Supplementary Information

Chiral bifunctional sulfide-catalyzed asymmetric bromoaminocyclizations

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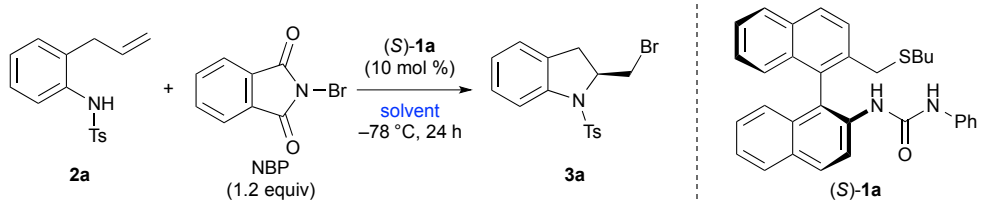
General Information

^{1}H, ^{13}C, and ^{19}F NMR spectra were measured on a JEOL JNM-AL 400 NMR instrument (400 MHz for ^{1}H NMR, 100 MHz for ^{13}C NMR, and 376 Hz for ^{19}F NMR). Tetramethylsilane (TMS) served as the internal standard (0 ppm) for ^{1}H NMR, $CDCl_3$ served as the internal standard (77.0 ppm) for ^{13}C NMR, and hexafluorobenzene served as the external standard (–164.9 ppm) for ^{19}F NMR. The following abbreviations were used to express the multiplicities: s = singlet; d = doublet; t = triplet; m = multiplet; br = broad. High-resolution mass spectra (HRMS) were measured on a JEOL JMS-700N. Infrared spectra (IR) were measured on a JASCO FT/IR-4200 spectrometer. Optical rotations were measured on a JASCO P-2100 polarimeter. High performance liquid chromatography (HPLC) was performed on Shimadzu LC-20AT and SPD-20A instruments using Daicel Chiralpak AD-3, IC-3, IE-3, or Chiralcel OD-3 columns (4.6 mm × 250 mm). All reactions were monitored by thin-layer chromatography using Merck precoated TLC plates (silica gel 60GF-254, 0.25 mm), with visualization by the use of UV lamp (254 nm), or dyes such as $KMnO_4$. The products were purified by flash column chromatography on silica gel. Dehydrated solvents were purchased from Kanto Chemical.

Table S1 Optimization of the reaction solvents[a]



Entry	Solvent	Yield[b] (%)	er[c]
1	CH_2Cl_2 (2 mL)	80	78:22
2	toluene (2 mL)	26	63:37
3	toluene (1 mL)-CH_2Cl_2 (1 mL)	81	75:25
4	hexane (1 mL)-CH_2Cl_2 (1 mL)	82	77:23

[a] Reaction conditions: **2a** (0.10 mmol), NBP (0.12 mmol), (*S*)-**1a** (10 mol %, 0.010 mmol), solvent (2 mL), –78 °C, 24 h. [b] Yield of isolated product **3a**. [c] Enantiomeric ratio (er) was determined by HPLC analysis on a chiral stationary phase.

Experimental Section

1. Details of computational method.

All calculations were performed with the Gaussian 09 package.[1] As a preliminary study, various TS models were explored at the SMD(CH_2Cl_2)-B3LYP/6-31G* level. The promising TS models were further optimized at the SMD(CH_2Cl_2)-ωB97XD/6-31G* level. Frequency analyses were also carried out to identify the stationary points (TS: one imaginary frequency) and to estimate thermodynamic properties at 298.15 K and 1 atm and Gibbs free energies. Single-point energy calculations of the optimized structures were evaluated at the SMD(CH_2Cl_2)-ωB97-XD/def2TZVP level. The molecular structures were depicted by using the CYLview v1.0.561 β.[2]

To identify the promising TS model, various concerted **TS1** models consisting of (*S*)-**1a**, NBS, and **2g** were explored based on our previous study (Fig. S1).[3] We found a wide variety of coordination modes among (*S*)-**1a**, NBS, and **2g** through the hydrogen bonding network. The energetically favored **TS1r-1** involving multi-point coordinated succinimide anion found to be the most stable TS model. While **TS1s-1** having similar structural features with **TS1r-1** was not found as a stationary point at the SMD(CH_2Cl_2)-B3LYP/6-31G* level, it was predicted to be more stable by the corresponding approximate TS model partially optimized. The consideration of dispersion interactions was found to be crucial to obtain the promising TS models and reaction pathways. Consequently, we located two distinct concerted (**TS1s**) and stepwise (**TS2r**/**TS3r**) pathways leading to the major and minor enantiomers, respectively.

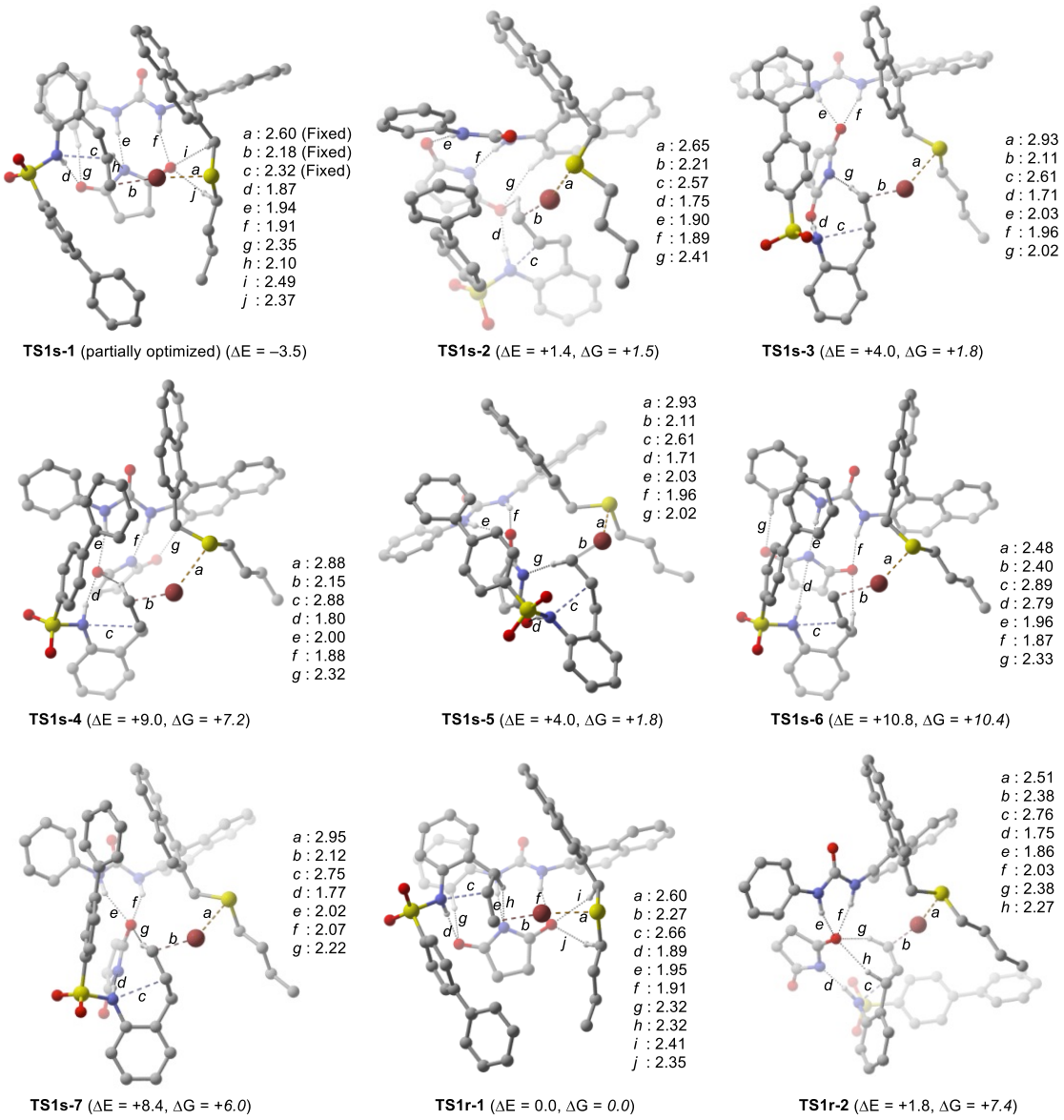


Fig. S1 3D structures and the relative Gibbs free energies (**TS1r-1** is set to zero, kcal mol^{-1}) of various TS models. Distances are shown in Å.

To clarify the details of the cooperative functions of urea and sulfide moieties in (*S*)-**1a** and the succinimide anion in the energy difference between **TS1s** and **TS3r**, partially defected TS models (**TS-d1** and **-d2**: the sulfide group and the Ph group of the urea moiety are exchanged with H atom, **TS-d3**: the succinimide anion is removed) were investigated (Fig. S2). The **TS-d1** model indicates that the sulfide moiety in (*S*)-**1a** has a

great impact on stabilizing **TS1s**. Removing the sulfide moiety significantly destabilizes **TS1s**. In contrast, **TS-d2** and **-d3** models indicate that the π/π, CH/π, and hydrogen bonding interactions around the succinimide anion and the terminal Ph group of the urea moiety in (*S*)-**1a** exist similarly between **TS1s** and **TS3r**. Removing those moieties rarely changes the relative stabilities of **TS1s** and **TS3r**.

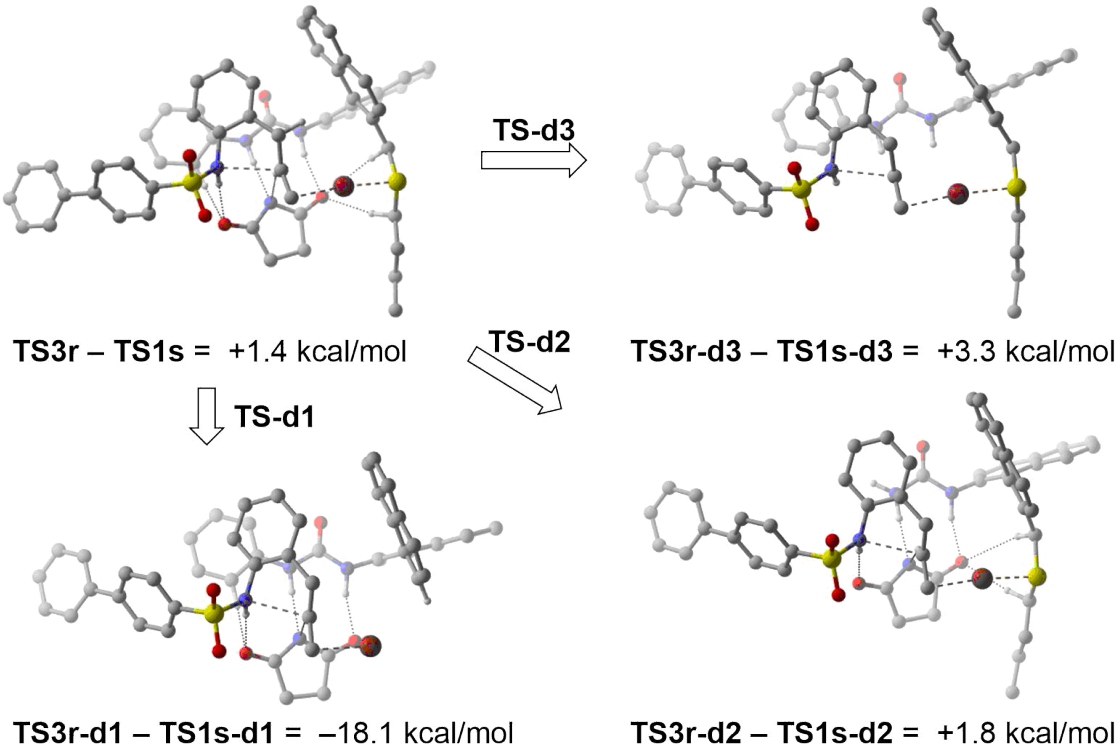
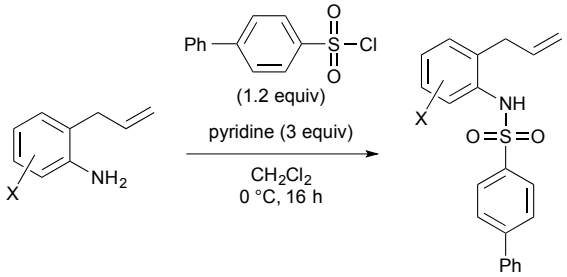


Fig. S2 3D structures and the energy differences between **TS3r** and **TS1s** of the partially defected TS models (**TS-d1**, **TS-d2**, and **TS-d3**).

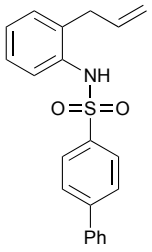
2. Synthesis of catalysts.

Catalysts (*S*)-**1** and (*S*)-**4** were prepared according to the literature.[3]

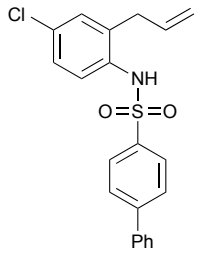
3. Synthesis of substrates.[4]



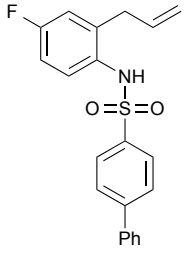
A solution of 2-allylaniline[4] (5.0 mmol) in dichloromethane (10 mL) was cooled to 0 °C. 4-Biphenylsulfonyl chloride (6.0 mmol) and pyridine (15 mmol) was added to the cooled solution of 2-allylaniline, and stirred for 16 h at 0 °C. The reaction mixture was quenched with water (10 mL) at 0 °C. The organic materials were extracted with dichloromethane for three times (5 mL × 3). The combined extracts were dried over Na_2SO_4 and concentrated. The residue was purified by flash column chromatography on silica gel (hexane/ethyl acetate as eluent) to give substrate.



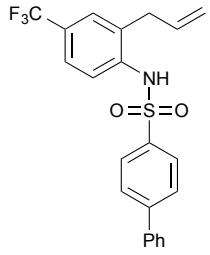
2g: 90% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (td, *J* = 2.0, 8.8 Hz, 2H), 7.65 (td, *J* = 2.0, 8.8 Hz, 2H), 7.60–7.56 (m, 2H), 7.49–7.38 (m, 4H), 7.23 (dt, *J* = 1.6, 7.6 Hz, 1H), 7.16–7.07 (m, 2H), 6.59 (s, 1H), 5.84–5.74 (m, 1H), 5.14–5.10 (m, 1H), 4.98–4.93 (m, 1H), 3.05 (d, *J* = 5.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.8, 139.0, 138.2, 135.5, 134.8, 132.1, 130.5, 129.0, 128.5, 127.7, 127.6, 127.5, 127.2, 126.4, 124.6, 117.1, 36.1; IR (neat): 3281, 1331, 1157, 1094, 913, 761, 670 cm^{-1}; HRMS (FAB) calcd for $C_{21}H_{20}NO_2S$: 350.1215 ($[M+H]^+$), found 350.1216.



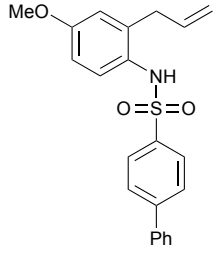
5a: 83% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, *J* = 8.4 Hz, 2H), 7.67 (d, *J* = 8.4 Hz, 2H), 7.59 (d, *J* = 8.4 Hz, 2H), 7.50–7.38 (m, 4H), 7.21 (dd, *J* = 2.4, 8.4 Hz, 1H), 7.09 (d, *J* = 2.4 Hz, 1H), 6.49 (s, 1H), 5.80–5.70 (m, 1H), 5.17–5.13 (m, 1H), 4.98–4.93 (m, 1H), 3.00 (d, *J* = 6.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.0, 138.9, 137.9, 134.6, 134.3, 133.3, 131.9, 130.3, 129.1, 128.6, 127.7, 127.64, 127.56, 127.3, 126.2, 117.7, 35.8; IR (neat): 3277, 1482, 1331, 1160, 1094, 912, 763, 671 cm^{-1}; HRMS (FAB) calcd for $C_{21}H_{19}ClNO_2S$: 384.0825 ($[M+H]^+$), found 384.0825.



5b: 81% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 8.4 Hz, 2H), 7.67 (d, *J* = 8.0 Hz, 2H), 7.61–7.57 (m, 2H), 7.50–7.40 (m, 3H), 7.36 (dd, *J* = 5.2, 8.8 Hz, 1H), 6.92 (dt, *J* = 2.8, 8.4 Hz, 1H), 6.82 (dd, *J* = 2.8, 9.2 Hz, 1H), 6.39 (s, 1H), 5.77–5.68 (m, 1H), 5.15–5.11 (m, 1H), 4.97–4.92 (m, 1H), 2.99 (d, *J* = 6.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.1 (d, *J* = 246 Hz), 145.9, 139.0, 138.0, 136.3 (d, *J* = 7.4 Hz), 134.7, 130.4 (d, *J* = 2.1 Hz), 129.1, 128.6, 127.9 (d, *J* = 8.2 Hz), 127.60, 127.59, 127.3, 117.6, 117.0 (d, *J* = 23.0 Hz), 114.4 (d, *J* = 22.2 Hz), 35.9; IR (neat): 3273, 1494, 1330, 1158, 1094, 913, 763, 671 cm^{-1}; HRMS (FAB) calcd for $C_{21}H_{19}FNO_2S$: 368.1121 ($[M+H]^+$), found 368.1120.

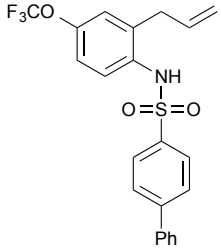


5c: 84% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, *J* = 8.8 Hz, 2H), 7.68 (d, *J* = 8.8 Hz, 2H), 7.64–7.57 (m, 3H), 7.50–7.40 (m, 4H), 7.35 (s, 1H), 6.78 (s, 1H), 5.86–5.76 (m, 1H), 5.23–5.20 (m, 1H), 5.03–4.99 (m, 1H), 3.17 (d, *J* = 6.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.3, 138.9, 138.3, 137.8, 134.3, 130.8, 129.1, 128.7, 127.8, 127.60 (q, *J* = 4.1 Hz), 127.58, 127.51 (q, *J* = 33.0 Hz), 127.3, 124.9 (q, *J* = 3.8 Hz), 123.8 (q, *J* = 270 Hz), 122.4, 118.1, 36.1; IR (neat): 3291, 1329, 1158, 1119, 1092, 914, 840, 763, 671 cm^{-1}; HRMS (FAB) calcd for $C_{22}H_{19}F_3NO_2S$: 418.1089 ($[M+H]^+$), found 418.1089.

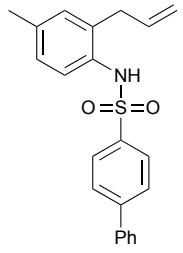


5d: 87% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 8.4 Hz, 2H), 7.66 (d, *J* = 8.0 Hz, 2H), 7.60 (d, *J* = 8.0 Hz, 2H), 7.50–7.39 (m, 3H), 7.26 (d, *J* = 8.4 Hz, 1H), 6.74 (dd, *J* = 3.2, 8.8 Hz, 1H), 6.63 (d, *J* = 2.8 Hz, 1H), 6.29 (s, 1H), 5.78–5.69 (m, 1H), 5.10–5.07 (m, 1H), 4.96–

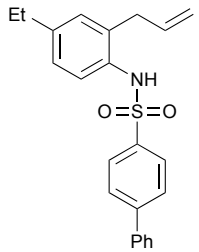
4.91 (m, 1H), 3.78 (s, 3H), 2.96 (d, J = 6.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.5, 145.7, 139.1, 138.3, 136.1, 135.5, 129.0, 128.5, 128.3, 127.6, 127.5, 127.3, 127.1, 116.9, 115.8, 112.4, 55.3, 36.2; IR (neat): 3274, 1497, 1327, 1156, 1094, 1038, 913, 763, 671 cm^{-1}; HRMS (FAB) calcd for $C_{22}H_{21}NO_3S$: 379.1242 ($[M]^+$), found 379.1242.



5e: 80% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (td, J = 2.0, 8.8 Hz, 2H), 7.68 (td, J = 2.0, 8.8 Hz, 2H), 7.61–7.57 (m, 2H), 7.50–7.40 (m, 4H), 7.09 (dd, J = 2.0, 8.8 Hz, 1H), 6.96 (d, J = 2.8 Hz, 1H), 6.55 (s, 1H), 5.81–5.71 (m, 1H), 5.18–5.15 (m, 1H), 5.00–4.95 (m, 1H), 3.05 (d, J = 6.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.1 (q, J = 1.7 Hz), 146.1, 138.9, 138.0, 134.7, 134.5, 133.3, 129.1, 128.7, 127.7, 127.6, 127.3, 126.2, 122.8, 120.3 (q, J = 256 Hz), 119.9, 117.9, 35.9; IR (neat): 3275, 1496, 1252, 1220, 1152, 1094, 917, 763, 696, 671 cm^{-1}; HRMS (FAB) calcd for $C_{22}H_{19}F_3NO_3S$: 434.1038 ($[M+H]^+$), found 434.1038.

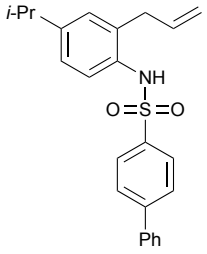


5f: 91% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, J = 8.0 Hz, 2H), 7.65 (d, J = 8.8 Hz, 2H), 7.59 (d, J = 8.8 Hz, 2H), 7.49–7.39 (m, 3H), 7.29 (d, J = 8.4 Hz, 1H), 7.03 (d, J = 8.4 Hz, 1H), 6.89 (s, 1H), 6.43 (s, 1H), 5.82–5.71 (m, 1H), 5.12–5.08 (m, 1H), 4.97–4.91 (m, 1H), 2.98 (d, J = 6.0 Hz, 2H), 2.28 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.6, 139.1, 138.3, 136.5, 135.7, 132.7, 132.0, 131.1, 129.0, 128.5, 128.3, 127.6, 127.5, 127.2, 125.3, 116.8, 36.0, 20.9; IR (neat): 3273, 1498, 1395, 1329, 1160, 1094, 913, 763, 671 cm^{-1}; HRMS (FAB) calcd for $C_{22}H_{21}NO_2S$: 363.1293 ($[M]^+$), found 363.1293.

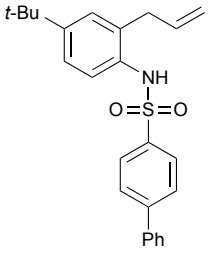


5g: 89% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, J = 8.8 Hz, 2H), 7.65 (d, J = 8.4 Hz, 2H), 7.59 (dd, J = 1.2, 8.8 Hz, 2H), 7.49–7.39 (m, 3H), 7.31 (d, J = 8.4 Hz, 1H), 7.05 (dd, J = 1.6, 8.4 Hz, 1H), 6.91 (d, J = 1.6 Hz, 1H), 6.45 (s, 1H), 5.83–5.73 (m, 1H), 5.12–5.08 (m, 1H), 4.98–4.93 (m, 1H), 3.01 (d, J = 6.4 Hz, 2H), 2.58 (q, J = 7.2 Hz, 2H), 1.20 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.7, 142.8, 139.1, 138.4, 135.8, 132.7, 132.2, 129.9, 129.0, 128.5, 127.6, 127.5, 127.3, 127.0, 125.3, 116.9, 36.2, 28.2,

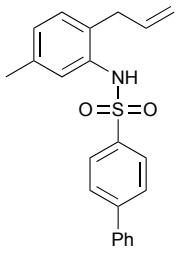
15.3; IR (neat): 3258, 1396, 1327, 1159, 1094, 913, 839, 762, 673 cm^{-1}; HRMS (FAB) calcd for $C_{23}H_{23}NO_2S$: 377.1449 ($[M]^+$), found 377.1450.



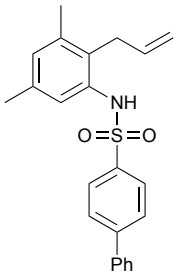
5h: 88% yield; ^1H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, J = 8.0 Hz, 2H), 7.65 (d, J = 8.4 Hz, 2H), 7.60 (d, J = 8.4 Hz, 2H), 7.49–7.39 (m, 3H), 7.31 (d, J = 8.0 Hz, 1H), 7.08 (dd, J = 2.0, 8.4 Hz, 1H), 6.89 (d, J = 2.0 Hz, 1H), 6.46 (s, 1H), 5.84–5.74 (m, 1H), 5.13–5.09 (m, 1H), 4.99–4.94 (m, 1H), 3.03 (d, J = 6.0 Hz, 2H), 2.84 (septet, J = 6.8 Hz, 1H), 1.21 (d, J = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.4, 145.7, 139.2, 138.5, 135.9, 132.5, 132.3, 129.0, 128.6, 128.5, 127.6, 127.5, 127.3, 125.6, 125.1, 116.9, 36.4, 33.6, 23.9; IR (neat): 3275, 2960, 1498, 1396, 1331, 1161, 1095, 913, 763, 671 cm^{-1}; HRMS (FAB) calcd for $C_{24}H_{25}NO_2S$: 391.1606 ($[M]^+$), found 391.1606.



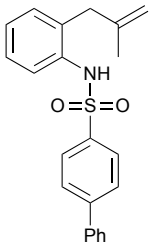
5i: 87% yield; ^1H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, J = 8.4 Hz, 2H), 7.66 (d, J = 8.8 Hz, 2H), 7.59 (d, J = 7.2 Hz, 2H), 7.49–7.39 (m, 3H), 7.31 (d, J = 8.8 Hz, 1H), 7.22 (dd, J = 2.0, 8.4 Hz, 1H), 7.08 (d, J = 2.0 Hz, 1H), 6.51 (s, 1H), 5.84–5.75 (m, 1H), 5.13–5.09 (m, 1H), 4.99–4.94 (m, 1H), 3.06 (d, J = 6.0 Hz, 2H), 1.27 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.6, 145.6, 139.1, 138.6, 135.9, 132.04, 131.97, 129.0, 128.5, 127.6, 127.5, 127.4, 127.2, 124.6, 124.5, 116.8, 36.5, 34.4, 31.3; IR (neat): 3275, 2963, 1499, 1395, 1331, 1161, 1094, 910, 839, 762, 730, 696, 670 cm^{-1}; HRMS (FAB) calcd for $C_{25}H_{27}NO_2S$: 405.1762 ($[M]^+$), found 405.1763.



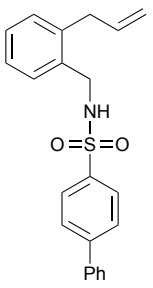
5j: 90% yield; ^1H NMR (400 MHz, $CDCl_3$) δ 7.77 (td, J = 2.0, 8.8 Hz, 2H), 7.65 (td, J = 2.0, 8.8 Hz, 2H), 7.60–7.56 (m, 2H), 7.49–7.38 (m, 3H), 7.29 (s, 1H), 6.96–6.94 (m, 2H), 6.53–6.52 (m, 1H), 5.81–5.71 (m, 1H), 5.11–5.08 (m, 1H), 4.96–4.90 (m, 1H), 2.96 (d, J = 6.0 Hz, 2H), 2.31 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.7, 139.1, 138.3, 137.6, 135.8, 134.6, 130.3, 129.0, 128.5, 127.55, 127.47, 127.23, 127.19, 125.3, 116.8, 35.7, 21.0; IR (neat): 3279, 1395, 1329, 1165, 1155, 1094, 908, 840, 762, 722, 696, 670 cm^{-1}; HRMS (FAB) calcd for $C_{22}H_{22}NO_2S$: 364.1371 ($[M+H]^+$), found 364.1370.



5k: 89% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, J = 8.4 Hz, 2H), 7.65 (td, J = 2.0, 8.4 Hz, 2H), 7.61–7.57 (m, 2H), 7.50–7.38 (m, 3H), 7.13 (s, 1H), 6.85 (s, 1H), 6.44 (s, 1H), 5.81–5.72 (m, 1H), 5.05–5.01 (m, 1H), 4.82–4.75 (m, 1H), 3.03 (d, J = 5.2 Hz, 2H), 2.26 (s, 3H), 2.17 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.6, 139.2, 138.4, 137.4, 136.8, 134.8, 134.7, 129.2, 129.0, 128.5, 127.6, 127.5, 127.2, 122.9, 116.1, 31.2, 21.0, 19.9; IR (neat): 3289, 1395, 1328, 1163, 910, 841, 763, 672 cm^{-1}; HRMS (FAB) calcd for $C_{23}H_{24}NO_2S$: 378.1528 ([M+H]$^+$), found 378.1528.



7: 80% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, J = 8.8 Hz, 2H), 7.64 (d, J = 8.4 Hz, 2H), 7.58 (d, J = 8.4 Hz, 2H), 7.52–7.38 (m, 4H), 7.24 (dt, J = 1.6, 8.0 Hz, 1H), 7.12 (dt, J = 0.8, 8.0 Hz, 1H), 7.05 (dd, J = 1.6, 7.6 Hz, 1H), 6.76 (s, 1H), 4.89 (s, 1H), 4.63 (m, 1H), 2.95 (s, 2H), 1.57 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.7, 143.5, 139.0, 138.3, 135.2, 131.4, 130.9, 129.0, 128.5, 127.7, 127.5, 127.2, 126.0, 124.1, 112.9, 40.8, 22.1; IR (neat): 3290, 1780, 1335, 1160, 1094, 923, 902, 840, 763, 671 cm^{-1}; HRMS (FAB) calcd for $C_{22}H_{22}NO_2S$: 364.1371 ([M+H]$^+$), found 364.1371.

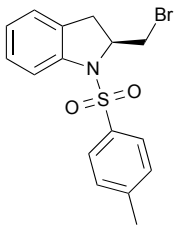


9: 32% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, J = 8.4 Hz, 2H), 7.72 (d, J = 8.4 Hz, 2H), 7.62 (d, J = 8.0 Hz, 2H), 7.52–7.41 (m, 3H), 7.25–7.13 (m, 4H), 5.94–5.83 (m, 1H), 5.05–5.01 (m, 1H), 4.89–4.83 (m, 1H), 4.59 (t, J = 6.0 Hz, 1H), 4.16 (d, J = 5.6 Hz, 2H), 3.33 (d, J = 5.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.7, 139.3, 138.2, 138.1, 136.9, 133.8, 130.2, 129.6, 129.0, 128.5, 127.7, 127.3, 126.8, 116.1, 45.0, 36.7; IR (neat): 3276, 1326, 1156, 1096, 839, 762, 670 cm^{-1}; HRMS (FAB) calcd for $C_{22}H_{22}NO_2S$: 364.1371 ([M+H]$^+$), found 364.1371.

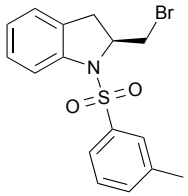
4. General procedure for asymmetric bromoaminocyclizations.

A solution of substrate (0.10 mmol) and catalyst (*S*)-**1a** (10 mol %, 0.010 mmol) in dichloromethane (2 mL) was cooled to –90 °C (or –78 °C). After stirring for 5 min at –90 °C (or –78 °C), *N*-bromophthalimide (NBP) (0.12 mmol) was added to the cooled

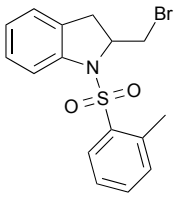
reaction solution. The reaction mixture was stirred for 24 h at –90 °C (or –78 °C). After 24 h, the reaction mixture was quenched with saturated aqueous Na_2SO_3 (4 mL) at –90 °C (or –78 °C) and stirred for 10 min at –90 °C (or –78 °C). The quenched reaction mixture was diluted with dichloromethane (2 mL) and water (2 mL), and warmed to room temperature. The organic materials were extracted with dichloromethane for three times (5 mL × 3). The combined extracts were dried over Na_2SO_4 and concentrated. The residue was purified by flash column chromatography on silica gel (hexane/ethyl acetate as eluent) to give bromoaminocyclization product. The enantioselectivity of the product was determined by HPLC analysis on a chiral stationary phase.



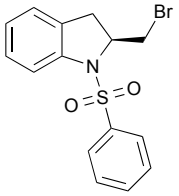
3a:[4d] $[\alpha]^{19}_D$ +56.1 (*c* = 1.0, $CHCl_3$, 78:22 er); HPLC analysis: Daicel Chiralcel OD-3, hexane/2-propanol = 20:1, flow rate = 0.5 mL/min, 254 nm; retention time: 13.6 min (major) and 14.8 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 8.4 Hz, 1H), 7.57 (d, *J* = 8.4 Hz, 2H), 7.25–7.17 (m, 3H), 7.08–7.02 (m, 2H), 4.46–4.40 (m, 1H), 3.82 (dd, *J* = 3.6, 10.0 Hz, 1H), 3.41 (t, *J* = 10.0 Hz, 1H), 2.94–2.91 (m, 2H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.3, 141.1, 134.5, 130.6, 129.7, 127.9, 127.0, 125.2, 124.9, 116.8, 62.1, 35.9, 33.2, 21.5; IR (neat): 1479, 1460, 1354, 1166, 1091, 1026, 758, 670 cm^{-1}.



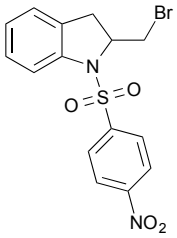
3b: $[\alpha]^{24}_D$ +30.9 (*c* = 0.78, $CHCl_3$, 68:32 er); HPLC analysis: Daicel Chiralpak IE-3, hexane/2-propanol = 20:1, flow rate = 0.5 mL/min, 254 nm; retention time: 31.0 min (major) and 33.1 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 7.6 Hz, 1H), 7.50 (s, 1H), 7.47 (d, *J* = 7.6 Hz, 1H), 7.34 (d, *J* = 7.2 Hz, 1H), 7.29–7.21 (m, 2H), 7.09–7.02 (m, 2H), 4.48–4.41 (m, 1H), 3.82 (dd, *J* = 3.6, 10.0 Hz, 1H), 3.42 (t, *J* = 10.0 Hz, 1H), 2.97–2.88 (m, 2H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.0, 139.3, 137.3, 134.1, 130.6, 128.9, 127.9, 127.4, 125.2, 125.0, 124.1, 116.8, 62.1, 35.9, 33.2, 21.3; IR (neat): 1487, 1459, 1355, 1162, 1100, 1025, 758, 698, 687 cm^{-1}; HRMS (FAB) calcd for $C_{16}H_{16}BrNO_2S$: 365.0085 ($[M]^+$), found 365.0084.



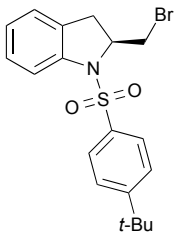
3c: $[\alpha]^{26}_{D}$ +2.3 (*c* = 0.60, $CHCl_3$, 58:42 er); HPLC analysis: Daicel Chiralpak IE-3, hexane/2-propanol = 20:1, flow rate = 0.5 mL/min, 254 nm; retention time: 27.8 min (major) and 31.1 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (dd, *J* = 1.6, 8.8 Hz, 1H), 7.46–7.37 (m, 2H), 7.29–7.25 (m, 2H), 7.18–7.13 (m, 2H), 7.03 (dt, *J* = 0.8, 7.6 Hz, 1H), 4.61–4.54 (m, 1H), 3.77 (dd, *J* = 3.2, 10.0 Hz, 1H), 3.38 (t, *J* = 10.0 Hz, 1H), 3.19 (dd, *J* = 9.6, 16.8 Hz, 1H), 3.07 (dd, *J* = 2.8, 16.8 Hz, 1H), 2.51 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.2, 137.9, 137.2, 133.1, 133.0, 129.7, 129.4, 127.9, 126.3, 125.4, 124.5, 116.0, 62.1, 35.2, 33.1, 20.8; IR (neat): 1478, 1460, 1342, 1163, 756, 710, 692 cm^{-1}; HRMS (FAB) calcd for $C_{16}H_{16}BrNO_2S$: 365.0085 ($[M]^+$), found 365.0085.



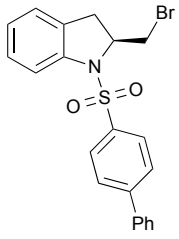
3d:[4d] $[\alpha]^{23}_{D}$ +37.5 (*c* = 0.95, $CHCl_3$, 70:30 er); HPLC analysis: Daicel Chiralpak IE-3, hexane/2-propanol = 20:1, flow rate = 0.5 mL/min, 254 nm; retention time: 33.1 min (major) and 41.2 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71–7.65 (m, 3H), 7.54 (tt, *J* = 1.6, 7.6 Hz, 1H), 7.41 (t, *J* = 7.6 Hz, 2H), 7.26–7.21 (m, 1H), 7.10–7.03 (m, 2H), 4.48–4.41 (m, 1H), 3.82 (dd, *J* = 3.6, 10.0 Hz, 1H), 3.42 (t, *J* = 10.0 Hz, 1H), 2.98–2.85 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.0, 137.4, 133.3, 130.6, 129.1, 128.0, 127.0, 125.3, 125.1, 116.8, 62.2, 35.8, 33.1; IR (neat): 1479, 1446, 1355, 1168, 1102, 1091, 1026, 757, 719, 688 cm^{-1}.



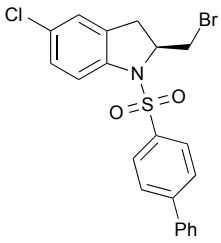
3e:[4d] HPLC analysis: Daicel Chiralpak AD-3, hexane/2-propanol = 20:1, flow rate = 0.5 mL/min, 254 nm; retention time: 42.5 min and 56.7 min. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (d, *J* = 8.8 Hz, 2H), 7.89 (d, *J* = 9.2 Hz, 2H), 7.66 (d, *J* = 8.4 Hz, 1H), 7.29–7.24 (m, 1H), 7.11–7.07 (m, 2H), 4.48–4.42 (m, 1H), 3.80 (dd, *J* = 3.6, 10.0 Hz, 1H), 3.44 (t, *J* = 10.0 Hz, 1H), 3.02–2.89 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.5, 143.0, 140.1, 130.5, 128.3, 128.2, 125.8, 125.7, 124.4, 116.6, 62.5, 35.4, 33.1; IR (neat): 1530, 1349, 1171, 745, 735, 614 cm^{-1}.



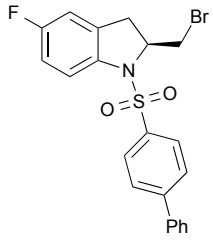
3f: $[\alpha]^{26}_{D}$ +63.4 (*c* = 1.0, $CHCl_3$, 81:19 er); HPLC analysis: Daicel Chiralcel OD-3, hexane/2-propanol = 20:1, flow rate = 0.5 mL/min, 254 nm; retention time: 10.5 min (major) and 11.8 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 8.0 Hz, 1H), 7.61 (d, *J* = 8.8 Hz, 2H), 7.40 (d, *J* = 8.4 Hz, 2H), 7.23 (t, *J* = 7.6 Hz, 1H), 7.10–7.03 (m, 2H), 4.47–4.40 (m, 1H), 3.84 (dd, *J* = 3.6, 10.0 Hz, 1H), 3.42 (t, *J* = 10.0 Hz, 1H), 2.95 (d, *J* = 6.4 Hz, 2H), 1.28 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.2, 141.2, 134.5, 130.4, 128.0, 126.9, 126.1, 125.2, 124.8, 116.6, 62.1, 35.9, 35.1, 32.2, 31.0; IR (neat): 1479, 1170, 1114, 1086, 1026, 761, 637 cm^{-1}; HRMS (FAB) calcd for $C_{19}H_{22}BrNO_2S$: 407.0555 ($[M]^+$), found 407.0554.



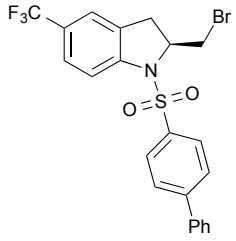
3g: $[\alpha]^{23}_{D}$ +98.8 (*c* = 1.1, $CHCl_3$, 95: 5 er); HPLC analysis: Daicel Chiralcel OD-3, hexane/2-propanol = 20:1, flow rate = 0.5 mL/min, 254 nm; retention time: 20.8 min (major) and 24.2 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (td, *J* = 2.0, 8.8 Hz, 2H), 7.70 (d, *J* = 8.0 Hz, 1H), 7.61 (td, *J* = 2.0, 8.4 Hz, 2H), 7.56–7.53 (m, 2H), 7.47–7.38 (m, 3H), 7.27–7.23 (m, 1H), 7.10–7.04 (m, 2H), 4.51–4.45 (m, 1H), 3.85 (dd, *J* = 4.0, 9.6 Hz, 1H), 3.44 (t, *J* = 9.6 Hz, 1H), 2.97 (d, *J* = 6.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.1, 141.0, 138.9, 135.9, 130.6, 129.0, 128.6, 128.0, 127.6, 127.5, 127.2, 125.3, 125.1, 116.8, 62.2, 35.9, 32.2; IR (neat): 1478, 1355, 1166, 1094, 1025, 760, 673 cm^{-1}; HRMS (FAB) calcd for $C_{21}H_{18}BrNO_2S$: 427.0242 ($[M]^+$), found 427.0242.



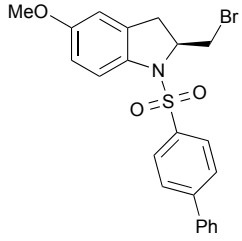
6a: $[\alpha]^{20}_{D}$ +125.4 (*c* = 1.0, $CHCl_3$, 88:12 er); HPLC analysis: Daicel Chiralcel OD-3, hexane/2-propanol = 20:1, flow rate = 0.5 mL/min, 254 nm; retention time: 25.0 min (major) and 28.3 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 8.4 Hz, 2H), 7.65–7.61 (m, 3H), 7.56 (d, *J* = 7.6 Hz, 2H), 7.48–7.39 (m, 3H), 7.22 (dd, *J* = 1.6, 8.4 Hz, 1H), 7.06 (s, 1H), 4.51–4.45 (m, 1H), 3.82 (dd, *J* = 3.6, 10.0 Hz, 1H), 3.45 (t, *J* = 10.0 Hz, 1H), 2.95 (d, *J* = 6.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.4, 139.8, 138.8, 135.6, 132.5, 130.3, 129.1, 128.7, 128.1, 127.8, 127.5, 127.2, 125.5, 117.7, 62.4, 35.8, 33.1; IR (neat): 1473, 1359, 1168, 763, 697, 672, 612 cm^{-1}; HRMS (FAB) calcd for $C_{21}H_{17}BrClNO_2S$: 460.9852 ($[M]^+$), found 460.9853.



6b: $[\alpha]^{24}_{D}$ +106.8 (*c* = 1.0, $CHCl_3$, 94: 6 er); HPLC analysis: Daicel Chiralcel OD-3, hexane/2-propanol = 20:1, flow rate = 0.5 mL/min, 254 nm; retention time: 26.2 min (major) and 29.7 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (td, *J* = 2.0, 8.8 Hz, 2H), 7.66–7.61 (m, 3H), 7.57–7.54 (m, 2H), 7.48–7.38 (m, 3H), 6.95 (dt, *J* = 2.8, 8.8 Hz, 1H), 6.79 (dd, *J* = 2.8, 8.4 Hz, 1H), 4.53–4.46 (m, 1H), 3.81 (dd, *J* = 3.6, 10.0 Hz, 1H), 3.44 (t, *J* = 10.0 Hz, 1H), 2.96–2.86 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.5 (d, *J* = 242 Hz), 146.3, 138.8, 137.0 (d, *J* = 2.5 Hz), 135.5, 132.9 (d, *J* = 8.2 Hz), 129.1, 128.7, 127.7, 127.6, 127.2, 118.1 (d, *J* = 8.2 Hz), 114.8 (d, *J* = 23.1 Hz), 112.5 (d, *J* = 23.8 Hz), 62.6, 35.7, 33.2 (d, *J* = 1.6 Hz); IR (neat): 1480, 1357, 1167, 1094, 1027, 761, 672 cm^{-1}; HRMS (FAB) calcd for $C_{21}H_{17}BrFNO_2S$: 445.0147 ($[M]^+$), found 445.0148.

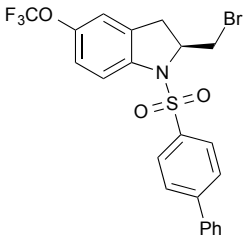


6c: $[\alpha]^{27}_{D}$ +61.0 (*c* = 0.94, $CHCl_3$, 77:23 er); HPLC analysis: Daicel Chiralcel OD-3, hexane/2-propanol = 20:1, flow rate = 0.5 mL/min, 254 nm; retention time: 24.2 min (major) and 28.6 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80–7.75 (m, 3H), 7.66 (td, *J* = 2.0, 8.8 Hz, 2H), 7.57–7.39 (m, 6H), 7.35 (s, 1H), 4.59–4.53 (m, 1H), 3.86 (dd, *J* = 3.6, 10.0 Hz, 1H), 3.51 (t, *J* = 10.0 Hz, 1H), 3.13–3.01 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.7, 144.2, 138.7, 135.7, 131.0, 129.1, 128.8, 127.9, 127.5, 127.2, 127.0 (q, *J* = 32.9 Hz), 125.7 (q, *J* = 4.1 Hz), 124.0 (q, *J* = 270 Hz), 122.6 (q, *J* = 3.3 Hz), 115.9, 62.4, 35.8, 33.1; IR (neat): 1361, 1331, 1167, 1116, 671, 608 cm^{-1}; HRMS (FAB) calcd for $C_{22}H_{17}BrF_3NO_2S$: 495.0115 ($[M]^+$), found 495.0117.

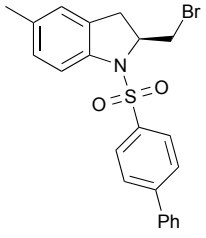


6d: $[\alpha]^{18}_{D}$ +144.5 (*c* = 0.99, $CHCl_3$, 89:11 er); HPLC analysis: Daicel Chiralpak IC-3, hexane/2-propanol = 5:1, flow rate = 0.5 mL/min, 254 nm; retention time: 34.7 min (major) and 38.5 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.4 Hz, 2H), 7.62–7.59 (m, 3H), 7.55 (d, *J* = 7.6 Hz, 2H), 7.48–7.38 (m, 3H), 6.79 (dd, *J* = 2.4, 8.8 Hz, 1H), 6.62 (d, *J* = 2.0 Hz, 1H), 4.49–4.41 (m, 1H), 3.80 (dd, *J* = 3.6, 10.0 Hz, 1H), 3.77 (s, 3H), 3.40 (t, *J* = 10.0 Hz, 1H), 2.91–2.79 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.7, 146.0, 138.9, 135.6, 134.2, 132.6, 129.0, 128.6, 127.60, 127.56,

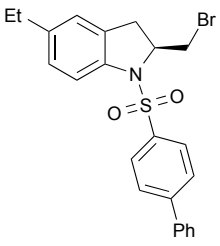
127.2, 118.2, 113.2, 110.9, 62.6, 55.6, 35.7, 33.3; IR (neat): 1487, 1354, 1166, 1031, 763, 673 cm^{-1}; HRMS (FAB) calcd for $C_{22}H_{20}BrNO_3S$: 457.0347 ($[M]^+$), found 457.0347.



6e: $[\alpha]^{28}_D$ +76.8 (*c* = 0.97, $CHCl_3$, 84:16 er); HPLC analysis: Daicel Chiralcel OD-3, hexane/2-propanol = 20:1, flow rate = 0.5 mL/min, 254 nm; retention time: 20.0 min (major) and 23.0 min (minor). ^1H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 8.8 Hz, 2H), 7.69 (d, *J* = 8.8 Hz, 1H), 7.65 (d, *J* = 8.4 Hz, 2H), 7.56 (d, *J* = 7.6 Hz, 2H), 7.48–7.39 (m, 3H), 7.11 (d, *J* = 8.8 Hz, 1H), 6.65 (s, 1H), 4.56–4.48 (m, 1H), 3.84 (dd, *J* = 3.6, 10.0 Hz, 1H), 3.47 (t, *J* = 10.0 Hz, 1H), 2.99 (d, *J* = 6.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.5, 146.3 (q, *J* = 1.6 Hz), 139.7, 138.8, 135.6, 132.4, 129.1, 128.7, 127.8, 127.5, 127.2, 120.9, 120.4 (q, *J* = 256 Hz), 118.4, 117.3, 62.6, 35.7, 33.2; ^{19}F NMR (376 MHz, $CDCl_3$) δ –61.0; IR (neat): 1481, 1360, 1258, 1220, 1166, 763, 673, 607 cm^{-1}; HRMS (FAB) calcd for $C_{22}H_{17}BrF_3NO_3S$: 511.0065 ($[M]^+$), found 511.0065.

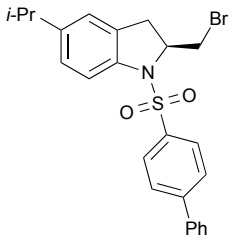


6f: $[\alpha]^{21}_D$ +136.8 (*c* = 0.99, $CHCl_3$, 93: 7 er); HPLC analysis: Daicel Chiralcel OD-3, hexane/2-propanol = 50:1, flow rate = 0.5 mL/min, 254 nm; retention time: 24.4 min (major) and 27.3 min (minor). ^1H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 8.4 Hz, 2H), 7.62–7.53 (m, 5H), 7.47–7.37 (m, 3H), 7.05 (d, *J* = 8.0 Hz, 1H), 6.89 (s, 1H), 4.49–4.42 (m, 1H), 3.83 (dd, *J* = 3.6, 10.0 Hz, 1H), 3.42 (t, *J* = 10.0 Hz, 1H), 2.90 (d, *J* = 6.4 Hz, 2H), 2.29 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.0, 138.9, 138.6, 135.9, 134.9, 130.7, 129.0, 128.62, 128.57, 127.59, 127.55, 127.2, 125.9, 116.7, 62.3, 35.9, 33.1, 21.0; IR (neat): 1486, 1356, 1167, 763, 673, 623 cm^{-1}; HRMS (FAB) calcd for $C_{22}H_{20}BrNO_2S$: 441.0398 ($[M]^+$), found 441.0401.

