

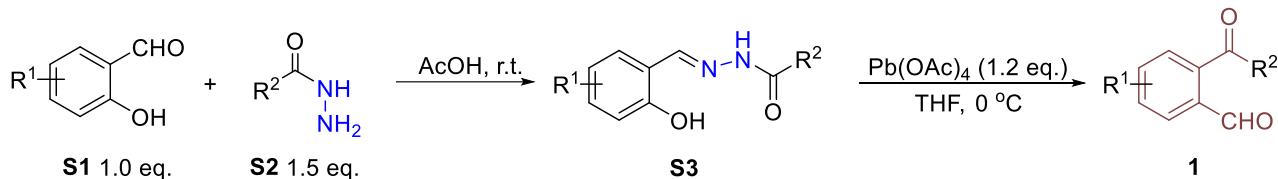
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General Information

Unless otherwise noted, all starting materials were purchased from commercial sources and used without any further purification. Toluene, Chlorobenzene, DCM, CHCl₃, CCl₄, THF, D₂O, H₂¹⁸O, 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 KMnO₄ followed by heating. Abbreviations are reported as follows: DCM = dichloromethane, THF = tetrahydrofuran, EA = ethyl acetate, PE = petroleum ether, D₂O = deuterium oxide, H₂¹⁸O = heavy-oxygen water, TLC = thin layer chromatograph, ee = enantiomeric excess, dr = diastereomeric ratio, rt = room temperature. ¹H NMR, ¹⁹F NMR and ¹³C 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



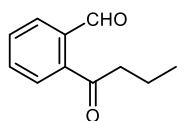
The 2-acetylbenzaldehyde were synthesized according to the literature^[1] with the modifications.

Procedure 1: The salicylaldehyde **S1** (1.0 ml, 10 mmol, 1.0 equiv.) was added to a solution containing the acetylhydrazine **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 CH₂Cl₂. The organic layer was washed with brine, dried over anhydrous MgSO₄, and evaporated under reduced 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 NaHCO₃ and brine. The organic layer was dried over anhydrous MgSO₄ and evaporated under reduced pressure. The crude product was purified by column chromatography over silica gel (PE: EA = 10:1) to afford the desired product.

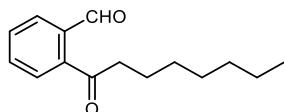
The characterizations of unknown products were as following:

2-butryrylbenzaldehyde (**1c'**)



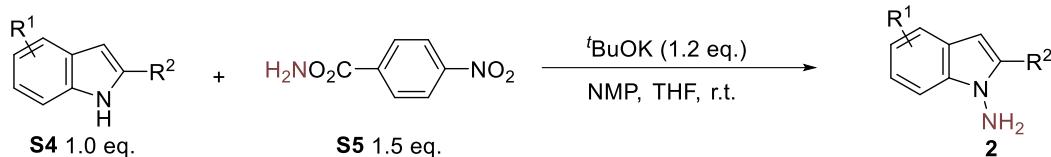
¹H NMR (500 MHz, CDCl₃) ¹H NMR (500 MHz, Chloroform-*d*) δ 10.19 (s, 1H), 7.96 – 7.88 (m, 1H), 7.71 – 7.62 (m, 3H), 2.94 (t, *J* = 7.3 Hz, 2H), 1.82 (q, *J* = 7.4 Hz, 2H), 1.04 (t, *J* = 7.4 Hz, 3H). ¹³C NMR (126 MHz, CDCl₃) δ 204.02, 192.02, 141.32, 135.88, 133.14, 131.37, 129.93, 127.83, 43.29, 17.69, 13.76. HRMS (APCI) m/z: calculated for [C₁₁H₁₂O₂+Na]⁺ 199.0729, found 199.0732.

2-octanoylbenzaldehyde (1d')



¹H NMR (500 MHz, CDCl₃) ¹H NMR (500 MHz, Chloroform-*d*) δ 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). ¹³C NMR (126 MHz, CDCl₃) δ 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 [C₁₅H₂₀O₂+Na]⁺ 255.1355, found 255.1366.

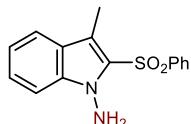
Synthesis of 2-(phenylsulfonyl)-1*H*-indol-1-amine



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

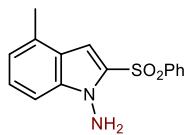
Procedure 3: To a stirred solution of the **S4** (10 mmol, 1.0 eq.) in 50 mL *N*-methylpyrrolidone (NMP) was added 12 mL ^tBuOK (1M in THF) and the reaction mixture was stirred at rt for 0.5 h. Then, a solution of **S5** (15 mmol, 1.5 eq.) was added to the mixture, which was stirred at rt for 2 h. After 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 Na₂SO₄ 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)



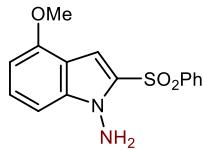
¹H NMR (500 MHz, CDCl₃) ¹H NMR (500 MHz, Chloroform-*d*) δ 7.98 – 7.93 (m, 2H), 7.64 (dt, *J* = 8.2, 0.9 Hz, 1H), 7.62 – 7.55 (m, 1H), 7.55 – 7.48 (m, 3H), 7.41 – 7.33 (m, 1H), 7.16 (ddd, *J* = 8.0, 6.9, 1.0 Hz, 1H), 4.82 (s, 2H), 2.72 (s, 3H). ¹³C NMR (126 MHz, CDCl₃) δ 142.43, 138.63, 133.47, 129.47, 128.73, 126.90, 126.63, 124.05, 120.76, 120.54, 119.56, 110.46, 9.73. HRMS (APCI) m/z: calculated for [C₁₅H₁₄N₂O₂S+H]⁺ 287.0848, found 287.0844.

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



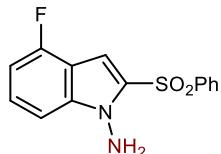
¹H NMR (500 MHz, CDCl₃) δ 8.04 – 7.98 (m, 2H), 7.64 – 7.57 (m, 1H), 7.53 (dd, *J* = 8.5, 7.0 Hz, 2H), 7.42 (s, 1H), 7.38 (d, *J* = 8.5 Hz, 1H), 7.20 (dd, *J* = 8.6, 1.6 Hz, 1H), 7.17 (s, 1H), 4.77 (s, 2H), 2.43 (s, 3H). ¹³C NMR (126 MHz, CDCl₃) δ 138.03, 134.13, 133.60, 130.98, 129.40, 128.18, 127.86, 122.99, 121.84, 110.02, 107.94, 21.40. HRMS (APCI) m/z: calculated for [C₁₅H₁₄N₂O₂S+Na]⁺ 309.0668 found 309.0677.

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



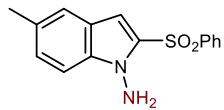
¹H NMR (500 MHz, CDCl₃) δ 8.01 (dd, *J* = 8.4, 1.4 Hz, 2H), 7.63 – 7.57 (m, 1H), 7.53 (dd, *J* = 8.4, 7.0 Hz, 2H), 7.35 (s, 1H), 7.29 (d, *J* = 7.9 Hz, 1H), 7.08 (d, *J* = 8.4 Hz, 1H), 6.52 (d, *J* = 7.7 Hz, 1H), 4.81 (s, 2H), 3.94 (d, *J* = 1.2 Hz, 3H). ¹³C NMR (126 MHz, CDCl₃) δ 154.49, 141.16, 140.89, 133.59, 133.01, 129.39, 127.89, 127.31, 106.26, 103.11, 100.46, 55.48. HRMS (APCI) m/z: calculated for [C₁₅H₁₄N₂O₃S+H]⁺ 303.0797, found 303.0792.

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



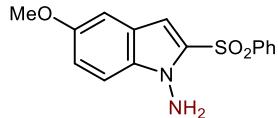
¹H NMR (500 MHz, CDCl₃) δ 8.06 – 8.01 (m, 2H), 7.67 – 7.61 (m, 1H), 7.56 (dd, *J* = 8.5, 7.1 Hz, 2H), 7.31 – 7.24 (m, 3H), 6.82 (ddd, *J* = 9.9, 5.1, 3.3 Hz, 1H), 4.86 (s, 2H). ¹³C NMR (126 MHz, CDCl₃) δ 156.99 (d, *J* = 252.3 Hz), 141.54 (d, *J* = 9.5 Hz), 140.53, 134.91, 133.93, 129.51, 128.01, 126.75 (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 [C₁₄H₁₁FN₂O₂S+Na]⁺ 313.0417, found 313.0427.

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



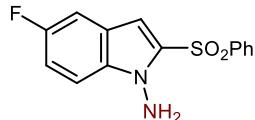
¹H NMR (500 MHz, CDCl₃) δ 8.03 – 7.98 (m, 2H), 7.63 – 7.56 (m, 1H), 7.52 (dd, *J* = 8.4, 6.9 Hz, 2H), 7.41 (s, 1H), 7.38 (d, *J* = 8.6 Hz, 1H), 7.20 (dd, *J* = 8.7, 1.6 Hz, 1H), 7.16 (s, 1H), 4.77 (s, 2H), 2.42 (s, 3H). ¹³C NMR (126 MHz, CDCl₃) δ 141.11, 138.00, 134.12, 133.57, 130.94, 129.36, 128.15, 127.83, 122.96, 121.81, 109.99, 107.90, 21.37. HRMS (APCI) m/z: calculated for [C₁₅H₁₄N₂O₂S+H]⁺ 287.0848, found 287.0845.

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



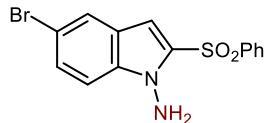
¹H NMR (500 MHz, CDCl₃) δ 8.04 – 7.95 (m, 2H), 7.65 – 7.58 (m, 1H), 7.54 (dd, *J* = 8.5, 7.1 Hz, 2H), 7.40 (d, *J* = 9.0 Hz, 1H), 7.17 (s, 1H), 7.05 (dd, *J* = 9.0, 2.4 Hz, 1H), 7.02 (d, *J* = 2.3 Hz, 1H), 4.79 (s, 2H), 3.83 (s, 3H). ¹³C NMR (126 MHz, CDCl₃) δ 155.23, 134.95, 134.15, 133.60, 129.41, 127.79, 122.97, 117.97, 111.40, 107.73, 102.37, 55.74. HRMS (APCI) m/z: calculated for [C₁₅H₁₄N₂O₃S+H]⁺ 303.0797, found 303.0788.

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



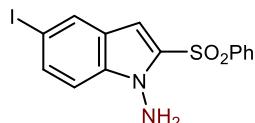
¹H NMR (500 MHz, CDCl₃) δ 8.04 – 7.99 (m, 2H), 7.63 (t, *J* = 7.4 Hz, 1H), 7.55 (dd, *J* = 8.5, 6.9 Hz, 2H), 7.45 (dd, *J* = 9.1, 4.4 Hz, 1H), 7.30 – 7.24 (m, 1H), 7.16 (s, 1H), 7.13 (td, *J* = 9.1, 2.5 Hz, 1H), 4.84 (s, 2H). ¹³C NMR (126 MHz, CDCl₃) δ 158.46 (d, *J* = 238.1 Hz), 140.66, 136.14, 135.68, 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). ¹⁹F NMR (471 MHz, CDCl₃) δ -121.69. HRMS (APCI) m/z: calculated for [C₁₄H₁₁FN₂O₂S+Na]⁺ 313.0417, found 313.0439.

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



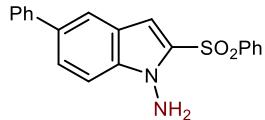
¹H NMR (500 MHz, CDCl₃) δ 8.04 – 7.96 (m, 2H), 7.78 (d, *J* = 1.8 Hz, 1H), 7.68 – 7.61 (m, 1H), 7.57 (dd, *J* = 8.6, 7.2 Hz, 2H), 7.45 (dd, *J* = 8.9, 1.8 Hz, 1H), 7.40 (d, *J* = 8.8 Hz, 1H), 7.15 (s, 1H), 4.83 (s, 2H). ¹³C NMR (126 MHz, CDCl₃) δ 140.56, 138.09, 135.48, 133.95, 129.55, 129.22, 127.93, 124.88, 124.02, 114.61, 112.11, 107.38. HRMS (APCI) m/z: calculated for [C₁₄H₁₁BrN₂O₂S+Na]⁺ 372.9616, found 374.9605.

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



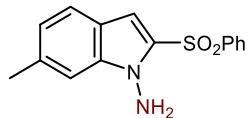
¹H NMR (500 MHz, CDCl₃) δ 8.04 – 7.91 (m, 3H), 7.67 – 7.62 (m, 1H), 7.61 (dd, *J* = 8.8, 1.6 Hz, 1H), 7.56 (dd, *J* = 8.5, 7.1 Hz, 2H), 7.30 (d, *J* = 8.8 Hz, 1H), 7.14 (d, *J* = 0.8 Hz, 1H), 4.82 (s, 2H). ¹³C NMR (126 MHz, CDCl₃) δ 140.55, 138.51, 135.10, 134.50, 133.95, 131.26, 129.54, 127.91, 124.87, 112.46, 107.12, 84.79. HRMS (APCI) m/z: calculated for [C₁₄H₁₁IN₂O₂S+Na]⁺ 420.9478, found 420.9475.

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



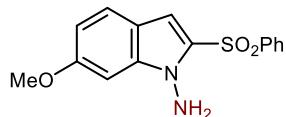
¹H NMR (500 MHz, CDCl₃) δ 8.04 (dd, *J* = 8.4, 1.3 Hz, 2H), 7.84 (d, *J* = 1.6 Hz, 1H), 7.66 – 7.61 (m, 4H), 7.60 – 7.53 (m, 5H), 7.44 (t, *J* = 7.7 Hz, 2H), 7.37 – 7.31 (m, 1H), 7.30 (s, 1H), 4.84 (s, 2H). ¹³C NMR (126 MHz, CDCl₃) δ 141.44, 140.92, 138.97, 135.16, 134.91, 133.74, 129.46, 128.81, 127.89, 127.33, 126.93, 126.22, 123.17, 120.81, 110.69, 108.70. HRMS (APCI) m/z: calculated for [C₂₀H₁₆N₂O₂S+H]⁺ 349.1005, found 349.1005.

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



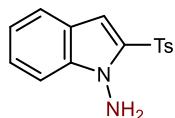
¹H NMR (500 MHz, CDCl₃) δ 8.04 – 7.98 (m, 2H), 7.60 (td, *J* = 7.2, 1.5 Hz, 1H), 7.53 (td, *J* = 8.0, 7.6, 1.9 Hz, 3H), 7.29 (s, 1H), 7.21 (s, 1H), 7.00 (dd, *J* = 8.2, 1.6 Hz, 1H), 4.76 (s, 2H), 2.47 (s, 3H). ¹³C NMR (126 MHz, CDCl₃) δ 141.18, 139.93, 136.67, 133.54, 129.37, 127.79, 123.64, 122.24, 120.69, 109.86, 108.56, 22.10. HRMS (APCI) m/z: calculated for [C₁₅H₁₄N₂O₂S+Na]⁺ 309.0668, found 309.0693.

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



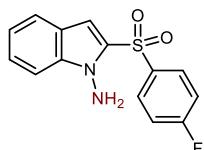
¹H NMR (500 MHz, CDCl₃) δ 7.99 (dt, *J* = 7.2, 1.3 Hz, 2H), 7.63 – 7.57 (m, 1H), 7.56 – 7.46 (m, 3H), 7.21 – 7.18 (m, 1H), 6.90 (d, *J* = 2.3 Hz, 1H), 6.81 (dd, *J* = 8.8, 2.3 Hz, 1H), 4.78 (s, 2H), 3.85 (s, 3H). ¹³C NMR (126 MHz, CDCl₃) δ 159.54, 141.36, 140.84, 133.48, 132.53, 129.42, 127.63, 123.49, 116.94, 113.45, 109.18, 91.85, 55.56. HRMS (APCI) m/z: calculated for [C₁₅H₁₄N₂O₃S+Na]⁺ 325.0617, found 325.0627.

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



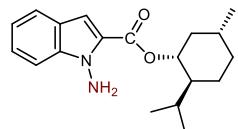
¹H NMR (500 MHz, CDCl₃) δ 7.89 – 7.84 (m, 2H), 7.62 – 7.56 (m, 1H), 7.38 (dd, *J* = 8.5, 1.1 Hz, 1H), 7.33 (d, *J* = 8.2 Hz, 2H), 7.25 (ddd, *J* = 8.3, 6.9, 1.1 Hz, 1H), 7.08 (d, *J* = 0.9 Hz, 1H), 7.05 (ddd, *J* = 7.9, 6.8, 1.0 Hz, 1H), 5.87 (s, 2H), 2.28 (s, 3H). ¹³C NMR (126 MHz, CDCl₃) δ 144.63, 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 [C₁₅H₁₄N₂O₂S+Na]⁺ 309.0668, found 309.0676.

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



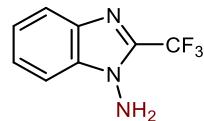
¹H NMR (500 MHz, DMSO-*d*₆) δ 8.09 – 8.02 (m, 2H), 7.65 (d, *J* = 8.1 Hz, 1H), 7.48 (d, *J* = 8.4 Hz, 1H), 7.38 (ddd, *J* = 8.3, 6.9, 1.1 Hz, 1H), 7.23 – 7.15 (m, 4H), 4.80 (s, 2H). ¹³C NMR (126 MHz, DMSO-*d*₆) δ 165.68 (d, *J* = 257.0 Hz), 139.42, 137.01 (d, *J* = 3.2 Hz), 134.43, 130.96 (d, *J* = 9.6 Hz), 126.26, 122.77, 122.70, 121.62, 116.63 (d, *J* = 22.7 Hz), 110.12, 108.31. ¹⁹F NMR (471 MHz, CDCl₃) δ -103.25. HRMS (APCI) m/z: calculated for [C₁₄H₁₁FN₂O₂S+Na]⁺ 313.0417, found 313.0434.

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



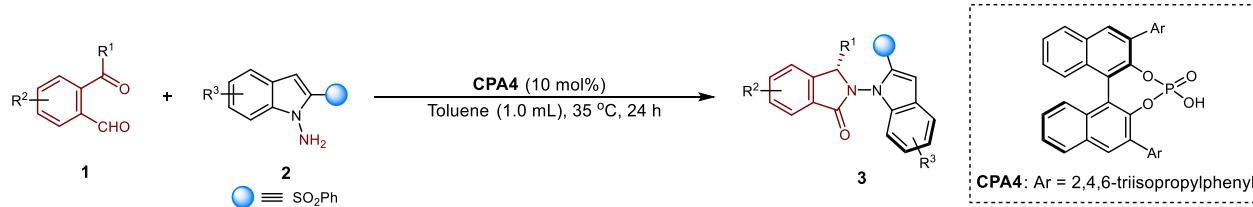
¹H NMR (500 MHz, CDCl₃) δ 7.62 (t, *J* = 7.6 Hz, 2H), 7.34 (dd, *J* = 8.6, 6.8 Hz, 1H), 7.17 (s, 1H), 7.12 (t, *J* = 7.7 Hz, 1H), 5.35 (d, *J* = 2.0 Hz, 2H), 4.94 (td, *J* = 10.9, 4.3 Hz, 1H), 2.16 – 2.10 (m, 1H), 1.99 (pd, *J* = 6.9, 2.4 Hz, 1H), 1.74 (dt, *J* = 14.7, 3.8 Hz, 2H), 1.63 – 1.52 (m, 2H), 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). ¹³C NMR (126 MHz, CDCl₃) δ 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 [C₁₉H₂₆N₂O₂+H]⁺ 315.2067, found 315.2075.

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



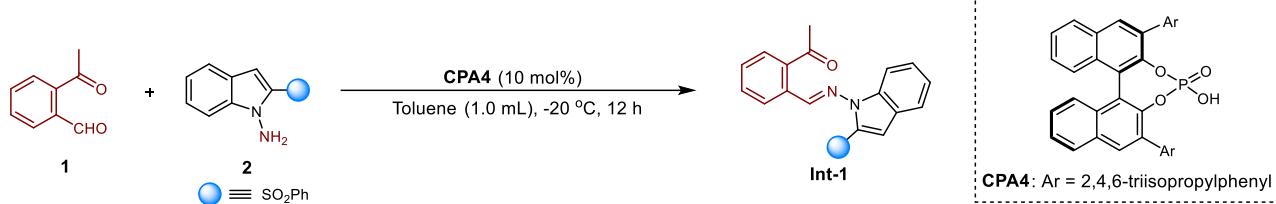
¹H NMR (500 MHz, CDCl₃) δ 7.84 (d, *J* = 8.1 Hz, 1H), 7.55 (d, *J* = 8.1 Hz, 1H), 7.50 – 7.44 (m, 1H), 7.42 – 7.35 (m, 1H), 4.94 (s, 2H). ¹³C NMR (126 MHz, CDCl₃) δ 140.77, 138.82, 136.01, 125.73, 123.96, 121.73, 118.76 (d, *J* = 271.5 Hz), 109.65. ¹⁹F NMR (471 MHz, CDCl₃) δ -62.91. HRMS (APCI) m/z: calculated for [C₈H₆F₃N₃+H]⁺ 202.0586, found 202.0579.

General procedure for synthesis of products 3

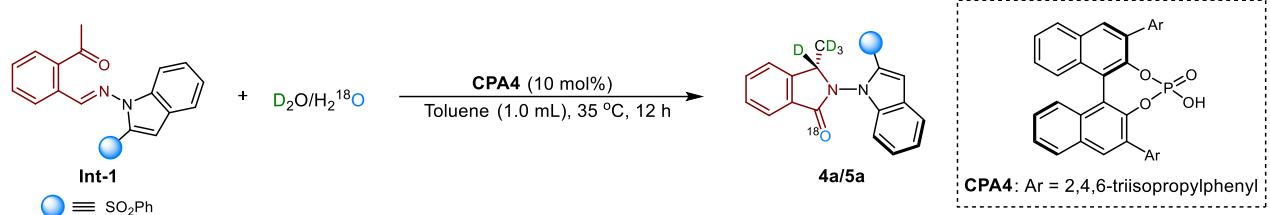


Procedure 4: To a 4 mL vial equipped with a stirring bar was added **1** (0.2 mmol, 1.0 eq.), **2** (0.1 mmol, 1.0 eq.) and toluene (1 mL). **CPA4** (0.01 mmol, 0.1 eq.) was then added to the vial and the reaction mixture was stirred at 35 °C for 24 h. After the completion of the reaction which was indicated 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



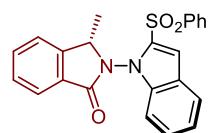
Procedure 5: To a test tube equipped with a stirring bar was added **1** (0.2 mmol, 1.0 eq.), **2** (0.1 mmol, 1.0 eq.) and **CPA4** (0.01 mmol, 0.1 eq.). Toluene (1 mL) was then added to the vial and the reaction mixture was stirred at -20 °C for 12 h. After the completion of the reaction which was 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 µL 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 °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.

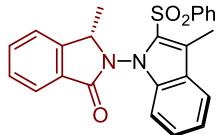
Products characterization for chiral isoindolinones

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



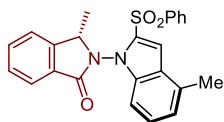
Following the **Procedure 4**, **3a** was obtained as faint yellow solid (36.6 mg, 91% yield). 1H NMR (500 MHz, $CDCl_3$) δ 7.96 (dd, J = 7.6, 1.6 Hz, 2H), 7.85 (d, J = 7.6 Hz, 1H), 7.74 – 7.66 (m, 2H), 7.54 (td, J = 7.4, 1.9 Hz, 2H), 7.50 (d, J = 7.5 Hz, 1H), 7.47 – 7.40 (m, 3H), 7.30 (ddd, J = 8.4, 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}C NMR (126 MHz, $CDCl_3$) δ 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), tr = 35.670 min (minor), 42.083 min (major); ee = 95%. HRMS (ESI) m/z: calculated for $[C_{23}H_{18}N_2O_3S+Na]^+$ 425.0930, found 425.0943.

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



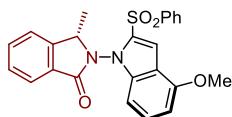
Following the general **Procedure 4**, **3b** was obtained as faint yellow solid (33.3 mg, 80% yield). ¹H NMR (500 MHz, CDCl₃) δ 8.17 (dd, *J* = 7.4, 1.9 Hz, 2H), 7.98 (d, *J* = 7.6 Hz, 1H), 7.68 (dd, *J* = 8.3, 6.6 Hz, 2H), 7.59 – 7.51 (m, 2H), 7.51 – 7.44 (m, 3H), 7.35 (ddd, *J* = 8.3, 7.0, 1.1 Hz, 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). ¹³C NMR (126 MHz, CDCl₃) δ 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), tr = 21.467 min (minor), 38.017 min (major); ee = 86%. HRMS (ESI) m/z: calculated for [C₂₄H₂₀N₂O₃S+H]⁺ 417.1267, found 417.1259.

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



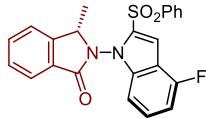
Following the **Procedure 4**, **3c** was obtained as faint yellow solid (27.4 mg, 66% yield). ¹H NMR (500 MHz, CDCl₃) δ 7.99 – 7.94 (m, 2H), 7.83 (d, *J* = 7.6 Hz, 1H), 7.68 (td, *J* = 7.6, 1.1 Hz, 1H), 7.57 – 7.47 (m, 4H), 7.43 (t, *J* = 7.7 Hz, 2H), 7.19 (dd, *J* = 8.4, 7.2 Hz, 1H), 7.01 (d, *J* = 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). ¹³C NMR (126 MHz, CDCl₃) δ 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), tr = 31.693 min (minor), 36.210 min (major); ee = 94%. HRMS (ESI) m/z: calculated for [C₂₄H₂₀N₂O₃S+H]⁺ 417.1267, found 417.1255.

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



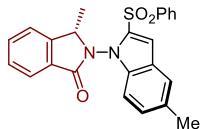
Following the **Procedure 4**, **3d** was obtained as faint yellow solid (32.4 mg, 75% yield). ¹H NMR (500 MHz, CDCl₃) δ 7.98 – 7.90 (m, 2H), 7.85 (d, *J* = 7.6 Hz, 1H), 7.67 (td, *J* = 7.6, 1.1 Hz, 1H), 7.56 (s, 1H), 7.52 (t, *J* = 7.9 Hz, 2H), 7.48 (d, *J* = 7.6 Hz, 1H), 7.42 (t, *J* = 7.7 Hz, 2H), 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). ¹³C NMR (126 MHz, CDCl₃) δ 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), tr = 46.300 min (minor), 53.200 min (major); ee = 94%. HRMS (ESI) m/z: calculated for [C₂₄H₂₀N₂O₄S+Na]⁺ 455.1036, found 455.1048.

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



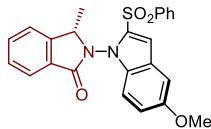
Following the **Procedure 4**, **3e** was obtained as faint yellow solid (26.0 mg, 62% yield). ¹H NMR (500 MHz, CDCl₃) δ 8.00 – 7.93 (m, 2H), 7.85 (d, *J* = 7.6 Hz, 1H), 7.73 (t, *J* = 7.5 Hz, 1H), 7.62 – 7.53 (m, 2H), 7.53 (d, *J* = 8.8 Hz, 2H), 7.47 (t, *J* = 7.7 Hz, 2H), 7.23 (dd, *J* = 8.1, 4.9 Hz, 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). ¹³C NMR (126 MHz, CDCl₃) δ 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. ¹⁹F NMR (470 MHz, CDCl₃) δ -119.16 (dd, *J* = 9.7, 5.0 Hz). HPLC (Chiraldak IC column, 80:20 hexanes/isopropanol, 1 mL/min), tr = 20.297 min (minor), 24.937 min (major); ee = 94%. HRMS (ESI) m/z: calculated for [C₂₃H₁₇FN₂O₃S+H]⁺ 421.1016, found 421.0999.

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



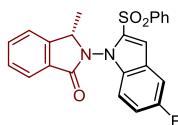
Following the **Procedure 4**, **3f** was obtained as faint yellow solid (31.2 mg, 75% yield). ¹H NMR (500 MHz, CDCl₃) δ 7.95 (dd, *J* = 7.5, 1.7 Hz, 2H), 7.84 (d, *J* = 7.6 Hz, 1H), 7.70 – 7.66 (m, 1H), 7.53 (t, *J* = 7.4 Hz, 2H), 7.51 – 7.47 (m, 2H), 7.42 (t, *J* = 7.7 Hz, 2H), 7.37 (s, 1H), 7.12 (dd, *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). ¹³C NMR (126 MHz, CDCl₃) δ 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 (Chiraldak IC column, 80:20 hexanes/isopropanol, 1 mL/min), tr = 39.520 min (minor), 51.073 min (major); ee = 95%. HRMS (ESI) m/z: calculated for [C₂₄H₂₀N₂O₃S+H]⁺ 417.1267, found 417.1255.

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



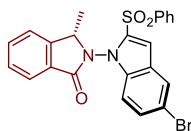
Following the **Procedure 4**, **3g** was obtained as faint yellow solid (39.3 mg, 91% yield). ¹H NMR (500 MHz, CDCl₃) δ 7.99 – 7.91 (m, 2H), 7.84 (d, *J* = 7.6 Hz, 1H), 7.67 (t, *J* = 7.5 Hz, 1H), 7.52 (td, *J* = 7.5, 3.7 Hz, 2H), 7.48 (d, *J* = 7.7 Hz, 1H), 7.42 (t, *J* = 7.8 Hz, 2H), 7.37 (s, 1H), 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). ¹³C NMR (126 MHz, CDCl₃) δ 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 (Chiraldak IC column, 70:30 hexanes/isopropanol, 1 mL/min), tr = 30.660 min (minor), 45.857 min (major); ee = 94%. HRMS (ESI) m/z: calculated for [C₂₄H₂₀N₂O₄S+H]⁺ 433.1216, found 433.1201.

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



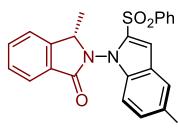
Following the **Procedure 4**, **3h** was obtained as faint yellow solid (27.7 mg, 66% yield). ^1H NMR (500 MHz, CDCl_3) δ 7.95 (d, $J = 7.8$ Hz, 2H), 7.83 (d, $J = 7.6$ Hz, 1H), 7.69 (t, $J = 7.5$ Hz, 1H), 7.55 (dt, $J = 10.1, 7.5$ Hz, 2H), 7.50 (d, $J = 7.6$ Hz, 1H), 7.44 (t, $J = 7.7$ Hz, 2H), 7.39 (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}C NMR (126 MHz, CDCl_3) δ 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), tr = 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)



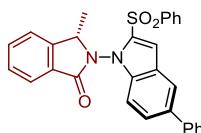
Following the **Procedure 4**, **3i** was obtained as faint yellow solid (38.9.7 mg, 81% yield). ^1H NMR (500 MHz, CDCl_3) δ 7.96 – 7.91 (m, 2H), 7.84 (d, $J = 1.8$ Hz, 1H), 7.82 (d, $J = 7.6$ Hz, 1H), 7.72 – 7.67 (m, 1H), 7.54 (dt, $J = 9.7, 7.5$ Hz, 2H), 7.50 (d, $J = 7.5$ Hz, 1H), 7.43 (t, $J = 7.8$ 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}C NMR (126 MHz, CDCl_3) δ 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), tr = 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)



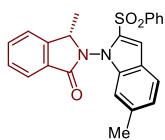
Following the **Procedure 4**, **3j** was obtained as faint yellow solid (32.2 mg, 61% yield). ^1H NMR (500 MHz, CDCl_3) δ 8.06 (s, 1H), 7.93 (d, $J = 7.8$ Hz, 2H), 7.82 (d, $J = 7.7$ Hz, 1H), 7.71 (t, $J = 7.6$ Hz, 1H), 7.55 (q, $J = 7.8$ Hz, 2H), 7.54 – 7.48 (m, 2H), 7.44 (t, $J = 7.7$ Hz, 2H), 7.36 (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}C NMR (126 MHz, CDCl_3) δ 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), tr = 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)



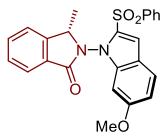
Following the **Procedure 4**, **3k** was obtained as faint yellow solid (33.5 mg, 70% yield). ^1H NMR (500 MHz, CDCl_3) δ 8.02 (d, $J = 7.8$ Hz, 2H), 7.96 – 7.92 (m, 1H), 7.90 (d, $J = 7.6$ Hz, 1H), 7.73 (t, $J = 7.5$ Hz, 1H), 7.58 (t, $J = 5.5$ Hz, 4H), 7.55 (t, $J = 6.0$ Hz, 3H), 7.47 (q, $J = 7.8$ 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}C NMR (126 MHz, CDCl_3) δ 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 (Chiraldak OD column, 80:20 hexanes/isopropanol, 1 mL/min), tr = 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**)



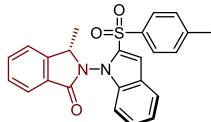
Following the **Procedure 4**, **3l** was obtained as faint yellow solid (25.8 mg, 62% yield). ^1H NMR (500 MHz, CDCl_3) δ 7.98 – 7.93 (m, 2H), 7.87 (d, $J = 7.6$ Hz, 1H), 7.71 (td, $J = 7.5, 1.2$ Hz, 1H), 7.60 (d, $J = 8.3$ Hz, 1H), 7.58 – 7.55 (m, 1H), 7.52 (dd, $J = 8.3, 7.1$ Hz, 2H), 7.46 – 7.42 (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}C NMR (126 MHz, CDCl_3) δ 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 (Chiraldak IC column, 80:20 hexanes/isopropanol, 1 mL/min), tr = 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**)



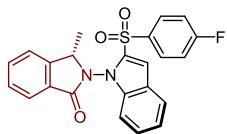
Following the **Procedure 4**, **3m** was obtained as faint yellow solid (27.2 mg, 63% yield). ^1H NMR (500 MHz, CDCl_3) δ 7.59 (t, $J = 8.3$ Hz, 2H), 7.53 (dd, $J = 10.3, 7.5$ Hz, 2H), 7.46 (t, $J = 7.9$ Hz, 2H), 7.99 – 7.94 (m, 2H), 7.91 (d, $J = 7.6$ Hz, 1H), 7.72 (td, $J = 7.6, 1.2$ Hz, 1H), 7.40 (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}C NMR (126 MHz, CDCl_3) δ 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 (Chiraldak IC column, 80:20 hexanes/isopropanol, 1 mL/min), tr = 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**)



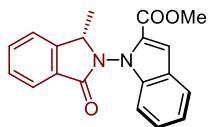
Following the **Procedure 4**, **3n** was obtained as faint yellow solid (30.4 mg, 73% yield). ^1H NMR (500 MHz, CDCl_3) δ 7.87 (d, $J = 7.6$ Hz, 1H), 7.84 (d, $J = 8.0$ Hz, 2H), 7.73 – 7.66 (m, 2H), 7.54 (t, $J = 7.5$ Hz, 1H), 7.49 (d, $J = 7.6$ Hz, 1H), 7.41 (s, 1H), 7.28 (t, $J = 7.7$ Hz, 1H), 7.24 (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}C NMR (126 MHz, CDCl_3) δ 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), tr = 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)-1*H*-indol-1-yl)-3-methylisoindolin-1-one (**3o**)



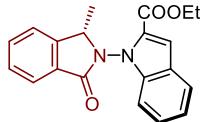
Following the **Procedure 4**, **3o** was obtained as faint yellow solid (29.4 mg, 70% yield). ^1H NMR (500 MHz, CDCl_3) δ 7.97 (dd, $J = 8.7, 5.0$ Hz, 2H), 7.86 (d, $J = 7.6$ Hz, 1H), 7.75 – 7.66 (m, 2H), 7.55 (t, $J = 7.6$ Hz, 1H), 7.51 (d, $J = 7.6$ Hz, 1H), 7.46 (s, 1H), 7.30 (t, $J = 7.7$ Hz, 1H), 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}C NMR (126 MHz, CDCl_3) δ 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}F NMR (471 MHz, CDCl_3) δ -103.70. HPLC (Chiralpak IC column, 90:10 hexanes/isopropanol, 1 mL/min), tr = 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-oxoisodolin-2-yl)-1*H*-indole-2-carboxylate (**3p**)



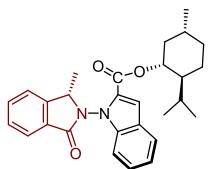
Following the **Procedure 4**, **3p** was obtained as white solid (26.2 mg, 82% yield). ^1H NMR (500 MHz, CDCl_3) δ 7.95 (d, $J = 7.6$ Hz, 1H), 7.71 (dd, $J = 8.3, 0.9$ Hz, 1H), 7.68 (td, $J = 7.5, 1.1$ Hz, 1H), 7.54 (t, $J = 7.6$ Hz, 1H), 7.50 (d, $J = 7.5$ Hz, 1H), 7.45 (s, 1H), 7.36 (dd, $J = 5.9, 1.2$ 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}C NMR (126 MHz, CDCl_3) δ 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), tr = 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-oxoisodolin-2-yl)-1*H*-indole-2-carboxylate (**3q**)



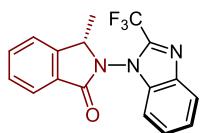
Following the **Procedure 4**, **3q** was obtained as white solid (22.0 mg, 66% yield). ^1H NMR (500 MHz, CDCl_3) δ 7.94 (d, $J = 7.6$ Hz, 1H), 7.70 (d, $J = 8.1$ Hz, 1H), 7.66 (t, $J = 7.6$ Hz, 1H), 7.52 (t, $J = 7.6$ Hz, 1H), 7.49 (d, $J = 9.6$ Hz, 2H), 7.36 – 7.32 (m, 2H), 7.21 (ddd, $J = 8.1, 5.1, 2.9$ 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}C NMR (126 MHz, CDCl_3) δ 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), $\text{tr} = 24.733$ 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

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



Following the **Procedure 4**, **3r** was obtained as white solid (29.3 mg, 66% yield). ^1H NMR (500 MHz, CDCl_3) δ 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}C NMR (126 MHz, CDCl_3) δ 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), $\text{tr} = 10.377$ 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.

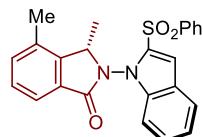
(S)-3-methyl-2-(2-(trifluoromethyl)-1*H*-benzo[d]imidazol-1-yl)isoindolin-1-one (3s)



Following the **Procedure 4**, **3s** was obtained as viscous oil (13.9 mg, 42% yield). ^1H NMR (500 MHz, CDCl_3) δ 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}C NMR (126 MHz, CDCl_3) δ 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,

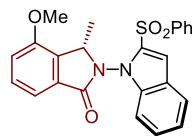
1 mL/min), tr = 9.007 min (major), 18.940 min (minor); ee = 82%. HRMS (ESI) m/z: calculated for [C₁₇H₁₂F₃N₃O +Na]⁺ 354.0824, found 354.0844.

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



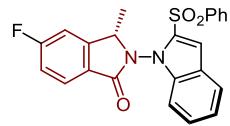
Following the **Procedure 4**, **3t** was obtained as faint yellow solid (30.8 mg, 74% yield). ¹H NMR (500 MHz, CDCl₃) δ 7.95 (d, *J* = 7.8 Hz, 2H), 7.70 (d, *J* = 8.0 Hz, 1H), 7.65 (s, 1H), 7.53 (t, *J* = 7.5 Hz, 1H), 7.49 (d, *J* = 7.8 Hz, 1H), 7.46 – 7.40 (m, 3H), 7.38 (d, *J* = 7.8 Hz, 1H), 7.27 (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). ¹³C NMR (126 MHz, CDCl₃) δ 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), tr = 41.520 min (minor), 52.810 min (major); ee = 94%. HRMS (ESI) m/z: calculated for [C₂₄H₂₀N₂O₃S+H]⁺ 433.1216, found 433.1257.

(S)-4-methoxy-3-methyl-2-(phenylsulfonyl)-1*H*-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, CDCl₃) δ 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). ¹³C NMR (126 MHz, CDCl₃) δ 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), tr = 42.467 min (minor), 61.543 min (major); ee = 88%. HRMS (ESI) m/z: calculated for [C₂₄H₂₀N₂O₄S+Na]⁺ 455.1036, found 455.1050.

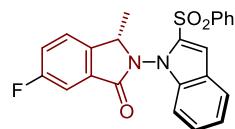
(S)-5-fluoro-3-methyl-2-(phenylsulfonyl)-1*H*-indol-1-yl)isoindolin-1-one (3v)



Following the **Procedure 4**, **3v** was obtained as faint yellow solid (25.2 mg, 60% yield). ¹H NMR (500 MHz, CDCl₃) δ 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). ¹³C NMR (126 MHz, CDCl₃) δ 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. ¹⁹F NMR (470 MHz, CDCl₃) δ -

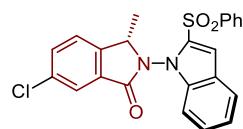
103.71 (td, $J = 8.6, 5.1$ Hz). HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min), tr = 39.323 min (major), 48.370 min (minor); ee = 93%. HRMS (ESI) m/z: calculated for [C₂₃H₁₇FN₂O₃S+H]⁺ 421.1016, found 421.0999.

(S)-6-fluoro-3-methyl-2-(phenylsulfonyl)-1*H*-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, CDCl₃) δ 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). ¹³C NMR (126 MHz, CDCl₃) δ 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. ¹⁹F NMR (470 MHz, CDCl₃) δ -111.46. HPLC (Chiralpak IA column, 80:20 hexanes/isopropanol, 1 mL/min), tr = 29.967 min (major), 37.487 min (minor); ee = 95%. HRMS (ESI) m/z: calculated for [C₂₃H₁₇FN₂O₃S+H]⁺ 421.1016, found 421.0995.

(S)-6-chloro-3-methyl-2-(phenylsulfonyl)-1*H*-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, CDCl₃) δ 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). ¹³C NMR (126 MHz, CDCl₃) δ 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), tr = 30.870 min (minor), 42.590 min (major); ee = 96%. HRMS (ESI) m/z: calculated for [C₂₃H₁₇ClN₂O₃S+H]⁺ 437.0721, found 437.0699.

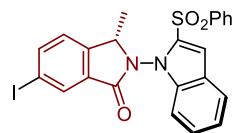
(S)-6-bromo-3-methyl-2-(phenylsulfonyl)-1*H*-indol-1-yl)isoindolin-1-one (3y)



Following the **Procedure 4**, **3y** was obtained as faint yellow solid (19.7 mg, 41% yield). ¹H NMR (500 MHz, CDCl₃) δ 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). ¹³C NMR (126 MHz, CDCl₃) δ 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,

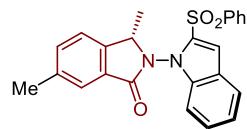
57.95, 17.18. HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min), tr = 29.000 min (minor), 40.167 min (major); ee = 98%. HRMS (ESI) m/z: calculated for $[C_{23}H_{17}BrN_2O_3S+H]^+$ 481.0216, found 481.0193.

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



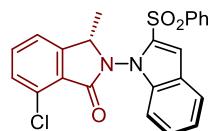
Following the **Procedure 4**, **3z** was obtained as faint yellow solid (17.4 mg, 33% yield). 1H NMR (500 MHz, $CDCl_3$) δ 8.21 (d, J = 1.6 Hz, 1H), 8.01 (dd, J = 8.0, 1.7 Hz, 1H), 7.97 – 7.94 (m, 2H), 7.73 (d, J = 8.0 Hz, 1H), 7.57 (tt, J = 7.0, 1.3 Hz, 1H), 7.48 – 7.43 (m, 3H), 7.32 (ddd, J = 8.3, 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, $CDCl_3$) δ 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), tr = 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-(phenylsulfonyl)-1*H*-indol-1-one (3a')



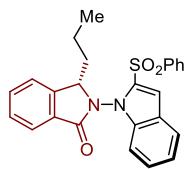
Following the **Procedure 4**, **3a'** was obtained as faint yellow solid (25.4 mg, 61% yield). 1H NMR (500 MHz, $CDCl_3$) δ 8.02 (dd, J = 8.3, 1.3 Hz, 2H), 7.73 (dd, J = 5.9, 2.9 Hz, 1H), 7.71 (d, J = 8.1 Hz, 1H), 7.57 – 7.51 (m, 1H), 7.48 – 7.42 (m, 5H), 7.31 (ddd, J = 8.3, 7.1, 1.1 Hz, 1H), 7.21 (d, 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, $CDCl_3$) δ 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), tr = 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-(phenylsulfonyl)-1*H*-indol-1-one (3b')



Following the **Procedure 4**, **3b'** was obtained as faint yellow solid (16.1 mg, 37% yield). 1H NMR (500 MHz, $CDCl_3$) δ 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, $CDCl_3$) δ 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), tr = 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)-1*H*-indol-1-yl)-3-propylisoindolin-1-one (3c')



Following the **Procedure 4**, **3c'** was obtained as orange viscous oil (29.2 mg, 68% yield). ^1H NMR (500 MHz, CDCl_3) δ 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}C NMR (126 MHz, CDCl_3) δ 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), tr = 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)-1*H*-indol-1-yl)isoindolin-1-one (3d')



Following the **Procedure 4**, **3d'** was obtained as orange viscous oil (34.5 mg, 71% yield). ^1H NMR (500 MHz, CDCl_3) δ 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}C NMR (126 MHz, CDCl_3) δ 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), tr = 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.

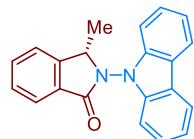
(E)-1-(((2-(phenylsulfonyl)-1*H*-indol-1-yl)imino)methyl)phenyl)ethan-1-one (Int-1a)



Following the **Procedure 5**, **Int-1a** was obtained as gray solid (31.0 mg, 77% yield). ^1H NMR (500 MHz, CDCl_3) δ 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}C NMR (126 MHz, CDCl_3) δ 200.61, 155.33, 141.14, 137.06, 135.05, 133.81, 133.29, 133.23,

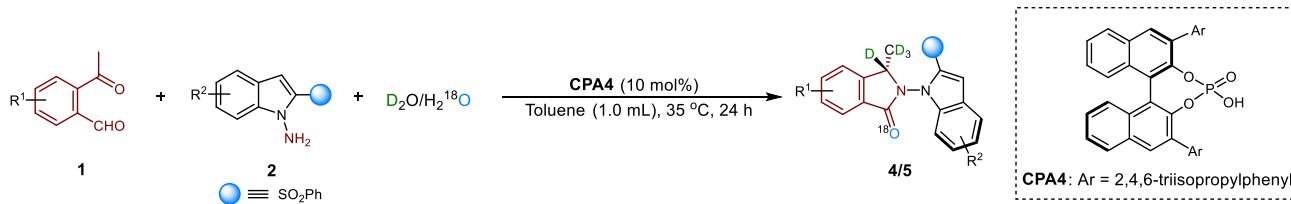
132.68, 130.71, 130.07, 128.83, 128.66, 128.33, 127.17, 124.89, 123.31, 122.41, 111.97, 110.68, 28.62. HRMS (ESI) m/z: calculated for [C₂₃H₁₈N₂O₃S+Na]⁺ 425.0930, found 425.0942.

(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, CDCl₃) δ 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 (dd, 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). ¹³C NMR (126 MHz, CDCl₃) δ 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), tr = 25.680 min (major), 33.510 min (minor); ee = 7%. HRMS (ESI) m/z: calculated for [C₂₁H₁₆N₂O+Na]⁺ 335.1154, found 335.1182.

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



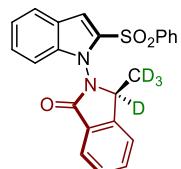
Procedure 7: The reaction was proceeded in the glovebox under argon atmosphere. To a 4 mL dry bottle equipped with a stirring bar was added **1** (0.2 mmol, 1.0 eq.), **2** (0.1 mmol, 1.0 eq.), **CPA4** (0.01mmol, 0.1 eq.) and dry toluene (1 mL). The 50 µL of deuterium oxide (D₂O) or heavy-oxygen water (H₂¹⁸O) was then added to the flask 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.

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

$$\text{isotopic ratio} = \frac{\text{intensity}_{\text{labeled}}}{\text{intensity}_{\text{total}}} = \frac{\text{intensity}_{\text{labeled}}}{\text{intensity}_{\text{labeled}} + \text{intensity}_{\text{unlabeled}}}$$

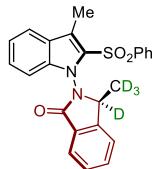
Isotopic ratio analysis

(S)-3-(methyl-d₃)-2-(phenylsulfonyl)-1*H*-indol-1-yl)isoindolin-1-one-3-*d* (**4a**)



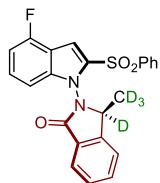
Following the **Procedure 7**, **4a** was obtained as faint yellow solid (26.8 mg, 66% yield). ^1H NMR (500 MHz, CDCl_3) δ 7.98 (dd, $J = 7.4, 1.8$ Hz, 2H), 7.87 (d, $J = 7.6$ Hz, 1H), 7.74 (d, $J = 7.9$ Hz, 1H), 7.70 (td, $J = 7.6, 1.1$ Hz, 1H), 7.55 (h, $J = 4.1$ Hz, 2H), 7.51 (d, $J = 7.6$ Hz, 1H), 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), tr = 35.663 min (minor), 41.980 min (major); ee = 95%.

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



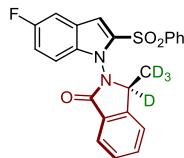
Following the **Procedure 7**, **4b** was obtained as faint yellow solid (33.2 mg, 79% yield). ^1H NMR (500 MHz, CDCl_3) δ 8.19 (d, $J = 7.5$ Hz, 2H), 7.99 (d, $J = 7.6$ Hz, 1H), 7.68 (t, $J = 7.4$ Hz, 2H), 7.58 – 7.51 (m, 2H), 7.52 – 7.46 (m, 4H), 7.35 (t, $J = 7.7$ Hz, 1H), 7.24 (q, $J = 7.5, 7.0$ 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), tr = 21.193 min (minor), 36.850 min (major); ee = 93%.

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



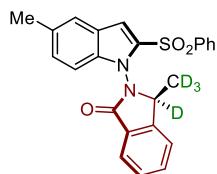
Following the **Procedure 7**, **4c** was obtained as faint yellow solid (38.2 mg, 90% yield). ^1H NMR (500 MHz, CDCl_3) δ 7.97 (d, $J = 8.1$ Hz, 2H), 7.86 (d, $J = 7.8$ Hz, 1H), 7.73 (t, $J = 7.7$ Hz, 1H), 7.61 – 7.56 (m, 2H), 7.53 (d, $J = 5.5$ Hz, 2H), 7.47 (t, $J = 7.8$ Hz, 2H), 7.24 (q, $J = 9.2, 7.8$ 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), tr = 20.023 min (minor), 24.663 min (major); ee = 94%.

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



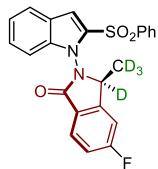
Following the **Procedure 7**, **4d** was obtained as faint yellow solid (34.3 mg, 81% yield). ^1H NMR (500 MHz, CDCl_3) δ 7.98 – 7.93 (m, 2H), 7.85 (d, $J = 7.6$ Hz, 1H), 7.73 – 7.68 (m, 1H), 7.57 (td, $J = 7.5, 1.8$ Hz, 2H), 7.52 (t, $J = 7.2$ Hz, 1H), 7.48 – 7.43 (m, 2H), 7.40 (s, 1H), 7.38 (dd, $J = 8.6, 2.5$ 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), tr = 40.533 min (major), 51.327 min (minor); ee = 91%.

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



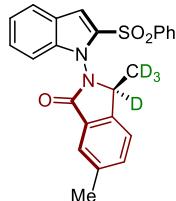
Following the **Procedure 7**, **4e** was obtained as faint yellow solid (33.6 mg, 80% yield). ^1H NMR (500 MHz, CDCl_3) δ 8.00 – 7.95 (m, 2H), 7.86 (d, J = 7.5 Hz, 1H), 7.69 (td, J = 7.5, 1.2 Hz, 1H), 7.57 – 7.52 (m, 2H), 7.52 – 7.49 (m, 2H), 7.48 – 7.41 (m, 2H), 7.39 (s, 1H), 7.13 (dd, J = 8.5, 1.7 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 (Chiraldak IC column, 80:20 hexanes/isopropanol, 1 mL/min), tr = 40.090 min (minor), 52.667 min (major); ee = 94%.

(S)-5-fluoro-3-(methyl-d3)-2-(2-(phenylsulfonyl)-1H-indol-1-yl)isoindolin-1-one-3-d (4f)



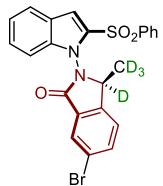
Following the **Procedure 7**, **4f** was obtained as faint yellow solid (26.3 mg, 62% yield). ^1H NMR (500 MHz, CDCl_3) δ 7.99 – 7.94 (m, 2H), 7.86 (dd, J = 8.4, 4.9 Hz, 1H), 7.74 (d, J = 7.9 Hz, 1H), 7.56 (t, J = 7.4 Hz, 1H), 7.48 – 7.44 (m, 3H), 7.32 (t, J = 7.5 Hz, 1H), 7.25 (td, J = 7.5, 5.0, 2.4 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 (Chiraldak IC column, 80:20 hexanes/isopropanol, 1 mL/min), tr = 38.647 min (major), 48.400 min (minor); ee = 99%.

(S)-6-methyl-3-(methyl-d3)-2-(2-(phenylsulfonyl)-1H-indol-1-yl)isoindolin-1-one-3-d (4g)



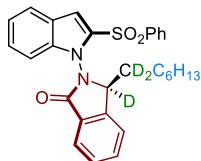
Following the **Procedure 7**, **4g** was obtained as faint yellow solid (24.4 mg, 58% yield). ^1H NMR (500 MHz, CDCl_3) δ 7.99 – 7.95 (m, 2H), 7.73 (d, J = 7.9 Hz, 1H), 7.67 (s, 1H), 7.58 – 7.54 (m, 1H), 7.52 (dd, J = 7.8, 1.7 Hz, 1H), 7.48 – 7.43 (m, 3H), 7.40 (d, J = 7.8 Hz, 1H), 7.30 (td, J = 7.6, 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 (Chiraldak IC column, 80:20 hexanes/isopropanol, 1 mL/min), tr = 40.490 min (minor), 50.473 min (major); ee = 94%.

(S)-6-bromo-3-(methyl-d3)-2-(2-(phenylsulfonyl)-1H-indol-1-yl)isoindolin-1-one-3-d (4h)



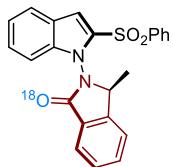
Following the **Procedure 7**, **4h** was obtained as faint yellow solid (32.9 mg, 68% yield). ^1H NMR (500 MHz, CDCl_3) δ 7.99 (s, 1H), 7.95 (d, J = 8.2 Hz, 2H), 7.75 (dd, J = 35.1, 8.7 Hz, 2H), 7.54 (d, J = 7.6 Hz, 1H), 7.44 (s, 3H), 7.37 (d, J = 8.9 Hz, 1H), 7.29 (d, J = 8.4 Hz, 1H), 7.25 – 7.18 (m, 1H), 6.93 (d, J = 8.9 Hz, 1H), 5.06 (s, 0.3H), 1.56 (s, 0.28H). HPLC (Chiraldak IC column, 80:20 hexanes/isopropanol, 1 mL/min), tr = 30.247 min (minor), 39.377 min (major); ee = 98%.

(S)-3-(heptyl-1,1-d₂)-2-(2-(phenylsulfonyl)-1*H*-indol-1-yl)isoindolin-1-one-3-*d* (4i**)**



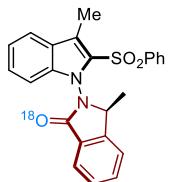
Following the **Procedure 7**, **4i** was obtained as orange viscous oil (20.0 mg, 41% yield). ¹H NMR (500 MHz, CDCl₃) δ 8.00 (d, *J* = 7.8 Hz, 2H), 7.88 (d, *J* = 7.6 Hz, 1H), 7.74 (d, *J* = 8.1 Hz, 1H), 7.70 (t, *J* = 7.6 Hz, 1H), 7.57 (dd, *J* = 10.9, 7.4 Hz, 3H), 7.47 (d, *J* = 8.8 Hz, 3H), 7.31 (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-¹⁸O (5a**)**



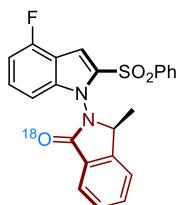
Following the **Procedure 7**, **5a** was obtained as faint yellow solid (35.6 mg, 88% yield). HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min), tr = 35.810 min (minor), 42.290 min (major); ee = 91%. HRMS (APCI) m/z: calculated for [C₂₃H₁₈N₂O₂¹⁶OS+H]⁺ 403.1111, found 403.1053, [C₂₃H₁₈N₂O₂¹⁸OS+H]⁺ 405.1153, found 405.1148. The ratio of relative peak intensities for the relevant isotopologues was 79:21 (C₂₃H₁₈N₂O₂¹⁸OS:C₂₃H₁₈N₂O₂¹⁶OS).

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



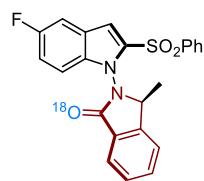
Following the **Procedure 7**, **5b** was obtained as faint yellow solid (34.7 mg, 83% yield). HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min), tr = 21.303 min (minor), 37.293 min (major); ee = 91%. HRMS (APCI) m/z: calculated for [C₂₄H₂₀N₂O₂¹⁶OS+H]⁺ 417.1267, found 417.1242, [C₂₄H₂₀N₂O₂¹⁸OS+H]⁺ 419.1309, found 419.1294. The ratio of relative peak intensities for the relevant isotopologues was 70:30 (C₂₄H₂₀N₂O₂¹⁸OS:C₂₄H₂₀N₂O₂¹⁶OS).

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



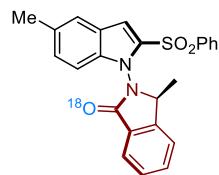
Following the **Procedure 7**, **5c** was obtained as faint yellow solid (30.0 mg, 71% yield). HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min), tr = 19.983 min (minor), 24.637 min (major); ee = 95%. HRMS (APCI) m/z: calculated for [C₂₃H₁₇FN₂O₂¹⁶OS+H]⁺ 421.1017, found 421.0993, [C₂₃H₁₇FN₂O₂¹⁸OS+H]⁺ 423.1059, found 423.1059. The ratio of relative peak intensities for the relevant isotopologues was 82:18 (C₂₃H₁₇FN₂O₂¹⁸OS: C₂₃H₁₇FN₂O₂¹⁶OS).

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



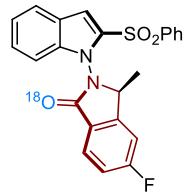
Following the **Procedure 7**, **5d** was obtained as faint yellow solid (27.0 mg, 64% yield). HPLC (Chiralpak AD column, 80:20 hexanes/isopropanol, 1 mL/min), t_r = 39.640 min (major), 50.423 min (minor); ee = 93%. HRMS (APCI) m/z: calculated for $[C_{23}H_{17}FN_2O_2^{16}OS+H]^+$ 421.1017, found 421.1001, $[C_{23}H_{17}FN_2O_2^{18}OS+H]^+$ 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)-1*H*-indol-1-yl)isoindolin-1-one-¹⁸O (5e)



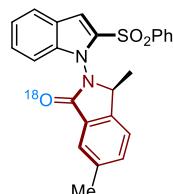
Following the **Procedure 7**, **5e** was obtained as faint yellow solid (28.8 mg, 69% yield). HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min), t_r = 40.420 min (minor), 50.493 min (major); ee = 94%. HRMS (APCI) m/z: calculated for $[C_{24}H_{20}N_2O_2^{16}OS+H]^+$ 417.1267, found 417.1194,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



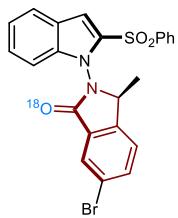
Following the **Procedure 7**, **5f** was obtained as faint yellow solid (32.5 mg, 77% yield). HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min), t_r = 40.037 min (major), 49.117 min (minor); ee = 98%. HRMS (APCI) m/z: calculated for $[C_{23}H_{17}FN_2O_2^{16}OS+H]^+$ 421.1017, found 421.0989, $[C_{23}H_{17}FN_2O_2^{18}OS+H]^+$ 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)-1*H*-indol-1-yl)isoindolin-1-one-¹⁸O (5g)



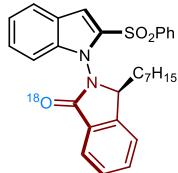
Following the **Procedure 7**, **5g** was obtained as faint yellow solid (32.2 mg, 77% yield). HPLC (Chiralpak IC column, 80:20 hexanes/isopropanol, 1 mL/min), t_r = 40.420 min (minor), 50.493 min (major); ee = 94%. HRMS (APCI) m/z: calculated for $[C_{24}H_{20}N_2O_2^{16}OS+H]^+$ 417.1267, found 417.1194, $[C_{24}H_{20}N_2O_2^{18}OS+H]^+$ 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)-1*H*-indol-1-yl)isoindolin-1-one-¹⁸O (5h)



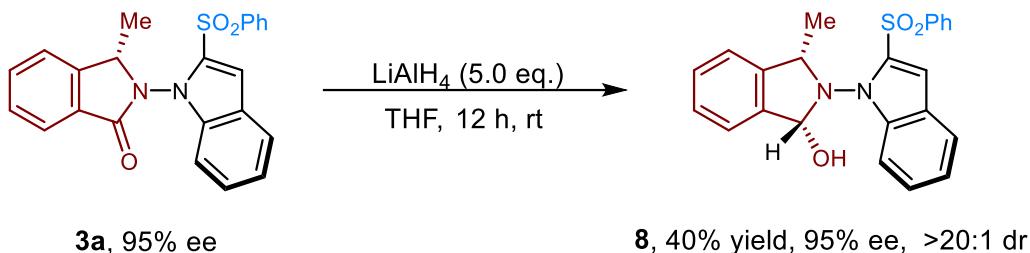
Following the **Procedure 7**, **5h** was obtained as faint yellow solid (31.3 mg, 65% yield). HPLC (Chiraldpak IC column, 80:20 hexanes/isopropanol, 1 mL/min), $\text{tr} = 28.633$ min (minor), 39.330 min (major); ee = 99%. HRMS (APCI) m/z: calculated for $[\text{C}_{23}\text{H}_{17}\text{BrN}_2\text{O}_2{}^{16}\text{OS}+\text{H}]^+$ 481.0216, found 481.0156, $[\text{C}_{23}\text{H}_{17}\text{BrN}_2\text{O}_2{}^{18}\text{OS}+\text{H}]^+$ 483.0258, found 483.0242. The ratio of relative peak intensities for the relevant isotopologues was 91:9 ($\text{C}_{23}\text{H}_{17}\text{BrN}_2\text{O}_2{}^{18}\text{OS}$: $\text{C}_{23}\text{H}_{17}\text{BrN}_2\text{O}_2{}^{16}\text{OS}$).

(S)-3-heptyl-2-(2-(phenylsulfonyl)-1H-indol-1-yl)isoindolin-1-one- ^{18}O (5i)



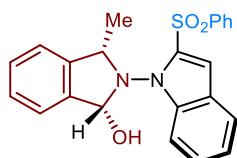
Following the **Procedure 7**, **5i** was obtained as orange viscous oil (30.7 mg, 63% yield). HPLC (Chiraldpak IC column, 80:20 hexanes/isopropanol, 1 mL/min), $\text{tr} = 20.920$ min (minor), 32.467 min (major); ee = 94%. HRMS (APCI) m/z: calculated for $[\text{C}_{29}\text{H}_{30}\text{N}_2\text{O}_2{}^{16}\text{OS}+\text{H}]^+$ 487.2049, found 487.1987, $[\text{C}_{29}\text{H}_{30}\text{N}_2\text{O}_2{}^{18}\text{OS}+\text{H}]^+$ 489.2092, found 489.2080. The ratio of relative peak intensities for the relevant isotopologues was 83:17 ($\text{C}_{29}\text{H}_{30}\text{N}_2\text{O}_2{}^{18}\text{OS}$: $\text{C}_{29}\text{H}_{30}\text{N}_2\text{O}_2{}^{16}\text{OS}$).

Synthetic applications of 3a

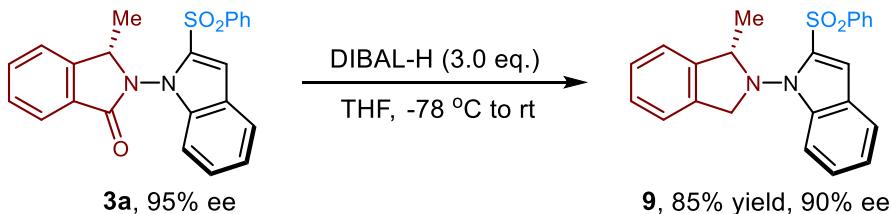


The reaction was proceeded in the glovebox under argon atmosphere. To a solution of **3a** (80.4 mg, 0.2 mmol, 1.0 eq.) in THF (1 mL) was added LiAlH₄ (38.0 mg, 1.0 mmol, 5.0 eq.) slowly. Then the mixture was stirred at room temperature for 12 h. The mixture was quenched with triethylamine and water. Then the mixture was extracted with EA (5 mL x 3). The combined organic layers were dried over anhydrous Na₂SO₄, 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.

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

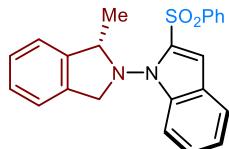


Following the above procedure, compound **8** was obtained as red solid (32.3 mg, 40% yield). ^1H NMR (500 MHz, CDCl_3) δ 8.08 – 8.03 (m, 2H), 7.74 (dd, J = 7.1, 1.8 Hz, 1H), 7.64 – 7.59 (m, 1H), 7.54 – 7.48 (m, 3H), 7.44 – 7.40 (m, 2H), 7.26 (s, 1H), 7.20 (qd, J = 7.4, 1.4 Hz, 2H), 7.13 (dd, J = 5.0, 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). ^{13}C NMR (126 MHz, CDCl_3) 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), $\text{tr} = 23.357$ min (minor), 39.050 min (major); ee = 95%. HRMS (APCI) m/z: calculated for $[\text{C}_{23}\text{H}_{20}\text{N}_2\text{O}_3\text{S}+\text{Na}]^+$ 427.1086, found 427.1092.

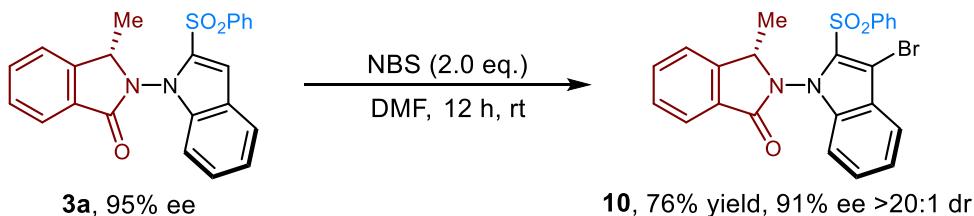


The reaction was proceeded under argon atmosphere. A solution of **3a** (80.4 mg, 0.2 mmol, 1.0 eq.) in THF (1 mL) was cooled at -78 °C. Then $[(\text{CH}_3)_2\text{CHCH}_2]_2\text{AlH}$ (1 M in THF, 0.6 mL, 0.6 mmol, 3.0 eq.) was added to the mixture, and the mixture stirred at -78 °C for 12 h. After 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_2SO_4 , 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)



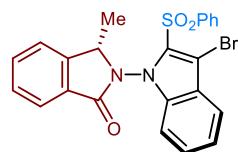
Following the above procedure, compound **9** was obtained as red solid (66.0 mg, 85% yield). ^1H NMR (500 MHz, CDCl_3) δ 7.97 (dd, $J = 8.3, 1.4$ Hz, 2H), 7.79 – 7.74 (m, 1H), 7.59 – 7.52 (m, 1H), 7.42 (t, $J = 7.8$ Hz, 2H), 7.35 (s, 1H), 7.32 (d, $J = 7.4$ Hz, 1H), 7.28 (t, $J = 7.3$ Hz, 1H), 7.18 (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). ^{13}C NMR (126 MHz, CDCl_3) 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 $[\text{C}_{23}\text{H}_{20}\text{N}_2\text{O}_2\text{S}+\text{Na}]^+$ 411.1137, found 411.1130.



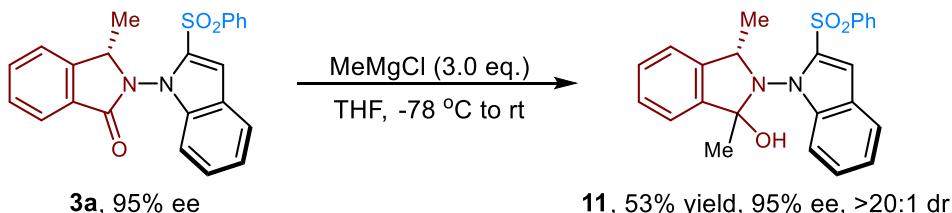
To a solution of **3a** (80.4 mg, 0.2 mmol, 1.0 eq.) in DMF (1 mL) was added *N*-bromosuccinimide (71.2 mg, 0.4 mmol, 2.0 eq.) slowly. Then the mixture was stirred at room temperature for 12 h. The mixture was quenched with water.

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) and the product **10** (73.0 mg, 76% yield) was given.

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

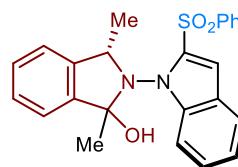


Following the above procedure, compound **10** was obtained as white solid (73.0 mg, 76% yield). ^1H NMR (500 MHz, CDCl_3) δ 8.30 (dd, $J = 7.8, 1.7$ Hz, 2H), 8.03 (d, $J = 7.6$ Hz, 1H), 7.74 – 7.70 (m, 1H), 7.68 (d, $J = 8.1$ Hz, 1H), 7.59 (t, $J = 7.5$ Hz, 2H), 7.55 – 7.50 (m, 3H), 7.44 – 7.40 (m, 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). ^{13}C NMR (126 MHz, CDCl_3) 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), tr = 15.870 min (major), 23.587 min (minor); ee = 91%. HRMS (APCI) m/z: calculated for $[\text{C}_{23}\text{H}_{17}\text{BrN}_2\text{O}_3\text{S}+\text{Na}]^+$ 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 Na₂SO₄, 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.

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



Following the above procedure, compound **11** was obtained as red solid (44.3 mg, 53% yield). ^1H NMR (500 MHz, CDCl_3) 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}C NMR (126 MHz, CDCl_3) δ 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 IA column, 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

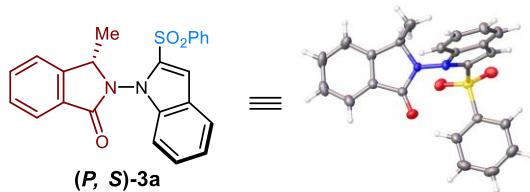


Table S1. Crystal data and structure refinement for CCDC 2359270

Identification code	CCDC 2359270
Empirical formula	C ₂₃ H ₁₈ N ₂ O ₃ 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 ³	981.56(17)
Z	2
ρcalcg/cm ³	1.362
μ/mm ⁻¹	1.693
F(000)	420.0
Crystal size/mm ³	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 [Rint = 0.0289, Rsigma = 0.0343]
Data/restraints/parameters	3435/1/264
Goodness-of-fit on F ²	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 ⁻³	0.28/-0.19
Flack parameter	0.090(4)

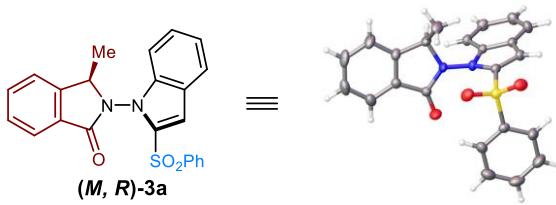


Table S2. Crystal data and structure refinement for CCDC 2362138

Identification code	CCDC 2362138
Empirical formula	C ₂₃ H ₁₈ N ₂ O ₃ 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 ³	982.28(8)
Z	2
ρcalcg/cm ³	1.361
μ/mm ⁻¹	1.691
F(000)	420.0
Crystal size/mm ³	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 [Rint = 0.0257, Rsigma = 0.0326]
Data/restraints/parameters	3365/1/263
Goodness-of-fit on F ²	1.098
Final R indexes [I>=2σ (I)]	R1 = 0.0266, wR2 = 0.0666
Final R indexes [all data]	R1 = 0.0267, wR2 = 0.0667
Largest diff. peak/hole / e Å ⁻³	0.20/-0.40
Flack parameter	0.074(5)

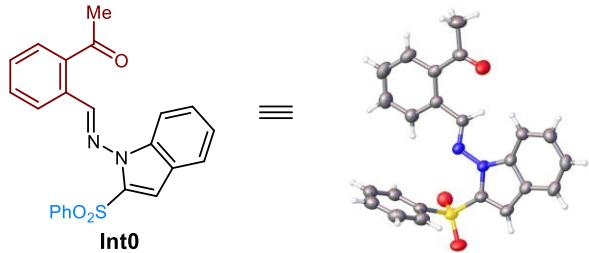


Table S3. Crystal data and structure refinement for CCDC 2354174

Identification code	CCDC 2354174
Empirical formula	C ₂₃ H ₁₈ N ₂ O ₃ S
Formula weight	402.45
Temperature/K	223.00
Crystal system	monoclinic
Space group	P21/c
a/Å	11.0123(12)
b/Å	12.1777(14)
c/Å	14.8173(17)
α/°	90
β/°	104.644(4)
γ/°	90
Volume/Å ³	1922.5(4)
Z	4
ρcalcg/cm ³	1.390
μ/mm ⁻¹	1.728
F(000)	840.0
Crystal size/mm ³	0.13 × 0.11 × 0.1
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	8.298 to 137.162
Index ranges	-13 ≤ h ≤ 13, -14 ≤ k ≤ 14, -17 ≤ l ≤ 17
Reflections collected	41027
Independent reflections	3524 [Rint = 0.0334, Rsigma = 0.0201]
Data/restraints/parameters	3524/0/263
Goodness-of-fit on F ²	1.047
Final R indexes [I>=2σ (I)]	R1 = 0.0313, wR2 = 0.0828
Final R indexes [all data]	R1 = 0.0327, wR2 = 0.0835
Largest diff. peak/hole / e Å ⁻³	0.19/-0.38

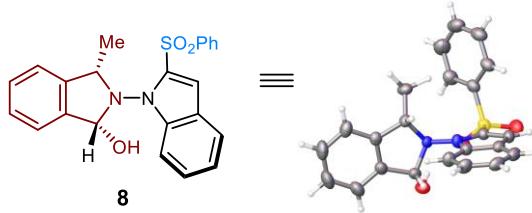


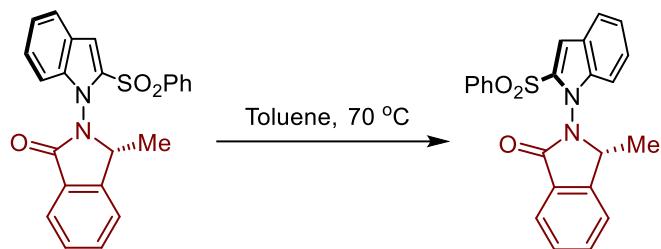
Table S4. Crystal data and structure refinement for CCDC 2393057

Identification code	CCDC 2393057
Empirical formula	C ₂₃ H ₂₀ N ₂ O ₃ 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 ³	1968.03(4)
Z	4
ρcalcg/cm ³	1.365
μ/mm ⁻¹	1.689
F(000)	848.0
Crystal size/mm ³	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 [Rint = 0.0329, Rsigma = 0.0216]
Data/restraints/parameters	3603/0/272
Goodness-of-fit on F ²	1.075
Final R indexes [I>=2σ (I)]	R1 = 0.0251, wR2 = 0.0668
Final R indexes [all data]	R1 = 0.0255, wR2 = 0.0672
Largest diff. peak/hole / e Å ⁻³	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 µL) 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 $k_B = 1.38066 \times 10^{-23} \text{ J} \cdot \text{K}^{-1}$ ($-\ln \text{ee} = \ln/\{(1+M/P)/(1-M/P)\}$).



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

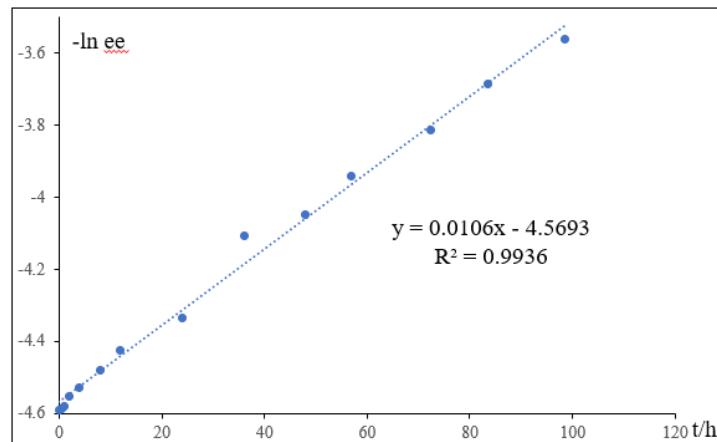


Figure S1. Racemization experiments.

k racemization = 0.01060 h⁻¹; **k** enantiomerization = 0.00530 h⁻¹

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

ΔG^{343K} = 29.33 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.

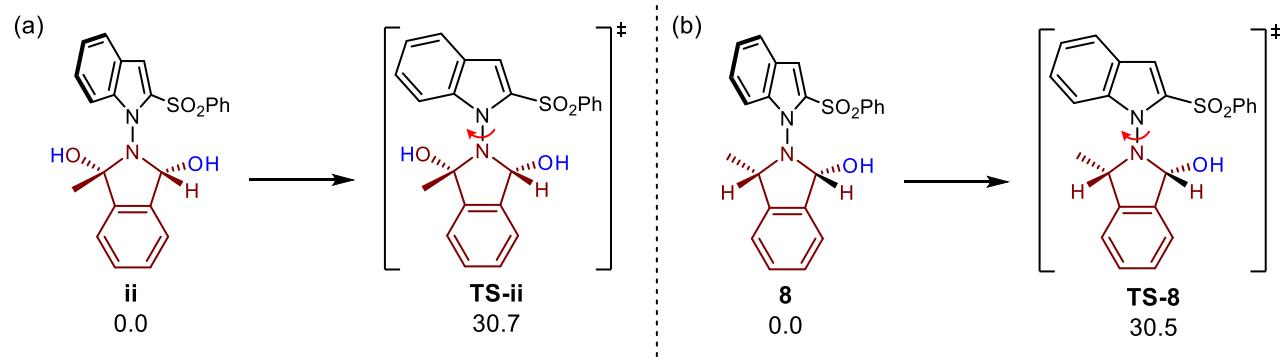


Figure S2. The rotational energy barriers of **ii** and **8** (in kcal/mol).

Computational methods

The Gaussian 16 program was used for all the DFT calculations.^[4] Geometry optimizations were optimized at the M06-2X^[5] and def2-SVP^[6] 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)^[7-8] calculations were performed to confirm the connection between transition state and its reactant and product.

