

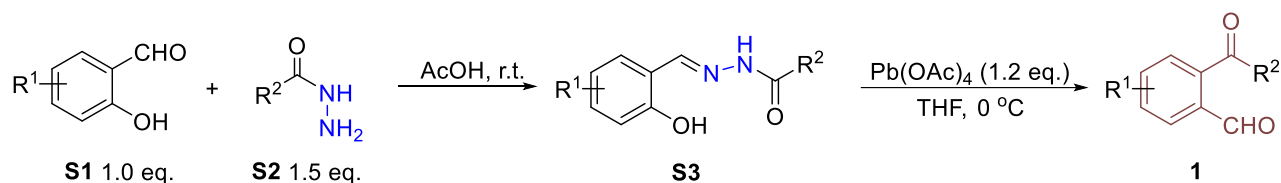
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## General Information

Unless otherwise noted, all starting materials were purchased from commercial sources and used without any further purification. Toluene, Chlorobenzene, DCM,  $\text{CHCl}_3$ ,  $\text{CCl}_4$ , THF,  $\text{D}_2\text{O}$ ,  $\text{H}_2^{18}\text{O}$ , EA and PE were obtained from commercial sources. The analytical data for the known compounds were found to match with the literature data. TLC plates were visualized under UV light (254 nm) or by staining with phosphomolybdic acid or  $\text{KMnO}_4$  followed by heating. Abbreviations are reported as follows: DCM = dichloromethane, THF = tetrahydrofuran, EA = ethyl acetate, PE = petroleum ether,  $\text{D}_2\text{O}$  = deuterium oxide,  $\text{H}_2^{18}\text{O}$  = heavy-oxygen water, TLC = thin layer chromatograph, ee = enantiomeric excess, dr = diastereomeric ratio, rt = room temperature.  $^1\text{H}$  NMR,  $^{19}\text{F}$  NMR and  $^{13}\text{C}$  NMR spectra were recorded on Bruker-*AVANCE* 500 spectrometer, and chemical shifts are reported in ppm. Multiplicities are reported using the following abbreviations: s = singlet, d = doublet, t = triplet, q = quartet, p = pentet, m = multiplet. High resolution mass spectra were obtained by using the UHD Accurate-Mass Q-TOF. Enantiomeric excess (ee) and diastereomeric ratio (dr) were determined on a Thermo Fisher UltiMate 3000 Chiral HPLC using AD, OD, IA and IC column. X-ray crystallographic analysis was carried out by Bruker APEX-II CCD. Reflections were merged by SHEXL according to the crystal class for calculation of statistics and refinement.

## Synthesis of 2-acetylbenzaldehyde



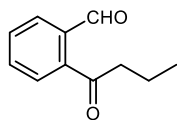
The 2-acetylbenzaldehyde were synthesized according to the literature<sup>[1]</sup> with the modifications.

**Procedure 1:** The salicylaldehyde **S1** (1.0 ml, 10 mmol, 1.0 equiv.) was added to a solution containing the acylhydrazine **S2** (1.11 g, 15 mmol, 1.5 equiv.) in AcOH (30 mL) at room temperature. The reaction mixture was stirred at room temperature for 2 h. Then, the resulting solution was poured into ice water and extracted with  $\text{CH}_2\text{Cl}_2$ . The organic layer was washed with brine, dried over anhydrous  $\text{MgSO}_4$ , and evaporated under reduce pressure to give the title compound **S3**. The product could be used for the next step without further purification.

**Procedure 2:** To a solution containing the **S3** (10 mmol, 1.0 equiv.) in anhydrous THF (30 mL) was added lead tetraacetate (5.4 g, 12 mmol, 1.2 equiv.) at 0 °C. The reaction mixture was stirred at 0 °C and monitored by TLC. After completion (3 h), the resulting reaction was filtered through celite and washed with EA (3 × 20 mL). The filtrate was washed with saturated aqueous solution of  $\text{NaHCO}_3$  and brine. The organic layer was dried over anhydrous  $\text{MgSO}_4$  and evaporated under reduce pressure. The crude product was purified by column chromatography over silica gel (PE: EA= 10:1) to afford the desired product.

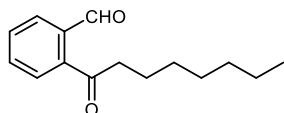
The characterizations of unknown products were as following:

### 2-butyrylbenzaldehyde (1c')



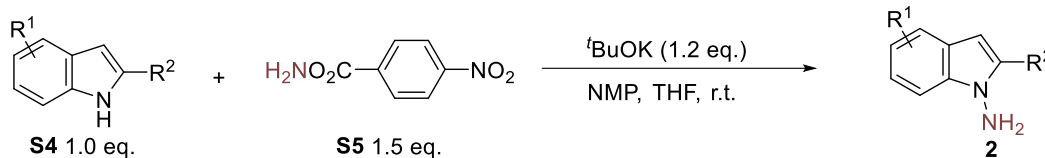
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $^1\text{H}$  NMR (500 MHz, Chloroform-*d*)  $\delta$  10.19 (s, 1H), 7.96 – 7.88 (m, 1H), 7.71 – 7.62 (m, 3H), 2.94 (t,  $J = 7.3$  Hz, 2H), 1.82 (q,  $J = 7.4$  Hz, 2H), 1.04 (t,  $J = 7.4$  Hz, 3H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  204.02, 192.02, 141.32, 135.88, 133.14, 131.37, 129.93, 127.83, 43.29, 17.69, 13.76. HRMS (APCI)  $m/z$ : calculated for  $[\text{C}_{11}\text{H}_{12}\text{O}_2+\text{Na}]^+$  199.0729, found 199.0732.

### 2-octanoylbenzaldehyde (1d')



$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $^1\text{H}$  NMR (500 MHz, Chloroform-*d*)  $\delta$  10.16 (s, 1H), 7.91 – 7.86 (m, 1H), 7.68 – 7.59 (m, 3H), 2.93 (t,  $J = 7.4$  Hz, 2H), 1.76 (p,  $J = 7.4$  Hz, 2H), 1.45 – 1.23 (m, 8H), 0.89 (t,  $J = 6.7$  Hz, 3H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  204.12, 191.97, 141.35, 135.89, 133.12, 131.35, 129.90, 127.82, 41.45, 31.68, 29.20, 29.10, 24.27, 22.61, 14.08. HRMS (APCI)  $m/z$ : calculated for  $[\text{C}_{15}\text{H}_{20}\text{O}_2+\text{Na}]^+$  255.1355, found 255.1366.

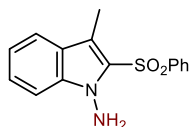
### Synthesis of 2-(phenylsulfonyl)-1*H*-indol-1-amine



The 2-(phenylsulfonyl)-1*H*-indole were synthesized according to the literature<sup>[2]</sup> with the modifications. The 2-(phenylsulfonyl)-1*H*-indol-1-amine were synthesized according to the literature<sup>[3]</sup> with the modifications.

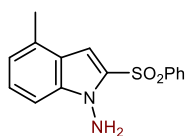
**Procedure 3:** To a stirred solution of the **S4** (10 mmol, 1.0 eq.) in 50 mL *N*-methylpyrrolidone (NMP) was added 12 mL *t*BuOK (1M in THF) and the reaction mixture was stirred at rt for 0.5 h. Then, a solution of **S5** (15 mmol, 1.5 eq.) was added to the mixture, which was stirred at rt for 2 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was quenched with brine and the aqueous layer was extracted with EtOAc (3×20 mL). The combined organic layers were dried over anhydrous  $\text{Na}_2\text{SO}_4$  and then concentrated under reduced pressure. The crude product was purified by column chromatography over silica gel (PE: EA= 4:1) to afford the desired product.

### 3-methyl-2-(phenylsulfonyl)-1*H*-indol-1-amine (2b)



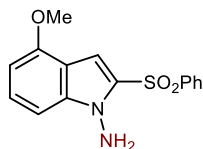
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $^1\text{H}$  NMR (500 MHz, Chloroform-*d*)  $\delta$  7.98 – 7.93 (m, 2H), 7.64 (dt,  $J = 8.2, 0.9$  Hz, 1H), 7.62 – 7.55 (m, 1H), 7.55 – 7.48 (m, 3H), 7.41 – 7.33 (m, 1H), 7.16 (ddd,  $J = 8.0, 6.9, 1.0$  Hz, 1H), 4.82 (s, 2H), 2.72 (s, 3H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  142.43, 138.63, 133.47, 129.47, 128.73, 126.90, 126.63, 124.05, 120.76, 120.54, 119.56, 110.46, 9.73. HRMS (APCI)  $m/z$ : calculated for  $[\text{C}_{15}\text{H}_{14}\text{N}_2\text{O}_2\text{S}+\text{H}]^+$  287.0848, found 287.0844.

#### 4-methyl-2-(phenylsulfonyl)-1H-indol-1-amine (2c)



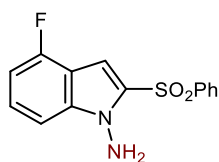
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.04 – 7.98 (m, 2H), 7.64 – 7.57 (m, 1H), 7.53 (dd,  $J$  = 8.5, 7.0 Hz, 2H), 7.42 (s, 1H), 7.38 (d,  $J$  = 8.5 Hz, 1H), 7.20 (dd,  $J$  = 8.6, 1.6 Hz, 1H), 7.17 (s, 1H), 4.77 (s, 2H), 2.43 (s, 3H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  138.03, 134.13, 133.60, 130.98, 129.40, 128.18, 127.86, 122.99, 121.84, 110.02, 107.94, 21.40. HRMS (APCI)  $m/z$ : calculated for  $[\text{C}_{15}\text{H}_{14}\text{N}_2\text{O}_2\text{S}+\text{Na}]^+$  309.0668 found 309.0677.

#### 4-methoxy-2-(phenylsulfonyl)-1H-indol-1-amine (2d)



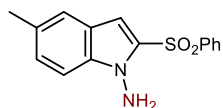
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.01 (dd,  $J$  = 8.4, 1.4 Hz, 2H), 7.63 – 7.57 (m, 1H), 7.53 (dd,  $J$  = 8.4, 7.0 Hz, 2H), 7.35 (s, 1H), 7.29 (d,  $J$  = 7.9 Hz, 1H), 7.08 (d,  $J$  = 8.4 Hz, 1H), 6.52 (d,  $J$  = 7.7 Hz, 1H), 4.81 (s, 2H), 3.94 (d,  $J$  = 1.2 Hz, 3H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  154.49, 141.16, 140.89, 133.59, 133.01, 129.39, 127.89, 127.31, 106.26, 103.11, 100.46, 55.48. HRMS (APCI)  $m/z$ : calculated for  $[\text{C}_{15}\text{H}_{14}\text{N}_2\text{O}_3\text{S}+\text{H}]^+$  303.0797, found 303.0792.

#### 4-fluoro-2-(phenylsulfonyl)-1H-indol-1-amine (2e)



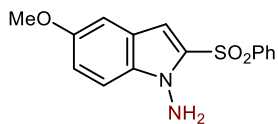
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.06 – 8.01 (m, 2H), 7.67 – 7.61 (m, 1H), 7.56 (dd,  $J$  = 8.5, 7.1 Hz, 2H), 7.31 – 7.24 (m, 3H), 6.82 (ddd,  $J$  = 9.9, 5.1, 3.3 Hz, 1H), 4.86 (s, 2H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  156.99 (d,  $J$  = 252.3 Hz), 141.54 (d,  $J$  = 9.5 Hz), 140.53, 134.91, 133.93, 129.51, 128.01, 126.75 (d,  $J$  = 7.9 Hz), 112.64 (d,  $J$  = 23.5 Hz), 106.48 (d,  $J$  = 4.1 Hz), 105.89 (d,  $J$  = 18.6 Hz), 104.28. HRMS (APCI)  $m/z$ : calculated for  $[\text{C}_{14}\text{H}_{11}\text{FN}_2\text{O}_2\text{S}+\text{Na}]^+$  313.0417, found 313.0427.

#### 5-methyl-2-(phenylsulfonyl)-1H-indol-1-amine (2f)



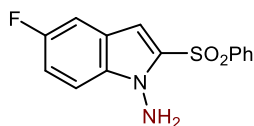
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.03 – 7.98 (m, 2H), 7.63 – 7.56 (m, 1H), 7.52 (dd,  $J$  = 8.4, 6.9 Hz, 2H), 7.41 (s, 1H), 7.38 (d,  $J$  = 8.6 Hz, 1H), 7.20 (dd,  $J$  = 8.7, 1.6 Hz, 1H), 7.16 (s, 1H), 4.77 (s, 2H), 2.42 (s, 3H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  141.11, 138.00, 134.12, 133.57, 130.94, 129.36, 128.15, 127.83, 122.96, 121.81, 109.99, 107.90, 21.37. HRMS (APCI)  $m/z$ : calculated for  $[\text{C}_{15}\text{H}_{14}\text{N}_2\text{O}_2\text{S}+\text{H}]^+$  287.0848, found 287.0845.

#### 5-methoxy-2-(phenylsulfonyl)-1H-indol-1-amine (2g)



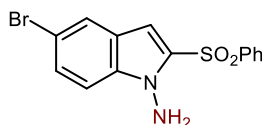
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.04 – 7.95 (m, 2H), 7.65 – 7.58 (m, 1H), 7.54 (dd,  $J = 8.5, 7.1$  Hz, 2H), 7.40 (d,  $J = 9.0$  Hz, 1H), 7.17 (s, 1H), 7.05 (dd,  $J = 9.0, 2.4$  Hz, 1H), 7.02 (d,  $J = 2.3$  Hz, 1H), 4.79 (s, 2H), 3.83 (s, 3H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  155.23, 134.95, 134.15, 133.60, 129.41, 127.79, 122.97, 117.97, 111.40, 107.73, 102.37, 55.74. HRMS (APCI)  $m/z$ : calculated for  $[\text{C}_{15}\text{H}_{14}\text{N}_2\text{O}_3\text{S}+\text{H}]^+$  303.0797, found 303.0788.

#### 5-fluoro-2-(phenylsulfonyl)-1H-indol-1-amine (2h)



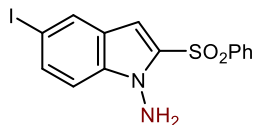
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.04 – 7.99 (m, 2H), 7.63 (t,  $J = 7.4$  Hz, 1H), 7.55 (dd,  $J = 8.5, 6.9$  Hz, 2H), 7.45 (dd,  $J = 9.1, 4.4$  Hz, 1H), 7.30 – 7.24 (m, 1H), 7.16 (s, 1H), 7.13 (td,  $J = 9.1, 2.5$  Hz, 1H), 4.84 (s, 2H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  158.46 (d,  $J = 238.1$  Hz), 140.66, 136.14, 135.68, 133.87, 129.50, 127.92, 122.62 (d,  $J = 10.5$  Hz), 115.39 (d,  $J = 27.1$  Hz), 111.69 (d,  $J = 9.4$  Hz), 107.77 (d,  $J = 5.2$  Hz), 106.83 (d,  $J = 23.8$  Hz).  $^{19}\text{F}$  NMR (471 MHz,  $\text{CDCl}_3$ )  $\delta$  -121.69. HRMS (APCI)  $m/z$ : calculated for  $[\text{C}_{14}\text{H}_{11}\text{FN}_2\text{O}_2\text{S}+\text{Na}]^+$  313.0417, found 313.0439.

#### 5-bromo-2-(phenylsulfonyl)-1H-indol-1-amine (2i)



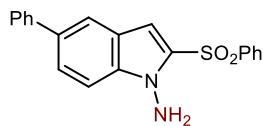
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.04 – 7.96 (m, 2H), 7.78 (d,  $J = 1.8$  Hz, 1H), 7.68 – 7.61 (m, 1H), 7.57 (dd,  $J = 8.6, 7.2$  Hz, 2H), 7.45 (dd,  $J = 8.9, 1.8$  Hz, 1H), 7.40 (d,  $J = 8.8$  Hz, 1H), 7.15 (s, 1H), 4.83 (s, 2H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  140.56, 138.09, 135.48, 133.95, 129.55, 129.22, 127.93, 124.88, 124.02, 114.61, 112.11, 107.38. HRMS (APCI)  $m/z$ : calculated for  $[\text{C}_{14}\text{H}_{11}\text{BrN}_2\text{O}_2\text{S}+\text{Na}]^+$  372.9616, found 374.9605.

#### 5-iodo-2-(phenylsulfonyl)-1H-indol-1-amine (2j)



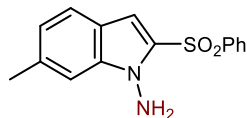
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.04 – 7.91 (m, 3H), 7.67 – 7.62 (m, 1H), 7.61 (dd,  $J = 8.8, 1.6$  Hz, 1H), 7.56 (dd,  $J = 8.5, 7.1$  Hz, 2H), 7.30 (d,  $J = 8.8$  Hz, 1H), 7.14 (d,  $J = 0.8$  Hz, 1H), 4.82 (s, 2H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  140.55, 138.51, 135.10, 134.50, 133.95, 131.26, 129.54, 127.91, 124.87, 112.46, 107.12, 84.79. HRMS (APCI)  $m/z$ : calculated for  $[\text{C}_{14}\text{H}_{11}\text{IN}_2\text{O}_2\text{S}+\text{Na}]^+$  420.9478, found 420.9475.

#### 5-phenyl-2-(phenylsulfonyl)-1H-indol-1-amine (2k)



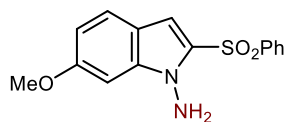
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.04 (dd,  $J = 8.4, 1.3$  Hz, 2H), 7.84 (d,  $J = 1.6$  Hz, 1H), 7.66 – 7.61 (m, 4H), 7.60 – 7.53 (m, 5H), 7.44 (t,  $J = 7.7$  Hz, 2H), 7.37 – 7.31 (m, 1H), 7.30 (s, 1H), 4.84 (s, 2H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  141.44, 140.92, 138.97, 135.16, 134.91, 133.74, 129.46, 128.81, 127.89, 127.33, 126.93, 126.22, 123.17, 120.81, 110.69, 108.70. HRMS (APCI)  $m/z$ : calculated for  $[\text{C}_{20}\text{H}_{16}\text{N}_2\text{O}_2\text{S}+\text{H}]^+$  349.1005, found 349.1005.

#### 6-methyl-2-(phenylsulfonyl)-1H-indol-1-amine (2l)



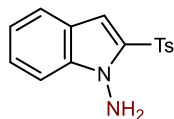
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.04 – 7.98 (m, 2H), 7.60 (td,  $J = 7.2, 1.5$  Hz, 1H), 7.53 (td,  $J = 8.0, 7.6, 1.9$  Hz, 3H), 7.29 (s, 1H), 7.21 (s, 1H), 7.00 (dd,  $J = 8.2, 1.6$  Hz, 1H), 4.76 (s, 2H), 2.47 (s, 3H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  141.18, 139.93, 136.67, 133.54, 129.37, 127.79, 123.64, 122.24, 120.69, 109.86, 108.56, 22.10. HRMS (APCI)  $m/z$ : calculated for  $[\text{C}_{15}\text{H}_{14}\text{N}_2\text{O}_2\text{S}+\text{Na}]^+$  309.0668, found 309.0693.

#### 6-methoxy-2-(phenylsulfonyl)-1H-indol-1-amine (2m)



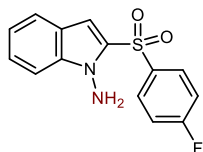
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.99 (dt,  $J = 7.2, 1.3$  Hz, 2H), 7.63 – 7.57 (m, 1H), 7.56 – 7.46 (m, 3H), 7.21 – 7.18 (m, 1H), 6.90 (d,  $J = 2.3$  Hz, 1H), 6.81 (dd,  $J = 8.8, 2.3$  Hz, 1H), 4.78 (s, 2H), 3.85 (s, 3H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  159.54, 141.36, 140.84, 133.48, 132.53, 129.42, 127.63, 123.49, 116.94, 113.45, 109.18, 91.85, 55.56. HRMS (APCI)  $m/z$ : calculated for  $[\text{C}_{15}\text{H}_{14}\text{N}_2\text{O}_3\text{S}+\text{Na}]^+$  325.0617, found 325.0627.

#### 2-tosyl-1H-indol-1-amine (2n)



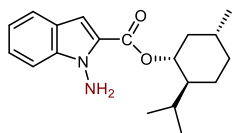
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.89 – 7.84 (m, 2H), 7.62 – 7.56 (m, 1H), 7.38 (dd,  $J = 8.5, 1.1$  Hz, 1H), 7.33 (d,  $J = 8.2$  Hz, 2H), 7.25 (ddd,  $J = 8.3, 6.9, 1.1$  Hz, 1H), 7.08 (d,  $J = 0.9$  Hz, 1H), 7.05 (ddd,  $J = 7.9, 6.8, 1.0$  Hz, 1H), 5.87 (s, 2H), 2.28 (s, 3H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  144.63, 139.33, 138.57, 136.36, 130.12, 128.72, 125.48, 122.91, 122.73, 121.39, 111.37, 106.13, 21.54. HRMS (APCI)  $m/z$ : calculated for  $[\text{C}_{15}\text{H}_{14}\text{N}_2\text{O}_2\text{S}+\text{Na}]^+$  309.0668, found 309.0676.

#### 2-((4-fluorophenyl)sulfonyl)-1H-indol-1-amine (2o)



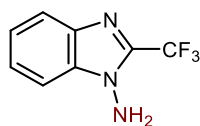
$^1\text{H}$  NMR (500 MHz,  $\text{DMSO-}d_6$ )  $\delta$  8.09 – 8.02 (m, 2H), 7.65 (d,  $J$  = 8.1 Hz, 1H), 7.48 (d,  $J$  = 8.4 Hz, 1H), 7.38 (ddd,  $J$  = 8.3, 6.9, 1.1 Hz, 1H), 7.23 – 7.15 (m, 4H), 4.80 (s, 2H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{DMSO-}d_6$ )  $\delta$  165.68 (d,  $J$  = 257.0 Hz), 139.42, 137.01 (d,  $J$  = 3.2 Hz), 134.43, 130.96 (d,  $J$  = 9.6 Hz), 126.26, 122.77, 122.70, 121.62, 116.63 (d,  $J$  = 22.7 Hz), 110.12, 108.31.  $^{19}\text{F}$  NMR (471 MHz,  $\text{CDCl}_3$ )  $\delta$  -103.25. HRMS (APCI)  $m/z$ : calculated for  $[\text{C}_{14}\text{H}_{11}\text{FN}_2\text{O}_2\text{S}+\text{Na}]^+$  313.0417, found 313.0434.

**(1*R*,2*S*,5*R*)-2-isopropyl-5-methylcyclohexyl 1-amino-1*H*-indole-2-carboxylate (2r)**



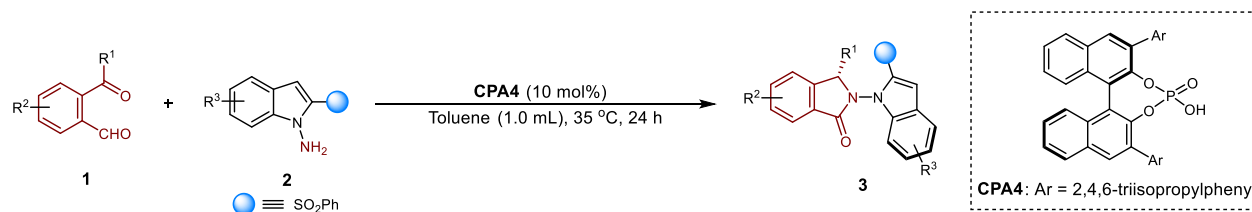
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.62 (t,  $J$  = 7.6 Hz, 2H), 7.34 (dd,  $J$  = 8.6, 6.8 Hz, 1H), 7.17 (s, 1H), 7.12 (t,  $J$  = 7.7 Hz, 1H), 5.35 (d,  $J$  = 2.0 Hz, 2H), 4.94 (td,  $J$  = 10.9, 4.3 Hz, 1H), 2.16 – 2.10 (m, 1H), 1.99 (pd,  $J$  = 6.9, 2.4 Hz, 1H), 1.74 (dt,  $J$  = 14.7, 3.8 Hz, 2H), 1.63 – 1.52 (m, 2H), 1.20 – 1.09 (m, 2H), 0.94 (dd,  $J$  = 7.6, 5.7 Hz, 7H), 0.82 (dd,  $J$  = 6.9, 2.0 Hz, 3H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  162.20, 139.30, 126.52, 125.35, 123.03, 122.20, 120.78, 110.80, 107.75, 74.72, 47.27, 41.08, 34.29, 31.53, 26.61, 23.75, 22.07, 20.74, 16.64. HRMS (APCI)  $m/z$ : calculated for  $[\text{C}_{19}\text{H}_{26}\text{N}_2\text{O}_2+\text{H}]^+$  315.2067, found 315.2075.

**2-(trifluoromethyl)-1*H*-benzo[*d*]imidazol-1-amine (2s)**



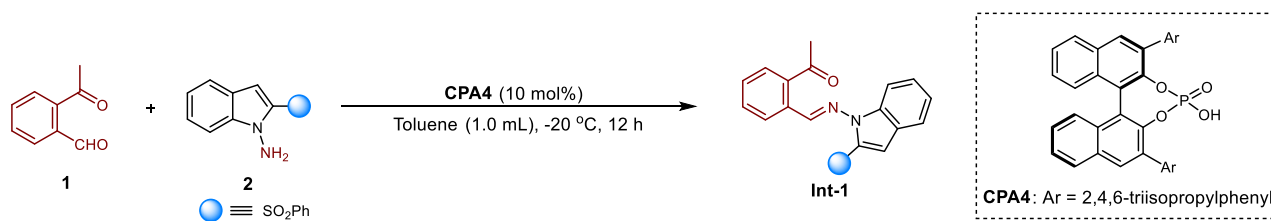
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.84 (d,  $J$  = 8.1 Hz, 1H), 7.55 (d,  $J$  = 8.1 Hz, 1H), 7.50 – 7.44 (m, 1H), 7.42 – 7.35 (m, 1H), 4.94 (s, 2H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  140.77, 138.82, 136.01, 125.73, 123.96, 121.73, 118.76 (d,  $J$  = 271.5 Hz), 109.65.  $^{19}\text{F}$  NMR (471 MHz,  $\text{CDCl}_3$ )  $\delta$  -62.91. HRMS (APCI)  $m/z$ : calculated for  $[\text{C}_8\text{H}_6\text{F}_3\text{N}_3+\text{H}]^+$  202.0586, found 202.0579.

**General procedure for synthesis of products 3**

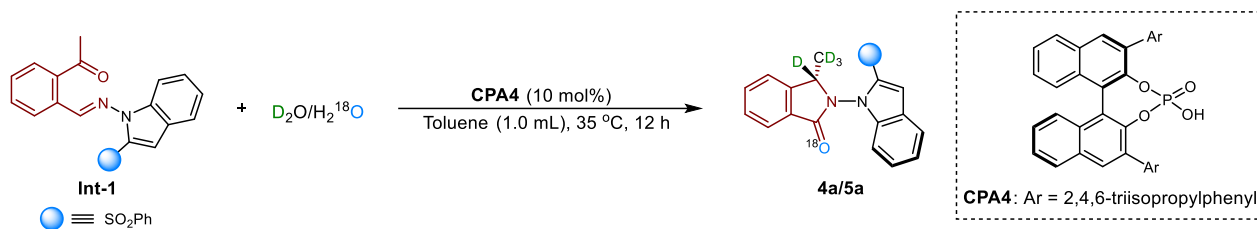


**Procedure 4:** To a 4 mL vial equipped with a stirring bar was added **1** (0.2 mmol, 1.0 eq.), **2** (0.1 mmol, 1.0 eq.) and toluene (1 mL). **CPA4** (0.01 mmol, 0.1 eq.) was then added to the vial and the reaction mixture was stirred at 35 °C for 24 h. After the completion of the reaction which was indicated by TLC, the crude product was purified by column chromatography on silica gel (PE/EA as the eluent) and the desired product was afforded.

## General procedure for synthesis of products 4a/5a



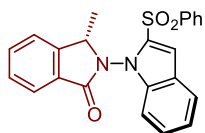
**Procedure 5:** To a test tube equipped with a stirring bar was added **1** (0.2 mmol, 1.0 eq.), **2** (0.1 mmol, 1.0 eq.) and **CPA4** (0.01 mmol, 0.1 eq.). Toluene (1 mL) was then added to the vial and the reaction mixture was stirred at  $-20\text{ }^{\circ}\text{C}$  for 12 h. After the completion of the reaction which was indicated by TLC, the crude product was purified by column chromatography on silica gel (PE/EA as the eluent) and the desired product was afforded.



**Procedure 6:** The reaction was proceeded in the glovebox under argon atmosphere. To a 4 mL dry vial equipped with a stirring bar was added **Int-1** (0.01 mmol, 0.1 eq.), **CPA4** (0.01 mmol, 0.1 eq.) and dry toluene (1 mL). The 50  $\mu\text{L}$  of deuterium oxide ( $\text{D}_2\text{O}$ ) or heavy-oxygen water ( $\text{H}_2^{18}\text{O}$ ) was then added to the flask and the reaction mixture was stirred at  $35\text{ }^{\circ}\text{C}$  for 12 h. After the completion of the reaction which was indicated by TLC, the crude product was purified by column chromatography on silica gel (PE/EA as the eluent) and the desired product was afforded.

## Products characterization for chiral isoindolinones

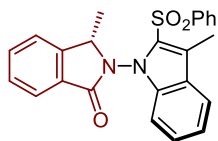
### (*S*)-3-methyl-2-(2-(phenylsulfonyl)-1*H*-indol-1-yl)isoindolin-1-one (**3a**)



Following the **Procedure 4**, **3a** was obtained as faint yellow solid (36.6 mg, 91% yield).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.96 (dd,  $J = 7.6, 1.6$  Hz, 2H), 7.85 (d,  $J = 7.6$  Hz, 1H), 7.74 – 7.66 (m, 2H), 7.54 (td,  $J = 7.4, 1.9$  Hz, 2H), 7.50 (d,  $J = 7.5$  Hz, 1H), 7.47 – 7.40 (m, 3H), 7.30 (ddd,  $J = 8.4, 7.0, 1.2$  Hz, 1H), 7.22 (t,  $J = 7.7$  Hz, 1H), 6.94 (d,  $J = 8.3$  Hz, 1H), 5.13 (q,  $J = 6.8$  Hz, 1H), 1.65 (d,  $J = 6.9$  Hz, 3H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  166.66, 145.64, 140.83, 138.13, 136.75, 133.59, 133.39, 128.97, 128.74, 128.47, 128.32, 127.00, 124.53, 124.19, 123.49, 122.77, 122.65, 112.33, 110.04, 58.12, 17.41. HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min),  $t_r = 35.670$  min (minor), 42.083 min (major); ee = 95%. HRMS (ESI)  $m/z$ : calculated for  $[\text{C}_{23}\text{H}_{18}\text{N}_2\text{O}_3\text{S}+\text{Na}]^+$  425.0930, found 425.0943.

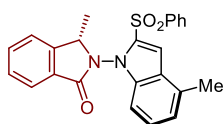
### (*S*)-3-methyl-2-(3-methyl-2-(phenylsulfonyl)-1*H*-indol-1-yl)isoindolin-1-one (**3b**)





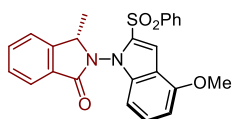
Following the general **Procedure 4**, **3b** was obtained as faint yellow solid (33.3 mg, 80% yield).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.17 (dd,  $J = 7.4, 1.9$  Hz, 2H), 7.98 (d,  $J = 7.6$  Hz, 1H), 7.68 (dd,  $J = 8.3, 6.6$  Hz, 2H), 7.59 – 7.51 (m, 2H), 7.51 – 7.44 (m, 3H), 7.35 (ddd,  $J = 8.3, 7.0, 1.1$  Hz, 1H), 7.23 (t,  $J = 8.0$  Hz, 1H), 7.04 (d,  $J = 8.3$  Hz, 1H), 5.06 (q,  $J = 6.7$  Hz, 1H), 2.55 (s, 3H), 1.60 (d,  $J = 6.8$  Hz, 3H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  166.75, 145.56, 142.14, 137.51, 133.28, 133.05, 130.90, 129.01, 128.94, 128.62, 127.73, 127.44, 125.72, 124.65, 122.47, 122.29, 122.16, 121.22, 110.16, 57.56, 17.00, 10.03. HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min),  $t_r = 21.467$  min (minor), 38.017 min (major); ee = 86%. HRMS (ESI)  $m/z$ : calculated for  $[\text{C}_{24}\text{H}_{20}\text{N}_2\text{O}_3\text{S}+\text{H}]^+$  417.1267, found 417.1259.

**(S)-3-methyl-2-(4-methyl-2-(phenylsulfonyl)-1H-indol-1-yl)isoindolin-1-one (3c)**



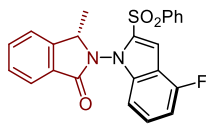
Following the **Procedure 4**, **3c** was obtained as faint yellow solid (27.4 mg, 66% yield).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.99 – 7.94 (m, 2H), 7.83 (d,  $J = 7.6$  Hz, 1H), 7.68 (td,  $J = 7.6, 1.1$  Hz, 1H), 7.57 – 7.47 (m, 4H), 7.43 (t,  $J = 7.7$  Hz, 2H), 7.19 (dd,  $J = 8.4, 7.2$  Hz, 1H), 7.01 (d,  $J = 7.2$  Hz, 1H), 6.74 (d,  $J = 8.3$  Hz, 1H), 5.13 (q,  $J = 6.8$  Hz, 1H), 2.57 (s, 3H), 1.65 (d,  $J = 6.8$  Hz, 3H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  166.75, 145.70, 140.90, 138.09, 136.05, 133.58, 133.44 (d,  $J = 3.9$  Hz), 129.01, 128.75, 128.50, 128.33, 127.28, 124.53, 124.28, 122.89, 122.69, 111.02, 107.54, 58.16, 18.27, 17.46, 1.12. HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min),  $t_r = 31.693$  min (minor), 36.210 min (major); ee = 94%. HRMS (ESI)  $m/z$ : calculated for  $[\text{C}_{24}\text{H}_{20}\text{N}_2\text{O}_3\text{S}+\text{H}]^+$  417.1267, found 417.1255.

**(S)-2-(4-methoxy-2-(phenylsulfonyl)-1H-indol-1-yl)-3-methylisoindolin-1-one (3d)**



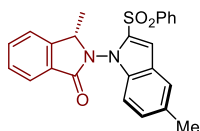
Following the **Procedure 4**, **3d** was obtained as faint yellow solid (32.4 mg, 75% yield).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.98 – 7.90 (m, 2H), 7.85 (d,  $J = 7.6$  Hz, 1H), 7.67 (td,  $J = 7.6, 1.1$  Hz, 1H), 7.56 (s, 1H), 7.52 (t,  $J = 7.9$  Hz, 2H), 7.48 (d,  $J = 7.6$  Hz, 1H), 7.42 (t,  $J = 7.7$  Hz, 2H), 7.20 (t,  $J = 8.1$  Hz, 1H), 6.56 (d,  $J = 7.9$  Hz, 1H), 6.51 (d,  $J = 8.4$  Hz, 1H), 5.10 (q,  $J = 6.7$  Hz, 1H), 3.92 (s, 3H), 1.63 (d,  $J = 6.8$  Hz, 3H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  166.63, 155.07, 145.68, 141.13, 139.55, 135.17, 133.50, 133.39, 128.97, 128.73, 128.54, 128.40, 128.27, 124.53, 122.68, 115.56, 110.17, 102.68, 102.09, 58.07, 55.66, 17.36. HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min),  $t_r = 46.300$  min (minor), 53.200 min (major); ee = 94%. HRMS (ESI)  $m/z$ : calculated for  $[\text{C}_{24}\text{H}_{20}\text{N}_2\text{O}_4\text{S}+\text{Na}]^+$  455.1036, found 455.1048.

**(S)-2-(4-fluoro-2-(phenylsulfonyl)-1H-indol-1-yl)-3-methylisoindolin-1-one (3e)**



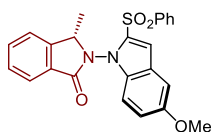
Following the **Procedure 4**, **3e** was obtained as faint yellow solid (26.0 mg, 62% yield).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.00 – 7.93 (m, 2H), 7.85 (d,  $J = 7.6$  Hz, 1H), 7.73 (t,  $J = 7.5$  Hz, 1H), 7.62 – 7.53 (m, 2H), 7.53 (d,  $J = 8.8$  Hz, 2H), 7.47 (t,  $J = 7.7$  Hz, 2H), 7.23 (dd,  $J = 8.1, 4.9$  Hz, 1H), 6.90 (dd,  $J = 9.7, 7.9$  Hz, 1H), 6.73 (d,  $J = 8.4$  Hz, 1H), 5.14 (q,  $J = 6.8$  Hz, 1H), 1.69 (d,  $J = 6.8$  Hz, 3H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  166.62, 157.47 (d,  $J = 253.9$  Hz), 145.60, 140.48, 140.01 (d,  $J = 9.5$  Hz), 137.28, 133.82, 133.56, 129.06, 128.85, 128.45, 128.27, 127.83 (d,  $J = 7.7$  Hz), 124.62, 122.67, 114.07 (d,  $J = 23.6$  Hz), 107.99, 107.51 (d,  $J = 18.6$  Hz), 106.03 (d,  $J = 4.3$  Hz), 58.22, 17.45.  $^{19}\text{F}$  NMR (470 MHz,  $\text{CDCl}_3$ )  $\delta$  -119.16 (dd,  $J = 9.7, 5.0$  Hz). HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min),  $t_r = 20.297$  min (minor), 24.937 min (major); ee = 94%. HRMS (ESI)  $m/z$ : calculated for  $[\text{C}_{23}\text{H}_{17}\text{FN}_2\text{O}_3\text{S}+\text{H}]^+$  421.1016, found 421.0999.

**(S)-3-methyl-2-(5-methyl-2-(phenylsulfonyl)-1H-indol-1-yl)isoindolin-1-one (3f)**



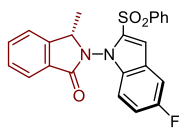
Following the **Procedure 4**, **3f** was obtained as faint yellow solid (31.2 mg, 75% yield).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.95 (dd,  $J = 7.5, 1.7$  Hz, 2H), 7.84 (d,  $J = 7.6$  Hz, 1H), 7.70 – 7.66 (m, 1H), 7.53 (t,  $J = 7.4$  Hz, 2H), 7.51 – 7.47 (m, 2H), 7.42 (t,  $J = 7.7$  Hz, 2H), 7.37 (s, 1H), 7.12 (dd,  $J = 8.5, 1.6$  Hz, 1H), 6.83 (d,  $J = 8.5$  Hz, 1H), 5.10 (q,  $J = 6.8$  Hz, 1H), 2.40 (s, 3H), 1.62 (d,  $J = 6.8$  Hz, 3H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  166.66, 145.67, 141.00, 136.66, 136.60, 133.55, 133.37, 132.41, 128.97, 128.86, 128.74, 128.58, 128.29, 124.53, 124.48, 122.87, 122.67, 112.06, 109.80, 58.08, 21.39, 17.38. HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min),  $t_r = 39.520$  min (minor), 51.073 min (major); ee = 95%. HRMS (ESI)  $m/z$ : calculated for  $[\text{C}_{24}\text{H}_{20}\text{N}_2\text{O}_3\text{S}+\text{H}]^+$  417.1267, found 417.1255.

**(S)-2-(5-methoxy-2-(phenylsulfonyl)-1H-indol-1-yl)-3-methylisoindolin-1-one (3g)**



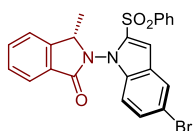
Following the **Procedure 4**, **3g** was obtained as faint yellow solid (39.3 mg, 91% yield).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.99 – 7.91 (m, 2H), 7.84 (d,  $J = 7.6$  Hz, 1H), 7.67 (t,  $J = 7.5$  Hz, 1H), 7.52 (td,  $J = 7.5, 3.7$  Hz, 2H), 7.48 (d,  $J = 7.7$  Hz, 1H), 7.42 (t,  $J = 7.8$  Hz, 2H), 7.37 (s, 1H), 7.10 (d,  $J = 2.4$  Hz, 1H), 6.95 (dd,  $J = 9.0, 2.4$  Hz, 1H), 6.84 (d,  $J = 9.0$  Hz, 1H), 5.09 (q,  $J = 6.8$  Hz, 1H), 3.79 (s, 3H), 1.63 (d,  $J = 6.8$  Hz, 3H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  166.68, 156.14, 145.64, 141.00, 136.87, 133.56, 133.40, 133.36, 128.98, 128.76, 128.50, 128.27, 124.78, 124.51, 122.68, 118.33, 111.94, 111.06, 103.81, 58.22, 55.86, 17.38. HPLC (Chiralpak IC column, 70:30 hexanes/isopropanol, 1 mL/min),  $t_r = 30.660$  min (minor), 45.857 min (major); ee = 94%. HRMS (ESI)  $m/z$ : calculated for  $[\text{C}_{24}\text{H}_{20}\text{N}_2\text{O}_4\text{S}+\text{H}]^+$  433.1216, found 433.1201.

**(S)-2-(5-fluoro-2-(phenylsulfonyl)-1H-indol-1-yl)-3-methylisoindolin-1-one (3h)**



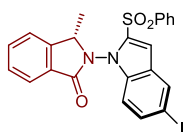
Following the **Procedure 4**, **3h** was obtained as faint yellow solid (27.7 mg, 66% yield).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.95 (d,  $J = 7.8$  Hz, 2H), 7.83 (d,  $J = 7.6$  Hz, 1H), 7.69 (t,  $J = 7.5$  Hz, 1H), 7.55 (dt,  $J = 10.1, 7.5$  Hz, 2H), 7.50 (d,  $J = 7.6$  Hz, 1H), 7.44 (t,  $J = 7.7$  Hz, 2H), 7.39 (s, 1H), 7.36 (dd,  $J = 8.7, 2.5$  Hz, 1H), 7.04 (td,  $J = 9.0, 2.5$  Hz, 1H), 6.88 (dd,  $J = 9.0, 4.1$  Hz, 1H), 5.10 (q,  $J = 6.8$  Hz, 1H), 1.65 (d,  $J = 6.8$  Hz, 3H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  166.76, 165.71 (d,  $J = 256.0$  Hz), 145.65, 138.18, 136.96 (d,  $J = 3.1$  Hz), 136.54, 133.50, 131.28 (d,  $J = 9.7$  Hz), 128.83, 128.37, 127.18, 124.51, 124.16, 123.53, 122.88, 122.70, 116.27 (d,  $J = 22.7$  Hz), 112.47, 110.06, 58.12, 17.40. HPLC (Chiralpak AD column, 80:20 hexanes/isopropanol, 1 mL/min),  $t_r = 40.040$  min (major), 50.857 min (minor); ee = 96%. HRMS (ESI)  $m/z$ : calculated for  $[\text{C}_{23}\text{H}_{17}\text{FN}_2\text{O}_3\text{S}+\text{H}]^+$  421.1016, found 421.0997.

**(S)-2-(5-bromo-2-(phenylsulfonyl)-1H-indol-1-yl)-3-methylisoindolin-1-one (3i)**



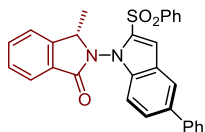
Following the **Procedure 4**, **3i** was obtained as faint yellow solid (38.9.7 mg, 81% yield).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.96 – 7.91 (m, 2H), 7.84 (d,  $J = 1.8$  Hz, 1H), 7.82 (d,  $J = 7.6$  Hz, 1H), 7.72 – 7.67 (m, 1H), 7.54 (dt,  $J = 9.7, 7.5$  Hz, 2H), 7.50 (d,  $J = 7.5$  Hz, 1H), 7.43 (t,  $J = 7.8$  Hz, 2H), 7.36 (s, 1H), 7.34 (dd,  $J = 8.8, 1.8$  Hz, 1H), 6.81 (d,  $J = 8.8$  Hz, 1H), 5.09 (q,  $J = 6.8$  Hz, 1H), 1.65 (d,  $J = 6.8$  Hz, 3H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  166.61, 145.55, 140.43, 138.06, 136.70, 133.88, 133.61, 129.93, 129.08, 128.89, 128.43, 128.21, 125.89, 125.66, 124.58, 122.75, 115.88, 111.59, 111.19, 58.32, 17.45. HPLC (Chiralpak AD column, 70:30 hexanes/isopropanol, 1 mL/min),  $t_r = 35.100$  min (major), 40.730 min (minor); ee = 95%. HRMS (ESI)  $m/z$ : calculated for  $[\text{C}_{23}\text{H}_{17}\text{BrN}_2\text{O}_3\text{S}+\text{H}]^+$  481.02160, found 481.0206.

**(S)-2-(5-iodo-2-(phenylsulfonyl)-1H-indol-1-yl)-3-methylisoindolin-1-one (3j)**



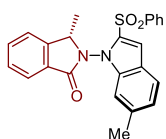
Following the **Procedure 4**, **3j** was obtained as faint yellow solid (32.2 mg, 61% yield).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.06 (s, 1H), 7.93 (d,  $J = 7.8$  Hz, 2H), 7.82 (d,  $J = 7.7$  Hz, 1H), 7.71 (t,  $J = 7.6$  Hz, 1H), 7.55 (q,  $J = 7.8$  Hz, 2H), 7.54 – 7.48 (m, 2H), 7.44 (t,  $J = 7.7$  Hz, 2H), 7.36 (s, 1H), 6.72 (d,  $J = 8.7$  Hz, 1H), 5.09 (q,  $J = 6.8$  Hz, 1H), 1.66 (d,  $J = 6.8$  Hz, 3H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  166.58, 145.55, 140.45 (d,  $J = 2.9$  Hz), 137.69, 137.19, 135.26, 133.85, 133.58, 132.18, 129.07, 128.88, 128.42, 128.23, 126.40, 124.59, 122.72, 111.91, 110.91, 86.12, 58.30, 17.44. HPLC (Chiralpak AD column, 70:30 hexanes/isopropanol, 1 mL/min),  $t_r = 35.940$  min (major), 49.160 min (minor); ee = 92%. HRMS (ESI)  $m/z$ : calculated for  $[\text{C}_{23}\text{H}_{17}\text{IN}_2\text{O}_3\text{S}+\text{H}]^+$  529.0077, found 529.0062.

**(S)-3-methyl-2-(5-phenyl-2-(phenylsulfonyl)-1H-indol-1-yl)isoindolin-1-one (3k)**



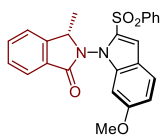
Following the **Procedure 4**, **3k** was obtained as faint yellow solid (33.5 mg, 70% yield).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.02 (d,  $J = 7.8$  Hz, 2H), 7.96 – 7.92 (m, 1H), 7.90 (d,  $J = 7.6$  Hz, 1H), 7.73 (t,  $J = 7.5$  Hz, 1H), 7.58 (t,  $J = 5.5$  Hz, 4H), 7.55 (t,  $J = 6.0$  Hz, 3H), 7.47 (q,  $J = 7.8$  Hz, 4H), 7.36 (t,  $J = 7.5$  Hz, 1H), 7.04 (d,  $J = 8.7$  Hz, 1H), 5.20 (q,  $J = 6.5$  Hz, 1H), 1.72 (d,  $J = 6.8$  Hz, 3H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  166.75, 145.69, 141.13, 140.81, 137.61, 137.39, 136.57, 133.69, 133.50, 129.04, 128.93, 128.81, 128.45, 128.37, 127.45, 127.24, 126.98, 124.72, 124.55, 122.75, 121.78, 112.54, 110.39, 58.31, 17.48. HPLC (Chiralpak OD column, 80:20 hexanes/isopropanol, 1 mL/min),  $t_r = 12.567$  min (minor), 24.573 min (major); ee = 92%. HRMS (ESI)  $m/z$ : calculated for  $[\text{C}_{29}\text{H}_{22}\text{N}_2\text{O}_3\text{S}+\text{H}]^+$  501.1243, found 501.1244.

**(S)-3-methyl-2-(6-methyl-2-(phenylsulfonyl)-1H-indol-1-yl)isoindolin-1-one (3l)**



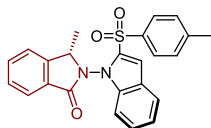
Following the **Procedure 4**, **3l** was obtained as faint yellow solid (25.8 mg, 62% yield).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.98 – 7.93 (m, 2H), 7.87 (d,  $J = 7.6$  Hz, 1H), 7.71 (td,  $J = 7.5, 1.2$  Hz, 1H), 7.60 (d,  $J = 8.3$  Hz, 1H), 7.58 – 7.55 (m, 1H), 7.52 (dd,  $J = 8.3, 7.1$  Hz, 2H), 7.46 – 7.42 (m, 2H), 7.40 (d,  $J = 0.9$  Hz, 1H), 7.06 (dd,  $J = 8.3, 1.4$  Hz, 1H), 6.72 (s, 1H), 5.13 (q,  $J = 6.8$  Hz, 1H), 2.36 (s, 3H), 1.65 (d,  $J = 6.8$  Hz, 3H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  166.60, 145.64, 141.07, 138.64, 137.77, 135.87, 133.45, 133.31, 128.92, 128.70, 128.60, 128.21, 124.80, 124.57, 123.11, 122.64, 122.12, 112.56, 109.65, 57.97, 22.02, 17.33. HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min),  $t_r = 37.603$  min (minor), 45.353 min (major); ee = 57%. HRMS (ESI)  $m/z$ : calculated for  $[\text{C}_{24}\text{H}_{20}\text{N}_2\text{O}_3\text{S}+\text{Na}]^+$  439.1086, found 439.1096.

**(S)-2-(6-methoxy-2-(phenylsulfonyl)-1H-indol-1-yl)-3-methylisoindolin-1-one (3m)**



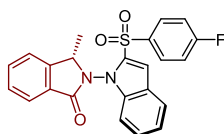
Following the **Procedure 4**, **3m** was obtained as faint yellow solid (27.2 mg, 63% yield).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.59 (t,  $J = 8.3$  Hz, 2H), 7.53 (dd,  $J = 10.3, 7.5$  Hz, 2H), 7.46 (t,  $J = 7.9$  Hz, 2H), 7.99 – 7.94 (m, 2H), 7.91 (d,  $J = 7.6$  Hz, 1H), 7.72 (td,  $J = 7.6, 1.2$  Hz, 1H), 7.40 (s, 1H), 6.89 (dd,  $J = 8.8, 2.2$  Hz, 1H), 6.33 (d,  $J = 2.2$  Hz, 1H), 5.12 (q,  $J = 6.8$  Hz, 1H), 3.72 (s, 3H), 1.64 (d,  $J = 6.8$  Hz, 3H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  166.33, 160.19, 145.60, 139.70, 135.15, 133.33, 133.27, 128.91, 128.71, 128.13, 124.63, 124.39, 122.62, 118.43, 113.50, 113.18, 92.70, 57.54, 55.78, 29.74, 17.21. HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min),  $t_r = 50.300$  min (minor), 69.517 min (major); ee = 23%. HRMS (ESI)  $m/z$ : calculated for  $[\text{C}_{24}\text{H}_{20}\text{N}_2\text{O}_4\text{S}+\text{H}]^+$  433.1216, found 433.1202.

**(S)-3-methyl-2-(2-tosyl-1H-indol-1-yl)isoindolin-1-one (3n)**



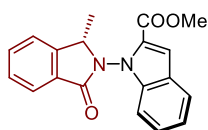
Following the **Procedure 4**, **3n** was obtained as faint yellow solid (30.4 mg, 73% yield).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.87 (d,  $J = 7.6$  Hz, 1H), 7.84 (d,  $J = 8.0$  Hz, 2H), 7.73 – 7.66 (m, 2H), 7.54 (t,  $J = 7.5$  Hz, 1H), 7.49 (d,  $J = 7.6$  Hz, 1H), 7.41 (s, 1H), 7.28 (t,  $J = 7.7$  Hz, 1H), 7.24 (s, 1H), 7.22 (d,  $J = 8.0$  Hz, 2H), 6.94 (d,  $J = 8.3$  Hz, 1H), 5.12 (q,  $J = 6.8$  Hz, 1H), 2.37 (s, 3H), 1.63 (d,  $J = 6.9$  Hz, 3H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  166.57, 145.65, 144.56, 138.10, 138.00, 137.18, 133.33, 129.61, 128.70, 128.60, 128.38, 126.87, 124.49, 124.23, 123.42, 122.71, 122.64, 112.05, 110.05, 58.05, 21.71, 17.34. HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min),  $t_r = 47.630$  min (minor), 55.903 min (major); ee = 90%. HRMS (ESI)  $m/z$ : calculated for  $[\text{C}_{24}\text{H}_{20}\text{N}_2\text{O}_3\text{S}+\text{Na}]^+$  439.1086, found 439.1120.

**(S)-2-(2-((4-fluorophenyl)sulfonyl)-1H-indol-1-yl)-3-methylisoindolin-1-one (3o)**



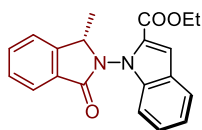
Following the **Procedure 4**, **3o** was obtained as faint yellow solid (29.4 mg, 70% yield).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.97 (dd,  $J = 8.7, 5.0$  Hz, 2H), 7.86 (d,  $J = 7.6$  Hz, 1H), 7.75 – 7.66 (m, 2H), 7.55 (t,  $J = 7.6$  Hz, 1H), 7.51 (d,  $J = 7.6$  Hz, 1H), 7.46 (s, 1H), 7.30 (t,  $J = 7.7$  Hz, 1H), 7.26 – 7.19 (m, 1H), 7.10 (t,  $J = 8.4$  Hz, 2H), 6.95 (d,  $J = 8.3$  Hz, 1H), 5.13 (q,  $J = 6.8$  Hz, 1H), 1.64 (d,  $J = 6.8$  Hz, 3H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  166.76, 165.71 (d,  $J = 256.0$  Hz), 145.65, 138.18, 136.96 (d,  $J = 3.1$  Hz), 136.54, 133.50, 131.28 (d,  $J = 9.7$  Hz), 128.83, 128.37, 127.18, 124.51, 124.16, 123.53, 122.88, 122.70, 116.27 (d,  $J = 22.7$  Hz), 112.47, 110.06, 58.12, 17.40.  $^{19}\text{F}$  NMR (471 MHz,  $\text{CDCl}_3$ )  $\delta$  -103.70. HPLC (Chiralpak IC column, 90:10 hexanes/isopropanol, 1 mL/min),  $t_r = 46.083$  min (minor), 50.427 min (major); ee = 93%. HRMS (ESI)  $m/z$ : calculated for  $[\text{C}_{23}\text{H}_{17}\text{FN}_2\text{O}_3\text{S}+\text{H}]^+$  421.1016, found 421.1000.

**methyl (S)-1-(1-methyl-3-oxoisindolin-2-yl)-1H-indole-2-carboxylate (3p)**



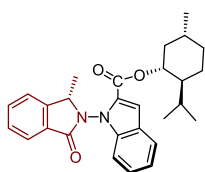
Following the **Procedure 4**, **3p** was obtained as white solid (26.2 mg, 82% yield).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.95 (d,  $J = 7.6$  Hz, 1H), 7.71 (dd,  $J = 8.3, 0.9$  Hz, 1H), 7.68 (td,  $J = 7.5, 1.1$  Hz, 1H), 7.54 (t,  $J = 7.6$  Hz, 1H), 7.50 (d,  $J = 7.5$  Hz, 1H), 7.45 (s, 1H), 7.36 (dd,  $J = 5.9, 1.2$  Hz, 2H), 7.22 (ddd,  $J = 8.0, 5.8, 2.1$  Hz, 1H), 5.17 (q,  $J = 6.8$  Hz, 1H), 3.77 (s, 3H), 1.57 (d,  $J = 6.8$  Hz, 3H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  167.84, 160.93, 145.91, 140.15, 133.03, 129.11, 128.48, 126.66, 126.30, 124.52, 124.09, 122.90, 122.35, 122.10, 111.79, 110.23, 59.85, 51.88, 17.94. HPLC (Chiralpak ID column, 80:20 hexanes/isopropanol, 1 mL/min),  $t_r = 23.823$  min (major), 34.137 min (minor); ee = 94%. HRMS (ESI)  $m/z$ : calculated for  $[\text{C}_{19}\text{H}_{16}\text{N}_2\text{O}_3+\text{Na}]^+$  343.1053, found 343.1087.

**ethyl (S)-1-(1-methyl-3-oxoisindolin-2-yl)-1H-indole-2-carboxylate (3q)**



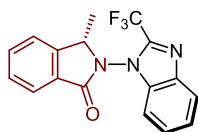
Following the **Procedure 4**, **3q** was obtained as white solid (22.0 mg, 66% yield).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.94 (d,  $J = 7.6$  Hz, 1H), 7.70 (d,  $J = 8.1$  Hz, 1H), 7.66 (t,  $J = 7.6$  Hz, 1H), 7.52 (t,  $J = 7.6$  Hz, 1H), 7.49 (d,  $J = 9.6$  Hz, 2H), 7.36 – 7.32 (m, 2H), 7.21 (ddd,  $J = 8.1, 5.1, 2.9$  Hz, 1H), 5.15 (q,  $J = 6.8$  Hz, 1H), 4.21 (q,  $J = 7.1$  Hz, 2H), 1.55 (d,  $J = 6.8$  Hz, 3H), 1.17 (t,  $J = 7.1$  Hz, 3H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  167.83, 160.48, 145.94, 140.16, 133.07, 129.22, 128.53, 126.88, 126.60, 124.51, 124.16, 122.88, 122.39, 122.09, 111.89, 110.26, 60.88, 59.93, 18.00, 14.07. HPLC (Chiralpak ID column, 80:20 hexanes/isopropanol, 1 mL/min),  $t_r = 24.733$  min (major), 30.817 min (minor); ee = 95%. HRMS (ESI)  $m/z$ : calculated for  $[\text{C}_{20}\text{H}_{18}\text{N}_2\text{O}_3 + \text{Na}]^+$  357.1209, found 357.1237

**(1R,2S,5R)-2-isopropyl-5-methylcyclohexyl 1-((S)-1-methyl-3-oxoisindolin-2-yl)-1H-indole-2-carboxylate (3r)**



Following the **Procedure 4**, **3r** was obtained as white solid (29.3 mg, 66% yield).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.95 (d,  $J = 7.6$  Hz, 1H), 7.72 – 7.64 (m, 2H), 7.53 (td,  $J = 7.6, 2.5$  Hz, 1H), 7.49 (dd,  $J = 12.1, 4.5$  Hz, 2H), 7.37 – 7.32 (m, 2H), 7.20 (dt,  $J = 8.0, 3.9$  Hz, 1H), 5.12 (qd,  $J = 6.7, 2.9$  Hz, 1H), 4.80 (tdd,  $J = 11.0, 7.1, 4.4$  Hz, 1H), 1.99 (td,  $J = 12.9, 10.3, 5.8$  Hz, 1H), 1.89 (dtt,  $J = 18.3, 7.0, 3.4$  Hz, 1H), 1.61 (dt,  $J = 13.7, 3.1$  Hz, 2H), 1.55 (dd,  $J = 6.8, 4.8$  Hz, 3H), 1.39 (tdd,  $J = 11.9, 6.5, 3.3$  Hz, 1H), 1.18 (dddd,  $J = 14.1, 11.6, 5.9, 3.0$  Hz, 1H), 1.05 – 0.93 (m, 1H), 0.84 (ddd,  $J = 16.2, 7.2, 4.7$  Hz, 7H), 0.78 – 0.66 (m, 4H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  167.61 (d,  $J = 6.0$  Hz), 160.05 (d,  $J = 5.3$  Hz), 145.95 (d,  $J = 7.1$  Hz), 140.13, 133.01 (d,  $J = 1.8$  Hz), 129.33 (d,  $J = 11.2$  Hz), 128.52, 127.33, 126.50 (d,  $J = 5.8$  Hz), 124.59 (d,  $J = 6.0$  Hz), 124.18, 122.80 (d,  $J = 2.7$  Hz), 122.39 (d,  $J = 3.6$  Hz), 122.03, 111.93 (d,  $J = 15.1$  Hz), 110.27 (d,  $J = 3.1$  Hz), 74.77 (d,  $J = 16.6$  Hz), 59.97 (d,  $J = 2.7$  Hz), 47.11, 40.79 (d,  $J = 7.8$  Hz), 34.22, 31.40, 26.31 (d,  $J = 21.3$  Hz), 23.40 (d,  $J = 3.7$  Hz), 22.02 (d,  $J = 6.5$  Hz), 20.85, 18.16, 16.39. HPLC (Chiralpak ID column, 80:20 hexanes/isopropanol, 1 mL/min),  $t_r = 10.377$  min (minor), 12.957 min (major); ee = 97%. HRMS (ESI)  $m/z$ : calculated for  $[\text{C}_{28}\text{H}_{32}\text{N}_2\text{O}_3 + \text{Na}]^+$  467.2305, found 467.2310.

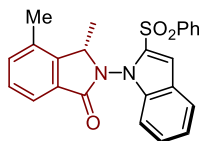
**(S)-3-methyl-2-(2-(trifluoromethyl)-1H-benzo[d]imidazol-1-yl)isoindolin-1-one (3s)**



Following the **Procedure 4**, **3s** was obtained as viscous oil (13.9 mg, 42% yield).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.97 (d,  $J = 7.7$  Hz, 1H), 7.94 (d,  $J = 7.9$  Hz, 1H), 7.76 (t,  $J = 7.6$  Hz, 1H), 7.60 (t,  $J = 7.6$  Hz, 1H), 7.56 (d,  $J = 7.7$  Hz, 1H), 7.40 (dt,  $J = 19.1, 7.5$  Hz, 2H), 7.11 (d,  $J = 8.1$  Hz, 1H), 5.24 (q,  $J = 6.7$  Hz, 1H), 1.58 (d,  $J = 6.4$  Hz, 3H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  166.55, 145.36, 141.54 (q,  $J = 40.32$  Hz), 139.30, 134.03, 133.78, 129.20, 127.69, 126.62, 125.01, 124.81, 122.78, 122.53, 118.22 (d,  $J = 272.2$  Hz), 109.63, 58.01, 17.43. HPLC (Chiralpak AD column, 90:10 hexanes/isopropanol,

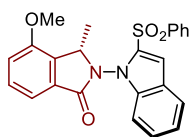
1 mL/min),  $t_r = 9.007$  min (major), 18.940 min (minor); ee = 82%. HRMS (ESI)  $m/z$ : calculated for  $[C_{17}H_{12}F_3N_3O + Na]^+$  354.0824, found 354.0844.

**(S)-3,4-dimethyl-2-(2-(phenylsulfonyl)-1H-indol-1-yl)isoindolin-1-one (3t)**



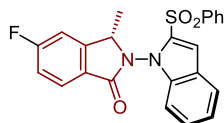
Following the **Procedure 4**, **3t** was obtained as faint yellow solid (30.8 mg, 74% yield).  $^1H$  NMR (500 MHz,  $CDCl_3$ )  $\delta$  7.95 (d,  $J = 7.8$  Hz, 2H), 7.70 (d,  $J = 8.0$  Hz, 1H), 7.65 (s, 1H), 7.53 (t,  $J = 7.5$  Hz, 1H), 7.49 (d,  $J = 7.8$  Hz, 1H), 7.46 – 7.40 (m, 3H), 7.38 (d,  $J = 7.8$  Hz, 1H), 7.27 (t,  $J = 7.7$  Hz, 1H), 7.20 (t,  $J = 7.5$  Hz, 1H), 6.91 (d,  $J = 8.3$  Hz, 1H), 5.08 (q,  $J = 6.9$  Hz, 1H), 2.46 (s, 3H), 1.62 (d,  $J = 6.8$  Hz, 3H).  $^{13}C$  NMR (126 MHz,  $CDCl_3$ )  $\delta$  166.95, 143.02, 140.92, 138.90, 138.16, 136.80, 134.43, 133.58, 128.98, 128.52, 128.34, 126.98, 124.64, 124.20, 123.49, 122.75, 122.47, 112.24, 110.07, 58.11, 21.43, 17.57. HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min),  $t_r = 41.520$  min (minor), 52.810 min (major); ee = 94%. HRMS (ESI)  $m/z$ : calculated for  $[C_{24}H_{20}N_2O_3S+H]^+$  433.1216, found 433.1257.

**(S)-4-methoxy-3-methyl-2-(2-(phenylsulfonyl)-1H-indol-1-yl)isoindolin-1-one (3u)**



Following the **Procedure 4**, **3u** was obtained as yellow solid (21.6 mg, 50% yield).  $^1H$  NMR (500 MHz,  $CDCl_3$ )  $\delta$  8.06 – 8.01 (m, 2H), 7.72 (d,  $J = 8.0$  Hz, 1H), 7.56 (t,  $J = 7.4$  Hz, 1H), 7.52 – 7.44 (m, 5H), 7.32 (t,  $J = 7.8$  Hz, 1H), 7.23 (t,  $J = 7.6$  Hz, 1H), 7.15 (dd,  $J = 7.2, 1.7$  Hz, 1H), 7.00 (d,  $J = 8.3$  Hz, 1H), 5.16 (q,  $J = 6.7$  Hz, 1H), 3.92 (s, 3H), 1.69 (d,  $J = 6.8$  Hz, 3H).  $^{13}C$  NMR (126 MHz,  $CDCl_3$ )  $\delta$  166.42, 155.14, 141.14, 138.39, 136.74, 133.56, 133.11, 130.38, 130.26, 128.98, 128.35, 127.01, 124.22, 123.40, 122.77, 116.41, 114.70, 112.53, 110.21, 57.19, 55.67, 16.04. HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min),  $t_r = 42.467$  min (minor), 61.543 min (major); ee = 88%. HRMS (ESI)  $m/z$ : calculated for  $[C_{24}H_{20}N_2O_4S+Na]^+$  455.1036, found 455.1050.

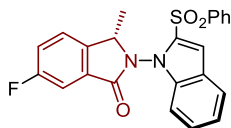
**(S)-5-fluoro-3-methyl-2-(2-(phenylsulfonyl)-1H-indol-1-yl)isoindolin-1-one (3v)**



Following the **Procedure 4**, **3v** was obtained as faint yellow solid (25.2 mg, 60% yield).  $^1H$  NMR (500 MHz,  $CDCl_3$ )  $\delta$  7.99 – 7.94 (m, 2H), 7.87 (dd,  $J = 8.4, 5.0$  Hz, 1H), 7.73 (d,  $J = 8.1$  Hz, 1H), 7.56 (t,  $J = 7.4$  Hz, 1H), 7.49 – 7.43 (m, 3H), 7.33 (t,  $J = 7.8$  Hz, 1H), 7.28 – 7.23 (m, 2H), 7.20 (dd,  $J = 8.0, 2.2$  Hz, 1H), 6.95 (d,  $J = 8.4$  Hz, 1H), 5.11 (q,  $J = 6.9$  Hz, 1H), 1.66 (d,  $J = 6.9$  Hz, 3H).  $^{13}C$  NMR (126 MHz,  $CDCl_3$ )  $\delta$  166.26 (d,  $J = 254.4$  Hz), 165.62, 148.15 (d,  $J = 9.8$  Hz), 138.09, 136.73, 133.60, 128.97, 128.29, 127.81, 127.08, 126.99 (d,  $J = 9.7$  Hz), 124.63, 124.24, 123.57, 122.86, 116.74 (d,  $J = 23.5$  Hz), 112.48, 110.17 (d,  $J = 24.2$  Hz), 109.92, 57.82 (d,  $J = 2.6$  Hz), 17.31.  $^{19}F$  NMR (470 MHz,  $CDCl_3$ )  $\delta$  -

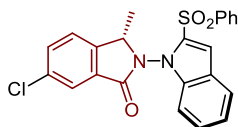
103.71 (td,  $J = 8.6, 5.1$  Hz). HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min),  $t_r = 39.323$  min (major), 48.370 min (minor); ee = 93%. HRMS (ESI)  $m/z$ : calculated for  $[C_{23}H_{17}FN_2O_3S+H]^+$  421.1016, found 421.0999.

**(S)-6-fluoro-3-methyl-2-(2-(phenylsulfonyl)-1H-indol-1-yl)isoindolin-1-one (3w)**



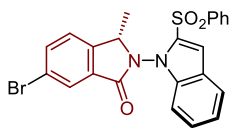
Following the **Procedure 4**, **3w** was obtained as faint yellow solid (35.3 mg, 84% yield).  $^1H$  NMR (500 MHz,  $CDCl_3$ )  $\delta$  7.98 – 7.94 (m, 2H), 7.73 (d,  $J = 8.0$  Hz, 1H), 7.60 – 7.52 (m, 2H), 7.51 – 7.44 (m, 4H), 7.41 (td,  $J = 8.7, 2.5$  Hz, 1H), 7.33 (t,  $J = 7.7$  Hz, 1H), 7.26 – 7.22 (m, 1H), 6.95 (d,  $J = 8.3$  Hz, 1H), 5.11 (q,  $J = 6.8$  Hz, 1H), 1.64 (d,  $J = 6.7$  Hz, 3H).  $^{13}C$  NMR (126 MHz,  $CDCl_3$ )  $\delta$  165.61, 163.00 (d,  $J = 248.9$  Hz), 141.13 (d,  $J = 2.7$  Hz), 140.86, 138.12, 136.65, 133.67, 130.56 (d,  $J = 8.4$  Hz), 129.02, 128.29, 127.13, 124.49 (d,  $J = 8.5$  Hz), 124.23, 123.56, 122.90, 120.98 (d,  $J = 23.5$  Hz), 112.59, 111.27 (d,  $J = 23.6$  Hz), 109.95, 57.88, 17.38.  $^{19}F$  NMR (470 MHz,  $CDCl_3$ )  $\delta$  -111.46. HPLC (Chiralpak IA column, 80:20 hexanes/isopropanol, 1 mL/min),  $t_r = 29.967$  min (major), 37.487 min (minor); ee = 95%. HRMS (ESI)  $m/z$ : calculated for  $[C_{23}H_{17}FN_2O_3S+H]^+$  421.1016, found 421.0995.

**(S)-6-chloro-3-methyl-2-(2-(phenylsulfonyl)-1H-indol-1-yl)isoindolin-1-one (3x)**



Following the **Procedure 4**, **3x** was obtained as faint yellow solid (30.1 mg, 69% yield).  $^1H$  NMR (500 MHz,  $CDCl_3$ )  $\delta$  7.99 – 7.93 (m, 2H), 7.86 (d,  $J = 2.0$  Hz, 1H), 7.74 (d,  $J = 8.0$  Hz, 1H), 7.67 (dd,  $J = 8.2, 2.0$  Hz, 1H), 7.57 (t,  $J = 7.5$  Hz, 1H), 7.50 – 7.44 (m, 4H), 7.33 (t,  $J = 7.6$  Hz, 1H), 7.24 (d,  $J = 7.7$  Hz, 1H), 6.95 (d,  $J = 8.3$  Hz, 1H), 5.12 (q,  $J = 6.8$  Hz, 1H), 1.64 (d,  $J = 6.8$  Hz, 3H).  $^{13}C$  NMR (126 MHz,  $CDCl_3$ )  $\delta$  165.34, 143.71, 140.84, 138.09, 136.63, 135.16, 133.68, 133.55, 130.29, 129.03, 128.28, 127.15, 124.66, 124.24, 124.09, 123.58, 122.92, 112.62, 109.92, 57.90, 17.26. HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min),  $t_r = 30.870$  min (minor), 42.590 min (major); ee = 96%. HRMS (ESI)  $m/z$ : calculated for  $[C_{23}H_{17}ClN_2O_3S+H]^+$  437.0721, found 437.0699.

**(S)-6-bromo-3-methyl-2-(2-(phenylsulfonyl)-1H-indol-1-yl)isoindolin-1-one (3y)**

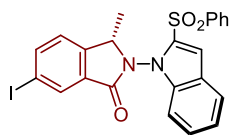


Following the **Procedure 4**, **3y** was obtained as faint yellow solid (19.7 mg, 41% yield).  $^1H$  NMR (500 MHz,  $CDCl_3$ )  $\delta$  8.01 (d,  $J = 1.9$  Hz, 1H), 7.96 (d,  $J = 7.9$  Hz, 2H), 7.82 (dd,  $J = 8.1, 1.9$  Hz, 1H), 7.73 (d,  $J = 8.1$  Hz, 1H), 7.57 (t,  $J = 7.3$  Hz, 1H), 7.49 – 7.44 (m, 3H), 7.40 (d,  $J = 8.1$  Hz, 1H), 7.33 (t,  $J = 7.7$  Hz, 1H), 7.26 – 7.22 (m, 1H), 6.94 (d,  $J = 8.3$  Hz, 1H), 5.09 (q,  $J = 6.8$  Hz, 1H), 1.64 (d,  $J = 6.8$  Hz, 3H).  $^{13}C$  NMR (126 MHz,  $CDCl_3$ )  $\delta$  165.18, 144.19, 140.84, 138.09, 136.65, 136.35, 133.67, 130.55, 129.02, 128.27, 127.67, 127.14, 124.36, 124.25, 123.57, 122.92, 122.88, 112.62, 109.91,



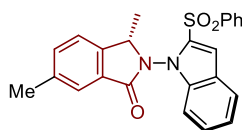
57.95, 17.18. HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min),  $t_r$  = 29.000 min (minor), 40.167 min (major); ee = 98%. HRMS (ESI)  $m/z$ : calculated for  $[C_{23}H_{17}BrN_2O_3S+H]^+$  481.0216, found 481.0193.

**(S)-6-iodo-3-methyl-2-(2-(phenylsulfonyl)-1H-indol-1-yl)isoindolin-1-one (3z)**



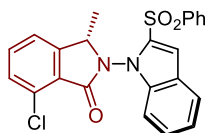
Following the **Procedure 4**, **3z** was obtained as faint yellow solid (17.4 mg, 33% yield).  $^1H$  NMR (500 MHz,  $CDCl_3$ )  $\delta$  8.21 (d,  $J$  = 1.6 Hz, 1H), 8.01 (dd,  $J$  = 8.0, 1.7 Hz, 1H), 7.97 – 7.94 (m, 2H), 7.73 (d,  $J$  = 8.0 Hz, 1H), 7.57 (tt,  $J$  = 7.0, 1.3 Hz, 1H), 7.48 – 7.43 (m, 3H), 7.32 (ddd,  $J$  = 8.3, 7.1, 1.2 Hz, 1H), 7.28 (d,  $J$  = 8.0 Hz, 1H), 7.24 – 7.20 (m, 1H), 6.96 – 6.92 (m, 1H), 5.08 (q,  $J$  = 6.8 Hz, 1H), 1.62 (d,  $J$  = 6.9 Hz, 3H).  $^{13}C$  NMR (126 MHz,  $CDCl_3$ )  $\delta$  165.04, 144.85, 142.10, 140.82, 138.08, 136.59, 133.71, 133.59, 130.60, 129.05, 128.28, 127.17, 124.56, 124.23, 123.59, 122.94, 112.64, 109.94, 93.85, 58.00, 17.15. HPLC (Chiralpak AD column, 70:30 hexanes/isopropanol, 1 mL/min),  $t_r$  = 48.850 min (minor), 57.410 min (major); ee = 92%. HRMS (ESI)  $m/z$ : calculated for  $[C_{23}H_{17}IN_2O_3S+H]^+$  529.0077, found 529.0071.

**(S)-3,6-dimethyl-2-(2-(phenylsulfonyl)-1H-indol-1-yl)isoindolin-1-one (3a')**



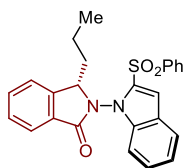
Following the **Procedure 4**, **3a'** was obtained as faint yellow solid (25.4 mg, 61% yield).  $^1H$  NMR (500 MHz,  $CDCl_3$ )  $\delta$  8.02 (dd,  $J$  = 8.3, 1.3 Hz, 2H), 7.73 (dd,  $J$  = 5.9, 2.9 Hz, 1H), 7.71 (d,  $J$  = 8.1 Hz, 1H), 7.57 – 7.51 (m, 1H), 7.48 – 7.42 (m, 5H), 7.31 (ddd,  $J$  = 8.3, 7.1, 1.1 Hz, 1H), 7.21 (d,  $J$  = 7.4 Hz, 1H), 7.00 (d,  $J$  = 8.3 Hz, 1H), 5.12 (q,  $J$  = 6.7 Hz, 1H), 2.43 (s, 3H), 1.65 (d,  $J$  = 6.7 Hz, 3H).  $^{13}C$  NMR (126 MHz,  $CDCl_3$ )  $\delta$  166.47, 143.60, 141.23, 138.39, 136.76, 135.00, 133.60, 133.30, 129.01, 128.92, 128.84, 128.34, 127.07, 124.26, 123.44, 122.84, 122.25, 112.67, 110.25, 57.91, 18.81, 16.31. HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min),  $t_r$  = 40.217 min (minor), 50.453 min (major); ee = 94%. HRMS (ESI)  $m/z$ : calculated for  $[C_{24}H_{20}N_2O_3S+Na]^+$  439.1086, found 439.1105.

**(S)-7-chloro-3-methyl-2-(2-(phenylsulfonyl)-1H-indol-1-yl)isoindolin-1-one (3b')**



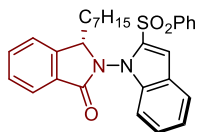
Following the **Procedure 4**, **3b'** was obtained as faint yellow solid (16.1 mg, 37% yield).  $^1H$  NMR (500 MHz,  $CDCl_3$ )  $\delta$  7.95 – 7.90 (m, 2H), 7.72 (d,  $J$  = 8.0 Hz, 1H), 7.58 (dt,  $J$  = 15.9, 7.7 Hz, 2H), 7.46 (t,  $J$  = 4.0 Hz, 2H), 7.43 (t,  $J$  = 7.7 Hz, 2H), 7.39 (d,  $J$  = 7.6 Hz, 1H), 7.30 (t,  $J$  = 7.5 Hz, 1H), 7.22 (t,  $J$  = 7.5 Hz, 1H), 6.93 (d,  $J$  = 8.3 Hz, 1H), 5.10 (q,  $J$  = 6.8 Hz, 1H), 1.67 (d,  $J$  = 6.8 Hz, 3H).  $^{13}C$  NMR (126 MHz,  $CDCl_3$ )  $\delta$  164.03, 147.91, 140.44, 138.13, 137.03, 134.03, 133.71, 132.35, 130.32, 129.02, 128.43, 127.02, 125.00, 124.27, 123.54, 122.79, 121.15, 112.24, 109.97, 57.02, 17.46. HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min),  $t_r$  = 43.040 min (major), 55.340 min (minor); ee = 60%. HRMS (ESI)  $m/z$ : calculated for  $[C_{23}H_{17}ClN_2O_3S+H]^+$  437.0721, found 437.0700.

**(S)-2-(2-(phenylsulfonyl)-1H-indol-1-yl)-3-propylisoindolin-1-one (3c')**



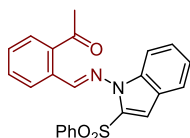
Following the **Procedure 4**, **3c'** was obtained as orange viscous oil (29.2 mg, 68% yield).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.00 – 7.95 (m, 2H), 7.85 (d,  $J = 7.6$  Hz, 1H), 7.72 (d,  $J = 8.0$  Hz, 1H), 7.67 (d,  $J = 7.5$  Hz, 1H), 7.55 (dd,  $J = 13.2, 5.4$  Hz, 3H), 7.47 – 7.42 (m, 3H), 7.29 (t,  $J = 7.7$  Hz, 1H), 7.21 (t,  $J = 7.6$  Hz, 1H), 6.92 (d,  $J = 8.3$  Hz, 1H), 5.06 (t,  $J = 6.4$  Hz, 1H), 2.20 – 2.09 (m, 1H), 2.04 (ddt,  $J = 13.9, 11.0, 5.5$  Hz, 1H), 1.27 (q,  $J = 6.9, 6.4$  Hz, 2H), 0.88 (t,  $J = 7.2$  Hz, 3H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  166.95, 144.95, 140.89, 137.85, 136.65, 133.58, 133.22, 128.96, 128.67, 128.64, 128.34, 126.99, 124.58, 124.11, 123.49, 123.20, 122.67, 112.26, 109.97, 62.13, 34.34, 19.73, 14.04. HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min),  $t_r = 27.463$  min (minor), 41.750 min (major); ee = 94%. HRMS (ESI)  $m/z$ : calculated for  $[\text{C}_{25}\text{H}_{22}\text{N}_2\text{O}_3\text{S}+\text{Na}]^+$  453.1243, found 453.1254.

**(S)-3-heptyl-2-(2-(phenylsulfonyl)-1H-indol-1-yl)isoindolin-1-one (3d')**



Following the **Procedure 4**, **3d'** was obtained as orange viscous oil (34.5 mg, 71% yield).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.03 – 7.98 (m, 2H), 7.88 (d,  $J = 7.6$  Hz, 1H), 7.74 (d,  $J = 7.8$  Hz, 1H), 7.71 – 7.66 (m, 1H), 7.57 (dd,  $J = 14.3, 7.5$  Hz, 3H), 7.50 – 7.43 (m, 3H), 7.31 (t,  $J = 7.7$  Hz, 1H), 7.23 (t,  $J = 7.5$  Hz, 1H), 6.95 (d,  $J = 8.3$  Hz, 1H), 5.07 (t,  $J = 6.4$  Hz, 1H), 2.19 (dddd,  $J = 14.5, 10.8, 6.7, 4.4$  Hz, 1H), 2.08 (tt,  $J = 14.6, 5.9$  Hz, 1H), 1.34 – 1.10 (m, 10H), 0.85 (t,  $J = 7.1$  Hz, 3H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  166.92, 145.06, 141.01, 137.92, 136.74, 133.59, 133.24, 128.98, 128.70 (d,  $J = 2.9$  Hz), 128.37, 127.83, 127.02, 124.61, 124.17, 123.51, 123.24 (d,  $J = 4.1$  Hz), 122.71, 112.33, 110.05, 62.16, 32.29, 31.71, 29.45, 29.03, 26.35, 22.60, 14.12 (d,  $J = 6.5$  Hz). HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min),  $t_r = 21.360$  min (minor), 33.497 min (major); ee = 92%. HRMS (ESI)  $m/z$ : calculated for  $[\text{C}_{29}\text{H}_{30}\text{N}_2\text{O}_3\text{S}+\text{H}]^+$  487.2049, found 487.2046.

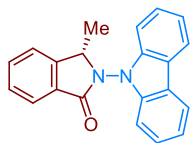
**(E)-1-(2-(((2-(phenylsulfonyl)-1H-indol-1-yl)imino)methyl)phenyl)ethan-1-one (Int-1a)**



Following the **Procedure 5**, **Int-1a** was obtained as gray solid (31.0 mg, 77% yield).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  9.42 (s, 1H), 8.18 (dd,  $J = 7.8, 1.3$  Hz, 1H), 8.11 – 8.04 (m, 3H), 7.88 (dd,  $J = 7.9, 1.3$  Hz, 1H), 7.73 (d,  $J = 8.0$  Hz, 1H), 7.66 (td,  $J = 7.7, 1.3$  Hz, 1H), 7.57 (td,  $J = 7.6, 1.4$  Hz, 1H), 7.54 – 7.46 (m, 3H), 7.43 (dd,  $J = 8.5, 7.1$  Hz, 2H), 7.27 – 7.21 (m, 1H), 2.66 (s, 3H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  200.61, 155.33, 141.14, 137.06, 135.05, 133.81, 133.29, 133.23,

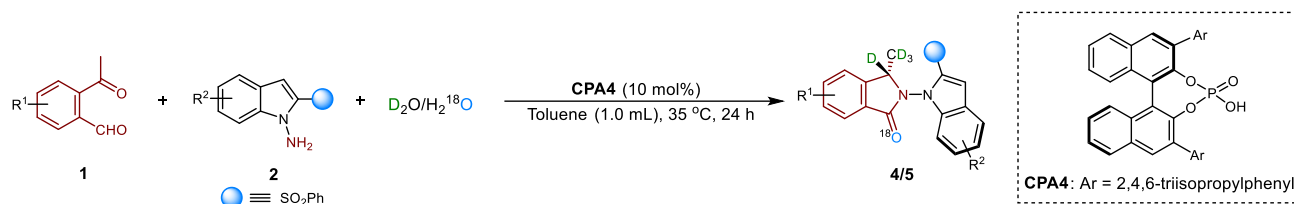
132.68, 130.71, 130.07, 128.83, 128.66, 128.33, 127.17, 124.89, 123.31, 122.41, 111.97, 110.68, 28.62. HRMS (ESI)  $m/z$ : calculated for  $[C_{23}H_{18}N_2O_3S+Na]^+$  425.0930, found 425.0942.

### (S)-2-(9H-carbazol-9-yl)-3-methylisoindolin-1-one (7)



Following the **Procedure 4**, **7** was obtained as red solid (24.0 mg, 77% yield).  $^1H$  NMR (500 MHz,  $CDCl_3$ )  $\delta$  8.11 (dd,  $J = 11.4, 7.7$  Hz, 2H), 8.03 (d,  $J = 7.6$  Hz, 1H), 7.72 (td,  $J = 7.6, 1.2$  Hz, 1H), 7.59 (t,  $J = 7.6$  Hz, 1H), 7.53 (d,  $J = 7.6$  Hz, 1H), 7.41 (dddd,  $J = 12.3, 8.1, 7.1, 1.2$  Hz, 2H), 7.34 (d,  $J = 8.1$  Hz, 1H), 7.32 – 7.27 (m, 2H), 7.13 (d,  $J = 8.1$  Hz, 1H), 5.22 (q,  $J = 6.7$  Hz, 1H), 1.48 (d,  $J = 6.7$  Hz, 3H).  $^{13}C$  NMR (126 MHz,  $CDCl_3$ )  $\delta$  166.46, 145.70, 140.75, 139.22, 133.09, 129.23, 128.78, 126.54, 126.33, 124.76, 122.54, 122.30, 121.86, 120.92, 120.82, 120.77, 120.54, 109.13, 108.44, 57.55, 18.62. HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min),  $t_r = 25.680$  min (major), 33.510 min (minor); ee = 7%. HRMS (ESI)  $m/z$ : calculated for  $[C_{21}H_{16}N_2O+Na]^+$  335.1154, found 335.1182.

### General procedure for synthesis of products 4 and 5



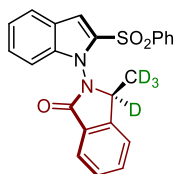
**Procedure 7:** The reaction was proceeded in the glovebox under argon atmosphere. To a 4 mL dry bottle equipped with a stirring bar was added **1** (0.2 mmol, 1.0 eq.), **2** (0.1 mmol, 1.0 eq.), **CPA4** (0.01mmol, 0.1 eq.) and dry toluene (1 mL). The 50  $\mu$ L of deuterium oxide ( $D_2O$ ) or heavy-oxygen water ( $H_2^{18}O$ ) was then added to the flask and the reaction mixture was stirred at 35  $^{\circ}C$  for 24 h. After the completion of the reaction which was indicated by TLC, the crude product was purified by column chromatography on silica gel (PE/EA as the eluent) and the desired product was afforded.

The deuterium incorporation rates of deuterated products were calculated by  $^1H$  NMR. The isotopic ratios of  $^{18}O$  products were obtained by the following formula:

$$isotopic\ ratio = \frac{intensity_{labeled}}{intensity_{total}} = \frac{intensity_{labeled}}{intensity_{labeled} + intensity_{unlabeled}}$$

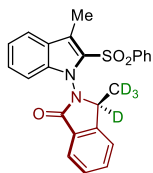
### Isotopic ratio analysis

#### (S)-3-(methyl- $d_3$ )-2-(2-(phenylsulfonyl)-1H-indol-1-yl)isoindolin-1-one-3- $d$ (4a)



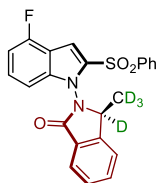
Following the **Procedure 7**, **4a** was obtained as faint yellow solid (26.8 mg, 66% yield).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.98 (dd,  $J = 7.4, 1.8$  Hz, 2H), 7.87 (d,  $J = 7.6$  Hz, 1H), 7.74 (d,  $J = 7.9$  Hz, 1H), 7.70 (td,  $J = 7.6, 1.1$  Hz, 1H), 7.55 (h,  $J = 4.1$  Hz, 2H), 7.51 (d,  $J = 7.6$  Hz, 1H), 7.49 – 7.43 (m, 3H), 7.34 – 7.27 (m, 1H), 7.24 (d,  $J = 7.6$  Hz, 1H), 6.95 (d,  $J = 8.4$  Hz, 1H), 5.13 (d,  $J = 5.8$  Hz, 0.37H), 1.63 (d,  $J = 7.6$  Hz, 0.28H). HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min),  $t_r = 35.663$  min (minor), 41.980 min (major); ee = 95%.

**(S)-3-(methyl- $d_3$ )-2-(3-methyl-2-(phenylsulfonyl)-1H-indol-1-yl)isoindolin-1-one-3- $d$**  (**4b**)



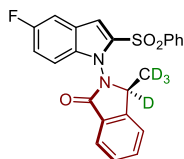
Following the **Procedure 7**, **4b** was obtained as faint yellow solid (33.2 mg, 79% yield).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.19 (d,  $J = 7.5$  Hz, 2H), 7.99 (d,  $J = 7.6$  Hz, 1H), 7.68 (t,  $J = 7.4$  Hz, 2H), 7.58 – 7.51 (m, 2H), 7.52 – 7.46 (m, 4H), 7.35 (t,  $J = 7.7$  Hz, 1H), 7.24 (q,  $J = 7.5, 7.0$  Hz, 1H), 7.04 (d,  $J = 8.4$  Hz, 1H), 5.06 (d,  $J = 4.4$  Hz, 0.37H), 2.57 (s, 3H), 1.57 (d,  $J = 7.6$  Hz, 0.26H). HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min),  $t_r = 21.193$  min (minor), 36.850 min (major); ee = 93%.

**(S)-2-(4-fluoro-2-(phenylsulfonyl)-1H-indol-1-yl)-3-(methyl- $d_3$ )isoindolin-1-one-3- $d$**  (**4c**)



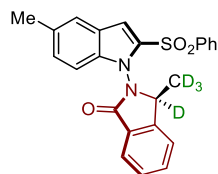
Following the **Procedure 7**, **4c** was obtained as faint yellow solid (38.2 mg, 90% yield).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.97 (d,  $J = 8.1$  Hz, 2H), 7.86 (d,  $J = 7.8$  Hz, 1H), 7.73 (t,  $J = 7.7$  Hz, 1H), 7.61 – 7.56 (m, 2H), 7.53 (d,  $J = 5.5$  Hz, 2H), 7.47 (t,  $J = 7.8$  Hz, 2H), 7.24 (q,  $J = 9.2, 7.8$  Hz, 1H), 6.90 (t,  $J = 8.9$  Hz, 1H), 6.73 (d,  $J = 8.5$  Hz, 1H), 5.15 (d,  $J = 21.7$  Hz, 0.35H), 1.66 (d,  $J = 7.9$  Hz, 0.34H). HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min),  $t_r = 20.023$  min (minor), 24.663 min (major); ee = 94%.

**(S)-2-(5-fluoro-2-(phenylsulfonyl)-1H-indol-1-yl)-3-(methyl- $d_3$ )isoindolin-1-one-3- $d$**  (**4d**)



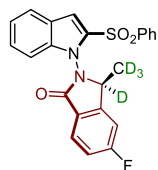
Following the **Procedure 7**, **4d** was obtained as faint yellow solid (34.3 mg, 81% yield).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.98 – 7.93 (m, 2H), 7.85 (d,  $J = 7.6$  Hz, 1H), 7.73 – 7.68 (m, 1H), 7.57 (td,  $J = 7.5, 1.8$  Hz, 2H), 7.52 (t,  $J = 7.2$  Hz, 1H), 7.48 – 7.43 (m, 2H), 7.40 (s, 1H), 7.38 (dd,  $J = 8.6, 2.5$  Hz, 1H), 7.06 (td,  $J = 8.9, 2.4$  Hz, 1H), 6.89 (dd,  $J = 9.0, 4.1$  Hz, 1H), 5.11 (d,  $J = 5.8$  Hz, 0.32H), 1.64 (d,  $J = 7.6$  Hz, 0.26H). HPLC (Chiralpak AD column, 80:20 hexanes/isopropanol, 1 mL/min),  $t_r = 40.533$  min (major), 51.327 min (minor); ee = 91%.

**(S)-3-(methyl- $d_3$ )-2-(5-methyl-2-(phenylsulfonyl)-1H-indol-1-yl)isoindolin-1-one-3- $d$**  (**4e**)



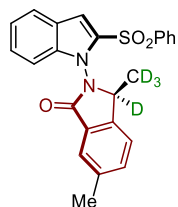
Following the **Procedure 7**, **4e** was obtained as faint yellow solid (33.6 mg, 80% yield).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.00 – 7.95 (m, 2H), 7.86 (d,  $J = 7.5$  Hz, 1H), 7.69 (td,  $J = 7.5, 1.2$  Hz, 1H), 7.57 – 7.52 (m, 2H), 7.52 – 7.49 (m, 2H), 7.48 – 7.41 (m, 2H), 7.39 (s, 1H), 7.13 (dd,  $J = 8.5, 1.7$  Hz, 1H), 6.85 (d,  $J = 8.5$  Hz, 1H), 5.11 (d,  $J = 6.0$  Hz, 0.33H), 2.42 (s, 3H), 1.61 (d,  $J = 7.6$  Hz, 0.26H). HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min),  $t_r = 40.090$  min (minor), 52.667 min (major); ee = 94%.

**(S)-5-fluoro-3-(methyl- $d_3$ )-2-(2-(phenylsulfonyl)-1H-indol-1-yl)isoindolin-1-one-3-d (4f)**



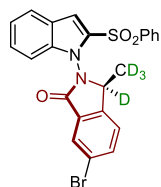
Following the **Procedure 7**, **4f** was obtained as faint yellow solid (26.3 mg, 62% yield).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.99 – 7.94 (m, 2H), 7.86 (dd,  $J = 8.4, 4.9$  Hz, 1H), 7.74 (d,  $J = 7.9$  Hz, 1H), 7.56 (t,  $J = 7.4$  Hz, 1H), 7.48 – 7.44 (m, 3H), 7.32 (t,  $J = 7.5$  Hz, 1H), 7.25 (dtd,  $J = 7.5, 5.0, 2.4$  Hz, 2H), 7.21 (dd,  $J = 8.1, 2.4$  Hz, 1H), 6.95 (d,  $J = 8.4$  Hz, 1H), 5.11 (d,  $J = 6.0$  Hz, 0.36H), 1.62 (d,  $J = 7.6$  Hz, 0.32H). HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min),  $t_r = 38.647$  min (major), 48.400 min (minor); ee = 99%.

**(S)-6-methyl-3-(methyl- $d_3$ )-2-(2-(phenylsulfonyl)-1H-indol-1-yl)isoindolin-1-one-3-d (4g)**



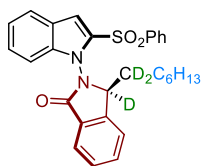
Following the **Procedure 7**, **4g** was obtained as faint yellow solid (24.4 mg, 58% yield).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.99 – 7.95 (m, 2H), 7.73 (d,  $J = 7.9$  Hz, 1H), 7.67 (s, 1H), 7.58 – 7.54 (m, 1H), 7.52 (dd,  $J = 7.8, 1.7$  Hz, 1H), 7.48 – 7.43 (m, 3H), 7.40 (d,  $J = 7.8$  Hz, 1H), 7.30 (td,  $J = 7.6, 6.9, 1.1$  Hz, 1H), 7.23 (t,  $J = 7.4$  Hz, 1H), 6.93 (d,  $J = 8.4$  Hz, 1H), 5.09 (d,  $J = 5.8$  Hz, 0.33H), 2.49 (s, 3H), 1.61 (d,  $J = 7.6$  Hz, 0.28H). HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min),  $t_r = 40.490$  min (minor), 50.473 min (major); ee = 94%.

**(S)-6-bromo-3-(methyl- $d_3$ )-2-(2-(phenylsulfonyl)-1H-indol-1-yl)isoindolin-1-one-3-d (4h)**



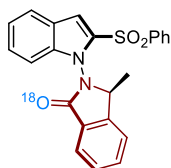
Following the **Procedure 7**, **4h** was obtained as faint yellow solid (32.9 mg, 68% yield).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.99 (s, 1H), 7.95 (d,  $J = 8.2$  Hz, 2H), 7.75 (dd,  $J = 35.1, 8.7$  Hz, 2H), 7.54 (d,  $J = 7.6$  Hz, 1H), 7.44 (s, 3H), 7.37 (d,  $J = 8.9$  Hz, 1H), 7.29 (d,  $J = 8.4$  Hz, 1H), 7.25 – 7.18 (m, 1H), 6.93 (d,  $J = 8.9$  Hz, 1H), 5.06 (s, 0.3H), 1.56 (s, 0.28H). HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min),  $t_r = 30.247$  min (minor), 39.377 min (major); ee = 98%.

**(S)-3-(heptyl-1,1-*d*<sub>2</sub>)-2-(2-(phenylsulfonyl)-1*H*-indol-1-yl)isoindolin-1-one-3-*d*** (**4i**)



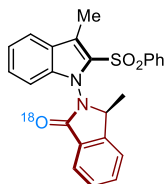
Following the **Procedure 7**, **4i** was obtained as orange viscous oil (20.0 mg, 41% yield). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.00 (d, *J* = 7.8 Hz, 2H), 7.88 (d, *J* = 7.6 Hz, 1H), 7.74 (d, *J* = 8.1 Hz, 1H), 7.70 (t, *J* = 7.6 Hz, 1H), 7.57 (dd, *J* = 10.9, 7.4 Hz, 3H), 7.47 (d, *J* = 8.8 Hz, 3H), 7.31 (t, *J* = 7.8 Hz, 1H), 7.23 (d, *J* = 7.5 Hz, 1H), 6.95 (d, *J* = 8.3 Hz, 1H), 5.06 (d, *J* = 6.3 Hz, 0.3H), 2.17 (td, *J* = 12.9, 11.7, 5.3 Hz, 0.27H), 2.06 (q, *J* = 6.8, 6.2 Hz, 0.48H), 1.32 – 1.12 (m, 10H), 0.85 (t, *J* = 7.1 Hz, 3H). HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min), *tr* = 20.723 min (minor), 33.933 min (major); ee = 93%.

**(S)-3-methyl-2-(2-(phenylsulfonyl)-1*H*-indol-1-yl)isoindolin-1-one-<sup>18</sup>O** (**5a**)



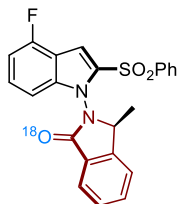
Following the **Procedure 7**, **5a** was obtained as faint yellow solid (35.6 mg, 88% yield). HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min), *tr* = 35.810 min (minor), 42.290 min (major); ee = 91%. HRMS (APCI) *m/z*: calculated for [C<sub>23</sub>H<sub>18</sub>N<sub>2</sub>O<sub>2</sub><sup>16</sup>OS+H]<sup>+</sup> 403.1111, found 403.1053, [C<sub>23</sub>H<sub>18</sub>N<sub>2</sub>O<sub>2</sub><sup>18</sup>OS+H]<sup>+</sup> 405.1153, found 405.1148. The ratio of relative peak intensities for the relevant isotopologues was 79:21 (C<sub>23</sub>H<sub>18</sub>N<sub>2</sub>O<sub>2</sub><sup>18</sup>OS:C<sub>23</sub>H<sub>18</sub>N<sub>2</sub>O<sub>2</sub><sup>16</sup>OS).

**(S)-3-methyl-2-(3-methyl-2-(phenylsulfonyl)-1*H*-indol-1-yl)isoindolin-1-one-<sup>18</sup>O** (**5b**)



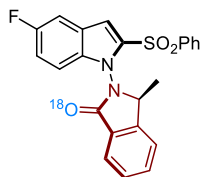
Following the **Procedure 7**, **5b** was obtained as faint yellow solid (34.7 mg, 83% yield). HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min), *tr* = 21.303 min (minor), 37.293 min (major); ee = 91%. HRMS (APCI) *m/z*: calculated for [C<sub>24</sub>H<sub>20</sub>N<sub>2</sub>O<sub>2</sub><sup>16</sup>OS+H]<sup>+</sup> 417.1267, found 417.1242, [C<sub>24</sub>H<sub>20</sub>N<sub>2</sub>O<sub>2</sub><sup>18</sup>OS+H]<sup>+</sup> 419.1309, found 419.1294. The ratio of relative peak intensities for the relevant isotopologues was 70:30 (C<sub>24</sub>H<sub>20</sub>N<sub>2</sub>O<sub>2</sub><sup>18</sup>OS:C<sub>24</sub>H<sub>20</sub>N<sub>2</sub>O<sub>2</sub><sup>16</sup>OS).

**(S)-2-(4-fluoro-2-(phenylsulfonyl)-1*H*-indol-1-yl)-3-methylisoindolin-1-one-<sup>18</sup>O** (**5c**)



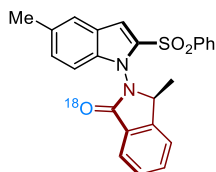
Following the **Procedure 7**, **5c** was obtained as faint yellow solid (30.0 mg, 71% yield). HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min), *tr* = 19.983 min (minor), 24.637 min (major); ee = 95%. HRMS (APCI) *m/z*: calculated for [C<sub>23</sub>H<sub>17</sub>FN<sub>2</sub>O<sub>2</sub><sup>16</sup>OS+H]<sup>+</sup> 421.1017, found 421.0993, [C<sub>23</sub>H<sub>17</sub>FN<sub>2</sub>O<sub>2</sub><sup>18</sup>OS+H]<sup>+</sup> 423.1059, found 423.1059. The ratio of relative peak intensities for the relevant isotopologues was 82:18 (C<sub>23</sub>H<sub>17</sub>FN<sub>2</sub>O<sub>2</sub><sup>18</sup>OS: C<sub>23</sub>H<sub>17</sub>FN<sub>2</sub>O<sub>2</sub><sup>16</sup>OS).

**(S)-2-(5-fluoro-2-(phenylsulfonyl)-1H-indol-1-yl)-3-methylisoindolin-1-one-<sup>18</sup>O (5d)**



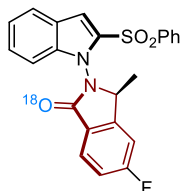
Following the **Procedure 7**, **5d** was obtained as faint yellow solid (27.0 mg, 64% yield). HPLC (Chiralpak AD column, 80:20 hexanes/isopropanol, 1 mL/min),  $t_r = 39.640$  min (major), 50.423 min (minor); ee = 93%. HRMS (APCI)  $m/z$ : calculated for  $[C_{23}H_{17}FN_2O_2^{16}OS+H]^+$  421.1017, found 421.1001,  $[C_{23}H_{17}FN_2O_2^{18}OS+H]^+$  423.1059, found 423.1059. The ratio of relative peak intensities for the relevant isotopologues was 86:14 ( $C_{23}H_{17}FN_2O_2^{18}OS$ :  $C_{23}H_{17}FN_2O_2^{16}OS$ ).

**(S)-3-methyl-2-(5-methyl-2-(phenylsulfonyl)-1H-indol-1-yl)isoindolin-1-one-<sup>18</sup>O (5e)**



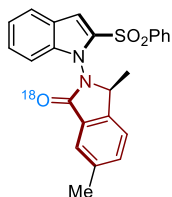
Following the **Procedure 7**, **5e** was obtained as faint yellow solid (28.8 mg, 69% yield). HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min),  $t_r = 40.420$  min (minor), 50.493 min (major); ee = 94%. HRMS (APCI)  $m/z$ : calculated for  $[C_{24}H_{20}N_2O_2^{16}OS+H]^+$  417.1267, found 417.1194,  $[C_{24}H_{20}N_2O_2^{18}OS+H]^+$  419.1309, found 419.1283. The ratio of relative peak intensities for the relevant isotopologues was 80:20 ( $C_{24}H_{20}N_2O_2^{18}OS$ :  $C_{24}H_{20}N_2O_2^{16}OS$ ).

**(S)-5-fluoro-3-methyl-2-(2-(phenylsulfonyl)-1H-indol-1-yl)isoindolin-1-one-<sup>18</sup>O (5f)**



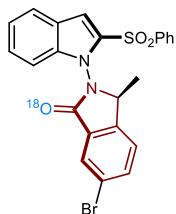
Following the **Procedure 7**, **5f** was obtained as faint yellow solid (32.5 mg, 77% yield). HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min),  $t_r = 40.037$  min (major), 49.117 min (minor); ee = 98%. HRMS (APCI)  $m/z$ : calculated for  $[C_{23}H_{17}FN_2O_2^{16}OS+H]^+$  421.1017, found 421.0989,  $[C_{23}H_{17}FN_2O_2^{18}OS+H]^+$  423.1059, found 423.1057. The ratio of relative peak intensities for the relevant isotopologues was 82:18 ( $C_{23}H_{17}FN_2O_2^{18}OS$ :  $C_{23}H_{17}FN_2O_2^{16}OS$ ).

**(S)-3,6-dimethyl-2-(2-(phenylsulfonyl)-1H-indol-1-yl)isoindolin-1-one-<sup>18</sup>O (5g)**

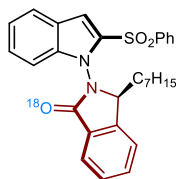


Following the **Procedure 7**, **5g** was obtained as faint yellow solid (32.2 mg, 77% yield). HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min),  $t_r = 40.420$  min (minor), 50.493 min (major); ee = 94%. HRMS (APCI)  $m/z$ : calculated for  $[C_{24}H_{20}N_2O_2^{16}OS+H]^+$  417.1267, found 417.1194,  $[C_{24}H_{20}N_2O_2^{18}OS+H]^+$  419.1309, found 419.1303. The ratio of relative peak intensities for the relevant isotopologues was 82:18 ( $C_{24}H_{20}N_2O_2^{18}OS$ :  $C_{24}H_{20}N_2O_2^{16}OS$ ).

**(S)-6-bromo-3-methyl-2-(2-(phenylsulfonyl)-1H-indol-1-yl)isoindolin-1-one-<sup>18</sup>O (5h)**

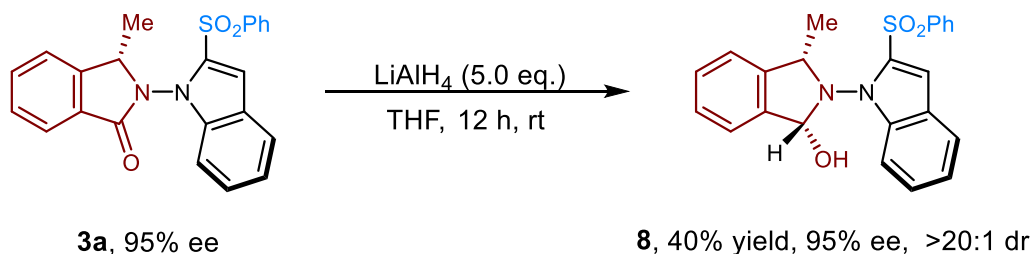


Following the **Procedure 7**, **5h** was obtained as faint yellow solid (31.3 mg, 65% yield). HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min),  $t_r$  = 28.633 min (minor), 39.330 min (major); ee = 99%. HRMS (APCI)  $m/z$ : calculated for  $[C_{23}H_{17}BrN_2O_2^{16}OS+H]^+$  481.0216, found 481.0156,  $[C_{23}H_{17}BrN_2O_2^{18}OS+H]^+$  483.0258, found 483.0242. The ratio of relative peak intensities for the relevant isotopologues was 91:9 ( $C_{23}H_{17}BrN_2O_2^{18}OS$ :  $C_{23}H_{17}BrN_2O_2^{16}OS$ ).  
**(S)-3-heptyl-2-(2-(phenylsulfonyl)-1H-indol-1-yl)isoindolin-1-one- $^{18}O$  (5i)**



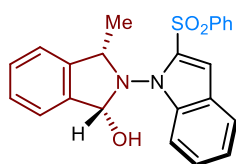
Following the **Procedure 7**, **5i** was obtained as orange viscous oil (30.7 mg, 63% yield). HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min),  $t_r$  = 20.920 min (minor), 32.467 min (major); ee = 94%. HRMS (APCI)  $m/z$ : calculated for  $[C_{29}H_{30}N_2O_2^{16}OS+H]^+$  487.2049, found 487.1987,  $[C_{29}H_{30}N_2O_2^{18}OS+H]^+$  489.2092, found 489.2080. The ratio of relative peak intensities for the relevant isotopologues was 83:17 ( $C_{29}H_{30}N_2O_2^{18}OS$ : $C_{29}H_{30}N_2O_2^{16}OS$ ).

### Synthetic applications of **3a**



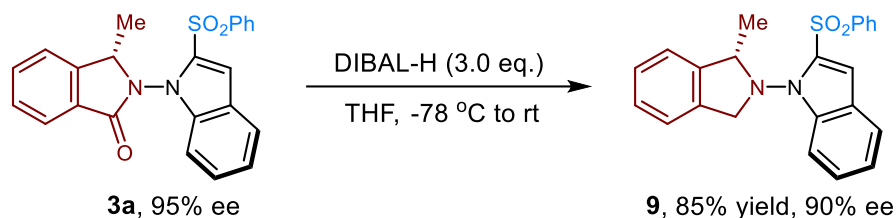
The reaction was proceeded in the glovebox under argon atmosphere. To a solution of **3a** (80.4 mg, 0.2 mmol, 1.0 eq.) in THF (1 mL) was added  $LiAlH_4$  (38.0 mg, 1.0 mmol, 5.0 eq.) slowly. Then the mixture was stirred at room temperature for 12 h. The mixture was quenched with triethylamine and water. Then the mixture was extracted with EA (5 mL x 3). The combined organic layers were dried over anhydrous  $Na_2SO_4$ , filtered and concentrated in vacuo. The residue was purified by column chromatography on silica gel (PE/EA as eluent, a small amount of triethylamine was required to be added to the eluent) and the product **8** (32.3 mg, 40% yield) was given.

### **(1R,3S)-3-methyl-2-(2-(phenylsulfonyl)-1H-indol-1-yl)isoindolin-1-ol (8)**



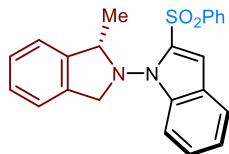


Following the above procedure, compound **8** was obtained as red solid (32.3 mg, 40% yield). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.08 – 8.03 (m, 2H), 7.74 (dd, *J* = 7.1, 1.8 Hz, 1H), 7.64 – 7.59 (m, 1H), 7.54 – 7.48 (m, 3H), 7.44 – 7.40 (m, 2H), 7.26 (s, 1H), 7.20 (qd, *J* = 7.4, 1.4 Hz, 2H), 7.13 (dd, *J* = 5.0, 3.5 Hz, 1H), 6.94 – 6.90 (m, 1H), 6.37 (s, 1H), 5.00 (q, *J* = 6.5 Hz, 1H), 4.26 (s, 1H), 0.75 (d, *J* = 6.5 Hz, 3H). <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 140.86, 140.58, 138.25, 137.14, 135.60, 133.92, 129.45, 129.18, 129.03, 128.45, 125.95, 124.52, 124.06, 123.93, 122.07, 121.95, 111.32, 109.50, 92.12, 63.38, 19.83. HPLC (Chiralpak IA column, 85:15 hexanes/isopropanol, 1 mL/min), *tr* = 23.357 min (minor), 39.050 min (major); *ee* = 95%. HRMS (APCI) *m/z*: calculated for [C<sub>23</sub>H<sub>20</sub>N<sub>2</sub>O<sub>3</sub>S+Na]<sup>+</sup> 427.1086, found 427.1092.

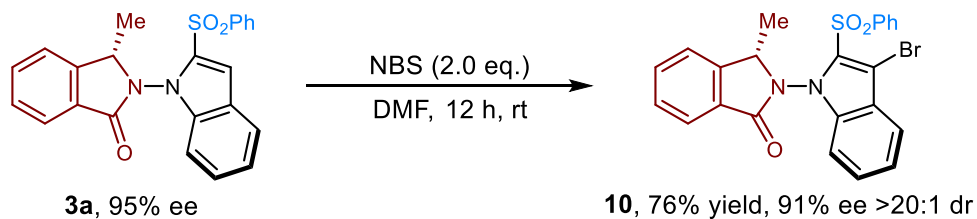


The reaction was proceeded under argon atmosphere. A solution of **3a** (80.4 mg, 0.2 mmol, 1.0 eq.) in THF (1 mL) was cooled at -78 °C. Then [(CH<sub>3</sub>)<sub>2</sub>CHCH<sub>2</sub>]<sub>2</sub>AlH (1 M in THF, 0.6 mL, 0.6 mmol, 3.0 eq.) was added to the mixture, and the mixture stirred at -78 °C for 12 h. After the mixture stirred at room temperature for a while, the mixture was quenched with water. Then the mixture was extracted with EA (5 mL x 3). The combined organic layers were dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>, filtered and concentrated in vacuo. The residue was purified by column chromatography on silica gel (PE/EA as eluent) and the product **9** (66.0 mg, 85% yield) was given.

#### (S)-1-(1-methylisoindolin-2-yl)-2-(phenylsulfonyl)-1H-indole (**9**)



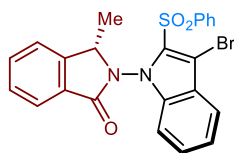
Following the above procedure, compound **9** was obtained as red solid (66.0 mg, 85% yield). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.97 (dd, *J* = 8.3, 1.4 Hz, 2H), 7.79 – 7.74 (m, 1H), 7.59 – 7.52 (m, 1H), 7.42 (t, *J* = 7.8 Hz, 2H), 7.35 (s, 1H), 7.32 (d, *J* = 7.4 Hz, 1H), 7.28 (t, *J* = 7.3 Hz, 1H), 7.18 (qd, *J* = 7.4, 1.5 Hz, 3H), 7.10 – 7.06 (m, 2H), 5.20 (q, *J* = 6.6 Hz, 1H), 4.41 (d, *J* = 13.1 Hz, 1H), 3.52 – 3.46 (m, 1H), 1.26 (d, *J* = 6.4 Hz, 3H). <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 141.70, 140.89, 137.66, 136.28, 134.66, 133.19, 129.07, 128.80, 127.76, 127.62, 125.13, 124.95, 124.06, 122.34, 122.30, 121.49, 111.86, 107.75, 64.39, 57.52, 19.40. HPLC (Chiralpak IA column, 85:15 hexanes/isopropanol, 1 mL/min), *tr* = 8.647 min (major), 14.747 min (minor); *ee* = 90%. HRMS (APCI) *m/z*: calculated for [C<sub>23</sub>H<sub>20</sub>N<sub>2</sub>O<sub>2</sub>S+Na]<sup>+</sup> 411.1137, found 411.1130.



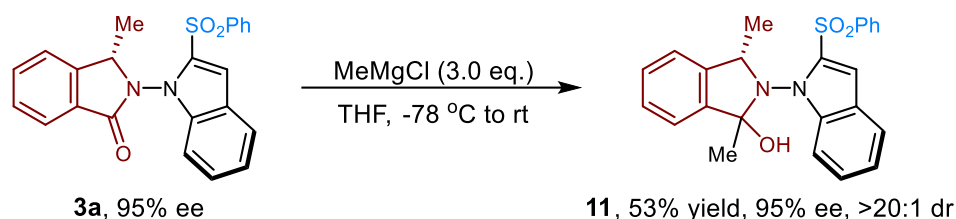
To a solution of **3a** (80.4 mg, 0.2 mmol, 1.0 eq.) in DMF (1 mL) was added *N*-bromosuccinimide (71.2 mg, 0.4 mmol, 2.0 eq.) slowly. Then the mixture was stirred at room temperature for 12 h. The mixture was quenched water.

Then the mixture was extracted with EA (5 mL x 3). The combined organic layers were dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>, filtered and concentrated in vacuo. The residue was purified by column chromatography on silica gel (PE/EA as eluent) and the product **10** (73.0 mg, 76% yield) was given.

**(S)-2-(3-bromo-2-(phenylsulfonyl)-1H-indol-1-yl)-3-methylisoindolin-1-one (10)**

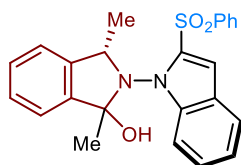


Following the above procedure, compound **10** was obtained as white solid (73.0 mg, 76% yield). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.30 (dd, *J* = 7.8, 1.7 Hz, 2H), 8.03 (d, *J* = 7.6 Hz, 1H), 7.74 – 7.70 (m, 1H), 7.68 (d, *J* = 8.1 Hz, 1H), 7.59 (t, *J* = 7.5 Hz, 2H), 7.55 – 7.50 (m, 3H), 7.44 – 7.40 (m, 1H), 7.31 (t, *J* = 7.6 Hz, 1H), 7.11 (d, *J* = 8.3 Hz, 1H), 5.11 (q, *J* = 6.8 Hz, 1H), 1.63 (d, *J* = 6.8 Hz, 3H). <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 166.56, 145.45, 140.88, 137.11, 133.88, 133.29, 132.01, 128.83, 128.79, 128.76, 128.70, 128.35, 125.19, 124.83, 123.51, 122.55, 121.89, 110.28, 101.54, 57.72, 16.86. HPLC (Chiralpak AD column, 80:20 hexanes/isopropanol, 1 mL/min), *t*<sub>r</sub> = 15.870 min (major), 23.587 min (minor); ee = 91%. HRMS (APCI) *m/z*: calculated for [C<sub>23</sub>H<sub>17</sub>BrN<sub>2</sub>O<sub>3</sub>S+Na]<sup>+</sup> 503.0035, found 503.0043.



The reaction was proceeded under argon atmosphere. A solution of **3a** (80.4 mg, 0.2 mmol, 1.0 eq.) in THF (1 mL) was cooled at -78 °C. Then MeMgCl (1 M in THF, 0.6 mL, 0.6 mmol, 3.0 eq.) was added to the mixture, and the mixture stirred at -78 °C for 0.5 h. After the mixture stirred at room temperature for 12 h, the mixture was quenched with triethylamine water. Then the mixture was extracted with EA (5 mL x 3). The combined organic layers were dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>, filtered and concentrated in vacuo. The residue was purified by column chromatography on silica gel (PE/EA as eluent, a small amount of triethylamine was required to be added to the eluent) and the product **9** (44.3 mg, 53% yield) was given. The absolute configuration of **11** regarding the quaternary carbon stereocenters was not determined.

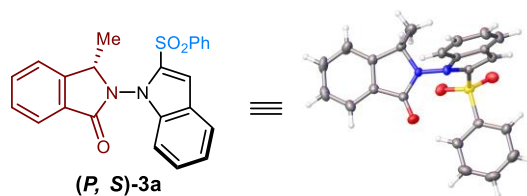
**(3S)-1,3-dimethyl-2-(2-(phenylsulfonyl)-1H-indol-1-yl)isoindolin-1-ol (11)**



Following the above procedure, compound **11** was obtained as red solid (44.3 mg, 53% yield). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.06 – 8.01 (m, 2H), 7.75 – 7.71 (m, 1H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.51 (t, *J* = 7.7 Hz, 2H), 7.48 – 7.46 (m, 1H), 7.42 – 7.38 (m, 3H), 7.20 – 7.15 (m, 2H), 7.14 – 7.11 (m, 1H), 6.73 – 6.68 (m, 1H), 5.06 (s, 1H), 4.91 (q, *J* = 6.6

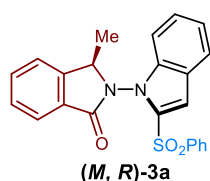
Hz, 1H), 1.57 (s, 3H), 0.58 (d,  $J = 6.6$  Hz, 3H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  142.50, 141.32, 140.58, 137.36, 136.83, 133.79, 129.22, 129.17, 128.81, 128.39, 126.13, 124.15, 123.87, 122.69, 121.89, 121.71, 112.35, 109.87, 97.13, 63.93, 24.13, 21.17. HPLC (Chiralpak IAcolumn, 80:20 hexanes/isopropanol, 1 mL/min),  $t_r = 8.953$  min (major), 22.577 min (minor); ee = 95%. HRMS (APCI)  $m/z$ : calculated for  $[\text{C}_{24}\text{H}_{22}\text{N}_2\text{O}_3\text{S}+\text{Na}]^+$  441.1243, found 441.1269.

X-ray structures of (*P, S*)-3a, (*M, R*)-3a, Int0 and 8

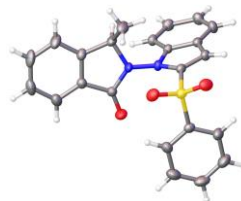


**Table S1. Crystal data and structure refinement for CCDC 2359270**

Identification code	<b>CCDC 2359270</b>
Empirical formula	C <sub>23</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub> S
Formula weight	402.45
Temperature/K	193.00
Crystal system	monoclinic
Space group	P21
a/Å	8.3879(8)
b/Å	12.8676(13)
c/Å	9.7824(10)
α/°	90
β/°	111.619(3)
γ/°	90
Volume/Å <sup>3</sup>	981.56(17)
Z	2
ρ <sub>calc</sub> /cm <sup>3</sup>	1.362
μ/mm <sup>-1</sup>	1.693
F(000)	420.0
Crystal size/mm <sup>3</sup>	0.13 × 0.11 × 0.1
Radiation	CuKα (λ = 1.54178)
2θ range for data collection/°	11.346 to 136.904
Index ranges	-10 ≤ h ≤ 10, -15 ≤ k ≤ 15, -11 ≤ l ≤ 11
Reflections collected	16483
Independent reflections	3435 [R <sub>int</sub> = 0.0289, R <sub>sigma</sub> = 0.0343]
Data/restraints/parameters	3435/1/264
Goodness-of-fit on F <sup>2</sup>	1.076
Final R indexes [I ≥ 2σ (I)]	R1 = 0.0246, wR2 = 0.0596
Final R indexes [all data]	R1 = 0.0247, wR2 = 0.0596
Largest diff. peak/hole / e Å <sup>-3</sup>	0.28/-0.19
Flack parameter	0.090(4)

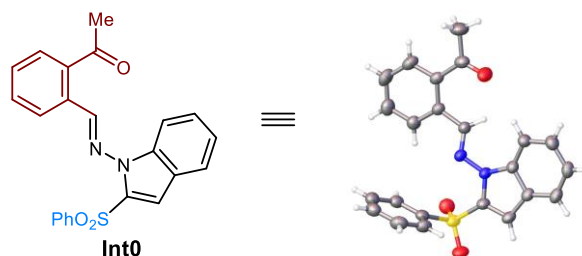


≡



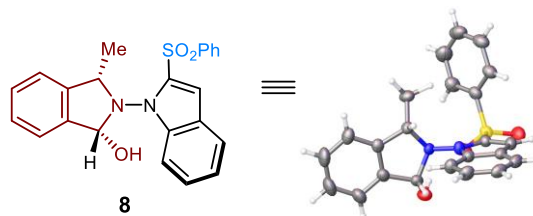
**Table S2. Crystal data and structure refinement for CCDC 2362138**

Identification code	<b>CCDC 2362138</b>
Empirical formula	C <sub>23</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub> S
Formula weight	402.45
Temperature/K	193.00
Crystal system	monoclinic
Space group	P21
a/Å	8.3907(4)
b/Å	12.8791(6)
c/Å	9.7624(4)
α/°	90
β/°	111.3930(10)
γ/°	90
Volume/Å <sup>3</sup>	982.28(8)
Z	2
ρ <sub>calc</sub> /cm <sup>3</sup>	1.361
μ/mm <sup>-1</sup>	1.691
F(000)	420.0
Crystal size/mm <sup>3</sup>	0.14 × 0.13 × 0.1
Radiation	CuKα (λ = 1.54178)
2θ range for data collection/°	9.73 to 136.548
Index ranges	-10 ≤ h ≤ 10, -14 ≤ k ≤ 15, -11 ≤ l ≤ 11
Reflections collected	15494
Independent reflections	3365 [R <sub>int</sub> = 0.0257, R <sub>sigma</sub> = 0.0326]
Data/restraints/parameters	3365/1/263
Goodness-of-fit on F <sup>2</sup>	1.098
Final R indexes [I ≥ 2σ (I)]	R <sub>1</sub> = 0.0266, wR <sub>2</sub> = 0.0666
Final R indexes [all data]	R <sub>1</sub> = 0.0267, wR <sub>2</sub> = 0.0667
Largest diff. peak/hole / e Å <sup>-3</sup>	0.20/-0.40
Flack parameter	0.074(5)



**Table S3. Crystal data and structure refinement for CCDC 2354174**

Identification code	<b>CCDC 2354174</b>
Empirical formula	$C_{23}H_{18}N_2O_3S$
Formula weight	402.45
Temperature/K	223.00
Crystal system	monoclinic
Space group	P21/c
$a/\text{\AA}$	11.0123(12)
$b/\text{\AA}$	12.1777(14)
$c/\text{\AA}$	14.8173(17)
$\alpha/^\circ$	90
$\beta/^\circ$	104.644(4)
$\gamma/^\circ$	90
Volume/ $\text{\AA}^3$	1922.5(4)
Z	4
$\rho_{\text{calc}}/\text{cm}^3$	1.390
$\mu/\text{mm}^{-1}$	1.728
F(000)	840.0
Crystal size/ $\text{mm}^3$	$0.13 \times 0.11 \times 0.1$
Radiation	CuK $\alpha$ ( $\lambda = 1.54178$ )
$2\theta$ range for data collection/ $^\circ$	8.298 to 137.162
Index ranges	$-13 \leq h \leq 13, -14 \leq k \leq 14, -17 \leq l \leq 17$
Reflections collected	41027
Independent reflections	3524 [Rint = 0.0334, Rsigma = 0.0201]
Data/restraints/parameters	3524/0/263
Goodness-of-fit on F2	1.047
Final R indexes [ $I \geq 2\sigma(I)$ ]	R1 = 0.0313, wR2 = 0.0828
Final R indexes [all data]	R1 = 0.0327, wR2 = 0.0835
Largest diff. peak/hole / $e \text{\AA}^{-3}$	0.19/-0.38



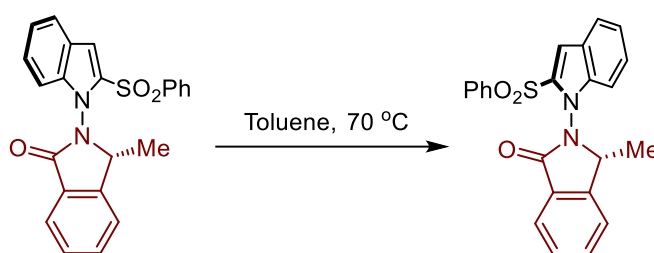
**Table S4. Crystal data and structure refinement for CCDC 2393057**

Identification code	<b>CCDC 2393057</b>
Empirical formula	C <sub>23</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub> S
Formula weight	404.47
Temperature/K	193.15
Crystal system	orthorhombic
Space group	P212121
a/Å	8.84300(10)
b/Å	12.3300(2)
c/Å	18.0497(2)
α/°	90
β/°	90
γ/°	90
Volume/Å <sup>3</sup>	1968.03(4)
Z	4
ρ <sub>calc</sub> /cm <sup>3</sup>	1.365
μ/mm <sup>-1</sup>	1.689
F(000)	848.0
Crystal size/mm <sup>3</sup>	0.1 × 0.1 × 0.1
Radiation	CuKα (λ = 1.54184)
2θ range for data collection/°	8.686 to 136.434
Index ranges	-10 ≤ h ≤ 10, -14 ≤ k ≤ 14, -21 ≤ l ≤ 21
Reflections collected	40924
Independent reflections	3603 [R <sub>int</sub> = 0.0329, R <sub>sigma</sub> = 0.0216]
Data/restraints/parameters	3603/0/272
Goodness-of-fit on F <sup>2</sup>	1.075
Final R indexes [I ≥ 2σ (I)]	R <sub>1</sub> = 0.0251, wR <sub>2</sub> = 0.0668
Final R indexes [all data]	R <sub>1</sub> = 0.0255, wR <sub>2</sub> = 0.0672
Largest diff. peak/hole / e Å <sup>-3</sup>	0.14/-0.38
Flack parameter	0.034(3)

## Racemization experiment

Compound **3a** (0.1 mmol) were added to a vial equipped with a magnetic stirring bar. The vial was then charged with toluene (1.0 mL). The vial was sealed, and the mixture was stirred at 70 °C. The ee of the obtained compound **3a** was detected directly. At given interval of time, small samples (5  $\mu$ L) was removed via syringe and subjected into the HPLC to measure the enantiomeric excess.

The enantiomerisation barrier, corresponding to barrier to rotation for **3a** atropisomers, was obtained by kinetic of racemization of an enantiomer. The slope of the first-order kinetic line gives the racemization constant ( $k_{\text{racemization}} = 2 \times k_{\text{enantiomerisation}}$ ). Eyring equation gives the enantiomerisation barrier from enantiomerisation constant ( $k_{\text{enantiomerisation}}$ ),  $R = 8.31451 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$ ,  $h = 6.62608 \times 10^{-34} \text{ J} \cdot \text{s}$  and  $k_B = 1.38066 \times 10^{-23} \text{ J} \cdot \text{K}^{-1}$  ( $-\ln ee = \ln\{(1+M/P)/(1-M/P)\}$ ).



Time/h	ee (%)	-ln ee	Time/h	ee (%)	-ln ee
0	98.54	-4.59046	24	76.26	-4.33414
0.5	98.30	-4.58802	36	60.70	-4.10594
1	97.38	-4.57862	48	57.22	-4.04690
2	94.76	-4.55134	57	51.50	-3.94158
4	92.60	-4.52828	72.5	43.38	-3.8133
8	88.20	-4.47960	83.5	39.96	-3.68637
12	83.58	-4.42580	98.5	35.23	-3.56189

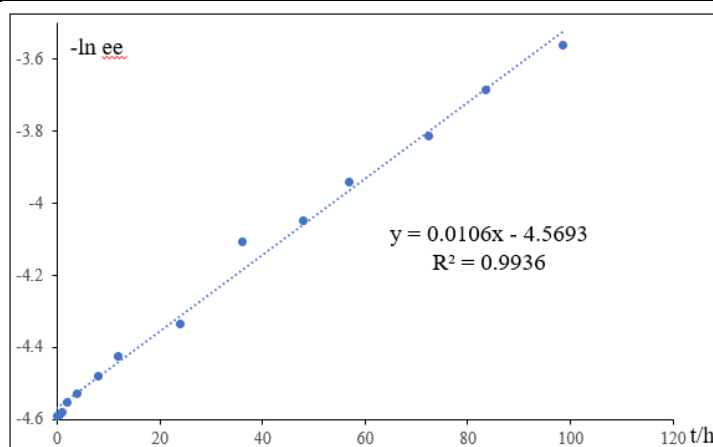


Figure S1. Racemization experiments.

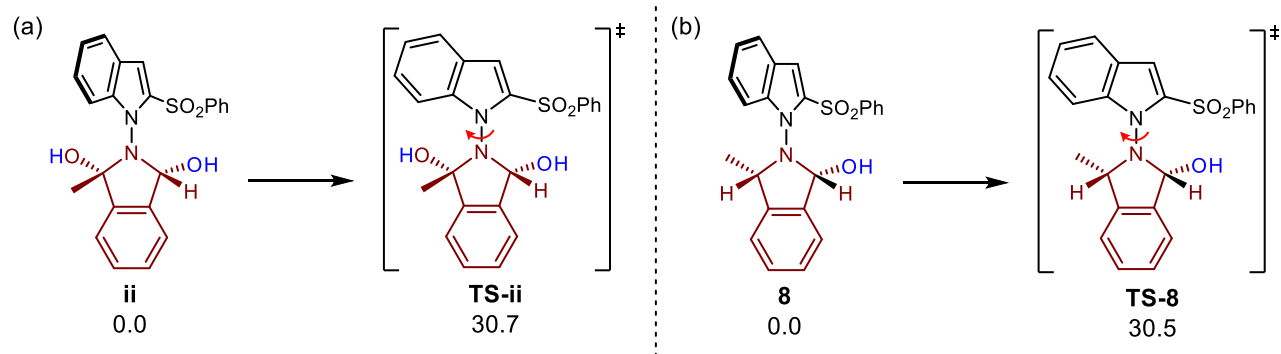


$k_{\text{racemization}} = 0.01060 \text{ h}^{-1}$ ;  $k_{\text{enantiomerization}} = 0.00530 \text{ h}^{-1}$

Half-life time  $t_{1/2}$  (343K) = 65.39 h

$\Delta G^{343\text{K}} = 29.33 \text{ kcal/mol}$

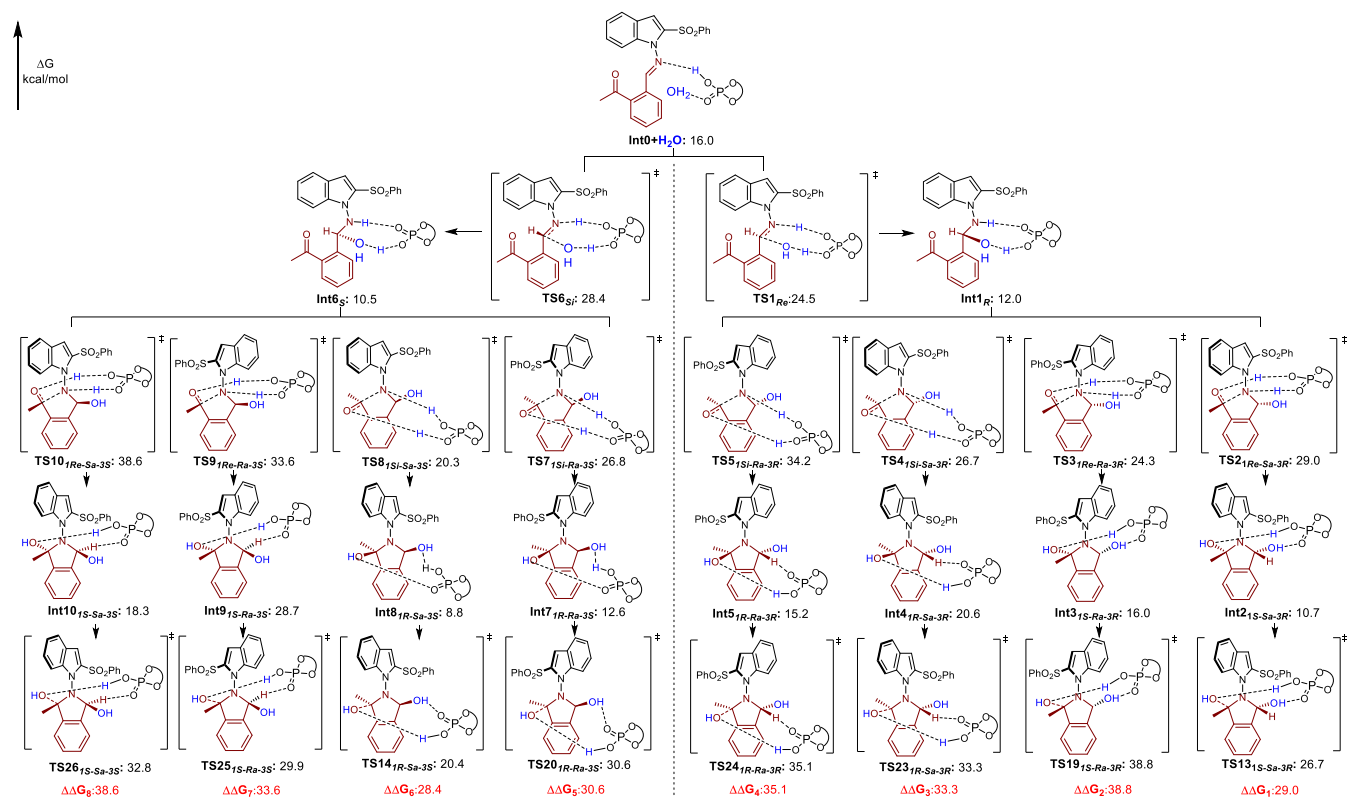
In addition, we calculated the rotational barriers of **ii** and **8** about the N-N axis, as shown in **Figure S2**. The calculated rotational barriers were 30.7 and 30.5 kcal/mol, respectively. This result indicated that the axial chirality was generated in the annulation process.



**Figure S2.** The rotational energy barriers of **Int2**<sub>1S-5a-3R</sub>, **8** and **9** (in kcal/mol).

## Computational methods

The Gaussian 16 program was used for all the DFT calculations.<sup>[4]</sup> Geometry optimizations were optimized at the M06-2X<sup>[5]</sup> and def2-SVP<sup>[6]</sup> basis set level of theory. The single-point energies in toluene were calculated using the SMD solvation model at the M06-2X and def2-TZVPP basis set level of theory. Vibrational frequency calculations were performed at the same level to obtain thermal energy correction, and to confirm the stationary point is an energy minimum or a transition state. Intrinsic reaction coordinate (IRC)<sup>[7-8]</sup> calculations were performed to confirm the connection between transition state and its reactant and product.



**Figure S3.** Free energy diagrams of chiral phosphoric acid-catalyzed stepwise mechanism in asymmetric annulation and dehydration. The meaning for the corner mark in the structure name: **Re**: the rectus face; **Si**: the sinister face; **Ra**: the potential **R**-configuration for the *N-N* axis; **Sa**: the potential **S**-configuration for the *N-N* axis; **R**: the **R**-configuration for the central chirality; **S**: the **S**-configuration for the central chirality.

