Electronic Supplementary Material (ESI) for ChemComm.

Enantioselective gold(I)-catalyzed cyclization/intermolecular nucleophilic additions of 1,5-enyne derivatives

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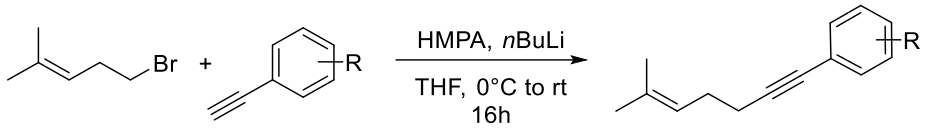
I. General information:

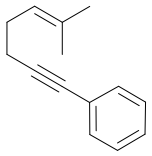
Reactions were performed using oven dried glassware under an atmosphere of argon. All separations were carried out under flash-chromatographic conditions on silica gel (Redi Sep® prepacked column, 230–400 mesh) at medium pressure (20 psi) with use of a CombiFlash Companion. Reactions were monitored by thin-layer chromatography on Merck silica gel plates (60 F_{254} aluminum sheets) which were rendered visible by ultraviolet and spraying with vanillin (15%) + sulfuric acid (2.5%) in EtOH, followed by heating. Reagent-grade chemicals were obtained from diverse commercial suppliers and used as received. ^{1}H NMR (500 or 300 MHz) and ^{13}C NMR (125 or 75 MHz) spectra were recorded on Brüker Avance spectrometers at 298 K unless otherwise stated. Chemical shifts are given in ppm (δ) and are referenced to the internal solvent signal. Multiplicities are declared as follow: s (singlet), bs (broad singlet), d (doublet), t (triplet), q (quadruplet), dd (doublet of doublet), dt (doublet of triplet), m (multiplet). Coupling constants *J* are given in Hz. Carbon multiplicities were determined by DEPT-135 experiment. Infrared spectra (IR) were recorded on a Perkin-Elmer FT-IR system using diamond window Dura SamplIR II and the data are reported in reciprocal centimeters (cm^{-1}). Melting points were recorded in open capillary tubes on a Büchi B-540 apparatus and are uncorrected. High-resolution mass spectrometry (HRMS) was performed using electrospray ionization (ESI) and time-of-flight (TOF) analyzer, in positive-ion or negative-ion detection mode. Supercritical fluid chromatography (SFC) separation was performed with Investigator SFC System (Waters) equipped with a diode array UV detector. Data are reported as follows: column type, temperature, eluent, flow rate, pressure in column, retention time.

II. Experimental procedures:

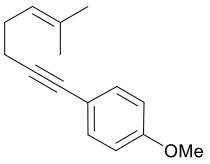
Procedure I: synthesis of substrates **1a-d**:



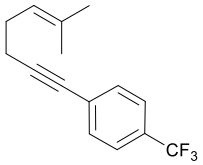
To a solution of phenylacetylene derivatives (1.0 equiv.) in THF was added *n*BuLi (1.6 M, 1.2 equiv.) dropwise at 0°C, and the mixture was stirred for 1 hour at this temperature. Then HMPA (2.0 equiv.) and 5-bromo-2-methyl-2-pentene (1.1 equiv.) were added at 0°C. The reaction mixture was then warmed to room temperature and stirred overnight. The reaction was quenched at 0°C with saturated NH_4Cl aq., extracted with petroleum ether. After evaporation of the organic layer, the crude product was purified by flash chromatography on silica gel using petroleum ether/EtOAc as the eluent (from 0% to 2% EtOAc), to yield the target products.



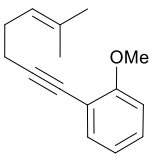
II.1. (6-Methylhept-5-en-1-yn-1-yl)benzene[1] (1a) (207 mg, 61% yield). Colorless oil; R_f 0.35 (*n*-heptane); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.39 (d, J = 6.1 Hz, 2H), 7.33-7.23 (m, 3H), 5.24 (t, J = 6.6 Hz, 1H), 2.42 (t, J = 7.3 Hz, 2H), 2.30 (q, J = 7.2 Hz, 2H), 1.73 (s, 3H), 1.67 (s, 3H).



II.2. (6-Methylhept-5-en-1-yn-1-yl)benzene (1b) (224 mg, 27% yield). Colorless oil; R_f 0.71 (*n*-heptane); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33 (d, J = 8.4 Hz, 2H), 6.81 (d, J = 8.4 Hz, 2H), 5.27-5.20 (m, 1H), 3.80 (s, 3H), 2.45-2.37 (m, 2H), 2.29 (q, J = 7.2 Hz, 2H), 1.73 (d, J = 0.5 Hz, 3H), 1.66 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.2 (C), 133.8 (C), 133.0 (CH x 2), 123.1 (CH), 116.4 (C), 114.0 (CH x 2), 88.7 (C), 80.4 (C), 55.4 (CH_3), 27.8 (CH_2), 25.8 (CH_3), 20.1 (CH_2), 17.9 (CH_3); IR: ν_{max} = 2966, 2913, 2837, 1607, 1508, 1442, 1377, 1289, 1246, 1172, 1106, 1034, 830, 737 cm^{-1}; HRMS (ESI) Calcd. For $C_{15}H_{19}O$ $[M+H]^+$: 215.1436, found: 215.1430.



II.3. 1-(6-Methylhept-5-en-1-yn-1-yl)-4-(trifluoromethyl)benzene (1c) (526 mg, 52% yield). Colorless oil; R_f 0.60 (*n*-heptane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.53 (d, J = 8.4 Hz, 2H), 7.48 (d, J = 8.4 Hz, 2H), 5.26-5.18 (m, 1H), 2.48-2.34 (m, 2H), 2.36-2.26 (m, 2H), 1.73 (s, 3H), 1.67 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 133.5 (C), 131.9 (CH x 2), 129.4 (q, J = 32.2 Hz, C), 128.1 (C), 125.2 (q, J = 3.8 Hz, CH x 2), 124.2 (q, J = 270.0 Hz, C), 122.7 (CH), 93.3 (C), 79.7 (C), 27.5 (CH_2), 25.9 (CH_3), 20.1 (CH_2), 18.0 (CH_3); ^{19}F NMR (282 MHz, $CDCl_3$) δ -62.7; IR: ν_{max} = 2971, 2918, 1617, 1378, 1324, 1267, 1167, 1127, 1105, 1068, 1018, 842, 741 cm^{-1}; HRMS (ESI) Calcd. For $C_{15}H_{16}F_3$ $[M+H]^+$: 253.1204, found: 253.1215.



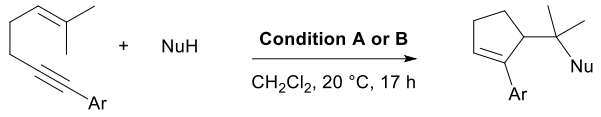
II.4. 1-Methoxy-2-(6-methylhept-5-en-1-yn-1-yl)benzene (1d) (240 mg, 37% yield). Colorless oil; R_f 0.63 (5 % EtOAc/*n*-heptane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.30 (dd, J = 7.5, 1.7 Hz, 1H), 7.21-7.13 (m, 1H), 6.80 (m, 2H), 5.21-5.15 (m, 1H), 3.80 (s, 3H), 2.45-2.36 (m, 2H), 2.28-2.22 (m, 2H), 1.65 (d, J = 0.8 Hz, 3H), 1.58 (s, 3H);

[1] K. Speck, K. Karaghiosoff, T. Magauer, *Org. Lett.* 2015, **17**, 1982.

^{13}C NMR (75 MHz, $CDCl_3$) δ 160.0 (C), 133.8 (CH), 133.0 (C), 129.0 (CH), 123.1 (CH), 120.5 (CH), 113.3 (C), 110.7 (CH), 94.6 (C), 77.2 (C), 55.9 (CH_3), 27.8 (CH_2), 25.9 (CH_3), 20.5 (CH_2), 18.0 (CH_3); IR: ν_{max} = 2967, 2914, 1596, 1492, 1464, 1434, 1292, 1262, 1237, 1117, 1049, 1026, 748, 735, 703 cm^{-1}; HRMS (ESI) Calcd. For $C_{15}H_{19}O$ $[M+H]^+$: 215.1436, found: 215.1430.

Procedure II: synthesis of racemic mixture of compounds **3a-3v**

In a Schlenk tube, substrates **1a-d** (0.10 mmol, 1.0 equiv), nucleophile (0.20 mmol, 2.0 equiv.), gold catalyst (5 mol %) and distillated CH_2Cl_2 (0.5 M) were added. The reaction mixture was then reacted at 20 °C for 17 h (2 h in some cases). The crude reaction mixture was concentrated and purified by automatic flash chromatography using 4g silica gel pre-packed column and EtOAc/*n*-heptane (or PE) as eluent (5-10% EtOAc). Alternatively, prepared TLC (5-10% EtOAc/heptane) could be used for the purification. For **condition A**, $Ph_3PAuCl/AgBF_4$ was used as catalyst. For **condition B**, [(2-biphenyl)di-*tert*-butylphosphineAuSbF$_6$.CH_3CN] was used as gold catalyst.



Condition A: $Ph_3PAuCl/AgBF_4$ (5 mol %)

Condition B: [(2-biphenyl)di-*tert*-butylphosphineAuSbF$_6$.CH_3CN] (5 mol %)

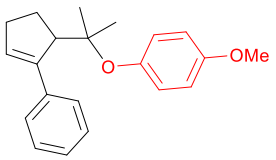
entry	NuH	Ar	Condition A or B	Isolated yield (%)
1	*p*-MeO-C_6H_4OH	Ph	A	80 (**3a**)
2	*p*-MeO-C_6H_4OH	*o*-MeO-C_6H_4	B	18 (**3b**)
3	*p*-MeO-C_6H_4OH	*p*-MeO-C_6H_4	B	47 (**3c**)
4	*p*-MeO-C_6H_4OH	*p*-CF_3-C_6H_4	B	62 (**3d**)
5	*o*-MeO-C_6H_4OH	Ph	B	39 (**3e**)
6	*m*-MeO-C_6H_4OH	Ph	B	32 (**3f**)
7	*p*-Me-C_6H_4OH	Ph	B	52 (**3g**)
8	allyl alcohol	*p*-MeO-C_6H_4	B	88 (**3h**)
9	propargyl alcohol	*p*-MeO-C_6H_4	B	30 (**3i**)
10	MeOH	*p*-MeO-C_6H_4	A	81 (**3j**)
11	H_2O	Ph	B	99 (**3k**)
12	H_2O	*o*-MeO-C_6H_4	B	61 (**3l**)
13	H_2O	*p*-MeO-C_6H_4	A	78 (**3m**)
14	H_2O	*p*-CF_3-C_6H_4	B	81 (**3n**)
15	*p*-NO_2-$C_6H_4NH_2$	Ph	A	99 (**3o**)
16	EtO_2CNH_2	Ph	A	75 (**3p**)
17	*N*-Me-indole	Ph	B	75 (**3q**)
18	*N*-Me-indole	*p*-MeO-C_6H_4	A	82 (**3r**)
19	*N*-Me-indole	*o*-MeO-C_6H_4	B	64 (**3s**)
20	indole	Ph	B	66 (**3t**)
21	MeOH	Ph	A	93 (**3u**)
22	$C_6H_5CH_2OH$	Ph	A	99 (**3v**)

Table S1. Reaction scope of the racemic gold(I)-catalyzed cyclization/nucleophilic addition.

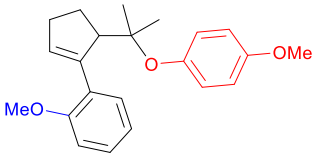
Procedure III: Synthesis of enantioenriched compounds **3a-3t**

In a Schlenk tube, substrates **1a-d** (0.05 mmol, 1.0 equiv) and the corresponding nucleophile (0.1 mmol, 2.0 equiv.) were added. Chiral gold catalyst (**VII**) (2 mol %), $AgPF_6$ (2 mol %) and distillated DCE (0.5 M) were added to another reaction tube, stirred for 15 minutes at 20°C, filtrated and transferred in the previous Schlenk tube. The reaction mixture was then reacted at -20 °C for 24 h. The crude reaction mixture was concentrated and purified by automatic flash chromatography using 4g silica gel pre-packed column and EtOAc/heptane (or PE) as eluent (5-10% EtOAc). Alternatively, prepared TLC (5-10% EtOAc/heptane) could be used for the purification.

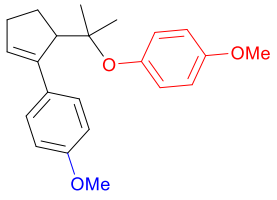
II.5. 1-Methoxy-4-((2-(2-phenylcyclopent-2-en-1-yl)propan-2-yl)oxy)benzene (3a) (24.6 mg, 80% yield). Colorless oil; R_f 0.27 (5% EtOAc/*n*-heptane); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.38-7.34 (m, 2H), 7.27 (t, J = 7.5 Hz, 2H), 7.19 (t, J = 7.3 Hz, 1H), 6.79-6.72 (m, 4H), 6.02 (bs, 1H), 3.76 (s, 3H), 3.55 (d, J = 9.3 Hz, 1H), 2.58-2.40 (m, 3H), 2.29-2.22 (m, 1H), 1.19 (s, 3H), 0.91 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 155.7 (C), 148.5 (C), 145.6 (C), 139.6 (C), 132.3 (CH), 128.1 (CH x 2), 127.1 (CH x 2), 126.7 (CH), 125.3 (CH x 2), 113.9 (CH x 2), 84.1 (C), 55.6 (CH_3), 55.4 (CH), 32.4 (CH_2), 27.9 (CH_2), 26.2 (CH_3), 23.5 (CH_3); IR: ν_{max} = 2977, 2935, 1503, 1442, 1366, 1265, 1216, 1180, 1136, 1121, 1035, 911, 886, 840, 763, 697 cm^{-1}; HRMS (ESI) Calcd. For $C_{21}H_{25}O_2$ $[M+H]^+$: 309.1855, found: 309.1862. For asymmetric synthesis of compound **3a** (12.2 mg, 81% yield); SFC Analysis: 93:7 e.r. [CHIRALPAK® IC, 30°C, 5% *i*PrOH, 4.0 mL/min, 100 bar, retention times: 6.0 min (major) and 8.9 min (minor)].



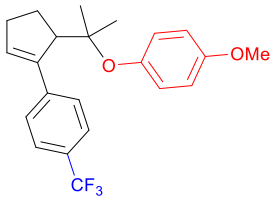
II.6. 1-Methoxy-2-(5-(2-(4-methoxyphenoxy)propan-2-yl)cyclopent-1-en-1-yl)benzene (3b) (6.0 mg, 18% yield). Colorless oil; R_f 0.52 (5% EtOAc/*n*-heptane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.24-7.16 (m, 2H), 6.89 (t, J = 7.4 Hz, 1H), 6.83-6.69 (m, 5H), 5.92 (d, J = 1.9 Hz, 1H), 3.83-3.78 (m, 1H), 3.78 (s, 3H), 3.75 (s, 3H), 2.52-2.45 (m, 2H), 2.40-2.25 (m, 2H), 1.11 (s, 3H), 0.87 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 157.0 (C), 155.5 (C), 148.8 (C), 143.5 (C), 133.6 (CH), 130.0 (CH), 129.5 (C), 128.1 (CH), 125.2 (CH x 2), 120.6 (CH), 113.8 (CH x 2), 110.7 (CH), 83.7 (C), 55.9 (CH_3), 55.6 (CH), 55.4 (CH_3), 31.8 (CH_2), 27.0 (CH_2), 25.2 (CH_3), 23.0 (CH_3); IR: ν_{max} = 2972, 2836, 1596, 1505, 1464, 1265, 1240, 1219, 1124, 1032, 842, 738, 704 cm^{-1}; HRMS (ESI) Calcd. For $C_{22}H_{26}NaO_3$ $[M+Na]^+$: 361.1780, found: 361.1766. For asymmetric synthesis of compound **3b** (6.2 mg, 37% yield); SFC Analysis: 96:4 e.r. [CHIRALPAK® IC, 30°C, 5% *i*PrOH, 4.0 mL/min, 100 bar, retention times: 7.3 min (major) and 11.3 min (minor)].



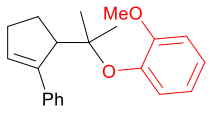
II.7. 1-Methoxy-4-(5-(2-(4-methoxyphenoxy)propan-2-yl)cyclopent-1-en-1-yl)benzene (3c) (15.9 mg, 47% yield). Colorless solid, Mp = 53-55°C; R_f 0.29 (5 % EtOAc/*n*-heptane); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.27 (d J = 8.5 Hz, 2H), 6.81 (d, J = 8.6 Hz, 2H), 6.80-6.72 (m, 4H), 5.94 (s, 1H), 3.79 (s, 3H), 3.76 (s, 3H), 3.49 (d, J = 9.3 Hz, 1H), 2.56-2.39 (m, 3H), 2.25-2.21 (m, 1H), 1.17 (s, 3H), 0.91 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.6 (C), 155.7 (C), 148.6 (C), 145.0 (C), 132.2 (C), 130.8 (CH), 128.1 (CH x 2), 125.4 (CH x 2), 113.9 (CH x 2), 113.5 (CH x 2), 84.2 (C), 55.6 (CH), 55.3 (CH_3 x 2), 32.4 (CH_2), 27.9 (CH_2), 26.4 (CH_3), 23.4 (CH_3); IR: ν_{max} = 2975, 2836, 1606, 1502, 1464, 1366, 1292, 1247, 1217, 1177, 1121, 1035, 887, 833, 811, 785, 742 cm^{-1}; HRMS (ESI)



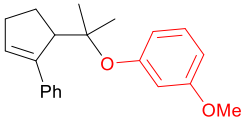
Calcd. For $C_{22}H_{27}O_3[M+H]^+$: 339.1960, found: 339.1944. For asymmetric synthesis of compound **3c** (12.1 mg, 72% yield); SFC Analysis: 94:6 e.r. [CHIRALPAK® IC, 30°C, 5% *i*PrOH, 4.0 mL/min, 100 bar, retention times: 11.0 min (major) and 16.0 min (minor)].

II.8. 1-Methoxy-4-((2-(2-(4-(trifluoromethyl)phenyl)cyclopent-2-en-1-yl)propan-2-yl)oxy)benzene (3d) (23.0 mg, 62% yield). Colorless oil; R_f 0.55 (5 % EtOAc/*n*-heptane); 

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.52 (d, J = 8.7 Hz, 2H), 7.47 (d, J = 8.7 Hz, 2H), 6.78-6.63 (m, 4H), 6.12 (bs, 1H), 3.75 (s, 3H), 3.61-3.53 (m, 1H), 2.63-2.42 (m, 2H), 2.42-2.22 (m, 2H), 1.20 (s, 3H), 0.91 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 155.8 (C), 148.3 (C), 144.7 (C), 143.3 (C), 134.4 (CH), 128.6 (q, J = 31.5 Hz, C), 127.3 (CH x 2), 125.1 (CH x 2), 125.0 (q, J = 4.5 Hz, CH x 2), 124.5 (q, J = 271.7 Hz, C), 114.0 (CH x 2), 83.9 (C), 55.7 (CH_3), 55.6 (CH), 32.5 (CH_2), 27.9 (CH_2), 25.2 (CH_3), 24.1 (CH_3); ^{19}F NMR (282 MHz, $CDCl_3$) δ -62.3; IR: ν_{max} = 2983, 2934, 1615, 1505, 1367, 1328, 1265, 1218, 1164, 1123, 1109, 1069, 1038, 840, 737, 704 cm^{-1}; HRMS (ESI) Calcd. For $C_{22}H_{24}F_3O_2$ $[M+H]^+$: 377.1728, found: 377.1745. For asymmetric synthesis of compound **3d** (12.9 mg, 69% yield); SFC Analysis: 82:18 e.r. [CHIRALPAK® IC, 30°C, 5% *i*PrOH, 4.0 mL/min, 100 bar, retention times: 3.0 min (major) and 3.8 min (minor)].

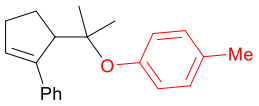
II.9. 1-Methoxy-2-((2-(2-phenylcyclopent-2-en-1-yl)propan-2-yl)oxy)benzene (3e) (12.0 mg, 39% yield). Colorless oil; R_f 0.33 (5% EtOAc/*n*-heptane); 

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.38-7.32 (m, 2H), 7.28-7.21 (m, 2H), 7.20-7.12 (m, 1H), 7.00 (dt, J = 7.8, 1.8 Hz, 1H), 6.91 (dd, J = 7.9, 1.7 Hz, 1H), 6.84 (dd, J = 8.0, 1.7 Hz, 1H), 6.79 (dt, J = 8.1, 1.7 Hz, 1H), 6.01 (bs, 1H), 3.76 (s, 3H), 3.64 (d, J = 9.4 Hz, 1H), 2.69-2.37 (m, 3H), 2.232-2.17 (m, 1H), 1.15 (s, 3H), 0.91 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 154.5 (C), 145.6 (C), 144.5 (C), 139.6 (C), 132.6 (CH), 128.2 (CH x 2), 127.1 (CH x 2), 127.0 (CH), 125.9 (CH), 124.1 (CH), 120.4 (CH), 112.4 (CH), 85.8 (C), 55.9 (CH), 55.7 (CH_3), 32.6 (CH_2), 27.7 (CH_2), 26.8 (CH_3), 22.6 (CH_3); IR: ν_{max} = 2977, 2935, 1505, 1464, 1442, 1382, 1366, 1217, 1136, 1121, 1035, 911, 886, 840, 763, 739, 697 cm^{-1}; HRMS (ESI) Calcd. For $C_{21}H_{24}NaO_2$ $[M+Na]^+$: 331.1674, found: 331.1661. For asymmetric synthesis of compound **3e** (11.6 mg, 77% yield); SFC Analysis: 91:9 e.r. [CHIRALPAK® IC, 30°C, 5% *i*PrOH, 4.0 mL/min, 100 bar, retention times: 4.7 min (major) and 5.7 min (minor)].

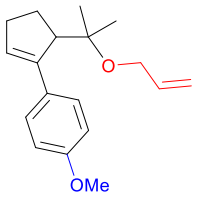
II.10. 1-Methoxy-3-((2-(2-phenylcyclopent-2-en-1-yl)propan-2-yl)oxy)benzene (3f) (9.9 mg, 32% yield). Colorless oil; R_f 0.46 (5% EtOAc/*n*-heptane); 

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37 (d, J = 7.5 Hz, 2H), 7.27 (t, J = 7.5 Hz, 2H), 7.19 (t, J = 7.5 Hz, 1H), 7.10 (t, J = 8.2 Hz, 1H), 6.58 (dd, J = 8.2, 1.5 Hz, 1H), 6.46 (d, J = 8.0 Hz, 1H), 6.30 (bs, 1H), 6.02 (bs, 1H), 3.72 (s, 3H), 3.62 (d, J = 9.3 Hz, 1H), 2.58-2.43 (m, 2H), 2.39-2.34 (m, 1H), 2.28-2.20 (m, 1H), 1.26 (s, 3H), 0.99 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.2 (C), 156.6 (C), 145.6 (C), 139.6 (C), 132.3 (CH), 129.1 (CH), 128.1 (CH x 2), 127.1 (CH x 2), 126.7 (CH), 116.2 (CH), 109.8 (CH), 108.8 (CH), 84.6 (C), 55.7 (CH), 55.4 (CH_3), 32.4 (CH_2), 27.8 (CH_2), 25.7 (CH_3), 24.1 (CH_3); IR: ν_{max} = 2978, 2938, 1597, 1587, 1484, 1382, 1367, 1279, 1263, 1195, 1143, 1135, 1119, 1041, 959, 762, 732, 698 cm^{-1}; HRMS (ESI) Calcd. For $C_{21}H_{25}O_2$ $[M+H]^+$: 309.1855, found: 309.1856. For asymmetric synthesis of compound **3f** (12.5 mg, 81% yield); SFC Analysis: 88.5:11.5 e.r. [CHIRALPAK® AD-H, 30°C, 3% *i*PrOH, 4.0 mL/min, 100 bar, retention times: 6.8 min (major) and 9.1 min (minor)].

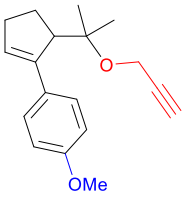
II.11. 1-Methyl-4-((2-(2-phenylcyclopent-2-en-1-yl)propan-2-yl)oxy)benzene (3g) (15.2 mg, 52% yield). Colorless oil; R_f 0.45 (5% EtOAc/*n*-heptane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.36-7.31 (m, 2H), 7.29-7.22 (m, 3H), 6.98 (d, J = 8.1 Hz, 2H), 6.68 (d, J = 8.1 Hz, 2H), 6.00 (bs, 1H), 3.56 (d, J = 9.1 Hz, 1H), 2.60-2.35 (m, 3H), 2.34-2.20 (m, 1H), 2.26 (s, 3H), 1.19 (s, 3H), 0.92 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 152.8 (C), 145.6 (C), 139.6 (C), 132.6 (C), 132.3 (CH), 129.4 (CH x 2), 128.1 (CH x 2), 127.1 (CH x 2), 126.7 (CH), 124.1 (CH x 2), 84.1 (C), 55.5 (CH), 32.4 (CH_2), 27.8 (CH_2), 26.2 (CH_3), 23.6 (CH_3), 20.9 (CH_3); IR: ν_{max} = 3027, 2978, 1610, 1506, 1445, 1382, 1366, 1265, 1224, 1136, 1122, 1032, 949, 885, 836, 762, 736, 698 cm^{-1}; HRMS(ESI) Calcd. For $C_{14}H_{17}$ [M-O-*p*Me-C_6H_4]$^+$: 185.1330, found: 185.1320. For asymmetric synthesis of compound **3g** (14.6 mg, 99% yield); SFC Analysis: 88:12 e.r. [CHIRALPAK® IC, 30°C, 5% *i*PrOH, 4.0 mL/min, 100 bar, retention times: 3.4 min (major) and 5.2 min (minor)].



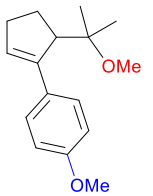
II.12. 1-(5-(2-(Allyloxy)propan-2-yl)cyclopent-1-en-1-yl)-4-methoxybenzene (3h) (24.0 mg, 88% yield). Colorless oil; R_f 0.40 (5 % EtOAc/*n*-heptane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.30-7.20 (m, 2H), 6.87-6.74 (m, 2H), 5.90-5.71 (m, 2H), 5.19 (dq, J = 17.1, 1.5 Hz, 1H), 5.06 (dq, J = 10.2, 1.5 Hz, 1H), 3.90-3.84 (m, 2H), 3.80 (s, 3H), 3.40 (d, J = 9.3 Hz, 1H), 2.48-2.33 (m, 2H), 2.30-2.04 (m, 2H), 1.07 (s, 3H), 0.92 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.6 (C), 145.2 (C), 136.4 (CH), 132.3 (C), 130.5 (CH), 128.1 (CH x 2), 115.5 (CH_2), 113.5 (CH x 2), 78.9 (C), 62.6 (CH_2), 55.4 (CH_3), 54.3 (CH), 32.4 (CH_2), 26.9 (CH_2), 25.4 (CH_3), 22.6 (CH_3); IR: ν_{max} = 2972, 2936, 1728, 1668, 1600, 1510, 1463, 1367, 1246, 1174, 1031, 829, 736, 702 cm^{-1}; HRMS (ESI) Calcd. For $C_{15}H_{19}O_2$ [M-allyl]$^+$: 231.1385, found: 231.1392. For asymmetric synthesis of compound **3h** (10.9 mg, 80% yield); SFC Analysis: 86:14 e.r. [CHIRALPAK® AD-H, 30°C, 2% *i*PrOH, 4.0 mL/min, 100 bar, retention times: 3.9 min (minor) and 4.7 min (major)].



II.13. 1-Methoxy-4-(5-(2-(prop-2-yn-1-yloxy)propan-2-yl)cyclopent-1-en-1-yl)benzene (3i) (8.0 mg, 30% yield). Colorless oil; R_f 0.22 (5 % EtOAc / *n*-heptane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.25 (d, J = 8.7 Hz, 2H), 6.82 (d, J = 8.7 Hz, 2H), 5.89-5.83 (m, 1H), 4.04 (d, J = 2.4 Hz, 2H), 3.80 (s, 3H), 3.38 (bd, J = 9.3 Hz, 1H), 2.46-2.38 (m, 2H), 2.34 (t, J = 2.4 Hz, 1H), 2.31-2.02 (m, 2H), 1.09 (s, 3H), 0.93 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.6 (C), 144.9 (C), 132.0 (C), 130.7 (CH), 128.1 (CH x 2), 113.6 (CH x 2), 81.9 (C), 80.2 (C), 72.9 (CH), 55.4 (CH_3), 54.2 (CH), 50.0 (CH_2), 32.4 (CH_2), 27.0 (CH_2), 25.5 (CH_3), 22.5 (CH_3); IR: ν_{max} = 3286, 2972, 2937, 1729, 1668, 1599, 1510, 1463, 1368, 1244, 1173, 1059, 1031, 831, 735 cm^{-1}; HRMS (ESI) Calcd. For $C_{15}H_{19}O_2$ [M-propargyl]$^+$: 231.1385, found: 231.1382. For asymmetric synthesis of compound **3i** (8.0 mg, 59% yield); SFC Analysis: 87:13 e.r. [CHIRALPAK® AD-H, 30°C, 3% *i*PrOH, 4.0 mL/min, 100 bar, retention times: 4.2 min (minor) and 5.0 min (major)].

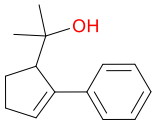


II.14. 1-Methoxy-4-(5-(2-methoxypropan-2-yl)cyclopent-1-en-1-yl)benzene (3j) (20.0 mg, 81% yield). Colorless oil; R_f 0.27 (5% EtOAc/*n*-heptane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.25 (d, J = 8.7 Hz, 2H), 6.82 (d, J = 8.7 Hz, 2H), 5.85 (bs, 1H), 3.80 (s, 3H), 3.37 (d, J = 9.0 Hz, 1H), 3.16 (s, 3H), 2.44-2.37 (m, 2H), 2.26-2.01 (m, 2H), 1.03 (s, 3H), 0.88 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.6 (C), 145.2 (C), 132.2 (C), 130.4 (CH), 128.1 (CH x 2), 113.5 (CH x 2), 78.5 (C), 55.4 (CH_3), 53.7 (CH), 49.1 (CH_3), 32.4 (CH_2), 26.7 (CH_2), 24.9 (CH_3), 22.1 (CH_3); IR: ν_{max} = 2972, 2936, 2902, 1606, 1509, 1464, 1380, 1292,

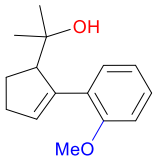


1253, 1176, 1147, 1076, 1038, 836, 819, 798, 736 cm^{-1}; HRMS (ESI) Calcd. For $C_{15}H_{19}O$ [M-OMe]$^+$: 215.1436, found: 215.1430. For asymmetric synthesis of compound **3j** (10.5 mg, 85% yield); SFC Analysis: 86:14 e.r. [CHIRALPAK® AD-H, 30°C, 2% *i*PrOH, 4.0 mL/min, 100 bar, retention times: 4.3 min (minor) and 6.5 min (major)].

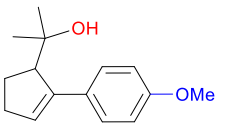
II.15. 2-(2-Phenylcyclopent-2-en-1-yl)propan-2-ol (3k) (20.0 mg, 99% yield). Colorless oil; R_f 0.32 (20 % EtOAc/*n*-heptane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.45-7.36 (m, 2H), 7.35-7.27 (m, 2H), 7.26-7.17 (m, 1H), 6.06-6.01 (m, 1H), 3.36 (bd, J = 9.4 Hz, 1H), 2.49-2.42 (m, 2H), 2.27-2.15 (m, 1H), 2.08-1.94 (m, 1H), 1.30 (bs, OH), 1.15 (s, 3H), 1.08 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 145.0 (C), 139.1 (C), 131.9 (CH), 128.5 (CH x 2), 127.2 (CH), 127.0 (CH x 2), 75.2 (C), 56.8 (CH), 32.4 (CH_2), 28.3 (CH_3), 27.9 (CH_2), 27.1 (CH_3); IR: ν_{max} = 3424, 2971, 2931, 1598, 1493, 1466, 1444, 1371, 1143, 1120, 1031, 951, 917, 865, 843, 809, 762, 696 cm^{-1}; HRMS(ESI) Calcd. For $C_{14}H_{17}$ [M-OH]$^+$: 185.1330, found: 185.1322. For asymmetric synthesis of compound **3k** (9.9 mg, 98% yield); SFC Analysis: 90:10 e.r. [CHIRALPAK® IA, 30°C, 5% *i*PrOH, 4.0 mL/min, 100 bar, retention times: 4.6 min (major) and 7.1 min (minor)].



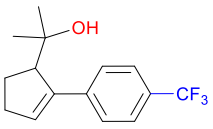
II.16. 2-(2-(2-Methoxyphenyl)cyclopent-2-en-1-yl)propan-2-ol (3l) (14.0 mg, 61% yield). Light yellow oil; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.26-7.16 (m, 1H), 7.20 (d, J = 7.5 Hz, 1H), 6.92 (td, J = 7.5, 0.9 Hz, 1H), 6.85 (d, J = 8.1 Hz, 1H), 5.90 (dd, J = 4.0, 2.4 Hz, 1H), 3.84 (s, 3H), 3.52-3.46 (m, 1H), 2.53-2.33 (m, 2H), 2.26-2.11 (m, 1H), 2.02-1.88 (m, 1H), 1.63 (s, OH), 1.07 (s, 3H), 1.03 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 156.7 (C), 142.9 (C), 133.7 (CH), 130.0 (CH), 129.2 (C), 128.5 (CH), 121.0 (CH), 111.0 (CH), 74.4 (C), 57.9 (CH), 55.5 (CH_3), 31.8 (CH_3), 28.0 (CH_3), 27.2 (CH_2), 26.7 (CH_3); IR: ν_{max} = 3442, 2933, 1596, 1578, 1488, 1463, 1435, 1266, 1237, 1179, 1152, 1115, 1027, 948, 920, 785, 749, 740 cm^{-1}; HRMS (ESI) Calcd. For $C_{15}H_{19}O$ [M-OH]$^+$: 215.1436, found: 215.1430. For asymmetric synthesis of compound **3l** (7.1 mg, 61% yield); SFC Analysis: 97:3 e.r. [CHIRALPAK® IB, 30°C, 2% *i*PrOH, 4.0 mL/min, 100 bar, retention times: 5.0 min (major) and 5.5 min (minor)].



II.17. 2-(2-(4-Methoxyphenyl)cyclopent-2-en-1-yl)propan-2-ol (3m) (18.0 mg, 78% yield). Colorless oil; R_f 0.34 (25 % EtOAc/*n*-heptane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.34 (d, J = 8.7 Hz, 2H), 6.84 (d, J = 8.7 Hz, 2H), 5.95 (bs, 1H), 3.80 (s, 3H), 3.30 (d, J = 9.4 Hz, 1H), 2.48-2.38 (m, 2H), 2.21-2.14 (m, 1H), 2.07-1.89 (m, 1H), 1.59 (bs, OH), 1.16 (s, 3H), 1.07 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.9 (C), 144.4 (C), 131.6 (C), 130.3 (CH), 128.2 (CH x 2), 114.0 (CH x 2), 75.2 (C), 56.8 (CH), 55.4 (CH_3), 32.3 (CH_2), 28.4 (CH_3), 28.0 (CH_2), 26.9 (CH_3); IR: ν_{max} = 3419, 2969, 1739, 1605, 1510, 1464, 1293, 1250, 1178, 1034, 847, 830, 805, 736 cm^{-1}; HRMS (ESI) Calcd. For $C_{15}H_{19}O$ [M-OH]$^+$: 215.1436, found: 215.1434. For asymmetric synthesis of compound **3m** (9.5 mg, 75% yield); SFC Analysis: 95:5 e.r. [CHIRALPAK® IC, 30°C, 2% *i*PrOH, 4.0 mL/min, 100 bar, retention times: 23.8 min (minor) and 25.7 min (major)].

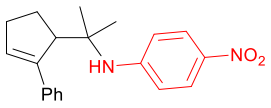


II.18. 2-(2-(4-(Trifluoromethyl)phenyl)cyclopent-2-en-1-yl)propan-2-ol (3n) (22.0 mg, 81% yield). White solid, Mp = 68-70°C; R_f 0.12 (5% EtOAc/*n*-heptane); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.57 (d, J = 8.0 Hz, 2H), 7.52 (d, J = 8.2 Hz, 2H), 6.14 (s, 1H), 3.35 (d, J = 9.5 Hz, 1H), 2.56-2.39 (m, 2H), 2.25-2.18 (m, 1H), 2.11-

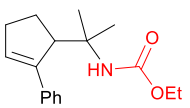


1.98 (m, 1H), 1.15 (s, 3H), 1.07 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 144.1 (C), 142.8 (C), 134.2 (CH), 128.6 (q, J = 32.7 Hz, C), 127.1 (CH x 2), 125.3 (q, J = 2.3 Hz, CH x 2), 124.4 (q, J = 271.2 Hz, C), 75.0 (C), 56.7 (CH), 32.5 (CH_2), 28.4 (CH_3), 27.9 (CH_2), 27.3 (CH_3); ^{19}F NMR (282 MHz, $CDCl_3$) δ -62.5; IR: ν_{max} = 3050, 2964, 2930, 1598, 1544, 1485, 1464, 1362, 1329, 1265, 1224, 1152, 1106, 1019, 993, 816, 760, 735, 698 cm^{-1}; HRMS (ESI) Calcd. For $C_{15}H_{16}F_3$ [M-OH]$^+$: 253.1204, found: 253.1203. For asymmetric synthesis of compound **3n** (12.6 mg, 93% yield); SFC Analysis: 82:18 e.r. [CHIRALPAK® IA, 30°C, 5% *i*PrOH, 4.0 mL/min, 100 bar, retention times: 3.2 min (major) and 5.1 min (minor)].

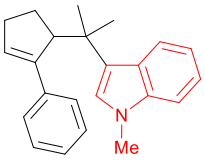
II.19. 4-Nitro-N-(2-(5-phenylcyclopent-1-en-1-yl)propan-2-yl)aniline (3o) (32.0 mg, 99% yield). Yellow oil; R_f 0.27 (15 % EtOAc / *n*-heptane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.95 (d, J = 9.3 Hz, 2H), 7.26-7.15 (m, 5H), 6.28 (d, J = 9.3 Hz, 2H), 6.04-5.91 (m, 1H), 4.37 (bs, NH), 3.77 (d, J = 9.6 Hz, 1H), 2.53-2.42 (m, 2H), 2.36-2.14 (m, 1H), 2.04-1.93 (m, 1H), 1.42 (s, 3H), 1.22 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 179.8 (C), 152.2 (C), 145.2 (C), 139.3 (C), 132.8 (CH), 128.5 (CH x 2), 127.2 (CH), 126.8 (CH x 2), 126.2 (CH x 2), 113.0 (CH x 2), 58.5 (C), 54.2 (CH), 32.3 (CH_2), 27.3 (CH_2), 26.4 (CH_3), 25.2 (CH_3); IR: ν_{max} = 3409, 3379, 2981, 2850, 1595, 1504, 1474, 1317, 1304, 1266, 1184, 1110, 968, 831, 734, 698, 673 cm^{-1}; HRMS (ESI) Calcd. For $C_{20}H_{23}N_2O_2$[M+H]$^+$: 323.1760, found: 323.1738. For asymmetric synthesis of compound **3o** (10.7 mg, 66% yield); SFC Analysis: 89:11 e.r. [CHIRALPAK® IB, 30°C, 10% MeOH, 4.0 mL/min, 100 bar, retention times: 6.9 min (major) and 7.8 min (minor)].



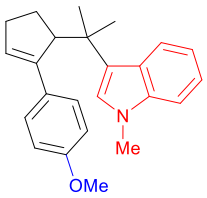
II.20. Ethyl (2-(2-phenylcyclopent-2-en-1-yl)propan-2-yl)carbamate (3p) (20.5 mg, 75% yield). Yellow oil; R_f 0.30 (5% EtOAc/*n*-heptane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.26-7.06 (m, 5H), 5.87-5.80 (m, 1H), 4.25 (bs, NH), 3.93-3.70 (m, 3H), 2.34-2.16 (m, 2H), 2.19-2.01 (m, 1H), 1.91-1.79 (m, 1H), 1.19 (s, 3H), 1.03 (t, J = 7.0 Hz, 3H), 0.98 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 145.8 (C), 139.7 (C), 132.2 (CH), 128.3 (CH x 2), 126.8 (CH), 126.7 (CH x 2), 60.0 (CH_2), 56.8 (C), 52.9 (CH), 32.3 (CH_2), 27.6 (CH_2), 25.4 (CH_3 x 2), 14.7 (CH_3); IR: ν_{max} = 3430, 3345, 2978, 2931, 1711, 1506, 1386, 1366, 1320, 1263, 1241, 1215, 1165, 1088, 1034, 764, 736, 701 cm^{-1}; HRMS (ESI) Calcd. For $C_{17}H_{24}NO_2$[M+H]$^+$: 274.1807, found: 274.1804. For asymmetric synthesis of compound **3p** (11.0 mg, 81% yield); SFC Analysis: 93:7 e.r. [CHIRALPAK® AD-H, 30°C, 2% *i*PrOH, 4.0 mL/min, 100 bar, retention times: 6.0 min (major) and 7.0 min (minor)].