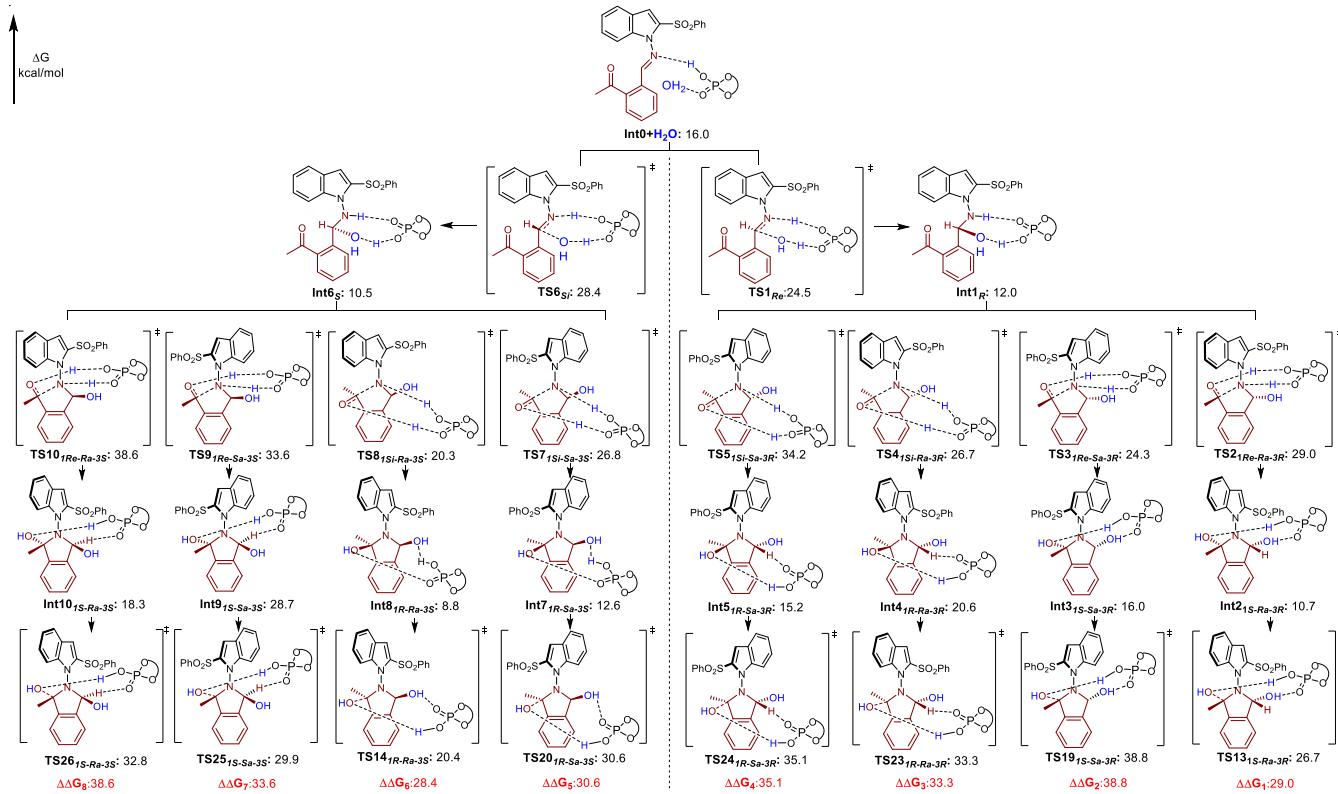


Figure S3. Free energy diagrams of chiral phosphoric acid-catalyzed stepwise mechanism in asymmetric annulation and dehydration. The meaning for the corner mark in the structure name: **Re**: the rectus face; **Si**: the sinister face; **Ra**: the (potential) **R**-configuration for the *N-N* axis; **Sa**: 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
H₂O	0.003949	-76.433213	TS11_{IRe-Ra-3Re}	1.235706	-4279.052964
CPA	0.867742	-2582.036042	TS12_{ISi-Ra-3Si}	1.238793	-4279.054653
Int0	1.205454	-4202.630730	TS13_{IS-Ra-3R}	1.239669	-4279.051586
Int0+H₂O	1.231781	-4279.060820	TS14_{IR-Ra-3S}	1.237124	-4279.059093
TS1_{Re}	1.233156	-4279.048592	TS15_{P-Re}	1.206928	-4202.589283
Int1_R	1.238581	-4279.073964	TS16_{P-Si}	1.210572	-4202.587333
TS2_{1Re-Ra-3R}	1.241509	-4279.049869	Int11_P	1.211006	-4202.618837
TS3_{1Re-Sa-3R}	1.242254	-4279.057850	(P,R)-3a	0.314580	-1620.620748
TS4_{1Si-Ra-3R}	1.240384	-4279.052382	(P,S)-3a	0.313841	-1620.621035
TS5_{1Si-Sa-3R}	1.239710	-4279.039820	TS17_{1Re-Sa-3Re}	1.239719	-4279.058216
Int2_{1S-Ra-3R}	1.239899	-4279.077374	TS18_{1Si-Sa-3Si}	1.241763	-4279.047623
Int3_{1S-Sa-3R}	1.245549	-4279.074633	TS19_{1S-Sa-3R}	1.238808	-4279.031563
Int4_{IR-Ra-3R}	1.240917	-4279.062622	TS20_{IR-Sa-3S}	1.240898	-4279.046617
Int5_{IR-Sa-3R}	1.240375	-4279.070664	TS21_{M-Re}	1.203059	-4202.586698
TS6_{Si}	1.237785	-4279.047129	TS22_{M-Si}	1.208337	-4202.588708
Int6_S	1.236214	-4279.074054	Int12_M	1.207652	-4202.612865
TS7_{1Si-Sa-3S}	1.241408	-4279.053245	(M,R)-3a	0.314835	-1620.623487
TS8_{1Si-Ra-3S}	1.237443	-4279.059684	(M,S)-3a	0.314751	-1620.626210
TS9_{1Re-Sa-3S}	1.242373	-4279.043349	TS23_{IR-Ra-3R}	1.240180	-4279.041600
TS10_{1Re-Ra-3S}	1.240434	-4279.033492	TS24_{IR-Sa-3R}	1.239553	-4279.038123
Int7_{IR-Sa-3S}	1.243725	-4279.078221	TS25_{IS-Sa-3S}	1.240206	-4279.047135
Int8_{IR-Ra-3S}	1.242056	-4279.082552	TS26_{IS-Ra-3S}	1.240383	-4279.042596
Int9_{IS-Sa-3S}	1.243909	-4279.052691			
Int10_{IS-Ra-3S}	1.243293	-4279.068737			

Cartesian coordinates for all optimized geometries

H₂O

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
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O	1.04185900	0.13358400	0.98158000
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O	0.93950200	-1.65576900	-0.85465800
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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
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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
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 H 2.94091600 -1.55035100 -4.27967800
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 H 4.62570200 -5.15573700 -0.64179500
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Int0

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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
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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
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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

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 O -2.29736800 -0.15776300 -2.08402700
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 C -1.32156800 -4.81624700 -1.44770800
 C -1.41037700 -6.34647300 -1.41940800
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 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
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 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+H₂O

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 -2.38687500 -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

TS1_{Re}

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	0.58644500	-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_R

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-Ra-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 -3.511149000 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_{IRe-Sa-3R}

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 -3.277446200 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_{1Si-Ra-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

TS5_{ISi-Sa-3R}

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_{IS-Ra-3R}

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_{1S-Sa-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 1.400005800 -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	3.3865700	-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-Ra-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

Int5_{IR-Sa-3R}

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

TS6_{Si}

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

Int6s

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_{1Si-Sa-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

TS8_{1Si-Ra-3S}

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_{IRe-Sa-3S}

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 -1.511181400 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_{IRe-Ra-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_{IR-Sa-3s}

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 -0.28555500
 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	3.4981600	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_{IR-Ra-3S}

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_{1S-Sa-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_{IS-Ra-3S}

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_{IRe-Ra-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_{ISi-Ra-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
TS13_{IS-Ra-3R}			
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_{IR-Ra-3S}

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_{P-Re}

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_{p-Si}

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
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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
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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
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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
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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
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 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
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 C -1.91616200 3.03717100 -3.67796400
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 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
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 H -1.36125500 5.65350700 2.82861300
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 H 3.97834800 1.94049500 -1.08332900
 H 5.52786200 2.78815700 -0.76312500
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 H 4.01965300 6.27538800 -0.94057700
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 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

Int11_P

S -2.55923900 0.13235600 1.62791800
 O -1.96864700 1.48040500 1.71201900
 O -1.91937200 -0.83607800 0.74487800
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 C -2.79728200 -0.31064400 5.61916000
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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
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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
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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
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C	6.70608200	-2.19005200	2.42122700
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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
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O	2.28335100	0.49225700	-0.82973000
P	0.81016400	0.04918000	-0.33705000
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C	-0.95416000	-3.97751600	0.20961700

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 C -2.14791600 -3.23188200 -2.19831900
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 C 3.89838200 3.64122200 3.74864300
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 C 4.74817000 3.74837000 -2.66344100
 C 2.52657200 2.66242400 -3.20087700
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 H 5.53514400 3.87049900 -1.90486600
 H 5.19696500 3.29095700 -3.55791300
 H 4.38819200 4.75121900 -2.94052500
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 H 2.11158200 3.62012600 -3.55116700
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 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_{IRe-Sa-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-Sa-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-Sa-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-Sa-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_{M-Re}

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	-1.844439500	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
TS22_{M-Si}			
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
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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_M

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
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 C -5.54598100 1.36963500 1.55314400
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 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-Ra-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_{IR-Sa-3R}

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_{1S-Sa-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	-0.940004200	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_{IS-Ra-3S}

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
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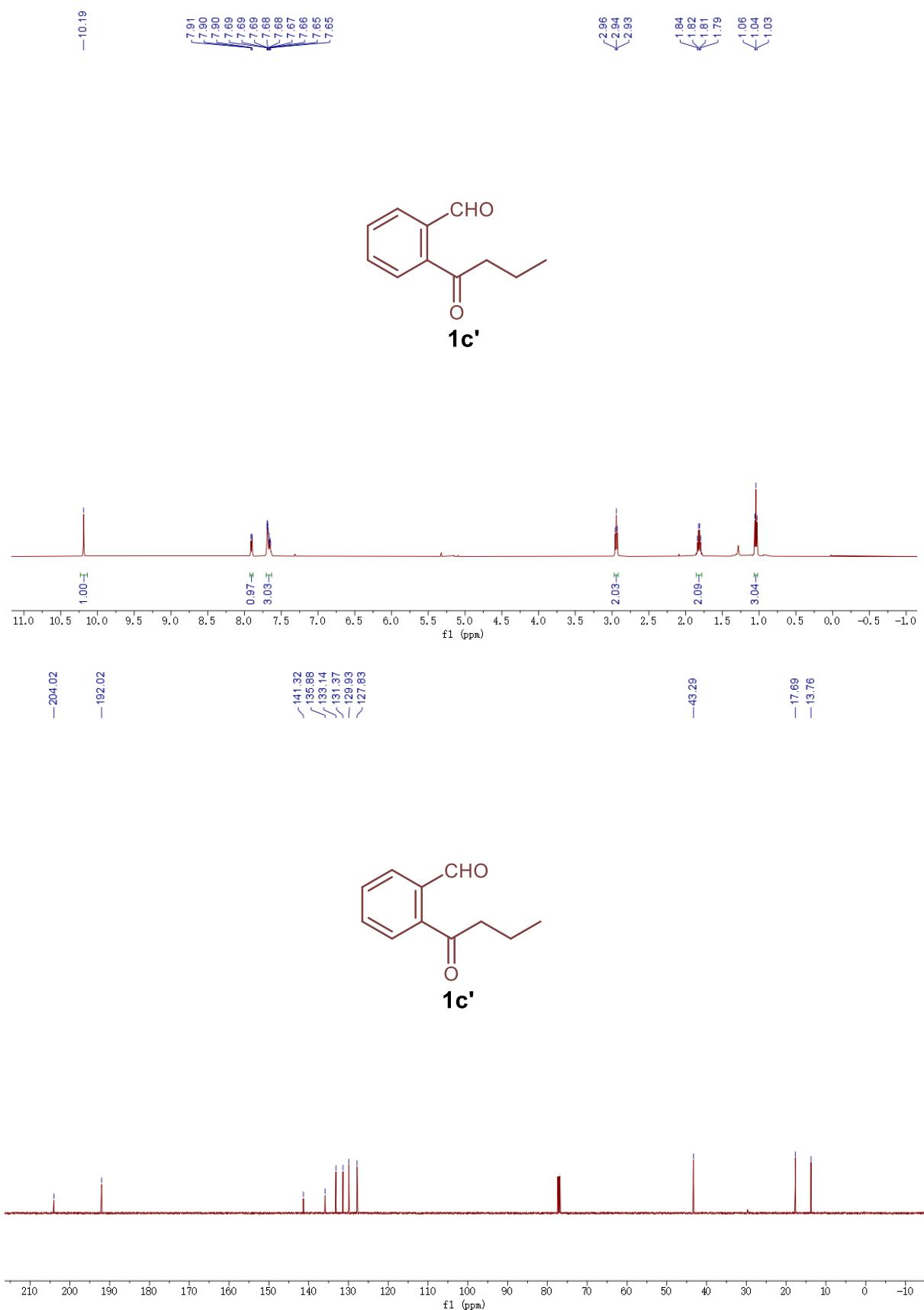
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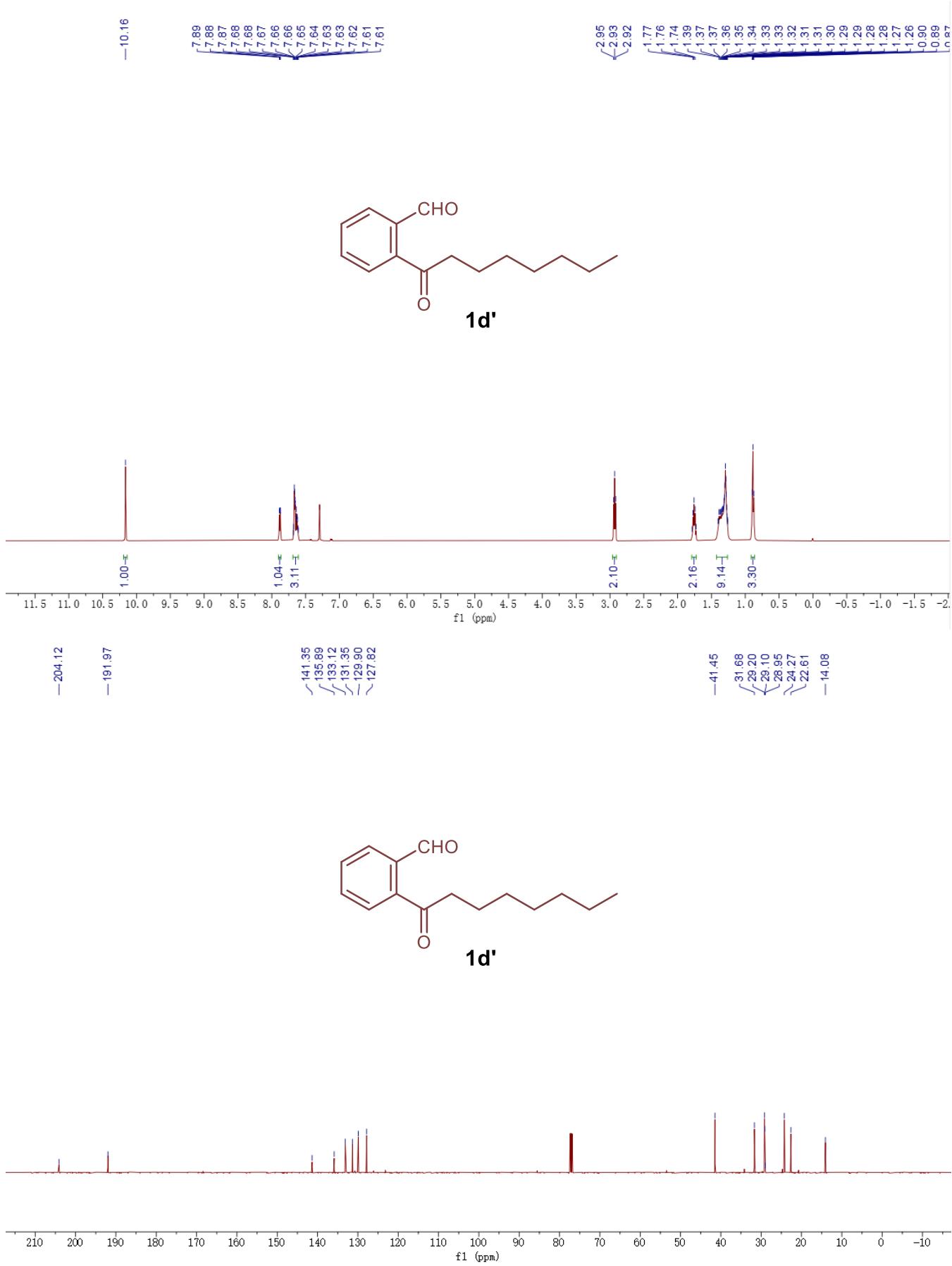
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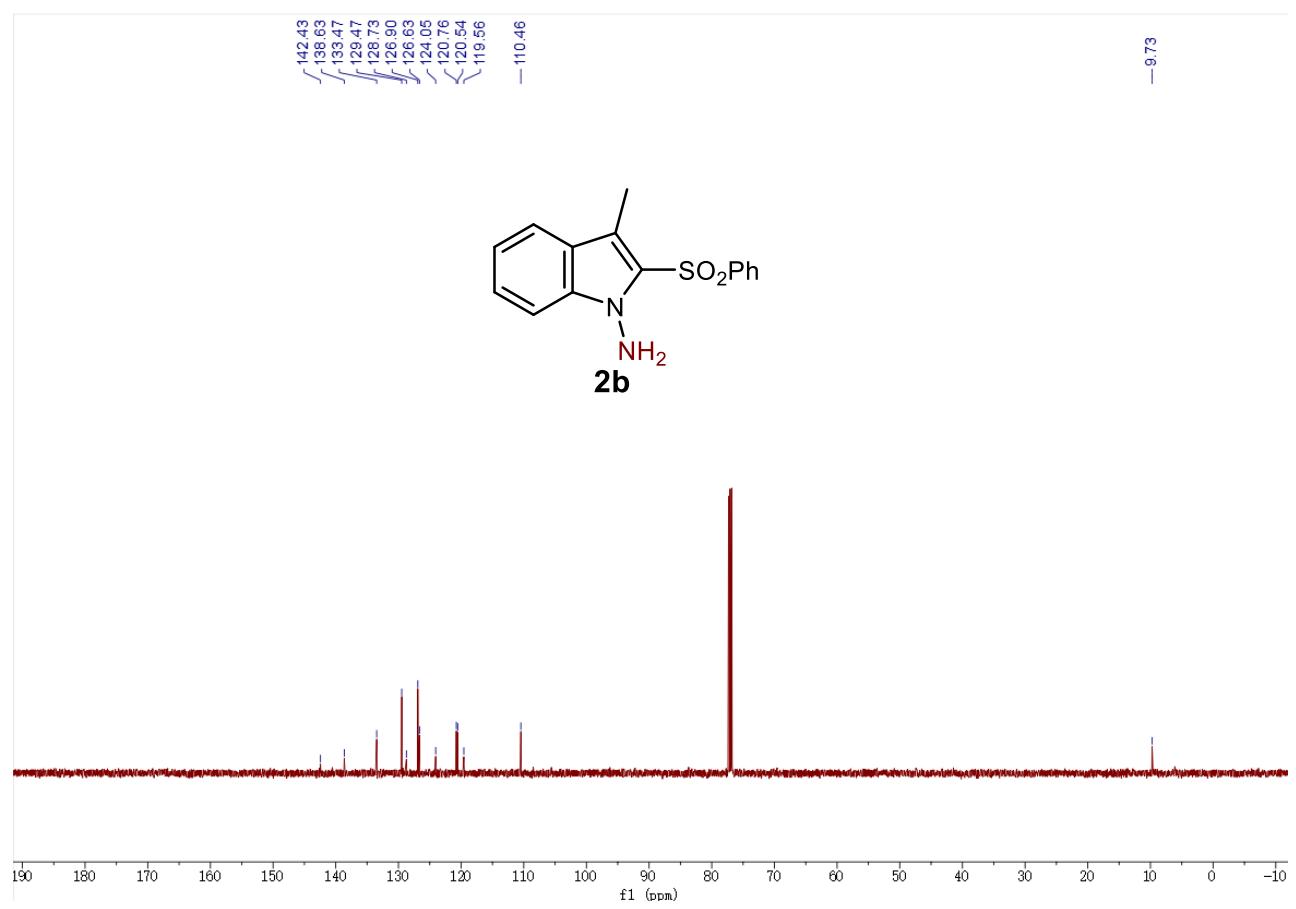
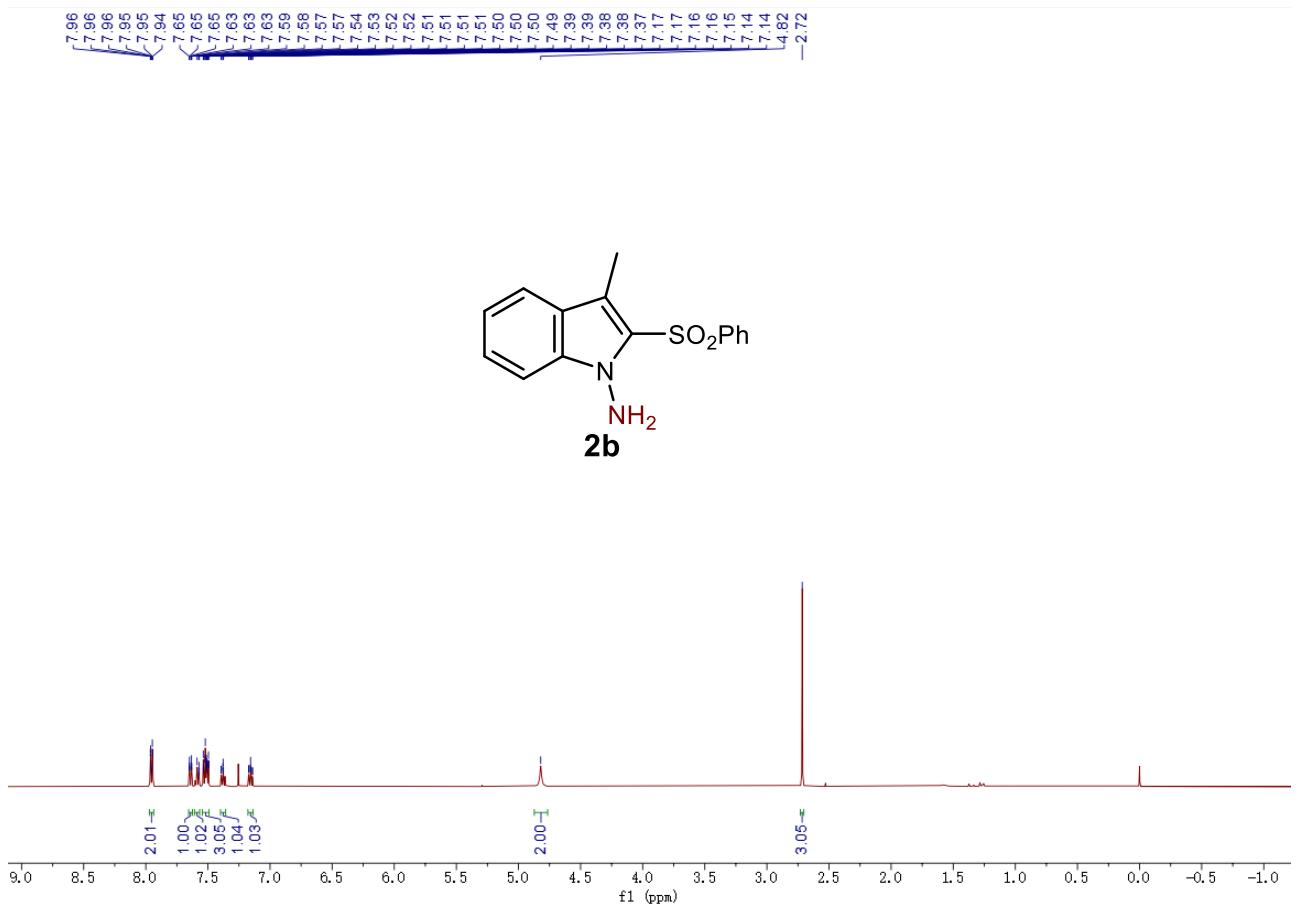
References

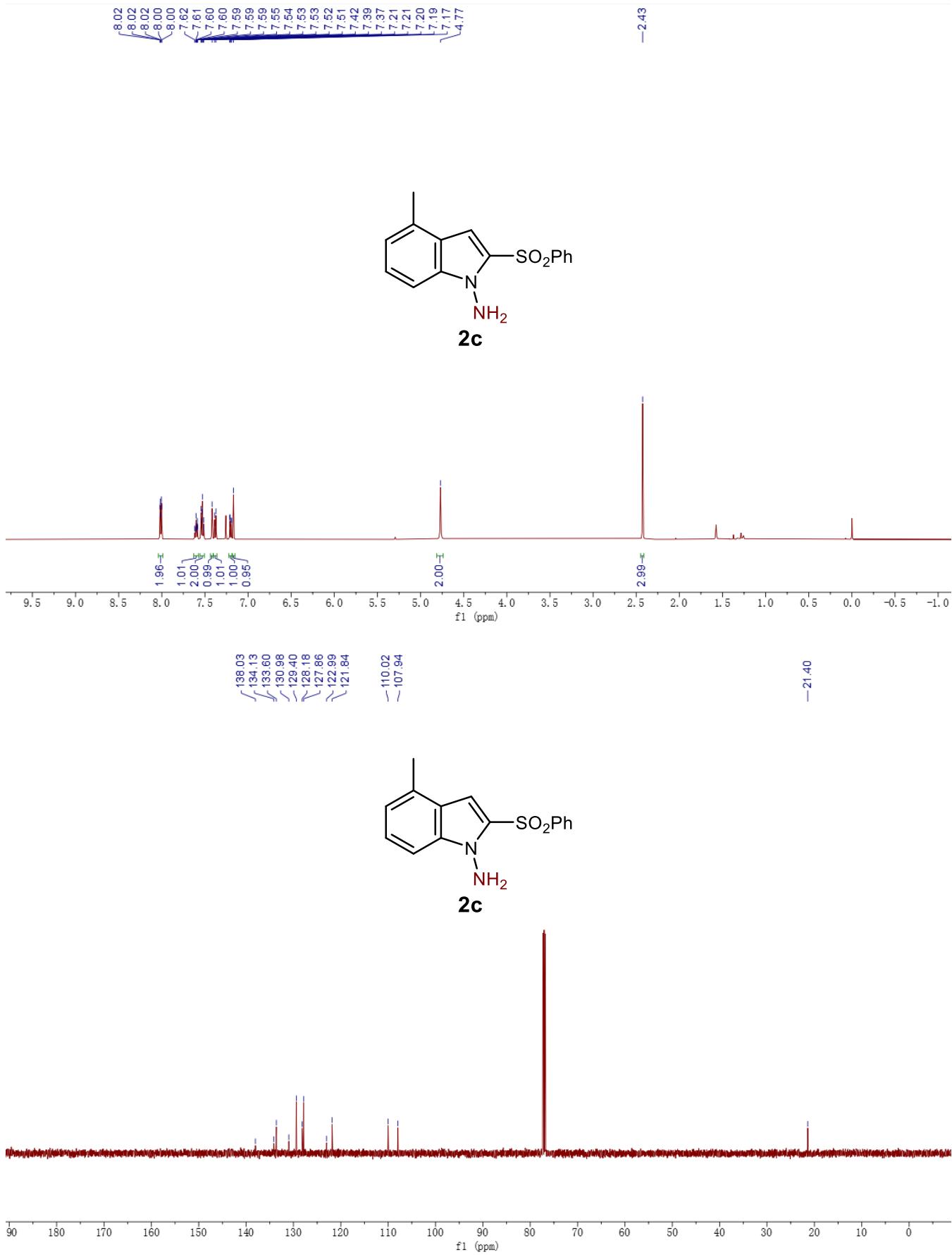
- [1] Rungsima H., Sanit T., Sittisak O., Duangduan C., Jutatip B., Somsak R. Facile synthesis of 1-substituted 4-H phthalazine, a versatile scaffold for chemically diverse phthalazines. *Tetrahedron*, **121**, 132920 (2022).
- [2] Katrun, P., Mueangkaew, C., Pohmakotr, M., Reutrakul, V., Jaipetch, T., Soorukram, D., and Kuhakarn. C. Regioselective C2 sulfonylation of indoles mediated by molecular iodine. *J. Org. Chem.*, **79**, 1778-1785. (2014).
- [3] Chen K.-W., Chen Z.-H., Yang S., Wu S.-F., Zhang Y.-C., Shi F. Organocatalytic Atroposelective Synthesis of N–N Axially Chiral Indoles and Pyrroles by De Novo Ring Formation. *Angew. Chem. Int. Ed.*, **61**, e202116829. (2022).
- [4] Gaussian 16, Revision C.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2016.
- [5] Zhao, Y. & Truhlar, D. G. The M06 Suite of Density Functionals for Main Group Thermochemistry, Thermo-chemical Kinetics, Noncovalent Interactions, Excited States, and Transition Elements: Two New Functionals and Systematic Testing of Four M06-class Functionals and 12 other Functionals. *Theor. Chem. Acc.*, **120**, 215–241. (2007).
- [6] Weigend, F. & Ahlrichs, R. Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for H to Rn: Design and assessment of accuracy. *Phys. Chem. Chem. Phys.*, **7**, 3297-3305 (2005).
- [7] Fukui K. The Path of Chemical Reactions-The IRC Approach. *Acc. Chem. Res.*, **14**, **12**, 363–368. (1981).
- [8] Fukui K. Formulation of the Reaction Coordinate. *J. Phys. Chem.*, **74**, **23**, 4161–4163. (1970).

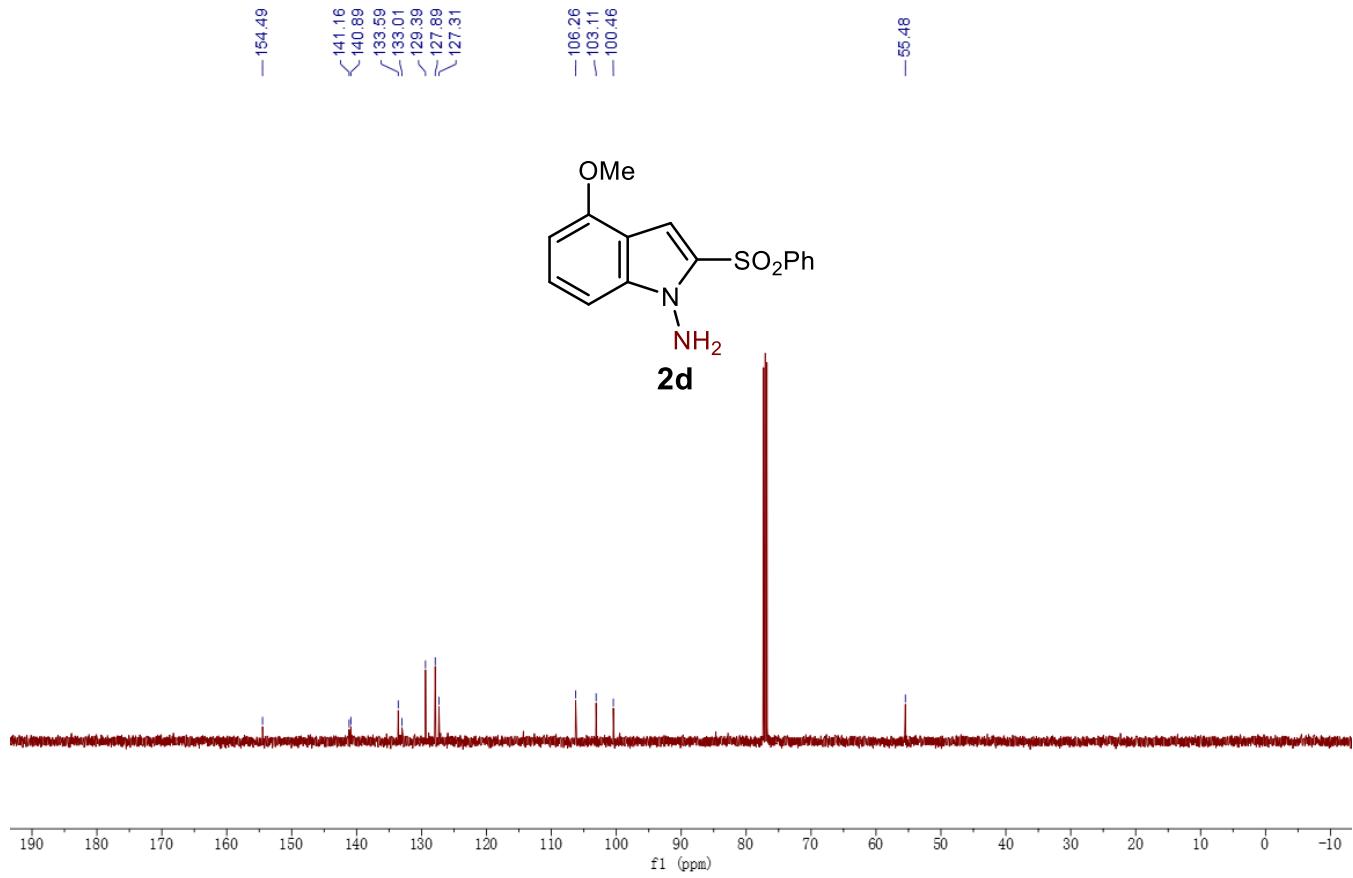
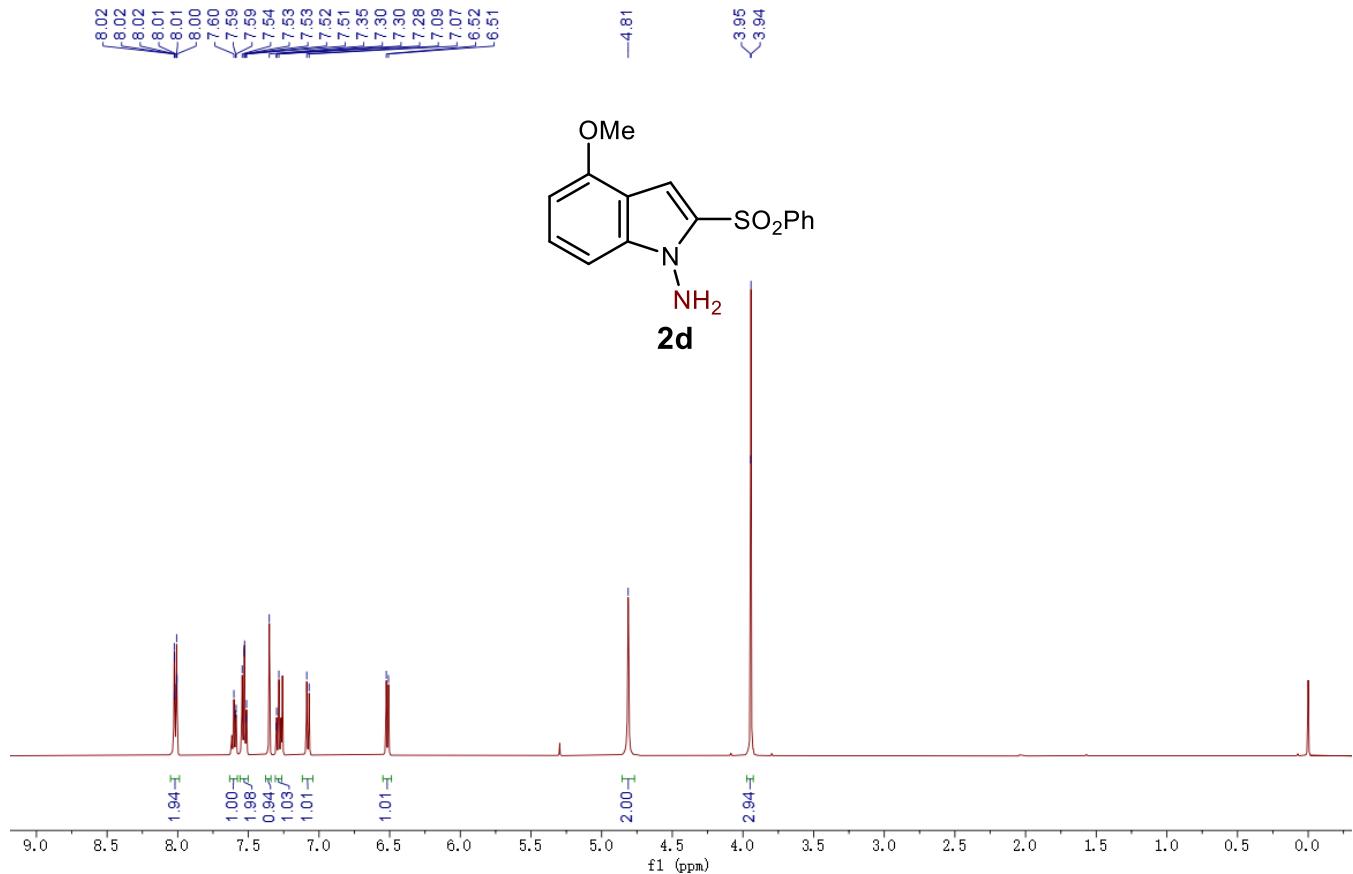
NMR spectrums





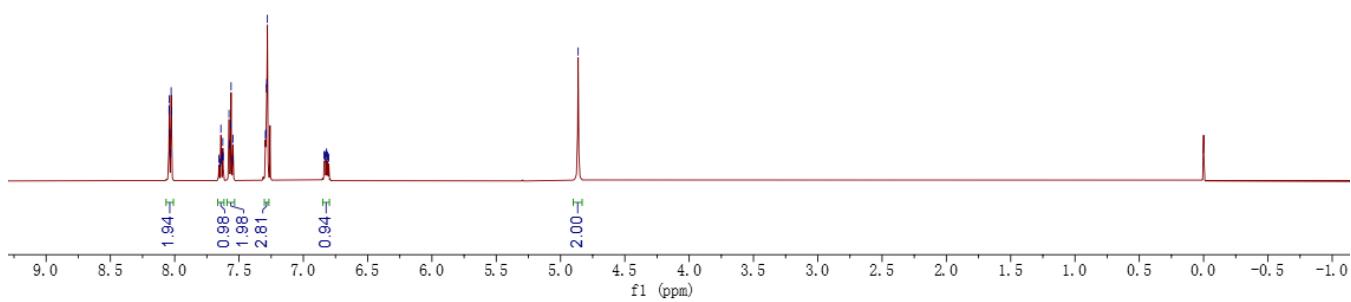




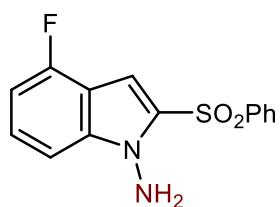




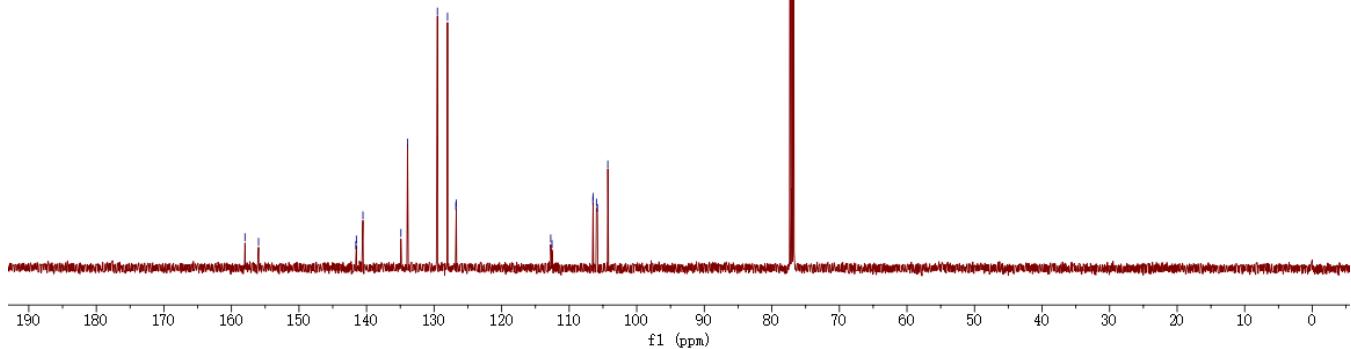
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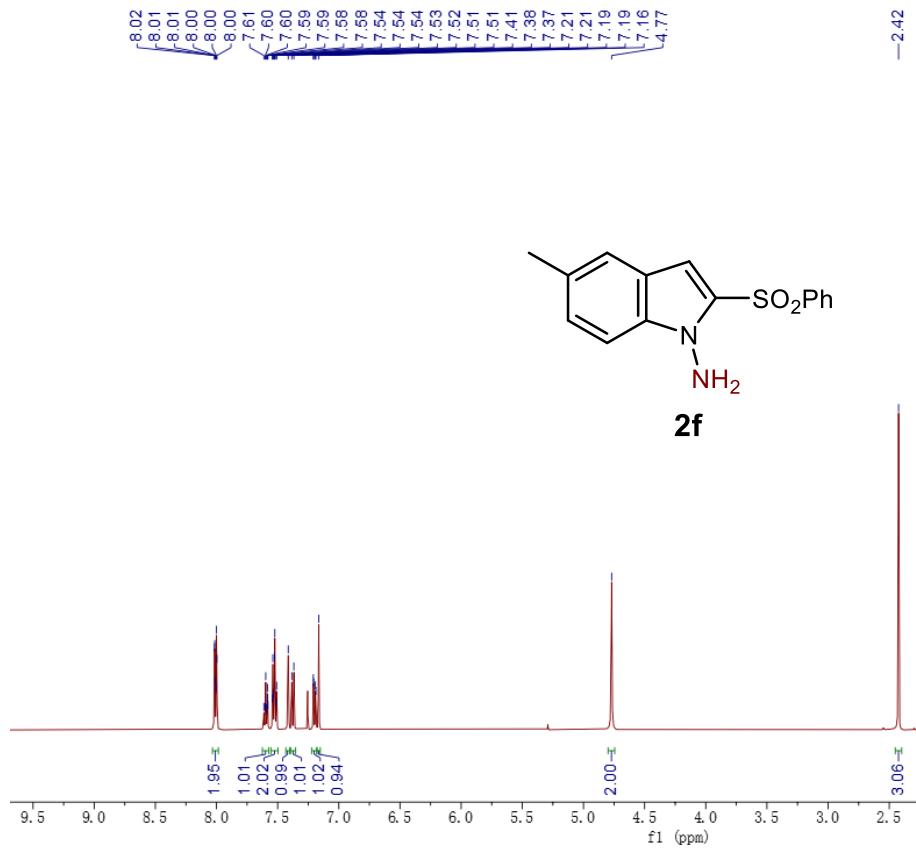
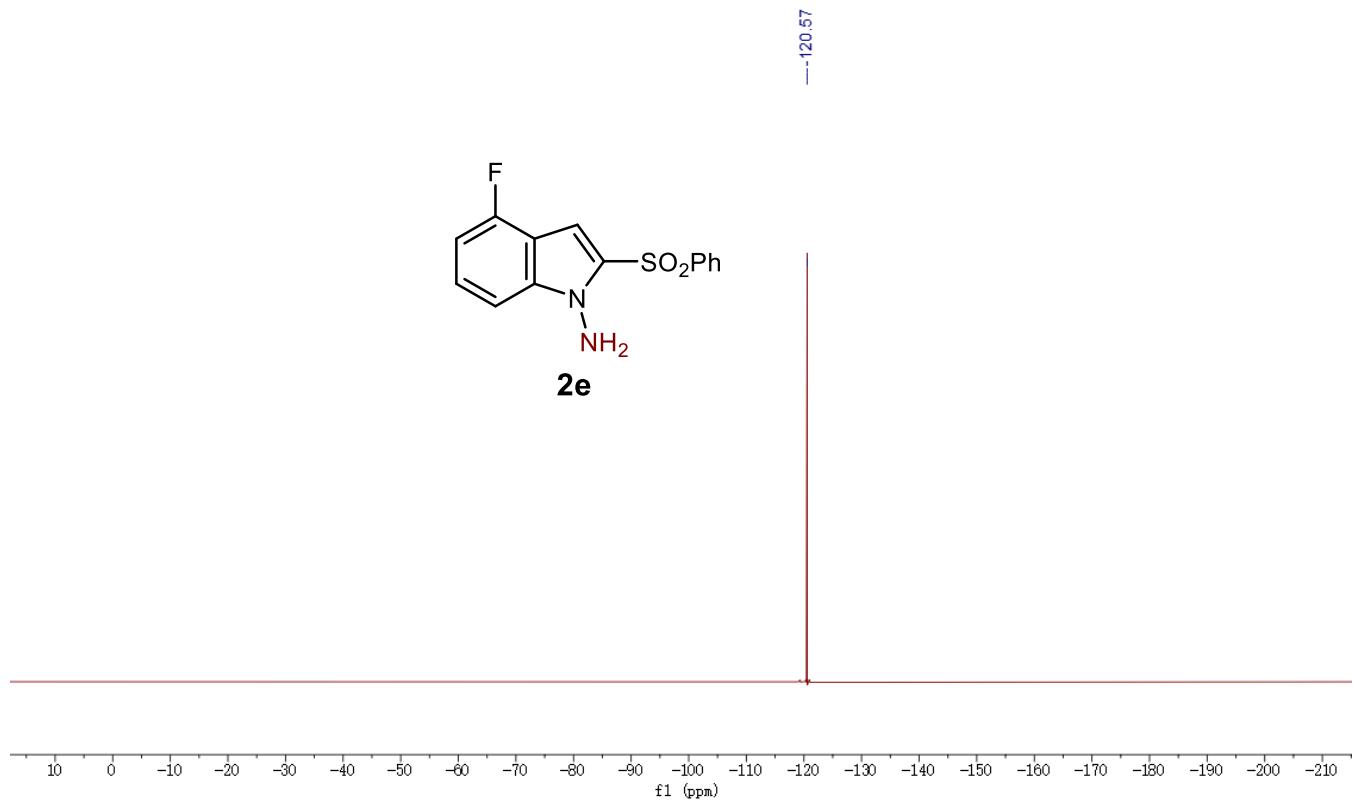


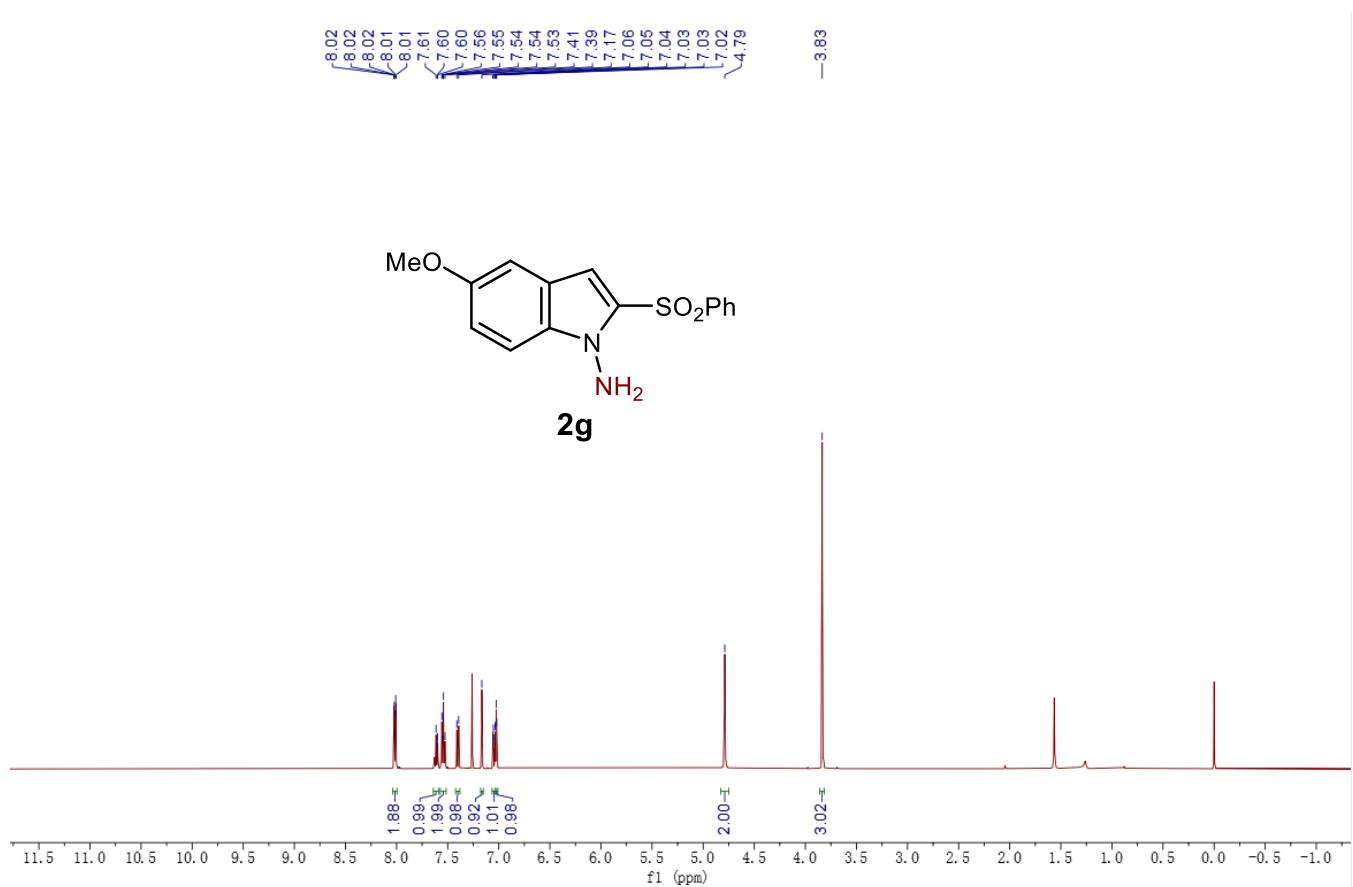
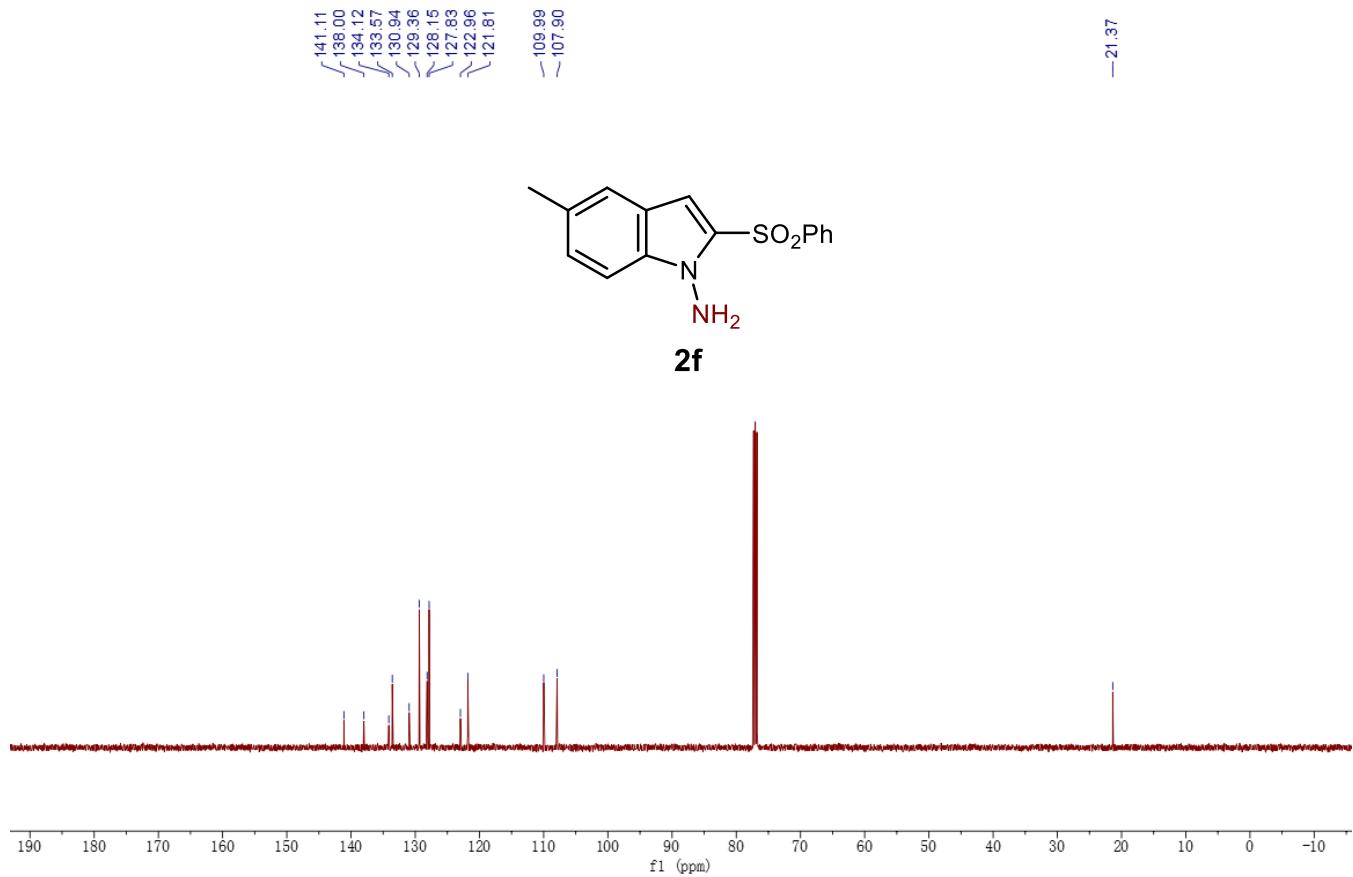
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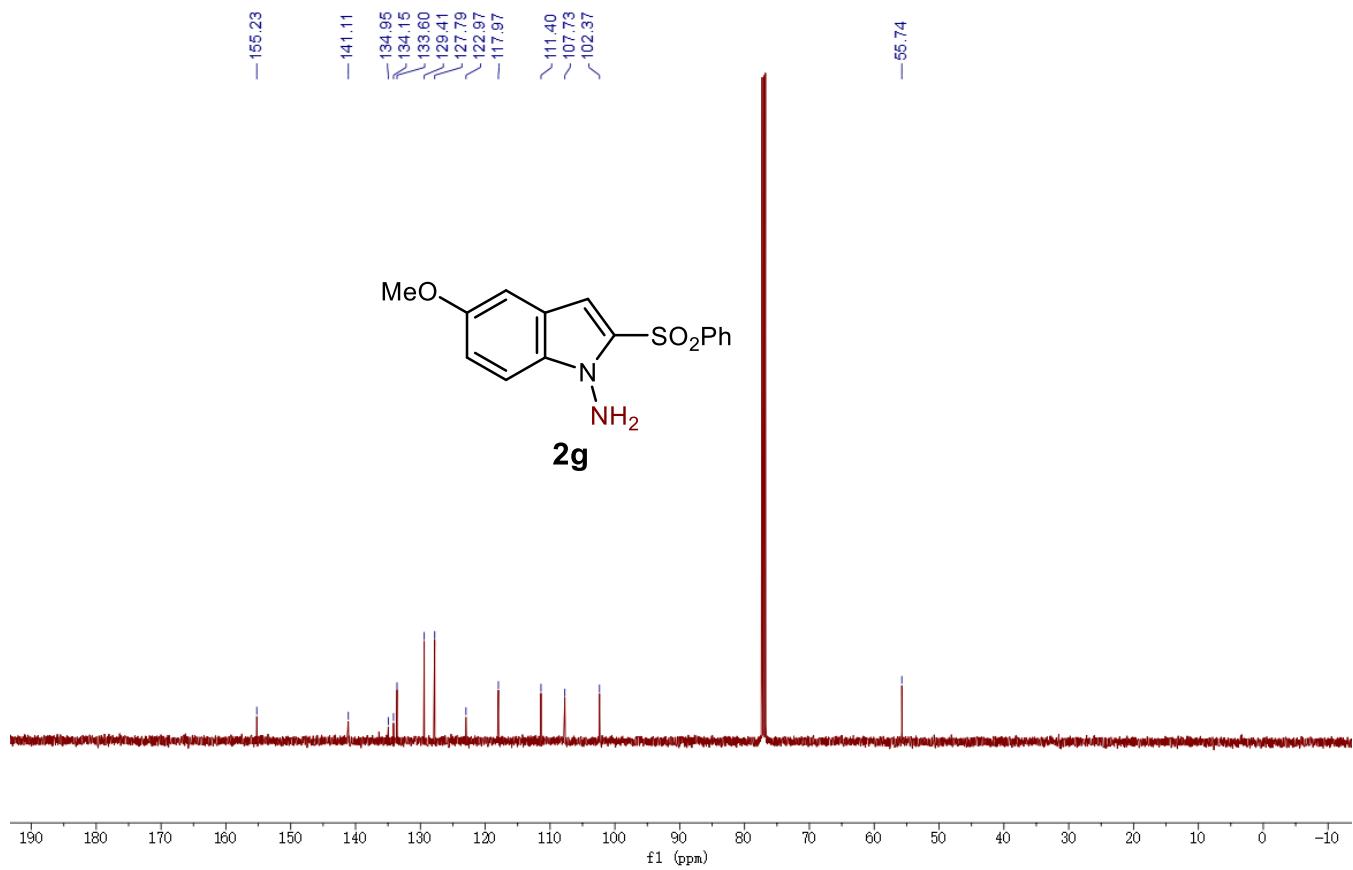


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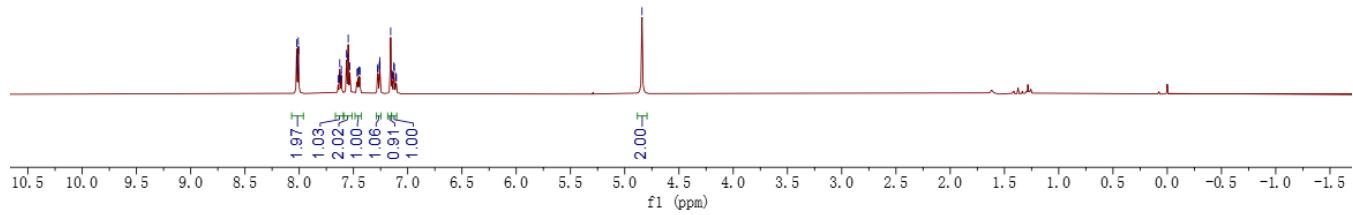
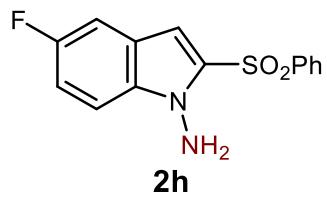


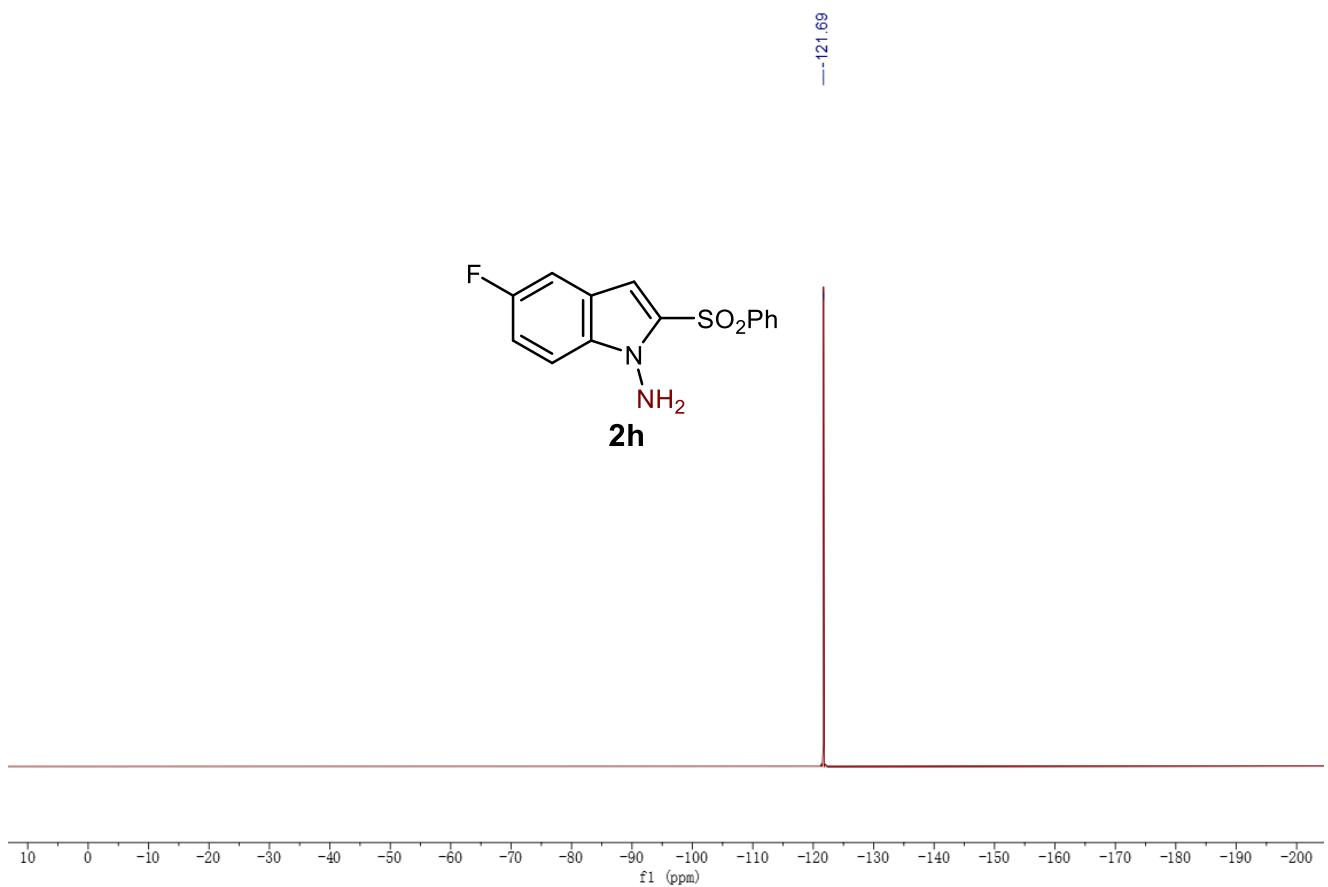
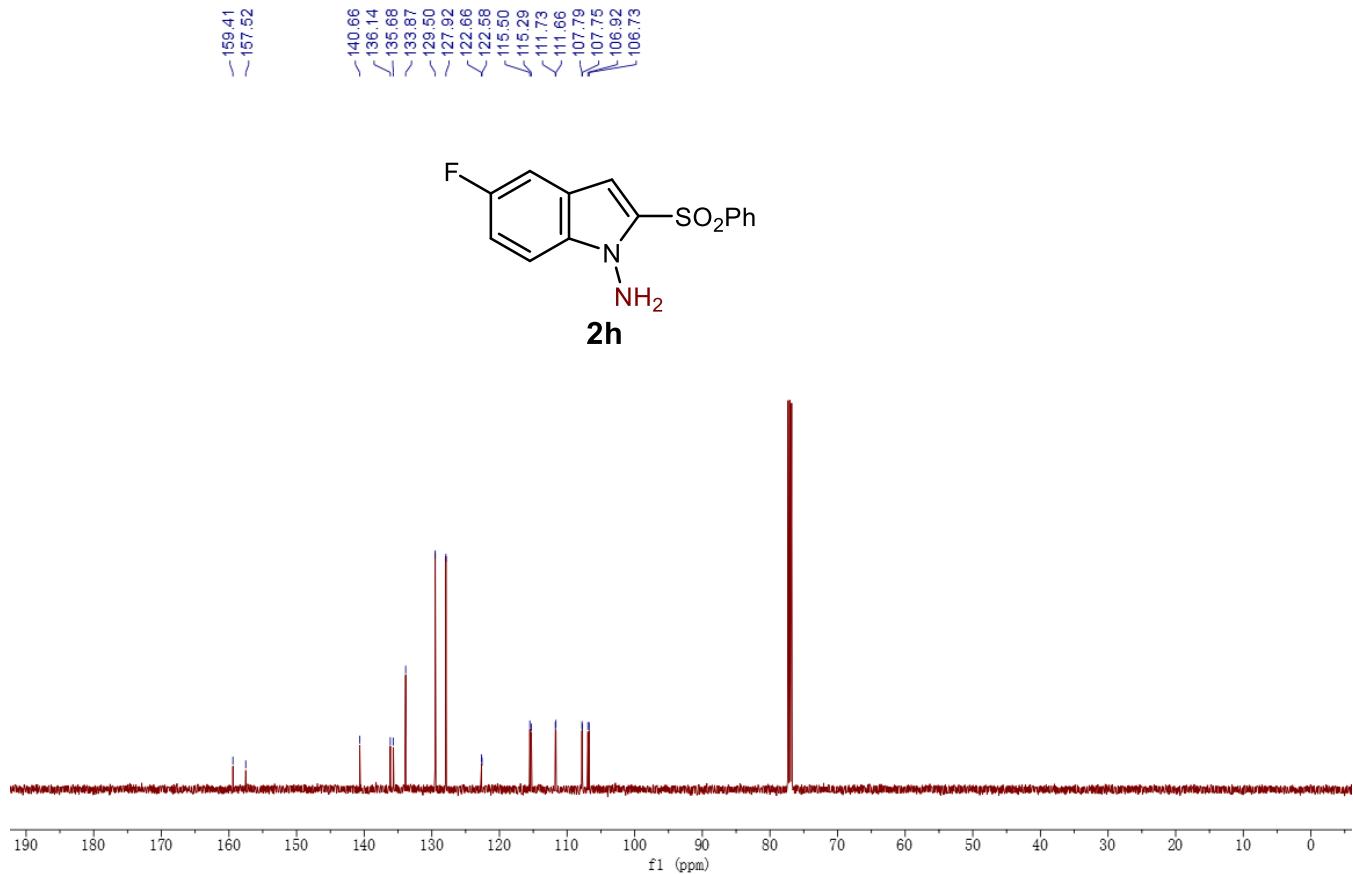






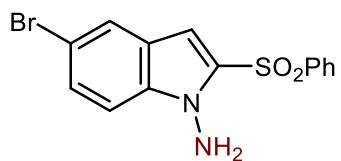
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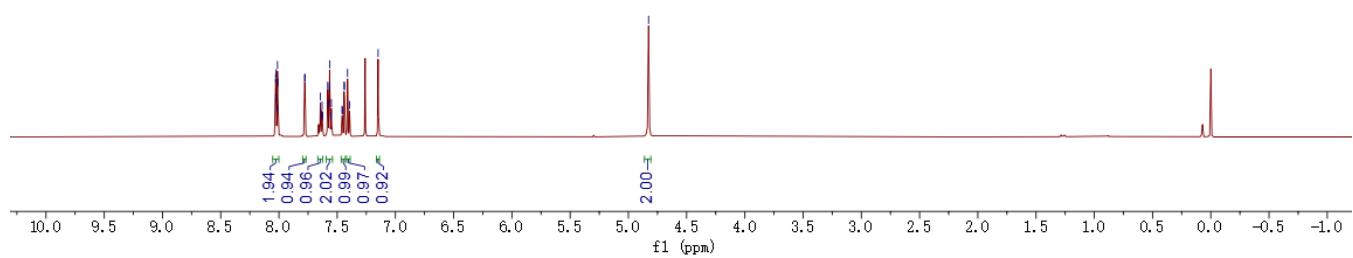


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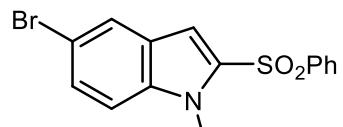
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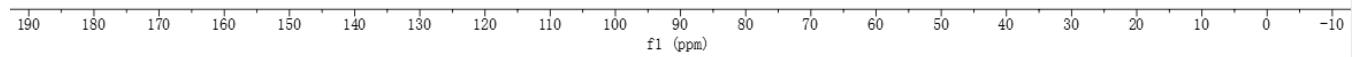
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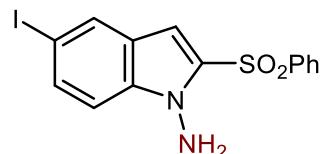


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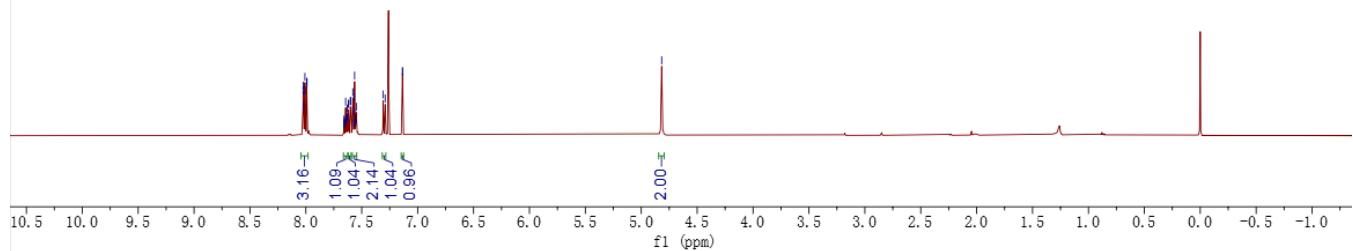


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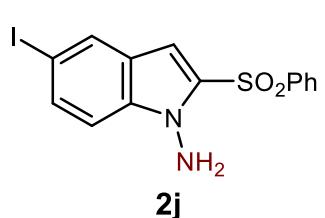




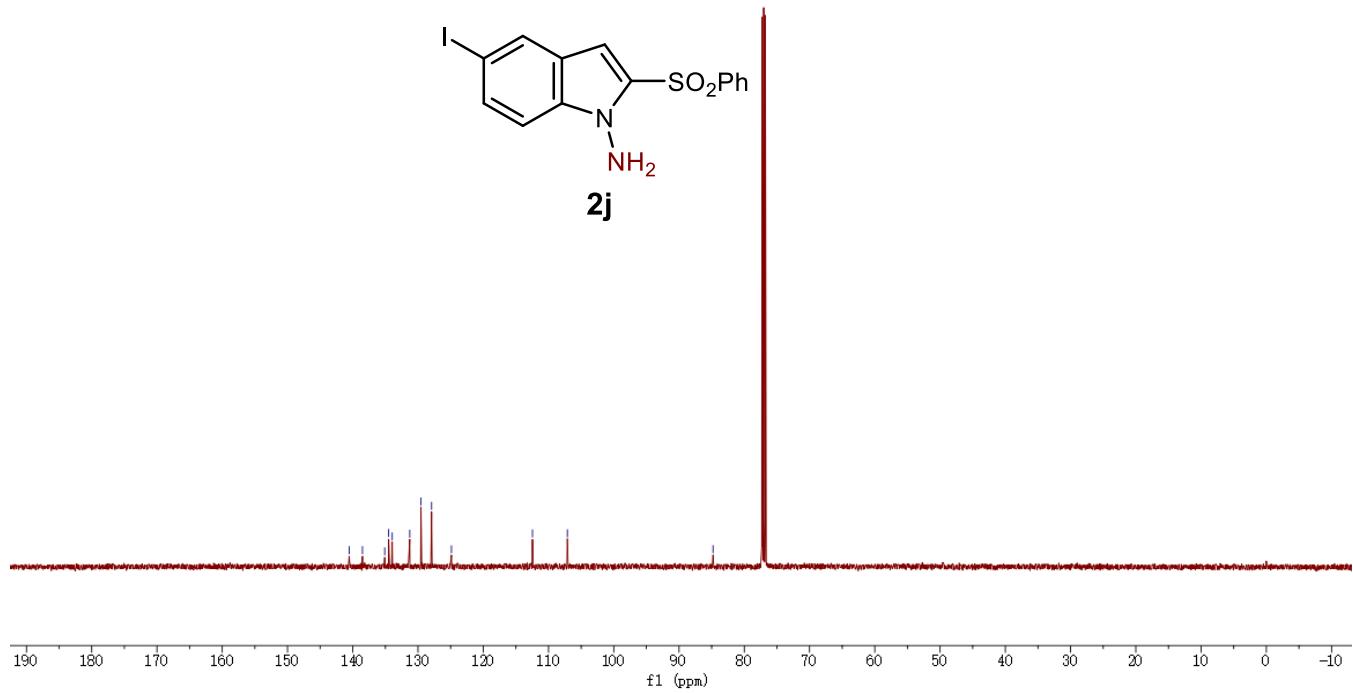
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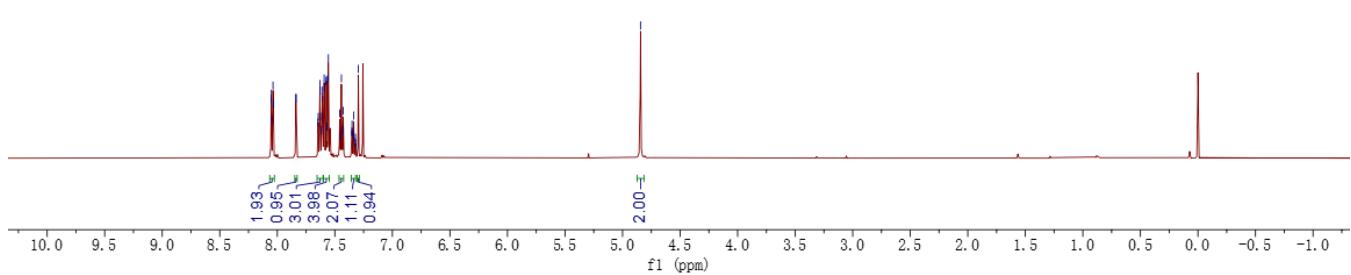
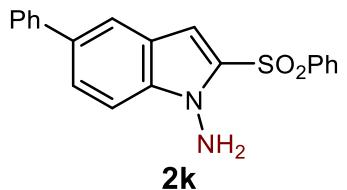


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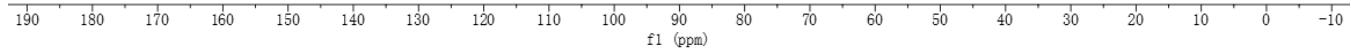
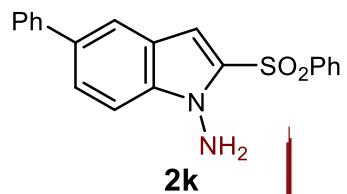


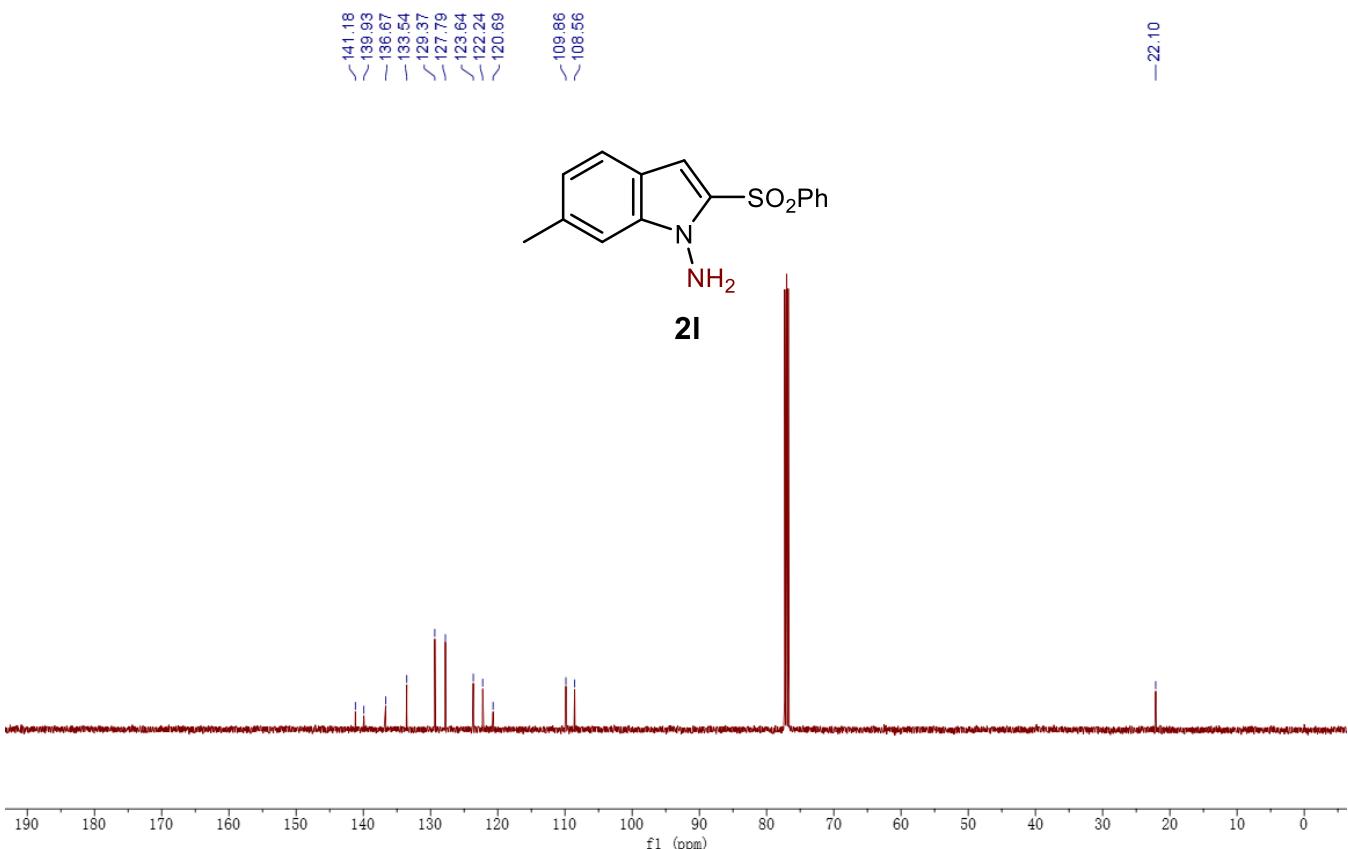
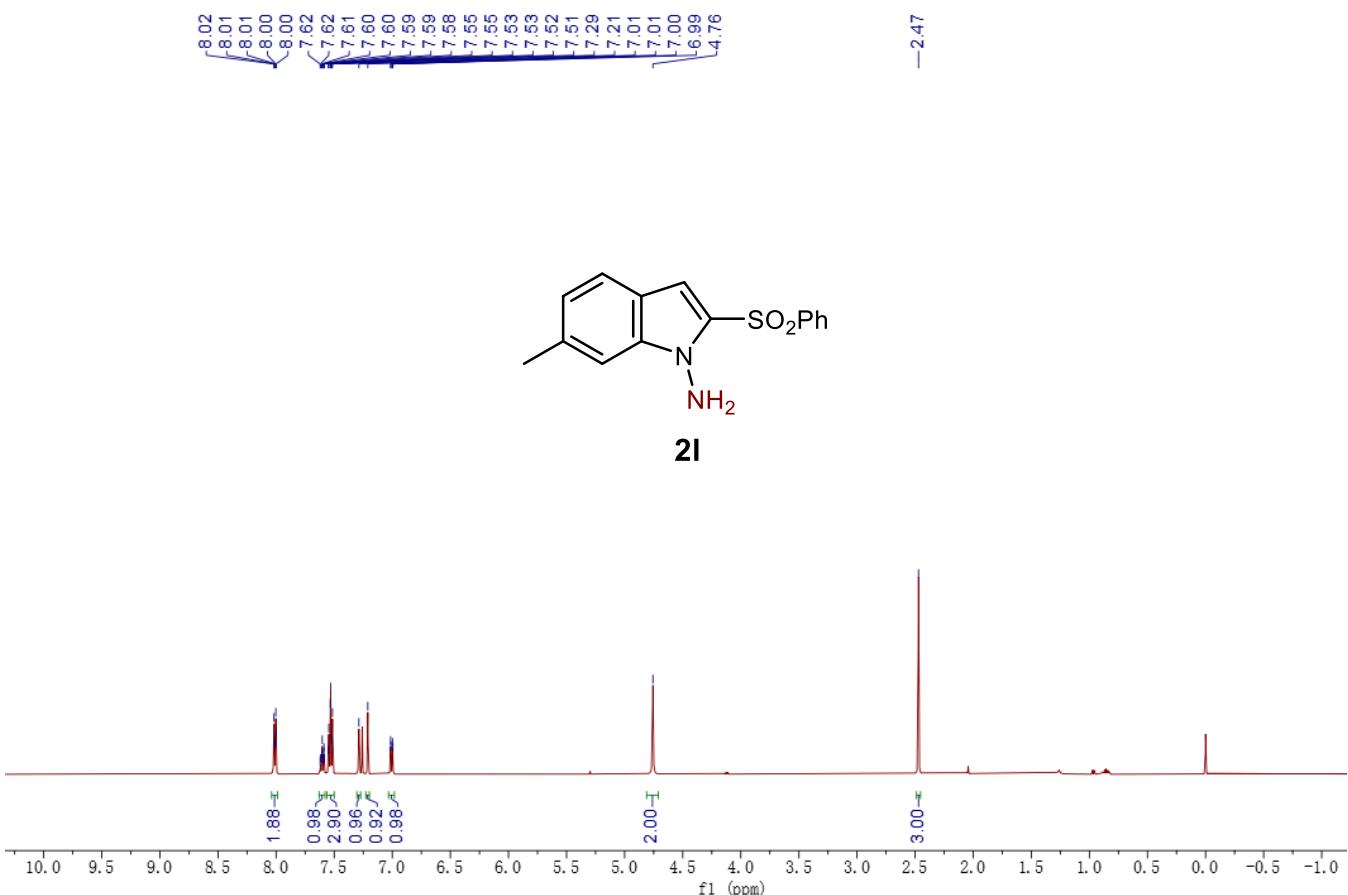
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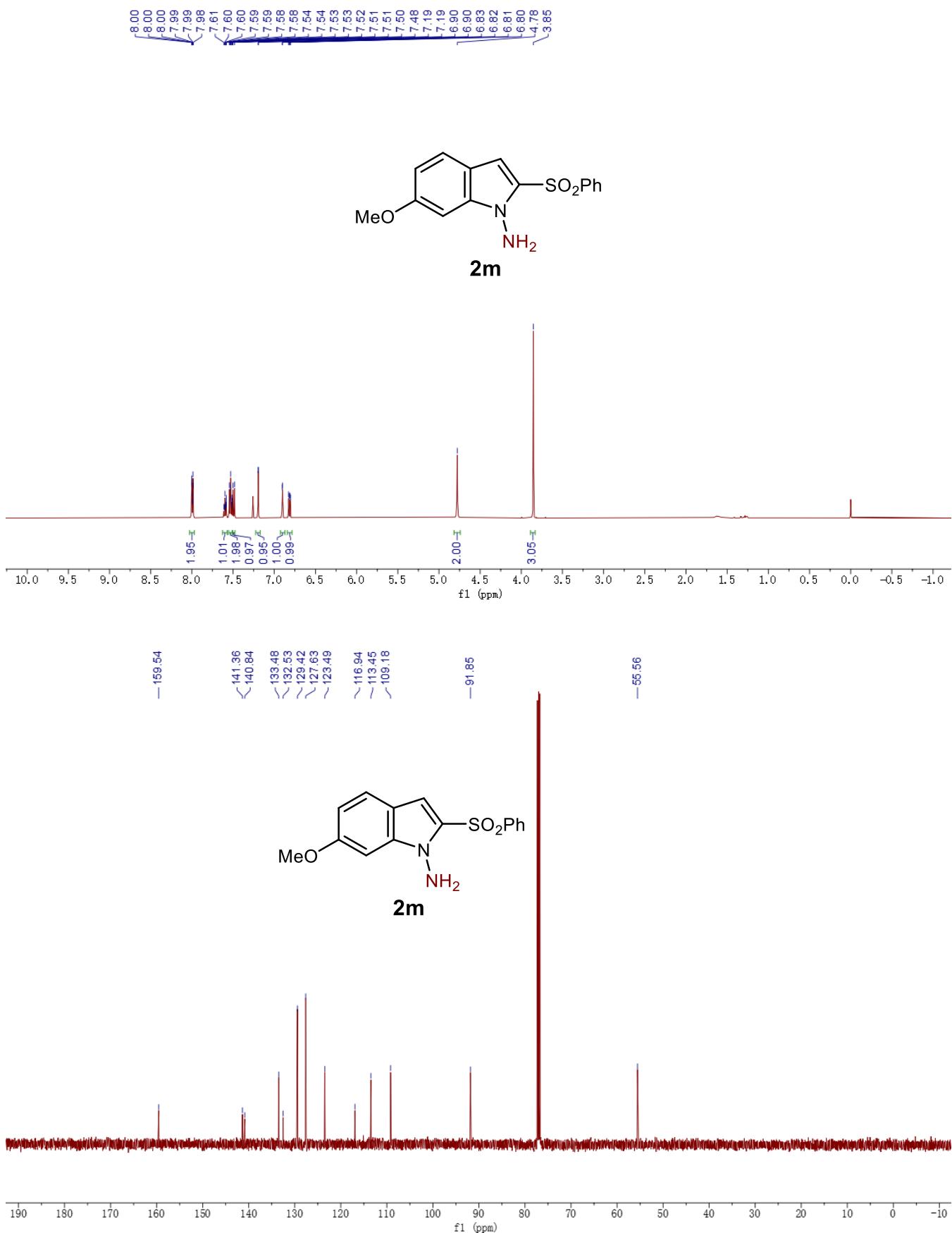


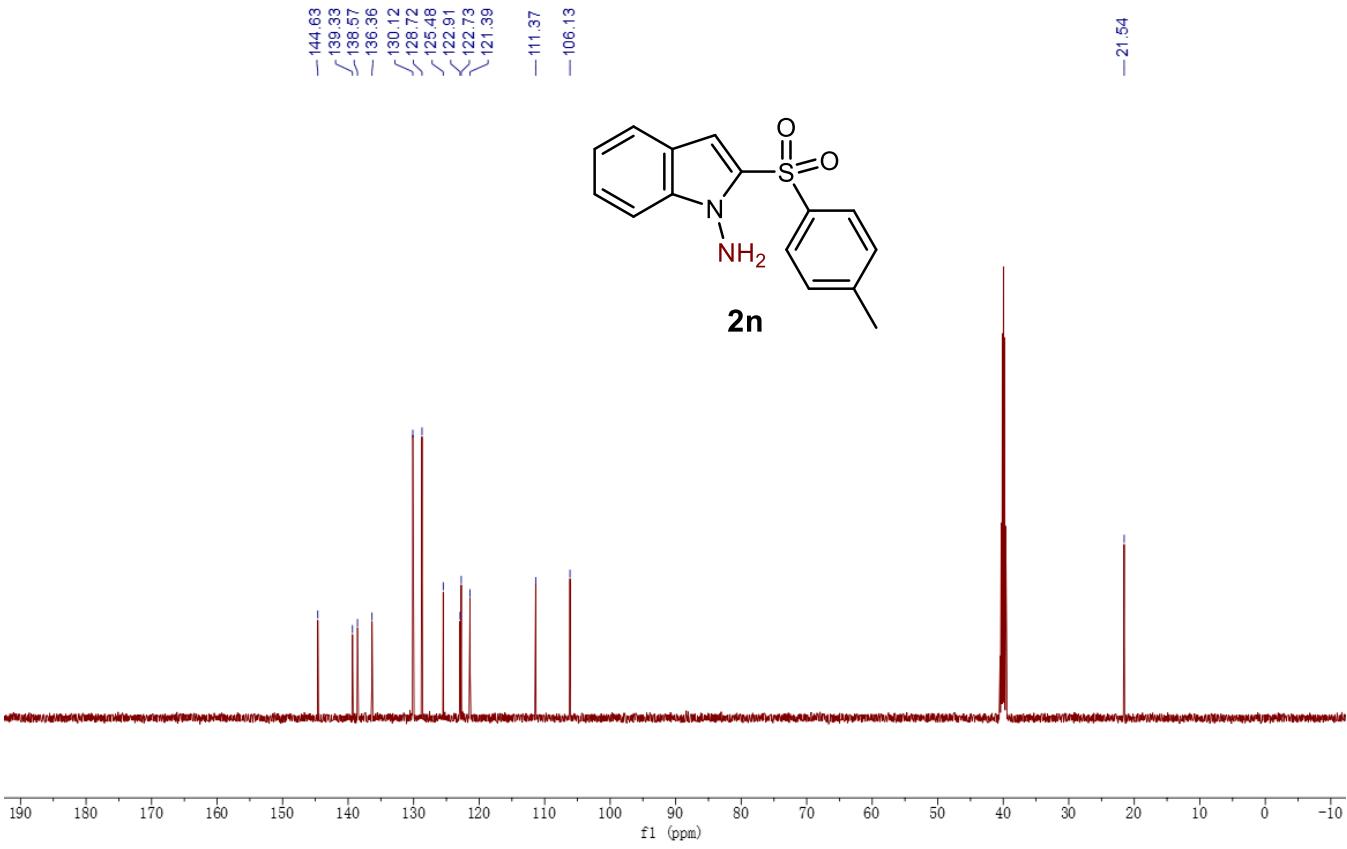
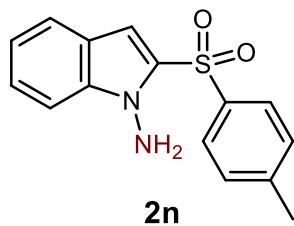
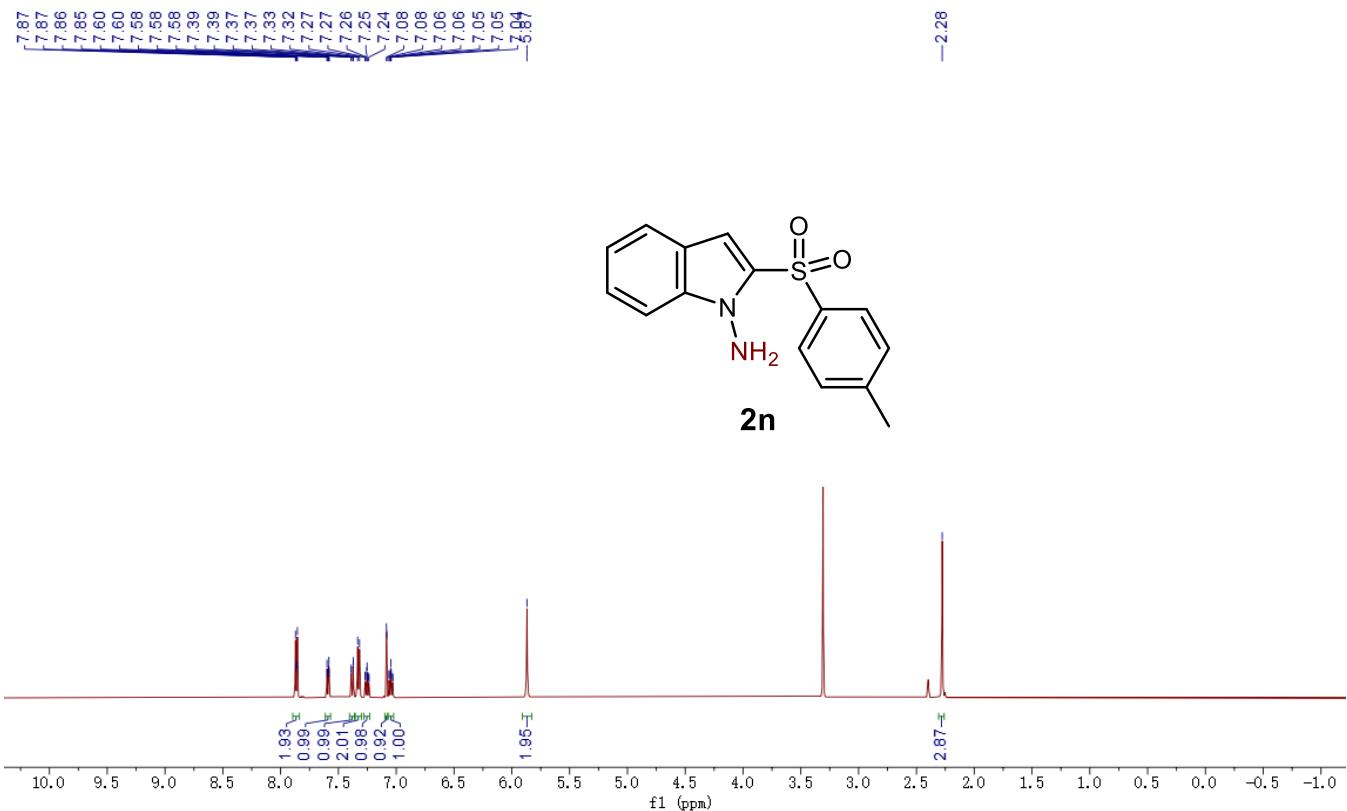


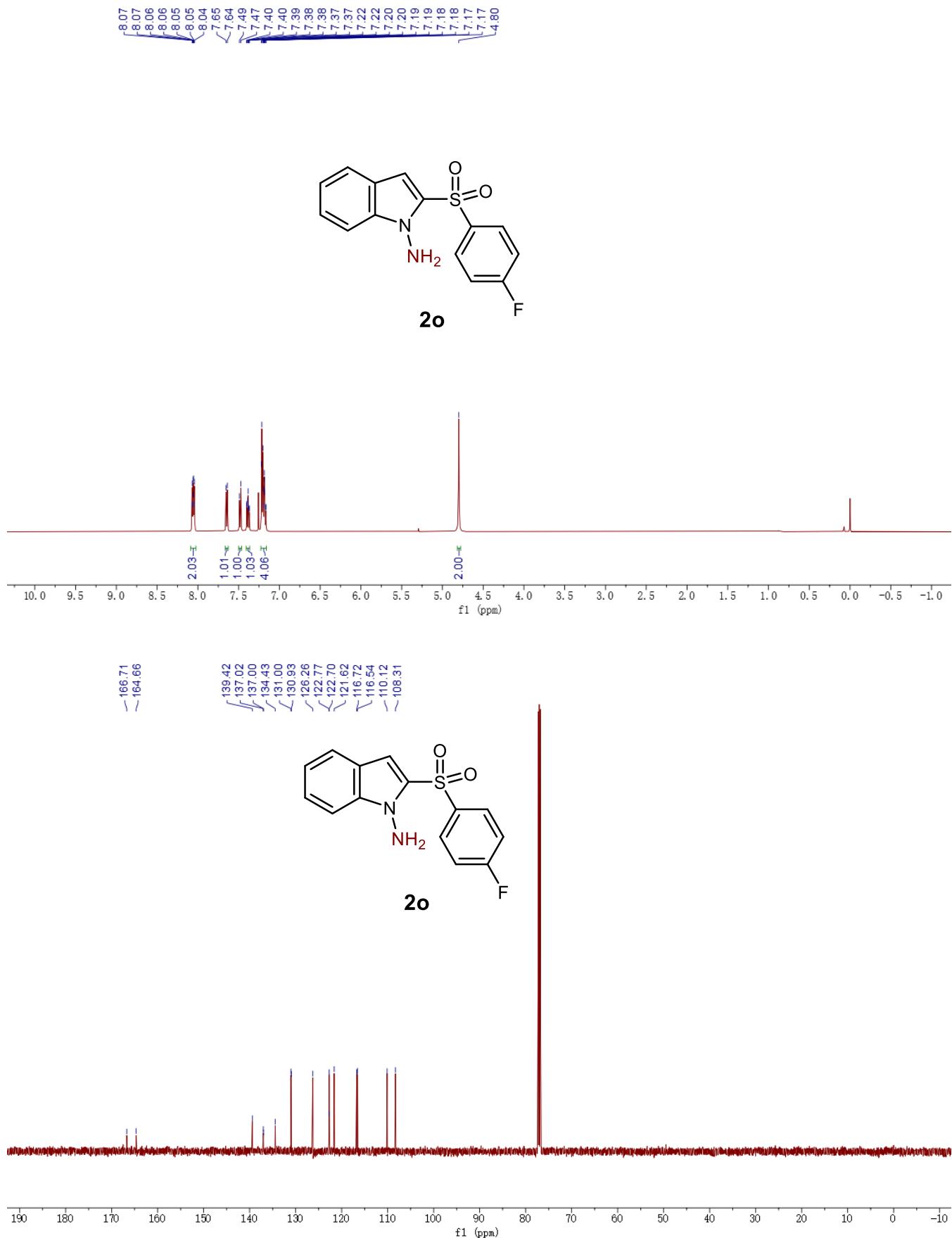
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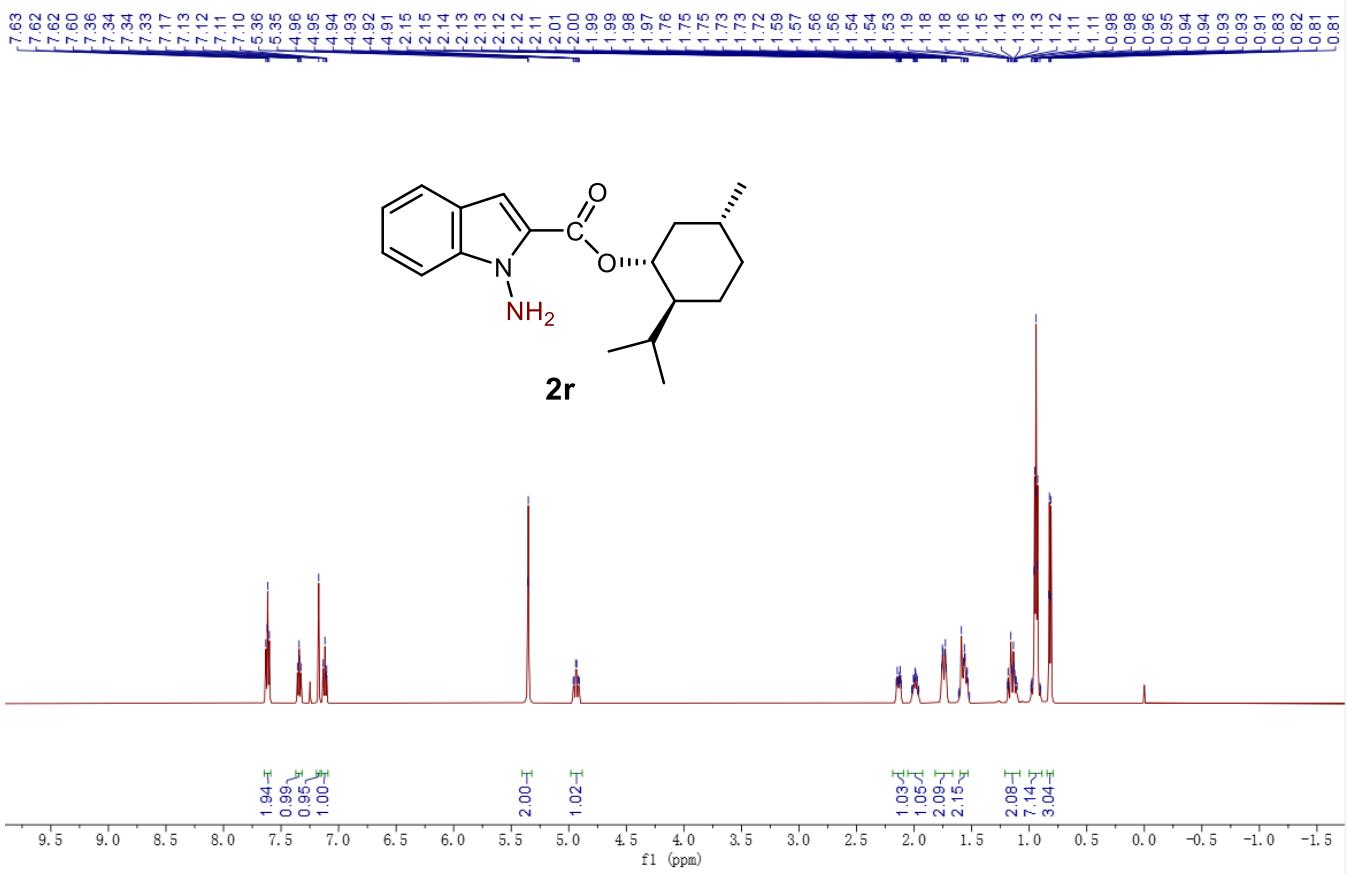
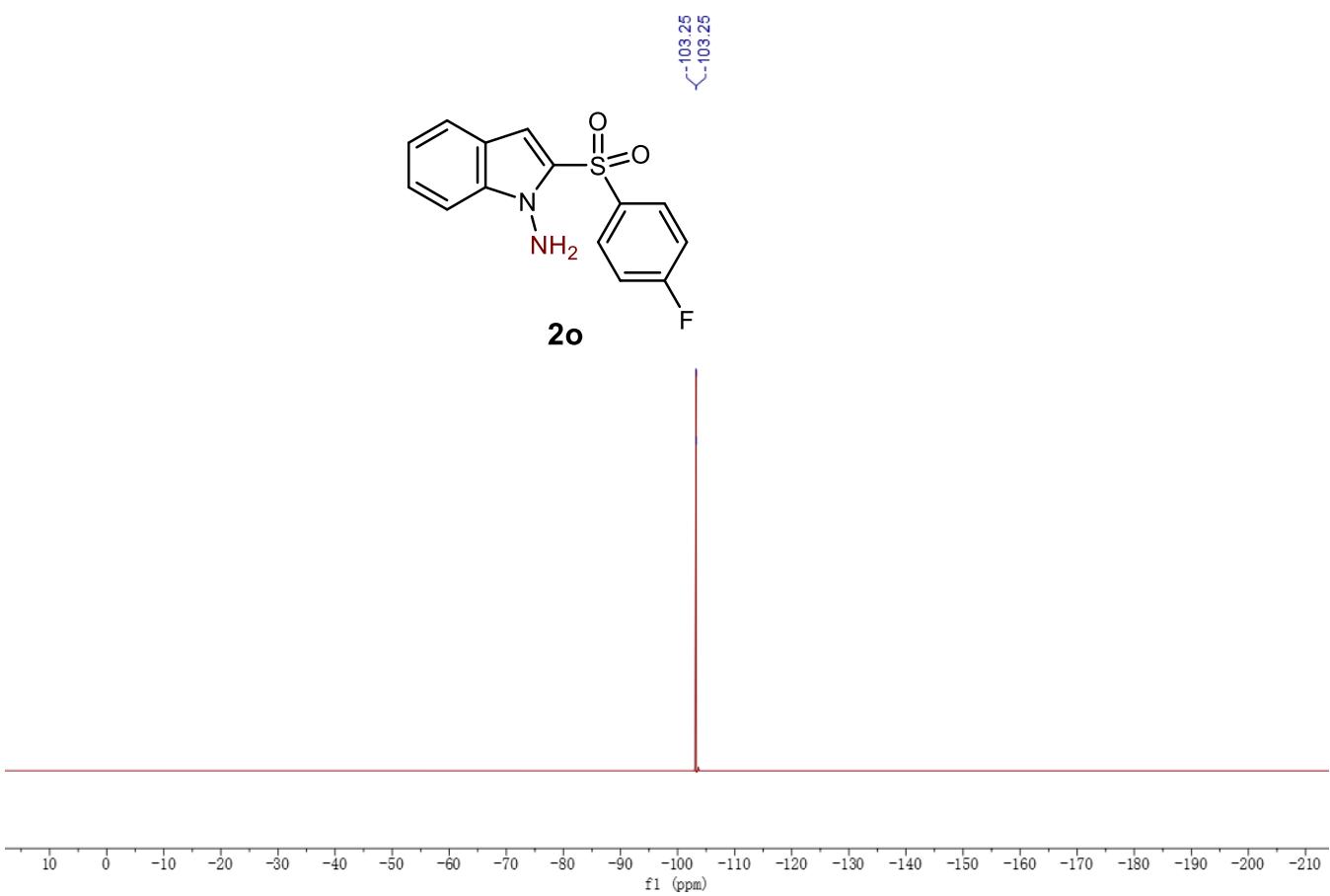


