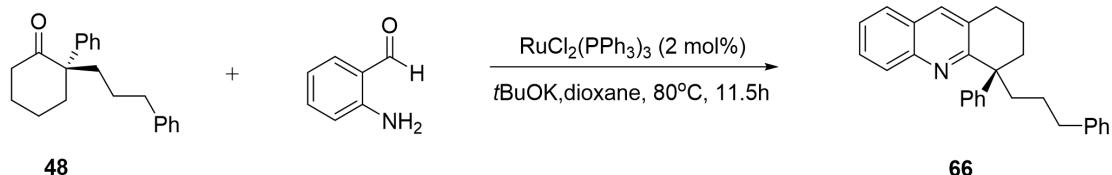
¹H NMR (400 MHz, CDCl₃) δ 7.43 – 7.33 (m, 2H), 7.30 – 7.25 (m, 3H), 6.03 (s, 1H), 2.55 – 2.50 (m, 1H), 2.36 – 2.31 (m, 1H), 2.12 – 2.01 (m, 1H), 1.96 – 1.88 (m, 1H), 1.86 – 1.77 (m, 1H), 1.76 – 1.46 (m, 5H), 1.23 – 1.14 (m, 3H), 1.05 – 0.96 (m, 1H), 0.81 (t, *J* = 7.1 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 178.5, 143.2, 128.7, 126.6, 126.2, 61.1, 47.5, 39.2, 37.1, 25.5, 25.0, 23.3, 22.7, 13.9.

HRMS (ESI) *m/z* calcd. for C₁₆H₂₄NO [M + H]⁺ 246.1582, found 246.1582.

HPLC (ChiralPak AD-H column), hexane/*i*-PrOH = 95:5, flow rate = 0.5 mL/min, λ = 220 nm, *t_R* = 18.475 min (major), *t_R* = 17.564 min (minor)

(S)-4-phenyl-4-(3-phenylpropyl)-1,2,3,4-tetrahydroacridine (**66**)⁸



Under N₂, to an oven-dried Schlenk tube were added RuCl₂(PPh₃)₃ (3.8 mg, 2 mol%), 'BuOK (22.4 mg, 0.2 mmol), 2-aminobenzaldehyde (48.5 mg, 0.4 mmol), and a solution of **48** (58.5 mg, 0.2 mmol) in anhydrous dioxane (1 mL). The mixture was stirred at 80 °C and the reaction progress was monitored by TLC. Upon completion (11.5 h), the reaction was cooled to room temperature, filtrated through a short pad of silica gel (petroleum ether: ethyl acetate), and concentrated. The residue was purified by silica gel flash column chromatography (petroleum ether: hexanes/ethyl acetate = 50:1) to afford **66**.

Colorless oil, *R*_f = 0.9 (petroleum ether/ethyl acetate = 10/1), 60% yield, 95:5 e.r.

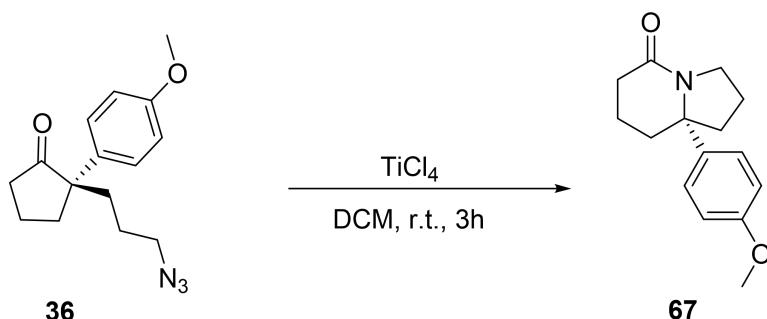
¹H NMR (400 MHz, CDCl₃) δ 8.08 (d, *J* = 8.4 Hz, 1H), 7.85 (d, *J* = 1.3 Hz, 1H), 7.76 (dd, *J* = 8.1, 1.5 Hz, 1H), 7.65 (ddd, *J* = 8.5, 6.8, 1.5 Hz, 1H), 7.50 (ddd, *J* = 8.1, 6.8, 1.2 Hz, 1H), 7.25 – 7.10 (m, 8H), 7.04 – 6.98 (m, 2H), 3.01 – 2.81 (m, 2H), 2.77 – 2.61 (m, 3H), 2.45 – 2.35 (m, 1H), 2.33 – 2.23 (m, 1H), 2.23 – 2.11 (m, 1H), 1.88 – 1.65 (m, 3H), 1.58 – 1.43 (m, 1H).

¹³C NMR (101 MHz, CDCl₃) δ 162.7, 148.9, 146.8, 142.9, 134.8, 132.0, 129.5, 128.5, 128.2, 128.1, 127.9, 127.4, 127.1, 126.7, 125.9, 125.6, 125.5, 49.8, 42.0, 36.8, 34.4, 29.3, 27.2, 18.7.

HRMS (ESI) *m/z* calcd. for C₂₈H₂₈N [M + H]⁺ 378.2216, found 378.2215.

HPLC (ChiralPak AD-H column), hexane/*i*-PrOH = 100:0, flow rate = 0.5 mL/min, λ = 220 nm, *t_R* = 17.455 min (major), *t_R* = 21.398 min (minor)

(R)-8a-(4-methoxyphenyl)hexahydroindolin-5(1H)-one (**67**)⁹



To a solution of the above azide **36** (54.7 mg, 0.2 mmol) in CH₂Cl₂ (2 mL) was added TiCl₄ (110 µL, 1 mmol, 5 equiv). After 3 h, the reaction was quenched with saturated NaHCO₃ (2 mL) and extracted with CH₂Cl₂ (3x). The combined organics were dried (Na₂SO₄), concentrated and chromatographed to give the ketoamide **67** (218 mg, 81% yield, 92:8 e.r.) as a colorless oil.

Colorless oil. $R_f = 0.1$ (petroleum ether/ethyl acetate (Et_2N) = 1/1), 86% yield, 92.8 e.r.

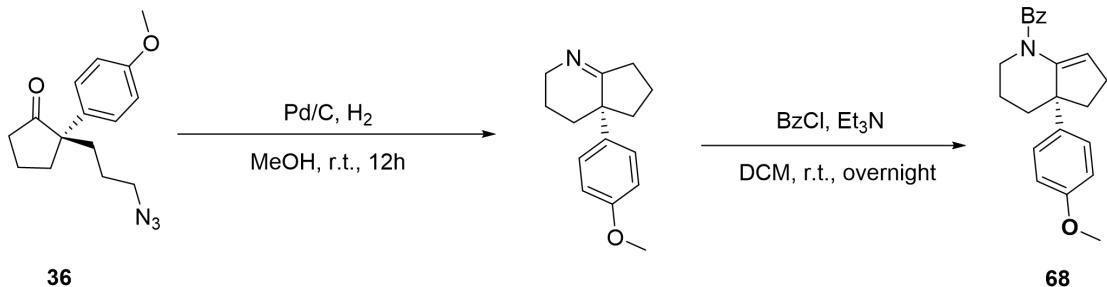
¹H NMR (400 MHz, CDCl₃) δ 7.08 – 7.02 (m, 2H), 6.87 – 6.81 (m, 2H), 3.78 (s, 4H), 3.53 – 3.43 (m, 1H), 2.44 – 2.16 (m, 4H), 1.93 – 1.57 (m, 4H), 1.50 – 1.21 (m, 2H).

¹³C NMR (101 MHz, CDCl₃) δ 170.1, 158.5, 135.9, 126.7, 113.7, 68.7, 55.3, 45.0, 42.0, 36.8, 30.5, 20.0, 17.4.

HRMS (ESI) m/z calcd. for $C_{15}H_{20}NO_2 [M + H]^+$ 246.1489, found 246.1489.

HPLC (ChiralPak AD-H column), hexane/*i*-PrOH = 95:5, flow rate = 1 mL/min, λ = 220 nm, t_R = 22.438 min (major), t_R = 20.405 min (minor)

(S)-(4a-(4-methoxyphenyl)-2,3,4,4a,5,6-hexahydro-1H-cyclopenta[b]pyridin-1-yl)(phenyl)methanone (68)^{10,11}



Introduce 0.2 mmol of the compound **36** into a Schlenk tube, dissolving it in 1 ml of MeOH. Following this, incorporate 10 mol% of Pd/C catalyst. Proceed to inflate a hydrogen balloon and, using a long needle, carefully introduce the hydrogen gas beneath the liquid surface, maintaining a steady rate of bubble release at two per second. Once the gas is introduced, allow the reaction mixture to stir at ambient temperature for a duration of 12 hours. Upon completion of the reaction, employ vacuum distillation to remove the solvent, leaving behind the dried residue. Finally, purify the reaction products through column chromatography using a silica gel medium.

In a nitrogen atmosphere, the synthesized compound is dissolved in 1 ml of DCM and transferred into a Schlenk tube. Subsequently, BzCl (1.5 eq.) and triethylamine (2.0 eq.) are added to the mixture. The reaction mixture is then stirred at room temperature throughout the night. Following the completion of the reaction, it is quenched with NaHCO_3 (aq.) solution, and the product is extracted with DCM. The combined organic layers are evaporated to dryness under vacuum, and the resulting compound is purified using column chromatography with a silica gel stationary phase.

Colorless oil, $R_f = 0.3$ (petroleum ether/ethyl acetate = 10/1), 85% yield, 95:5 e.r.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.57 – 7.33 (m, 5H), 7.27 (d, $J = 6.4$ Hz, 2H), 6.92 – 6.85 (m, 2H), 5.83 (s, 1H), 3.90 (d, $J = 13.0$ Hz, 1H), 3.81 (s, 3H), 3.12 – 3.00 (m, 1H), 2.67 – 2.59 (m, 1H), 2.28 – 2.21 (m, 2H), 2.07 – 1.87 (m, 2H), 1.76 – 1.64 (m, 1H), 1.61 – 1.45 (m, 2H).

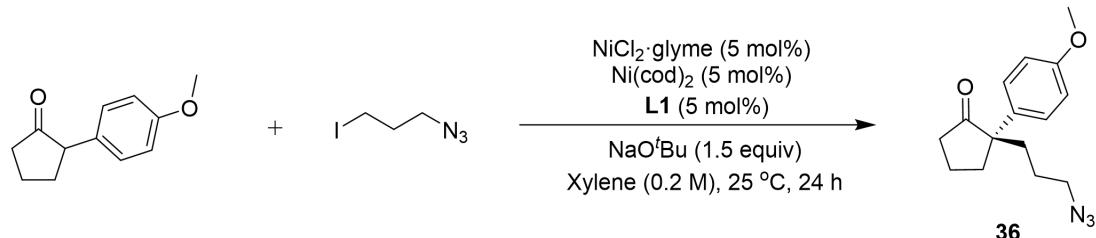
$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 171.0, 157.9, 137.0, 136.7, 129.6, 128.2, 127.9, 127.1, 121.9, 113.7, 55.2, 52.2, 48.4, 41.6, 38.2, 27.8, 21.7.

HRMS (ESI) m/z calcd. for $\text{C}_{22}\text{H}_{24}\text{NO}_2$ [$\text{M} + \text{H}]^+$ 334.1802, found 334.1804.

HPLC (ChiralPak AD-H column), hexane/*i*-PrOH = 85:15, flow rate = 1 mL/min, $\lambda = 220$ nm, t_R = 15.506 min (major), t_R = 12.696 min (minor)

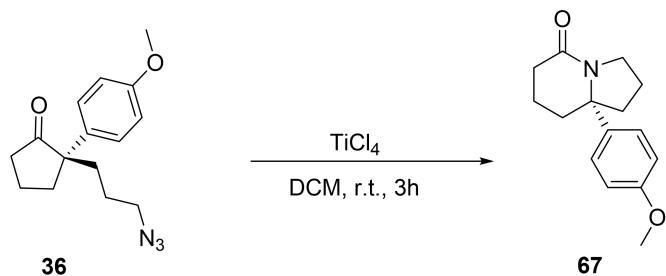
8. Scale-up Synthesis

a) scale-up synthesis of **36**.



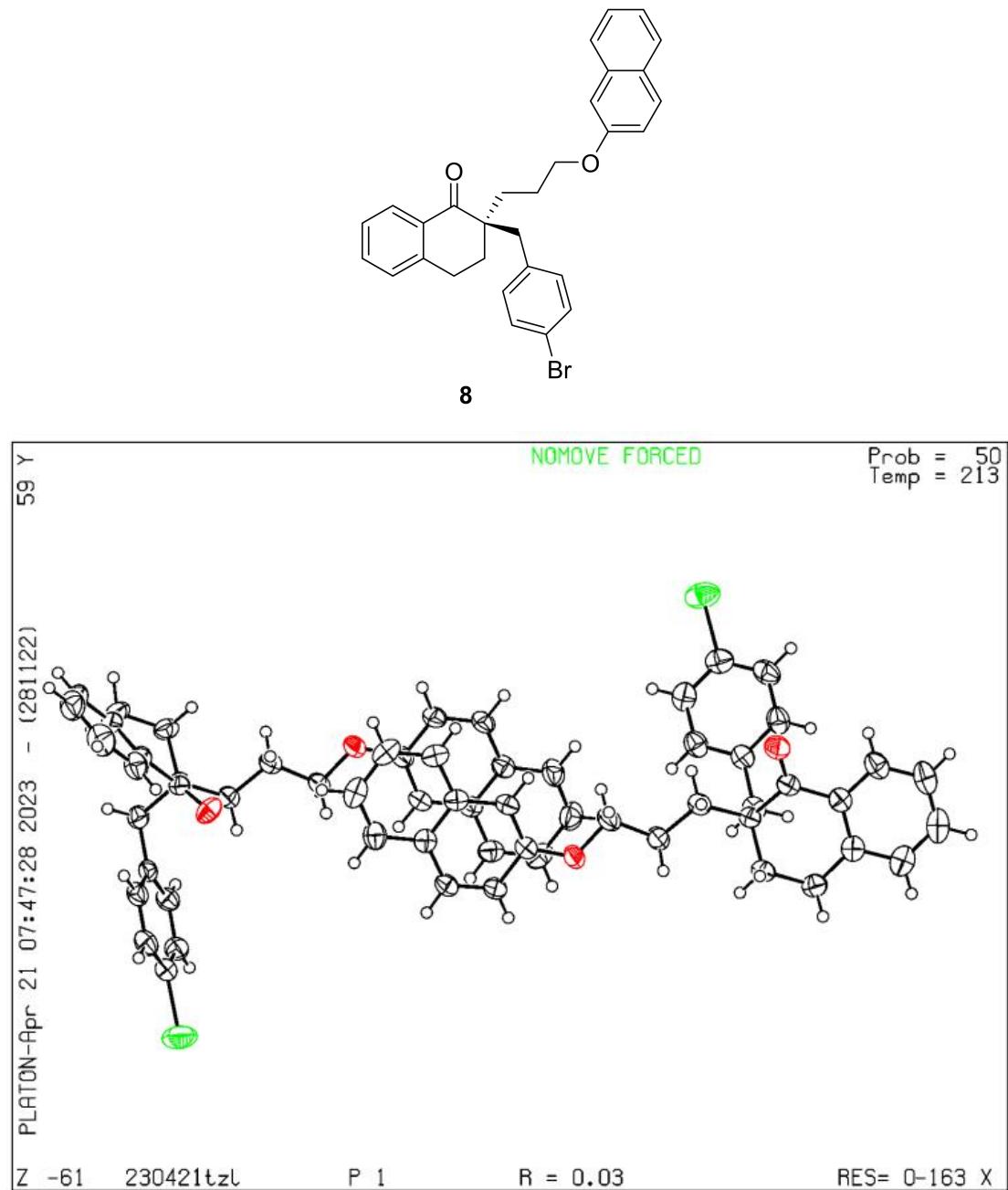
Prepared following the modified General Procedure C. The $\text{Ni}(\text{cod})_2$ (13.8 mg, 0.05 mmol, 5 mol %), $\text{NiCl}_2\text{-glyme}$ (11.0 mg, 0.05 mmol, 5 mol %), **L** (0.05 mmol, 5 mol %) and $^\text{t}\text{BuONa}$ (144.2 mg, 1.5 mmol, 1.5 equiv) were introduced into a flame-dried two-necked round-bottomed flask in an N_2 -filled glove box. After taking out from the glove box, two-necked round-bottomed flask was connected to Schlenk line under N_2 . 5 mL dry Xylene was injected into the round-bottomed flask, the mixture was stirred at r.t. for 30 min. The ketone (190.2 mg, 1 mmol, 1.0 equiv) was then added rapidly under nitrogen. After 30 min, alkyl iodide (316.5 mg, 1.5 mmol, 1.5 equiv) was introduced into the system by a syringe under N_2 . The resulting mixture was stirred under room temperature for 24 hours. The reaction mixture was quenched with saturated NH_4Cl (aq.) solution and extracted with EtOAc (3x). The organic phase was washed with brine, dried over anhydrous Na_2SO_4 , filtered, and concentrated under reduced pressure. The crude material was purified using column chromatography to give the enantioenriched product **36** (161 mg, 0.59 mmol, 59% yield, 95:5 e.r.).

b) scale-up synthesis of **67**.



To a solution of the above azide **36** (300.6 mg, 1.1 mmol) in CH_2Cl_2 (10 mL) was added TiCl_4 (603 μL , 5.5 mmol, 5 equiv). After 3 h, the reaction was quenched with saturated NaHCO_3 (10 mL) and extracted with CH_2Cl_2 (3x). The combined organics were dried (Na_2SO_4), concentrated and chromatographed to give the ketoamide **67** (218 mg, 81% yield, 92:8 e.r.) as a colorless oil.

9. X-ray Crystallography

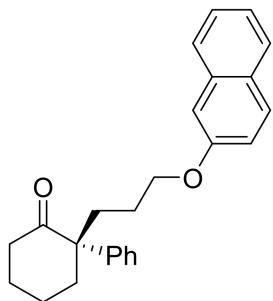


Supplementary Fig. S1 The X-ray structure of **8** (CCDC 2282206).

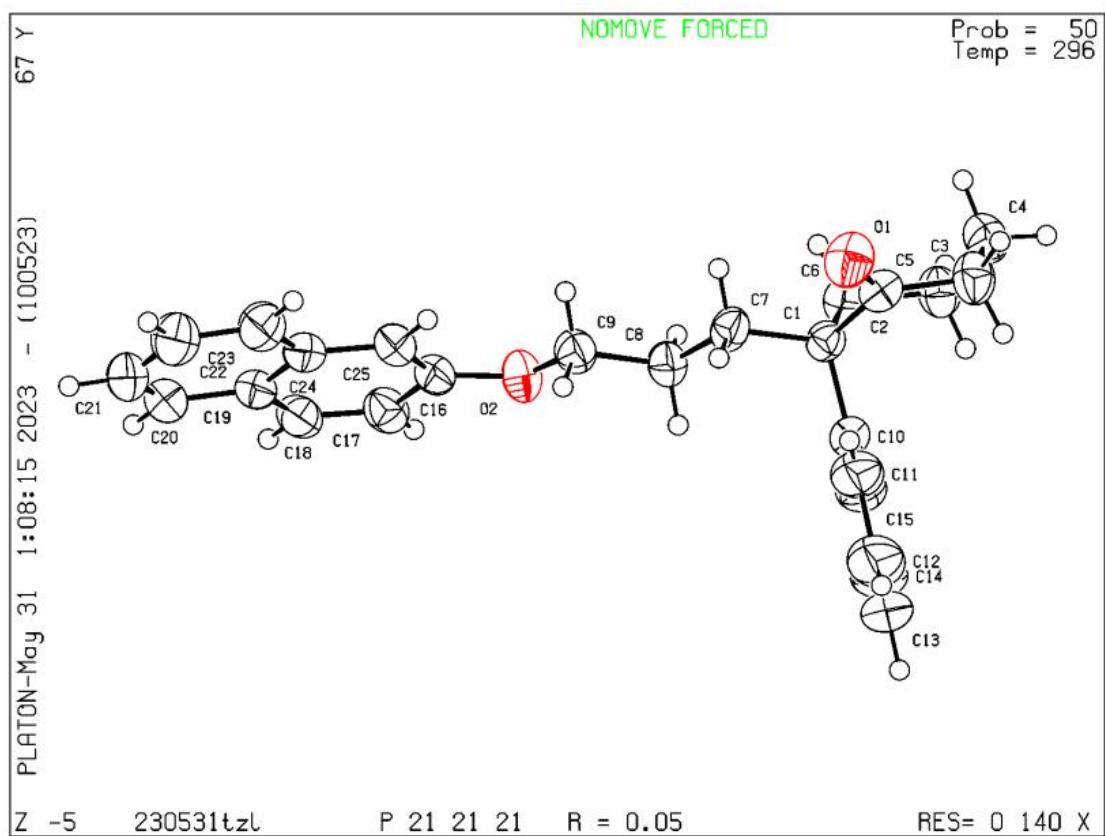
Table S4. Crystal data and structure refinement for CCDC 2282206.

Identification code	CCDC 2282206	
Empirical formula	C30 H27 Br O2	
Formula weight	499.42	
Temperature	213 K	
Wavelength	1.34139 Å	
Crystal system	Triclinic	
Space group	P1	
Unit cell dimensions	a = 8.1211(2) Å	α= 90.9670(10)°.
	b = 8.1420(2) Å	β= 99.9990(10)°.
	c = 18.9532(4) Å	γ=103.2620(10)°.
Volume	1199.17(5) Å ³	
Z	2	
Density (calculated)	1.383 Mg/m ³	
Absorption coefficient	1.661 mm ⁻¹	
F(000)	516	
Crystal size	0.07 x 0.07 x 0.05 mm ³	
Theta range for data collection	4.128 to 55.199°.	
Index ranges	-9<=h<=9, -9<=k<=9, -23<=l<=23	
Reflections collected	38765	
Independent reflections	9020 [R(int) = 0.0420]	
Completeness to theta = 53.594°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7508 and 0.6184	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	9020 / 3 / 595	

Goodness-of-fit on F ²	1.035
Final R indices [I>2sigma(I)]	R1 = 0.0290, wR2 = 0.0716
R indices (all data)	R1 = 0.0328, wR2 = 0.0740
Absolute structure parameter	0.017(6)
Extinction coefficient	n/a
Largest diff. peak and hole	0.333 and -0.453 e. \AA^{-3}



24



Supplementary Fig. S2 The X-ray structure of **24** (CCDC 2282207).

Table S5. Crystal data and structure refinement for CCDC 2282207.

Identification code	CCDC 2282207
Empirical formula	C ₂₅ H ₂₆ O ₂
Formula weight	358.46
Temperature	296 K

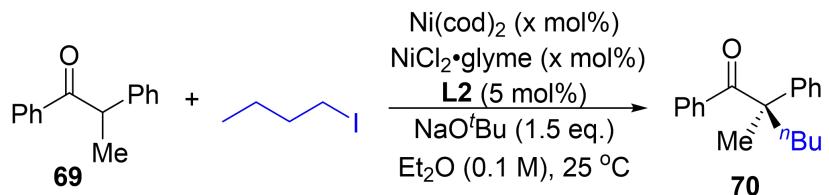
Wavelength	1.34139 Å	
Crystal system	Orthorhombic	
Space group	P2 ₁ 2 ₁ 2 ₁	
Unit cell dimensions	a = 6.3710(2) Å	α= 90°.
	b = 10.0598(2) Å	β= 90°.
	c = 31.1131(7) Å	γ = 90°.
Volume	1994.07(9) Å ³	
Z	4	
Density (calculated)	1.194 Mg/m ³	
Absorption coefficient	0.367 mm ⁻¹	
F(000)	768	
Crystal size	0.07 x 0.07 x 0.05 mm ³	
Theta range for data collection	4.018 to 54.927°.	
Index ranges	-7<=h<=7, -12<=k<=12, -37<=l<=37	
Reflections collected	23258	
Independent reflections	3789 [R(int) = 0.0559]	
Completeness to theta = 53.594°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7508 and 0.4302	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	3789 / 0 / 244	
Goodness-of-fit on F ²	1.071	
Final R indices [I>2sigma(I)]	R1 = 0.0475, wR2 = 0.1239	
R indices (all data)	R1 = 0.0532, wR2 = 0.1305	
Absolute structure parameter	0.02(12)	
Extinction coefficient	n/a	

Largest diff. peak and hole	0.182 and -0.212 e. \AA^{-3}
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All the other configurations are uncertain and based on the assumption that the configuration follows that of **8** or **24**.

10. Mechanistic Study

10.1 Kinetic Experiments



General Kinetics Experimental Procedure: The $\text{Ni}(\text{cod})_2$ (x mol\%), $\text{NiCl}_2\text{-glyme}$ (x mol\%), **L2** (0.01 mmol, 5 mol%) and 'BuONa (29.0 mg, 0.3 mmol, 1.5 equiv) were introduced into a flame-dried Schlenk tube in an nitrogen-filled glove box (note: $\text{Ni}/\text{L}=2\text{x}/5$). After taking out from the glove box, Schlenk tube was connected to Schlenk line under N_2 . 2 mL dry Et_2O was injected into the Schlenk tube, the mixture was stirred at r.t. for 30 min. The ketone (0.2 mmol, 1.0 equiv) was then added rapidly under nitrogen. Following this, n-dodecane (0.2 mmol, 1.0 equiv) as internal standard was introduced using a microliter syringe under N_2 . After 30 min, alkyl iodide (0.3 mmol, 1.5 equiv) was introduced into the system by a microliter syringe under N_2 . The reaction progress was monitored by removing aliquots ($\sim 10 \mu\text{L}$) from the reaction mixture via syringe under N_2 . Each aliquot was quenched by ethyl acetate (4.0 mL) in an 8.0 mL tube. The mixture was filtered with a filter head into 2.0 mL GC vial and analyzed by gas chromatography.

Supplementary Table S6

kinetic experiments with varying ligand/nickel ratios

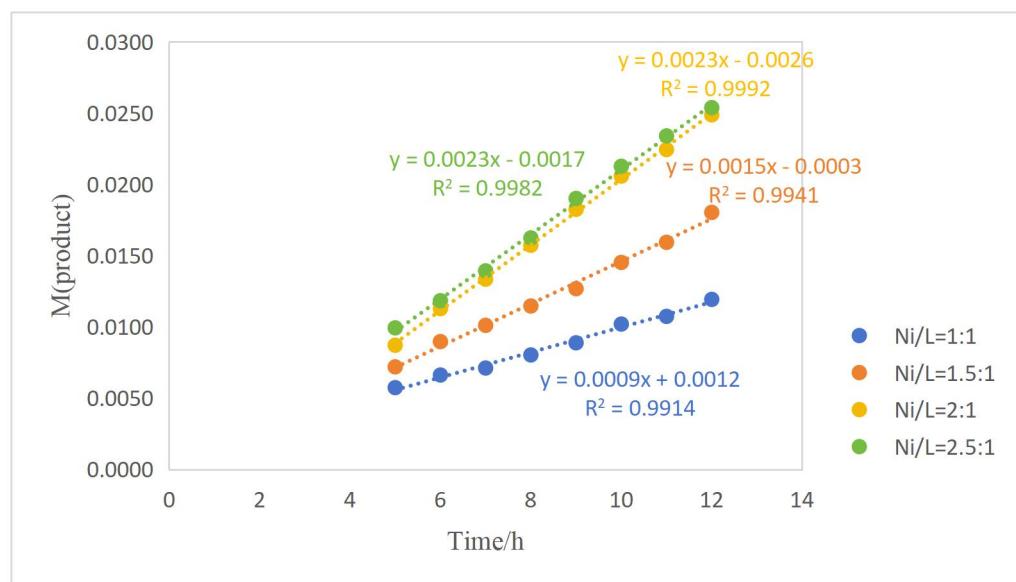
The molar concentration of product **70** in different ligand/nickel ratios at different time intervals

Time(h)	M($\text{Ni}/\text{L}=1:1$)	M($\text{Ni}/\text{L}=1.5:1$)	M($\text{Ni}/\text{L}=2:1$)	M($\text{Ni}/\text{L}=2.5:1$)
1	0.0021	0.0019	0.0020	0.0022
2	0.0028	0.0032	0.0035	0.0035
3	0.0038	0.0046	0.0057	0.0053
4	0.0050	0.0064	0.0072	0.0078
5	0.0057	0.0072	0.0087	0.0099
6	0.0066	0.0090	0.0113	0.0118
7	0.0071	0.0101	0.0133	0.0139
8	0.0080	0.0115	0.0157	0.0162
9	0.0089	0.0127	0.0182	0.0190
10	0.0102	0.0145	0.0206	0.0213
11	0.0107	0.0159	0.0224	0.0234
12	0.0119	0.0180	0.0249	0.0254

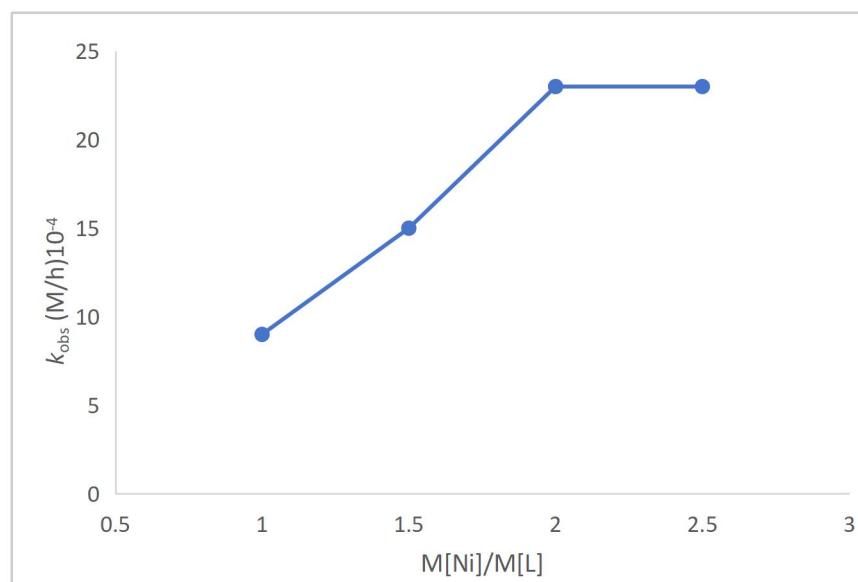
Supplementary Table S7

The k value of product **70** in different ligand/nickel ratios.

$M[Ni]/M[L]$	$k_{obs} (M \cdot h^{-1})$
1: 1	0. 0009
1. 5: 1	0. 0015
2: 1	0. 0023
2. 5:1	0. 0023

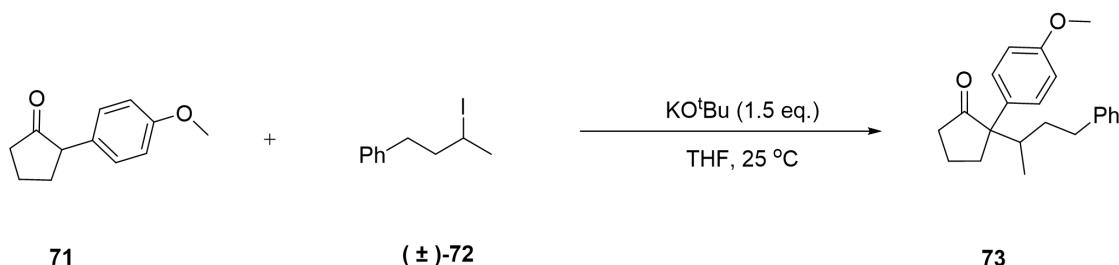


Supplementary Fig. S3 Time-course for the product **70** in different concentrations of ligand/nickel ratios



Supplementary Fig. S4 The reaction rate course in different concentrations of ligand/nickel ratios

10.2 Research on the Mechanism of Nucleophilic Substitution Reaction



General procedure E for racemates: To a flame-dried 10-mL Schlenk tube was added **71** (39.2 mg, 0.2 mmol) and anhydrous THF (1 mL) under N₂. The reaction mixture was stirred at room temperature for 30 minutes. Then (4-iodo-3-methylbutyl)benzene (1.5 equiv) was introduced into the system by a microsyringe and the mixture was stirred at room temperature for 12 h. The reaction mixture was quenched by the addition of saturated NH₄Cl (aq.) solution. The aqueous layer was extracted with ethyl acetate, and the organic layers were combined, washed with brine, dried over anhydrous Na₂SO₄ and concentrated under reduced pressure. The crude product was purified by column chromatography to afford target product.

2-(4-methoxyphenyl)-2-(4-phenylbutan-2-yl)cyclopentan-1-one (73)

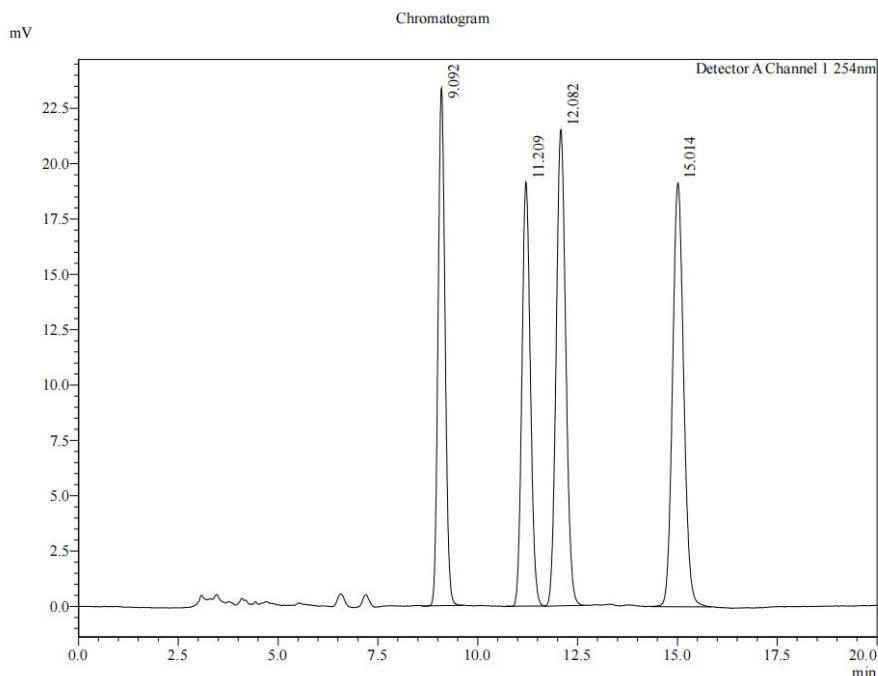
Colorless oil, $R_f = 0.2$ (petroleum ether/ethyl acetate = 10/1), 70% yield, 1:1.14 d.r.

¹H NMR (400 MHz, CDCl₃) δ 7.39 – 7.24 (m, 3H), 7.21 – 7.10 (m, 3H), 6.98 – 6.92 (m, 1H), 6.90 – 6.80 (m, 2H), 3.80 (s, 3H), 2.83 – 2.39 (m, 2.68H), 2.33 – 2.15 (m, 2.59H), 2.14 – 1.84 (m, 3.27H), 1.82 – 1.69 (m, 1.08H), 1.46 – 1.29 (m, 1.65H), 1.16 – 1.02 (m, 0.52H), 0.95 (d, $J = 6.7$ Hz, 1.38H, minor), 0.69 (d, $J = 6.8$ Hz, 1.61H, major).

¹³C NMR (101 MHz, CDCl₃) δ 219.8, 219.8, 158.4, 158.4, 142.6, 142.2, 130.1, 129.8, 128.5, 128.46, 128.4, 128.3, 128.3, 128.2, 125.7, 125.6, 113.8, 61.0, 60.6, 55.2, 40.5, 39.4, 38.4, 38.3, 36.0, 34.8, 33.8, 33.3, 27.7, 27.2, 18.6, 18.5, 15.5, 14.9.

HRMS (ESI) *m/z* calcd. for C₂₂H₂₇O₂ [M + H]⁺ 322.2006, found 322.2006.

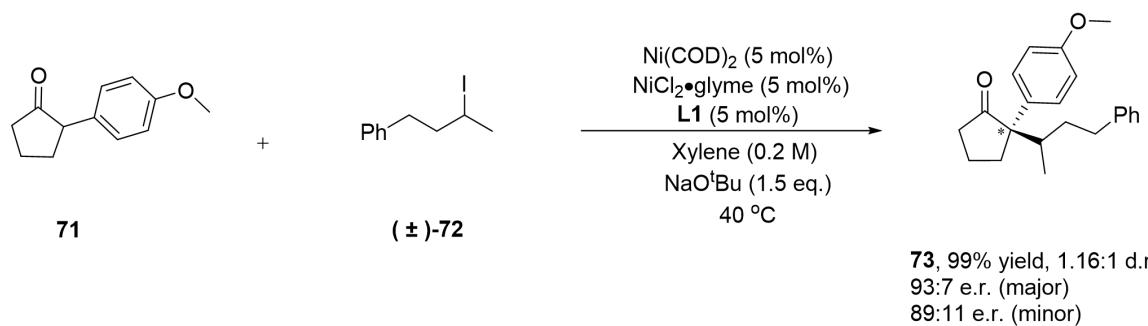
HPLC (ChiralPak AD-H column), hexane/*i*-PrOH = 99:1, flow rate = 1 mL/min, $\lambda = 254$ nm, $t_R = 9.092$ min, $t_R = 11.209$ min, $t_R = 12.082$ min, $t_R = 15.014$ min.



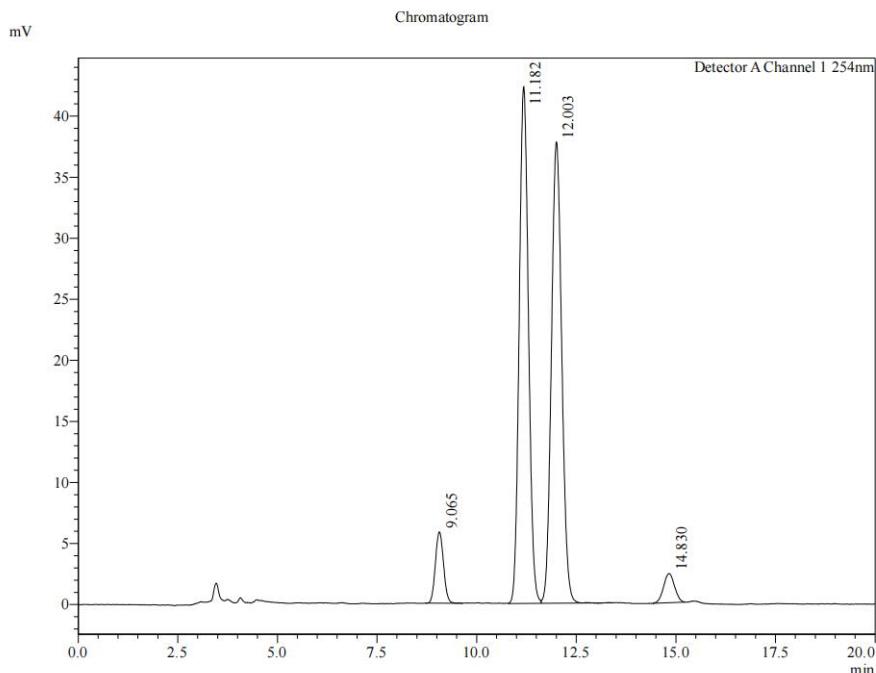
Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	9.092	284888	23363	21.924	28.092
2	11.209	282307	19146	21.726	23.021
3	12.082	361238	21508	27.800	25.861
4	15.014	370984	19149	28.550	23.025
Total		1299417	83167	100.000	100.000



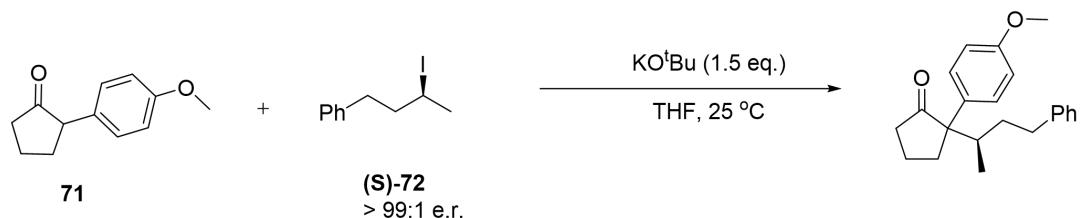
Synthesis through General procedure C.



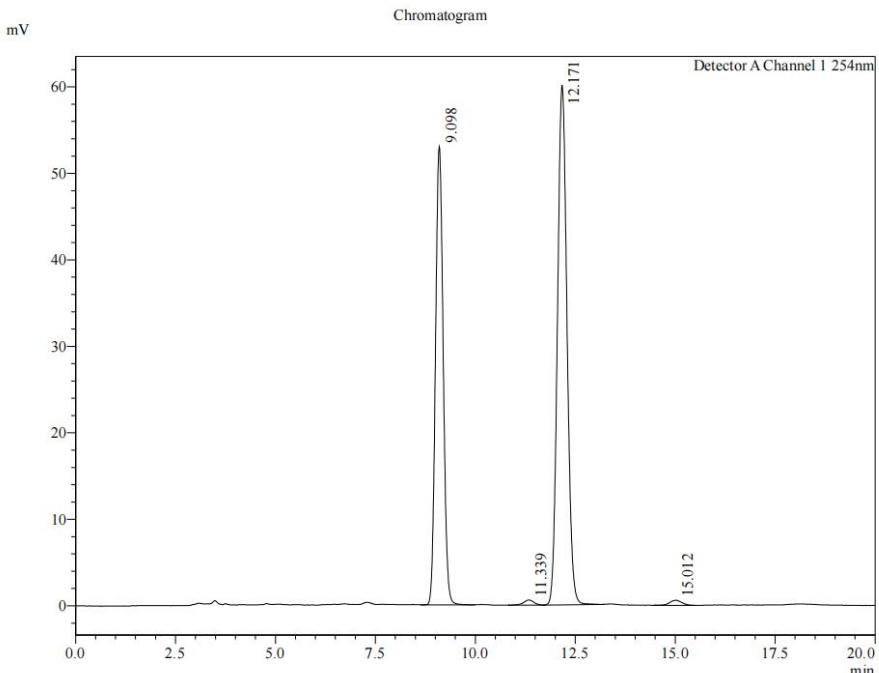
Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	9.065	82955	5845	5.559	6.621
2	11.182	683314	42286	45.795	47.895
3	12.003	680199	37775	45.586	42.786
4	14.830	45663	2383	3.060	2.699
Total		1492130	88289	100.000	100.000



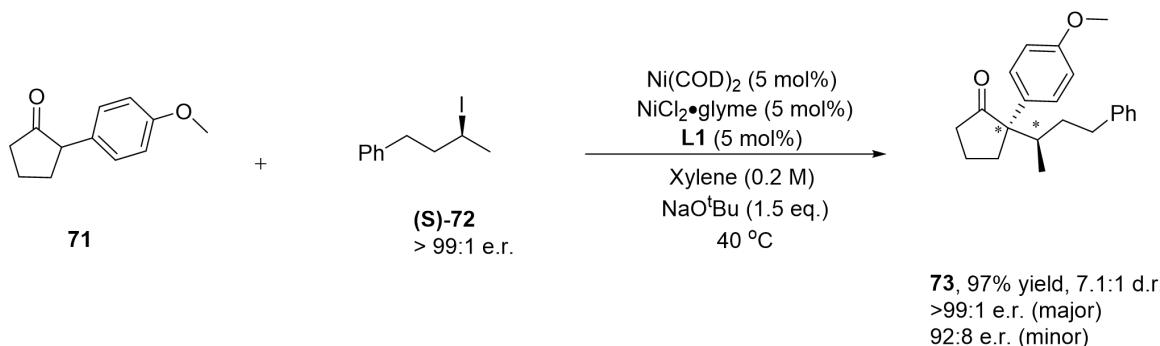
Synthesis through General procedure E.



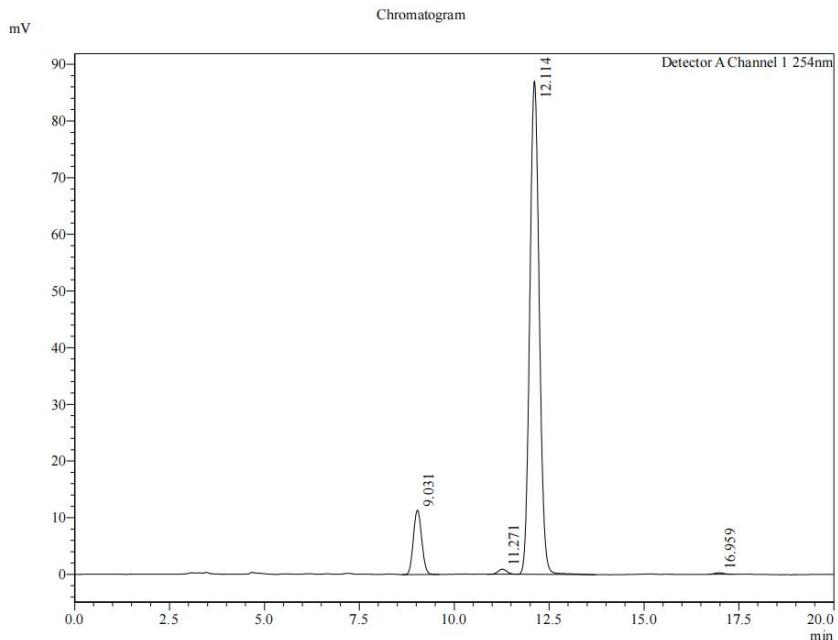
Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	9.098	709077	53005	41.025	46.403
2	11.339	10598	594	0.613	0.520
3	12.171	996434	60046	57.650	52.568
4	15.012	12312	582	0.712	0.509
Total		1728422	114226	100.000	100.000



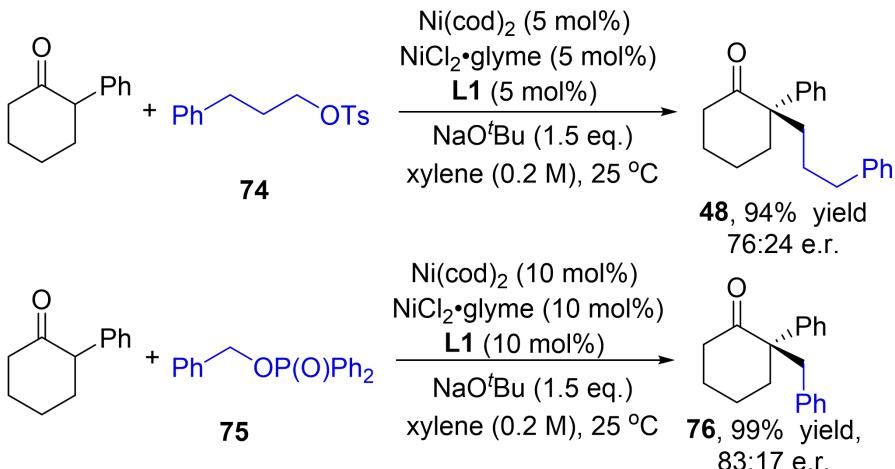
Synthesis through General procedure C.



Peak Table

Detector A Channel 1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	9.031	173095	11323	10.151	11.385
2	11.271	14107	886	0.827	0.891
3	12.114	1513804	86998	88.773	87.470
4	16.959	4240	253	0.249	0.255
Total		1705247	99460	100.000	100.000

Other type of alkyl electrophiles



Synthesis through General procedure C.

(R)-2-benzyl-2-phenylcyclohexan-1-one (76)

Colorless oil, $R_f = 0.4$ (petroleum ether/Ether = 20/1), 99% yield, 83:17 e.r.

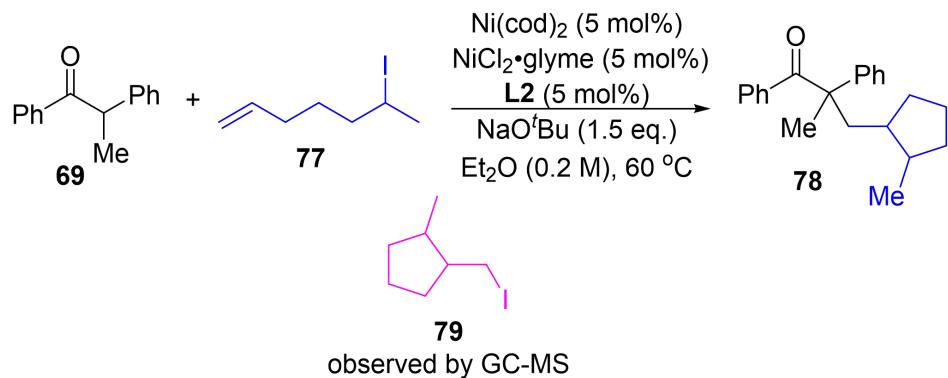
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.33 – 7.20 (m, 3H), 7.17 – 7.01 (m, 3H), 6.95 (dd, $J = 8.1, 1.6$ Hz, 2H), 6.58 – 6.52 (m, 2H), 3.12 (d, $J = 13.5$ Hz, 1H), 2.98 (d, $J = 13.4$ Hz, 1H), 2.53 – 2.44 (m, 1H), 2.44 – 2.33 (m, 2H), 2.00 – 1.90 (m, 1H), 1.77 – 1.55 (m, 4H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 213.3, 139.9, 137.2, 130.8, 128.6, 127.4, 127.3, 126.8, 126.0, 58.0, 46.3, 40.2, 34.7, 28.3, 21.4.

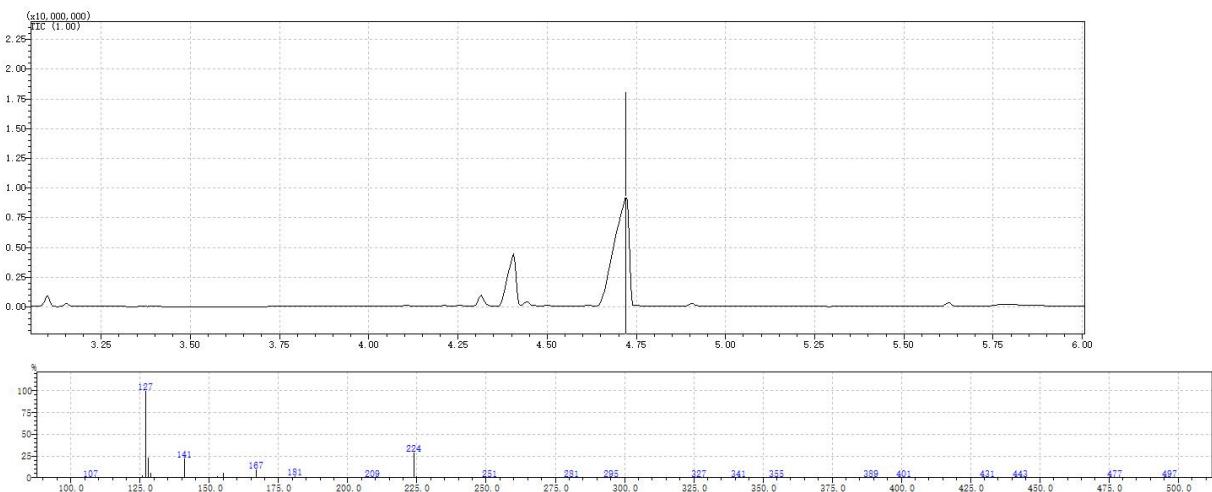
HRMS (ESI) *m/z* calcd. for C₁₉H₂₁O [M + H]⁺ 265.1587, found 265.1592.

HPLC (ChiralPak AD-H column), hexane/i-PrOH = 99:1, flow rate = 1 mL/min, λ = 220 nm, t_R = 7.026 min (major), t_R = 8.047 min (minor)

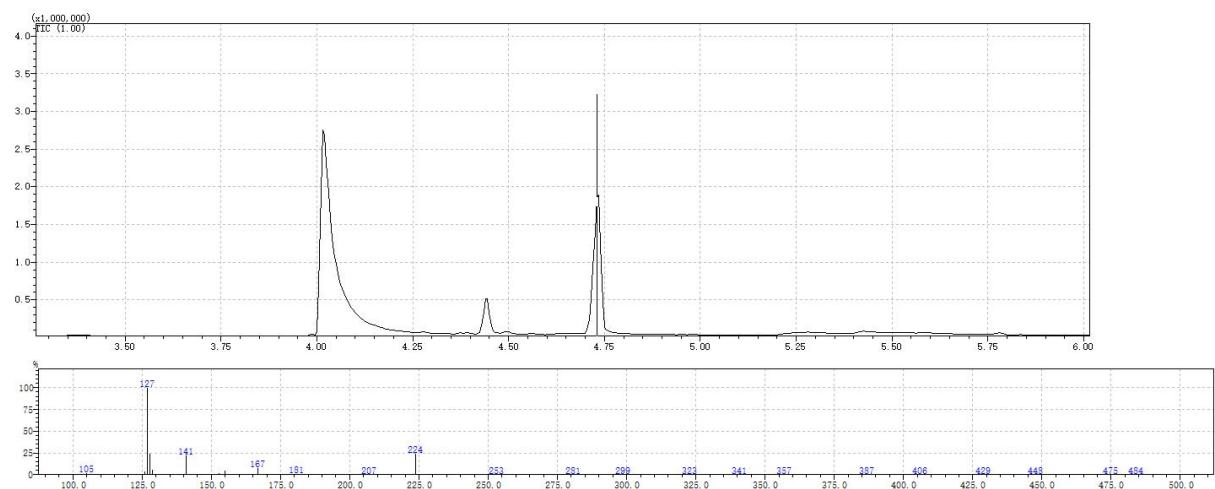
10.3 Cyclization of Olefin-tethered Alkyl Iodide



The Ni(cod)₂ (2.9 mg, 0.01 mmol, 5 mol%), NiCl₂•glyme (2.2 mg, 0.01 mmol, 5 mol%), **L2** (0.01 mmol, 5 mol%) and 'BuONa (29.0 mg, 0.3 mmol, 1.5 equiv) were introduced into a flame-dried Schlenk tube in an nitrogen-filled glove box. After taking out from the glove box, Schlenk tube was connected to Schlenk line under N₂. 1 mL dry Et₂O was injected into the Schlenk tube, the mixture was stirred at r.t. for 30 min. The ketone **69** (0.2 mmol, 1.0 equiv) was then added rapidly under nitrogen. After 30 min, 6-iodohept-1-ene **77** (0.3 mmol, 1.5 equiv) was introduced into the system by a microsyringe under N₂. The resulting mixture was stirred under 60 °C. The reaction progress was monitored by removing aliquots (~10 μL) from the reaction mixture via syringe under N₂. Each aliquot was quenched by EA (4.0 mL) in an 8.0 mL tube. The mixture was filtered with a filter head into 2.0 mL GC-MS vial and analyzed by gas chromatography.



Supplementary Fig. S5 standard samples 1-(iodomethyl)-2-methylcyclopentane **79** in GC-MS



Supplementary Fig. S6 GC-MS evaluation of the 18-hour reaction.

11. DFT Calculations

11.1 Computational Details.

Complete reference for Gaussian 09

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Men-nucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Ko-bayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyen-gar, J. T omasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cio-slowski, D. J. Fox, Gaussian 09, revision D.01; Gaussian, Inc.: Wallingford, CT, **2013**.

Computational methods

All of the density functional theory (DFT) calculations were performed with the Gaussian 09 series of programs. The B3LYP-D3 functional¹²⁻¹⁵ with the standard 6-31G(d) basis set (SDD basis set for Ni) was used for the geometry optimizations. Harmonic vibrational frequency calculations were performed for all of the stationary points to determine whether they are local minima or transition structures and to derive the thermochemical corrections for the enthalpies and free energies. The M06 functional¹⁶ with the 6-311+G(d,p) basis set (SDD basis set for Ni) was used to calculate the single-point energies in diethyl ether solvent to provide more accurate energy information. The solvent effect was considered by single-point calculations based on the solution-phase stationary points with the SMD^{17,18} continuum solvation model. The Gibbs free energies ($\Delta G_{(Et_2O)}$) reported in this paper were obtained using Eq. (1), $\Delta G_{(Et_2O)} = \Delta G_{M06(Et_2O)} + \Delta G_{B3LYP-D3(\text{correction})}$ (1) where $\Delta G_{B3LYP-D3(\text{correction})}$ is the thermochemical correction for the Gibbs free energy calculated at the B3LYP-D3/6-31G(d) (SDD basis set for Ni) level in the gas phase, and $\Delta E_{M06L(Et_2O)}$ is the single-point energy calculated at the M06/6-311+G(d,p) (SDD basis set for Ni) level in diethyl ether solvent relative to stationary points. The $\Delta G_{(Et_2O)}$ values are used to discuss the energies. The 3D images of the calculated structures were prepared using CYLview.¹⁹

Supplementary Table S8

B3LYP-D3 and M06 calculated absolute energies, enthalpies, and free energies for all structures

Geometry	$E_{(\text{elec-B3LYP-D3})}^1$	$H_{(\text{corr-B3LYP-D3})}^2$	$G_{(\text{cor-B3LYP-D3})}^3$	$E_{(\text{solv-M06})}^4$	IF ⁵
³INT-1	-3406.7033	0.765202	0.630158	-3405.6311	
³INT-2	-3601.1592	1.014785	0.854394	-3599.7325	
³TS-3-S	-3601.1592	1.014785	0.854394	-3599.7325	277.87 <i>i</i>

³TS-3-R	-3770.446	1.147946	0.970934	-3768.8872	294.75 <i>i</i>
³INT-4	-3770.4991	1.152345	0.978226	-3768.9535	
<i>t</i>BuO-	-233.04406	0.127898	0.091853	-233.04039	
<i>t</i>BuOH	-233.67727	0.144086	0.107628	-233.5853	
A	-654.68493	0.248565	0.194025	-654.42449	
70	-812.5193	0.383329	0.315836	-812.09248	
I-Bu	-169.27924	0.13153	0.090954	-169.15398	
Cl	-460.24873	0.00236	-0.015023	-460.34543	
I-	-11.51891	0.00236	-0.016848	-11.553415	

¹The electronic energy calculated by B3LYP-D3 in gas phase. ²The thermal correction to enthalpy calculated by B3LYP-D3 in gas phase. ³The thermal correction to Gibbs free energy calculated by B3LYP-D3 in gas phase. ⁴The electronic energy calculated by M06 in diethyl ether solvent. ⁵The B3LYP-D3 calculated imaginary frequencies for the transition states.

11.2 B3LYP-D3 geometries for all the optimized compounds and transition states in gas phase

³INT-1

C	-2.277235	-3.259054	0.547993
C	-0.000117	-3.306667	-0.000213
C	-0.000098	-4.749405	-0.000146
C	-1.224418	-5.400411	0.289216
C	-2.366014	-4.651730	0.563200
C	1.224233	-5.400409	-0.289419
H	-1.260652	-6.485928	0.295316
H	-3.315442	-5.124889	0.788483
C	2.365830	-4.651720	-0.563415
C	2.277008	-3.259049	-0.548331
H	1.260489	-6.485925	-0.295422
H	3.315288	-5.124865	-0.788591
N	-1.115880	-2.602502	0.268556
N	1.115630	-2.602490	-0.269054
C	-4.497536	-0.453367	1.191339
C	-5.510241	-1.661860	1.158931
C	5.510153	-1.661921	-1.158743
C	4.497471	-0.453409	-1.191366
N	-3.227738	-1.061701	0.778081
C	3.376973	-2.352594	-0.819940
O	4.597521	-2.826188	-1.119261

C	6.327155	-1.755575	-2.439189
H	5.670891	-1.815982	-3.313075
H	6.976009	-2.636993	-2.426099
C	6.387619	-1.745427	0.086022
H	6.956590	-2.680267	0.068626
H	5.788379	-1.716504	0.998321
H	4.366918	-0.163283	-2.242347
C	-3.377143	-2.352589	0.819715
O	-4.597679	-2.826167	1.119161
C	-6.388046	-1.745263	-0.085591
H	-6.957040	-2.680088	-0.068121
H	-5.789054	-1.716273	-0.998053
C	-6.326883	-1.755561	2.439610
H	-5.670357	-1.816050	3.313293
H	-6.975780	-2.636948	2.426651
H	-4.366781	-0.163189	2.242280
N	3.227575	-1.061708	-0.778327
Ni	-1.262194	-0.541545	0.308632
Ni	1.262079	-0.541525	-0.308574
C	7.481973	4.949044	-1.057753
C	6.893841	3.806788	-1.563039
C	6.203980	2.908860	-0.714724
C	6.102163	3.180130	0.678093
C	6.717959	4.357748	1.165546
C	7.391998	5.221718	0.320914
C	5.609809	1.720290	-1.240702
C	5.370624	2.243952	1.521328
C	4.798174	1.056829	0.955479
C	4.951367	0.804652	-0.467442
C	4.086113	0.180823	1.812705
H	3.614503	-0.698251	1.399363
C	3.933717	0.443316	3.160006
C	4.501150	1.601221	3.714381
C	5.201683	2.476669	2.906763
H	5.703515	1.546899	-2.311344
H	8.010295	5.632788	-1.716289
H	6.953926	3.579885	-2.625085
H	6.669587	4.600835	2.220929
H	7.853641	6.117904	0.726487
H	3.353670	-0.237165	3.775493
H	4.381239	1.817761	4.772299
H	5.621270	3.369714	3.355772
C	-3.933977	0.443193	-3.160086
C	-4.086364	0.180719	-1.812785

C	-4.798251	1.056840	-0.955526
C	-5.370515	2.244062	-1.521344
C	-5.201593	2.476755	-2.906792
C	-4.501240	1.601196	-3.714437
C	-4.951438	0.804688	0.467405
C	-6.101846	3.180378	-0.678073
C	-6.203750	2.909069	0.714729
C	-5.609766	1.720392	1.240676
C	-6.893453	3.807091	1.563073
H	-6.953616	3.580142	2.625105
C	-7.481323	4.949502	1.057833
C	-7.391211	5.222253	-0.320808
C	-6.717329	4.358186	-1.165468
H	-3.354081	-0.237379	-3.775616
H	-3.614901	-0.698444	-1.399466
H	-5.621080	3.369852	-3.355788
H	-4.381333	1.817708	-4.772362
H	-5.703485	1.547000	2.311318
H	-8.009525	5.633316	1.716392
H	-7.852611	6.118583	-0.726339
H	-6.668816	4.601365	-2.220821
Cl	-0.438567	0.130776	-1.846132
Cl	0.438482	0.129390	1.846366
H	7.087902	-0.905414	0.111533
H	6.955628	-0.863022	-2.534207
H	-6.955285	-0.862983	2.534865
H	-7.088317	-0.905230	-0.110843

³INT-2

C	-2.176607	3.573677	-0.997373
C	0.034147	3.610294	-0.212676
C	0.001098	5.052834	-0.130039
C	-1.179409	5.710291	-0.556424
C	-2.267477	4.965083	-0.996379
C	1.145035	5.705722	0.383783
H	-1.225219	6.794896	-0.524244
H	-3.189528	5.438019	-1.316446
C	2.245607	4.958850	0.792192
C	2.205231	3.572669	0.646730
H	1.147351	6.788746	0.466246
H	3.130031	5.427160	1.209896
N	-1.047866	2.904669	-0.604767
N	1.133895	2.907840	0.123521
C	-4.427398	0.743886	-1.249491

C	-5.393743	1.934459	-1.607761
C	5.365281	2.001517	1.621022
C	4.435414	0.775626	1.267414
N	-3.108417	1.393322	-1.262132
C	3.289613	2.677183	1.000555
O	4.431996	3.145687	1.528593
C	5.860153	1.930203	3.059786
H	5.017115	1.841868	3.752520
H	6.436714	2.823296	3.320734
C	6.501230	2.268161	0.640223
H	7.014841	3.195203	0.913905
H	6.131542	2.361637	-0.382855
H	4.169126	0.276400	2.204884
C	-3.278387	2.677075	-1.285113
O	-4.534933	3.132821	-1.407312
C	-6.615421	2.083716	-0.716822
H	-7.192215	2.967821	-1.007281
H	-6.333576	2.172323	0.334145
C	-5.753212	1.904623	-3.091263
H	-4.848352	1.821663	-3.702974
H	-6.288361	2.815681	-3.376942
H	-4.453165	0.019936	-2.067691
N	3.199384	1.401024	0.783710
C	7.322652	-4.631799	0.509670
C	6.769332	-3.536316	1.141640
C	6.201535	-2.477449	0.394222
C	6.191469	-2.533049	-1.027418
C	6.766080	-3.669664	-1.645006
C	7.318869	-4.694081	-0.897259
C	5.606311	-1.358289	1.052418
C	5.596390	-1.427086	-1.765838
C	5.045042	-0.303958	-1.064896
C	5.038567	-0.308200	0.387021
C	4.516990	0.767957	-1.829915
H	4.104941	1.629579	-1.326325
C	4.489781	0.736607	-3.210587
C	5.006030	-0.375583	-3.893864
C	5.551581	-1.425436	-3.180431
H	5.585933	-1.372304	2.140821
H	7.755677	-5.441095	1.090778
H	6.759425	-3.472923	2.227443
H	6.779928	-3.754434	-2.725652
H	7.751099	-5.553859	-1.401737
H	4.056399	1.568005	-3.758481

H	4.979270	-0.413152	-4.979195
H	5.951662	-2.269401	-3.730354
C	-3.477227	2.113005	2.886174
C	-3.938944	1.725011	1.641567
C	-4.294296	0.383407	1.354542
C	-4.251395	-0.564204	2.426464
C	-3.766508	-0.138528	3.685414
C	-3.366213	1.164921	3.915169
C	-4.662791	-0.066943	0.023313
C	-4.713946	-1.928373	2.212127
C	-5.191211	-2.289198	0.922896
C	-5.106104	-1.345371	-0.147840
C	-5.679648	-3.595695	0.690953
H	-6.020007	-3.850640	-0.307754
C	-5.690556	-4.537888	1.700373
C	-5.205418	-4.192570	2.976044
C	-4.729761	-2.916986	3.223999
H	-3.208135	3.151197	3.061357
H	-4.050413	2.487744	0.885707
H	-3.700788	-0.849151	4.501430
H	-2.990918	1.454676	4.892846
H	-5.329752	-1.709639	-1.147528
H	-6.062792	-5.541052	1.510945
H	-5.203918	-4.930787	3.773666
H	-4.367561	-2.685686	4.219484
Ni	-1.245422	0.855966	-0.619905
Ni	1.593426	0.956963	-0.317580
H	6.505011	1.052399	3.181127
H	7.220360	1.444123	0.668206
H	-7.251667	1.199514	-0.822658
H	-6.391800	1.039793	-3.302148
O	-1.802252	-0.806877	0.046283
C	-1.111626	-1.910956	0.293454
C	-1.465423	-3.120921	-0.255799
C	0.008418	-1.719906	1.264243
C	-0.182953	-0.856837	2.358918
C	1.278307	-2.291599	1.078060
C	0.844595	-0.624806	3.271793
H	-1.152025	-0.383951	2.484939
C	2.305431	-2.066202	1.996536
H	1.456485	-2.909325	0.203113
C	2.088855	-1.241292	3.103224
H	0.670451	0.029524	4.122868
H	3.275133	-2.527401	1.836649

H	2.883918	-1.075637	3.827330
C	-2.460043	-3.191460	-1.348577
C	-3.312577	-4.303639	-1.498672
C	-2.559022	-2.180205	-2.332998
C	-4.247477	-4.379454	-2.534203
H	-3.271071	-5.113559	-0.778564
C	-3.483281	-2.258882	-3.370312
H	-1.888531	-1.333735	-2.283247
C	-4.351461	-3.353280	-3.473418
H	-4.897070	-5.249618	-2.603495
H	-3.516646	-1.464308	-4.113553
H	-5.074443	-3.414112	-4.283087
C	-0.974375	-4.440918	0.298980
H	-0.549052	-5.085787	-0.482583
H	-0.225533	-4.311134	1.081164
H	-1.802267	-5.003560	0.755314
Cl	0.451176	0.261968	-2.118779

³TS-3-R

C	-3.825681	-3.199986	0.008113
C	-1.585007	-3.797444	-0.289105
C	-1.957042	-5.013541	-0.964349
C	-3.345385	-5.255540	-1.138588
C	-4.277812	-4.333661	-0.675099
C	-0.908618	-5.851133	-1.410490
H	-3.667635	-6.153723	-1.657124
H	-5.342004	-4.477909	-0.828657
C	0.420236	-5.461487	-1.241146
C	0.688234	-4.225519	-0.654806
H	-1.148350	-6.790027	-1.901123
H	1.241677	-6.076551	-1.591853
N	-2.501068	-2.969474	0.239498
N	-0.297568	-3.415080	-0.181268
C	-5.112389	-0.089983	1.374986
C	-6.438450	-0.907588	1.161486
C	4.223254	-3.206383	-0.762517
C	3.469646	-1.908073	-0.277253
N	-4.076532	-1.096342	1.097911
C	1.993274	-3.582016	-0.575203
O	3.139660	-4.245046	-0.743359
C	4.633256	-3.065895	-2.224515
H	3.776808	-2.767427	-2.837764
H	5.030311	-4.013613	-2.602302
C	5.368771	-3.685680	0.111265

H	5.775820	-4.623630	-0.279675
H	5.062422	-3.834528	1.147467
H	3.612788	-1.153711	-1.057031
C	-4.640172	-2.116034	0.514992
O	-5.975727	-2.069667	0.355128
C	-7.572890	-0.213289	0.426992
H	-8.416214	-0.900376	0.304881
H	-7.269154	0.150948	-0.554137
C	-6.906566	-1.488304	2.497562
H	-6.080530	-1.995607	3.007744
H	-7.714320	-2.208461	2.336229
H	-5.056788	0.162463	2.437817
N	2.059917	-2.316411	-0.311482
C	4.913919	3.145022	2.940771
C	4.911092	2.247894	1.891604
C	4.405942	0.936966	2.058234
C	3.918902	0.517229	3.327456
C	3.928007	1.461678	4.381544
C	4.410481	2.745641	4.193770
C	4.305560	0.052458	0.938855
C	3.440626	-0.851138	3.474904
C	3.395091	-1.720093	2.338043
C	3.787697	-1.207878	1.037586
C	2.953272	-3.052936	2.530454
H	2.932316	-3.740544	1.696611
C	2.556583	-3.518255	3.768752
C	2.582966	-2.659353	4.878610
C	3.021684	-1.358153	4.727194
H	4.602766	0.433694	-0.036165
H	5.292276	4.153381	2.799744
H	5.286322	2.539656	0.915138
H	3.545023	1.190663	5.359062
H	4.399591	3.449420	5.021861
H	2.219004	-4.545102	3.877154
H	2.265216	-3.015065	5.854644
H	3.050185	-0.717494	5.601250
C	-4.886639	0.388864	-3.072383
C	-5.001501	0.258238	-1.701444
C	-4.732441	1.335200	-0.819043
C	-4.340023	2.590143	-1.390702
C	-4.219886	2.683329	-2.797977
C	-4.481029	1.611303	-3.628633
C	-4.830920	1.210617	0.627021
C	-4.065422	3.735167	-0.532859

C	-4.165212	3.569768	0.875637
C	-4.545223	2.297429	1.405494
C	-3.885746	4.654841	1.738104
H	-3.949928	4.499358	2.812087
C	-3.529393	5.887743	1.230604
C	-3.445588	6.065167	-0.163093
C	-3.703326	5.012425	-1.023071
H	-5.100115	-0.461005	-3.714359
H	-5.317218	-0.696709	-1.310295
H	-3.907998	3.618668	-3.247461
H	-4.372323	1.717263	-4.703983
H	-4.586395	2.203826	2.488883
H	-3.309614	6.713849	1.900153
H	-3.168120	7.033883	-0.569484
H	-3.625276	5.186913	-2.090108
Ni	-2.156314	-1.394361	1.463369
Ni	0.314205	-1.555879	0.393408
H	5.392814	-2.285351	-2.329440
H	6.161359	-2.930830	0.096289
H	-7.909417	0.643893	1.019074
H	-7.275491	-0.686828	3.146963
O	0.604109	0.378152	0.330262
C	0.192428	0.989448	-0.729426
C	0.127594	2.386629	-0.862551
C	-0.232392	0.038231	-1.825234
C	0.696525	-0.556056	-2.697761
C	-1.566175	-0.399834	-1.845123
C	0.293275	-1.575884	-3.560608
H	1.735149	-0.242818	-2.700407
C	-1.960219	-1.428858	-2.702016
H	-2.286226	0.052885	-1.171642
C	-1.031535	-2.022839	-3.557233
H	1.022518	-2.024910	-4.229740
H	-2.991736	-1.766094	-2.688736
H	-1.337091	-2.828397	-4.219805
C	0.275383	3.295487	0.294090
C	-0.180100	4.628808	0.201530
C	0.917156	2.923018	1.502364
C	-0.007002	5.536370	1.245305
H	-0.696333	4.967139	-0.688411
C	1.091647	3.836334	2.540674
H	1.290704	1.916204	1.617716
C	0.635054	5.150784	2.422999
H	-0.381064	6.550945	1.132301

H	1.608542	3.511267	3.439623
H	0.778900	5.861976	3.232461
C	-0.516767	2.937750	-2.122462
H	-0.503917	2.204044	-2.931223
H	-1.565016	3.209354	-1.946747
H	-0.003395	3.833333	-2.485169
Cl	-0.293713	-1.516217	2.661579
I	4.639645	0.898268	-3.148928
C	2.485862	2.128419	-1.647754
C	3.101314	3.357491	-1.073349
H	2.020627	2.121939	-2.620104
H	2.544178	1.209834	-1.087276
C	2.884568	4.638503	-1.880585
H	2.723026	3.482791	-0.048562
H	4.175749	3.173125	-0.954832
C	3.475026	5.859407	-1.170020
H	3.333465	4.516118	-2.874962
H	1.810083	4.795810	-2.027735
H	3.336411	6.772045	-1.760784
H	2.991127	6.008917	-0.196795
H	4.551269	5.733157	-0.997144

³TS-3-S

C	1.413567	4.188636	0.440994
C	-0.576553	3.613239	-0.628550
C	-0.577854	4.848902	-1.369018
C	0.473100	5.753987	-1.112075
C	1.465036	5.432841	-0.184319
C	-1.627405	5.047835	-2.309105
H	0.500763	6.701972	-1.641562
H	2.273032	6.118561	0.045494
C	-2.580798	4.057548	-2.501879
C	-2.529570	2.902132	-1.716490
H	-1.651587	5.962513	-2.893703
H	-3.359667	4.156616	-3.250470
N	0.427332	3.284735	0.199909
N	-1.581061	2.718614	-0.745676
C	3.417196	2.204524	2.749157
C	4.075623	3.627720	2.900677
C	-4.957454	0.316330	-2.625399
C	-4.218435	-0.298342	-1.372564
N	2.277924	2.466445	1.854101
C	-3.386523	1.749241	-1.838384
O	-4.421147	1.703150	-2.685645

C	-4.495590	-0.375419	-3.905833
H	-3.401404	-0.395085	-3.960459
H	-4.880646	0.144684	-4.788159
C	-6.471396	0.403482	-2.533727
H	-6.875899	0.883727	-3.430289
H	-6.786446	0.968234	-1.654944
H	-3.701254	-1.205930	-1.699504
C	2.386820	3.674482	1.395900
O	3.438168	4.402393	1.800652
C	5.585352	3.702756	2.743774
H	5.919830	4.741968	2.823625
H	5.920697	3.293787	1.790496
C	3.607698	4.285725	4.198630
H	2.515835	4.247204	4.279216
H	3.925462	5.332245	4.233634
H	3.005054	1.933133	3.725861
N	-3.187081	0.704056	-1.085038
C	-6.608961	-4.542382	2.428445
C	-5.986880	-4.000889	1.321264
C	-5.844295	-2.600584	1.181234
C	-6.352253	-1.728293	2.183003
C	-6.979909	-2.313730	3.308267
C	-7.105091	-3.686340	3.430479
C	-5.166890	-2.049348	0.050388
C	-6.214334	-0.289901	1.994010
C	-5.594499	0.222897	0.809318
C	-5.031800	-0.706573	-0.153493
C	-5.553799	1.628715	0.631554
H	-5.145067	2.047267	-0.276018
C	-6.048877	2.500203	1.582702
C	-6.613366	1.996214	2.764817
C	-6.699540	0.630214	2.952591
H	-4.709362	-2.746601	-0.646989
H	-6.714807	-5.619004	2.528521
H	-5.591958	-4.643448	0.539398
H	-7.378778	-1.687250	4.097972
H	-7.592331	-4.104708	4.306944
H	-5.996973	3.571930	1.411775
H	-6.991563	2.673970	3.524838
H	-7.154615	0.263211	3.865251
C	5.230241	1.666977	-1.298285
C	4.736388	1.862606	-0.020615
C	4.715018	0.815505	0.935065
C	5.224797	-0.465783	0.546161

C	5.672782	-0.644016	-0.784077
C	5.677025	0.396757	-1.693325
C	4.219134	0.996429	2.289041
C	5.287501	-1.554718	1.513162
C	4.920583	-1.291475	2.862272
C	4.364758	-0.016794	3.194633
C	5.028193	-2.310175	3.837248
H	4.747418	-2.085514	4.863689
C	5.451297	-3.577555	3.486093
C	5.760254	-3.858853	2.141551
C	5.684636	-2.870099	1.175450
H	5.271520	2.501093	-1.993512
H	4.391810	2.850686	0.249305
H	6.013737	-1.615949	-1.114506
H	6.030210	0.223302	-2.705186
H	3.993749	0.115941	4.209513
H	5.521225	-4.359489	4.237051
H	6.052400	-4.863542	1.850195
H	5.890016	-3.134814	0.145069
Ni	0.941344	1.414819	0.868446
Ni	-1.841050	1.037592	0.367594
H	-4.856532	-1.409663	-3.920842
H	-6.888712	-0.605235	-2.457245
H	6.057051	3.124447	3.544624
H	4.036674	3.759627	5.058617
Cl	-2.062275	0.487670	2.494141
O	-0.096274	0.085021	-0.155115
C	-0.002685	-0.297072	-1.408779
C	-0.343889	-1.608553	-1.816397
C	0.520853	0.739045	-2.348525
C	1.775647	1.326107	-2.131452
C	-0.301112	1.237480	-3.369353
C	2.186310	2.405556	-2.913286
H	2.437572	0.938187	-1.362991
C	0.105809	2.325000	-4.139459
H	-1.276024	0.791146	-3.534392
C	1.350416	2.915205	-3.907975
H	3.159968	2.848172	-2.737084
H	-0.552622	2.716874	-4.909142
H	1.669546	3.765176	-4.504718
C	-1.169193	-2.535079	-0.969727
C	-1.761951	-3.670729	-1.565165
C	-1.363355	-2.374232	0.419561
C	-2.473227	-4.605782	-0.812312

H	-1.660290	-3.852767	-2.627640
C	-2.088964	-3.300418	1.165830
H	-0.942253	-1.530791	0.938444
C	-2.633302	-4.433231	0.563145
H	-2.893826	-5.476464	-1.309069
H	-2.221421	-3.121205	2.228450
H	-3.184074	-5.159666	1.152835
C	-0.350731	-1.889829	-3.316153
H	0.359353	-1.258149	-3.848852
H	-1.346969	-1.720639	-3.744448
H	-0.072398	-2.924440	-3.528696
I	4.220320	-3.786862	-2.496695
C	1.671098	-2.236249	-1.439758
C	1.958455	-2.243913	0.028400
H	1.392007	-3.166869	-1.916527
H	2.181396	-1.533651	-2.086516
C	1.793285	-3.618515	0.693244
H	1.302506	-1.513696	0.528025
H	2.972823	-1.863751	0.185523
C	1.798327	-3.520443	2.219570
H	2.604423	-4.266594	0.343997
H	0.853542	-4.072627	0.356947
H	1.722086	-4.512243	2.679757
H	0.952070	-2.918933	2.577044
H	2.721089	-3.056512	2.581538

³INT-4

C	-4.282585	-2.939023	0.107583
C	-2.085672	-3.714874	-0.092394
C	-2.532729	-4.935392	-0.711307
C	-3.932702	-5.091101	-0.899322
C	-4.802996	-4.079044	-0.515988
C	-1.540667	-5.859410	-1.110450
H	-4.308094	-5.993228	-1.373103
H	-5.871282	-4.153220	-0.688987
C	-0.191043	-5.542503	-0.965823
C	0.152699	-4.299297	-0.434429
H	-1.839921	-6.802511	-1.558350
H	0.591496	-6.215589	-1.297698
N	-2.950128	-2.789707	0.361262
N	-0.776286	-3.418356	0.018368
C	-5.336527	0.375155	1.136335
C	-6.721699	-0.296765	0.810684
C	3.733190	-3.513870	-0.732833

C	3.086744	-2.141991	-0.294673
N	-4.406739	-0.761251	1.066236
C	1.494600	-3.729044	-0.422557
O	2.578401	-4.472933	-0.612325
C	4.098971	-3.490567	-2.210345
H	3.235140	-3.188994	-2.812034
H	4.435406	-4.480084	-2.536843
C	4.862796	-4.023242	0.142656
H	5.195378	-5.006807	-0.203768
H	4.566827	-4.094052	1.190955
H	3.224861	-1.447340	-1.130562
C	-5.023356	-1.760104	0.498368
O	-6.319743	-1.589129	0.193661
C	-7.628075	0.442877	-0.158838
H	-8.538059	-0.137587	-0.340011
H	-7.135930	0.635850	-1.112527
C	-7.446606	-0.656419	2.107765
H	-6.779380	-1.202504	2.783567
H	-8.318676	-1.282090	1.895500
H	-5.375211	0.715344	2.175145
N	1.650067	-2.457018	-0.219292
C	5.654994	2.764352	2.399257
C	5.371663	1.831049	1.421551
C	4.671591	0.643330	1.742015
C	4.261348	0.388910	3.080404
C	4.572546	1.362864	4.059535
C	5.249105	2.524280	3.726498
C	4.298584	-0.265335	0.703864
C	3.545996	-0.848178	3.367039
C	3.229620	-1.756743	2.304629
C	3.577261	-1.400310	0.941235
C	2.588673	-2.976825	2.636324
H	2.381530	-3.701980	1.862033
C	2.232186	-3.285666	3.934766
C	2.506945	-2.376617	4.968618
C	3.157884	-1.191442	4.683247
H	4.572272	-0.007823	-0.318100
H	6.182710	3.679619	2.146860
H	5.662821	1.997282	0.387809
H	4.275944	1.214352	5.092178
H	5.466952	3.257135	4.498902
H	1.736152	-4.228011	4.149340
H	2.220661	-2.606538	5.991045
H	3.381251	-0.515095	5.500622

