Electronic Supplementary Information

Synthesis of 8-membered trifluoromethyl benzoxazocines via a Pd-catalyzed ring-expansion reaction of trifluoromethyl benzoxazinones with 2-methylidenetrimethylene carbonate and mechanistic investigations

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General Methods. Solvents and reagents were used as purchased without further purification. The reaction progress was monitored by thin-layer chromatography (TLC) on silica gel GF_{254} precoated plates. Visualization of the developed plates was performed under a UV lamp. Chromatographic purification was performed with silica gel (100-200 mesh size). Melting points were uncorrected. Nuclear magnetic resonance spectra (^1H and ^{13}C NMR) were recorded on Bruker DPX 400 MHz and 100 MHz spectrometers in $CDCl_3$ with the chemical shift (δ) given in parts per million (ppm). Multiplicities were indicated as follows: s (singlet), d (doublet), t (triplet), m (multiplet), dd (doublet of doublets) and so forth; the coupling constant (*J*) was given in hertz (Hz). High-resolution mass spectra (HRMS) were recorded on an Agilent Q-TOF mass spectrometer. 4-Trifluoromethyl benzoxazinones **1** and 2-methylidenetrimethylene carbonate **2** were prepared according to literature procedures.[1,2]

General Procedure for the Synthesis of Compound 3. To a solution of 4-trifluoromethyl benzoxazinones **1** (0.1 mmol) and 2-methylidenetrimethylene carbonate **2** (0.2 mmol) in THF (1 mL) was added $Pd_2(dba)_3{\cdot}CHCl_3$ (10 mol%) and P(*p*-Tol)$_3$ (20 mol%). The reaction mixture was stirred at 50 °C for 5-15 min under nitrogen. When the reaction was completed, the solvent was removed and the residue was extracted with DCM (3 × 5 mL). The combined organic layers were washed with brine, dried over Na_2SO_4, filtered and concentrated. The residue was purified by chromatography on silica gel to afford the compound **3**.

3-Methylene-1-tosyl-6-(trifluoromethyl)-1,3,4,6-tetrahydro-2H-benzo[c][1,5]oxazocine (3a). White solid (32.6 mg, 82% yield), ethyl acetate/petroleum ether = 1:10, mp 102-103 ºC. ^1H NMR (400 MHz, $CDCl_3$) δ: 7.64 (d, *J* = 7.6 Hz, 2H), 7.56 (d, *J* = 7.6 Hz, 1H), 7.38-7.28 (m, 4H), 6.89 (d, *J* = 7.6 Hz, 1H), 5.16 (s, 1H), 5.12 (q, *J* = 7.2 Hz, 1H), 5.05 (s, 1H), 4.90 (d, *J* =

14.0 Hz, 1H), 4.45 and 4.33 (ABq, *J* = 12.8 Hz, 2H), 3.67 (d, *J* = 14.0 Hz, 1H), 2.46 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 144.3, 141.6, 139.6, 136.5, 136.0, 130.3, 130.0, 129.5, 128.9, 127.6, 127.3 (d, *J* = 3.1 Hz), 124.4 (q, *J* = 280.2 Hz), 121.8, 76.3 (q, *J* = 31.7 Hz), 75.1, 58.1, 21.7. HRMS (ESI) m/z calcd. for $C_{19}H_{19}F_3NO_3S$ $[M + H]^+$ 398.1032; found 398.1039.

8-Methyl-3-methylene-1-tosyl-6-(trifluoromethyl)-1,3,4,6-tetrahydro-2H-benzo[c][1,5] oxazocine (3b). White solid (33.3 mg, 81% yield), ethyl acetate/petroleum ether = 1:10, mp 104-105 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.64 (d, *J* = 8.4 Hz, 2H), 7.34-7.31 (m, 3H), 7.09 (d, *J* = 8.0 Hz, 1H), 6.74 (d, *J* = 8.0 Hz, 1H), 5.16 (s, 1H), 5.11 (q, *J* = 7.2 Hz, 1H), 5.05 (s, 1H), 4.89 (d, *J* = 14.0 Hz, 1H), 4.44 and 4.31 (ABq, *J* = 12.4 Hz, 2H), 3.65 (d, *J* = 14.0 Hz, 1H), 2.46 (s, 3H), 2.34 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 144.2, 141.7, 139.7, 136.8, 136.6, 135.6, 130.9, 130.0, 128.5, 127.8 (d, *J* = 2.9 Hz), 127.6, 124.5 (q, *J* = 279.9 Hz), 121.8, 76.4 (q, *J* = 31.6 Hz), 75.0, 58.1, 21.6, 21.6. HRMS (ESI) m/z calcd. for $C_{20}H_{21}F_3NO_3S$ $[M + H]^+$ 412.1189; found 412.1183.

8-Methoxy-3-methylene-1-tosyl-6-(trifluoromethyl)-1,3,4,6-tetrahydro-2H-benzo[c][1, 5]oxazocine (3c). White solid (30.2 mg, 71% yield), ethyl acetate/petroleum ether = 1:10, mp 90-91 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.63 (d, *J* = 7.6 Hz, 2H), 7.32 (d, *J* = 7.6 Hz, 2H), 7.05 (s, 1H), 6.79 (s, 2H), 5.17 (s, 1H), 5.09-5.03 (m, 2H), 4.89 (d, *J* = 14.0 Hz, 1H), 4.44 and 4.30 (ABq, *J* = 12.8 Hz, 2H), 3.78 (s, 3H), 3.64 (d, *J* = 13.6 Hz, 1H), 2.45 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 159.7, 144.1, 141.6, 137.0, 136.5, 131.6, 129.9, 129.8, 127.6, 124.3 (q, *J* = 279.7 Hz), 122.0, 115.2, 112.7 (d, *J* = 2.9 Hz), 76.3 (q, *J* = 31.6 Hz), 75.0, 58.1, 55.5, 21.6. HRMS (ESI) m/z calcd. for $C_{20}H_{20}F_3NNaO_4S$ $[M + Na]^+$ 450.0957; found 450.0968.

8-Chloro-3-methylene-1-tosyl-6-(trifluoromethyl)-1,3,4,6-tetrahydro-2H-benzo[c][1,5]

oxazocine (3d). White solid (25.6 mg, 59% yield), ethyl acetate/petroleum ether = 1:10, mp 109-110 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.62 (d, *J* = 7.6 Hz, 2H), 7.52 (s, 1H), 7.33 (d, *J* = 8.0 Hz, 2H), 7.28 (d, *J* = 10.0 Hz, 1H), 6.82 (d, *J* = 8.4 Hz, 1H), 5.19 (s, 1H), 5.07 (s, 1H), 5.05 (q, *J* = 7.2 Hz, 1H), 4.89 (d, *J* = 14.0 Hz, 1H), 4.46 and 4.29 (ABq, *J* = 12.8 Hz, 2H), 3.64 (d, *J* = 14.0 Hz, 1H), 2.46 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 144.6, 141.1, 138.0, 137.8, 136.2, 135.4, 130.5, 130.2, 130.1, 127.8, 127.6, 124.1 (q, *J* = 279.9 Hz), 122.4, 76.0 (q, *J* = 32.1 Hz), 75.2, 58.1, 21.7. HRMS (ESI) m/z calcd. for $C_{19}H_{17}ClF_3NNaO_3S$ $[M + Na]^+$ 454.0462; found 454.0471.

8-Bromo-3-methylene-1-tosyl-6-(trifluoromethyl)-1,3,4,6-tetrahydro-2H-benzo[c][1,5] oxazocine (3e). White solid (34.3 mg, 72% yield), ethyl acetate/petroleum ether = 1:10, mp 104-105 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.67 (s, 1H), 7.63 (d, *J* = 7.6 Hz, 2H), 7.44 (d, *J* = 8.0 Hz, 1H), 7.34 (d, *J* = 8.0 Hz, 2H), 6.75 (d, *J* = 8.4 Hz, 1H), 5.19 (s, 1H), 5.08 (s, 1H), 5.05 (q, *J* = 7.2 Hz, 1H), 4.89 (d, *J* = 13.6 Hz, 1H), 4.46 and 4.29 (ABq, *J* = 12.8 Hz, 2H), 3.64 (d, *J* = 14.0 Hz, 1H), 2.46 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 144.6, 141.1, 138.5, 138.1, 136.2, 133.5, 130.6 (d, *J* = 3.4 Hz), 130.5, 130.1, 127.6, 124.1 (q, *J* = 279.9 Hz), 123.5, 122.5, 76.0 (q, *J* = 31.9 Hz), 75.2, 58.1, 21.7. HRMS (ESI) m/z calcd. for $C_{19}H_{17}BrF_3NNaO_3S$ $[M + Na]^+$ 497.9957; found 497.9955.

3-Methylene-1-tosyl-6,8-bis(trifluoromethyl)-1,3,4,6-tetrahydro-2H-benzo[c][1,5]oxazocine (3f). White solid (16.8 mg, 36% yield), ethyl acetate/petroleum ether = 1:10, mp 139-140 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.79 (s, 1H), 7.64 (d, *J* = 7.6 Hz, 2H), 7.59 (d, *J* = 8.4 Hz, 1H), 7.35 (d, *J* = 8.0 Hz, 2H), 7.04 (d, *J* = 8.4 Hz, 1H), 5.20 (s, 1H), 5.13-5.08 (m, 2H), 4.92 (d, *J* = 14.0 Hz, 1H), 4.49 and 4.33 (ABq, *J* = 12.8 Hz, 2H), 3.68 (d, *J* = 14.0 Hz, 1H),

2.47 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 144.8, 143.0, 140.8, 137.3, 136.1, 131.6 (q, *J* = 32.7 Hz), 130.2, 129.7, 127.6, 127.3 (d, *J* = 3.9 Hz), 124.5, 124.1 (q, *J* = 279.9 Hz), 123.3 (q, *J* = 271.3 Hz), 122.5, 76.0 (q, *J* = 32.0 Hz), 75.3, 58.1, 21.7. HRMS (ESI) m/z calcd. for $C_{20}H_{17}F_6NNaO_3S$ $[M + Na]^+$ 488.0726; found 488.0733.

9-Methyl-3-methylene-1-tosyl-6-(trifluoromethyl)-1,3,4,6-tetrahydro-2H-benzo[c][1,5] oxazocine (3g). White solid (31.5 mg, 77% yield), ethyl acetate/petroleum ether = 1:10, mp 97-98 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.65 (d, *J* = 7.6 Hz, 2H), 7.42 (d, *J* = 8.0 Hz, 1H), 7.33 (d, *J* = 7.6 Hz, 2H), 7.16 (d, *J* = 8.0 Hz, 1H), 6.71 (s, 1H), 5.16 (s, 1H), 5.06 (s, 1H), 5.02 (q, *J* = 8.4 Hz, 1H), 4.87 (d, *J* = 14.0 Hz, 1H), 4.41 and 4.28 (ABq, *J* = 12.8 Hz, 2H), 3.66 (d, *J* = 14.0 Hz, 1H), 2.46 (s, 3H), 2.25 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 144.3, 141.6, 140.6, 139.4, 136.6, 132.8, 130.2, 129.9, 129.5, 127.7, 127.0 (d, *J* = 2.9 Hz), 124.5 (q, *J* = 280.0 Hz), 121.9, 76.4 (q, *J* = 31.5 Hz), 74.8, 58.1, 21.7, 21.1. HRMS (ESI) m/z calcd. for $C_{20}H_{20}F_3NNaO_3S$ $[M + Na]^+$ 434.1008; found 434.1025.

9-Fluoro-3-methylene-1-tosyl-6-(trifluoromethyl)-1,3,4,6-tetrahydro-2H-benzo[c][1,5] oxazocine (3h). White solid (26.0 mg, 63% yield), ethyl acetate/petroleum ether = 1:10, mp 103-104 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.65 (d, *J* = 8.0 Hz, 2H), 7.54 (t, *J* = 7.6 Hz, 1H), 7.35 (d, *J* = 7.6 Hz, 2H), 7.08 (t, *J* = 8.4 Hz, 1H), 6.64 (d, *J* = 8.8 Hz, 1H), 5.19 (s, 1H), 5.09 (s, 1H), 5.04 (q, *J* = 7.2 Hz, 1H), 4.88 (d, *J* = 14.0 Hz, 1H), 4.44 and 4.29 (ABq, *J* = 12.8 Hz, 2H), 3.65 (d, *J* = 13.6 Hz, 1H), 2.46 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 162.9 (d, *J* = 250.6 Hz), 144.7, 141.2, 141.1, 136.1, 132.4 (d, *J* = 3.8 Hz), 130.1, 128.8 (dd, *J* = 3.0, 8.6 Hz), 127.6, 124.3 (q, *J* = 280.0 Hz), 122.4, 116.6 (d, *J* = 20.9 Hz), 116.4 (d, *J* = 21.8 Hz), 75.8 (q, *J* = 31.8 Hz), 74.9, 58.1, 21.7. HRMS (ESI) m/z calcd. for $C_{19}H_{18}F_4NO_3S$ $[M + H]^+$ 416.0938; found

416.0931.

3-Methylene-1-tosyl-6,9-bis(trifluoromethyl)-1,3,4,6-tetrahydro-2H-benzo[c][1,5]oxazocine (3i). White solid (21.0 mg, 45% yield), ethyl acetate/petroleum ether = 1:10, mp 104-105 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.71-7.62 (m, 4H), 7.36 (d, *J* = 8.0 Hz, 2H), 7.02 (s, 1H), 5.24-5.19 (m, 2H), 5.08 (s, 1H), 4.91 (d, *J* = 14.0 Hz, 1H), 4.52 and 4.37 (ABq, *J* = 12.8 Hz, 2H), 3.66 (d, *J* = 14.4 Hz, 1H), 2.48 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 144.9, 141.0, 140.3, 140.2, 135.8, 132.4 (q, *J* = 33.1 Hz), 130.2, 128.0 (d, *J* = 3.2 Hz), 127.7, 126.3 (d, *J* = 4.0Hz), 126.0 (d, *J* = 3.8 Hz), 124.1 (q, *J* = 280.0 Hz), 123.1 (q, *J* = 271.0 Hz), 122.3, 76.2 (q, *J* = 32.2 Hz), 75.5, 58.0, 21.7. HRMS (ESI) m/z calcd. for $C_{20}H_{17}F_6NNaO_3S$ $[M + Na]^+$ 488.0726; found 488.0731.

3-Methylene-1-(phenylsulfonyl)-6-(trifluoromethyl)-1,3,4,6-tetrahydro-2H-benzo [c][1, 5]oxazocine (3j). White solid (30.5 mg, 80% yield), ethyl acetate/petroleum ether = 1:10, mp 90-91 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.77 (d, *J* = 8.0 Hz, 2H), 7.65 (t, *J* = 7.6 Hz, 1H), 7.58-7.52 (m, 3H), 7.37 (t, *J* = 7.2 Hz, 1H), 7.30 (t, *J* = 7.6 Hz, 1H), 6.87 (d, *J* = 7.6 Hz, 1H), 5.17 (s, 1H), 5.12 (q, *J* = 7.2 Hz, 1H), 5.07 (s, 1H), 4.92 (d, *J* = 14.0 Hz, 1H), 4.45 and 4.33 (ABq, *J* = 12.8 Hz, 2H), 3.69 (d, *J* = 14.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 141.5, 139.4, 139.4, 136.0, 133.3, 130.3, 129.6, 129.3, 128.8, 127.5, 127.3 (d, *J* = 3.0 Hz), 124.4 (q, *J* = 279.7 Hz), 121.8, 76.3 (q, *J* = 31.7 Hz), 75.0, 58.1. HRMS (ESI) m/z calcd. for $C_{18}H_{16}F_3NNaO_3S$ $[M + Na]^+$ 406.0695; found 406.0685.