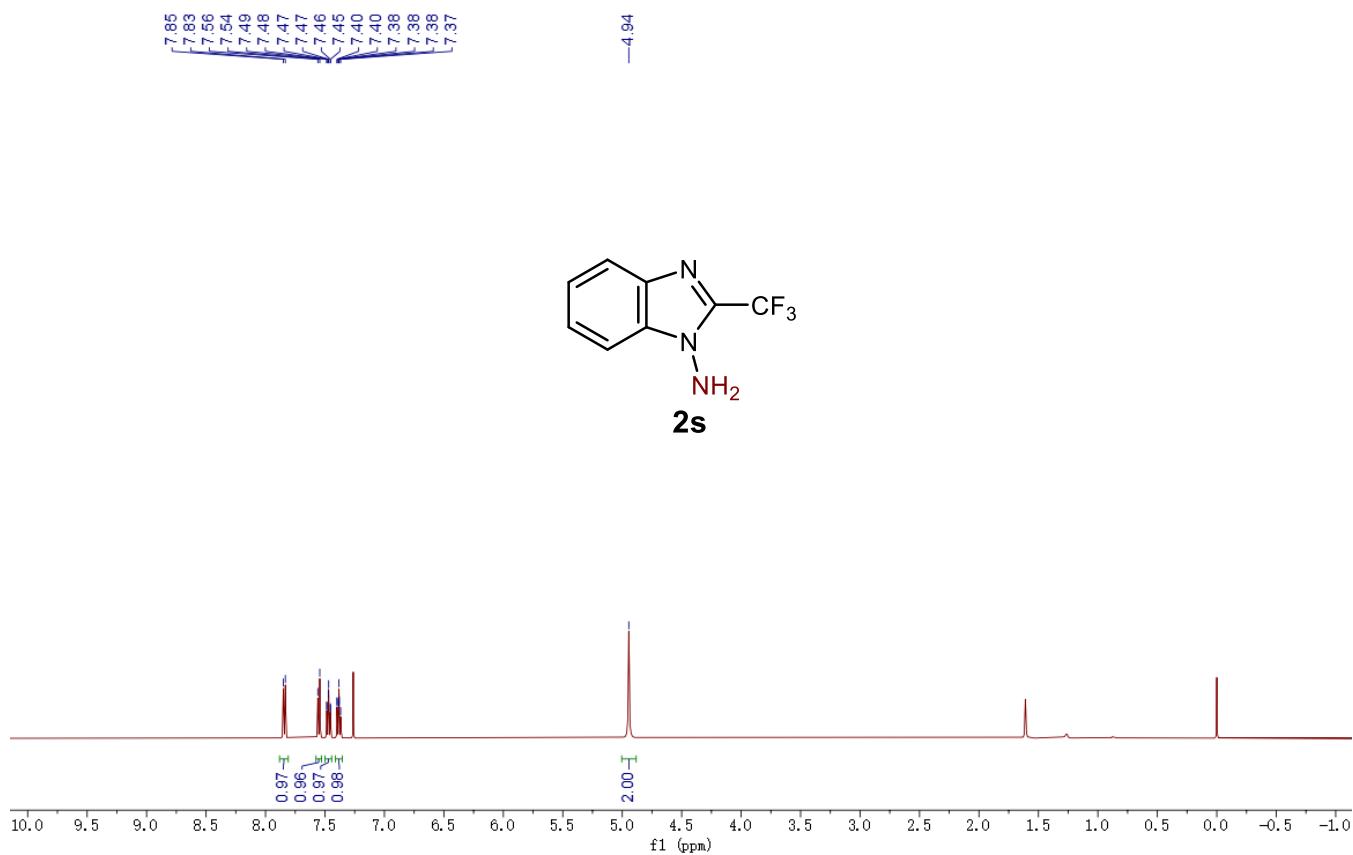
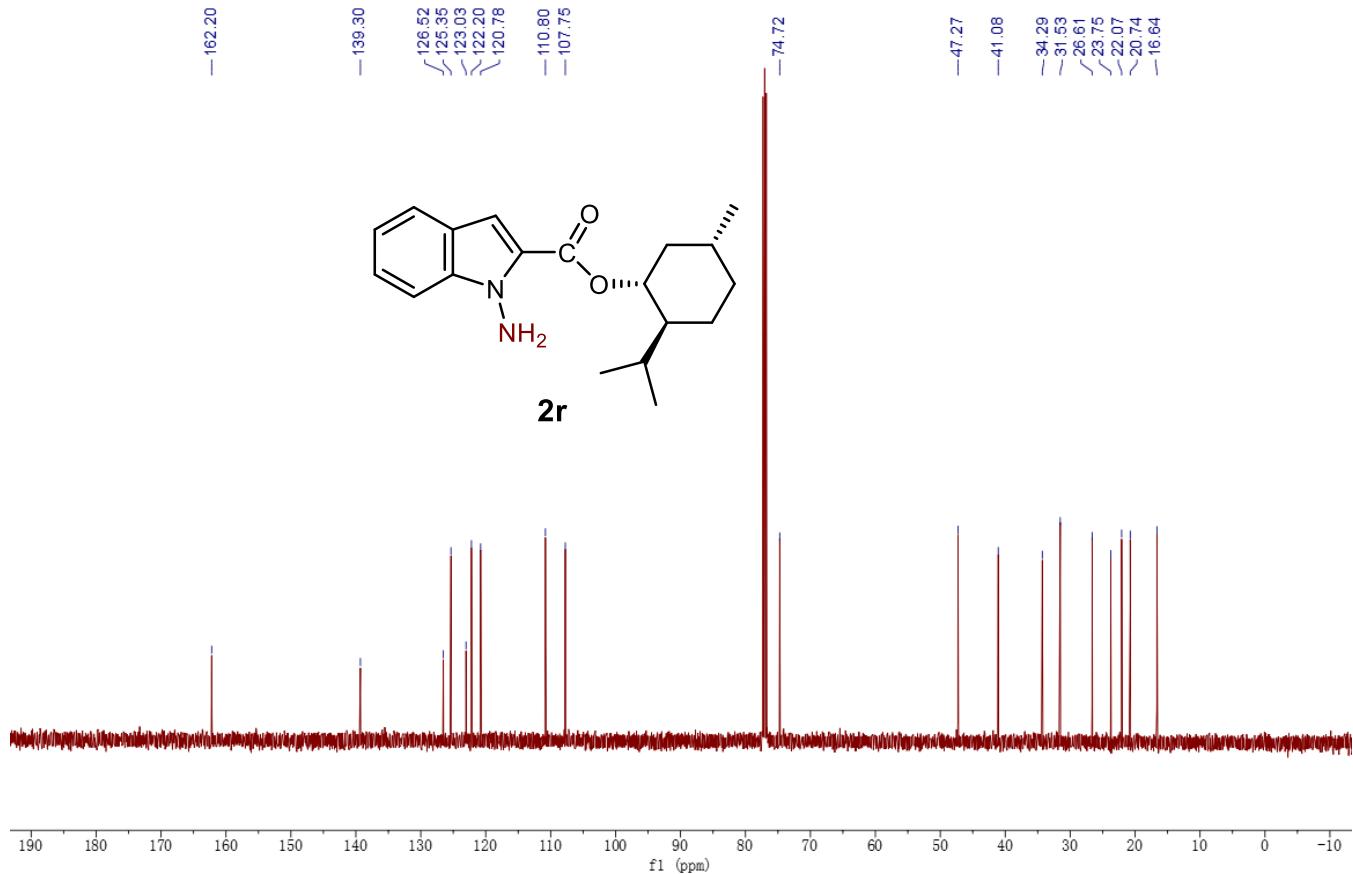


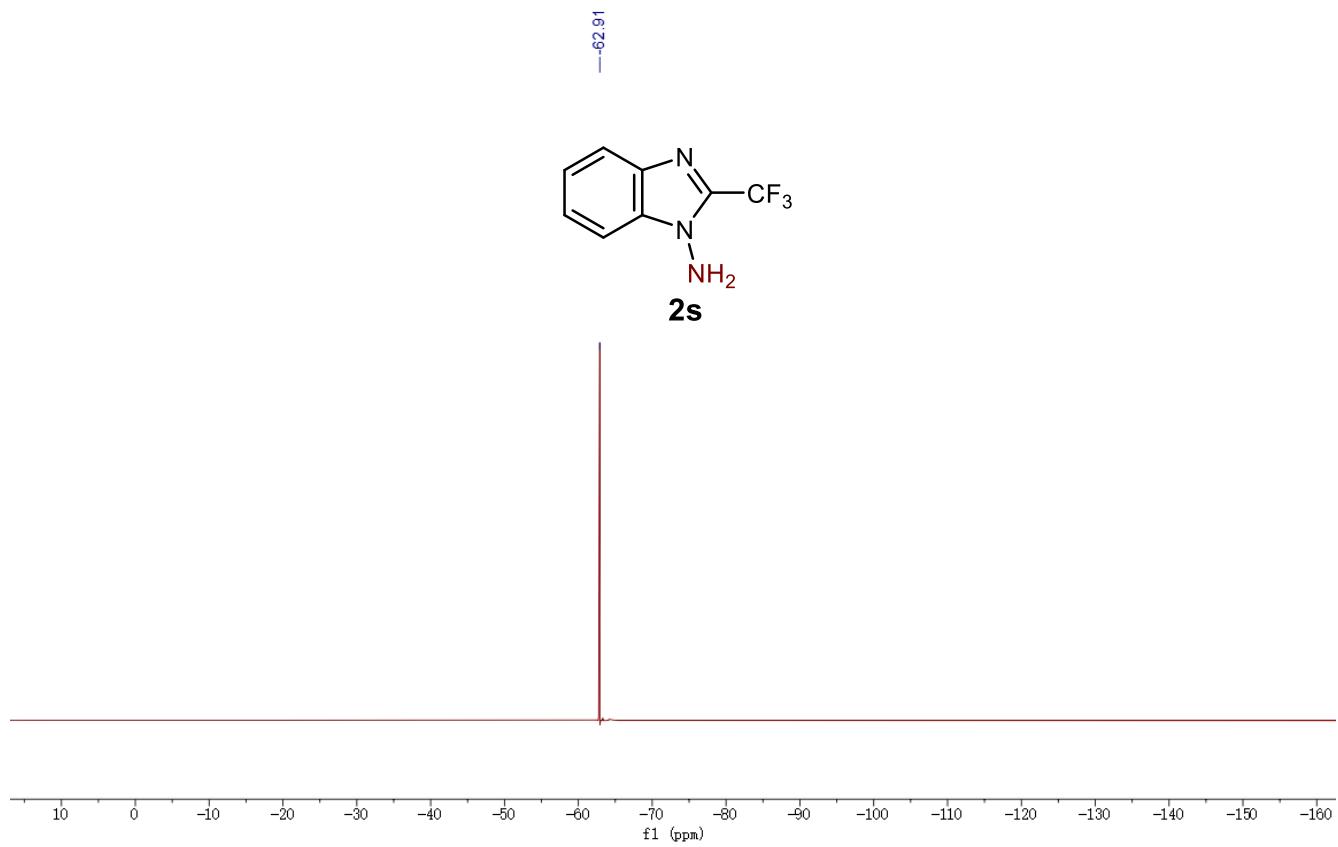
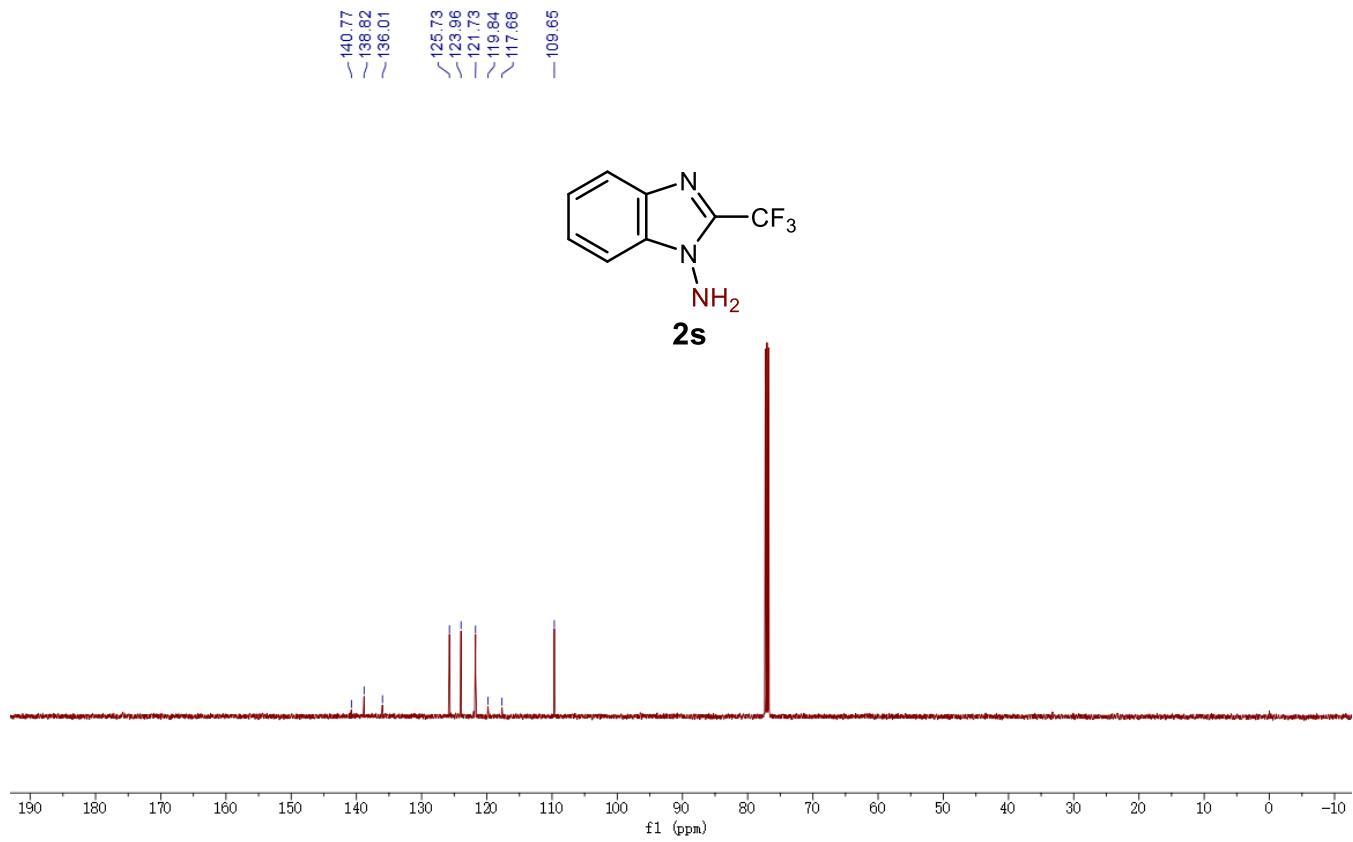


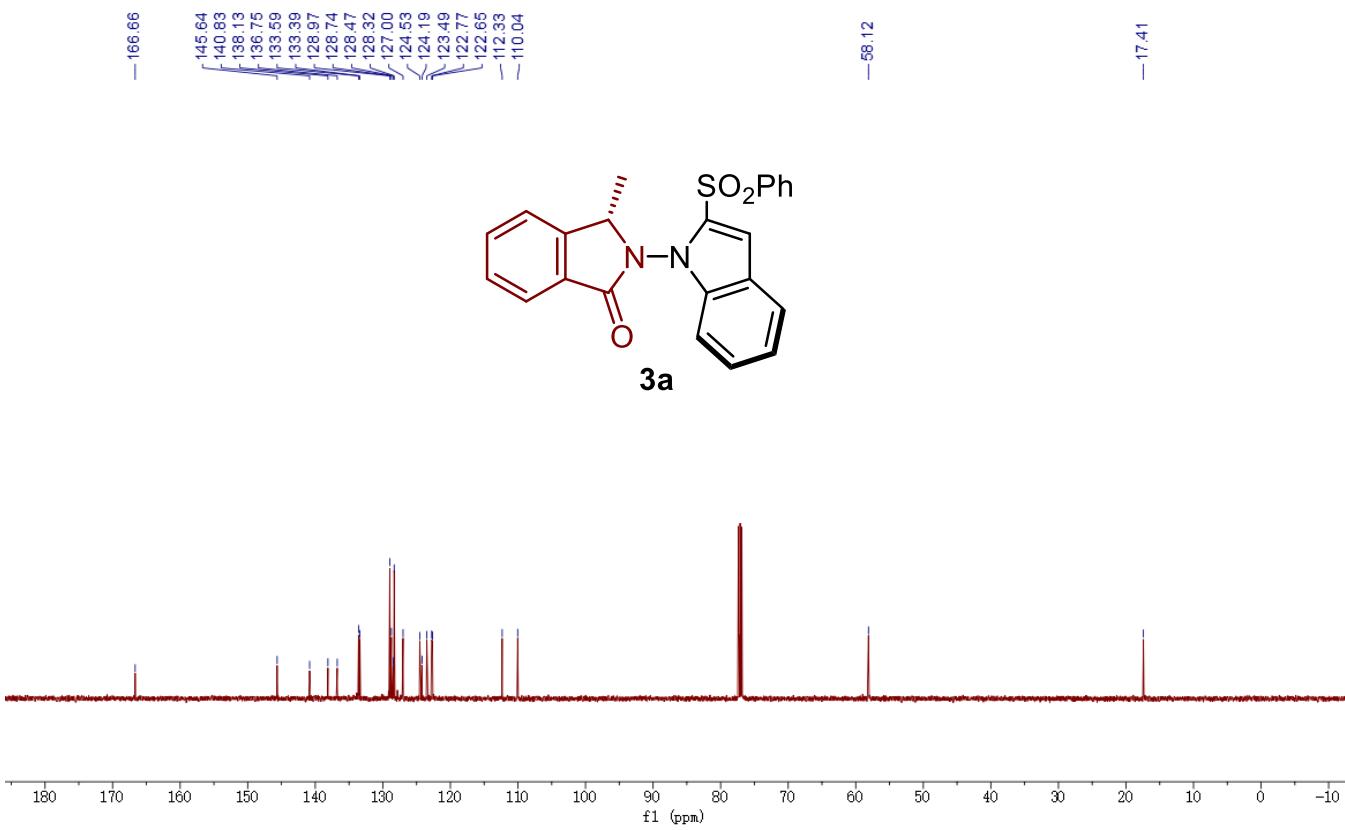
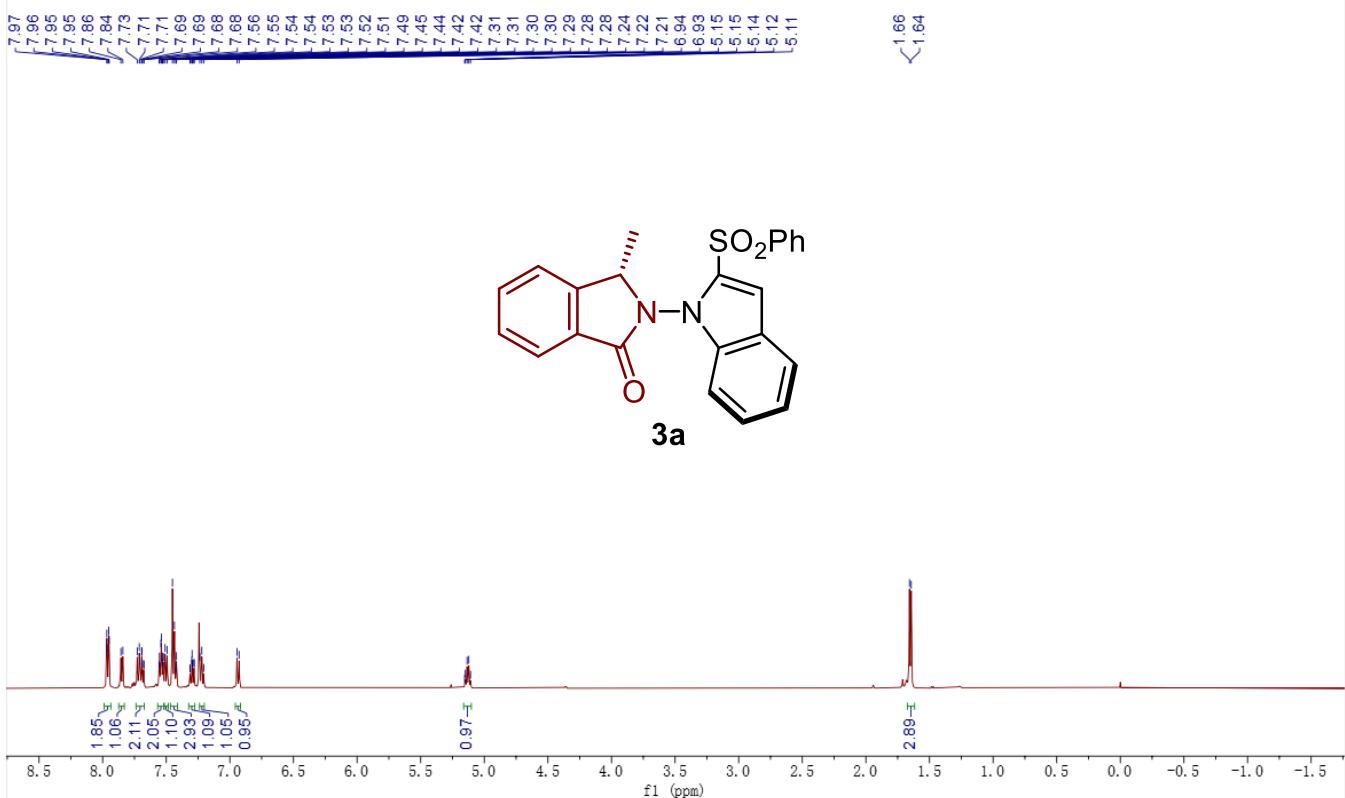


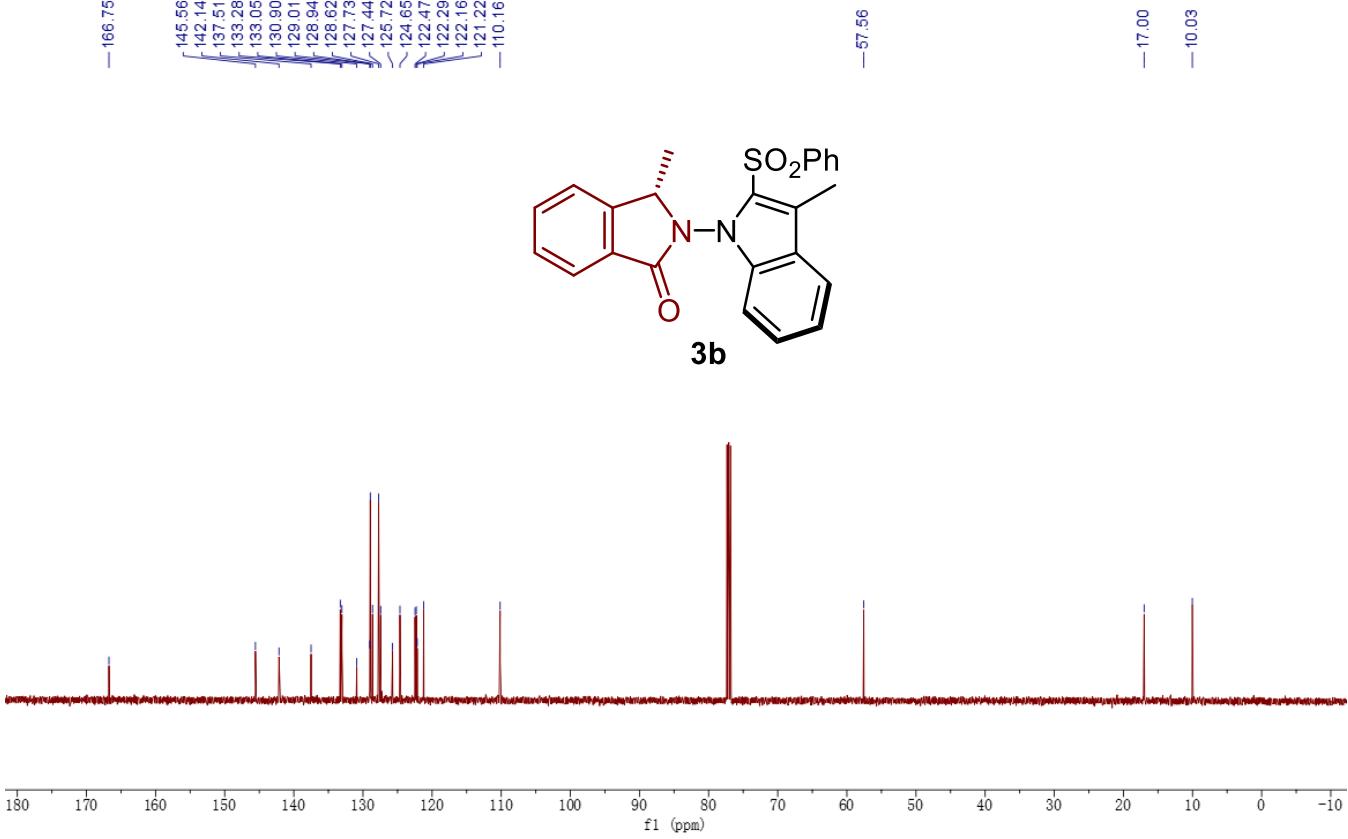
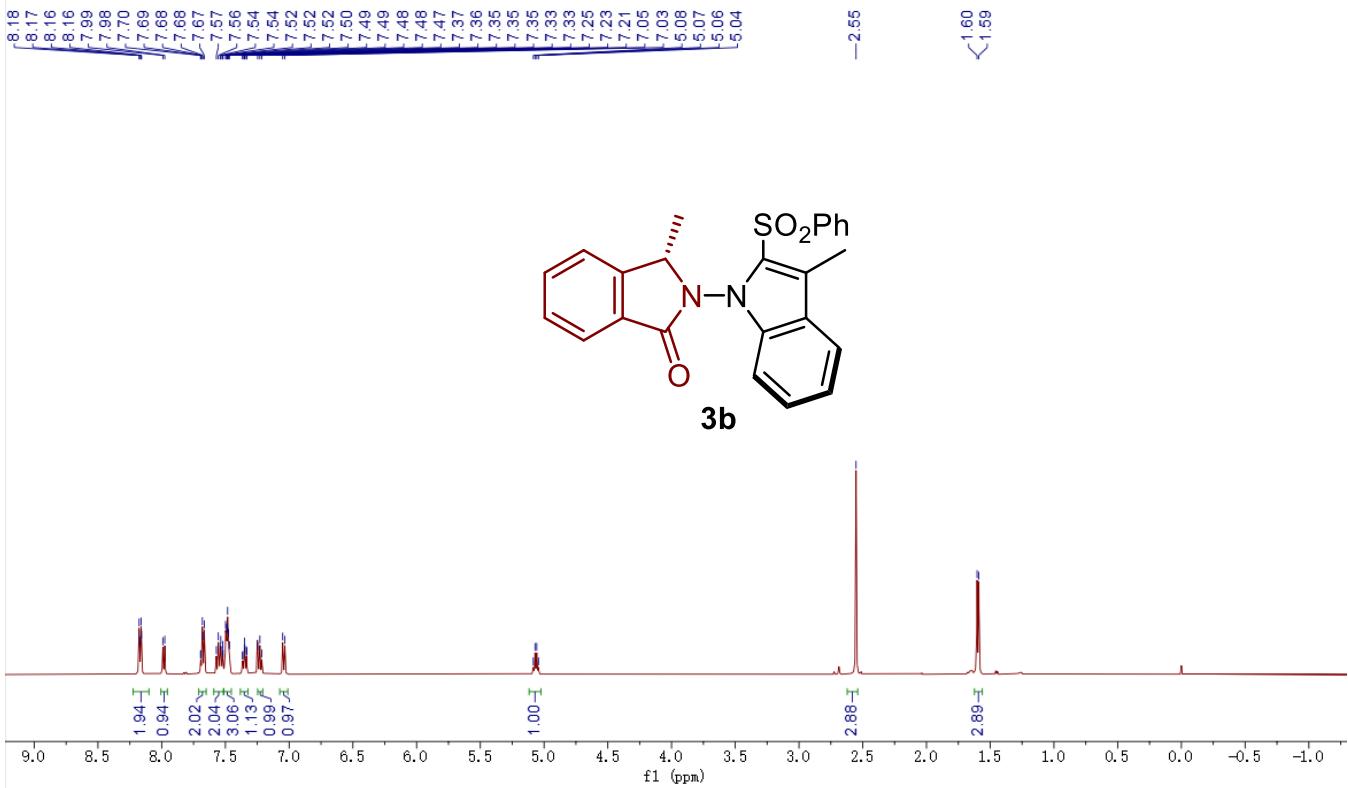


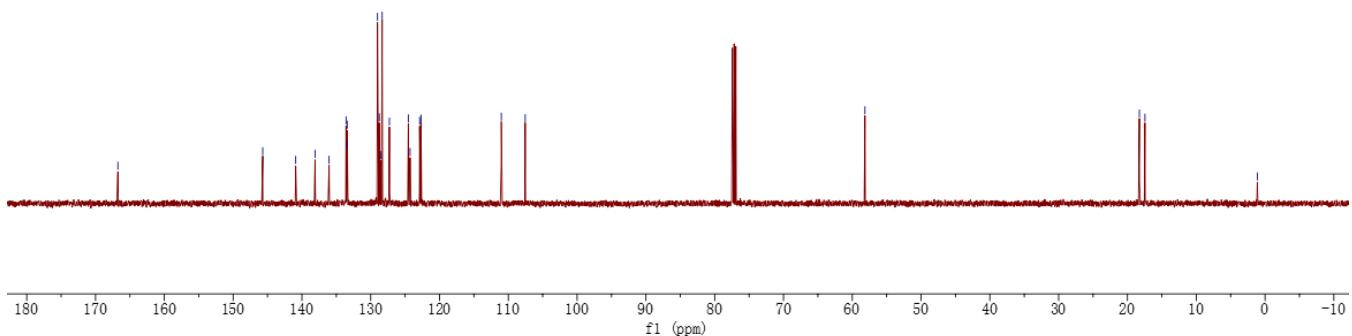
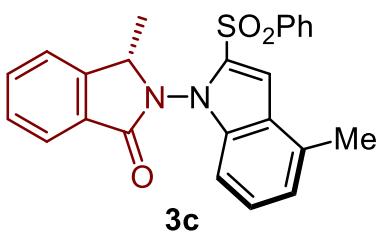
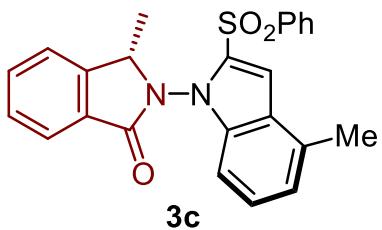
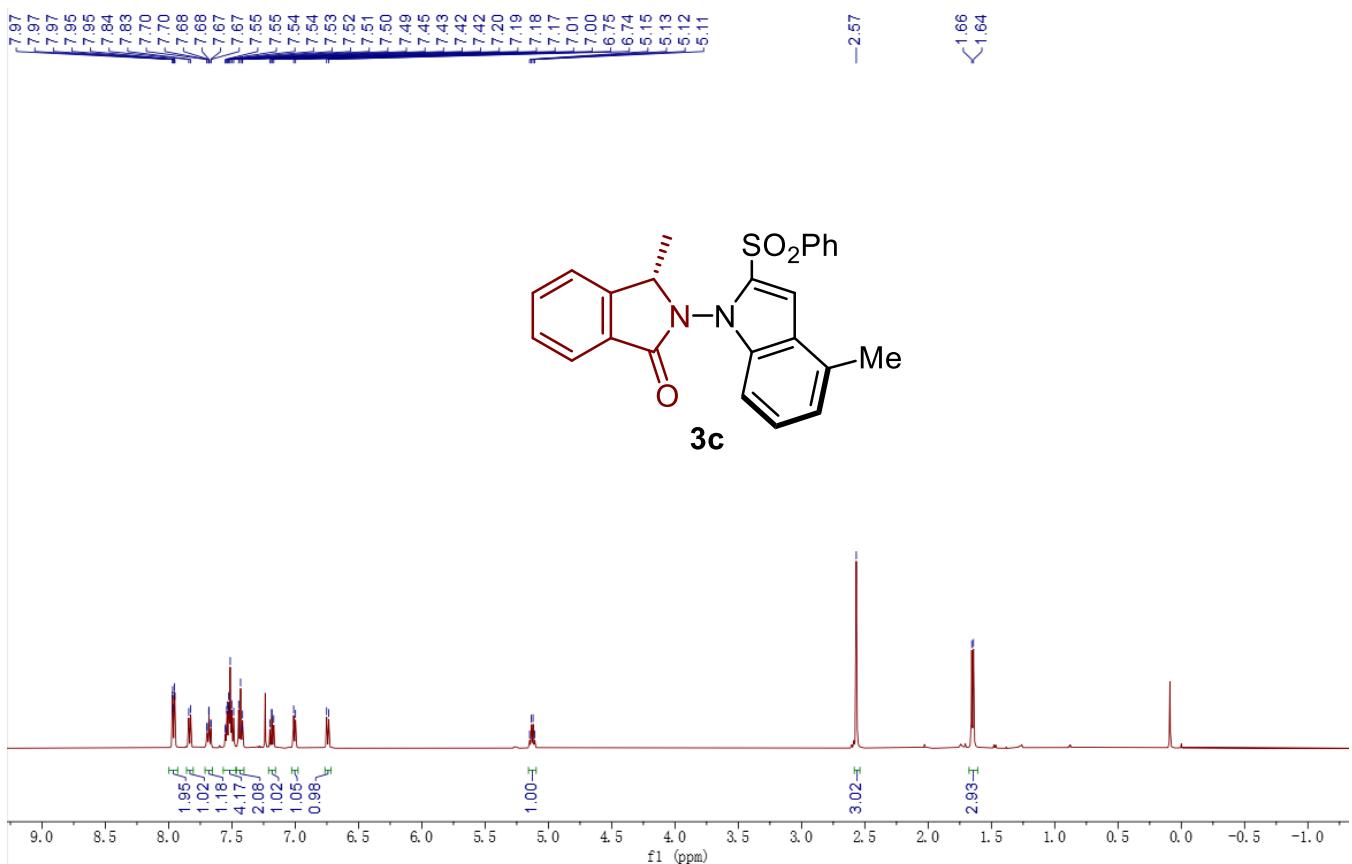


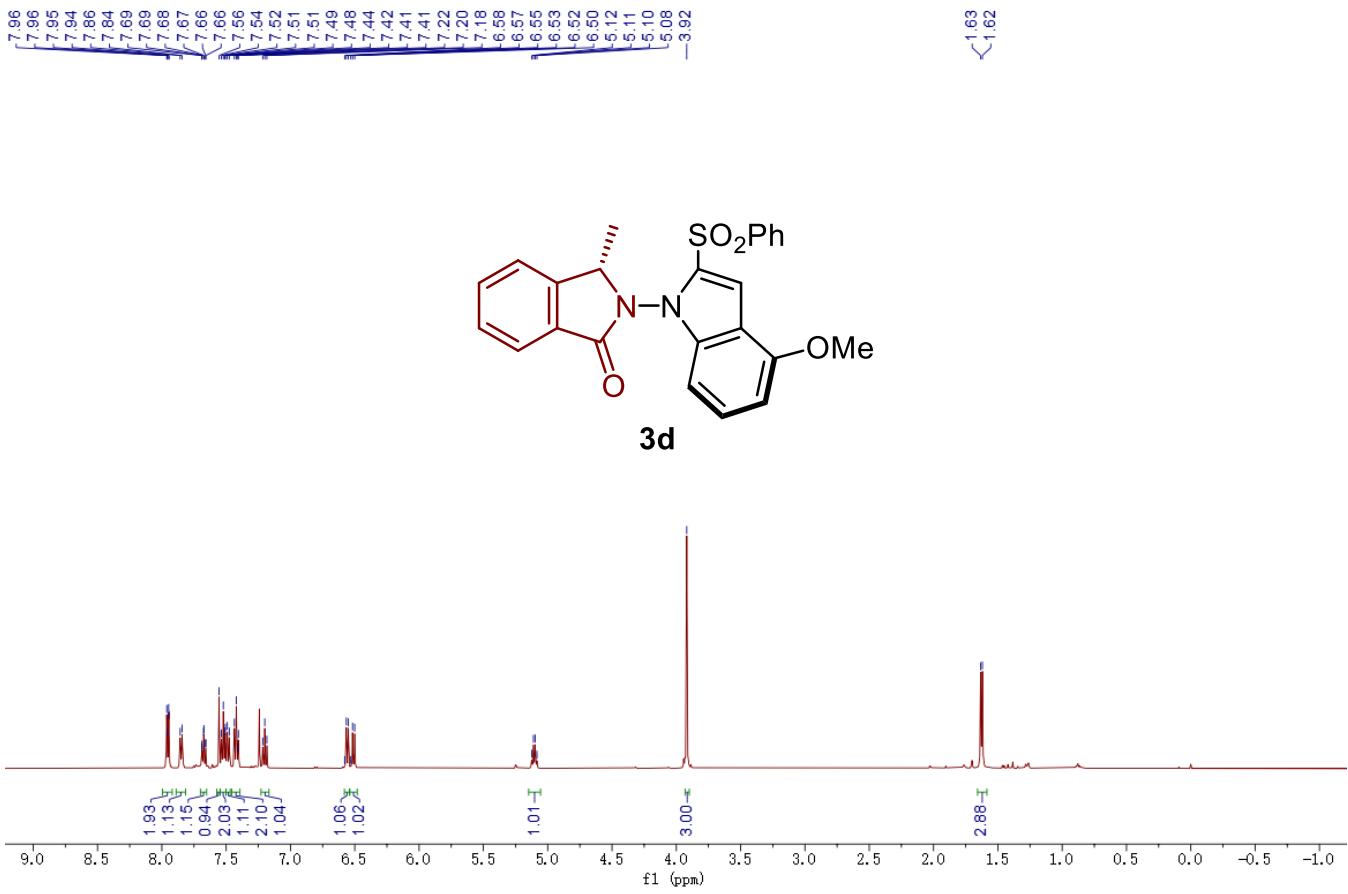




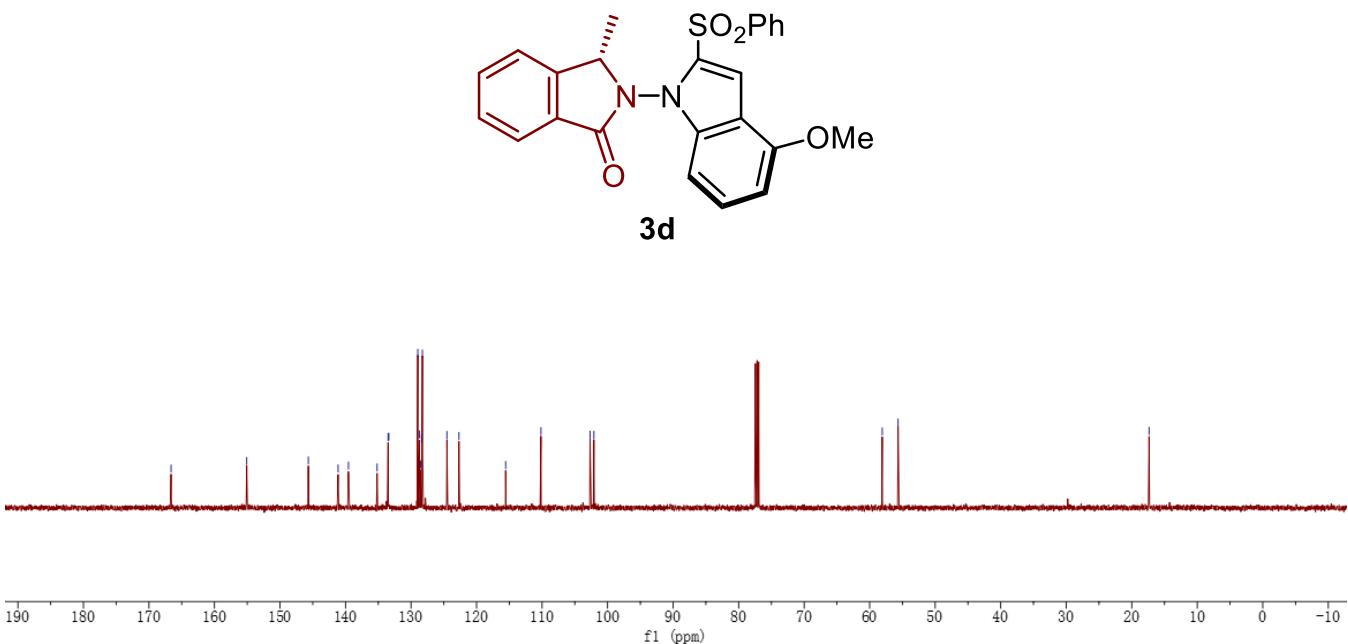


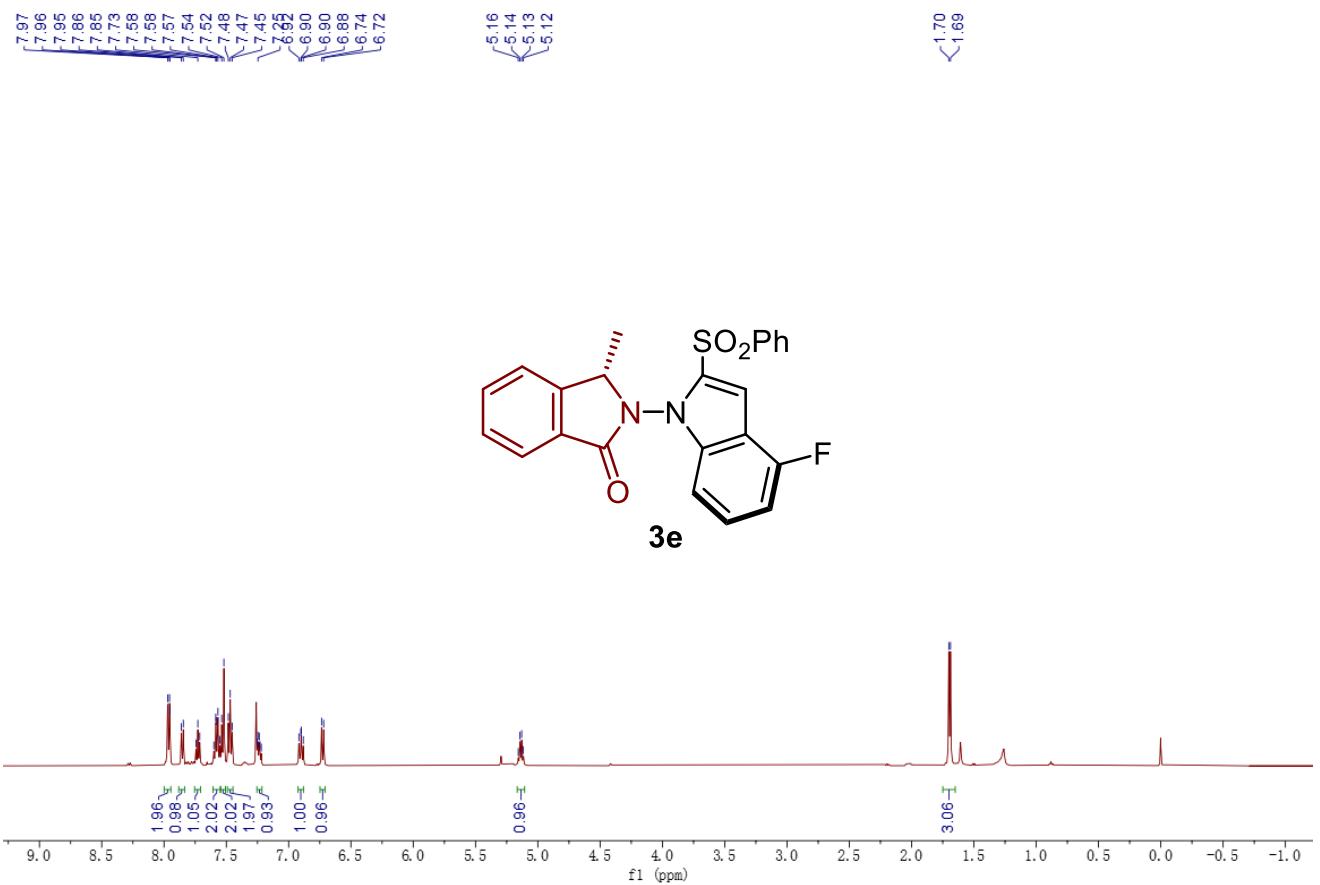


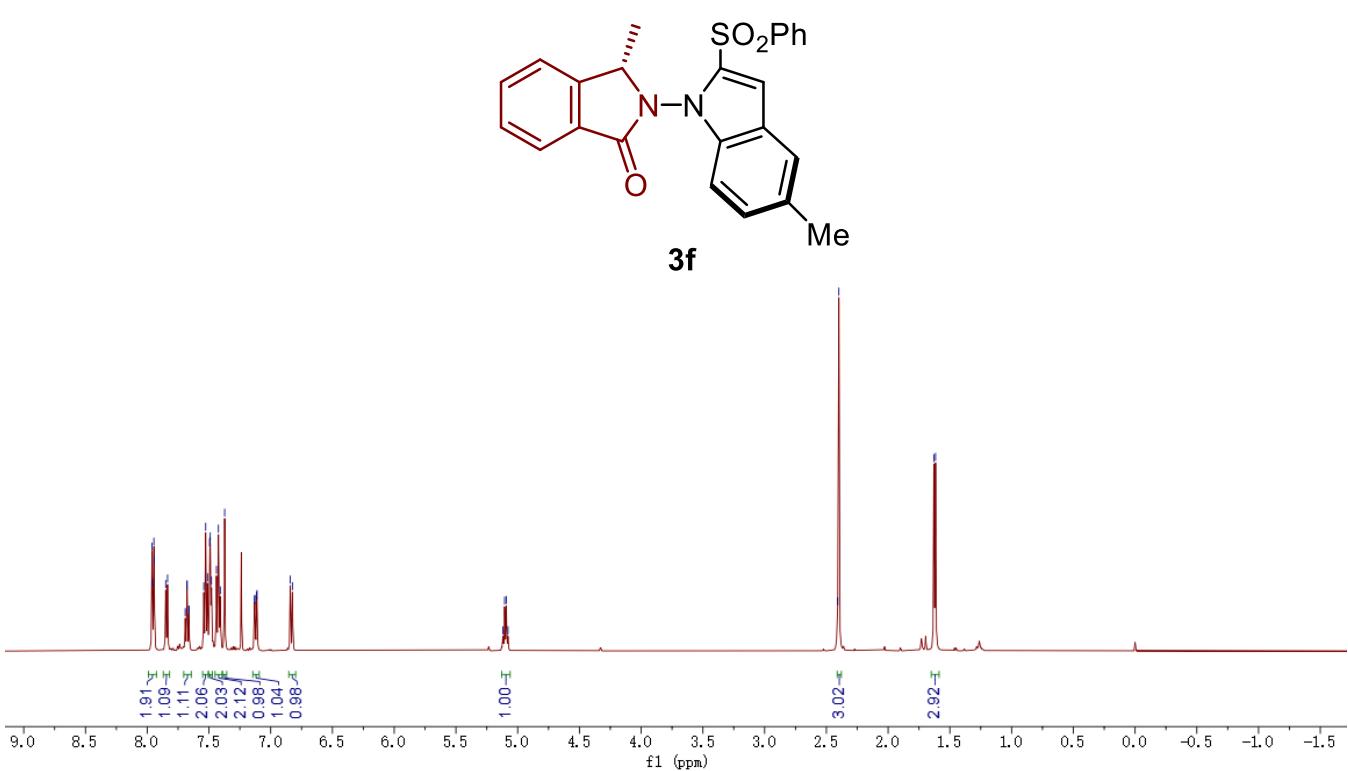
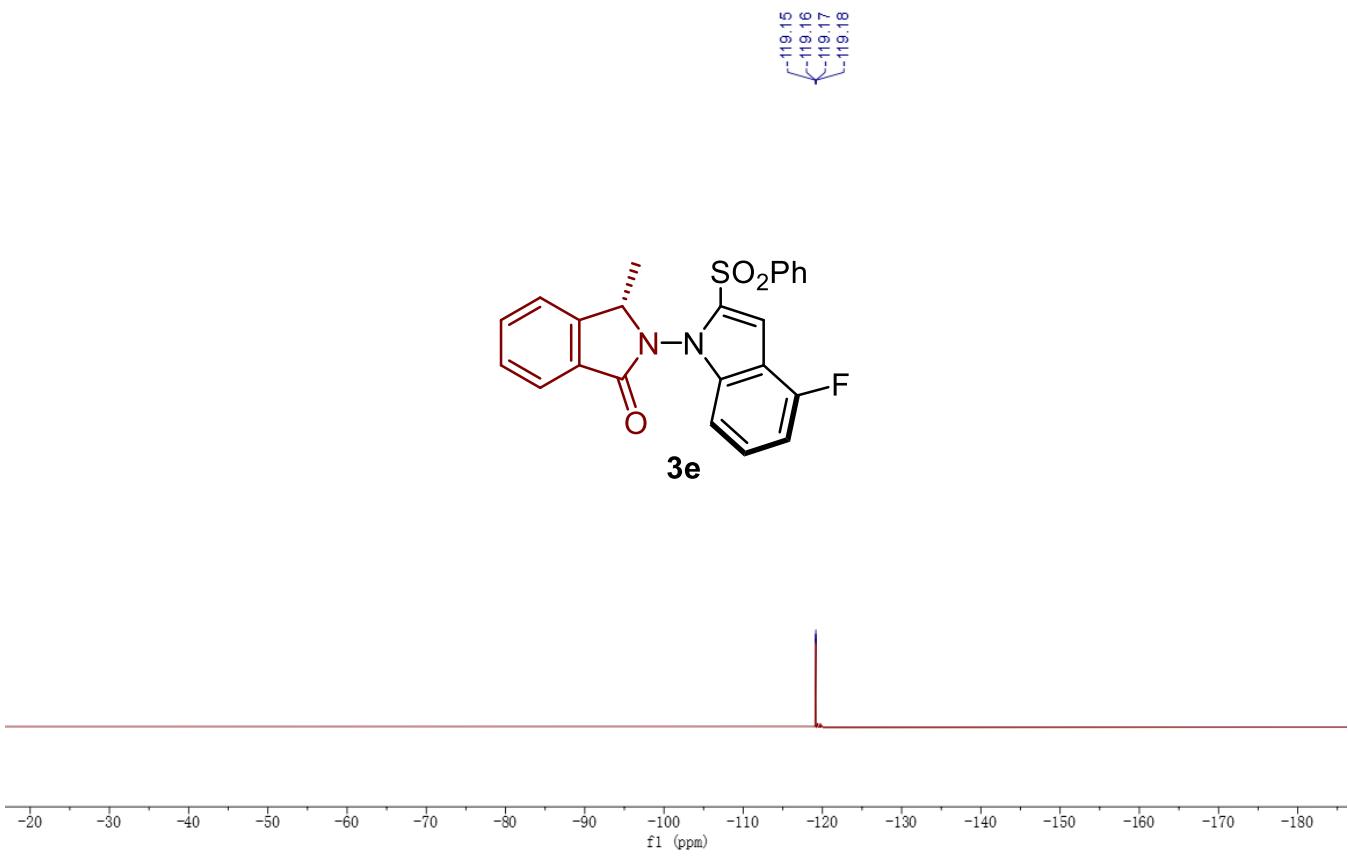


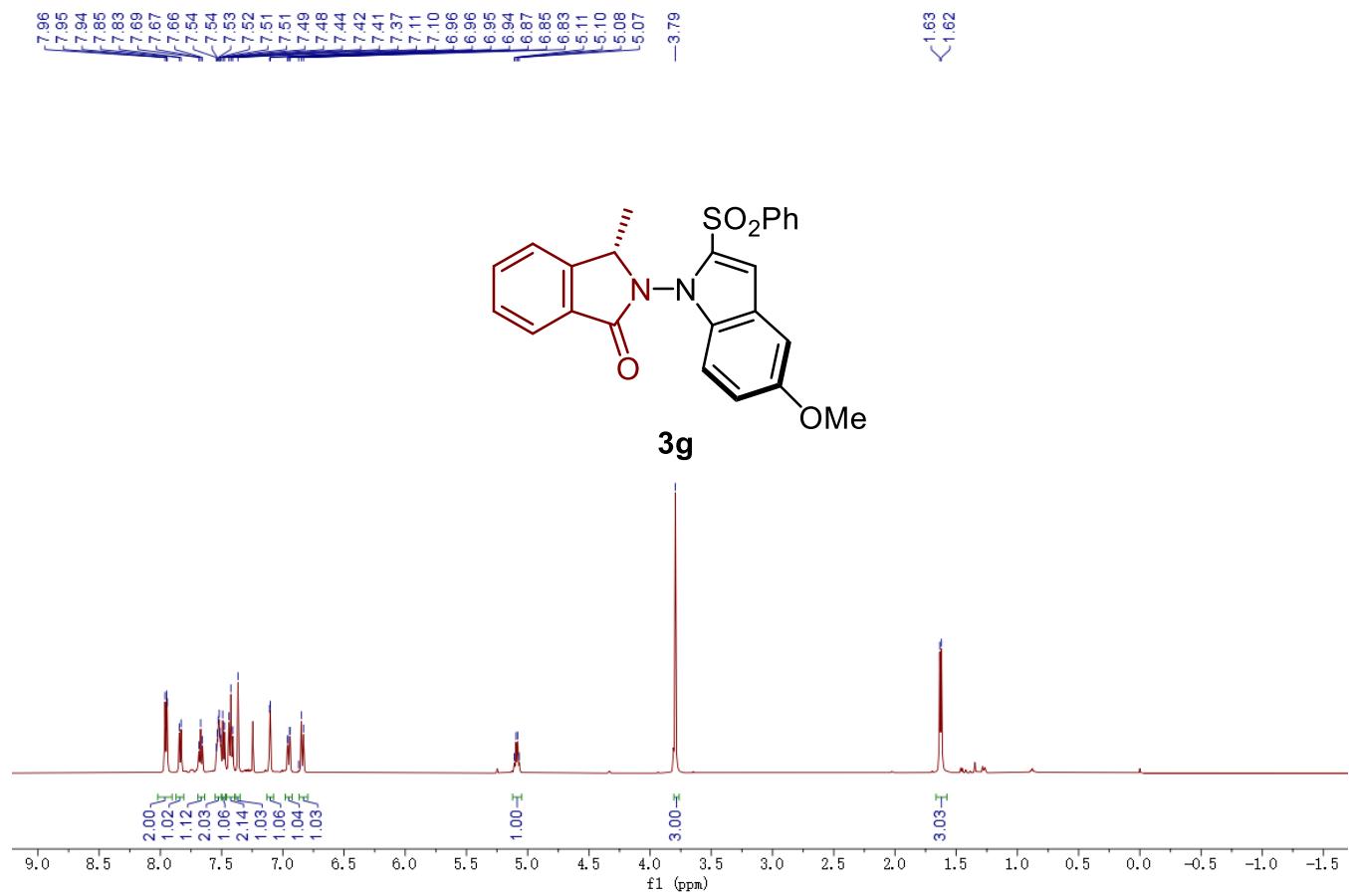
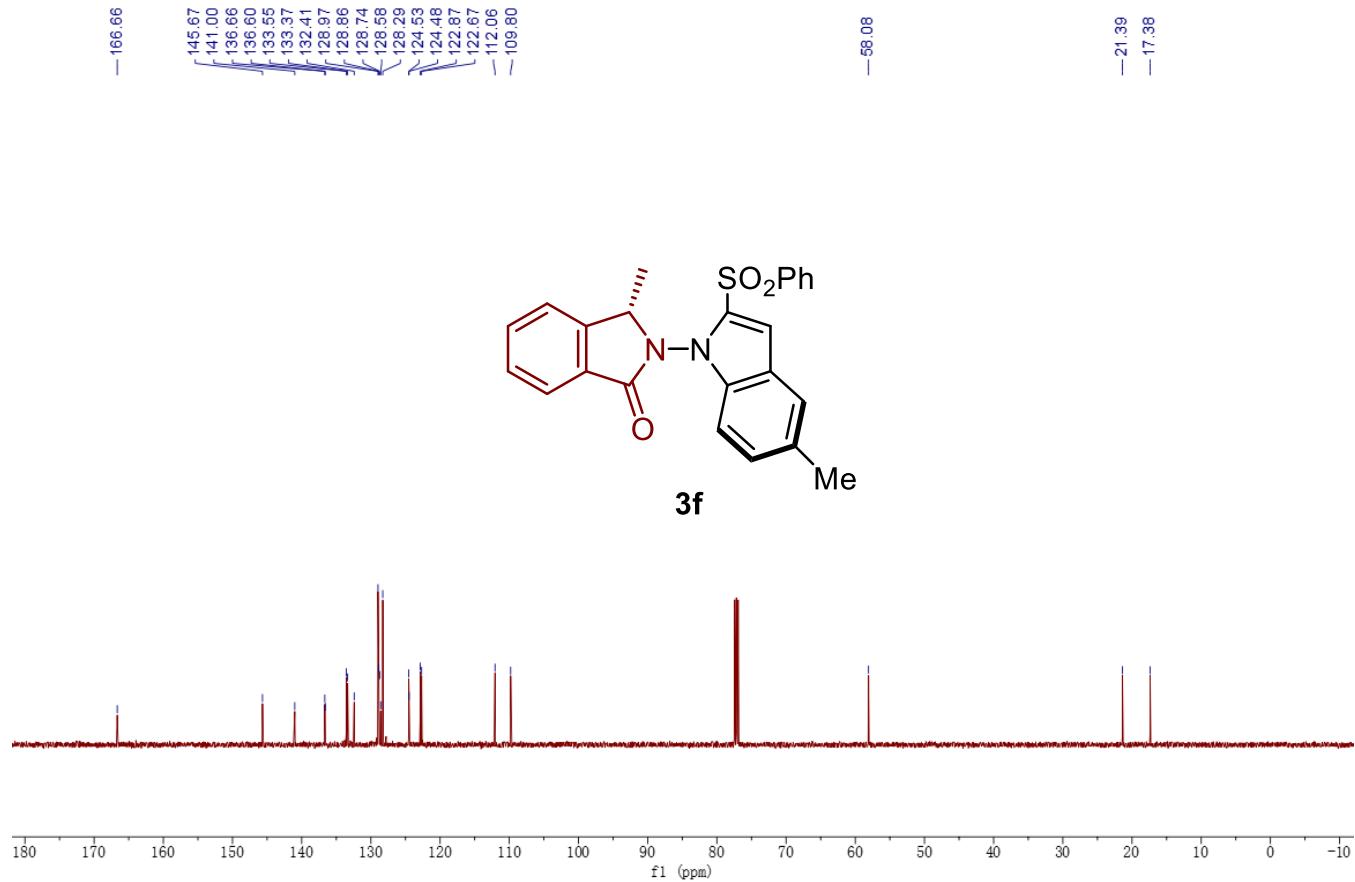


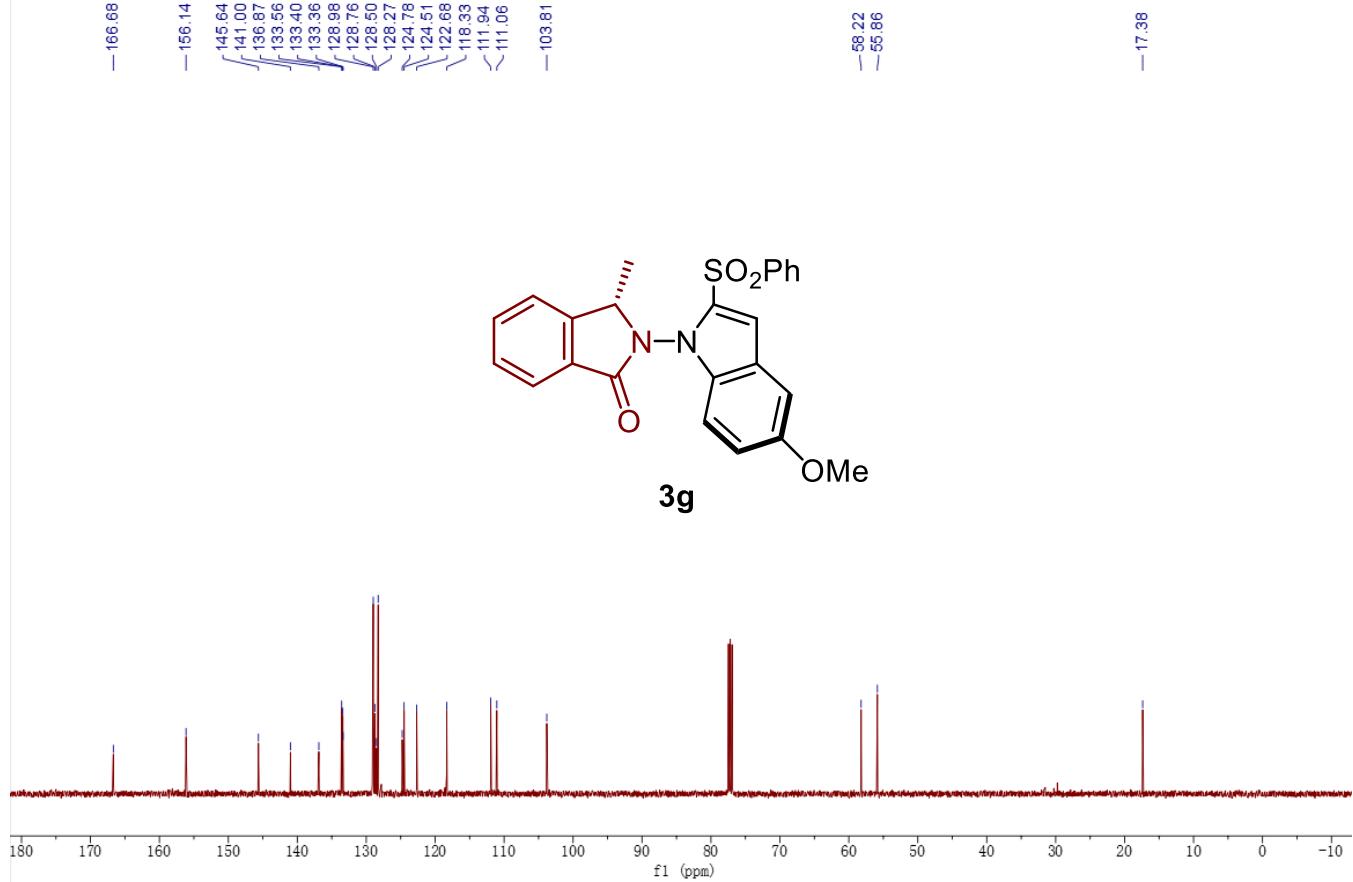
¹H NMR chemical shifts (δ, ppm): 166.63, 155.07, 145.68, 141.13, 139.55, 135.17, 133.50, 133.39, 128.97, 128.73, 128.54, 128.40, 128.27, 124.53, 122.68, 110.17, 102.68, <102.09, 3.00, 2.88, 1.62.

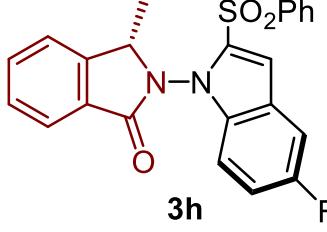




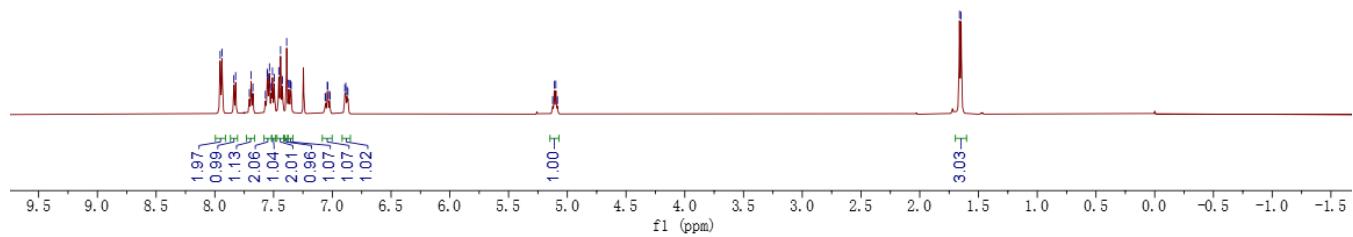


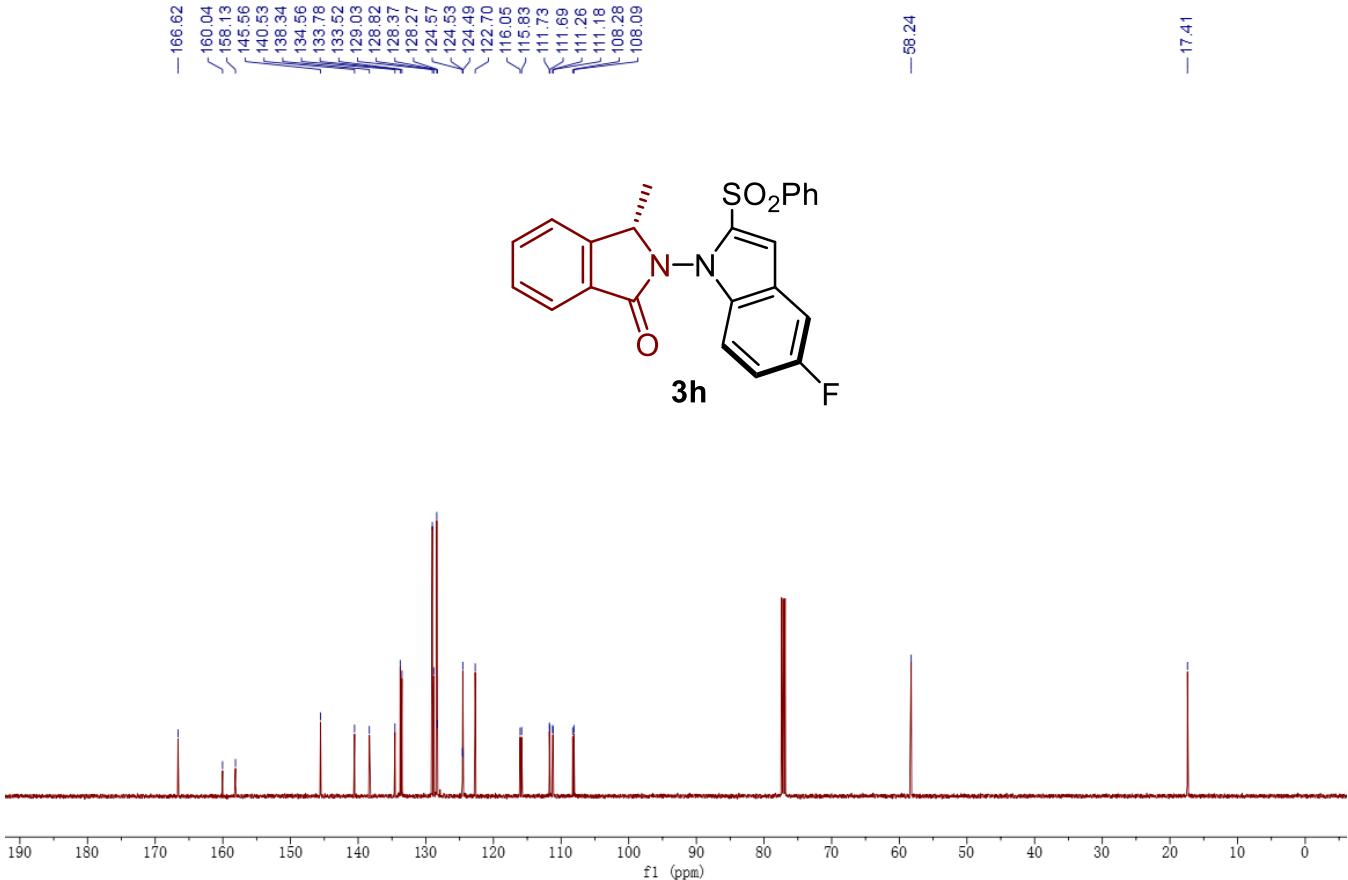




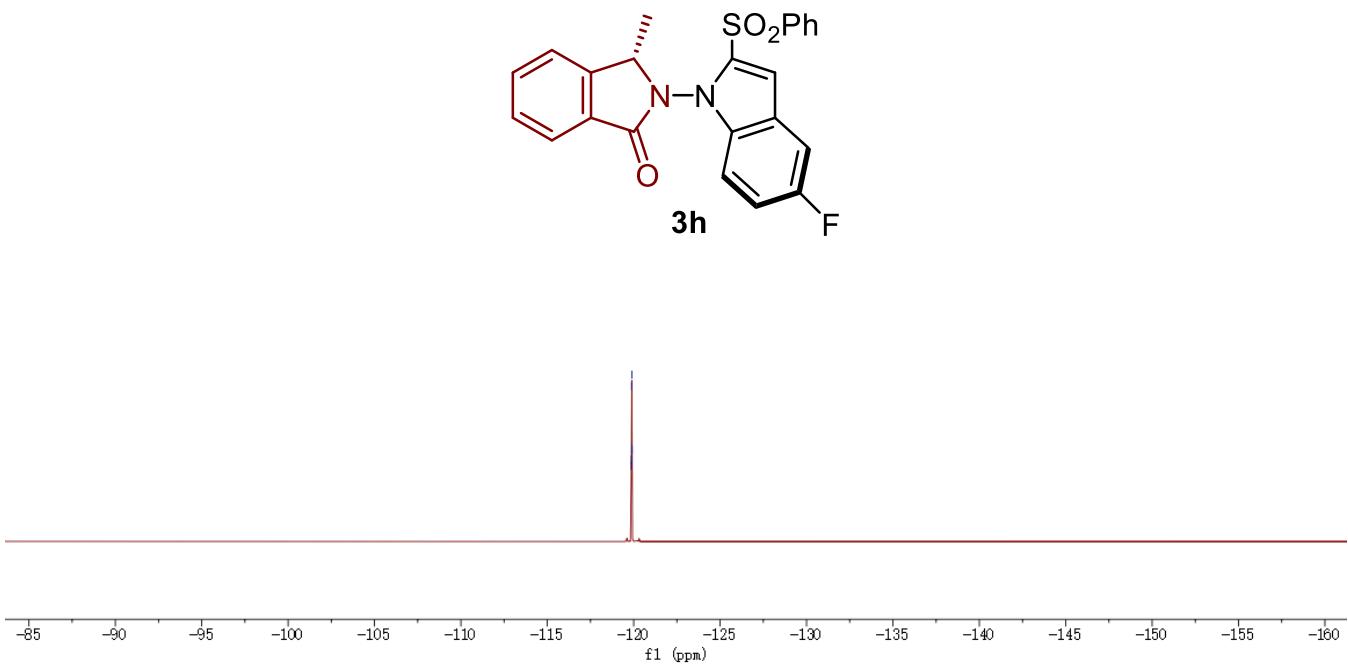


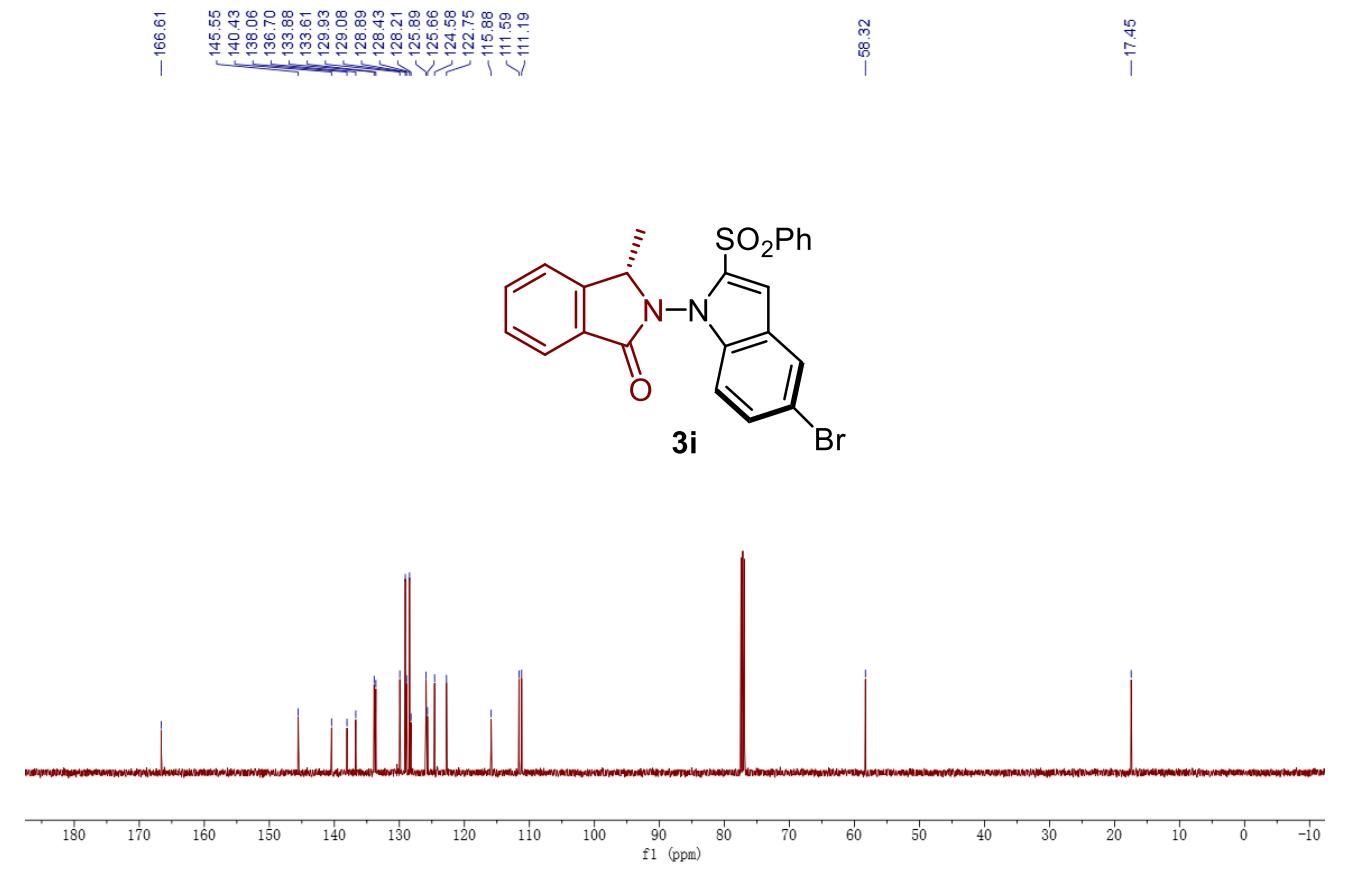
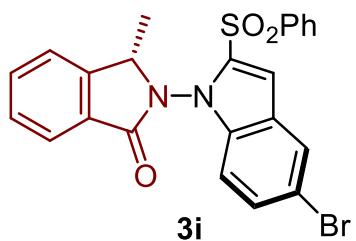
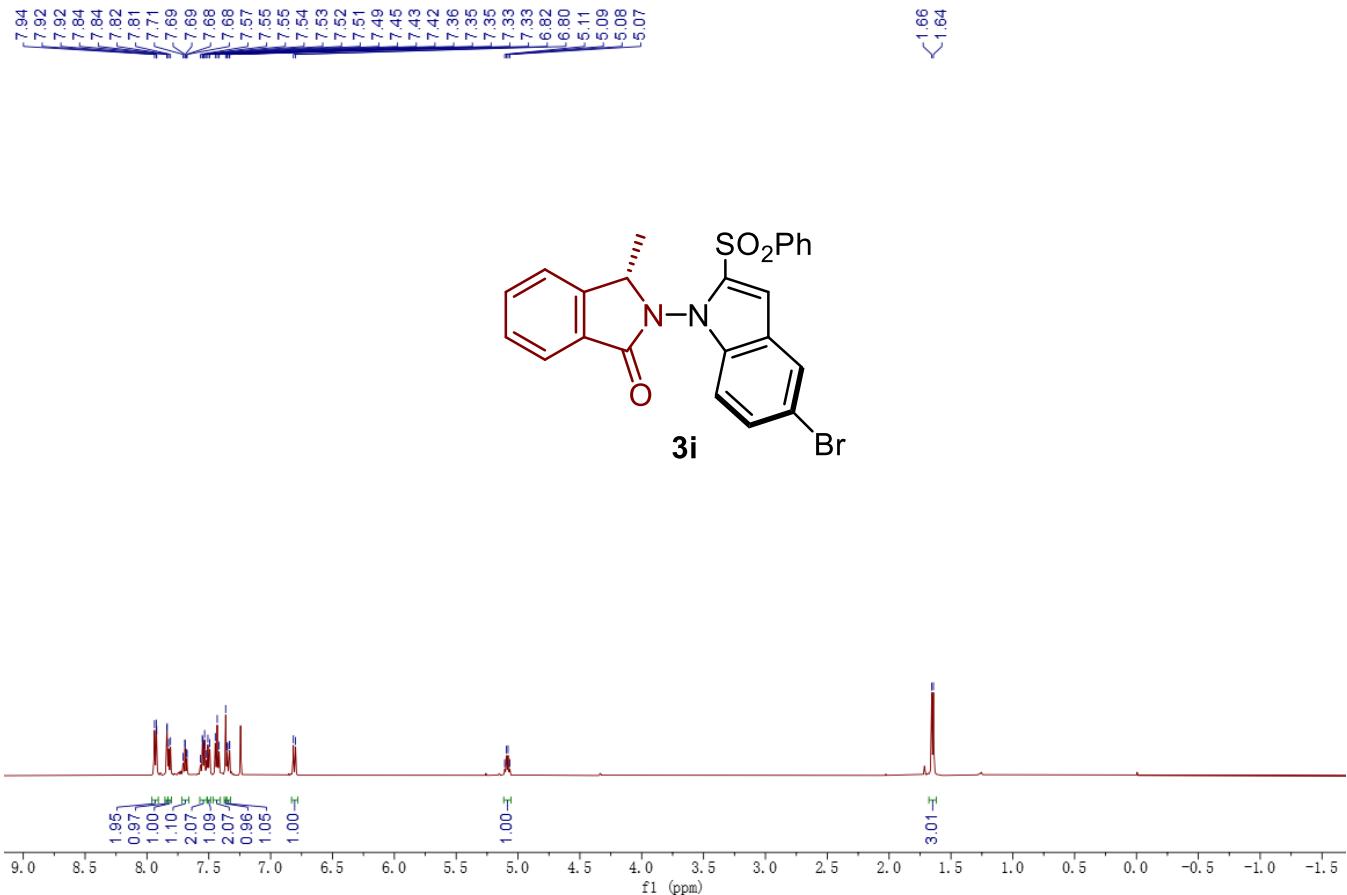
3h

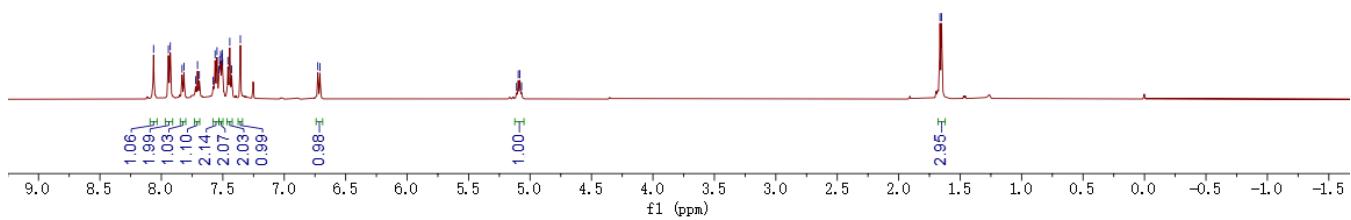
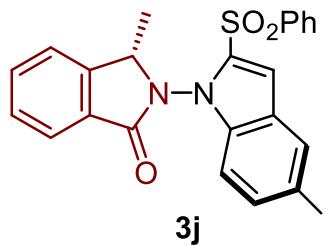




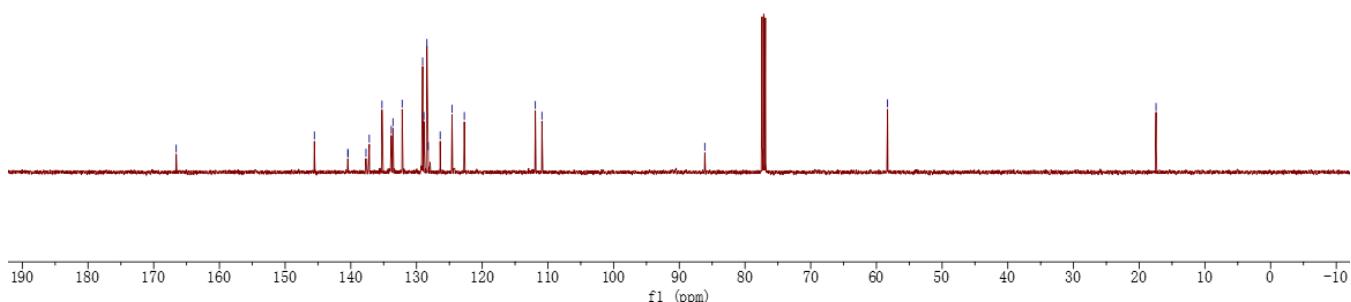
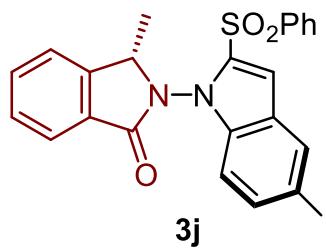
119.86
 119.87
 119.88
 119.89
 119.90
 119.91





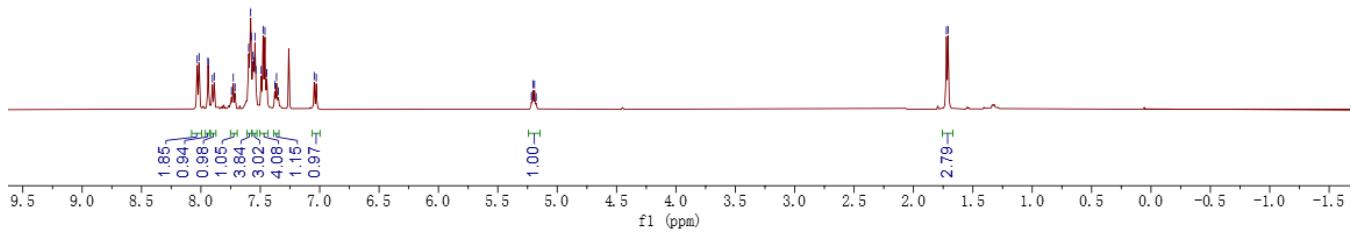
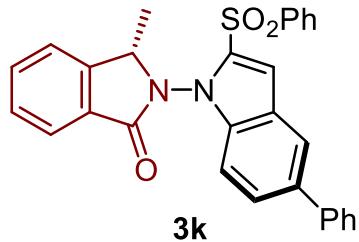


—166.58 —145.55 —140.46 —140.43 —137.69 —137.19 —135.26 —133.85 —133.58 —132.18 —129.07 —128.88 —128.42 —128.23 —126.40 —124.59 —122.72 —111.91 —110.91
—86.12 —58.30 —17.44





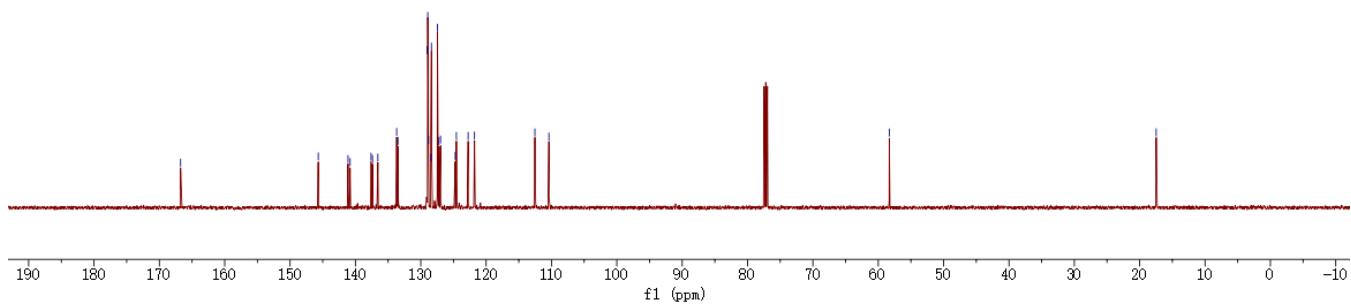
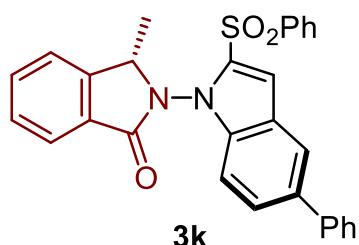
$<^{1.72}$
 $^{1.71}$