C	-4.277807	0.319804	-3.212280
C	-4.661238	0.361292	-1.885478
C	-4.451219	1.508858	-1.078693
C	-3.848970	2.657217	-1.689694
C	-3.447492	2.570475	-3.044704
C	-3.646032	1.428708	-3.795399
C	-4.825034	1.563883	0.326730
C	-3.660657	3.882420	-0.923745
C	-4.059906	3.901563	0.440706
C	-4.620661	2.722280	1.022567
C	-3.883516	5.072437	1.213935
H	-4.187173	5.060024	2.257741
C	-3.328015	6.209142	0.660758
C	-2.931618	6.199330	-0.690455
C	-3.096422	5.063211	-1.463121
H	-4.459135	-0.577027	-3.797583
H	-5.157071	-0.505395	-1.477115
H	-2.966598	3.419074	-3.516399
H	-3.318584	1.394103	-4.830068
H	-4.874008	2.762482	2.080107
H	-3.192474	7.103274	1.262152
H	-2.489782	7.088341	-1.131118
H	-2.777763	5.093743	-2.498390
Ni	-2.541609	-1.184948	1.526586
Ni	-0.020436	-1.586785	0.553120
H	4.886410	-2.752593	-2.393477
H	5.703281	-3.326210	0.069881
H	-7.913143	1.405276	0.278121
H	-7.783575	0.254778	2.614024
O	0.432012	0.416177	0.495091
C	0.510686	0.992375	-0.600865
C	0.905554	2.469441	-0.676958
C	0.173270	0.163030	-1.799845
C	1.108322	-0.136750	-2.798902
C	-1.083763	-0.472963	-1.798994
C	0.797526	-1.096471	-3.763491
H	2.101917	0.302748	-2.806878
C	-1.390574	-1.413503	-2.782379
H	-1.830167	-0.209940	-1.052316
C	-0.445038	-1.737360	-3.757710
H	1.548686	-1.342453	-4.508845
H	-2.365489	-1.891035	-2.773218
H	-0.676664	-2.483773	-4.513019
C	0.734248	3.092308	0.714413

C	-0.263048	4.035058	0.991605
C	1.583987	2.700241	1.762677
C	-0.397736	4.579731	2.272969
H	-0.948724	4.362616	0.219712
C	1.452028	3.240689	3.038862
H	2.356626	1.962834	1.584220
C	0.457928	4.187326	3.300497
H	-1.178736	5.312368	2.454995
H	2.133419	2.919137	3.820815
H	0.354004	4.613710	4.295134
C	0.011568	3.124459	-1.755924
H	0.218843	2.685925	-2.735272
H	-1.050362	2.977639	-1.542779
H	0.202651	4.196610	-1.815934
Cl	-0.724505	-1.419758	2.771184
I	4.923059	0.318407	-3.171284
C	2.414781	2.476268	-1.143721
C	3.258251	3.720033	-0.821489
H	2.440991	2.311287	-2.223673
H	2.931658	1.615925	-0.708750
C	2.733553	5.060914	-1.345521
H	3.416233	3.797531	0.259949
H	4.242930	3.521451	-1.266455
C	3.744018	6.192156	-1.126181
H	2.501710	4.975197	-2.416520
H	1.796013	5.313077	-0.833511
H	3.359412	7.153131	-1.487901
H	3.977676	6.304599	-0.059893
H	4.683779	5.985740	-1.652488

*t*BuOH

C	0.686090	1.267756	-0.508647
C	-0.005099	-0.000049	0.015243
H	0.202275	2.158472	-0.094751
H	1.743300	1.282923	-0.211798
H	0.646665	1.322865	-1.602794
C	0.696432	-1.261581	-0.509808
C	-1.488450	-0.005846	-0.360309
H	0.220168	-2.156650	-0.096499
H	0.657332	-1.316178	-1.603991
H	1.753864	-1.268134	-0.213327
H	-1.614737	-0.004966	-1.448225
H	-1.977879	-0.895179	0.050104
H	-1.985134	0.878369	0.052428

O	0.010160	-0.000580	1.452026
H	0.939033	0.001443	1.733771

tBuO-

C	-0.658829	-1.304965	-0.436878
C	0.000262	0.000102	0.162481
H	-0.107210	-2.177108	-0.057662
H	-1.687707	-1.379572	-0.056614
H	-0.688694	-1.362317	-1.541256
C	-0.801457	1.222223	-0.437715
C	1.459045	0.082077	-0.438898
H	-0.350408	2.151162	-0.060508
H	-0.839442	1.274800	-1.542139
H	-1.831478	1.181083	-0.055601
H	1.522717	0.083957	-1.543315
H	1.938497	0.996418	-0.060919
H	2.038552	-0.771122	-0.058320
O	0.001381	0.000759	1.485299

A

O	0.270514	-1.825824	-0.136724
C	0.460987	-0.584232	0.038630
C	-0.514564	0.422839	0.234935
C	1.942572	-0.210761	0.002039
C	2.854235	-1.054344	0.658086
C	2.464896	0.835494	-0.774189
C	4.228111	-0.831977	0.587949
H	2.450703	-1.900871	1.205983
C	3.843067	1.051523	-0.867880
H	1.776971	1.477677	-1.317736
C	4.732958	0.225692	-0.178091
H	4.912476	-1.489638	1.122251
H	4.222004	1.864399	-1.485841
H	5.806261	0.394921	-0.244349
C	-1.937114	0.167122	0.089576
C	-2.894046	1.215898	0.233466
C	-2.486940	-1.114847	-0.221913
C	-4.264142	1.005689	0.086616
H	-2.556919	2.223969	0.453067
C	-3.855144	-1.310924	-0.366484
H	-1.792817	-1.936844	-0.337645
C	-4.771591	-0.260566	-0.213927
H	-4.944310	1.849865	0.207230
H	-4.218714	-2.311925	-0.602077

H	-5.841888	-0.425566	-0.325581
C	-0.122177	1.818205	0.683725
H	0.935910	1.883791	0.946240
H	-0.316993	2.607150	-0.066943
H	-0.683436	2.120794	1.583952

70

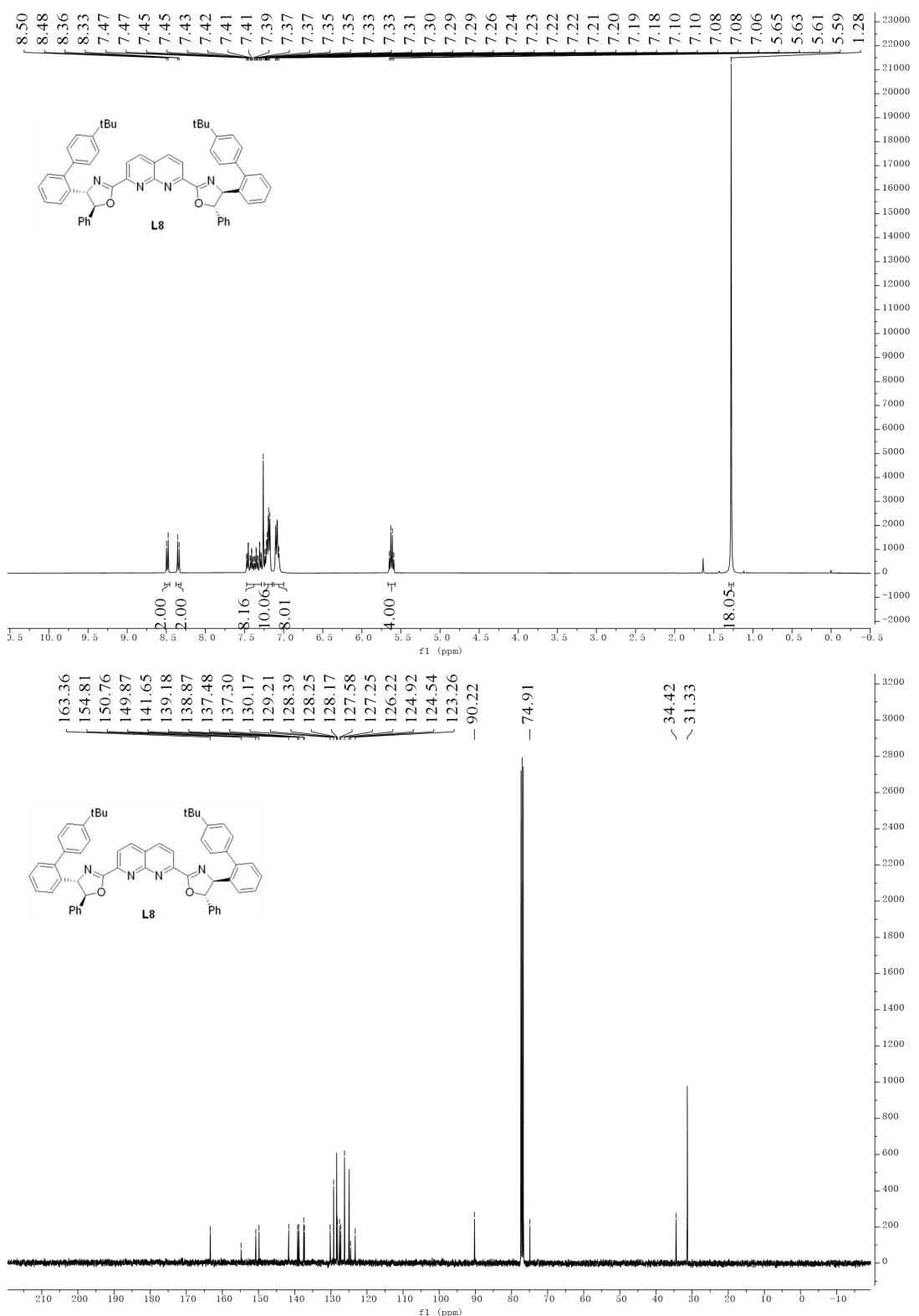
O	-0.901147	-1.817860	-0.857392
C	-1.068578	-0.728852	-0.334284
C	0.157429	0.122576	0.150552
C	-2.494588	-0.268711	-0.128355
C	-2.934480	1.063931	-0.150287
C	-3.450389	-1.286086	0.042374
C	-4.288108	1.369252	-0.001579
H	-2.233404	1.873281	-0.308646
C	-4.797767	-0.980772	0.214182
H	-3.113156	-2.317132	0.035331
C	-5.222341	0.350518	0.190736
H	-4.610668	2.406304	-0.036667
H	-5.518342	-1.780973	0.359843
H	-6.274356	0.591553	0.317627
C	1.395652	-0.786513	0.153867
C	2.099692	-1.097654	1.323291
C	1.870693	-1.327103	-1.054592
C	3.240725	-1.906511	1.291112
H	1.770927	-0.713746	2.282203
C	3.006814	-2.130814	-1.092748
H	1.338053	-1.120910	-1.976261
C	3.701645	-2.425100	0.083703
H	3.765577	-2.126298	2.217307
H	3.347864	-2.532384	-2.043440
H	4.588758	-3.052275	0.056195
C	-0.165807	0.668326	1.561521
H	-1.009832	1.358628	1.534305
H	-0.432174	-0.142557	2.248343
H	0.684734	1.206351	1.983522
C	0.359316	1.304866	-0.873228
C	1.762314	1.932232	-0.989006
H	-0.342774	2.105470	-0.617275
H	0.070416	0.957504	-1.873496
C	2.341415	2.549170	0.289759
H	2.470888	1.191009	-1.374780
H	1.692474	2.716183	-1.757559

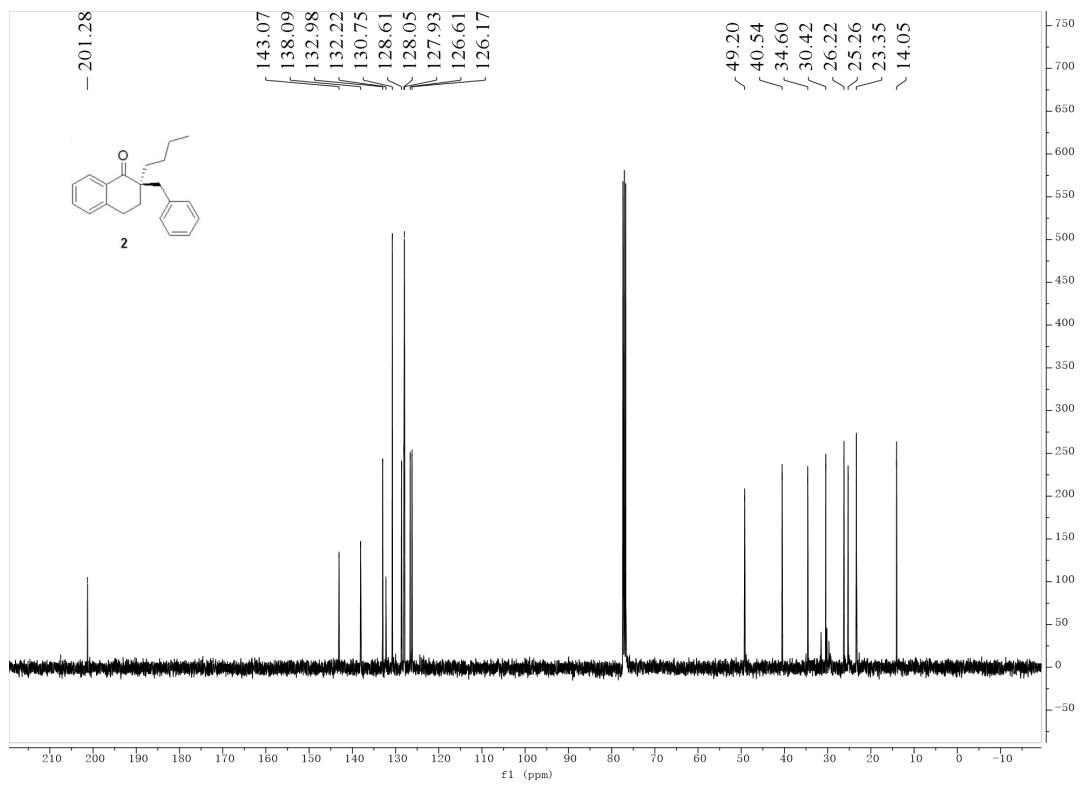
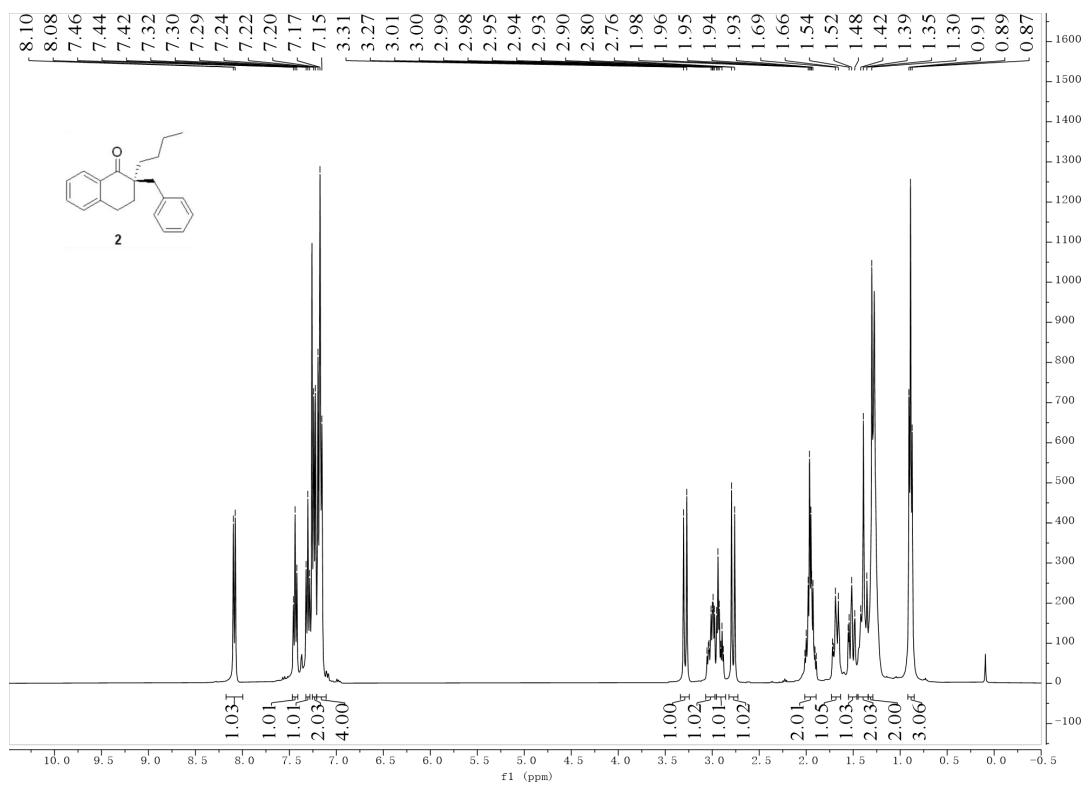
C	3.642405	3.313642	0.022409
H	1.601828	3.222706	0.746354
H	2.538313	1.754553	1.018695
H	4.058637	3.732673	0.945689
H	4.400017	2.652584	-0.416240
H	3.479146	4.141982	-0.678480

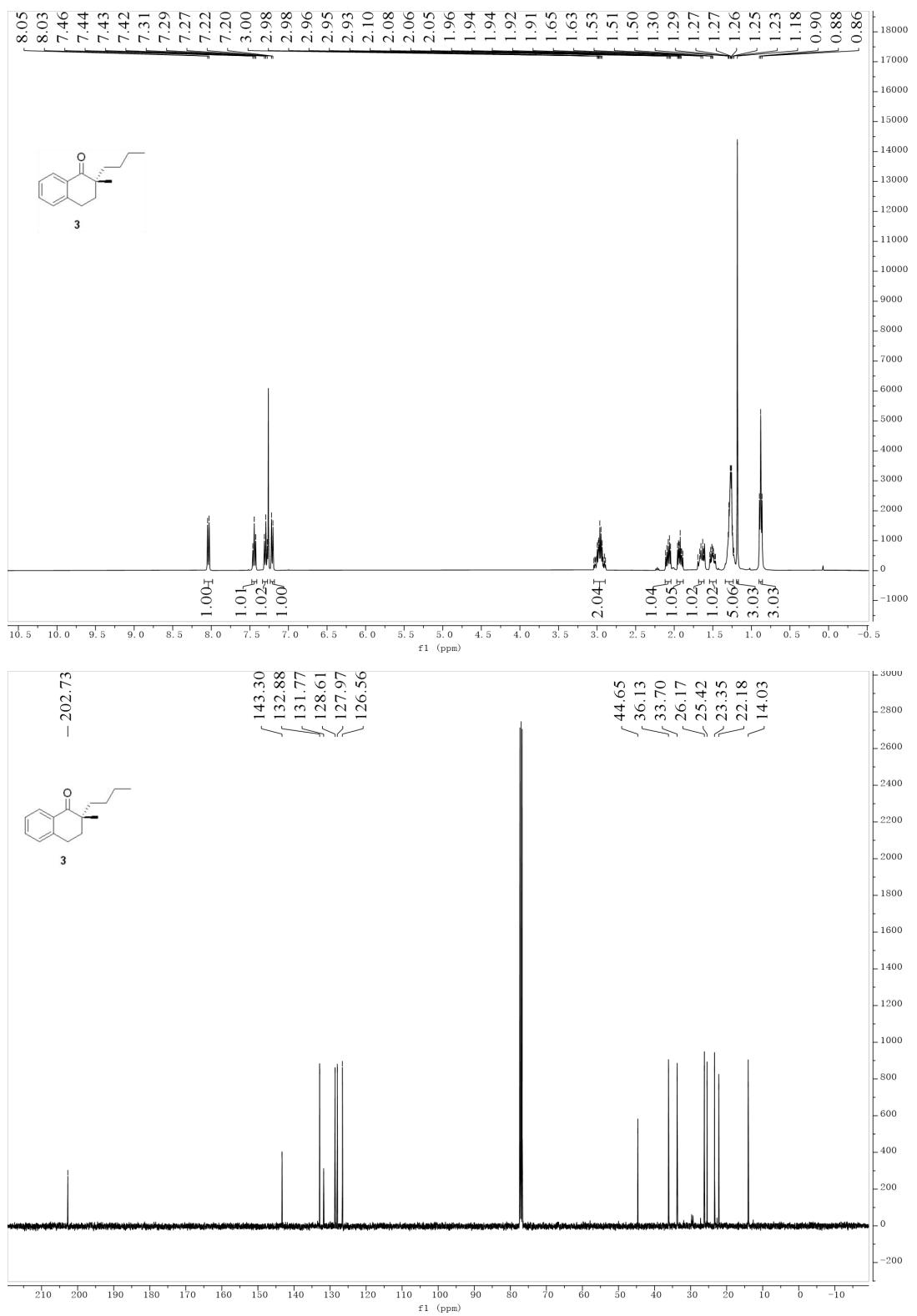
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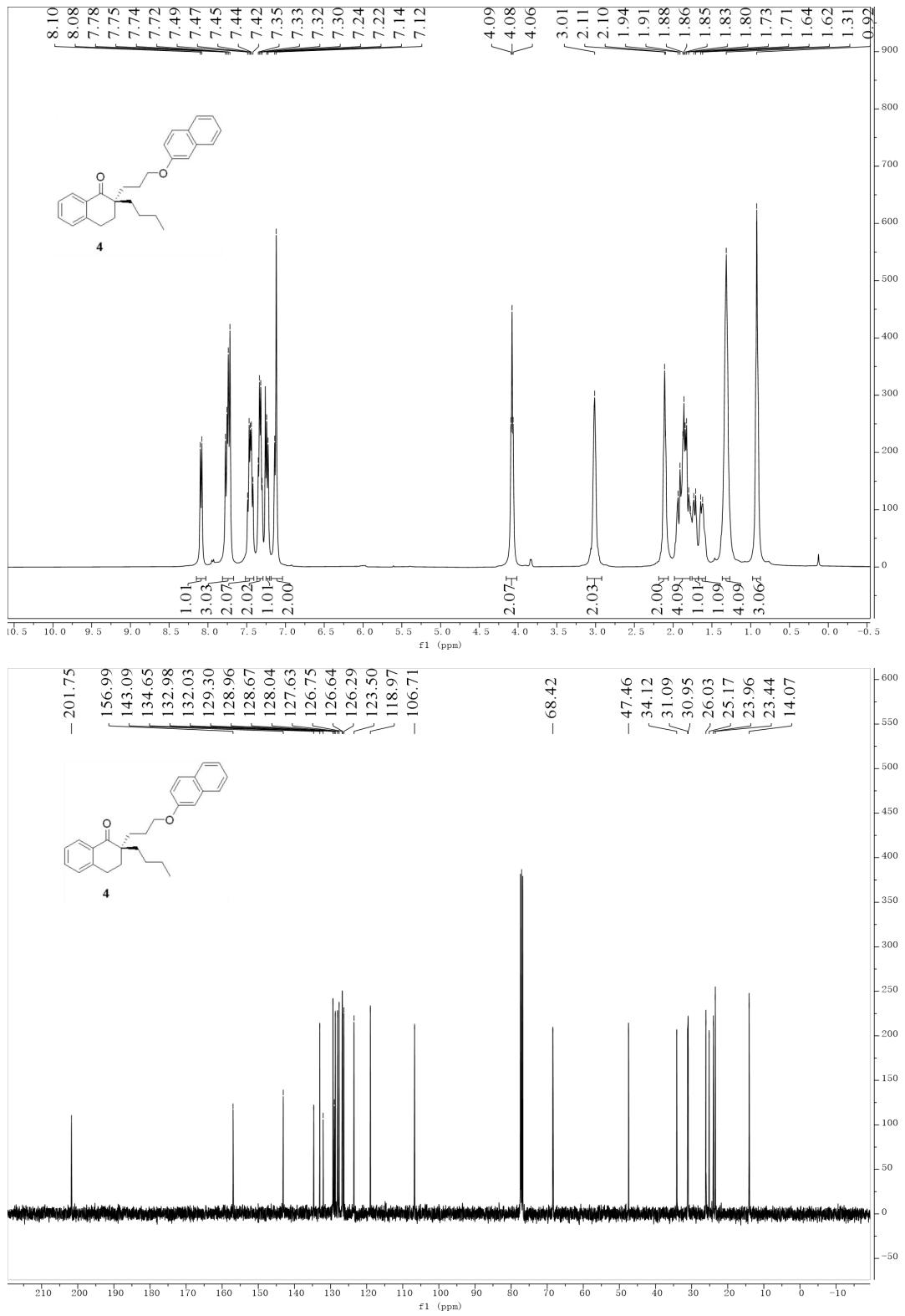
C	-0.518844	0.842885	0.000046
C	-1.631684	-0.191243	0.000256
H	-0.524356	1.470562	-0.891832
H	-0.524188	1.470710	0.891815
C	-3.011772	0.490111	-0.000060
H	-1.538751	-0.838559	-0.880124
H	-1.538808	-0.838090	0.880983
C	-4.158230	-0.527658	-0.000092
H	-3.097090	1.142928	0.879585
H	-3.096749	1.142639	-0.879956
H	-5.132678	-0.026890	-0.000120
H	-4.111589	-1.173171	-0.885424
H	-4.111636	-1.173154	0.885254
I	1.501868	-0.091727	-0.000020

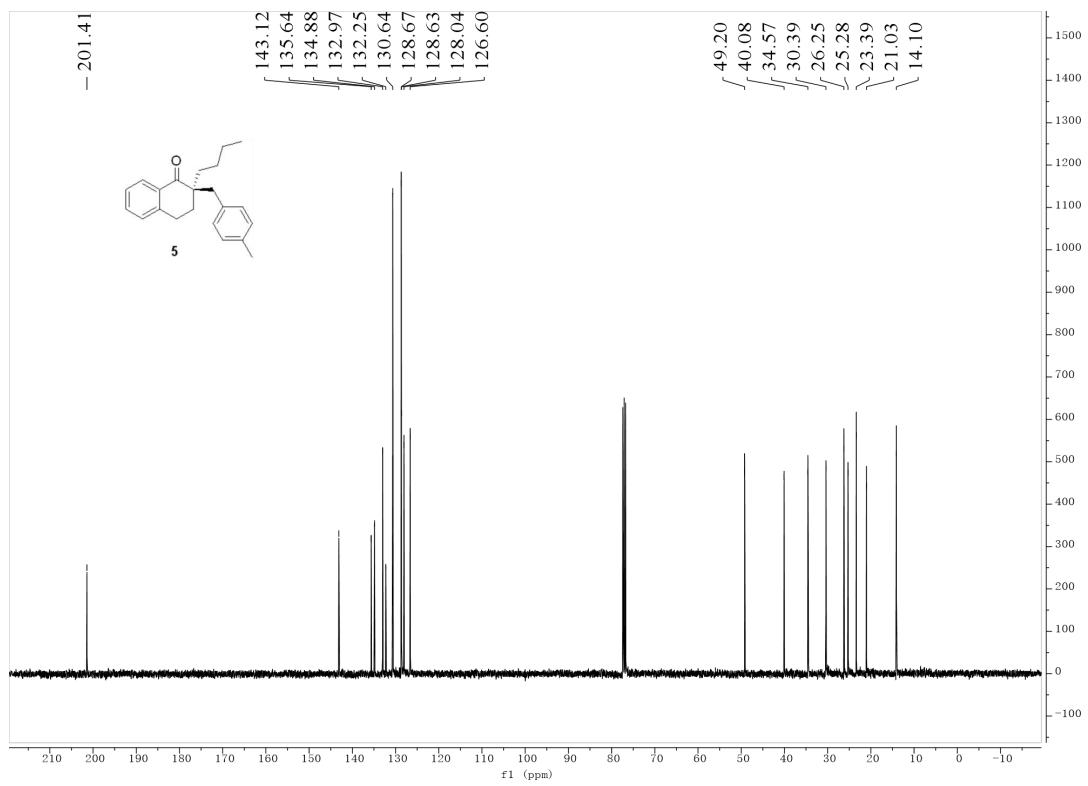
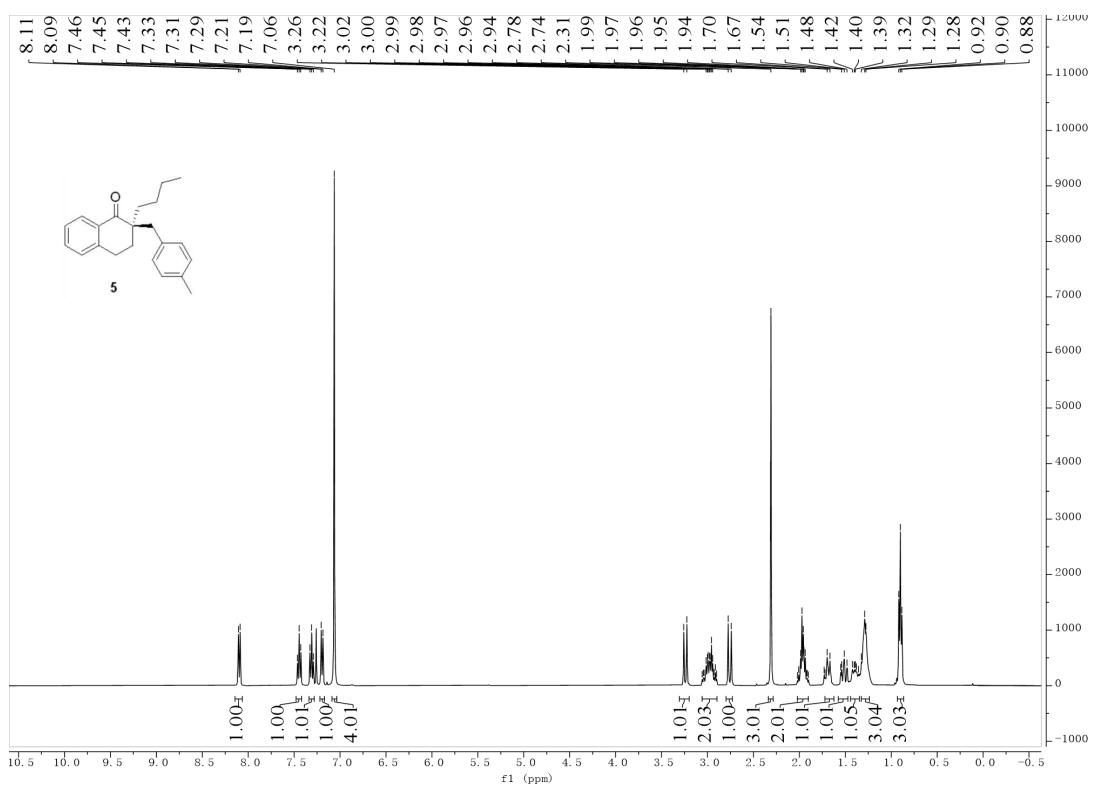
12. NMR Spectra

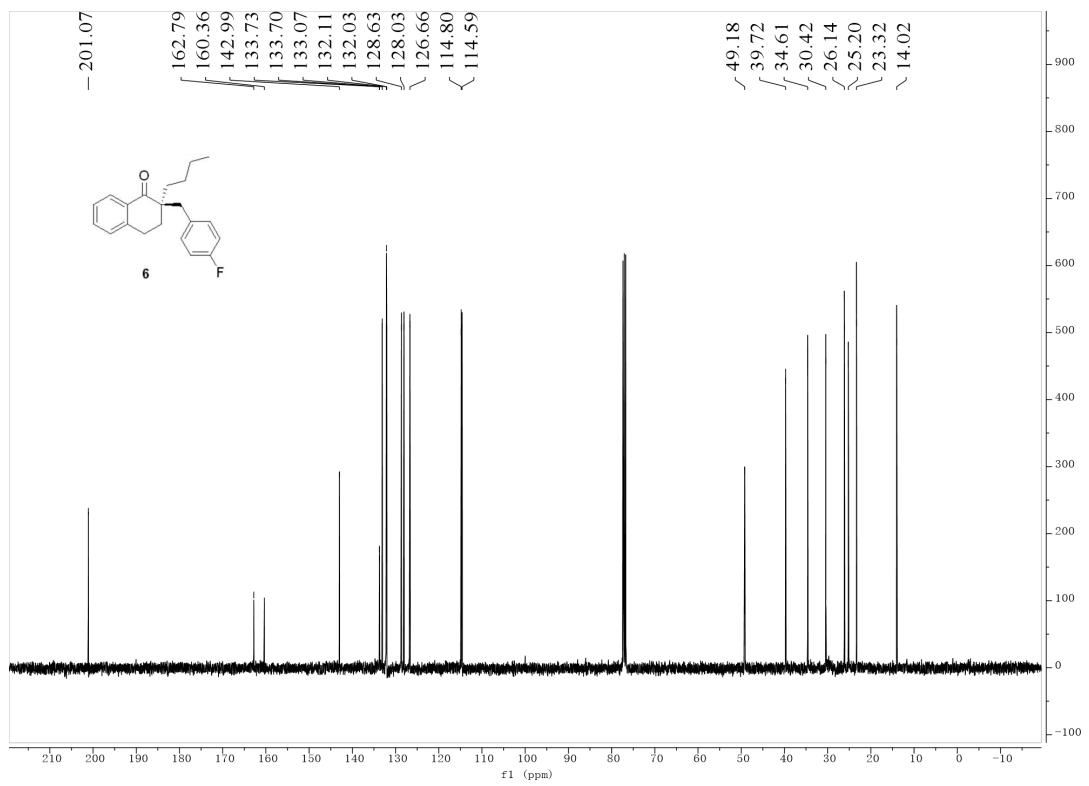
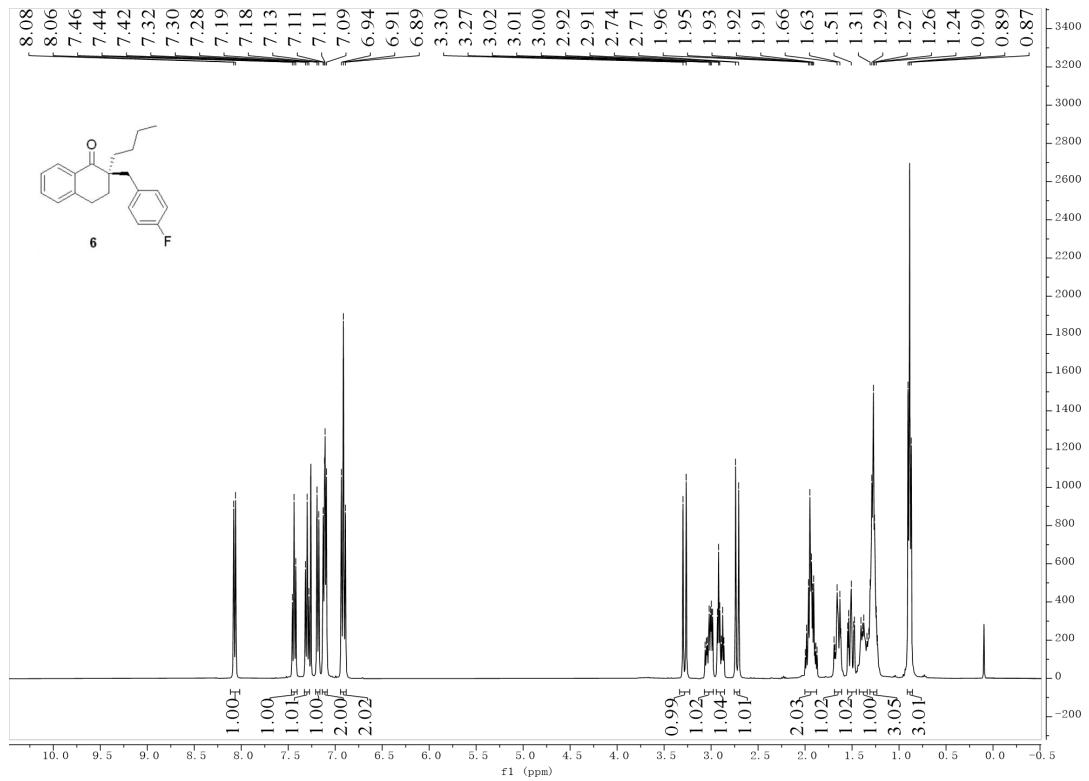


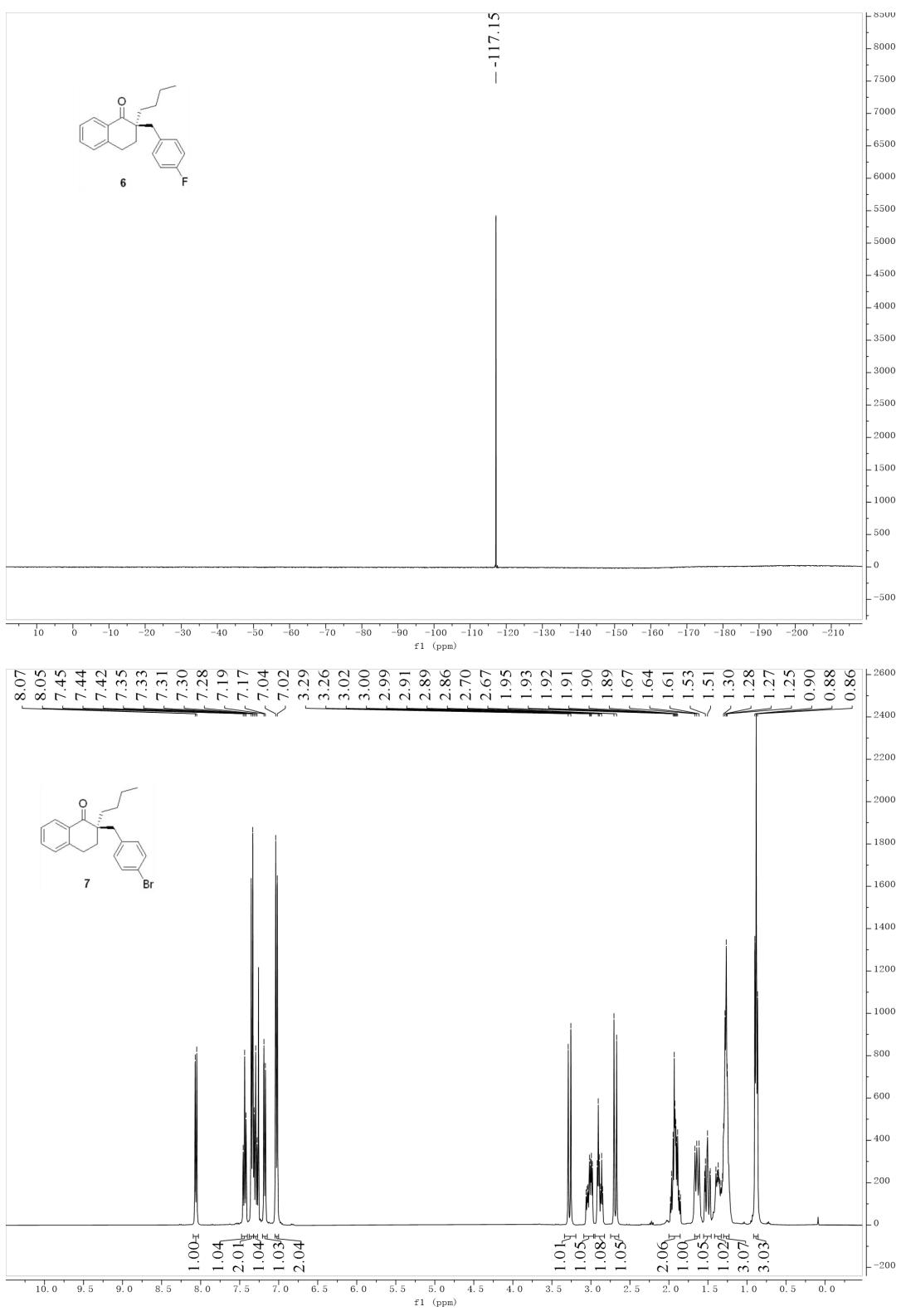


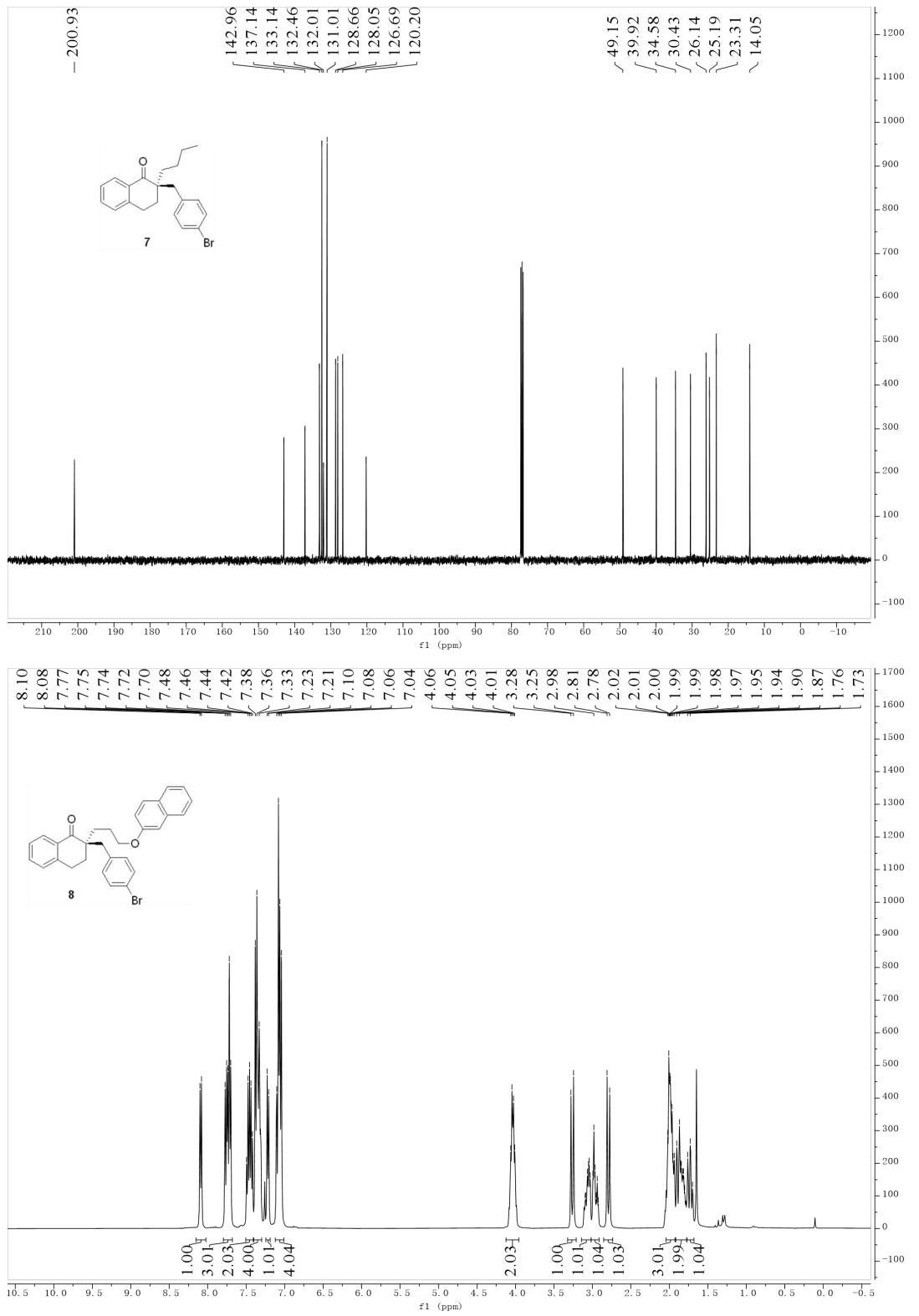


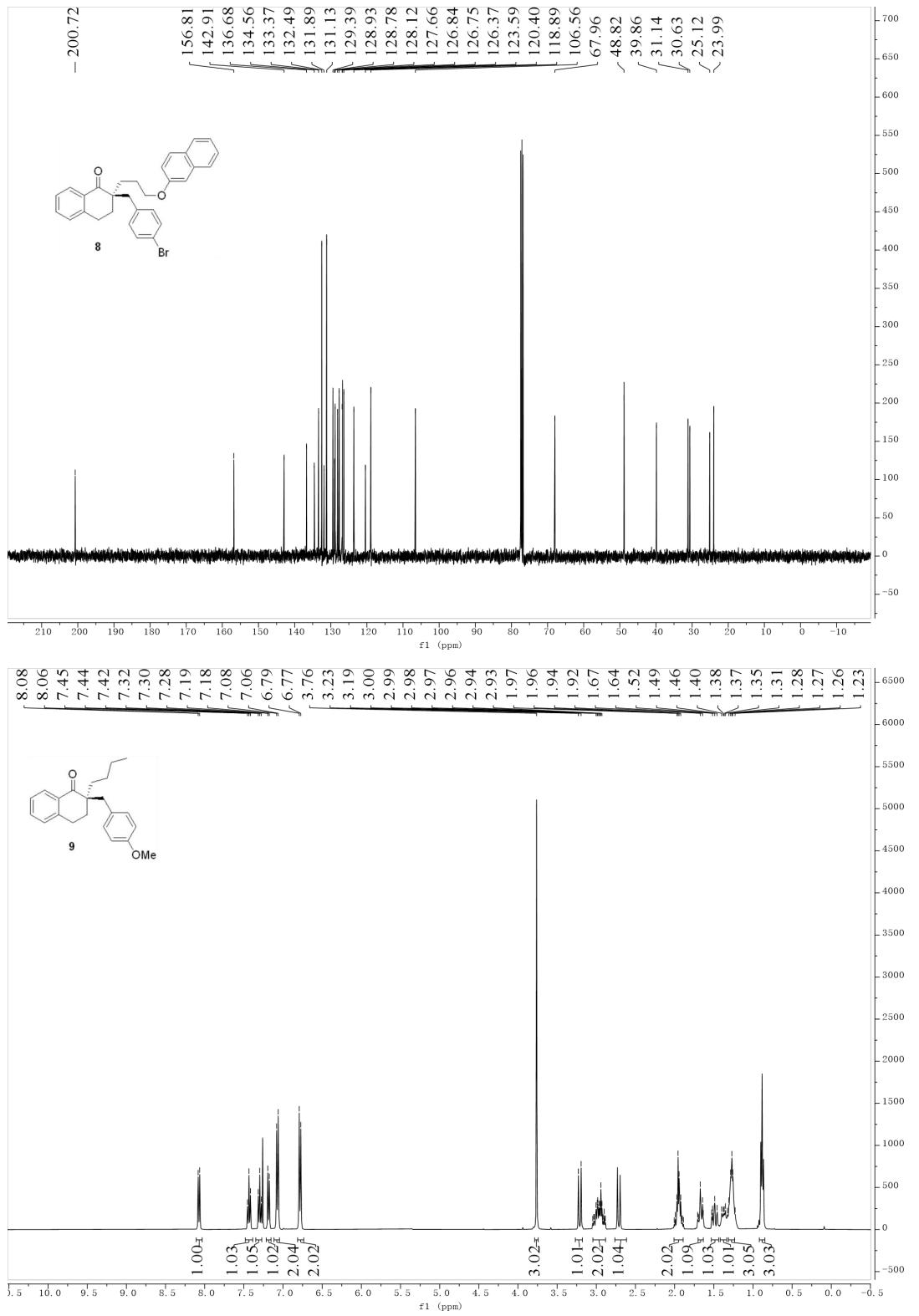


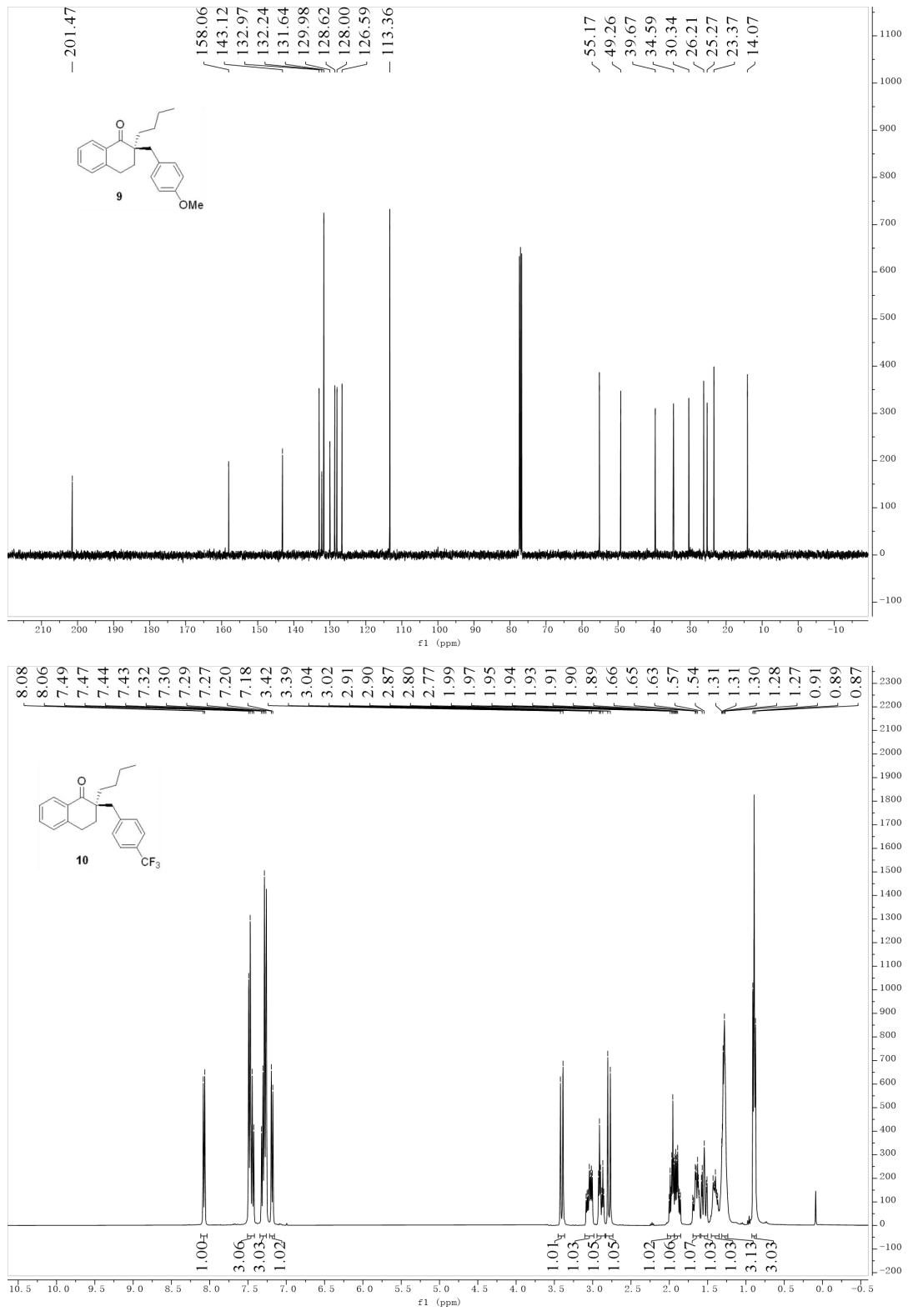


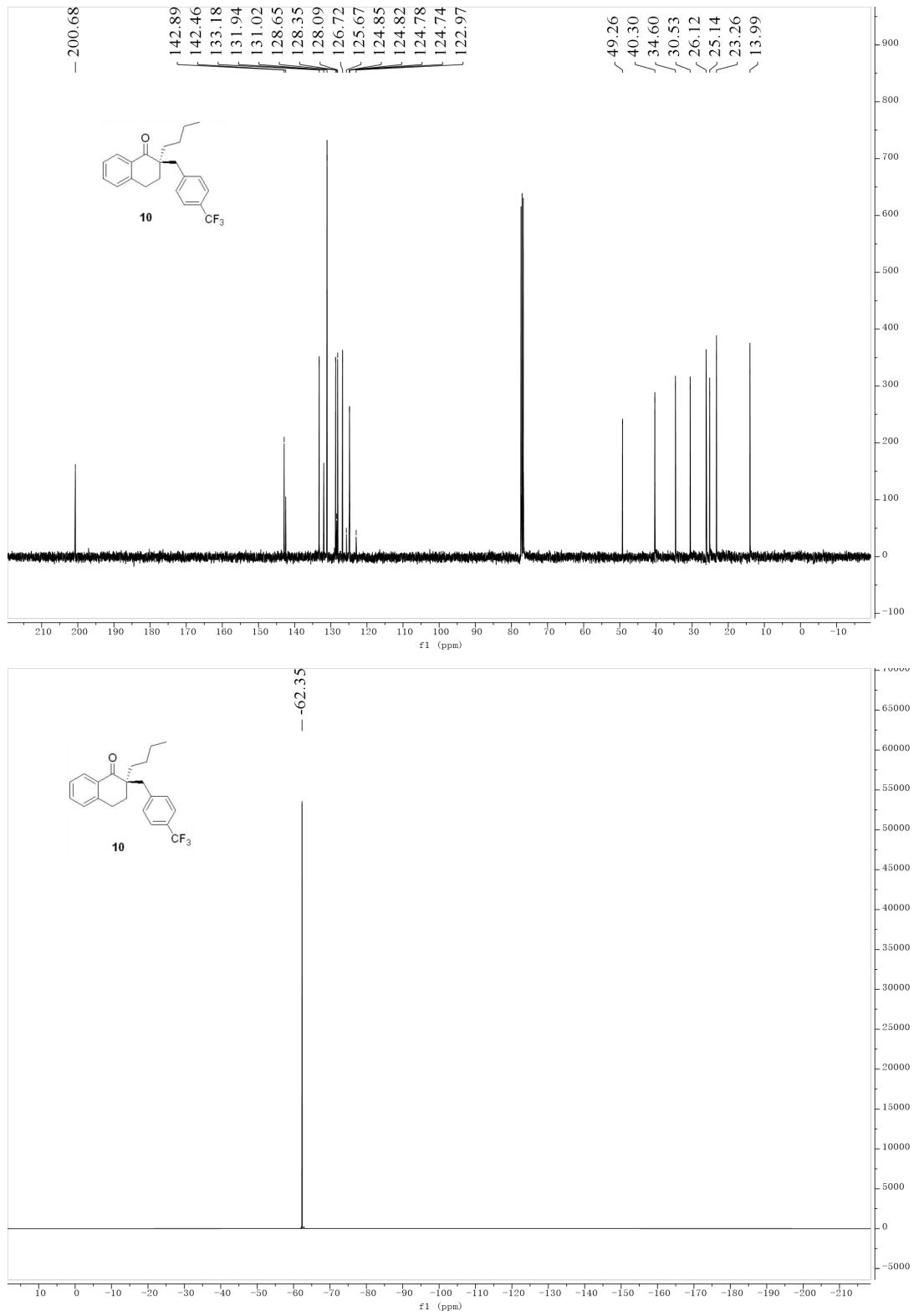


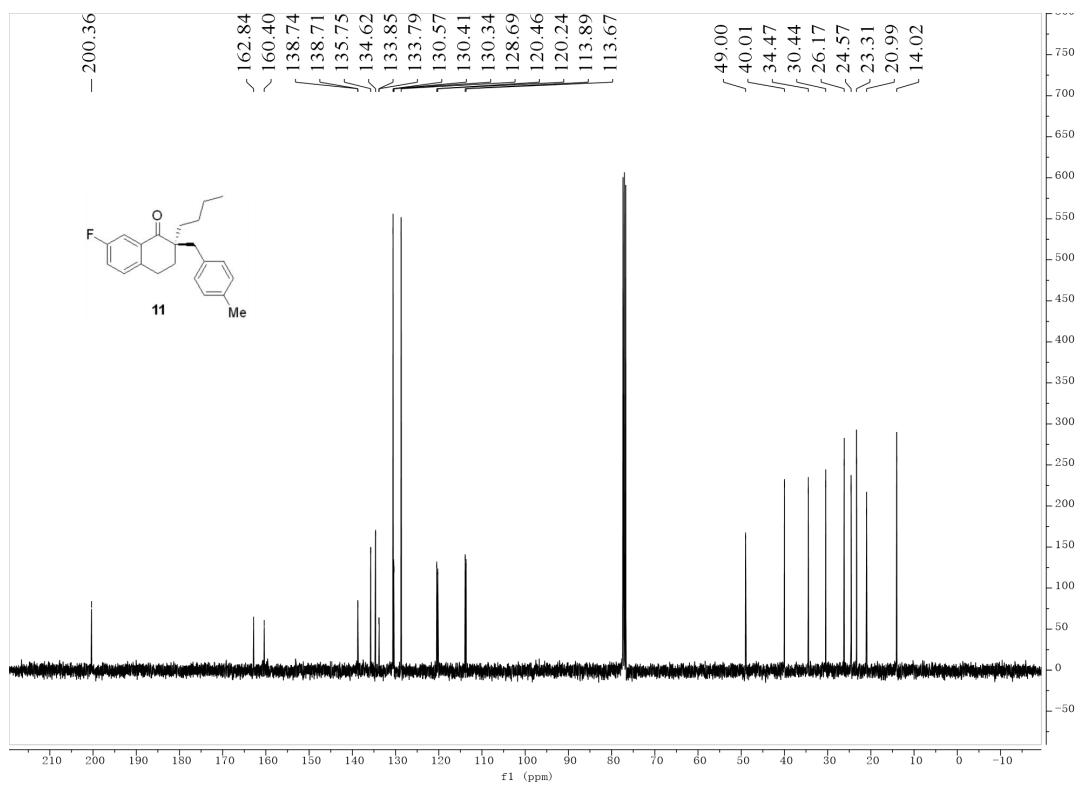
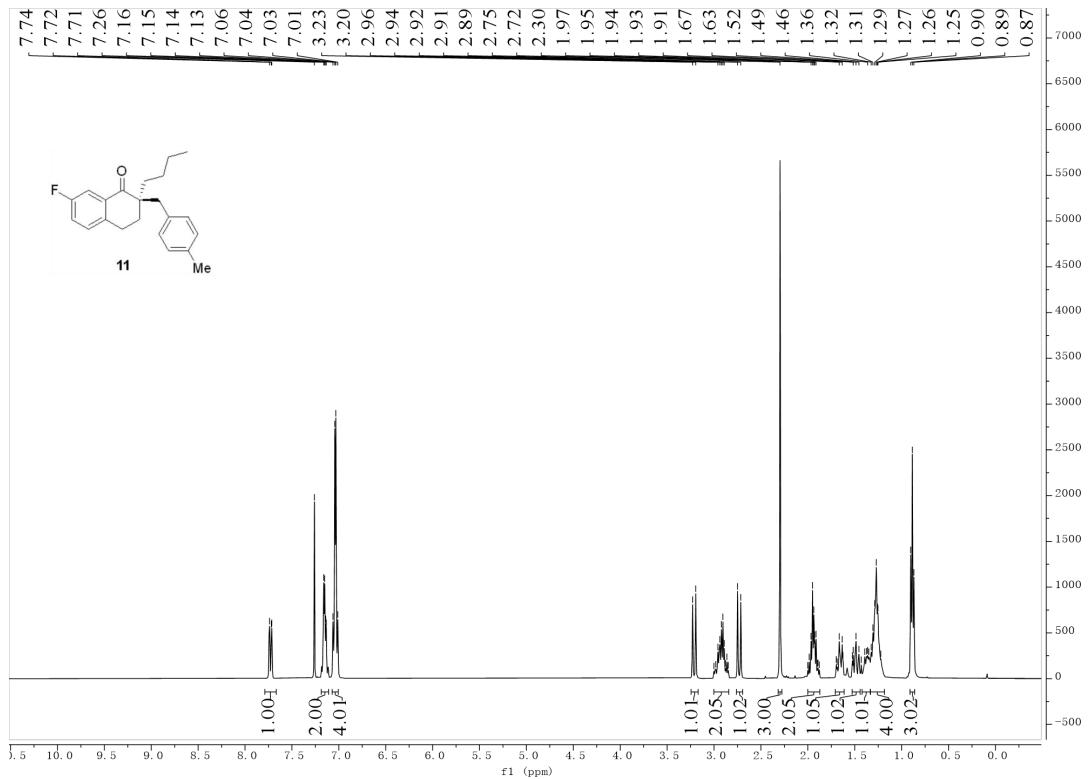


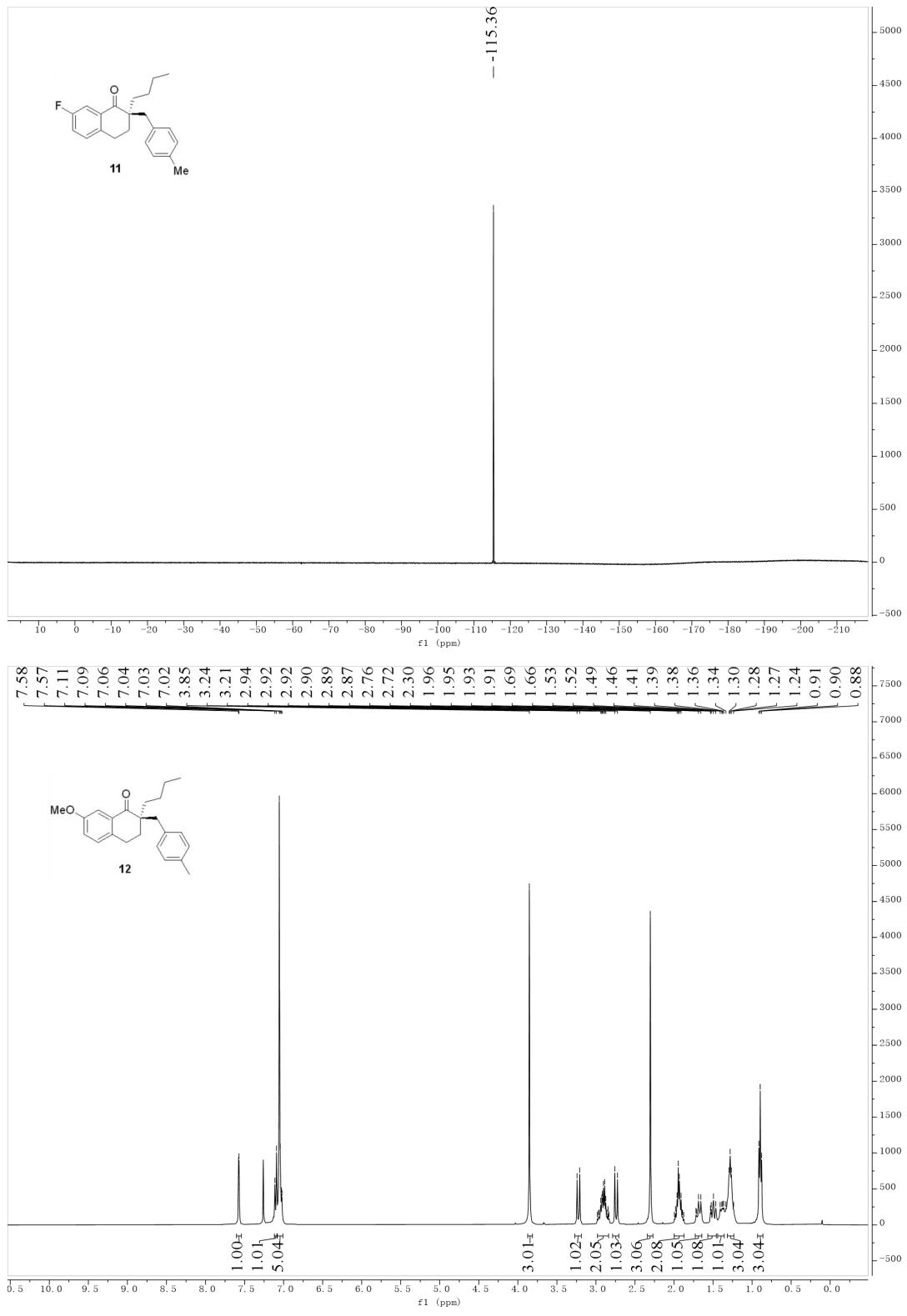


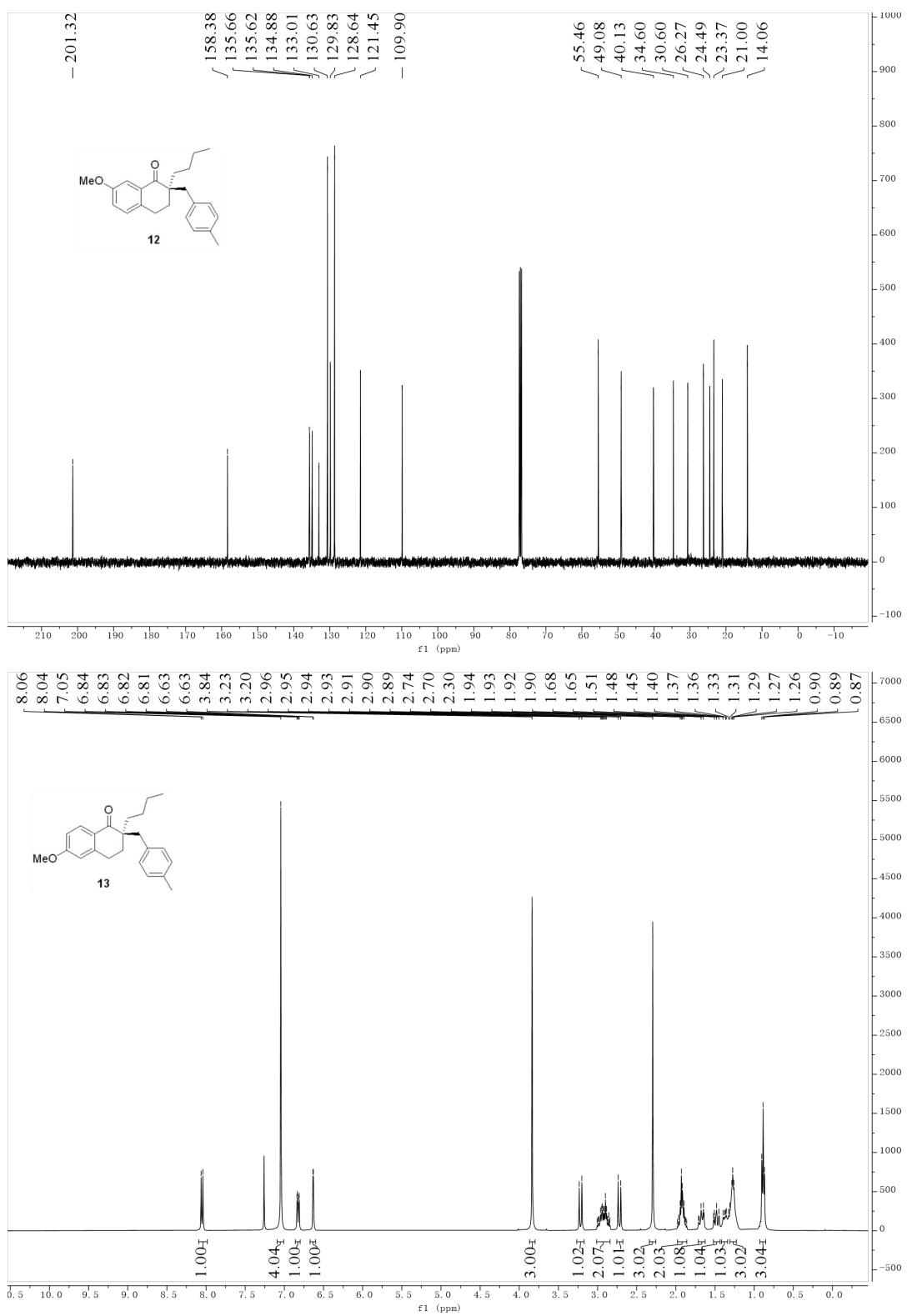


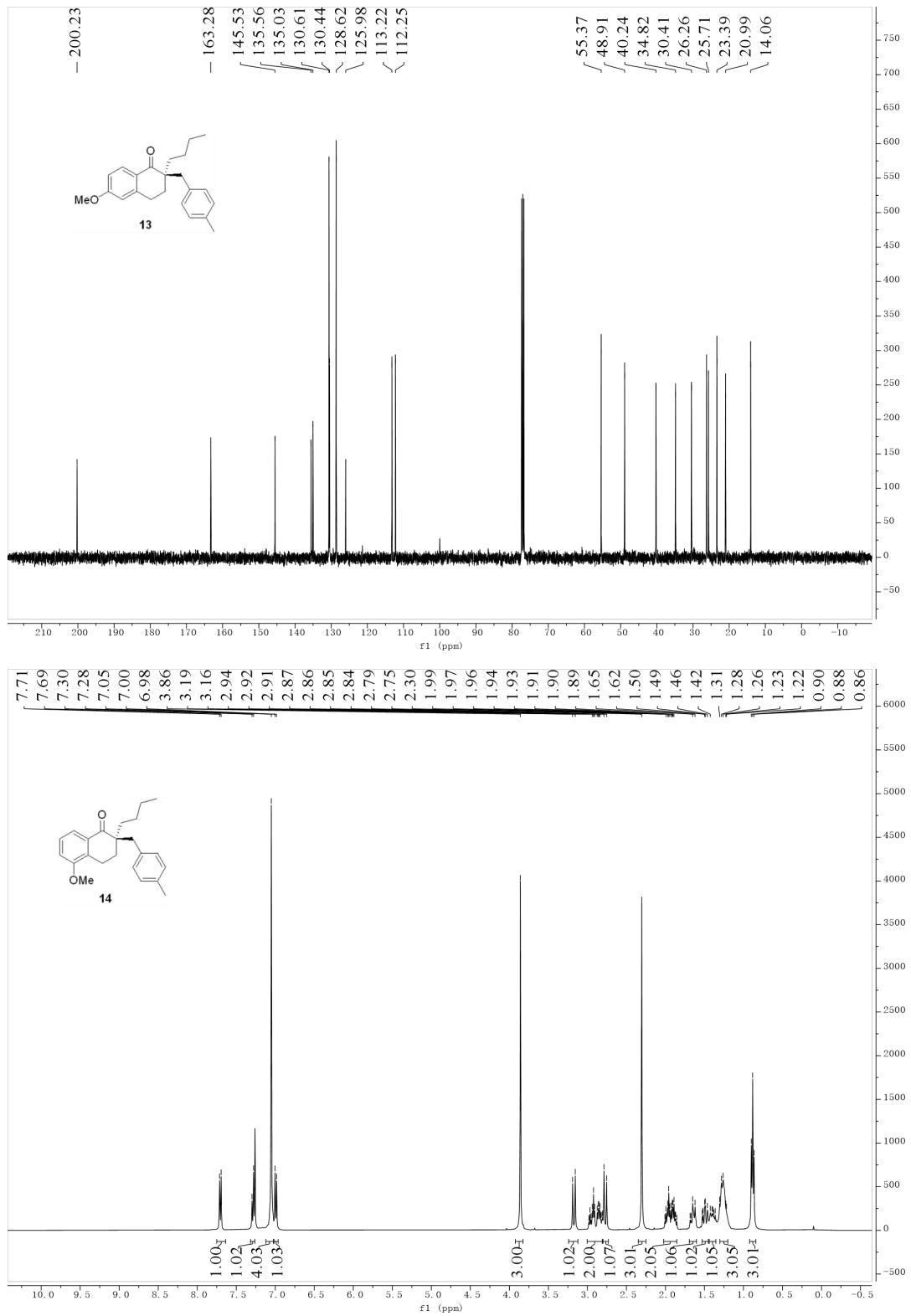


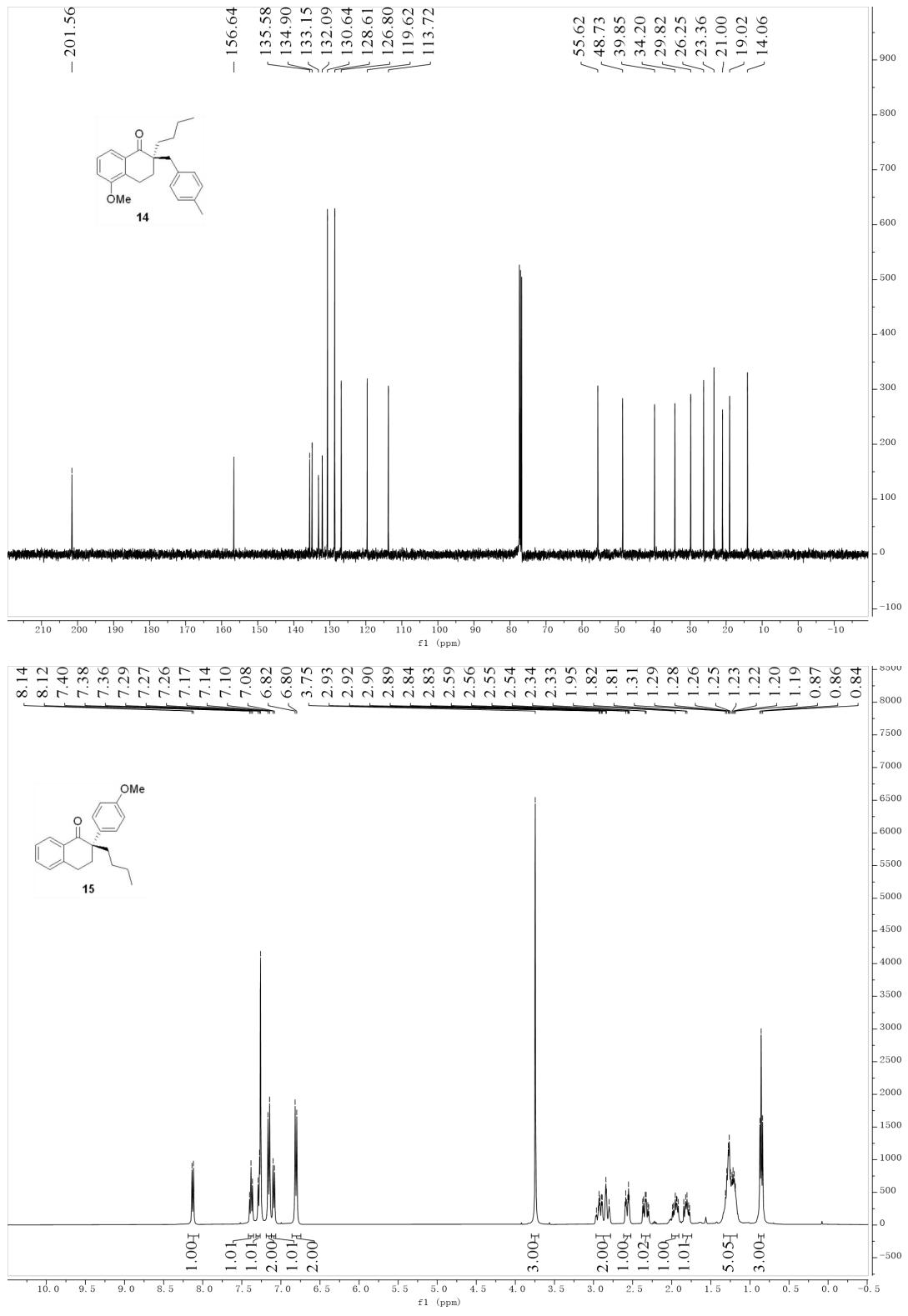


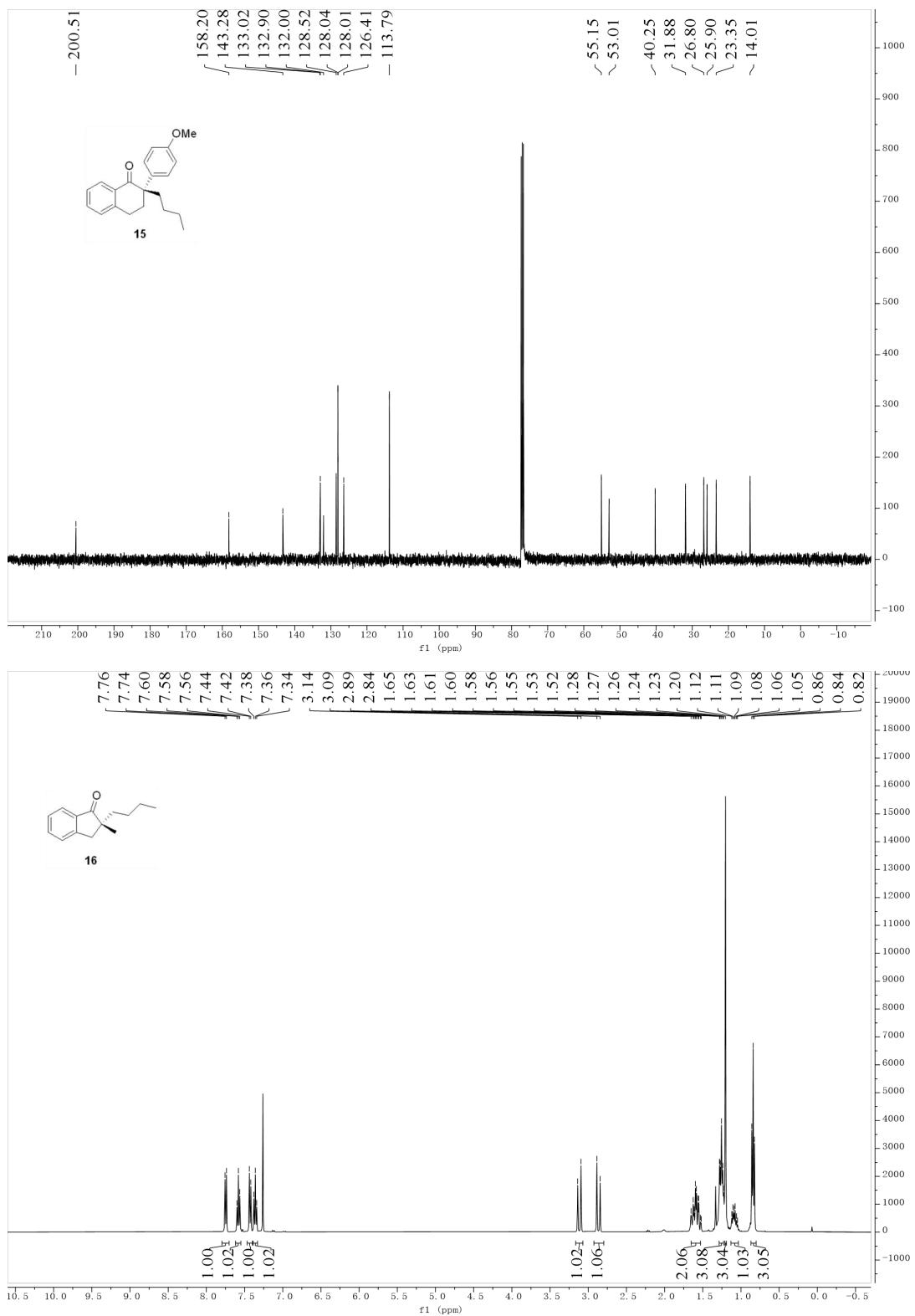


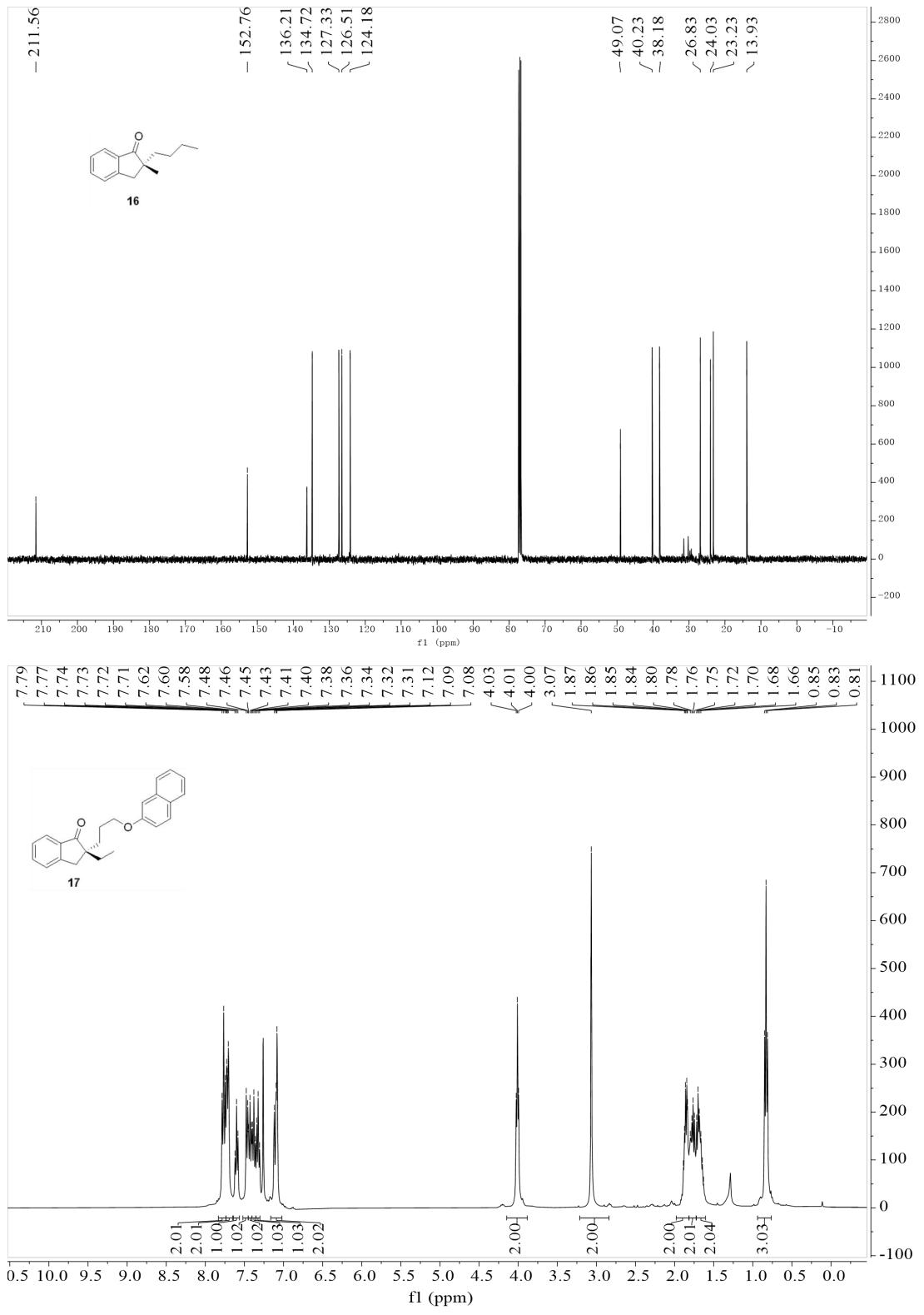


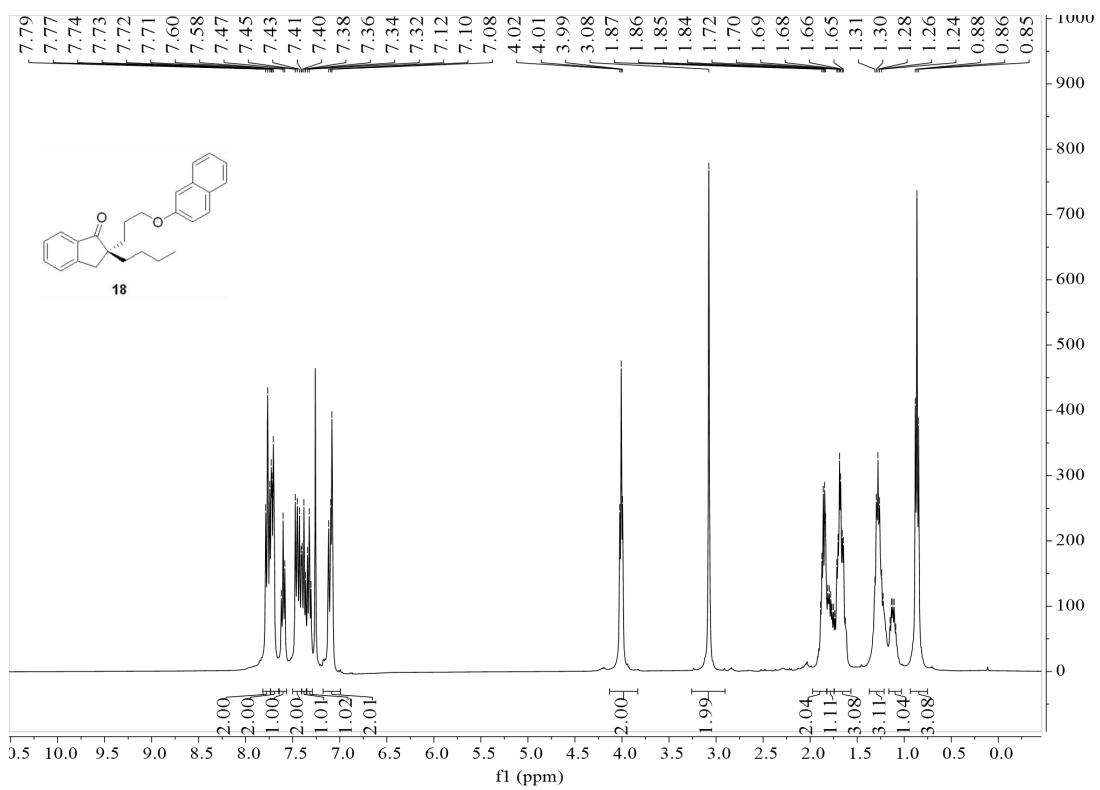
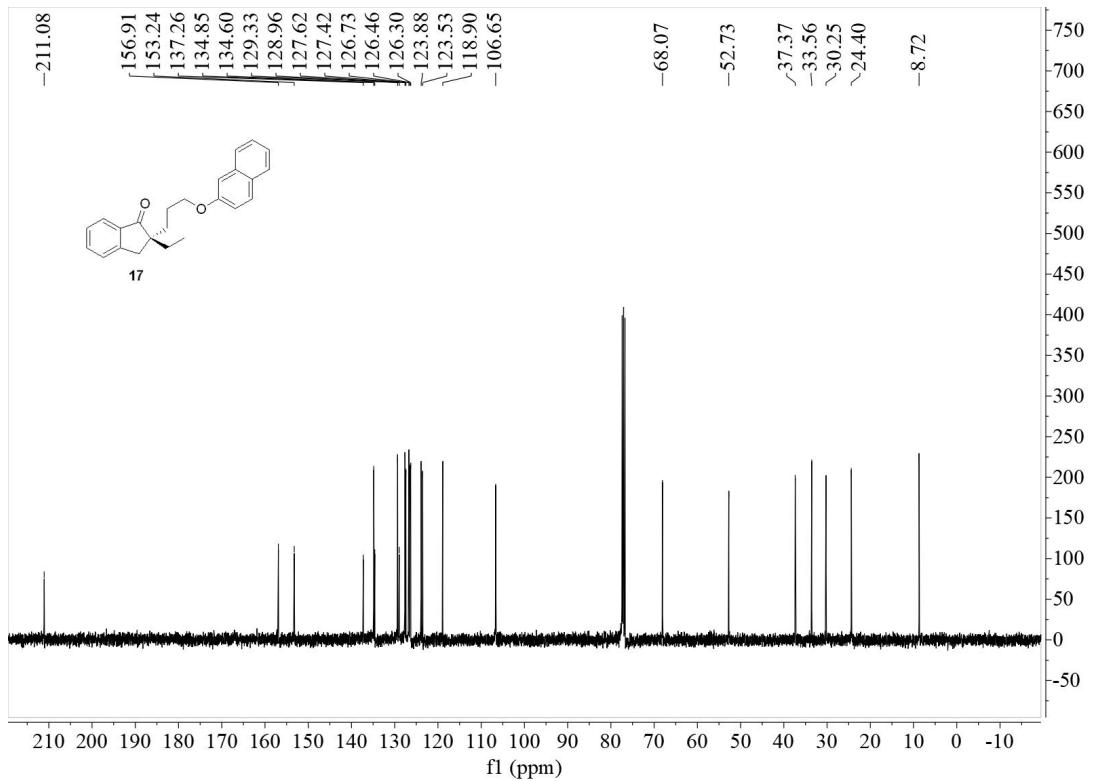