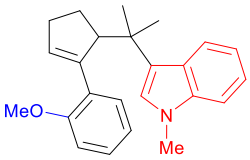
II.21. 1-Methyl-3-(2-(2-phenylcyclopent-2-en-1-yl)propan-2-yl)-3a,7a-dihydro-1H-indole (3q) (23.6 mg, 75% yield). Colorless oil; R_f 0.26 (5 % EtOAc/*n*-heptane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.90 (d, J = 7.9 Hz, 1H), 7.24-7.18 (m, 2H), 7.15-7.02 (m, 6H), 6.45 (s, 1H), 5.92-5.87 (m, 1H), 4.02 (dd, J = 9.3, 1.3 Hz, 1H), 3.54 (s, 3H), 2.41-2.32 (m, 2H), 2.12-1.88 (m, 2H), 1.43 (s, 3H), 1.19 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 146.9 (C), 140.2 (C), 137.8 (C), 131.2 (CH), 127.5 (CH x 2), 126.6 (CH x 2), 125.9 (CH), 125.82 (CH), 125.76 (C), 124.5 (C), 121.6 (CH), 120.9 (CH), 118.2 (CH), 109.3 (CH), 54.1 (CH), 39.7 (C), 32.5 (CH_2), 32.4 (CH_3), 28.3 (CH_2), 27.2 (CH_3), 25.3 (CH_3); IR: ν_{max} =3050, 2964, 2932, 2847, 1687, 1485, 1362, 1329, 1265, 1152, 1106, 1019, 993, 816, 760, 733, 697, 733, 697 cm^{-1}. For asymmetric synthesis of compound **3q** (12.7 mg, 84% yield); SFC Analysis: 92.5:7.5 e.r. [CHIRALPAK® AD-H, 30°C, 3% *i*PrOH, 4.0 mL/min, 100 bar, retention times: 7.0 min (major) and 8.1 min (minor)].



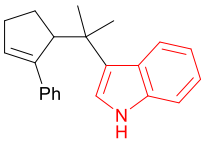
II.22. 3-(2-(2-(4-Methoxyphenyl)cyclopent-2-en-1-yl)propan-2-yl)- 1-methyl-3a,7a-dihydro-1H-indole (3r) (26.0 mg, 82% yield). Yellow oil; R_f 0.45 (5 % EtOAc/*n*-heptane); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.88 (d, J = 7.8 Hz, 1H), 7.23-7.18 (m, 2H), 7.13-7.06 (m, 1H), 7.02 (d, J = 8.7 Hz, 2H), 6.61 (d, J = 8.7 Hz, 2H), 6.47 (s, 1H), 5.82 (bs, 1H), 3.94 (d, J = 9.3 Hz, 1H), 3.76 (s, 3H), 3.56 (s, 3H), 2.37-2.29 (m, 2H), 2.10-1.87 (m, 2H), 1.40 (s, 3H), 1.18 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.1 (C), 146.4 (C), 137.9 (C), 133.0 (C), 129.8 (CH), 127.7 (CH x 2), 126.6 (C), 125.9 (CH), 124.6 (C), 121.6 (CH), 121.0 (CH), 118.2 (CH), 112.9 (CH x 2), 109.3 (CH), 55.4 (CH), 54.2 (CH_3), 39.7 (C), 32.45 (CH_2), 32.43 (CH_3), 28.3 (CH_2), 27.3 (CH_3), 25.4 (CH_3); IR: ν_{max} = 2962, 2932, 1685, 1606, 1509, 1465, 1328, 1292, 1248, 1177, 1152, 1036, 906, 832, 810, 732 cm^{-1}. For asymmetric synthesis of compound **3r** (14.6 mg, 84% yield); SFC Analysis: 92.5:7.5 e.r. [CHIRALPAK® IA, 30°C, 5% *i*PrOH, 4.0 mL/min, 100 bar, retention times: 8.6 min (minor) and 10.5 min (major)].



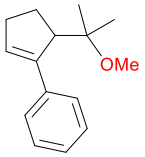
II. 23. 3-(2-(2-(2-Methoxyphenyl)cyclopent-2-en-1-yl)propan-2-yl)-1-methyl-1H-indole (3s) (20 mg, 64% yield) Colorless oil; R_f 0.32 (10% EtOAc/*n*-heptane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.85 (d, J = 7.9 Hz, 1H), 7.18-7.00 (m, 5H), 6.77 (t, J = 7.3 Hz, 1H), 6.34 (d, J = 8.0 Hz, 1H), 6.23 (s, 1H), 5.79 (d, J = 1.7 Hz, 1H), 4.35-4.25 (m, 1H), 3.47 (s, 3H), 3.24 (s, 3H), 2.41-2.35 (m, 2H), 2.13-2.05 (m, 1H), 1.96-1.89 (m, 1H), 1.40 (s, 3H), 1.15 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 156.5 (C), 145.5 (C), 137.5 (C), 132.0 (CH), 129.8 (CH), 127.0 (CH + C), 126.7 (C), 125.8 (CH), 124.3 (C), 121.9 (CH), 120.6 (CH), 119.6 (CH), 117.9 (CH), 109.3 (CH), 109.0 (CH), 54.4 (CH_3), 54.1 (CH), 38.9 (C), 32.3 (CH_3), 31.7 (CH_2), 27.2 (CH_2), 26.1 (CH_3), 24.9 (CH_3); IR: ν_{max} = 3051, 2963, 2931, 2849, 2253, 1595, 1578, 1545, 1487, 1464, 1435, 1362, 1330, 1265, 1239, 1181, 1115, 1029, 993, 907 cm^{-1}; HRMS(ESI) Calcd. For $C_{24}H_{28}NO$ $[M+H]^+$: 346.2171, found: 346.2162. For asymmetric synthesis of compound **3s** (15.7 mg, 91% yield); SFC Analysis: 96:4 e.r. [CHIRALPAK® AD-H, 30°C, 3% *i*PrOH, 4.0 mL/min, 100 bar, retention times: 6.8 min (major) and 8.3 min (minor)].



II.24. 3-(2-(2-Phenylcyclopent-2-en-1-yl)propan-2-yl)-3a,7a-dihydro-1H-indole (3t) (20.0 mg, 66% yield). Colorless oil; R_f 0.51 (20 % EtOAc/*n*-heptane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.98 (d, J = 7.6 Hz, 1H), 7.73 (bs, NH), 7.35 (dd, J = 6.9, 1.2 Hz, 1H), 7.29-7.16 (m, 7H), 6.77 (d, J = 2.4 Hz, 1H), 5.97 (bs, 1H), 4.09 (d, J = 9.2 Hz, 1H), 2.42-2.35 (m, 2H), 2.17-1.88 (m, 2H), 1.44 (s, 3H), 1.24 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 146.7 (C), 140.3 (C), 137.3 (C), 131.5 (CH), 127.8 (CH x 2), 126.7 (CH x 2), 126.2 (CH + C), 121.6 (CH), 121.5 (CH), 120.7 (CH + C), 118.9 (CH), 111.4 (CH), 53.7 (CH), 40.0 (C), 32.5 (CH_2), 28.5 (CH_2), 28.0 (CH_3), 24.8 (CH_3); IR: ν_{max} = 3424, 3054, 2966, 1459, 1416, 1363, 1335, 1265, 1103, 1017, 896, 737, 700 cm^{-1}; HRMS(ESI) Calcd. For $C_{22}H_{24}N$ $[M+H]^+$: 302.1909, found: 302.1907. For asymmetric synthesis of compound **3t** (11.5 mg, 78% yield); SFC Analysis: 88:12 e.r. [CHIRALPAK® IA, 30°C, 10% *i*PrOH, 4.0 mL/min, 100 bar, retention times: 10.5 min (minor) and 13.0 min (major)].

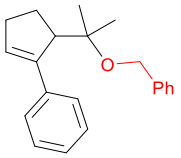


II.25. (5-(2-Methoxypropan-2-yl)cyclopent-1-en-1-yl)benzene (3u) (20.0 mg, 93% yield). Colorless oil; R_f 0.36 (5% EtOAc/*n*-heptane); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33 (d, J = 7.5 Hz, 2H), 7.28 (t, J = 7.5 Hz, 2H), 7.21 (t, J = 7.5 Hz, 1H), 5.94 (s, 1H), 3.44 (d, J = 9.4 Hz, 1H), 3.16 (s, 3H), 2.47-2.40 (m, 2H), 2.23-2.19 (m, 1H), 2.16-2.10 (m,

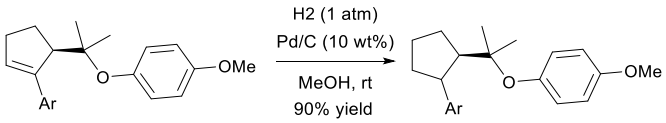


1H), 1.05 (s, 3H), 0.88 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 145.8 (C), 139.6 (C), 131.9 (CH), 128.1 (CH x 2), 127.0 (CH x 2), 126.7 (CH), 78.4 (C), 53.8 (CH), 49.0 (CH_3), 32.5 (CH_2), 26.7 (CH_2), 24.8 (CH_3), 22.1 (CH_3); IR: ν_{max} = 2975, 2939, 1469, 1444, 1381, 1365, 1265, 1129, 1075, 909, 825, 797, 762, 735, 698 cm^{-1}; HRMS(ESI) Calcd. For $C_{14}H_{17}$ [M-OMe]$^+$:185.1330, found: 185.1369.

II.26. (5-(2-(Benzyloxy)propan-2-yl)cyclopent-1-en-1-yl)benzene (3v) (29.0 mg, 99% yield). Colorless oil; R_f 0.50 (5 % EtOAc/*n*-heptane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.37-7.31 (m, 2H), 7.31-7.14 (m, 8H), 5.94 (bs, 1H), 4.39 (s, 2H), 3.53 (d, J = 8.7 Hz, 1H), 2.51-2.40 (m, 2H), 2.39-2.25 (m, 1H), 2.16 (dq, J = 13.5, 9.3 Hz, 1H), 1.14 (s, 3H), 1.00 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 145.8 (C), 134.0 (C), 139.7 (C), 132.0 (CH), 128.3 (CH x 2), 128.2 (CH x 2), 127.4 (CH x 2), 127.1 (CH x 3), 126.7 (CH), 79.2 (C), 63.6 (CH_2), 54.6 (CH), 32.6 (CH_2), 27.1 (CH_2), 25.0 (CH_3), 22.8 (CH_3); IR: ν_{max} = 2975, 2898, 1706, 1494, 1452, 1385, 1365, 1265, 1145, 1062, 1027, 910, 733, 696 cm^{-1}; HRMS(ESI) Calcd. For $C_{21}H_{24}NaO$ [M+Na]$^+$: 315.1725, found: 315.1720.



II.27. Hydrogenation of compound 3c.



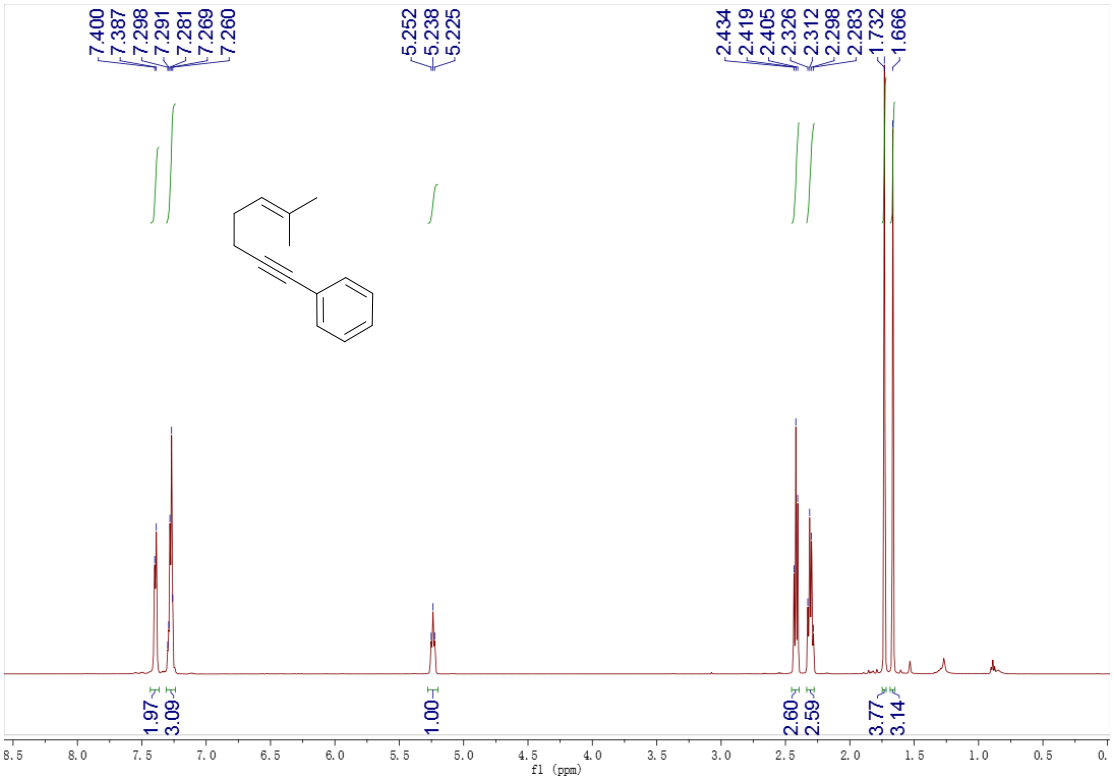
3c, Ar = *p*OMe-C_6H_4 **4**

1-Methoxy-4-(2-(2-(4-methoxyphenoxy)propan-2-yl)cyclopentyl)benzene (4).

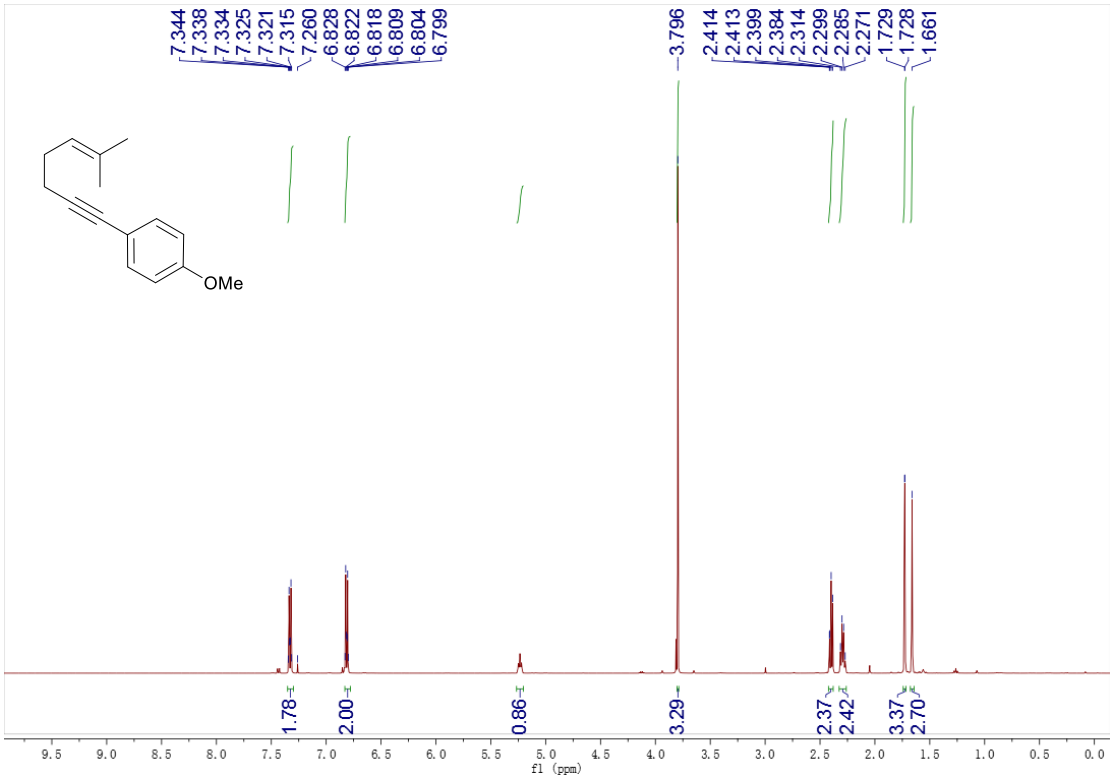
Pd/C (10 wt%, 2 mg) and compound **3c** (20 mg, 0.6 mmol, 90:10 e.r.) were added to a schlenk tube, and methanol (0.5 mL) was added. The reaction system was flushed three times with H_2. The mixture was stirred under H_2 atmosphere for 17 hours. The reaction mixture was then filtrated through silica pad, evaporated and dried under vacuum to possess pure target compound **4** (18 mg, 90% yield). Colorless oil; R_f 0.33 (10% EtOAc/*n*-heptane); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.21 (d, J = 8.6 Hz, 2H), 6.85 (d, J = 8.5 Hz, 2H), 6.79-6.71 (m, 4H), 3.80 (s, 3H), 3.76 (s, 3H), 3.41 (dd, J = 7.0, 6.0 Hz, 1H), 2.40 (q, J = 7.5 Hz, 1H), 2.28-2.14 (m, 1H), 2.12-1.93 (m, 3H), 1.93-1.82 (m, 2H), 0.92 (s, 3H), 0.89 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 157.9 (C), 155.7 (C), 148.4 (C), 138.3 (C), 130.6 (CH x 2), 125.7 (CH x 2), 113.8 (CH x 2), 113.3 (CH x 2), 82.0 (C), 56.1 (CH), 55.6 (CH_3), 55.4 (CH_3), 46.1 (CH), 34.1 (CH_2), 26.1 (CH_2), 25.9 (CH_3), 24.4 (CH_3), 23.1 (CH_2); IR: ν_{max} = 3054, 2954, 2835, 2062, 1610, 1583, 1503, 1464, 1442, 1265, 1247, 1218, 1180, 1143, 1121, 1037, 938, 806, 788, 736, 703; HRMS(ESI) Calcd. For $C_{15}H_{21}O$ [M-O-*p*OMe-C_6H_4]$^+$: 217.1592, found: 217.1580; SFC Analysis: 90:10 e.r. [CHIRALPAK® IC, 30°C, 10% *i*PrOH, 4.0 mL/min, 100 bar, retention times: 4.3 min (minor) and 5.1 min (major)].

III. NMR Spectra (^{1}H, ^{13}C and ^{19}F NMR):

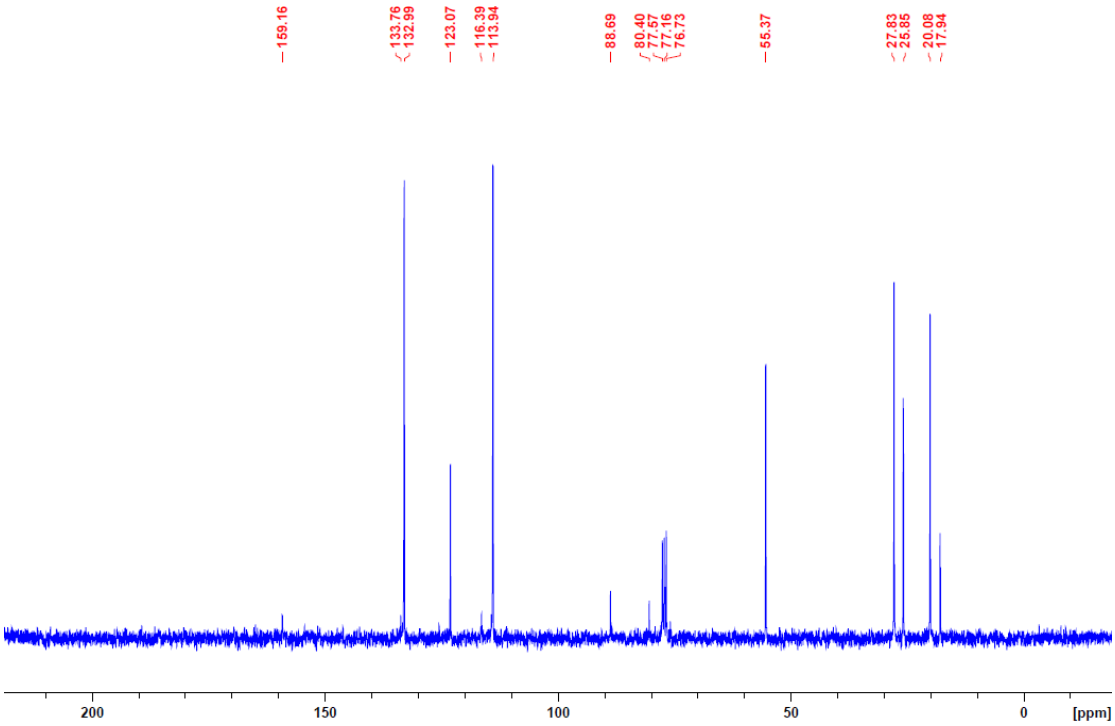
III.1. ^{1}H NMR ($CDCl_3$, 300 MHz) (**1a**)[1]



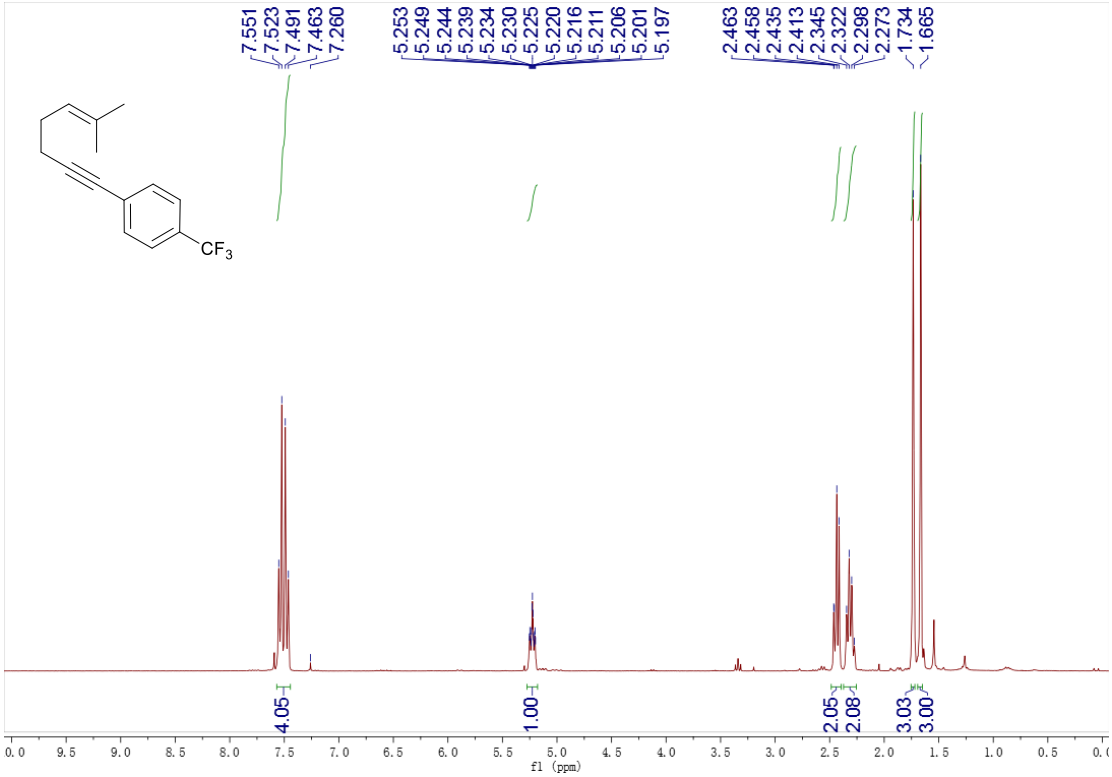
III.2. ^{1}H NMR ($CDCl_3$, 500 MHz) (**1b**)



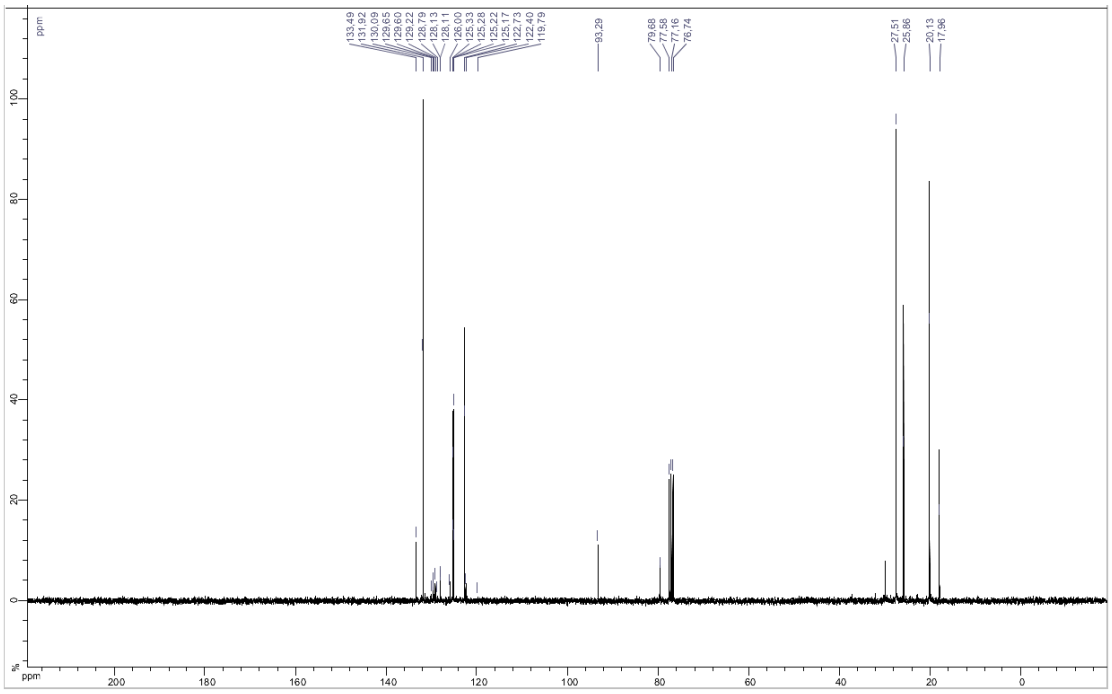
^{13}C NMR ($CDCl_3$, 75 MHz)



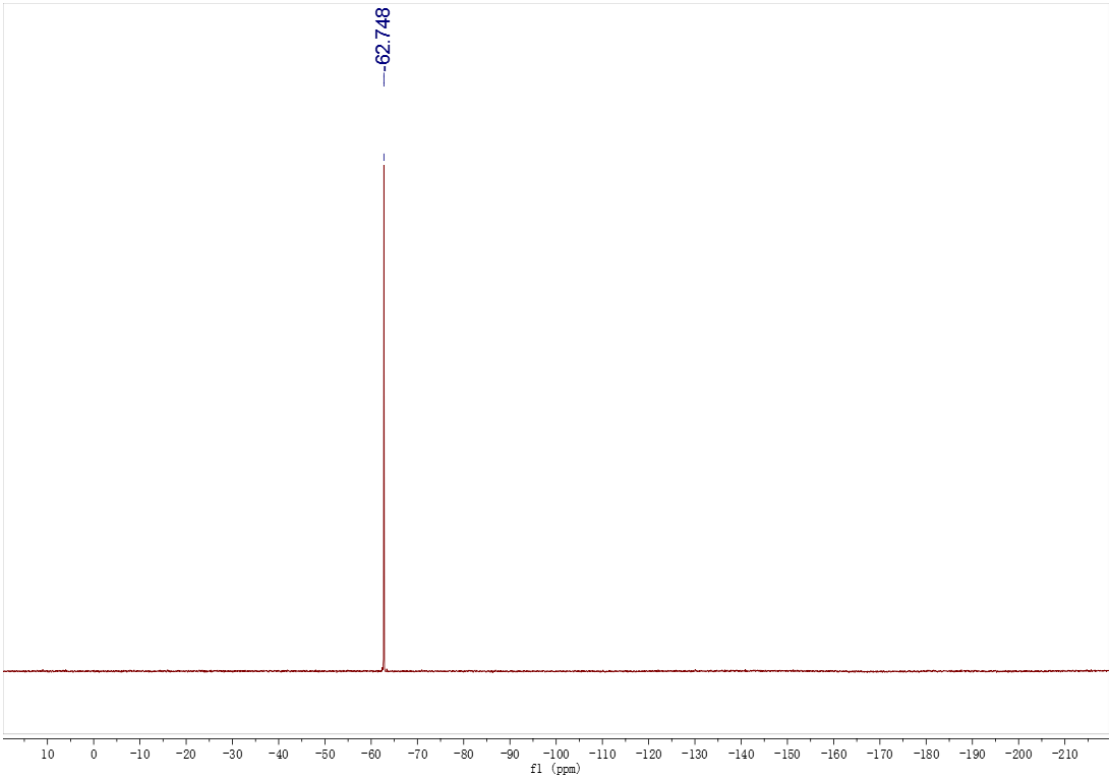
III.3. ^{1}H NMR ($CDCl_3$, 300 MHz) (**1c**)



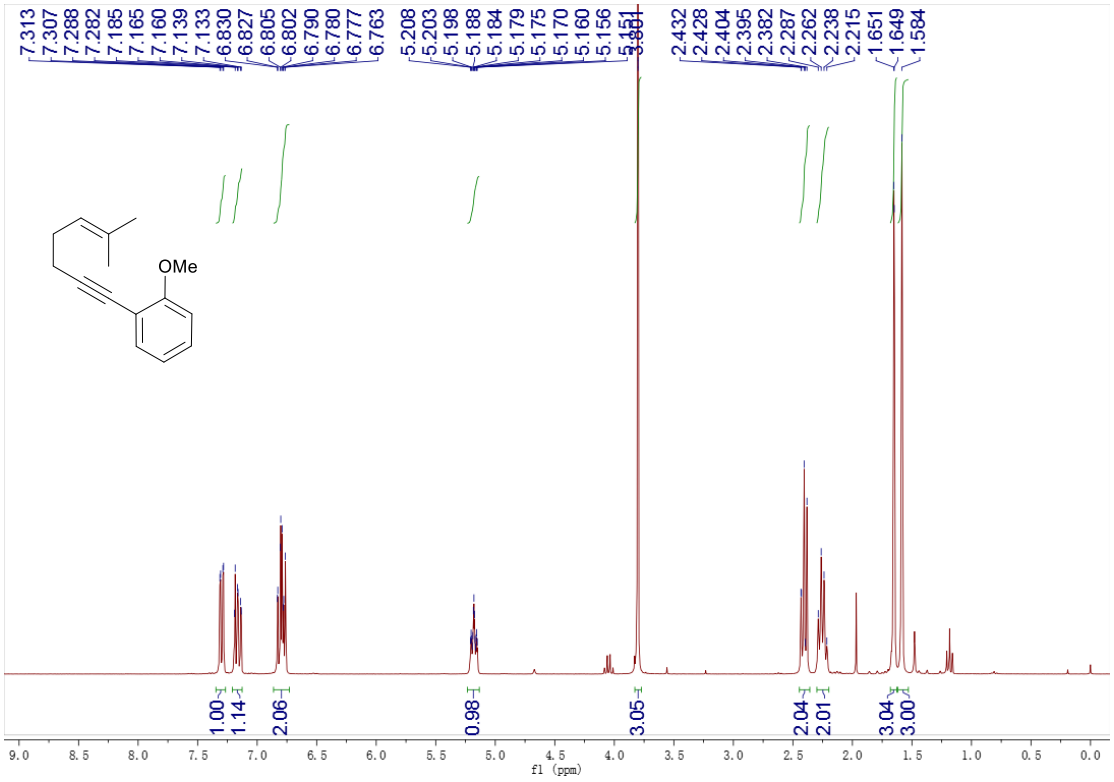
^{13}C NMR ($CDCl_3$, 75 MHz)



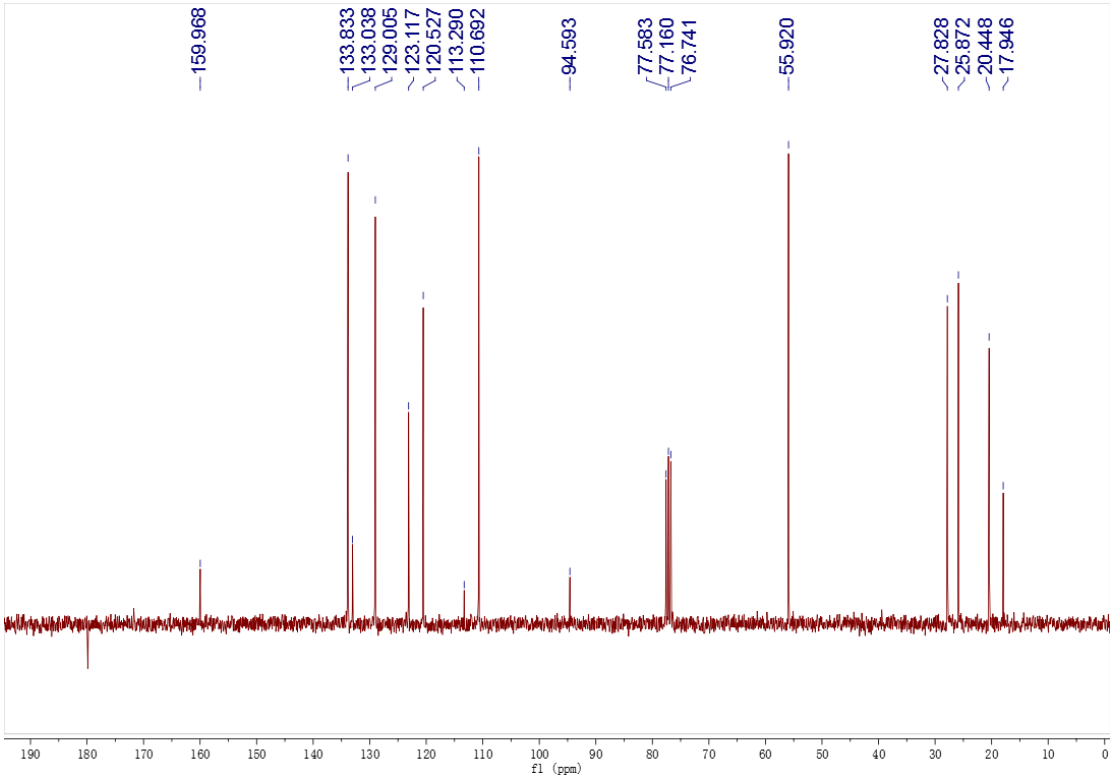
^{19}F NMR (282 MHz, $CDCl_3$)



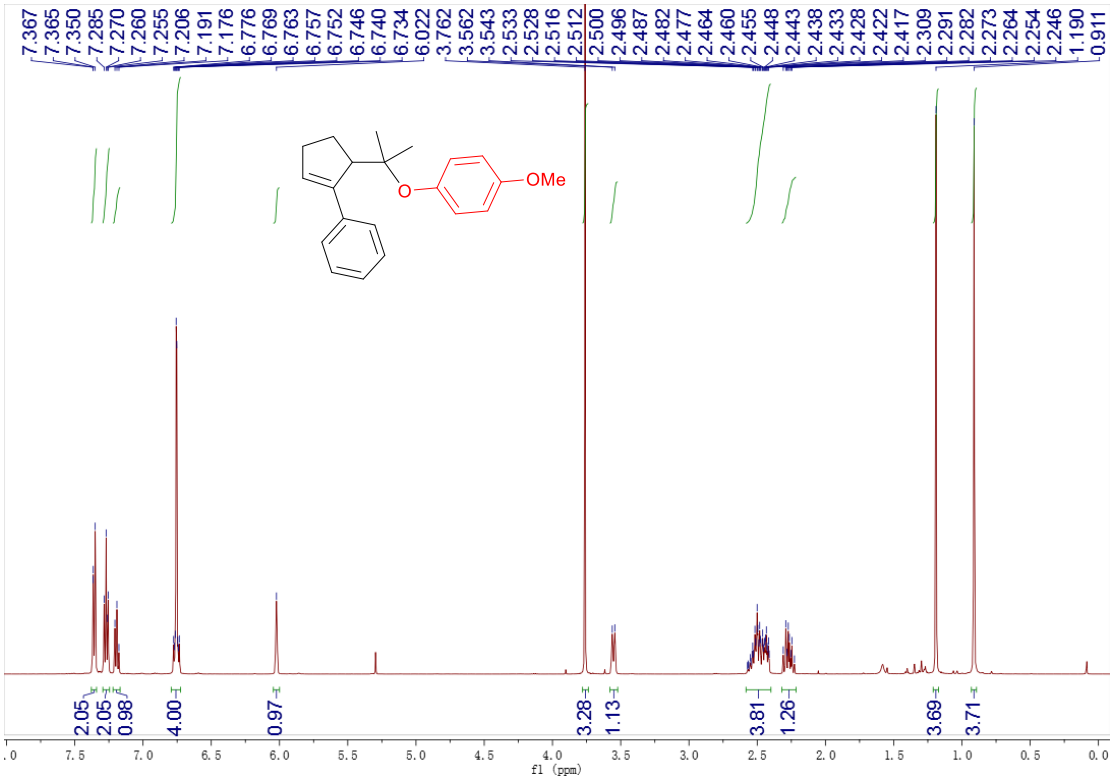
III.4. ^{1}H NMR ($CDCl_3$, 300 MHz) (**1d**)



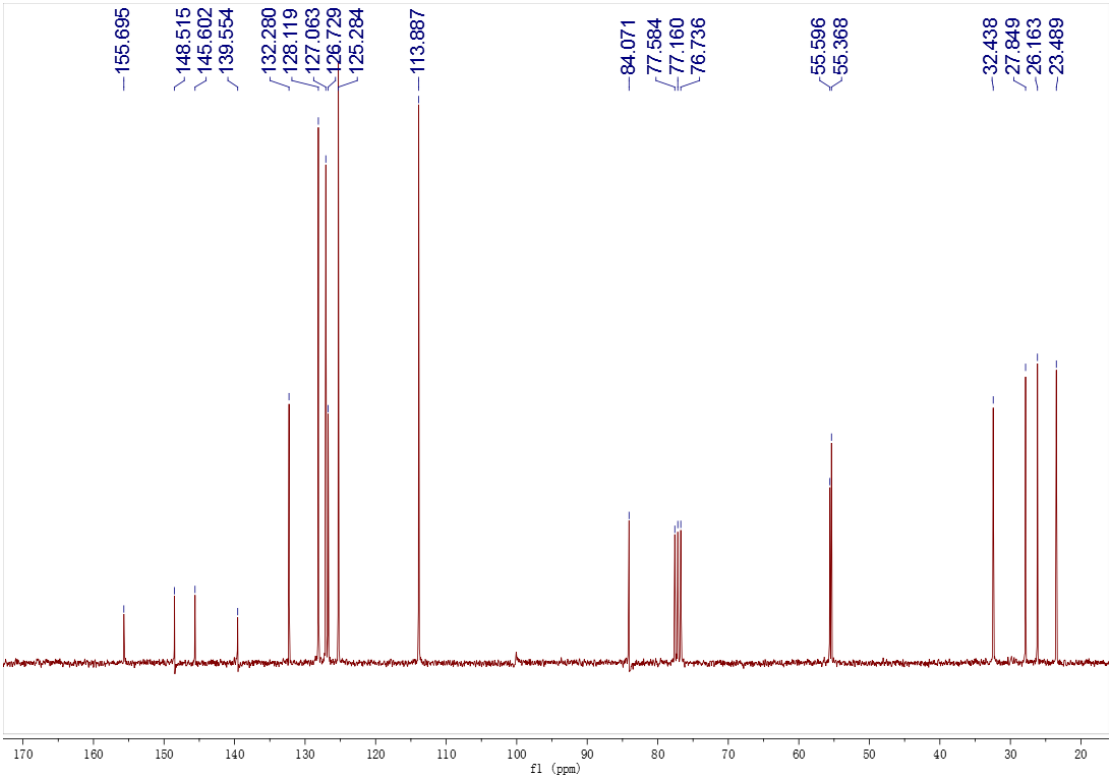
^{13}C NMR ($CDCl_3$, 75 MHz)



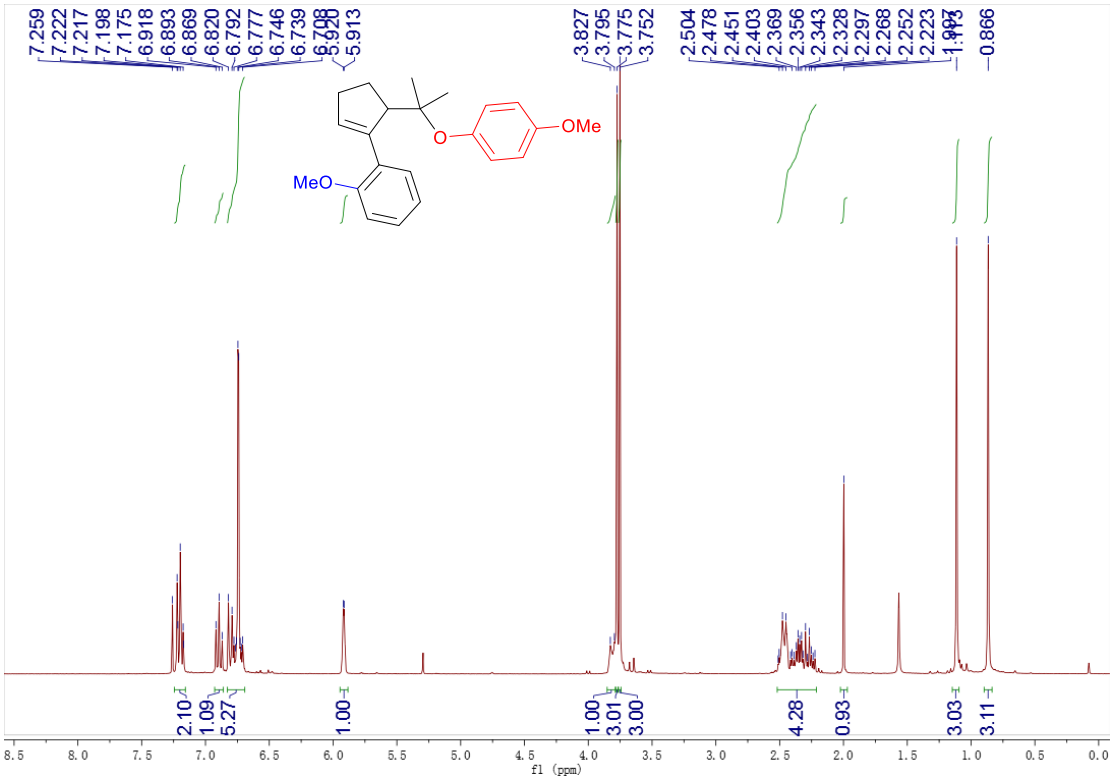
III.5. ^{1}H NMR ($CDCl_3$, 300 MHz) (**3a**)