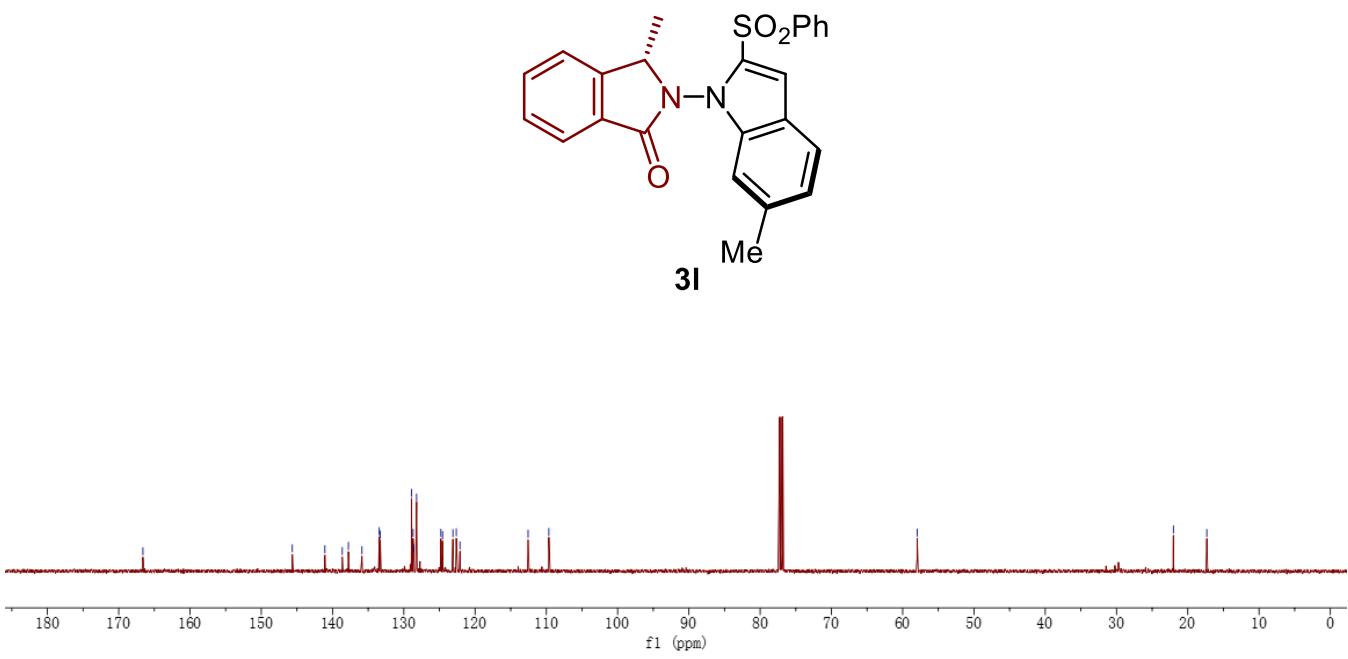
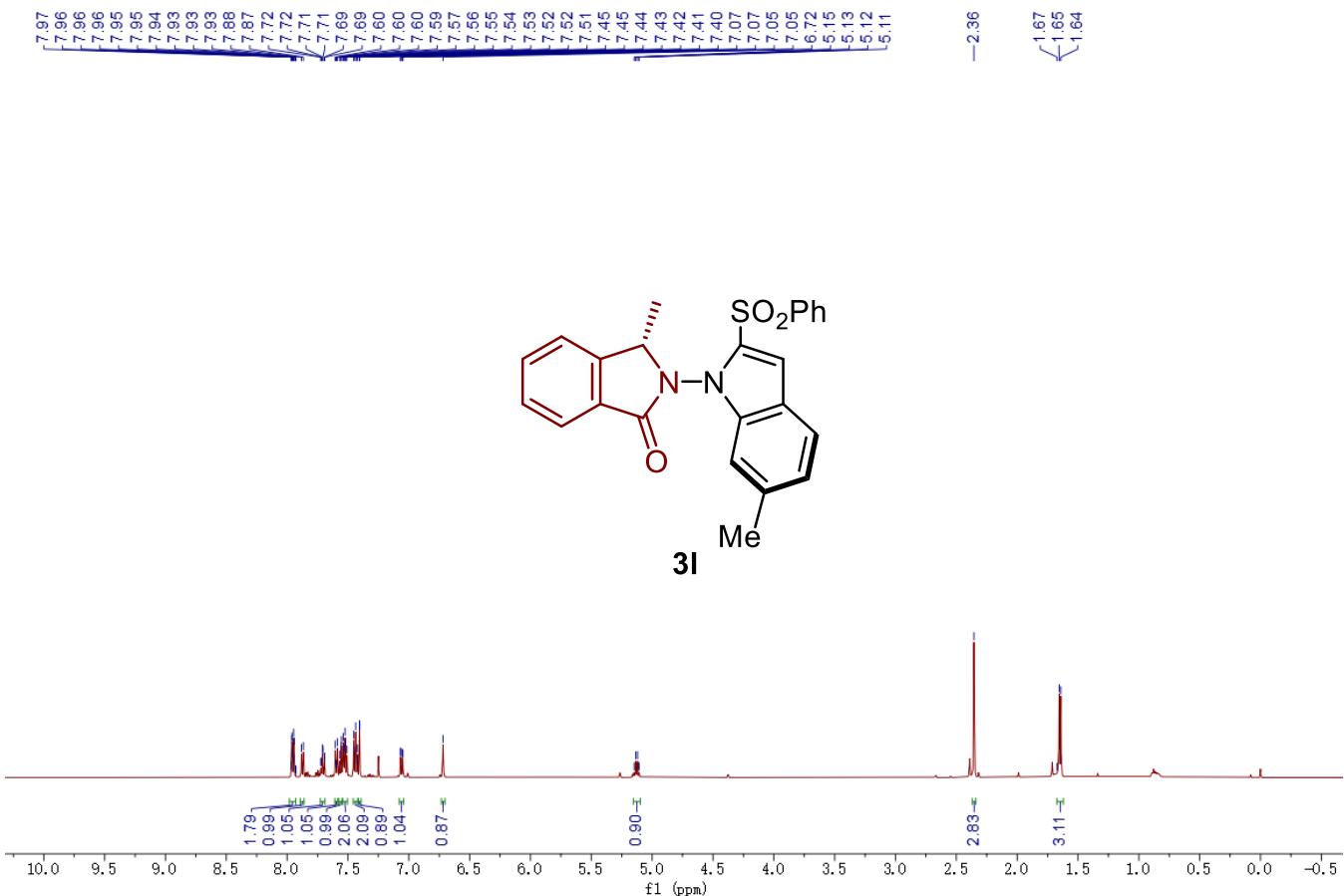


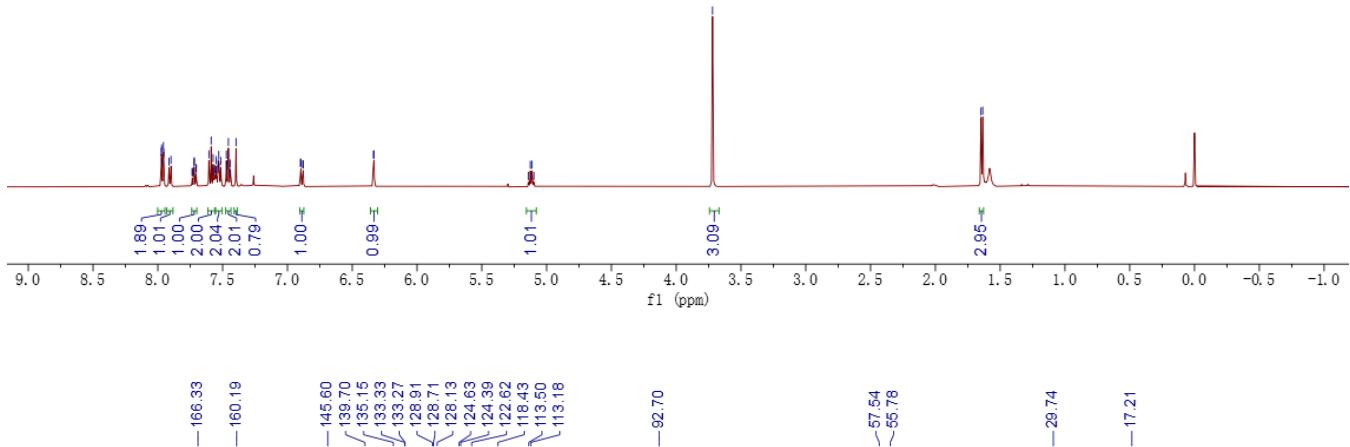
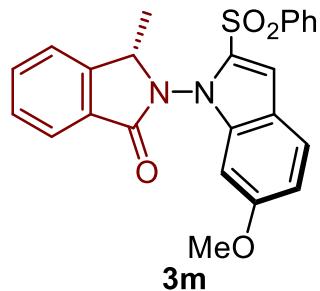
166.75
145.69
141.13
137.61
137.39
136.57
133.69
133.50
129.04
128.93
128.81
128.45
128.37
127.45
127.24
126.98
124.72
124.55
122.75
121.78
112.54
-110.39

-58.31

-17.48







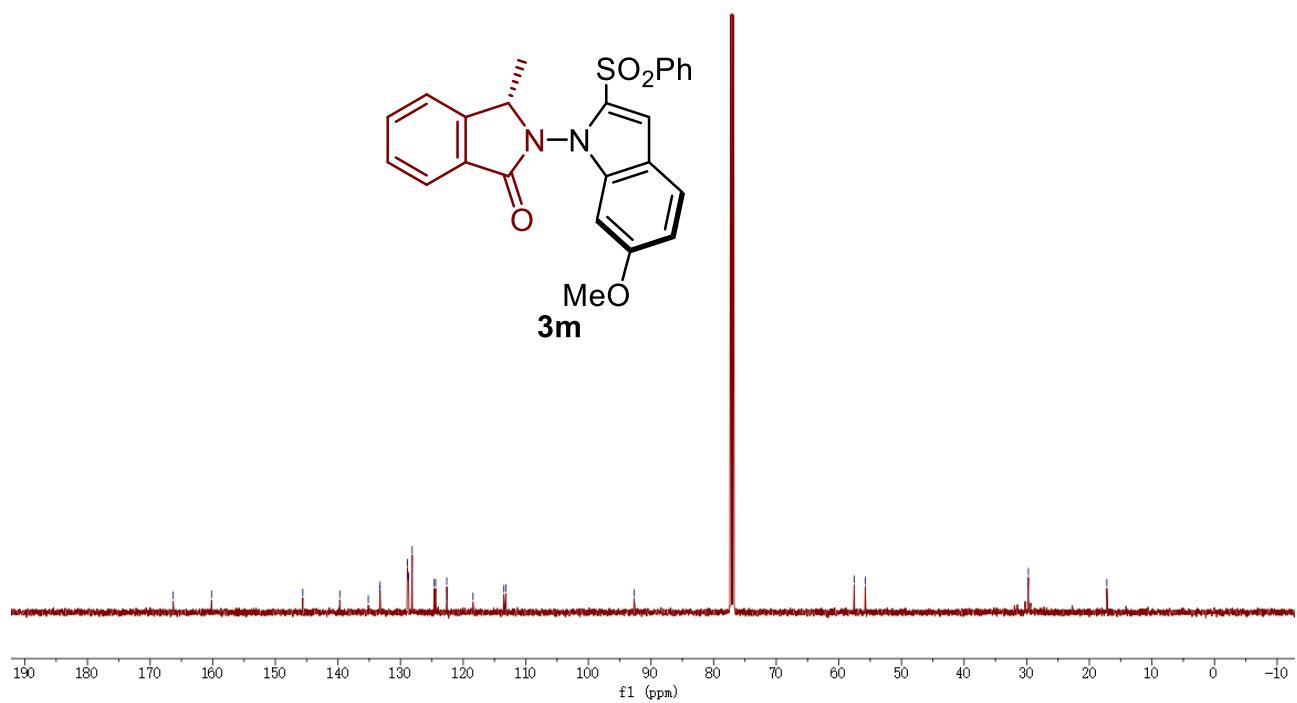
-166.33
-160.19

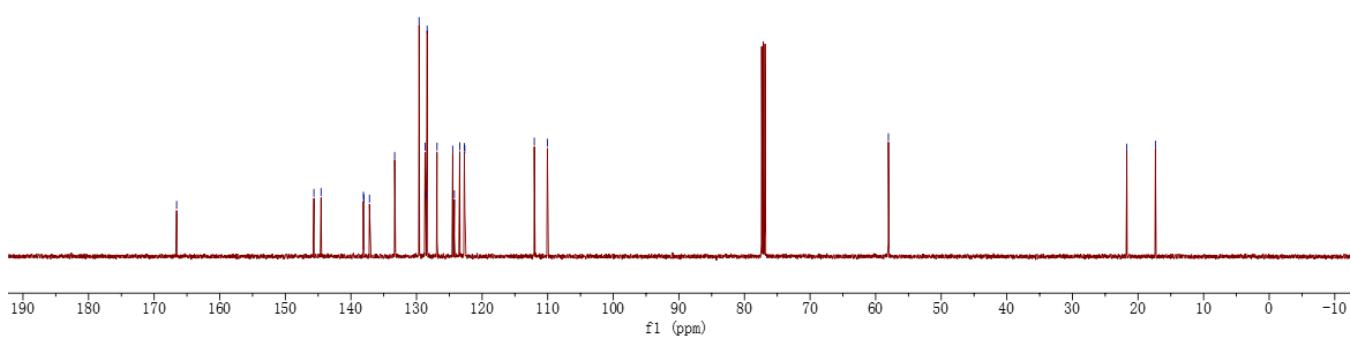
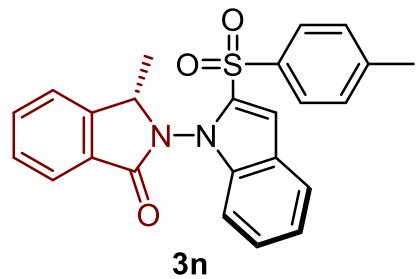
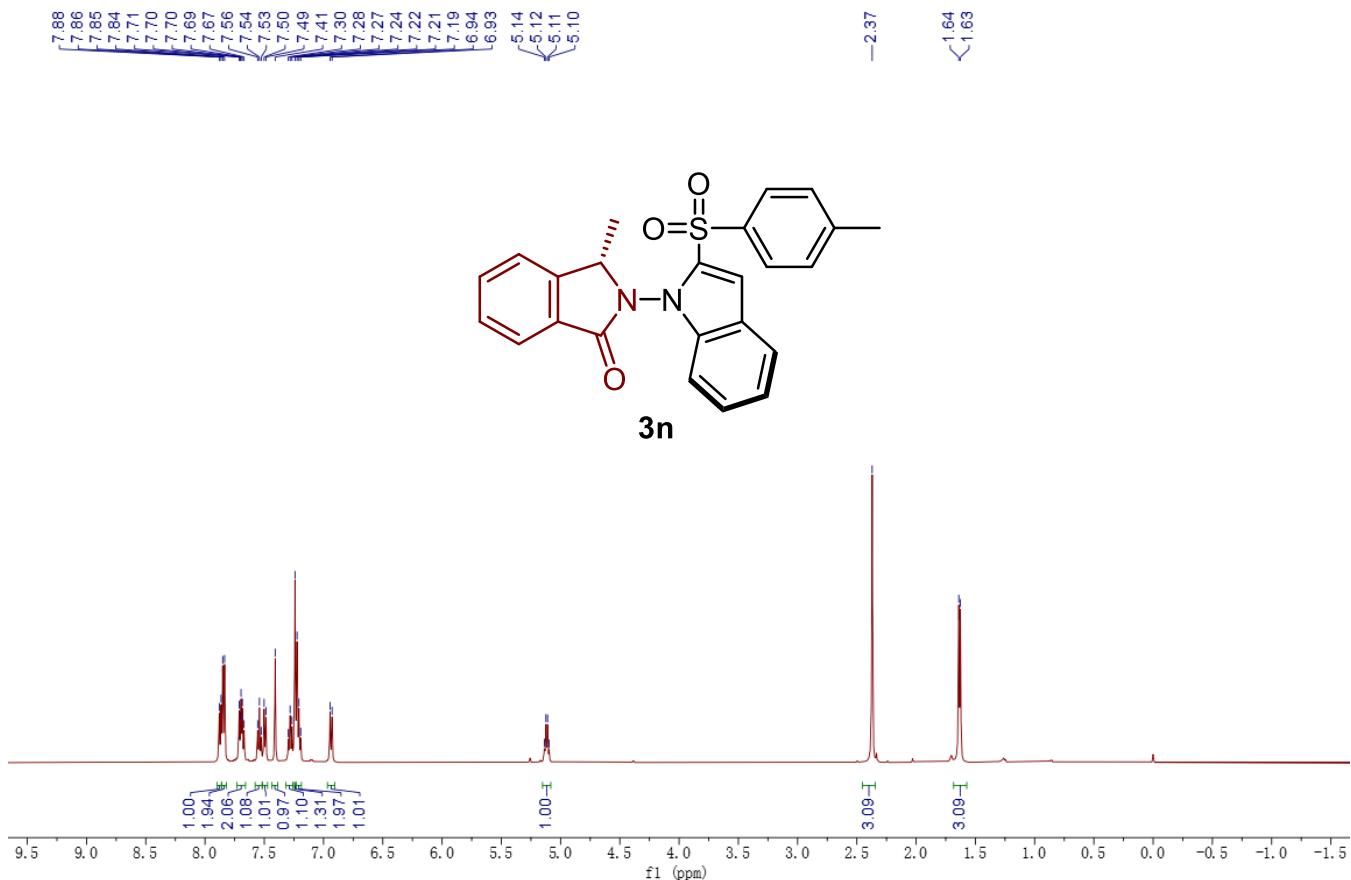
-145.60
-139.70
-135.15
-133.33
-133.27
-128.91
-128.71
-128.13
-124.63
-124.39
-122.62
-118.43
-113.50
-113.18

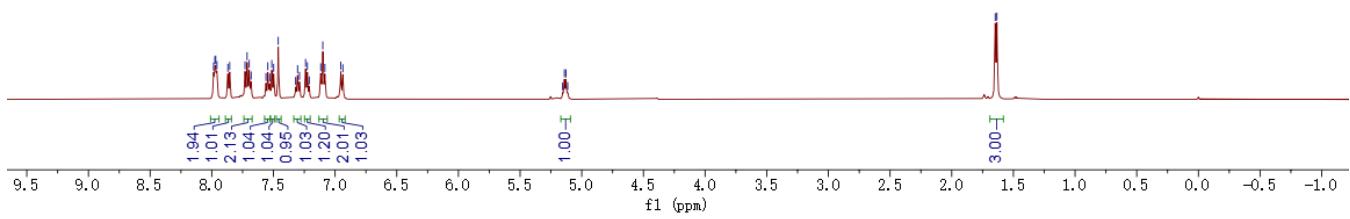
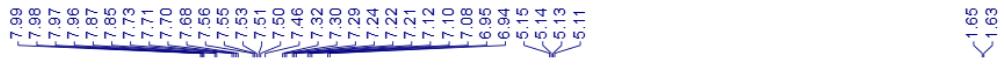
-92.70

-57.54
-55.78

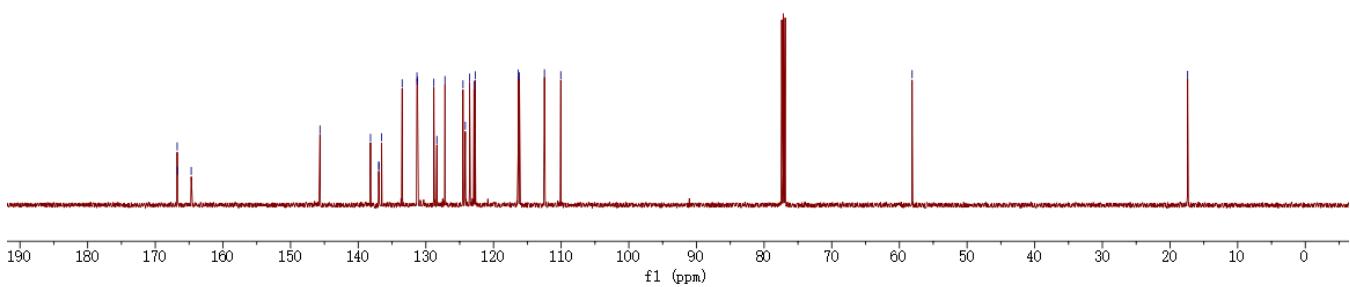
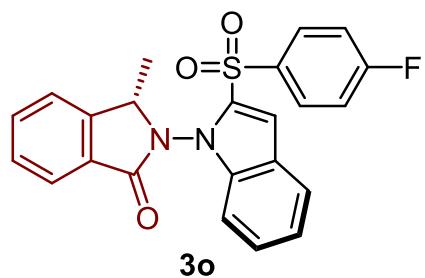
-29.74
-17.21

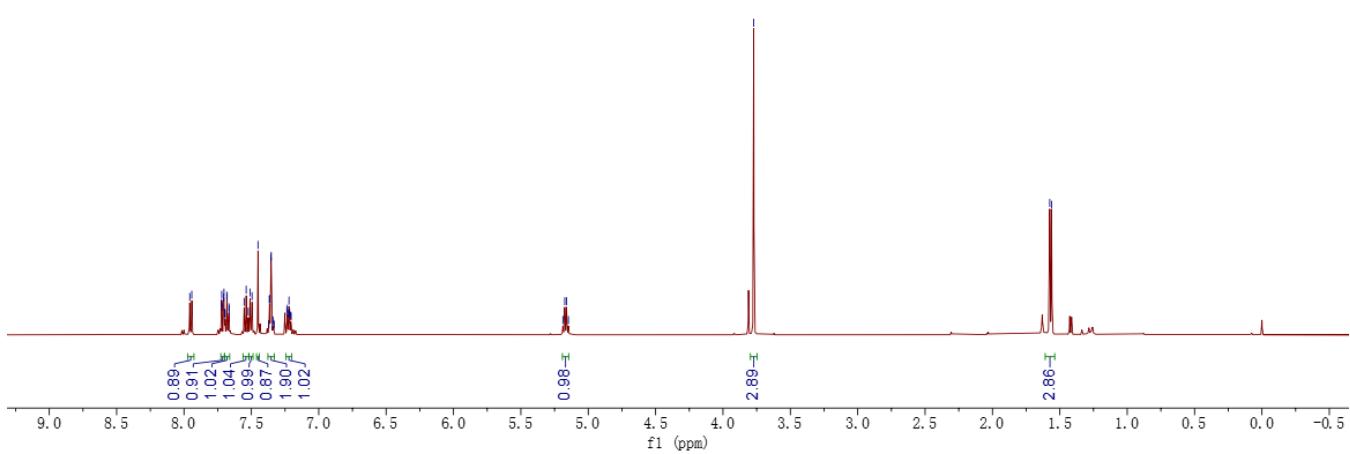
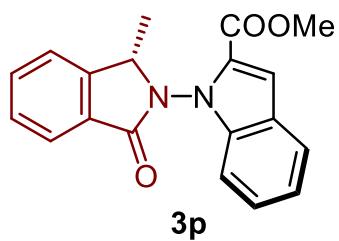
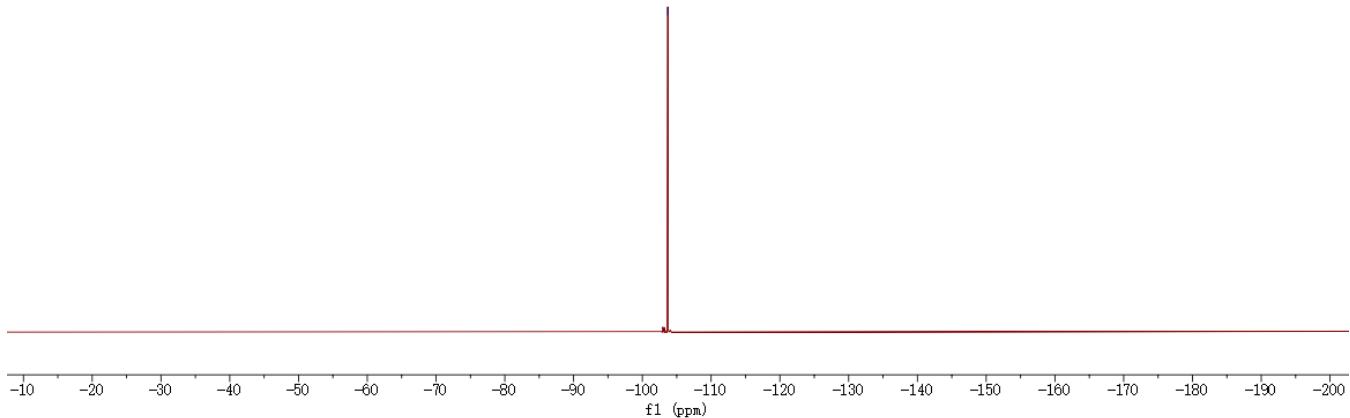
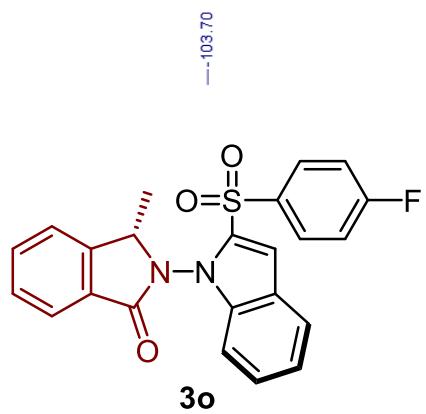


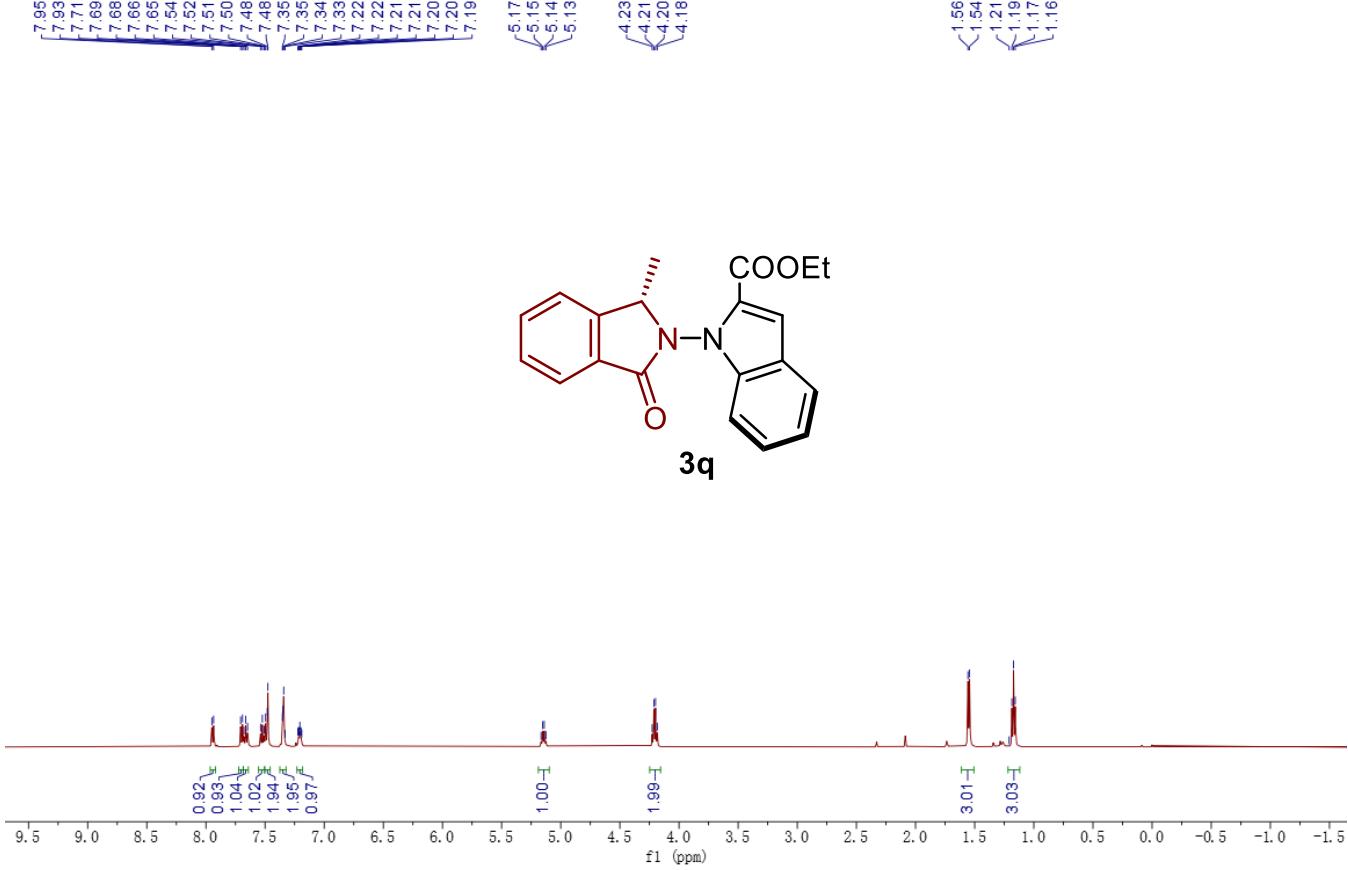
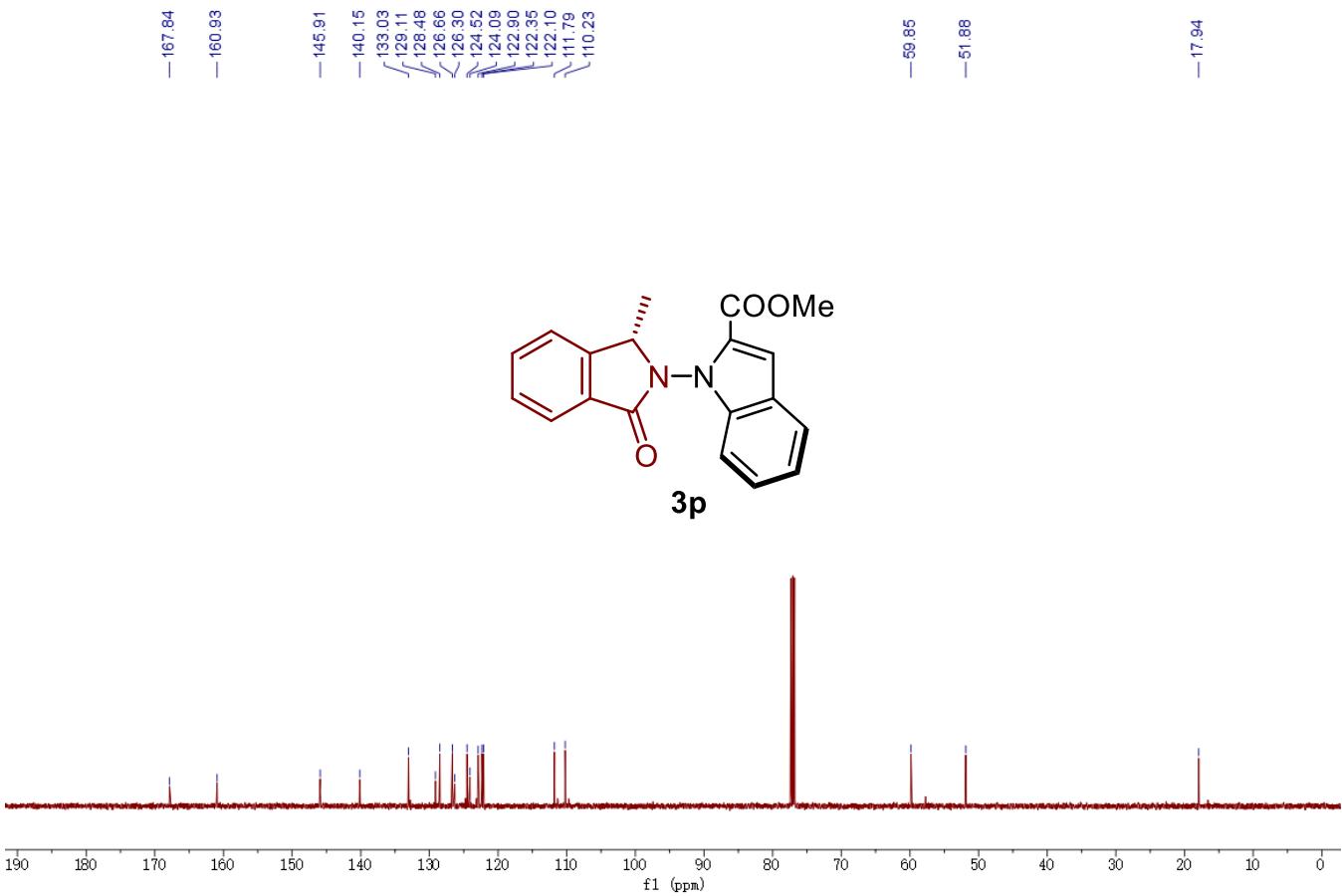


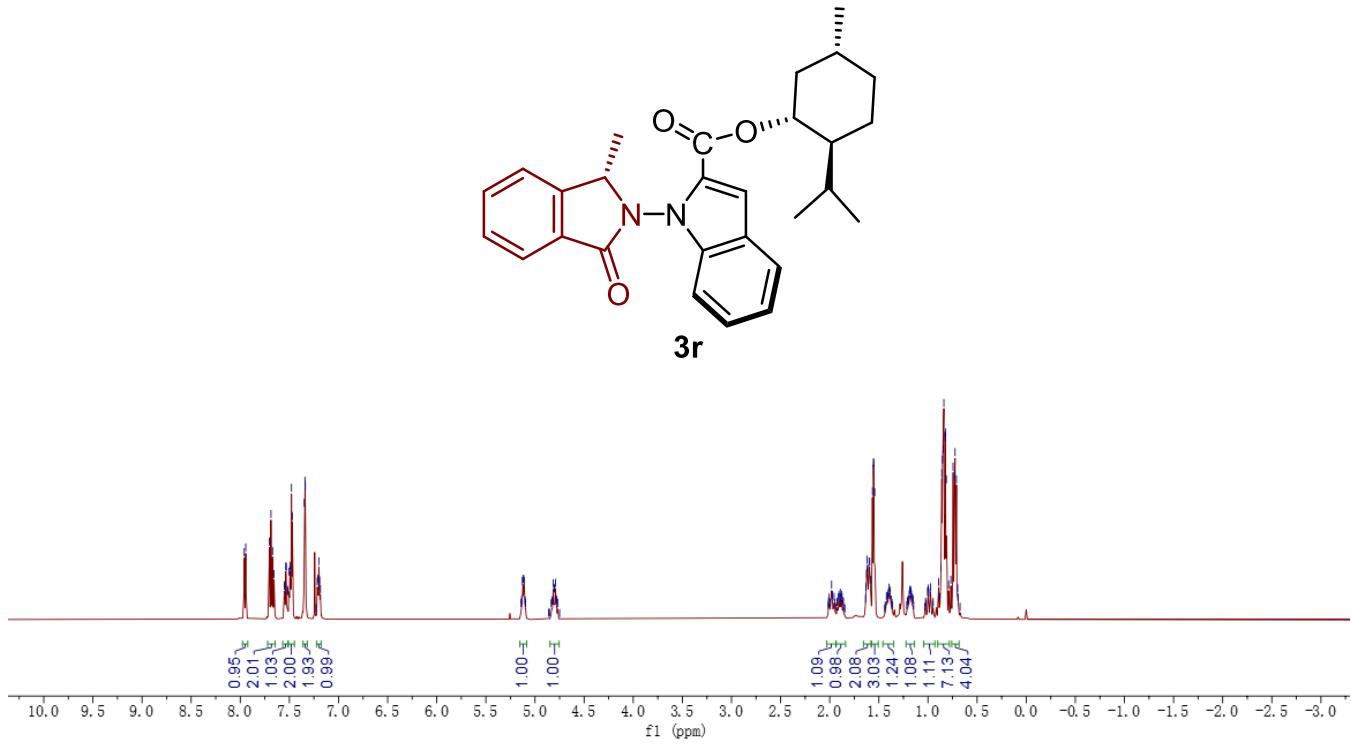
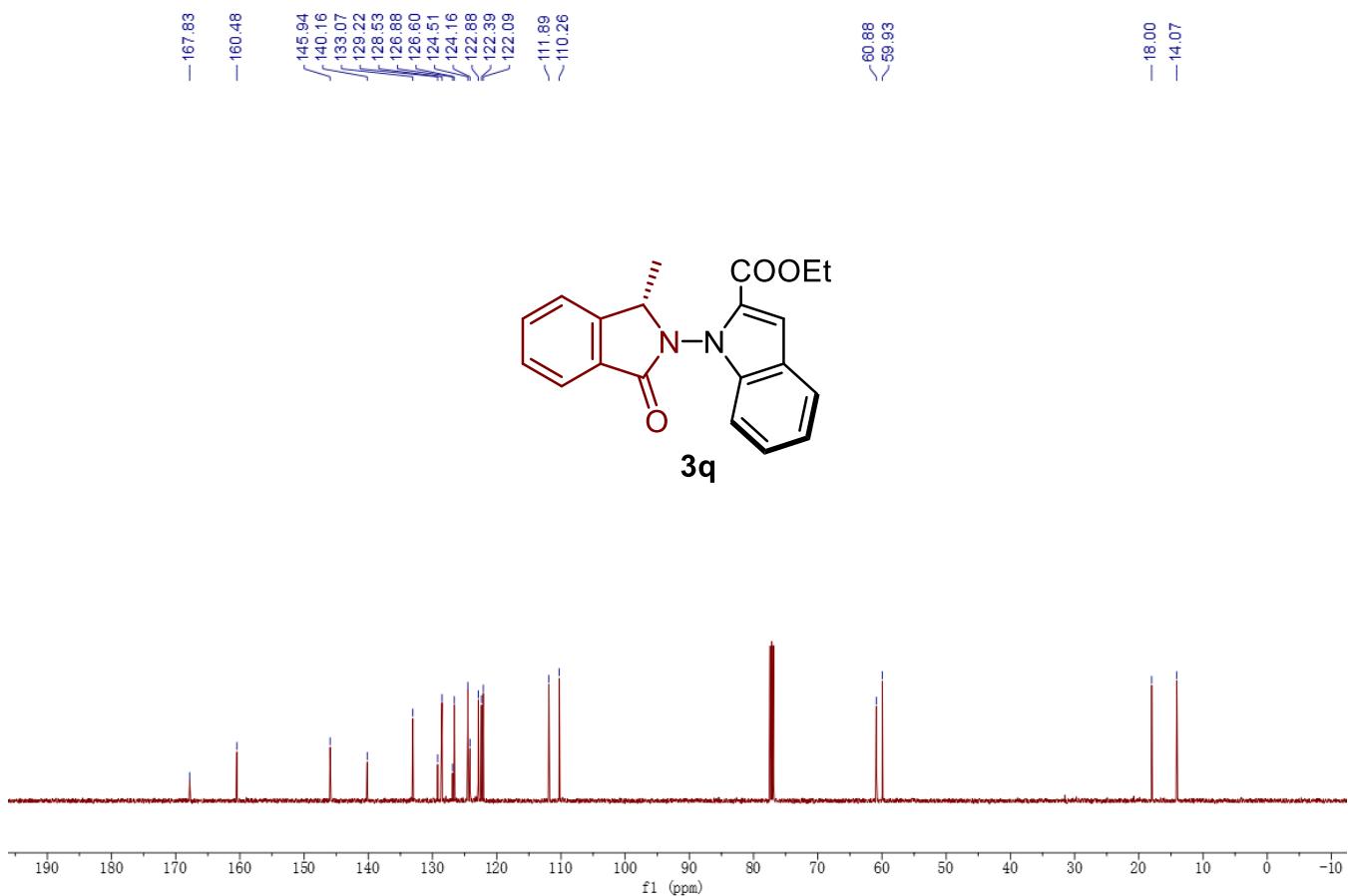


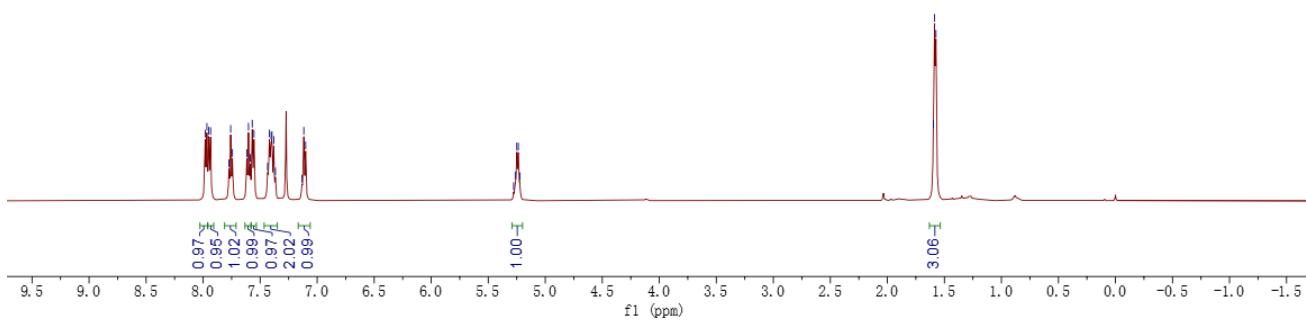
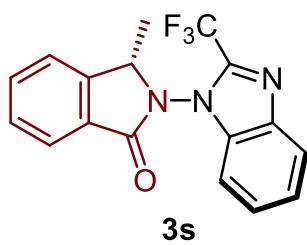
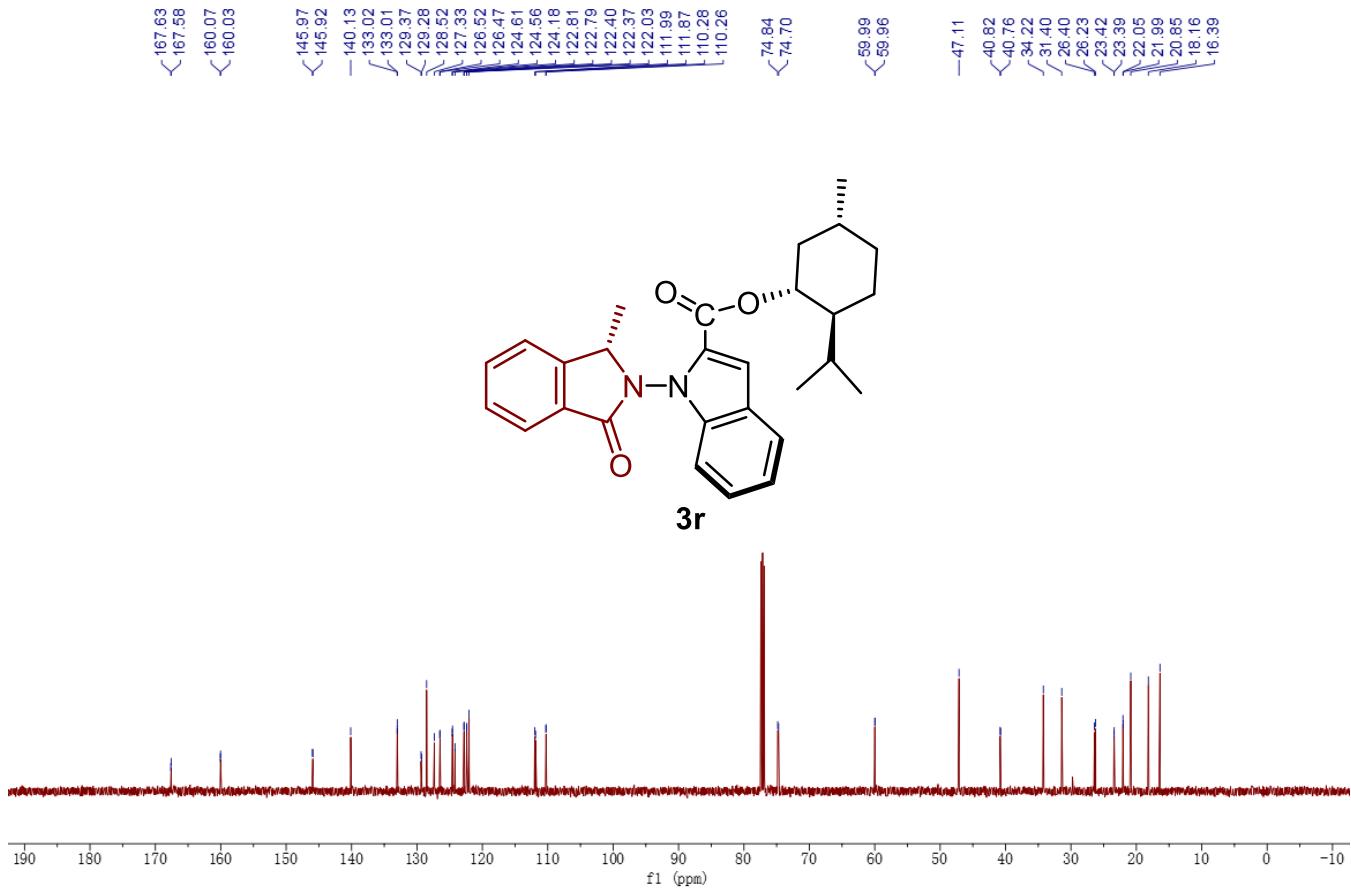
166.76
166.72
164.69
145.65
138.18
136.97
136.94
136.54
133.50
131.32
131.24
128.83
128.37
127.18
124.51
124.16
123.53
122.88
122.70
116.36
116.18
112.47
110.06
— 58.12
— 17.40

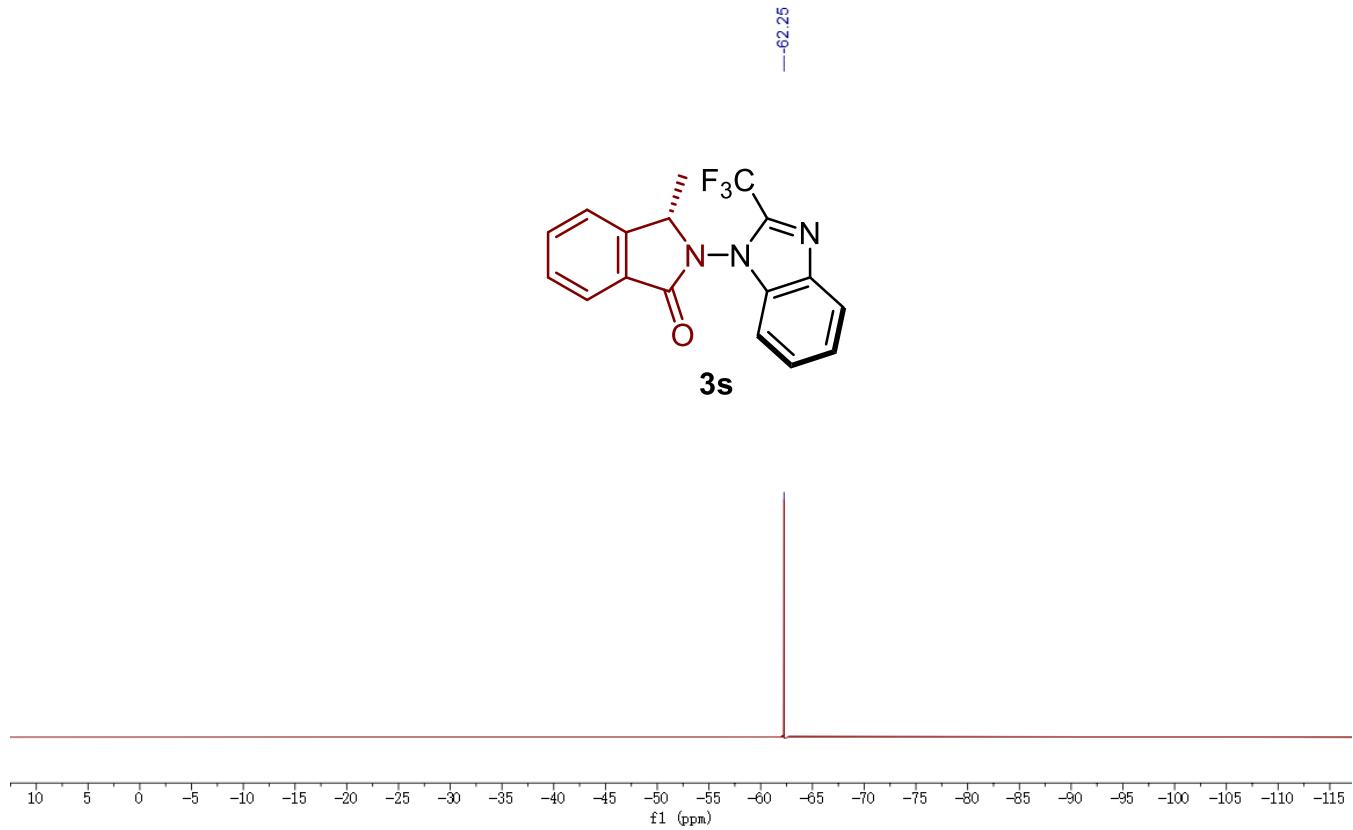
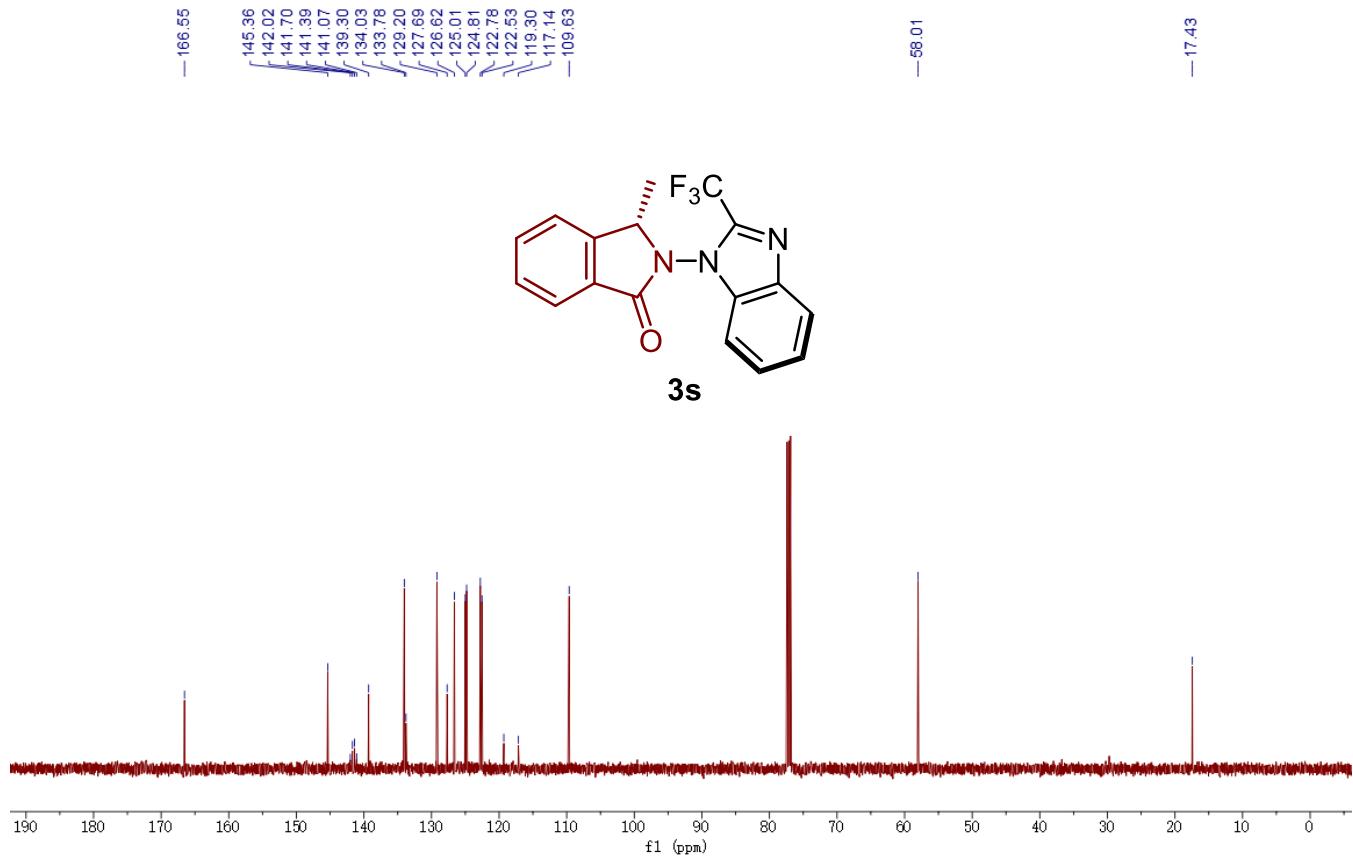


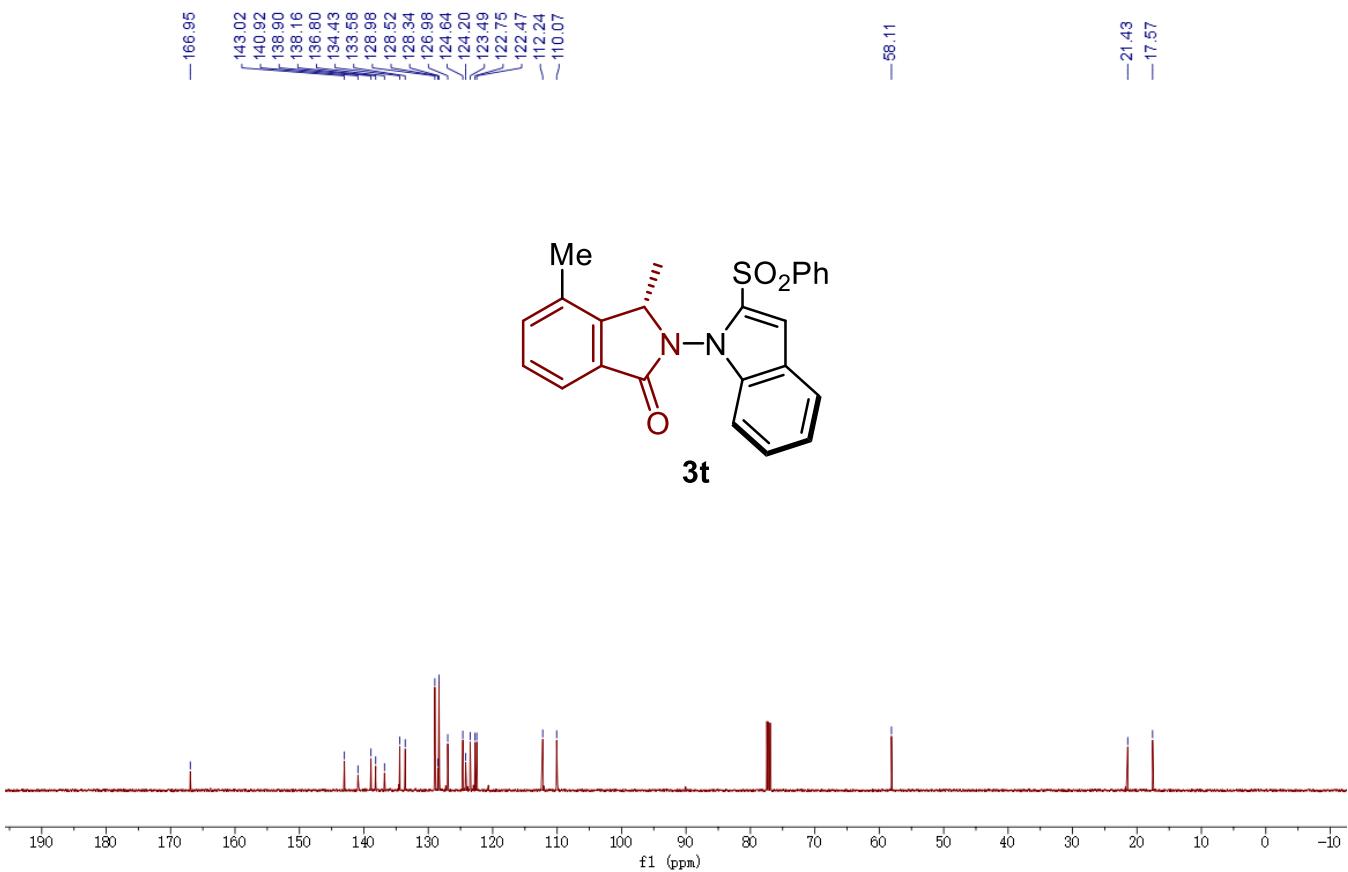
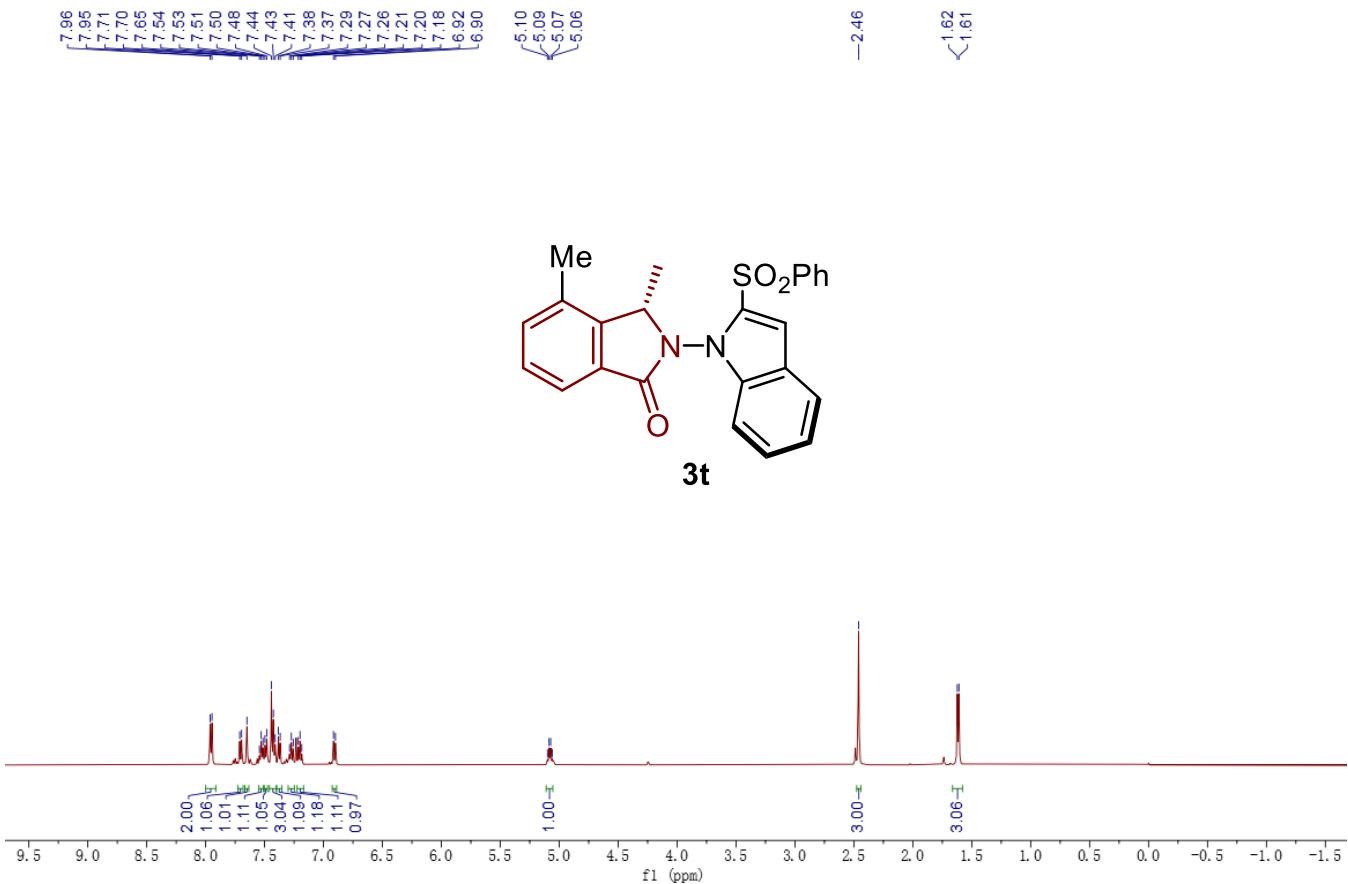


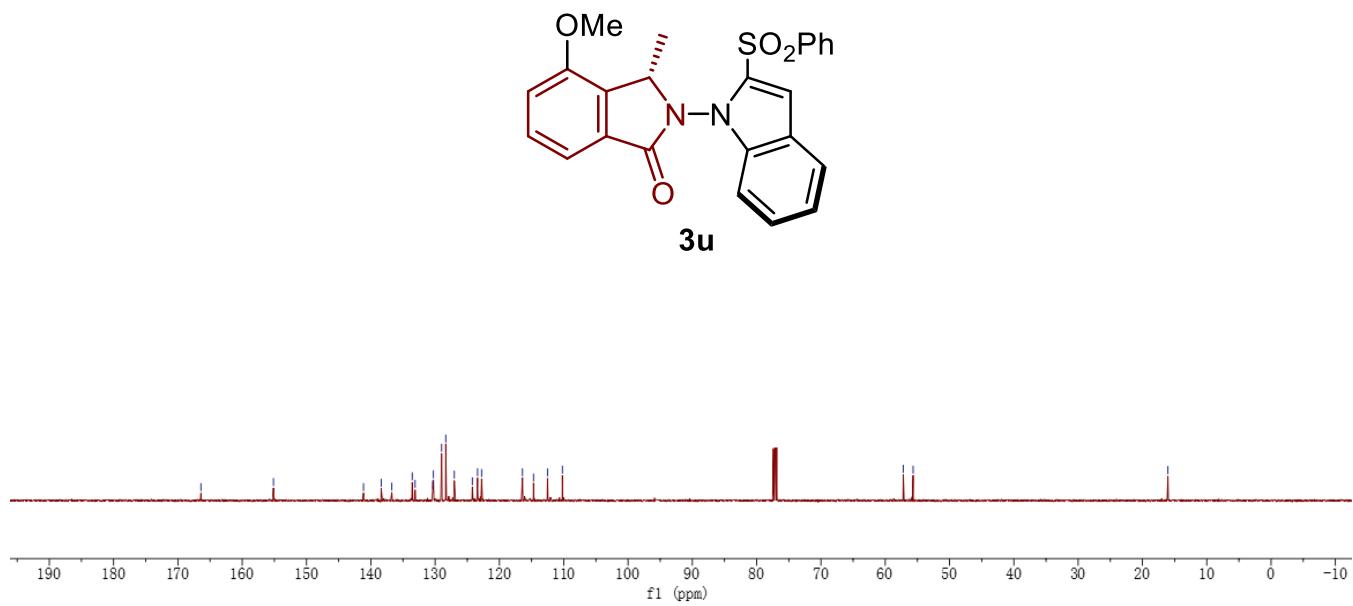
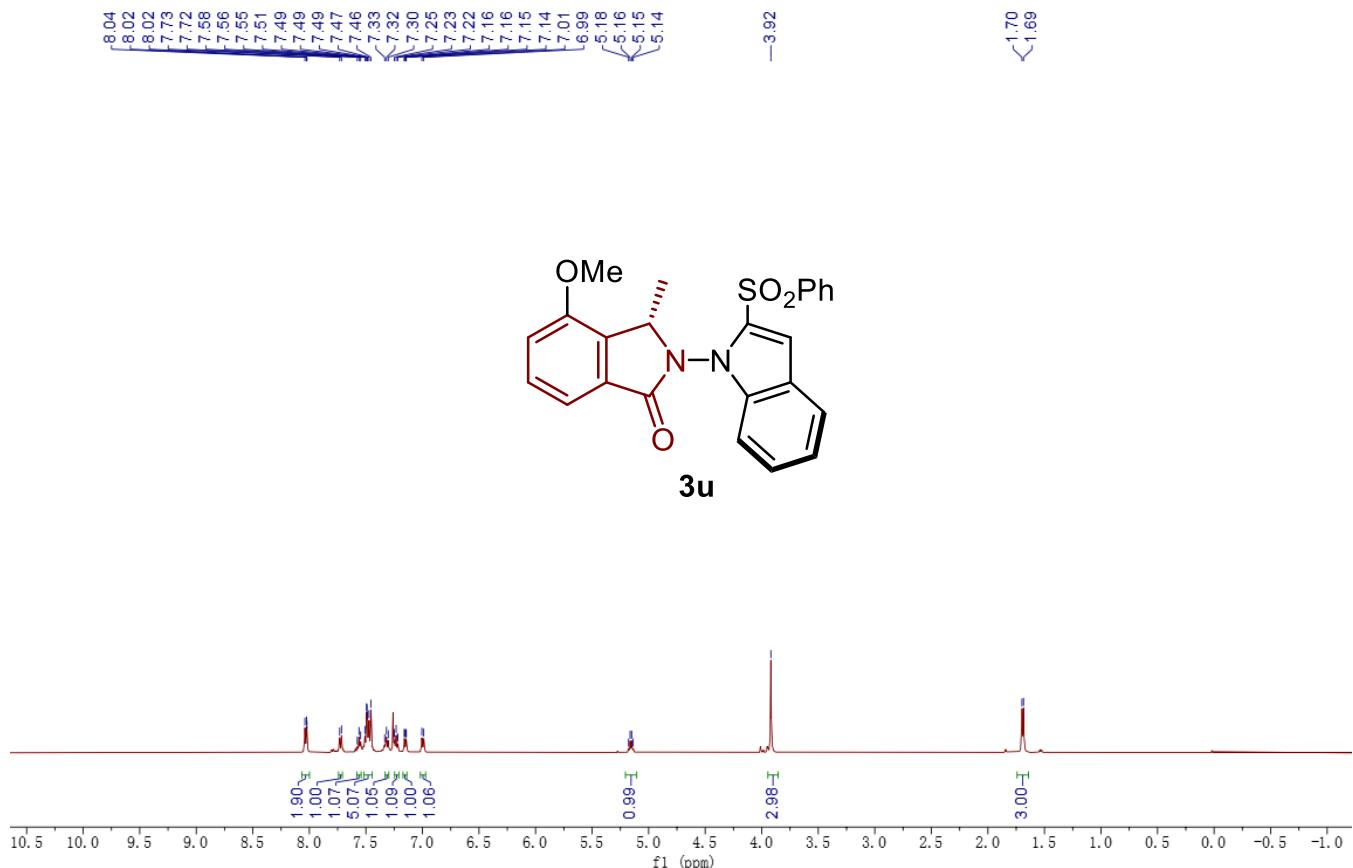


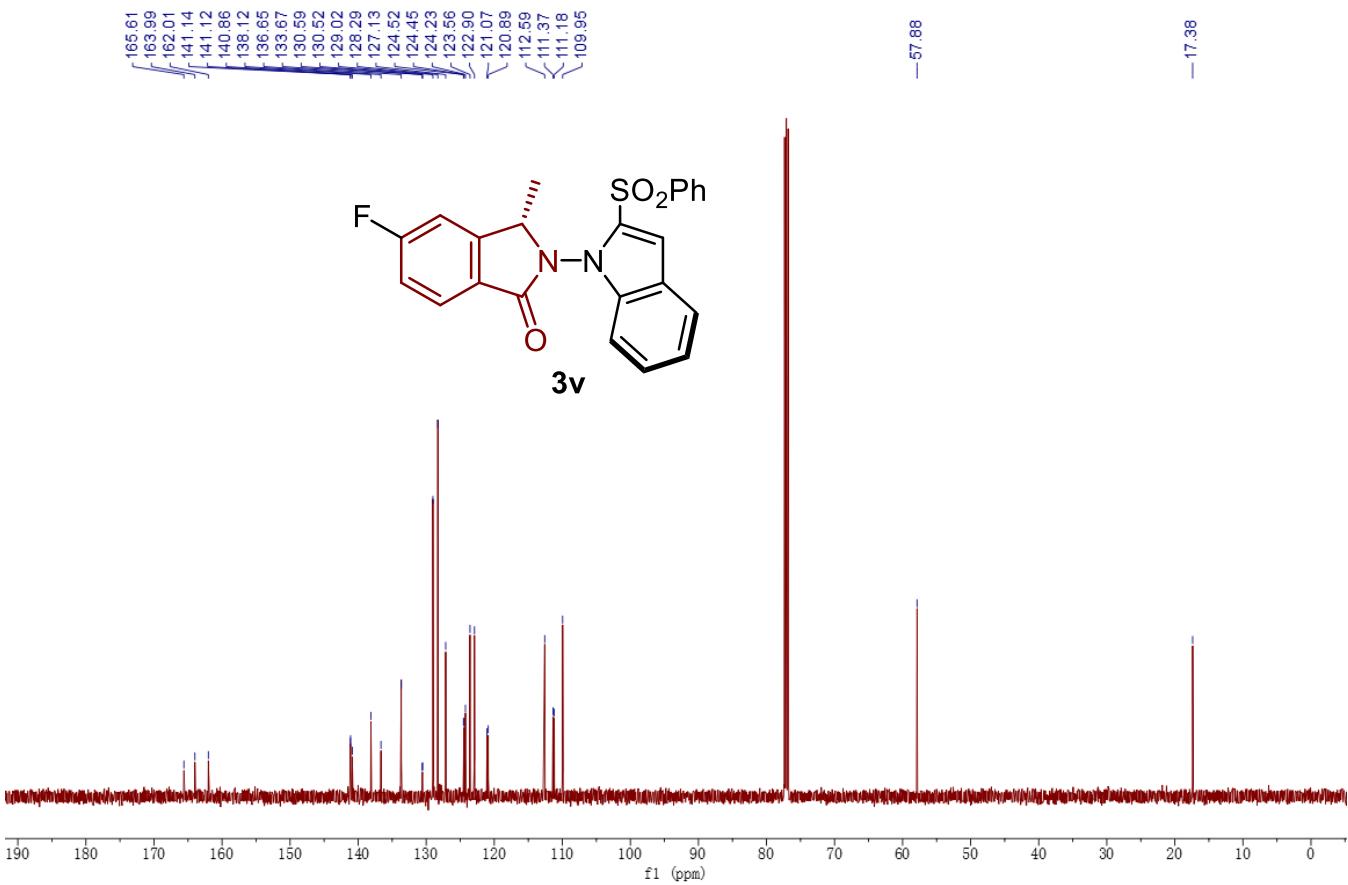
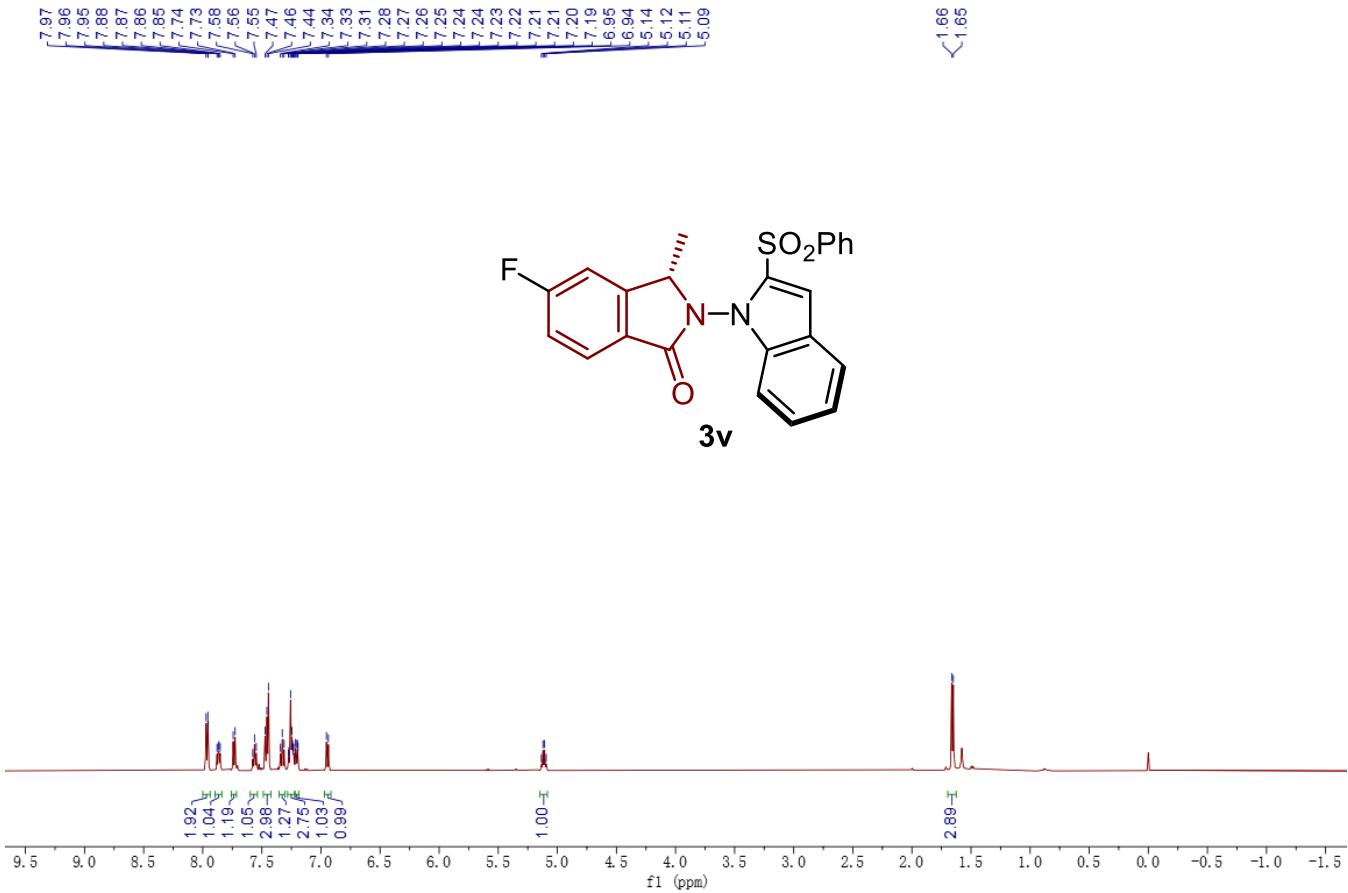




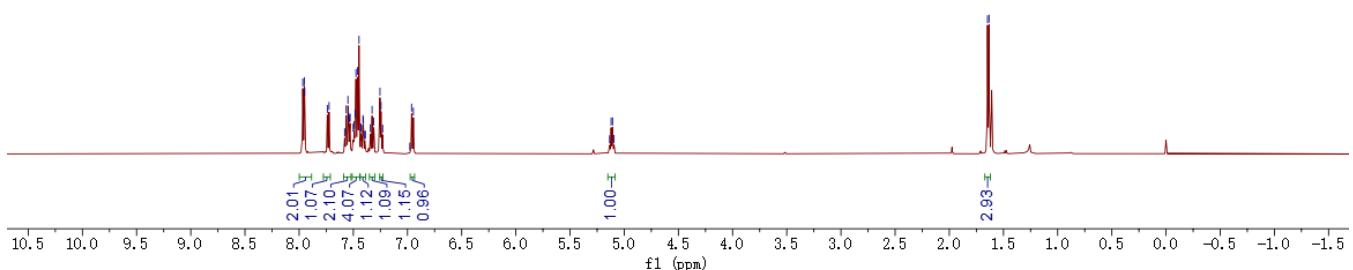
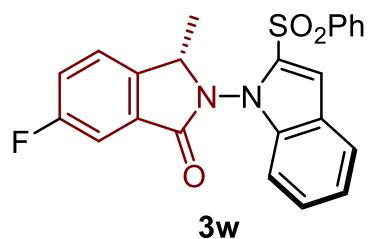
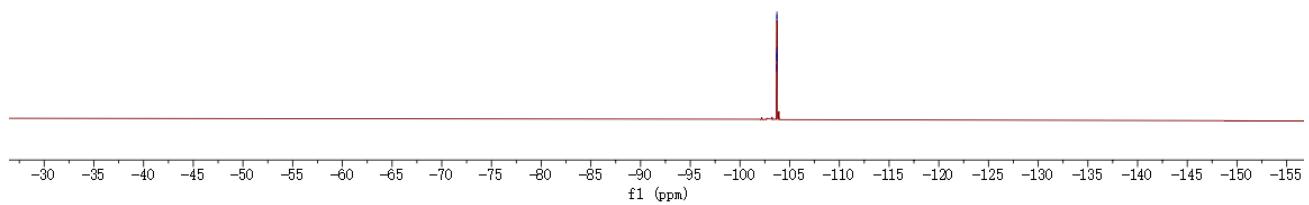
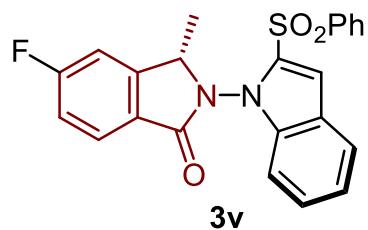


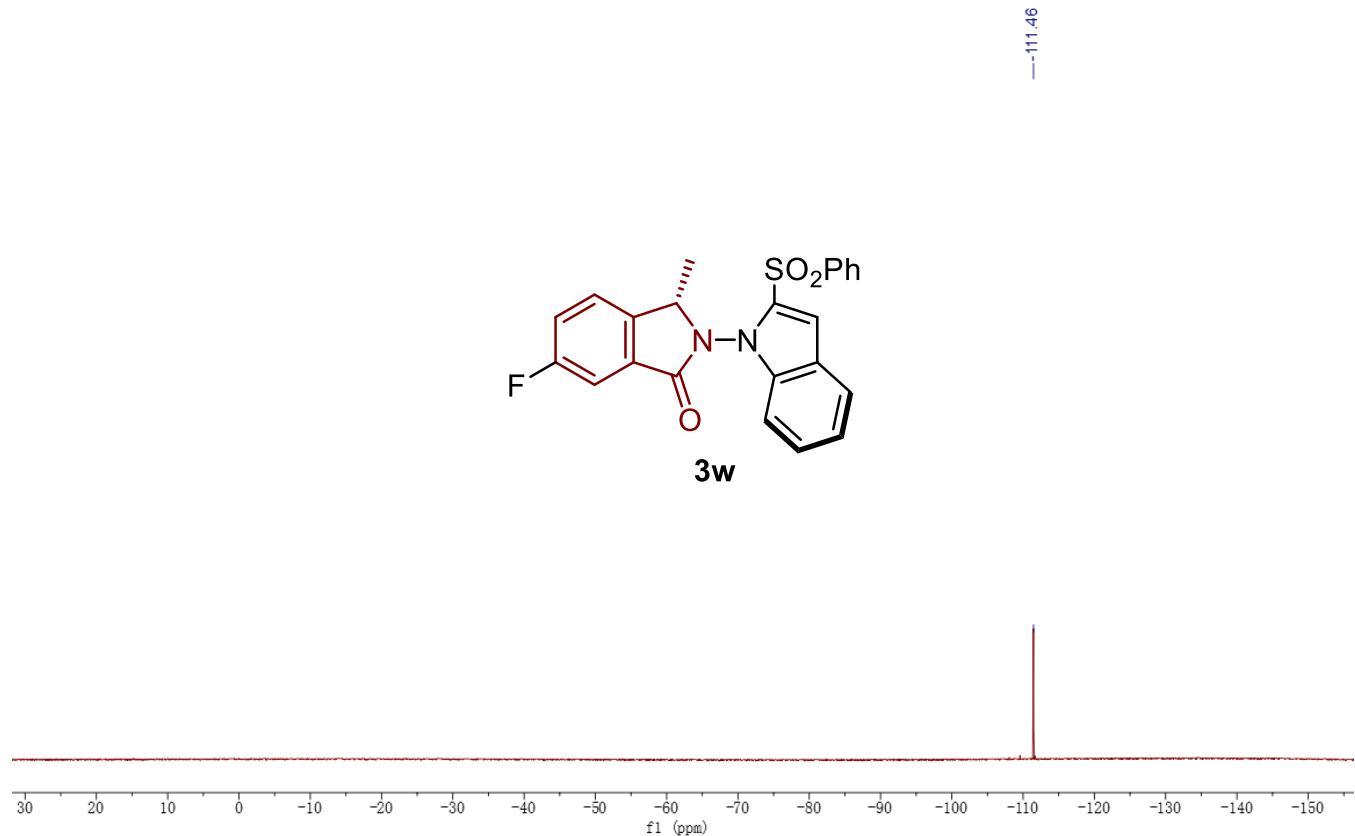
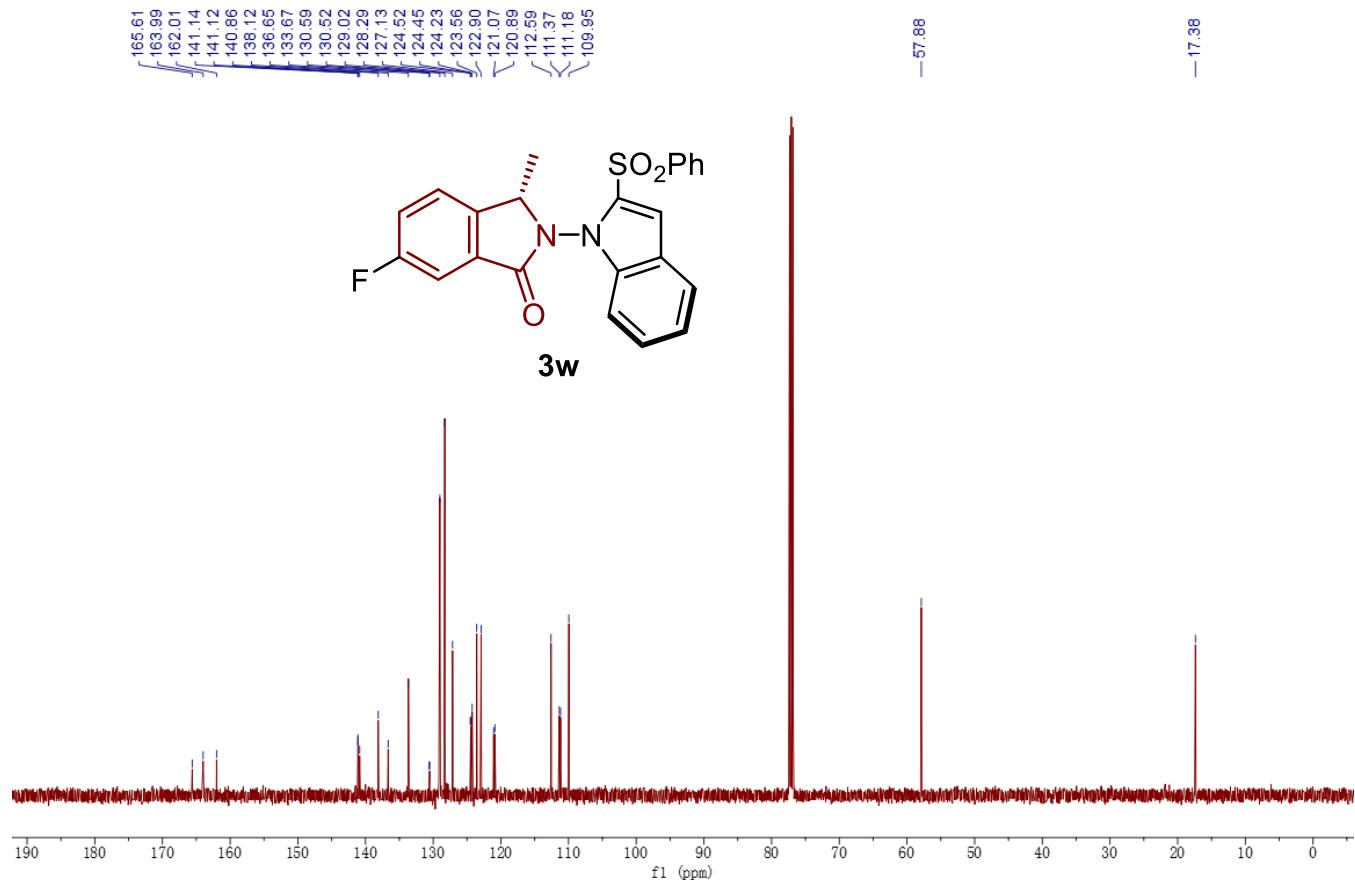


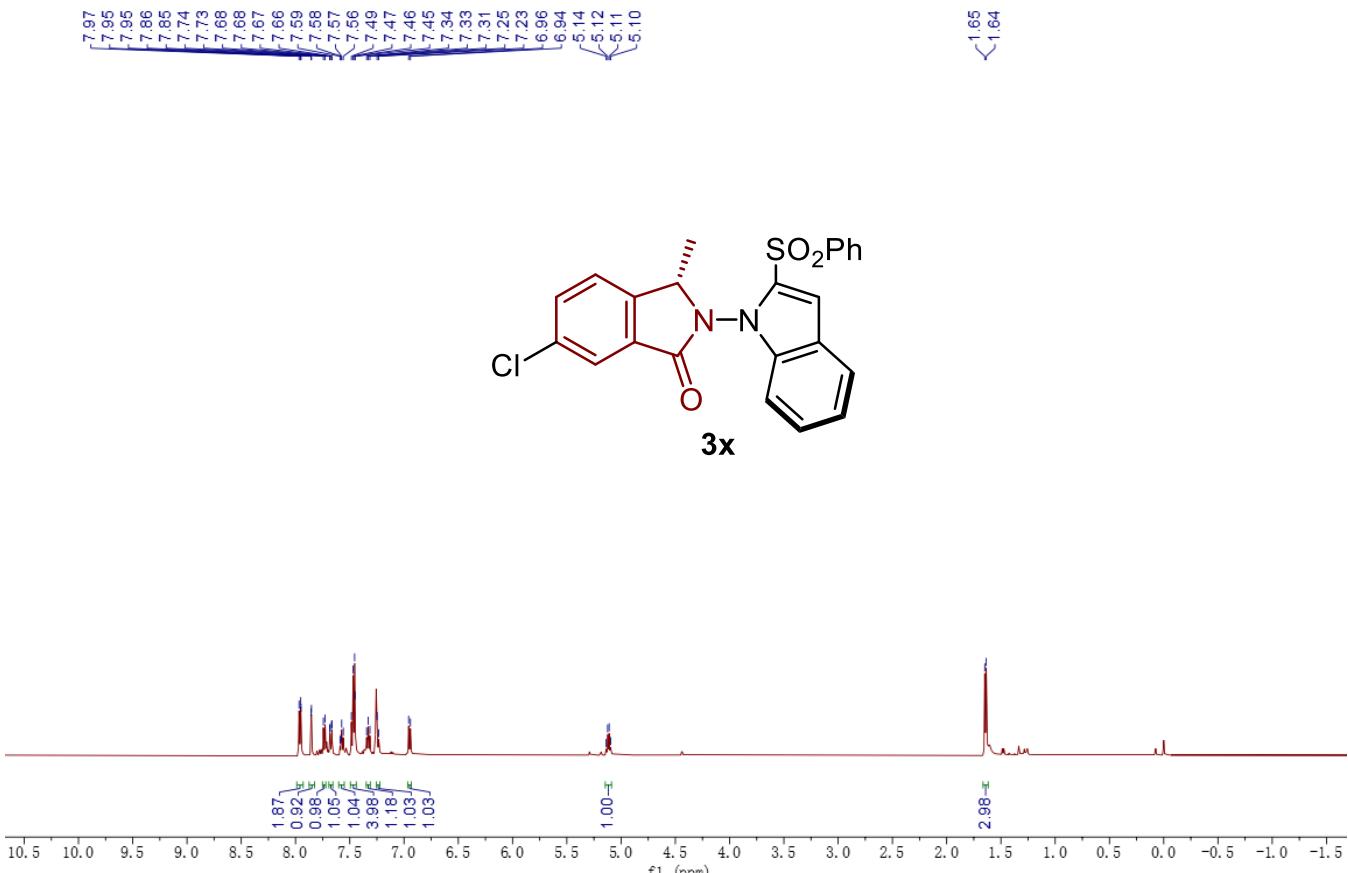




¹H NMR assignments:
-103.69
-103.70
-103.72
-103.73





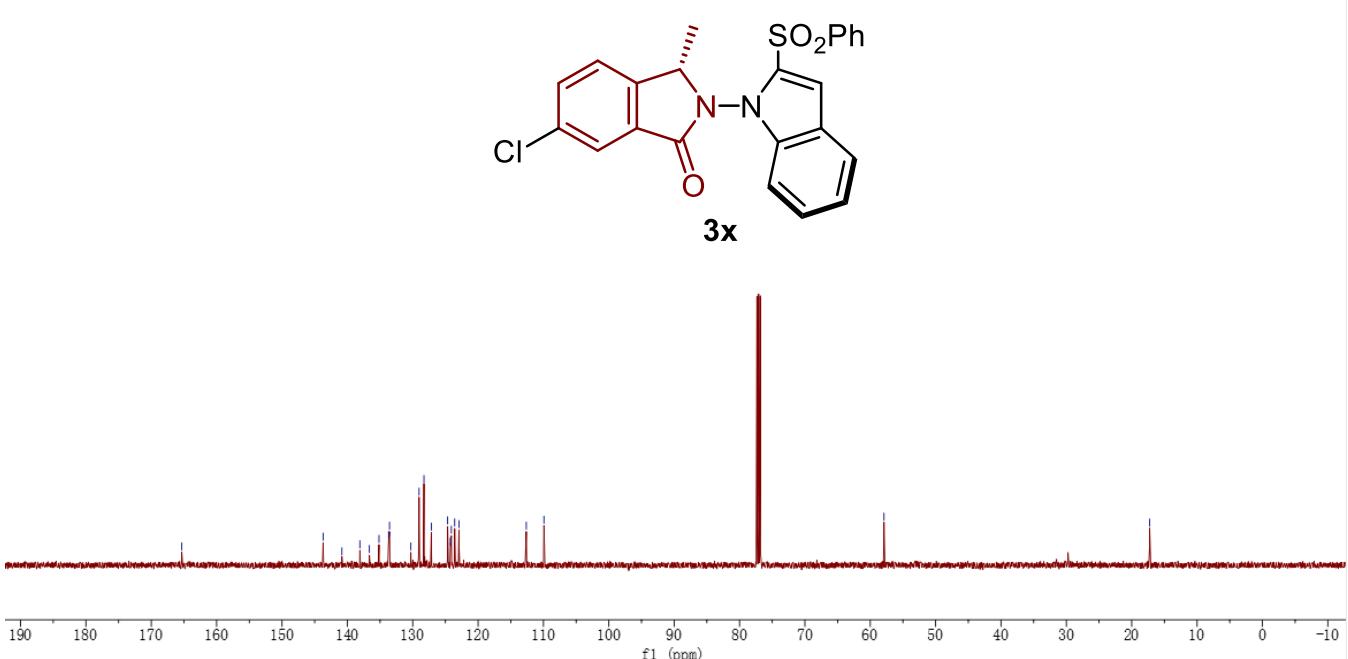


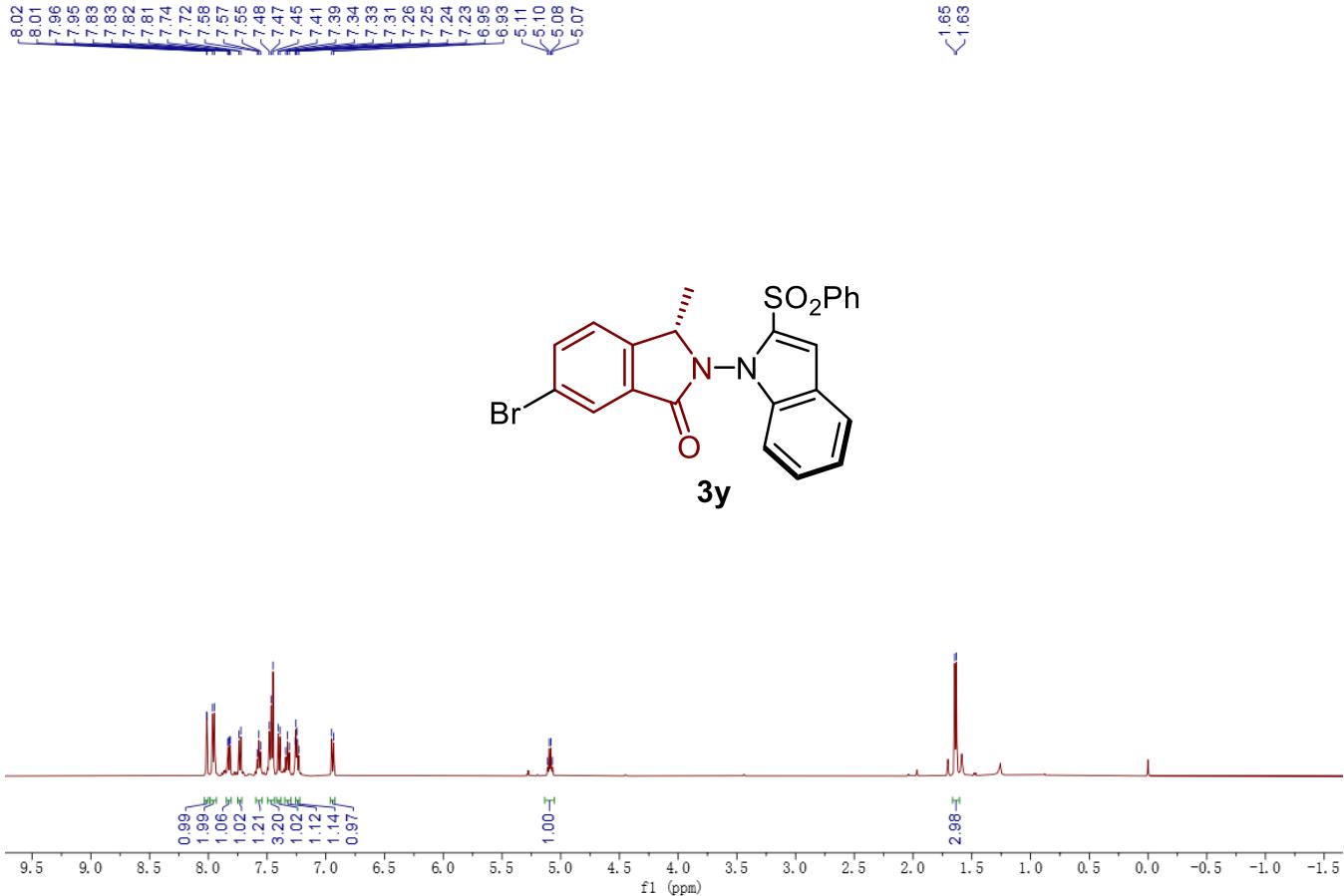
— 165.34

— 143.71
 — 140.84
 — 138.09
 — 136.63
 — 135.16
 — 133.68
 — 133.55
 — 130.29
 — 129.03
 — 128.28
 — 127.15
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 — 124.24
 — 124.09
 — 123.58
 — 122.92
 — 112.62
 — 109.92