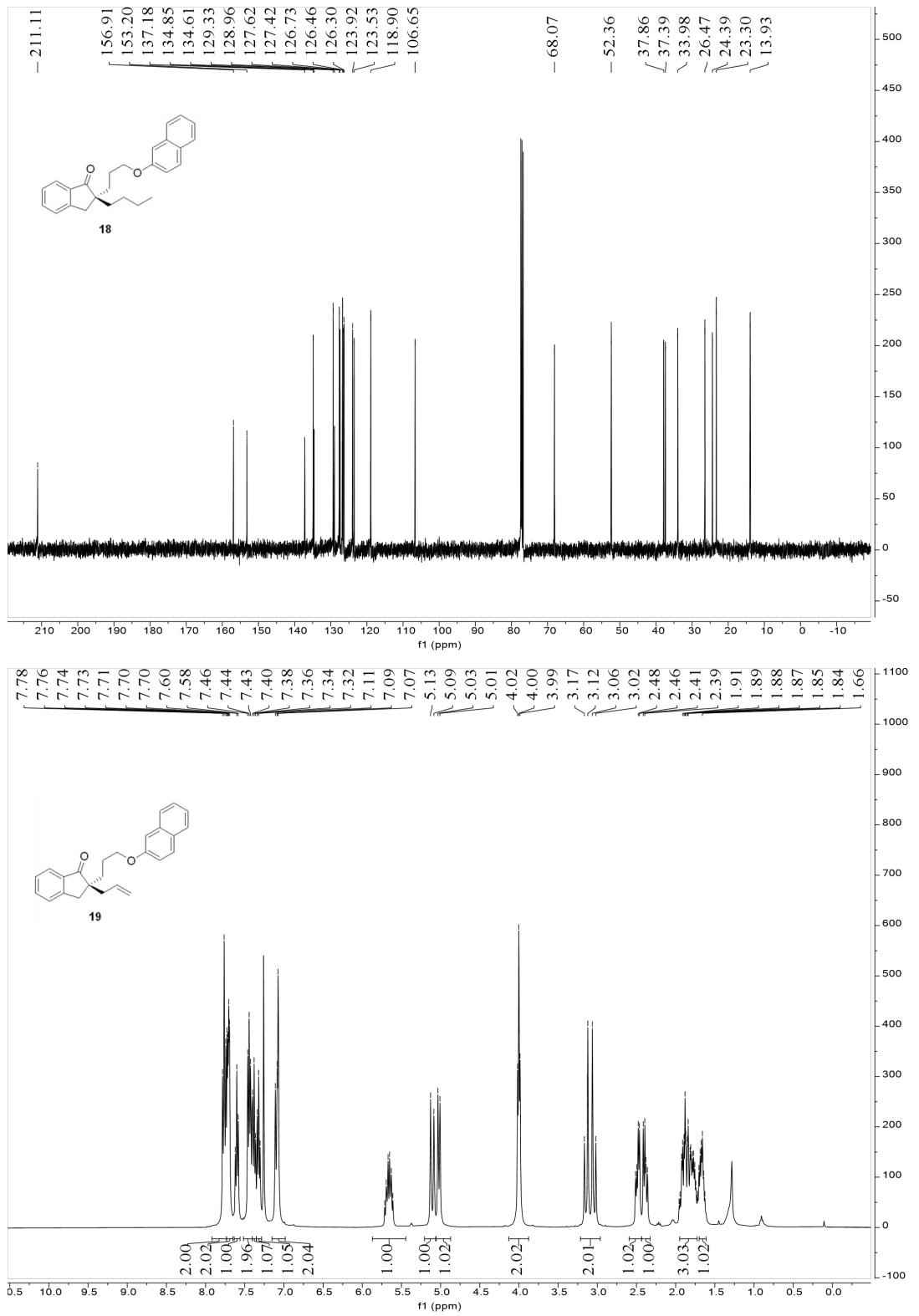


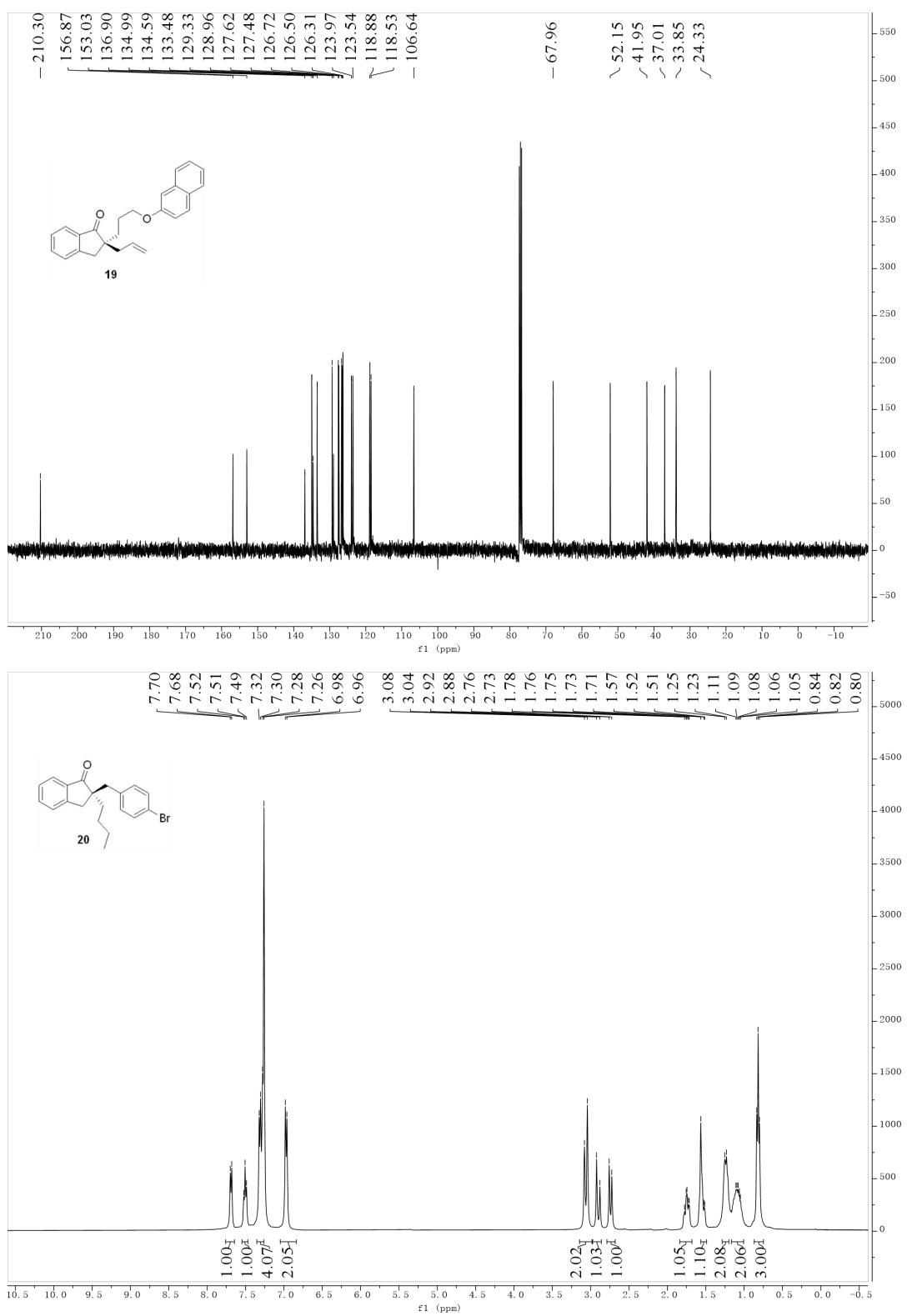


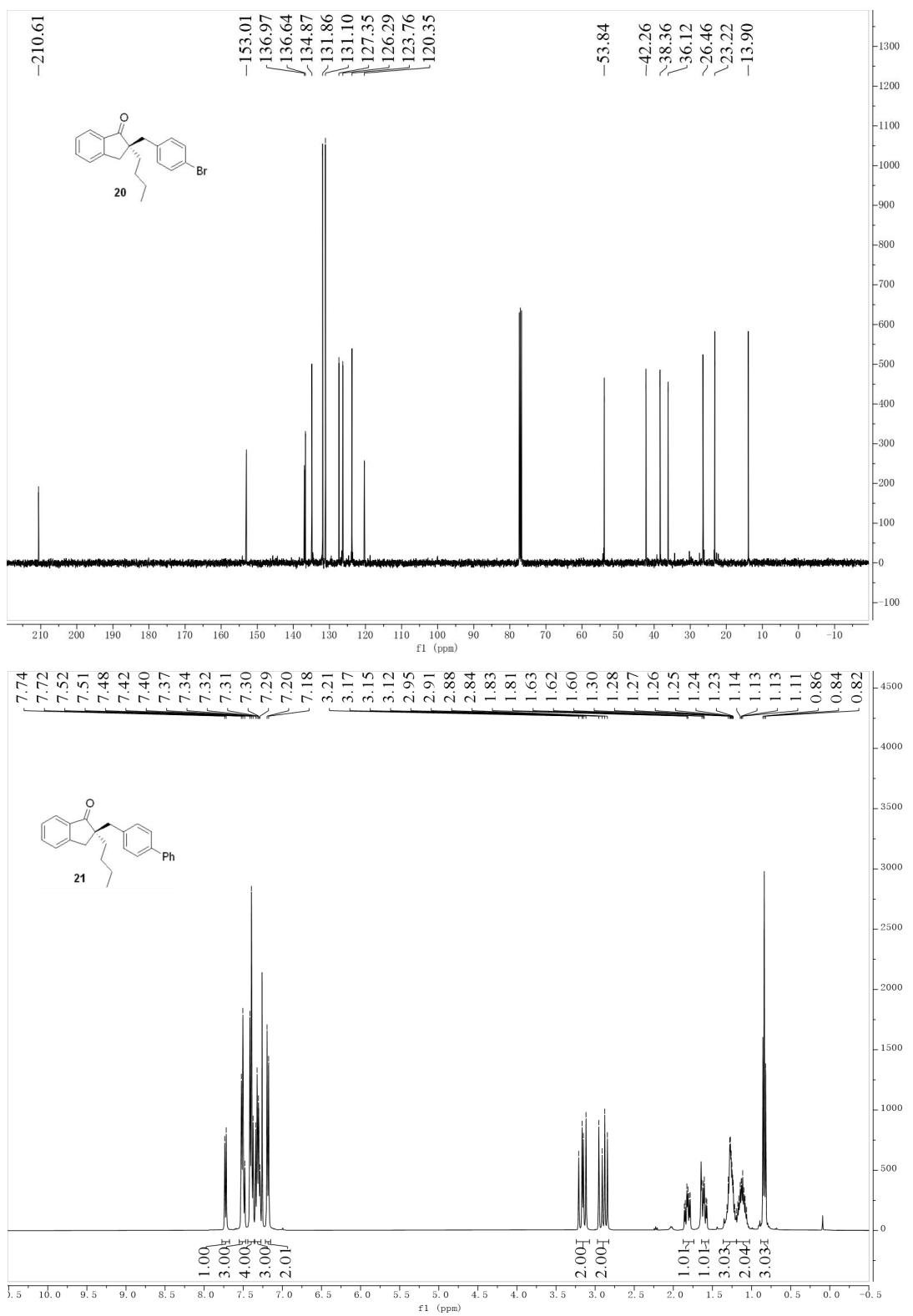


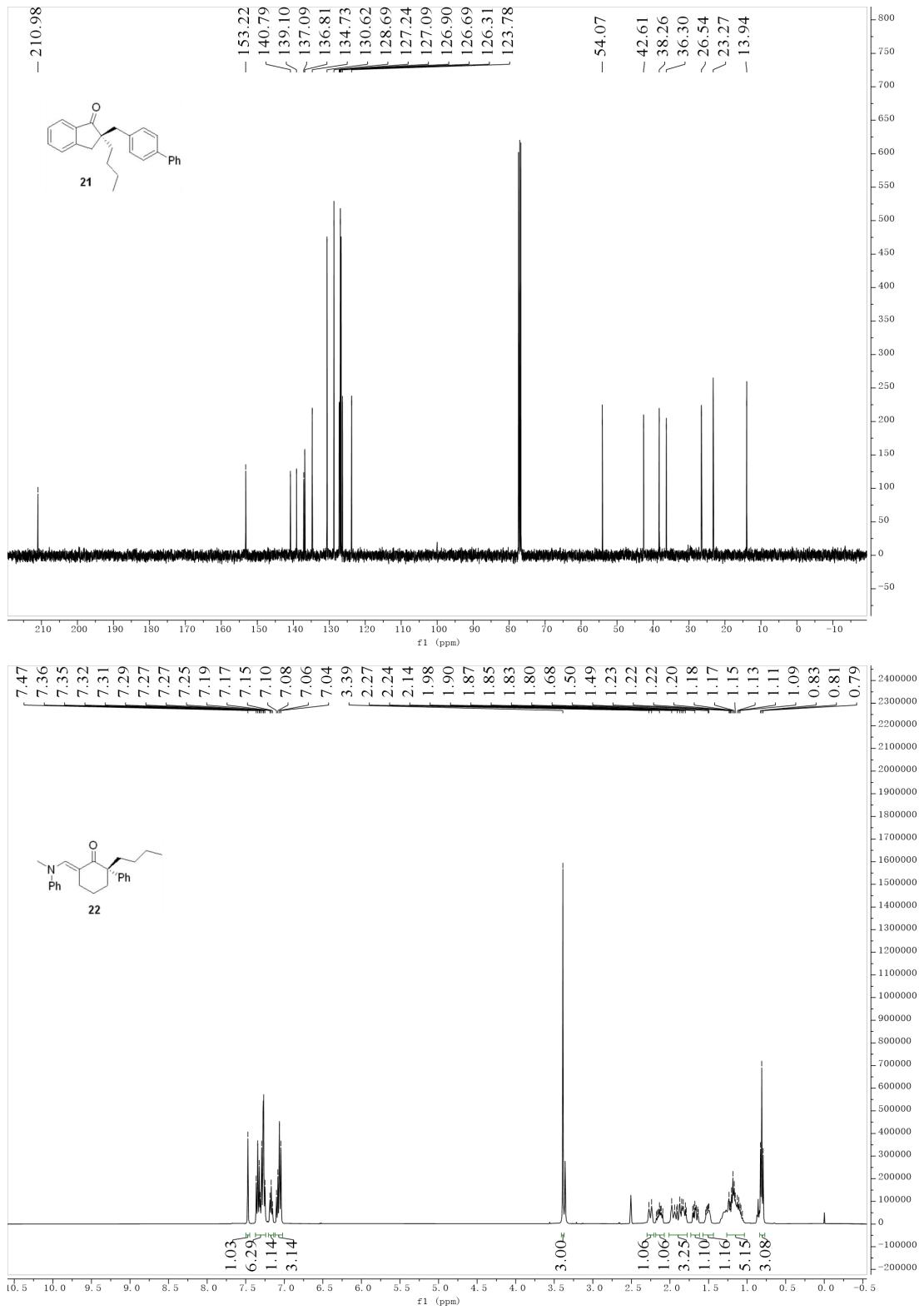


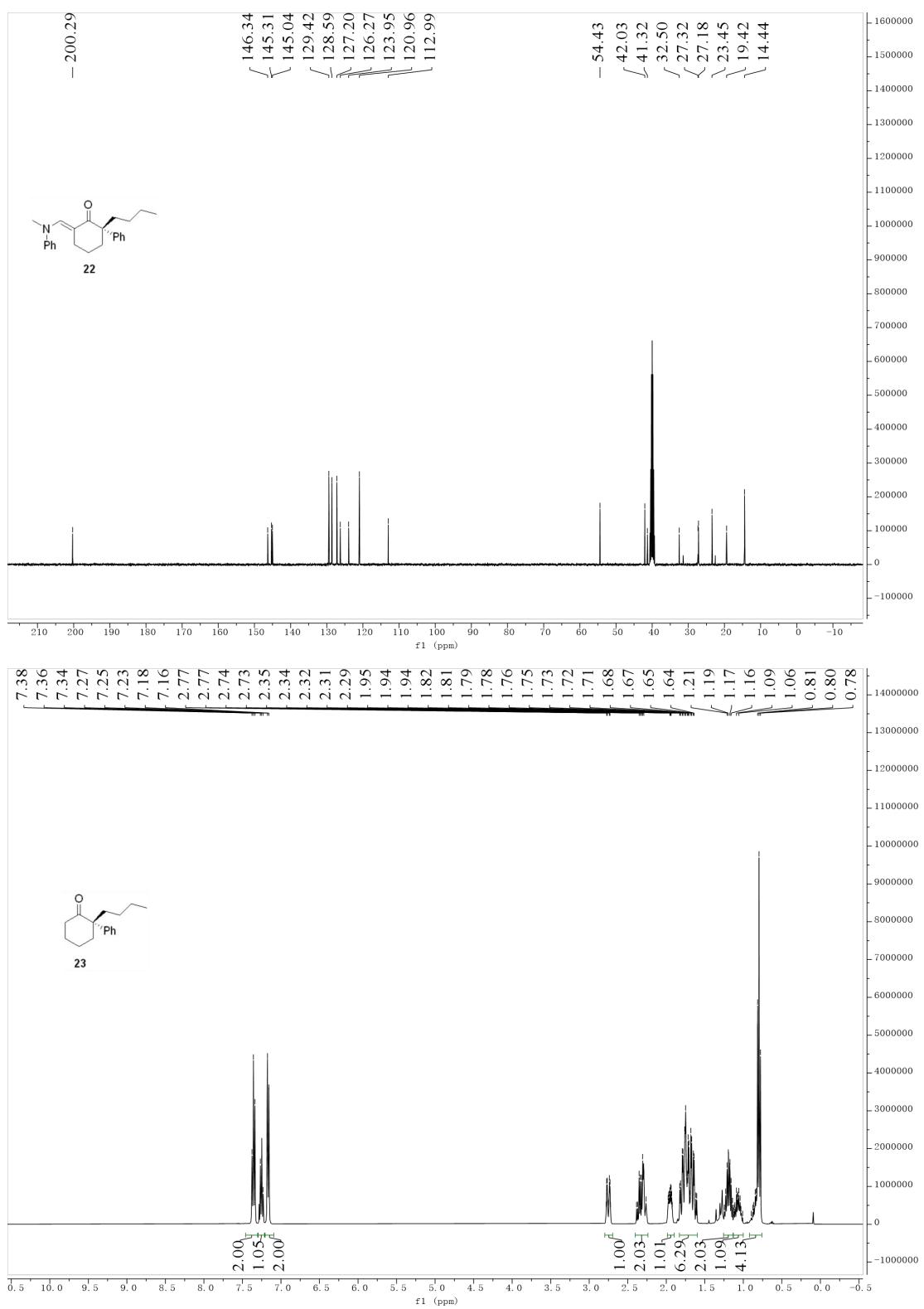




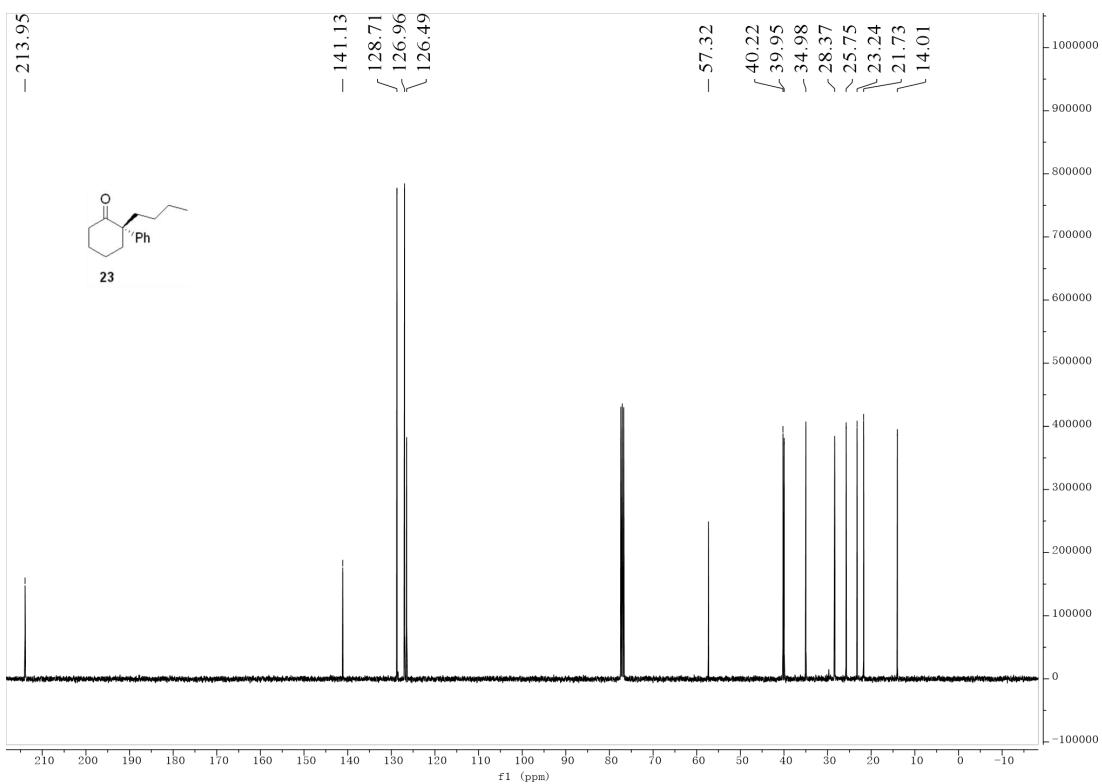








- 213.95



7.78

7.76

7.73

7.72

7.71

7.70

7.46

7.44

7.42

7.40

7.38

7.36

7.34

7.31

7.29

7.24

7.22

7.21

7.12

7.11

7.09

7.08

7.05

7.04

3.97

3.96

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2.03

2.02

2.00

1.99

1.86

1.83

1.80

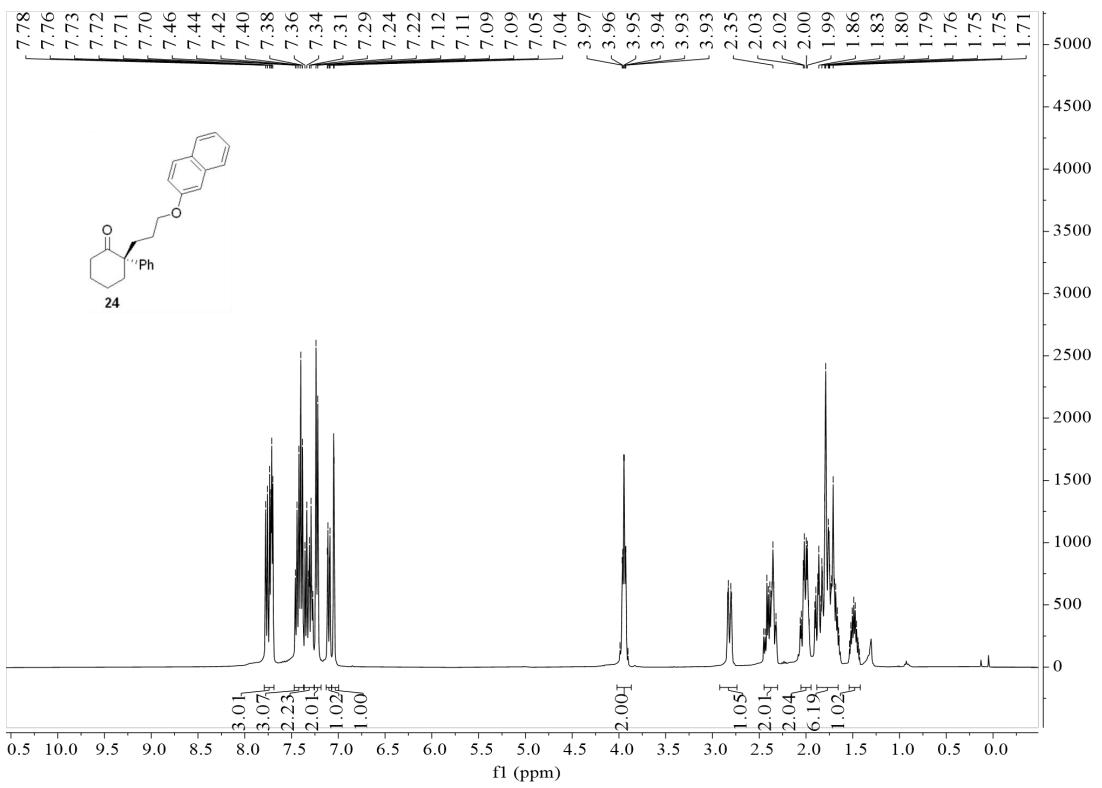
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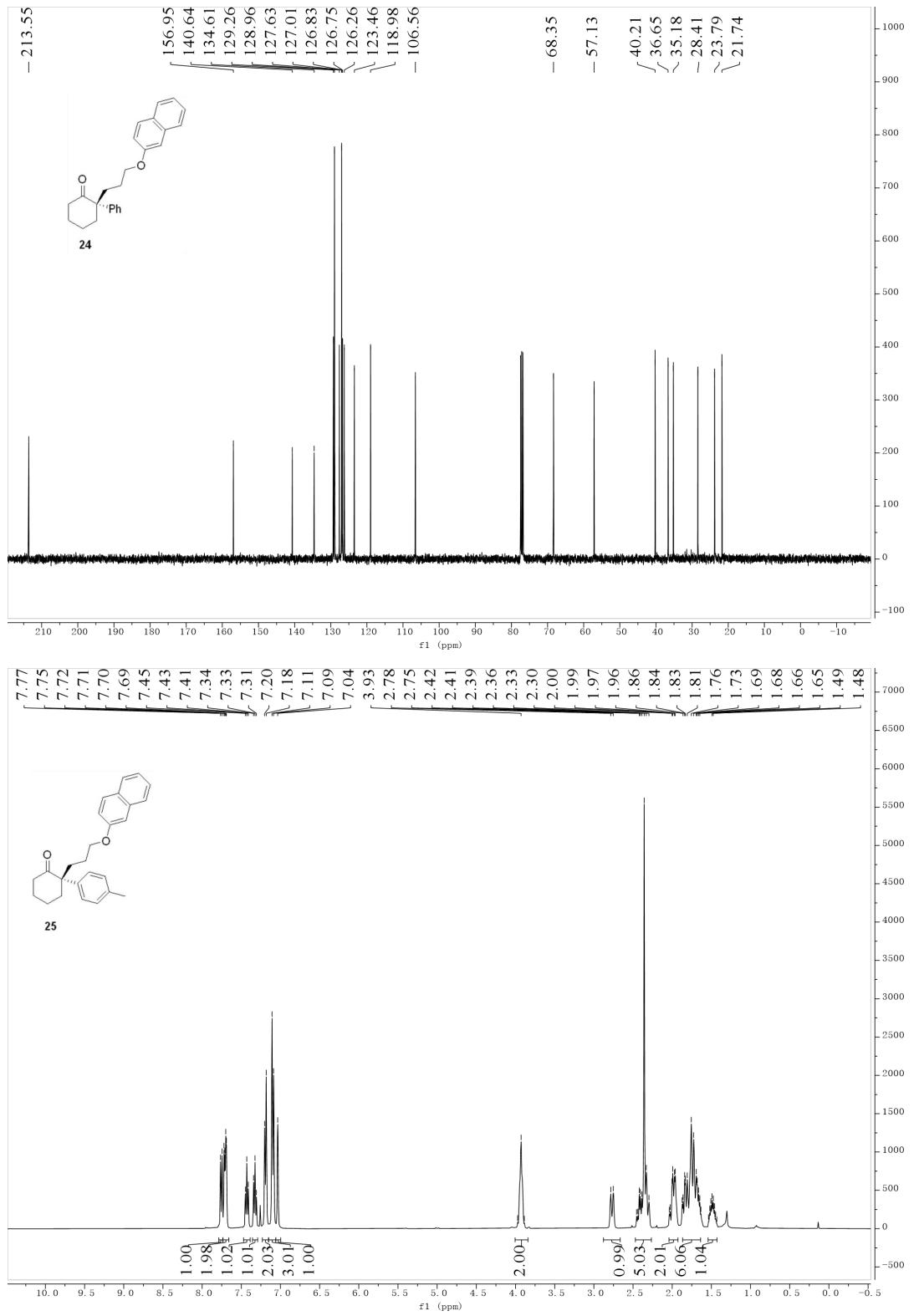
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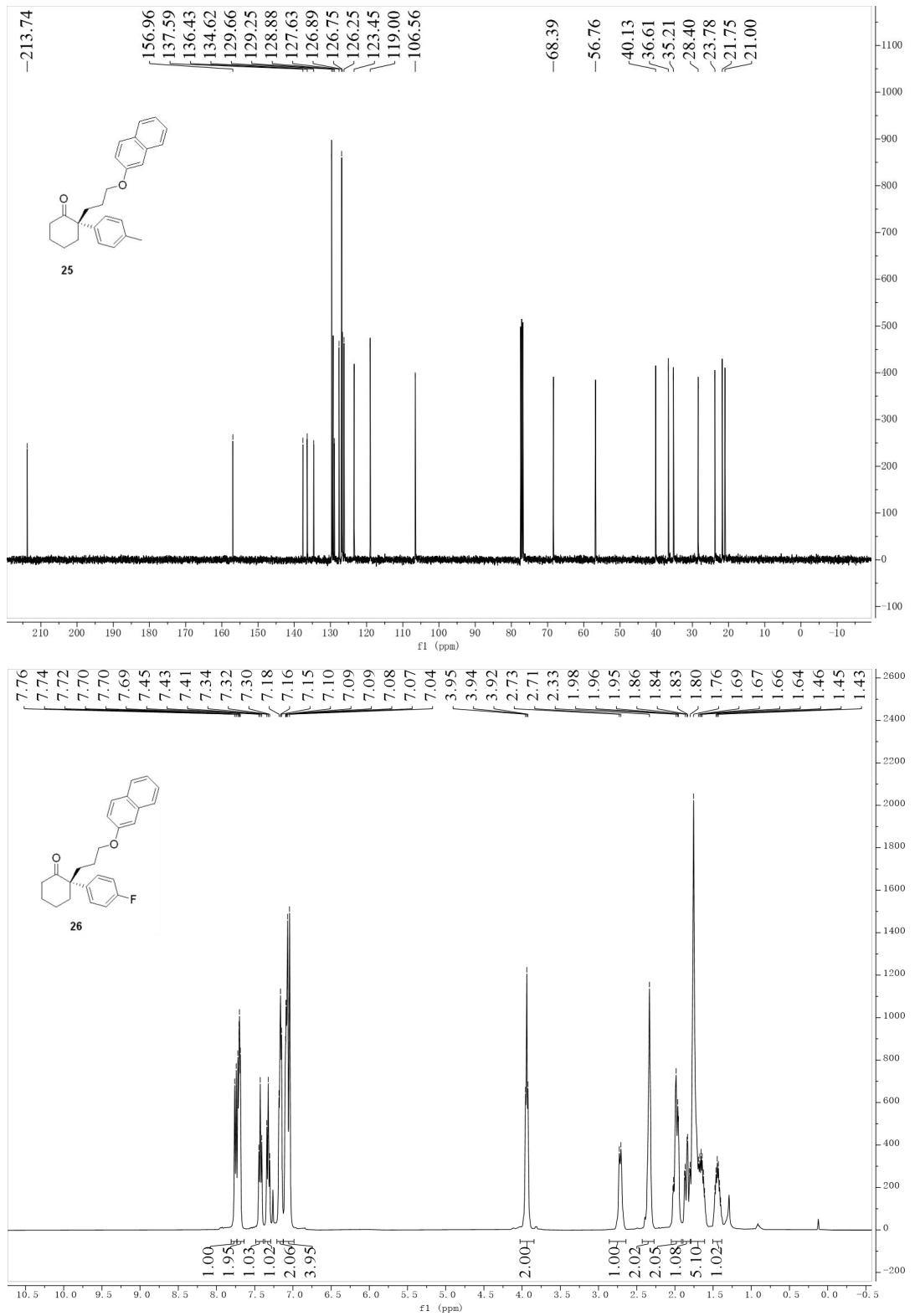
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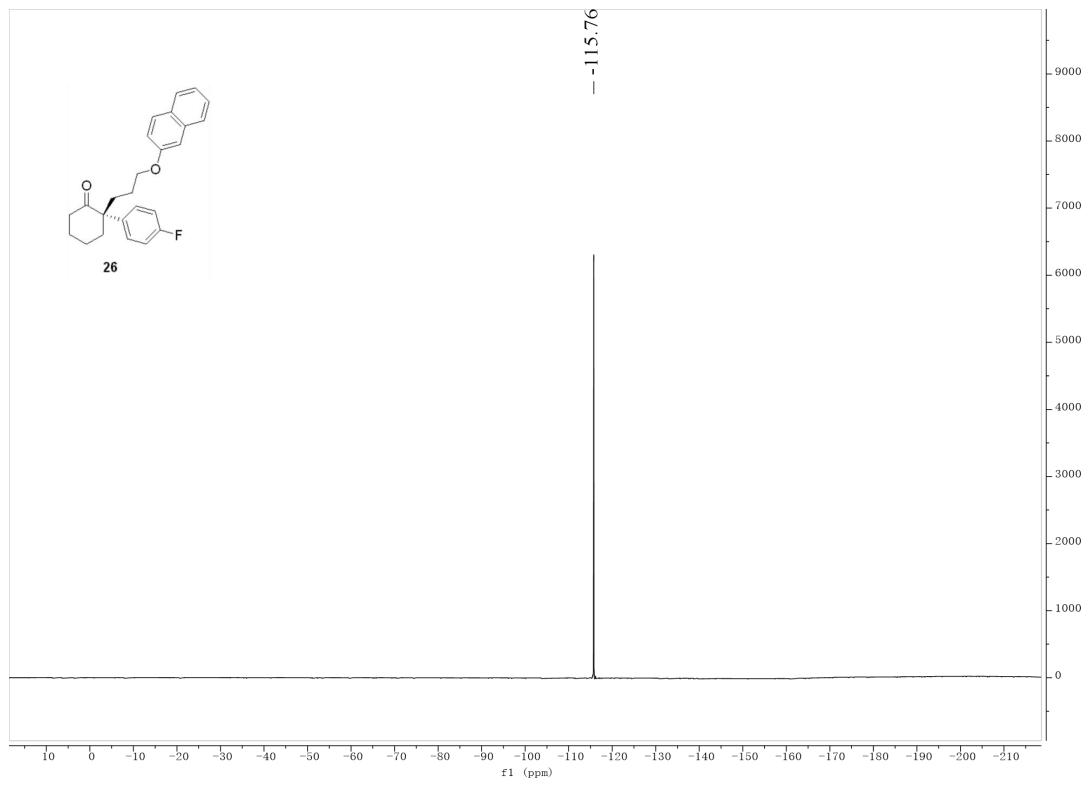
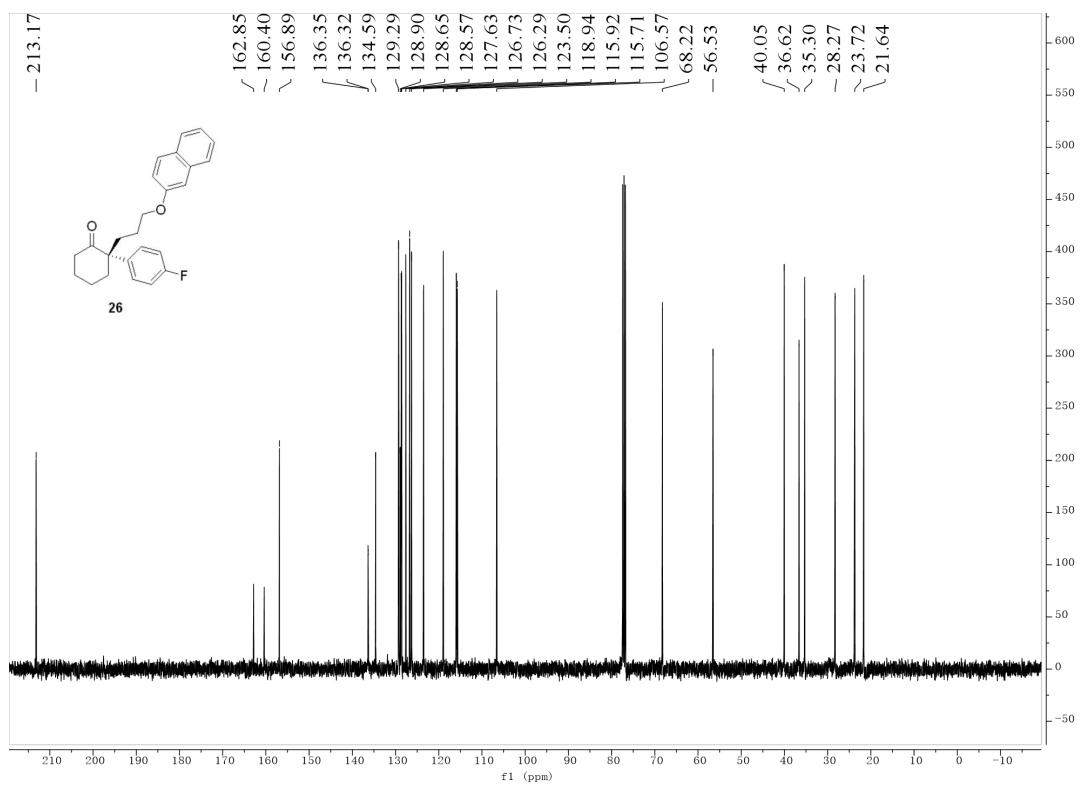
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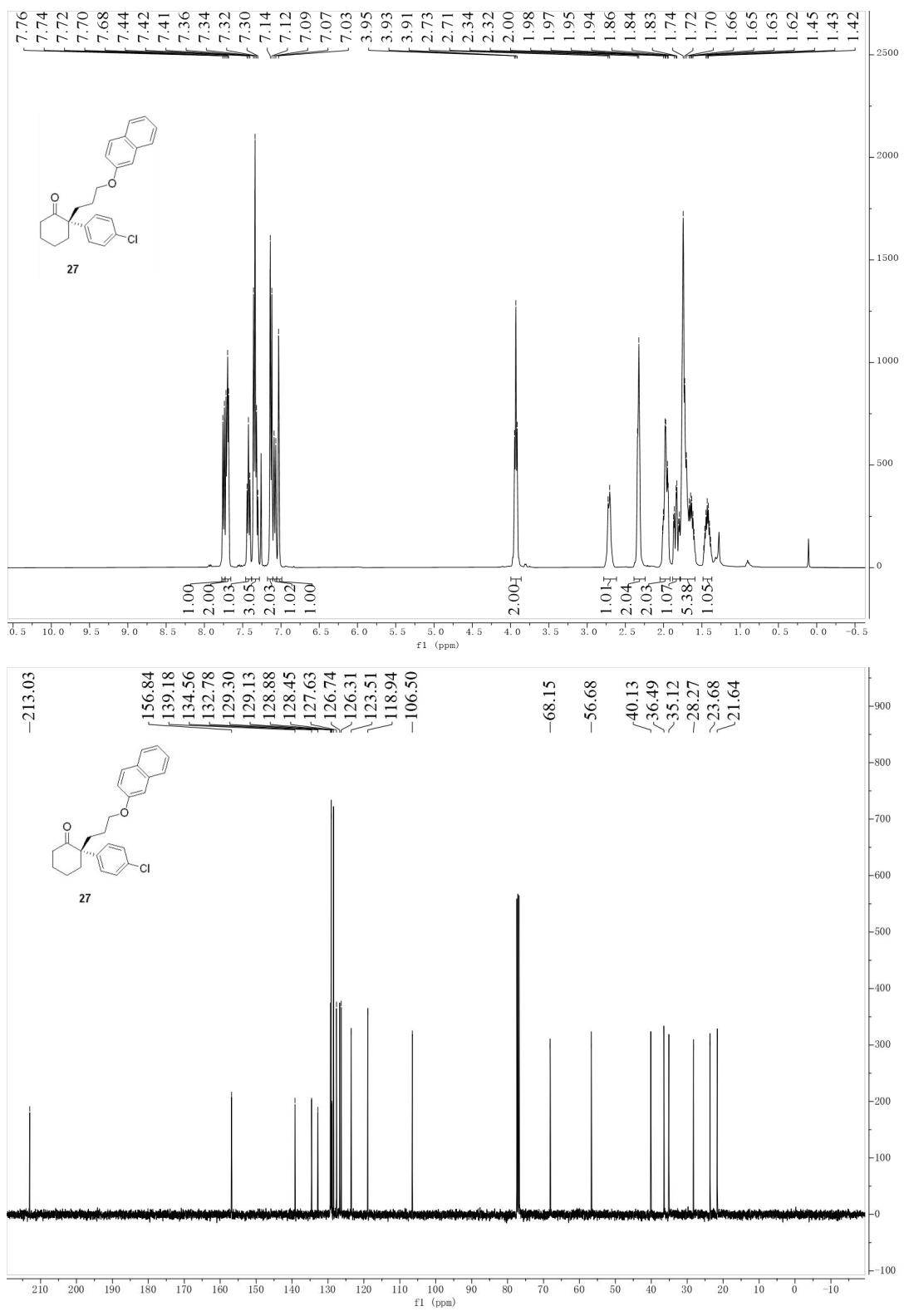
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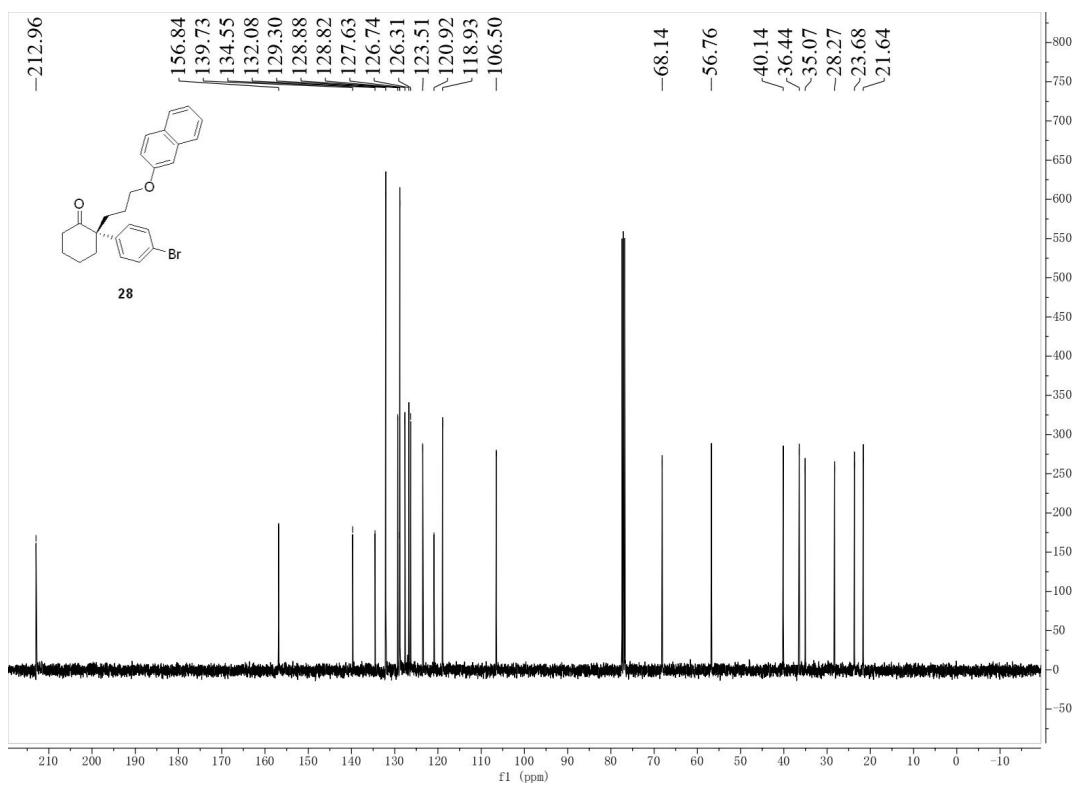
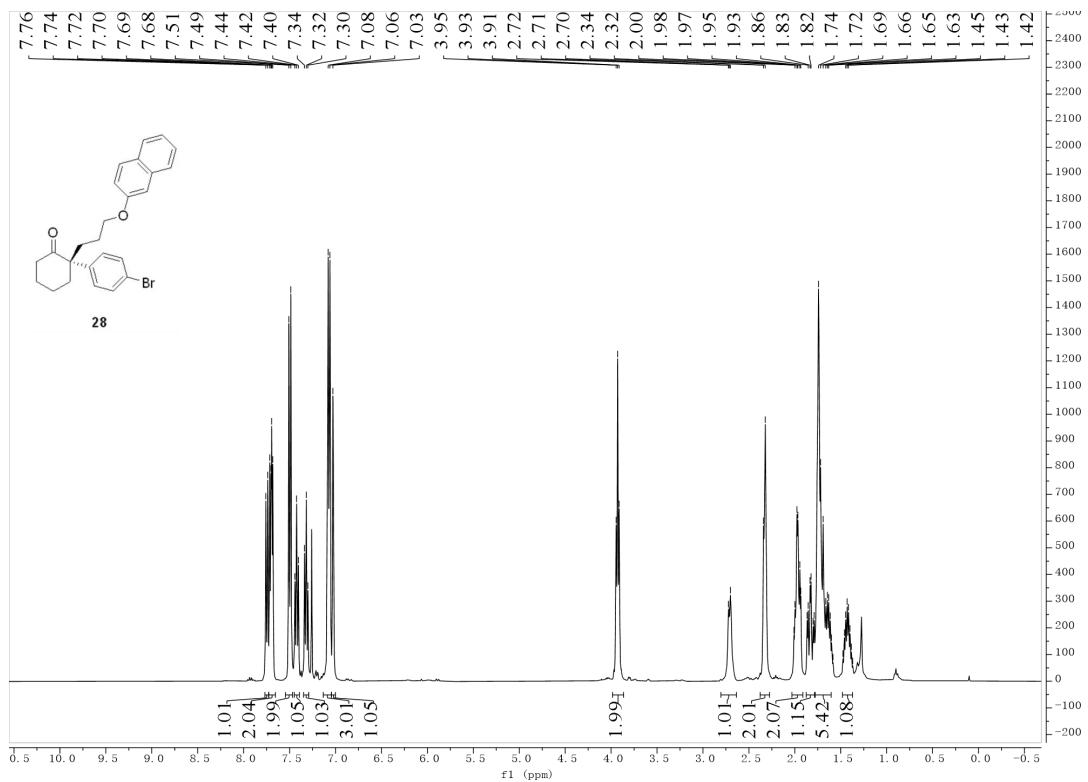


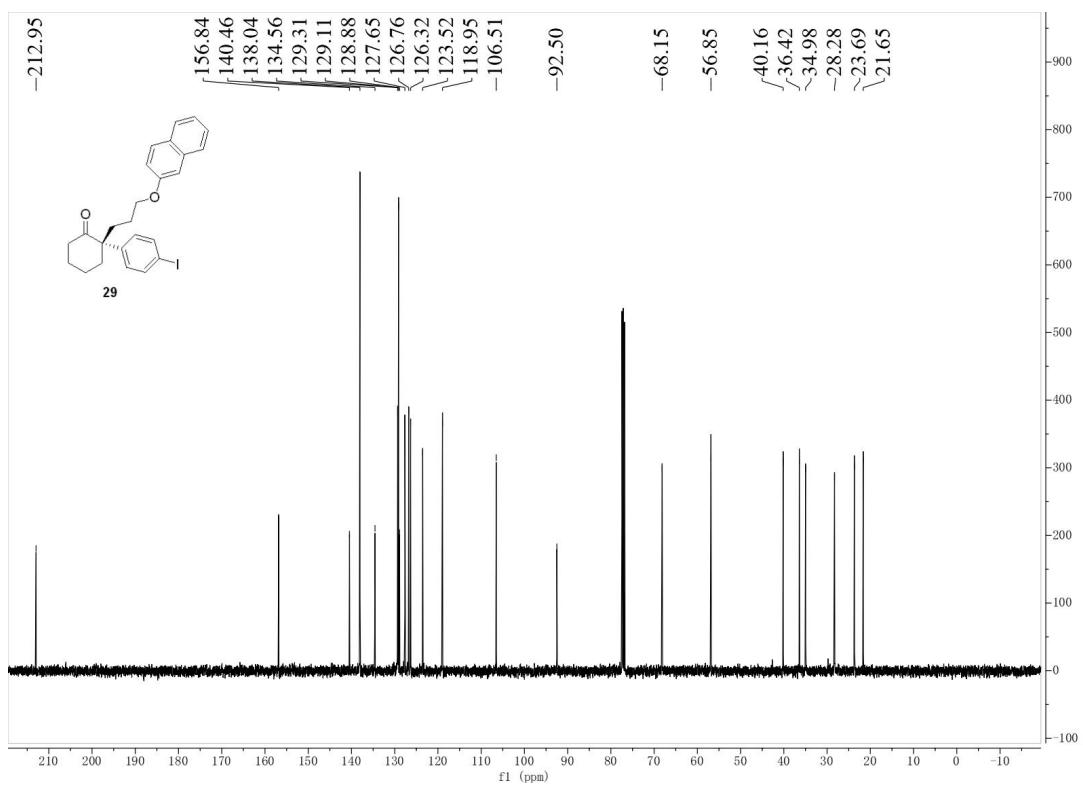
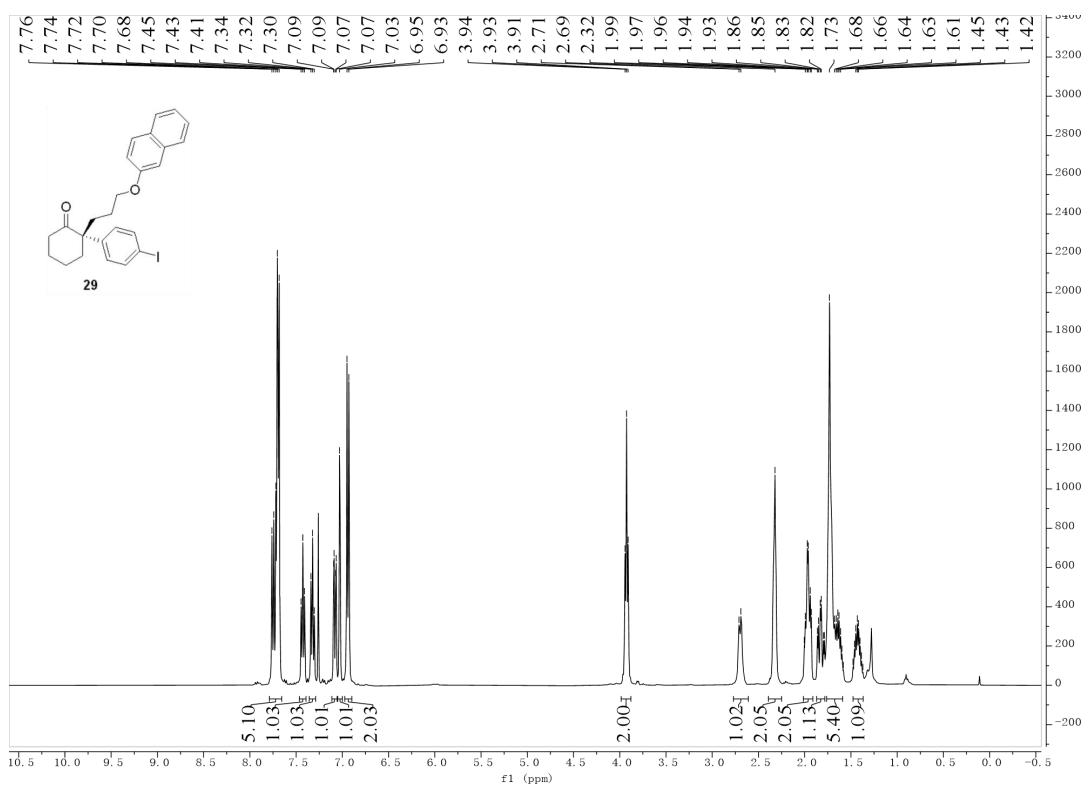


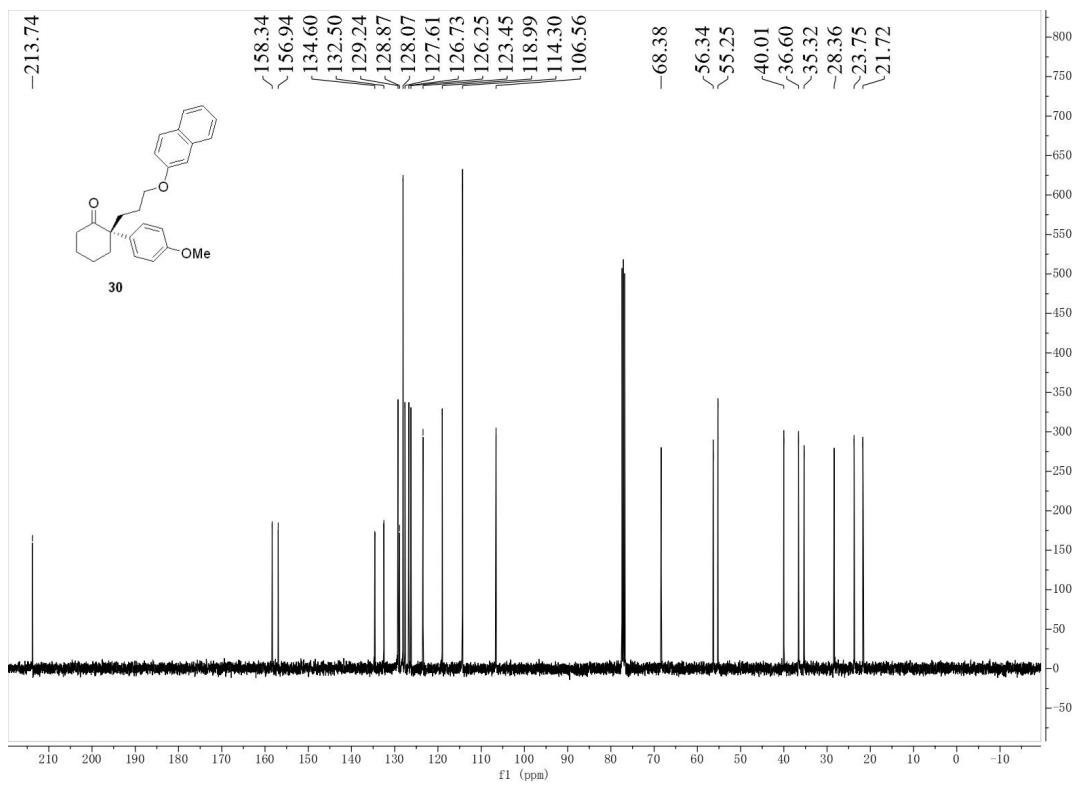
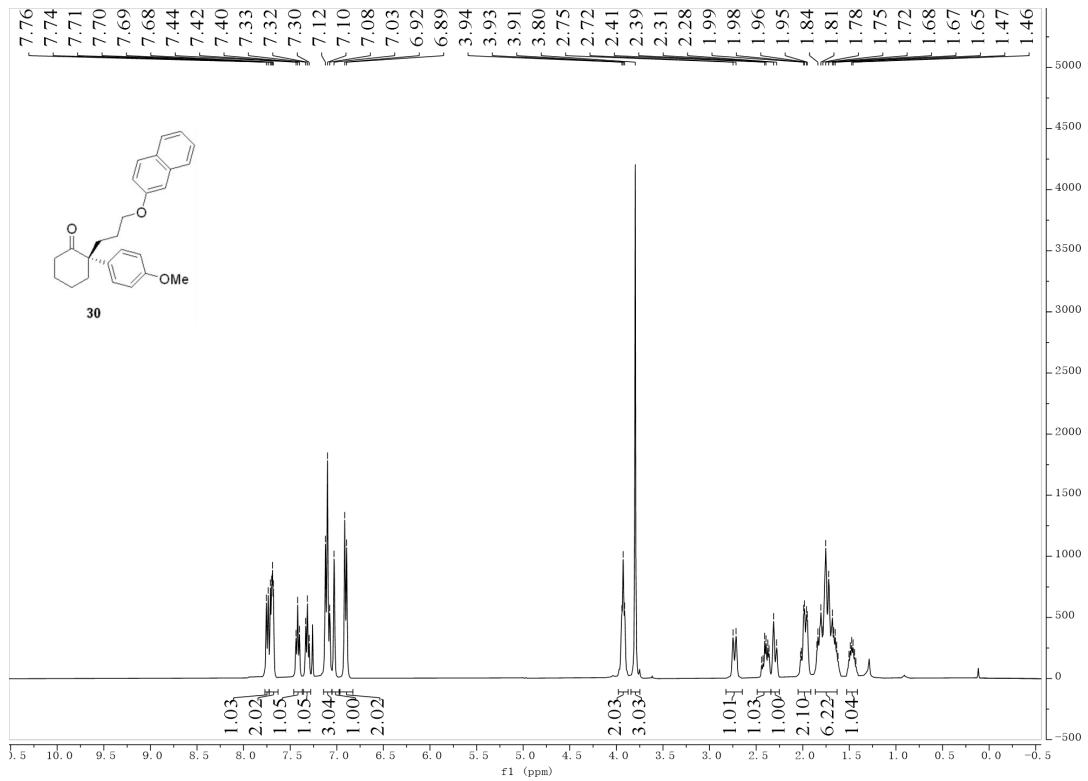


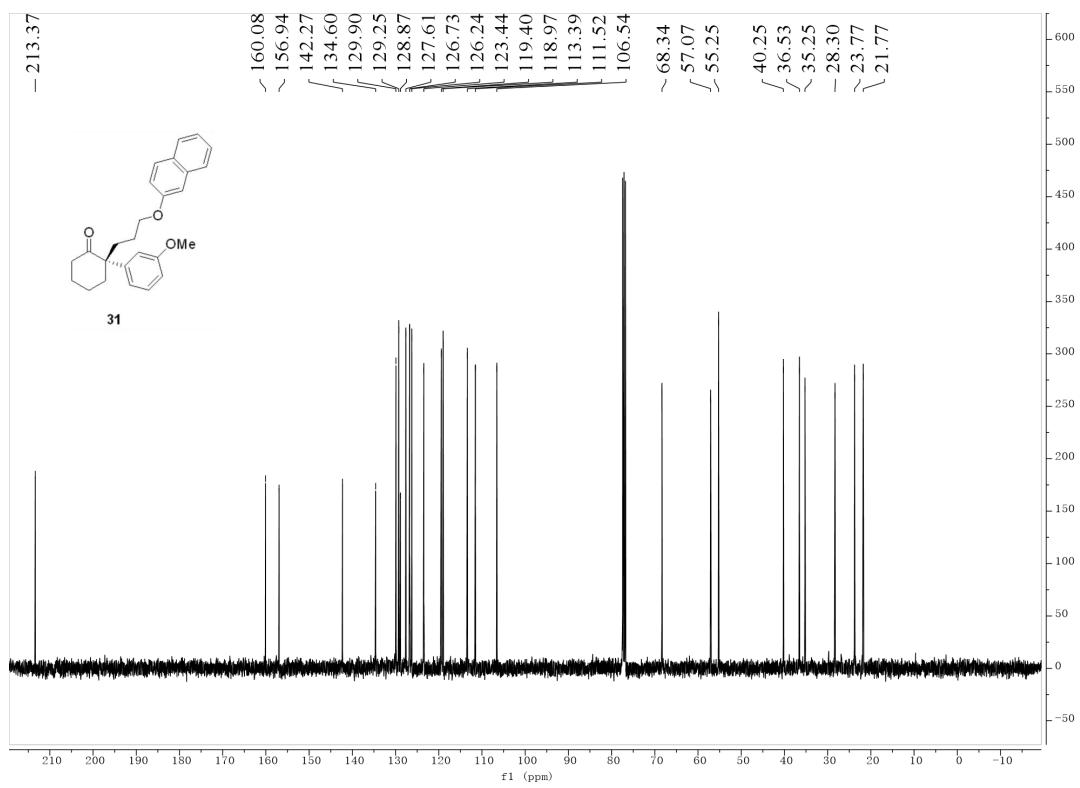
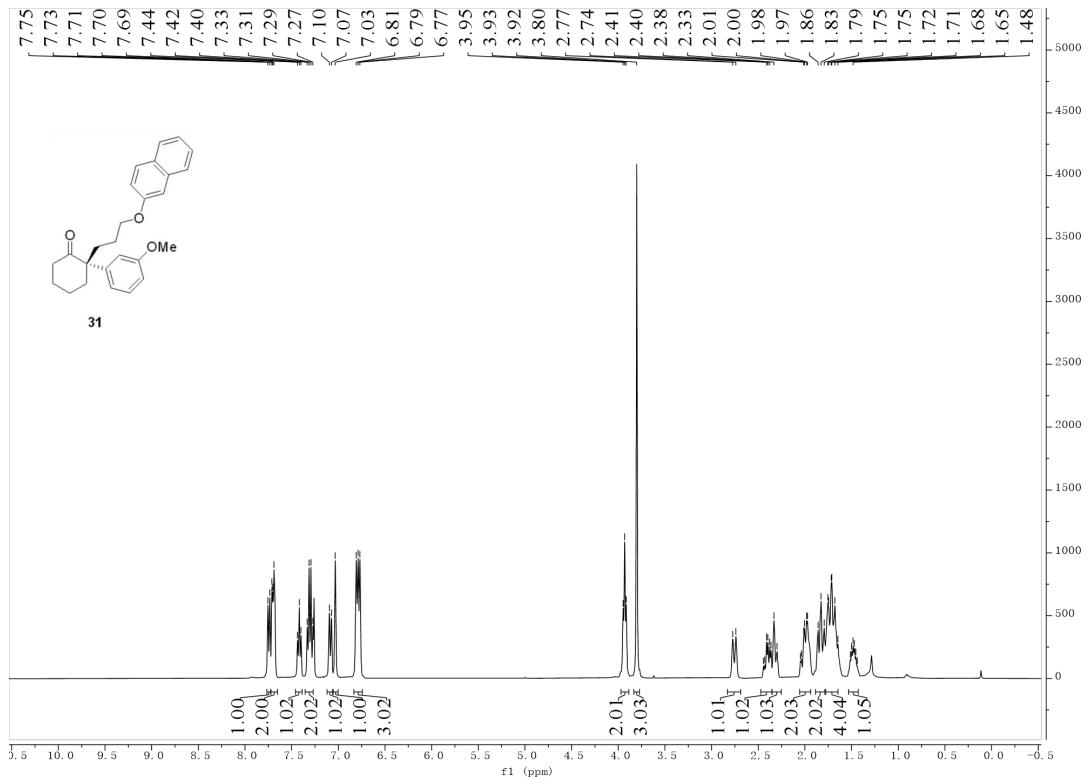


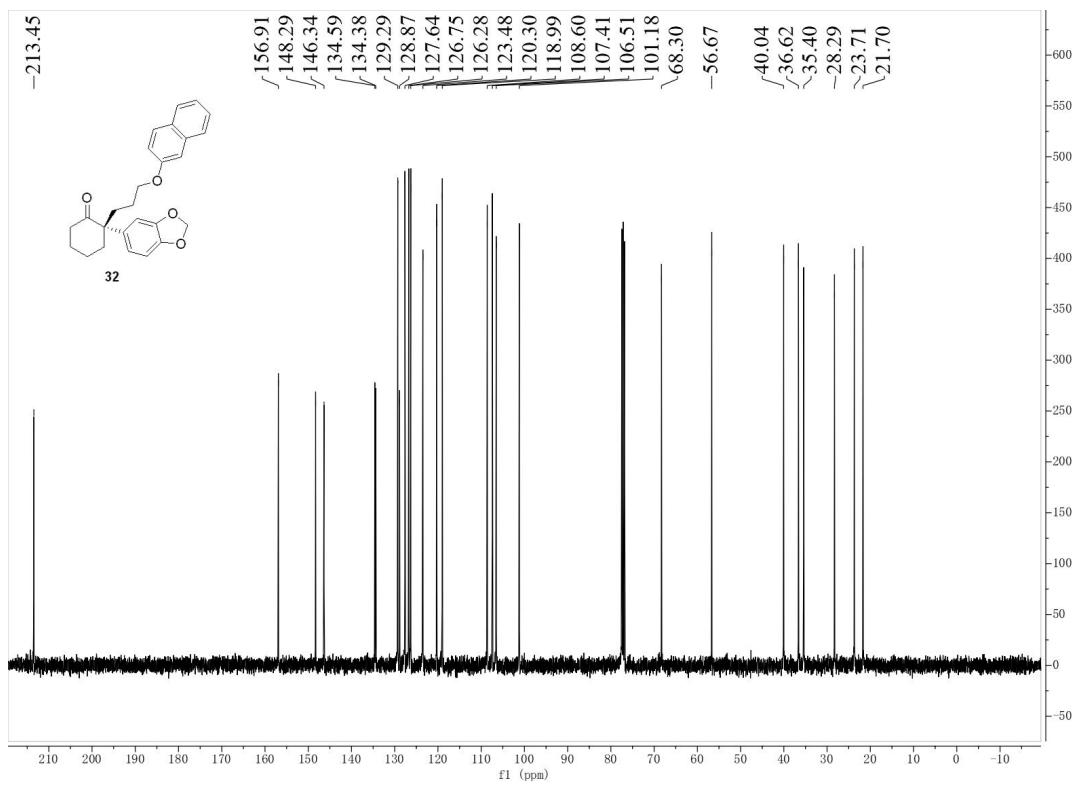
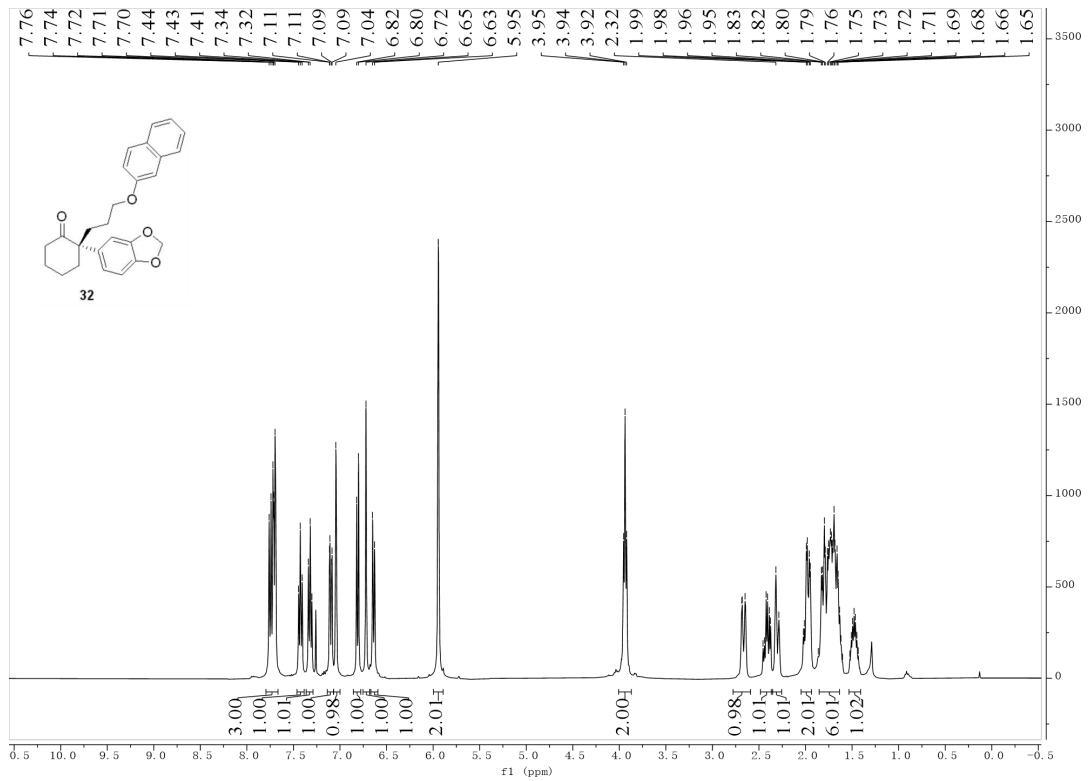


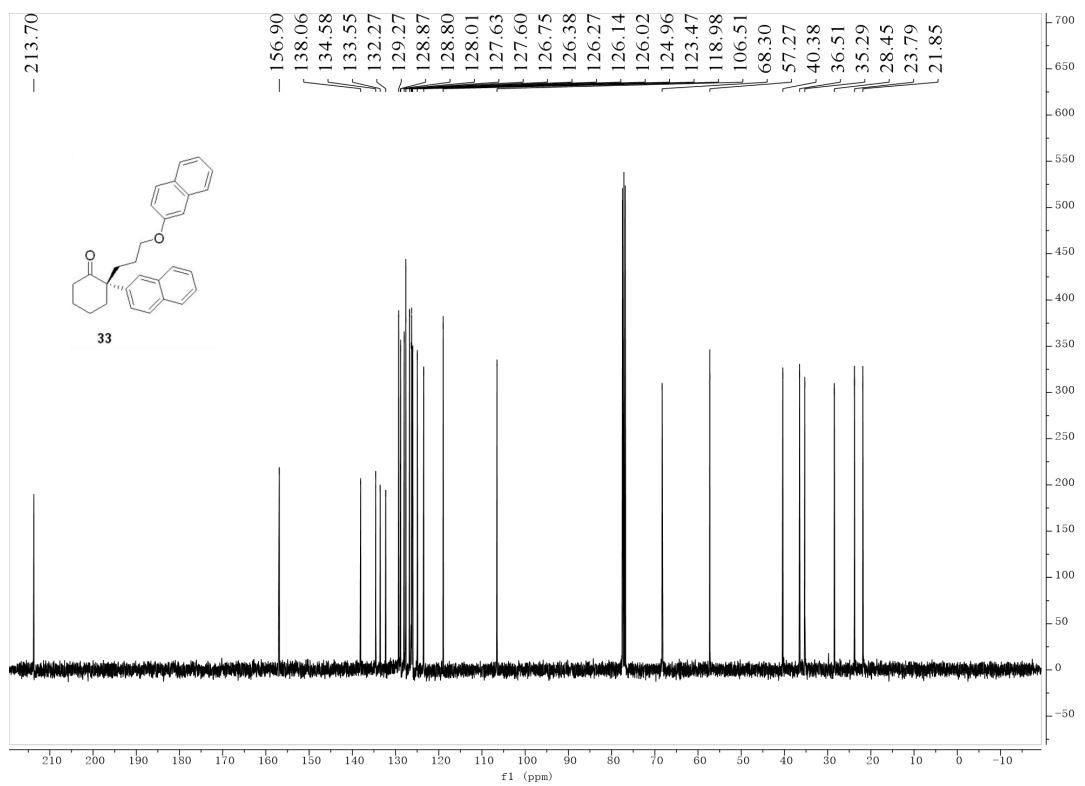
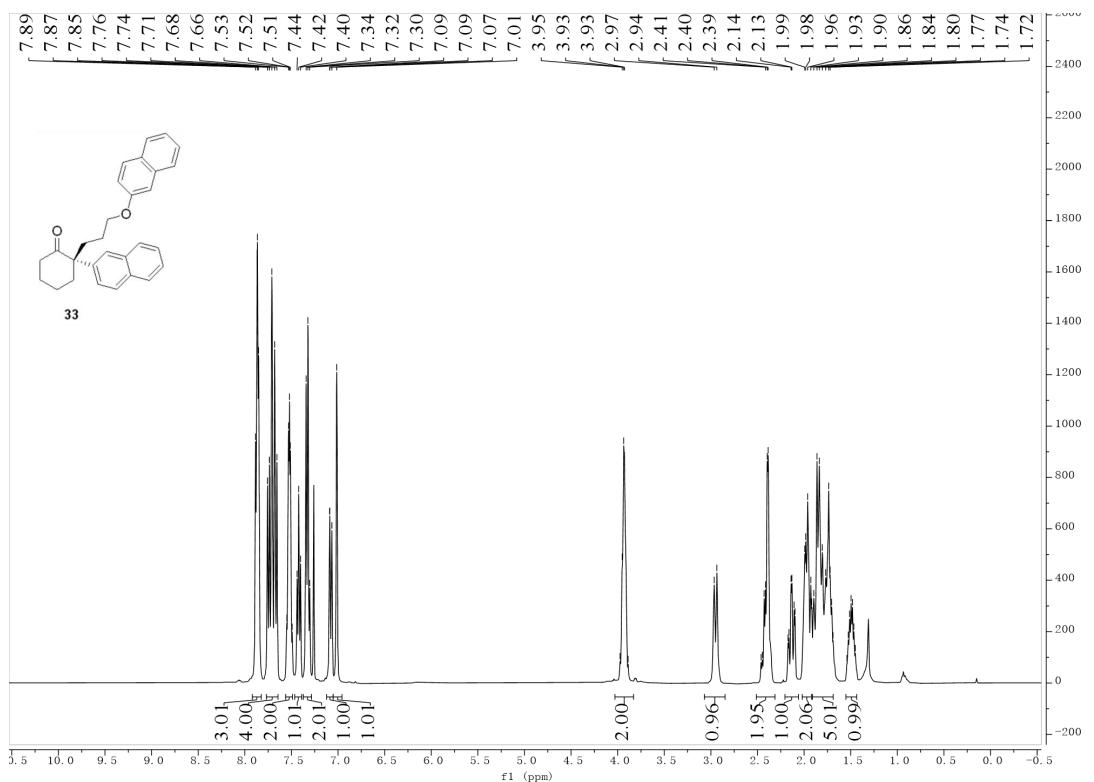