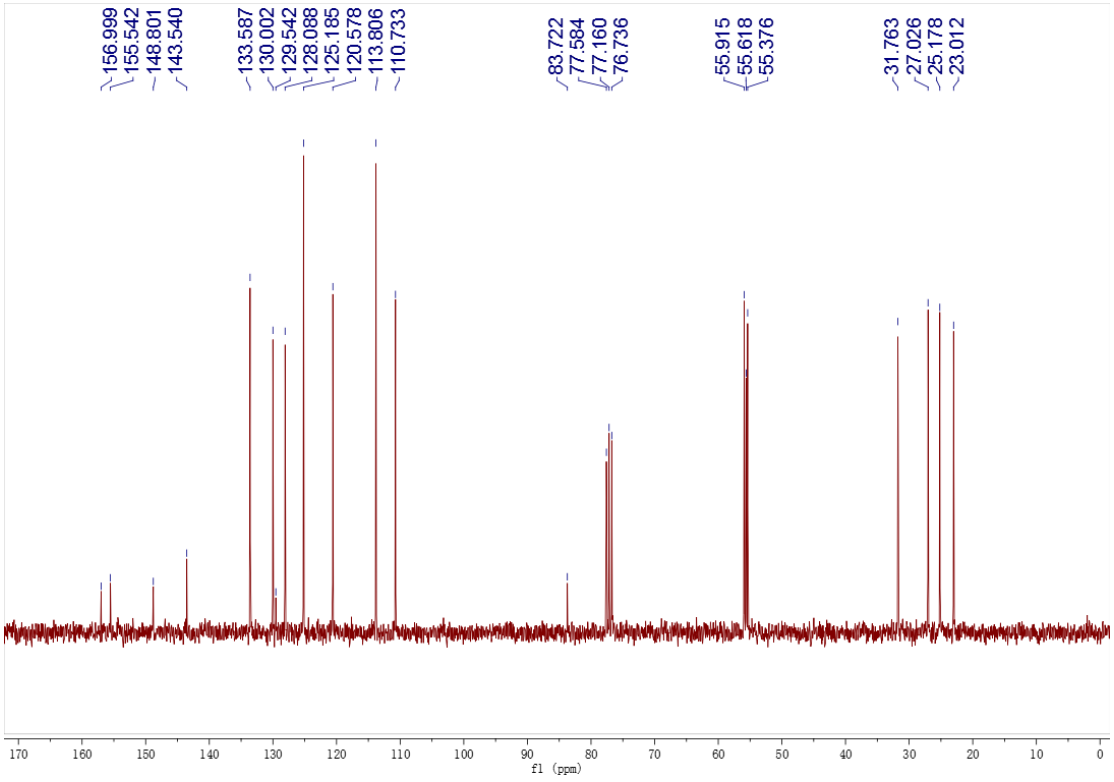
^{13}C NMR ($CDCl_3$, 75 MHz)



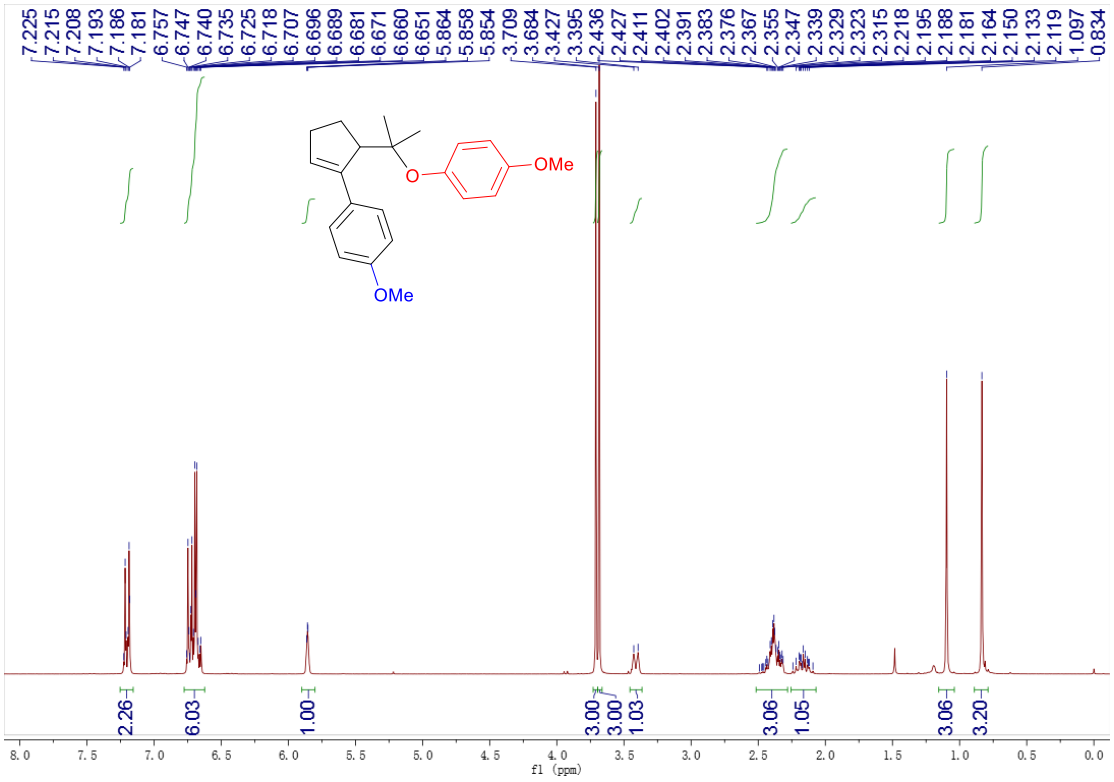
III.6. ^{1}H NMR ($CDCl_3$, 300 MHz) (**3b**)



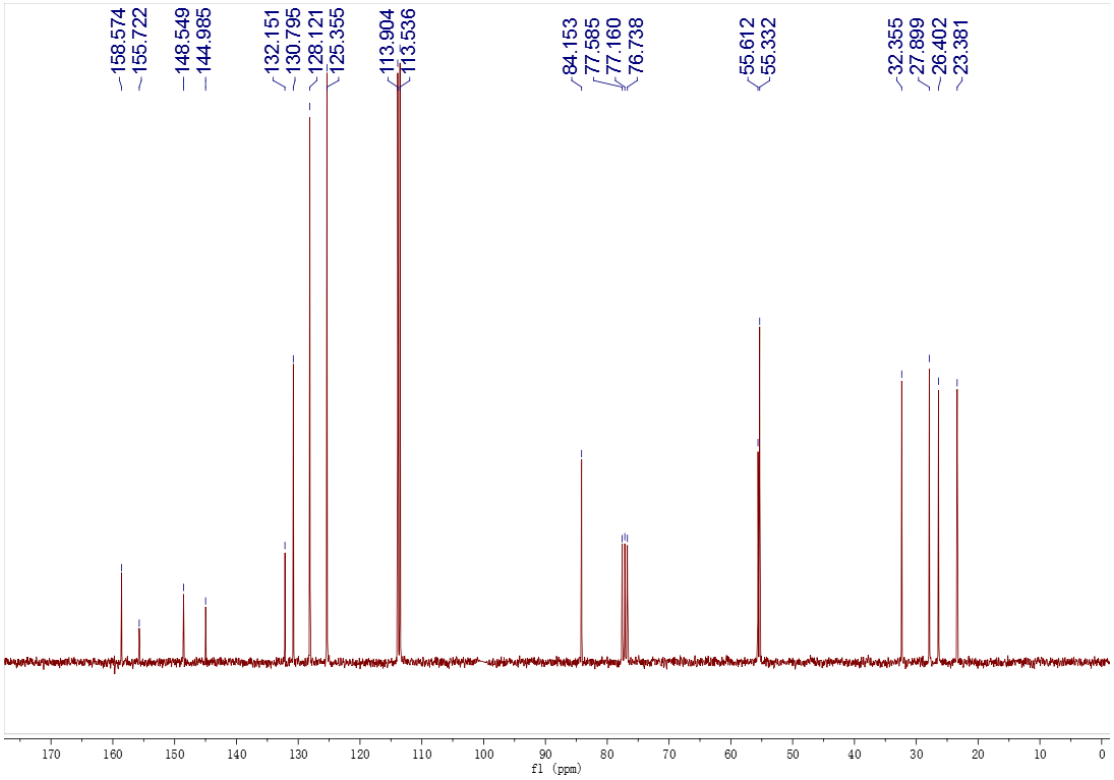
^{13}C NMR ($CDCl_3$, 75 MHz)



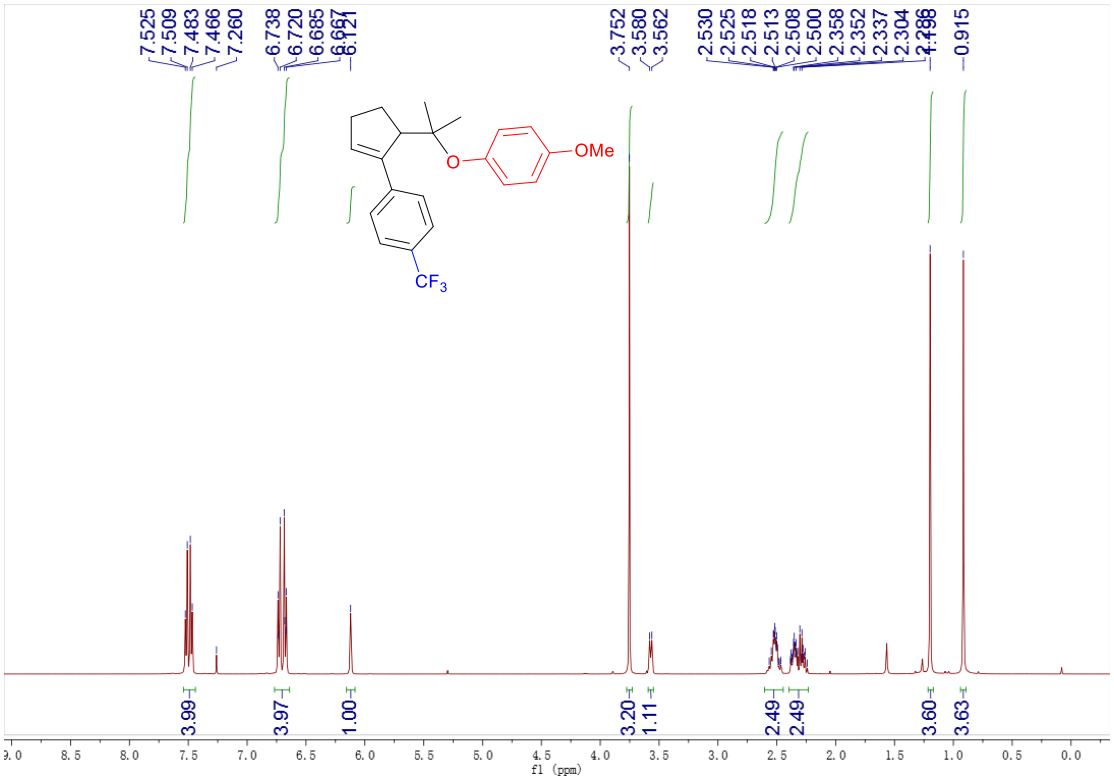
III.7. ^{1}H NMR ($CDCl_3$, 500 MHz) (**3c**)



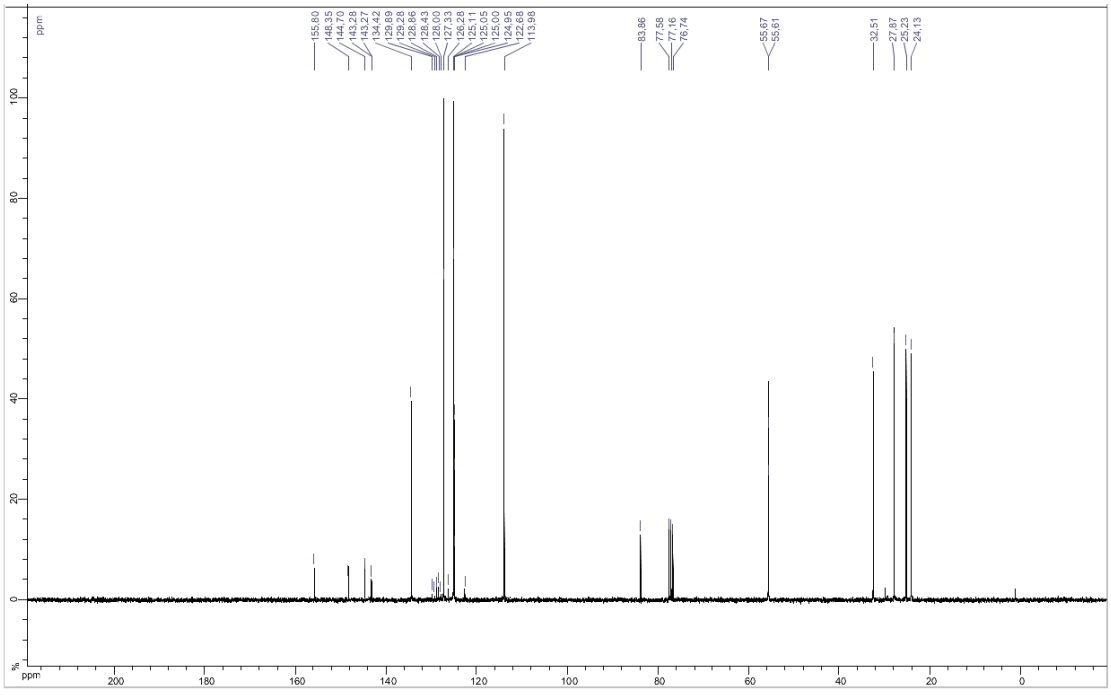
^{13}C NMR ($CDCl_3$, 75 MHz)



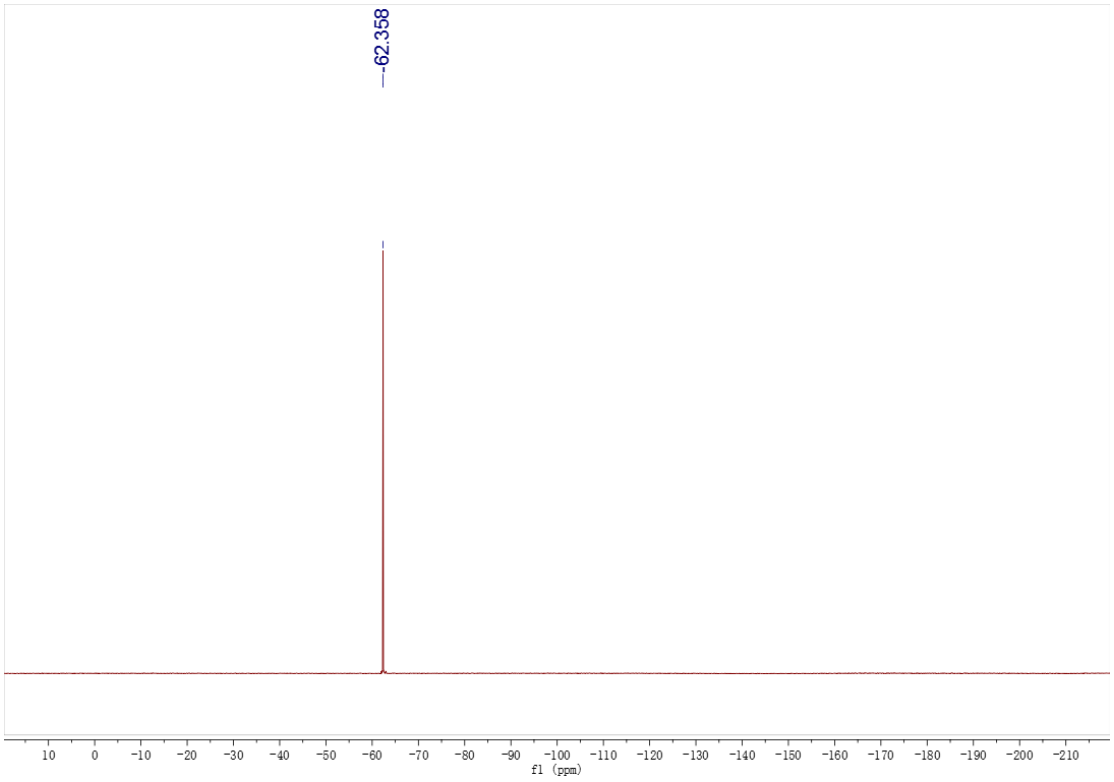
III.8. ^{1}H NMR ($CDCl_3$, 500 MHz) (**3d**)



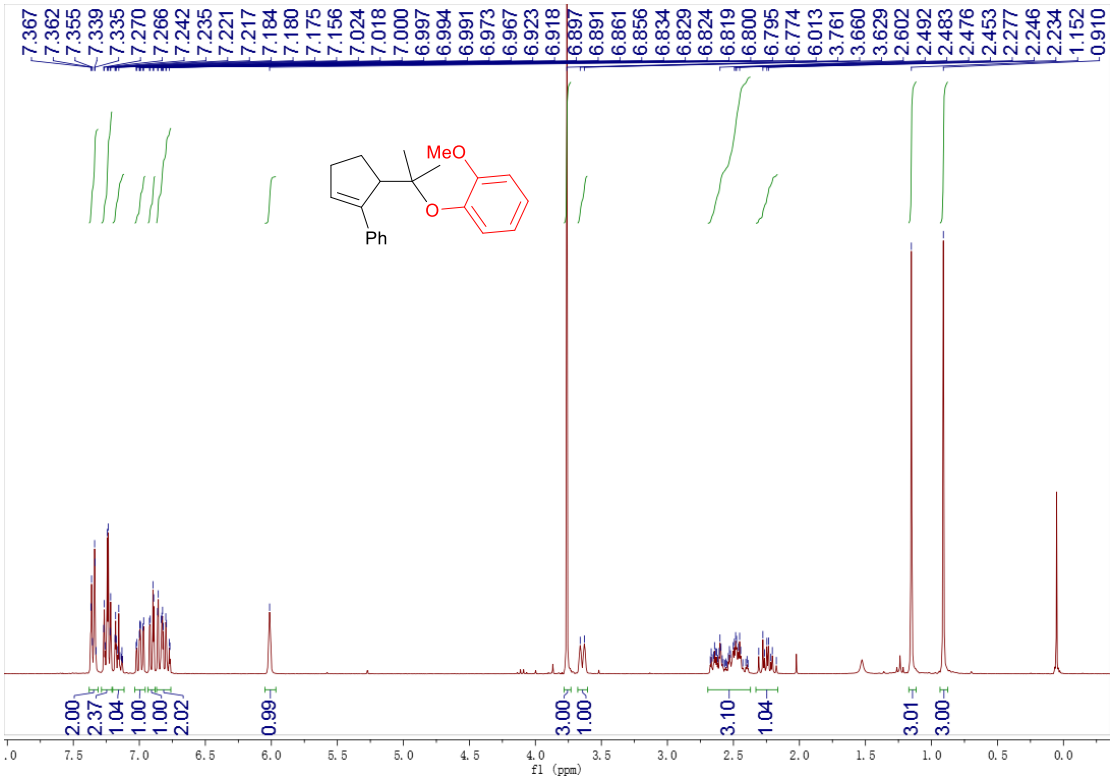
^{13}C NMR ($CDCl_3$, 75 MHz)



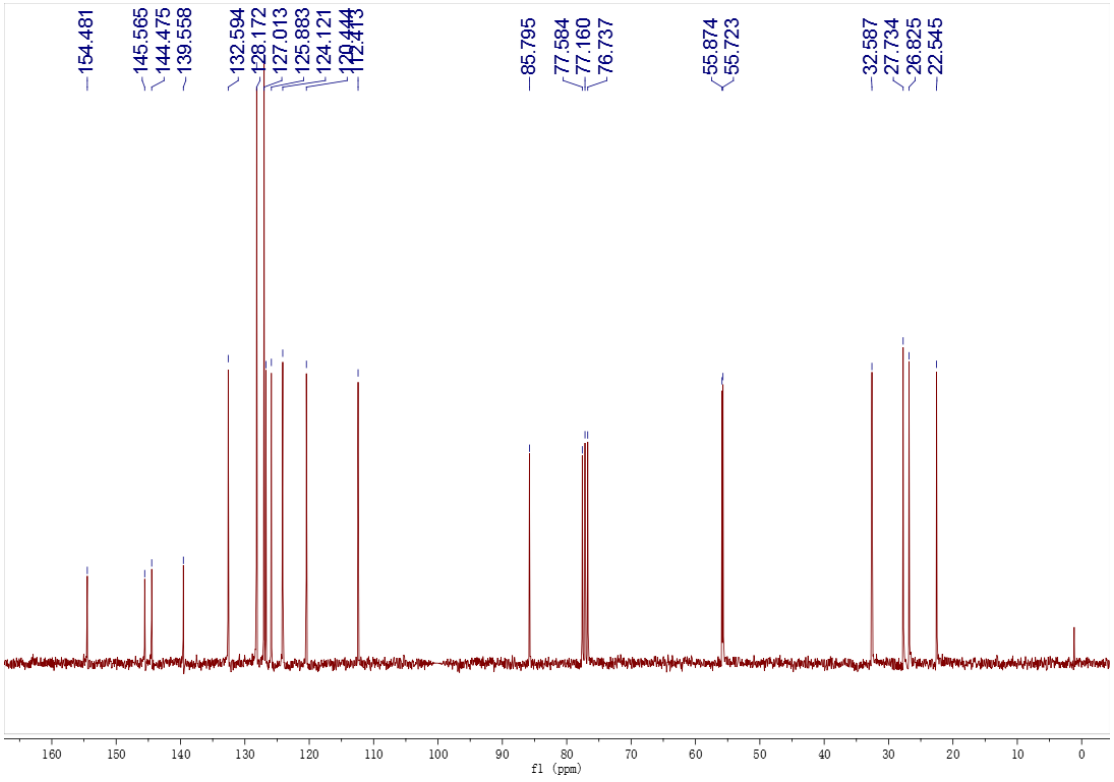
^{19}F NMR (282 MHz, $CDCl_3$)



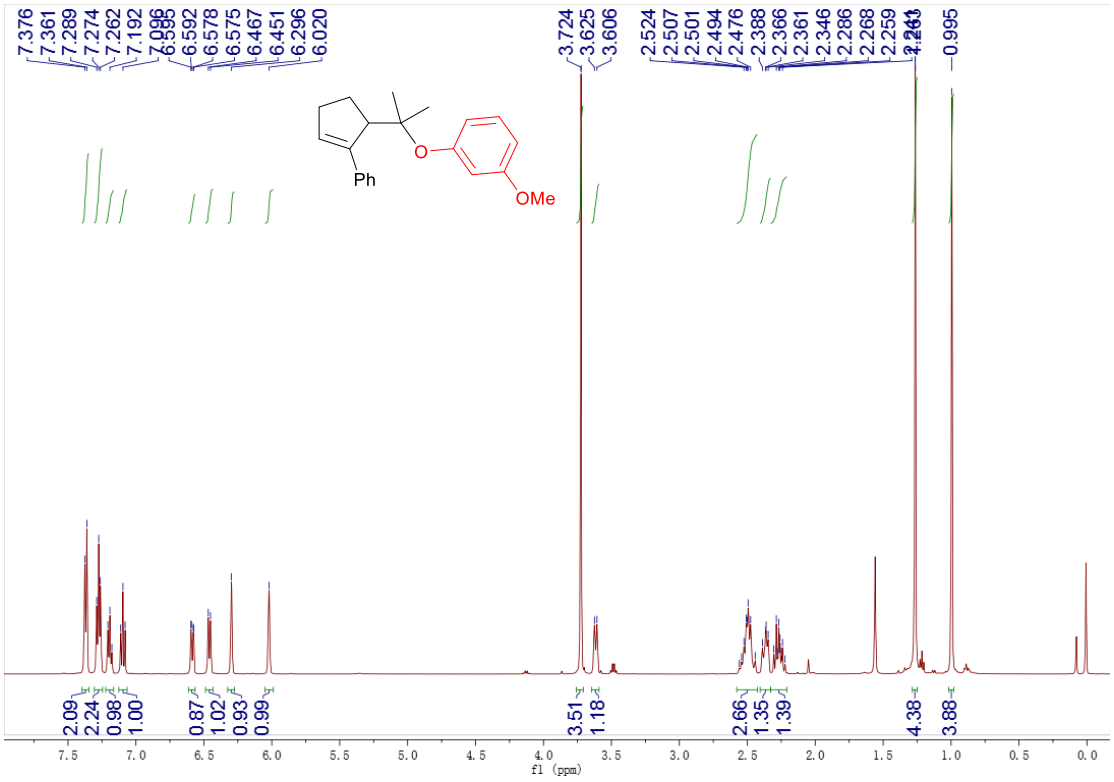
III.9. ^{1}H NMR ($CDCl_3$, 300 MHz) (**3e**)



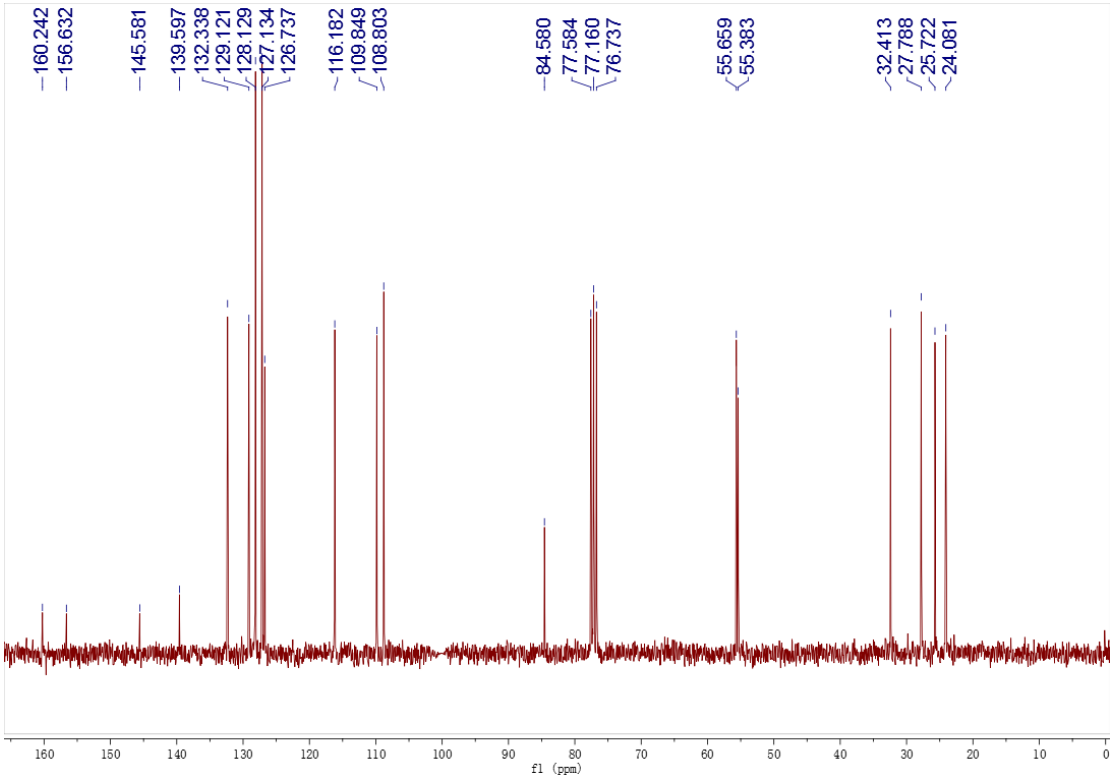
^{13}C NMR ($CDCl_3$, 75 MHz)



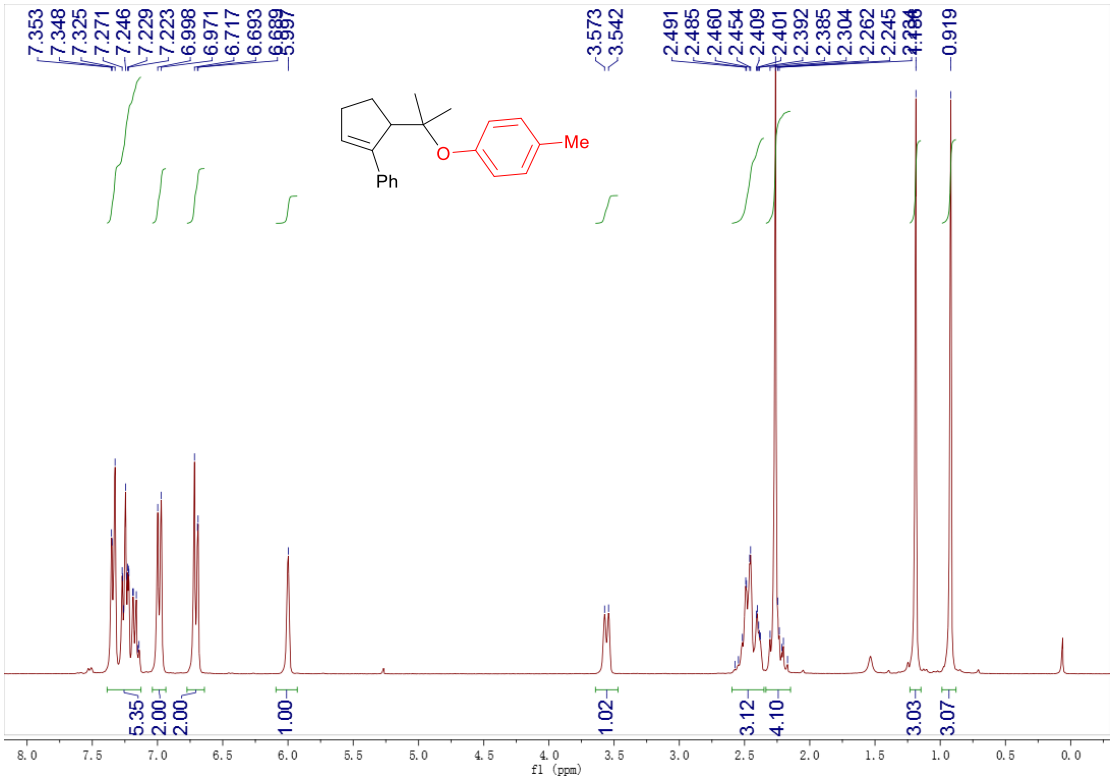
III.10. ^{1}H NMR ($CDCl_3$, 500 MHz) (**3f**)



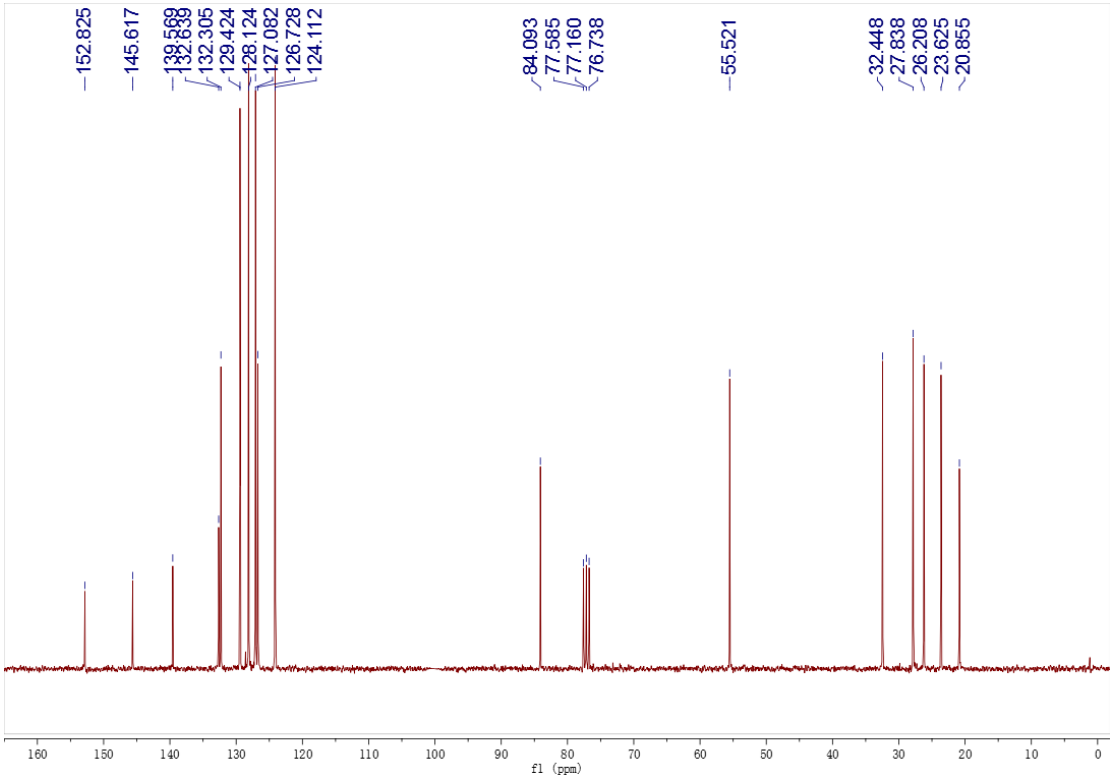
^{13}C NMR ($CDCl_3$, 75 MHz)



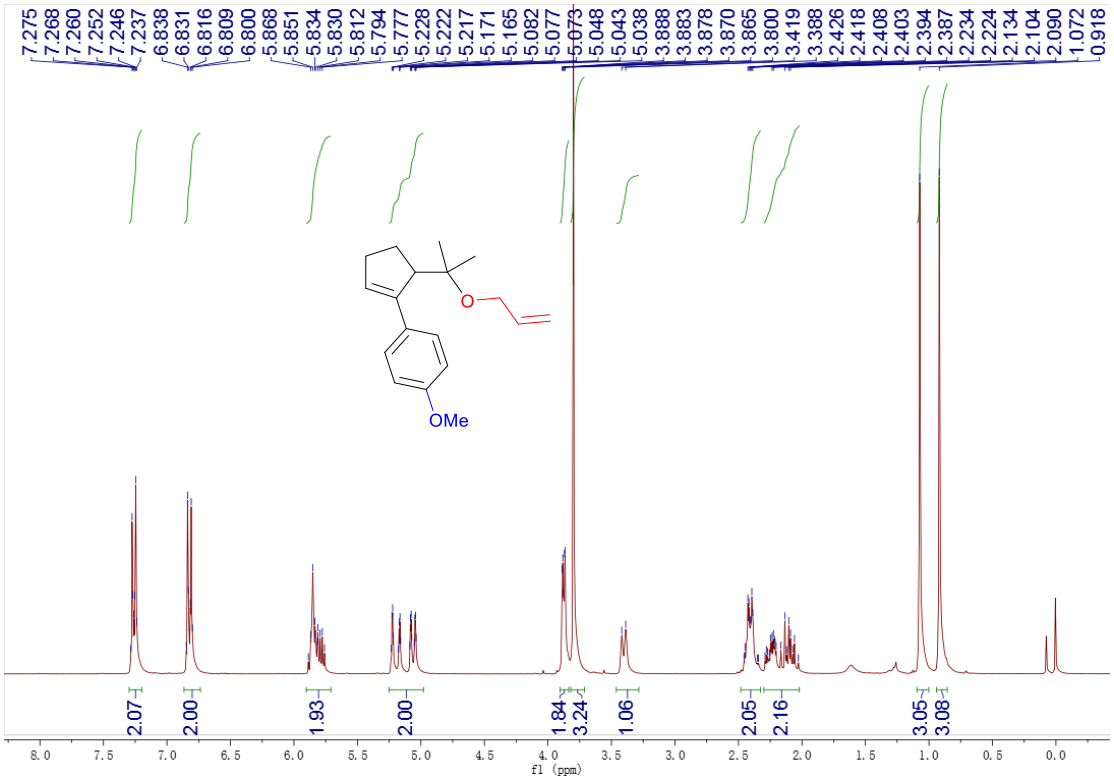
III.11. ^{1}H NMR ($CDCl_3$, 300 MHz) (**3g**)



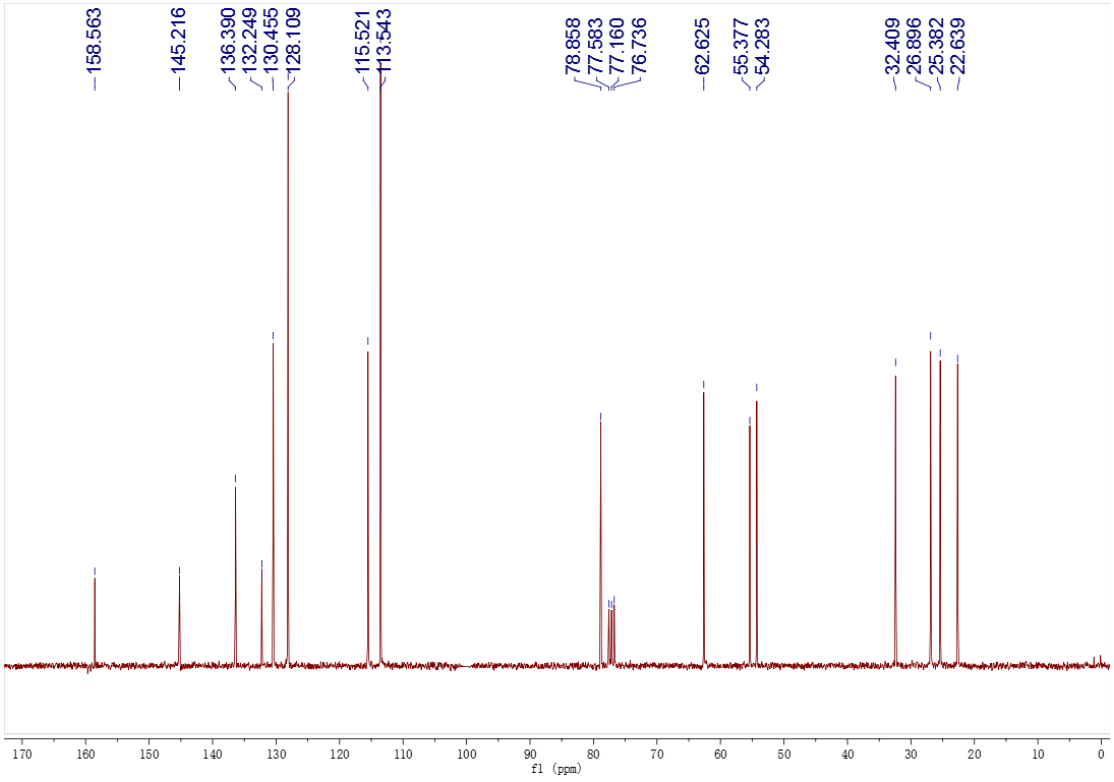
^{13}C NMR ($CDCl_3$, 75 MHz)



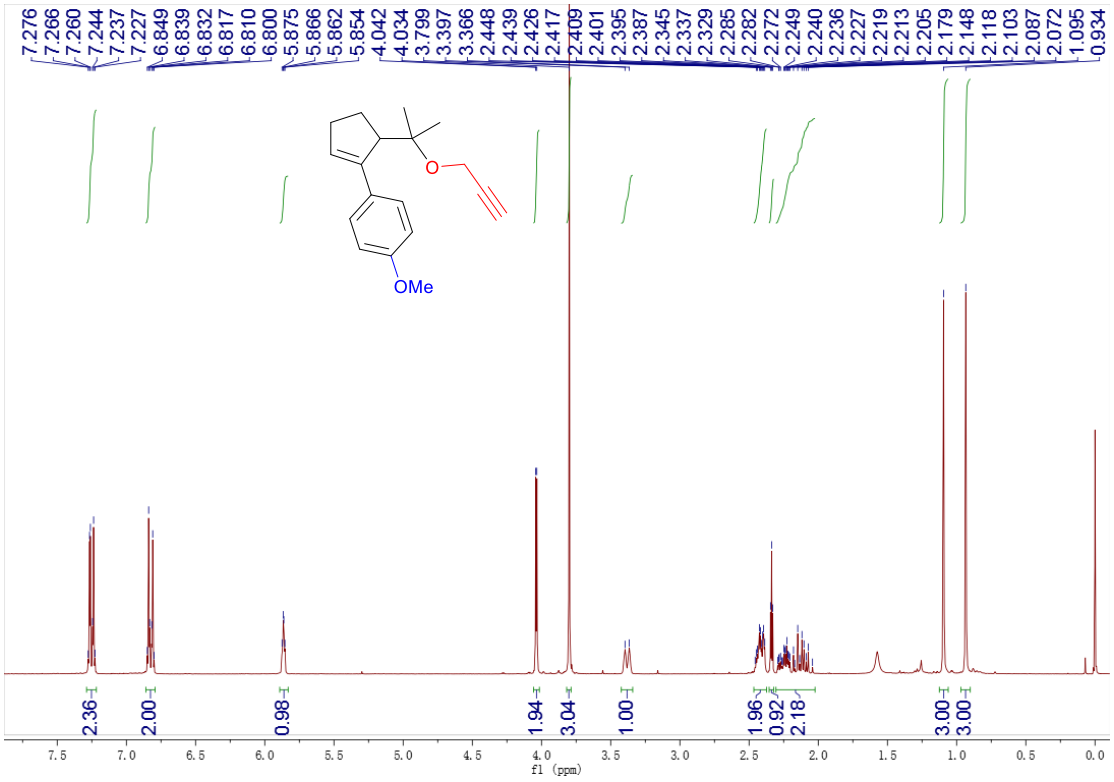
III.12. ^{1}H NMR ($CDCl_3$, 300 MHz) (**3h**)