— 57.90

— 17.26

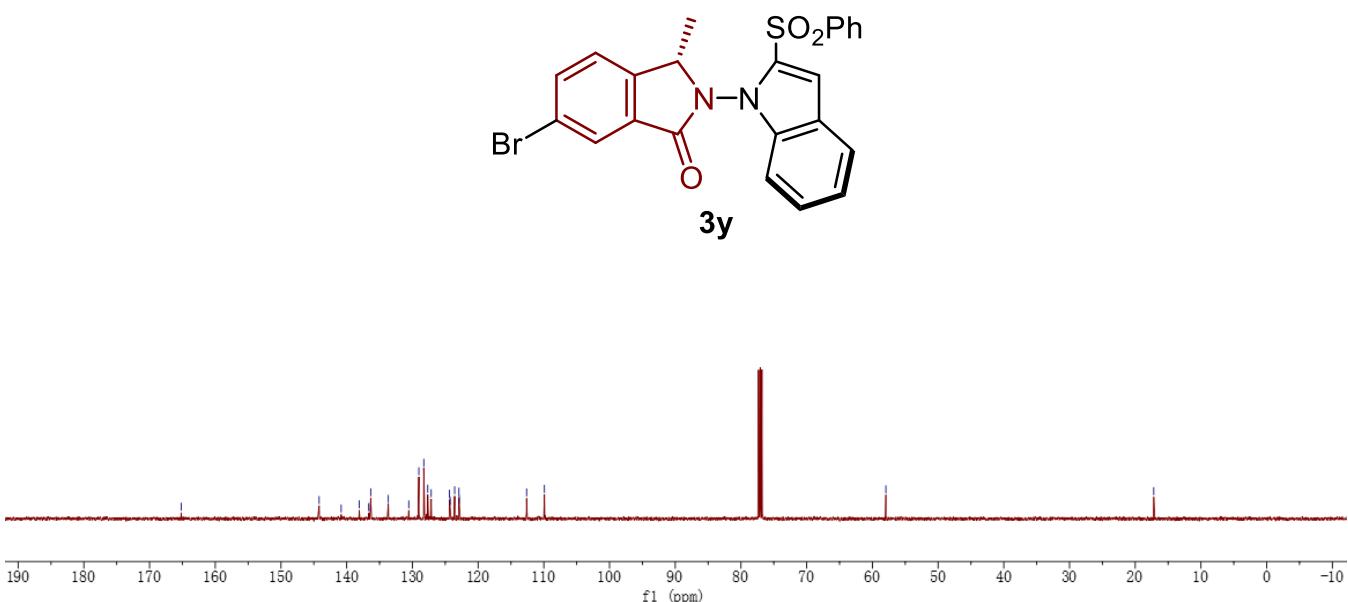


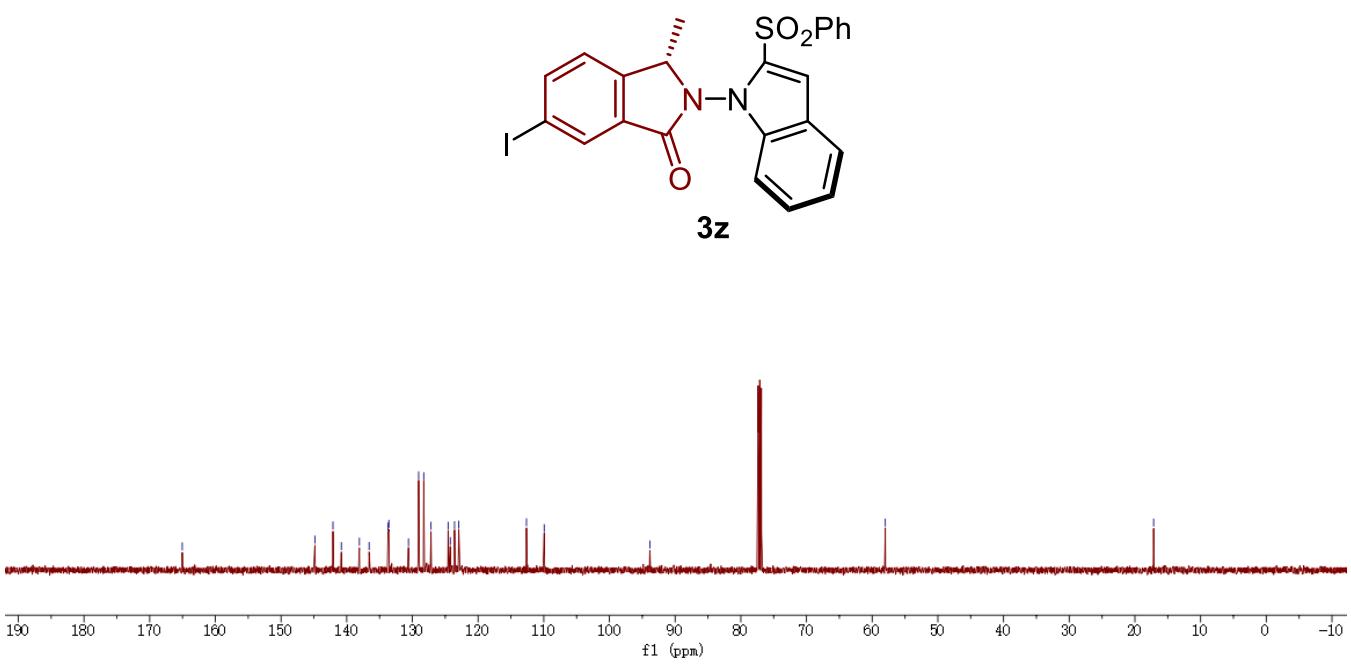
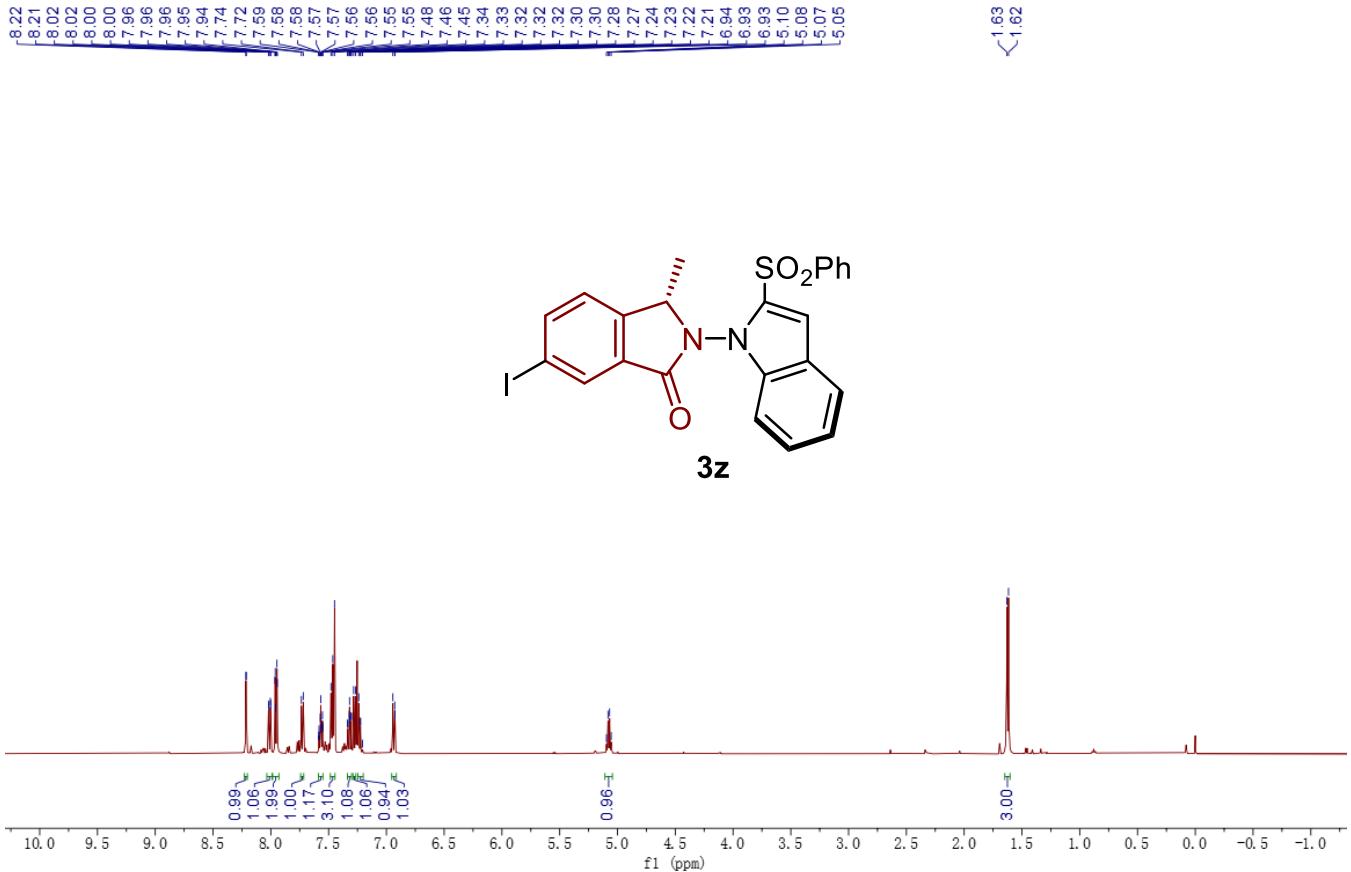


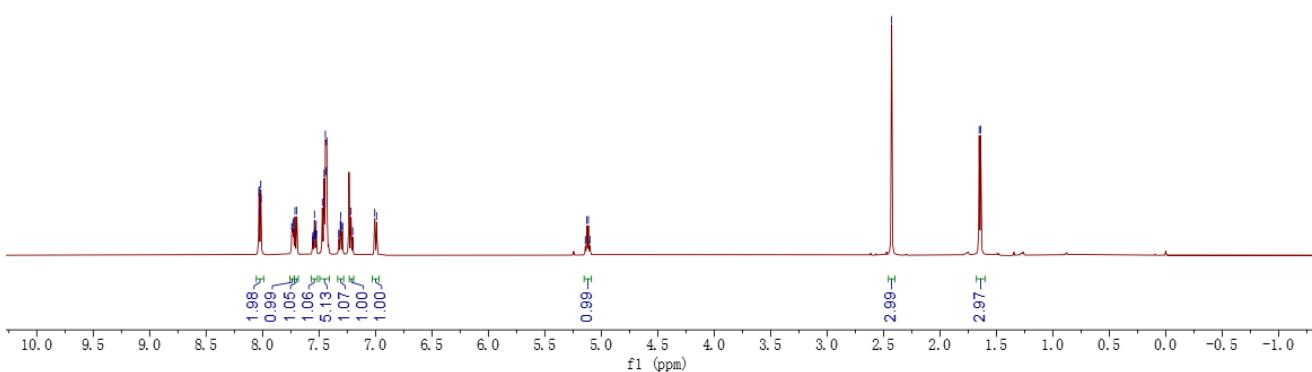
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136.65
136.35
133.67
130.55
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124.25
123.57
122.92
122.88
112.62
109.91

-57.95

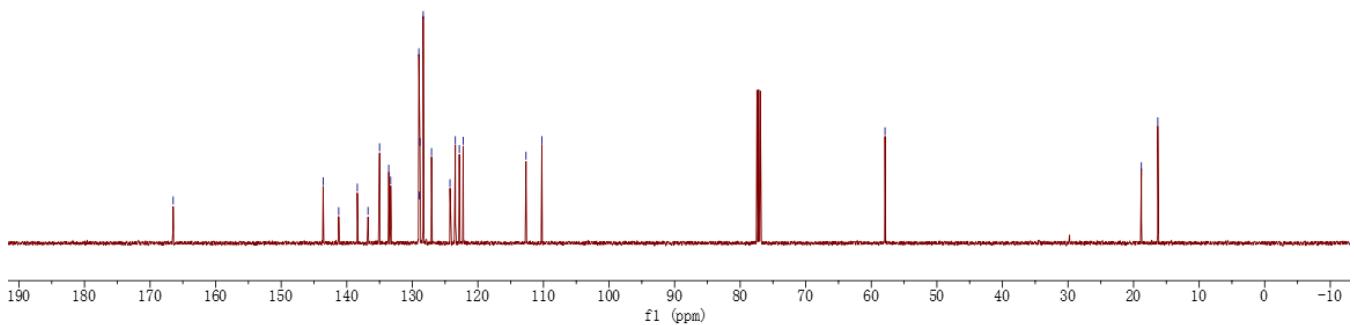
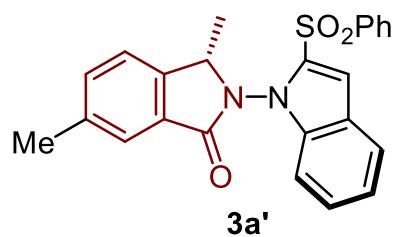
-17.18

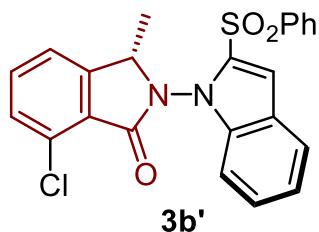
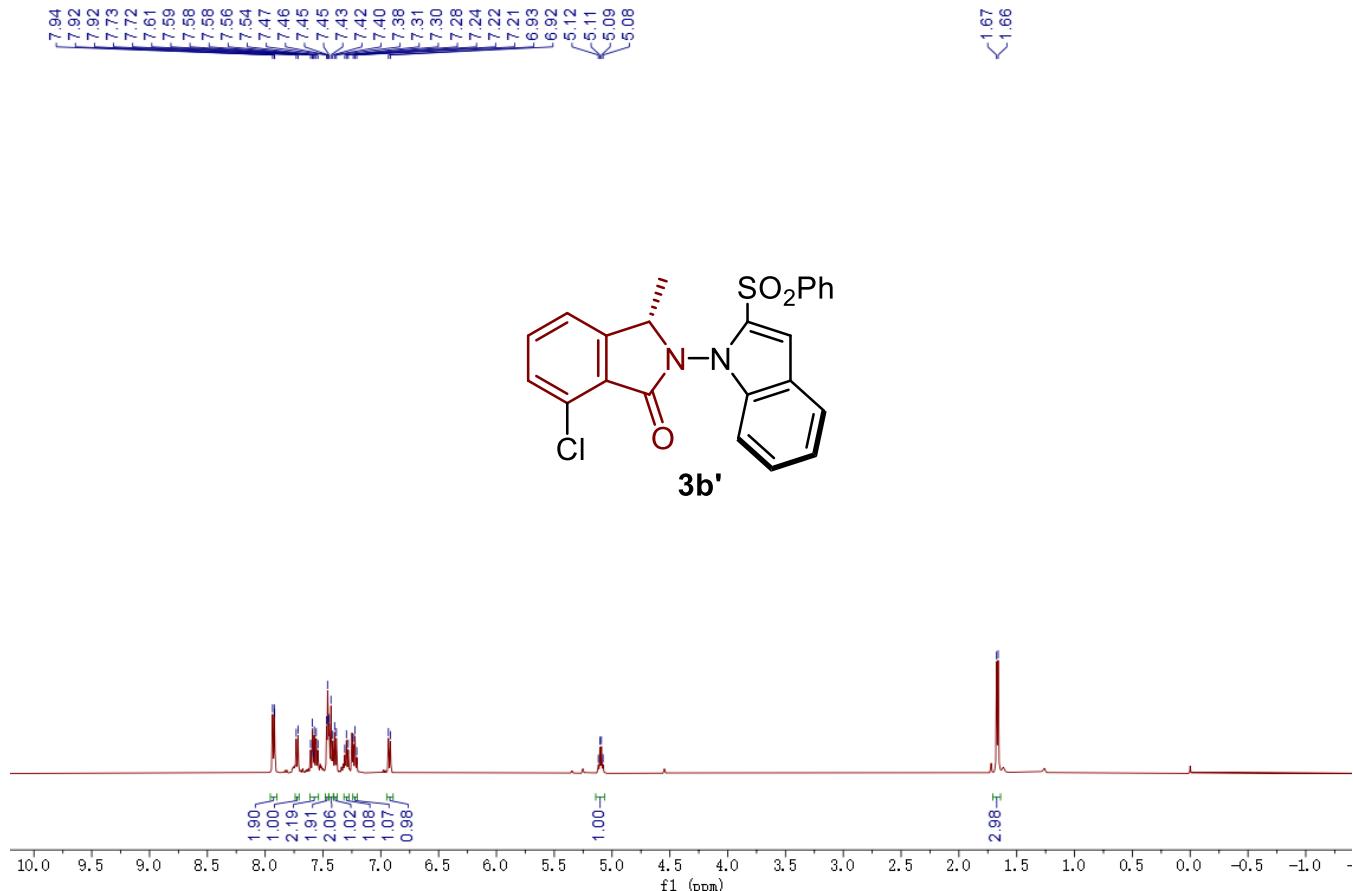




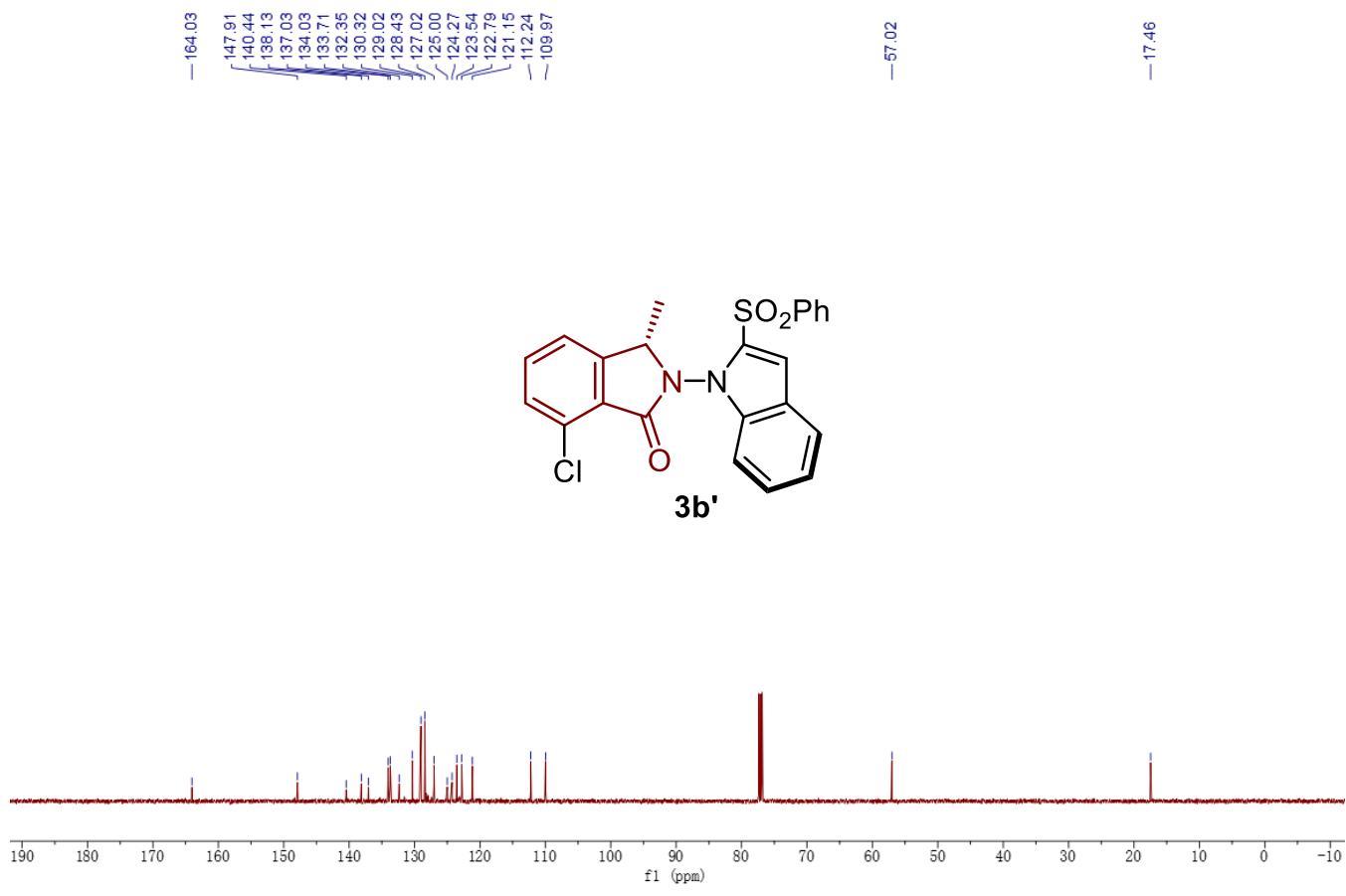


—166.47
—143.60 [141.23 138.39 136.76 135.00 133.60 133.30 129.01 128.92 128.84 128.34 127.07 124.26 123.44 122.84 122.25 112.67 110.25]
—57.91
—2.99 ±
—2.97 ±
—18.81
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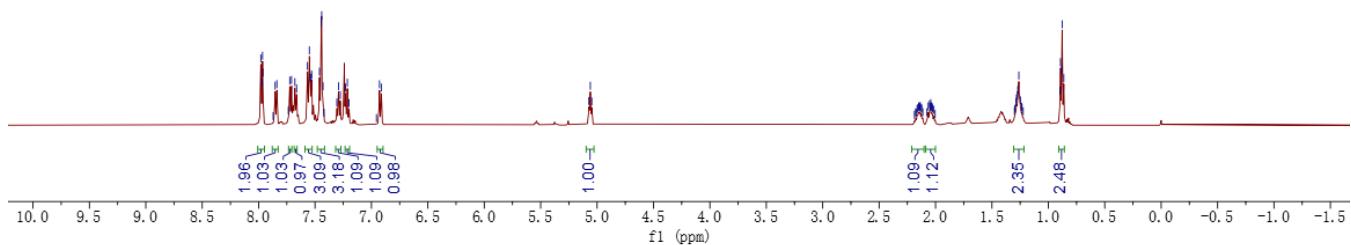
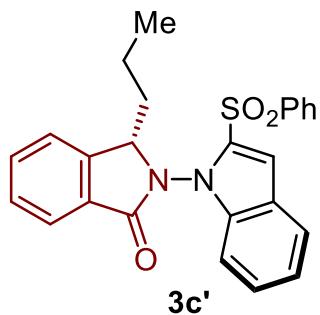




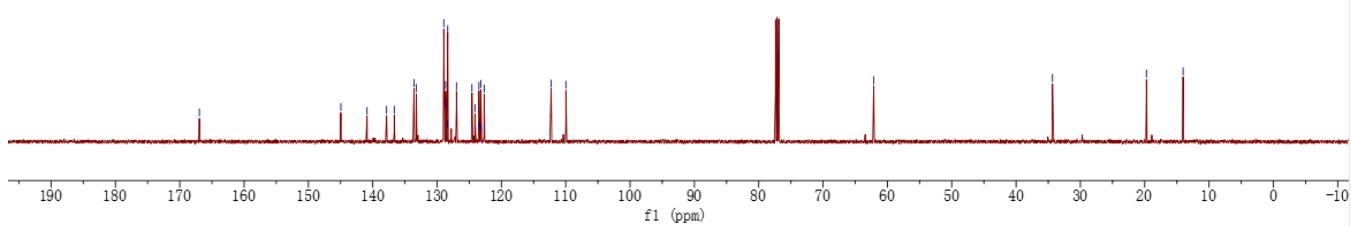
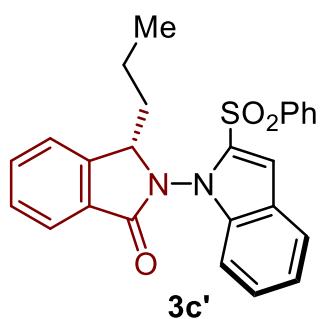
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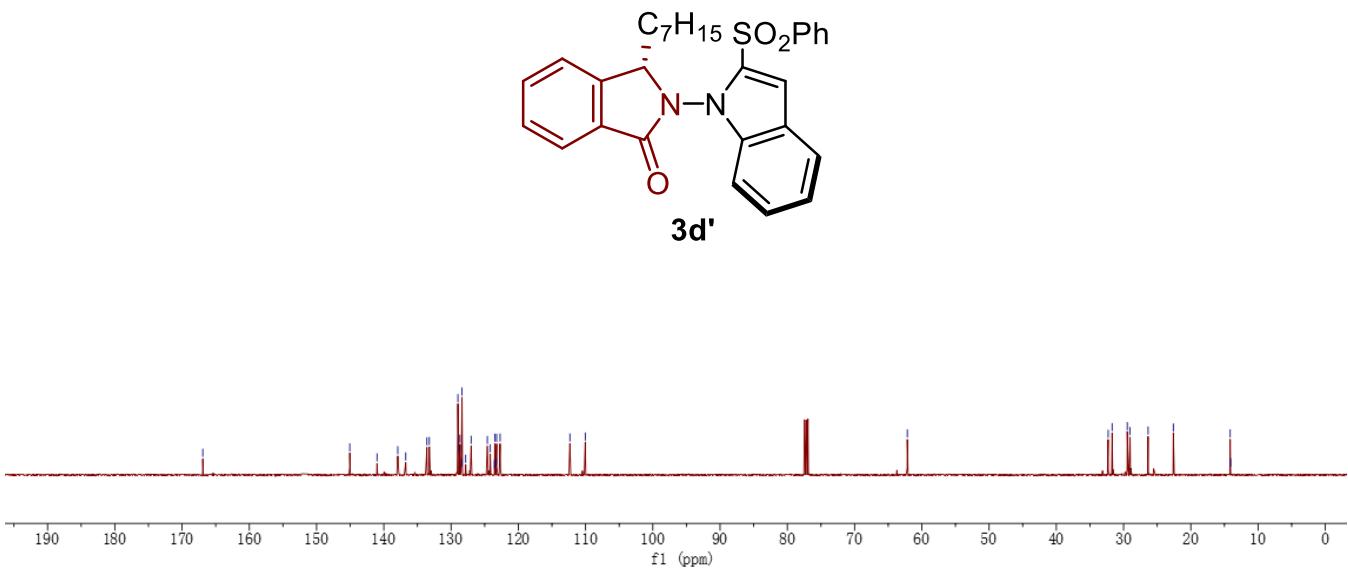
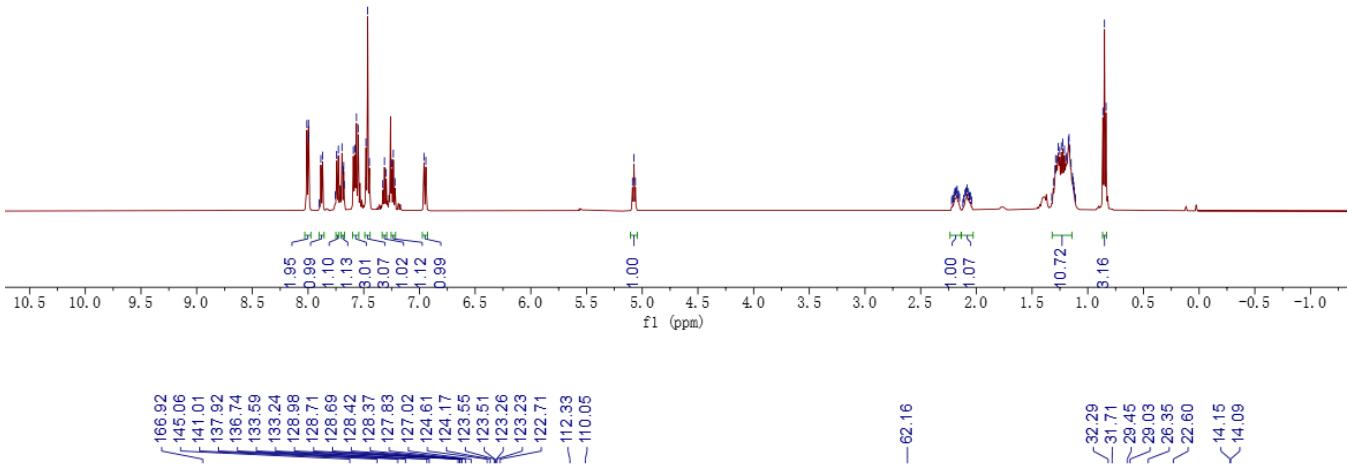


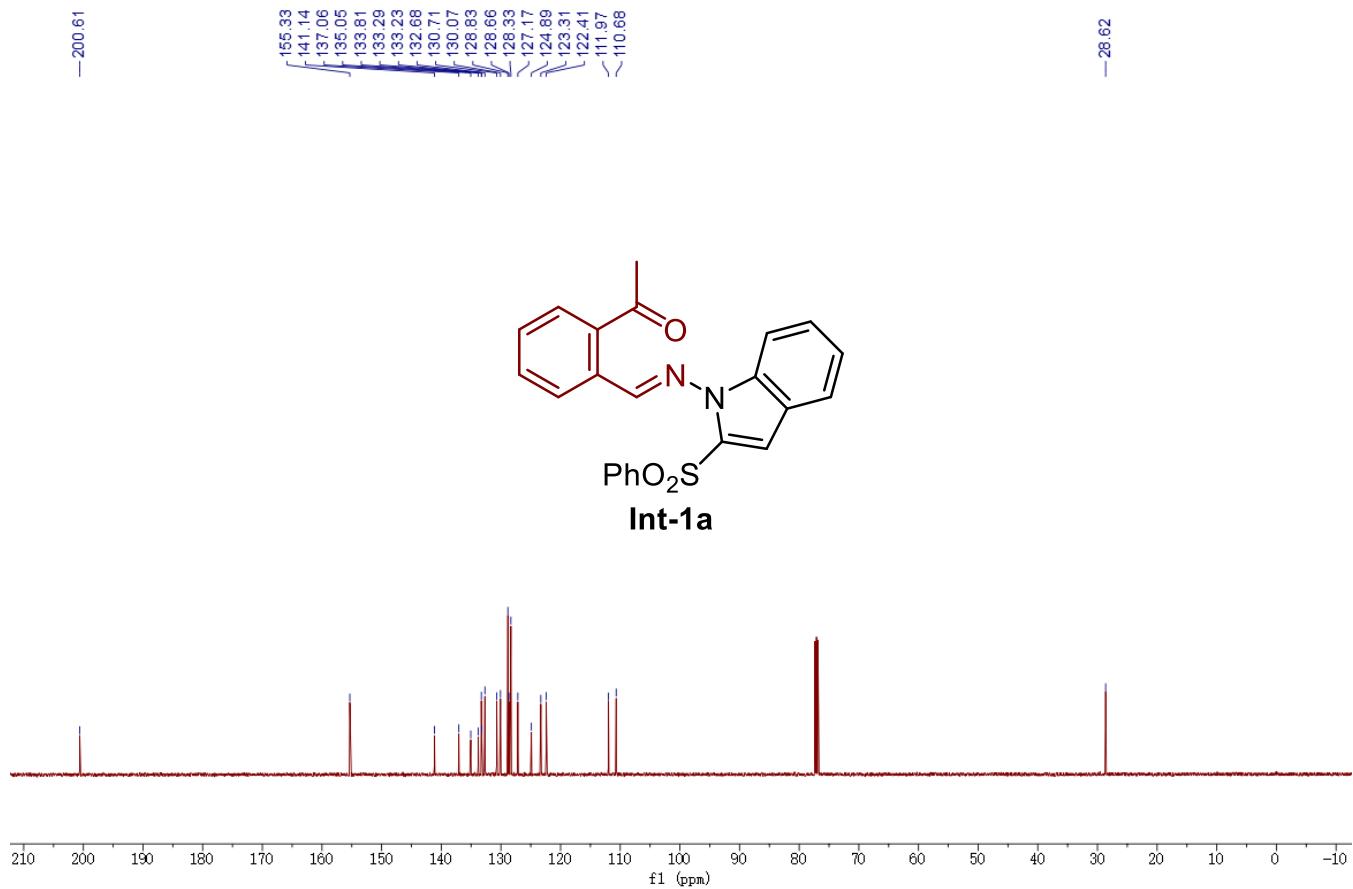
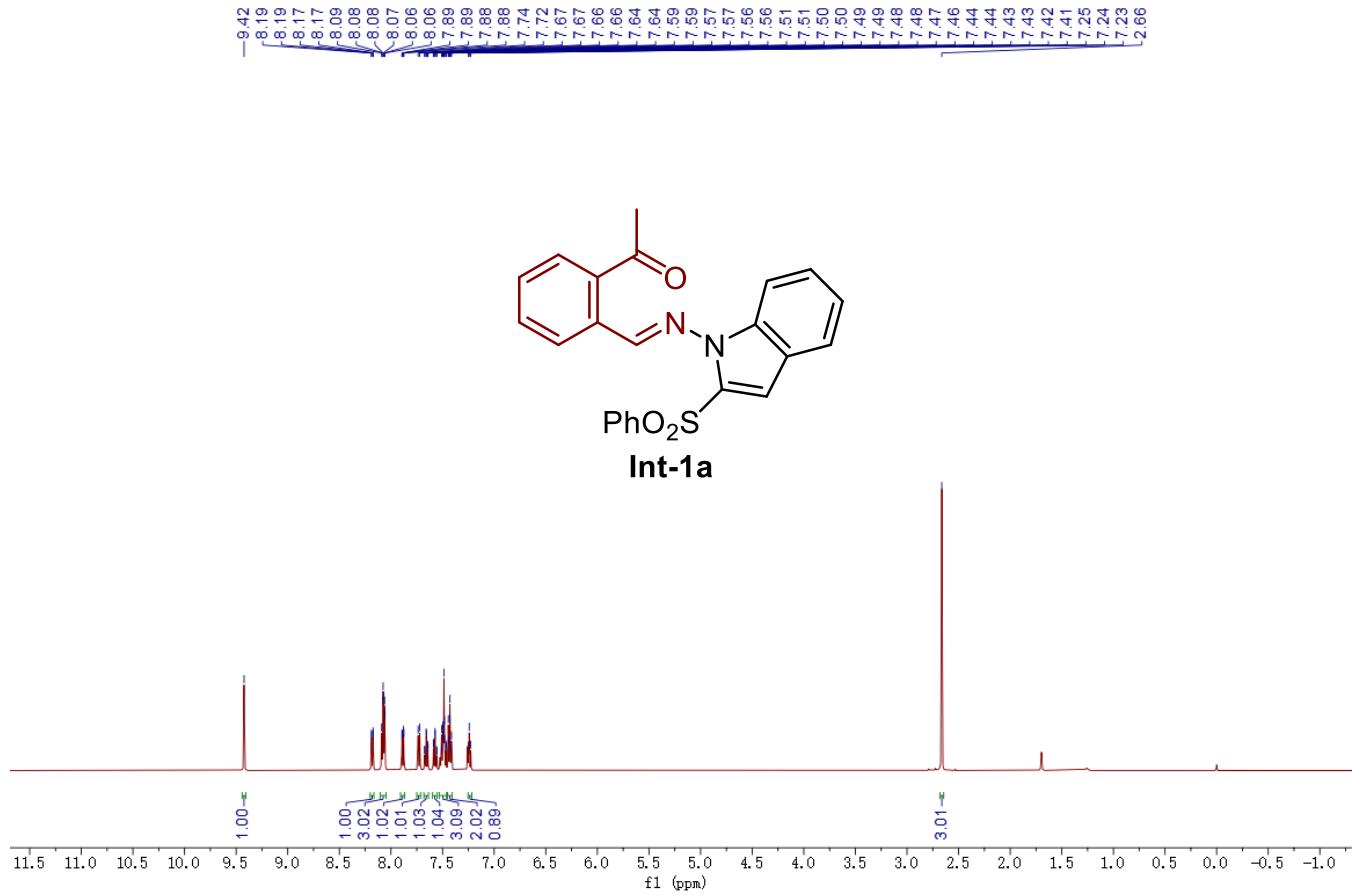
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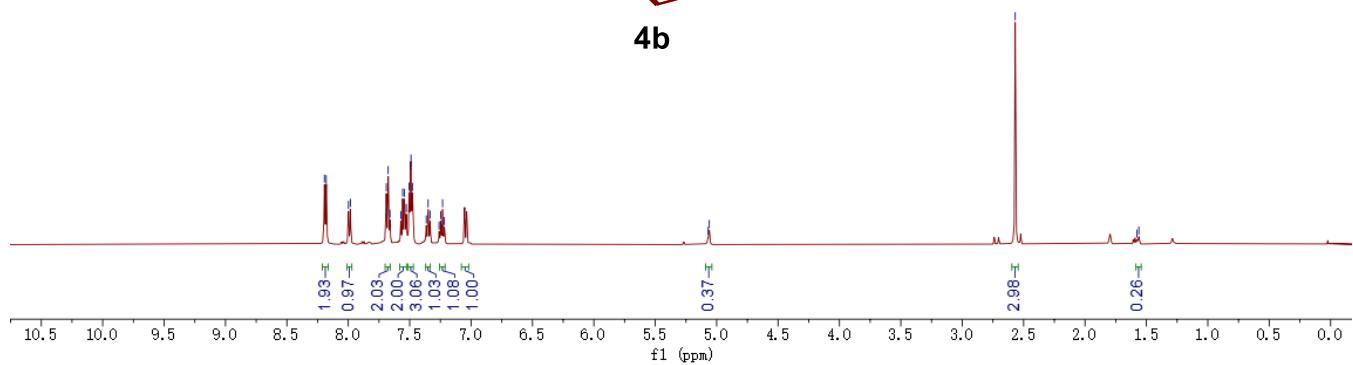
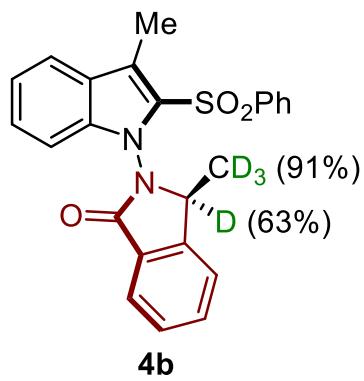
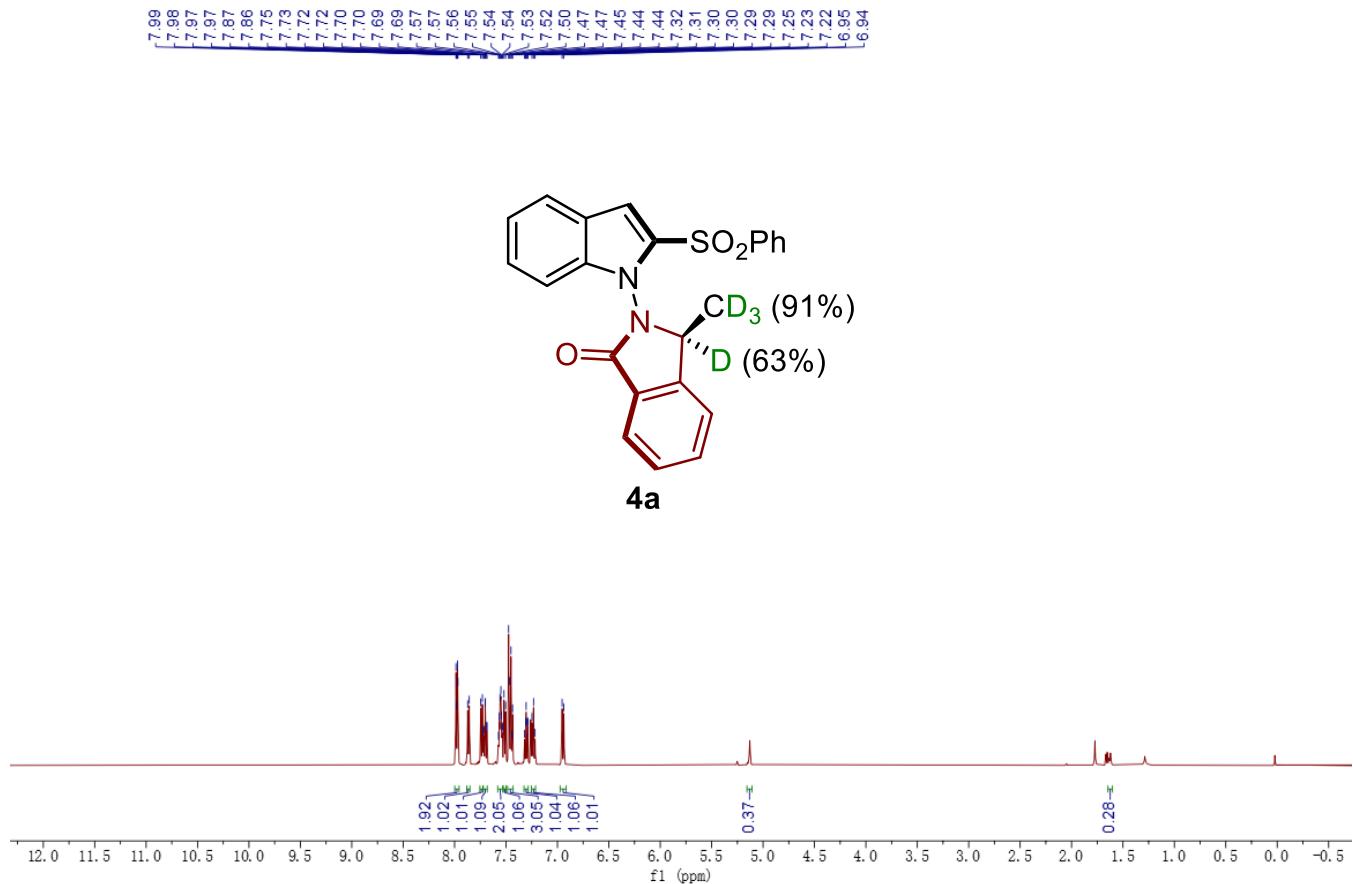


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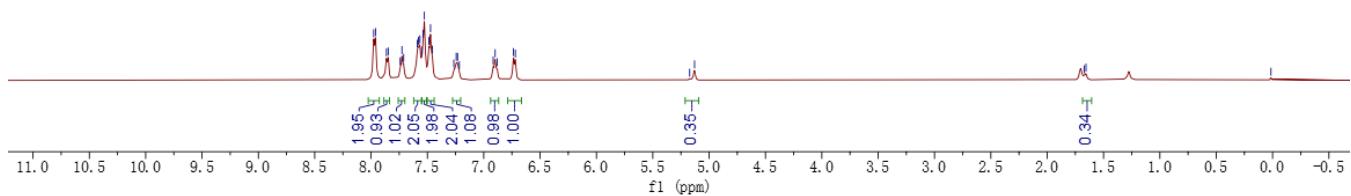
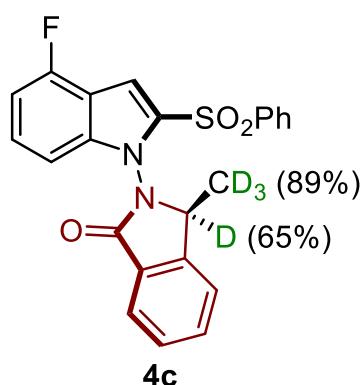


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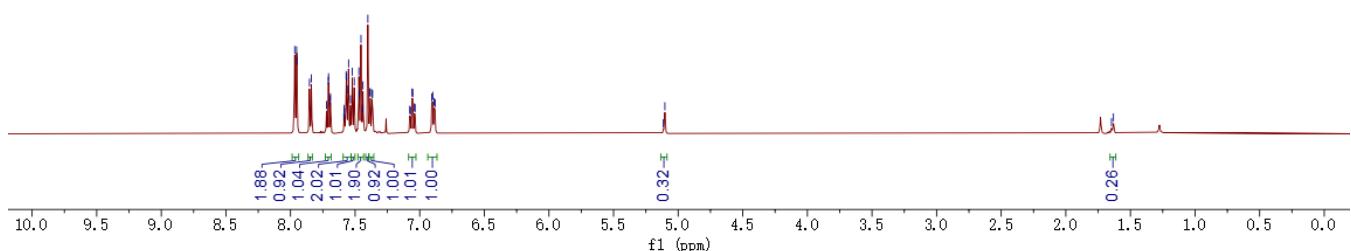
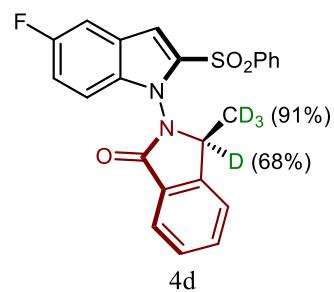
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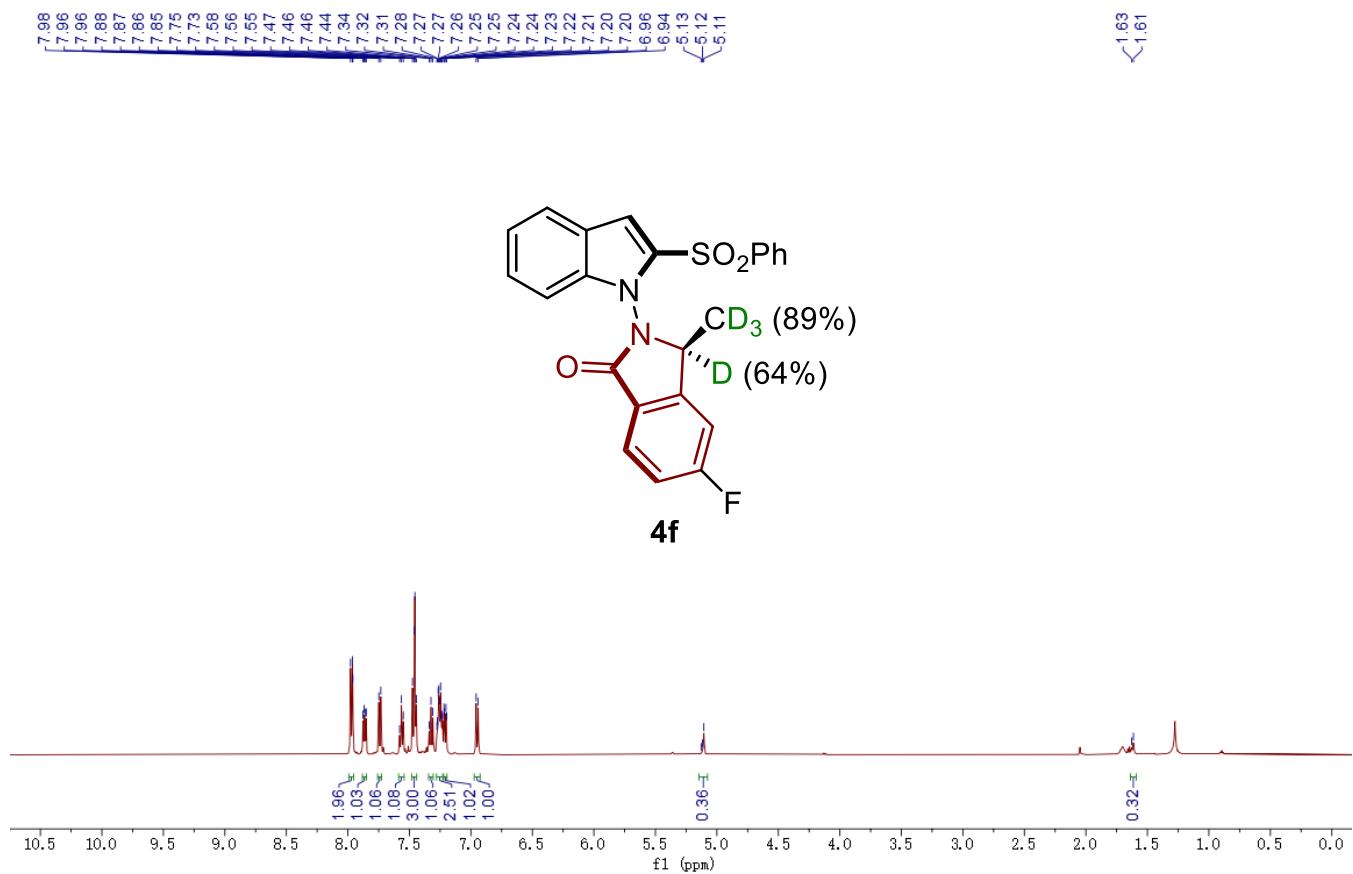
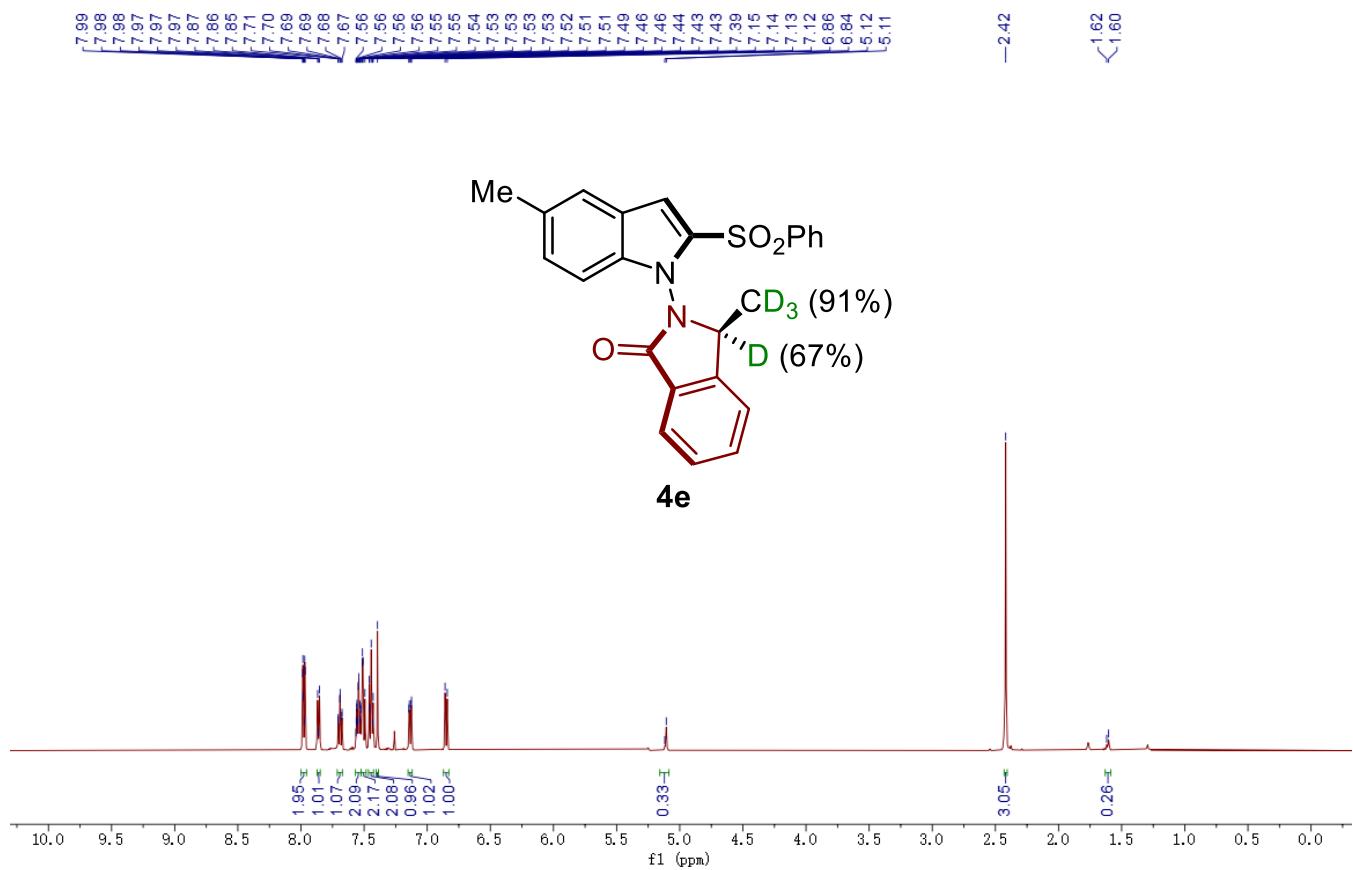
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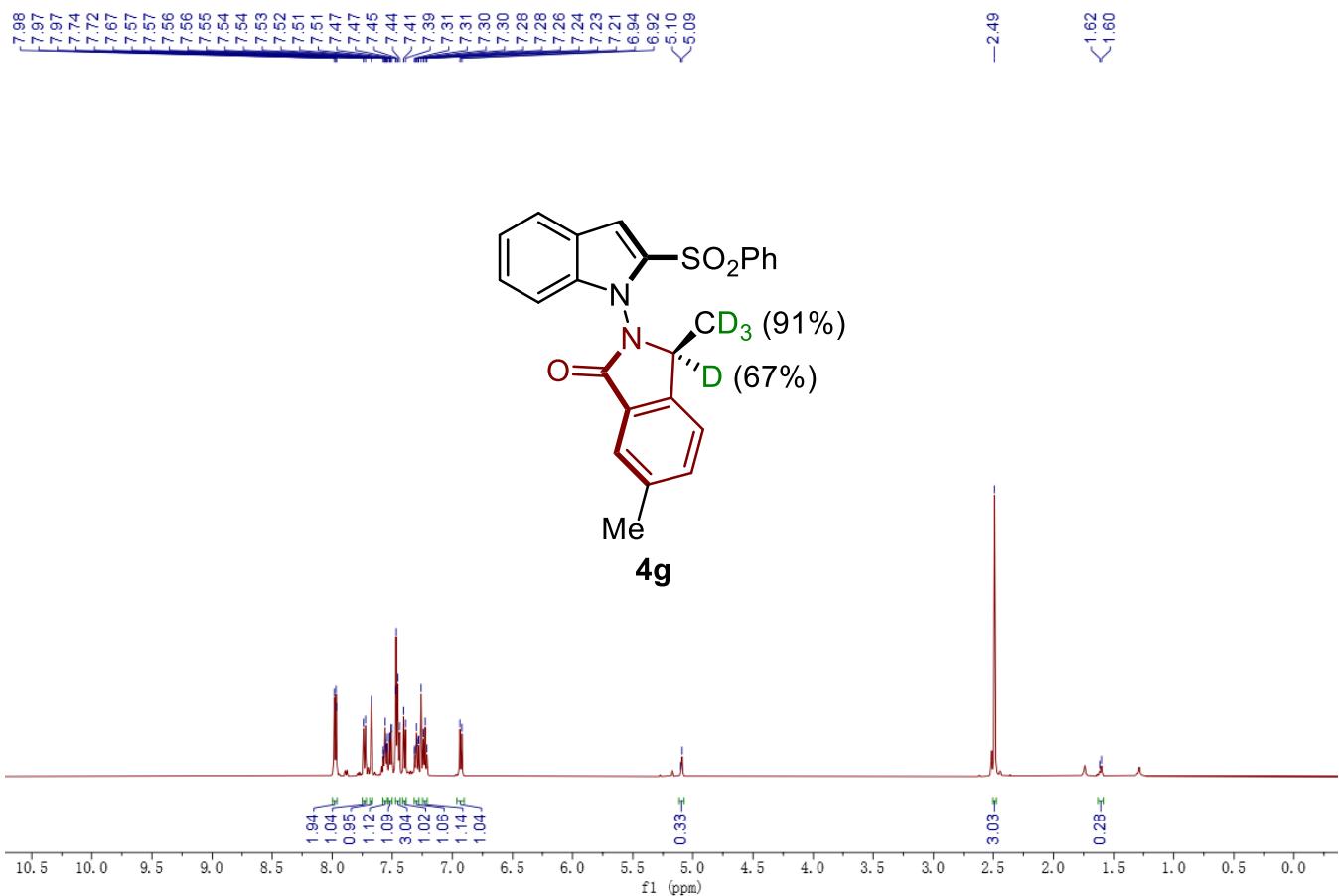


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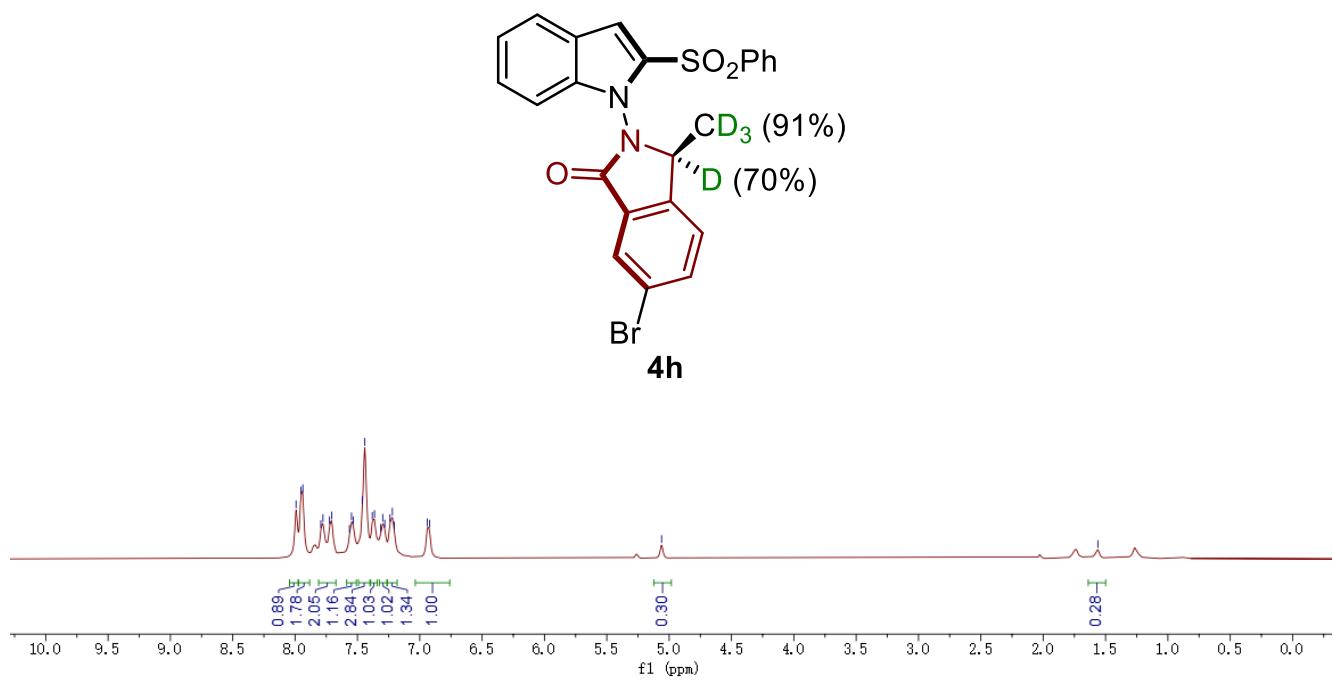


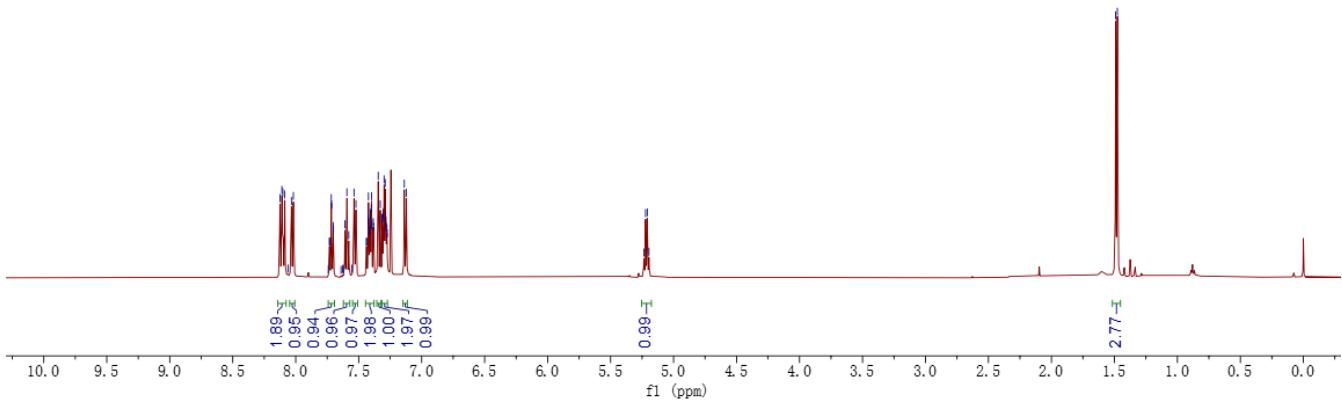
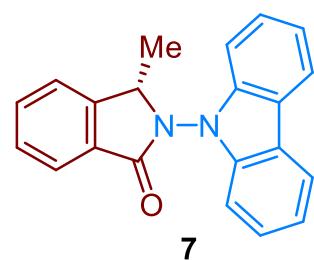
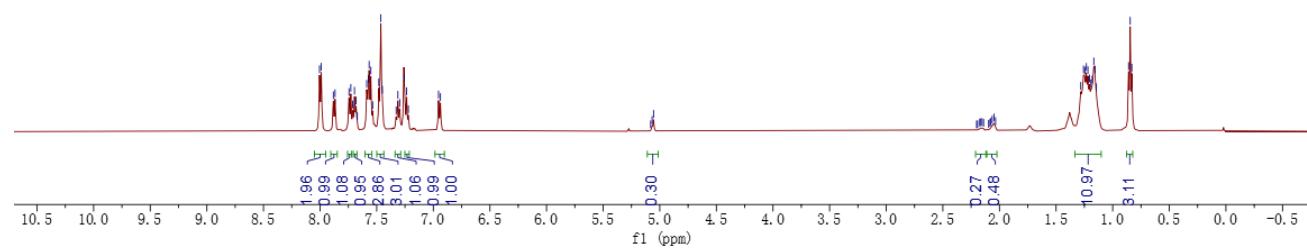


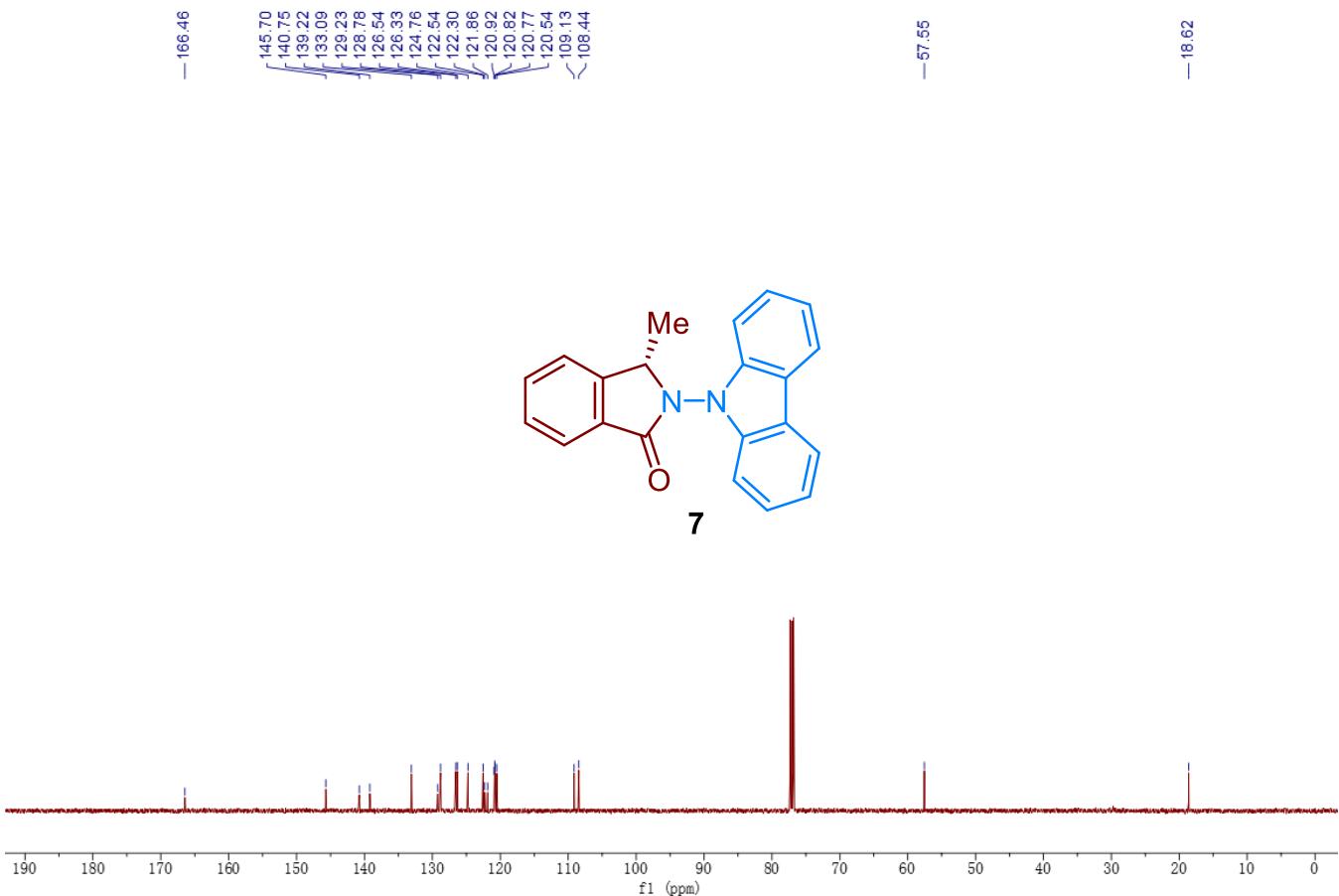


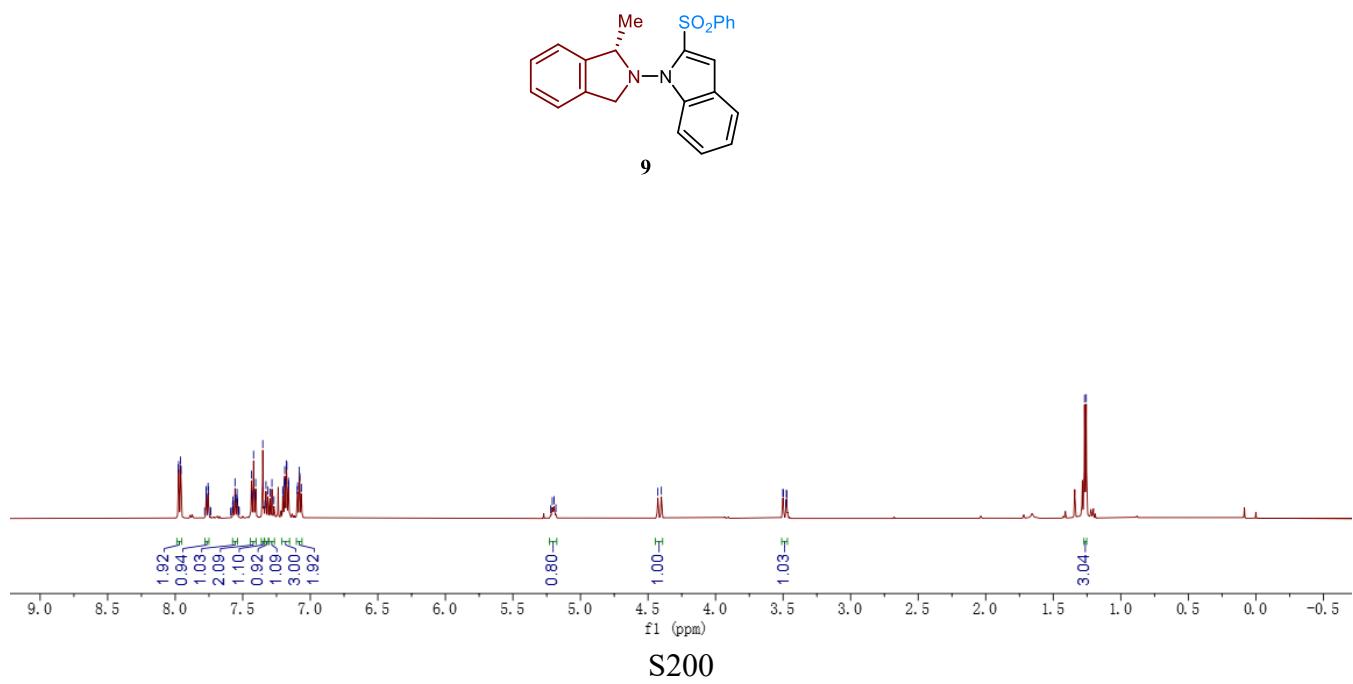
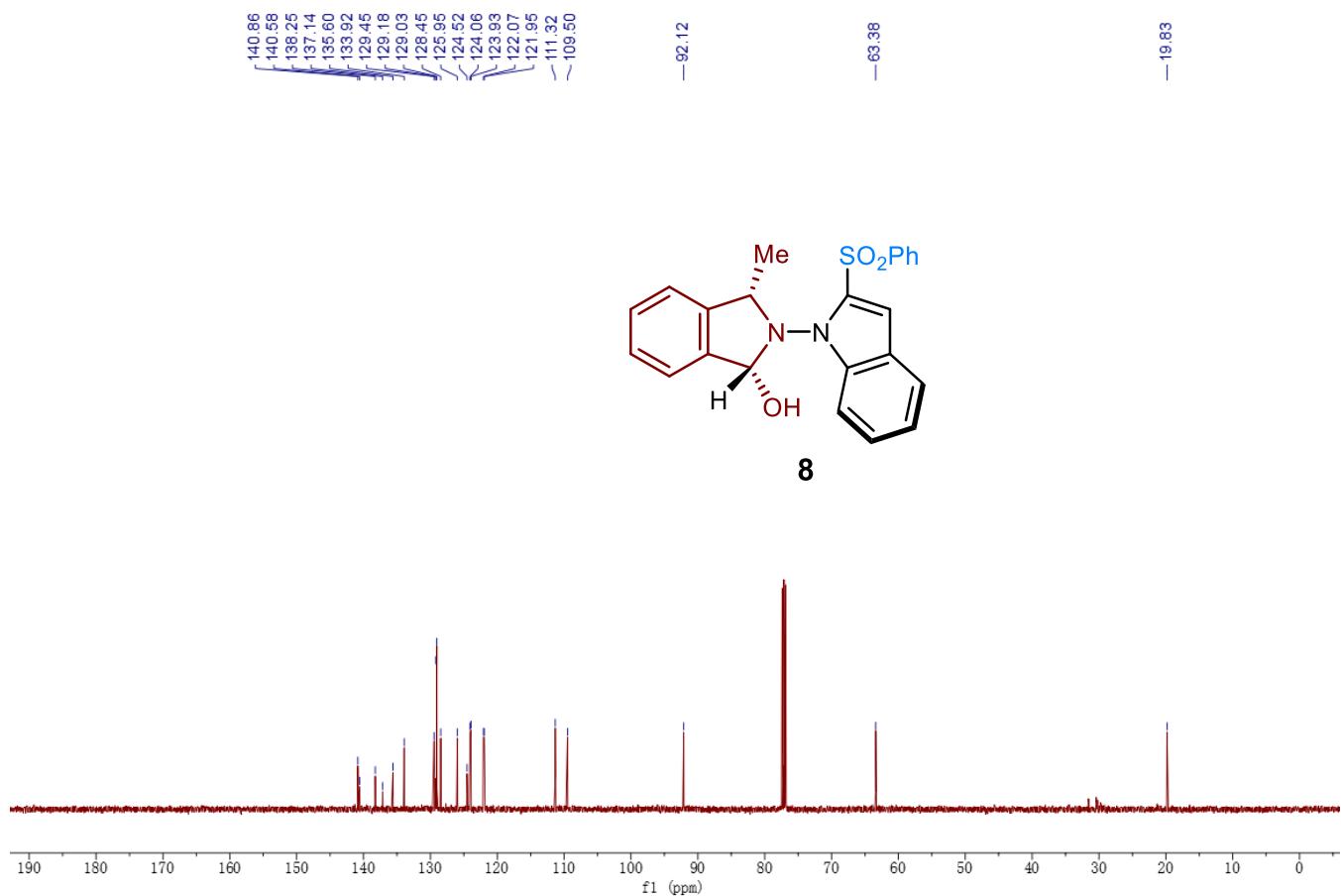
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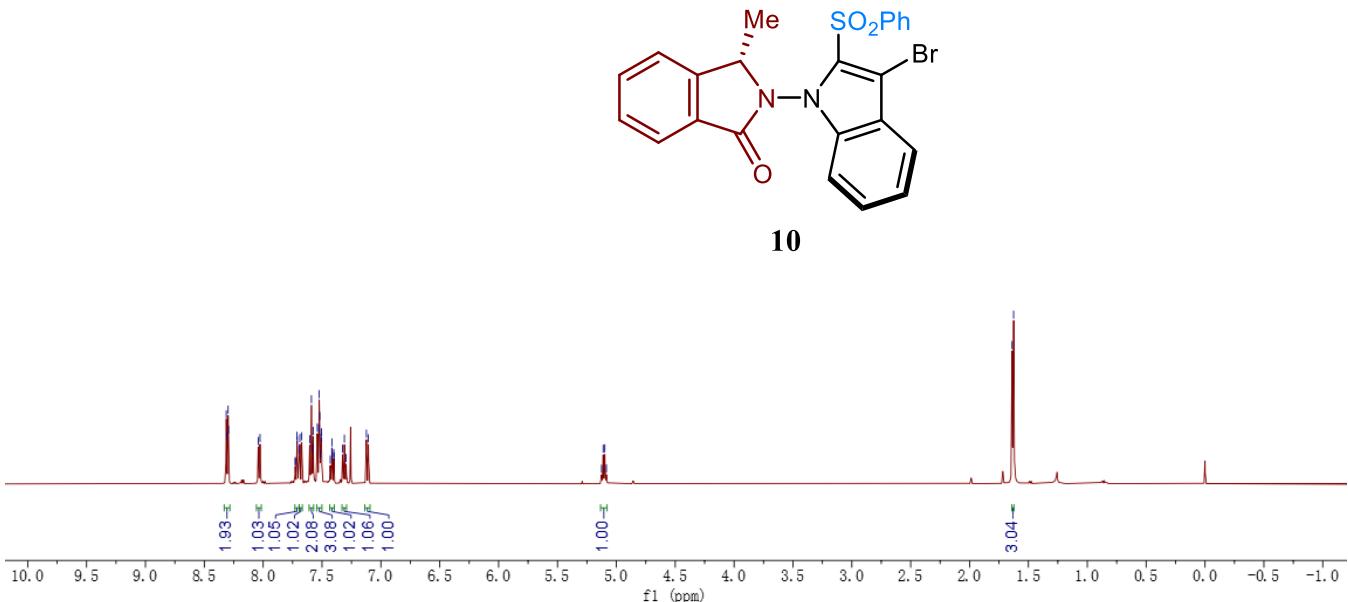
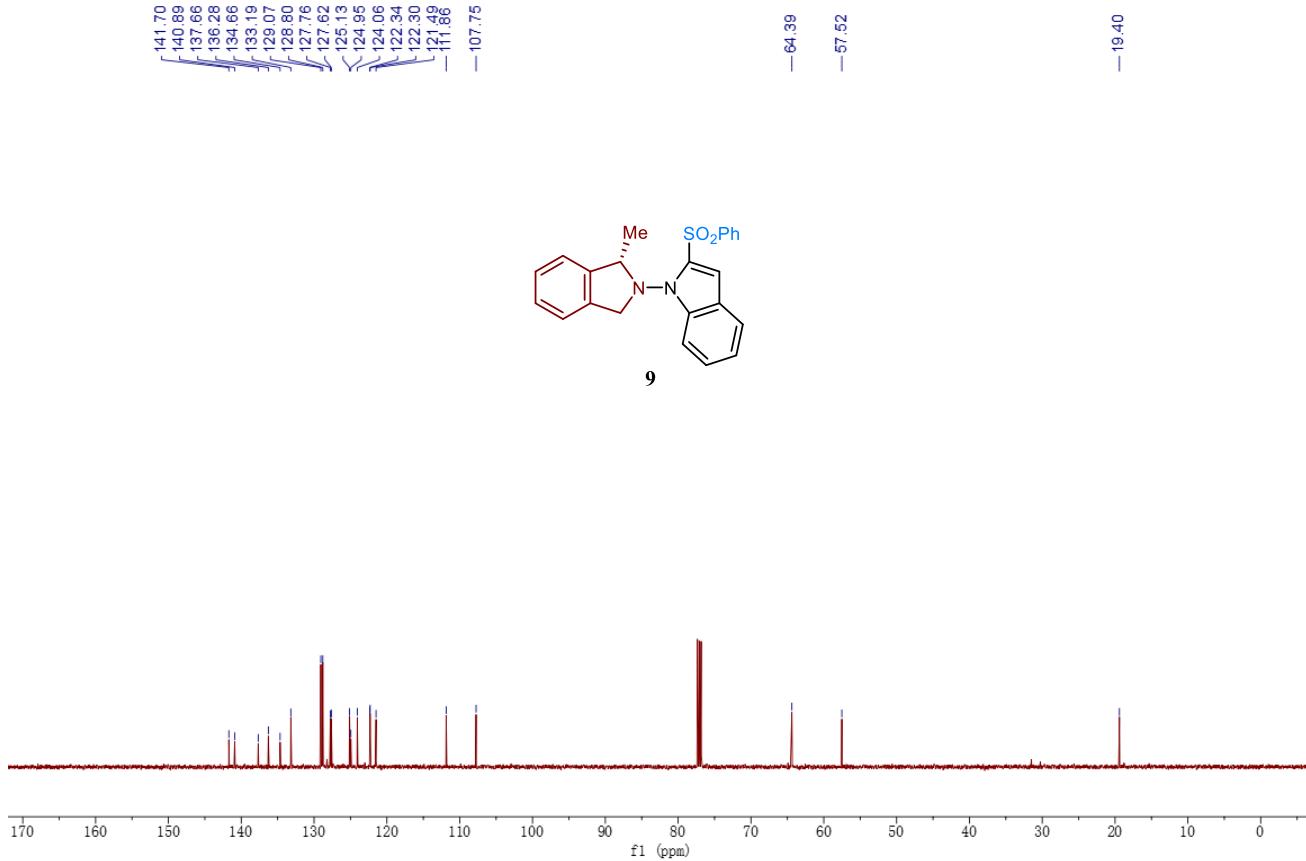
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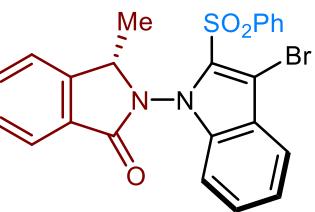
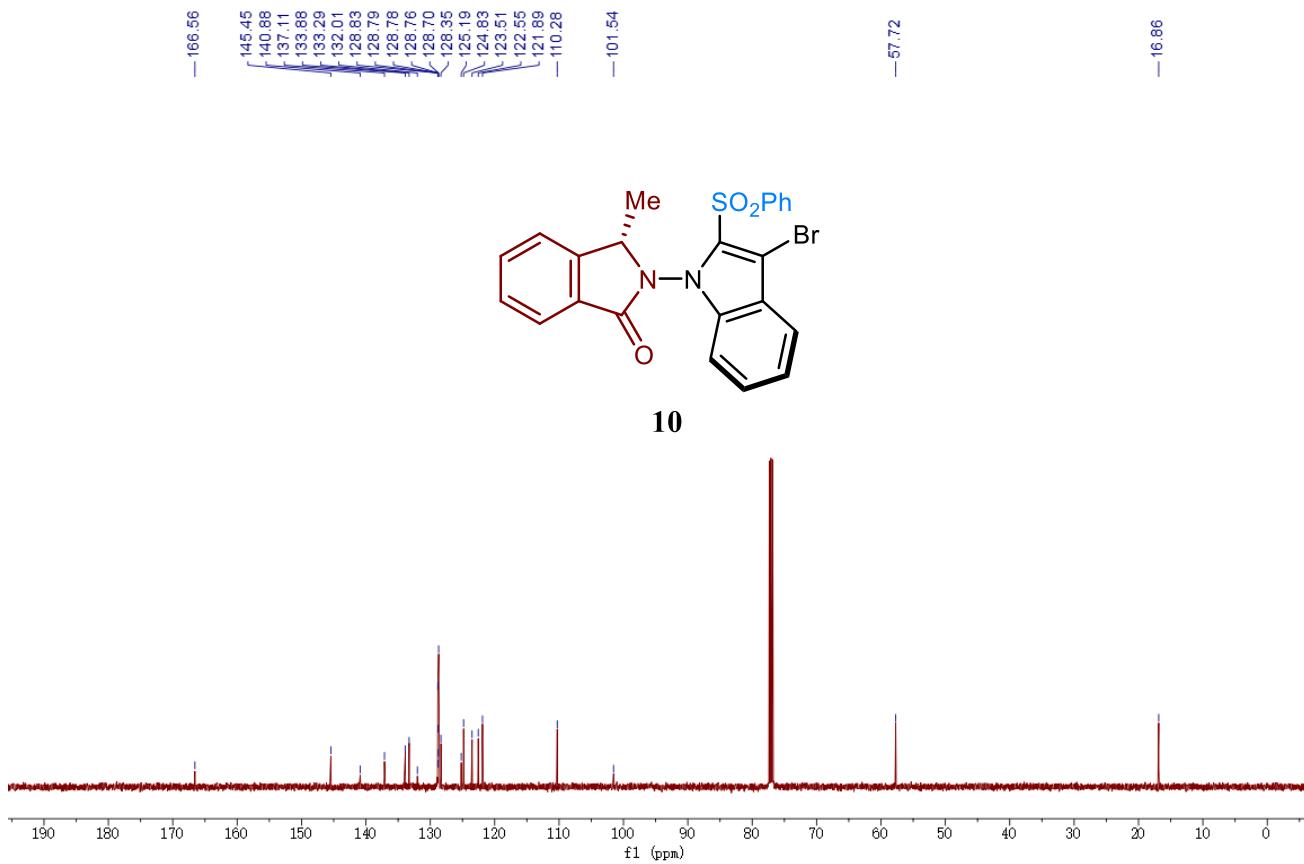