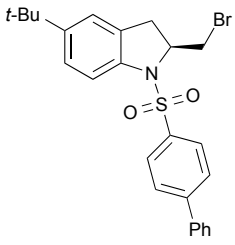


6g: $[\alpha]^{28}_D$ +126.2 (*c* = 0.99, $CHCl_3$, 92: 8 er); HPLC analysis: Daicel Chiralcel OD-3, hexane/2-propanol = 20:1, flow rate = 0.5 mL/min, 254 nm; retention time: 17.4 min (major) and 19.8 min (minor). ^1H NMR (400 MHz, $CDCl_3$) δ 7.74 (td, *J* = 2.0, 8.8 Hz, 2H), 7.62–7.52 (m, 5H), 7.47–7.37 (m, 3H), 7.07 (d, *J* = 8.4 Hz, 1H), 6.91 (s, 1H), 4.50–4.42 (m, 1H), 3.83 (dd, *J* = 4.0, 9.6 Hz, 1H), 3.42 (t, *J* = 10.0 Hz, 1H), 2.92 (d, *J* =

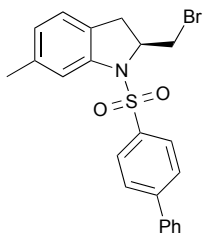
6.0 Hz, 2H), 2.58 (q, J = 8.0 Hz, 2H), 1.20 (t, J = 8.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.0, 141.4, 138.9, 138.7, 135.9, 130.7, 129.0, 128.6, 127.60, 127.57, 127.50, 127.2, 124.7, 116.7, 62.4, 35.9, 33.2, 28.3, 15.6; IR (neat): 1484, 1355, 1166, 763, 672, 622 cm^{-1}; HRMS (FAB) calcd for $C_{23}H_{22}BrNO_2S$: 455.0555 ([M]$^+$), found 455.0555.



6h: [α]$^{22}_D$ +109.8 (c = 0.99, $CHCl_3$, 87:13 er); HPLC analysis: Daicel Chiralcel OD-3, hexane/2-propanol = 20:1, flow rate = 0.5 mL/min, 254 nm; retention time: 16.4 min (major) and 18.1 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (td, J = 2.0, 8.0 Hz, 2H), 7.63–7.52 (m, 5H), 7.47–7.37 (m, 3H), 7.09 (dd, J = 1.2, 8.0 Hz, 1H), 6.94 (d, J = 0.8 Hz, 1H), 4.50–4.42 (m, 1H), 3.85 (dd, J = 4.0, 9.6 Hz, 1H), 3.42 (t, J = 9.6 Hz, 1H), 2.93 (d, J = 6.0 Hz, 2H), 2.85 (septet, J = 6.8 Hz, 1H), 1.21 (d, J = 7.2 Hz, 3H), 1.20 (d, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.03, 146.00, 138.9, 138.7, 136.0, 130.5, 129.0, 128.6, 127.6, 127.2, 126.2, 123.2, 116.5, 62.4, 35.8, 33.6, 33.2, 24.1, 24.0; IR (neat): 2959, 1486, 1355, 1165, 1094, 763, 729, 671, 620 cm^{-1}; HRMS (FAB) calcd for $C_{24}H_{24}BrNO_2S$: 469.0711 ([M]$^+$), found 469.0711.

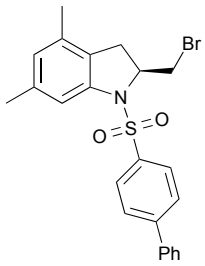


6i: [α]$^{22}_D$ +132.8 (c = 1.0, $CHCl_3$, 93: 7 er); HPLC analysis: Daicel Chiralcel OD-3, hexane/2-propanol = 20:1, flow rate = 0.5 mL/min, 254 nm; retention time: 14.8 min (major) and 17.4 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, J = 8.4 Hz, 2H), 7.63–7.53 (m, 5H), 7.48–7.37 (m, 3H), 7.28–7.24 (m, 1H), 7.09 (d, J = 0.8 Hz, 1H), 4.50–4.43 (m, 1H), 3.86 (dd, J = 3.6, 9.6 Hz, 1H), 3.42 (t, J = 9.6 Hz, 1H), 2.95 (d, J = 6.0 Hz, 2H), 1.28 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.3, 146.0, 138.9, 138.4, 136.0, 130.1, 129.0, 128.6, 127.6, 127.2, 125.0, 122.3, 116.1, 62.4, 35.8, 34.5, 33.4, 31.4; IR (neat): 2962, 1489, 1357, 1168, 763, 672, 617 cm^{-1}; HRMS (FAB) calcd for $C_{25}H_{26}BrNO_2S$: 483.0868 ([M]$^+$), found 483.0867.

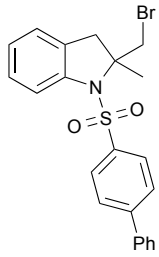


6j: [α]$^{19}_D$ +84.9 (c = 0.96, $CHCl_3$, 73:27 er); HPLC analysis: Daicel Chiralcel OD-3, hexane/2-propanol = 20:1, flow rate = 0.5 mL/min, 254 nm; retention time: 17.6 min (major) and 19.7 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, J = 8.4 Hz, 2H), 7.62 (d, J = 8.4

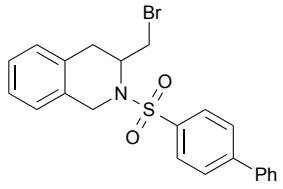
Hz, 2H), 7.57–7.53 (m, 3H), 7.47–7.38 (m, 3H), 6.96 (d, J = 7.6 Hz, 1H), 6.88 (d, J = 8.0 Hz, 1H), 4.50–4.43 (m, 1H), 3.82 (dd, J = 4.0, 10.0 Hz, 1H), 3.42 (t, J = 10.0 Hz, 1H), 2.90 (d, J = 6.0 Hz, 2H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.1, 141.1, 138.9, 138.1, 136.0, 129.0, 128.6, 127.63, 127.59, 127.50, 127.2, 125.9, 124.9, 117.4, 62.5, 35.9, 32.9, 21.6; IR (neat): 1355, 1166, 763, 672, 606 cm^{-1}; HRMS (FAB) calcd for $C_{22}H_{20}BrNO_2S$: 441.0398 ([M]$^+$), found 441.0396.



6k: $[\alpha]^{22}_D$ +79.5 (c = 1.0, $CHCl_3$, 75:25 er); HPLC analysis: Daicel Chiralpak IE-3, hexane/2-propanol = 20:1, flow rate = 0.5 mL/min, 254 nm; retention time: 48.2 min (major) and 52.7 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, J = 8.0 Hz, 2H), 7.62 (d, J = 8.4 Hz, 2H), 7.56 (d, J = 8.4 Hz, 2H), 7.48–7.36 (m, 4H), 6.71 (s, 1H), 4.51–4.44 (m, 1H), 3.86 (dd, J = 3.6, 10.0 Hz, 1H), 3.43 (t, J = 10.0 Hz, 1H), 2.83 (d, J = 6.0 Hz, 2H), 2.35 (s, 3H), 2.10 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.0, 140.8, 139.0, 138.2, 136.0, 134.4, 129.0, 128.6, 127.61, 127.55, 127.2, 126.8, 126.2, 114.5, 62.4, 36.3, 32.0, 21.5, 18.6; IR (neat): 1355, 1167, 1096, 763, 724, 672, 610 cm^{-1}; HRMS (FAB) calcd for $C_{23}H_{22}BrNO_2S$: 455.0555 ([M]$^+$), found 455.0554.



8: $[\alpha]^{26}_D$ +12.8 (c = 1.0, $CHCl_3$, 61:39 er); HPLC analysis: Daicel Chiralpak AD-3, hexane/2-propanol = 20:1, flow rate = 0.5 mL/min, 254 nm; retention time: 33.8 min (minor) and 37.6 min (major). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (td, J = 1.6, 8.0 Hz, 2H), 7.67 (td, J = 2.0, 8.4 Hz, 2H), 7.57 (d, J = 7.2 Hz, 2H), 7.51–7.38 (m, 4H), 7.19–7.13 (m, 2H), 6.99 (t, J = 7.6 Hz, 1H), 3.99 (d, J = 10.4 Hz, 1H), 3.95 (d, J = 10.0 Hz, 1H), 3.53 (d, J = 16.4 Hz, 1H), 2.95 (d, J = 16.8 Hz, 1H), 1.83 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.9, 141.7, 139.9, 139.1, 129.0, 128.5, 127.9, 127.7, 127.5, 127.3, 127.2, 125.1, 123.3, 114.0, 71.6, 42.6, 40.8, 24.5; IR (neat): 1479, 1351, 1337, 1164, 996, 762, 751, 692 cm^{-1}; HRMS (FAB) calcd for $C_{22}H_{20}BrNO_2S$: 441.0398 ([M]$^+$), found 441.0397.

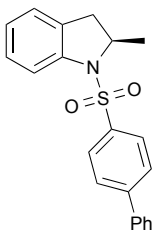


10: $[\alpha]^{29}_D$ –9.6 (c = 0.80, $CHCl_3$, 67:33 er); HPLC analysis: Daicel Chiralpak IE-3, hexane/2-propanol = 2:1, flow rate = 0.5 mL/min, 254 nm; retention time: 27.3 min (major) and 34.0 min

(minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.0 Hz, 2H), 7.65 (d, *J* = 8.4 Hz, 2H), 7.57 (d, *J* = 7.2 Hz, 2H), 7.50–7.39 (m, 3H), 7.20–7.14 (m, 2H), 7.11–7.06 (m, 2H), 4.48 (d, *J* = 15.2 Hz, 1H), 4.41 (d, *J* = 15.2 Hz, 1H), 4.41–4.34 (m, 1H), 3.54 (dd, *J* = 4.0, 10.0 Hz, 1H), 3.17 (t, *J* = 9.6 Hz, 1H), 3.06 (dd, *J* = 4.0, 15.6 Hz, 1H), 2.84 (dd, *J* = 6.0, 15.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.8, 139.1, 137.2, 132.0, 131.9, 129.0, 128.9, 128.5, 127.7, 127.6, 127.3, 126.8, 126.1, 53.7, 45.0, 33.5, 30.8; IR (neat): 1335, 1158, 1093, 1030, 911, 722, 670 cm^{-1}; HRMS (FAB) calcd for $C_{22}H_{21}BrNO_2S$: 442.0476 ($[M+H]^+$), found 442.0476.

5. Transformations of product 3g.

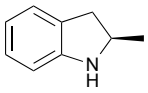
To a solution of bromoaminocyclization product **3g** (0.10 mmol) in toluene (2 mL) was added 2,2'-azobis(isobutyronitrile) (AIBN) (0.030 mmol) and tributyltin hydride (0.25 mmol). The reaction mixture was warmed to 80 °C and stirred for 16 h. After 16 h, the reaction mixture was cooled to room temperature and quenched with saturated aqueous $NaHCO_3$ (10 mL). The organic materials were extracted with ethyl acetate for three times (5 mL × 3). The combined extracts were dried over Na_2SO_4 and concentrated. The residue was purified by flash column chromatography on silica gel (hexane/ethyl acetate = 50:1–10:1 as eluent) to give product **11**.



11: $[\alpha]^{27}_D$ +221.5 (*c* = 1.1, $CHCl_3$, 95: 5 er); HPLC analysis: Daicel Chiralpak IC-3, hexane/2-propanol = 5:1, flow rate = 0.5 mL/min, 254 nm; retention time: 35.0 min (major) and 38.2 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75–7.68 (m, 3H), 7.60–7.52 (m, 4H), 7.47–7.36 (m, 3H), 7.26–7.21 (m, 1H), 7.08–7.01 (m, 2H), 4.44–4.36 (m, 1H), 2.95 (dd, *J* = 10.0, 16.4 Hz, 1H), 2.47 (dd, *J* = 2.4, 16.4 Hz, 1H), 1.46 (d, *J* = 6.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.6, 140.9, 139.1, 136.8, 131.6, 129.0, 128.5, 127.7, 127.43, 127.41, 127.2, 125.3, 124.5, 117.1, 58.5, 36.2, 23.4; IR (neat): 1350, 1165, 1093, 1023, 759, 723, 696, 670 cm^{-1}; HRMS (FAB) calcd for $C_{21}H_{19}NO_2S$: 349.1136 ($[M]^+$), found 349.1138.

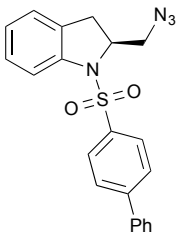
To a mixture of **11** (0.050 mmol) and magnesium powder (0.50 mmol) in THF

(1 mL) was added titanium(IV) isopropoxide (0.15 mmol) and trimethylsilyl chloride (0.25 mmol) under nitrogen atmosphere. The reaction mixture was warmed to 50 °C and stirred for 17 h. After 17 h, the reaction mixture was cooled to room temperature and quenched with 1M aqueous NaOH (2 mL). The resulting mixture was stirred for 30 min at room temperature. The resulting mixture was diluted with ethyl acetate and filtered over celite. The filtrate was diluted with water. The solution was extracted with ethyl acetate (5 mL × 3). The combined extracts were dried over Na_2SO_4 and concentrated. The residue was purified by flash column chromatography on silica gel (hexane/ethyl acetate = 30:1–5:1 as eluent) to give product **12**.



12:[4d,5] $[\alpha]^{26}_D$ +14.2 (*c* = 0.14, benzene, 95: 5 er); HPLC analysis: Daicel Chiralcel OD-3, hexane/2-propanol = 20:1, flow rate = 0.5 mL/min, 254 nm; retention time: 14.0 min (major) and 15.8 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.08 (d, *J* = 7.2 Hz, 1H), 7.02 (t, *J* = 7.2 Hz, 1H), 6.71 (t, *J* = 7.2 Hz, 1H), 6.64 (d, *J* = 7.6 Hz, 1H), 4.06–3.96 (m, 1H), 3.15 (dd, *J* = 8.8, 15.2 Hz, 1H), 2.65 (dd, *J* = 8.0, 15.2 Hz, 1H), 1.31 (d, *J* = 6.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.9, 128.8, 127.1, 124.6, 118.4, 109.1, 55.1, 37.7, 22.2; IR (neat): 3369, 2961, 1608, 1484, 1466, 1246, 744, 713 cm^{-1}.

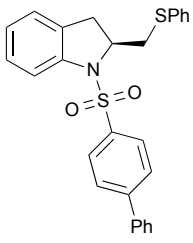
To a solution of bromoaminocyclization product **3g** (0.10 mmol) in DMF (2 mL) was added NaN_3 (0.30 mmol). The reaction mixture was warmed to 60 °C and stirred for 17 h. After 17 h, the reaction mixture was cooled to room temperature and quenched with water (20 mL). The organic materials were extracted with ethyl acetate for three times (10 mL × 3). The combined extracts were dried over Na_2SO_4 and concentrated. The residue was purified by flash column chromatography on silica gel (hexane/ethyl acetate = 50:1–5:1 as eluent) to give product **13**.



13: $[\alpha]^{27}_D$ +164.7 (*c* = 1.0, $CHCl_3$, 95: 5 er); HPLC analysis: Daicel Chiralcel OD-3, hexane/2-propanol = 20:1, flow rate = 0.5 mL/min, 254 nm; retention time: 28.5 min (major) and 34.8 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74–7.71 (m, 3H), 7.60 (d, *J* = 8.8 Hz, 2H), 7.54 (d, *J* =

7.6 Hz, 2H), 7.47–7.37 (m, 3H), 7.29–7.22 (m, 1H), 7.10–7.04 (m, 2H), 4.41–4.35 (m, 1H), 3.65 (dd, J = 4.4, 12.4 Hz, 1H), 3.55 (dd, J = 7.2, 12.4 Hz, 1H), 2.89 (dd, J = 9.6, 16.4 Hz, 1H), 2.75 (dd, J = 3.2, 16.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.1, 141.1, 138.9, 136.0, 131.1, 129.0, 128.6, 128.0, 127.6, 127.5, 127.2, 125.22, 125.16, 117.2, 61.0, 55.2, 32.1; IR (neat): 2101, 1479, 1354, 1166, 1095, 761, 672 cm^{-1}; HRMS (FAB) calcd for $C_{21}H_{19}N_4O_2S$: 391.1229 ($[M+H]^+$), found 391.1229.

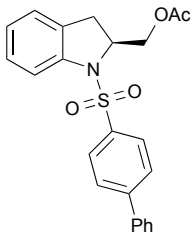
To a solution of bromoaminocyclization product **3g** (0.10 mmol) in CH_3CN (1 mL) was added K_2CO_3 (0.20 mmol) and thiophenol (0.30 mmol). The reaction mixture was warmed to 75 °C and stirred for 24 h. After 24 h, the reaction mixture was cooled to room temperature and quenched with saturated aqueous NH_4Cl (5 mL). The organic materials were extracted with ethyl acetate for three times (5 mL × 3). The combined extracts were dried over Na_2SO_4 and concentrated. The residue was purified by flash column chromatography on silica gel (hexane/ethyl acetate = 50:1–5:1 as eluent) to give product **14**.



14: $[\alpha]^{27}_D$ –32.3 (c = 0.60, $CHCl_3$, 95: 5 er); HPLC analysis: Daicel Chiralpak IC-3, hexane/2-propanol = 5:1, flow rate = 0.5 mL/min, 254 nm; retention time: 22.3 min (major) and 25.2 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, J = 8.0 Hz, 1H), 7.59 (d, J = 8.8 Hz, 2H), 7.54–7.35 (m, 11H), 7.28–7.21 (m, 2H), 7.08–7.02 (m, 2H), 4.34–4.27 (m, 1H), 3.75 (dd, J = 3.6, 13.6 Hz, 1H), 2.97–2.84 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.9, 141.1, 138.9, 136.0, 134.8, 131.0, 129.11, 129.02, 128.98, 128.5, 127.9, 127.50, 127.42, 127.2, 126.2, 125.4, 124.9, 117.0, 60.8, 38.5, 33.3; IR (neat): 1478, 1354, 1165, 1093, 1024, 760, 740, 693, 670 cm^{-1}; HRMS (FAB) calcd for $C_{27}H_{24}NO_2S_2$: 458.1248 ($[M+H]^+$), found 458.1249.

To a solution of bromoaminocyclization product **3g** (0.050 mmol) in DMF (2.5 mL) was added KOAc (0.20 mmol) and 18-crown-6 ether (0.10 mmol). The reaction mixture was warmed to 50 °C and stirred for 7 h. After 7 h, the reaction mixture was

cooled to room temperature and quenched with water (20 mL). The organic materials were extracted with ethyl acetate for three times (10 mL × 3). The combined extracts were dried over Na_2SO_4 and concentrated. The residue was purified by flash column chromatography on silica gel (hexane/ethyl acetate = 30:1–3:1 as eluent) to give product **15**.



15: $[\alpha]^{26}_D$ +191.2 (*c* = 0.93, $CHCl_3$, 95: 5 er); HPLC analysis: Daicel Chiralcel OD-3, hexane/2-propanol = 10:1, flow rate = 0.5 mL/min, 254 nm; retention time: 31.3 min (major) and 33.9 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73–7.68 (m, 3H), 7.58 (td, *J* = 1.6, 8.8 Hz, 2H), 7.55–7.52 (m, 2H), 7.47–7.37 (m, 3H), 7.28–7.22 (m, 1H), 7.06 (d, *J* = 4.0 Hz, 2H), 4.60–4.53 (m, 1H), 4.22 (dd, *J* = 6.4, 11.2 Hz, 1H), 4.17 (dd, *J* = 6.4, 11.2 Hz, 1H), 2.82 (dd, *J* = 10.0, 16.4 Hz, 1H), 2.60 (dd, *J* = 2.4, 16.4 Hz, 1H), 2.07 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.0, 145.9, 141.1, 138.9, 136.3, 131.5, 129.0, 128.6, 128.0, 127.5, 127.2, 125.1, 117.8, 65.7, 60.1, 31.5, 20.8; IR (neat): 1739, 1478, 1354, 1229, 1165, 1096, 1044, 761, 671 cm^{-1}; HRMS (FAB) calcd for $C_{23}H_{22}NO_4S$: 408.1270 ($[M+H]^+$), found 408.1270.

6. Determination of the absolute configuration of products.

The absolute configurations of products **3a**,[4d] **3d**,[4d] and **12**[4d,5] were confirmed by comparison of an optical rotation value with the literature.[4d,5]