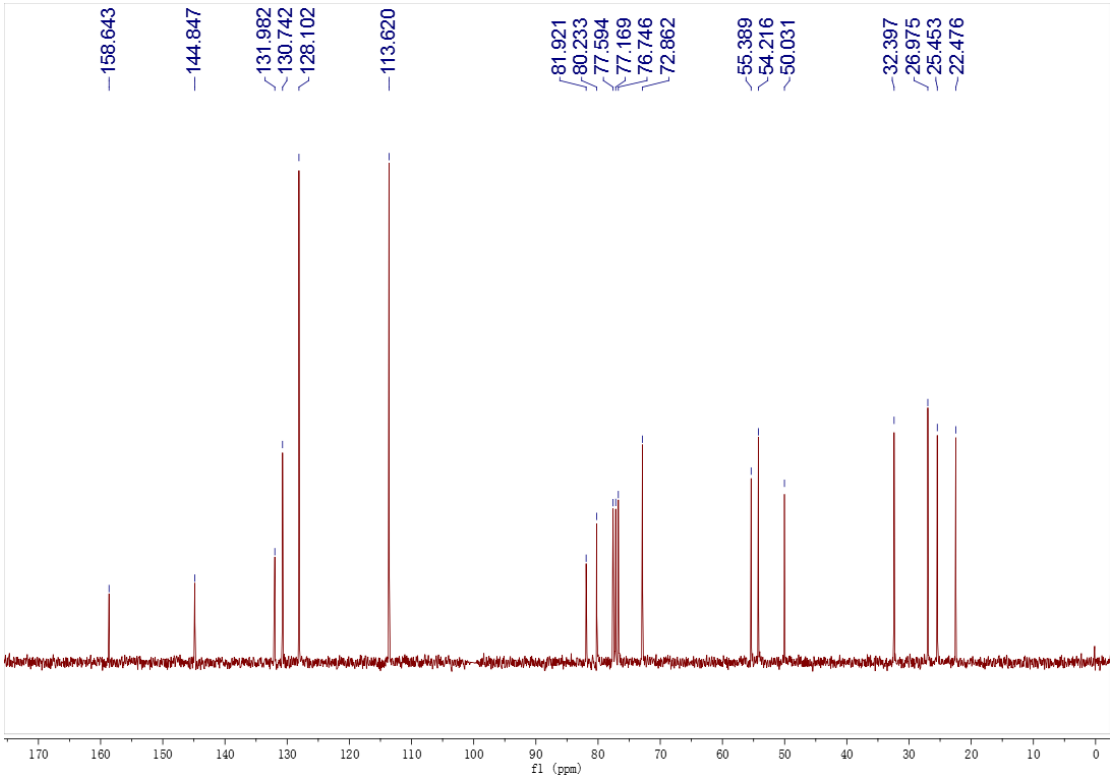
^{13}C NMR ($CDCl_3$, 75 MHz)



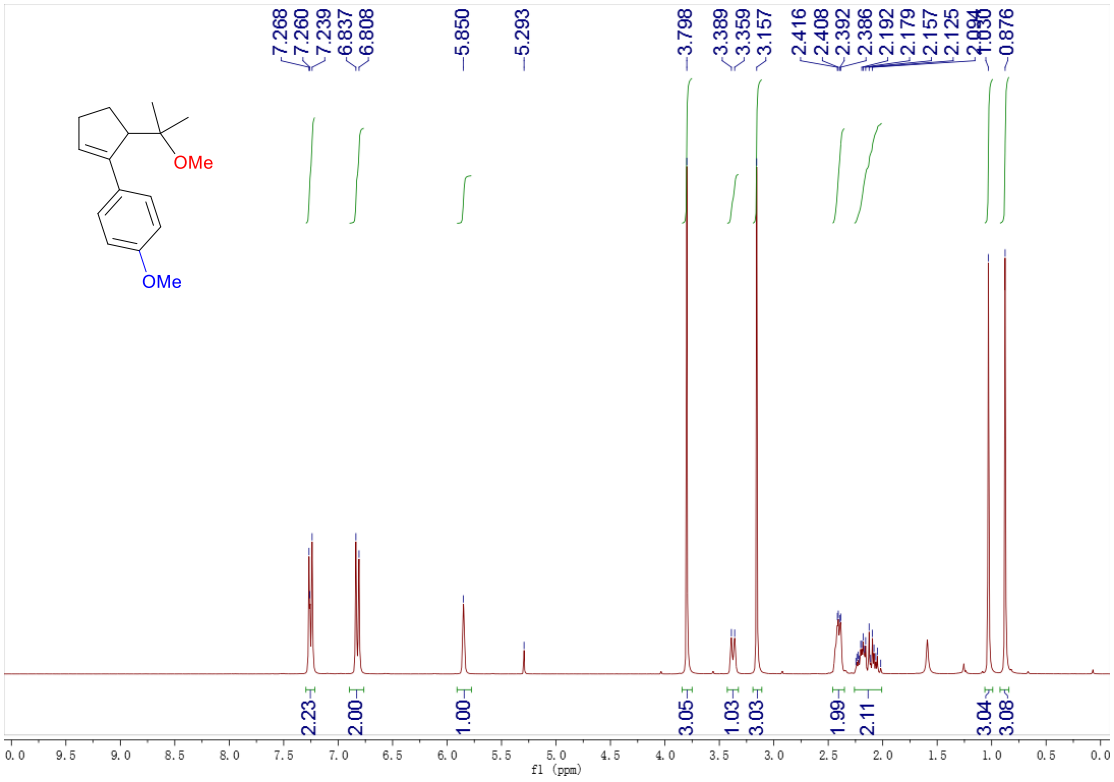
III.13. ^{1}H NMR ($CDCl_3$, 300 MHz) (**3i**)



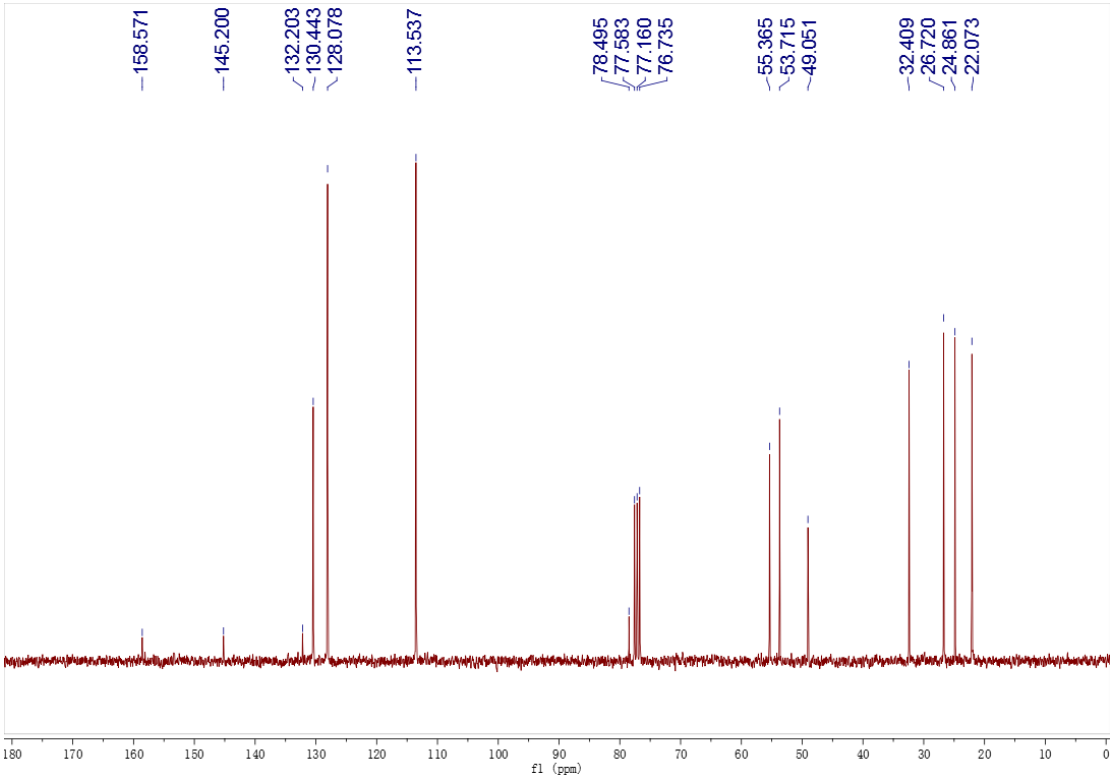
^{13}C NMR ($CDCl_3$, 75 MHz)



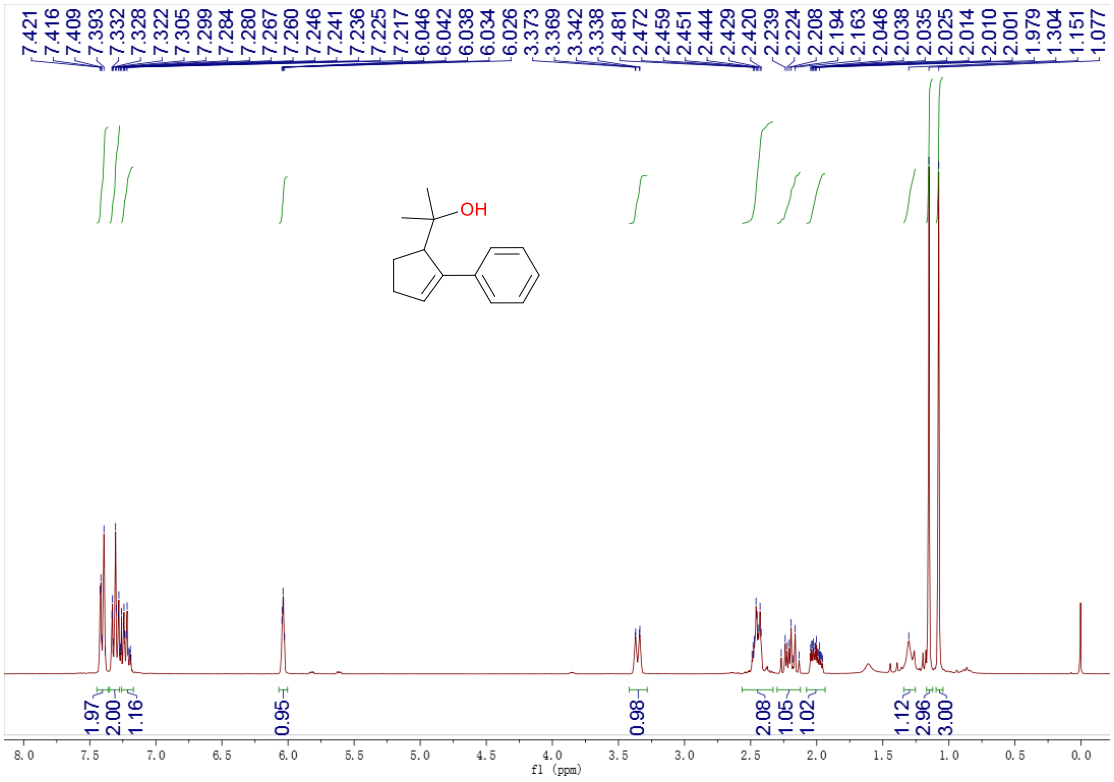
III.14. ^{1}H NMR ($CDCl_3$, 300 MHz) (**3j**)



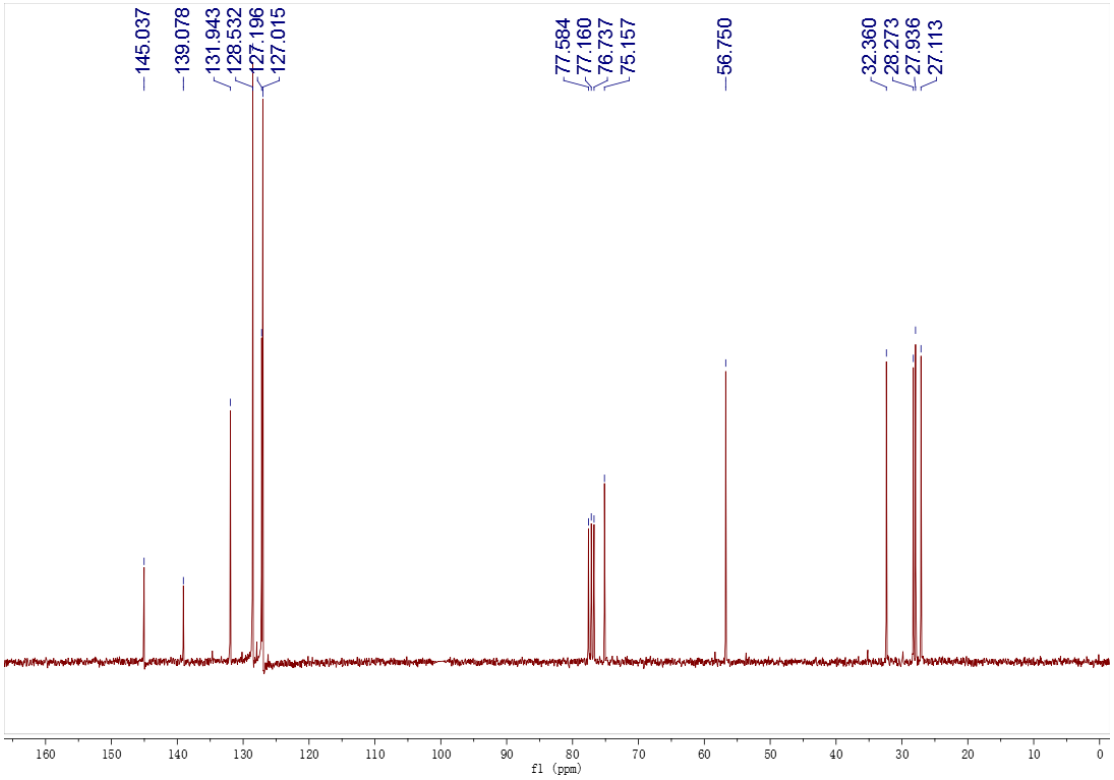
^{13}C NMR ($CDCl_3$, 75 MHz)



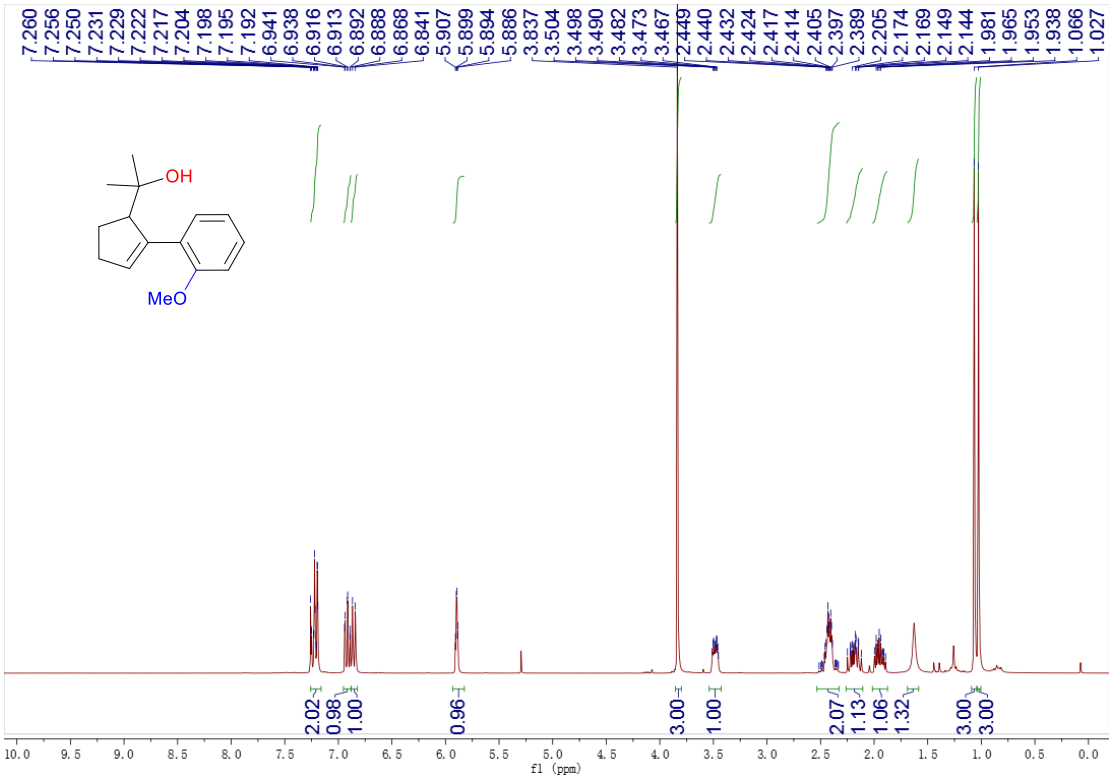
III.15. ^{1}H NMR ($CDCl_3$, 300 MHz) (**3k**)



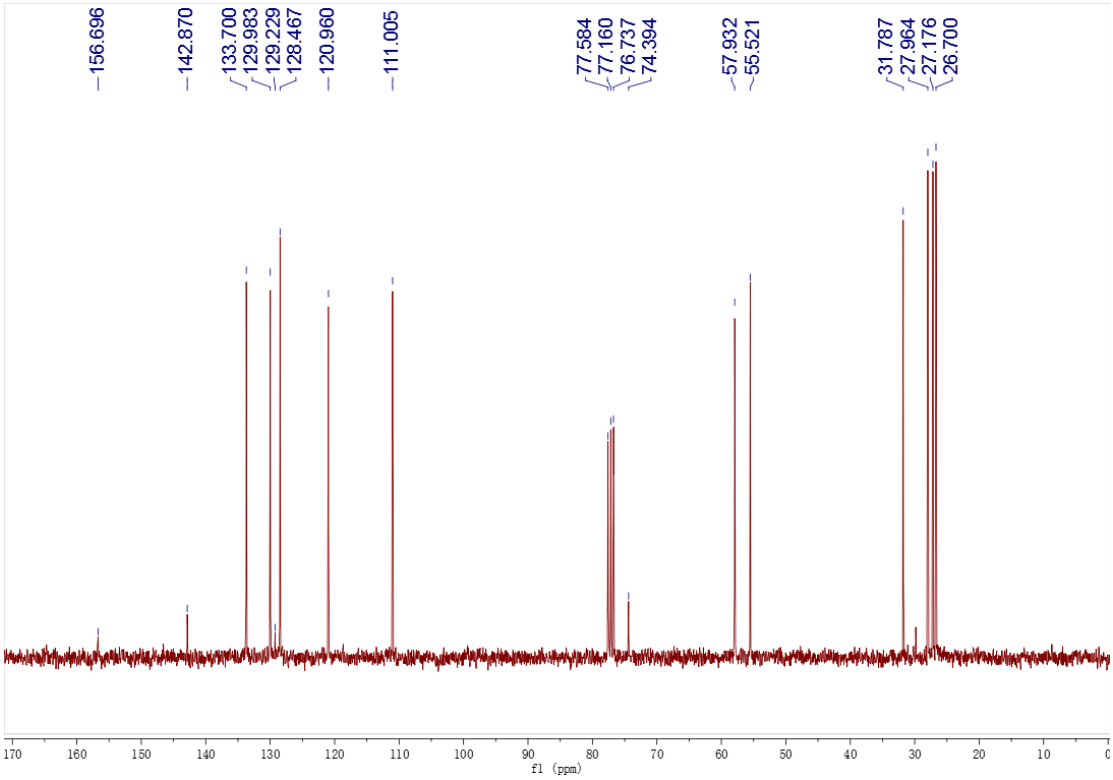
^{13}C NMR ($CDCl_3$, 75 MHz)



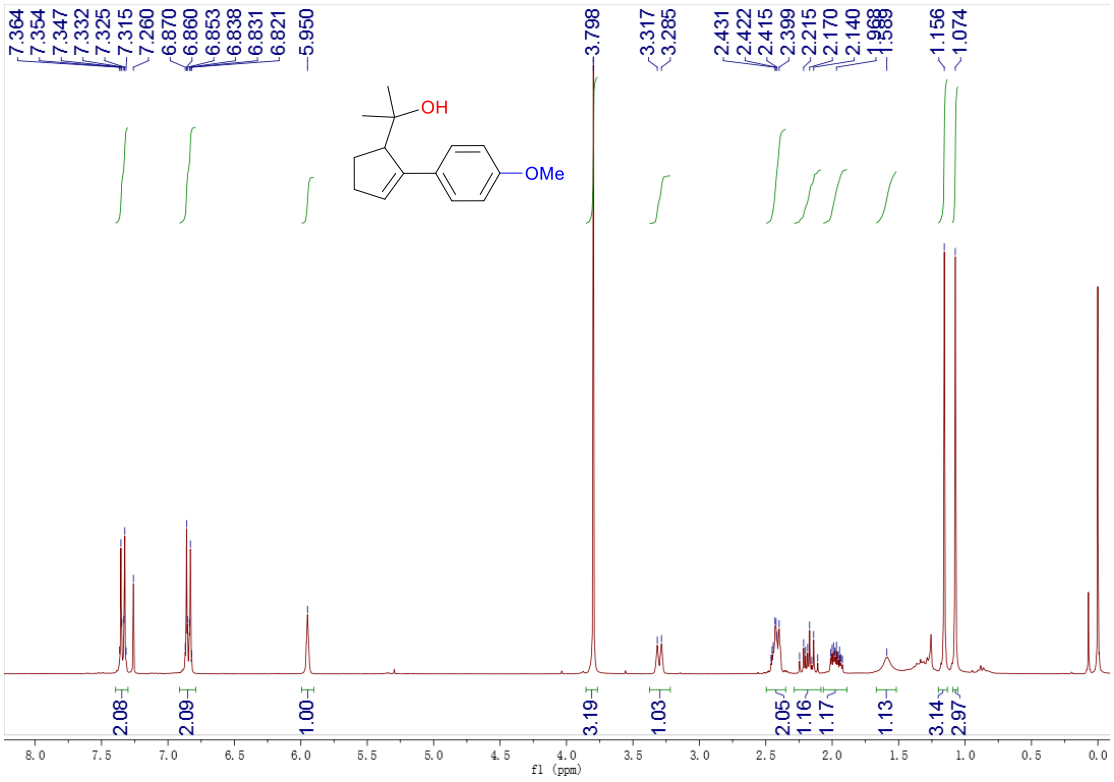
III.16. ^{1}H NMR ($CDCl_3$, 300 MHz) (**3l**)



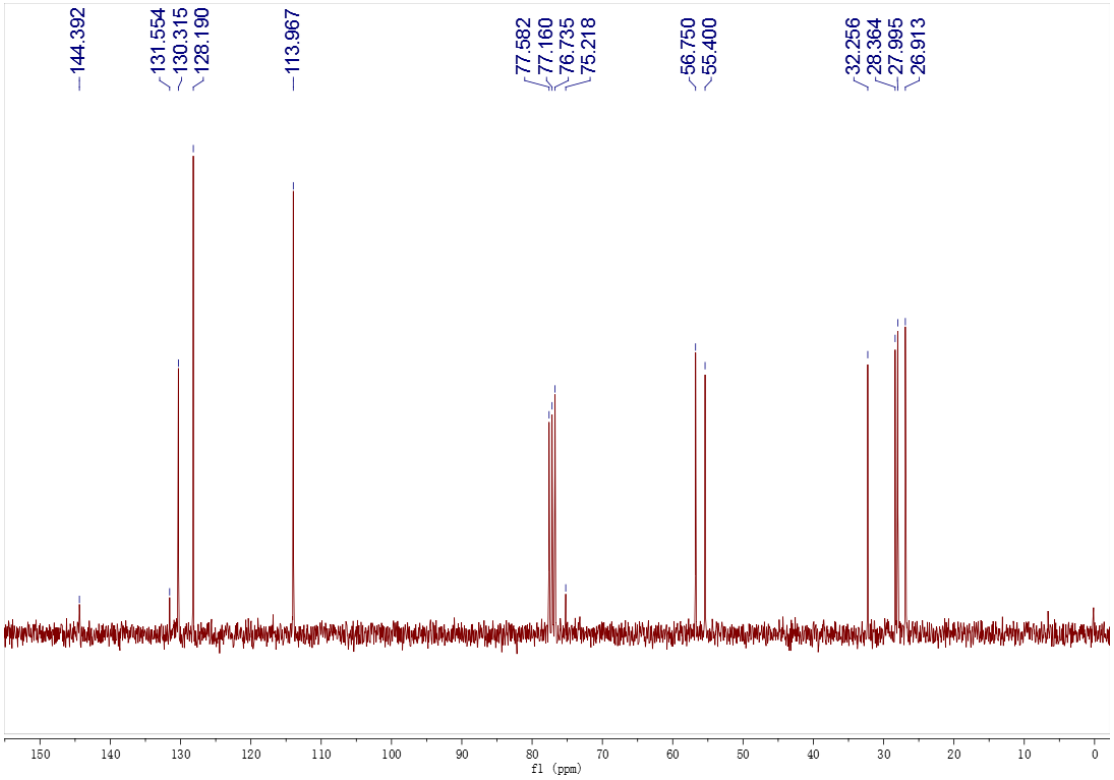
^{13}C NMR ($CDCl_3$, 75 MHz)



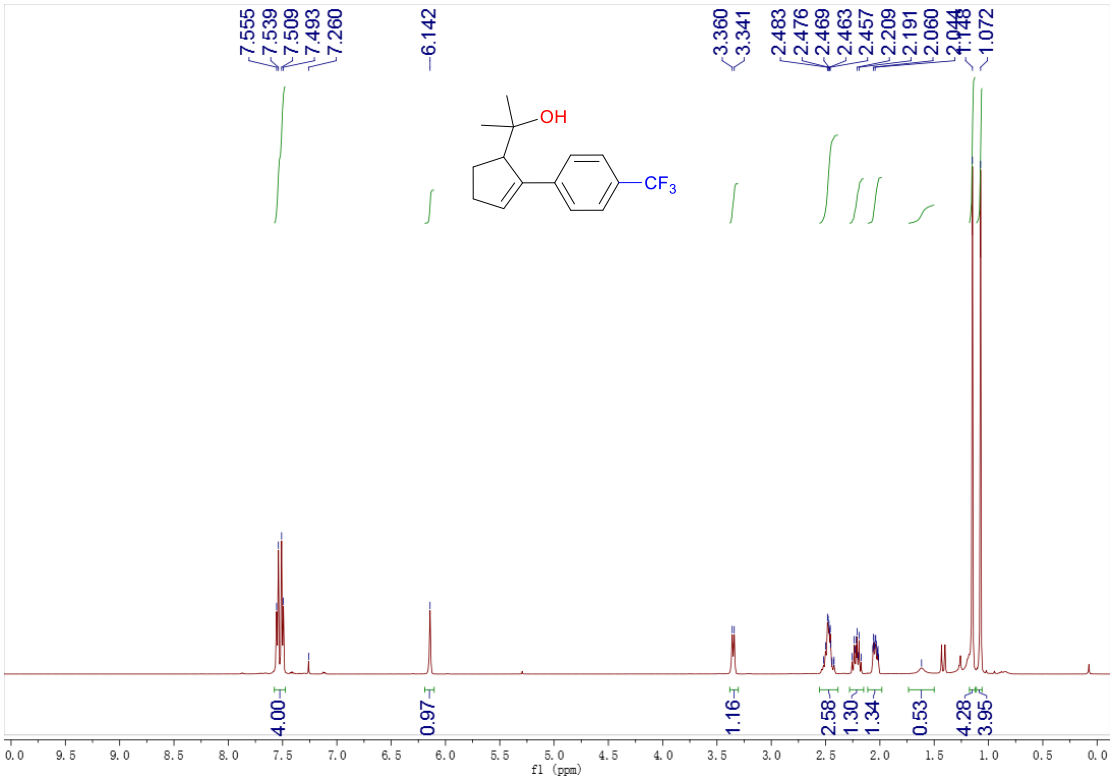
III.17. ^{1}H NMR ($CDCl_3$, 300 MHz) (**3m**)



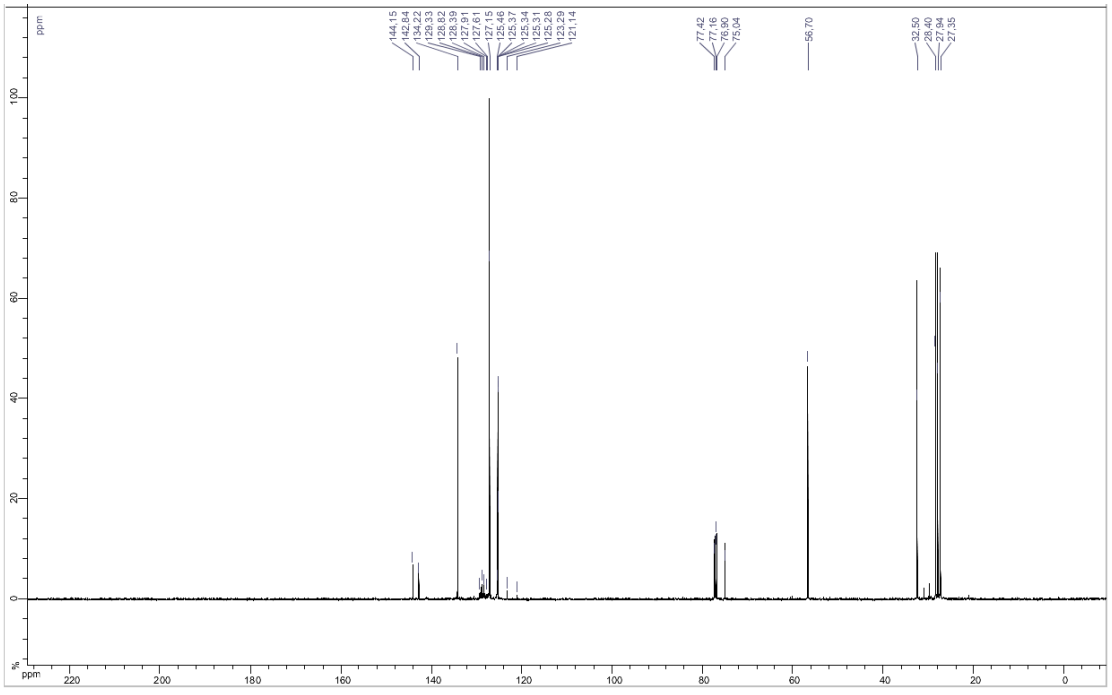
^{13}C NMR ($CDCl_3$, 75 MHz)



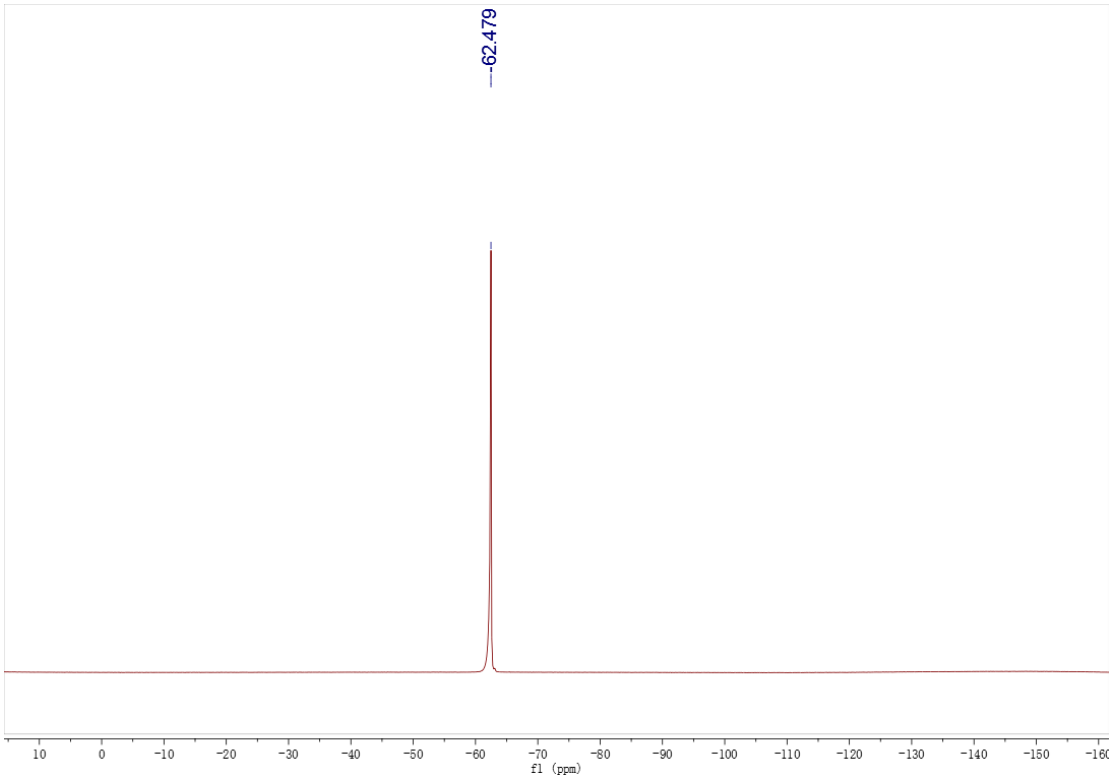
III.18. ^{1}H NMR ($CDCl_3$, 300 MHz) (**3n**)



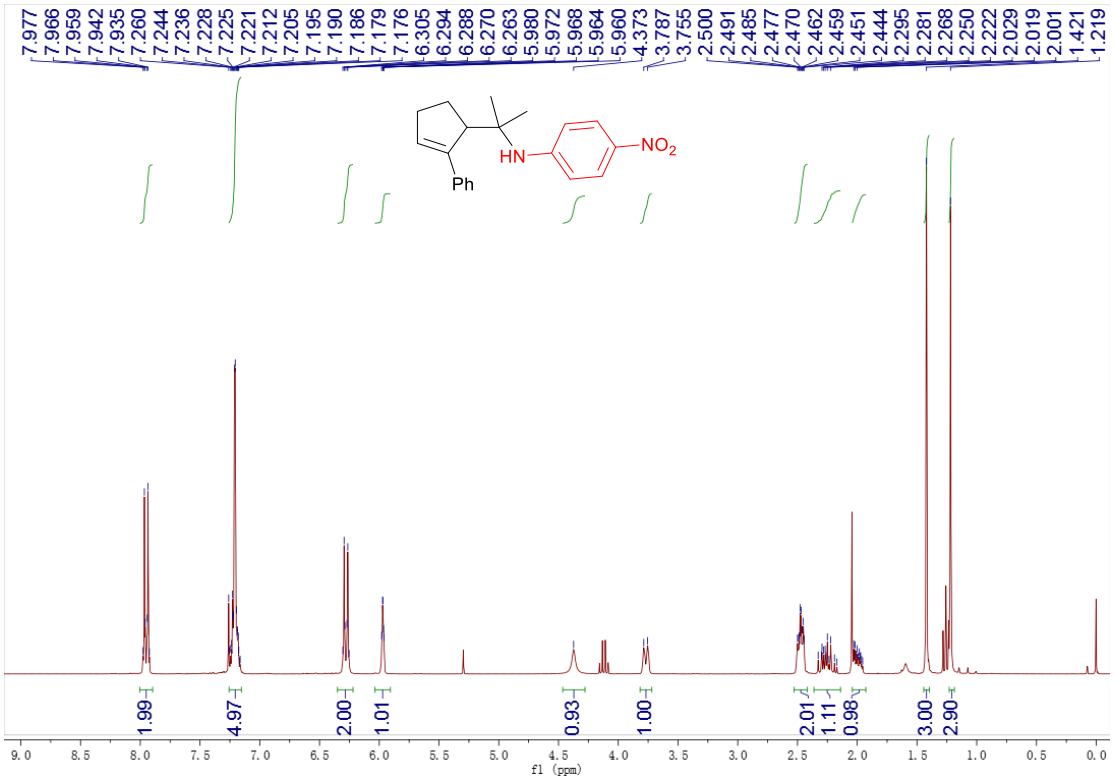
^{13}C NMR ($CDCl_3$, 125 MHz)



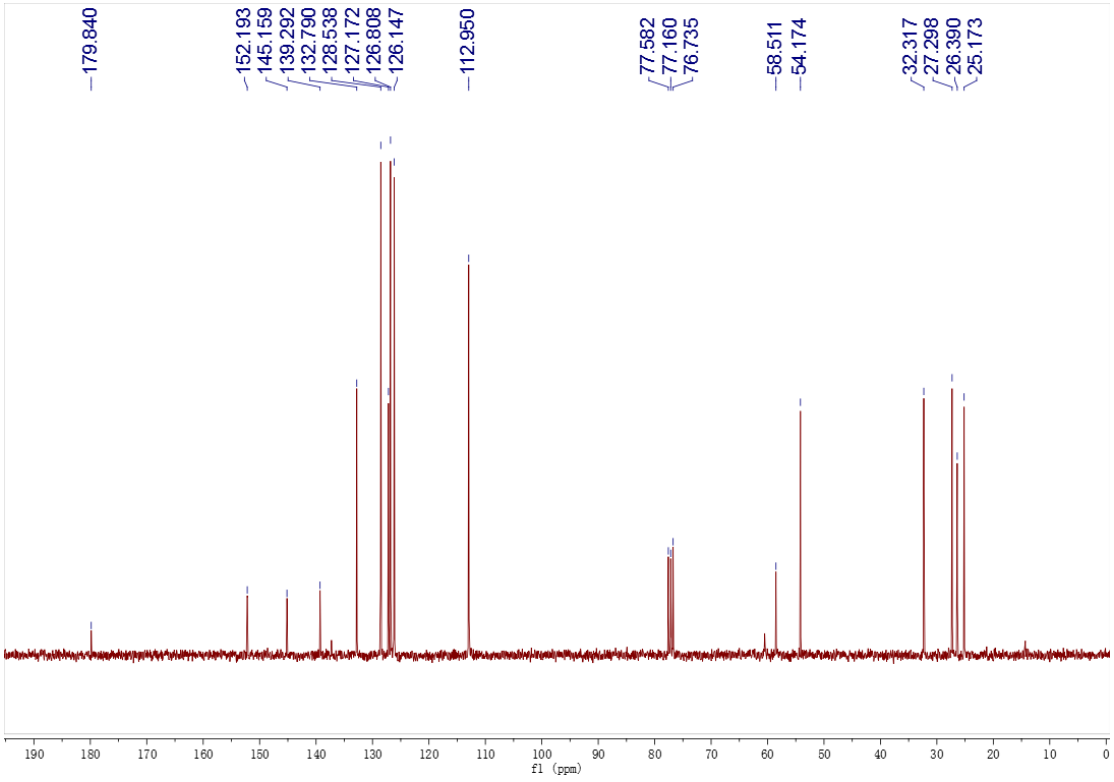
^{19}F NMR (282 MHz, $CDCl_3$)



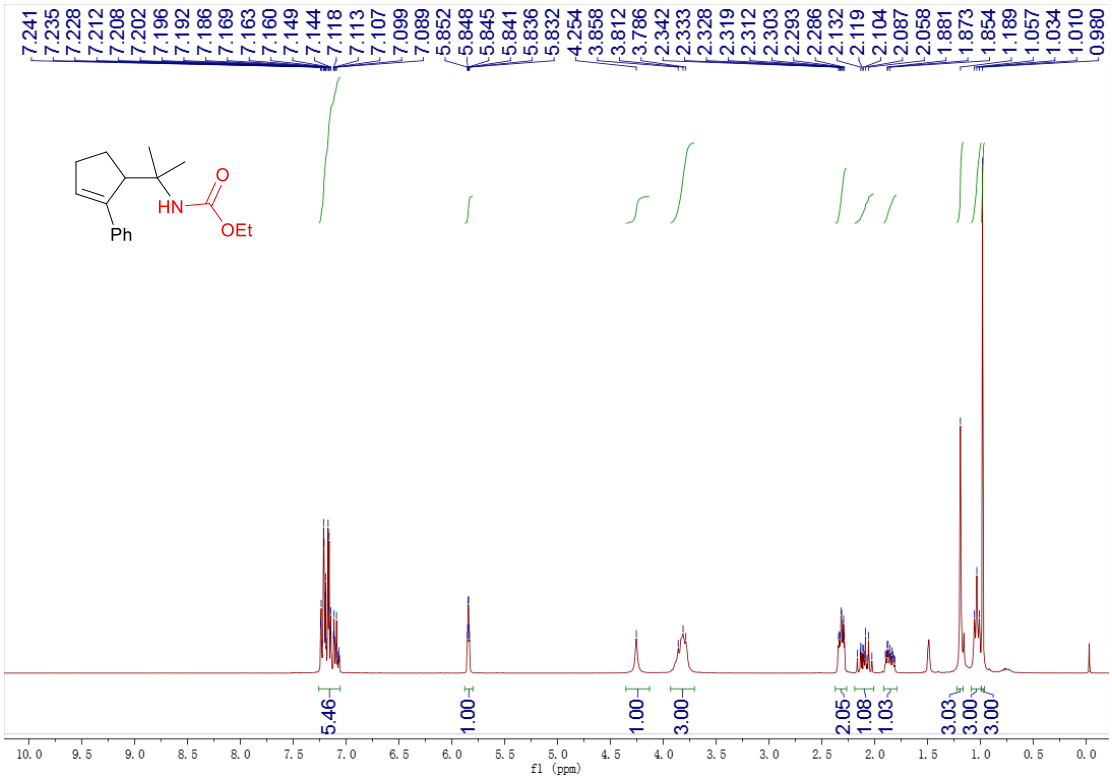
III.19. ^{1}H NMR ($CDCl_3$, 300 MHz) (**3o**)