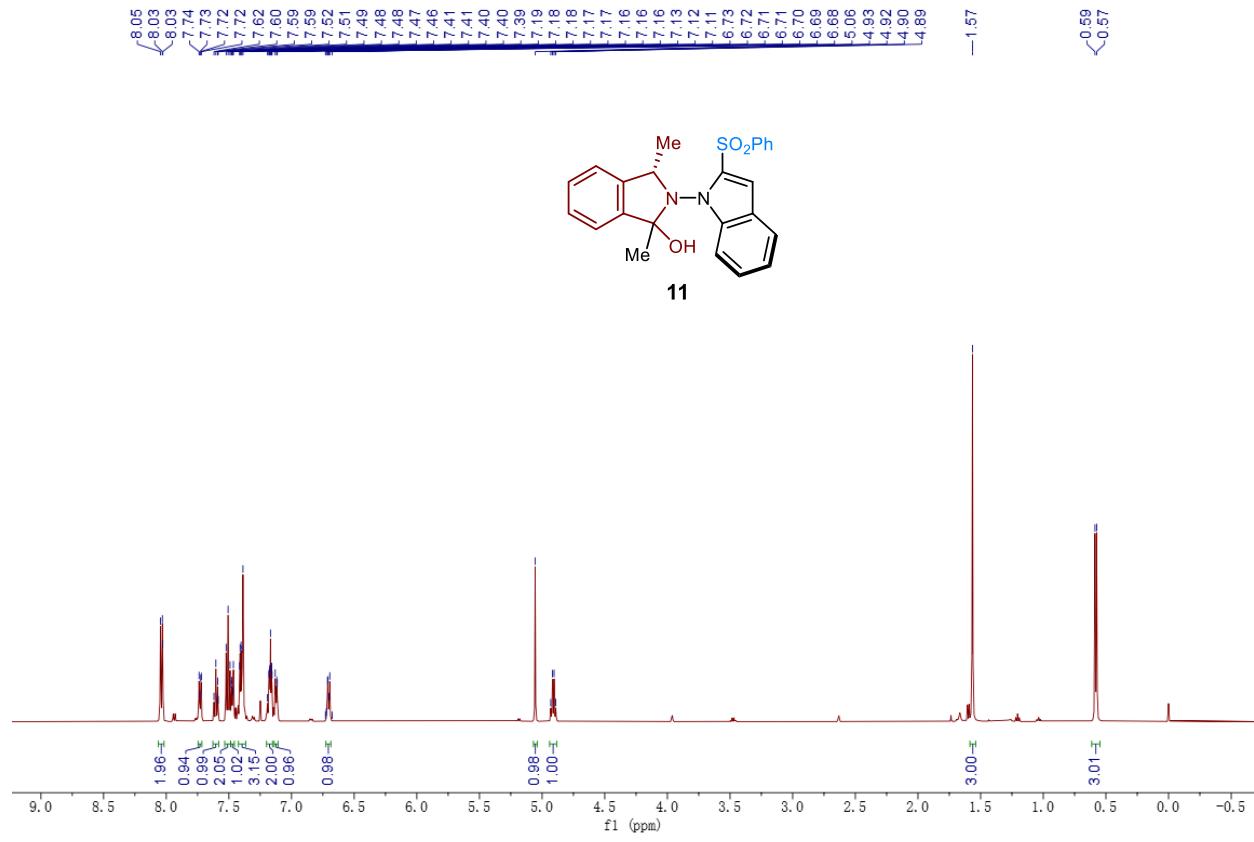




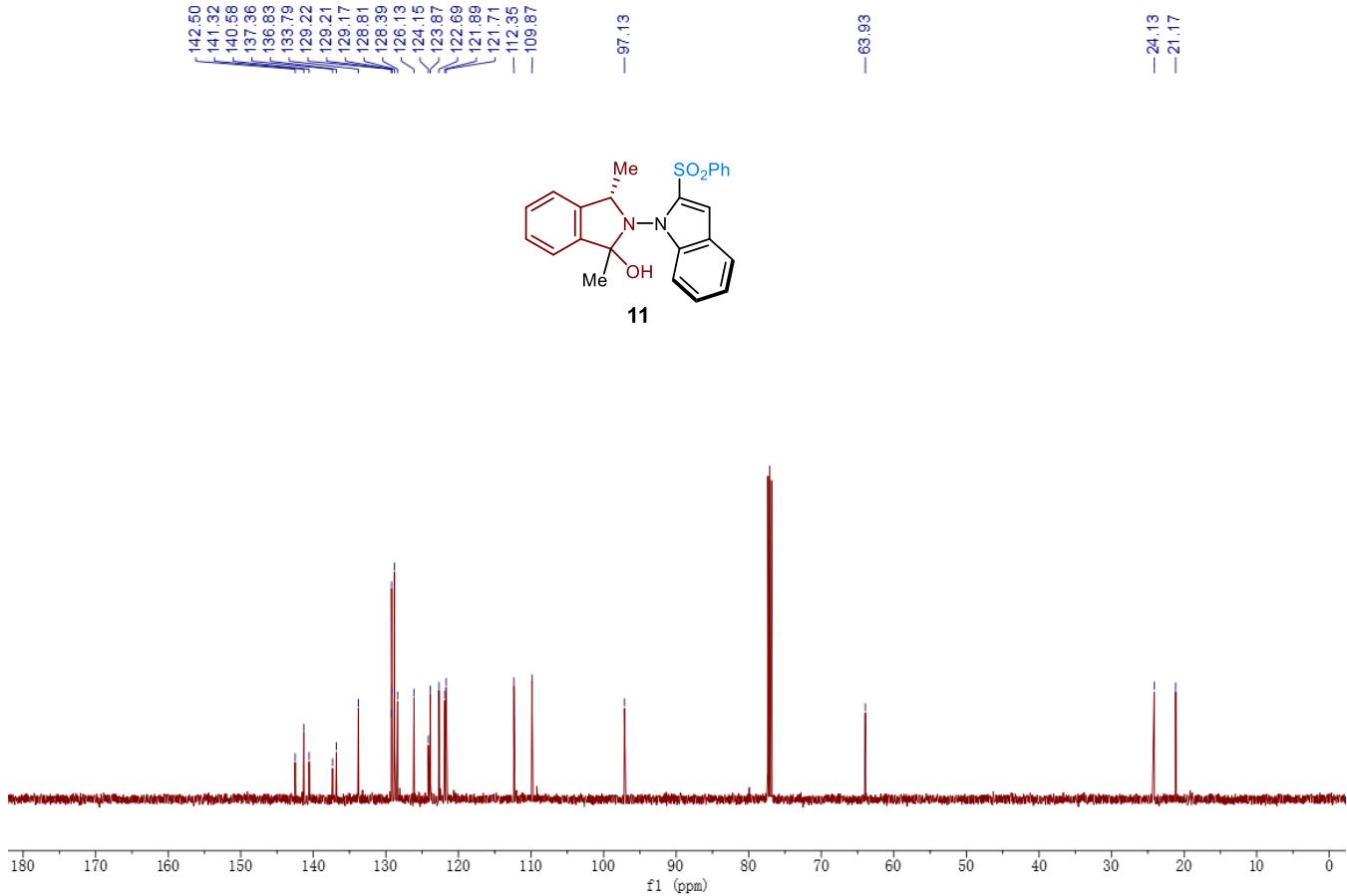




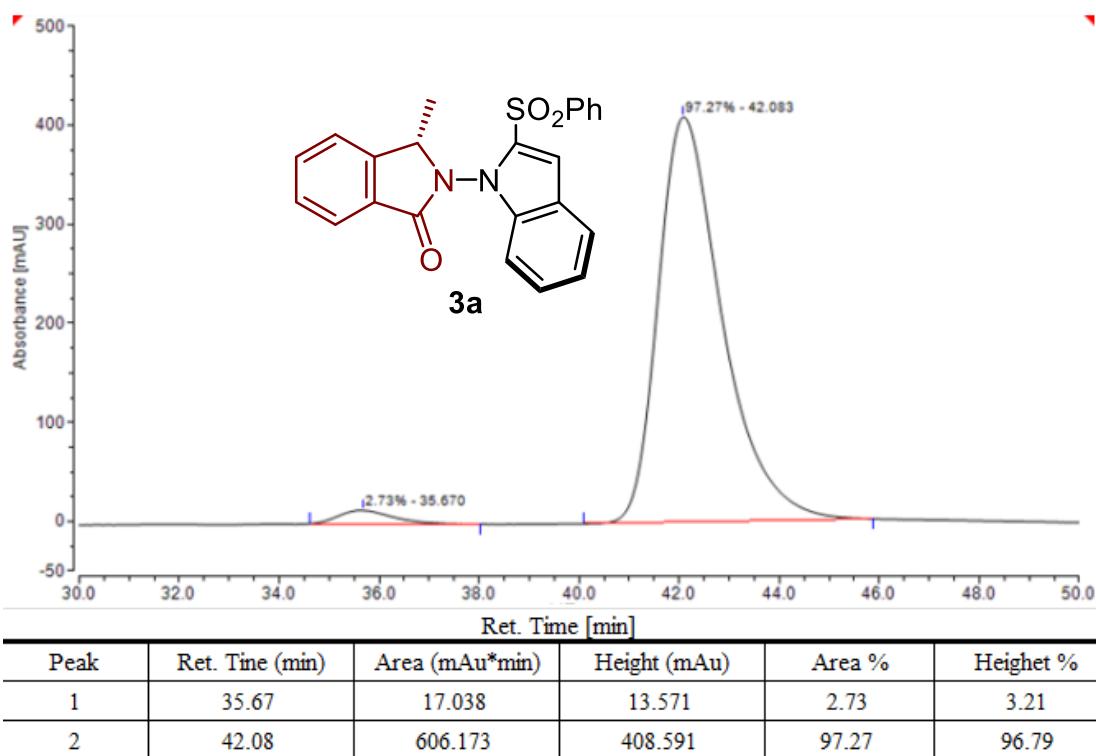
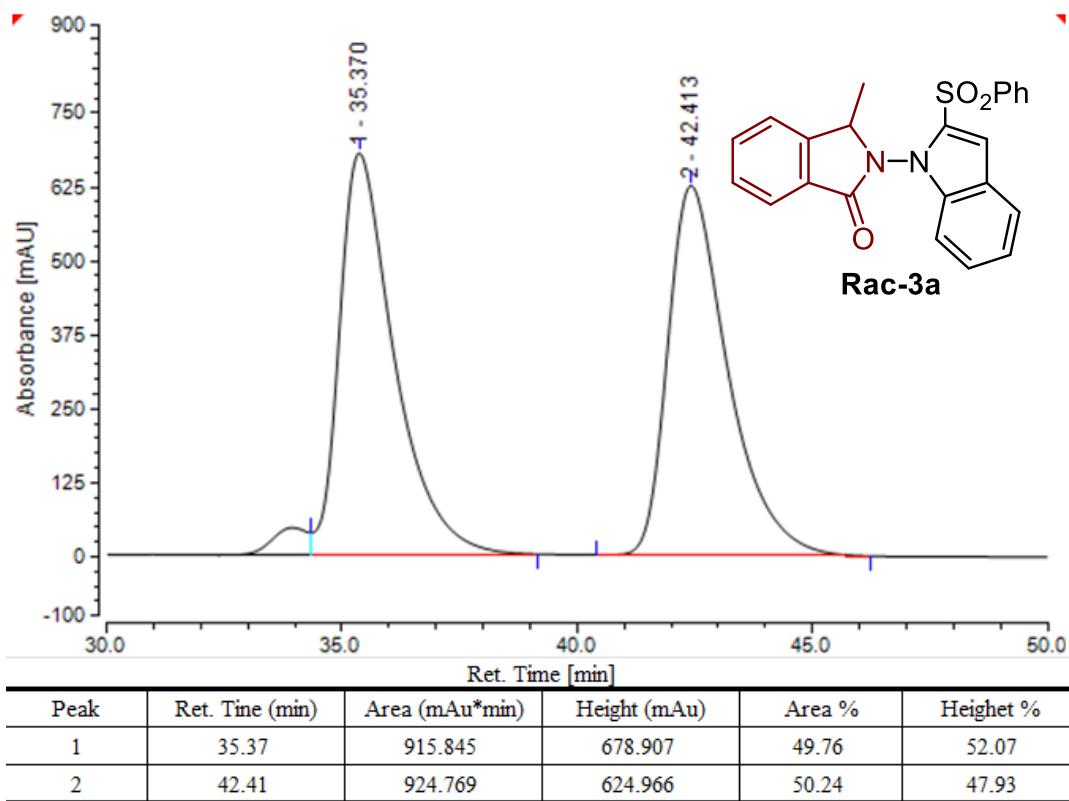
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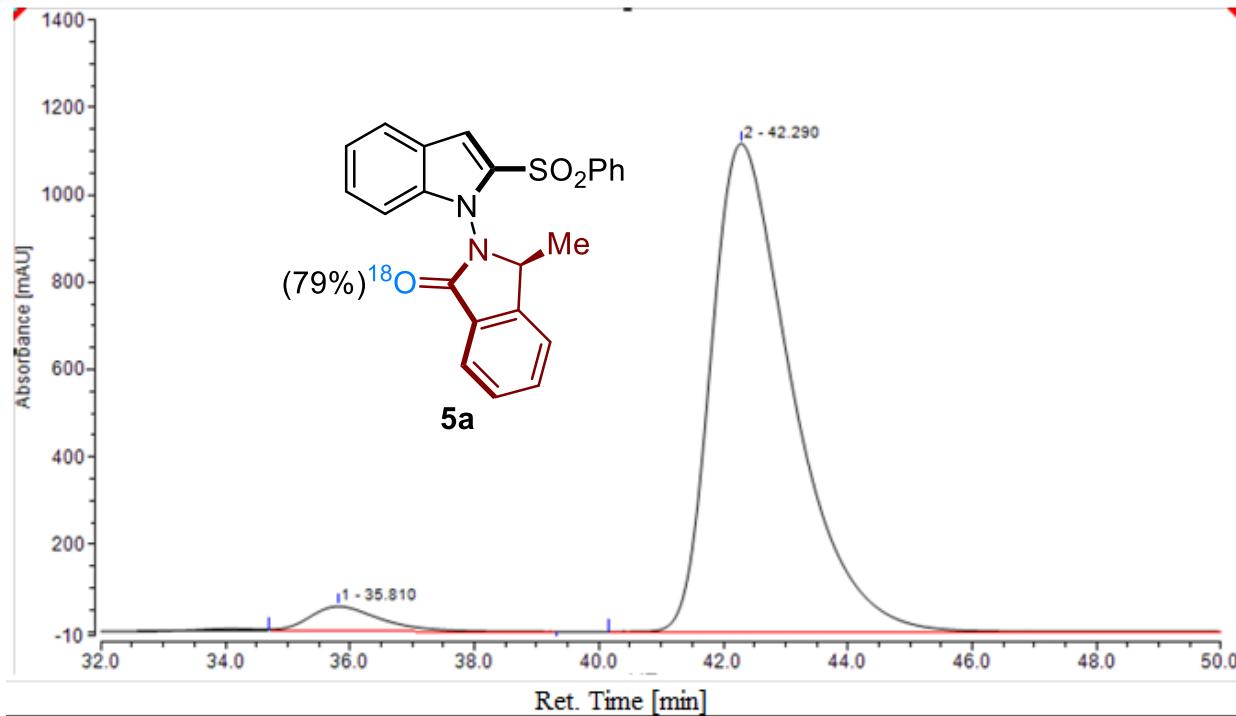
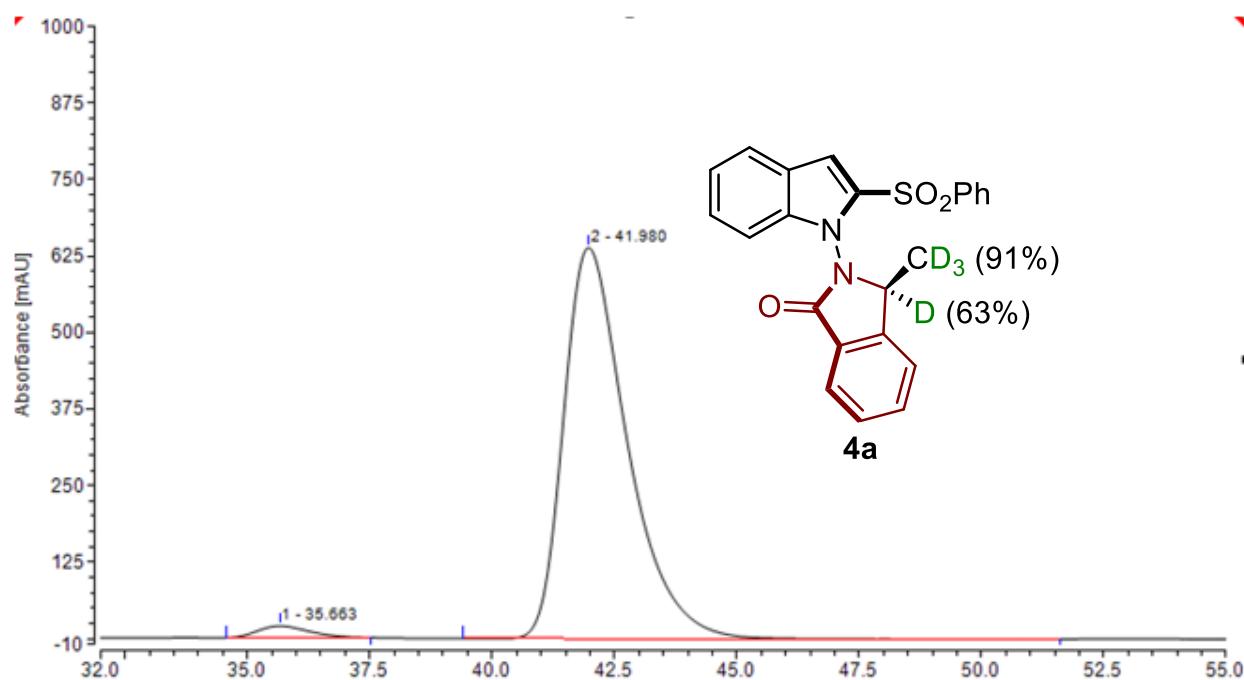


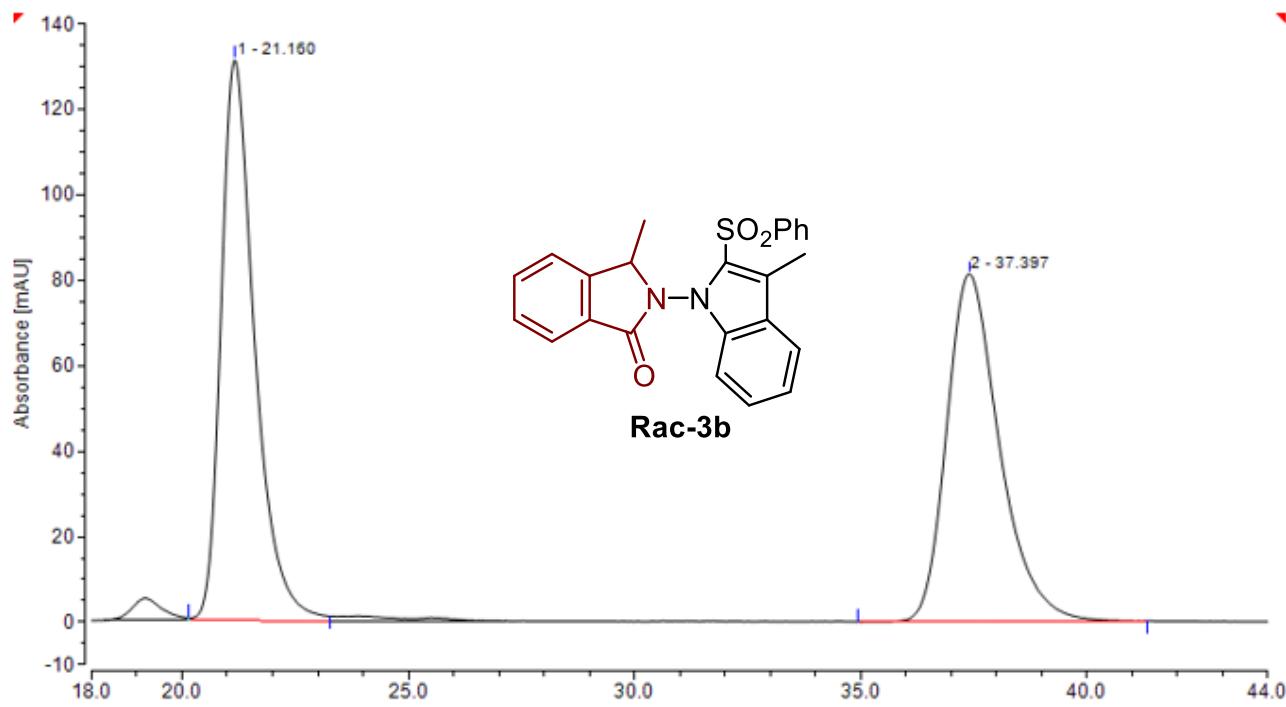
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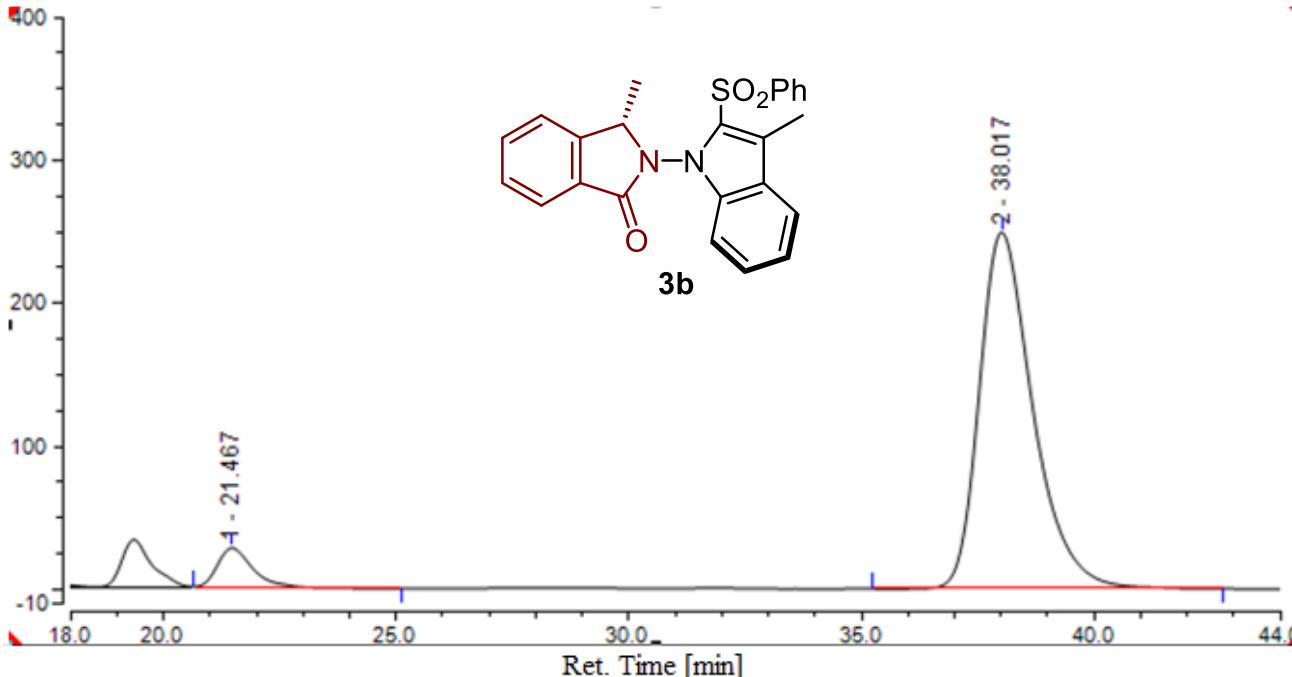
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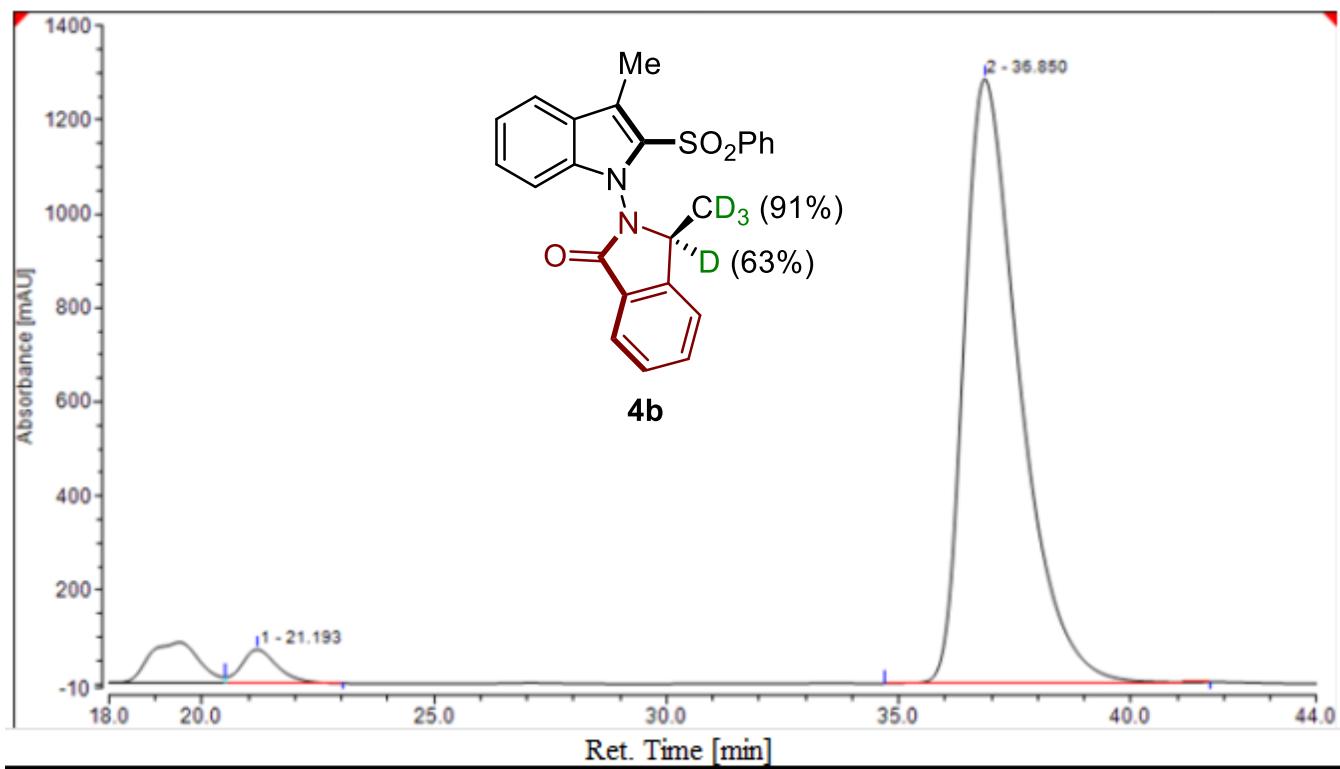




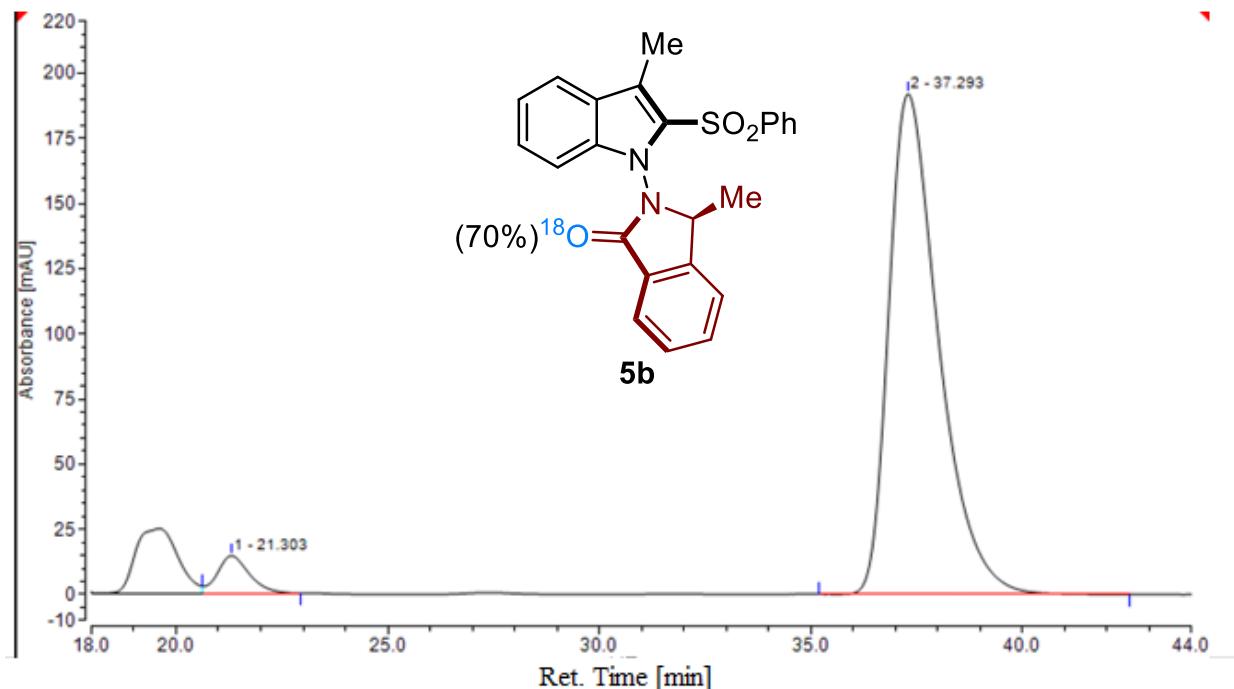
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Heighet %
1	21.16	113.362	131.266	50.80	61.75
2	37.40	109.770	81.327	49.20	38.25



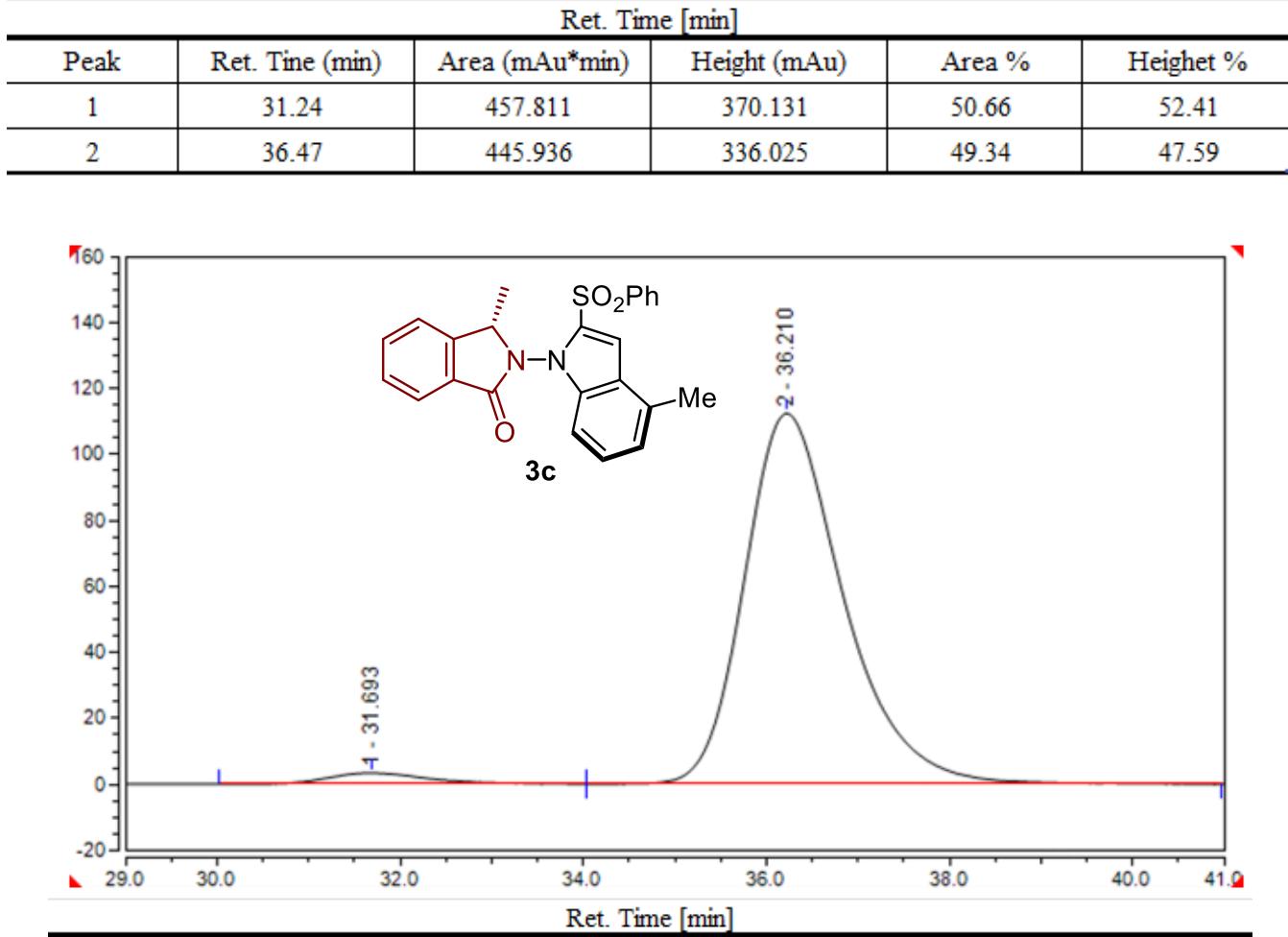
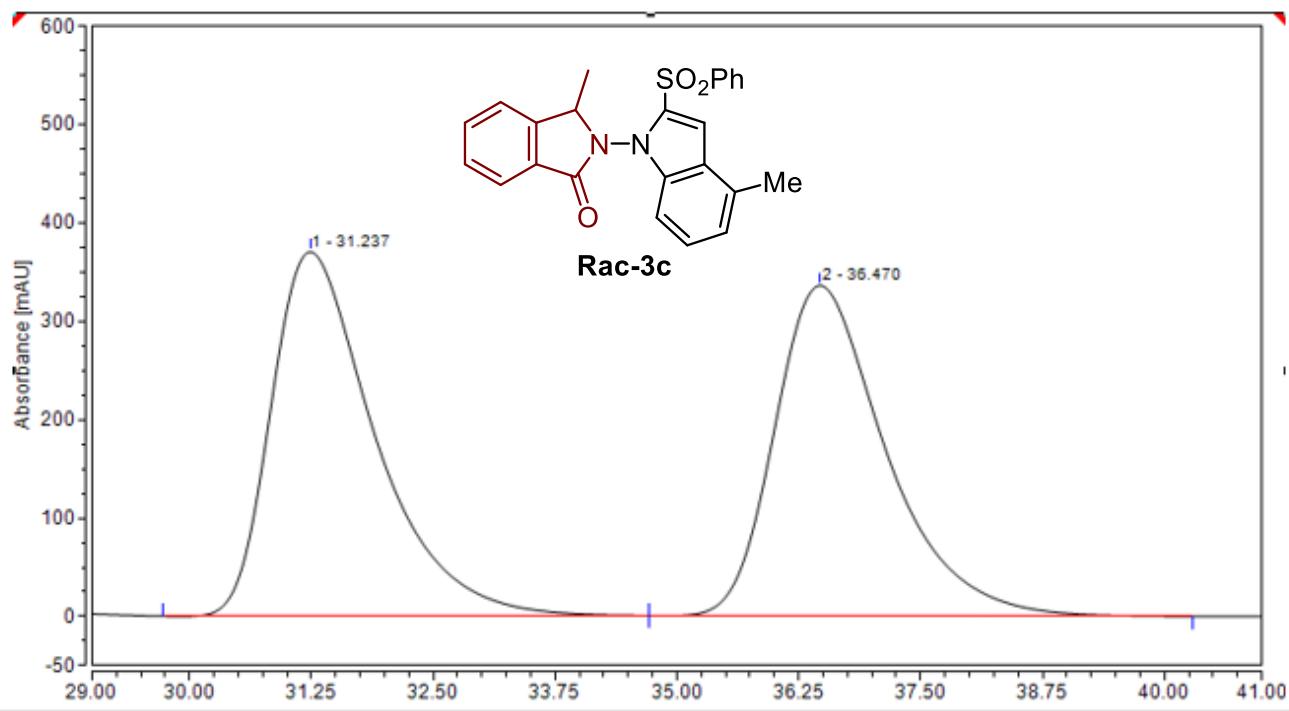
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Heighet %
1	21.47	25.606	28.210	7.16	10.17
2	38.02	332.140	249.201	92.84	89.83

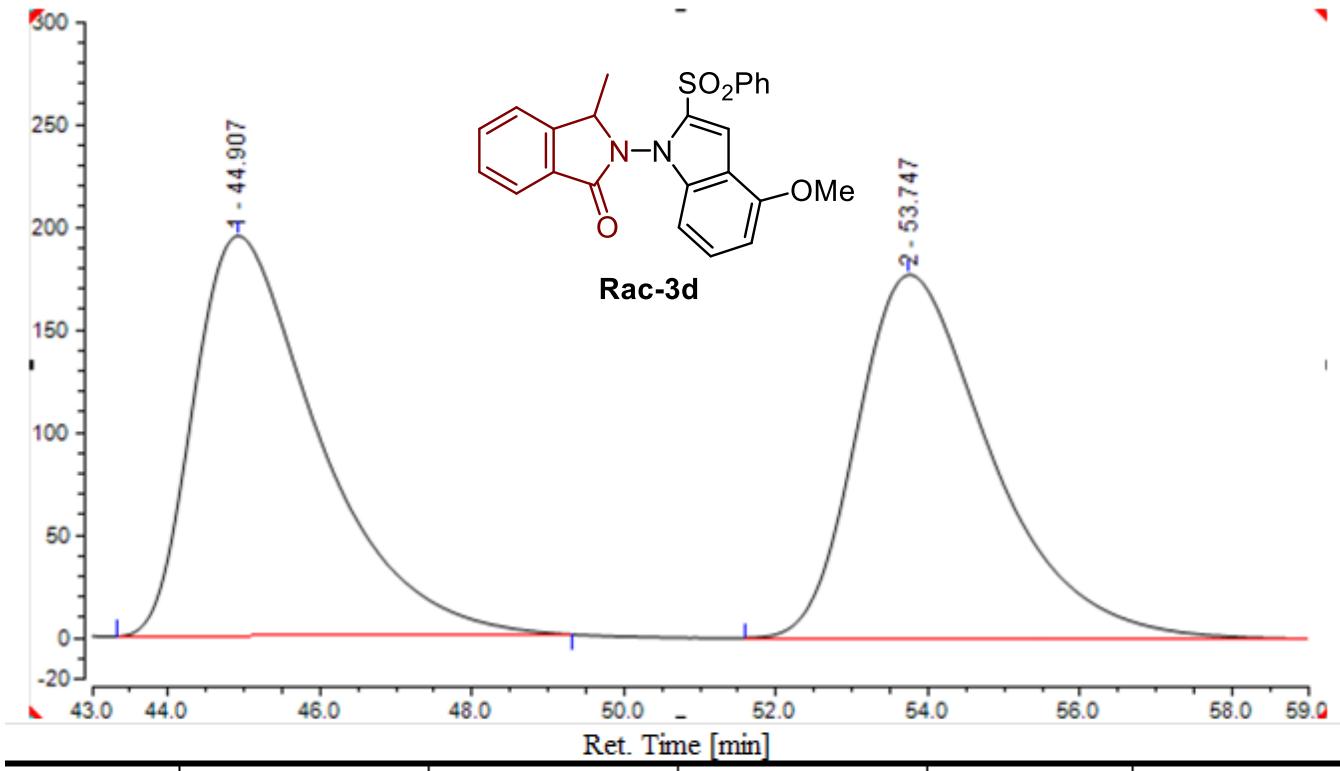
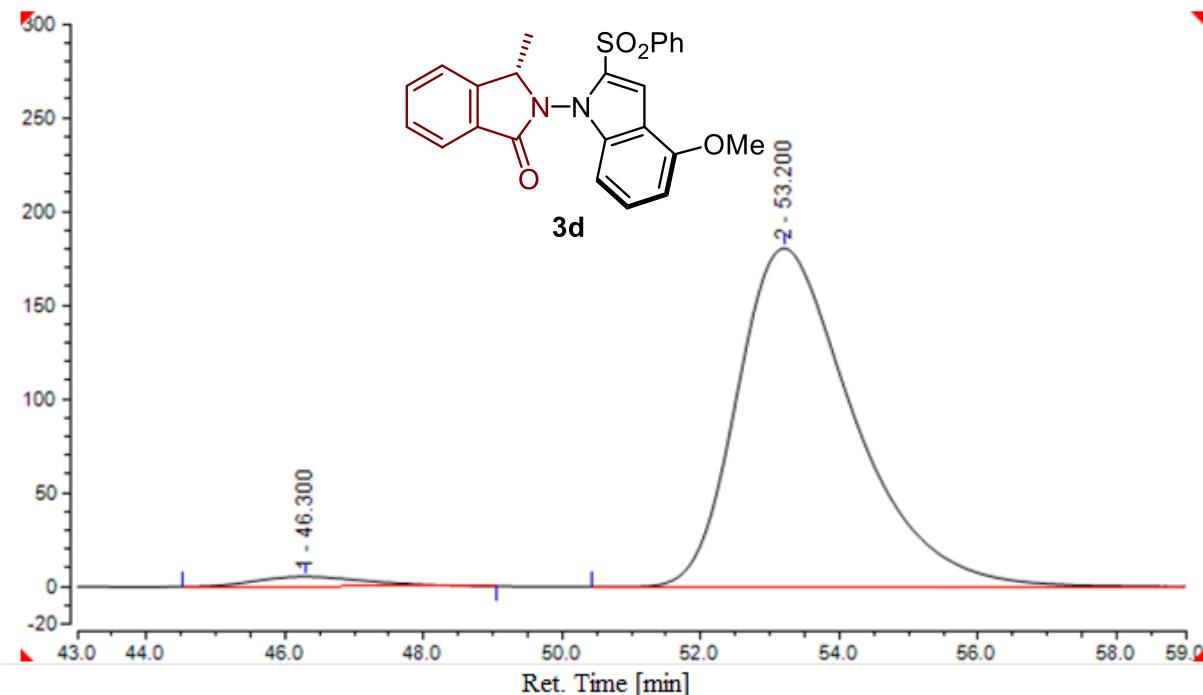


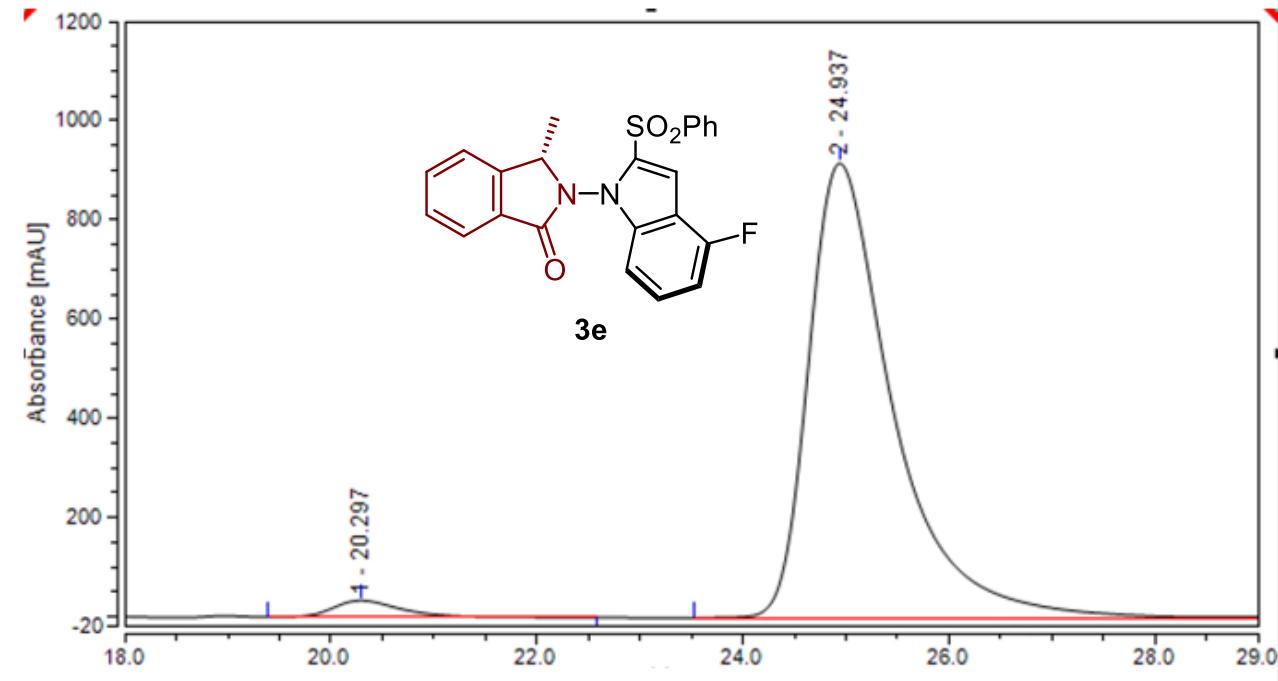
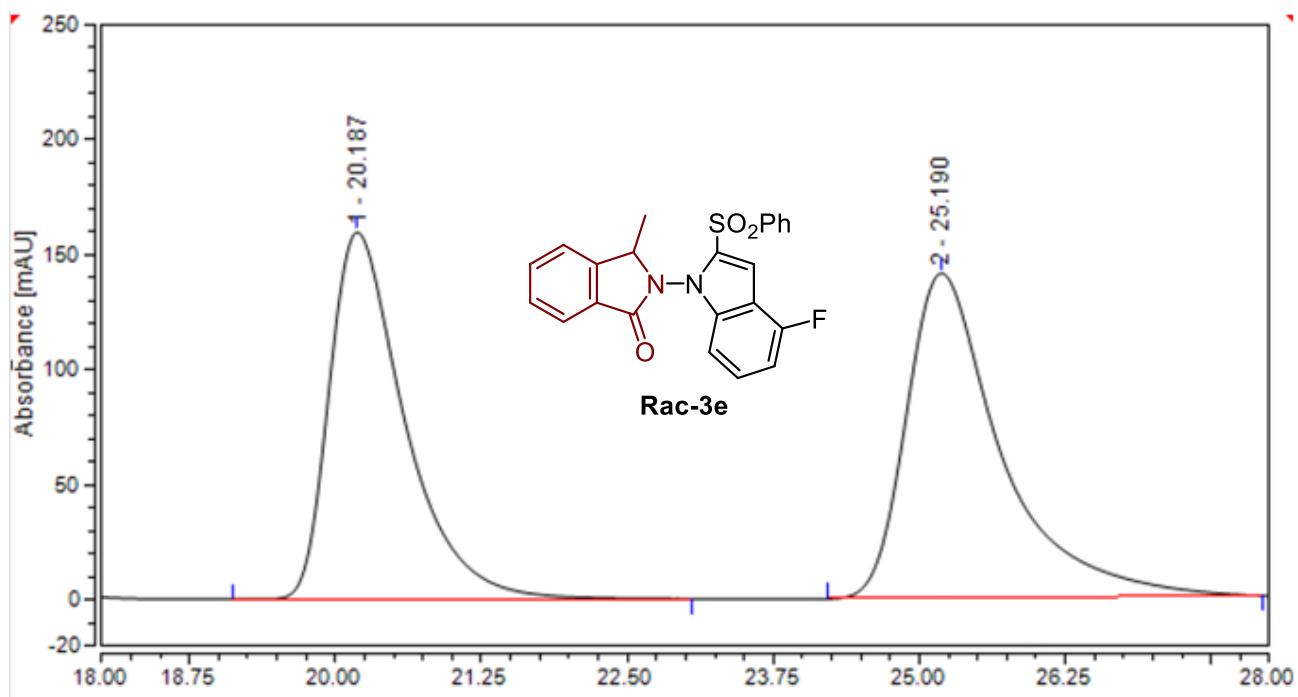
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Heighet %
1	21.19	64.358	72.033	3.50	5.31
2	36.85	1773.571	1284.940	96.50	94.69



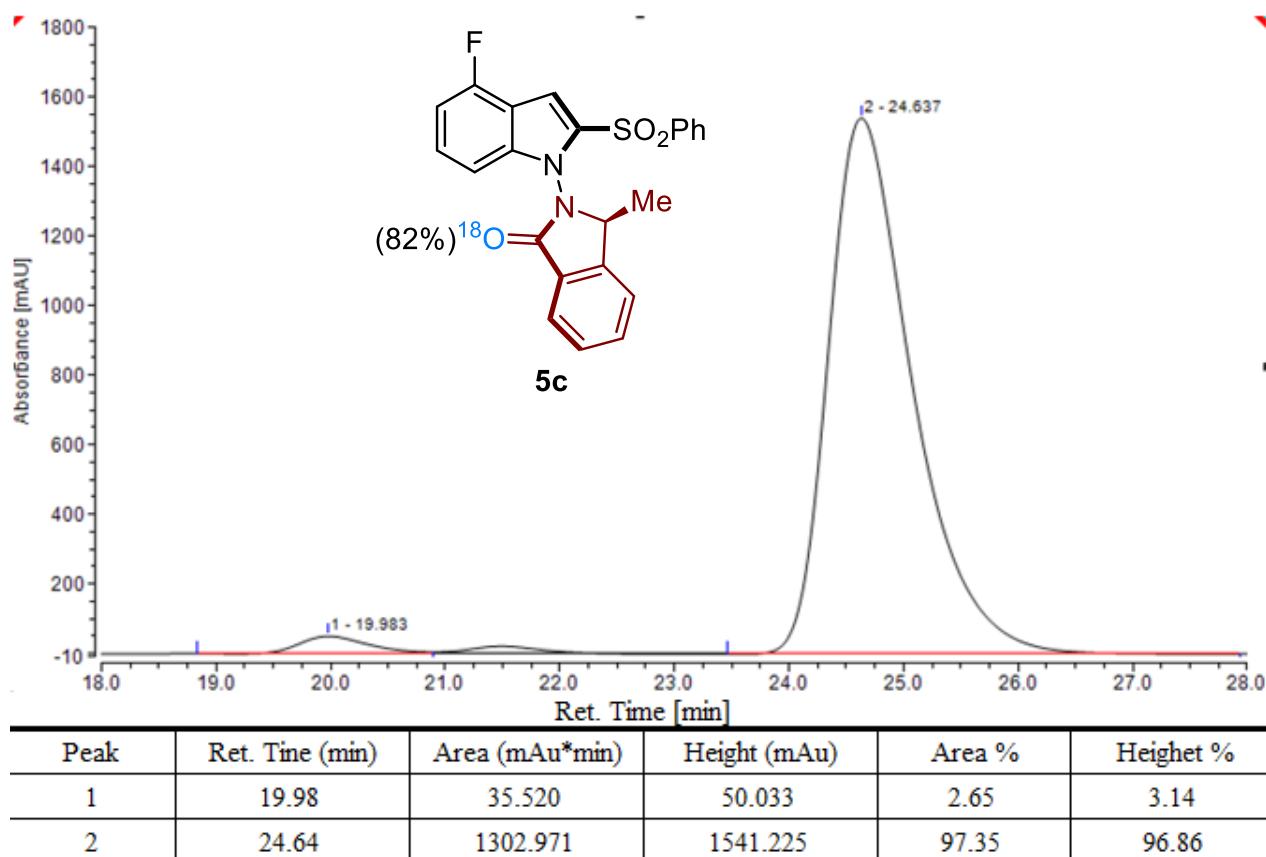
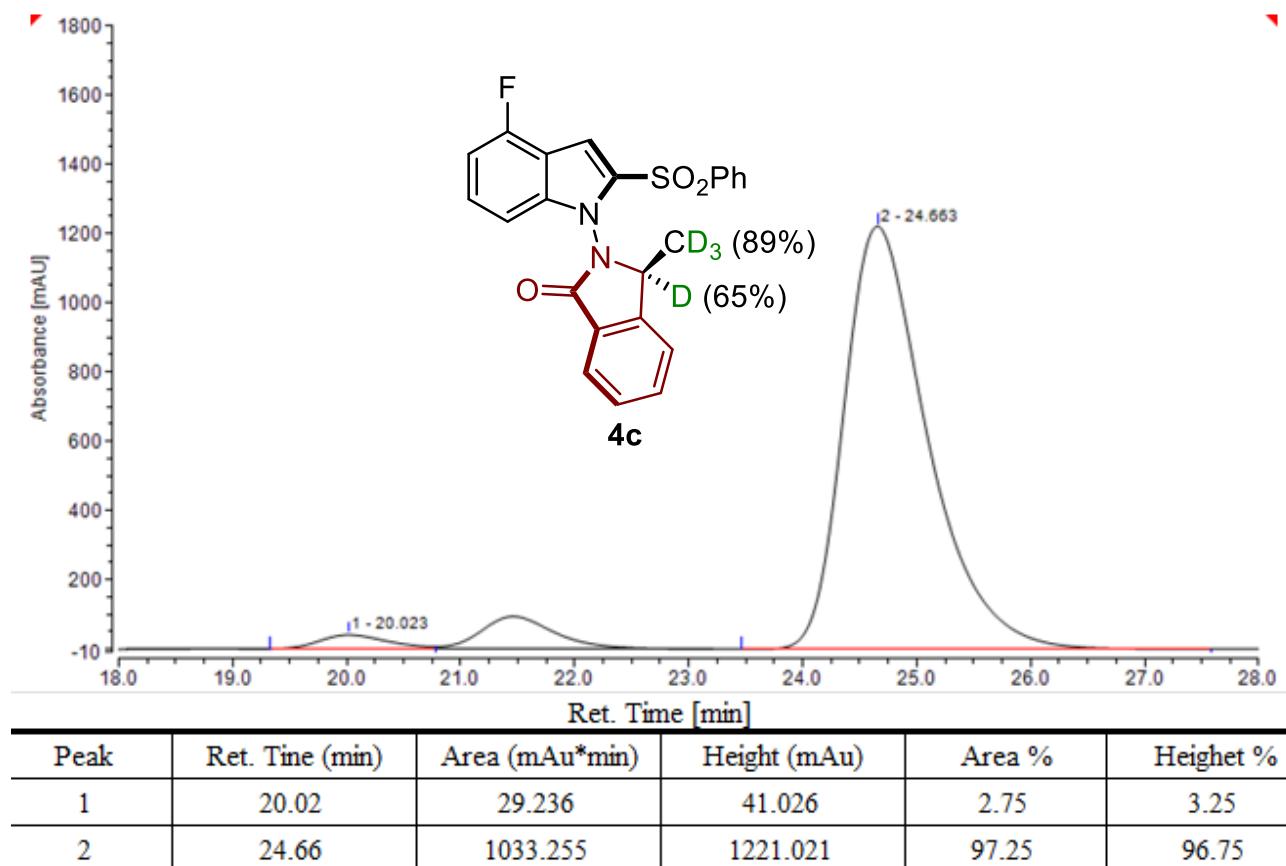
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Heighet %
1	21.30	12.495	14.383	4.56	6.97
2	37.29	261.777	192.045	95.44	93.03

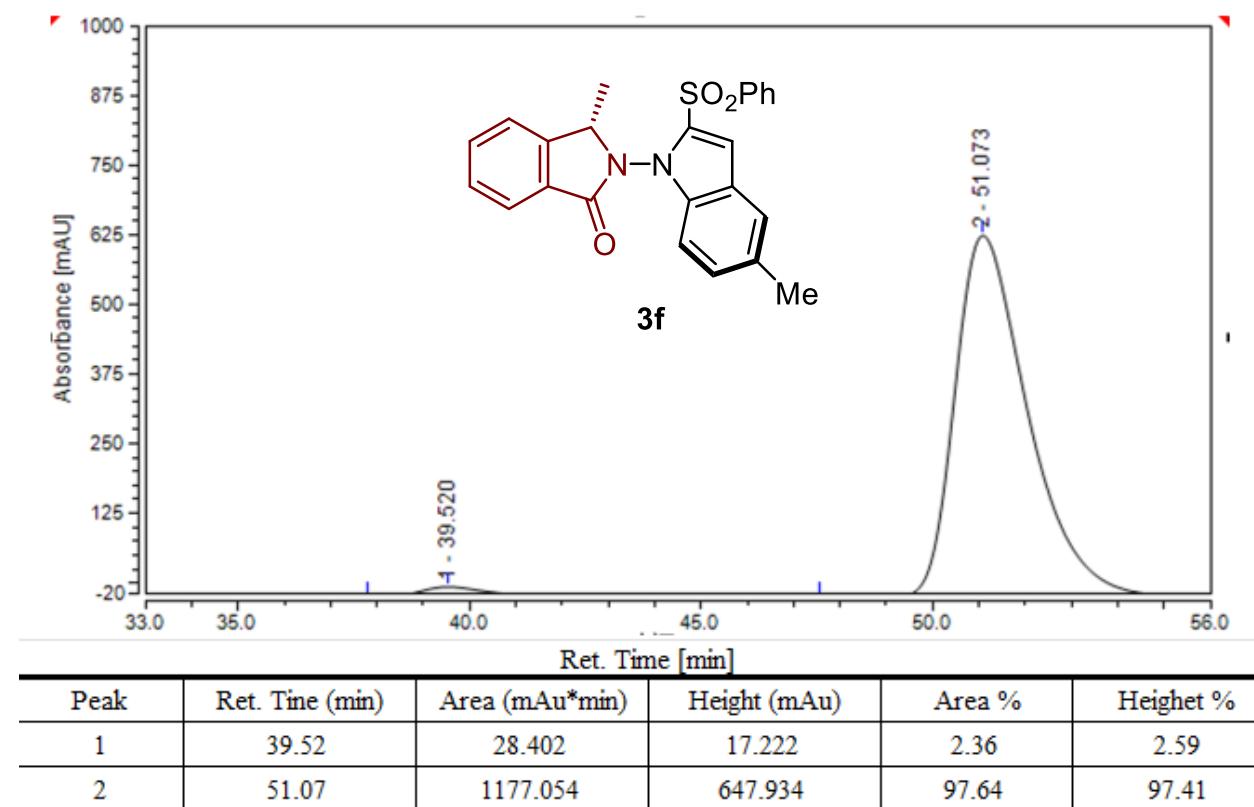
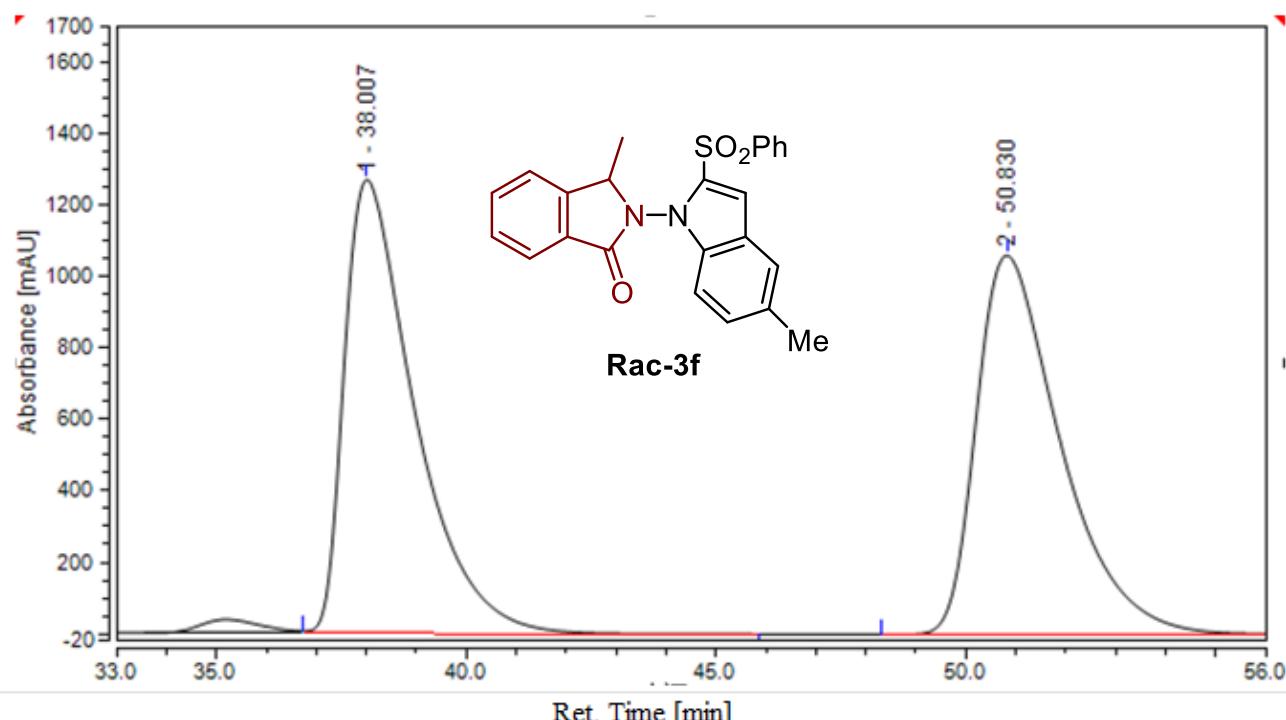


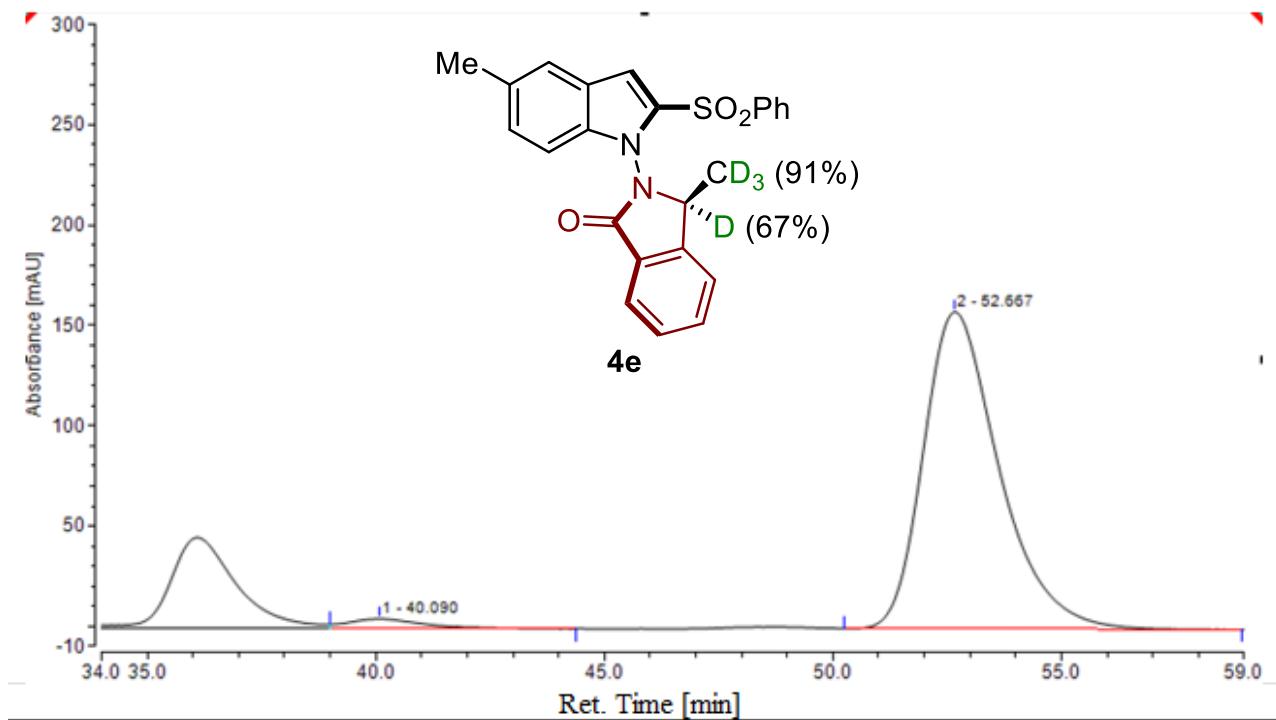





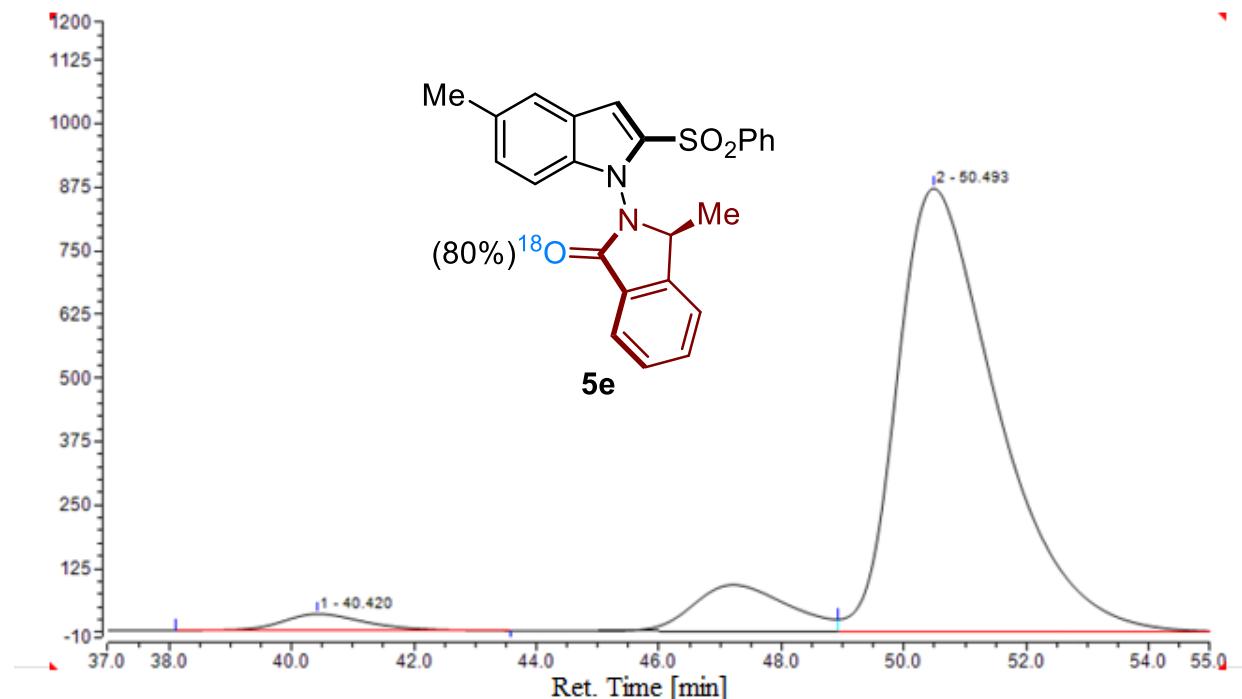
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Heighet %
1	20.30	26.275	33.712	2.93	3.55
2	24.94	870.214	916.240	97.07	96.45



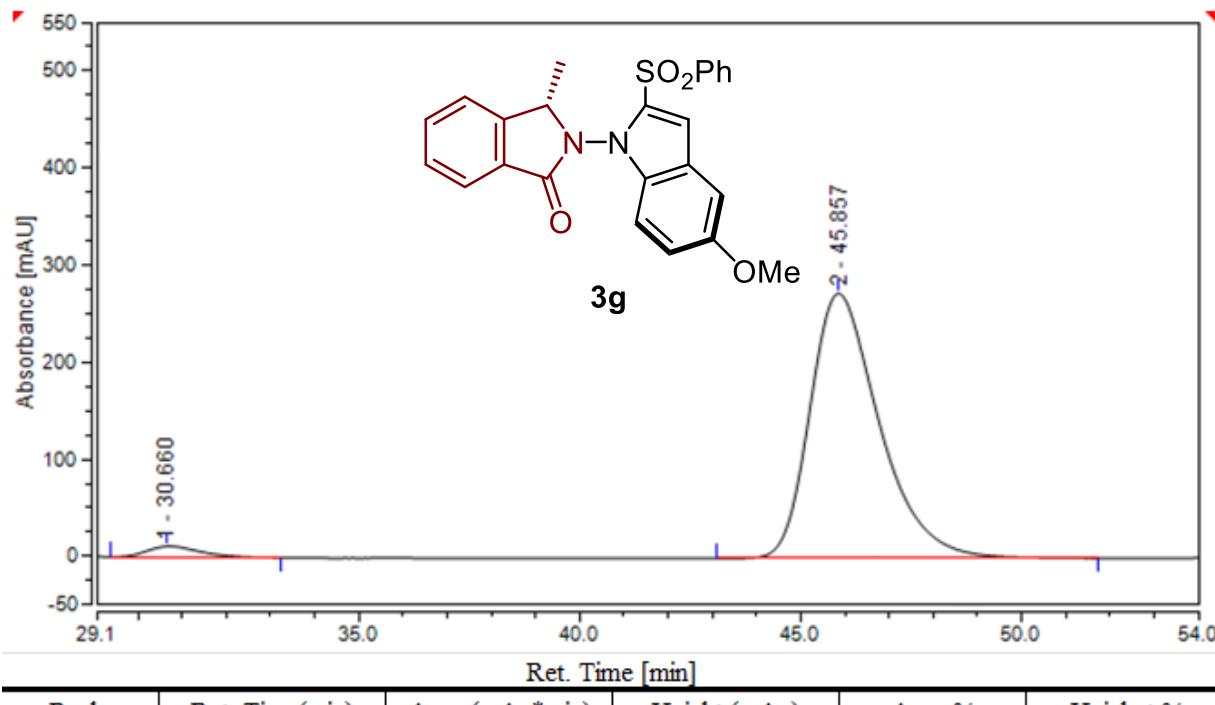
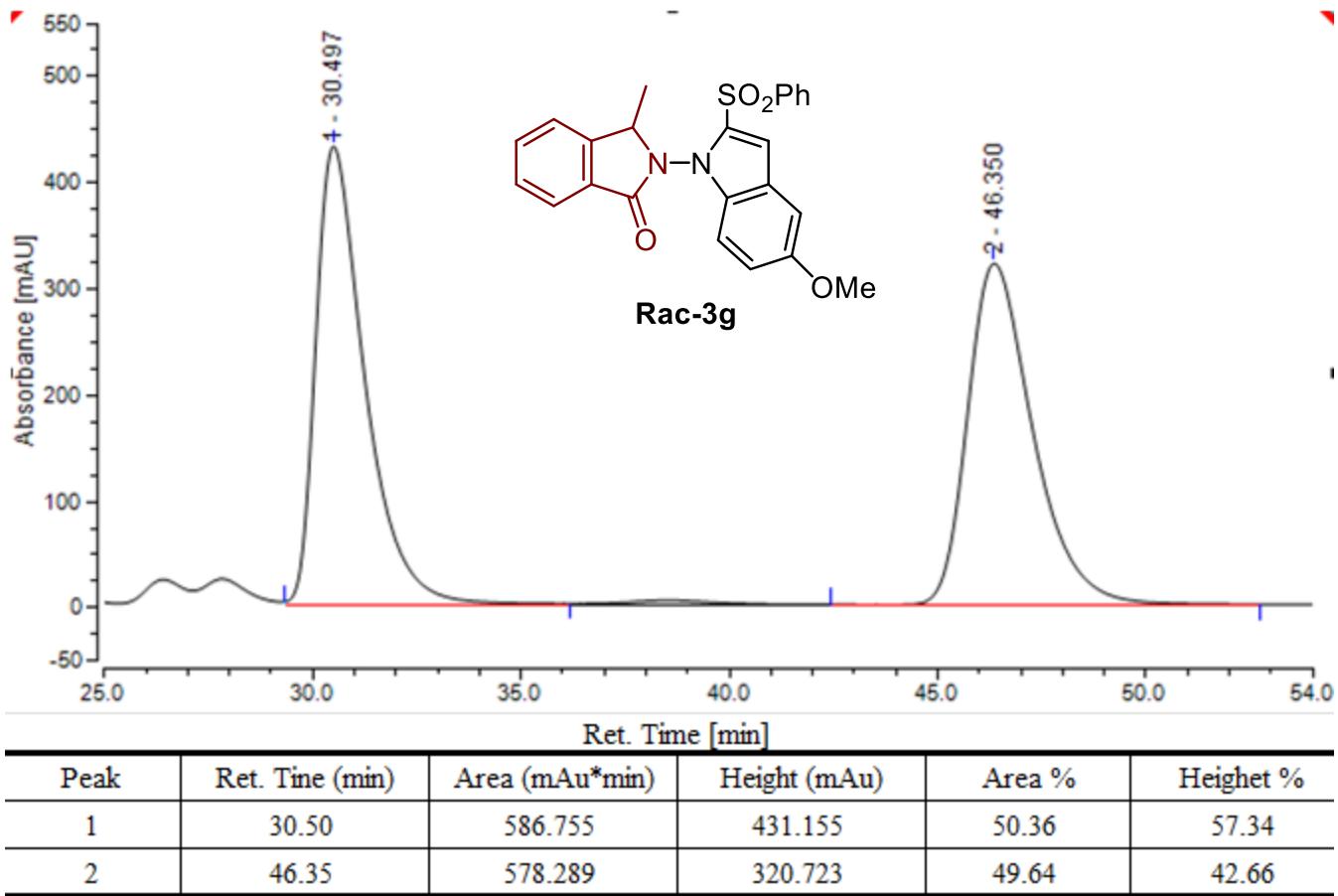


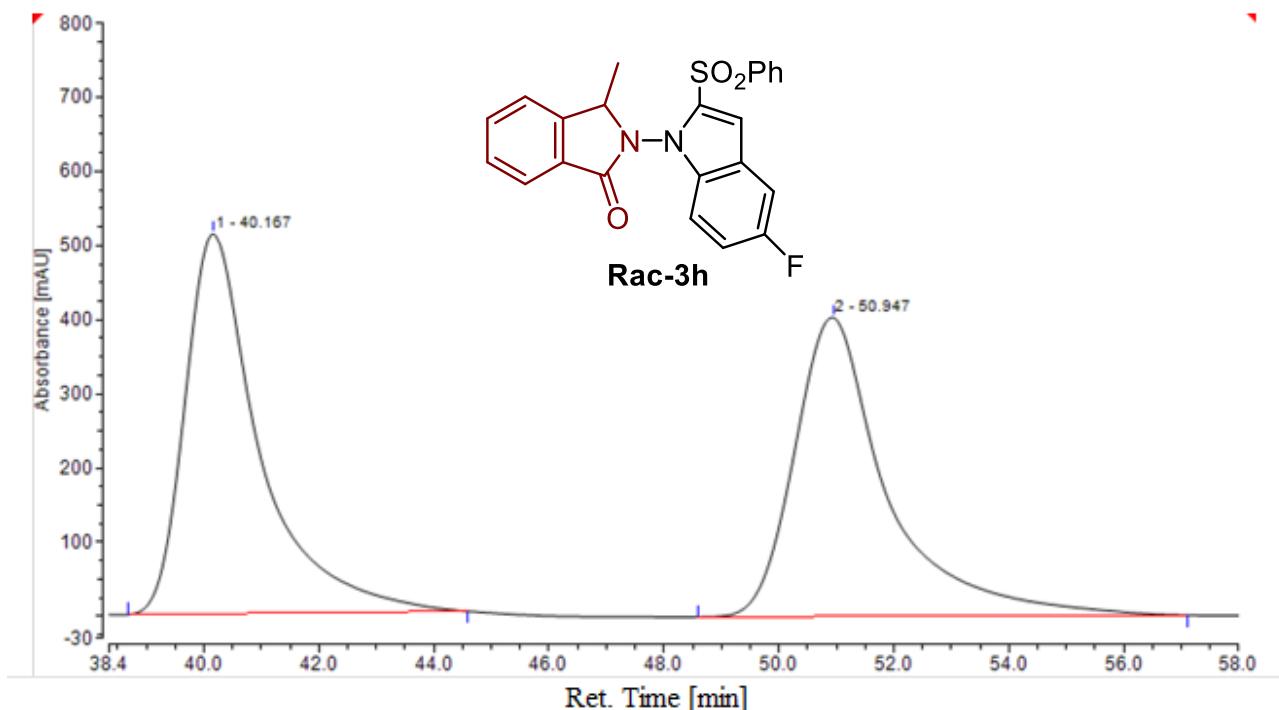


Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Heighet %
1	40.090	9.269	4.847	2.97	2.98
2	52.667	302.843	158.017	97.03	97.02

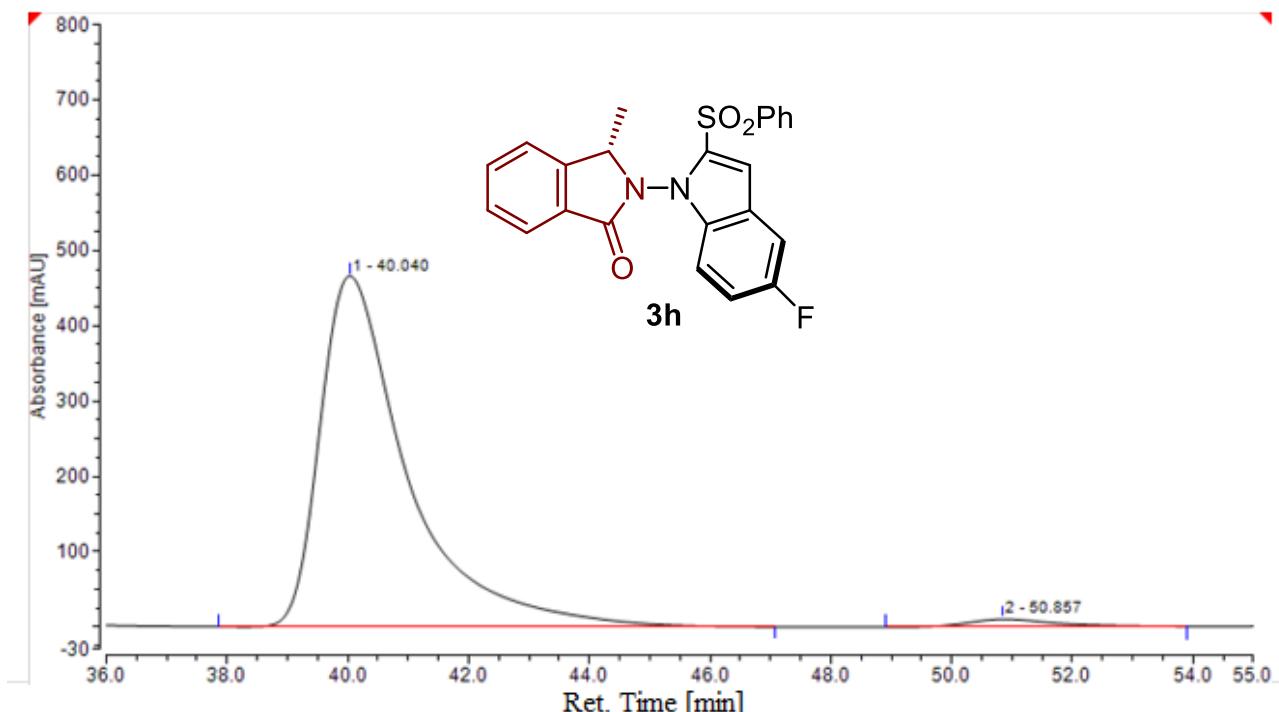


Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Heighet %
1	40.420	52.762	32.177	3.09	3.63
2	50.493	1653.888	871.207	96.91	96.37

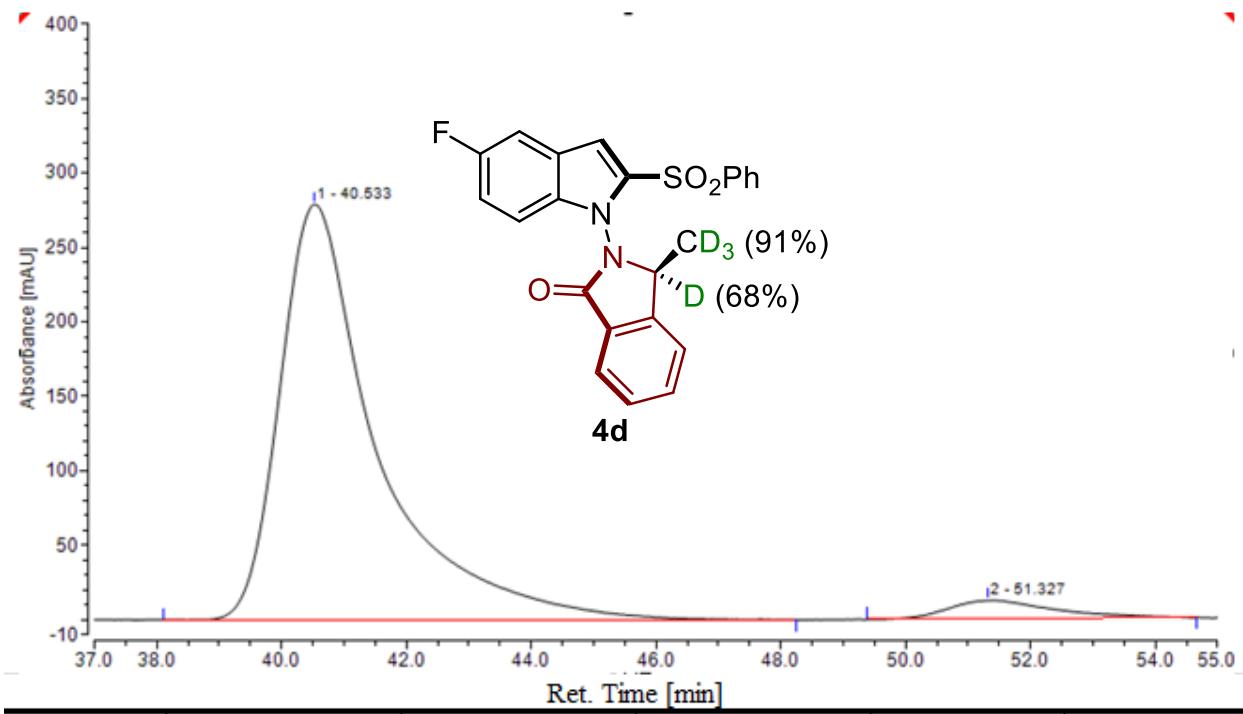




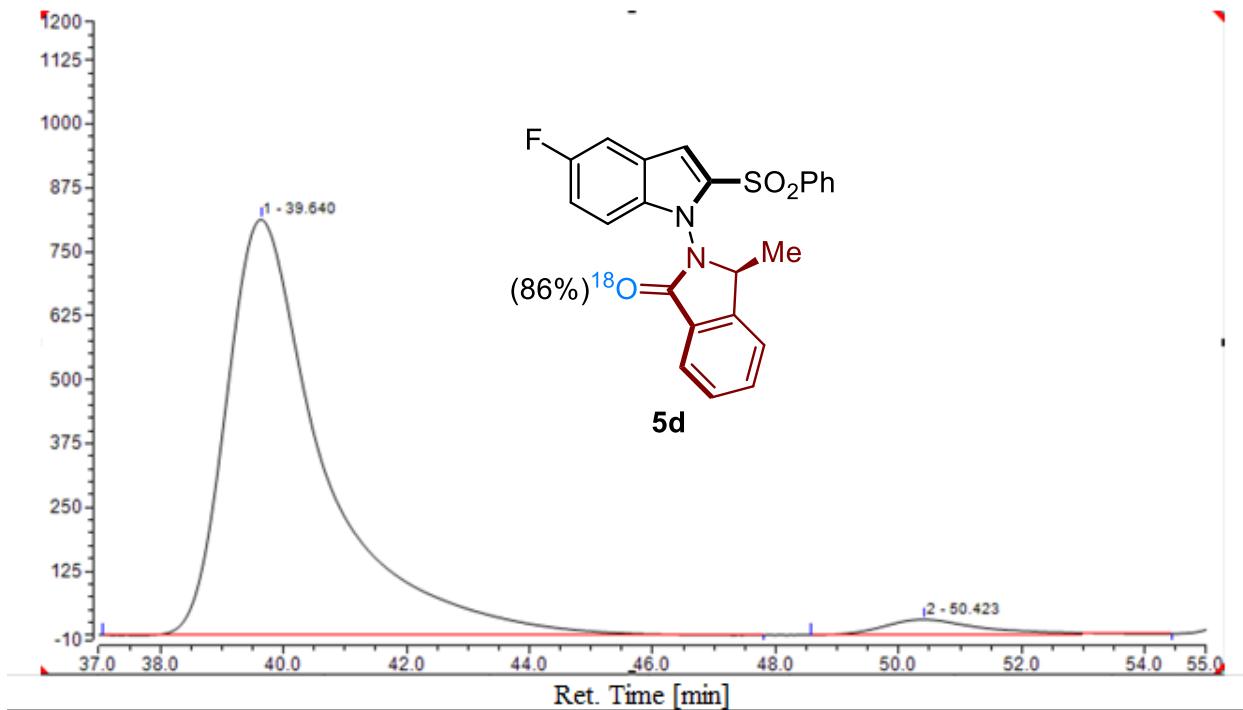
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Heighet %
1	40.167	768.554	512.251	50.48	55.94
2	50.947	753.857	403.402	49.52	44.06



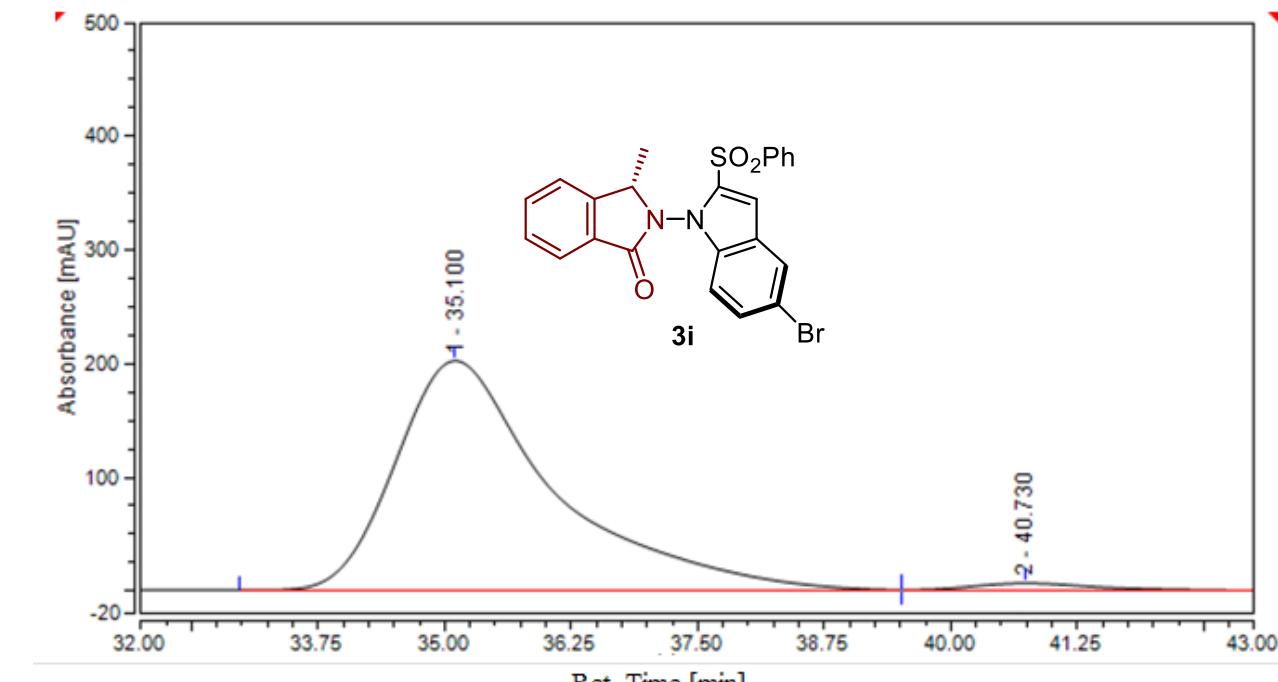
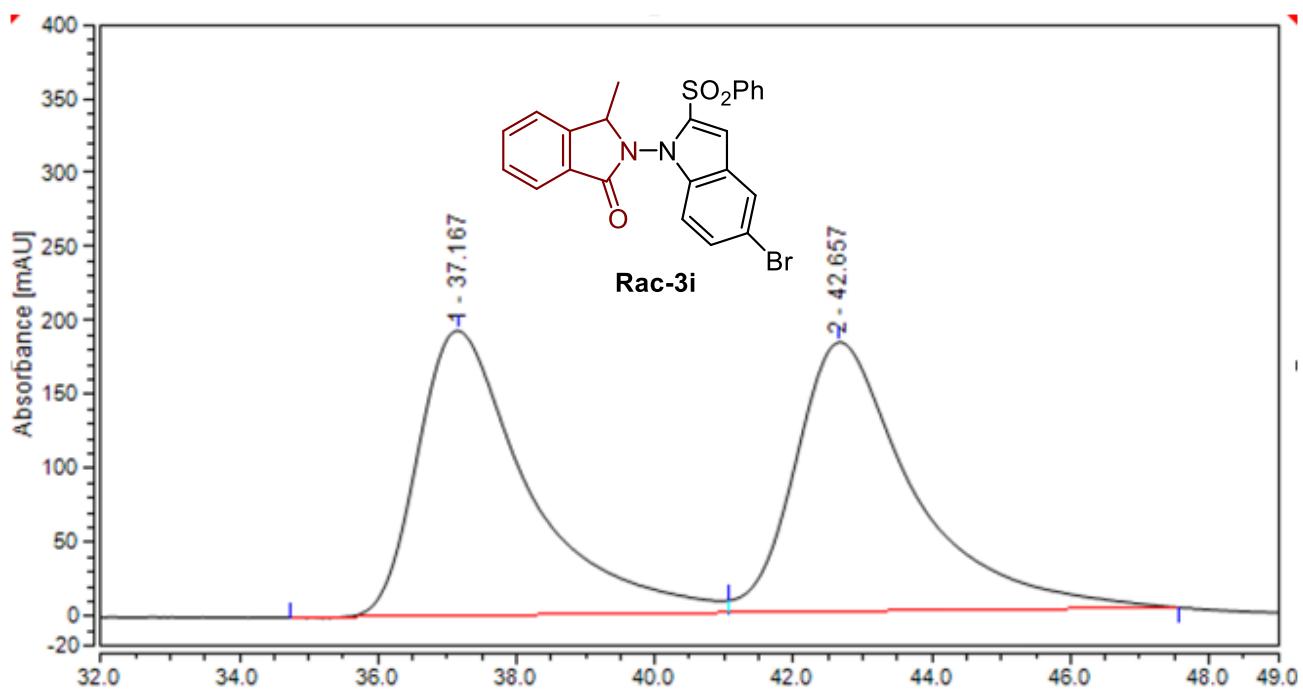
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Heighet %
1	40.040	782.646	466.134	97.91	97.89
2	50.857	16.743	10.043	2.09	2.11