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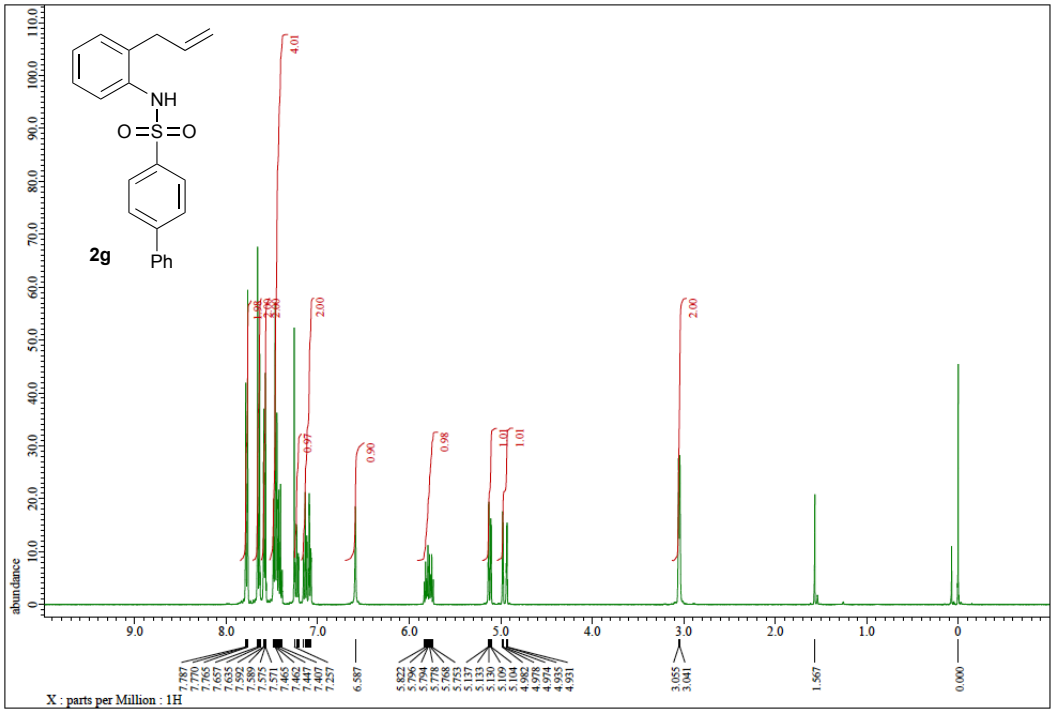
NMR Charts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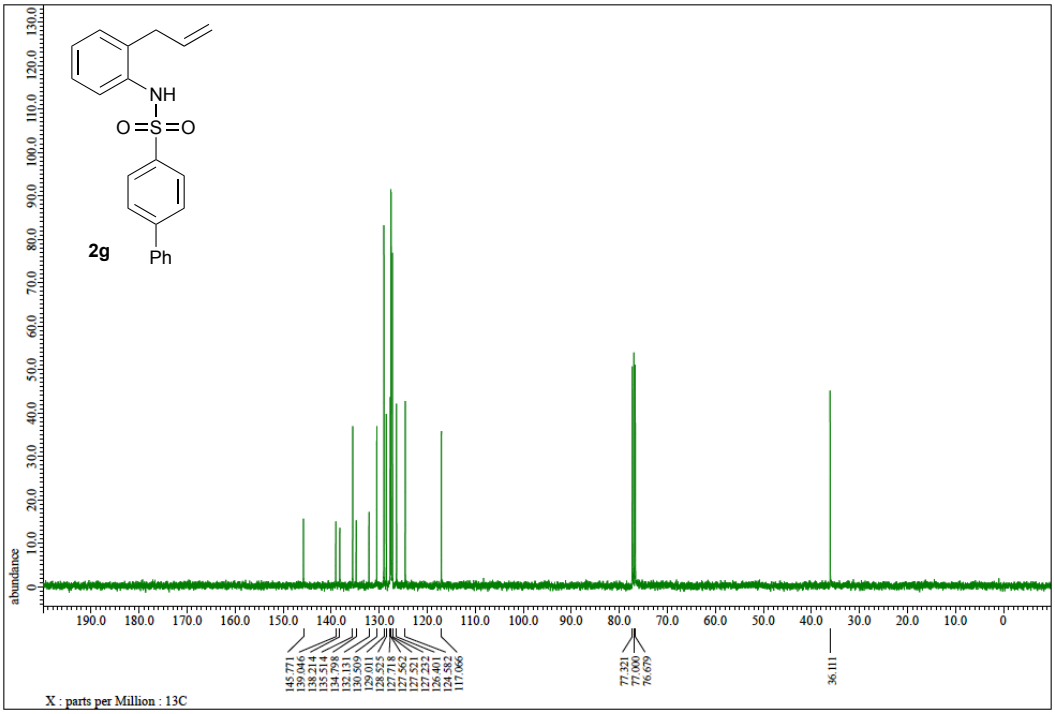
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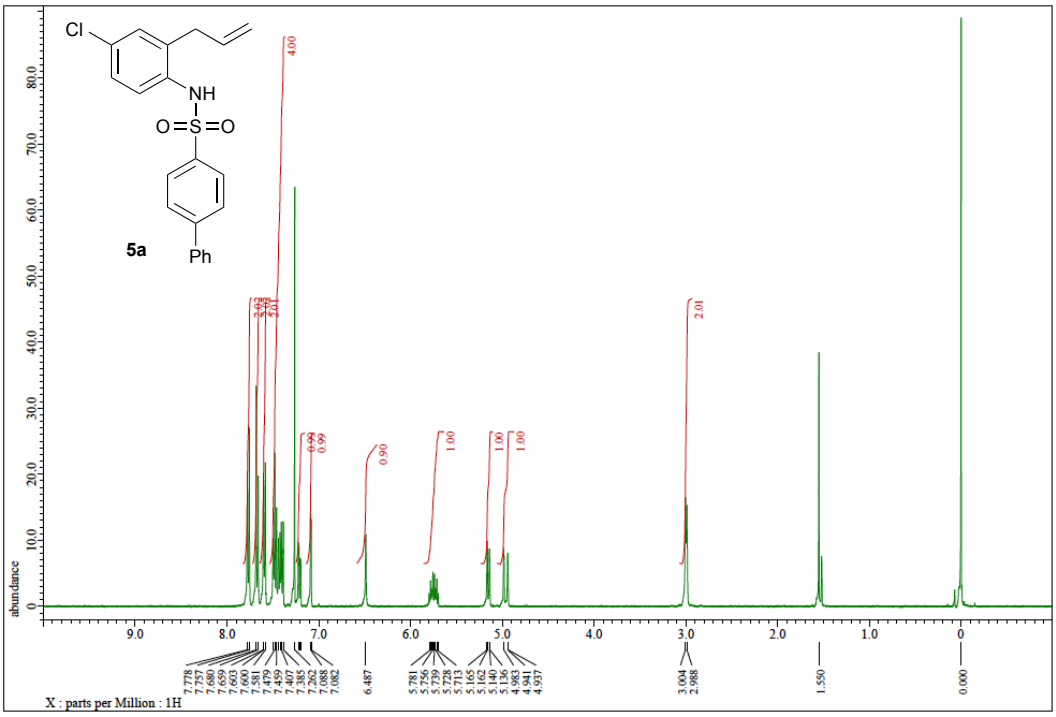
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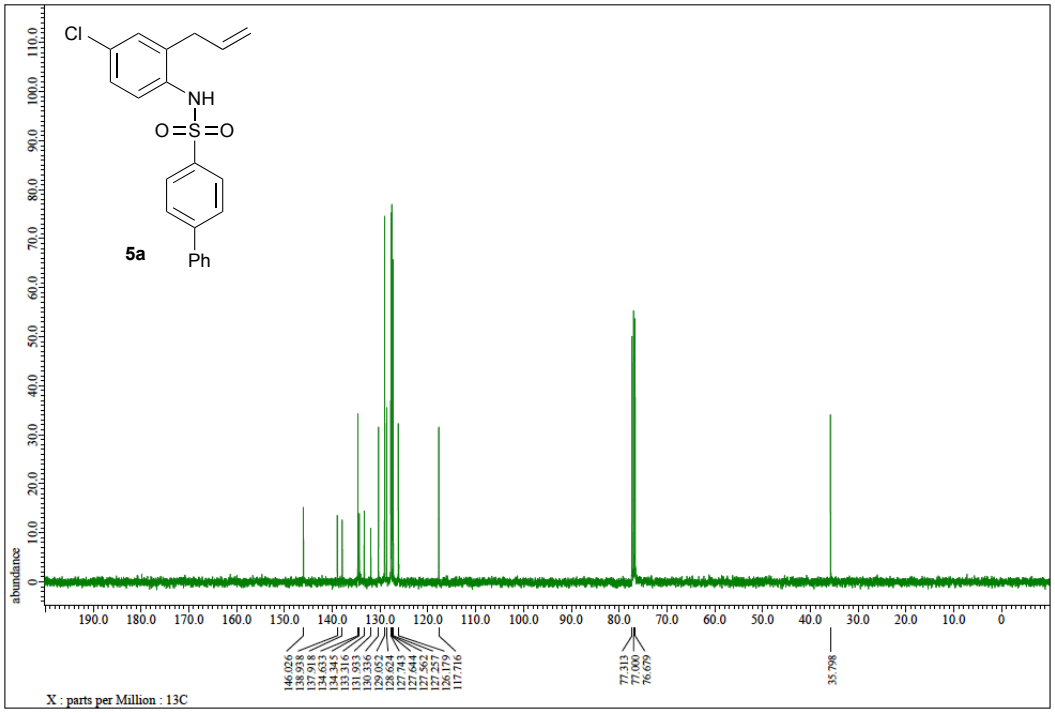
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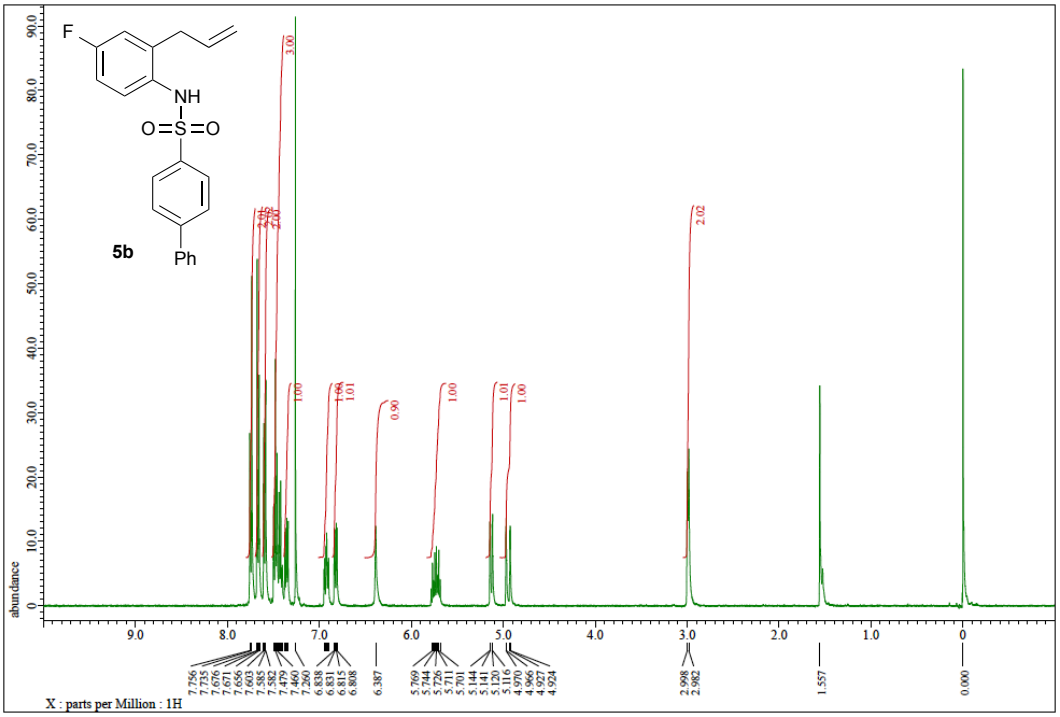
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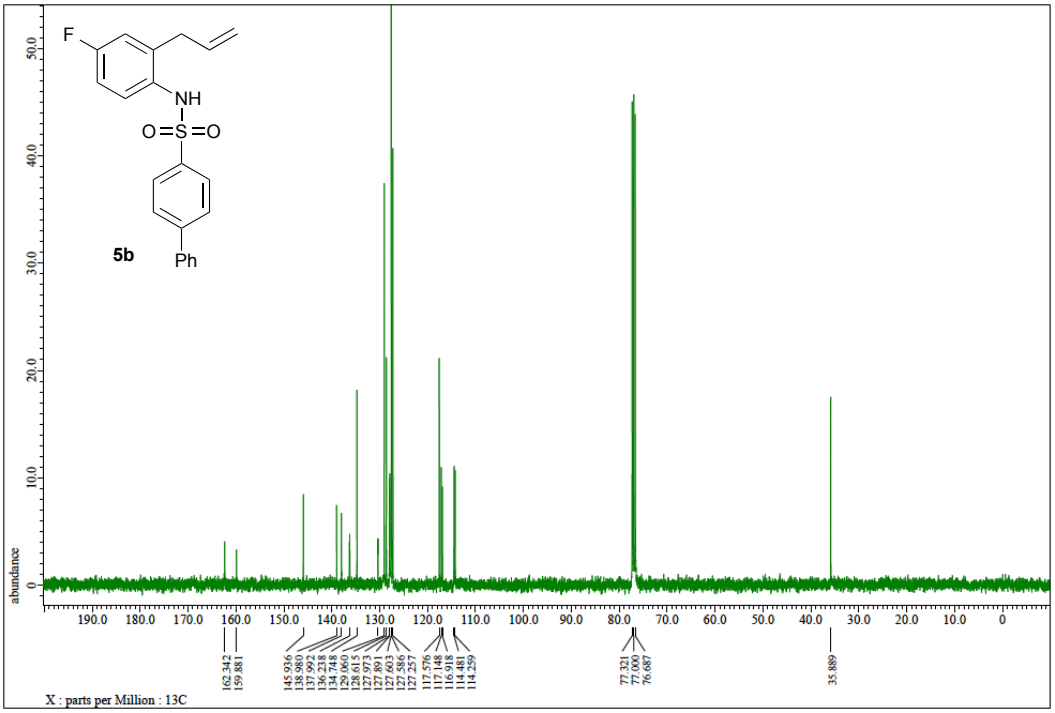
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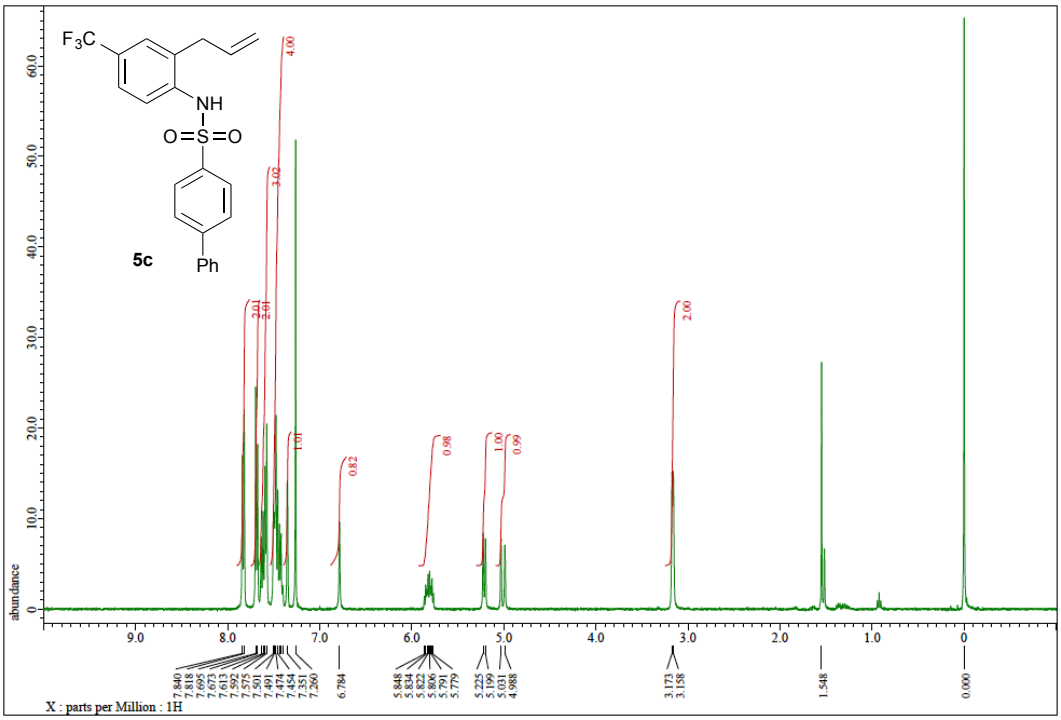
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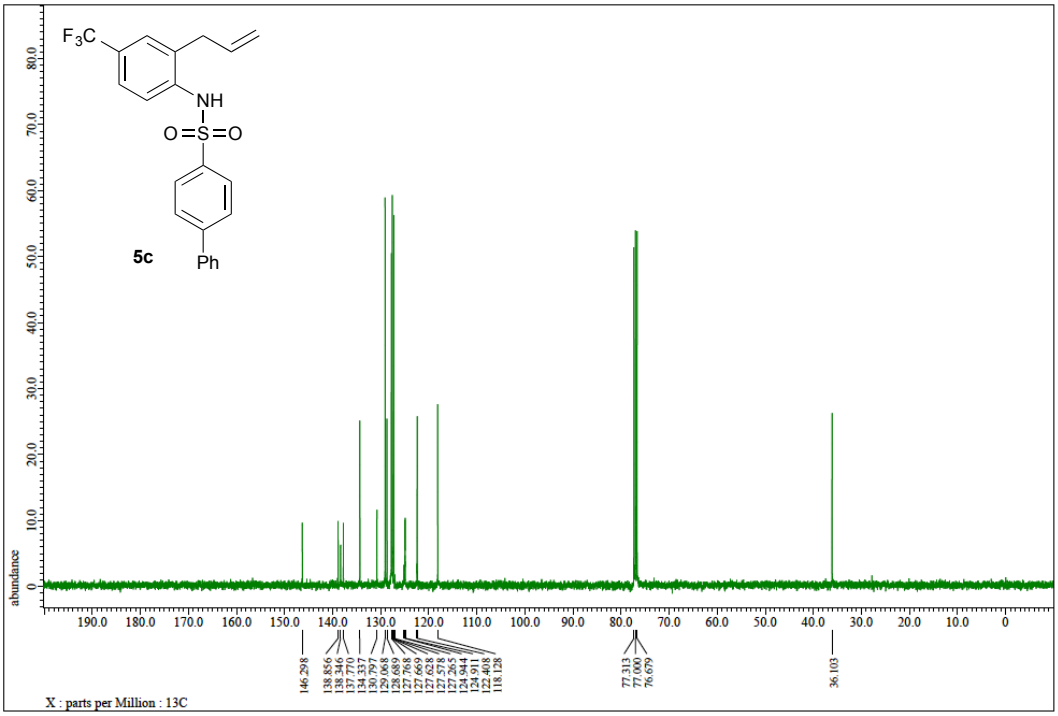
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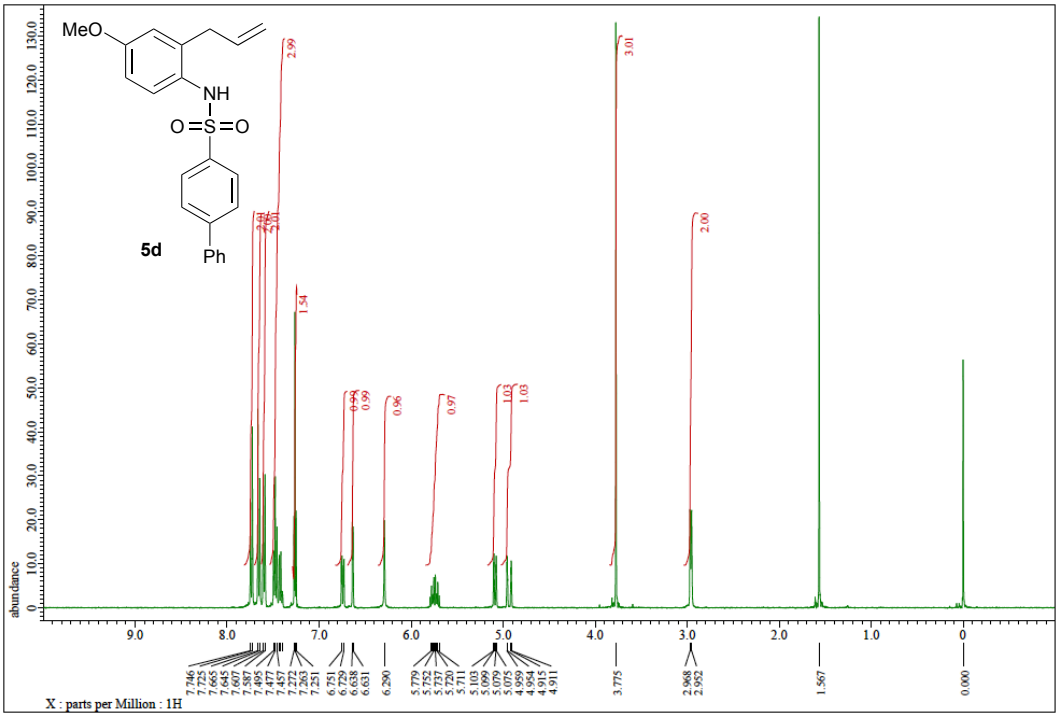
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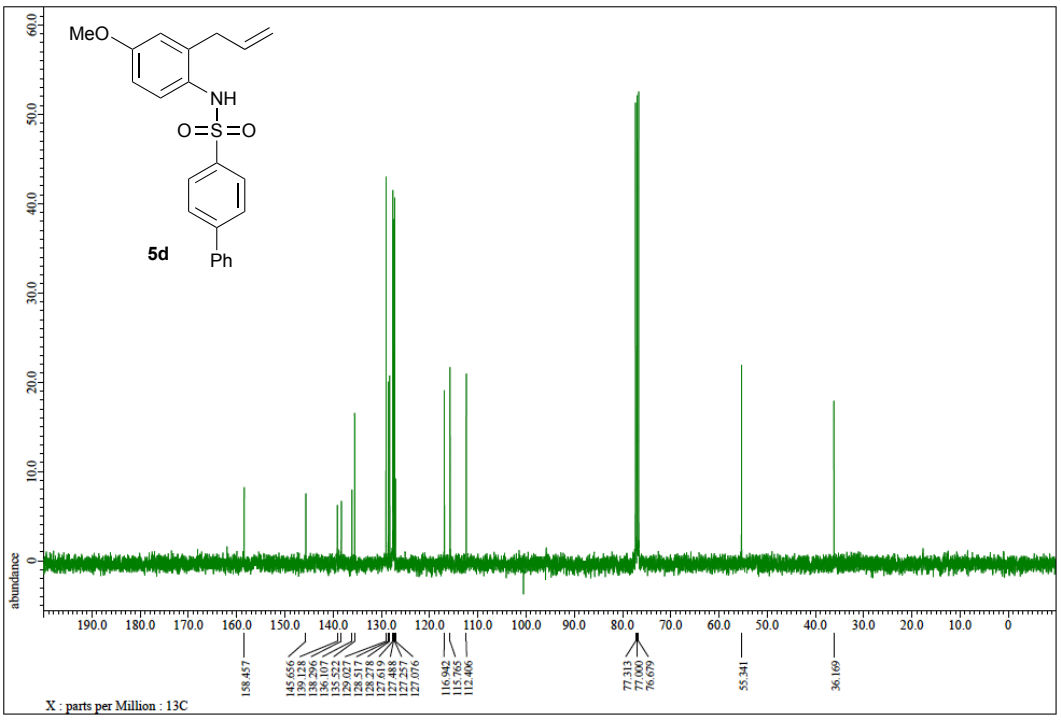
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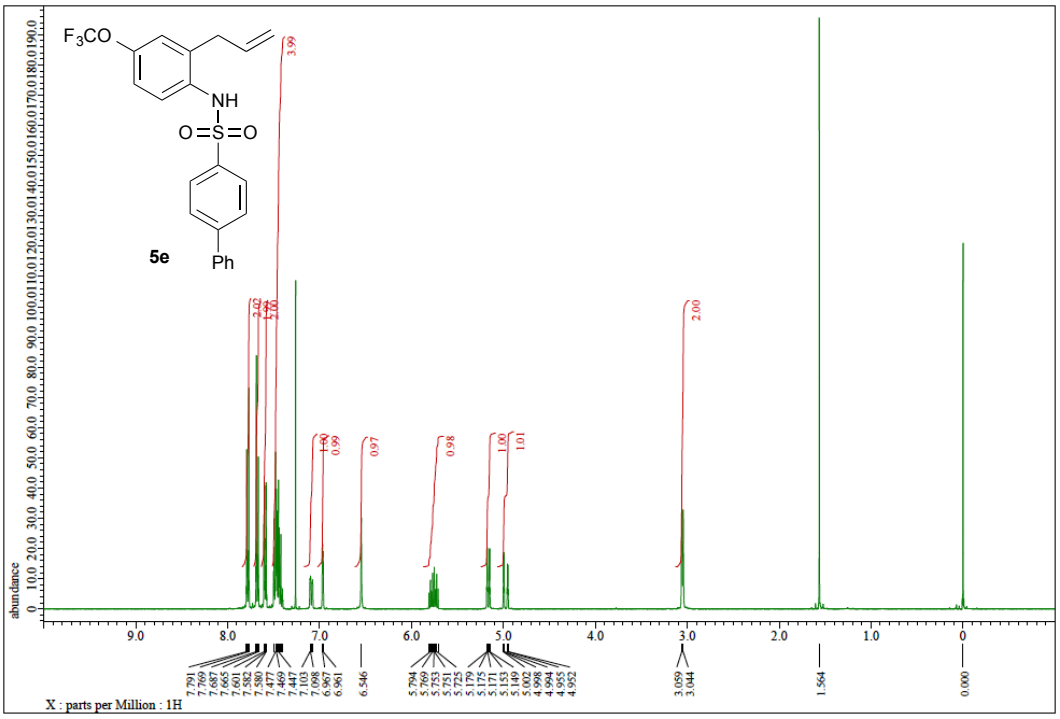
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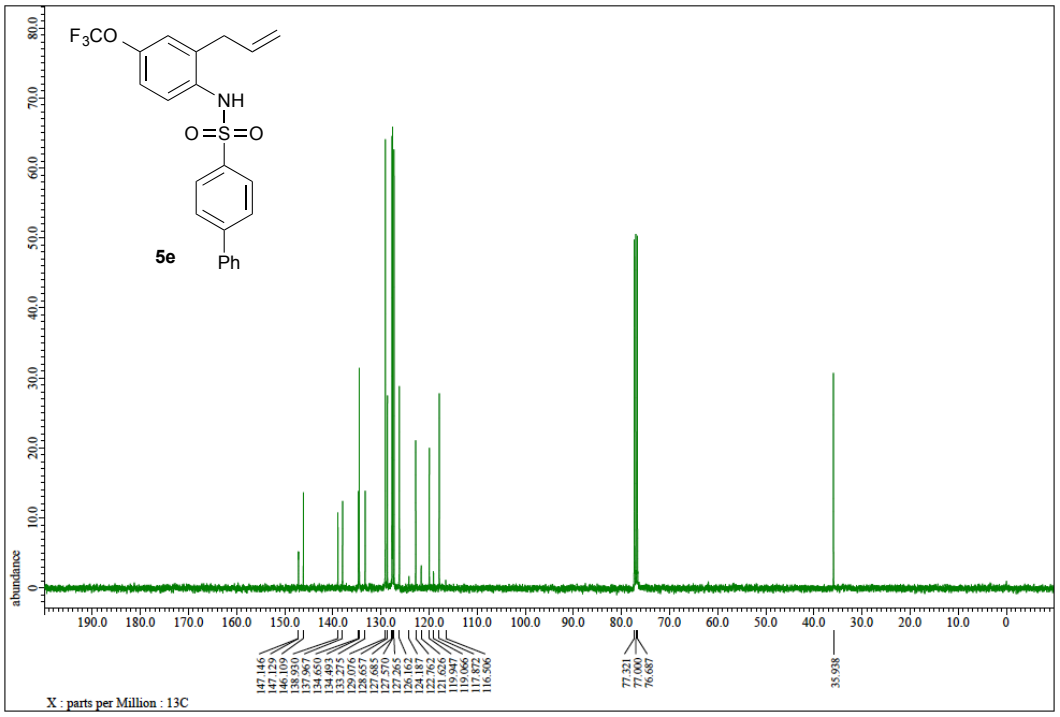
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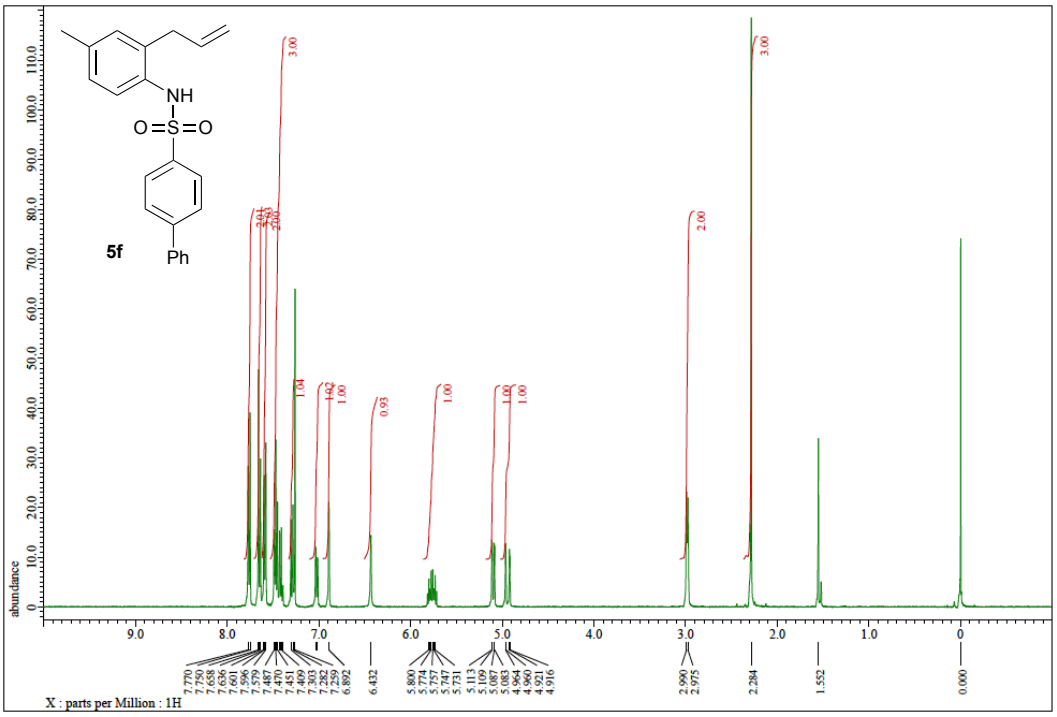
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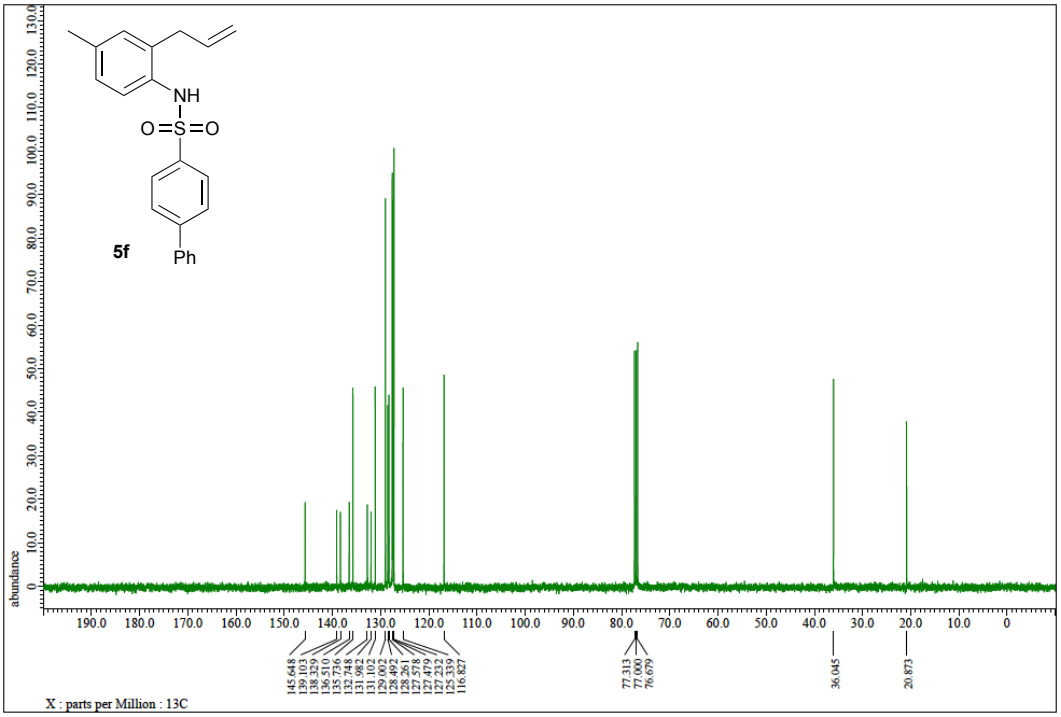
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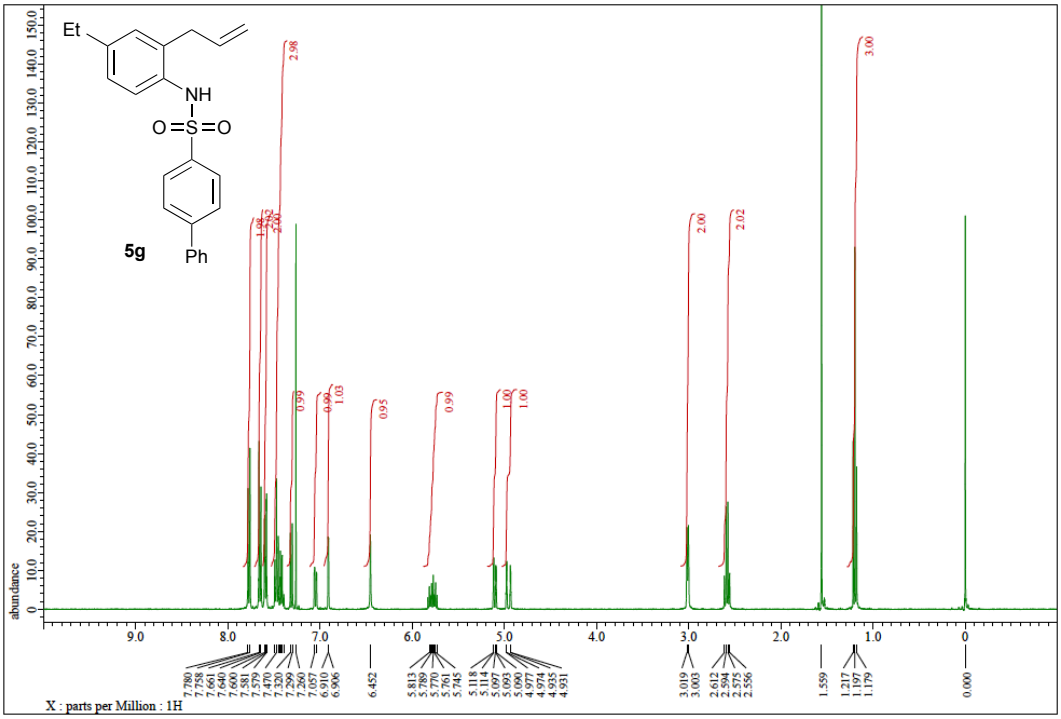
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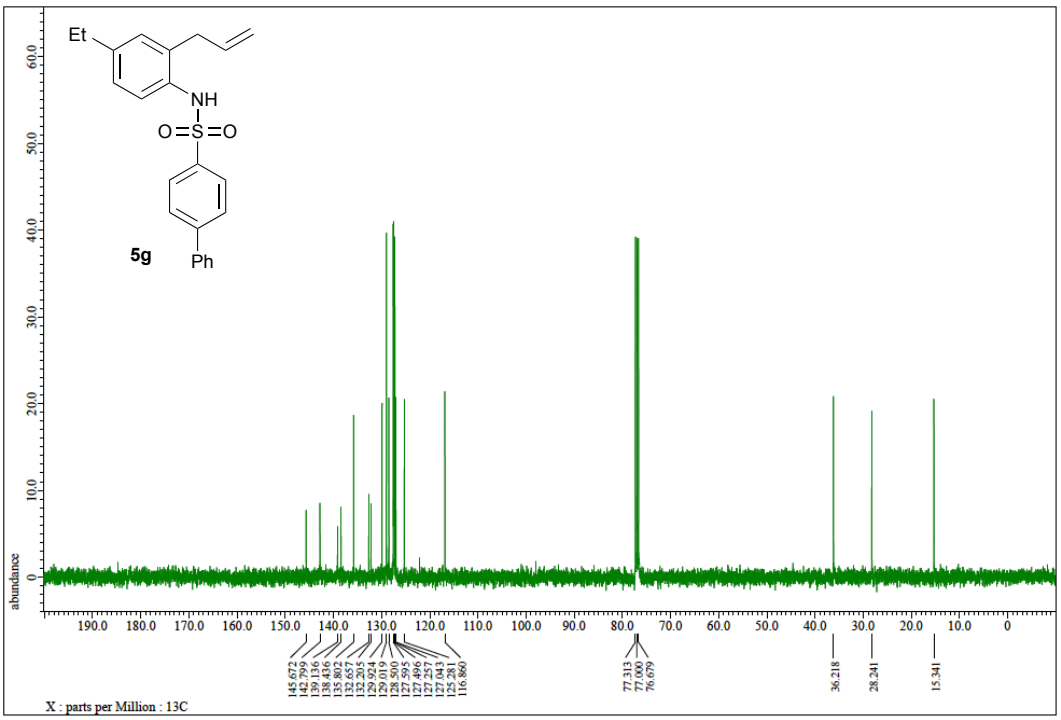
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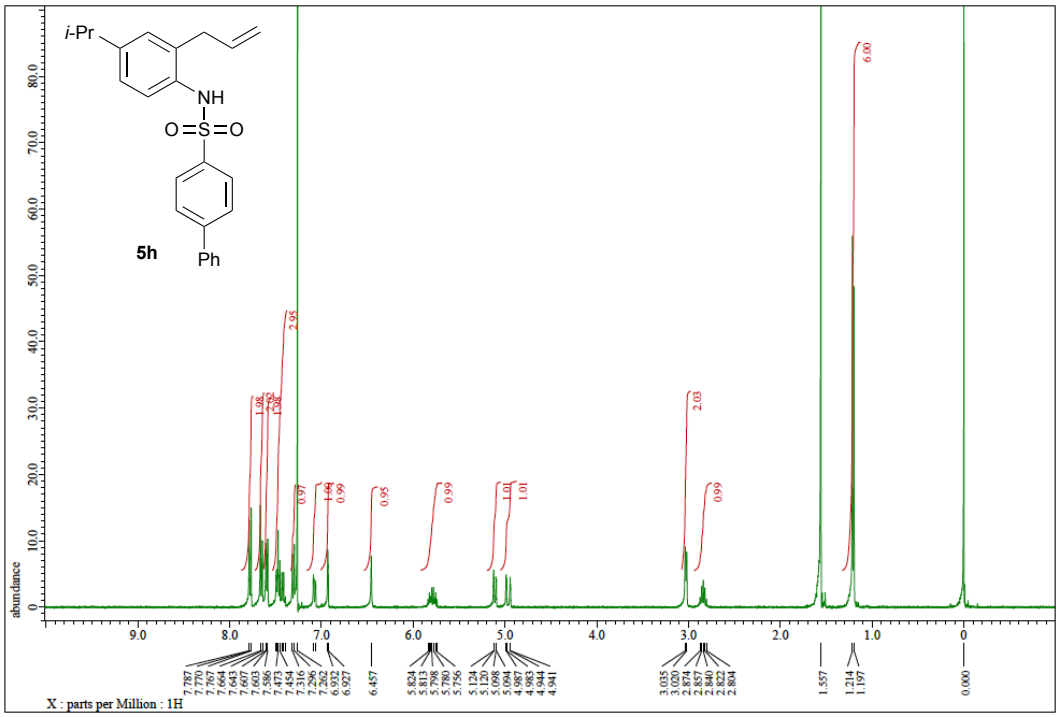
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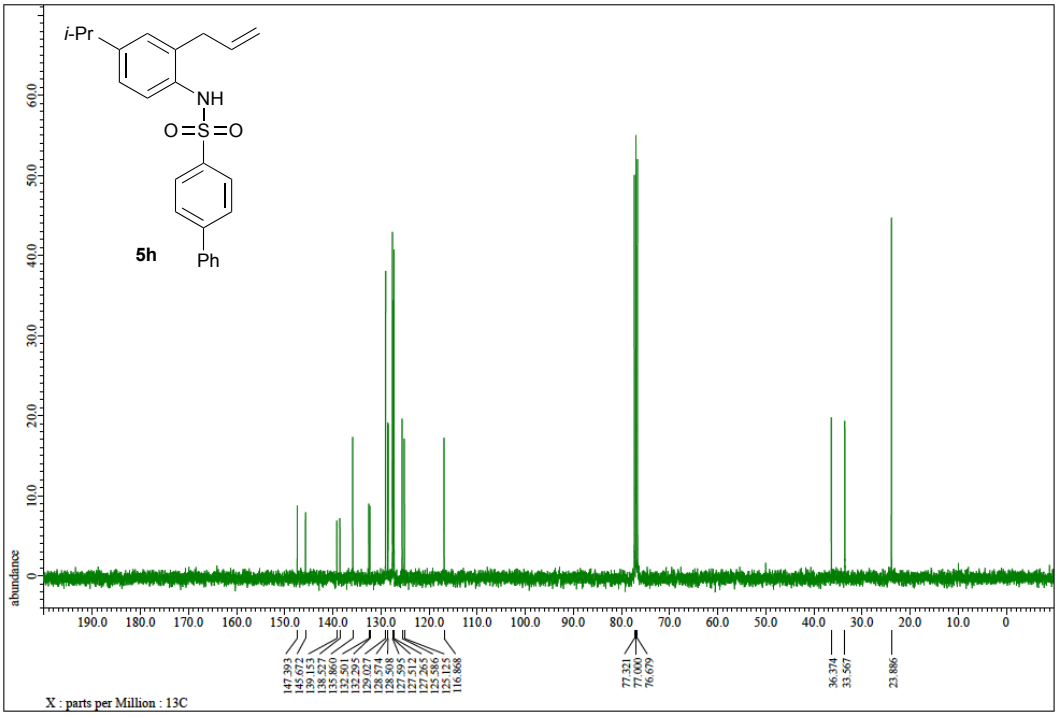
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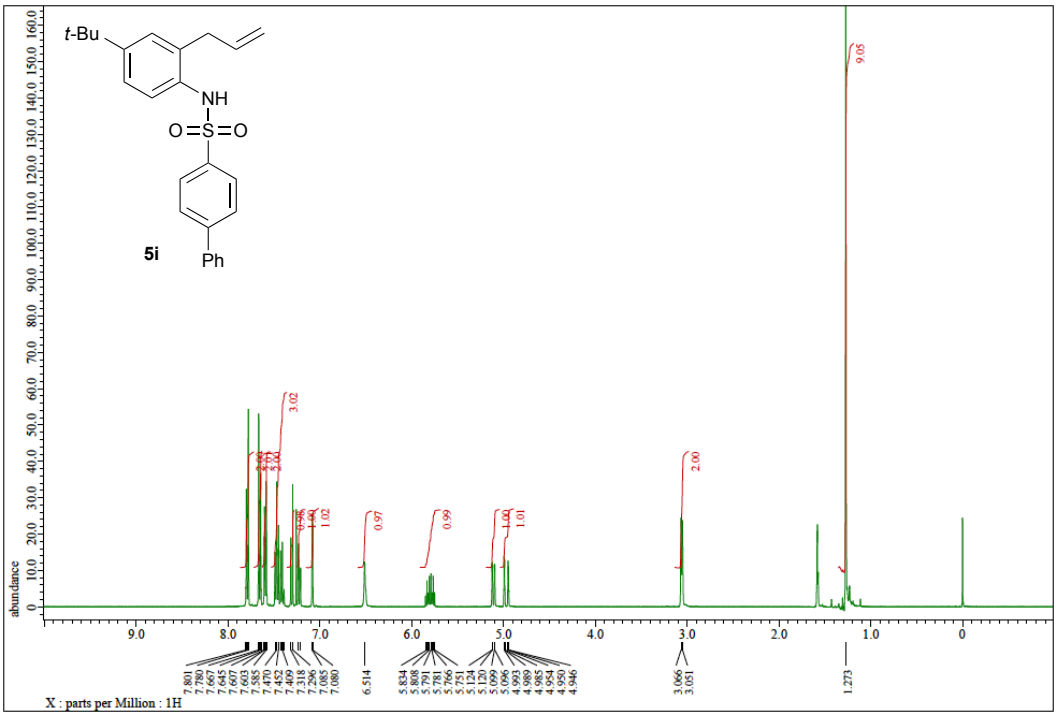
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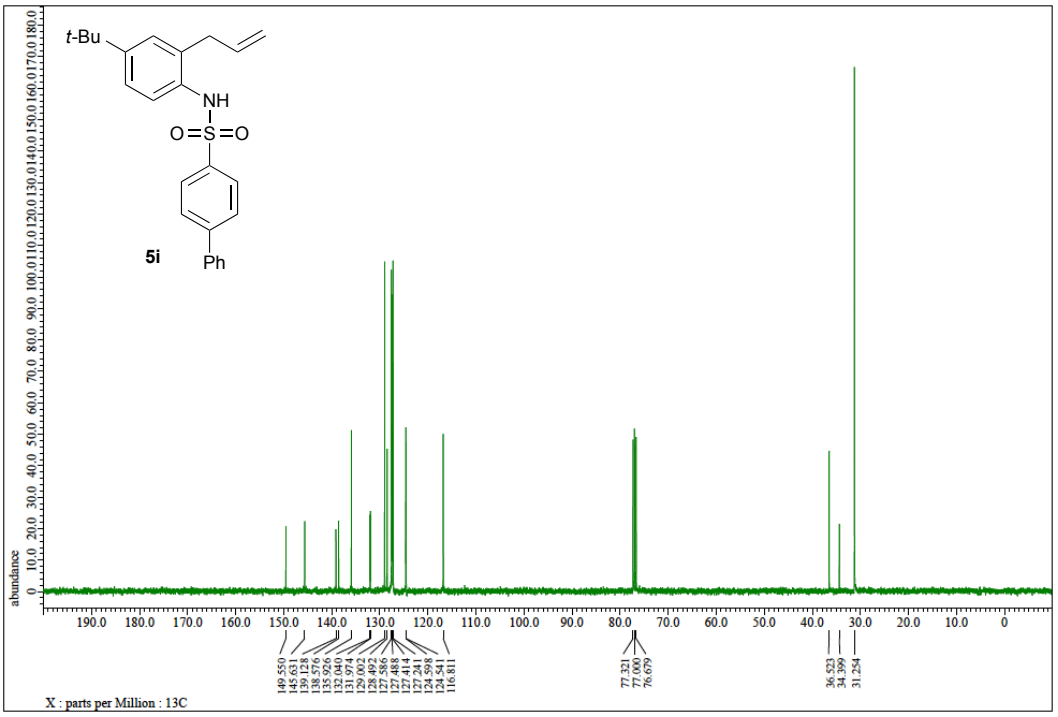
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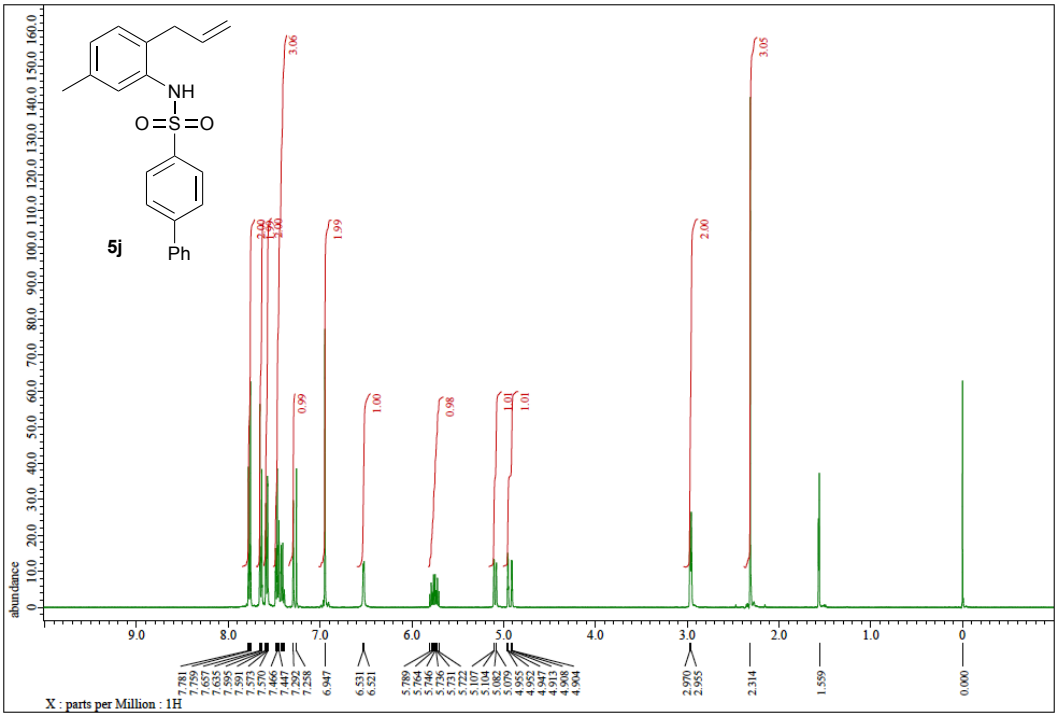
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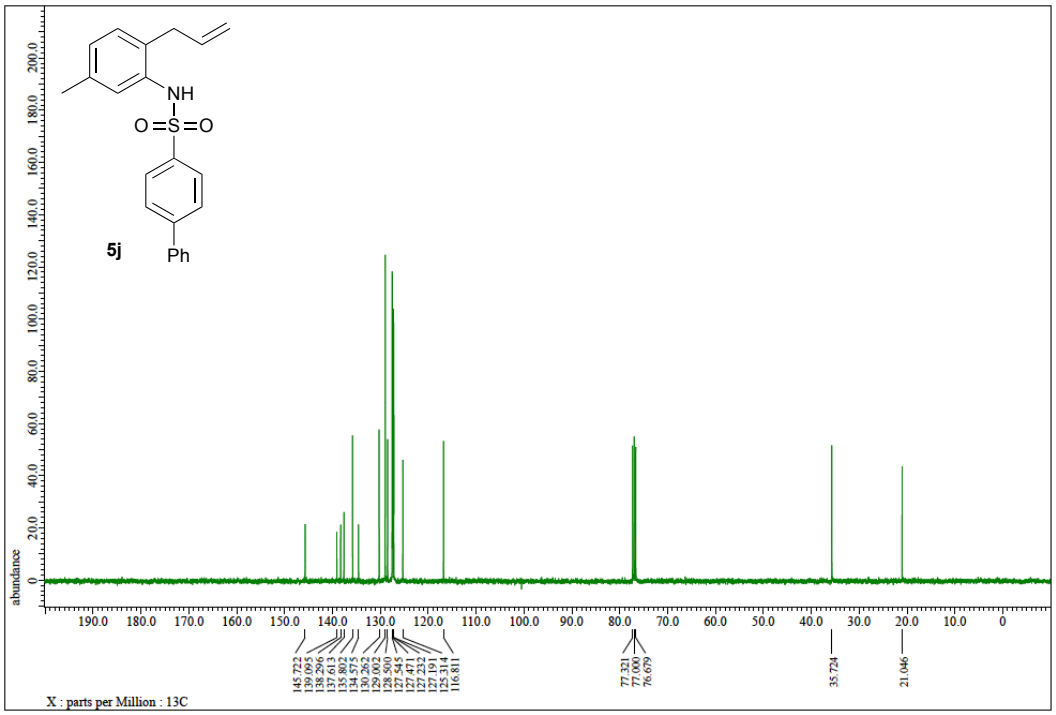
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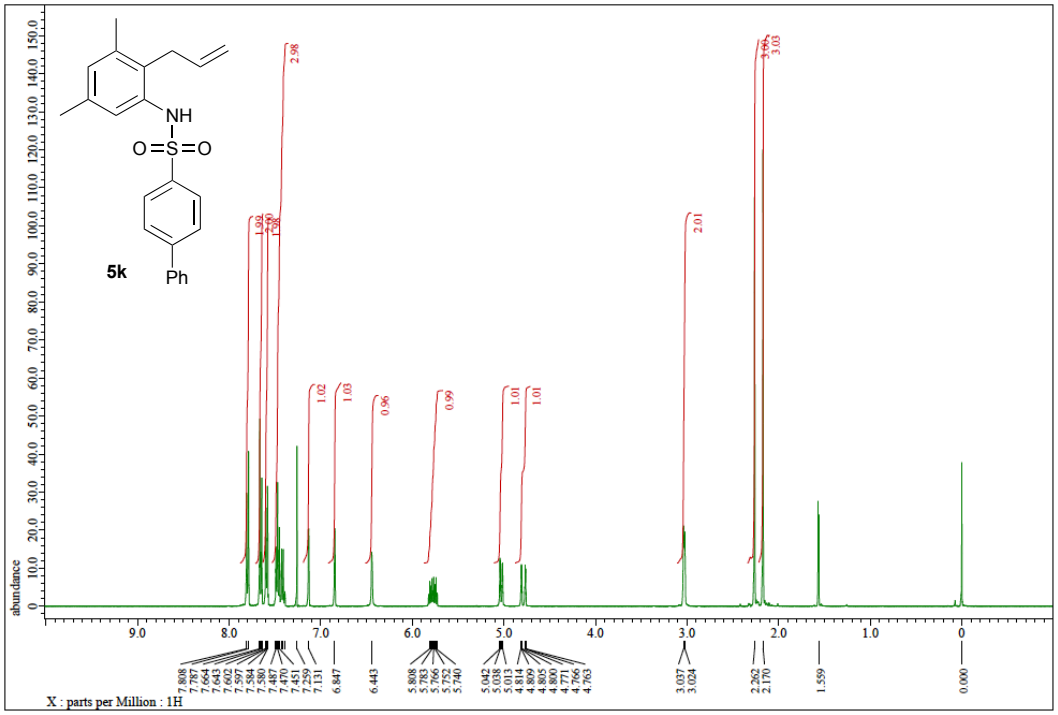
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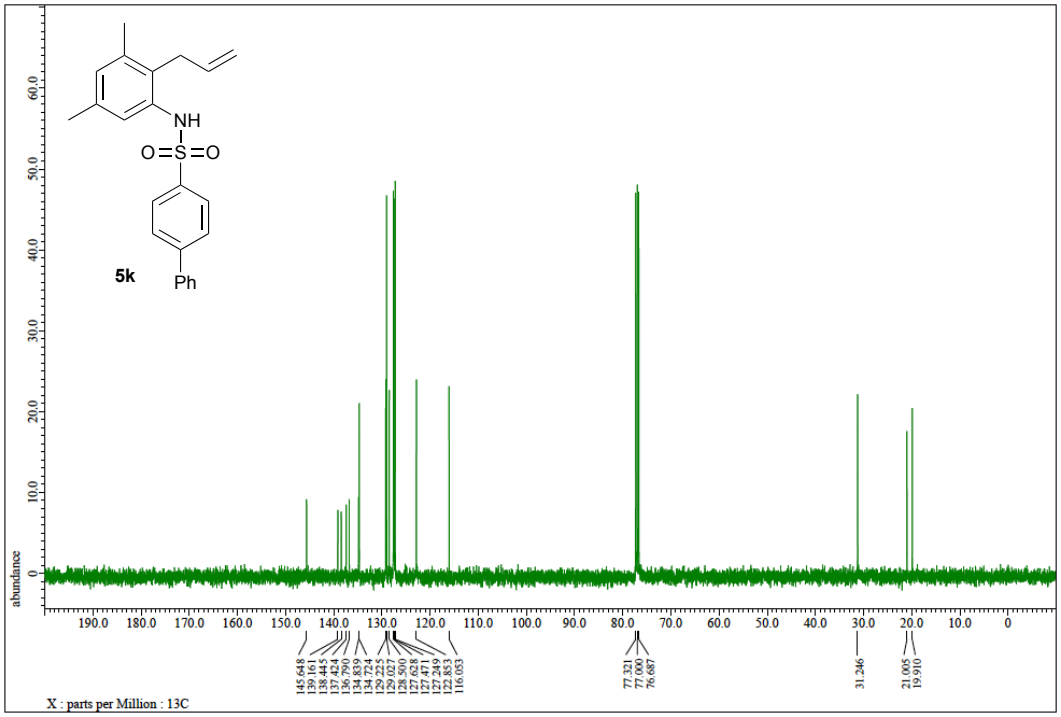
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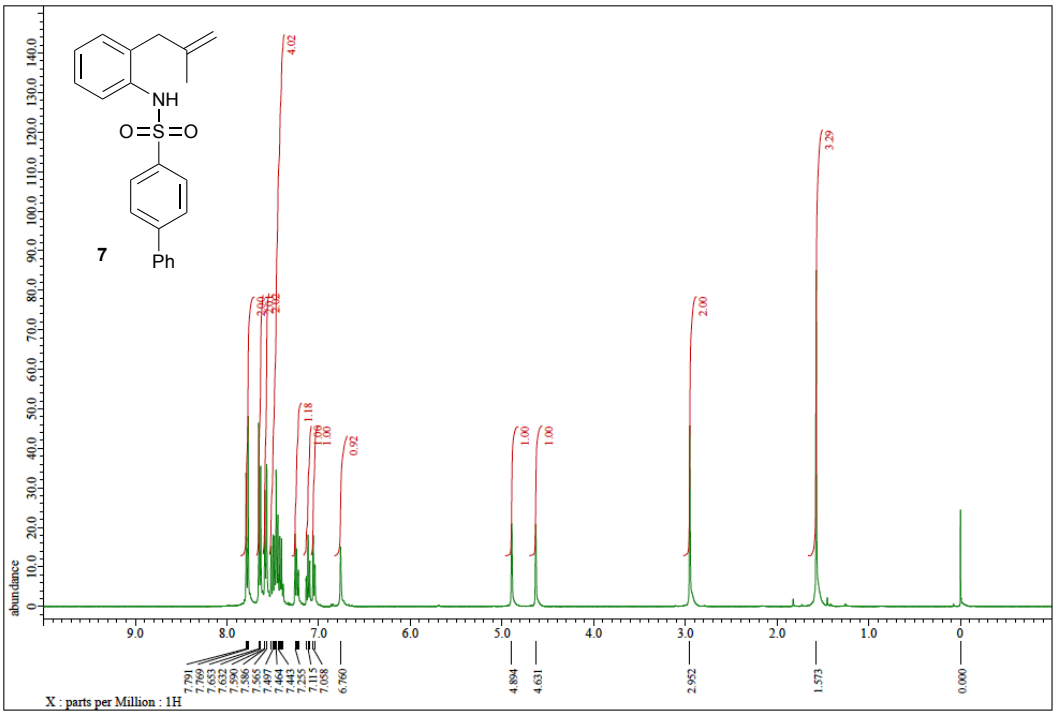
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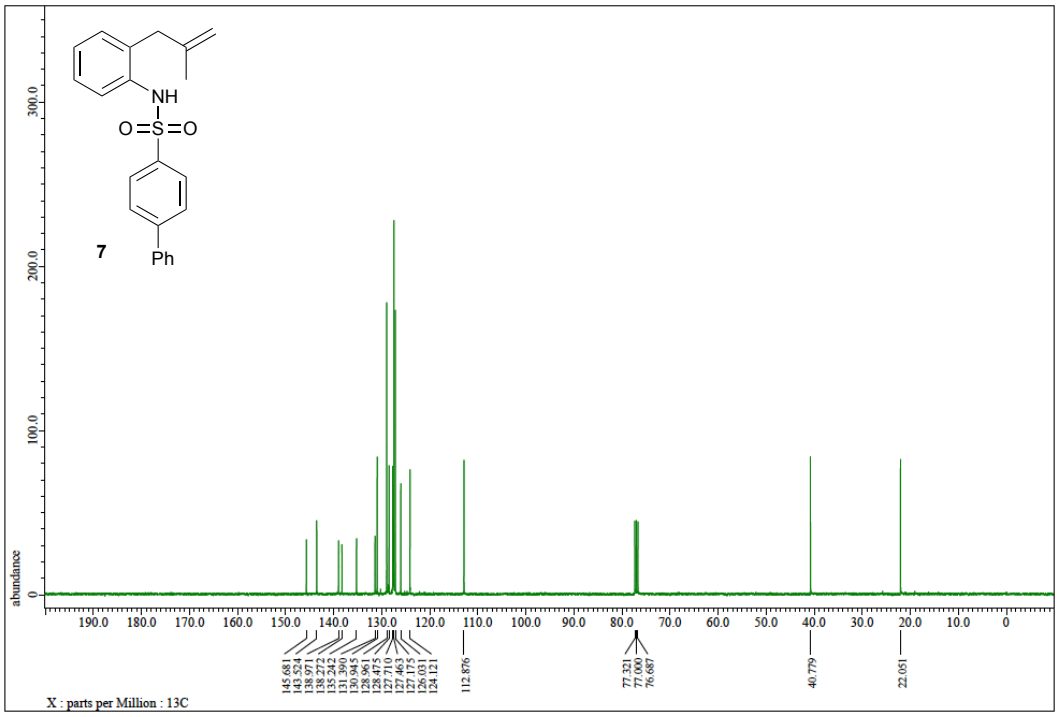
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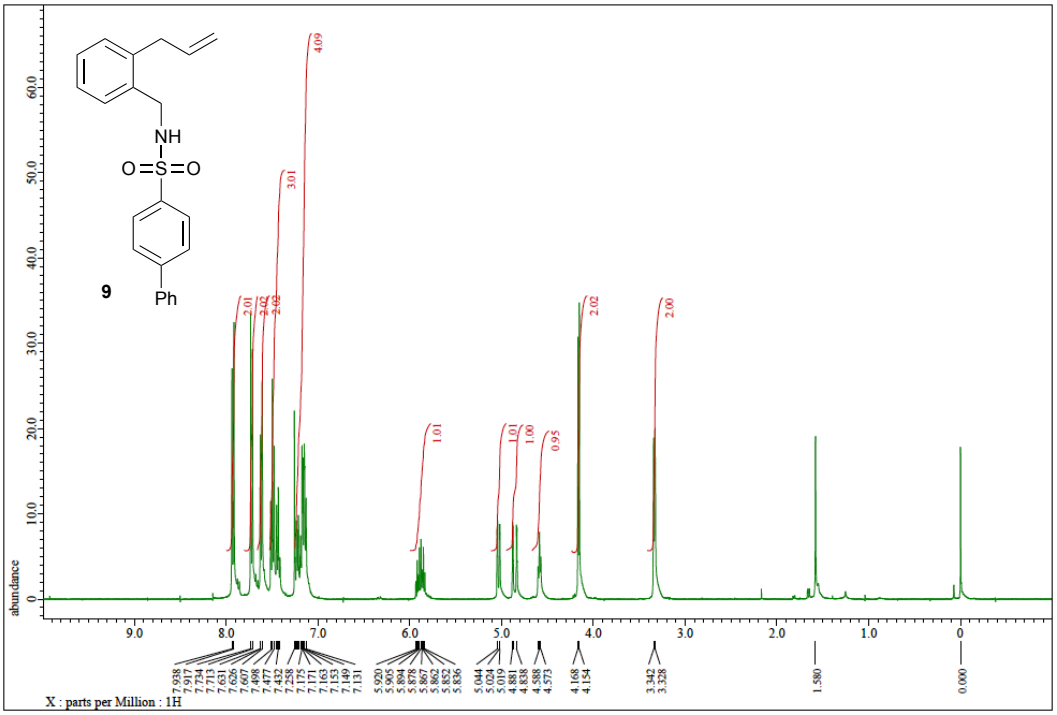
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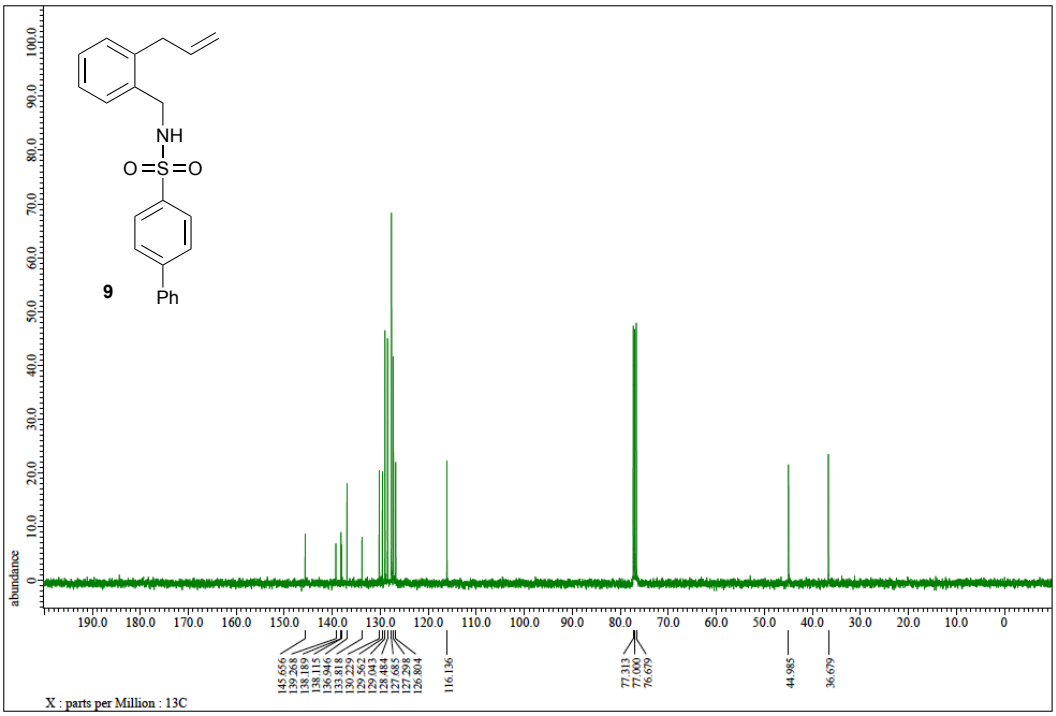
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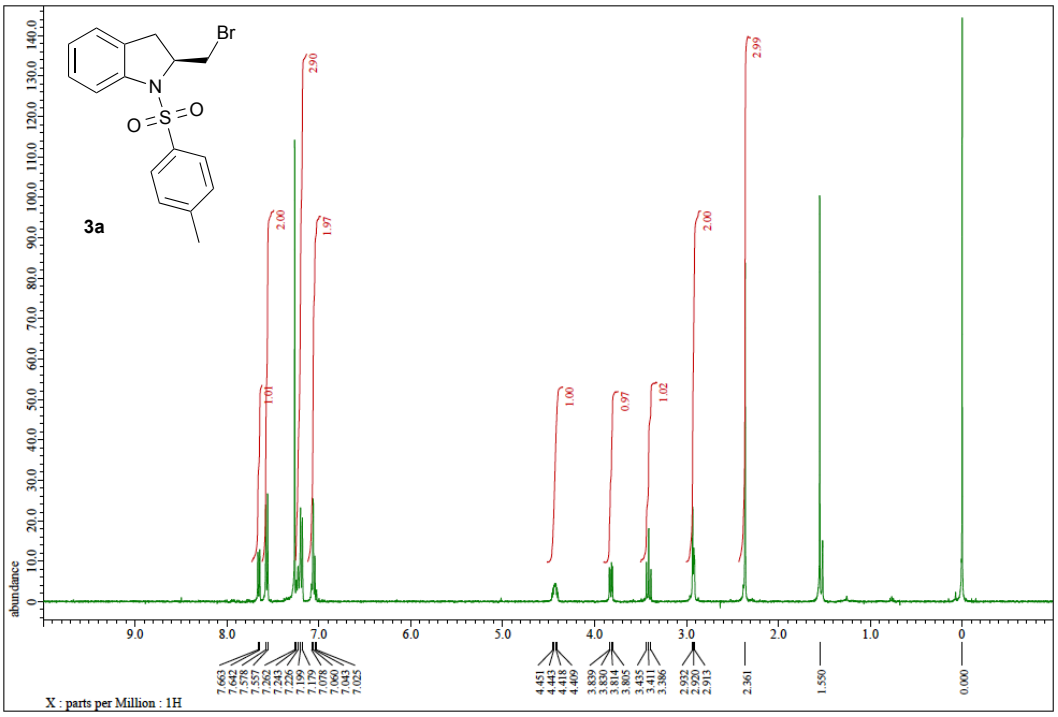
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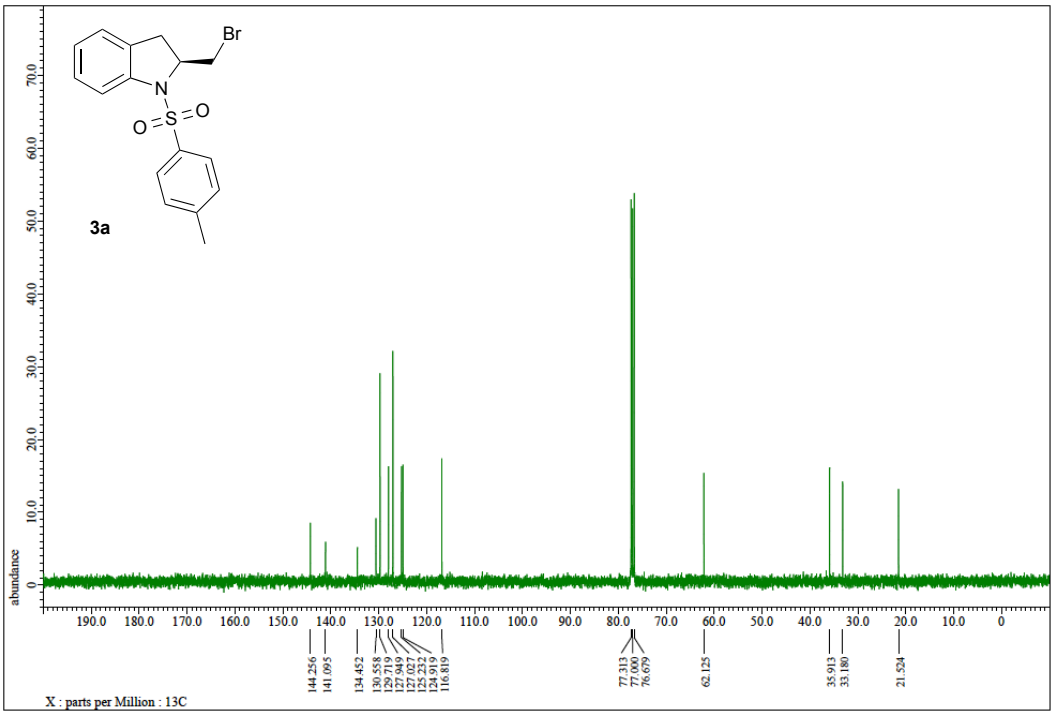
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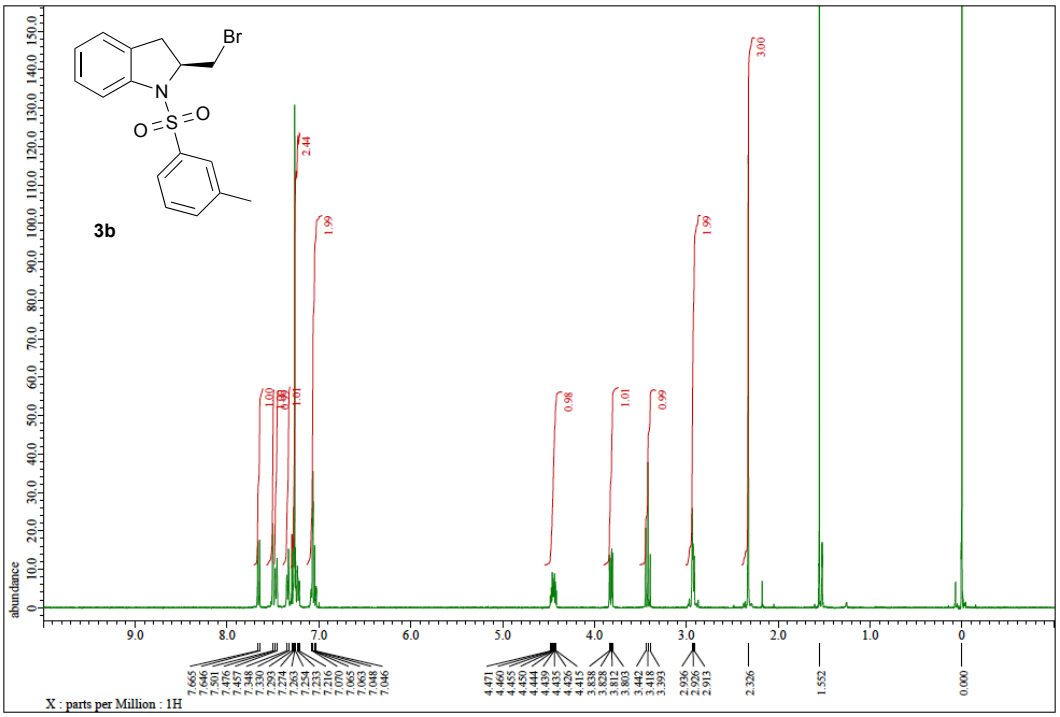
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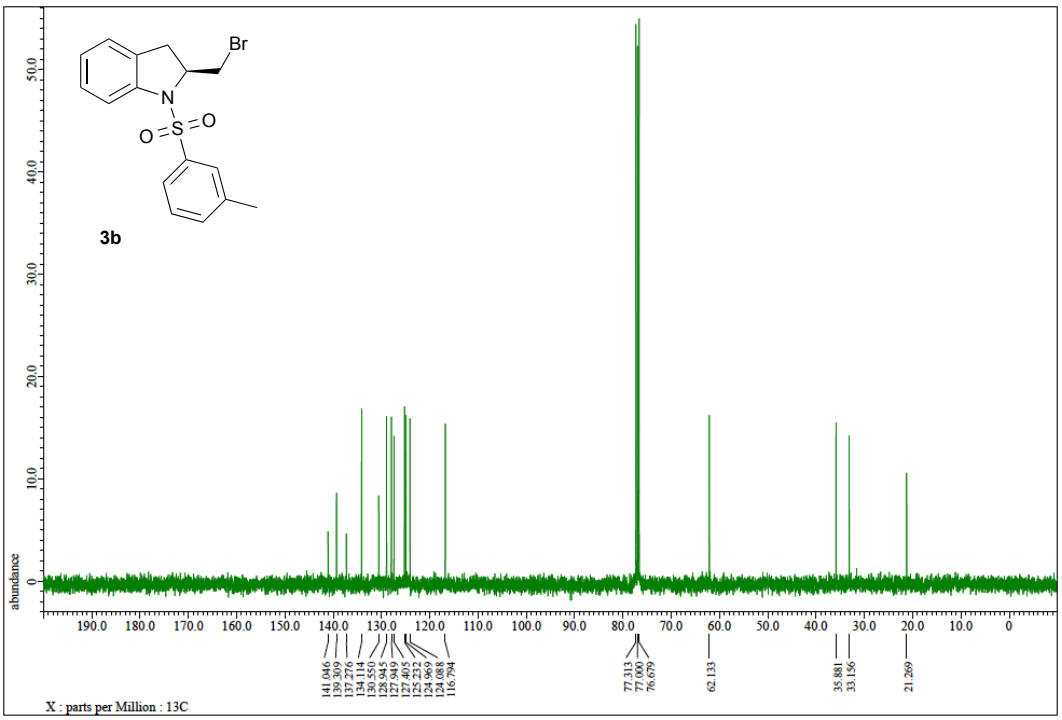
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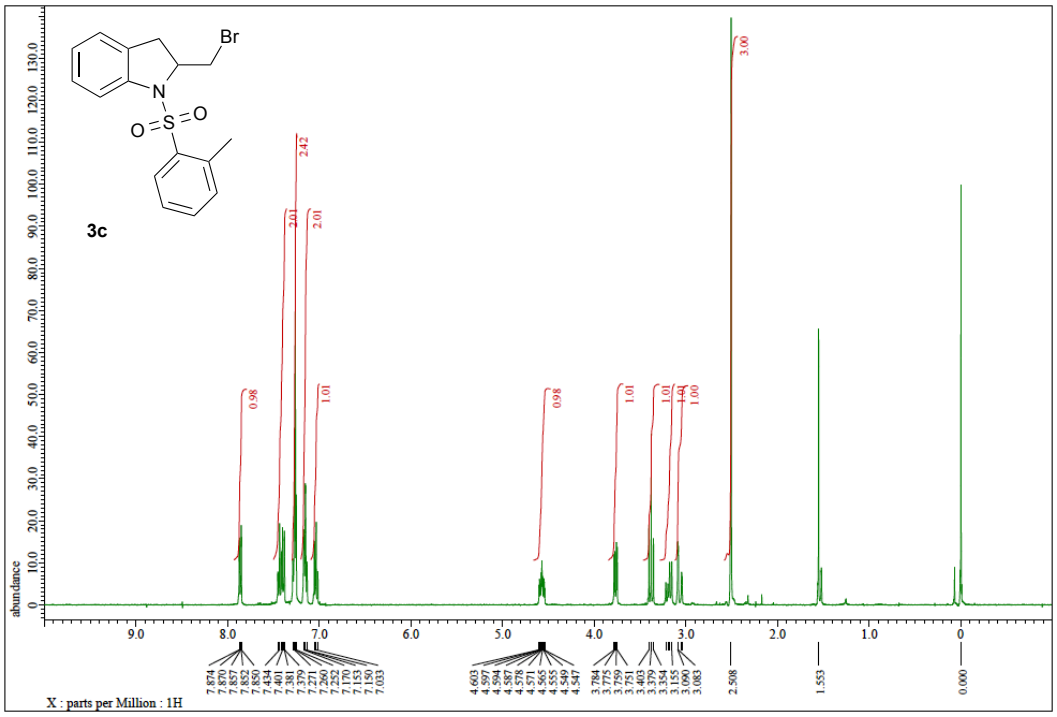
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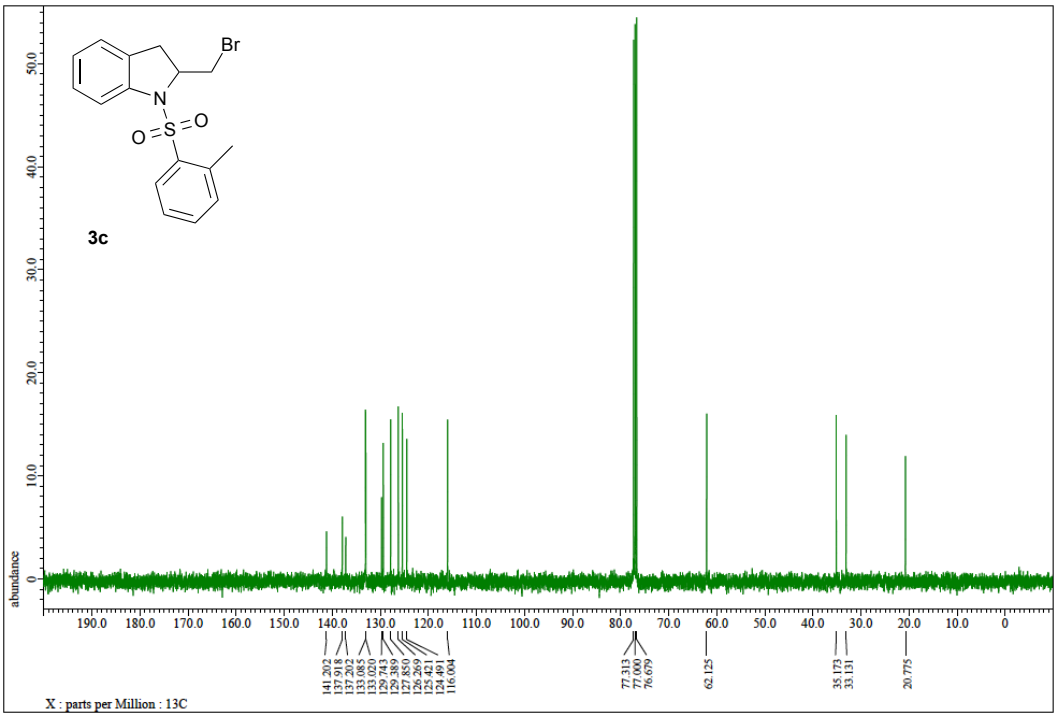
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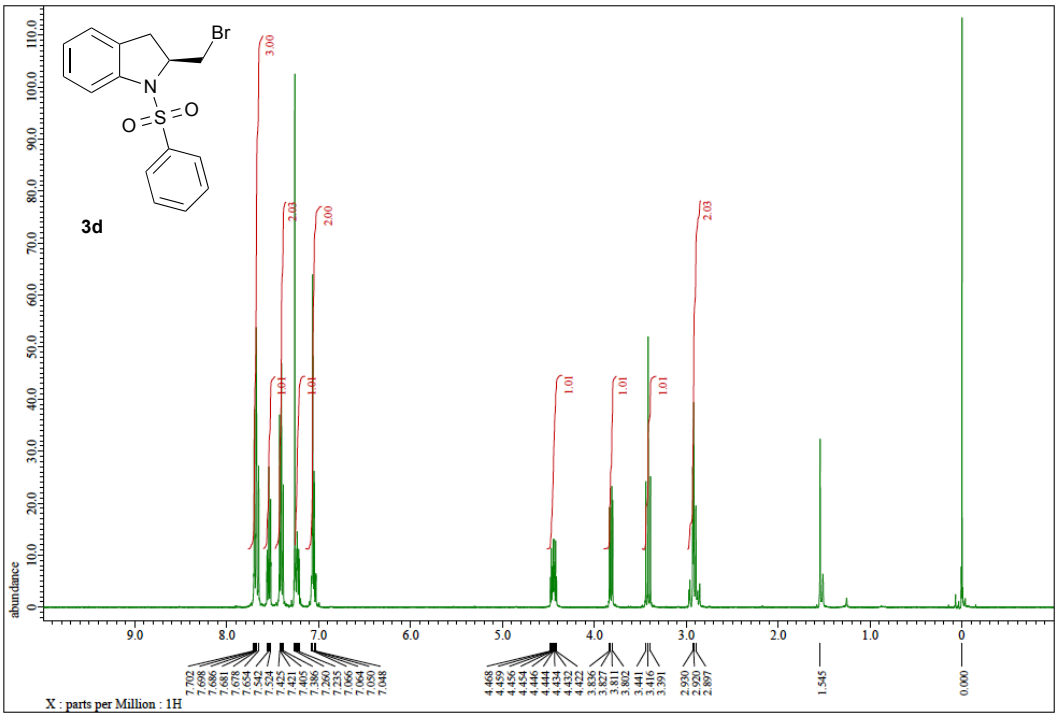
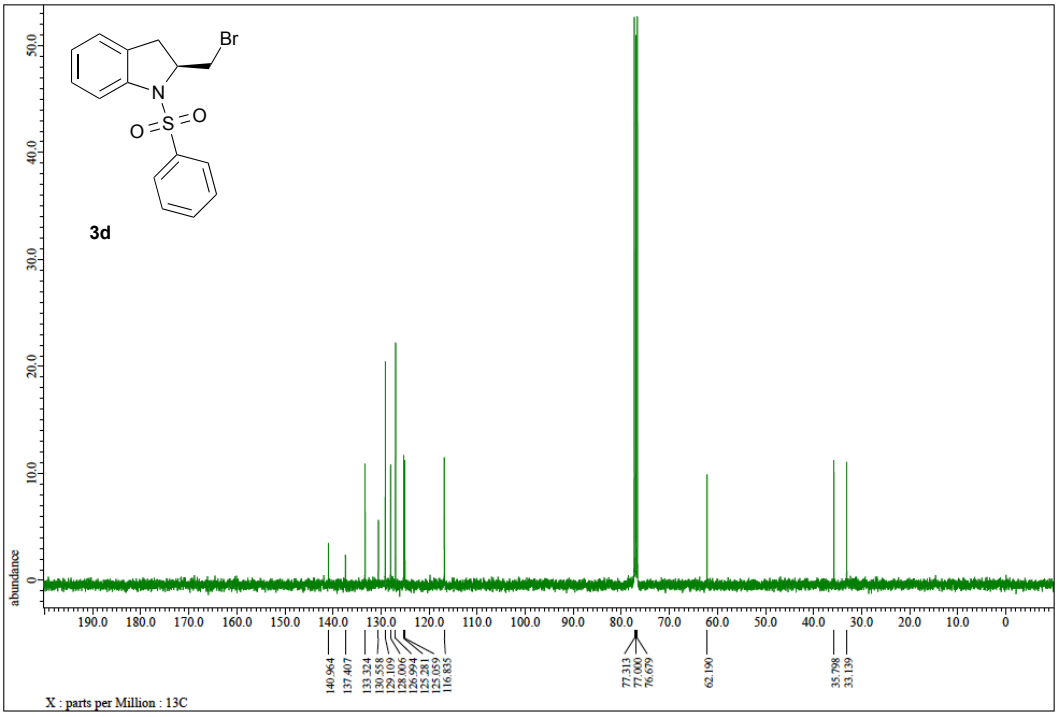
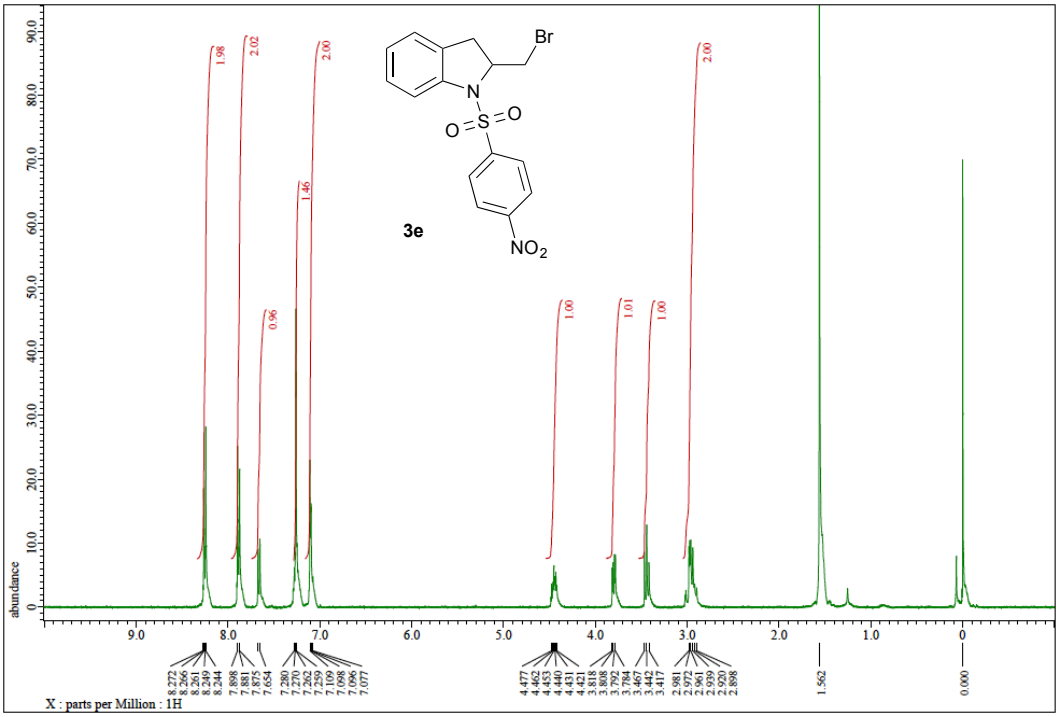
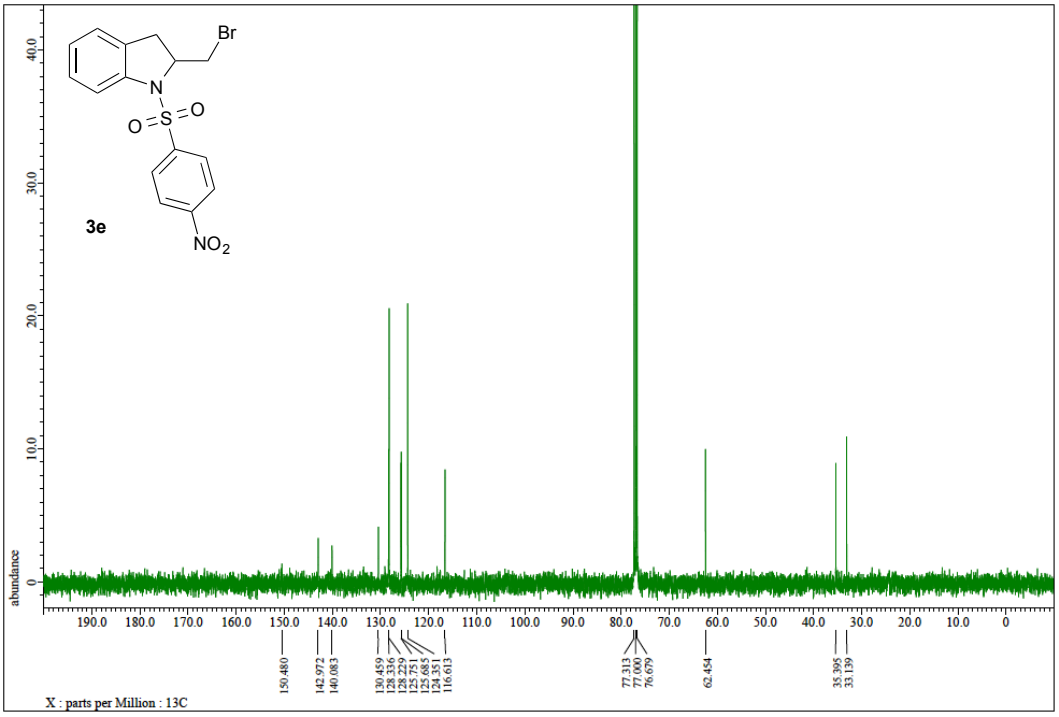
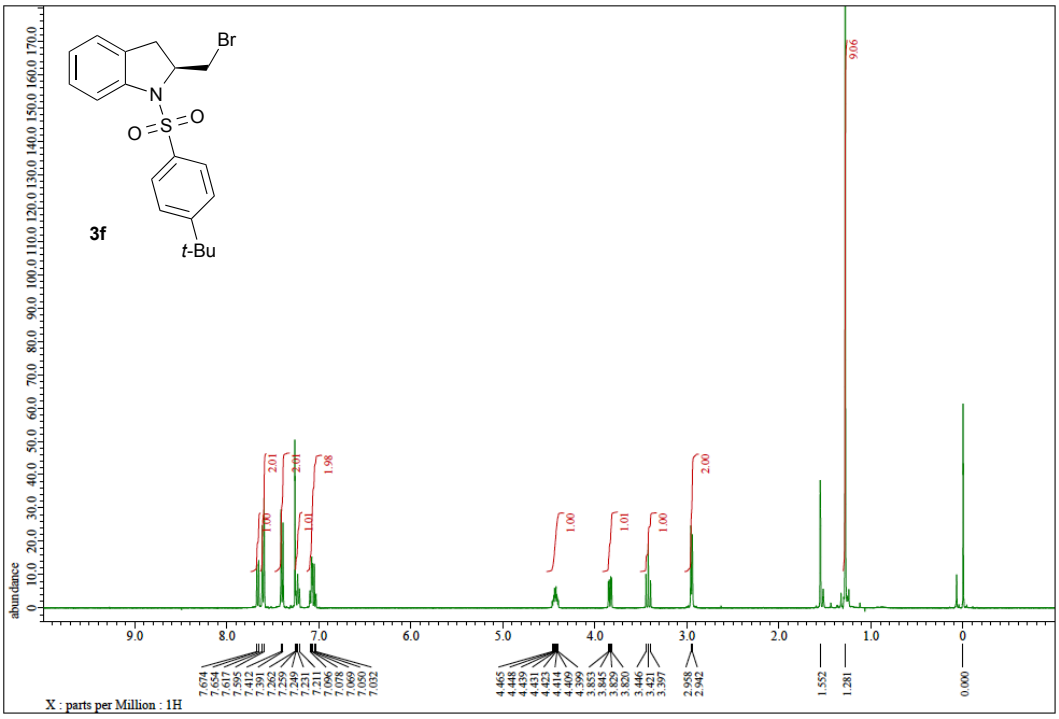
abundance
X : parts per Million : 13C