1-((4-Fluorophenyl)sulfonyl)-3-methylene-6-(trifluoromethyl)-1,3,4,6-tetrahydro-2H-benzo[c][1,5]oxazocine (3k). White solid (30.6 mg, 76% yield), ethyl acetate/petroleum ether = 1:10, mp 110-111 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.79-7.75 (m, 2H), 7.58 (d, *J* = 8.0 Hz,

1H), 7.38 (t, *J* = 7.6 Hz, 1H), 7.32 (t, *J* = 7.6 Hz, 1H), 7.21 (t, *J* = 8.0 Hz, 2H), 6.86 (d, *J* = 7.6 Hz, 1H), 5.19 (s, 1H), 5.12 (q, *J* = 7.2 Hz, 1H), 5.09 (s, 1H), 4.91 (d, *J* = 14.0 Hz, 1H), 4.46 and 4.34 (ABq, *J* = 12.8 Hz, 2H), 3.68 (d, *J* = 14.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 165.5 (d, *J* = 254.8 Hz), 141.4, 139.3, 136.0, 135.6 (d, *J* = 3.3 Hz), 130.4, 130.4, 130.3, 129.8, 128.8, 127.5 (d, *J* = 3.2 Hz), 124.4 (q, *J* = 279.9 Hz), 122.1, 116.6 (d, *J* = 22.5 Hz), 76.3 (q, *J* = 31.7 Hz), 75.0, 58.1. HRMS (ESI) m/z calcd. for $C_{18}H_{16}F_4NO_3S$ $[M + H]^+$ 402.0782; found 402.0774.

1-((4-Chlorophenyl)sulfonyl)-3-methylene-6-(trifluoromethyl)-1,3,4,6-tetrahydro-2H-benzo[c][1,5]oxazocine (3l). White solid (32.1 mg, 77% yield), ethyl acetate/petroleum ether = 1:10, mp 119-120 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.70 (d, *J* = 8.0 Hz, 2H), 7.59 (d, *J* = 8.0 Hz, 1H), 7.52 (d, *J* = 8.0 Hz, 2H), 7.39 (t, *J* = 8.0 Hz, 1H), 7.32 (t, *J* = 8.0 Hz, 1H), 6.84 (d, *J* = 7.6 Hz, 1H), 5.19 (s, 1H), 5.14 (q, *J* = 7.2 Hz, 1H), 5.08 (s, 1H), 4.90 (d, *J* = 14.0 Hz, 1H), 4.46 and 4.34 (ABq, *J* = 12.8 Hz, 2H), 3.68 (d, *J* = 14.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 141.3, 140.0, 139.2, 137.9, 136.0, 130.4, 129.8, 129.7, 129.0, 128.6, 127.5 (d, *J* = 3.2 Hz), 124.4 (q, *J* = 280.2 Hz), 122.2, 76.3 (q, *J* = 31.7 Hz), 75.0, 58.2. HRMS (ESI) m/z calcd. for $C_{18}H_{15}ClF_3NNaO_3S$ $[M + Na]^+$ 440.0305; found 440.0316.

1-((4-Bromophenyl)sulfonyl)-3-methylene-6-(trifluoromethyl)-1,3,4,6-tetrahydro-2H-benzo[c][1,5]oxazocine (3m). White solid (30.3 mg, 66% yield), ethyl acetate/petroleum ether = 1:8, mp 125-126 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.68 (d, *J* = 8.0 Hz, 2H), 7.61 (d, *J* = 8.4 Hz, 2H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.39 (t, *J* = 7.6 Hz, 1H), 7.32 (t, *J* = 8.0 Hz, 1H), 6.84 (d, *J* = 8.0 Hz, 1H), 5.19 (s, 1H), 5.14 (q, *J* = 7.6 Hz, 1H), 5.08 (s, 1H), 4.89 (d, *J* = 14.0 Hz, 1H), 4.46 and 4.34 (ABq, *J* = 12.8 Hz, 2H), 3.68 (d, *J* = 13.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$)

δ: 141.3, 139.2, 138.5, 136.0, 132.7, 130.4, 129.8, 129.1, 128.7, 128.4, 127.5 (d, *J* = 3.1 Hz), 124.4 (q, *J* = 279.9 Hz), 122.1, 76.3 (q, *J* = 31.8 Hz), 75.0, 58.2. HRMS (ESI) m/z calcd. for $C_{18}H_{16}BrF_3NO_3S$ $[M + H]^+$ 461.9981; found 461.9978.

1-((4-(tert-Butyl)phenyl)sulfonyl)-3-methylene-6-(trifluoromethyl)-1,3,4,6-tetrahydro-2H-benzo[c][1,5]oxazocine (3n). White solid (26.4 mg, 60% yield), ethyl acetate/petroleum ether = 1:10, mp 89-90 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.66 (d, *J* = 8.0 Hz, 2H), 7.53-7.51 (m, 3H), 7.39-7.34 (m, 2H), 7.04 (d, *J* = 6.8 Hz, 1H), 5.18 (s, 1H), 5.10 (s, 1H), 4.97-4.90 (m, 2H), 4.44 and 4.30 (ABq, *J* = 12.8 Hz, 2H), 3.70 (d, *J* = 14.0 Hz, 1H), 1.35 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 157.3, 141.6, 139.6, 136.4, 135.8, 130.3, 129.5, 129.4, 127.4, 127.2 (d, *J* = 2.9 Hz), 126.3, 124.4 (q, *J* = 280.1 Hz), 121.8, 76.1 (q, *J* = 31.6 Hz), 75.0, 58.0, 35.3, 31.1. HRMS (ESI) m/z calcd. for $C_{22}H_{25}F_3NO_3S$ $[M + H]^+$ 440.1502; found 440.1514.

1-((3-Chlorophenyl)sulfonyl)-3-methylene-6-(trifluoromethyl)-1,3,4,6-tetrahydro-2H-benzo[c][1,5]oxazocine (3o). White solid (30.7 mg, 73% yield), ethyl acetate/petroleum ether = 1:10, mp 99-100 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.76 (s, 1H), 7.65-7.58 (m, 3H), 7.48 (t, *J* = 8.0 Hz, 1H), 7.40 (t, *J* = 7.6 Hz, 1H), 7.33 (t, *J* = 7.6 Hz, 1H), 6.86 (d, *J* = 8.0 Hz, 1H), 5.20 (s, 1H), 5.14-5.08 (m, 2H), 4.91 (d, *J* = 14.0 Hz, 1H), 4.46 and 4.34 (ABq, *J* = 12.8 Hz, 2H), 3.71 (d, *J* = 14.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 141.2, 141.2, 139.1, 135.9, 135.7, 133.4, 130. 7, 130.4, 129.9, 128.8, 127.6, 127.5 (d, *J* = 3.1 Hz), 125.8, 124.4 (q, *J* = 280.0 Hz), 122.2, 76.3 (q, *J* = 31.9 Hz), 75.0, 58.3. HRMS (ESI) m/z calcd. for $C_{18}H_{16}ClF_3NO_3S$ $[M + H]^+$ 418.0486; found 418.0484.

1-((3-Chloro-4-methylphenyl)sulfonyl)-3-methylene-6-(trifluoromethyl)-1,3,4,6-tetra-hydro-2H-benzo[c][1,5]oxazocine (3p). White solid (35.1 mg, 81% yield), ethyl

acetate/petroleum ether = 1:8, mp 103-104 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.75 (s, 1H), 7.58 (d, *J* = 7.6 Hz, 1H), 7.53 (d, *J* = 8.0 Hz, 1H), 7.40-7.37 (m, 2H), 7.33 (t, *J* = 7.6 Hz, 1H), 6.89 (d, *J* = 7.6 Hz, 1H), 5.19 (s, 1H), 5.14-5.09 (m, 2H), 4.90 (d, *J* = 14.4 Hz, 1H), 4.45 and 4.33 (ABq, *J* = 12.8 Hz, 2H), 3.69 (d, *J* = 14.0 Hz, 1H), 2.48 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 142.3, 141.4, 139.2, 138.4, 136.0, 135.6, 131.7, 130.4, 129.8, 128.8, 128.1, 127.4 (d, *J* = 3.1 Hz), 125.7, 124.4 (q, *J* = 280.2 Hz), 122.1, 76.3 (q, *J* = 31.8 Hz), 75.0, 58.2, 20.4. HRMS (ESI) m/z calcd. for $C_{19}H_{18}ClF_3NO_3S$ $[M + H]^+$ 432.0643; found 432.0638.

3-Methylene-1-(naphthalen-2-ylsulfonyl)-6-(trifluoromethyl)-1,3,4,6-tetrahydro-2H-benzo[c][1,5]oxazocine (3q). White solid (28.6 mg, 66% yield), ethyl acetate/petroleum ether = 1:10, mp 143-144 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.32 (s, 1H), 8.02 (d, *J* = 8.4 Hz, 1H), 7.97-7.92 (m, 2H), 7.79 (d, *J* = 8.8 Hz, 1H), 7.69 (t, *J* = 7.2 Hz, 1H), 7.63 (t, *J* = 7.6 Hz, 1H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.36 (t, *J* = 7.6 Hz, 1H), 7.24 (t, *J* = 7.6 Hz, 1H), 6.80 (d, *J* = 8.0 Hz, 1H), 5.27 (q, *J* = 7.2 Hz, 1H), 5.18 (s, 1H), 5.06 (s, 1H), 4.99 (d, *J* = 14.0 Hz, 1H), 4.47 and 4.37 (ABq, *J* = 12.8 Hz, 2H), 3.73 (d, *J* = 14.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 141.5, 139.4, 136.3, 136.1, 135.0, 132.2, 130.3, 129.7, 129.6, 129.4, 129.2, 129.2, 128.7, 128.0, 127.9, 127.3 (d, *J* = 3.0 Hz), 124.4 (q, *J* = 279.6 Hz), 122.5, 121.9, 76.4 (q, *J* = 31.6 Hz), 75.0, 58.4. HRMS (ESI) m/z calcd. for $C_{22}H_{19}F_3NO_3S$ $[M + H]^+$ 434.1032; found 434.1024.

3-Methylene-1-(thiophen-2-ylsulfonyl)-6-(trifluoromethyl)-1,3,4,6-tetrahydro-2H-benzo[c][1,5]oxazocine (3r). White solid (27.7 mg, 71% yield), ethyl acetate/petroleum ether = 1:10, mp 94-95 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.68 (d, *J* = 5.2 Hz, 1H), 7.59 (d, *J* = 7.6 Hz, 1H), 7.52-7.51 (m, 1H), 7.41-7.32 (m, 2H), 7.14 (t, *J* = 3.6 Hz, 1H), 6.95 (d, *J* = 7.6 Hz, 1H), 5.19-5.14 (m, 2H), 5.10 (s, 1H), 4.89 (d, *J* = 14.0 Hz, 1H), 4.48 and 4.36 (ABq, *J* = 12.8

Hz, 2H), 3.73 (d, *J* = 14.0 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 141.3, 139.9, 139.4, 136.0, 133.3, 132.7, 130.4, 129.7, 128.5, 127.8, 127.4 (d, *J* = 3.0 Hz), 124.4 (q, *J* = 280.2 Hz), 121.9, 76.5 (q, *J* = 31.7 Hz), 75.2, 58.1. HRMS (ESI) m/z calcd. for $C_{16}H_{14}F_3NNaO_3S_2$ $[M + Na]^+$ 412.0259; found 412.0255.

1-((4-Fluorophenyl)sulfonyl)-8-methyl-3-methylene-6-(trifluoromethyl)-1,3,4,6-tetra-hydro-2H-benzo[c][1,5]oxazocine (3s). Yellow solid (32.2 mg, 77% yield), ethyl acetate/petroleum ether = 1:10, mp 99-100 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.79-7.75 (m, 2H), 7.36 (s, 1H), 7.21 (t, *J* = 8.4 Hz, 2H), 7.10 (d, *J* = 8.4 Hz, 1H), 6.72 (d, *J* = 8.0 Hz, 1H), 5.19 (s, 1H), 5.13-5.08 (m, 2H), 4.90 (d, *J* = 14.0 Hz, 1H), 4.44 and 4.32 (ABq, *J* = 12.8 Hz, 2H), 3.66 (d, *J* = 14.0 Hz, 1H), 2.35 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 165.5 (d, *J* = 254.6 Hz), 141.4, 140.0, 136.4, 135.6 (d, *J* = 3.2 Hz), 135.6, 131.0, 130.4, 130.3, 128.3, 128.0 (d, *J* = 2.9 Hz), 124.4 (q, *J* = 280.2 Hz), 122.2, 116.6 (d, *J* = 22.5 Hz), 76.3 (q, *J* = 31.7 Hz), 75.0, 58.1, 21.6. HRMS (ESI) m/z calcd. for $C_{19}H_{17}F_4NNaO_3S$ $[M + Na]^+$ 438.0757; found 438.0766.

1-((4-Chlorophenyl)sulfonyl)-8-methyl-3-methylene-6-(trifluoromethyl)-1,3,4,6-tetra-hydro-2H-benzo[c][1,5]oxazocine (3t). White solid (29.4 mg, 68% yield), ethyl acetate/petroleum ether = 1:10, mp 103-104 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.70 (d, *J* = 8.0 Hz, 2H), 7.51 (d, *J* = 7.6 Hz, 2H), 7.37 (s, 1H), 7.10 (d, *J* = 8.0 Hz, 1H), 6.70 (d, *J* = 8.0 Hz, 1H), 5.19 (s, 1H), 5.12 (q, *J* = 7.2 Hz, 1H), 5.08 (s, 1H), 4.89 (d, *J* = 13.6 Hz, 1H), 4.45 and 4.33 (ABq, *J* = 12.4 Hz, 2H), 3.66 (d, *J* = 14.0 Hz, 1H), 2.35 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 141.4, 140.1, 139.9, 138.0, 136.3, 135.6, 131.0, 129.7, 129.1, 128.3, 128.1 (d, *J* = 2.9 Hz), 124.4 (q, *J* = 280.3 Hz), 122.2, 76.3 (q, *J* = 31.9 Hz), 75.0, 58.2, 21.6. HRMS (ESI) m/z calcd. for $C_{19}H_{17}ClF_3NNaO_3S$ $[M + Na]^+$ 454.0462; found 454.0464.

1-((4-Bromophenyl)sulfonyl)-8-methyl-3-methylene-6-(trifluoromethyl)-1,3,4,6-tetra-hydro-2H-benzo[c][1,5]oxazocine (3u). White solid (30.0 mg, 63% yield), ethyl acetate/petroleum ether = 1:10, mp 101-102 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.68 (d, *J* = 8.0 Hz, 2H), 7.62 (d, *J* = 8.0 Hz, 2H), 7.37 (s, 1H), 7.10 (d, *J* = 8.0 Hz, 1H), 6.69 (d, *J* = 8.0 Hz, 1H), 5.19 (s, 1H), 5.12 (q, *J* = 7.6 Hz, 1H), 5.07 (s, 1H), 4.88 (d, *J* = 14.0 Hz, 1H), 4.45 and 4.33 (ABq, *J* = 12.4 Hz, 2H), 3.65 (d, *J* = 13.6 Hz, 1H), 2.35 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 141.3, 140.1, 138.5, 136.3, 135.6, 132.7, 131.0, 129.1, 128.4, 128.2, 128.1 (d, *J* = 2.9 Hz), 124.4 (q, *J* = 279.9 Hz), 122.3, 76.3 (q, *J* = 31.6 Hz), 75.0, 58.2, 21.6. HRMS (ESI) m/z calcd. for $C_{19}H_{18}BrF_3NO_3S$ $[M + H]^+$ 476.0137; found 476.0139.