**Table S6. Thermal correction of Gibbs free energy (TCG, hartree) and total electronic energies (E, hartree) in toluene solvent for all species involved in the DFT study**

Compounds	TCG	E	Compounds	TCG	E
<b>H<sub>2</sub>O</b>	0.003949	-76.433213	<b>TS11</b> <i>IRe-Sa-3Re</i>	1.235706	-4279.052964
<b>CPA</b>	0.867742	-2582.036042	<b>TS12</b> <i>ISi-Sa-3Si</i>	1.238793	-4279.054653
<b>Int0</b>	1.205454	-4202.630730	<b>TS13</b> <i>IS-Sa-3R</i>	1.239669	-4279.051586
<b>Int0+H<sub>2</sub>O</b>	1.231781	-4279.060820	<b>TS14</b> <i>IR-Sa-3S</i>	1.237124	-4279.059093
<b>TS1</b> <i>Re</i>	1.233156	-4279.048592	<b>TS15</b> <i>P-Re</i>	1.206928	-4202.589283
<b>Int1</b> <i>R</i>	1.238581	-4279.073964	<b>TS16</b> <i>P-Si</i>	1.210572	-4202.587333
<b>TS2</b> <i>1Re-Sa-3R</i>	1.241509	-4279.049869	<b>Int11</b> <i>P</i>	1.211006	-4202.618837
<b>TS3</b> <i>1Re-Ra-3R</i>	1.242254	-4279.057850	<b>(P,R)</b> - <b>3a</b>	0.314580	-1620.620748
<b>TS4</b> <i>1Si-Sa-3R</i>	1.240384	-4279.052382	<b>(P,S)</b> - <b>3a</b>	0.313841	-1620.621035
<b>TS5</b> <i>1Si-Ra-3R</i>	1.239710	-4279.039820	<b>TS17</b> <i>1Re-Ra-3Re</i>	1.239719	-4279.058216
<b>Int2</b> <i>IS-Sa-3R</i>	1.239899	-4279.077374	<b>TS18</b> <i>1Si-Ra-3Si</i>	1.241763	-4279.047623
<b>Int3</b> <i>IS-Ra-3R</i>	1.245549	-4279.074633	<b>TS19</b> <i>IS-Ra-3R</i>	1.238808	-4279.031563
<b>Int4</b> <i>IR-Sa-3R</i>	1.240917	-4279.062622	<b>TS20</b> <i>1R-Ra-3S</i>	1.240898	-4279.046617
<b>Int5</b> <i>IR-Ra-3R</i>	1.240375	-4279.070664	<b>TS21</b> <i>M-Re</i>	1.203059	-4202.586698
<b>TS6</b> <i>Si</i>	1.237785	-4279.047129	<b>TS22</b> <i>M-Si</i>	1.208337	-4202.588708
<b>Int6</b> <i>S</i>	1.236214	-4279.074054	<b>Int12</b> <i>M</i>	1.207652	-4202.612865
<b>TS7</b> <i>1Si-Ra-3S</i>	1.241408	-4279.053245	<b>(M,R)</b> - <b>3a</b>	0.314835	-1620.623487
<b>TS8</b> <i>1Si-Sa-3S</i>	1.237443	-4279.059684	<b>(M,S)</b> - <b>3a</b>	0.314751	-1620.626210
<b>TS9</b> <i>1Re-Ra-3S</i>	1.242373	-4279.043349	<b>TS23</b> <i>1R-Sa-3R</i>	1.240180	-4279.041600
<b>TS10</b> <i>1Re-Sa-3S</i>	1.240434	-4279.033492	<b>TS24</b> <i>1Si-Ra-3R</i>	1.239553	-4279.038123
<b>Int7</b> <i>IR-Ra-3S</i>	1.243725	-4279.078221	<b>TS25</b> <i>IS-Ra-3S</i>	1.240206	-4279.047135
<b>Int8</b> <i>IR-Sa-3S</i>	1.242056	-4279.082552	<b>TS26</b> <i>IS-Sa-3S</i>	1.240383	-4279.042596
<b>Int9</b> <i>IS-Ra-3S</i>	1.243909	-4279.052691			
<b>Int10</b> <i>IS-Sa-3S</i>	1.243293	-4279.068737			

## Cartesian coordinates for all optimized geometries

### H<sub>2</sub>O

O	0.00000000	0.00000000	0.11916800
H	0.00000000	0.75600100	-0.47667000
H	0.00000000	-0.75600100	-0.47667000

### CPA

C	1.52903200	1.14288900	0.17921100
C	0.68603600	2.17113300	-0.19057200
C	1.21758500	3.20733300	-1.03261500
C	2.60852600	3.19263800	-1.34609400
C	3.42000600	2.10791000	-0.91447700
C	2.89599000	1.05211100	-0.20945100
H	-0.66292700	4.23281600	-1.40342800
C	0.40999800	4.23534500	-1.59398900
C	3.15438000	4.23482800	-2.14469200
H	4.47372900	2.09587100	-1.19914900
C	2.35444800	5.23184900	-2.64436500
C	0.96429600	5.21948700	-2.37686700
H	4.22359200	4.21568700	-2.36511600
H	2.78233800	6.02346200	-3.26078300
H	0.32526600	5.99515300	-2.80098200
C	-0.73863600	2.13323400	0.24276700
C	-1.36809400	3.23647100	0.91434700
C	-1.49104700	0.99239400	0.02576100
C	-0.64864900	4.38992200	1.33515800
C	-2.76166100	3.16565800	1.20290100
C	-2.87182200	0.88238400	0.34685700
C	-1.28923700	5.43008900	1.96420300
H	0.42640000	4.43884000	1.16242100
C	-3.39898800	4.26595800	1.83935000
C	-3.48758400	1.98599100	0.88522100
C	-2.68310900	5.37736900	2.20768600
H	-0.71696600	6.30168000	2.28475000
H	-4.46974800	4.20022100	2.04219800
H	-4.55750600	1.94975800	1.09997500
H	-3.18039500	6.21315000	2.70156300
O	-0.90127300	-0.11291400	-0.56574400
O	1.04185900	0.13358400	0.98158000
P	0.09574700	-1.00610800	0.33199400
O	0.93950200	-1.65576900	-0.85465800
H	1.68104200	-2.19724700	-0.53695600
O	-0.44986700	-1.89194800	1.36075000
C	-3.59937600	-0.39723300	0.08404400
C	-3.98563200	-0.72245800	-1.23163500
C	-3.88082700	-1.27580800	1.14982100
C	-4.69527400	-1.90383900	-1.45279900
C	-4.59695000	-2.44576800	0.87644600
C	-5.01936100	-2.77470300	-0.41072400
H	-4.99998100	-2.15332700	-2.47343700
H	-4.82620300	-3.13315000	1.69371500
C	3.64894800	-0.20660800	0.08169700
C	4.00477700	-1.06831700	-0.98696800
C	3.92402800	-0.58265600	1.41157200
C	4.63693600	-2.27875000	-0.68942600
C	4.56652800	-1.80203400	1.65296400
C	4.92972500	-2.66513000	0.62214900
H	4.91489800	-2.94307100	-1.51132100
H	4.78770100	-2.09100300	2.68379800
C	-3.64656200	0.16593600	-2.41926200
C	-4.91291200	0.68580300	-3.10647400
C	-2.73131500	-0.56270200	-3.40871400
H	-3.09606900	1.04200200	-2.04731400
H	-5.55196500	1.23167600	-2.39748000
H	-4.65395000	1.36423300	-3.93293500

H	-5.50517100	-0.14230500	-3.52507100
H	-1.81478500	-0.90565900	-2.90914600
H	-3.23733800	-1.43885400	-3.84277900
H	-2.44868100	0.10588100	-4.23567800
C	-3.44516500	-0.97719500	2.57827500
C	-2.94131300	-2.21856600	3.31831100
C	-4.58159900	-0.31352400	3.36541500
H	-2.60231500	-0.27148900	2.52592800
H	-2.16022700	-2.72292600	2.73655400
H	-2.51218400	-1.92097900	4.28650100
H	-3.75828300	-2.92536900	3.52948500
H	-4.91382400	0.62275700	2.89646900
H	-5.45036300	-0.98815400	3.42002500
H	-4.25951200	-0.08687100	4.39278700
C	-5.79062400	-4.05409100	-0.67650100
C	-5.00166600	-5.00163800	-1.58483500
C	-7.17774200	-3.76350600	-1.25612700
H	-5.92813500	-4.55463700	0.29564400
H	-4.01384600	-5.22635400	-1.15897000
H	-5.54427300	-5.94827800	-1.72627700
H	-4.84615900	-4.55142400	-2.57741800
H	-7.75284800	-3.09996800	-0.59514300
H	-7.09638200	-3.27282800	-2.23828100
H	-7.74590500	-4.69562800	-1.39318600
C	3.74244500	-0.72113000	-2.44845700
C	3.18847400	-1.89315100	-3.26461700
C	5.02462700	-0.19255300	-3.10469300
H	2.98583100	0.07505900	-2.47657800
H	2.27121400	-2.29951400	-2.81846900
H	2.94091600	-1.55035100	-4.27967800
H	3.92225700	-2.70623100	-3.36829400
H	5.43812500	0.66896000	-2.56288300
H	5.79761700	-0.97680500	-3.11585700
H	4.83203800	0.11224300	-4.14398600
C	3.58099600	0.30499200	2.59787800
C	4.85946500	0.88190700	3.21647800
C	2.73858300	-0.43267900	3.64261300
H	2.98502900	1.15217300	2.23268300
H	5.43931200	1.44753500	2.47283100
H	4.61409800	1.55612900	4.05028800
H	5.50328800	0.07931000	3.60814100
H	1.83388600	-0.86097500	3.18977600
H	3.31001200	-1.24440700	4.11813100
H	2.43027500	0.26188900	4.43776200
C	5.61775100	-3.98609800	0.90931300
C	7.01403500	-4.03633200	0.28236500
C	4.76412500	-5.17186900	0.45036900
H	5.73452100	-4.05644700	2.00270900
H	7.63366800	-3.19586300	0.62504100
H	7.52433900	-4.97438200	0.54598600
H	6.95257900	-3.98524300	-0.81560200
H	3.76993300	-5.15078800	0.91877700
H	4.62570200	-5.15573700	-0.64179500
H	5.24878800	-6.12398300	0.71182700
<b>Int0</b>			
S	5.77245400	0.82835200	2.05155100
O	6.57863700	-0.21194600	2.67787000
O	4.49031500	1.22518900	2.61963800
O	1.20306600	2.36820400	-2.78712300
N	4.60663600	0.82304900	-0.47660200
N	3.83298200	1.88839400	-0.10480300
C	6.79038800	2.28635400	1.90853800
C	8.14253200	2.17572300	2.22229800
H	8.54126400	1.21001400	2.53510400
C	8.94273300	3.31370000	2.13683900
H	10.00357600	3.25017100	2.38219900

C	8.38605700	4.53034000	1.74206400
H	9.01676800	5.41817700	1.67525100
C	7.02753200	4.62061200	1.43305000
H	6.59862700	5.57492200	1.12510500
C	6.21245300	3.49436100	1.51996000
H	5.15089500	3.53293300	1.27115200
C	5.53701700	0.28221600	0.38340900
C	6.17031200	-0.78407700	-0.19632900
H	6.92758700	-1.39539600	0.28610600
C	5.61612300	-0.90776800	-1.51098500
C	4.62965000	0.10467900	-1.65670000
C	3.91220100	0.28491900	-2.85274800
H	3.15886000	1.06502600	-2.96605500
C	4.20221100	-0.58260100	-3.89143600
H	3.66329200	-0.47341300	-4.83389600
C	5.17333200	-1.60236800	-3.76720300
H	5.36380900	-2.26213600	-4.61508700
C	5.88058800	-1.77126700	-2.59214200
H	6.63827900	-2.55130100	-2.49858600
C	2.61006200	1.88438500	-0.46661300
H	2.14735800	1.07473900	-1.04135200
C	1.75980600	2.99874000	-0.00403800
C	2.04401200	3.58904600	1.23393400
H	2.86050400	3.17263400	1.82927400
C	1.28010600	4.65710600	1.69721900
H	1.51664000	5.11516400	2.65867200
C	0.20531300	5.12708200	0.94230600
H	-0.39658900	5.96368900	1.30311400
C	-0.11928500	4.50574300	-0.26022400
H	-0.98365100	4.85043500	-0.82963900
C	0.65846100	3.45317200	-0.75217300
C	0.34444000	2.85437200	-2.08882400
C	-1.09602500	2.91189400	-2.55067400
H	-1.36769200	3.93916900	-2.83934400
H	-1.79525600	2.61896500	-1.75050000
H	-1.19172600	2.28463800	-3.44845100
C	-3.59752900	-0.18832300	0.60572400
C	-3.76247300	-1.44220900	1.15314000
C	-5.09912900	-1.96495200	1.24853100
C	-6.19447800	-1.11984200	0.90723300
C	-5.94816600	0.19628400	0.42915300
C	-4.67265200	0.66478800	0.23036000
H	-4.54731900	-3.97548100	1.86628900
C	-5.37561900	-3.30362600	1.64244200
C	-7.52174500	-1.61450900	1.02681200
H	-6.79899100	0.84248400	0.20514800
C	-7.75780200	-2.90379900	1.43423900
C	-6.66947900	-3.75899500	1.73046000
H	-8.35011300	-0.94954600	0.77435200
H	-8.77967400	-3.27614000	1.51674100
H	-6.85857700	-4.79149100	2.02705400
C	-2.57662300	-2.22827500	1.59088600
C	-2.48885400	-2.78326600	2.91299100
C	-1.52932800	-2.45666900	0.71832100
C	-3.41787100	-2.46421300	3.94220500
C	-1.41599000	-3.66861900	3.21840600
C	-0.46130900	-3.35954600	0.98887500
C	-3.30034500	-3.01970100	5.19357000
H	-4.22372600	-1.76030800	3.73337900
C	-1.33079500	-4.23945600	4.51795900
C	-0.44791900	-3.96552200	2.22299500
C	-2.25295100	-3.92694100	5.48503500
H	-4.01717600	-2.75387700	5.97164900
H	-0.50731000	-4.92316500	4.73283100
H	0.34173400	-4.68558300	2.45013200
H	-2.17477700	-4.36433600	6.48112300

O	-1.54979800	-1.87134400	-0.53739900
O	-2.31858000	0.31007900	0.44029200
P	-1.41880400	-0.28632300	-0.75772300
O	-2.29736800	-0.15776300	-2.08402700
H	-1.97590900	0.56644000	-2.64137200
O	-0.09864500	0.35435300	-0.80962600
C	0.54404600	-3.68760300	-0.06645200
C	0.11651500	-4.36216700	-1.23200700
C	1.90456000	-3.35207900	0.10262400
C	1.05830900	-4.68015500	-2.21038800
C	2.80397900	-3.67467200	-0.92098400
C	2.40504900	-4.33922200	-2.07942900
H	0.72775000	-5.21868900	-3.10280900
H	3.85397100	-3.38912300	-0.81942400
C	-4.39380600	2.03520900	-0.29819400
C	-4.66489700	2.35807900	-1.64824600
C	-3.86867600	3.01223500	0.56918900
C	-4.45402500	3.66967700	-2.07625200
C	-3.66784300	4.31275300	0.08835000
C	-3.97183400	4.66970900	-1.22437700
H	-4.66749500	3.92741500	-3.11745600
H	-3.26986400	5.06160700	0.77625400
C	-1.32156800	-4.81624700	-1.44770800
C	-1.41037700	-6.34647300	-1.41940800
C	-1.91436800	-4.24936800	-2.74096500
H	-1.93837200	-4.44685600	-0.61739600
H	-1.01425200	-6.74687500	-0.47502000
H	-2.45473800	-6.67627300	-1.52565700
H	-0.82986900	-6.79015400	-2.24271600
H	-1.87216500	-3.15184900	-2.74176700
H	-1.37200800	-4.61944900	-3.62439700
H	-2.96637100	-4.55497700	-2.84418600
C	2.40898800	-2.55659700	1.30080700
C	2.39131500	-1.06799300	0.94483900
C	3.80337200	-2.97599000	1.76965000
H	1.71936000	-2.71142800	2.14089500
H	1.37361000	-0.70718000	0.74106900
H	2.83973500	-0.45294500	1.74087400
H	2.97579100	-0.92617000	0.02320300
H	3.85943400	-4.05551100	1.97414600
H	4.57115300	-2.72490900	1.02309500
H	4.07179800	-2.42856600	2.68499300
C	3.41160300	-4.71780300	-3.14893000
C	2.98658500	-4.23255700	-4.53640600
C	3.66323200	-6.22934900	-3.14787700
H	4.35562500	-4.21250600	-2.89020100
H	2.78883900	-3.15131700	-4.53175600
H	3.77369200	-4.44134300	-5.27723700
H	2.07258700	-4.74518100	-4.87399500
H	4.00342200	-6.57309600	-2.16090400
H	2.73962000	-6.77603700	-3.39462000
H	4.42647500	-6.50035800	-3.89294600
C	-5.18664100	1.32483500	-2.63826600
C	-4.49913200	1.41705200	-4.00415100
C	-6.70376500	1.45073200	-2.82250900
H	-4.96696200	0.32978000	-2.22557500
H	-3.40494800	1.46544100	-3.91181100
H	-4.75077400	0.53913200	-4.61567300
H	-4.82021000	2.30928800	-4.56228900
H	-7.24306200	1.31842300	-1.87562000
H	-6.95890300	2.44666900	-3.21686900
H	-7.07127600	0.69616100	-3.53365600
C	-3.56670600	2.72009300	2.03161900
C	-4.55633400	3.45740300	2.94062200
C	-2.11868600	3.05128600	2.39611600
H	-3.70824100	1.64598100	2.20717800

H	-5.59406500	3.17976200	2.70511600
H	-4.36387500	3.21510500	3.99614800
H	-4.46258700	4.54793700	2.82146600
H	-1.41229200	2.56114000	1.70971700
H	-1.93602000	4.13562800	2.35874300
H	-1.89749600	2.71424500	3.41953000
C	-3.82747100	6.08922500	-1.75428200
C	-3.10258700	7.04062500	-0.80568700
C	-5.20472200	6.66250400	-2.11408900
H	-3.23915400	6.02435000	-2.68741500
H	-2.10299600	6.67619300	-0.52851800
H	-2.98011100	8.02451000	-1.27934500
H	-3.67987800	7.18770200	0.11983800
H	-5.73424900	6.02695000	-2.83682000
H	-5.82887800	6.73617200	-1.21056500
H	-5.10646500	7.66802700	-2.54861700

### Int0+H<sub>2</sub>O

S	5.14617500	0.24916300	-0.85346200
O	5.40539600	-0.27773100	0.48764000
O	4.71185300	1.63398400	-1.01255000
O	3.52301300	-3.25368000	3.06114400
N	2.80277300	-1.18420800	-1.04323100
N	2.28464800	-0.60198300	0.10789800
C	6.60200100	0.01861800	-1.84472400
C	7.45785200	-1.03840400	-1.54343900
H	7.23270600	-1.69455200	-0.70143300
C	8.59048400	-1.21899900	-2.33291900
H	9.27734800	-2.03828800	-2.11813400
C	8.84717500	-0.34892700	-3.39487600
H	9.73607500	-0.49577000	-4.01010100
C	7.98186200	0.70990000	-3.67300300
H	8.19539600	1.38962200	-4.49858400
C	6.84438100	0.90476200	-2.89088900
H	6.15216300	1.72856700	-3.07150300
C	3.98442900	-0.82045500	-1.65678200
C	4.04906300	-1.36512100	-2.91501900
H	4.88081000	-1.27288300	-3.60815400
C	2.82743200	-2.09102900	-3.10318000
C	2.06537000	-1.95165500	-1.91750100
C	0.80999800	-2.55621300	-1.73954400
H	0.27602300	-2.49608600	-0.78919900
C	0.32305200	-3.28240300	-2.81037200
H	-0.64930000	-3.76618700	-2.71256700
C	1.05649600	-3.42928300	-4.01208600
H	0.62880200	-4.01771500	-4.82466600
C	2.30324200	-2.85562700	-4.16549600
H	2.87273400	-2.98398900	-5.08702400
C	2.78014900	-1.04975200	1.19999300
H	3.53152300	-1.84157000	1.14714800
C	2.42488400	-0.50176900	2.51171100
C	1.55896300	0.59214300	2.63406100
H	1.13139700	1.05861400	1.74501800
C	1.27538100	1.12565000	3.88753500
H	0.58099200	1.96107000	3.96252100
C	1.88979100	0.60815000	5.02548500
H	1.67221500	1.03363000	6.00610400
C	2.78952700	-0.45030800	4.91279000
H	3.27118100	-0.85240300	5.80579100
C	3.04204100	-1.02619900	3.66783100
C	3.92417100	-2.24304800	3.59284400
C	5.31666700	-2.12638300	4.14951100
H	5.78758500	-3.11504600	4.18066100
H	5.32361400	-1.65665800	5.14185400
H	5.88069300	-1.46336500	3.47321000
C	-2.23090900	2.22816300	-0.19281300
C	-3.41654800	1.97714400	-0.85755800



C	-3.78539100	2.85667300	-1.93484900
C	-3.00042300	4.02127100	-2.17635700
C	-1.81985300	4.24404100	-1.41793400
C	-1.38518700	3.33857500	-0.48478300
H	-5.46836800	1.68519600	-2.65728000
C	-4.88747100	2.59670300	-2.79644800
C	-3.37639700	4.91369800	-3.21691200
H	-1.20947500	5.12460900	-1.63228400
C	-4.46412200	4.65079000	-4.01189900
C	-5.21642900	3.46971500	-3.80590500
H	-2.76955100	5.80658400	-3.38034700
H	-4.73989400	5.33860300	-4.81234800
H	-6.06099800	3.24539300	-4.45885500
C	-4.23486600	0.79036000	-0.48383300
C	-5.63787400	0.87872000	-0.18009200
C	-3.63321400	-0.44908100	-0.39318500
C	-6.32455400	2.12073800	-0.07818500
C	-6.37285200	-0.32051400	0.05319900
C	-4.33344100	-1.64782800	-0.07222300
C	-7.67103700	2.16360100	0.19387700
H	-5.76716600	3.04784700	-0.21147700
C	-7.76767100	-0.24348600	0.31717700
C	-5.69338300	-1.56976900	0.08582600
C	-8.40767000	0.96923300	0.37992900
H	-8.17501800	3.12781500	0.27346600
H	-8.31679400	-1.17235600	0.48416700
H	-6.26370700	-2.47514900	0.30477400
H	-9.47717900	1.01675500	0.58895100
O	-2.28774100	-0.57110200	-0.66829500
O	-1.82496600	1.37021200	0.81694200
P	-1.16155000	-0.04147600	0.35823900
O	0.00612100	0.31561500	-0.60966100
H	0.93777700	0.05095200	-0.25073900
O	-0.83004900	-0.89828100	1.51477700
C	-3.51114600	-2.87025300	0.17373100
C	-3.06626500	-3.68062200	-0.89507500
C	-3.06231200	-3.11560500	1.49025900
C	-2.14213400	-4.69430000	-0.62652700
C	-2.11346700	-4.12663100	1.68706600
C	-1.61942000	-4.91043300	0.64946100
H	-1.81332500	-5.33098500	-1.45248400
H	-1.73135200	-4.29584900	2.69789400
C	-0.08923100	3.48705400	0.24402800
C	1.15070800	3.16307200	-0.34741000
C	-0.14149600	3.92723600	1.58976100
C	2.30026900	3.23375200	0.46079900
C	1.03957800	4.04040400	2.31931600
C	2.27337900	3.66589000	1.78197100
H	3.24578000	2.90832600	0.02553300
H	0.99954000	4.39929200	3.35318800
C	-3.58365900	-3.57806100	-2.32918600
C	-3.37328600	-2.23377000	-3.03705400
C	-5.04515900	-4.02970800	-2.43372300
H	-2.99009300	-4.31702800	-2.89278800
H	-2.36251700	-1.83779100	-2.86995400
H	-3.52022600	-2.36867500	-4.11937200
H	-4.09733900	-1.47625200	-2.70523600
H	-5.18870700	-5.01780200	-1.97374200
H	-5.71303100	-3.31482800	-1.93237000
H	-5.35172500	-4.08986900	-3.48908700
C	-3.60199400	-2.46119000	2.76771400
C	-4.88855700	-3.18141300	3.19748100
C	-3.79989500	-0.94217500	2.84162700
H	-2.84023000	-2.69241500	3.52844700
H	-4.74306300	-4.27027900	3.23676400
H	-5.21016900	-2.83493700	4.19141400

H	-5.70436200	-2.97250500	2.48951200
H	-2.90831400	-0.39957100	2.50900900
H	-4.67153900	-0.58913300	2.27523700
H	-3.97354800	-0.67304000	3.89506200
C	-0.59135300	-5.99254700	0.91596100
C	0.55953200	-5.96885100	-0.09021200
C	-1.26458600	-7.36865500	0.96314700
H	-0.16436200	-5.77793500	1.90836400
H	1.04121300	-4.98232200	-0.08715400
H	1.30948400	-6.73003000	0.17343500
H	0.21007400	-6.19258400	-1.11062200
H	-2.06579500	-7.39591700	1.71571600
H	-1.71259000	-7.61104600	-0.01341300
H	-0.53272100	-8.15413000	1.20498800
C	1.44437400	2.71715800	-1.79017800
C	2.39184000	3.73201700	-2.45154700
C	0.30849400	2.41960700	-2.77275700
H	2.01843600	1.78065000	-1.67017000
H	2.65896300	3.39115200	-3.46313700
H	1.89519200	4.71123100	-2.54262200
H	3.32066700	3.86585900	-1.88286700
H	-0.46941000	1.76984300	-2.36070900
H	-0.16044300	3.34150000	-3.14453100
H	0.74470300	1.90397800	-3.64169500
C	-1.45250300	4.31346100	2.26280100
C	-1.49131300	5.81849900	2.54718500
C	-1.70804100	3.49782100	3.53290000
H	-2.27609500	4.09433800	1.57045900
H	-1.35420000	6.39696500	1.62218400
H	-2.45434600	6.10495500	2.99562000
H	-0.69177700	6.10781100	3.24665400
H	-1.68571900	2.42052800	3.31357400
H	-0.95738800	3.71886000	4.30902000
H	-2.69459500	3.74159100	3.95405600
C	3.53376200	3.75872600	2.62295400
C	4.14880200	5.15784500	2.49468700
C	4.56548700	2.67978100	2.29253700
H	3.22315100	3.62162300	3.67368600
H	3.42529800	5.93866500	2.76975100
H	5.03371700	5.25911200	3.14093100
H	4.45980200	5.33753400	1.45413000
H	4.13103200	1.67059400	2.34540600
H	4.97517000	2.80238700	1.27901800
H	5.40581400	2.73018400	3.00075400
O	0.98691000	-3.12461800	1.48682400
H	1.56822500	-3.22466300	2.25254200
H	0.31616300	-2.45993600	1.72111200
<b>TS1<sub>Re</sub></b>			
S	-5.42266400	-0.58012800	-0.43773000
O	-5.45198600	-0.06188100	0.93502300
O	-5.03288800	-1.96010900	-0.67621800
O	-3.44770800	2.21182800	3.15998200
N	-3.03219600	0.55017100	-1.17561400
N	-2.41941300	-0.11043500	-0.13732900
C	-7.01762400	-0.29307400	-1.16342300
C	-7.79163800	0.76568000	-0.69391200
H	-7.41919400	1.38977600	0.11968900
C	-9.03335900	0.99051700	-1.28372200
H	-9.65941800	1.81267500	-0.93540800
C	-9.47650200	0.15996400	-2.31507500
H	-10.45047100	0.34023300	-2.77238600
C	-8.68913900	-0.90208700	-2.76288700
H	-9.04781800	-1.55052500	-3.56290300
C	-7.44360100	-1.13864300	-2.18423200
H	-6.80500600	-1.96431300	-2.50188500
C	-4.39056100	0.48625200	-1.41471200

C	-4.72711800	1.31995200	-2.44799300
H	-5.72400700	1.46443400	-2.85506600
C	-3.50519200	1.93677700	-2.88064100
C	-2.46114000	1.44218300	-2.06055300
C	-1.12384300	1.83478600	-2.21211900
H	-0.33485200	1.44057800	-1.57143000
C	-0.86016000	2.73814600	-3.22652100
H	0.16937800	3.05912800	-3.38653700
C	-1.88155900	3.25379200	-4.05680700
H	-1.62004700	3.96537300	-4.84090800
C	-3.19810800	2.86576800	-3.89383700
H	-3.98591400	3.26150300	-4.53633000
C	-2.62176900	0.39104000	1.08820800
H	-3.46420600	1.07736800	1.13756000
C	-2.40119900	-0.44772600	2.28774500
C	-1.61893100	-1.60464000	2.24135100
H	-1.11322300	-1.90481700	1.31858800
C	-1.48402800	-2.39645900	3.37966200
H	-0.85515500	-3.28376400	3.33161000
C	-2.14594300	-2.05914100	4.55716100
H	-2.03810700	-2.68392800	5.44459700
C	-2.95280000	-0.92478300	4.60056700
H	-3.47305200	-0.66458900	5.52353400
C	-3.07194600	-0.10223400	3.47926300
C	-3.88892400	1.15739900	3.57091600
C	-5.28234900	1.04592300	4.12044200
H	-5.69265500	2.04703800	4.29213500
H	-5.32377100	0.44234800	5.03582300
H	-5.87233700	0.52209400	3.35023700
C	3.09462200	-1.79725700	-0.17744400
C	4.16018700	-1.05217300	-0.64507800
C	4.98222800	-1.62314000	-1.68030500
C	4.76962800	-2.97976900	-2.06301700
C	3.66935100	-3.69854300	-1.52095200
C	2.78546200	-3.10414800	-0.65755600
H	6.13006200	0.16940100	-2.12349000
C	5.98889900	-0.88417800	-2.36268200
C	5.60962400	-3.56928300	-3.04658000
H	3.48598800	-4.72033100	-1.86016700
C	6.59728900	-2.83935200	-3.66001700
C	6.77337100	-1.47610100	-3.32387100
H	5.43840300	-4.61316700	-3.31761000
H	7.23162100	-3.29951600	-4.41881800
H	7.53381800	-0.88601500	-3.83729400
C	4.38714100	0.32130900	-0.11877300
C	5.67447600	0.76127000	0.34835200
C	3.33380800	1.21860800	-0.07448600
C	6.77152700	-0.12786300	0.52455900
C	5.86396700	2.13572400	0.67167300
C	3.49569300	2.58272800	0.31457600
C	7.99332800	0.33223800	0.95385600
H	6.63096600	-1.18979400	0.32346700
C	7.14375000	2.58477300	1.09767000
C	4.75683100	3.02530000	0.62080000
C	8.19027700	1.70651900	1.23072400
H	8.81695100	-0.37021200	1.08922700
H	7.27158000	3.64361400	1.33202100
H	4.90771400	4.07217100	0.89482000
H	9.16672400	2.05995800	1.56469000
O	2.08451300	0.82493200	-0.48790300
O	2.29425600	-1.28493900	0.81830700
P	1.16070900	-0.17994100	0.42315900
O	0.11192200	-0.74069300	-0.49207200
H	-1.50521300	-0.58507100	-0.36699900
O	0.72193700	0.47744400	1.70715600
C	2.27184200	3.43124800	0.41793000

C	1.69772200	4.00072400	-0.74422400
C	1.64061200	3.58129900	1.66982200
C	0.45193300	4.62165600	-0.64183600
C	0.39560900	4.22874300	1.70749800
C	-0.23732000	4.71377400	0.56903600
H	-0.00040900	5.03602200	-1.54757300
H	-0.10533700	4.33660300	2.67571100
C	1.49870100	-3.73391300	-0.24218100
C	0.40682500	-3.77949200	-1.13662100
C	1.35754400	-4.20642000	1.07840200
C	-0.81099700	-4.28434600	-0.66101500
C	0.13451100	-4.74575600	1.48149700
C	-0.97574700	-4.76737600	0.63681400
H	-1.66548400	-4.28962200	-1.34321700
H	0.03641800	-5.14871100	2.49478800
C	2.40157400	4.08890200	-2.09884400
C	2.85129200	2.77639700	-2.75460900
C	3.56150400	5.09138600	-2.04615300
H	1.64779600	4.52995600	-2.77130800
H	2.09872800	1.98203200	-2.65620600
H	3.03393600	2.95367100	-3.82551600
H	3.79092800	2.40311200	-2.32418300
H	3.23041900	6.05920800	-1.64354800
H	4.37589600	4.71310600	-1.41199100
H	3.97026100	5.25532800	-3.05489800
C	2.22374700	3.21925800	3.04178600
C	2.98342900	4.43728100	3.58914200
C	3.06815500	1.95286700	3.22857500
H	1.33778700	3.08122500	3.68251800
H	2.36169400	5.34380400	3.57233100
H	3.31009900	4.25460400	4.62406900
H	3.88056300	4.63139800	2.98150900
H	2.61409600	1.08409600	2.74052300
H	4.09853100	2.07296900	2.87153800
H	3.12425000	1.74017700	4.30728800
C	-1.62831200	5.31647900	0.62977000
C	-2.61576700	4.52289700	-0.23432000
C	-1.61711800	6.79624400	0.23602600
H	-1.96534500	5.24630700	1.67777500
H	-2.63849300	3.46787400	0.07296300
H	-3.63004100	4.94131000	-0.14785900
H	-2.32550400	4.55036300	-1.29771300
H	-0.92518200	7.37076800	0.86802900
H	-1.29854000	6.91743000	-0.81075300
H	-2.62222500	7.23315500	0.33341300
C	0.40981000	-3.38038000	-2.61661900
C	0.71800000	-4.61036800	-3.48297400
C	1.24027300	-2.17925800	-3.08657300
H	-0.63941600	-3.11046100	-2.81643800
H	0.58645500	-4.37023300	-4.54887300
H	1.75967400	-4.93438400	-3.33914700
H	0.06220300	-5.45645100	-3.23194500
H	1.15512600	-1.33387800	-2.39459900
H	2.30080900	-2.42431100	-3.22600700
H	0.85285600	-1.85751900	-4.06545900
C	2.50558600	-4.16100500	2.07544000
C	3.02090000	-5.57238400	2.37472100
C	2.11649500	-3.42158400	3.35834800
H	3.33264500	-3.60085400	1.61877900
H	3.34858100	-6.07579600	1.45365800
H	3.87171100	-5.53626400	3.07147300
H	2.23249200	-6.18930000	2.83357500
H	1.71352700	-2.42486800	3.12676500
H	1.36361200	-3.98511800	3.93308700
H	2.99502300	-3.29604300	4.00847800
C	-2.30409700	-5.32394000	1.11647700

C	-2.48666700	-6.76621300	0.62979000
C	-3.49423800	-4.45377200	0.70940300
H	-2.25981100	-5.34445900	2.21918100
H	-1.65496200	-7.40586800	0.95781900
H	-3.42697900	-7.19259600	1.01044500
H	-2.51950100	-6.79381400	-0.47038100
H	-3.36251300	-3.40397100	1.00688700
H	-3.65155900	-4.46119100	-0.37904600
H	-4.41944800	-4.82620800	1.17344800
O	-1.36289900	1.78079700	1.34537700
H	-1.70233900	2.24392300	2.13213700
H	-0.45467200	1.31178800	1.56837800

**Int1<sub>R</sub>**

S	5.54154000	0.87687800	-0.29288000
O	5.45194800	0.25593200	1.03190100
O	5.22899700	2.28616500	-0.46396200
O	3.23404100	-2.28899200	2.82239900
N	3.21538800	-0.16075200	-1.27114100
N	2.57013900	0.45975900	-0.21991400
C	7.18726000	0.59056400	-0.90920500
C	7.89583500	-0.51951600	-0.45621900
H	7.44202000	-1.18537200	0.27921900
C	9.17587500	-0.74131300	-0.95940500
H	9.75134700	-1.60357100	-0.62064200
C	9.72195800	0.14296800	-1.89195100
H	10.72525100	-0.03497600	-2.28196500
C	8.99919500	1.25562300	-2.32500700
H	9.43715500	1.94584800	-3.04691000
C	7.71696200	1.48919300	-1.83099100
H	7.12628700	2.35343100	-2.13846000
C	4.57909400	-0.09393500	-1.42835300
C	4.98590800	-0.88650100	-2.47172700
H	6.00660700	-1.02000700	-2.81867500
C	3.79292000	-1.48394400	-2.99941700
C	2.70439100	-1.02238500	-2.21610200
C	1.37974400	-1.42238500	-2.44794000
H	0.56407000	-1.05882900	-1.82213600
C	1.17209500	-2.29841400	-3.49865100
H	0.15543900	-2.62706900	-3.71886800
C	2.23913800	-2.77794900	-4.29423700
H	2.02422400	-3.46797400	-5.11128900
C	3.54202300	-2.38127700	-4.05640800
H	4.36305600	-2.75118400	-4.67249300
C	2.51279000	-0.35866400	0.95362300
H	3.46675900	-0.89281700	0.98966800
C	2.36327200	0.45899700	2.21830500
C	1.65197100	1.65959000	2.22942500
H	1.18673500	2.03698400	1.31373000
C	1.52350900	2.38744200	3.41123900
H	0.95162000	3.31538500	3.40361400
C	2.11907300	1.93469100	4.58673700
H	2.02046400	2.50753800	5.50951300
C	2.84239400	0.74586000	4.58023500
H	3.30361600	0.39148800	5.50318800
C	2.95152300	-0.00981400	3.40759800
C	3.67444000	-1.32556300	3.42190400
C	4.99703500	-1.39276600	4.13386800
H	5.33748000	-2.43289600	4.18000200
H	4.95619800	-0.95324600	5.13836300
H	5.70068200	-0.79006900	3.53685800
C	-3.41490900	1.61006500	-0.07504100
C	-4.40345600	0.76157900	-0.53159300
C	-5.35365700	1.29565600	-1.47342200
C	-5.33577900	2.69370800	-1.75491000
C	-4.29168700	3.50721300	-1.23353000
C	-3.27879900	2.96892400	-0.48214100

H	-6.29239500	-0.59351700	-1.99861400
C	-6.30111600	0.48444200	-2.15737000
C	-6.30762000	3.24047800	-2.63648700
H	-4.25630100	4.56297300	-1.50814600
C	-7.23461100	2.43571300	-3.25100900
C	-7.21530200	1.03959200	-3.02093300
H	-6.28629400	4.31471800	-2.83098200
H	-7.97052600	2.86498400	-3.93212000
H	-7.92737600	0.39579300	-3.53897600
C	-4.42227800	-0.66182400	-0.09045800
C	-5.61347600	-1.29823500	0.40810900
C	-3.26207200	-1.41424300	-0.13750700
C	-6.81004300	-0.57948600	0.68326100
C	-5.59617000	-2.69990700	0.66477500
C	-3.20368700	-2.79546200	0.21429500
C	-7.93486500	-1.22579300	1.13733300
H	-6.82616900	0.50066000	0.54016500
C	-6.78057500	-3.34304000	1.11671000
C	-4.37789700	-3.42243000	0.54249100
C	-7.92943100	-2.62622500	1.34187700
H	-8.83792600	-0.65165700	1.34897300
H	-6.75089500	-4.41935900	1.29793100
H	-4.36776600	-4.48662300	0.79016900
H	-8.83103400	-3.12813200	1.69533100
O	-2.09115700	-0.84262100	-0.59225500
O	-2.48898900	1.14242900	0.84196300
P	-1.27533400	0.23471100	0.30015500
O	-0.23631600	0.88368500	-0.52726200
H	1.66590000	0.84697900	-0.51109900
O	-0.78947400	-0.44604900	1.61973700
C	-1.86083900	-3.44816700	0.28953200
C	-1.20416400	-3.88844800	-0.88691000
C	-1.21087600	-3.53296300	1.53840700
C	0.11789600	-4.32456200	-0.79619000
C	0.11761500	-3.99330800	1.56451700
C	0.81212300	-4.35866900	0.41620900
H	0.62476500	-4.64148100	-1.71186800
H	0.63140700	-4.04801000	2.53084600
C	-2.00493800	3.67603100	-0.15481300
C	-1.01649800	3.83149900	-1.15375300
C	-1.73951500	4.05872600	1.17490500
C	0.22267200	4.36121000	-0.77343400
C	-0.49701000	4.61366800	1.48852300
C	0.51244300	4.74886900	0.53484400
H	0.99808100	4.45342500	-1.53792700
H	-0.30238100	4.94042900	2.51464300
C	-1.88323100	-4.03902600	-2.24840700
C	-2.49807800	-2.78450500	-2.88122500
C	-2.90086600	-5.18665500	-2.22401300
H	-1.07317300	-4.35760700	-2.92380100
H	-1.83999900	-1.90971800	-2.79326400
H	-2.68102300	-2.97674900	-3.94945300
H	-3.46644800	-2.52554000	-2.43052000
H	-2.44705300	-6.11022000	-1.83747700
H	-3.76265100	-4.93319100	-1.58997200
H	-3.27803600	-5.38327300	-3.23903800
C	-1.82116600	-3.28292800	2.92500400
C	-2.30830700	-4.62565700	3.49170800
C	-2.90310600	-2.21741300	3.14403100
H	-0.96356800	-2.96730300	3.54075000
H	-1.51674900	-5.38777000	3.46737600
H	-2.64720900	-4.50499700	4.53162300
H	-3.15744100	-5.00194900	2.90037200
H	-2.68873800	-1.28001900	2.62069700
H	-3.90197000	-2.56490700	2.85308100
H	-2.94207000	-1.99315200	4.22070700

C	2.26277900	-4.80403200	0.47730100
C	3.15963300	-3.97167700	-0.44573900
C	2.38549100	-6.29765000	0.15828800
H	2.60835900	-4.64371000	1.51200500
H	3.13208100	-2.90590200	-0.17731800
H	4.20292600	-4.31453200	-0.37941700
H	2.84270800	-4.04834000	-1.49885000
H	1.75921200	-6.90025600	0.83127200
H	2.06460000	-6.50090000	-0.87509500
H	3.42839800	-6.63274100	0.25992800
C	-1.16247200	3.49847900	-2.64277700
C	-1.79076300	4.67155400	-3.40780300
C	-1.82180100	2.17245400	-3.04431000
H	-0.12241000	3.42375300	-2.99619800
H	-1.71800100	4.49941200	-4.49229100
H	-2.85649400	4.78072300	-3.16077600
H	-1.28585000	5.61936000	-3.17214100
H	-1.43095400	1.33756200	-2.45063500
H	-2.91642300	2.19130700	-2.96022700
H	-1.58482400	1.97434300	-4.10072900
C	-2.77438100	3.89396300	2.27702900
C	-3.35882200	5.25358600	2.67455000
C	-2.20876800	3.15202400	3.49076800
H	-3.59987700	3.28601300	1.88090900
H	-3.81311600	5.75618000	1.80842100
H	-4.12968600	5.13500700	3.45071000
H	-2.57304000	5.91409900	3.07305500
H	-1.74438500	2.20179200	3.18956600
H	-1.45351300	3.75763000	4.01607600
H	-3.01018900	2.93293200	4.21184100
C	1.86745900	5.31948000	0.91324400
C	1.93697400	6.80829800	0.55317900
C	3.03588800	4.55025700	0.29368700
H	1.95130700	5.23570700	2.01043500
H	1.12686500	7.37473900	1.03452700
H	2.89938100	7.24077500	0.86508400
H	1.84013500	6.94035300	-0.53565600
H	2.98649800	3.47037200	0.49138200
H	3.07207400	4.68343900	-0.79819700
H	3.99309100	4.91511600	0.69302800
O	1.47037700	-1.34112000	0.87759700
H	1.75719300	-2.09834400	1.42081600
H	0.12314000	-0.86650300	1.43781300

**TS2***1Re-Sa-3R*

S	-2.93152600	0.22843000	1.93524700
O	-2.22521000	1.12897500	2.82491500
O	-2.20128900	-0.53352900	0.91506500
O	-1.02230100	2.83112500	0.70398400
N	-3.97138900	1.57047600	-0.27102500
N	-2.71448800	1.57812700	-0.87440000
C	-3.86869900	-0.89519100	2.94685800
C	-3.62268600	-0.88245400	4.31595600
H	-2.93653000	-0.14302700	4.73057500
C	-4.25705200	-1.83527300	5.11315000
H	-4.07375700	-1.85008400	6.18796900
C	-5.11885200	-2.76734500	4.53612900
H	-5.61053200	-3.51149000	5.16438400
C	-5.36028500	-2.75520600	3.15952200
H	-6.03688200	-3.48563600	2.71335500
C	-4.72729100	-1.81594500	2.35134500
H	-4.88969400	-1.79525700	1.27334300
C	-4.18683000	1.09394400	1.01432100
C	-5.46164300	1.37608900	1.41990200
H	-5.90396600	1.08802100	2.36977100
C	-6.07798100	2.08966100	0.34731100
C	-5.11435700	2.22976600	-0.68794900

C	-5.41732800	2.96177800	-1.85387500
H	-4.69203400	3.14311300	-2.64293400
C	-6.68854400	3.49456100	-1.97029800
H	-6.93675300	4.06516300	-2.86606900
C	-7.66487200	3.32787700	-0.96471700
H	-8.65548600	3.76189400	-1.10219400
C	-7.36631800	2.63620000	0.19148800
H	-8.10620400	2.51751800	0.98420500
C	-2.59651600	1.29734500	-2.33643900
H	-3.46501600	1.72397100	-2.84909100
C	-1.29907800	2.00320300	-2.68802500
C	-0.59240700	1.71935300	-3.85155800
H	-1.03223200	1.06431000	-4.60600800
C	0.70283600	2.21457300	-4.00360900
H	1.26707500	1.98656700	-4.90909800
C	1.29911000	2.95173800	-2.97937100
H	2.32956900	3.29907900	-3.07633300
C	0.59171400	3.22972300	-1.81013000
H	1.06008800	3.76546000	-0.98415400
C	-0.71983200	2.78205200	-1.68643800
C	-1.51006300	3.07072400	-0.43594400
C	-2.48392900	4.22189700	-0.50578000
H	-3.21049200	4.14460200	0.31509700
H	-2.99514100	4.27769100	-1.47381400
H	-1.90044000	5.14340500	-0.36701600
C	1.61608200	-2.46827300	-0.13380900
C	2.99426700	-2.39893800	-0.20080700
C	3.69817900	-3.39730100	-0.96005700
C	2.97338000	-4.51055400	-1.47300400
C	1.55991700	-4.54002500	-1.34156100
C	0.86760500	-3.50386300	-0.76559900
H	5.65215000	-2.44481500	-0.89947300
C	5.09102200	-3.31440700	-1.24095100
C	3.66522300	-5.53167000	-2.18016100
H	1.00484700	-5.37345100	-1.77722300
C	5.01595900	-5.43932800	-2.40599400
C	5.73007900	-4.30752700	-1.94396600
H	3.09349000	-6.38266500	-2.55624300
H	5.53719400	-6.22392200	-2.95617200
H	6.79694200	-4.21873500	-2.15361400
C	3.70320000	-1.28072100	0.47087200
C	4.79917900	-1.51726900	1.37088200
C	3.29380400	0.02197000	0.24264300
C	5.16910300	-2.82028300	1.80875100
C	5.53384600	-0.40698600	1.87271800
C	3.98395500	1.14065800	0.79597100
C	6.23350200	-3.00420300	2.65828600
H	4.58999900	-3.67954000	1.47150900
C	6.63977700	-0.62837100	2.73814900
C	5.10801800	0.90698600	1.54757200
C	6.98984800	-1.89953900	3.11924000
H	6.49308900	-4.01163000	2.98663900
H	7.19543200	0.23722800	3.10465700
H	5.65018800	1.75750800	1.96876700
H	7.83614800	-2.06082900	3.78832100
O	2.22102000	0.26093600	-0.58785600
O	0.92879800	-1.51622400	0.59484500
P	0.69159000	-0.06046800	-0.09340500
O	0.36656100	0.89554800	1.05773300
C	3.48140600	2.53537400	0.61608300
C	3.88414800	3.29761700	-0.50476000
C	2.66123900	3.11210100	1.61312100
C	3.45171900	4.62488800	-0.61465600
C	2.21192800	4.42392600	1.40947100
C	2.59880400	5.20506300	0.32352900
H	3.79443800	5.20795500	-1.47226900



H	1.54568200	4.86224000	2.15921700
C	-0.61796600	-3.42393600	-0.84853300
C	-1.23466600	-3.08942900	-2.07667600
C	-1.39457400	-3.68236900	0.29569900
C	-2.63069200	-3.01676800	-2.10393000
C	-2.78770800	-3.62765400	0.20017700
C	-3.42440700	-3.27595900	-0.98692600
H	-3.11169600	-2.72079000	-3.04076700
H	-3.38954500	-3.84915500	1.08591600
C	4.86893600	2.82908800	-1.57845100
C	4.65627500	1.43671400	-2.18475600
C	6.31649500	2.99327600	-1.09664900
H	4.73458400	3.54698300	-2.40470500
H	3.59296300	1.21303300	-2.34682600
H	5.17606500	1.38561900	-3.15337000
H	5.07815300	0.64419700	-1.55141300
H	6.50220800	4.01411300	-0.73326000
H	6.53405200	2.29057300	-0.27923600
H	7.01874800	2.78234000	-1.91743900
C	2.26178600	2.53093700	2.98141100
C	2.97980800	3.33988100	4.07688900
C	2.43168000	1.04598700	3.31879300
H	1.18174400	2.74027600	3.05761600
H	2.79753000	4.41964100	3.99393400
H	2.64889300	3.00924000	5.07246800
H	4.06741100	3.17705200	4.01104500
H	2.02474000	0.37605600	2.55777800
H	3.47977400	0.78023900	3.50995000
H	1.87277800	0.85531300	4.24731700
C	2.04956700	6.61701600	0.19358900
C	0.54905200	6.57480100	-0.12184700
C	2.78903800	7.47720200	-0.82651800
H	2.16610400	7.09042700	1.18331100
H	0.01055200	5.95602900	0.61139400
H	0.11520800	7.58608000	-0.11090000
H	0.38287800	6.14126900	-1.12120500
H	3.86959700	7.50555200	-0.62622900
H	2.64029900	7.09466600	-1.84811300
H	2.40818800	8.50812500	-0.80224300
C	-0.55014700	-2.84307300	-3.42922500
C	-0.50880400	-4.14366100	-4.24489700
C	0.81273700	-2.14128000	-3.48347100
H	-1.24954300	-2.17019000	-3.95343500
H	-0.17446000	-3.93922700	-5.27330300
H	0.19936400	-4.85861400	-3.80059500
H	-1.49686100	-4.62382200	-4.28800400
H	0.84162300	-1.25419600	-2.83992200
H	1.64542100	-2.80441100	-3.21494400
H	0.98661200	-1.81337000	-4.52043800
C	-0.76013900	-4.06320200	1.62468300
C	-1.01152900	-5.54243000	1.93506500
C	-1.23340500	-3.16322700	2.76856400
H	0.32634200	-3.92660000	1.53587300
H	-0.62482300	-6.18600700	1.13134900
H	-0.52178600	-5.83182000	2.87704800
H	-2.08987000	-5.74187100	2.03722300
H	-1.05663200	-2.10711000	2.52167500
H	-2.30895700	-3.30126900	2.97002600
H	-0.68976300	-3.40617200	3.69411300
C	-4.93087300	-3.11705600	-1.06867600
C	-5.55874600	-4.05406000	-2.10336300
C	-5.29654500	-1.65508400	-1.35794000
H	-5.34044800	-3.39557200	-0.08173900
H	-5.31679700	-5.10383700	-1.88587200
H	-6.65346000	-3.94335200	-2.11709000
H	-5.18615700	-3.82319900	-3.11263800

H	-4.78395200	-0.97052800	-0.66430900
H	-4.96357700	-1.36793300	-2.36630100
H	-6.38292700	-1.49144000	-1.28656100
O	-2.59140500	-0.04802800	-2.62126800
H	-1.77543600	-0.42910200	-2.22975200
H	-0.25775600	1.82883700	0.86964800
O	-0.22249700	-0.10452000	-1.26244500
H	-2.16303100	0.82225600	-0.42880000

**TS3<sub>1Re-Ra-3R</sub>**

S	5.69369800	-1.36797600	-1.46209900
O	5.34735100	-0.33015200	-2.44079500
O	5.45286000	-2.76817400	-1.79448600
O	1.08957900	-2.34985900	1.28240900
N	3.54587400	-0.55578200	0.19602100
N	2.43019700	-0.99319100	-0.51977900
C	7.41029100	-1.18838000	-1.06152100
C	7.99701300	0.07042900	-1.17437500
H	7.39986700	0.92088700	-1.50673700
C	9.34775700	0.19784900	-0.86238700
H	9.83355300	1.17062000	-0.94381200
C	10.07886000	-0.91973500	-0.45256500
H	11.13701100	-0.81256300	-0.20983300
C	9.47277100	-2.17314300	-0.35912200
H	10.05463700	-3.04185800	-0.04975200
C	8.12180700	-2.31920100	-0.66998800
H	7.61953400	-3.28637700	-0.62362300
C	4.88110000	-0.93886200	0.06089200
C	5.55429200	-0.70273800	1.23288700
H	6.62303000	-0.82304900	1.38442700
C	4.60527800	-0.19457400	2.17280200
C	3.36718700	-0.10913000	1.50284900
C	2.20861500	0.36983200	2.13007700
H	1.25682500	0.45657000	1.60786000
C	2.32918600	0.74885800	3.45337500
H	1.44692400	1.13602600	3.96451700
C	3.55773300	0.66063300	4.14867800
H	3.60012600	0.96843900	5.19425500
C	4.69959600	0.20461700	3.52114000
H	5.65225400	0.14736200	4.04908400
C	2.53777500	-1.24854200	-1.99315000
H	3.39556500	-1.91974700	-2.14847000
C	1.26547800	-2.01724900	-2.23818000
C	0.57270100	-2.02583900	-3.43741800
H	0.95828000	-1.46709500	-4.29066800
C	-0.63464500	-2.72487300	-3.50104900
H	-1.20035200	-2.74687400	-4.43365800
C	-1.14525800	-3.35934300	-2.36932600
H	-2.10228300	-3.87679900	-2.42223200
C	-0.46015100	-3.31721700	-1.15214400
H	-0.89128100	-3.75835500	-0.25139800
C	0.76658200	-2.66752100	-1.11002600
C	1.62804400	-2.55865400	0.11771500
C	2.80911500	-3.49410400	0.20855500
H	3.44729700	-3.18665800	1.04964800
H	3.39779200	-3.54989200	-0.71530900
H	2.40442700	-4.49229300	0.43086900
C	-2.02843100	2.33905500	-0.17851400
C	-3.27746200	2.20420600	-0.75356600
C	-3.65011100	3.11711000	-1.79824200
C	-2.79527600	4.21899100	-2.08685000
C	-1.55412100	4.34047300	-1.40547400
C	-1.12388000	3.38823000	-0.51581300
H	-5.47452400	2.09535500	-2.38678800
C	-4.83242900	2.95682600	-2.57253700
C	-3.17296200	5.14927500	-3.09318200
H	-0.90107900	5.18267000	-1.64441300

C	-4.33294600	4.98116400	-3.80831900
C	-5.16306300	3.86347100	-3.55131600
H	-2.51062400	5.99336700	-3.29650800
H	-4.60953900	5.69672500	-4.58385500
H	-6.07012400	3.71688700	-4.13940400
C	-4.18027400	1.12941800	-0.26325700
C	-5.51309400	1.42084300	0.19382300
C	-3.71278300	-0.16983100	-0.16518000
C	-6.02472300	2.74658800	0.28909200
C	-6.35532000	0.34888400	0.60639600
C	-4.52250300	-1.23492700	0.32963200
C	-7.31011900	2.98084800	0.71505300
H	-5.38148600	3.58667200	0.03037400
C	-7.68517600	0.62068600	1.02945700
C	-5.82814300	-0.96806800	0.65553600
C	-8.15995800	1.90736600	1.07512400
H	-7.67564000	4.00640900	0.78410800
H	-8.31596700	-0.21791300	1.33153100
H	-6.46122200	-1.77662200	1.02925100
H	-9.18017800	2.10728900	1.40538500
O	-2.43974700	-0.47196300	-0.59382000
O	-1.64004400	1.44120900	0.79142700
P	-1.11429300	-0.01535600	0.25388600
O	-0.90849100	-0.90322300	1.45746300
C	-3.93010400	-2.58606300	0.55480500
C	-3.96447400	-3.56595700	-0.45990400
C	-3.35418700	-2.88015600	1.81107900
C	-3.38820900	-4.81874000	-0.21338700
C	-2.74782600	-4.13128900	1.97738100
C	-2.74827500	-5.11443400	0.98985900
H	-3.43849400	-5.57402100	-1.00184700
H	-2.27868300	-4.35515500	2.94120300
C	0.23388300	3.43303900	0.10067500
C	1.39551300	3.20771600	-0.67259400
C	0.34953300	3.70771900	1.48005800
C	2.63454700	3.25670000	-0.01976400
C	1.61650700	3.80517400	2.06083300
C	2.78109100	3.57605400	1.33074100
H	3.52763800	3.04347100	-0.61543000
H	1.68108800	4.04886400	3.12230000
C	-4.68088600	-3.40038500	-1.80106500
C	-4.45195500	-2.08936200	-2.56615200
C	-6.18126800	-3.68620000	-1.65520400
H	-4.27663100	-4.20747500	-2.43501300
H	-3.41718200	-1.73062800	-2.47422400
H	-4.67168300	-2.25149900	-3.63241700
H	-5.12072100	-1.29127000	-2.21580300
H	-6.35694600	-4.65937100	-1.17498400
H	-6.66497900	-2.90833000	-1.04711500
H	-6.66714800	-3.69144300	-2.64276200
C	-3.45530800	-2.05383400	3.10079800
C	-4.60271000	-2.63900300	3.94174900
C	-3.59194000	-0.52843900	3.07988200
H	-2.51220900	-2.26364800	3.62972000
H	-4.48933300	-3.72137800	4.09478500
H	-4.64797100	-2.14854300	4.92565600
H	-5.56581400	-2.46899300	3.43494000
H	-2.84550400	-0.04416900	2.44527500
H	-4.59287400	-0.19480700	2.77681300
H	-3.42880300	-0.16647400	4.10679900
C	-2.02927900	-6.42871800	1.24628500
C	-0.51865000	-6.26633600	1.02797200
C	-2.56833300	-7.59556400	0.42225600
H	-2.18540800	-6.66621800	2.31185000
H	-0.12008900	-5.42166600	1.61039100
H	0.01945200	-7.17933500	1.32463900

H	-0.30624100	-6.07618800	-0.03609500
H	-3.65706300	-7.69945300	0.53368000
H	-2.34507800	-7.46371500	-0.64744800
H	-2.09692000	-8.53666300	0.73994700
C	1.49137800	2.98604800	-2.18739700
C	1.87959300	4.30442900	-2.87421600
C	0.34941800	2.30969900	-2.95255000
H	2.34941900	2.30529700	-2.29216500
H	2.07657200	4.13301400	-3.94333800
H	1.06238600	5.03808000	-2.79850000
H	2.77570700	4.75292600	-2.42128700
H	-0.07458600	1.47030400	-2.39042200
H	-0.45302800	3.00974900	-3.21948400
H	0.76388600	1.91027600	-3.89064000
C	-0.86107400	3.94475200	2.37262300
C	-0.89872900	5.39267600	2.87251100
C	-0.90106000	2.94987000	3.53684800
H	-1.77062600	3.78576800	1.77970100
H	-0.91169700	6.09939200	2.03016700
H	-1.79608200	5.56732800	3.48479300
H	-0.01765500	5.62182700	3.49166400
H	-0.85882000	1.91591700	3.16435800
H	-0.06052600	3.11609400	4.22992500
H	-1.83170100	3.06812100	4.11188300
C	4.16876800	3.62959200	1.95585000
C	4.16427000	4.06799600	3.41804500
C	5.11057900	4.53410700	1.15184700
H	4.56798000	2.59887100	1.91708800
H	3.54670600	3.40924100	4.04263800
H	5.18724600	4.04921800	3.82133400
H	3.78048700	5.09582500	3.51641400
H	5.19961800	4.21645300	0.10443600
H	4.73746100	5.56988300	1.15731200
H	6.11858400	4.53111600	1.59285200
O	2.63495000	-0.11367700	-2.74984400
H	3.58127800	0.08041100	-2.86709300
H	0.20143500	-1.78114500	1.31845100
O	0.05006800	0.16702400	-0.67030100
H	1.62626700	-0.30261700	-0.43130100

**TS4***ISI-Sa-3R*

S	5.64001600	-0.36198200	-0.25886600
O	5.07489400	0.15235000	-1.50200400
O	5.91526700	-1.77575600	-0.05779300
O	1.05249200	2.61242500	-0.57433200
N	3.28029600	0.51022100	1.16747800
N	2.30689200	0.48780200	0.17818900
C	7.19545200	0.47982700	0.00897900
C	7.37490100	1.76619900	-0.49437900
H	6.56981400	2.25529400	-1.04433100
C	8.60085900	2.39668300	-0.29634400
H	8.76142400	3.40357900	-0.68318200
C	9.62491500	1.73646600	0.38551300
H	10.58367500	2.23471700	0.53614700
C	9.43493600	0.43971500	0.86337500
H	10.24390600	-0.07766800	1.38046300
C	8.21282400	-0.20294200	0.67082800
H	8.03717800	-1.22366600	1.01303900
C	4.65782200	0.28560700	1.10196600
C	5.22457200	0.61862500	2.30445200
H	6.27983300	0.53089700	2.54689900
C	4.18611200	1.11003000	3.15449800
C	2.98650900	1.05073900	2.41373100
C	1.76509800	1.51899200	2.92545500
H	0.84062600	1.48131600	2.34992200
C	1.78307400	2.01904800	4.21643100
H	0.85120600	2.38683400	4.64772700

C	2.96699000	2.06617900	4.98530900
H	2.92911400	2.46743000	5.99861800
C	4.16736700	1.61961100	4.46701000
H	5.08641500	1.66334600	5.05287800
C	2.24209600	-0.73039900	-0.72732200
H	1.26272800	-1.19558700	-0.51418600
C	2.25788200	-0.16057600	-2.12121300
C	2.31721600	-0.93930400	-3.27085900
H	2.40992200	-2.02271800	-3.18271000
C	2.25629800	-0.31478100	-4.51464000
H	2.30121200	-0.91446900	-5.42474100
C	2.13041300	1.07356100	-4.60314800
H	2.07124700	1.55316000	-5.58097400
C	2.08292800	1.85036500	-3.44723100
H	1.98805200	2.93645200	-3.50908300
C	2.15997900	1.22193800	-2.20552800
C	2.16128000	1.99800100	-0.91662500
C	3.39494200	2.79428700	-0.59854200
H	3.39924300	3.08376300	0.46244000
H	3.35199600	3.71072000	-1.20580200
H	4.29326000	2.22716500	-0.85985700
C	-2.54654400	-1.97500800	0.17102400
C	-3.83108800	-1.63864600	0.56493500
C	-4.52919800	-2.54332900	1.43980900
C	-3.97046300	-3.82758000	1.69837300
C	-2.68898100	-4.14833600	1.17808200
C	-1.93816700	-3.22376900	0.49572900
H	-6.17380300	-1.20854600	1.92766800
C	-5.75573100	-2.20398800	2.07643100
C	-4.67783200	-4.74822200	2.51894700
H	-2.27057700	-5.13719900	1.37432300
C	-5.87382000	-4.40078100	3.09592600
C	-6.40696500	-3.10671000	2.88265800
H	-4.23866300	-5.73250400	2.69497300
H	-6.40526400	-5.11028400	3.73152100
H	-7.34089700	-2.82006600	3.36804900
C	-4.45543400	-0.37239000	0.09156600
C	-5.76664900	-0.33956900	-0.50419300
C	-3.76233400	0.81779600	0.19160500
C	-6.49559600	-1.51698100	-0.83135100
C	-6.35914400	0.92169900	-0.80565600
C	-4.30257600	2.07761500	-0.20501500
C	-7.75566200	-1.44242900	-1.37585900
H	-6.04003000	-2.49106400	-0.65580900
C	-7.67042500	0.96645200	-1.35215500
C	-5.60469000	2.11482200	-0.63009600
C	-8.36110200	-0.18809900	-1.62528100
H	-8.29011400	-2.36030700	-1.62481500
H	-8.11028600	1.94261300	-1.56658700
H	-6.05479200	3.07001300	-0.91003500
H	-9.36442500	-0.14238800	-2.05080800
O	-2.51051900	0.82717000	0.75340000
O	-1.82825100	-1.12733500	-0.63605400
P	-1.20709200	0.26284800	-0.03783100
O	-0.81205400	1.08947400	-1.23222500
C	-3.36157200	3.23650200	-0.22997000
C	-3.04320600	3.94458100	0.95272100
C	-2.67325500	3.50554800	-1.43160900
C	-1.99168700	4.86183700	0.92132400
C	-1.62479600	4.43629200	-1.39647400
C	-1.24561700	5.09955800	-0.23537300
H	-1.74436200	5.39953200	1.84081700
H	-1.06800000	4.62872600	-2.31859500
C	-0.53187100	-3.53095300	0.09607000
C	0.46918900	-3.71173000	1.07680100
C	-0.21700000	-3.70625000	-1.27236500

C	1.74161100	-4.13133300	0.65180200
C	1.07078900	-4.10981500	-1.63712000
C	2.06559600	-4.35470700	-0.68804800
H	2.50935700	-4.30669400	1.41432800
H	1.28992900	-4.26797200	-2.69657400
C	-3.82847900	3.83759800	2.25921100
C	-3.85908200	2.46228700	2.93606200
C	-5.24563800	4.40253900	2.10570400
H	-3.29862000	4.50631400	2.95616600
H	-2.86370300	2.00082000	2.96582200
H	-4.22434200	2.57834000	3.96772000
H	-4.54083600	1.76601500	2.42777500
H	-5.22531000	5.41182300	1.67024800
H	-5.85719200	3.75890200	1.45756800
H	-5.74235000	4.45798200	3.08631700
C	-3.01467300	2.95985600	-2.82392000
C	-4.08639600	3.85770800	-3.45989900
C	-3.38340000	1.48392900	-3.02333400
H	-2.08830700	3.10766400	-3.40094000
H	-3.79812200	4.91800700	-3.42242600
H	-4.25091300	3.57600200	-4.51102500
H	-5.04405200	3.74814700	-2.92866900
H	-2.68579000	0.81566800	-2.50737200
H	-4.40912900	1.25079600	-2.71051200
H	-3.31942600	1.26351900	-4.10022200
C	-0.07825600	6.06775100	-0.23456100
C	0.93017300	5.74504900	0.87098400
C	-0.56600000	7.51658500	-0.13470100
H	0.43431800	5.94629400	-1.20333800
H	1.24661000	4.69533700	0.80631500
H	1.81545600	6.39398900	0.78829700
H	0.49210100	5.91146800	1.86707700
H	-1.26027000	7.75899800	-0.95167800
H	-1.09619900	7.67906300	0.81657200
H	0.27977600	8.21958600	-0.17544600
C	0.32088900	-3.53639600	2.59309800
C	0.05576400	-4.87931000	3.28840700
C	-0.63228400	-2.45438900	3.11139600
H	1.32820900	-3.22312400	2.91340800
H	0.14462900	-4.76057900	4.37849400
H	-0.96154500	-5.23868800	3.07768400
H	0.76756000	-5.65274500	2.96541100
H	-0.55762100	-1.53213100	2.52112700
H	-1.67952100	-2.78389400	3.12018700
H	-0.35756900	-2.21874600	4.15078200
C	-1.25165000	-3.52672700	-2.37420500
C	-1.53878000	-4.86033500	-3.07263300
C	-0.82638600	-2.44863700	-3.37451700
H	-2.19166600	-3.19411400	-1.91765200
H	-1.87663400	-5.61950200	-2.35228500
H	-2.32298400	-4.73287900	-3.83337500
H	-0.64061600	-5.24855900	-3.57718300
H	-0.60313200	-1.49966900	-2.86516000
H	0.06596700	-2.75898300	-3.94117800
H	-1.63238600	-2.26429900	-4.10037600
C	3.43325900	-4.89797900	-1.06810200
C	4.06612900	-4.20506300	-2.27600400
C	3.33298200	-6.41217500	-1.29250500
H	4.09851800	-4.72660700	-0.20510100
H	4.21107600	-3.13268400	-2.08941300
H	5.05016500	-4.64881000	-2.48522200
H	3.45160000	-4.33642900	-3.18106400
H	2.91434800	-6.91936800	-0.41171400
H	2.67643200	-6.62860000	-2.14965300
H	4.32387200	-6.84035300	-1.50398000
O	3.25892100	-1.60893900	-0.47677900

H	2.94051300	-2.32673500	0.09053600
H	0.22349900	2.09332900	-0.91418500
O	-0.15152600	0.00869300	1.00535100
H	1.35617800	0.46977200	0.66048100
<b>TS5<sub>1Si-Ra-3R</sub></b>			
S	-2.94293100	-0.31099700	1.82110400
O	-2.30952300	0.97702200	1.44452200
O	-2.16601800	-1.52964800	1.66524000
O	-2.05622600	-2.65864900	-1.01674700
N	-4.47531200	-0.33319000	-0.39143500
N	-3.32187800	-0.38894200	-1.09637200
C	-3.44647100	-0.17231100	3.51880900
C	-3.78357500	1.08072300	4.02718300
H	-3.72467300	1.96187700	3.38599300
C	-4.18484600	1.16846200	5.35776000
H	-4.45221300	2.13709700	5.78127200
C	-4.23724300	0.01838200	6.14854500
H	-4.55047500	0.09415200	7.19084200
C	-3.88593500	-1.22486400	5.62154300
H	-3.92036500	-2.11571700	6.24945900
C	-3.48220400	-1.32982100	4.29135400
H	-3.18653300	-2.28327400	3.85050900
C	-4.48729100	-0.37866400	0.98355900
C	-5.76330500	-0.40286600	1.48241100
H	-6.05213800	-0.42431700	2.52950000
C	-6.61954100	-0.37935800	0.33262800
C	-5.78942700	-0.33415100	-0.81735800
C	-6.32839200	-0.31209500	-2.11314700
H	-5.68140900	-0.28019300	-2.98786400
C	-7.70458600	-0.33080200	-2.23557200
H	-8.15137400	-0.31294000	-3.23066800
C	-8.54848000	-0.36810200	-1.10072800
H	-9.62986300	-0.37765500	-1.24124600
C	-8.02047100	-0.39211700	0.17511000
H	-8.67105000	-0.42140300	1.05053400
C	-2.83238400	0.76292800	-1.80445400
H	-2.30164300	1.44789800	-1.11803000
C	-1.90226900	0.16787900	-2.83924200
C	-1.11087500	0.92108100	-3.70082700
H	-1.07749000	2.00692200	-3.58901000
C	-0.34919300	0.27479800	-4.67479700
H	0.28502600	0.85994100	-5.34299600
C	-0.38563900	-1.11597900	-4.79028800
H	0.21334100	-1.61574300	-5.55359900
C	-1.17315500	-1.87071400	-3.92076600
H	-1.19415300	-2.96072000	-3.99583200
C	-1.93221200	-1.22249400	-2.94884800
C	-2.74426900	-1.96416800	-1.92435200
C	-3.94777200	-2.73629700	-2.38416000
H	-3.60745900	-3.70944800	-2.77038400
H	-4.49396900	-2.20730800	-3.17173900
H	-4.61393800	-2.92277500	-1.52940800
C	2.63199700	1.79332300	0.16617700
C	3.83472000	1.24310100	0.56661000
C	4.70001700	2.04380900	1.39135800
C	4.36834200	3.41013400	1.62281600
C	3.15153900	3.93473300	1.10930000
C	2.25209700	3.13855600	0.44942500
H	6.11000500	0.46408800	1.88159200
C	5.86700700	1.51848500	2.01282800
C	5.23669400	4.21558800	2.40904900
H	2.90140400	4.98104400	1.30069600
C	6.37037500	3.68592800	2.97361100
C	6.67777100	2.31745000	2.78311200
H	4.97311600	5.26340100	2.56686200
H	7.02588100	4.31102500	3.58144000

H	7.56262000	1.89054100	3.25718300
C	4.18809200	-0.14264400	0.15547000
C	5.43951700	-0.45352400	-0.48427700
C	3.28304300	-1.16954800	0.33632800
C	6.36886500	0.54636900	-0.88634500
C	5.75959100	-1.81603400	-0.75310700
C	3.54433200	-2.52327800	-0.02573100
C	7.56491400	0.20605300	-1.47184200
H	6.12032100	1.59628900	-0.73426200
C	7.01213300	-2.13752200	-1.34380500
C	4.79521900	-2.82865800	-0.49669400
C	7.90166300	-1.15122700	-1.69008000
H	8.25797300	0.99110800	-1.77740300
H	7.24343900	-3.18801400	-1.53174600
H	5.03877200	-3.86429900	-0.74233900
H	8.85731800	-1.40795800	-2.14897900
O	2.07170400	-0.91638200	0.94070300
O	1.74263500	1.02941000	-0.57050900
P	0.88398400	-0.09668400	0.22481300
O	-0.01544800	-0.83359200	-0.68296000
C	2.39557300	-3.47684400	0.01320000
C	1.97942000	-4.07798300	1.22262000
C	1.63950600	-3.64780600	-1.16830300
C	0.77079600	-4.77760600	1.23983500
C	0.44128400	-4.36774900	-1.08530400
C	-0.03301900	-4.90703300	0.10631100
H	0.44516600	-5.22641100	2.18227700
H	-0.16715400	-4.47825600	-1.98669800
C	0.91645100	3.60630900	-0.02566600
C	-0.19991400	3.68827300	0.83619400
C	0.77029400	3.87238900	-1.40454000
C	-1.44564800	3.96033500	0.25492600
C	-0.48815100	4.19852900	-1.91544600
C	-1.62192700	4.22795500	-1.10278000
H	-2.32696800	3.96453900	0.90378900
H	-0.57891300	4.42381900	-2.98035600
C	2.79804500	-4.07887300	2.51281900
C	3.05445900	-2.71294400	3.15946900
C	4.10522200	-4.86423500	2.35392500
H	2.18088700	-4.64192100	3.23077600
H	2.13881700	-2.10990600	3.20899000
H	3.43176700	-2.86421400	4.18221400
H	3.81494500	-2.13409900	2.61653200
H	3.92065700	-5.85798300	1.92124400
H	4.81148400	-4.32962800	1.70308800
H	4.59010700	-4.99792500	3.33289700
C	2.03803000	-3.18053000	-2.57356100
C	3.08789500	-4.11525800	-3.19005600
C	2.42436500	-1.71185000	-2.78238200
H	1.12028600	-3.32029800	-3.16562500
H	2.80079600	-5.17011200	-3.07281300
H	3.19866300	-3.90304200	-4.26449200
H	4.07247400	-3.97211400	-2.72350800
H	1.67008400	-1.03707500	-2.35598000
H	3.41416200	-1.46107900	-2.37659600
H	2.46352600	-1.51341000	-3.86512100
C	-1.36641200	-5.62732200	0.15925900
C	-2.27789200	-5.06041800	1.25087800
C	-1.16783500	-7.13709300	0.32676600
H	-1.85891500	-5.44614400	-0.80950200
H	-2.40882500	-3.97722000	1.12300500
H	-3.26481600	-5.54693800	1.21238400
H	-1.85631600	-5.24731100	2.25138400
H	-0.54374400	-7.54913000	-0.47915100
H	-0.66942200	-7.35769400	1.28371400
H	-2.13507600	-7.66209000	0.32095500



C	-0.23321400	3.57642200	2.36906000
C	-0.61808600	4.94715700	2.95293000
C	0.97466300	3.05545000	3.15458600
H	-1.06664900	2.88297800	2.57442000
H	-0.72759600	4.88076200	4.04592100
H	0.17264200	5.68242800	2.73583600
H	-1.55648500	5.33413200	2.53348100
H	1.40249800	2.13728400	2.74088000
H	1.76824400	3.81101600	3.23051500
H	0.63901200	2.83650600	4.17975500
C	1.96114000	3.86101900	-2.35503900
C	2.23611700	5.27054100	-2.89021200
C	1.78315000	2.85645400	-3.49513100
H	2.85119900	3.55273200	-1.79048700
H	2.40439300	5.97965600	-2.06677700
H	3.12626500	5.27233800	-3.53693700
H	1.38622700	5.64047300	-3.48429300
H	1.59252400	1.84839500	-3.10028500
H	0.94140500	3.14125700	-4.14754700
H	2.68851700	2.82257800	-4.11989400
C	-3.00897300	4.57763000	-1.61892300
C	-3.10879400	4.60895300	-3.14023900
C	-3.47458000	5.91432400	-1.02748400
H	-3.68643200	3.78278800	-1.26568600
H	-2.78480400	3.65534400	-3.57830000
H	-4.15211300	4.77732400	-3.44312200
H	-2.50210700	5.42381800	-3.56598600
H	-3.45998200	5.89974200	0.07151600
H	-2.81367200	6.72954400	-1.36074200
H	-4.49940000	6.14715600	-1.35289600
O	-3.82564100	1.56593200	-2.40661400
H	-4.08856600	1.15716100	-3.24021900
H	-1.27385800	-2.13697700	-0.72295800
O	0.24722600	0.60337600	1.46975600
H	-0.72975800	0.81255200	1.38999400

**Int2**<sub>IS-Sa-3R</sub>

S	-3.22628200	-0.25956200	1.71400000
O	-2.26286000	0.54517400	2.43827600
O	-2.79947700	-1.19735800	0.66281600
O	-1.71799700	2.74140100	0.65344400
N	-4.27932200	1.30875800	-0.27504500
N	-3.04964700	1.45172300	-0.84997200
C	-4.13921800	-1.22187100	2.89989900
C	-4.11324400	-0.82151800	4.23185200
H	-3.55024300	0.06910400	4.51459700
C	-4.79927300	-1.59287800	5.17001900
H	-4.79202700	-1.30141900	6.22082300
C	-5.48241800	-2.73954200	4.76556100
H	-6.01308700	-3.34160900	5.50456900
C	-5.48707700	-3.12955500	3.42371900
H	-6.01548400	-4.03289500	3.11675800
C	-4.80875500	-2.36884100	2.47565600
H	-4.78630400	-2.65613100	1.42268400
C	-4.50163400	0.71631400	0.95418600
C	-5.81740100	0.82424300	1.31420600
H	-6.27210500	0.41656100	2.21278700
C	-6.46864100	1.52661300	0.24369900
C	-5.48409100	1.80940000	-0.73268500
C	-5.78941800	2.46207200	-1.93601200
H	-5.02042100	2.66260000	-2.68242600
C	-7.10692500	2.83605000	-2.13585500
H	-7.38172500	3.34364800	-3.06145900
C	-8.10451500	2.57340300	-1.17042800
H	-9.13034800	2.88661800	-1.36716500
C	-7.79968600	1.92353400	0.01154900
H	-8.57312000	1.71688400	0.75270400

C	-2.74875400	0.74975000	-2.07675900
H	-3.64939600	0.65741400	-2.70952900
C	-1.65076800	1.59972600	-2.66260500
C	-0.91325800	1.37066200	-3.82039900
H	-1.19010800	0.57295500	-4.51260300
C	0.22021500	2.15157200	-4.04794800
H	0.81914800	1.98836400	-4.94499300
C	0.61795200	3.11345200	-3.11301500
H	1.52993500	3.69142000	-3.27851100
C	-0.13046000	3.33729100	-1.95682300
H	0.18957700	4.05850200	-1.20644500
C	-1.28186900	2.58777700	-1.75925800
C	-2.26440200	2.70322900	-0.60865000
C	-3.10597300	3.97077400	-0.73122400
H	-3.90633000	3.96220200	0.02227800
H	-3.53543300	4.08569100	-1.73325000
H	-2.44861700	4.82538600	-0.52175500
C	2.19626100	-2.35684000	-0.08716300
C	3.51550000	-1.97201100	0.01399700
C	4.51614500	-2.86194600	-0.51483200
C	4.12192000	-4.16324900	-0.94174500
C	2.74242100	-4.51152700	-0.96723300
C	1.76999200	-3.60356200	-0.63655600
H	6.19280200	-1.48943800	-0.35655100
C	5.88439600	-2.49606600	-0.63921600
C	5.10921400	-5.07034700	-1.41319900
H	2.45515600	-5.49966900	-1.33123300
C	6.42829300	-4.69726900	-1.49488600
C	6.81382000	-3.38914800	-1.11768900
H	4.79207300	-6.06681900	-1.72766000
H	7.17634700	-5.39912800	-1.86590300
H	7.85676900	-3.08383300	-1.21256600
C	3.85777300	-0.67683400	0.66267000
C	4.83901800	-0.61885500	1.71469600
C	3.21789600	0.49687400	0.29494500
C	5.39819600	-1.78365600	2.31342100
C	5.25273800	0.65009400	2.20836900
C	3.58006800	1.76865900	0.82579700
C	6.34542000	-1.68423500	3.30382100
H	5.05808600	-2.76646400	1.98942200
C	6.24859300	0.72301500	3.22080500
C	4.61967400	1.82194600	1.72161900
C	6.79186000	-0.41827400	3.75428600
H	6.75128900	-2.59167000	3.75308200
H	6.55837300	1.70816200	3.57535900
H	4.92846800	2.79273300	2.11660400
H	7.55019300	-0.35480900	4.53574600
O	2.23061500	0.47509000	-0.67248100
O	1.21877600	-1.52475100	0.41174700
P	0.78656400	-0.20290100	-0.41114900
O	-0.20602100	0.56354500	0.36154800
C	2.83798800	3.02652800	0.49845300
C	3.20791000	3.81521500	-0.62045100
C	1.85346500	3.48837200	1.39764400
C	2.60034900	5.06075400	-0.79290900
C	1.24904800	4.73140000	1.14189000
C	1.61762800	5.54266200	0.07660500
H	2.91475100	5.67641200	-1.64120300
H	0.46934500	5.07702400	1.82692300
C	0.31030900	-3.80206800	-0.87050500
C	-0.20887000	-3.78432900	-2.18314300
C	-0.56520000	-3.85146400	0.23928900
C	-1.60380600	-3.77684800	-2.34060400
C	-1.93820500	-3.86627100	0.01833600
C	-2.48473500	-3.78978900	-1.26365200
H	-1.99820100	-3.71328900	-3.35630100

H	-2.60914000	-3.86336300	0.88113500
C	4.31786800	3.46919600	-1.61445900
C	4.26939900	2.07927000	-2.25704700
C	5.70685500	3.75155600	-1.02695700
H	4.17905300	4.18902700	-2.43766400
H	3.24916300	1.79585400	-2.54813600
H	4.90431000	2.07806500	-3.15582200
H	4.66047000	1.30004500	-1.58814400
H	5.76530500	4.77040600	-0.61768200
H	5.94575200	3.04127000	-0.22256900
H	6.47684500	3.64658700	-1.80629700
C	1.44698200	2.86661100	2.74179800
C	2.19865100	3.59568800	3.86748400
C	1.53125200	1.35578900	2.97702200
H	0.37988700	3.12445700	2.84020000
H	2.08154900	4.68635200	3.79882300
H	1.82865100	3.26544000	4.84954600
H	3.27433500	3.36515600	3.81937200
H	1.05154400	0.78394300	2.17744200
H	2.56044700	1.00001000	3.11957500
H	0.97757300	1.12941000	3.90065600
C	0.99078400	6.91032900	-0.12640500
C	0.33530800	7.05306300	-1.50288800
C	2.02282000	8.01906700	0.10413900
H	0.20259600	7.01723100	0.63649900
H	-0.43982000	6.29045700	-1.66341900
H	-0.13139300	8.04384800	-1.60690200
H	1.07938400	6.94961400	-2.30793200
H	2.47644200	7.93569200	1.10171300
H	2.83169700	7.95701500	-0.64023600
H	1.55682100	9.01171600	0.01472700
C	0.58469100	-3.78255600	-3.49581100
C	0.85514700	-5.21907400	-3.96384800
C	1.85387100	-2.92680300	-3.61080500
H	-0.12218600	-3.35340700	-4.22343500
H	1.29013500	-5.21652100	-4.97487800
H	1.56784200	-5.72299400	-3.29493000
H	-0.06887700	-5.81444200	-3.98349700
H	1.73940800	-1.95839800	-3.10919900
H	2.74301000	-3.42717300	-3.20826600
H	2.04824000	-2.73719400	-4.67751600
C	-0.06263200	-3.90189400	1.67544200
C	-0.25801600	-5.30950300	2.25032800
C	-0.71931600	-2.84315600	2.56744100
H	1.01734100	-3.70069100	1.67187100
H	0.25790500	-6.06323700	1.63772000
H	0.13384000	-5.36838900	3.27692900
H	-1.32719300	-5.57223000	2.27838600
H	-0.62225400	-1.83886200	2.13264500
H	-1.79164500	-3.05274900	2.71488600
H	-0.24577000	-2.84280300	3.56074500
C	-3.99047700	-3.65095600	-1.41626400
C	-4.71820300	-4.90264200	-0.91397700
C	-4.43442500	-3.29201900	-2.83067100
H	-4.26976800	-2.80475000	-0.76133500
H	-4.43582000	-5.14896000	0.12021000
H	-5.80937700	-4.76329500	-0.95038800
H	-4.46206800	-5.76897700	-1.54292600
H	-3.92282500	-2.38404100	-3.18041300
H	-4.21511300	-4.10865900	-3.53596000
H	-5.51895600	-3.11325900	-2.85589900
O	-2.23389500	-0.56620700	-1.88372700
H	-2.47098000	-0.87882700	-0.97895700
H	-1.14456400	1.95614900	0.76399200
O	0.36415800	-0.64002500	-1.85080100
H	-0.64888900	-0.65815300	-1.94413900

**Int3***IS-Ra-3R*

S	-5.65192400	0.61458000	-1.28814400
O	-5.10185400	-0.68697800	-1.70050800
O	-5.53358700	1.75497600	-2.19098900
O	-1.35172900	2.91426900	0.92254400
N	-3.55274800	0.88356500	0.49232000
N	-2.51225300	1.24236700	-0.34276800
C	-7.36876200	0.38888100	-0.90498400
C	-7.81924500	-0.88610100	-0.57137100
H	-7.11614200	-1.72071600	-0.55921100
C	-9.16816000	-1.05093800	-0.26634100
H	-9.54823000	-2.03874600	-0.00362700
C	-10.03149900	0.04637100	-0.30302800
H	-11.08702800	-0.08906400	-0.06272900
C	-9.55995200	1.31272500	-0.65214700
H	-10.24396000	2.16119100	-0.68865100
C	-8.21341900	1.49391100	-0.96315000
H	-7.81416900	2.46600700	-1.25597400
C	-4.93053100	0.96159600	0.29020300
C	-5.59800700	0.83786400	1.48319600
H	-6.67523500	0.76674300	1.60677600
C	-4.60249400	0.71358600	2.50135100
C	-3.34754600	0.70352600	1.85236600
C	-2.14780500	0.51242500	2.55519000
H	-1.19275000	0.49448000	2.03260600
C	-2.24608800	0.34912500	3.92483200
H	-1.33349300	0.19415100	4.50241300
C	-3.49109600	0.38509900	4.59929500
H	-3.51409700	0.26372600	5.68299200
C	-4.66866700	0.56182300	3.90175600
H	-5.63263200	0.57269100	4.41259400
C	-2.48459000	0.74600800	-1.71127500
H	-3.42395800	0.89796600	-2.25888100
C	-1.40456600	1.59358600	-2.31946900
C	-0.69387900	1.36756200	-3.49221900
H	-0.93191200	0.51851300	-4.13490200
C	0.36670700	2.22377200	-3.78697600
H	0.95398300	2.06728200	-4.69313900
C	0.71505100	3.25402000	-2.90635800
H	1.57885000	3.88421500	-3.12646800
C	-0.00960300	3.47068700	-1.73355000
H	0.28840600	4.23679100	-1.01908100
C	-1.09410700	2.64288700	-1.47090700
C	-2.00950600	2.65572000	-0.26263900
C	-3.15183700	3.65723600	-0.38102800
H	-3.76448100	3.60554500	0.53154300
H	-3.78033700	3.43870100	-1.25631500
H	-2.73979500	4.67171100	-0.46523800
C	2.20491100	-2.40499600	0.05499100
C	3.52624600	-2.28229900	-0.32203500
C	4.10987900	-3.36451000	-1.06979100
C	3.36549300	-4.56879100	-1.23264300
C	2.02302400	-4.64098500	-0.76635300
C	1.40005800	-3.55696200	-0.20359500
H	5.95778100	-2.34755000	-1.58697000
C	5.39611300	-3.27831300	-1.66875700
C	3.95175800	-5.66053300	-1.92853700
H	1.45777700	-5.56064400	-0.93104700
C	5.20803700	-5.55648800	-2.47342600
C	5.92914800	-4.34493700	-2.35322100
H	3.37282200	-6.58012300	-2.03650200
H	5.64482500	-6.39805500	-3.01264000
H	6.91435300	-4.25387000	-2.81253800
C	4.28887900	-1.06076100	0.06527000
C	5.55276400	-1.15728900	0.74949700
C	3.76394800	0.20205100	-0.15371300

C	6.09591200	-2.39385700	1.20057100
C	6.28577400	0.03323500	1.02315900
C	4.43148200	1.40268200	0.22532400
C	7.31775400	-2.44399300	1.82765400
H	5.52736900	-3.31155700	1.05643100
C	7.55577400	-0.05173300	1.65682700
C	5.69982800	1.29479700	0.73851800
C	8.06905600	-1.26397700	2.04379700
H	7.70774800	-3.40362300	2.16972800
H	8.10510900	0.87291700	1.84528400
H	6.24541600	2.20251200	1.00620800
H	9.04110000	-1.31945800	2.53548700
O	2.55274700	0.34489400	-0.79908600
O	1.61071600	-1.36730700	0.74452400
P	1.15662800	-0.06984000	-0.11114800
O	0.53514600	0.93121100	0.77777800
C	3.72220800	2.72096000	0.19636100
C	3.72429300	3.54909100	-0.94638900
C	3.08686000	3.15500800	1.38538600
C	3.10495100	4.80520500	-0.87445300
C	2.44928000	4.40009200	1.37779800
C	2.45807700	5.25351300	0.27563000
H	3.15271700	5.45088400	-1.75482000
H	1.95917700	4.73731000	2.29672600
C	-0.05866300	-3.49567400	0.11298600
C	-1.03621000	-3.53023400	-0.90803700
C	-0.45842900	-3.29105900	1.45394500
C	-2.37626700	-3.33048700	-0.54277700
C	-1.80389300	-3.07068800	1.75095400
C	-2.78932500	-3.05923800	0.76170800
H	-3.12448500	-3.35674800	-1.34193000
H	-2.08000800	-2.89336100	2.79011700
C	4.46583400	3.23640900	-2.24565600
C	4.19547200	1.87107100	-2.88507800
C	5.97299300	3.47886500	-2.09291700
H	4.10060200	3.98951800	-2.96339000
H	3.12570700	1.62414500	-2.88570900
H	4.55425300	1.88479300	-3.92548800
H	4.73246400	1.06170900	-2.37105700
H	6.17554000	4.48144100	-1.68967200
H	6.42049000	2.73701600	-1.41585300
H	6.47522000	3.38865700	-3.06800500
C	3.15438900	2.48762800	2.76684700
C	4.37467600	3.02274900	3.53204600
C	3.08285000	0.96426000	2.90482300
H	2.26310700	2.87106000	3.28816600
H	4.40650800	4.12140200	3.52193900
H	4.34694700	2.68364300	4.57852100
H	5.30781800	2.64874700	3.08512500
H	2.24788400	0.54116600	2.33711100
H	4.01300700	0.45803600	2.61375800
H	2.90883000	0.72653700	3.96564800
C	1.78824400	6.61518600	0.38922800
C	0.26116200	6.51712600	0.26437400
C	2.33918500	7.64954700	-0.58933800
H	2.00784300	6.97008700	1.41013300
H	-0.14916100	5.70186300	0.87893100
H	-0.21075300	7.46116400	0.57480100
H	-0.02761100	6.33162600	-0.78166200
H	3.43355300	7.72994200	-0.52141400
H	2.07864400	7.39203200	-1.62746200
H	1.90626900	8.63849200	-0.38099900
C	-0.83124900	-3.79227000	-2.40681700
C	-1.09148600	-5.27251500	-2.72028500
C	0.44877200	-3.31684500	-3.10733600
H	-1.64848700	-3.22456800	-2.87931800

H	-1.07047100	-5.44263700	-3.80723300
H	-0.31822300	-5.90917800	-2.26461600
H	-2.06695800	-5.60143500	-2.33479500
H	0.80935900	-2.35731200	-2.71787700
H	1.26450500	-4.04680600	-3.03646200
H	0.22663000	-3.18830200	-4.17744800
C	0.52582100	-3.36790200	2.61312200
C	0.34880300	-4.69876800	3.35431800
C	0.40448800	-2.18091000	3.57077200
H	1.54621300	-3.35877000	2.20922600
H	0.48909400	-5.55140200	2.67409600
H	1.07721600	-4.78570100	4.17441800
H	-0.66164500	-4.77306500	3.78519100
H	0.46883100	-1.22945300	3.02331500
H	-0.54839100	-2.20323200	4.12149900
H	1.21605700	-2.20871400	4.31320100
C	-4.24743000	-2.73443200	1.06536400
C	-4.55165700	-2.69220900	2.56007500
C	-5.20768700	-3.69143900	0.35046900
H	-4.42949300	-1.72086900	0.65918900
H	-3.92634600	-1.95936700	3.08739200
H	-5.60036100	-2.40186400	2.72241600
H	-4.39364300	-3.68127600	3.01984900
H	-5.16731700	-3.58273800	-0.74206600
H	-4.97459100	-4.73718700	0.60371400
H	-6.24323500	-3.49416700	0.66735000
O	-2.14786500	-0.61465000	-1.77789100
H	-2.93052400	-1.14781700	-1.55836600
H	-0.56813000	2.33120100	0.95720600
O	0.38055100	-0.60614300	-1.35130200
H	-0.62239800	-0.70215900	-1.34189100

**Int4***IR-Sa-3R*

S	5.55010200	-0.44718500	-0.09139200
O	5.24982300	0.10921100	-1.40546900
O	5.70238700	-1.87914800	0.13018800
O	1.21489400	2.73756500	-0.81352900
N	3.07860300	0.66312900	0.92340100
N	2.26720700	0.67978700	-0.19834800
C	7.08914200	0.29134500	0.45092700
C	7.38526900	1.60210500	0.08319500
H	6.67813100	2.17424400	-0.51899100
C	8.59576600	2.15477200	0.49259900
H	8.84480400	3.17980600	0.21576600
C	9.49205700	1.39518400	1.24780300
H	10.44002000	1.83284400	1.56414400
C	9.18743100	0.07841200	1.59094400
H	9.89674500	-0.51513100	2.16907800
C	7.97761000	-0.48650500	1.18750700
H	7.71392400	-1.51821500	1.42341600
C	4.40208900	0.24724400	1.10650100
C	4.77537100	0.47282100	2.40557200
H	5.74834400	0.24029400	2.83013200
C	3.67669100	1.10588300	3.06676500
C	2.64848200	1.24039200	2.10892300
C	1.46703700	1.95070700	2.38267100
H	0.72265700	2.14275000	1.61108500
C	1.31448100	2.44930700	3.66456400
H	0.40840700	3.00751200	3.90599500
C	2.30721800	2.27460400	4.65464600
H	2.14435800	2.68490300	5.65192000
C	3.48932000	1.61995600	4.36482000
H	4.27270800	1.51344300	5.11657900
C	2.21210800	-0.58384500	-1.02710700
H	1.22969400	-1.06679400	-0.87176700
C	2.30277300	-0.05597900	-2.42932000
C	2.32456000	-0.79978300	-3.60322100

H	2.33441900	-1.89050600	-3.56431800
C	2.33755900	-0.11497300	-4.81763300
H	2.36034700	-0.67331200	-5.75456400
C	2.31702200	1.28365000	-4.84607700
H	2.31722400	1.80279300	-5.80564700
C	2.30094900	2.01901600	-3.66112800
H	2.28513200	3.11064200	-3.67807400
C	2.30981000	1.32896500	-2.45302600
C	2.31945600	1.92946400	-1.06302600
C	3.55305300	2.77097300	-0.78559600
H	3.55437100	3.11156400	0.26026200
H	3.50627100	3.65463600	-1.43561200
H	4.45854700	2.19807100	-1.01070900
C	-2.56733800	-2.02163300	0.09480800
C	-3.82734000	-1.65659900	0.53524400
C	-4.50740500	-2.55697000	1.43165000
C	-3.96291300	-3.85427400	1.65577700
C	-2.69823900	-4.18862400	1.10300500
C	-1.95354700	-3.26896900	0.40830200
H	-6.10081700	-1.19481100	2.01053600
C	-5.69796100	-2.20065900	2.12467900
C	-4.65638800	-4.77156400	2.49175000
H	-2.28148100	-5.17908400	1.29406200
C	-5.82181000	-4.40849000	3.11917100
C	-6.33458600	-3.10078100	2.94546800
H	-4.22920400	-5.76550500	2.63998700
H	-6.34212000	-5.11560100	3.76641300
H	-7.24034900	-2.80048600	3.47391400
C	-4.44149800	-0.36331900	0.12077000
C	-5.78924100	-0.26891100	-0.37961600
C	-3.71708000	0.80730000	0.20778200
C	-6.57005800	-1.41199500	-0.70590400
C	-6.36450200	1.02074000	-0.57944900
C	-4.23991700	2.10055200	-0.08357400
C	-7.86188000	-1.28099800	-1.15691900
H	-6.12948900	-2.40355800	-0.60482400
C	-7.70949100	1.12229800	-1.02832300
C	-5.57001300	2.18817600	-0.40229000
C	-8.44774700	-0.00147500	-1.30505700
H	-8.43777400	-2.17232500	-1.40943800
H	-8.13718500	2.11736400	-1.16615100
H	-6.01746800	3.16567500	-0.59440600
H	-9.47640200	0.08875000	-1.65635500
O	-2.41221700	0.76375000	0.65685500
O	-1.85886200	-1.19774800	-0.75757000
P	-1.23520300	0.21097500	-0.28407900
O	-0.80499200	0.99568000	-1.46158600
C	-3.24688900	3.21637300	-0.12646000
C	-2.76427900	3.80820300	1.06328000
C	-2.64213700	3.51415200	-1.36830500
C	-1.63542500	4.62969400	0.99474400
C	-1.51783800	4.34942700	-1.37012700
C	-0.97323500	4.88657600	-0.20708000
H	-1.26084500	5.07266400	1.92073000
H	-1.02564700	4.56005400	-2.32453500
C	-0.53867400	-3.55081700	0.01954800
C	0.45956000	-3.66210900	1.01446900
C	-0.20326500	-3.73670300	-1.34082100
C	1.75575300	-4.01703100	0.60801100
C	1.10735200	-4.07960900	-1.68732900
C	2.10511400	-4.24659200	-0.72531900
H	2.52928900	-4.12388600	1.37685700
H	1.34683400	-4.23897400	-2.74151600
C	-3.43144600	3.66256000	2.43059500
C	-3.40304600	2.26293100	3.05692000
C	-4.85196500	4.23852300	2.43686000

H	-2.83290600	4.30283400	3.09809100
H	-2.40460800	1.80985100	2.99497400
H	-3.68847000	2.33725100	4.11710400
H	-4.11785000	1.57912500	2.57721300
H	-4.86771800	5.25827100	2.02643600
H	-5.53528500	3.61616400	1.84219300
H	-5.24304000	4.27362300	3.46494300
C	-3.14861600	3.08584100	-2.75086600
C	-4.27117800	4.03241400	-3.19925200
C	-3.54810000	1.62723300	-3.01074600
H	-2.29193800	3.27312900	-3.41640700
H	-3.96787100	5.08504800	-3.10749700
H	-4.54208400	3.83677500	-4.24779200
H	-5.17305400	3.88442300	-2.58691100
H	-2.79137300	0.92783300	-2.63826100
H	-4.52636800	1.36421100	-2.58869100
H	-3.62091100	1.48371200	-4.09964900
C	0.26257500	5.76302400	-0.28037300
C	1.20624400	5.56821400	0.90512900
C	-0.13803500	7.23483200	-0.43453500
H	0.80502800	5.45134700	-1.18725700
H	1.45723400	4.50558900	1.02576200
H	2.13763500	6.13201200	0.74551100
H	0.76185700	5.93574400	1.84316900
H	-0.77715100	7.38379700	-1.31661200
H	-0.70153000	7.57192000	0.44949700
H	0.75138600	7.87471000	-0.53732600
C	0.28454400	-3.47332900	2.52650800
C	0.03450000	-4.81435100	3.23097000
C	-0.69736300	-2.40720900	3.02557500
H	1.27960900	-3.13663800	2.85930400
H	0.10869200	-4.68552800	4.32101100
H	-0.97318800	-5.19524000	3.01151900
H	0.76481400	-5.57587600	2.92197800
H	-0.61800300	-1.47817100	2.44853100
H	-1.74106800	-2.74694900	3.00627700
H	-0.45270500	-2.17287800	4.07238600
C	-1.23528600	-3.62074000	-2.45291500
C	-1.47893400	-4.98323400	-3.11082300
C	-0.83385700	-2.56392300	-3.48585000
H	-2.18748400	-3.30147900	-2.01039100
H	-1.80495800	-5.72775100	-2.37006400
H	-2.25577700	-4.90264900	-3.88544000
H	-0.56284100	-5.36165500	-3.58968500
H	-0.62646900	-1.59490200	-3.00824000
H	0.06283400	-2.87297000	-4.04539000
H	-1.64359900	-2.41750400	-4.21600300
C	3.51508100	-4.69644900	-1.07184400
C	4.06044900	-4.10477200	-2.37117200
C	3.56344500	-6.22970200	-1.09990500
H	4.17217200	-4.34704800	-0.25800300
H	4.08545700	-3.00808400	-2.32202300
H	5.08835600	-4.45891900	-2.53438400
H	3.46530400	-4.42009200	-3.24306400
H	3.21382000	-6.65864100	-0.14992700
H	2.91742000	-6.61772900	-1.90291100
H	4.58890200	-6.58207100	-1.28437700
O	3.19384900	-1.48226800	-0.69233300
H	2.83676000	-2.15607300	-0.09671100
H	0.41093600	2.30507100	-1.16634300
O	-0.10916700	-0.05176600	0.77435000
H	0.77851500	0.34863300	0.46554600
<b>Int5<sub>IR-Ra-3R</sub></b>			
S	2.80357200	0.37397700	1.76054500
O	2.25285800	-0.98013800	1.50677000
O	1.95475400	1.51960000	1.48098200



O	2.46979800	2.22641800	-1.17719600
N	4.46740100	0.08169900	-0.41159100
N	3.46328800	0.07060200	-1.32350200
C	3.28301700	0.45027700	3.46766700
C	3.62986700	-0.72505900	4.13079600
H	3.60161800	-1.67777000	3.59945300
C	4.00264100	-0.64165000	5.46974500
H	4.27660900	-1.54591900	6.01409400
C	4.01945100	0.59760200	6.11412800
H	4.31201600	0.65589100	7.16351500
C	3.65843500	1.76039800	5.43249000
H	3.66477900	2.72177300	5.94695900
C	3.27954900	1.69456400	4.09251600
H	2.97569800	2.58131800	3.53311100
C	4.36019700	0.40074900	0.93145700
C	5.59718000	0.47285600	1.51757500
H	5.80194800	0.66412000	2.56710000
C	6.54664100	0.19182800	0.48092700
C	5.81103400	-0.05763100	-0.69991600
C	6.43587200	-0.38454900	-1.91151200
H	5.84634400	-0.58151700	-2.80552000
C	7.81628400	-0.45705100	-1.91317700
H	8.33568000	-0.71527600	-2.83709200
C	8.57240800	-0.21025800	-0.74333500
H	9.65976300	-0.27903700	-0.78864300
C	7.95345200	0.11074900	0.44928600
H	8.53692700	0.29730700	1.35200300
C	2.75887200	-1.15224600	-1.67936300
H	2.18881500	-1.55826900	-0.82867300
C	1.88058200	-0.64249200	-2.79498300
C	0.97347500	-1.36606000	-3.55898400
H	0.78439200	-2.41918600	-3.34199000
C	0.29133300	-0.70437400	-4.58227700
H	-0.43452500	-1.24942100	-5.18829900
C	0.51897400	0.65221400	-4.82891400
H	-0.02440300	1.15375200	-5.63187700
C	1.42366400	1.37429200	-4.04776600
H	1.59451200	2.43798100	-4.22870100
C	2.10095400	0.70936300	-3.03358900
C	3.06884800	1.30423900	-2.02788500
C	4.24441900	2.03190000	-2.66495100
H	3.87061700	2.93941100	-3.15781600
H	4.75396200	1.40280300	-3.40485600
H	4.95891300	2.33760500	-1.88671900
C	-2.83279700	-1.59666600	0.24955900
C	-3.95007500	-0.87078700	0.61580500
C	-4.90439700	-1.50268600	1.48801600
C	-4.74978300	-2.88458300	1.80069600
C	-3.61255100	-3.59169900	1.32388900
C	-2.62253200	-2.95854000	0.61914300
H	-6.09343700	0.27247400	1.88517400
C	-5.98839400	-0.79511900	2.07803000
C	-5.70933000	-3.52309800	2.63279100
H	-3.49664700	-4.64699300	1.58243200
C	-6.76094600	-2.81900400	3.16476100
C	-6.88987400	-1.43576100	2.89417200
H	-5.58220600	-4.58510900	2.85256800
H	-7.48732900	-3.31732600	3.80812500
H	-7.70822000	-0.87066300	3.34242100
C	-4.12147400	0.52342400	0.12269800
C	-5.32709900	0.96015500	-0.53135100
C	-3.08628500	1.43075000	0.23672600
C	-6.38589900	0.07153800	-0.86983100
C	-5.46508400	2.33468300	-0.88250700
C	-3.16809400	2.78332800	-0.20467600
C	-7.53167200	0.53294600	-1.47273500

H	-6.27843900	-0.99115100	-0.65446700
C	-6.66949700	2.78464300	-1.48920100
C	-4.37218400	3.22361500	-0.69057100
C	-7.68635900	1.90741500	-1.77289400
H	-8.32626800	-0.16935800	-1.72848700
H	-6.76021100	3.84342500	-1.74045600
H	-4.47869000	4.26579100	-0.99844500
H	-8.60378300	2.26170000	-2.24470000
O	-1.91148800	1.05797600	0.84832500
O	-1.85975900	-1.00271300	-0.53441300
P	-0.84920400	0.04162000	0.19117600
O	0.15578500	0.57459800	-0.74597200
C	-1.90194700	3.57644500	-0.22794000
C	-1.39592800	4.19534700	0.93736700
C	-1.14441000	3.57256100	-1.42128000
C	-0.11257900	4.74632000	0.89880800
C	0.13393400	4.14299500	-1.39354800
C	0.68370700	4.70620800	-0.24609900
H	0.27661400	5.21534600	1.80675600
H	0.74206000	4.11222900	-2.30105500
C	-1.35067800	-3.61006800	0.18475500
C	-0.24877500	-3.75856600	1.05676600
C	-1.23204500	-3.97114500	-1.17513100
C	0.96207600	-4.19263400	0.50049500
C	-0.01501900	-4.45819900	-1.65783500
C	1.10954700	-4.55617200	-0.83814600
H	1.83763500	-4.25735500	1.15444300
H	0.05207300	-4.75408100	-2.70728300
C	-2.18298000	4.36937100	2.23540700
C	-2.57297300	3.08129100	2.96925600
C	-3.39793000	5.28578400	2.04981500
H	-1.49136500	4.90171700	2.90756400
H	-1.72918900	2.38224400	3.03426000
H	-2.90277700	3.33259100	3.98881800
H	-3.40776000	2.56148700	2.47811400
H	-3.11244200	6.22782700	1.55999100
H	-4.17181400	4.79962300	1.43931900
H	-3.84606300	5.52573300	3.02609700
C	-1.61527800	3.06792100	-2.79069500
C	-2.54726600	4.08324000	-3.46634400
C	-2.18290900	1.64843200	-2.89912100
H	-0.69410700	3.05188800	-3.39310100
H	-2.13079300	5.09971900	-3.41892500
H	-2.69223300	3.81684000	-4.52458500
H	-3.53839300	4.09408400	-2.99187600
H	-1.50928100	0.91500600	-2.43583400
H	-3.18971100	1.54781100	-2.47070200
H	-2.26248000	1.38628800	-3.96601700
C	2.08389200	5.28917600	-0.26270700
C	2.95245200	4.74388600	0.87315400
C	2.03398800	6.82037600	-0.24013000
H	2.54477000	4.96592100	-1.20919000
H	2.98624300	3.64725200	0.82858600
H	3.97691000	5.13874400	0.79175100
H	2.55686400	5.04954900	1.85544800
H	1.44105300	7.21192300	-1.07913100
H	1.57151900	7.17852900	0.69313300
H	3.04694200	7.24650100	-0.30124100
C	-0.20188000	-3.55786300	2.58029200
C	0.03789500	-4.92378000	3.24726000
C	-1.34787700	-2.86743200	3.32658600
H	0.70013400	-2.94403900	2.74971000
H	0.15314500	-4.80424800	4.33502600
H	-0.82553800	-5.58357100	3.06824600
H	0.93094100	-5.43078300	2.85803800
H	-1.67693900	-1.93558600	2.85703500

H	-2.21595100	-3.53051600	3.44110000
H	-0.99145500	-2.62605300	4.33961700
C	-2.41234700	-3.88420000	-2.13456000
C	-2.84569800	-5.28444500	-2.58205100
C	-2.11856700	-2.98103800	-3.33422300
H	-3.26169200	-3.44071100	-1.59789700
H	-3.09716900	-5.91523700	-1.71714500
H	-3.72789100	-5.22599000	-3.23694100
H	-2.04168200	-5.78640400	-3.14216700
H	-1.81361300	-1.97839000	-3.00231600
H	-1.31478900	-3.40099400	-3.96129000
H	-3.01357100	-2.88319600	-3.96704800
C	2.44808200	-5.09170800	-1.31969400
C	2.57519700	-5.15128200	-2.83838900
C	2.71572400	-6.47198100	-0.70613900
H	3.21547400	-4.38990200	-0.95596600
H	2.37101400	-4.17143000	-3.29121100
H	3.59676500	-5.44640400	-3.11835300
H	1.88622700	-5.89305900	-3.27210900
H	2.68002500	-6.43983300	0.39209400
H	1.95675600	-7.19412300	-1.04510300
H	3.70574200	-6.84655900	-1.00644700
O	3.61894600	-2.18844400	-2.07244200
H	3.94095100	-1.99339400	-2.96184400
H	1.64249700	1.84764300	-0.81918800
O	-0.32279100	-0.66995600	1.48554100
H	0.64578200	-0.90407000	1.45484900
<b>TS6<sub>Si</sub></b>			
S	-5.06759300	0.16579000	-1.21299500
O	-4.37142100	-0.67141000	-2.17585800
O	-4.92104200	1.62438300	-1.27144600
O	-2.93700600	4.30347400	0.53368600
N	-3.28614400	-0.31502500	0.78802000
N	-2.31762400	0.24833600	-0.00662400
C	-6.80001100	-0.22042200	-1.24744000
C	-7.18648200	-1.48081500	-1.69714000
H	-6.42864400	-2.18791300	-2.03879100
C	-8.54414000	-1.79339300	-1.70321400
H	-8.87413200	-2.77245400	-2.05205200
C	-9.47909000	-0.85231400	-1.26789100
H	-10.54083000	-1.10313100	-1.27515700
C	-9.07029400	0.40828600	-0.82870200
H	-9.80916100	1.13907600	-0.49812500
C	-7.71608700	0.73636300	-0.81747800
H	-7.36230400	1.71455600	-0.48867100
C	-4.61651600	-0.35419000	0.42118300
C	-5.38777800	-0.78198500	1.46737500
H	-6.46521700	-0.92280900	1.45264200
C	-4.48512300	-1.00751500	2.56301300
C	-3.17821500	-0.70597800	2.10916500
C	-2.04344700	-0.81297600	2.92308800
H	-1.05028800	-0.55927700	2.54910600
C	-2.25818800	-1.22685200	4.22726600
H	-1.40234800	-1.31812700	4.89763800
C	-3.55283800	-1.52345700	4.71303500
H	-3.67112600	-1.84098300	5.74970300
C	-4.66454200	-1.42095300	3.89747600
H	-5.66123700	-1.65740300	4.27277800
C	-2.27222200	1.58303600	-0.05810200
H	-3.14266700	2.06073600	0.38511500
C	-1.68541700	2.28218200	-1.23407900
C	-0.77089200	1.65839900	-2.08917000
H	-0.41108300	0.65344300	-1.86884800
C	-0.32745000	2.30484000	-3.24122300
H	0.39191100	1.80457000	-3.89035300
C	-0.81705200	3.56431000	-3.57391100

H	-0.48055100	4.06521200	-4.48289300
C	-1.75667700	4.17677300	-2.74902700
H	-2.14936400	5.15834600	-3.01810300
C	-2.17973700	3.56024000	-1.56931800
C	-3.13612700	4.28403100	-0.66149900
C	-4.34400700	4.92887500	-1.28350800
H	-4.89691300	5.47807800	-0.51361900
H	-4.96440100	4.11958000	-1.69965100
H	-4.07182200	5.60088900	-2.10827000
C	2.74864400	-2.30192200	-0.01459800
C	3.93693600	-1.78947000	-0.49879900
C	4.68281000	-2.59337900	-1.43336100
C	4.25875400	-3.93166900	-1.68394300
C	3.01926200	-4.38908000	-1.15578300
C	2.21176000	-3.56274600	-0.41770200
H	6.12093500	-1.06872000	-2.00847100
C	5.81710100	-2.10669700	-2.14049500
C	5.02351000	-4.75565300	-2.55349800
H	2.66791100	-5.38757600	-1.42266200
C	6.13916100	-4.26826000	-3.18848900
C	6.52507300	-2.92132500	-2.99232900
H	4.68952600	-5.78142400	-2.72325500
H	6.71403000	-4.90746900	-3.85994300
H	7.38793900	-2.52192500	-3.52717000
C	4.36626500	-0.42330100	-0.08839900
C	5.69980600	-0.14493600	0.37774700
C	3.45922000	0.62394600	-0.12597500
C	6.64738400	-1.17090100	0.65214300
C	6.09144100	1.20646000	0.60348300
C	3.80988000	1.96307300	0.21710100
C	7.92090700	-0.86617200	1.06934500
H	6.34937700	-2.21269000	0.53775700
C	7.42144400	1.49199500	1.01643200
C	5.12282400	2.24120300	0.49950500
C	8.32280100	0.48070400	1.23733800
H	8.62581100	-1.67147900	1.28064200
H	7.70436000	2.53497800	1.17326000
H	5.41824000	3.26713400	0.73206900
H	9.33887400	0.70945800	1.56157100
O	2.17327800	0.41212800	-0.55597200
O	2.02964600	-1.57843900	0.90946400
P	1.07435500	-0.37334600	0.37491100
O	0.00275500	-0.86131300	-0.55352300
H	-1.50886300	-0.36002200	-0.31715300
O	0.67619400	0.44876000	1.57225500
C	2.73427500	2.98932700	0.36865100
C	2.23068900	3.70659400	-0.73712900
C	2.22411500	3.23317400	1.66589900
C	1.22810300	4.66539400	-0.52757400
C	1.22179500	4.20052500	1.80934900
C	0.71996600	4.94836300	0.74092200
H	0.86940000	5.22469000	-1.39462200
H	0.83917600	4.39522500	2.81639100
C	0.77425500	-3.83758900	-0.12403800
C	-0.17899800	-3.70957800	-1.16254900
C	0.35068200	-4.04413700	1.20096000
C	-1.53100900	-3.80105600	-0.82305600
C	-1.01592200	-4.14733200	1.48076200
C	-1.97962700	-4.01638500	0.48228300
H	-2.26966700	-3.65273000	-1.61600200
H	-1.32355400	-4.31215400	2.51405400
C	2.82309300	3.66551800	-2.14626300
C	3.15856400	2.30385300	-2.76316300
C	4.04781900	4.58924500	-2.20910400
H	2.04705900	4.11454000	-2.78763400
H	2.37748500	1.55814700	-2.57171600

H	3.27090700	2.42596700	-3.85160500
H	4.10916300	1.90347500	-2.38455400
H	3.80321100	5.60245700	-1.85991800
H	4.85562600	4.19331800	-1.57523300
H	4.42858400	4.65600100	-3.23957400
C	2.75278100	2.67224000	2.99472000
C	3.76726200	3.66894800	3.57829700
C	3.31653500	1.25063200	3.09718400
H	1.87083700	2.68772200	3.65510000
H	3.35926400	4.68910100	3.62016600
H	4.05896700	3.36637400	4.59507700
H	4.67847000	3.69259700	2.96130300
H	2.66197300	0.51265000	2.62404800
H	4.32830900	1.15992800	2.68198200
H	3.38578900	0.99616300	4.16597800
C	-0.27767500	6.06705500	1.01852000
C	-0.77015200	6.77820700	-0.23763500
C	0.32826600	7.09523200	1.98345800
H	-1.15451600	5.61295500	1.51057400
H	-1.18551900	6.07553100	-0.97123400
H	-1.55171200	7.50646000	0.02225800
H	0.05096600	7.32500200	-0.72752900
H	0.63463700	6.63805600	2.93378000
H	1.21726000	7.56165000	1.53157500
H	-0.40021700	7.88810800	2.20849200
C	0.10433500	-3.47323800	-2.65084400
C	0.31881800	-4.80248800	-3.38756900
C	1.17707600	-2.45249200	-3.05606500
H	-0.84430700	-3.06222800	-3.02974100
H	0.34619300	-4.63520100	-4.47518300
H	1.27385800	-5.26483300	-3.09901900
H	-0.48698400	-5.51697500	-3.16592000
H	1.12886300	-1.55145100	-2.43309900
H	2.19558400	-2.85874900	-3.00942100
H	0.99764000	-2.15970600	-4.10232000
C	1.34093000	-4.17910800	2.34792800
C	1.40902900	-5.63342100	2.82696100
C	1.02006300	-3.22786200	3.50392600
H	2.33813300	-3.91040100	1.97193900
H	1.68811400	-6.30695100	2.00372100
H	2.15009300	-5.74460000	3.63286700
H	0.43229300	-5.96237800	3.21471500
H	0.96251200	-2.18905100	3.14801900
H	0.06391300	-3.48789200	3.98425700
H	1.80446300	-3.28570900	4.27351600
C	-3.47491600	-4.06784900	0.76510500
C	-3.80255100	-4.32201900	2.23243000
C	-4.17746600	-5.10746000	-0.11566100
H	-3.87741100	-3.07296500	0.49519200
H	-3.32519100	-3.58599700	2.89280900
H	-4.88881500	-4.26282300	2.39648500
H	-3.46702900	-5.32662600	2.53647400
H	-4.01465800	-4.92178700	-1.18579800
H	-3.79913200	-6.11592600	0.11246000
H	-5.26228800	-5.09880100	0.07000100
O	-1.17931700	2.15674700	1.38265700
H	-0.88004000	3.06573800	1.21400600
H	-0.36452600	1.53729900	1.46018500
<b>Int6s</b>			
S	-5.30870000	0.27959400	-1.09598600
O	-4.79659800	-0.87124900	-1.83066400
O	-5.00542100	1.63872200	-1.53391300
O	-1.91503000	4.57068700	0.43856200
N	-3.48240900	0.06130600	0.86894700
N	-2.55929800	0.41432300	-0.08371100
C	-7.07633300	0.11264000	-0.97104000

C	-7.63302900	-1.16237200	-1.04065300
H	-6.98431700	-2.02572600	-1.19953100
C	-9.01446000	-1.29117900	-0.91313500
H	-9.47511500	-2.27832000	-0.96546300
C	-9.80698800	-0.15702900	-0.72509300
H	-10.88832900	-0.26399800	-0.62683000
C	-9.23011200	1.11271400	-0.66853600
H	-9.85822200	1.99357800	-0.53066900
C	-7.84938500	1.25671600	-0.79392300
H	-7.36446100	2.23358200	-0.76619500
C	-4.82863600	0.11084700	0.60220300
C	-5.56295800	-0.06720900	1.74499400
H	-6.64664500	-0.10357200	1.81561200
C	-4.60272800	-0.24184500	2.80029400
C	-3.31266200	-0.15441300	2.21884200
C	-2.13380700	-0.32161500	2.95809800
H	-1.15529500	-0.24989500	2.48284300
C	-2.27640800	-0.57592800	4.31092700
H	-1.38291800	-0.71511900	4.92143700
C	-3.55127500	-0.65572100	4.91991500
H	-3.61599100	-0.85469400	5.99034900
C	-4.70975700	-0.49116700	4.18291500
H	-5.69004600	-0.56516300	4.65623800
C	-2.20918000	1.80025300	-0.09123500
H	-3.12062900	2.34476500	0.20282300
C	-1.81035600	2.29290500	-1.47876900
C	-1.58882000	1.38484900	-2.51546100
H	-1.70343200	0.32120600	-2.32254000
C	-1.22858000	1.81899900	-3.78790700
H	-1.04123200	1.08316000	-4.57118400
C	-1.12106800	3.18023100	-4.06271700
H	-0.83842300	3.52576800	-5.05766400
C	-1.41047800	4.09881400	-3.06192700
H	-1.36645000	5.16435100	-3.28910400
C	-1.74801900	3.67546300	-1.76715400
C	-2.10446700	4.72009500	-0.75684500
C	-2.76422400	5.98661700	-1.24794600
H	-3.07369300	6.57682000	-0.37856400
H	-3.63039100	5.74015300	-1.87771600
H	-2.06772800	6.58055000	-1.85525300
C	2.31099500	-2.38559000	-0.13097600
C	3.60970900	-2.19672600	-0.55813100
C	4.13911100	-3.12725300	-1.52054800
C	3.36590800	-4.27367700	-1.86764700
C	2.04359500	-4.41434500	-1.36345800
C	1.47354800	-3.45130600	-0.57045300
H	5.97265000	-2.04215900	-1.95235200
C	5.39277300	-2.93970400	-2.16585200
C	3.89826700	-5.22293200	-2.78204500
H	1.44677100	-5.27341700	-1.67716500
C	5.12791300	-5.03115700	-3.36165100
C	5.87284500	-3.86624600	-3.06069100
H	3.29743400	-6.10084400	-3.02797300
H	5.52339900	-5.76257400	-4.06766000
H	6.83382100	-3.69728300	-3.54847100
C	4.38496200	-1.02793900	-0.05848200
C	5.71179400	-1.16098900	0.48322400
C	3.82256900	0.23549100	-0.08237400
C	6.31384200	-2.42569100	0.73455000
C	6.45194700	0.01290100	0.80831200
C	4.51727400	1.41021500	0.32641700
C	7.59238000	-2.51440000	1.23067600
H	5.74431900	-3.33374500	0.53827900
C	7.77878900	-0.11115000	1.30363900
C	5.82997800	1.28648700	0.70253600
C	8.34324900	-1.34601700	1.50429900

H	8.02932300	-3.49540400	1.42222300
H	8.33361400	0.79980800	1.53715500
H	6.39322100	2.17663500	0.99203100
H	9.35969700	-1.43045800	1.89088600
O	2.55044400	0.42519000	-0.57780300
O	1.76596000	-1.49084800	0.77771600
P	1.20943800	-0.11491500	0.14011700
O	0.10380300	-0.22837200	-0.82979700
H	-1.79428500	-0.25430200	-0.20912200
O	0.89491500	0.74565800	1.40871400
C	3.73463800	2.67815200	0.42591900
C	3.50331700	3.48952200	-0.70528700
C	3.12897700	2.98932700	1.66521000
C	2.64173300	4.58535500	-0.58205300
C	2.26451100	4.08845800	1.71883000
C	1.99822900	4.89721900	0.61462700
H	2.47311400	5.20317500	-1.46562500
H	1.78292300	4.32403700	2.67354400
C	0.03163300	-3.44321300	-0.18473200
C	-0.96958800	-3.11812200	-1.13083800
C	-0.31647800	-3.67758800	1.16023800
C	-2.29497800	-3.04834500	-0.68509800
C	-1.66162800	-3.64824100	1.53845500
C	-2.67144800	-3.34009400	0.62919600
H	-3.07000200	-2.74810100	-1.39805500
H	-1.91515300	-3.86421400	2.57717100
C	4.18356600	3.30476600	-2.06137700
C	3.89134700	1.98943700	-2.79237200
C	5.69169800	3.57180700	-1.98880500
H	3.75781900	4.10056800	-2.69275400
H	2.82035300	1.74847600	-2.78069400
H	4.21910100	2.08020700	-3.83896900
H	4.43695700	1.14148400	-2.35516700
H	5.90185000	4.53200600	-1.49596100
H	6.20995800	2.77713000	-1.43434400
H	6.11914000	3.60345600	-3.00243400
C	3.41497800	2.32072900	3.01644300
C	4.60855800	3.02857500	3.67561300
C	3.59369000	0.80105700	3.12551300
H	2.52777700	2.55752600	3.62460900
H	4.46201300	4.11748300	3.70975100
H	4.75438900	2.66192000	4.70283600
H	5.53249000	2.82791900	3.11226600
H	2.81782100	0.24596500	2.58859400
H	4.57756800	0.45897300	2.78041000
H	3.51437700	0.52724000	4.18869900
C	1.07566200	6.09509900	0.76886900
C	0.63554700	6.69882700	-0.56159600
C	1.73211300	7.16856000	1.64609700
H	0.17073000	5.73800900	1.28814500
H	0.23946700	5.93065000	-1.24321000
H	-0.14217400	7.45857000	-0.39463700
H	1.47735800	7.19263400	-1.07164800
H	2.00655700	6.76951500	2.63237100
H	2.65026000	7.54130400	1.16654400
H	1.05141600	8.01957700	1.79779700
C	-0.79646700	-2.90214900	-2.63950500
C	-1.08718400	-4.21798400	-3.37730200
C	0.48232000	-2.26475400	-3.19631400
H	-1.61624900	-2.21241100	-2.89904100
H	-1.09287200	-4.05534000	-4.46573500
H	-0.31146000	-4.96629000	-3.15324300
H	-2.05843300	-4.63920600	-3.08189000
H	0.81028800	-1.41021000	-2.59436600
H	1.30963300	-2.98052200	-3.28304400
H	0.26819700	-1.90132300	-4.21357100

C	0.71991500	-4.00909000	2.22480900
C	0.58852700	-5.47006300	2.66888900
C	0.63317800	-3.05401400	3.41879500
H	1.72081000	-3.89303500	1.78711500
H	0.69326600	-6.15255800	1.81302400
H	1.36131100	-5.72232600	3.41045600
H	-0.39516700	-5.65352700	3.12784500
H	0.74079300	-2.01068700	3.08892400
H	-0.32923100	-3.15507500	3.94399900
H	1.43387100	-3.27153200	4.14162200
C	-4.14419700	-3.34019300	1.00470900
C	-4.39535100	-3.58982400	2.48849200
C	-4.92070500	-4.35455900	0.15565100
H	-4.53307700	-2.34121400	0.75040100
H	-3.82734400	-2.89708500	3.12528700
H	-5.46277700	-3.45733900	2.71966000
H	-4.11599700	-4.61972100	2.76400400
H	-4.82323500	-4.14185000	-0.91813700
H	-4.54641200	-5.37415200	0.33678000
H	-5.99069400	-4.33280100	0.41448000
O	-1.20445900	2.08677800	0.88583200
H	-1.20350600	3.06243900	0.98369100
H	0.07320200	1.32708600	1.22466700

**TS7***ISi-Ra-3S*

S	2.61097000	-0.20643700	1.79465700
O	1.47133000	-0.25544000	2.69267200
O	2.47368700	0.24208900	0.40917400
O	2.20227800	-0.79114000	-2.28802100
N	3.01348400	-2.71353300	0.67978400
N	1.96127800	-2.55603400	-0.21519000
C	3.87662600	0.77147300	2.57377200
C	3.63151800	1.27747700	3.84543200
H	2.69813200	1.02621600	4.35133000
C	4.58834700	2.11441500	4.42119000
H	4.41618000	2.53109700	5.41417000
C	5.75810600	2.42018900	3.72640800
H	6.50154500	3.07618900	4.18167100
C	5.98660200	1.89586400	2.45070900
H	6.90226600	2.14276300	1.91170500
C	5.03663400	1.06812800	1.86067800
H	5.17701300	0.66113500	0.85834200
C	3.37357800	-1.81299400	1.66903500
C	4.42140800	-2.30305200	2.39907900
H	4.92291900	-1.78767900	3.21362400
C	4.73398600	-3.58640800	1.84904600
C	3.83926500	-3.81641800	0.77177400
C	3.89182500	-5.00491000	0.02072900
H	3.21113000	-5.19904200	-0.80589800
C	4.85453900	-5.93831200	0.36347300
H	4.91549100	-6.86638000	-0.20633200
C	5.75510900	-5.72071400	1.42842100
H	6.49676800	-6.48400500	1.66527300
C	5.70216600	-4.55625800	2.17006100
H	6.39422800	-4.38416600	2.99553100
C	0.89061700	-3.58904300	-0.14128700
H	1.37935100	-4.57028900	-0.06497100
C	0.19371000	-3.44759400	-1.47804100
C	-1.07457700	-3.97588800	-1.70737500
H	-1.59521600	-4.48467800	-0.89425500
C	-1.67717200	-3.80401600	-2.95073000
H	-2.67449300	-4.20991000	-3.12377200
C	-1.02877700	-3.08754600	-3.95882300
H	-1.51677200	-2.93680600	-4.92262700
C	0.22120600	-2.52703300	-3.71965500
H	0.71250300	-1.91724500	-4.48034400
C	0.83651200	-2.72277200	-2.48035300



C	2.15548200	-2.05433600	-2.21029900
C	3.43724200	-2.77134900	-2.52419200
H	3.70970200	-2.50531000	-3.55707900
H	3.32709100	-3.85754700	-2.45554300
H	4.23946300	-2.42448100	-1.85852600
C	-2.86061900	0.71700200	0.40297900
C	-2.82966400	2.01791900	0.87904200
C	-3.53824900	2.32429700	2.09266400
C	-4.39801600	1.34089100	2.65624200
C	-4.44964900	0.05041900	2.07141100
C	-3.64471100	-0.30437800	1.01565100
H	-2.70893300	4.31324900	2.38746300
C	-3.40175400	3.56651900	2.77438900
C	-5.14210400	1.64519300	3.82914700
H	-5.10455500	-0.70374400	2.51225700
C	-5.01245200	2.86424700	4.44580700
C	-4.11789800	3.82670300	3.91800700
H	-5.80480100	0.87962500	4.23822300
H	-5.58031600	3.08748200	5.35004800
H	-3.98954500	4.78232500	4.42832300
C	-2.05654500	3.06160600	0.15664800
C	-2.63571700	4.33036400	-0.20082600
C	-0.74599200	2.81593100	-0.20094300
C	-4.02180500	4.61524900	-0.05112300
C	-1.79661800	5.34465900	-0.74556100
C	0.07241600	3.78564300	-0.85578400
C	-4.53000300	5.85021100	-0.37695000
H	-4.68774600	3.83621700	0.31918100
C	-2.34752300	6.61748200	-1.05649600
C	-0.44016100	5.04267800	-1.04657700
C	-3.68369900	6.87165400	-0.87028900
H	-5.59767600	6.04151600	-0.26040200
H	-1.68583400	7.38438300	-1.46454500
H	0.18075700	5.81087800	-1.51299000
H	-4.09817700	7.84967200	-1.11850700
O	-0.16649500	1.61825200	0.13743500
O	-2.15181500	0.39086300	-0.73684200
P	-0.53194700	0.22393900	-0.61289000
O	0.01563200	0.21105300	-2.03213200
C	1.38274000	3.33356700	-1.40557100
C	2.53419400	3.24558000	-0.59587800
C	1.40583900	2.87274900	-2.74184400
C	3.67410600	2.63137600	-1.12087600
C	2.56834600	2.24292700	-3.19716700
C	3.69417000	2.07468700	-2.39738400
H	4.55560900	2.55087300	-0.47971600
H	2.57827000	1.83291500	-4.21191200
C	-3.65228500	-1.72699400	0.55988800
C	-3.20820700	-2.74980000	1.42728500
C	-4.25771100	-2.05924800	-0.67526700
C	-3.44801700	-4.08079400	1.05110400
C	-4.48178700	-3.40105100	-0.98787400
C	-4.10808500	-4.43217900	-0.12256600
H	-3.11008200	-4.87542500	1.72395700
H	-4.99080200	-3.64262200	-1.92596800
C	2.65547100	3.84259700	0.80516800
C	1.60406100	3.42777300	1.84128100
C	2.76242100	5.37093000	0.73070700
H	3.62178700	3.47306500	1.18779600
H	1.40269600	2.34914600	1.81827100
H	1.96790800	3.69733200	2.84520500
H	0.64882500	3.95122800	1.69234700
H	3.56479100	5.68101700	0.04603200
H	1.81782400	5.80701800	0.37295400
H	2.97130400	5.79138500	1.72644900
C	0.30975300	3.06860000	-3.79737200

C	0.47252600	4.44993800	-4.44887300
C	-1.16406100	2.82178200	-3.45055700
H	0.55447700	2.32521100	-4.57250400
H	1.50479200	4.61374100	-4.78989100
H	-0.20173700	4.54839800	-5.31325900
H	0.21901200	5.24729800	-3.73462000
H	-1.30549400	1.87551900	-2.91747200
H	-1.61026900	3.63563500	-2.86471800
H	-1.72866300	2.76128400	-4.39404200
C	4.88347400	1.28973000	-2.91521000
C	5.48868100	0.39035100	-1.83542800
C	5.94205200	2.21300300	-3.52596300
H	4.49584300	0.63517900	-3.71313900
H	4.68982900	-0.13942900	-1.29259100
H	6.17942300	-0.34386400	-2.27710900
H	6.07105400	0.98486000	-1.11285000
H	5.51770800	2.81580400	-4.34120100
H	6.32783600	2.90639800	-2.76234400
H	6.79017500	1.63558800	-3.92493000
C	-2.51906700	-2.59484000	2.79168500
C	-3.50526000	-2.87855800	3.93473600
C	-1.71392800	-1.32752300	3.10055400
H	-1.78916900	-3.42123100	2.79685100
H	-2.96490300	-2.93708500	4.89128300
H	-4.24558900	-2.06926500	4.02215100
H	-4.04786900	-3.82292500	3.78485800
H	-1.09815300	-0.98582700	2.25982200
H	-2.35195700	-0.49291800	3.42048900
H	-1.02622600	-1.54825800	3.93038200
C	-4.73958300	-0.99926200	-1.65619000
C	-6.25245300	-1.08997700	-1.87972400
C	-3.96970900	-1.08180200	-2.97699600
H	-4.53840200	-0.01041800	-1.22605800
H	-6.79736200	-1.01189300	-0.92771600
H	-6.59163300	-0.27756300	-2.53940300
H	-6.53333000	-2.04343200	-2.35288300
H	-2.88823100	-0.98895400	-2.80423800
H	-4.16061300	-2.04136100	-3.48529800
H	-4.28325500	-0.27362100	-3.65498400
C	-4.46140700	-5.88149400	-0.40807000
C	-4.01625600	-6.35243600	-1.79355800
C	-5.96600300	-6.10420700	-0.21697300
H	-3.93249800	-6.49327100	0.34101300
H	-2.93134300	-6.23902700	-1.93081500
H	-4.26774400	-7.41351600	-1.93800300
H	-4.52495900	-5.78483100	-2.58877500
H	-6.28446800	-5.79989400	0.78978700
H	-6.53835500	-5.50825500	-0.94477500
H	-6.22826700	-7.16305000	-0.36150800
O	0.07453100	-3.47671100	0.95777800
H	-0.38872400	-2.61640400	0.88647500
H	1.18068700	-0.27391400	-2.18074200
O	-0.16400800	-0.92269200	0.27235600
H	1.47579100	-1.66316000	-0.00399500
<b>TS8<sub>ISI-Sa-3S</sub></b>			
S	-5.95421100	1.00691600	0.32260500
O	-5.75942800	1.22453300	-1.10881100
O	-5.70451300	2.10508000	1.24572500
O	-1.53482300	-1.41711100	-1.97722700
N	-3.59837500	-0.44242500	0.81414000
N	-2.72805200	0.18993700	-0.07105600
C	-7.61091500	0.41956000	0.57744900
C	-8.22860800	-0.31854000	-0.42921000
H	-7.69563900	-0.52092600	-1.35948600
C	-9.52861100	-0.77072200	-0.21542800
H	-10.03574100	-1.35071900	-0.98717100

C	-10.18297800	-0.47386400	0.98197000
H	-11.20185400	-0.82935800	1.14251400
C	-9.55022000	0.28011000	1.97149900
H	-10.07330400	0.51667500	2.89865500
C	-8.24887200	0.73801000	1.77324600
H	-7.72475800	1.33794800	2.51882300
C	-4.98304900	-0.39226800	0.84914300
C	-5.47139400	-1.45045600	1.57819600
H	-6.51446100	-1.62301900	1.82622000
C	-4.34441900	-2.22952100	1.98694200
C	-3.19201000	-1.57699100	1.49156000
C	-1.89550000	-2.07751900	1.70088900
H	-1.00436500	-1.57985000	1.31680200
C	-1.78860800	-3.23813900	2.44546200
H	-0.79474700	-3.64378300	2.63823900
C	-2.92591500	-3.90579800	2.95610700
H	-2.79097500	-4.81956200	3.53655300
C	-4.19897900	-3.41610200	2.73268600
H	-5.07685400	-3.93064300	3.12571100
C	-2.69684100	1.66767900	-0.14895800
H	-3.72013200	2.05645800	-0.12226900
C	-2.08957800	1.91900400	-1.51618600
C	-1.58765400	3.17288200	-1.85909300
H	-1.61887200	3.97441200	-1.11920900
C	-1.02180300	3.37453600	-3.11491600
H	-0.62407300	4.35665900	-3.37440600
C	-0.93654700	2.32081000	-4.02666700
H	-0.47626100	2.47765300	-5.00316900
C	-1.40542000	1.05931600	-3.67507300
H	-1.30091700	0.21764500	-4.36286900
C	-1.99573200	0.86243900	-2.42297300
C	-2.42403600	-0.52913600	-2.03847800
C	-3.83327700	-0.97656200	-2.28890800
H	-4.08974700	-1.78536300	-1.58884300
H	-3.86391900	-1.38867700	-3.31017700
H	-4.54425700	-0.14928100	-2.20184200
C	3.09156000	1.32020600	0.39796100
C	4.03701800	0.42153500	0.85804400
C	4.83700300	0.79495000	1.99368200
C	4.75179600	2.12735800	2.48808500
C	3.81867600	3.02661200	1.91026500
C	2.94183700	2.63320100	0.92837000
H	5.74307000	-1.15417800	2.32996300
C	5.69859500	-0.11805800	2.66451200
C	5.56635200	2.52246700	3.58455300
H	3.76127700	4.04782400	2.29244400
C	6.40790500	1.62555300	4.19329900
C	6.46005800	0.28713300	3.73437600
H	5.49437600	3.55180000	3.94177000
H	7.02330800	1.93472500	5.03915400
H	7.10610100	-0.43244500	4.23909100
C	4.19295800	-0.90866300	0.20972500
C	5.47082700	-1.39541200	-0.23637900
C	3.09071600	-1.71990500	0.03066500
C	6.63624000	-0.57981700	-0.26338100
C	5.57733400	-2.74055500	-0.69378200
C	3.17142600	-3.05348200	-0.46340800
C	7.84231600	-1.08536500	-0.68619400
H	6.56314800	0.46254400	0.04664900
C	6.84166100	-3.23861200	-1.11124500
C	4.41148200	-3.55040900	-0.77056100
C	7.95341300	-2.43337800	-1.10342600
H	8.72079600	-0.43894100	-0.70650700
H	6.90625500	-4.27428400	-1.45099300
H	4.50112600	-4.57409200	-1.14260000
H	8.91787200	-2.82353800	-1.43112600