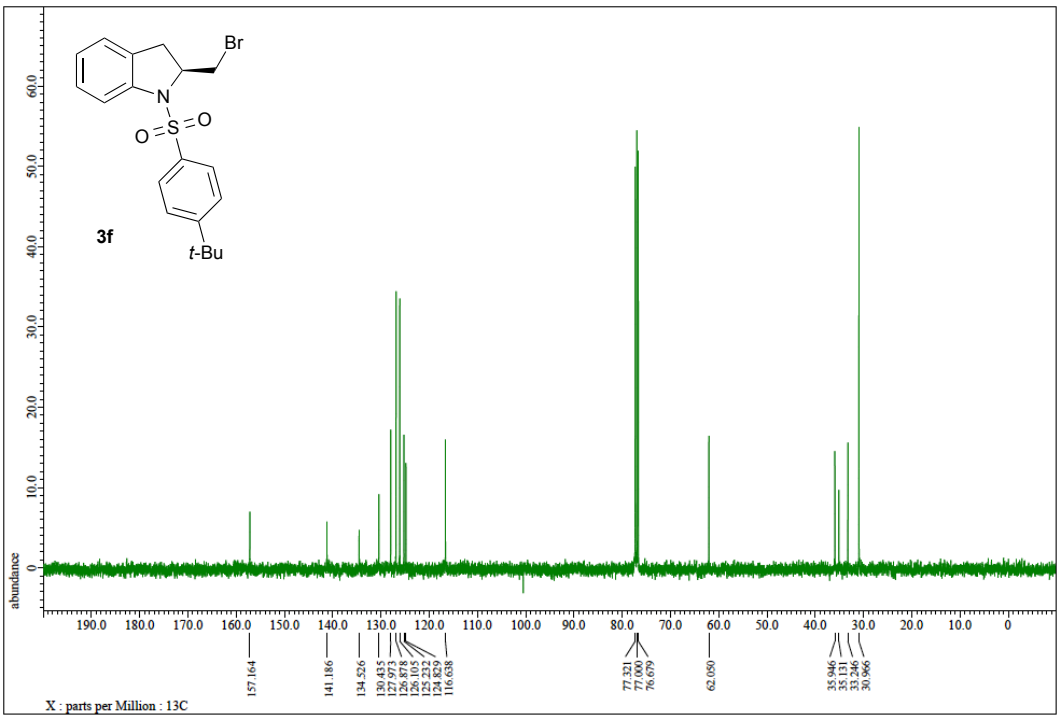

Br
N
O=S=O
3d
3.00
2.03
2.00
1.01
1.01
1.01
1.01
2.03
abundance
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.702
7.698
7.686
7.681
7.678
7.648
7.542
7.524
7.425
7.421
7.405
7.386
7.260
7.235
7.066
7.064
7.050
7.048
4.468
4.459
4.456
4.454
4.446
4.444
4.438
4.433
4.422
3.836
3.827
3.811
3.802
3.441
3.416
3.391
2.930
2.920
2.897
1.545
0.000
X : parts per Million : 1H

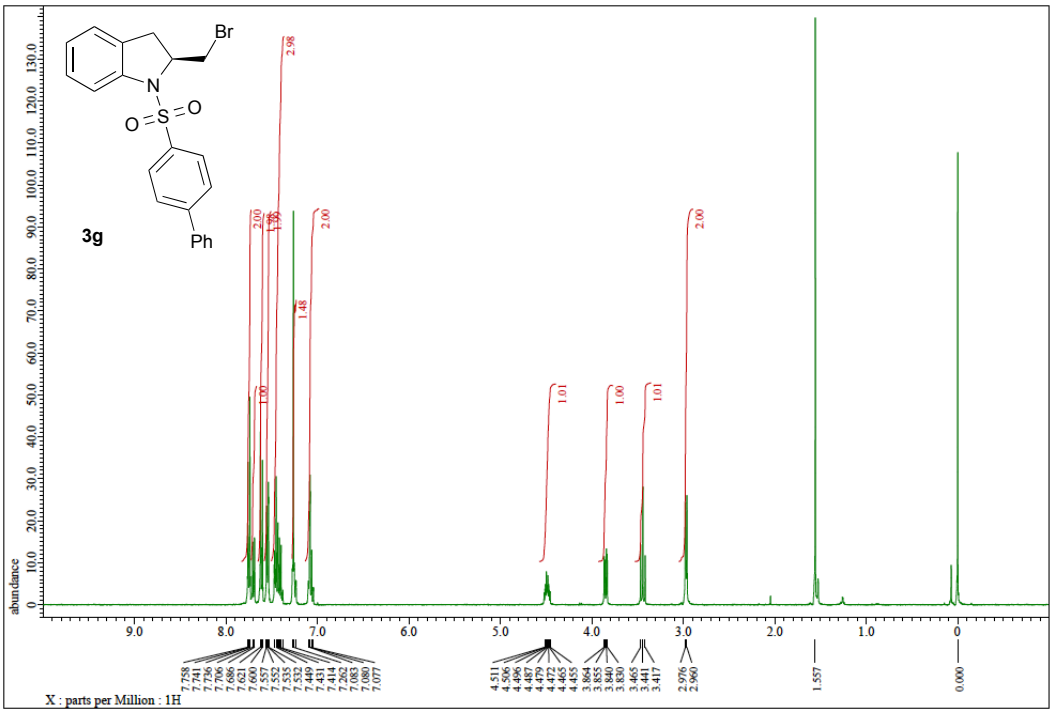

Br
N
O=S=O
3d
abundance
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
140.964
137.407
133.524
130.558
129.109
128.106
125.994
125.281
125.059
116.835
77.313
77.000
76.679
62.190
35.798
33.139
X : parts per Million : 13C

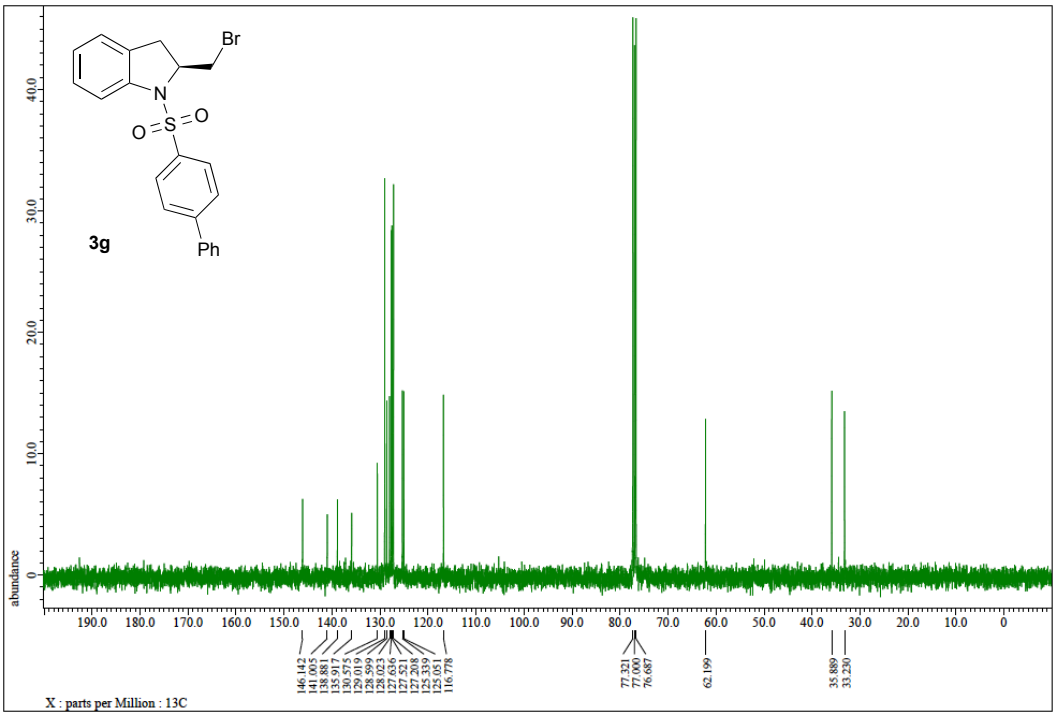

Br
N
O
S
O
3e
NO2
abundance
X : parts per Million : 1H

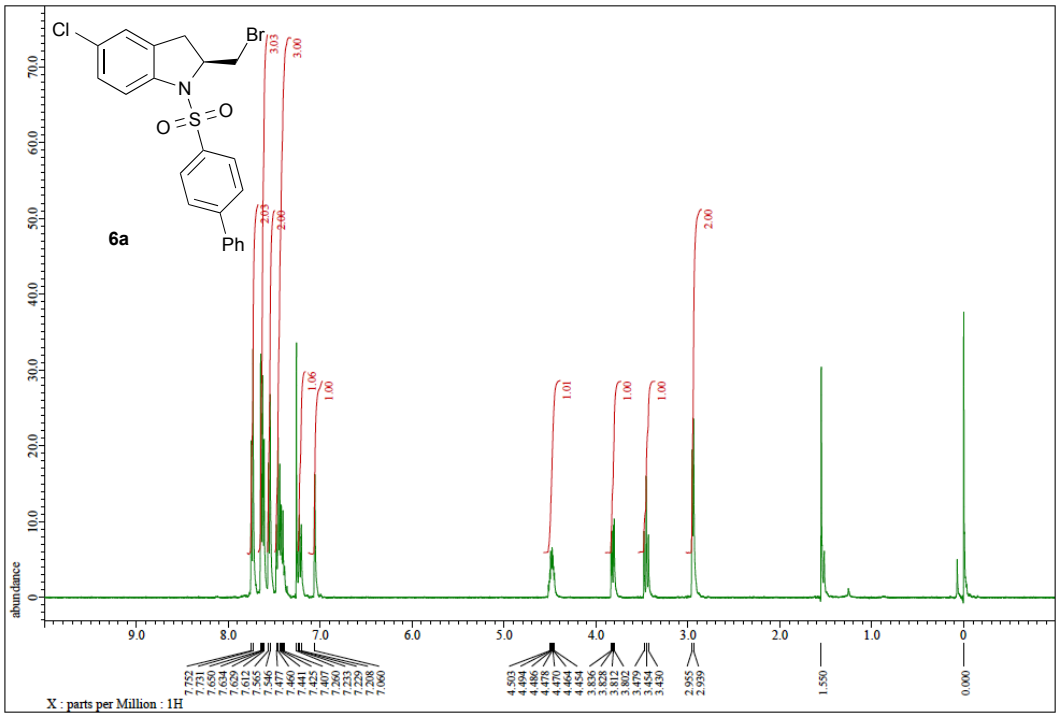

Br
N
O
S
O
3e
NO2
abundance
X : parts per Million : 13C

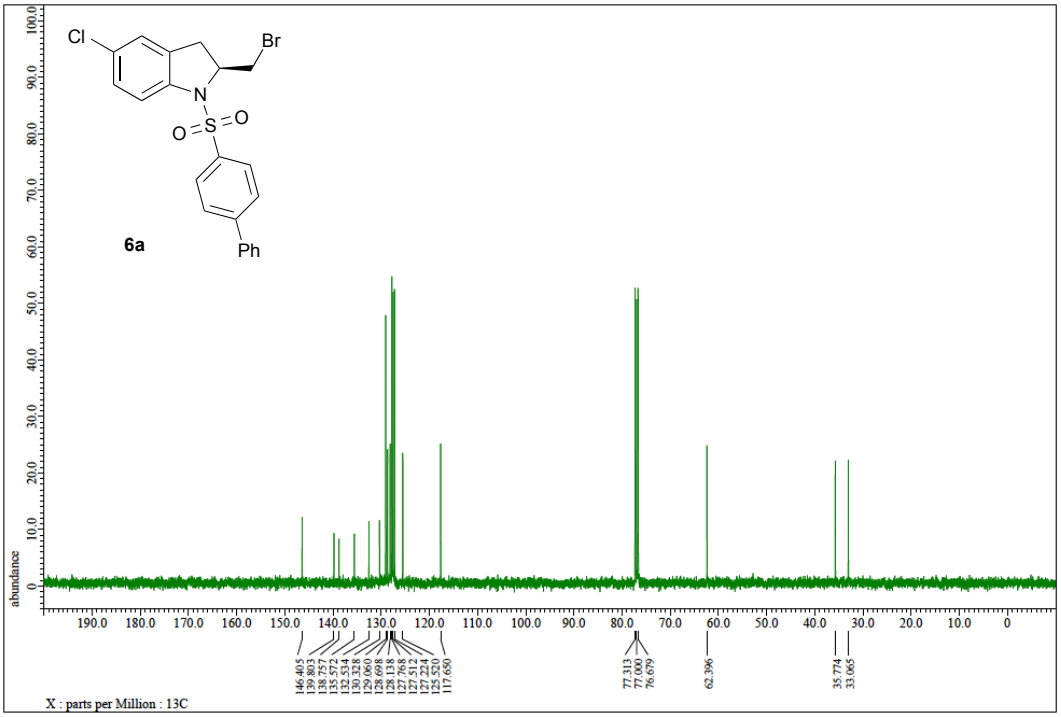

Br
N
O
S
O
3f
t-Bu
abundance
X : parts per Million : 1H

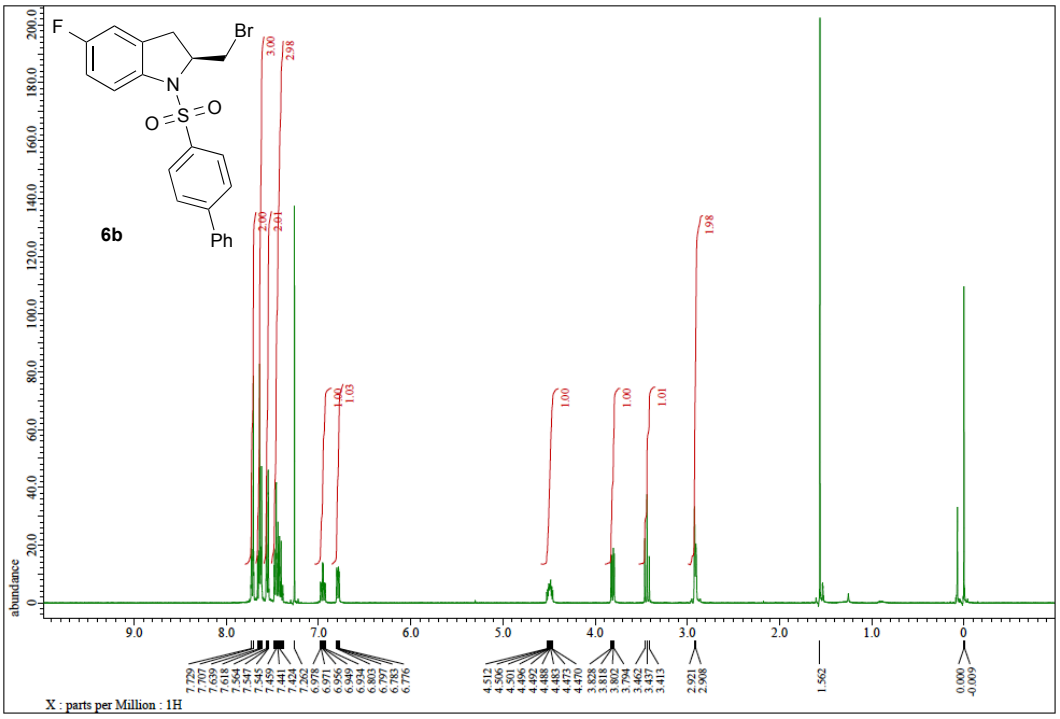

Br
N
O
S
O
3f
t-Bu
abundance
X : parts per Million : 13C

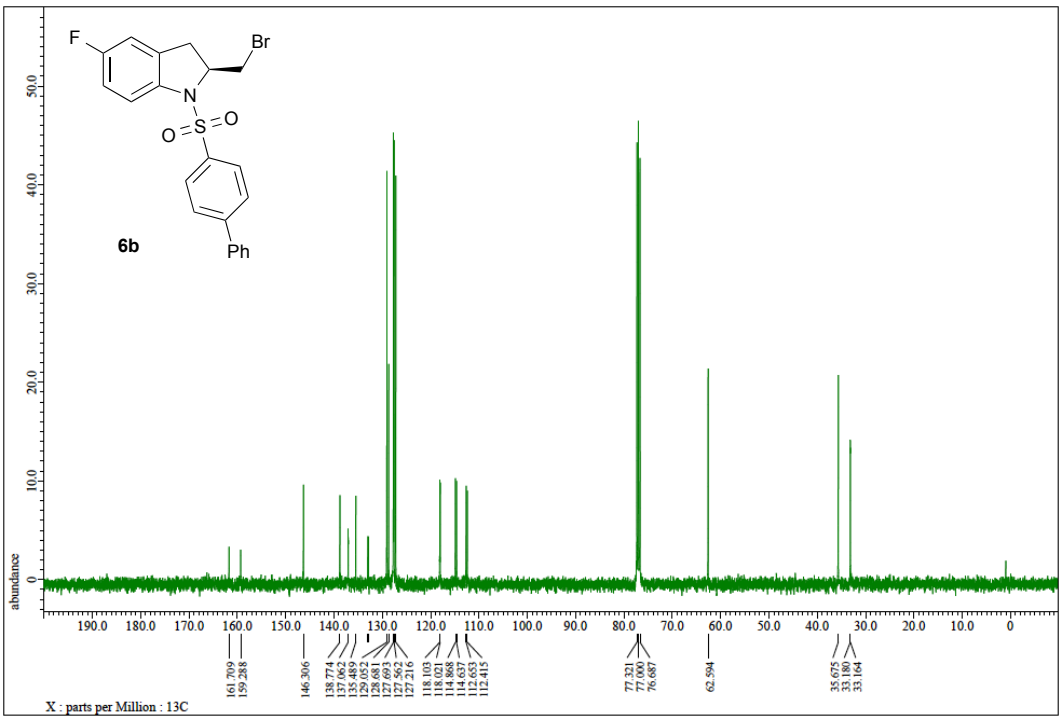

Br
N
O
S
O
3g
Ph
abundance
X : parts per Million : 1H

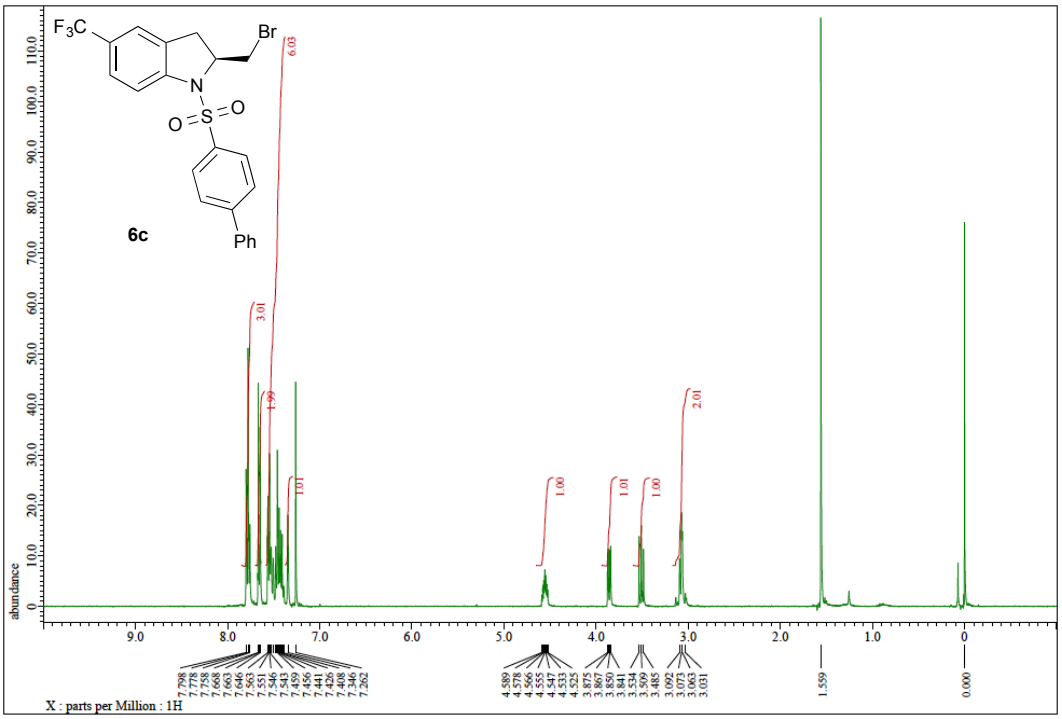

Br
N
O
S
O
3g
Ph
abundance
X : parts per Million : 13C

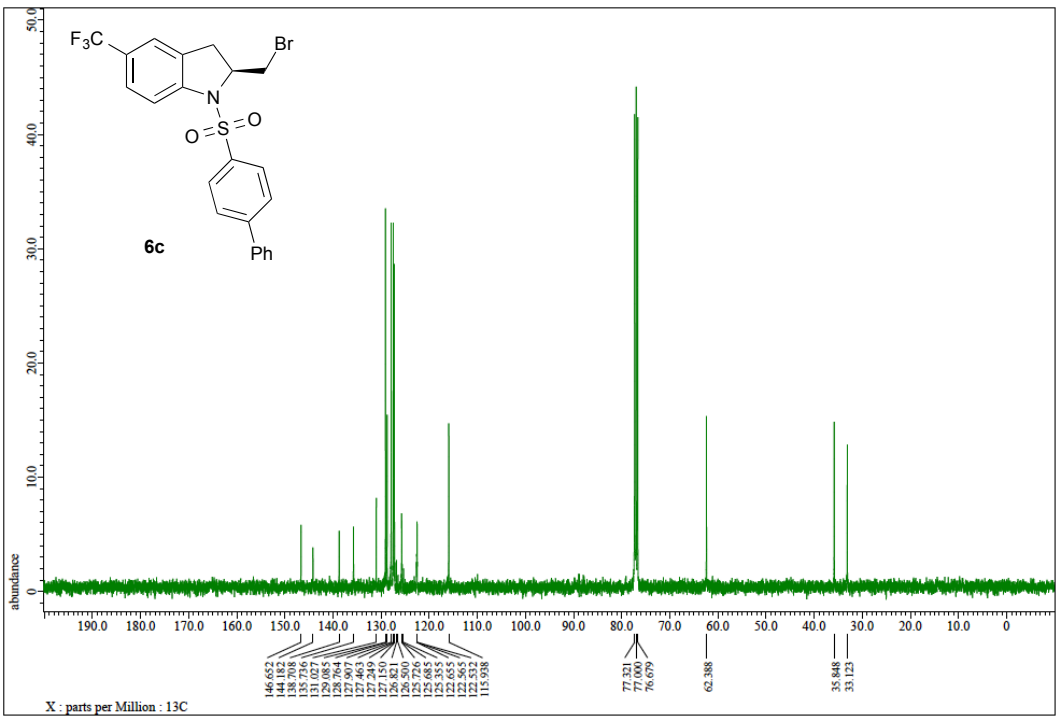

Cl
Br
N
O
S
O
6a
Ph
abundance
X : parts per Million : 1H

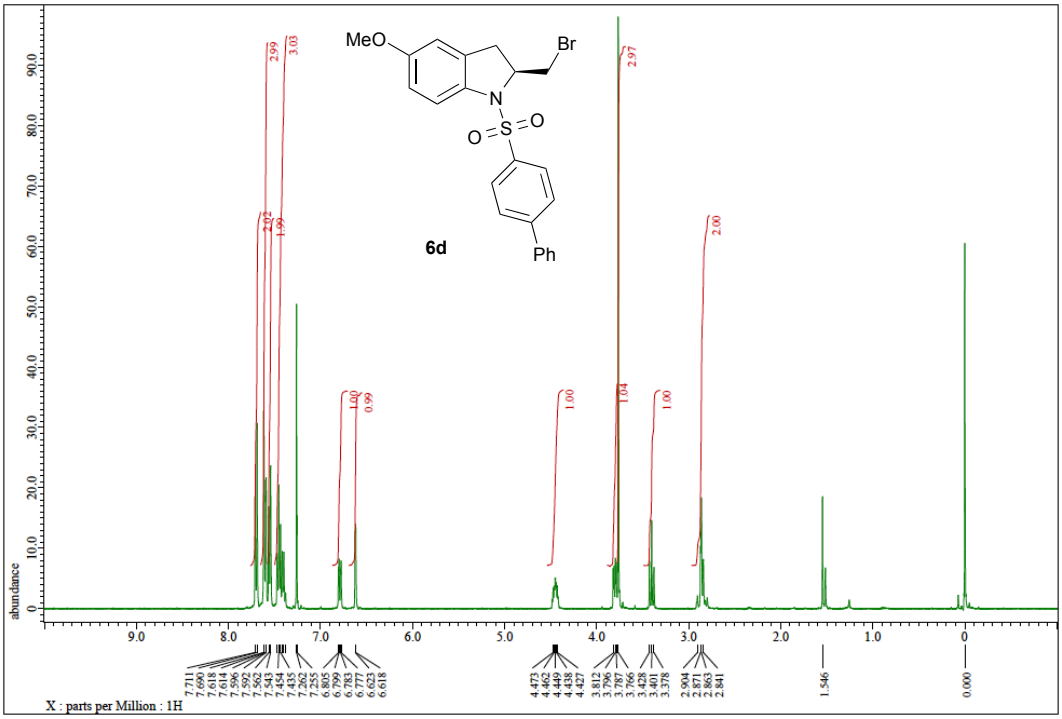

Cl
Br
N
O
S
O
6a
Ph
abundance
X : parts per Million : 13C

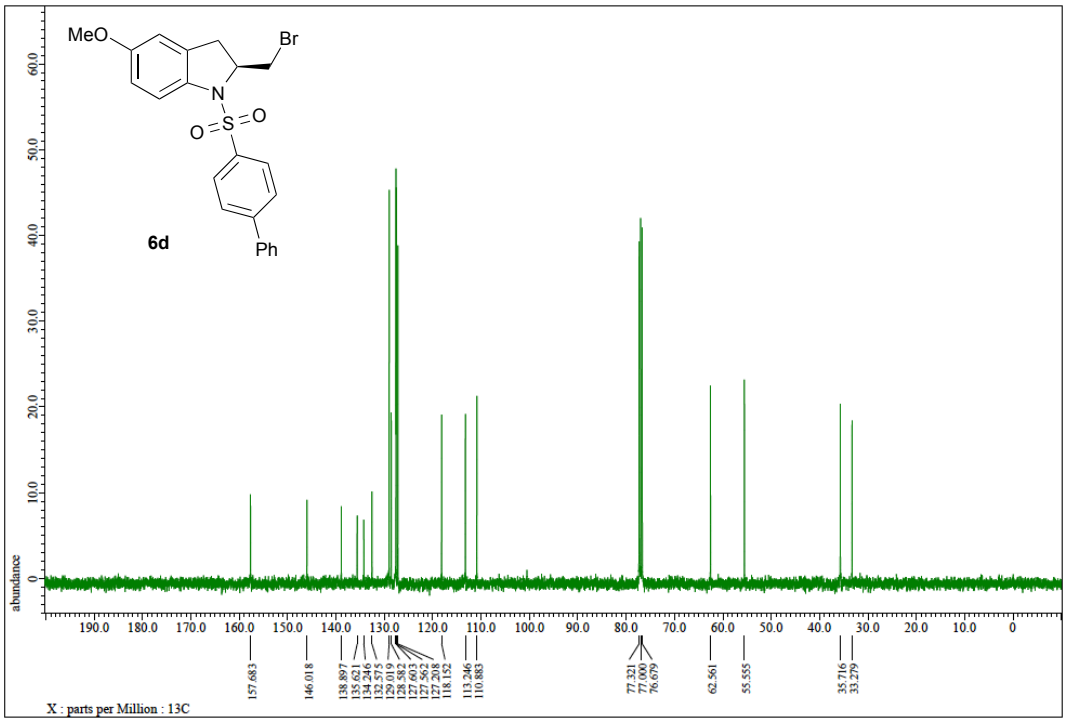

F
Br
N
O
S
O
Ph
6b
abundance
X : parts per Million : 1H

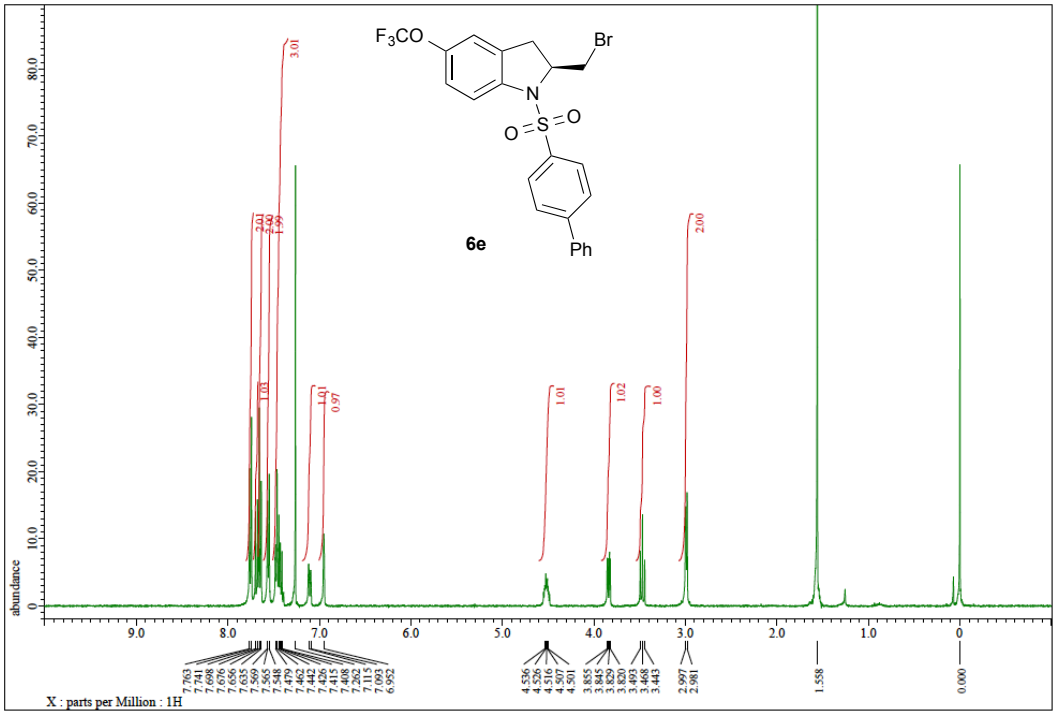

F
Br
N
O
S
O
Ph
6b
abundance
X : parts per Million : 13C

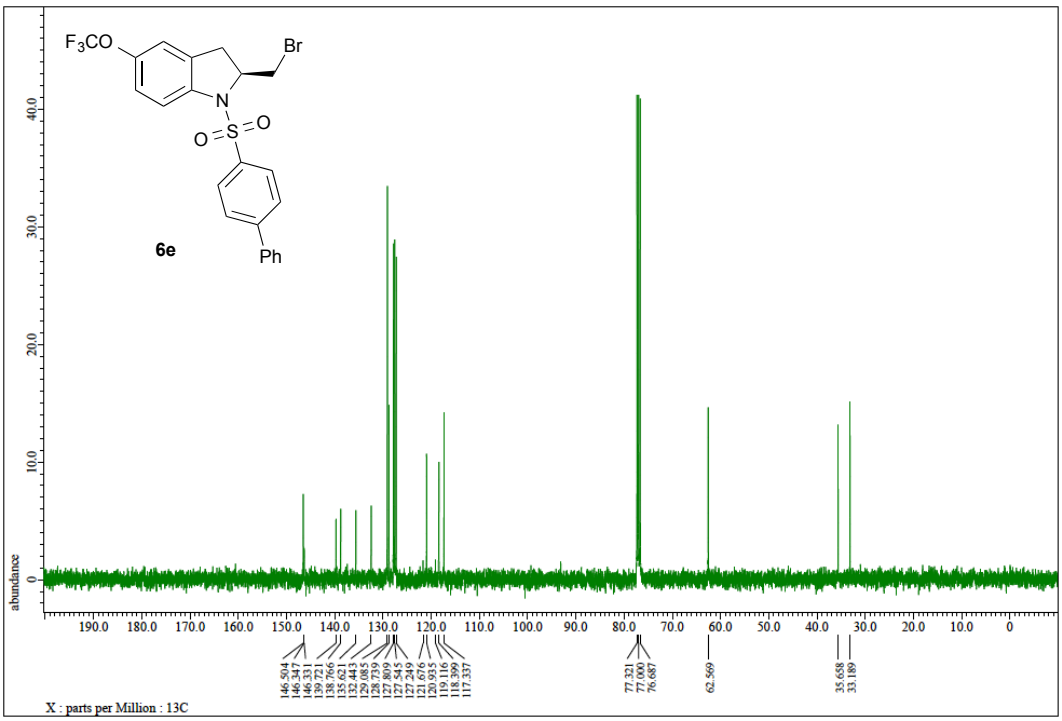

F3C
Br
N
O
S
O
6c
Ph
6.03
3.01
1.99
1.01
1.00
1.01
1.00
2.01
abundance
X : parts per Million : 1H