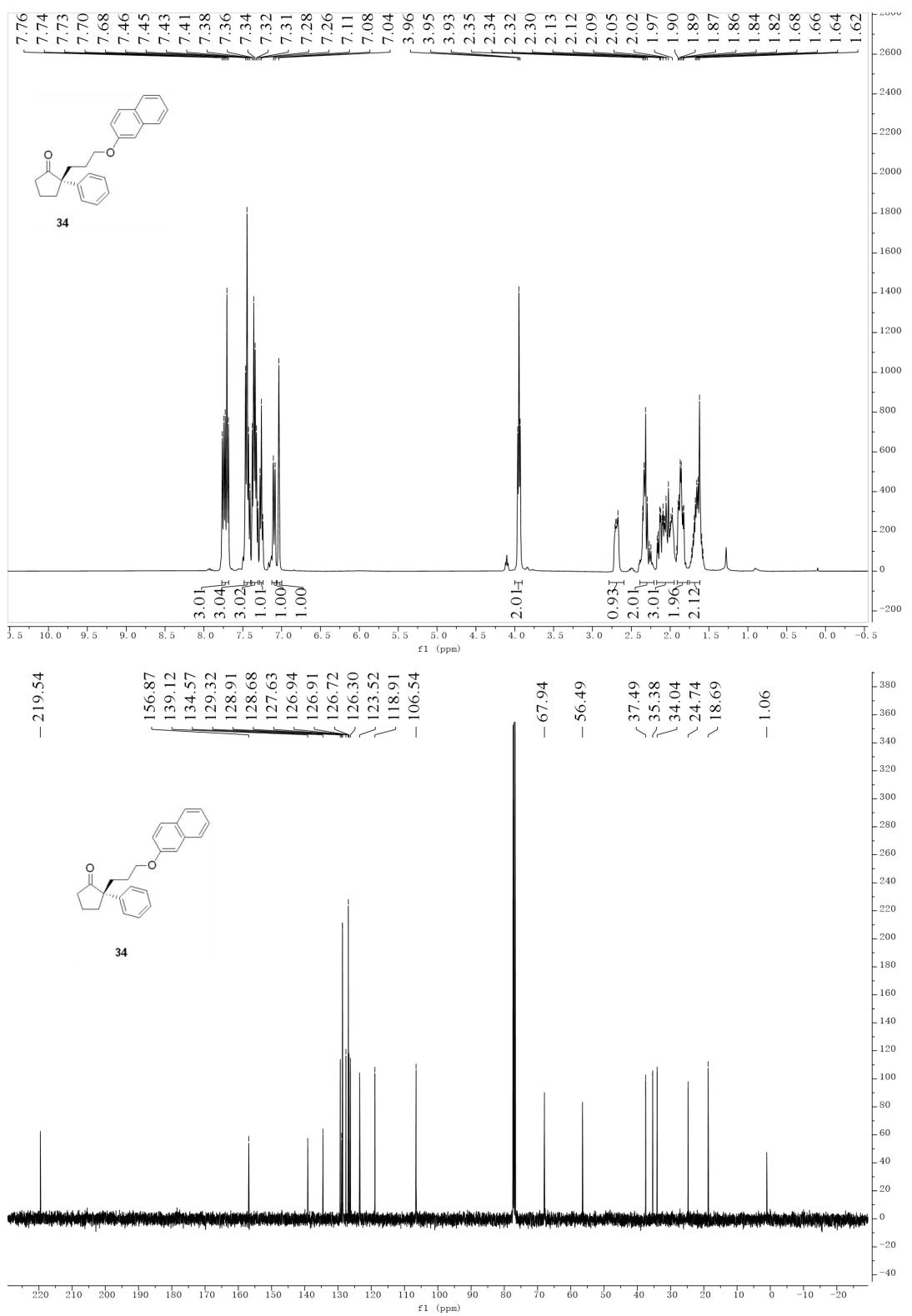


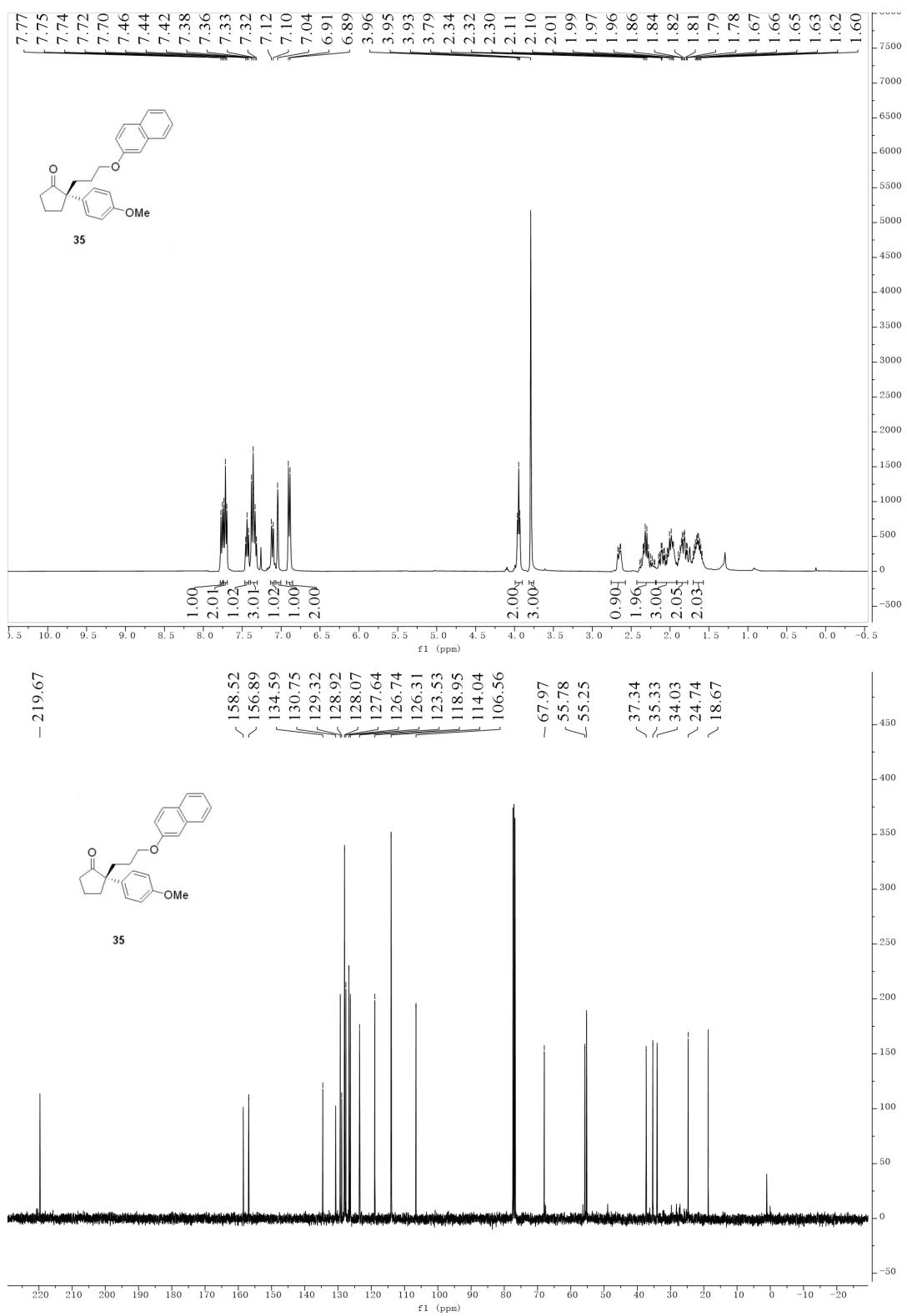


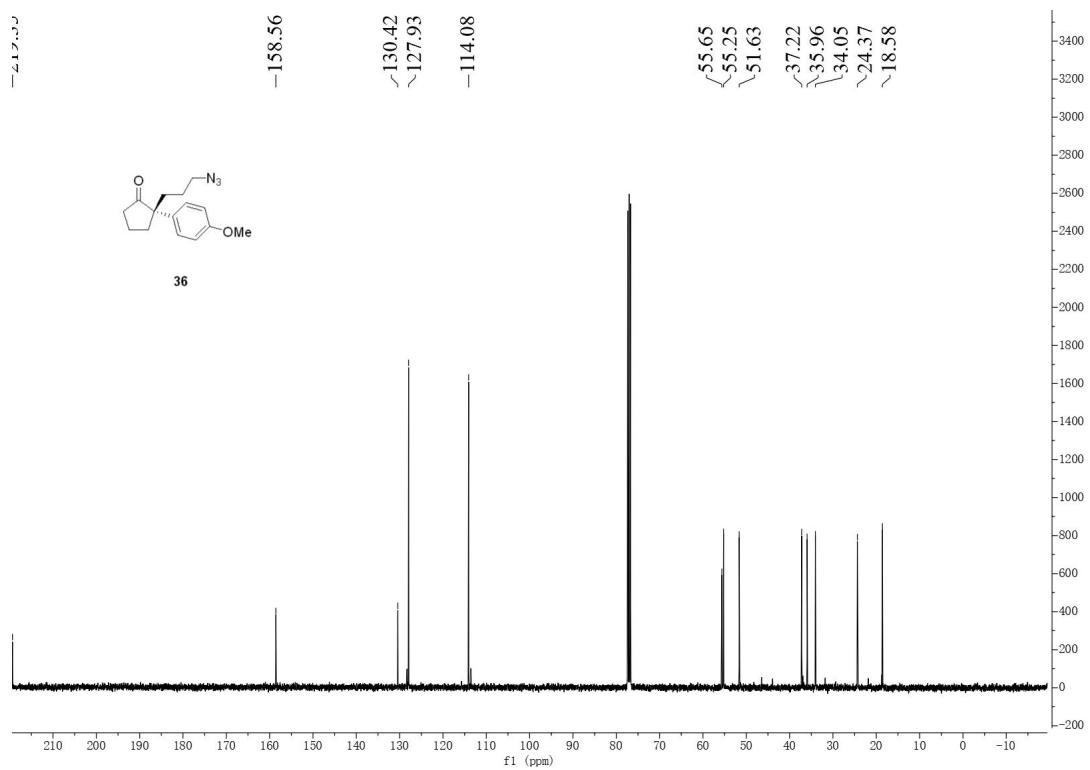
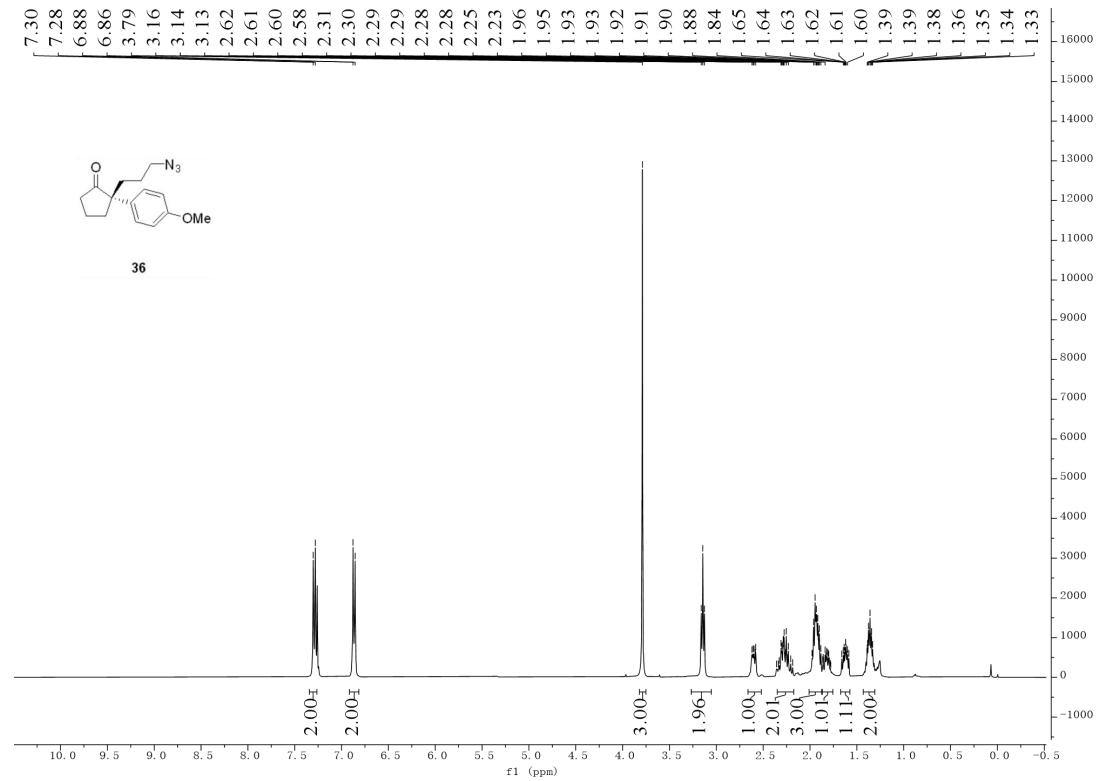


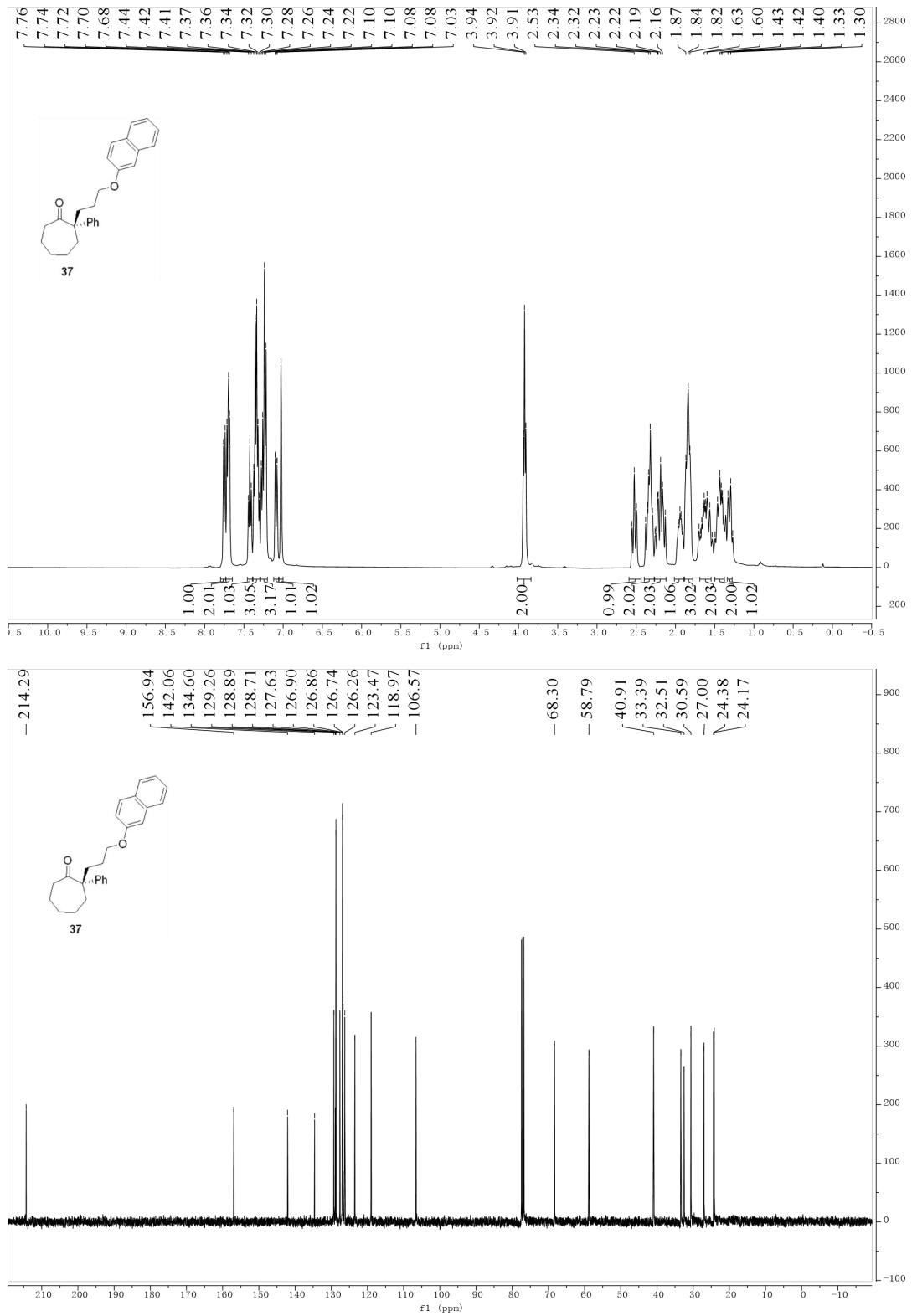


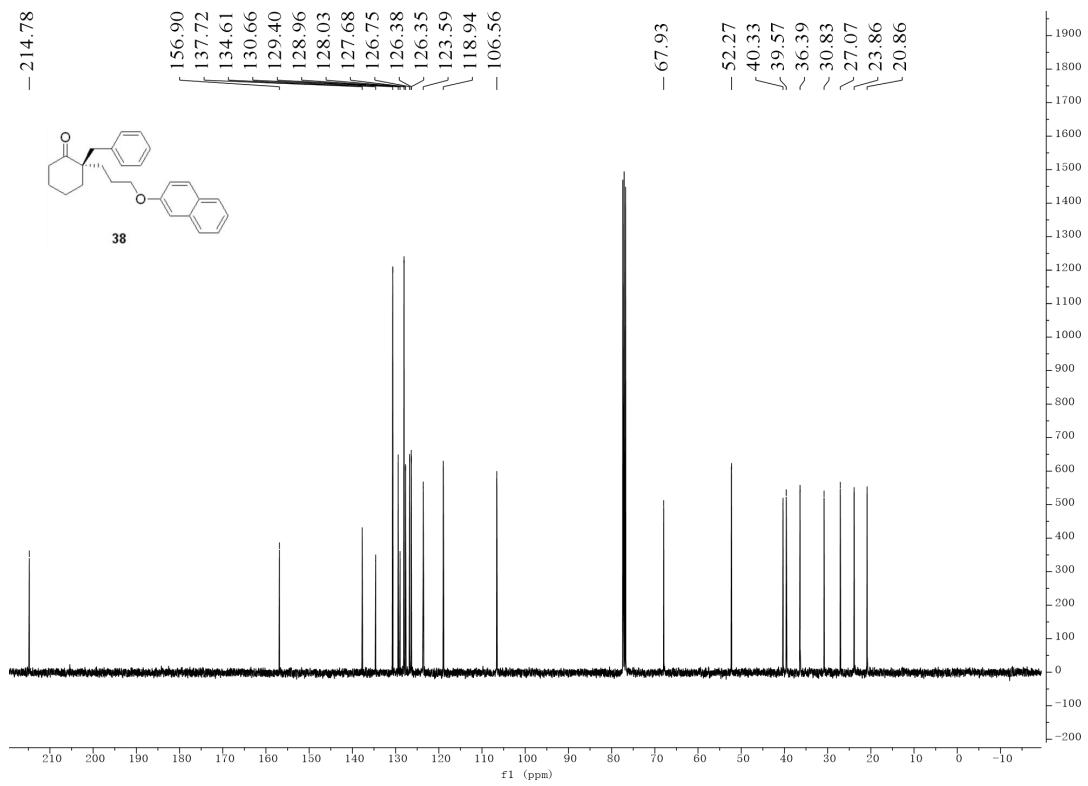
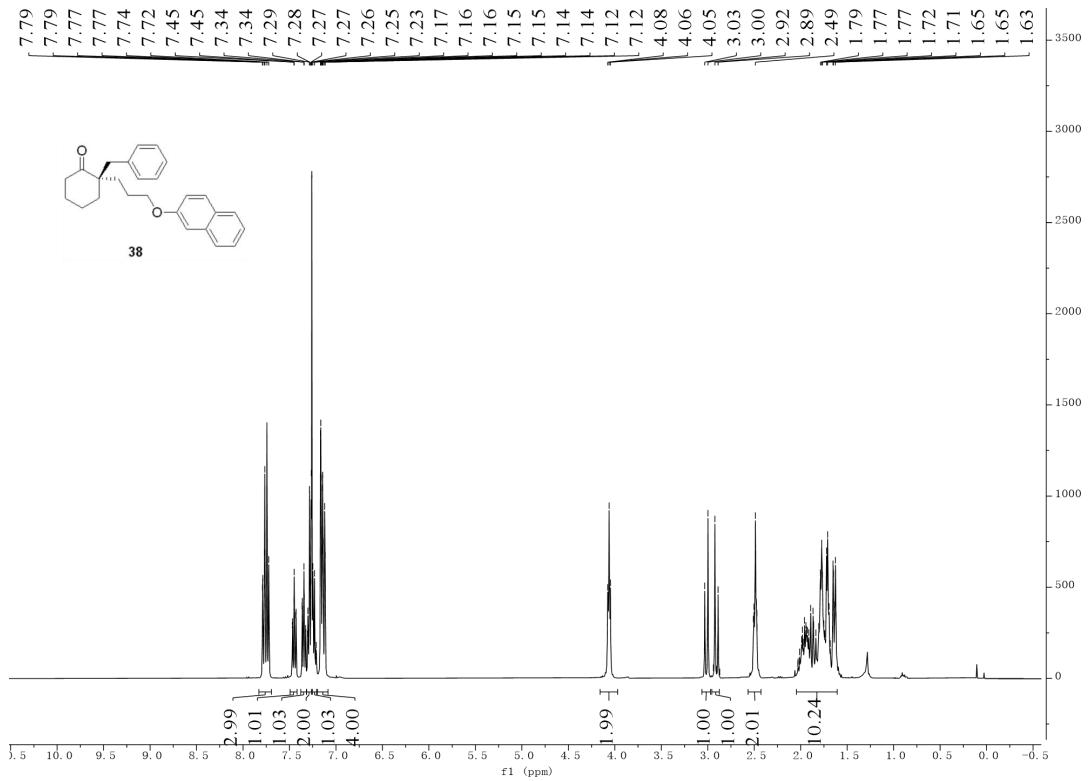


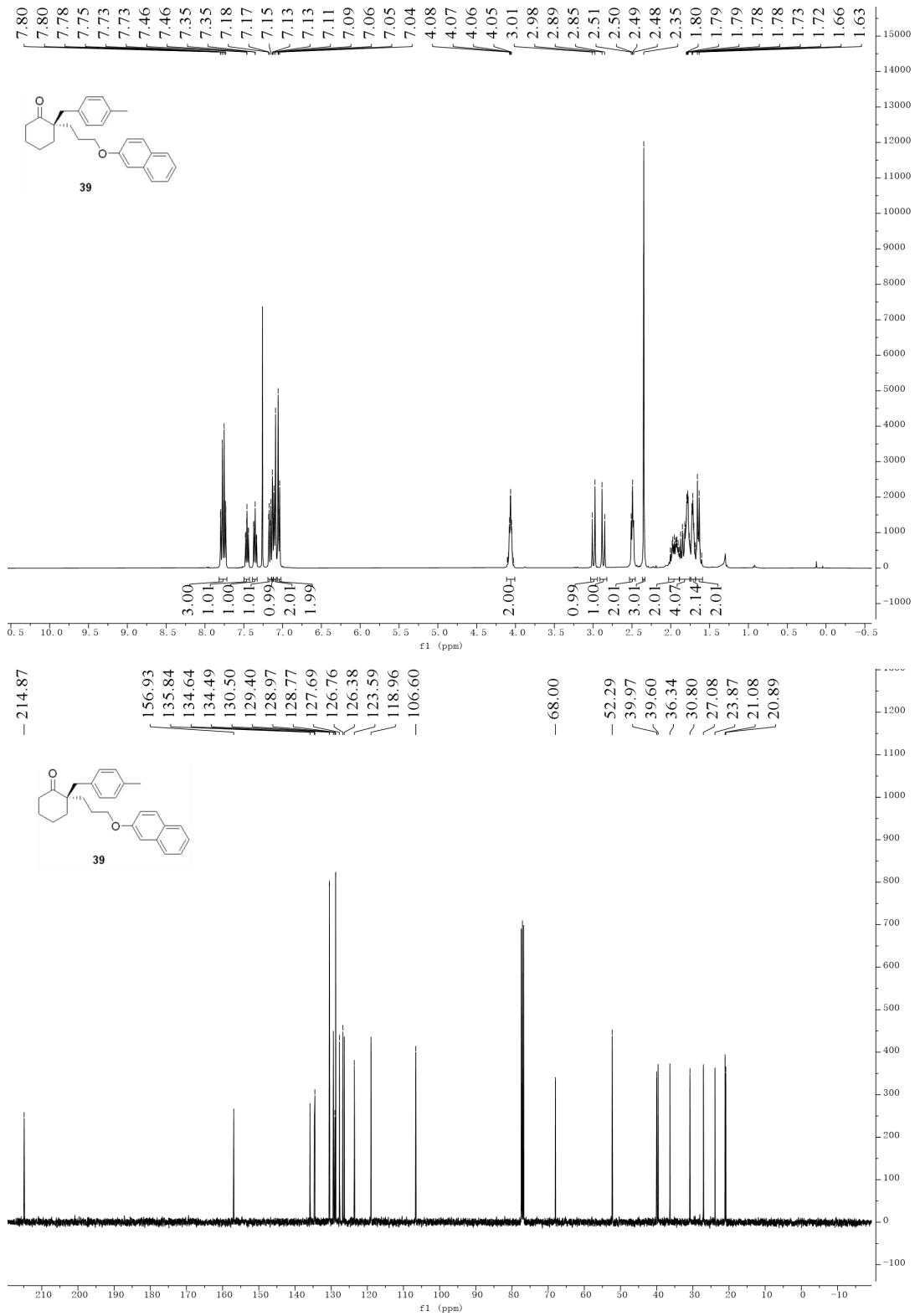


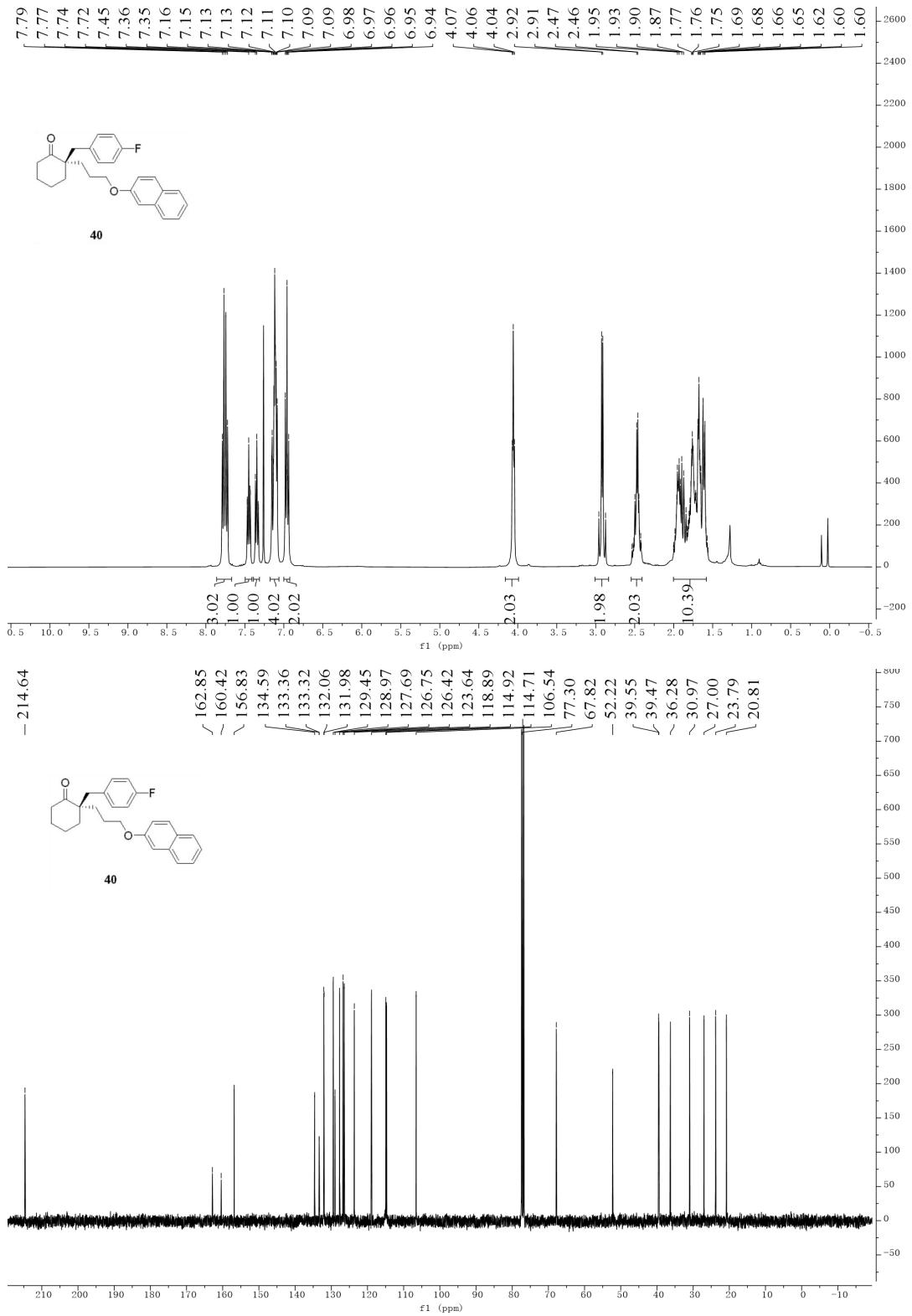


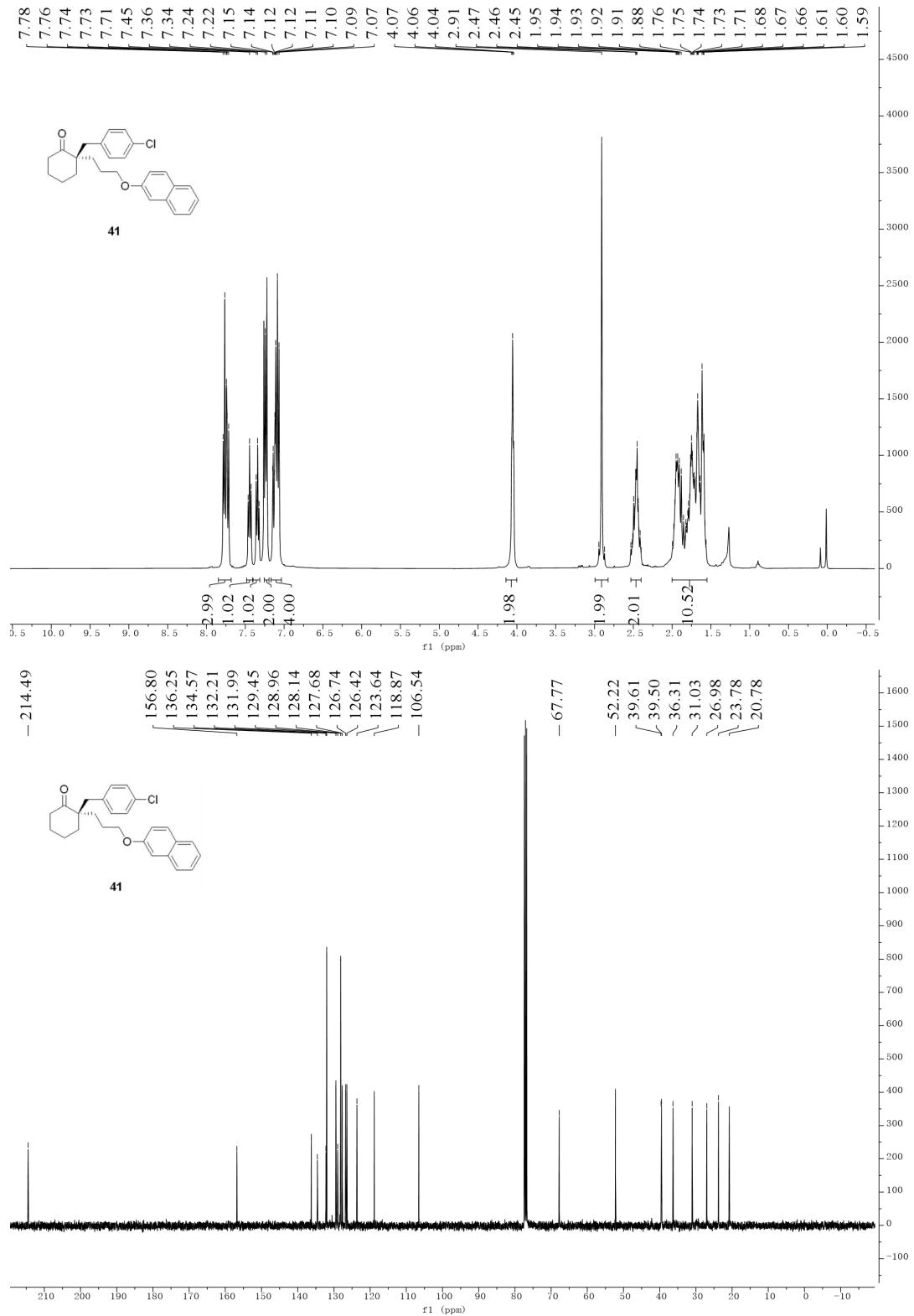


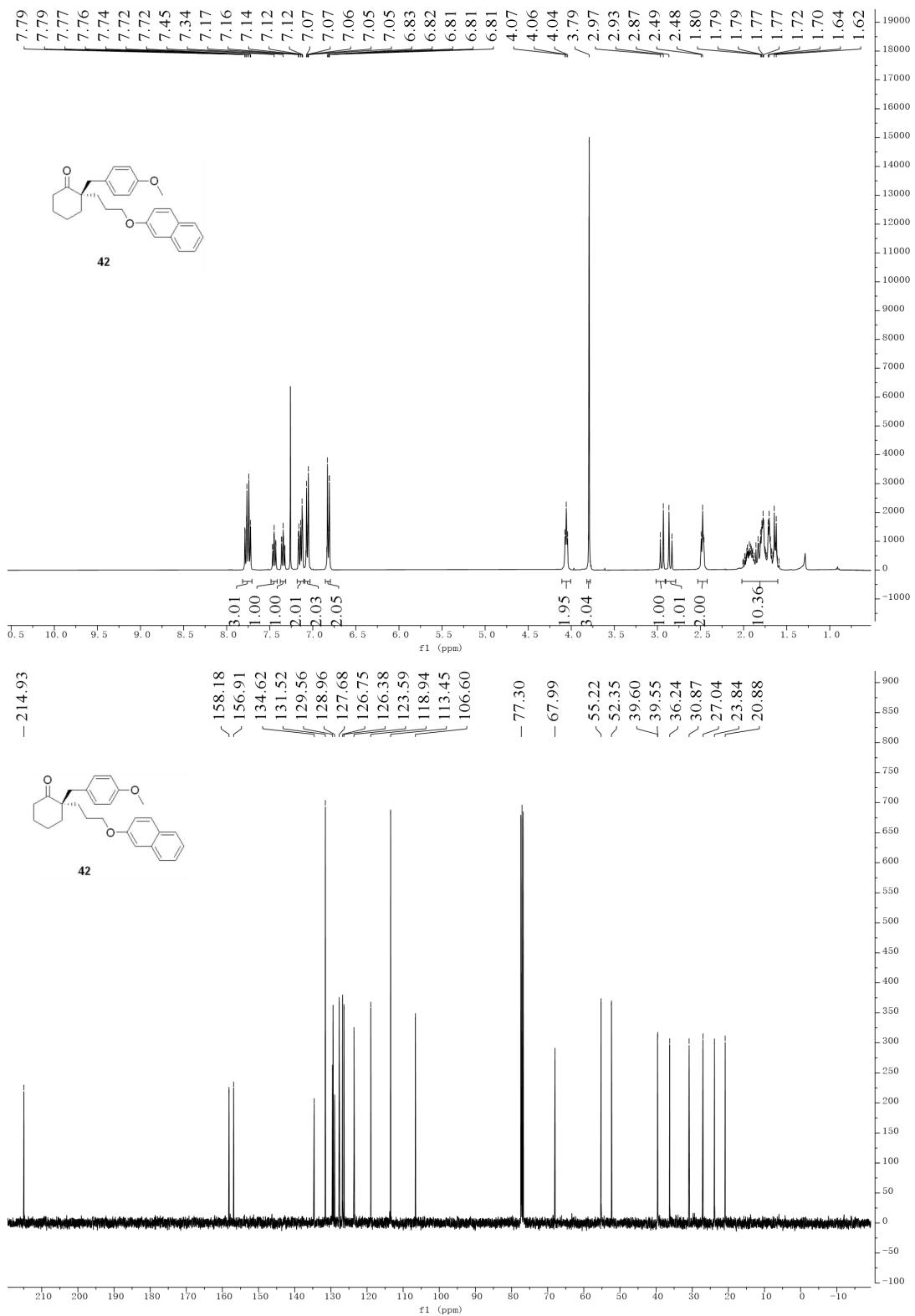


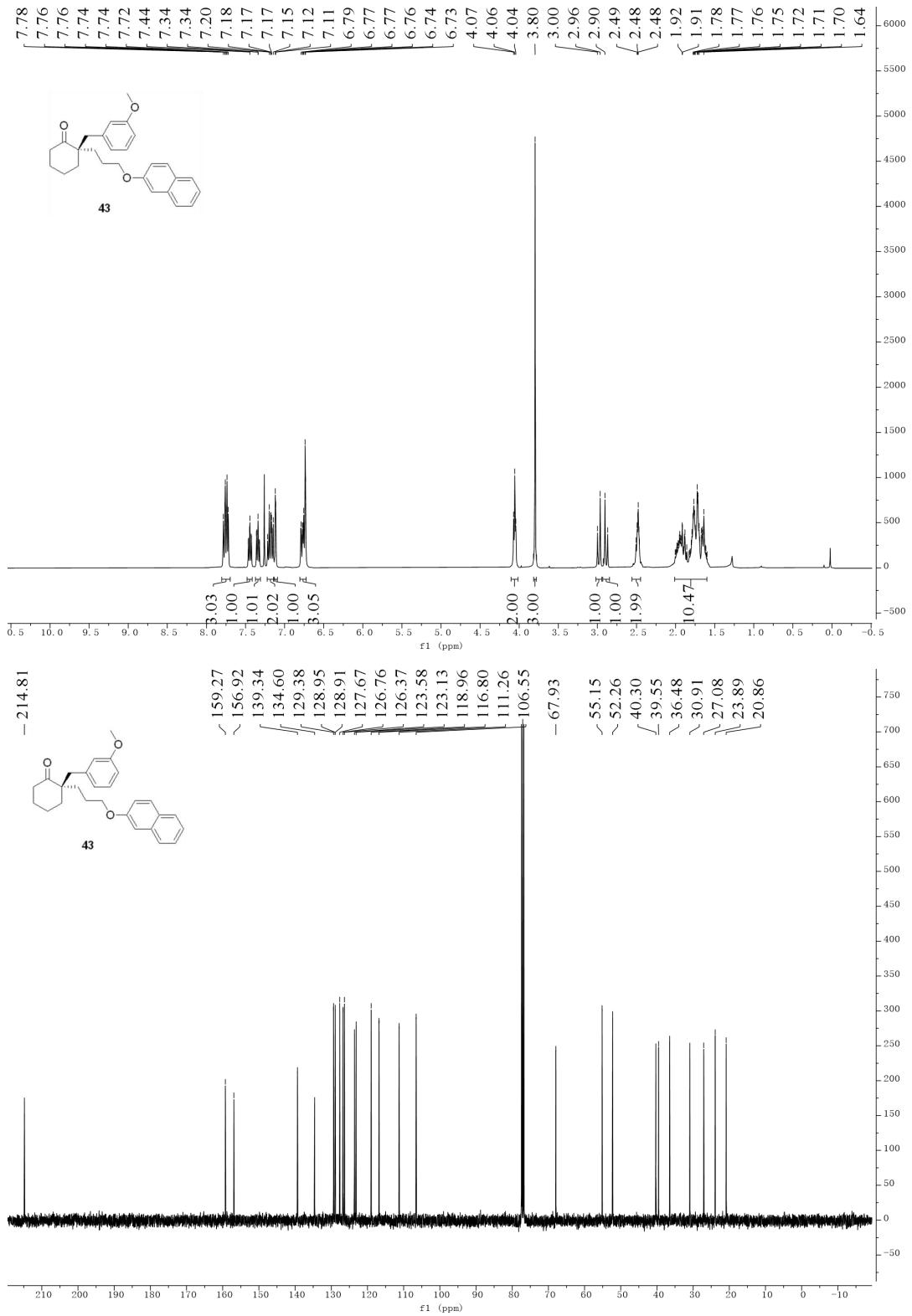


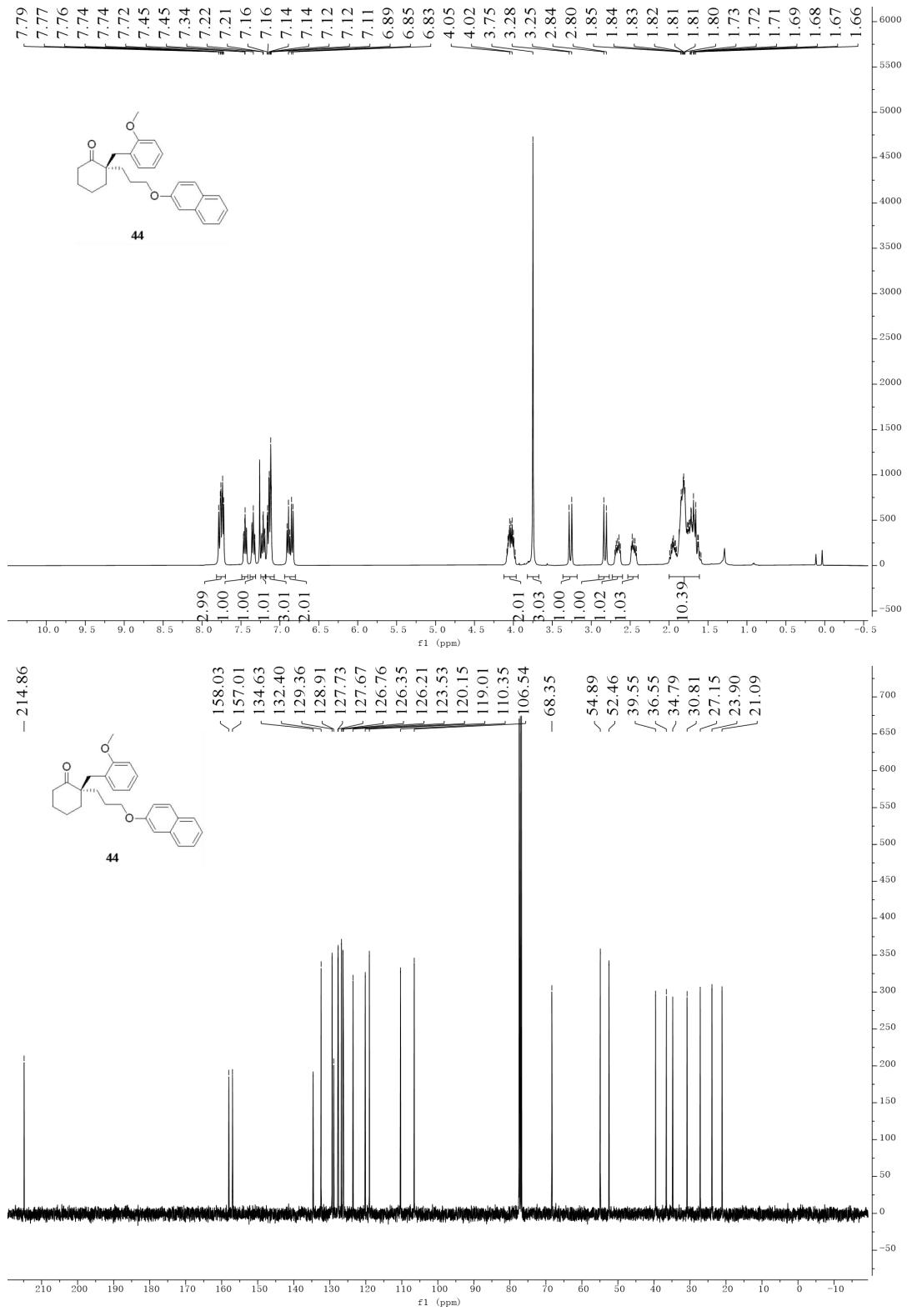


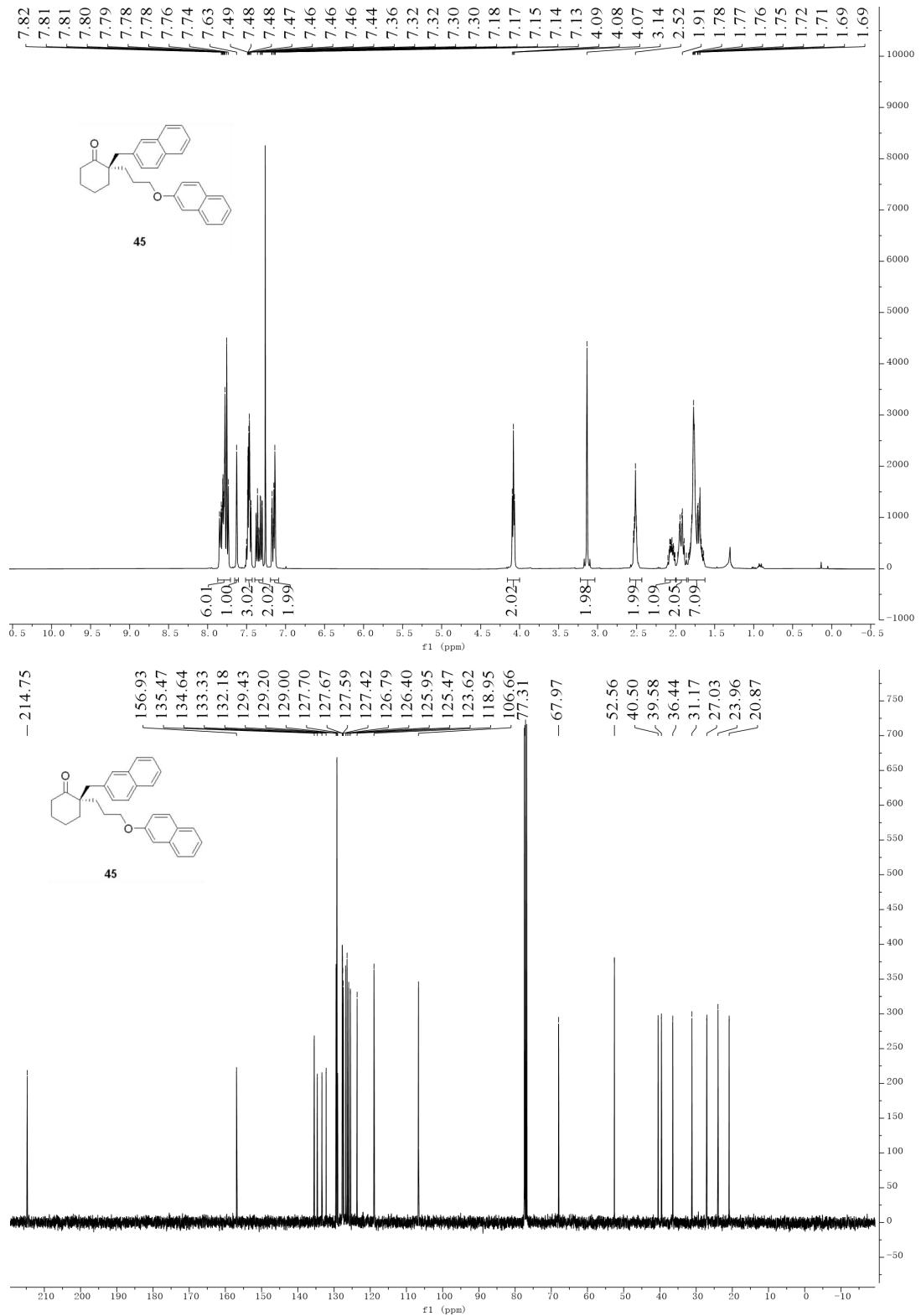


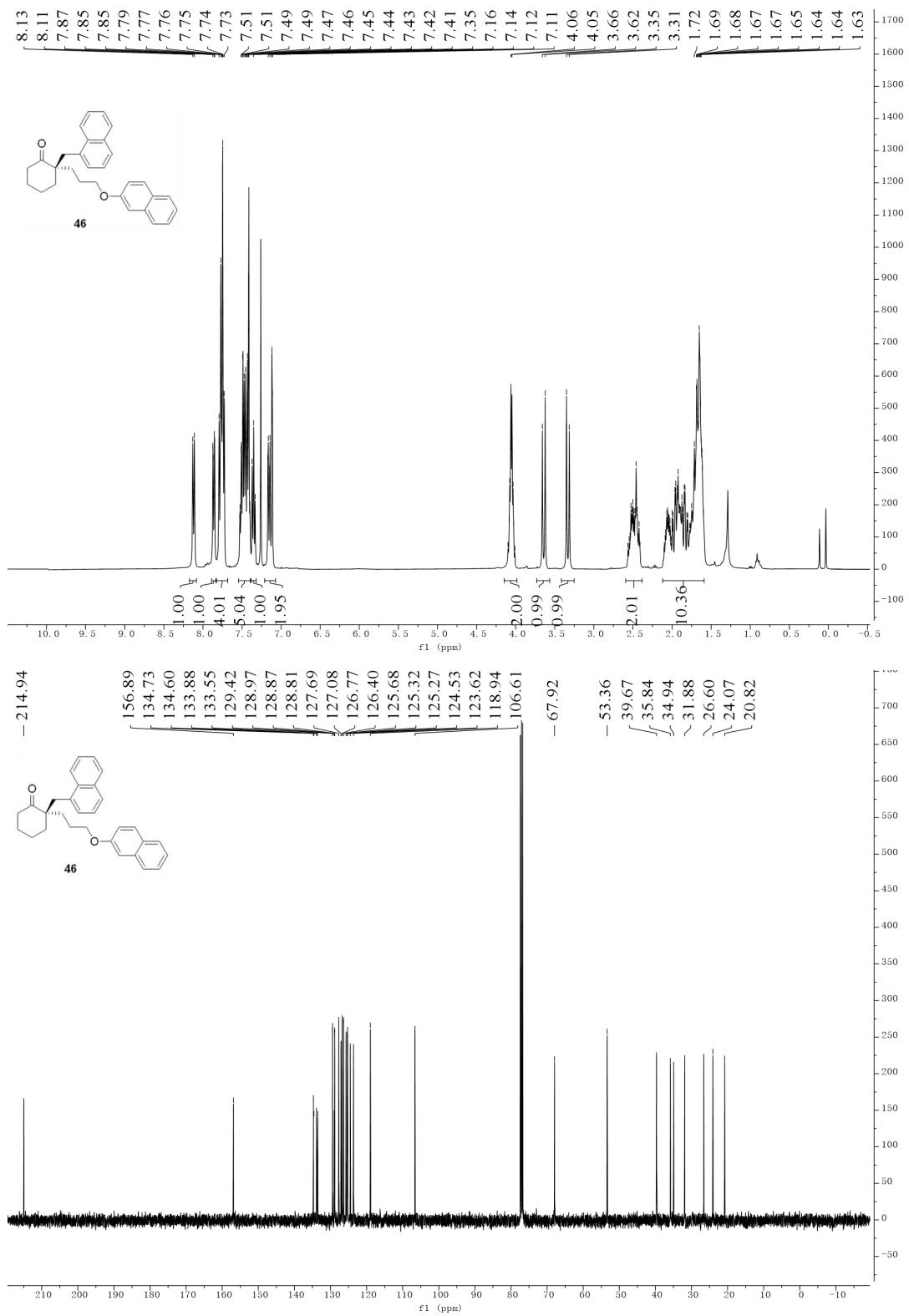


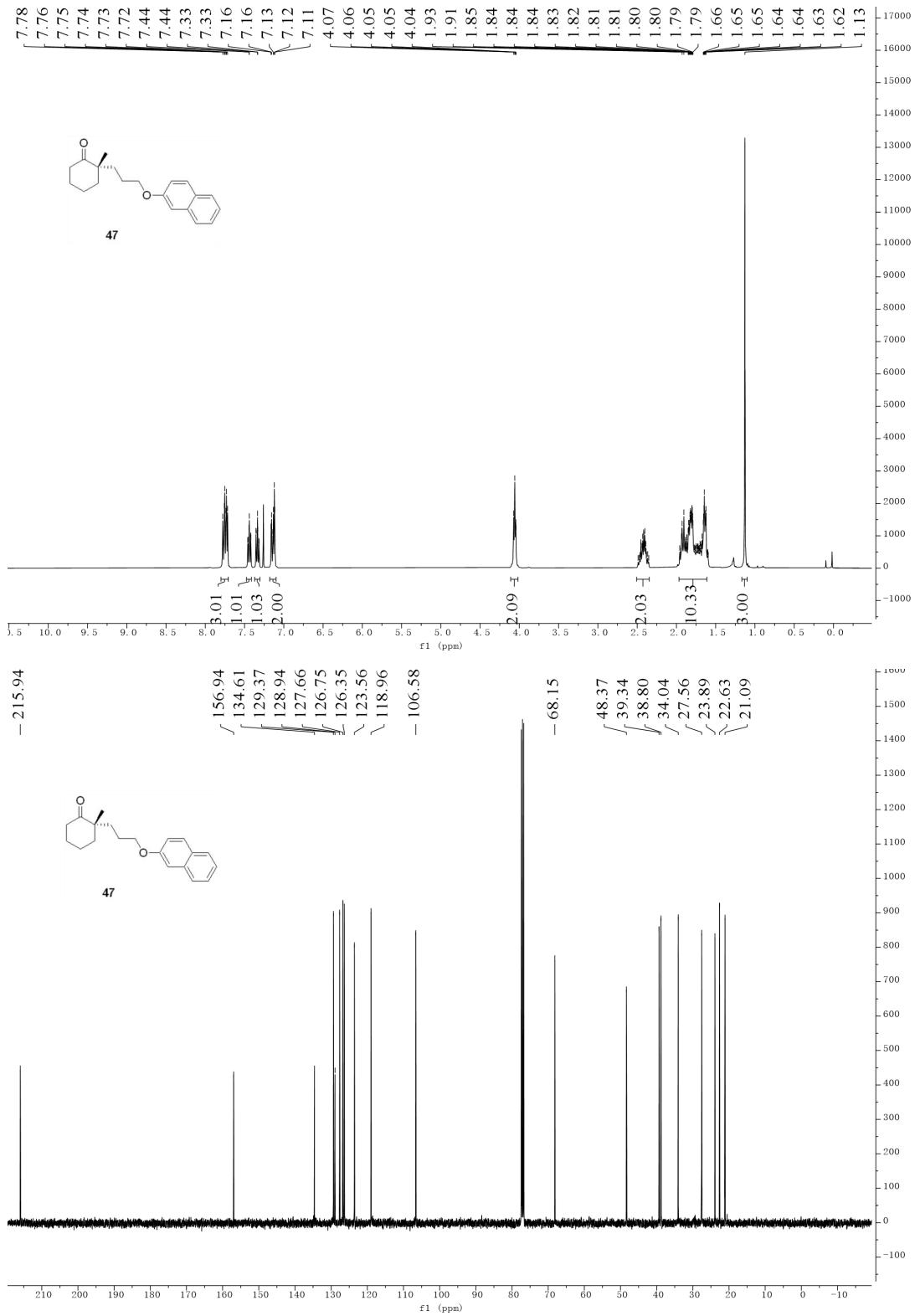


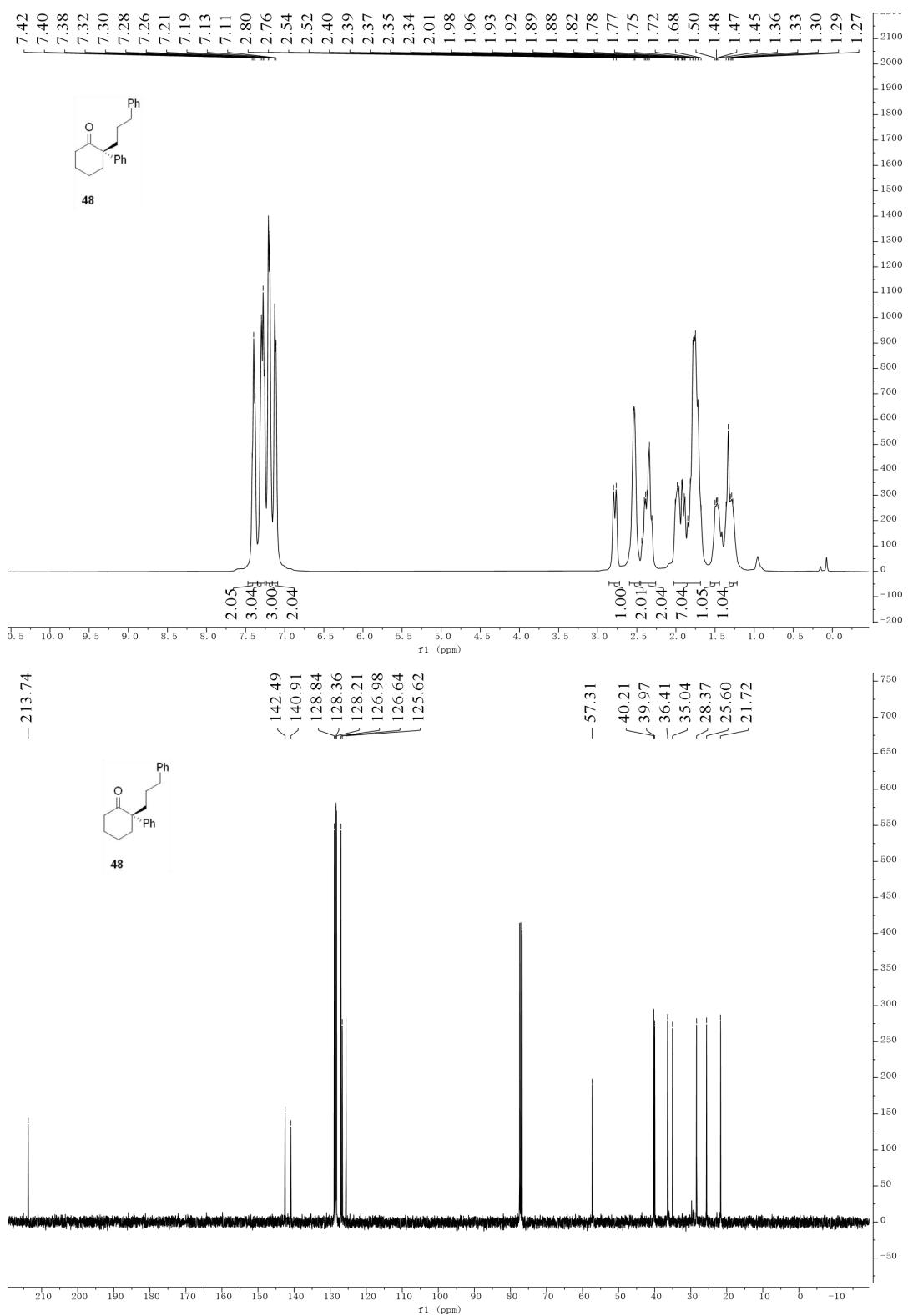


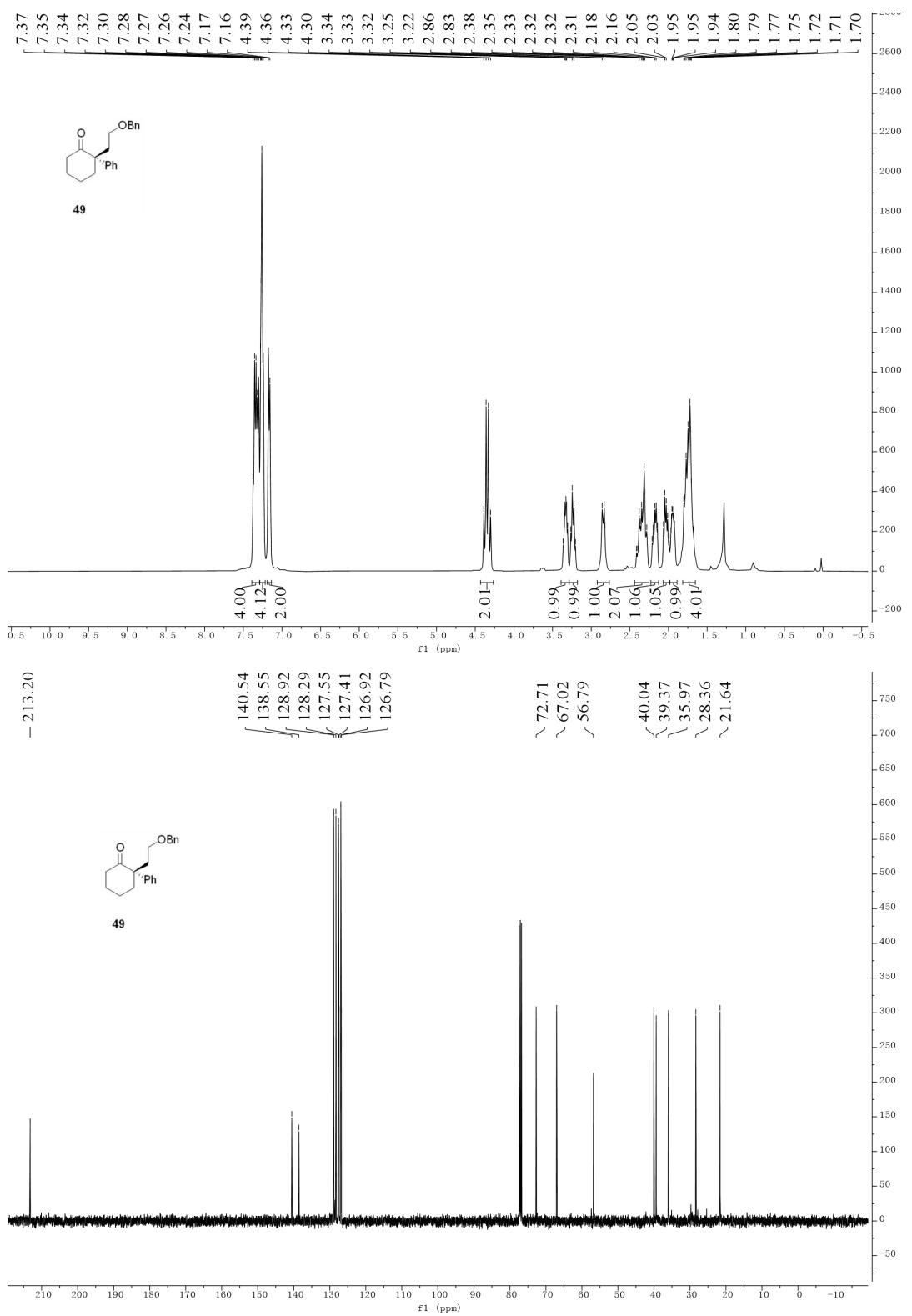


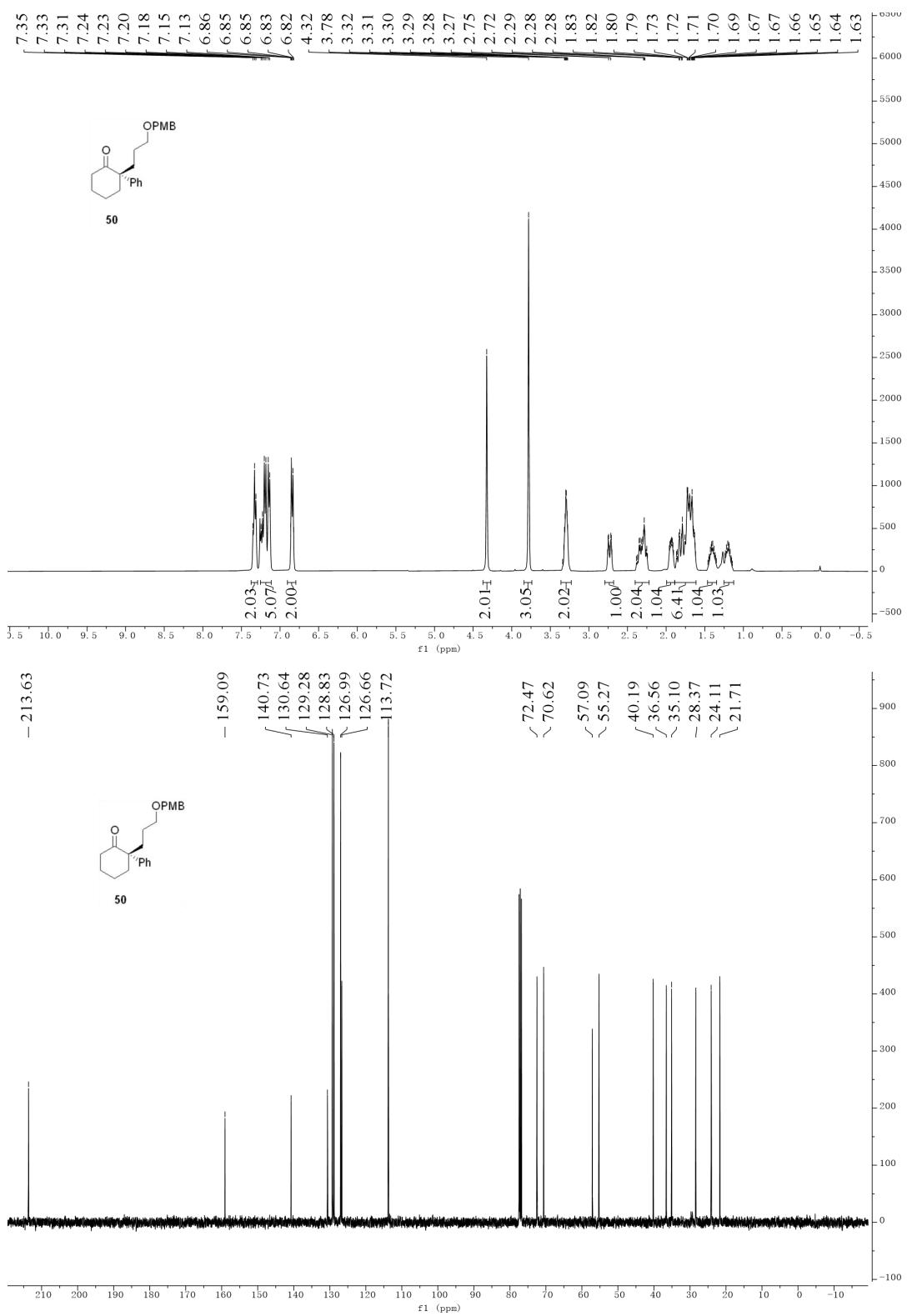


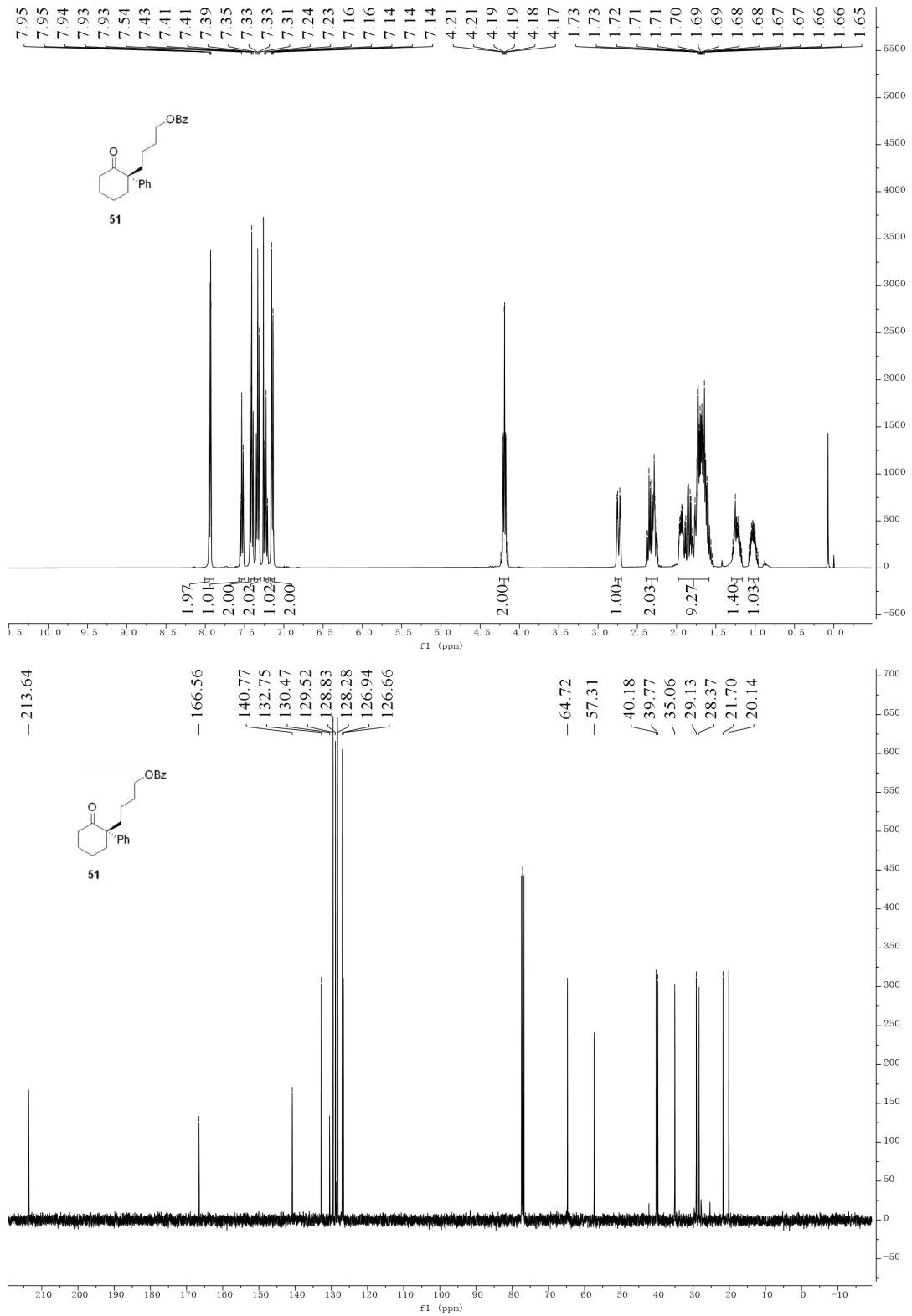


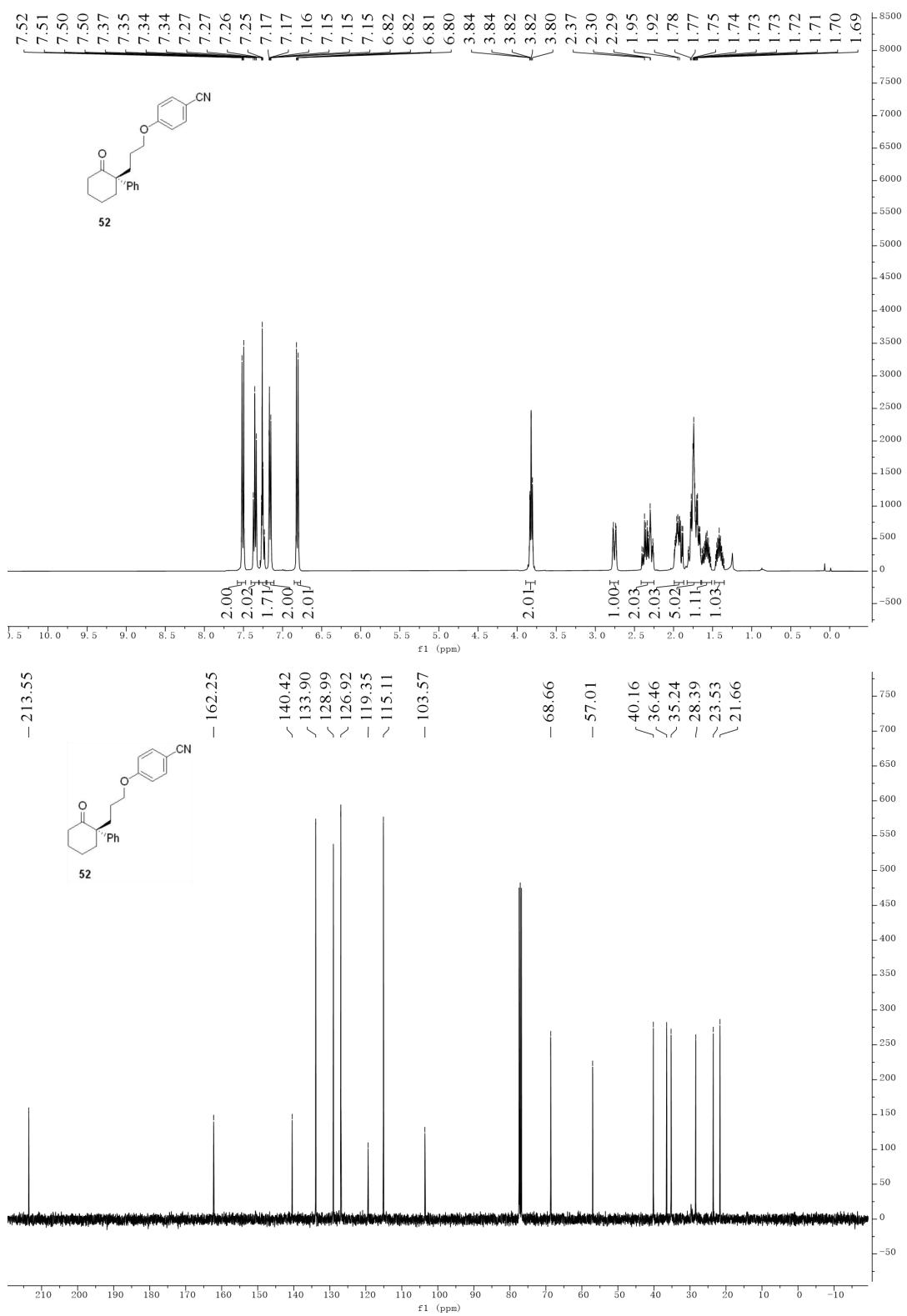


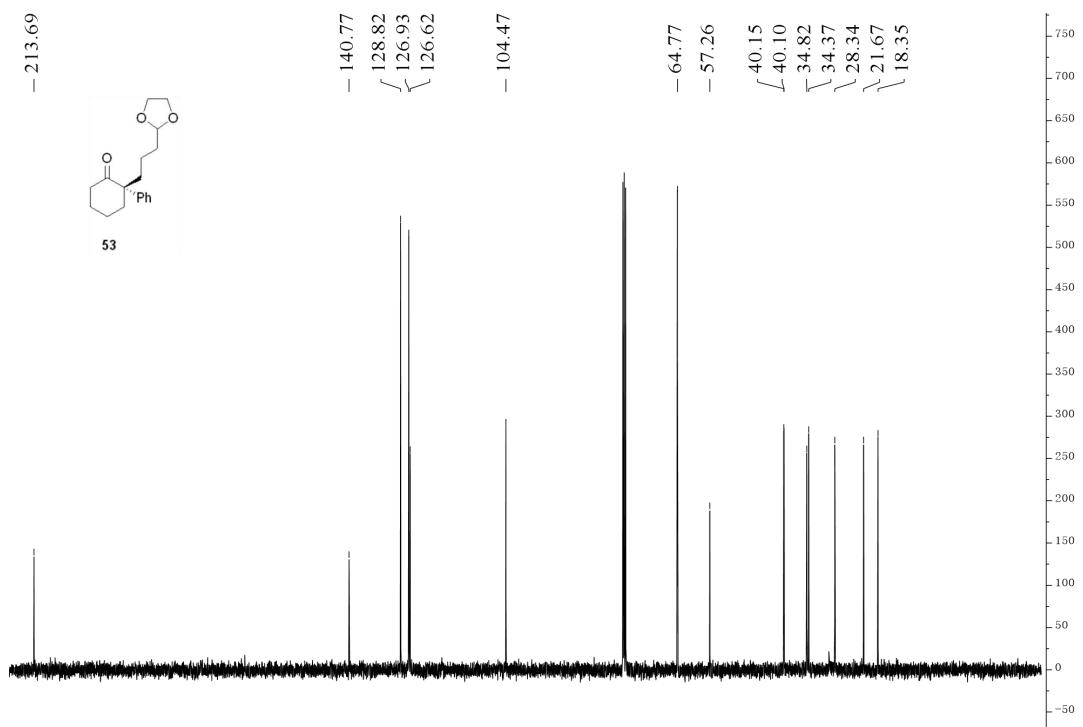
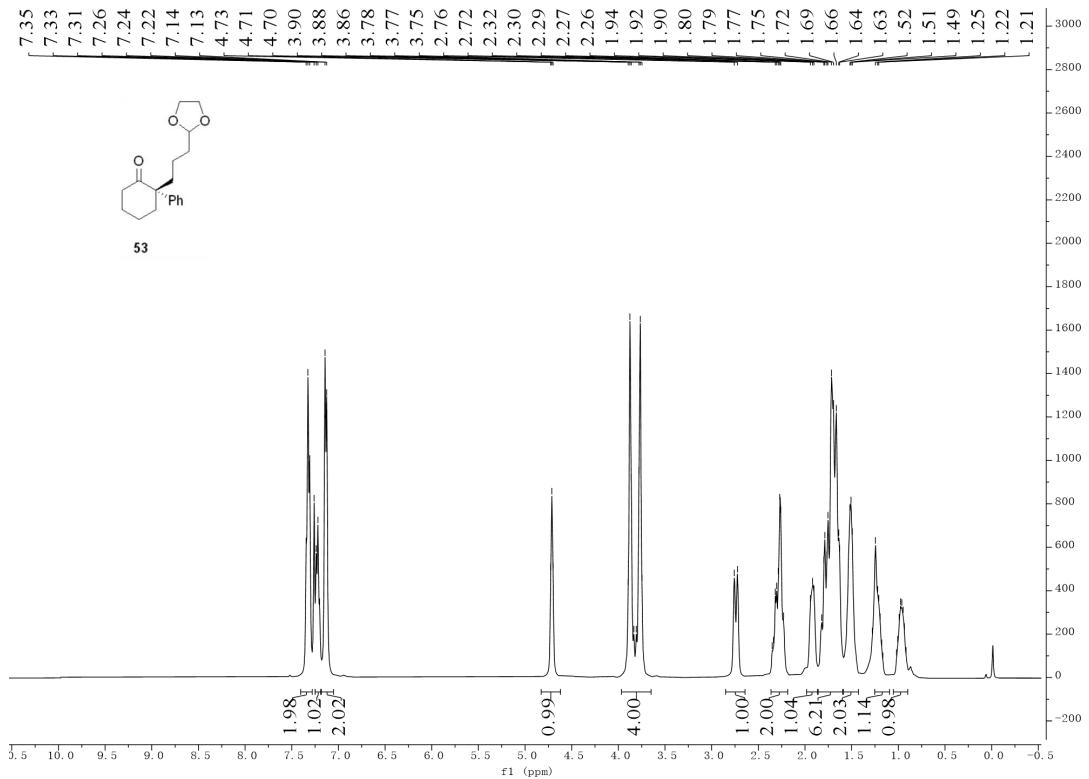