O	1.84807700	-1.25899900	0.40773800
O	2.28289600	0.96602500	-0.66818100
P	1.08844500	-0.09811900	-0.43381600
O	0.73218600	-0.59786000	-1.83942900
C	1.90172200	-3.81718600	-0.64344000
C	1.32714500	-4.49668000	0.45601700
C	1.23482900	-3.78442200	-1.88737600
C	0.07579700	-5.09938100	0.29739100
C	-0.03472000	-4.37153700	-1.96609200
C	-0.64072400	-5.02246900	-0.89590800
H	-0.35059400	-5.63565300	1.14737000
H	-0.57263200	-4.31633100	-2.91827800
C	1.90493000	3.59211300	0.44012200
C	0.86649900	4.02336400	1.29424200
C	2.05677300	4.17476600	-0.84032700
C	0.04502900	5.07251300	0.85432100
C	1.22231800	5.22913900	-1.21418000
C	0.22115500	5.71298200	-0.36872400
H	-0.76233400	5.40660500	1.51343300
H	1.37867800	5.70052400	-2.18892300
C	2.01371100	-4.71466800	1.80578300
C	2.51728900	-3.47201400	2.55155800
C	3.12091600	-5.77068800	1.70101800
H	1.22862800	-5.15274600	2.44381700
H	1.80518100	-2.63722600	2.49109000
H	2.66477500	-3.72454200	3.61226500
H	3.48544900	-3.12368900	2.16594300
H	2.74677300	-6.69241400	1.23329400
H	3.96199000	-5.39548700	1.10042200
H	3.50772200	-6.02007500	2.70085300
C	1.77113700	-3.27376900	-3.23370000
C	2.14777400	-4.49315300	-4.09197000
C	2.91483300	-2.25710600	-3.31369700
H	0.89956200	-2.79103500	-3.70620500
H	1.31603000	-5.20476500	-4.18528800
H	2.45156200	-4.17623900	-5.10097900
H	2.99557300	-5.02654900	-3.63375300
H	2.77951500	-1.39991100	-2.64706300
H	3.89218800	-2.71411600	-3.11258100
H	2.94499900	-1.86864600	-4.34301700
C	-2.04415100	-5.58122300	-1.05517200
C	-3.06356600	-4.43570100	-1.04030600
C	-2.41044400	-6.63847100	-0.01753700
H	-2.08244800	-6.05265000	-2.05212000
H	-2.78043600	-3.65410600	-1.75843000
H	-4.07279100	-4.80378300	-1.28220600
H	-3.09463500	-3.97276000	-0.04053700
H	-1.66716200	-7.44798600	0.02231800
H	-2.48944700	-6.18952500	0.98492200
H	-3.38887400	-7.07996800	-0.25554800
C	0.54208600	3.51311900	2.70453300
C	1.06763500	4.48765800	3.76841800
C	0.90782300	2.07461900	3.08447600
H	-0.55855900	3.56301800	2.74600400
H	0.69233800	4.20172500	4.76226100
H	2.16706900	4.46538100	3.80868300
H	0.75438800	5.52126500	3.56419900
H	0.67480700	1.35825500	2.28711000
H	1.96735100	1.96450500	3.35092600
H	0.31863500	1.79122000	3.96944700
C	3.14750800	3.73830400	-1.80897900
C	4.12902900	4.88040200	-2.09108600
C	2.54879600	3.17825200	-3.10193000
H	3.72425500	2.92897300	-1.34337200
H	4.57126800	5.26001800	-1.15850300
H	4.94373100	4.53463100	-2.74450600

H	3.62979700	5.72209800	-2.59506500
H	1.87101900	2.33987700	-2.88800800
H	1.98102800	3.95237300	-3.64319300
H	3.34670200	2.81908900	-3.76922600
C	-0.60305200	6.93893600	-0.72209200
C	-1.19987300	6.89379700	-2.12936200
C	0.24244900	8.20421100	-0.53293300
H	-1.43806200	6.98113000	-0.00385200
H	-1.85254600	6.02026500	-2.26695800
H	-1.80021900	7.79579600	-2.31791000
H	-0.41130600	6.86070500	-2.89754300
H	0.64326200	8.26181800	0.48871900
H	1.09560800	8.20275100	-1.22917400
H	-0.35475400	9.10801800	-0.72551900
O	-2.01421000	2.27606000	0.88618500
H	-1.07815100	2.01502600	0.81409100
H	-0.33106500	-0.99759600	-1.93376900
O	-0.03469700	0.40243200	0.41142100
H	-1.77167500	-0.06444500	0.22213000

**TS9<sub>IrRe-Ra-3S</sub>**

S	-5.23118900	-1.99805900	1.68287600
O	-4.42270700	-1.24441700	2.64867300
O	-5.63317500	-3.36040300	1.99501600
O	-0.30303200	-2.96982600	-1.43824800
N	-3.08580100	-1.63649000	-0.21041200
N	-1.89128400	-1.98306900	0.43687300
C	-6.71538100	-1.05269500	1.40983700
C	-6.66784000	0.32954900	1.57499000
H	-5.73531700	0.80984400	1.87673400
C	-7.83500500	1.06266500	1.37389400
H	-7.82141600	2.14624900	1.49941800
C	-9.01954300	0.40925700	1.02689500
H	-9.93075600	0.98836300	0.87106000
C	-9.05156200	-0.97978600	0.89638500
H	-9.98546900	-1.48491800	0.64737400
C	-7.89192100	-1.72752300	1.09629900
H	-7.88702700	-2.81637200	1.02436300
C	-4.41967700	-1.93974800	0.08700100
C	-5.17244800	-1.85829300	-1.05621300
H	-6.25472300	-1.94514000	-1.10325500
C	-4.30154100	-1.49937700	-2.12895500
C	-3.01964800	-1.32620700	-1.57080000
C	-1.94240500	-0.85550600	-2.33592300
H	-0.95885400	-0.67276400	-1.91342200
C	-2.17608100	-0.61715800	-3.67675200
H	-1.35558600	-0.24272300	-4.28986700
C	-3.44270800	-0.83425800	-4.26422000
H	-3.57646100	-0.64658800	-5.33051100
C	-4.51186100	-1.25824400	-3.50109200
H	-5.50189300	-1.39507800	-3.93906800
C	-1.89471200	-2.33077600	1.88538800
H	-2.12282100	-1.43085200	2.47545200
C	-0.47926100	-2.81543300	2.07241600
C	0.25473600	-2.73729500	3.24636800
H	-0.18301900	-2.30144100	4.14624200
C	1.57255300	-3.19719500	3.24215700
H	2.17080600	-3.14097700	4.15279800
C	2.14553100	-3.68469200	2.06732700
H	3.18732500	-4.00446400	2.06249200
C	1.40904400	-3.74140400	0.88175700
H	1.87584500	-4.08011900	-0.04546200
C	0.07864000	-3.33480200	0.90742900
C	-0.82522800	-3.33447300	-0.29644300
C	-1.79990500	-4.47020600	-0.47462600
H	-2.55250100	-4.17603500	-1.22163400
H	-2.28170700	-4.75560100	0.46389200

H	-1.22970600	-5.31738800	-0.88196100
C	1.01592300	2.40286400	0.12172400
C	2.15434200	2.76710700	0.81653300
C	2.02682500	3.71733600	1.88631900
C	0.77228000	4.35966600	2.08964900
C	-0.33943200	3.99619100	1.28344100
C	-0.26391200	2.99098500	0.35058900
H	4.05087800	3.51472100	2.65024900
C	3.09675400	4.02827600	2.77059800
C	0.64169800	5.32425900	3.12574100
H	-1.29608600	4.49815100	1.44691600
C	1.69961500	5.62055200	3.94917800
C	2.93593300	4.95314800	3.77466400
H	-0.32431100	5.81525000	3.26128500
H	1.58732900	6.35734400	4.74571100
H	3.76727200	5.17046000	4.44676700
C	3.46255800	2.16664900	0.43490700
C	4.59812300	2.98906100	0.11152400
C	3.59095000	0.79401500	0.32126000
C	4.52497100	4.40872100	0.03016300
C	5.84851600	2.36602600	-0.16742200
C	4.81269000	0.16133500	-0.05357600
C	5.63895900	5.15939000	-0.26029300
H	3.56759500	4.90321700	0.19121000
C	6.98678300	3.16962800	-0.44980400
C	5.92233600	0.94888800	-0.22955800
C	6.89029900	4.53807600	-0.48835900
H	5.55506900	6.24526400	-0.32309100
H	7.93748400	2.67161800	-0.65127600
H	6.87454000	0.48102000	-0.49015000
H	7.76772700	5.14642400	-0.71163900
O	2.52983900	-0.02163000	0.62434000
O	1.11889100	1.43042100	-0.85033200
P	1.17268600	-0.09979300	-0.27101600
O	1.31740200	-1.04901800	-1.42847100
C	4.84094300	-1.30383400	-0.34761500
C	5.07337500	-2.25464400	0.67026100
C	4.65891300	-1.72345000	-1.68505600
C	5.11605900	-3.61076100	0.32732100
C	4.67709100	-3.09785400	-1.95685300
C	4.90894600	-4.05915700	-0.97711400
H	5.33240600	-4.33556300	1.11771900
H	4.53177800	-3.42508800	-2.99092700
C	-1.47585400	2.57927000	-0.42228300
C	-2.60393300	2.01227800	0.21785500
C	-1.52988300	2.85847900	-1.80817700
C	-3.74728300	1.77652300	-0.55667700
C	-2.72087400	2.65309000	-2.51165400
C	-3.85938900	2.13620300	-1.89783600
H	-4.61488800	1.31619800	-0.06996500
H	-2.75122600	2.91994100	-3.56951300
C	5.40978100	-1.91536300	2.12238000
C	4.50889700	-0.90301100	2.83818800
C	6.88513200	-1.51528700	2.25437000
H	5.29420000	-2.86858800	2.66549700
H	3.44675600	-1.06763600	2.61463500
H	4.65870100	-0.99693200	3.92472300
H	4.75916000	0.13222100	2.56751100
H	7.54524700	-2.27364700	1.80971400
H	7.07094600	-0.55662400	1.74837000
H	7.15658900	-1.39451500	3.31409900
C	4.59648900	-0.82540200	-2.92735800
C	6.02084500	-0.58669700	-3.45155300
C	3.82358900	0.49636800	-2.89206900
H	4.08267500	-1.44625400	-3.67810100
H	6.57230200	-1.53073500	-3.56685600

H	5.98793100	-0.07965100	-4.42763200
H	6.58457300	0.05690600	-2.75988100
H	2.81909600	0.36742000	-2.47634600
H	4.34710500	1.28876900	-2.34046200
H	3.70816800	0.84998100	-3.92836900
C	4.91579600	-5.53566200	-1.33197500
C	3.55509000	-6.17456900	-1.03361700
C	6.04130000	-6.30897900	-0.64335200
H	5.08188200	-5.59791100	-2.41983100
H	2.75034800	-5.66888400	-1.58724700
H	3.54985000	-7.23820000	-1.31573600
H	3.32581500	-6.10756500	0.04222000
H	7.01723600	-5.83404600	-0.81667600
H	5.87976200	-6.36817300	0.44360700
H	6.08492500	-7.34023400	-1.02279500
C	-2.80346300	1.66653300	1.70219000
C	-3.77293800	2.67245000	2.34501700
C	-1.61262300	1.45797000	2.64308600
H	-3.33218400	0.69761600	1.67082300
H	-4.06774700	2.32817600	3.34834200
H	-3.28918000	3.65552000	2.45474200
H	-4.68079900	2.82082700	1.74122200
H	-0.79596800	0.90038700	2.17112000
H	-1.21030100	2.40627900	3.02400700
H	-1.97207100	0.89071900	3.51758000
C	-0.35563700	3.44819100	-2.57892600
C	-0.69231100	4.83822400	-3.12935300
C	0.10207400	2.50107000	-3.69236600
H	0.49079800	3.57589400	-1.89368900
H	-0.99939900	5.51813500	-2.32143200
H	0.18360000	5.27362800	-3.63292500
H	-1.51181400	4.79261200	-3.86272000
H	0.36336000	1.51661800	-3.27865100
H	-0.68778000	2.36925000	-4.44919200
H	0.99022300	2.90588100	-4.20050800
C	-5.20940300	2.02030900	-2.58857800
C	-5.16201900	2.30907200	-4.08535600
C	-6.22779800	2.94572600	-1.90836000
H	-5.55483100	0.98237400	-2.44549300
H	-4.42783400	1.67332500	-4.59795600
H	-6.14767100	2.13147500	-4.53957200
H	-4.89500400	3.36102200	-4.27224900
H	-6.32821800	2.71657900	-0.83784100
H	-5.90941900	3.99549800	-2.00106900
H	-7.21956800	2.84279300	-2.37423800
O	-2.80773400	-3.35089400	2.12118500
H	-3.36111600	-3.12098600	2.87846100
H	0.43191000	-2.24695000	-1.39214000
O	0.01061500	-0.29925400	0.66191800
H	-1.19244000	-1.15637600	0.38674500

**TS10***1Re-Sa-3S*

S	-3.16783200	-0.27614100	1.36957800
O	-2.37286800	0.52473400	2.28556900
O	-2.53109000	-0.88674500	0.18797100
O	-1.56594400	2.89468900	0.74315100
N	-4.50268400	1.62267000	-0.07225600
N	-3.37161700	1.74994500	-0.80420500
C	-3.90434900	-1.59390300	2.31081800
C	-3.82206700	-1.53383300	3.69758800
H	-3.32725500	-0.68296800	4.16791900
C	-4.35864900	-2.58591800	4.43951400
H	-4.29999700	-2.56739200	5.52834100
C	-4.96300700	-3.66138900	3.78856400
H	-5.38046800	-4.48247600	4.37325800
C	-5.03506300	-3.70014500	2.39349200
H	-5.50306500	-4.55035700	1.89504500

C	-4.49718300	-2.65915700	1.64096900
H	-4.50511500	-2.66601800	0.54933200
C	-4.59964300	0.65616600	0.90334700
C	-5.81668100	0.69932000	1.53168500
H	-6.14999000	0.06145500	2.34559500
C	-6.53628800	1.76891500	0.90489300
C	-5.69310300	2.33000800	-0.08878400
C	-6.10213200	3.41173100	-0.88553300
H	-5.44718300	3.79938100	-1.66240500
C	-7.36630000	3.92277700	-0.65654900
H	-7.71438400	4.76554900	-1.25585100
C	-8.22340500	3.37867700	0.32862800
H	-9.21386900	3.81246100	0.47225000
C	-7.82335800	2.30842400	1.10437000
H	-8.48402300	1.88648000	1.86338300
C	-3.36237200	1.44162100	-2.18508500
H	-3.68169500	0.39405900	-2.36059600
C	-1.90941700	1.65075600	-2.54782900
C	-1.25793700	1.10924300	-3.64884700
H	-1.79738000	0.46239900	-4.34570400
C	0.10182200	1.37197500	-3.84088900
H	0.62280700	0.94323800	-4.69836900
C	0.79945300	2.14902100	-2.91901200
H	1.86740700	2.33536700	-3.04799300
C	0.14446900	2.68571600	-1.80702000
H	0.69191200	3.26125500	-1.06510600
C	-1.21373700	2.45325200	-1.63694800
C	-2.02517700	3.01192800	-0.49595900
C	-2.64450400	4.36427500	-0.72474500
H	-3.41908400	4.54320900	0.03386600
H	-3.07388700	4.42340700	-1.73154400
H	-1.85600100	5.12531100	-0.60777800
C	2.12651000	-2.28321700	0.14201400
C	3.45700500	-1.91722600	0.19219600
C	4.43086100	-2.76633800	-0.43940500
C	4.01025600	-4.02650600	-0.95242900
C	2.62719900	-4.34267000	-0.96788700
C	1.67509300	-3.45792400	-0.52177100
H	6.13123800	-1.42053800	-0.25425600
C	5.79824600	-2.40102000	-0.59297800
C	4.96819100	-4.90598500	-1.52762500
H	2.30400700	-5.28197100	-1.42095900
C	6.28662900	-4.53910500	-1.62848300
C	6.69837900	-3.26411300	-1.17046100
H	4.62687200	-5.87234700	-1.90466100
H	7.01398700	-5.21659000	-2.07764200
H	7.73989700	-2.95997100	-1.28290000
C	3.84130400	-0.63026500	0.82532600
C	4.87537700	-0.55628900	1.81996600
C	3.20292700	0.53564100	0.44224500
C	5.45754400	-1.71379700	2.40866700
C	5.32057000	0.72137100	2.25879400
C	3.61408600	1.82083700	0.90022300
C	6.44979300	-1.59996300	3.35215800
H	5.09925900	-2.69942200	2.11184700
C	6.35967200	0.80820700	3.22552000
C	4.68631100	1.88597400	1.75494800
C	6.91804300	-0.32648100	3.75831500
H	6.87593300	-2.49958500	3.79826300
H	6.69349600	1.79758600	3.54443100
H	5.02016600	2.86478400	2.10827500
H	7.71015700	-0.25172100	4.50447900
O	2.14466700	0.45712600	-0.46129900
O	1.18840900	-1.49194500	0.78092200
P	0.73662800	-0.07931700	0.13401800
O	0.09546900	0.81162300	1.11554100



C	2.91592400	3.07035200	0.47283200
C	3.31060800	3.69705200	-0.73857400
C	1.91603000	3.64844200	1.28363600
C	2.66611300	4.87124900	-1.12878800
C	1.26862200	4.80175600	0.80132600
C	1.62141900	5.42912000	-0.38611000
H	2.98270900	5.35299500	-2.05844700
H	0.44309700	5.21386700	1.38795300
C	0.23676300	-3.70468300	-0.83116800
C	-0.19991400	-3.59852000	-2.17382500
C	-0.65281800	-4.11830200	0.17621000
C	-1.50722700	-3.99543100	-2.46006500
C	-1.95085300	-4.51808300	-0.17262700
C	-2.38315800	-4.50408900	-1.49768500
H	-1.84986600	-3.93466600	-3.49856800
H	-2.61871600	-4.87000900	0.61763700
C	4.48994800	3.26708000	-1.61647600
C	4.66667900	1.77856700	-1.94431700
C	5.79878400	3.84521400	-1.06133400
H	4.30768000	3.77025300	-2.57972900
H	3.71041600	1.27354500	-2.14002900
H	5.29211500	1.68682700	-2.84479800
H	5.18107500	1.23781000	-1.13832500
H	5.72276800	4.93143700	-0.91173100
H	6.04544600	3.38094800	-0.09491000
H	6.63089100	3.64521100	-1.75331800
C	1.45028600	3.22362300	2.68654400
C	1.76730100	4.35972200	3.67627000
C	1.92644200	1.91750100	3.32817000
H	0.35419000	3.14716400	2.59519100
H	1.34181100	5.32423700	3.37085700
H	1.37234500	4.11275700	4.67248300
H	2.85794400	4.48683600	3.76640800
H	1.80792400	1.04318200	2.68385600
H	2.97088300	1.98008900	3.66348200
H	1.30550300	1.74361300	4.21925900
C	0.89885000	6.67363200	-0.86544200
C	0.34273400	6.49971200	-2.28174000
C	1.80770900	7.90379700	-0.77929400
H	0.04885800	6.83346100	-0.18131200
H	-0.28990300	5.60335300	-2.35906600
H	-0.25600700	7.37562500	-2.57272400
H	1.15745600	6.39548900	-3.01457900
H	2.17982800	8.05058600	0.24431300
H	2.67930000	7.78761900	-1.44202100
H	1.26742400	8.81130100	-1.08740300
C	0.62470200	-3.15847500	-3.39286200
C	1.19914100	-4.37415900	-4.13604600
C	1.70402500	-2.08157100	-3.23251300
H	-0.13067100	-2.71830200	-4.06460100
H	1.59922700	-4.06612700	-5.11373600
H	2.02584900	-4.82702600	-3.56993300
H	0.43304100	-5.14525900	-4.30195600
H	1.33978400	-1.21441200	-2.66998200
H	2.61938900	-2.45811600	-2.75686300
H	1.98946900	-1.73226300	-4.23711900
C	-0.21078200	-4.21312300	1.62842700
C	-0.20410800	-5.66763100	2.10877600
C	-1.06687900	-3.32996700	2.53715500
H	0.82112500	-3.84297300	1.69375400
H	0.44165000	-6.29154900	1.47368400
H	0.16318400	-5.73099600	3.14390100
H	-1.21826800	-6.09570500	2.08448900
H	-1.08774200	-2.29261800	2.17239800
H	-2.10275700	-3.70179400	2.58874200
H	-0.66251100	-3.32592600	3.56065400

C	-3.70787500	-5.08568300	-1.96990000
C	-4.70067200	-5.39026700	-0.85430400
C	-3.44900300	-6.35591600	-2.79244500
H	-4.16766200	-4.33948200	-2.64056500
H	-4.94151700	-4.49336900	-0.27095500
H	-5.63775800	-5.78016900	-1.27626400
H	-4.30275100	-6.15241200	-0.16622900
H	-2.77544300	-6.16091900	-3.63813600
H	-2.97890500	-7.12421600	-2.15952800
H	-4.39098100	-6.76358900	-3.18855300
O	-4.20852400	2.31697800	-2.92746600
H	-4.13802700	2.09058100	-3.86239900
H	-1.06151600	2.05835400	0.89381400
O	-0.10751400	-0.44005400	-1.14253700
H	-1.05490400	-0.56046000	-0.88171200

**Int7<sub>IR-Ra-3S</sub>**

S	-2.87173600	-0.19650400	1.78649200
O	-2.21375200	0.80599800	2.63931000
O	-2.13663400	-0.82552600	0.69885500
O	-2.87276300	0.11383000	-1.91252700
N	-4.20667900	1.71404400	0.37152000
N	-3.11265900	1.95307400	-0.40722600
C	-3.51443900	-1.45478100	2.85512600
C	-3.71838300	-1.16795500	4.20270600
H	-3.47691600	-0.17626000	4.58758100
C	-4.21557800	-2.17947000	5.02172900
H	-4.38172800	-1.98620900	6.08202500
C	-4.49003100	-3.44082900	4.48803800
H	-4.87606900	-4.22821700	5.13715200
C	-4.26660200	-3.70726900	3.13613400
H	-4.47145800	-4.69883600	2.72961700
C	-3.76956200	-2.70617700	2.30437300
H	-3.55750900	-2.87435300	1.24731100
C	-4.33921300	0.61603000	1.20416100
C	-5.60351900	0.54432900	1.71916600
H	-5.96651400	-0.19303900	2.43001800
C	-6.31868900	1.66846600	1.17939100
C	-5.41800100	2.38554200	0.35700800
C	-5.77934300	3.57775100	-0.28555000
H	-5.06486500	4.12855200	-0.89735100
C	-7.07447200	4.02971700	-0.09944000
H	-7.38887500	4.95746400	-0.57939100
C	-7.99626800	3.32060000	0.70236300
H	-9.00773600	3.71034400	0.82133200
C	-7.63157000	2.15036000	1.34290900
H	-8.34198800	1.61042300	1.97051500
C	-2.20198700	3.02111500	-0.07043000
H	-2.75318900	3.93891300	0.20933700
C	-1.41380200	3.15678400	-1.34415700
C	-0.25934900	3.90484400	-1.55266600
H	0.16644100	4.51835400	-0.75512200
C	0.36380900	3.81208300	-2.79665200
H	1.27307600	4.38472700	-2.98307100
C	-0.14681100	2.97309000	-3.79335900
H	0.37017500	2.90270200	-4.75183500
C	-1.28066200	2.19856900	-3.55858700
H	-1.64983000	1.49586300	-4.30797500
C	-1.90707200	2.30467300	-2.32228900
C	-3.07435200	1.47710600	-1.82150900
C	-4.36610400	1.75187100	-2.58321800
H	-4.24330100	1.36292700	-3.60246100
H	-4.59155700	2.82298300	-2.63572900
H	-5.20417500	1.21760500	-2.11228900
C	3.18601500	0.07237500	0.44895200
C	3.56123900	-1.21514100	0.78867800
C	4.47833600	-1.39054100	1.88163300

C	5.10769400	-0.24460900	2.44468500
C	4.75477100	1.04758600	1.97356100
C	3.76191900	1.23436600	1.04366700
H	4.26987500	-3.54749300	2.04245700
C	4.77393500	-2.66570200	2.43847700
C	6.04641700	-0.40980900	3.49950000
H	5.25073100	1.92017100	2.40394500
C	6.32815400	-1.65622400	4.00118800
C	5.67204900	-2.79330400	3.47102300
H	6.52709500	0.47933700	3.91286100
H	7.04397500	-1.77238600	4.81604800
H	5.87650000	-3.77966600	3.88972900
C	3.03222400	-2.36863300	0.01174200
C	3.90928400	-3.34793000	-0.57490000
C	1.67536100	-2.48438400	-0.22279200
C	5.32805300	-3.22960800	-0.55224000
C	3.34225900	-4.47466100	-1.23819800
C	1.10219000	-3.54792500	-0.97850900
C	6.12849700	-4.20028700	-1.10522300
H	5.78319400	-2.34985000	-0.09897200
C	4.19644600	-5.47093600	-1.78553900
C	1.93496200	-4.54743800	-1.41441500
C	5.56101400	-5.34502700	-1.71462200
H	7.21270700	-4.08212300	-1.08060900
H	3.74043800	-6.33127300	-2.27967900
H	1.51453900	-5.38867800	-1.97022900
H	6.20828700	-6.11147000	-2.14287600
O	0.81227000	-1.55850800	0.32092100
O	2.26227100	0.26685300	-0.55601900
P	0.69344700	-0.05753900	-0.25986100
O	-0.11748000	0.13917200	-1.47664800
C	-0.33350100	-3.46059800	-1.38140200
C	-1.37148200	-3.95247800	-0.55950300
C	-0.63505100	-2.81537700	-2.60206800
C	-2.69329600	-3.75296600	-0.96448100
C	-1.98140400	-2.58799000	-2.91398800
C	-3.02418700	-3.01936400	-2.10290600
H	-3.49572900	-4.17051900	-0.34920700
H	-2.22124600	-2.02845300	-3.82205600
C	3.34043800	2.61035800	0.64269800
C	2.74138400	3.48981600	1.57136900
C	3.62489400	3.05824200	-0.67088400
C	2.46861200	4.80188700	1.15362100
C	3.35141600	4.38157500	-1.01916500
C	2.78080500	5.27989000	-0.11522100
H	2.00479900	5.48635000	1.87137800
H	3.61630800	4.72351700	-2.02381700
C	-1.15864000	-4.69815100	0.75577600
C	-0.47949000	-3.86310600	1.84823500
C	-0.47771600	-6.06055800	0.58633200
H	-2.17781300	-4.91052400	1.12050600
H	-0.87343300	-2.83762000	1.86683700
H	-0.64747100	-4.33105100	2.83074700
H	0.60768000	-3.80050300	1.69577900
H	-0.97344200	-6.65858300	-0.19219200
H	0.58093000	-5.94811800	0.31604100
H	-0.52054600	-6.62253400	1.53183600
C	0.35540400	-2.43825700	-3.71179800
C	0.56816000	-3.65868900	-4.62055700
C	1.70618200	-1.79298900	-3.38419000
H	-0.18761500	-1.68747300	-4.30710400
H	-0.38958800	-4.08797700	-4.94734500
H	1.14885500	-3.37743900	-5.51216900
H	1.12913000	-4.44212800	-4.08893200
H	1.59877200	-0.93400000	-2.71398300
H	2.43294400	-2.49758200	-2.95880100

H	2.13826900	-1.41857800	-4.32531800
C	-4.46550200	-2.69531400	-2.44254900
C	-5.19602500	-2.08335600	-1.24430500
C	-5.20265200	-3.92474600	-2.98114700
H	-4.43374500	-1.92940300	-3.23353600
H	-4.60572700	-1.24961100	-0.83850800
H	-6.18697600	-1.70642600	-1.54104900
H	-5.35733400	-2.82983700	-0.44898100
H	-4.70069000	-4.33187800	-3.87037800
H	-5.23392900	-4.72016300	-2.21980800
H	-6.23971500	-3.67406800	-3.25118000
C	2.38619400	3.22056100	3.04109400
C	3.42322400	3.87764800	3.96459700
C	2.09452000	1.79406100	3.51832400
H	1.44556600	3.77855500	3.17953800
H	3.09866800	3.80497700	5.01345300
H	4.39534900	3.36874100	3.88016400
H	3.57611600	4.93841200	3.72071300
H	1.51065700	1.21915300	2.79148200
H	3.00890000	1.23350300	3.75077700
H	1.50964800	1.85683300	4.44850700
C	4.29395500	2.17271200	-1.71441800
C	5.68954400	2.70045300	-2.06476500
C	3.42193100	2.01840600	-2.96339400
H	4.43157200	1.17075200	-1.29046900
H	6.32044300	2.77503200	-1.16705100
H	6.18540000	2.02856700	-2.78109100
H	5.63536700	3.69978500	-2.52341800
H	2.41660500	1.66272700	-2.69731400
H	3.32181600	2.97658900	-3.49908400
H	3.87536400	1.29540600	-3.65819900
C	2.58730400	6.74753200	-0.45475300
C	1.93285600	6.98094400	-1.81673900
C	3.93037400	7.48238800	-0.36618100
H	1.92165200	7.16953300	0.31626200
H	0.95329900	6.48783600	-1.88808600
H	1.78603400	8.05709400	-1.99032700
H	2.56615700	6.60289900	-2.63450400
H	4.38780200	7.35122800	0.62445900
H	4.63277300	7.08575100	-1.11569800
H	3.80254900	8.55924200	-0.55273800
O	-1.31340400	2.72503200	0.99132500
H	-1.80059500	2.38234000	1.76686400
H	-1.97051900	-0.10678200	-1.60216800
O	0.32661700	0.75666200	1.01683500
H	-0.30262600	1.53821700	0.88711900

**Int8<sub>IR-Sa-3S</sub>**

S	5.70605500	0.57923600	-0.19035000
O	5.71892000	0.28864400	1.23979100
O	5.38145400	1.93560700	-0.62948500
O	1.67877500	-2.45826200	1.45819400
N	3.30620200	-0.78988200	-0.61468000
N	2.71852500	-0.49265800	0.58369300
C	7.28540200	0.14398700	-0.87893500
C	7.97708900	-0.93939100	-0.34149500
H	7.54743900	-1.50124700	0.48962800
C	9.21487000	-1.27069100	-0.88619000
H	9.77651900	-2.11458000	-0.48425800
C	9.73800700	-0.51888000	-1.94091500
H	10.70902900	-0.78306900	-2.36230300
C	9.03419900	0.56999500	-2.45603000
H	9.45446500	1.15702400	-3.27339500
C	7.79282500	0.91313900	-1.92201400
H	7.21714100	1.76320400	-2.29087100
C	4.61543900	-0.55037700	-1.01629300
C	4.84389200	-1.10646500	-2.24868800

H	5.76691900	-1.03841700	-2.81838700
C	3.63041700	-1.75854700	-2.63572700
C	2.69234300	-1.54605200	-1.59862700
C	1.39523300	-2.08311600	-1.64539700
H	0.71282900	-1.98400100	-0.80341800
C	1.05099800	-2.78989700	-2.78199100
H	0.04784900	-3.21336300	-2.84890700
C	1.96574900	-2.99498600	-3.84165900
H	1.64839300	-3.56404400	-4.71635800
C	3.25238500	-2.49900500	-3.77453600
H	3.96548500	-2.66866100	-4.58260700
C	2.63421700	0.87279200	1.02584200
H	3.56516900	1.43516100	0.86114000
C	2.35271900	0.70593800	2.49513400
C	2.04501700	1.68871000	3.42893600
H	1.96986000	2.73767600	3.13414300
C	1.80457300	1.29729800	4.74645800
H	1.56067100	2.04912900	5.49878900
C	1.85598700	-0.05228200	5.10904600
H	1.65460900	-0.33967600	6.14212300
C	2.14870100	-1.03315400	4.16075300
H	2.16286700	-2.09121200	4.42932400
C	2.40833400	-0.63269700	2.85506300
C	2.68672400	-1.52101000	1.65940500
C	3.98959000	-2.29986500	1.75641400
H	4.16745600	-2.83293600	0.80960600
H	3.88874600	-3.04936600	2.55252800
H	4.82815800	-1.62893400	1.97160400
C	-2.88193500	1.85580500	-0.24634600
C	-4.04042900	1.26153300	-0.71229600
C	-4.85776500	2.01008200	-1.63066500
C	-4.55114800	3.38055700	-1.86889700
C	-3.37455500	3.94406300	-1.30664700
C	-2.49155700	3.18664400	-0.57874700
H	-6.17360100	0.37529800	-2.19670400
C	-5.95544700	1.43480000	-2.32901400
C	-5.38404700	4.14467500	-2.73110500
H	-3.13452800	4.98722900	-1.52116400
C	-6.45575400	3.56816100	-3.36627100
C	-6.73065500	2.19306500	-3.17358400
H	-5.14020200	5.19673000	-2.89278600
H	-7.08391900	4.16026700	-4.03302800
H	-7.56171100	1.72807500	-3.70556300
C	-4.40137400	-0.11581600	-0.27461600
C	-5.70643100	-0.43760100	0.24332600
C	-3.46205100	-1.12766600	-0.32109100
C	-6.69213000	0.55100200	0.51889500
C	-6.02467800	-1.79896400	0.52147000
C	-3.72784500	-2.47214900	0.06839900
C	-7.93542500	0.19979300	0.98801100
H	-6.45050300	1.60209600	0.36478400
C	-7.32522100	-2.13257700	0.98861300
C	-5.01558600	-2.79473300	0.41165100
C	-8.26623400	-1.15817900	1.20986400
H	-8.67105400	0.97725300	1.19866200
H	-7.55274100	-3.18215000	1.18559200
H	-5.25795600	-3.82477500	0.68224100
H	-9.25905800	-1.42418400	1.57491500
O	-2.19640400	-0.86228300	-0.80329300
O	-2.06558800	1.16848000	0.62842900
P	-1.12998800	-0.03041000	0.07026400
O	-0.46203700	-0.72413000	1.18949600
C	-2.56736800	-3.40202200	0.20843700
C	-2.02637300	-4.08842400	-0.90319000
C	-1.95220300	-3.49896900	1.47624800
C	-0.85530300	-4.83063700	-0.72718200

C	-0.77373200	-4.24972300	1.58235300
C	-0.19510200	-4.90466500	0.50083800
H	-0.44232500	-5.36333200	-1.58875500
H	-0.27436900	-4.30435700	2.55340900
C	-1.15692900	3.71725600	-0.16653500
C	-0.17533300	4.02584000	-1.13945300
C	-0.88354000	3.93226500	1.20214000
C	1.04151700	4.56381700	-0.69633100
C	0.34454400	4.48233100	1.58334100
C	1.32592400	4.81340700	0.64900900
H	1.80189000	4.80913400	-1.44546600
H	0.52124300	4.67125100	2.64403300
C	-2.68979300	-4.16337600	-2.27800600
C	-2.96896700	-2.83480500	-2.99056300
C	-3.95417500	-5.03014500	-2.23111300
H	-1.96377500	-4.70255000	-2.90898600
H	-2.11006400	-2.15243200	-2.94267900
H	-3.19629000	-3.03595000	-4.04831700
H	-3.83976400	-2.31493400	-2.56707000
H	-3.74628800	-6.00988700	-1.77813700
H	-4.74219900	-4.53816900	-1.64266200
H	-4.34596900	-5.19232100	-3.24674200
C	-2.49724800	-2.96089800	2.80620700
C	-3.46703700	-3.98769500	3.40962600
C	-3.10135800	-1.55428300	2.89468600
H	-1.61297400	-2.93673900	3.46218600
H	-3.02034400	-4.99165100	3.43937700
H	-3.74453800	-3.69768800	4.43436500
H	-4.39165800	-4.04375300	2.81583800
H	-2.45421100	-0.80052300	2.43329800
H	-4.10701000	-1.48548500	2.45975500
H	-3.19632800	-1.29357400	3.96007100
C	1.08350100	-5.70312000	0.66823100
C	2.17261600	-5.26433500	-0.31229700
C	0.80271200	-7.20520600	0.55466700
H	1.45150800	-5.49572500	1.68583700
H	2.38151500	-4.19376100	-0.18680400
H	3.09791100	-5.83417600	-0.13573800
H	1.86838600	-5.43493900	-1.35725500
H	0.04111500	-7.52489400	1.28036700
H	0.43438200	-7.45555400	-0.45253100
H	1.71915400	-7.78785000	0.73236100
C	-0.28874600	3.89069100	-2.66449400
C	-0.65213300	5.24120000	-3.29886500
C	-1.14408400	2.77005800	-3.26781500
H	0.74526600	3.67431500	-2.97780400
H	-0.57705900	5.17593400	-4.39449100
H	-1.68572400	5.52520300	-3.05279400
H	0.01268300	6.04529400	-2.95254700
H	-1.04534300	1.82939800	-2.71398900
H	-2.20747200	3.03367100	-3.32396100
H	-0.80072400	2.59317200	-4.29800900
C	-1.90258300	3.64166600	2.29379700
C	-2.39169300	4.94419200	2.93658300
C	-1.34267700	2.67457200	3.34043400
H	-2.77604700	3.16138100	1.83622600
H	-2.83128500	5.61641000	2.18538400
H	-3.15500100	4.73235600	3.69984800
H	-1.56421200	5.47988900	3.42696100
H	-0.93021600	1.77106000	2.86846900
H	-0.54240800	3.14729900	3.93170600
H	-2.13430100	2.36987100	4.04106700
C	2.68299100	5.38375400	1.03165900
C	3.77408300	4.31096200	0.92179300
C	2.70538900	6.02947300	2.41461000
H	2.91083900	6.16566000	0.28797900

H	3.79550800	3.82379300	-0.06420900
H	4.77183900	4.74126300	1.09118600
H	3.62740200	3.53080600	1.68735600
H	1.90643100	6.77583800	2.52894800
H	2.58545400	5.27523300	3.20814600
H	3.67063100	6.52662000	2.58450600
O	1.60890500	1.56825800	0.32750100
H	1.79315200	2.51881500	0.26381500
H	0.82291900	-1.98485200	1.42598000
O	-0.22619800	0.54597300	-1.06871300
H	0.60953500	0.93404100	-0.65156900

**Int9***IS-Ra-3S*

S	5.21098400	-1.98508500	-1.54020000
O	4.58502200	-1.04979100	-2.49396300
O	5.33303400	-3.39367400	-1.87297300
O	0.86222000	-3.04457600	1.64652900
N	3.06824500	-1.45593400	0.31682800
N	1.87851600	-1.93583000	-0.24786300
C	6.85728400	-1.36532900	-1.25224200
C	7.09896400	0.00221100	-1.36566600
H	6.28696100	0.67514600	-1.64747400
C	8.38943500	0.46975400	-1.13198500
H	8.60228100	1.53647000	-1.21203600
C	9.40882200	-0.42784200	-0.80404800
H	10.41807600	-0.05589700	-0.62180200
C	9.15050400	-1.79613300	-0.72088100
H	9.95503500	-2.49207200	-0.48071200
C	7.86229900	-2.27893900	-0.95118800
H	7.62629100	-3.34311000	-0.90578300
C	4.41808000	-1.74418400	0.04048900
C	5.18909100	-1.46696100	1.13947900
H	6.27362600	-1.50001200	1.18215700
C	4.32247800	-1.01189700	2.17350400
C	3.02287800	-0.98217600	1.63352800
C	1.94284800	-0.52429500	2.40286800
H	0.92392400	-0.51404500	2.03657500
C	2.20053500	-0.11770500	3.69782500
H	1.36774600	0.23289700	4.30769200
C	3.49893000	-0.15355000	4.25167700
H	3.65324700	0.16874300	5.28258400
C	4.56536900	-0.59312400	3.49584300
H	5.57877300	-0.61573200	3.90084100
C	1.69616400	-2.01342400	-1.73304100
H	1.67015600	-0.98678000	-2.13026400
C	0.37050800	-2.73438700	-1.78177000
C	-0.56771900	-2.77293800	-2.80508000
H	-0.43685600	-2.17885800	-3.71122700
C	-1.69029600	-3.58491300	-2.63355300
H	-2.44946200	-3.63037200	-3.41661100
C	-1.86220000	-4.33040900	-1.46246100
H	-2.75492500	-4.94478100	-1.34333600
C	-0.91763300	-4.27722500	-0.43714100
H	-1.05706800	-4.82854200	0.49488100
C	0.20647200	-3.48202800	-0.62609500
C	1.32538000	-3.22805700	0.36158800
C	2.40140600	-4.30150700	0.40468500
H	3.13948200	-4.02973200	1.17400800
H	2.89794400	-4.39916200	-0.56932000
H	1.94099500	-5.25593900	0.69146000
C	-1.12865000	2.48010700	-0.07629300
C	-2.32393700	2.76538900	-0.70561000
C	-2.31511400	3.68305800	-1.81317200
C	-1.11008200	4.37636900	-2.11825600
C	0.07144500	4.07603400	-1.39093300
C	0.10873400	3.09565300	-0.42975100
H	-4.36978300	3.35553900	-2.44857500

C	-3.45176700	3.91129600	-2.63806400
C	-1.09222400	5.31363200	-3.18696800
H	0.99622600	4.59811000	-1.64800700
C	-2.21351700	5.53311100	-3.94774200
C	-3.40010100	4.81065500	-3.67626300
H	-0.16143300	5.84359000	-3.39933000
H	-2.18900200	6.24882400	-4.77051500
H	-4.28100500	4.96364300	-4.30115300
C	-3.57706400	2.10009800	-0.25979500
C	-4.75332600	2.86205000	0.06178600
C	-3.63688500	0.72343300	-0.15214600
C	-4.74477700	4.28147000	0.16534400
C	-5.97662300	2.17595600	0.30360000
C	-4.84027300	0.02092900	0.14262000
C	-5.89593900	4.97389900	0.45448400
H	-3.80820900	4.82039000	0.02276900
C	-7.15511600	2.92027000	0.58427500
C	-5.98804600	0.75631500	0.30640800
C	-7.12008000	4.29040200	0.65330000
H	-5.86457500	6.06108500	0.53796800
H	-8.08567300	2.37603800	0.75779100
H	-6.92888600	0.23600200	0.49859300
H	-8.02719200	4.85376000	0.87575800
O	-2.51068600	-0.03359400	-0.41132900
O	-1.13262800	1.55321600	0.95735200
P	-1.19420600	-0.00477100	0.51675900
O	-1.17062400	-0.93700300	1.66454800
C	-4.84702800	-1.46095200	0.33373700
C	-4.98889400	-2.33492800	-0.76451400
C	-4.77238300	-1.97583400	1.64982300
C	-5.05356900	-3.71336800	-0.52349200
C	-4.80975600	-3.36341100	1.81896200
C	-4.95471700	-4.25405800	0.75602400
H	-5.19826800	-4.37415700	-1.38115800
H	-4.75450000	-3.76344900	2.83658400
C	1.40771800	2.73203500	0.21326700
C	2.44993500	2.13107500	-0.53348200
C	1.62996700	3.09917500	1.55889800
C	3.67907300	1.93491600	0.10756000
C	2.90214600	2.94031600	2.11854400
C	3.95748200	2.38444600	1.39795100
H	4.47502200	1.43726200	-0.45728300
H	3.06561800	3.27849400	3.14336300
C	-5.20978400	-1.90067800	-2.21419400
C	-4.23814300	-0.87179100	-2.80189200
C	-6.66370900	-1.46496200	-2.43833300
H	-5.06507300	-2.82267100	-2.80052500
H	-3.19919900	-1.08079400	-2.51545000
H	-4.31051300	-0.89927900	-3.89984500
H	-4.48301100	0.15383600	-2.49160200
H	-7.36786700	-2.23290500	-2.08749900
H	-6.87696500	-0.52976800	-1.90020300
H	-6.84905700	-1.28634200	-3.50839600
C	-4.79982200	-1.16307900	2.95067700
C	-6.25183200	-0.92206800	3.38958000
C	-3.99302700	0.13491000	3.05123700
H	-4.35774200	-1.84204700	3.69671600
H	-6.83313500	-1.85512200	3.38692800
H	-6.27611800	-0.49925000	4.40520500
H	-6.74926400	-0.20552400	2.71980500
H	-2.96290600	-0.00692300	2.70506400
H	-4.45327500	0.97218400	2.50963700
H	-3.94472400	0.42823700	4.11107200
C	-5.00123200	-5.74812700	1.03626300
C	-3.61682400	-6.27714700	1.43084800
C	-5.57775600	-6.57205600	-0.11198100



H	-5.66374900	-5.87770300	1.90887300
H	-3.18119500	-5.69386000	2.25430400
H	-3.67730600	-7.32938000	1.74600200
H	-2.92733600	-6.22232200	0.57441100
H	-6.56340200	-6.19962400	-0.42524600
H	-4.91178500	-6.55308300	-0.98909200
H	-5.68652700	-7.62294100	0.19140100
C	2.47166000	1.72237700	-2.01595400
C	3.39800100	2.66817100	-2.79886000
C	1.17740400	1.54396700	-2.81930100
H	2.97989200	0.74283600	-2.00660300
H	3.51182200	2.31534500	-3.83455800
H	2.97355300	3.68416300	-2.82984800
H	4.39739700	2.73726800	-2.34698100
H	0.37579100	1.06169200	-2.25077900
H	0.79691400	2.49829600	-3.20671500
H	1.40621800	0.91658300	-3.69590200
C	0.55109800	3.75313000	2.41262700
C	0.94868400	5.17889900	2.80956200
C	0.21721100	2.90288400	3.64073200
H	-0.36723500	3.83371300	1.81691700
H	1.16639200	5.78909900	1.92095600
H	0.13557200	5.66281100	3.37082900
H	1.84465300	5.18105600	3.44879800
H	-0.12554700	1.90415600	3.33565200
H	1.09661300	2.78734300	4.29392800
H	-0.58215700	3.37690100	4.22985600
C	5.38963300	2.32984000	1.91031800
C	5.54269800	2.77602100	3.36114300
C	6.30308100	3.17432800	1.01045700
H	5.72133900	1.28037300	1.83077400
H	4.89519500	2.19915500	4.03422000
H	6.58386900	2.64766100	3.69105300
H	5.28912100	3.84234200	3.46927700
H	6.25310300	2.85092400	-0.03922500
H	6.00236900	4.23269300	1.04823700
H	7.34990900	3.10107900	1.34262800
O	2.61965900	-2.80172800	-2.39607500
H	3.22300700	-2.22857400	-2.89157900
H	0.07206500	-2.47046800	1.65373800
O	-0.02856000	-0.17314600	-0.50689300
H	0.72479500	-0.81144200	-0.21935100

### Int10<sub>IS-Sa-3S</sub>

S	-3.04883200	-0.46761000	1.58968300
O	-2.33912300	0.20291800	2.66122500
O	-2.37776000	-0.80049800	0.31987800
O	-2.24424700	2.23320200	0.63130900
N	-4.72650400	1.16246700	0.04355100
N	-3.83590300	1.42881800	-0.94162600
C	-3.67491300	-1.98999600	2.27583200
C	-3.62493300	-2.15008900	3.65696800
H	-3.22196400	-1.34661200	4.27484400
C	-4.06759400	-3.35407000	4.20419300
H	-4.03146800	-3.50440600	5.28377200
C	-4.54495800	-4.36524900	3.37114800
H	-4.88912600	-5.30611700	3.80302800
C	-4.58135800	-4.18599200	1.98577000
H	-4.95018200	-4.98471900	1.34129800
C	-4.13869900	-2.99005600	1.42650800
H	-4.13086500	-2.82925500	0.34683800
C	-4.54603300	0.39637200	1.18471500
C	-5.68381300	0.40486600	1.94944600
H	-5.82337000	-0.12322300	2.88939300
C	-6.63854200	1.21815800	1.25391300
C	-6.00691400	1.67203900	0.07402100
C	-6.64818800	2.48415200	-0.87205500

H	-6.12056600	2.79400500	-1.77519700
C	-7.95649400	2.84262900	-0.59982800
H	-8.49603500	3.47496400	-1.30645700
C	-8.61274400	2.40765100	0.57608400
H	-9.64428300	2.71514800	0.75185800
C	-7.97249600	1.60191000	1.49978800
H	-8.48638700	1.26839700	2.40255300
C	-3.68197800	0.50810600	-2.04308000
H	-3.72526700	-0.53339100	-1.67157900
C	-2.30491300	0.86953500	-2.53422600
C	-1.61764600	0.34272100	-3.62308000
H	-2.07642200	-0.42573800	-4.24755600
C	-0.33426300	0.82081000	-3.89448200
H	0.22716100	0.41602100	-4.73820600
C	0.24432000	1.80277100	-3.08513900
H	1.25629500	2.15714500	-3.29217100
C	-0.45668800	2.33904600	-2.00398500
H	-0.00297300	3.09462500	-1.36442900
C	-1.74123100	1.87151900	-1.74868900
C	-2.70008600	2.34683300	-0.67354900
C	-3.13951100	3.79285700	-0.86778800
H	-3.90818900	4.03225200	-0.11763000
H	-3.54813300	3.94045500	-1.87636500
H	-2.27844600	4.45787800	-0.71208300
C	2.58917200	-1.95171800	0.29543700
C	3.82327800	-1.33938000	0.38456100
C	4.96886500	-2.02339800	-0.15395900
C	4.81270800	-3.36240600	-0.61504500
C	3.51101800	-3.92299900	-0.69547500
C	2.39190100	-3.20645000	-0.34739400
H	6.38313700	-0.37908800	0.02488800
C	6.25305000	-1.42007300	-0.26856300
C	5.94526800	-4.07758100	-1.09194000
H	3.38890500	-4.91751000	-1.12881600
C	7.17925700	-3.48003500	-1.15213900
C	7.32593000	-2.12980400	-0.75261300
H	5.80627600	-5.10690400	-1.42920400
H	8.04152700	-4.03335300	-1.52640400
H	8.29905700	-1.64406100	-0.83604500
C	3.92233100	0.03528600	0.94005100
C	4.87493000	0.37886600	1.95918800
C	3.09013200	1.02820200	0.45349100
C	5.64140100	-0.59945200	2.65215300
C	5.04349700	1.74615800	2.31466500
C	3.21787500	2.39582100	0.82918000
C	6.54835700	-0.23011500	3.61588100
H	5.49373600	-1.65382500	2.41853300
C	6.00091300	2.09950300	3.30477400
C	4.21812800	2.72838000	1.70826300
C	6.74278700	1.13493600	3.93928500
H	7.11874600	-0.99659200	4.14229400
H	6.12227300	3.15432300	3.55902900
H	4.33827700	3.77450900	2.00072900
H	7.47021000	1.41397700	4.70268600
O	2.10096500	0.69147100	-0.46741900
O	1.48955800	-1.33141700	0.85838700
P	0.80238500	-0.05696700	0.14163600
O	-0.01370500	0.74216800	1.06913500
C	2.29239100	3.43994200	0.29445000
C	2.58148600	4.03567900	-0.96176900
C	1.17315500	3.86015300	1.04511200
C	1.72717900	5.02471500	-1.44947600
C	0.32725500	4.82739200	0.46947900
C	0.58118800	5.42641200	-0.75745300
H	1.96600900	5.48988700	-2.41004300
H	-0.57449300	5.11502500	1.01671800

C	1.03908100	-3.67653400	-0.76711100
C	0.71529400	-3.65693900	-2.14618300
C	0.11087800	-4.15676600	0.17367600
C	-0.50627200	-4.21222700	-2.53186200
C	-1.10416500	-4.69690500	-0.27069500
C	-1.41326000	-4.76941800	-1.62796700
H	-0.75950000	-4.22126700	-3.59731300
H	-1.80581700	-5.08612600	0.47156000
C	3.84351100	3.78493300	-1.79269400
C	4.27687400	2.33641000	-2.05240700
C	5.01818100	4.60350700	-1.24063700
H	3.60372000	4.20883500	-2.78078600
H	3.42293100	1.67381600	-2.25012100
H	4.93783100	2.31632000	-2.93171100
H	4.84800700	1.91864500	-1.21209300
H	4.74987300	5.66451800	-1.13808000
H	5.32220100	4.22771000	-0.25257100
H	5.88716800	4.52693200	-1.91170500
C	0.74838500	3.43778600	2.46273600
C	0.76085400	4.67617100	3.37758700
C	1.47137000	2.31703800	3.21532900
H	-0.29723800	3.10879700	2.34192800
H	0.14484300	5.50021600	2.99585000
H	0.38750200	4.40825500	4.37664200
H	1.79084800	5.05083900	3.49034300
H	1.58482500	1.39854100	2.63501900
H	2.45709600	2.63656700	3.58185000
H	0.85879600	2.06438600	4.09316800
C	-0.34339300	6.48633600	-1.32588600
C	-0.81210200	6.13931700	-2.74166500
C	0.32242000	7.86584200	-1.28977500
H	-1.23001500	6.52387500	-0.67136500
H	-1.26820800	5.13948100	-2.78052200
H	-1.55197300	6.87316900	-3.09426400
H	0.03057000	6.15107400	-3.44971300
H	0.62724500	8.13192900	-0.26794200
H	1.22219700	7.87720400	-1.92426600
H	-0.36410600	8.64075500	-1.66210800
C	1.57392400	-3.11167900	-3.29642000
C	2.45014600	-4.20482400	-3.92552400
C	2.39036000	-1.83462400	-3.06696600
H	0.82734100	-2.84517300	-4.06209600
H	2.86137200	-3.85209100	-4.88328800
H	3.30089400	-4.45642500	-3.27664200
H	1.87481500	-5.12283800	-4.11385400
H	1.79409900	-1.05280500	-2.58110500
H	3.30237800	-2.00547400	-2.47903300
H	2.71178100	-1.44949900	-4.04728900
C	0.42000300	-4.15968300	1.66255200
C	0.57923500	-5.59100000	2.18503100
C	-0.63749400	-3.39191800	2.45712500
H	1.37951900	-3.64679700	1.81220500
H	1.36459300	-6.12835400	1.63372100
H	0.84717200	-5.58585400	3.25206700
H	-0.35908000	-6.15660300	2.07476900
H	-0.76119300	-2.36956900	2.06986600
H	-1.61390700	-3.90101000	2.41195900
H	-0.34807800	-3.32125100	3.51652500
C	-2.63046000	-5.49282200	-2.17977900
C	-3.78633000	-5.62097400	-1.19465900
C	-2.21429400	-6.87724700	-2.69484500
H	-2.98610100	-4.90729000	-3.04429800
H	-4.09728800	-4.63803200	-0.81659600
H	-4.65274200	-6.09140500	-1.68136700
H	-3.50837700	-6.24977300	-0.33453300
H	-1.41635400	-6.79941900	-3.44633500

H	-1.83376200	-7.49035700	-1.86346300
H	-3.06899300	-7.40109100	-3.14847000
O	-4.62245200	0.68530800	-3.07064100
H	-5.47019300	0.34263300	-2.76341300
H	-1.47484700	1.63220300	0.72246400
O	0.07343200	-0.62600900	-1.13185400
H	-0.88539200	-0.72189500	-0.94251300

**TS11***Re-Sa-3Re*

S	-3.61204600	-0.34554900	1.66045200
O	-2.56791900	0.40506000	2.33116800
O	-3.28021900	-1.35927300	0.64429500
O	-1.48042000	2.75061000	0.80907700
N	-4.40156600	1.34403600	-0.27733000
N	-3.10523700	1.33594200	-0.68822100
C	-4.59818900	-1.16164700	2.89480100
C	-4.57686600	-0.65529800	4.19119900
H	-3.95308000	0.21021300	4.41942600
C	-5.34772600	-1.28969400	5.16432100
H	-5.34613500	-0.91361900	6.18795400
C	-6.11131400	-2.40840700	4.82971300
H	-6.71034300	-2.90286700	5.59584700
C	-6.10985400	-2.90712700	3.52503500
H	-6.70176100	-3.78828700	3.27515800
C	-5.34575600	-2.28349100	2.54175900
H	-5.31607500	-2.65531300	1.51616700
C	-4.79334300	0.72678700	0.88764900
C	-6.12060700	0.94663300	1.14651300
H	-6.68911900	0.55627400	1.98609900
C	-6.59601400	1.75857500	0.06075000
C	-5.50026700	1.98464000	-0.81200300
C	-5.62813500	2.71761100	-2.00196200
H	-4.77719300	2.86508900	-2.66833000
C	-6.87706300	3.23658700	-2.29455200
H	-7.01466800	3.81072800	-3.21187200
C	-7.98029000	3.03567800	-1.43377300
H	-8.94755300	3.46222600	-1.70166200
C	-7.85266500	2.30426100	-0.26703500
H	-8.70941600	2.14597300	0.38980000
C	-2.77613700	0.74682200	-1.94138800
H	-3.64986400	0.67375700	-2.61413500
C	-1.65374100	1.59204200	-2.49759900
C	-0.97675800	1.33303800	-3.68690500
H	-1.34414200	0.56328700	-4.36876900
C	0.20441600	2.02039000	-3.96206700
H	0.74691500	1.82009500	-4.88705900
C	0.72004200	2.92800800	-3.03357900
H	1.66812000	3.43481700	-3.22611500
C	0.03497000	3.19162700	-1.84786800
H	0.44128500	3.88166200	-1.10928700
C	-1.17390900	2.54585600	-1.60180100
C	-2.02509600	2.83501300	-0.39394500
C	-2.91807700	4.04348100	-0.48772900
H	-3.72890300	3.96126100	0.25010500
H	-3.33392700	4.17307900	-1.49178500
H	-2.30926100	4.92362300	-0.23030800
C	2.18710900	-2.39950500	0.01934500
C	3.51622300	-2.05033500	0.12353700
C	4.49475600	-2.96852900	-0.40031400
C	4.06658400	-4.26143700	-0.82034100
C	2.67745700	-4.56441100	-0.86551500
C	1.72994000	-3.62391600	-0.55192500
H	6.20943300	-1.64074500	-0.25593300
C	5.87282400	-2.64127800	-0.52715500
C	5.02975600	-5.20049000	-1.27918500
H	2.36180200	-5.54085900	-1.23692400
C	6.35897700	-4.86537700	-1.35895300

C	6.77849500	-3.56411900	-0.99458200
H	4.68528400	-6.18984400	-1.58739100
H	7.08864500	-5.59112400	-1.72047400
H	7.82930700	-3.28753600	-1.09085200
C	3.89692500	-0.75616200	0.75232300
C	4.90021200	-0.70672200	1.78383100
C	3.29167800	0.43106600	0.36800300
C	5.42048000	-1.87601500	2.40775600
C	5.38013900	0.55745200	2.22652000
C	3.72513100	1.70214400	0.84552800
C	6.39113300	-1.78775300	3.37622600
H	5.03074300	-2.85198700	2.12071800
C	6.39931900	0.61795700	3.21628000
C	4.79040600	1.73972400	1.71127200
C	6.90191100	-0.52921300	3.77651100
H	6.76583200	-2.69759900	3.84710400
H	6.75993600	1.59886700	3.53246300
H	5.15393900	2.70852900	2.06201200
H	7.67802900	-0.47500200	4.54101700
O	2.27749600	0.42419600	-0.57188500
O	1.23235400	-1.55142000	0.53415900
P	0.82114100	-0.20567200	-0.25549000
O	-0.08958800	0.58624700	0.59424500
C	3.03201400	2.97871600	0.48648100
C	3.39011400	3.69261300	-0.68553400
C	2.10598700	3.52987300	1.39749700
C	2.81973300	4.94828000	-0.90594200
C	1.53983200	4.78116500	1.09703900
C	1.88962400	5.51459600	-0.02939200
H	3.12018400	5.50363100	-1.79967700
H	0.80824600	5.19861800	1.79532000
C	0.27899100	-3.77503300	-0.86241800
C	-0.15534600	-3.72850700	-2.20663800
C	-0.66327600	-3.84116600	0.18818400
C	-1.53584300	-3.74668300	-2.45343200
C	-2.02071600	-3.87679800	-0.12135800
C	-2.48332400	-3.80740700	-1.43522600
H	-1.86822600	-3.67041000	-3.49070800
H	-2.75023900	-3.89953700	0.69197400
C	4.45814200	3.25918500	-1.69164400
C	4.35378900	1.84186500	-2.26421900
C	5.86972300	3.52664900	-1.15277000
H	4.31907100	3.94199800	-2.54582600
H	3.31949300	1.57351500	-2.51699300
H	4.96515200	1.78045900	-3.17701800
H	4.74123300	1.08457200	-1.56871600
H	5.97053100	4.56293300	-0.79944000
H	6.10532700	2.85174900	-0.31745600
H	6.61631200	3.35553600	-1.94298700
C	1.73073700	2.99634200	2.78781500
C	2.55652900	3.74826300	3.84426000
C	1.76163300	1.49642600	3.09642500
H	0.68085600	3.30672600	2.91450200
H	2.48296300	4.83811000	3.72247200
H	2.21165700	3.48550200	4.85535300
H	3.61868500	3.46833100	3.76906400
H	1.23794100	0.90363400	2.34026000
H	2.78015500	1.10735900	3.22547300
H	1.23206200	1.33905400	4.04807500
C	1.28641000	6.88010700	-0.30277600
C	0.49973200	6.90226900	-1.61674700
C	2.36125600	7.97113900	-0.28958400
H	0.58139700	7.08927000	0.51820100
H	-0.30527100	6.15364900	-1.61769800
H	0.05011200	7.89247200	-1.78316500
H	1.15775300	6.68451100	-2.47250100

H	2.91424900	7.97059400	0.66017000
H	3.08665300	7.81420900	-1.10265300
H	1.90976900	8.96454500	-0.42932200
C	0.72197600	-3.65790700	-3.46399400
C	1.07806900	-5.06156700	-3.97258300
C	1.95927100	-2.74966900	-3.46355300
H	0.04754500	-3.22603900	-4.22023900
H	1.54529700	-4.99845300	-4.96713100
H	1.79402800	-5.55707300	-3.30155300
H	0.18488800	-5.69821700	-4.04808100
H	1.75769100	-1.78981900	-2.97306600
H	2.83083200	-3.21346200	-2.98505800
H	2.23932100	-2.54567200	-4.50845000
C	-0.25570400	-3.88744500	1.65360000
C	-0.50594300	-5.28530600	2.23038100
C	-0.96086300	-2.80915400	2.48370200
H	0.82448000	-3.69799900	1.71851400
H	0.03956900	-6.05268900	1.66187000
H	-0.18235000	-5.33576800	3.28092400
H	-1.57763300	-5.53565800	2.19268200
H	-0.82364400	-1.80957400	2.04823800
H	-2.04375700	-3.00230600	2.55220200
H	-0.56023200	-2.80033700	3.50857200
C	-3.97966000	-3.77100000	-1.69133100
C	-4.59045800	-5.16729400	-1.52629600
C	-4.35273700	-3.16599400	-3.04238500
H	-4.39784600	-3.11790200	-0.90552000
H	-4.36525800	-5.58791800	-0.53565500
H	-5.68364000	-5.13627400	-1.65059000
H	-4.17823700	-5.85314900	-2.28239100
H	-3.86732600	-2.18858000	-3.17716500
H	-4.04714600	-3.82179600	-3.87229000
H	-5.44190100	-3.03285200	-3.11364600
O	-2.23954000	-0.58518300	-1.80366400
H	-2.60848600	-0.98328700	-0.98266300
H	-0.93024200	1.92597600	0.86083400
O	0.31376700	-0.59507000	-1.67318700
H	-0.71468200	-0.63032300	-1.74725300

**TS12***1Si-Sa-3Si*

S	-5.86155500	0.75538400	0.32359900
O	-5.70313700	0.73099200	-1.12884800
O	-5.62449600	2.00877100	1.03317200
O	-1.70805500	-2.09856100	-1.64738600
N	-3.49107000	-0.64411100	0.82149600
N	-2.69966100	-0.16492000	-0.17970300
C	-7.50241000	0.19828700	0.72229100
C	-8.10909500	-0.75094500	-0.09695900
H	-7.57783300	-1.13506800	-0.96934600
C	-9.39426400	-1.17991800	0.22428800
H	-9.89120900	-1.92257200	-0.40079400
C	-10.04699200	-0.65427600	1.34169900
H	-11.05431400	-0.99355100	1.58767300
C	-9.42600600	0.30509500	2.14212100
H	-9.94669000	0.71693100	3.00735100
C	-8.13888900	0.74336500	1.83346500
H	-7.62385600	1.49857900	2.42901000
C	-4.85600900	-0.51459900	1.04892000
C	-5.25406600	-1.35871900	2.05918600
H	-6.25679400	-1.43123200	2.47134700
C	-4.09239600	-2.08748300	2.46585400
C	-3.01756900	-1.61852500	1.67636500
C	-1.71567000	-2.13132500	1.78981400
H	-0.92222800	-1.78413900	1.13058300
C	-1.51051100	-3.10313700	2.75026200
H	-0.50924400	-3.51886000	2.87428500
C	-2.56648100	-3.58046500	3.56432400

H	-2.35802600	-4.35230100	4.30647400
C	-3.85127600	-3.09177800	3.42682300
H	-4.66504000	-3.46777900	4.04879600
C	-2.69032500	1.21636200	-0.50034300
H	-3.61013100	1.76156300	-0.24176900
C	-2.41513000	1.26860200	-1.98561900
C	-2.18747900	2.43752000	-2.70541400
H	-2.25936600	3.40889200	-2.21094800
C	-1.86358100	2.35686000	-4.05865500
H	-1.68596700	3.26887100	-4.63215700
C	-1.75548600	1.11144400	-4.68198100
H	-1.48749200	1.05406500	-5.73785500
C	-1.99310500	-0.05831200	-3.96144800
H	-1.90785000	-1.03602100	-4.44016300
C	-2.34379800	0.02903700	-2.61529200
C	-2.65435800	-1.16589000	-1.75974300
C	-4.01250700	-1.78998100	-1.90529700
H	-4.21505000	-2.42507100	-1.02896200
H	-3.99430400	-2.43695800	-2.79561000
H	-4.78793500	-1.02504200	-2.00868600
C	3.07909500	1.60314200	0.32510700
C	4.15210400	0.86952000	0.79646200
C	5.00676200	1.48567900	1.77726300
C	4.83335700	2.86815000	2.07402300
C	3.74919400	3.58014800	1.49460000
C	2.82416700	2.95562800	0.69612200
H	6.12589500	-0.30197800	2.30246600
C	6.01178600	0.76684900	2.48204000
C	5.70450900	3.49912900	3.00360700
H	3.61236700	4.63316400	1.74903600
C	6.68492200	2.78435600	3.64555800
C	6.82572800	1.39906100	3.39138200
H	5.56362900	4.56206500	3.21025800
H	7.34284900	3.27508900	4.36392400
H	7.58299600	0.82532700	3.92734600
C	4.39320300	-0.51274400	0.29530400
C	5.68120600	-0.92963600	-0.19770800
C	3.36252900	-1.43187100	0.25309700
C	6.76382500	-0.02601200	-0.38903300
C	5.88298000	-2.29950000	-0.53654100
C	3.51861200	-2.77527800	-0.19551300
C	7.98582100	-0.46924000	-0.83559200
H	6.61513200	1.03429600	-0.18767300
C	7.16368900	-2.73093200	-0.97777900
C	4.78356900	-3.20037700	-0.51057800
C	8.19813700	-1.83978300	-1.11731800
H	8.79733800	0.24504100	-0.98124100
H	7.30038000	-3.78647800	-1.22139700
H	4.94119000	-4.23560800	-0.82073700
H	9.17511100	-2.17966900	-1.46331400
O	2.10975600	-1.07793900	0.70669700
O	2.21939600	1.04191300	-0.59574800
P	1.15290200	-0.07626900	-0.11259400
O	0.44933300	-0.61631700	-1.29710500
C	2.28342900	-3.58346200	-0.42576800
C	1.62600400	-4.25707300	0.62945300
C	1.72259100	-3.56877400	-1.72284100
C	0.39298600	-4.86321500	0.37229600
C	0.48274300	-4.19215100	-1.91247800
C	-0.21245800	-4.81928200	-0.88436400
H	-0.11395300	-5.38024600	1.19159400
H	0.02831600	-4.16028500	-2.90665800
C	1.58437800	3.65563300	0.24327600
C	0.60599300	4.06480300	1.18138200
C	1.39901500	3.93520600	-1.12955100
C	-0.50001600	4.78537000	0.70787400

C	0.28129400	4.66849200	-1.54026800
C	-0.67779900	5.12505800	-0.63577800
H	-1.25855800	5.09121100	1.43499900
H	0.17115300	4.88798300	-2.60342100
C	2.21100300	-4.45024500	2.02792000
C	2.50474200	-3.17808900	2.83136600
C	3.43454100	-5.37422500	2.00205000
H	1.42690300	-4.98969000	2.58453300
H	1.67425900	-2.46090900	2.78563700
H	2.67543900	-3.44851800	3.88437200
H	3.41150400	-2.66718000	2.47793000
H	3.21287800	-6.31019000	1.46973400
H	4.28514200	-4.88667300	1.50479200
H	3.74551000	-5.62393100	3.02779700
C	2.37789400	-3.02238600	-2.99834100
C	3.31207600	-4.08251200	-3.59912400
C	3.06813100	-1.65308700	-2.98418700
H	1.53604400	-2.91424700	-3.70014000
H	2.80745100	-5.05486500	-3.69028800
H	3.65241600	-3.77047600	-4.59814200
H	4.20419700	-4.21811600	-2.97034000
H	2.44179800	-0.88705500	-2.51298800
H	4.05137700	-1.66875500	-2.49593500
H	3.23523300	-1.34430100	-4.02767800
C	-1.56151300	-5.46211100	-1.14173300
C	-2.61665700	-5.02540700	-0.12434100
C	-1.43310500	-6.98838200	-1.18947000
H	-1.89010900	-5.11213500	-2.13387500
H	-2.68412100	-3.92959100	-0.09102400
H	-3.60159500	-5.43760800	-0.39241400
H	-2.37347900	-5.37845500	0.89011400
H	-0.70308200	-7.30366500	-1.94869700
H	-1.09524800	-7.37627100	-0.21576600
H	-2.40189500	-7.45556200	-1.42227800
C	0.60648100	3.84969000	2.70143400
C	1.04887600	5.13237700	3.42073200
C	1.31798000	2.63306700	3.30400000
H	-0.46167400	3.71278300	2.93567000
H	0.90829300	5.02532300	4.50649700
H	2.11560100	5.33281000	3.24049500
H	0.47797900	6.00848600	3.08136000
H	1.17722900	1.72747900	2.70302800
H	2.39368000	2.79852900	3.44229500
H	0.88971800	2.44538000	4.29985000
C	2.39767300	3.51815100	-2.19953200
C	3.07266100	4.74533800	-2.82214800
C	1.73478500	2.64144300	-3.26718200
H	3.18885900	2.92336300	-1.72776600
H	3.57714900	5.35165900	-2.05582600
H	3.82192200	4.43451800	-3.56517700
H	2.33887300	5.38763500	-3.33298200
H	1.20091100	1.79319300	-2.81422500
H	1.01231200	3.21967500	-3.86447500
H	2.49332300	2.24329300	-3.95761500
C	-1.87524500	5.97251900	-1.04883500
C	-1.95688600	6.23673500	-2.55070600
C	-1.87456300	7.30754100	-0.29235000
H	-2.78411400	5.41965300	-0.74766800
H	-2.00151500	5.31156900	-3.14257900
H	-2.85760900	6.82224800	-2.78070800
H	-1.08416100	6.81428500	-2.89204700
H	-1.87435200	7.16407200	0.79625100
H	-0.97854400	7.88942600	-0.55695000
H	-2.76188000	7.90078000	-0.55643100
O	-1.63313400	1.86223700	0.24557400
H	-1.41638700	2.74418200	-0.10016700



H	-0.82362100	-1.66440500	-1.55509700
O	0.30044600	0.50702600	1.04709800
H	-0.53650400	1.02700300	0.73399200
<b>TS13<sub>IS-Sa-3R</sub></b>			
S	-2.80629400	0.04213700	1.89034300
O	-2.19514700	1.11492500	2.68714100
O	-2.06461100	-0.65424000	0.85599100
N	-4.13057600	1.75080300	0.20461800
N	-2.98014800	2.05577400	-0.46433200
C	-3.47938200	-1.13793100	3.02499200
C	-3.80189900	-0.73861800	4.32019800
H	-3.62765200	0.29270600	4.62984800
C	-4.32612100	-1.69212000	5.18979600
H	-4.58444600	-1.41120600	6.21131900
C	-4.50761600	-3.00832200	4.75786800
H	-4.91412200	-3.74998800	5.44706400
C	-4.16432700	-3.38712500	3.45904200
H	-4.29549400	-4.42033800	3.13389800
C	-3.64141400	-2.44464600	2.57584600
H	-3.34035000	-2.70000900	1.55782000
C	-4.26067300	0.75959700	1.16588200
C	-5.57680700	0.55665000	1.46190100
H	-5.96257900	-0.14336600	2.19809300
C	-6.32828100	1.44099800	0.61023000
C	-5.39835900	2.16170800	-0.17261700
C	-5.78684900	3.09986100	-1.13691100
H	-5.05184900	3.63386300	-1.74214200
C	-7.14740200	3.31315700	-1.29325600
H	-7.49173800	4.03451700	-2.03527100
C	-8.09592400	2.61550900	-0.51572800
H	-9.15708400	2.81322900	-0.66962800
C	-7.70186200	1.68471000	0.43053300
H	-8.43975700	1.14425600	1.02478700
C	-2.25486900	3.17469500	-0.20997200
C	-1.35639900	3.33638200	-1.37525800
C	-0.29895800	4.22682400	-1.55694300
H	-0.01889100	4.94012200	-0.77918500
C	0.42789000	4.12757800	-2.73980400
H	1.27360500	4.79456800	-2.90623200
C	0.11582600	3.15635700	-3.70104500
H	0.71953800	3.09087000	-4.60740400
C	-0.91890800	2.24926900	-3.49525300
H	-1.12978800	1.45159600	-4.20804500
C	-1.65211900	2.35879900	-2.32101500
C	3.22044500	-0.03902200	0.24546900
C	3.57833800	-1.32643500	0.60821100
C	4.49176400	-1.50500500	1.70379600
C	5.12116100	-0.36033700	2.27027500
C	4.75117000	0.93292600	1.81685100
C	3.76492600	1.11797100	0.87935300
H	4.27329200	-3.66071600	1.87828400
C	4.78168200	-2.77907200	2.26808200
C	6.05929700	-0.52596000	3.32552300
H	5.22027900	1.80676600	2.27476800
C	6.34073900	-1.77200800	3.82809200
C	5.68008300	-2.90751300	3.30035200
H	6.53893900	0.36364400	3.73941500
H	7.05684000	-1.88859400	4.64275400
H	5.88026200	-3.89390600	3.72130800
C	2.98617100	-2.48034000	-0.11945800
C	3.79950600	-3.52344900	-0.68306100
C	1.61364600	-2.54394600	-0.29407500
C	5.22164600	-3.46007200	-0.71544600
C	3.16662200	-4.66269400	-1.25905200
C	0.97639400	-3.63697900	-0.95458100
C	5.96485900	-4.48851300	-1.24303700

H	5.72278200	-2.57567900	-0.32285400
C	3.96244600	-5.71808700	-1.78297400
C	1.75090900	-4.69219800	-1.36610100
C	5.33262700	-5.64051700	-1.77024100
H	7.05301500	-4.41227200	-1.26227600
H	3.45704100	-6.58620000	-2.21141500
H	1.27500600	-5.54931100	-1.84869600
H	5.93457200	-6.45265400	-2.18025000
O	0.81458900	-1.56261400	0.22544500
O	2.32903800	0.14342400	-0.78255000
P	0.73174200	-0.06091700	-0.42750300
O	-0.02908900	-0.04952700	-1.71512200
C	-0.47681400	-3.53599300	-1.28388100
C	-1.47713800	-3.92855900	-0.36503300
C	-0.83447200	-2.99068200	-2.53588100
C	-2.81548800	-3.72869600	-0.70983800
C	-2.19378500	-2.76512800	-2.79589700
C	-3.19673100	-3.10135800	-1.89628000
H	-3.59102300	-4.06466500	-0.01420600
H	-2.47287600	-2.28957500	-3.74027900
C	3.30216600	2.49935000	0.54892000
C	2.63572600	3.28362400	1.51604300
C	3.62544300	3.05687800	-0.71024800
C	2.35323000	4.61983300	1.19448800
C	3.35097600	4.40376800	-0.95839800
C	2.72892000	5.21411900	-0.00677000
H	1.83951300	5.23185700	1.94342300
H	3.65896300	4.83191300	-1.91679600
C	-1.20442000	-4.58557100	0.98671000
C	-0.42629000	-3.71059300	1.97731800
C	-0.58509100	-5.98271200	0.86889500
H	-2.20541900	-4.73592000	1.42643000
H	-0.76895600	-2.66707500	1.94718500
H	-0.55432300	-4.10539900	2.99740800
H	0.65103700	-3.70963700	1.75853600
H	-1.15477700	-6.61247500	0.17000900
H	0.45474800	-5.92945100	0.51951500
H	-0.58028500	-6.47614800	1.85291800
C	0.09674200	-2.72420800	-3.72655000
C	0.16526700	-3.99657000	-4.58572500
C	1.50813600	-2.15970800	-3.52850400
H	-0.44159600	-1.96613100	-4.31776700
H	-0.83787900	-4.37128600	-4.83464200
H	0.70931200	-3.80006000	-5.52210300
H	0.70139800	-4.79272600	-4.04687000
H	1.51164000	-1.28776700	-2.86725100
H	2.22061400	-2.90471000	-3.15156700
H	1.87928500	-1.83248200	-4.51252700
C	-4.65056600	-2.77271600	-2.17393300
C	-5.19853700	-1.81519800	-1.11034400
C	-5.51090700	-4.03347000	-2.28877100
H	-4.67933600	-2.24746100	-3.14223200
H	-4.54407500	-0.93594200	-1.02888900
H	-6.21992800	-1.48635000	-1.35881600
H	-5.23865900	-2.30736000	-0.12370500
H	-5.13167500	-4.70377000	-3.07308100
H	-5.51231500	-4.59299100	-1.34026400
H	-6.55391300	-3.77496400	-2.52624200
C	2.21872600	2.88898700	2.94122800
C	3.17421000	3.52765300	3.96129900
C	1.98219200	1.42053100	3.31029500
H	1.24245200	3.38782700	3.06040600
H	2.80184200	3.36581400	4.98406800
H	4.17190300	3.06755800	3.89354500
H	3.28976700	4.60898100	3.80033900
H	1.44157400	0.87997600	2.52593800

H	2.91619900	0.88856100	3.53289000
H	1.37008500	1.39566000	4.22526500
C	4.32749900	2.25388600	-1.79670900
C	5.70713900	2.83714100	-2.11829100
C	3.45563900	2.14405300	-3.05006200
H	4.48814400	1.23421900	-1.42561700
H	6.33369600	2.88826300	-1.21598200
H	6.22391500	2.21309400	-2.86255900
H	5.62708800	3.85423700	-2.53222800
H	2.47856800	1.70581300	-2.80210600
H	3.29338400	3.13540800	-3.50539900
H	3.94264300	1.50504400	-3.80223900
C	2.57055900	6.71471100	-0.19217000
C	2.08553500	7.13535800	-1.57937700
C	3.89542800	7.41118800	0.14483400
H	1.82029400	7.05120100	0.54327600
H	1.09544600	6.71914900	-1.81265800
H	2.00979900	8.23095700	-1.63984900
H	2.78737400	6.81477000	-2.36483200
H	4.23293900	7.14513700	1.15619800
H	4.67914500	7.09937600	-0.56289200
H	3.79330200	8.50533800	0.08553400
H	-0.27836100	2.10194900	0.83687000
O	0.37741700	0.87387000	0.69062500
O	-2.60671400	0.14147100	-1.91210300
H	-1.64348300	-0.08477300	-1.74654500
C	-2.77868100	1.47489300	-1.85384200
C	-2.87161900	4.31198000	0.54069500
H	-3.65683400	4.76267800	-0.08439000
H	-3.32900800	3.95306100	1.47218100
H	-2.10767400	5.05972600	0.77303900
H	-3.72144700	1.71669700	-2.37987900
O	-0.87978100	2.90187600	1.14876900
H	-1.33746200	2.46976100	1.89884200

**TS14<sub>IR-Sa-3S</sub>**

S	6.16157200	1.12424100	-0.75668600
O	6.15446900	2.54296800	-0.41183200
O	5.63684900	0.69675100	-2.04926700
N	3.90649700	0.40096700	0.60984000
N	3.14860500	1.23834600	-0.14879800
C	7.80835000	0.49661800	-0.56805700
C	8.66776100	1.13066200	0.32625900
H	8.32722000	2.01112100	0.87310300
C	9.95363000	0.61814000	0.48304800
H	10.64790000	1.09539300	1.17539400
C	10.35359500	-0.49958500	-0.25196600
H	11.36242300	-0.89521700	-0.12577500
C	9.47978600	-1.11121000	-1.15280300
H	9.80581200	-1.97665400	-1.73048600
C	8.18970200	-0.61207800	-1.32018100
H	7.48467900	-1.05567100	-2.02517000
C	5.28055900	0.23931500	0.49877800
C	5.71221100	-0.69859400	1.39429400
H	6.73999800	-1.03014800	1.51787200
C	4.54749000	-1.15839800	2.10476200
C	3.43362900	-0.46896200	1.57828900
C	2.12465800	-0.68421100	2.00979900
H	1.26952700	-0.19625200	1.55221900
C	1.94408500	-1.60186200	3.02837800
H	0.92057300	-1.78858200	3.35995500
C	3.03945900	-2.29518300	3.59197700
H	2.85791200	-3.01512100	4.39174400
C	4.33194700	-2.09379500	3.13727300
H	5.17033700	-2.64357500	3.56741700
C	2.53725800	0.77879500	-1.44780200
H	3.38150300	0.45355500	-2.07480200

C	1.96006300	2.09551100	-1.91440700
C	1.31888600	2.38518300	-3.11040500
H	1.14136400	1.60639300	-3.85342200
C	0.92064500	3.70511200	-3.33433800
H	0.42363900	3.96453200	-4.27062500
C	1.13971400	4.70235500	-2.37657600
H	0.81398700	5.72351700	-2.57982000
C	1.74715000	4.40033000	-1.15842400
H	1.89184200	5.16607200	-0.39445100
C	2.15652100	3.08734700	-0.95305700
C	2.81939200	2.48092400	0.21936000
C	3.58354100	3.21300600	1.26167300
H	3.75439300	2.57083000	2.13605100
H	3.03866700	4.11337400	1.56289100
H	4.55905900	3.47362500	0.82337100
C	-2.57446500	-2.19372800	-0.10179000
C	-3.92380200	-1.91171900	-0.01557000
C	-4.80340200	-2.97048600	0.40532600
C	-4.28746400	-4.29419800	0.51524300
C	-2.90355700	-4.53338100	0.28816900
C	-2.02789100	-3.50434800	0.05490500
H	-6.56667900	-1.73510700	0.69180900
C	-6.16938900	-2.74960900	0.73264500
C	-5.15907900	-5.35312400	0.88803300
H	-2.52890200	-5.55675300	0.35005400
C	-6.47997400	-5.11189800	1.17590300
C	-6.98356700	-3.79106300	1.11048600
H	-4.74990800	-6.36330900	0.95663900
H	-7.13765900	-5.93116400	1.46955700
H	-8.02563100	-3.59571300	1.36749700
C	-4.42999000	-0.56035500	-0.38834600
C	-5.51086700	-0.41126600	-1.33157800
C	-3.85484800	0.59123600	0.12126800
C	-6.03425800	-1.50184800	-2.08260700
C	-6.07248300	0.87945300	-1.55373700
C	-4.36494100	1.89716800	-0.15164000
C	-7.08129700	-1.32612000	-2.95589700
H	-5.58710200	-2.48883700	-1.97090900
C	-7.16739300	1.02719700	-2.44786900
C	-5.48964800	2.01293400	-0.92486500
C	-7.67035900	-0.05167800	-3.13134400
H	-7.45604100	-2.17839800	-3.52455000
H	-7.58914500	2.02429600	-2.59142100
H	-5.91654200	3.00061800	-1.11286700
H	-8.50648400	0.07283700	-3.82074300
O	-2.81344500	0.53854700	0.99953500
O	-1.70041000	-1.18739300	-0.42566200
P	-1.33175900	-0.09401100	0.73738300
O	-0.42045700	0.88713600	-0.00666400
C	-3.58188000	3.06718100	0.34667300
C	-3.71208100	3.53363900	1.67558200
C	-2.63392500	3.64749800	-0.52136000
C	-2.85456100	4.54464100	2.11783200
C	-1.80685900	4.66174800	-0.02015300
C	-1.88258000	5.11302900	1.29247200
H	-2.95477200	4.89226200	3.14983900
H	-1.06808400	5.10894300	-0.69059300
C	-0.55178200	-3.68133200	-0.08919200
C	0.26327500	-4.04258500	1.00476200
C	0.03495600	-3.41293800	-1.35015900
C	1.65058000	-4.09237800	0.80254800
C	1.41994300	-3.47436400	-1.48860700
C	2.25174600	-3.79144500	-0.41462000
H	2.29068100	-4.34627500	1.65334000
H	1.86140500	-3.24696700	-2.46197300
C	-4.79288900	3.07496700	2.65388200

C	-4.83524800	1.58049000	2.99210800
C	-6.17683800	3.57748900	2.22429100
H	-4.55056000	3.59228200	3.59585600
H	-3.83499800	1.17664000	3.19279400
H	-5.46019600	1.43510200	3.88614000
H	-5.28455200	0.98700100	2.18363600
H	-6.16617700	4.66095500	2.03709400
H	-6.51054900	3.07116000	1.30732200
H	-6.91819800	3.36881600	3.01050900
C	-2.46708400	3.34232200	-2.01301200
C	-3.48152000	4.13582600	-2.84752700
C	-2.41059900	1.88094100	-2.47185300
H	-1.47719700	3.75929900	-2.25058200
H	-3.48489100	5.19972800	-2.56927000
H	-3.23790300	4.05622100	-3.91838700
H	-4.49842700	3.74146100	-2.70975000
H	-1.75747200	1.28299000	-1.82369900
H	-3.40045000	1.40642400	-2.52085300
H	-1.99104400	1.85247700	-3.49094500
C	-0.91050400	6.15667700	1.80894100
C	0.10411900	5.51486200	2.76179000
C	-1.61539800	7.34438500	2.46660100
H	-0.35816400	6.53621800	0.93226400
H	0.58936900	4.65024900	2.28578800
H	0.87076300	6.24252600	3.07094200
H	-0.40217700	5.15169900	3.66996000
H	-2.33833600	7.80773400	1.78056100
H	-2.16012800	7.02941500	3.36939600
H	-0.88521300	8.10908900	2.77091600
C	-0.19648900	-4.43648900	2.41175600
C	-0.39231800	-5.95546000	2.51365600
C	-1.37792200	-3.68530700	3.03657000
H	0.67661200	-4.20267700	3.04344300
H	-0.58002300	-6.24640900	3.55853000
H	-1.25618400	-6.28214600	1.91689900
H	0.49266100	-6.49969500	2.15347400
H	-1.35569300	-2.61437600	2.79259100
H	-2.34754000	-4.09151100	2.72072700
H	-1.32493400	-3.79583400	4.13107200
C	-0.79845100	-3.12482400	-2.59364800
C	-0.72754200	-4.31819200	-3.55438000
C	-0.39631800	-1.82572600	-3.29619000
H	-1.84974300	-3.01803500	-2.29550700
H	-1.05590900	-5.24336200	-3.05868900
H	-1.36825000	-4.14860400	-4.43291600
H	0.30290400	-4.47429000	-3.90977500
H	-0.48999100	-0.97099900	-2.61429000
H	0.64382700	-1.86521700	-3.65453300
H	-1.04789200	-1.65292500	-4.16647700
C	3.76150600	-3.82510700	-0.56004000
C	4.29526900	-2.59590500	-1.29834300
C	4.21842500	-5.11919200	-1.24088200
H	4.17722400	-3.80791400	0.46202100
H	3.87773400	-1.67586800	-0.86704100
H	5.39388600	-2.55162700	-1.23856600
H	4.01979900	-2.61467200	-2.36427200
H	3.87817500	-6.00216000	-0.68171200
H	3.79962500	-5.18336300	-2.25730200
H	5.31579100	-5.15831600	-1.32053100
O	1.67419800	-0.26069400	-1.29365000
H	0.83468200	0.06386000	-0.88366800
O	-0.85465400	-0.66217800	2.01897800
O	1.13196800	2.39276200	1.30461700
H	0.42840600	1.86714900	0.76921800
H	1.22237900	1.89957300	2.13430100

TS15<sub>P-Re</sub>

S	-5.56802500	0.16370300	0.32149500
O	-5.88267200	1.22290600	1.27238200
O	-5.11120700	-1.13439900	0.79815900
N	-3.10032300	1.10326100	-0.41646400
N	-2.64935700	0.71186800	0.80297500
C	-6.97961200	-0.09171200	-0.72774800
C	-7.90952200	0.93554700	-0.86393400
H	-7.76734400	1.86639900	-0.31278600
C	-9.00561800	0.73034100	-1.69972400
H	-9.75017500	1.51766600	-1.82264100
C	-9.15228600	-0.48428900	-2.37207000
H	-10.01293500	-0.63976700	-3.02437900
C	-8.21322300	-1.50520500	-2.21233100
H	-8.34210900	-2.45406900	-2.73418300
C	-7.11238300	-1.31536200	-1.37971200
H	-6.36480500	-2.09476000	-1.22207300
C	-4.38477700	0.80999100	-0.84079400
C	-4.53957000	1.13863900	-2.15647600
H	-5.44690700	1.02719300	-2.74363400
C	-3.27313000	1.66229600	-2.59075300
C	-2.38835400	1.62357700	-1.48494800
C	-1.07197800	2.09538500	-1.56111300
H	-0.42081300	2.13274800	-0.68563500
C	-0.64732200	2.55857700	-2.79602700
H	0.37584800	2.91981600	-2.89441600
C	-1.50355700	2.59063100	-3.91677600
H	-1.12306000	2.96909600	-4.86619800
C	-2.81507600	2.16183200	-3.82309700
H	-3.48409400	2.20109000	-4.68389700
C	-2.32358200	-0.59837700	1.07113600
C	-2.18895900	-0.65675900	2.53254200
C	-2.01287400	-1.76569800	3.35301000
H	-1.96497700	-2.76444400	2.91603500
C	-1.90694400	-1.54472300	4.72306200
H	-1.78097500	-2.38677600	5.40488000
C	-1.96066600	-0.24035600	5.23727100
H	-1.88045700	-0.09068900	6.31540600
C	-2.11762600	0.86785100	4.40605300
H	-2.15055400	1.87573400	4.82349700
C	-2.23836200	0.65052300	3.03351400
C	-2.33971200	1.61062600	1.90587000
C	-3.14612900	2.87343800	1.99140600
H	-2.99176100	3.48816000	1.09213700
H	-2.81373500	3.45945300	2.85957700
H	-4.21758400	2.64525000	2.09197300
C	2.79983100	-1.90000700	-0.18271900
C	3.93167700	-1.23956400	-0.61628300
C	4.81201500	-1.93422300	-1.51653600
C	4.57524300	-3.31412500	-1.78150000
C	3.41323800	-3.94351100	-1.25694400
C	2.47968600	-3.24271800	-0.53574000
H	6.07003700	-0.23201800	-2.00863800
C	5.90418500	-1.29766800	-2.16795700
C	5.46794100	-4.02323200	-2.63062900
H	3.22753300	-4.99257500	-1.49562200
C	6.53120900	-3.38771400	-3.22278700
C	6.73955800	-2.00568800	-2.99875800
H	5.27835400	-5.08239400	-2.81634400
H	7.20550800	-3.93958200	-3.87894500
H	7.56658300	-1.49601100	-3.49487500
C	4.19251700	0.14942000	-0.14913700
C	5.44619100	0.52520700	0.45070900
C	3.19782700	1.10583300	-0.22974300
C	6.47257400	-0.41657200	0.74366600
C	5.66471400	1.88786000	0.80495000
C	3.37266000	2.45265900	0.19961700

C	7.66127400	-0.01514900	1.30434900
H	6.30557200	-1.47162400	0.53028800
C	6.91100700	2.27531800	1.36887200
C	4.61021400	2.82759300	0.65610700
C	7.89409100	1.34792400	1.60671900
H	8.42962000	-0.75701900	1.52609400
H	7.06232700	3.32626800	1.62315200
H	4.77039300	3.85870000	0.98058300
H	8.84500900	1.65343200	2.04505800
O	1.96765700	0.76578200	-0.77656500
O	1.93264100	-1.25382100	0.68040700
P	0.94274100	-0.11741900	0.10547700
O	0.27521100	0.59658200	1.22088100
C	2.20636600	3.38525500	0.18726700
C	1.89886100	4.11827600	-0.98501400
C	1.39610000	3.50570700	1.33543700
C	0.76213000	4.92735400	-0.99245800
C	0.23986600	4.30069700	1.24513400
C	-0.10239400	5.01154100	0.10095600
H	0.53214100	5.49080400	-1.90158200
H	-0.40950900	4.37248600	2.12355300
C	1.15218600	-3.80272900	-0.14830500
C	0.16293300	-4.05069300	-1.12917100
C	0.86953800	-4.02462800	1.21617800
C	-1.08666100	-4.51132800	-0.69822800
C	-0.38845700	-4.50847300	1.58105900
C	-1.39040700	-4.74287800	0.64222800
H	-1.85949900	-4.67981900	-1.45386800
H	-0.59741900	-4.70232000	2.63746200
C	2.77839300	4.17570400	-2.23566200
C	3.28732600	2.85074900	-2.81990800
C	3.94298000	5.15281400	-2.02919300
H	2.12933300	4.62150400	-3.00736500
H	2.52303300	2.06137700	-2.79459500
H	3.57865500	3.01249800	-3.86840100
H	4.17686100	2.48258500	-2.29087900
H	3.58323600	6.13495700	-1.69149900
H	4.64366200	4.76441700	-1.27558400
H	4.50051500	5.28896300	-2.96820200
C	1.67217500	2.96873800	2.74779900
C	2.17547500	4.13917300	3.60954700
C	2.58270400	1.76138900	2.99162700
H	0.67732500	2.67926200	3.12874200
H	1.49176300	4.99868500	3.57789100
H	2.29207800	3.82336200	4.65693000
H	3.15841000	4.47811500	3.24601600
H	2.35202400	0.90726400	2.34851300
H	3.64642600	2.01028800	2.88484200
H	2.42813700	1.43171100	4.03001700
C	-1.34925200	5.87462200	0.04759400
C	-2.28178600	5.46980100	-1.09802500
C	-0.98126200	7.35910700	-0.04503900
H	-1.88778800	5.71967700	0.99735100
H	-2.58051800	4.41354300	-1.02667700
H	-3.19031200	6.09027400	-1.09174800
H	-1.79017500	5.60224000	-2.07440300
H	-0.33167600	7.66008400	0.78895400
H	-0.44462500	7.56811000	-0.98337600
H	-1.88486100	7.98634100	-0.02704100
C	0.30461100	-3.91446100	-2.65107600
C	0.67482900	-5.26882700	-3.27251800
C	1.17900700	-2.80132600	-3.24330000
H	-0.72088800	-3.69181700	-2.98574500
H	0.63766400	-5.20884200	-4.37078800
H	1.69598800	-5.56355200	-2.98828900
H	-0.00984000	-6.06328900	-2.94316300

H	1.07807700	-1.85843600	-2.69339800
H	2.24120900	-3.07258800	-3.28312000
H	0.85407200	-2.62236800	-4.27932600
C	1.90254900	-3.79729400	2.31056700
C	2.37221900	-5.13601100	2.89072000
C	1.37773000	-2.86726200	3.40774100
H	2.78186100	-3.31360000	1.86475900
H	2.79313000	-5.78084300	2.10559900
H	3.14333400	-4.97661900	3.65929000
H	1.53441100	-5.67663700	3.35750700
H	0.99879300	-1.92637900	2.98315800
H	0.56054000	-3.33886300	3.97566100
H	2.17985200	-2.62786000	4.12199600
C	-2.75938600	-5.24215700	1.06378100
C	-2.97355200	-6.69040700	0.61151300
C	-3.88466700	-4.33289100	0.56282000
H	-2.77859300	-5.22896800	2.16694300
H	-2.18470900	-7.35102500	0.99866500
H	-3.94679300	-7.06775300	0.95951400
H	-2.95880500	-6.75611400	-0.48763400
H	-3.73638400	-3.28692300	0.86195700
H	-3.93958100	-4.35339900	-0.53725300
H	-4.85527700	-4.67637800	0.95136700
O	-2.14018500	-1.46367200	0.22104300
H	-0.85217700	-1.10349500	-0.64953500
H	-0.81136600	1.77515700	1.64773300
O	0.03475100	-0.75298000	-0.99495100

**TS16<sub>P-Si</sub>**

S	2.67529300	-0.00398600	1.80418300
O	2.08879300	-1.30435700	2.11160800
O	1.91625200	1.07254400	1.18579400
N	4.07311900	-0.73047500	-0.48066500
N	3.02638600	-1.32646700	-1.10220400
C	3.38667700	0.62610900	3.31195500
C	3.70492600	-0.26802800	4.33054800
H	3.50192200	-1.33114100	4.19491100
C	4.26585800	0.23278400	5.50398900
H	4.52074400	-0.44732000	6.31754600
C	4.49384300	1.60330300	5.63930400
H	4.93102500	1.98994900	6.56112100
C	4.16005000	2.48491500	4.60944600
H	4.33098400	3.55561300	4.72689600
C	3.59892100	1.99770600	3.43093300
H	3.30981300	2.66033100	2.61323700
C	4.13693300	-0.25650700	0.82025900
C	5.42268400	0.09936300	1.12328000
H	5.75773900	0.53318300	2.06112600
C	6.21384500	-0.16200900	-0.04755800
C	5.34206300	-0.68163500	-1.02756900
C	5.76906800	-1.04933200	-2.30833300
H	5.06629300	-1.44361600	-3.04375900
C	7.11307600	-0.87304200	-2.59279000
H	7.48885600	-1.13963300	-3.58148500
C	8.00718100	-0.34781100	-1.63360300
H	9.05691500	-0.22077600	-1.90039000
C	7.57360900	0.00834900	-0.36832100
H	8.26818300	0.41514800	0.36796500
C	2.23207800	-0.67889400	-2.02739400
C	1.42295600	-1.75416600	-2.64594100
C	0.53164500	-1.67975900	-3.71137100
H	0.30948500	-0.72392800	-4.18664000
C	-0.06712600	-2.86318100	-4.13864500
H	-0.77428500	-2.84577400	-4.96872800
C	0.23994100	-4.07937900	-3.51543500
H	-0.23480100	-4.99578400	-3.87221100
C	1.13559600	-4.14288200	-2.44830500



H	1.36561700	-5.09375000	-1.96739300
C	1.71965600	-2.95996100	-2.00928100
C	2.67854000	-2.72091400	-0.89592000
C	3.84677500	-3.65492600	-0.71147900
H	4.46277900	-3.34386900	0.14397000
H	4.47827900	-3.67995600	-1.61340500
H	3.47507500	-4.66846400	-0.51098400
C	-2.24490300	2.16864400	-0.17633000
C	-3.54553900	1.71784100	-0.06872100
C	-4.60092500	2.56159600	-0.56109400
C	-4.28693700	3.88359400	-0.98760700
C	-2.93051000	4.30828800	-1.01292500
C	-1.90555600	3.45816100	-0.68708500
H	-6.19711400	1.09897700	-0.37629200
C	-5.94974700	2.12169800	-0.66140200
C	-5.32932800	4.73577200	-1.44282800
H	-2.69705500	5.31375400	-1.37211800
C	-6.62685100	4.29059800	-1.50446400
C	-6.93450600	2.96327400	-1.12145000
H	-5.07266600	5.74937700	-1.75768700
H	-7.41833000	4.95054600	-1.86214500
H	-7.96103800	2.60222000	-1.19803200
C	-3.80450800	0.38865500	0.54398900
C	-4.71899800	0.23084700	1.64198300
C	-3.09703900	-0.71742100	0.10763800
C	-5.36354300	1.32986900	2.27807000
C	-4.97369000	-1.07735500	2.14336400
C	-3.25688300	-2.01147000	0.67835100
C	-6.24877400	1.12867900	3.30945400
H	-5.14144700	2.34362700	1.94704200
C	-5.90737200	-1.25590900	3.20114200
C	-4.23221000	-2.17346500	1.63237200
C	-6.54028400	-0.17892400	3.76841300
H	-6.72547400	1.98708600	3.78479400
H	-6.09567700	-2.26882400	3.56289900
H	-4.39576900	-3.16580300	2.05880700
H	-7.25058100	-0.32370700	4.58349000
O	-2.20755300	-0.57675400	-0.94057300
O	-1.20739200	1.36004800	0.25497800
P	-0.76690300	0.11238400	-0.68315100
O	0.26764000	-0.75667400	-0.10833700
C	-2.32845600	-3.14157800	0.36487600
C	-2.57460300	-4.02248600	-0.71081500
C	-1.24133100	-3.37331700	1.24209000
C	-1.75237400	-5.14511600	-0.86710900
C	-0.42853800	-4.48796500	0.99950400
C	-0.67897800	-5.40571700	-0.01901400
H	-1.97930500	-5.83303800	-1.68399300
H	0.41087100	-4.66801200	1.67982500
C	-0.46294200	3.79003600	-0.86010000
C	0.13413700	3.79175800	-2.13450100
C	0.32155400	3.98449400	0.30328200
C	1.53093500	3.92601900	-2.19800300
C	1.69819600	4.13190600	0.17606000
C	2.32827500	4.07553700	-1.07091600
H	2.01329500	3.88551900	-3.17943000
H	2.30518200	4.26492600	1.07400200
C	-3.75343000	-3.91958500	-1.67861700
C	-3.92211400	-2.58436500	-2.40844700
C	-5.06918300	-4.35766600	-1.02285600
H	-3.53200500	-4.66503600	-2.45942200
H	-2.96286500	-2.20145700	-2.78059000
H	-4.60193600	-2.72430200	-3.26257600
H	-4.36768100	-1.81352200	-1.76490400
H	-4.96395400	-5.33972400	-0.53941700
H	-5.39294700	-3.63163600	-0.26374700

H	-5.86538100	-4.42832400	-1.77947000
C	-0.93114600	-2.65240400	2.56380600
C	-1.63054300	-3.40078700	3.71092900
C	-1.14364700	-1.14530200	2.72644900
H	0.15265400	-2.79494800	2.69551000
H	-1.43577800	-4.48234400	3.66898100
H	-1.27949100	-3.02051200	4.68201300
H	-2.71980300	-3.24881100	3.66932800
H	-0.60295200	-0.57801600	1.96300300
H	-2.20122700	-0.84771700	2.74168100
H	-0.71562300	-0.85587000	3.69911600
C	0.17296900	-6.66262700	-0.11713400
C	-0.04746500	-7.46672500	-1.39624000
C	-0.06245000	-7.55840500	1.10638600
H	1.22973300	-6.33875900	-0.08893000
H	0.08721500	-6.85763200	-2.30204100
H	0.65704000	-8.30913500	-1.44362100
H	-1.06548300	-7.88407500	-1.42319800
H	0.13843900	-7.02207200	2.04380400
H	-1.11036600	-7.89414100	1.12948700
H	0.58452300	-8.44768600	1.07152800
C	-0.55412700	3.72145100	-3.50460800
C	-0.62307800	5.13840100	-4.09549100
C	-1.91616200	3.03717100	-3.67796400
H	0.15399200	3.15052600	-4.12801000
H	-1.01797100	5.11017600	-5.12237500
H	-1.29416600	5.76817300	-3.49063200
H	0.36405200	5.62085100	-4.11319200
H	-2.00809300	2.11515900	-3.09373300
H	-2.75040500	3.70056200	-3.41741000
H	-2.03361000	2.77798400	-4.74128300
C	-0.34838500	4.10956500	1.66496700
C	-0.84001200	5.54878500	1.86502900
C	0.52780500	3.66329000	2.83276500
H	-1.22990600	3.45355000	1.66916400
H	-1.53149800	5.84866600	1.06431200
H	-1.36125500	5.65350700	2.82861300
H	0.01210600	6.24610100	1.85517000
H	0.91652900	2.65189900	2.65426000
H	1.37539600	4.34964800	2.99267500
H	-0.06107900	3.65830600	3.76165400
C	3.83904000	4.11140700	-1.18709100
C	4.43718500	2.82344800	-0.61333500
C	4.44691400	5.35066800	-0.52717800
H	4.07895700	4.14681100	-2.26213800
H	3.97834800	1.94049500	-1.08332900
H	5.52786200	2.78815700	-0.76312500
H	4.23952300	2.76262000	0.46885900
H	4.01965300	6.27538800	-0.94057700
H	4.26296000	5.34989200	0.55852400
H	5.53654000	5.37357300	-0.67765000
O	2.24294400	0.51456800	-2.26421800
H	0.49412100	0.90995700	-2.23767600
H	1.79902100	-2.73957600	0.37222100
O	-0.47103400	0.72753200	-2.10994300
<b>Int11<sub>p</sub></b>			
S	-2.55923900	0.13235600	1.62791800
O	-1.96864700	1.48040500	1.71201900
O	-1.91937200	-0.83607800	0.74487800
N	-4.58283700	0.94565400	-0.00265600
N	-3.74086300	1.65325500	-0.80333900
C	-2.65823100	-0.57099200	3.24808400
C	-2.72126300	0.27083100	4.35568000
H	-2.69791600	1.35306200	4.21843500
C	-2.79728200	-0.31064400	5.61916000
H	-2.84304900	0.32206400	6.50602400

C	-2.80435600	-1.70124500	5.74874600
H	-2.86021800	-2.14909400	6.74198300
C	-2.73077900	-2.52470600	4.62371000
H	-2.72311600	-3.60956600	4.73648400
C	-2.65405500	-1.96067200	3.35202600
H	-2.57270100	-2.57014700	2.44813700
C	-4.25230600	0.33356200	1.18976100
C	-5.37504700	-0.15297800	1.80211300
H	-5.40261000	-0.70903700	2.73543200
C	-6.47718900	0.17838400	0.94267500
C	-5.94672300	0.85974000	-0.17630800
C	-6.73633600	1.33349000	-1.23107400
H	-6.28583600	1.85911200	-2.07431500
C	-8.09564900	1.08953000	-1.14262600
H	-8.75196400	1.43259700	-1.94346300
C	-8.65530800	0.40101300	-0.04104500
H	-9.73179200	0.22879400	-0.01600100
C	-7.86537400	-0.05396100	0.99884700
H	-8.30345900	-0.58438600	1.84532900
C	-3.68696500	3.04073400	-0.81081400
C	-2.79590300	3.36643200	-1.82109600
C	-2.32353300	4.61767900	-2.33371500
H	-2.66954800	5.55897100	-1.90138100
C	-1.44234100	4.61228400	-3.37788700
H	-1.08679000	5.56043400	-3.78624100
C	-0.96049200	3.38767400	-3.96061400
H	-0.24936000	3.44133500	-4.78623700
C	-1.37055600	2.17317300	-3.49208800
H	-0.99494900	1.23847100	-3.91043700
C	-2.31118200	2.14036100	-2.41955800
C	3.37752500	0.38301000	0.00670800
C	3.92523200	-0.86123900	0.25669200
C	5.07026500	-0.93462800	1.12751600
C	5.71109800	0.27296800	1.52570000
C	5.12412000	1.52018900	1.18421500
C	3.92358000	1.59547400	0.52353000
H	5.08011000	-3.09523000	1.37202200
C	5.58717900	-2.16398400	1.62309700
C	6.87936300	0.21358000	2.33347300
H	5.60158800	2.44060000	1.52511200
C	7.37380700	-0.99114800	2.76773500
C	6.70608200	-2.19005200	2.42122700
H	7.36290600	1.15043800	2.61808600
H	8.26595600	-1.02658100	3.39436100
H	7.07849000	-3.14439700	2.79612400
C	3.32729600	-2.08086900	-0.34918300
C	4.13256200	-3.05445500	-1.03965900
C	1.96278000	-2.29817100	-0.27918200
C	5.50257500	-2.83632100	-1.35869400
C	3.53614200	-4.28149200	-1.44911700
C	1.33540500	-3.47355500	-0.78045300
C	6.24273900	-3.80260000	-1.99639700
H	5.96398300	-1.88318700	-1.10272200
C	4.33230500	-5.27062600	-2.08933600
C	2.13784000	-4.46551700	-1.28653200
C	5.65980300	-5.04299700	-2.35156900
H	7.28834100	-3.60747300	-2.23846600
H	3.85752600	-6.20828400	-2.38539500
H	1.68036900	-5.39106900	-1.64356900
H	6.26115900	-5.80400100	-2.85058000
O	1.15331600	-1.37361600	0.34738900
O	2.28335100	0.49225700	-0.82973000
P	0.81016400	0.04918000	-0.33705000
O	-0.15773600	0.04449500	-1.44831100
C	-0.15350100	-3.54750500	-0.87442600
C	-0.95416000	-3.97751600	0.20961700

C	-0.74985400	-3.18190100	-2.10140400
C	-2.33887500	-4.03311400	0.03705800
C	-2.14791600	-3.23188200	-2.19831900
C	-2.96019300	-3.65411900	-1.15397800
H	-2.95300100	-4.39164500	0.86936400
H	-2.61764600	-2.92787400	-3.13791800
C	3.18429000	2.88493200	0.39955700
C	2.64185200	3.49623100	1.55577200
C	3.01873600	3.48677700	-0.86348200
C	1.97619300	4.71468000	1.39558500
C	2.34300700	4.70790500	-0.96103800
C	1.82335800	5.34770100	0.16129900
H	1.54751600	5.19160400	2.28346700
H	2.22595600	5.16239700	-1.94643400
C	-0.41285000	-4.46193600	1.55414700
C	0.41611900	-3.44178200	2.34240800
C	0.32177100	-5.80303600	1.44201500
H	-1.31511600	-4.65825900	2.15869200
H	-0.03199400	-2.43978800	2.30322700
H	0.48725800	-3.76120800	3.39377000
H	1.44243600	-3.36263500	1.95716000
H	-0.28992600	-6.54673000	0.91127100
H	1.27299700	-5.68942200	0.90381200
H	0.55054300	-6.19526400	2.44469500
C	-0.03878300	-2.85806200	-3.42430400
C	0.12795100	-4.15268700	-4.23506100
C	1.27039000	-2.06144000	-3.45079000
H	-0.76952300	-2.23650800	-3.96644900
H	-0.81952500	-4.70418700	-4.31442000
H	0.48609400	-3.92466700	-5.25021300
H	0.86884400	-4.81315300	-3.75963600
H	1.21059900	-1.14958100	-2.84789700
H	2.14162900	-2.65016800	-3.13580100
H	1.45465400	-1.75260800	-4.49129700
C	-4.46827100	-3.67280900	-1.30294200
C	-5.09326800	-2.56415000	-0.45455900
C	-5.07027700	-5.04023800	-0.97402700
H	-4.68706000	-3.44950500	-2.35939800
H	-4.64411100	-1.59547500	-0.71681900
H	-6.18264800	-2.50669200	-0.60613600
H	-4.90870600	-2.75068400	0.61655900
H	-4.61919500	-5.83371800	-1.58668400
H	-4.91192600	-5.29912600	0.08426800
H	-6.15548200	-5.03704400	-1.15443700
C	2.72067100	2.99495700	3.00513300
C	3.89838200	3.64122200	3.74864300
C	2.67239900	1.48809100	3.28809200
H	1.80865400	3.40815700	3.46498900
H	3.83724900	3.41803400	4.82466400
H	4.85873300	3.24908000	3.38373500
H	3.90515900	4.73307000	3.61997100
H	1.94108900	0.97584900	2.65260400
H	3.64691400	0.99955300	3.16215000
H	2.37446300	1.34222200	4.33780900
C	3.60068300	2.88180500	-2.13270600
C	4.74817000	3.74837000	-2.66344100
C	2.52657200	2.66242400	-3.20087700
H	4.02521900	1.89961300	-1.88642000
H	5.53514400	3.87049900	-1.90486600
H	5.19696500	3.29095700	-3.55791300
H	4.38819200	4.75121900	-2.94052500
H	1.69601000	2.05806800	-2.81017000
H	2.11158200	3.62012600	-3.55116700
H	2.95509400	2.14481900	-4.07258500
C	1.14228000	6.70500100	0.10609700
C	0.67878600	7.10603800	-1.29079800

C	2.06440100	7.77988600	0.69592500
H	0.25027700	6.63584600	0.75199800
H	0.04850200	6.32765300	-1.74223200
H	0.10118300	8.04072700	-1.24520100
H	1.53759900	7.28373700	-1.95660800
H	2.36756300	7.53147100	1.72285700
H	2.97809100	7.86756500	0.08813300
H	1.56474100	8.76018100	0.71017400
H	-0.38067800	1.32279100	1.03639500
O	0.52738400	0.95663800	0.91112300
O	-2.85736000	-0.23906800	-1.89798900
H	-1.94930300	-0.51938300	-1.64353200
C	-2.92209700	1.08591800	-1.76440700
C	-4.44646500	3.85375500	0.17809600
H	-5.53775800	3.73350700	0.08084100
H	-4.16561800	3.58619800	1.20982500
H	-4.20904800	4.91430000	0.02978700

**(P,R)-3a**

C	3.55652600	0.14213800	0.15019900
C	2.54669000	-0.84677700	0.21984700
C	2.81818900	-2.17987000	0.55164200
C	4.13564900	-2.50271800	0.82856200
C	5.16078700	-1.53185600	0.77988800
C	4.88582900	-0.21925600	0.44117900
C	2.92604800	1.36873800	-0.25353300
H	2.02592800	-2.92799800	0.56672200
H	4.38989100	-3.53316200	1.08072000
H	6.18563700	-1.82961100	1.00381700
H	5.68142900	0.52540400	0.39170000
H	3.37998700	2.33618000	-0.44951500
C	1.59798200	1.08939900	-0.40304400
N	1.34732000	-0.24115900	-0.10225200
C	-1.96905300	-1.53344200	0.48929500
C	-1.76611300	-1.84611100	-0.85304200
C	-3.18589200	-1.82449100	1.09888700
C	-2.75213200	-2.44287100	-1.63123300
C	-4.18483300	-2.42060700	0.32631700
H	-3.36387600	-1.58601200	2.14944100
C	-3.97440700	-2.72670200	-1.02467200
H	-2.55635400	-2.66967800	-2.68037600
H	-5.14850100	-2.65283700	0.78260100
H	-4.77490400	-3.19134300	-1.60164300
N	0.12692700	-0.83087500	-0.10961500
C	-0.39364400	-1.43419700	-1.26181500
O	0.17860400	-1.57270900	-2.30361900
C	-0.73124900	-0.89998500	1.08045900
H	-0.95655300	0.12047400	1.43343200
C	-0.11981400	-1.70193500	2.22436700
H	0.83815200	-1.26280500	2.53745200
H	-0.80035400	-1.69102400	3.08736400
H	0.04436200	-2.74566100	1.92274700
S	0.41802700	2.18818200	-1.13774500
O	-0.10191500	1.57268700	-2.34742000
O	1.07981600	3.48331300	-1.15775200
C	-0.93093600	2.26710700	0.02504100
C	-2.15373300	1.71251700	-0.33877800
C	-0.72861700	2.88531300	1.25835500
C	-3.20206100	1.74991000	0.58128500
H	-2.26112000	1.25047600	-1.32199200
C	-1.78046300	2.90862200	2.17026200
H	0.23967700	3.33355700	1.48972600
C	-3.01142100	2.33720300	1.83205300
H	-4.16588500	1.31025600	0.32083900
H	-1.64553400	3.38017700	3.14444700
H	-3.83216400	2.35984000	2.55071000

**(P,S)-3a**

C	-1.31826700	2.89313000	0.12590200
C	-0.05748600	2.48805100	-0.36918800
C	0.80952500	3.35744300	-1.04326300
C	0.37416900	4.65910200	-1.22287300
C	-0.88536800	5.08897800	-0.74653800
C	-1.73274100	4.22363200	-0.07835700
C	-1.90231100	1.75087800	0.76906300
H	1.77251700	3.00918400	-1.41789500
H	1.01415600	5.36849900	-1.74932400
H	-1.19042200	6.12273400	-0.91242600
H	-2.70378800	4.56109400	0.28651100
H	-2.87351900	1.68067500	1.25228700
C	-1.00588900	0.72557800	0.64628800
N	0.11522200	1.15688100	-0.05253700
C	3.31997200	-0.43455800	0.33190500
C	2.78247200	-1.11322400	-0.75947100
C	4.56608900	-0.79642400	0.83399700
C	3.44956000	-2.16136200	-1.38268700
C	5.24564200	-1.84826600	0.21610600
H	5.00516600	-0.27908200	1.68901700
C	4.69714500	-2.52540800	-0.88042000
H	2.99372000	-2.67152900	-2.23237000
H	6.22279000	-2.15051900	0.59616000
H	5.25270900	-3.34415700	-1.33925900
N	1.29538000	0.50351000	-0.19082400
C	1.45226500	-0.54283500	-1.09097100
O	0.65954300	-0.86924000	-1.93677900
C	2.37003900	0.64128900	0.80380100
H	2.83636100	1.63582200	0.68431300
C	1.88941800	0.47757800	2.24105400
H	2.73611200	0.61591900	2.92764900
H	1.13250500	1.23909200	2.48322400
H	1.45846700	-0.52001400	2.39026500
S	-1.27197600	-0.93259800	1.23266800
O	-1.81904200	-0.80234400	2.57491000
O	-0.05764200	-1.70342800	0.98909200
C	-2.56342400	-1.56807100	0.18328400
C	-3.83889700	-1.70551100	0.72500000
C	-2.25862000	-1.94061100	-1.12538300
C	-4.85043200	-2.22589400	-0.08057300
H	-4.01622000	-1.41697300	1.76180400
C	-3.28424300	-2.45385000	-1.91621300
H	-1.24563900	-1.81708900	-1.51528700
C	-4.57243200	-2.59595000	-1.39639800
H	-5.85662400	-2.34677200	0.32258400
H	-3.07337000	-2.74801800	-2.94495100
H	-5.36749900	-3.00212700	-2.02364400

**TS17***1Re-Ra-3Re*

S	-6.25791300	1.19205000	-0.99564200
O	-5.80703800	0.39878600	-2.13661300
O	-6.11662100	2.64117000	-0.99406000
O	-1.62013300	2.36833600	1.22515600
N	-4.13472800	0.46962100	0.51804100
N	-3.36323000	1.10713800	-0.40316700
C	-7.97459400	0.81082800	-0.71004400
C	-8.46892600	-0.42006000	-1.13455400
H	-7.80600000	-1.11473700	-1.65295200
C	-9.80747300	-0.71897400	-0.89001000
H	-10.21927700	-1.67526200	-1.21476800
C	-10.62143200	0.20835900	-0.23613400
H	-11.66925100	-0.03046800	-0.04779400
C	-10.10932300	1.44093400	0.17171600
H	-10.75500000	2.16319900	0.67262700
C	-8.77195100	1.75345000	-0.06721900
H	-8.34004900	2.71174800	0.22507700
C	-5.51102700	0.50386700	0.45797700

C	-6.07358800	-0.12008300	1.53872700
H	-7.13517400	-0.25444600	1.72727700
C	-4.97349700	-0.56073400	2.34825200
C	-3.77569000	-0.18602600	1.68394500
C	-2.50824100	-0.46711300	2.21535500
H	-1.59658600	-0.18346000	1.69000700
C	-2.47109100	-1.10933100	3.44095300
H	-1.50173500	-1.32644400	3.88894200
C	-3.64950700	-1.49022000	4.12274100
H	-3.56851100	-1.99384600	5.08708100
C	-4.89694500	-1.22881300	3.58607300
H	-5.80791600	-1.52199200	4.11039400
C	-2.73401400	0.36354500	-1.42865600
H	-3.47256600	-0.04307900	-2.13977700
C	-1.76863200	1.34918100	-2.04031000
C	-1.08905400	1.16854300	-3.24066400
H	-1.34739300	0.33402800	-3.89569200
C	-0.04717700	2.03458300	-3.57034200
H	0.49955700	1.89648500	-4.50419400
C	0.32446200	3.05418900	-2.69118600
H	1.16700600	3.70554200	-2.93163800
C	-0.37083100	3.24567500	-1.49676600
H	-0.07138200	4.03198400	-0.80106700
C	-1.43498600	2.40170200	-1.18658400
C	-2.25572200	2.53995600	0.06691200
C	-3.23471900	3.67758300	0.12993600
H	-3.89575000	3.52840500	0.99521500
H	-3.84347000	3.72304000	-0.77822800
H	-2.67470300	4.61468500	0.27538400
C	2.60553100	-2.24106000	-0.03808000
C	3.90842300	-1.92099100	-0.35620800
C	4.64001800	-2.83852600	-1.19055100
C	4.05430000	-4.09868400	-1.50604700
C	2.72381900	-4.38404300	-1.09138200
C	1.96137500	-3.45253500	-0.43553700
H	6.35977100	-1.55651300	-1.53753400
C	5.91813200	-2.53359700	-1.73339800
C	4.78465700	-5.02992300	-2.29271100
H	2.28036000	-5.34390600	-1.36553500
C	6.02973500	-4.71695000	-2.78002600
C	6.59262700	-3.44766800	-2.50806300
H	4.32586400	-5.99526500	-2.51627600
H	6.57853000	-5.43605100	-3.38948300
H	7.56829700	-3.18880000	-2.92147500
C	4.50513800	-0.65442600	0.15385000
C	5.76705400	-0.64788000	0.84757400
C	3.84495100	0.55209200	0.00255200
C	6.43784600	-1.84224500	1.23462100
C	6.36587000	0.59850300	1.19014300
C	4.39843800	1.80206400	0.40278400
C	7.65133200	-1.79530600	1.87795600
H	5.97407200	-2.80591100	1.02653300
C	7.63037800	0.61523900	1.83985700
C	5.66377200	1.80606700	0.93223000
C	8.26636700	-0.55464700	2.17157600
H	8.14140700	-2.72456700	2.17166100
H	8.07675700	1.58144600	2.08346000
H	6.12149300	2.75568800	1.21826700
H	9.23325900	-0.53222000	2.67583700
O	2.61643400	0.60375800	-0.62135900
O	1.87146000	-1.35735700	0.73073600
P	1.27563300	-0.05102700	-0.01867000
O	0.48667800	0.75885600	0.93694500
C	3.56284300	3.03857700	0.32020500
C	3.49523500	3.80198100	-0.86483300
C	2.82012200	3.42410100	1.46096200

C	2.67888300	4.94008200	-0.88654700
C	1.99528900	4.54999400	1.36312300
C	1.90771800	5.32547000	0.20797900
H	2.64569000	5.53007800	-1.80512100
H	1.39968300	4.83576500	2.23591800
C	0.51123700	-3.63597600	-0.12972000
C	-0.46003400	-3.68183700	-1.14935900
C	0.11144600	-3.68709500	1.23118600
C	-1.81560100	-3.74800900	-0.76998700
C	-1.24262700	-3.72583000	1.54494900
C	-2.23399700	-3.73259800	0.55634900
H	-2.56298400	-3.77338900	-1.56854900
H	-1.55256000	-3.73800000	2.59358100
C	4.31558100	3.53363000	-2.12656500
C	4.17500800	2.14211400	-2.75401400
C	5.79175700	3.90034700	-1.92995000
H	3.91665800	4.24289900	-2.87000500
H	3.12803400	1.81160100	-2.78607100
H	4.56592700	2.17094400	-3.78224400
H	4.75546700	1.38297900	-2.21114000
H	5.89814500	4.91867700	-1.52945200
H	6.28162600	3.20254300	-1.23605800
H	6.32728600	3.84837600	-2.88995500
C	2.92365300	2.81443800	2.86459200
C	4.05956200	3.50296200	3.63595800
C	3.01469500	1.29496200	3.04114600
H	1.98338000	3.11157900	3.35480600
H	3.96769000	4.59761100	3.59426900
H	4.04819900	3.19140400	4.69118900
H	5.03784100	3.22560700	3.21598400
H	2.24870200	0.77133200	2.45862300
H	4.00407100	0.88893900	2.79198600
H	2.83076700	1.06297000	4.10130900
C	1.01239300	6.55382600	0.19638700
C	0.63863500	7.03247800	-1.20487300
C	1.66065100	7.69018900	0.99718400
H	0.08167600	6.26730300	0.71691900
H	0.21206700	6.22238100	-1.81507100
H	-0.10394500	7.84052300	-1.14383500
H	1.51622100	7.43355900	-1.73458900
H	1.88758500	7.37655000	2.02567400
H	2.60529300	7.99556700	0.52165100
H	0.99709400	8.56655700	1.04089700
C	-0.24186400	-3.70468400	-2.66832600
C	-0.36694400	-5.14649000	-3.18262700
C	0.98739900	-3.03307400	-3.29355300
H	-1.11205200	-3.15266400	-3.06005700
H	-0.33275200	-5.16547700	-4.28217200
H	0.46550000	-5.76153500	-2.80790300
H	-1.30493900	-5.61639900	-2.85492300
H	1.25842600	-2.09757200	-2.79095500
H	1.86537300	-3.69080500	-3.30260900
H	0.75187100	-2.80052700	-4.34317700
C	1.12782100	-3.77317800	2.36131400
C	1.18464000	-5.20948500	2.89549000
C	0.85697100	-2.77318000	3.48568700
H	2.12144200	-3.54248100	1.95737200
H	1.43817500	-5.91908600	2.09450900
H	1.94079000	-5.29846400	3.68978200
H	0.21108500	-5.50729800	3.31473900
H	0.74535600	-1.75543500	3.08424600
H	-0.05270200	-3.03765900	4.04656300
H	1.69250900	-2.77292500	4.20099100
C	-3.69659900	-3.76097900	0.96677000
C	-4.12531400	-5.19890900	1.28455800
C	-4.64854500	-3.13237200	-0.05117300



H	-3.76763200	-3.17239100	1.89671500
H	-3.47606100	-5.64616000	2.05039100
H	-5.16188700	-5.22446000	1.65204000
H	-4.06258200	-5.82573700	0.38143000
H	-4.37772700	-2.09314800	-0.30504100
H	-4.69258000	-3.71450400	-0.98473900
H	-5.66653600	-3.09581700	0.36385000
O	-1.90555700	-0.72676800	-0.97052900
H	-2.40659700	-1.47985100	-0.62182700
H	-0.82668400	1.79249000	1.11670100
O	0.57086700	-0.53757600	-1.31706700
H	-0.43682000	-0.67199700	-1.19889200

**TS18***ISI-Ra-3Si*

S	-2.41524900	-0.92550700	1.85842600
O	-1.89634200	0.20748600	2.61447000
O	-1.67999100	-1.48299400	0.72537400
O	-2.49024100	-0.95128500	-2.08919400
N	-4.20484100	0.54583500	0.44187900
N	-3.18457700	0.91619000	-0.38141600
C	-2.72212700	-2.24907300	3.00761400
C	-2.94462500	-1.94028000	4.34721500
H	-2.93053000	-0.89767500	4.66868600
C	-3.16309700	-2.98758500	5.24026000
H	-3.33877900	-2.77400800	6.29526600
C	-3.14368500	-4.30852300	4.78719700
H	-3.31025600	-5.12368600	5.49307500
C	-2.90264000	-4.59603200	3.44262300
H	-2.87521300	-5.63120800	3.09882600
C	-2.68735400	-3.55791100	2.53817700
H	-2.47363300	-3.73455100	1.48304900
C	-4.06164700	-0.46462500	1.36722200
C	-5.26392000	-0.78148700	1.94171800
H	-5.43157000	-1.52203100	2.71869900
C	-6.22988500	0.09291300	1.33782500
C	-5.53785100	0.90883600	0.40668000
C	-6.19219400	1.89354600	-0.35026500
H	-5.65067400	2.51579100	-1.06386500
C	-7.55515000	2.04318200	-0.15907000
H	-8.09326500	2.80120700	-0.73001000
C	-8.26397300	1.23855200	0.76045300
H	-9.33716600	1.38911000	0.88256600
C	-7.61657300	0.26977700	1.50598400
H	-8.16649800	-0.34813800	2.21753000
C	-2.80341500	2.28320900	-0.44385700
H	-3.61265800	2.97094400	-0.13575900
C	-2.37963400	2.50825900	-1.88009700
C	-1.82343400	3.68837800	-2.36804900
H	-1.72972600	4.56249200	-1.71915800
C	-1.37515600	3.74016600	-3.68650300
H	-0.93764900	4.66068900	-4.07820900
C	-1.46813200	2.61180300	-4.50522900
H	-1.09715200	2.65320600	-5.53024000
C	-2.03016300	1.43353400	-4.01737300
H	-2.09659100	0.54339300	-4.64624500
C	-2.50361900	1.39514900	-2.70692300
C	-3.16728300	0.18802500	-2.10478300
C	-4.59869700	-0.06219400	-2.49773900
H	-4.58963800	-0.56582200	-3.47624400
H	-5.17641900	0.86362000	-2.57506900
H	-5.07005900	-0.73813800	-1.76942900
C	3.00677200	1.06166300	0.31262800
C	3.82650100	0.01300500	0.68411600
C	4.73907900	0.22161800	1.77701400
C	4.88303400	1.53285400	2.31439200
C	4.03687200	2.57669200	1.85324800
C	3.05072100	2.34781300	0.92698700

H	5.35760700	-1.85021200	1.99857600
C	5.49239200	-0.83253500	2.36420900
C	5.81548900	1.76129000	3.36265200
H	4.12629400	3.56736000	2.30480900
C	6.55168300	0.72808600	3.88716900
C	6.37280200	-0.58511200	3.39043100
H	5.91942900	2.77508900	3.75490100
H	7.25884500	0.91177700	4.69711700
H	6.93333300	-1.41092100	3.83064500
C	3.72476000	-1.28954600	-0.02930900
C	4.88282100	-1.95280100	-0.56835900
C	2.48867700	-1.87757500	-0.23020600
C	6.17342900	-1.35241200	-0.59249200
C	4.73850000	-3.25468600	-1.12969200
C	2.31707000	-3.13157100	-0.88556600
C	7.25962900	-2.02844300	-1.09403400
H	6.29563200	-0.33740800	-0.21581200
C	5.88425500	-3.93627100	-1.62438200
C	3.44242700	-3.82127200	-1.25944000
C	7.12139800	-3.34287600	-1.60123100
H	8.23664300	-1.54336400	-1.10792300
H	5.75343600	-4.93750900	-2.03994700
H	3.33795600	-4.80118200	-1.73045400
H	7.99319400	-3.87123700	-1.98930500
O	1.34946900	-1.27278500	0.25364300
O	2.10563800	0.88271200	-0.71542400
P	0.73389500	0.07223700	-0.38311700
O	-0.07084400	-0.04924800	-1.61955300
C	0.93290600	-3.55408800	-1.25602700
C	0.09342000	-4.24243800	-0.35279800
C	0.44610800	-3.15661500	-2.52273000
C	-1.23387200	-4.47262800	-0.72163800
C	-0.90687900	-3.37542200	-2.80811100
C	-1.77338000	-3.99259500	-1.91311300
H	-1.87643300	-5.02557400	-0.03082400
H	-1.30664700	-3.01377800	-3.75949000
C	2.04174500	3.39763600	0.59564900
C	1.12414300	3.84497200	1.57657600
C	2.01796600	3.96379400	-0.69872900
C	0.25057700	4.88614600	1.22872100
C	1.13502700	5.01106900	-0.98055000
C	0.25148600	5.50667300	-0.02247500
H	-0.46310000	5.22727900	1.98583700
H	1.15227400	5.44699100	-1.98098500
C	0.52515700	-4.76026200	1.01722700
C	0.88506700	-3.66099800	2.02436900
C	1.61406000	-5.83598700	0.94786100
H	-0.37368100	-5.25750600	1.41879000
H	0.17228800	-2.82690100	1.97093500
H	0.87594600	-4.07803400	3.04330100
H	1.89157200	-3.25624600	1.84398800
H	1.34599500	-6.62843700	0.23387200
H	2.57994700	-5.40902600	0.64527000
H	1.75120100	-6.29661000	1.93805000
C	1.27375300	-2.59039100	-3.68387800
C	1.92897500	-3.74338400	-4.45824500
C	2.29360000	-1.47262700	-3.43684700
H	0.51955100	-2.15056700	-4.35532200
H	1.19500000	-4.52008700	-4.71607500
H	2.38463500	-3.37014300	-5.38802700
H	2.72547300	-4.21058000	-3.86056200
H	1.86597000	-0.65331000	-2.84819200
H	3.21410300	-1.82472900	-2.95291700
H	2.58613300	-1.05628000	-4.41335300
C	-3.25391300	-4.11188400	-2.21487700
C	-4.10218900	-3.62885400	-1.03411600

C	-3.63099200	-5.53732900	-2.62801500
H	-3.45200500	-3.43747200	-3.06331000
H	-3.73220400	-2.65694600	-0.67475900
H	-5.15853100	-3.52782300	-1.32735500
H	-4.06718200	-4.34783700	-0.19942300
H	-3.05745400	-5.86176600	-3.50793000
H	-3.41881900	-6.24349100	-1.80985400
H	-4.70324800	-5.60732400	-2.86617200
C	0.95975200	3.36417000	3.02756900
C	1.53945900	4.41445100	3.98788500
C	1.42189300	1.96782200	3.45948600
H	-0.13379400	3.36614900	3.16786900
H	1.30986600	4.14369700	5.02902400
H	2.63482100	4.46328600	3.88828300
H	1.13922800	5.41993000	3.79426900
H	1.19608000	1.19991400	2.71305800
H	2.49250100	1.93547700	3.69820200
H	0.87534500	1.70435000	4.37707800
C	2.95661900	3.51579400	-1.80966400
C	3.94142800	4.63106200	-2.17700600
C	2.17340500	3.03284100	-3.03471100
H	3.55158700	2.67002200	-1.44511000
H	4.52515100	4.94821100	-1.30065500
H	4.64171500	4.28436700	-2.95133400
H	3.41507100	5.51424800	-2.57084400
H	1.42743500	2.27449600	-2.75588700
H	1.64767000	3.86798900	-3.52439700
H	2.85720300	2.59063300	-3.77470000
C	-0.67099900	6.69307000	-0.27198600
C	-0.64809000	7.20471000	-1.71034900
C	-0.33359400	7.84066000	0.68928200
H	-1.70015200	6.35975600	-0.04185500
H	-0.90279600	6.42312800	-2.44027400
H	-1.36912000	8.02502700	-1.83125300
H	0.34829300	7.59442200	-1.96857000
H	-0.39074800	7.52446800	1.73949200
H	0.68970400	8.19914800	0.50071700
H	-1.02629100	8.68298000	0.54696600
O	-1.70426100	2.51290400	0.45131900
H	-1.21987900	3.32385500	0.22247200
H	-1.54157900	-0.78160100	-1.85009000
O	0.12196400	0.76719800	0.85924700
H	-0.69482300	1.35370100	0.72574100

**TS19***IS-Ra-3R*

S	-5.93605600	0.42414100	-1.39530000
O	-5.73069400	-0.87186400	-2.04066900
O	-5.45775500	1.63001100	-2.06817600
N	-3.79857100	0.21524900	0.29313200
N	-2.87991700	0.65427200	-0.61418700
C	-7.65542100	0.60457700	-1.00844200
C	-8.44175800	-0.54195500	-0.92142800
H	-7.99417800	-1.51916300	-1.10892500
C	-9.79084400	-0.39509600	-0.60541400
H	-10.42992700	-1.27563100	-0.53286100
C	-10.32277700	0.87745400	-0.39025500
H	-11.38017000	0.98574500	-0.14462900
C	-9.51831100	2.01396400	-0.49417500
H	-9.94622900	3.00420800	-0.33512500
C	-8.16785600	1.88458700	-0.80949200
H	-7.51677800	2.75377600	-0.91346700
C	-5.18159400	0.32647700	0.20108700
C	-5.75509600	0.03491800	1.40799600
H	-6.82275200	-0.01277400	1.60773300
C	-4.67909100	-0.25022800	2.31939800
C	-3.47484800	-0.15172700	1.58956800
C	-2.21593800	-0.41342800	2.13652400