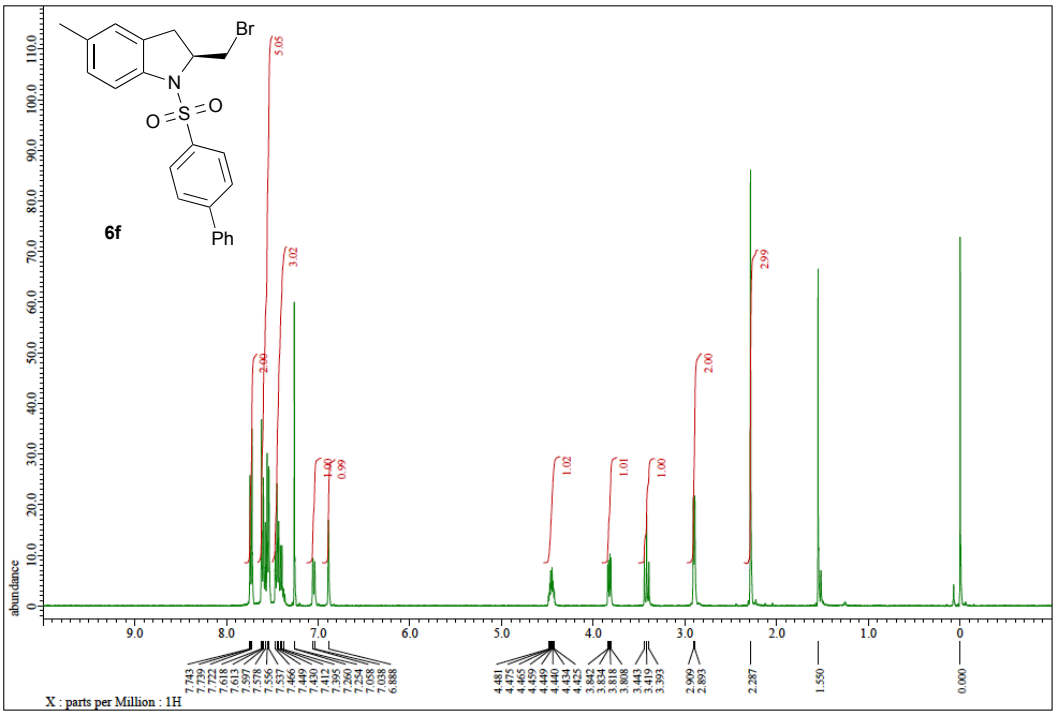

F3C
Br
N
O
S
O
6c
Ph
abundance
X : parts per Million : 13C

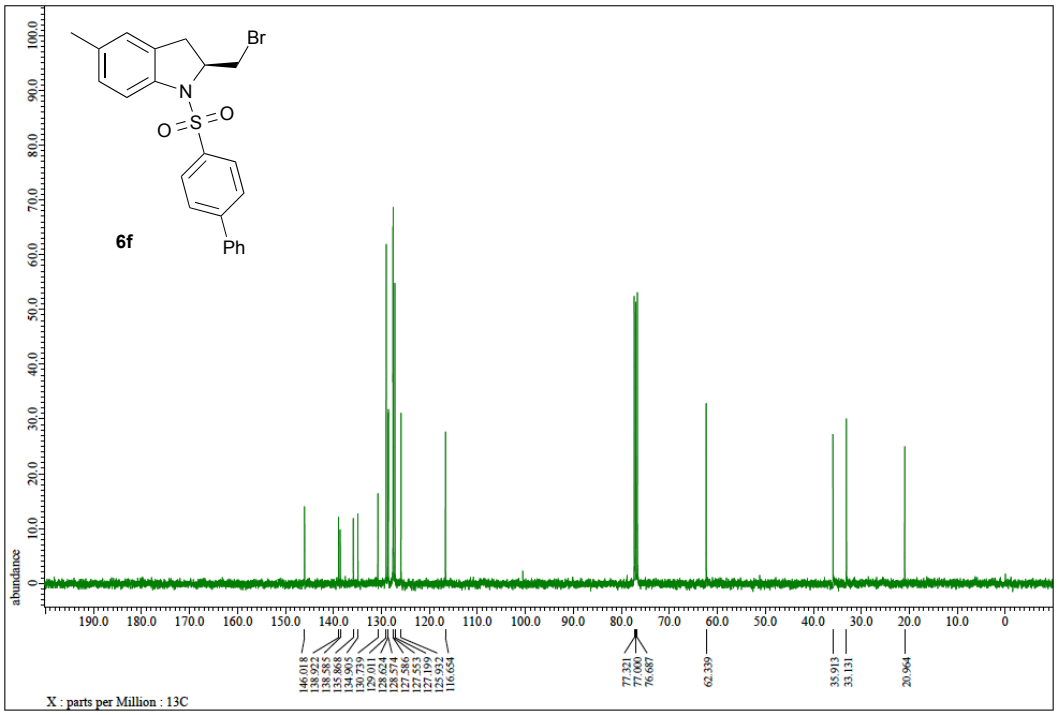

MeO
Br
N
O=S=O
Ph
6d
abundance
X : parts per Million : 1H

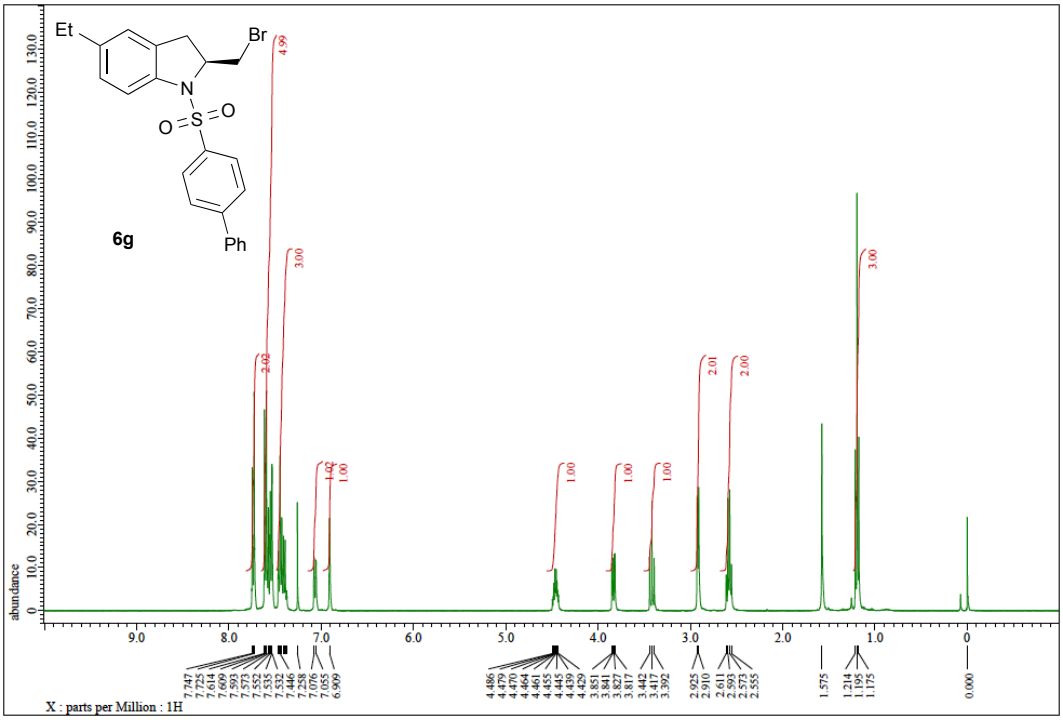

MeO
Br
N
O=S=O
Ph
6d
abundance
X : parts per Million : 13C

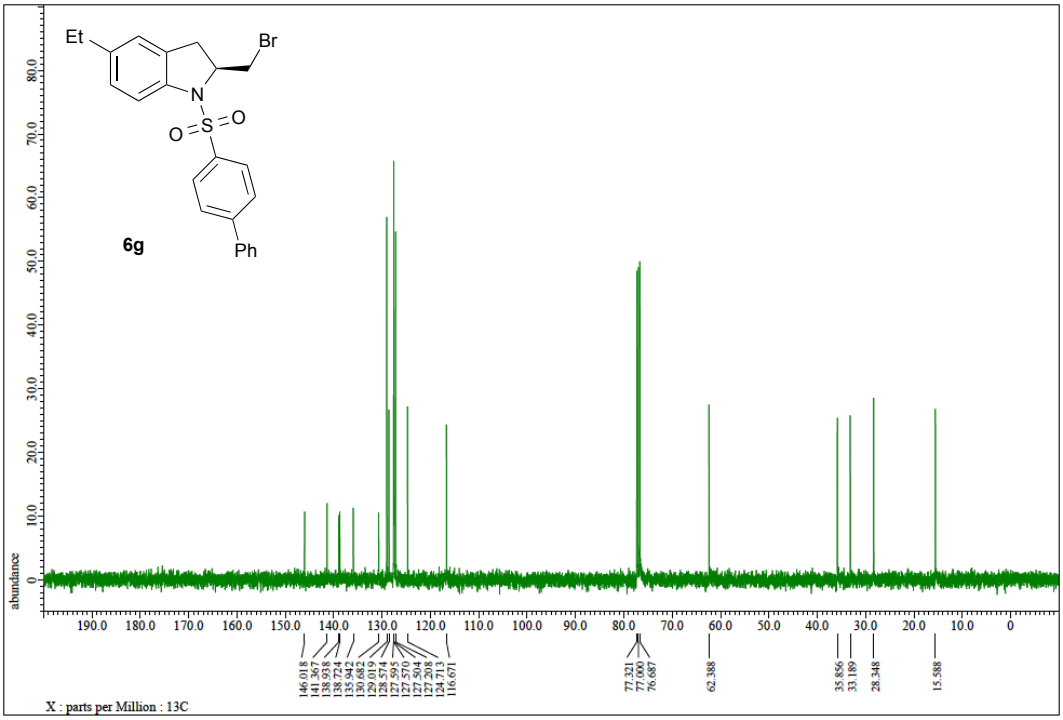

F3CO
Br
N
O=S=O
Ph
6e
abundance
X : parts per Million : 1H

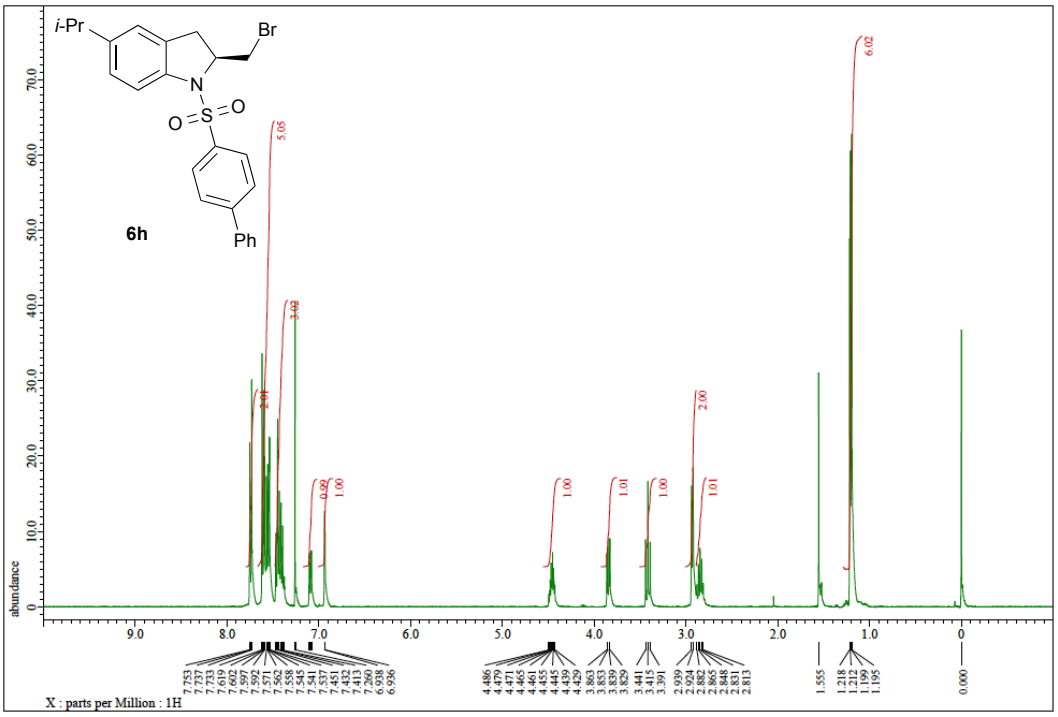

F3CO
Br
N
O=S=O
Ph
6e
abundance
X : parts per Million : 13C

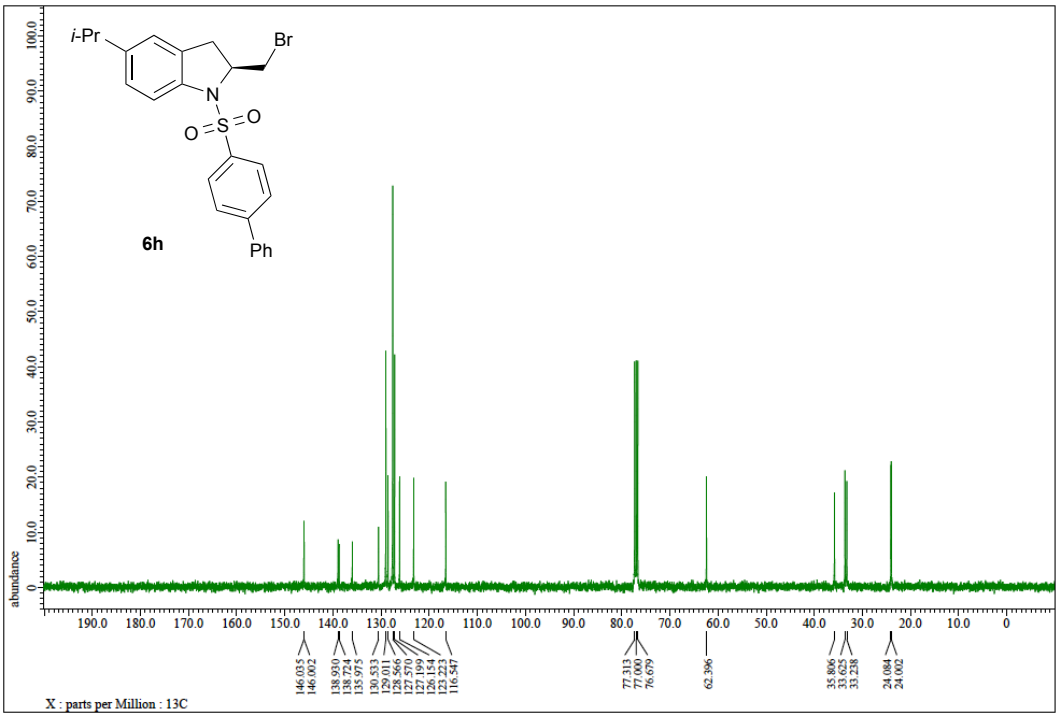

Br
N
O
S
O
O
Ph
6f
5.05
3.02
2.00
2.99
2.00
1.02
1.01
1.00
1.00
0.99
abundance
X : parts per Million : 1H

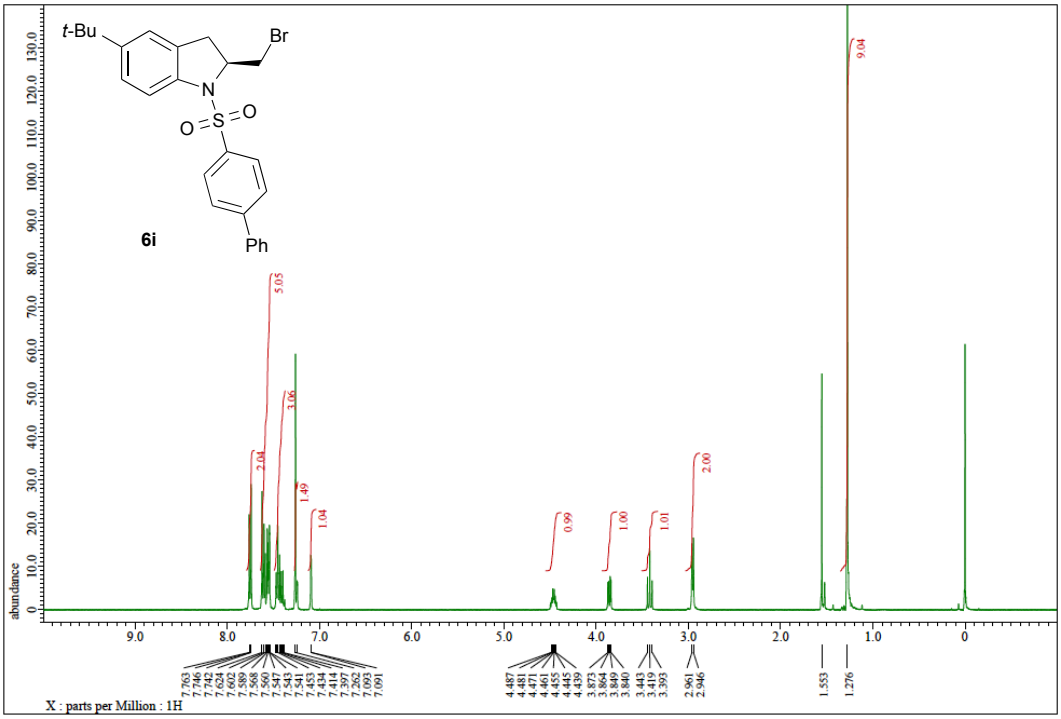

Br
N
O
S
O
O
Ph
6f
abundance
X : parts per Million : 13C

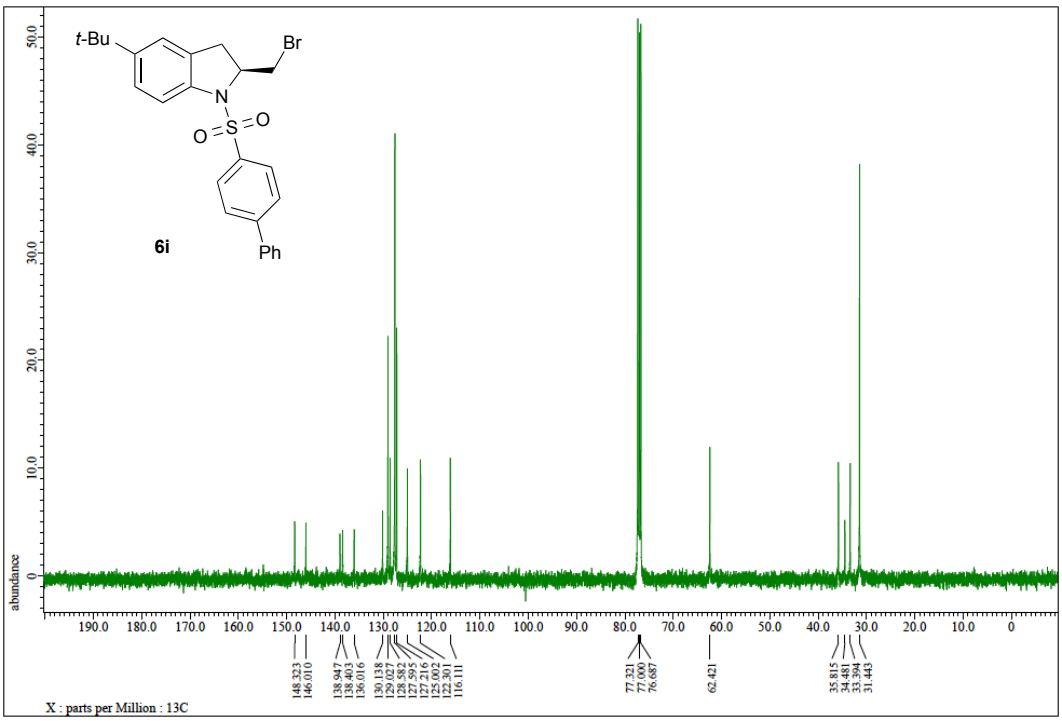

Et
Br
N
O
S
O
O
Ph
6g
abundance
X : parts per Million : 1H

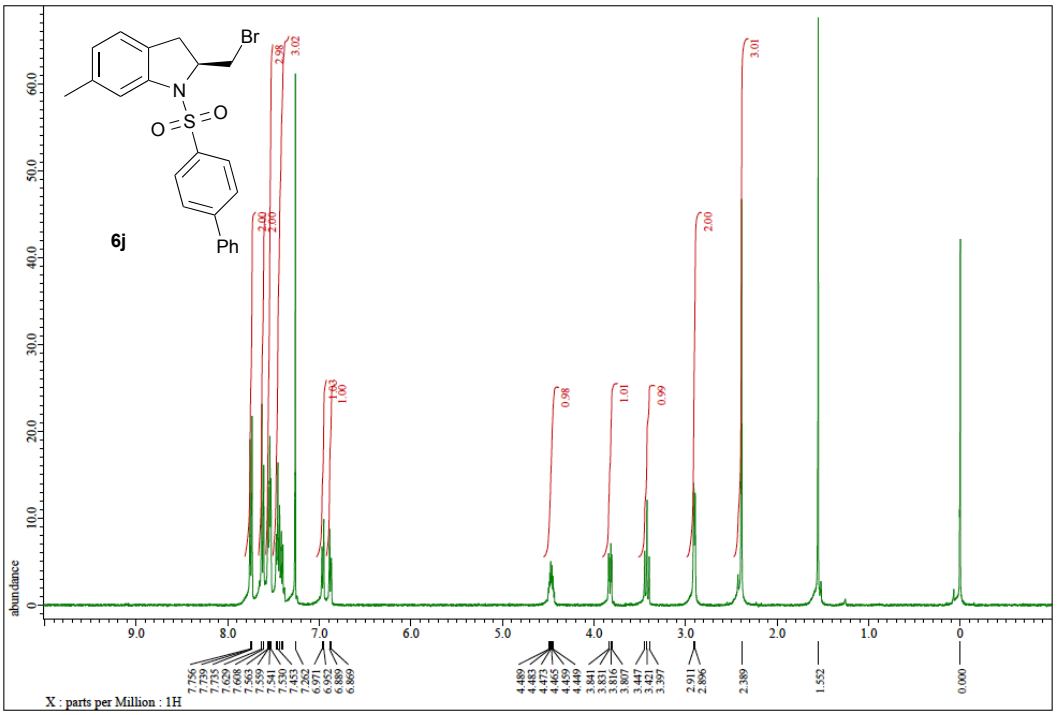

Et
Br
N
O
S
O
O
Ph
6g
abundance
X : parts per Million : 13C

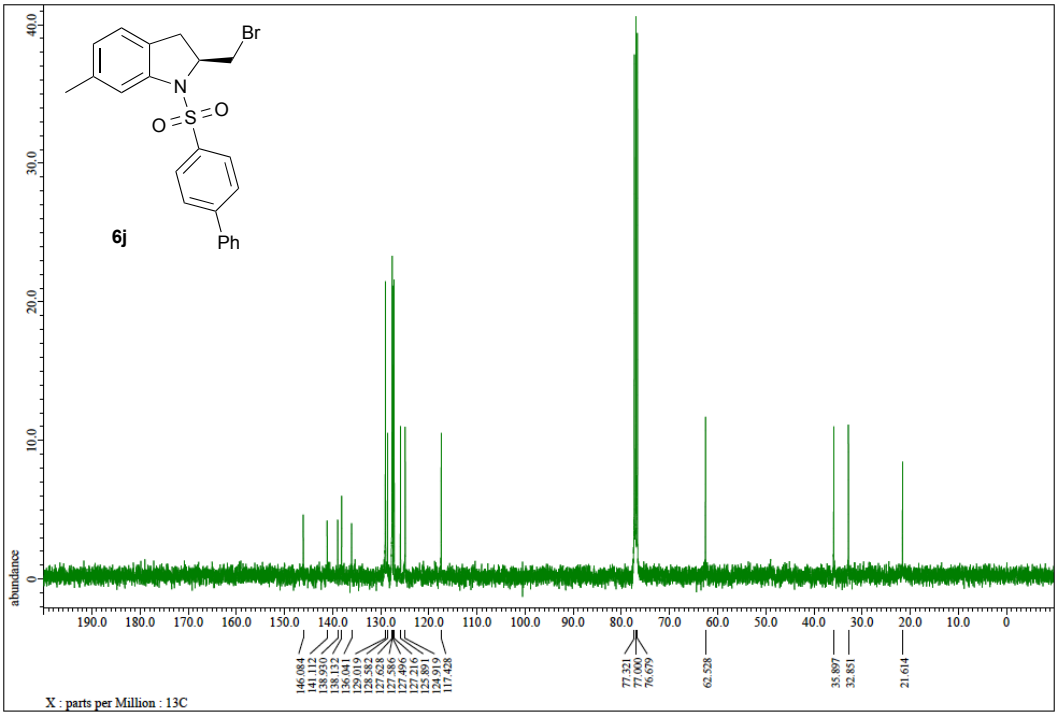

i-Pr
Br
N
O
S
O
O
Ph
6h
abundance
X : parts per Million : 1H

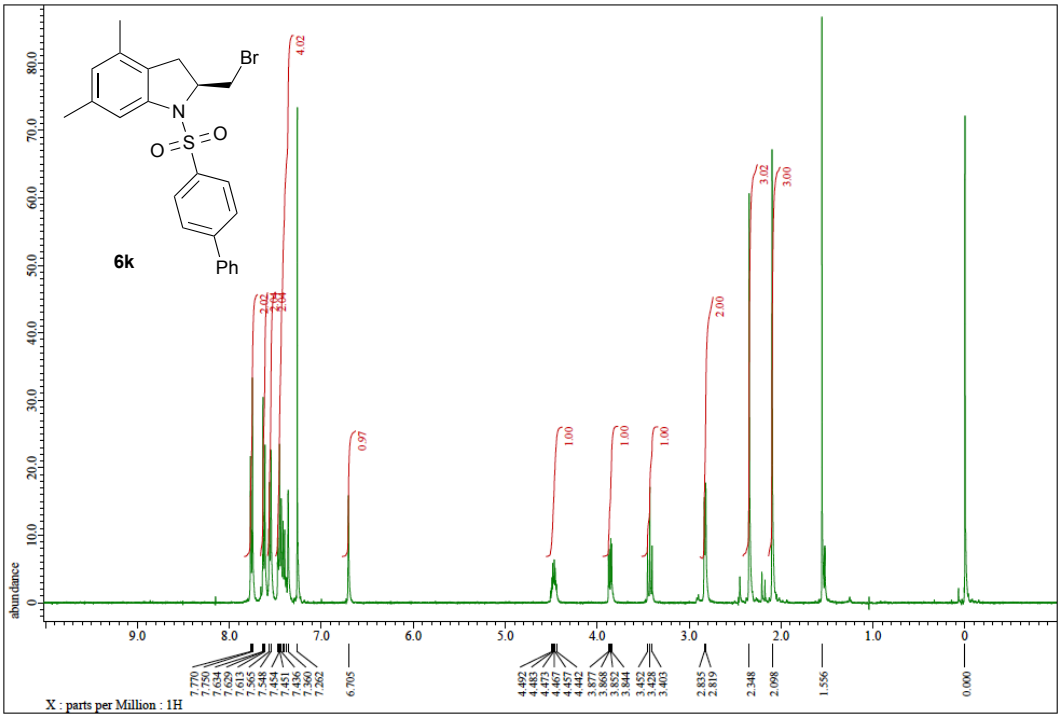

i-Pr
Br
N
O
S
O
O
Ph
6h
abundance
X : parts per Million : 13C

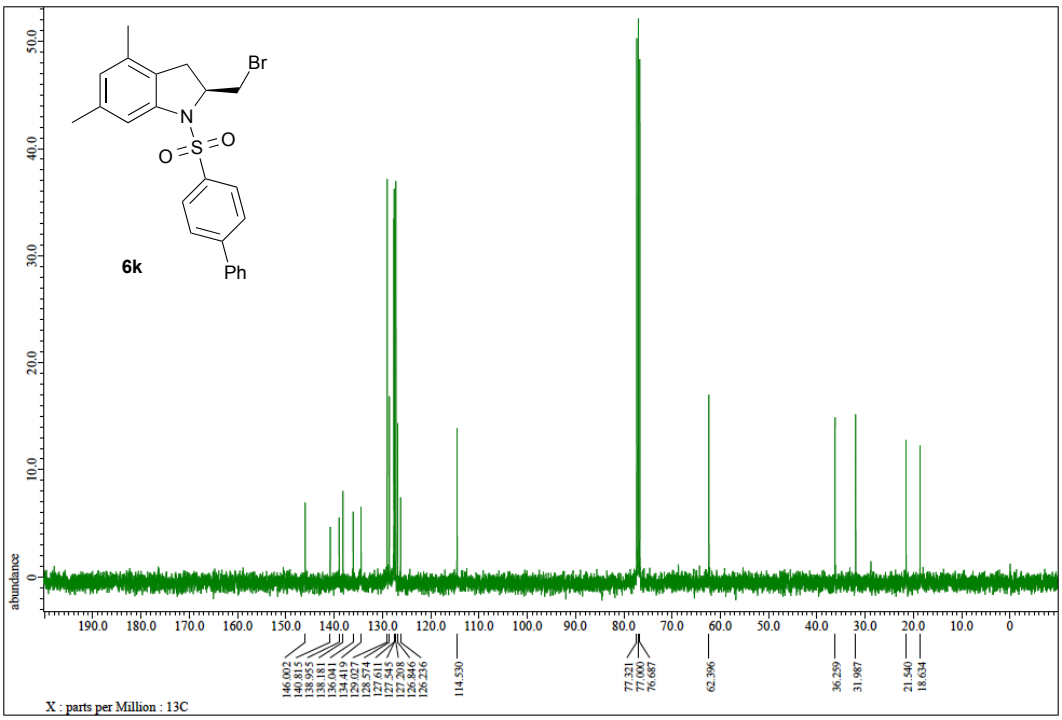

t-Bu
Br
N
O=S=O
Ph
6i
abundance
X : parts per Million : 1H

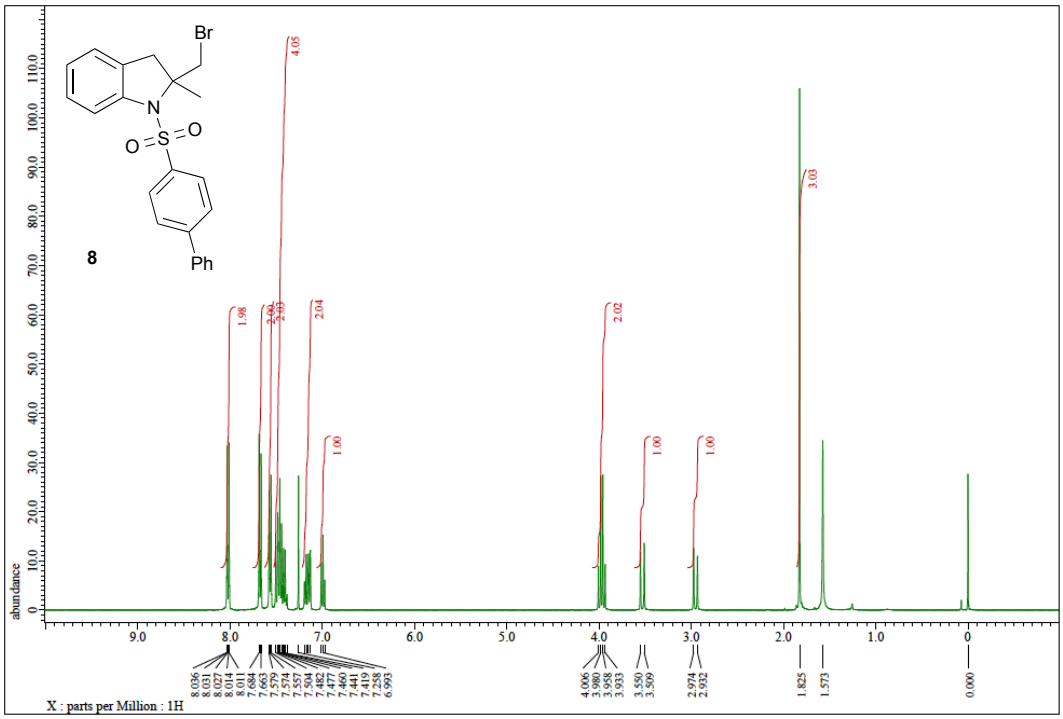

t-Bu
Br
N
O=S=O
Ph
6i
abundance
X : parts per Million : 13C

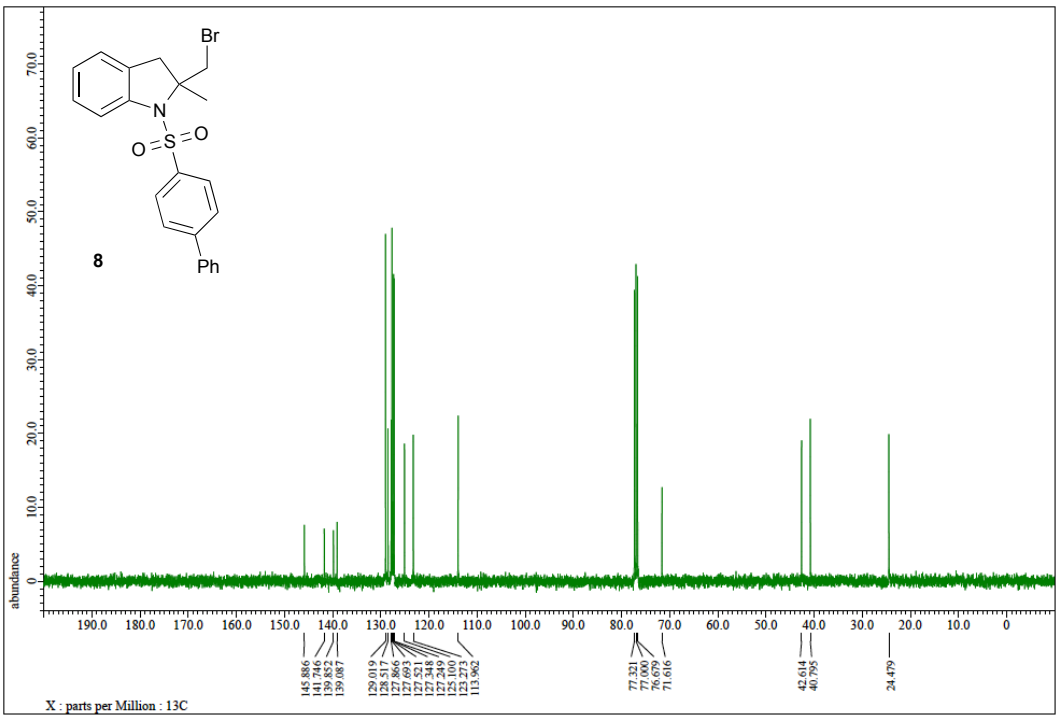

Br
N
O
S
O
O
Ph
6j
abundance
X : parts per Million : 1H


Br
N
O
S
O
O
Ph
6j
abundance
X : parts per Million : 13C

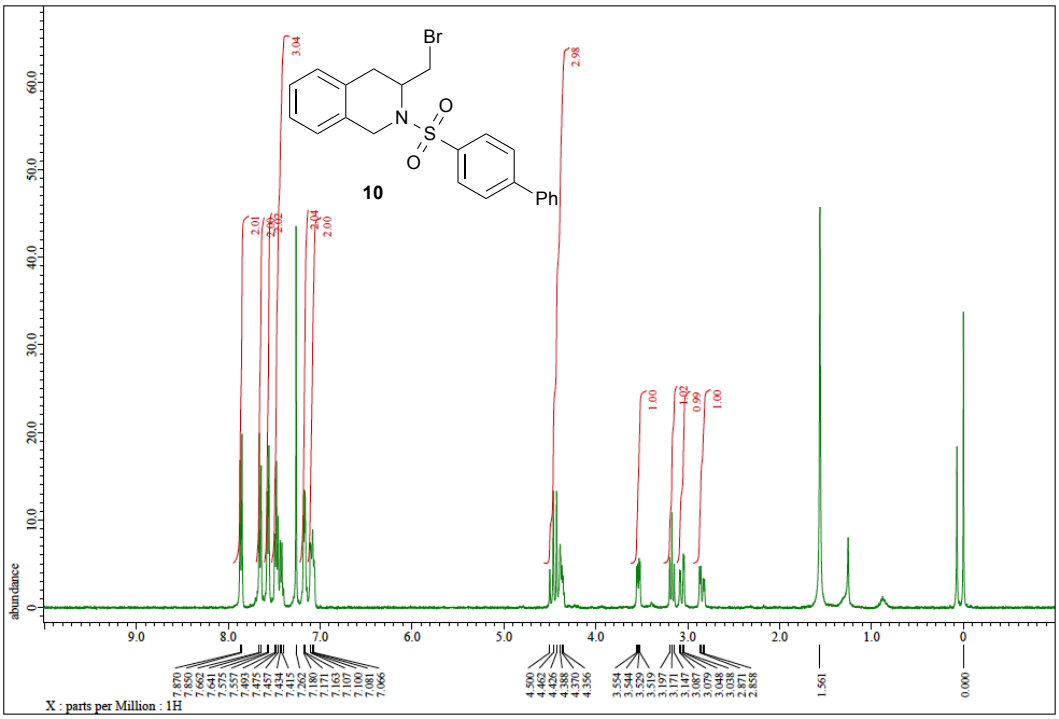

Br
N
O=S=O
Ph
6k
4.02
2.00
2.00
2.00
2.00
0.97
1.00
1.00
1.00
2.00
3.02
3.00
abundance
X : parts per Million : 1H