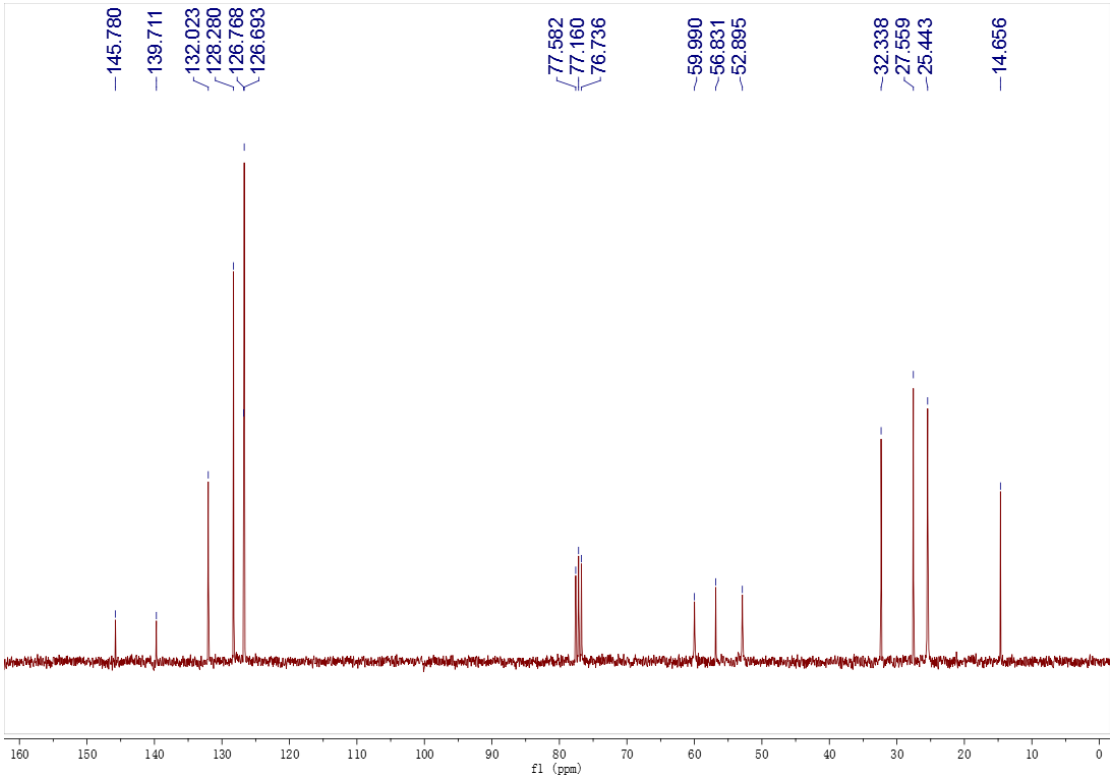
^{13}C NMR ($CDCl_3$, 75 MHz)



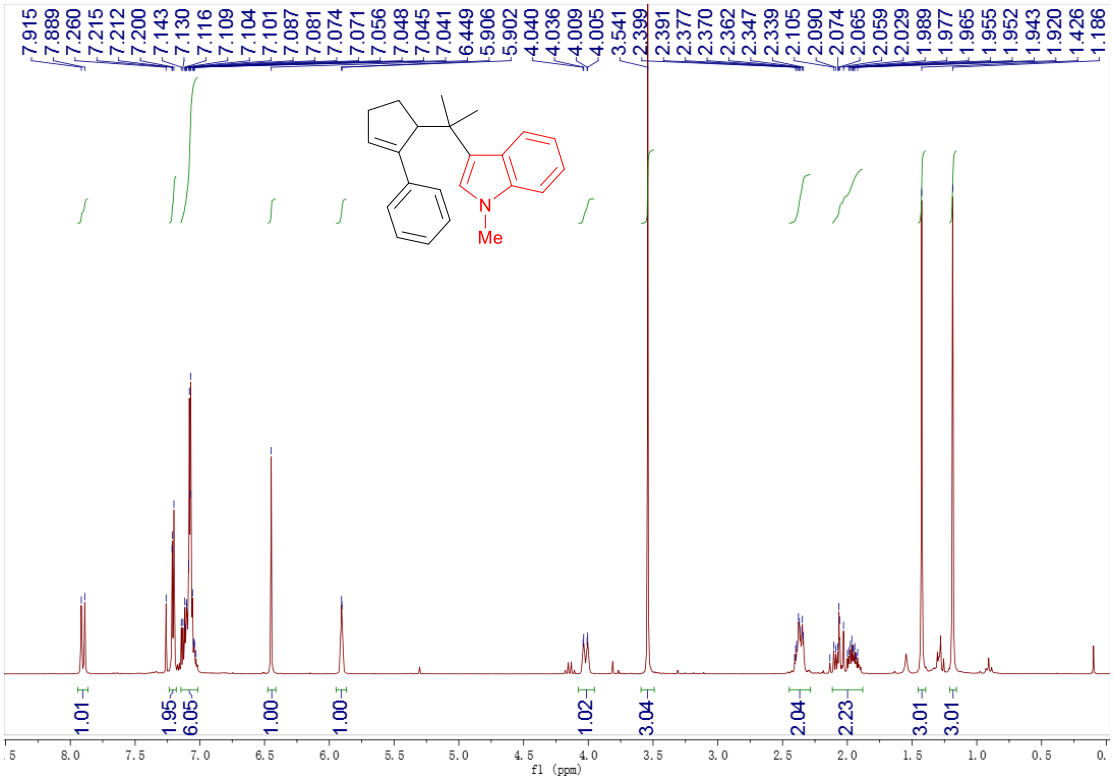
III.20. ^{1}H NMR ($CDCl_3$, 300 MHz) (**3p**)



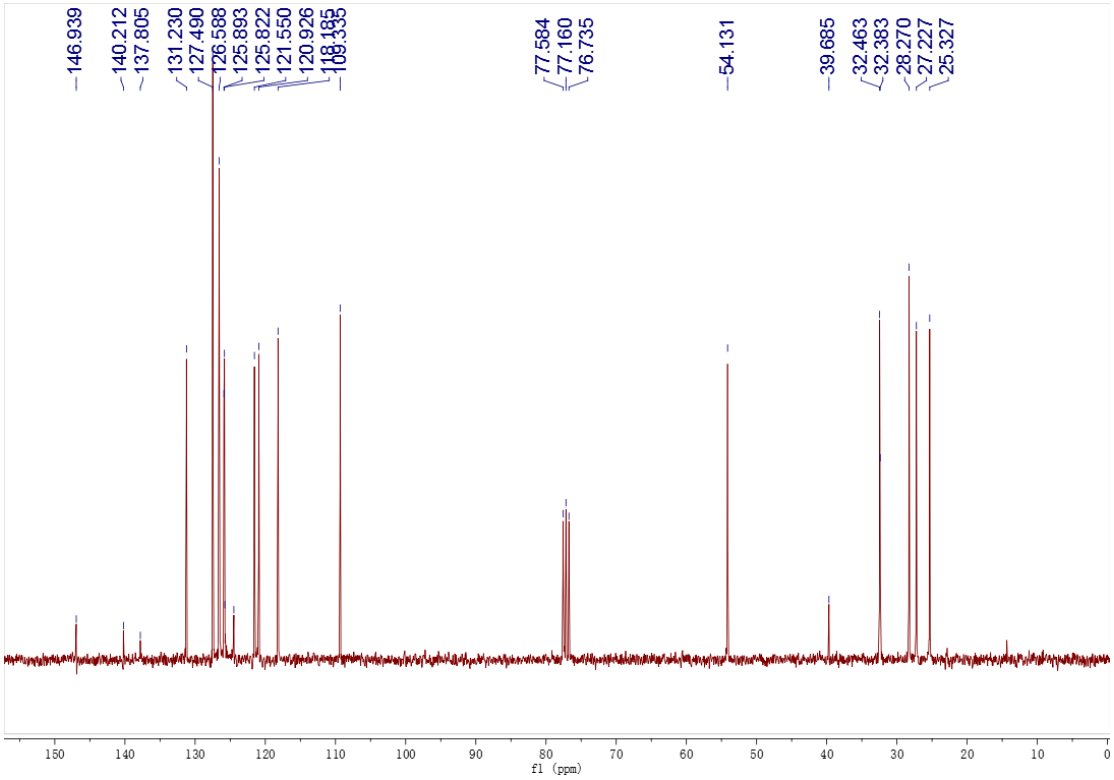
^{13}C NMR ($CDCl_3$, 75 MHz)



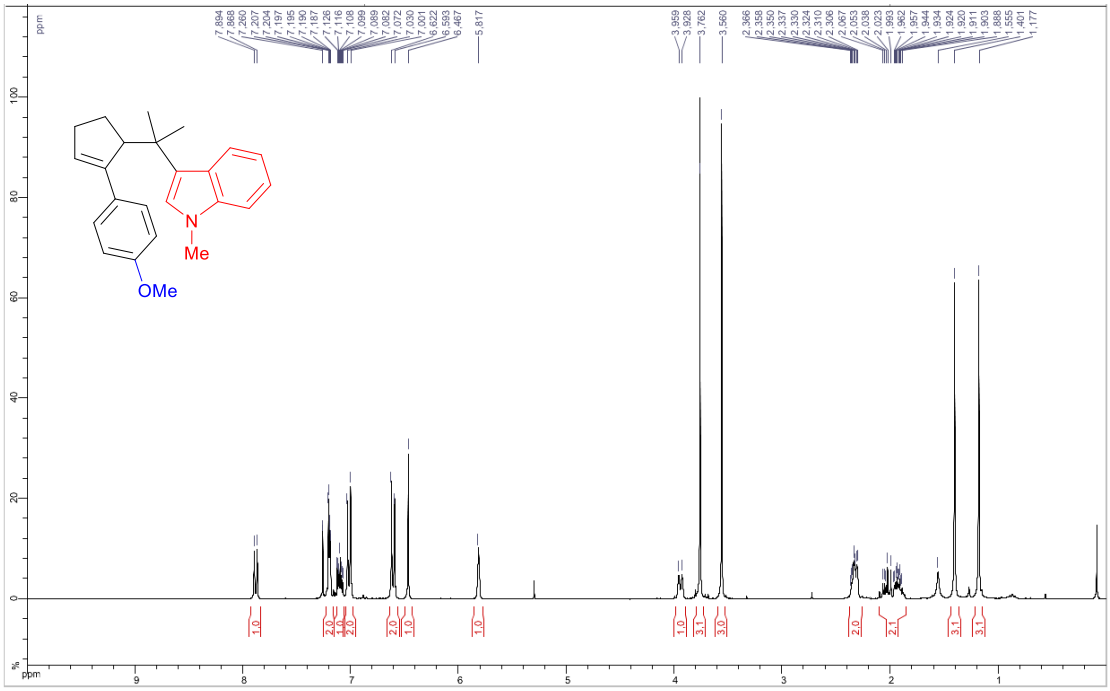
III.21. ^{1}H NMR ($CDCl_3$, 300 MHz) (**3q**)



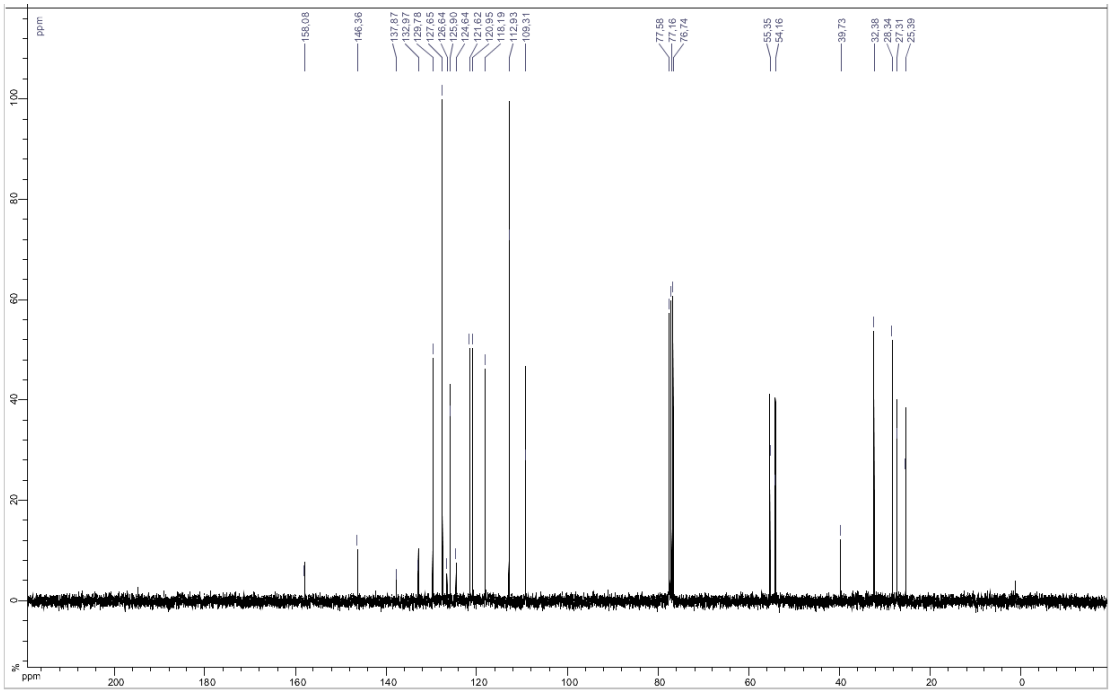
^{13}C NMR ($CDCl_3$, 75 MHz)



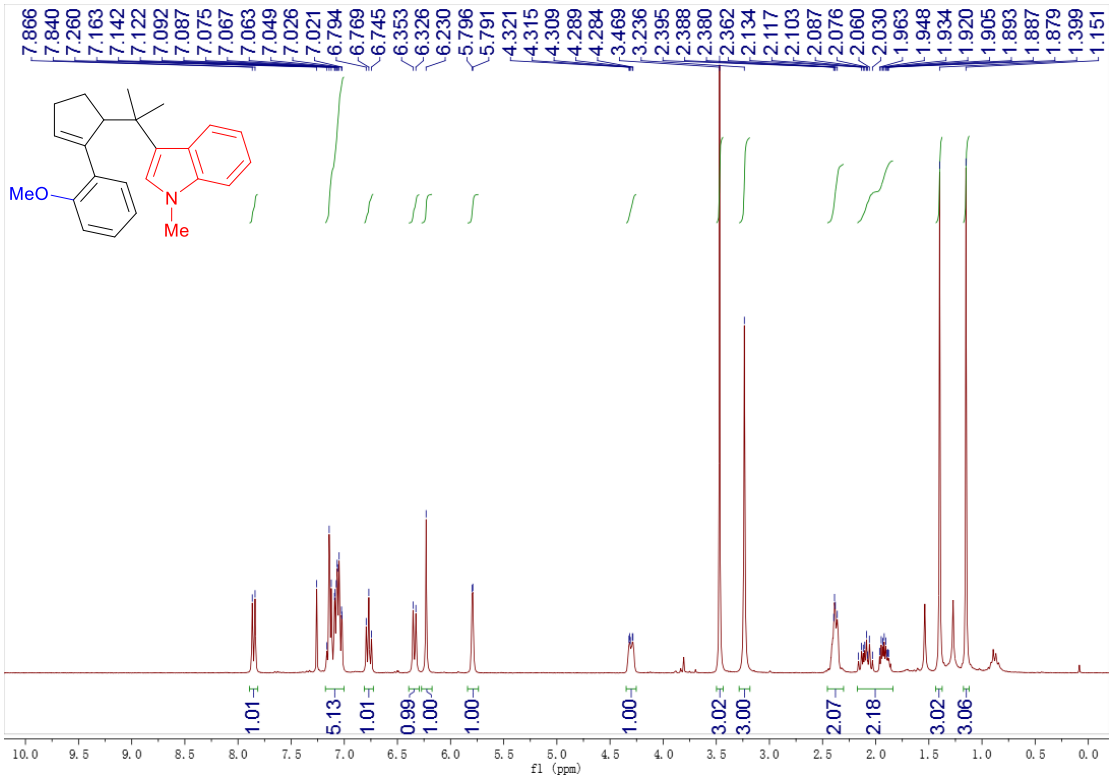
III.22. ^{1}H NMR ($CDCl_3$, 300 MHz) (**3r**)



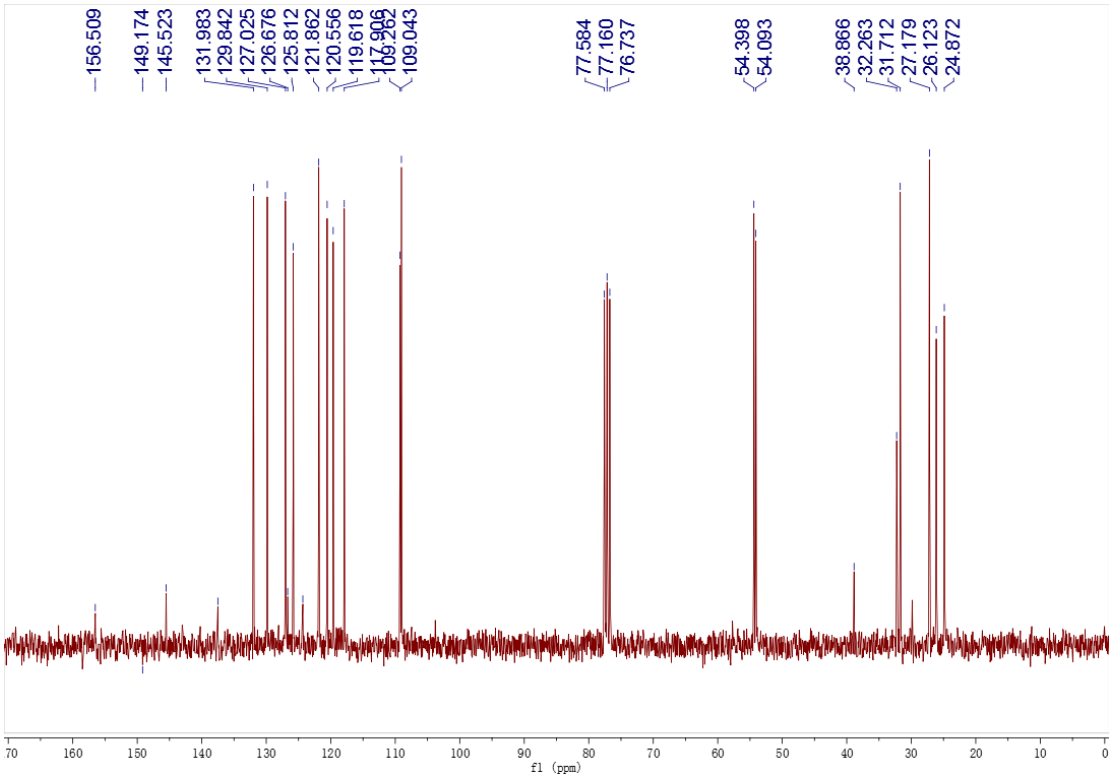
^{13}C NMR ($CDCl_3$, 75 MHz)



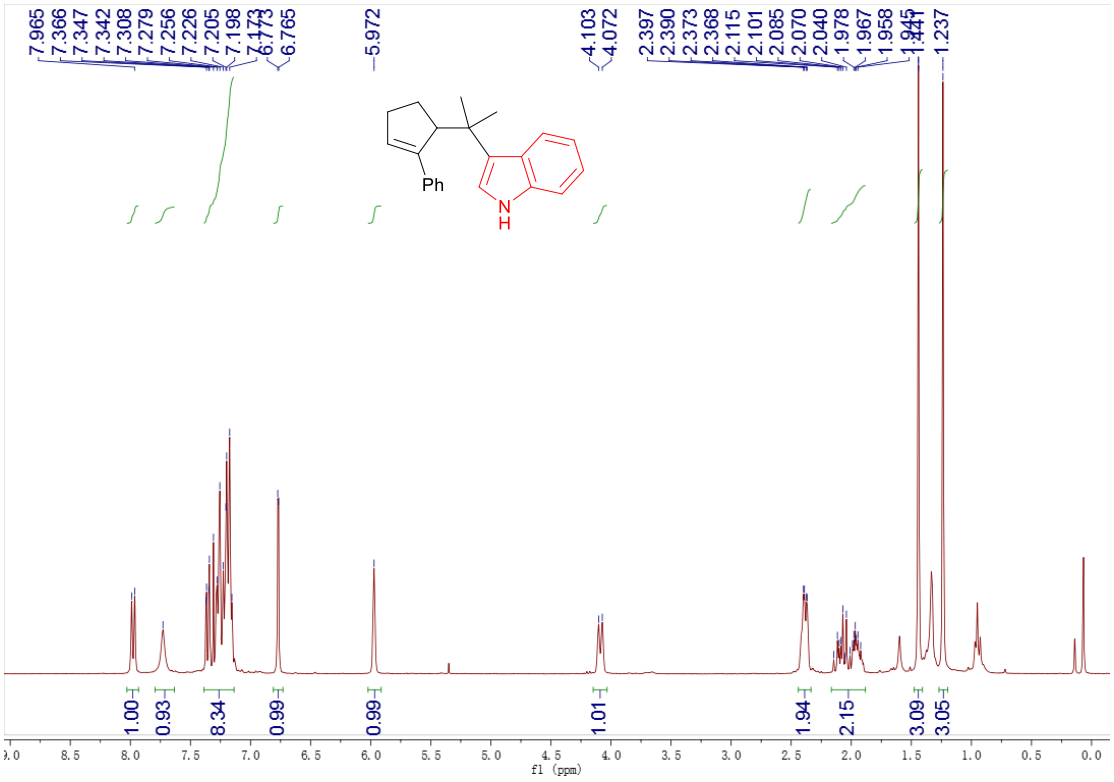
III.23. ^{1}H NMR ($CDCl_3$, 300 MHz) (**3s**)



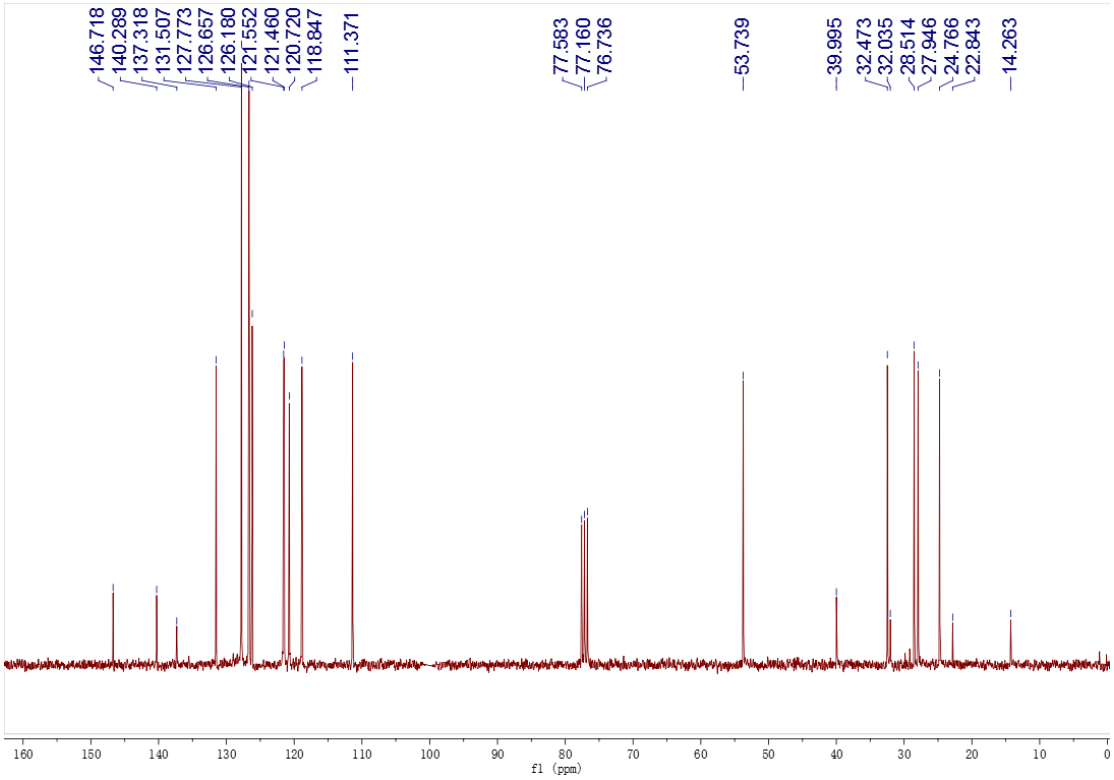
^{13}C NMR ($CDCl_3$, 75 MHz)



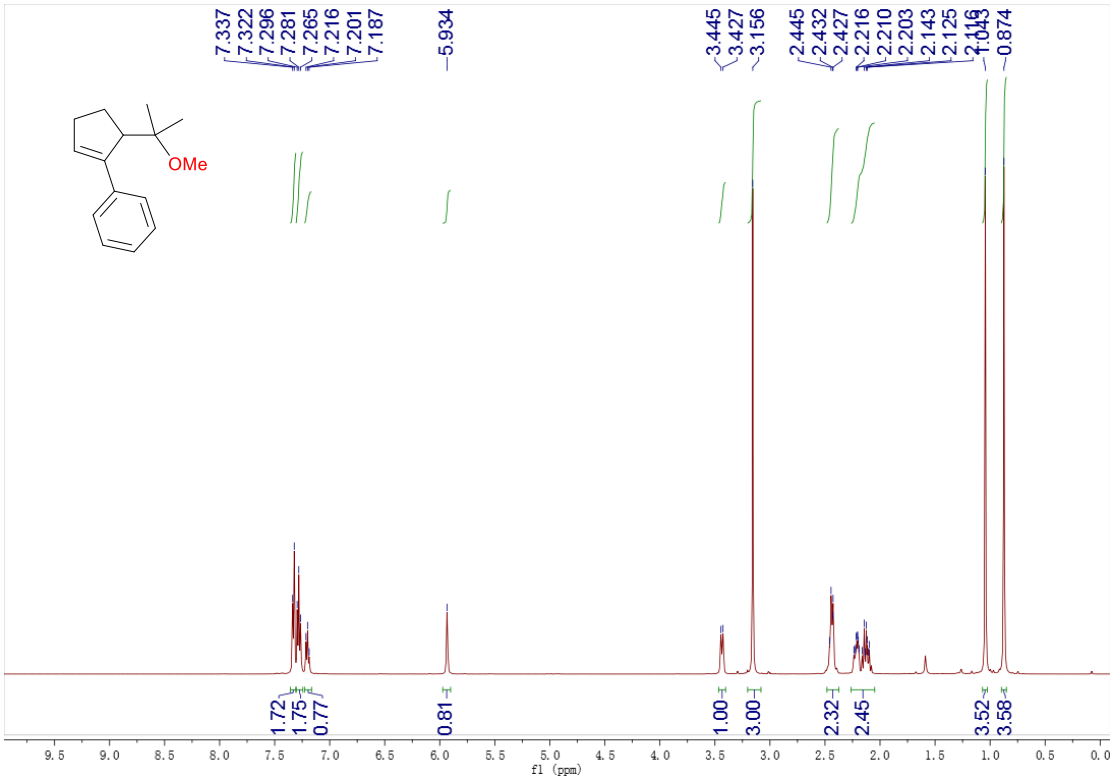
III.24. ^{1}H NMR ($CDCl_3$, 300 MHz) (**3t**)



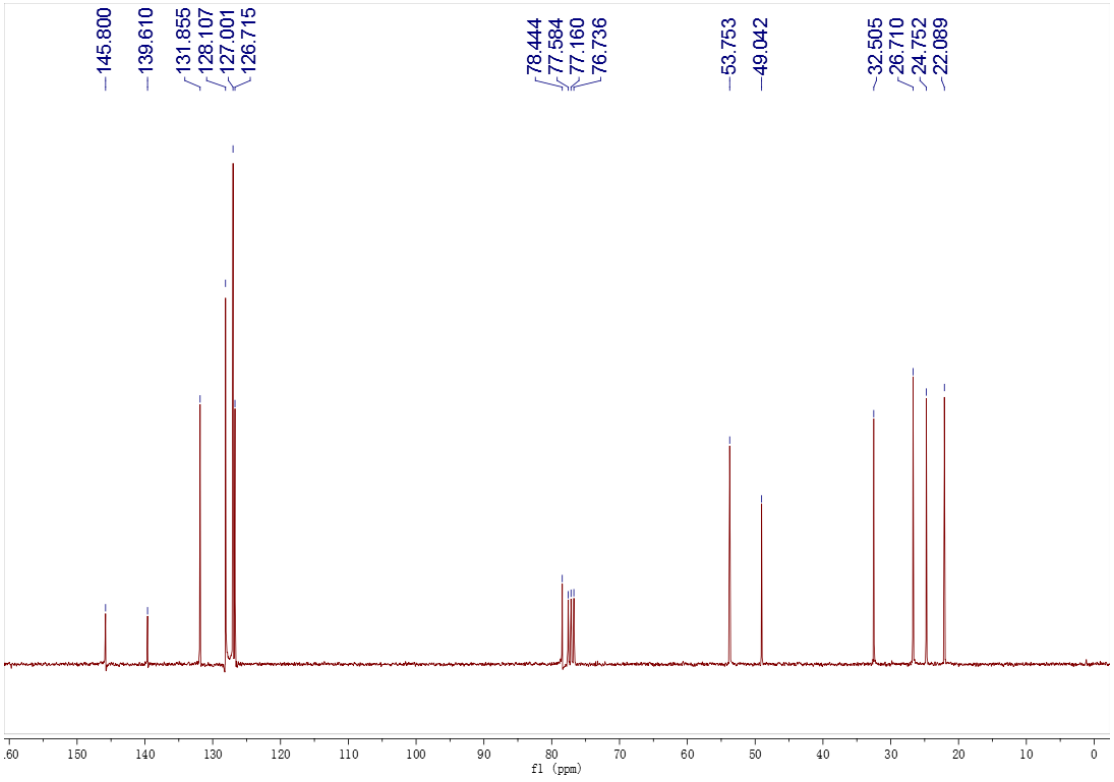
^{13}C NMR ($CDCl_3$, 75 MHz)



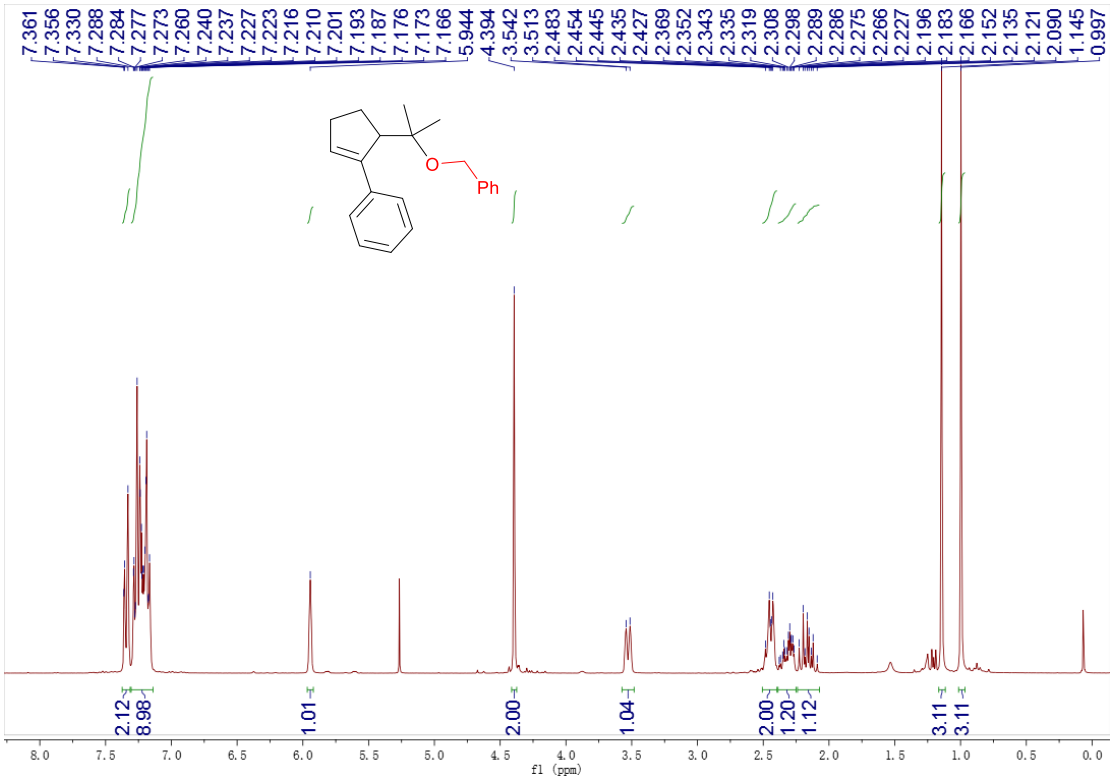
III.25. ^{1}H NMR ($CDCl_3$, 500 MHz) (**3u**)



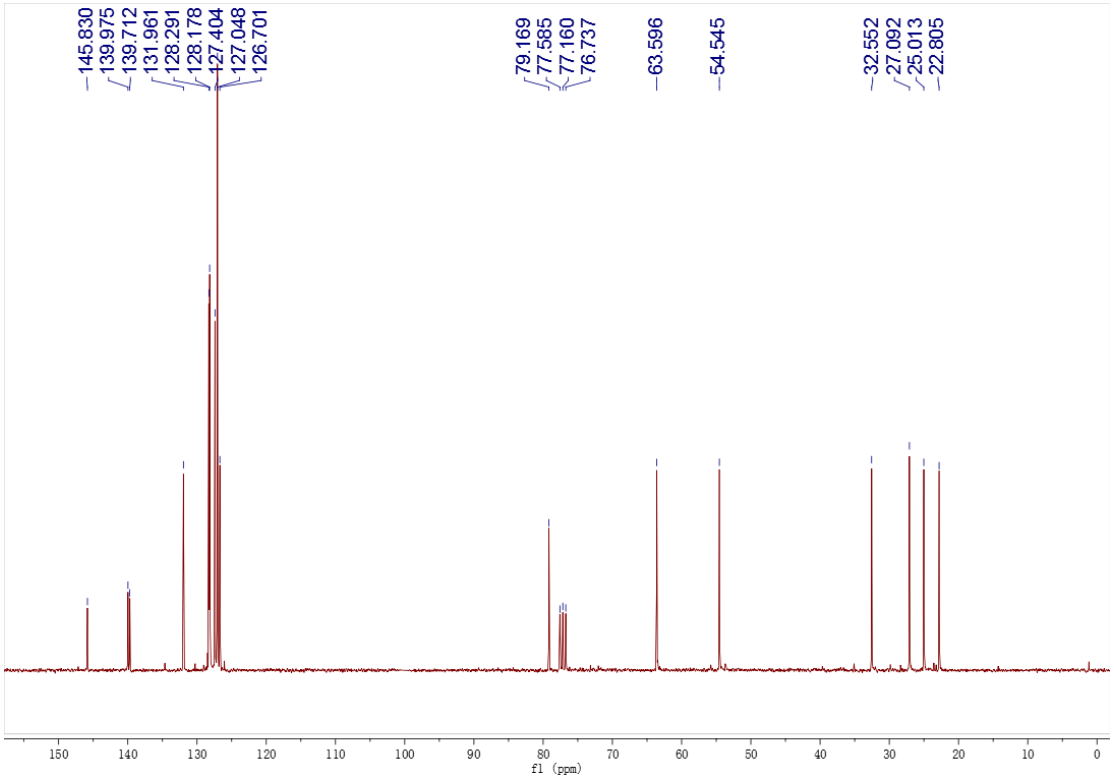
^{13}C NMR ($CDCl_3$, 75 MHz)



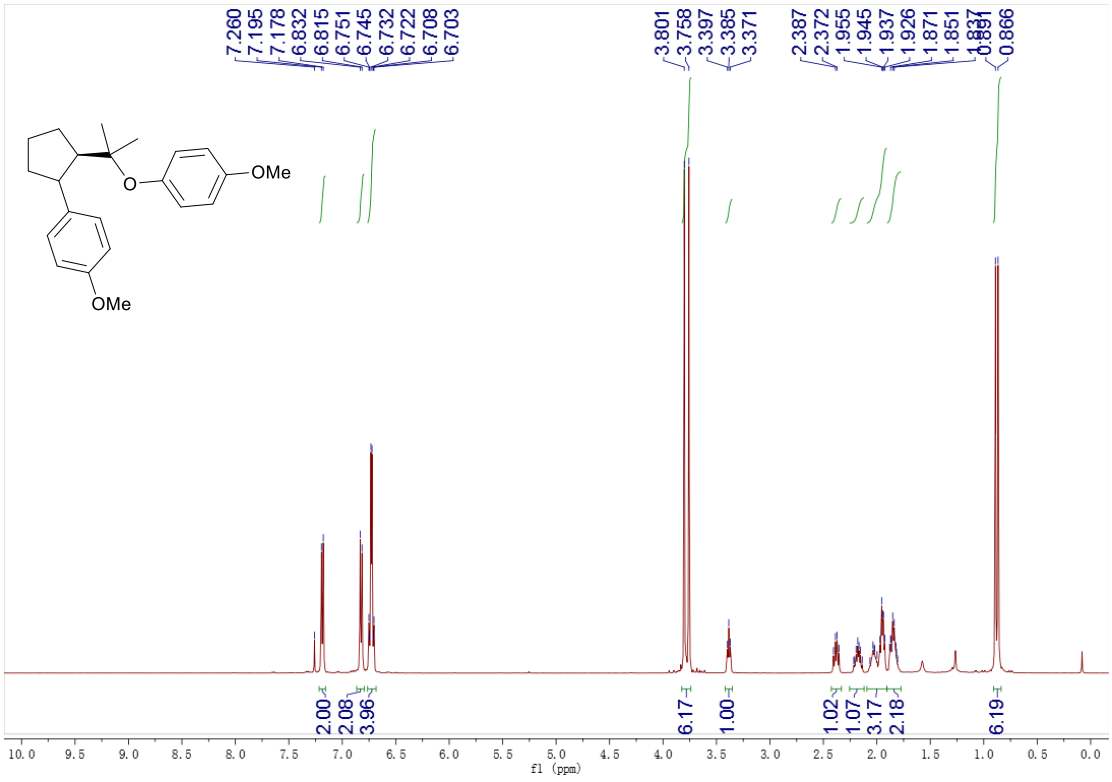
III.26. ^{1}H NMR ($CDCl_3$, 300 MHz) (**3v**)



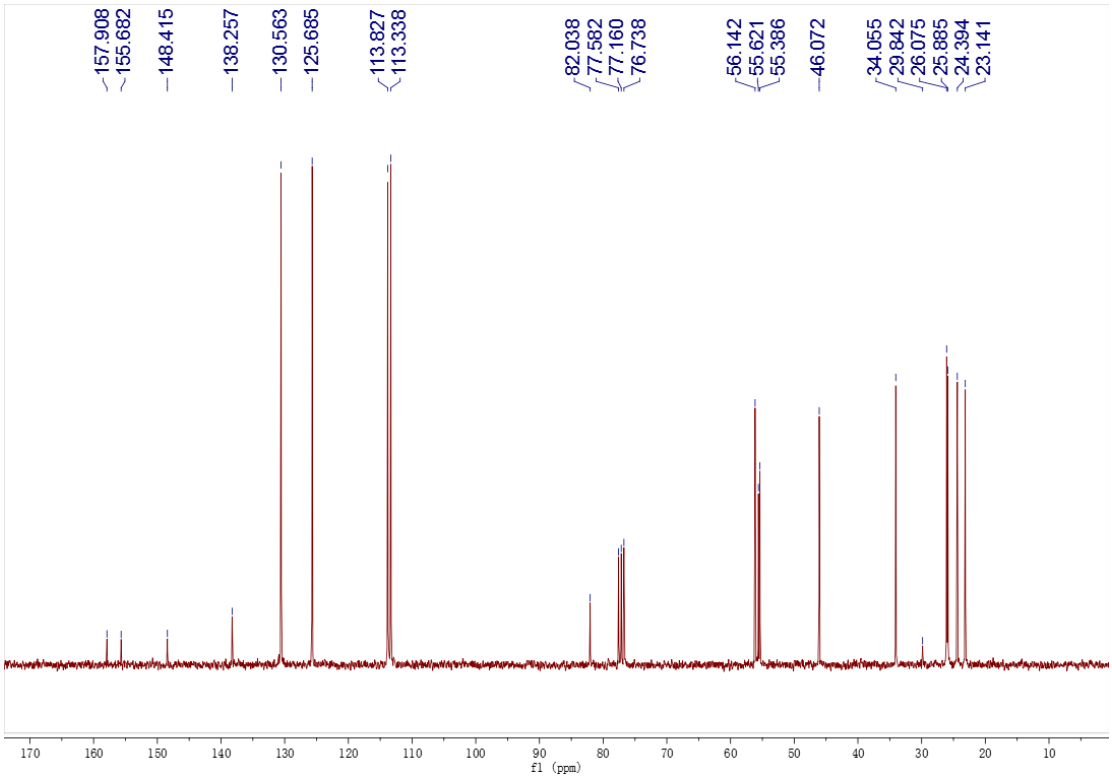
^{13}C NMR ($CDCl_3$, 75 MHz)



III.27. ^{1}H NMR ($CDCl_3$, 300 MHz) (**4**)



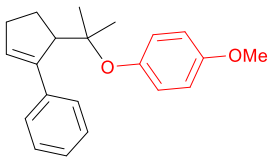
^{13}C NMR ($CDCl_3$, 75 MHz)

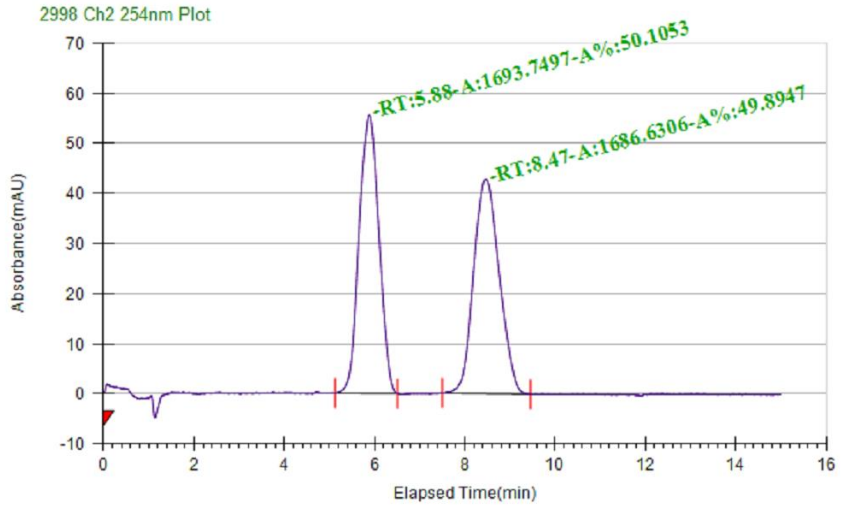


IV. Chiral SFC Data:

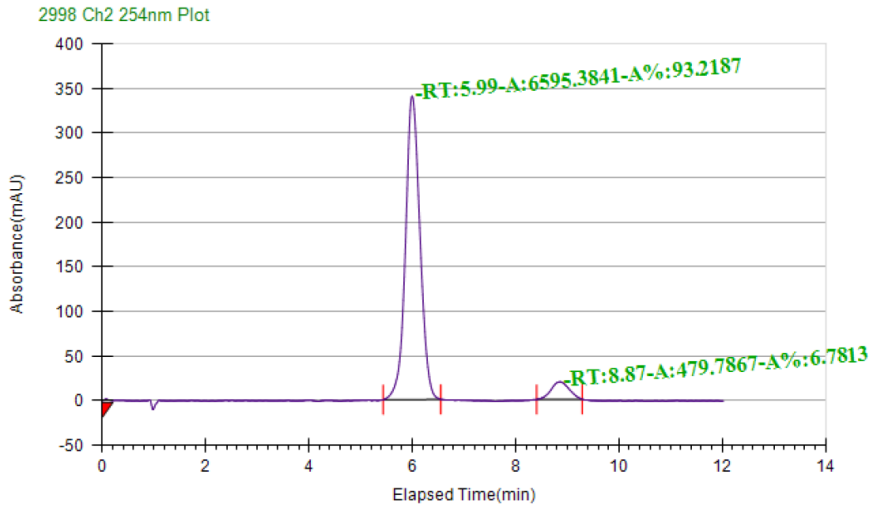
IV.1. Compound **3a**.