H	-1.31868200	-0.37007900	1.52114000
C	-2.19162300	-0.75899200	3.47647700
H	-1.23013400	-0.97809500	3.94205100
C	-3.37725500	-0.84806800	4.24229000
H	-3.30811600	-1.12697300	5.29454200
C	-4.61850900	-0.60855600	3.68079400
H	-5.53090900	-0.69839700	4.27176400
C	-2.59279200	-0.13708000	-1.85182300
H	-3.53082600	-0.09815200	-2.43395500
C	-1.62223200	0.78864900	-2.52566200
C	-0.87118700	0.58979700	-3.67497800
H	-0.85406000	-0.38233600	-4.16698900
C	-0.12243900	1.66178600	-4.15825300
H	0.49224100	1.52858100	-5.04976000
C	-0.13607800	2.90818200	-3.51750900
H	0.46159800	3.72688300	-3.92040700
C	-0.89081000	3.10385200	-2.36453800
H	-0.88758200	4.06699800	-1.84924600
C	-1.62826700	2.02467800	-1.88115800
C	-2.45346300	1.93178900	-0.66204800
C	-3.32933000	3.01821900	-0.13694100
H	-3.62162900	2.80902500	0.89989900
H	-4.21934100	3.04161100	-0.78395400
H	-2.81370900	3.98113300	-0.17827600
C	2.69139600	-2.02698000	-0.06251900
C	3.88679800	-1.56805700	-0.58962700
C	4.57543100	-2.40871400	-1.53282400
C	4.12454300	-3.74656500	-1.72373100
C	2.93349900	-4.18268100	-1.08278700
C	2.16217900	-3.32391100	-0.34074100
H	6.01597000	-0.92425100	-2.19614900
C	5.68782000	-1.95889000	-2.29707900
C	4.83393300	-4.60409100	-2.60828900
H	2.59206000	-5.20673000	-1.24214600
C	5.92276400	-4.14860200	-3.30986100
C	6.34108800	-2.80437400	-3.16200200
H	4.48014800	-5.62991700	-2.73258100
H	6.45444200	-4.81225800	-3.99316300
H	7.18619900	-2.43360800	-3.74385500
C	4.42280400	-0.24591900	-0.16311600
C	5.78142900	-0.08898700	0.29237300
C	3.59667300	0.86486800	-0.13850100
C	6.65860900	-1.19050100	0.50270400
C	6.27434800	1.21778200	0.57854200
C	4.04977900	2.15332300	0.27494000
C	7.95750200	-0.99763200	0.90930300
H	6.28745900	-2.20292200	0.34937500
C	7.62750200	1.38784800	0.97891200
C	5.38136800	2.32355300	0.55064600
C	8.45890800	0.30656300	1.13278500
H	8.60477600	-1.86109800	1.06954200
H	7.98568800	2.39956400	1.18100900
H	5.75336700	3.31074600	0.83497400
H	9.49388200	0.44676600	1.44755200
O	2.30701000	0.78170700	-0.57087300
O	1.99790400	-1.24932300	0.82358600
P	1.11375400	0.01654800	0.26571700
O	0.72602300	0.79903300	1.50472300
C	3.03371000	3.22030500	0.51900700
C	2.53312200	4.02925100	-0.52670600
C	2.55614900	3.38276700	1.83854800
C	1.56209600	4.99272600	-0.22716600
C	1.58534100	4.36611500	2.07452200
C	1.08540700	5.19041900	1.07185300
H	1.20683800	5.63704700	-1.03752500
H	1.22408300	4.50451400	3.09782800

C	0.80028700	-3.70176300	0.14137800
C	-0.24200500	-3.92801300	-0.78421900
C	0.55441300	-3.82841000	1.52865700
C	-1.49145800	-4.32106600	-0.28302000
C	-0.71409500	-4.20727200	1.96794700
C	-1.75318200	-4.47346900	1.07426300
H	-2.29873600	-4.51523400	-0.99769500
H	-0.89073300	-4.31271300	3.04245300
C	3.09288600	4.05349900	-1.94868300
C	3.24485700	2.71947500	-2.68622100
C	4.41353400	4.83510400	-1.97356600
H	2.36257500	4.64591100	-2.52511400
H	2.36889900	2.07294200	-2.55493000
H	3.37901800	2.92221300	-3.76056000
H	4.13159500	2.16451800	-2.34967200
H	4.29748200	5.83082000	-1.52210900
H	5.18972200	4.29158600	-1.41483200
H	4.76729300	4.95922300	-3.00830000
C	3.08002700	2.68976000	3.10356200
C	4.21809600	3.52930800	3.70438000
C	3.47684800	1.20967100	3.08126400
H	2.23302100	2.75378000	3.80452200
H	3.92895700	4.58420400	3.81731000
H	4.49944800	3.13655200	4.69299100
H	5.11018300	3.48622500	3.06184400
H	2.71616000	0.59222200	2.59240000
H	4.45106600	1.03245000	2.60727800
H	3.56277100	0.87030900	4.12528600
C	0.06453800	6.26469300	1.40053800
C	-1.33575700	5.83475000	0.96097800
C	0.43528500	7.62840900	0.81584100
H	0.05151200	6.36019400	2.49811600
H	-1.59155700	4.85719100	1.39425800
H	-2.09662700	6.56773400	1.26935800
H	-1.37897900	5.75358200	-0.13901100
H	1.44528000	7.93176800	1.12494100
H	0.40901800	7.61155900	-0.28433200
H	-0.27597700	8.39774500	1.15075300
C	-0.16843900	-3.80676100	-2.31084400
C	0.18895500	-5.13901200	-2.98402600
C	0.64465000	-2.64807700	-2.89494800
H	-1.21020300	-3.59331700	-2.59511500
H	0.00532400	-5.07282400	-4.06738200
H	1.25086400	-5.38647700	-2.84792400
H	-0.41188500	-5.96825200	-2.58249700
H	0.45537300	-1.72182100	-2.33501200
H	1.72476400	-2.84578900	-2.90761500
H	0.33726200	-2.50460100	-3.94402100
C	1.64356500	-3.62430900	2.57268100
C	1.98331000	-4.94935000	3.26427400
C	1.26080900	-2.54654200	3.59102400
H	2.55418700	-3.28343300	2.06450400
H	2.29454600	-5.70790600	2.53138800
H	2.80149800	-4.80992200	3.98678100
H	1.11332900	-5.34574900	3.81055100
H	1.01144000	-1.60332500	3.08371300
H	0.39944500	-2.86564800	4.19999200
H	2.09902800	-2.35513700	4.27794000
C	-3.11484000	-4.92961300	1.56312700
C	-3.75725900	-3.89788800	2.49187700
C	-3.02719200	-6.30084200	2.24006200
H	-3.75777900	-5.03363000	0.67325300
H	-3.82533000	-2.91253300	2.00794100
H	-4.76956300	-4.21276400	2.78888600
H	-3.16275100	-3.77144200	3.40988000
H	-2.58948900	-7.04915200	1.56444500

H	-2.39464200	-6.24922200	3.13968400
H	-4.02428300	-6.64981100	2.54851400
O	-2.21986600	-1.43084800	-1.64072500
H	-3.01536700	-1.97789300	-1.61225400
O	0.05101000	-0.34927300	-0.69843100
O	-1.08510700	2.30845500	0.72187300
H	-0.39596300	1.61306500	1.11135900
H	-0.49020700	2.99007900	0.36441500

**TS20***IR-Ra-3S*

S	-2.83696200	0.27872500	2.16516600
O	-2.27628000	0.59079700	3.46546400
O	-2.00870700	0.00028800	1.00383300
N	-4.02187300	2.24221300	0.50115300
N	-2.99228300	2.29216300	-0.38791800
C	-3.96056800	-1.08993600	2.38471200
C	-4.13237600	-1.60850300	3.66412200
H	-3.56414500	-1.18380600	4.49296100
C	-5.02557400	-2.66496000	3.83963900
H	-5.17053400	-3.09465100	4.83152400
C	-5.73709800	-3.16338600	2.74854600
H	-6.44605500	-3.98030500	2.89057800
C	-5.54357100	-2.62981300	1.47232100
H	-6.09839500	-3.04084100	0.62686300
C	-4.63239500	-1.59446600	1.27374400
H	-4.41776100	-1.19143000	0.27846000
C	-3.96120700	1.59957100	1.73937900
C	-4.92340800	2.09185300	2.56838200
H	-5.12331200	1.73688100	3.57630300
C	-5.59909200	3.14200500	1.85541600
C	-4.98005000	3.24666300	0.59106400
C	-5.31111500	4.24660600	-0.32931400
H	-4.77551500	4.35329900	-1.27333300
C	-6.33089200	5.11725800	0.02505700
H	-6.61643400	5.91266700	-0.66442100
C	-6.99983100	5.00068400	1.26088800
H	-7.80057500	5.70112200	1.49997600
C	-6.64101100	4.02853800	2.17990000
H	-7.14326700	3.95847500	3.14554600
C	-1.77170200	3.11561400	-0.02081300
H	-2.16826700	4.14985400	0.02651500
C	-0.98349900	2.93540400	-1.29613500
C	0.32316500	3.31106800	-1.57374100
H	0.96331500	3.75168500	-0.80621500
C	0.80808100	3.06653600	-2.85940500
H	1.83412900	3.34828900	-3.09599500
C	0.01336500	2.45903500	-3.83867100
H	0.42942100	2.27582400	-4.83008100
C	-1.28590700	2.05596700	-3.54704200
H	-1.89310200	1.53977700	-4.29345400
C	-1.76490300	2.30085000	-2.26344100
C	-3.01996500	1.83235400	-1.64127100
C	-4.31321600	1.62405400	-2.35838900
H	-4.16001500	1.03266500	-3.26773000
H	-4.71802500	2.60417300	-2.64781300
H	-5.03635800	1.11992600	-1.70523500
C	3.23263100	-0.15861700	0.47276000
C	3.41379600	-1.41838700	1.01853300
C	4.29115700	-1.55927600	2.14769000
C	5.07681300	-0.44462000	2.55527400
C	4.90792600	0.80300500	1.89859900
C	3.95775400	0.98486500	0.92505400
H	3.77063500	-3.61564700	2.61640200
C	4.39657800	-2.76678000	2.89249900
C	5.97664100	-0.58437100	3.64677500
H	5.50756300	1.65640000	2.22352300
C	6.07407600	-1.77062700	4.33109000

C	5.26277800	-2.86819200	3.95485500
H	6.57723800	0.27934200	3.93995300
H	6.76150900	-1.86566300	5.17277400
H	5.32023500	-3.80102400	4.51763400
C	2.71377400	-2.57794800	0.40538400
C	3.43329600	-3.74827100	-0.01997600
C	1.35418600	-2.49607700	0.14977700
C	4.85268200	-3.85490700	0.03840500
C	2.70482200	-4.84940000	-0.55401900
C	0.64829400	-3.53308000	-0.53159800
C	5.49329400	-5.00696900	-0.35021200
H	5.43751700	-3.00539100	0.38841600
C	3.39263200	-6.03526000	-0.93146700
C	1.31393100	-4.70571700	-0.79411300
C	4.75797400	-6.12028800	-0.82414200
H	6.58180000	-5.06011400	-0.29970900
H	2.81028100	-6.87050300	-1.32662900
H	0.77630800	-5.52566300	-1.27633800
H	5.27929700	-7.03120200	-1.12149000
O	0.65347200	-1.40907100	0.58646800
O	2.35099000	0.00431700	-0.56928800
P	0.75212000	0.05046300	-0.15830100
O	-0.06115100	0.01684700	-1.42128400
C	-0.72000300	-3.33144500	-1.10610400
C	-1.89630900	-3.57002200	-0.35592100
C	-0.81013900	-3.01315300	-2.48175600
C	-3.13233600	-3.50309000	-1.00641900
C	-2.08470400	-2.93293800	-3.06723900
C	-3.25445900	-3.18769100	-2.35935500
H	-4.02855900	-3.73443700	-0.42672700
H	-2.15114800	-2.70810900	-4.13727000
C	3.71490900	2.33532400	0.33942500
C	3.20127900	3.38860600	1.12600100
C	4.06931600	2.56732800	-1.01207000
C	3.07277100	4.65298900	0.52664400
C	3.93476200	3.84891700	-1.54601200
C	3.43888800	4.91391400	-0.78976100
H	2.66849800	5.47181700	1.13036200
H	4.24367100	4.02342600	-2.58164100
C	-1.92986800	-4.04804700	1.09564000
C	-1.11363400	-3.24839100	2.11378800
C	-1.59460400	-5.54323300	1.17970800
H	-2.98454500	-3.94272200	1.39996700
H	-1.23162000	-2.16697300	1.97392200
H	-1.44990700	-3.51800600	3.12704200
H	-0.04038700	-3.47687400	2.05499600
H	-2.22574900	-6.13384000	0.49959000
H	-0.54179300	-5.72180700	0.91734000
H	-1.75210300	-5.90968400	2.20537800
C	0.34256400	-2.87422200	-3.48785200
C	0.61924100	-4.22899900	-4.15850900
C	1.65773800	-2.21300500	-3.07135300
H	-0.07643600	-2.22136300	-4.27113100
H	-0.30545100	-4.69940500	-4.52318800
H	1.30152600	-4.09467300	-5.01130000
H	1.10308800	-4.92037200	-3.45358900
H	1.48280600	-1.27116700	-2.54161500
H	2.28955600	-2.86454700	-2.45307400
H	2.22896300	-1.98706400	-3.98532600
C	-4.60889500	-3.15135700	-3.04212800
C	-5.51605600	-2.08080500	-2.43196000
C	-5.28793600	-4.52309600	-3.01313500
H	-4.43140500	-2.88472100	-4.09733600
H	-5.02172300	-1.09967300	-2.42369400
H	-6.46117300	-1.99425100	-2.98833200
H	-5.76311500	-2.33145800	-1.38916200

H	-4.64897200	-5.28970000	-3.47273000
H	-5.49211100	-4.83337800	-1.97659200
H	-6.24614000	-4.49759400	-3.55322500
C	2.78603200	3.35738600	2.60428300
C	3.84861800	4.06781300	3.45709200
C	2.38057300	2.04073800	3.27515700
H	1.88330600	3.98977700	2.62576500
H	3.49964000	4.16230400	4.49621700
H	4.78318700	3.48589900	3.46977600
H	4.08315900	5.07216200	3.07653100
H	1.78149400	1.40663200	2.61251800
H	3.24678400	1.46985000	3.63394900
H	1.76658900	2.28427500	4.15535800
C	4.67481300	1.48308200	-1.89484700
C	6.12975800	1.81867700	-2.24045700
C	3.84144900	1.23768300	-3.15494500
H	4.68816700	0.54165500	-1.33249100
H	6.72859200	1.95764600	-1.32866900
H	6.58243500	1.00851400	-2.83151100
H	6.19566900	2.74527000	-2.83165800
H	2.80661300	0.97979300	-2.88870300
H	3.83323900	2.12510300	-3.80971500
H	4.26612100	0.40466900	-3.73523600
C	3.33382400	6.31206600	-1.37087600
C	2.45779200	6.35323200	-2.62511700
C	4.72394700	6.89013600	-1.65437000
H	2.85542700	6.94312800	-0.60422700
H	1.45101400	5.95992500	-2.42370100
H	2.35874600	7.38426100	-2.99625600
H	2.90037400	5.75140600	-3.43475000
H	5.34493800	6.88757300	-0.74770600
H	5.24381100	6.29292000	-2.41946900
H	4.65054200	7.92385700	-2.02425500
O	-1.24425200	2.80465800	1.17276300
H	-0.54436300	2.06435900	1.08250700
O	0.57923500	1.13303200	0.85929600
O	-2.60454200	-0.09177200	-1.55387500
H	-2.65716400	-0.60449900	-2.37609900
H	-1.60259600	-0.11683200	-1.33960300

**TS21<sub>M-Re</sub>**

S	-2.65496800	0.07434000	1.66765000
O	-1.63120100	0.97320900	2.23584900
O	-2.26430100	-0.72969400	0.51452700
N	-4.05192400	1.90180700	0.20754200
N	-2.97048900	2.21407100	-0.54841500
C	-3.22409600	-0.96354800	2.98233600
C	-3.06292700	-0.54034900	4.29925100
H	-2.59038200	0.42074300	4.50735600
C	-3.50672200	-1.38285500	5.31681800
H	-3.39198300	-1.08098900	6.35830200
C	-4.08710900	-2.61349000	5.00344700
H	-4.42781600	-3.26851400	5.80663200
C	-4.22851400	-3.01909900	3.67460800
H	-4.67127600	-3.98799600	3.43986300
C	-3.79193200	-2.18864800	2.64553500
H	-3.85899800	-2.47575600	1.59456300
C	-4.08036900	1.02077400	1.27096100
C	-5.30989100	1.02000900	1.87147000
H	-5.61002300	0.40707000	2.71689100
C	-6.09992200	1.98261300	1.15732500
C	-5.27821600	2.53164400	0.14571500
C	-5.71229300	3.55325700	-0.70888200
H	-5.04071700	3.98504300	-1.45098100
C	-7.01382700	3.99319100	-0.54692000
H	-7.39042800	4.79062900	-1.18892300
C	-7.86577700	3.44089000	0.43733200



H	-8.88537200	3.81684300	0.52818800
C	-7.42298500	2.44787500	1.29094700
H	-8.07797300	2.03588500	2.05983300
C	-2.05426100	3.19328900	-0.12941700
C	-1.14027000	3.33485800	-1.28606800
C	0.00061100	4.12625200	-1.40370000
H	0.35289500	4.71664600	-0.55485100
C	0.67009900	4.11685600	-2.62297700
H	1.57193100	4.71516900	-2.75150400
C	0.20130800	3.33246100	-3.68847900
H	0.74415700	3.34384600	-4.63555800
C	-0.91657200	2.51660900	-3.55041400
H	-1.24282800	1.87335000	-4.36950400
C	-1.58507600	2.51551000	-2.32595000
C	-2.69534400	1.64348900	-1.86379500
C	-3.88938800	1.43461600	-2.76053000
H	-3.56625700	0.92459100	-3.67830800
H	-4.36167000	2.38880700	-3.04428300
H	-4.64519800	0.80112400	-2.27494400
C	3.17402200	-0.20844100	0.25361300
C	3.40584900	-1.53748500	0.56008900
C	4.34749000	-1.84439500	1.60249100
C	5.13378900	-0.79309000	2.15211900
C	4.89706000	0.54322100	1.73665100
C	3.88758600	0.86492400	0.86258000
H	3.89317100	-3.96589700	1.74354900
C	4.51755500	-3.15738900	2.12376900
C	6.09977400	-1.09024700	3.15210300
H	5.49356500	1.34669700	2.17410600
C	6.25924600	-2.37218300	3.61628800
C	5.44648500	-3.41225100	3.10407300
H	6.70080400	-0.27222400	3.55462000
H	6.99760800	-2.58977500	4.38916800
H	5.55401600	-4.42487500	3.49526000
C	2.68400900	-2.60859300	-0.17792700
C	3.38359200	-3.69183000	-0.81543000
C	1.30849700	-2.55055600	-0.30135200
C	4.80349600	-3.75341300	-0.89714600
C	2.63026600	-4.73869500	-1.42027100
C	0.54953500	-3.53654400	-0.99562900
C	5.43115800	-4.81777700	-1.49844600
H	5.39729600	-2.93807700	-0.48536000
C	3.30817500	-5.83484200	-2.02087400
C	1.21600700	-4.63218100	-1.48531700
C	4.67923900	-5.88125000	-2.05353900
H	6.52035300	-4.83867000	-1.55510700
H	2.71205100	-6.63141900	-2.47065100
H	0.65085400	-5.40970500	-2.00520100
H	5.19092100	-6.72310200	-2.52179800
O	0.63095900	-1.50137600	0.29211000
O	2.24894300	0.11173200	-0.72422600
P	0.66742900	-0.03801400	-0.40692100
O	-0.15427000	0.07895000	-1.62833600
C	-0.89819900	-3.30517500	-1.28256700
C	-1.90687500	-3.73150800	-0.38665000
C	-1.24107800	-2.63626500	-2.47579700
C	-3.23831400	-3.45912300	-0.70037100
C	-2.59135500	-2.31316300	-2.68479500
C	-3.60130300	-2.70310800	-1.81601600
H	-4.02002300	-3.82758500	-0.02840800
H	-2.85763600	-1.74908300	-3.58435200
C	3.57187000	2.29555300	0.57609200
C	3.06428600	3.13159900	1.59370700
C	3.86866900	2.83079700	-0.69901700
C	2.90384400	4.49439200	1.30361100
C	3.71205300	4.20007100	-0.92003400

C	3.24313600	5.05793100	0.07712400
H	2.51002900	5.14770300	2.08874600
H	3.98735300	4.60850600	-1.89685300
C	-1.64588700	-4.47993100	0.91868300
C	-0.76642200	-3.71678000	1.91753600
C	-1.14626000	-5.91437200	0.71396800
H	-2.63963100	-4.56884000	1.38887100
H	-1.00710200	-2.64504400	1.91876700
H	-0.91935000	-4.11822900	2.93132400
H	0.30259400	-3.81927100	1.68164500
H	-1.79095400	-6.46271400	0.01188700
H	-0.11898600	-5.92815700	0.32537000
H	-1.14559100	-6.45317200	1.67380300
C	-0.33458000	-2.33167700	-3.67781900
C	-0.51470000	-3.47009900	-4.69636300
C	1.16188900	-2.03658600	-3.52963500
H	-0.77245700	-1.42085200	-4.11706200
H	-1.57410500	-3.64331500	-4.93191100
H	0.02030100	-3.24149000	-5.63033800
H	-0.10203900	-4.40761100	-4.29143800
H	1.37153200	-1.26328900	-2.78560100
H	1.75473900	-2.93079900	-3.29894100
H	1.52118100	-1.65620500	-4.49824500
C	-5.04229200	-2.29368000	-2.04820400
C	-5.55513600	-1.44767600	-0.87796300
C	-5.94992800	-3.49900000	-2.30317700
H	-5.05312900	-1.66108200	-2.95122600
H	-4.84208500	-0.64543800	-0.63724300
H	-6.53229600	-0.99530700	-1.10681200
H	-5.68031600	-2.06448300	0.02731500
H	-5.60266800	-4.08112200	-3.16819800
H	-5.96200900	-4.16895100	-1.42940400
H	-6.98446100	-3.17619100	-2.49313200
C	2.69614600	2.75320500	3.03590100
C	3.77960100	3.24588000	4.00720500
C	2.31218400	1.31097300	3.38683900
H	1.79634600	3.35779000	3.23385700
H	3.45431500	3.09843600	5.04803300
H	4.71283300	2.67967200	3.86536600
H	4.00606100	4.31145400	3.86244900
H	1.70788000	0.83707000	2.60690600
H	3.18816800	0.67762000	3.57742100
H	1.71773800	1.32896300	4.31281600
C	4.42369500	1.97615700	-1.83061800
C	5.84618300	2.40966000	-2.20046100
C	3.49752300	1.99048200	-3.04933300
H	4.48668900	0.93664300	-1.48420800
H	6.51158900	2.36839900	-1.32580800
H	6.25861900	1.75246000	-2.98050700
H	5.86116500	3.44014700	-2.58741600
H	2.48282800	1.66987600	-2.77457100
H	3.43289100	3.00038100	-3.48606300
H	3.87944600	1.31287200	-3.82802900
C	3.19209600	6.56393300	-0.11402800
C	2.51673400	6.99893600	-1.41449400
C	4.60752900	7.14629100	-0.01752800
H	2.60253700	6.97225900	0.72309600
H	1.48342800	6.63068700	-1.47852300
H	2.49067100	8.09645700	-1.48186900
H	3.06823700	6.63151000	-2.29424100
H	5.08478400	6.86877700	0.93279900
H	5.23676200	6.76033700	-0.83468100
H	4.58684900	8.24401700	-0.09093300
O	-2.08314200	3.74864100	0.93718500
H	-0.36815300	1.02520100	1.30663600
H	-1.84113300	0.35651200	-1.68306500

O	0.46501000	0.98844100	0.74971600
<b>TS22<sub>M-Si</sub></b>			
S	-5.67007700	1.57301300	-0.94139800
O	-5.00154500	0.94932200	-2.07401900
O	-5.57790100	3.01219600	-0.73050400
N	-3.77595700	0.55981600	0.75958700
N	-2.82111700	1.18232000	0.02172600
C	-7.39093500	1.12696400	-0.97784000
C	-7.75224600	-0.08221100	-1.56829900
H	-6.98294600	-0.71741100	-2.01135700
C	-9.09896200	-0.43711400	-1.57815600
H	-9.40942000	-1.37749300	-2.03490300
C	-10.04975000	0.41363300	-1.00942500
H	-11.10329800	0.13027300	-1.02123300
C	-9.66691000	1.62544500	-0.43293600
H	-10.41786500	2.28763000	-0.00051200
C	-8.32246400	1.99449800	-0.41521700
H	-7.98562400	2.93883900	0.01501100
C	-5.12908600	0.73341300	0.52991700
C	-5.86115700	0.13252700	1.51363000
H	-6.94544400	0.07993800	1.56301800
C	-4.91201700	-0.44142500	2.42760900
C	-3.61593500	-0.16497600	1.92715000
C	-2.44857500	-0.58830200	2.57368600
H	-1.46516000	-0.37837500	2.15267600
C	-2.61582500	-1.29593400	3.75393100
H	-1.73088700	-1.64180200	4.28925100
C	-3.89574200	-1.58817800	4.27464500
H	-3.97625200	-2.15139500	5.20525400
C	-5.04377000	-1.17363200	3.62193300
H	-6.03249100	-1.40408000	4.02136200
C	-2.24734200	0.61562800	-1.09391600
H	-0.95130900	1.77615800	1.27111800
C	-1.39834800	1.68124900	-1.65835500
C	-0.69767100	1.69907900	-2.86250500
H	-0.74832500	0.84845300	-3.54370200
C	0.05436700	2.83119000	-3.15497700
H	0.60550700	2.89411600	-4.09415300
C	0.11609800	3.89532900	-2.24101400
H	0.71890600	4.77223700	-2.48293900
C	-0.56571300	3.85751900	-1.02719400
H	-0.48068500	4.67839900	-0.31611600
C	-1.34649800	2.73745500	-0.74611300
C	-2.12188400	2.38342600	0.47016900
C	-2.95673400	3.40225200	1.19344900
H	-3.39665700	2.96629300	2.10220800
H	-3.76697200	3.76820600	0.54575800
H	-2.31949400	4.24288900	1.49913900
C	2.33790000	-2.43478000	-0.06500300
C	3.62393800	-2.07517700	-0.39488000
C	4.36645900	-2.96380800	-1.25223500
C	3.80476200	-4.23268600	-1.57798400
C	2.48328000	-4.55349400	-1.15713300
C	1.71054700	-3.64774500	-0.47992400
H	6.05354100	-1.63902400	-1.60020300
C	5.63070800	-2.62261300	-1.80522300
C	4.54626500	-5.13487200	-2.38733900
H	2.05084300	-5.51186000	-1.45412500
C	5.77825300	-4.78721500	-2.88482800
C	6.31623200	-3.51007400	-2.60113600
H	4.10610700	-6.10665200	-2.62016200
H	6.33509900	-5.48503700	-3.51150700
H	7.28086700	-3.22345200	-3.02206300
C	4.19877700	-0.80568700	0.13036000
C	5.46958600	-0.81281500	0.80758500
C	3.52882400	0.40165700	0.00514900

C	6.13535800	-2.01447900	1.18201900
C	6.08373300	0.42485900	1.14521100
C	4.11171200	1.64722300	0.38043500
C	7.35608700	-1.97852700	1.81196100
H	5.66209600	-2.97408100	0.97692600
C	7.35624000	0.43221100	1.77949800
C	5.38902000	1.63350600	0.88497100
C	7.98538200	-0.74375400	2.10183900
H	7.84163900	-2.91254700	2.09792900
H	7.81331600	1.39470500	2.01814300
H	5.86390800	2.58239500	1.14442700
H	8.95821600	-0.73136100	2.59490900
O	2.27542100	0.45885300	-0.57213700
O	1.59112300	-1.57205300	0.72200600
P	0.96028600	-0.28486100	-0.01563400
O	0.09499000	0.48299100	0.91082100
C	3.38685900	2.95634600	0.30746300
C	3.42654400	3.74468800	-0.86295600
C	2.80785200	3.47641200	1.48987100
C	2.92862000	5.05391900	-0.81170100
C	2.29295700	4.77764100	1.46371300
C	2.36877500	5.60041600	0.34034100
H	3.01769300	5.66624900	-1.71201200
H	1.86511300	5.18372800	2.38662900
C	0.25702600	-3.80937700	-0.18821400
C	-0.70792600	-3.67707800	-1.20692900
C	-0.14706400	-3.92214100	1.16487300
C	-2.05888100	-3.60534900	-0.82605700
C	-1.50100500	-3.87087600	1.47834200
C	-2.47812300	-3.68021200	0.49591900
H	-2.79810200	-3.43531400	-1.61149500
H	-1.81700300	-3.94027900	2.52334900
C	4.09638700	3.34544000	-2.17856900
C	3.75967500	1.96428400	-2.74763200
C	5.61531200	3.55221700	-2.11062200
H	3.71360700	4.07514600	-2.91071300
H	2.68950800	1.73575500	-2.66085400
H	4.03766800	1.93959300	-3.81208100
H	4.32479100	1.16238100	-2.25221100
H	5.86431900	4.56748200	-1.76966900
H	6.07673800	2.83277300	-1.41854400
H	6.06546100	3.39962300	-3.10316800
C	2.81285100	2.81619000	2.87472000
C	4.04232200	3.26778600	3.67708800
C	2.64399000	1.29850300	2.98213000
H	1.93490600	3.25113200	3.37903400
H	4.15005800	4.36171800	3.66907600
H	3.95636900	2.93412700	4.72208200
H	4.96137400	2.82800100	3.26273600
H	1.81955700	0.93695300	2.35650600
H	3.56094500	0.74767400	2.73214400
H	2.39522800	1.04934500	4.02489500
C	1.87942900	7.03894800	0.42533400
C	0.34958700	7.12511000	0.38955900
C	2.48479800	7.95253500	-0.63803000
H	2.20523200	7.41163000	1.41114200
H	-0.10922700	6.48205500	1.15501800
H	0.01497400	8.15784100	0.56704800
H	-0.03130200	6.81368300	-0.59550500
H	3.58215300	7.88978100	-0.64947700
H	2.11703300	7.69221100	-1.64251000
H	2.20049400	8.99714300	-0.44755700
C	-0.49740800	-3.60891300	-2.72710600
C	-0.89073800	-4.96171000	-3.34117000
C	0.83498000	-3.15544300	-3.33706900
H	-1.24898700	-2.87329300	-3.05940100

H	-0.85225600	-4.91250700	-4.43980700
H	-0.19055300	-5.74504300	-3.01049300
H	-1.90238000	-5.26762900	-3.04110300
H	1.29109200	-2.31357000	-2.80419700
H	1.56669500	-3.97185300	-3.39052200
H	0.64011500	-2.83482900	-4.37177900
C	0.86477100	-4.13591000	2.28150000
C	0.88374500	-5.61243800	2.69380000
C	0.62098300	-3.22691500	3.48695800
H	1.86468000	-3.89610400	1.89515500
H	1.12102800	-6.25769600	1.83552800
H	1.63298300	-5.79017200	3.47999400
H	-0.10063000	-5.91719700	3.08173100
H	0.54925400	-2.17501800	3.17311700
H	-0.30422300	-3.50193700	4.01624200
H	1.44845100	-3.31854800	4.20597500
C	-3.93614300	-3.57132700	0.90038800
C	-4.51930900	-4.96068300	1.18393100
C	-4.79267900	-2.81472900	-0.11387600
H	-3.94988800	-3.00415900	1.84603300
H	-3.93645400	-5.49125200	1.95060400
H	-5.55957700	-4.88202100	1.53454400
H	-4.50901500	-5.57332500	0.26895800
H	-4.32444300	-1.86190400	-0.40808900
H	-4.94365400	-3.41089100	-1.02836000
H	-5.78639200	-2.60822400	0.31220800
O	-2.35259400	-0.55168200	-1.44177100
H	-0.66534400	-0.90235200	-1.38614600
O	0.32504200	-0.78569000	-1.35909500

### Int12<sub>M</sub>

S	-6.81930200	0.58881900	-0.87628500
O	-7.32976000	-0.78818900	-0.85776300
O	-6.31937000	1.16222500	-2.11397900
N	-4.29106500	0.20381400	0.08693500
N	-3.95349600	-0.54319100	-0.99986600
C	-8.09062000	1.63054900	-0.20882200
C	-9.03351700	1.07799500	0.65451100
H	-8.99327400	0.01374400	0.89054300
C	-10.01578400	1.91347800	1.18247200
H	-10.76733000	1.50677000	1.85990400
C	-10.04169600	3.26569000	0.83657500
H	-10.81496300	3.91397800	1.25132000
C	-9.09387800	3.79545700	-0.04111100
H	-9.12959400	4.85063300	-0.31396800
C	-8.10377400	2.97409500	-0.57549600
H	-7.35381400	3.35043200	-1.27295000
C	-5.54188800	0.73000900	0.34283100
C	-5.54598100	1.36963500	1.55314400
H	-6.39208600	1.88739500	1.99678300
C	-4.21549300	1.24304900	2.08307300
C	-3.45438900	0.50781800	1.14420500
C	-2.09533300	0.21997800	1.31372200
H	-1.52637900	-0.33646900	0.56653600
C	-1.50773400	0.69192100	2.47544000
H	-0.45150600	0.48447700	2.65221000
C	-2.24191600	1.42407900	3.43695900
H	-1.73494400	1.77192400	4.33803000
C	-3.58465500	1.70451400	3.25526100
H	-4.14634700	2.27258400	3.99811200
C	-4.42552800	-1.82833400	-1.22017700
C	-3.81824200	-2.27140100	-2.37886500
C	-3.86459800	-3.52252500	-3.06560800
H	-4.50070700	-4.32624400	-2.69170100
C	-3.08951800	-3.68125200	-4.17924300
H	-3.10069700	-4.63020600	-4.71790200
C	-2.25131300	-2.61792800	-4.66682200

H	-1.65196200	-2.79195400	-5.56214900
C	-2.18603700	-1.40809700	-4.03414600
H	-1.53356100	-0.61606700	-4.40637800
C	-2.96619300	-1.20185700	-2.85439300
C	-3.07983000	-0.12504600	-1.98630700
C	-2.48277300	1.23882600	-1.98999300
H	-1.61380200	1.30916300	-1.31701300
H	-3.23331500	1.98954100	-1.69951500
H	-2.14063900	1.47738600	-3.00508900
C	2.78850300	-1.77673200	0.43728800
C	4.04814700	-1.66390400	-0.12228900
C	4.58065400	-2.81655800	-0.80170800
C	3.89462800	-4.06024500	-0.69165000
C	2.64114700	-4.11588300	-0.02544600
C	2.03409100	-2.98408600	0.45817000
H	6.26722800	-1.81116000	-1.73598900
C	5.75817800	-2.76491500	-1.59823800
C	4.44040600	-5.21683100	-1.31297000
H	2.11668200	-5.07047100	0.03960000
C	5.59632600	-5.14110500	-2.04916400
C	6.24999500	-3.89538900	-2.20577000
H	3.90614800	-6.16334700	-1.20879100
H	6.00153900	-6.03210100	-2.53044500
H	7.14858700	-3.82957600	-2.82067000
C	4.81226800	-0.38888500	-0.02163800
C	6.18198000	-0.35105700	0.42743300
C	4.21057200	0.81399300	-0.33176900
C	6.84756600	-1.48843900	0.96329000
C	6.90303800	0.87695700	0.35662000
C	4.88111000	2.07187500	-0.27618500
C	8.16466700	-1.42059700	1.35076800
H	6.29887300	-2.42273400	1.07583300
C	8.26973000	0.91062700	0.74552800
C	6.22514600	2.07234700	-0.01025100
C	8.89348000	-0.21434800	1.22469200
H	8.64975900	-2.30487300	1.76617800
H	8.80781400	1.85792000	0.67283300
H	6.77526000	3.01592300	0.00042800
H	9.94066000	-0.17655900	1.52740700
O	2.90667000	0.83848800	-0.78258600
O	2.21917700	-0.67871100	1.06771600
P	1.64278400	0.52083500	0.16535100
O	1.58690400	1.63883200	1.29807200
C	4.02453200	3.29179800	-0.37645800
C	3.56328400	3.76749700	-1.62727900
C	3.54339800	3.85898300	0.82455700
C	2.56449300	4.74302300	-1.64649800
C	2.53647900	4.83605900	0.73840900
C	2.01253000	5.27092800	-0.47665800
H	2.20189000	5.09381400	-2.61641200
H	2.15269900	5.27441400	1.66481500
C	0.62822500	-2.97854800	0.95697800
C	-0.44730600	-3.16002600	0.05355900
C	0.37884000	-2.76819100	2.32859600
C	-1.74530200	-3.14360300	0.57683600
C	-0.94062400	-2.74812700	2.79005300
C	-2.02077600	-2.92889100	1.92957200
H	-2.58298500	-3.27389700	-0.11578700
H	-1.12179200	-2.56995500	3.85180800
C	4.14882800	3.34813500	-2.97457700
C	3.99437100	1.87504300	-3.36834400
C	5.60790600	3.80142800	-3.10586200
H	3.57330500	3.92225800	-3.71764700
H	2.96879200	1.51662900	-3.21503300
H	4.24837500	1.76391900	-4.43294600
H	4.67331200	1.22151800	-2.80304500

H	5.71574700	4.87017800	-2.87172500
H	6.26011400	3.23092000	-2.42961600
H	5.96487400	3.63483400	-4.13310200
C	4.07244100	3.59272200	2.24089700
C	5.28464300	4.49977600	2.49923300
C	4.37677700	2.16371400	2.71275200
H	3.26578200	3.95416000	2.89842300
H	5.05875500	5.54990700	2.26597500
H	5.59338200	4.43395800	3.55313900
H	6.13793100	4.18905400	1.87851100
H	3.58943500	1.45309000	2.43849400
H	5.33664500	1.78667800	2.33949600
H	4.44360300	2.17797000	3.81108300
C	0.88147500	6.27993900	-0.52719700
C	-0.39272100	5.64358000	-1.09256200
C	1.26975900	7.53273400	-1.31665100
H	0.67614700	6.58502700	0.51178500
H	-0.69315900	4.76217700	-0.50766400
H	-1.22464300	6.36306900	-1.08309700
H	-0.23802800	5.31905100	-2.13297800
H	2.17910500	7.99488500	-0.90764300
H	1.45865300	7.29035600	-2.37338800
H	0.45888600	8.27507700	-1.28535400
C	-0.34854400	-3.38637700	-1.45995800
C	-0.26535300	-4.87601600	-1.81724100
C	0.68525000	-2.57107700	-2.24368300
H	-1.32564400	-3.04926900	-1.83743300
H	-0.42830900	-5.00376900	-2.89834300
H	0.72081300	-5.29980600	-1.57575000
H	-1.03279700	-5.45737100	-1.28554600
H	0.65820900	-1.51329600	-1.95009600
H	1.71113500	-2.94923800	-2.13585600
H	0.42738800	-2.62930300	-3.31167500
C	1.50254600	-2.61717000	3.34594500
C	1.53688100	-3.83018500	4.28291800
C	1.40295200	-1.31014200	4.13757700
H	2.46076300	-2.59873600	2.80803100
H	1.63953500	-4.76454300	3.71241400
H	2.38155400	-3.75671500	4.98431900
H	0.60998800	-3.89699600	4.87286900
H	1.46920400	-0.44215700	3.46671300
H	0.45674300	-1.24919700	4.69739600
H	2.22599300	-1.24051300	4.86471900
C	-3.46617700	-2.87309500	2.39256200
C	-3.64944100	-2.22682300	3.76231600
C	-4.10142900	-4.26692700	2.34822500
H	-4.00474600	-2.25694100	1.65492600
H	-3.18457500	-1.22986100	3.80188500
H	-4.72078800	-2.11252600	3.98317300
H	-3.21263300	-2.84505900	4.56283800
H	-4.03824400	-4.69721900	1.33927900
H	-3.59041300	-4.94687200	3.04797000
H	-5.16453000	-4.21540200	2.62717600
O	-5.23514300	-2.43834200	-0.34215200
H	-6.14455400	-2.09748700	-0.46995700
O	0.42099900	0.32493400	-0.62209600
H	1.37137000	2.52532400	0.96117000

**(M,R)-3a**

C	-3.43254500	-0.53695500	-0.23488700
C	-2.22320800	-1.27047000	-0.24860900
C	-2.13765000	-2.58332300	-0.72727900
C	-3.31272200	-3.16520800	-1.17390900
C	-4.53812100	-2.46401600	-1.15010600
C	-4.60900800	-1.16021400	-0.69065300
C	-3.12543800	0.77729300	0.26128100
H	-1.18514300	-3.11446700	-0.76089900

H	-3.29035800	-4.18596600	-1.55793200
H	-5.44034400	-2.95993400	-1.50955900
H	-5.55612500	-0.61900100	-0.68636500
H	-3.78931300	1.62546000	0.40295500
C	-1.78855800	0.78516000	0.53683900
N	-1.23288200	-0.45466300	0.26262000
C	2.02726400	-1.90775600	0.72305500
C	2.14232000	-1.30743900	-0.52944900
C	3.10869600	-2.59515100	1.26717300
C	3.30941300	-1.37600800	-1.28274700
C	4.28662100	-2.66912100	0.52112600
H	3.04448300	-3.06720300	2.24908600
C	4.39001500	-2.06835400	-0.74056500
H	3.35717100	-0.89378200	-2.26055300
H	5.14501800	-3.20522800	0.92892500
H	5.32483500	-2.14528700	-1.29721400
N	0.09017500	-0.75983900	0.28974100
C	0.86199900	-0.63630200	-0.87218800
O	0.51335600	-0.09815200	-1.88742000
C	0.65214000	-1.66620000	1.30333200
H	0.07378500	-2.60905400	1.28704000
C	0.64172300	-1.10076500	2.71374700
H	-0.37699400	-0.81480300	3.00774500
H	1.00832500	-1.86348200	3.41532700
H	1.26912700	-0.20429500	2.78500700
S	-0.89066000	2.16429500	1.19385600
O	-0.24721200	1.75875900	2.43706300
O	-1.83333000	3.27134000	1.16034400
C	0.38827100	2.45275200	-0.00748300
C	1.70053700	2.12089700	0.31500300
C	0.03433800	2.97283900	-1.24966600
C	2.68754200	2.29496300	-0.65349200
H	1.92787200	1.72732500	1.30665400
C	1.02999000	3.14224100	-2.20677000
H	-1.00646400	3.22722100	-1.45722200
C	2.34969400	2.79841900	-1.90984200
H	3.72213300	2.03417200	-0.42570800
H	0.77506100	3.53608300	-3.19099400
H	3.12407000	2.92574300	-2.66787100

**(M,S)-3a**

C	-3.50889800	-0.05948300	-0.16847000
C	-2.42355600	-0.96061000	-0.27704400
C	-2.55376000	-2.24041700	-0.82850300
C	-3.81737600	-2.61365300	-1.25389000
C	-4.92275400	-1.74148400	-1.13985400
C	-4.78141000	-0.47278600	-0.60626600
C	-2.99632900	1.15990300	0.39577900
H	-1.69231400	-2.90155100	-0.92539300
H	-3.96247200	-3.60225300	-1.69160200
H	-5.90102900	-2.07609600	-1.48654100
H	-5.63587400	0.20089000	-0.52882600
H	-3.52576600	2.07969900	0.62853000
C	-1.66384700	0.95531800	0.60671200
N	-1.30451700	-0.32976900	0.23045600
C	1.95251400	-1.78378500	0.77335200
C	2.02293600	-1.38629000	-0.56055700
C	3.05074100	-2.39045500	1.37727800
C	3.16513700	-1.57039400	-1.33176000
C	4.20377100	-2.58055700	0.61308200
H	3.01917300	-2.70723100	2.42133900
C	4.26438900	-2.17694100	-0.72750500
H	3.18053900	-1.23915100	-2.37148500
H	5.07580900	-3.05232000	1.06872900
H	5.18000900	-2.34099100	-1.29714000
N	-0.04164400	-0.82140000	0.19633100
C	0.74014800	-0.74564900	-0.95626300



O	0.40574400	-0.25498200	-2.00102800
C	0.59601900	-1.46029700	1.35482000
H	0.68467900	-0.71283000	2.16059700
C	-0.17756800	-2.67414500	1.85377000
H	0.31350800	-3.09188100	2.74346300
H	-1.20067300	-2.38463700	2.13373200
H	-0.22292100	-3.45191700	1.07845900
S	-0.53446900	2.10610700	1.33094800
O	0.09641200	1.47116000	2.48487000
O	-1.28283700	3.34422600	1.47035000
C	0.71566200	2.30730800	0.08075600
C	2.00332500	1.84889600	0.33923800
C	0.36204100	2.89464500	-1.13230800
C	2.96443200	1.96509900	-0.66431300
H	2.23172700	1.39961800	1.30743400
C	1.33016300	3.00107800	-2.12522600
H	-0.65901300	3.24515700	-1.29341700
C	2.62532000	2.53399700	-1.89129900
H	3.97754200	1.60104800	-0.48733500
H	1.07298700	3.44246400	-3.08840600
H	3.37756400	2.61342300	-2.67751400

**TS23***IR-Sa-3R*

S	-5.09310000	-0.18490500	-0.50331200
O	-5.08599700	0.27212400	0.88607600
O	-5.12286300	-1.59473700	-0.85690600
O	-0.86818100	2.79172000	1.83481000
N	-2.66575700	1.24058600	-0.68955800
N	-2.41284500	1.12742400	0.64115700
C	-6.51219000	0.55764600	-1.29645300
C	-7.03372200	1.74207600	-0.78231100
H	-6.58286800	2.19182100	0.10308100
C	-8.14582300	2.30814900	-1.40086600
H	-8.57166000	3.23366100	-1.01158000
C	-8.72127500	1.68474300	-2.50945700
H	-9.59275400	2.13146500	-2.99017000
C	-8.19881600	0.48667000	-2.99754500
H	-8.66440100	-0.00557700	-3.85222100
C	-7.08823900	-0.09208000	-2.38529000
H	-6.67307800	-1.04230000	-2.72463300
C	-3.73777800	0.62250100	-1.33431700
C	-3.61833500	0.78640200	-2.68339900
H	-4.32471100	0.43418600	-3.43094800
C	-2.42112800	1.54275300	-2.90901700
C	-1.83677600	1.80274000	-1.64941800
C	-0.65249400	2.54043800	-1.51153500
H	-0.19363100	2.73608500	-0.53931300
C	-0.06943900	3.00143100	-2.68018600
H	0.85786500	3.56820400	-2.60895800
C	-0.63077600	2.74738800	-3.95092800
H	-0.12693600	3.12751700	-4.84028500
C	-1.80079000	2.02506100	-4.07665500
H	-2.24012300	1.82578600	-5.05506900
C	-2.16835400	-0.20468100	1.29568200
H	-1.08718900	-0.31534200	1.42354800
C	-2.72789600	0.06954600	2.66356100
C	-2.96717800	-0.80343100	3.71287200
H	-2.84015800	-1.87695300	3.57336800
C	-3.39522700	-0.26392200	4.92853300
H	-3.61083500	-0.92994100	5.76519600
C	-3.55711000	1.11599300	5.09278200
H	-3.89303900	1.50888000	6.05299000
C	-3.30309700	1.99267100	4.03709700
H	-3.44012600	3.06888000	4.16110000
C	-2.89138100	1.44570200	2.82593300
C	-2.62752500	2.10699100	1.52648600
C	-3.28046800	3.37448200	1.09772800

H	-2.80524600	3.77158300	0.19252500
H	-3.23083700	4.12430000	1.89539800
H	-4.33323400	3.13196800	0.88744200
C	2.20549200	-2.25247100	-0.01390300
C	3.48133300	-2.00245600	-0.48887500
C	4.09688100	-2.97406200	-1.35183600
C	3.45753500	-4.23291400	-1.53543900
C	2.16725900	-4.44492300	-0.98259400
C	1.49306100	-3.45203600	-0.31462700
H	5.79287200	-1.75589000	-1.95712600
C	5.31506100	-2.73137900	-2.04630700
C	4.08208000	-5.22628300	-2.33829500
H	1.66713600	-5.39886300	-1.15995200
C	5.27460600	-4.97314000	-2.96925800
C	5.88596800	-3.70347900	-2.83255100
H	3.58069000	-6.18911600	-2.45801800
H	5.74226200	-5.73816000	-3.59052400
H	6.81595900	-3.49141000	-3.36195400
C	4.16760500	-0.73871400	-0.11084600
C	5.50196300	-0.73775500	0.42959100
C	3.50924800	0.47195600	-0.24575400
C	6.18981000	-1.93173900	0.78795000
C	6.16463500	0.50468400	0.64295100
C	4.12828200	1.71661500	0.07669500
C	7.47432300	-1.89040200	1.27495600
H	5.68225100	-2.88998100	0.68265800
C	7.49981200	0.51575300	1.13098400
C	5.45013000	1.71544500	0.44313200
C	8.14803600	-0.65551600	1.43350100
H	7.97638200	-2.81935800	1.54905200
H	7.99225000	1.47954900	1.27633200
H	5.94598200	2.66412500	0.66258800
H	9.17035200	-0.63756400	1.81358500
O	2.23593500	0.50937300	-0.75819200
O	1.60875600	-1.32958000	0.81092300
P	0.94481100	0.00489300	0.11247200
O	0.69512000	0.96583700	1.25934800
C	3.30539300	2.96100200	0.11712100
C	3.07807400	3.73283700	-1.04182200
C	2.75092000	3.35524200	1.35733200
C	2.27228000	4.87412300	-0.94460200
C	1.92570100	4.48551500	1.37913500
C	1.66285800	5.25550600	0.24835100
H	2.12115400	5.47613300	-1.84367500
H	1.48541400	4.79266200	2.33402300
C	0.05015600	-3.62677400	0.02754800
C	-0.90981500	-3.70945300	-1.00906400
C	-0.35081100	-3.77218200	1.37477500
C	-2.24056000	-3.97383100	-0.65235000
C	-1.69063000	-4.04259300	1.66751100
C	-2.65601800	-4.15226100	0.66508100
H	-2.99465500	-4.01147500	-1.44396200
H	-1.98583800	-4.17500800	2.71336600
C	3.73666700	3.48321800	-2.39899100
C	3.59342300	2.08110200	-3.00098800
C	5.20696500	3.92080300	-2.38107700
H	3.21676500	4.16767400	-3.09030600
H	2.57066500	1.69323900	-2.90682600
H	3.85612400	2.12384100	-4.06881300
H	4.27467600	1.35942400	-2.52949700
H	5.31170300	4.95045300	-2.00999800
H	5.80133800	3.25805800	-1.73584700
H	5.63179300	3.87154500	-3.39508100
C	3.06936000	2.77089900	2.74200800
C	4.22408400	3.57751700	3.35732600
C	3.32952600	1.27333500	2.94414700

H	2.16999800	2.99874600	3.33920200
H	4.02477500	4.65824600	3.33178900
H	4.39071900	3.27478300	4.40206400
H	5.15529100	3.39098800	2.80117000
H	2.57832400	0.65066400	2.44897200
H	4.32896500	0.96710200	2.61049500
H	3.27724100	1.06764200	4.02466900
C	0.70851400	6.43242300	0.34123000
C	-0.73605600	5.93054800	0.22811000
C	0.98349500	7.53335300	-0.68049600
H	0.83661100	6.86454300	1.34807700
H	-0.92893100	5.13963700	0.96659000
H	-1.45461400	6.75155400	0.37742600
H	-0.90600900	5.49715800	-0.77122300
H	2.03327500	7.85856600	-0.65197700
H	0.75801900	7.19279000	-1.70242000
H	0.34536500	8.40618500	-0.48064600
C	-0.67034100	-3.56462500	-2.51903400
C	-0.52084100	-4.93741000	-3.19070100
C	0.40907100	-2.59662100	-3.01610400
H	-1.62445000	-3.15082800	-2.88391400
H	-0.55537600	-4.82635800	-4.28501300
H	0.44478900	-5.39882800	-2.93772600
H	-1.32146400	-5.62717900	-2.88667300
H	0.38740400	-1.65400600	-2.45618200
H	1.41960800	-3.02279600	-2.96465700
H	0.20840500	-2.37235200	-4.07510800
C	0.64819100	-3.69887400	2.52106200
C	0.76935400	-5.05298500	3.22764300
C	0.29700600	-2.58432100	3.50962400
H	1.63470400	-3.46047200	2.10324800
H	1.05776800	-5.84202200	2.51822100
H	1.52865200	-5.00805200	4.02265600
H	-0.18600000	-5.34756300	3.68883000
H	0.23078800	-1.61280800	2.99745600
H	-0.65982400	-2.78690700	4.01617600
H	1.07161500	-2.50229300	4.28679100
C	-4.11197400	-4.44492600	0.97366900
C	-4.70098100	-3.48660200	2.00956100
C	-4.28570000	-5.90424700	1.40776200
H	-4.66863700	-4.29046000	0.03627700
H	-4.57049500	-2.44195200	1.69575100
H	-5.77656500	-3.68090600	2.13681500
H	-4.22680700	-3.62994200	2.99466400
H	-3.90415300	-6.59578500	0.64305600
H	-3.73348000	-6.09819300	2.34101100
H	-5.34650900	-6.13511500	1.58772000
O	-2.69527600	-1.22096500	0.57036800
H	-2.00197800	-1.55539400	-0.03003600
H	-0.69915300	2.95318600	2.77354200
O	-0.17947300	-0.37908600	-0.78340200
H	-0.18440700	2.02885000	1.55272400

**TS24<sub>ISi-Ra-3R</sub>**

S	-2.92192300	-1.06553200	1.61996700
O	-2.11528400	-0.03597100	2.24448300
O	-2.42336000	-1.94702500	0.56568600
O	-1.47843100	-1.73316400	-1.98313100
N	-4.34536700	0.29591600	-0.32007500
N	-3.24852400	0.54437900	-1.08977400
C	-3.59683600	-2.09626100	2.89986000
C	-3.62610400	-1.60322500	4.20142000
H	-3.23585000	-0.60597300	4.40989900
C	-4.13990500	-2.42076300	5.20726300
H	-4.17036900	-2.06047200	6.23603500
C	-4.60057000	-3.70109600	4.89881800
H	-4.99623800	-4.33803900	5.69125700

C	-4.54978000	-4.18053700	3.58762400
H	-4.89904500	-5.18787700	3.35832200
C	-4.04175500	-3.37571400	2.57145900
H	-3.97372300	-3.72826400	1.54077400
C	-4.37817100	-0.30830300	0.93073300
C	-5.64519700	-0.25574500	1.43527800
H	-5.96596800	-0.68238500	2.38195700
C	-6.45386200	0.43381200	0.46492100
C	-5.61069500	0.77729100	-0.61319300
C	-6.06797400	1.46796400	-1.74144200
H	-5.39700500	1.72578900	-2.56327500
C	-7.41088200	1.80732400	-1.76903600
H	-7.80726100	2.34617100	-2.63046600
C	-8.27656800	1.47220600	-0.70579300
H	-9.32682000	1.75857200	-0.76597700
C	-7.81346800	0.79128900	0.40656200
H	-8.48562400	0.53704900	1.22704300
C	-2.45883200	1.82095300	-0.90979500
H	-1.84550600	1.71684100	-0.00507000
C	-1.63274000	1.77057000	-2.17091900
C	-0.59636500	2.59918700	-2.57936800
H	-0.24504400	3.41590200	-1.94758900
C	0.00745200	2.32617200	-3.80939800
H	0.83036800	2.95701600	-4.14636700
C	-0.39665700	1.24966000	-4.60620200
H	0.11307200	1.05789900	-5.55048600
C	-1.40374200	0.39369600	-4.17717200
H	-1.67913700	-0.49127400	-4.75219700
C	-2.01073800	0.67710200	-2.95664900
C	-2.99050900	-0.11189800	-2.21555700
C	-3.90823300	-1.15916500	-2.72753100
H	-3.44089000	-1.69123200	-3.55975300
H	-4.84606400	-0.68174900	-3.05349100
H	-4.13172300	-1.87400400	-1.92536400
C	2.84544200	1.54062800	0.38519500
C	3.86097800	0.67240600	0.76246600
C	4.64506100	0.99860500	1.92682000
C	4.46913300	2.26593800	2.55515700
C	3.44330800	3.13154500	2.09614600
C	2.59927700	2.76313800	1.07976100
H	5.67846600	-0.91005900	2.10236400
C	5.57171600	0.09074000	2.51781000
C	5.26883000	2.61589000	3.67754200
H	3.28158200	4.08278100	2.60950700
C	6.18344400	1.73340100	4.19425800
C	6.31728200	0.44872800	3.61537400
H	5.12417000	3.59896700	4.13060500
H	6.78806200	2.00794600	5.05979100
H	7.01290800	-0.27078400	4.04977600
C	4.05307800	-0.62630900	0.06028300
C	5.33572600	-1.11018600	-0.36656100
C	2.95915300	-1.45299500	-0.11164400
C	6.49087200	-0.28220200	-0.41355300
C	5.46253300	-2.47505800	-0.75802100
C	3.05695500	-2.80400200	-0.55105000
C	7.70849300	-0.78883600	-0.80090400
H	6.39585200	0.76988400	-0.14201100
C	6.73886700	-2.97300900	-1.13780800
C	4.30877500	-3.30591400	-0.80041800
C	7.84015600	-2.15274900	-1.15730000
H	8.57992000	-0.13342700	-0.83858100
H	6.82171300	-4.02243300	-1.42902300
H	4.42515600	-4.35495200	-1.07900900
H	8.81271600	-2.54478600	-1.45820500
O	1.72744700	-1.01376000	0.26151000
O	2.05926500	1.26569100	-0.70048500

P	0.92190700	0.05878400	-0.70002200
O	0.83365800	-0.44341200	-2.11199400
C	1.79915700	-3.58996900	-0.72856200
C	0.97865300	-3.92582000	0.37567800
C	1.39823500	-3.95101100	-2.04144400
C	-0.21478300	-4.62123000	0.13653000
C	0.19223300	-4.63901200	-2.20457700
C	-0.63314800	-4.98366900	-1.13773200
H	-0.82996300	-4.88595300	1.00012600
H	-0.12247900	-4.90549500	-3.21876000
C	1.41536900	3.59792600	0.71838800
C	0.18423600	3.40226700	1.37649600
C	1.54329100	4.59077900	-0.27843100
C	-0.91222400	4.16812900	0.94942100
C	0.43197300	5.36273100	-0.62422600
C	-0.81816200	5.14419500	-0.03882500
H	-1.88318800	3.99812400	1.42570400
H	0.53985500	6.13472800	-1.39092300
C	1.22567200	-3.65202100	1.86915200
C	0.18157800	-2.66762000	2.42488200
C	2.62534300	-3.26787600	2.35481900
H	1.01556900	-4.62772700	2.34073600
H	-0.83542200	-3.07158300	2.31707200
H	0.36575000	-2.48748100	3.49556500
H	0.21952300	-1.70613600	1.89445800
H	3.41397900	-3.87650500	1.89291300
H	2.85227100	-2.20786500	2.18161600
H	2.66578300	-3.42915700	3.44252200
C	2.16092200	-3.70362400	-3.35244000
C	3.03737700	-4.91100400	-3.71406900
C	2.92858100	-2.38998700	-3.54635100
H	1.35730600	-3.67942300	-4.10569700
H	2.46825200	-5.85094600	-3.66869800
H	3.43916500	-4.79574900	-4.73240500
H	3.89281500	-4.99878900	-3.02917900
H	2.37798500	-1.53848000	-3.12641800
H	3.93392100	-2.41568100	-3.10777700
H	3.05477000	-2.22380800	-4.62794800
C	-1.96789700	-5.65839200	-1.39556600
C	-3.03075100	-4.59534400	-1.69673500
C	-2.42253100	-6.57499200	-0.26125400
H	-1.84466000	-6.27729600	-2.30014300
H	-2.71738200	-3.96327600	-2.53857200
H	-4.00362100	-5.05822400	-1.92670800
H	-3.14445000	-3.92895300	-0.82524700
H	-1.64276100	-7.30185200	0.00734500
H	-2.66976100	-5.99705800	0.64294700
H	-3.32675600	-7.12820300	-0.55492600
C	-0.07709000	2.54664700	2.62064900
C	-0.02251700	3.47315800	3.84692000
C	0.74385200	1.28656800	2.90360400
H	-1.11613300	2.19897800	2.50693000
H	-0.30646100	2.92204600	4.75612800
H	1.00173300	3.85292800	3.98891800
H	-0.69147400	4.33907800	3.73866900
H	0.78878500	0.62450000	2.03431900
H	1.76076100	1.50884200	3.25455100
H	0.23063600	0.72914000	3.70214700
C	2.85584300	4.80165700	-1.01884600
C	3.24918200	6.27685500	-1.12048700
C	2.78948900	4.14859900	-2.40405600
H	3.64613800	4.29057400	-0.45194100
H	3.26609900	6.75497500	-0.13055900
H	4.24979200	6.37231400	-1.56714000
H	2.55222700	6.84161500	-1.75827300
H	2.53306600	3.08214200	-2.31909800

H	2.02282500	4.65006700	-3.01937200
H	3.75388600	4.23881500	-2.92661000
C	-2.03474100	5.95959400	-0.43592300
C	-2.24947200	5.97886800	-1.95119000
C	-1.94154100	7.38436100	0.11894000
H	-2.90664500	5.46508200	0.02052900
H	-2.28219700	4.95807700	-2.36076500
H	-3.18965100	6.49104000	-2.20582300
H	-1.43489700	6.51224500	-2.46478500
H	-1.82875500	7.37380600	1.21204000
H	-1.06892100	7.90624400	-0.30372100
H	-2.84148400	7.96570800	-0.13298700
O	-3.31698700	2.89394000	-0.77451100
H	-3.61706500	3.19034700	-1.64324200
H	-0.58219400	-1.32301400	-2.13844400
O	-0.31360400	0.41388800	0.05067200
H	-1.47498000	-1.96691300	-1.03878000

**TS25***IS-Ra-3S*

S	-5.86153700	-0.19206400	-0.91951800
O	-5.94702900	-1.53456900	-1.46696700
O	-5.33926700	0.92748000	-1.69638300
O	-1.22727900	2.68041500	0.57639200
N	-3.63756300	0.18914900	0.74788600
N	-2.87129000	0.72354300	-0.23788500
C	-7.50169300	0.23543800	-0.35774900
C	-8.44310700	-0.78104000	-0.22128200
H	-8.16330300	-1.80692200	-0.46486800
C	-9.72763000	-0.44851800	0.20837400
H	-10.48062800	-1.22939900	0.32077300
C	-10.05011300	0.88016800	0.48276500
H	-11.05698900	1.13562000	0.81602400
C	-9.09664800	1.88853900	0.32450100
H	-9.35970500	2.92709800	0.52806400
C	-7.81080200	1.56990800	-0.10302400
H	-7.05529000	2.34327700	-0.24734700
C	-4.95536800	-0.23664500	0.61455400
C	-5.38212300	-0.78120300	1.79322600
H	-6.37331900	-1.18805600	1.97920100
C	-4.28157800	-0.70899400	2.71251200
C	-3.19788400	-0.11426500	2.02719400
C	-1.94734200	0.10958500	2.61613300
H	-1.11903800	0.53884600	2.05071300
C	-1.81844300	-0.27228300	3.94091700
H	-0.86133200	-0.11859800	4.44105200
C	-2.88216900	-0.86999600	4.65431000
H	-2.72760700	-1.15904400	5.69458700
C	-4.10850800	-1.09564100	4.05577600
H	-4.92709000	-1.56166800	4.60607900
C	-2.18293100	-0.16216900	-1.22562100
H	-1.29992800	-0.60921800	-0.74890400
C	-1.79367600	0.86563600	-2.25671200
C	-1.15664000	0.67730400	-3.47546100
H	-0.82231600	-0.31480600	-3.77521000
C	-0.94004200	1.79798000	-4.27676400
H	-0.44328900	1.67935700	-5.24063600
C	-1.34590000	3.07575000	-3.86858500
H	-1.17021500	3.93135000	-4.52168400
C	-1.97185700	3.26295800	-2.63897400
H	-2.29986100	4.25450200	-2.32316900
C	-2.18045200	2.13767900	-1.84408800
C	-2.80036500	2.02723000	-0.51185200
C	-3.75365600	2.99878400	0.08177100
H	-3.89541000	2.79607400	1.15024800
H	-4.70137600	2.86965400	-0.46181900
H	-3.38469500	4.02145400	-0.05053300
C	2.79499700	-2.04674300	-0.04911800

C	4.09744700	-1.64172600	-0.26306800
C	4.98259100	-2.56049500	-0.92760600
C	4.53408100	-3.89028900	-1.17962900
C	3.19357600	-4.25955100	-0.87048200
C	2.29564500	-3.34442400	-0.38658200
H	6.62369000	-1.16829800	-1.21101300
C	6.28525100	-2.19363400	-1.36259000
C	5.41729800	-4.81601100	-1.79799300
H	2.86656000	-5.27809900	-1.08940200
C	6.68040200	-4.43855900	-2.18414900
C	7.11058100	-3.10711200	-1.97515700
H	5.06261800	-5.83353100	-1.97574900
H	7.34605100	-5.15651800	-2.66521100
H	8.10325300	-2.80036000	-2.30784400
C	4.51763300	-0.29212300	0.21390500
C	5.67578300	-0.12179300	1.05310300
C	3.74668600	0.82699900	-0.06903100
C	6.42809800	-1.21830700	1.56369000
C	6.08206800	1.19288400	1.42583300
C	4.08447500	2.13229200	0.39934200
C	7.54425500	-1.01494600	2.33949200
H	6.10431500	-2.23462400	1.34366000
C	7.25104800	1.37299300	2.21464200
C	5.26664800	2.30101400	1.07346600
C	7.97632500	0.29506600	2.65655700
H	8.09746500	-1.87422700	2.72136000
H	7.54890500	2.39067400	2.47606900
H	5.55889000	3.29947100	1.40735600
H	8.86857100	0.44268600	3.26644300
O	2.64258300	0.74131600	-0.86273900
O	1.92288800	-1.17464800	0.54305600
P	1.26129400	-0.05406500	-0.46387900
O	0.38989500	0.79040100	0.43469400
C	3.09162800	3.24340300	0.25965000
C	2.99045900	4.01229500	-0.92020900
C	2.24344100	3.51974000	1.35906300
C	2.04113500	5.04215300	-0.97943100
C	1.32452100	4.56957000	1.24256100
C	1.20395400	5.34971300	0.09232200
H	1.99148400	5.63555400	-1.89382100
H	0.69388500	4.79953700	2.10778600
C	0.83272500	-3.58531200	-0.19468300
C	-0.04085000	-3.78130300	-1.28192200
C	0.30151100	-3.46692600	1.11350900
C	-1.42333300	-3.83588800	-1.02119100
C	-1.07810500	-3.47020200	1.30699000
C	-1.97563600	-3.64921800	0.24739200
H	-2.08099400	-4.02730400	-1.87330500
H	-1.46097300	-3.33394900	2.31981200
C	3.93141500	3.89730200	-2.11970900
C	4.02902200	2.52886300	-2.80015700
C	5.32586200	4.44040500	-1.78131100
H	3.50492400	4.58028800	-2.87168700
H	3.04126800	2.08102800	-2.96560000
H	4.52997100	2.65159400	-3.77236100
H	4.62624800	1.81716200	-2.21427700
H	5.26579600	5.44644200	-1.34128500
H	5.84180300	3.78112600	-1.06913700
H	5.94145500	4.49711900	-2.69173400
C	2.29511400	2.87050900	2.74865000
C	3.26306300	3.64620800	3.65393900
C	2.53999800	1.36389900	2.87740000
H	1.28287400	3.03872000	3.15119100
H	3.05479600	4.72576300	3.63822800
H	3.18022900	3.29013400	4.69184000
H	4.30306100	3.49219100	3.33096100

H	1.92481700	0.79124200	2.17444000
H	3.59348000	1.08587700	2.73885900
H	2.25954100	1.05748000	3.89762700
C	0.21192100	6.50555200	0.07585400
C	-1.22914000	5.99977100	0.20389200
C	0.34506200	7.41467900	-1.14193600
H	0.42767300	7.11069400	0.97308200
H	-1.36581400	5.36306300	1.09047900
H	-1.93880700	6.83763200	0.27249400
H	-1.49191100	5.40910000	-0.68903700
H	1.36535300	7.80968600	-1.24366400
H	0.09668100	6.87257700	-2.06790500
H	-0.34471700	8.26650200	-1.05891400
C	0.33479000	-4.00326400	-2.75084400
C	0.45543200	-5.50629200	-3.03979800
C	1.51866000	-3.23334200	-3.34961700
H	-0.55301900	-3.65334000	-3.30174900
H	0.60246300	-5.67723000	-4.11693700
H	1.31826000	-5.93695800	-2.51018800
H	-0.44275300	-6.05388400	-2.71950000
H	1.57320700	-2.21333500	-2.94903900
H	2.47856000	-3.73625700	-3.17880100
H	1.37656600	-3.17685200	-4.44002200
C	1.20468000	-3.40994800	2.33748500
C	1.22385700	-4.78180100	3.02301200
C	0.81264500	-2.30452500	3.31577100
H	2.22945500	-3.20210700	2.00623100
H	1.56091900	-5.56555800	2.32903700
H	1.90086000	-4.77225300	3.89053800
H	0.21698900	-5.05379300	3.37633700
H	0.72411500	-1.34363100	2.78944000
H	-0.14553000	-2.52383200	3.81158500
H	1.57674400	-2.20466800	4.10166900
C	-3.48434500	-3.59755400	0.47807000
C	-3.89853500	-4.24789900	1.80049900
C	-4.29912600	-4.18244600	-0.67623700
H	-3.75393800	-2.52797100	0.54862400
H	-3.44780600	-3.75190800	2.67058400
H	-4.99068300	-4.18748000	1.91969100
H	-3.60902000	-5.31032600	1.81850500
H	-4.19012600	-3.60979000	-1.60776200
H	-4.01334600	-5.22885100	-0.86674800
H	-5.36881800	-4.14901500	-0.42884600
O	-3.06012200	-1.12057400	-1.67573800
H	-2.72017600	-1.98942100	-1.41887400
H	-0.52783800	1.93300800	0.49512700
O	0.71413300	-0.66884400	-1.69828000
H	-0.78212300	3.44750700	0.18364600

**TS26<sub>IS-Sa-3S</sub>**

S	-3.67935900	0.43843000	1.91301400
O	-3.46812700	1.79396100	2.43929600
O	-2.54257900	-0.33834300	1.44477500
O	-1.47283400	2.75240700	0.76277200
N	-4.35726900	0.99146700	-0.67552000
N	-3.13161800	1.46192600	-1.02455700
C	-4.58985000	-0.47516200	3.12475200
C	-5.45277500	0.20979400	3.97859400
H	-5.54292100	1.29467000	3.90618400
C	-6.16842000	-0.52568300	4.92030700
H	-6.85063600	-0.01662200	5.60185300
C	-6.00071200	-1.91008700	5.00039100
H	-6.56078200	-2.47854700	5.74424300
C	-5.11528500	-2.57230900	4.14880100
H	-4.97733100	-3.65098100	4.22970100
C	-4.39615500	-1.85231400	3.19700200
H	-3.67934300	-2.33031800	2.52706700



C	-4.81005500	0.55892100	0.56245200
C	-6.13340700	0.23088300	0.48915100
H	-6.73346900	-0.16364600	1.30503800
C	-6.53977900	0.45741600	-0.87185300
C	-5.40826700	0.92400200	-1.57371700
C	-5.42313200	1.23094900	-2.93813200
H	-4.51589700	1.55268800	-3.45108800
C	-6.63007600	1.06232100	-3.59552300
H	-6.69045700	1.28001700	-4.66252700
C	-7.78202500	0.59981900	-2.92030700
H	-8.71024100	0.47747700	-3.47929800
C	-7.75033900	0.29272200	-1.57157300
H	-8.64126500	-0.07079200	-1.05798100
C	-2.04985300	0.60665800	-1.61788400
H	-1.51323800	0.20225000	-0.75025500
C	-1.22686900	1.68500700	-2.28228600
C	-0.21252900	1.57514300	-3.22423700
H	0.10306200	0.59556600	-3.57735700
C	0.38939700	2.75345400	-3.66778500
H	1.18251000	2.69937000	-4.41524800
C	0.00563400	4.00450600	-3.16966900
H	0.50742800	4.90126900	-3.53519100
C	-1.00113500	4.11300200	-2.21397000
H	-1.29823500	5.08347700	-1.81290800
C	-1.61672500	2.93451500	-1.80135500
C	-2.73999000	2.72954300	-0.87938700
C	-3.65948000	3.76878400	-0.35181400
H	-4.13708800	3.41892900	0.57285300
H	-4.43435200	3.96661600	-1.10888300
H	-3.09754100	4.68542800	-0.14624200
C	2.33366300	-2.33511100	0.00982900
C	3.68544400	-2.04765100	-0.03496800
C	4.56895000	-3.02226200	-0.61769200
C	4.04986800	-4.30241500	-0.96839200
C	2.65104800	-4.54155100	-0.87714200
C	1.78109900	-3.55528100	-0.48840200
H	6.34342600	-1.77021800	-0.66232000
C	5.94264000	-2.76044900	-0.87854400
C	4.92492000	-5.29152500	-1.49363500
H	2.25931400	-5.50741700	-1.20291000
C	6.25452800	-5.01868800	-1.70211400
C	6.76144900	-3.73111000	-1.40542600
H	4.51092800	-6.26989100	-1.74721200
H	6.91561000	-5.78288700	-2.11326100
H	7.81001200	-3.50359900	-1.60291900
C	4.16005300	-0.74134800	0.49696200
C	5.23806700	-0.65770700	1.44641200
C	3.51527500	0.42930700	0.12190600
C	5.83486500	-1.80597200	2.04121500
C	5.71835200	0.62346500	1.84341600
C	3.91644600	1.70870400	0.61204500
C	6.88061900	-1.68552800	2.92475200
H	5.44546000	-2.79378700	1.79763500
C	6.81281600	0.71682500	2.74601300
C	5.03785800	1.78762100	1.39893900
C	7.39172700	-0.41146000	3.27073100
H	7.31492200	-2.58176800	3.37025700
H	7.17078500	1.70966500	3.02675200
H	5.37185700	2.76432900	1.75795100
H	8.22700900	-0.32991100	3.96763200
O	2.48860600	0.39572100	-0.77810200
O	1.47477800	-1.42766700	0.56750600
P	0.98721600	-0.18052400	-0.39920300
O	0.24950300	0.79059100	0.47524600
C	3.05040100	2.90659200	0.38812300
C	3.17869800	3.72379100	-0.75524500

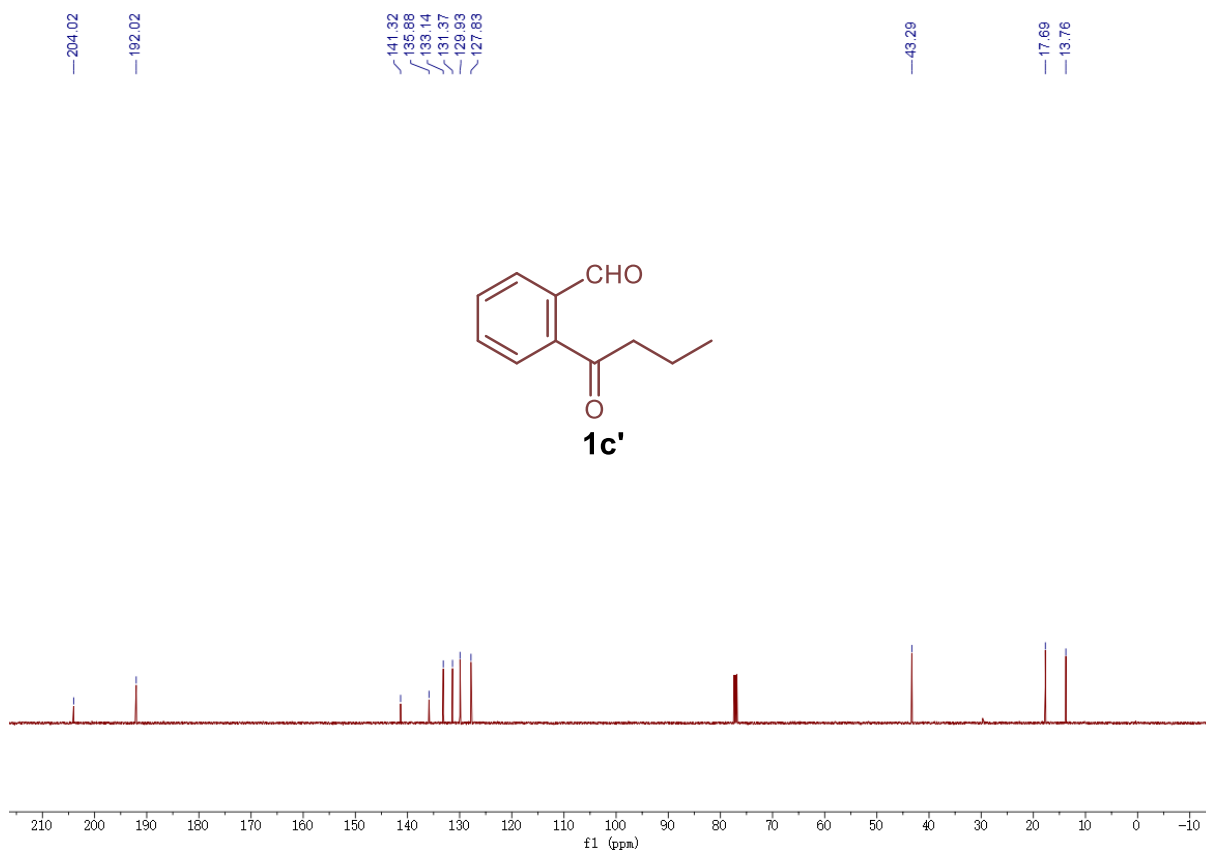
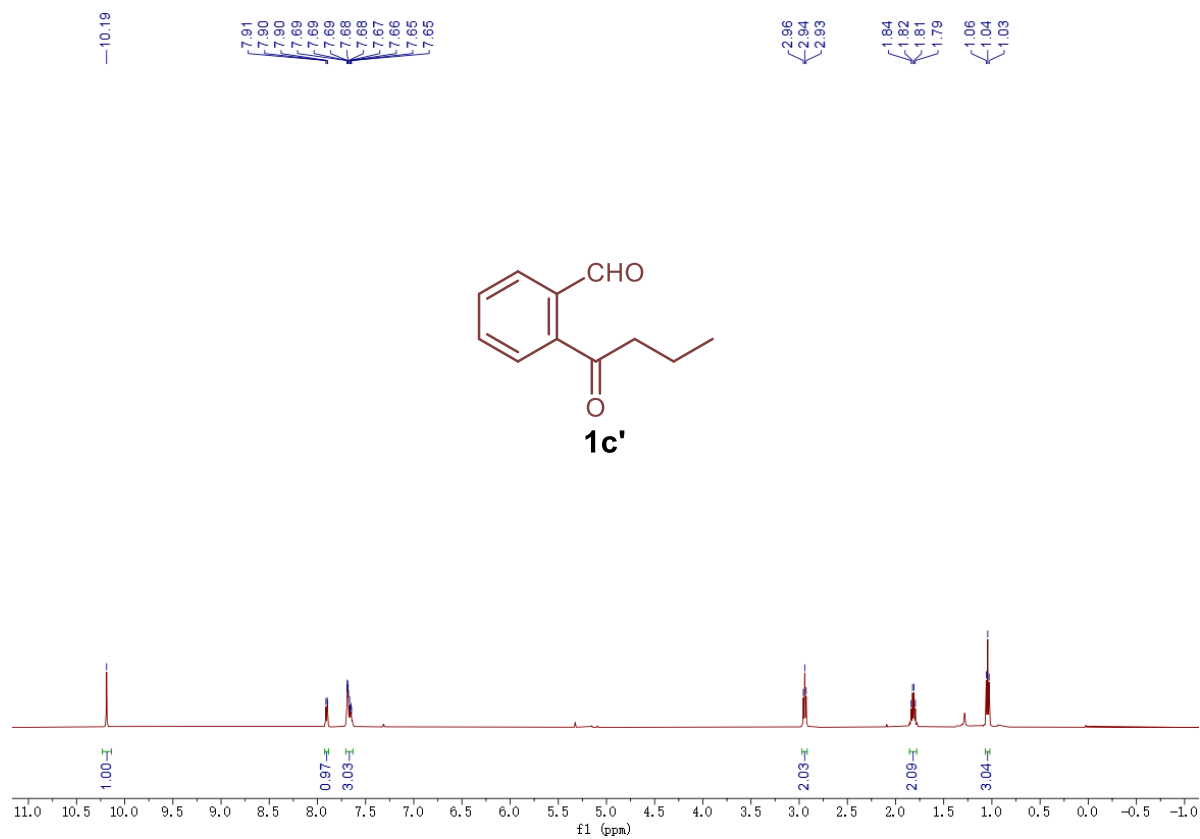
C	2.10043300	3.22745900	1.38619200
C	2.37217400	4.86432700	-0.86771100
C	1.29303000	4.35203100	1.19024100
C	1.42135600	5.19995400	0.09335600
H	2.50797900	5.50060600	-1.74492500
H	0.53940200	4.58271200	1.94900500
C	0.30071200	-3.67843700	-0.62990000
C	-0.28975500	-3.69728000	-1.91235000
C	-0.51272400	-3.69360500	0.52473000
C	-1.68963100	-3.76218900	-1.98973400
C	-1.90007500	-3.75587300	0.38647100
C	-2.51341000	-3.79976200	-0.86623500
H	-2.15429200	-3.79256000	-2.98123600
H	-2.51571500	-3.79020200	1.29005400
C	4.21682300	3.52200100	-1.85834700
C	4.24219700	2.14435100	-2.52686000
C	5.62012900	3.92988100	-1.39259800
H	3.92768200	4.23840500	-2.64502200
H	3.23071900	1.78152700	-2.75099800
H	4.81495200	2.20895400	-3.46471500
H	4.73359400	1.38957700	-1.89780200
H	5.61677500	4.94106700	-0.96043100
H	5.99820400	3.23058000	-0.63336600
H	6.32248300	3.91714900	-2.24007400
C	1.93576500	2.57539400	2.76762900
C	2.75759200	3.38155800	3.78646800
C	2.18023500	1.07970800	2.98925800
H	0.87205700	2.73887500	3.00752100
H	2.53049600	4.45616200	3.73439100
H	2.55560300	3.02865300	4.80912100
H	3.83377200	3.25225200	3.59342900
H	1.65647900	0.46242800	2.25396400
H	3.24572300	0.81513600	2.99371000
H	1.78259200	0.82039500	3.98304800
C	0.56417600	6.45550600	0.03012200
C	0.67344600	7.22201700	-1.28489900
C	0.89713300	7.39170300	1.19936500
H	-0.48381400	6.12585500	0.15686200
H	0.44257600	6.59194200	-2.15501800
H	-0.01757100	8.07728200	-1.28877100
H	1.69159100	7.61749500	-1.42150700
H	0.78022400	6.88743700	2.16797300
H	1.94120100	7.73162700	1.12188000
H	0.24439100	8.27768400	1.19099500
C	0.42048600	-3.69393600	-3.27230300
C	0.58646000	-5.12924900	-3.79204000
C	1.72201300	-2.90192000	-3.45051700
H	-0.31091900	-3.20826800	-3.93863400
H	0.95547500	-5.11794400	-4.82882100
H	1.31794300	-5.68179800	-3.18421800
H	-0.36321900	-5.68310100	-3.76632200
H	1.68728800	-1.95279400	-2.90291300
H	2.60775200	-3.46701400	-3.13490300
H	1.84646800	-2.68357400	-4.52260300
C	0.08029900	-3.69812000	1.92593300
C	-0.11202200	-5.06951100	2.58263600
C	-0.48568700	-2.57437400	2.79682800
H	1.16087700	-3.52815800	1.84141000
H	0.34593400	-5.86594100	1.97807100
H	0.34588700	-5.08734200	3.58311200
H	-1.18227700	-5.30564500	2.69488200
H	-0.42306000	-1.60573500	2.28301500
H	-1.54107700	-2.76157400	3.05348200
H	0.07288100	-2.51087700	3.74284600
C	-4.02197200	-3.87693600	-1.01219000
C	-4.68105800	-2.55241200	-0.62148800

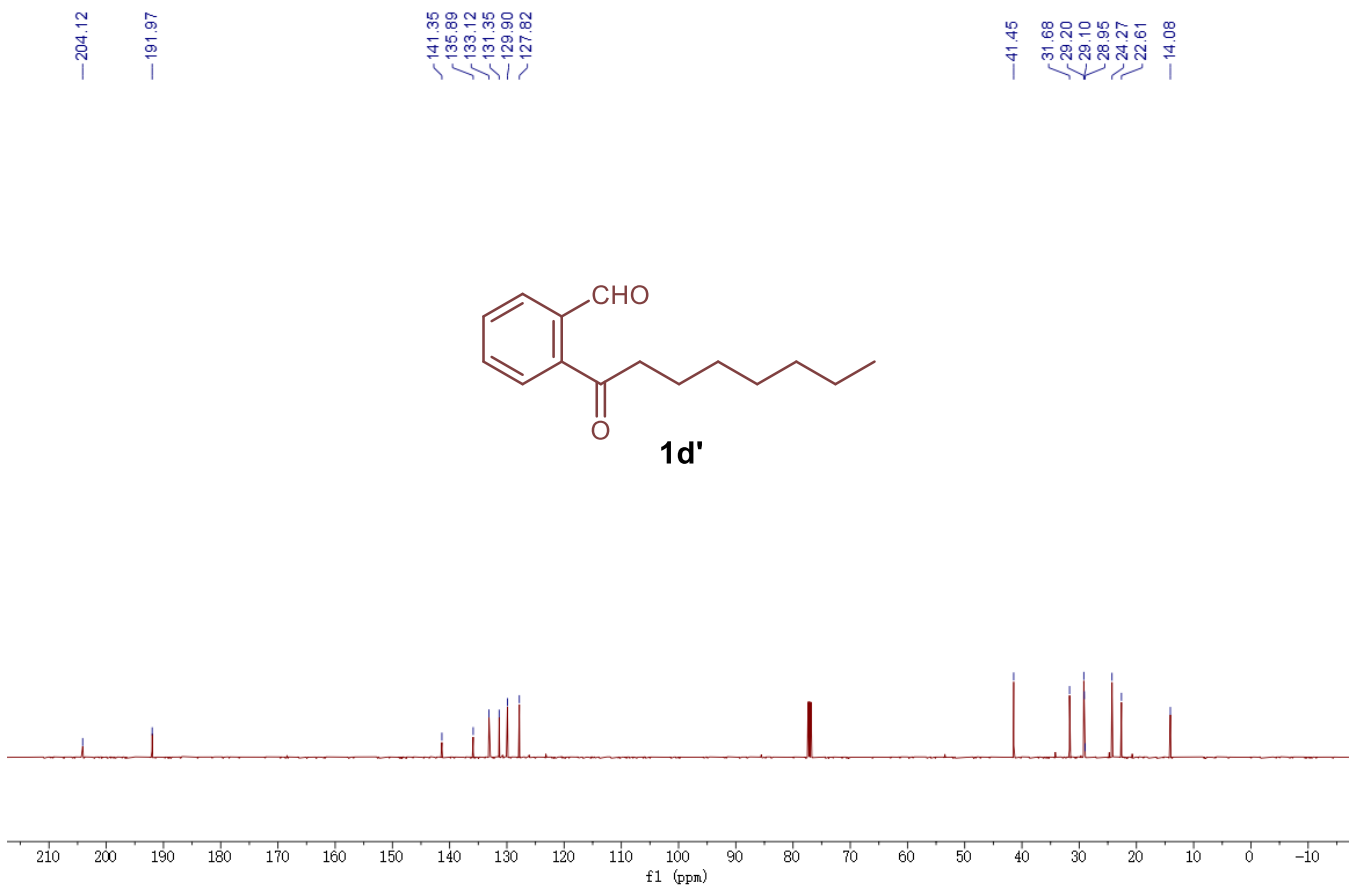
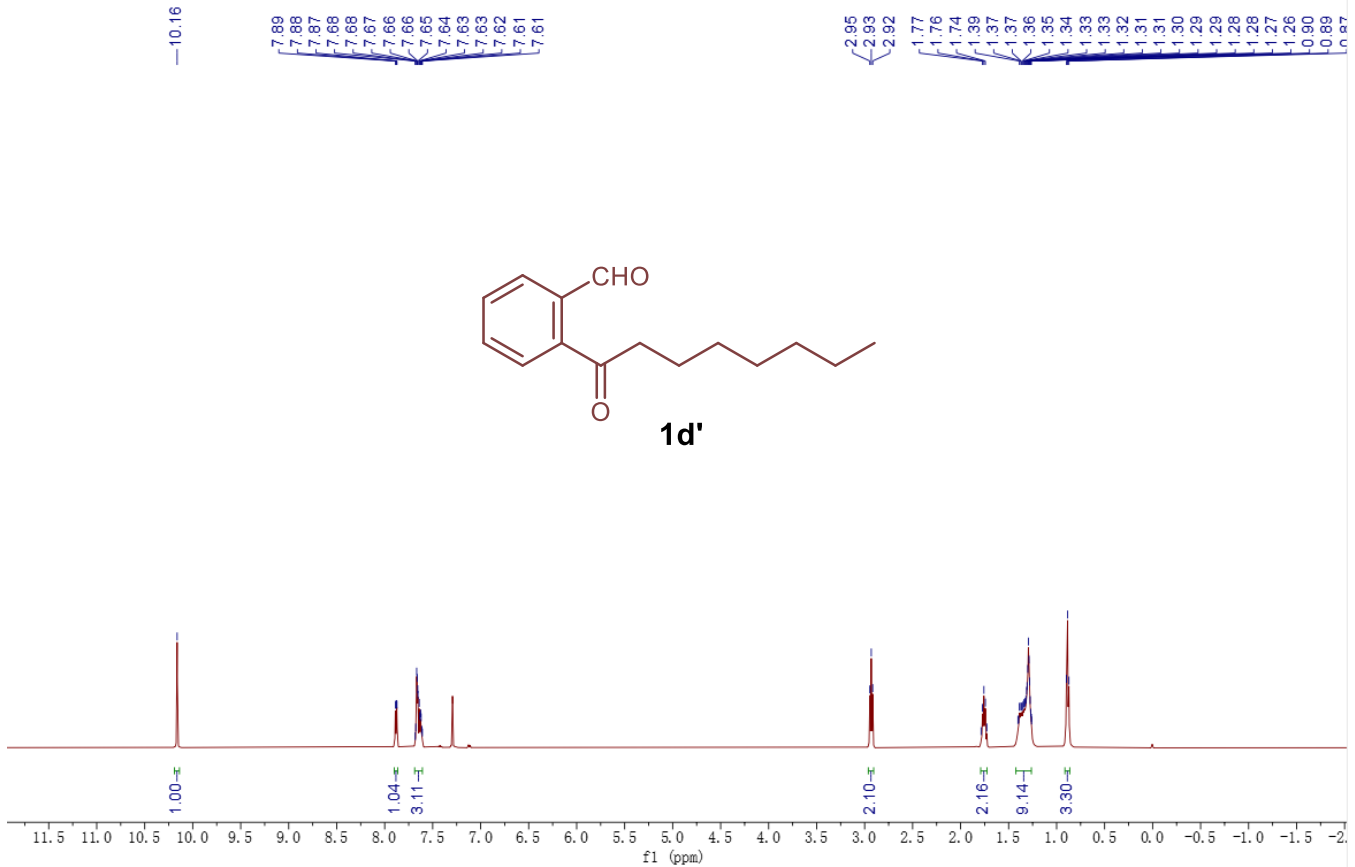
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H	-4.23241700	-4.05762400	-2.07887300
H	-4.28581300	-1.71858300	-1.22078800
H	-5.77317600	-2.59479900	-0.75771600
H	-4.47970200	-2.32829800	0.43717800
H	-4.13830400	-5.99203800	-0.47618600
H	-4.48483500	-4.88153300	0.86883400
H	-5.69748200	-5.12662700	-0.40460900
O	-2.56185400	-0.38081800	-2.41755200
H	-2.04034200	-1.18208100	-2.23427300
H	-0.74954900	2.06712000	0.63051500
O	0.36947000	-0.71613300	-1.64804700
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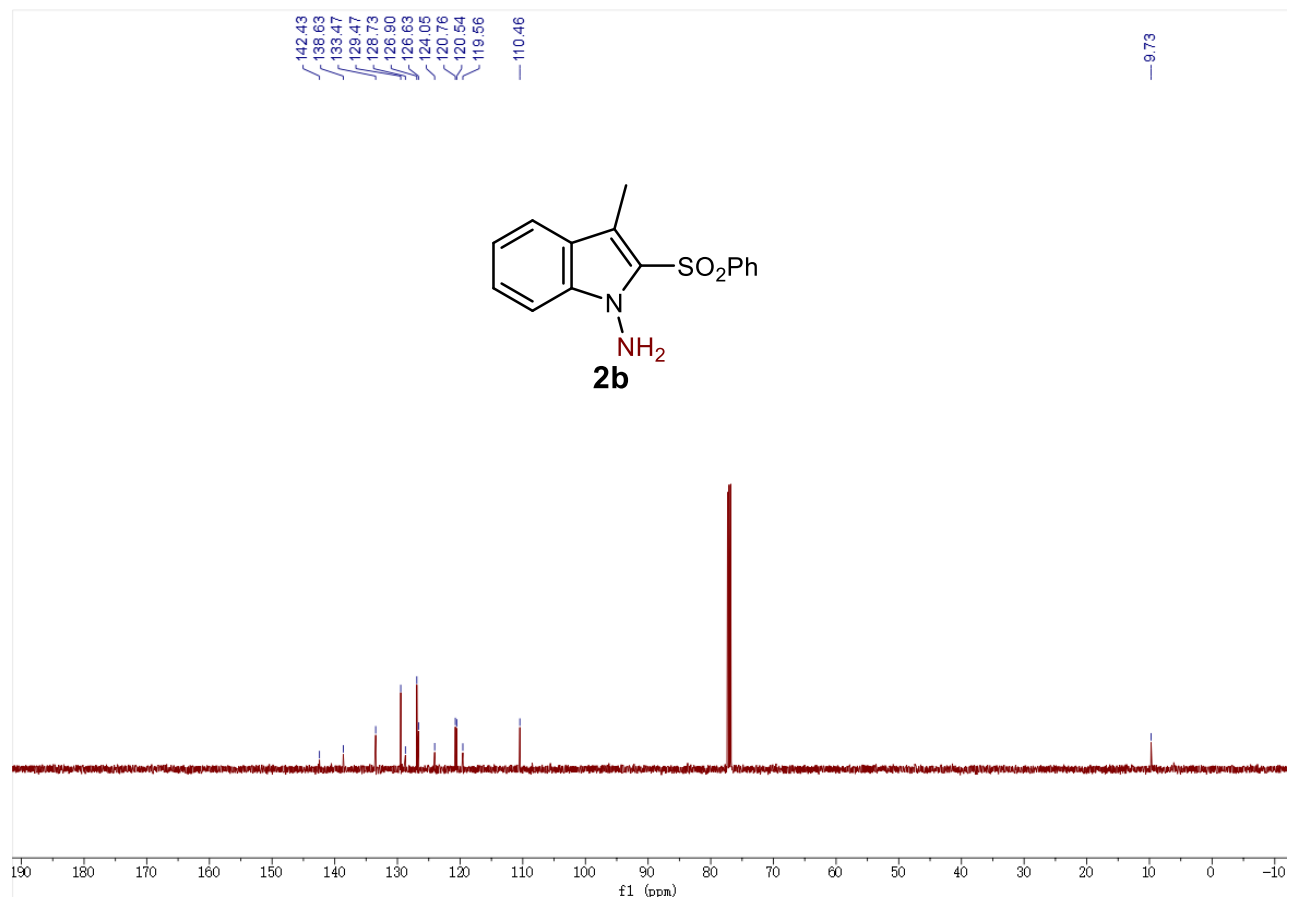
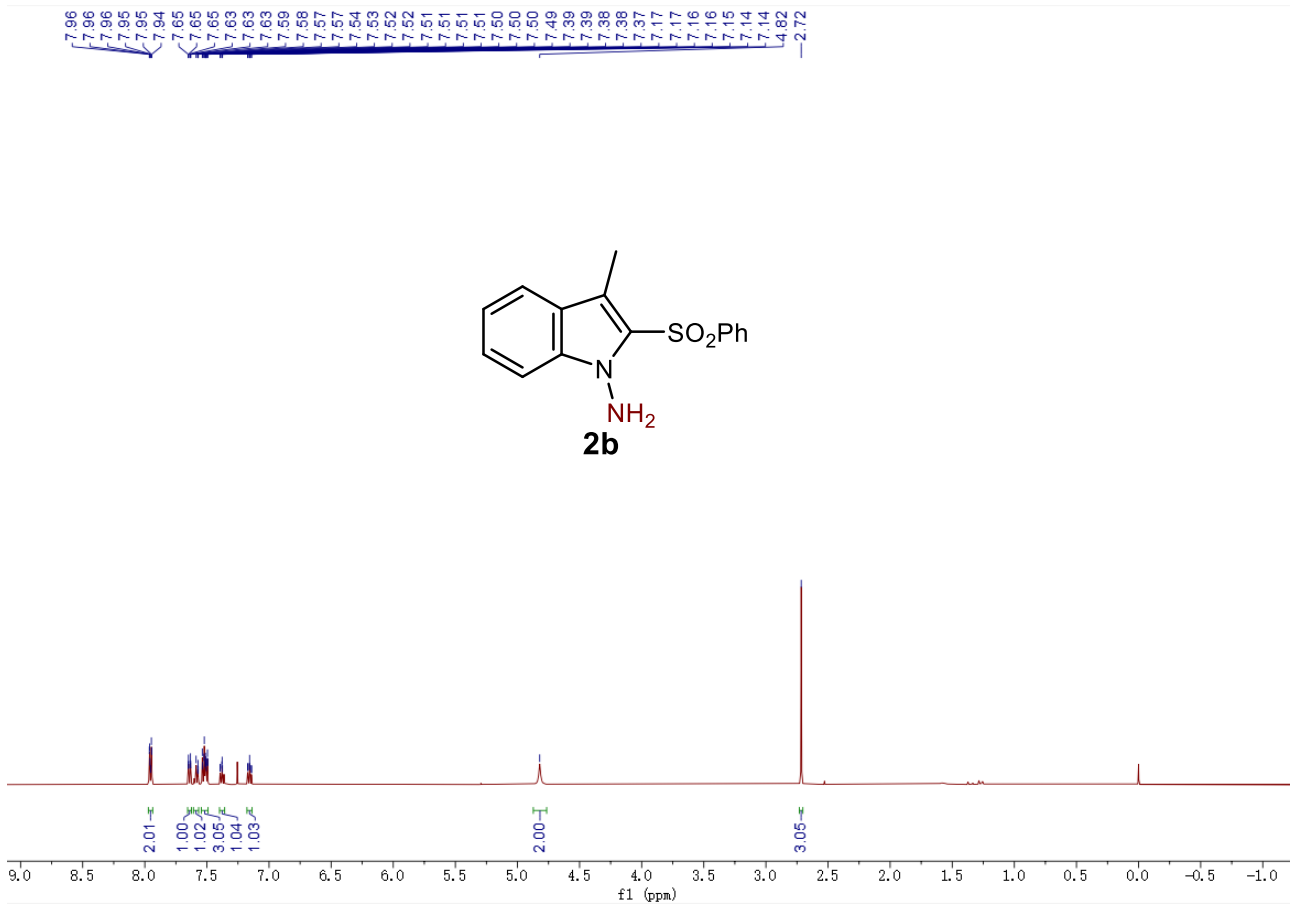
## References

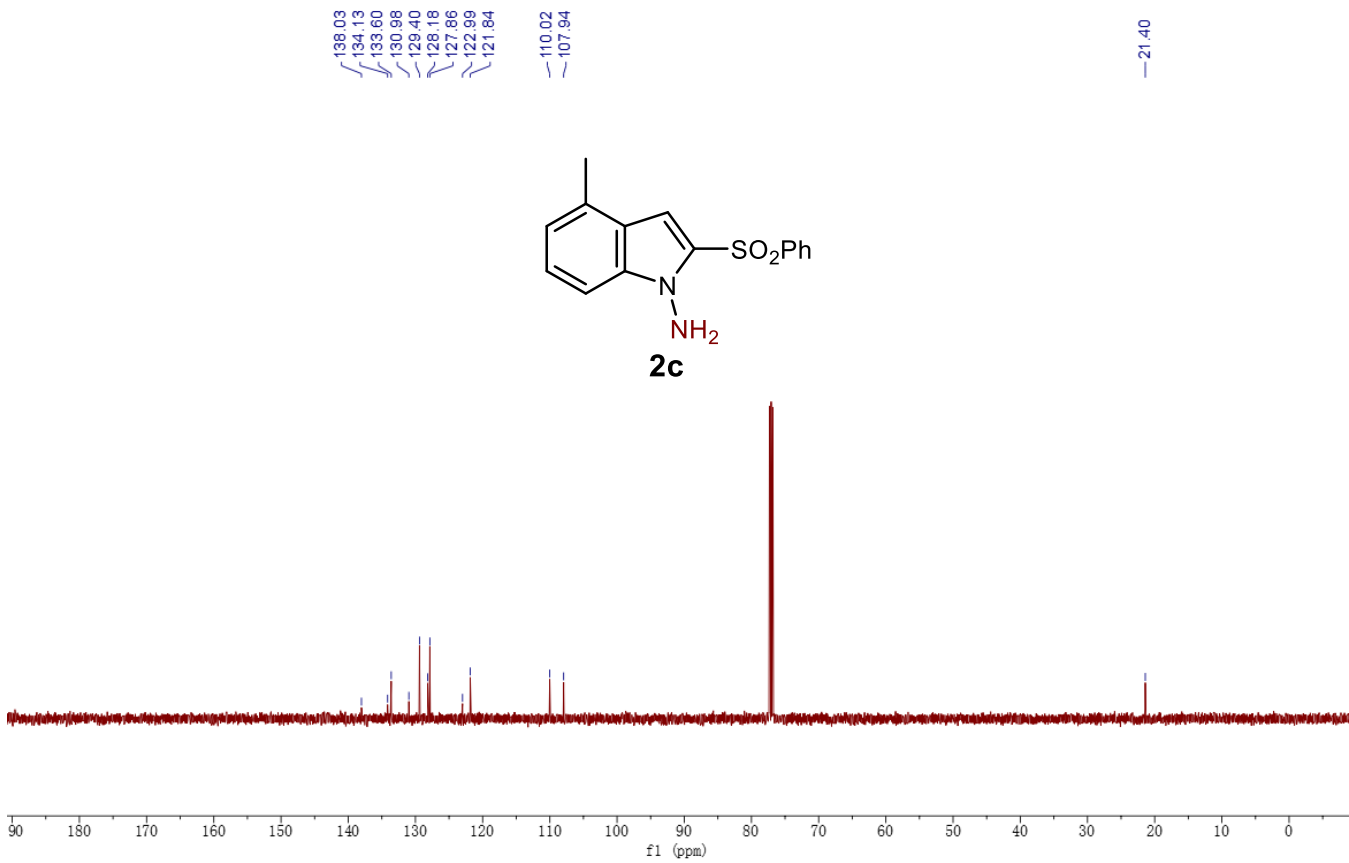
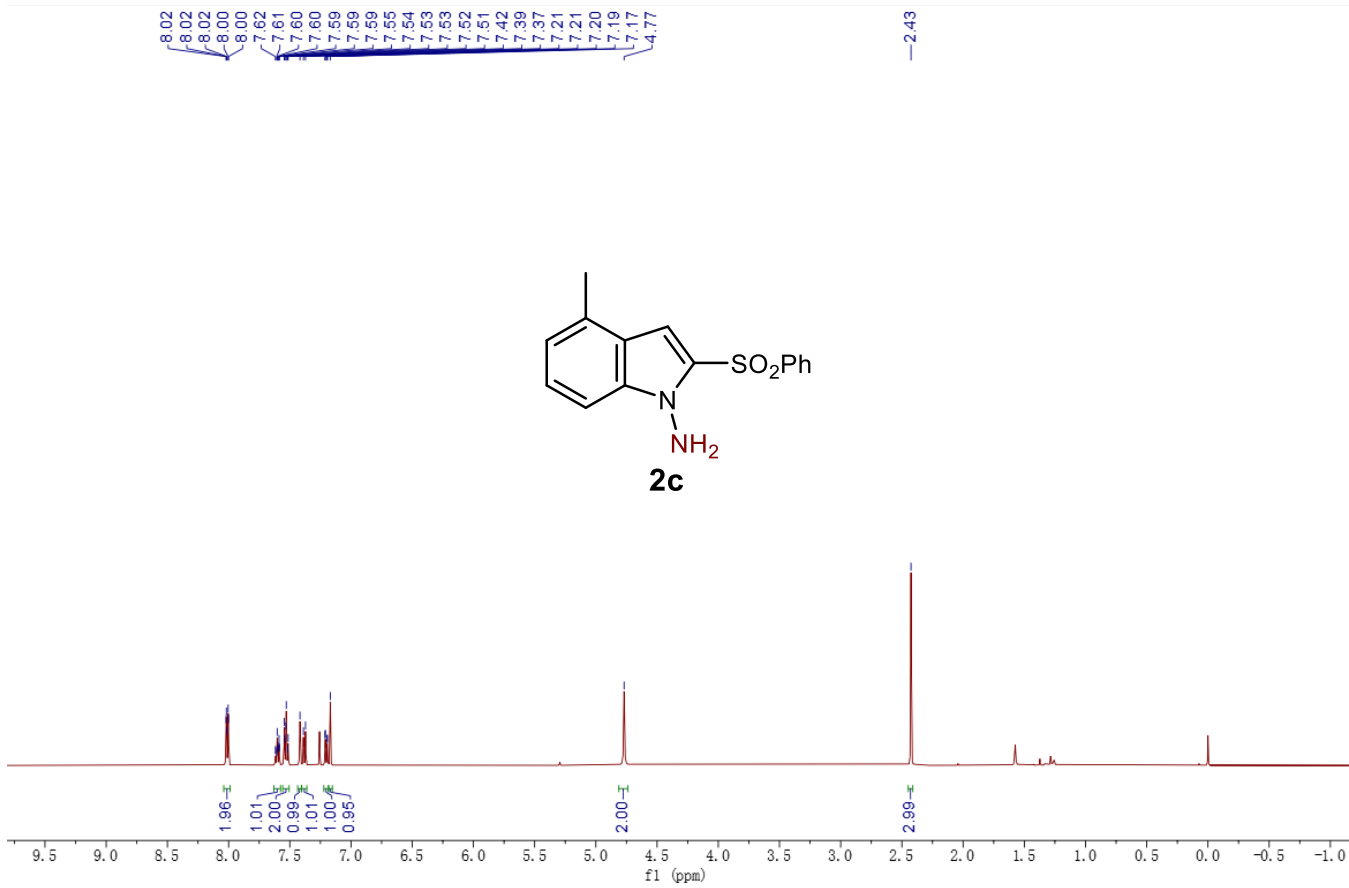
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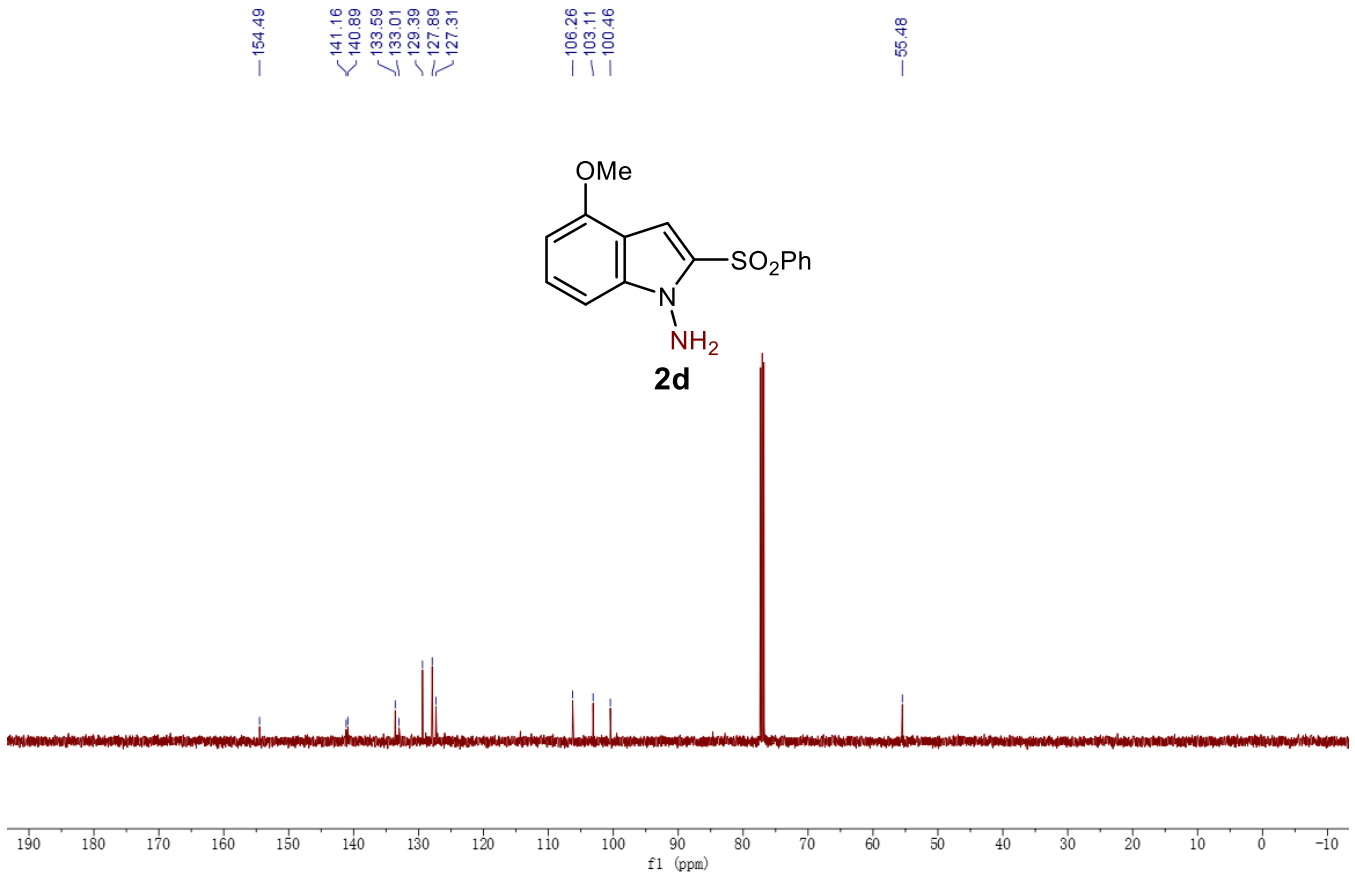
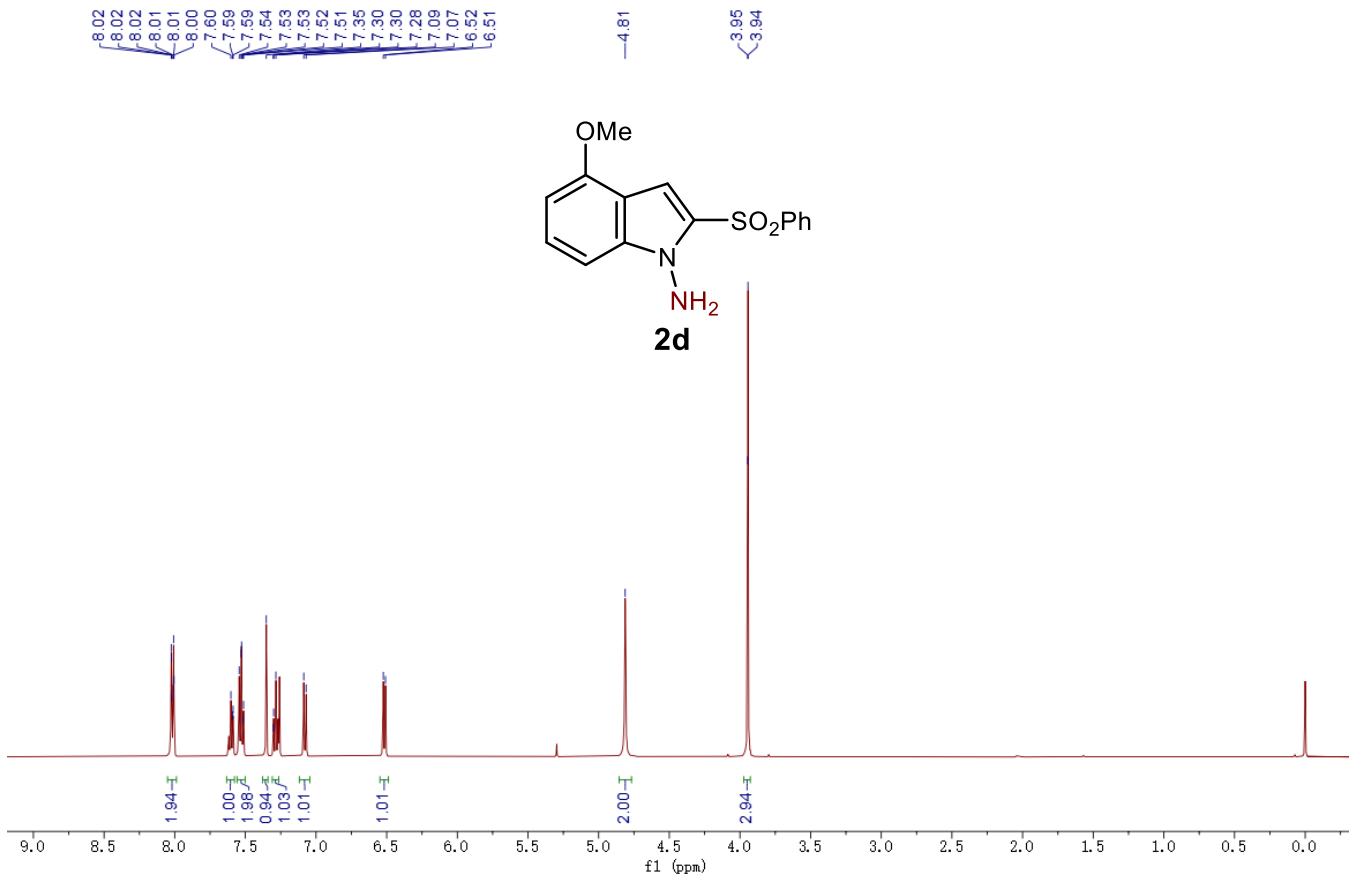
# NMR spectra





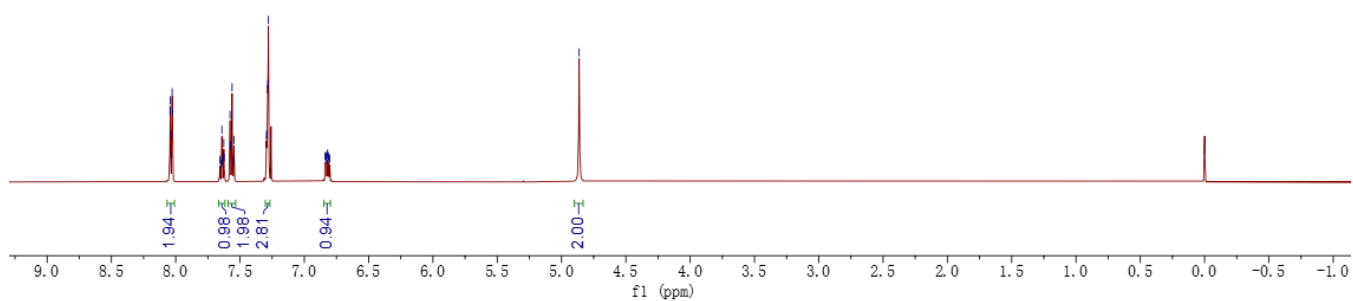
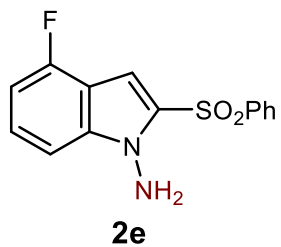




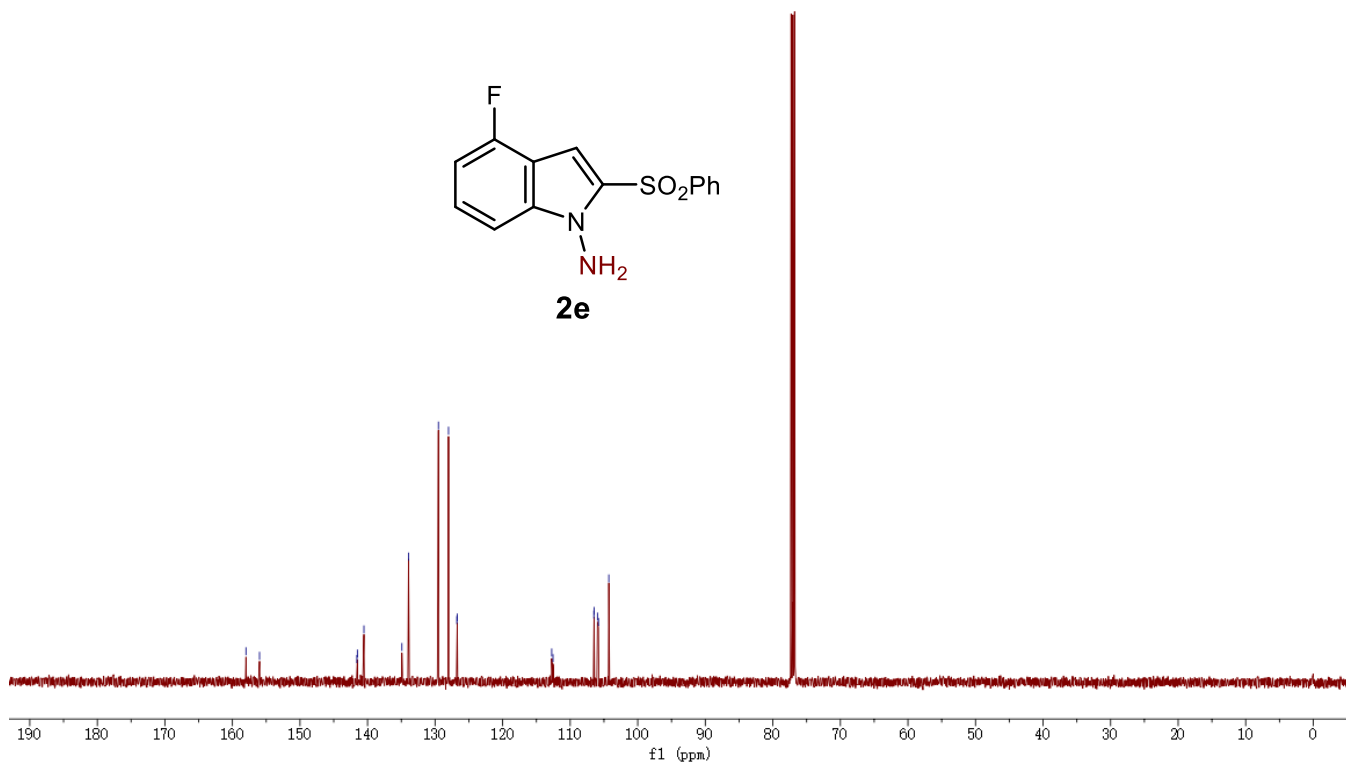
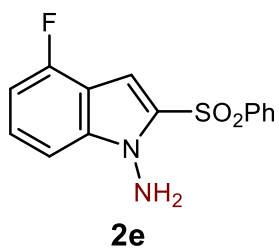


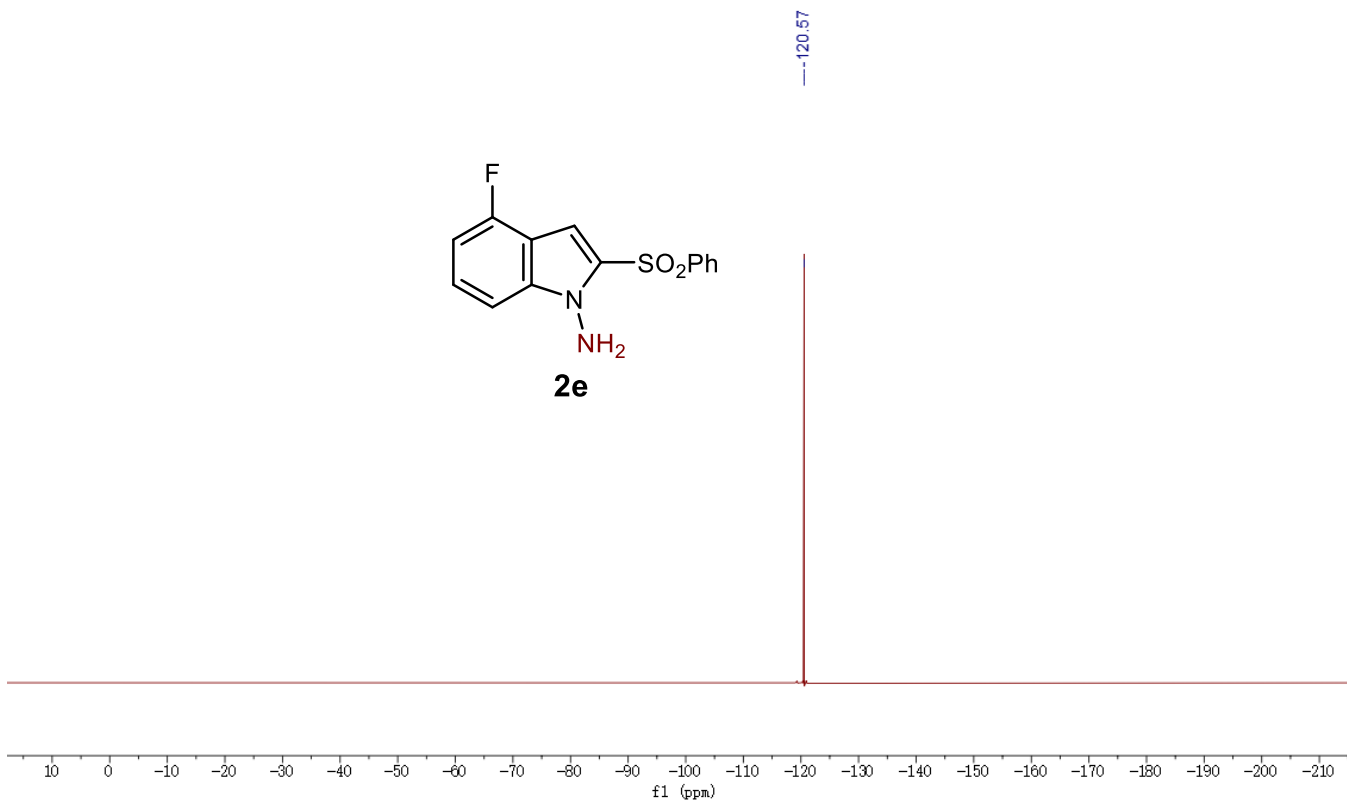


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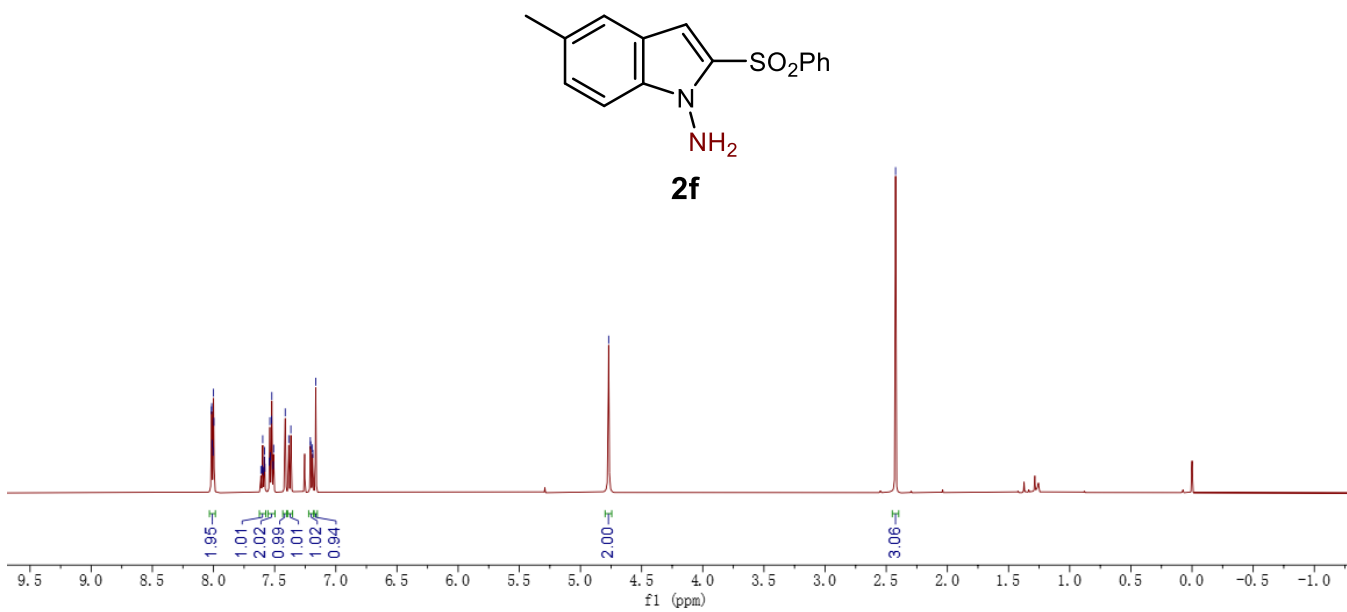
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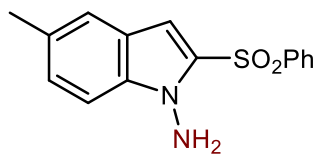
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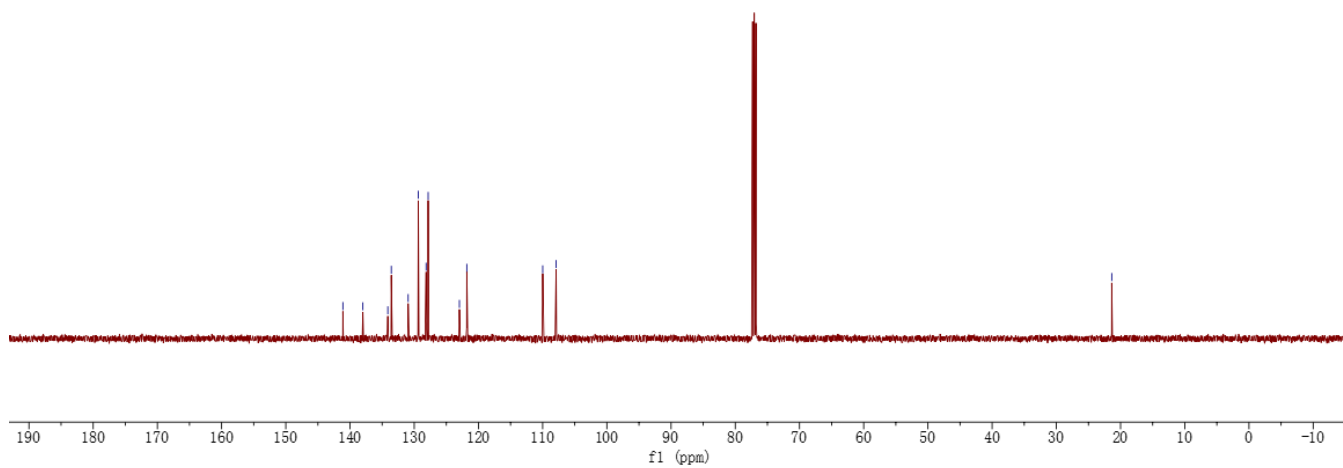


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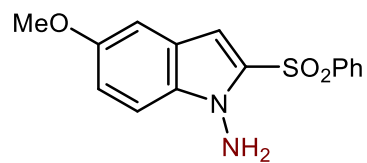
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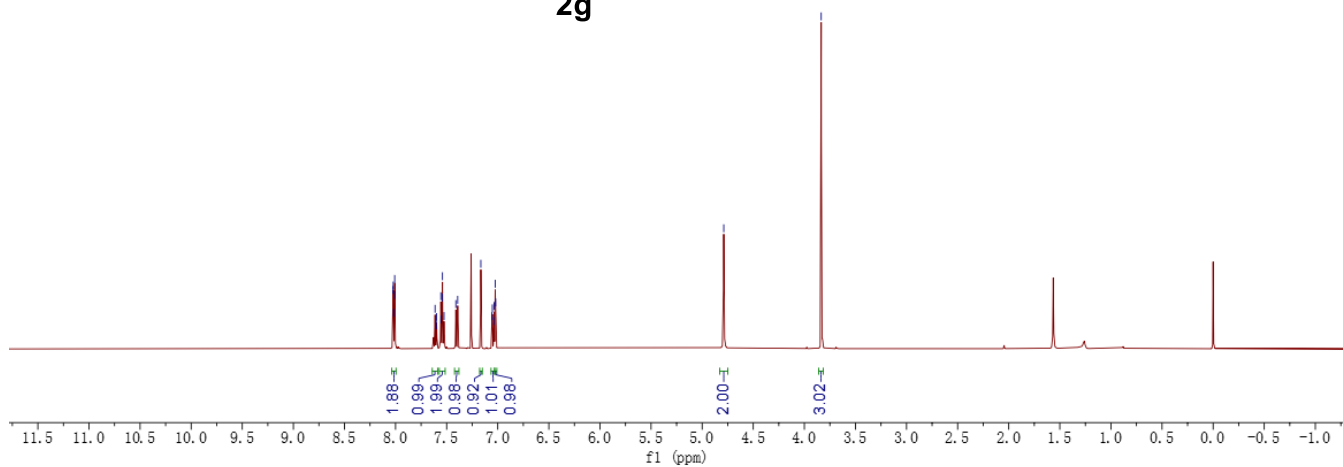
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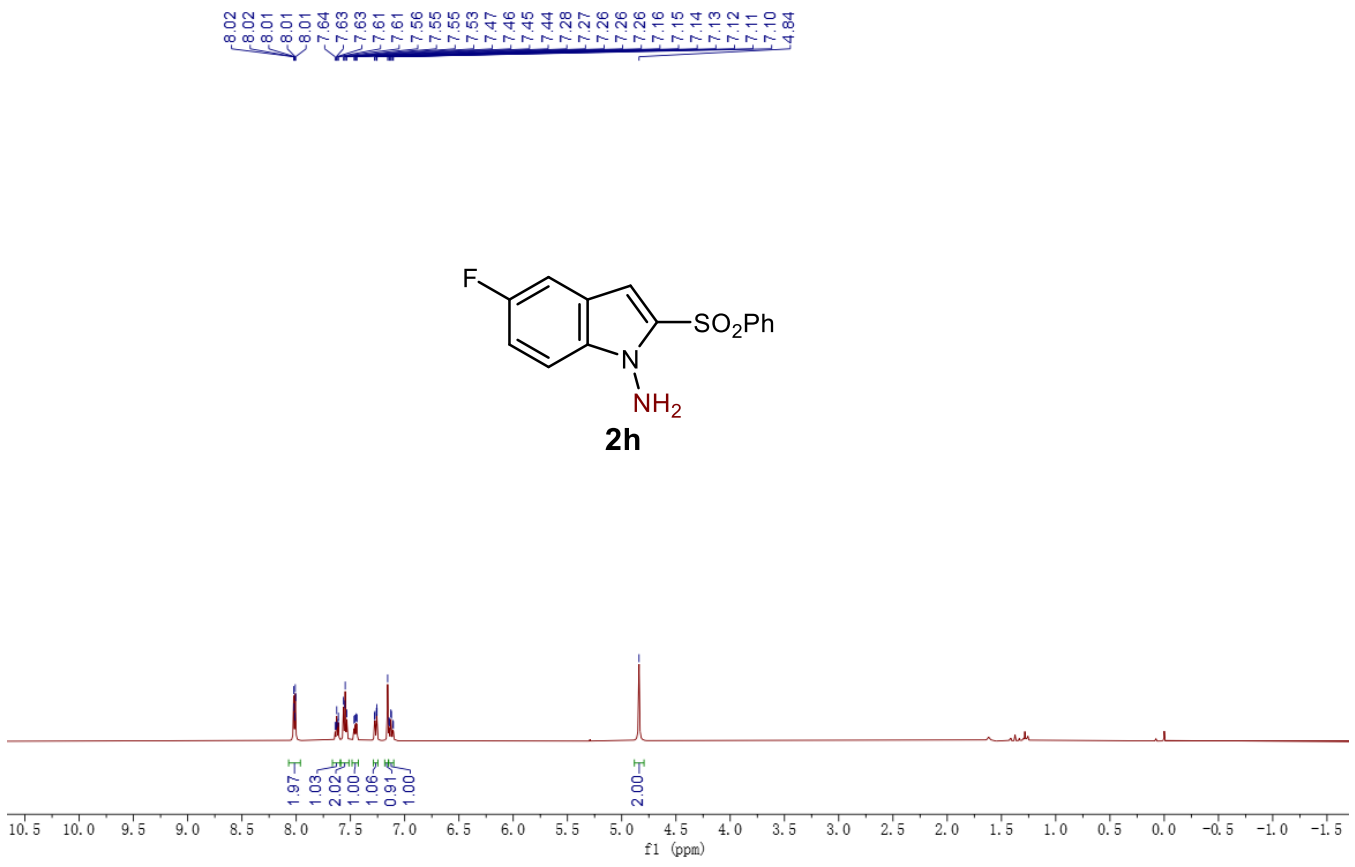
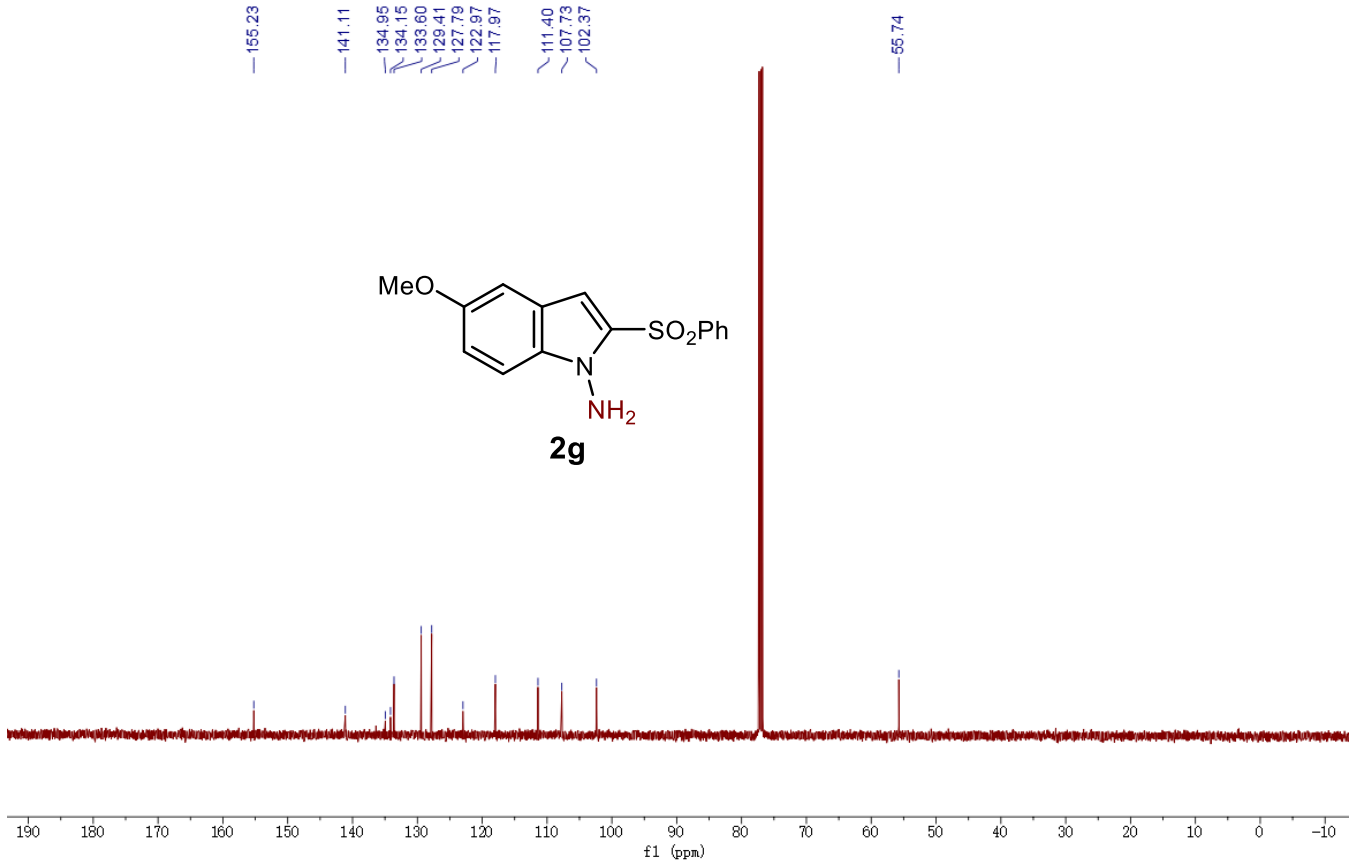