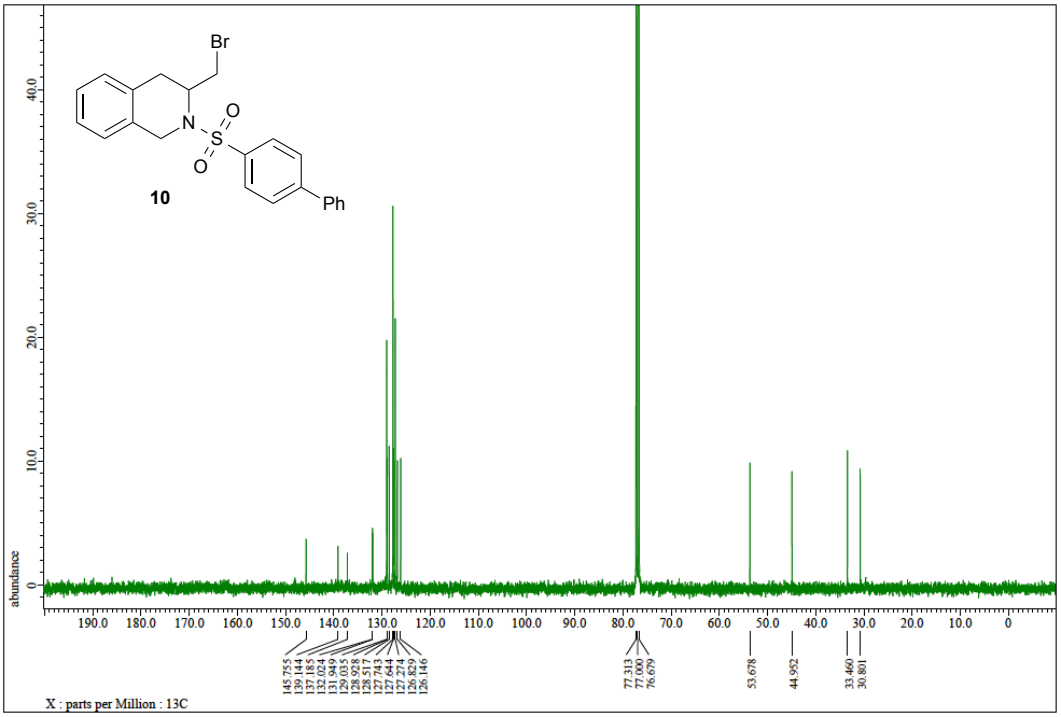

Br
N
O=S=O
Ph
6k
abundance
X : parts per Million : 13C

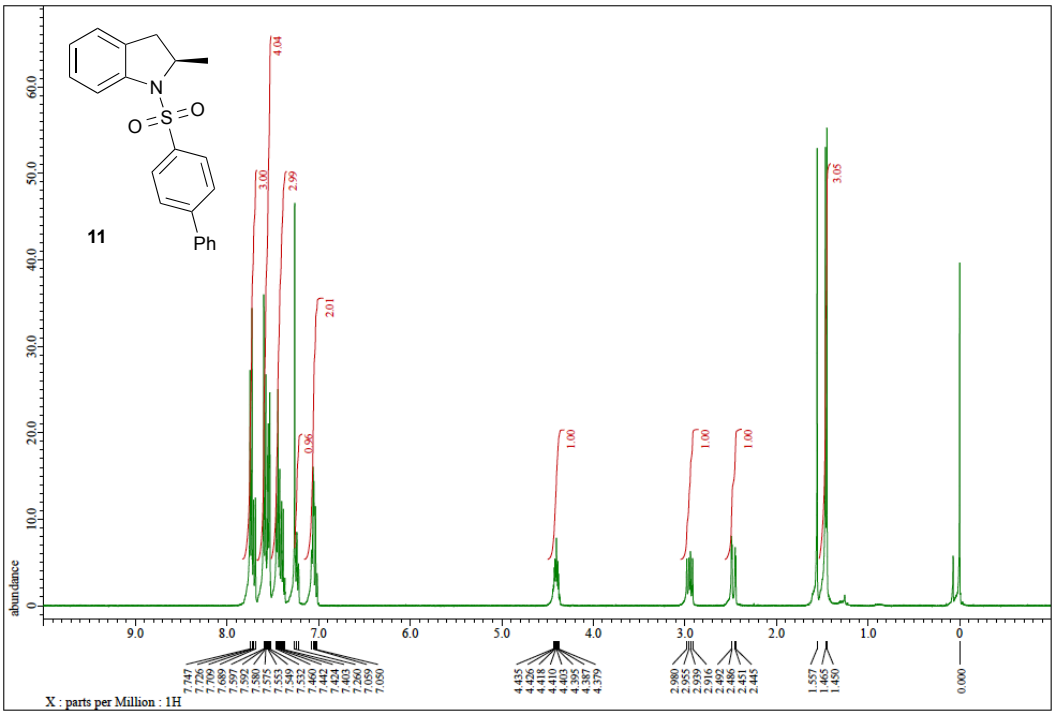

Br
N
O
S
O
Ph
8
abundance
X : parts per Million : 1H

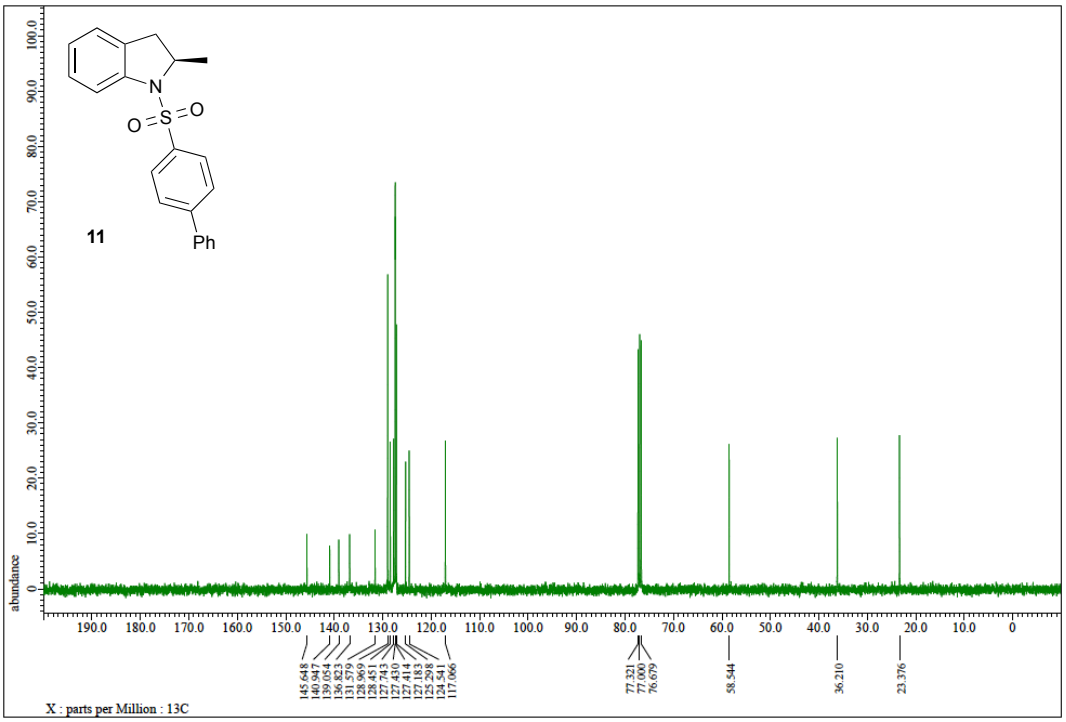

Br
N
O
S
O
Ph
8
abundance
X : parts per Million : 13C

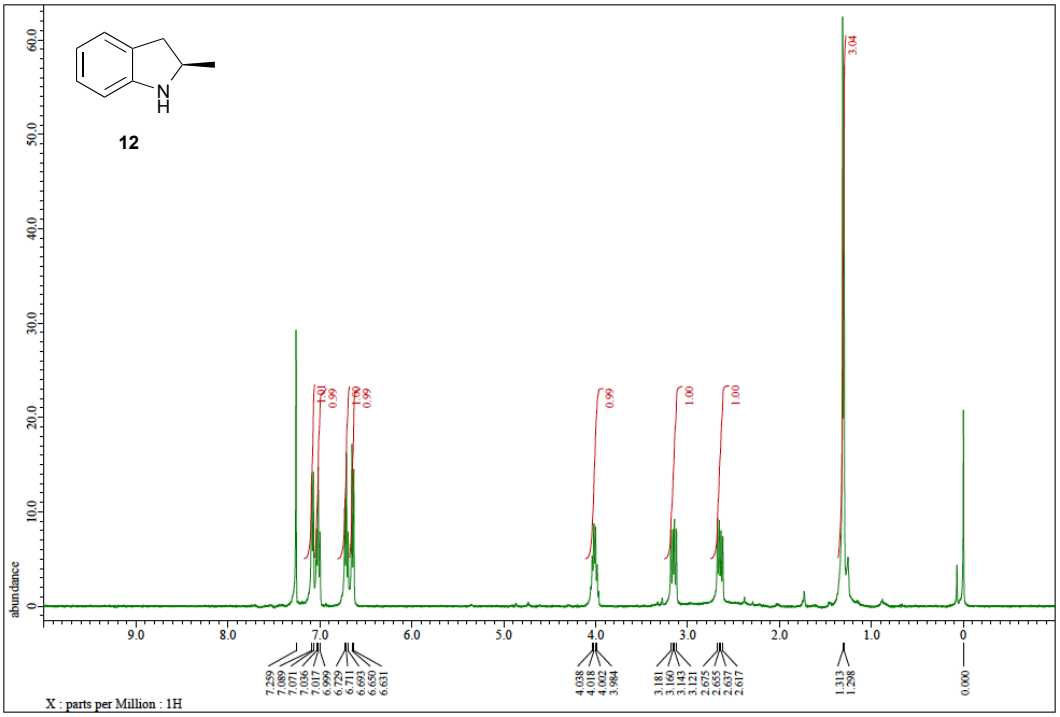
9

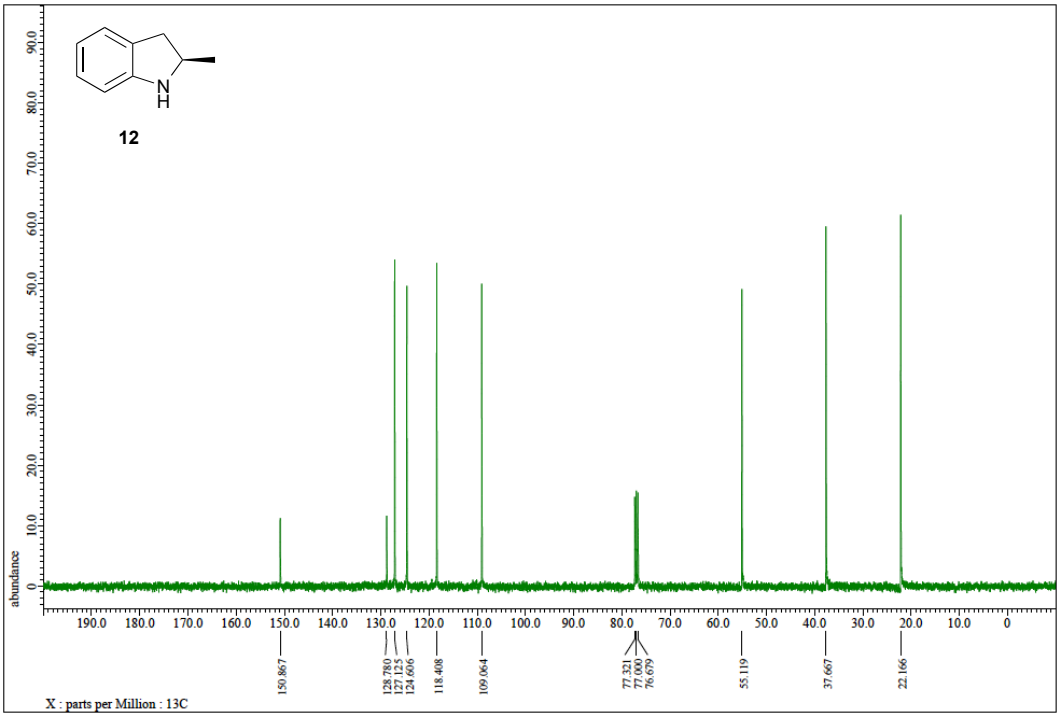

Br
N
O
S
O
O
Ph
10
abundance
X : parts per Million : 1H

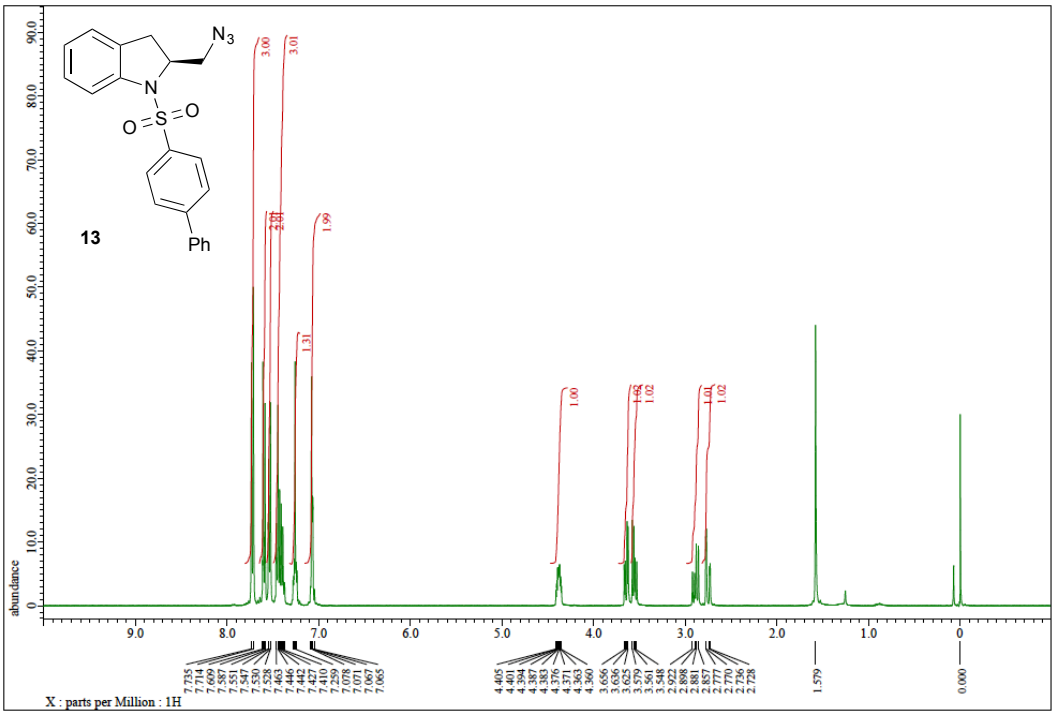

Br
N
O
S
O
O
Ph
10
abundance
X : parts per Million : 13C

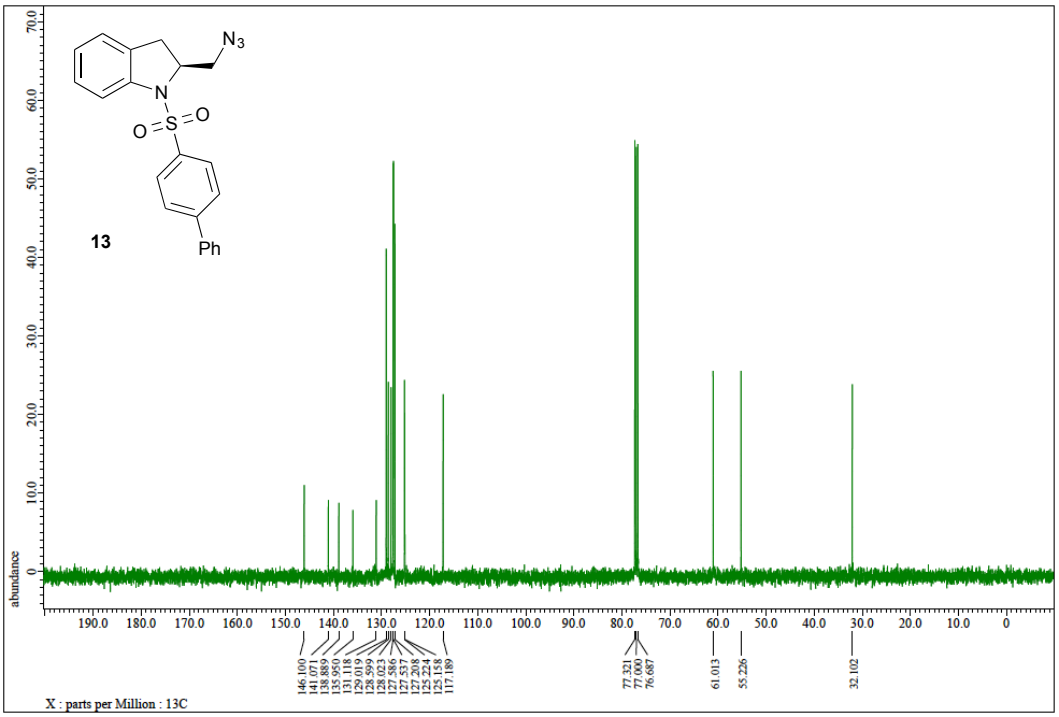

11
Ph
abundance
X : parts per Million : 1H

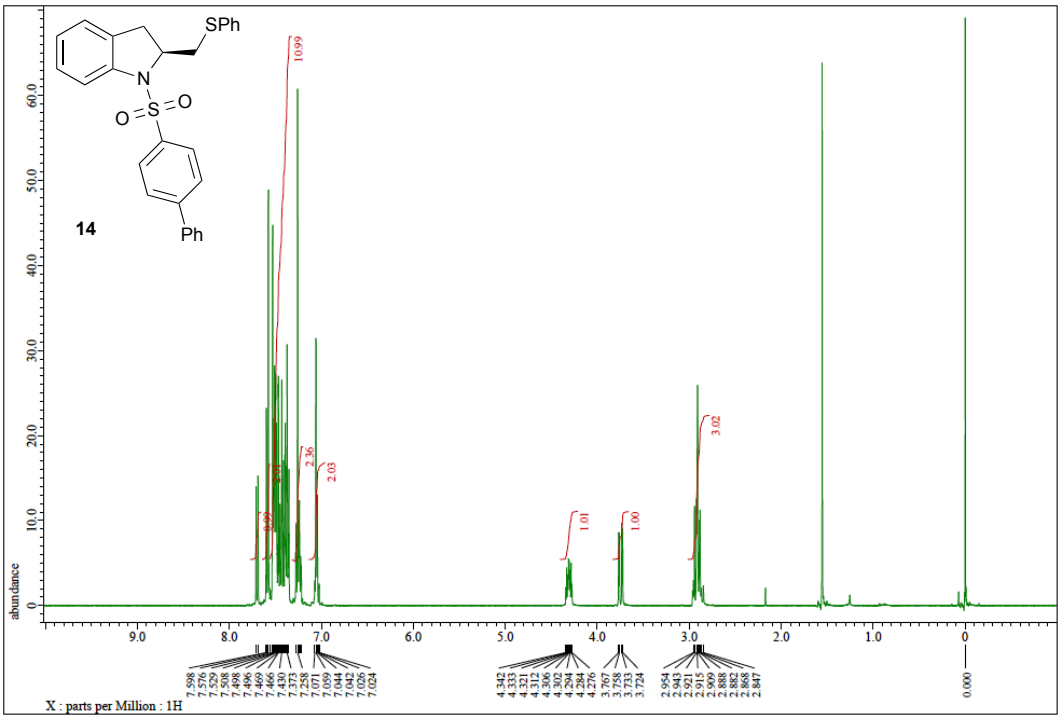

11
Ph
abundance
X : parts per Million : 13C

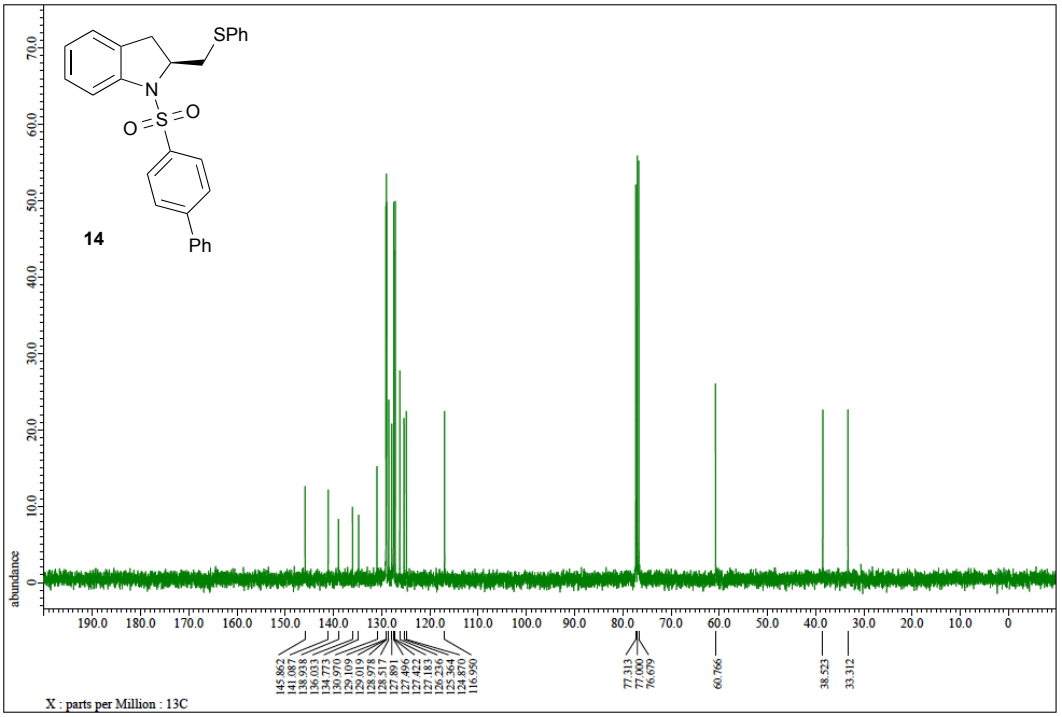

12
abundance
X : parts per Million : 1H

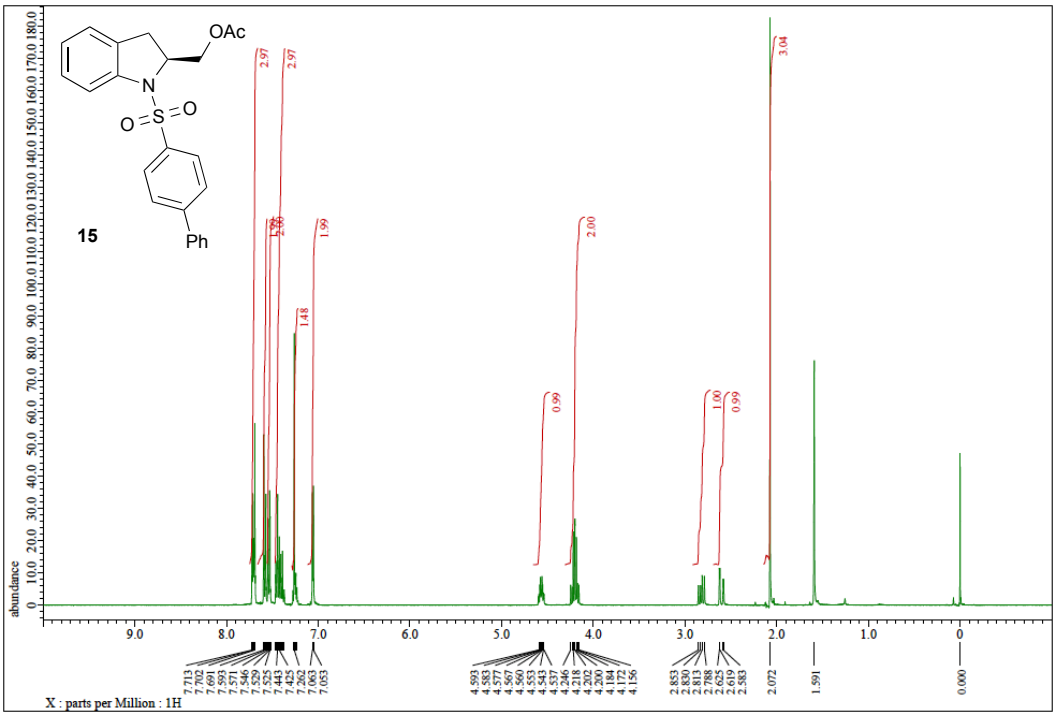

12
abundance
X : parts per Million : 13C

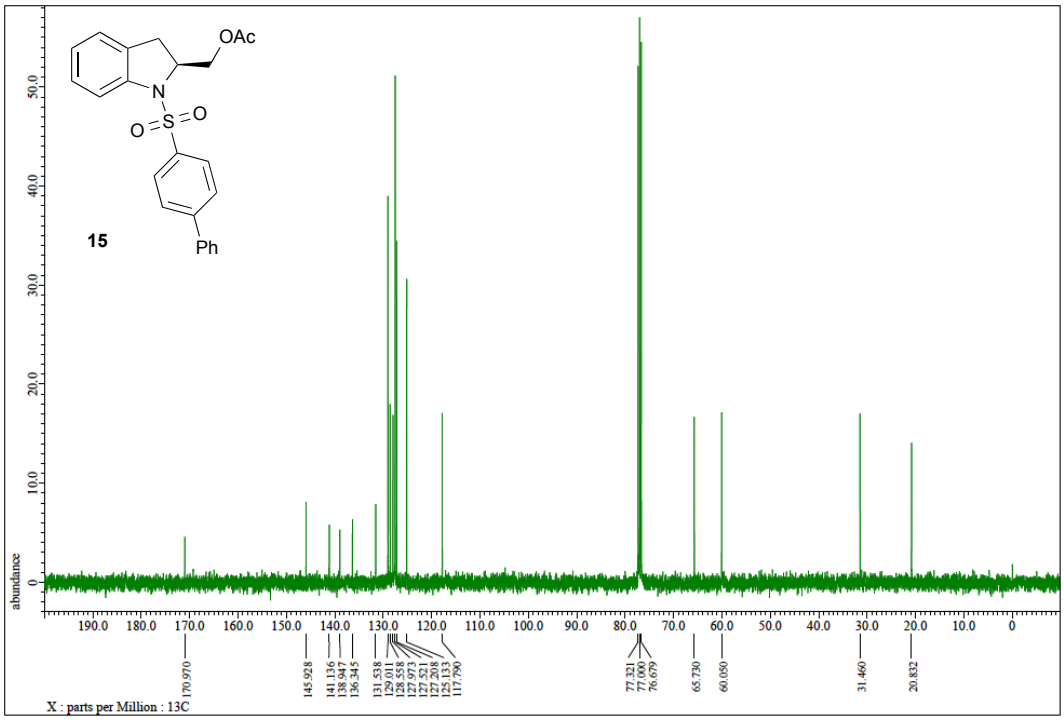

13
Ph
abundance
X : parts per Million : 1H


13
Ph
abundance
X : parts per Million : 13C

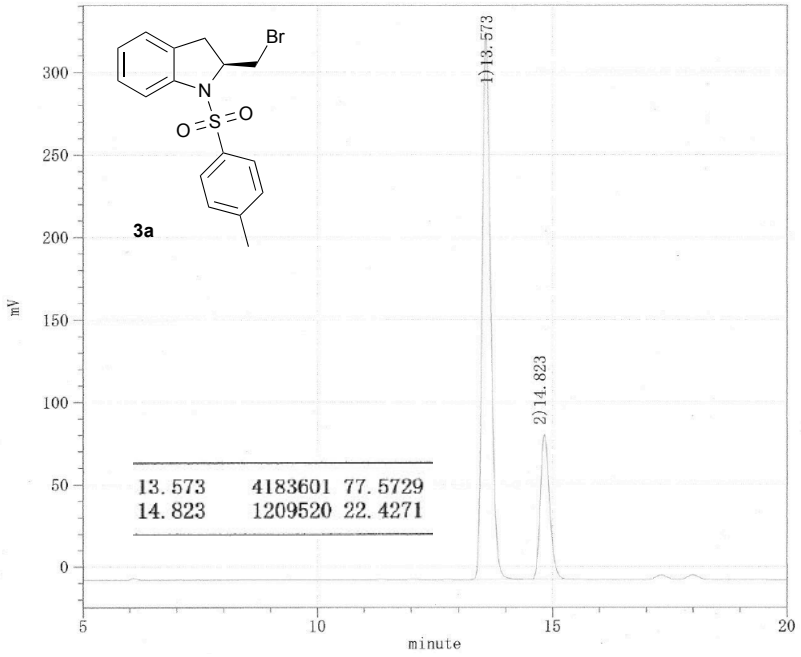

SPh
N
O
S
O
14
Ph
10.99
2.36
2.03
1.01
1.00
3.02
abundance
X : parts per Million : 1H

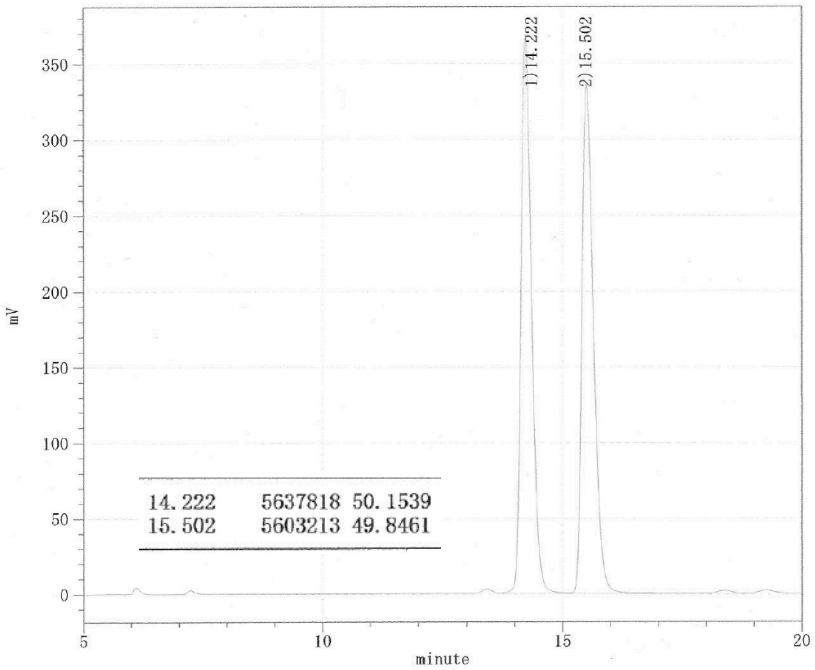

SPh
N
O
S
O
14
Ph
abundance
X : parts per Million : 13C

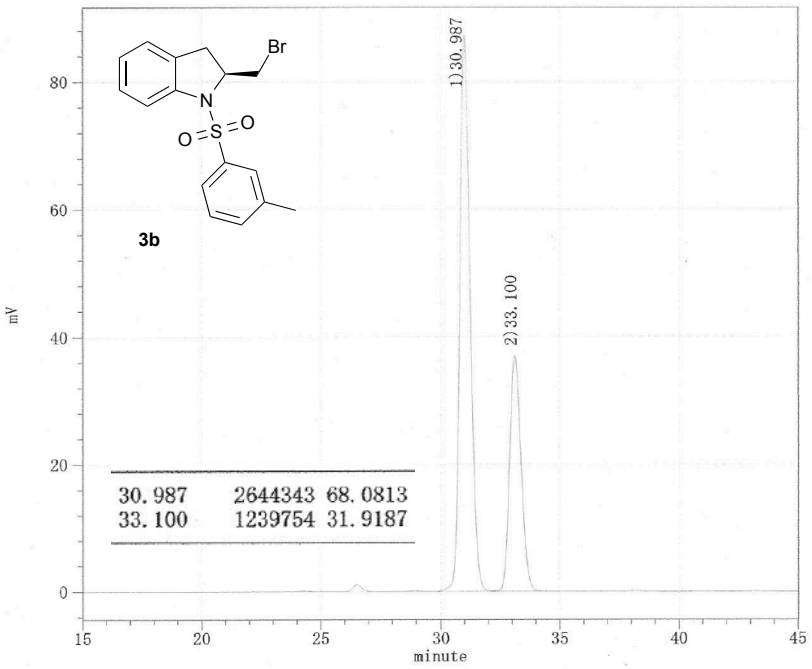

OAc
N
O=S=O
Ph
15
2.97
2.97
1.99
1.48
0.99
2.00
1.00
0.99
3.04
abundance
X : parts per Million : 1H

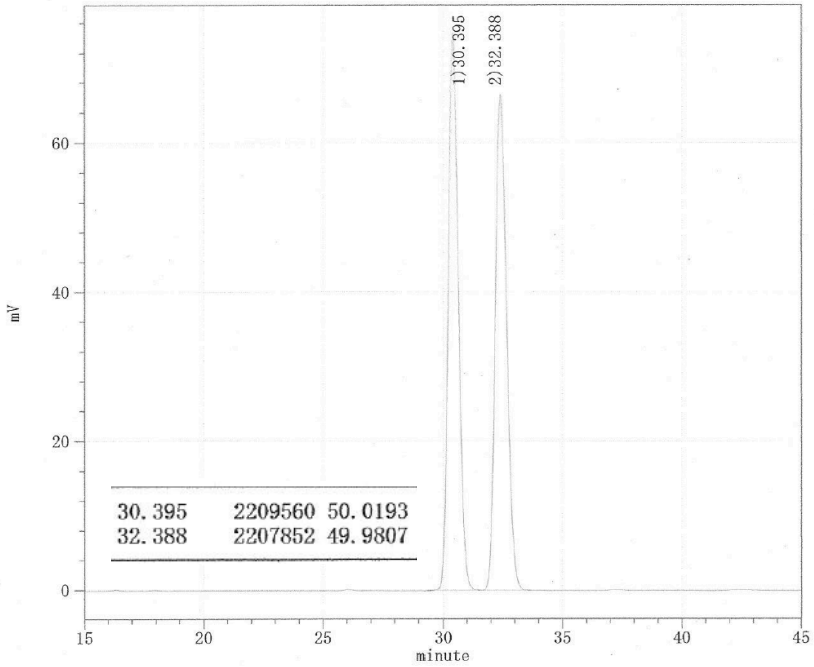

OAc
N
O=S=O
Ph
15
abundance
X : parts per Million : 13C

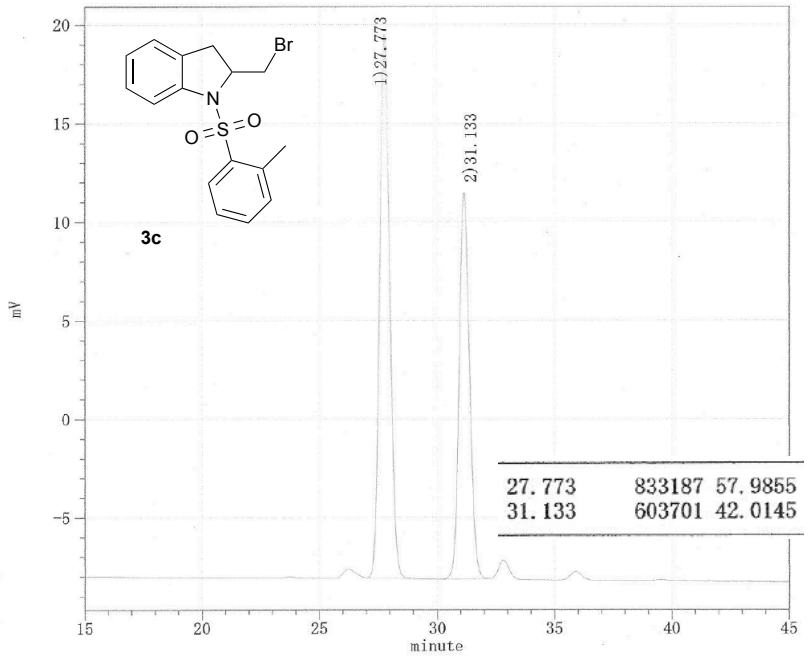
HPLC Charts

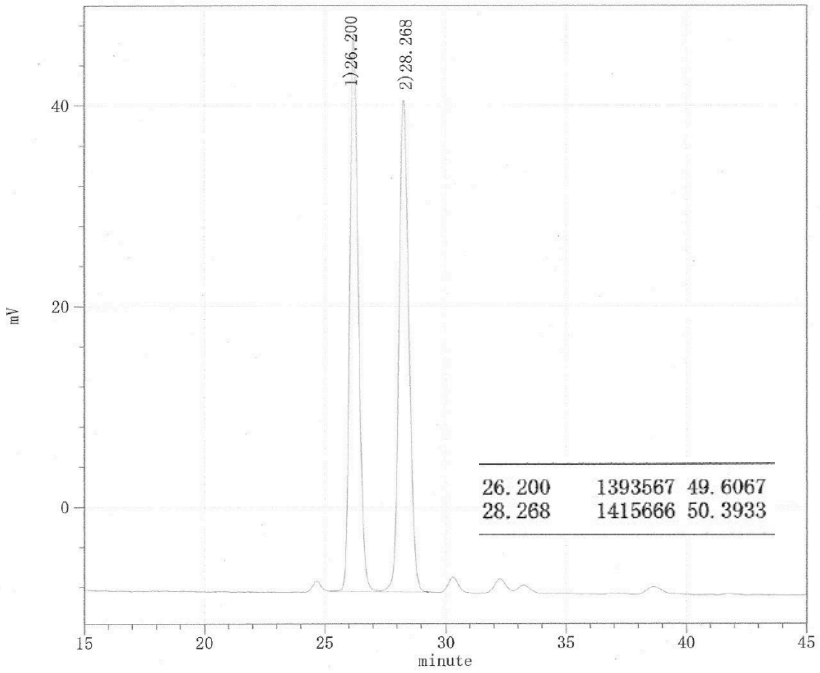

Br
N
O=S=O
3a
1) 13.573
2) 14.823
mV
minute
13.573 4183601 77.5729
14.823 1209520 22.4271

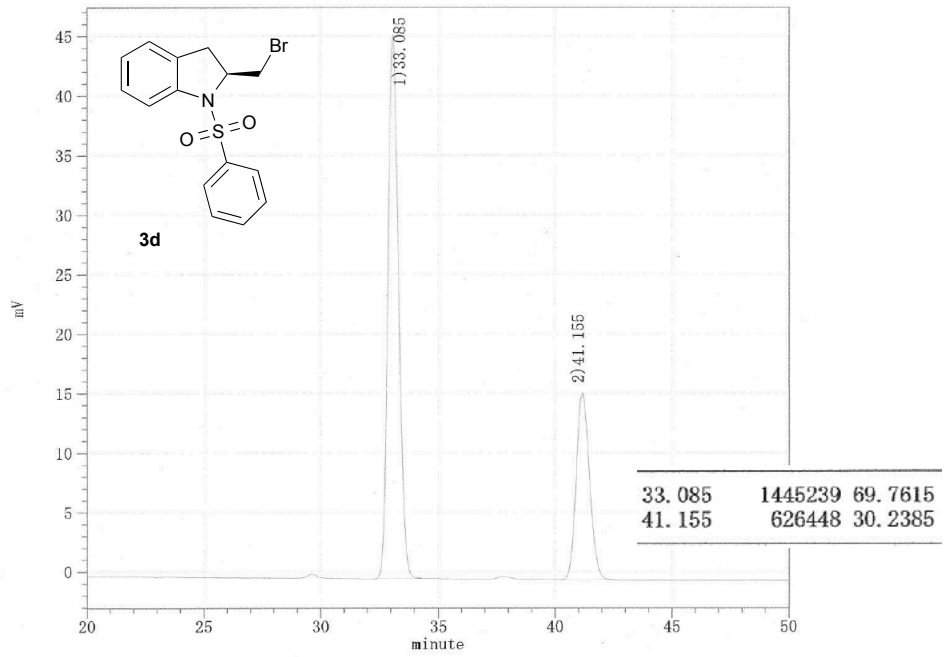

1) 14.222
2) 15.502
mV
minute
14.222 5637818 50.1539
15.502 5603213 49.8461

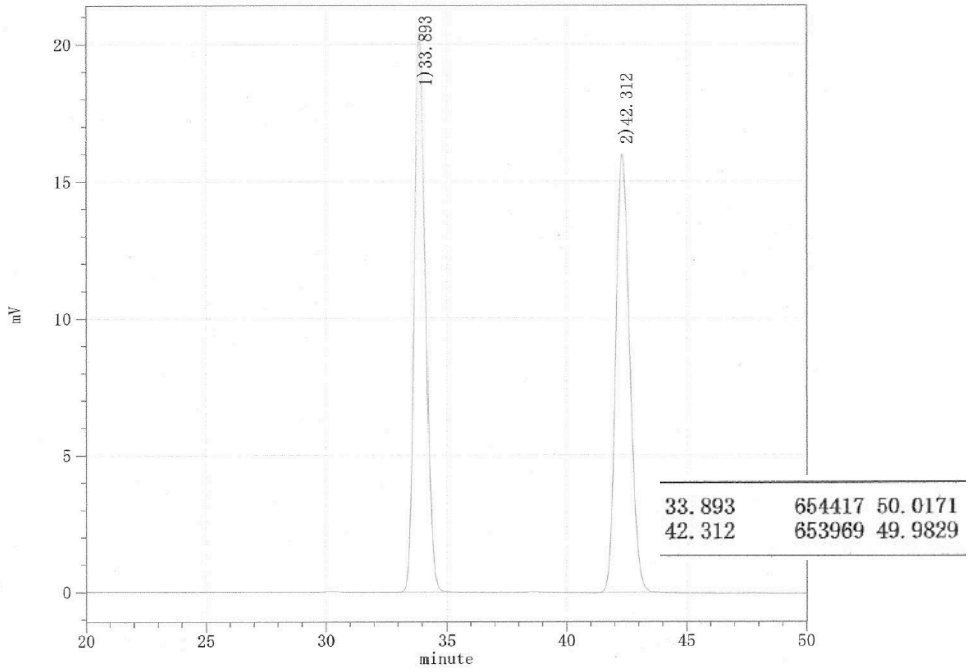

Br
N
O
S
O
3b
1)30.987
2)33.100
mV
80
60
40
20
0
15
20
25
30
35
40
45
minute
30.987 2644343 68.0813
33.100 1239754 31.9187

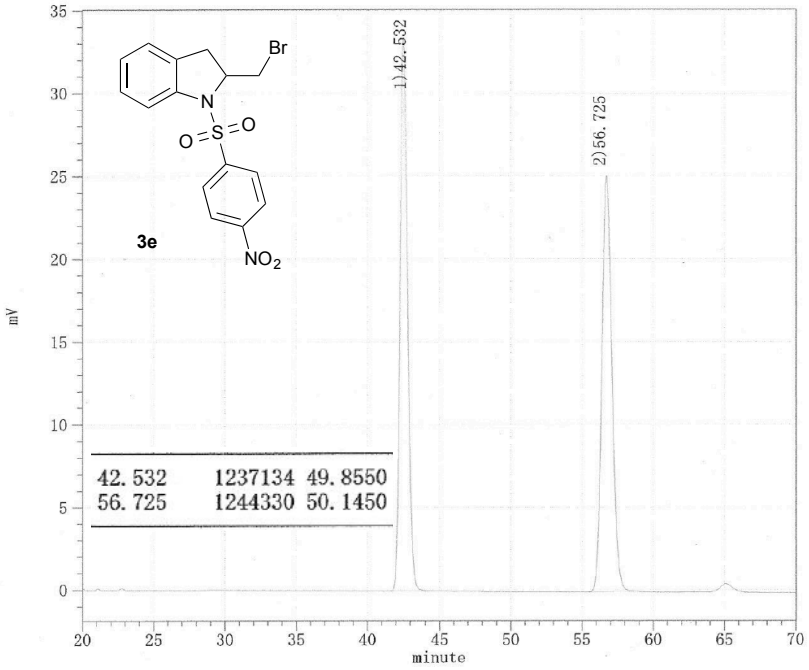

1)30.395
2)32.388
mV
60
40
20
0
15
20
25
30
35
40
45
minute
30.395 2209560 50.0193
32.388 2207852 49.9807

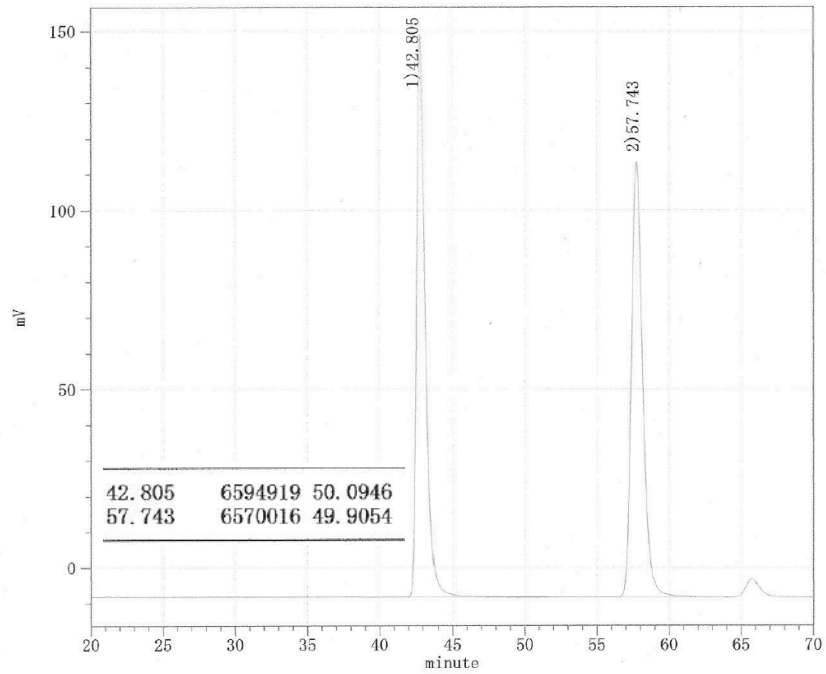

Br
N
O
S
O
3c
1) 27.773
2) 31.133
mV
minute
27.773 833187 57.9855
31.133 603701 42.0145

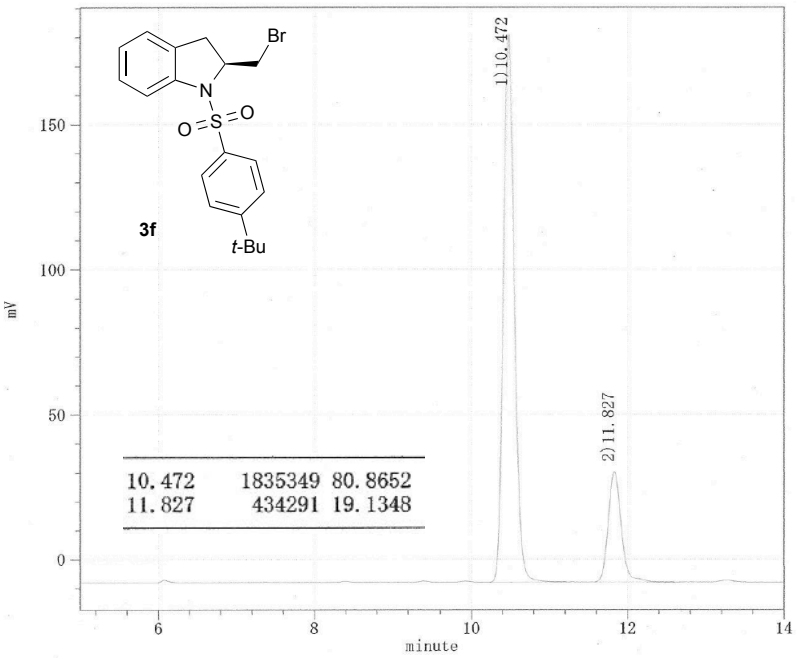

1) 26.200
2) 28.268
mV
minute
26.200 1393567 49.6067
28.268 1415666 50.3933

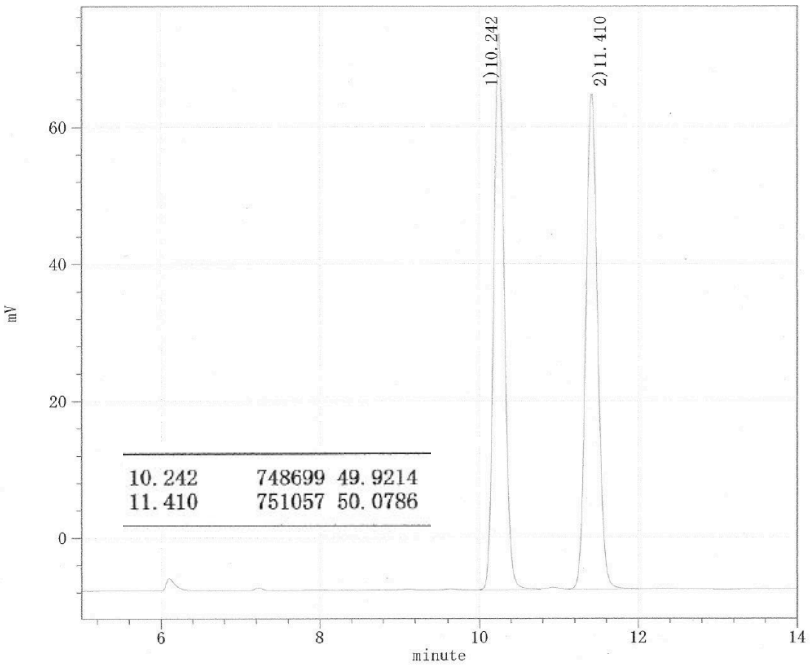

Br
N
O=S=O
3d
1)33.085
2)41.155
mV
minute
33.085 1445239 69.7615
41.155 626448 30.2385

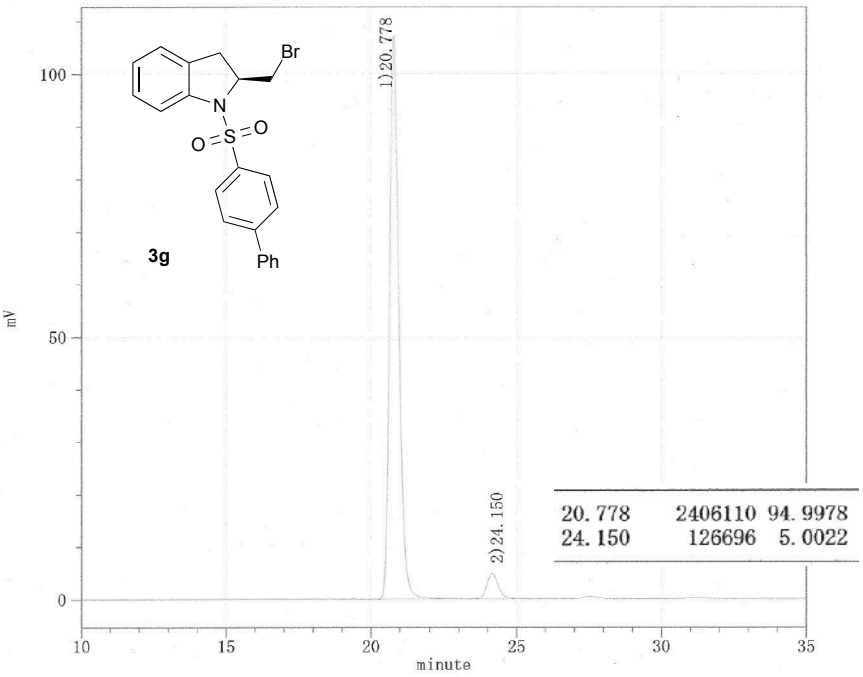

1)33.893
2)42.312
mV
minute
33.893 654417 50.0171
42.312 653969 49.9829

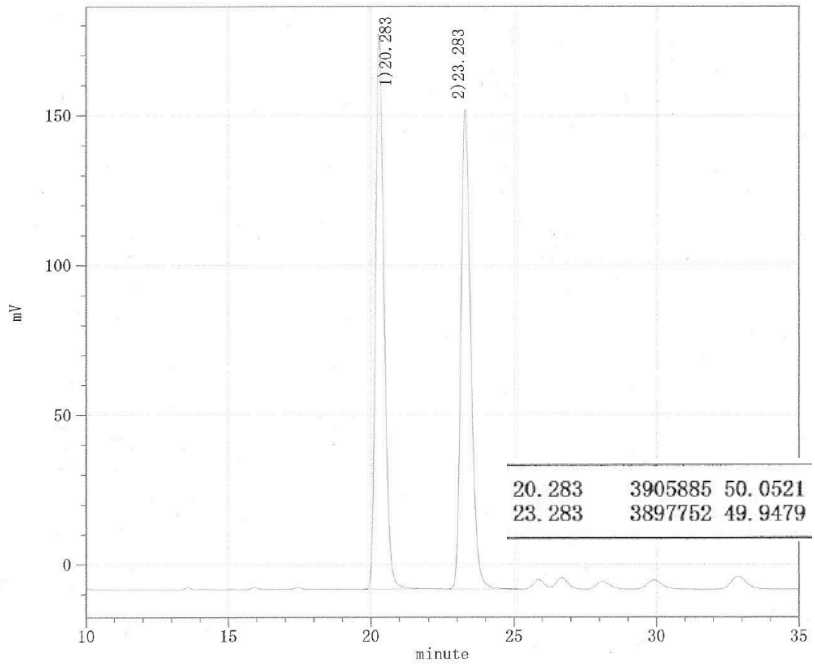

Br
N
O
S
O
O
NO2
3e
1) 42.532
2) 56.725
mV
minute
42.532 1237134 49.8550
56.725 1244330 50.1450

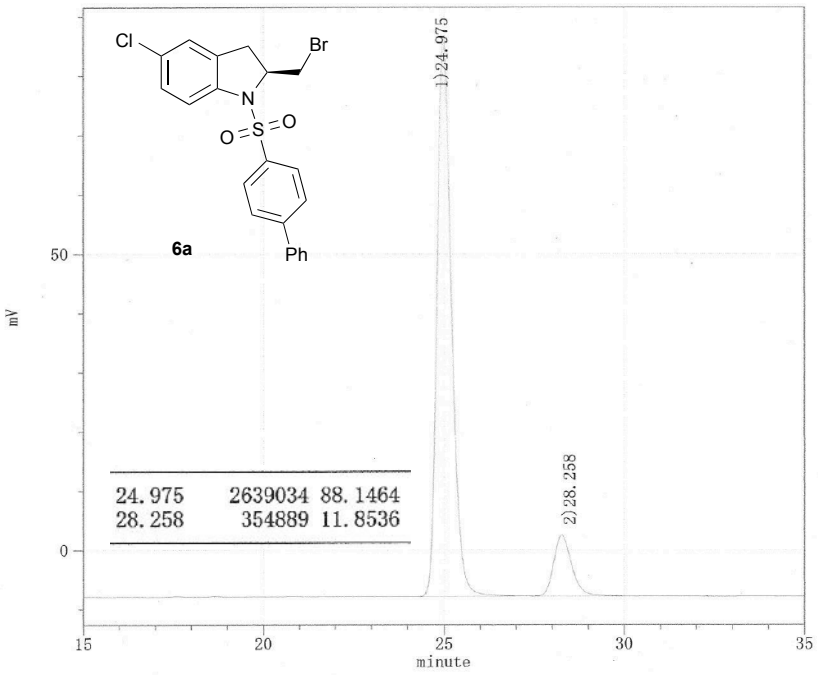

1) 42.805
2) 57.743
mV
minute
42.805 6594919 50.0946
57.743 6570016 49.9054

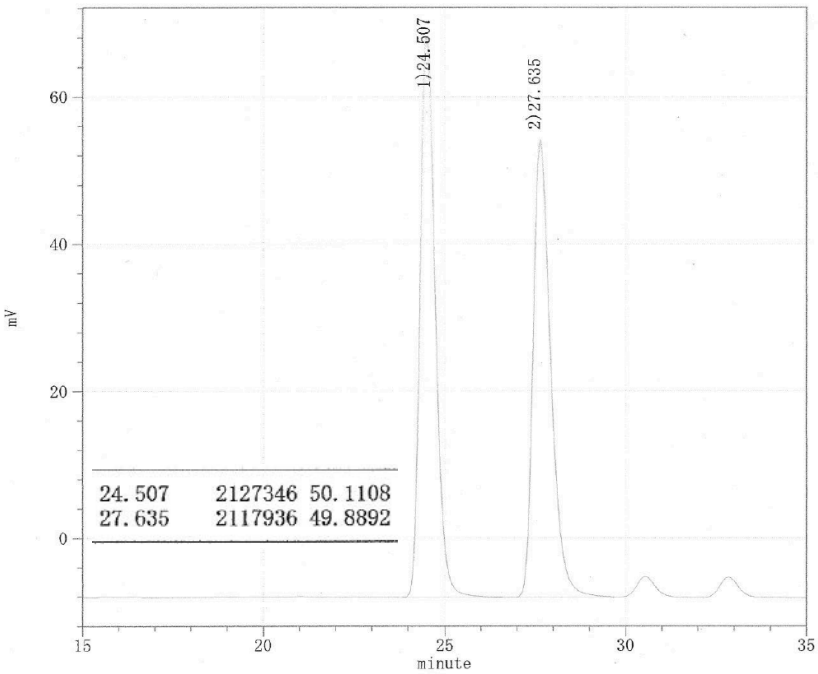

Br
N
O
S
O
3f
t-Bu
1)10.472
2)11.827
mV
150
100
50
0
6
8
10
12
14
minute
10.472 1835349 80.8652
11.827 434291 19.1348

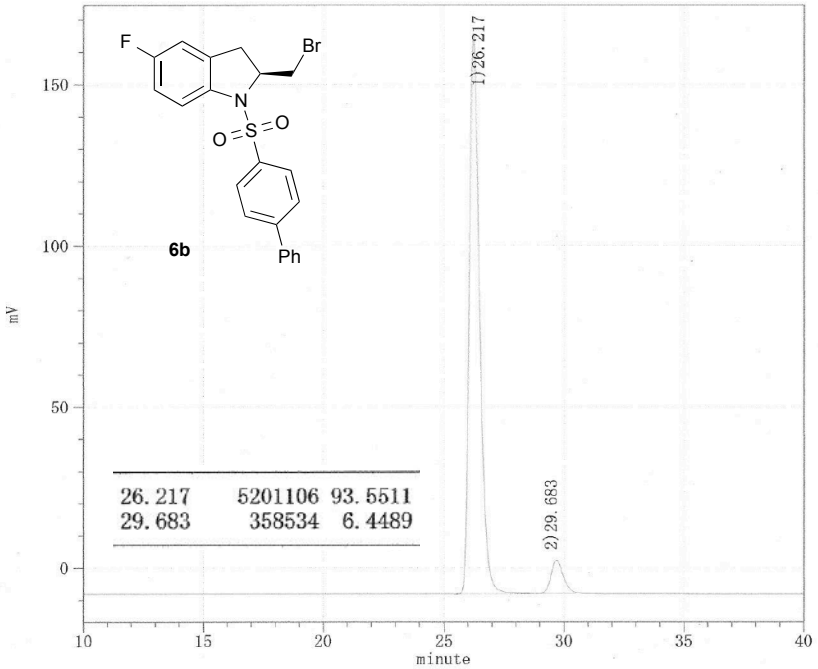

1)10.242
2)11.410
mV
60
40
20
0
6
8
10
12
14
minute
10.242 748699 49.9214
11.410 751057 50.0786

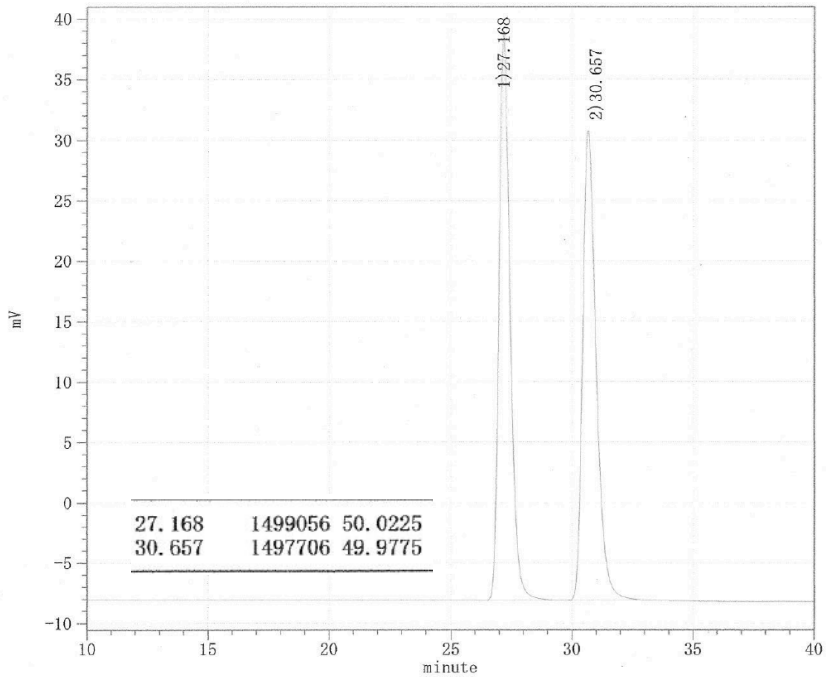

Br
N
O
S
O
3g
Ph
1)20.778
2)24.150
mV
100
50
0
10
15
20
25
30
35
minute
20.778 2406110 94.9978
24.150 126696 5.0022

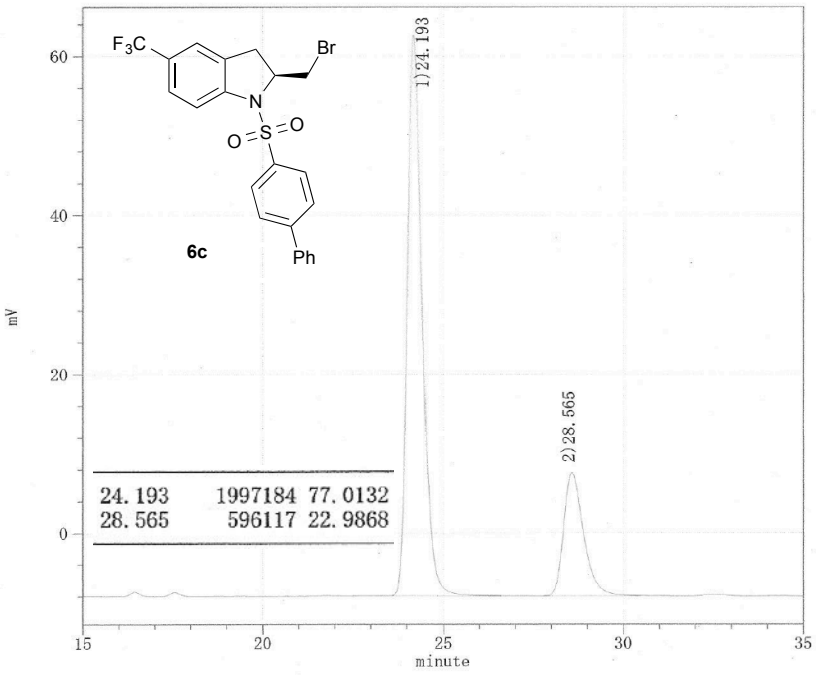

1)20.283
2)23.283
mV
150
100
50
0
10
15
20
25
30
35
minute
20.283 3905885 50.0521
23.283 3897752 49.9479

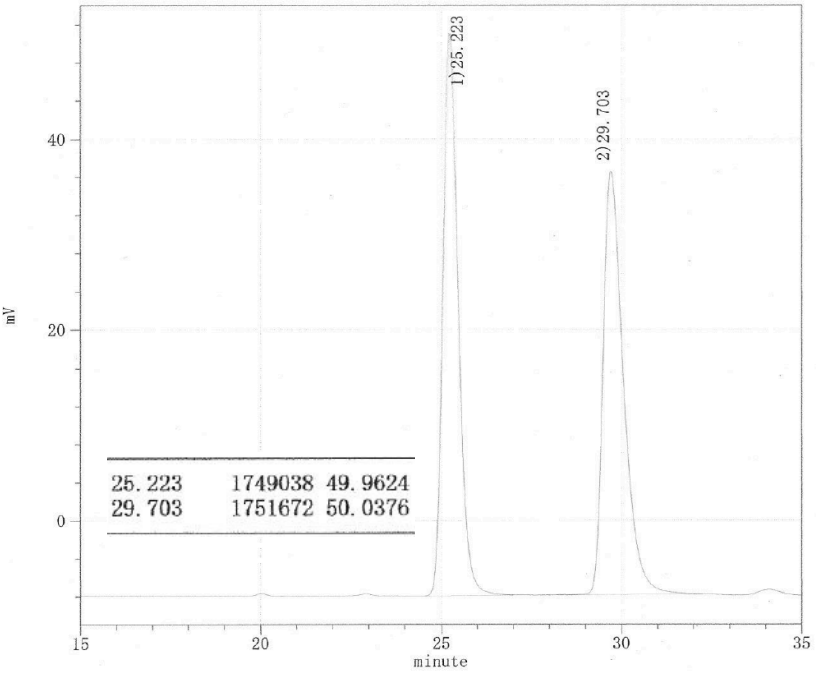

Cl
Br
N
O
S
O
O
Ph
6a
1)24.975
2)28.258
mV
50
0
15
20
25
30
35
minute
24.975 2639034 88.1464
28.258 354889 11.8536

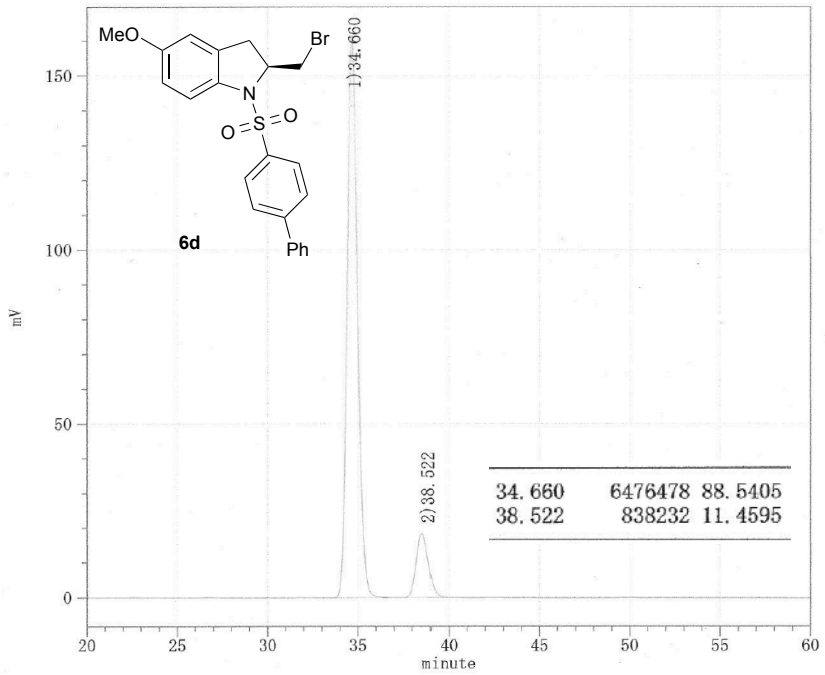

1)24.507
2)27.635
mV
60
40
20
0
15
20
25
30
35
minute
24.507 2127346 50.1108
27.635 2117936 49.8892

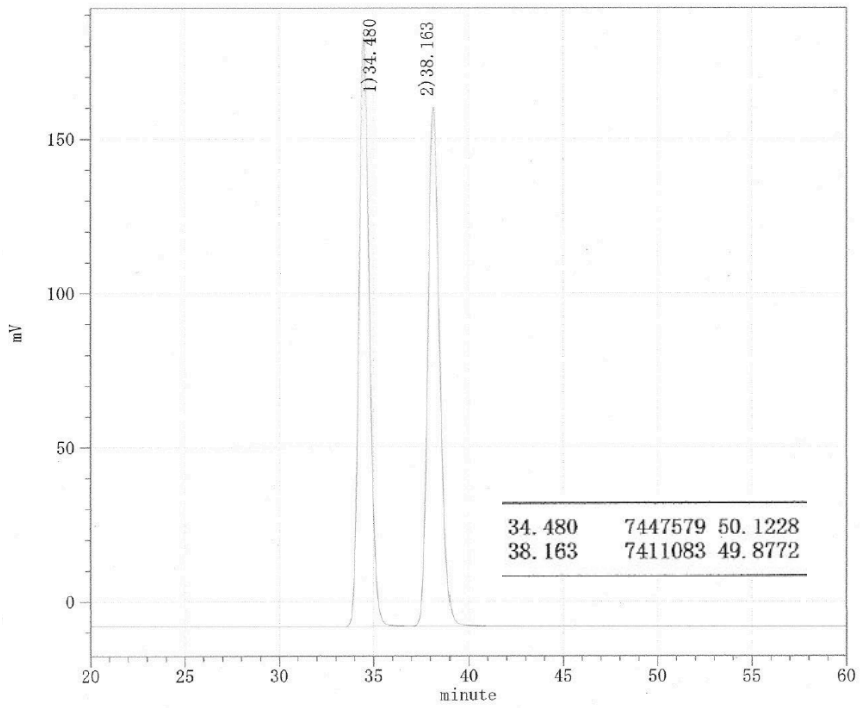

F
Br
N
O
S
O
Ph
6b
1)26.217
2)29.683
mV
150
100
50
0
10
15
20
25
30
35
40
minute
26.217 5201106 93.5511
29.683 358534 6.4489

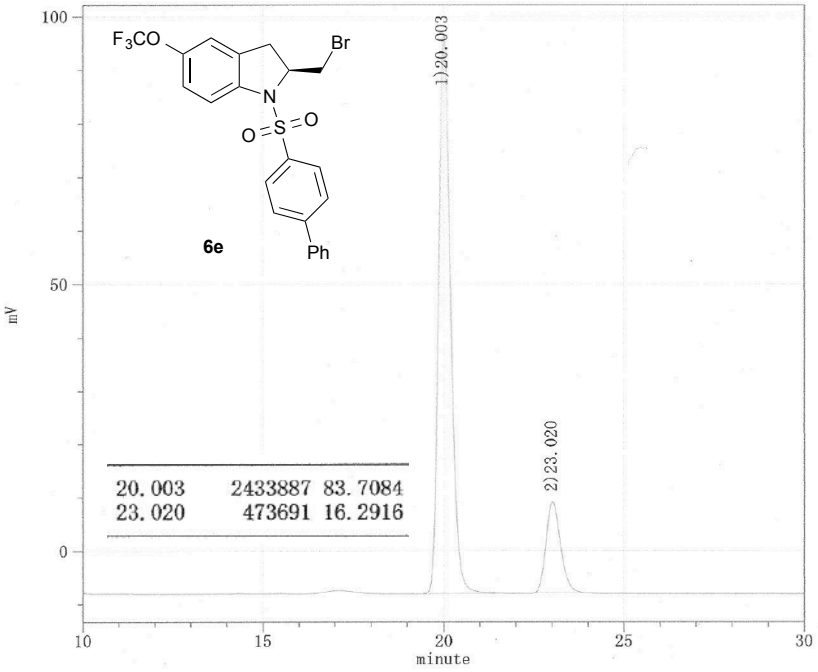

1)27.168
2)30.657
mV
40
35
30
25
20
15
10
5
0
−5
−10
10
15
20
25
30
35
40
minute
27.168 1499056 50.0225
30.657 1497706 49.9775