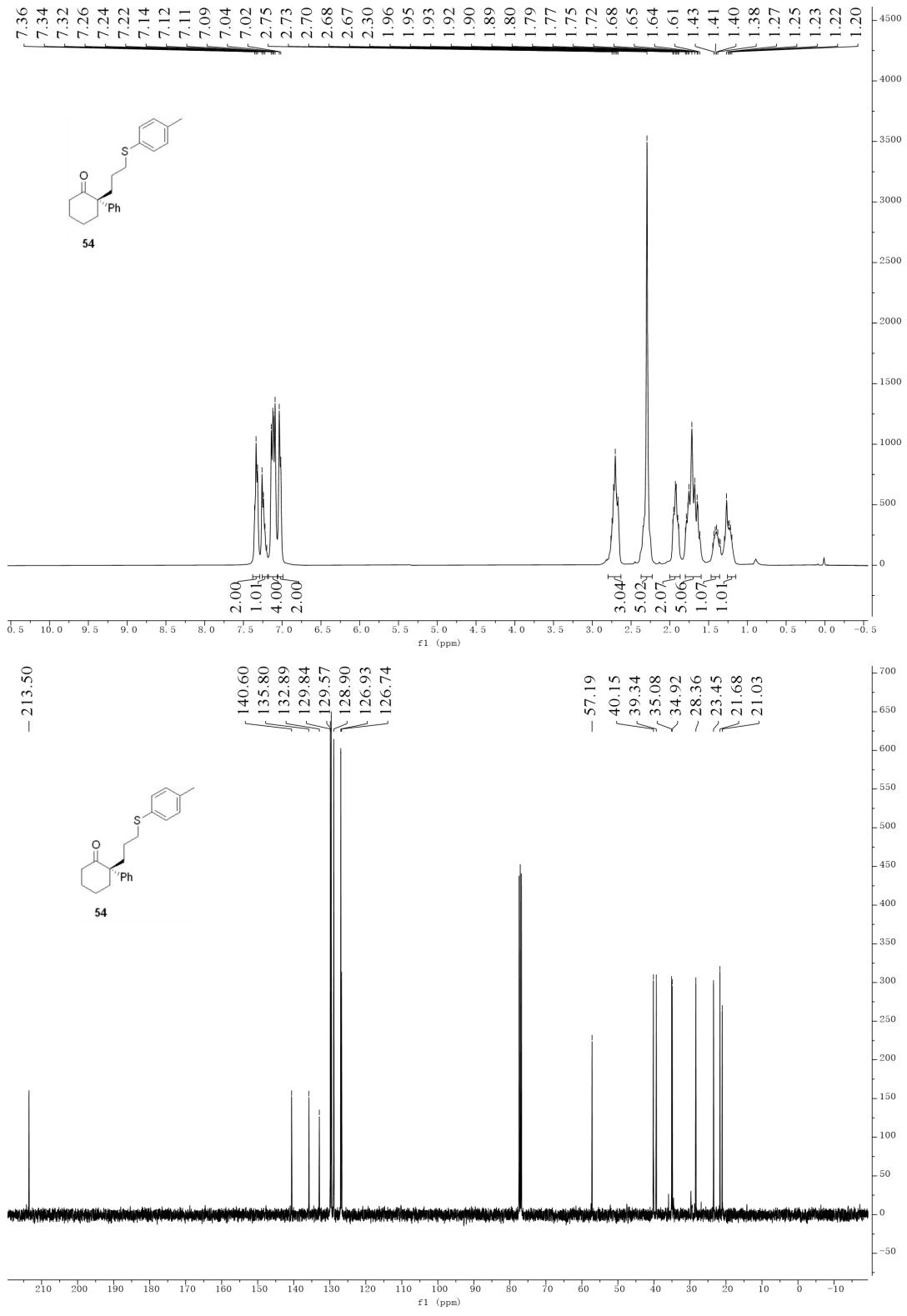


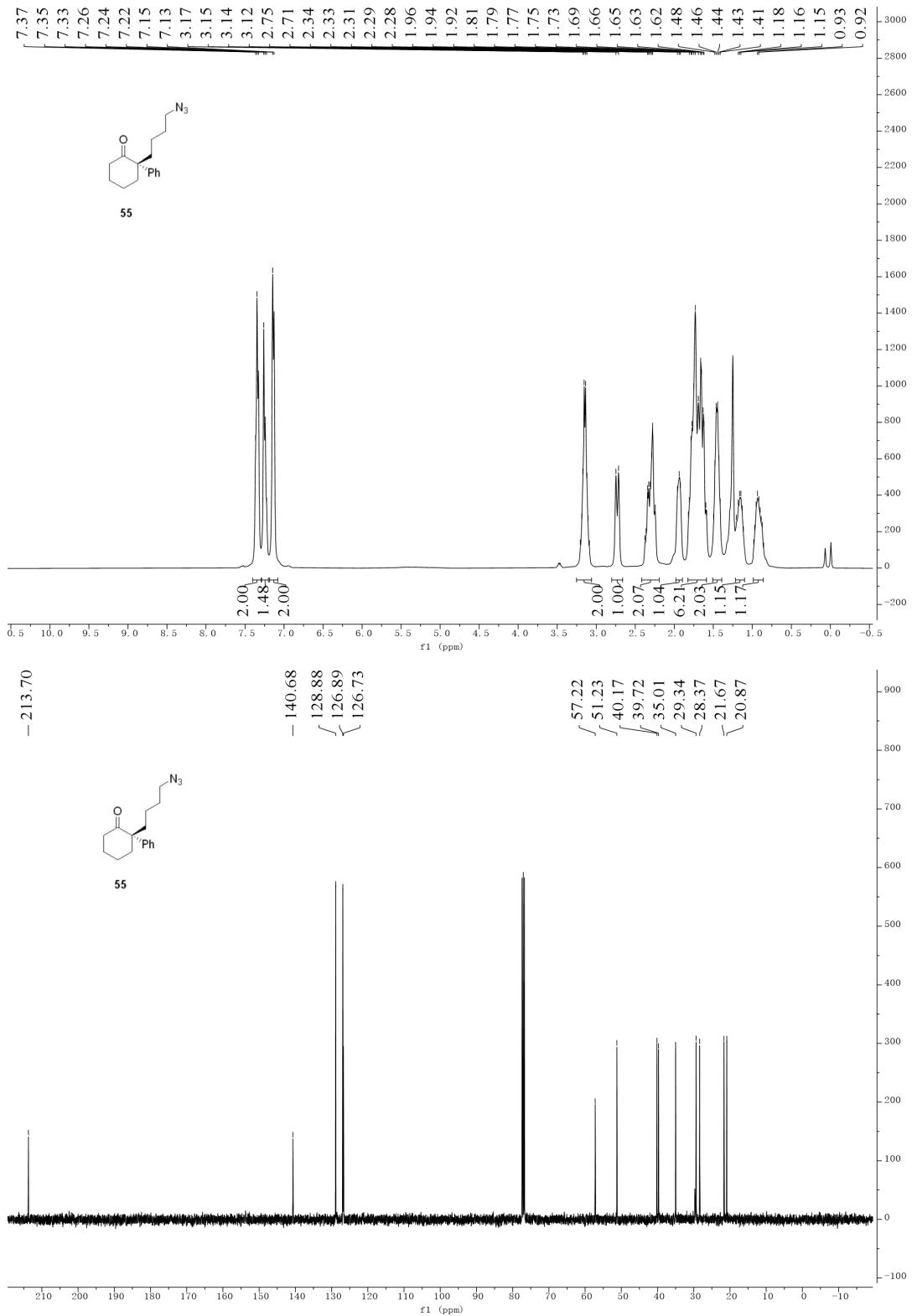


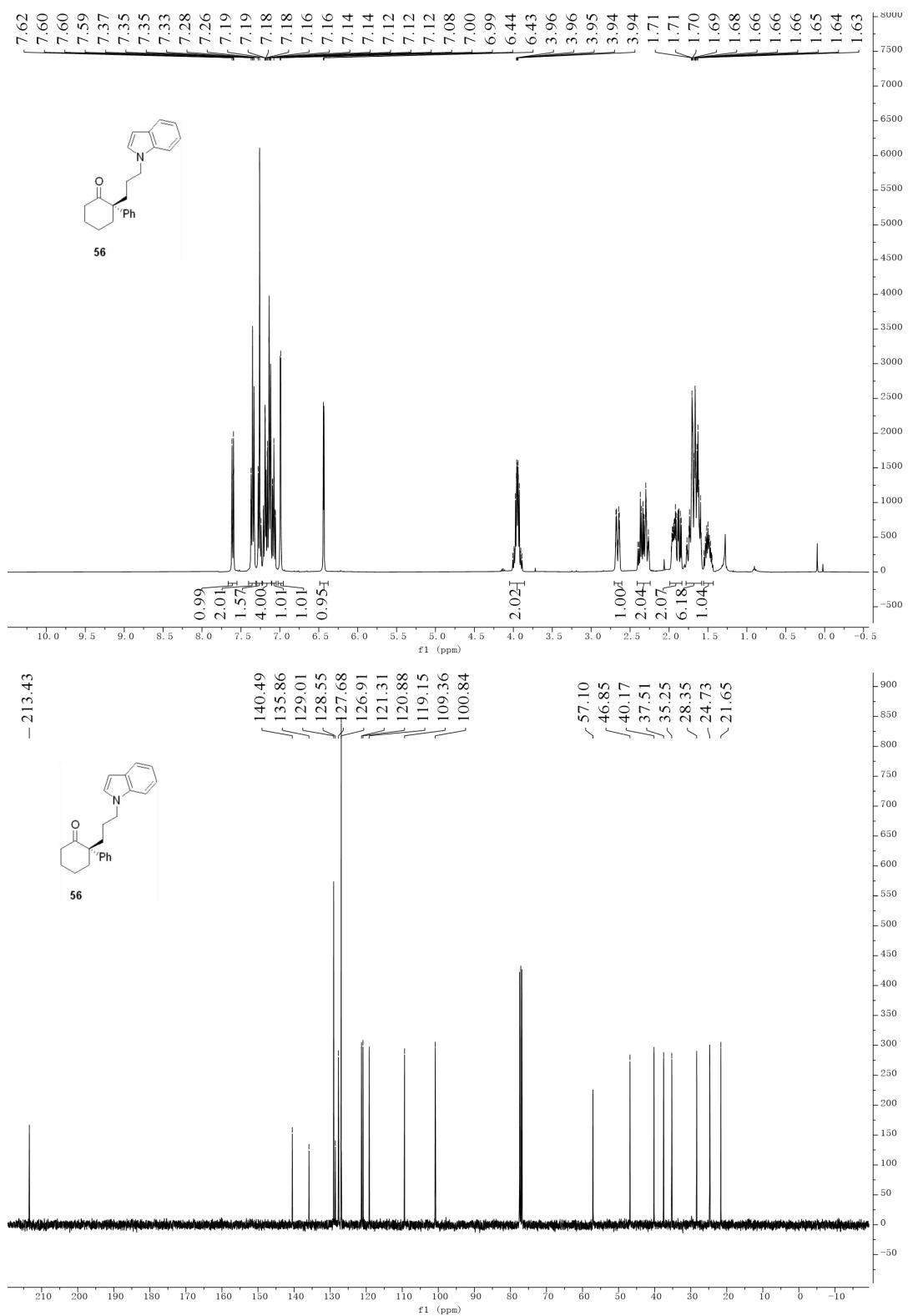


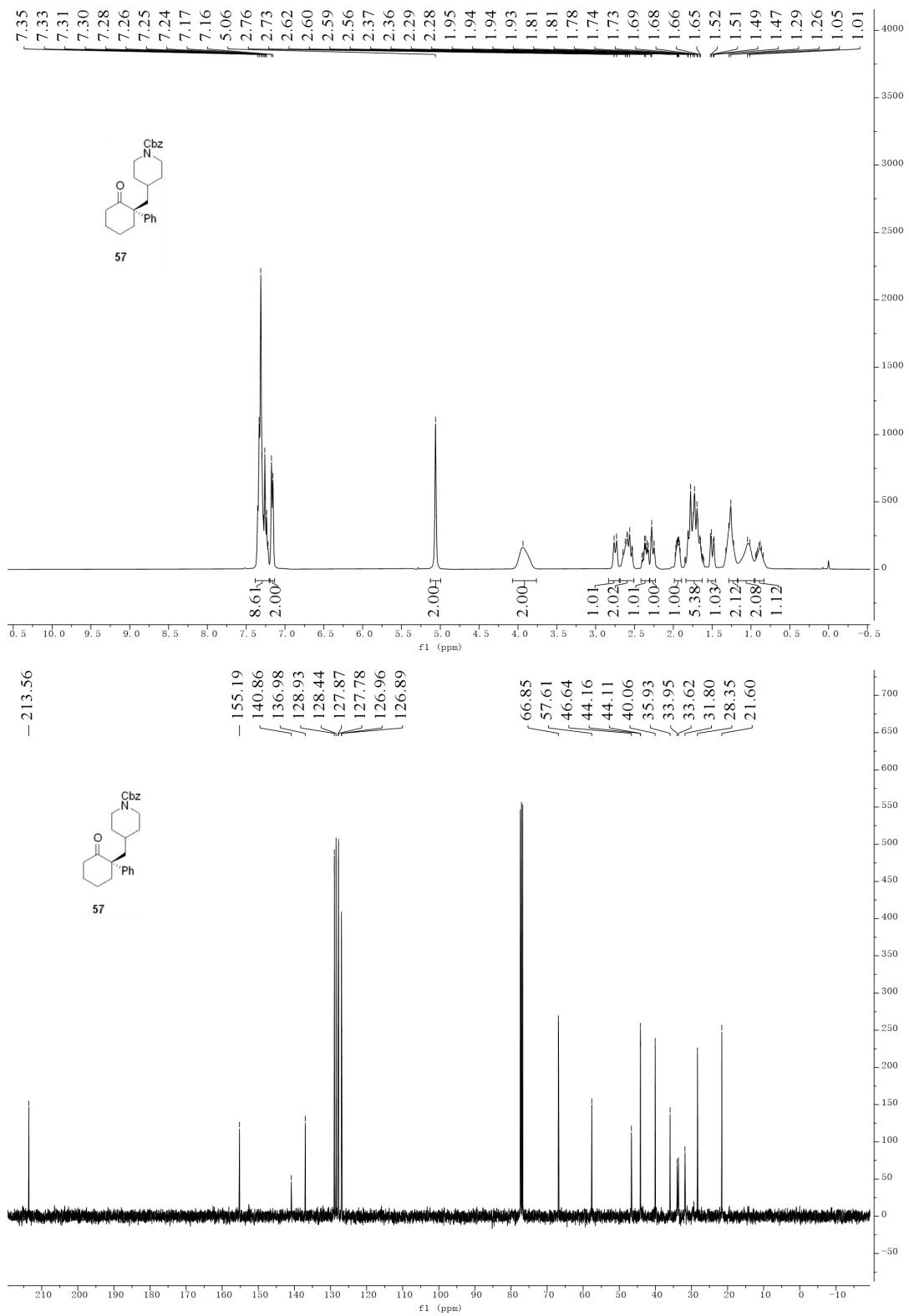


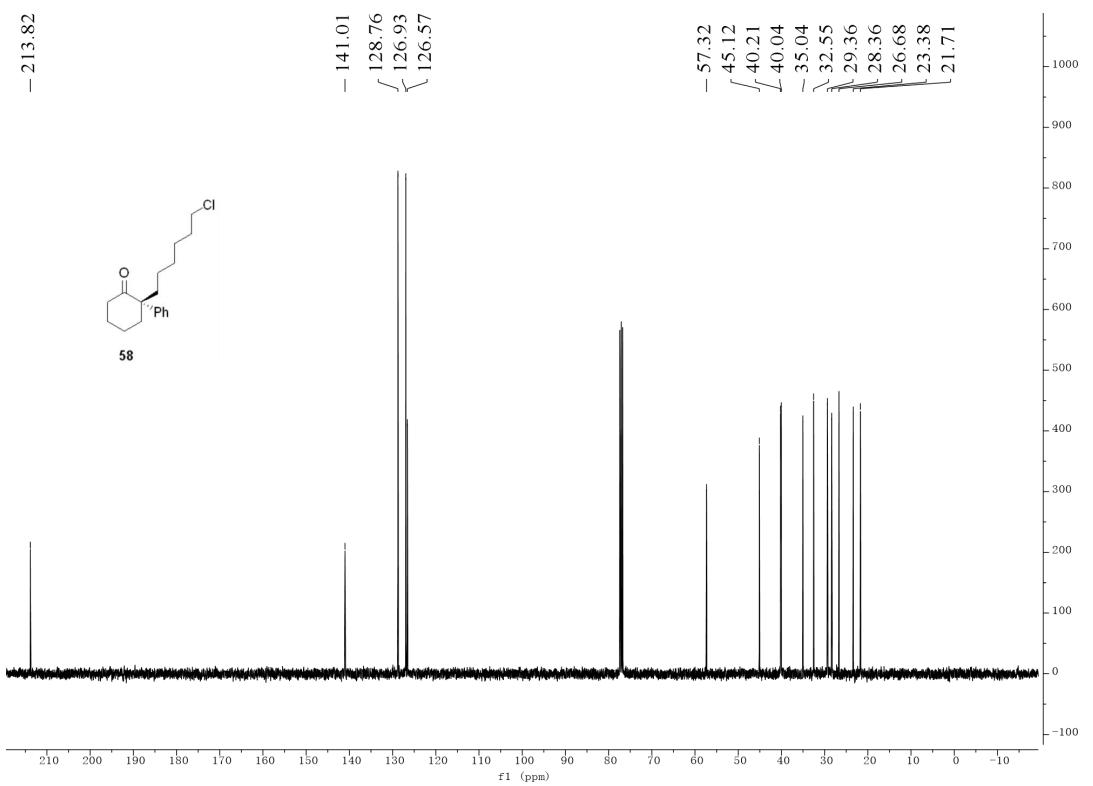
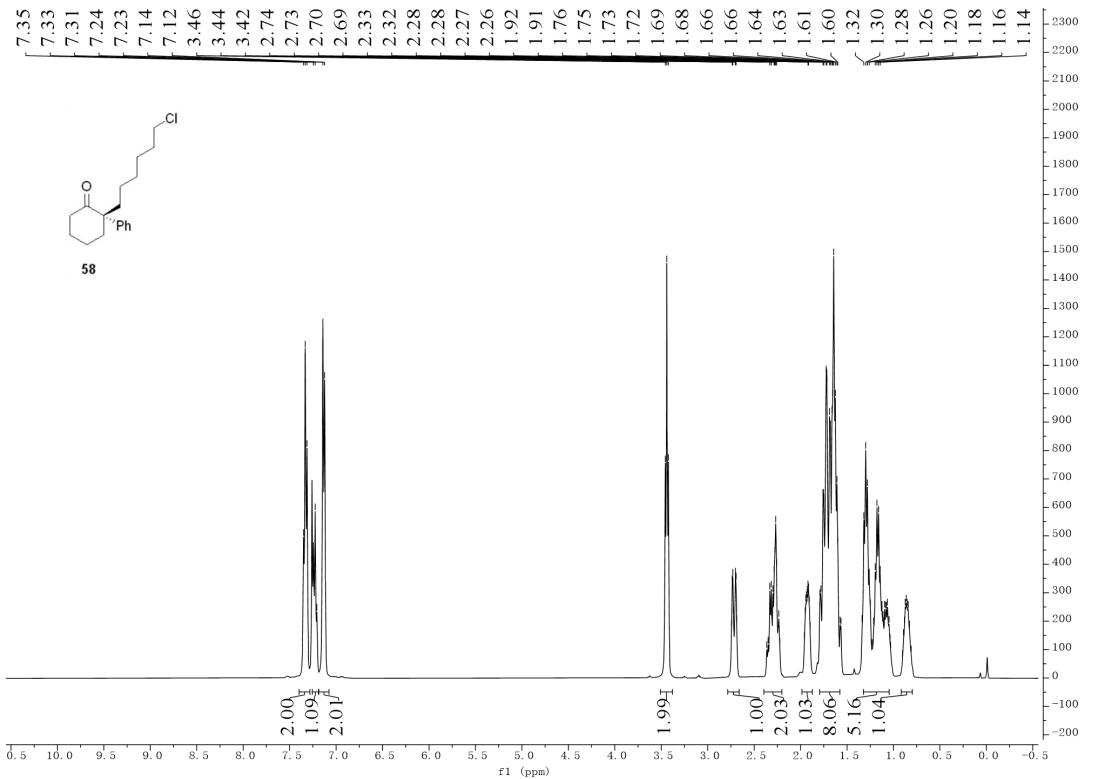


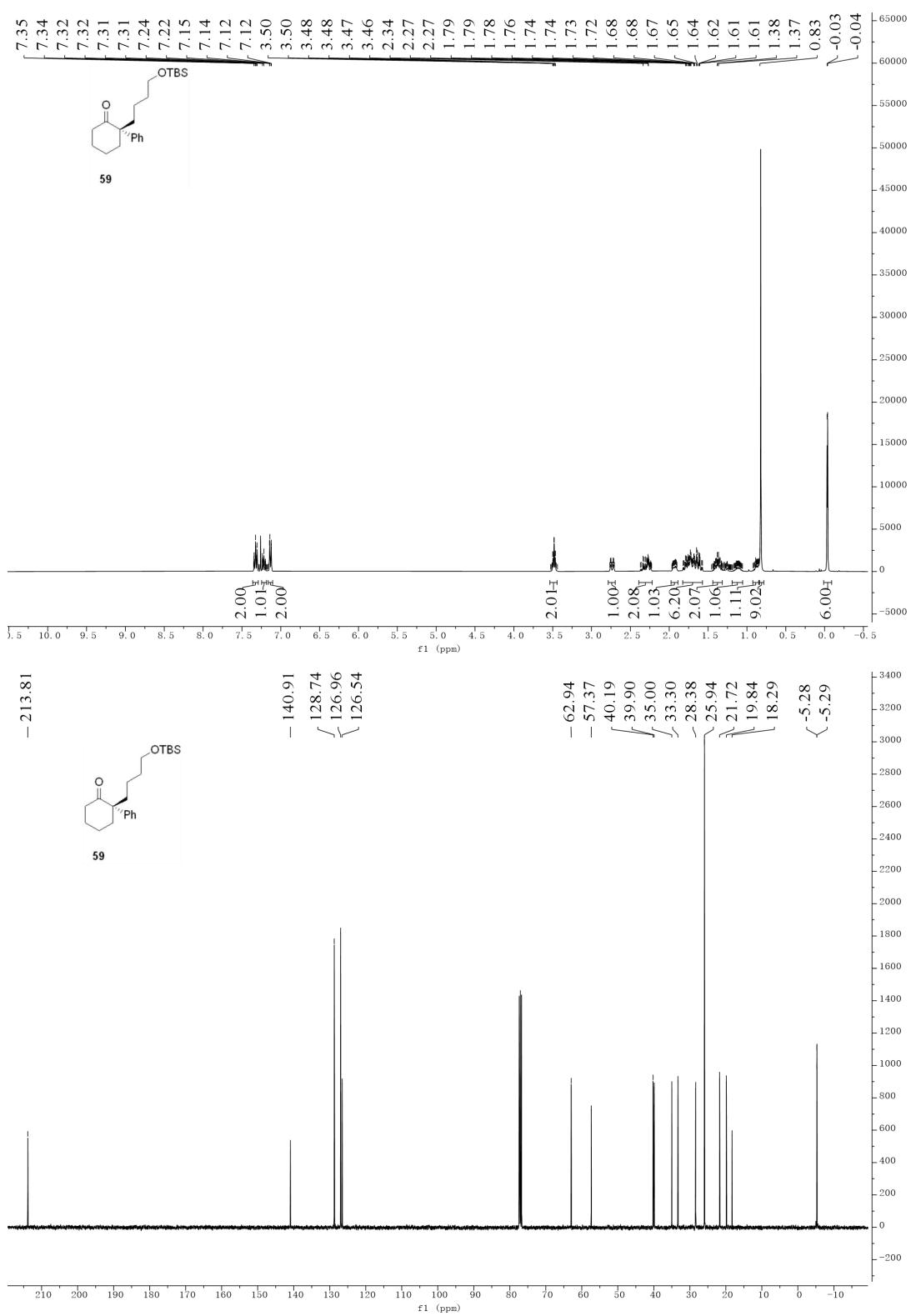


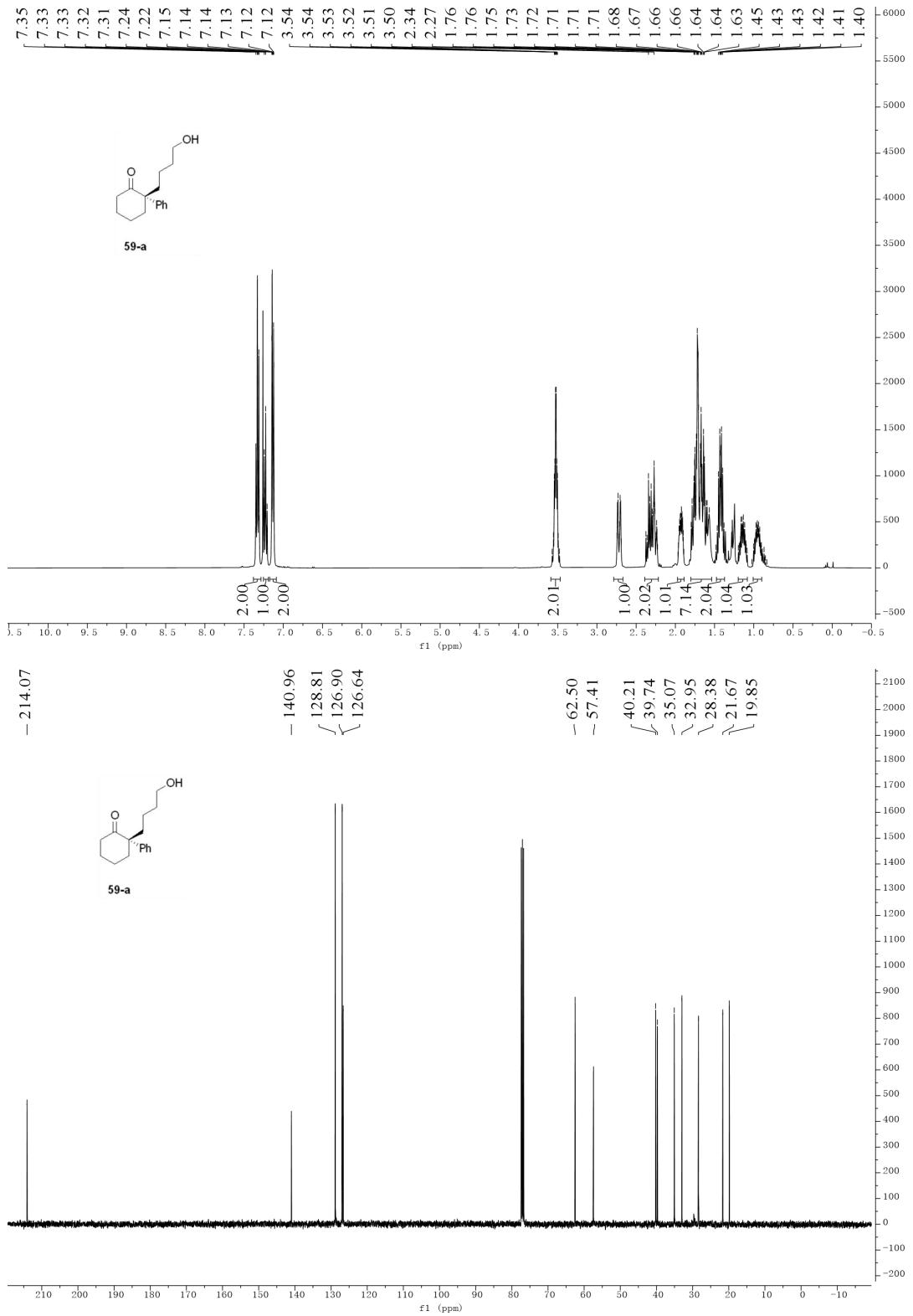


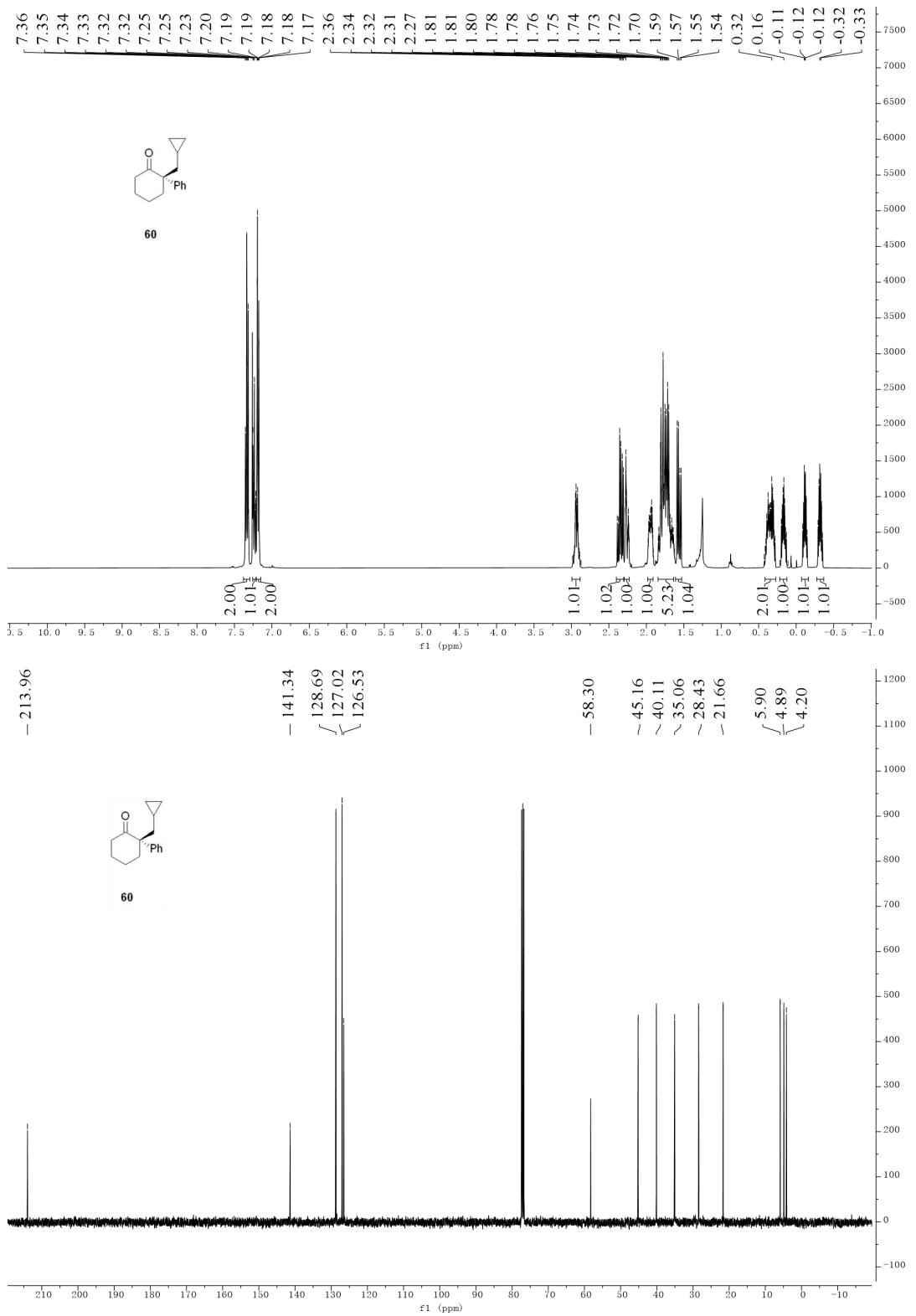


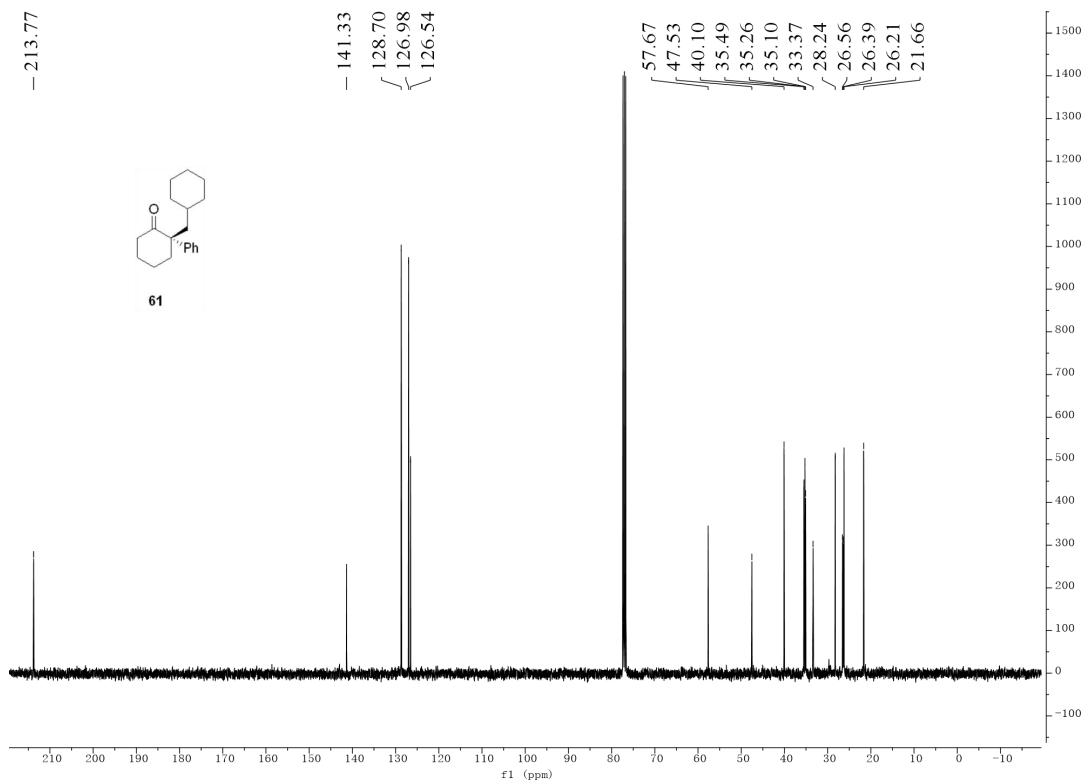
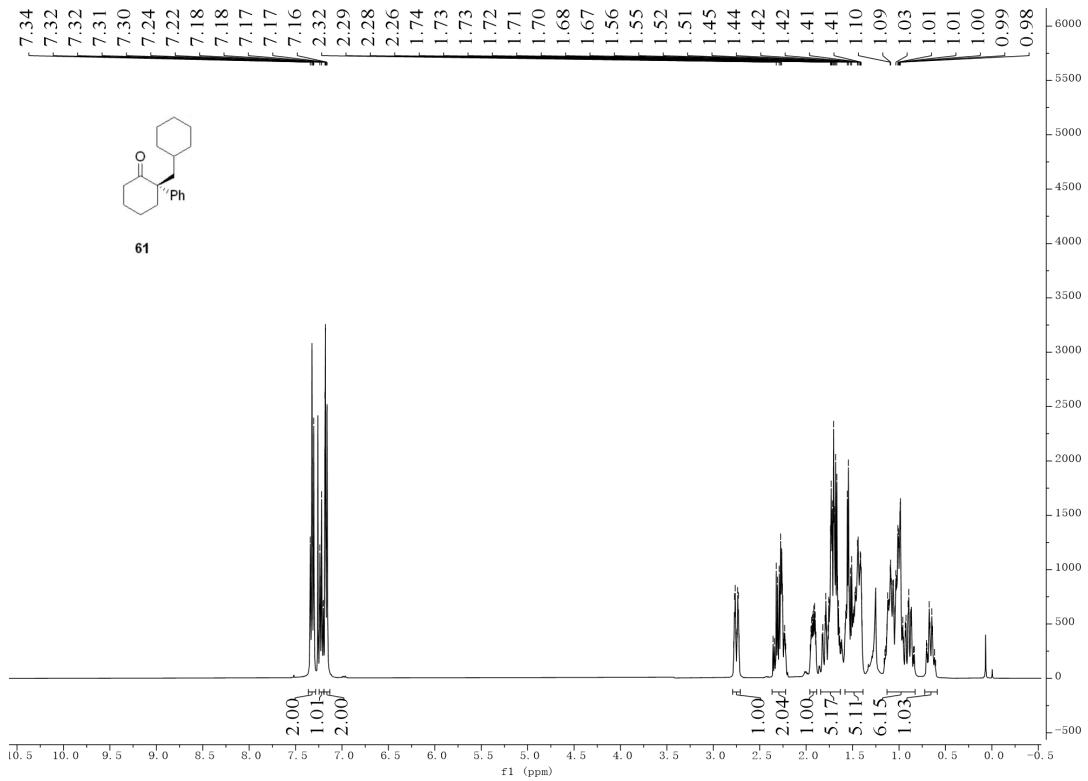


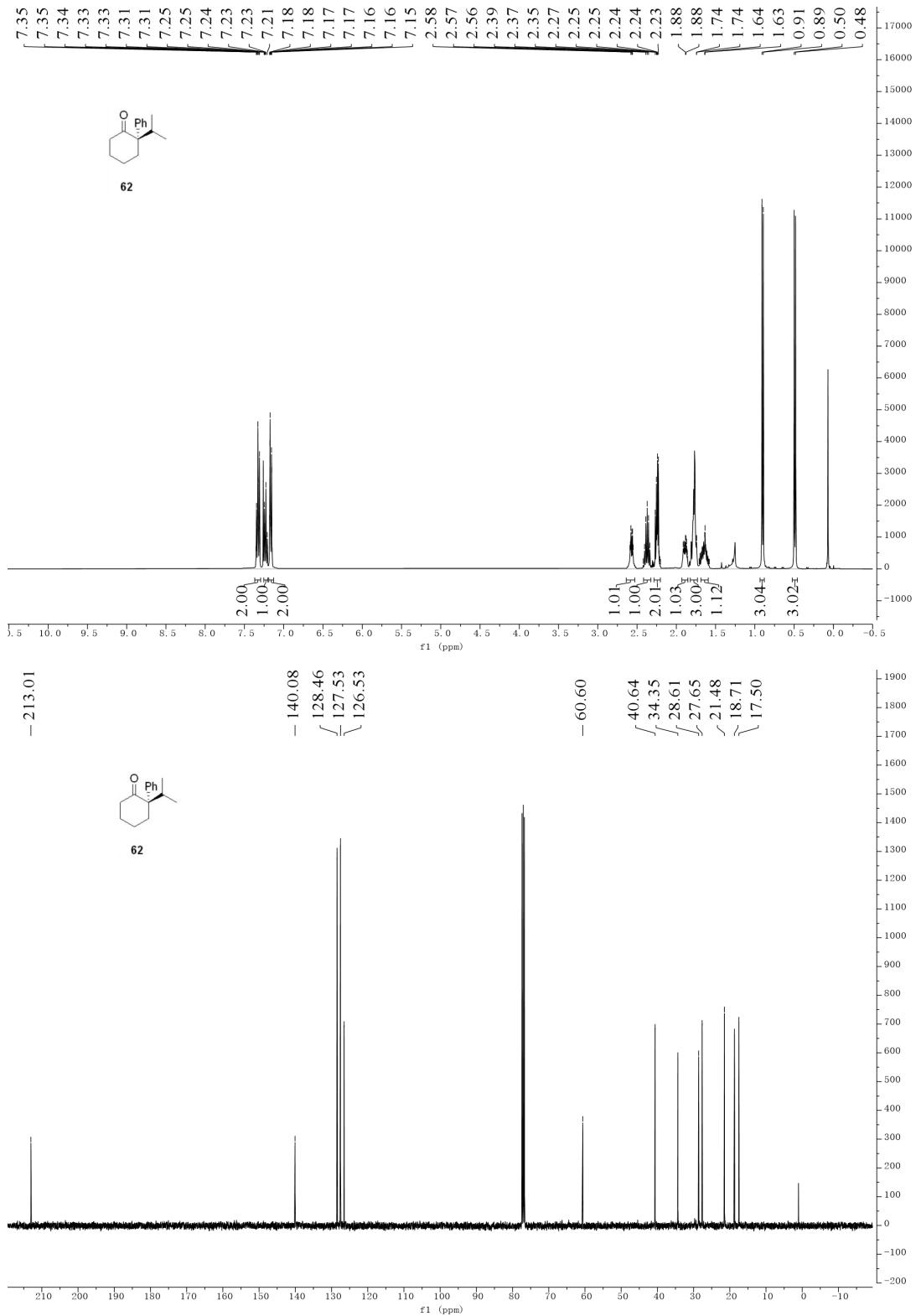


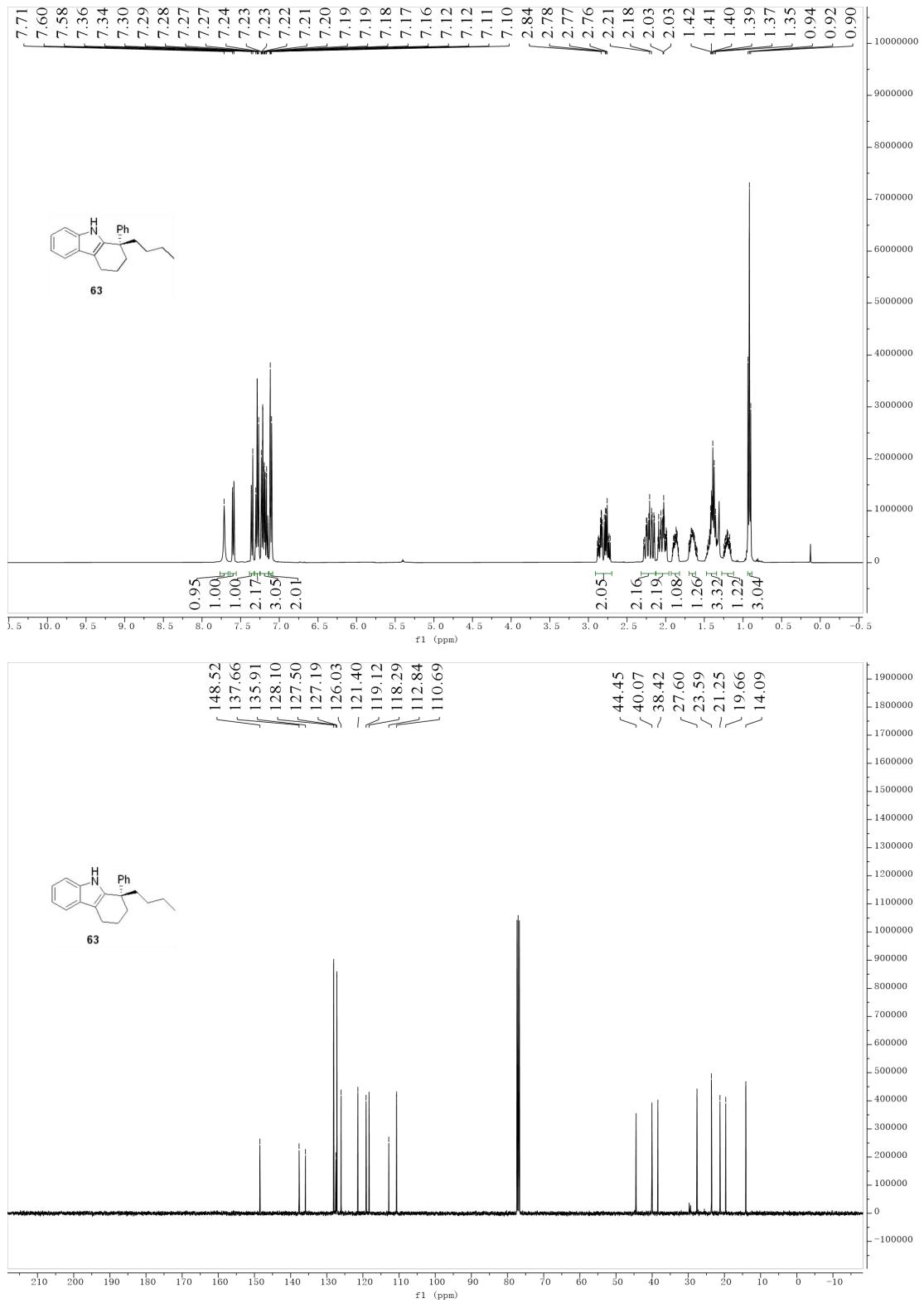


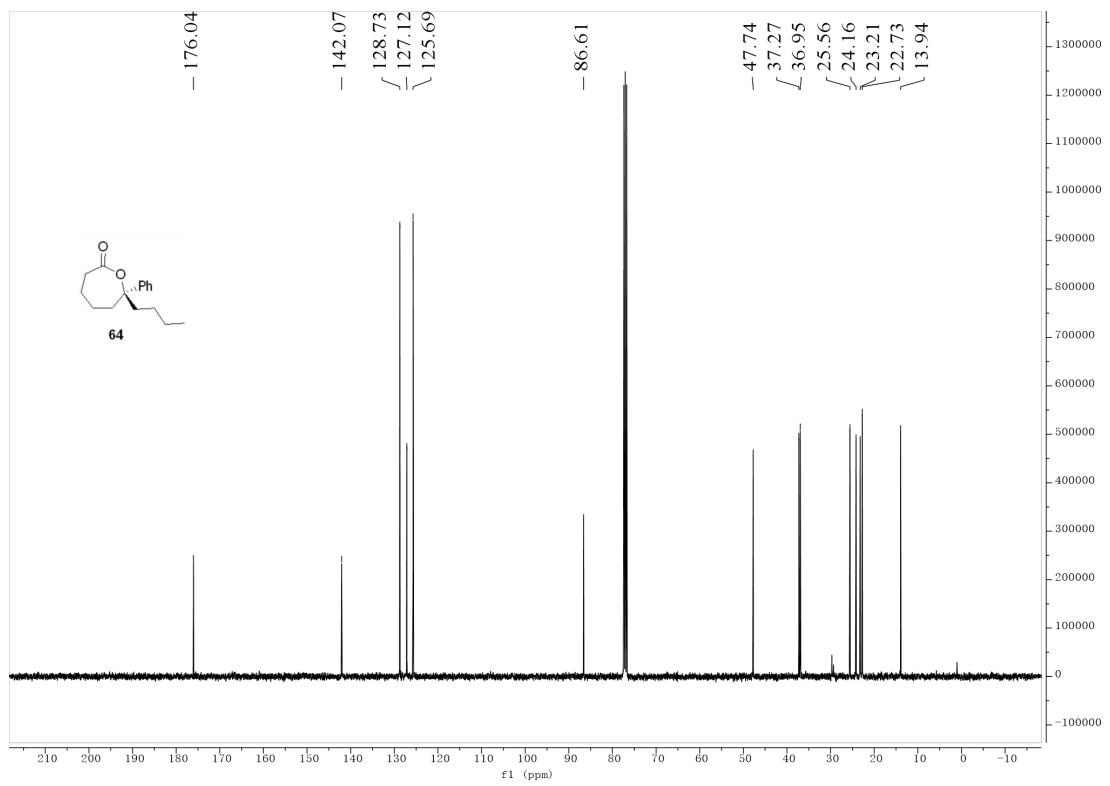
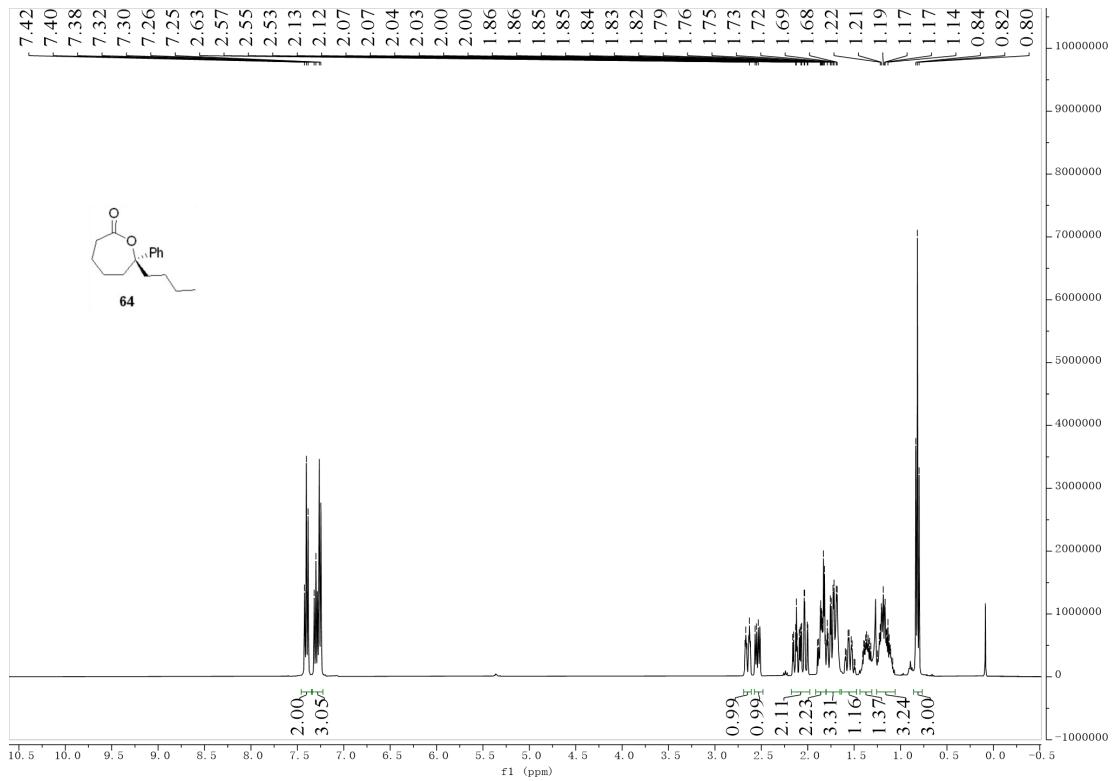


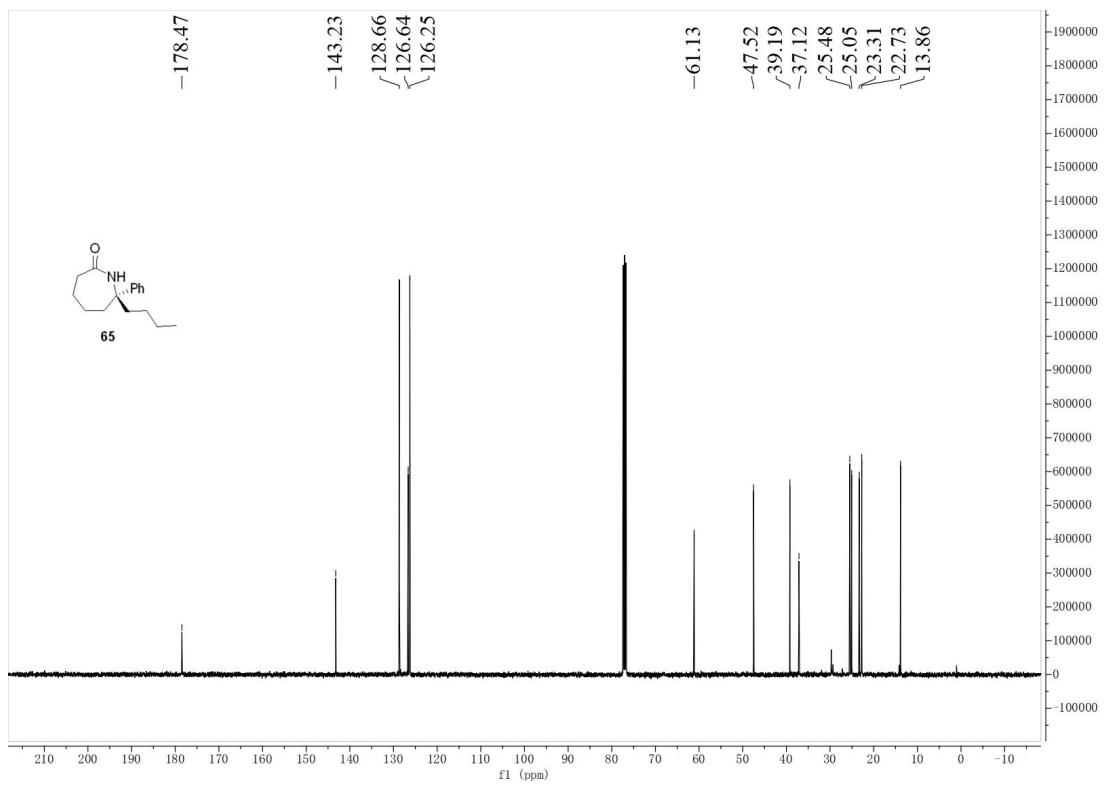
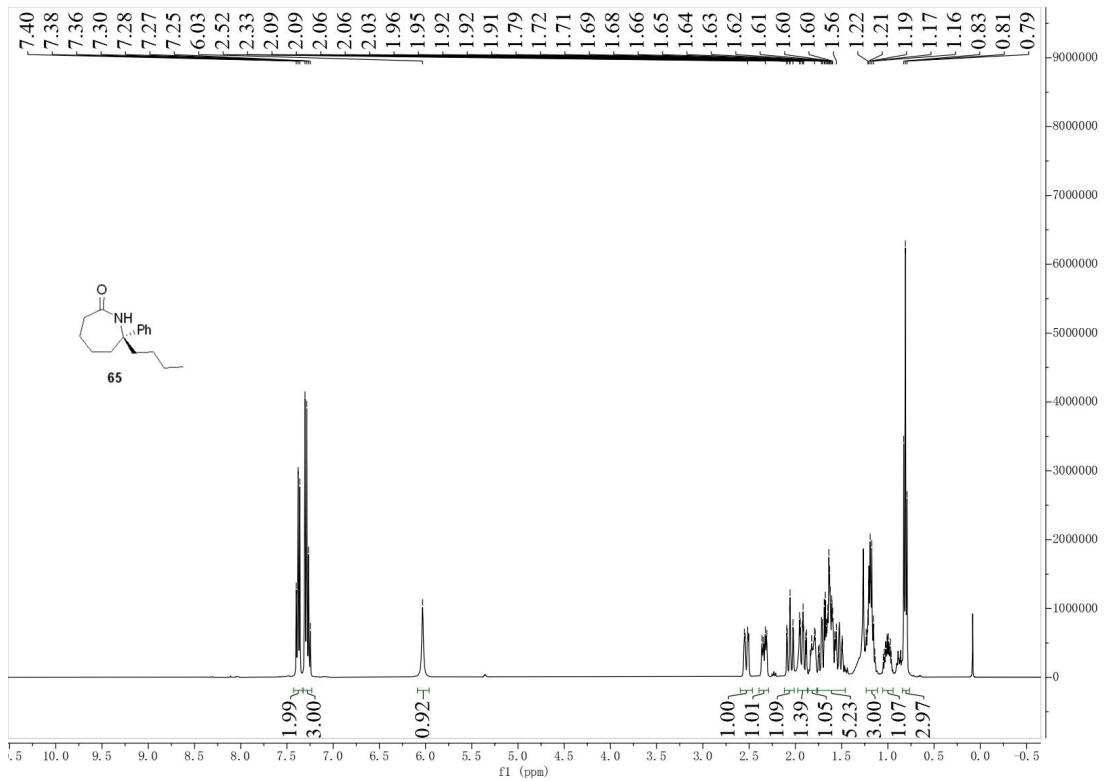


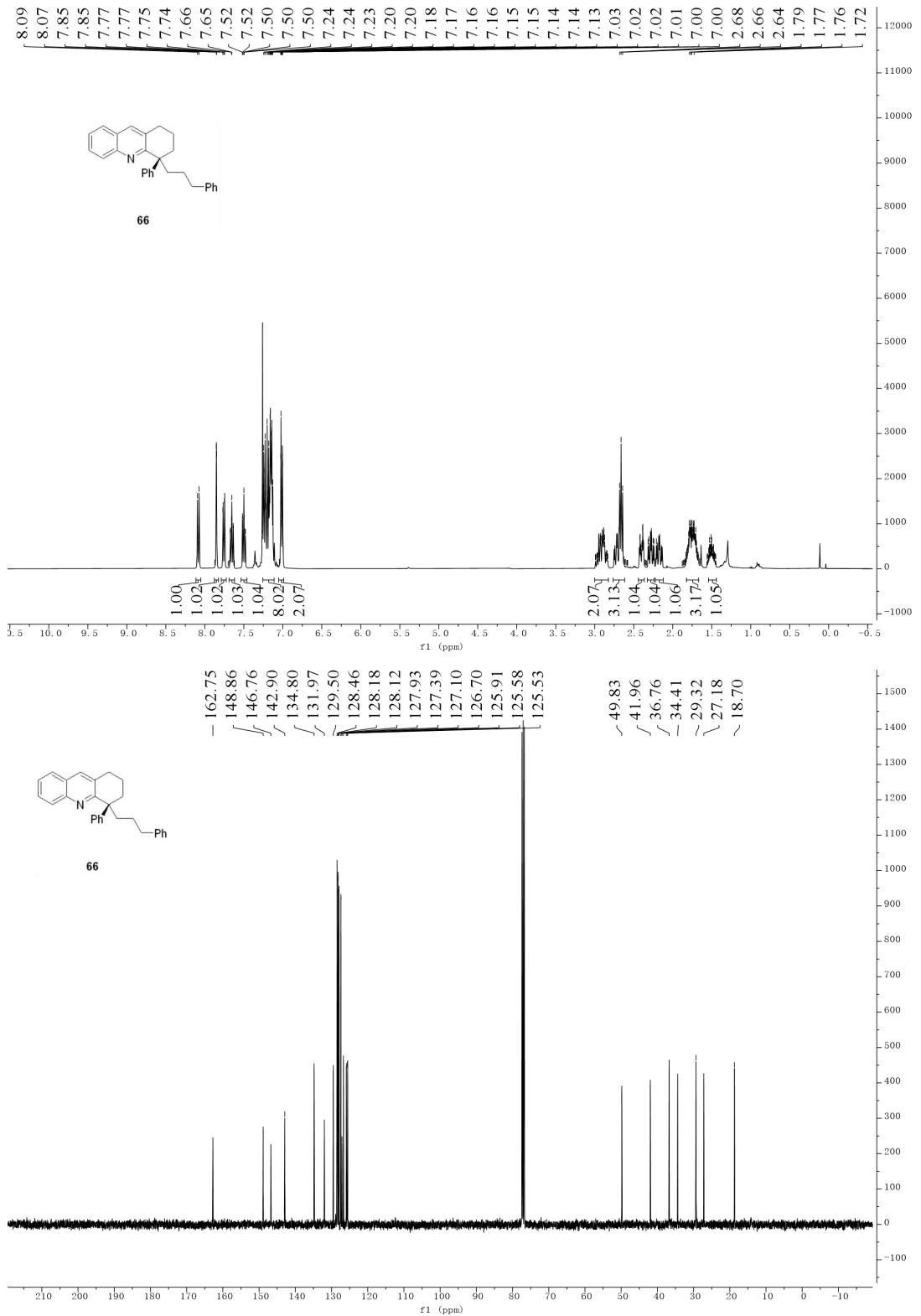


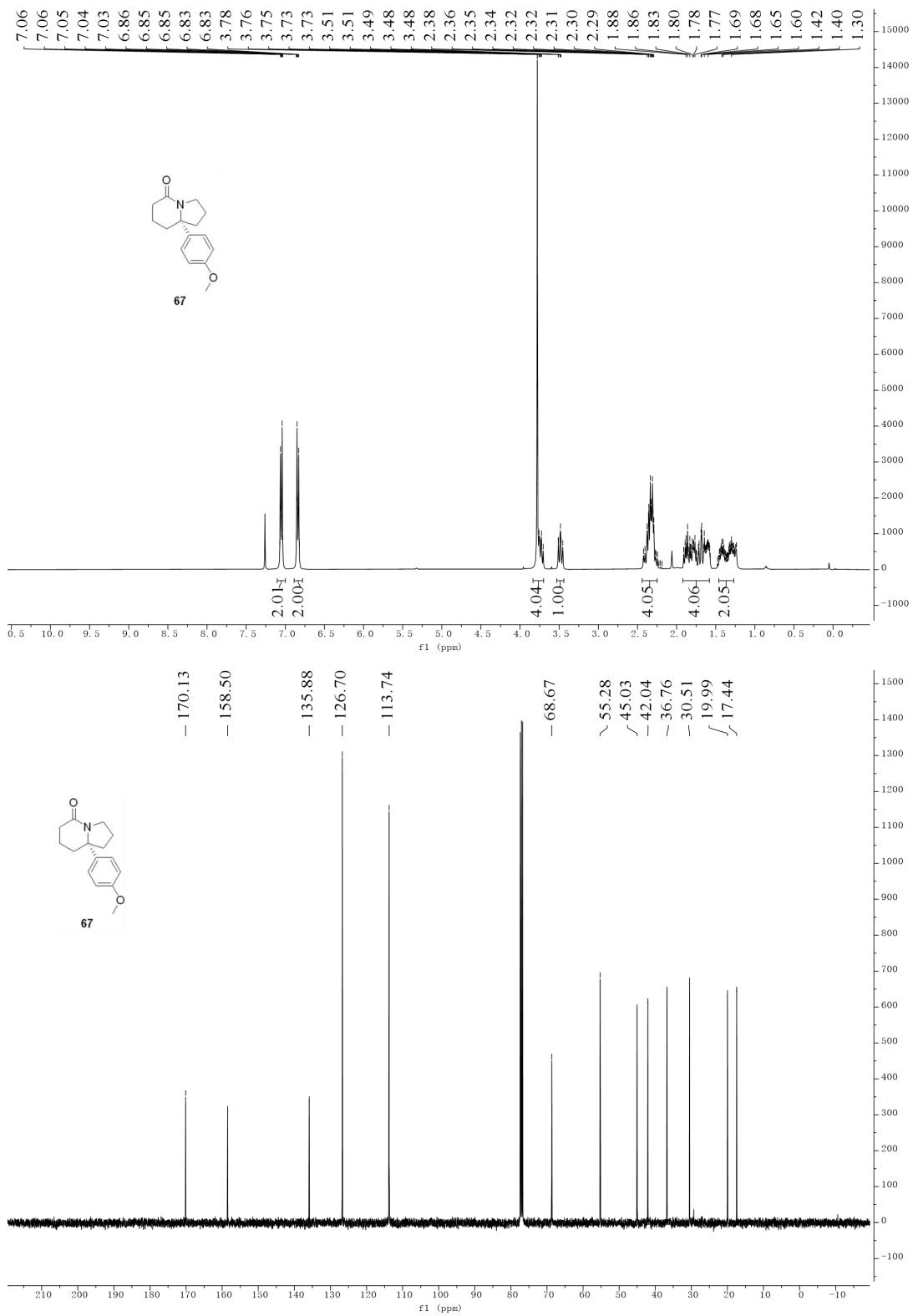


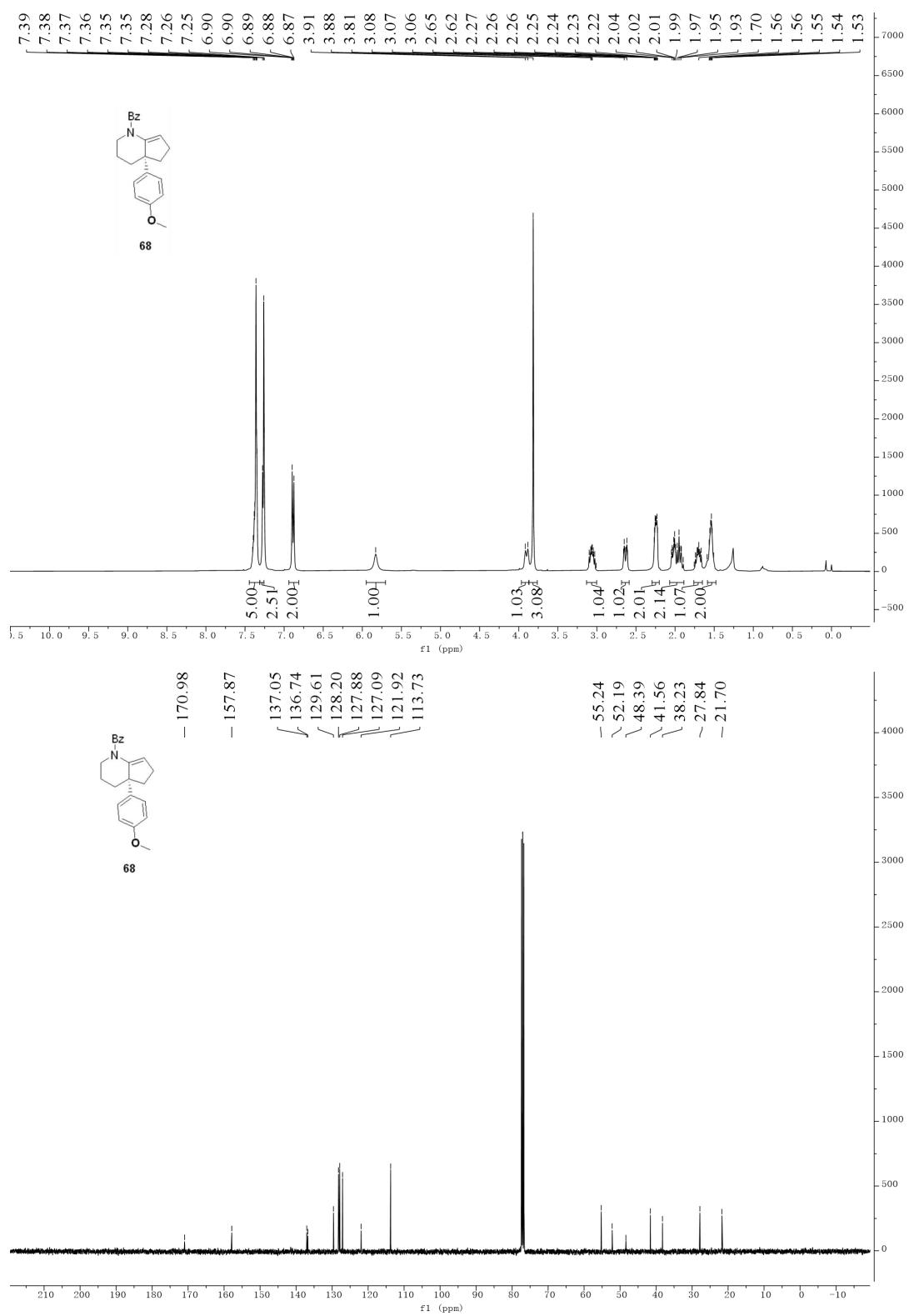


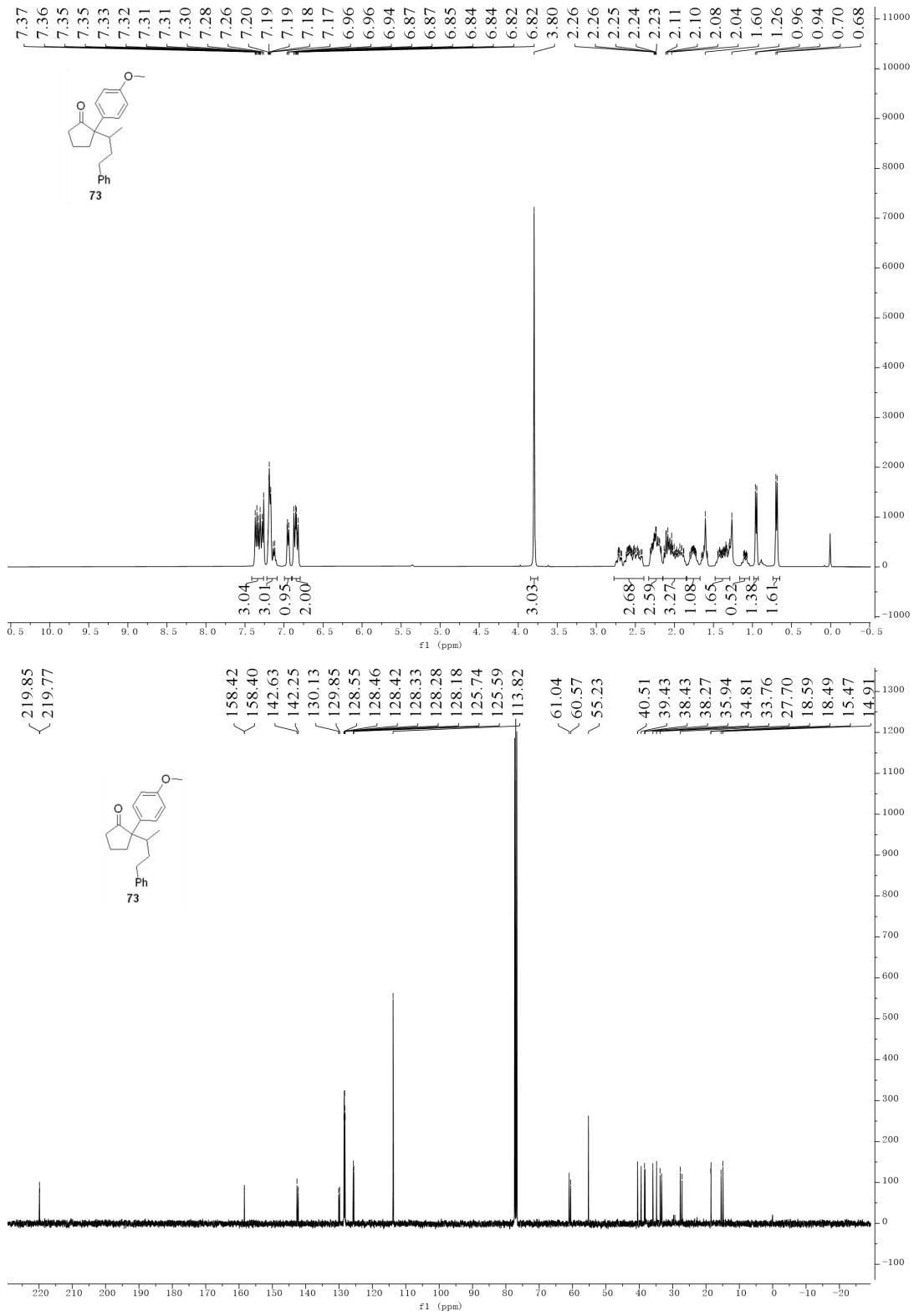


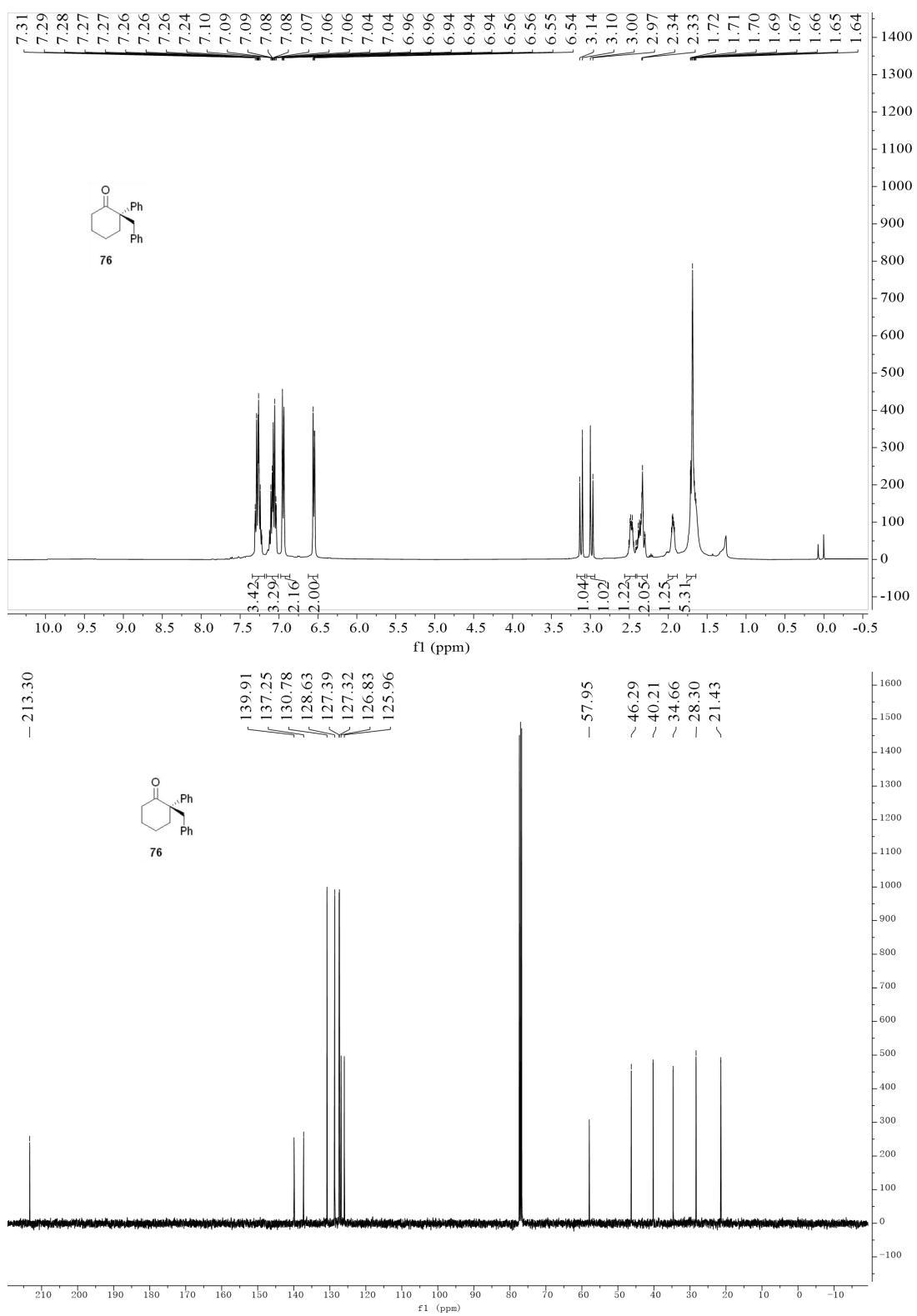




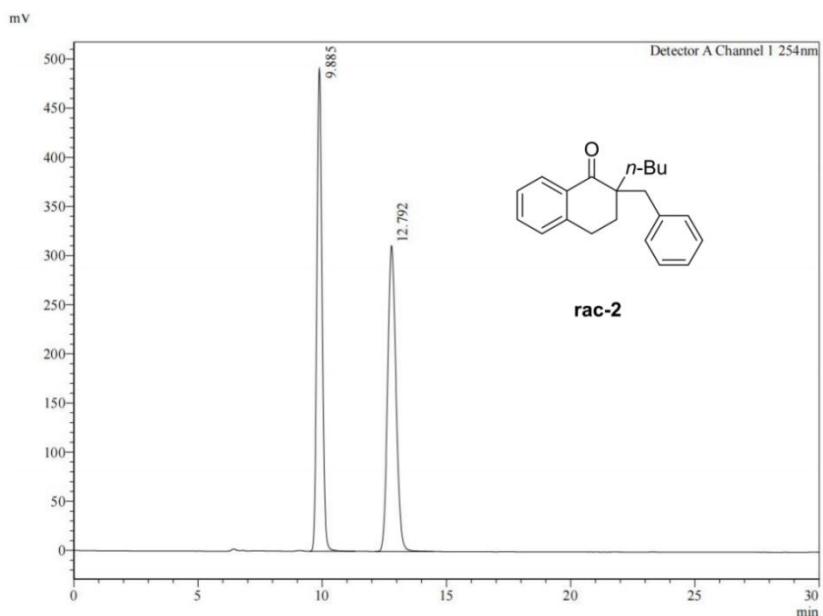








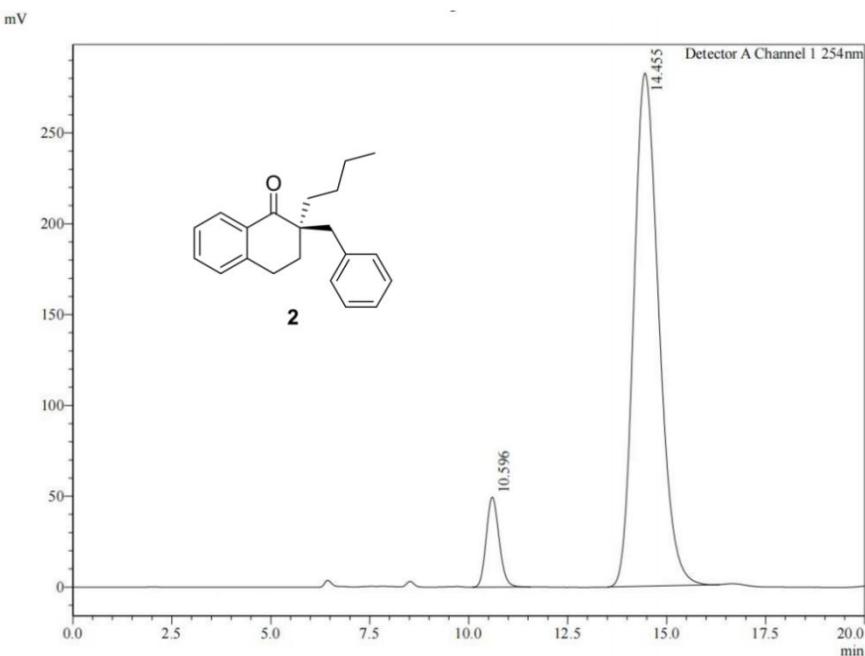
13. HPLC Spectra



Peak Table

Detector A Channel 1 254nm

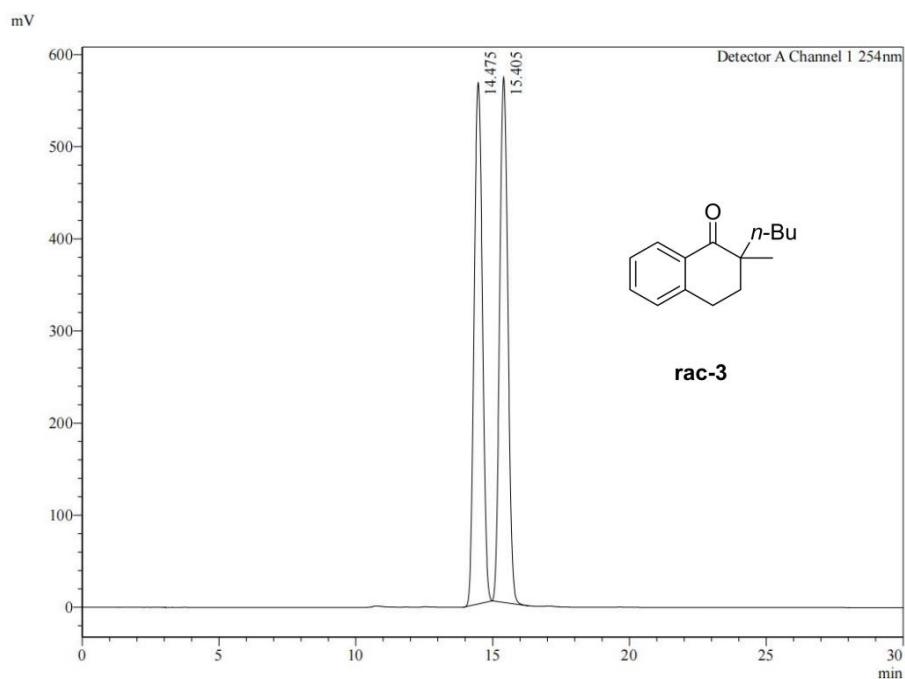
Peak#	Ret. Time	Area	Height	Area%	Height%
1	9.885	7187627	490786	49.657	61.226
2	12.792	7287020	310806	50.343	38.774
Total		14474648	801592	100.000	100.000



Peak Table

Detector A Channel 1 254nm

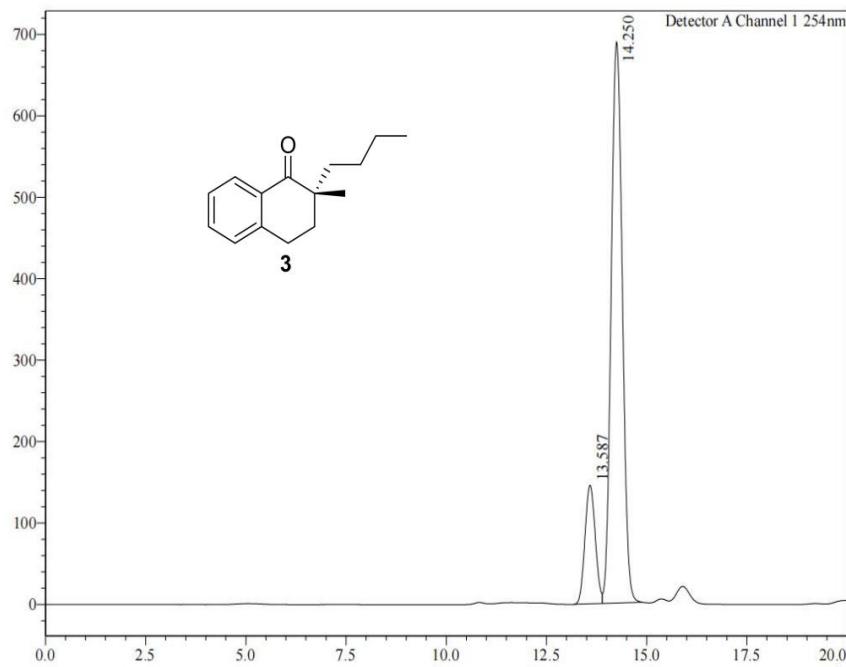
Peak#	Ret. Time	Area	Height	Area%	Height%
1	10.596	1119056	49470	8.280	14.905
2	14.455	12396496	282430	91.720	85.095
Total		13515552	331900	100.000	100.000



Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	14.475	11895973	565771	49.871	49.780
2	15.405	11957407	570761	50.129	50.220
Total		23853381	1136532	100.000	100.000