8-Methyl-3-methylene-1-(naphthalen-2-ylsulfonyl)-6-(trifluoromethyl)-1,3,4,6-tetra-hydro-2H-benzo[c][1,5]oxazocine (3v). White solid (34.2 mg, 76% yield), ethyl acetate/petroleum ether = 1:10, mp 137-138 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.32 (s, 1H), 8.01 (d, *J* = 8.4 Hz, 1H), 7.95 (t, *J* = 8.8 Hz, 2H), 7.79 (d, *J* = 8.4 Hz, 1H), 7.69 (t, *J* = 7.2 Hz, 1H), 7.63 (t, *J* = 7.6 Hz, 1H), 7.37 (s, 1H), 7.03 (d, *J* = 8.0 Hz, 1H), 6.65 (d, *J* = 8.0 Hz, 1H), 5.26 (q, *J* = 7.6 Hz, 1H), 5.18 (s, 1H), 5.05 (s, 1H), 4.99 (d, *J* = 13.6 Hz, 1H), 4.46 and 4.36 (ABq, *J* = 12.8 Hz, 2H), 3.71 (d, *J* = 14.0 Hz, 1H), 2.33 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 141.6, 139.9, 136.6, 136.4, 135.7, 135.1, 132.3, 130.9, 129.7, 129.4, 129.2, 129.2, 128.3, 128.1, 128.0 (d, *J* = 2.9 Hz), 127.9, 124.4 (q, *J* = 279.8 Hz), 122.6, 122.0, 76.5 (q, *J* = 31.7 Hz), 75.0, 58.4, 21.6. HRMS (ESI) m/z calcd. for $C_{23}H_{20}F_3NNaO_3S$ $[M + Na]^+$ 470.1008; found 470.1015.

8-Chloro-1-((4-fluorophenyl)sulfonyl)-3-methylene-6-(trifluoromethyl)-1,3,4,6-tetra-hydro-2H-benzo[c][1,5]oxazocine (3w). White solid (31.6 mg, 72% yield), ethyl

acetate/petroleum ether = 1:8, mp 124-125 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.79-7.75 (m, 2H), 7.54 (s, 1H), 7.30 (d, *J* = 8.8 Hz, 1H), 7.26-7.21 (m, 2H), 6.81 (d, *J* = 8.4 Hz, 1H), 5.22 (s, 1H), 5.12 (s, 1H), 5.04 (q, *J* = 7.2 Hz, 1H), 4.90 (d, *J* = 14.0 Hz, 1H), 4.47 and 4.31 (ABq, *J* = 12.8 Hz, 2H), 3.66 (d, *J* = 14.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 165.6 (d, *J* = 255.3 Hz), 140.8, 137.7, 137.6, 135.7, 135.3 (d, *J* = 3.3 Hz), 130.6, 130.4, 130.3, 130.1, 127.9 (d, *J* = 3.4 Hz), 124.0 (q, *J* = 279.9 Hz), 122.7, 116.8 (d, *J* = 22.5 Hz), 76.0 (q, *J* = 32.1 Hz), 75.2, 58.1. HRMS (ESI) m/z calcd. for $C_{18}H_{14}ClF_4NNaO_3S$ $[M + Na]^+$ 458.0211; found 458.0212.

8-Chloro-1-((4-chlorophenyl)sulfonyl)-3-methylene-6-(trifluoromethyl)-1,3,4,6-tetra-hydro-2H-benzo[c][1,5]oxazocine (3x). White solid (28.0 mg, 62% yield), ethyl acetate/petroleum ether = 1:10, mp 114-115 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.69 (d, *J* = 8.0 Hz, 2H), 7.55-7.51 (m, 3H), 7.29 (d, *J* = 8.4 Hz, 1H), 6.68 (d, *J* = 9.2 Hz, 1H), 5.22 (s, 1H), 5.11 (s, 1H), 5.06 (q, *J* = 7.2 Hz, 1H), 4.89 (d, *J* = 14.0 Hz, 1H), 4.47 and 4.31 (ABq, *J* = 12.8 Hz, 2H), 3.65 (d, *J* = 14.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 140.8, 140.2, 137.8, 137.6, 137.6, 135.7, 130.6, 130.0, 129.8, 129.0, 128.0 (d, *J* = 3.4 Hz), 124.1 (q, *J* = 280.1 Hz), 122.8, 76.0 (q, *J* = 32.1 Hz), 75.2, 58.2. HRMS (ESI) m/z calcd. for $C_{18}H_{14}Cl_2F_3NNaO_3S$ $[M + Na]^+$ 473.9916; found 473.9913.

8-Bromo-3-methylene-1-(naphthalen-2-ylsulfonyl)-6-(trifluoromethyl)-1,3,4,6-tetra-hydro-2H-benzo[c][1,5]oxazocine (3y). White solid (34.9 mg, 68% yield), ethyl acetate/petroleum ether = 1:8, mp 120-121 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.31 (s, 1H), 8.03 (d, *J* = 8.4 Hz, 1H), 7.95 (t, *J* = 8.0 Hz, 2H), 7.77 (d, *J* = 8.4 Hz, 1H), 7.73-7.63 (m, 3H), 7.37 (d, *J* = 8.4 Hz, 1H), 6.65 (d, *J* = 8.4 Hz, 1H), 5.21-5.17 (m, 2H), 5.08 (s, 1H), 4.99 (d, *J* = 13.6 Hz, 1H), 4.48 and 4.34 (ABq, *J* = 12.8 Hz, 2H), 3.70 (d, *J* = 14.0 Hz, 1H). ^{13}C NMR (100

MHz, $CDCl_3$) δ: 141.0, 138.4, 138.2, 136.0, 135.1, 133.5, 132.2, 130.8 (d, *J* = 3.2 Hz), 130.3, 129.9, 129.5, 129.3, 124.0 (q, *J* = 279.7 Hz), 123.7, 122.6, 122.4, 76.1 (q, *J* = 32.1 Hz), 75.2, 58.4. HRMS (ESI) m/z calcd. for $C_{22}H_{18}BrF_3NO_3S$ $[M + H]^+$ 512.0137; found 512.0141.

1-((4-Chlorophenyl)sulfonyl)-8-methoxy-3-methylene-6-(trifluoromethyl)-1,3,4,6-tetrahydro-2H-benzo[c][1,5]oxazocine (3z). White solid (35.5 mg, 79% yield), ethyl acetate/petroleum ether = 1:8, mp 88-89 ºC. ^1H NMR (400 MHz, $CDCl_3$) δ: 7.69 (d, *J* = 8.0 Hz, 2H), 7.51 (d, *J* = 8.0 Hz, 2H), 7.07 (s, 1H), 6.80 (d, *J* = 9.2 Hz, 1H), 6.74 (d, *J* = 8.4 Hz, 1H), 5.20 (s, 1H), 5.09-5.05 (m, 2H), 4.89 (d, *J* = 13.6 Hz, 1H), 4.45 and 4.32 (ABq, *J* = 12.8 Hz, 2H), 3.79 (s, 3H), 3.65 (d, *J* = 14.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 159.9, 141.3, 139.9, 138.0, 137.1, 131.2, 129.7, 129.0, 124.3 (q, *J* = 279.8 Hz), 122.4, 115.3, 113.0 (d, *J* = 3.2 Hz), 76.3 (q, *J* = 31.8 Hz), 75.0, 58.2, 55.6. HRMS (ESI) m/z calcd. for $C_{19}H_{17}ClF_3NNaO_4S$ $[M + Na]^+$ 470.0411; found 470.0415.

3-Methylene-6-(perfluoroethyl)-1-tosyl-1,3,4,6-tetrahydro-2H-benzo[c][1,5]oxazocine (3aa). White solid (31.9 mg, 71% yield), ethyl acetate/petroleum ether = 1:10, mp 108-109 ºC. ^1H NMR (400 MHz, $CDCl_3$) δ: 7.69-7.64 (m, 3H), 7.38-7.29 (m, 4H), 6.91 (d, *J* = 7.6 Hz, 1H), 5.35 (d, *J* = 23.6 Hz, 1H), 5.15 (s, 1H), 5.00 (s, 1H), 4.89 (d, *J* = 13.6 Hz, 1H), 4.37 and 4.22 (ABq, *J* = 12.4 Hz, 2H), 3.67 (d, *J* = 13.6 Hz, 1H), 2.45 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 144.3, 141.2, 139.5, 136.3, 135.9, 130.2, 129.9, 129.5, 128.7, 128.0 (dd, *J* = 2.6, 6.8 Hz), 127.6, 122.3, 74.7, 73.7 (dd, *J* = 18.6, 29.4 Hz), 58.3, 21.6. HRMS (ESI) m/z calcd. for $C_{20}H_{18}F_5NNaO_3S$ $[M + Na]^+$ 470.0820; found 470.0823.

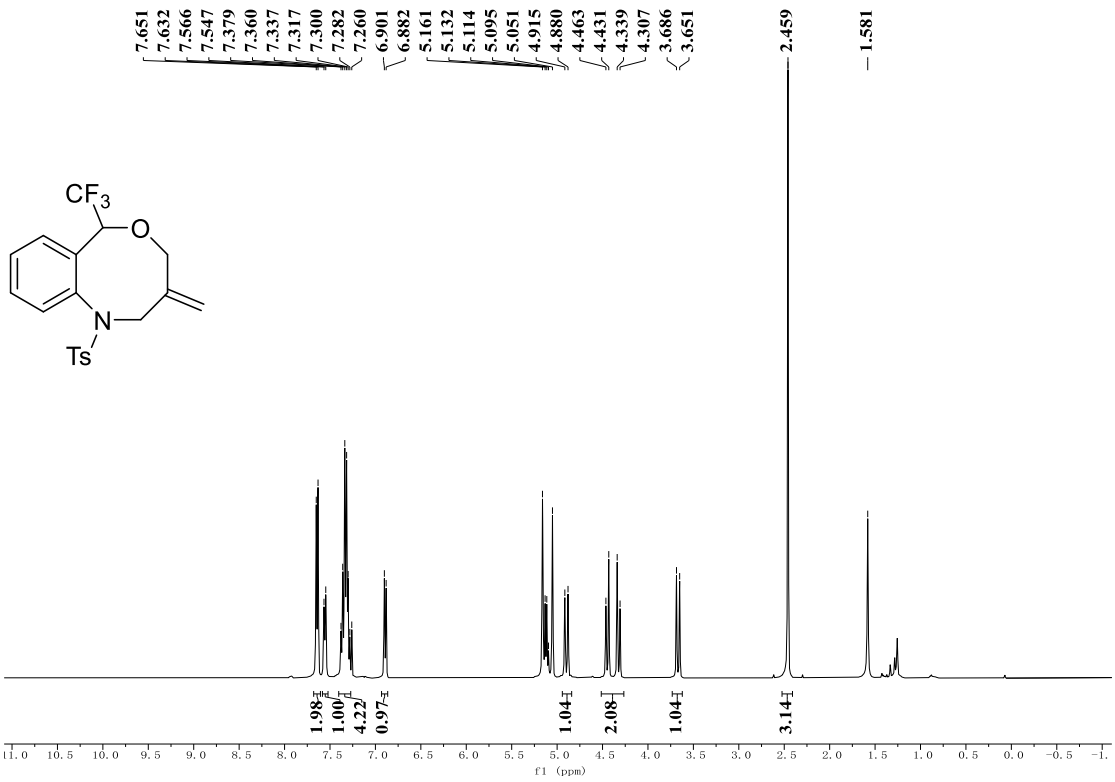
1-(2-(Hydroxymethyl)allyl)-4-(trifluoromethyl)-1,4-dihydro-2H-benzo[d][1,3]oxazin-2-one (3ad). White solid (23.4 mg, 82% yield), ethyl acetate/petroleum ether = 1:2, mp 99-100

ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.42 (t, *J* = 8.0 Hz, 1H), 7.25 (d, *J* = 7.2 Hz, 1H), 7.16 (t, *J* = 7.6 Hz, 1H), 7.05 (d, *J* = 8.0 Hz, 1H), 5.58 (q, *J* = 6.8 Hz, 1H), 5.24 (s, 1H), 5.01 (s, 1H), 4.67 and 4.56 (ABq, *J* = 17.2 Hz, 2H), 4.16 (s, 2H), 2.26 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 149.8, 142.1, 137.2, 131.3, 127.2, 124.2, 122.8 (q, *J* = 282.7 Hz), 114.7, 113.4, 112.9, 75.5 (q, *J* = 34.0 Hz), 64.1, 47.0. HRMS (ESI) m/z calcd. for $C_{13}H_{13}F_3NO_3$ $[M + H]^+$ 288.0842; found 288.0836.

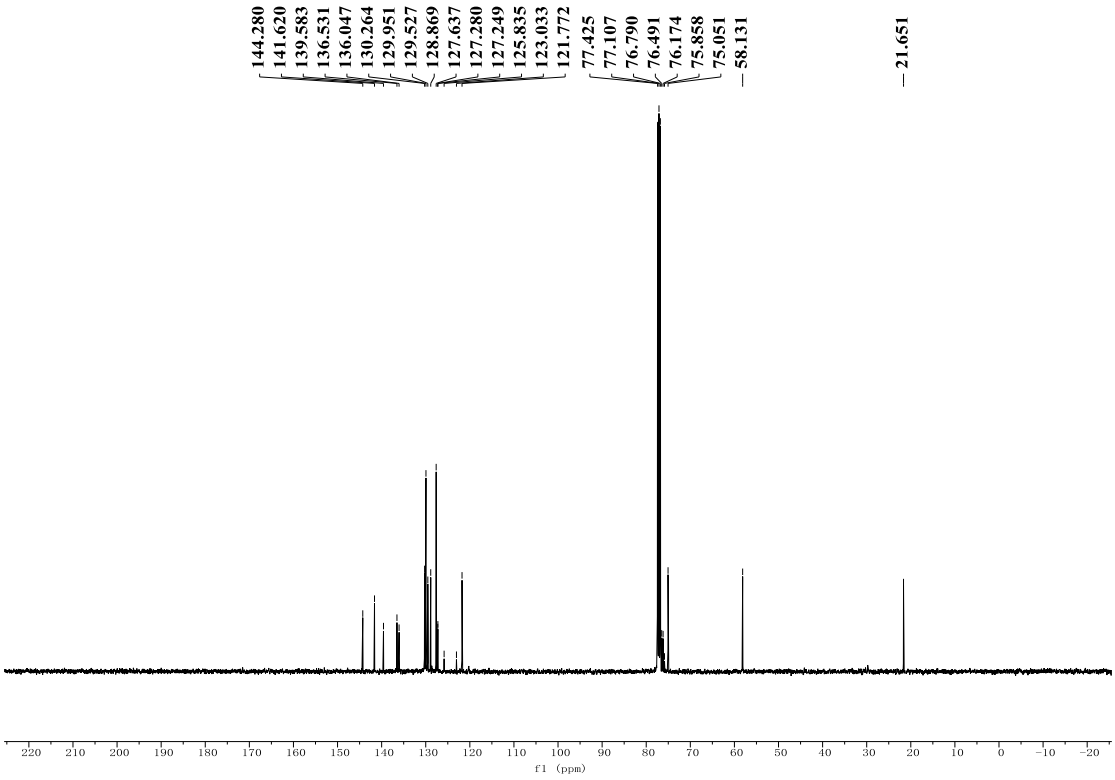
1.0 mmol Scale Synthesis of 3a with 10 mol% [Pd]. To a solution of 4-trifluoromethyl benzoxazinone **1a** (371 mg, 1.0 mmol) and 2-methylidenetrimethylene carbonate **2** (228 mg, 2.0 mmol) in THF (5 mL) was added $Pd_2(dba)_3{\cdot}CHCl_3$ (103.5 mg, 10 mol%) and P(*p*-Tol)$_3$ (60.8 mg, 20 mol%). The reaction mixture was stirred at 50 °C for 5 min under nitrogen. When the reaction was completed, the solvent was removed and the residue was extracted with DCM (3 × 10 mL). The combined organic layers were washed with brine, dried over Na_2SO_4, filtered and concentrated. The residue was purified by chromatography on silica gel to afford **3a** as a white solid (298 mg, 75% yield).

1.0 mmol Scale Synthesis of 3a with 5 mol% [Pd]. To a solution of 4-trifluoromethyl benzoxazinone **1a** (371 mg, 1.0 mmol) and 2-methylidenetrimethylene carbonate **2** (228 mg, 2.0 mmol) in THF (5 mL) was added $Pd_2(dba)_3{\cdot}CHCl_3$ (51.8 mg, 5 mol%) and P(*p*-Tol)$_3$ (60.8 mg, 20 mol%). The reaction mixture was stirred at 50 °C for 3 h under nitrogen. When the reaction was completed, the solvent was removed and the residue was extracted with DCM (3 × 10 mL). The combined organic layers were washed with brine, dried over Na_2SO_4, filtered and concentrated. The residue was purified by chromatography on silica gel to afford **3a** as a white solid (278 mg, 70% yield).