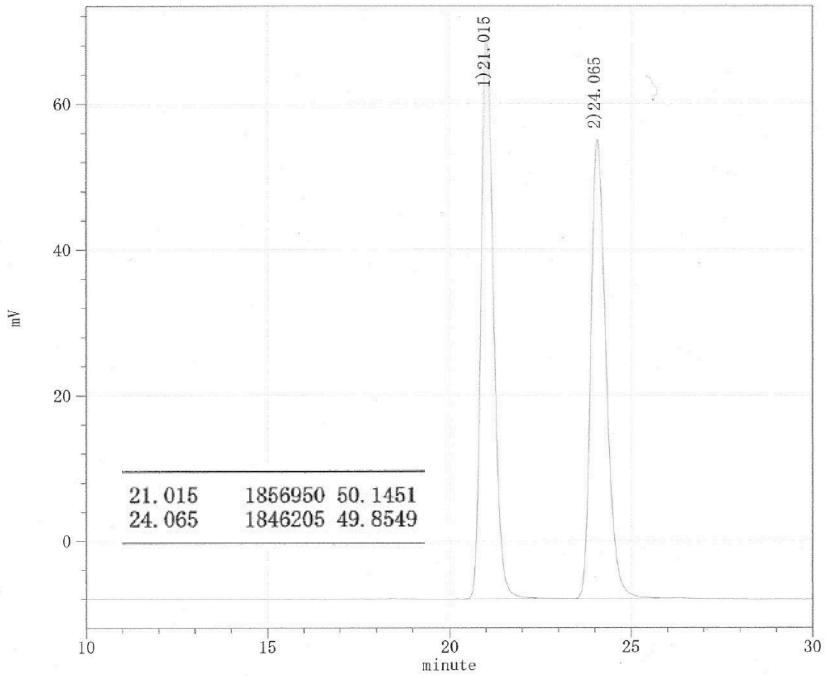

F3C
Br
N
O
S
O
Ph
6c
1)24.193
2)28.565
mV
60
40
20
0
15
20
25
30
35
minute
24.193 1997184 77.0132
28.565 596117 22.9868

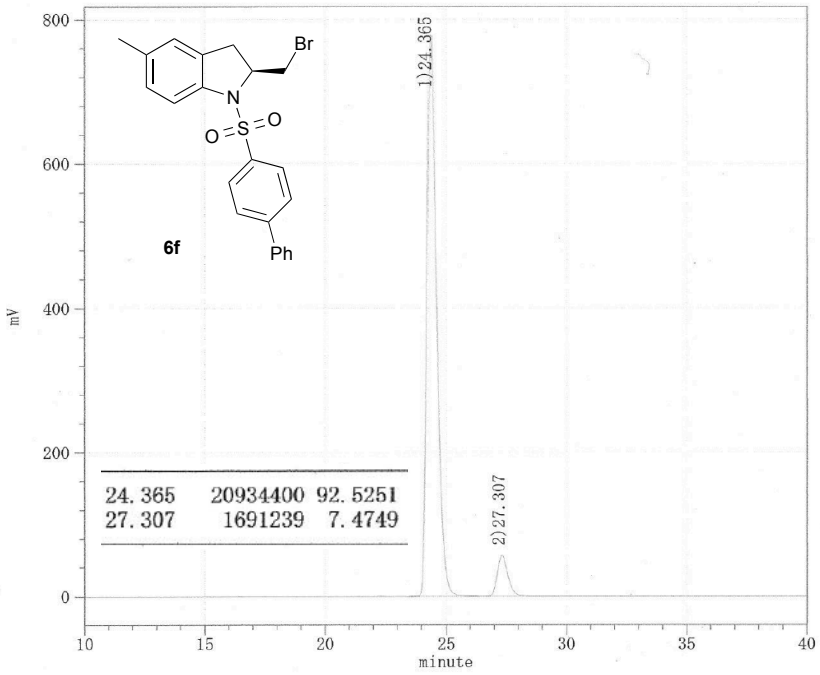

1)25.223
2)29.703
mV
40
20
0
15
20
25
30
35
minute
25.223 1749038 49.9624
29.703 1751672 50.0376

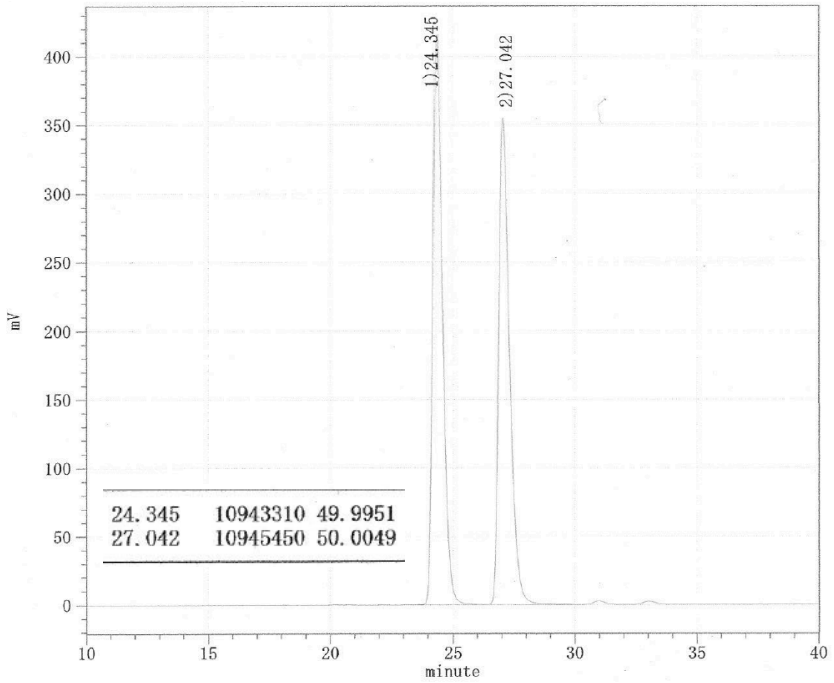

MeO
Br
N
O
S
O
Ph
6d
1)34.660
2)38.522
150
100
50
0
mV
20
25
30
35
40
45
50
55
60
minute
34.660 6476478 88.5405
38.522 838232 11.4595

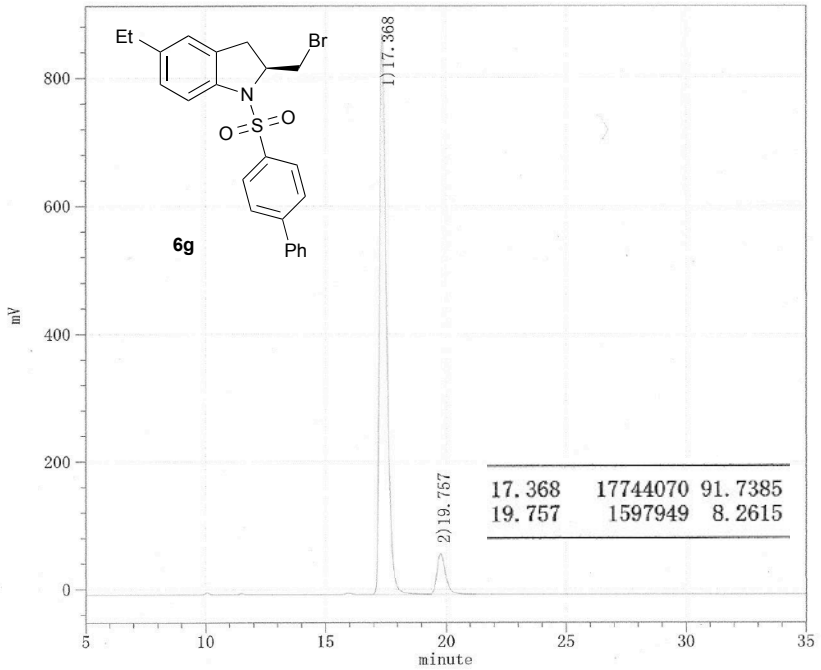

1)34.480
2)38.163
150
100
50
0
mV
20
25
30
35
40
45
50
55
60
minute
34.480 7447579 50.1228
38.163 7411083 49.8772

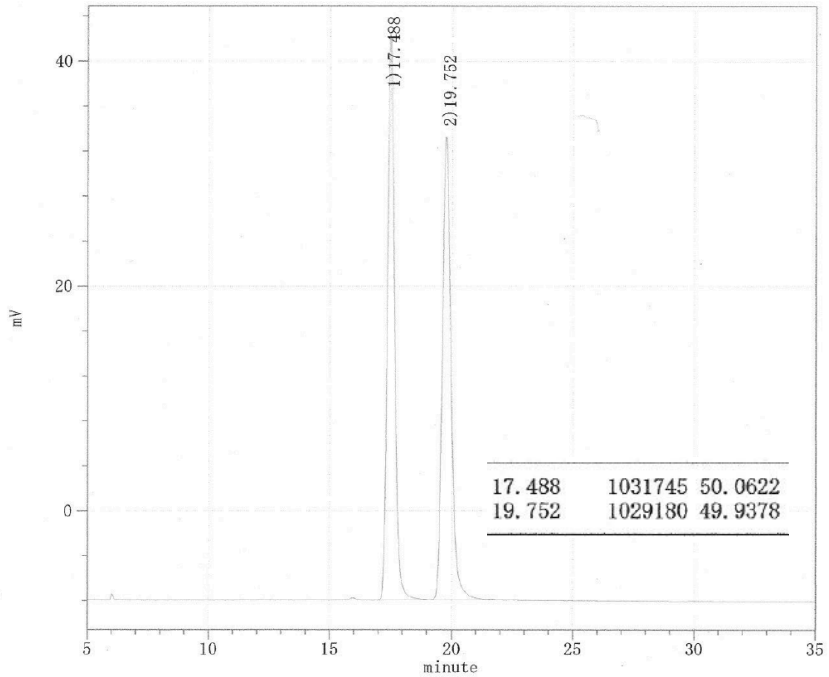

100
50
0
mV
10
15
20
25
30
minute
F3CO
Br
N
O=S=O
Ph
6e
1)20.003
2)23.020
20.003 2433887 83.7084
23.020 473691 16.2916

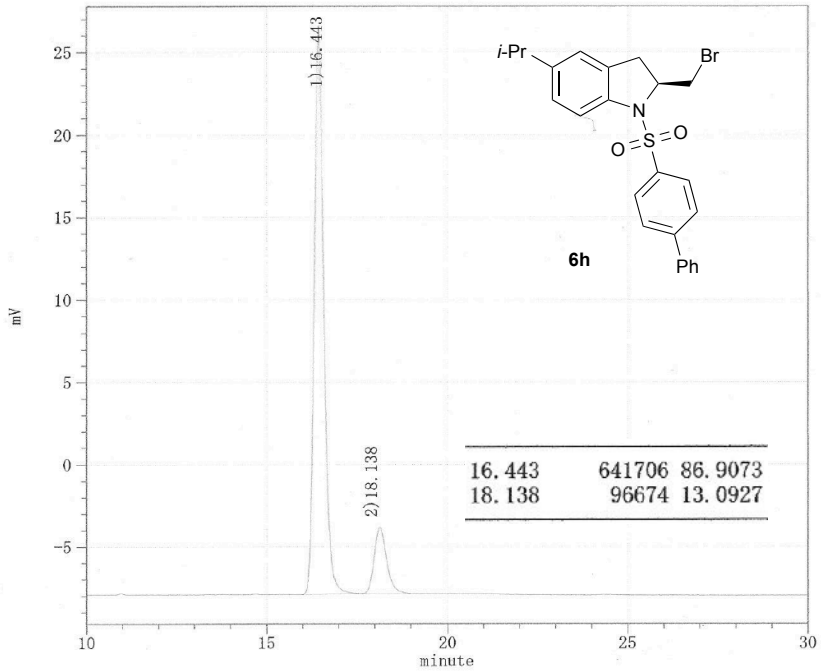

60
40
20
0
mV
10
15
20
25
30
minute
1)21.015
2)24.065
21.015 1856950 50.1451
24.065 1846205 49.8549

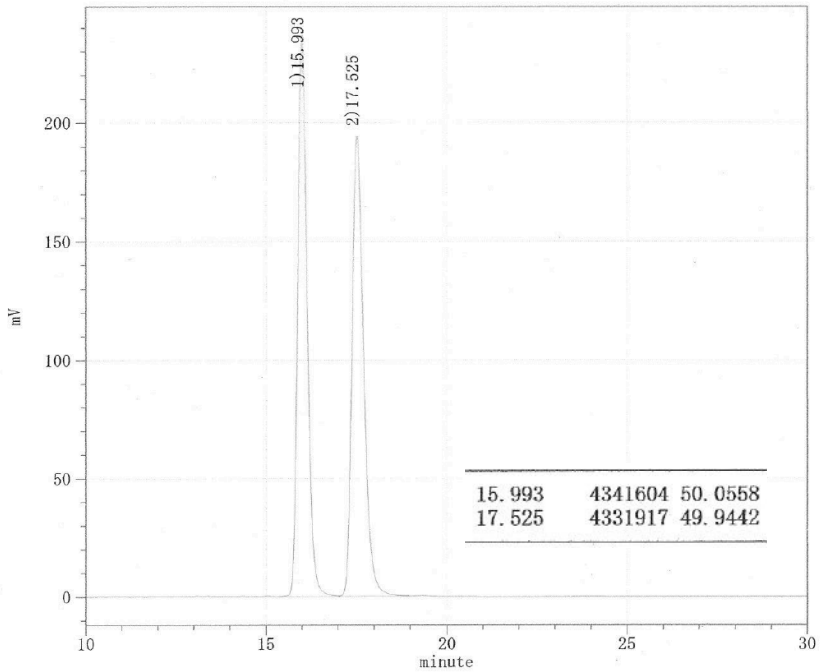

Br
N
O
S
O
Ph
6f
1)24.365
2)27.307
mV
minute
24.365 20934400 92.5251
27.307 1691239 7.4749

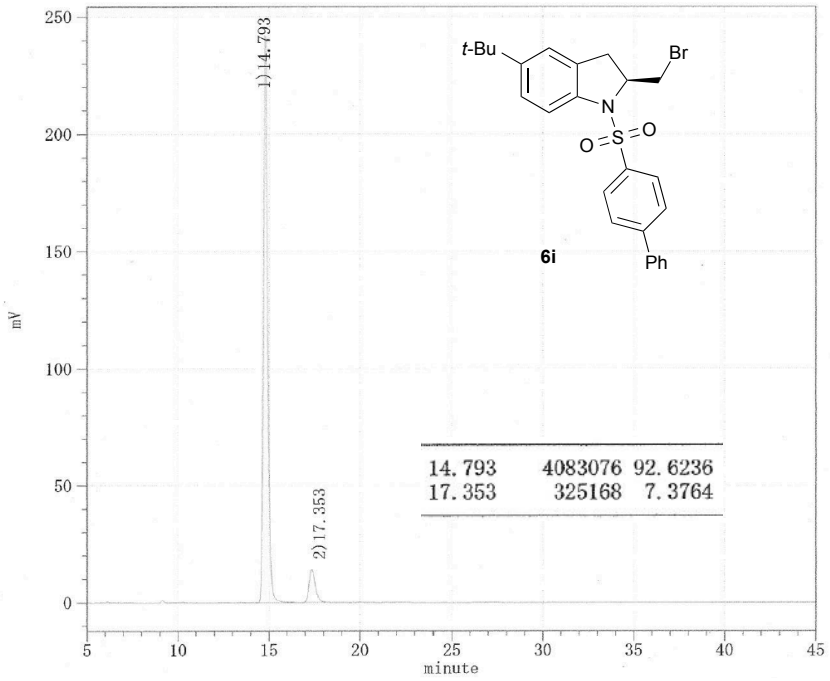

1)24.345
2)27.042
mV
minute
24.345 10943310 49.9951
27.042 10945450 50.0049

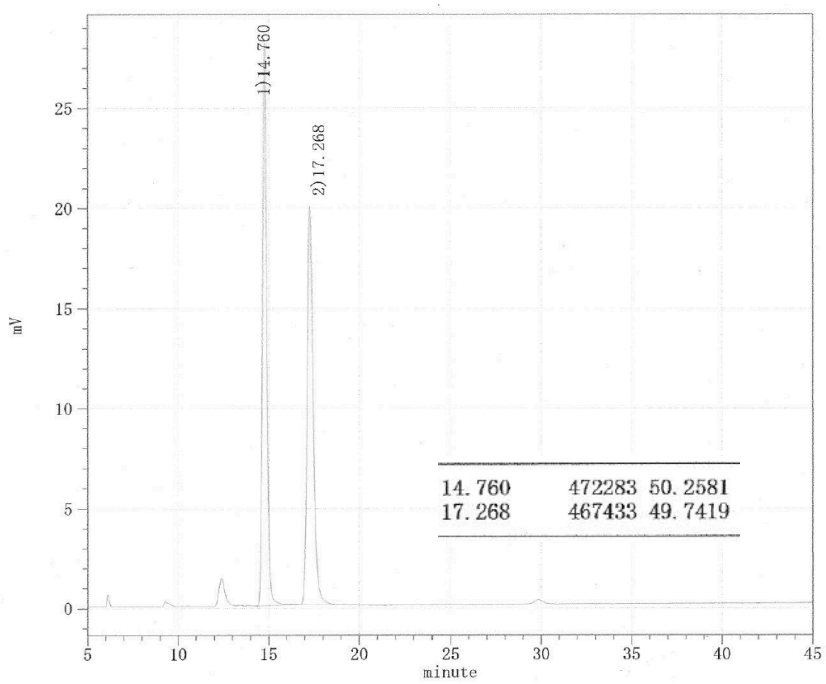

Et
Br
N
O=S=O
Ph
6g
1) 17.368
2) 19.757
mV
800
600
400
200
0
5
10
15
20
25
30
35
minute
17.368 17744070 91.7385
19.757 1597949 8.2615

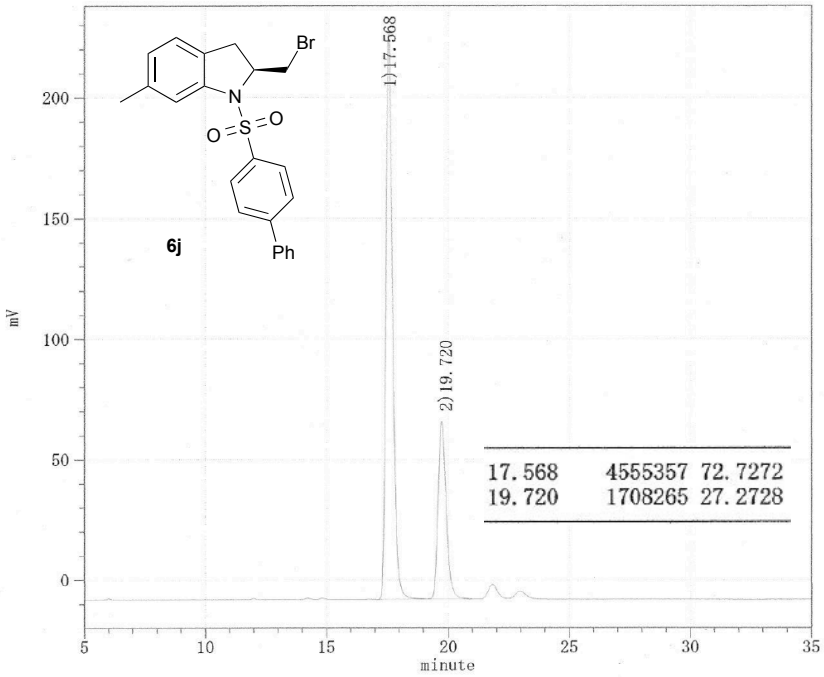

1) 17.488
2) 19.752
mV
40
20
0
5
10
15
20
25
30
35
minute
17.488 1031745 50.0622
19.752 1029180 49.9378

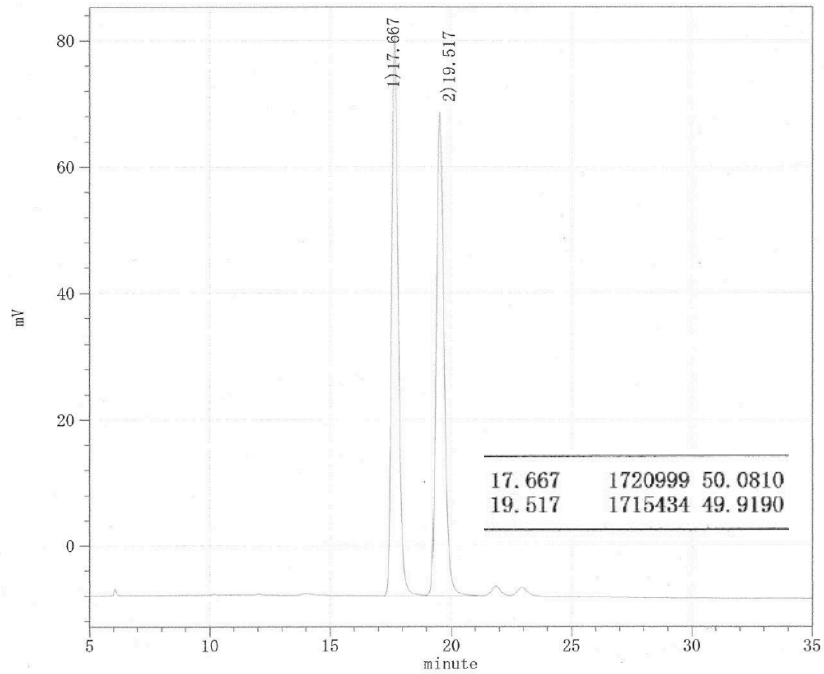

1) 16.443
2) 18.138
mV
minute
i-Pr
Br
N
O
S
O
Ph
6h
16.443 641706 86.9073
18.138 96674 13.0927

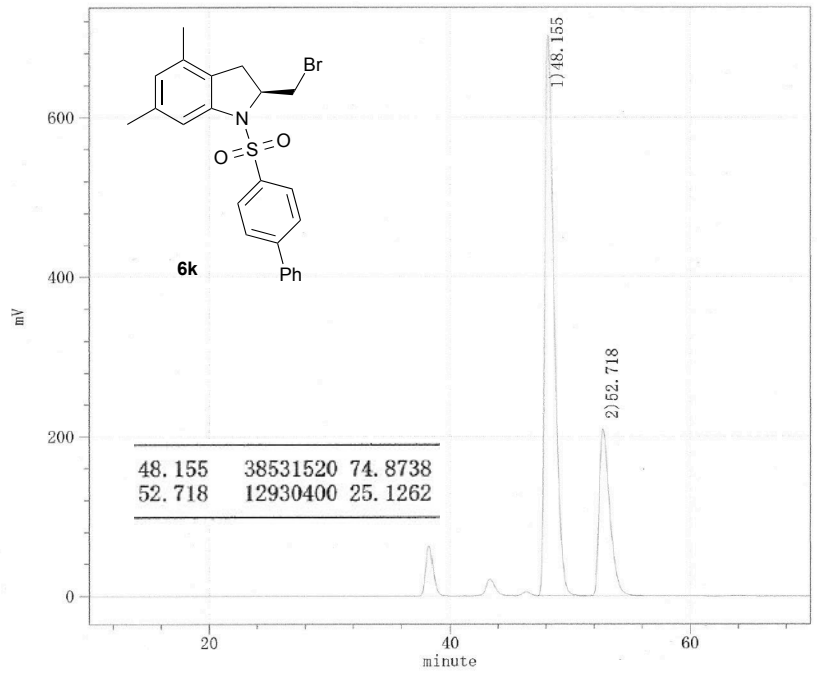

1) 15.993
2) 17.525
mV
minute
15.993 4341604 50.0558
17.525 4331917 49.9442

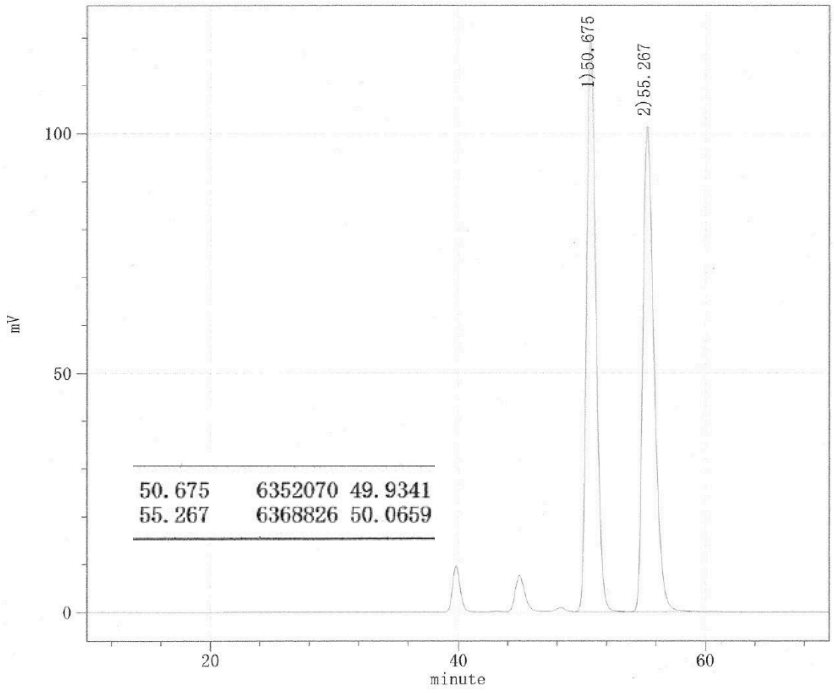

1) 14.793
2) 17.353
mV
minute
t-Bu
Br
N
O
S
O
Ph
6i
14.793 4083076 92.6236
17.353 325168 7.3764

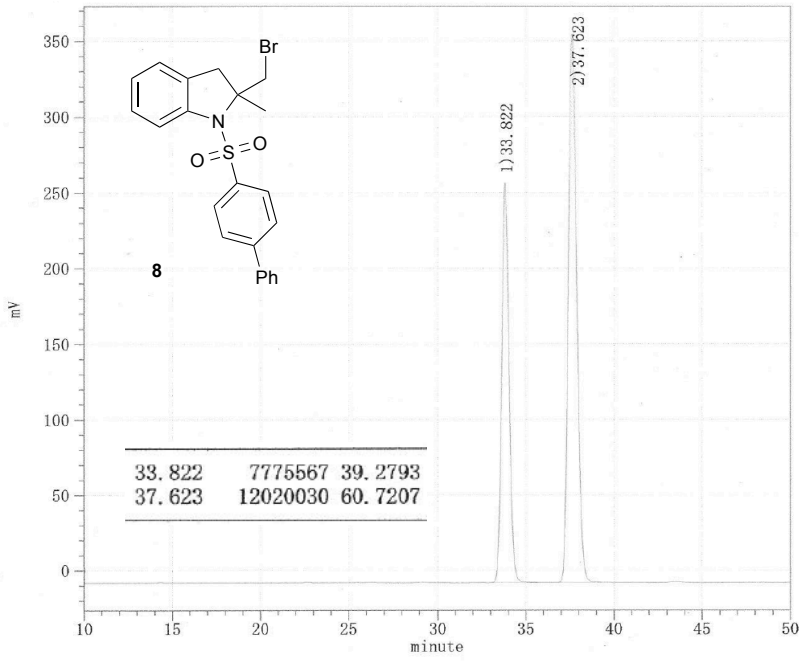

1) 14.760
2) 17.268
mV
minute
14.760 472283 50.2581
17.268 467433 49.7419

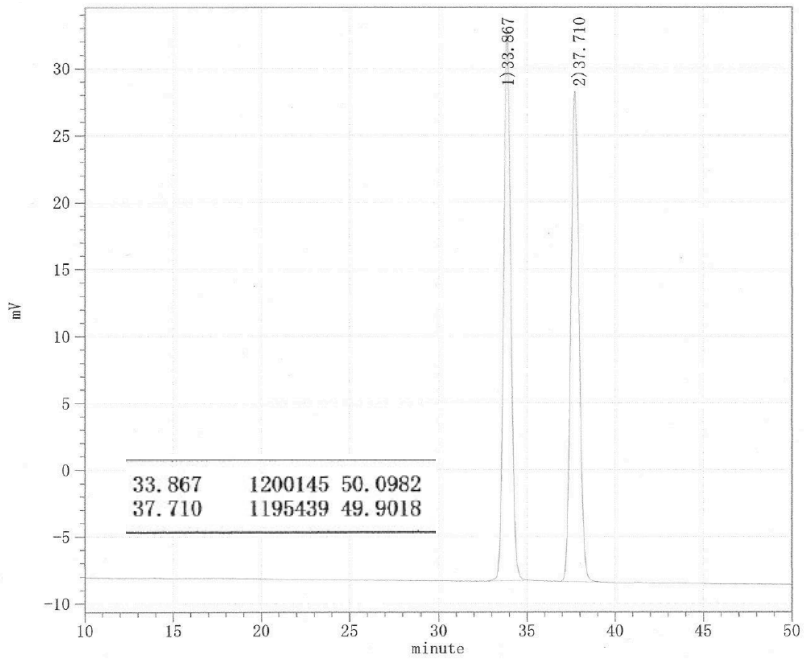

Br
N
O
S
O
6j
Ph
1)17.568
2)19.720
mV
200
150
100
50
0
5
10
15
20
25
30
35
minute
17.568 4555357 72.7272
19.720 1708265 27.2728

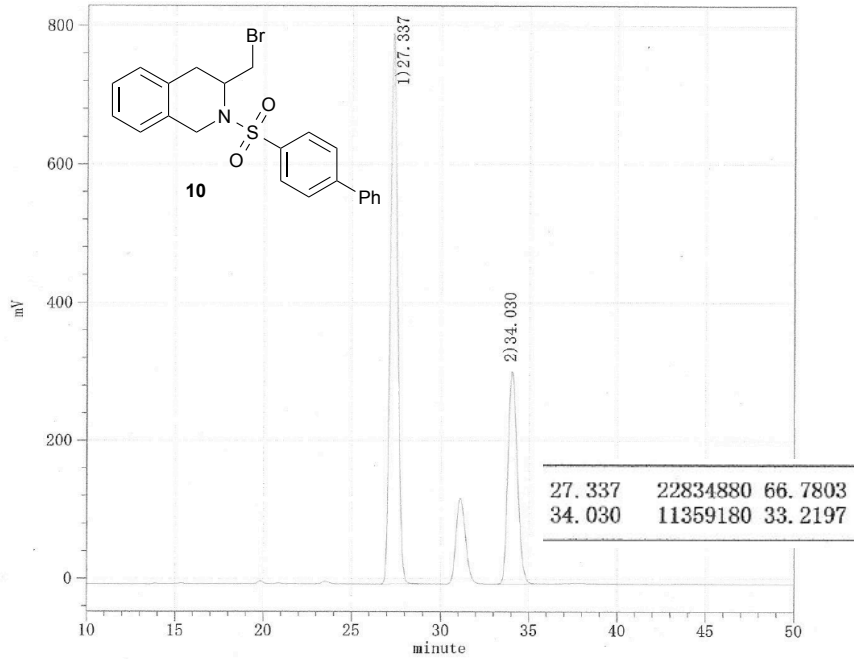

1)17.667
2)19.517
mV
80
60
40
20
0
5
10
15
20
25
30
35
minute
17.667 1720999 50.0810
19.517 1715434 49.9190

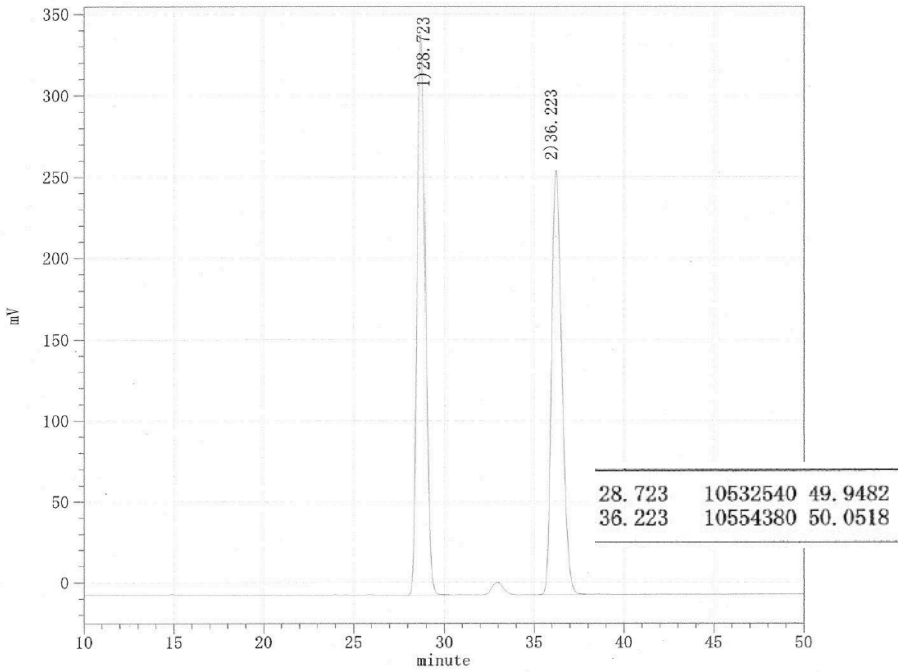

Br
N
O
S
O
6k
Ph
1)48.155
2)52.718
mV
600
400
200
0
20
40
60
minute
48.155 38531520 74.8738
52.718 12930400 25.1262

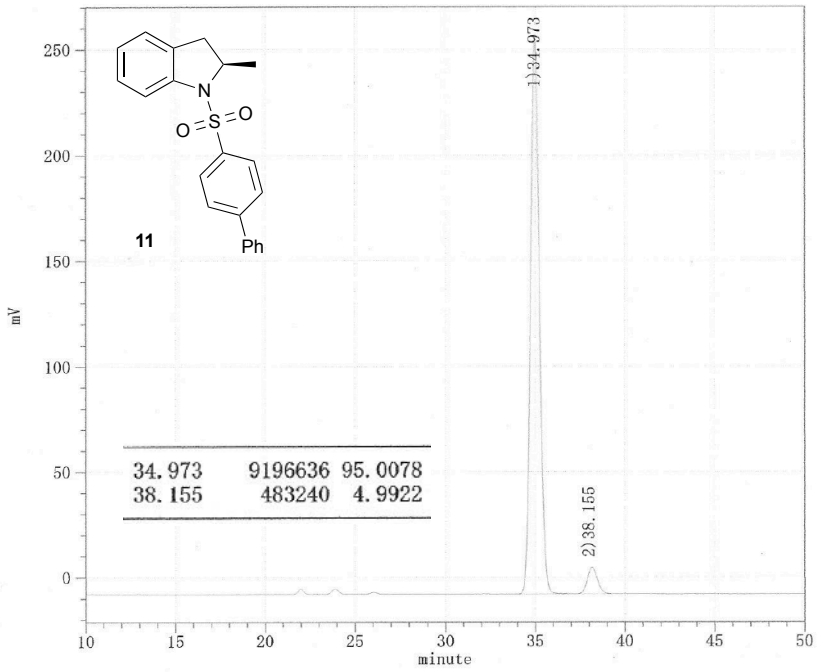

1)50.675
2)55.267
mV
100
50
0
20
40
60
minute
50.675 6352070 49.9341
55.267 6368826 50.0659

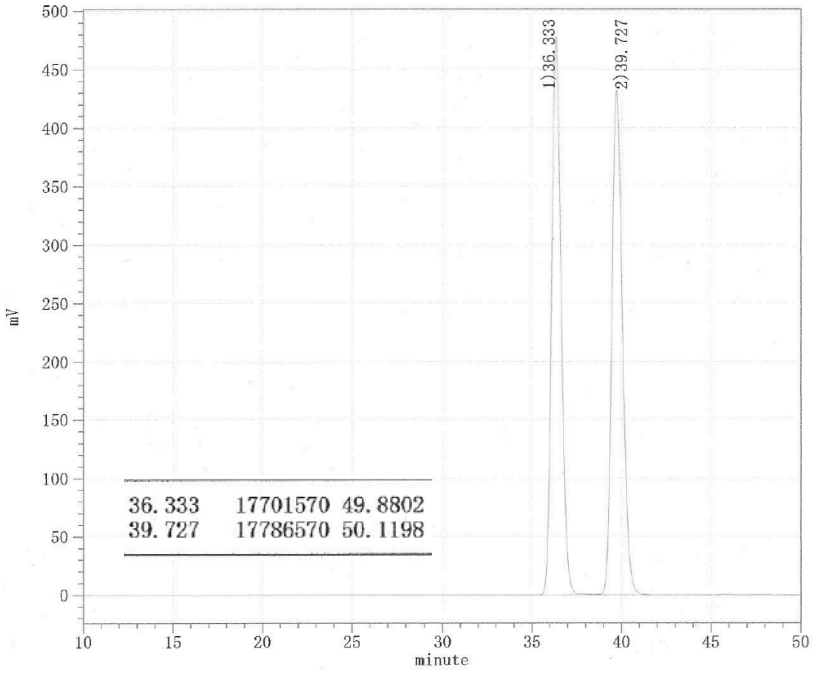

Br
N
O
S
O
Ph
8
1) 33.822
2) 37.623
mV
minute
33.822 7775567 39.2793
37.623 12020030 60.7207

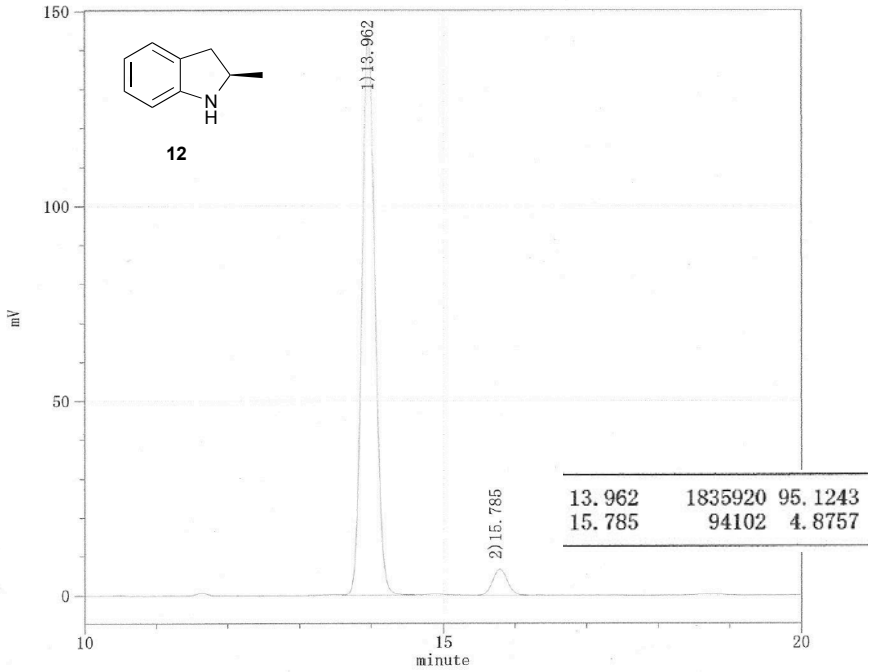

1) 33.867
2) 37.710
mV
minute
33.867 1200145 50.0982
37.710 1195439 49.9018

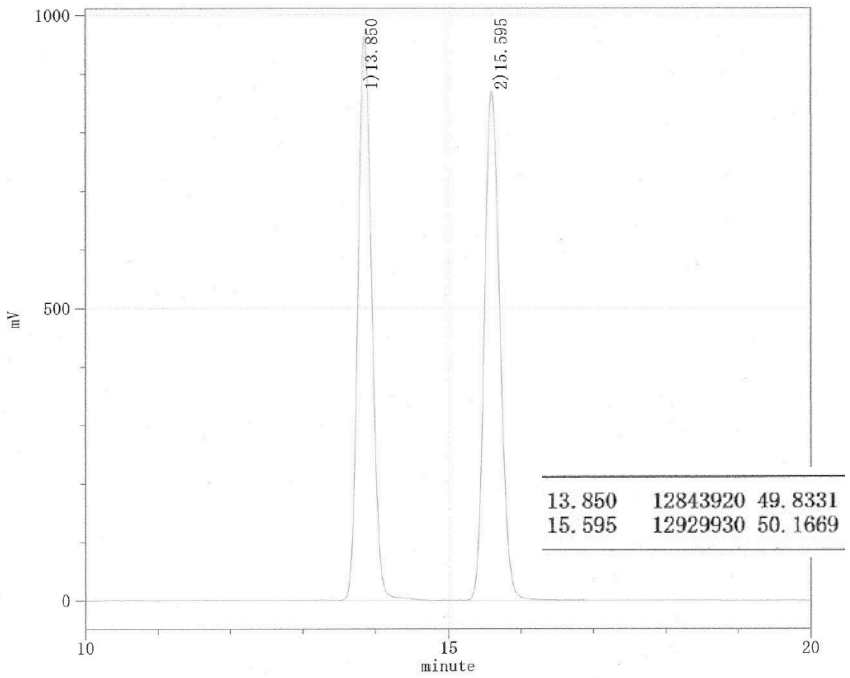

Br
N
S
O
O
Ph
10
1) 27.337
2) 34.030
mV
minute
27.337 22834880 66.7803
34.030 11359180 33.2197

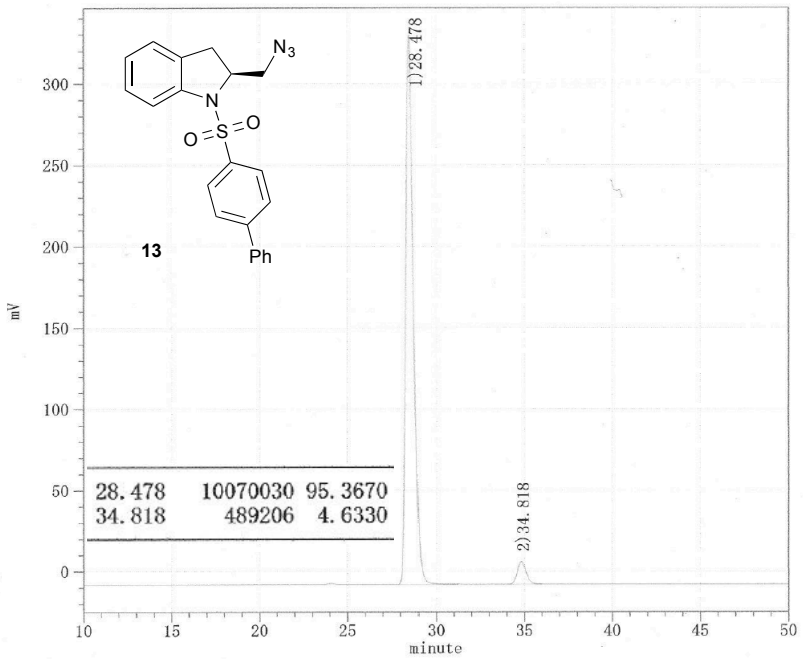

1) 28.723
2) 36.223
mV
minute
28.723 10532540 49.9482
36.223 10554380 50.0518

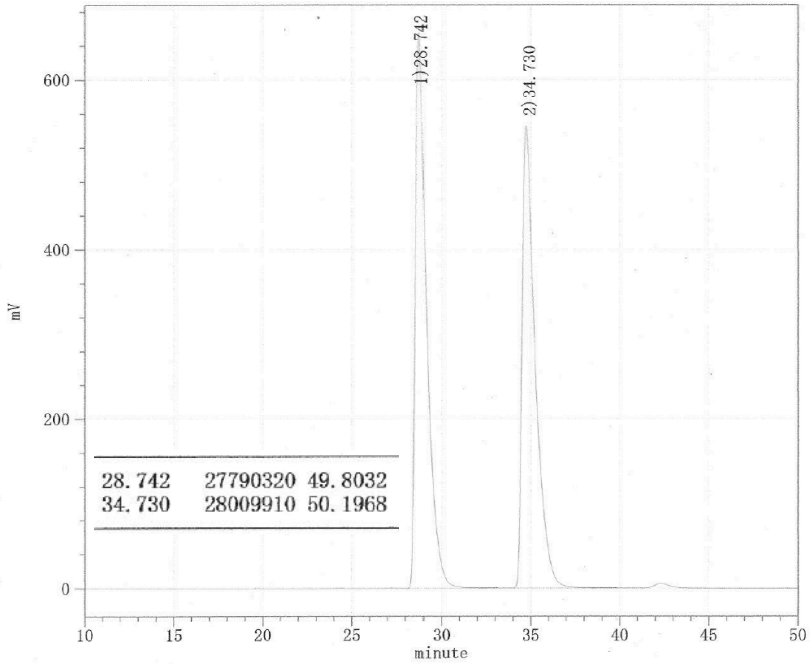

11
Ph
1) 34.973
2) 38.155
mV
minute
34.973 9196636 95.0078
38.155 483240 4.9922

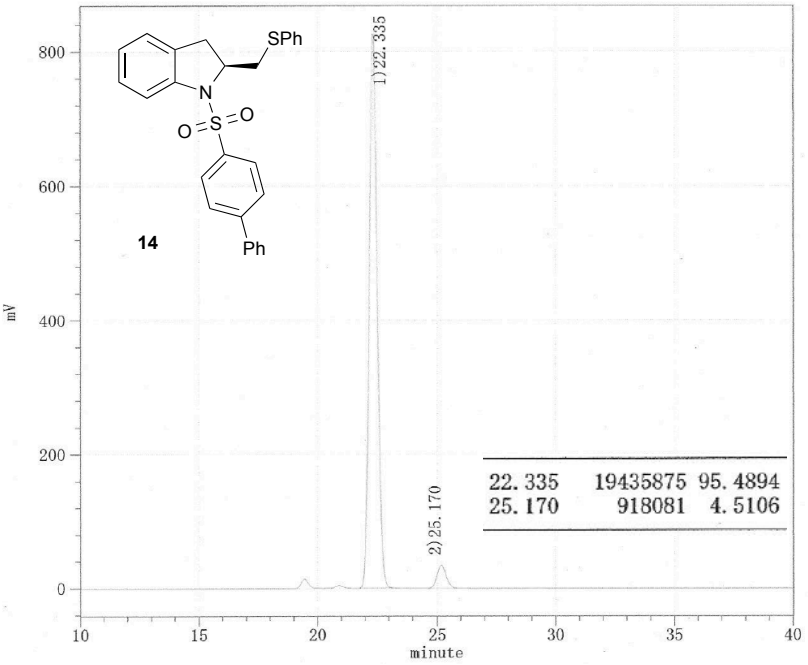

1) 36.333
2) 39.727
mV
minute
36.333 17701570 49.8802
39.727 17786570 50.1198

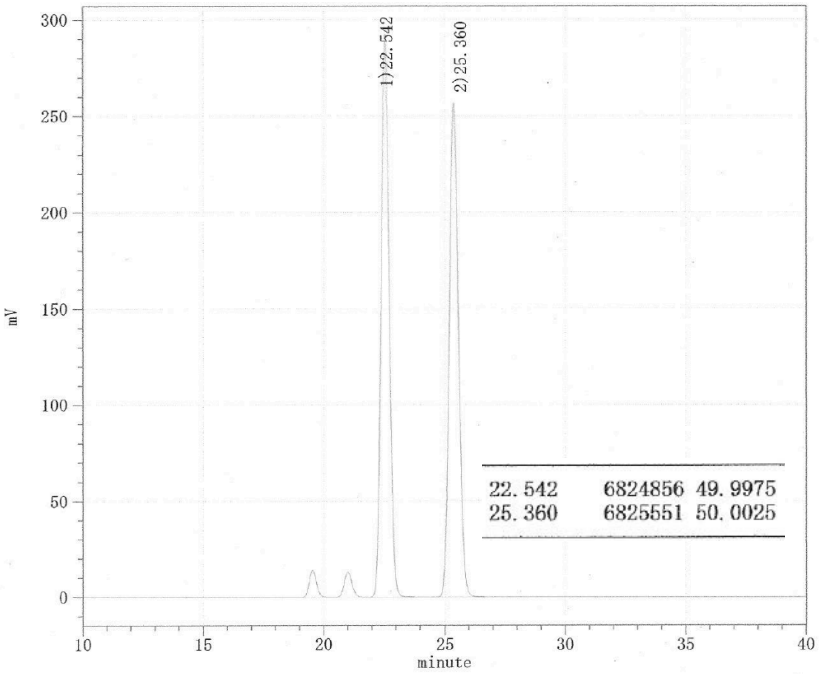

12
1)13.962
2)15.785
150
100
50
0
mV
10
15
20
minute
13.962 1835920 95.1243
15.785 94102 4.8757

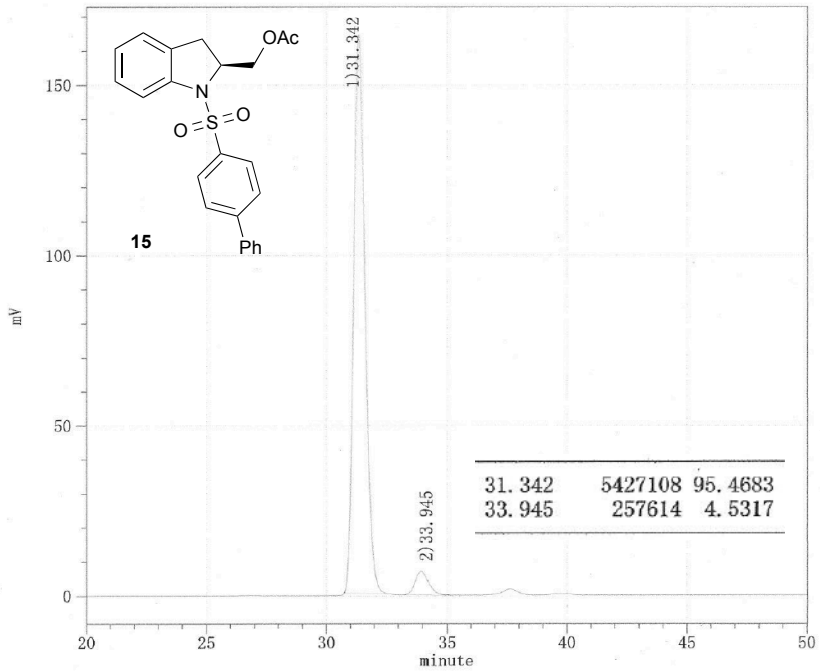

1)13.850
2)15.595
1000
500
0
mV
10
15
20
minute
13.850 12843920 49.8331
15.595 12929930 50.1669

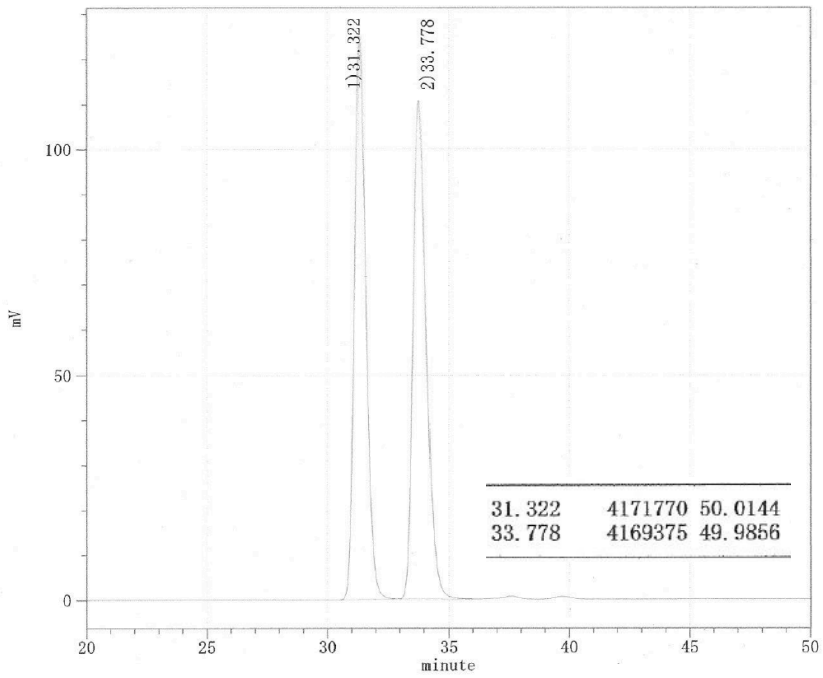

1) 28.478
2) 34.818
mV
minute
13
Ph
28.478 10070030 95.3670
34.818 489206 4.6330


1) 28.742
2) 34.730
mV
minute
28.742 27790320 49.8032
34.730 28009910 50.1968


SPh
N
O
S
O
Ph
14
1)22.335
2)25.170
mV
800
600
400
200
0
10
15
20
25
30
35
40
minute
22.335 19435875 95.4894
25.170 918081 4.5106

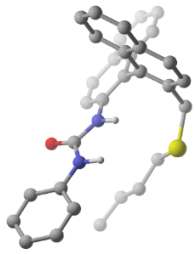

1)22.542
2)25.360
mV
300
250
200
150
100
50
0
10
15
20
25
30
35
40
minute
22.542 6824856 49.9975
25.360 6825551 50.0025


OAc
N
O
S
O
O
Ph
15
1)31.342
2)33.945
150
100
50
0
mV
20
25
30
35
40
45
50
minute
31.342 5427108 95.4683
33.945 257614 4.5317


1)31.322
2)33.778
100
50
0
mV
20
25
30
35
40
45
50
minute
31.322 4171770 50.0144
33.778 4169375 49.9856

Cartesian Coordinates

(*S*)-**1a**
SCF Done: E(RwB97XD) = -1820.55810244 A.U.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.601570	-3.442543	-2.014884
2	6	0	-2.371026	-2.210715	-1.455586
3	6	0	-2.202298	-2.066832	-0.051268
4	6	0	-2.282099	-3.232193	0.761402
5	6	0	-2.519402	-4.493234	0.154259
6	6	0	-2.673857	-4.599256	-1.204291
7	1	0	-2.729504	-3.532400	-3.089597
8	1	0	-2.318407	-1.331317	-2.089176
9	6	0	-1.950366	-0.793164	0.561298
10	6	0	-2.126792	-3.103418	2.166684
11	1	0	-2.575340	-5.374006	0.789054
12	1	0	-2.852915	-5.567518	-1.662271
13	6	0	-1.902457	-1.879126	2.730103
14	6	0	-1.807870	-0.704417	1.934402
15	1	0	-2.192305	-3.993465	2.787175
16	1	0	-1.789073	-1.788529	3.807516
17	6	0	-1.834398	0.408839	-0.321533
18	6	0	-2.991884	1.185373	-0.630148
19	6	0	-0.611541	0.740057	-0.887343
20	6	0	-4.267232	0.896440	-0.069884
21	6	0	-2.884082	2.282121	-1.530228
22	6	0	-0.507287	1.841993	-1.779565
23	6	0	-5.365029	1.654649	-0.391565
24	1	0	-4.366109	0.065226	0.621282
25	6	0	-4.038050	3.045485	-1.846271
26	6	0	-1.615999	2.578722	-2.091145
27	1	0	0.453677	2.077917	-2.214671
28	6	0	-5.254528	2.741472	-1.290592
29	1	0	-6.329790	1.419538	0.048747
30	1	0	-3.937929	3.876791	-2.539831
31	1	0	-1.528868	3.415019	-2.779894
32	1	0	-6.133489	3.329891	-1.536768
33	1	0	0.372804	-0.569984	0.327959
34	6	0	1.761080	-0.035590	-1.083241
35	8	0	2.042590	0.520622	-2.136170
36	1	0	2.329395	-1.115360	0.562566
37	6	0	4.022368	-0.978934	-0.574460
38	6	0	4.756968	-1.589730	0.451732
39	6	0	4.669161	-0.632509	-1.766555
40	6	0	6.111105	-1.850138	0.289664
41	1	0	4.259910	-1.856551	1.381412
42	6	0	6.029395	-0.897633	-1.911334
43	1	0	4.113615	-0.159251	-2.563730
44	6	0	6.759855	-1.505588	-0.894803
45	1	0	6.660129	-2.324368	1.098120
46	1	0	6.518701	-0.623551	-2.841827
47	1	0	7.819032	-1.707170	-1.021987
48	6	0	-1.514001	0.597767	2.633281
49	1	0	-1.827956	1.458889	2.039514
50	1	0	-2.047502	0.639880	3.586288
51	16	0	0.285946	0.789429	2.986874
52	6	0	0.695906	2.292567	2.026482
53	1	0	0.150356	2.253186	1.079695
54	1	0	0.358503	3.176886	2.576360
55	6	0	2.195770	2.358296	1.758185
56	1	0	2.747050	2.414700	2.706288
57	1	0	2.513162	1.433319	1.261526
58	6	0	2.564926	3.554519	0.878203
59	1	0	1.949963	3.534110	-0.031394
60	1	0	2.316645	4.486237	1.403149
61	6	0	4.041528	3.554062	0.489827
62	1	0	4.291615	4.426865	-0.123455
63	1	0	4.685267	3.572507	1.377564
64	1	0	4.292963	2.655977	-0.087022
65	7	0	2.655580	-0.763070	-0.328758
66	7	0	0.510533	-0.007411	-0.502413

NBS
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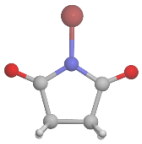
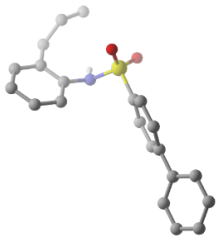


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.907983	1.181763	-0.000021
2	6	0	-0.907942	-1.181726	-0.000013
3	6	0	-2.364694	-0.766831	0.000024
4	6	0	-2.364715	0.766819	0.000066
5	1	0	-2.844609	-1.196081	0.883176
6	1	0	-2.844670	-1.196048	-0.883104
7	1	0	-2.844594	1.196014	0.883265
8	1	0	-2.844756	1.196101	-0.883000
9	8	0	-0.438555	2.291864	-0.000114
10	8	0	-0.438573	-2.291871	-0.000100
11	7	0	-0.159327	-0.000019	0.000050
12	35	0	1.679513	0.000001	0.000020

2g
SCF Done: E(RwB97XD) = -1415.11069861 A.U.