SFC Analysis: 93:7 e.r. [CHIRALPAK® IC, 30°C, 5% *i*PrOH, 4.0 mL/min, 100 bar, retention times: 6.0 min (major) and 8.9 min (minor)].





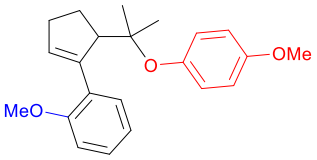
Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
50.1053	5.88 min	55.6645	1.3917 min	793.2592	5882.3333	1.0089	0	2.7421
49.8947	8.47 min	42.8813	1.9667 min	1044.3204	8465.6667	1.0956	-2.7421	0

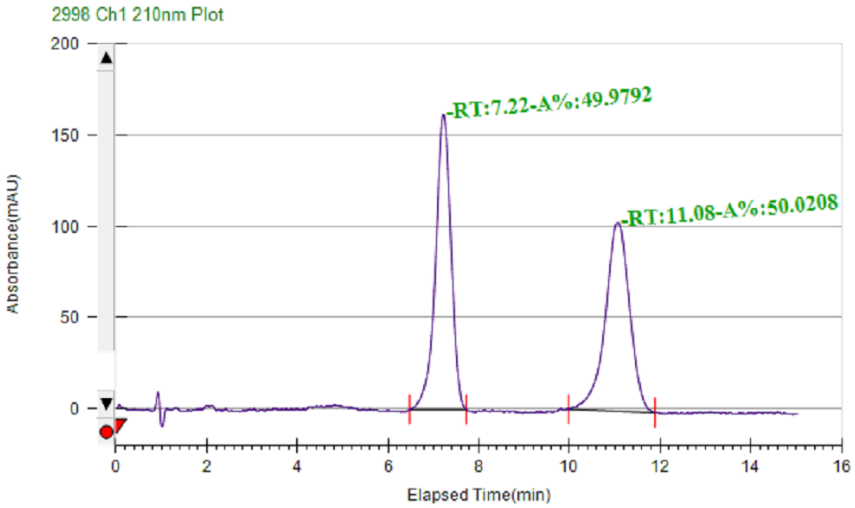


Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
93.2187	5.99 min	340.1032	1.125 min	2477.4775	0	1.0658	0	5.0735
6.7813	8.87 min	19.8065	0.8917 min	2963.9943	0	0.9894	-5.0735	0

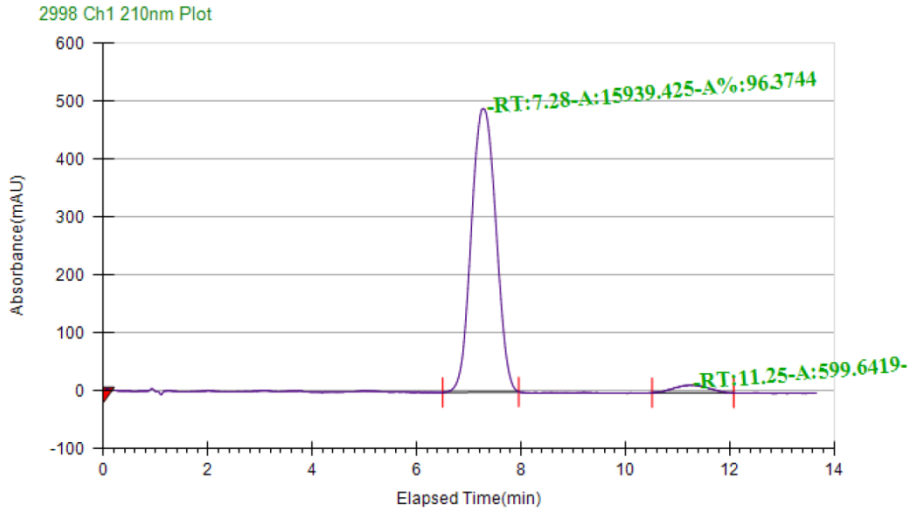
IV.2. Compound **3b**.

SFC Analysis: 96:4 e.r. [CHIRALPAK® IC, 30°C, 5% *i*PrOH, 4.0 mL/min, 100 bar, retention times: 7.3 min (major) and 11.3 min (minor)].





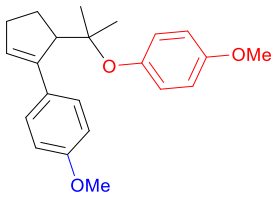
Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
49.9792	7.22 min	161.3529	1.2583 min	2360.7466	7224	0.8793	0	5.0327
50.0208	11.08 min	103.1602	1.9167 min	2246.3212	11074	0.907	-5.0327	0

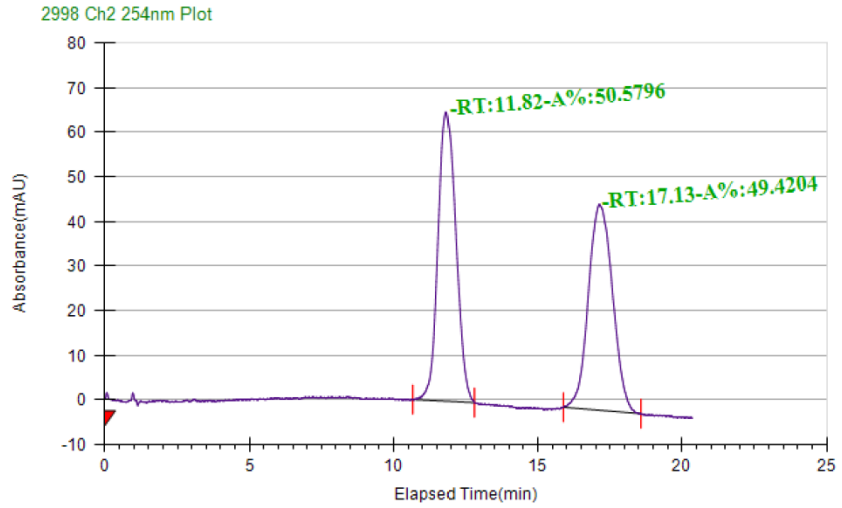


Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
96.3744	7.28 min	489.5758	1.4667 min	1100.9035	0	1.0259	0	3.6601
3.6256	11.25 min	13.0653	1.575 min	1219.2549	0	1.0195	-3.6601	0

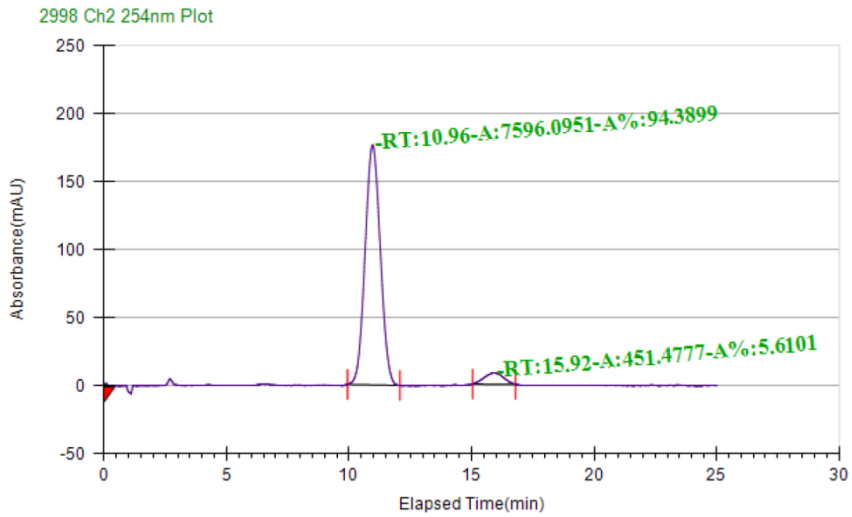
IV.3. Compound **3c**.

SFC Analysis: 94:6 e.r. [CHIRALPAK® IC, 30°C, 5% *i*PrOH, 4.0 mL/min, 100 bar, retention times: 11.0 min (major) and 16.0 min (minor)].





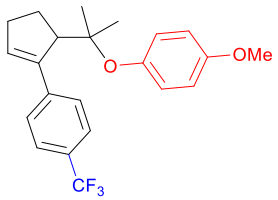
Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
50.5796	11.82 min	64.8369	2.1333 min	1784.876	11815.6667	1.1081	0	3.9714
49.4204	17.13 min	46.1843	2.7 min	1935.3995	17132.3333	1.0874	-3.9714	0

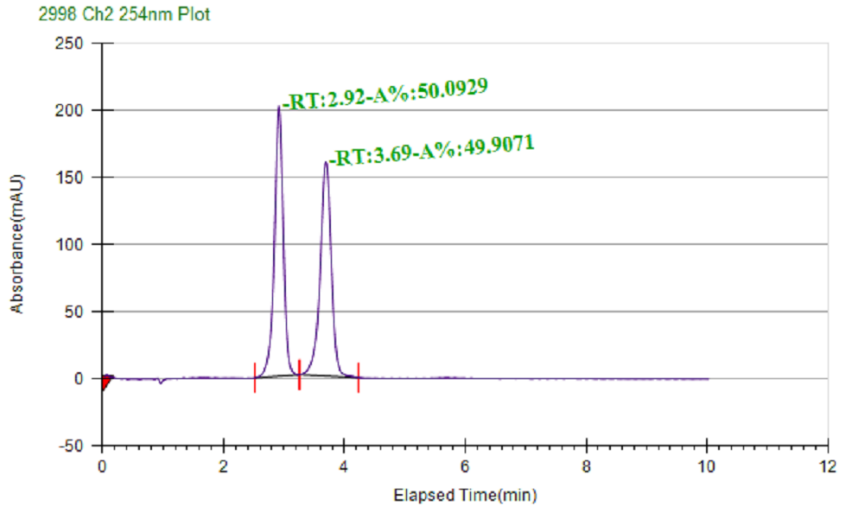


Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
94.3899	10.96 min	176.5191	2.15 min	1460.129	0	1.0438	0	3.7496
5.6101	15.92 min	8.3272	1.7583 min	1800.609	0	0.9898	-3.7496	0

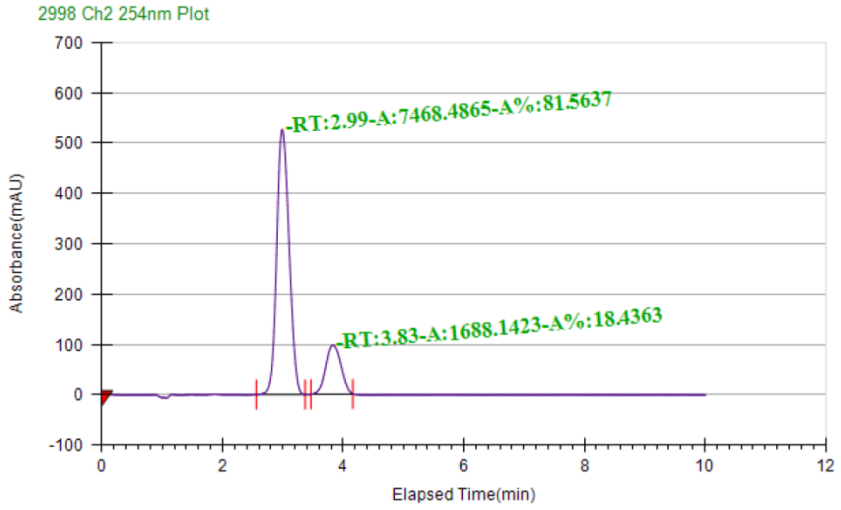
IV.4. Compound **3d**.

SFC Analysis: 82:18 e.r. [CHIRALPAK® IC, 30°C, 5% *i*PrOH, 4.0 mL/min, 100 bar, retention times: 3.0 min (major) and 3.8 min (minor)].





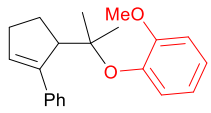
Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
50.0929	2.92 min	201.0436	0.7417 min	2094.5988	0	0.9167	0	2.7353
49.9071	3.69 min	159.2702	0.975 min	2246.3212	0	0.9333	-2.7353	0

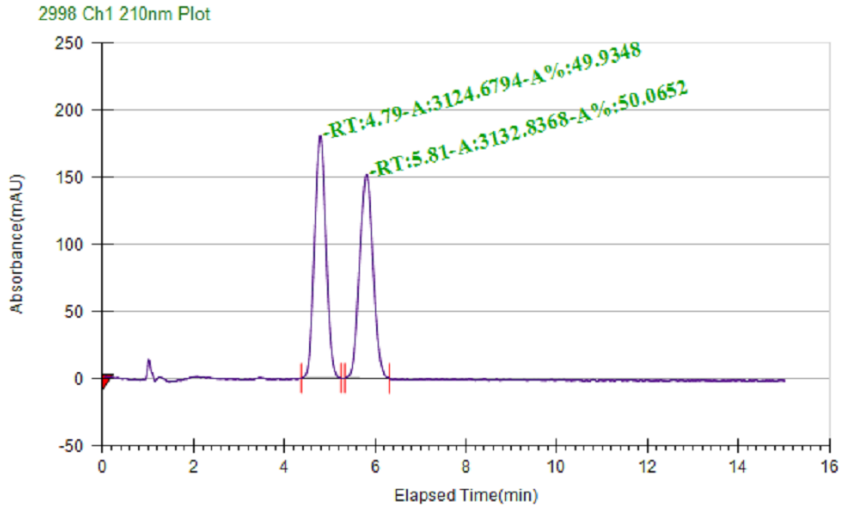


Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
81.5637	2.99 min	526.998	0.8167 min	1056.2141	0	1.125	0	2.014
18.4363	3.83 min	97.4375	0.7 min	1076.4591	0	1.0156	-2.014	0

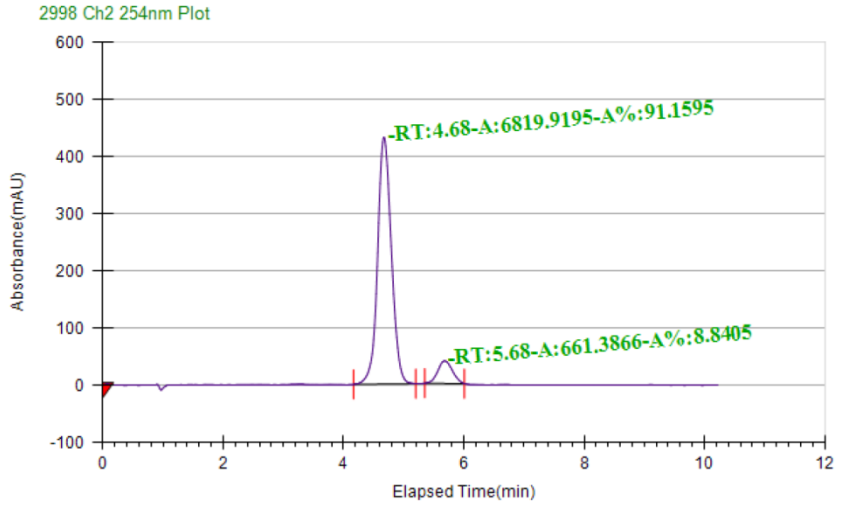
IV.5. Compound **3e**.

SFC Analysis: 91:9 e.r. [CHIRALPAK® IC, 30°C, 5% *i*PrOH, 4.0 mL/min, 100 bar, retention times: 4.7 min (major) and 5.7 min (minor)].





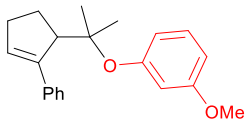
Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
49.9348	4.79 min	180.6649	0.8833 min	1681.9674	4790.6667	1.0469	0	1.9935
50.0652	5.81 min	152.2134	0.9833 min	1769.4818	5807.3333	1.0395	-1.9935	0

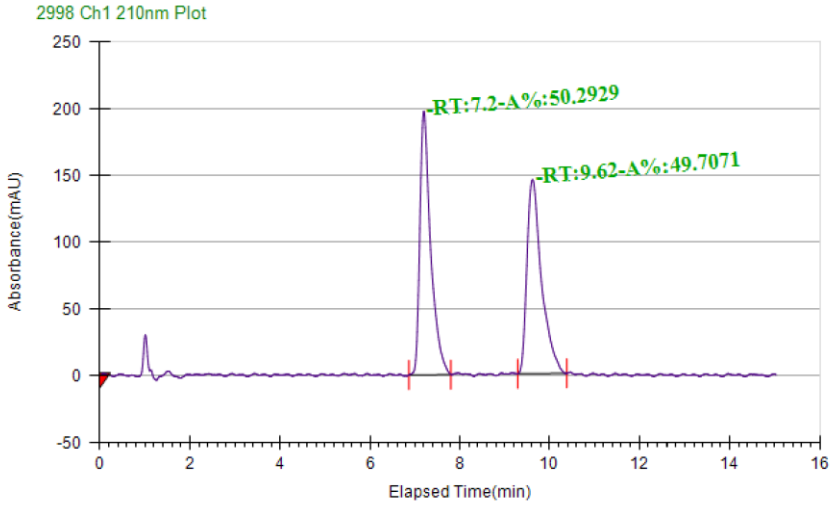


Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
91.1595	4.68 min	431.8225	1.0417 min	2223.9214	0	1.0484	0	2.4128
8.8405	5.68 min	39.4225	0.6667 min	2681.36	0	1.0667	-2.4128	0

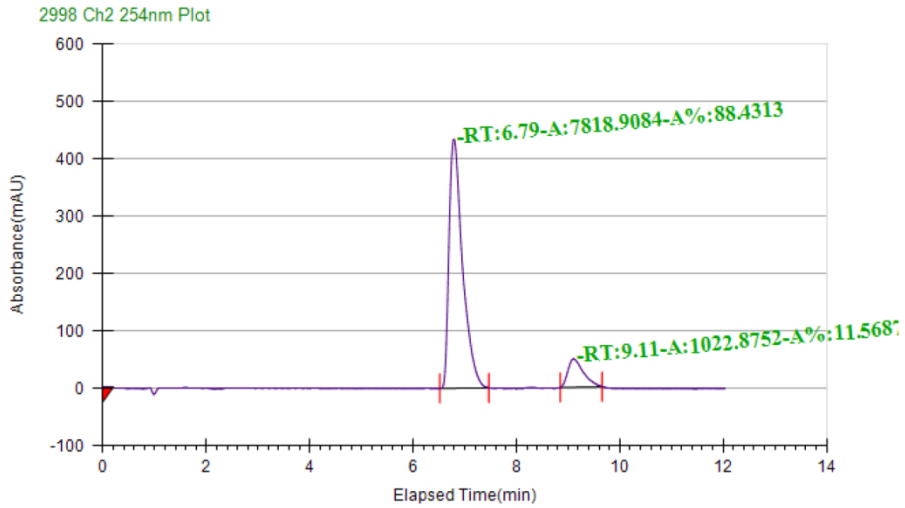
IV.6. Compound **3f**.

SFC Analysis: 88.5:11.5 e.r. [CHIRALPAK® AD-H, 30°C, 3% *i*PrOH, 4.0 mL/min, 100 bar, retention times: 6.8 min (major) and 9.1 min (minor)].





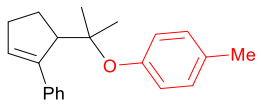
Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
50.2929	7.2 min	197.805	0.9417 min	5672.96	7199	1.7045	0	5.2489
49.7071	9.62 min	145.3034	1.1 min	5109.2151	9615.6667	1.6897	-5.2489	0

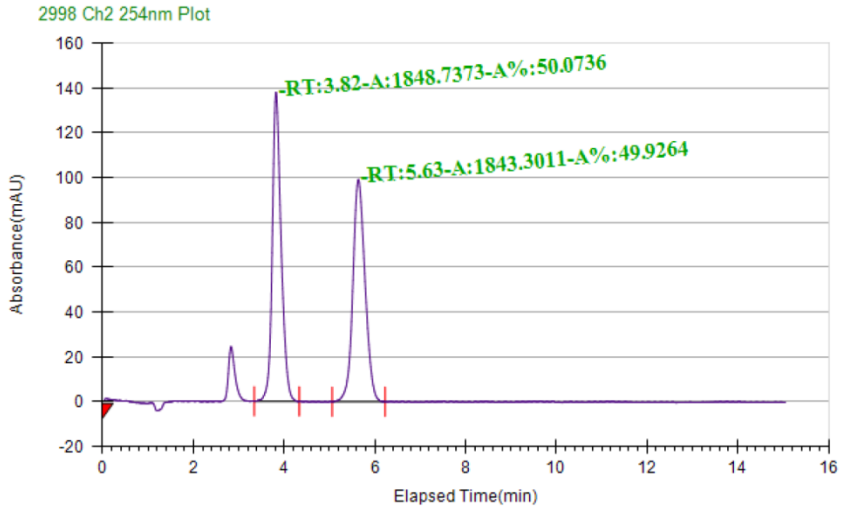


Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
88.4313	6.79 min	434.3199	0.9583 min	3829.1431	6790.6667	1.7857	0	4.8097
11.5687	9.11 min	49.5813	0.8167 min	4834.4452	9107.3333	1.6154	-4.8097	0

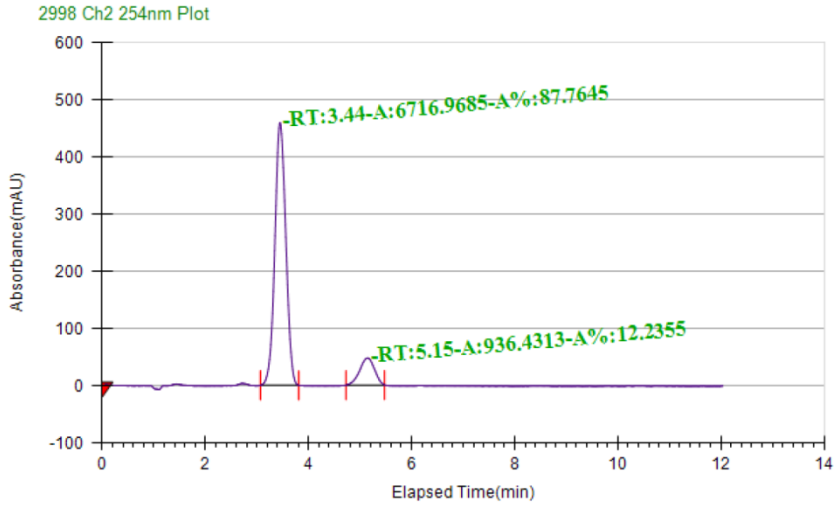
IV.7. Compound **3g**.

SFC Analysis: 88:12 e.r. [CHIRALPAK® IC, 30°C, 5% *i*PrOH, 4.0 mL/min, 100 bar, retention times: 3.4 min (major) and 5.2 min (minor)].





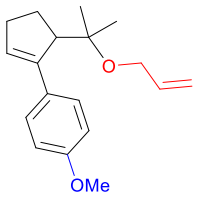
Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
50.0736	3.82 min	137.9422	1 min	2196.7723	3815.6667	1.2391	0	4.5798
49.9264	5.63 min	99.1836	1.175 min	2324.7448	5632.3333	1.1	-4.5798	0

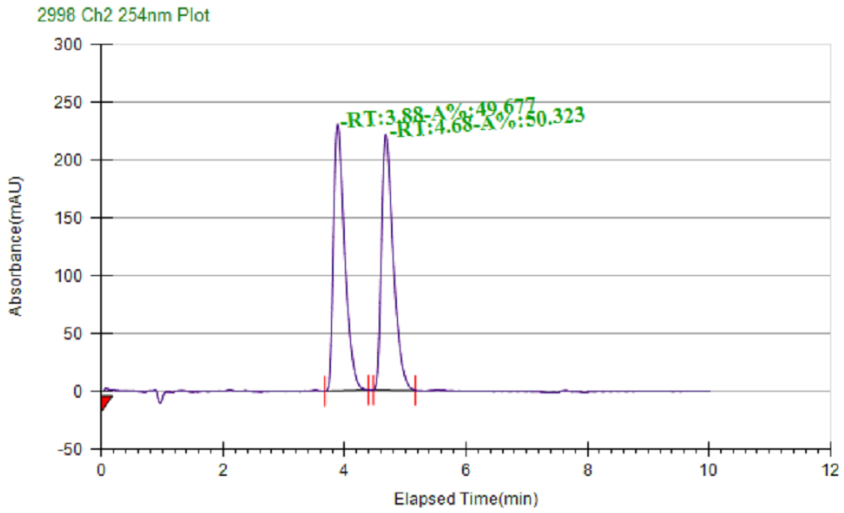


Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
87.7645	3.44 min	459.065	0.75 min	1296.2308	0	1.0357	0	3.7684
12.2355	5.15 min	47.3713	0.7583 min	1545.5507	0	0.9048	-3.7684	0

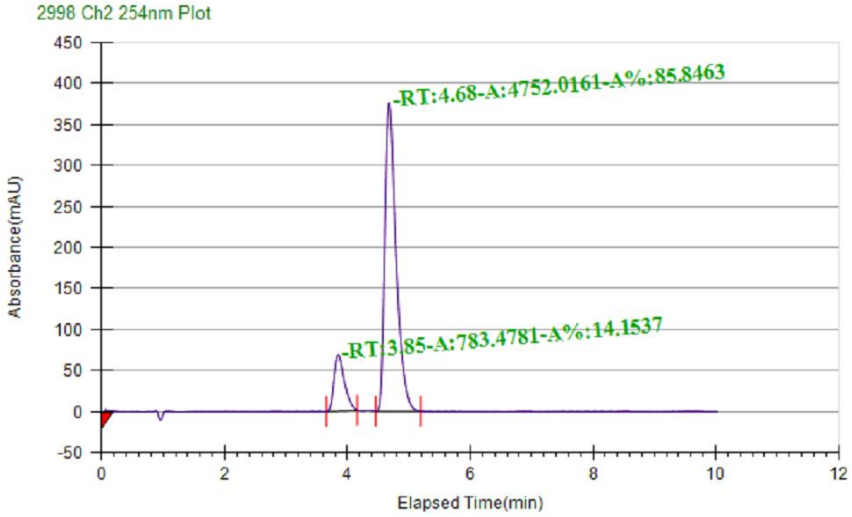
IV.8. Compound **3h**.

SFC Analysis: 86:14 e.r. [CHIRALPAK® AD-H, 30°C, 2% *i*PrOH, 4.0 mL/min, 100 bar, retention times: 3.9 min (minor) and 4.7 min (major)].





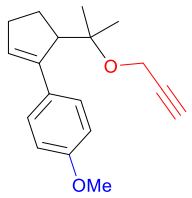
Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
49.677	3.88 min	230.1256	0.725 min	2485.6286	0	1.7	0	2.4552
50.323	4.68 min	221.136	0.7 min	3037.8051	0	1.6176	-2.4552	0

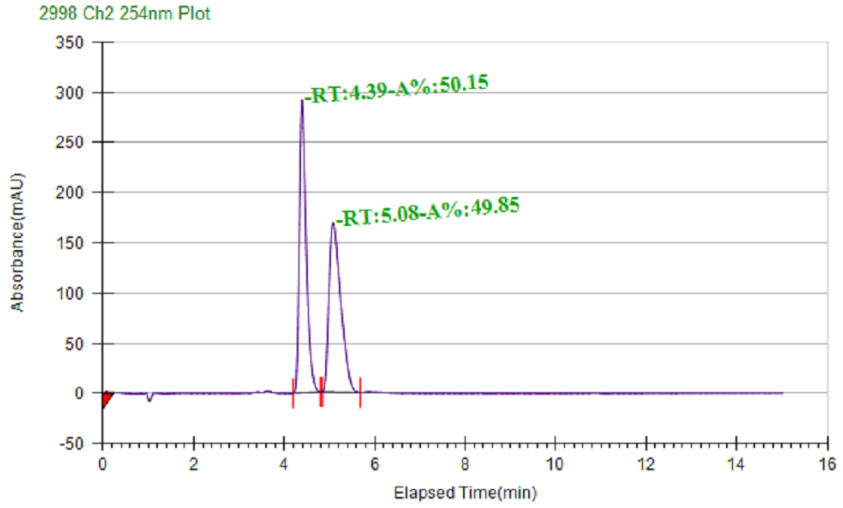


Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
14.1537	3.85 min	67.8877	0.5083 min	2681.36	0	1.4375	0	2.736
85.8463	4.68 min	376.076	0.7417 min	3615.2392	0	1.5294	-2.736	0

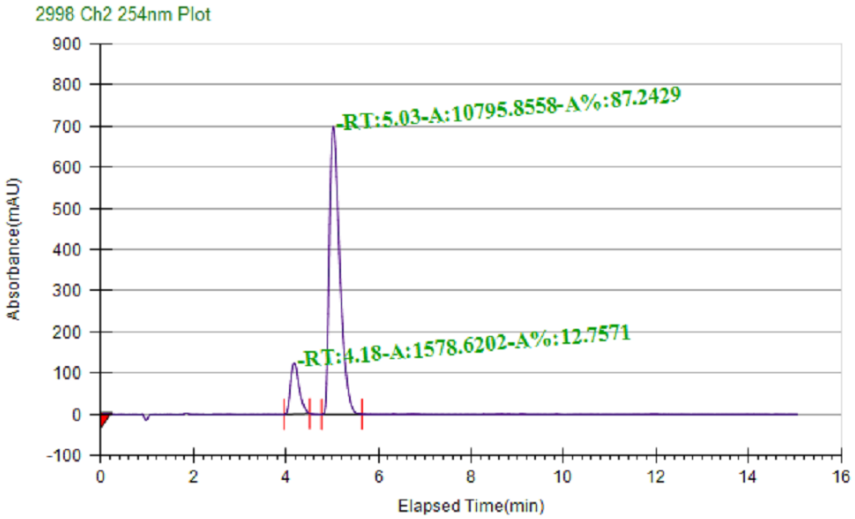
IV.9. Compound **3i**.

SFC Analysis: 87:13 e.r. [CHIRALPAK® AD-H, 30°C, 3% *i*PrOH, 4.0 mL/min, 100 bar, retention times: 4.2 min (minor) and 5.0 min (major)].





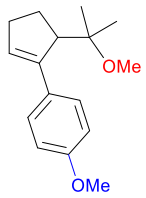
Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
50.15	4.39 min	292.4219	0.6167 min	4748.823	4390.6667	1.5714	0	1.9146
49.85	5.08 min	168.7892	0.85 min	1892.9605	5082.3333	1.5909	-1.9146	0

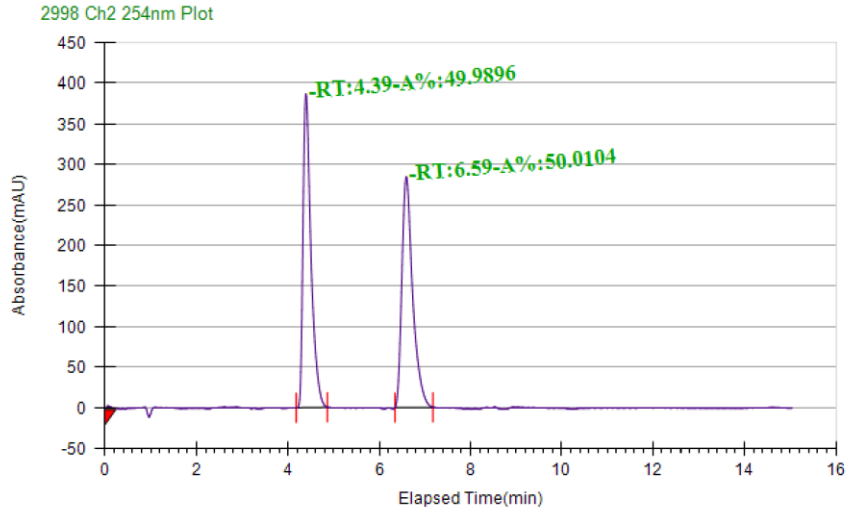


Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
12.7571	4.18 min	123.8746	0.5667 min	2873.028	0	1.3421	0	2.4
87.2429	5.03 min	698.2835	0.8833 min	2569.3799	0	1.6053	-2.4	0

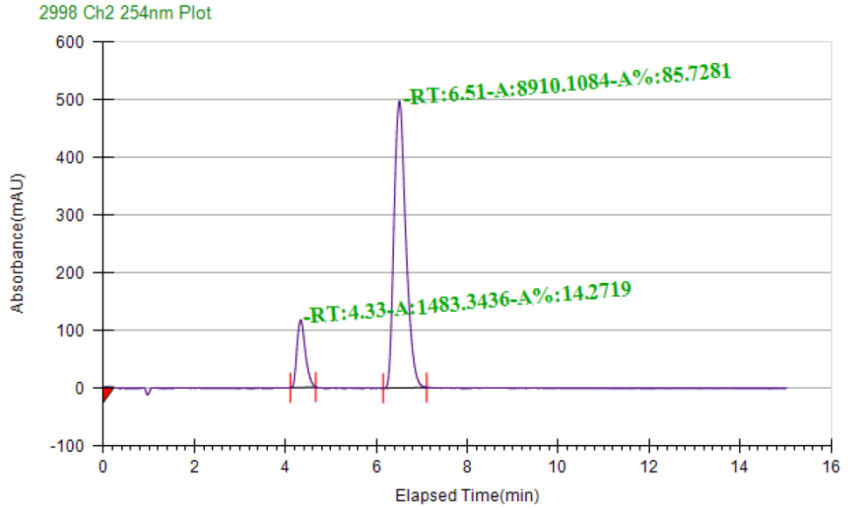
IV.10. Compound **3j**.

SFC Analysis: 86:14 e.r. [CHIRALPAK® AD-H, 30°C, 2% *i*PrOH, 4.0 mL/min, 100 bar, retention times: 4.3 min (minor) and 6.5 min (major)].





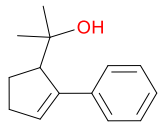
Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
49.9896	4.39 min	387.6946	0.6917 min	3846.5466	0	1.7	0	6.4706
50.0104	6.59 min	284.9395	0.8417 min	4421.2662	0	1.5217	-6.4706	0

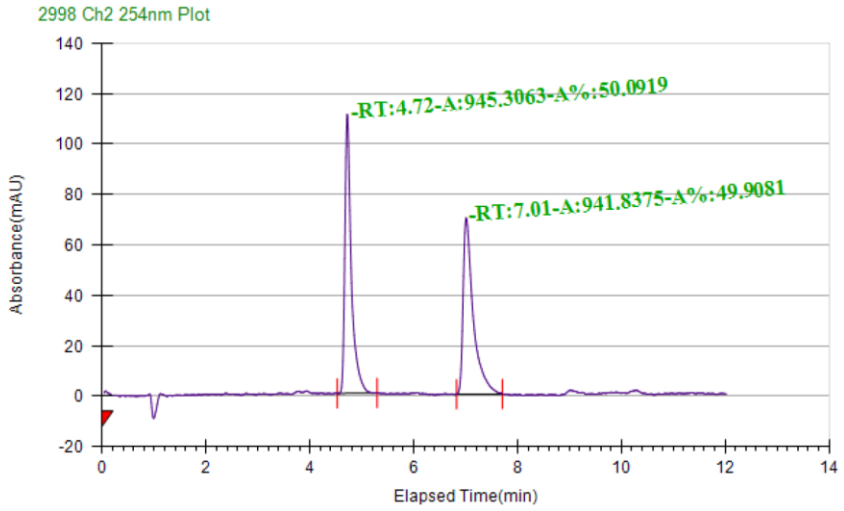


Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
14.2719	4.33 min	117.0265	0.5667 min	3095.0744	0	1.3158	0	5.5829
85.7281	6.51 min	497.1765	0.9667 min	3103.0156	0	1.2679	-5.5829	0

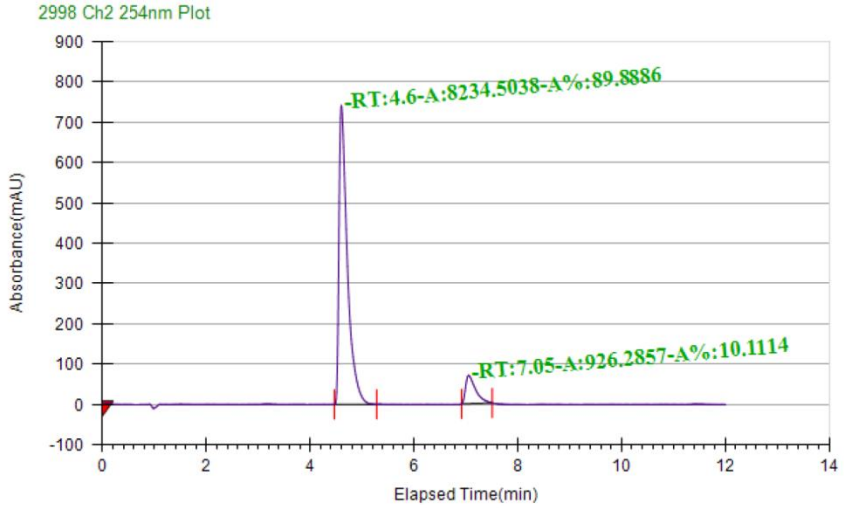
IV.11. Compound **3k**.

SFC Analysis: 90:10 e.r. [CHIRALPAK® IA, 30°C, 5% *i*PrOH, 4.0 mL/min, 100 bar, retention times: 4.6 min (major) and 7.1 min (minor)].