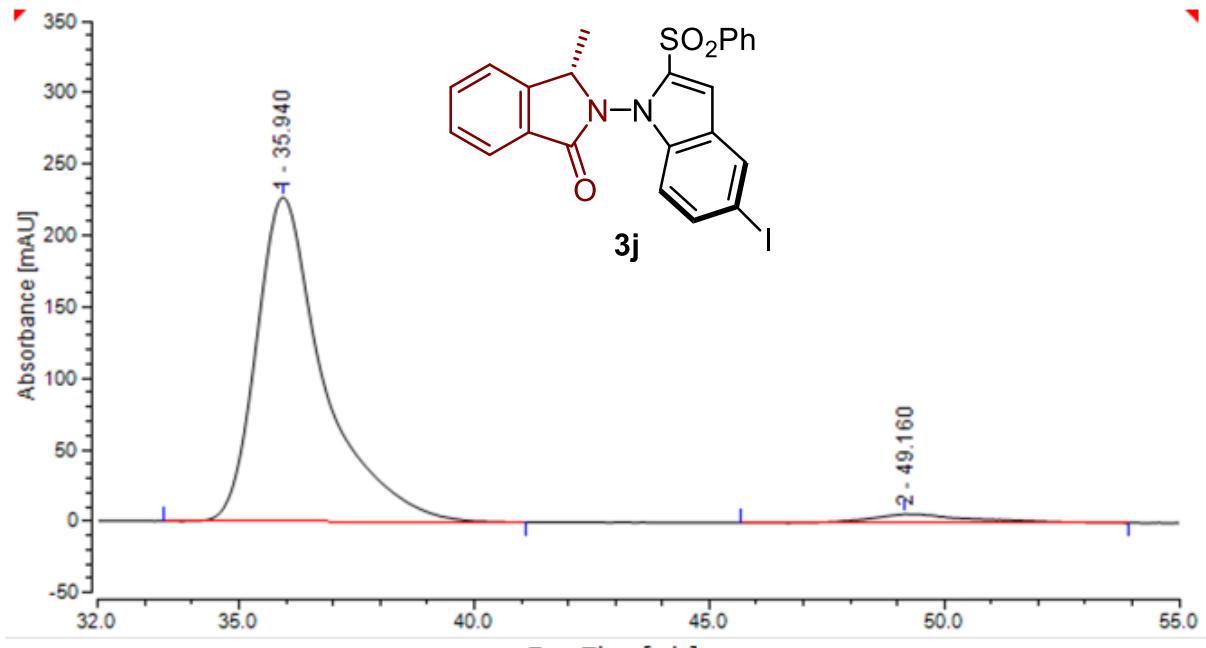
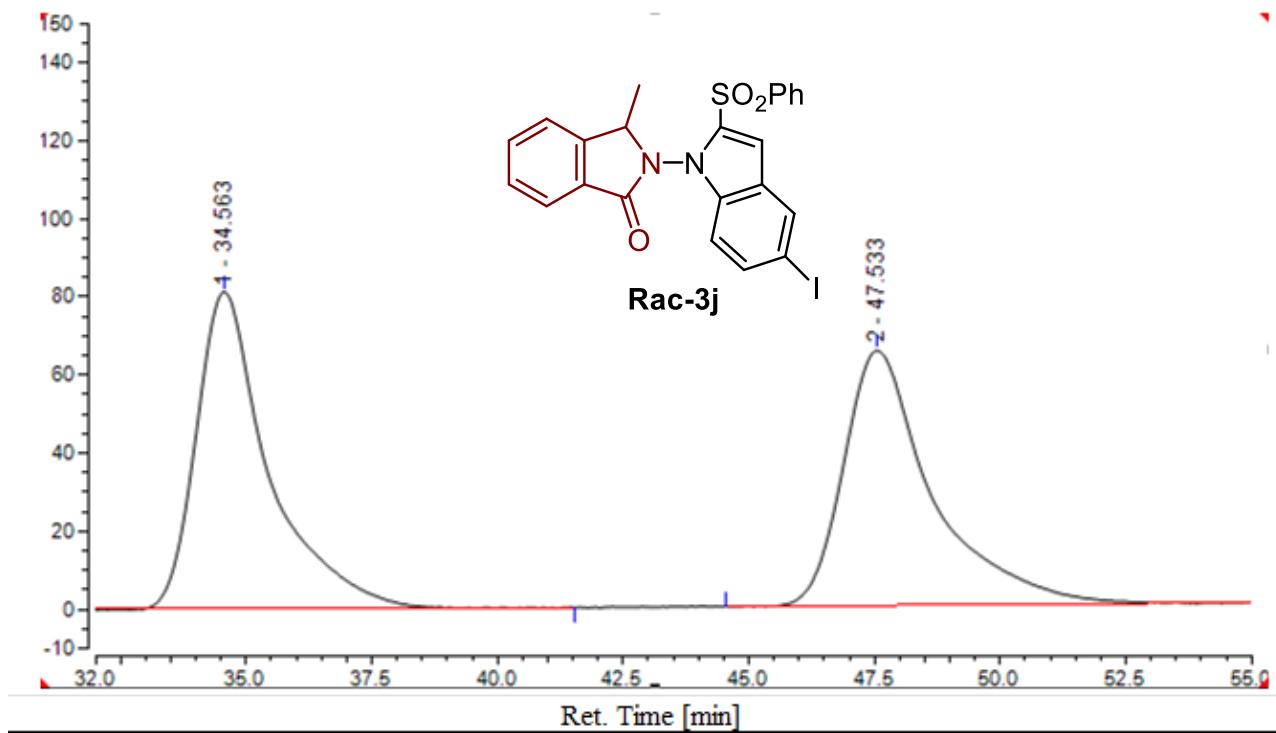


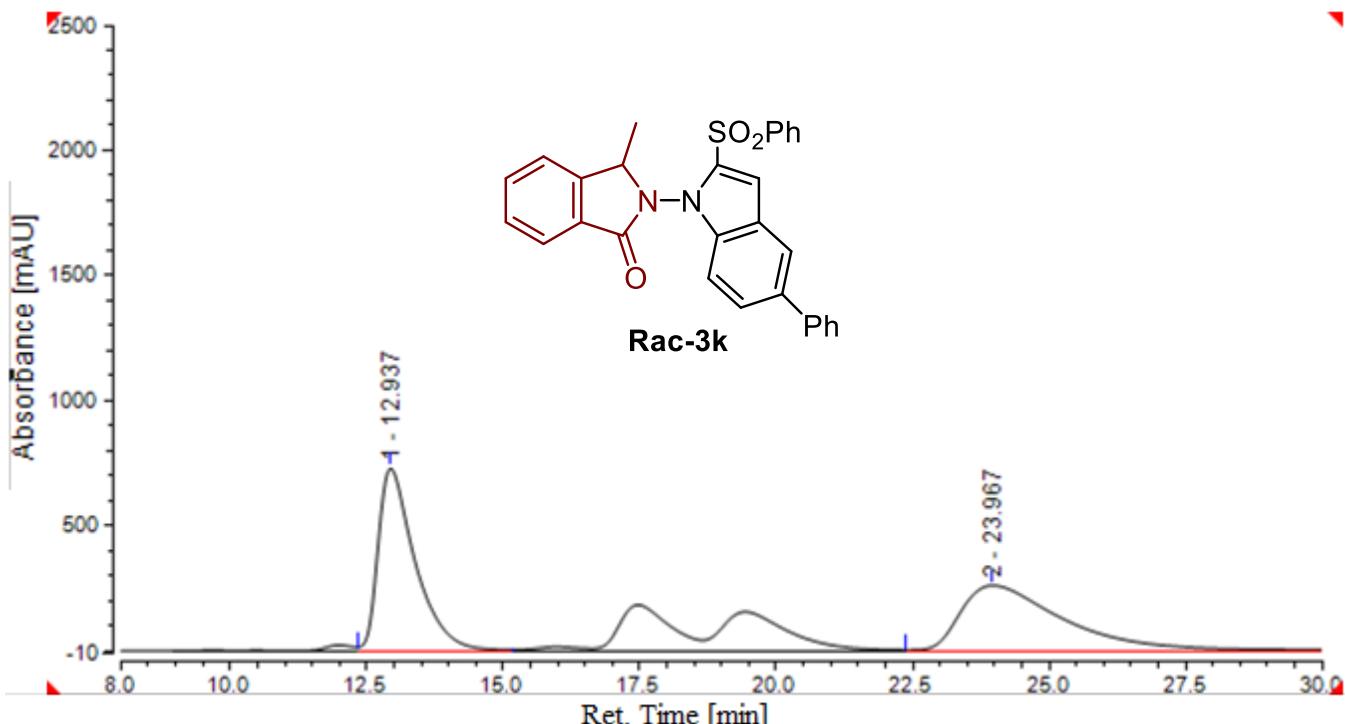
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Heighet %
1	40.533	501.535	278.743	95.44	95.78
2	51.327	23.955	12.267	4.56	4.22



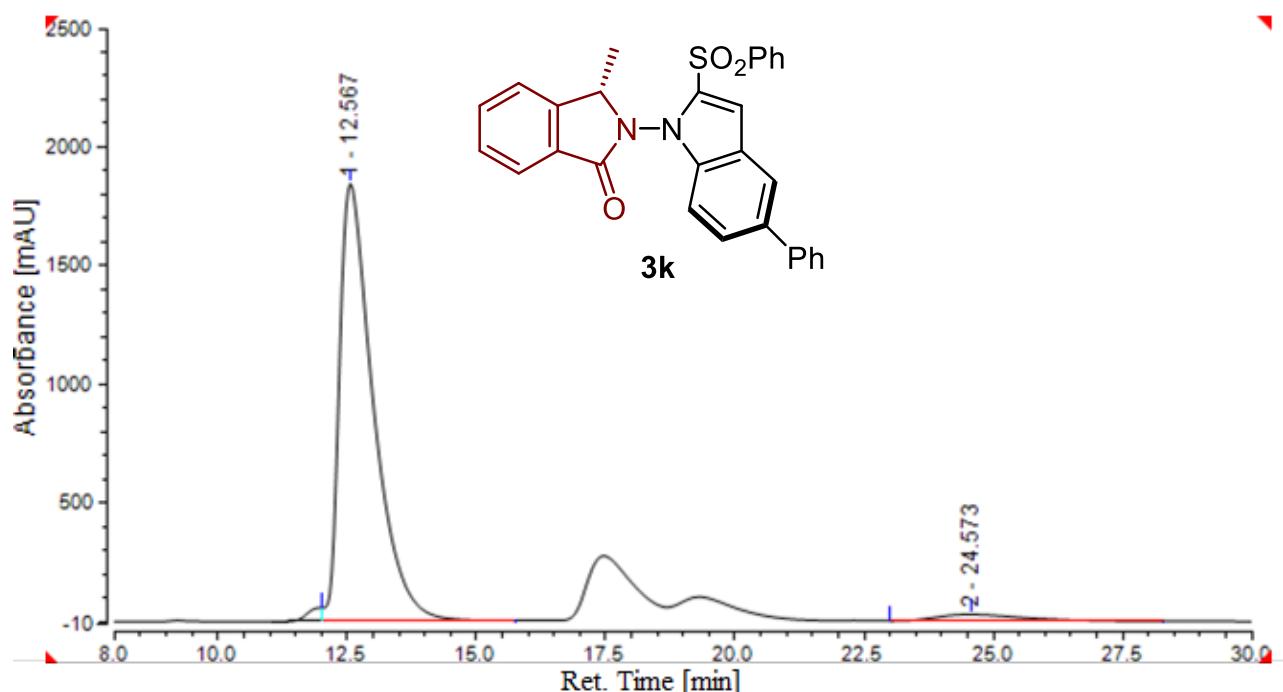
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Heighet %
1	39.640	1497.473	813.561	96.55	96.52
2	50.423	53.441	29.346	3.45	3.48



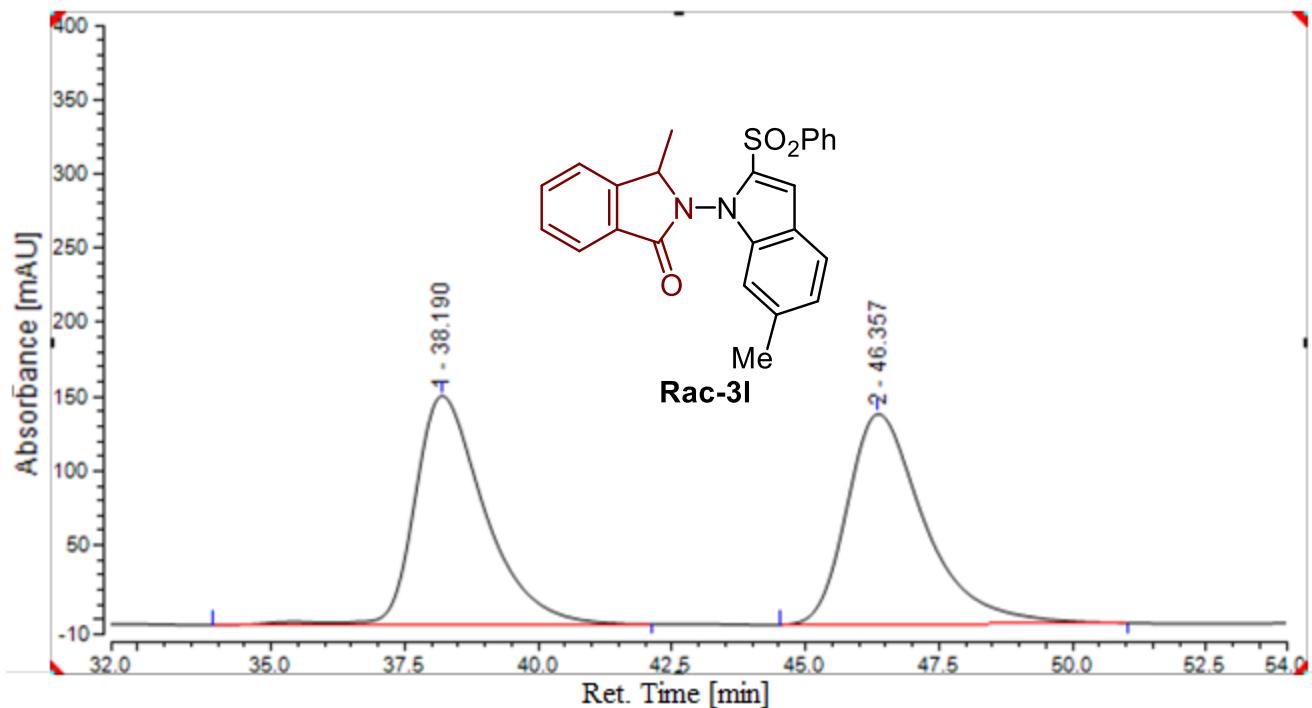




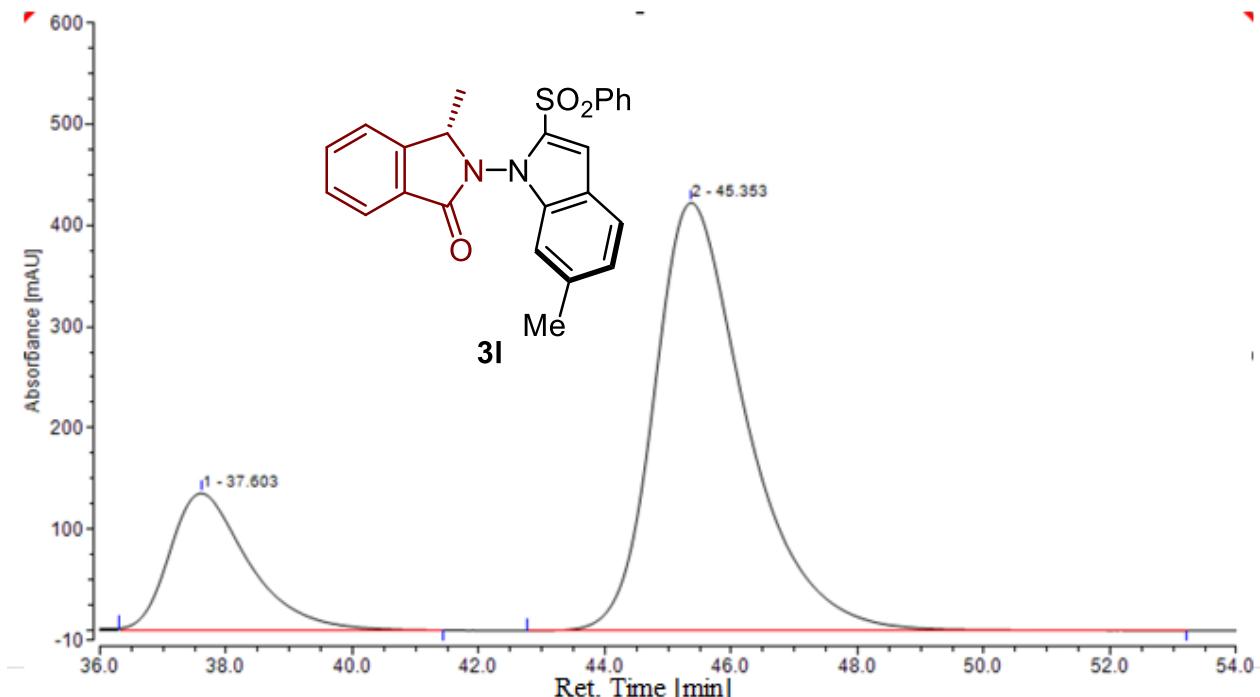
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Heighet %
1	12.940	574.239	729.857	49.73	73.62
2	23.970	580.502	261.516	50.27	26.38



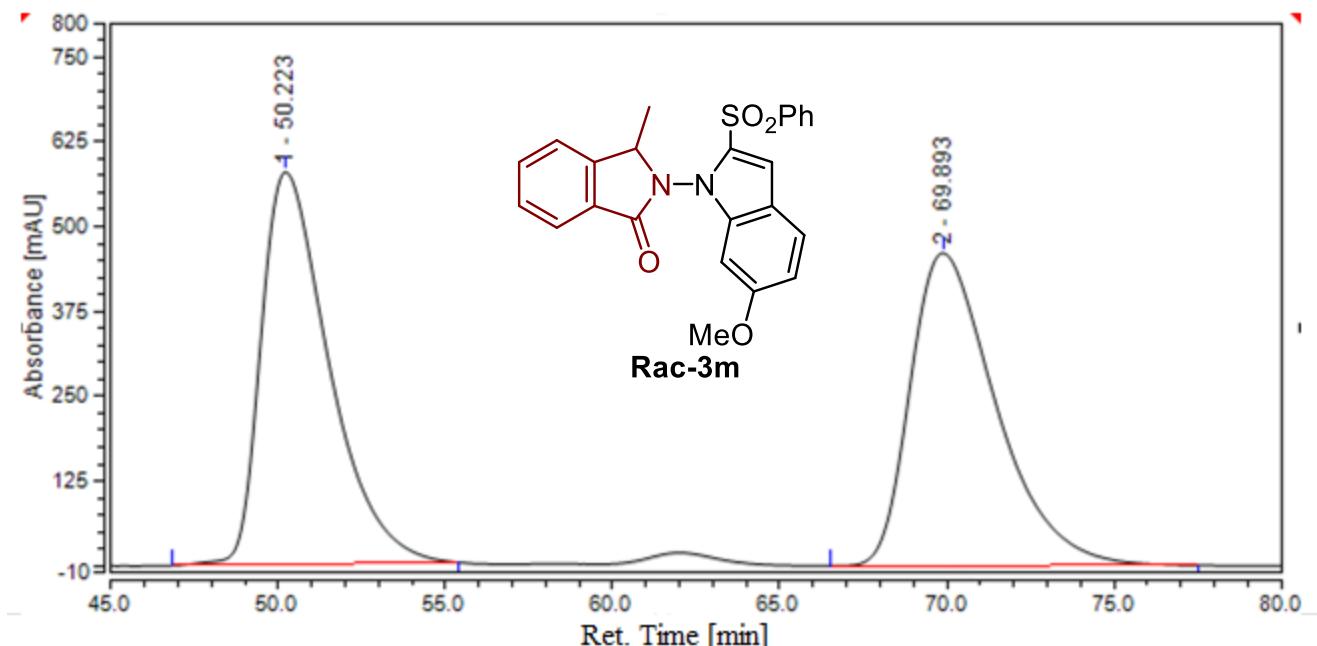
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Heighet %
1	12.567	1396.576	1844.393	96.26	98.53
2	24.573	54.268	27.490	3.74	1.47



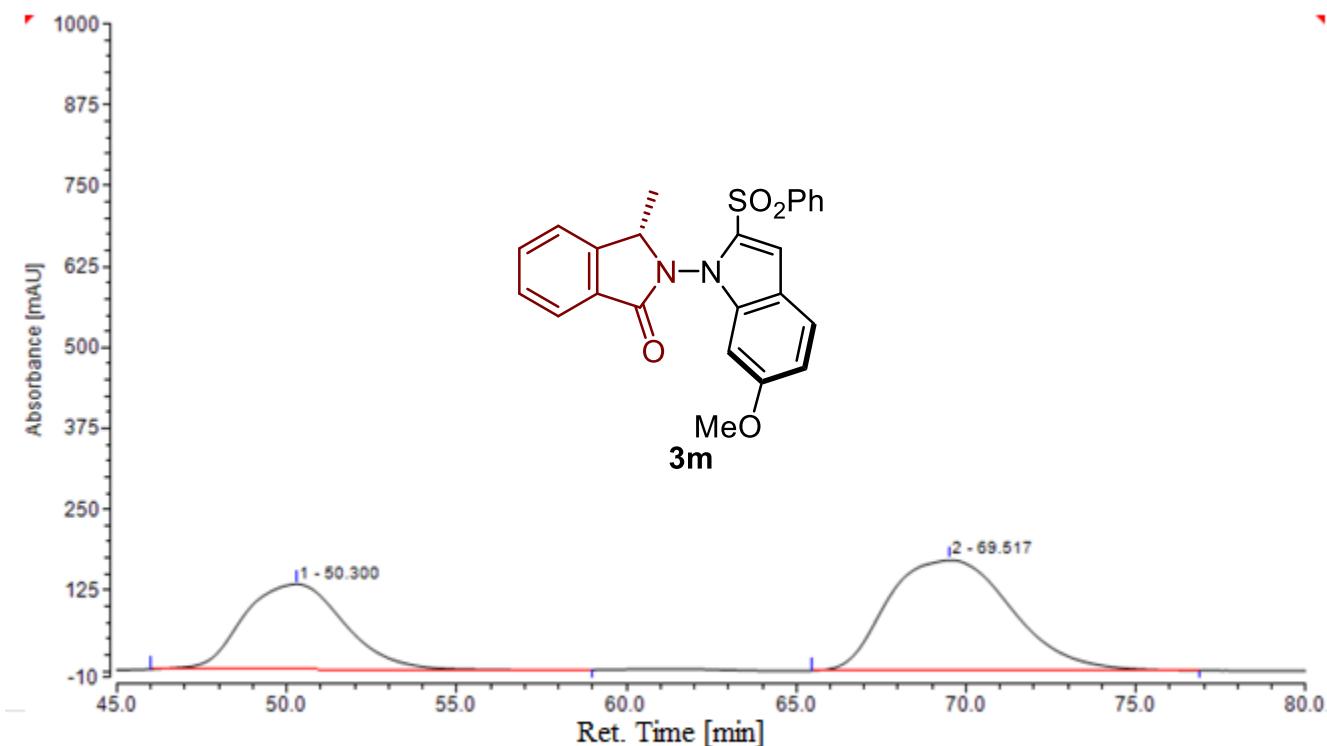
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Heighet %
1	38.19	234.075	154.168	49.58	52.10
2	46.36	238.051	141.760	50.42	47.90



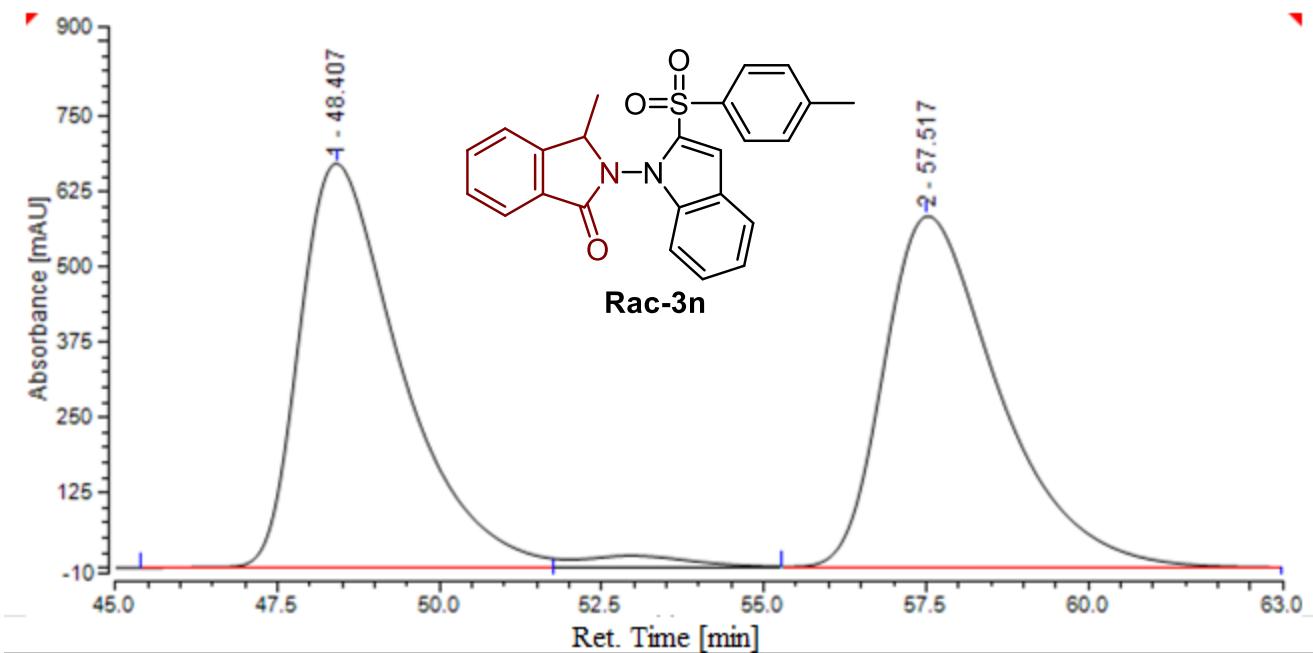
Peak	Ret. Tine (min)	Area (mAu*min)	Height (mAu)	Area %	Heighet %
1	37.60	196.292	135.300	21.49	24.26
2	45.35	717.196	422.511	78.51	75.74



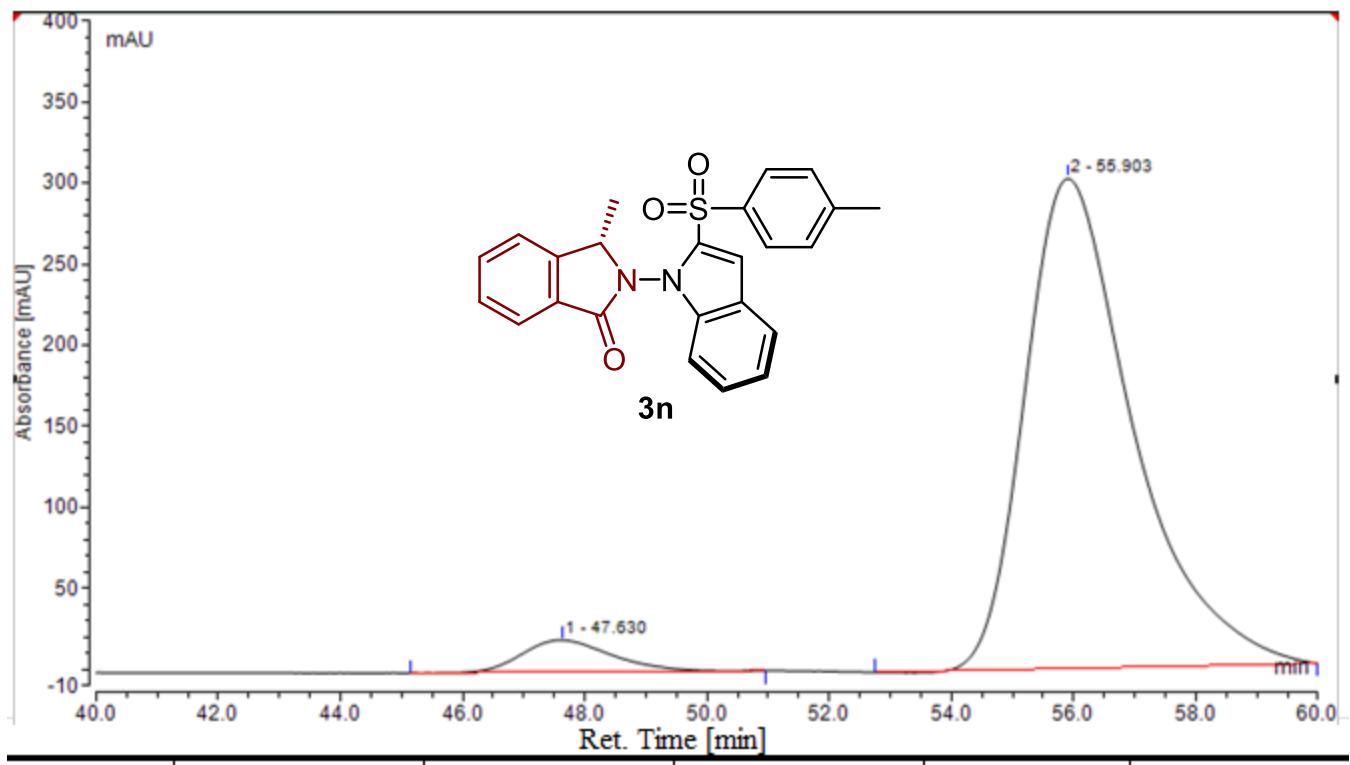
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Heighet %
1	50.22	1358.358	578.018	49.80	55.65
2	69.89	1369.488	460.578	50.20	44.35



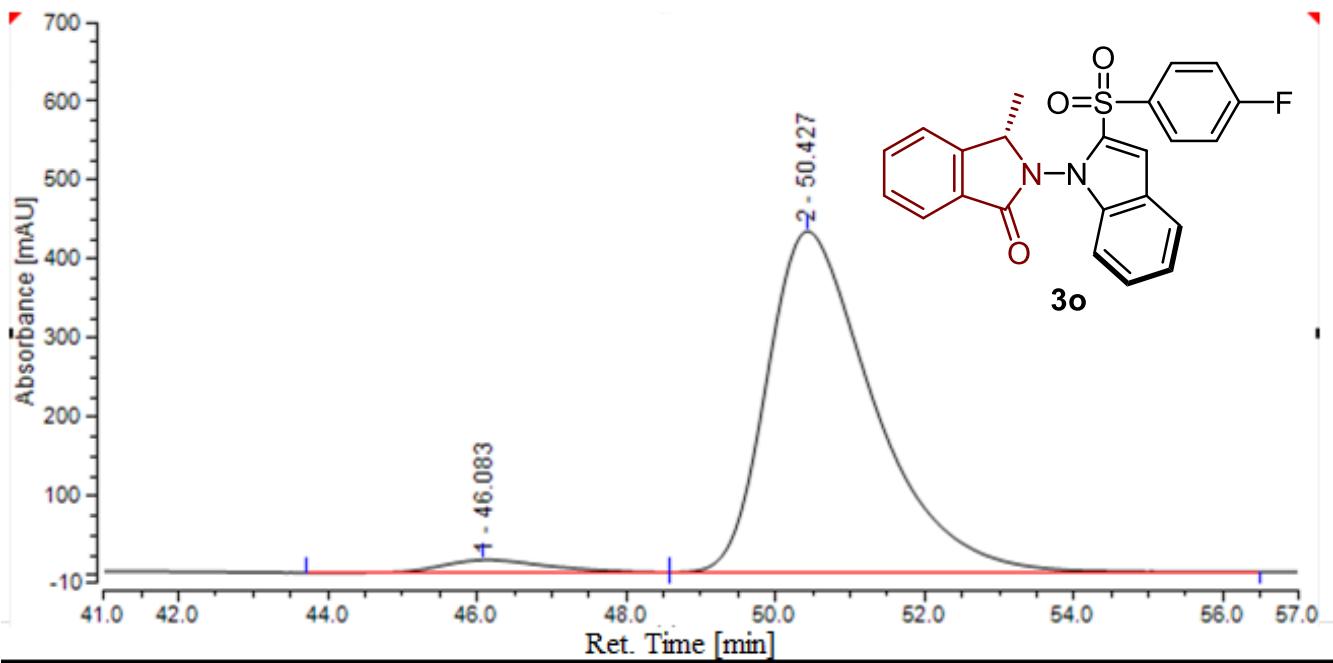
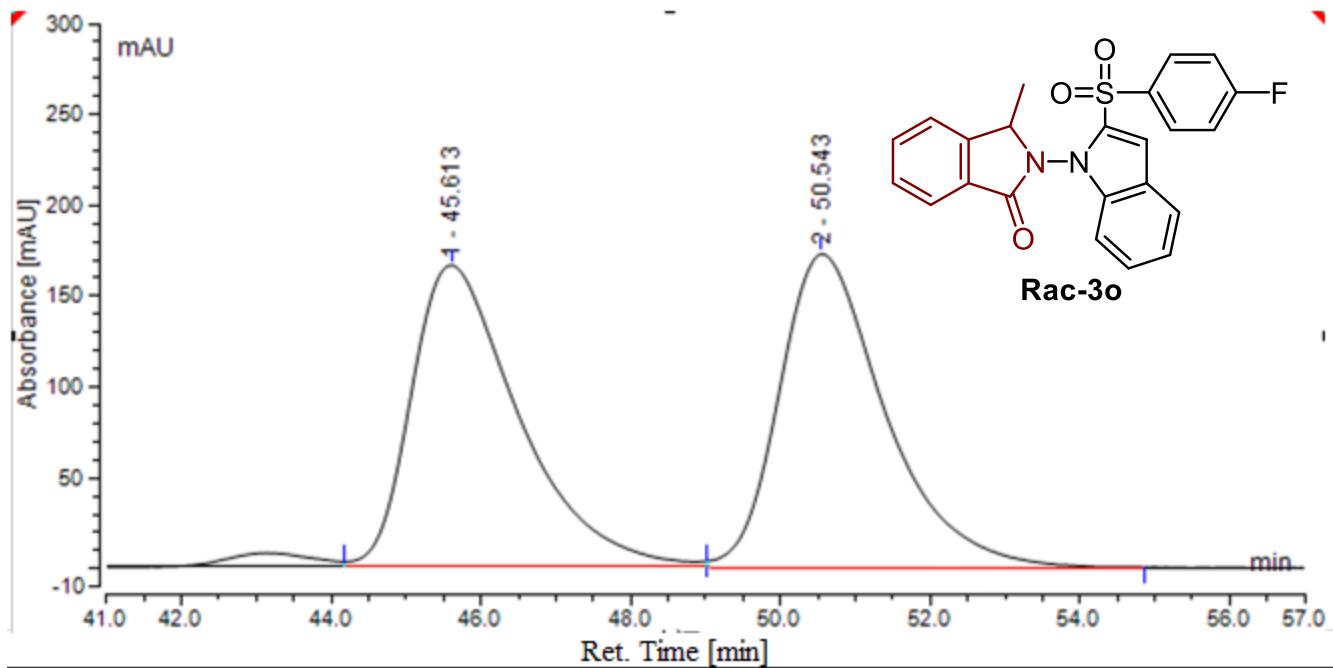
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Heighet %
1	50.30	449.690	131.769	38.42	43.59
2	69.52	720.666	170.547	61.58	56.41

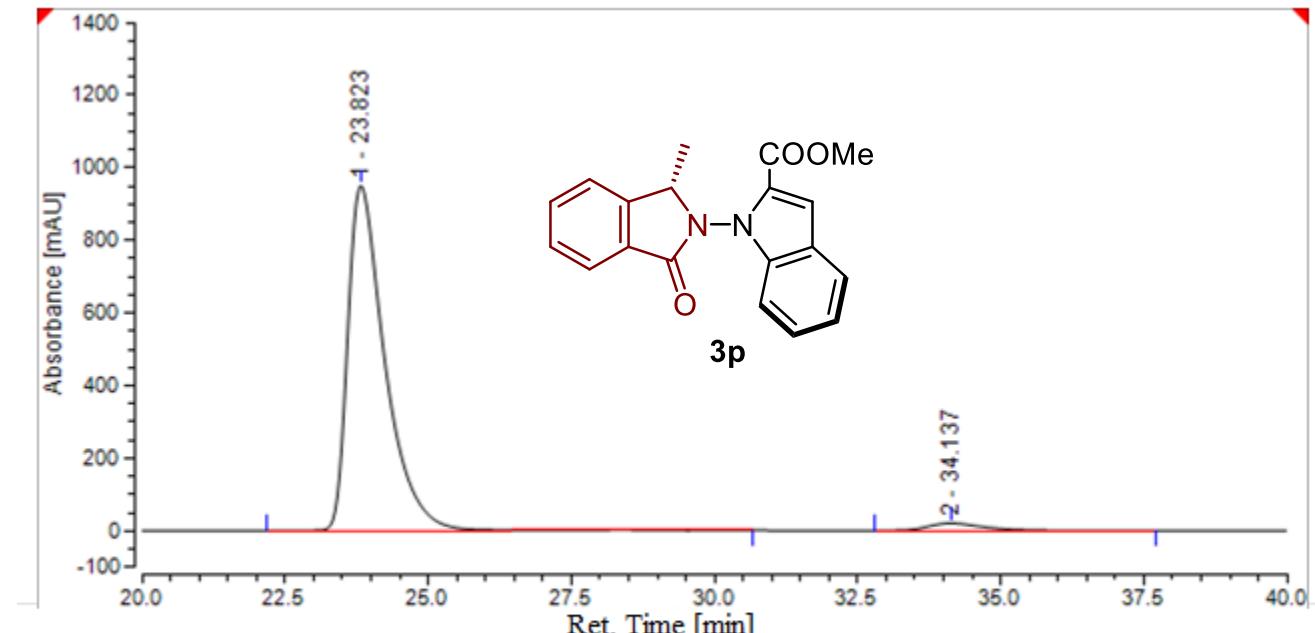
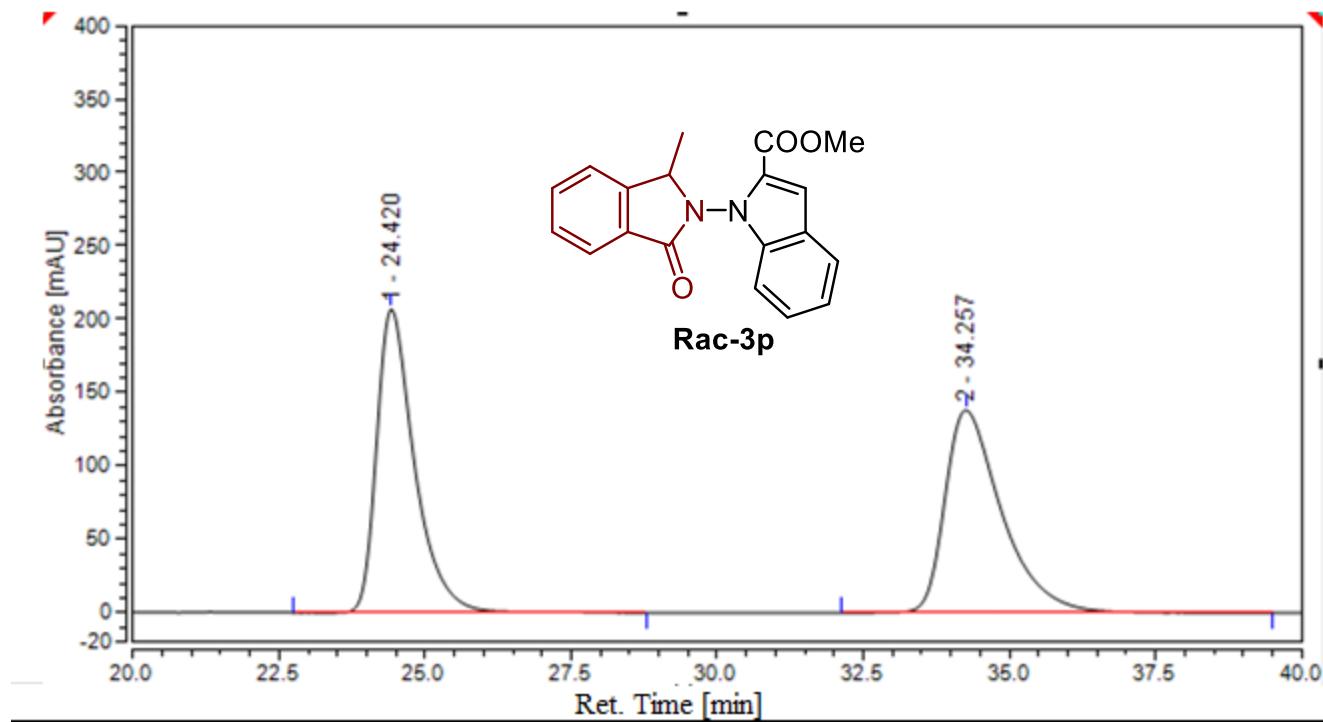


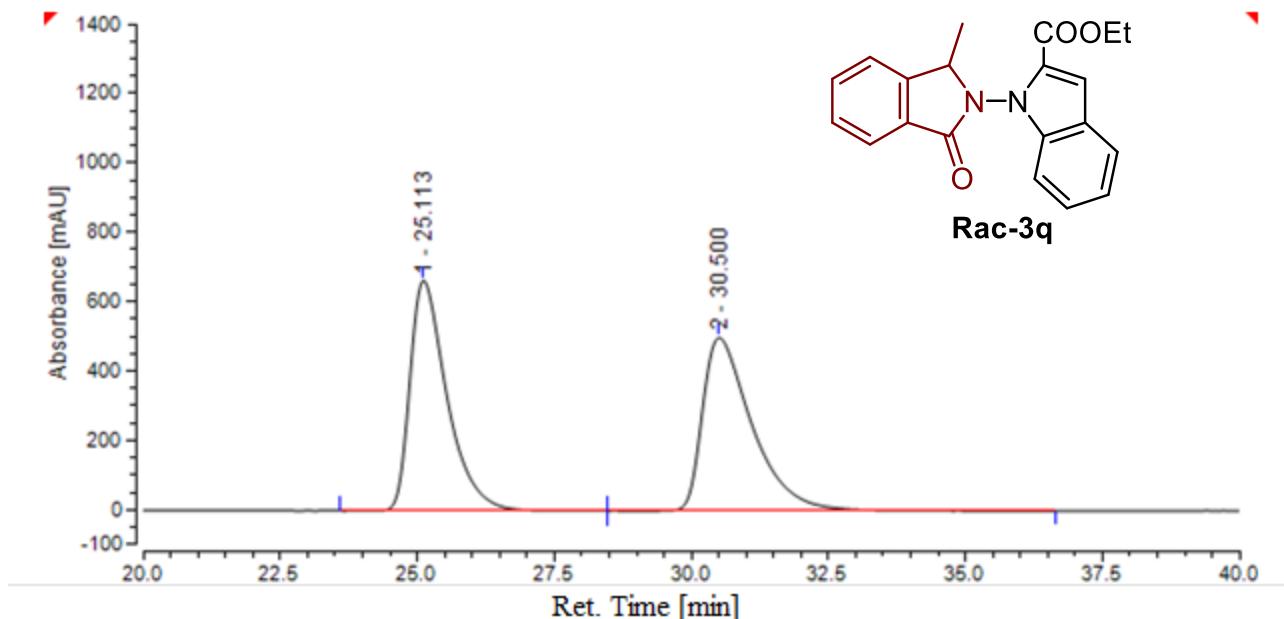
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Heighet %
1	48.41	1213.652	671.552	50.15	53.47
2	57.52	1206.493	584.302	49.85	46.53



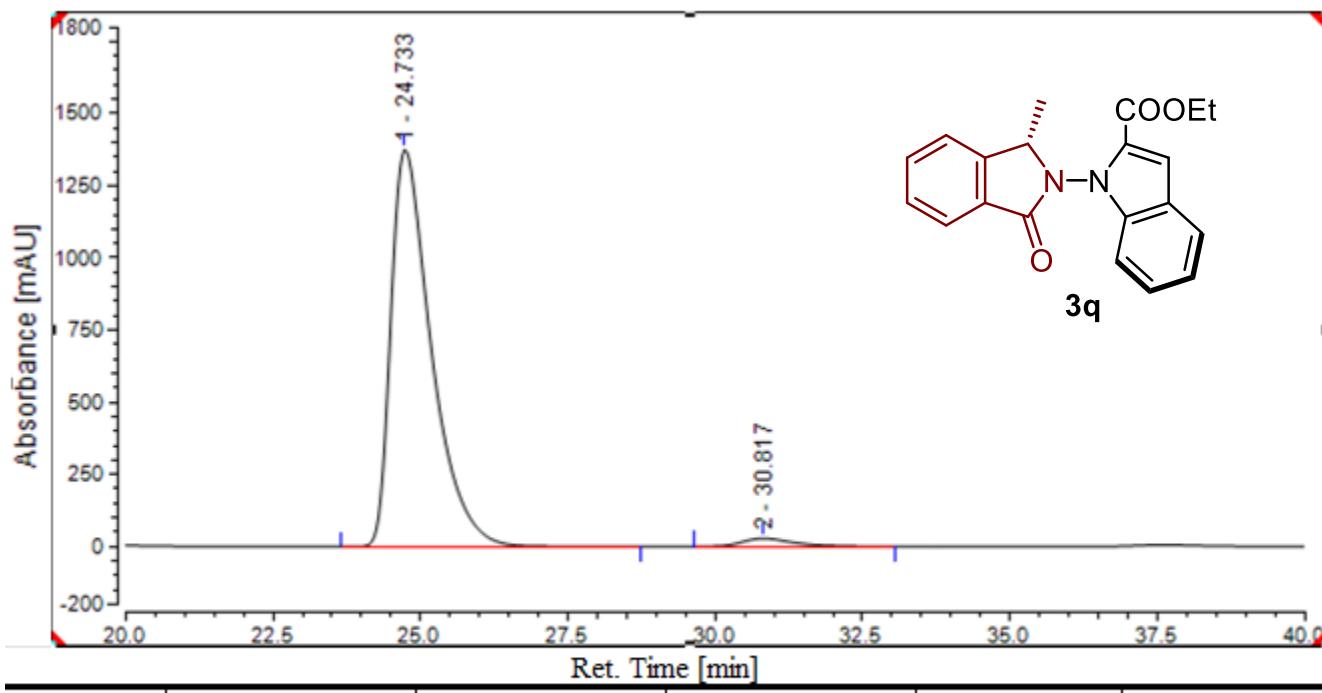
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Heighet %
1	47.63	33.532	19.764	5.15	6.14
2	55.90	617.123	301.969	94.85	93.86



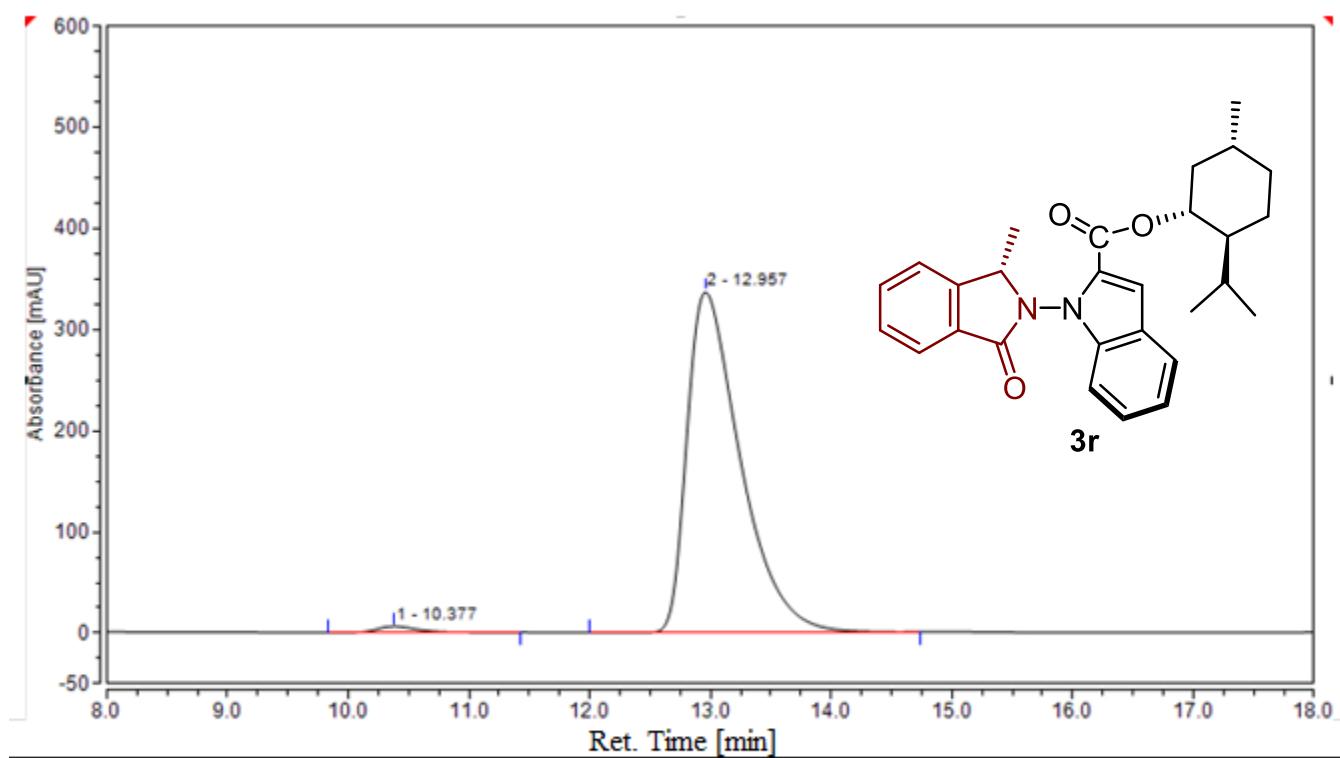
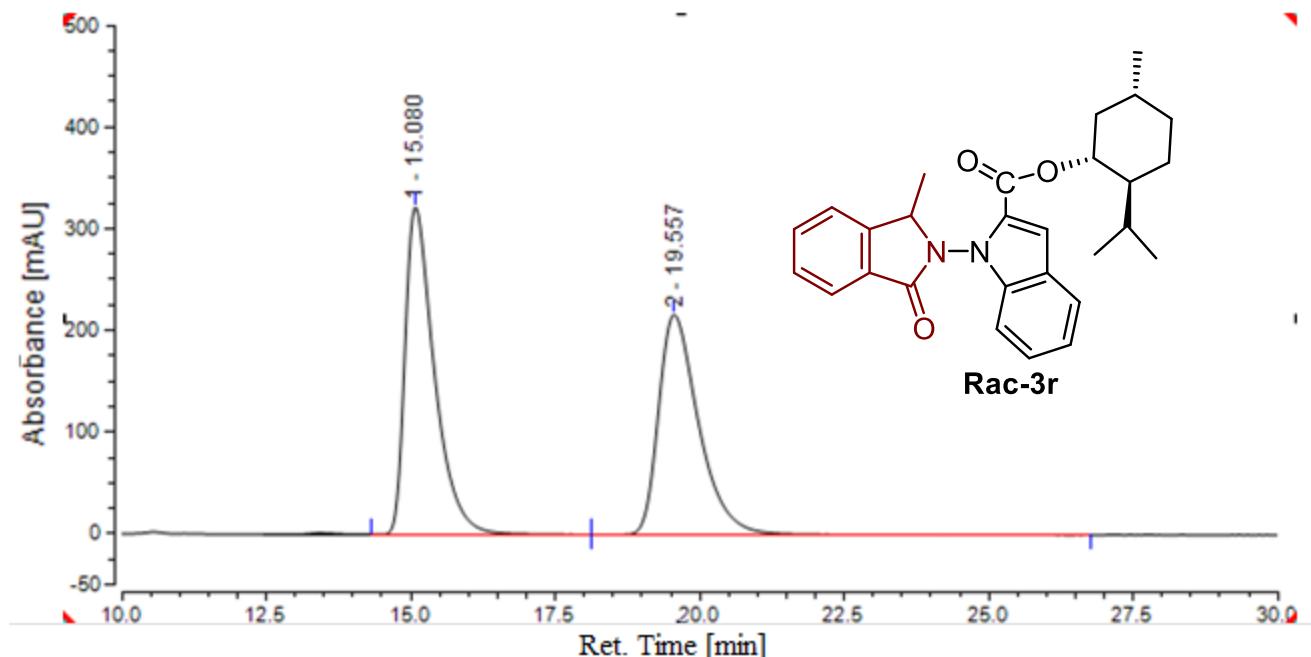


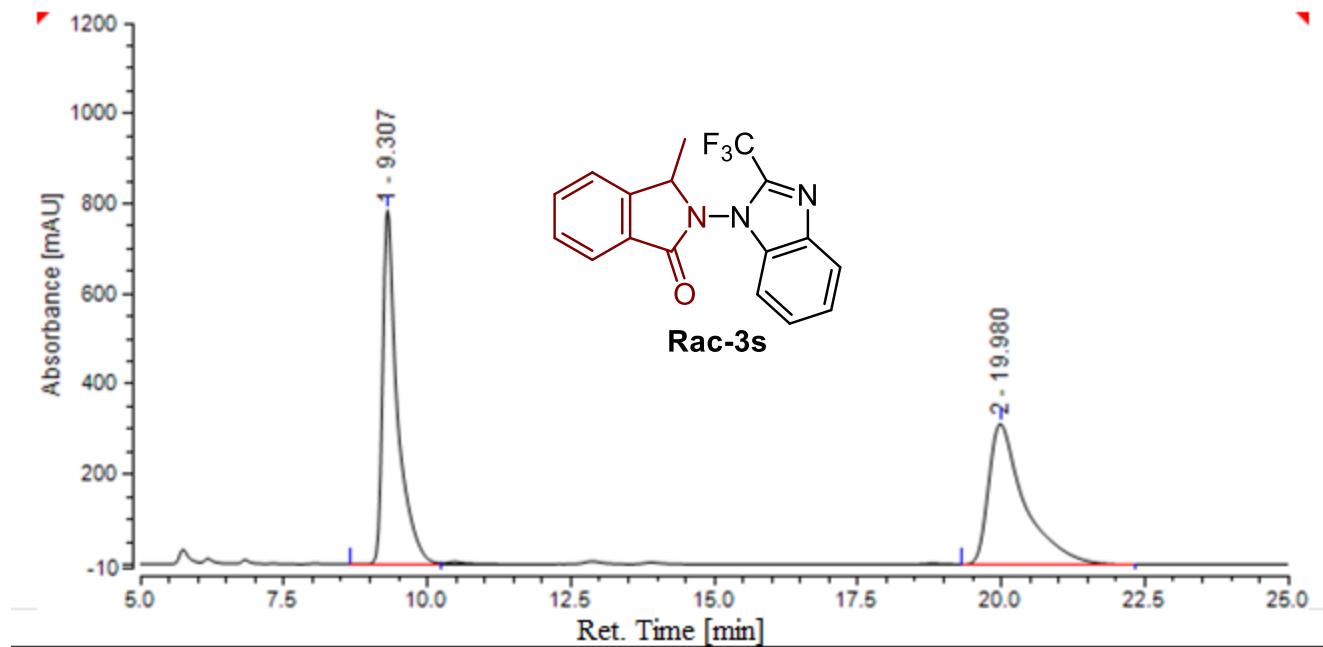


Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	25.11	517.470	663.531	49.84	57.09
2	30.50	520.759	498.722	50.16	42.91

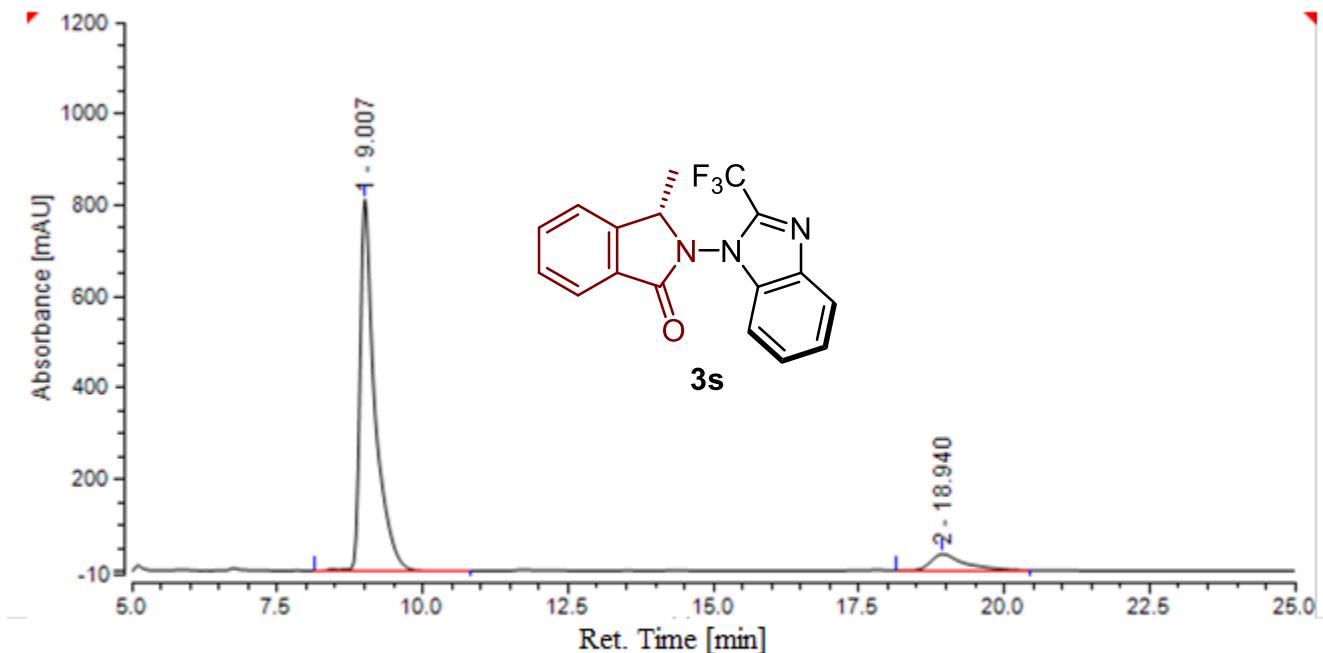


Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	24.73	1089.289	1374.710	97.50	98.02
2	30.82	27.875	27.818	2.50	1.98

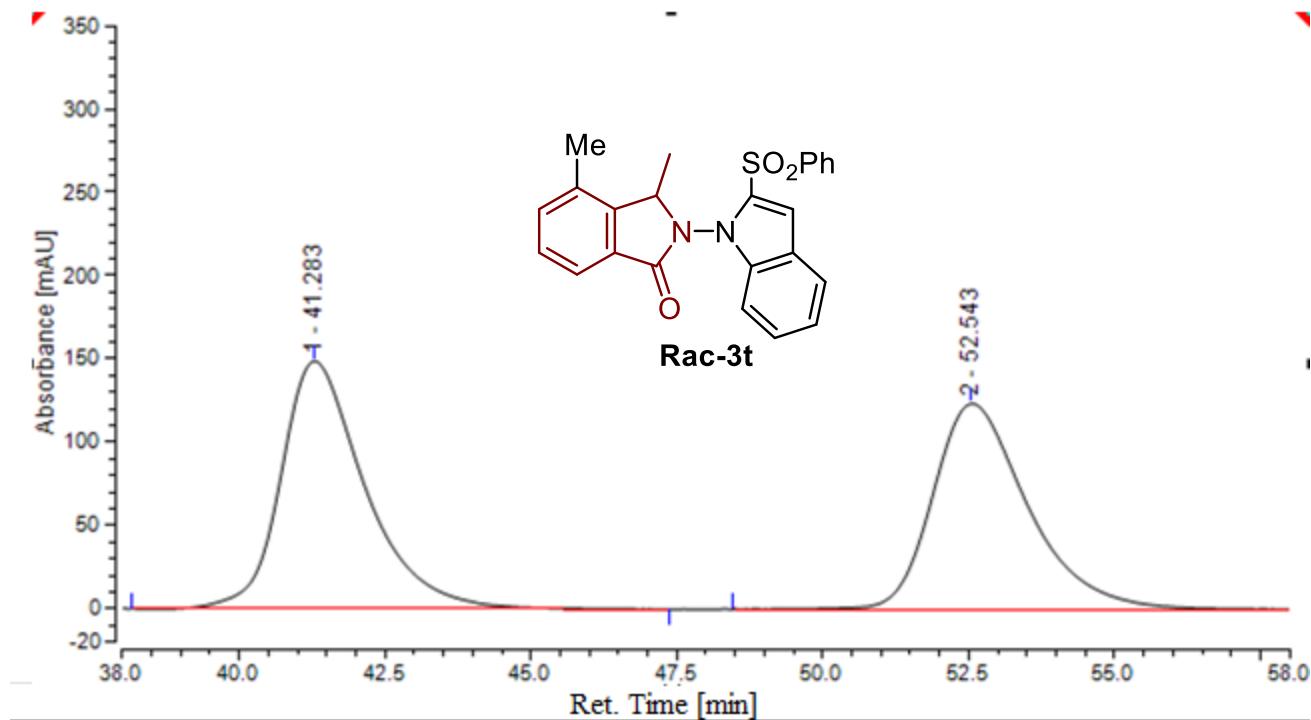




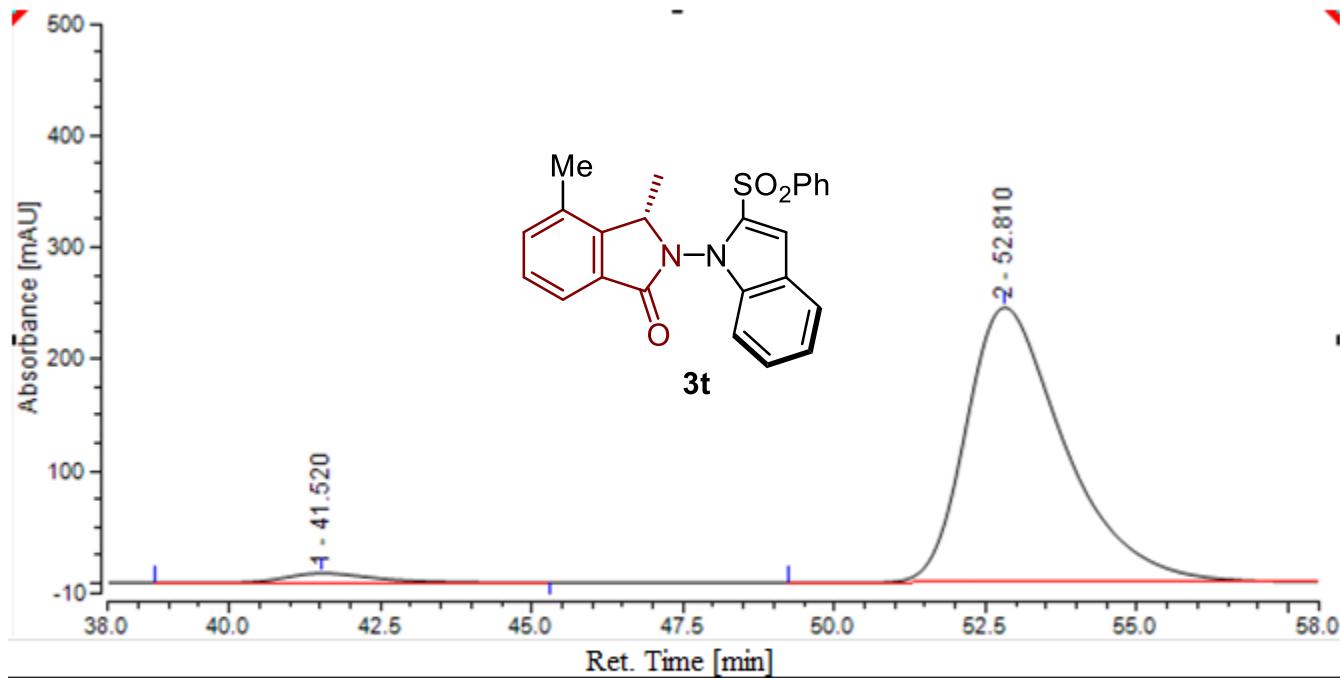
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Heighet %
1	9.31	232.812	785.073	50.71	71.54
2	19.98	226.301	312.268	49.29	28.46



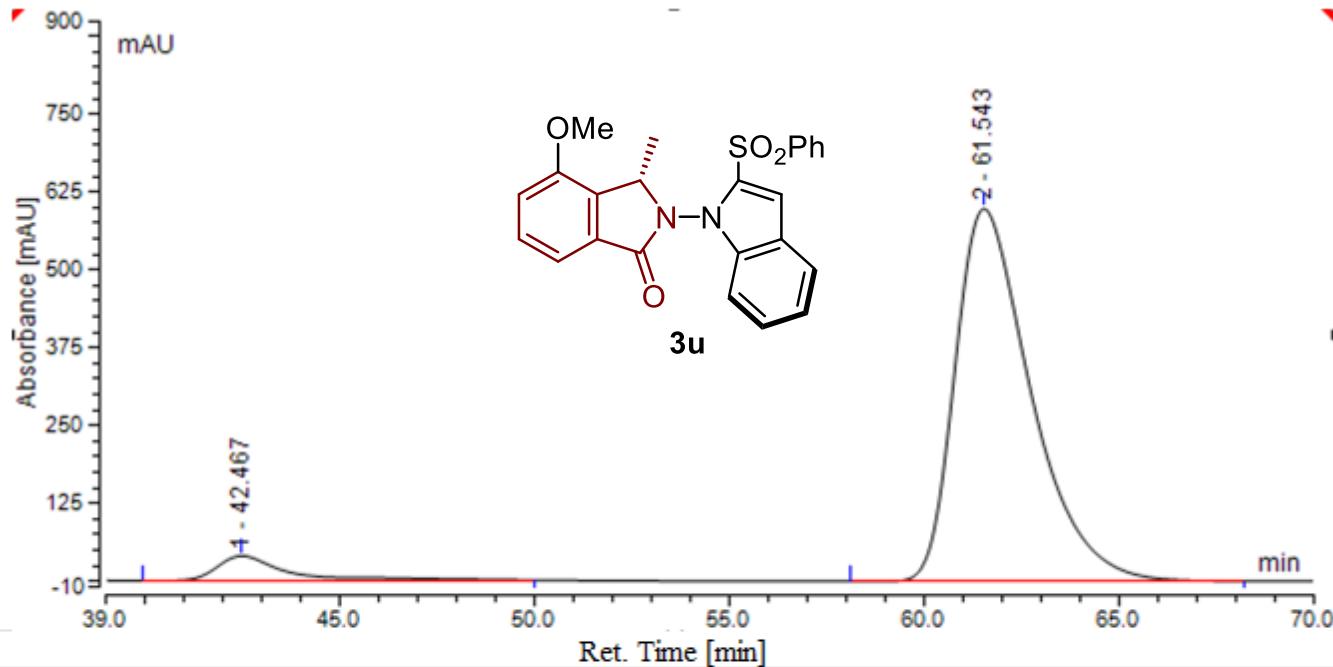
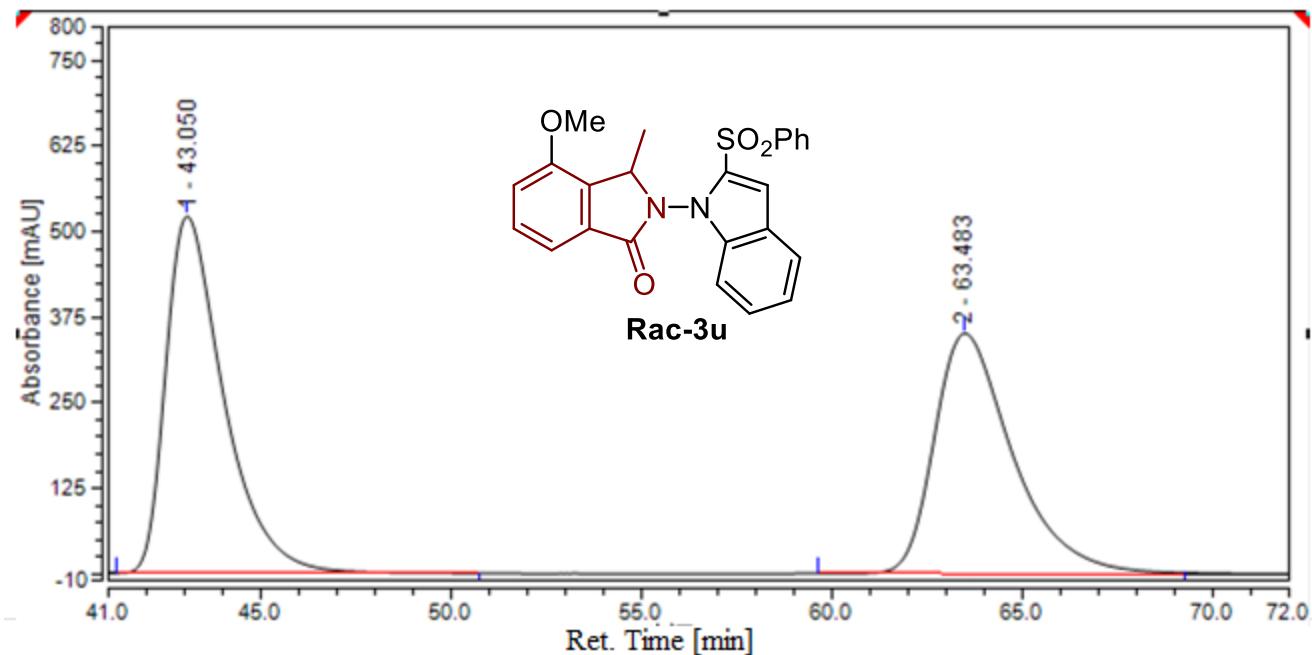
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Heighet %
1	9.01	238.787	812.691	91.00	95.79
2	18.94	23.602	35.724	9.00	4.21

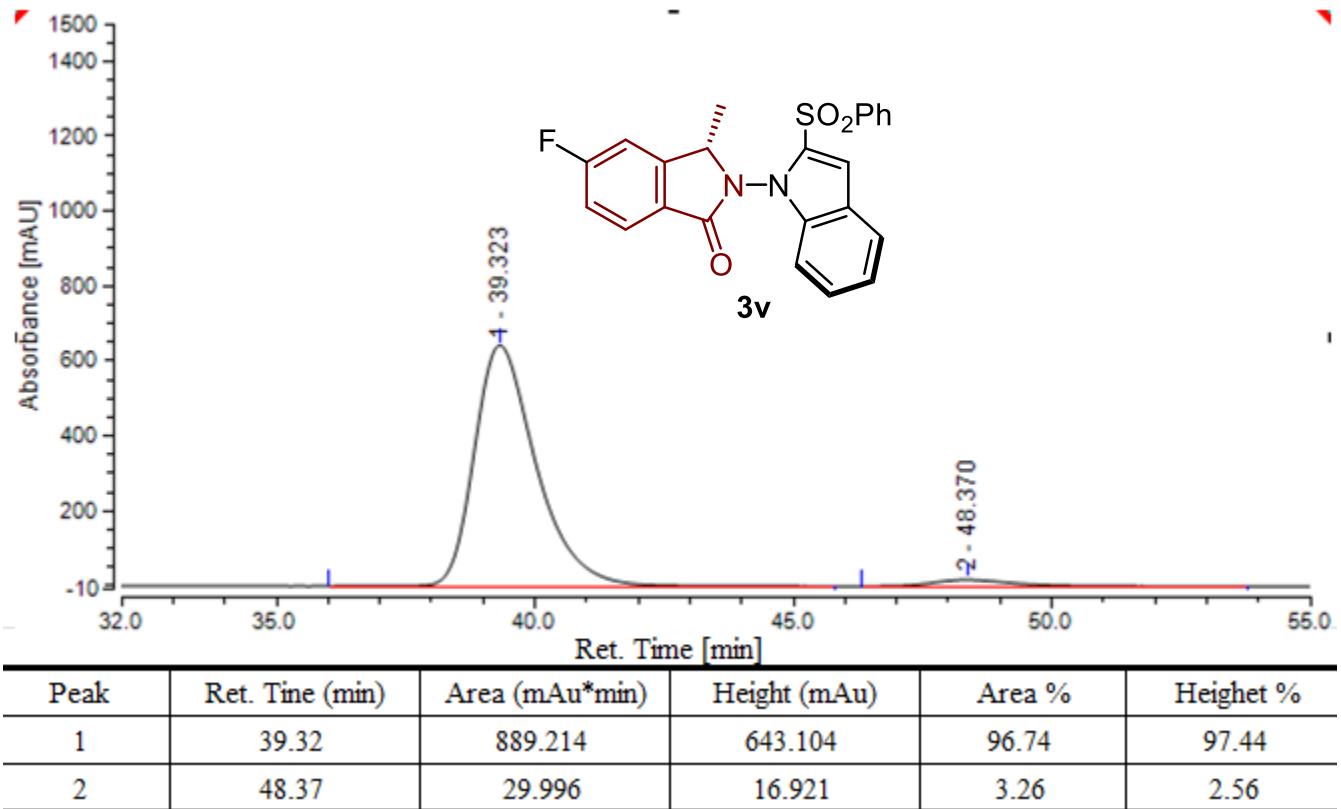
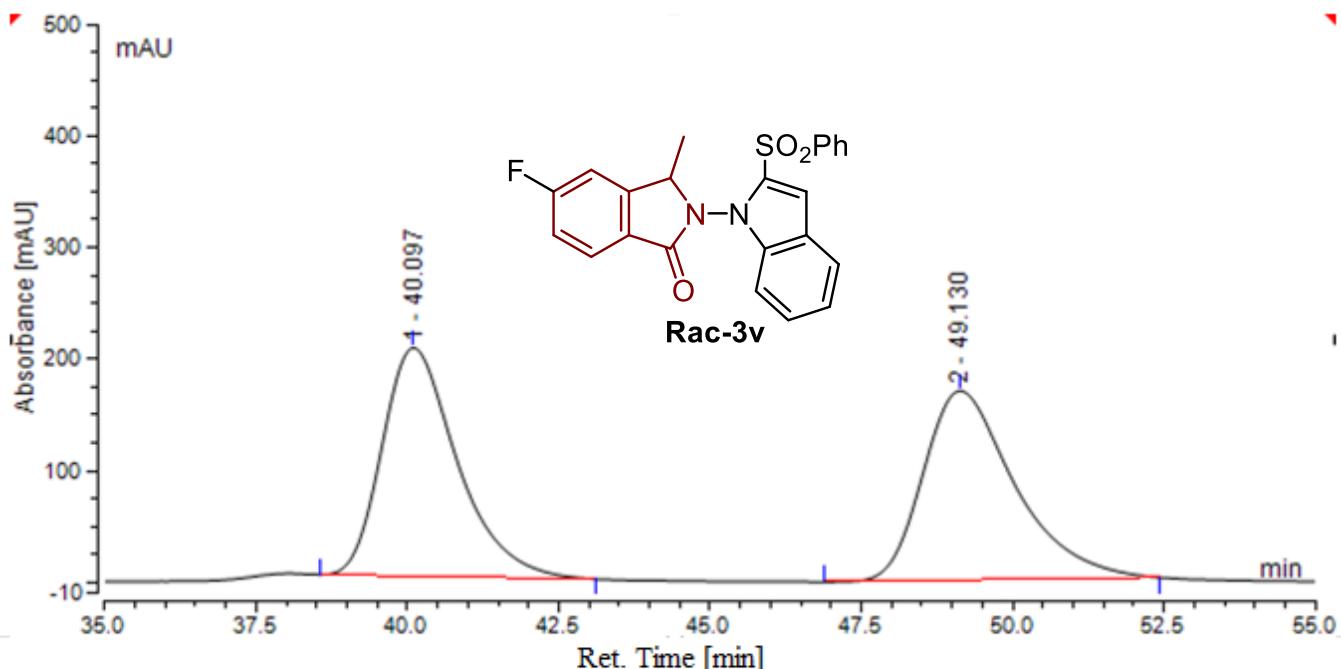


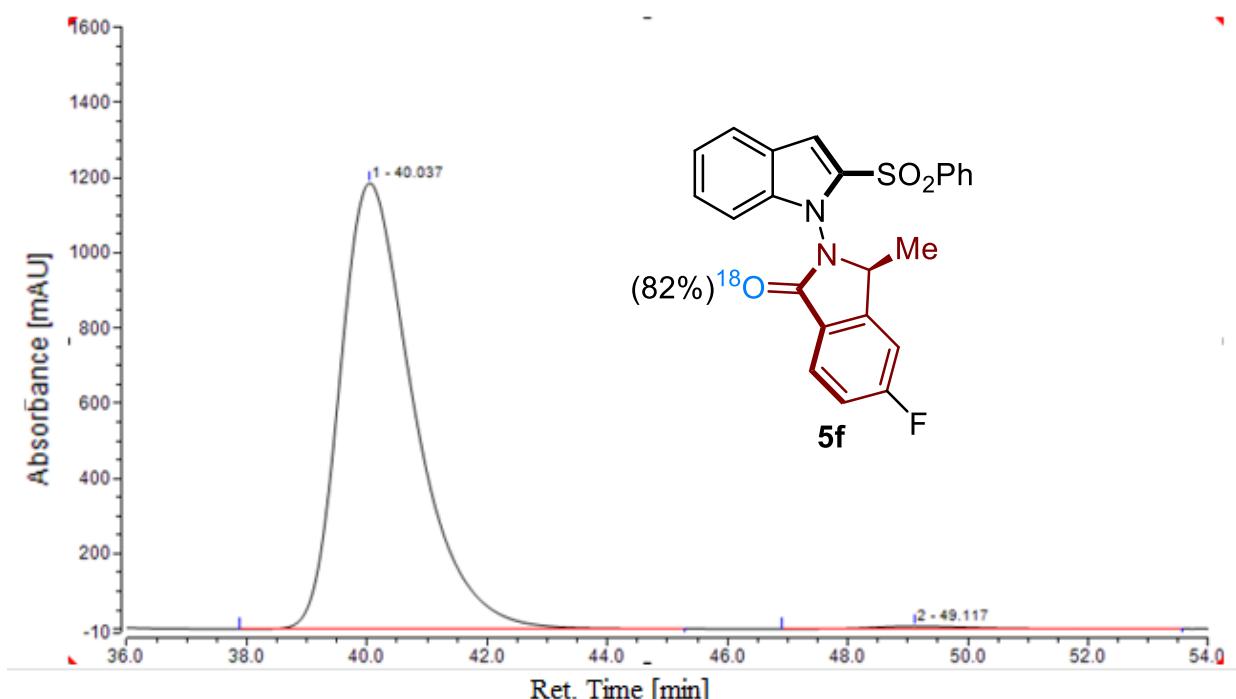
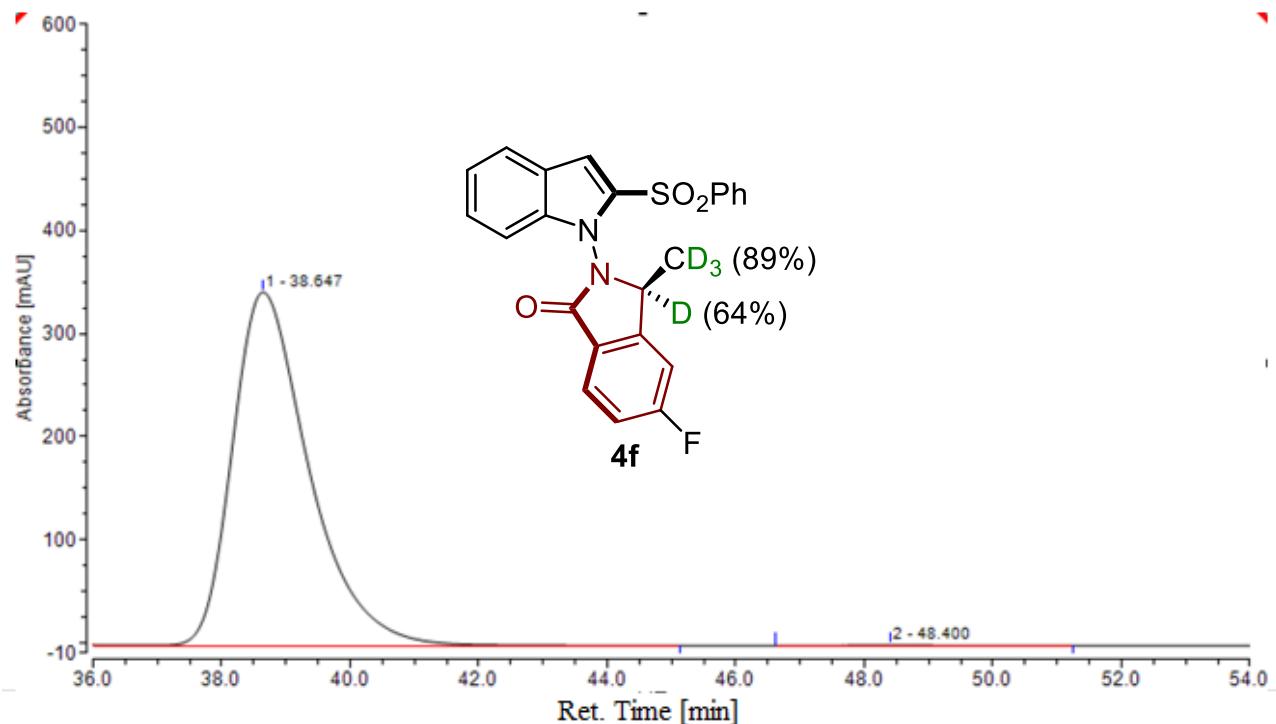
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Heighet %
1	41.28	248.288	148.596	51.66	54.66
2	52.54	232.304	123.283	48.34	45.34

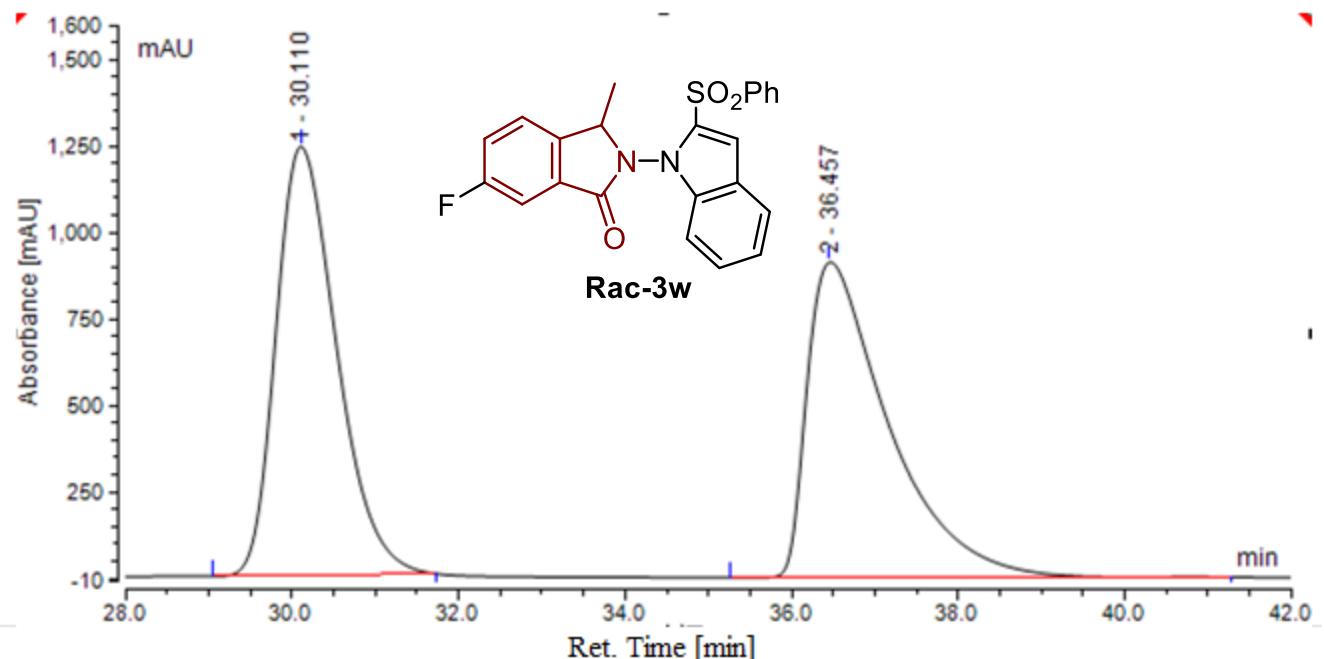


Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Heighet %
1	41.52	14.050	8.382	2.94	3.30
2	52.81	464.196	245.761	97.06	96.70

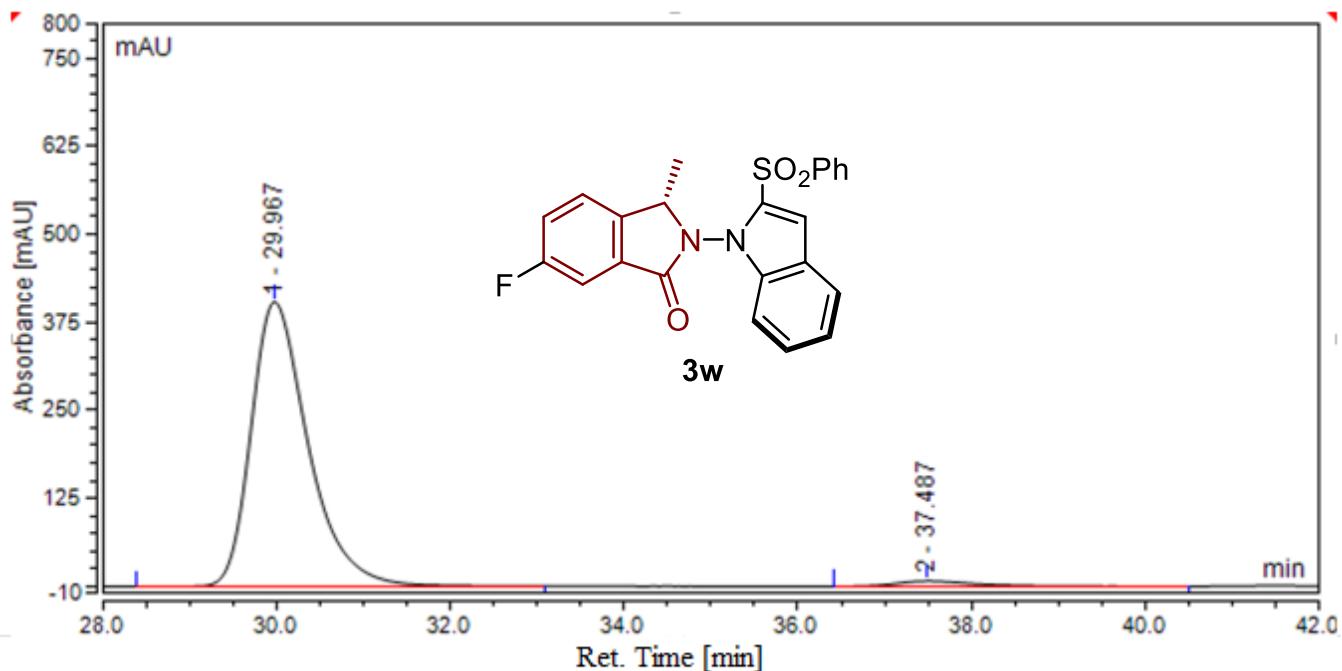




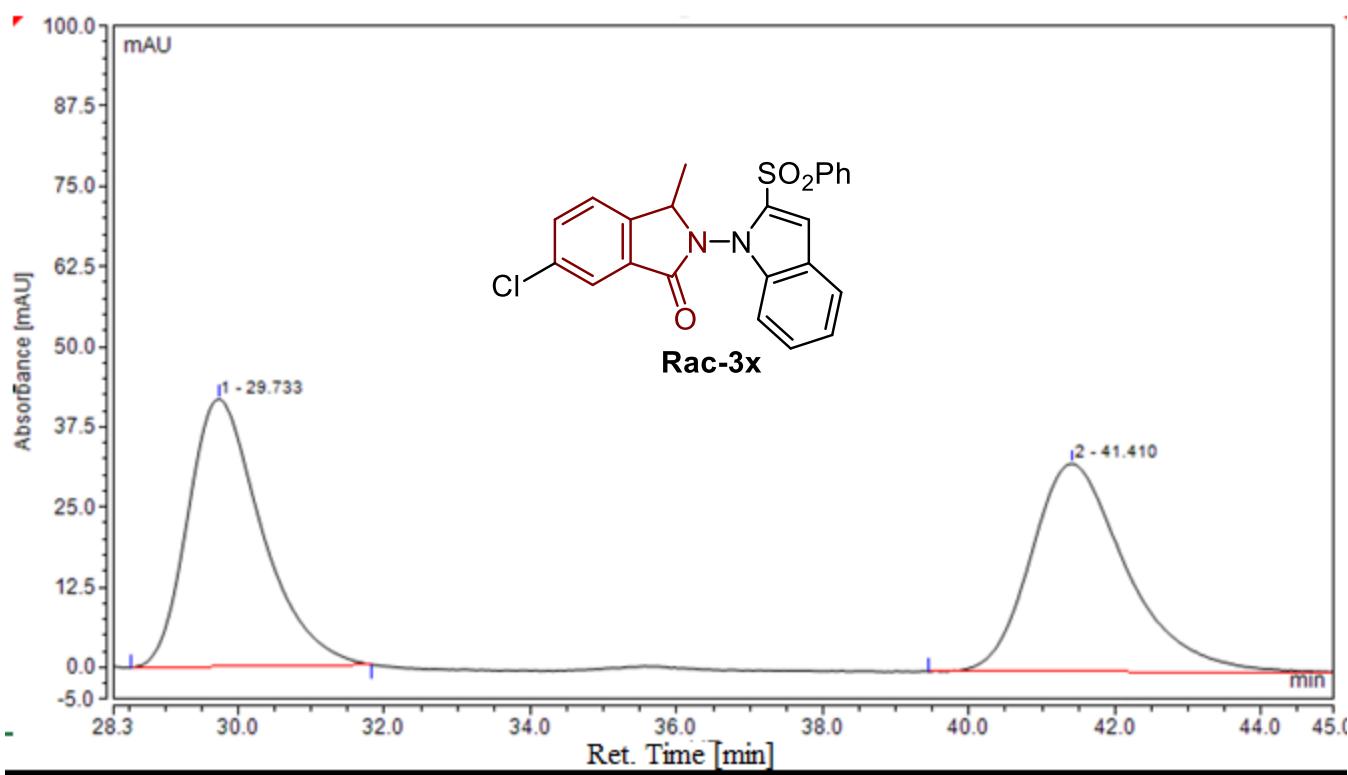




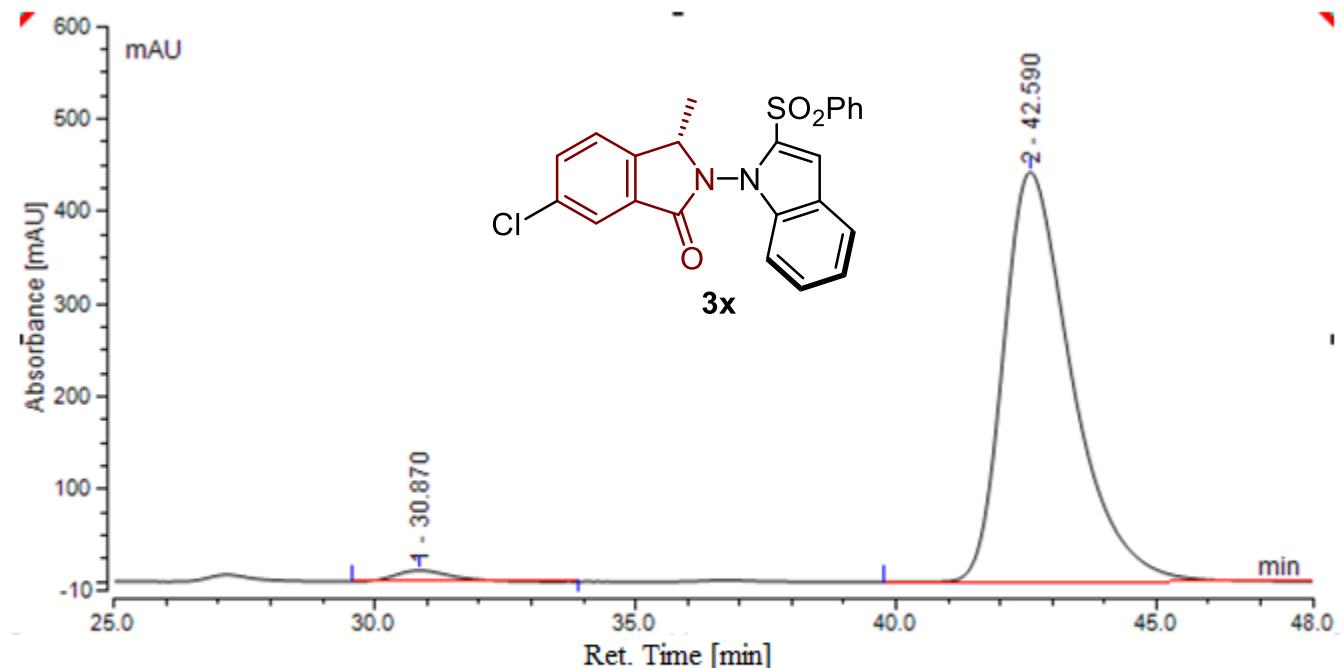
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	30.11	1043.754	1240.322	50.32	57.62
2	36.46	1030.470	912.443	49.68	42.38