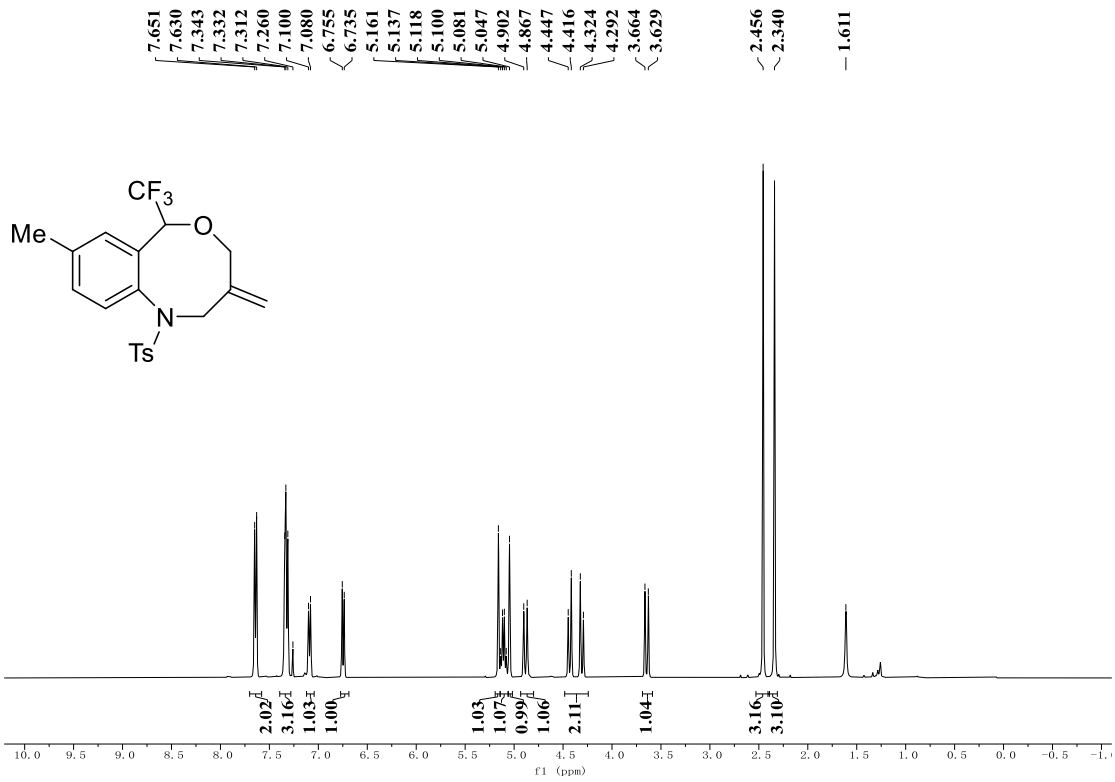
Synthesis of Compound 4. To a solution of $RuCl_3 \cdot H_2O$ (31 mg, 20 mol%) in MeCN (10 mL) was added a solution of $NaIO_4$ (850 mg, 4 mmol) in water (5 mL). After 2 min, a solution of **3a** (397 mg, 1.0 mmol) in ethyl acetate (10 mL) was added. The resulting mixture was stirred at room temperature for 5 min. After completion of the reaction, water (5 mL) was added and the mixture was extracted with ethyl acetate (3 × 5 mL). The combined organic layers were dried and concentrated under reduced pressure followed by silica gel column chromatography purification (ethyl acetate/petroleum ether = 1:10) to give the carbonyl compound **4** as a white solid (270 mg, 68% yield), mp 164-165 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.71 (d, *J* = 7.6 Hz, 2H), 7.55 (d, *J* = 7.2 Hz, 1H), 7.45-7.32 (m, 4H), 6.80 (d, *J* = 7.6 Hz, 1H), 5.53 (q, *J* = 7.2 Hz, 1H), 4.85 (d, *J* = 16.4 Hz, 1H), 4.57 (d, *J* = 16.4 Hz, 1H), 4.33 (d, *J* = 17.2 Hz, 1H), 3.86 (d, *J* = 17.2 Hz, 1H), 2.49 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 206.5, 145.0, 142.2, 136.0, 135.7, 130.5, 130.2, 129.6, 128.6, 127.9, 126.9, 124.4 (q, *J* = 280.7 Hz), 82.0 (q, *J* = 31.7 Hz), 80.1, 60.9, 21.7. HRMS (ESI) m/z calcd. for $C_{18}H_{16}F_3NNaO_4S$ $[M + Na]^+$ 422.0644; found 422.0650.



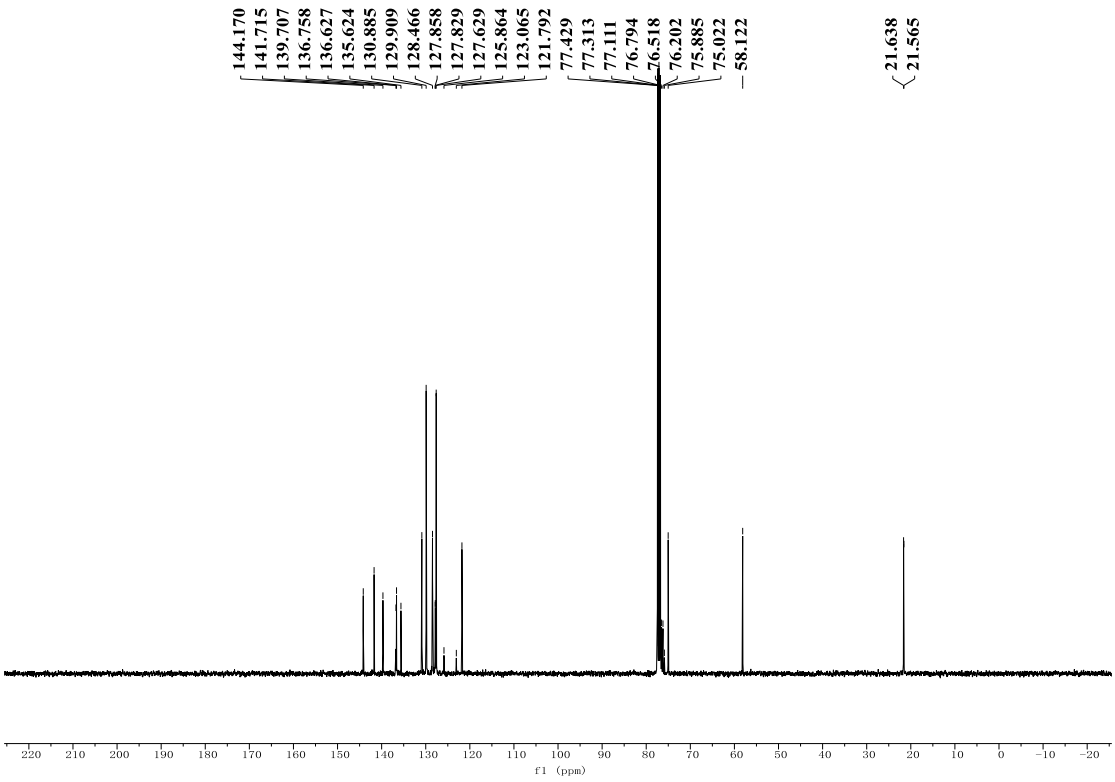
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of Compound **3a**



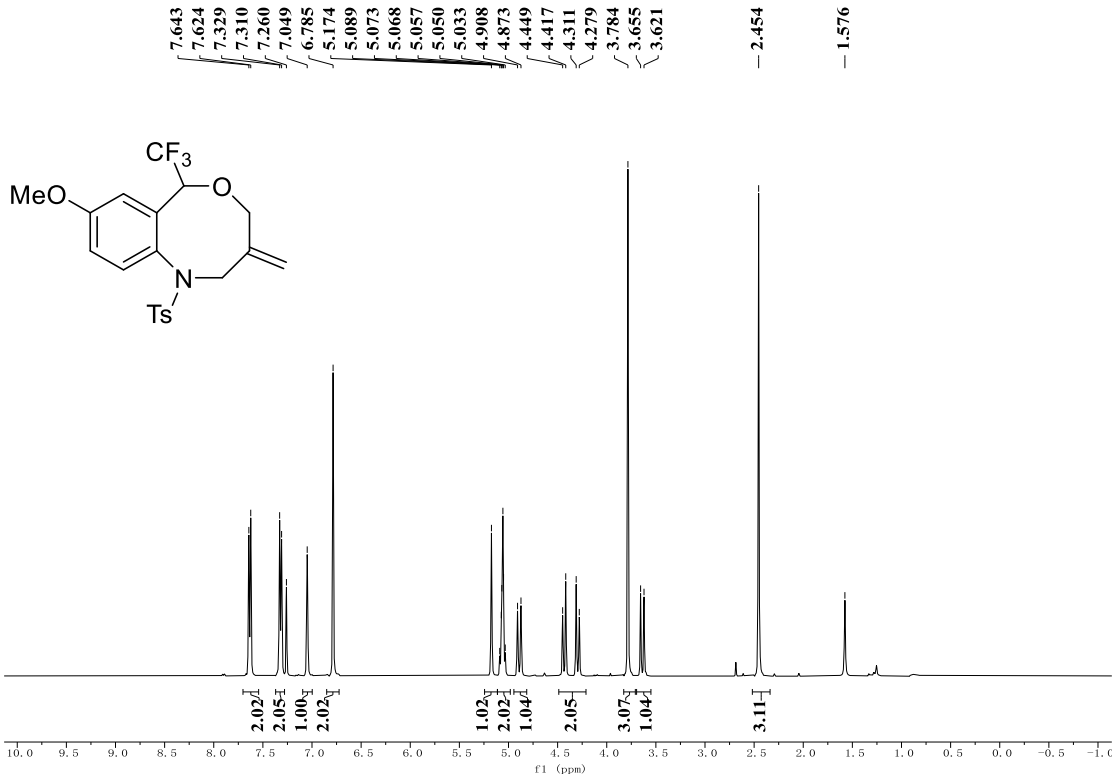
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of Compound **3a**



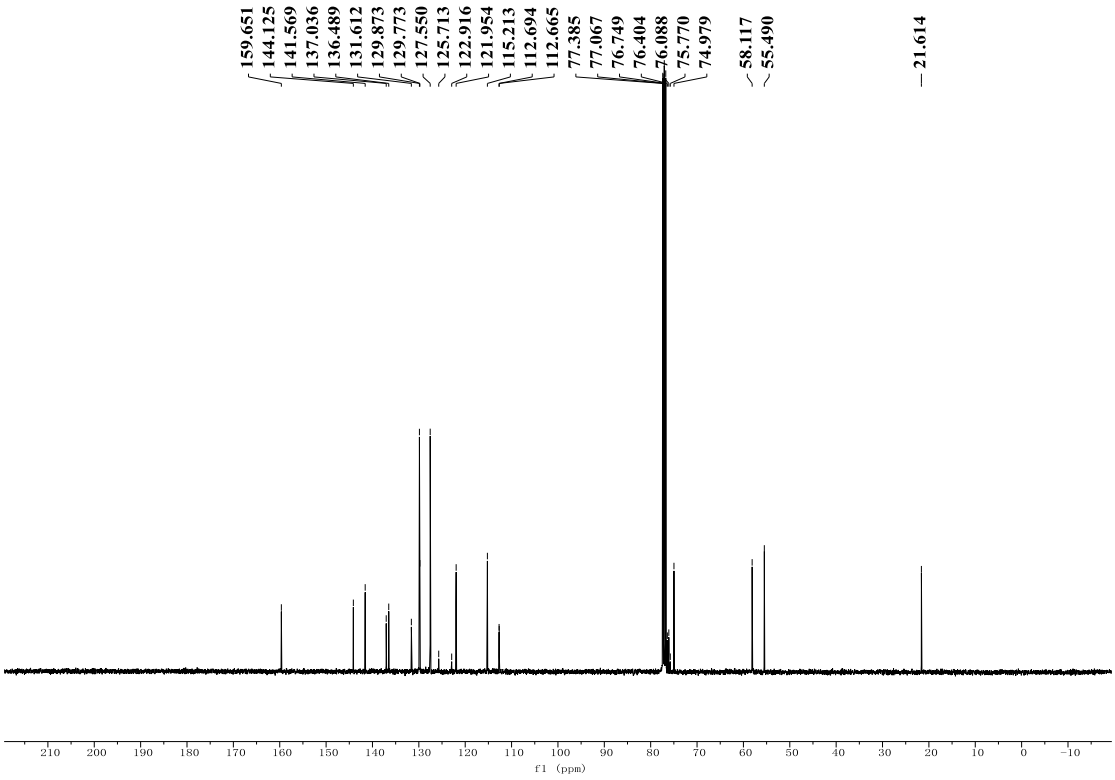
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of Compound **3b**



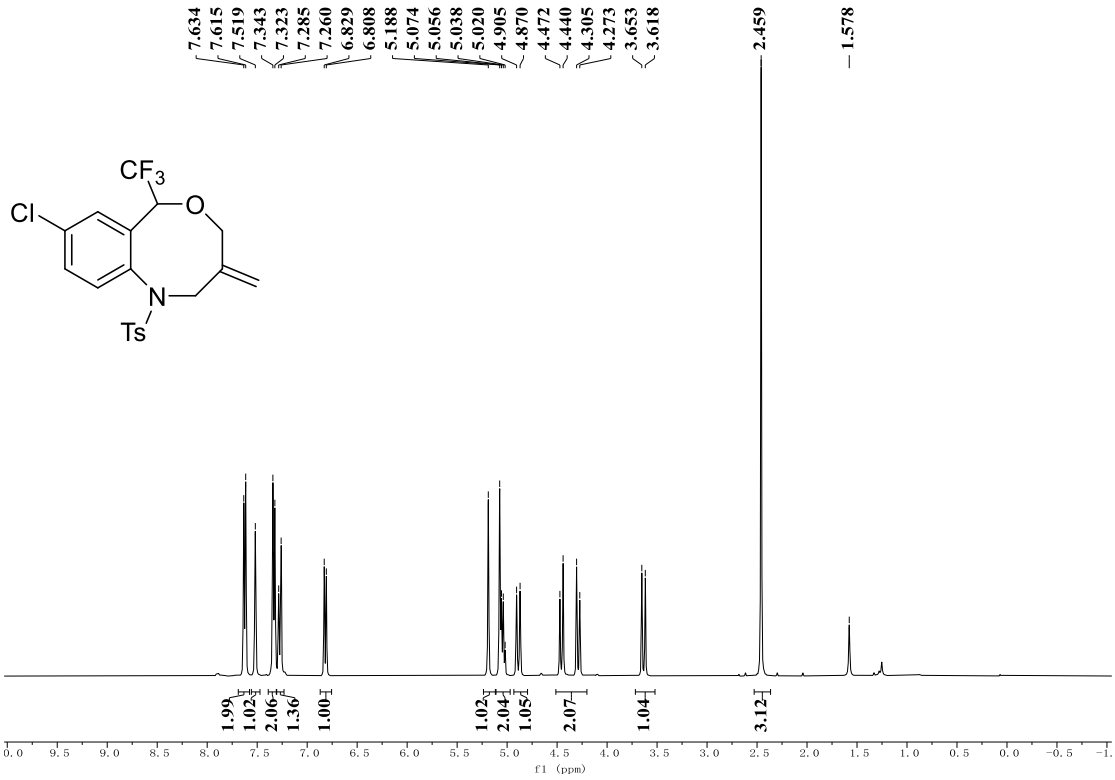
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of Compound **3b**