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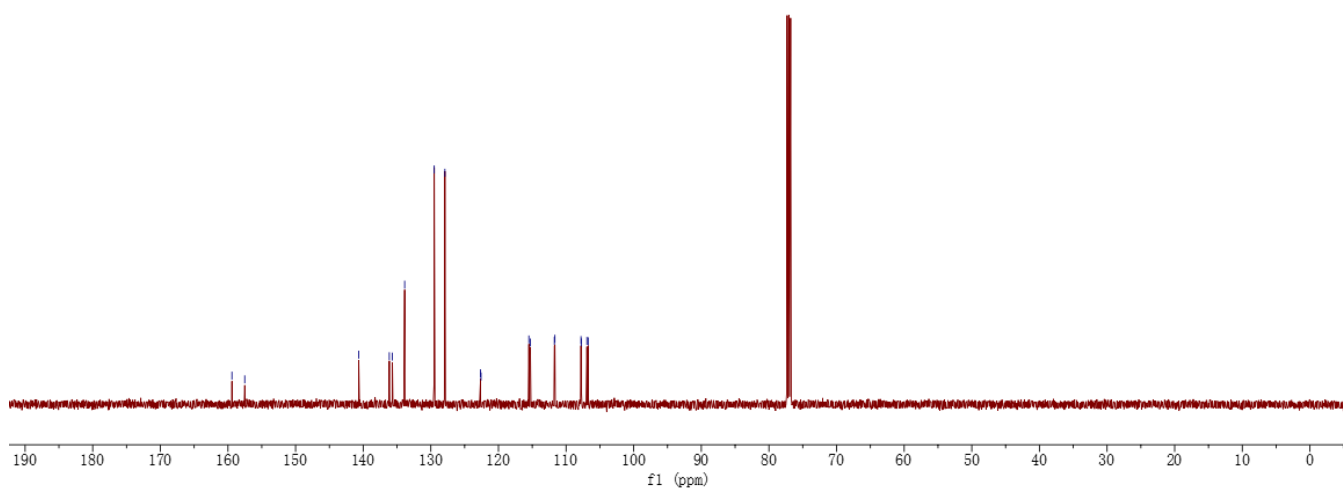
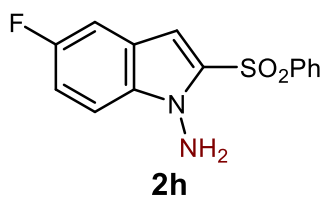
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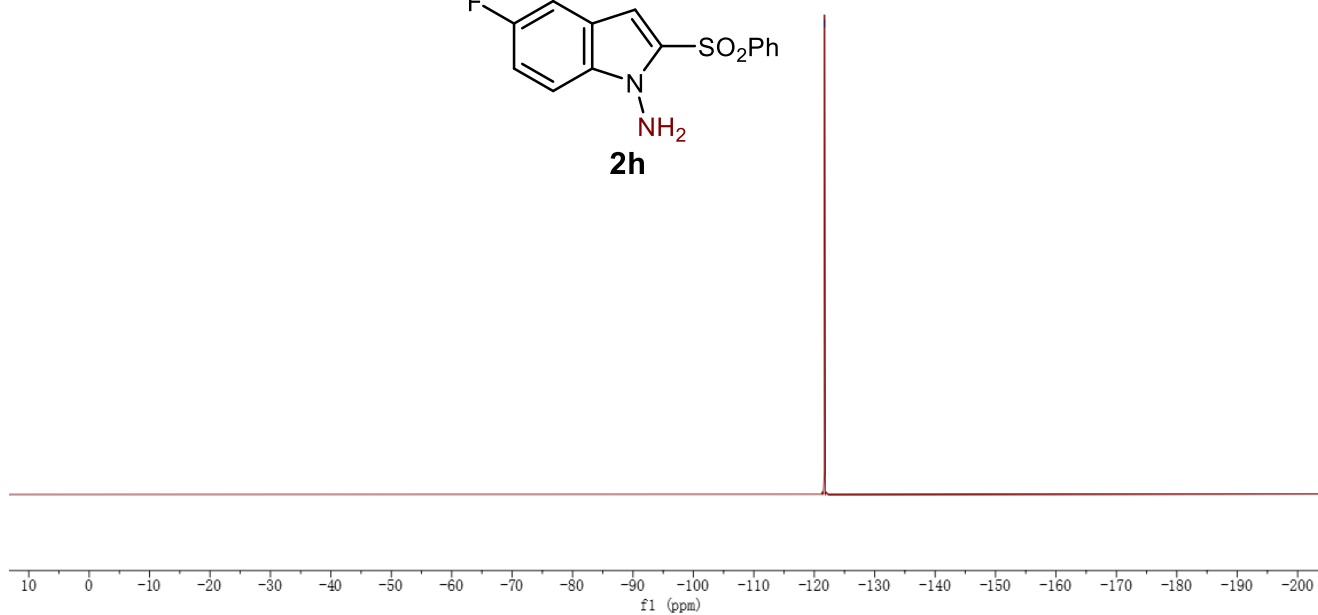
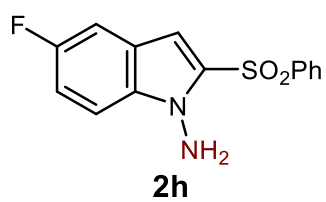


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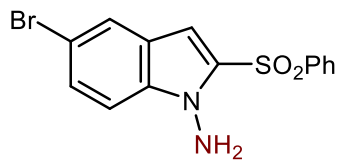


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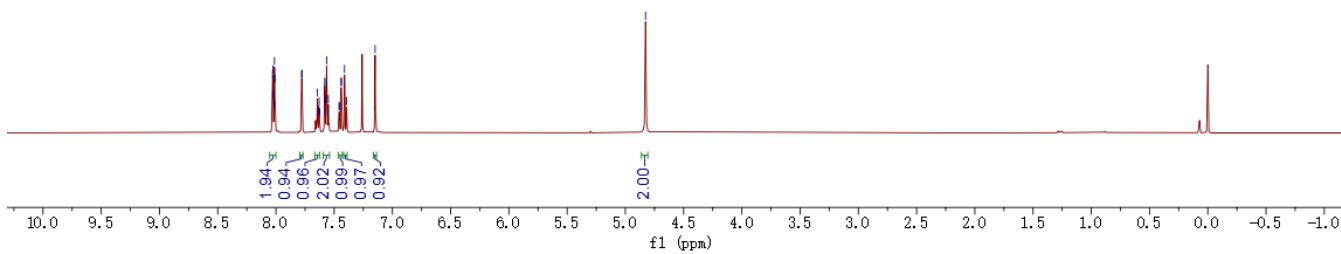


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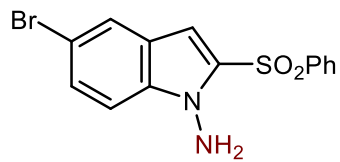
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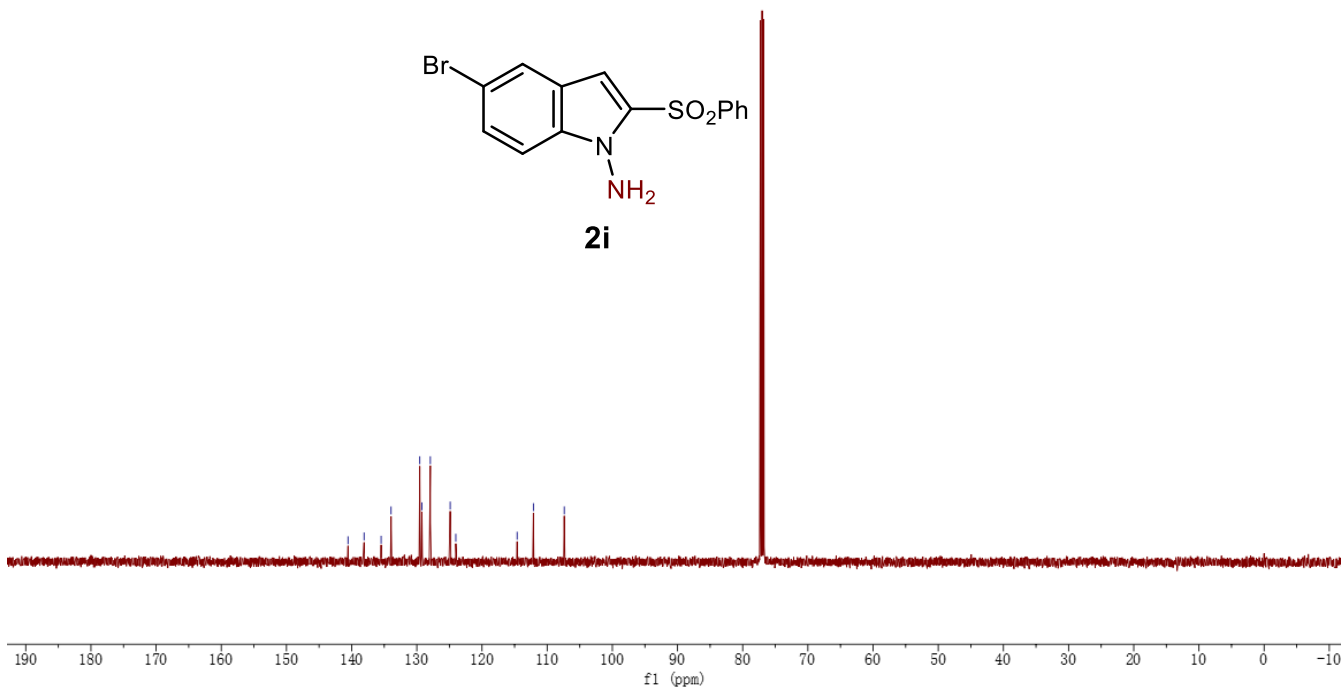
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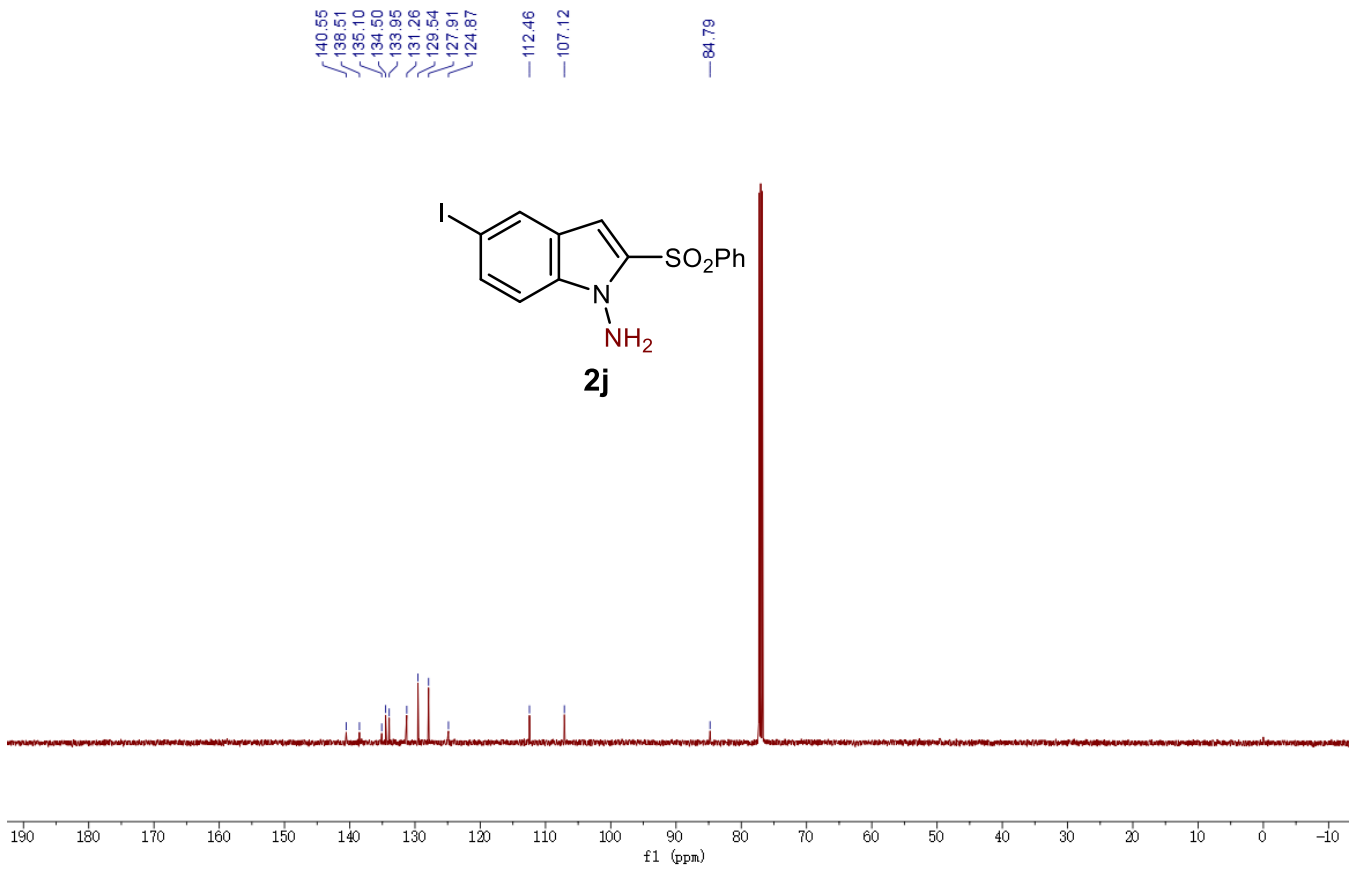
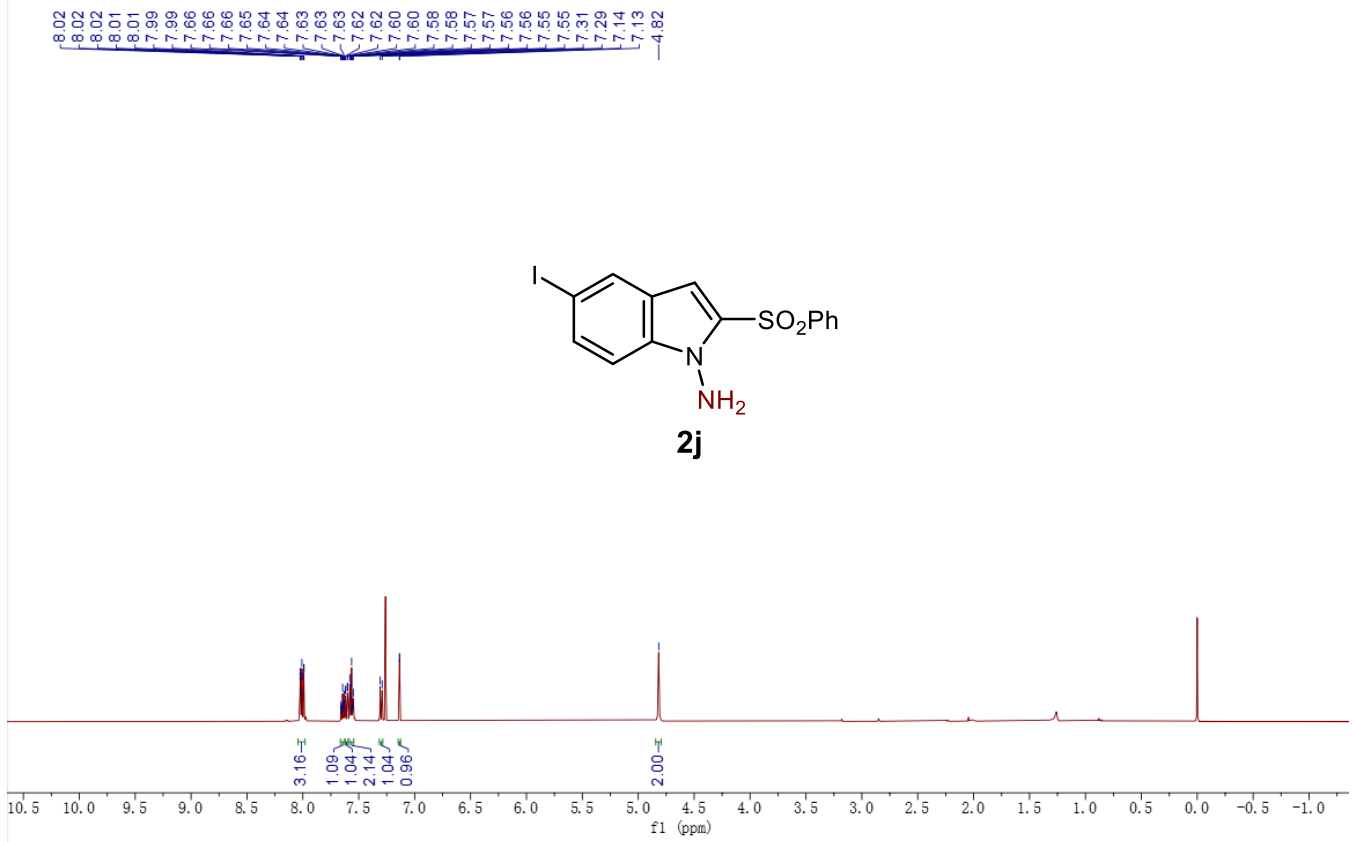


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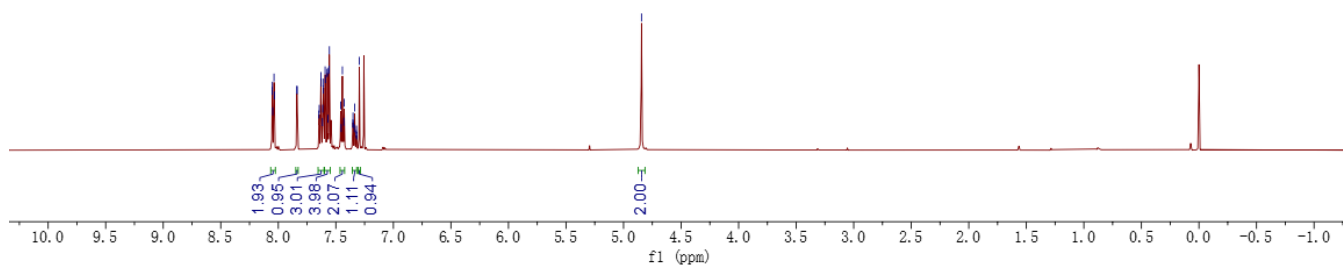
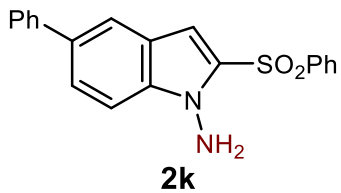


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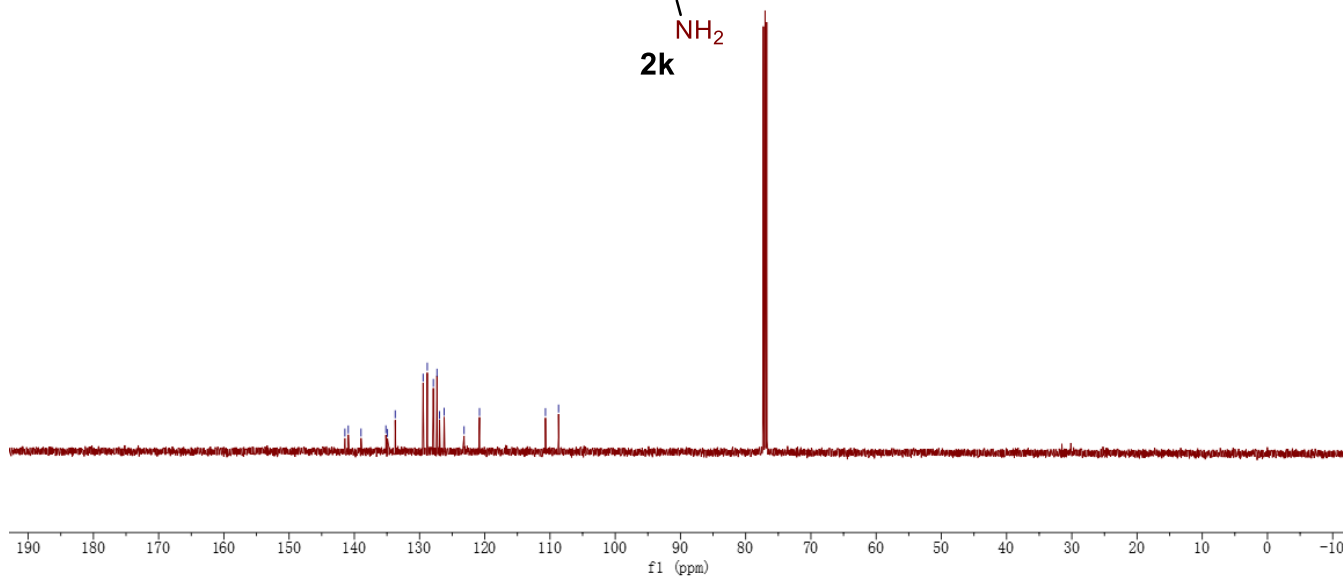
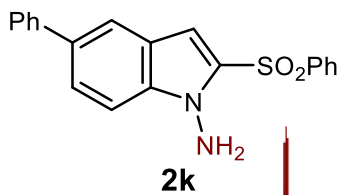




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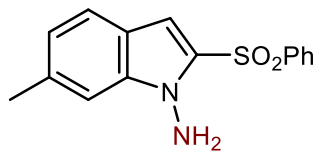
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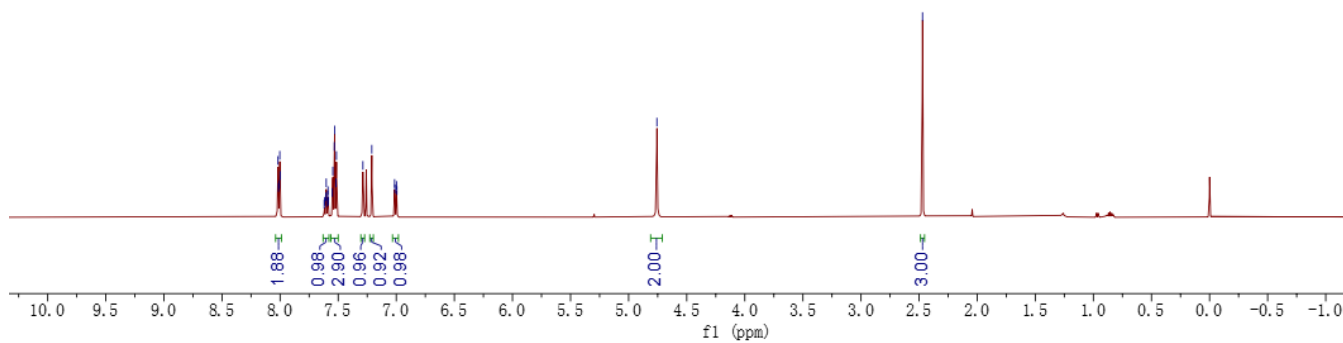


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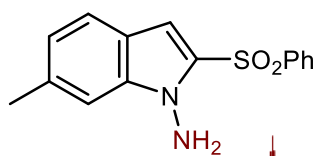


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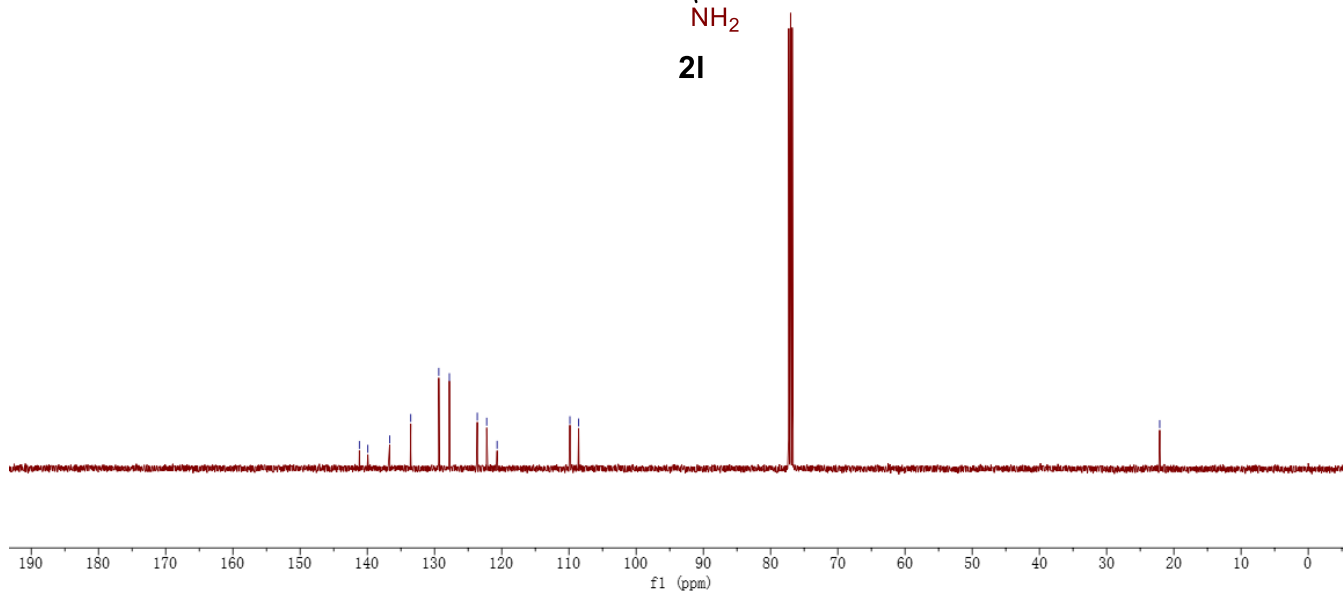


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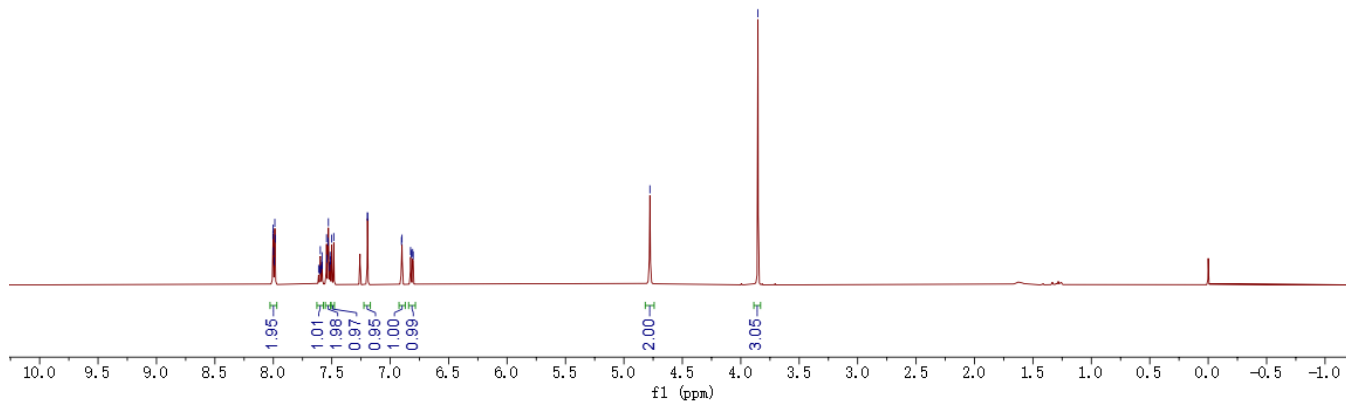
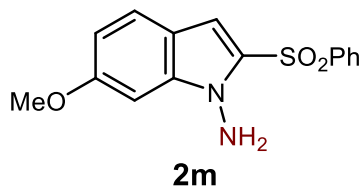
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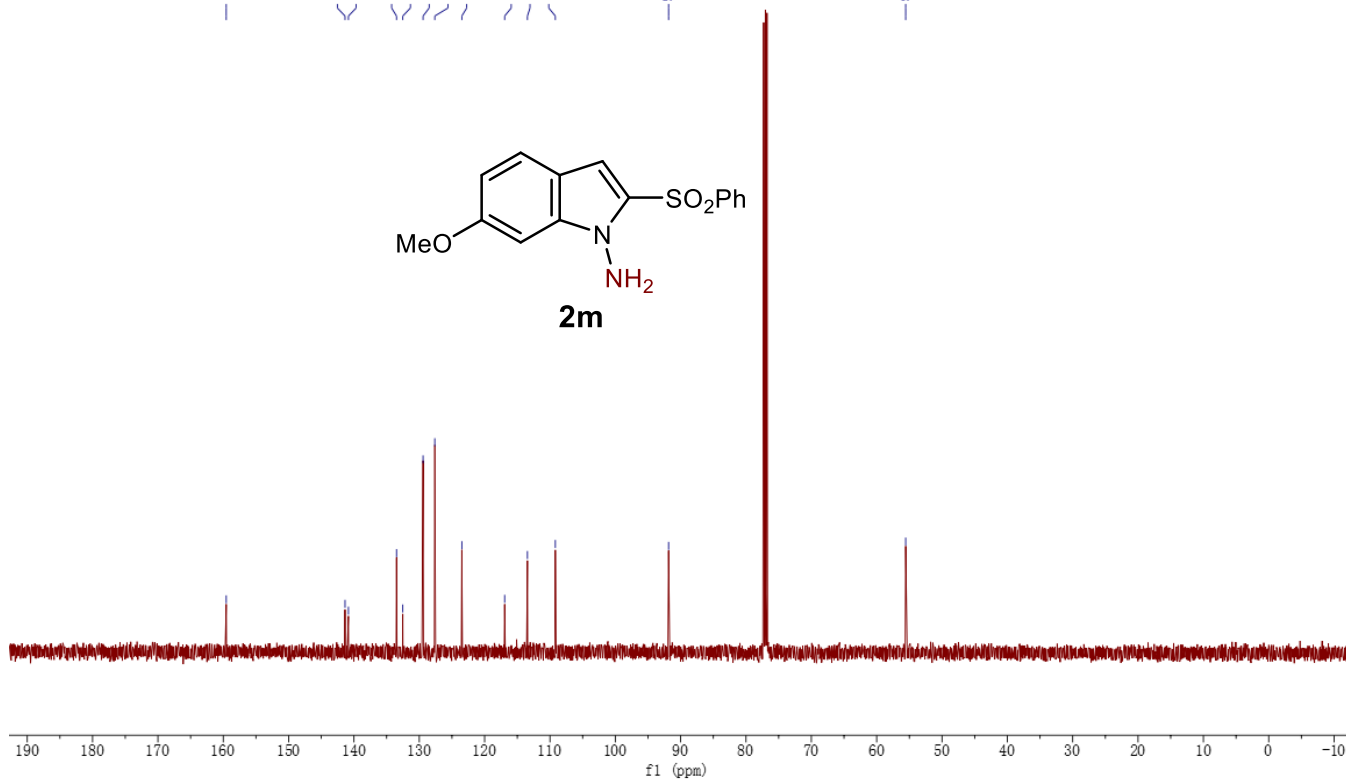
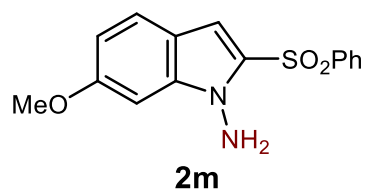
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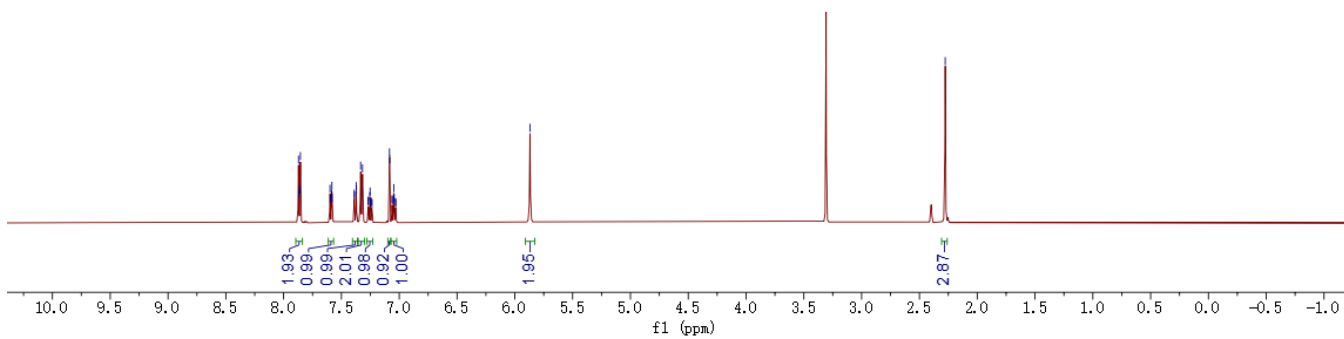
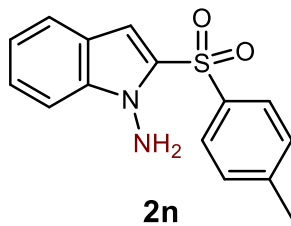


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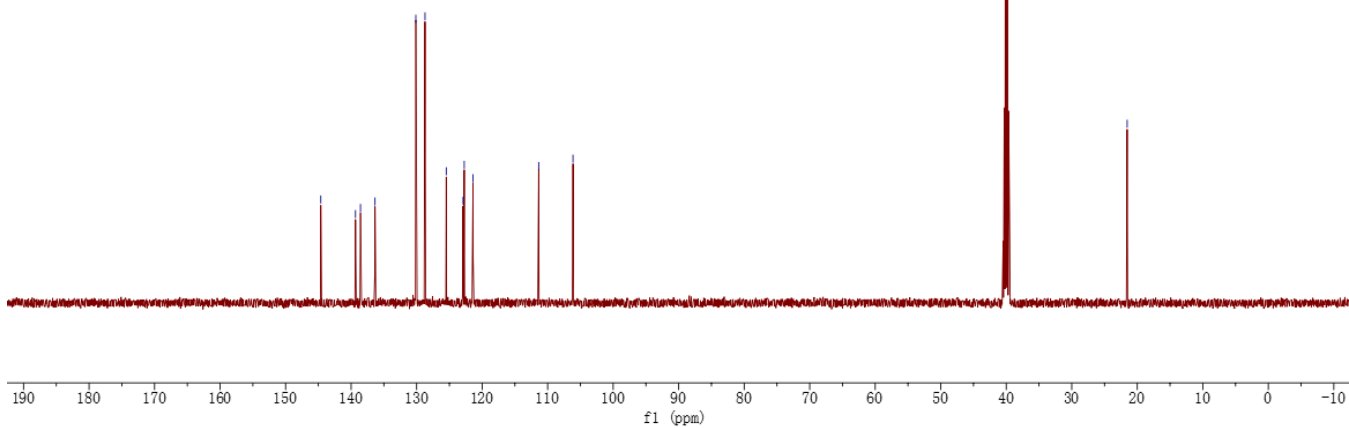
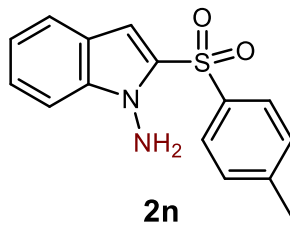
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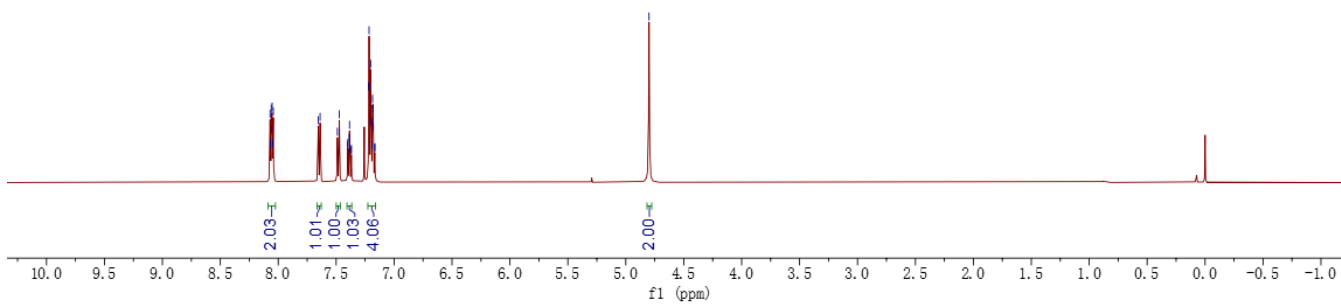
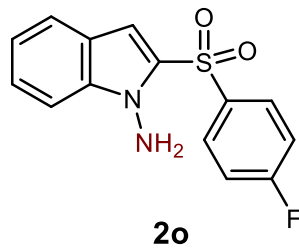


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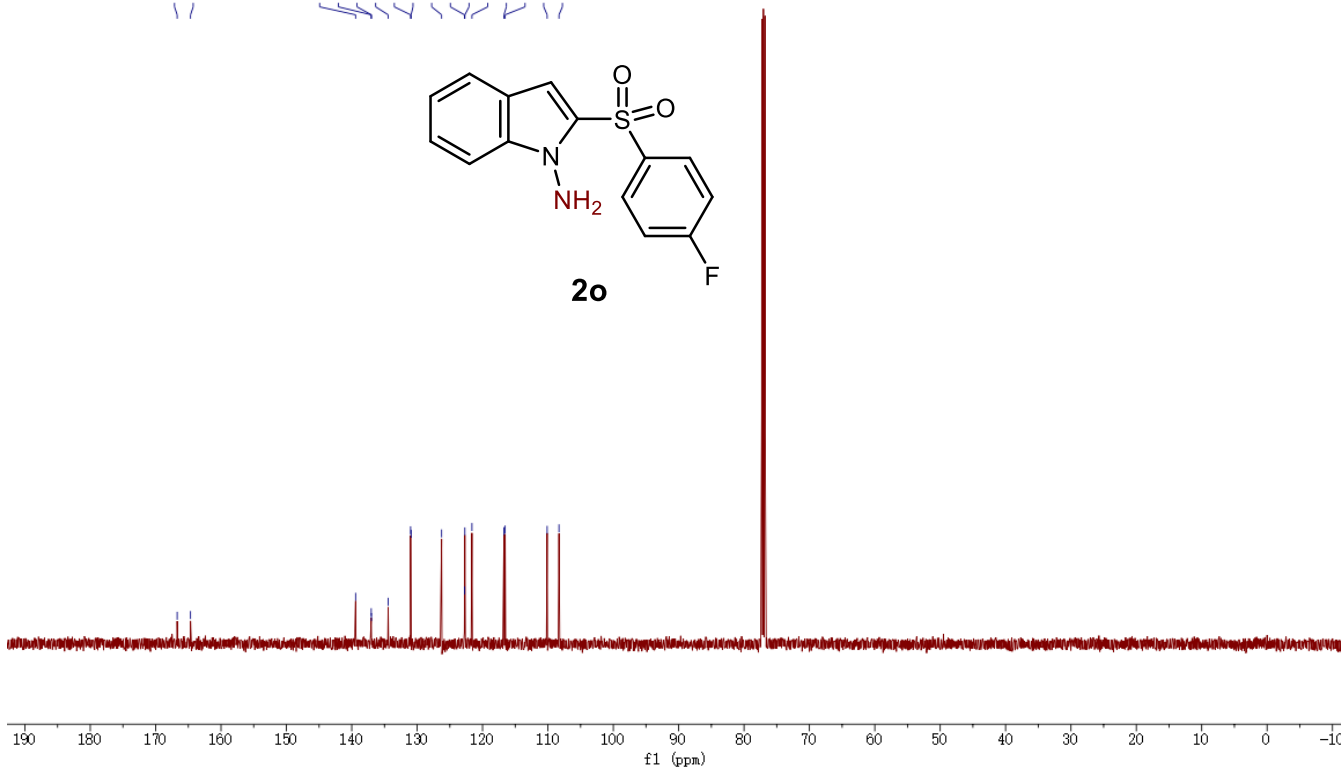
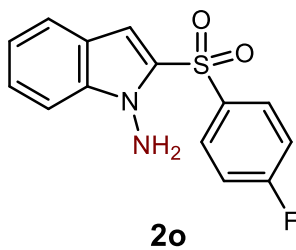
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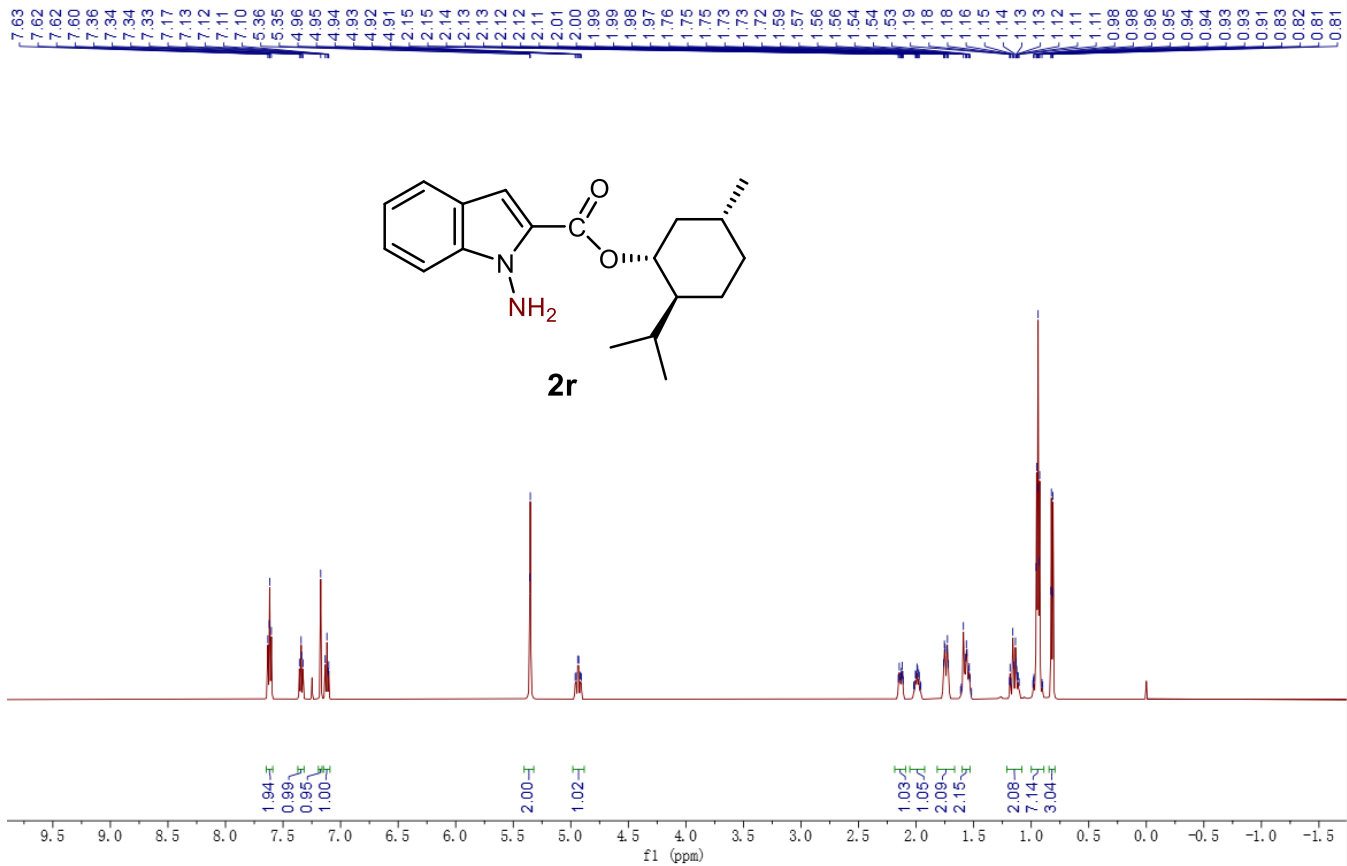
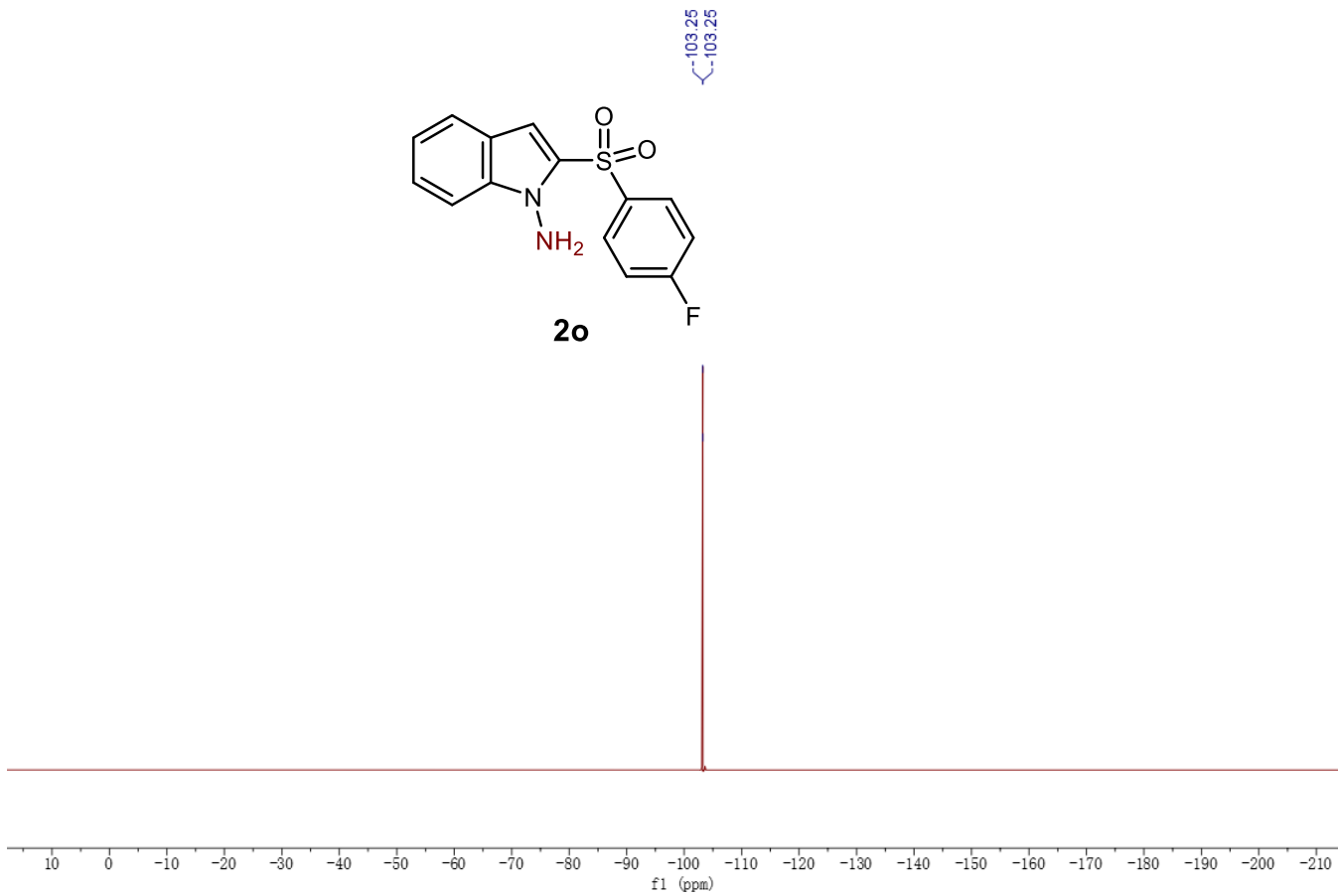


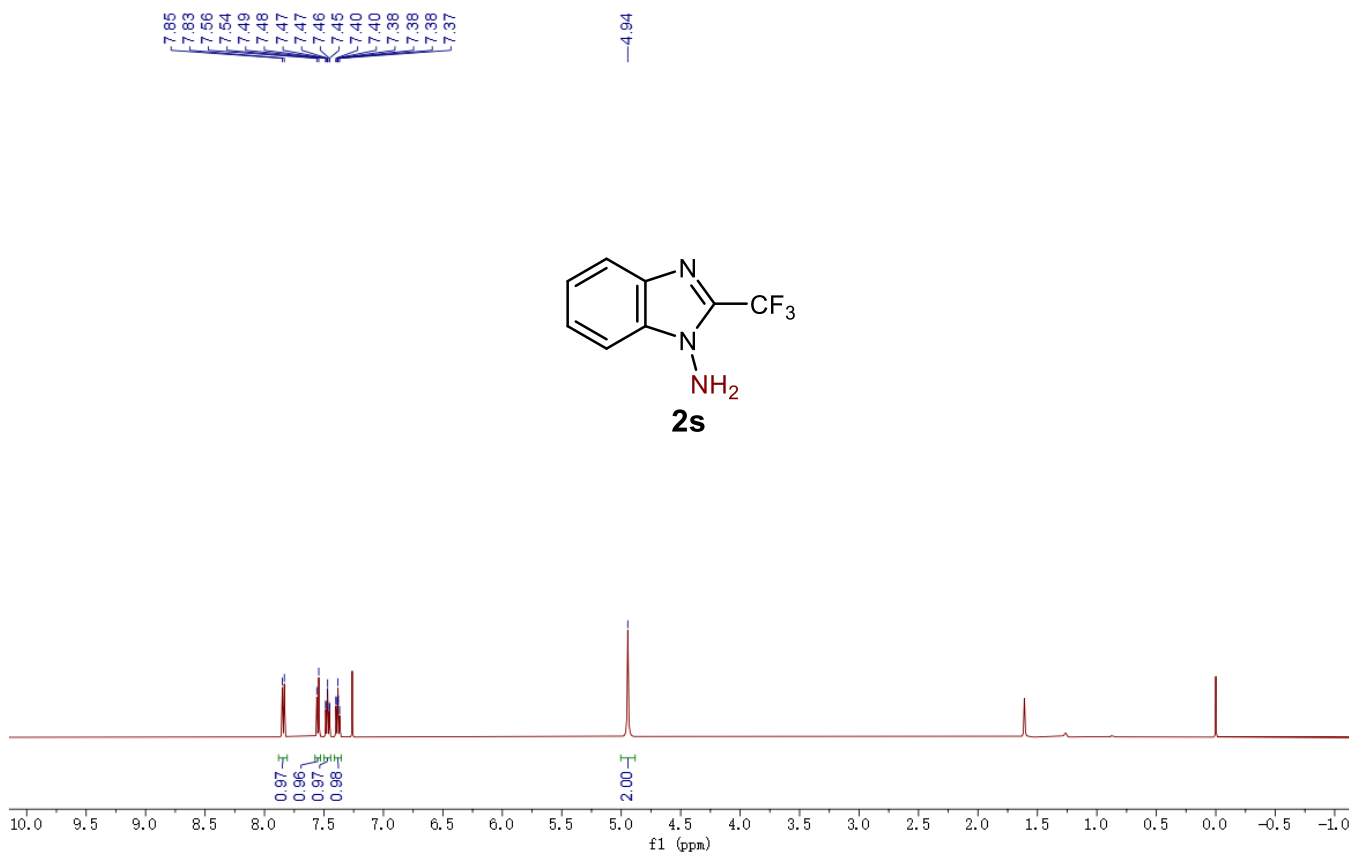
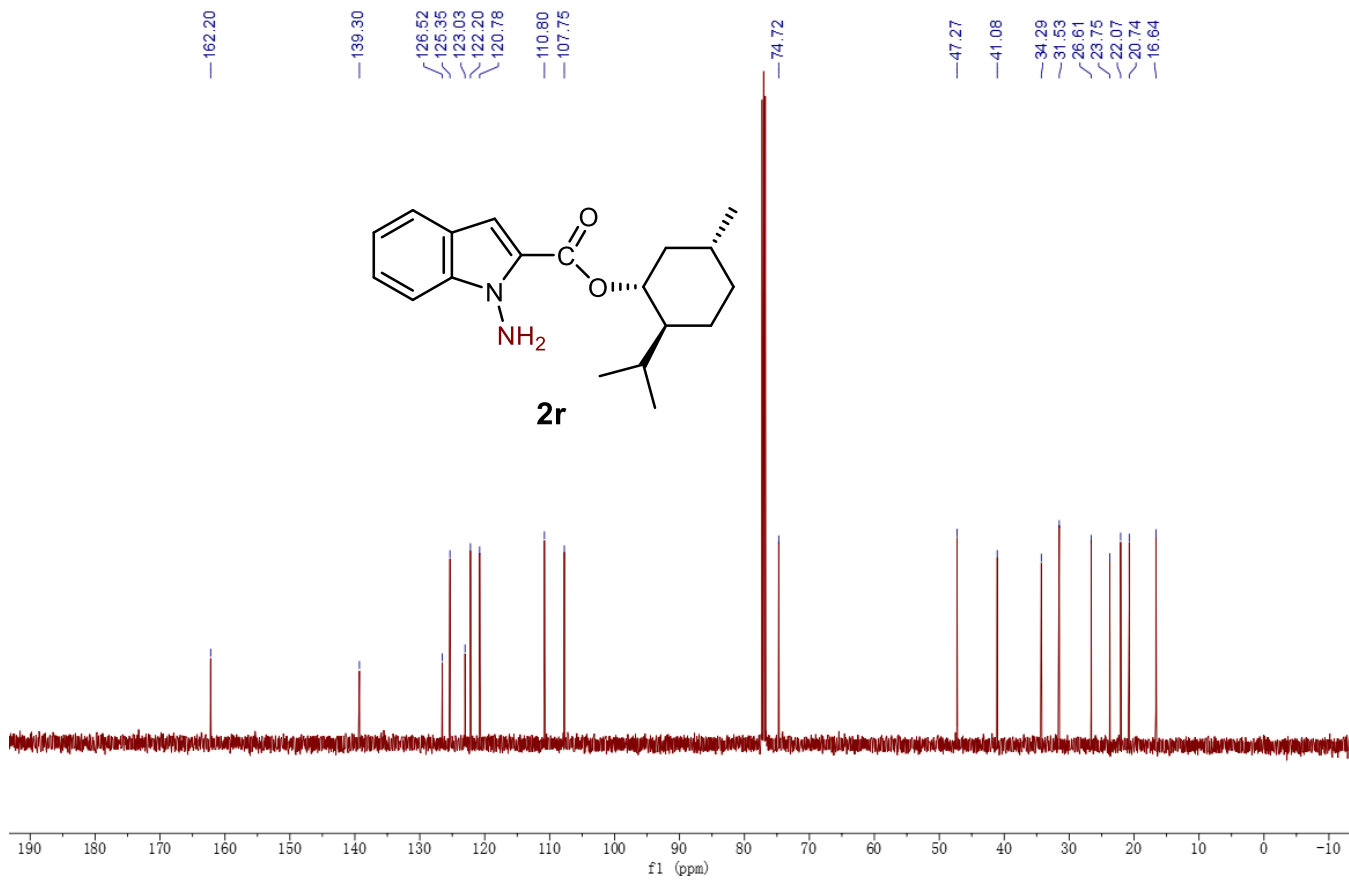
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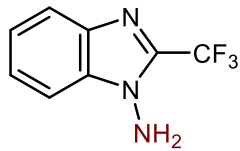
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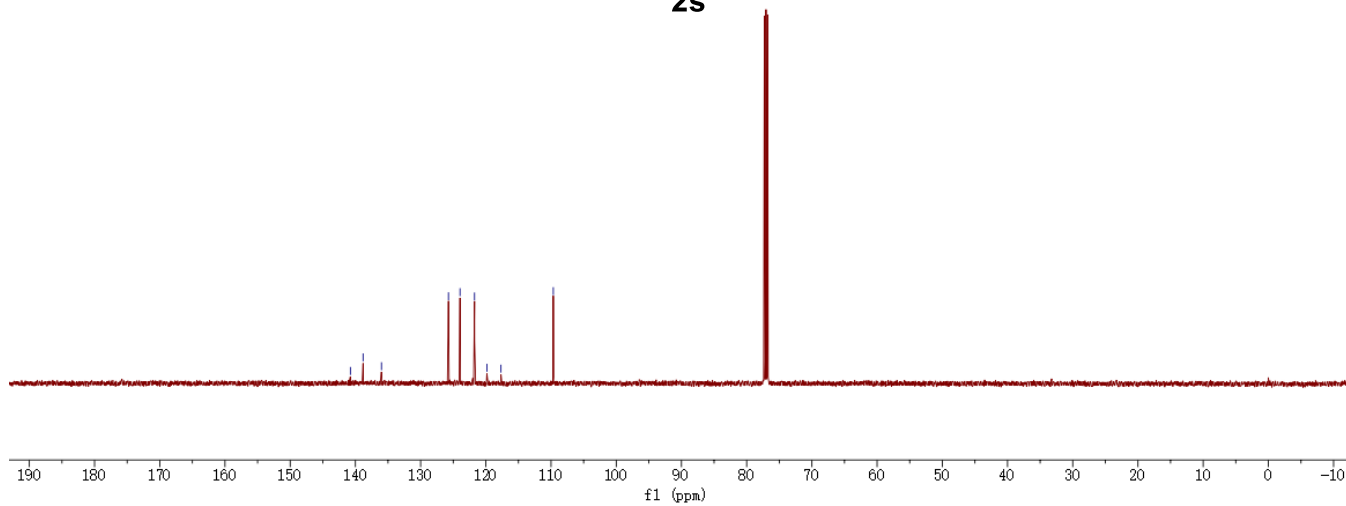




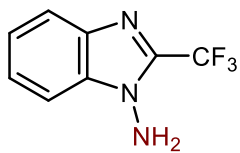
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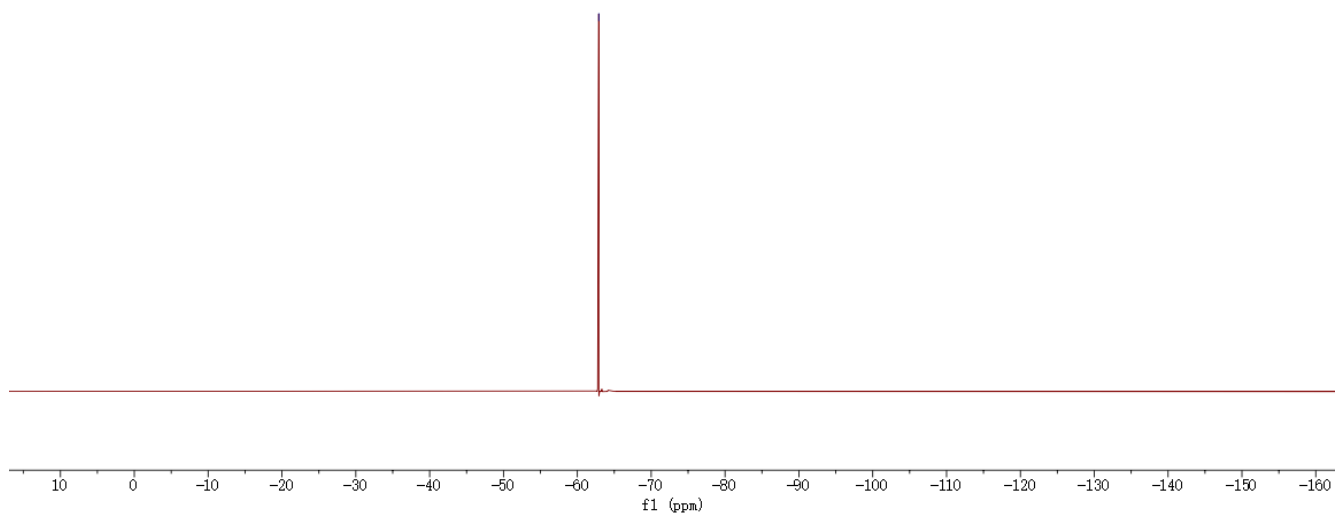
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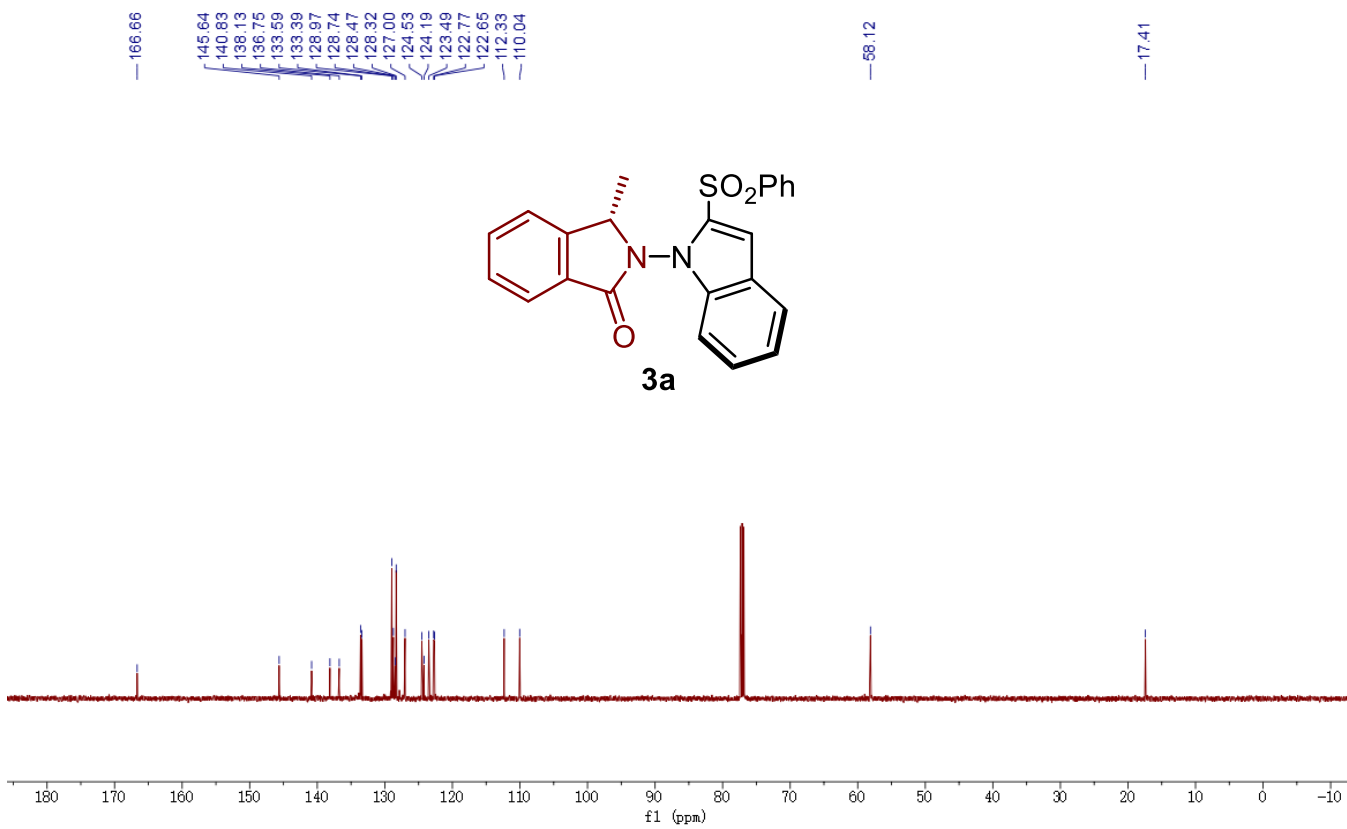
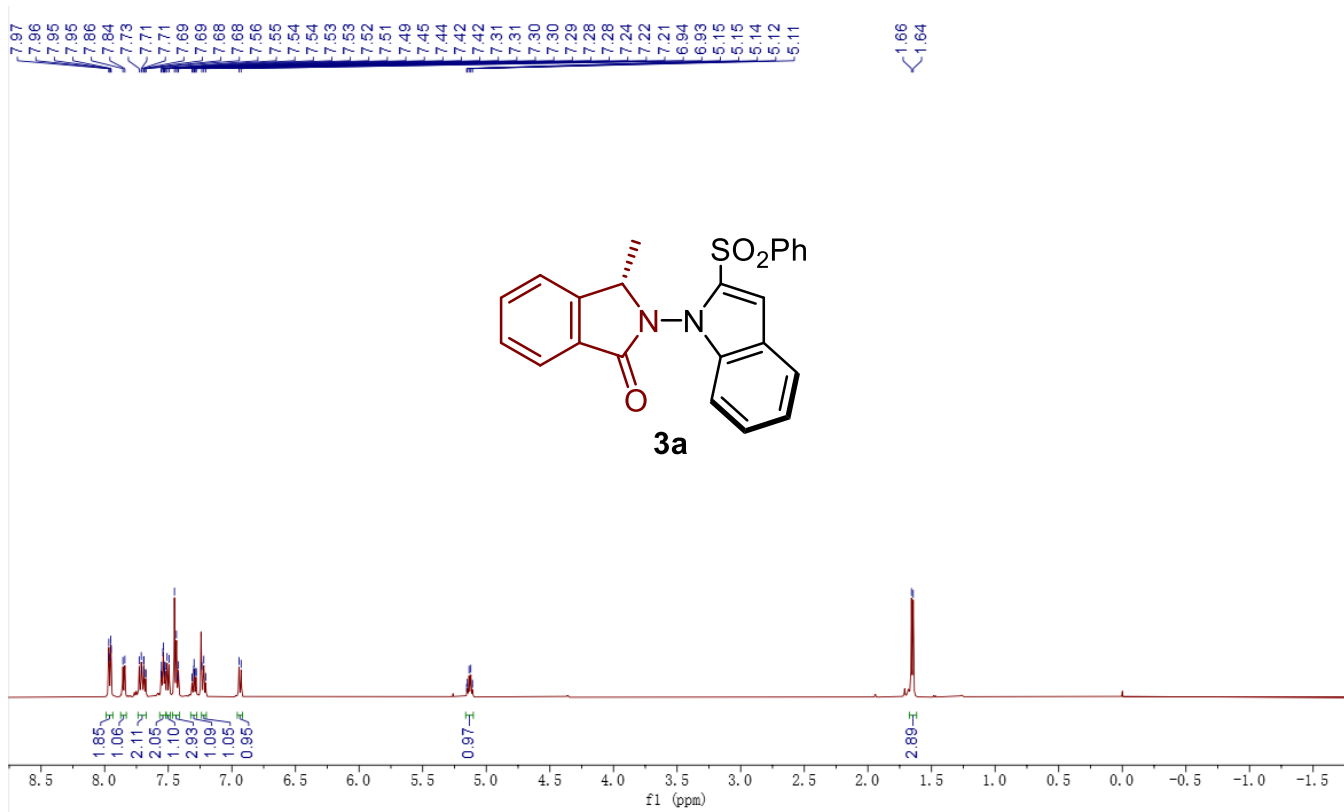


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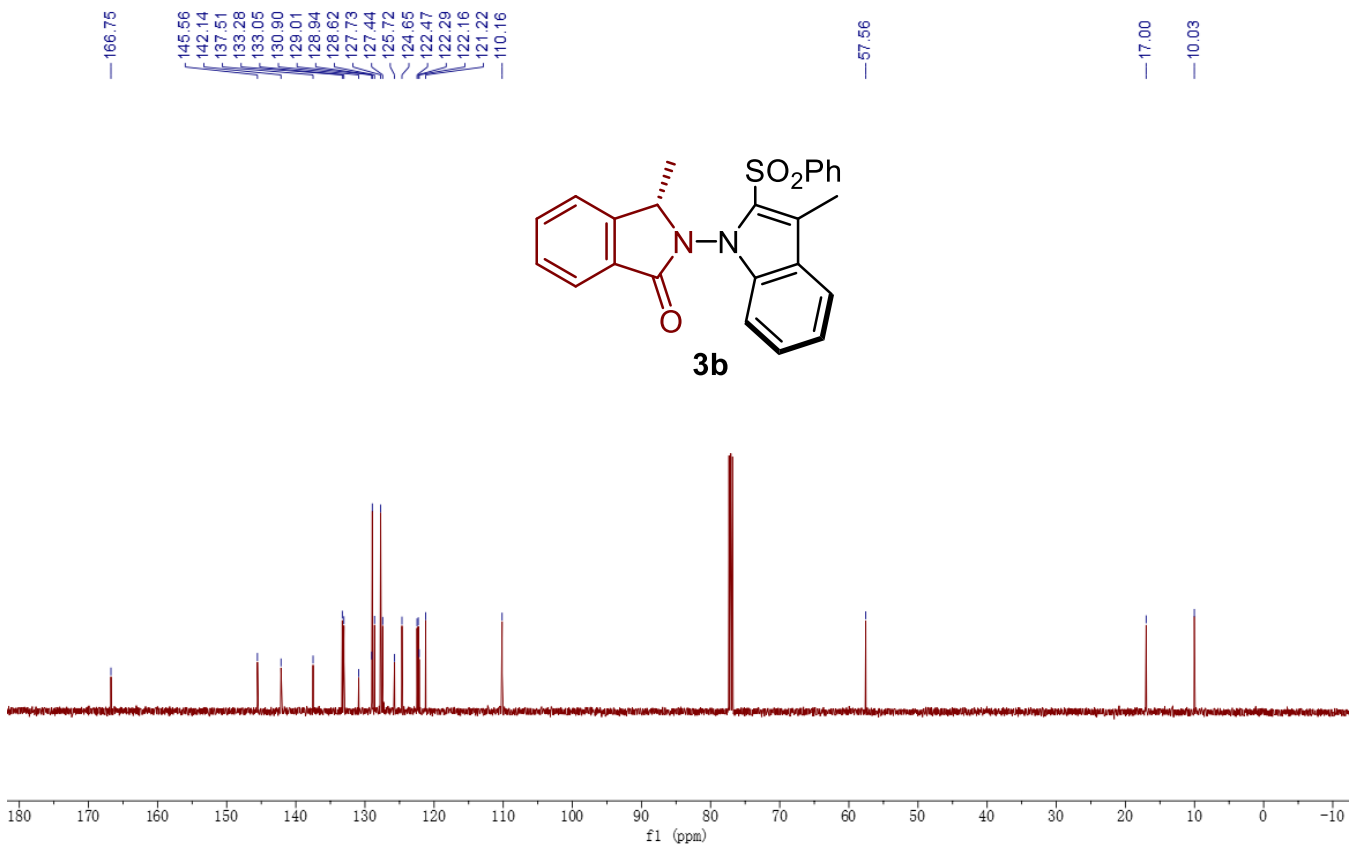
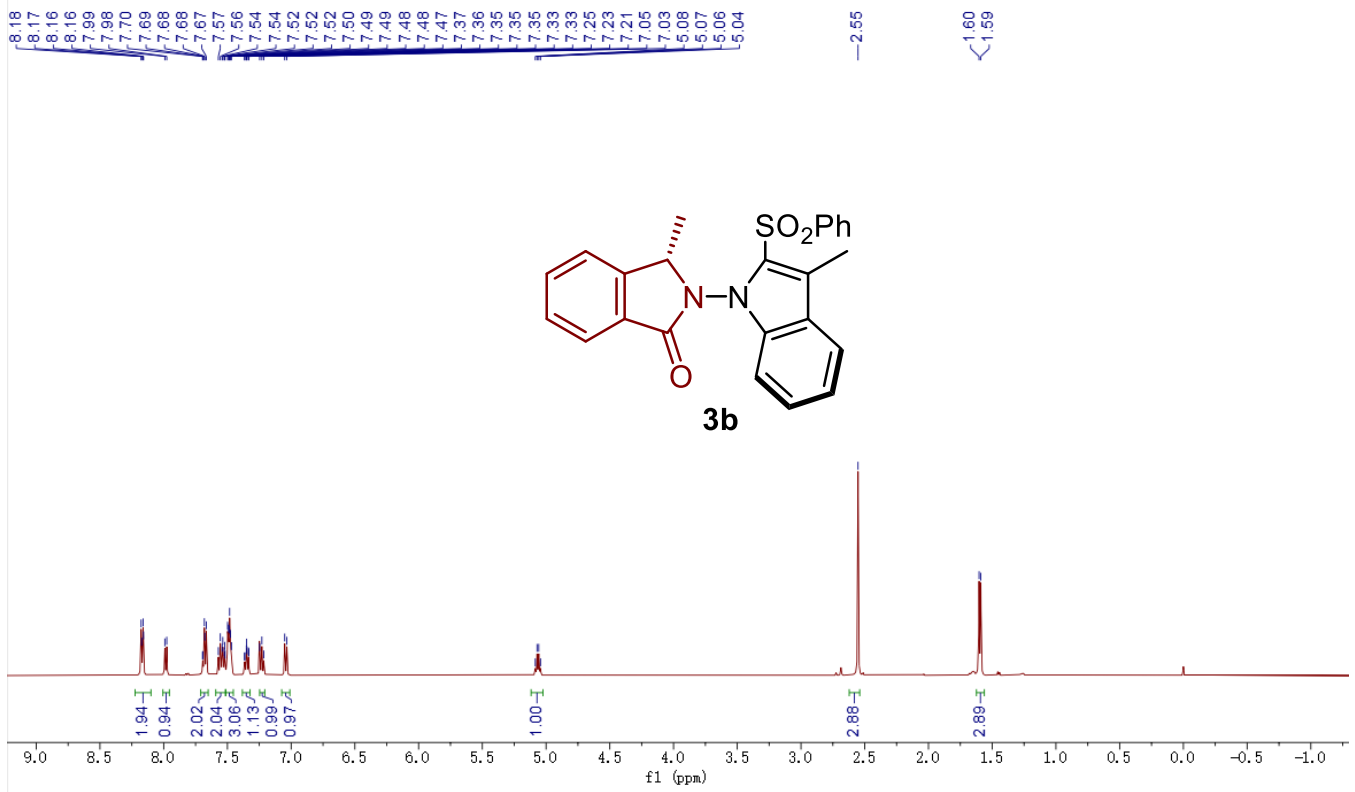


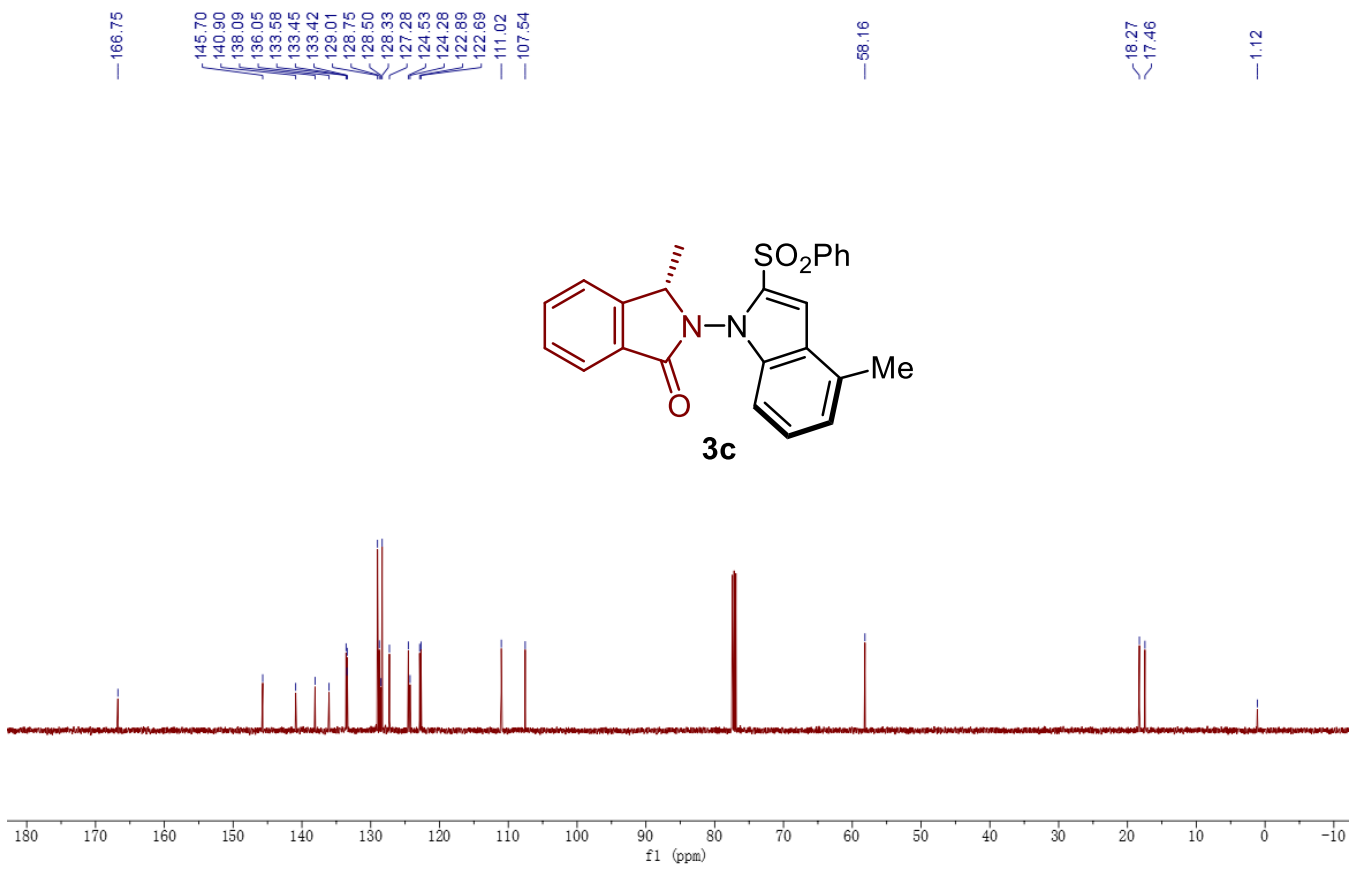
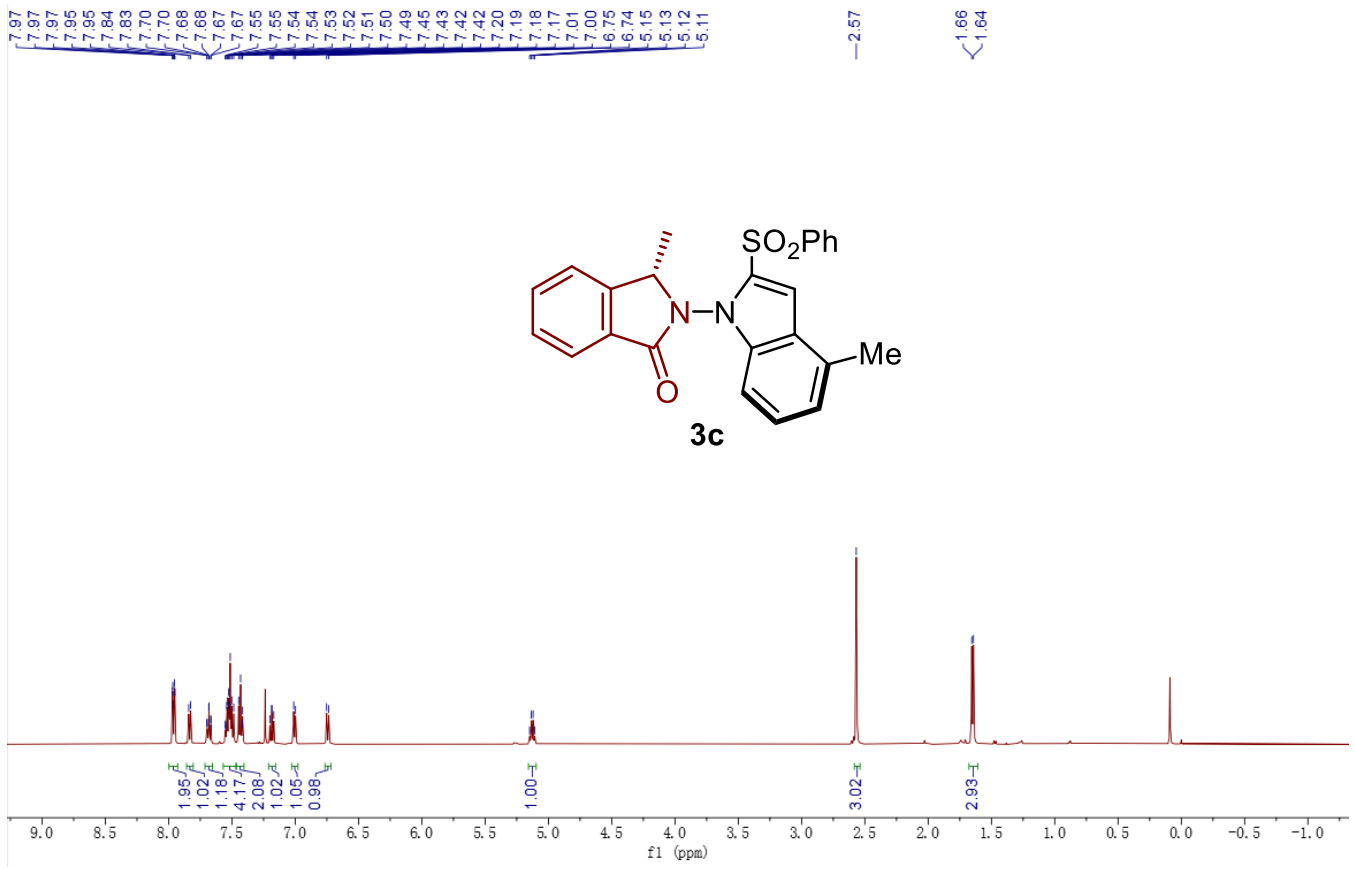
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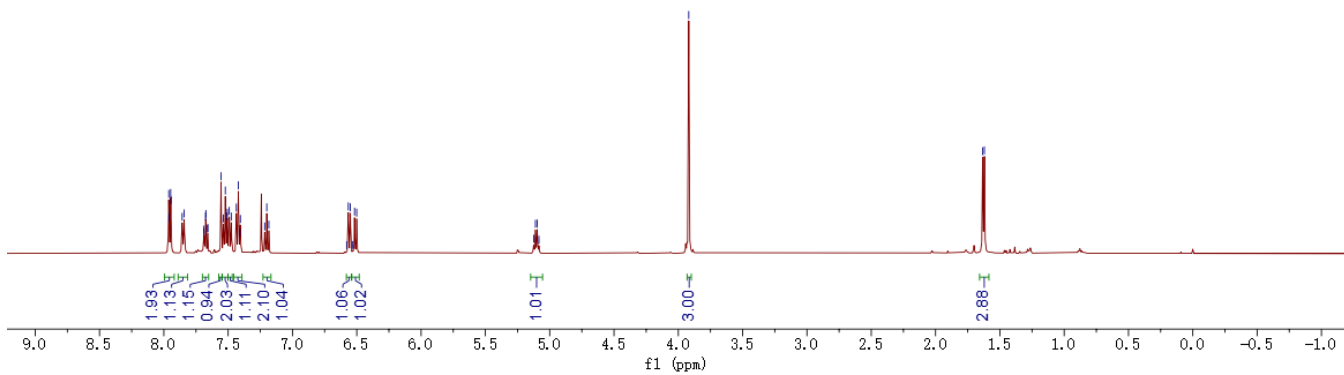
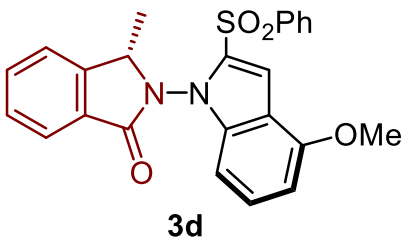




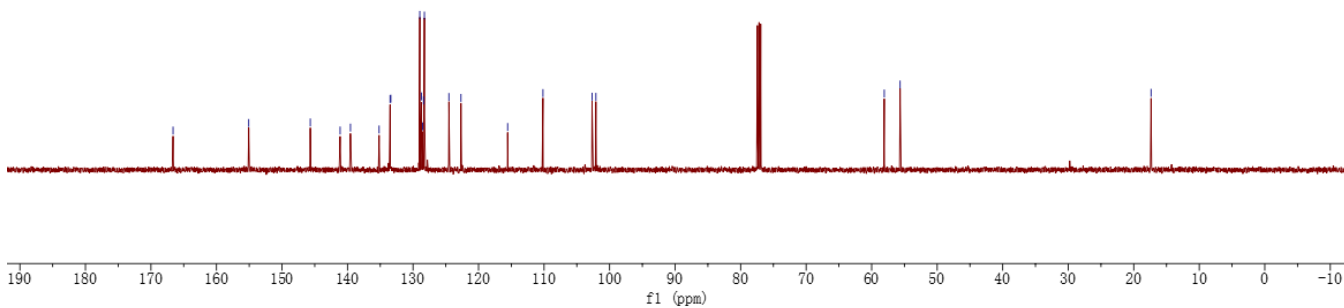
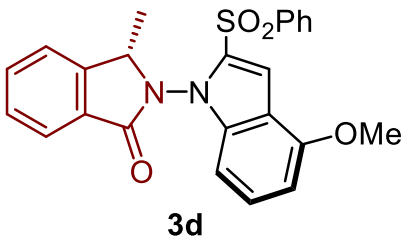


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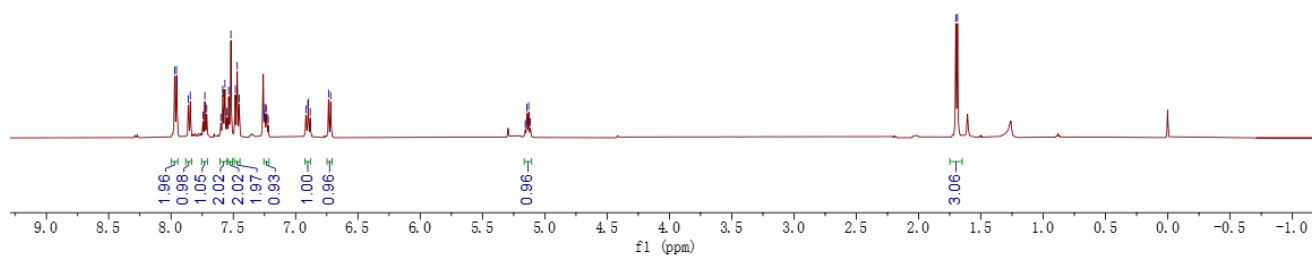
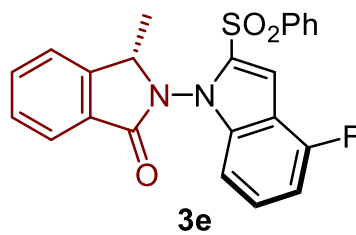
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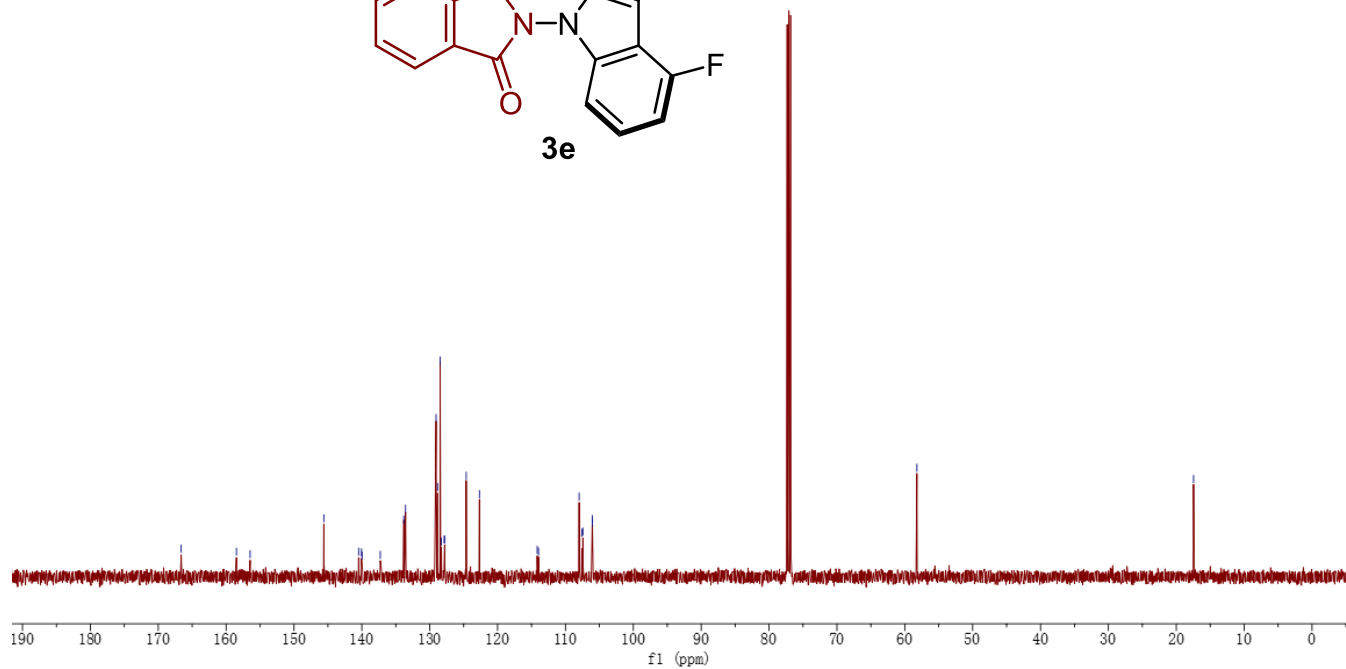
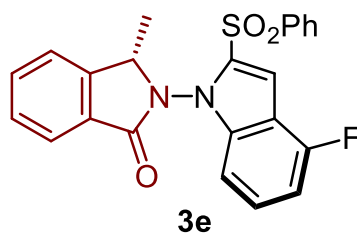
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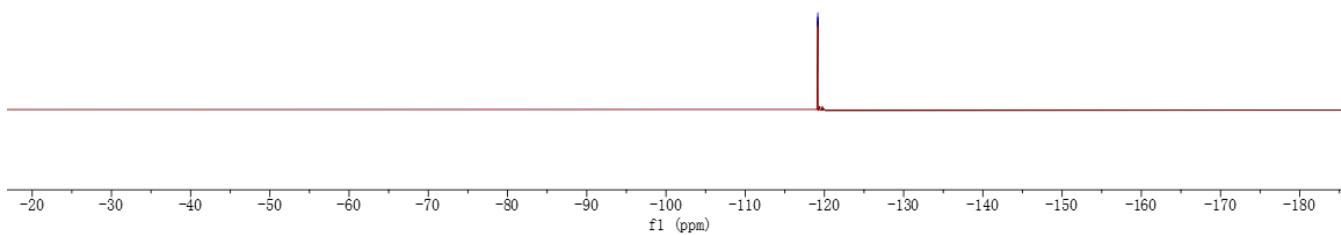
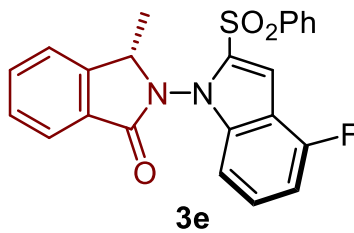
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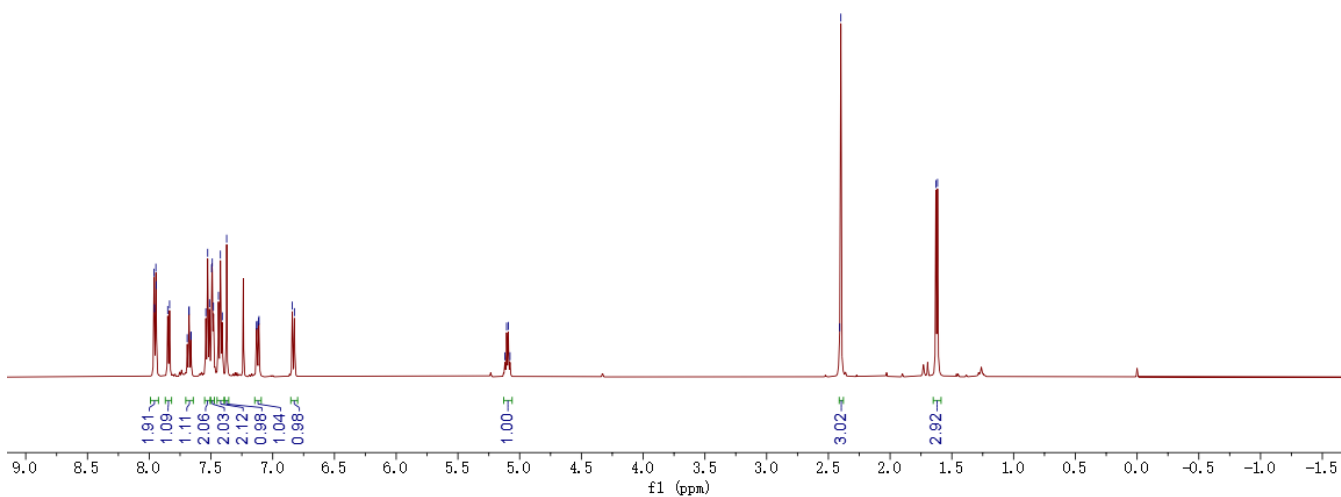
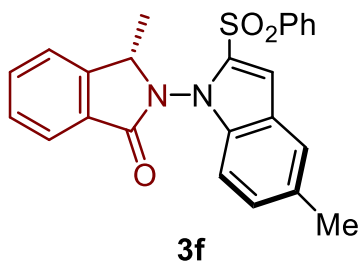
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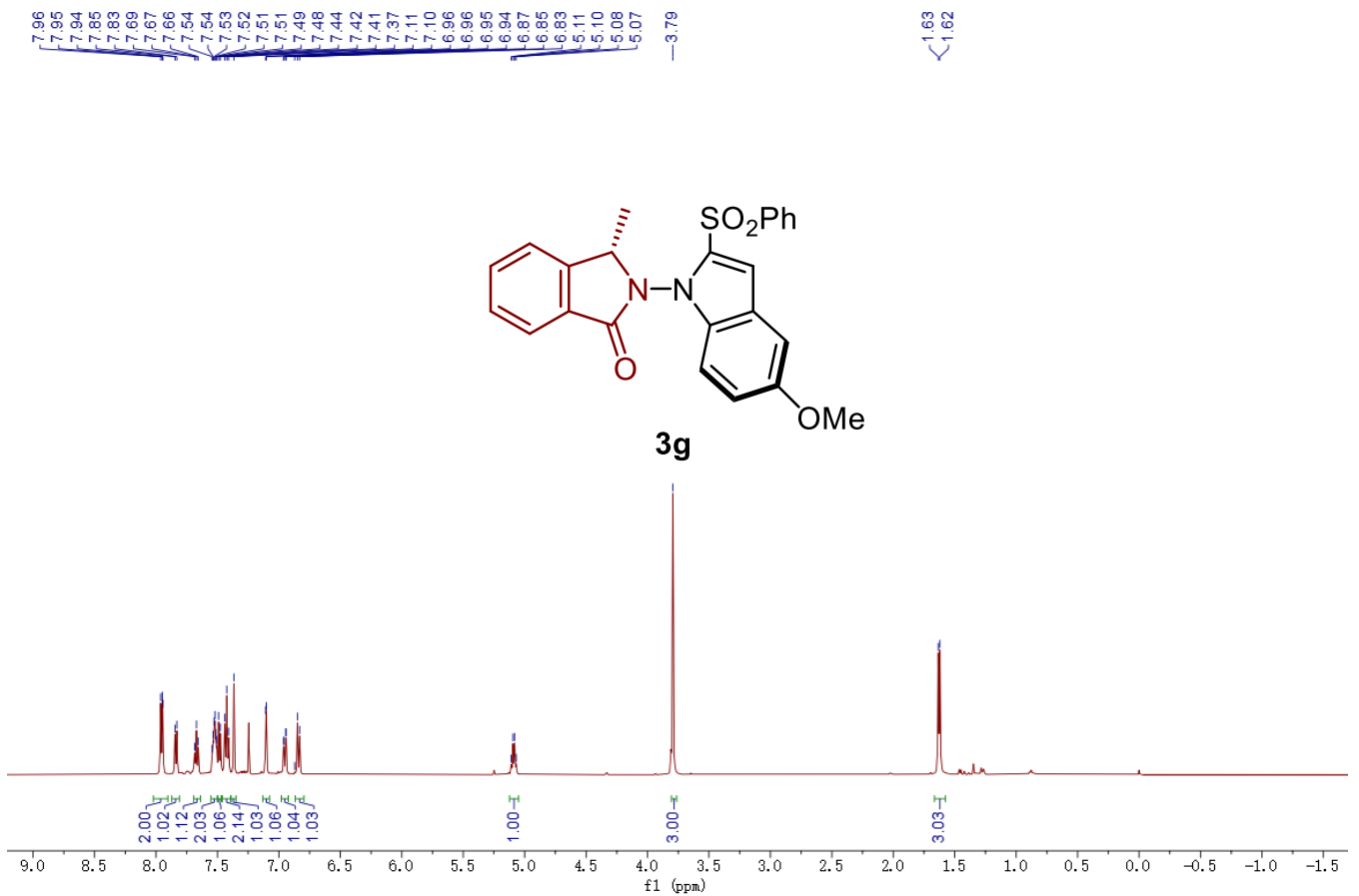
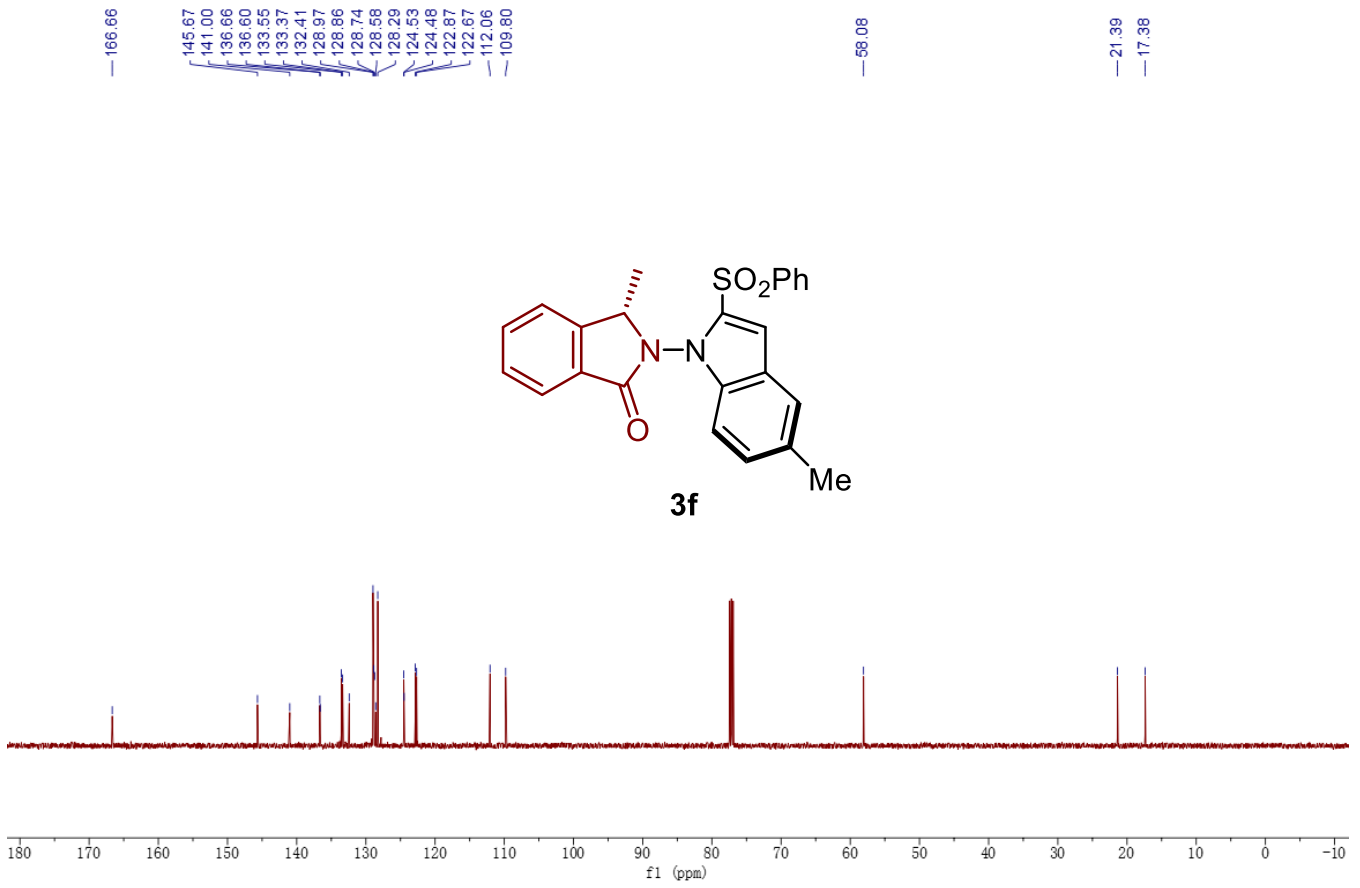


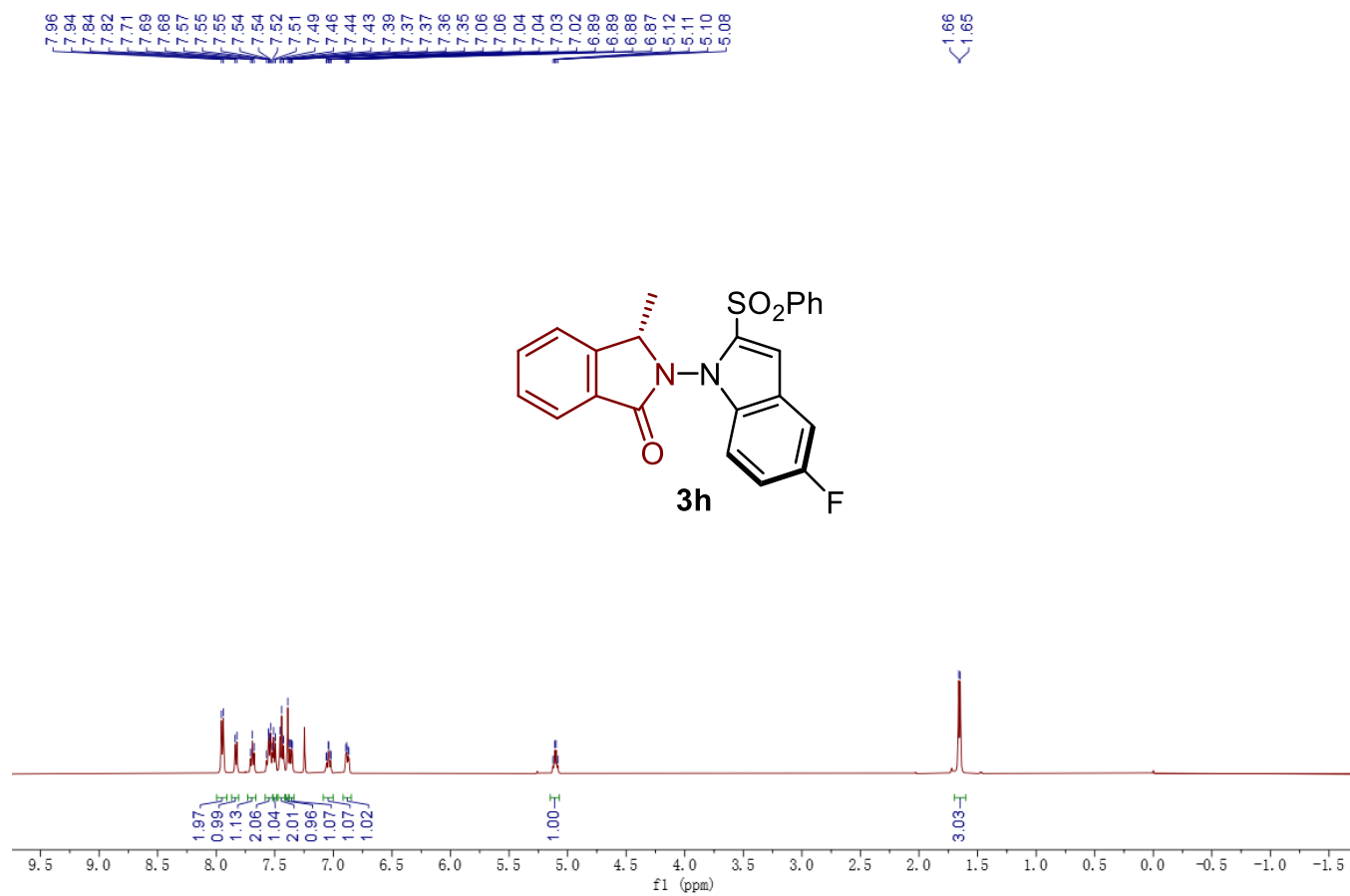
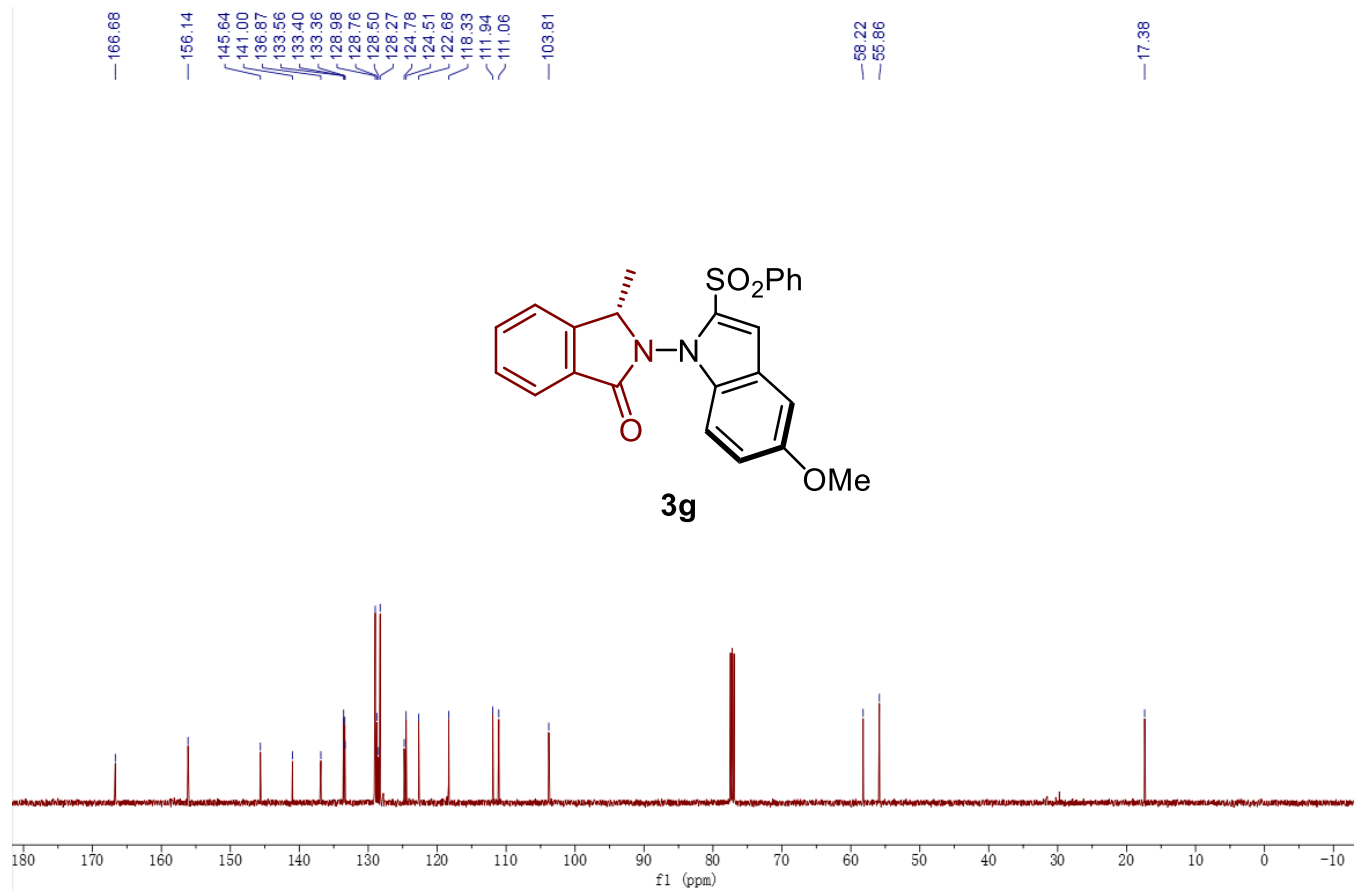
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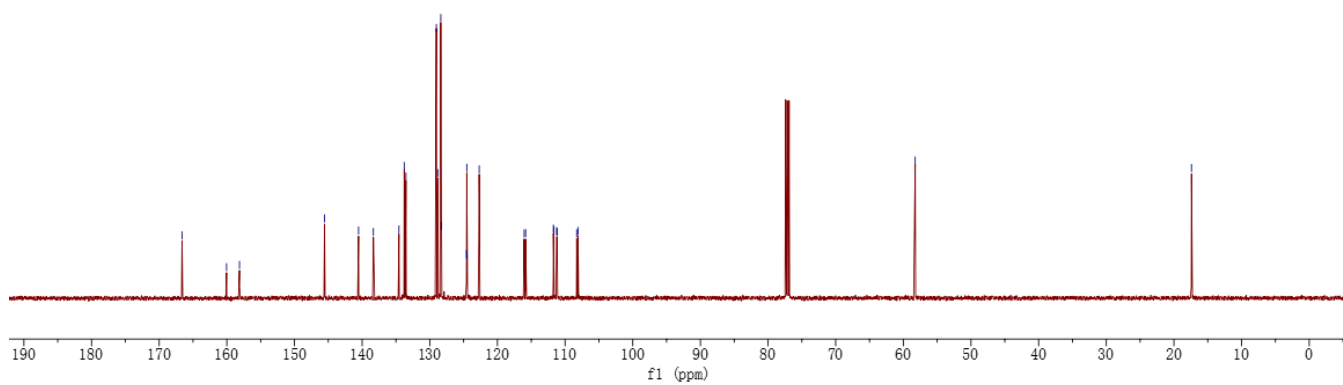
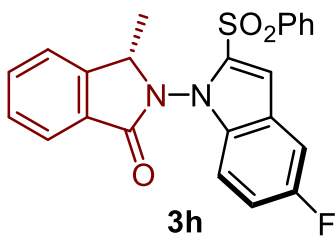




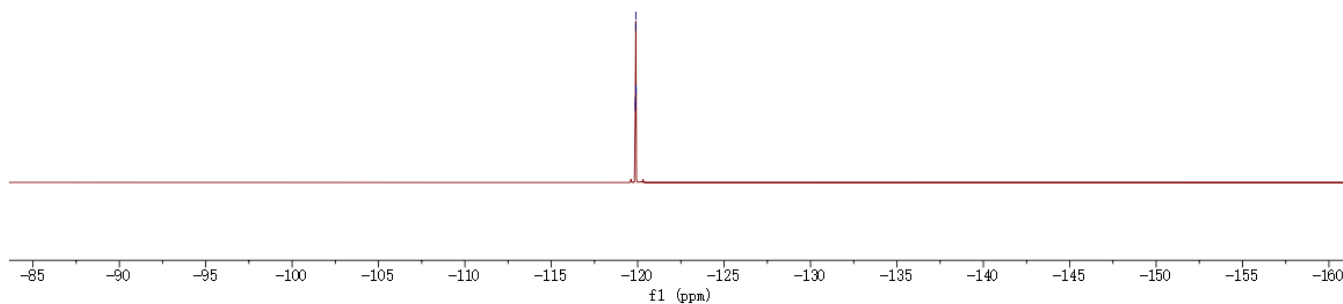
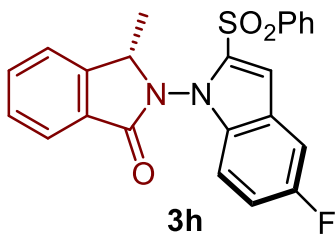
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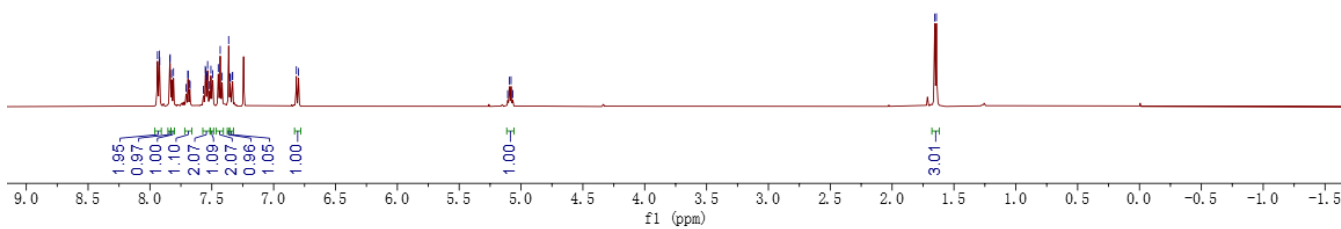
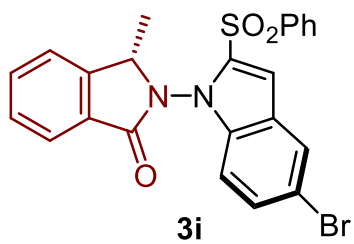
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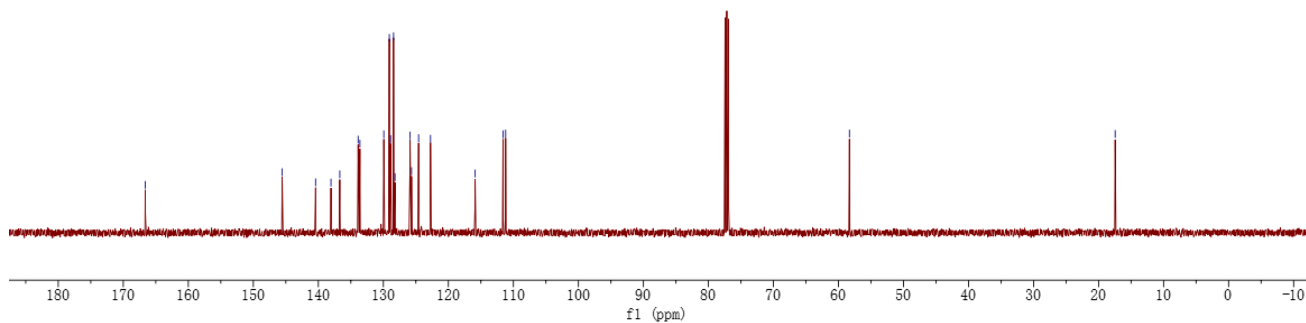
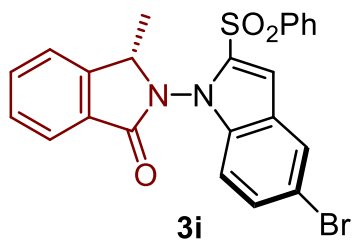
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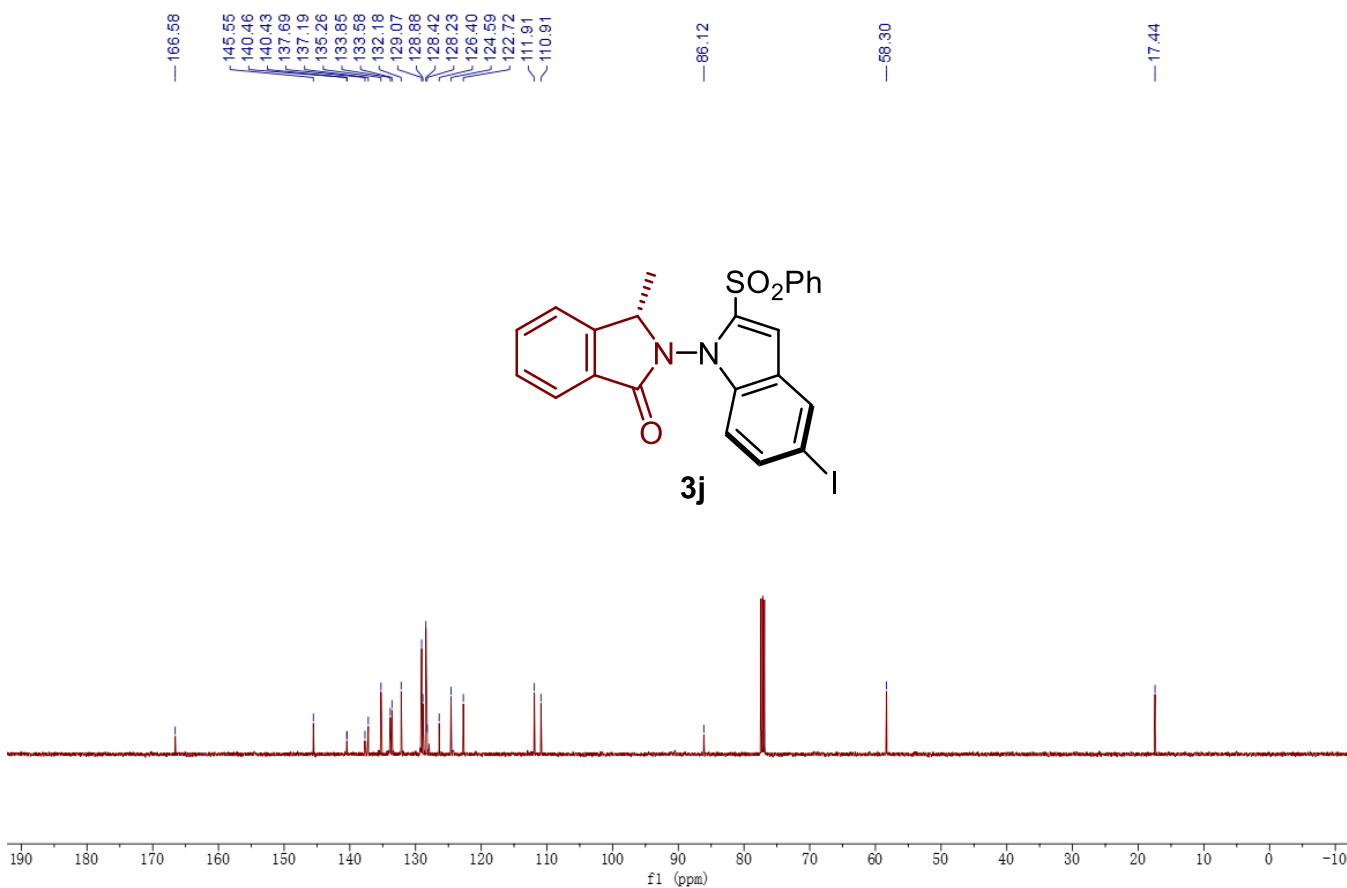
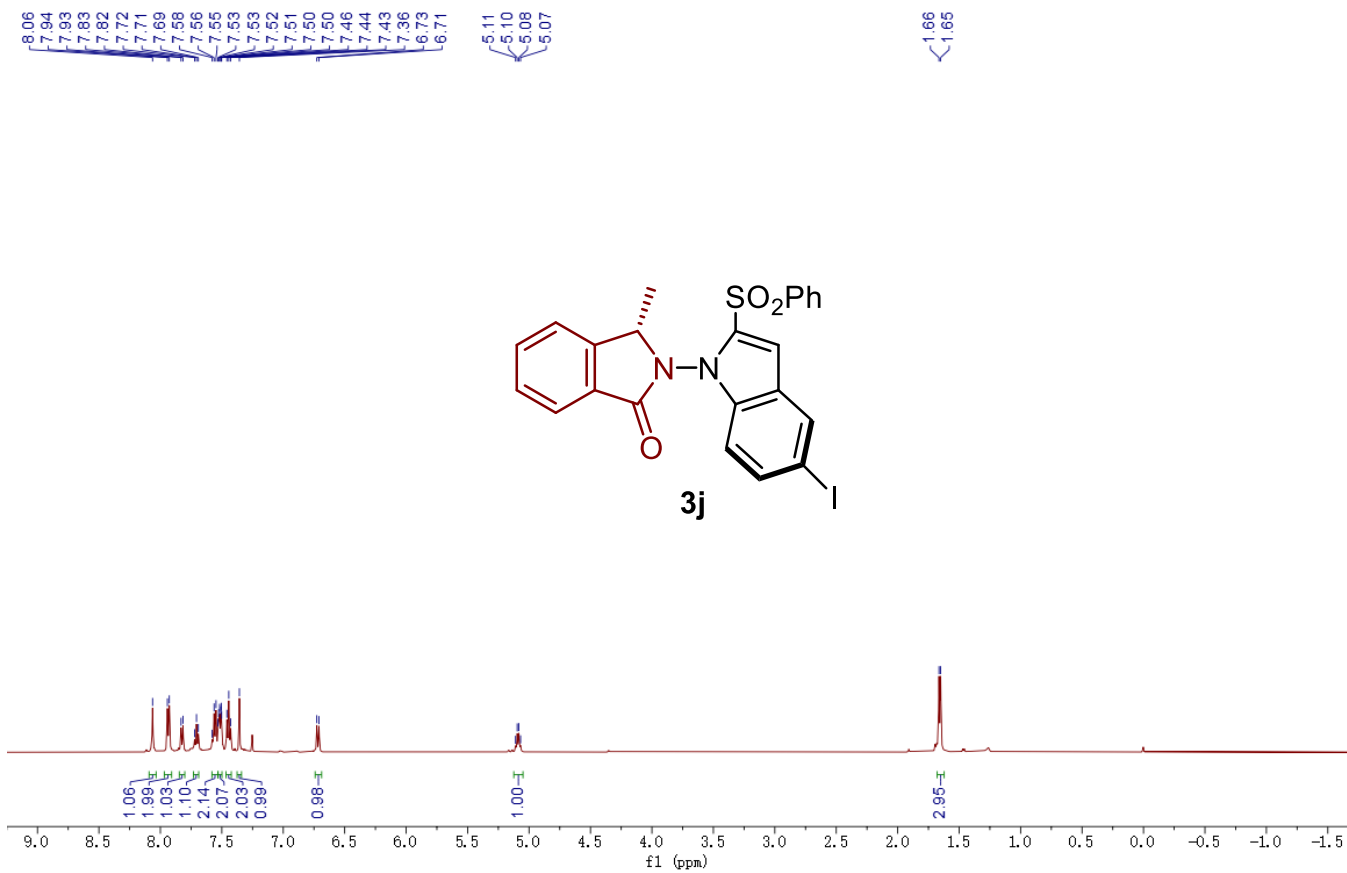


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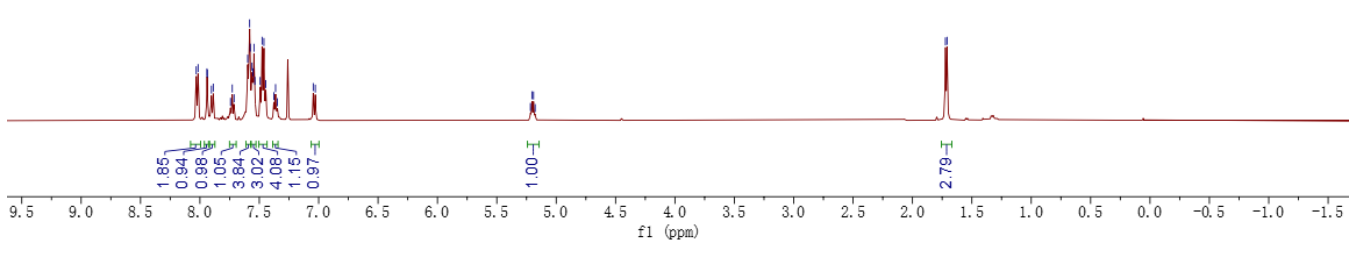
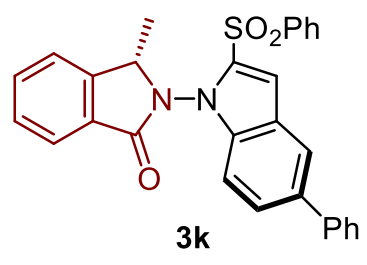
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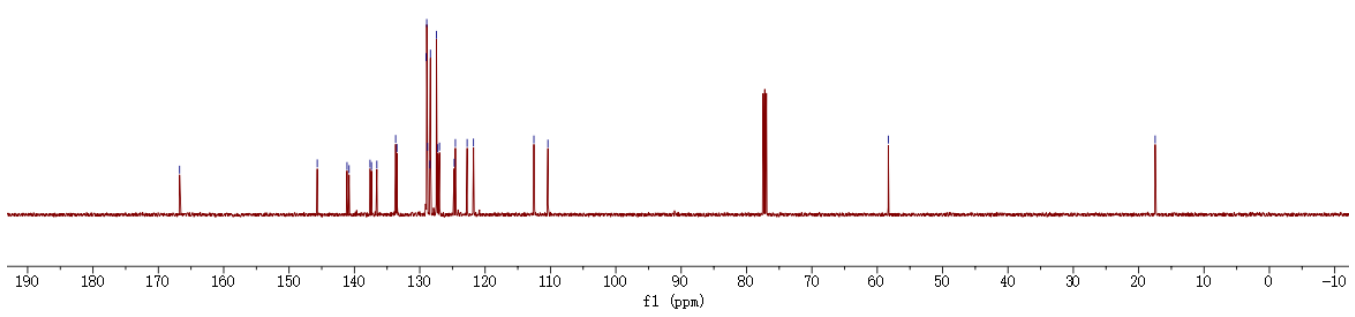
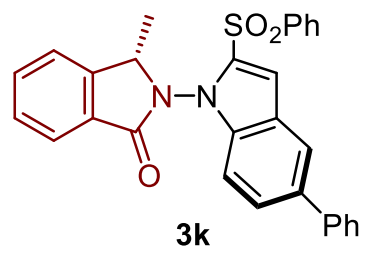
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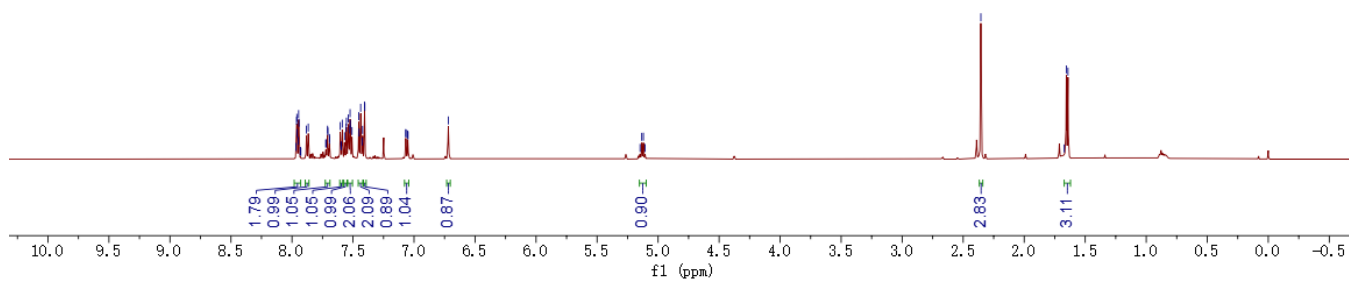
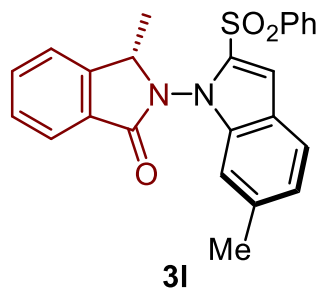
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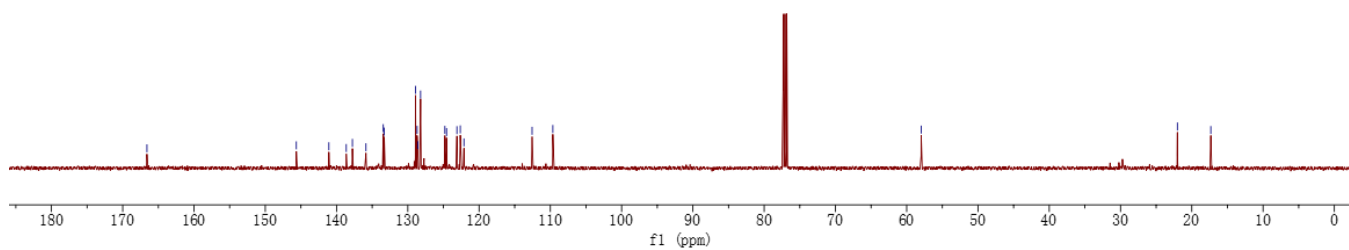
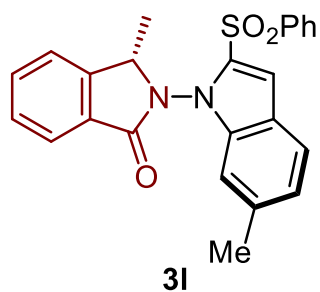
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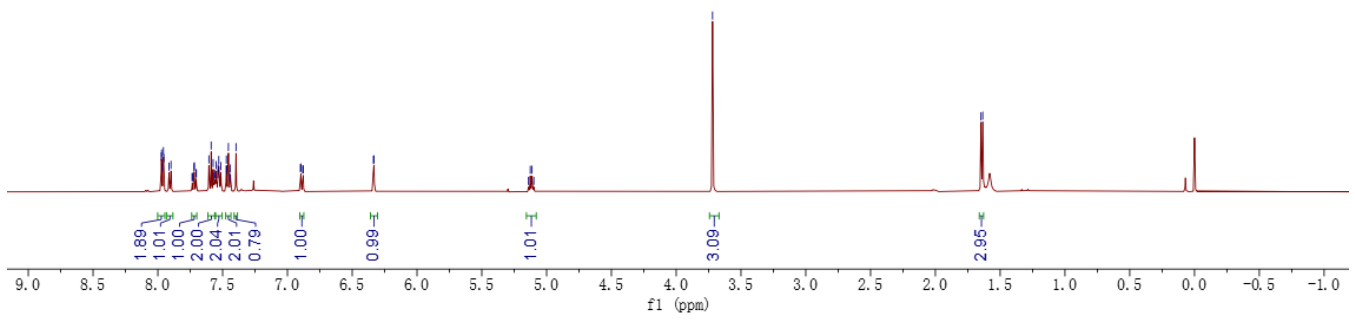
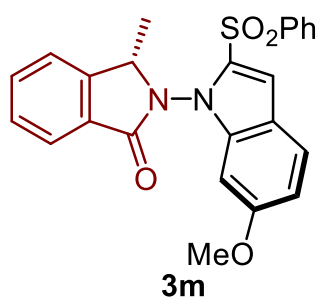
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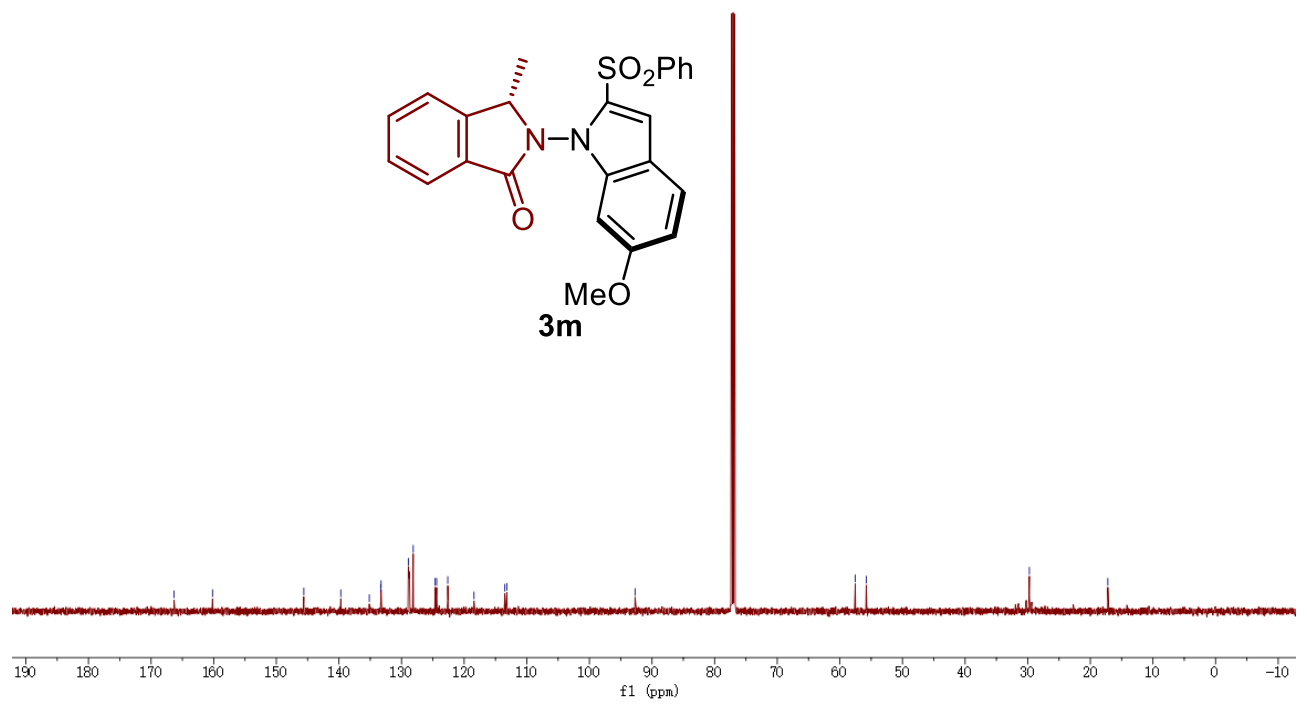
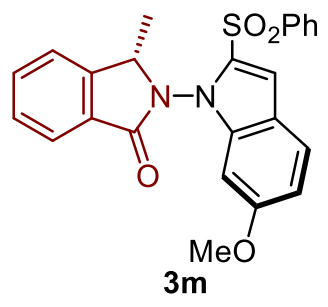