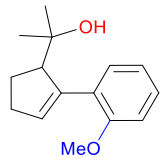
Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
50.0919	4.72 min	110.7787	0.775 min	10501.6109	0	1.9091	0	9.5156
49.9081	7.01 min	70.0094	0.8917 min	8885.1173	0	2.3929	-9.5156	0

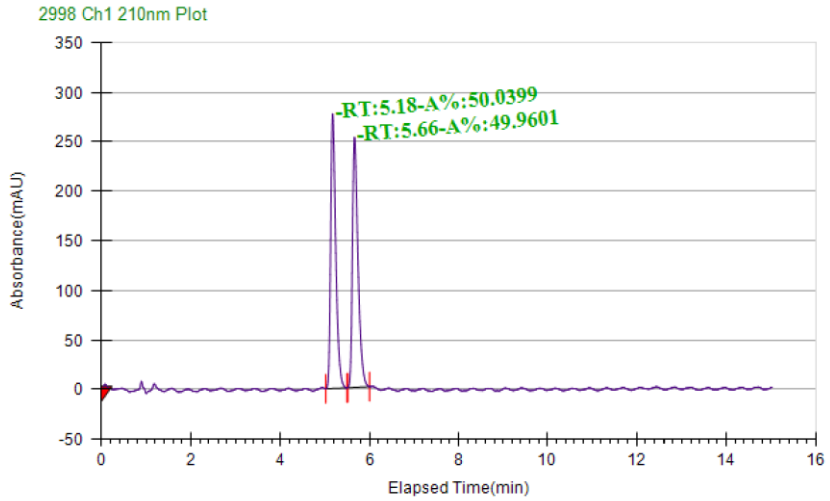


Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
89.8886	4.6 min	742.3366	0.825 min	4676.0669	0	2.5	0	8.4362
10.1114	7.05 min	70.1871	0.6 min	8192.2864	0	2.2308	-8.4362	0

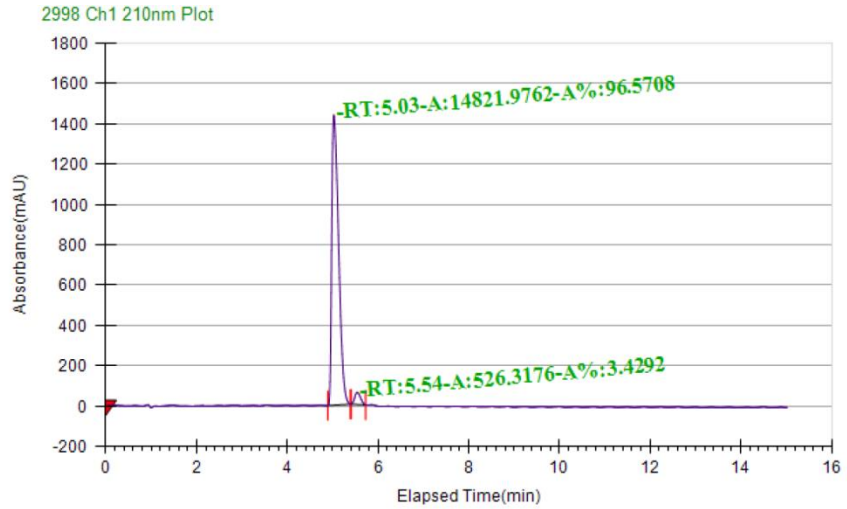
IV.12. Compound **3l**.

SFC Analysis: 97:3 e.r. [CHIRALPAK® IB, 30°C, 2% *i*PrOH, 4.0 mL/min, 100 bar, retention times: 5.0 min (major) and 5.5 min (minor)].





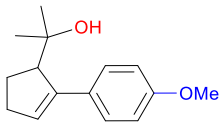
Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
50.0399	5.18 min	277.7882	0.4833 min	12641.7227	5174	1.4545	0	2.5272
49.9601	5.66 min	252.6035	0.5 min	13031.465	5657.3333	1.6364	-2.5272	0

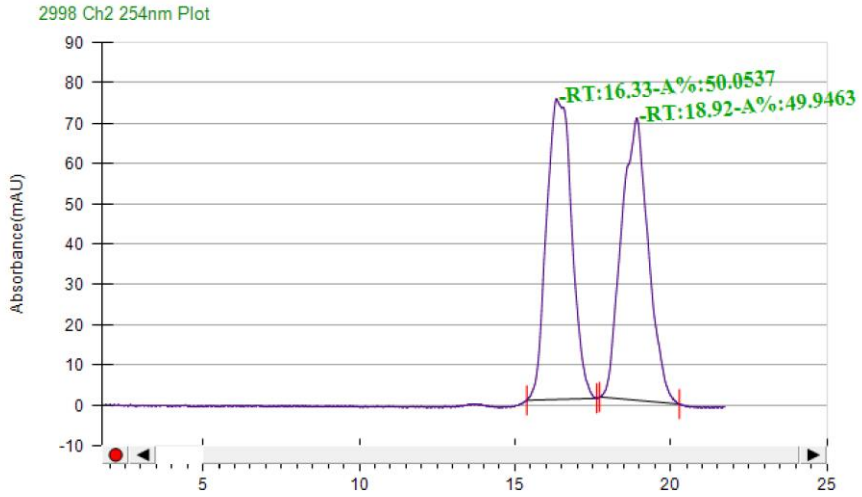


Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
96.5708	5.03 min	1440.307	0.5083 min	5580.0384	0	1.95	0	2.084
3.4292	5.54 min	60.9351	0.325 min	9570.0254	0	1.2308	-2.084	0

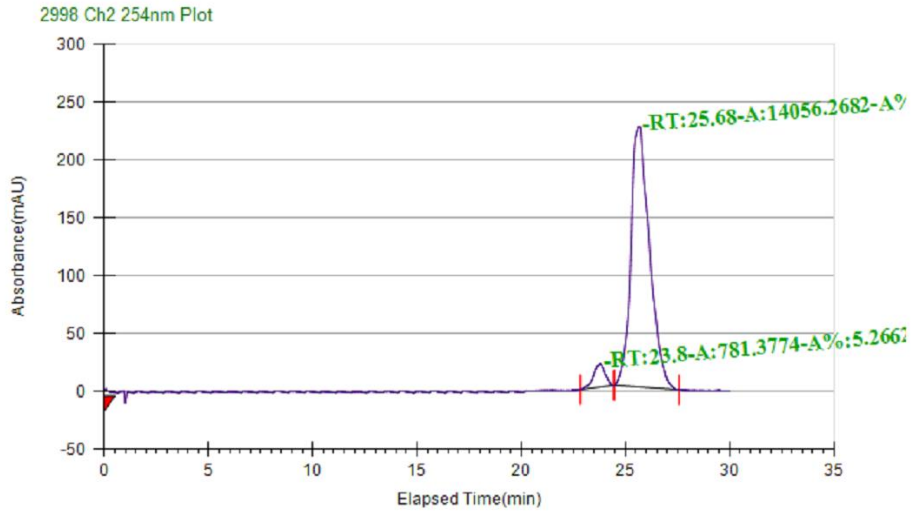
IV.13. Compound **3m**.

SFC Analysis: 95:5 e.r. [CHIRALPAK® IC, 30°C, 2% *i*PrOH, 4.0 mL/min, 100 bar, retention times: 23.8 min (minor) and 25.7 min (major)].





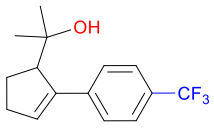
Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
50.0537	16.33 min	74.8074	2.2583 min	1824.6283	16332.3333	1.2083	0	1.6282
49.9463	18.92 min	70.1445	2.55 min	2121.512	18915.6667	1.0357	-1.6282	0

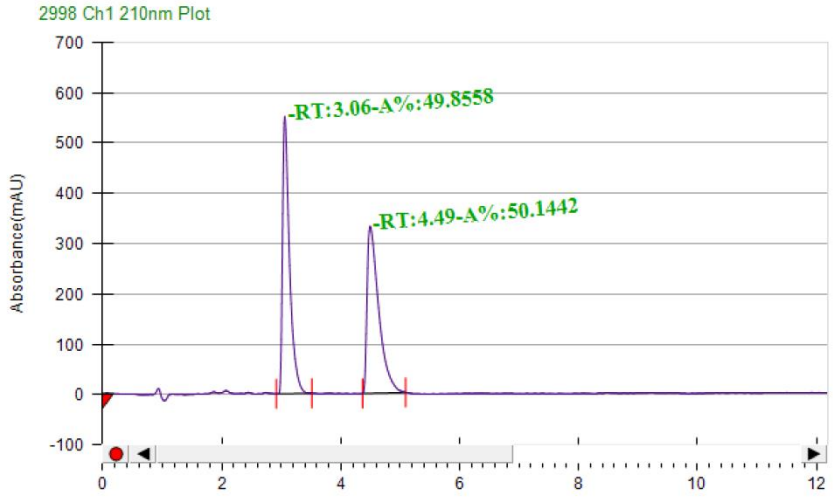


Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
5.2662	23.8 min	20.0609	1.6083 min	8716.8822	23799	0.8229	0	1.4386
94.7338	25.68 min	225.3001	3.1167 min	4192.346	25674	1.2196	-1.4386	0

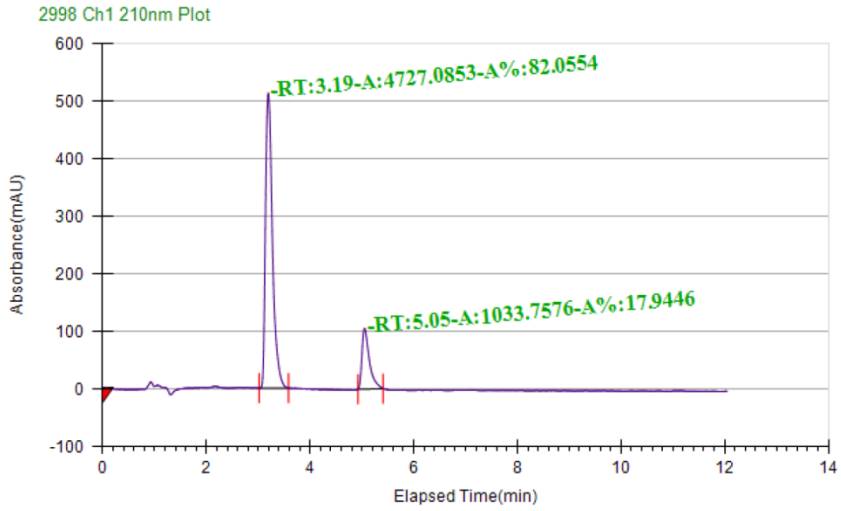
IV.14. Compound **3n**.

SFC Analysis: 82:18 e.r. [CHIRALPAK® IA, 30°C, 5% *i*PrOH, 4.0 mL/min, 100 bar, retention times: 3.2 min (major) and 5.1 min (minor)].





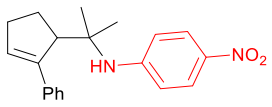
Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
49.8558	3.06 min	551.0516	0.6083 min	4415.2489	3057.3333	2.1875	0	5.6209
50.1442	4.49 min	332.0444	0.7333 min	3042.5073	4490.6667	2.6364	-5.6209	0

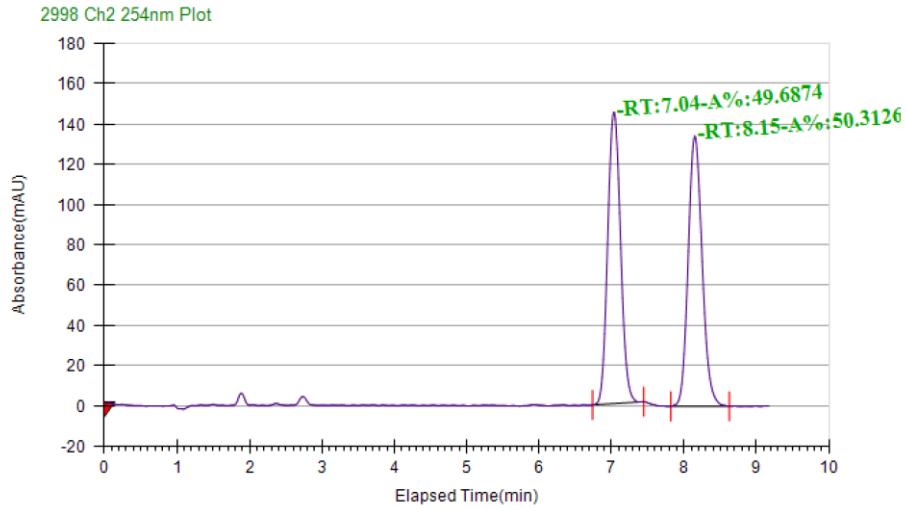


Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
82.0554	3.19 min	512.3718	0.575 min	3174.4416	0	1.5833	0	8.1985
17.9446	5.05 min	105.7109	0.4917 min	7947.2166	0	1.875	-8.1985	0

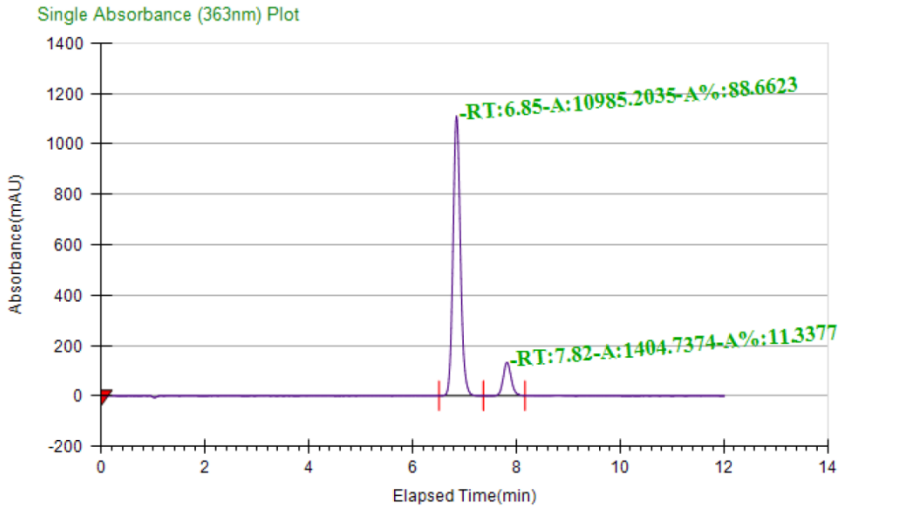
IV.15. Compound **3o**.

SFC Analysis: 89:11 e.r. [CHIRALPAK® IB, 30°C, 10% MeOH, 4.0 mL/min, 100 bar, retention times: 6.9 min (major) and 7.8 min (minor)].





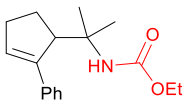
Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
49.6874	7.04 min	145.0772	0.7167 min	8172.9308	7040.6667	1.0682	0	3.4015
50.3126	8.15 min	134.4934	0.8083 min	9199.5162	8149	1.125	-3.4015	0

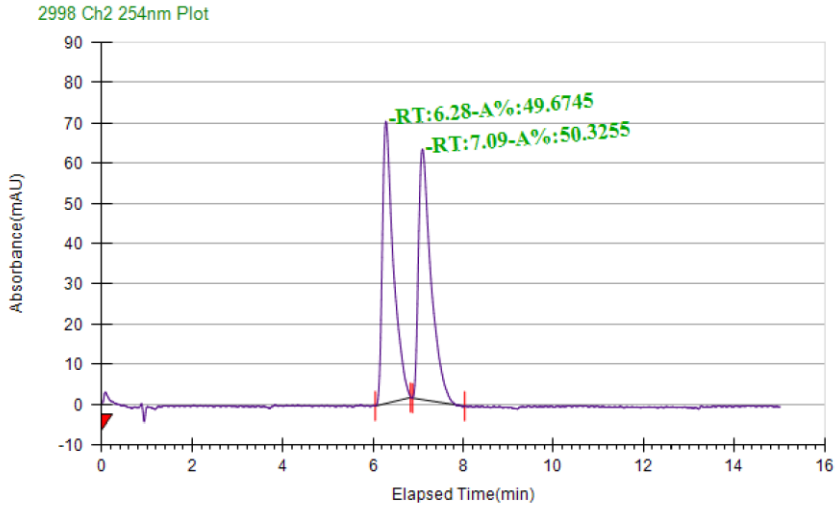


Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
88.6623	6.85 min	1110.0855	0.8667 min	12952.4953	0	1.1111	0	3.7908
11.3377	7.82 min	132.6671	0.8 min	13502.2	0	1.1579	-3.7908	0

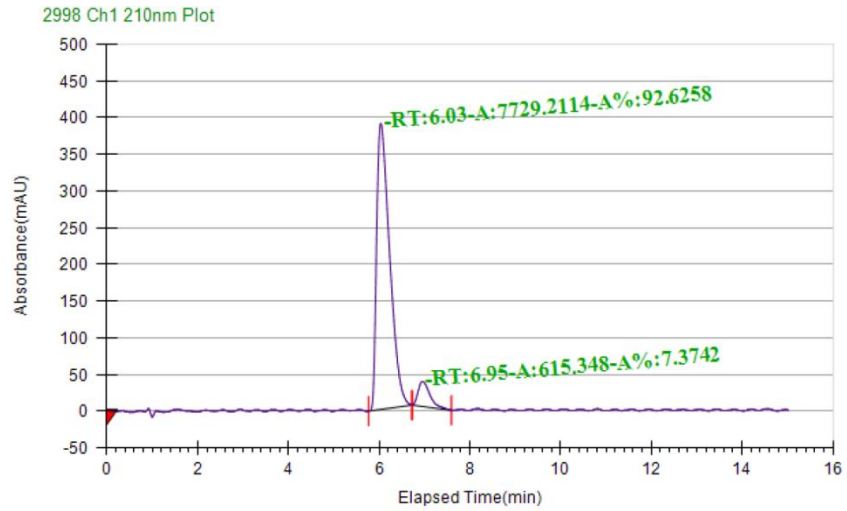
IV.16. Compound **3p**.

SFC Analysis: 93:7 e.r. [CHIRALPAK® AD-H, 30°C, 2% *i*PrOH, 4.0 mL/min, 100 bar, retention times: 6.0 min (major) and 7.0 min (minor)].





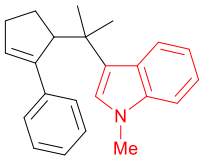
Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
49.6745	6.28 min	70.2928	0.7917 min	4017.3197	0	1.9211	0	1.8406
50.3255	7.09 min	62.3521	1.1667 min	3470.6519	0	2.2632	-1.8406	0

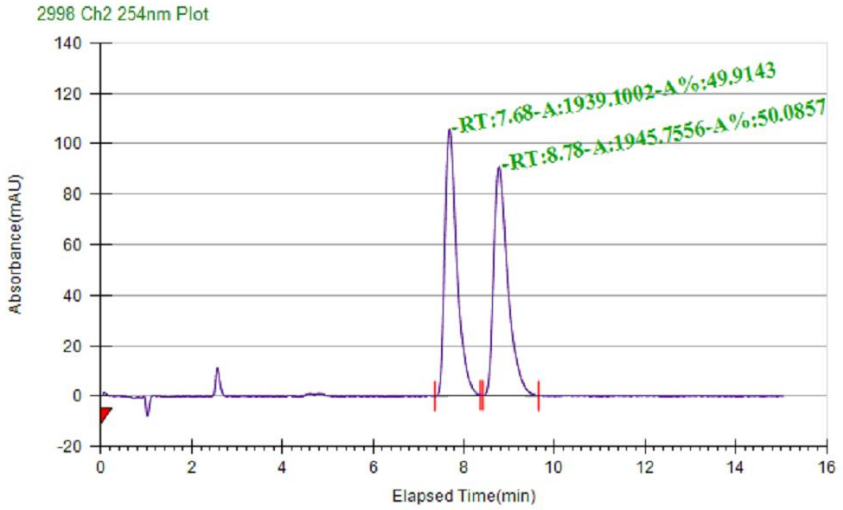


Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
92.6258	6.03 min	390.0752	0.9583 min	2240.6906	6032.3333	1.925	0	1.7974
7.3742	6.95 min	33.959	0.8667 min	2973.2872	6949	1.9773	-1.7974	0

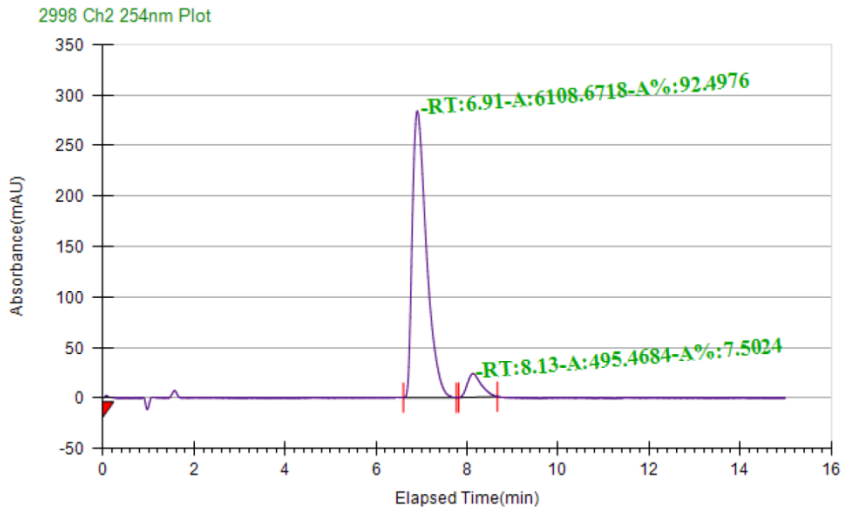
IV.17. Compound **3q**.

SFC Analysis: 92.5:7.5 e.r. [CHIRALPAK® AD-H, 30°C, 3% *i*PrOH, 4.0 mL/min, 100 bar, retention times: 7.0 min (major) and 8.1 min (minor)].





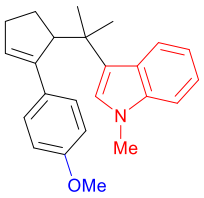
Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
49.9143	7.68 min	105.549	1.025 min	4599.0873	7682.3333	1.625	0	2.2336
50.0857	8.78 min	90.7336	1.2333 min	4487.0722	8774	1.6607	-2.2336	0

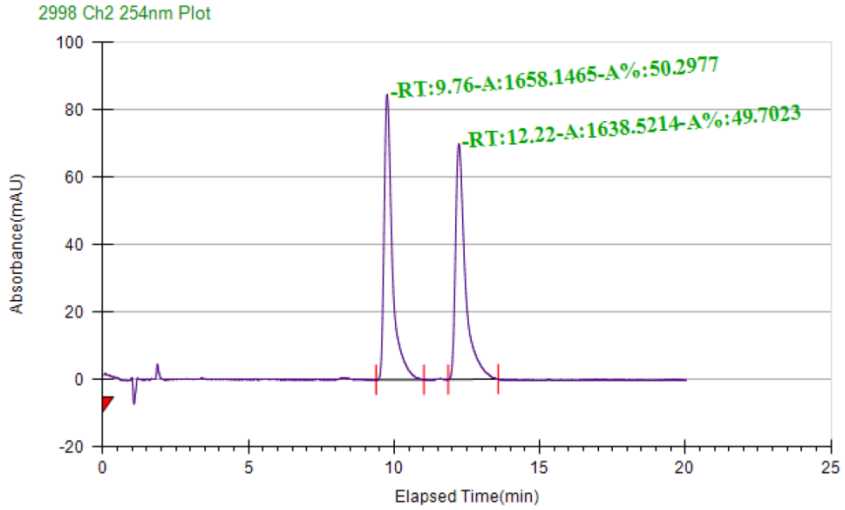


Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
92.4976	6.91 min	284.0194	1.175 min	2503.1658	0	1.76	0	2.246
7.5024	8.13 min	23.4565	0.8583 min	3654.6198	0	1.371	-2.246	0

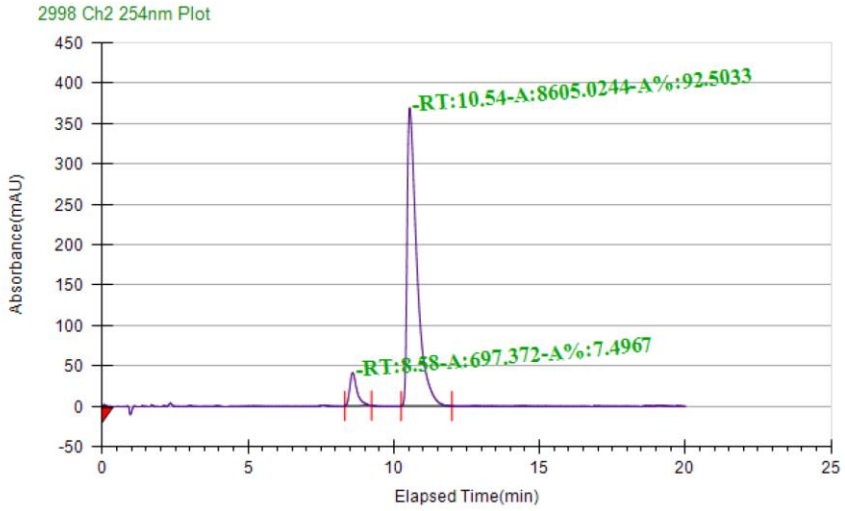
IV.18. Compound **3r**.

SFC Analysis: 92.5:7.5 e.r. [CHIRALPAK® IA, 30°C, 5% *i*PrOH, 4.0 mL/min, 100 bar, retention times: 8.6 min (minor) and 10.5 min (major)].





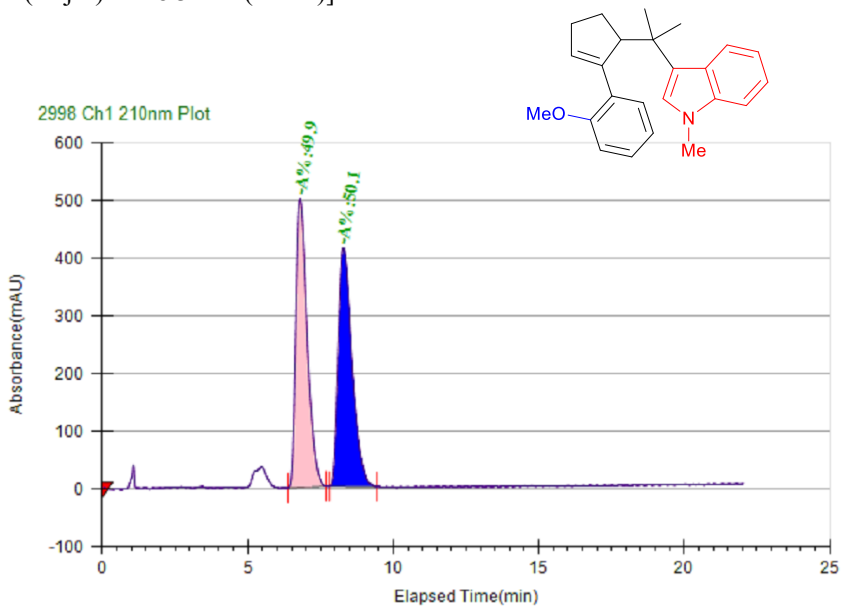
Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
50.2977	9.76 min	84.7159	1.65 min	7904.9689	9757.3333	2.06	0	5.1211
49.7023	12.22 min	69.8932	1.725 min	8708.965	12224	2.1786	-5.1211	0



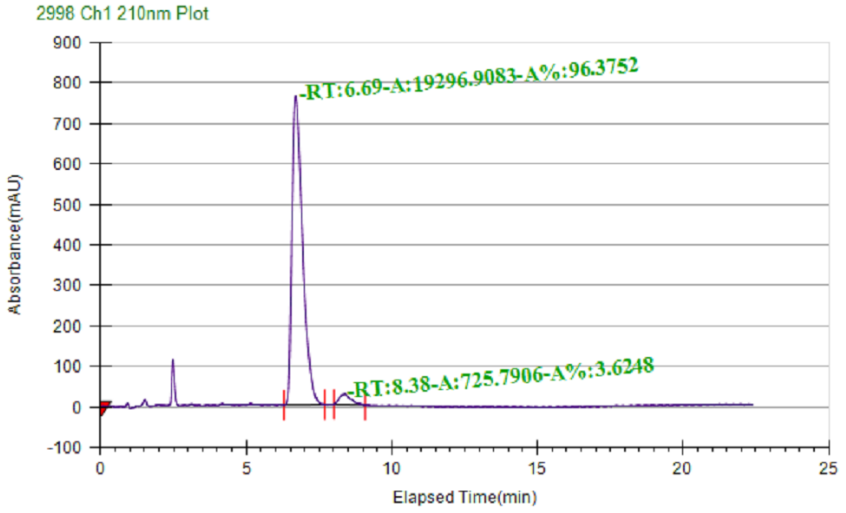
Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
7.4967	8.58 min	41.0015	0.925 min	7496.6658	0	1.6458	0	4.1264
92.5033	10.54 min	369.3066	1.75 min	5828.5644	0	2.725	-4.1264	0

IV.19. Compound **3s**.

SFC Analysis: 96:4 e.r. [CHIRALPAK® AD-H, 30°C, 3% *i*PrOH, 4.0 mL/min, 100 bar, retention times: 6.8 min (major) and 8.3 min (minor)].



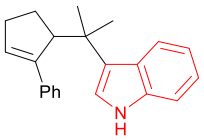
Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
49.9	6.79 min	499.504	1.325 min	1532.6141	0	1.5735	0	1.932
50.1	8.28 min	413.1401	1.65 min	1520.4776	0	1.5595	-1.932	0

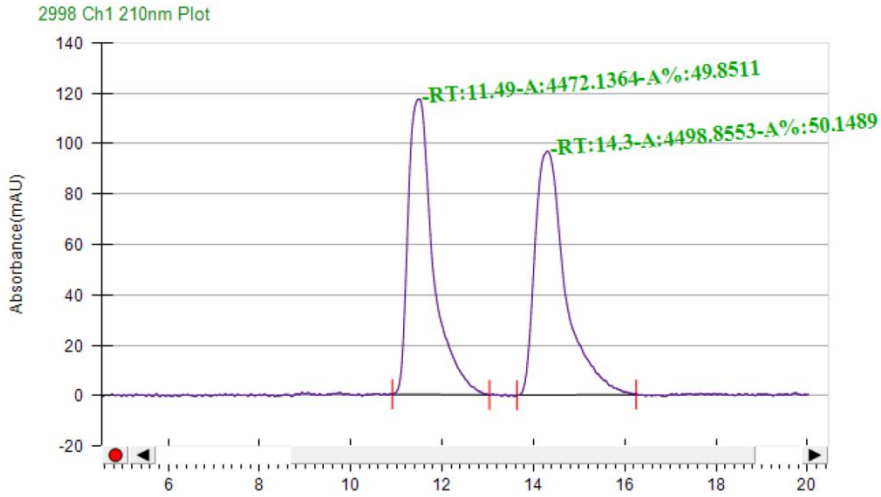


Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
96.3752	6.69 min	762.7962	1.4083 min	1688.205	0	1.7	0	2.3882
3.6248	8.38 min	26.3084	1.0833 min	1922.7296	0	1.4	-2.3882	0

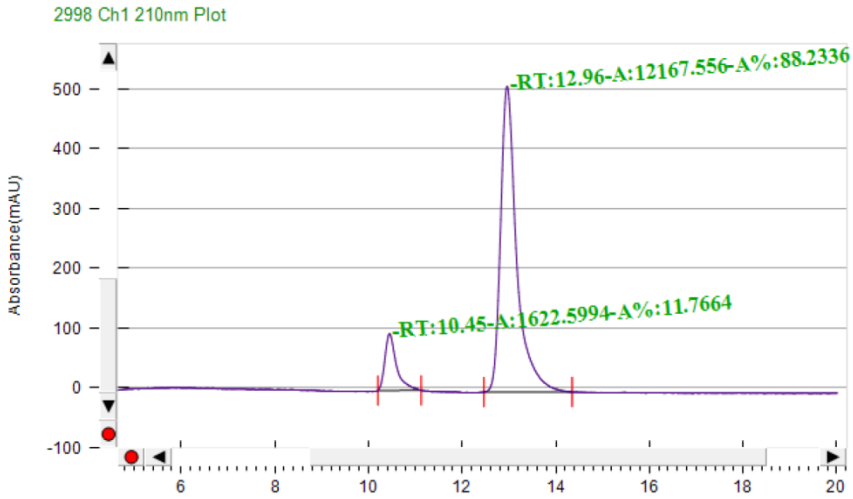
IV.20. Compound **3t**.

SFC Analysis: 88:12 e.r. [CHIRALPAK® IA, 30°C, 10% *i*PrOH, 4.0 mL/min, 100 bar, retention times: 10.5 min (minor) and 13.0 min (major)].





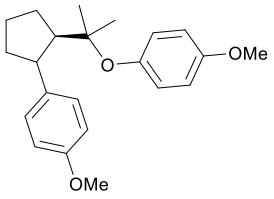
Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
49.8511	11.49 min	117.2849	2.1333 min	2740.6585	11490.6667	1.7653	0	2.873
50.1489	14.3 min	96.9098	2.6167 min	2824.3411	14299	1.8534	-2.873	0

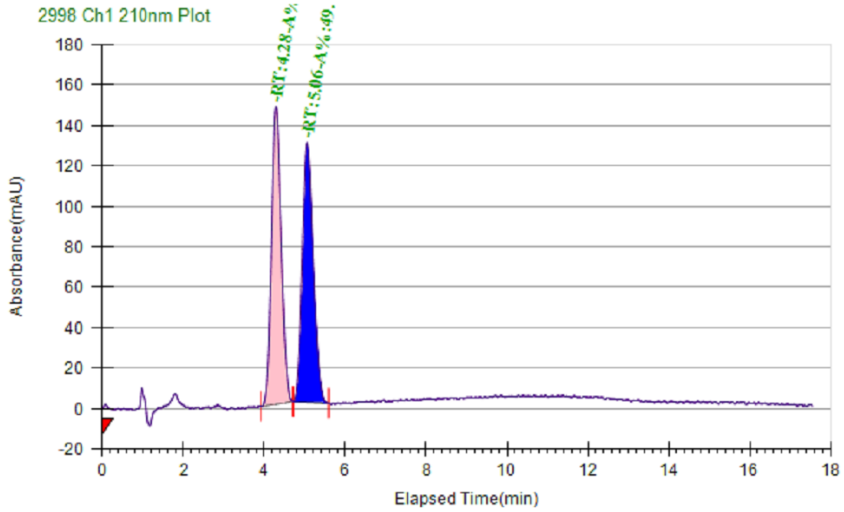


Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
11.7664	10.45 min	95.0578	0.9333 min	11950.2588	10449	1.68	0	5.448
88.2336	12.96 min	511.143	1.8917 min	9276.9103	12957.3333	1.6571	-5.448	0

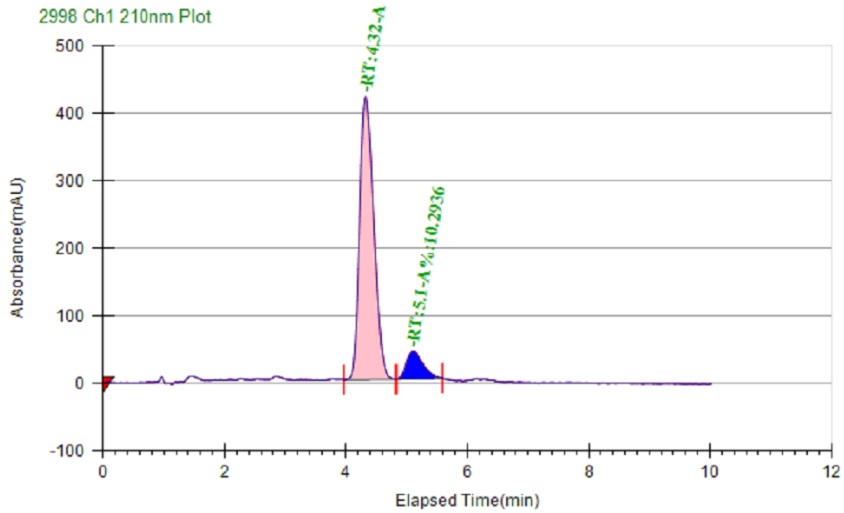
IV.21. Compound **4.**

SFC Analysis: 90:10 e.r. [CHIRALPAK® IC, 30°C, 10% *i*PrOH, 4.0 mL/min, 100 bar, retention times: 4.3 min (minor) and 5.1 min (major)].





Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
50.1094	4.28 min	146.9423	0.7917 min	1523.0446	4282.3333	1.1607	0	1.6833
49.8906	5.06 min	128.4133	0.8833 min	1765.7504	5057.3333	1.1935	-1.6833	0



Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
89.7064	4.32 min	418.8999	0.8583 min	1658.0666	4324	1.2708	0	1.7096
10.2936	5.1 min	40.6076	0.7583 min	1794.96	5099	1.4423	-1.7096	0

IV. Crystallographic data collection, structure determination and refinement:

Colourless large, thick crystalline plates were obtained for **compound 3c,** *from slow evaporation of dichloromethane/n-heptane* as a mixture of crystallization solvent. One 0.58 x 0.51 x 0.1 mm crystal was then selected dipped in Paratone® oil, picked up within a rayon loop and then quickly cryo-cooled in a LN2 stream upon the chi-partial goniostat of a RIGAKU Spider diffractometer constituted by a MM007 HF copper rotating-anode generator, equipped with Osmic CMF confocal optics. X-ray data were recorded at T=233K with a Rapid II curved Image Plate at 127.4 mm distance to the crystal, in a 2θ range of 4.3°-136.5°, following a six ω-scan strategy by the program *d*trek* [1] to provide the best coverage of Friedel pairs in a total of 193 four-degrees frames. Data reduction and scaling were carried out with an empirical absorption correction, as well as a treatment for Lorentz and polarization effects using the program *Fs_Process* implemented in the CrystalClear2.0 package. [2] The crystal structure was solved by intrinsic phasing methods (*SHELXT* program) [3] in the monoclinic space group $P2_1$, then refined by full-matrix least-squares methods on F^2 using *SHELX-L*[4] upon 230 parameters against 3148 reflections. All non-hydrogen atoms improved by anisotropic refinement. Most of the H atoms were identified in difference maps. Methyl H atoms were idealized and included as rigid groups allowed to rotate but not tip (AFIX 137) and refined with U_{iso} set to $1.5U_{eq}$(C) of the parent carbon atom. All other H atoms bound to carbon atoms were also refined as riding but with U_{iso} set to $1.2U_{eq}$(C). Despite the absence of strong anomalous scatterer, the Flack x parameter [5] was meaningfully determined using 1095 quotients [x = 0.01 (7)] [6] and altogether with the Bayesian-type analysis[7] of Bijvoet pairs as implemented within the PLATON[8] program [y = 0.04 (9)] for 1282 Friedel pairs (85% Friedel coverage), provided strong evidence that the absolute structure (C1 (*R*)) has been correctly assigned. Refinement converged to less then R1 = 4% (all data) after application the following weighted refinement scheme: $w = 1/[\sigma^2(F_o^2) + (0.0506P)^2 + 0.0191P]$ with $P = [\max(F_o^2,0) + 2F_o^2]/3$. X-ray crystallography data collection parameters and structure refinement statistics are reported in table ***1***. An Ortep view is shown in Figure 1.

CCDC 1979004 contains the supplementary crystallographic data for the **3c** compound. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

References

1 PlugrathJ.W.(2016) https://github.com/tlhrigaku/d-star-trek

2 CrystalClear2.0, Rigaku Corporation, Tokyo, Japan, 2011.

3 Sheldrick, G. M. (2015). *Acta Crystallogr.,* **A**71, 3-8.

4 Sheldrick, G. M. (2015). *Acta Crystallogr.,* **C**71, 3-8.

5 Flack, H.D. (1983). *Acta Crystallogr.*,A**39**,876-881.

6 Parsons, S., Flack, H.D. and Wagner, T.(2013). *Acta Crystallogr.*,B**69**,249-259.

7 Hooft, R. W. W., Straver, L. H. & Spek, A. L. (2008). *J. Appl. Cryst.* **41**, 96–103.

8 Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

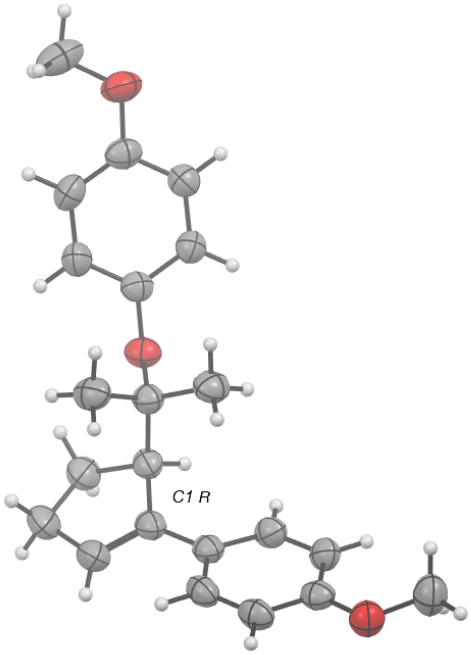


Figure 1 Ortep plot of ***3c*** showing the absolute (*R*)-configuration at the stereogenic center C1. Ellipsoids are drawn at 50% of probability and hydrogen atoms, with sphere radius of arbitrary size.