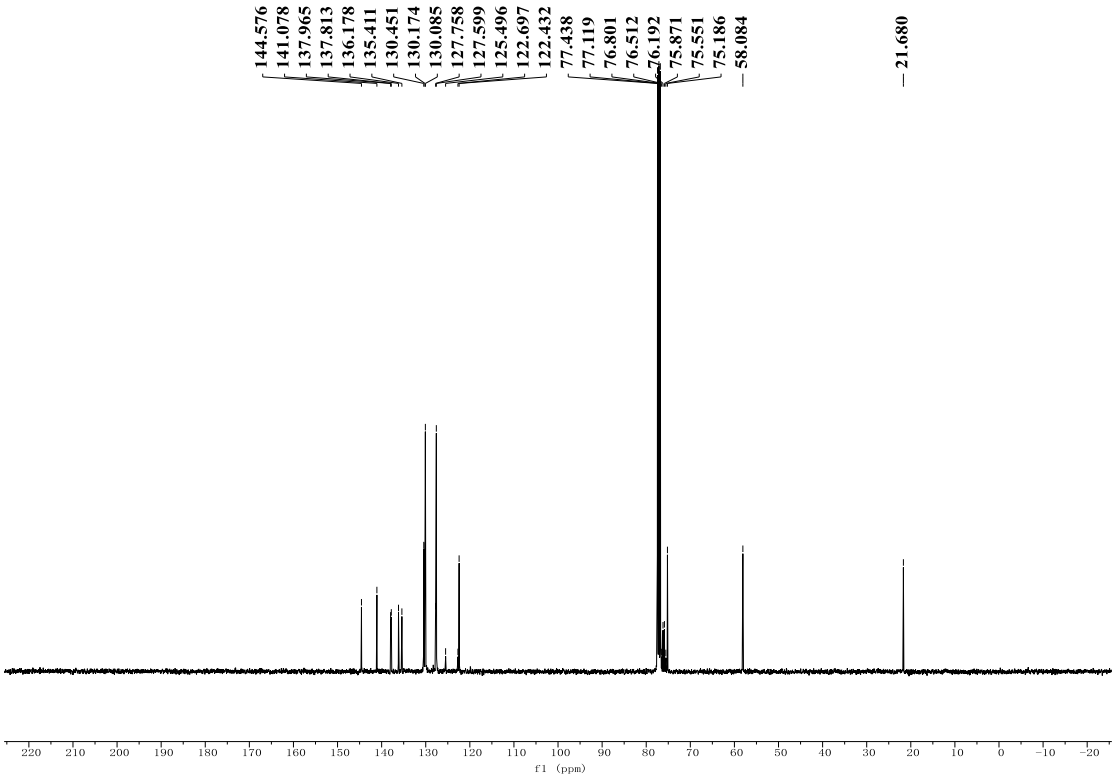
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of Compound **3c**



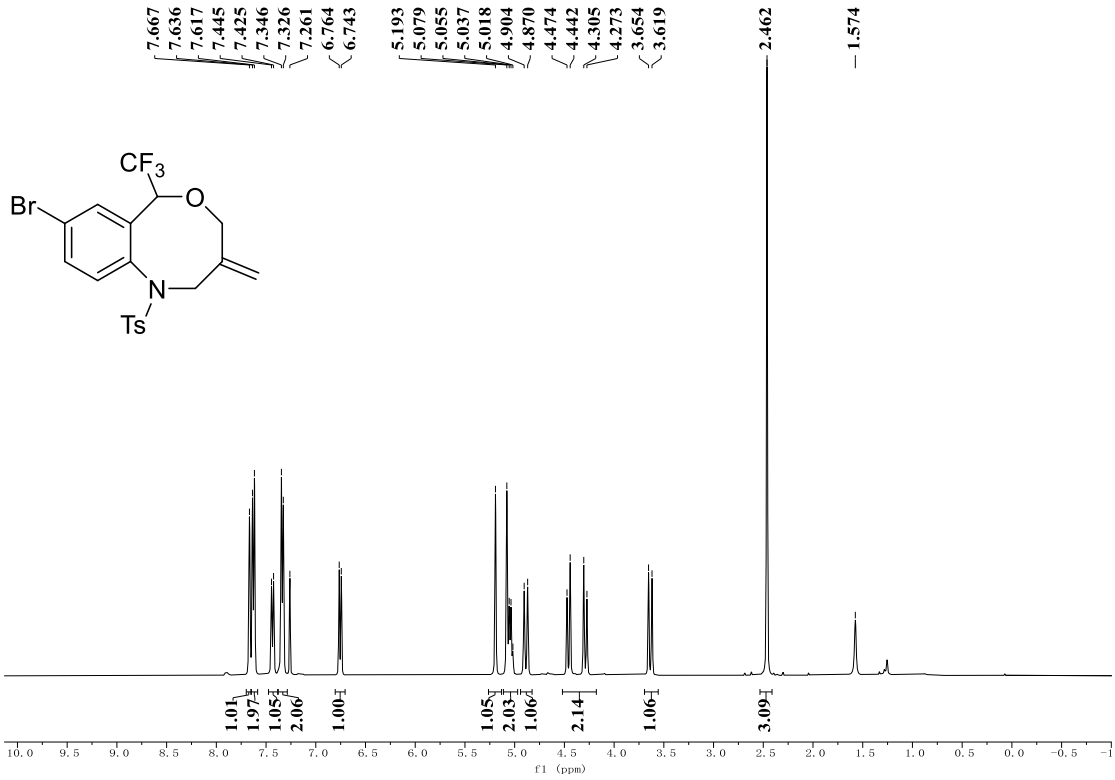
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of Compound **3c**



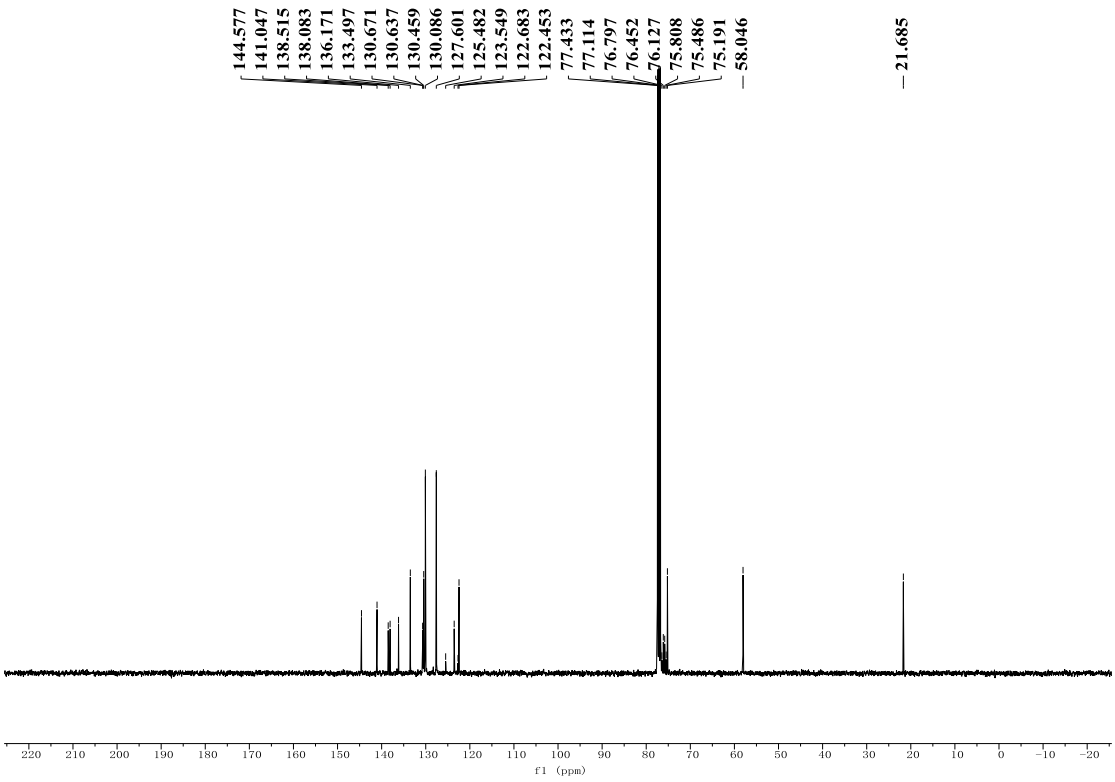
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of Compound **3d**



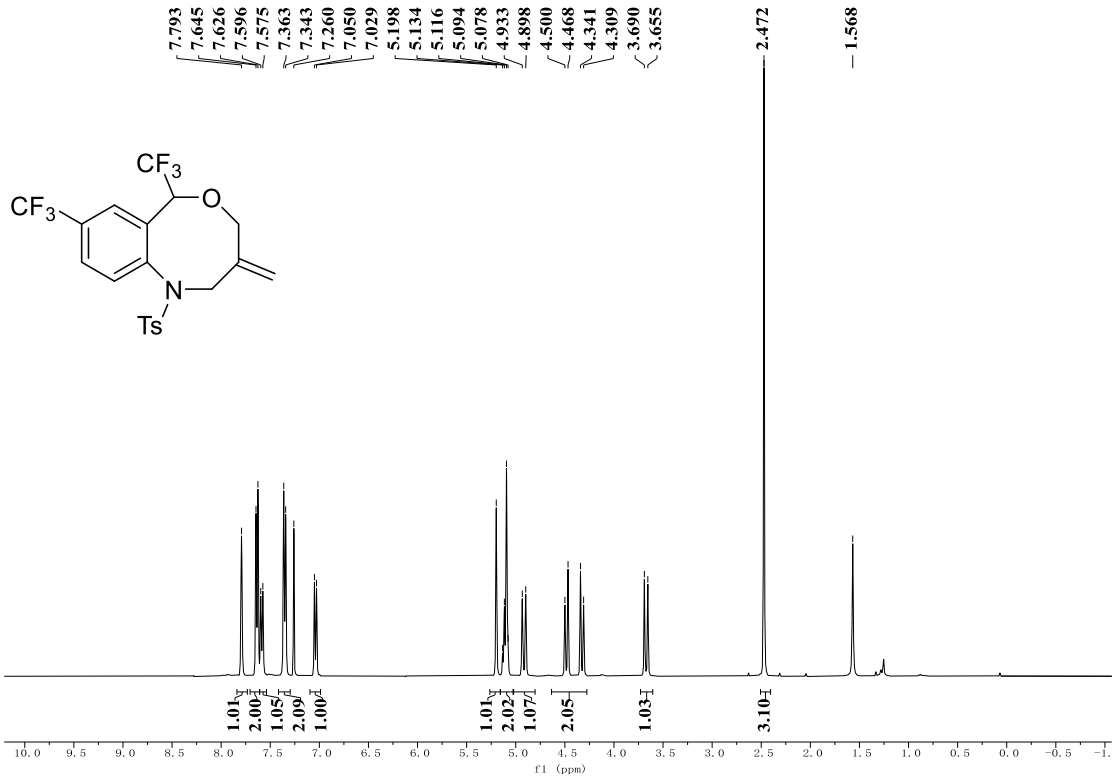
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of Compound **3d**



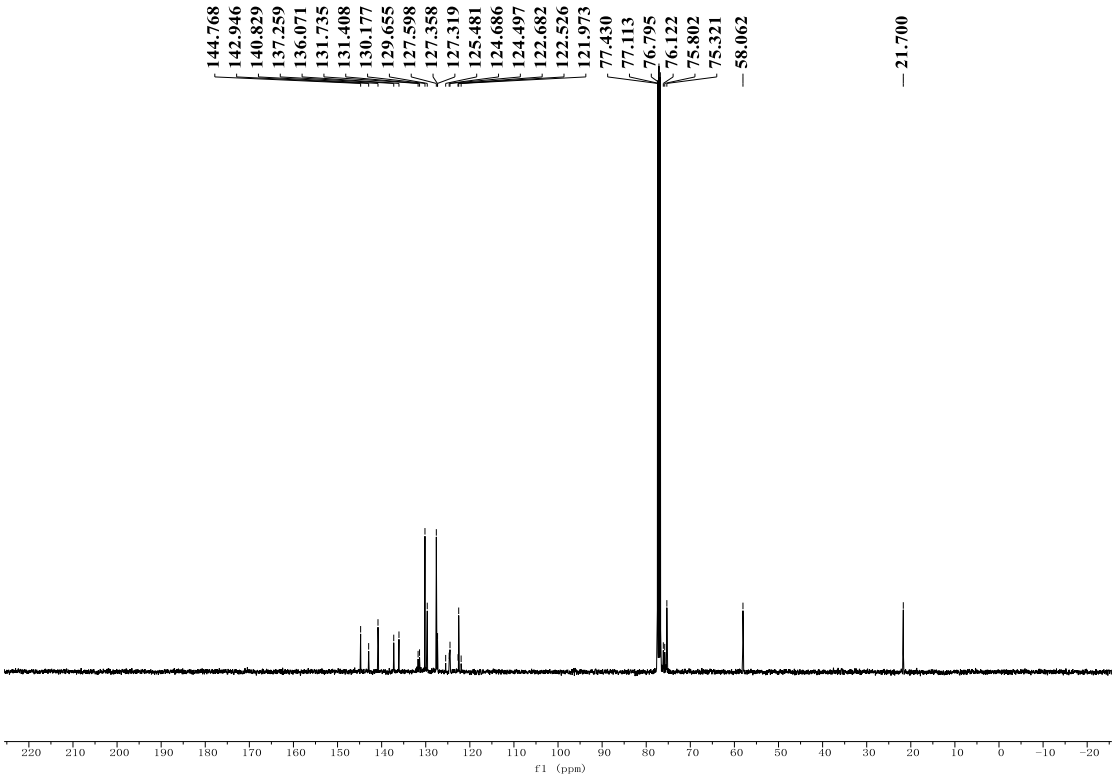
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of Compound **3e**



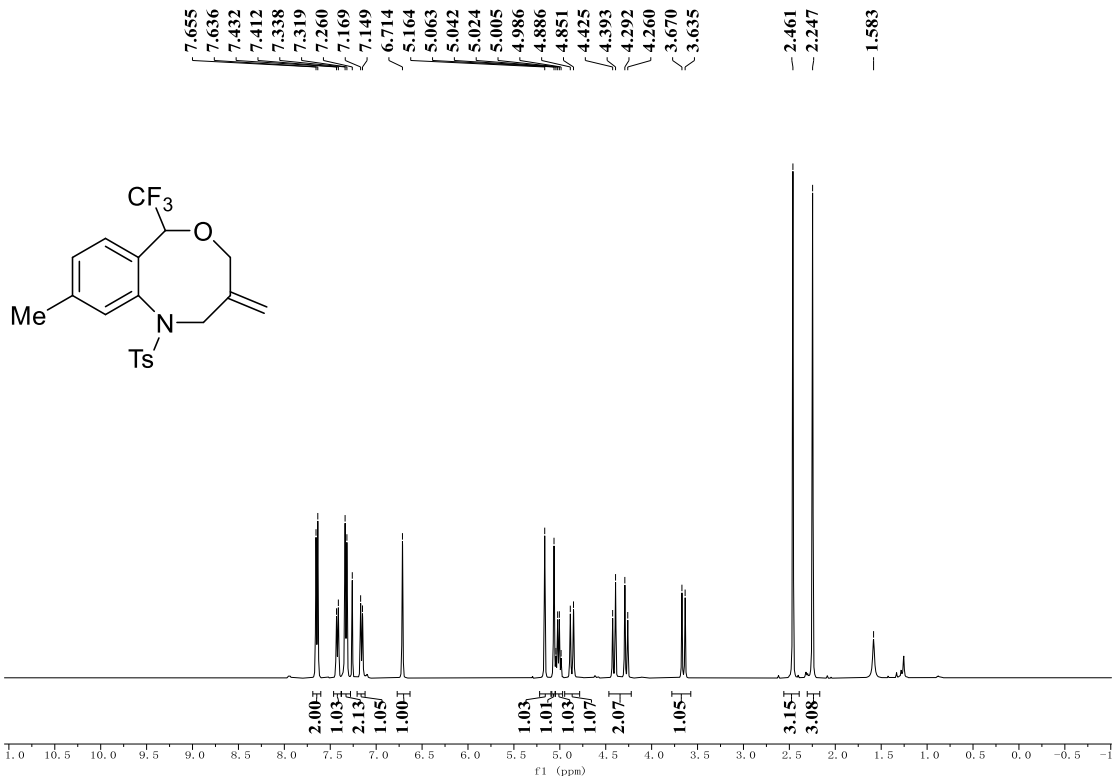
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of Compound **3e**