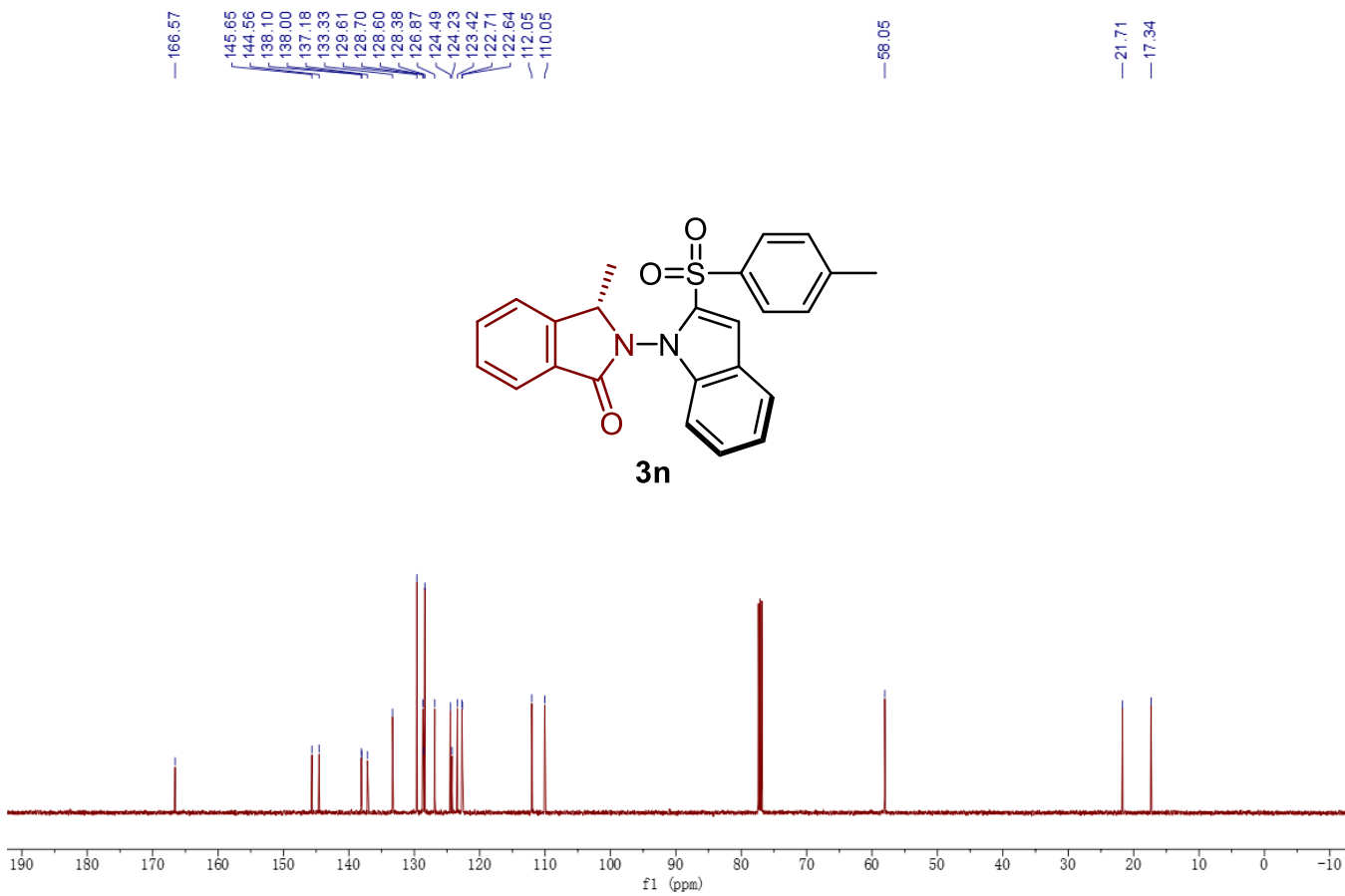
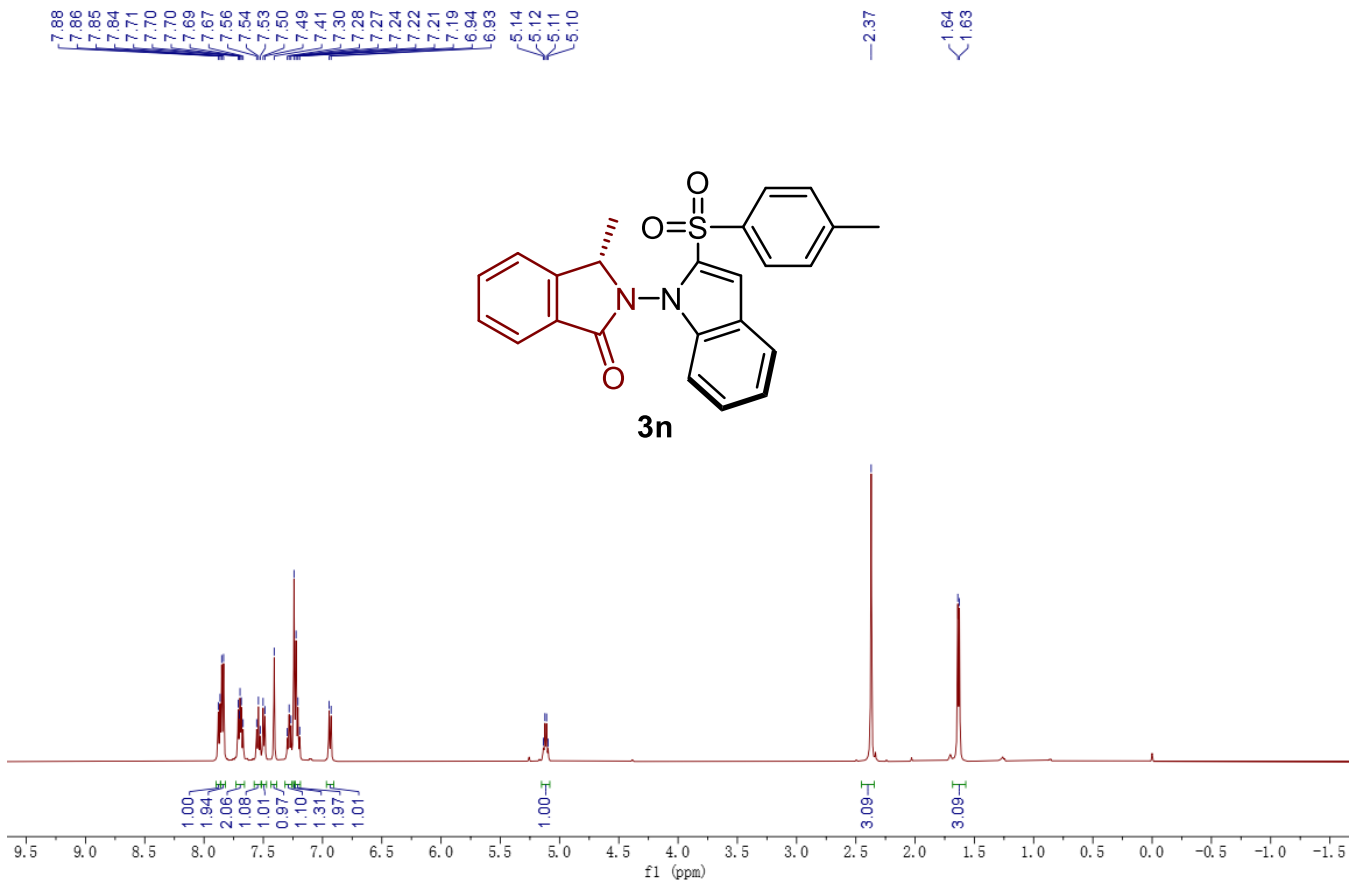
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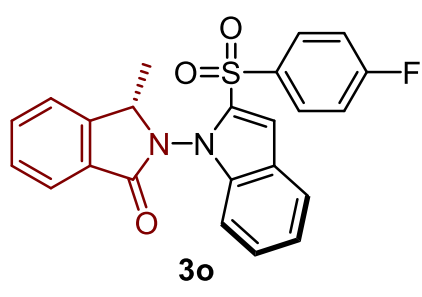
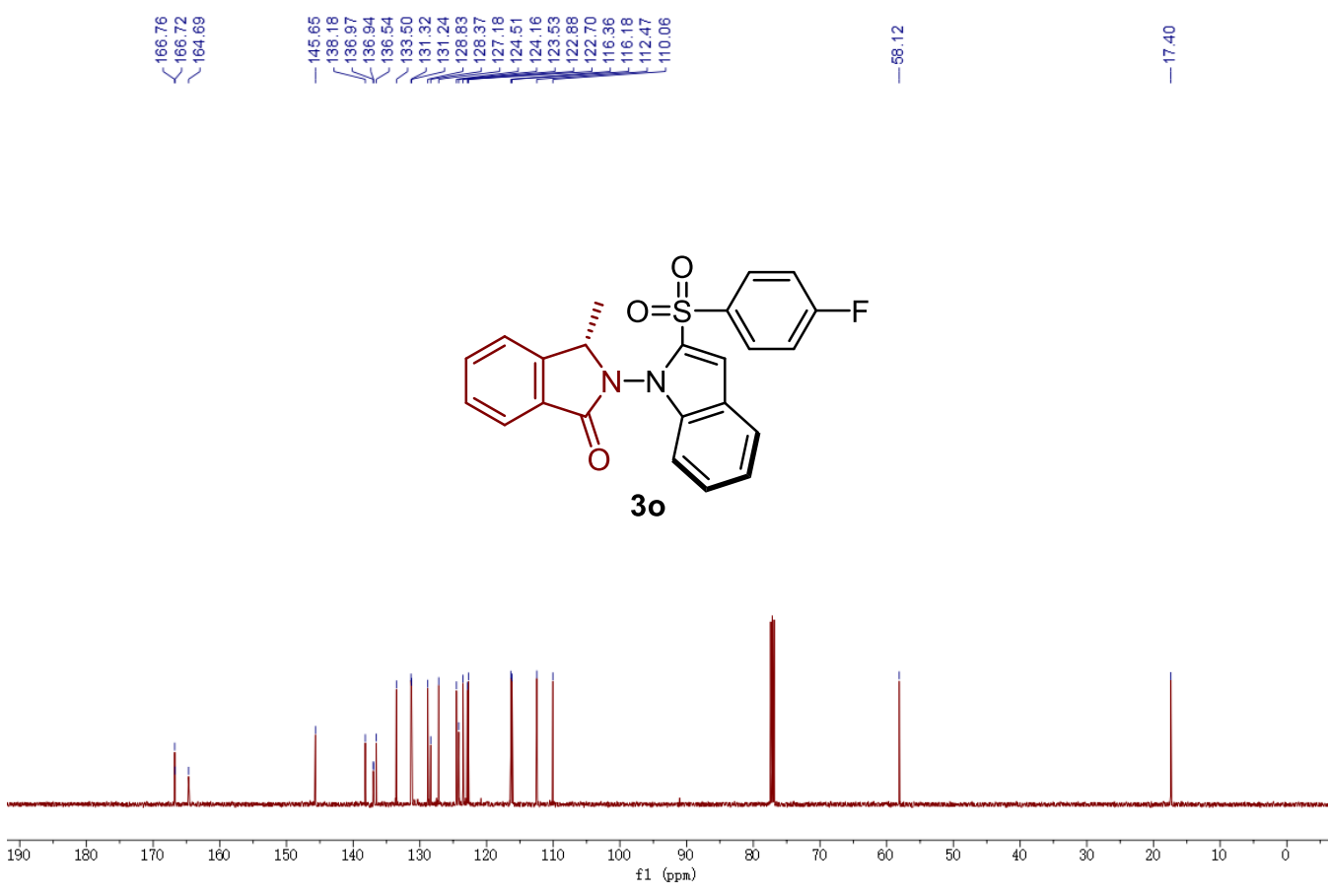
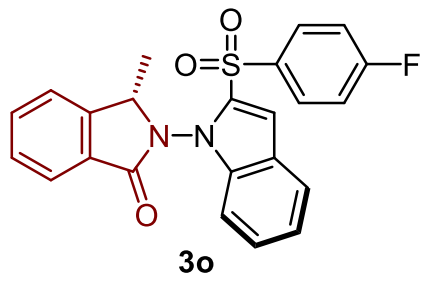
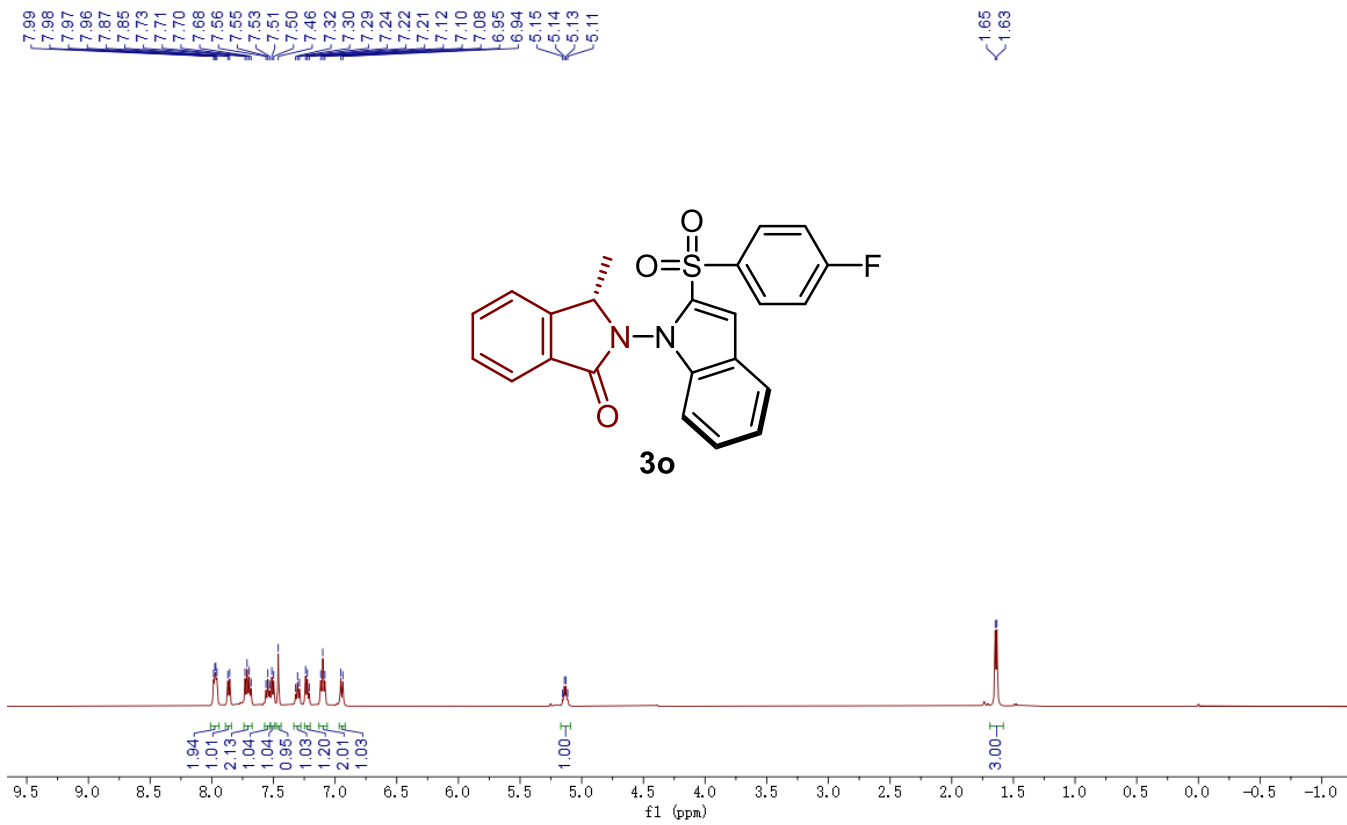
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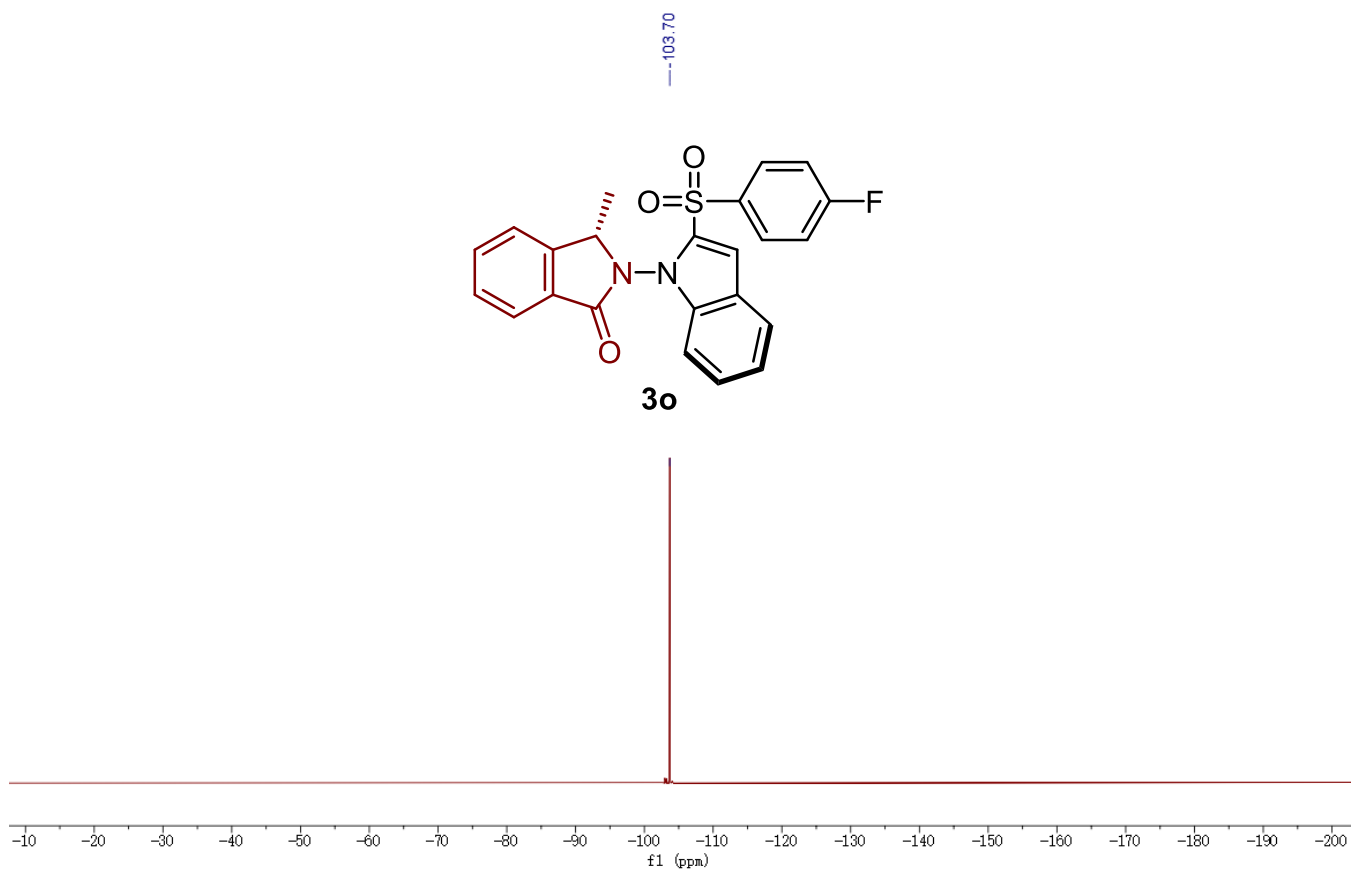
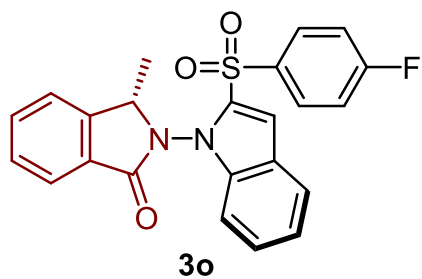


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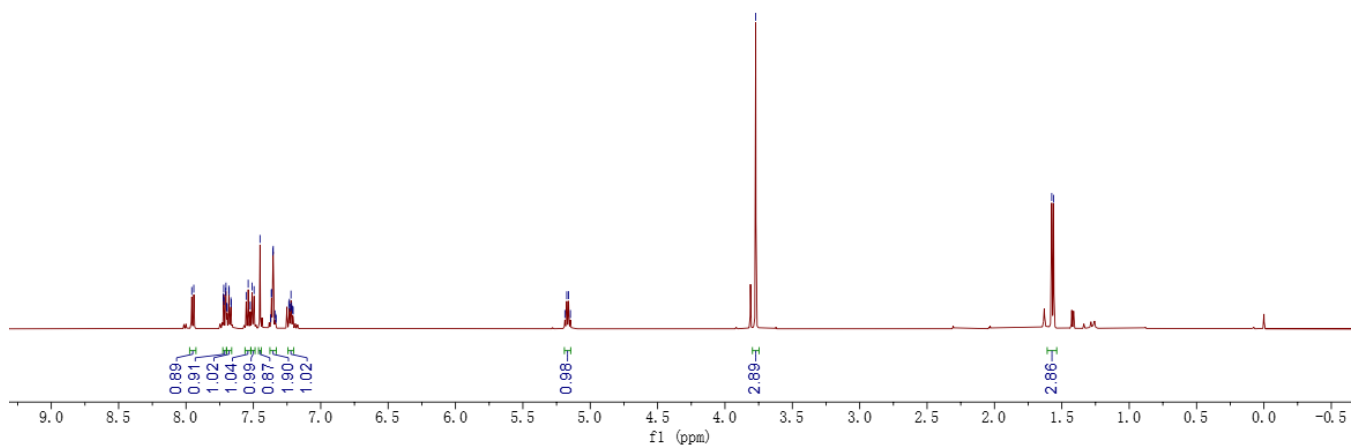
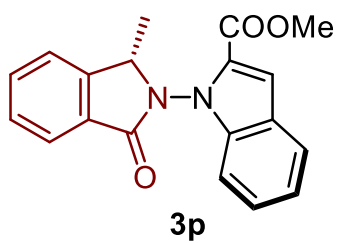








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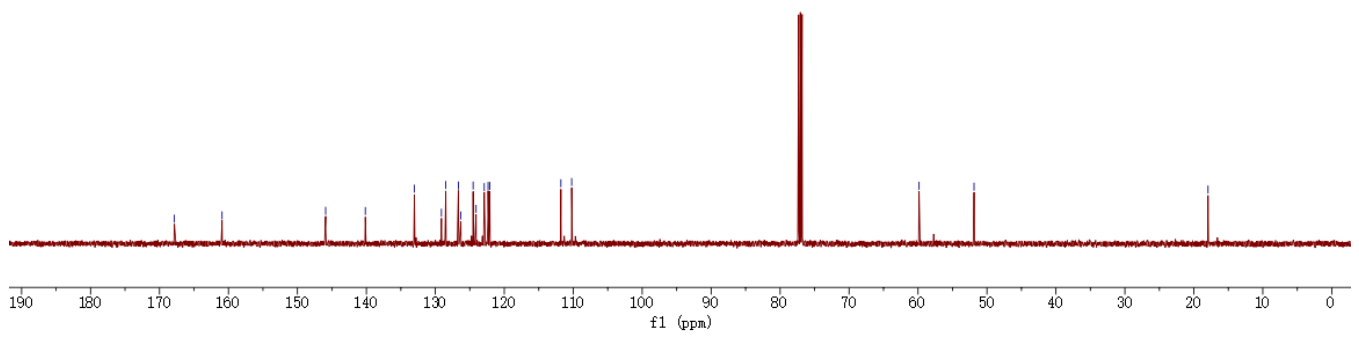
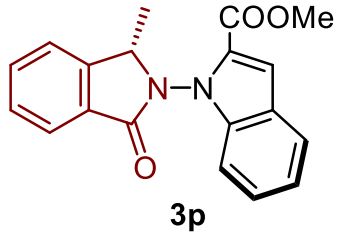


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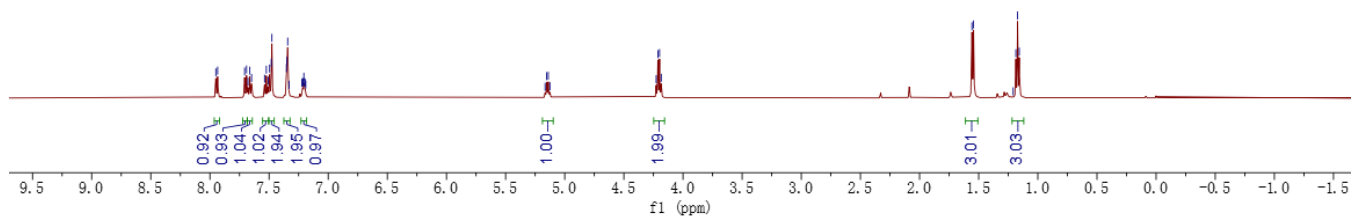
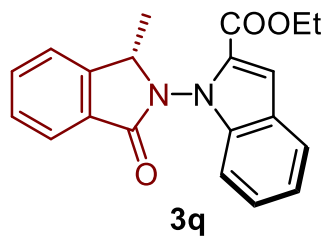


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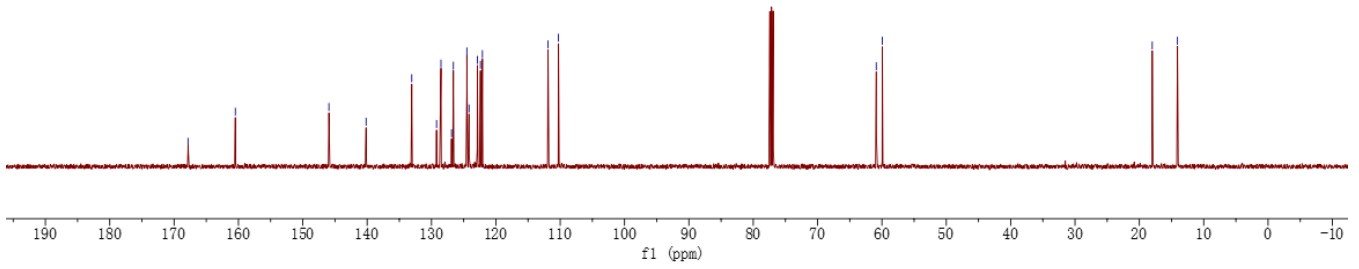
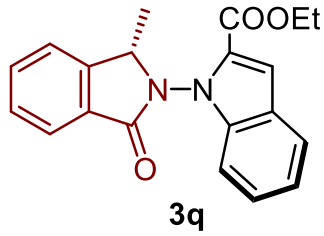
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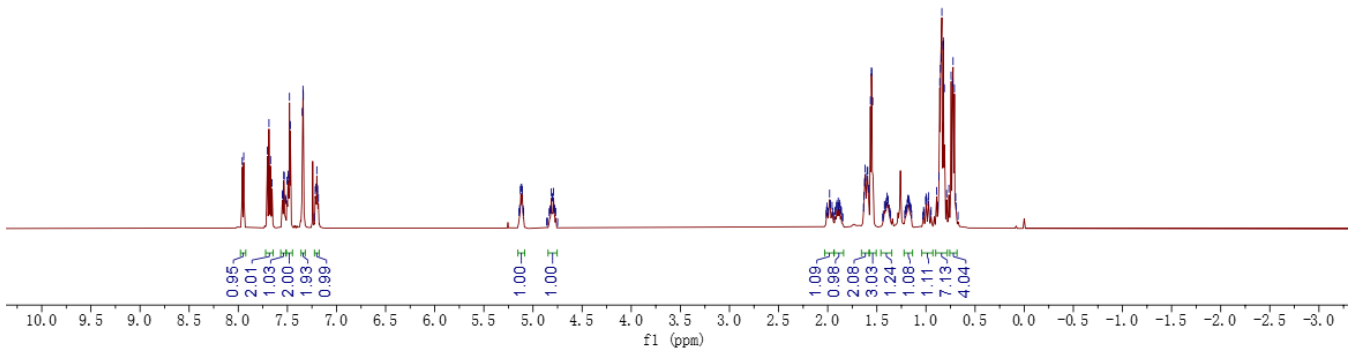
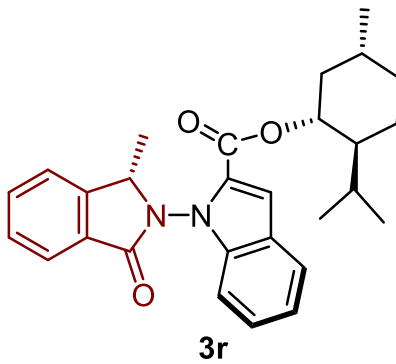
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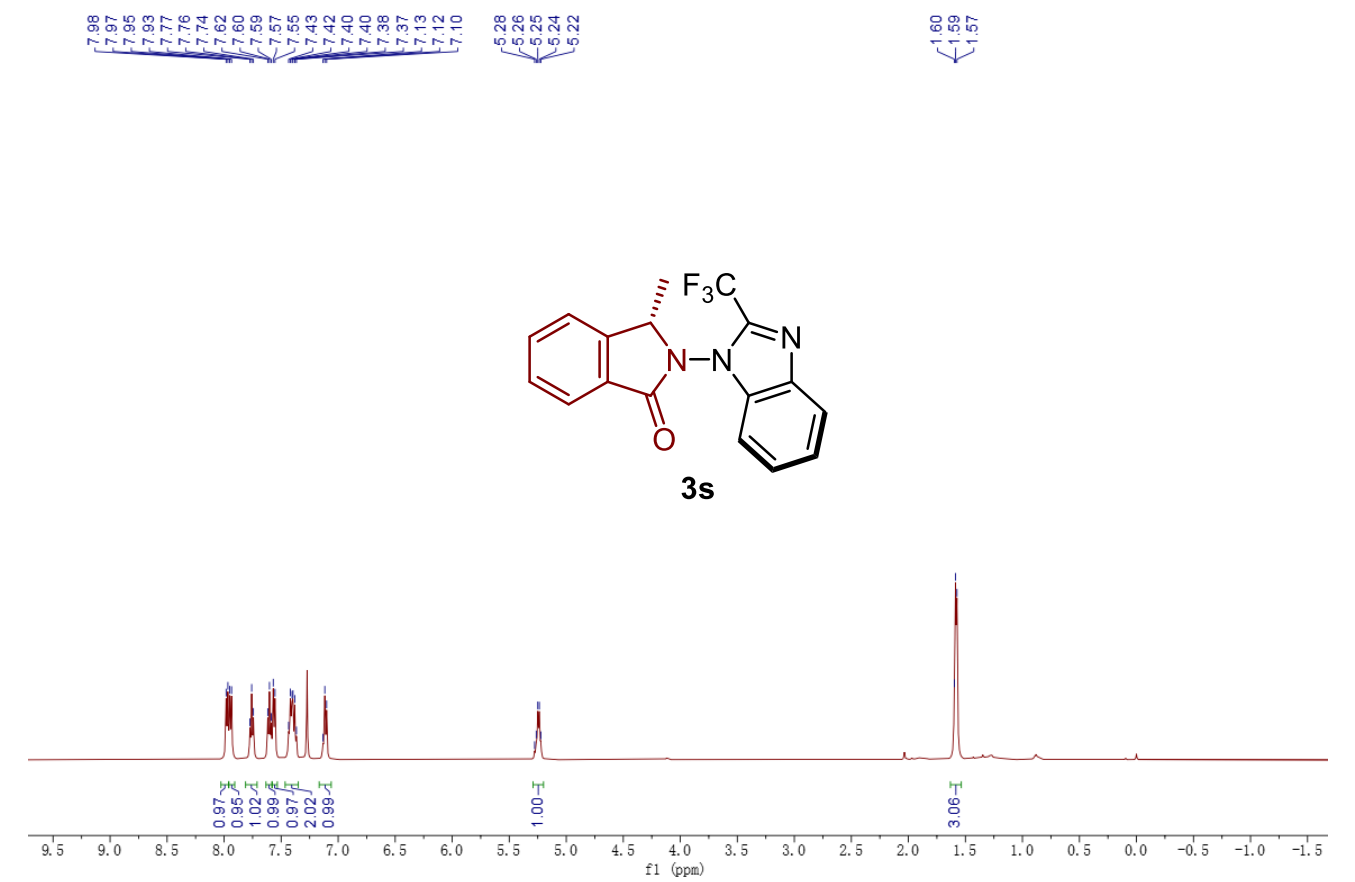
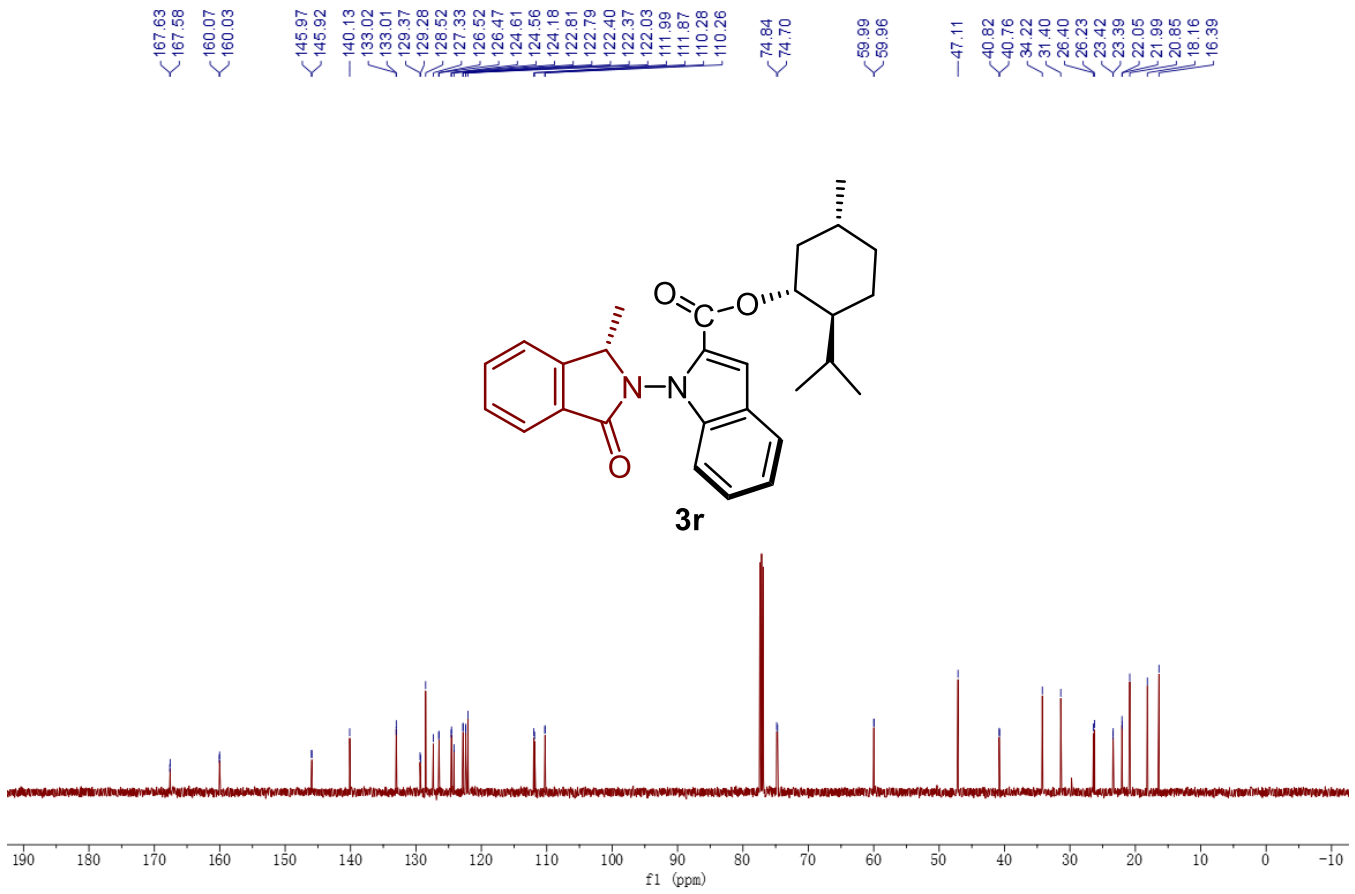
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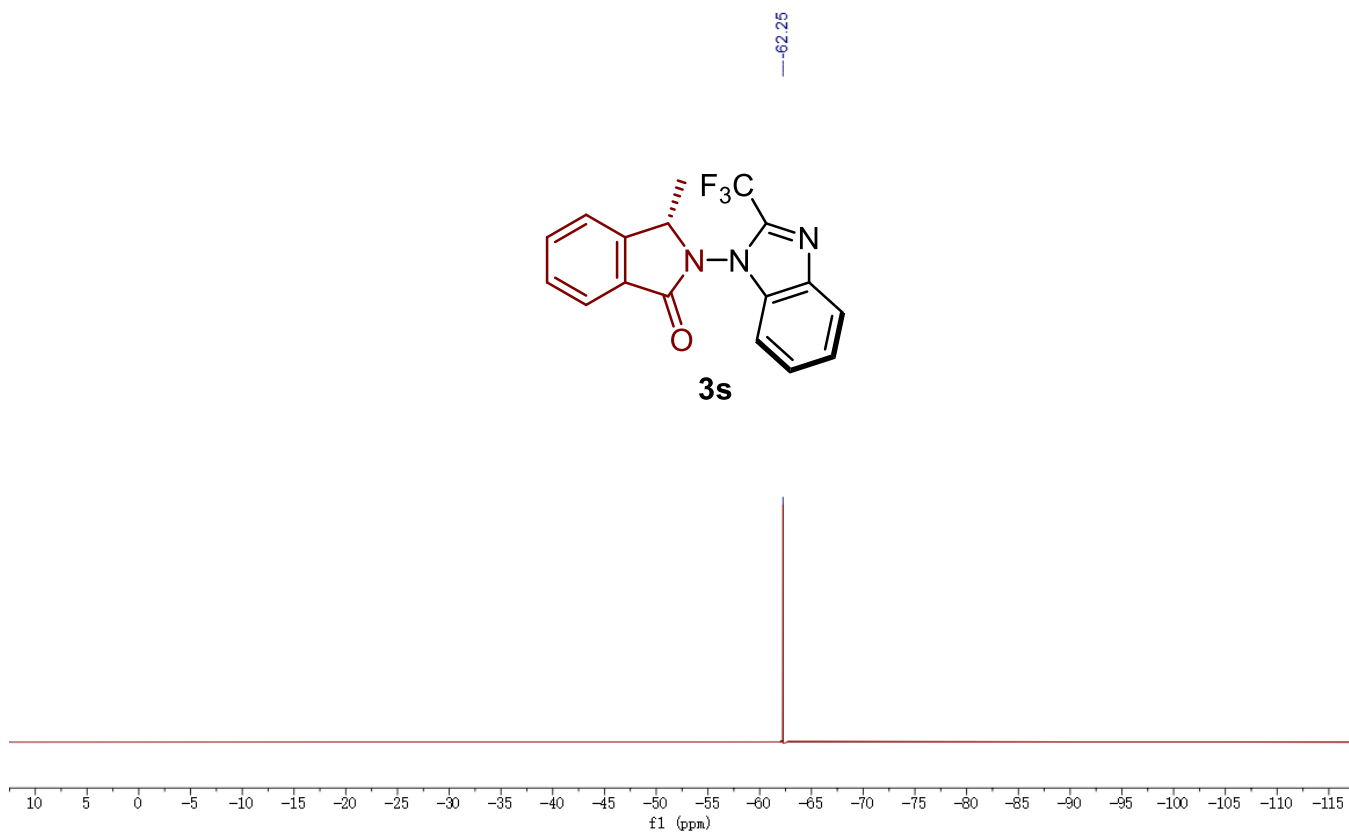
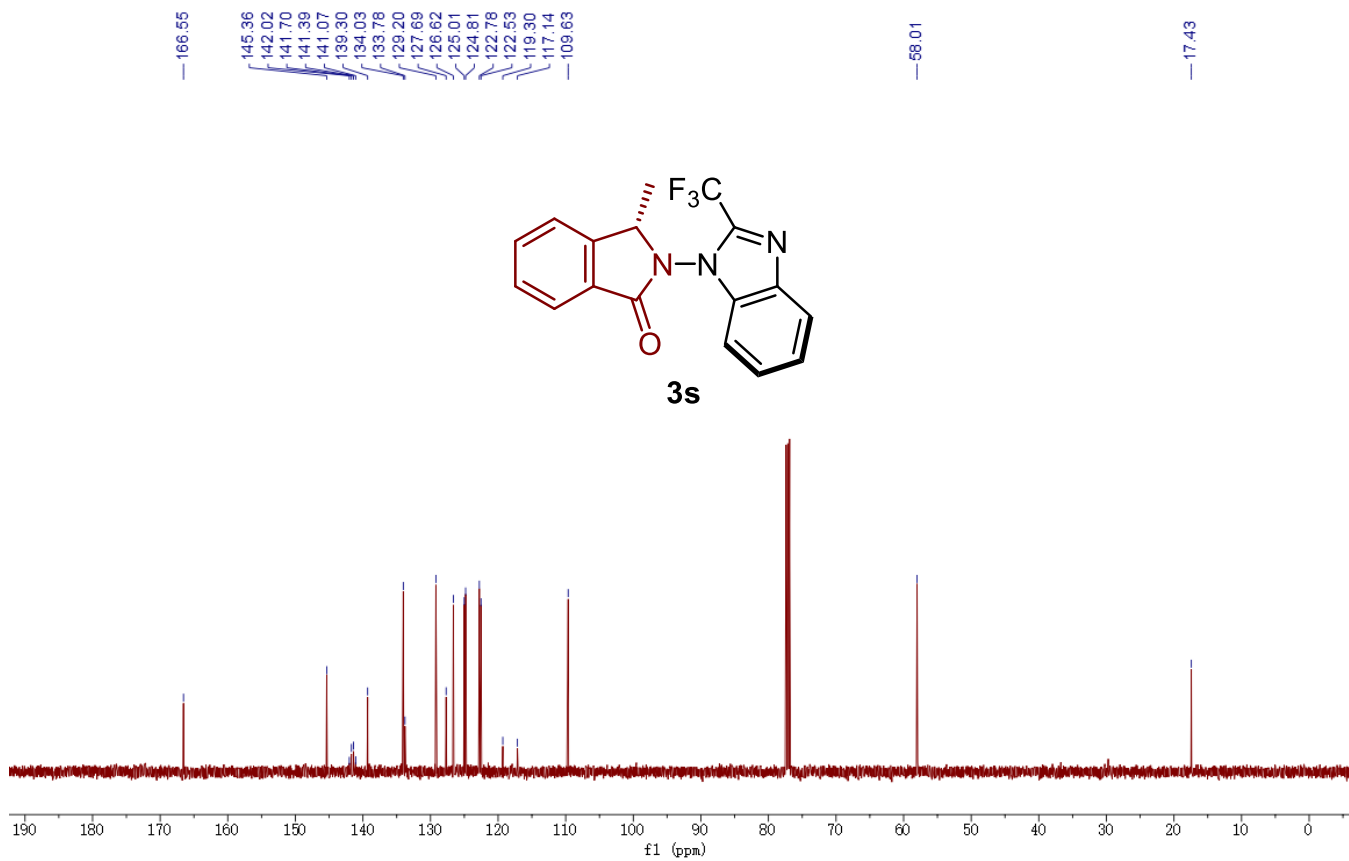
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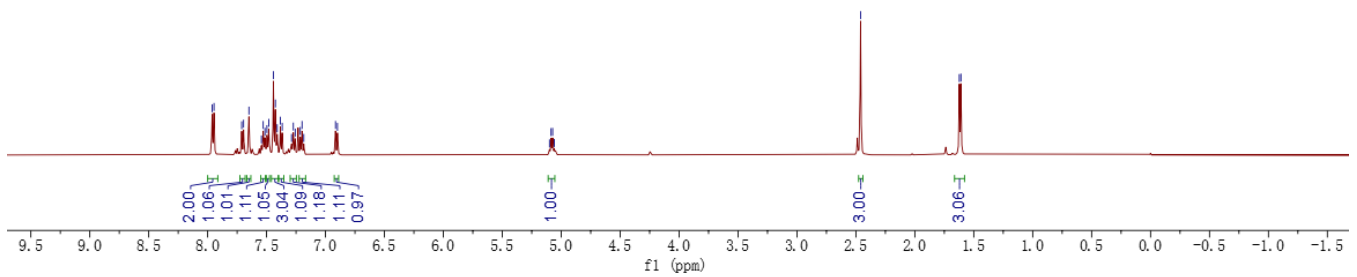
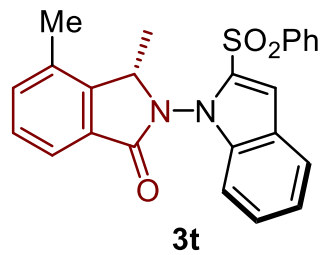


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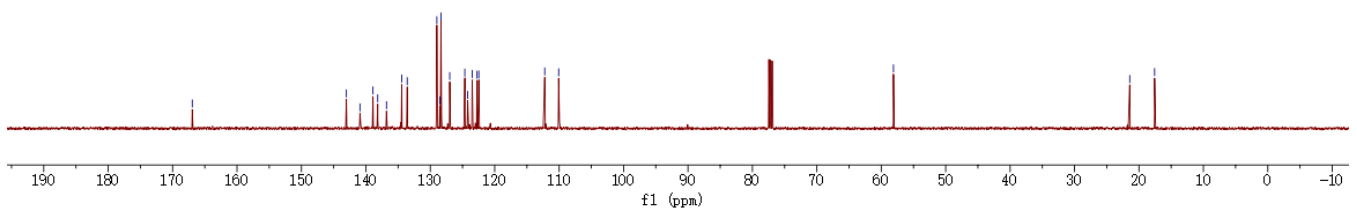
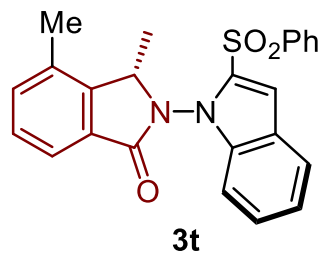
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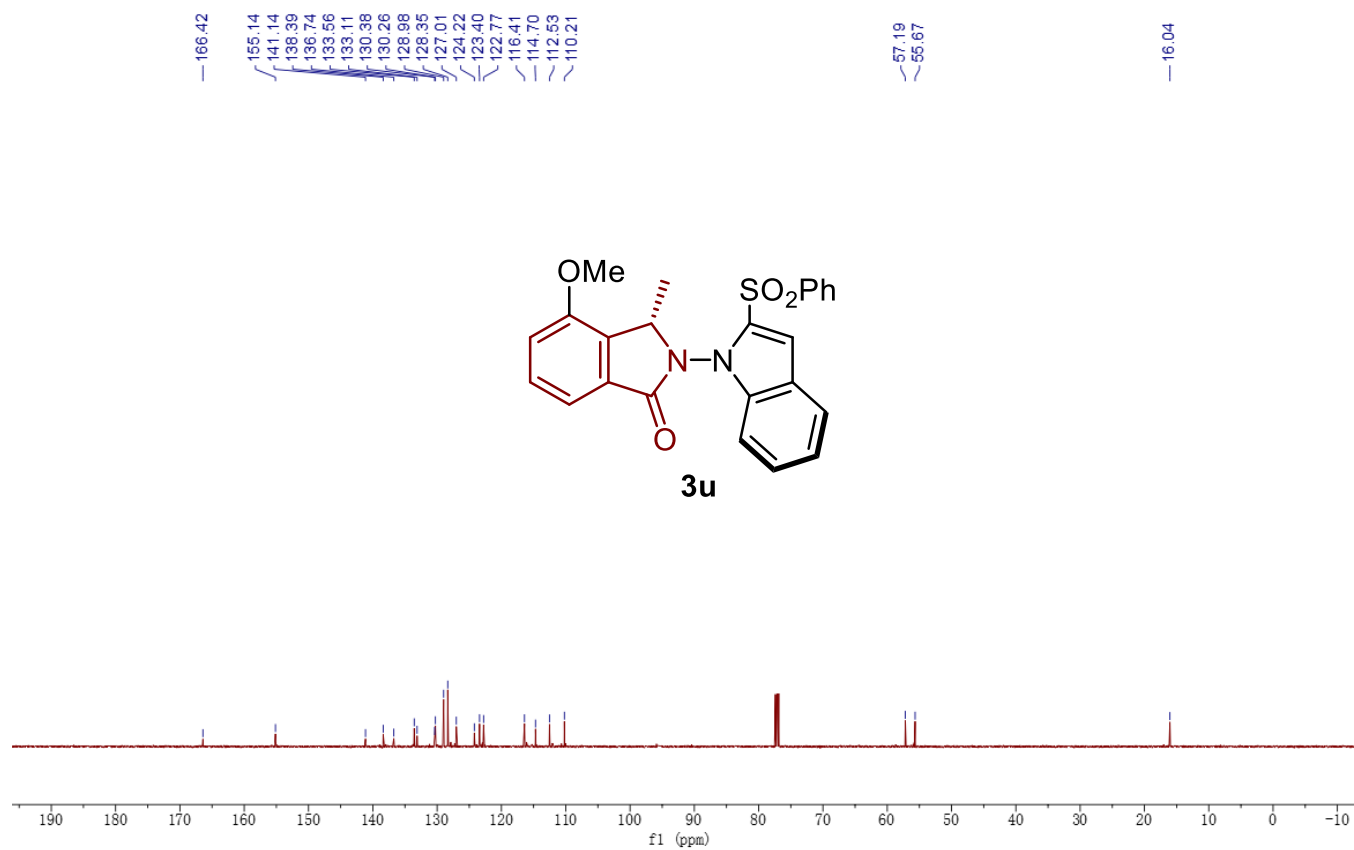
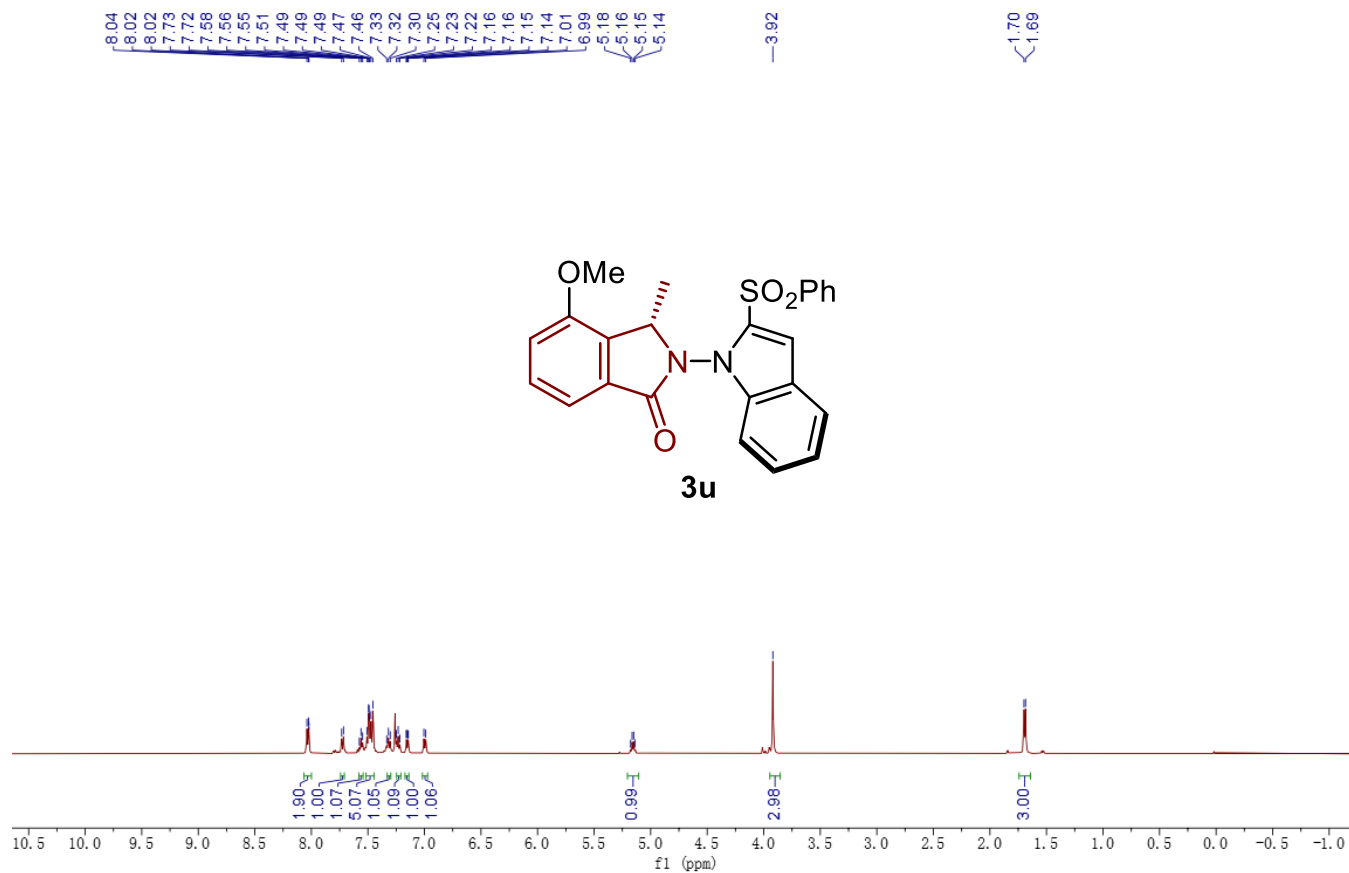


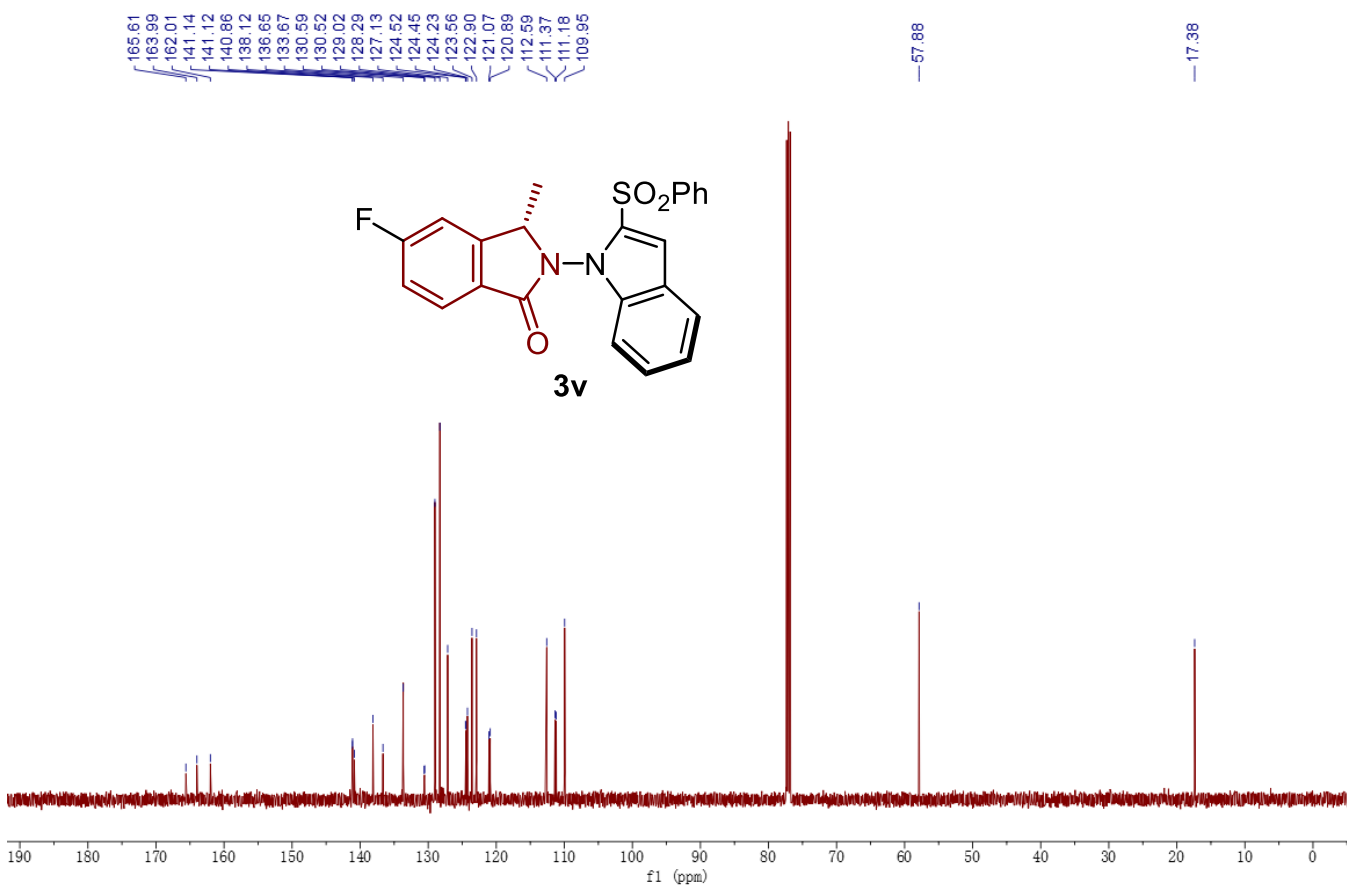
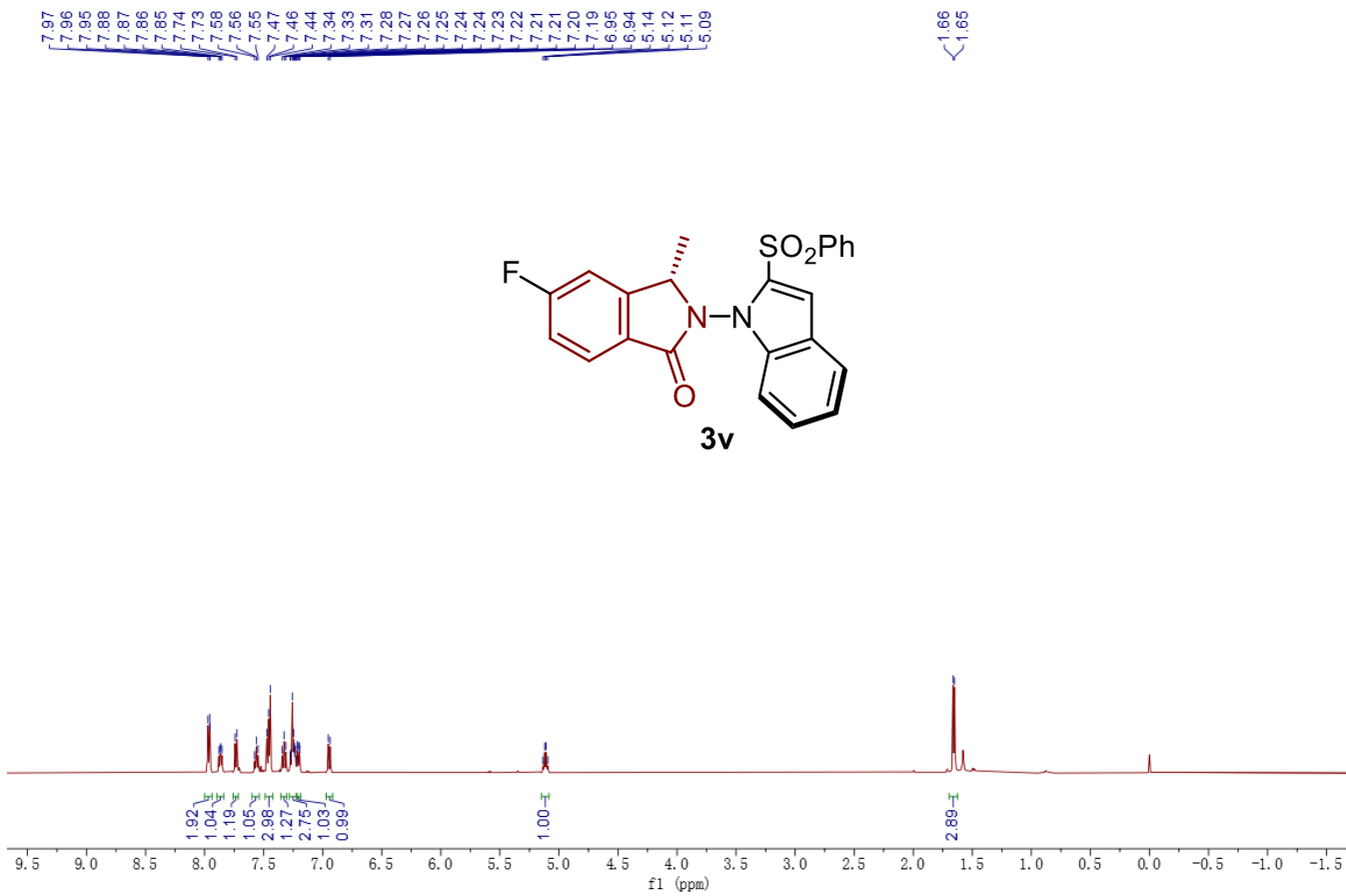
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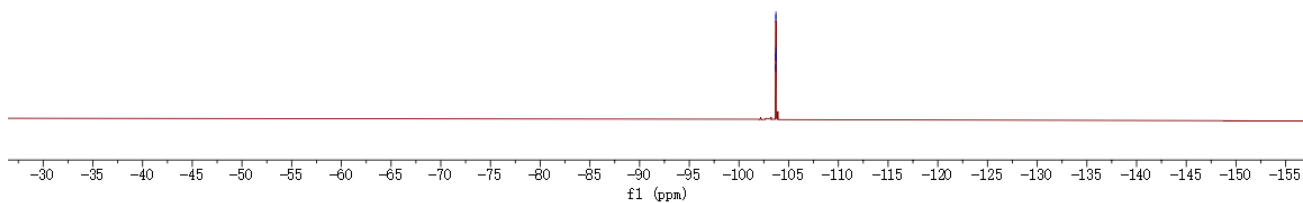
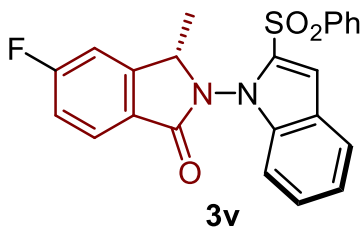
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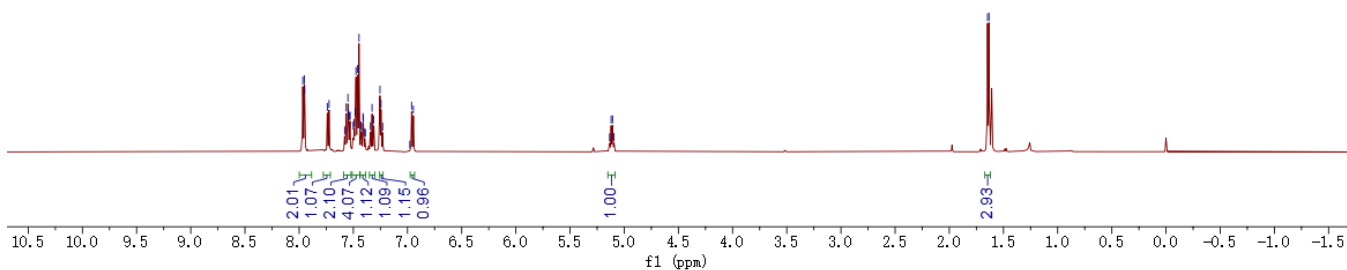
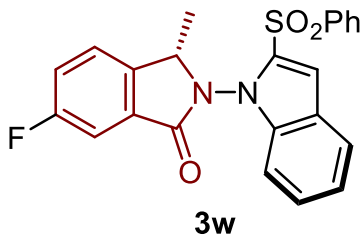


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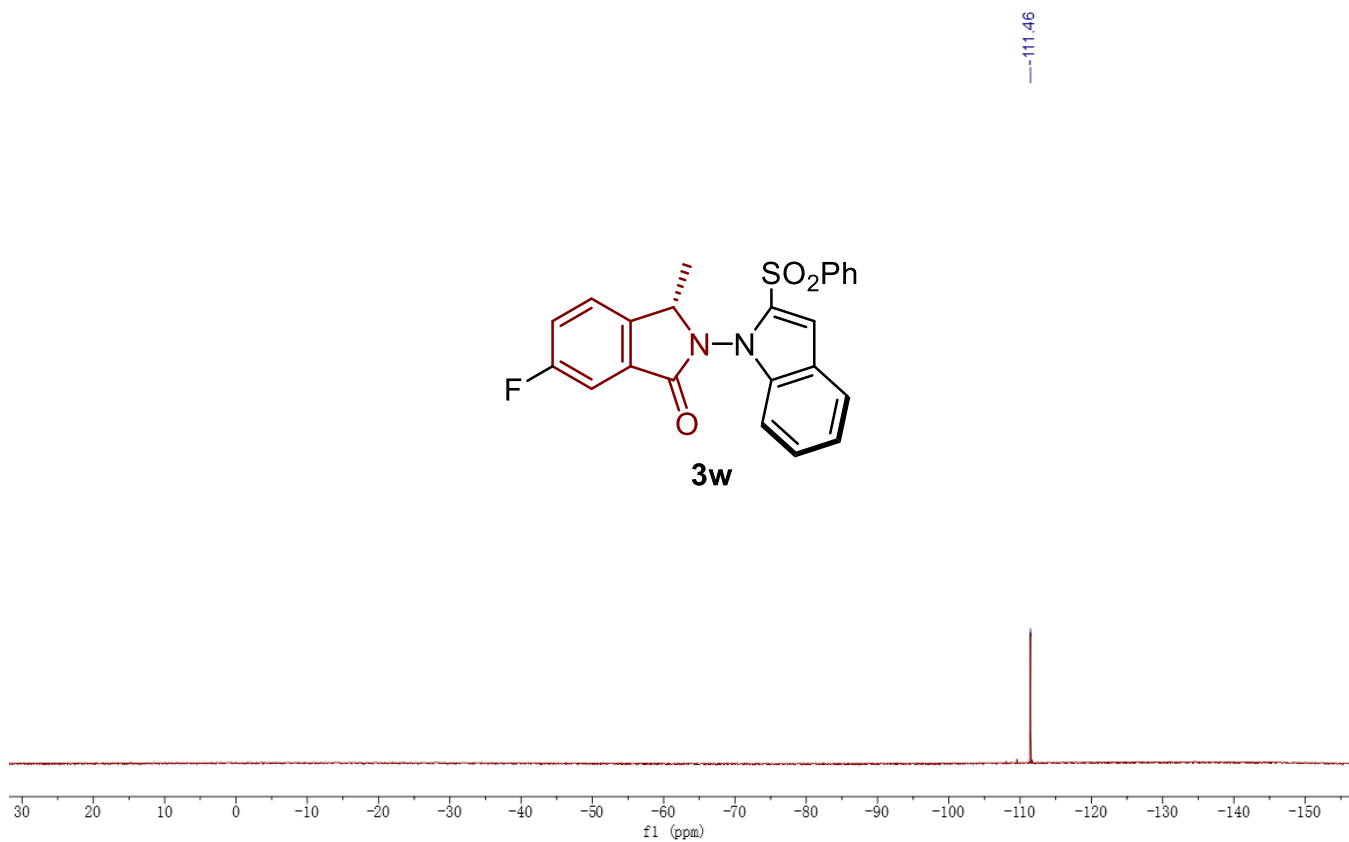
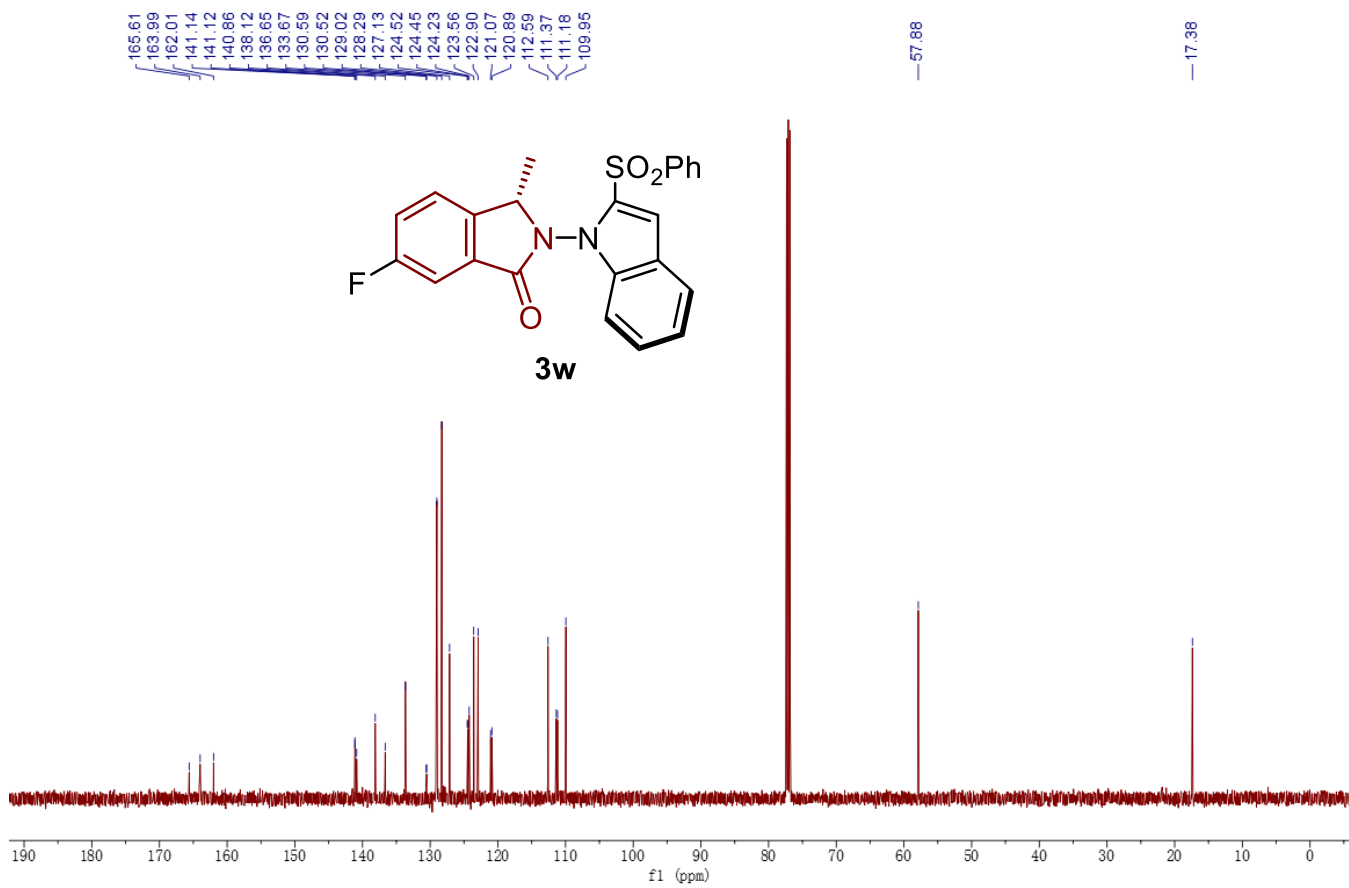


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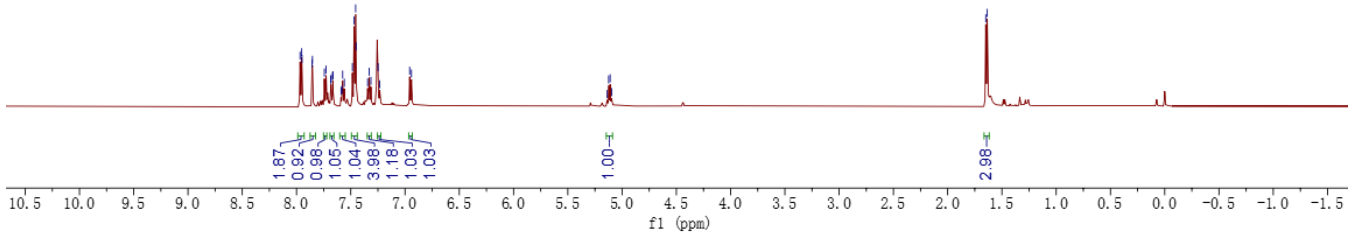
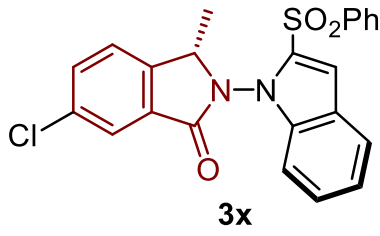






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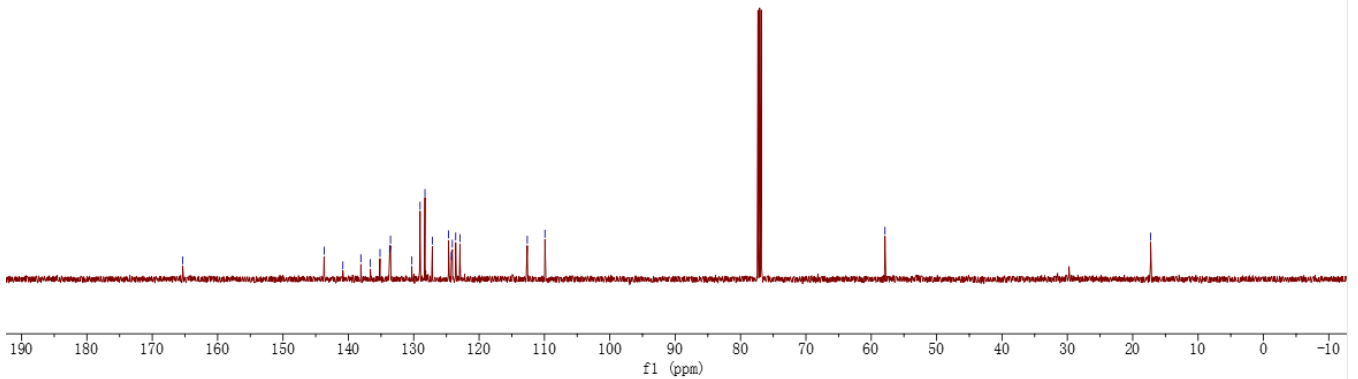
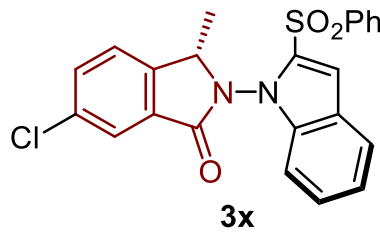
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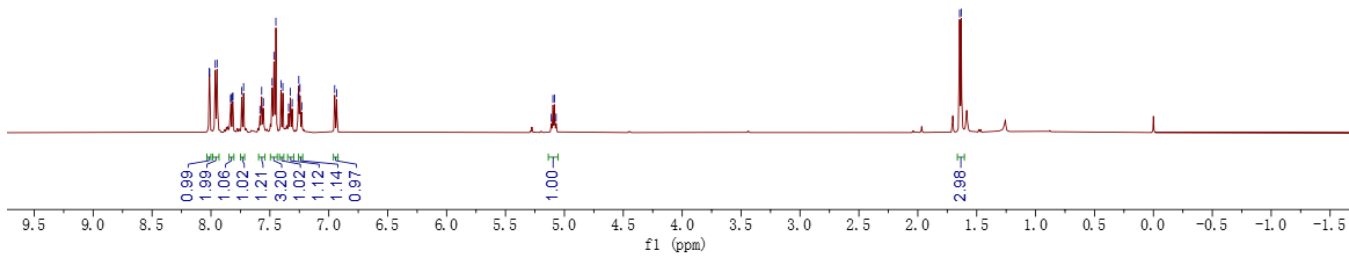
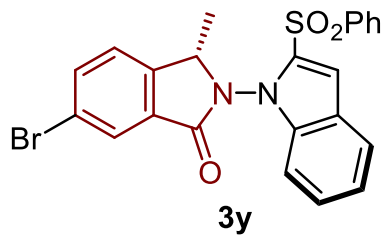
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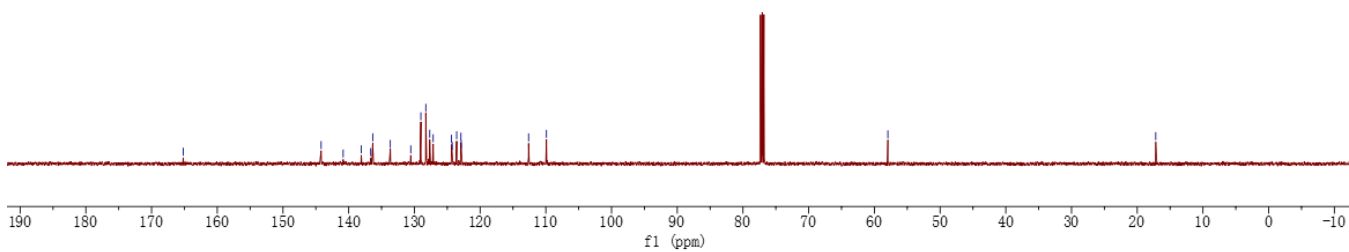
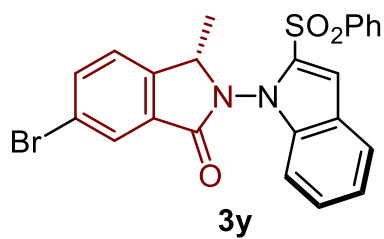
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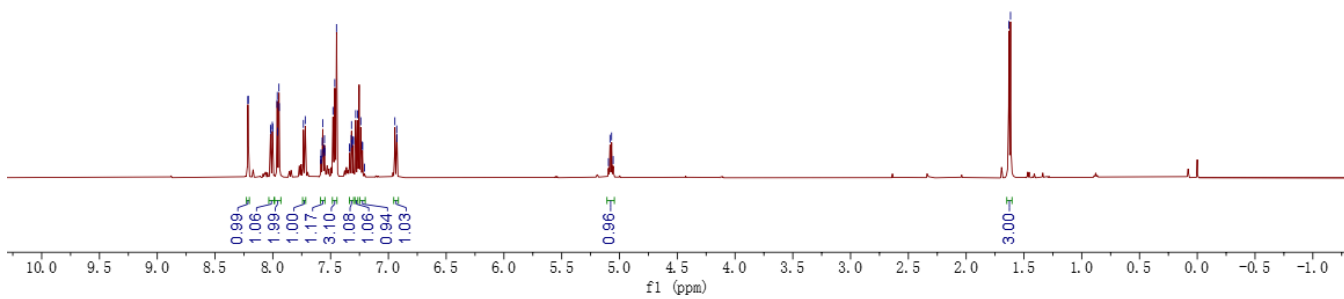
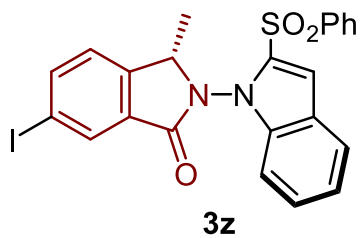
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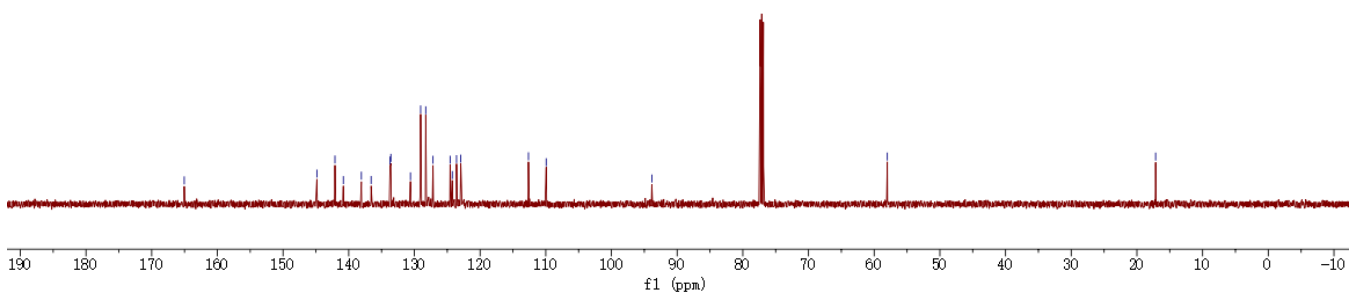
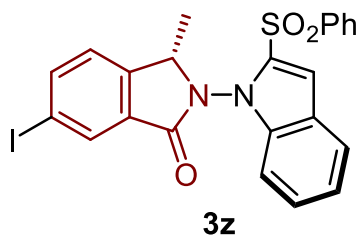


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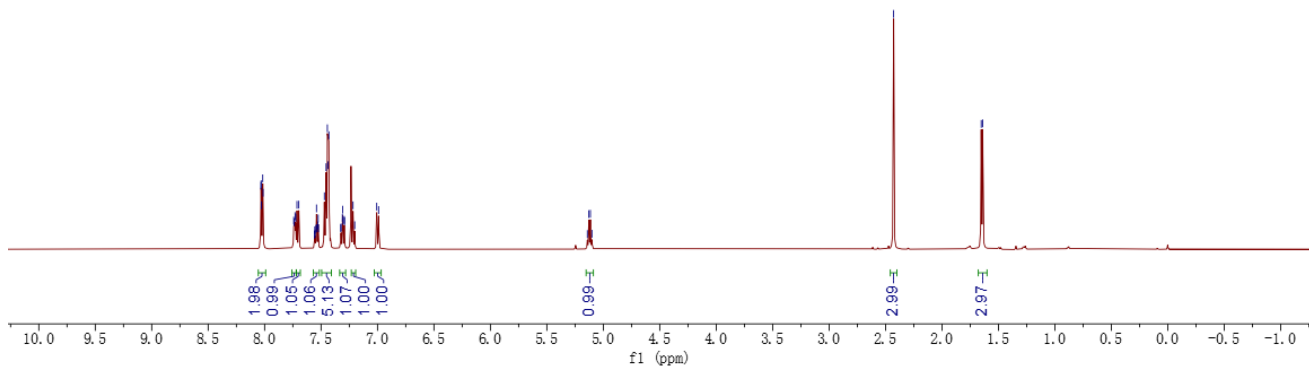
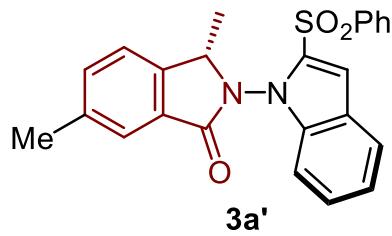
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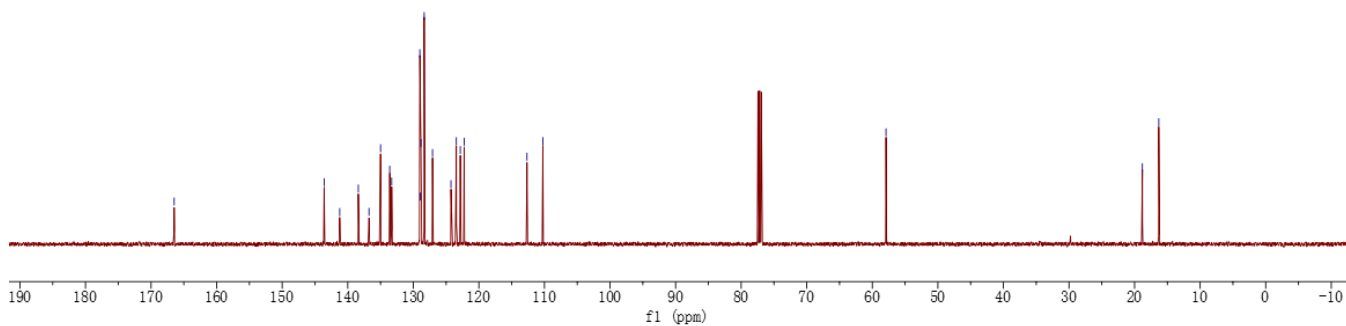
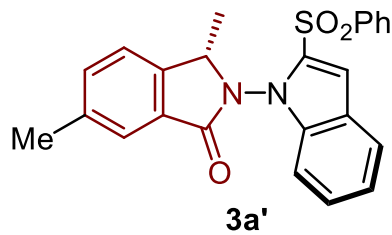


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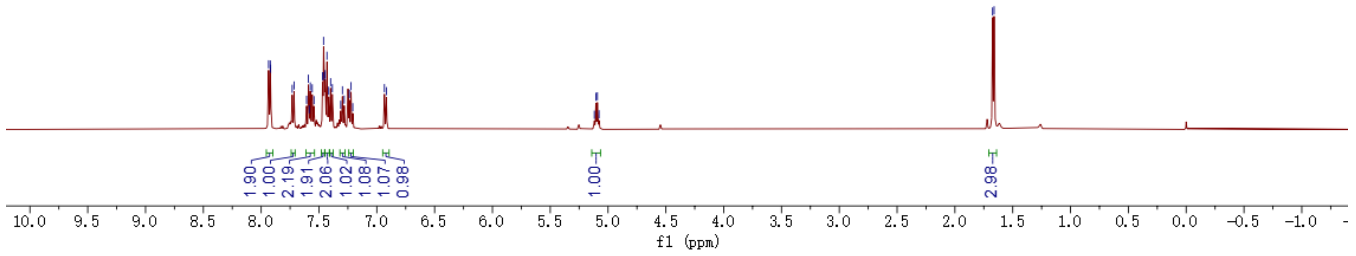
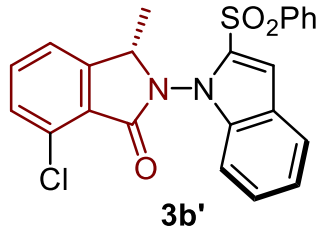
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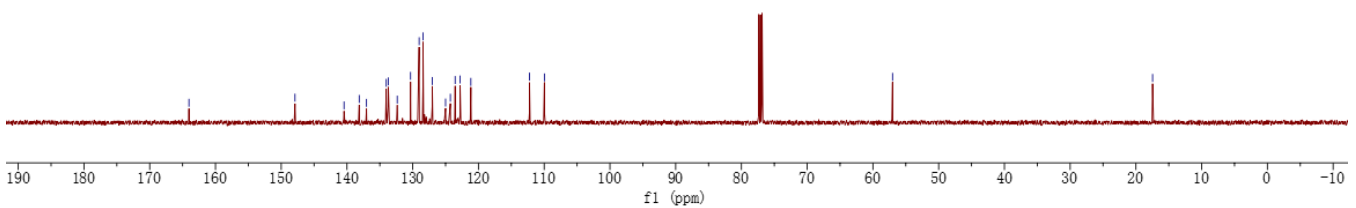
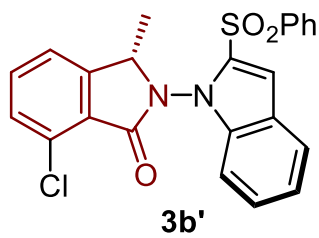
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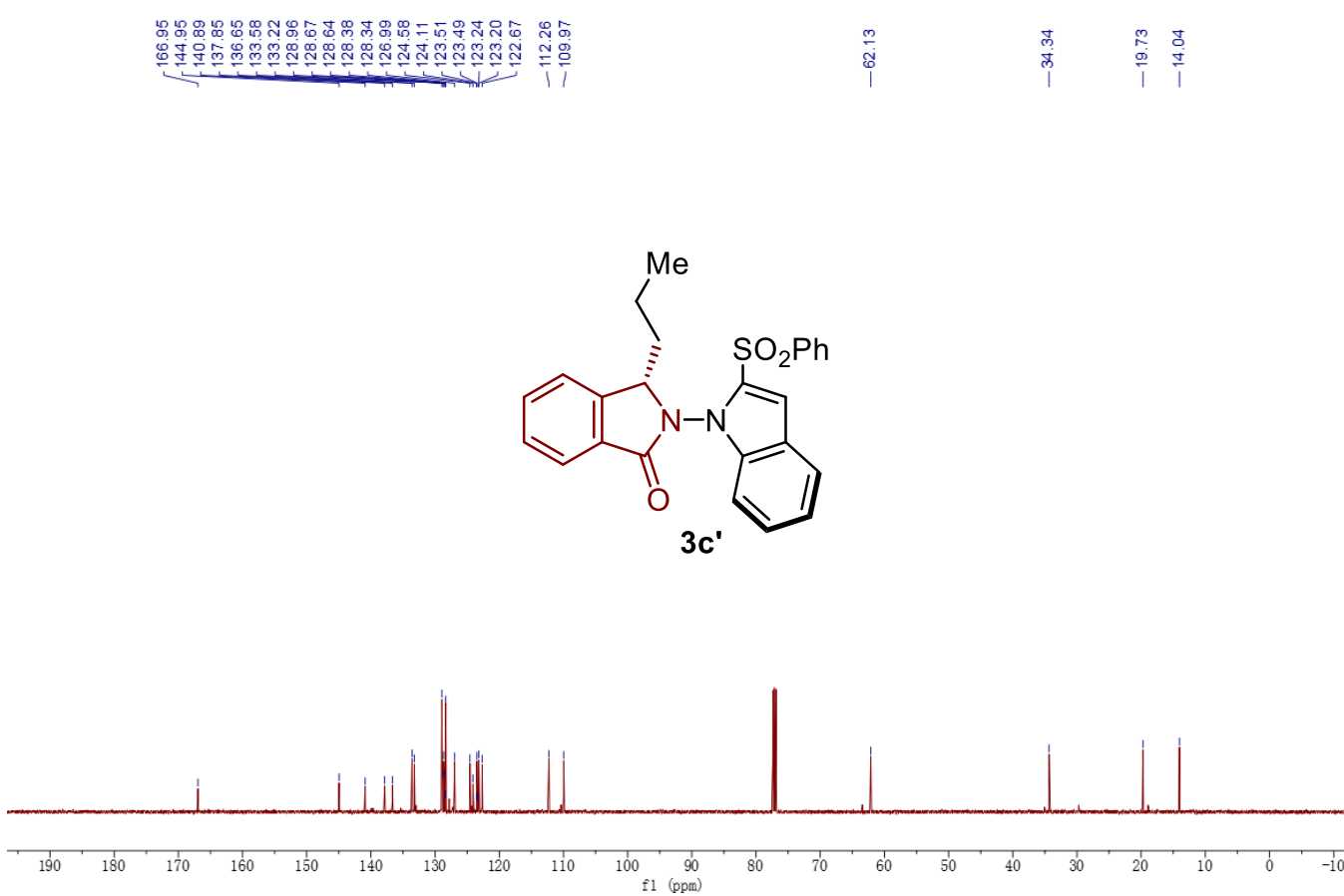
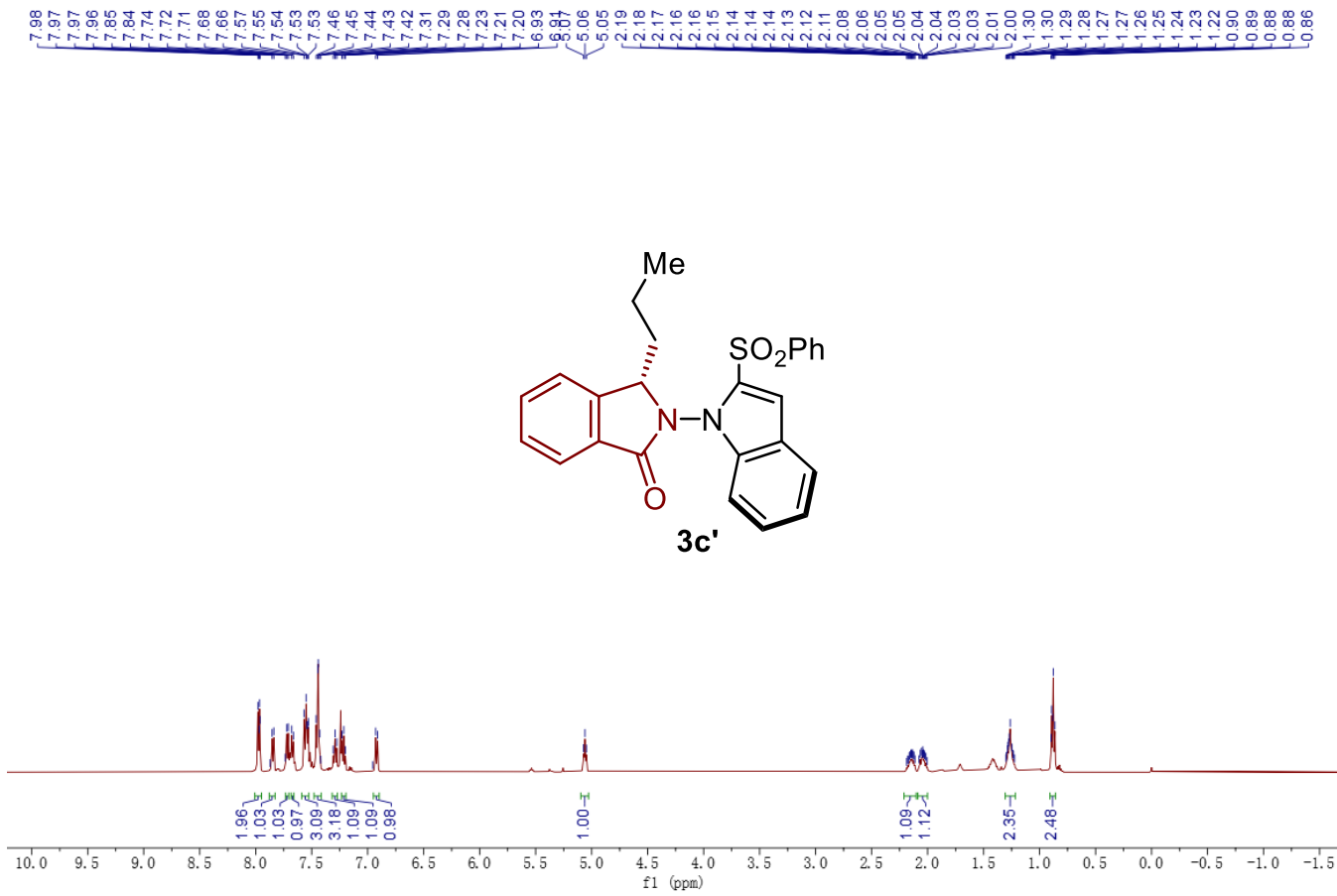


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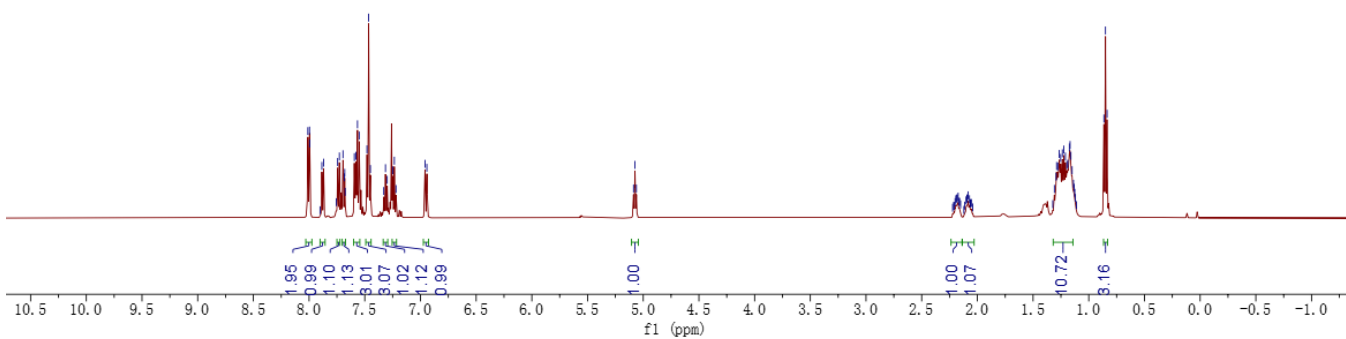
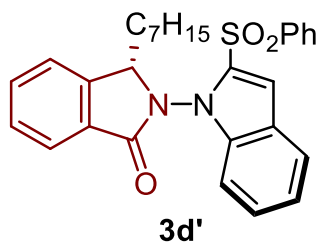
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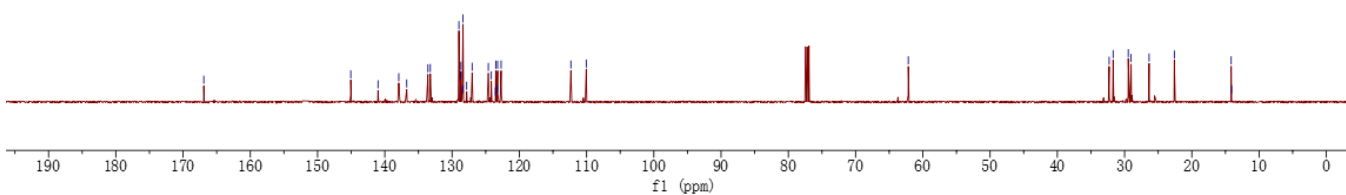
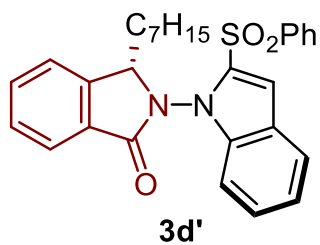




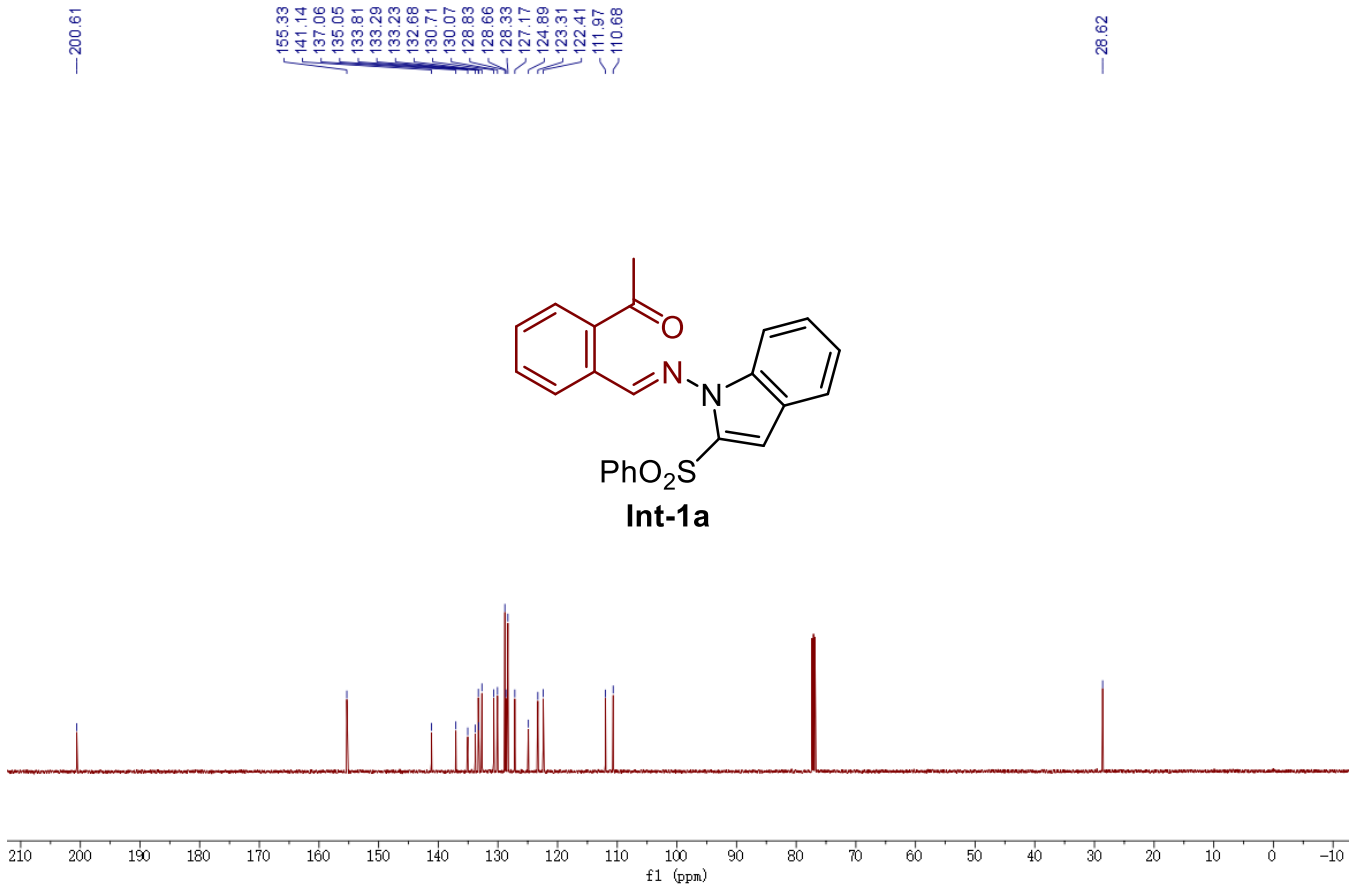
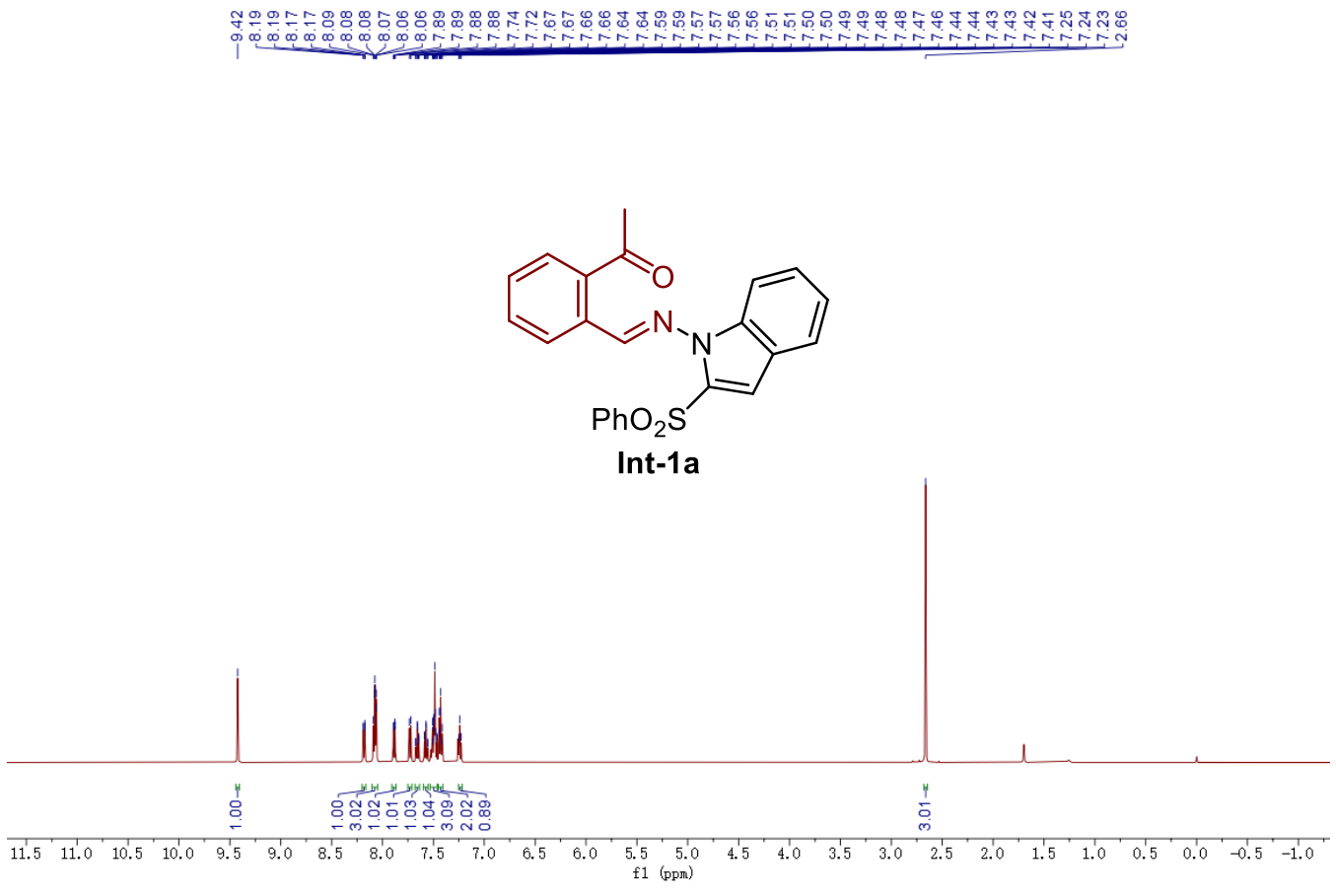
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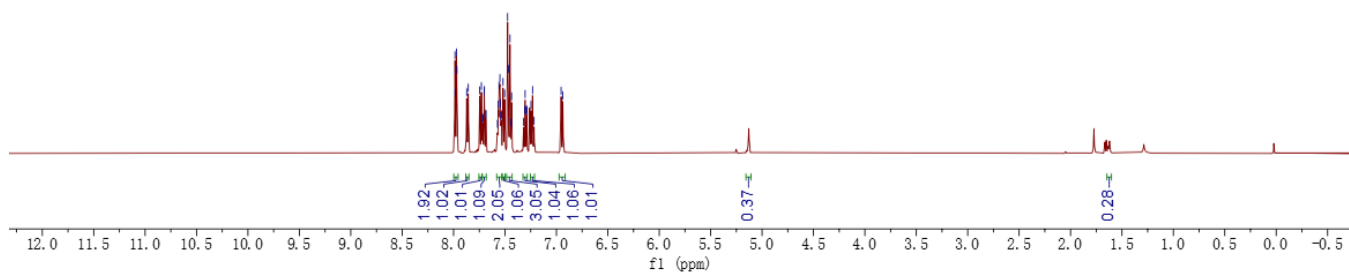
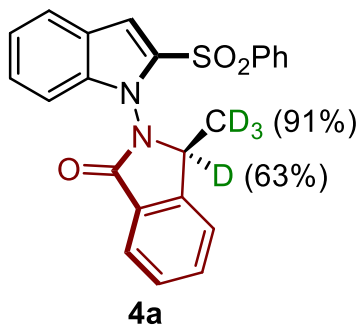
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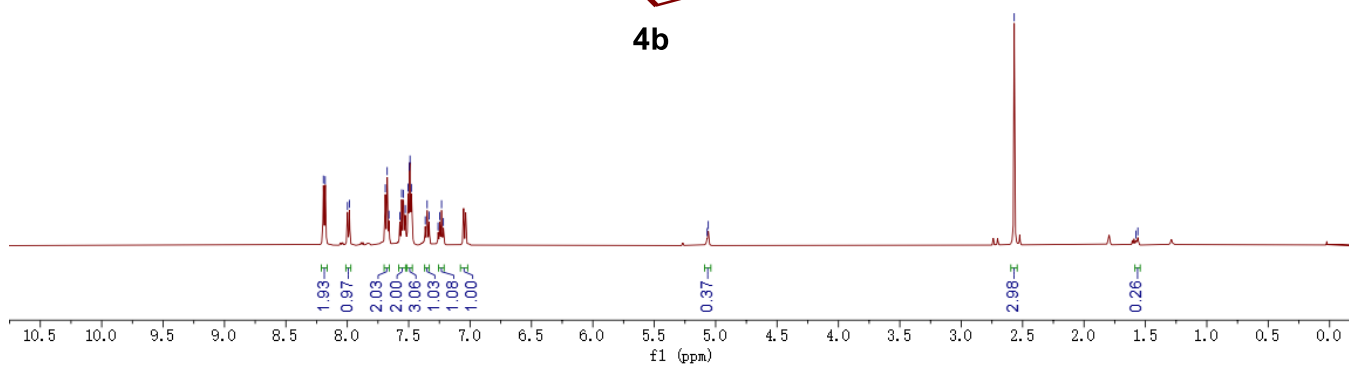
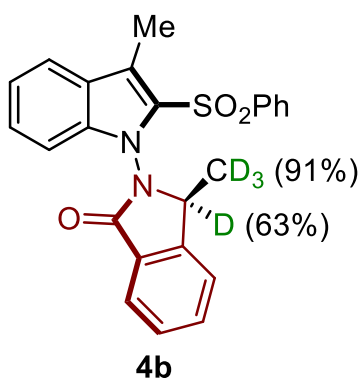


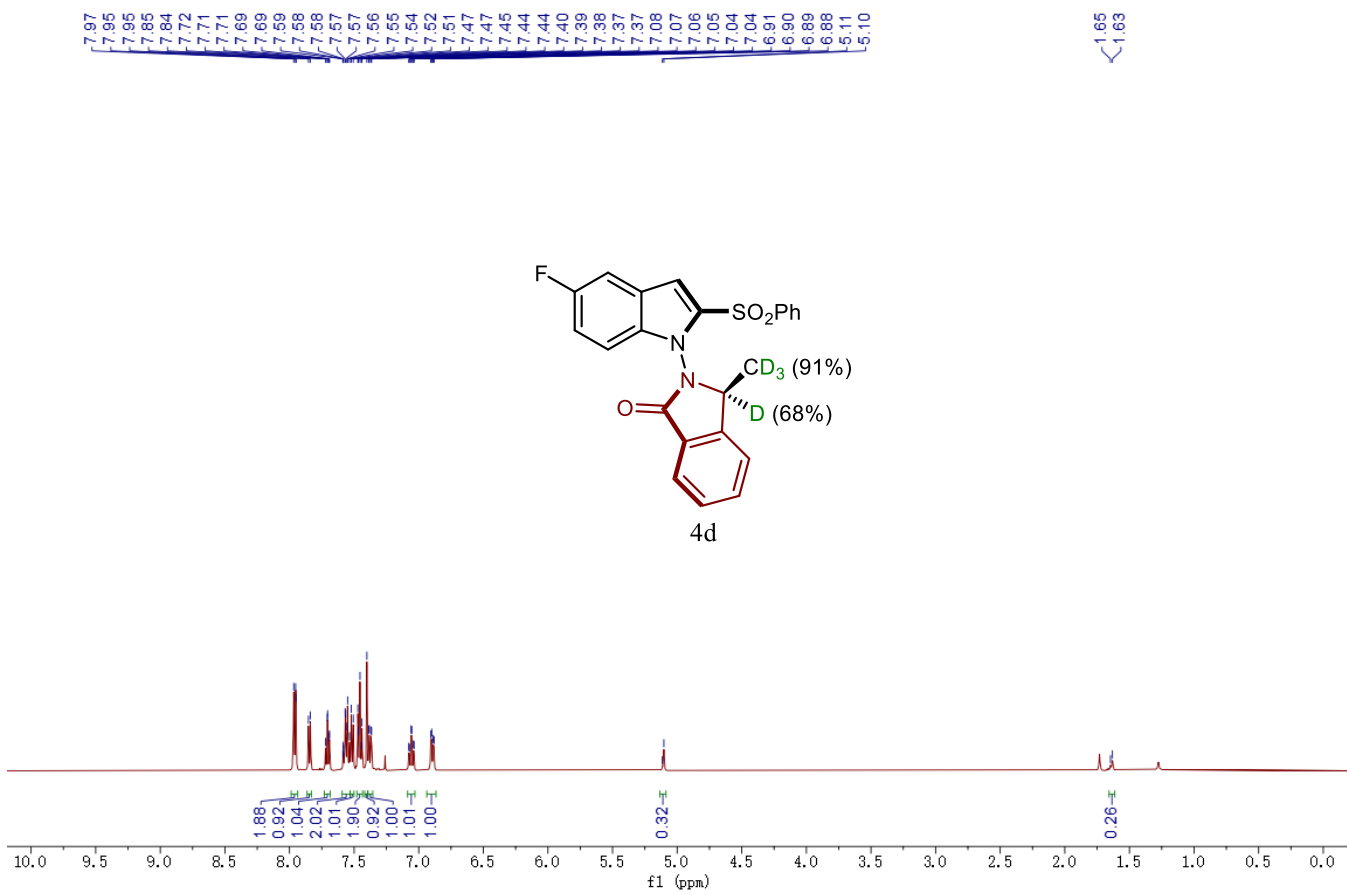
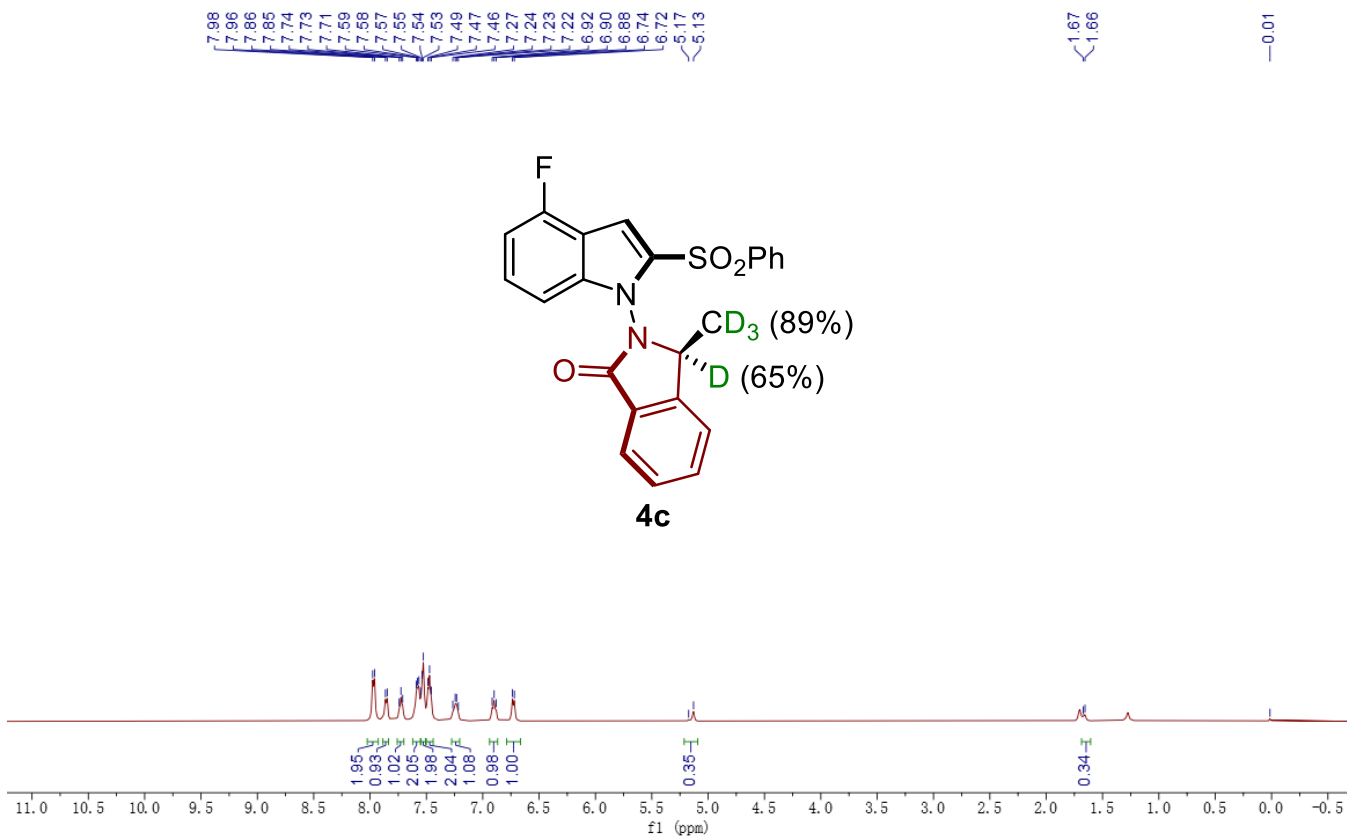


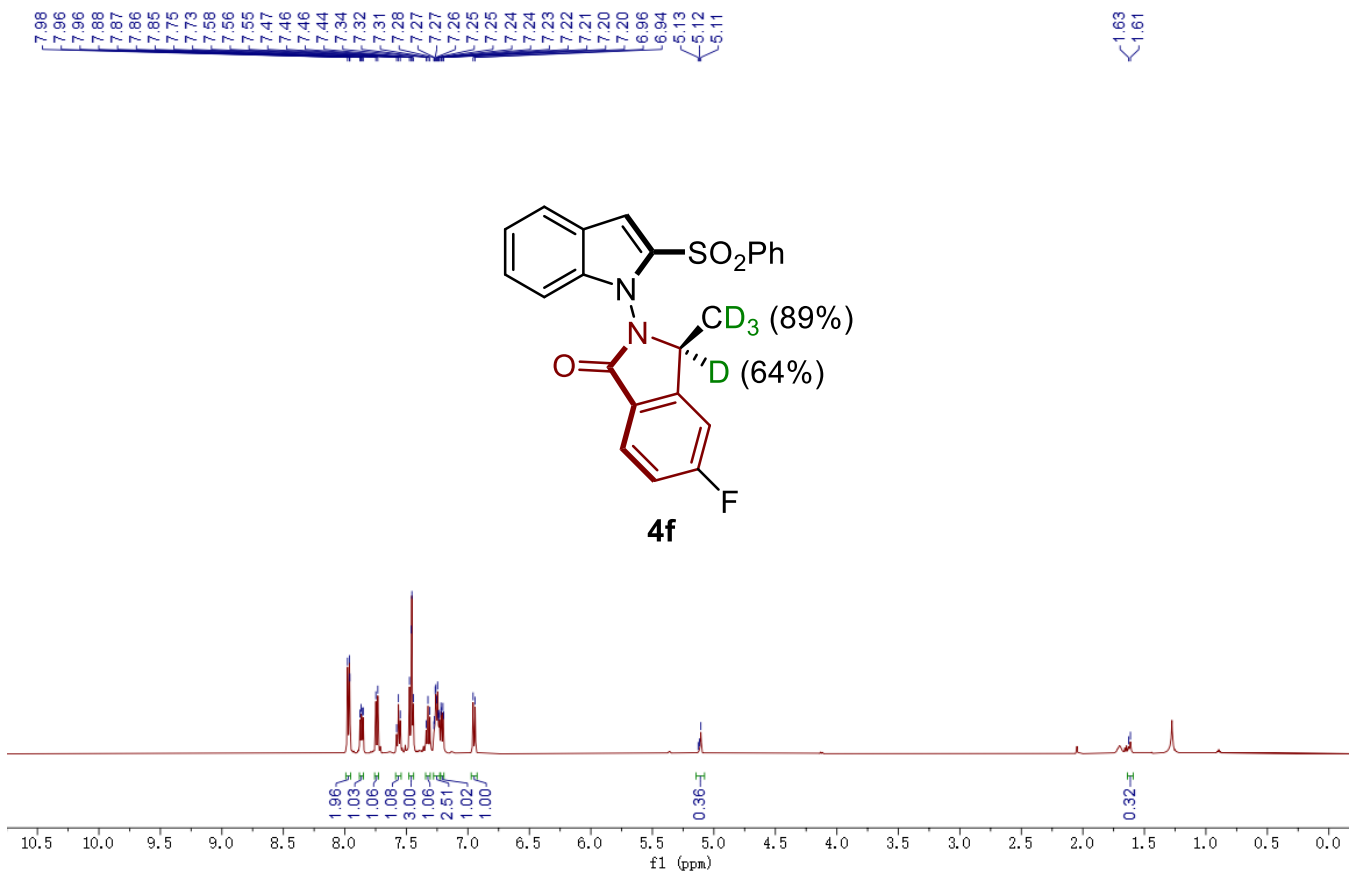
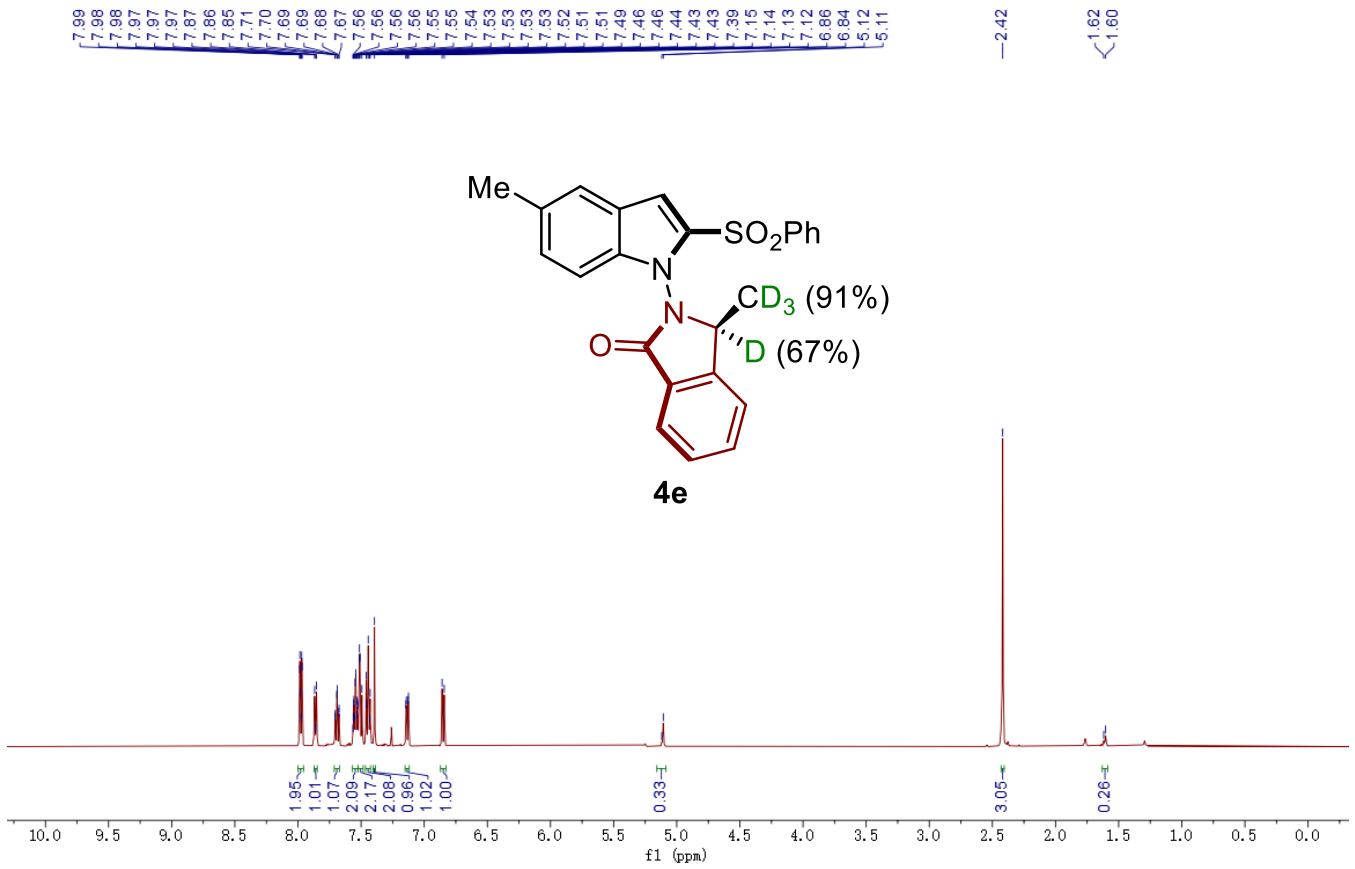
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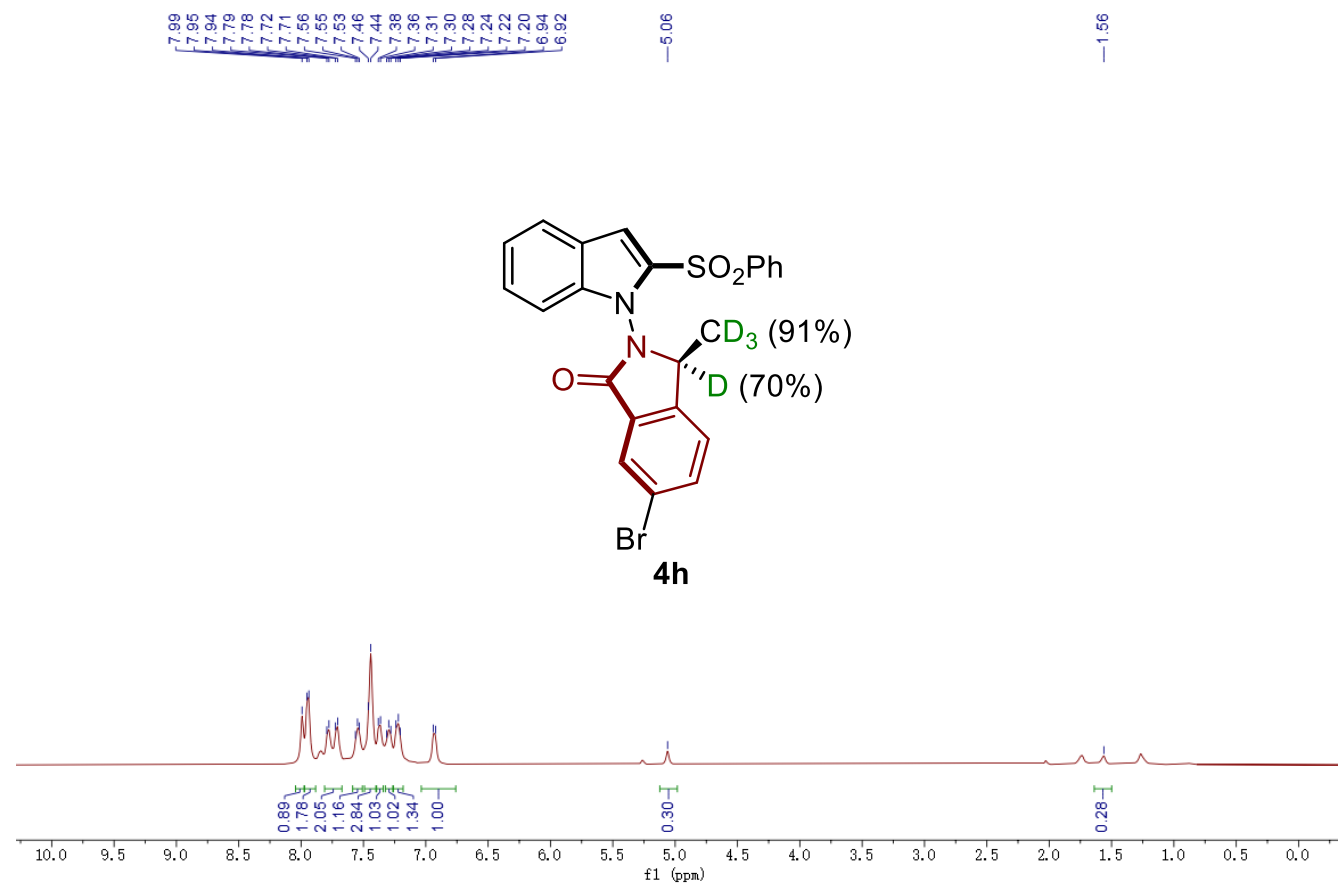
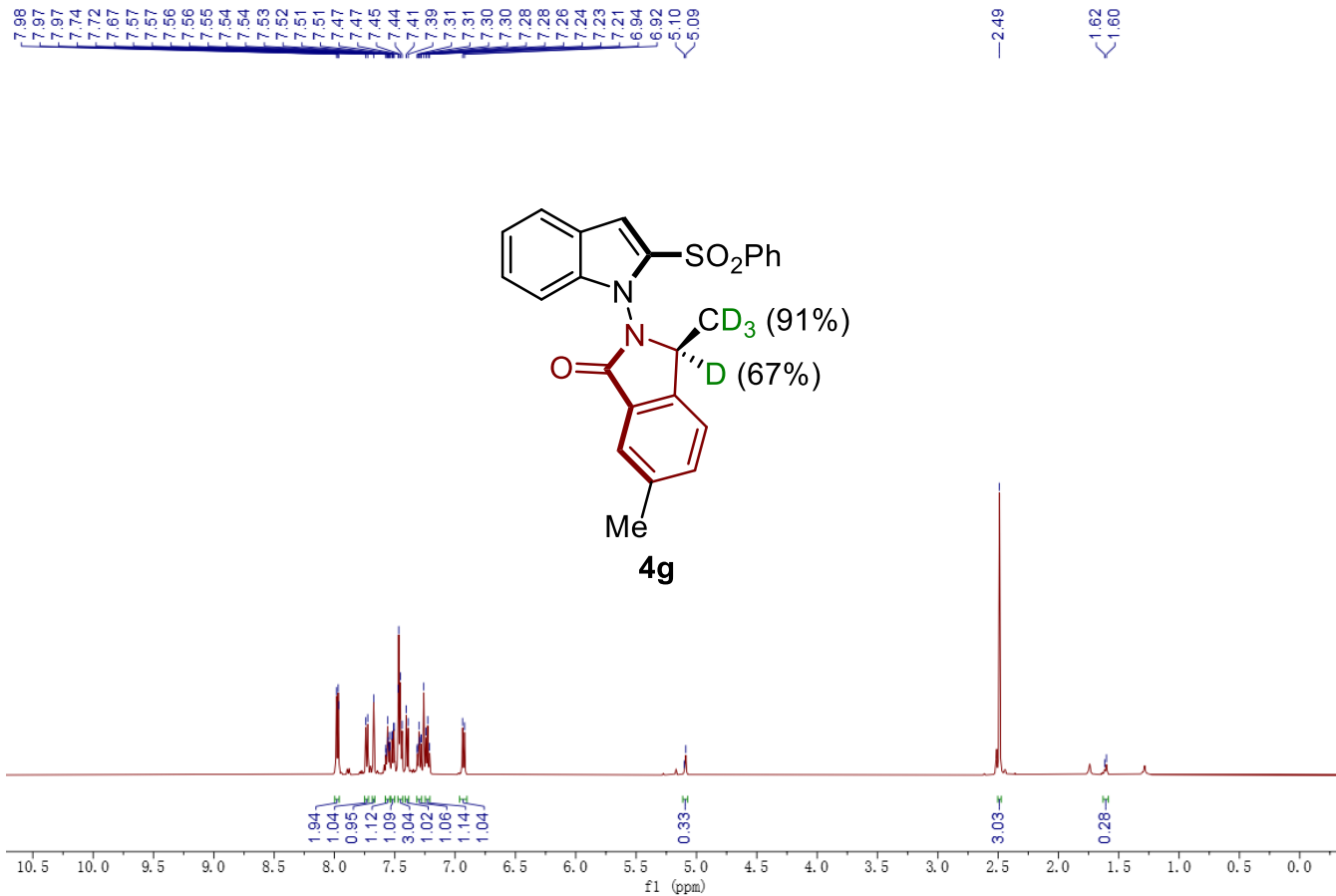


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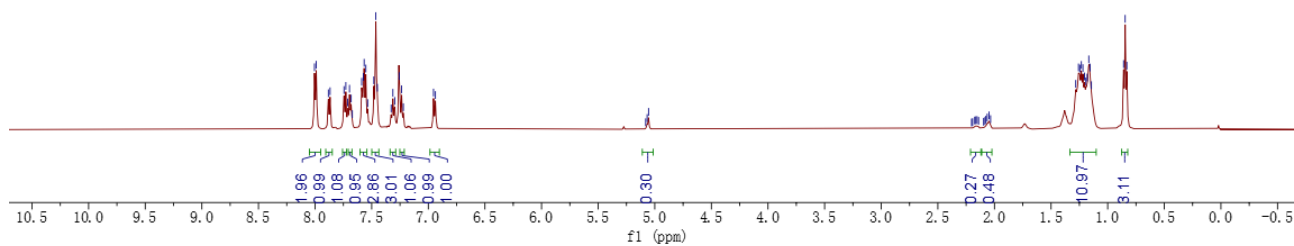
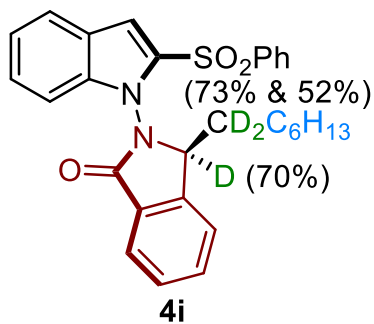




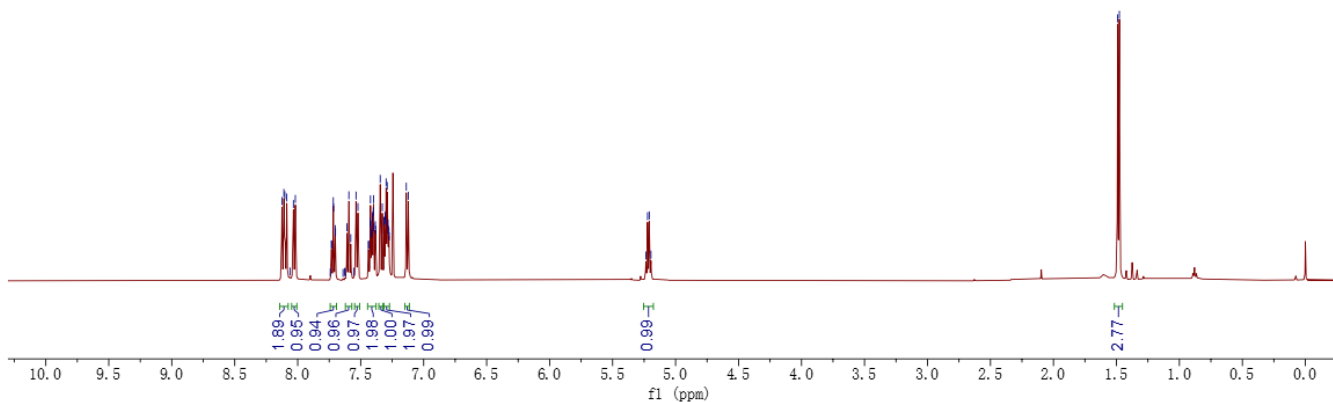
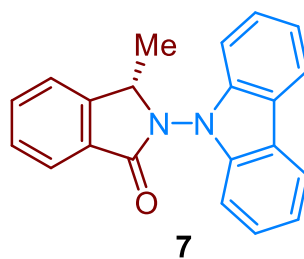


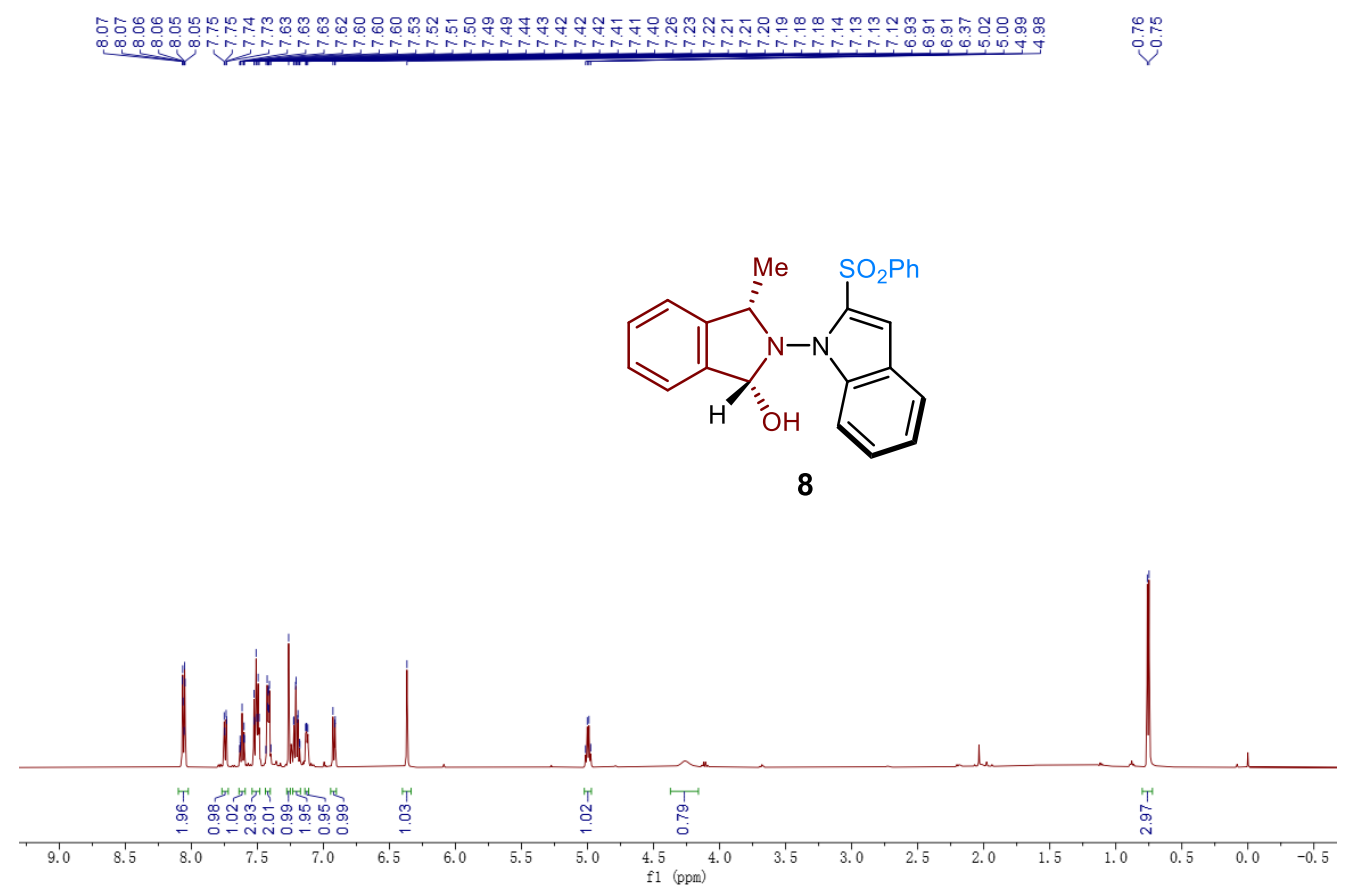
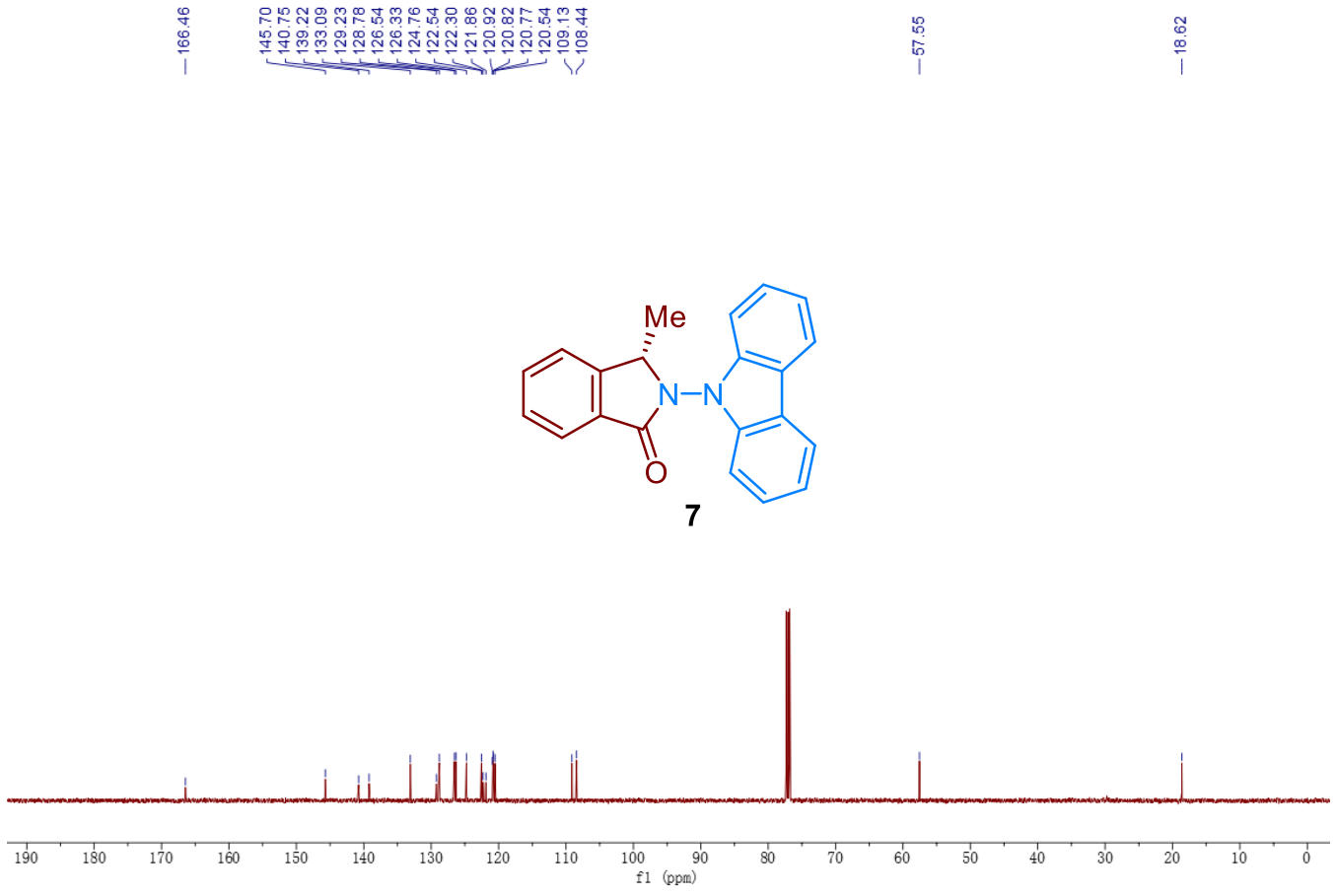


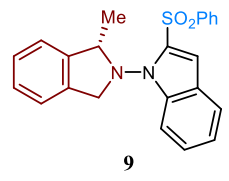
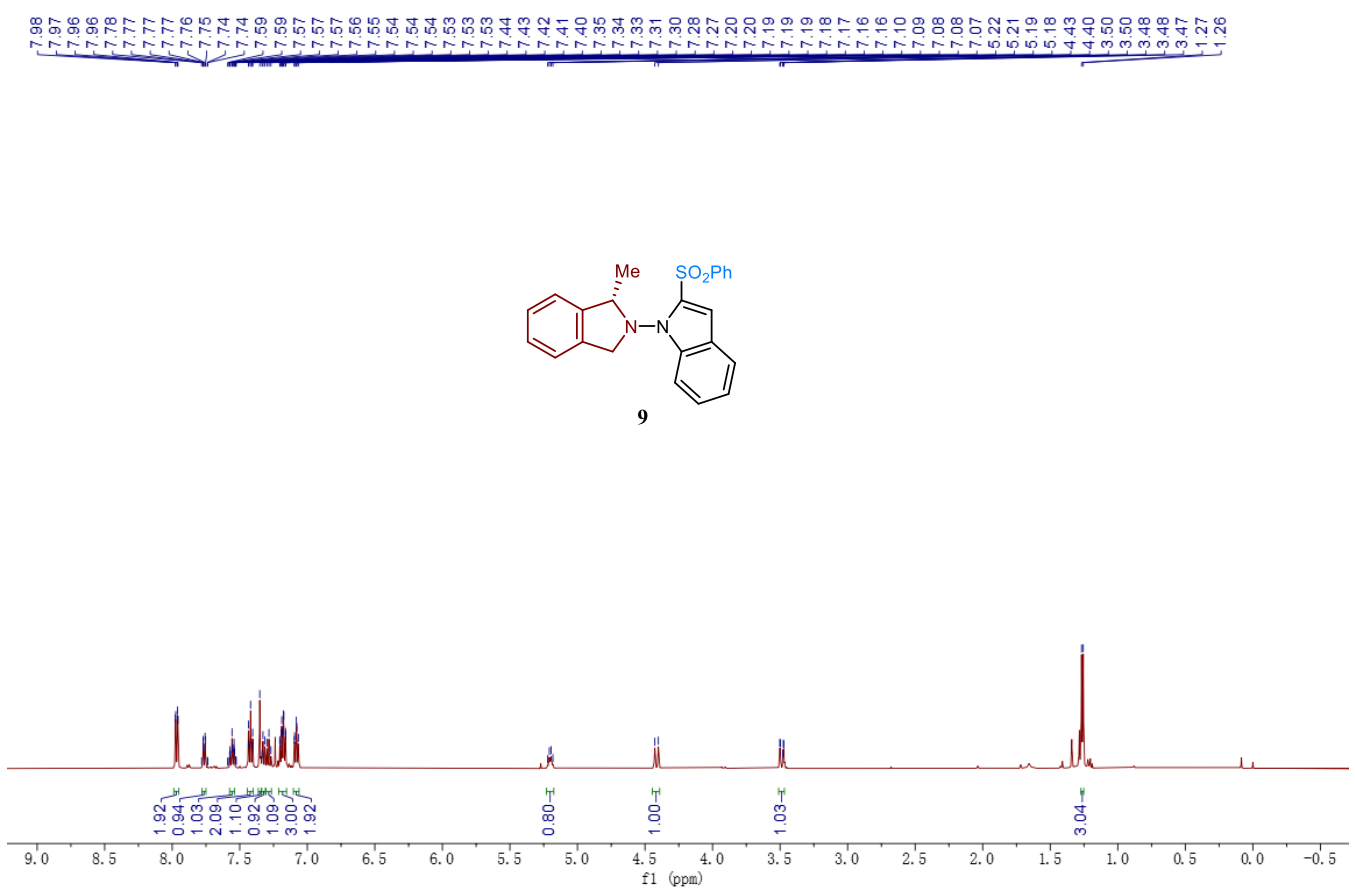
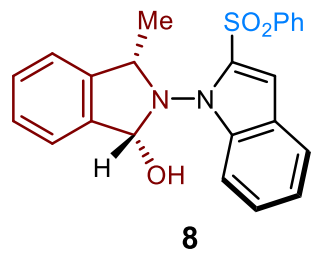
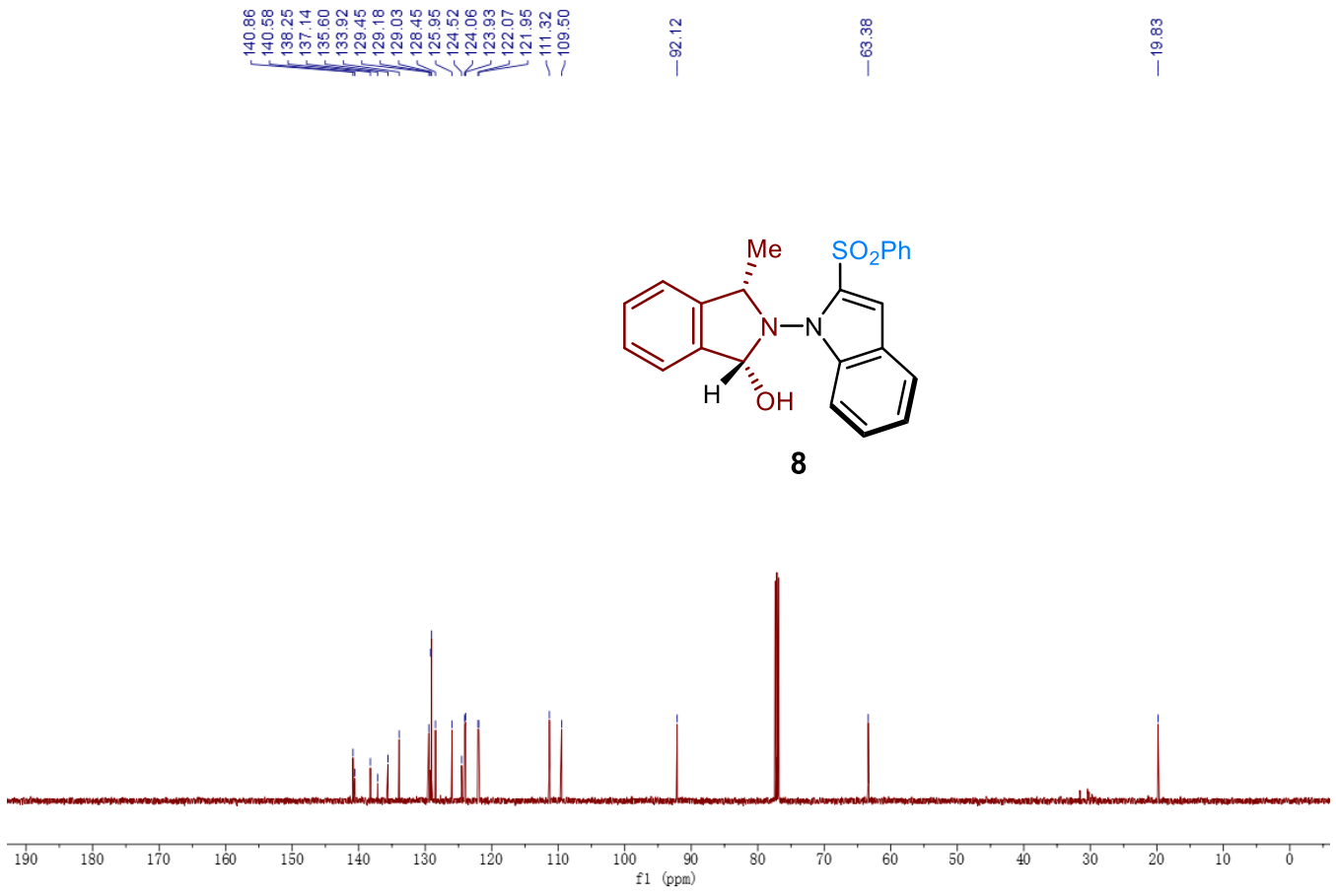
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S200