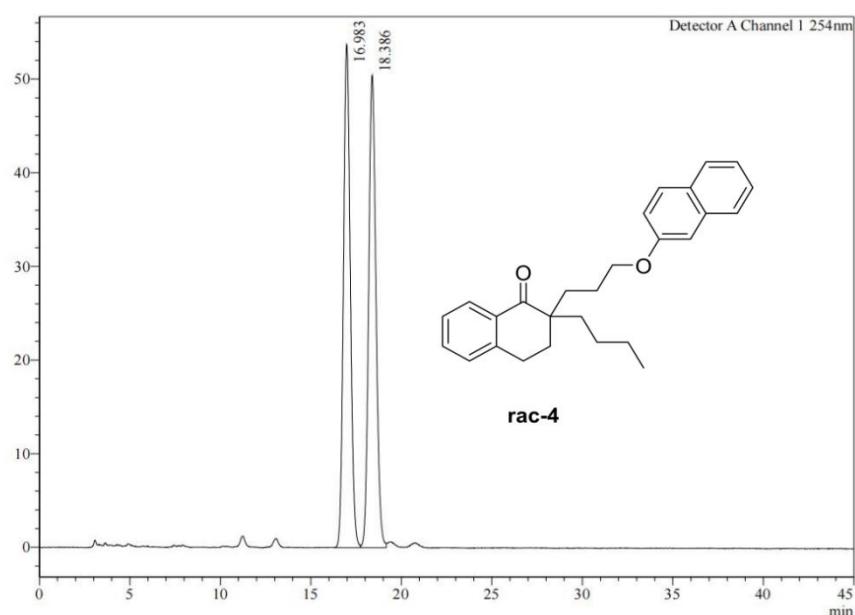


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	13.587	2614488	145535	16.432	17.449
2	14.250	13296022	688515	83.568	82.551
Total		15910511	834050	100.000	100.000

mV

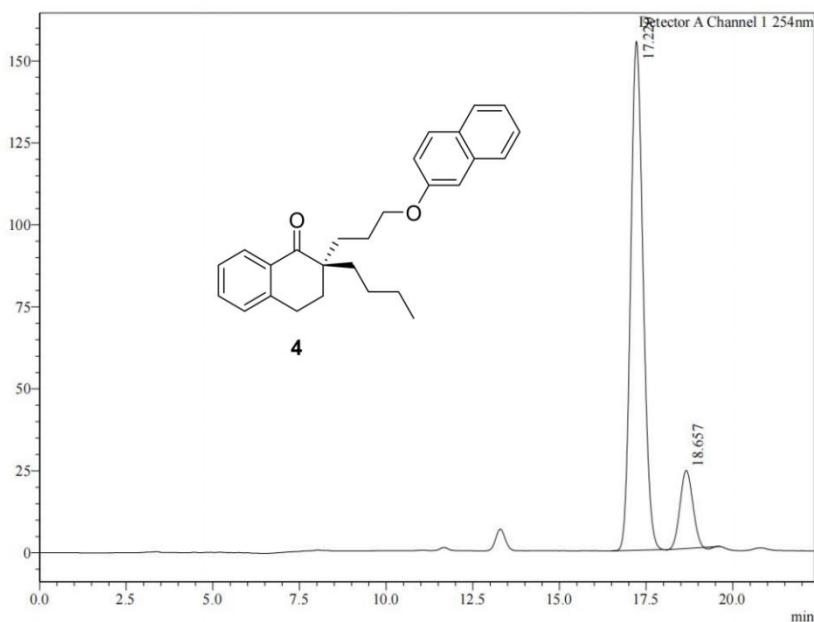


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	16.983	1410867	53701	49.892	51.582
2	18.386	1416975	50407	50.108	48.418
Total		2827841	104107	100.000	100.000

mV

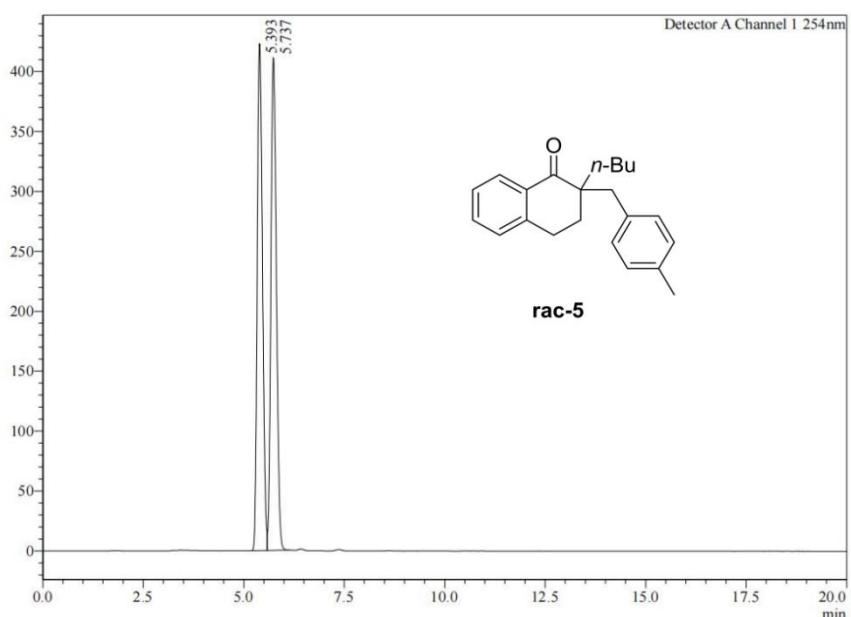


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	17.220	3866357	155140	86.403	86.696
2	18.657	608433	23807	13.597	13.304
Total		4474790	178947	100.000	100.000

mV

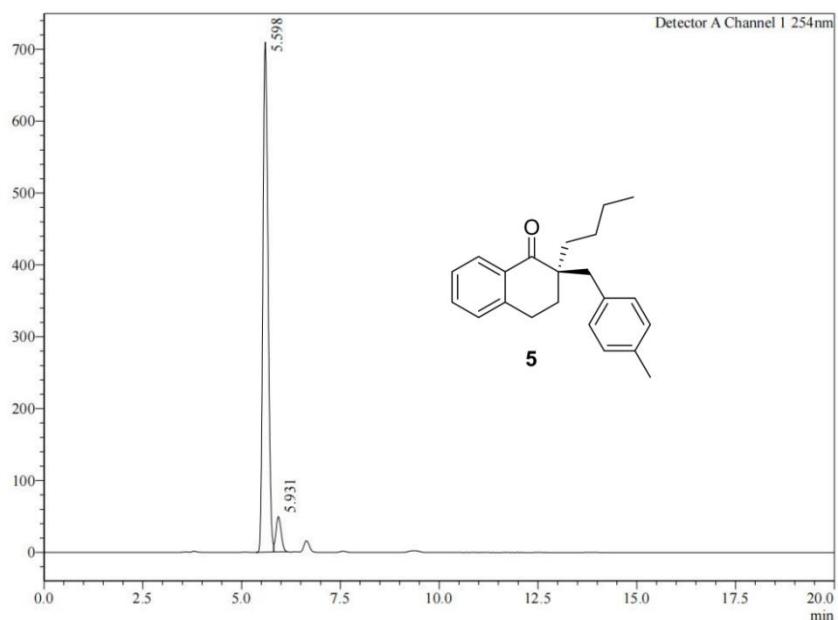


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	5.393	3856528	423220	49.749	50.741
2	5.737	3895499	410861	50.251	49.259
Total		7752027	834081	100.000	100.000

mV

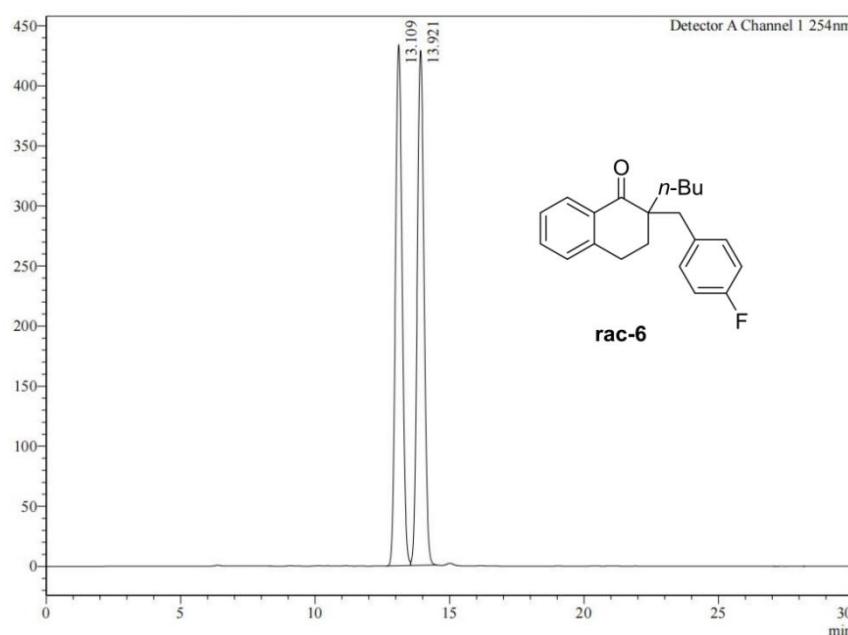


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	5.598	6428609	709716	93.461	93.556
2	5.931	449749	48884	6.539	6.444
Total		6878358	758600	100.000	100.000

mV

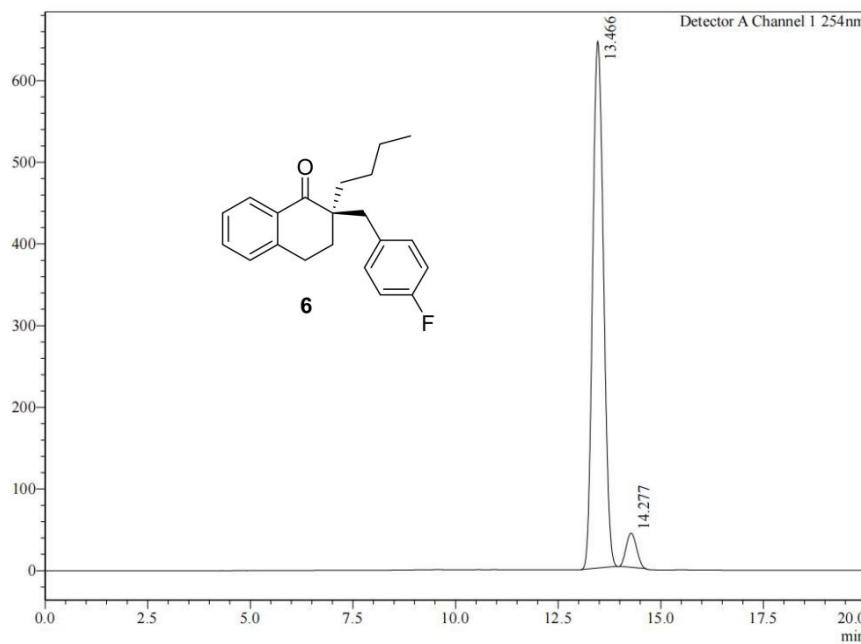


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	13.109	7528256	433176	49.861	50.271
2	13.921	7570241	428512	50.139	49.729
Total		15098497	861688	100.000	100.000

mV

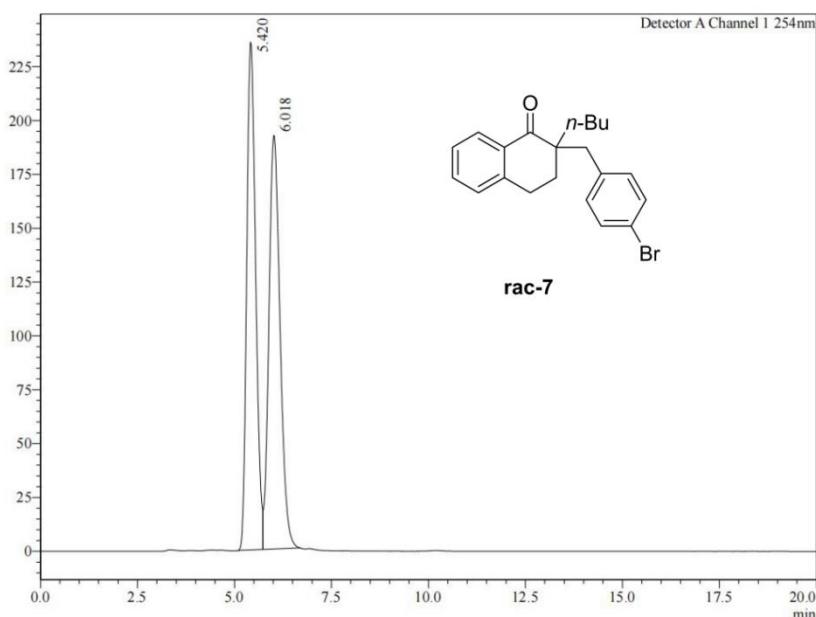


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	13.466	11867739	644746	94.131	93.910
2	14.277	739981	41814	5.869	6.090
Total		12607721	686560	100.000	100.000

mV

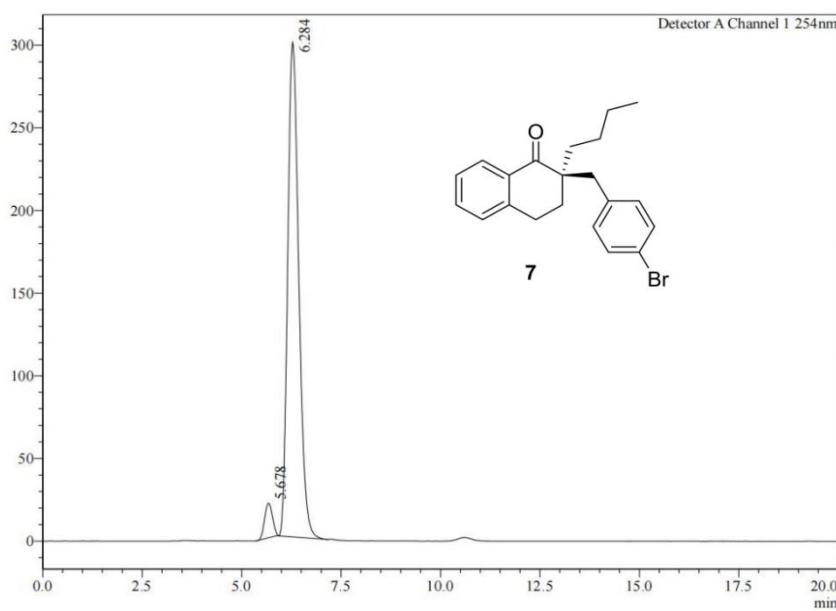


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	5.420	3778415	235639	49.576	55.106
2	6.018	3842989	191969	50.424	44.894
Total		7621404	427608	100.000	100.000

mV

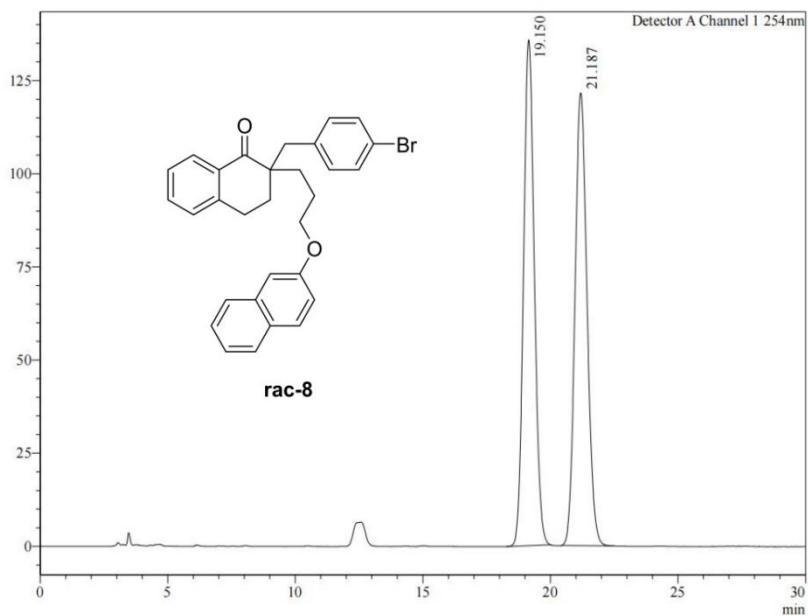


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	5.678	285643	20885	4.716	6.527
2	6.284	5771423	299100	95.284	93.473
Total		6057067	319985	100.000	100.000

mV

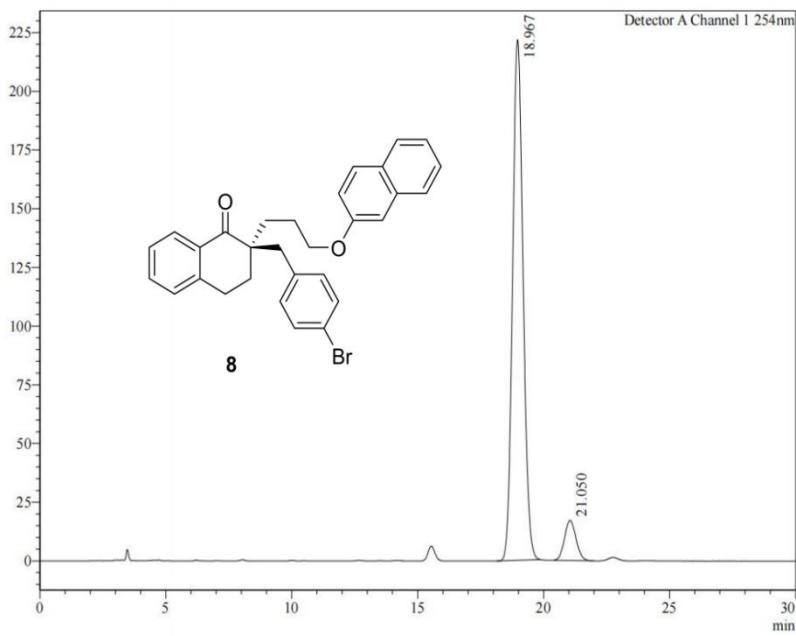


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	19.150	3979431	135676	49.977	52.755
2	21.187	3983055	121506	50.023	47.245
Total		7962486	257182	100.000	100.000

mV

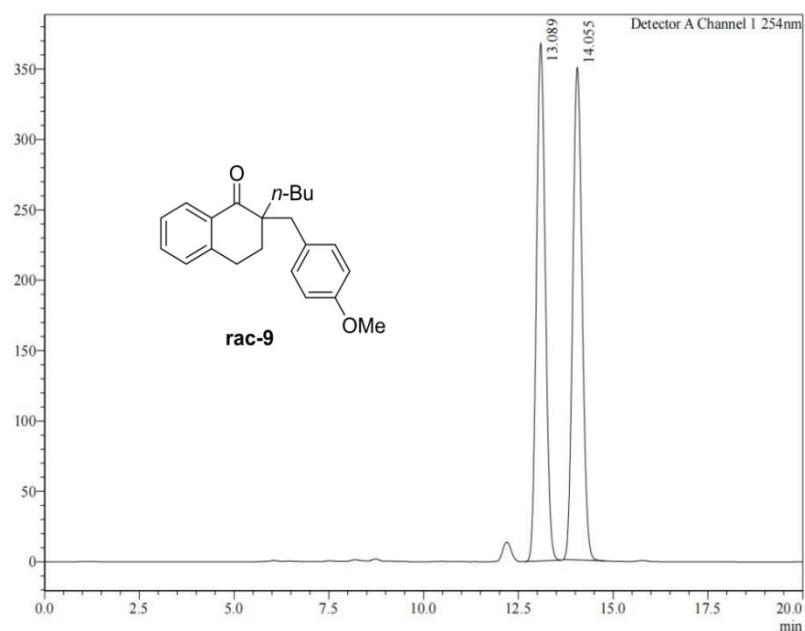


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	18.967	6412279	221643	92.215	92.855
2	21.050	541361	17054	7.785	7.145
Total		6953640	238697	100.000	100.000

mV

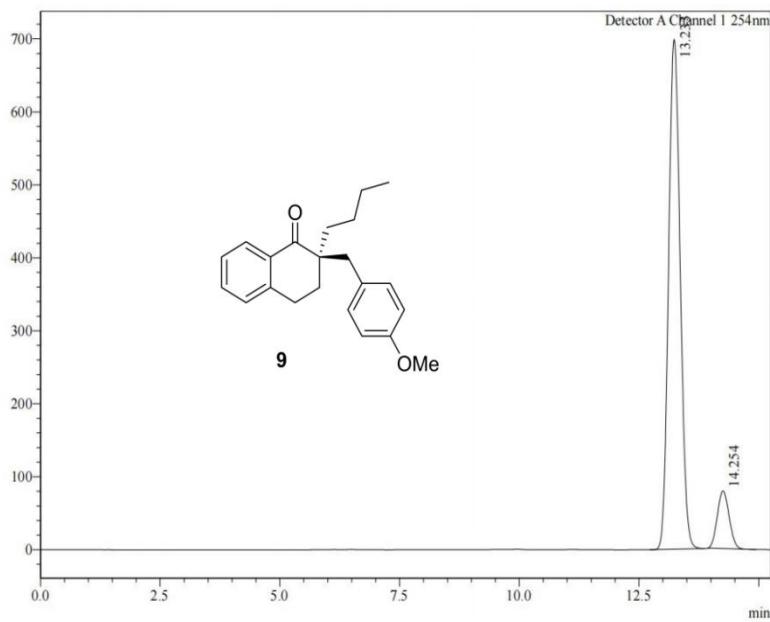


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	13.089	5999955	367621	49.924	51.222
2	14.055	6018221	350082	50.076	48.778
Total		12018176	717703	100.000	100.000

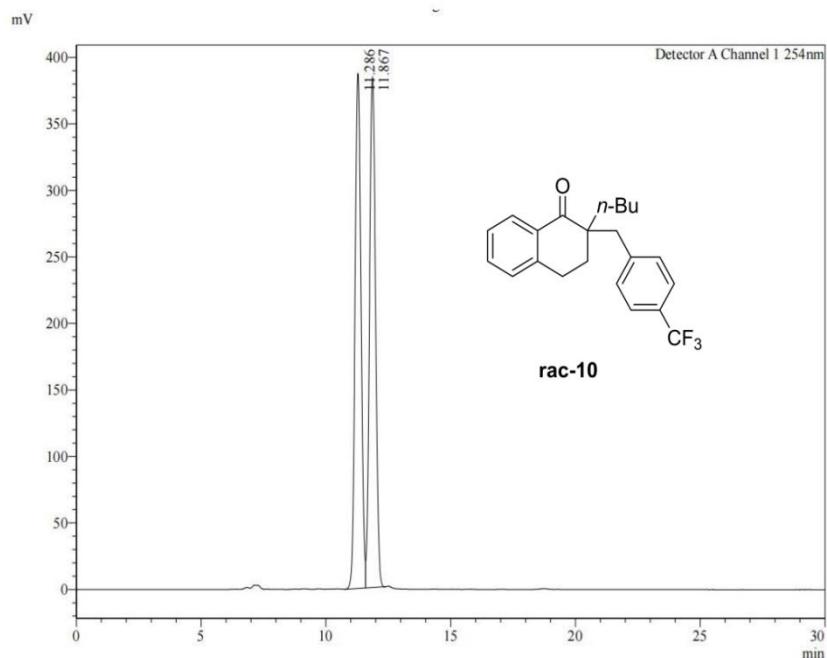
mV



Peak Table

Detector A Channel 1 254nm

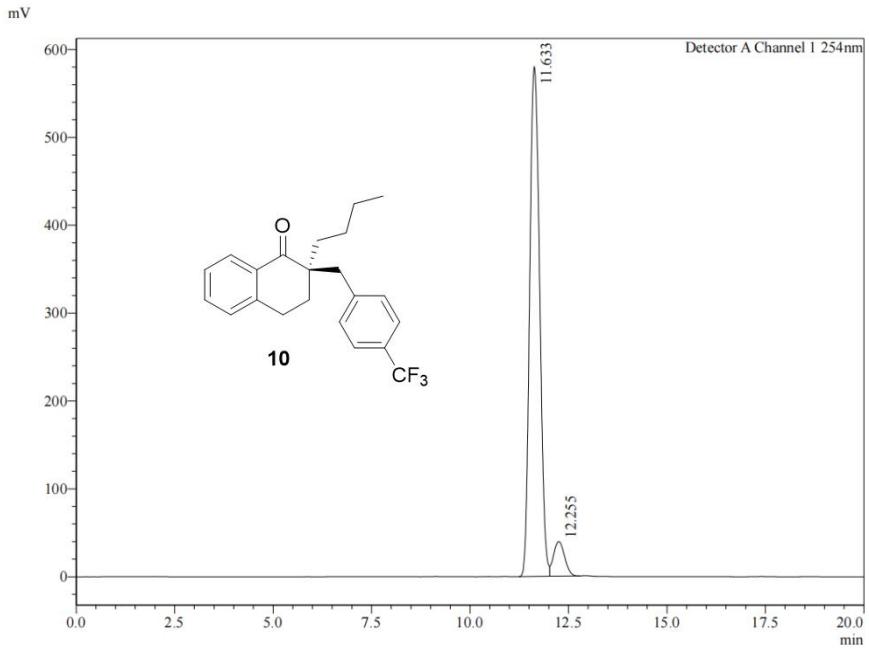
Peak#	Ret. Time	Area	Height	Area%	Height%
1	13.233	11764772	698154	89.715	89.865
2	14.254	1348652	78741	10.285	10.135
Total		13113424	776895	100.000	100.000



Peak Table

Detector A Channel 1 254nm

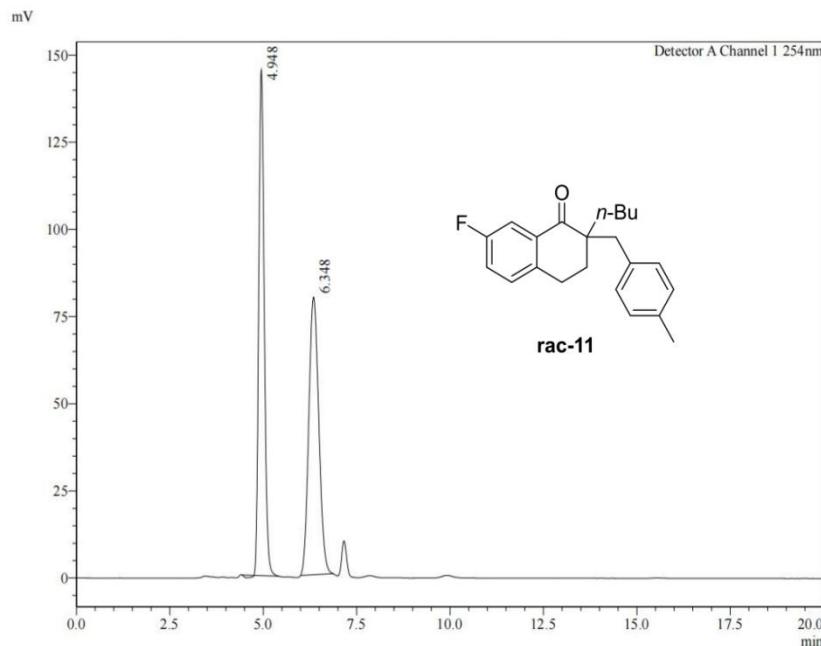
Peak#	Ret. Time	Area	Height	Area%	Height%
1	11.286	6448055	386899	50.003	50.218
2	11.867	6447202	383540	49.997	49.782
Total		12895257	770440	100.000	100.000



Peak Table

Detector A Channel 1 254nm

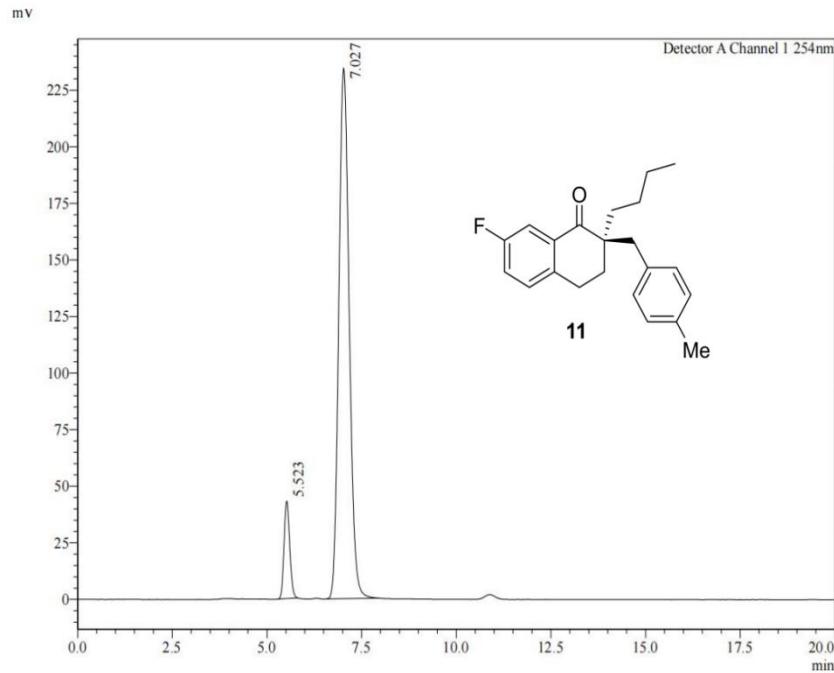
Peak#	Ret. Time	Area	Height	Area%	Height%
1	11.633	10221007	579886	92.947	93.638
2	12.255	775562	39401	7.053	6.362
Total		10996569	619287	100.000	100.000



Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	4.948	1480053	144980	49.992	64.538
2	6.348	1480545	79663	50.008	35.462
Total		2960598	224643	100.000	100.000

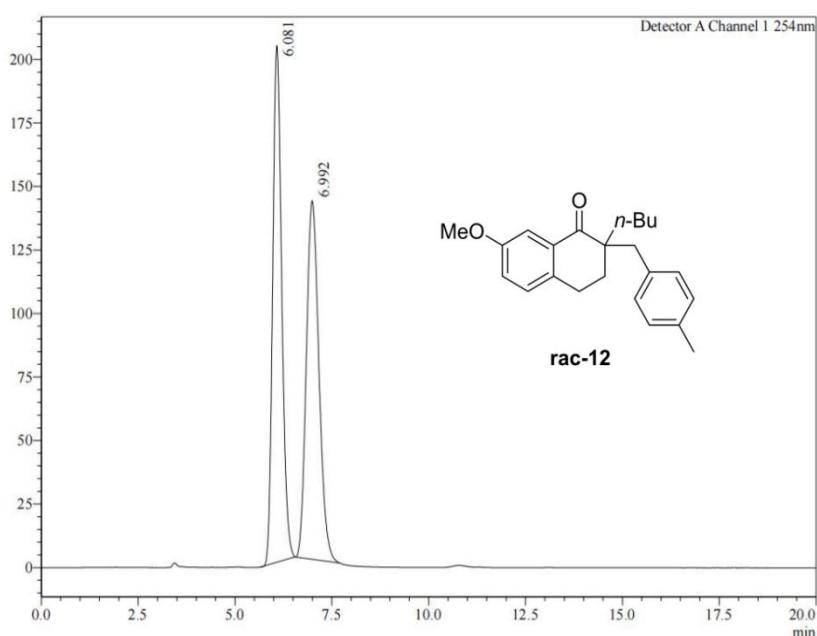


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	5.523	450723	42996	9.166	15.510
2	7.027	4466563	234209	90.834	84.490
Total		4917285	277204	100.000	100.000

mV

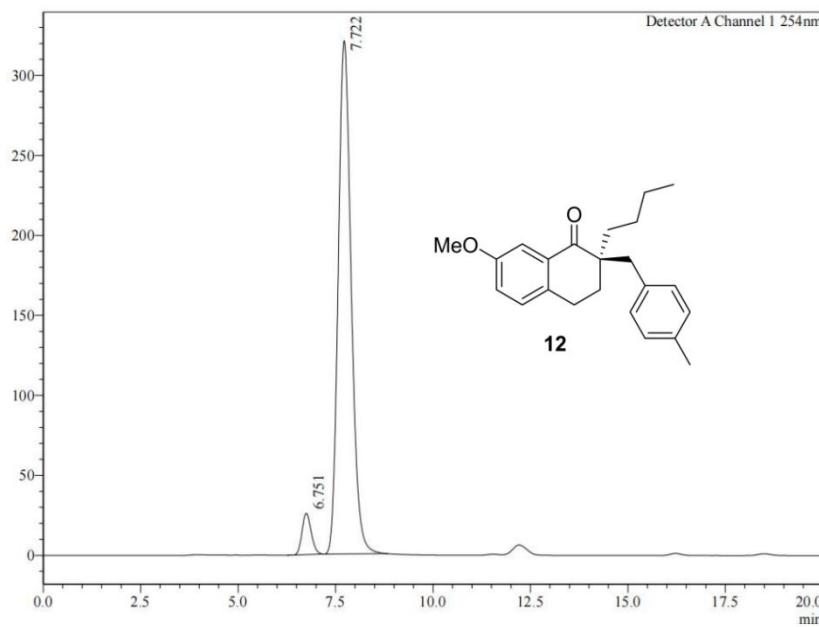


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	6.081	3285786	203202	50.812	59.020
2	6.992	3180828	141090	49.188	40.980
Total		6466614	344292	100.000	100.000

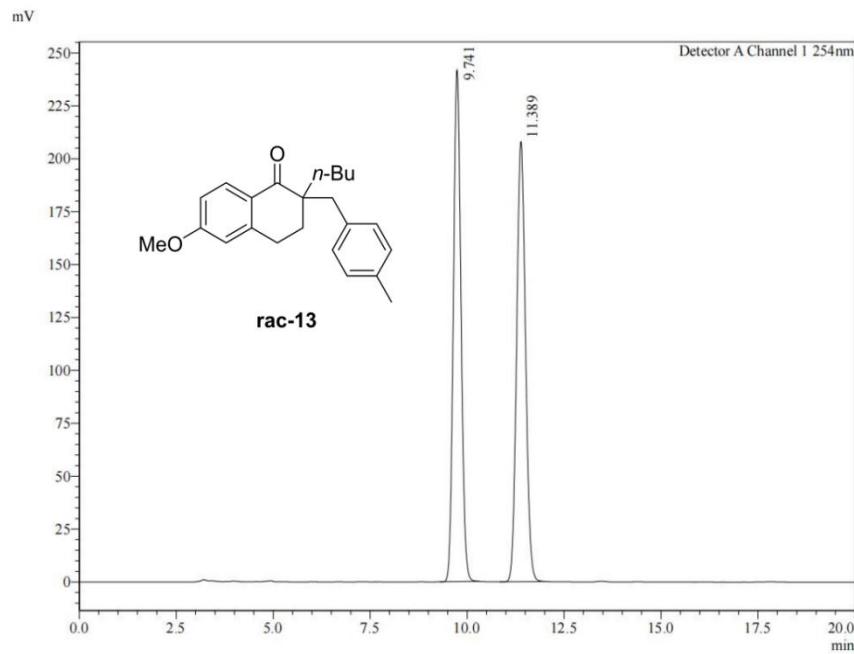
mV



Peak Table

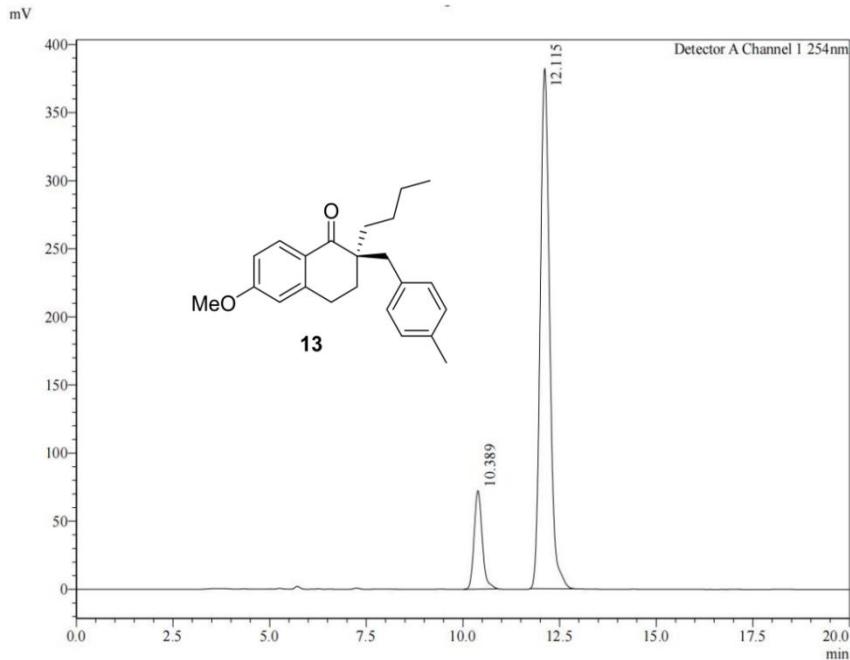
Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	6.751	421303	25778	5.361	7.438
2	7.722	7436884	320811	94.639	92.562
Total		7858186	346589	100.000	100.000



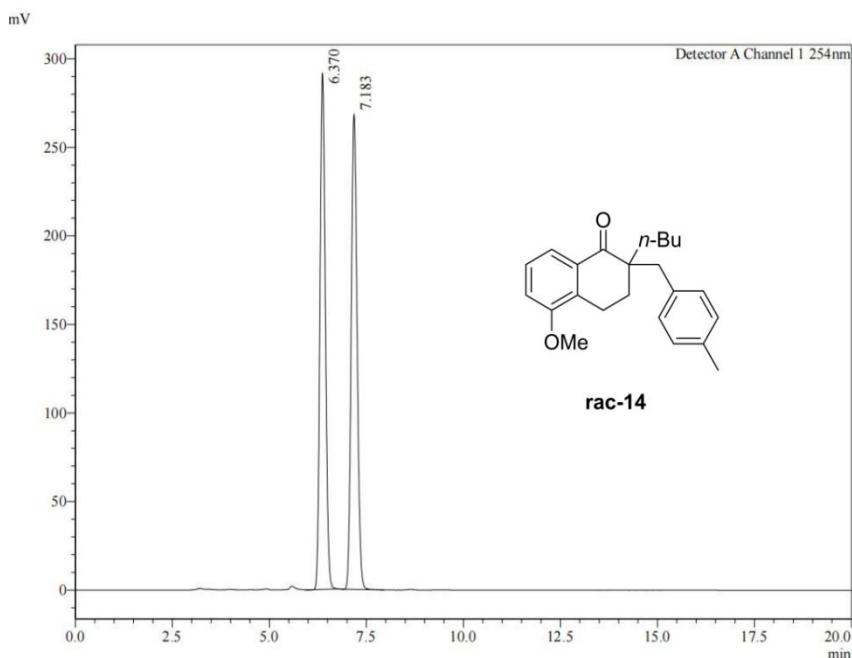
Peak Table

Detector A Channel 1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	9.741	3295785	241555	49.946	53.736
2	11.389	3302932	207965	50.054	46.264
Total		6598717	449519	100.000	100.000



Peak Table

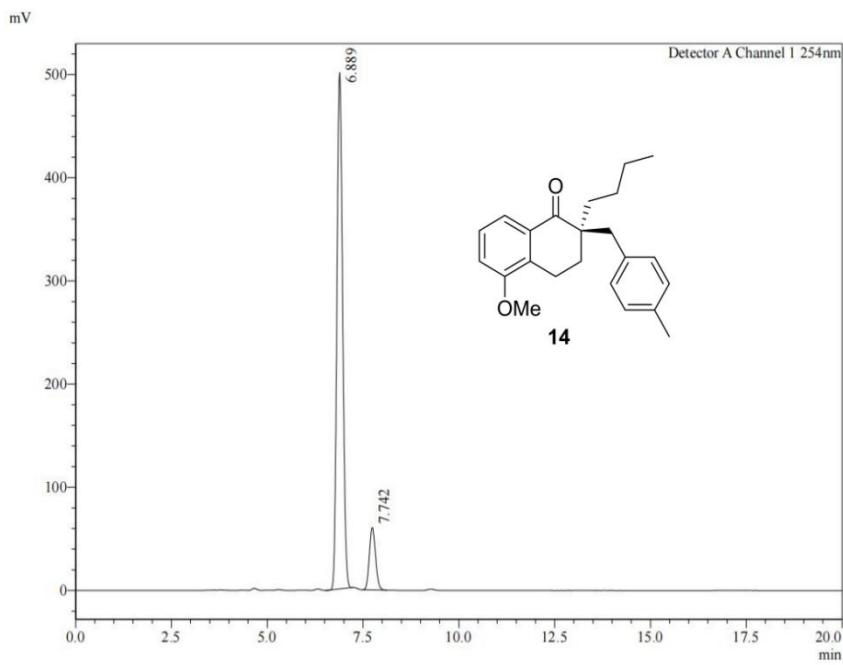
Detector A Channel 1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	10.389	1061453	72258	14.088	15.918
2	12.115	6473030	381682	85.912	84.082
Total		7534483	453941	100.000	100.000



Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	6.370	2828935	291263	49.912	52.034
2	7.183	2838964	268496	50.088	47.966
Total		5667898	559759	100.000	100.000

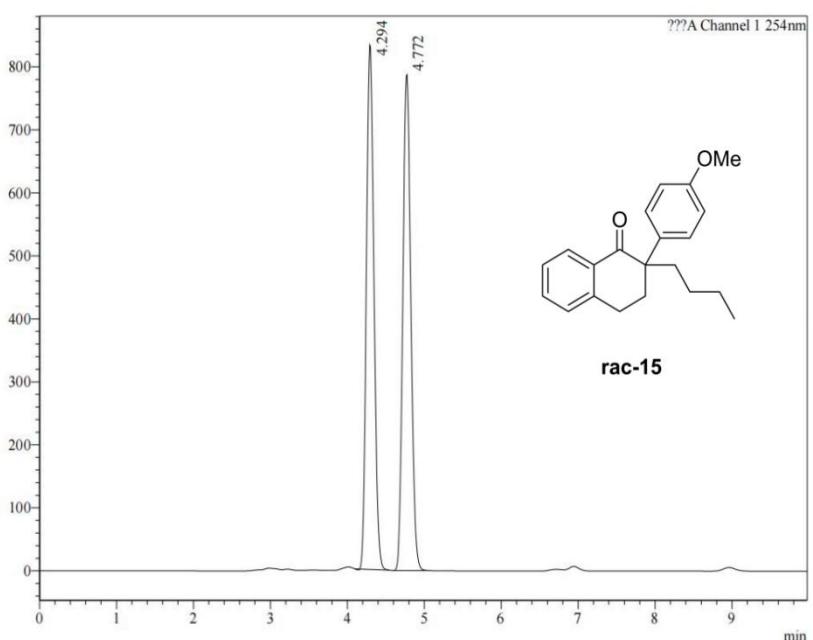


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	6.889	5183051	500581	88.409	89.220
2	7.742	679553	60484	11.591	10.780
Total		5862603	561065	100.000	100.000

mV

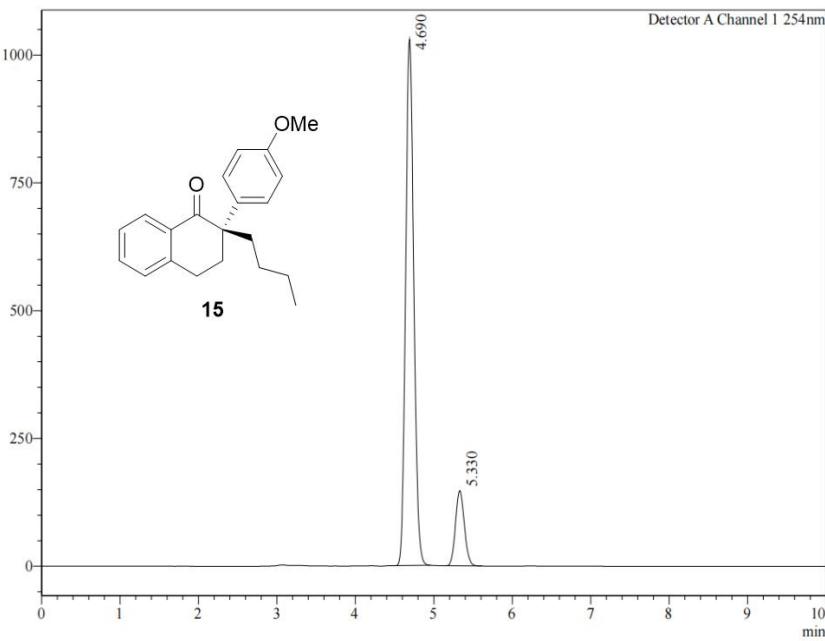


Peak Table

??A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	4.294	5659989	831750	49.846	51.393
2	4.772	5694940	786666	50.154	48.607
Total		11354929	1618417	100.000	100.000

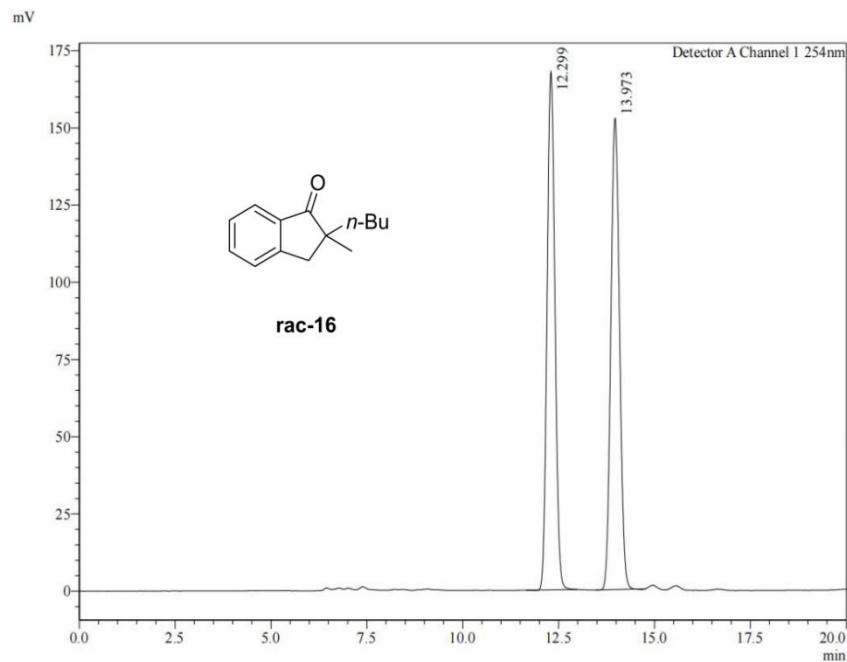
mV



Peak Table

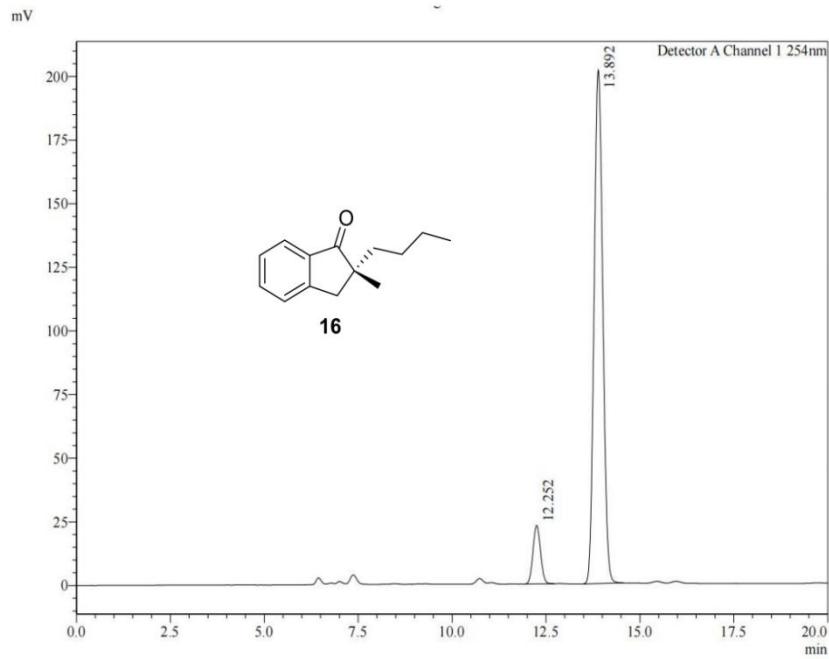
Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	4.690	7414370	1029078	86.428	87.460
2	5.330	1164275	147555	13.572	12.540
Total		8578645	1176633	100.000	100.000



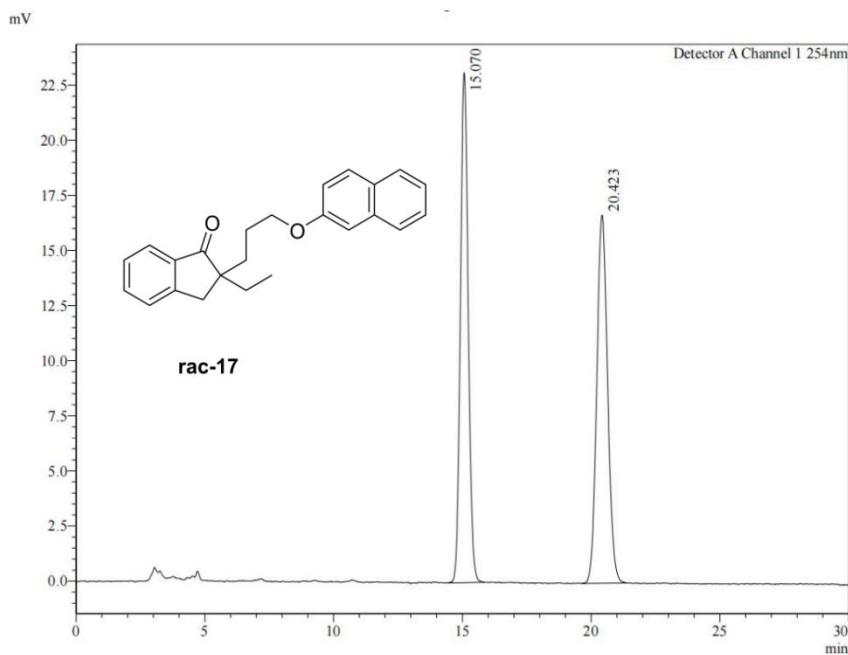
Peak Table

Detector A Channel 1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	12.299	2397326	167654	49.893	52.353
2	13.973	2407655	152581	50.107	47.647
Total		4804982	320235	100.000	100.000



Peak Table

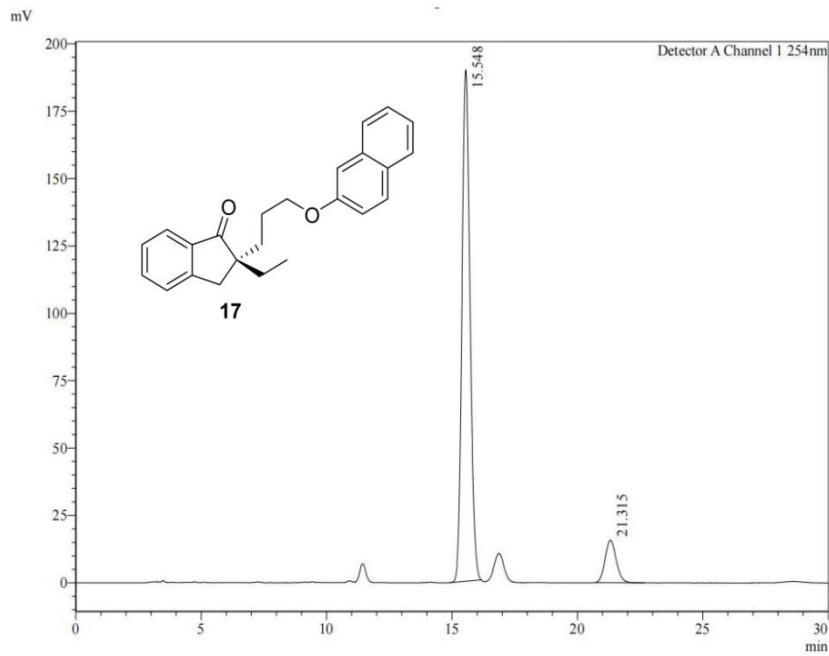
Detector A Channel 1 254nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	12.252	321548	22980	9.007	10.229
2	13.892	3248357	201685	90.993	89.771
Total		3569905	224666	100.000	100.000



Peak Table

Detector A Channel 1 254nm

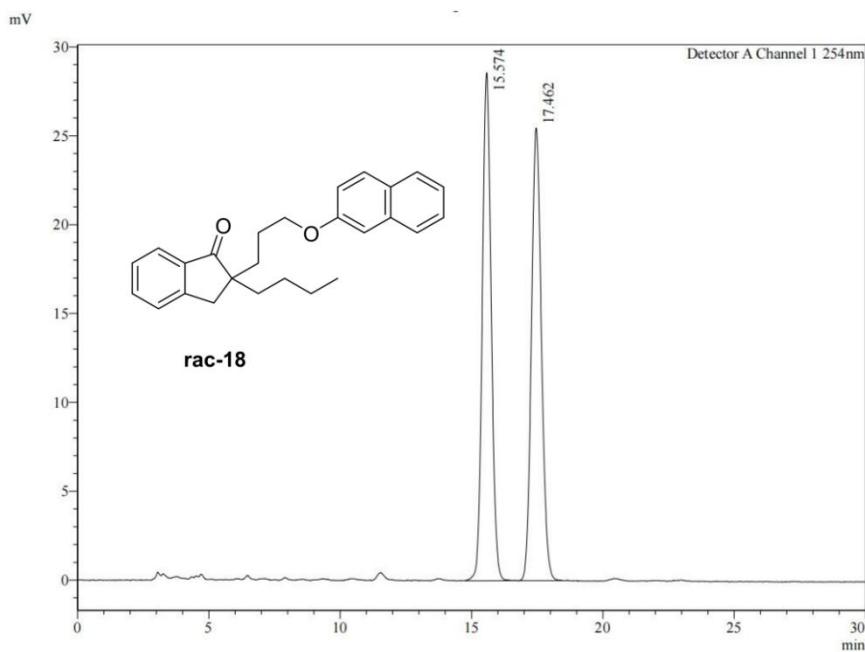
Peak#	Ret. Time	Area	Height	Area%	Height%
1	15.070	486649	23121	49.970	58.051
2	20.423	487243	16708	50.030	41.949
Total		973892	39829	100.000	100.000



Peak Table

Detector A Channel 1 254nm

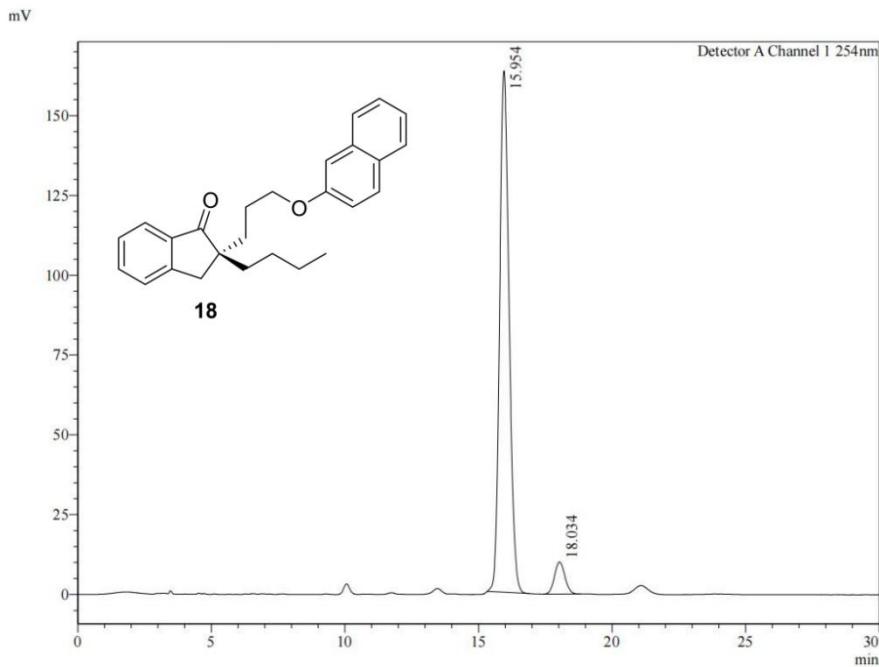
Peak#	Ret. Time	Area	Height	Area%	Height%
1	15.548	4231892	189651	89.729	92.323
2	21.315	484424	15771	10.271	7.677
Total		4716316	205422	100.000	100.000



Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	15.574	675131	28568	50.170	52.871
2	17.462	670568	25465	49.830	47.129
Total		1345699	54032	100.000	100.000

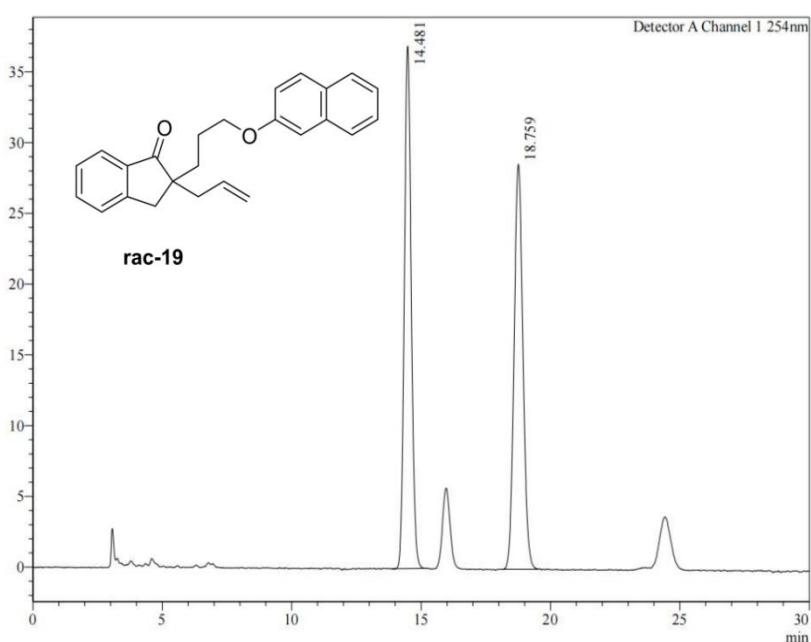


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	15.954	4026930	163324	93.671	94.200
2	18.034	272095	10056	6.329	5.800
Total		4299025	173379	100.000	100.000

mV

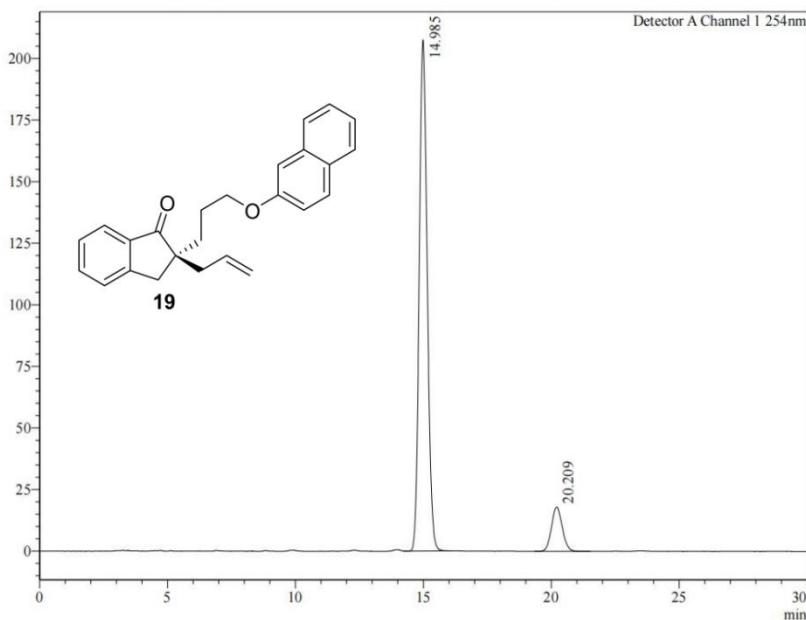


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	14.481	685477	36883	50.138	56.321
2	18.759	681707	28605	49.862	43.679
Total		1367185	65488	100.000	100.000

mV

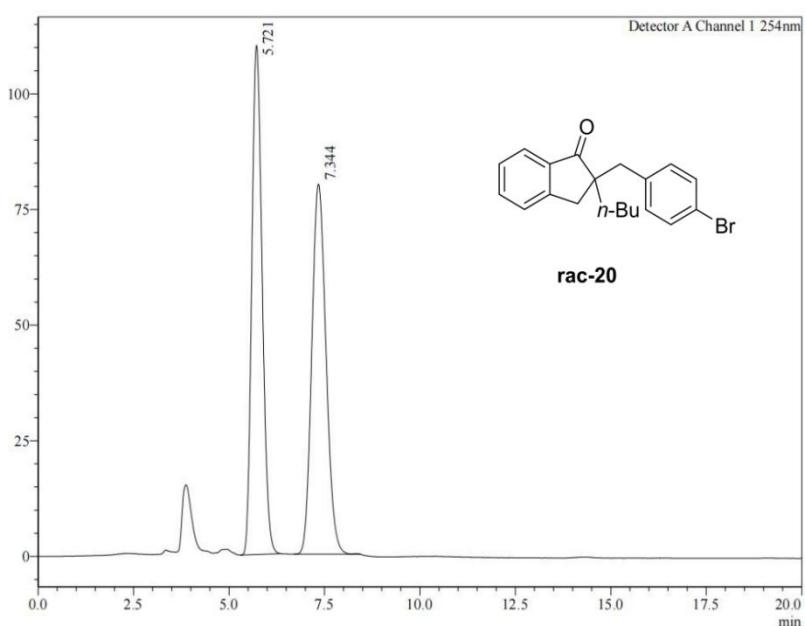


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	14.985	4496828	207285	89.541	92.032
2	20.209	525264	17945	10.459	7.968
Total		5022092	225231	100.000	100.000

mV

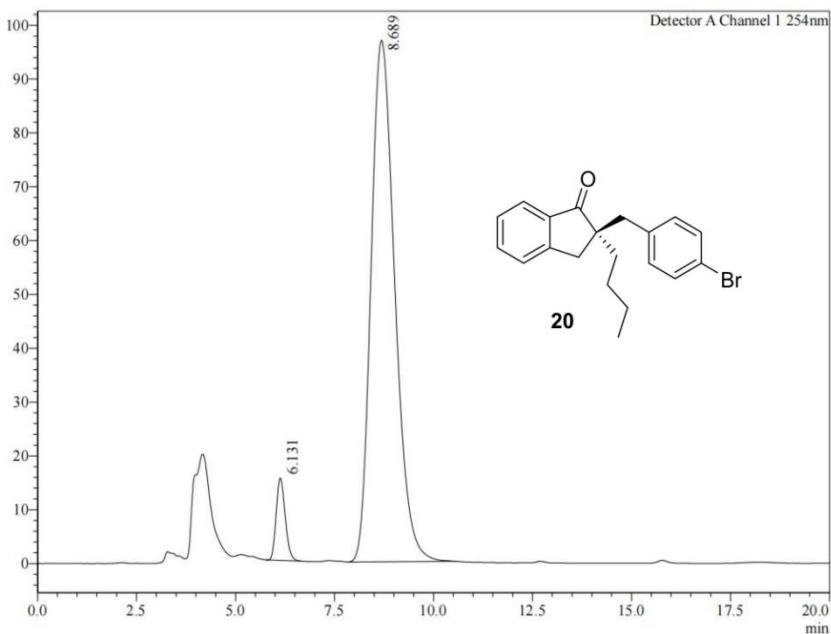


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	5.721	2078705	110055	50.124	57.912
2	7.344	2068397	79982	49.876	42.088
Total		4147101	190036	100.000	100.000

mV

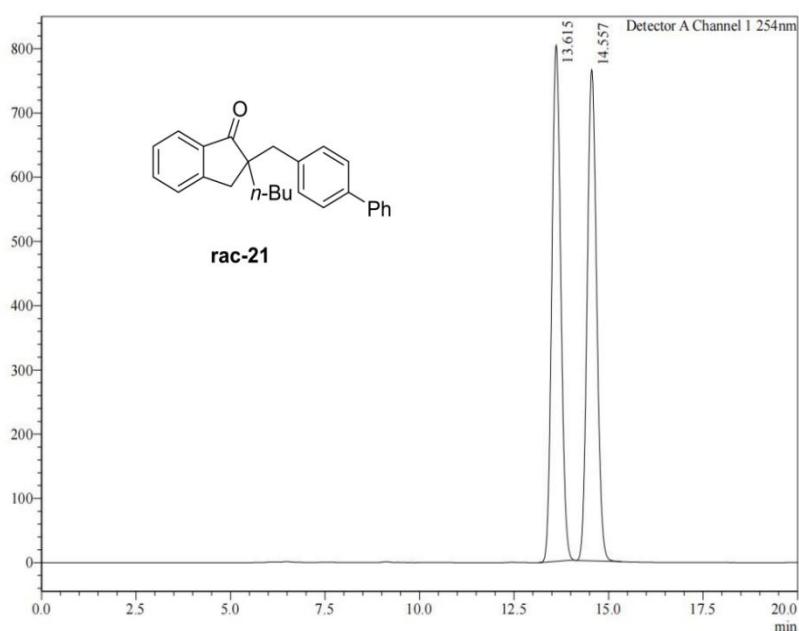


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	6.131	243127	15307	5.688	13.646
2	8.689	4031314	96867	94.312	86.354
Total		4274441	112174	100.000	100.000

mV

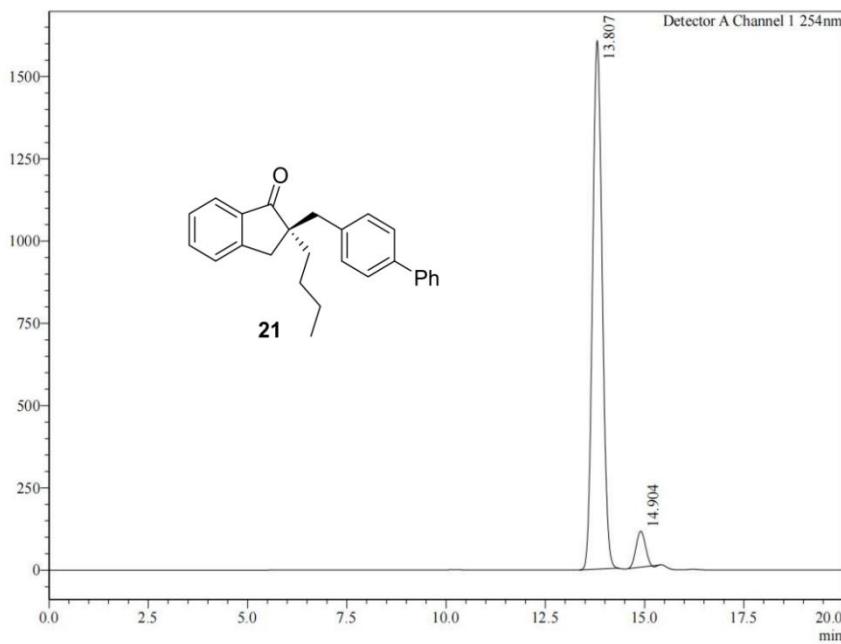


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	13.615	13258762	803128	49.906	51.227
2	14.557	13308922	764661	50.094	48.773
Total		26567684	1567789	100.000	100.000

mV

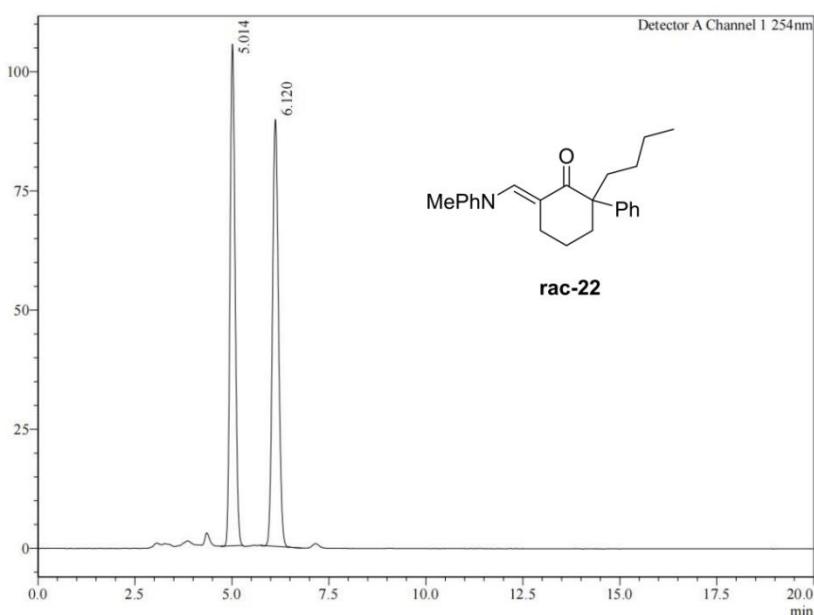


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	13.807	27250432	1605280	93.912	93.647
2	14.904	1766548	108904	6.088	6.353
Total		29016980	1714183	100.000	100.000

mV

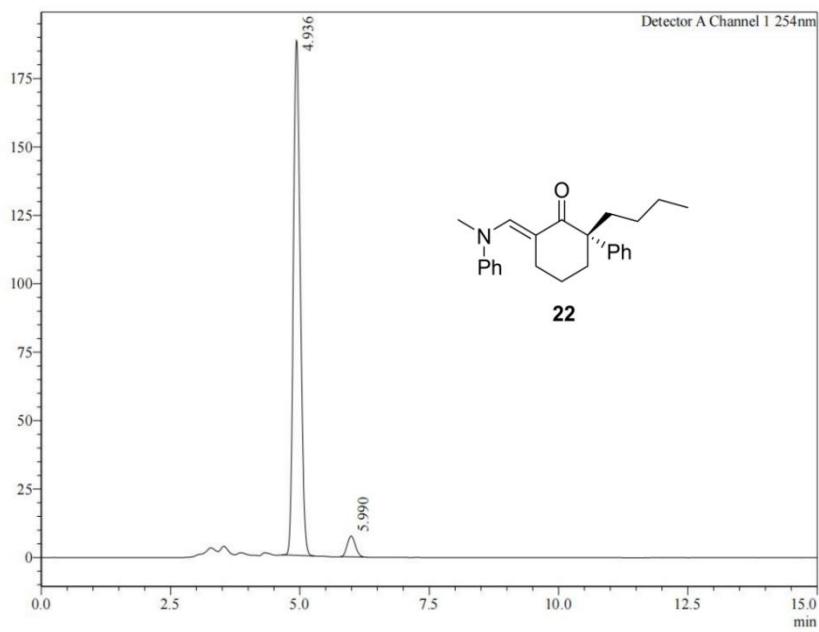


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	5.014	960454	105252	49.803	54.045
2	6.120	968042	89497	50.197	45.955
Total		1928496	194748	100.000	100.000

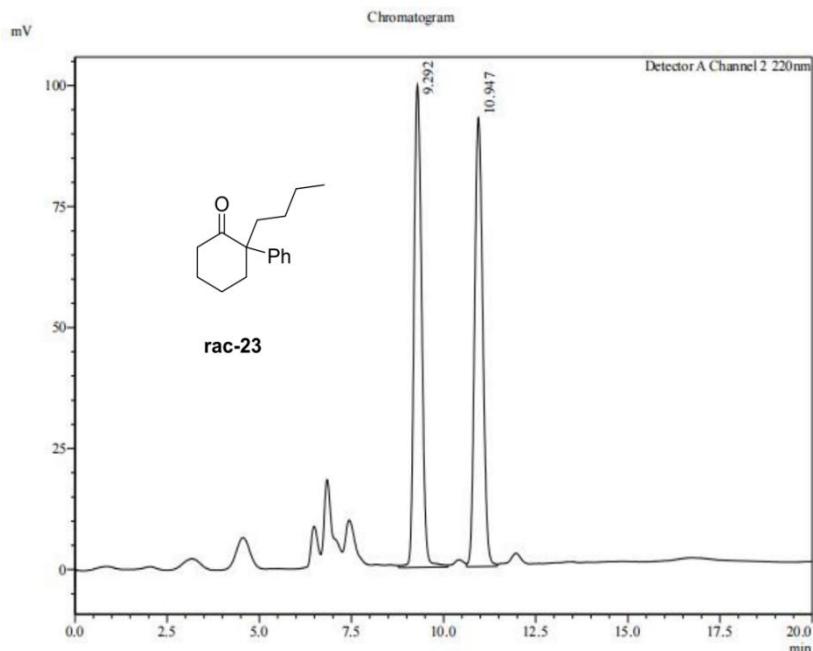
mV



Peak Table

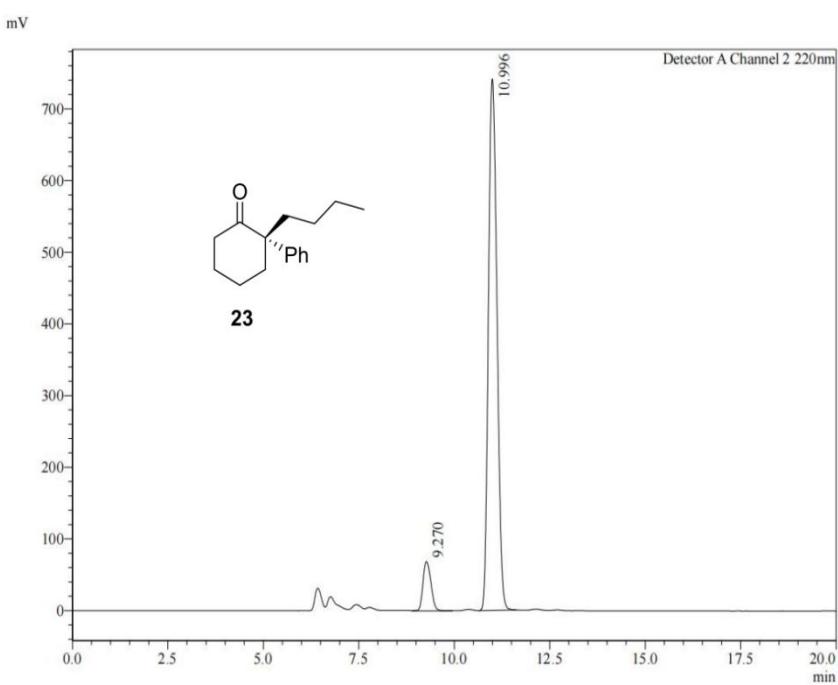
Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	4.936	1752454	187975	95.426	96.097
2	5.990	83992	7636	4.574	3.903
Total		1836446	195611	100.000	100.000



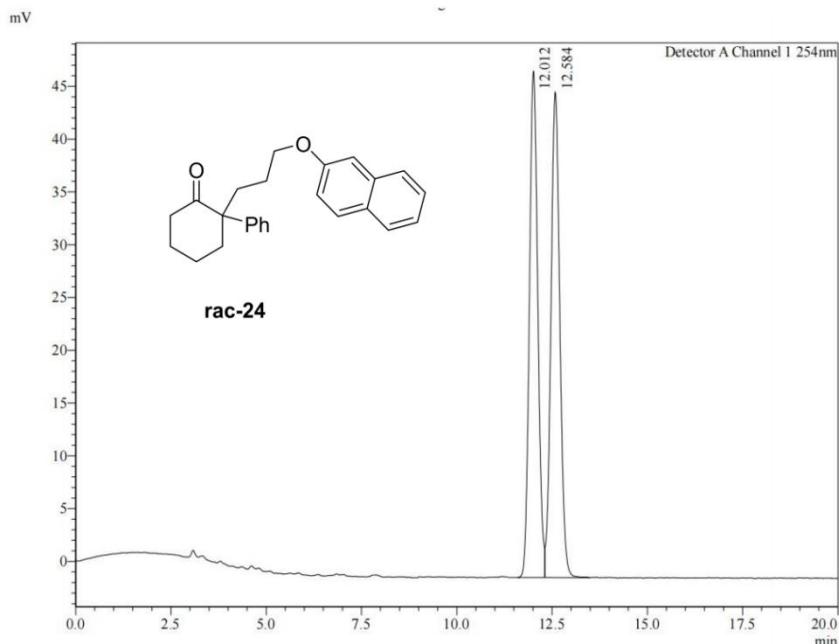
Peak Table

Detector A Channel 2 220nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	9.292	1440316	99669	50.276	51.813
2	10.947	1424492	92694	49.724	48.187
Total		2864808	192363	100.000	100.000



Peak Table

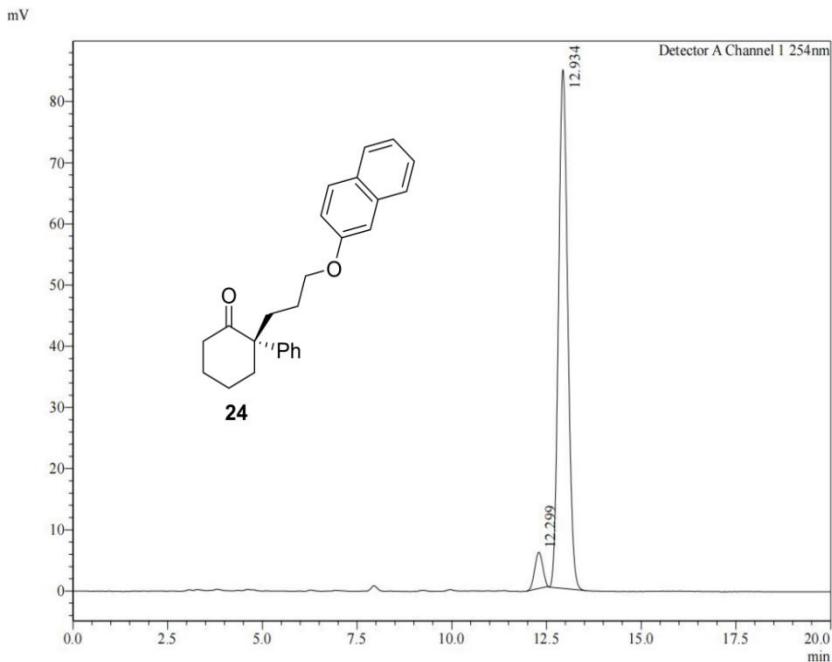
Detector A Channel 2 220nm					
Peak#	Ret. Time	Area	Height	Area%	Height%
1	9.270	997334	68531	7.955	8.464
2	10.996	11539706	741129	92.045	91.536
Total		12537040	809660	100.000	100.000



Peak Table

Detector A Channel 1 254nm

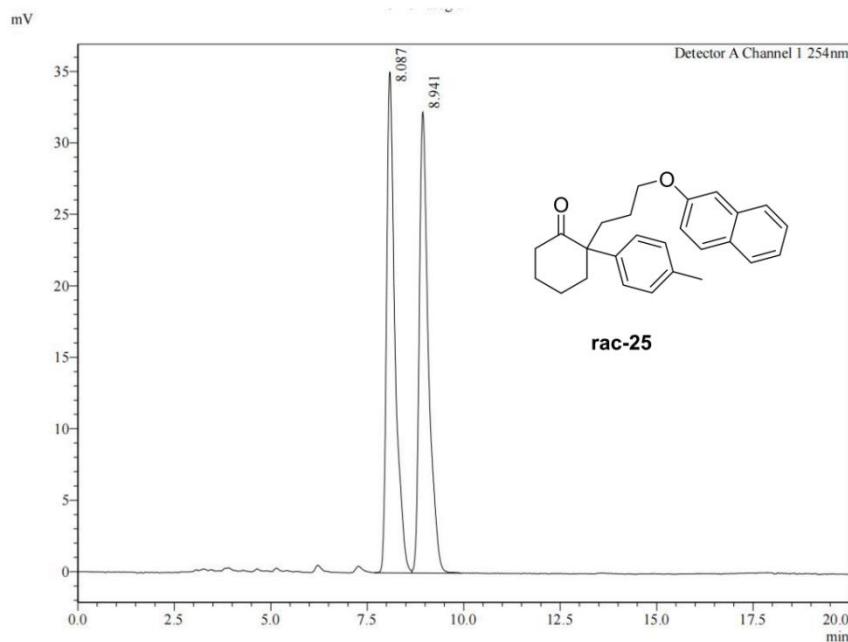
Peak#	Ret. Time	Area	Height	Area%	Height%
1	12.012	735704	47957	49.665	51.062
2	12.584	745622	45961	50.335	48.938
Total		1481326	93918	100.000	100.000



Peak Table

Detector A Channel 1 254nm

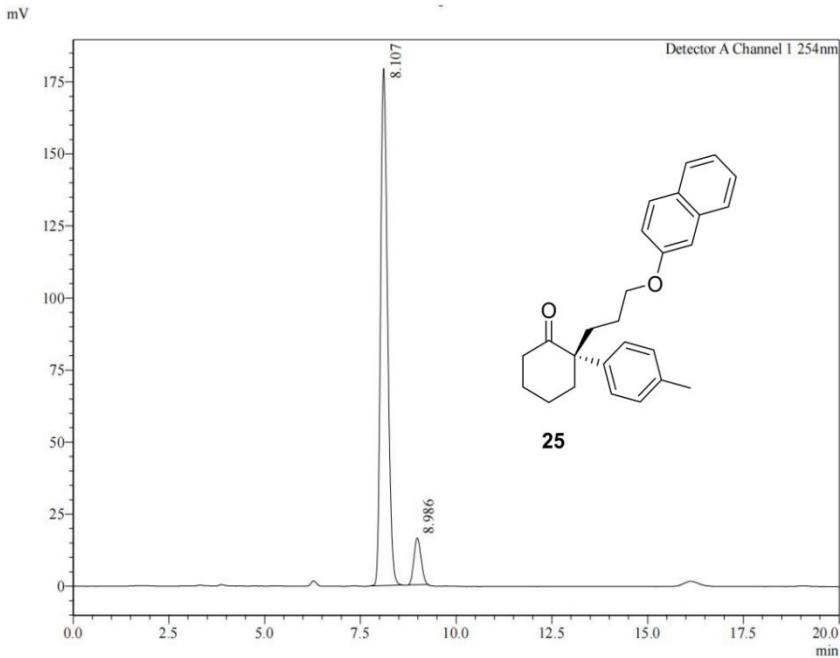
Peak#	Ret. Time	Area	Height	Area%	Height%
1	12.299	87503	5913	5.701	6.525
2	12.934	1447295	84715	94.299	93.475
Total		1534798	90628	100.000	100.000



Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	8.087	532596	35028	49.929	52.075
2	8.941	534104	32237	50.071	47.925
Total		1066700	67265	100.000	100.000