Table S2: Crystal data and structure refinement for **3c**

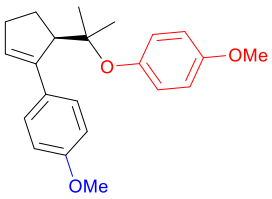
Identification code	(*R*)-1-methoxy-4-(5-(2-(4-methoxyphenoxy)propan-2-yl)cyclopent-1-en-1-yl)benzene	
Structure		
Empirical formula	C_{22} H_{26} O_3	
Formula weight	338.43	
Temperature	233(2) K	
Wavelength	1.54187 Å	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 7.7307(3) Å	α= 90°.
	b = 5.8517(2) Å	β= 92.530(7)°.
	c = 20.5811(14) Å	γ = 90°.
Volume	930.13(8) $Å^3$	
Z	2	
Density (calculated)	1.208 Mg/m^3	
Absorption coefficient	0.625 mm^{-1}	
F(000)	364	
Crystal size	0.58 x 0.51 x 0.10 mm^3	
θ range for data collection	2.149 to 68.248°.	
Index ranges	$-9 \le h \le 8$, $-6 \le k \le 7$, $-24 \le l \le 24$	
Reflections collected / Independent	9355 / 3157 [R(int) = 0.039]	
Completeness to θ = 67.7°	99.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000 and 0.755	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3148 / 1 / 230	
Goodness-of-fit on F^2	1.127	
Final R indices [I>2σ(I)]	R1 = 0.033, wR2 = 0.083	
R indices (all data)	R1 = 0.038, wR2 = 0.091	
Absolute structure parameter	x = 0.01(7)	
Largest diff. peak and hole	0.151 and -0.143 $e.Å^{-3}$	

Table S3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for vs171_deposit. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	2527(1)	3634(1)	5811(1)	23(1)
Cl(1)	4070(1)	3678(1)	2207(1)	21(1)
N(1)	3945(1)	7695(1)	6296(1)	17(1)
F(1)	2546(1)	7971(1)	7515(1)	22(1)
C(1)	2954(1)	6624(2)	6087(1)	15(1)
O(2)	4098(1)	6179(1)	4490(1)	23(1)
F(2)	3273(1)	5502(1)	7733(1)	26(1)
C(2)	2089(1)	7477(2)	5325(1)	16(1)
C(3)	1197(1)	6552(2)	4869(1)	23(1)
O(3)	3216(1)	3737(1)	4128(1)	31(1)
F(3)	1618(1)	5764(1)	7008(1)	27(1)
C(4)	395(1)	7320(2)	4185(1)	25(1)
C(5)	458(1)	9007(2)	3926(1)	23(1)
C(6)	1347(1)	9921(2)	4382(1)	25(1)
C(7)	2154(1)	9170(2)	5074(1)	22(1)
C(8)	-414(1)	9812(2)	3173(1)	33(1)
C(9)	3308(1)	4858(2)	5754(1)	18(1)
C(10)	3574(1)	5016(2)	4714(1)	20(1)
C(11)	2586(1)	6448(2)	7095(1)	19(1)
O(1W)	4703(2)	213(4)	4787(2)	47(1)

Table S4. Bond lengths [Å] and angles [°].

O(1)-C(9)	1.3995(15)
N(1)-C(1)	1.4999(15)
F(1)-C(11)	1.3404(15)
C(1)-C(2)	1.5242(16)
C(1)-C(11)	1.5454(17)
C(1)-C(9)	1.5621(17)
O(2)-C(10)	1.2086(17)
F(2)-C(11)	1.3414(15)
C(2)-C(7)	1.3897(18)
C(2)-C(3)	1.3950(18)
C(3)-C(4)	1.3886(19)
O(3)-C(10)	1.3184(16)
F(3)-C(11)	1.3283(15)
C(4)-C(5)	1.387(2)
C(5)-C(6)	1.387(2)
C(5)-C(8)	1.5073(18)
C(6)-C(7)	1.3934(18)
C(9)-C(10)	1.5304(18)
O(1W)-O(1W)#1	0.928(5)
N(1)-C(1)-C(2)	110.61(10)
N(1)-C(1)-C(11)	105.34(10)
C(2)-C(1)-C(11)	110.62(10)
N(1)-C(1)-C(9)	106.49(9)
C(2)-C(1)-C(9)	113.92(10)
C(11)-C(1)-C(9)	109.44(10)
C(7)-C(2)-C(3)	118.41(12)
C(7)-C(2)-C(1)	121.86(11)
C(3)-C(2)-C(1)	119.72(11)
C(4)-C(3)-C(2)	120.31(13)
C(5)-C(4)-C(3)	121.55(13)
C(6)-C(5)-C(4)	117.95(12)
C(6)-C(5)-C(8)	121.29(14)
C(4)-C(5)-C(8)	120.75(14)
C(5)-C(6)-C(7)	121.13(13)
C(2)-C(7)-C(6)	120.64(13)
O(1)-C(9)-C(10)	113.01(11)

O(1)-C(9)-C(1)	110.93(10)
C(10)-C(9)-C(1)	109.00(10)
O(2)-C(10)-O(3)	125.00(12)
O(2)-C(10)-C(9)	121.73(12)
O(3)-C(10)-C(9)	113.20(11)
F(3)-C(11)-F(1)	107.24(10)
F(3)-C(11)-F(2)	108.03(10)
F(1)-C(11)-F(2)	107.16(10)
F(3)-C(11)-C(1)	112.73(10)
F(1)-C(11)-C(1)	110.14(10)
F(2)-C(11)-C(1)	111.31(10)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z+1

Table S5. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for vs171_deposit. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	25(1)	17(1)	26(1)	4(1)	0(1)	-2(1)
Cl(1)	24(1)	17(1)	21(1)	-2(1)	-3(1)	3(1)
N(1)	14(1)	19(1)	17(1)	1(1)	1(1)	0(1)
F(1)	24(1)	26(1)	18(1)	-4(1)	5(1)	0(1)
C(1)	14(1)	17(1)	15(1)	0(1)	2(1)	0(1)
O(2)	22(1)	27(1)	22(1)	-1(1)	7(1)	1(1)
F(2)	29(1)	30(1)	17(1)	8(1)	3(1)	4(1)
C(2)	14(1)	20(1)	13(1)	0(1)	3(1)	3(1)
C(3)	20(1)	23(1)	24(1)	1(1)	-2(1)	-1(1)
O(3)	41(1)	30(1)	23(1)	-8(1)	8(1)	-5(1)
F(3)	22(1)	37(1)	23(1)	-1(1)	8(1)	-10(1)
C(4)	17(1)	34(1)	23(1)	0(1)	-2(1)	1(1)
C(5)	18(1)	34(1)	16(1)	2(1)	4(1)	11(1)
C(6)	28(1)	23(1)	23(1)	5(1)	2(1)	6(1)
C(7)	22(1)	21(1)	22(1)	2(1)	-1(1)	1(1)
C(8)	24(1)	49(1)	25(1)	9(1)	2(1)	16(1)
C(9)	18(1)	17(1)	18(1)	2(1)	1(1)	2(1)
C(10)	18(1)	22(1)	18(1)	-2(1)	1(1)	7(1)
C(11)	18(1)	22(1)	16(1)	1(1)	2(1)	-2(1)
O(1W)	37(2)	64(2)	45(2)	22(1)	19(1)	9(1)

Table S6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **3c**.

	x	y	z	U(eq)
H(1O)	2789	2877	6214	28
HN1	4460(14)	7210(20)	6738(13)	20
HN2	3833(12)	8720(20)	6547(11)	20
HN3	4195(13)	7830(20)	5743(13)	20
H(3)	1137	5392	5028	28
HO3	3390	3875	3571	46
H(4)	-211	6675	3886	30
H(6)	1406	11080	4219	30
H(7)	2755	9822	5378	27
H(8A)	-356	9426	2505	49
H(8B)	-338	11044	3209	49
H(8C)	-1115	9490	3314	49
H(9)	3978	4523	6221	22
H(1OW)	4780(40)	-380(50)	4270(20)	71
H(2OW)	4230(30)	940(50)	4510(30)	71

Table S7. Torsion angles [°] for **3c**.

N(1)-C(1)-C(2)-C(7)	-14.43(16)
C(11)-C(1)-C(2)-C(7)	101.89(13)
C(9)-C(1)-C(2)-C(7)	-134.34(12)
N(1)-C(1)-C(2)-C(3)	166.38(11)
C(11)-C(1)-C(2)-C(3)	-77.30(14)
C(9)-C(1)-C(2)-C(3)	46.47(15)
C(7)-C(2)-C(3)-C(4)	-0.2(2)
C(1)-C(2)-C(3)-C(4)	179.03(12)
C(2)-C(3)-C(4)-C(5)	0.6(2)
C(3)-C(4)-C(5)-C(6)	-0.7(2)
C(3)-C(4)-C(5)-C(8)	179.30(13)
C(4)-C(5)-C(6)-C(7)	0.3(2)
C(8)-C(5)-C(6)-C(7)	-179.68(13)

C(3)-C(2)-C(7)-C(6)	-0.19(19)
C(1)-C(2)-C(7)-C(6)	-179.39(12)
C(5)-C(6)-C(7)-C(2)	0.1(2)
N(1)-C(1)-C(9)-O(1)	163.25(10)
C(2)-C(1)-C(9)-O(1)	-74.55(13)
C(11)-C(1)-C(9)-O(1)	49.86(13)
N(1)-C(1)-C(9)-C(10)	-71.71(12)
C(2)-C(1)-C(9)-C(10)	50.50(13)
C(11)-C(1)-C(9)-C(10)	174.91(10)
O(1)-C(9)-C(10)-O(2)	168.09(11)
C(1)-C(9)-C(10)-O(2)	44.26(15)
O(1)-C(9)-C(10)-O(3)	-14.69(15)
C(1)-C(9)-C(10)-O(3)	-138.52(11)
N(1)-C(1)-C(11)-F(3)	169.64(10)
C(2)-C(1)-C(11)-F(3)	50.09(14)
C(9)-C(1)-C(11)-F(3)	-76.23(13)
N(1)-C(1)-C(11)-F(1)	49.91(12)
C(2)-C(1)-C(11)-F(1)	-69.64(13)
C(9)-C(1)-C(11)-F(1)	164.05(10)
N(1)-C(1)-C(11)-F(2)	-68.79(12)
C(2)-C(1)-C(11)-F(2)	171.65(10)
C(9)-C(1)-C(11)-F(2)	45.34(13)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z+1

Table S8. Hydrogen bonds [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1O)...Cl(1)#2	0.84	2.28	3.0725(10)	158.2
N(1)-HN1...Cl(1)#3	0.890(18)	2.251(18)	3.1322(11)	170.8(15)
N(1)-HN2...Cl(1)#4	0.903(18)	2.246(18)	3.1217(12)	163.3(14)
N(1)-HN3...O(2)	0.881(18)	2.143(17)	2.7893(15)	129.7(14)
N(1)-HN3...O(1W)#5	0.881(18)	2.451(17)	3.150(3)	136.6(14)
N(1)-HN3...O(1W)#3	0.881(18)	2.295(17)	2.975(3)	133.9(14)
O(3)-HO3...Cl(1)	0.84	2.21	3.0292(11)	166.3
C(9)-H(9)...Cl(1)#2	1.00	2.86	3.4656(13)	119.4
O(1W)-H(1OW)...Cl(1)#6	0.869(19)	2.81(3)	3.601(3)	152(5)
O(1W)-H(1OW)...F(2)#7	0.869(19)	2.57(4)	3.102(3)	121(3)
O(1W)-H(2OW)...O(3)	0.869(18)	2.562(19)	3.394(3)	161(4)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z+1 #2 x,-y+1/2,z+1/2 #3 -x+1,-y+1,-z+1

#4 x,-y+3/2,z+1/2 #5 x,y+1,z #6 -x+1,y-1/2,-z+1/2

#7 x,-y+1/2,z-1/2

IV. DFT Calculations:

DFT computations have been studied using the Gaussian 09 software package.[2] Minima and transition states were optimized using the B3LYP functional,[3] the LANL2DZ(ECP)[4] basis set for Au and the 6-31G(d,p) basis set for the other elements, at the temperature of 253.15 K. Single point calculations were performed with the M06 functional,[5] the def2-TZVP basis set for Au and the 6-311+G(2d,p) for the other elements. Solvation energies were obtained at the same level of theory with the CPCM model used for dichloroethane. The values presented are solvent-corrected ΔG_{253} in kcal/mol obtained from the M06 energies and applying the thermal corrections derived from the optimization level.

Table S9. Coordinates (x,y,z) and M06 energies of the computed species.

A E(RM06) = -3155.03043681				**$TS_{A\text{-}(R,S)\text{-}B}$** Frequency -268.5299 E(RM06) = -3155.01120621			
C	-1.048036	-1.126104	2.599597	C	5.517443	-1.508109	1.560496
C	-0.590828	-2.260336	3.289127	C	4.289991	-0.380761	0.457338
C	-0.733599	4.205322	2.331144	C	6.288996	-0.398685	1.8783
C	-4.425627	3.889134	-1.829139	C	3.163307	-0.552262	1.107514
C	-5.439078	3.502976	0.738296	C	-1.293108	-2.262492	-1.173062
C	-0.987252	3.055236	-1.314183	C	0.093099	-2.667953	-1.708371
C	0.006588	2.988859	-2.482936	C	0.491005	-2.165479	-2.958442
C	-3.087147	-4.486577	-4.293496	C	1.70475	-2.539672	-3.529828
C	-3.600522	-3.304658	-3.763533	C	2.546567	-3.437514	-2.867623
C	2.084132	-0.880626	-4.069192	C	2.161414	-3.945887	-1.628415
C	6.525258	-3.62288	2.147006	C	0.945431	-3.564453	-1.052395
C	3.16223	-2.224118	-2.383015	C	-1.479695	-2.512082	0.369259
C	3.245517	-1.4552	-3.542666	C	-1.141888	-4.475743	1.750447

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C	1.929601	-2.420584	-1.751548	C	-2.458151	-0.352749	1.621132
C	-2.118702	-1.225925	1.502675	C	-1.416329	-0.343801	2.750518
C	0.756182	-0.877502	4.757491	C	-1.301539	-1.404778	3.661871
C	-0.597782	0.135253	3.022199	C	-0.41233	-1.330941	4.736745
N	-1.73648	1.774413	-1.124218	C	0.367627	-0.190185	4.933161
C	1.372797	4.679986	1.26405	C	0.249082	0.877782	4.042497
C	-0.614348	-2.640986	-0.19748	C	-0.634566	0.80258	2.963925
C	-3.119053	1.610864	-3.227025	N	-1.109952	1.72036	-1.513118
C	0.563136	4.723373	2.397274	C	-2.447045	1.920771	-2.178395
C	-1.50923	-2.891599	-2.5927	C	-3.004577	3.321596	-1.925045
C	-0.99685	-4.077463	-3.141747	C	-2.947229	4.34182	-2.884104
C	0.896561	4.119677	0.073866	C	-3.47835	5.606626	-2.616241
C	-5.100976	-1.408228	3.947195	C	-4.083151	5.868199	-1.387719
C	-3.543964	-1.225305	2.090777	C	-4.155071	4.856829	-0.42647
C	-3.792804	-1.391063	3.457256	C	-3.620212	3.597474	-0.693737
C	3.417058	-0.948731	1.939992	C	0.008298	2.628653	-1.899721
C	4.694224	3.346751	0.130005	C	0.997682	1.961742	-2.869238
C	7.816099	-2.30346	0.405467	C	0.661433	3.315466	-0.692711
C	4.182326	2.114892	-1.913031	C	2.03515	3.592076	-0.656207
C	5.261187	4.277237	-2.028301	C	2.595862	4.306952	0.406423
C	4.158891	2.208117	-0.506282	C	1.796014	4.757776	1.455363
C	5.95488	-1.210453	1.627183	C	0.424828	4.492466	1.428237
C	0.30623	-2.13583	4.352576	C	-0.134633	3.78291	0.366145
C	6.695841	-2.312182	1.418485	C	-2.412977	1.517827	-3.658657
C	3.642036	1.136019	0.286303	C	-2.393138	-2.963921	-1.9907
C	-5.946959	-1.08625	1.715533	C	-2.293905	-4.336149	-2.267747
C	-1.781109	-4.868758	-3.978502	C	-3.290617	-4.989853	-2.989546
C	-5.793024	4.647437	0.018901	C	-4.401842	-4.285543	-3.4584
C	-4.578456	2.561146	0.176446	C	-4.504956	-2.920544	-3.198113
C	-0.40001	3.592032	-0.003061	C	-3.509153	-2.264688	-2.46944
C	-3.131779	1.67263	-1.694839	C	-2.732274	-1.75068	0.948671
C	0.441738	-4.607012	0.745596	C	-4.507875	-3.290024	1.402709
C	-2.818248	-2.513152	-2.918328	C	-3.814786	0.207416	2.097389
C	-1.998049	-2.464695	0.536145	C	-4.806229	0.502949	1.147491
C	-3.157747	-4.55562	0.638933	C	-6.051259	0.994979	1.537116
C	-4.641292	-1.072849	1.227457	C	-6.331867	1.199314	2.889613
C	-6.182433	-1.256016	3.081458	C	-5.356099	0.90749	3.840882
C	-1.209024	3.649131	1.145156	C	-4.10808	0.417004	3.449039
C	-4.056264	2.741597	-1.114555	C	3.171296	-1.280025	2.427464
C	-5.284204	4.836998	-1.264979	C	4.485567	-2.103754	2.498121
C	5.246818	4.371141	-0.633481	C	7.458563	-0.017511	1.028247
C	4.821819	-1.032036	2.600947	C	6.048066	0.459201	3.082629
C	4.728777	3.151181	-2.66437	C	4.860202	0.17354	-0.760277
C	0.857259	-1.077616	-3.439493	C	5.107307	1.555496	-0.872073

C	3.285045	0.202655	1.018606	C	5.646972	2.082963	-2.044642
C	0.298342	0.257948	4.087145	C	5.956984	1.238904	-3.114028
C	-0.634323	-2.046991	-1.652516	C	5.719139	-0.134887	-3.012388
C	0.761486	-1.845776	-2.267199	C	5.177807	-0.666983	-1.844216
H	5.700474	-3.62629	2.862706	H	-1.202963	3.600819	0.349367
H	3.774381	1.232858	-2.396468	Au	1.330371	0.002682	0.284351
H	-1.773539	3.763324	-1.597136	P	-0.857725	0.39947	-0.541362
H	0.85867	2.338809	-2.261638	O	-1.472143	-0.836287	-1.429308
H	0.929876	5.168342	3.317441	O	-1.600517	-3.910947	0.528006
H	-0.041196	-0.643482	-3.865237	O	-2.035633	0.596198	0.581643
H	2.377309	5.091199	1.293475	O	-3.397354	-2.548933	1.907349
H	-0.486847	2.601159	-3.375442	H	-0.569895	-2.163035	0.882827
P	-1.027747	0.42922	-0.477447	H	-3.414375	-1.543398	0.118788
O	-2.309859	-3.613243	1.296537	H	-1.069062	-5.55277	1.580601
H	1.277417	-3.980154	1.090364	H	-0.148945	-4.089825	2.024861
O	-0.254852	-3.998121	-0.336061	H	-1.837266	-4.283607	2.570303
H	-4.137747	1.469531	-3.600527	H	-5.28135	-2.615032	1.014656
H	4.778665	-1.855868	3.318941	H	-4.198279	-3.987331	0.617697
H	4.976144	-0.116097	3.186209	H	-4.915561	-3.847662	2.24839
H	-5.839805	3.339108	1.734404	H	-0.495173	3.428674	-2.453331
H	6.200215	-0.326526	1.037878	H	1.60552	1.199272	-2.371325
H	-2.223026	3.266314	1.102632	H	0.453221	1.481528	-3.68427
H	-1.366463	-5.783206	-4.39203	H	1.671505	2.701343	-3.311473
H	-0.221208	-4.809611	1.589027	H	-3.19388	-6.052347	-3.19245
H	-2.769803	-2.318174	-0.225443	H	-0.215809	4.851716	2.228646
O	-2.075187	0.010058	0.698062	H	2.230492	5.321562	2.275654
H	-3.32234	-5.368376	1.348991	H	3.660674	4.525481	0.403293
H	-0.96872	-3.236744	3.016445	H	2.681843	3.257965	-1.458929
H	-2.725955	2.523208	-3.682329	H	-3.118346	1.226571	-1.668111
H	-1.382962	4.24912	3.201048	H	-1.720695	2.127976	-4.244921
H	-5.558915	5.718953	-1.835846	H	-2.11115	0.472613	-3.7535
H	-2.507594	0.770245	-3.561999	H	-3.407784	1.632918	-4.099786
H	0.391326	3.985395	-2.718793	H	-2.501183	4.156651	-3.856149
H	5.667355	5.242942	-0.142027	H	-3.42427	6.382982	-3.373735
H	7.909251	-1.33639	-0.095713	H	-4.501627	6.848973	-1.182517
H	8.777204	-2.531903	0.883855	H	-4.635136	5.045673	0.529379
Au	1.213432	0.614718	0.176429	H	-3.683867	2.815556	0.057221
H	-0.966454	1.031041	2.538237	H	-3.594332	-1.200198	-2.29016
H	-2.969371	-1.511434	4.150315	H	-1.433837	-4.893762	-1.918105
H	-5.269264	-1.539976	5.01187	H	-0.165108	-1.484986	-3.490047
H	5.690613	5.080106	-2.619599	H	1.985074	-2.143628	-4.501541
H	-4.479131	-0.933265	0.163564	H	0.656223	-3.996788	-0.104921
H	0.621188	1.247029	4.398752	H	-3.366296	0.197636	4.207056
H	-3.225083	-1.588776	-2.527449	H	-5.56063	1.061292	4.896308

H	0.017111	-4.381642	-2.912839	H	-4.605282	0.35706	0.091216
H	6.353606	-4.438324	1.432439	H	-0.725782	1.64934	2.294896
H	7.442154	-3.88021	2.691789	H	0.8322	1.782594	4.18858
H	-4.311045	1.672345	0.740539	H	-1.938849	-2.271838	3.551063
H	2.131141	-0.293776	-4.982039	H	2.299001	-1.931156	2.52639
H	1.887504	-3.046984	-0.870965	H	3.076738	-0.551635	3.242367
H	-2.687897	-4.948595	-0.268052	H	5.918829	-2.160772	0.788301
O	-1.282518	-0.731509	-1.595284	H	7.574811	-0.660977	0.155534
H	0.165633	-2.114788	0.375109	H	7.3822	1.023422	0.694376
H	0.84041	-5.547923	0.359523	H	8.370347	-0.084946	1.636744
H	-4.12345	-4.099106	0.387934	H	4.868385	-2.160265	3.522548
H	4.746766	3.079589	-3.747461	H	6.888123	0.327888	3.778261
H	4.678559	3.409894	1.212967	H	5.127555	0.222379	3.613377
H	2.645567	-0.886396	2.713757	H	6.041076	1.519942	2.810093
H	7.662412	-3.074029	-0.361104	H	4.850818	2.206624	-0.042713
H	3.224722	-1.864765	1.369732	H	5.828027	3.150705	-2.123987
H	1.54715	4.109925	-0.793096	H	6.381344	1.650255	-4.024837
H	-3.508708	0.712228	-1.335269	H	5.95271	-0.789793	-3.846169
H	-4.060922	4.05043	-2.838594	H	4.973296	-1.730367	-1.770867
H	-6.465383	5.380766	0.453805	H	4.287848	-3.13034	2.178591
H	-3.693671	-5.101202	-4.951732	H	-0.348321	-2.162009	5.4335
H	-4.61057	-2.989447	-4.008456	H	1.043372	-0.127074	5.781428
H	4.200183	-1.318824	-4.042229	H	-7.300819	1.581632	3.196207
H	4.053749	-2.686264	-1.969452	H	-6.800061	1.219903	0.783271
H	1.439998	-0.78246	5.59613	H	3.48084	-3.75177	-3.324355
H	0.637359	-3.027491	4.877272	H	2.795663	-4.659594	-1.109726
H	-7.198335	-1.268334	3.464441	H	-5.35815	-2.357346	-3.56504
H	-6.778934	-0.962533	1.028567	H	-5.173956	-4.79555	-4.026579
	(*R*,*S*)-**B**				**TS**$_{\mathbf{A}\text{-}(S,R)\text{-}\mathbf{B}}$		
	E(RM06) =	-3155.03275089			Frequency	-266.3545	
					E(RM06) =	-3155.01430825	
C	5.429103	-0.537429	2.121025	C	-1.544523	-0.494633	2.720884
C	4.492443	-0.227235	0.885937	C	-1.444344	-1.567542	3.620305
C	5.390884	0.892621	1.812209	C	0.163571	4.473366	1.689074
C	3.150895	-0.322417	1.321736	C	-3.087043	4.316595	-2.787902
C	-1.228306	-2.406887	-0.904813	C	-4.394317	4.653355	-0.350358
C	0.183567	-2.856614	-1.319024	C	-0.056969	2.750116	-1.727488
C	0.644593	-2.495454	-2.595806	C	0.989731	2.218758	-2.718705
C	1.895169	-2.907475	-3.049809	C	-3.978409	-4.373327	-3.730641
C	2.70995	-3.703331	-2.240826	C	-4.158007	-3.018397	-3.459664
C	2.258782	-4.079509	-0.977411	C	1.978331	-2.310204	-3.546424
C	1.006304	-3.65958	-0.518231	C	5.834532	-2.726344	1.139773
C	-1.478542	-2.457322	0.648225	C	2.498629	-3.660744	-1.620439
C	-1.213625	-4.22655	2.283069	C	2.872468	-3.134548	-2.856147

C	-2.470045	-0.154444	1.586437	C	1.243163	-3.370888	-1.075871
C	-1.486422	-0.019299	2.760191	C	-2.515906	-0.524643	1.53098
C	-1.445002	-0.955517	3.805284	C	0.108168	-0.320206	5.003354
C	-0.625794	-0.75026	4.91797	C	-0.8188	0.674375	2.997941
C	0.154625	0.402781	5.020109	N	-1.134037	1.754909	-1.441367
C	0.112125	1.346581	3.992118	C	2.406465	4.20254	0.856836
C	-0.698384	1.136991	2.874173	C	-1.320833	-2.552591	0.258786
N	-1.025772	1.515246	-1.727486	C	-2.326633	1.576425	-3.653631
C	-2.379631	1.686935	-2.370107	C	1.539878	4.657239	1.848737
C	-2.86721	3.131686	-2.267605	C	-2.109175	-2.981836	-2.148309
C	-2.852554	4.013423	-3.356562	C	-1.930642	-4.343652	-2.438072
C	-3.31763	5.324639	-3.22143	C	1.907273	3.56344	-0.282487
C	-3.812178	5.771301	-1.997093	C	-5.614373	0.485716	3.603813
C	-3.841496	4.898557	-0.906307	C	-3.93172	-0.066546	1.939554
C	-3.372596	3.593062	-1.041588	C	-4.31648	0.08602	3.275813
C	0.100474	2.311528	-2.289986	C	3.239752	-1.074758	2.551071
C	1.024801	1.468729	-3.185431	C	5.465045	2.036235	-0.334162
C	0.833193	3.157127	-1.238751	C	7.365333	-0.853078	0.384332
C	2.160965	3.566801	-1.436857	C	4.665616	0.243385	-1.764238
C	2.797835	4.417467	-0.529157	C	5.794511	2.156434	-2.72658
C	2.11797	4.88292	0.596935	C	4.811135	0.796782	-0.476554
C	0.79138	4.496436	0.79804	C	5.624775	-0.391853	2.127564
C	0.157485	3.646848	-0.10985	C	-0.62097	-1.48255	4.745316
C	-2.412317	1.1064	-3.789922	C	6.232474	-1.286309	1.260863
C	-2.289772	-3.215587	-1.67033	C	4.27784	0.099727	0.678861
C	-2.168272	-4.609865	-1.773801	C	-6.177475	0.595389	1.265271
C	-3.132975	-5.359726	-2.443686	C	-2.859267	-5.032059	-3.216284
C	-4.233225	-4.732645	-3.032594	C	-4.36224	5.705135	-1.269673
C	-4.357825	-3.347588	-2.945069	C	-3.770502	3.442827	-0.648932
C	-3.394405	-2.594657	-2.268717	C	0.529896	3.36674	-0.450836
C	-2.741652	-1.619634	1.076915	C	-2.450226	1.906133	-2.160442
C	-4.553753	-3.078582	1.636556	C	-0.888585	-4.513945	1.612307
C	-3.83591	0.481272	1.923789	C	-3.23111	-2.327863	-2.674223
C	-4.775031	0.674375	0.897616	C	-2.656813	-1.908909	0.793938
C	-6.027292	1.226709	1.162832	C	-4.332722	-3.591784	1.07859
C	-6.368445	1.595805	2.465511	C	-4.882748	0.194054	0.939452
C	-5.445108	1.407399	3.492203	C	-6.549711	0.742252	2.603078
C	-4.189627	0.856243	3.224488	C	-0.33393	3.838376	0.552347
C	3.089961	-0.794571	2.741986	C	-3.104135	3.257172	-1.870892
C	4.537227	-1.046221	3.242758	C	-3.707596	5.532738	-2.488254
C	6.532387	1.483875	1.010814	C	5.952456	2.709526	-1.451659
C	4.675905	1.928509	2.656937	C	4.626283	-0.794588	3.192779
C	4.906159	-0.371268	-0.546184	C	5.147794	0.927796	-2.879767
C	4.516898	0.565343	-1.512893	C	0.726324	-2.027344	-3.005735

C	4.907905	0.411461	-2.843366	C	3.176212	-0.310038	1.254763
C	5.695679	-0.676898	-3.224325	C	0.001485	0.759574	4.125232
C	6.08548	-1.615207	-2.267702	C	-1.086707	-2.24361	-1.265576
C	5.691096	-1.464788	-0.936916	C	0.339336	-2.549789	-1.760547
H	-0.881026	3.379937	0.044333	H	5.044298	-3.021375	1.827804
Au	1.400598	0.000528	0.32756	H	4.152087	-0.705967	-1.880216
P	-0.790664	0.308076	-0.612721	H	-0.592737	3.563627	-2.228417
O	-1.402733	-1.023346	-1.347468	H	1.611436	1.433748	-2.277302
O	-1.618628	-3.822566	0.980469	H	1.927665	5.162409	2.728517
O	-1.975974	0.656712	0.464035	H	0.030627	-1.405833	-3.558881
O	-3.458683	-2.286033	2.096495	H	3.477717	4.351855	0.958144
H	-0.584336	-2.051428	1.14713	H	0.495877	1.801735	-3.597931
H	-3.38578	-1.506579	0.199832	P	-0.8487	0.410187	-0.512984
H	-1.138725	-5.316271	2.255366	O	-3.315377	-2.791351	1.679869
H	-0.231116	-3.808128	2.547074	H	0.057609	-4.059485	1.941365
H	-1.941692	-3.931742	3.041774	O	-1.330972	-3.959983	0.378786
H	-5.299243	-2.45257	1.129977	H	-3.308668	1.63943	-4.132471
H	-4.215311	-3.870732	0.961293	H	4.983493	-1.660307	3.76086
H	-5.007145	-3.522255	2.52522	H	4.532544	0.031743	3.902319
H	-0.404641	3.034269	-2.940737	H	-4.912465	4.77238	0.59681
H	1.661988	0.797787	-2.602241	H	6.126166	0.564692	2.256455
H	0.427162	0.862215	-3.86808	H	-1.405024	3.717922	0.433312
H	1.669736	2.107347	-3.795681	H	-2.703021	-6.085868	-3.427257
H	-3.019598	-6.437629	-2.511609	H	-1.634262	-4.391245	2.400389
H	0.238689	4.871289	1.654947	H	-3.305137	-1.714606	-0.065629
H	2.606334	5.556877	1.294681	O	-2.092824	0.48443	0.550277
H	3.821076	4.730796	-0.717622	H	-4.743139	-4.217043	1.874131
H	2.70722	3.243945	-2.315991	H	-2.041953	-2.454579	3.457752
H	-3.056854	1.088819	-1.757181	H	-1.658802	2.262126	-4.181486
H	-1.724682	1.617023	-4.46954	H	-0.526577	4.838715	2.444272
H	-2.144691	0.047914	-3.76611	H	-3.683101	6.340823	-3.213387
H	-3.418978	1.200439	-4.208455	H	-1.944039	0.561486	-3.779945
H	-2.49331	3.683594	-4.326233	H	1.647916	3.025266	-3.055387
H	-3.298639	5.99178	-4.078141	H	6.450468	3.666673	-1.331525
H	-4.179437	6.787996	-1.894323	H	7.602549	0.205659	0.490698
H	-4.238052	5.23211	0.048288	H	8.257132	-1.438723	0.642808
H	-3.407392	2.916669	-0.192652	Au	1.324229	0.129869	0.398854
H	-3.496023	-1.517453	-2.224377	H	-0.905667	1.532962	2.343511
H	-1.316641	-5.110337	-1.329614	H	-3.607912	-0.107531	4.071677
H	0.011133	-1.893229	-3.237937	H	-5.889533	0.596537	4.648513
H	2.230161	-2.616132	-4.040831	H	6.174544	2.682985	-3.59672
H	0.666443	-3.988014	0.454236	H	-4.6107	0.093464	-0.106052
H	-3.490837	0.718768	4.040309	H	0.54423	1.680664	4.317547
H	-5.696706	1.689696	4.510223	H	-3.374166	-1.271276	-2.485292

H	-4.527572	0.398962	-0.122167	H	-1.063826	-4.866032	-2.052508
H	-0.731233	1.889685	2.096548	H	5.511625	-2.946987	0.115534
H	0.694301	2.261337	4.063296	H	6.712341	-3.356847	1.328063
H	-2.088645	-1.823868	3.765209	H	-3.802172	2.629071	0.069459
H	2.51881	-1.733955	2.709222	H	2.247487	-1.904943	-4.517637
H	2.468027	-0.139018	3.36461	H	0.966298	-3.81597	-0.130547
H	6.352611	-1.06839	1.90342	H	-3.923916	-4.226649	0.286098
H	7.070038	0.742421	0.420415	O	-1.334871	-0.82111	-1.485875
H	6.190449	2.279509	0.342835	H	-0.468183	-2.144345	0.824325
H	7.235279	1.929701	1.725207	H	-0.726271	-5.57869	1.427797
H	4.744305	-0.530092	4.185052	H	-5.133138	-2.960805	0.671491
H	5.408843	2.364798	3.346231	H	5.02106	0.499533	-3.869421
H	3.855029	1.538396	3.255839	H	5.57598	2.470295	0.654941
H	4.290698	2.737322	2.029896	H	2.433577	-0.77865	3.227154
H	3.911464	1.416284	-1.217	H	7.147572	-1.062784	-0.669641
H	4.605647	1.147185	-3.582921	H	3.078712	-2.140993	2.345152
H	6.007009	-0.790215	-4.258262	H	2.607218	3.227693	-1.038504
H	6.697894	-2.464926	-2.55442	H	-3.099211	1.149914	-1.713181
H	5.994303	-2.203922	-0.200892	H	-2.602131	4.199783	-3.751838
H	4.712763	-2.111511	3.41302	H	-4.849808	6.647785	-1.039852
H	-0.61901	-1.48534	5.717684	H	-4.697149	-4.910557	-4.342072
H	0.770456	0.572355	5.898805	H	-5.017683	-2.490012	-3.861493
H	-7.343202	2.025528	2.675507	H	3.837899	-3.380479	-3.289469
H	-6.734207	1.369919	0.350972	H	3.172145	-4.322444	-1.082321
H	3.680894	-4.031873	-2.597722	H	0.733787	-0.249851	5.888625
H	2.872688	-4.71533	-0.345487	H	-0.566997	-2.323375	5.431068
H	-5.202591	-2.844709	-3.406806	H	-7.557603	1.053904	2.860078
H	-4.980141	-5.318336	-3.55996	H	-6.893488	0.794855	0.473385
		(*S*,*R*)-**B**					
	E(RM06) =	-3155.03770188					
C	-1.55434	-0.278707	2.713815				
C	-1.353938	-1.323465	3.626961				
C	0.690842	4.567215	1.215702				
C	-2.873096	4.332874	-2.886834				
C	-4.020663	4.850118	-0.400562				
C	0.095294	2.55824	-1.993515				
C	1.019796	1.831718	-2.981074				
C	-4.037591	-4.453042	-3.513986				
C	-4.169978	-3.080946	-3.310784				
C	1.939155	-2.695667	-3.492546				
C	4.550735	-2.613691	2.024796				
C	2.465602	-3.870342	-1.456468				
C	2.819822	-3.487669	-2.749277				
C	1.240095	-3.474512	-0.908708				

C	-2.49941	-0.406338	1.50992	
C	0.008421	0.10796	5.032156	
C	-0.966684	0.967551	2.988495	
N	-1.039682	1.698666	-1.54208	
C	2.838631	4.105625	0.228114	
C	-1.304641	-2.524201	0.371671	
C	-2.369417	1.506067	-3.680161	
C	2.082634	4.697501	1.238258	
C	-2.116165	-3.049144	-2.007074	
C	-1.985603	-4.429175	-2.227982	
C	2.213976	3.385297	-0.795664	
C	-5.665647	0.598559	3.474487	
C	-3.923829	0.067794	1.865932	
C	-4.357333	0.20126	3.189656	
C	3.213585	0.098764	2.927905	
C	5.653295	1.522194	-0.647087	
C	6.350799	-1.883467	0.420101	
C	4.278736	-0.207512	-1.624978	
C	5.438733	1.368623	-3.052556	
C	4.806237	0.416626	-0.486386	
C	5.488005	-0.15658	2.095097	
C	-0.571692	-1.133537	4.770028	
C	5.306497	-1.443844	1.426911	
C	4.463823	-0.066905	0.889447	
C	-6.14317	0.736526	1.117954	
C	-2.940018	-5.123385	-2.968993	
C	-3.957545	5.865311	-1.358756	
C	-3.506662	3.585798	-0.684965	
C	0.818571	3.246239	-0.827882	
C	-2.379989	1.9047	-2.198466	
C	-0.911135	-4.435738	1.81537	
C	-3.217182	-2.384169	-2.562625	
C	-2.633825	-1.836756	0.869036	
C	-4.329595	-3.473603	1.284556	
C	-4.837816	0.336283	0.834651	
C	-6.562974	0.869737	2.442735	
C	0.067807	3.853072	0.19393	
C	-2.921407	3.309315	-1.931249	
C	-3.383323	5.602629	-2.601471	
C	5.967818	1.995609	-1.922729	
C	4.70128	0.103036	3.370575	
C	4.593794	0.266975	-2.899004	
C	0.717304	-2.306915	-2.948458	
C	3.162442	0.033756	1.433719	

C	-0.195707	1.159351	4.135579	
C	-1.063585	-2.302656	-1.166203	
C	0.345721	-2.692493	-1.649377	
H	3.778618	-2.339319	2.741192	
H	3.625027	-1.067263	-1.516438	
H	-0.401606	3.364526	-2.543843	
H	1.600168	1.043589	-2.492463	
H	2.567381	5.268694	2.024762	
H	0.028751	-1.71578	-3.542672	
H	3.919856	4.208813	0.221076	
H	0.429176	1.37339	-3.776026	
P	-0.789529	0.39335	-0.550081	
O	-3.287707	-2.655609	1.817259	
H	0.022733	-3.958788	2.147596	
O	-1.34066	-3.923714	0.55977	
H	-3.37388	1.617465	-4.0998	
H	4.911207	-0.653491	4.132754	
H	4.977082	1.072396	3.793501	
H	-4.478419	5.040467	0.565892	
H	6.440082	0.348788	1.953335	
H	-1.01404	3.780639	0.173679	
H	-2.820591	-6.191121	-3.127295	
H	-1.672443	-4.303154	2.58741	
H	-3.285558	-1.699802	0.000724	
O	-2.059758	0.537168	0.472046	
H	-4.736302	-4.040001	2.1248	
H	-1.84628	-2.272916	3.466936	
H	-1.694136	2.121802	-4.279883	
H	0.086701	5.040621	1.984623	
H	-3.336575	6.382006	-3.356294	
H	-2.063456	0.462837	-3.785909	
H	1.722147	2.529662	-3.445764	
H	6.62586	2.852466	-2.03176	
H	6.928267	-1.053583	0.012989	
H	7.040938	-2.560433	0.937952	
Au	1.380474	0.230431	0.465435	
H	-1.127515	1.796789	2.309895	
H	-3.67882	-0.006439	4.008071	
H	-5.979753	0.695543	4.509501	
H	5.687572	1.732771	-4.044681	
H	-4.528495	0.239562	-0.200553	
H	0.230103	2.139054	4.334018	
H	-3.323824	-1.315259	-2.425996	
H	-1.135662	-4.960704	-1.818156	

H	4.091672	-3.213832	1.23448	
H	5.272807	-3.25264	2.547072	
H	-3.562974	2.799734	0.062236	
H	2.193811	-2.400759	-4.506509	
H	0.976927	-3.813981	0.083246	
H	-3.945484	-4.164302	0.526978	
O	-1.256954	-0.886368	-1.465851	
H	-0.445801	-2.102325	0.918406	
H	-0.729915	-5.502816	1.664755	
H	-5.125994	-2.854892	0.852185	
H	4.181641	-0.231722	-3.771003	
H	6.066848	2.018201	0.226548	
H	2.717965	1.04208	3.197398	
H	5.903455	-2.436046	-0.410988	
H	2.572813	-0.662863	3.390892	
H	2.830712	2.942402	-1.568904	
H	-3.050295	1.214829	-1.682542	
H	-2.450302	4.147451	-3.869135	
H	-4.35983	6.849876	-1.139912	
H	-4.776171	-4.995103	-4.096801	
H	-5.012498	-2.544168	-3.737024	
H	3.762008	-3.81284	-3.180495	
H	3.129337	-4.505206	-0.875498	
H	0.595129	0.260283	5.933622	
H	-0.440313	-1.955228	5.468429	
H	-7.578846	1.180961	2.666542	
H	-6.83006	0.945077	0.303028	