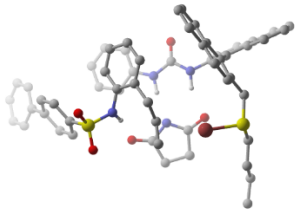


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.367559	2.500574	0.091346
2	6	0	3.981406	1.238277	-0.364096
3	6	0	2.613168	0.919889	-0.335330
4	6	0	1.676644	1.845042	0.127943
5	6	0	2.090828	3.085162	0.600401
6	6	0	3.441687	3.417648	0.579709
7	1	0	5.422790	2.761124	0.070484
8	1	0	0.620492	1.594726	0.109946
9	1	0	1.354402	3.793527	0.967546
10	1	0	3.775324	4.387064	0.937627
11	6	0	5.026046	0.252934	-0.853355
12	1	0	4.796441	-0.093269	-1.870269
13	6	0	5.184099	-0.934432	0.064215
14	1	0	5.383694	-0.699024	1.109159
15	6	0	5.088032	-2.205258	-0.319036
16	1	0	4.879688	-2.476046	-1.353057
17	1	0	5.211731	-3.022124	0.386858
18	1	0	5.983759	0.782645	-0.920942
19	7	0	2.153575	-0.342141	-0.813059
20	1	0	2.816462	-0.859353	-1.383097
21	16	0	1.413343	-1.430285	0.226630
22	8	0	1.852385	-1.236900	1.601952
23	8	0	1.590249	-2.724992	-0.421944
24	6	0	-0.301172	-0.970035	0.139793
25	6	0	-0.995862	-0.698949	1.312798
26	6	0	-0.931851	-0.922933	-1.102082
27	6	0	-2.344726	-0.369768	1.237397
28	1	0	-0.486209	-0.729282	2.269453
29	6	0	-2.277546	-0.593992	-1.162816
30	1	0	-0.379385	-1.136611	-2.011667
31	6	0	-3.003683	-0.313442	0.004279
32	1	0	-2.883894	-0.135277	2.150049
33	1	0	-2.775509	-0.571723	-2.127150
34	6	0	-4.444776	0.039796	-0.069385
35	6	0	-5.349800	-0.456293	0.877154
36	6	0	-4.924620	0.873509	-1.087026
37	6	0	-6.700274	-0.128171	0.806729
38	1	0	-4.998150	-1.121887	1.660720

39	6	0	-6.274584	1.204143	-1.154510
40	1	0	-4.233326	1.282696	-1.818747
41	6	0	-7.166876	0.703987	-0.208588
42	1	0	-7.390598	-0.528241	1.543709
43	1	0	-6.628537	1.859890	-1.944725
44	1	0	-8.220964	0.959732	-0.263869

CPs

SCF Done: E(RwB97XD) = -6169.96830804 A.U.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.333088	-4.523064	2.060651
2	6	0	-2.794854	-3.645685	1.112420
3	6	0	-3.460443	-2.449966	1.493861
4	6	0	-3.628370	-2.178249	2.880228
5	6	0	-3.148932	-3.110223	3.838006
6	6	0	-2.517388	-4.260193	3.438032
7	1	0	-1.816439	-5.426620	1.751239
8	1	0	-2.625608	-3.848768	0.060464
9	6	0	-3.964746	-1.518137	0.529681
10	6	0	-4.283735	-0.984014	3.276802
11	1	0	-3.290506	-2.893159	4.893576
12	1	0	-2.151720	-4.968589	4.175514
13	6	0	-4.722385	-0.088758	2.342650
14	6	0	-4.544515	-0.339152	0.956658
15	1	0	-4.433403	-0.788898	4.335018
16	1	0	-5.228234	0.813935	2.677039
17	6	0	-4.007762	-1.901329	-0.914274
18	6	0	-5.247571	-2.392277	-1.452260
19	6	0	-2.898069	-1.825907	-1.724931
20	6	0	-6.425695	-2.518142	-0.665738
21	6	0	-5.306962	-2.785446	-2.818484
22	6	0	-2.970129	-2.221598	-3.087722
23	6	0	-7.592674	-2.994598	-1.210567
24	1	0	-6.398524	-2.243965	0.383900
25	6	0	-6.527597	-3.271910	-3.354072
26	6	0	-4.136744	-2.689416	-3.618315
27	1	0	-2.077189	-2.141649	-3.698265
28	6	0	-7.649436	-3.372361	-2.570991
29	1	0	-8.479467	-3.085849	-0.590065
30	1	0	-6.555142	-3.565275	-4.400470
31	1	0	-4.187198	-2.986265	-4.662502
32	1	0	-8.578264	-3.748082	-2.989805
33	1	0	-1.641958	-0.271329	-1.242187
34	6	0	-0.524038	-2.032036	-1.387461
35	8	0	-0.560173	-3.243497	-1.593900
36	1	0	0.500315	-0.267216	-1.211041
37	6	0	1.933920	-1.729039	-1.502633
38	6	0	2.925383	-0.743498	-1.620414
39	6	0	2.306089	-3.078221	-1.579222
40	6	0	4.253850	-1.100015	-1.812707
41	1	0	2.656507	0.306212	-1.531304
42	6	0	3.643848	-3.418111	-1.768083
43	1	0	1.550808	-3.844855	-1.481552
44	6	0	4.627938	-2.440710	-1.887946
45	1	0	5.003448	-0.319677	-1.899331
46	1	0	3.912603	-4.470117	-1.821532
47	1	0	5.668108	-2.713735	-2.040993
48	6	0	-5.043062	0.632094	-0.084889
49	1	0	-4.477292	0.548796	-1.015060
50	1	0	-6.111391	0.507218	-0.301592
51	16	0	-4.927671	2.388001	0.432019
52	6	0	-4.774112	3.210563	-1.192070
53	1	0	-3.932185	2.726083	-1.702415
54	1	0	-5.712508	2.966514	-1.703567
55	6	0	-4.585111	4.712879	-1.031993
56	1	0	-5.443469	5.154118	-0.512101
57	1	0	-3.695680	4.909515	-0.420761
58	6	0	-4.411493	5.371468	-2.403112
59	1	0	-3.595662	4.873515	-2.941350
60	1	0	-5.322223	5.218646	-2.994870
61	6	0	-4.111521	6.862742	-2.282096
62	1	0	-4.001452	7.322029	-3.270024
63	1	0	-4.916768	7.387471	-1.754918
64	1	0	-3.180395	7.030680	-1.728304
65	7	0	0.622135	-1.286861	-1.284319
66	7	0	-1.681271	-1.295366	-1.218125
67	6	0	1.041837	2.596904	-1.195630
68	6	0	-1.066038	2.156468	-1.714242
69	6	0	-0.945152	3.651159	-1.999417
70	6	0	0.523585	3.940218	-1.706170
71	1	0	-1.629784	4.195672	-1.340440
72	1	0	-1.246062	3.856962	-3.030688
73	1	0	0.684957	4.708639	-0.945109
74	1	0	1.093694	4.230882	-2.593994
75	8	0	2.181865	2.435637	-0.746691
76	8	0	-2.121623	1.518746	-1.842563
77	7	0	0.097830	1.621155	-1.277388
78	6	0	0.214061	-1.781455	2.839818
79	6	0	0.717966	-0.501716	2.603916
80	6	0	1.979657	-0.390053	1.997579
81	6	0	2.713649	-1.528416	1.669517
82	6	0	2.206566	-2.794030	1.941208
83	6	0	0.948124	-2.919454	2.519351
84	1	0	-0.771491	-1.889190	3.283955
85	1	0	3.674873	-1.418222	1.178570
86	1	0	2.782814	-3.674783	1.675360
87	1	0	0.527644	-3.901607	2.713482
88	6	0	-0.089882	0.715331	3.007525
89	1	0	-1.110426	0.382062	3.238839
90	6	0	-0.161924	1.765491	1.936841
91	1	0	-0.159965	1.392447	0.914149
92	6	0	-0.226086	3.089981	2.143591
93	1	0	-0.207026	3.518767	3.143399
94	1	0	-0.221440	3.788333	1.309501
95	1	0	0.316417	1.152289	3.928192
96	7	0	2.482724	0.915616	1.697252
97	1	0	2.310286	1.326674	0.767105
98	16	0	3.787271	1.566679	2.451750
99	8	0	3.900751	0.937332	3.761878
100	8	0	3.661274	3.014668	2.342061
101	6	0	5.208297	1.100210	1.482011
102	6	0	5.971599	-0.001202	1.855666
103	6	0	5.488152	1.806800	0.314655
104	6	0	7.019659	-0.407811	1.038953
105	1	0	5.749441	-0.532535	2.775115
106	6	0	6.543248	1.394918	-0.488298
107	1	0	4.873915	2.653113	0.024957
108	6	0	7.314539	0.275703	-0.146736
109	1	0	7.622965	-1.260567	1.335063
110	1	0	6.744274	1.926698	-1.413591
111	6	0	8.399883	-0.197134	-1.043825
112	6	0	8.598758	-1.568211	-1.250659
113	6	0	9.230868	0.710556	-1.711777
114	6	0	9.598923	-2.019215	-2.106553
115	1	0	7.951353	-2.286103	-0.754402
116	6	0	10.232574	0.258793	-2.565606
117	1	0	9.103394	1.777361	-1.549577
118	6	0	10.419377	-1.107152	-2.766785
119	1	0	9.733270	-3.085655	-2.262554
120	1	0	10.872002	0.976495	-3.071493
121	1	0	11.198903	-1.458681	-3.436357
122	35	0	-2.857441	2.532407	1.232445

CPr

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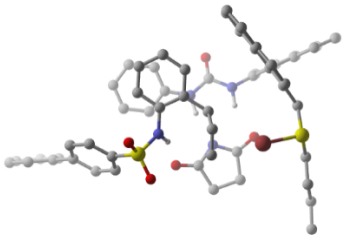

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3	6	0	3.534788	-2.555736	-1.205886
4	6	0	3.596551	-2.415047	-2.620648
5	6	0	3.126281	-3.467179	-3.449795
6	6	0	2.605306	-4.610183	-2.899621

7	1	0	2.099750	-5.646354	-1.064087
8	1	0	2.899391	-3.861845	0.407274
9	6	0	4.012745	-1.491802	-0.372466
10	6	0	4.139236	-1.227719	-3.174522
11	1	0	3.183011	-3.344881	-4.528135
12	1	0	2.243271	-5.409067	-3.540076
13	6	0	4.568638	-0.215629	-2.363999
14	6	0	4.480084	-0.326999	-0.951379
15	1	0	4.212278	-1.132256	-4.254157
16	1	0	4.992977	0.674728	-2.820577
17	6	0	4.129041	-1.707161	1.102336
18	6	0	5.415912	-2.023029	1.657122
19	6	0	3.032169	-1.635012	1.932178
20	6	0	6.589673	-2.120025	0.859801
21	6	0	5.532456	-2.256310	3.056357
22	6	0	3.156240	-1.888660	3.323216
23	6	0	7.807222	-2.406948	1.425698
24	1	0	6.518668	-1.970620	-0.212707
25	6	0	6.804568	-2.550422	3.612468
26	6	0	4.369603	-2.191968	3.869755
27	1	0	2.268075	-1.826494	3.943171
28	6	0	7.920899	-2.619246	2.818312
29	1	0	8.690766	-2.475808	0.797711
30	1	0	6.876635	-2.721843	4.683445
31	1	0	4.463052	-2.376315	4.936536
32	1	0	8.890119	-2.842342	3.254246
33	1	0	1.671368	-0.227124	1.296165
34	6	0	0.672422	-2.045522	1.575337
35	8	0	0.779966	-3.239979	1.843789
36	1	0	-0.458258	-0.359674	1.337072
37	6	0	-1.791877	-1.955640	1.308926
38	6	0	-2.892536	-1.091325	1.400723
39	6	0	-2.015074	-3.322400	1.098021
40	6	0	-4.185421	-1.584234	1.273545
41	1	0	-2.726534	-0.025766	1.539724
42	6	0	-3.317390	-3.800705	0.980869
43	1	0	-1.173364	-3.996347	1.019920
44	6	0	-4.411059	-2.943095	1.064603
45	1	0	-5.021715	-0.893994	1.332458
46	1	0	-3.471909	-4.863014	0.811025
47	1	0	-5.422995	-3.324875	0.964747
48	6	0	4.937727	0.786359	-0.039401
49	1	0	4.366949	0.798924	0.891497
50	1	0	6.010071	0.730648	0.188144
51	16	0	4.760907	2.459237	-0.767747
52	6	0	4.672232	3.484697	0.738379
53	1	0	3.893407	3.037866	1.367556
54	1	0	5.654815	3.341180	1.203938
55	6	0	4.410053	4.945685	0.399945
56	1	0	5.198859	5.334181	-0.255148
57	1	0	3.461226	5.036761	-0.142843
58	6	0	4.343338	5.777819	1.683408
59	1	0	3.584933	5.351277	2.351615
60	1	0	5.303592	5.707297	2.208811
61	6	0	4.013402	7.240120	1.397885
62	1	0	3.975769	7.819670	2.326081
63	1	0	4.767401	7.696002	0.745823
64	1	0	3.039834	7.334221	0.902876
65	7	0	-0.514538	-1.384299	1.387749
66	7	0	1.776620	-1.237846	1.405263
67	6	0	-1.009849	2.446326	1.213663
68	6	0	1.161511	2.207168	1.552582
69	6	0	0.959464	3.716913	1.654024
70	6	0	-0.553168	3.869203	1.526913
71	1	0	1.501586	4.198123	0.832745
72	1	0	1.378497	4.091307	2.592037
73	1	0	-0.873320	4.545830	0.730188
74	1	0	-1.031161	4.201175	2.454106
75	8	0	-2.169079	2.154619	0.899277
76	8	0	2.265799	1.654216	1.657545
77	7	0	0.005386	1.549405	1.304948
78	6	0	-0.278343	-2.268396	-2.307398
79	6	0	-0.696138	-0.978941	-1.976774
80	6	0	-2.074519	-0.730085	-1.879116
81	6	0	-2.992034	-1.752111	-2.124075
82	6	0	-2.553896	-3.020174	-2.486195
83	6	0	-1.190580	-3.284445	-2.569856
84	1	0	0.786833	-2.472822	-2.361441
85	1	0	-4.052468	-1.561527	-2.006992
86	1	0	-3.281411	-3.805235	-2.669717
87	1	0	-0.834930	-4.277645	-2.828472
88	6	0	0.326378	0.102205	-1.703505
89	1	0	0.150526	0.558631	-0.724212
90	6	0	0.349547	1.178595	-2.756153
91	1	0	0.702587	0.879047	-3.743158
92	6	0	-0.032953	2.448080	-2.553982
93	1	0	-0.448937	2.771102	-1.602758
94	1	0	-0.004604	3.183549	-3.353691
95	1	0	1.316528	-0.367599	-1.656028
96	7	0	-2.501453	0.570004	-1.497889
97	1	0	-2.190755	0.986095	-0.610673
98	16	0	-3.731014	1.407323	-2.192571
99	8	0	-3.950943	0.861462	-3.525585
100	8	0	-3.429054	2.821955	-2.020999
101	6	0	-5.178761	1.069713	-1.207266
102	6	0	-6.143240	0.185073	-1.675975
103	6	0	-5.306340	1.680856	0.038778
104	6	0	-7.245458	-0.102901	-0.879831
105	1	0	-6.031481	-0.279357	-2.650224
106	6	0	-6.417151	1.391311	0.820081
107	1	0	-4.540435	2.362394	0.395746
108	6	0	-7.399095	0.493307	0.377273
109	1	0	-7.984860	-0.813819	-1.235709
110	1	0	-6.528644	1.879062	1.783875
111	6	0	-8.572225	0.167847	1.229258
112	6	0	-9.843290	0.007014	0.664157
113	6	0	-8.426353	0.003650	2.612405
114	6	0	-10.939496	-0.310660	1.460309
115	1	0	-9.979844	0.151341	-0.404017
116	6	0	-9.522766	-0.315473	3.408024
117	1	0	-7.444618	0.104434	3.067039
118	6	0	-10.782684	-0.474094	2.834916
119	1	0	-11.918754	-0.425505	1.004726
120	1	0	-9.389106	-0.448761	4.477585
121	1	0	-11.637803	-0.724323	3.456128
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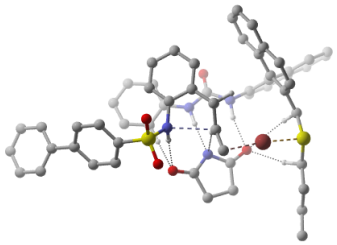

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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4	6	0	-3.511374	-2.246469	2.836165
5	6	0	-3.060179	-3.253945	3.729663
6	6	0	-2.540769	-4.430048	3.251481
7	1	0	-2.007405	-5.566564	1.483929
8	1	0	-2.776476	-3.859512	-0.096889
9	6	0	-3.933735	-1.470517	0.535793
10	6	0	-4.045111	-1.021176	3.311403
11	1	0	-3.132333	-3.072882	4.798978
12	1	0	-2.196389	-5.195468	3.940633
13	6	0	-4.474420	-0.063113	2.435687
14	6	0	-4.410787	-0.273055	1.033570
15	1	0	-4.113756	-0.853974	4.382855
16	1	0	-4.884840	0.861810	2.832028
17	6	0	-4.077401	-1.795810	-0.915800
18	6	0	-5.355942	-2.250451	-1.388332
19	6	0	-3.024573	-1.699175	-1.796484
20	6	0	-6.478646	-2.393556	-0.527470
21	6	0	-5.513011	-2.590019	-2.761203
22	6	0	-3.193290	-2.037776	-3.165591
23	6	0	-7.685567	-2.838094	-1.008008
24	1	0	-6.375701	-2.155498	0.526297
25	6	0	-6.773700	-3.043872	-3.229387
26	6	0	-4.399069	-2.471779	-3.634975
27	1	0	-2.342440	-1.941419	-3.831972
28	6	0	-7.839473	-3.164684	-2.374272
29	1	0	-8.528487	-2.943038	-0.331136
30	1	0	-6.877500	-3.295767	-4.281730
31	1	0	-4.523516	-2.725741	-4.684324
32	1	0	-8.799446	-3.515303	-2.741747
33	1	0	-1.694473	-0.181618	-1.391521
34	6	0	-0.643444	-1.978193	-1.573725
35	8	0	-0.723762	-3.186486	-1.783883
36	1	0	0.443222	-0.246430	-1.424363

37	6	0	1.826367	-1.753798	-1.719275
38	6	0	2.850100	-0.800413	-1.828426
39	6	0	2.156429	-3.113803	-1.789993
40	6	0	4.171170	-1.198023	-1.991255
41	1	0	2.612137	0.257581	-1.754120
42	6	0	3.485999	-3.495526	-1.954838
43	1	0	1.376123	-3.856398	-1.701541
44	6	0	4.503595	-2.550202	-2.054443
45	1	0	4.946563	-0.440647	-2.062658
46	1	0	3.722737	-4.555442	-2.002393
47	1	0	5.537107	-2.858399	-2.182727
48	6	0	-4.914473	0.763032	0.053537
49	1	0	-4.332302	0.734353	-0.870084
50	1	0	-5.970374	0.605913	-0.194695
51	16	0	-4.811015	2.484995	0.668337
52	6	0	-4.678071	3.380598	-0.918191
53	1	0	-3.873182	2.900078	-1.486897
54	1	0	-5.632984	3.223384	-1.430638
55	6	0	-4.403563	4.861079	-0.684484
56	1	0	-5.204812	5.310060	-0.084919
57	1	0	-3.471371	4.973367	-0.116383
58	6	0	-4.279667	5.602195	-2.017851
59	1	0	-3.521423	5.106731	-2.636925
60	1	0	-5.229270	5.525843	-2.561956
61	6	0	-3.906778	7.069667	-1.827165
62	1	0	-3.824227	7.582623	-2.791216
63	1	0	-4.659975	7.595879	-1.229208
64	1	0	-2.943335	7.166049	-1.312517
65	7	0	0.528880	-1.268634	-1.508214
66	7	0	-1.766721	-1.204148	-1.352727
67	6	0	1.115181	2.587653	-1.328786
68	6	0	-1.023098	2.237023	-1.801021
69	6	0	-0.854343	3.733357	-2.049094
70	6	0	0.632795	3.961307	-1.791444
71	1	0	-1.501936	4.283530	-1.358013
72	1	0	-1.175365	3.977807	-3.065672
73	1	0	0.845056	4.705600	-1.018895
74	1	0	1.187469	4.252152	-2.688942
75	8	0	2.260689	2.366789	-0.918381
76	8	0	-2.096909	1.635373	-1.929310
77	7	0	0.133473	1.651467	-1.402046
78	6	0	0.278212	-2.131245	2.555521
79	6	0	0.689378	-0.817928	2.334404
80	6	0	1.949642	-0.598743	1.760907
81	6	0	2.780632	-1.670116	1.439574
82	6	0	2.363710	-2.973355	1.687817
83	6	0	1.106950	-3.202761	2.239247
84	1	0	-0.704815	-2.315306	2.978003
85	1	0	3.741300	-1.482445	0.971675
86	1	0	3.010959	-3.804097	1.425119
87	1	0	0.761922	-4.217442	2.414832
88	6	0	-0.209129	0.340214	2.716225
89	1	0	-1.246108	-0.022896	2.739636
90	6	0	-0.132878	1.461850	1.735938
91	1	0	-0.060195	1.181574	0.686628
92	6	0	-0.224828	2.795755	2.036541
93	1	0	-0.249976	3.137079	3.068359
94	1	0	-0.001764	3.537665	1.275354
95	1	0	0.024654	0.702117	3.724322
96	7	0	2.331806	0.756699	1.495245
97	1	0	2.297266	1.107669	0.524836
98	16	0	3.534947	1.497333	2.361744
99	8	0	3.563022	0.882995	3.682330
100	8	0	3.321697	2.931399	2.224332
101	6	0	5.039418	1.091614	1.502167
102	6	0	5.862746	0.078120	1.981576
103	6	0	5.311350	1.737545	0.297771
104	6	0	6.969719	-0.302487	1.232315
105	1	0	5.640094	-0.407923	2.925560
106	6	0	6.422699	1.349556	-0.437386
107	1	0	4.643567	2.507472	-0.075800
108	6	0	7.257844	0.316662	0.010202
109	1	0	7.623113	-1.083824	1.608238
110	1	0	6.622694	1.830696	-1.390106
111	6	0	8.409412	-0.131610	-0.813626
112	6	0	8.706558	-1.495121	-0.933477
113	6	0	9.207880	0.793609	-1.496703
114	6	0	9.774209	-1.921614	-1.717424
115	1	0	8.084141	-2.227788	-0.426907
116	6	0	10.277584	0.366639	-2.277579
117	1	0	9.002496	1.856183	-1.399986
118	6	0	10.563548	-0.992250	-2.391393
119	1	0	9.984476	-2.983402	-1.807851
120	1	0	10.891664	1.098036	-2.795036
121	1	0	11.396653	-1.325166	-3.003520
122	35	0	-2.500139	2.500315	1.370005

TS2r

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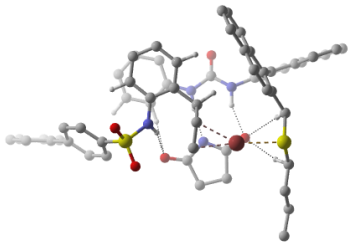

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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3	6	0	3.599919	-2.453590	-1.261188
4	6	0	3.569841	-2.281289	-2.673683
5	6	0	3.126692	-3.346870	-3.501149
6	6	0	2.720710	-4.536103	-2.952452
7	1	0	2.394596	-5.642764	-1.117303
8	1	0	3.143326	-3.833736	0.351073
9	6	0	4.050698	-1.375826	-0.429985
10	6	0	3.998915	-1.047628	-3.224875
11	1	0	3.111983	-3.197875	-4.577722
12	1	0	2.380191	-5.345678	-3.591319
13	6	0	4.405690	-0.026789	-2.412295
14	6	0	4.410639	-0.168102	-0.999743
15	1	0	4.003282	-0.923032	-4.304306
16	1	0	4.738843	0.902004	-2.867244
17	6	0	4.240932	-1.622367	1.032616
18	6	0	5.558686	-1.921030	1.519333
19	6	0	3.181249	-1.613352	1.912687
20	6	0	6.696624	-1.955139	0.667059
21	6	0	5.745283	-2.204512	2.901708
22	6	0	3.375463	-1.910886	3.286757
23	6	0	7.945147	-2.233668	1.165218
24	1	0	6.572522	-1.762475	-0.393668
25	6	0	7.048535	-2.487445	3.387615
26	6	0	4.619600	-2.200289	3.767999
27	1	0	2.515528	-1.894527	3.948325
28	6	0	8.127894	-2.498614	2.541388
29	1	0	8.799739	-2.253728	0.495120
30	1	0	7.174565	-2.696479	4.446838
31	1	0	4.765436	-2.419716	4.822292
32	1	0	9.121383	-2.714575	2.923073
33	1	0	1.757118	-0.219330	1.412402
34	6	0	0.813334	-2.074272	1.645424
35	8	0	0.953963	-3.276186	1.858269
36	1	0	-0.368656	-0.404500	1.510390
37	6	0	-1.667963	-2.014682	1.469299
38	6	0	-2.771270	-1.152785	1.564859
39	6	0	-1.891264	-3.382698	1.269122
40	6	0	-4.064493	-1.646239	1.448395
41	1	0	-2.608728	-0.086523	1.700796
42	6	0	-3.194558	-3.862517	1.163628
43	1	0	-1.048877	-4.056061	1.190329
44	6	0	-4.289531	-3.006592	1.247569
45	1	0	-4.900429	-0.954739	1.506956
46	1	0	-3.348539	-4.926167	1.001956
47	1	0	-5.300957	-3.391414	1.155202
48	6	0	4.844362	0.962988	-0.091133
49	1	0	4.243340	0.967596	0.821263
50	1	0	5.900572	0.869223	0.185232
51	16	0	4.664101	2.630934	-0.830272
52	6	0	4.513235	3.635206	0.684977
53	1	0	3.746872	3.160299	1.307016
54	1	0	5.480144	3.570683	1.195017
55	6	0	4.161835	5.078515	0.343020
56	1	0	4.929149	5.512788	-0.309913
57	1	0	3.216008	5.104296	-0.214473
58	6	0	4.029609	5.920754	1.613570
59	1	0	3.295109	5.453718	2.281540
60	1	0	4.987375	5.917595	2.148886
61	6	0	3.609702	7.357279	1.315047
62	1	0	3.522060	7.940494	2.237807
63	1	0	4.340406	7.857424	0.668703
64	1	0	2.638558	7.385592	0.806749
65	7	0	-0.395924	-1.431661	1.535399

66	7	0	1.890428	-1.233823	1.458916
67	6	0	-1.107035	2.409516	1.339462
68	6	0	1.070440	2.189597	1.662514
69	6	0	0.852982	3.695867	1.771056
70	6	0	-0.664116	3.831076	1.676393
71	1	0	1.371147	4.179588	0.935585
72	1	0	1.289504	4.077102	2.697796
73	1	0	-1.010583	4.523176	0.904428
74	1	0	-1.126386	4.132211	2.622036
75	8	0	-2.263758	2.110421	1.018159
76	8	0	2.176120	1.644734	1.764547
77	7	0	-0.083049	1.523216	1.408510
78	6	0	-0.252236	-2.407889	-2.072755
79	6	0	-0.651571	-1.104130	-1.780995
80	6	0	-2.022367	-0.812986	-1.729708
81	6	0	-2.958844	-1.815851	-1.978117
82	6	0	-2.541934	-3.101680	-2.302027
83	6	0	-1.184243	-3.403360	-2.341879
84	1	0	0.807588	-2.641141	-2.083714
85	1	0	-4.017228	-1.598576	-1.894968
86	1	0	-3.283475	-3.872144	-2.489957
87	1	0	-0.849087	-4.410856	-2.569243
88	6	0	0.389679	-0.055794	-1.452838
89	1	0	0.208586	0.372669	-0.463106
90	6	0	0.436313	1.051980	-2.457255
91	1	0	0.764518	0.799585	-3.464825
92	6	0	0.024123	2.349328	-2.205856
93	1	0	-0.465435	2.600760	-1.271953
94	1	0	-0.038632	3.072768	-3.012961
95	1	0	1.370349	-0.541822	-1.429928
96	7	0	-2.406755	0.517209	-1.397931
97	1	0	-2.210564	0.889585	-0.457191
98	16	0	-3.600610	1.359418	-2.162074
99	8	0	-3.745778	0.807095	-3.502119
100	8	0	-3.280177	2.769662	-1.983749
101	6	0	-5.096956	1.036597	-1.250310
102	6	0	-6.051604	0.170896	-1.772922
103	6	0	-5.262271	1.623432	0.002899
104	6	0	-7.180886	-0.127267	-1.019612
105	1	0	-5.909264	-0.274392	-2.752147
106	6	0	-6.399165	1.322200	0.740676
107	1	0	-4.504285	2.290785	0.401212
108	6	0	-7.369319	0.438115	0.247099
109	1	0	-7.912327	-0.825526	-1.414745
110	1	0	-6.539096	1.789159	1.711121
111	6	0	-8.565283	0.093947	1.058946
112	6	0	-9.821959	-0.051429	0.458591
113	6	0	-8.454227	-0.103222	2.441047
114	6	0	-10.938161	-0.384785	1.219877
115	1	0	-9.932236	0.117035	-0.609108
116	6	0	-9.570514	-0.438063	3.201634
117	1	0	-7.484080	-0.014988	2.922222
118	6	0	-10.816046	-0.579948	2.593906
119	1	0	-11.906145	-0.487315	0.738055
120	1	0	-9.463544	-0.596052	4.270865
121	1	0	-11.687111	-0.841577	3.187675
122	35	0	2.253282	2.379897	-1.619587

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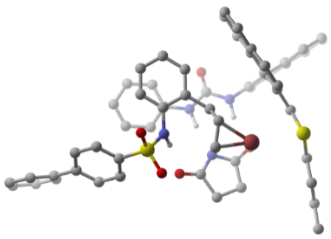

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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3	6	0	-3.546870	-2.425030	1.282625
4	6	0	-3.380183	-2.208613	2.679500
5	6	0	-2.950573	-3.280782	3.507002
6	6	0	-2.692924	-4.516511	2.972229
7	1	0	-2.625498	-5.708658	1.161563
8	1	0	-3.349177	-3.884785	-0.309500
9	6	0	-3.989702	-1.348120	0.451768
10	6	0	-3.654896	-0.923895	3.209035
11	1	0	-2.827403	-3.100563	4.571773
12	1	0	-2.364056	-5.331012	3.610905
13	6	0	-4.068943	0.094314	2.391863
14	6	0	-4.229978	-0.097391	0.995330
15	1	0	-3.544862	-0.757597	4.277458
16	1	0	-4.287812	1.061665	2.834370
17	6	0	-4.287874	-1.623592	-0.987653
18	6	0	-5.616443	-2.026484	-1.350885
19	6	0	-3.319641	-1.529021	-1.962266
20	6	0	-6.656613	-2.156210	-0.390583
21	6	0	-5.911003	-2.320755	-2.711474
22	6	0	-3.624153	-1.819334	-3.317641
23	6	0	-7.917088	-2.550864	-0.764574
24	1	0	-6.446668	-1.942283	0.652413
25	6	0	-7.224771	-2.723781	-3.068004
26	6	0	-4.882373	-2.204596	-3.683751
27	1	0	-2.834606	-1.724550	-4.056563
28	6	0	-8.207576	-2.837877	-2.118085
29	1	0	-8.697638	-2.644534	-0.015127
30	1	0	-7.435060	-2.942384	-4.111935
31	1	0	-5.111416	-2.423925	-4.723161
32	1	0	-9.209377	-3.147846	-2.400891
33	1	0	-1.875513	-0.072006	-1.699968
34	6	0	-0.938984	-1.942054	-1.782681
35	8	0	-1.084898	-3.154902	-1.909673
36	1	0	0.251859	-0.270916	-1.708662
37	6	0	1.550350	-1.873949	-1.666978
38	6	0	2.647207	-0.998195	-1.707897
39	6	0	1.785685	-3.247703	-1.524331
40	6	0	3.943985	-1.484675	-1.605613
41	1	0	2.476270	0.071727	-1.795936
42	6	0	3.093021	-3.718997	-1.430439
43	1	0	0.948838	-3.930955	-1.486690
44	6	0	4.180542	-2.850916	-1.467155
45	1	0	4.773782	-0.784141	-1.627317
46	1	0	3.255422	-4.787426	-1.315358
47	1	0	5.195022	-3.230008	-1.385614
48	6	0	-4.676153	1.014469	0.066990
49	1	0	-3.973718	1.089080	-0.768494
50	1	0	-5.663897	0.786118	-0.347589
51	16	0	-4.745165	2.674983	0.831200
52	6	0	-4.701946	3.691088	-0.685688
53	1	0	-3.930137	3.276101	-1.342834
54	1	0	-5.669511	3.603681	-1.190874
55	6	0	-4.400723	5.147027	-0.344796
56	1	0	-5.153456	5.535189	0.353943
57	1	0	-3.431843	5.211268	0.169476
58	6	0	-4.370477	6.022066	-1.599517
59	1	0	-3.636592	5.614653	-2.307195
60	1	0	-5.346377	5.970009	-2.098930
61	6	0	-4.029152	7.477131	-1.288620
62	1	0	-4.018189	8.084594	-2.200158
63	1	0	-4.762341	7.915982	-0.601371
64	1	0	-3.041407	7.559722	-0.819303
65	7	0	0.276080	-1.297246	-1.741869
66	7	0	-2.008396	-1.086343	-1.629564
67	6	0	1.006094	2.551130	-1.177903
68	6	0	-1.115588	2.335921	-1.762179
69	6	0	-0.915892	3.848251	-1.739478
70	6	0	0.569326	3.993481	-1.421897
71	1	0	-1.564521	4.278757	-0.968503
72	1	0	-1.217932	4.277576	-2.698341
73	1	0	0.783555	4.598953	-0.536323
74	1	0	1.150180	4.408336	-2.251419
75	8	0	2.130179	2.244837	-0.753431
76	8	0	-2.191114	1.789014	-2.026464
77	7	0	0.019453	1.662181	-1.437955
78	6	0	0.231810	-2.522582	1.810478
79	6	0	0.656617	-1.210246	1.608566
80	6	0	2.030904	-0.930083	1.641938
81	6	0	2.946114	-1.955509	1.871666
82	6	0	2.502216	-3.252666	2.101399
83	6	0	1.142114	-3.540823	2.067768
84	1	0	-0.827596	-2.746712	1.754388
85	1	0	4.008970	-1.745557	1.855581
86	1	0	3.227954	-4.040305	2.279192
87	1	0	0.787458	-4.554739	2.224931
88	6	0	-0.365042	-0.141092	1.272036
89	1	0	-0.141942	0.330613	0.311323
90	6	0	-0.436226	0.911565	2.332249
91	1	0	-0.797130	0.612595	3.315234
92	6	0	0.196768	2.203395	2.229190
93	1	0	0.805623	2.443041	1.364902
94	1	0	0.380054	2.774441	3.134418
95	1	0	-1.347061	-0.613761	1.191039
96	7	0	2.436103	0.415457	1.421789

97	1	0	2.247633	0.858993	0.508046
98	16	0	3.648510	1.176539	2.247554
99	8	0	3.784596	0.523537	3.541691
100	8	0	3.338651	2.599154	2.179150
101	6	0	5.133242	0.902627	1.307435
102	6	0	6.095671	0.020209	1.784852
103	6	0	5.282467	1.543810	0.078778
104	6	0	7.219135	-0.239134	1.009531
105	1	0	5.963477	-0.467343	2.745096
106	6	0	6.413057	1.278661	-0.681949
107	1	0	4.520619	2.228817	-0.281882
108	6	0	7.391744	0.379064	-0.234516
109	1	0	7.957476	-0.949526	1.368297
110	1	0	6.541287	1.784700	-1.634033
111	6	0	8.581380	0.072334	-1.070077
112	6	0	9.843092	-0.090204	-0.485000
113	6	0	8.459337	-0.075189	-2.457405
114	6	0	10.954048	-0.393735	-1.266002
115	1	0	9.960899	0.041787	0.586990
116	6	0	9.570450	-0.380999	-3.237612
117	1	0	7.485371	0.027598	-2.927945
118	6	0	10.820954	-0.541722	-2.644928
119	1	0	11.926014	-0.510093	-0.795535
120	1	0	9.455446	-0.502512	-4.310723
121	1	0	11.687498	-0.781561	-3.254246
122	35	0	-1.776222	2.437771	1.704582

TS3r

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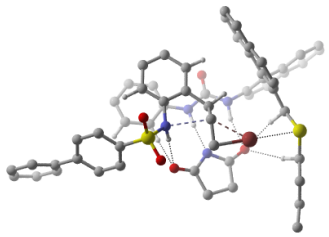

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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2	6	0	3.355303	-3.665552	-0.994423
3	6	0	3.586791	-2.337843	-1.452075
4	6	0	3.371621	-2.047665	-2.829060
5	6	0	2.931061	-3.079811	-3.700589
6	6	0	2.716974	-4.348776	-3.228990
7	1	0	2.751486	-5.647023	-1.492281
8	1	0	3.485737	-3.892347	0.057761
9	6	0	4.010602	-1.293869	-0.572293
10	6	0	3.602494	-0.729784	-3.293472
11	1	0	2.766479	-2.842991	-4.748669
12	1	0	2.378237	-5.131898	-3.900859
13	6	0	4.008103	0.254056	-2.431246
14	6	0	4.199949	-0.007637	-1.050910
15	1	0	3.459234	-0.509142	-4.348009
16	1	0	4.180247	1.252298	-2.820966
17	6	0	4.323181	-1.626065	0.852105
18	6	0	5.660443	-2.022587	1.191620
19	6	0	3.364028	-1.574796	1.838244
20	6	0	6.691694	-2.112798	0.217559
21	6	0	5.974236	-2.347928	2.540920
22	6	0	3.688257	-1.894033	3.182874
23	6	0	7.961035	-2.501305	0.567323
24	1	0	6.467352	-1.872816	-0.816652
25	6	0	7.296821	-2.742466	2.872863
26	6	0	4.955605	-2.268166	3.527136
27	1	0	2.905414	-1.829133	3.932292
28	6	0	8.270150	-2.819833	1.909588
29	1	0	8.734514	-2.565237	-0.192442
30	1	0	7.521515	-2.984176	3.908705
31	1	0	5.199020	-2.508366	4.558648
32	1	0	9.278988	-3.123730	2.173321
33	1	0	1.871648	-0.154162	1.714270
34	6	0	0.999239	-2.052489	1.678844
35	8	0	1.191017	-3.264945	1.710076
36	1	0	-0.249255	-0.423663	1.731318
37	6	0	-1.492325	-2.068941	1.722759
38	6	0	-2.614639	-1.224524	1.710787
39	6	0	-1.688649	-3.456106	1.705151
40	6	0	-3.897327	-1.754855	1.668706
41	1	0	-2.476175	-0.146128	1.709435
42	6	0	-2.982525	-3.971110	1.664374
43	1	0	-0.831325	-4.114506	1.711974
44	6	0	-4.094661	-3.134283	1.642617
45	1	0	-4.747581	-1.078489	1.645445
46	1	0	-3.115164	-5.049695	1.644797
47	1	0	-5.097831	-3.548684	1.605955
48	6	0	4.572745	1.075033	-0.057889
49	1	0	3.772153	1.159474	0.684700
50	1	0	5.487927	0.800964	0.475630
51	16	0	4.800602	2.748030	-0.764051
52	6	0	4.560032	3.732637	0.760251
53	1	0	3.836226	3.200476	1.387066
54	1	0	5.510260	3.781893	1.301109
55	6	0	4.045851	5.132743	0.438365
56	1	0	4.739923	5.652889	-0.234596
57	1	0	3.090423	5.049018	-0.097683
58	6	0	3.847668	5.958880	1.710597
59	1	0	3.217675	5.393827	2.409570
60	1	0	4.816572	6.096817	2.207401
61	6	0	3.210871	7.318439	1.434693
62	1	0	3.070970	7.884511	2.361940
63	1	0	3.835884	7.921140	0.764992
64	1	0	2.228430	7.203069	0.960903
65	7	0	-0.235513	-1.450451	1.745701
66	7	0	2.035986	-1.151027	1.538390
67	6	0	-1.138871	2.369299	1.484422
68	6	0	1.007286	2.210488	1.994777
69	6	0	0.714963	3.696294	2.174853
70	6	0	-0.797266	3.772320	1.978783
71	1	0	1.268153	4.253213	1.409445
72	1	0	1.070053	4.037968	3.150305
73	1	0	-1.126340	4.517881	1.250264
74	1	0	-1.336761	3.960575	2.912789
75	8	0	-2.239654	2.066619	0.996396
76	8	0	2.116860	1.698435	2.171762
77	7	0	-0.091955	1.519498	1.588223
78	6	0	-0.142507	-2.431226	-1.630067
79	6	0	-0.585418	-1.115511	-1.545454
80	6	0	-1.953615	-0.843538	-1.612127
81	6	0	-2.873158	-1.875082	-1.769592
82	6	0	-2.417422	-3.185169	-1.879618
83	6	0	-1.056125	-3.465394	-1.804597
84	1	0	0.917528	-2.644065	-1.547965
85	1	0	-3.936693	-1.669124	-1.790033
86	1	0	-3.136735	-3.988850	-2.001731
87	1	0	-0.701824	-4.489099	-1.873445
88	6	0	0.371476	0.029369	-1.283741
89	1	0	0.335012	0.343930	-0.236676
90	6	0	0.085813	1.188922	-2.163954
91	1	0	0.148389	1.014951	-3.239702
92	6	0	-0.187379	2.543788	-1.748461
93	1	0	-0.622408	2.696100	-0.770104
94	1	0	-0.537159	3.224979	-2.517562
95	1	0	1.385213	-0.317514	-1.514036
96	7	0	-2.295136	0.539747	-1.471727
97	1	0	-2.234866	0.922850	-0.508362
98	16	0	-3.542275	1.269181	-2.313118
99	8	0	-3.613988	0.637049	-3.620785
100	8	0	-3.277377	2.696517	-2.195243
101	6	0	-5.023874	0.906080	-1.402410
102	6	0	-5.971632	0.044000	-1.943475
103	6	0	-5.190915	1.473603	-0.140203
104	6	0	-7.101670	-0.267712	-1.197588
105	1	0	-5.822026	-0.388916	-2.927086
106	6	0	-6.327227	1.155058	0.589783
107	1	0	-4.440147	2.140748	0.272764
108	6	0	-7.293816	0.277103	0.077826
109	1	0	-7.829857	-0.962062	-1.604870
110	1	0	-6.470677	1.606064	1.566979
111	6	0	-8.492559	-0.078924	0.879654
112	6	0	-9.745636	-0.220049	0.270874
113	6	0	-8.387909	-0.288580	2.260340
114	6	0	-10.865313	-0.560794	1.023574
115	1	0	-9.851012	-0.041868	-0.795717
116	6	0	-9.507709	-0.631351	3.011958
117	1	0	-7.420523	-0.203512	2.747593
118	6	0	-10.749923	-0.768193	2.396365
119	1	0	-11.830821	-0.659477	0.536126
120	1	0	-9.406265	-0.798658	4.080257
121	1	0	-11.623974	-1.035205	2.983241
122	35	0	1.807373	2.721811	-1.579186