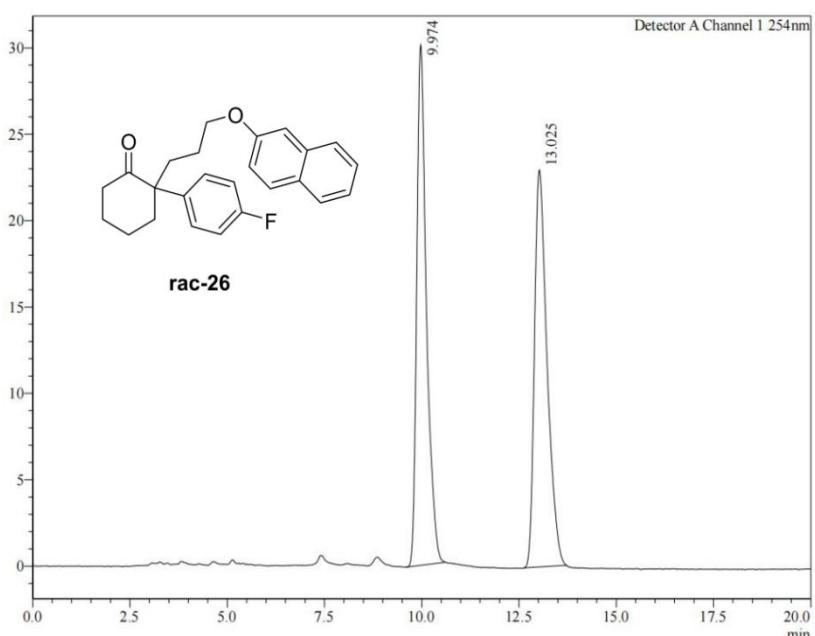


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	8.107	2273941	179422	91.478	91.706
2	8.986	211851	16226	8.522	8.294
Total		2485792	195648	100.000	100.000

mV

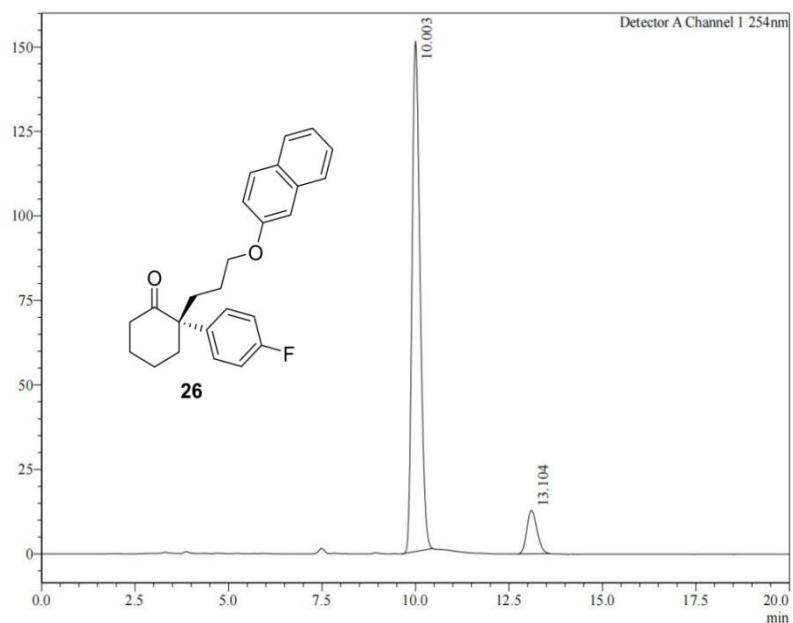


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	9.974	521664	30106	50.150	56.706
2	13.025	518540	22986	49.850	43.294
Total		1040203	53092	100.000	100.000

mV

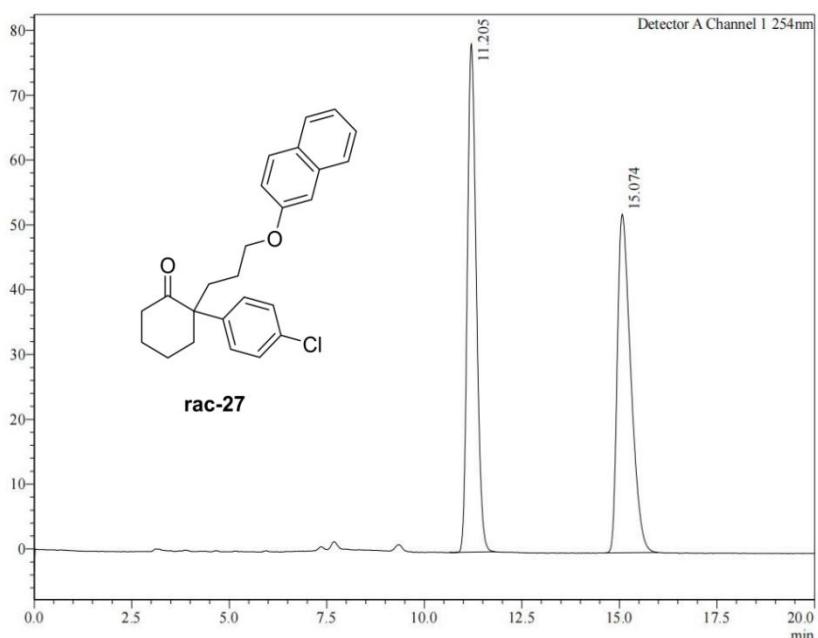


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	10.003	2249514	150874	90.258	92.173
2	13.104	242793	12812	9.742	7.827
Total		2492307	163686	100.000	100.000

mV

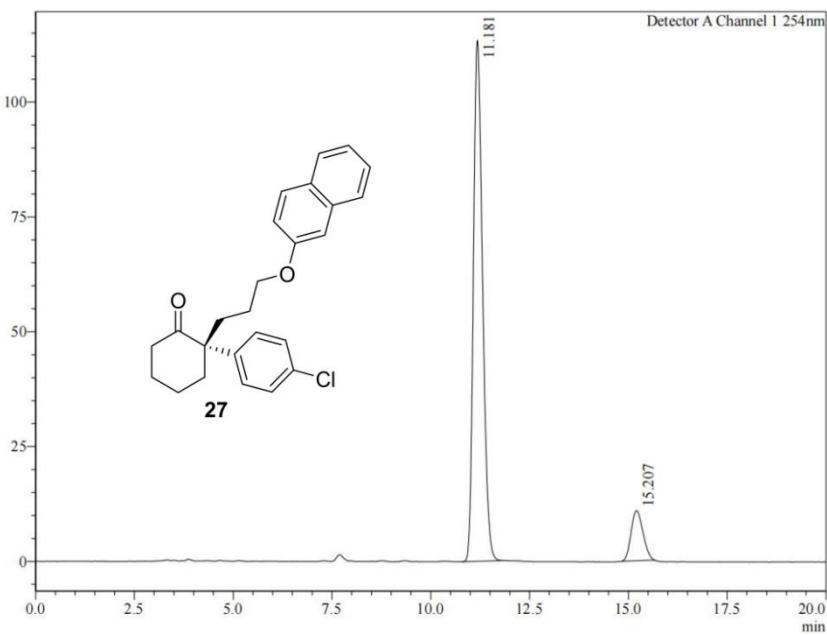


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	11.205	1249318	78387	49.933	60.023
2	15.074	1252677	52208	50.067	39.977
Total		2501996	130595	100.000	100.000

mV

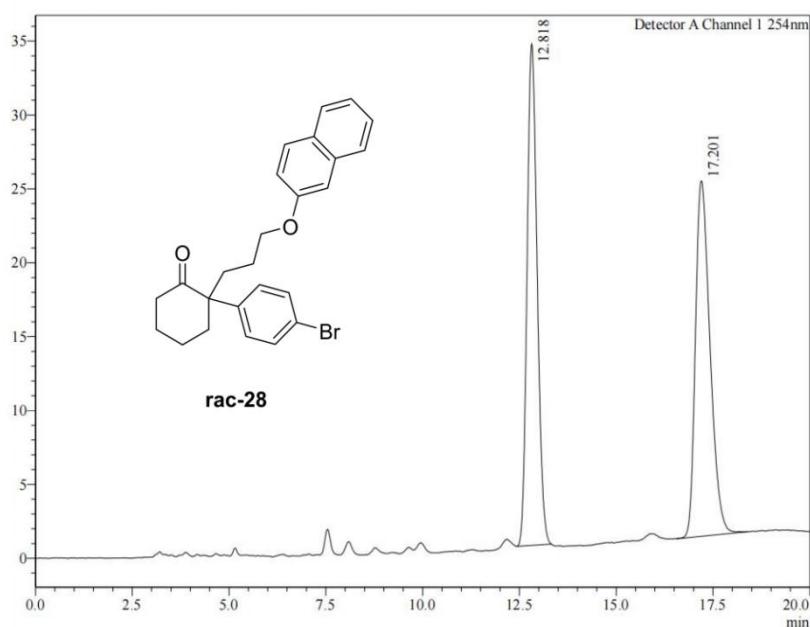


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	11.181	1826419	113345	88.869	91.206
2	15.207	228757	10929	11.131	8.794
Total		2055176	124274	100.000	100.000

mV

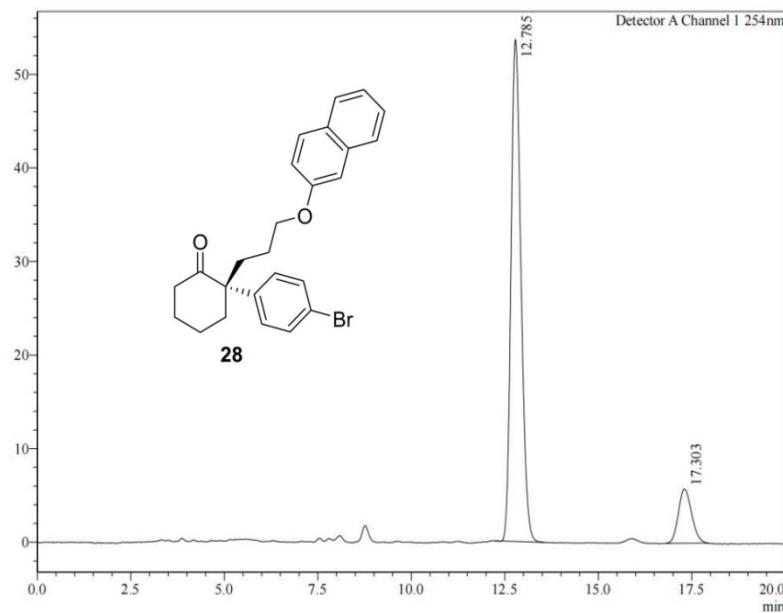


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	12.818	614103	33925	49.361	58.507
2	17.201	630000	24059	50.639	41.493
Total		1244103	57985	100.000	100.000

mV

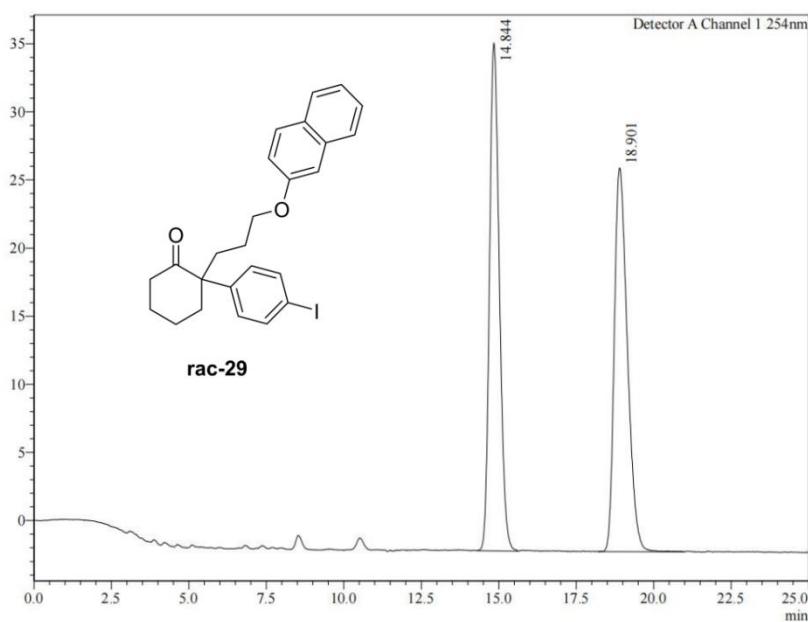


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	12.785	994047	53627	87.495	90.274
2	17.303	142065	5777	12.505	9.726
Total		1136112	59405	100.000	100.000

mV

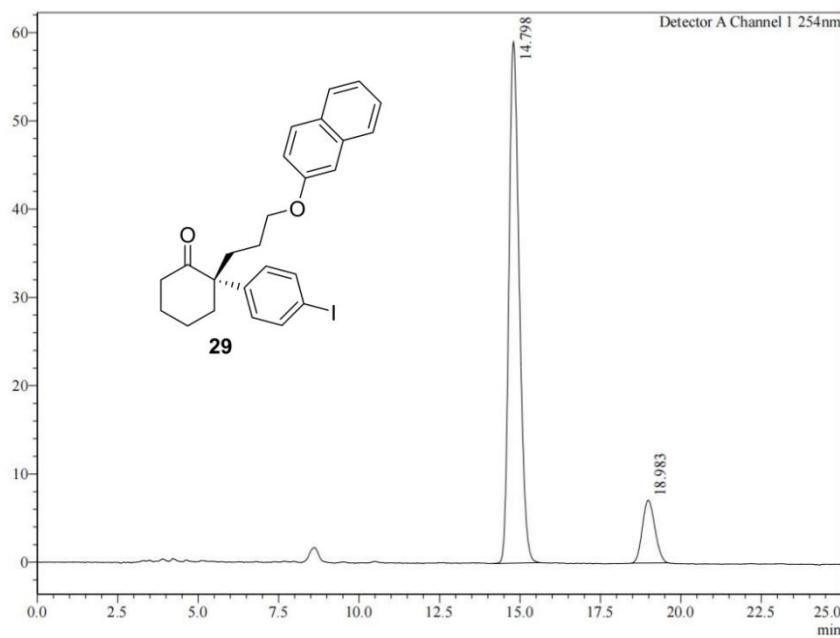


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	14.844	822757	37254	49.897	56.948
2	18.901	826160	28164	50.103	43.052
Total		1648917	65418	100.000	100.000

mV

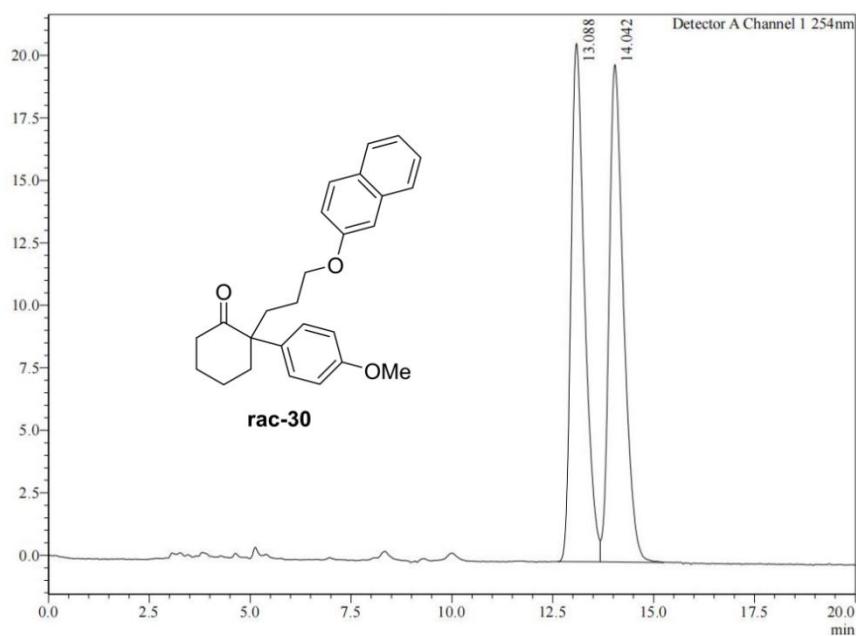


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	14.798	1317530	59064	87.189	89.245
2	18.983	193581	7118	12.811	10.755
Total		1511111	66182	100.000	100.000

mV

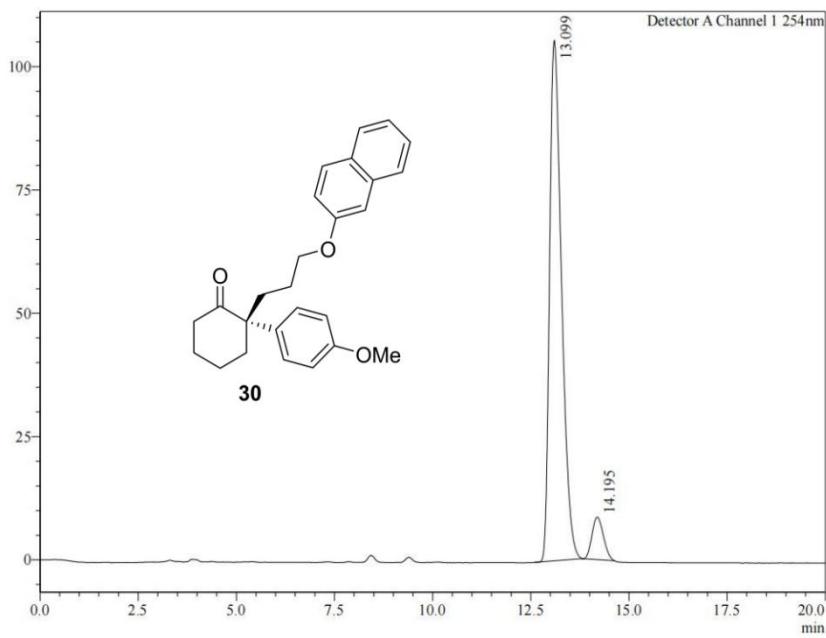


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	13.088	486884	20727	49.482	51.039
2	14.042	497083	19883	50.518	48.961
Total		983967	40610	100.000	100.000

mV

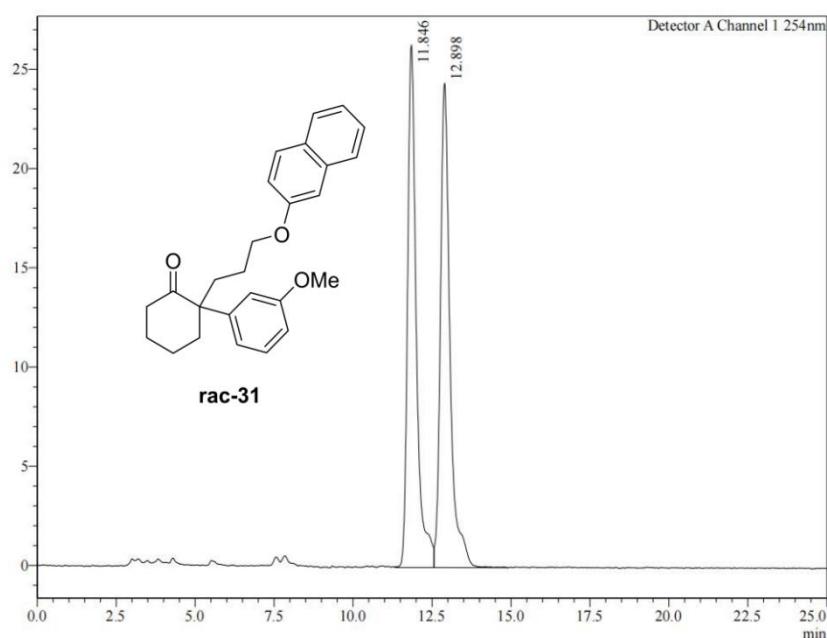


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	13.099	2229668	105495	92.695	92.441
2	14.195	175708	8626	7.305	7.559
Total		2405375	114122	100.000	100.000

mV

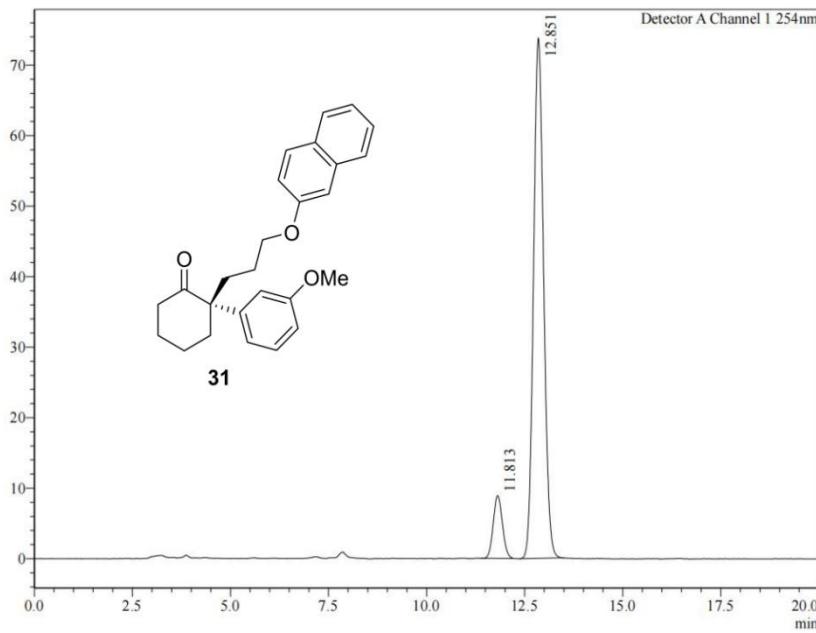


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	11.846	506871	26309	49.607	51.890
2	12.898	514893	24393	50.393	48.110
Total		1021765	50703	100.000	100.000

mV

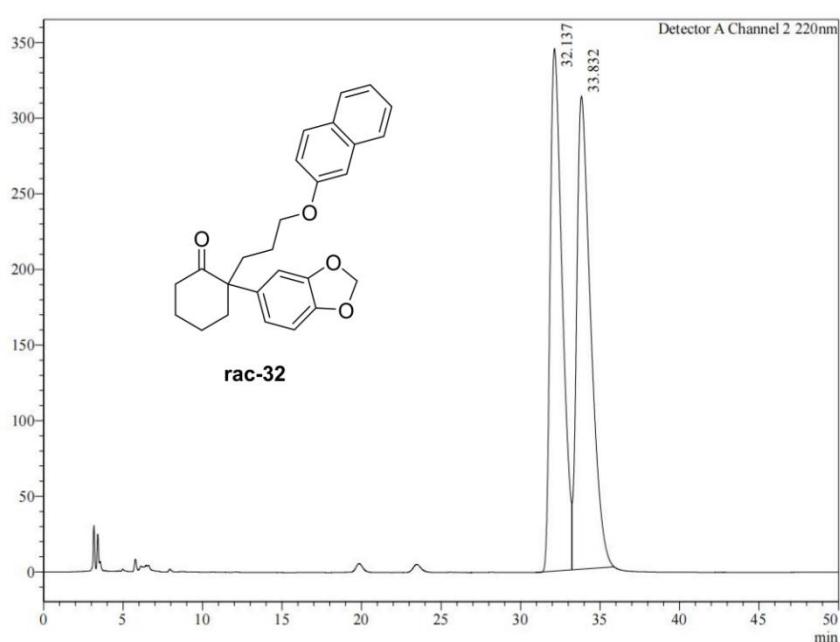


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	11.813	145180	8904	9.904	10.777
2	12.851	1320652	73717	90.096	89.223
Total		1465831	82621	100.000	100.000

mV

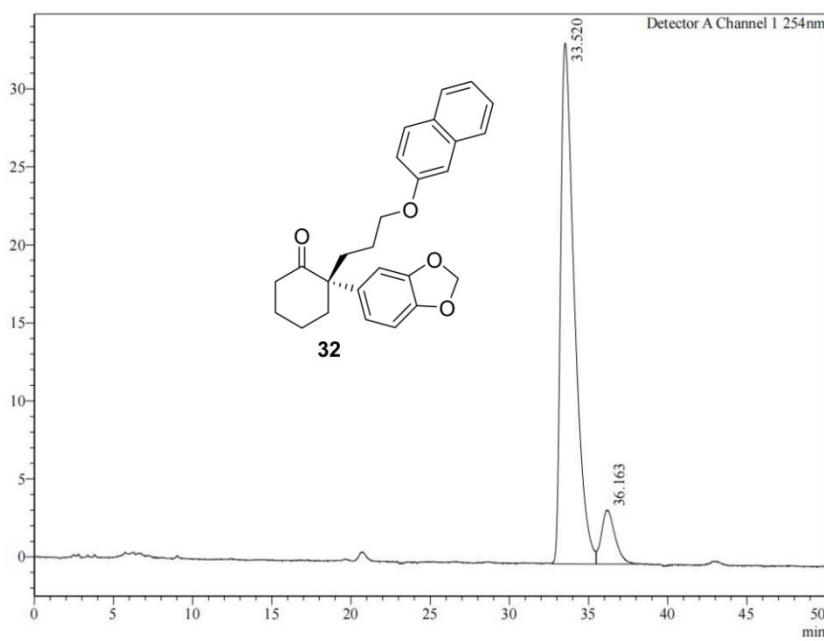


Peak Table

Detector A Channel 2 220nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	32.137	18205195	345296	48.738	52.492
2	33.832	19147727	312514	51.262	47.508
Total		37352922	657810	100.000	100.000

mV

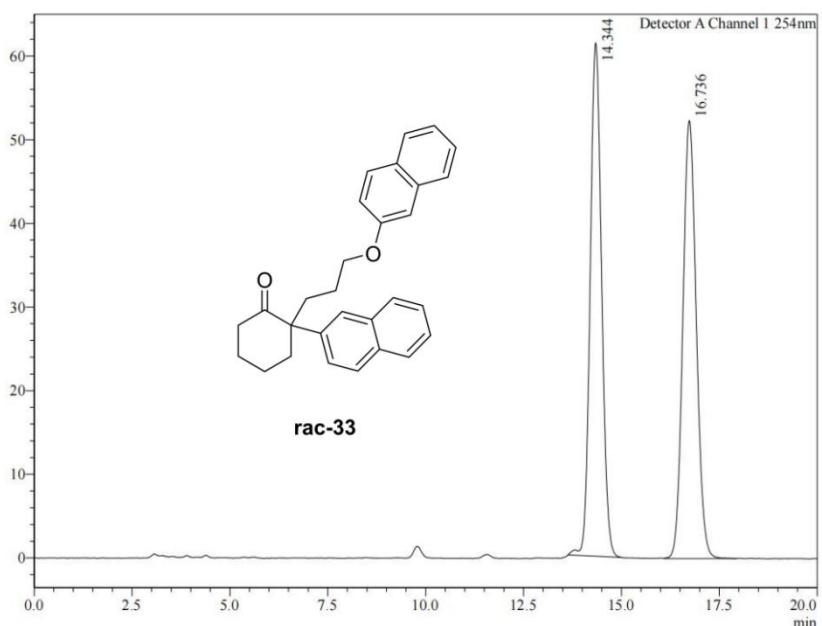


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	33.520	2016733	33378	90.640	90.615
2	36.163	208264	3457	9.360	9.385
Total		2224997	36835	100.000	100.000

mV

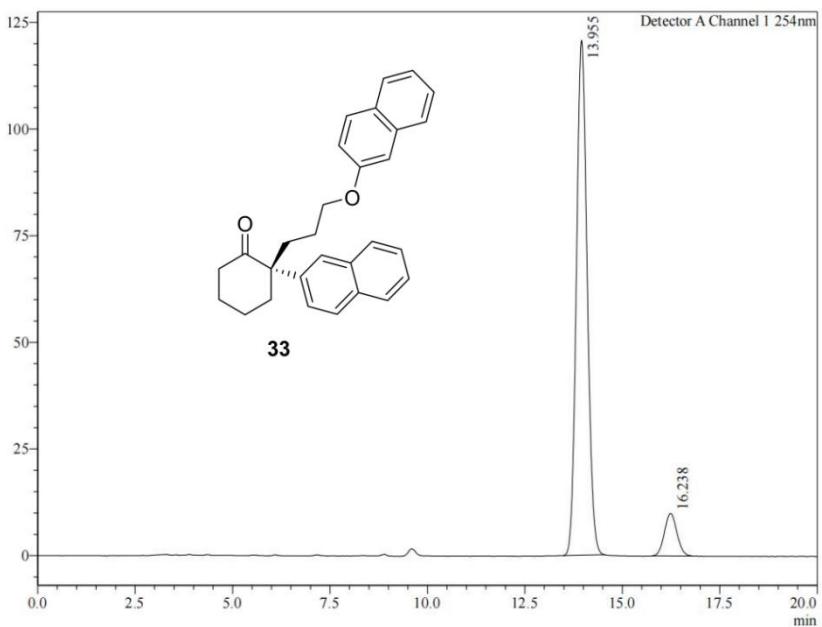


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	14.344	1240225	61333	49.833	53.960
2	16.736	1248547	52329	50.167	46.040
Total		2488772	113662	100.000	100.000

mV

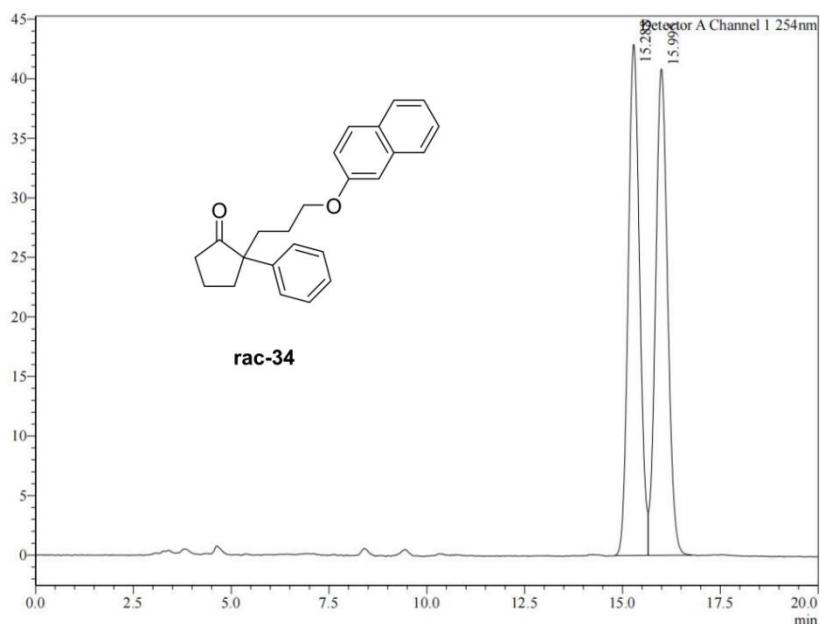


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	13.955	2311781	120602	91.226	92.374
2	16.238	222336	9957	8.774	7.626
Total		2534117	130559	100.000	100.000

mV

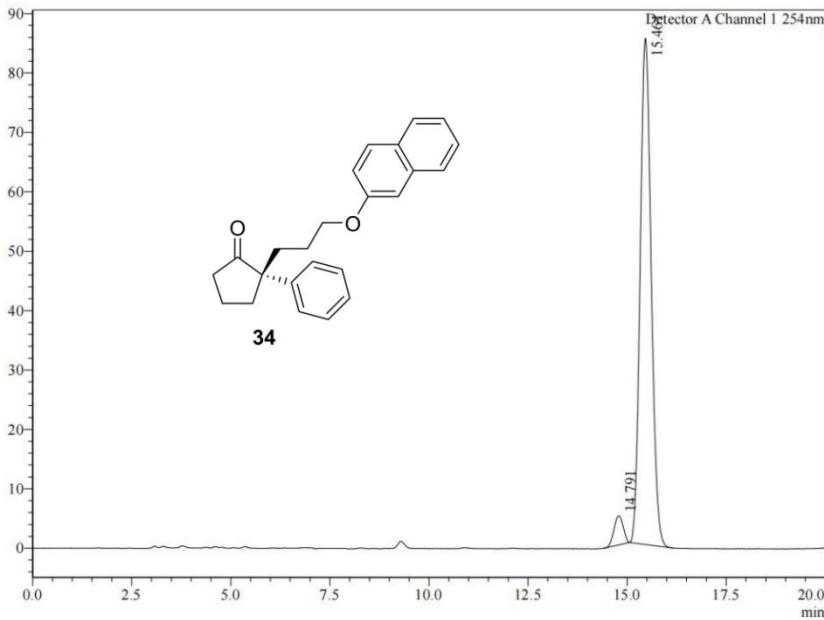


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	15.288	868737	42894	49.860	51.234
2	15.995	873611	40828	50.140	48.766
Total		1742347	83722	100.000	100.000

mV

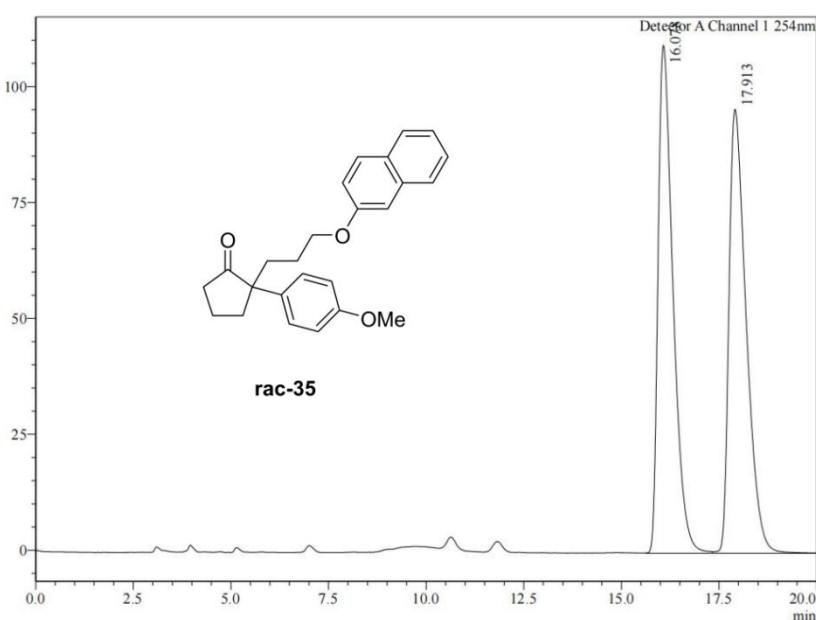


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	14.791	78988	4899	4.582	5.436
2	15.461	1645021	85218	95.418	94.564
Total		1724009	90117	100.000	100.000

mV

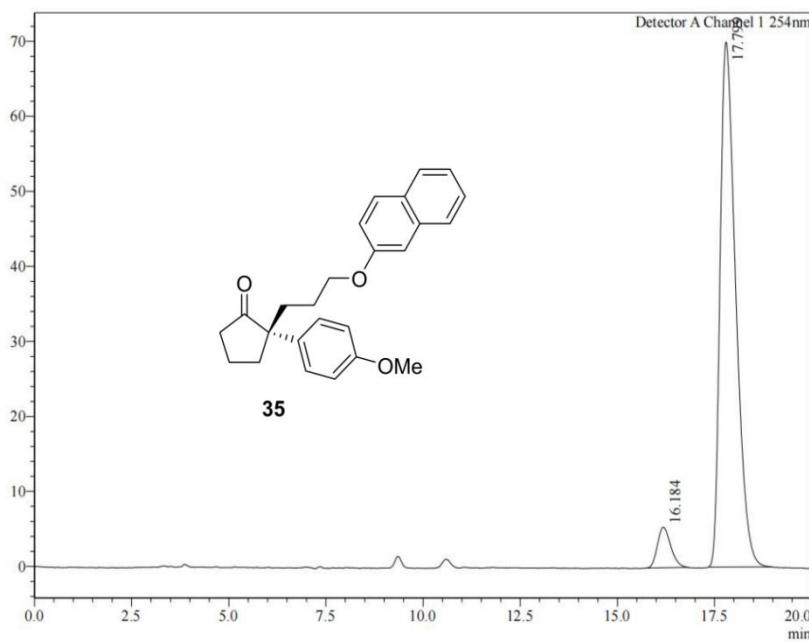


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	16.078	2915462	109543	49.905	53.372
2	17.913	2926522	95700	50.095	46.628
Total		5841985	205243	100.000	100.000

mV

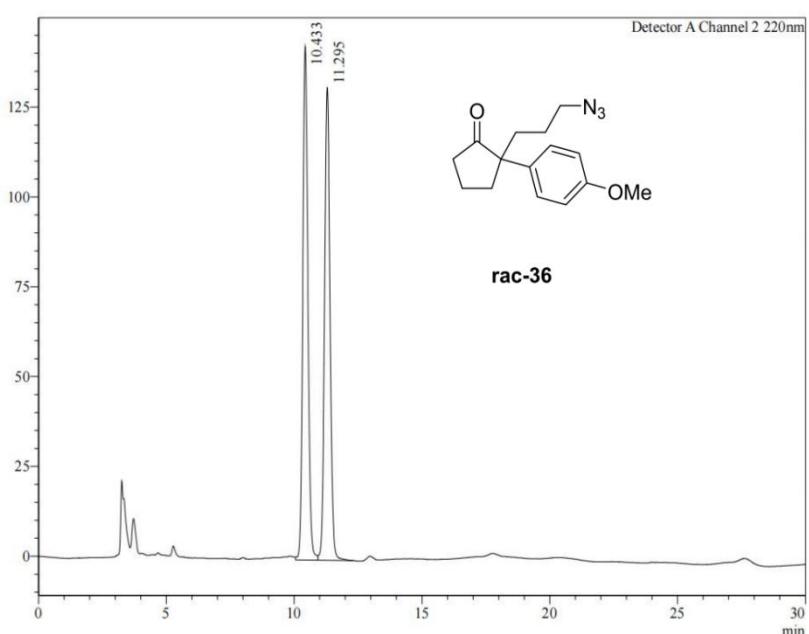


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	16.184	128701	5417	6.177	7.187
2	17.799	1954978	69955	93.823	92.813
Total		2083679	75372	100.000	100.000

mV

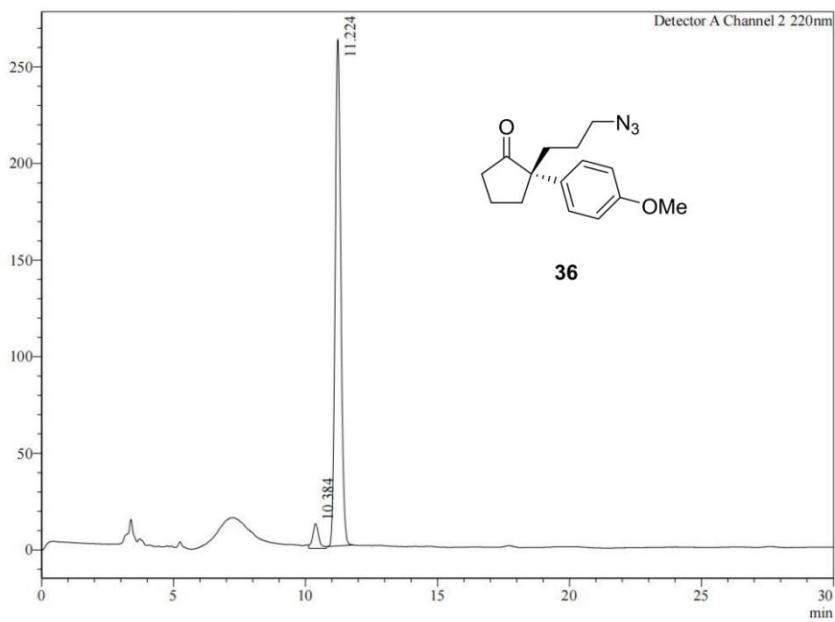


Peak Table

Detector A Channel 2 220nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	10.433	1978337	142860	50.316	52.066
2	11.295	1953521	131523	49.684	47.934
Total		3931859	274383	100.000	100.000

mV

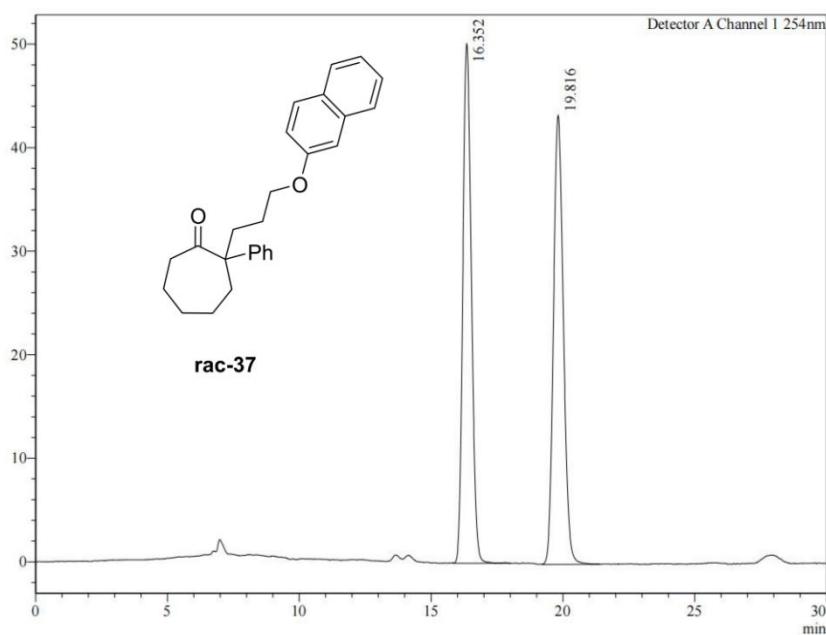


Peak Table

Detector A Channel 2 220nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	10.384	205042	12750	4.976	4.644
2	11.224	3915668	261801	95.024	95.356
Total		4120710	274551	100.000	100.000

mV

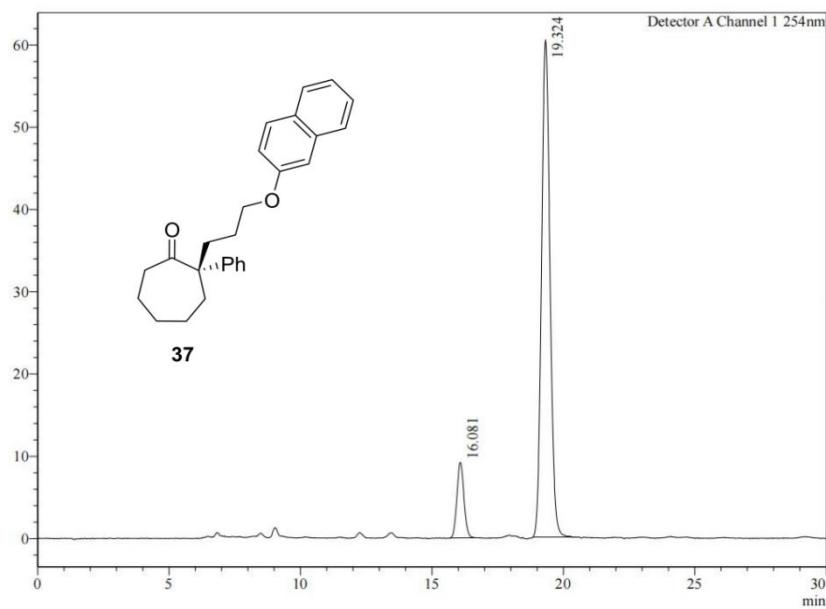


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	16.352	1126031	50175	49.877	53.653
2	19.816	1131604	43343	50.123	46.347
Total		2257635	93519	100.000	100.000

mV

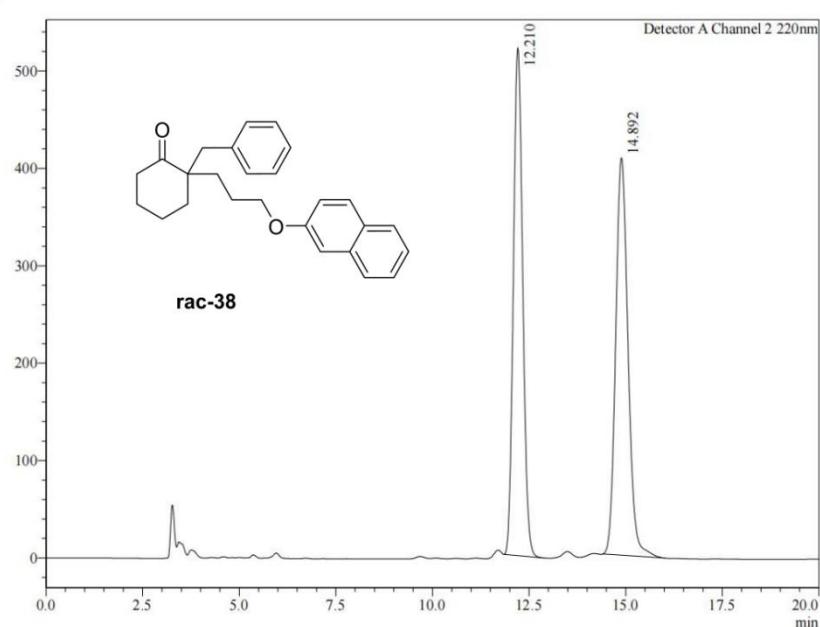


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	16.081	170562	9176	11.209	13.192
2	19.324	1351031	60384	88.791	86.808
Total		1521592	69561	100.000	100.000

mV

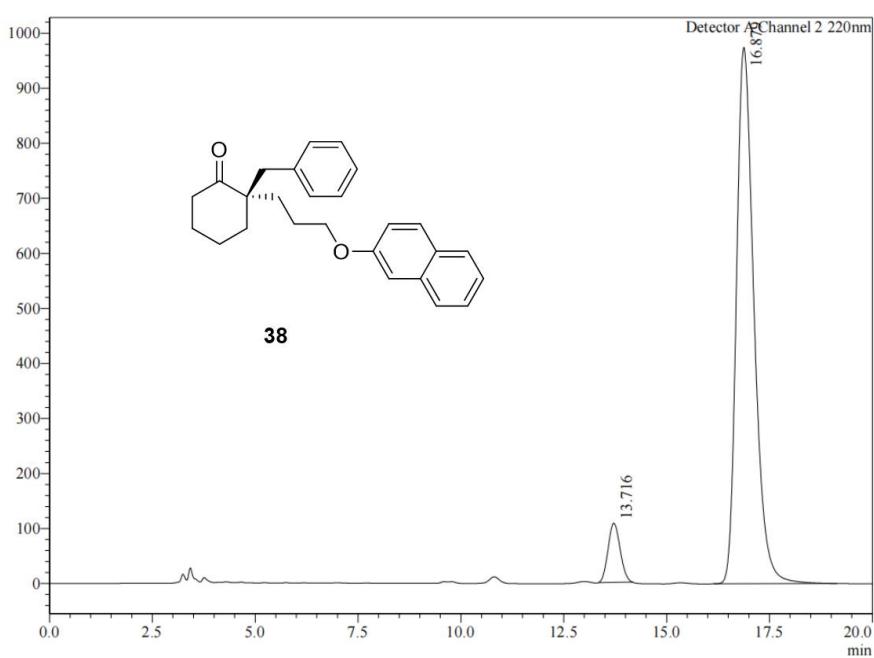


Peak Table

Detector A Channel 2 220nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	12.210	8755537	521017	49.203	56.088
2	14.892	9039353	407906	50.797	43.912
Total		17794891	928923	100.000	100.000

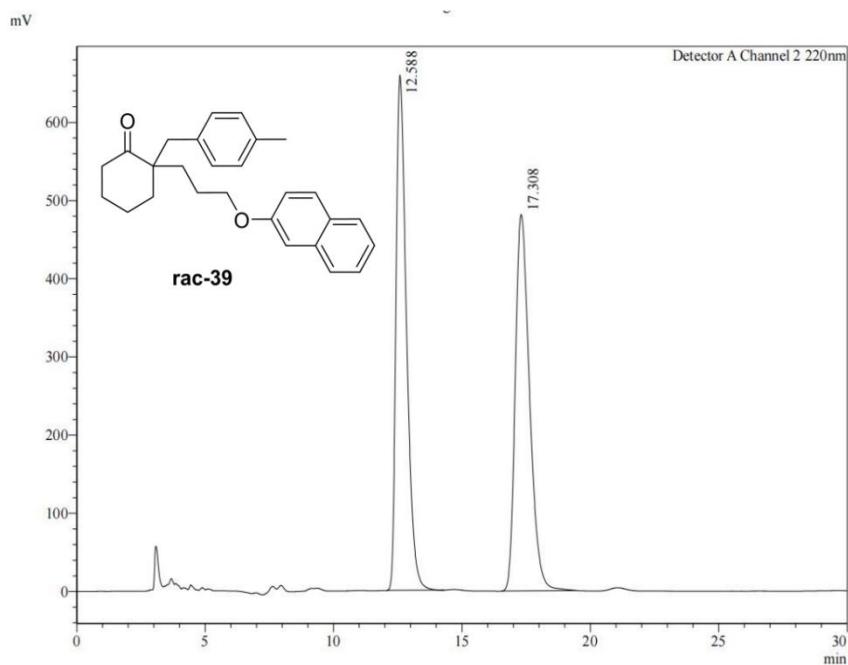
mV



Peak Table

Detector A Channel 2 220nm

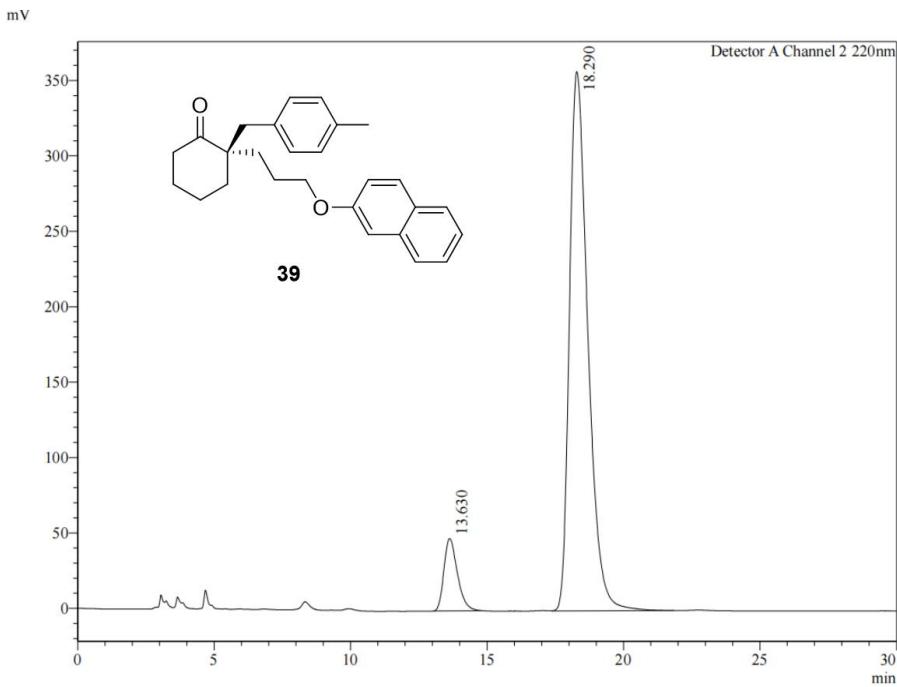
Peak#	Ret. Time	Area	Height	Area%	Height%
1	13.716	2196604	107509	7.069	9.937
2	16.879	28875163	974433	92.931	90.063
Total		31071766	1081941	100.000	100.000



Peak Table

Detector A Channel 2 220nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	12.588	18601778	658744	49.996	57.787
2	17.308	18604690	481203	50.004	42.213
Total		37206468	1139947	100.000	100.000

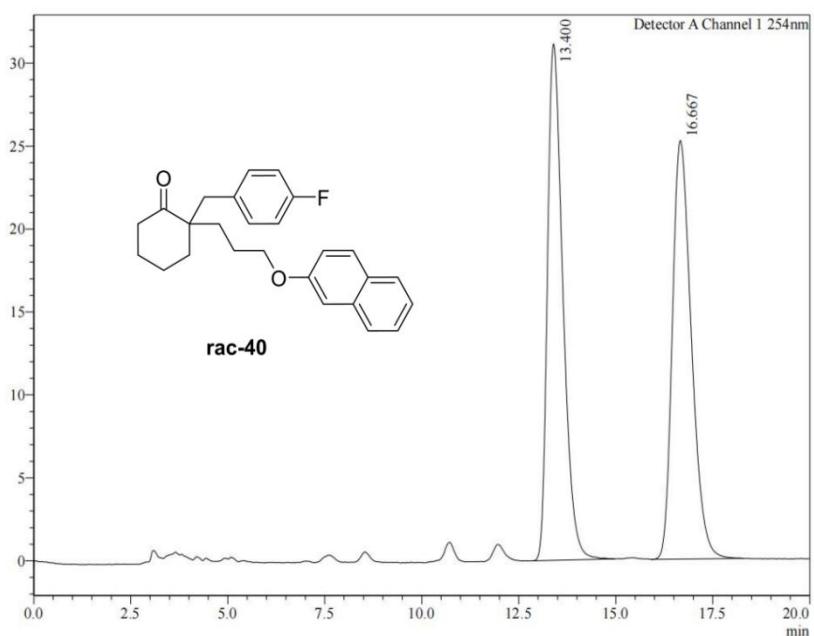


Peak Table

Detector A Channel 2 220nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	13.630	1641326	47865	8.936	11.806
2	18.290	16726442	357551	91.064	88.194
Total		18367768	405416	100.000	100.000

mV

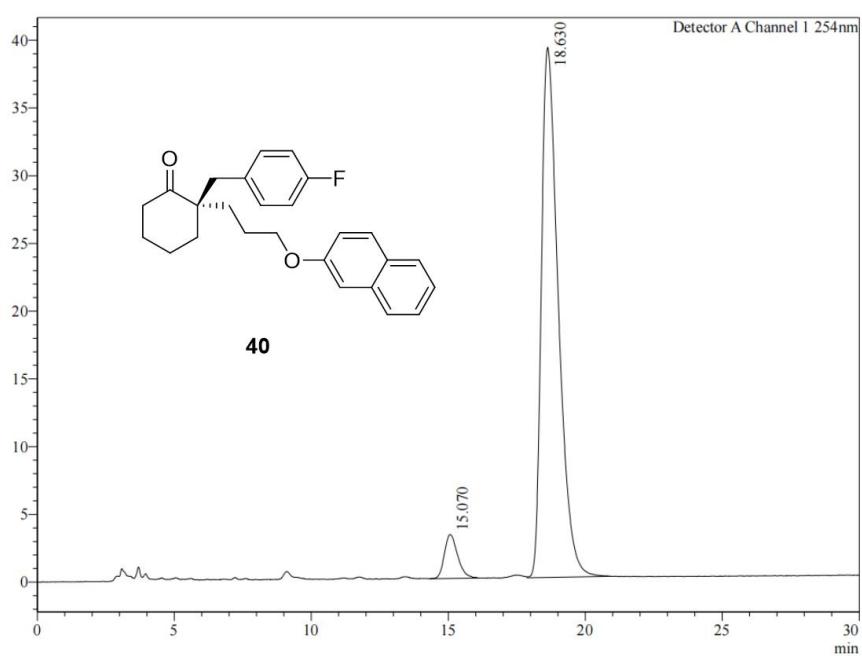


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	13.400	860992	31121	50.027	55.224
2	16.667	860076	25232	49.973	44.776
Total		1721068	56353	100.000	100.000

mV

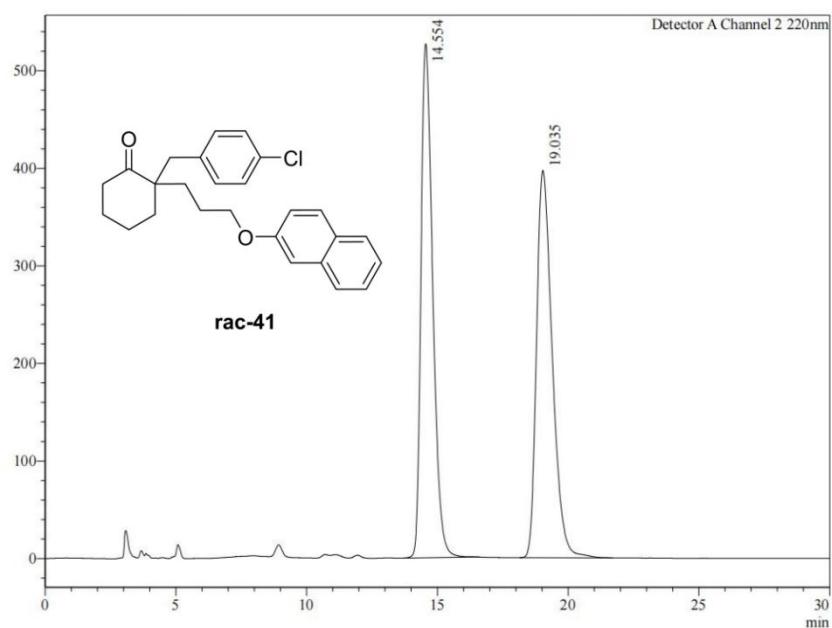


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	15.070	108554	3235	6.072	7.637
2	18.630	1679337	39118	93.928	92.363
Total		1787891	42352	100.000	100.000

mV

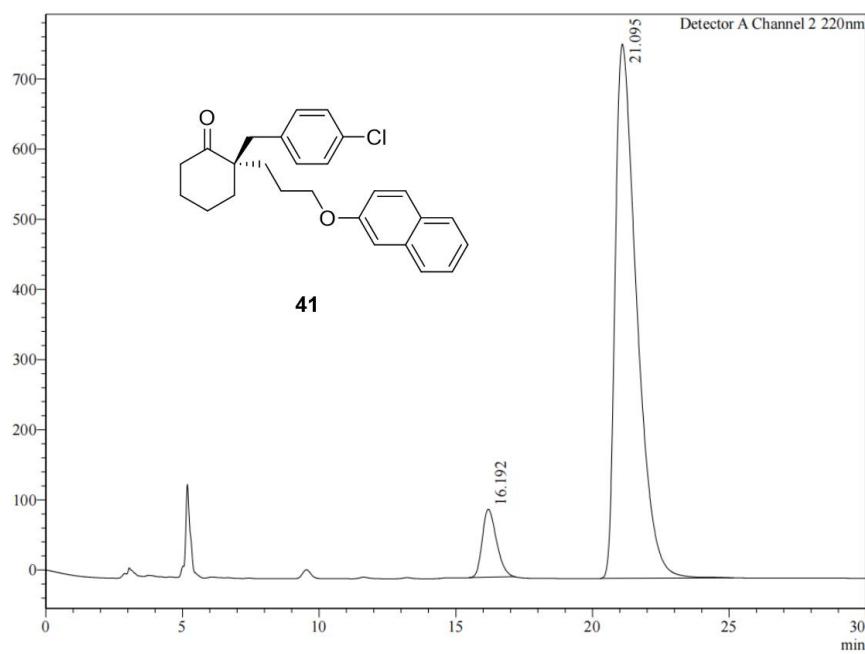


Peak Table

Detector A Channel 2 220nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	14.554	16440574	526674	49.826	57.019
2	19.035	16555278	397015	50.174	42.981
Total		32995852	923688	100.000	100.000

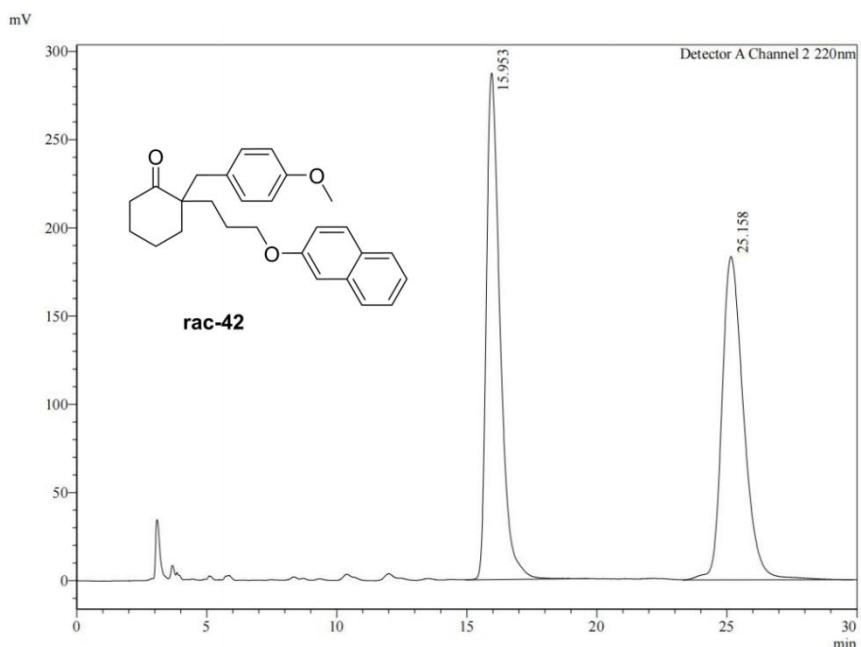
mV



Peak Table

Detector A Channel 2 220nm

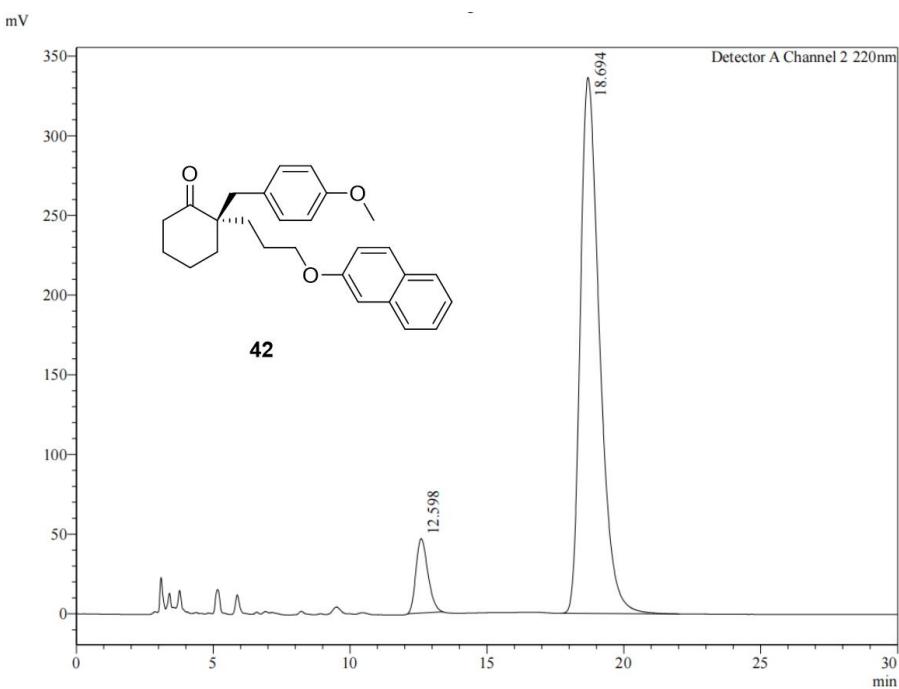
Peak#	Ret. Time	Area	Height	Area%	Height%
1	16.192	3516013	97082	7.784	11.306
2	21.095	41650892	761560	92.216	88.694
Total		45166905	858642	100.000	100.000



Peak Table

Detector A Channel 2 220nm

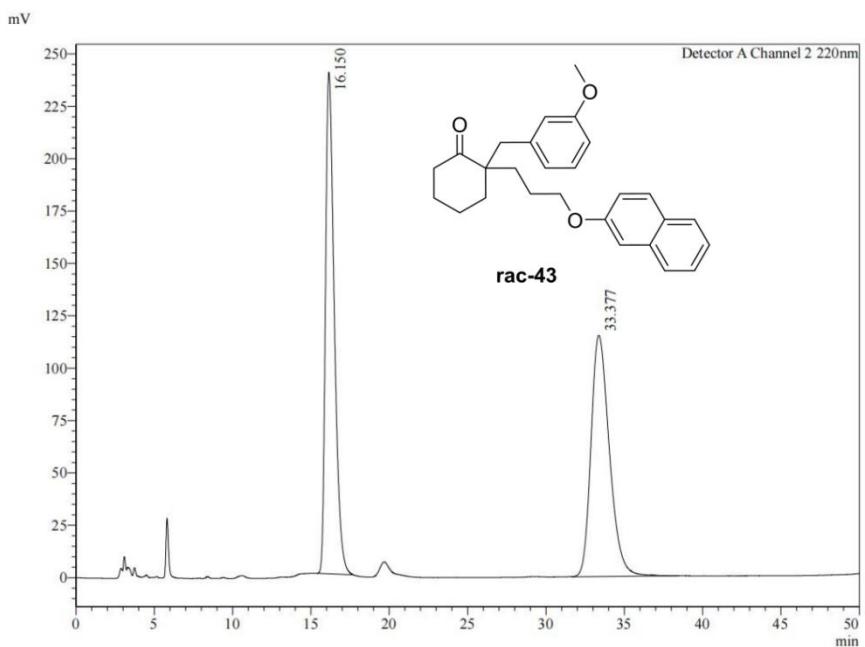
Peak#	Ret. Time	Area	Height	Area%	Height%
1	15.953	10563534	286996	49.861	61.036
2	25.158	10622287	183209	50.139	38.964
Total		21185821	470205	100.000	100.000



Peak Table

Detector A Channel 2 220nm

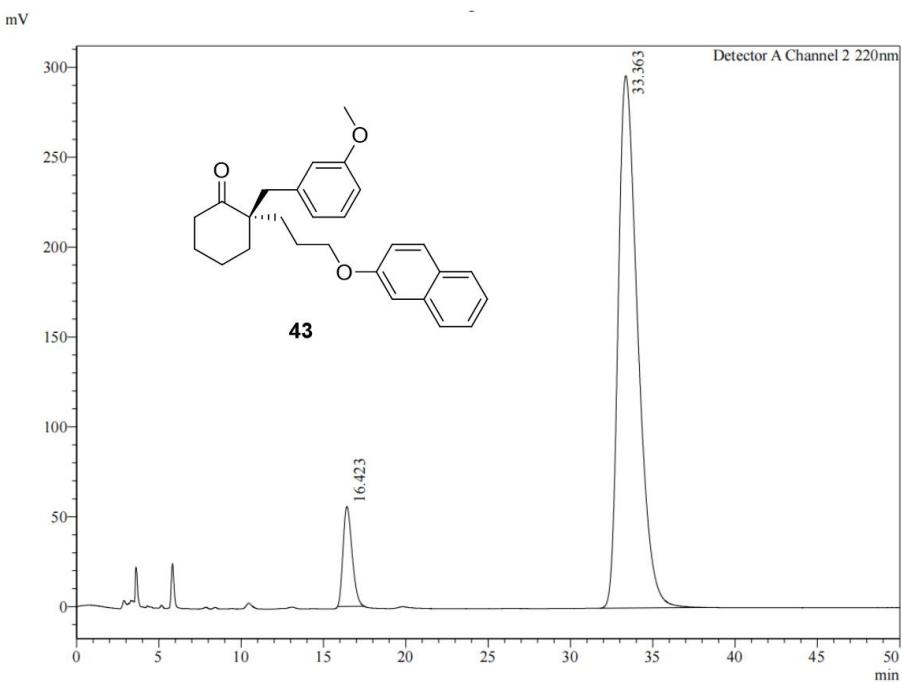
Peak#	Ret. Time	Area	Height	Area%	Height%
1	12.598	1420861	46751	7.958	12.204
2	18.694	16434393	336340	92.042	87.796
Total		17855254	383091	100.000	100.000



Peak Table

Detector A Channel 2 220nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	16.150	9345611	239319	49.879	67.503
2	33.377	9390785	115210	50.121	32.497
Total		18736396	354529	100.000	100.000

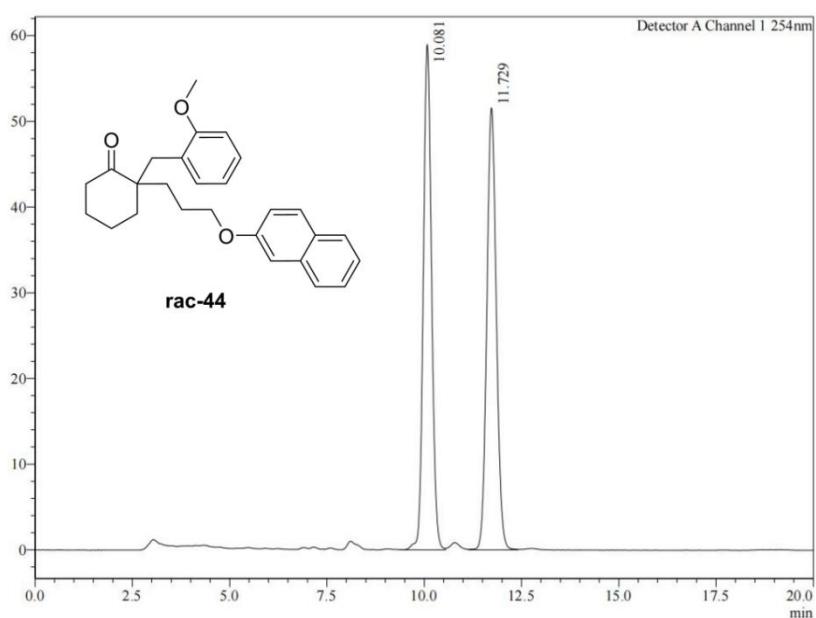


Peak Table

Detector A Channel 2 220nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	16.423	2125252	55571	7.993	15.802
2	33.363	24463072	296098	92.007	84.198
Total		26588324	351669	100.000	100.000

mV

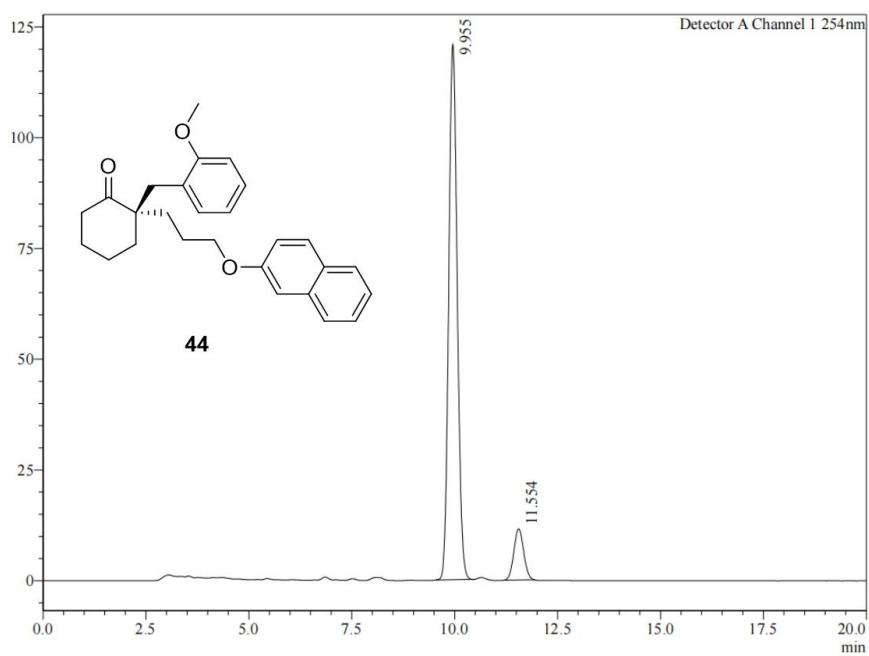


Peak Table

Detector A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	10.081	872038	58934	49.813	53.338
2	11.729	878573	51558	50.187	46.662
Total		1750612	110491	100.000	100.000

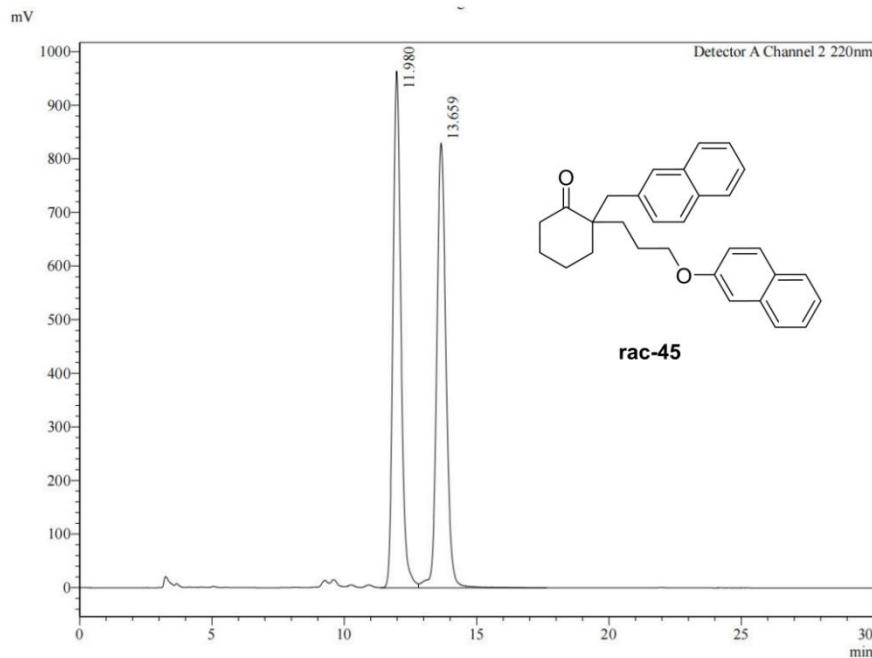
mV



Peak Table

Detector A Channel 1 254nm

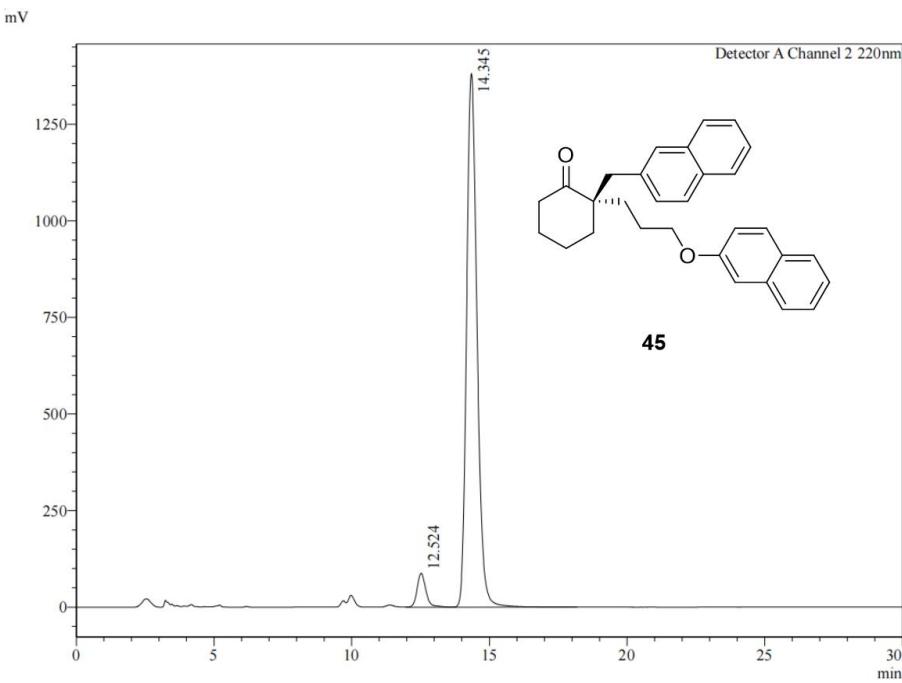
Peak#	Ret. Time	Area	Height	Area%	Height%
1	9.955	1735429	120807	90.004	91.248
2	11.554	192732	11586	9.996	8.752
Total		1928161	132393	100.000	100.000



Peak Table

Detector A Channel 2 220nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	11.980	20122448	963439	49.890	53.752
2	13.659	20211564	828931	50.110	46.248
Total		40334012	1792370	100.000	100.000

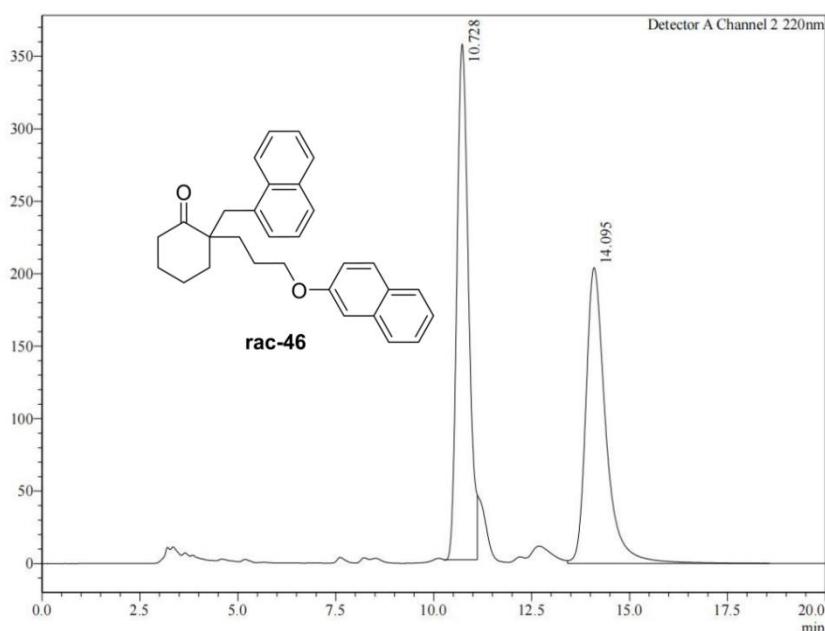


Peak Table

Detector A Channel 2 220nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	12.524	1953930	87557	5.108	5.963
2	14.345	36301782	1380702	94.892	94.037
Total		38255712	1468260	100.000	100.000

mV

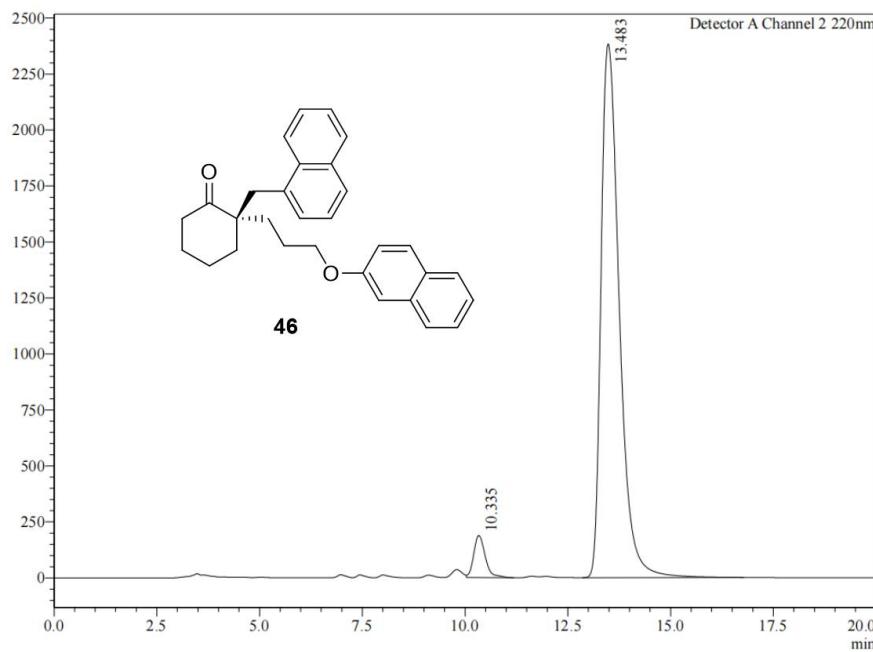


Peak Table

Detector A Channel 2 220nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	10.728	7336271	355676	50.571	63.544
2	14.095	7170549	204060	49.429	36.456
Total		14506820	559736	100.000	100.000

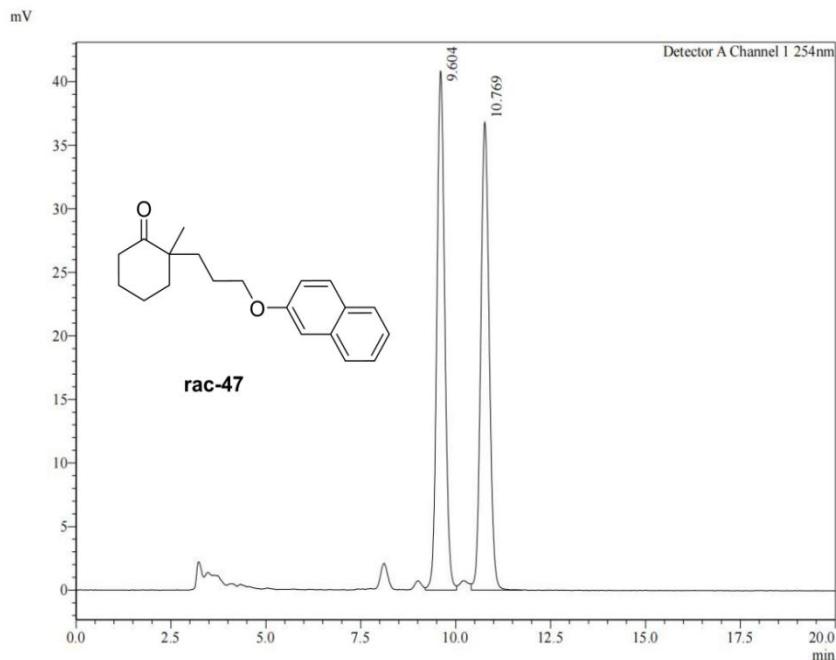
mV



Peak Table

Detector A Channel 2 220nm

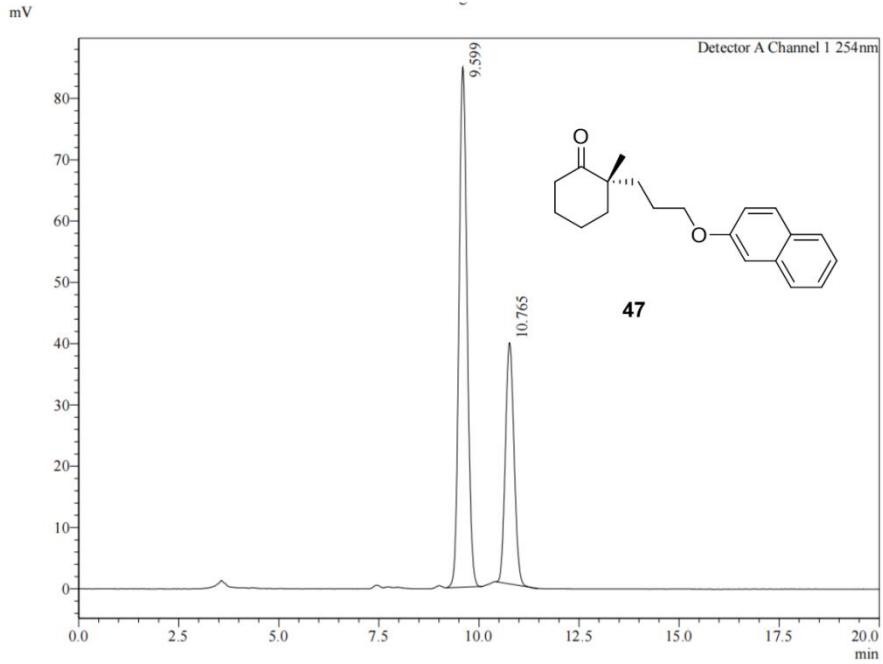
Peak#	Ret. Time	Area	Height	Area%	Height%
1	10.335	3684741	188194	4.776	7.319
2	13.483	73463315	2383213	95.224	92.681
Total		77148056	2571407	100.000	100.000



Peak Table

Detector A Channel 1 254nm

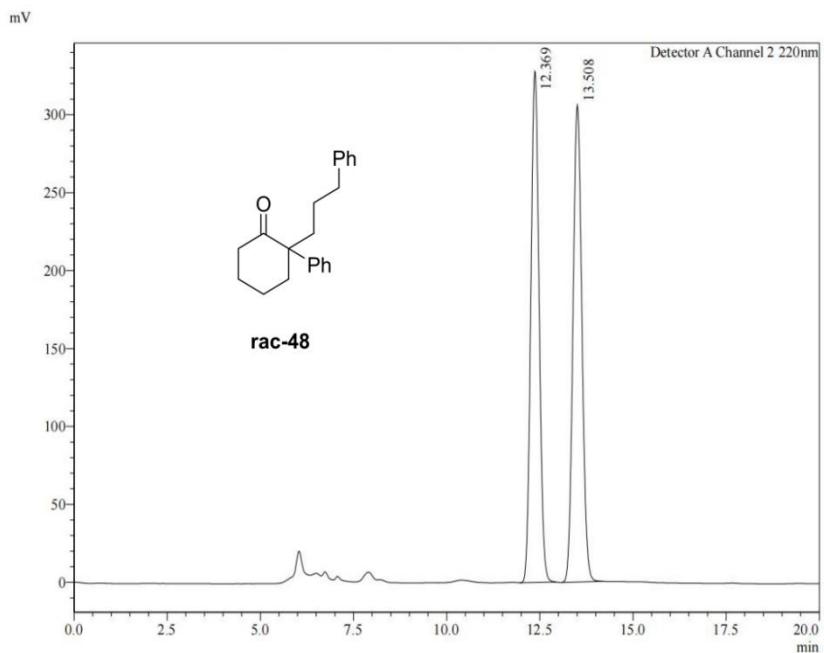
Peak#	Ret. Time	Area	Height	Area%	Height%
1	9.604	594029	40822	50.950	52.595
2	10.769	571870	36794	49.050	47.405
Total		1165899	77616	100.000	100.000



Peak Table

Detector A Channel 1 254nm

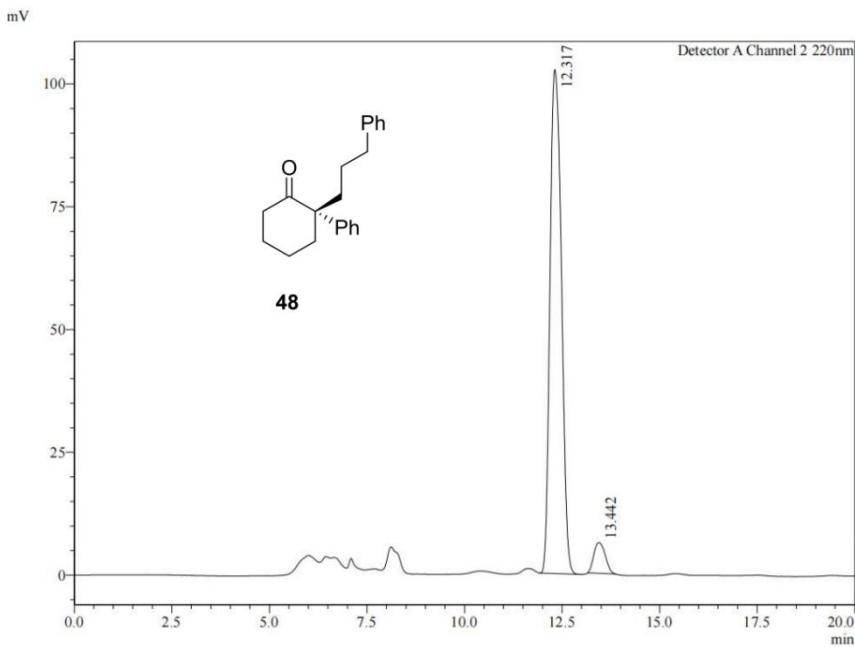
Peak#	Ret. Time	Area	Height	Area%	Height%
1	9.599	1200918	84808	67.032	68.301
2	10.765	590631	39360	32.968	31.699
Total		1791549	124167	100.000	100.000



Peak Table

Detector A Channel 2 220nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	12.369	5075307	327696	49.904	51.718
2	13.508	5094804	305919	50.096	48.282
Total		10170111	633615	100.000	100.000