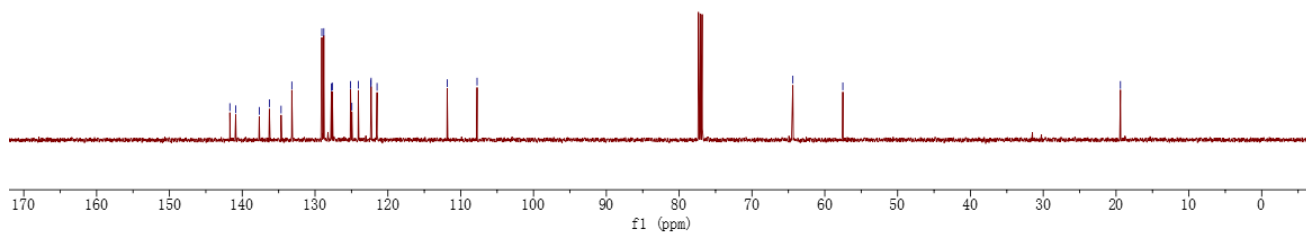
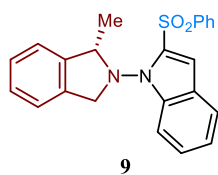


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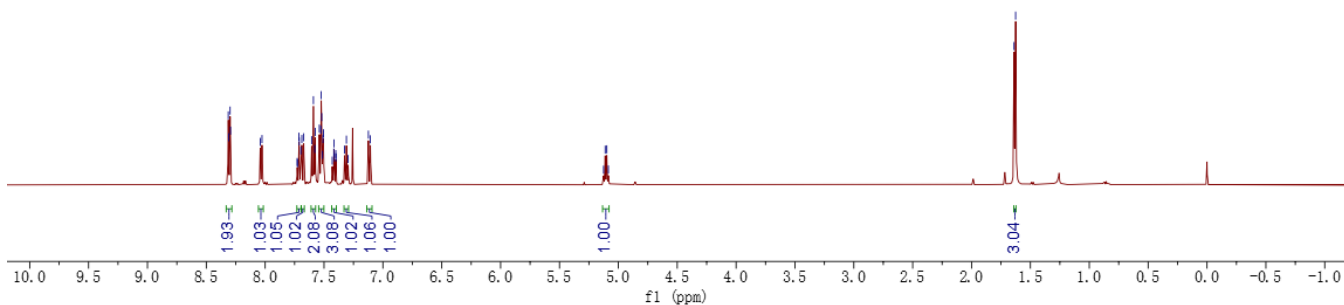
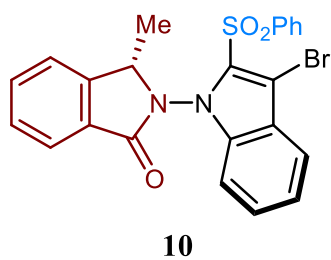
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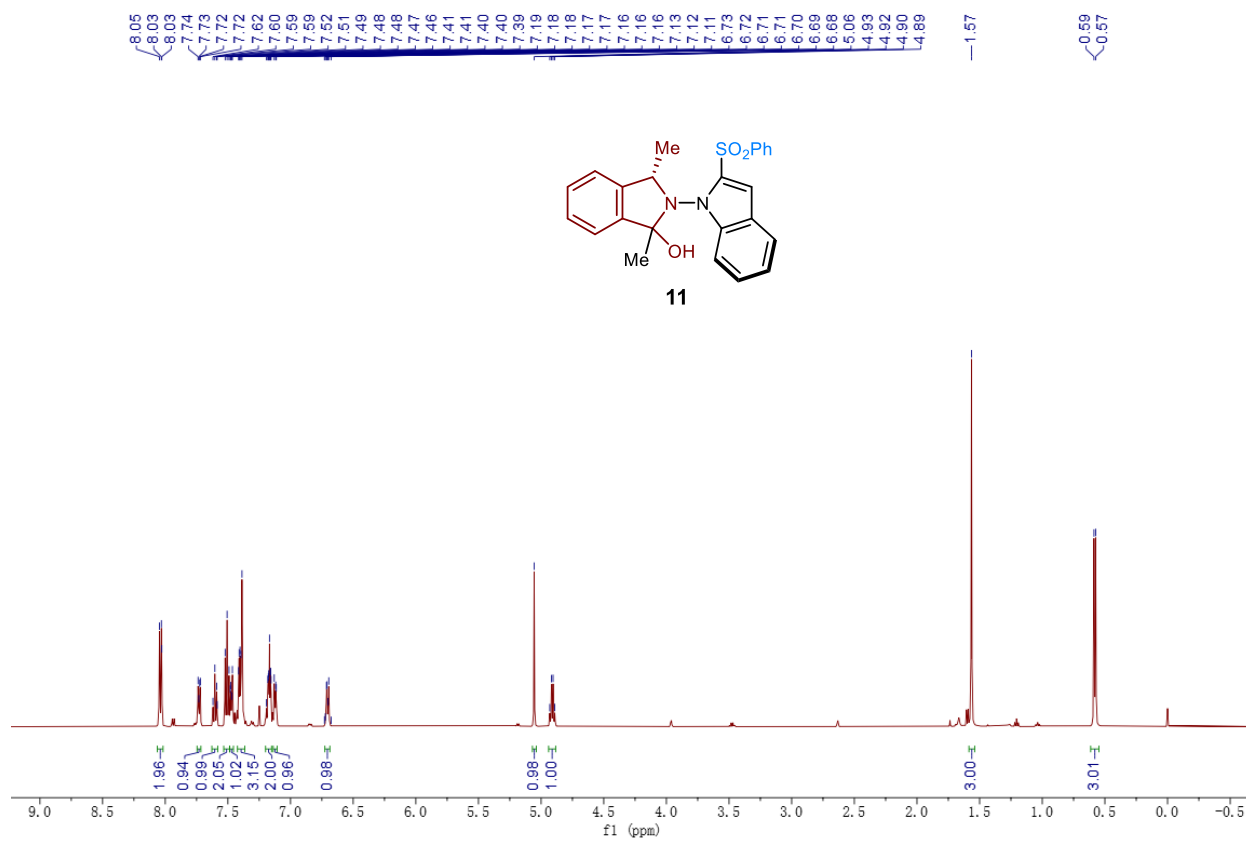
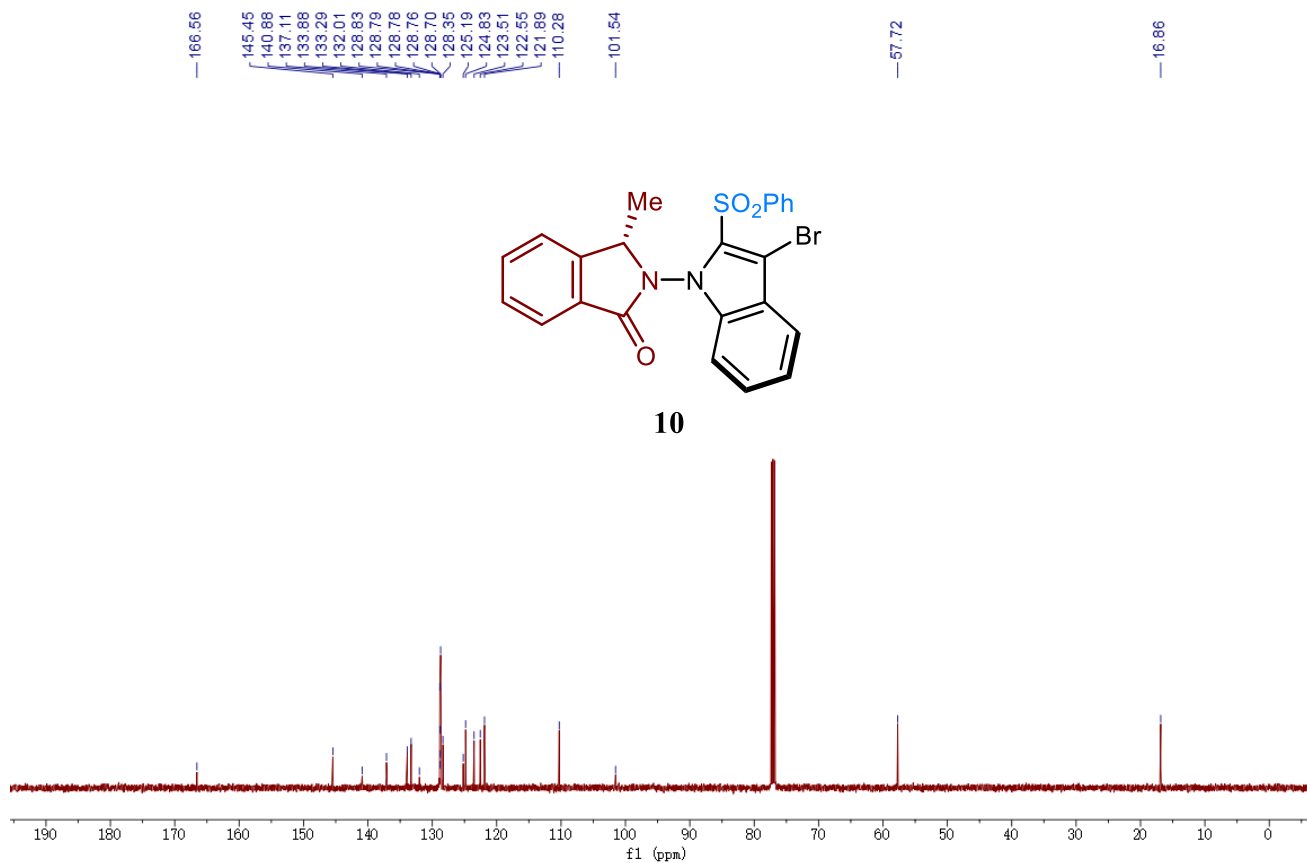
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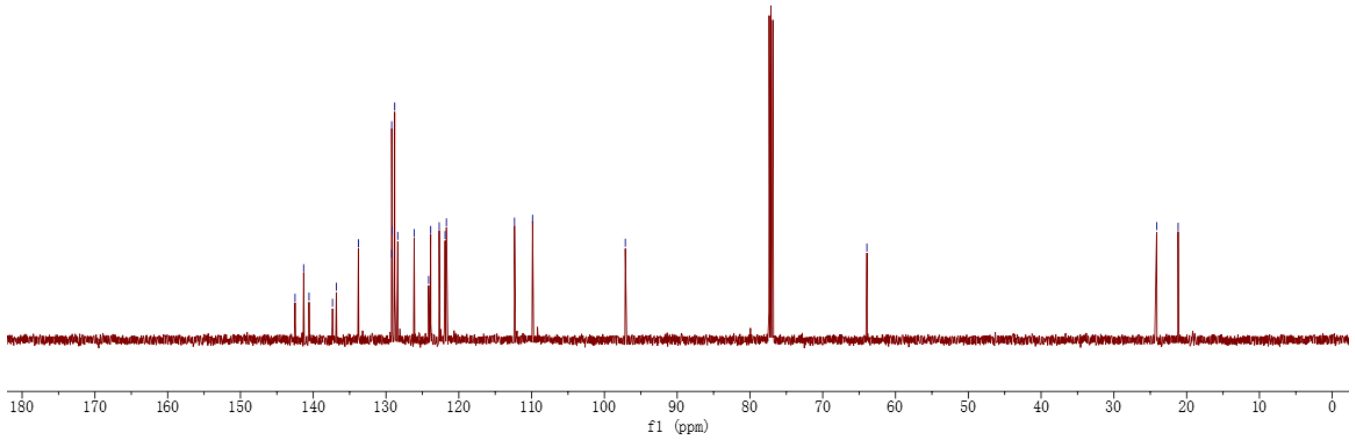
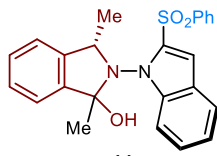


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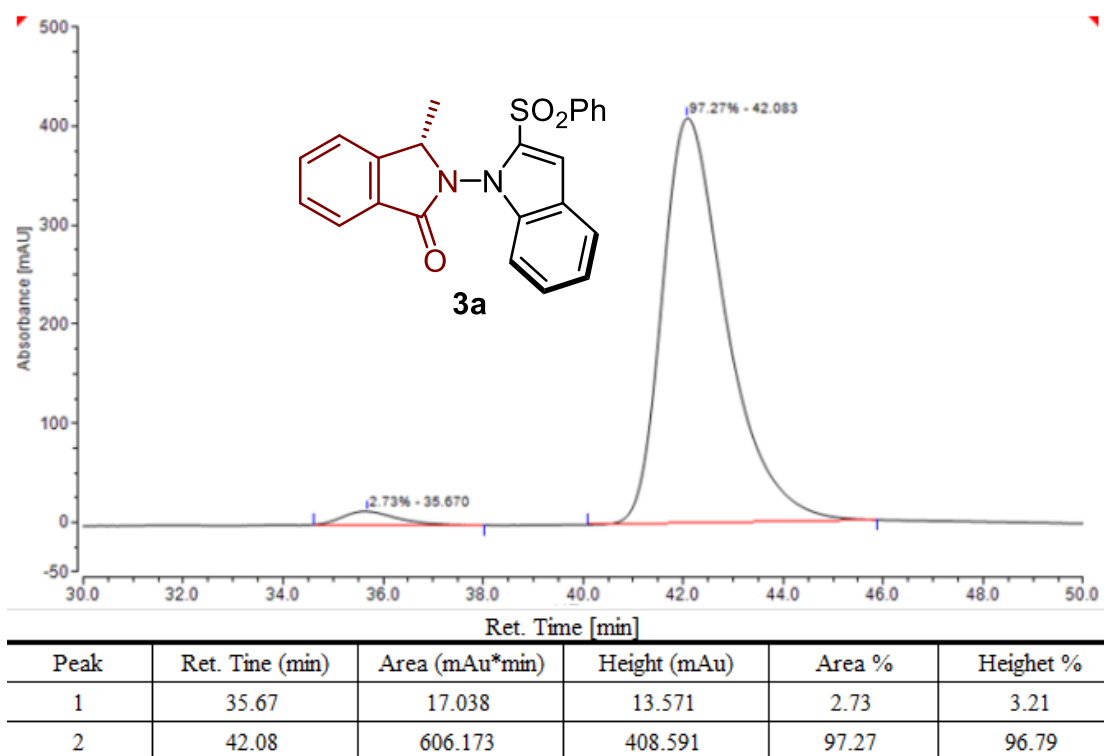
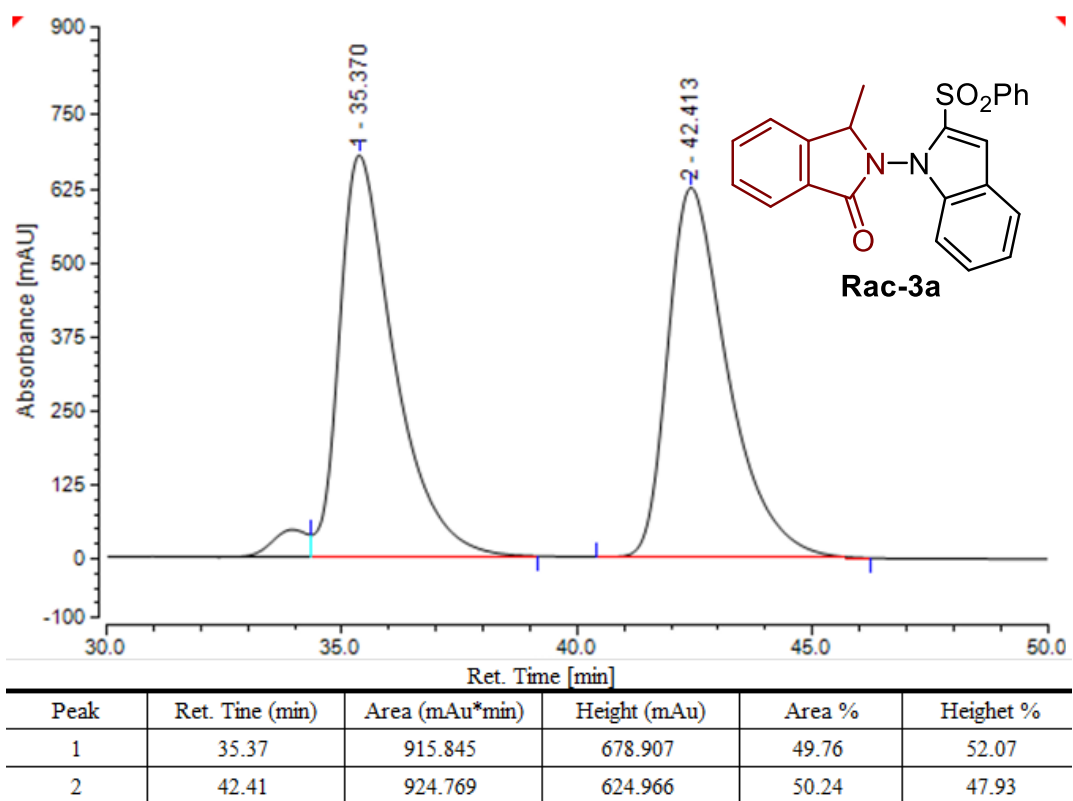
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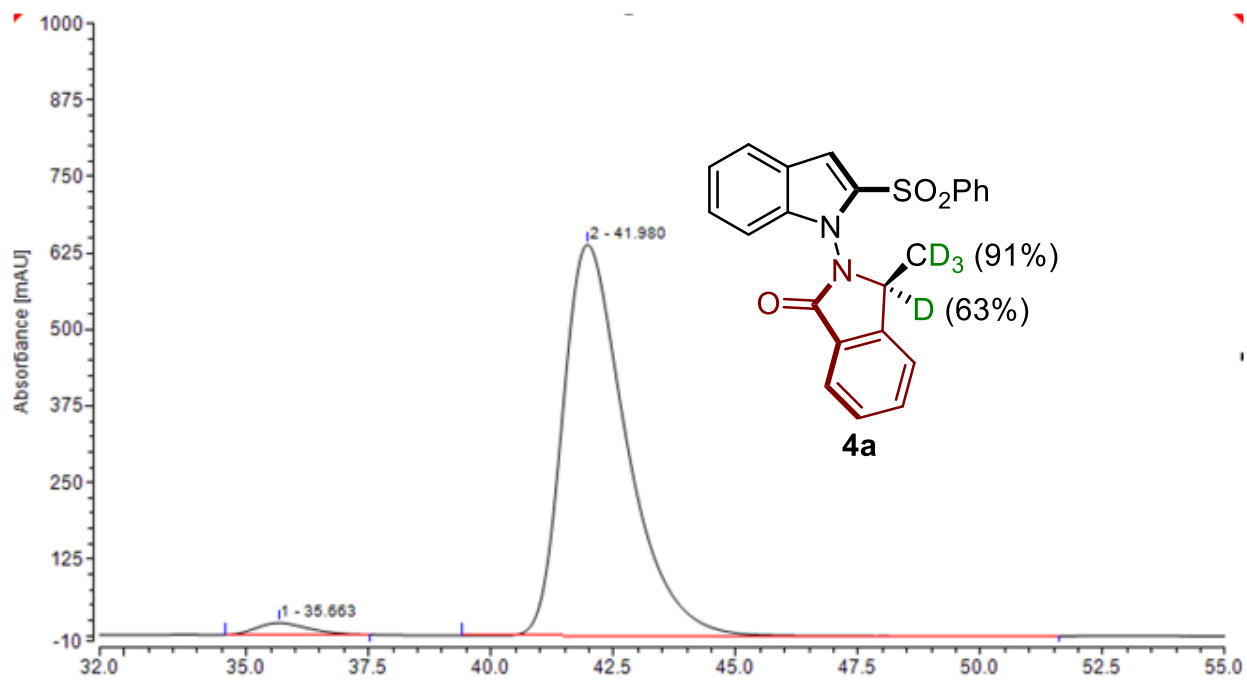
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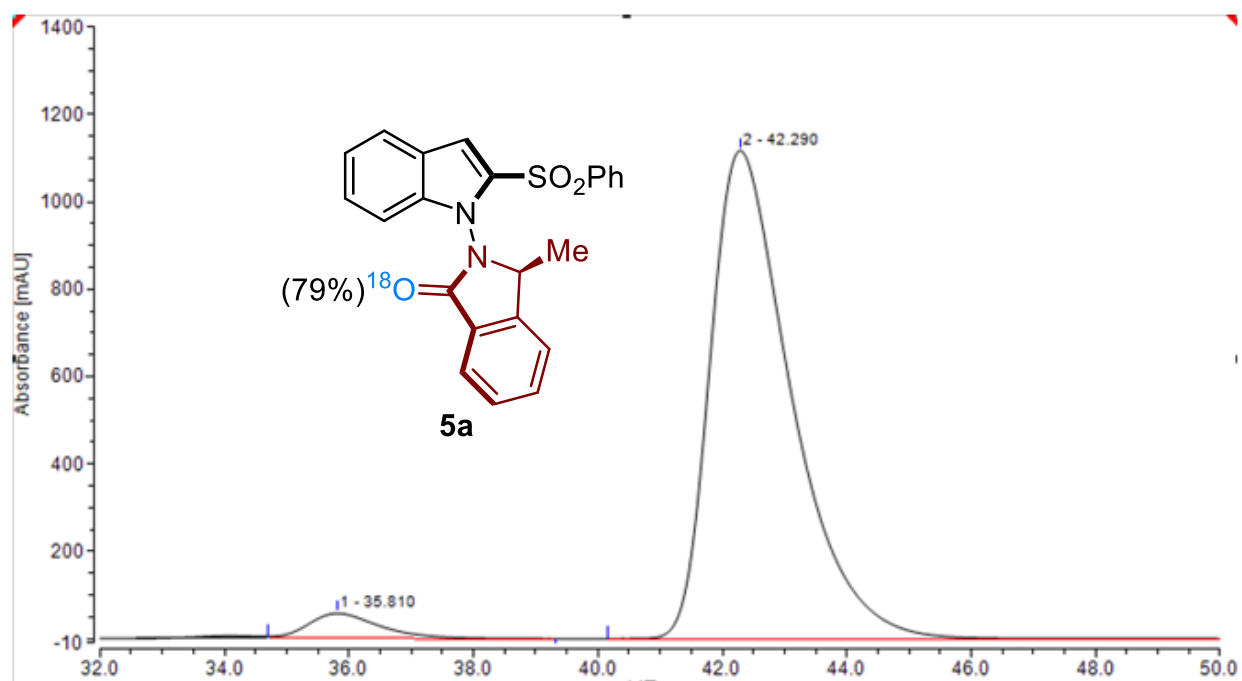


## HPLC data

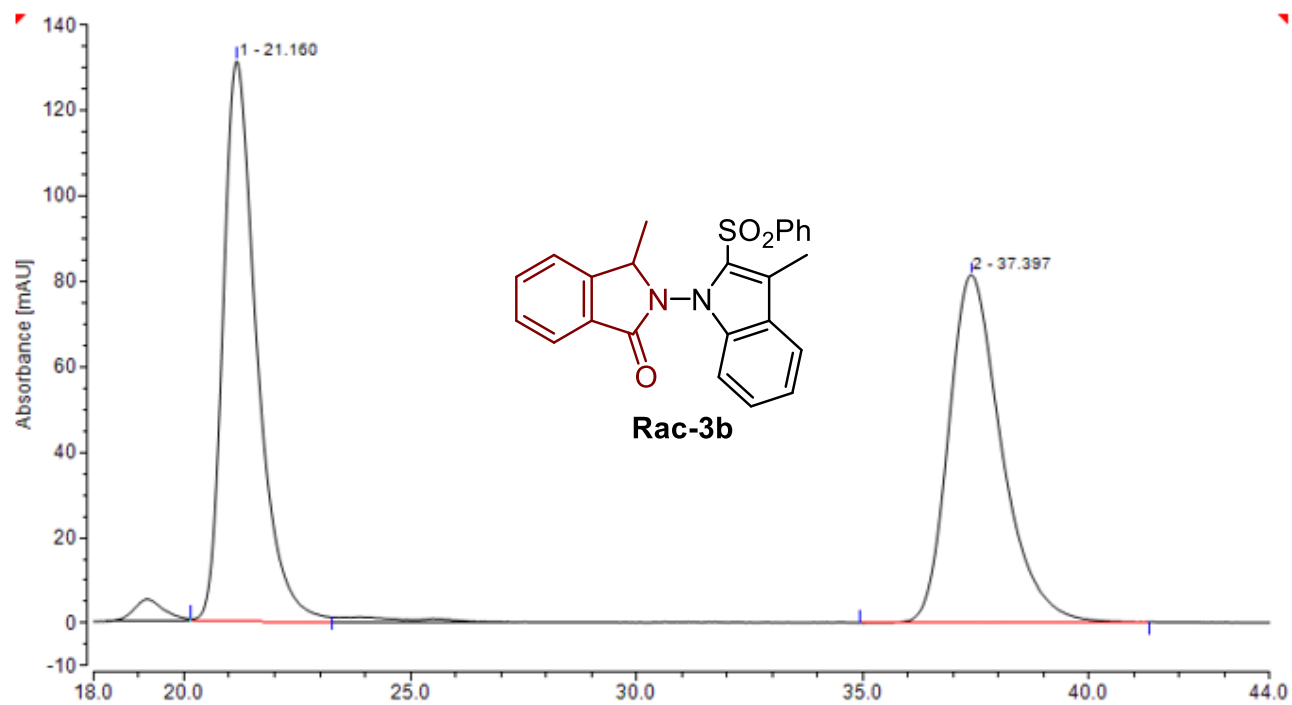




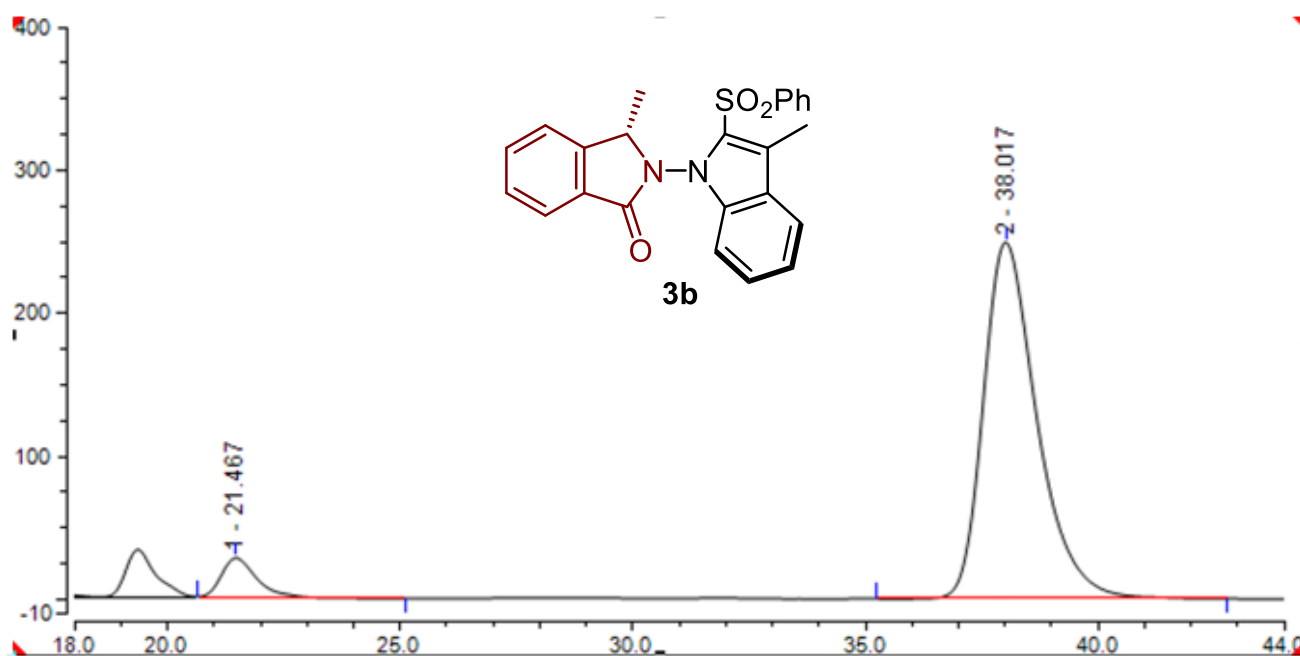
Ret. Time [min]					
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	35.66	23.802	19.301	2.47	2.93
2	41.98	958.447	638.975	97.58	97.07



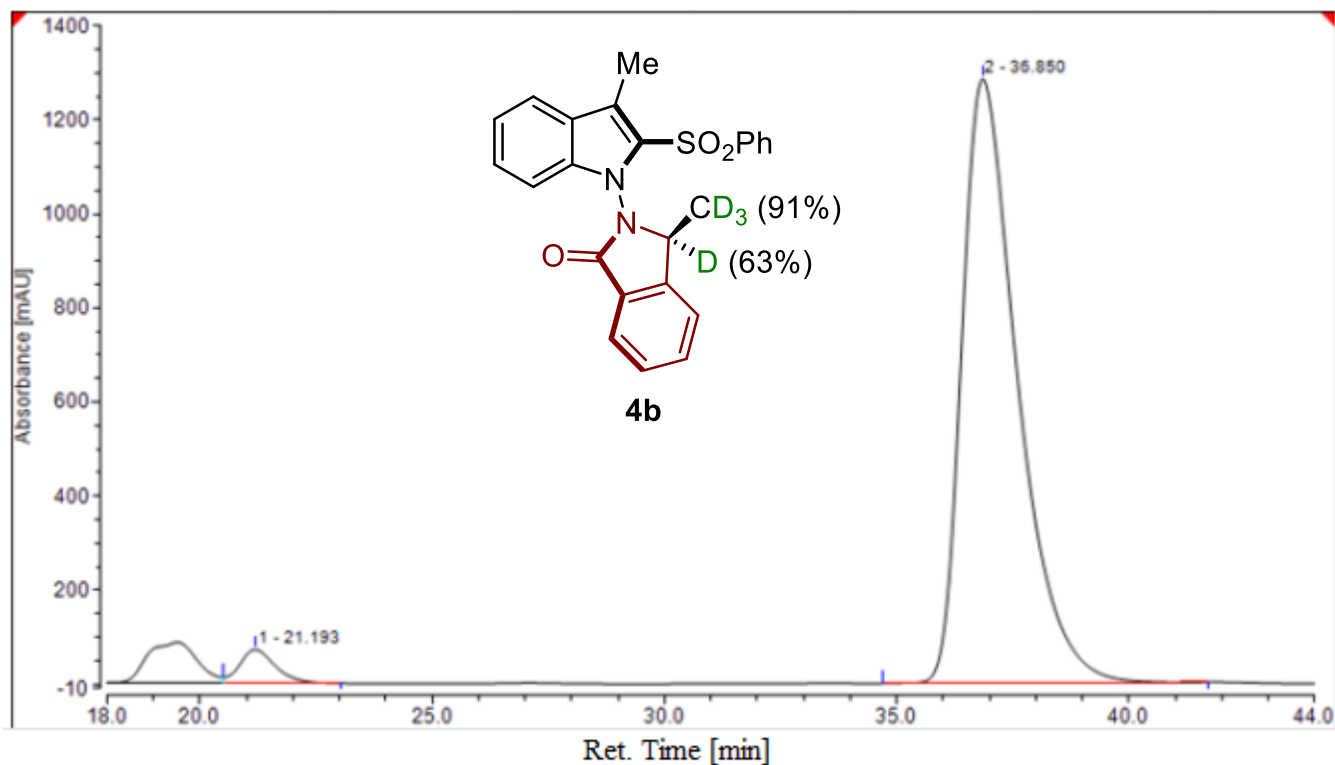
Ret. Time [min]					
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	35.81	77.528	57.589	4.42	4.90
2	42.29	1677.914	1117.331	95.58	95.10



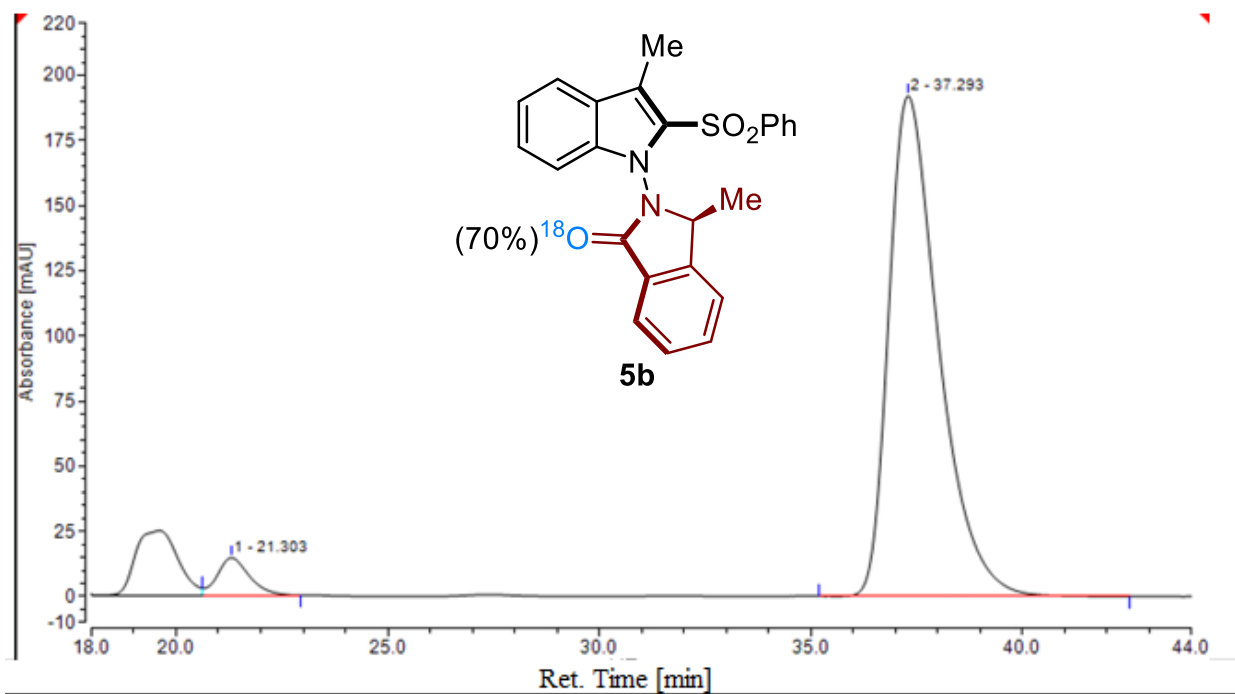
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	21.16	113.362	131.266	50.80	61.75
2	37.40	109.770	81.327	49.20	38.25



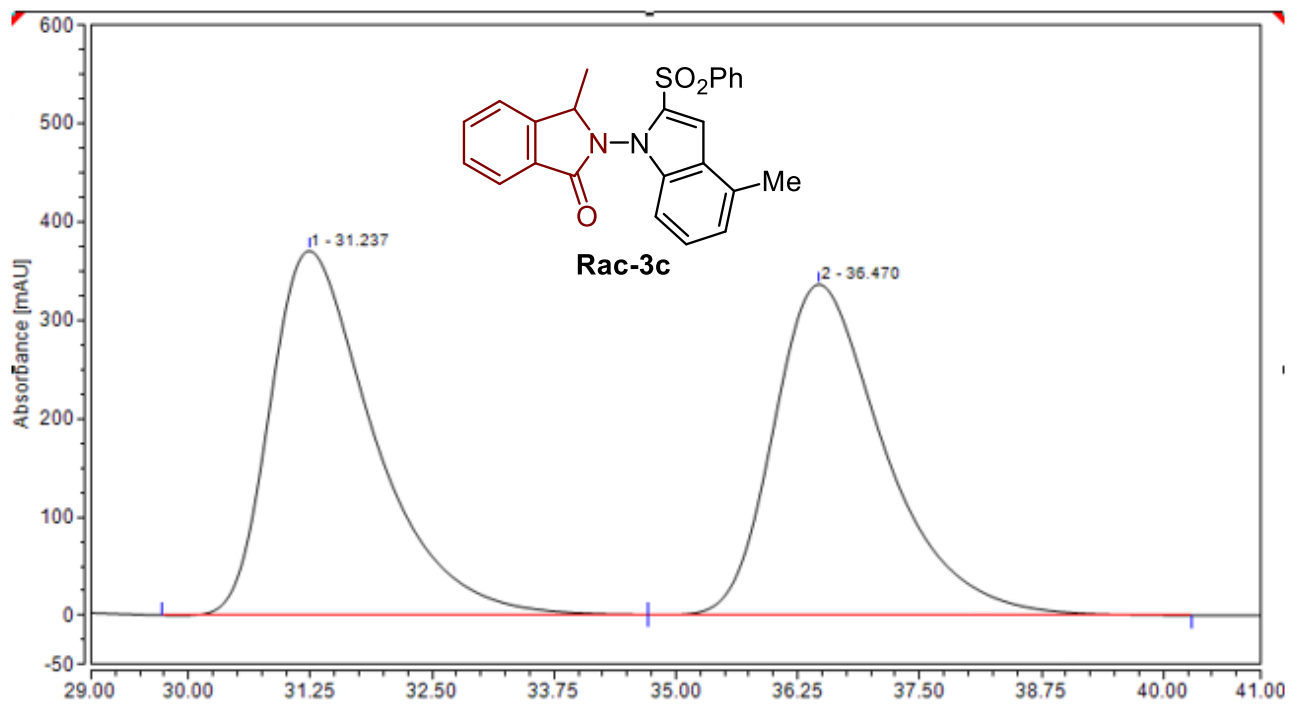
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	21.47	25.606	28.210	7.16	10.17
2	38.02	332.140	249.201	92.84	89.83



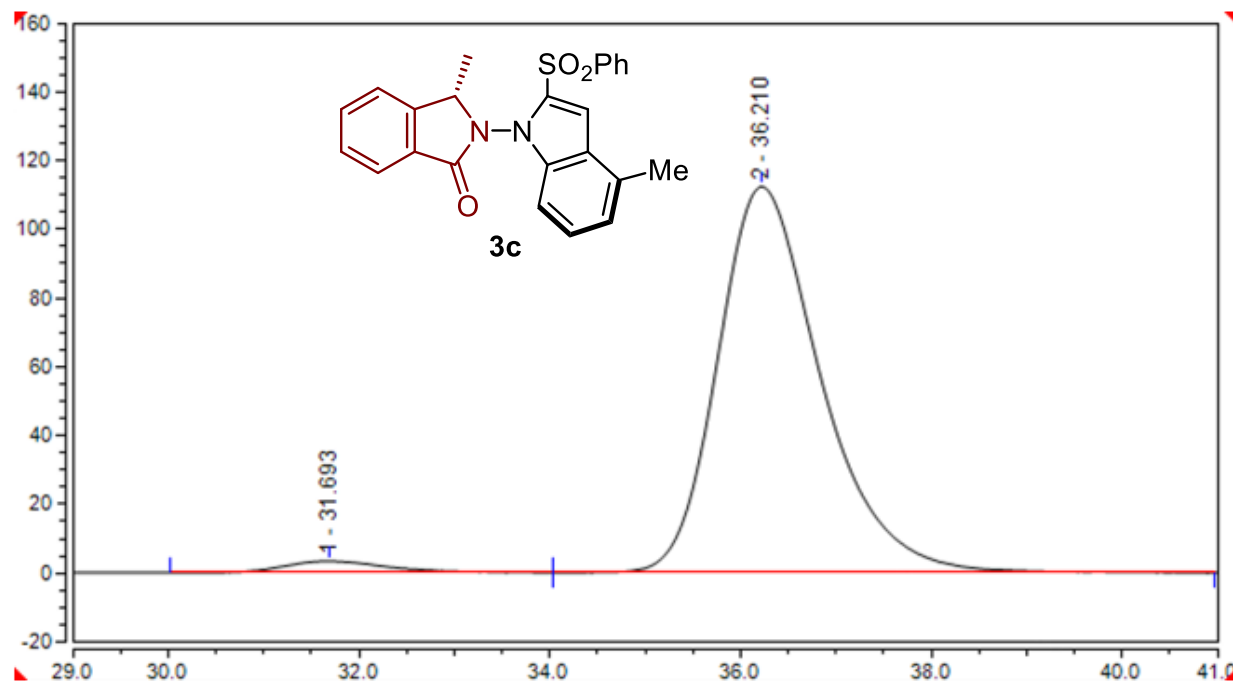
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	21.19	64.358	72.033	3.50	5.31
2	36.85	1773.571	1284.940	96.50	94.69



Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	21.30	12.495	14.383	4.56	6.97
2	37.29	261.777	192.045	95.44	93.03

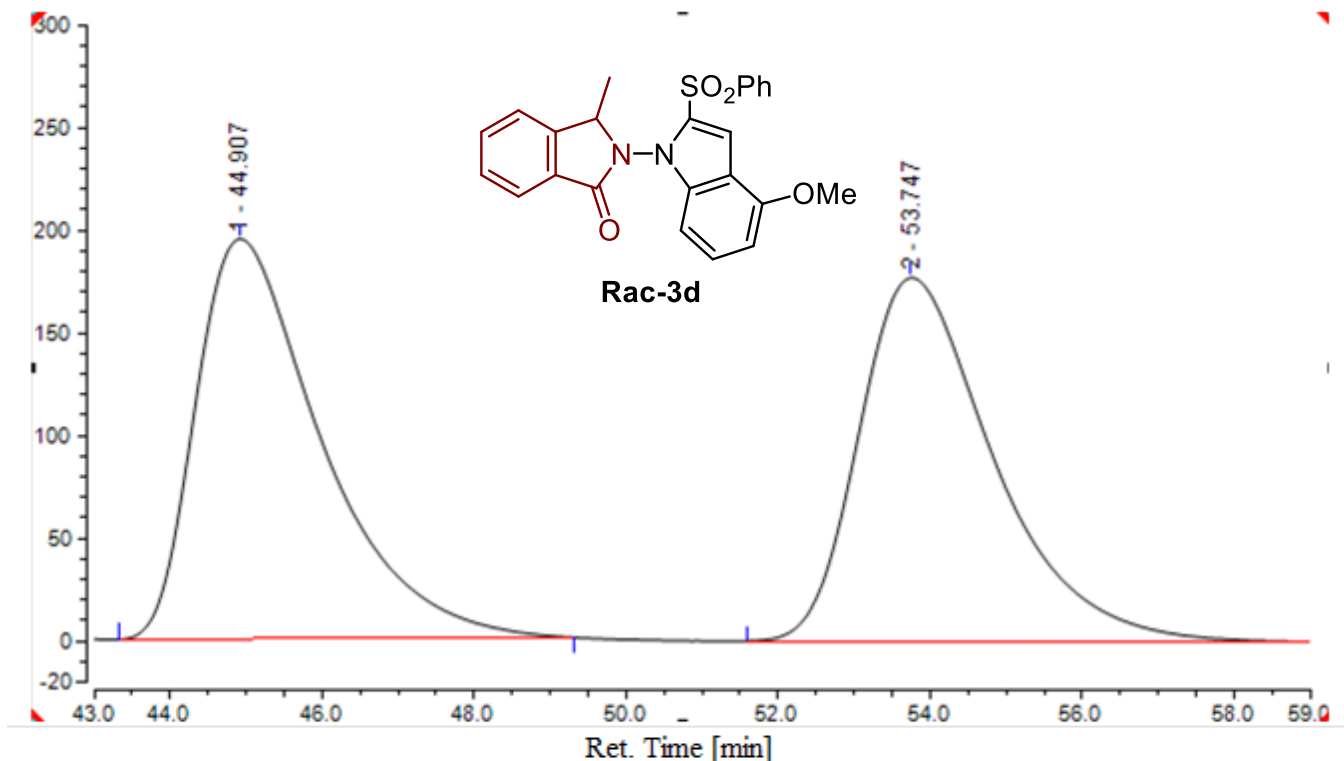


Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	31.24	457.811	370.131	50.66	52.41
2	36.47	445.936	336.025	49.34	47.59

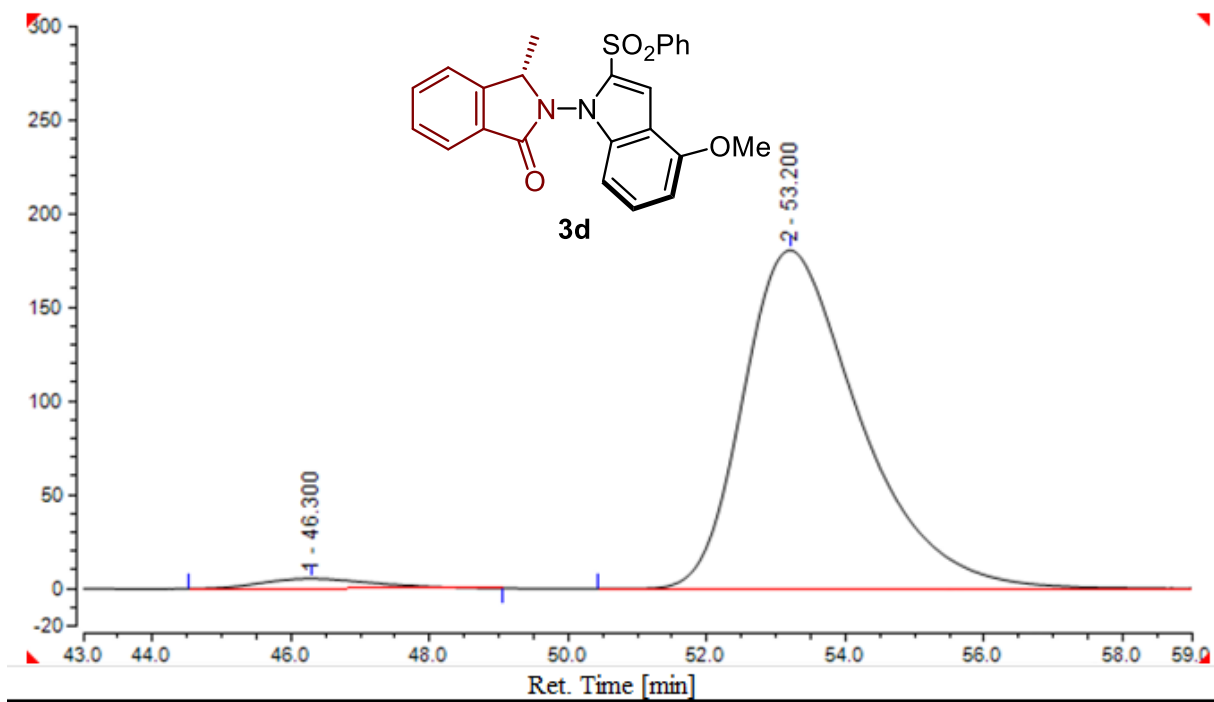


Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	31.69	4.265	3.381	2.94	2.92
2	36.21	140.892	112.285	97.06	97.08

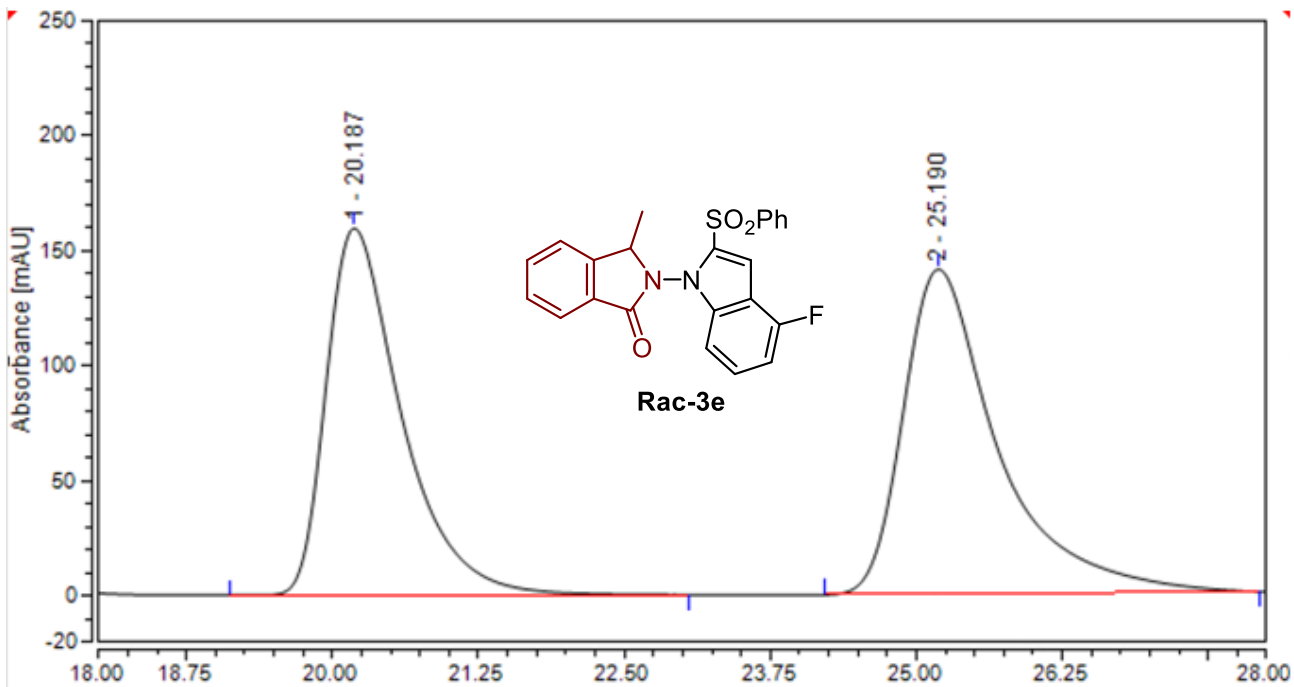




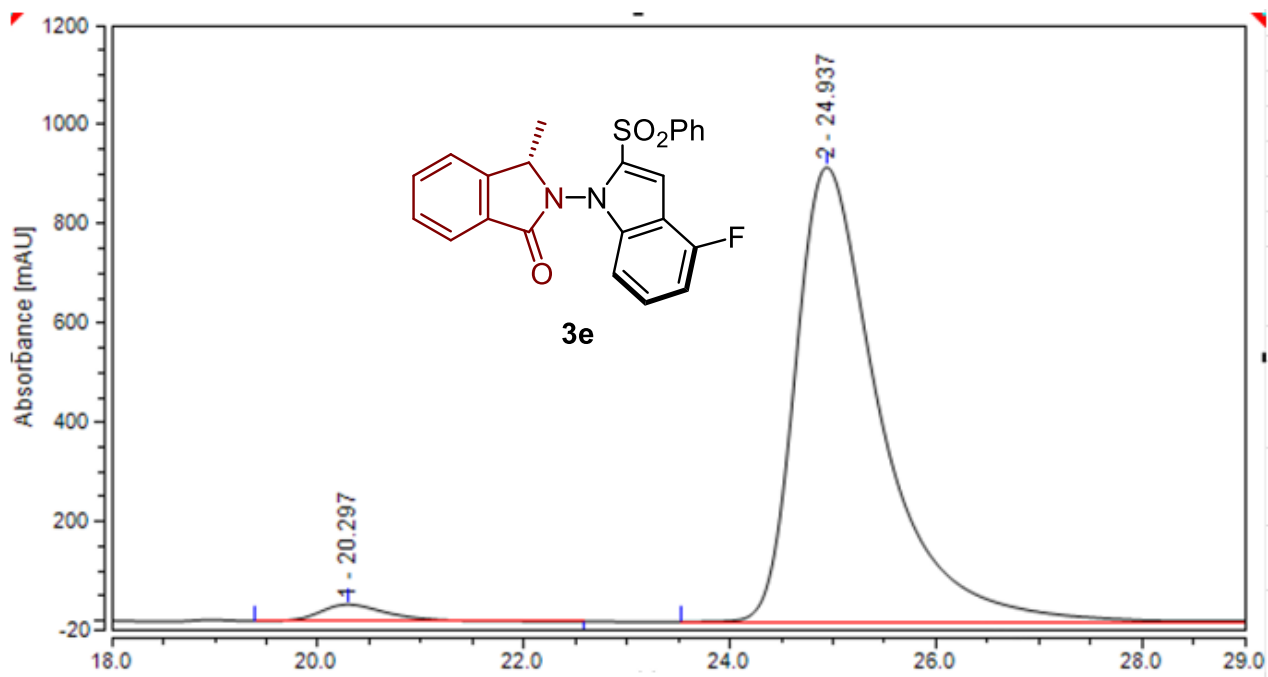
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	44.91	372.195	194.768	50.55	52.37
2	53.75	364.089	177.116	49.45	47.63



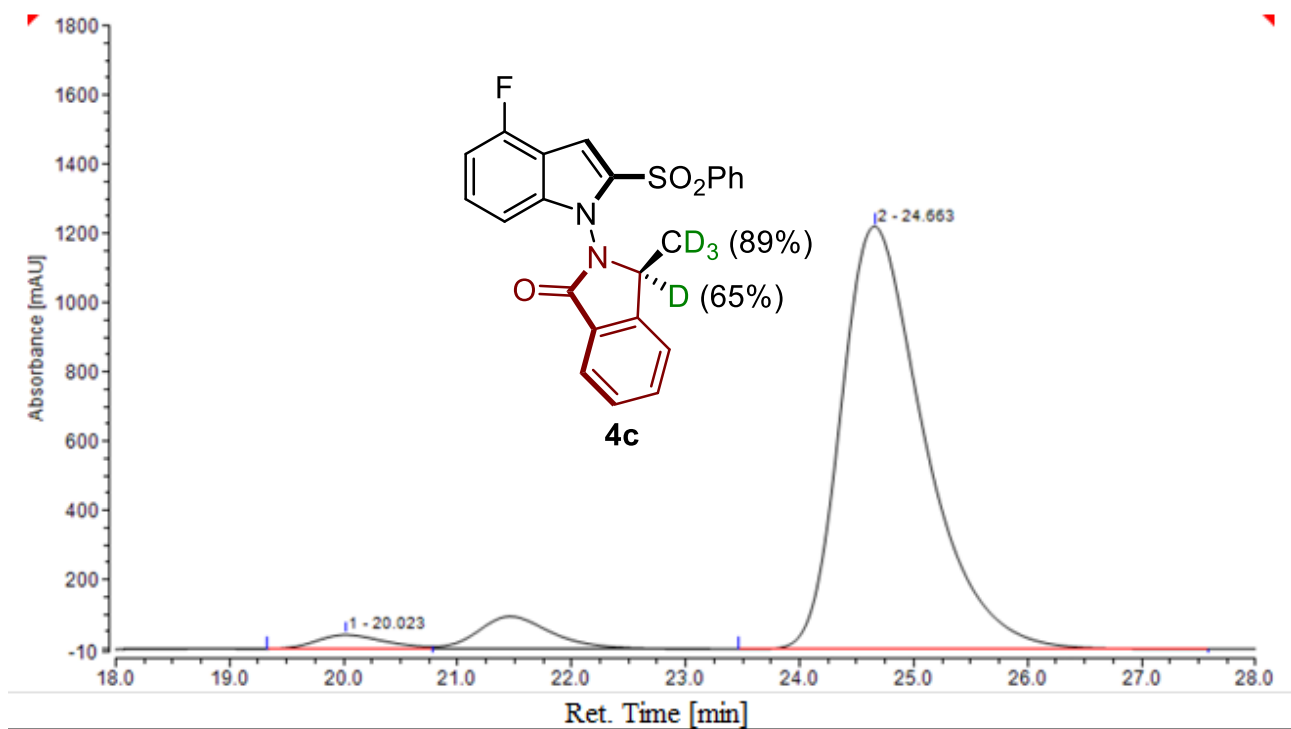
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	46.30	10.038	5.307	2.77	2.86
2	53.20	351.799	180.498	97.23	97.14



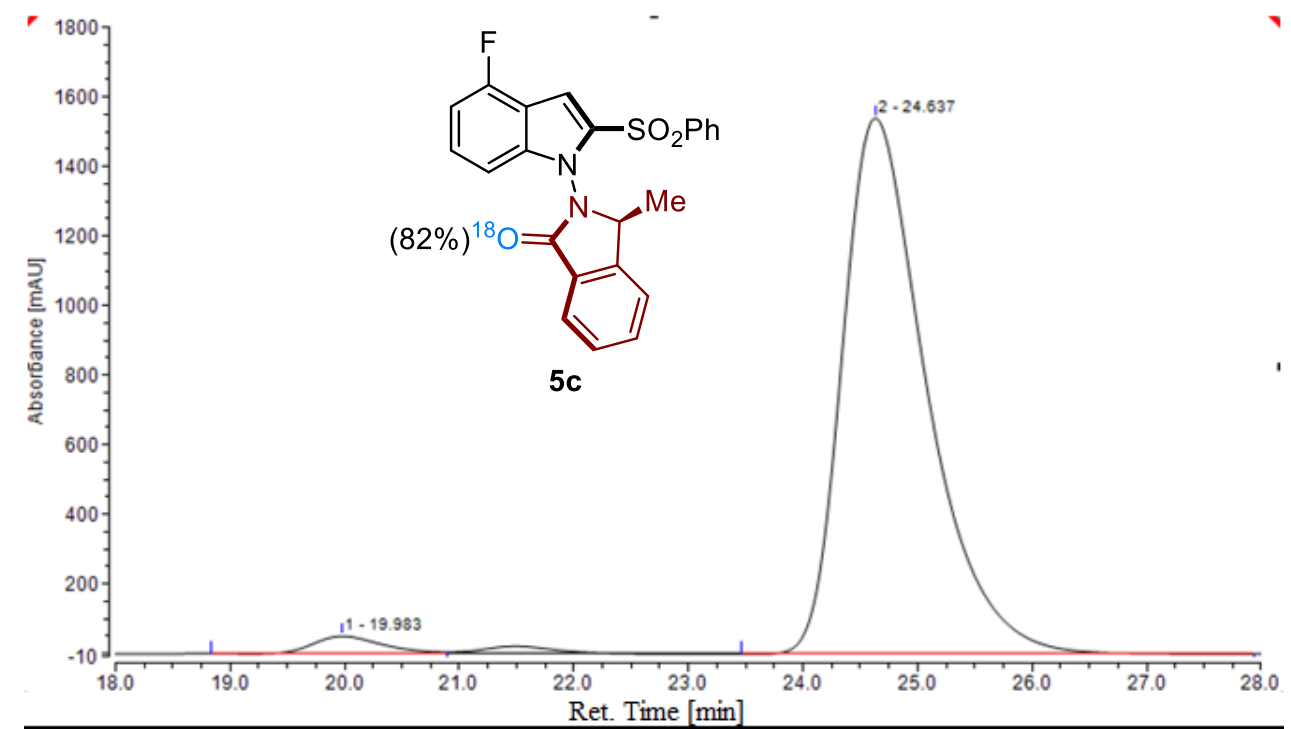
Ret. Time [min]					
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	20.19	118.600	159.153	47.25	53.04
2	25.19	132.398	140.905	52.75	46.96



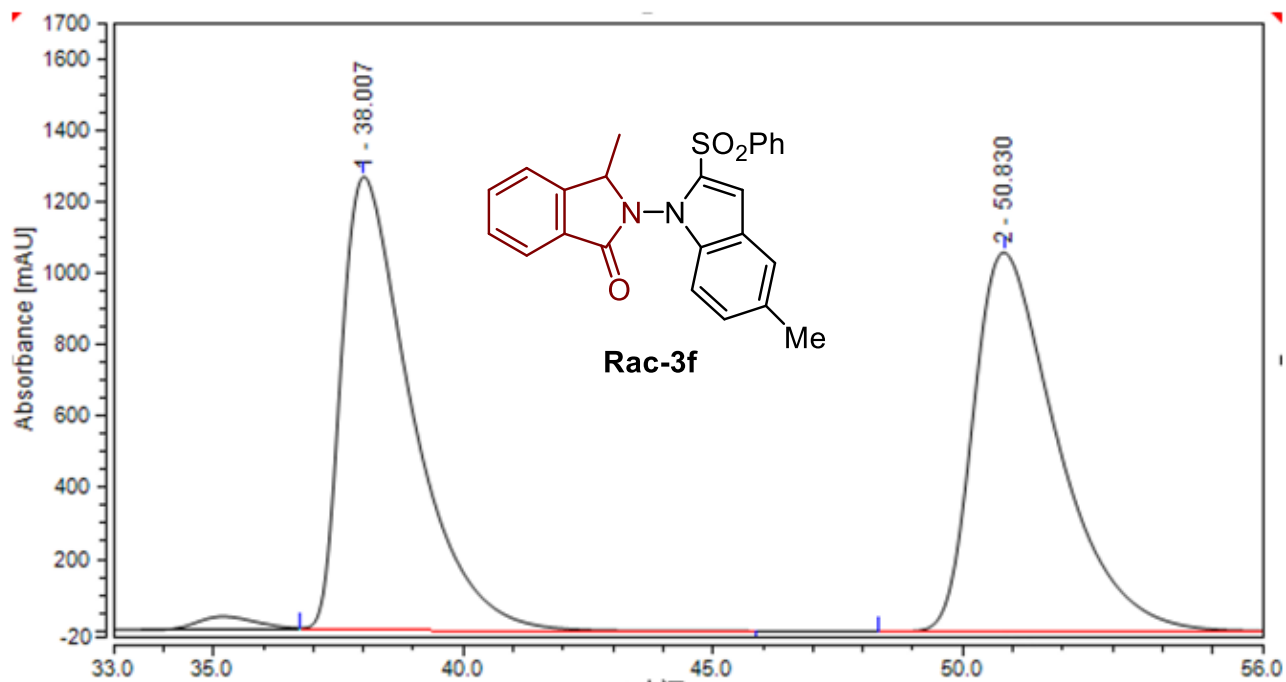
Ret. Time [min]					
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	20.30	26.275	33.712	2.93	3.55
2	24.94	870.214	916.240	97.07	96.45



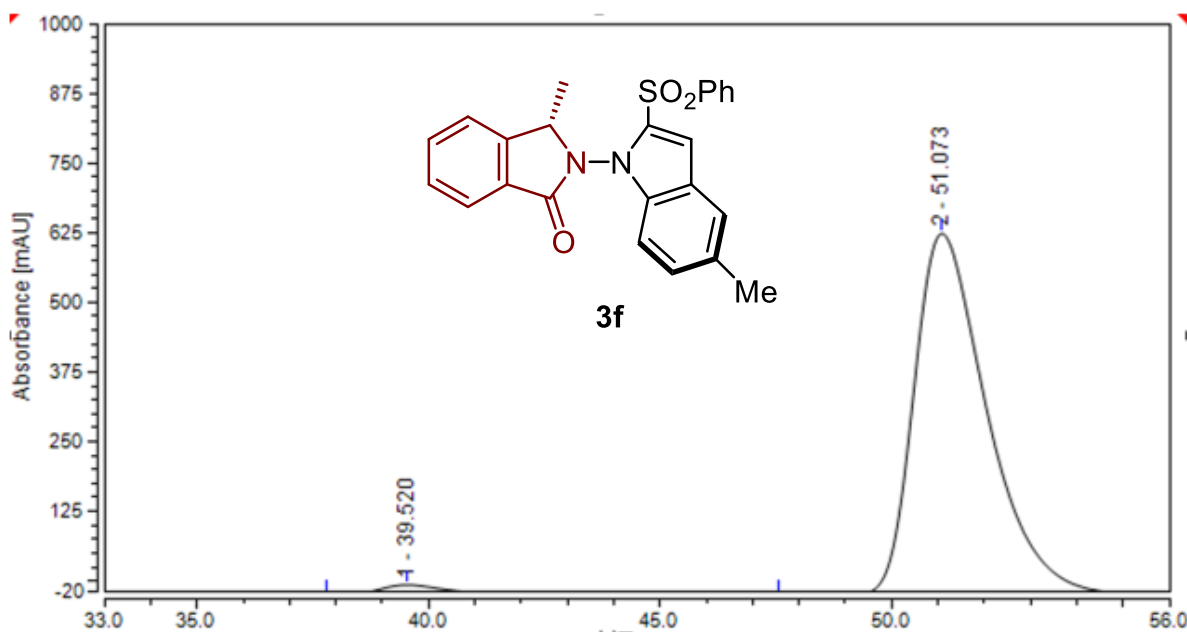
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	20.02	29.236	41.026	2.75	3.25
2	24.66	1033.255	1221.021	97.25	96.75



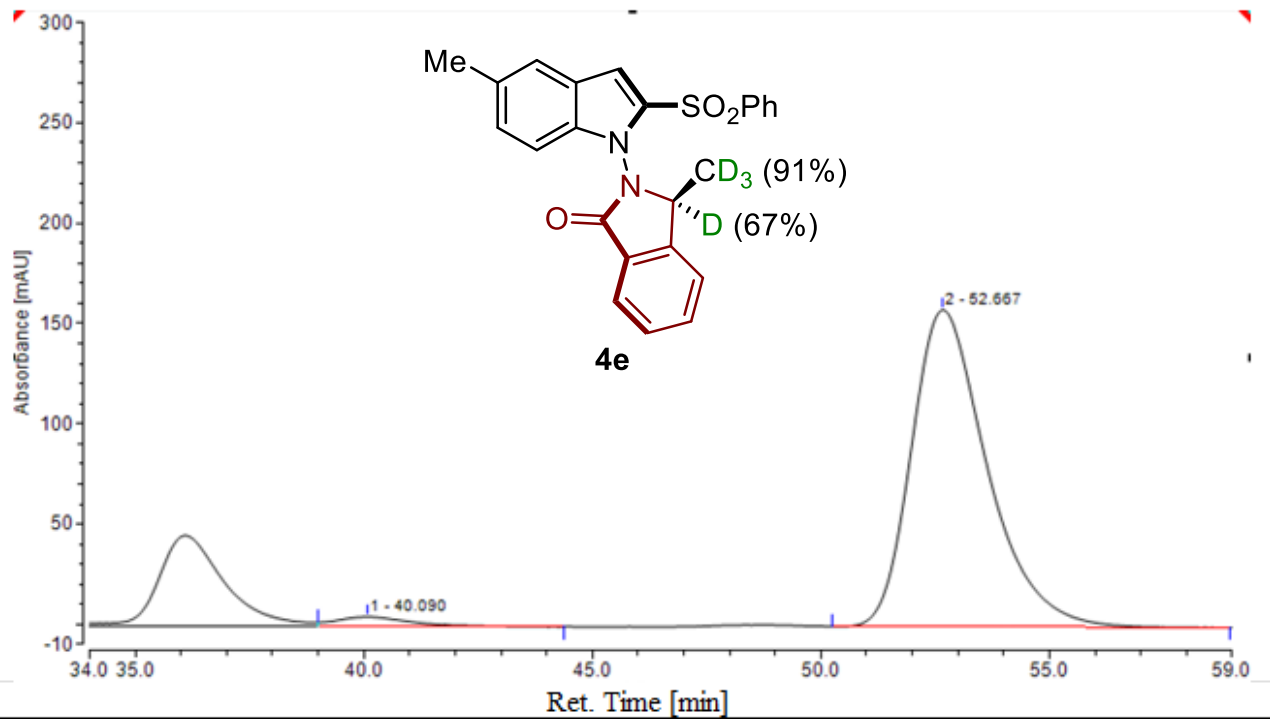
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	19.98	35.520	50.033	2.65	3.14
2	24.64	1302.971	1541.225	97.35	96.86



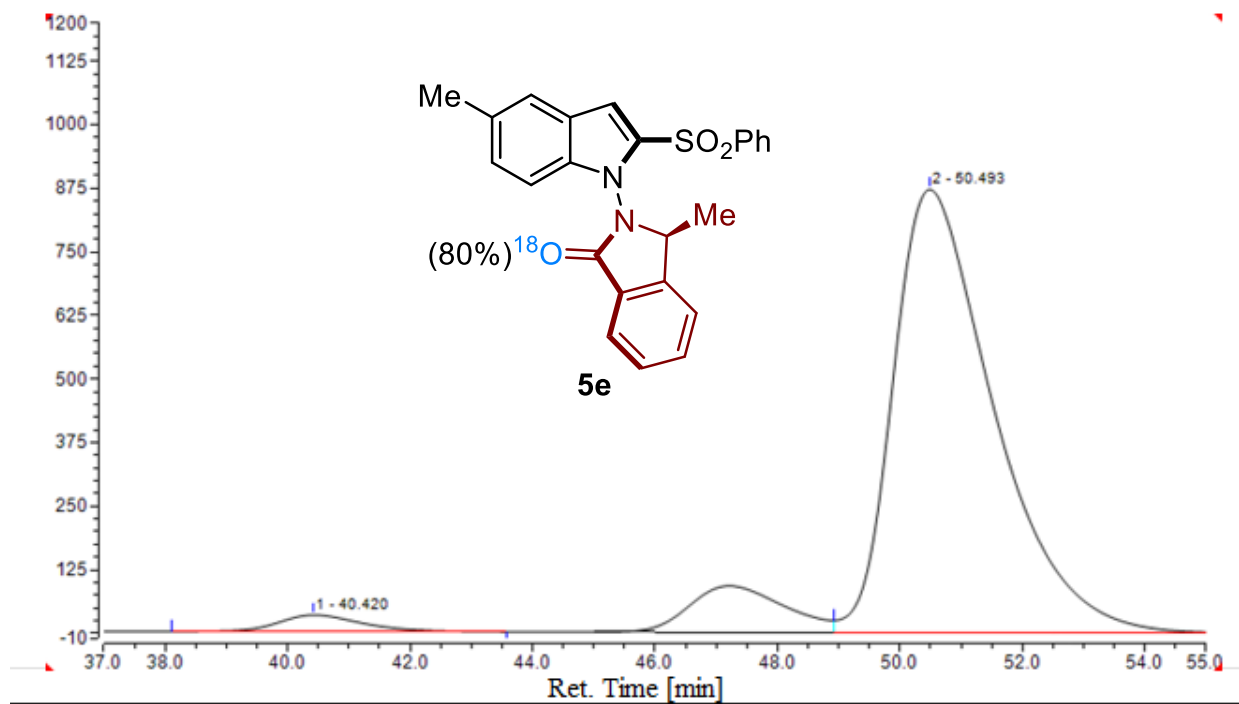
Ret. Time [min]					
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	38.01	2061.876	1269.205	49.93	54.48
2	50.83	2067.656	1060.375	50.07	45.52



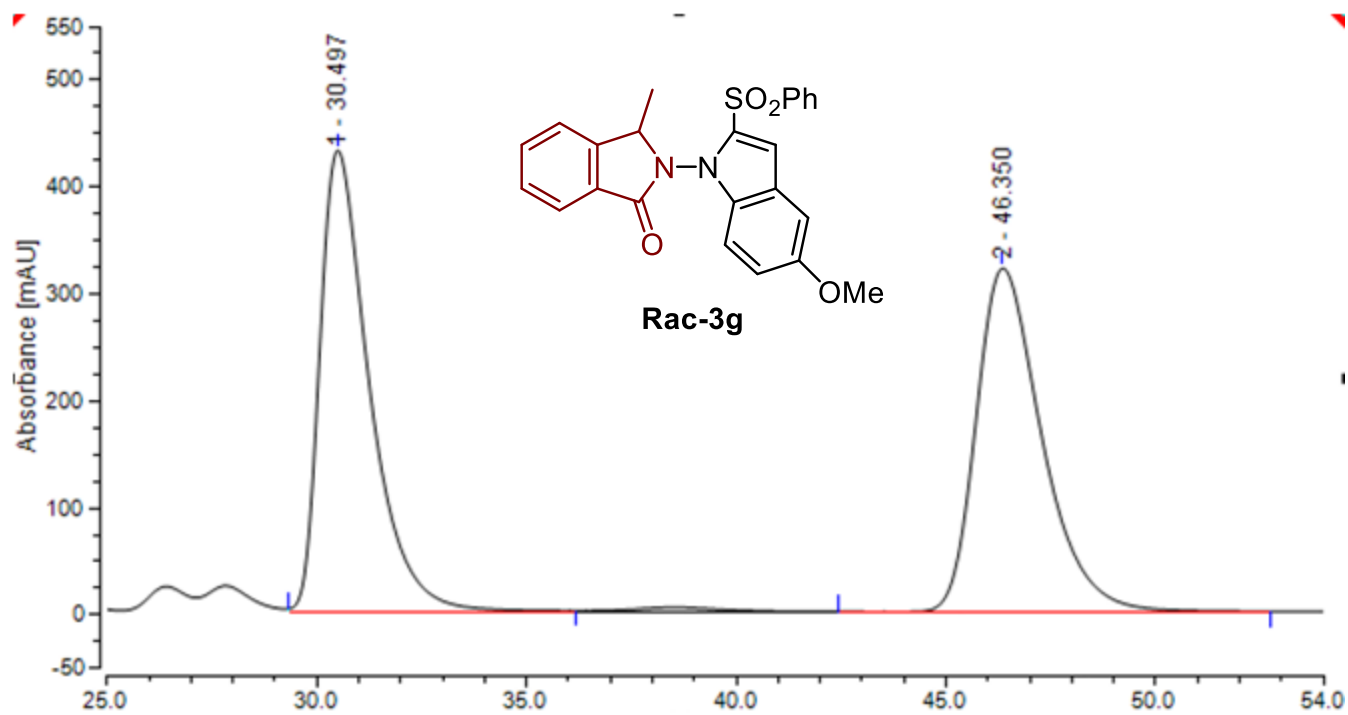
Ret. Time [min]					
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	39.52	28.402	17.222	2.36	2.59
2	51.07	1177.054	647.934	97.64	97.41



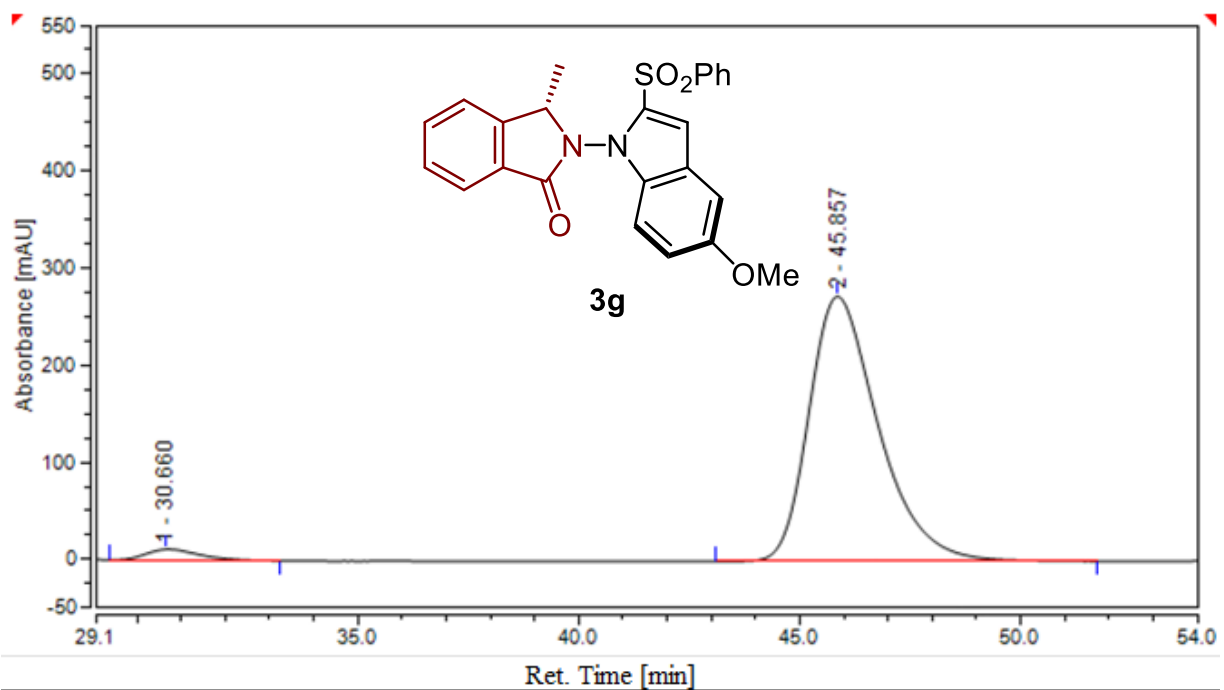
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	40.090	9.269	4.847	2.97	2.98
2	52.667	302.843	158.017	97.03	97.02



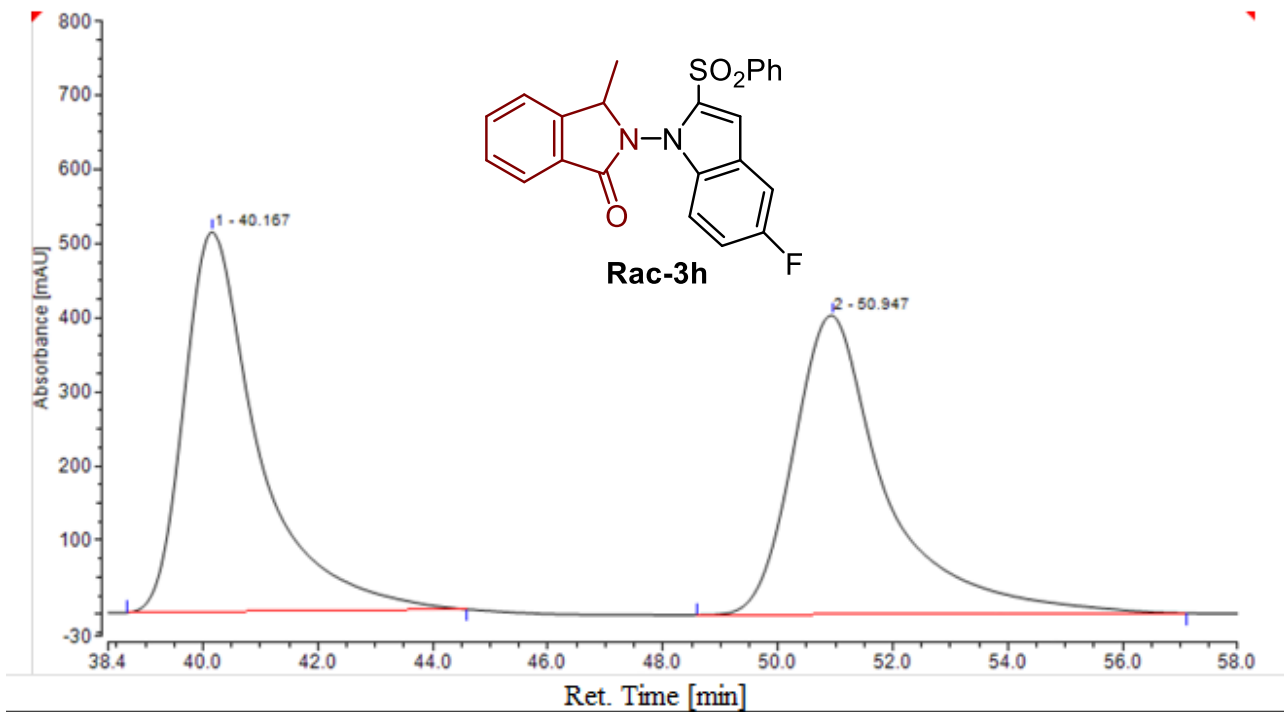
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	40.420	52.762	32.177	3.09	3.63
2	50.493	1653.888	871.207	96.91	96.37



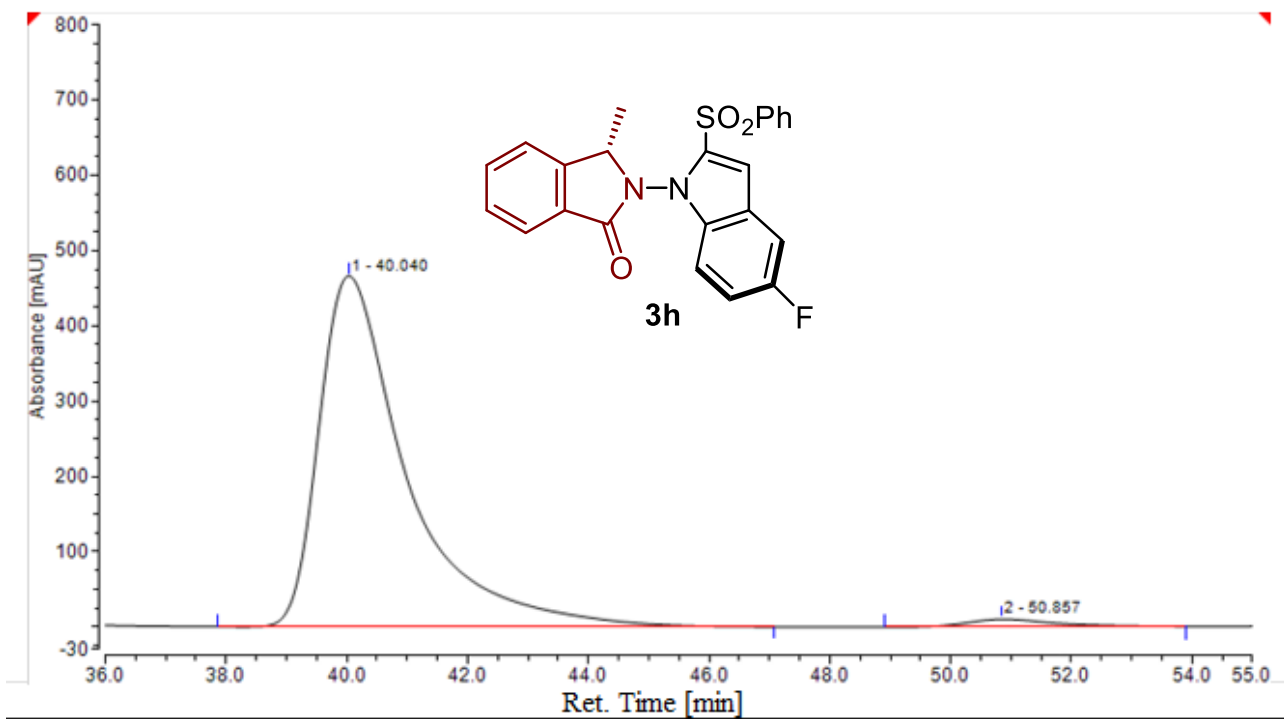
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	30.50	586.755	431.155	50.36	57.34
2	46.35	578.289	320.723	49.64	42.66



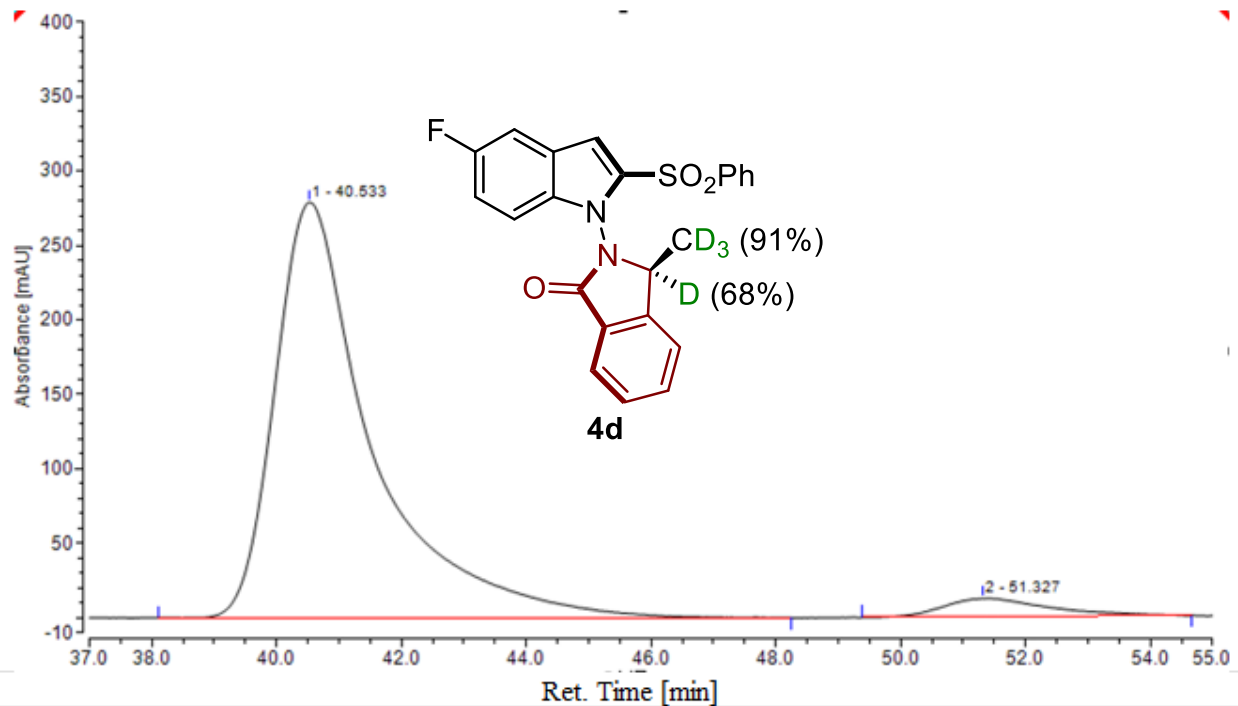
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	30.66	15.650	11.259	3.06	3.96
2	45.86	495.856	272.832	96.94	96.04



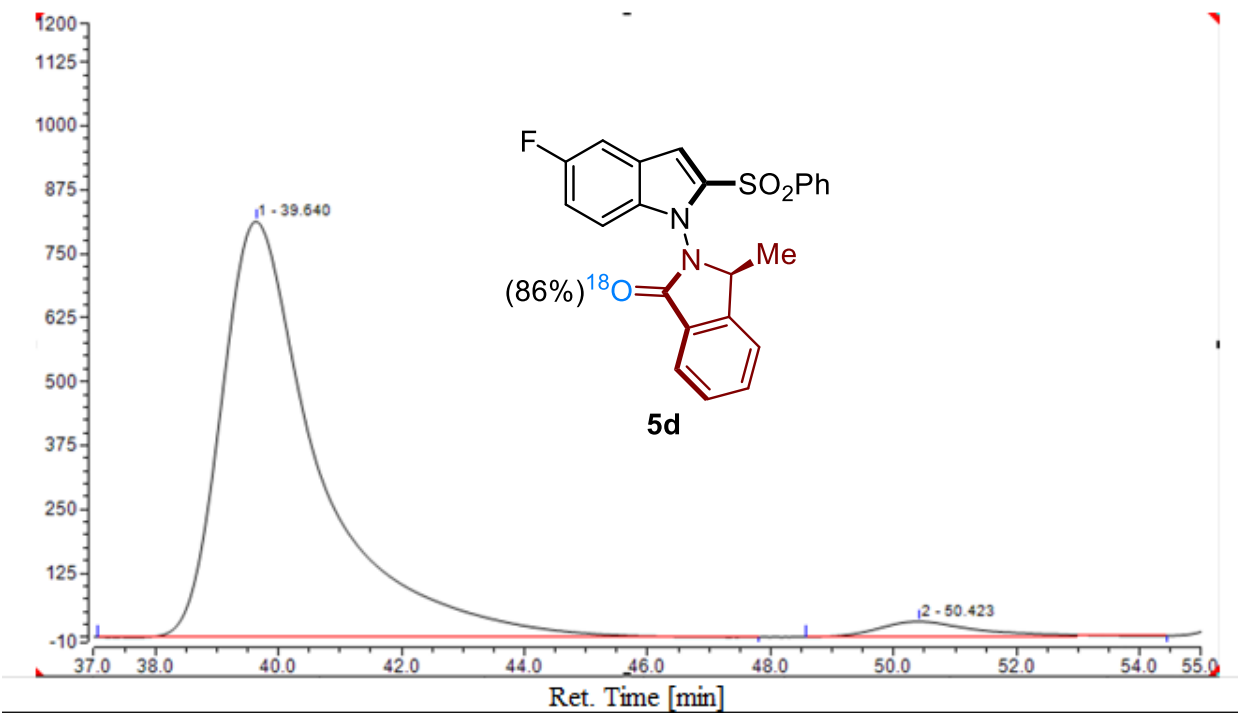
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	40.167	768.554	512.251	50.48	55.94
2	50.947	753.857	403.402	49.52	44.06



Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	40.040	782.646	466.134	97.91	97.89
2	50.857	16.743	10.043	2.09	2.11

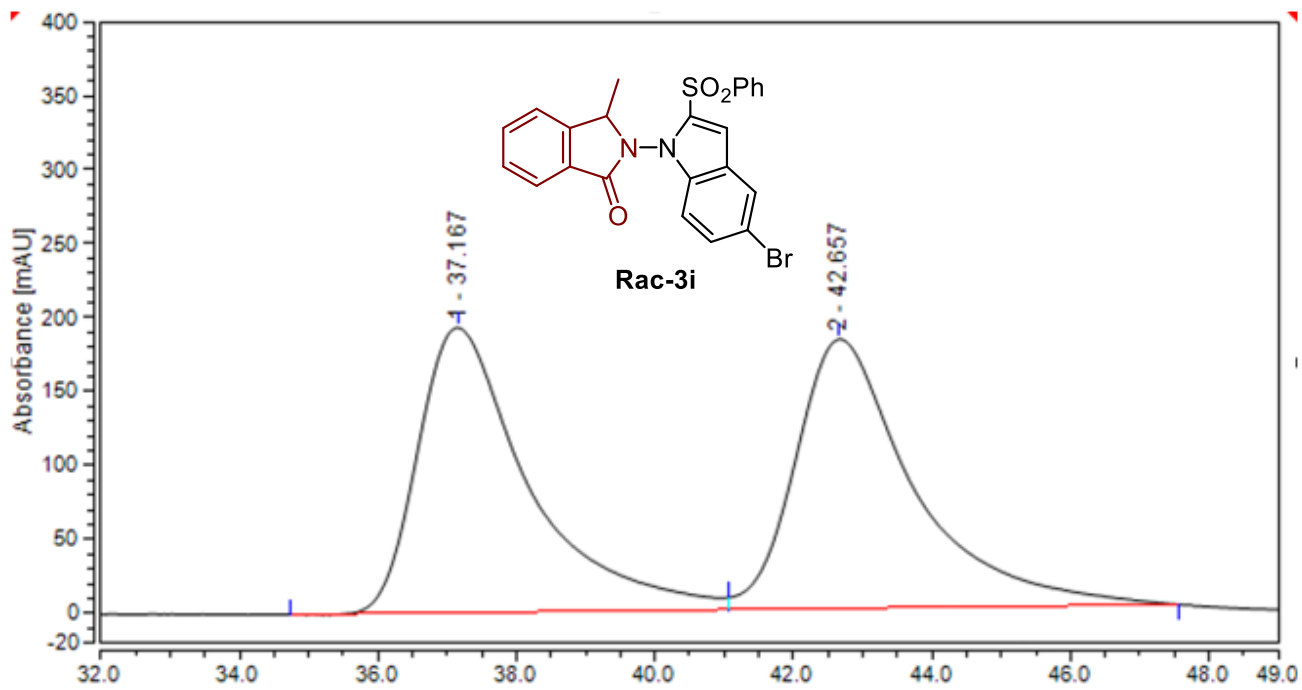


Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	40.533	501.535	278.743	95.44	95.78
2	51.327	23.955	12.267	4.56	4.22

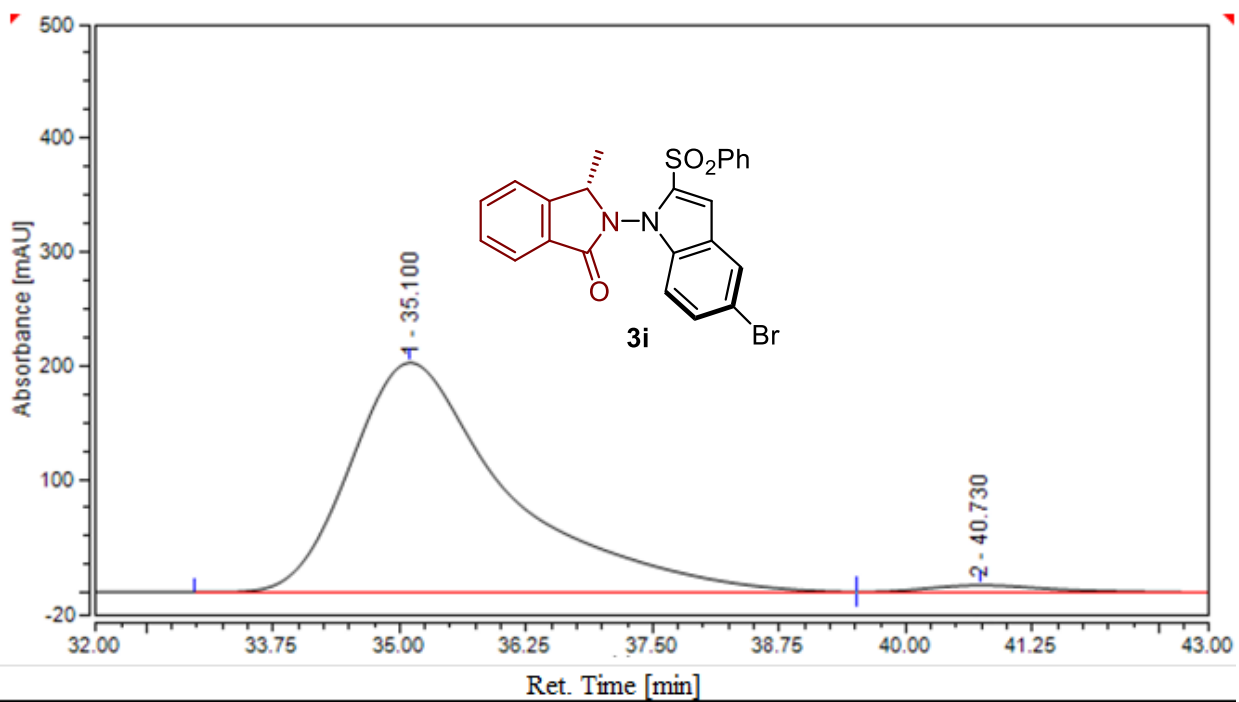


Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	39.640	1497.473	813.561	96.55	96.52
2	50.423	53.441	29.346	3.45	3.48

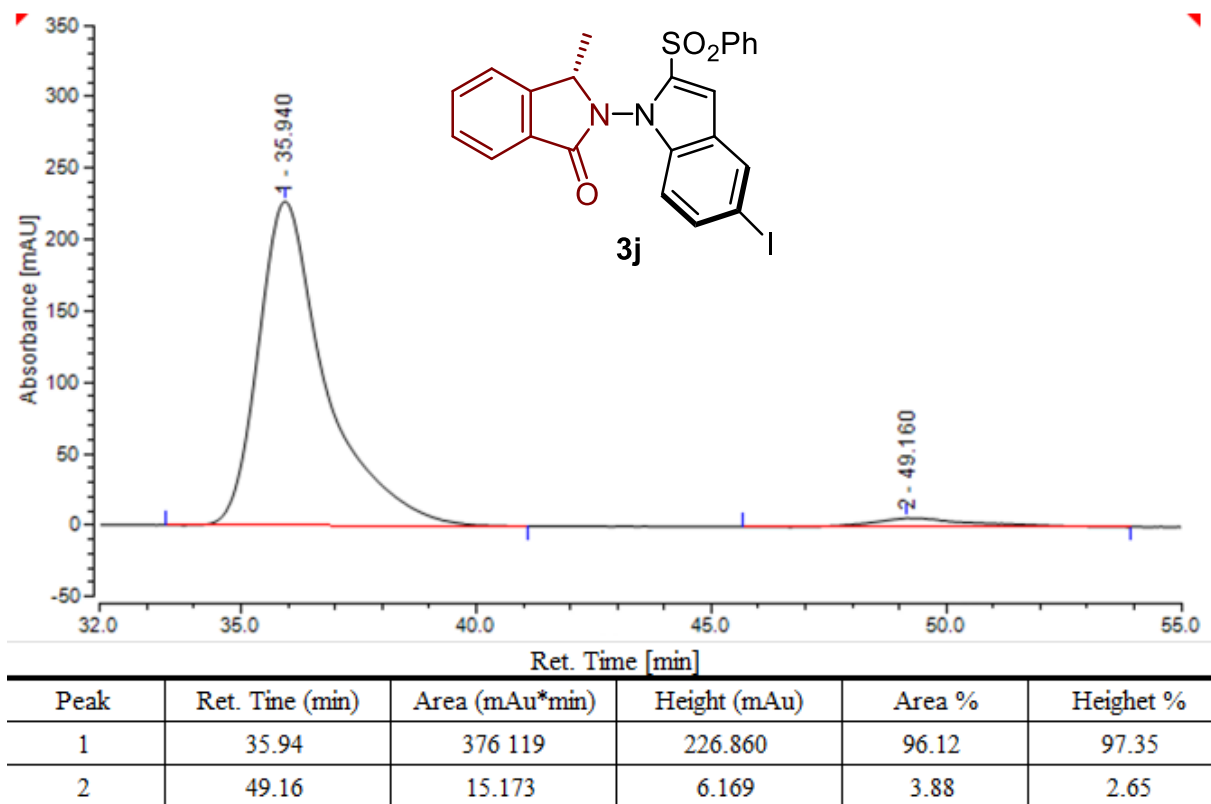
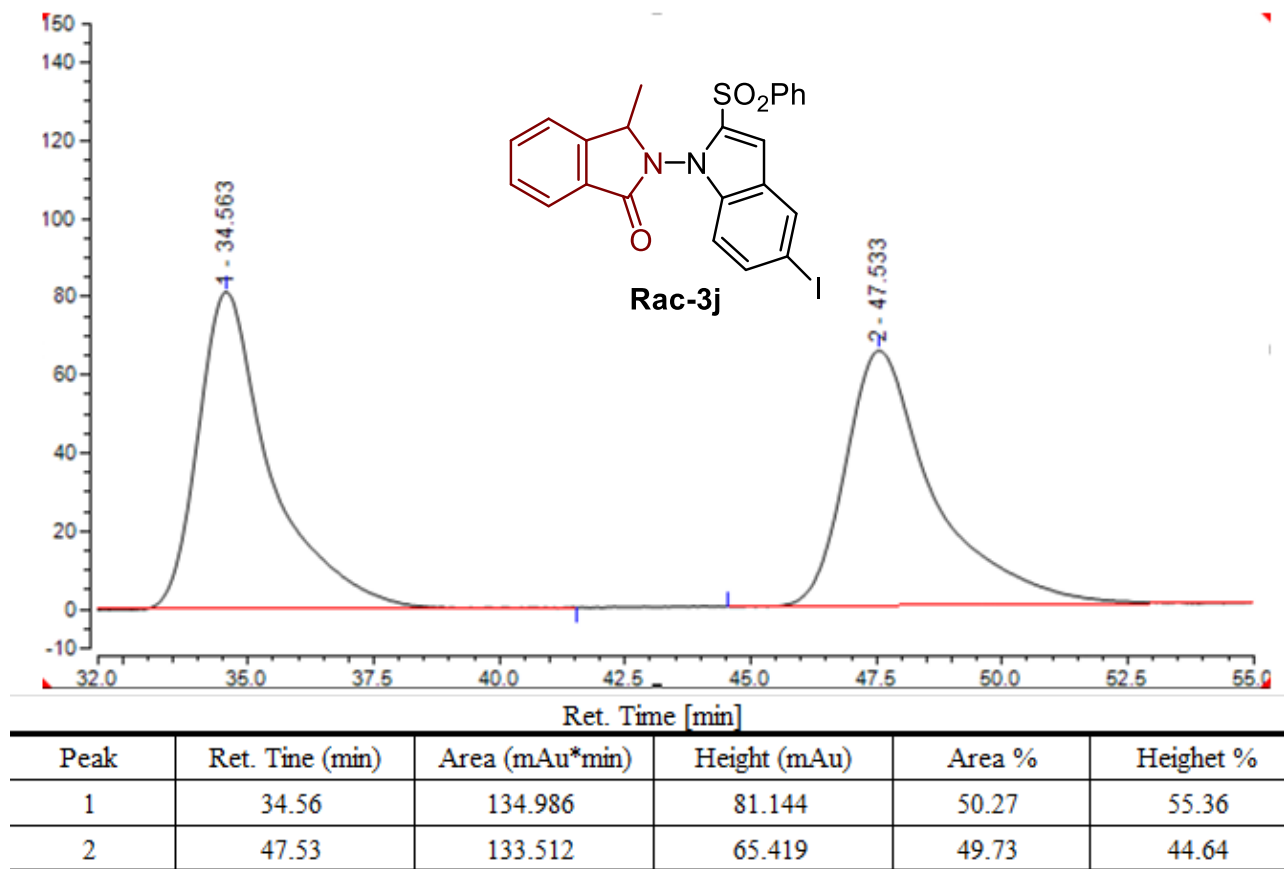


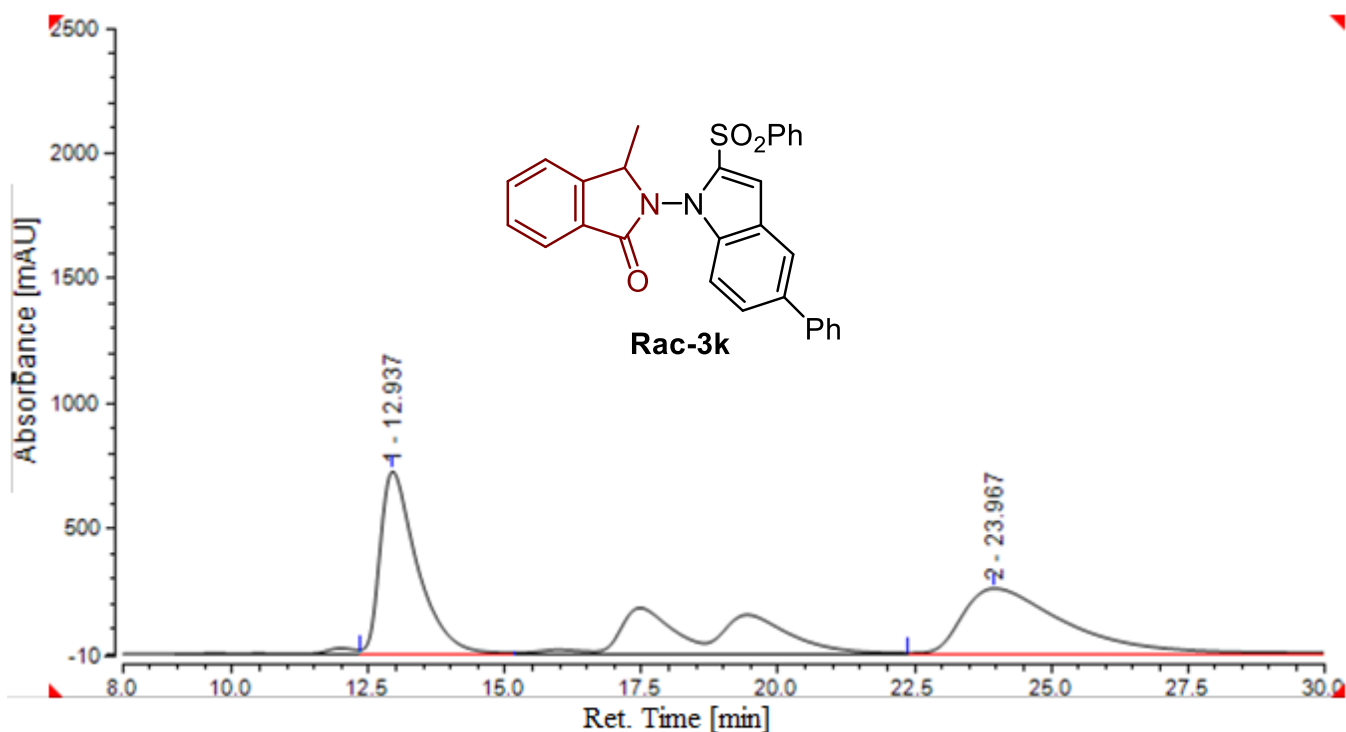


Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	37.17	357.105	192.645	49.84	51.43
2	42.66	359.417	181.960	50.16	48.57

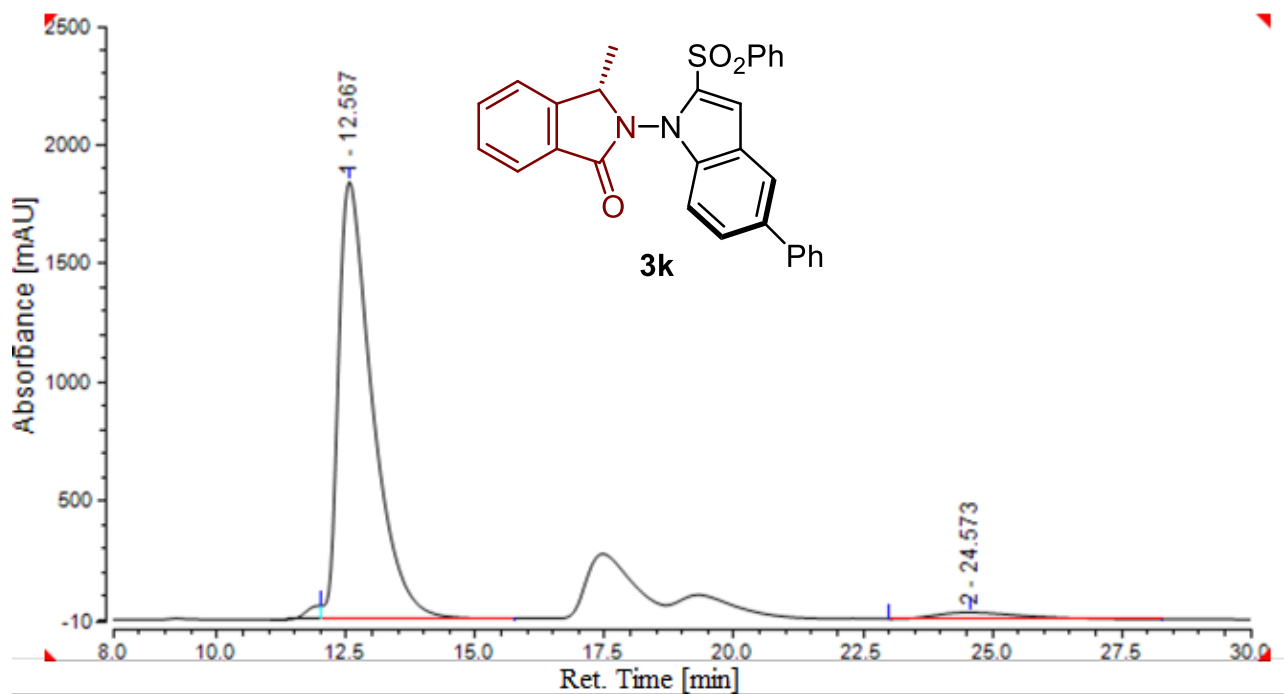


Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	35.10	364.086	201.747	97.56	96.97
2	40.73	9.103	6.296	2.44	3.03

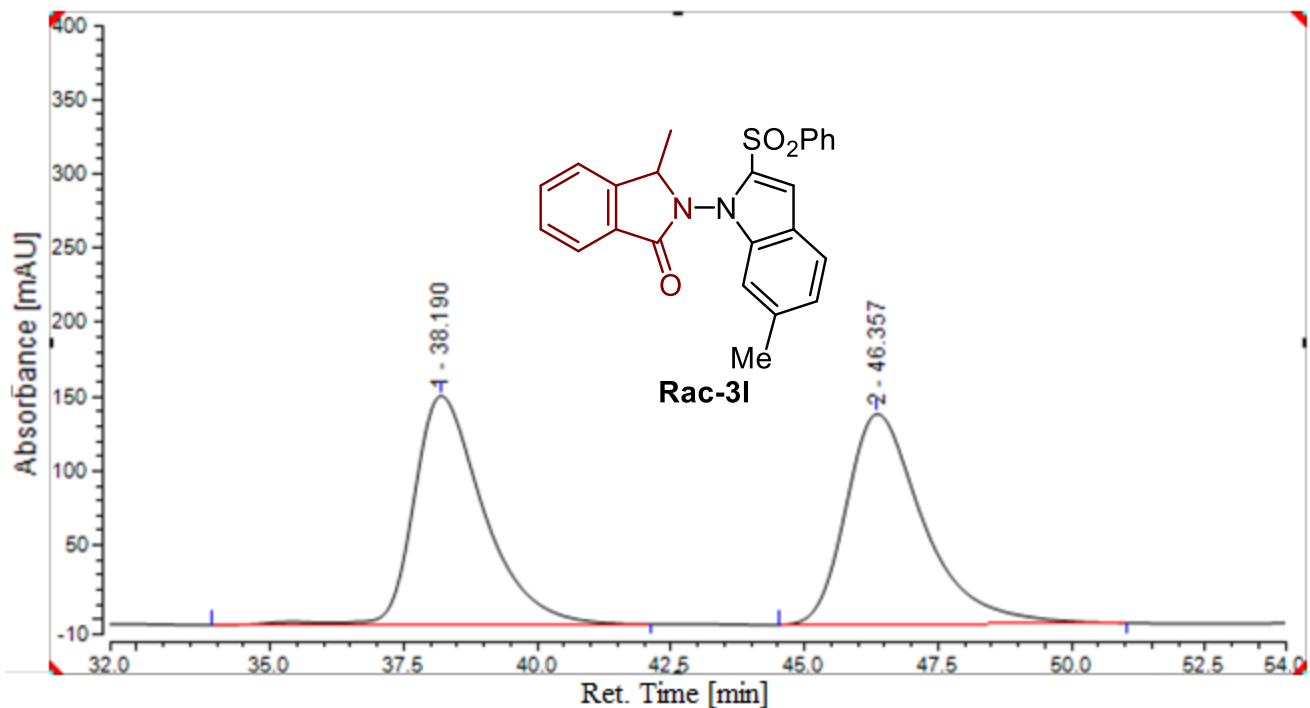




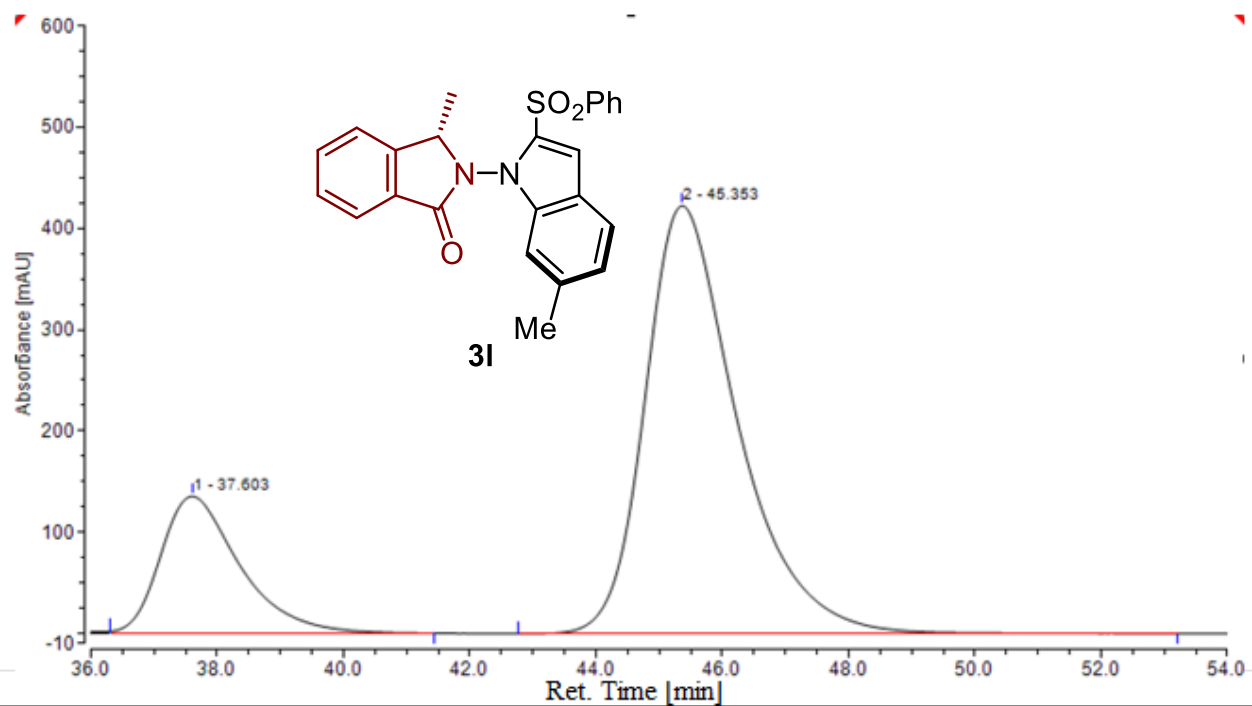
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	12.940	574.239	729.857	49.73	73.62
2	23.970	580.502	261.516	50.27	26.38



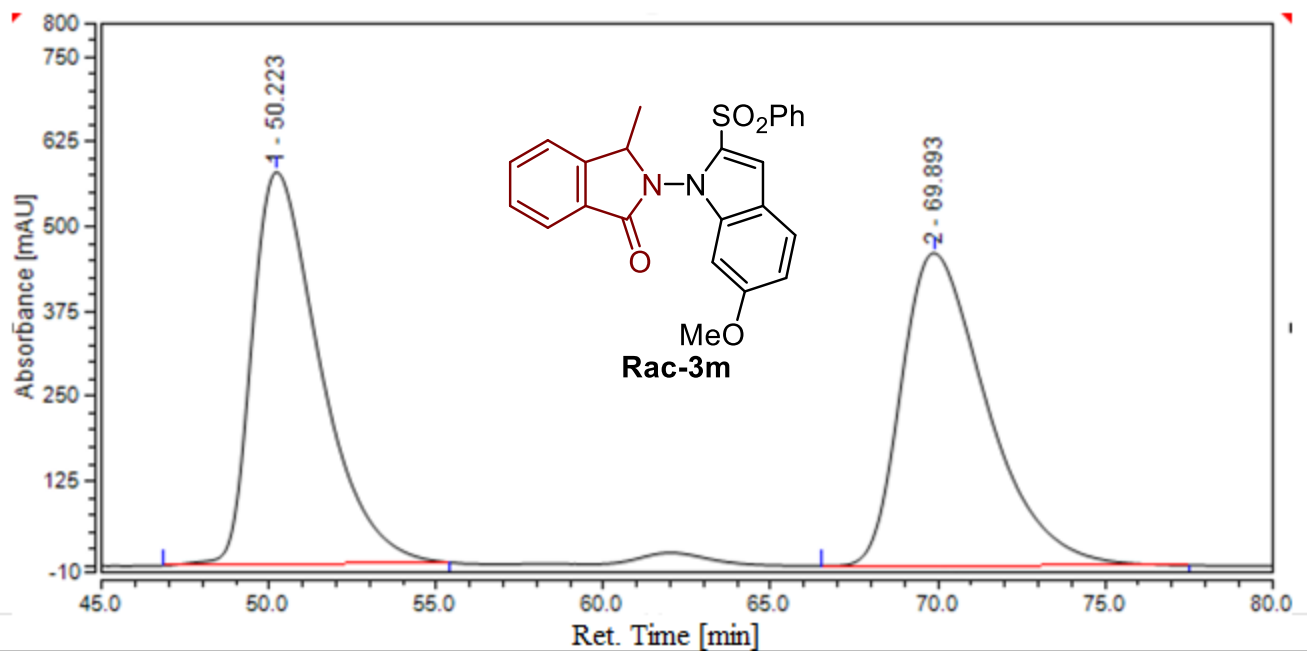
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	12.567	1396.576	1844.393	96.26	98.53
2	24.573	54.268	27.490	3.74	1.47



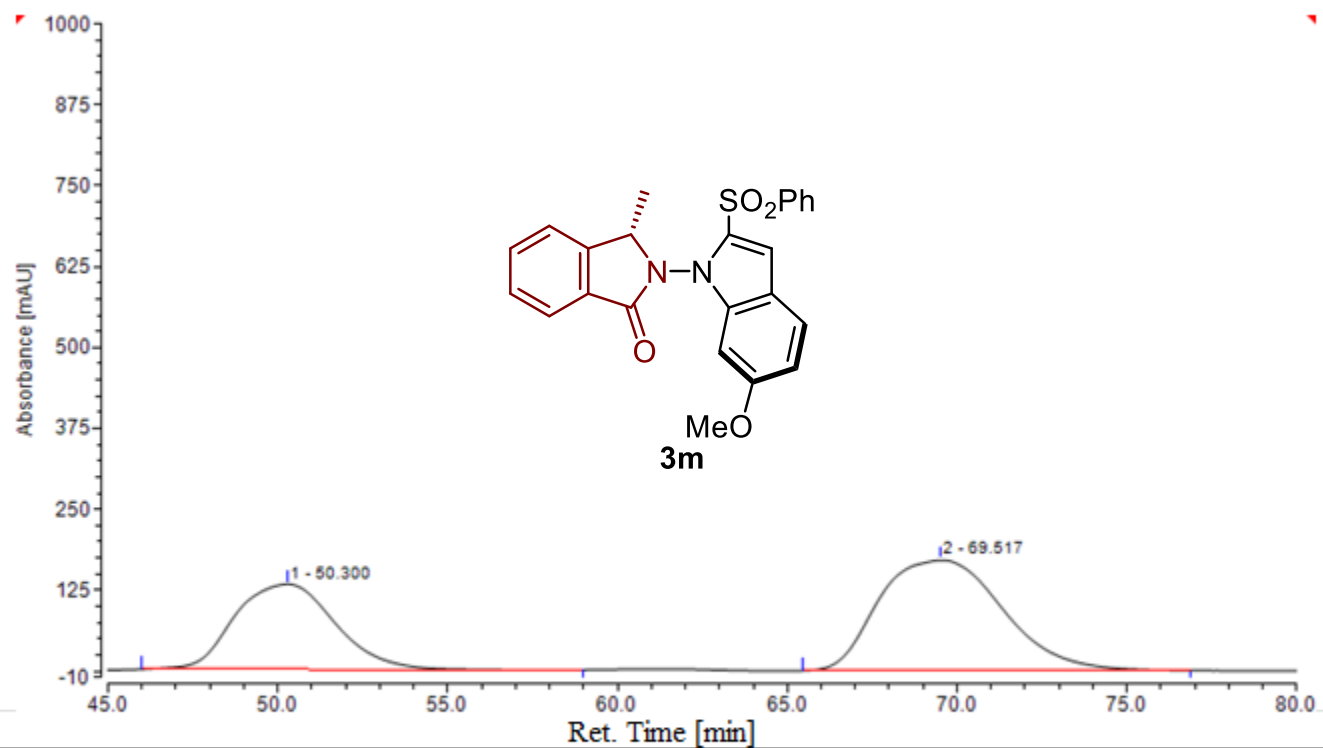
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	38.19	234.075	154.168	49.58	52.10
2	46.36	238.051	141.760	50.42	47.90



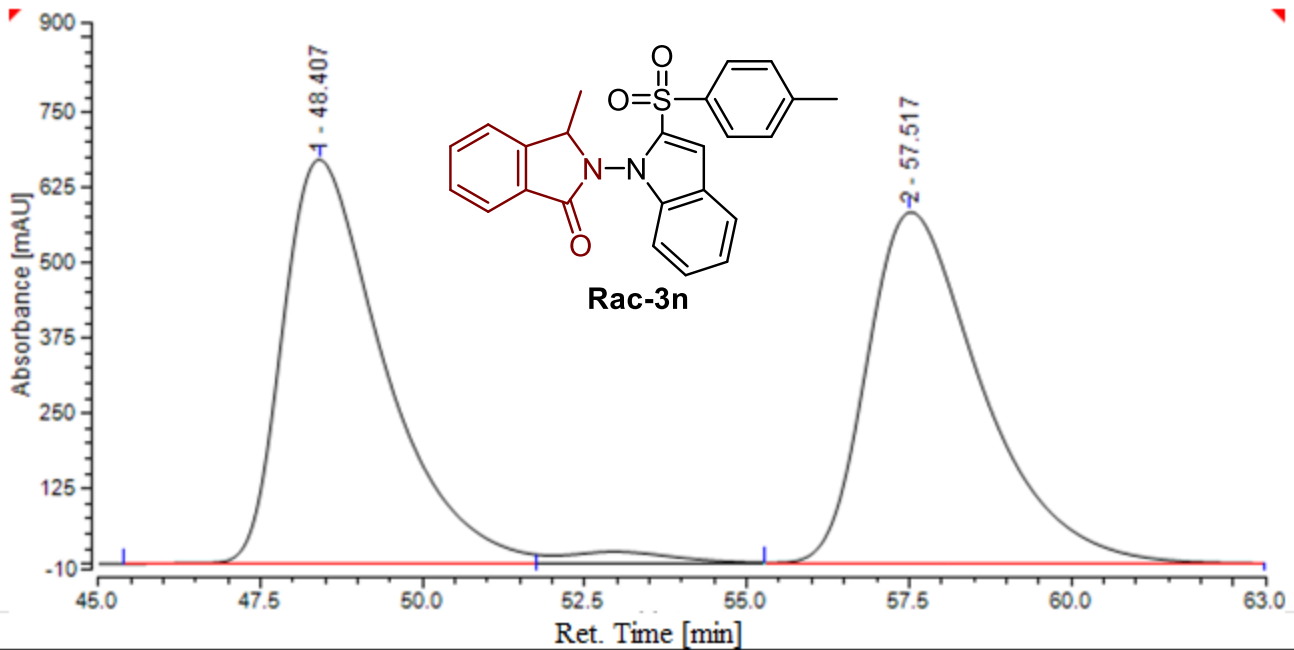
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	37.60	196.292	135.300	21.49	24.26
2	45.35	717.196	422.511	78.51	75.74



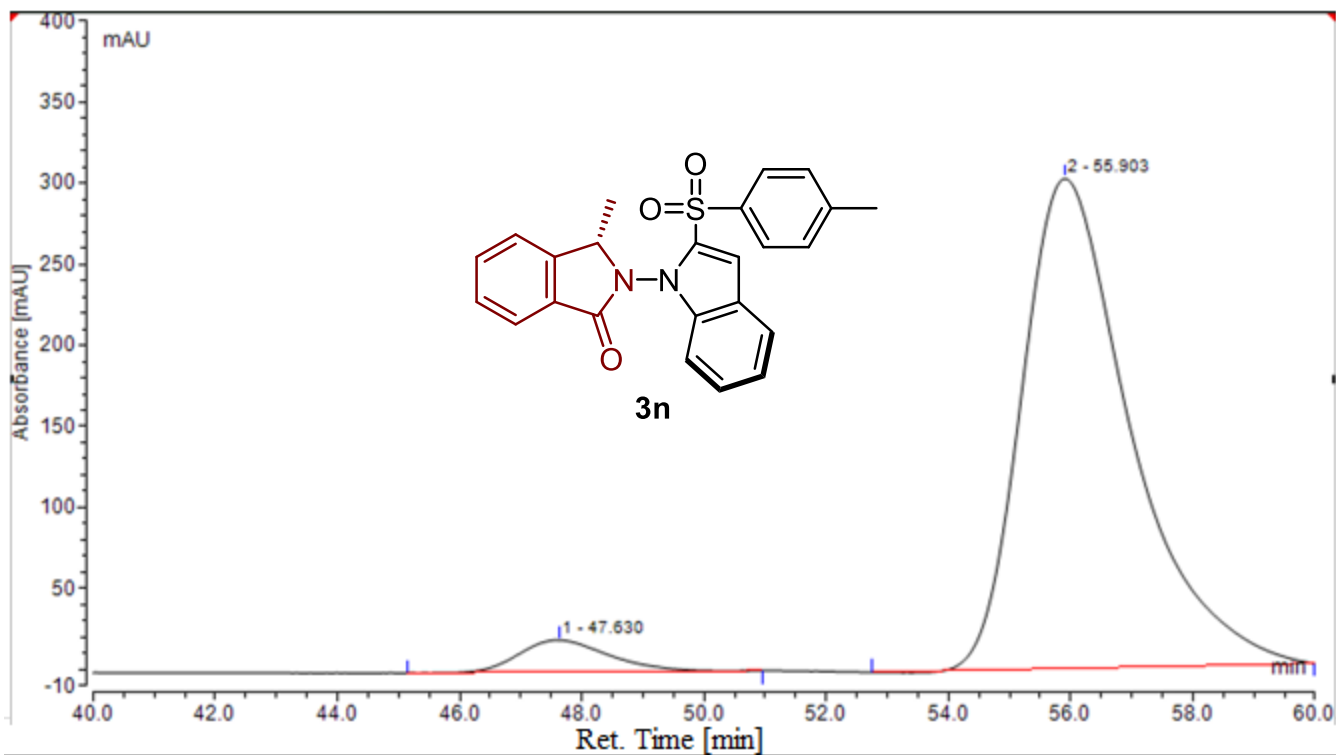
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	50.22	1358.358	578.018	49.80	55.65
2	69.89	1369.488	460.578	50.20	44.35



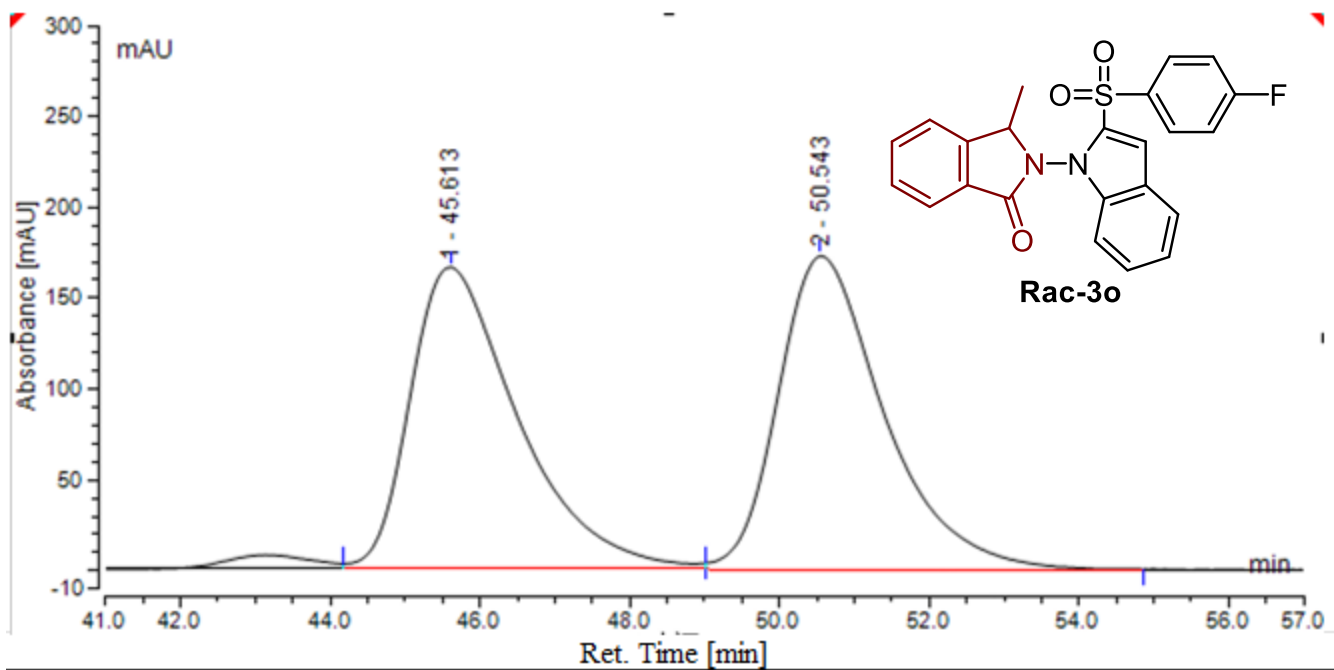
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	50.30	449.690	131.769	38.42	43.59
2	69.52	720.666	170.547	61.58	56.41



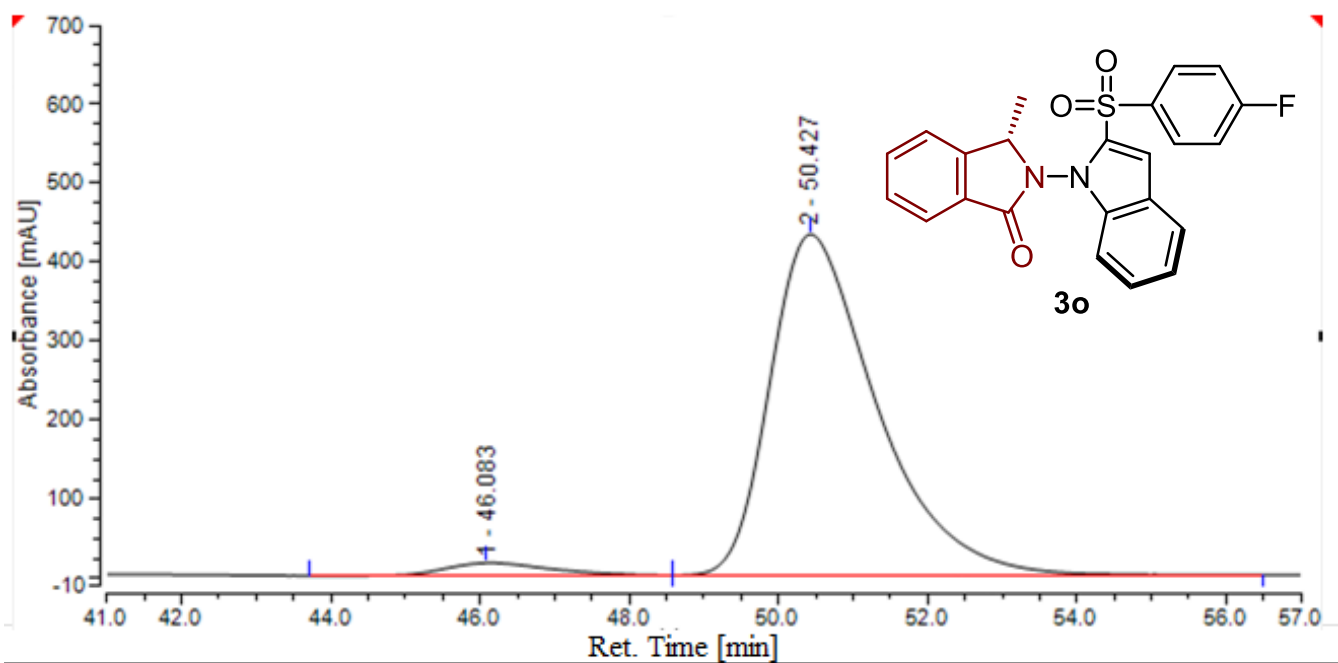
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	48.41	1213.652	671.552	50.15	53.47
2	57.52	1206.493	584.302	49.85	46.53



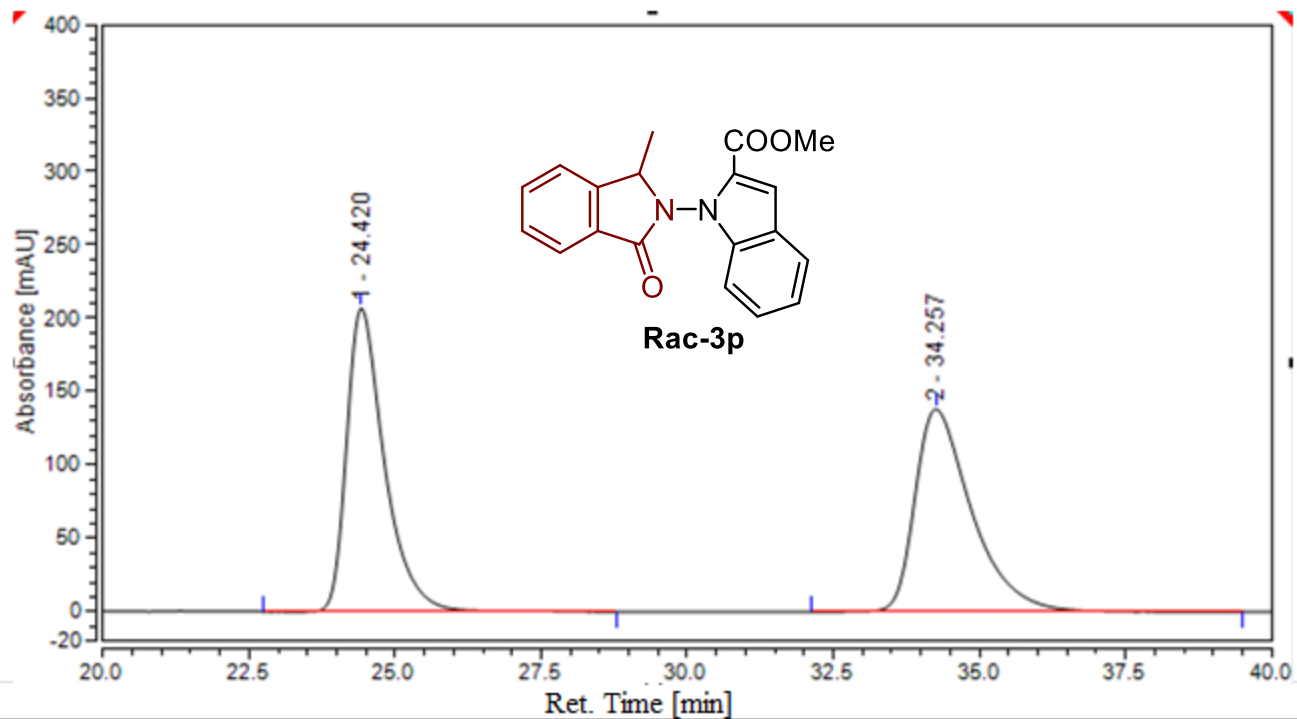
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	47.63	33.532	19.764	5.15	6.14
2	55.90	617.123	301.969	94.85	93.86



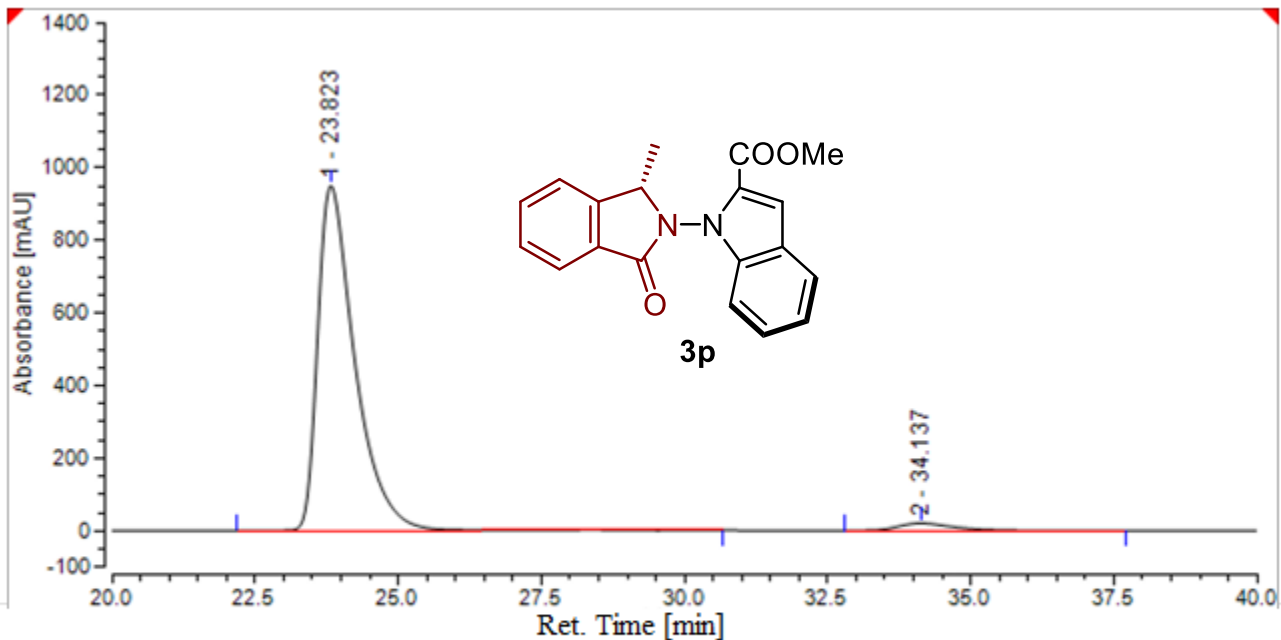
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	45.61	277.146	166.228	49.54	49.07
2	50.54	282.274	172.542	50.46	50.93



Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	46.08	25.978	16.136	3.51	3.60
2	50.43	713.425	431.866	96.49	96.40

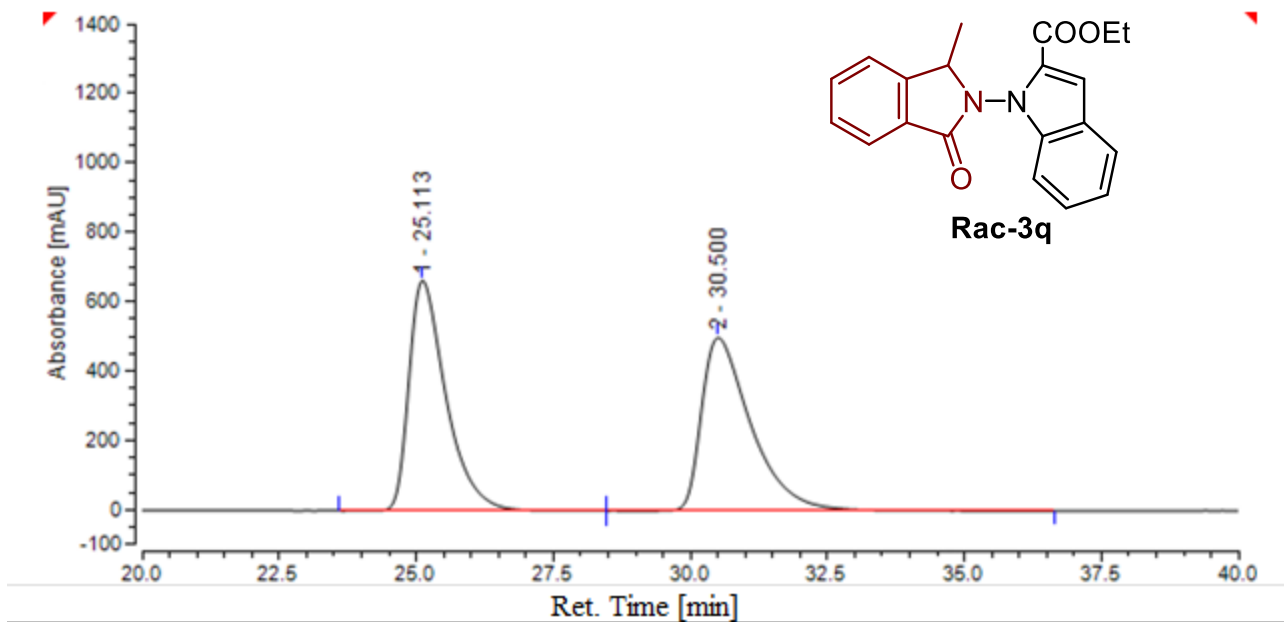


Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	24.42	155.907	206.911	50.05	59.99
2	34.26	155.602	138.012	49.95	40.01

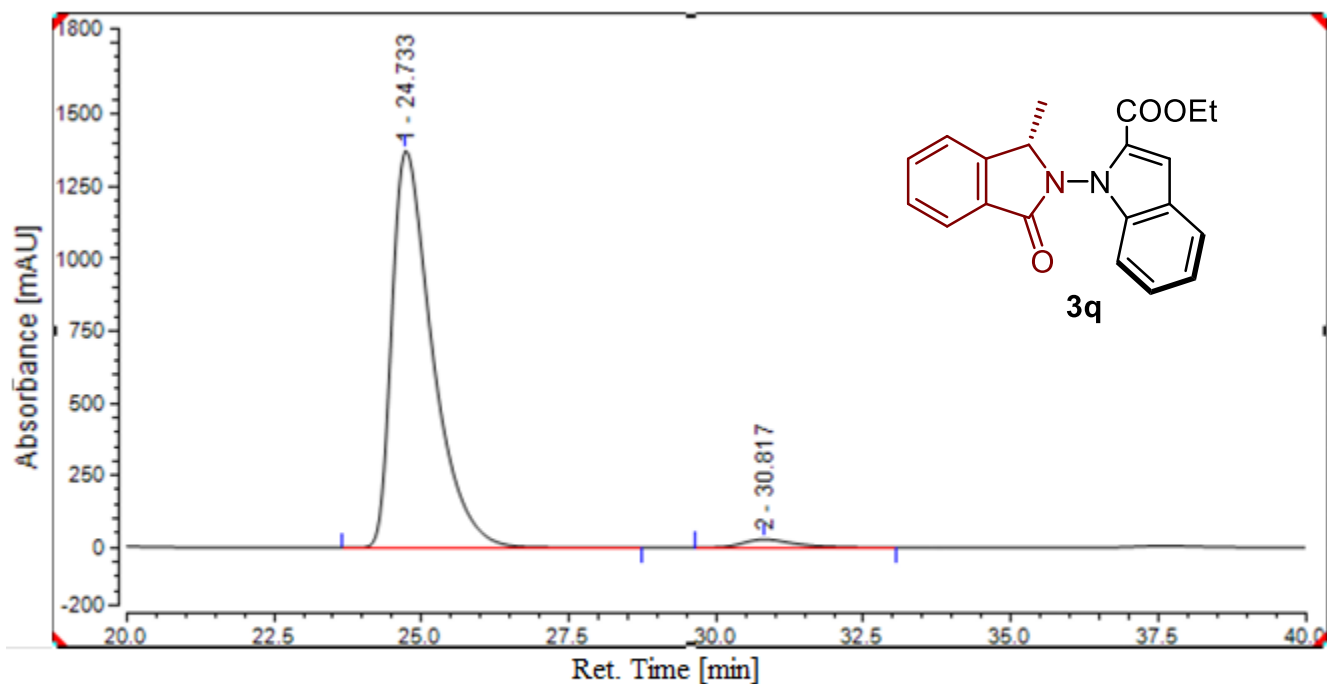


Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	23.82	713.143	950.632	96.94	97.92
2	34.14	22.523	20.237	3.06	2.08

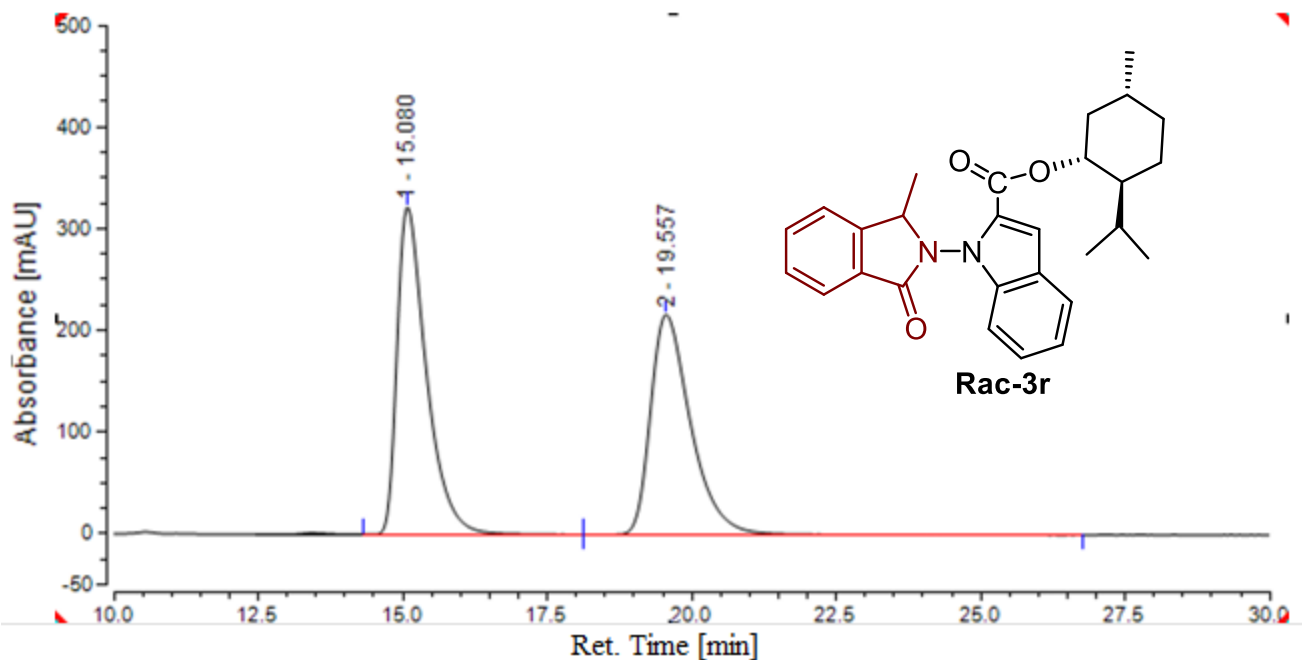




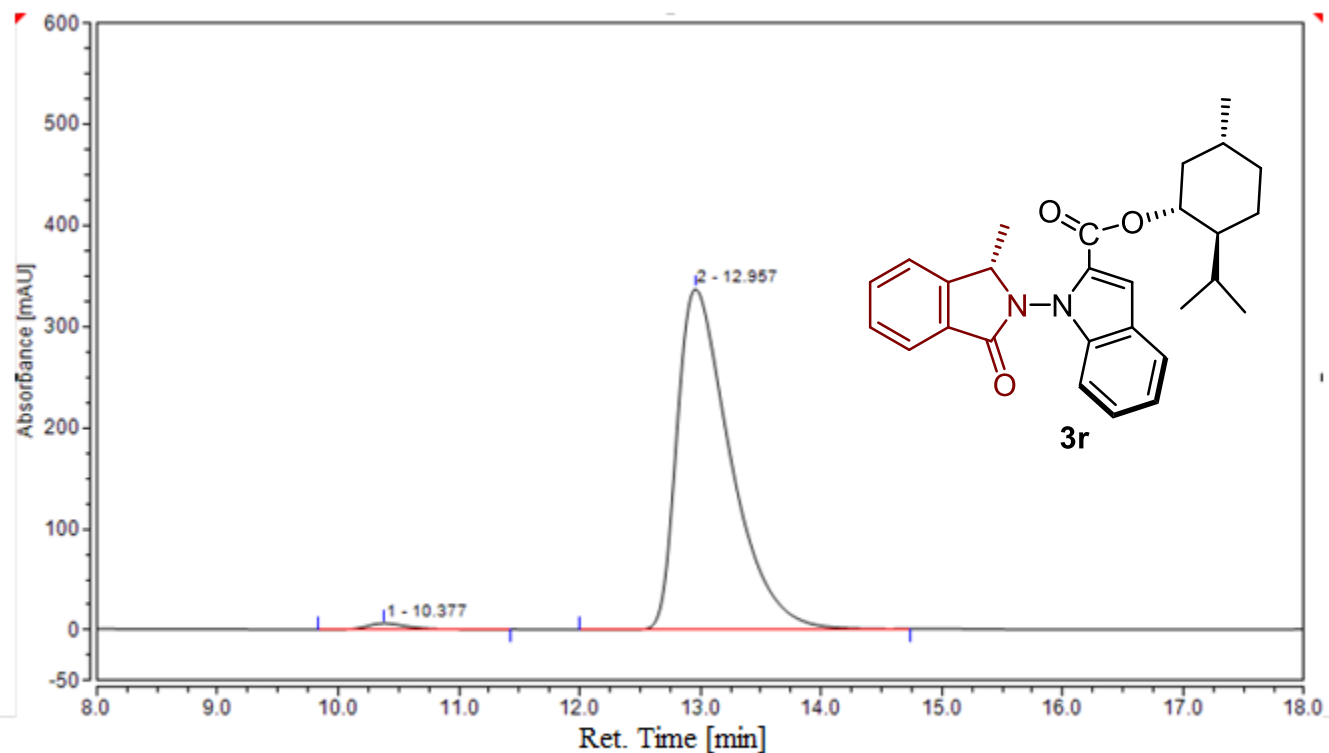
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	25.11	517.470	663.531	49.84	57.09
2	30.50	520.759	498.722	50.16	42.91



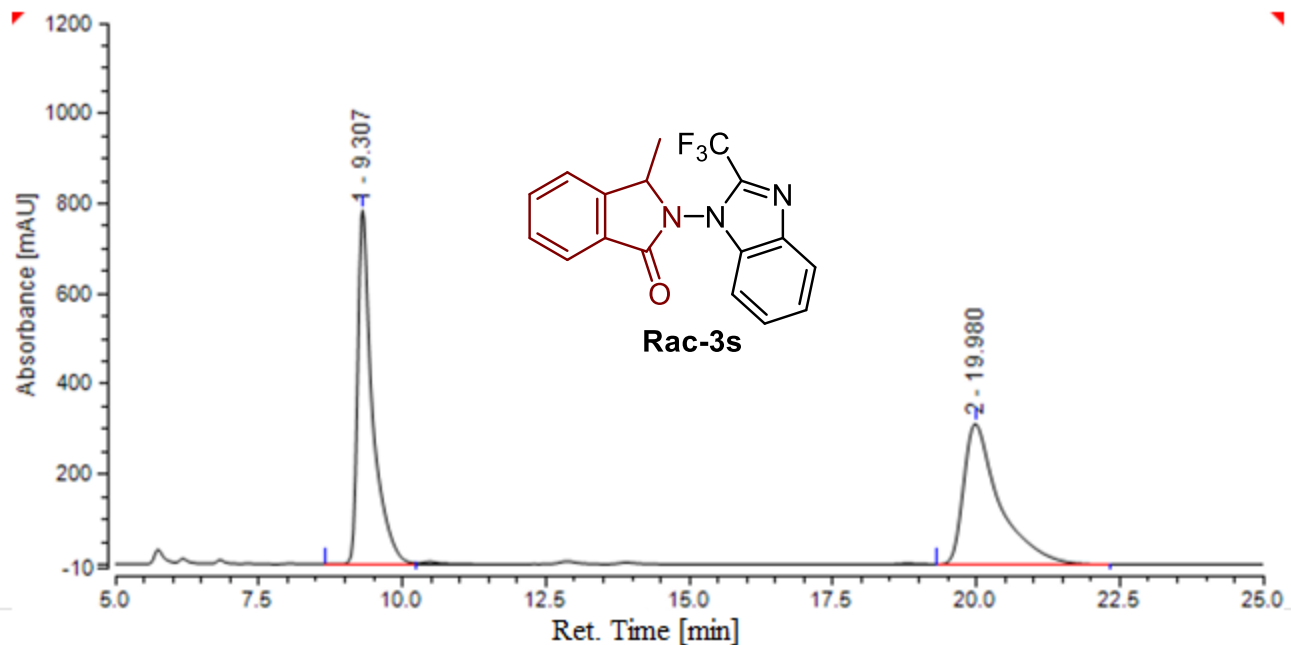
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	24.73	1089.289	1374.710	97.50	98.02
2	30.82	27.875	27.818	2.50	1.98



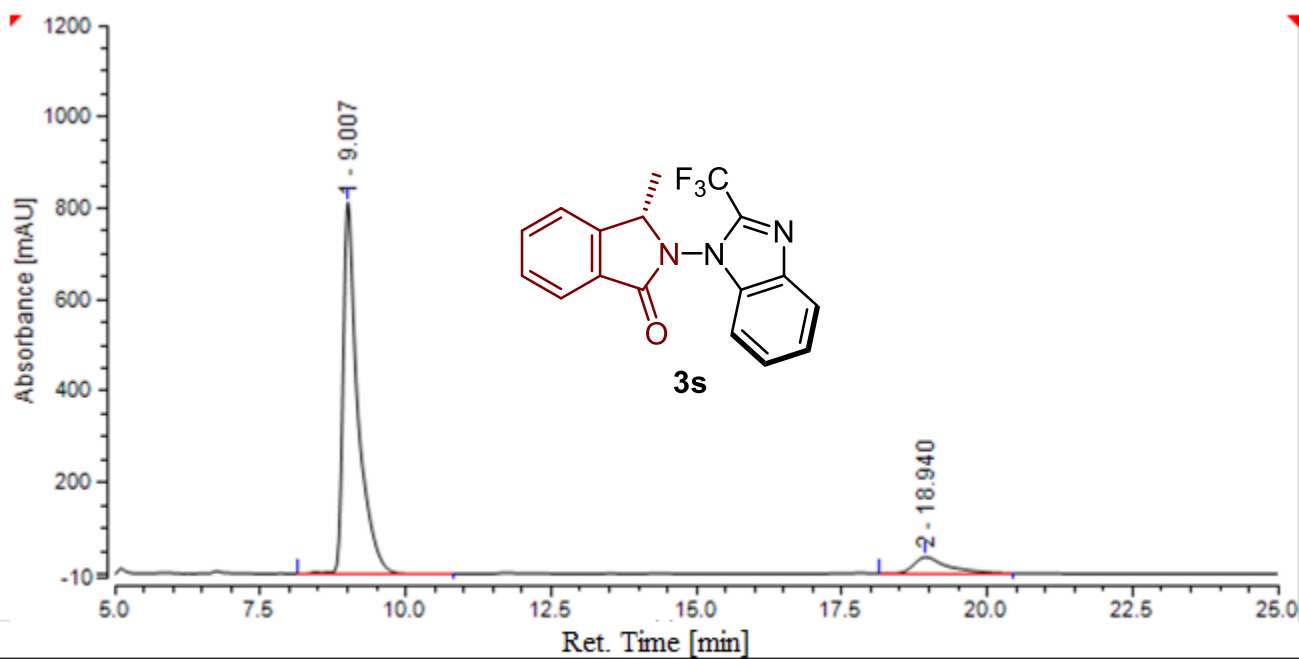
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	15.08	188 916	321.987	52.12	59.83
2	19.56	173.543	216.226	47.88	40.17



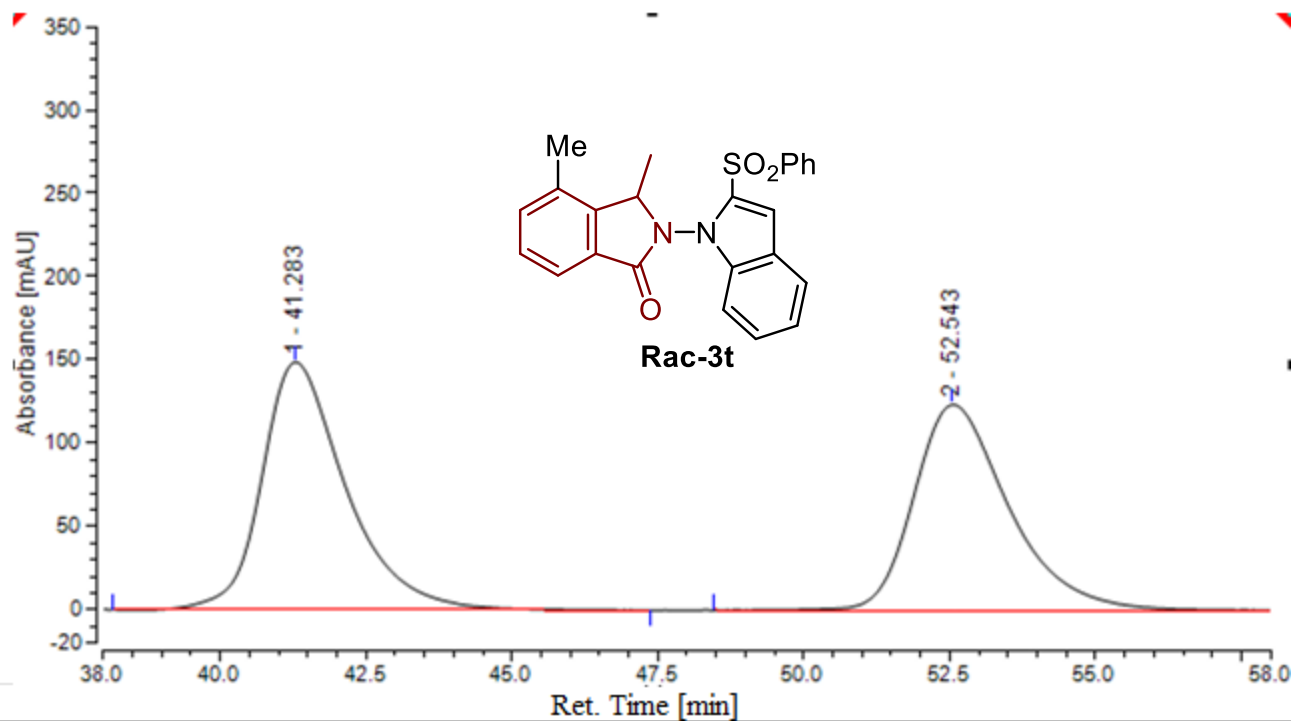
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	10.38	2.333	6.123	1.34	1.79
2	12.96	171.801	336.399	98.66	98.21



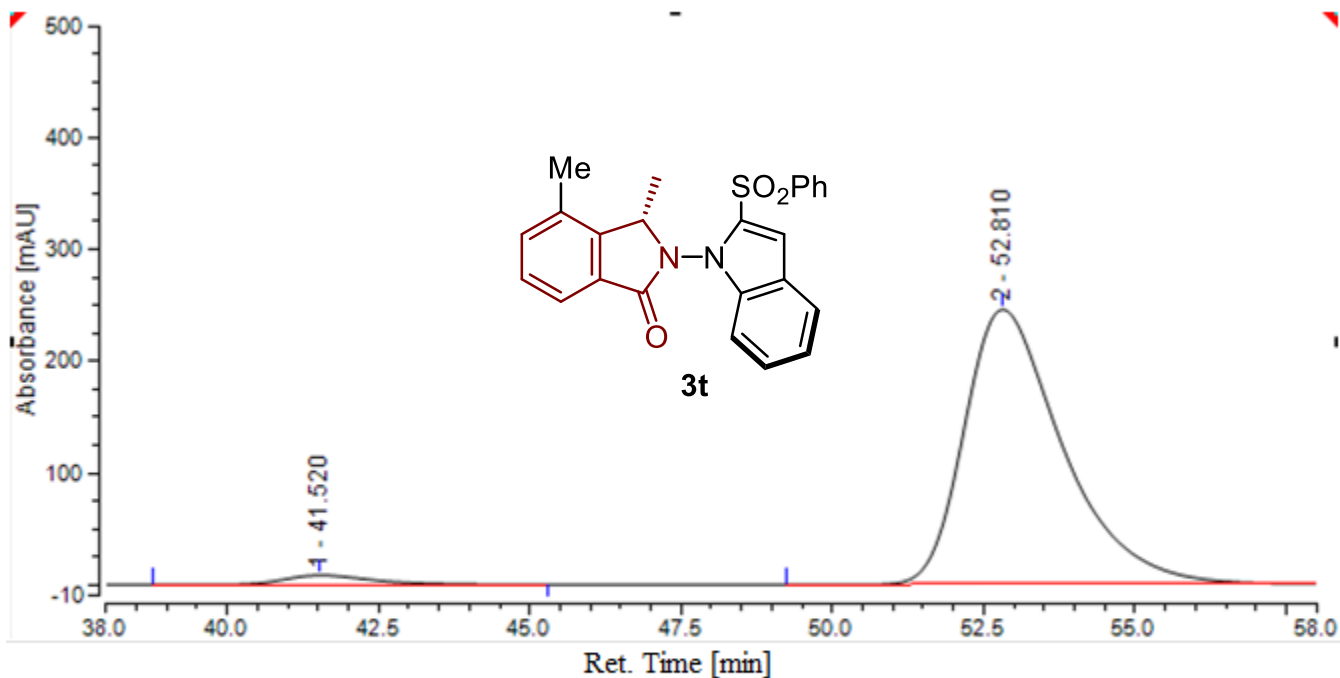
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	9.31	232.812	785.073	50.71	71.54
2	19.98	226.301	312.268	49.29	28.46



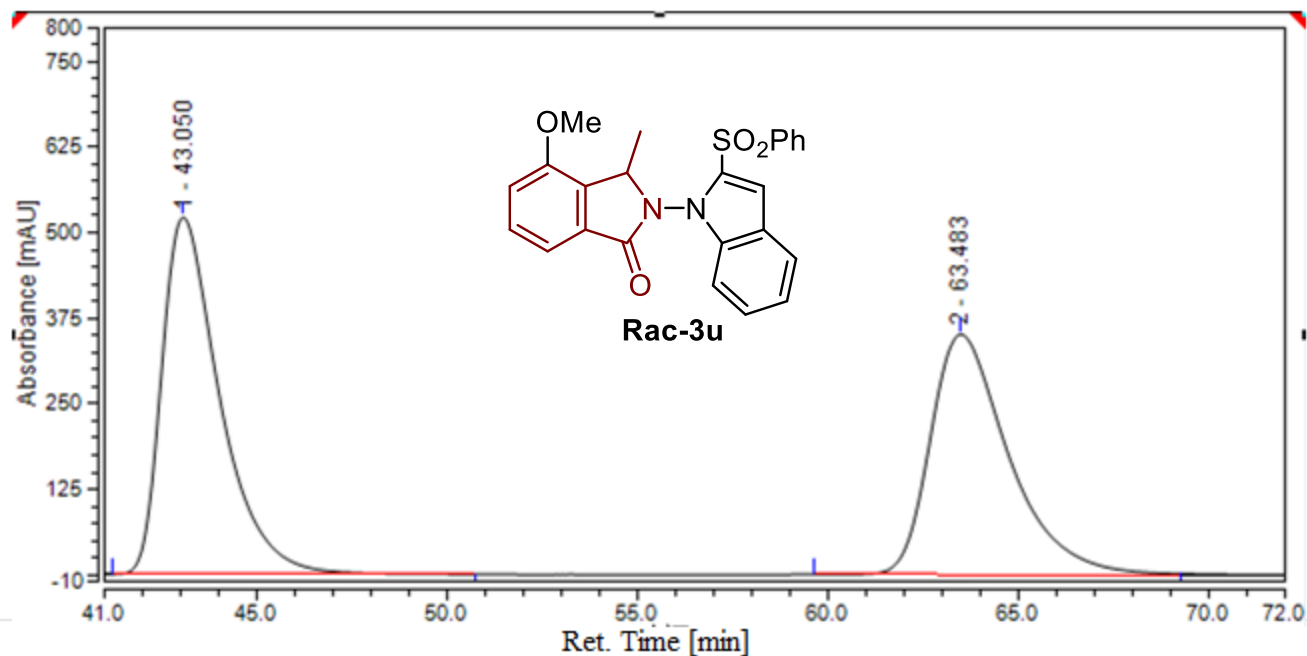
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	9.01	238.787	812.691	91.00	95.79
2	18.94	23.602	35.724	9.00	4.21



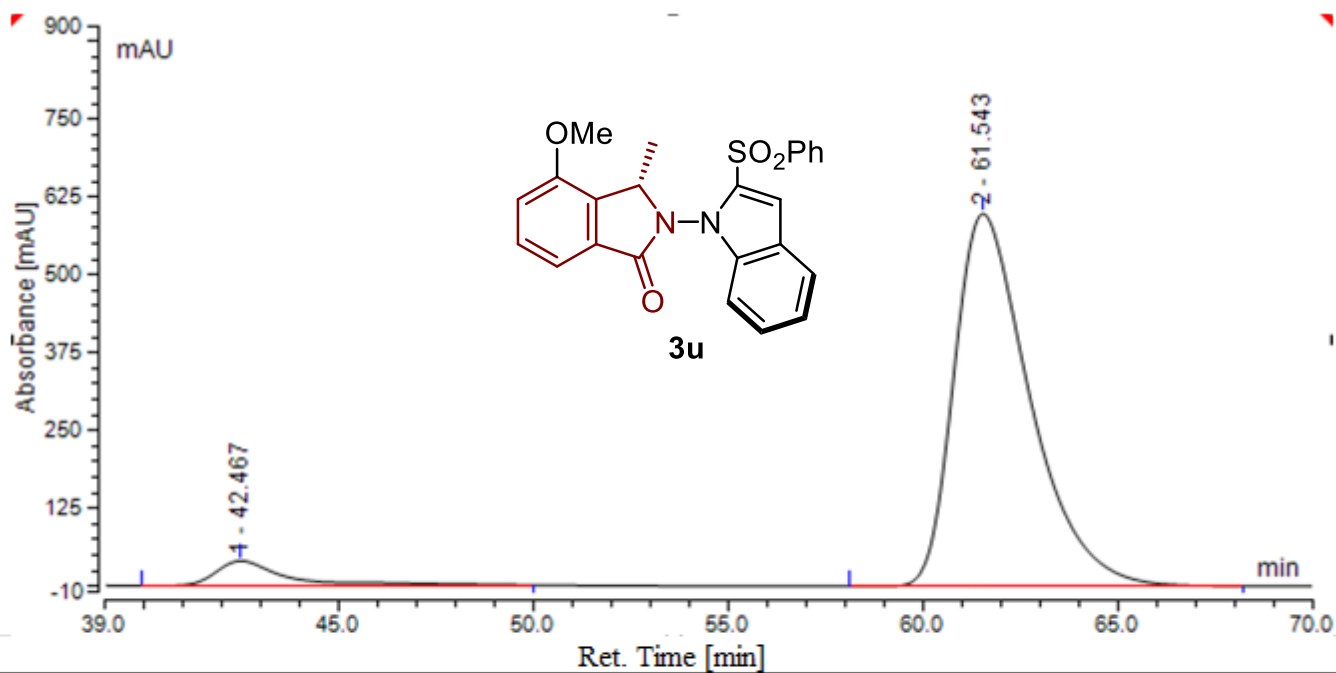
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	41.28	248.288	148.596	51.66	54.66
2	52.54	232.304	123.283	48.34	45.34



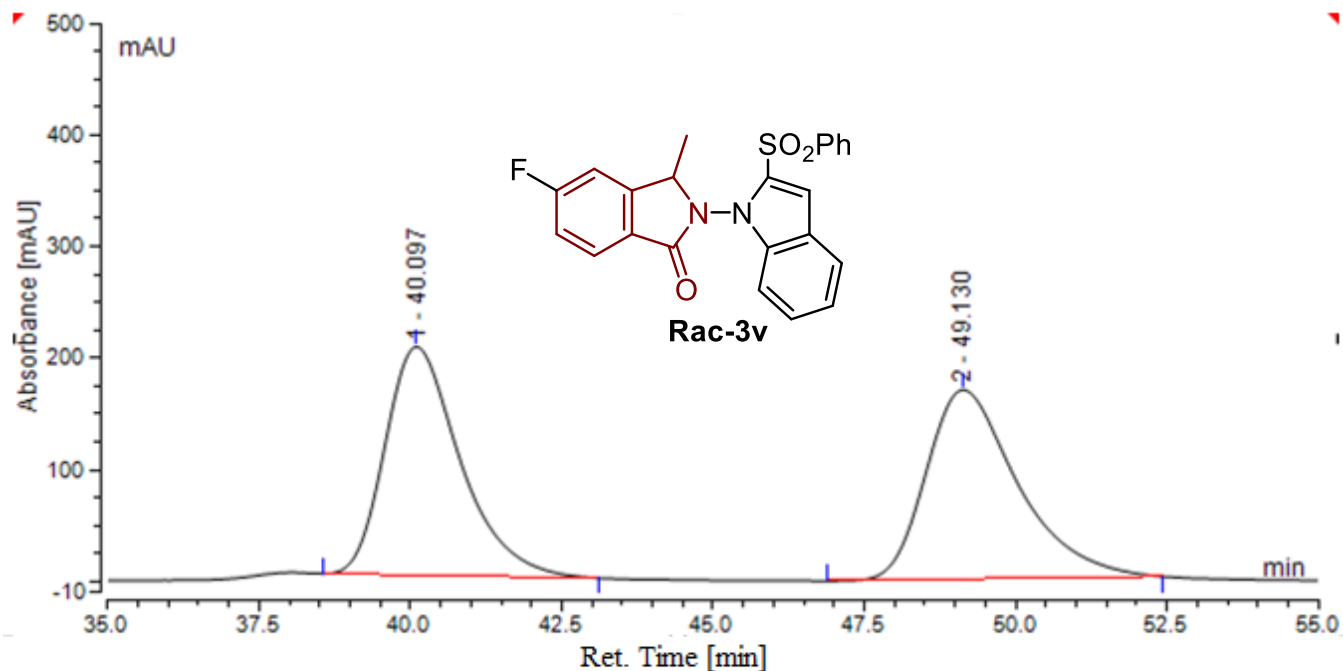
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	41.52	14.050	8.382	2.94	3.30
2	52.81	464.196	245.761	97.06	96.70



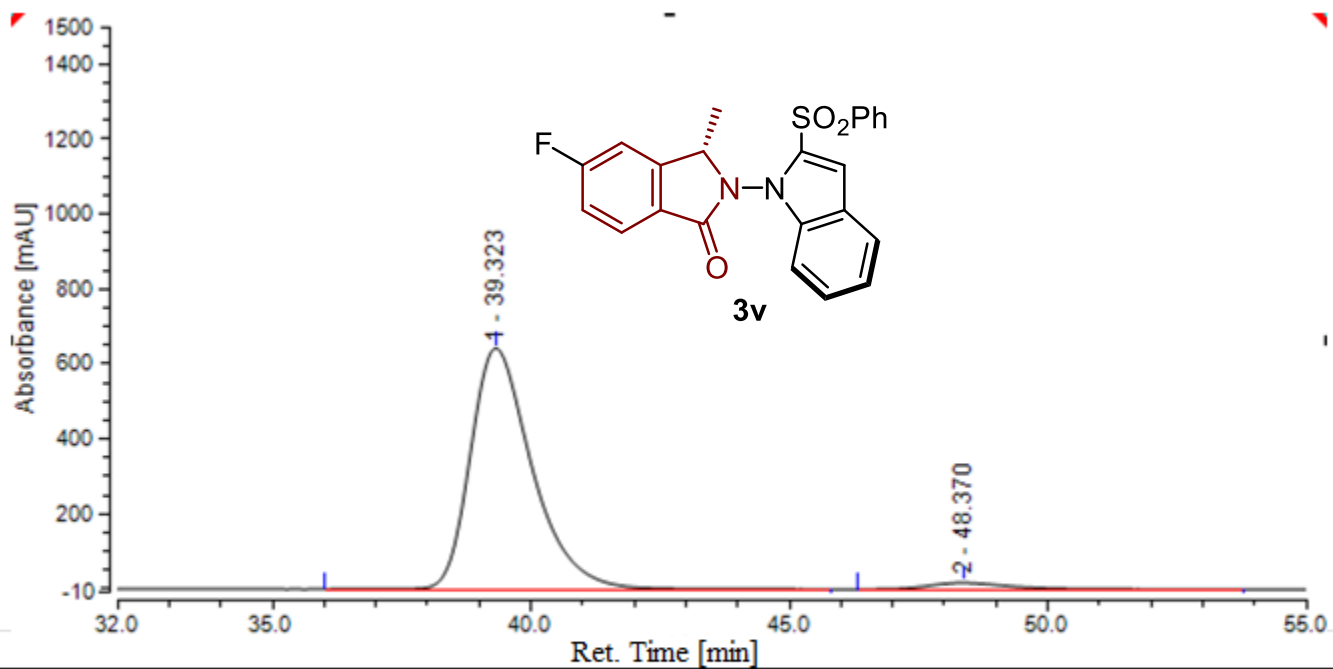
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	43.05	923.167	521.510	53.49	59.77
2	63.48	835.532	350.956	47.51	40.23



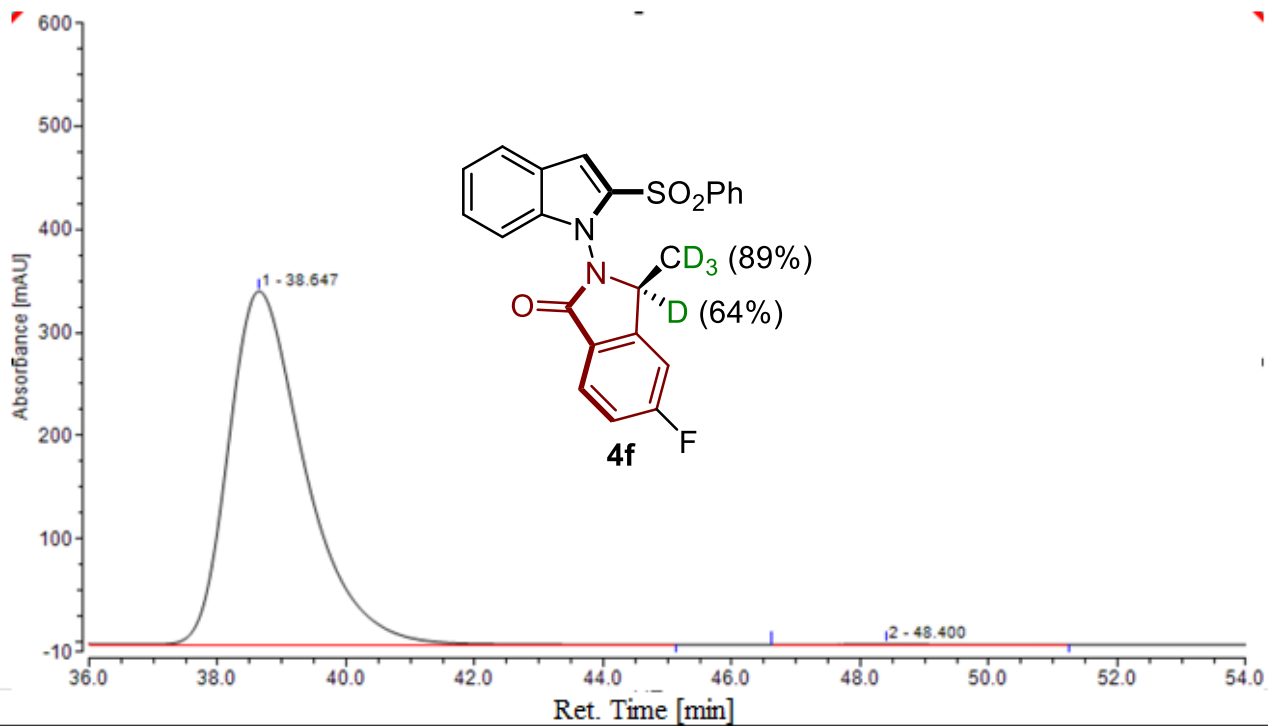
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	42.47	84.156	39.773	5.88	6.23
2	61.54	1347 885	598.282	94.12	93.77



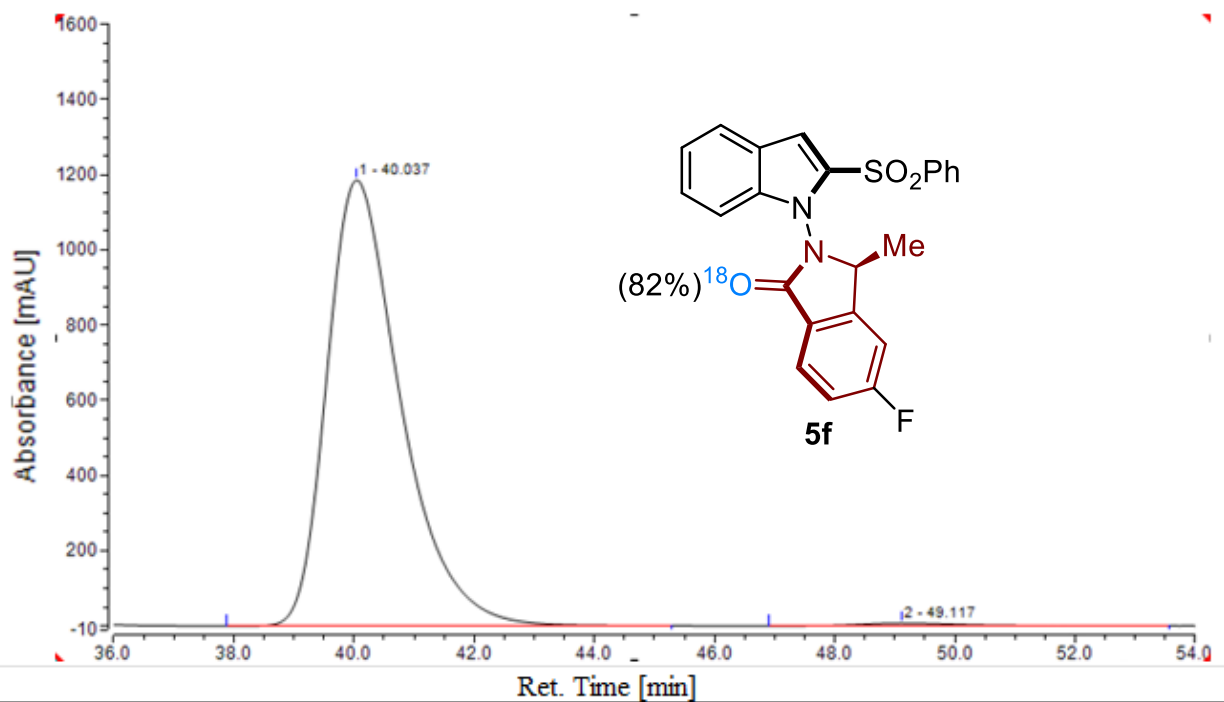
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	40.10	294.127	204.682	49.78	54.69
2	49.13	296.699	169.570	50.22	45.31



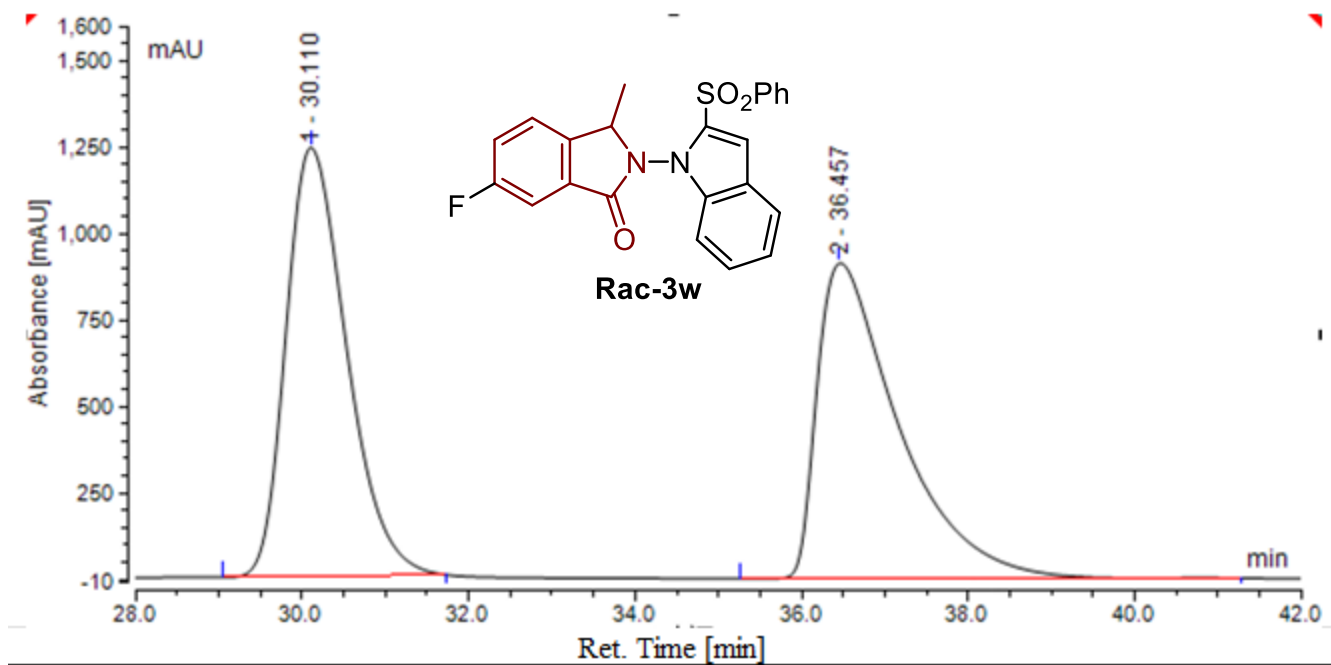
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	39.32	889.214	643.104	96.74	97.44
2	48.37	29.996	16.921	3.26	2.56



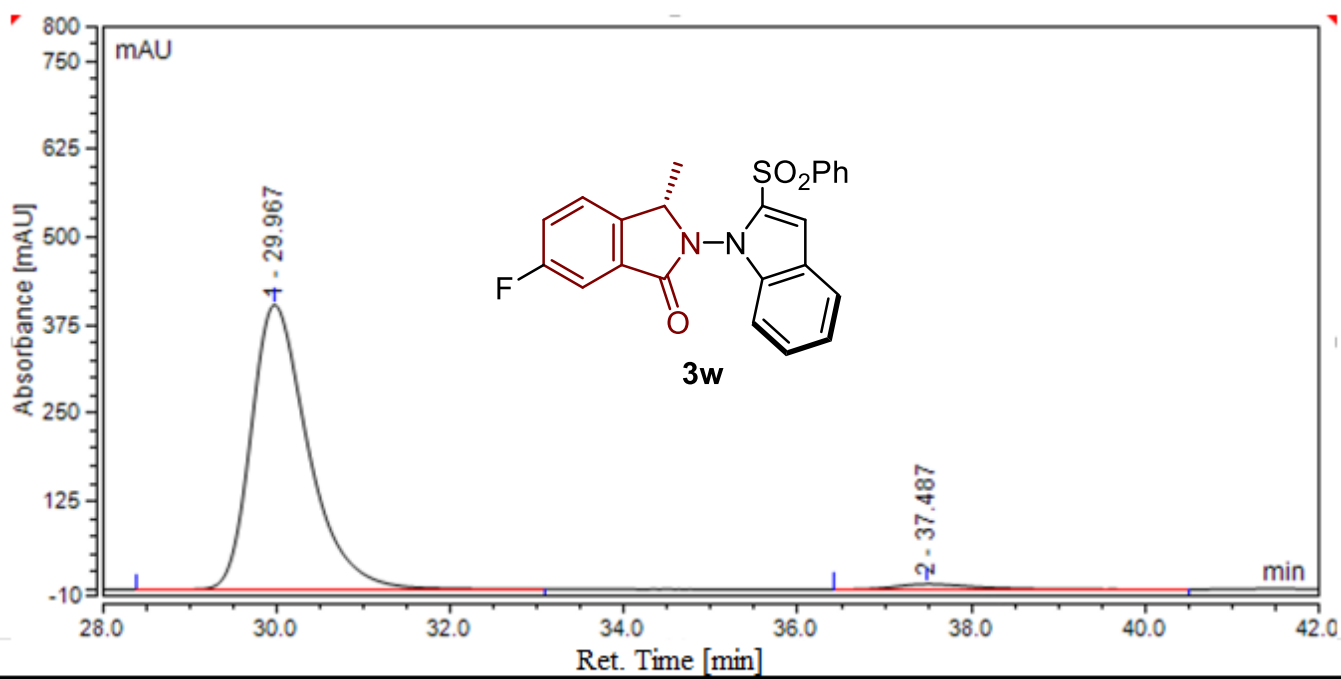
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	38.65	470.876	342.525	99.89	99.92
2	45.40	0.503	0.267	0.11	0.08



Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	40.04	1681.783	1185.105	99.21	99.40
2	49.12	13.341	7.116	0.79	0.60

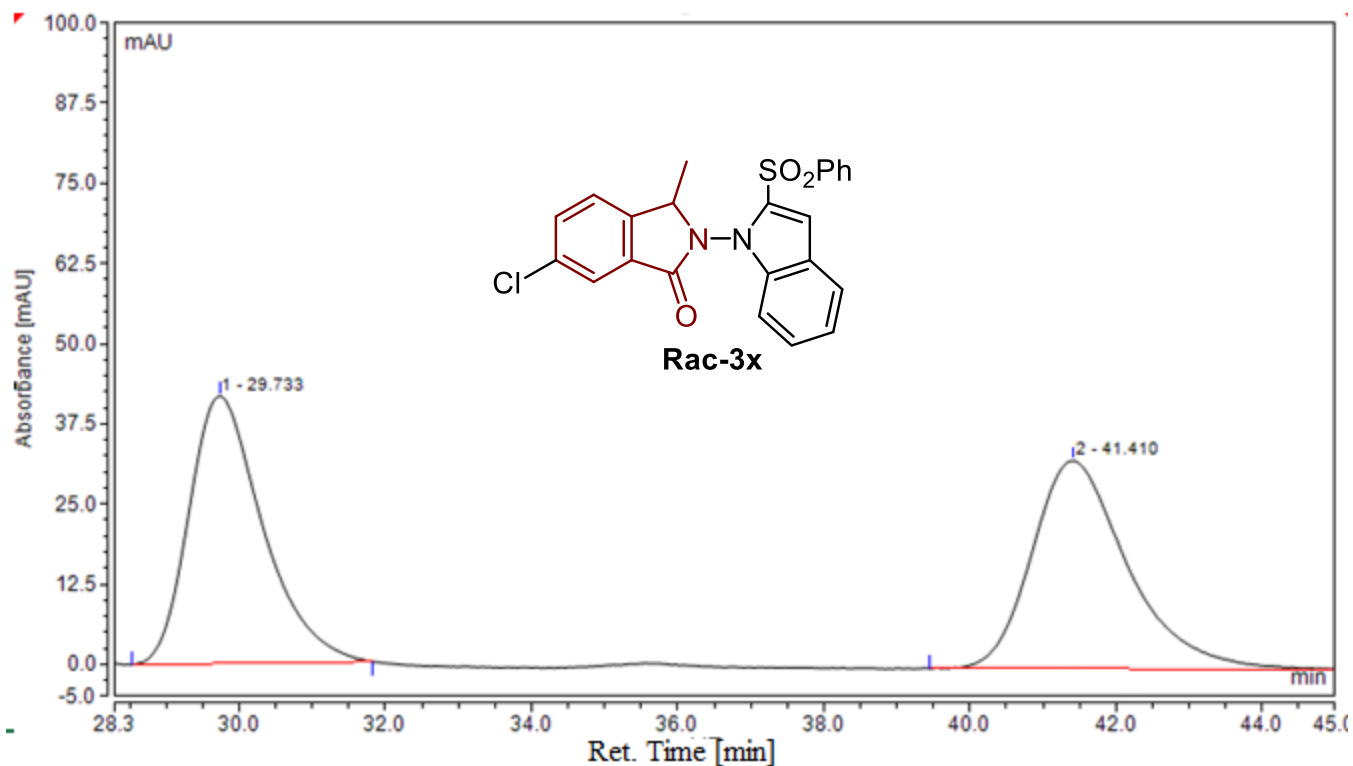


Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	30.11	1043.754	1240.322	50.32	57.62
2	36.46	1030.470	912.443	49.68	42.38

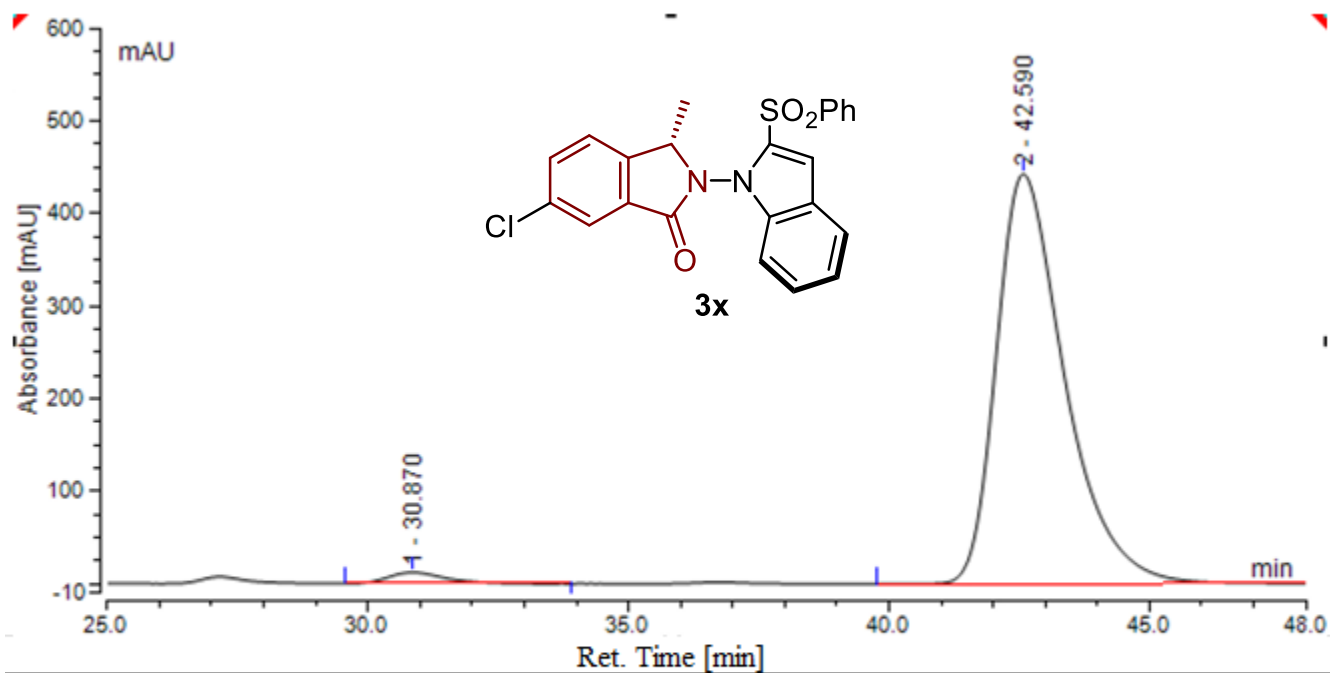


Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	29.97	306.996	403.867	97.41	98.17
2	37.49	8.176	7.515	2.59	1.83

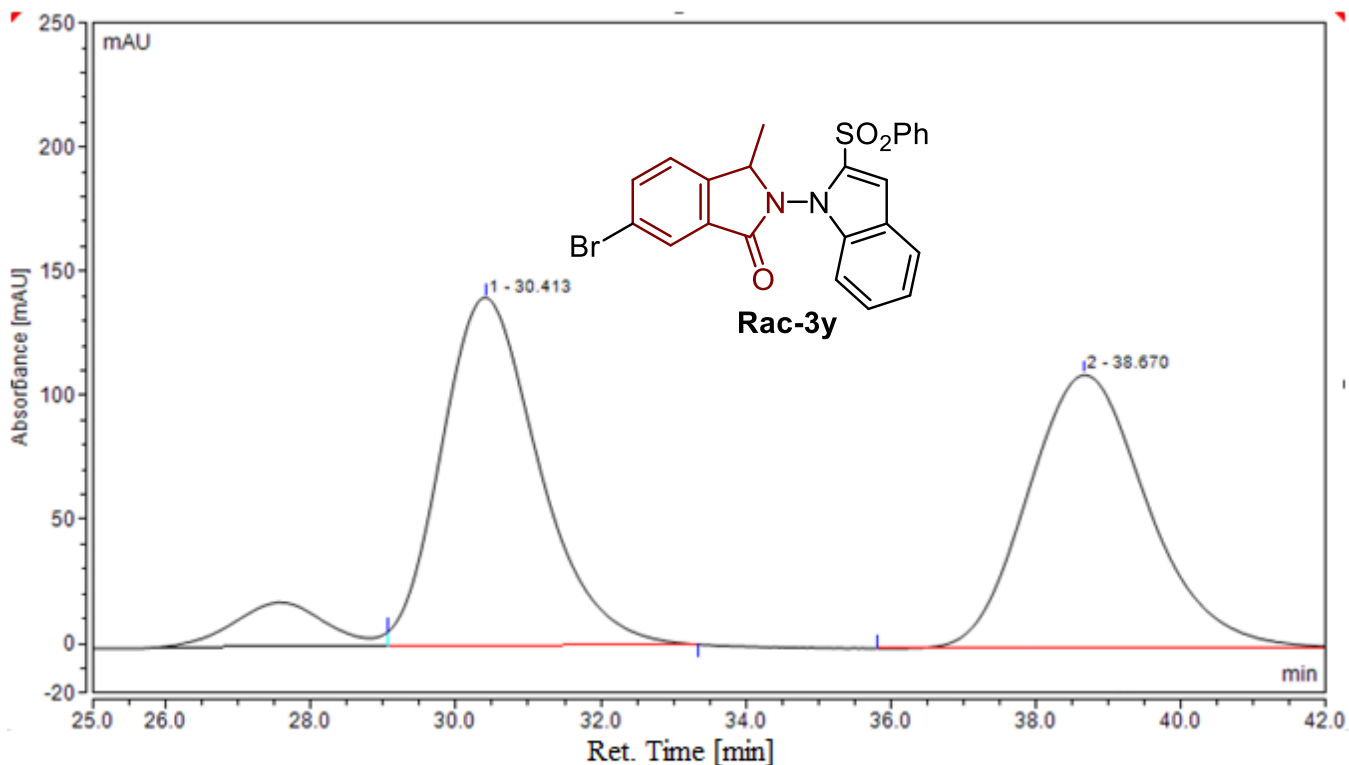




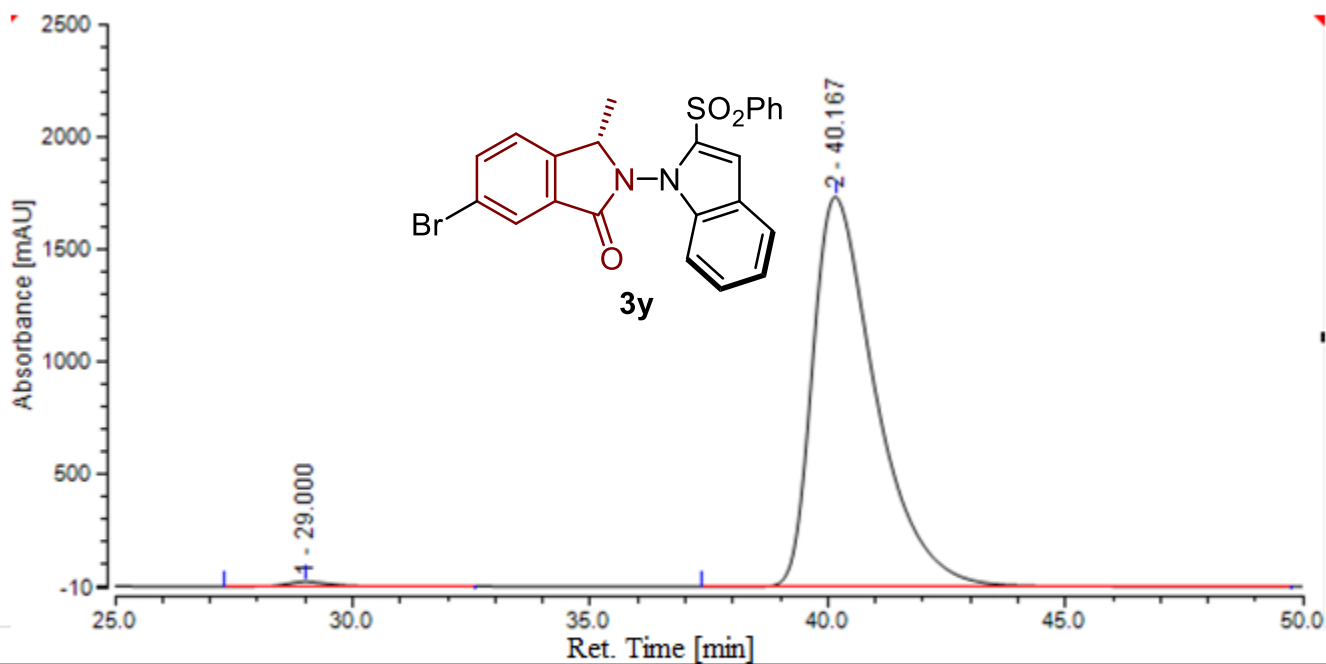
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	29.73	48.830	41.766	49.84	56.29
2	41.41	49.141	32.436	50.16	43.71



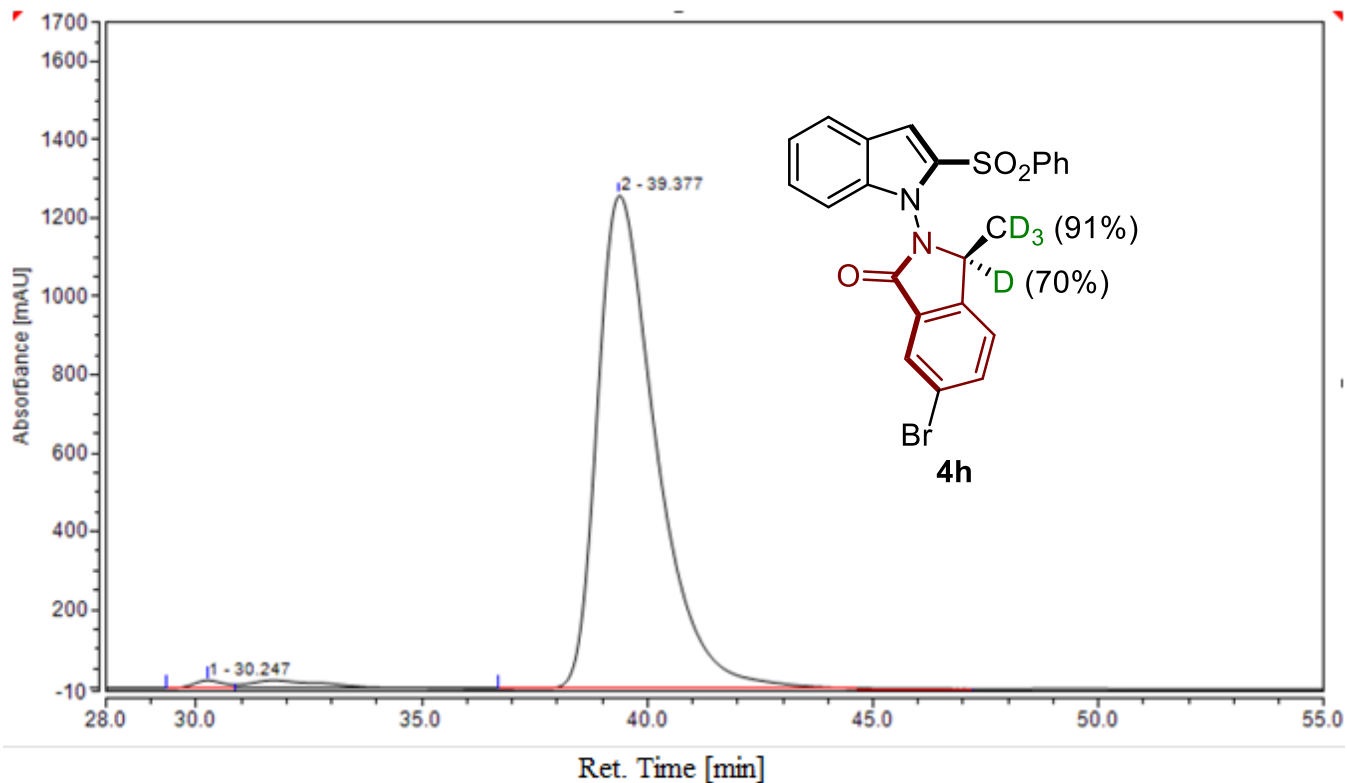
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	30.87	14.810	11.895	2.16	2.62
2	42.59	671.425	441.914	97.84	97.38



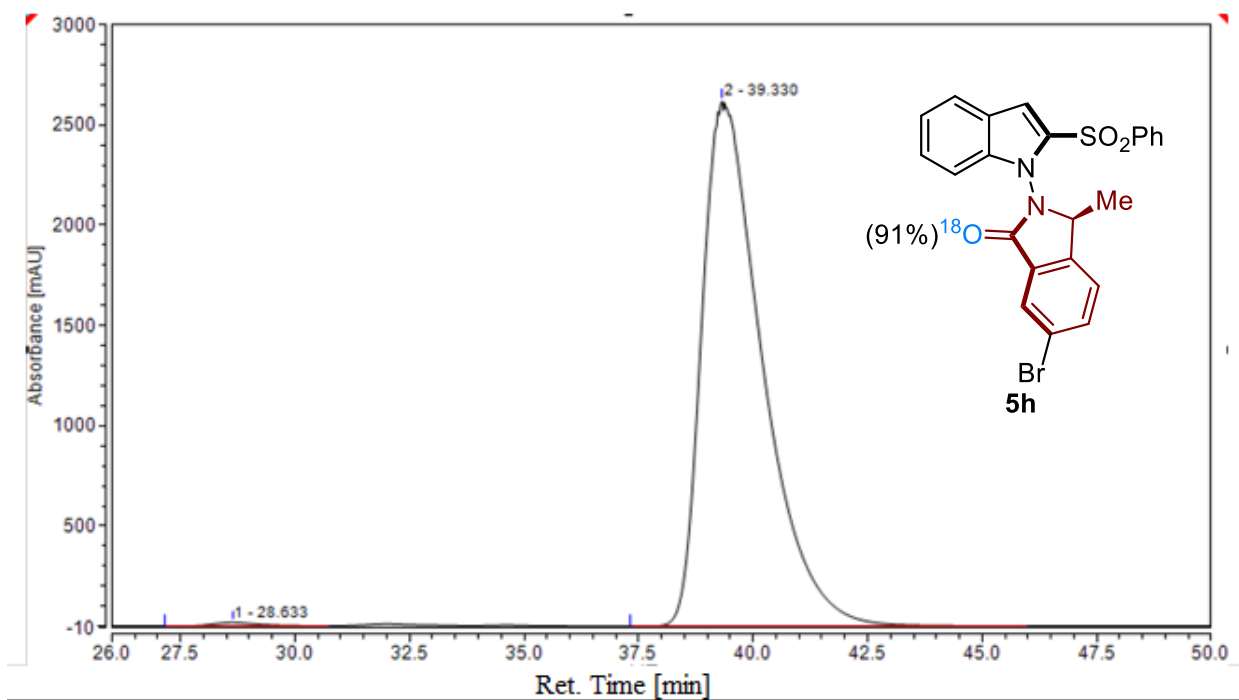
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	30.41	217.582	140.191	50.79	56.02
2	38.67	210.832	110.059	49.21	43.98



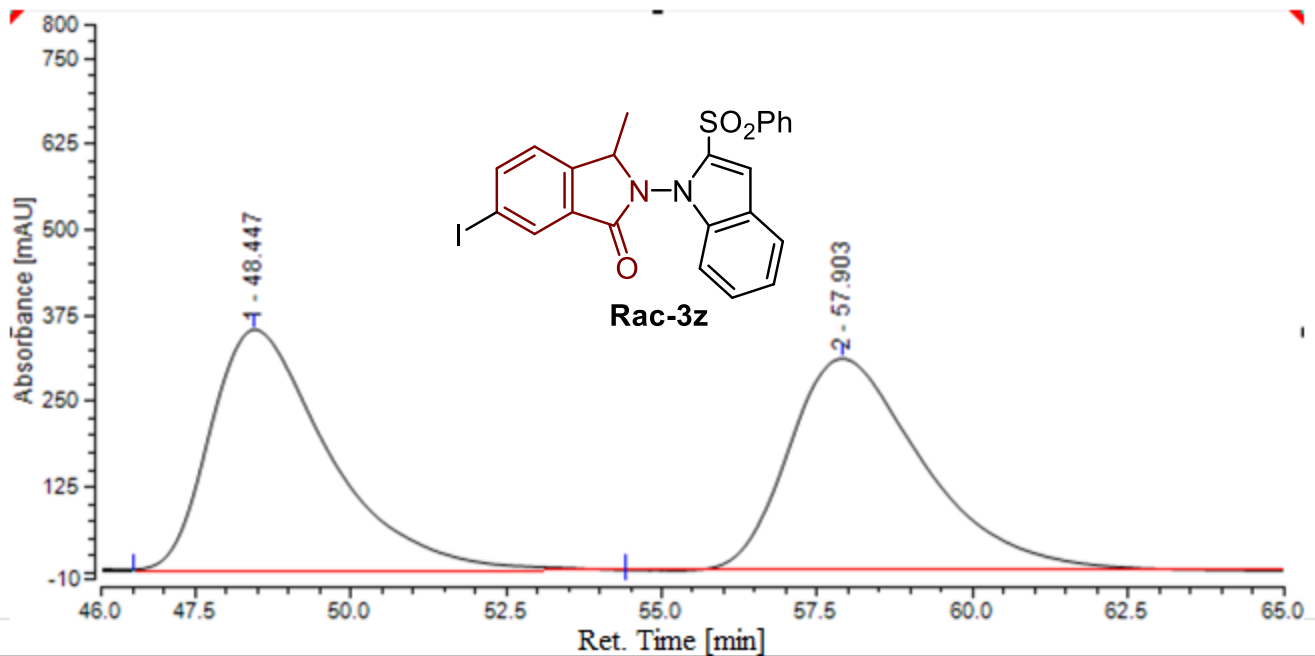
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	29.00	23.881	21.235	0.89	1.21
2	40.17	2651.331	1733.410	99.11	98.79



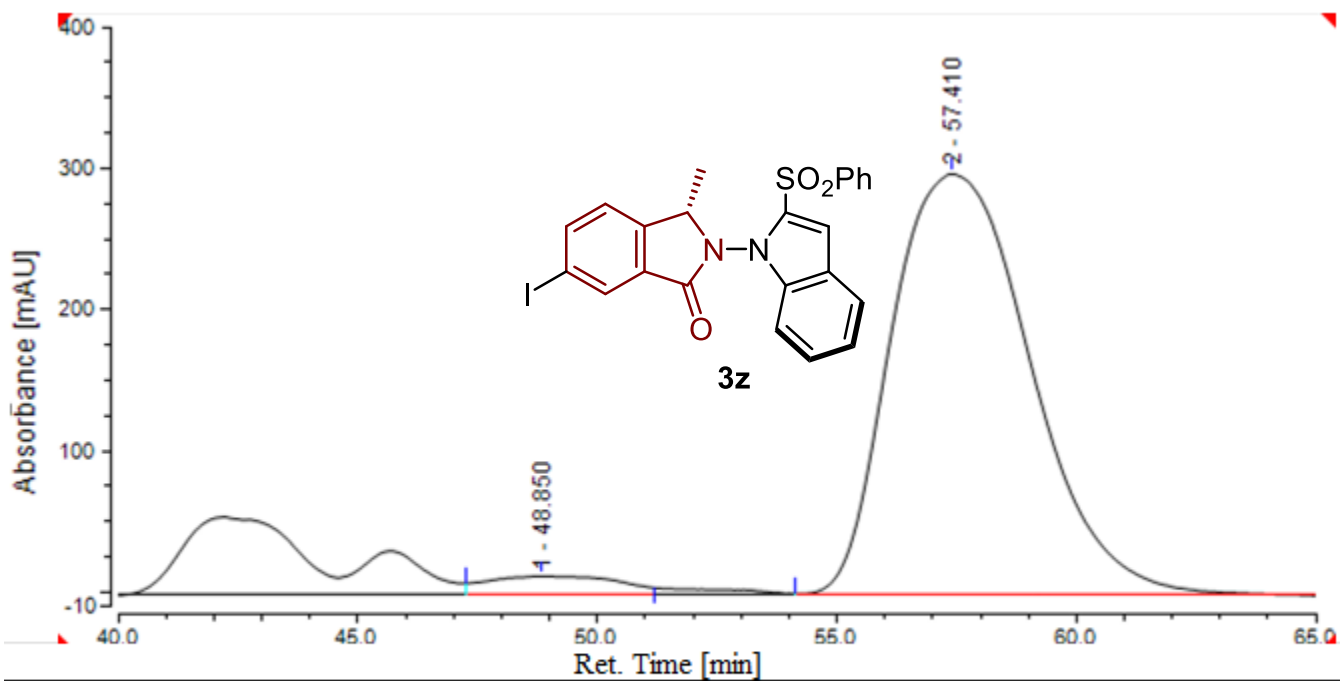
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	30.25	16.677	20.565	0.87	1.61
2	39.38	1904.451	1259.701	99.13	98.39



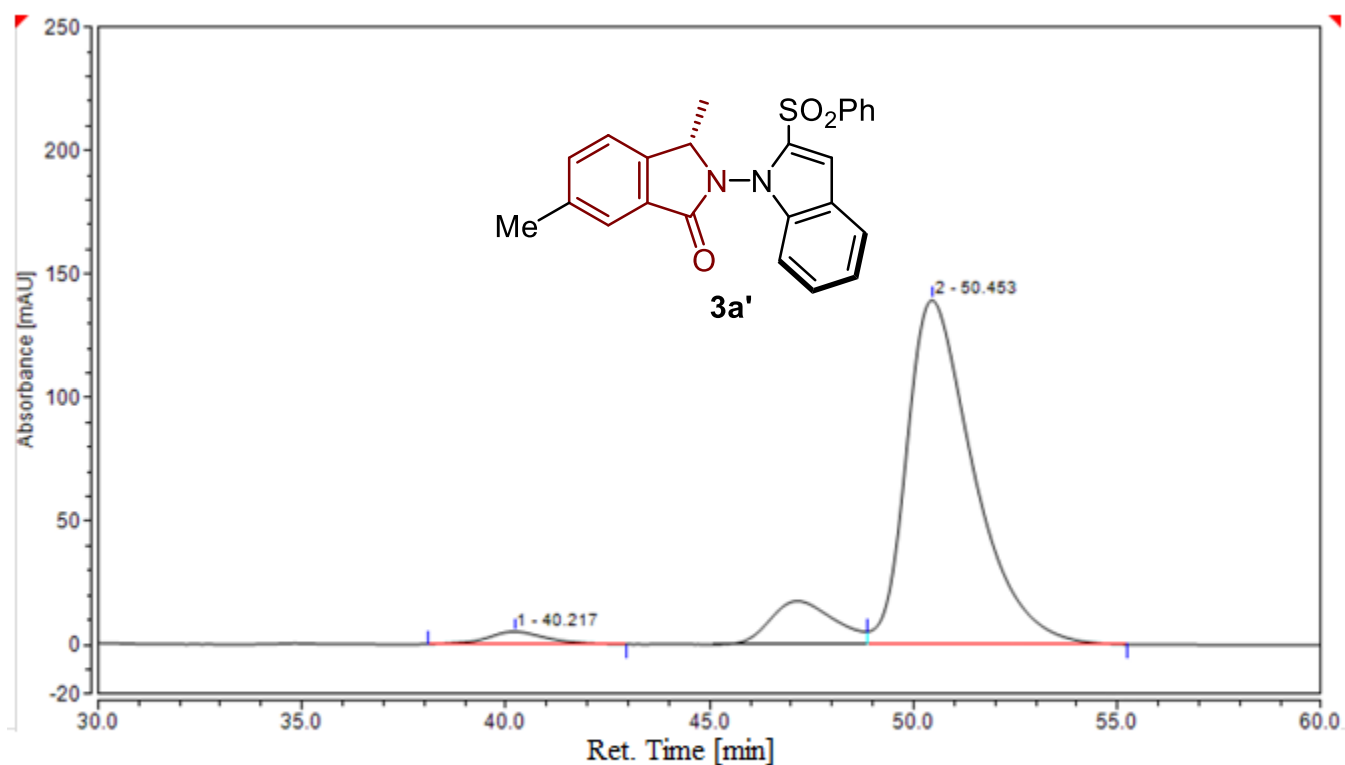
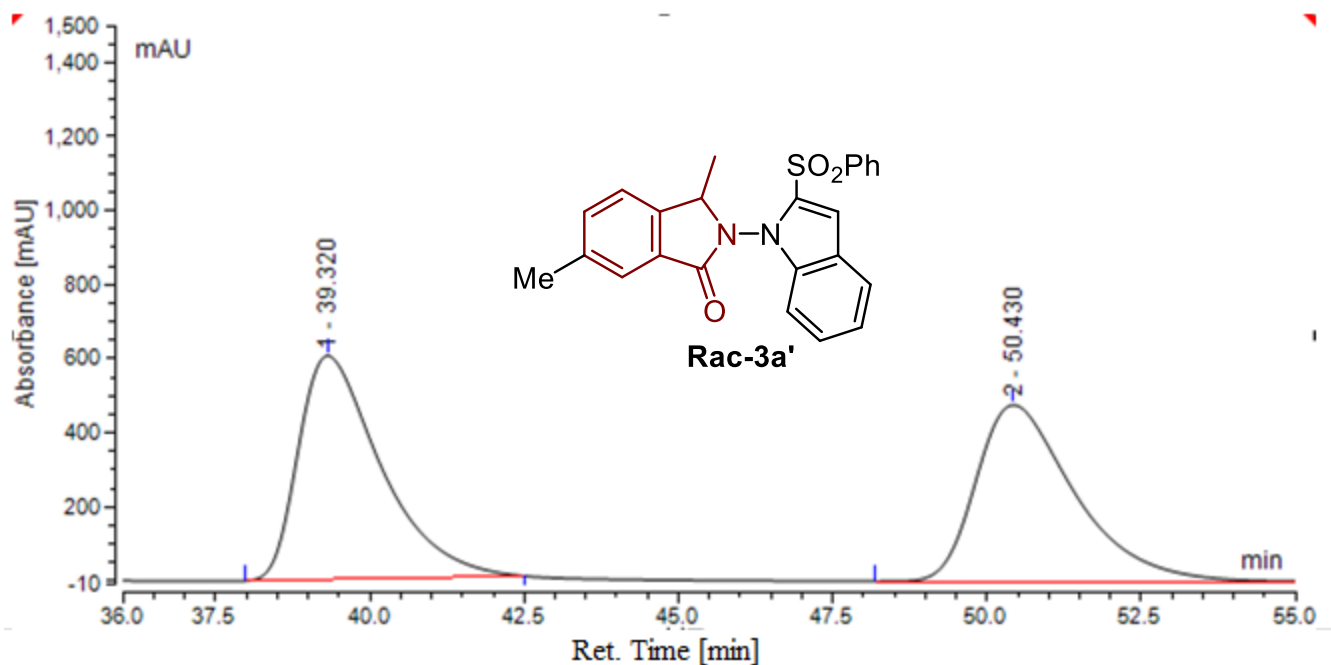
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	28.63	19.999	17.262	0.50	0.66
2	39.33	4000.542	2618.140	99.50	99.34

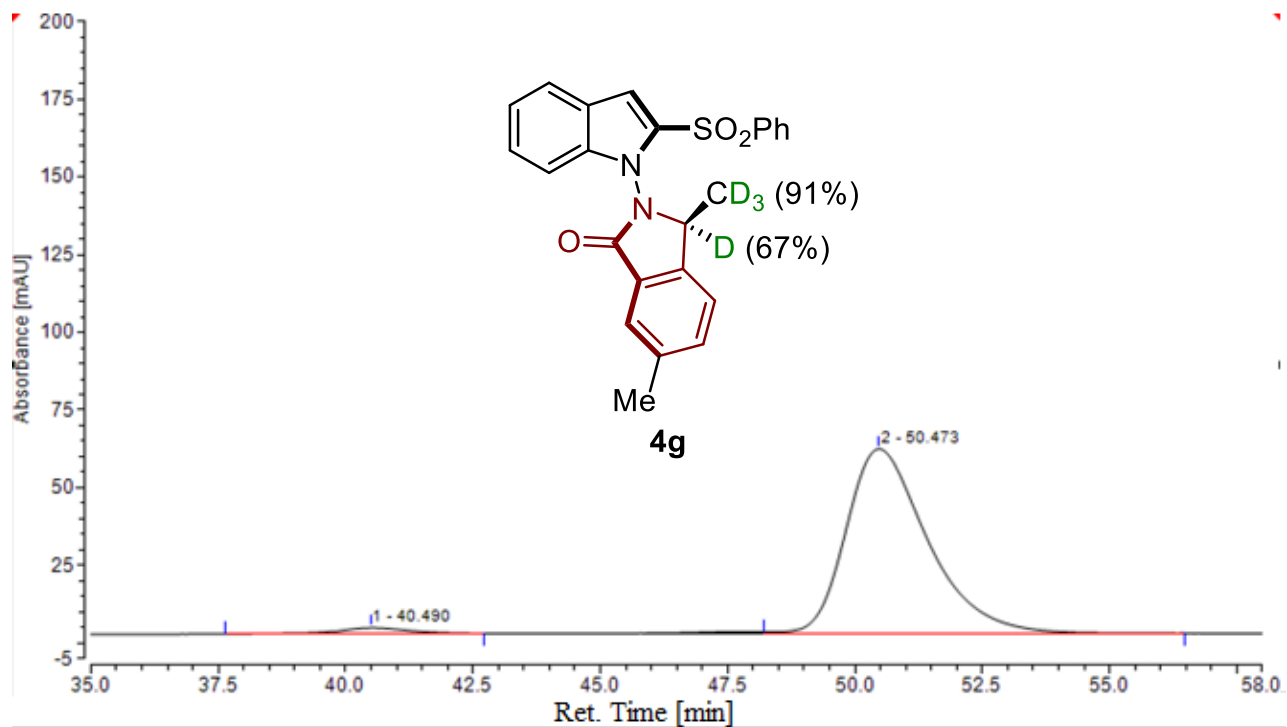


Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	48.45	780.109	352.186	50.25	53.31
2	57.90	763.124	308.424	49.45	46.69

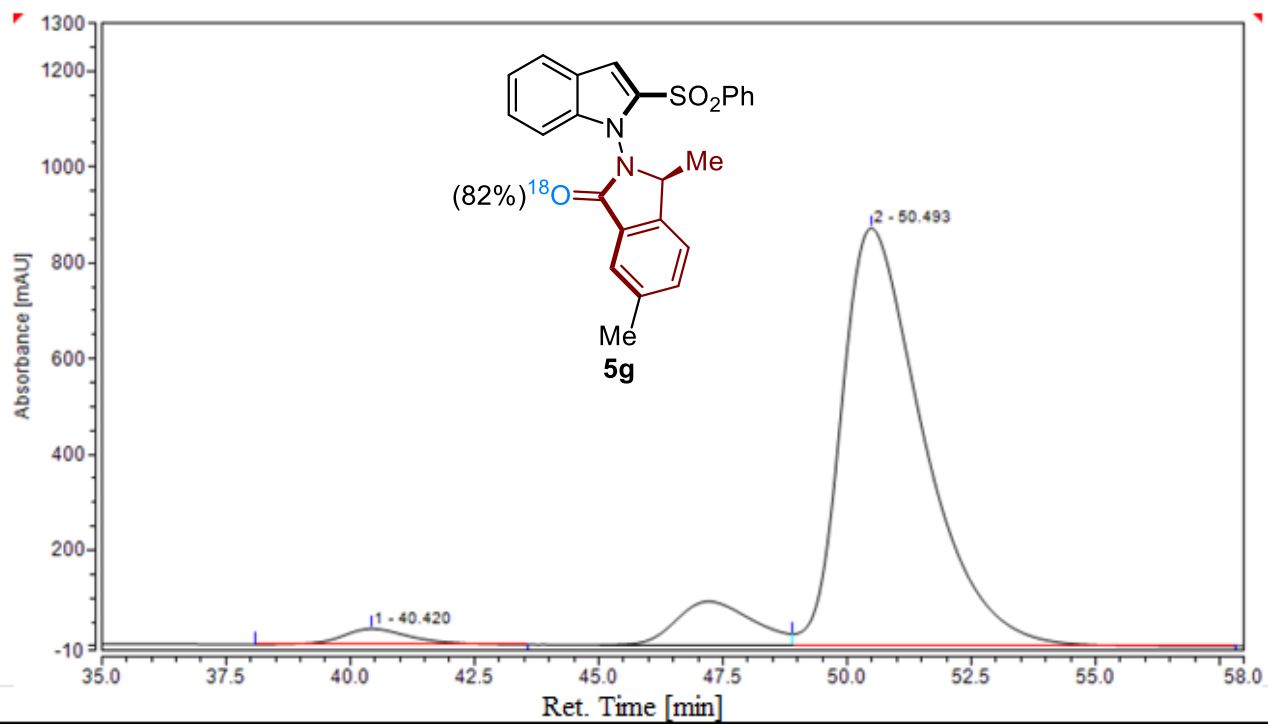


Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	48.85	43.368	13.591	4.14	4.36
2	57.41	1004.391	298.065	95.86	95.64

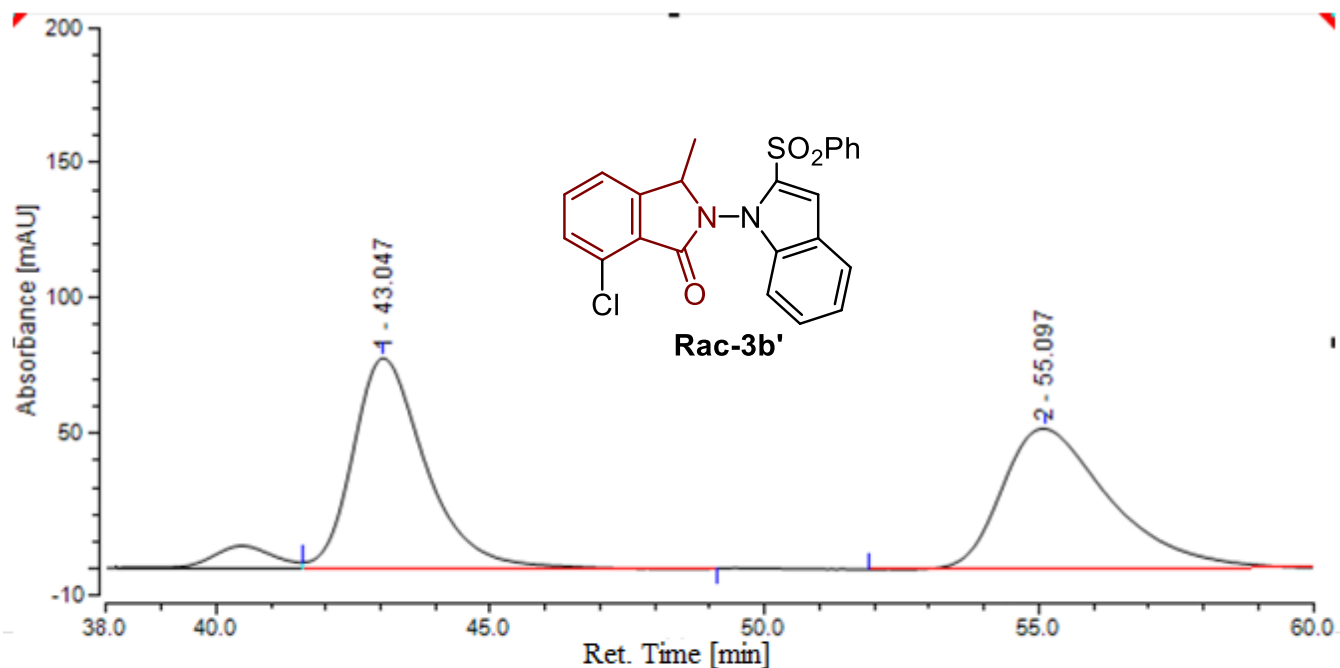




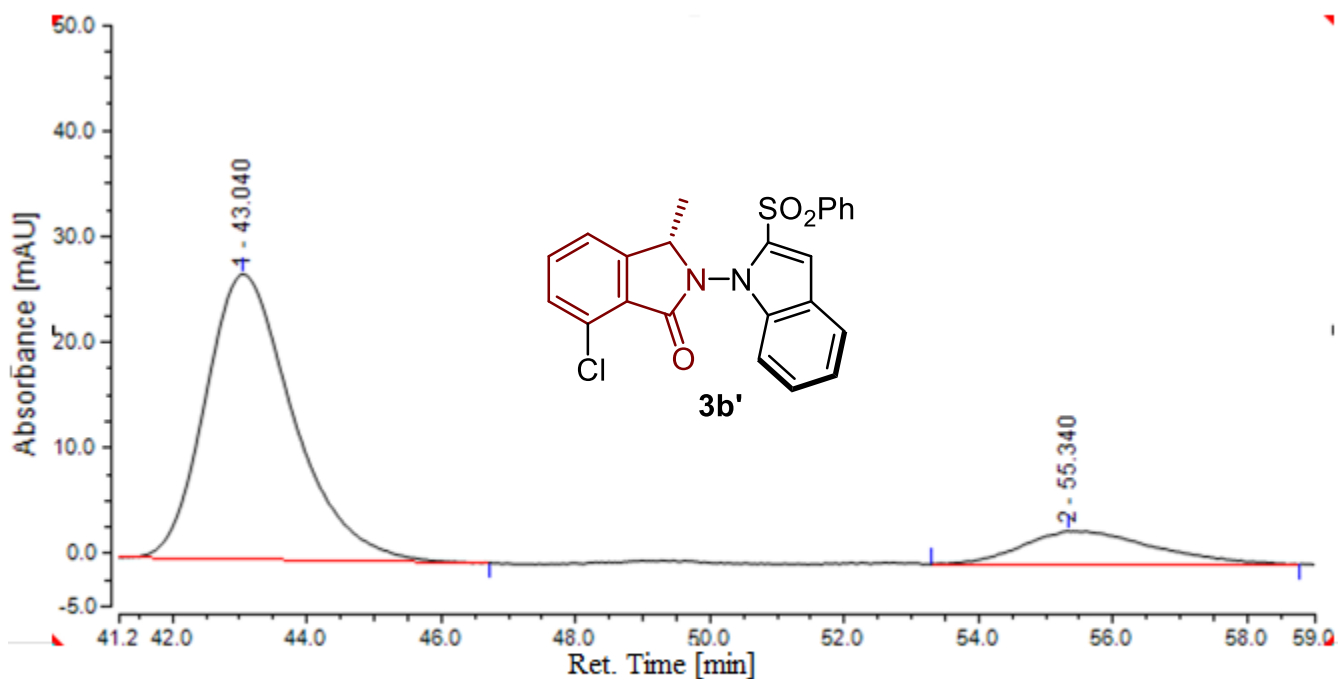
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	40.49	2.967	1.840	2.63	3.01
2	50.47	110.012	59.296	97.37	96.99



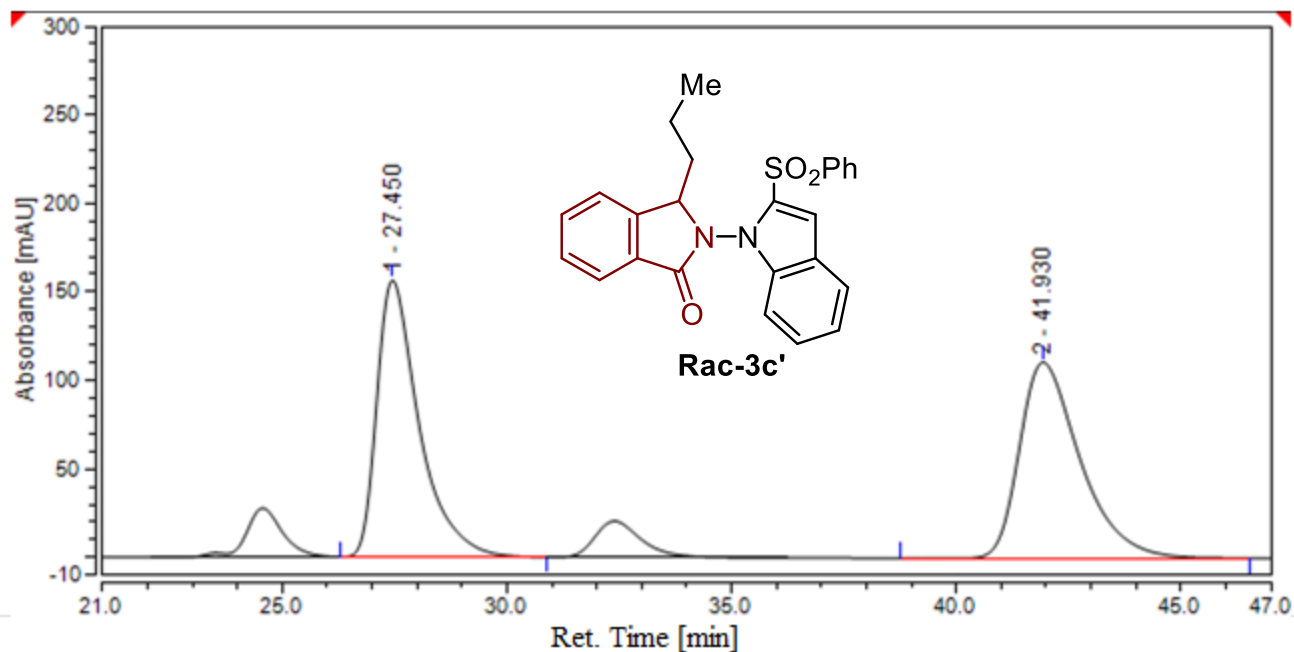
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	40.42	52.762	32.777	3.09	3.63
2	50.49	1653.888	871.207	96.91	96.37



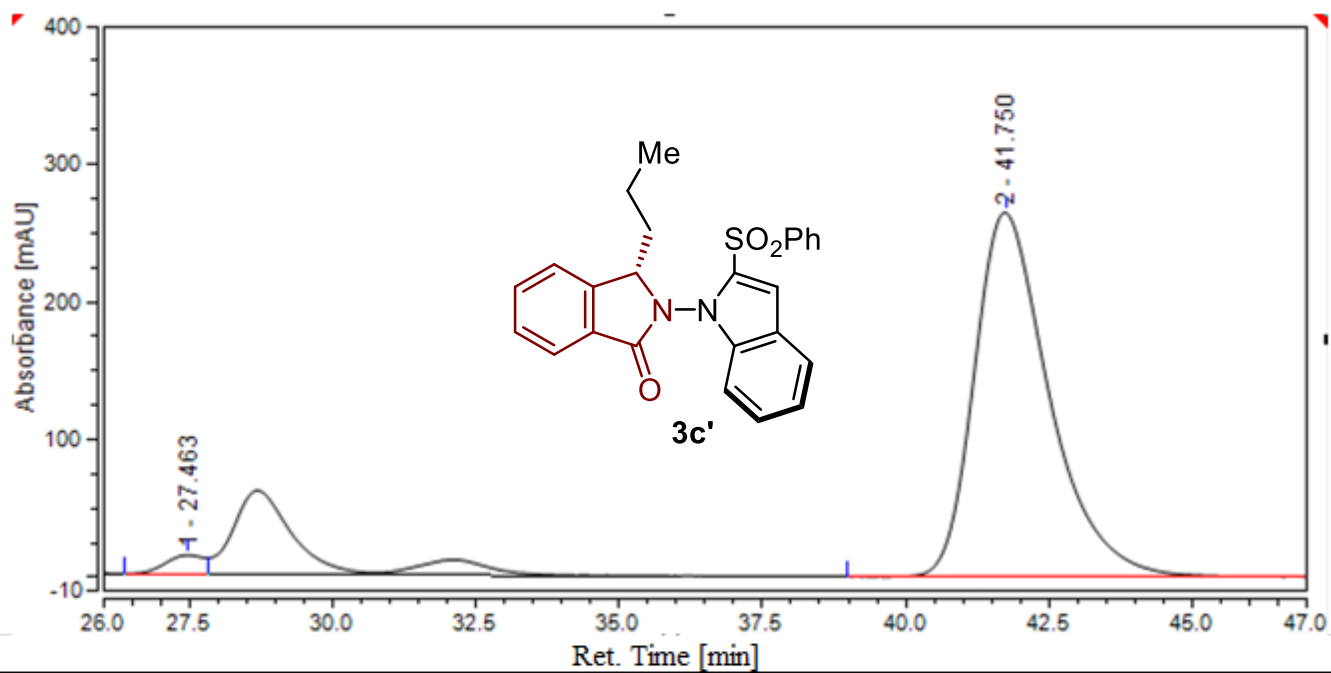
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	43.05	118 394	77.546	50.23	59.98
2	55.10	117.327	51.746	49.77	40.02



Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	43.04	40.777	26.976	85.14	89.47
2	55.34	7.116	3.176	14.86	10.53

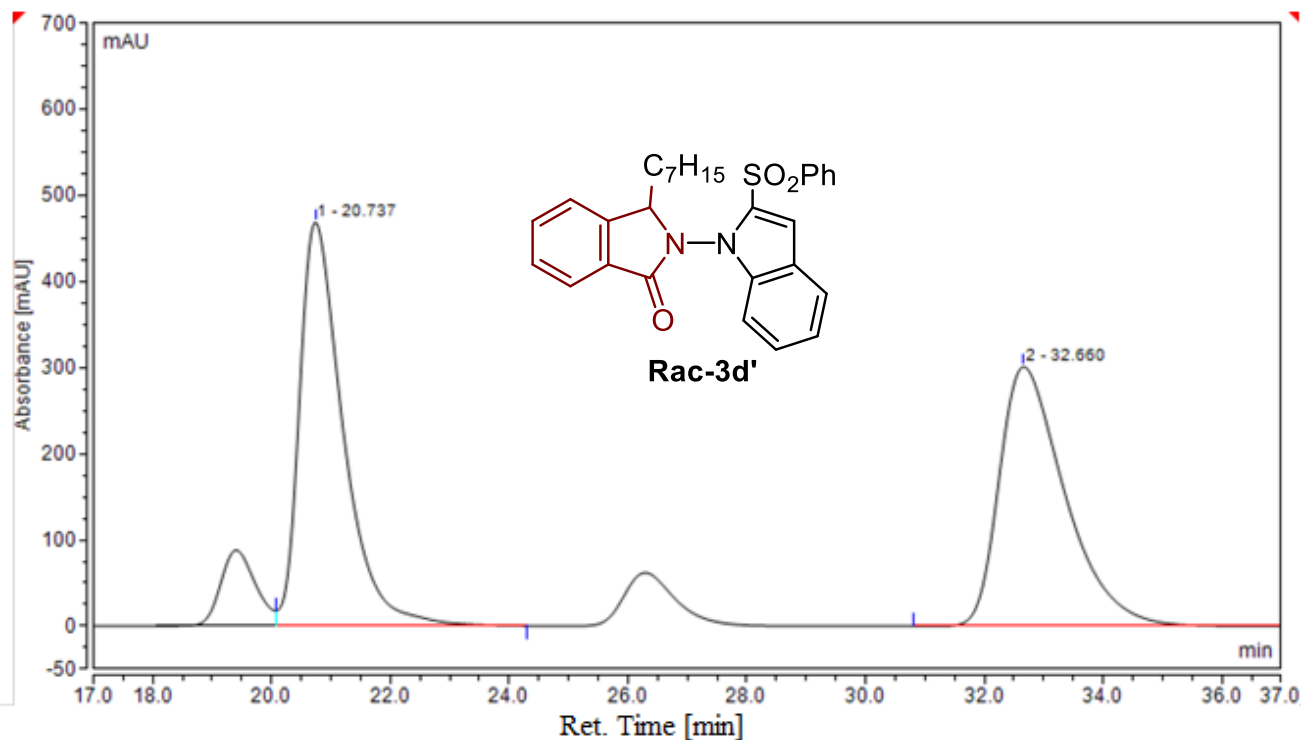


Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	27.45	171.243	156.623	49.80	58.61
2	41.93	172.645	110.622	50.20	41.39

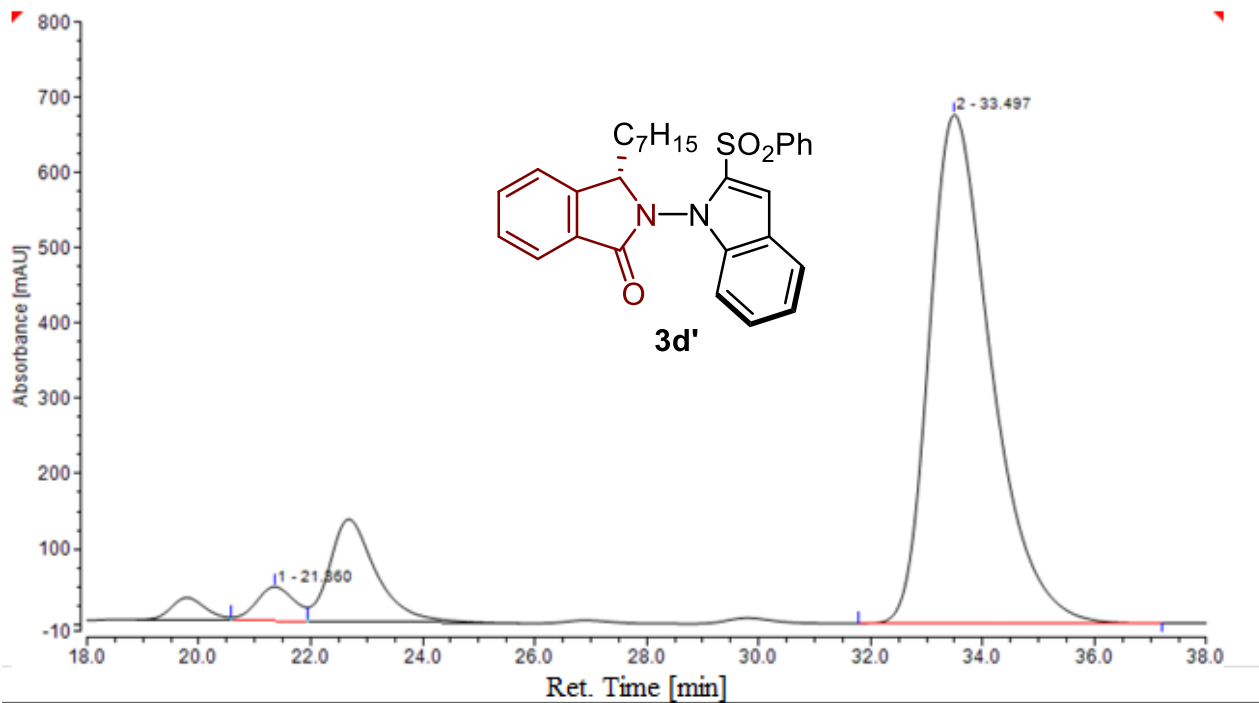


Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	27.46	11.547	14.171	2.81	5.09
2	41.75	399.032	264.164	97.19	94.91

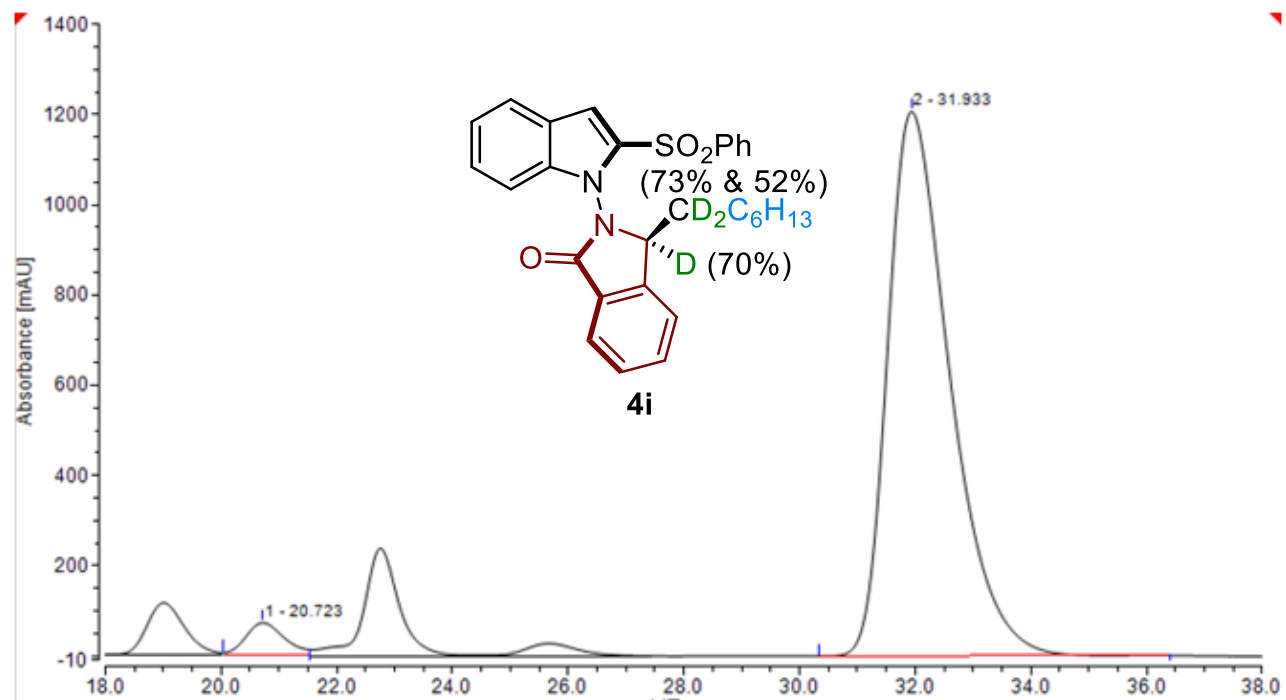




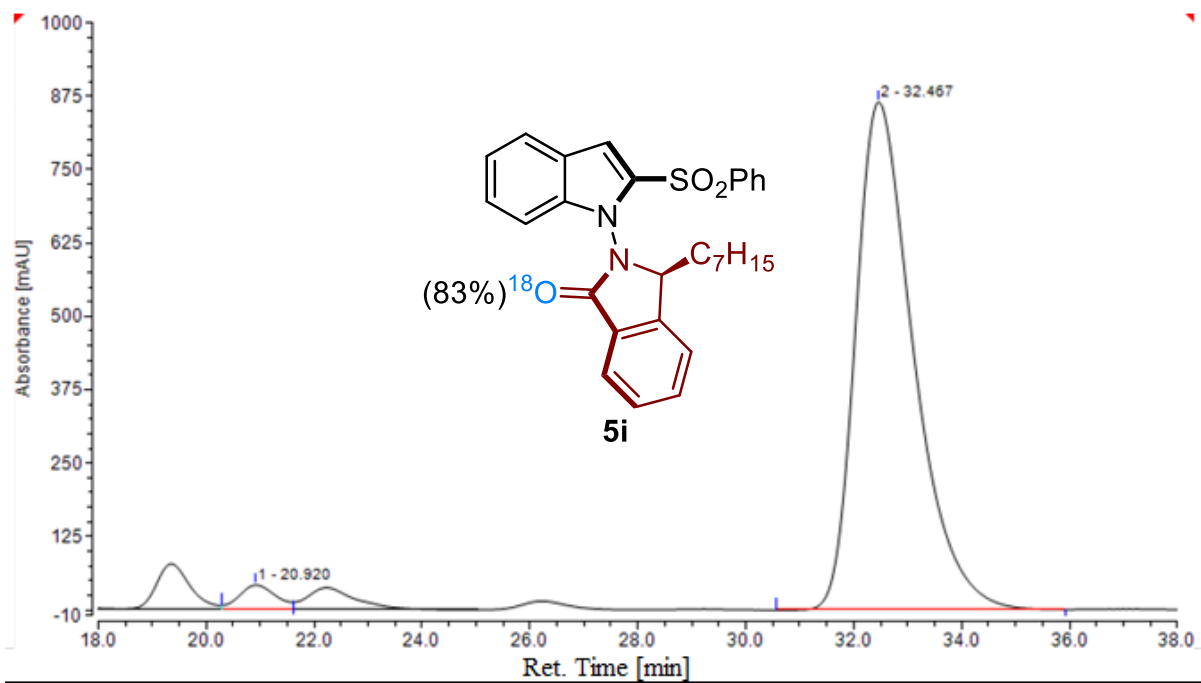
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	20.74	397.626	468.794	50.78	60.89
2	32.66	385.359	301.056	49.22	39.11



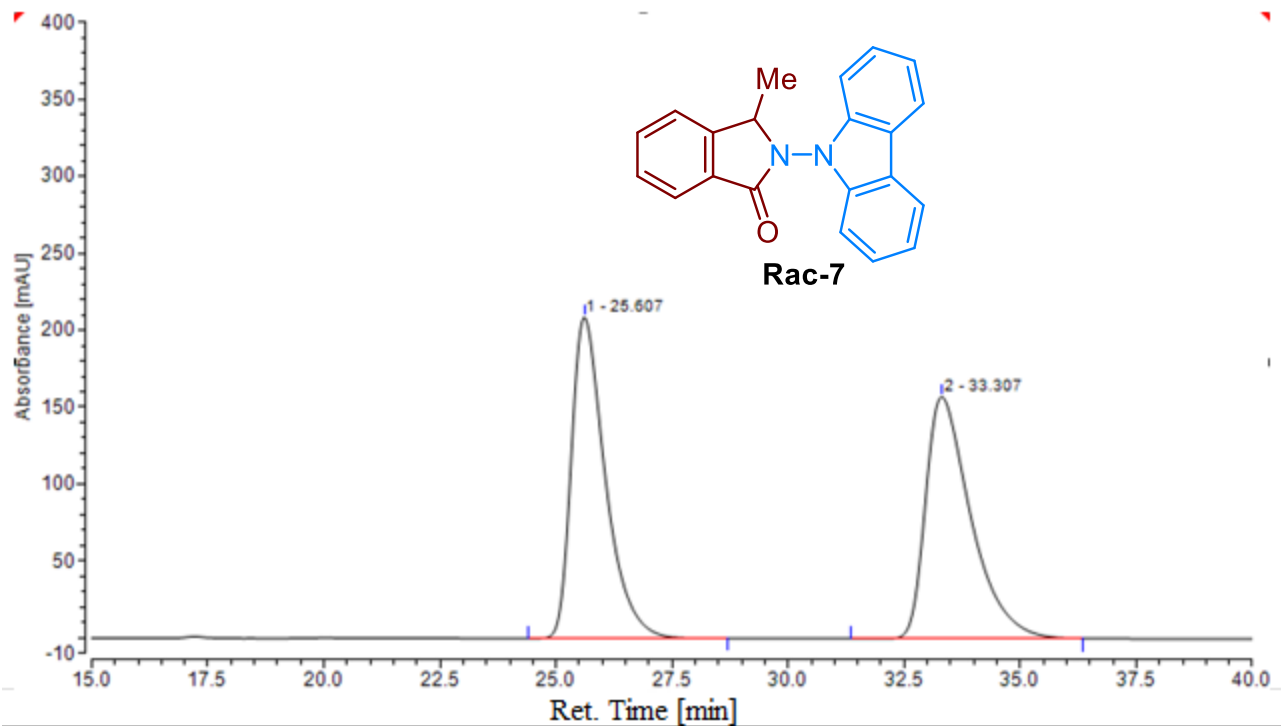
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	21.36	36.059	45.410	4.00	6.29
2	33.50	865.375	676.327	96.00	93.71



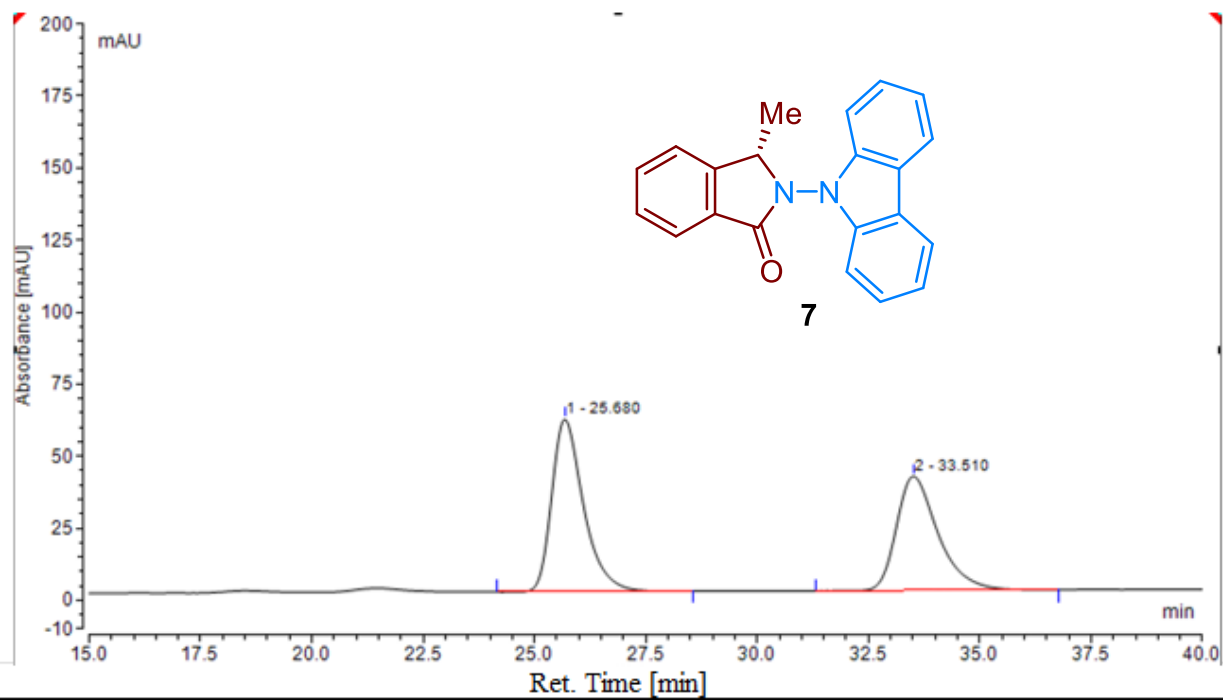
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	20.72	57.621	73.080	3.70	5.71
2	31.93	1498.545	1207.498	96.30	94.29



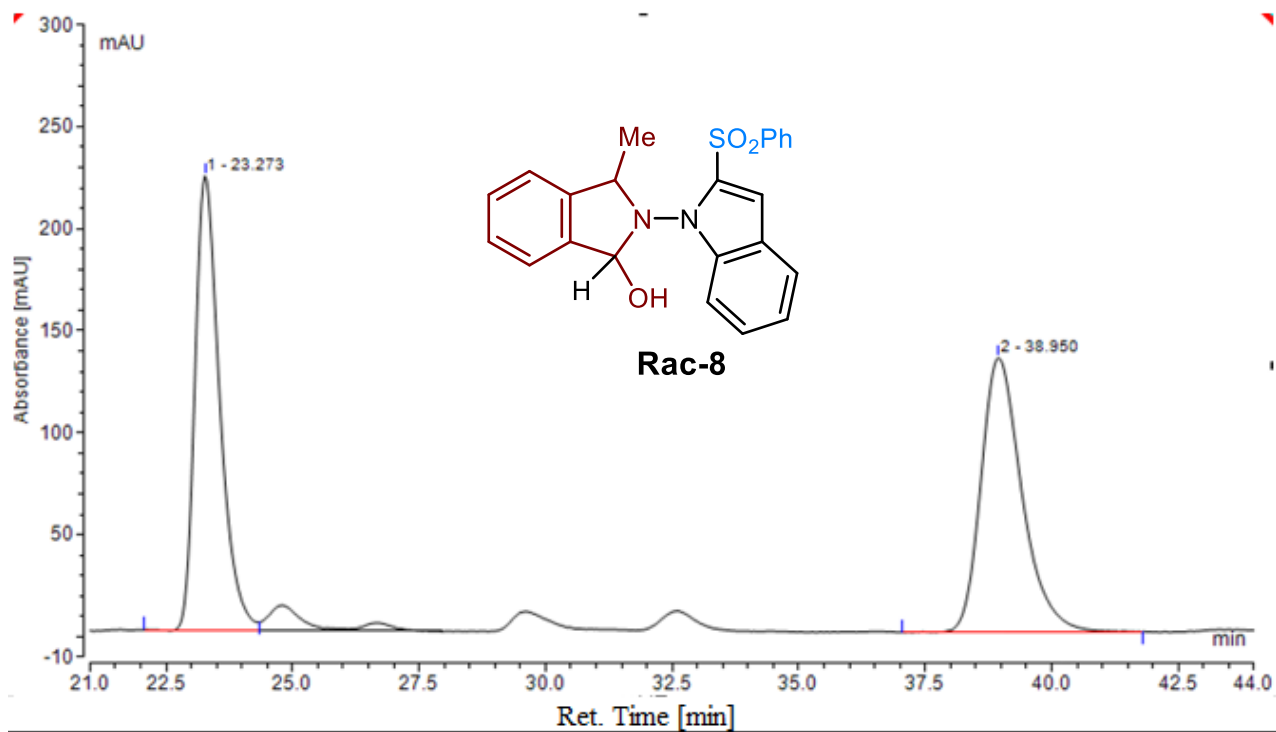
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	20.92	32.924	41.648	2.98	4.59
2	32.47	1071.239	865.622	97.02	95.41



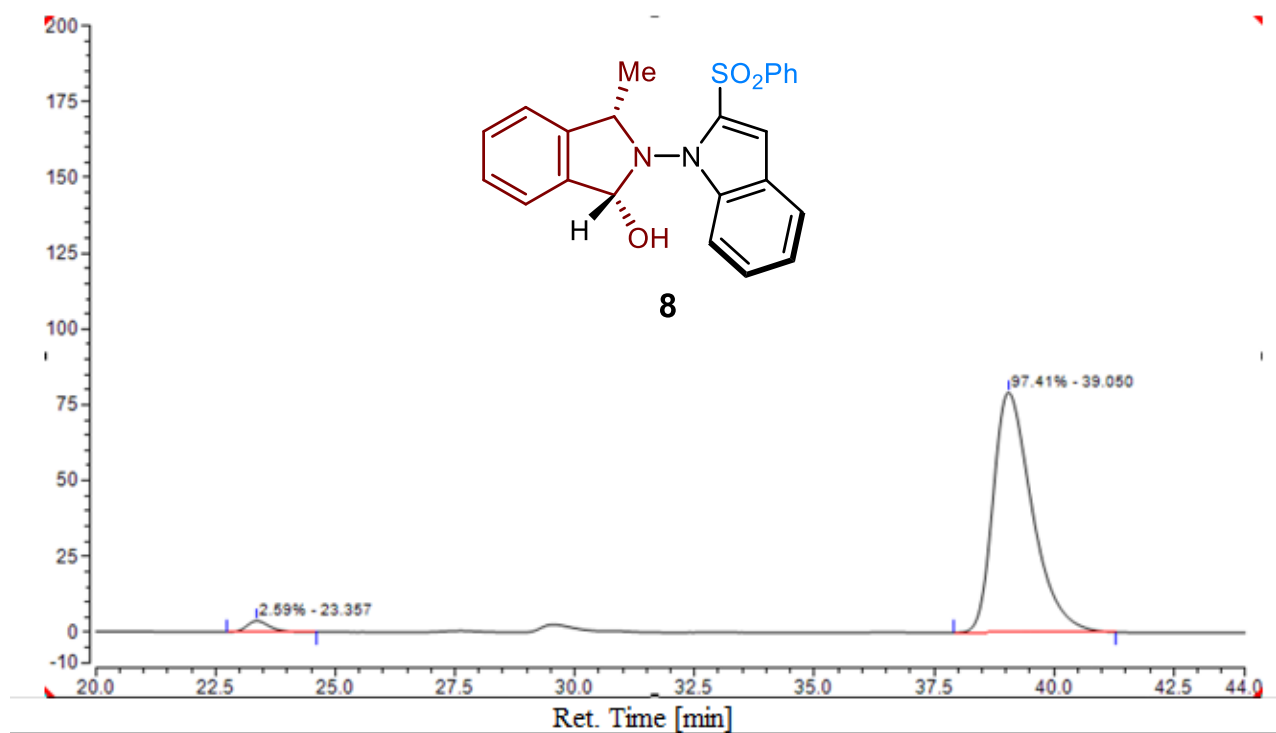
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	25.61	177.145	208.664	49.98	57.05
2	33.31	177.264	157.061	50.02	42.95



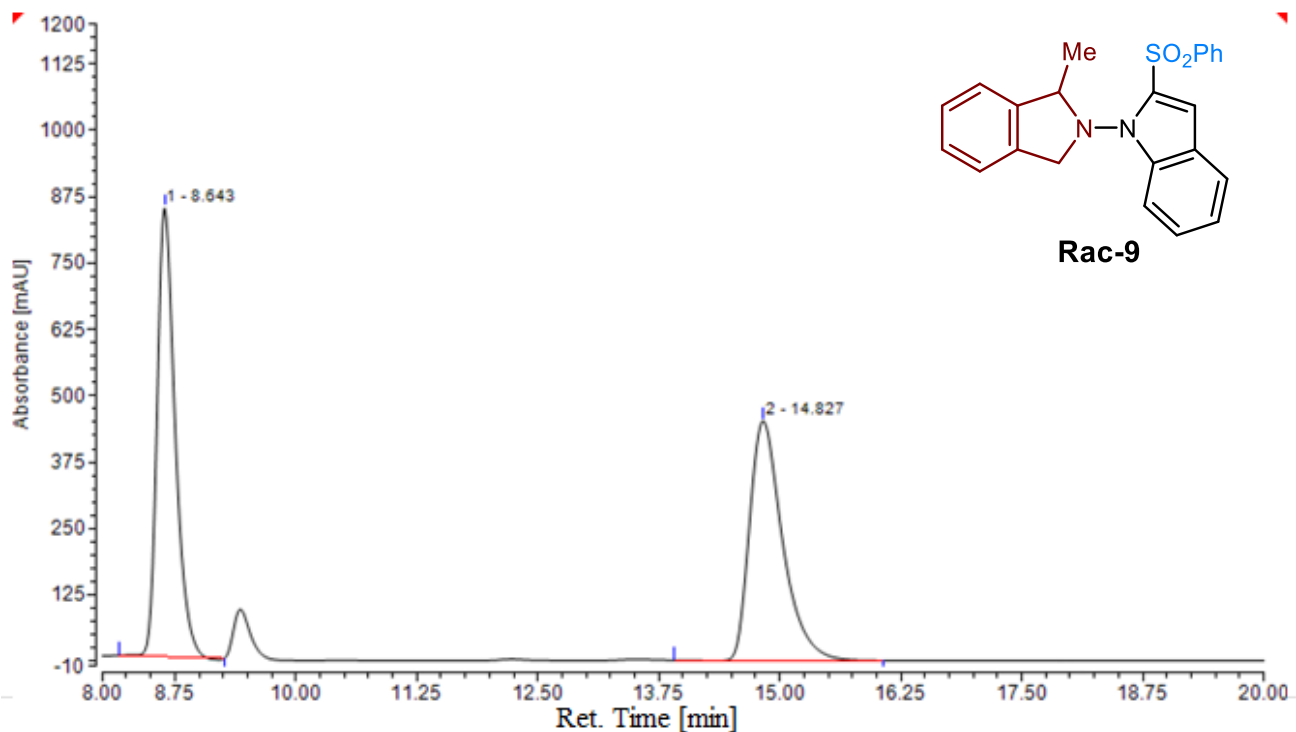
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	25.68	49.378	59.790	53.57	60.15
2	33.51	42.802	39.613	46.43	39.85



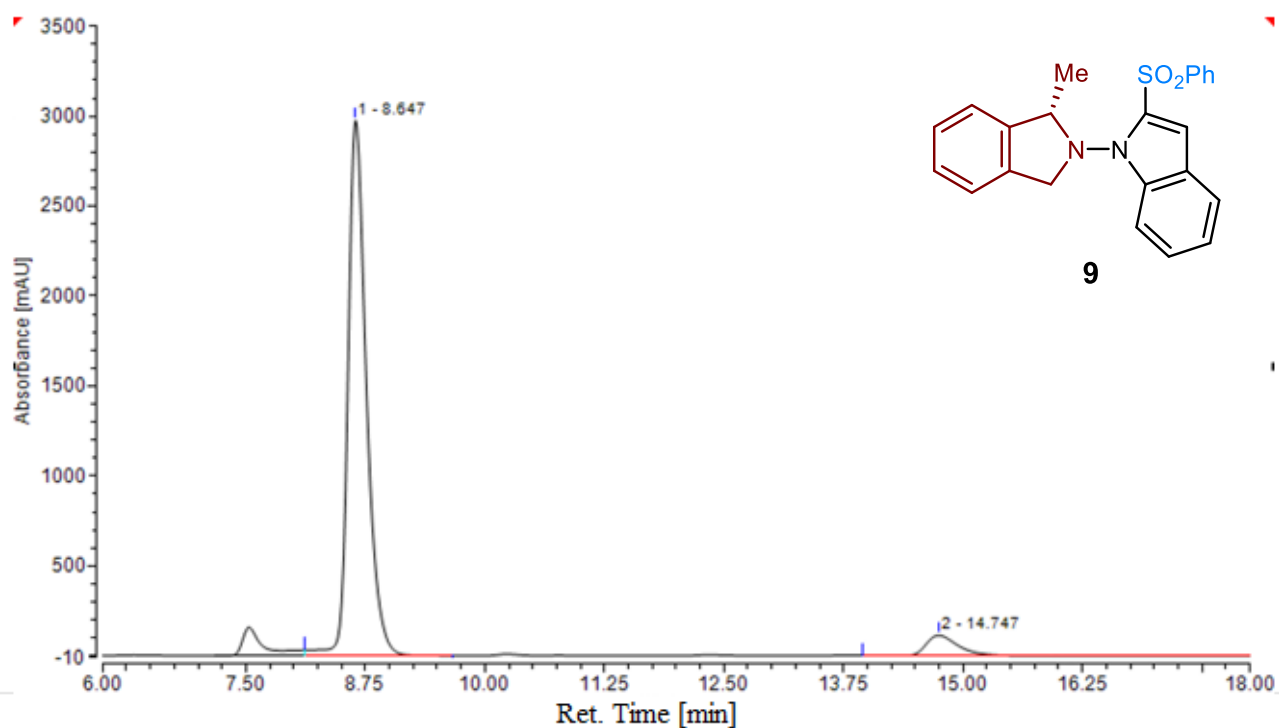
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	23.27	125.833	222.811	49.91	62.35
2	38.95	126.273	134.545	50.09	37.65



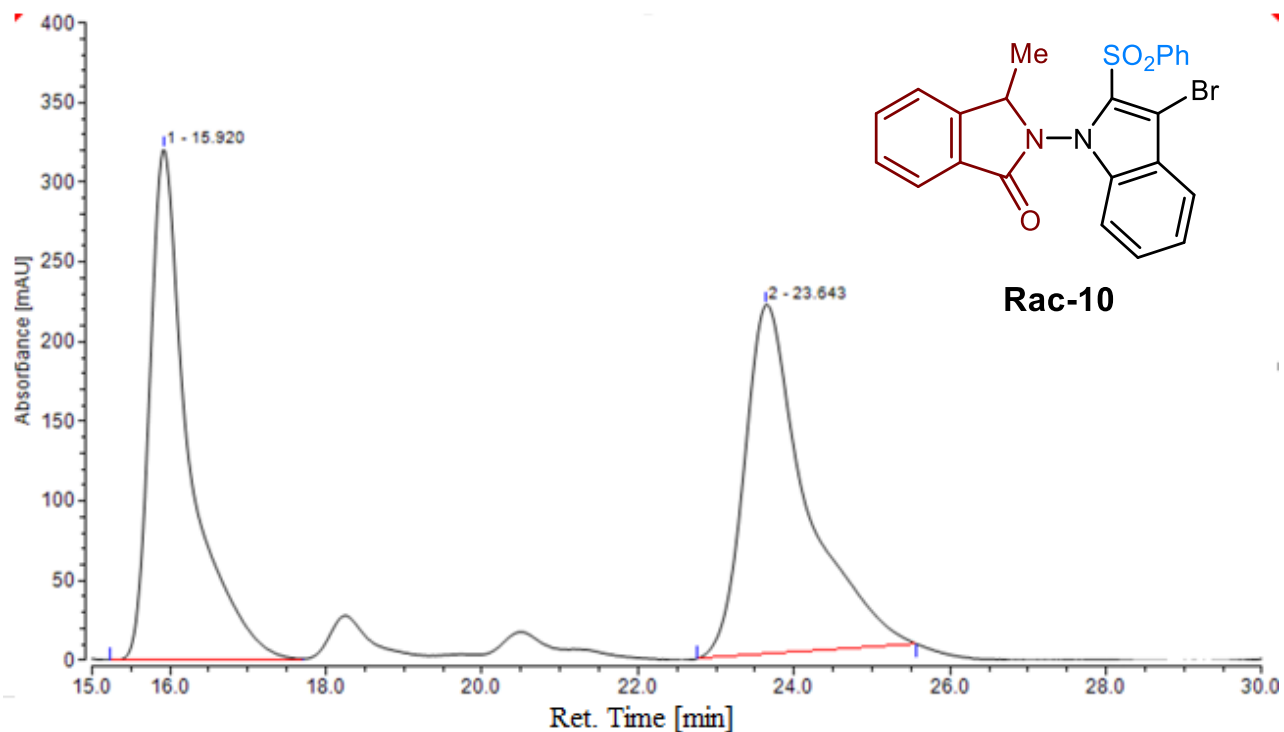
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	23.36	1.986	3.669	2.59	4.43
2	39.05	74.730	79.173	97.41	95.57



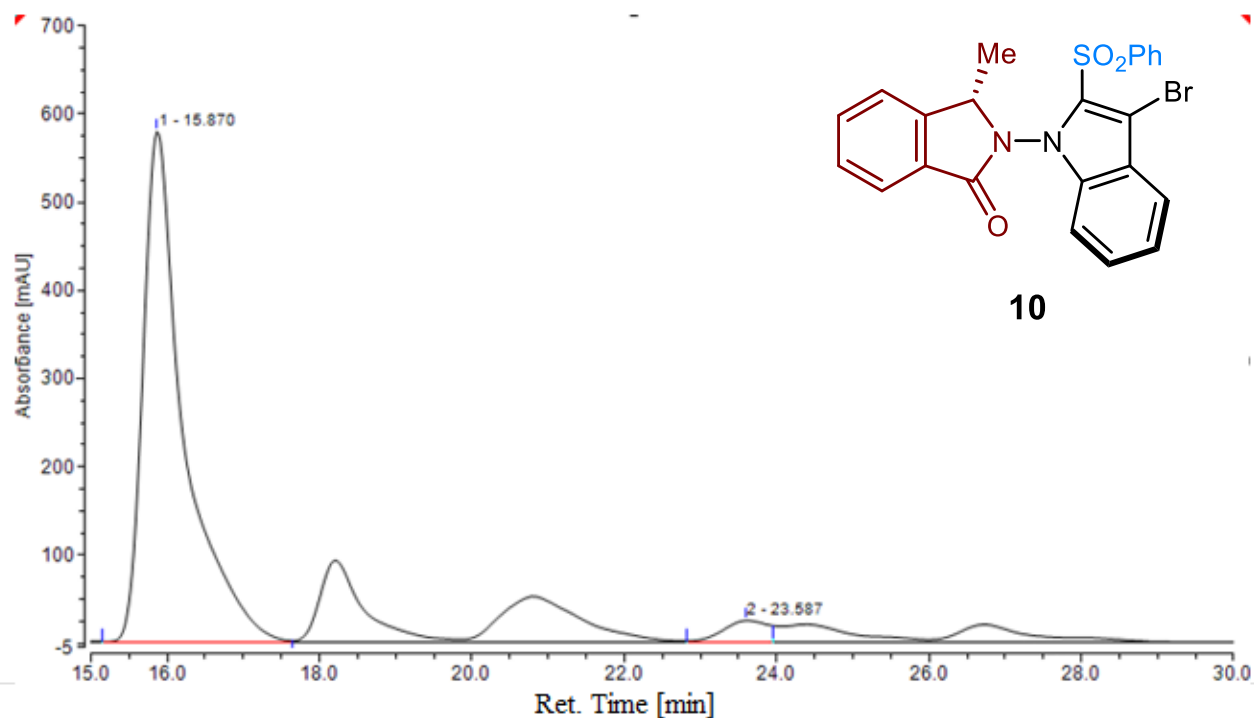
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	8.64	181.404	845.161	50.45	65.18
2	14.83	178.146	451.402	49.55	34.82



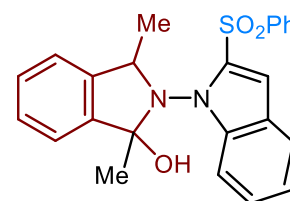
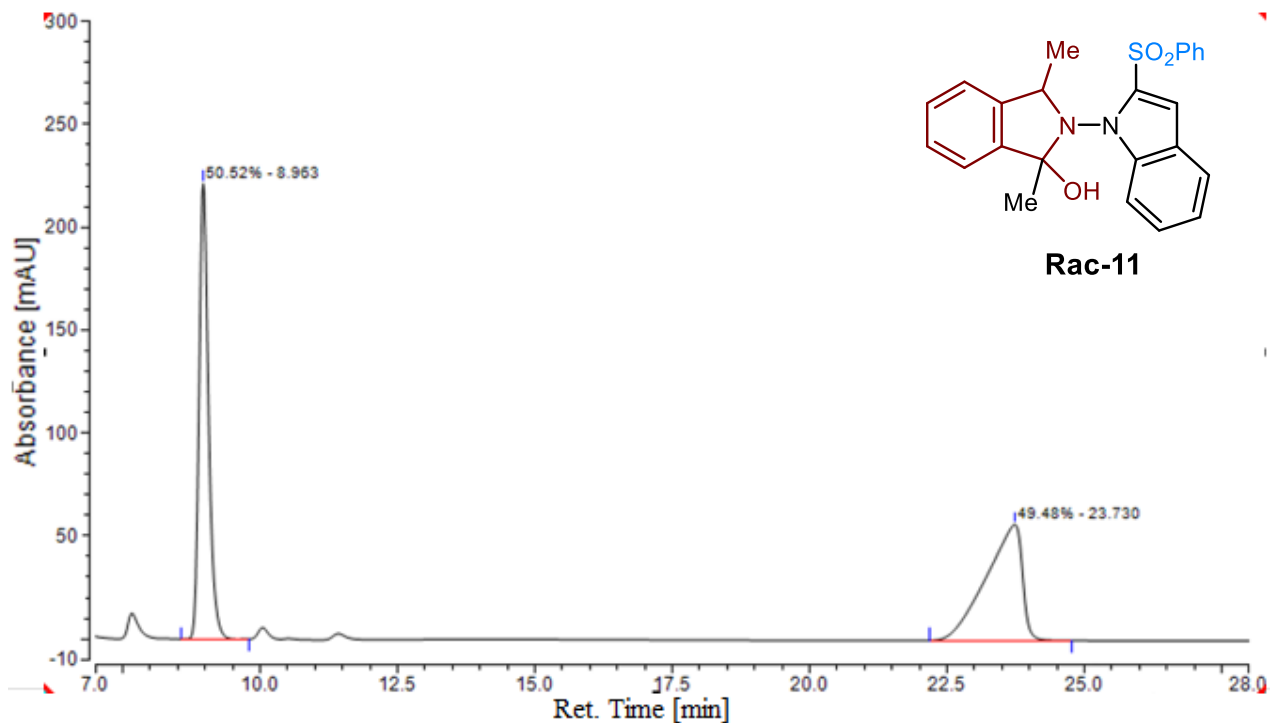
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	8.65	663.380	2975.563	94.34	96.34
2	14.75	40.044	112.884	5.69	3.66



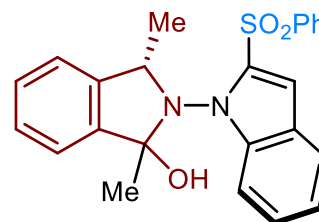
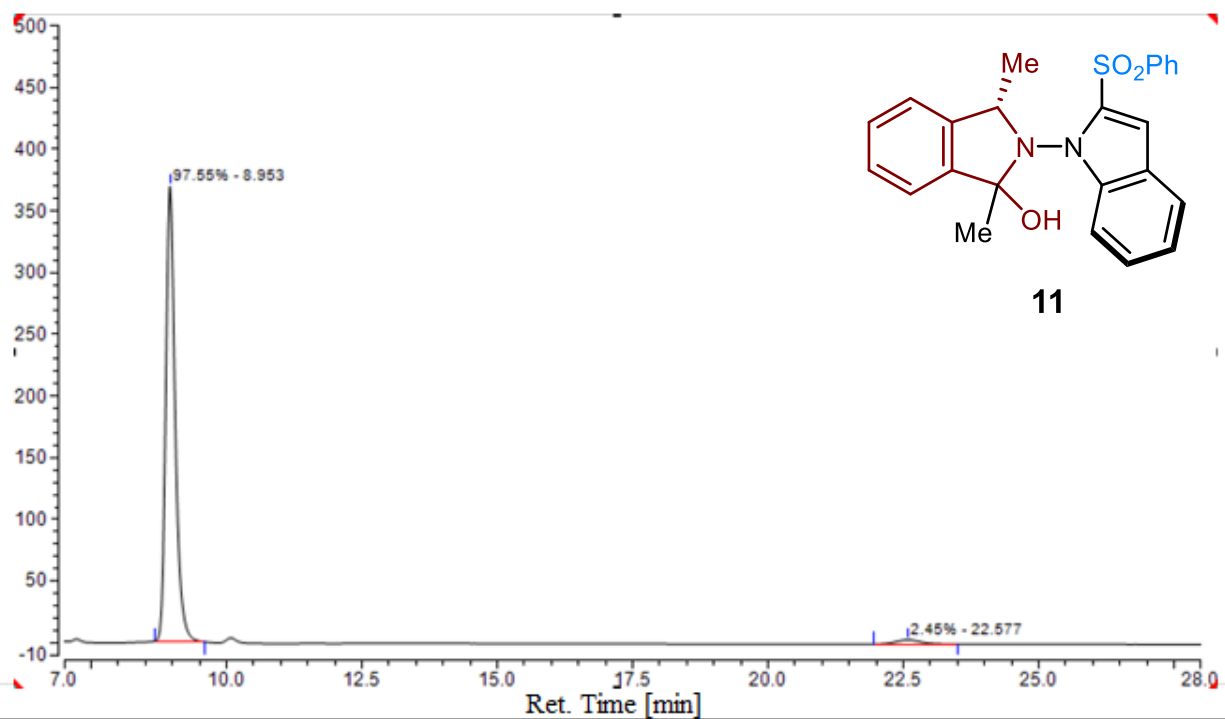
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	15.92	185.942	320.407	48.04	59.37
2	23.64	201.093	219.255	51.96	40.63



Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	15.87	357.821	578.969	95.45	95.86
2	23.59	17.068	24.997	4.55	4.14



**Rac-11**



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