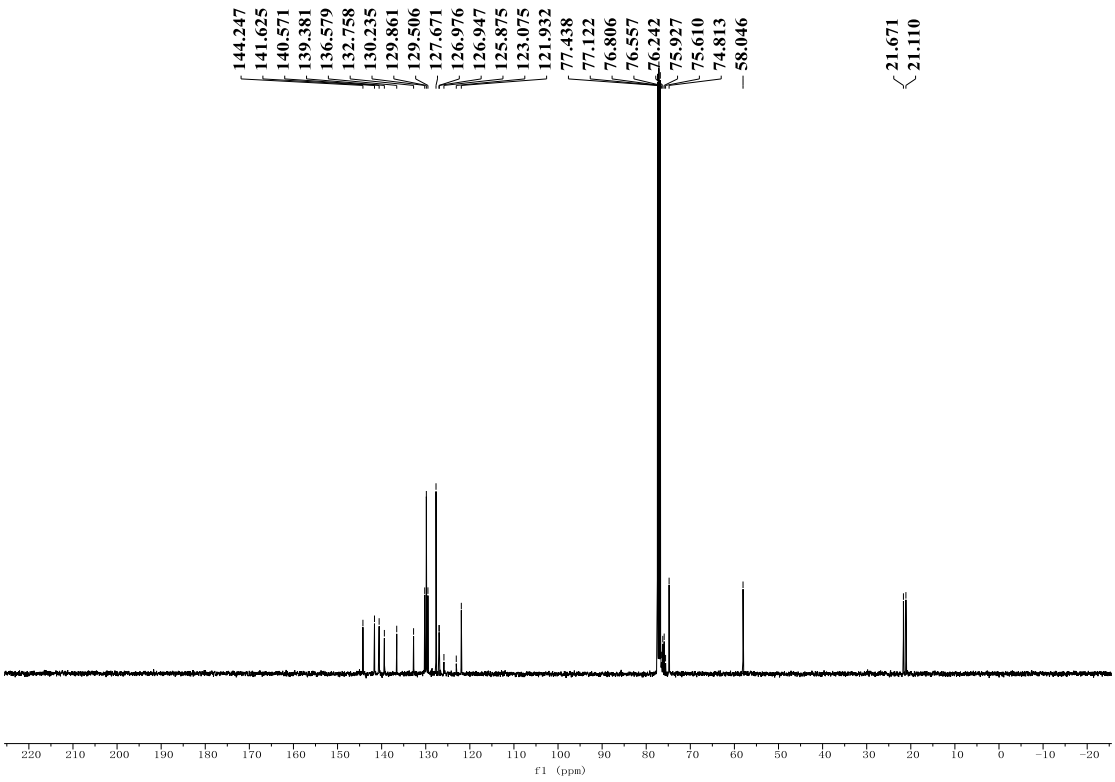
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of Compound **3f**



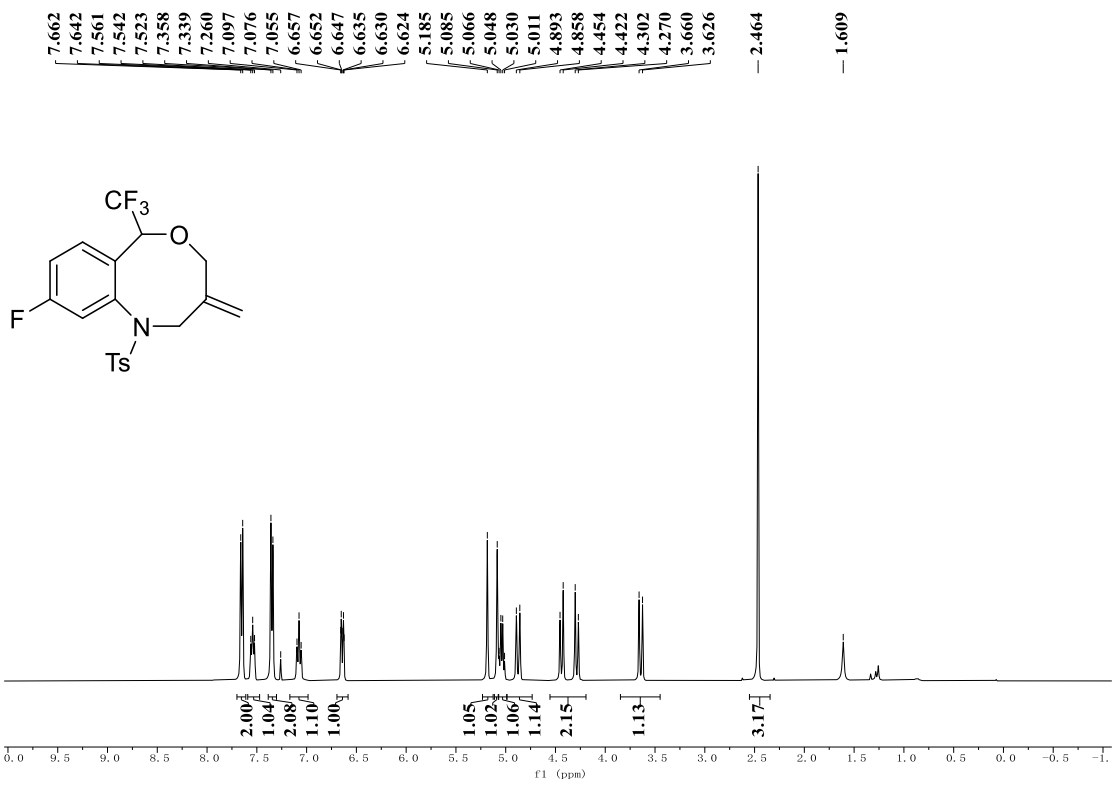
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of Compound **3f**



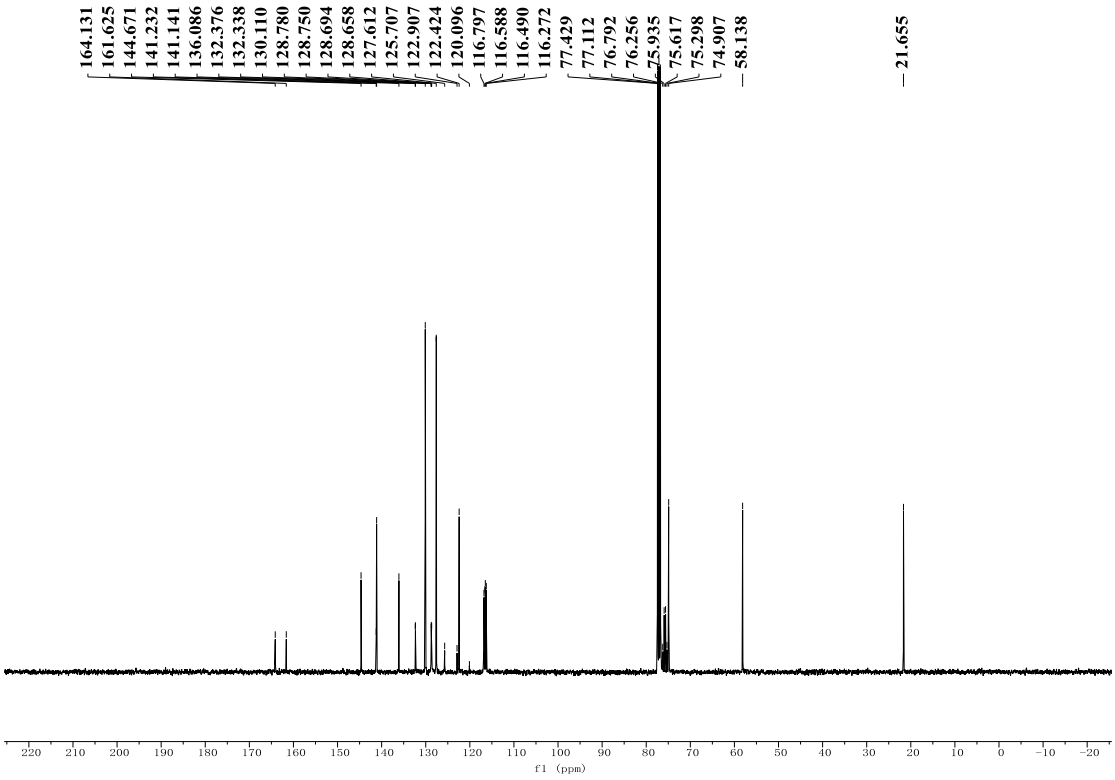
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of Compound **3g**



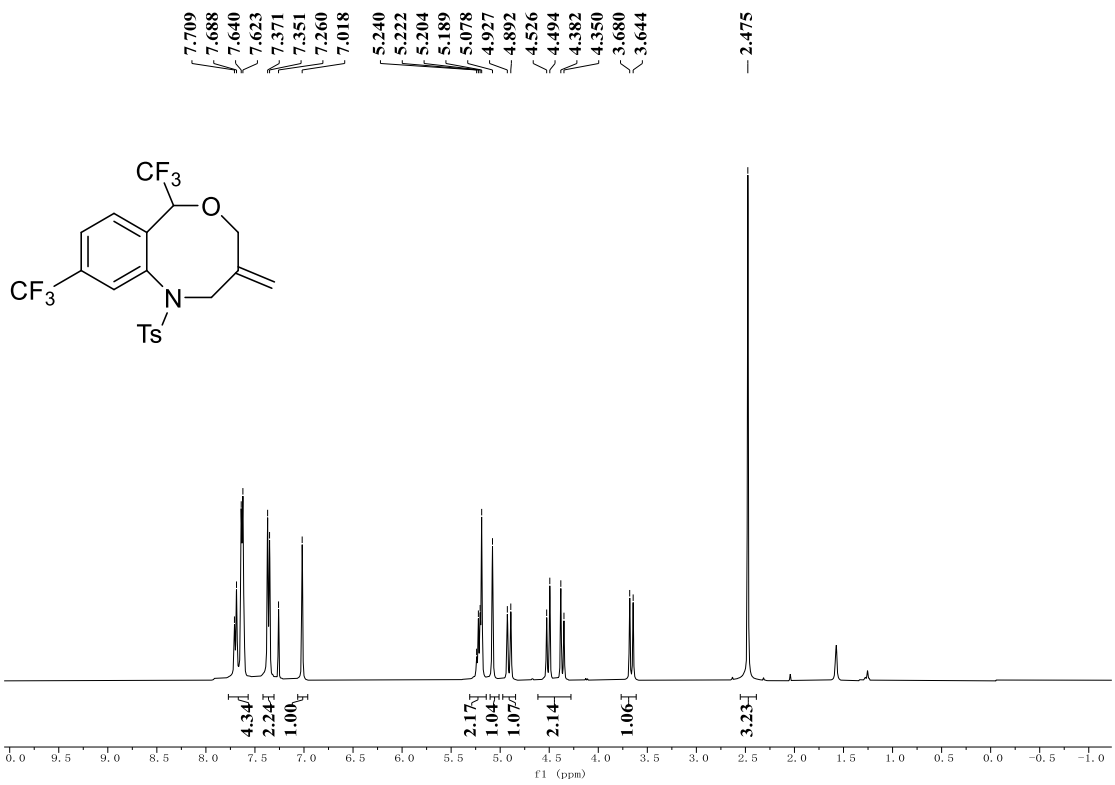
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of Compound **3g**



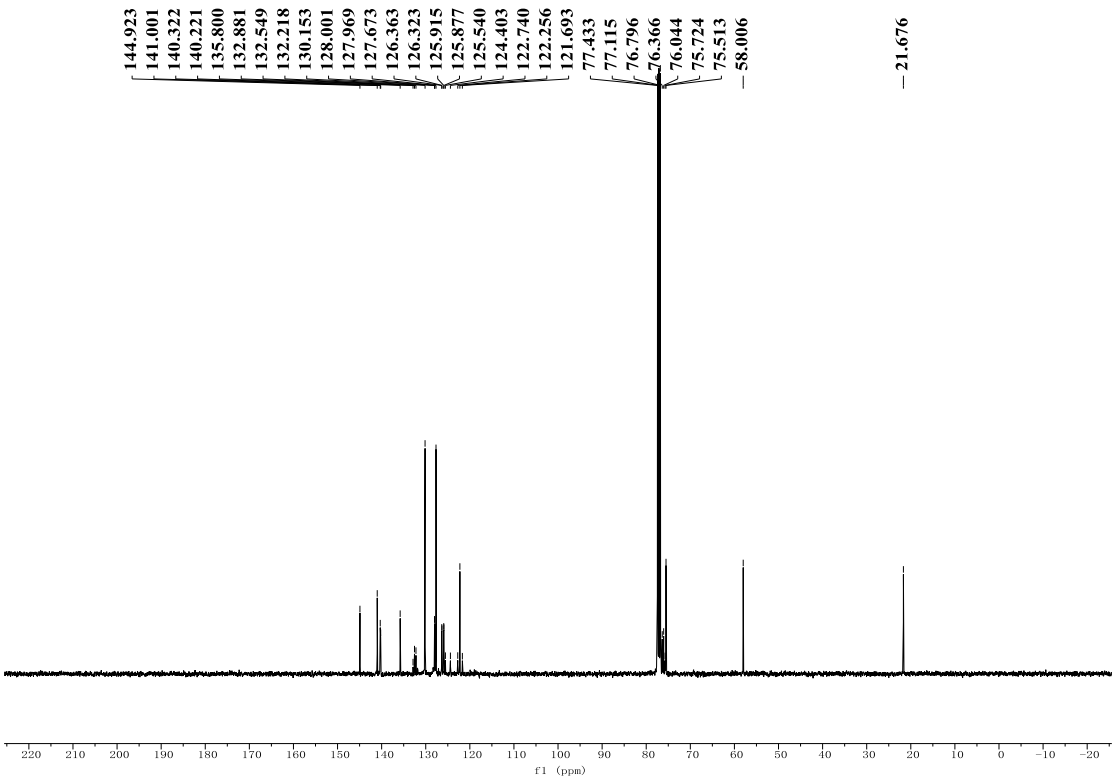
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of Compound **3h**



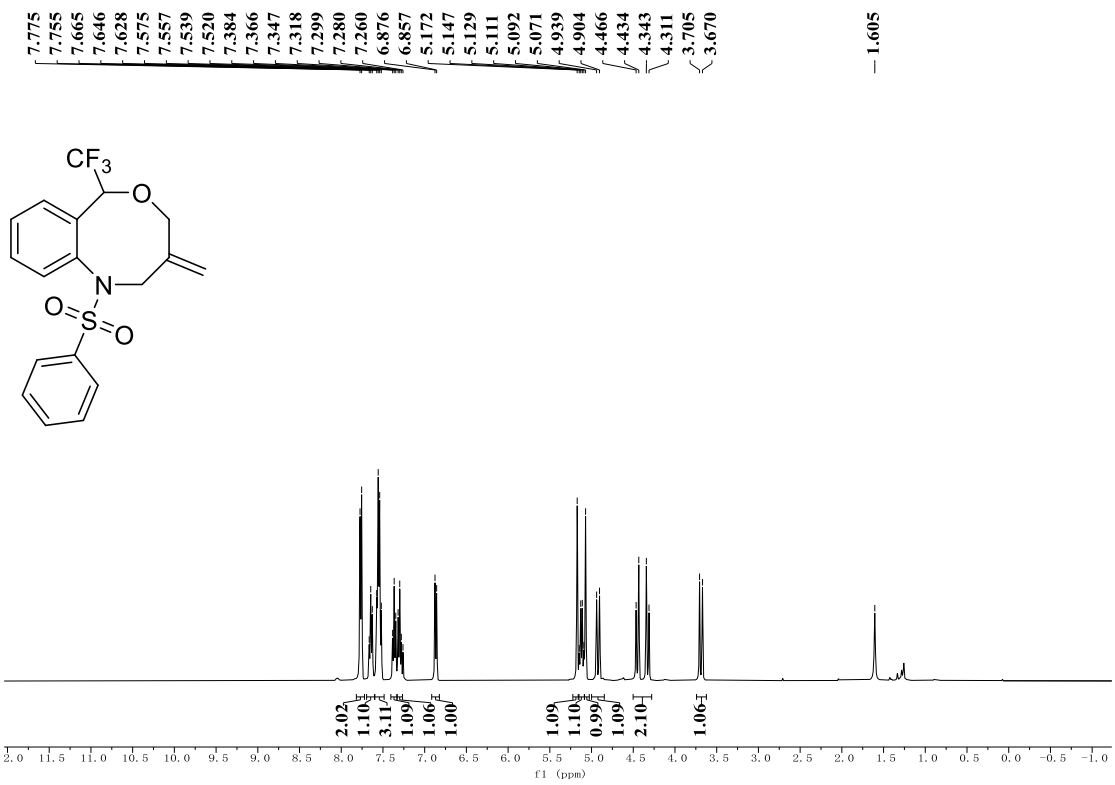
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of Compound **3h**