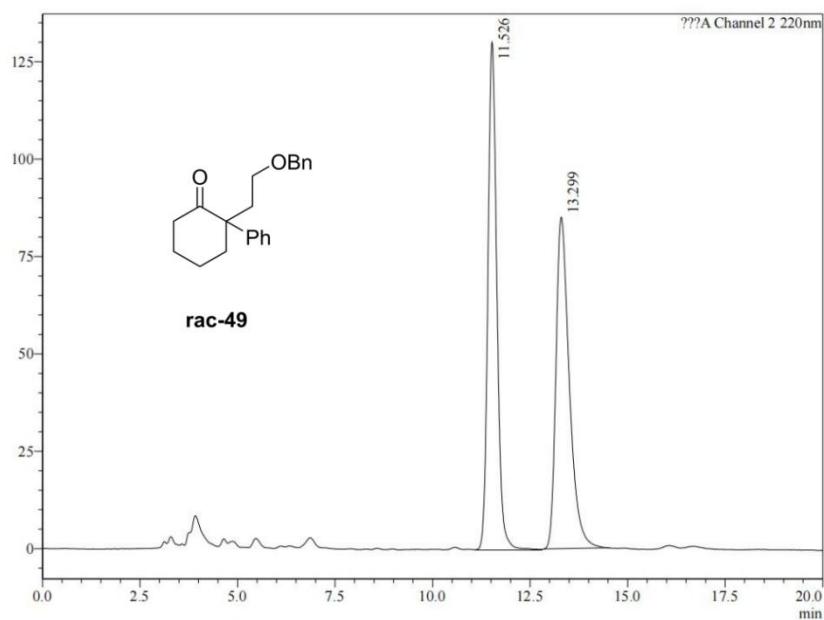


Peak Table

Detector A Channel 2 220nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	12.317	2080074	102596	94.217	94.239
2	13.442	127673	6272	5.783	5.761
Total		2207748	108869	100.000	100.000

mV

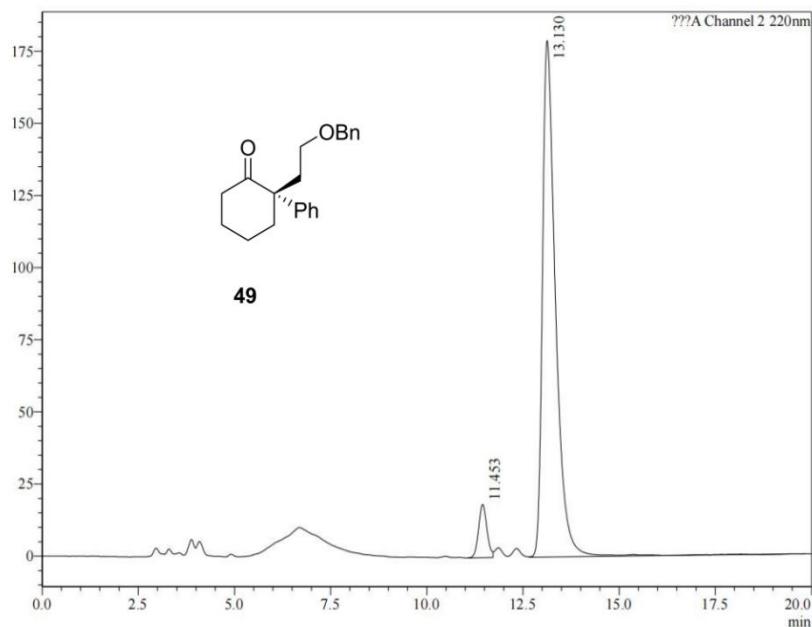


Peak Table

??A Channel 2 220nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	11.526	2084832	130353	50.657	60.483
2	13.299	2030753	85166	49.343	39.517
Total		4115586	215519	100.000	100.000

mV

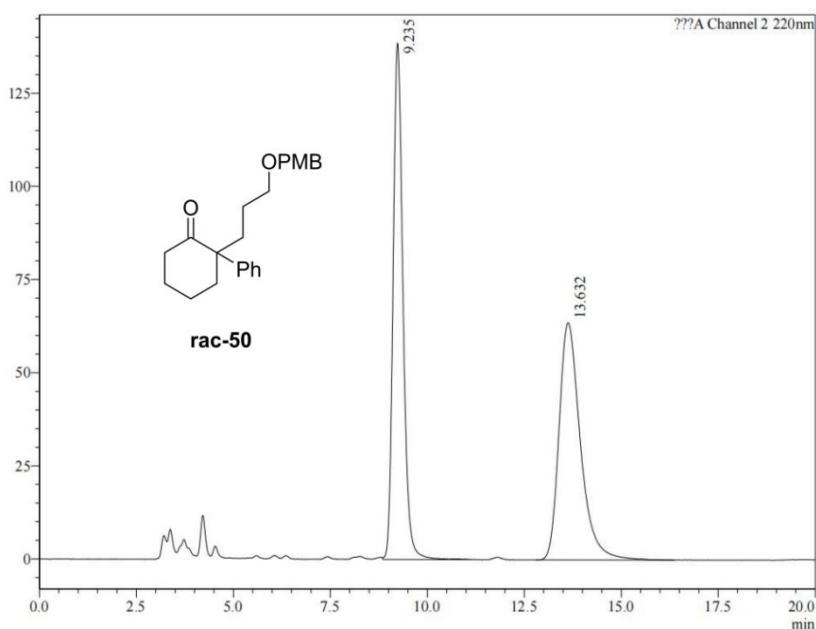


Peak Table

??A Channel 2 220nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	11.453	280204	18454	6.219	9.350
2	13.130	4225726	178915	93.781	90.650
Total		4505930	197368	100.000	100.000

mV

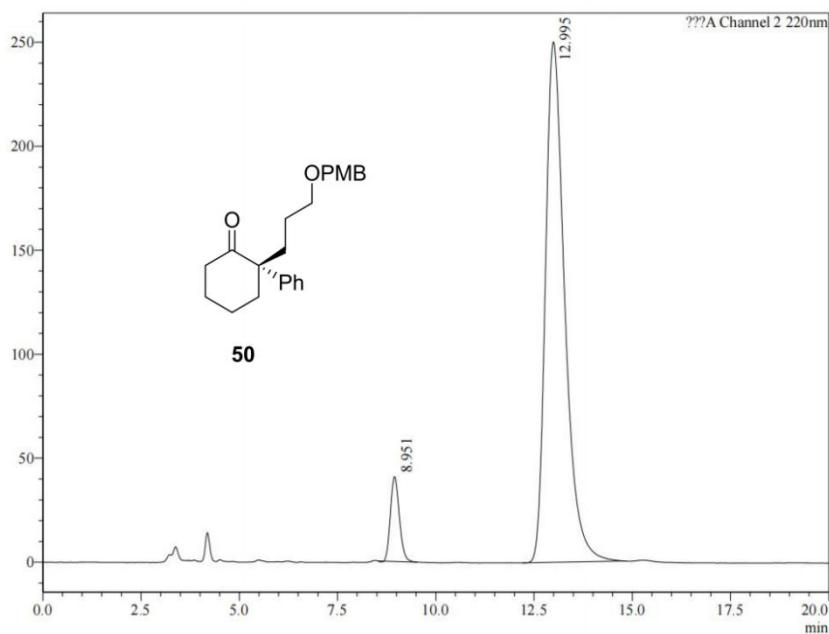


Peak Table

??A Channel 2 220nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	9.235	2454487	138436	50.143	68.499
2	13.632	2440458	63663	49.857	31.501
Total		4894946	202099	100.000	100.000

mV

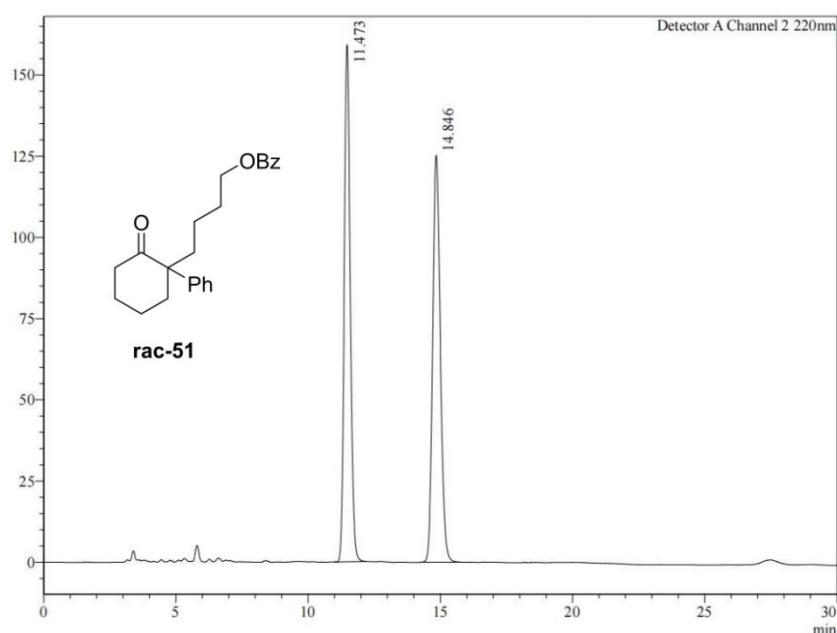


Peak Table

??A Channel 2 220nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	8.951	644289	40770	7.042	14.013
2	12.995	8504692	250170	92.958	85.987
Total		9148981	290940	100.000	100.000

mV

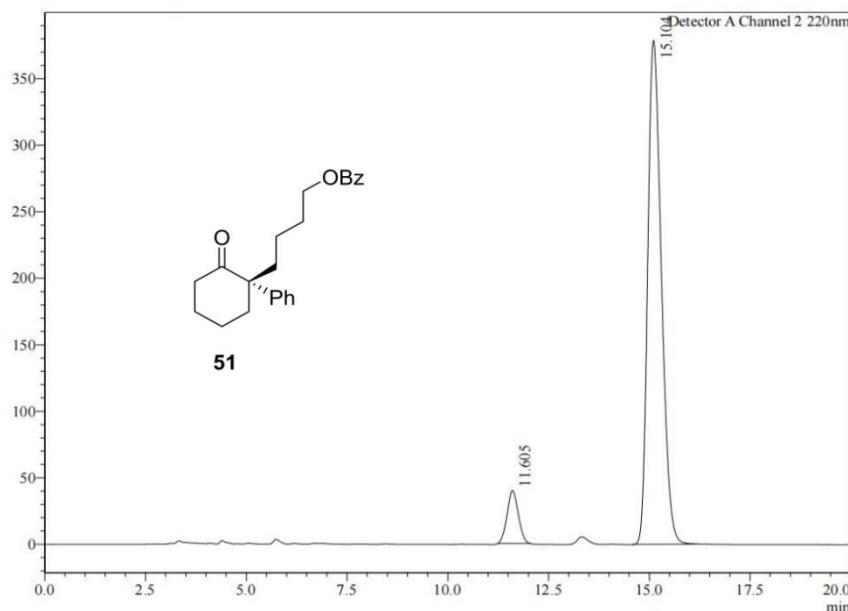


Peak Table

Detector A Channel 2 220nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	11.473	2508191	158948	49.847	55.929
2	14.846	2523564	125246	50.153	44.071
Total		5031754	284195	100.000	100.000

mV

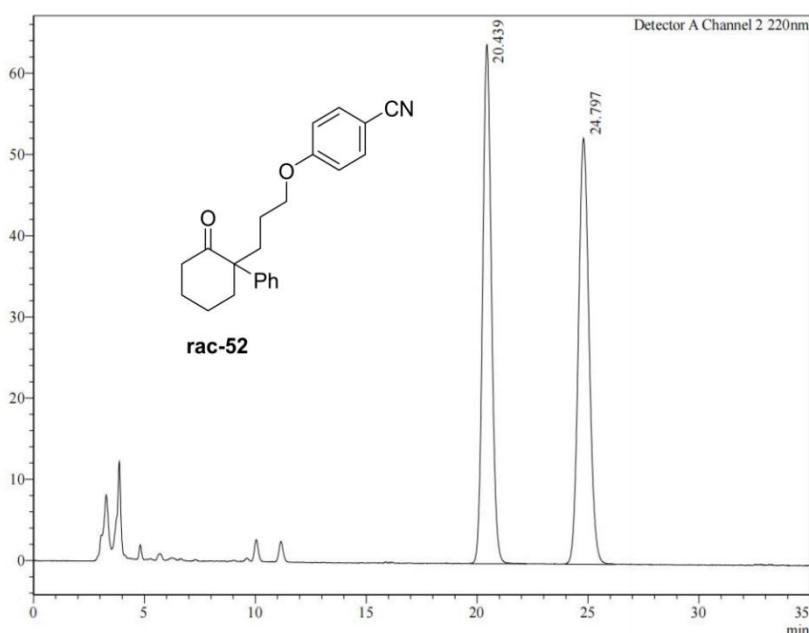


Peak Table

Detector A Channel 2 220nm

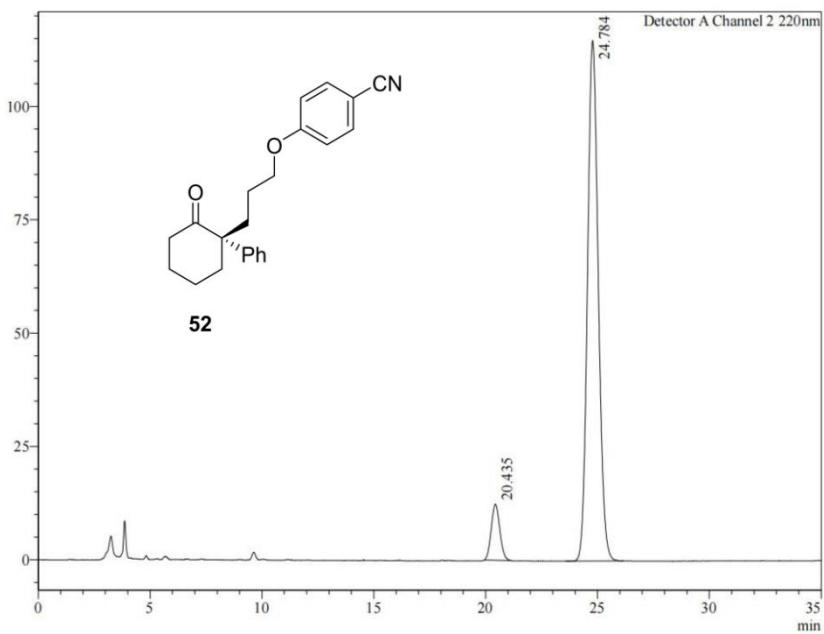
Peak#	Ret. Time	Area	Height	Area%	Height%
1	11.605	768445	39735	7.942	9.494
2	15.104	8906851	378783	92.058	90.506
Total		9675296	418518	100.000	100.000

mV

**Detector A Channel 2 220nm**

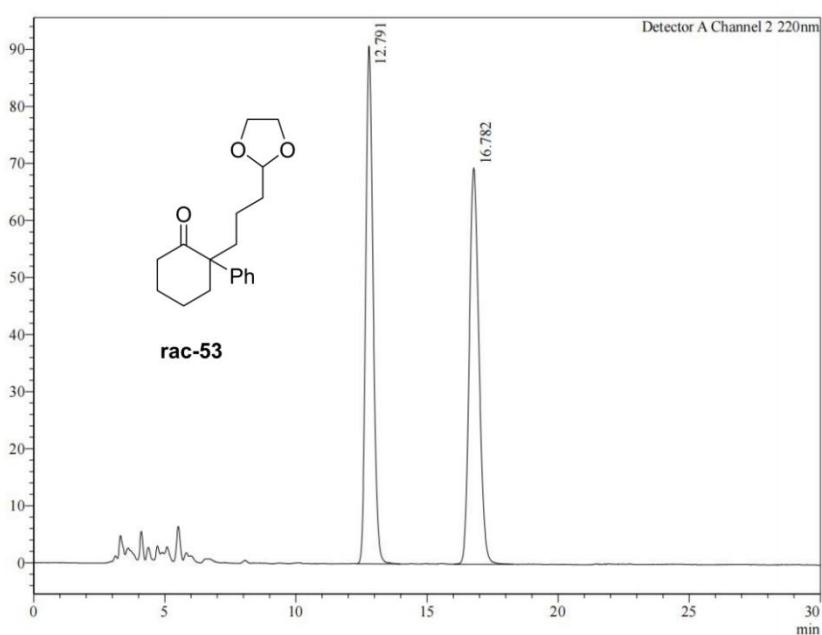
Peak#	Ret. Time	Area	Height	Area%	Height%
1	20.439	1750676	63910	50.049	54.946
2	24.797	1747281	52404	49.951	45.054
Total		3497957	116313	100.000	100.000

mV

**Detector A Channel 2 220nm**

Peak#	Ret. Time	Area	Height	Area%	Height%
1	20.435	330362	12386	7.935	9.739
2	24.784	3832923	114787	92.065	90.261
Total		4163285	127173	100.000	100.000

mV

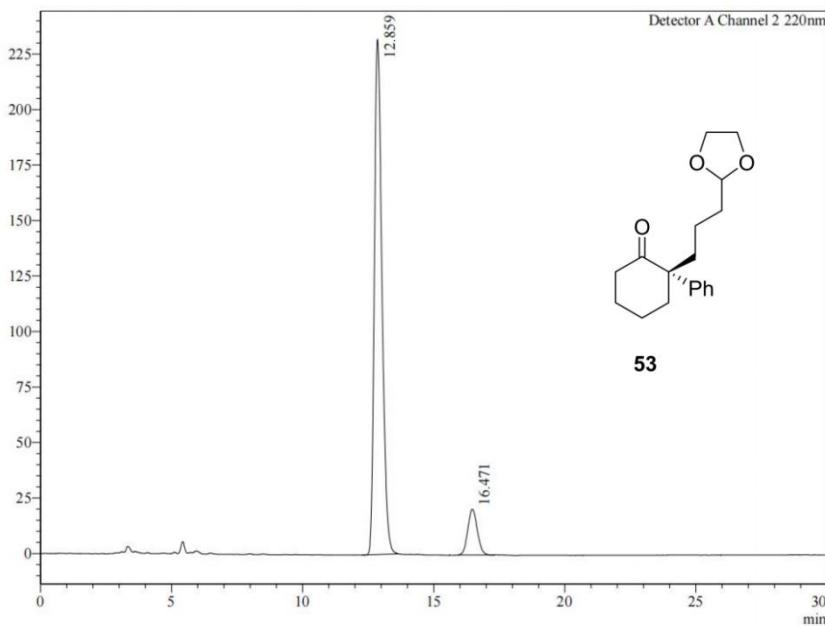


Peak Table

Detector A Channel 2 220nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	12.791	1777775	90701	49.883	56.639
2	16.782	1786122	69438	50.117	43.361
Total		3563898	160138	100.000	100.000

mV

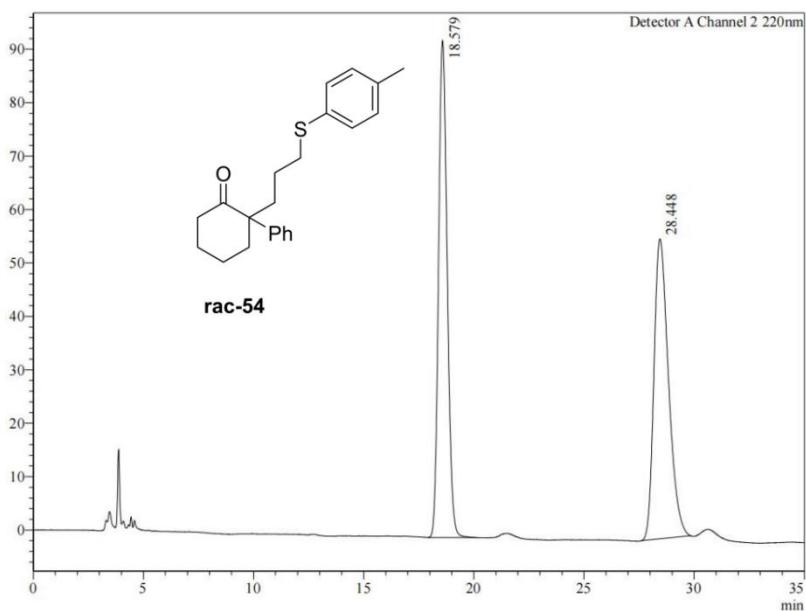


Peak Table

Detector A Channel 2 220nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	12.859	4683870	231847	90.028	91.835
2	16.471	518796	20613	9.972	8.165
Total		5202666	252460	100.000	100.000

mV

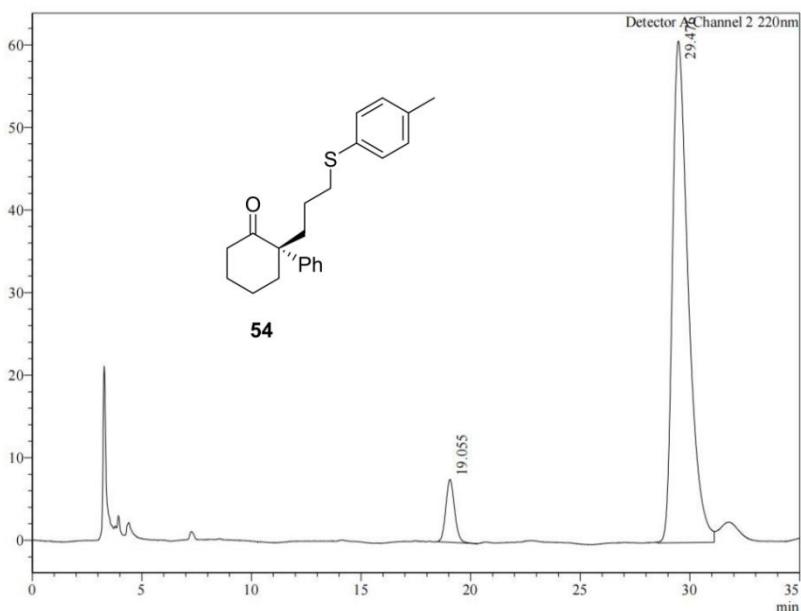


Peak Table

Detector A Channel 2 220nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	18.579	2548561	92963	49.818	62.346
2	28.448	2567151	56144	50.182	37.654
Total		5115713	149107	100.000	100.000

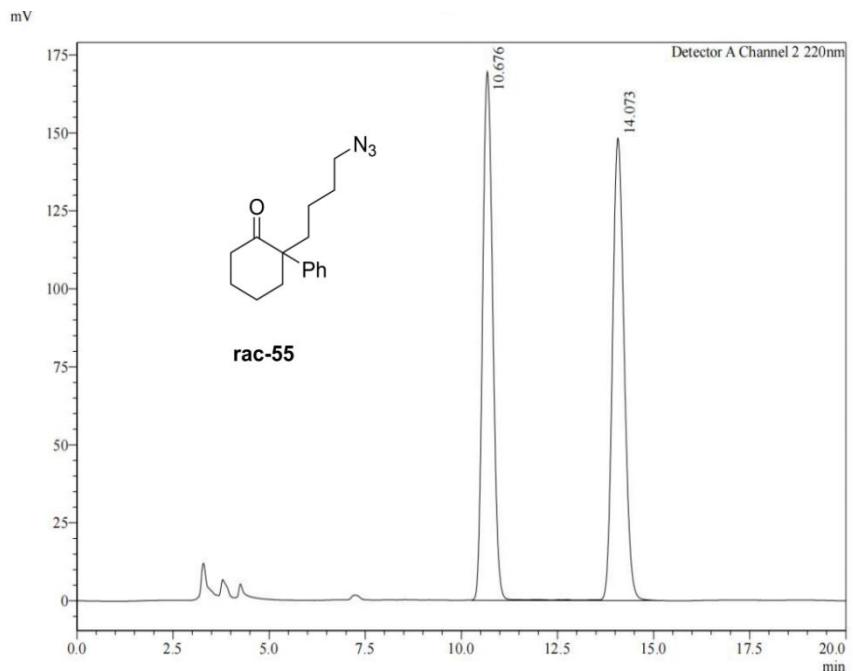
mV



Peak Table

Detector A Channel 2 220nm

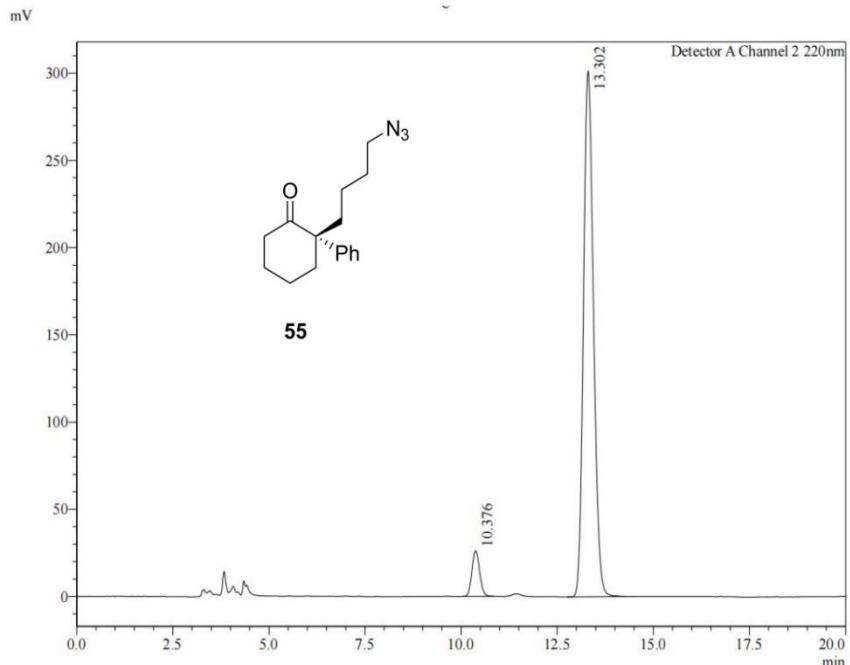
Peak#	Ret. Time	Area	Height	Area%	Height%
1	19.055	211725	7608	6.448	11.133
2	29.476	3071849	60729	93.552	88.867
Total		3283575	68337	100.000	100.000



Peak Table

Detector A Channel 2 220nm

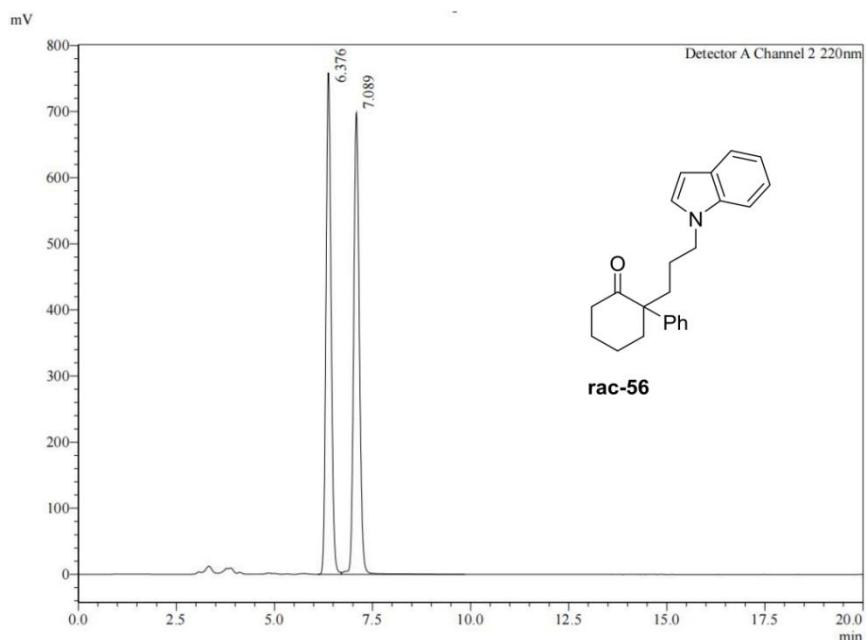
Peak#	Ret. Time	Area	Height	Area%	Height%
1	10.676	3114233	169400	50.040	53.340
2	14.073	3109282	148182	49.960	46.660
Total		6223515	317582	100.000	100.000



Peak Table

Detector A Channel 2 220nm

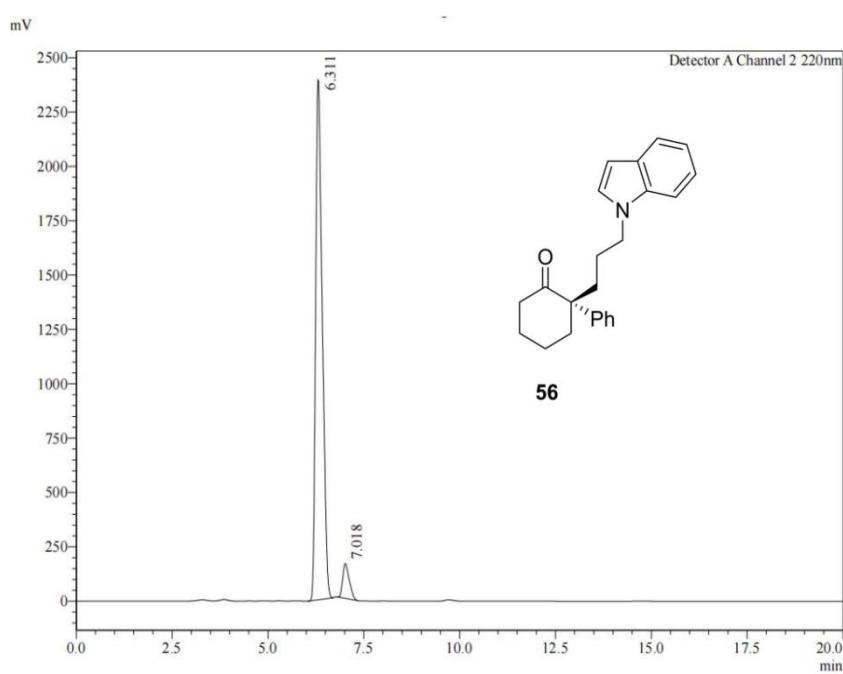
Peak#	Ret. Time	Area	Height	Area%	Height%
1	10.376	362862	26083	6.228	7.967
2	13.302	5463675	301305	93.772	92.033
Total		5826538	327388	100.000	100.000



Peak Table

Detector A Channel 2 220nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	6.376	6893415	758931	49.510	52.076
2	7.089	7029857	698415	50.490	47.924
Total		13923272	1457346	100.000	100.000

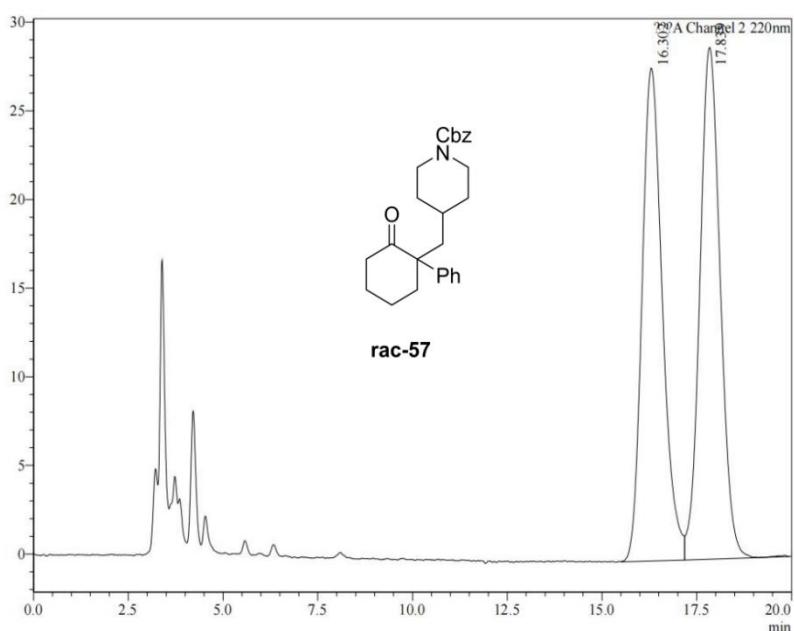


Peak Table

Detector A Channel 2 220nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	6.311	28723769	2390867	93.778	93.717
2	7.018	1905831	160292	6.222	6.283
Total		30629600	2551159	100.000	100.000

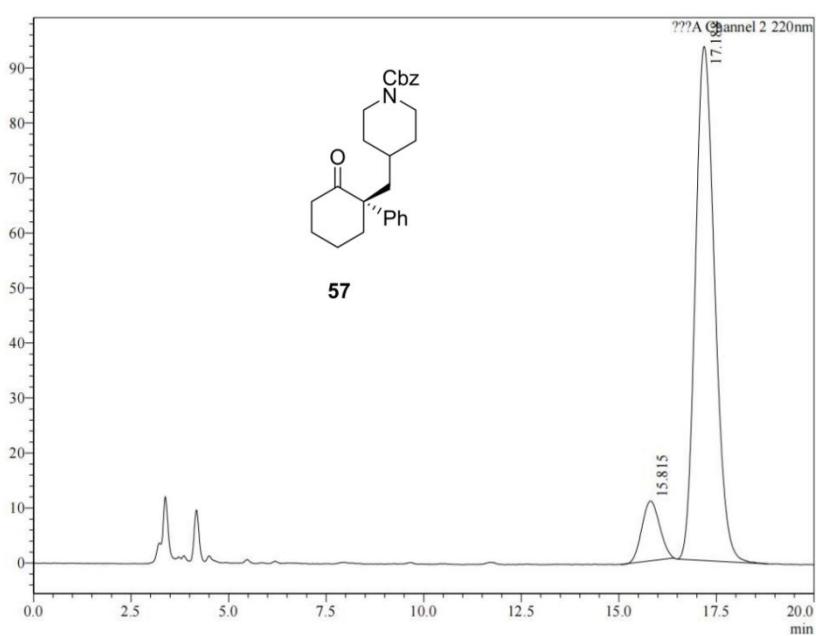
mV



Peak Table

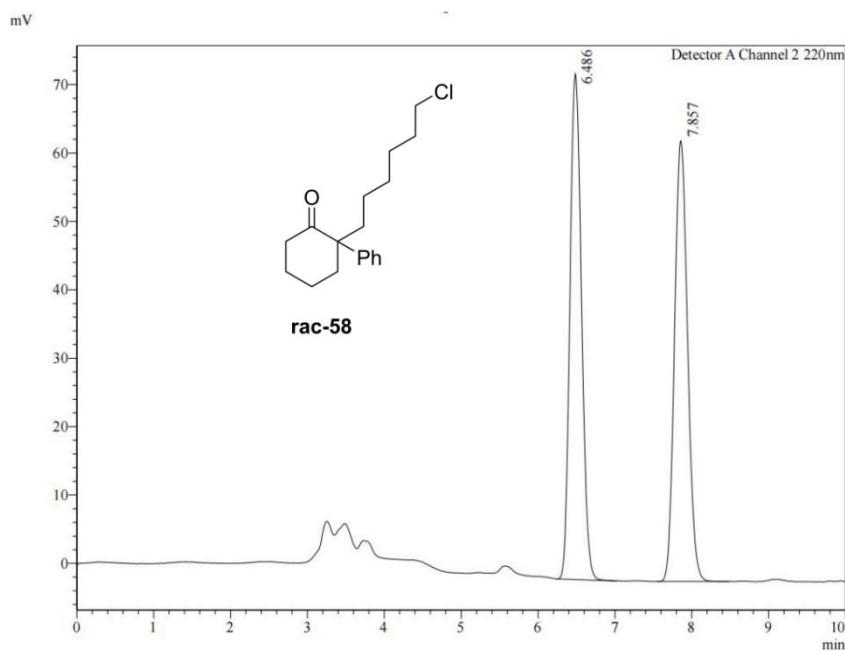
Peak#	Ret. Time	Area	Height	Area%	Height%
1	16.302	1037784	27809	49.054	49.070
2	17.839	1077796	28862	50.946	50.930
Total		2115580	56671	100.000	100.000

mV



Peak Table

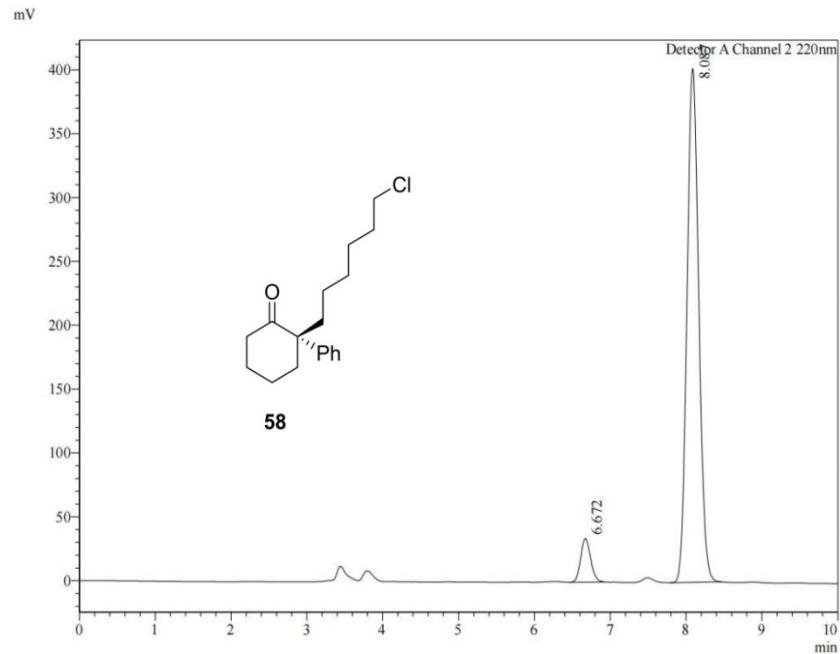
Peak#	Ret. Time	Area	Height	Area%	Height%
1	15.815	343693	10863	9.640	10.417
2	17.188	3221691	93417	90.360	89.583
Total		3565384	104279	100.000	100.000



Peak Table

Detector A Channel 2 220nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	6.486	771435	73913	50.392	53.451
2	7.857	759446	64369	49.608	46.549
Total		1530881	138282	100.000	100.000

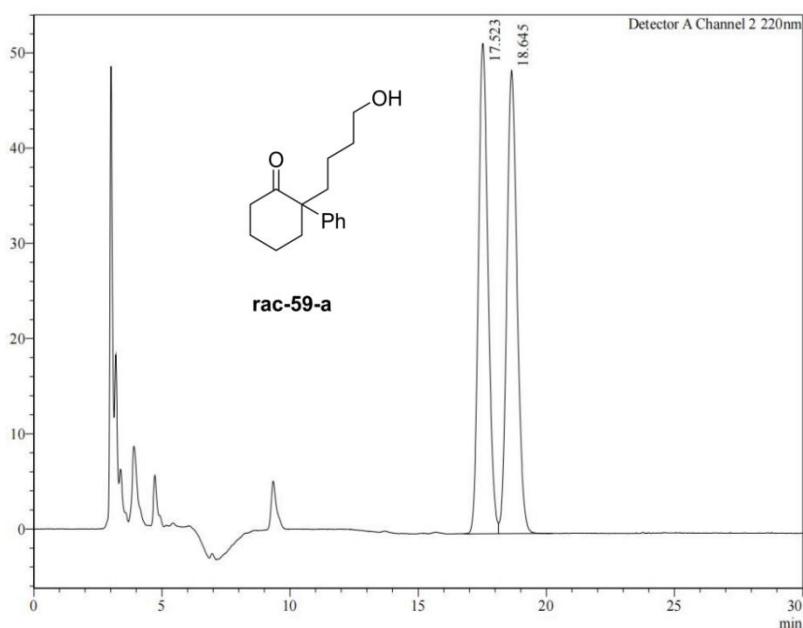


Peak Table

Detector A Channel 2 220nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	6.672	311844	34083	6.719	7.815
2	8.087	4329320	402013	93.281	92.185
Total		4641164	436096	100.000	100.000

mV

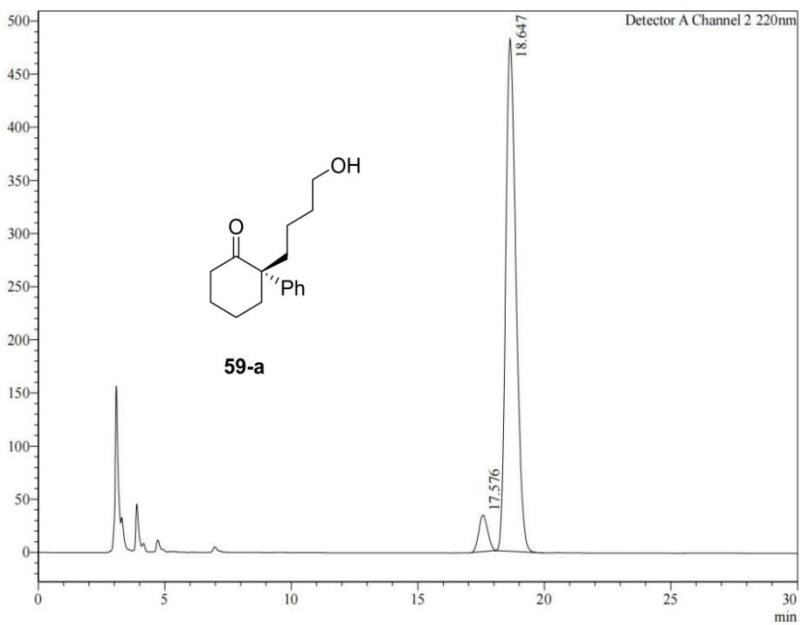


Peak Table

Detector A Channel 2 220nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	17.523	1345967	51498	49.898	51.426
2	18.645	1351472	48641	50.102	48.574
Total		2697439	100139	100.000	100.000

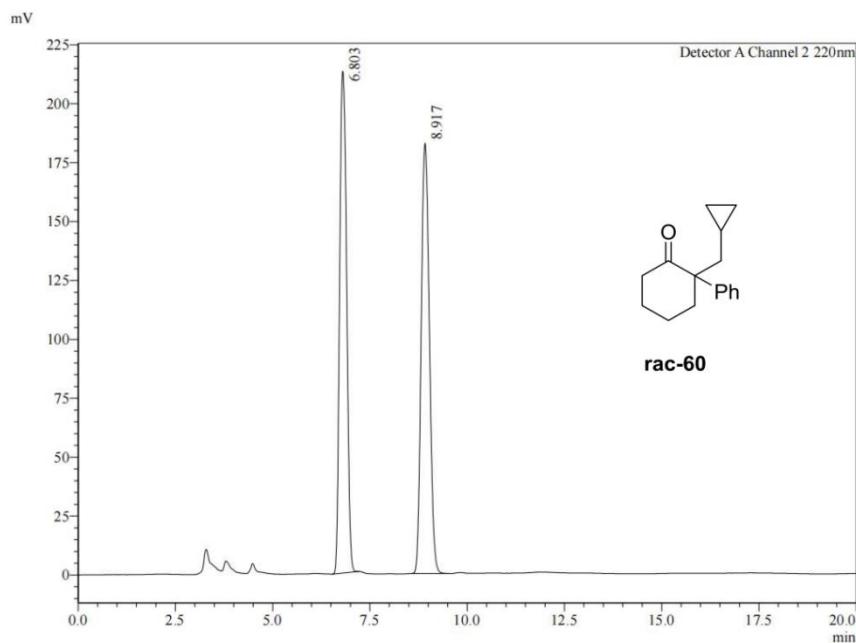
mV



Peak Table

Detector A Channel 2 220nm

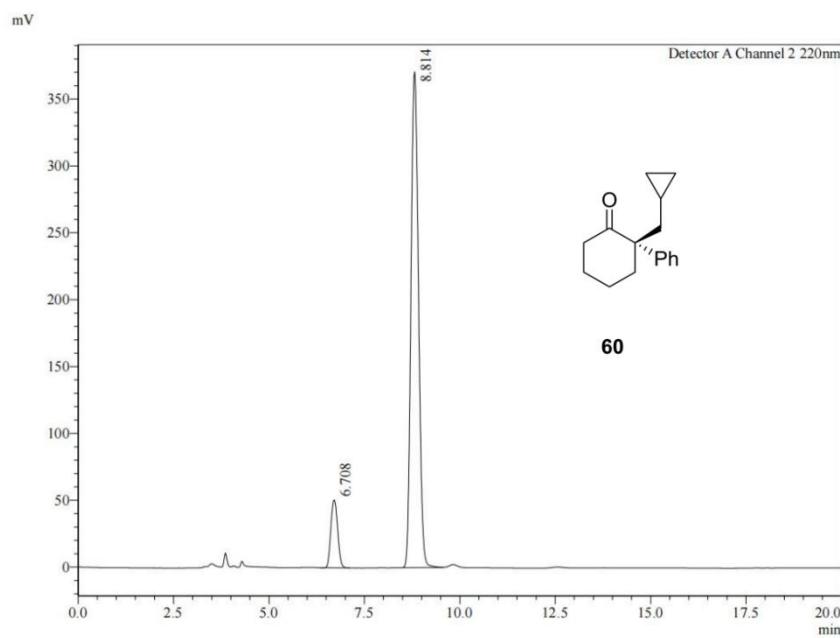
Peak#	Ret. Time	Area	Height	Area%	Height%
1	17.576	843360	34374	5.847	6.664
2	18.647	13579661	481478	94.153	93.336
Total		14423021	515851	100.000	100.000



Peak Table

Detector A Channel 2 220nm

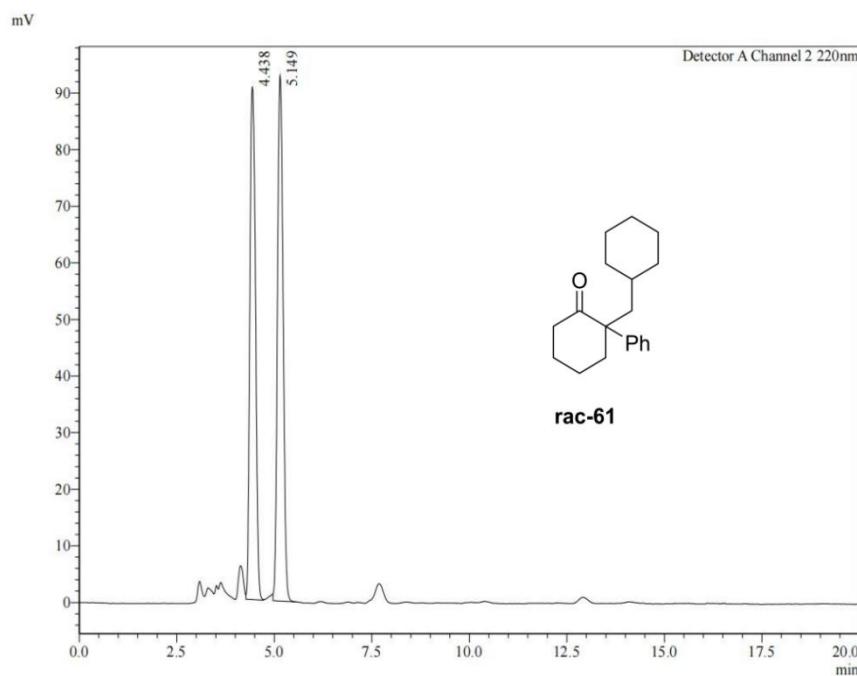
Peak#	Ret. Time	Area	Height	Area%	Height%
1	6.803	2661223	212883	49.892	53.850
2	8.917	2672731	182442	50.108	46.150
Total		5333954	395325	100.000	100.000



Peak Table

Detector A Channel 2 220nm

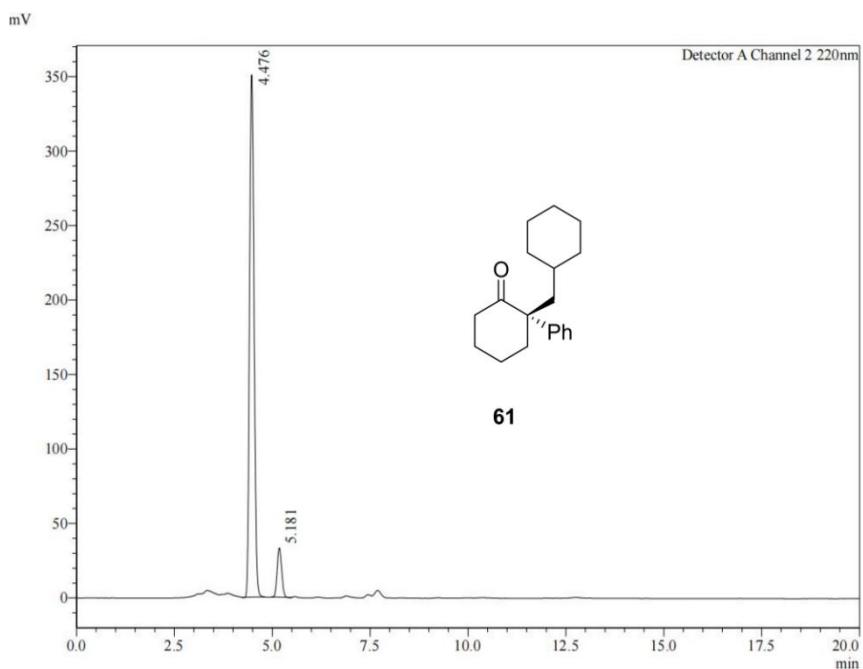
Peak#	Ret. Time	Area	Height	Area%	Height%
1	6.708	627734	50678	11.009	12.038
2	8.814	5074485	370310	88.991	87.962
Total		5702218	420988	100.000	100.000



Peak Table

Detector A Channel 2 220nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	4.438	912226	90606	49.444	49.405
2	5.149	932732	92788	50.556	50.595
Total		1844957	183394	100.000	100.000

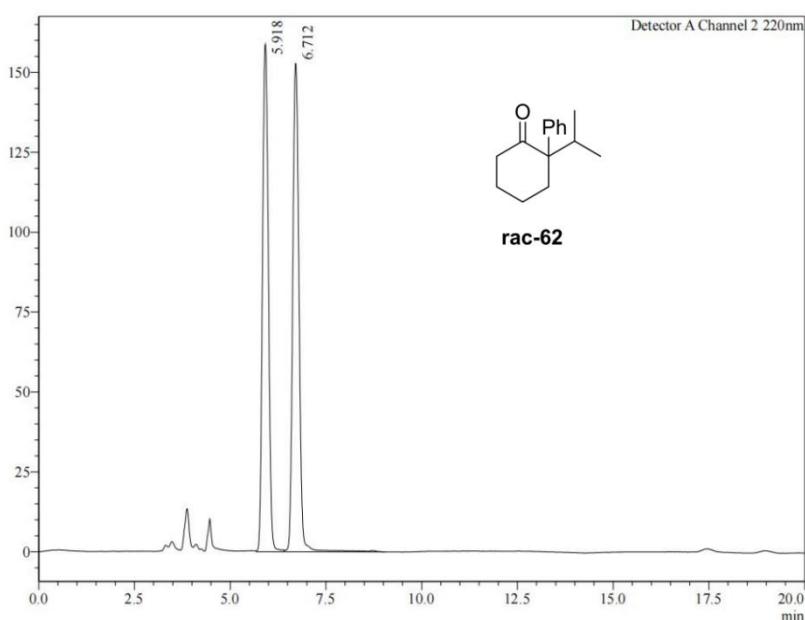


Peak Table

Detector A Channel 2 220nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	4.476	2809871	350651	91.418	91.385
2	5.181	263790	33057	8.582	8.615
Total		3073661	383708	100.000	100.000

mV

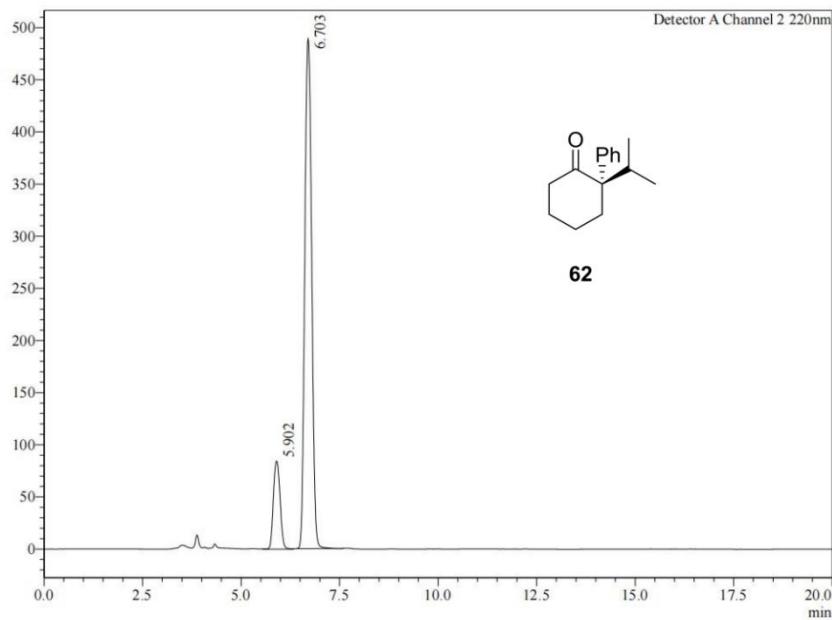


Peak Table

Detector A Channel 2 220nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	5.918	1702347	158612	49.367	50.939
2	6.712	1745983	152764	50.633	49.061
Total		3448330	311376	100.000	100.000

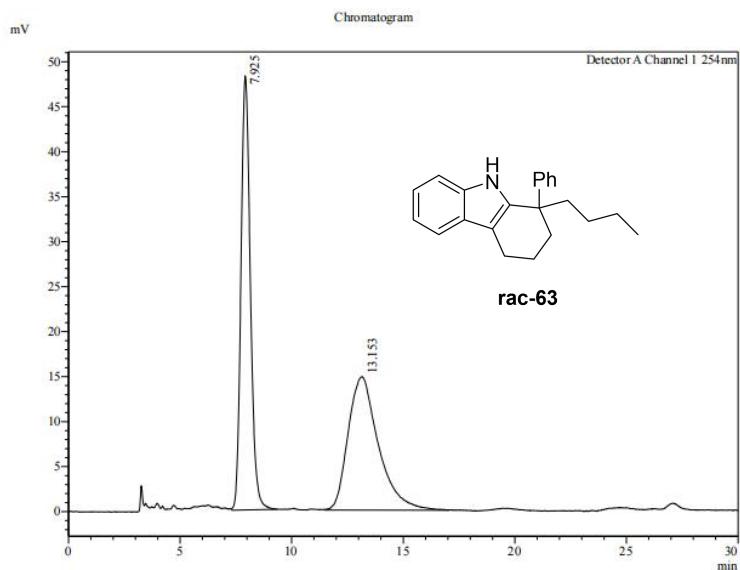
mV



Peak Table

Detector A Channel 2 220nm

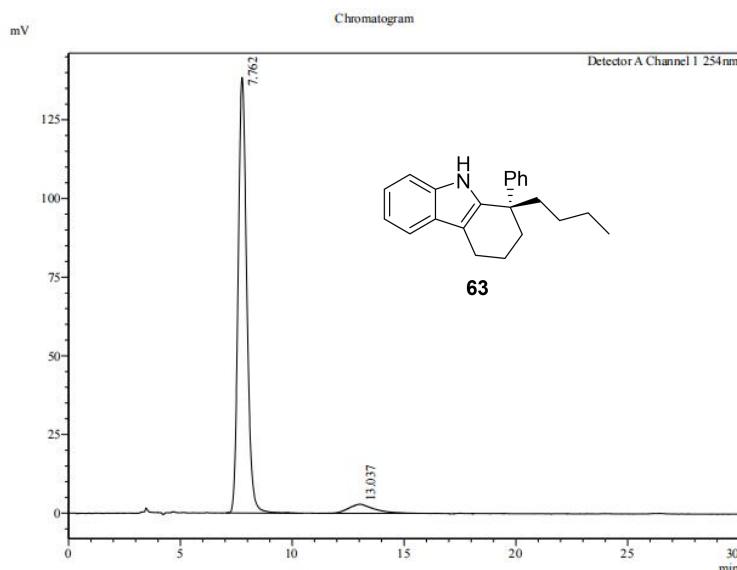
Peak#	Ret. Time	Area	Height	Area%	Height%
1	5.902	1008666	84527	14.514	14.744
2	6.703	5940802	488785	85.486	85.256
Total		6949468	573312	100.000	100.000



Peak Table

Detector A Channel 1 254nm

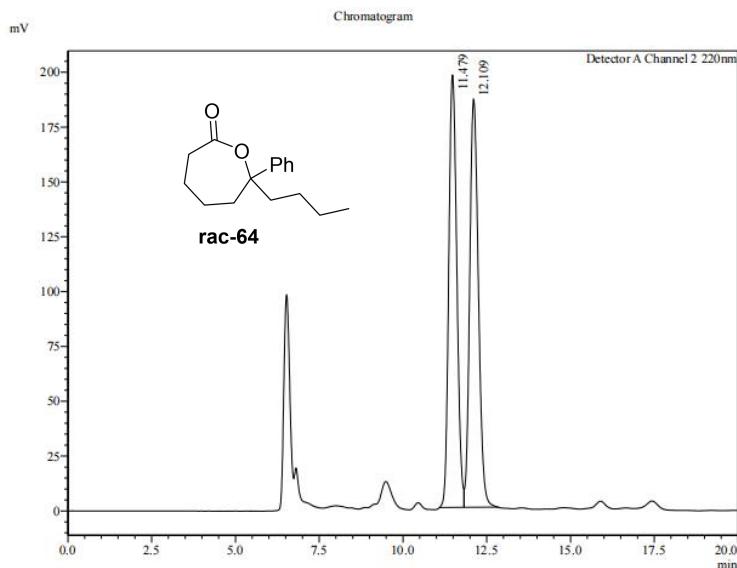
Peak#	Ret. Time	Area	Height	Area%	Height%
1	7.925	1408918	48200	50.163	76.489
2	13.153	1399784	14816	49.837	23.511
Total		2808701	63016	100.000	100.000



Peak Table

Detector A Channel 1 254nm

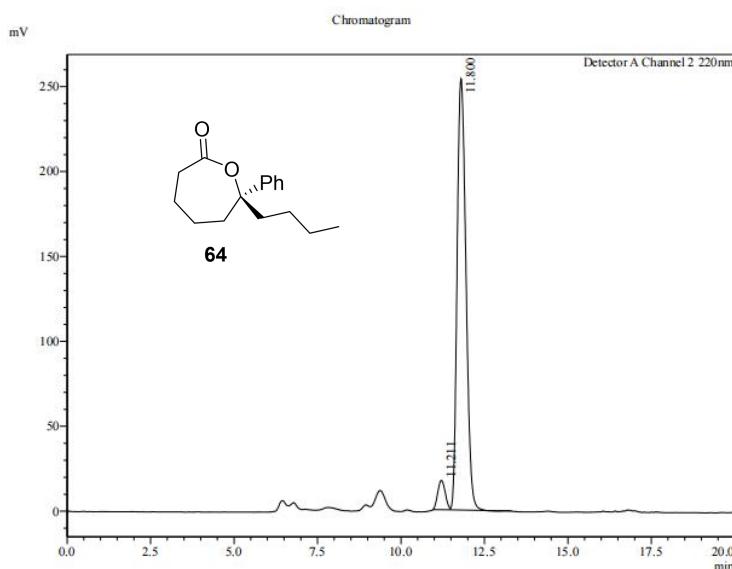
Peak#	Ret. Time	Area	Height	Area%	Height%
1	7.762	3706106	138394	94.228	97.968
2	13.037	227036	2870	5.772	2.032
Total		3933142	141264	100.000	100.000



Peak Table

Detector A Channel 2 220nm

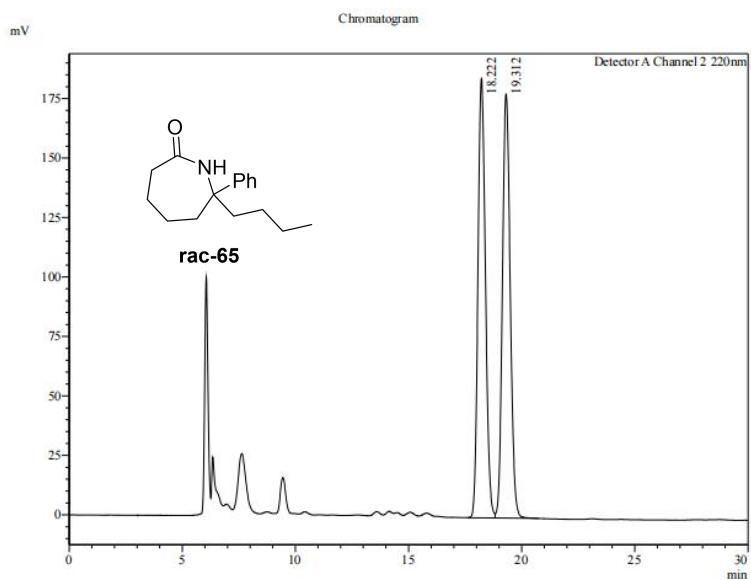
Peak#	Ret. Time	Area	Height	Area%	Height%
1	11.479	3296118	197061	49.575	51.434
2	12.109	3352651	186071	50.425	48.566
Total		6648769	383132	100.000	100.000



Peak Table

Detector A Channel 2 220nm

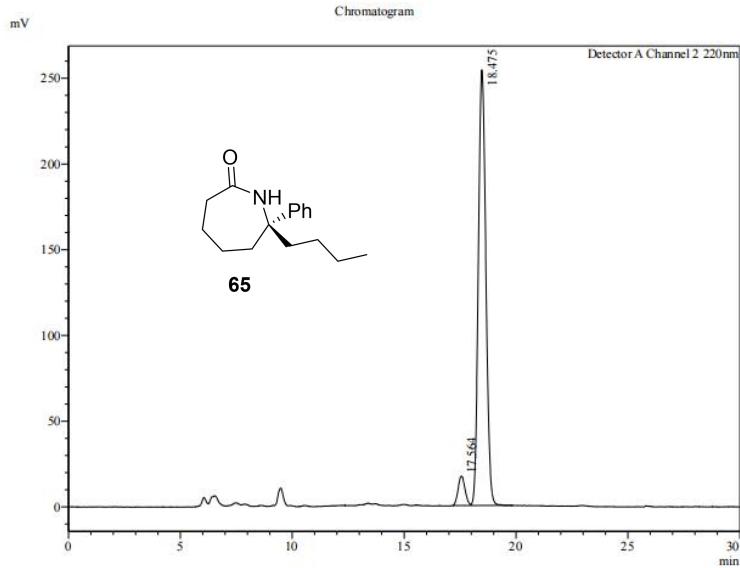
Peak#	Ret. Time	Area	Height	Area%	Height%
1	11.211	269270	17234	5.470	6.354
2	11.800	4653617	254004	94.530	93.646
Total		4922886	271238	100.000	100.000



Peak Table

Detector A Channel 2 220nm

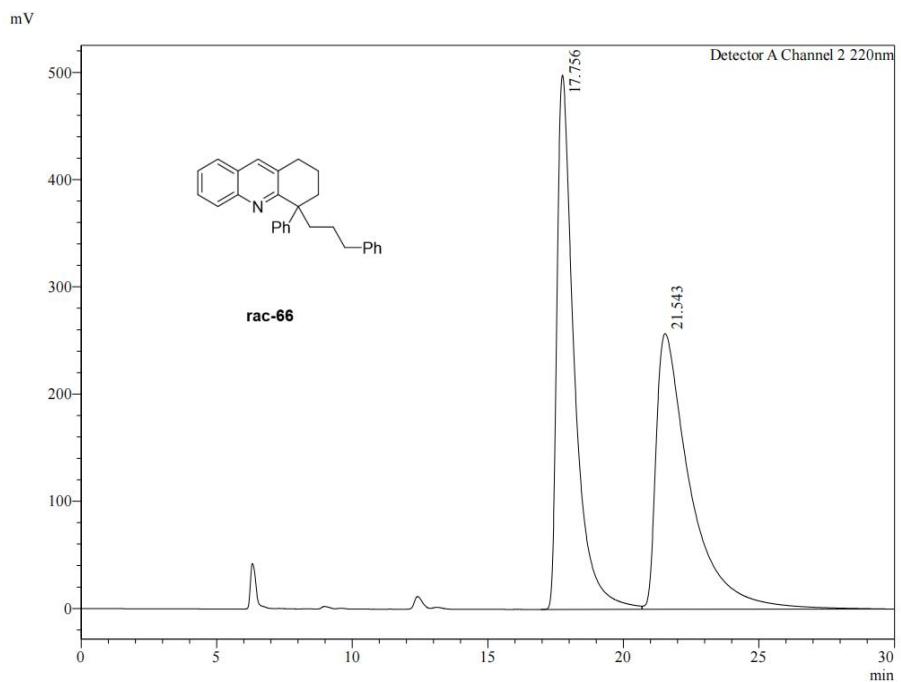
Peak#	Ret. Time	Area	Height	Area%	Height%
1	18.222	4243652	184757	49.873	50.898
2	19.312	4265230	178236	50.127	49.102
Total		8508882	362993	100.000	100.000



Peak Table

Detector A Channel 2 220nm

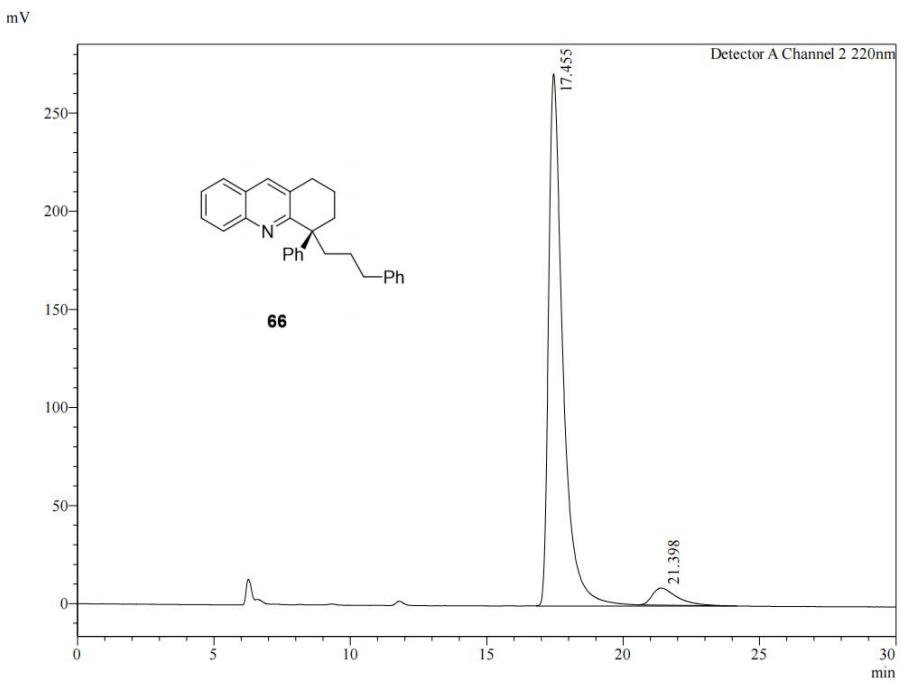
Peak#	Ret. Time	Area	Height	Area%	Height%
1	17.564	367336	17113	5.837	6.316
2	18.475	5925434	253817	94.163	93.684
Total		6292771	270930	100.000	100.000



Peak Table

Detector A Channel 2 220nm

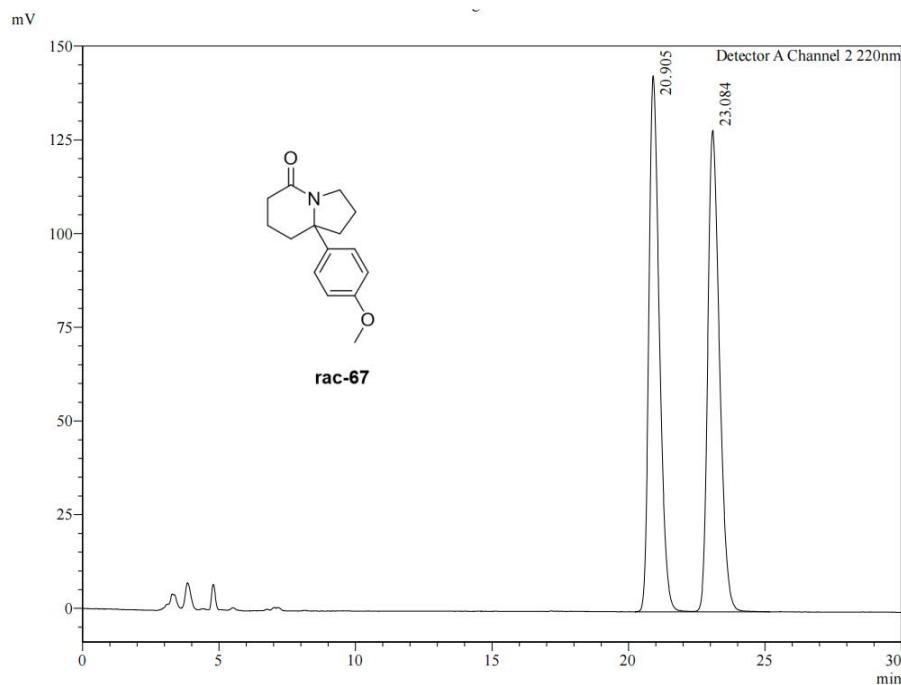
Peak#	Ret. Time	Area	Height	Area%	Height%
1	17.756	22248814	498320	49.754	65.967
2	21.543	22468452	257091	50.246	34.033
Total		44717266	755411	100.000	100.000



Peak Table

Detector A Channel 2 220nm

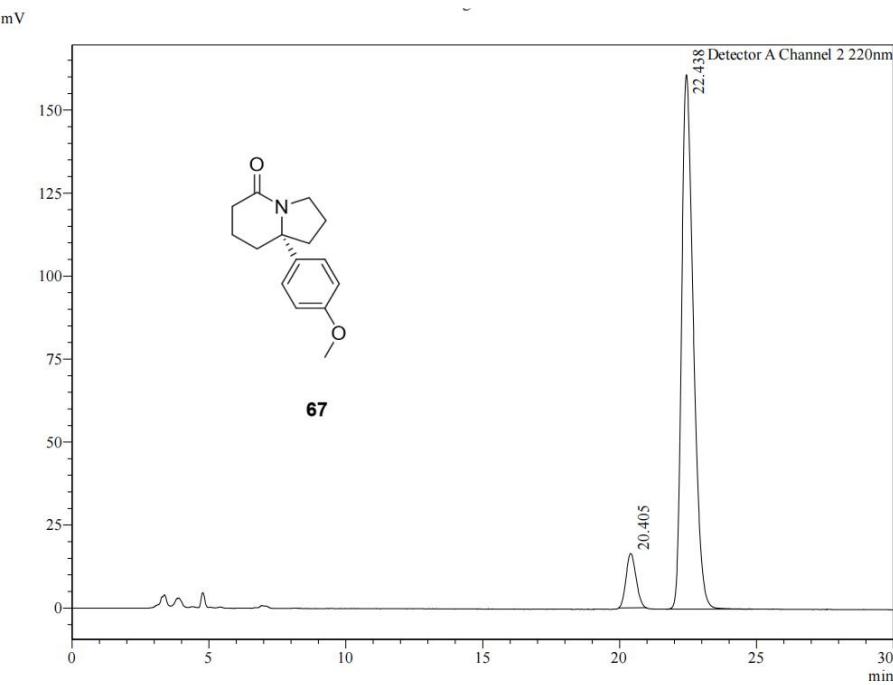
Peak#	Ret. Time	Area	Height	Area%	Height%
1	17.455	9992807	271179	94.817	96.895
2	21.398	546249	8690	5.183	3.105
Total		10539056	279869	100.000	100.000



Peak Table

Detector A Channel 2 220nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	20.905	3827176	142958	49.983	52.671
2	23.084	3829835	128459	50.017	47.329
Total		7657011	271417	100.000	100.000

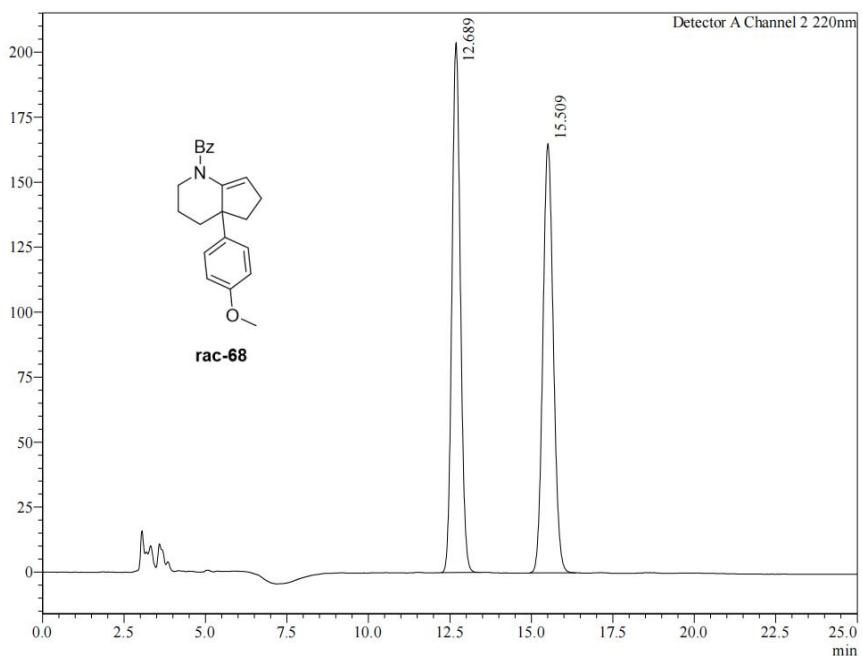


Peak Table

Detector A Channel 2 220nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	20.405	414482	16376	7.918	9.235
2	22.438	4820423	160947	92.082	90.765
Total		5234904	177324	100.000	100.000

mV

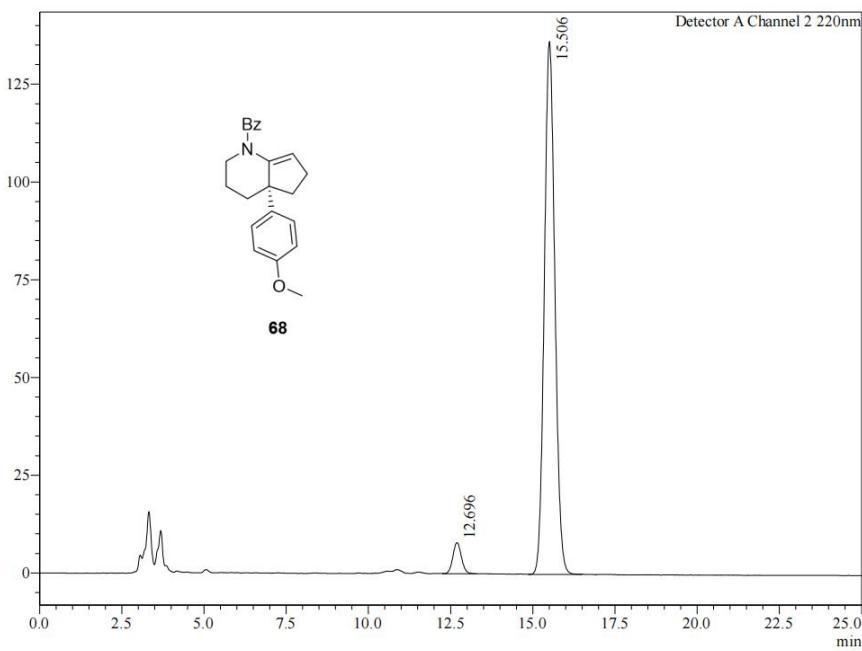


Peak Table

Detector A Channel 2 220nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	12.689	3669005	203667	49.946	55.231
2	15.509	3676952	165086	50.054	44.769
Total		7345957	368753	100.000	100.000

mV

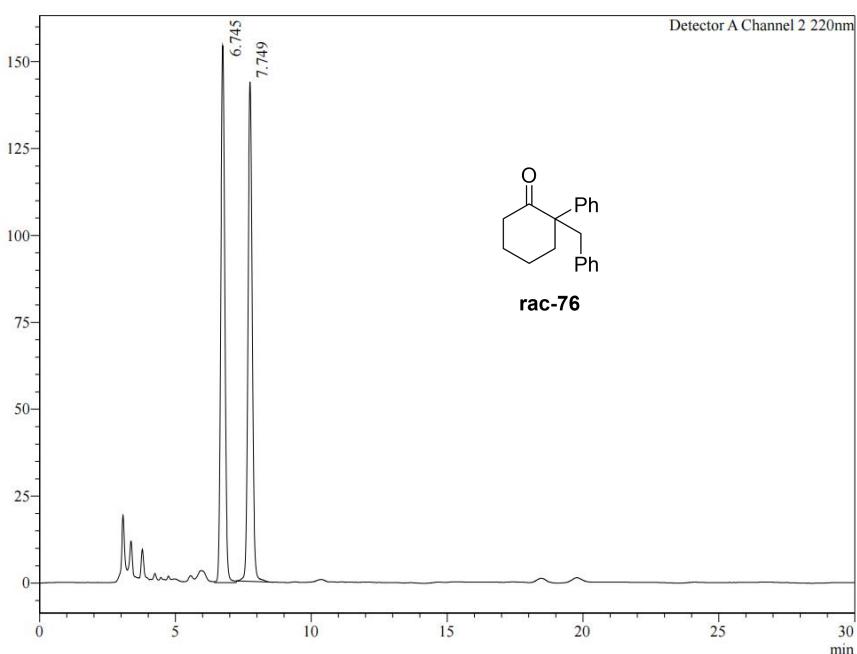


Peak Table

Detector A Channel 2 220nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	12.696	144088	7968	4.530	5.527
2	15.506	3036609	136203	95.470	94.473
Total		3180698	144171	100.000	100.000

mV

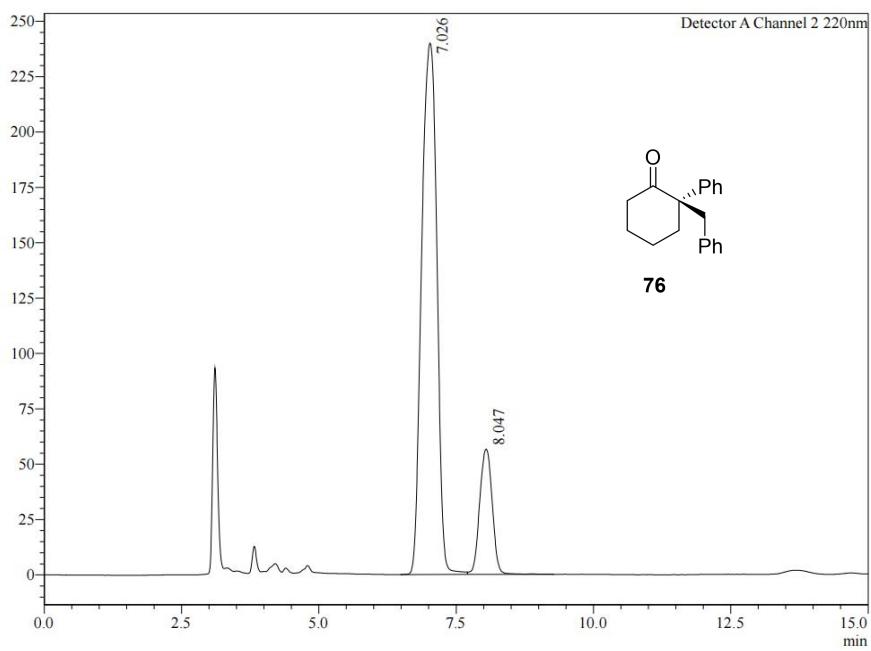


Peak Table

Detector A Channel 2 220nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	6.745	1592635	154455	50.376	51.805
2	7.749	1568887	143689	49.624	48.195
Total		3161522	298144	100.000	100.000

mV



Peak Table

Detector A Channel 2 220nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	7.026	4632707	240011	83.660	80.933
2	8.047	904817	56543	16.340	19.067
Total		5537524	296553	100.000	100.000

14. References

1. B. Shrestha, B. T. Rose, C. L. Olen, A. Roth, A. C. Kwong, Y. Wang and S. E. Denmark, A Unified Strategy for the Asymmetric Synthesis of Highly Substituted 1,2-Amino Alcohols Leading to Highly Substituted Bisoxazoline Ligands. *J. Org. Chem.*, 2021, **86**, 3490-3534.
2. M. J. Behlen and C. Uyeda, *C₂-Symmetric Dinickel Catalysts for Enantioselective [4+1]-Cycloadditions*. *J. Am. Chem. Soc.*, 2020, **142**, 17294-17300.
3. H. N. Tran, L. M. Stanley, Nickel-Catalyzed Enantioselective Hydroboration of Vinylarenes. *Org. Lett.*, 2022, **24**, 395-399.
4. X. Liao, L. M. Stanley, J. F. Hartwig, Enantioselective Total Syntheses of (-)-Taiwaniaquinone H and (-)-Taiwaniaquinol B by Iridium-Catalyzed Borylation and Palladium-Catalyzed Asymmetric alpha-Arylation. *J. Am. Chem. Soc.*, 2011, **133**, 2088-2091 .
5. M. López-Iglesias, E. Bustos, V. Gotor and V. Gotor-Fernández, Stereoselective Synthesis of 2,3-Disubstituted Indoline Diastereoisomers by Chemoenzymatic Processes. *J. Org. Chem.*, 2012, **77**, 8049-8055.
6. F.-F. Dang, C.-C. Wang, F. Han and Z.-W. Zhang, Synthesis of the ester side chains of homoharringtonine and harringtonine using lactones as building blocks. *Synth. Commun.*, 2021, **51**, 317-323.
7. J. Shi, D. Qiu, J. Wang, H. Xu, Y. Li, Domino Aryne Precursor: Efficient Construction of 2,4-Disubstituted Benzothiazoles. *J. Am. Chem. Soc.* 2015, **137**, 5670-5673.
8. D. Ma, C.-B. Miao and J. Sun, Catalytic EnantioselectiveHouse-Meinwald Rearrangement: Efficient Construction of All-Carbon Quaternary Stereocenters. *J. Am. Chem. Soc.* 2019, **141**, 13783-13787.
9. K. J. Frankowski, R. Liu, G. L. Milligan, K. D. Moeller and J. Aubé, Practical Electrochemical Anodic Oxidation of Polycyclic Lactams forLate Stage Functionalization. *Angew. Chem., Int. Ed.* 2015, **54**, 10555-10558.
10. H. Iwamoto, Y. Kondo, T. Kawatani, T. Haino and Y. Fukazawa, Magnetic shielding effect of amine and ammonium groups obtained from proton chemical shifts of androstane derivatives. *Tetrahedron letters*, 2003, **44**, 5975-5978.
11. R. Grigg, V. Sridharan, P. Stevenson and S. Sukirthalingam, The synthesis of spirocyclic compounds by regiospecific palladiumcatalysed cyclisation reactions. *Tetrahedron* 1989, **45**, 3557-3568.
12. A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648-5652.
13. C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B.*, 1988, **37**, 785.
14. S. Grimme, S. Ehrlich, L. Goerigk, *J. Comput. Chem.*, 2011, **32**, 1456-1465.
15. A. D. Becke and E. R. Johnson, *J. Chem. Phys.*, 2005, **123**, 154101.
16. Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215-241.
17. E. Cancès, B. Mennucci and J. Tomasi, A new integral equation formalism for the polarizable continuum model: Theoretical background and applications to isotropic and anisotropic dielectrics, *J. Chem. Phys.*, 1997, **107**, 3032.
18. M. Cossi, V. Barone, R. Cammi and J. Tomasi, Ab initio study of solvated molecules: a new implementation of the polarizable continuum model, *Chem. Phys. Lett.*, 1996, **255**, 327-335.
19. C. Y. Legault, CYLview, 1.0b; Universitéde Sherbrooke: 2009.