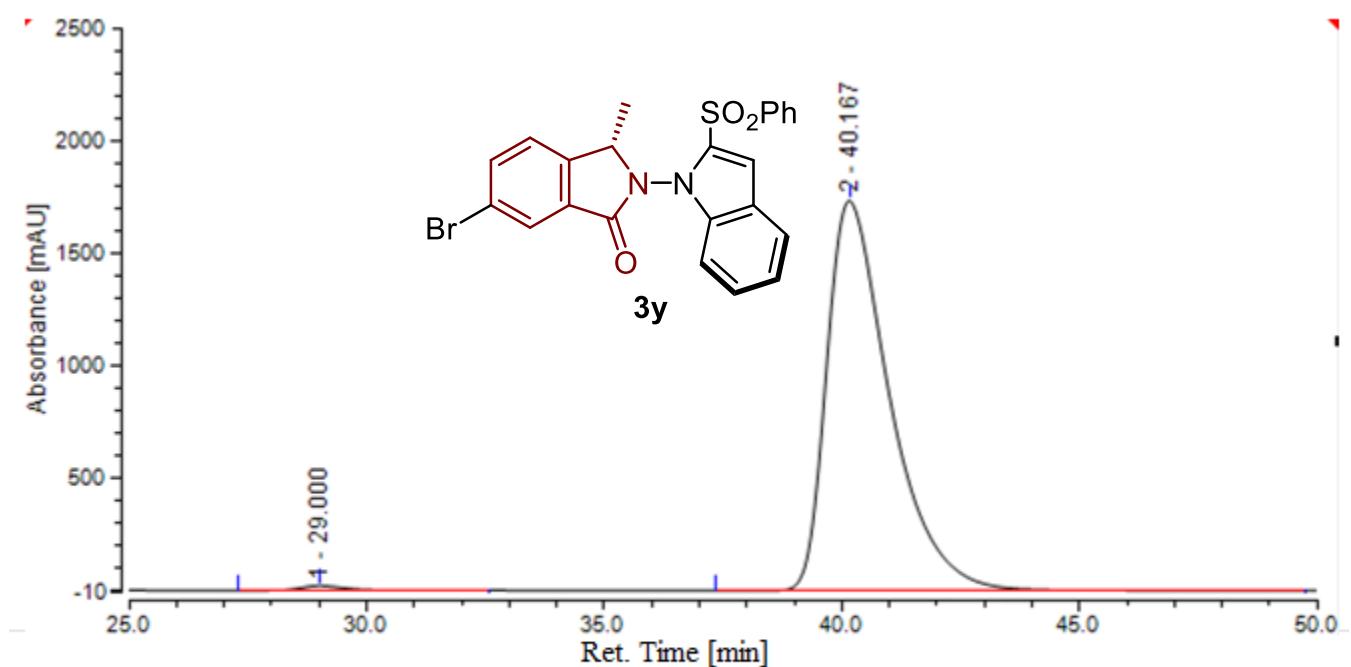
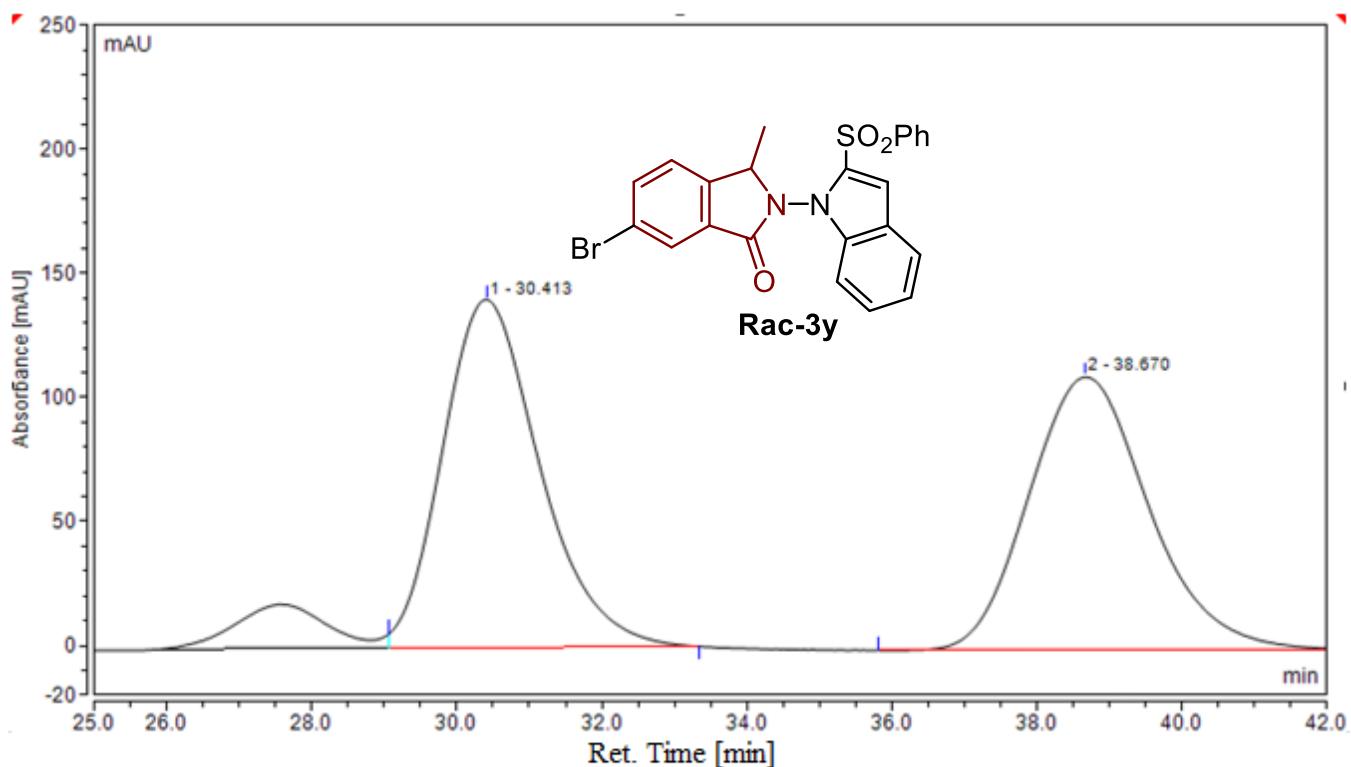
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Height %
1	29.97	306.996	403.867	97.41	98.17
2	37.49	8.176	7.515	2.59	1.83

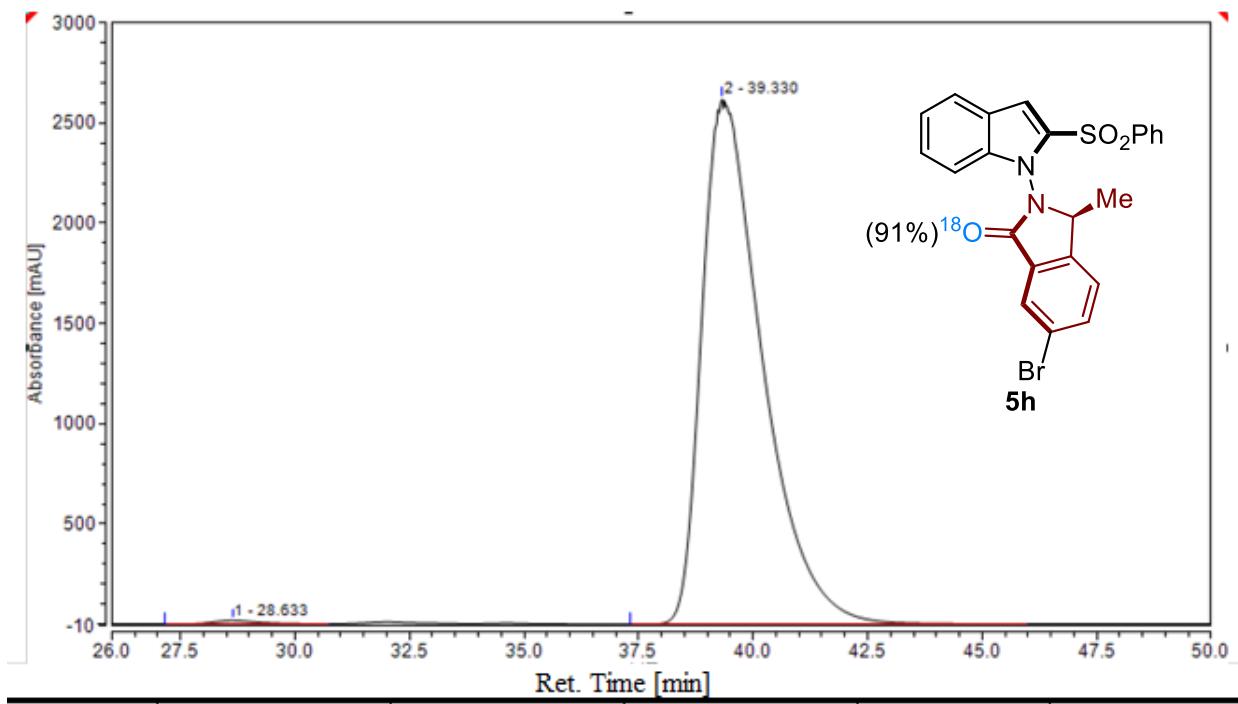
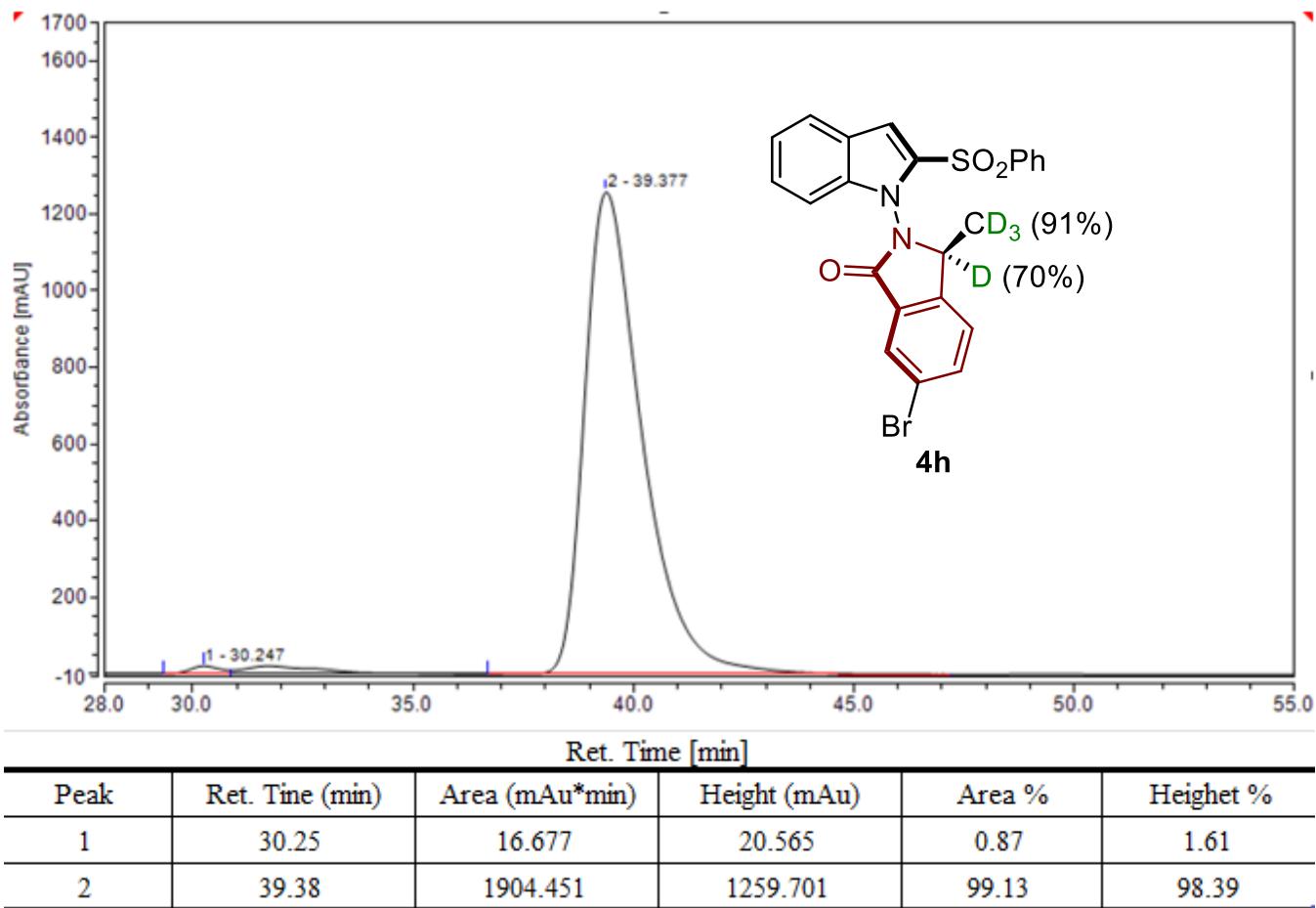


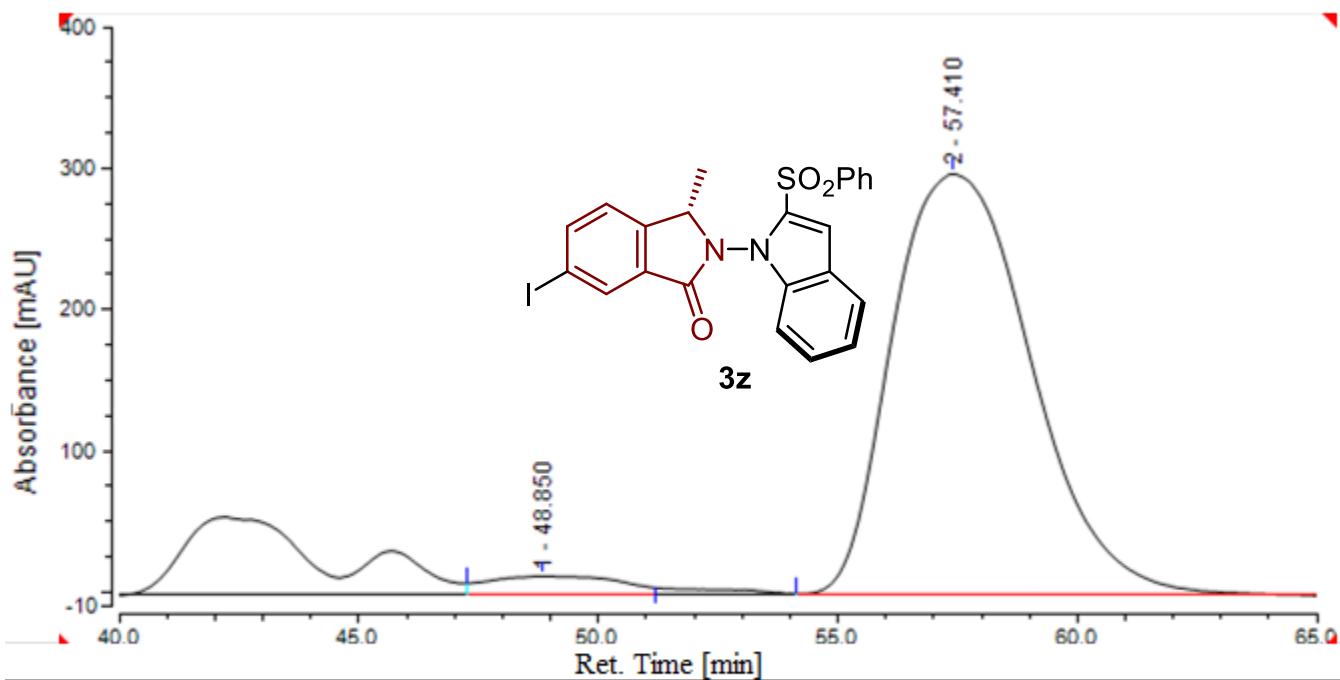
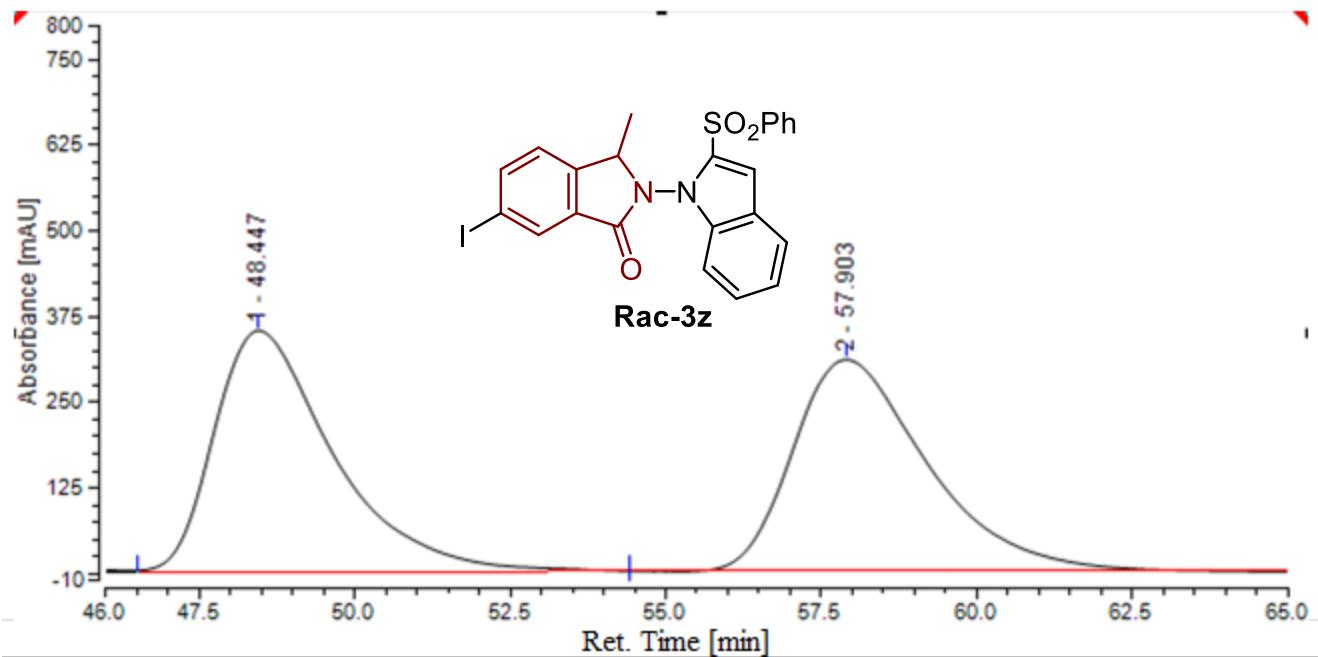
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Heighet %
1	29.73	48.830	41.766	49.84	56.29
2	41.41	49.141	32.436	50.16	43.71

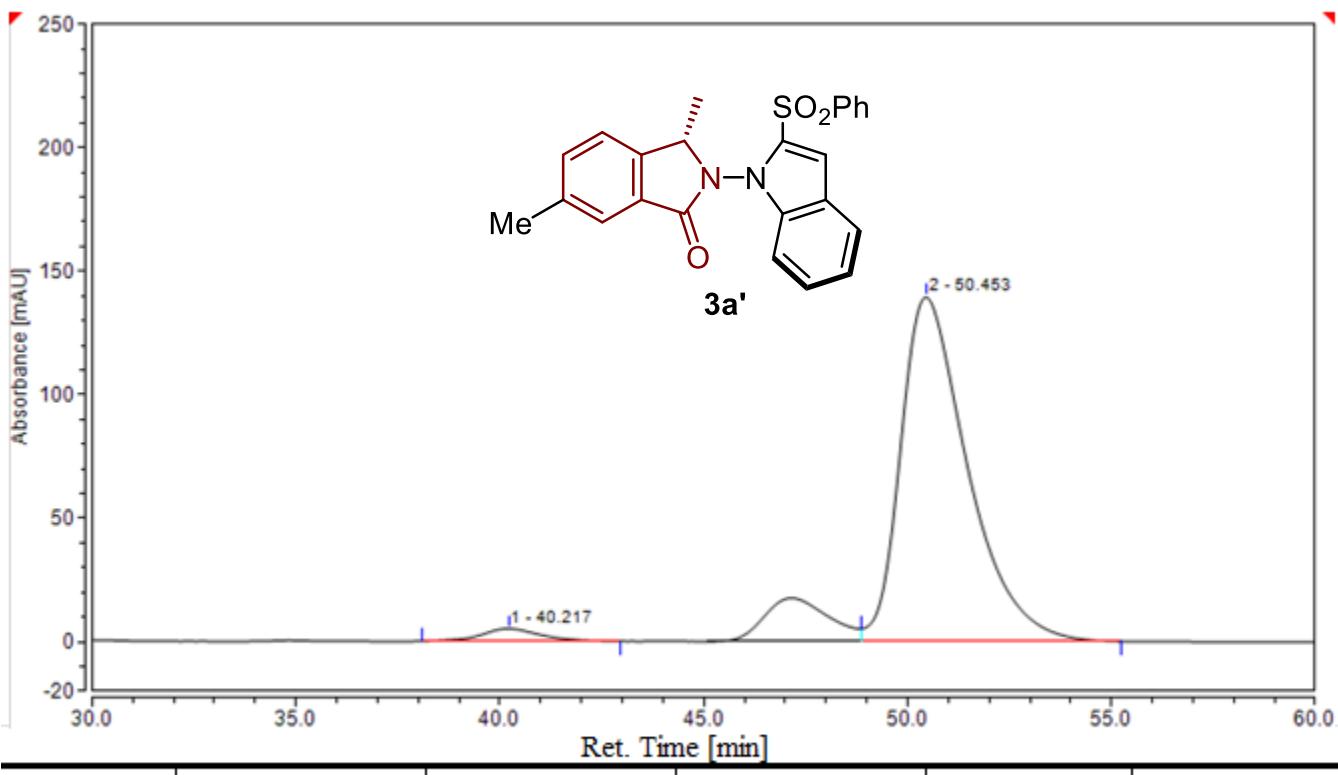
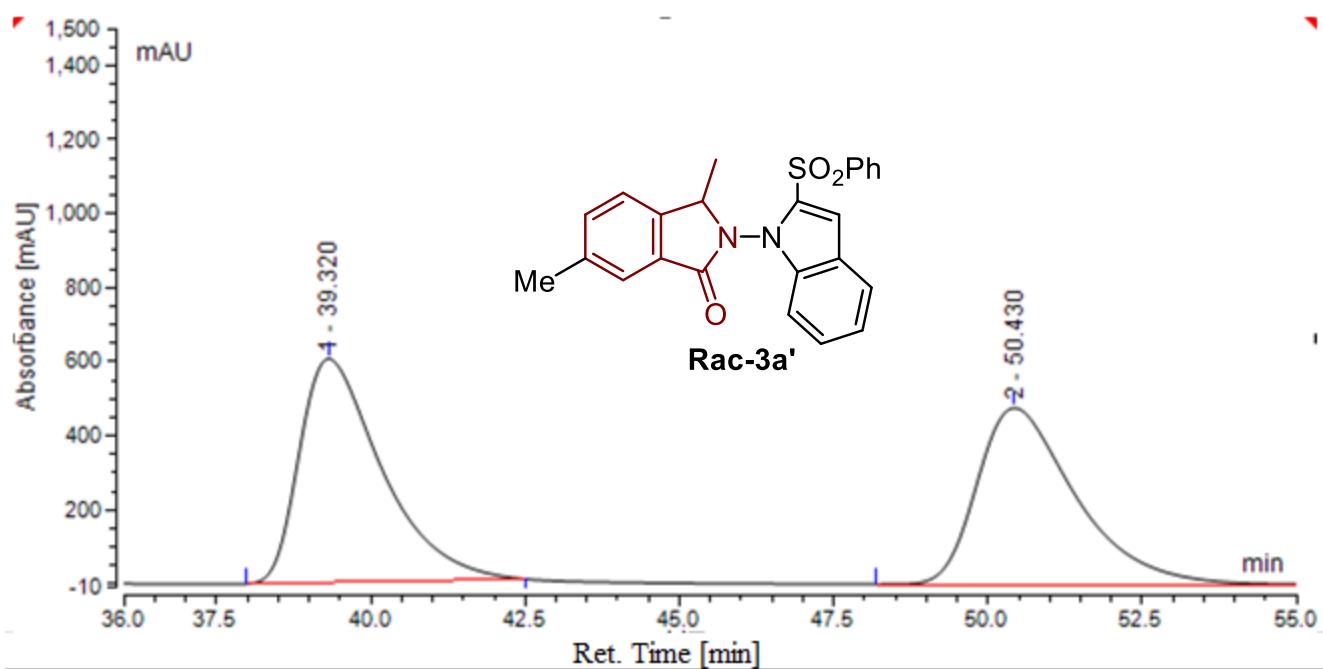


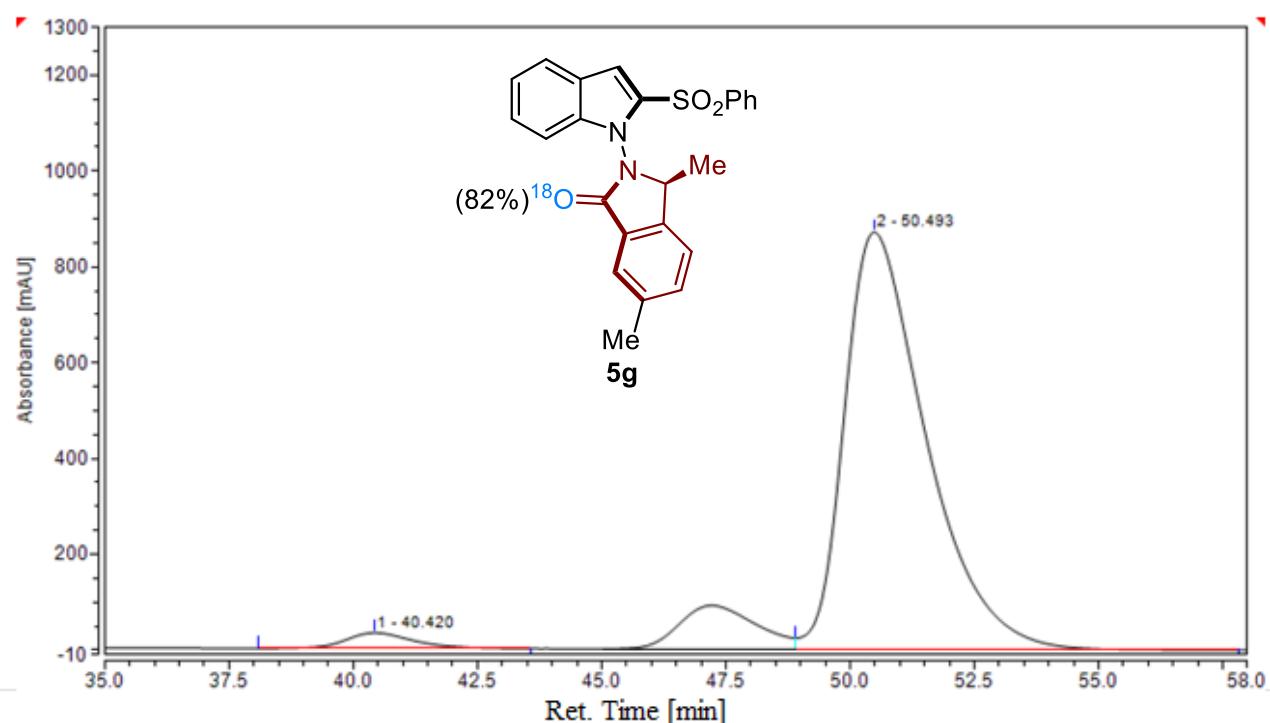
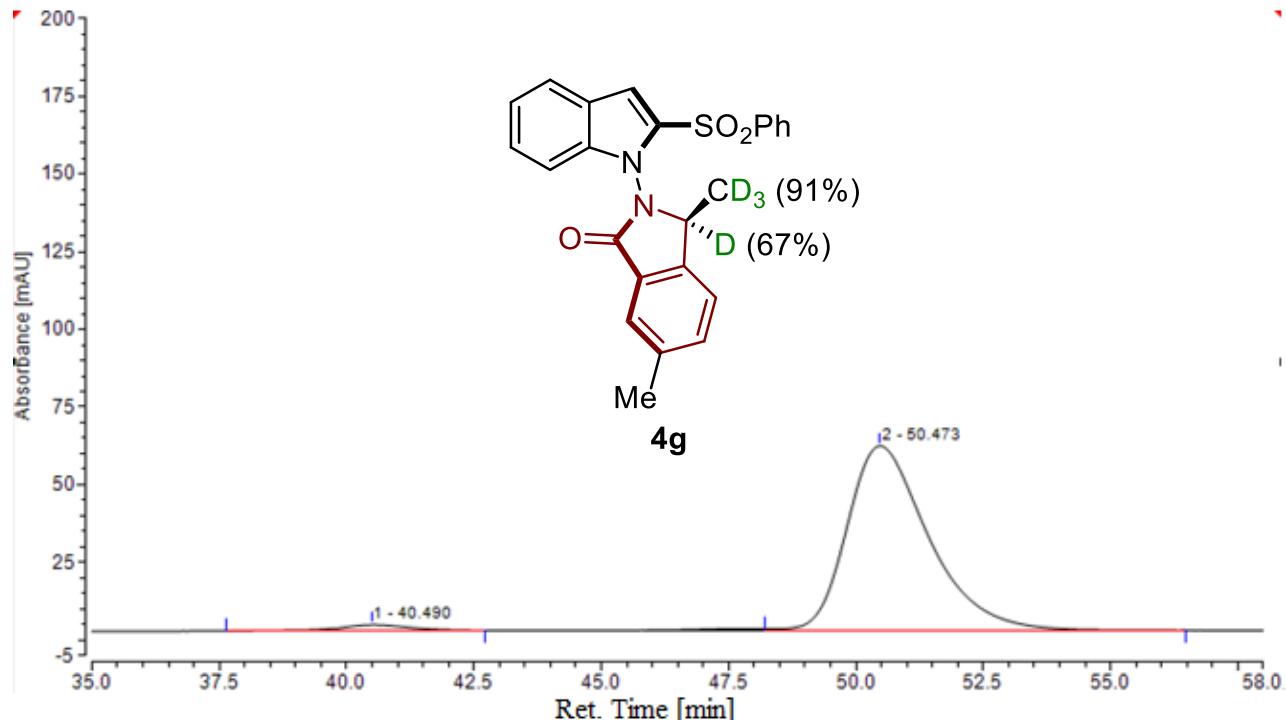
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Heighet %
1	30.87	14.810	11.895	2.16	2.62
2	42.59	671.425	441.914	97.84	97.38

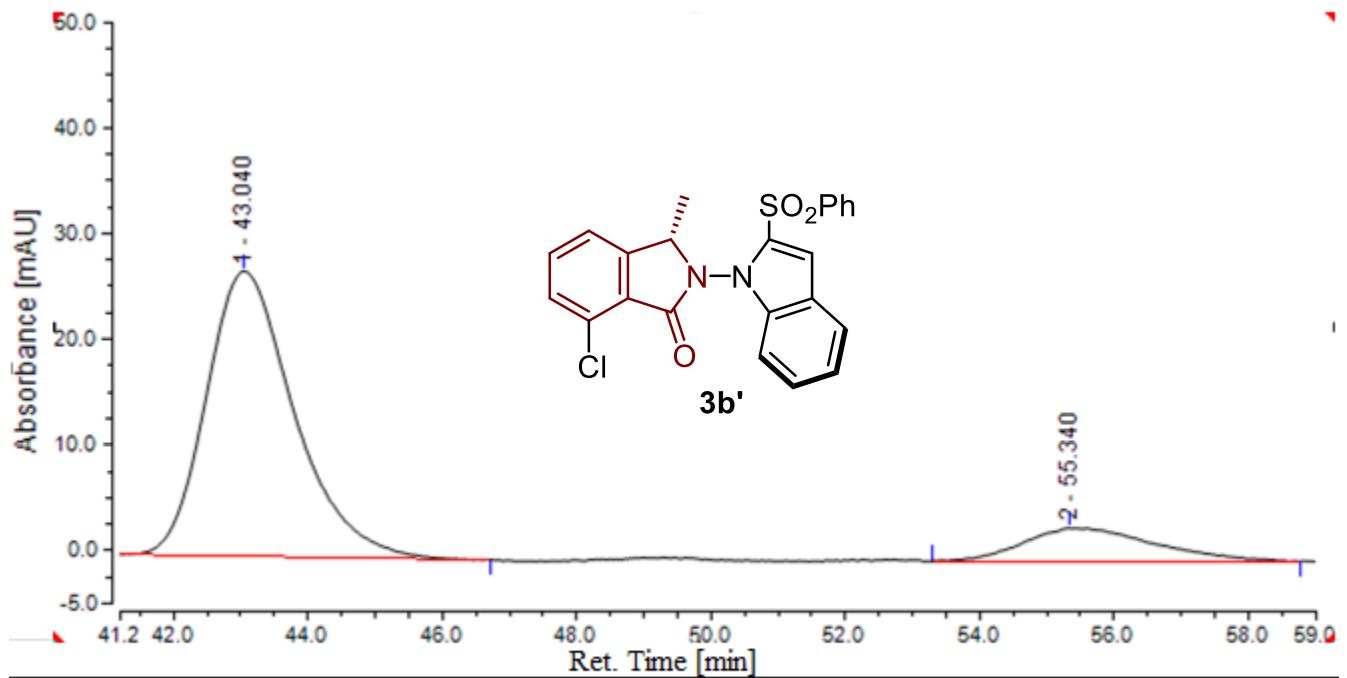
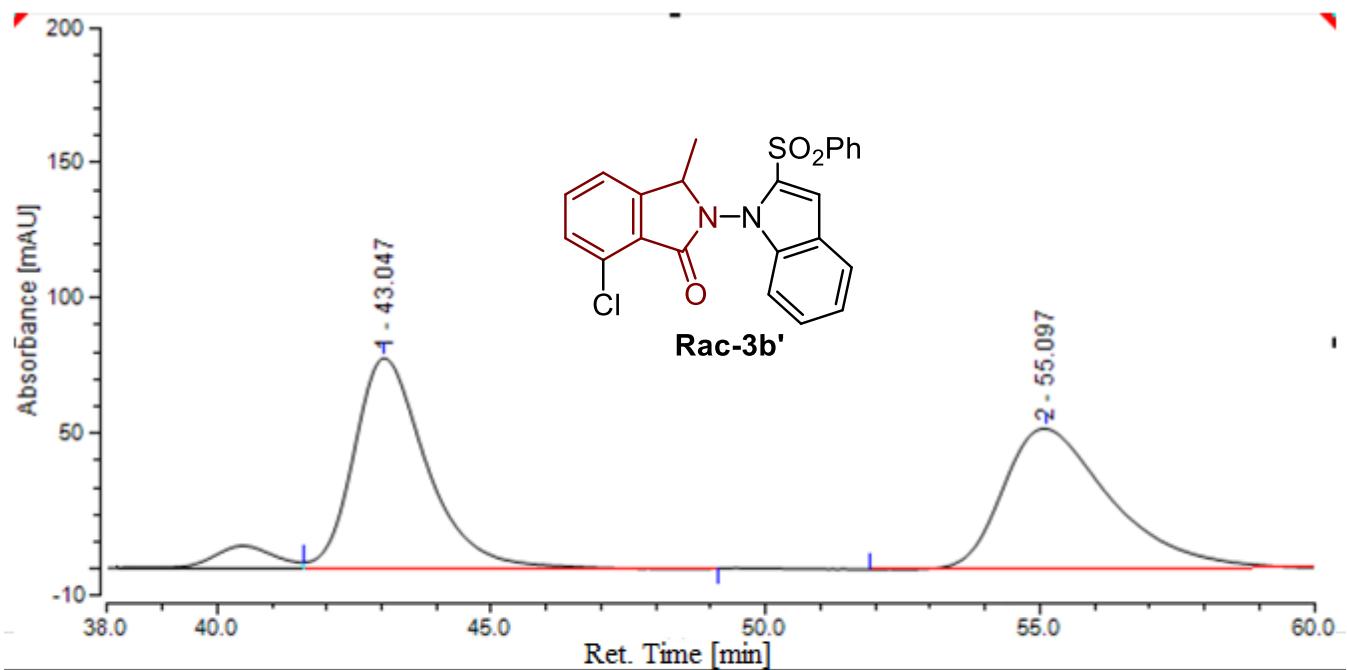


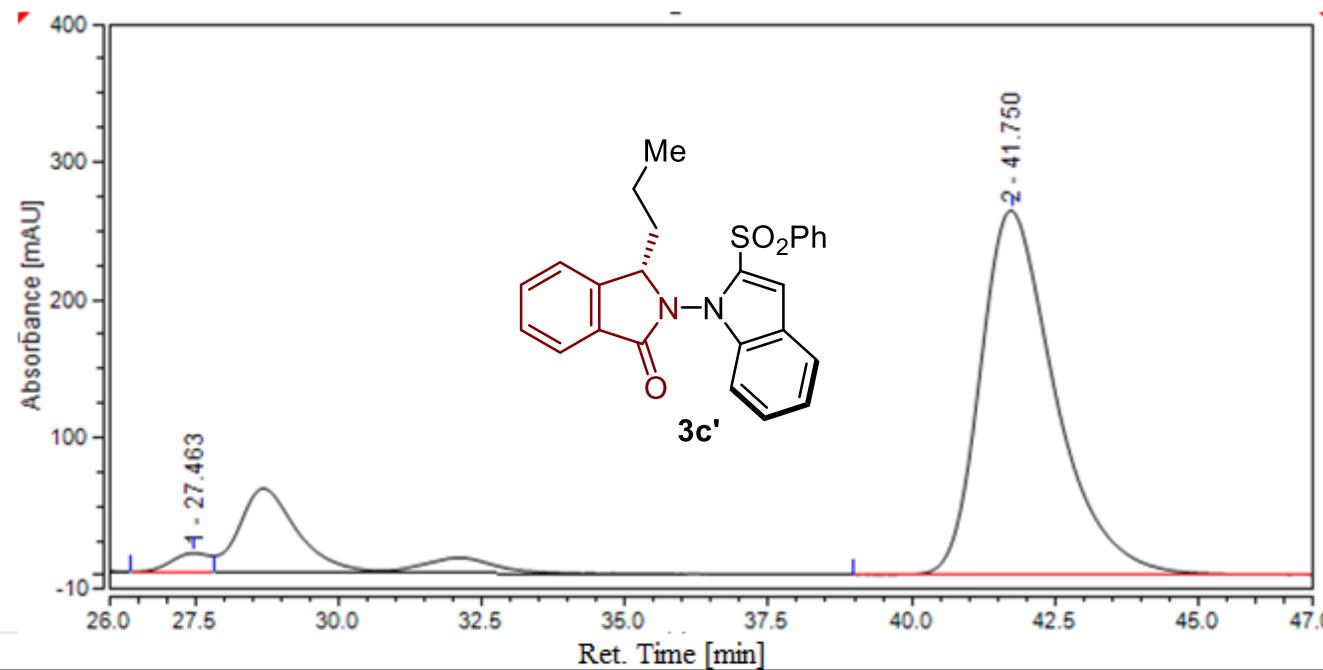
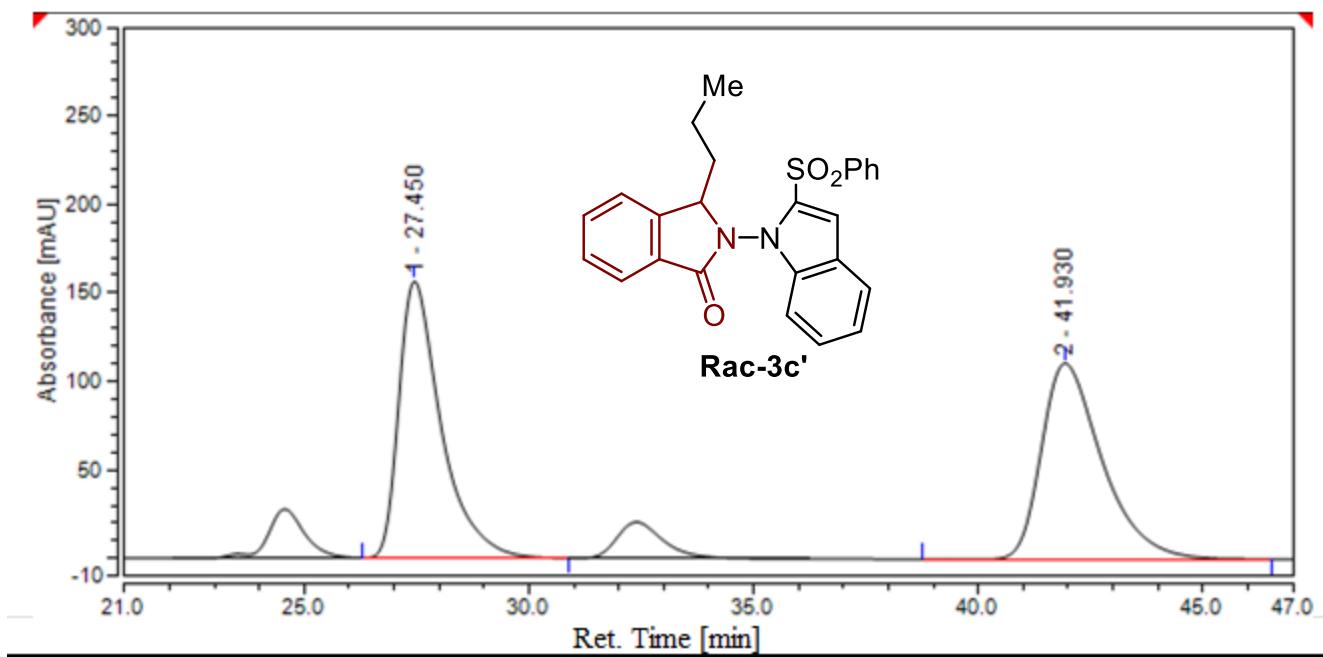


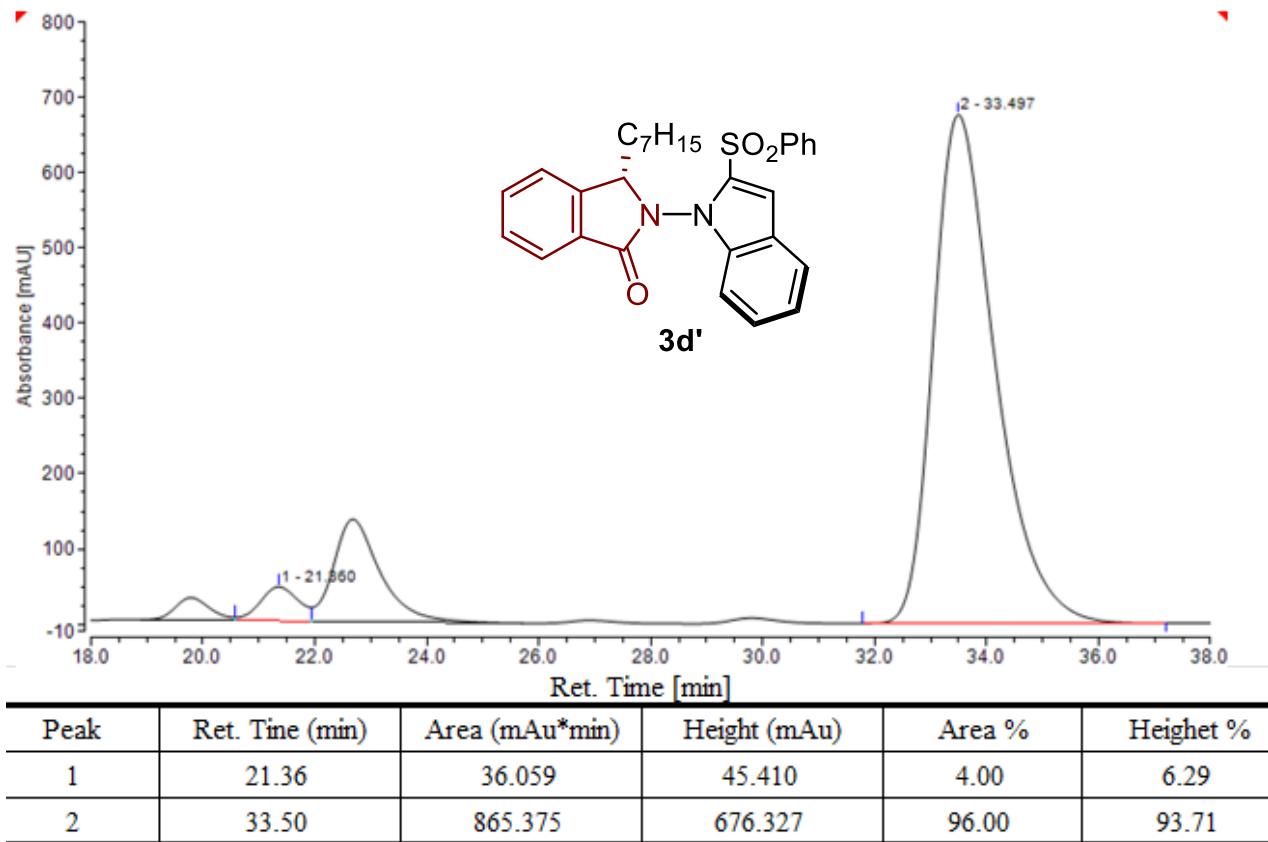
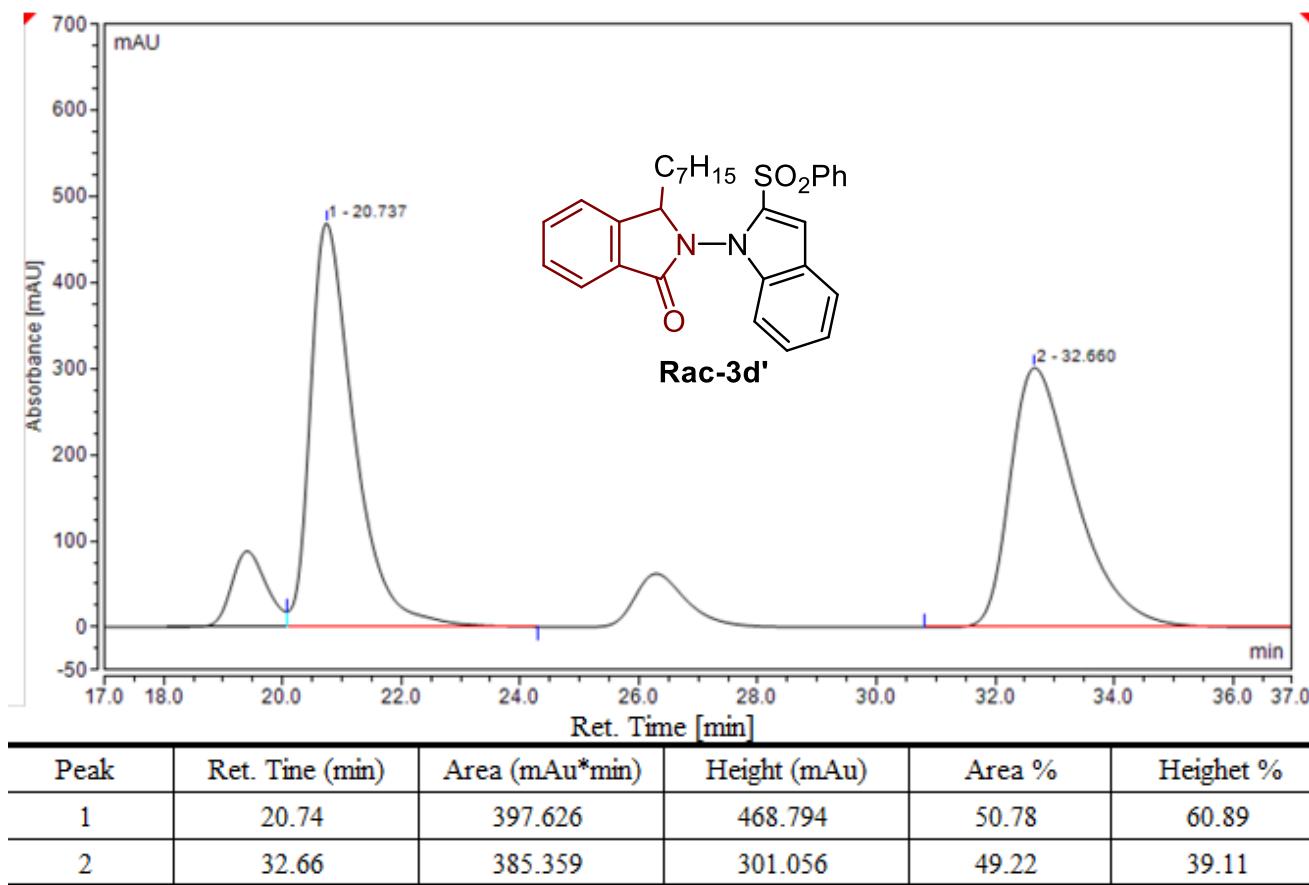


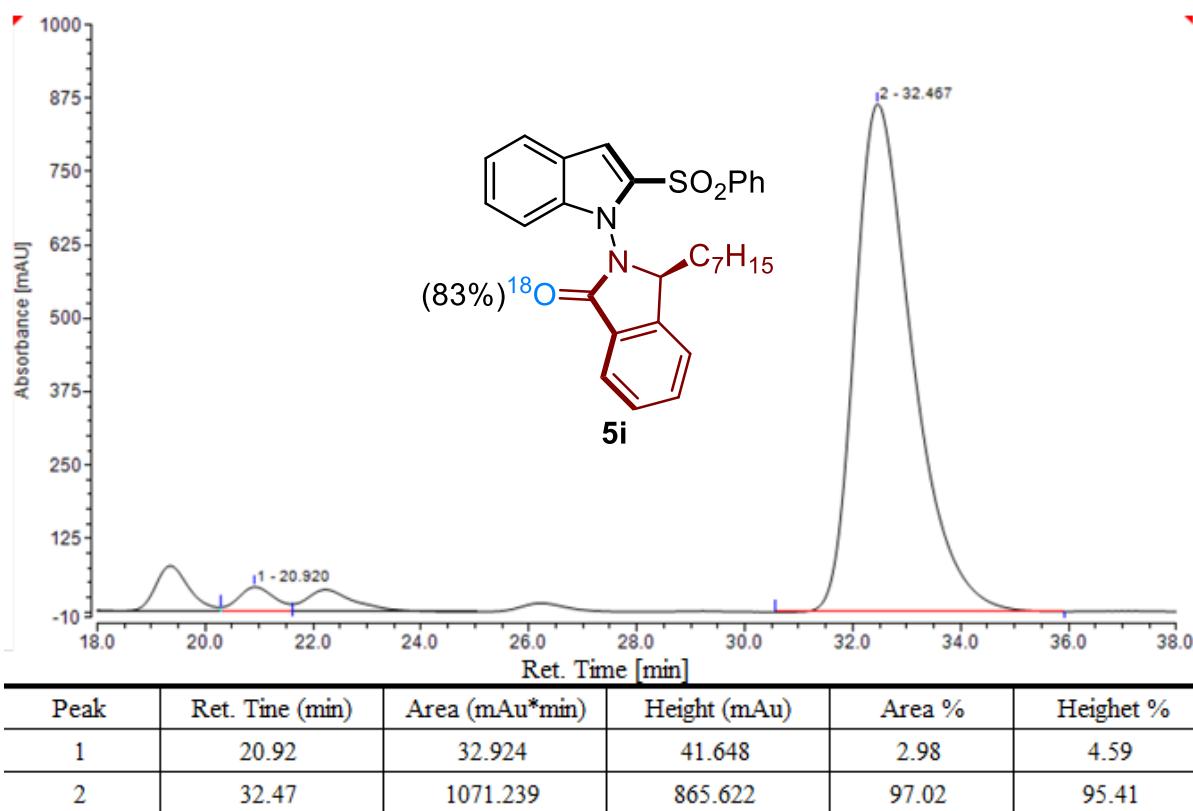
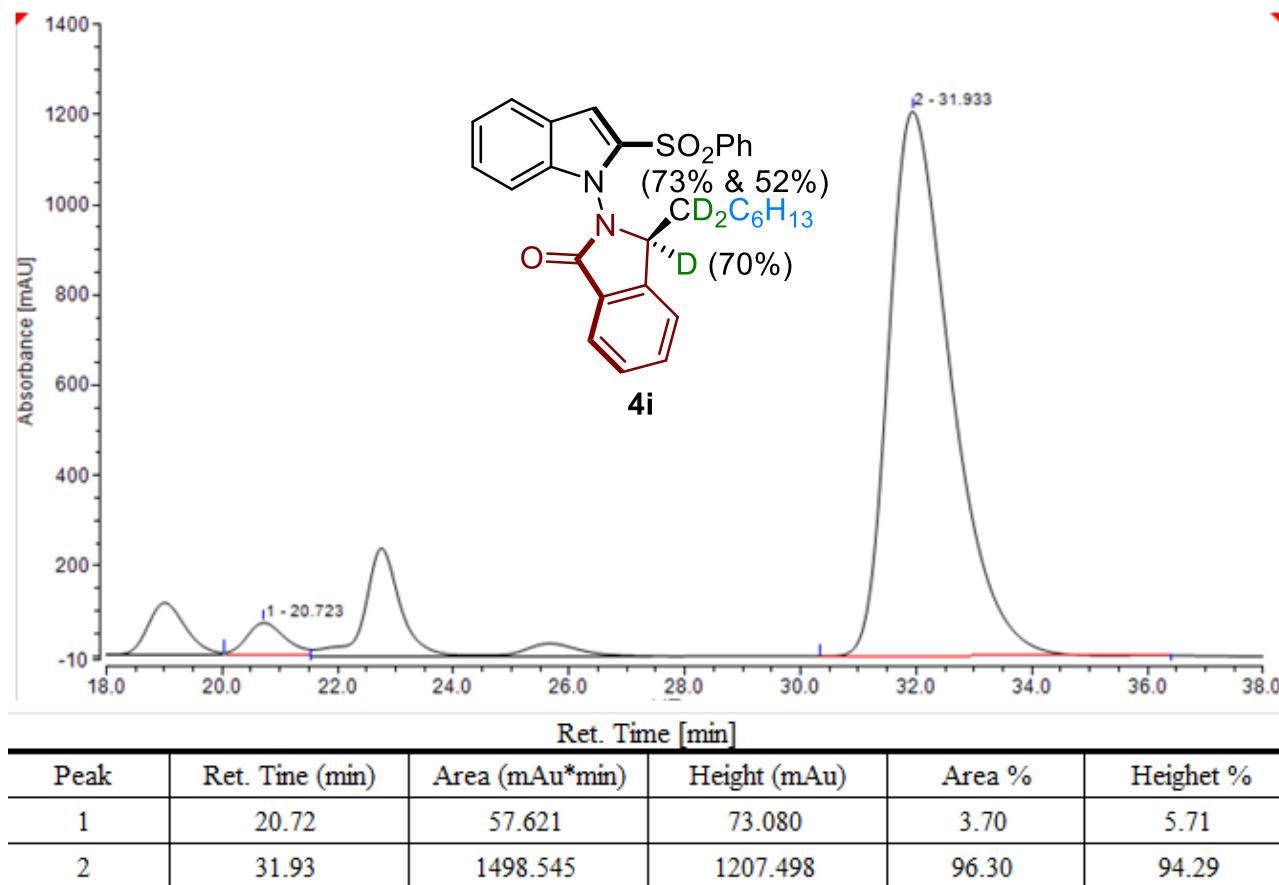


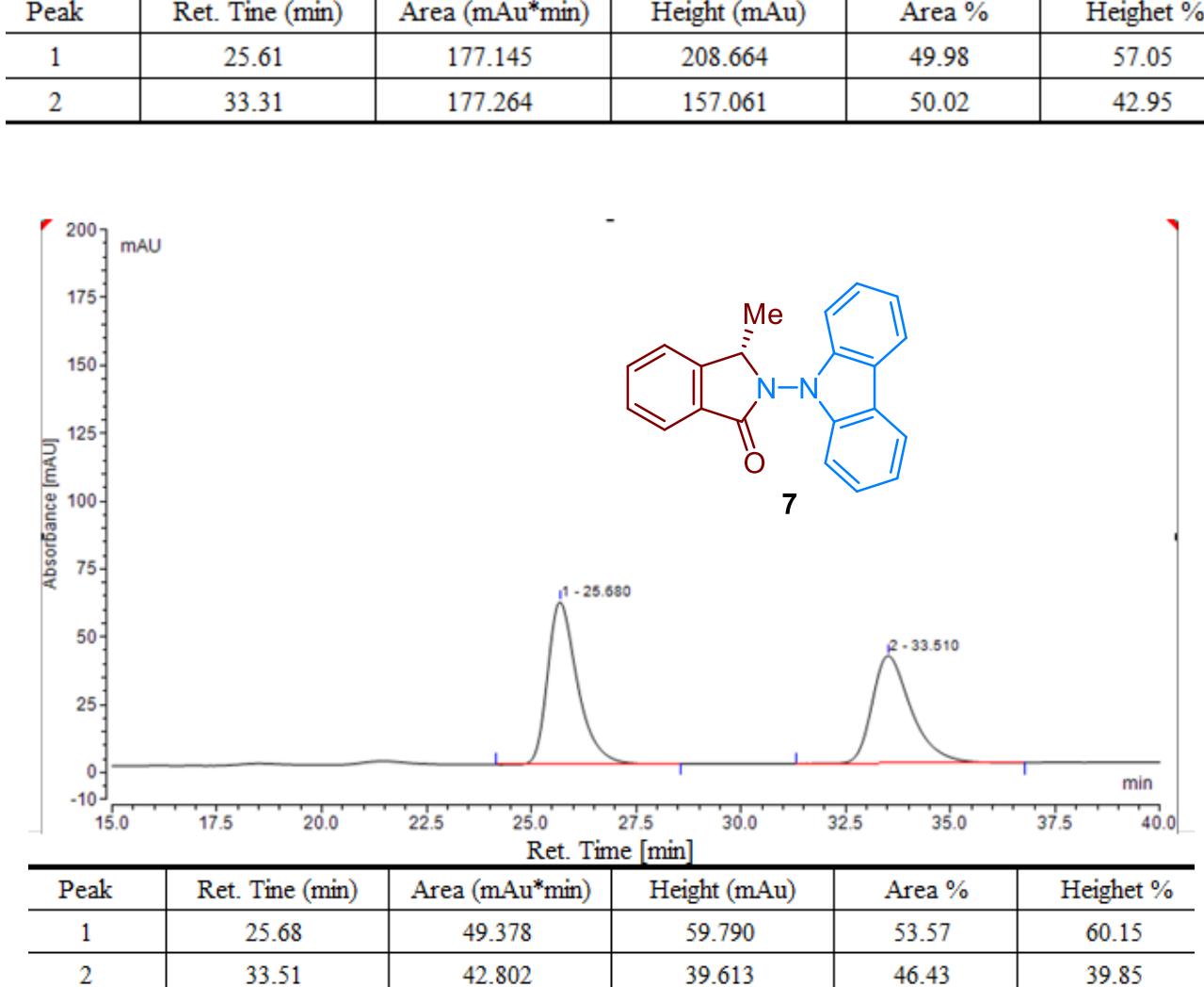
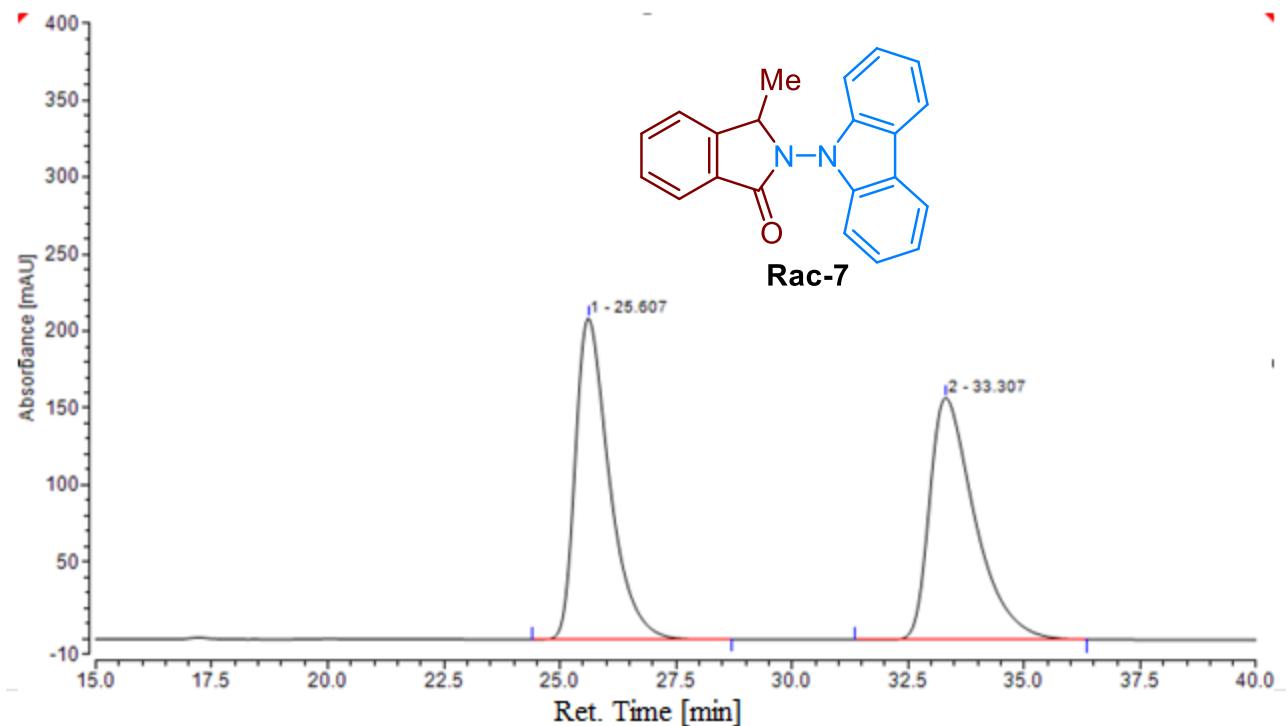


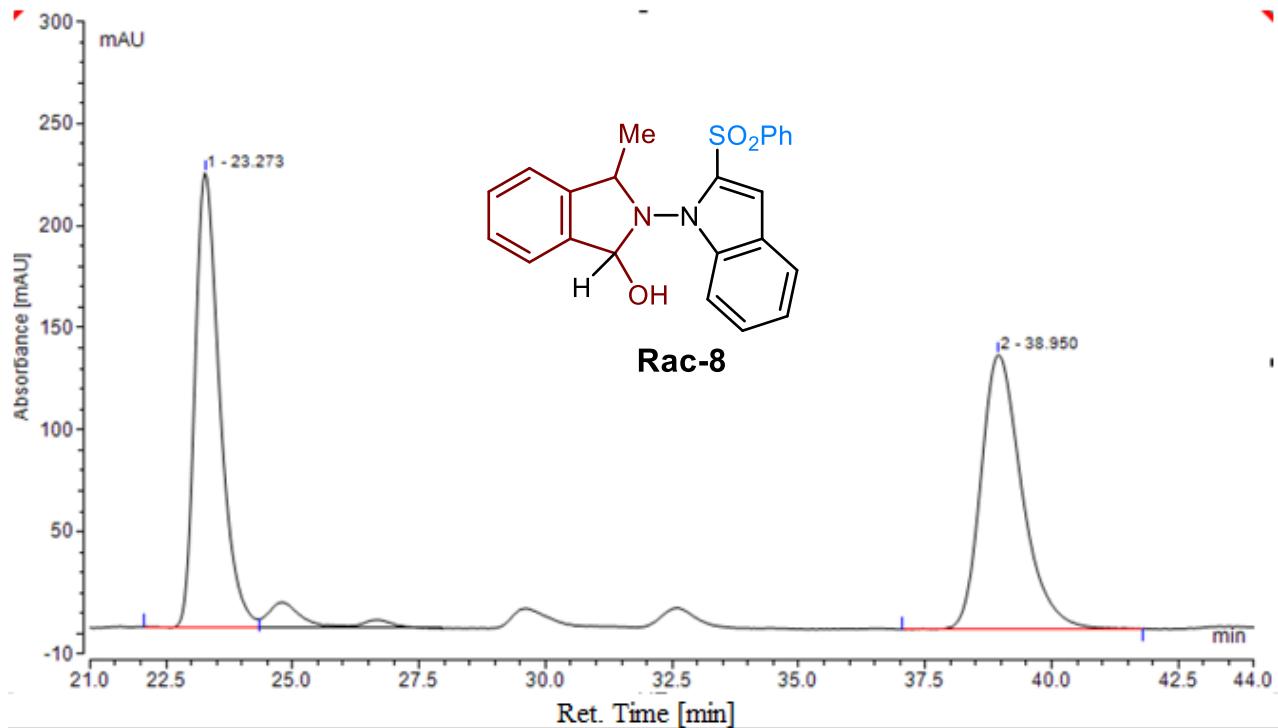




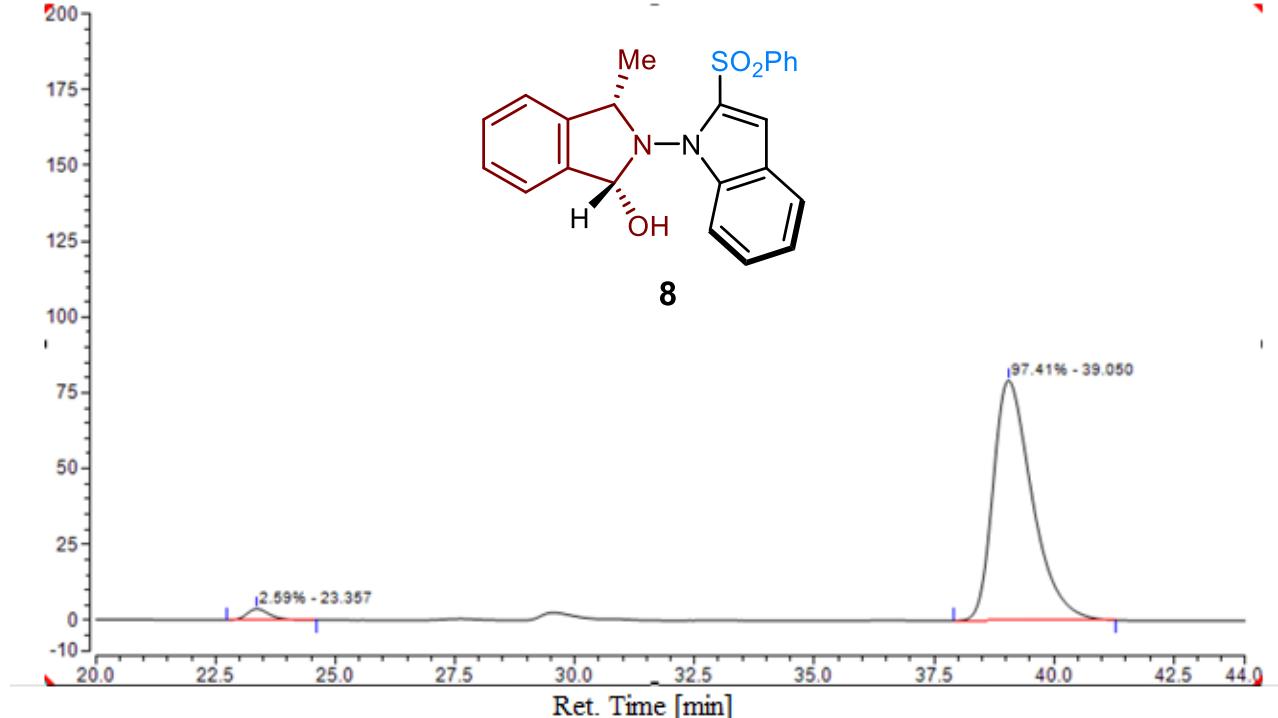




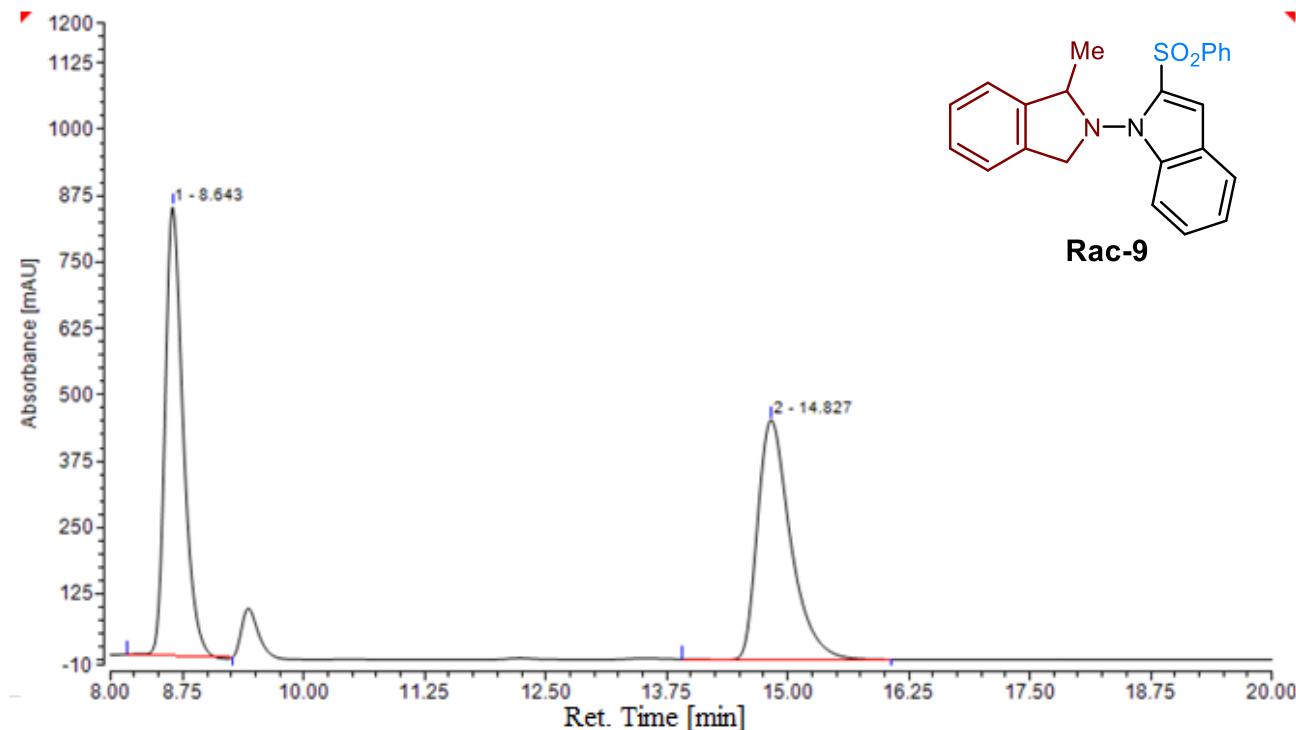




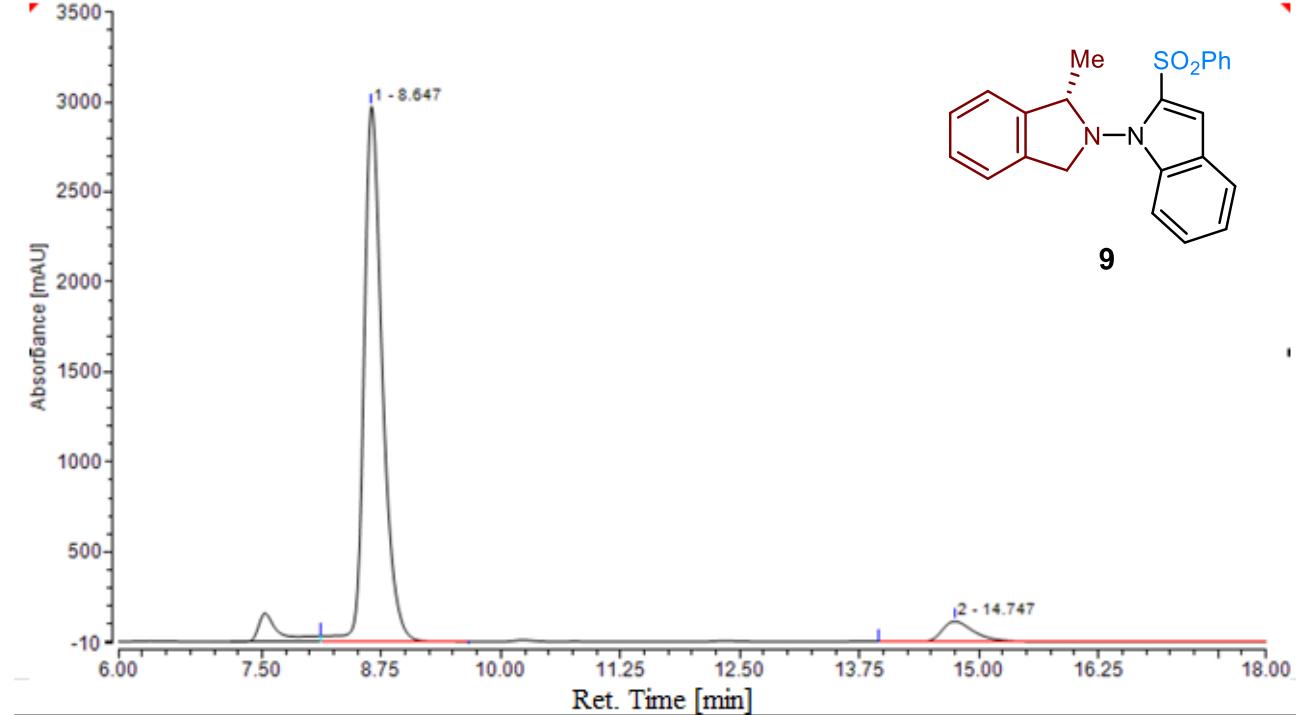
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Heighet %
1	23.27	125.833	222.811	49.91	62.35
2	38.95	126.273	134.545	50.09	37.65



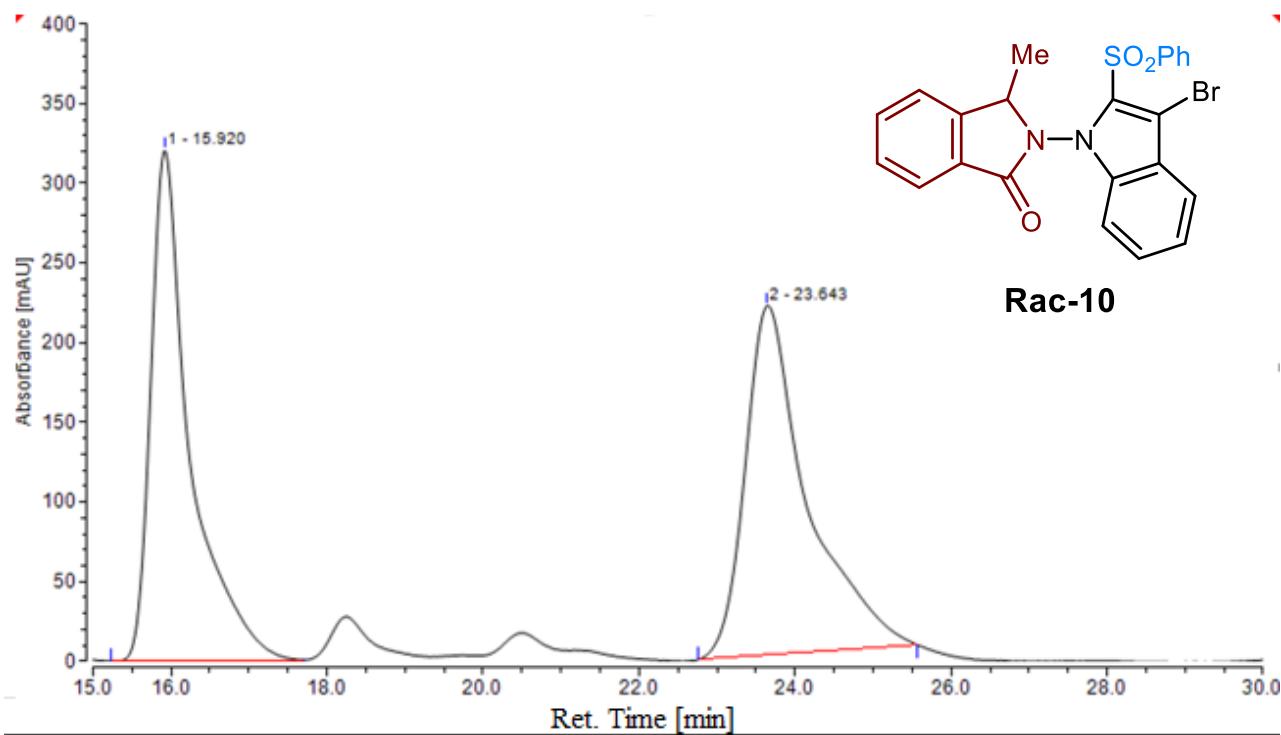
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Heighet %
1	23.36	1.986	3.669	2.59	4.43
2	39.05	74.730	79.173	97.41	95.57



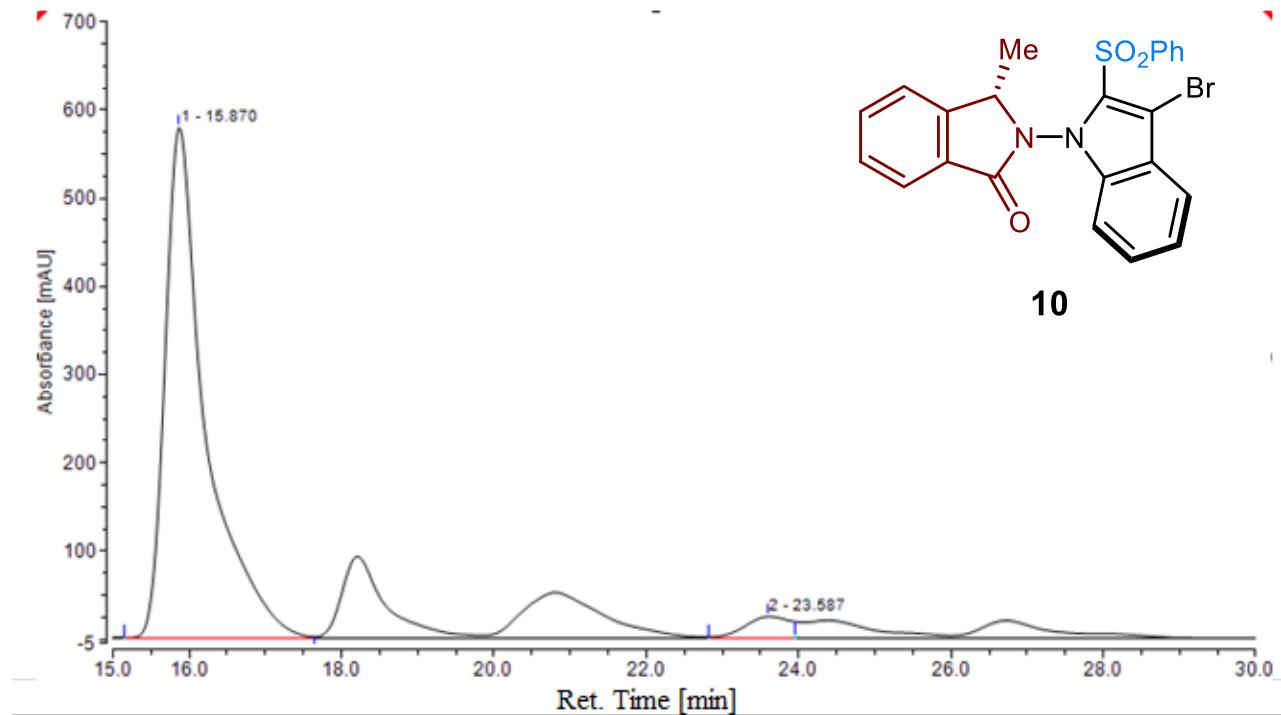
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Heighet %
1	8.64	181.404	845.161	50.45	65.18
2	14.83	178.146	451.402	49.55	34.82



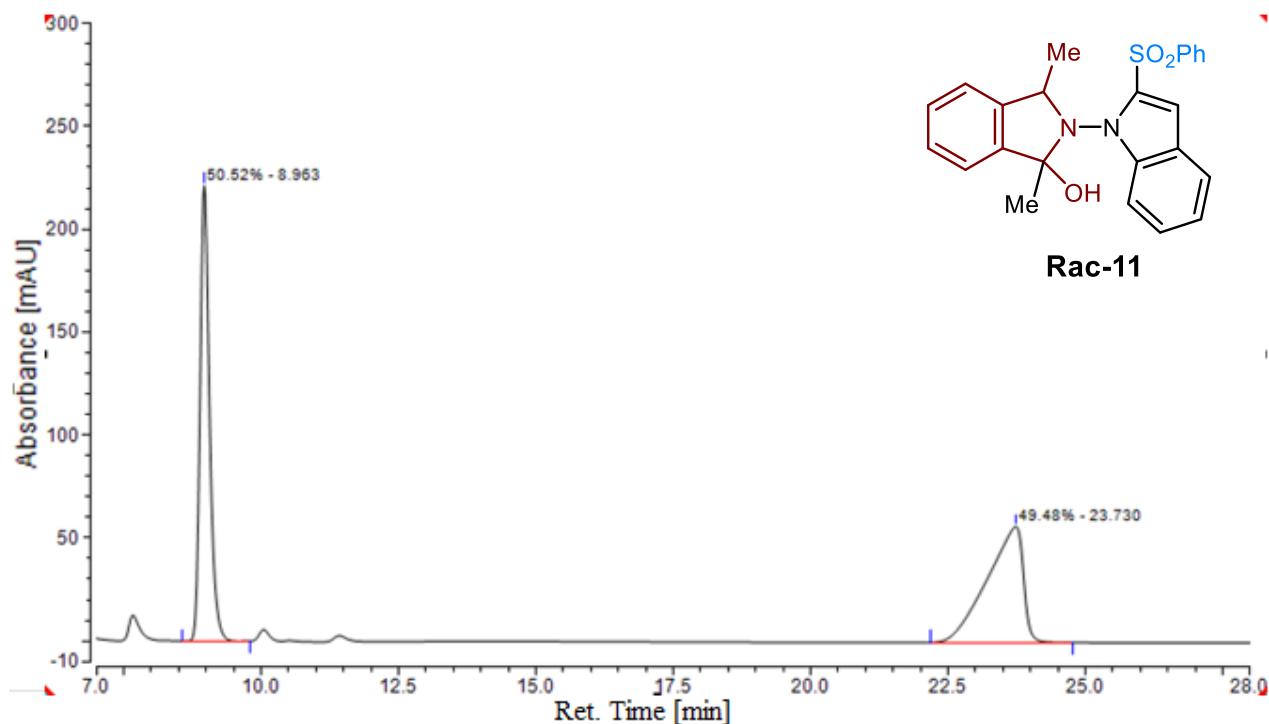
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Heighet %
1	8.65	663.380	2975.563	94.34	96.34
2	14.75	40.044	112.884	5.69	3.66



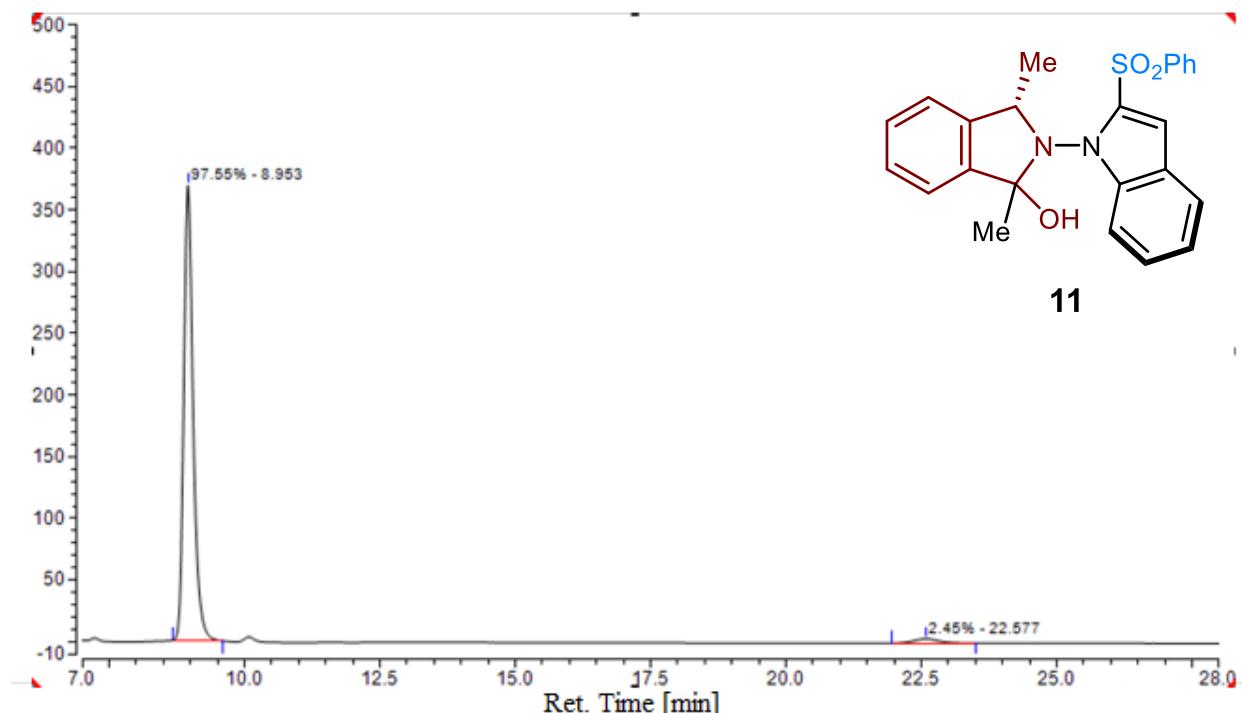
Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Heighet %
1	15.92	185.942	320.407	48.04	59.37
2	23.64	201.093	219.255	51.96	40.63



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



Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Heighet %
1	8.96	44.057	221.283	50.52	79.68
2	23.73	43.141	56.434	49.48	20.32



Peak	Ret. Time (min)	Area (mAu*min)	Height (mAu)	Area %	Heighet %
1	8.95	74.012	368.715	97.55	99.06
2	22.58	1.861	3.482	2.45	0.94