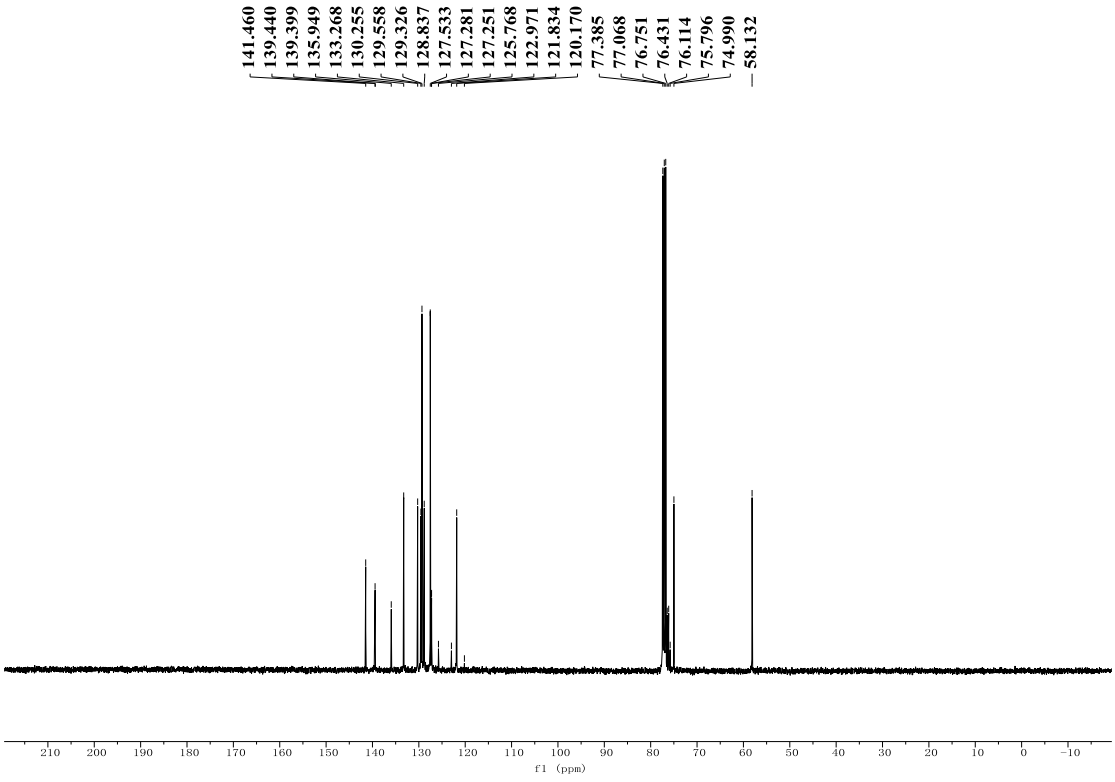
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of Compound **3i**



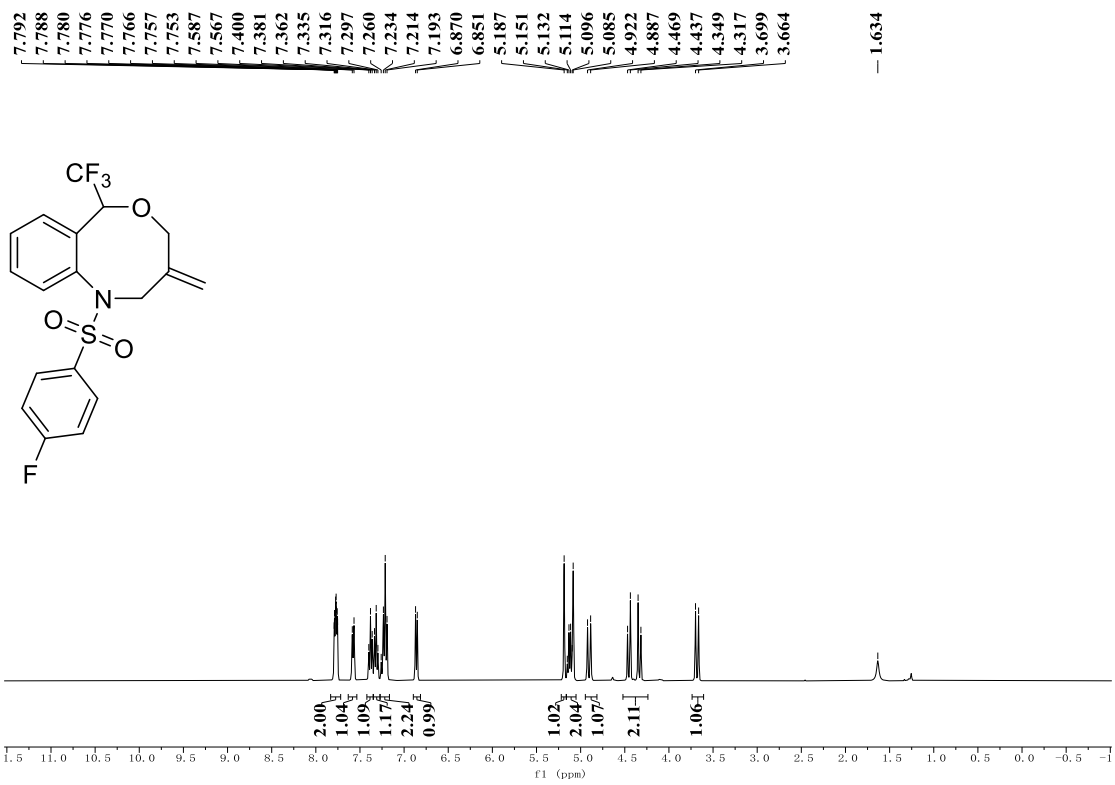
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of Compound **3i**



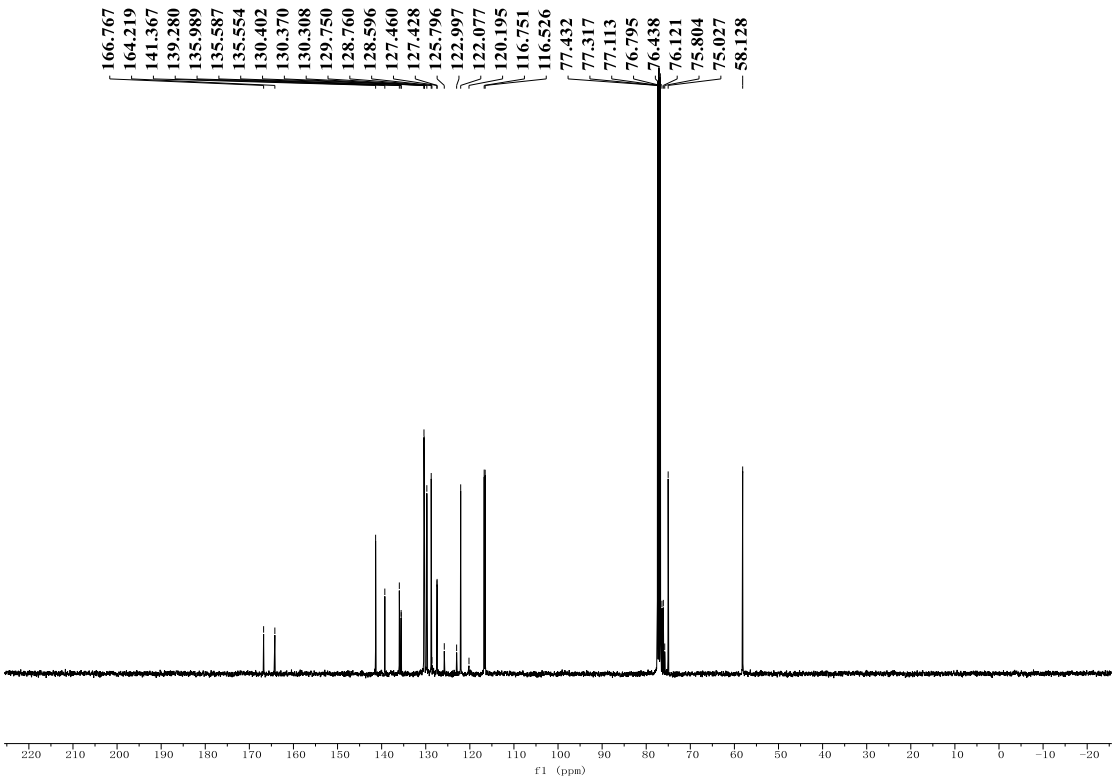
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of Compound **3j**



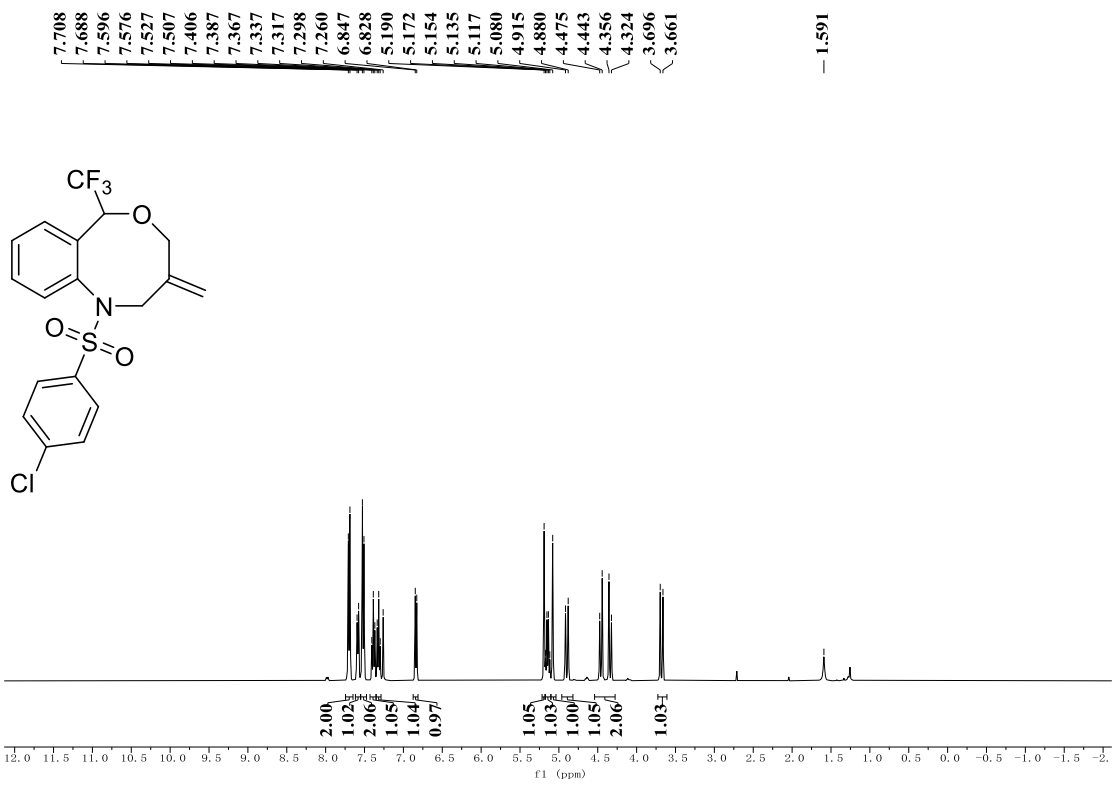
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of Compound **3j**



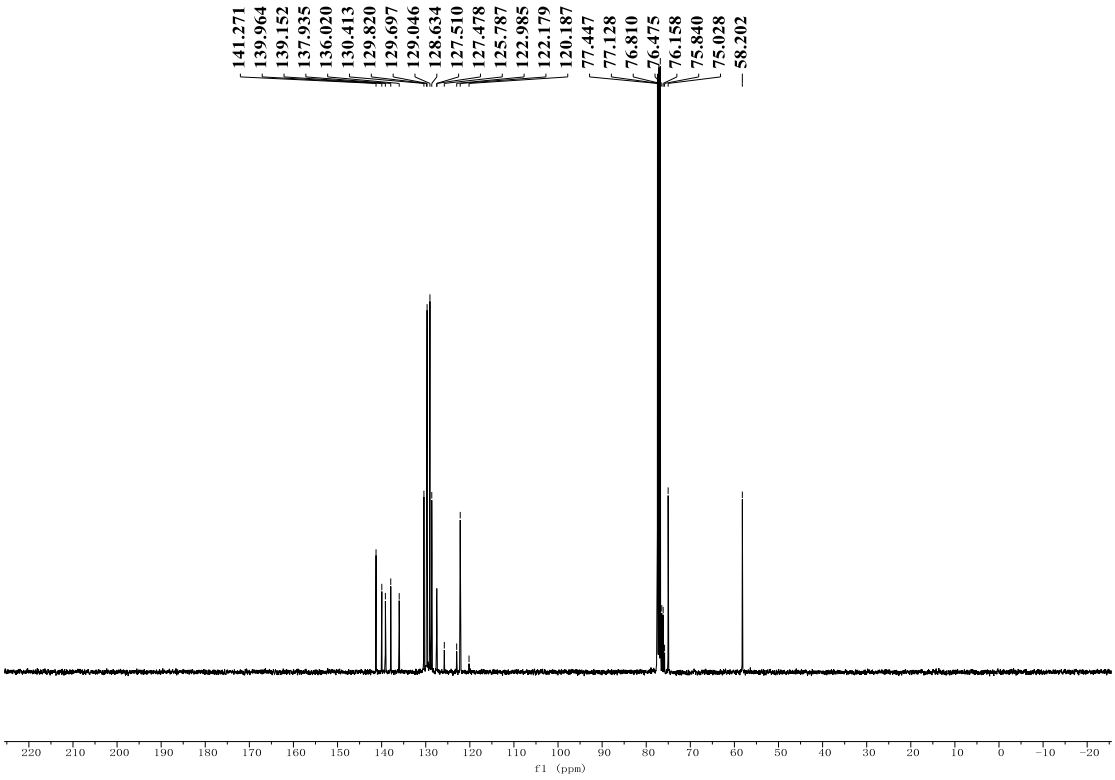
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of Compound **3k**



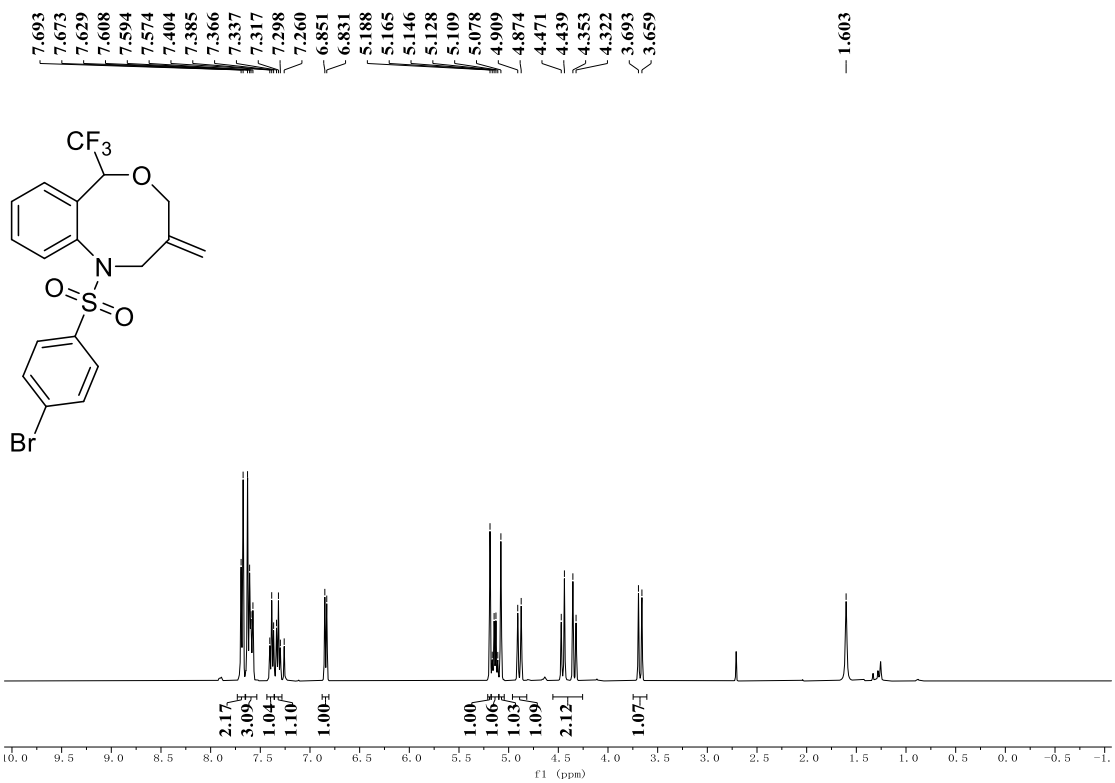
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of Compound **3k**



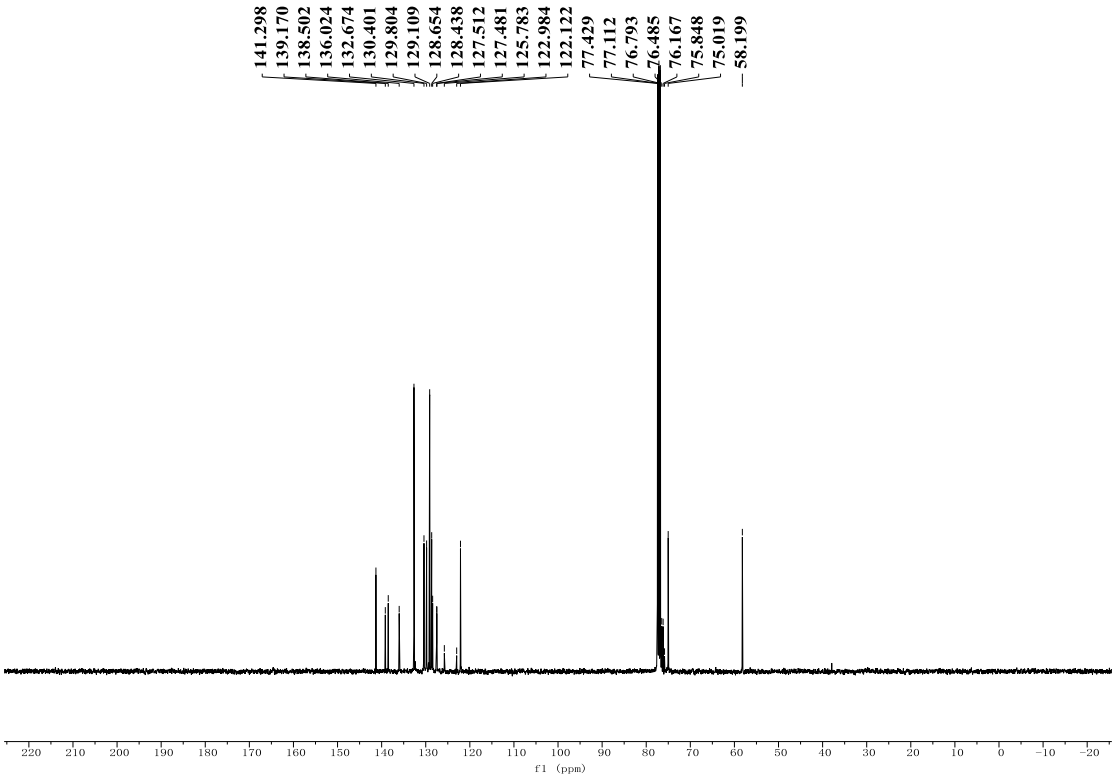
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of Compound **3l**



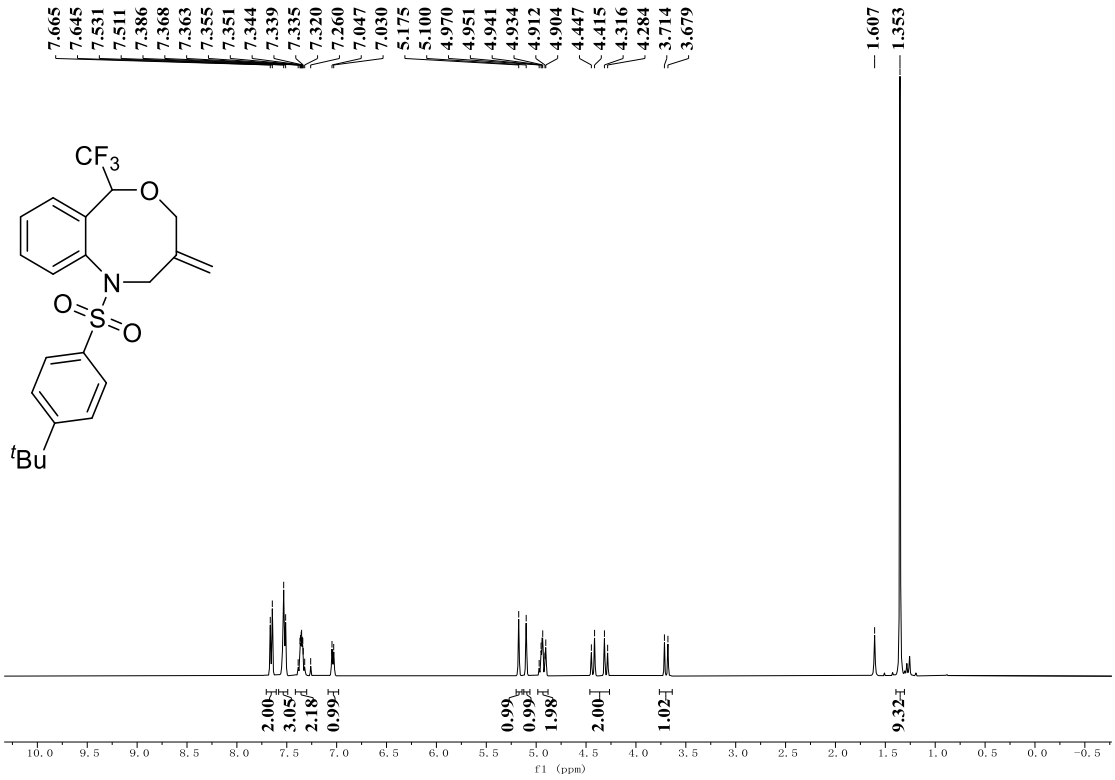
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of Compound **3l**



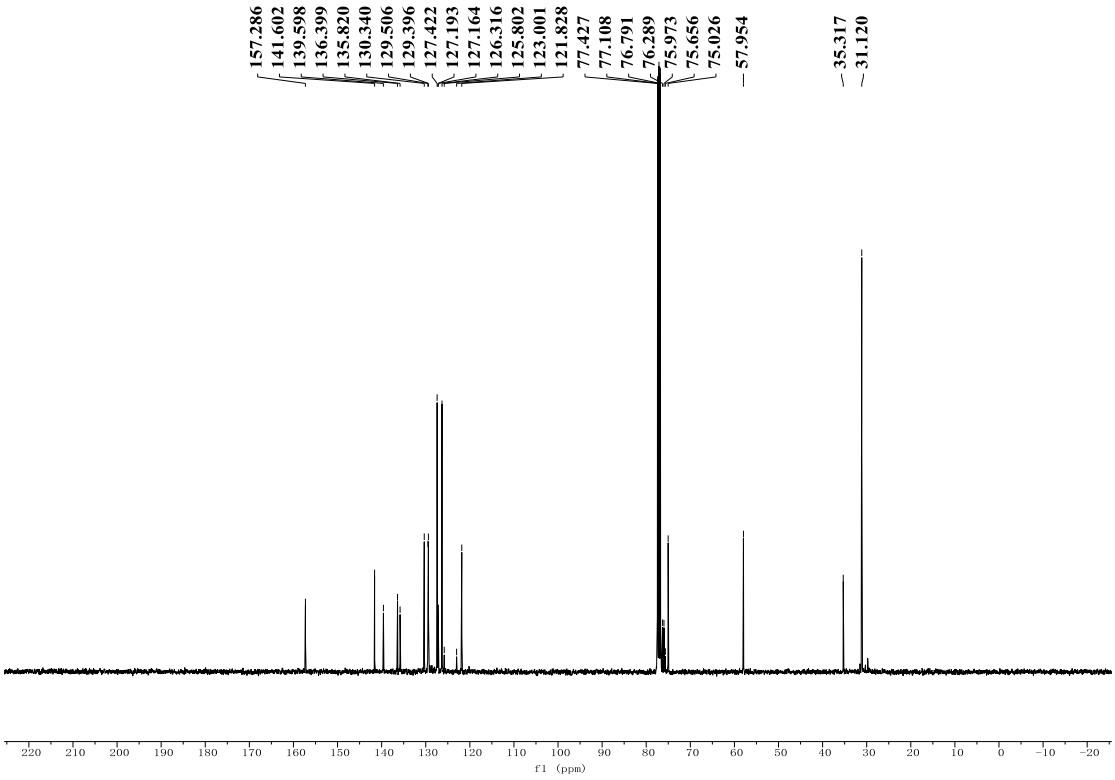
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of Compound **3m**



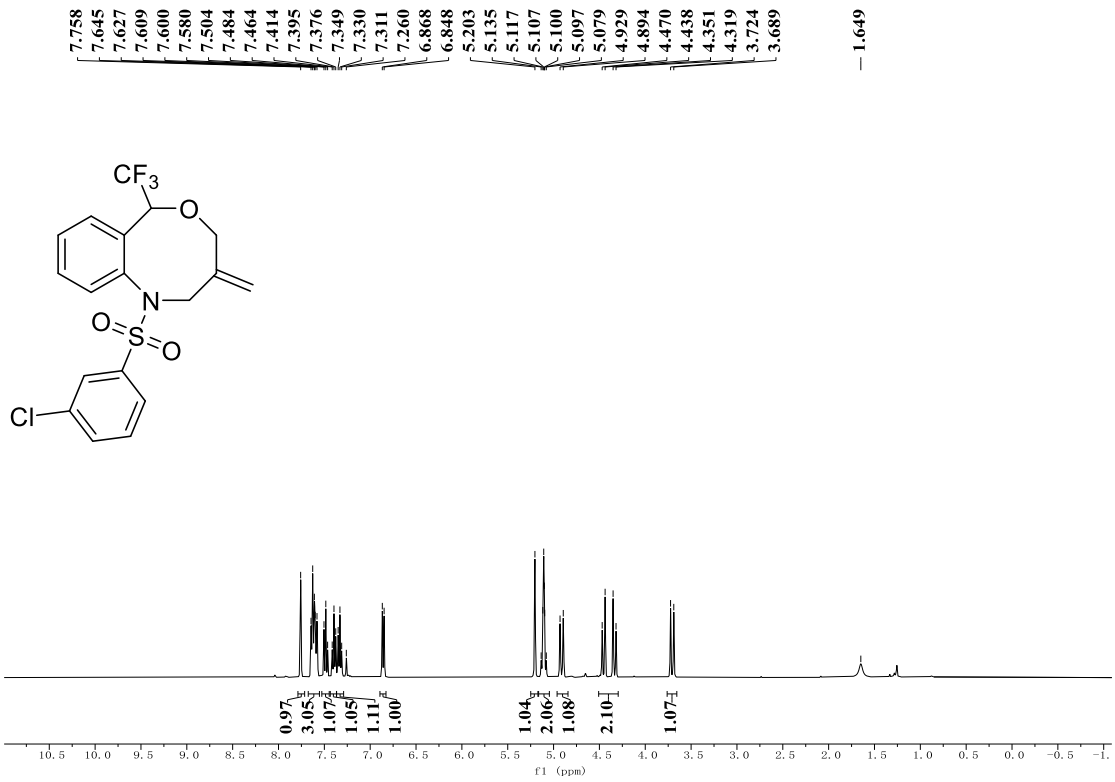
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of Compound **3m**



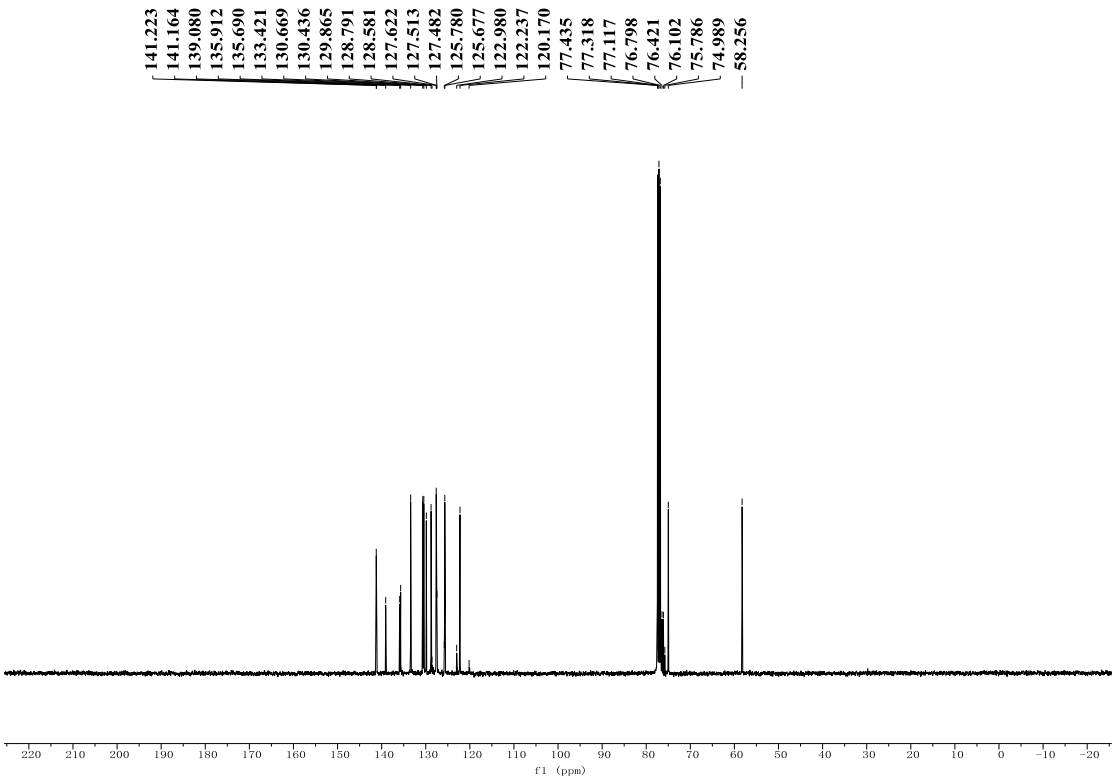
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of Compound **3n**



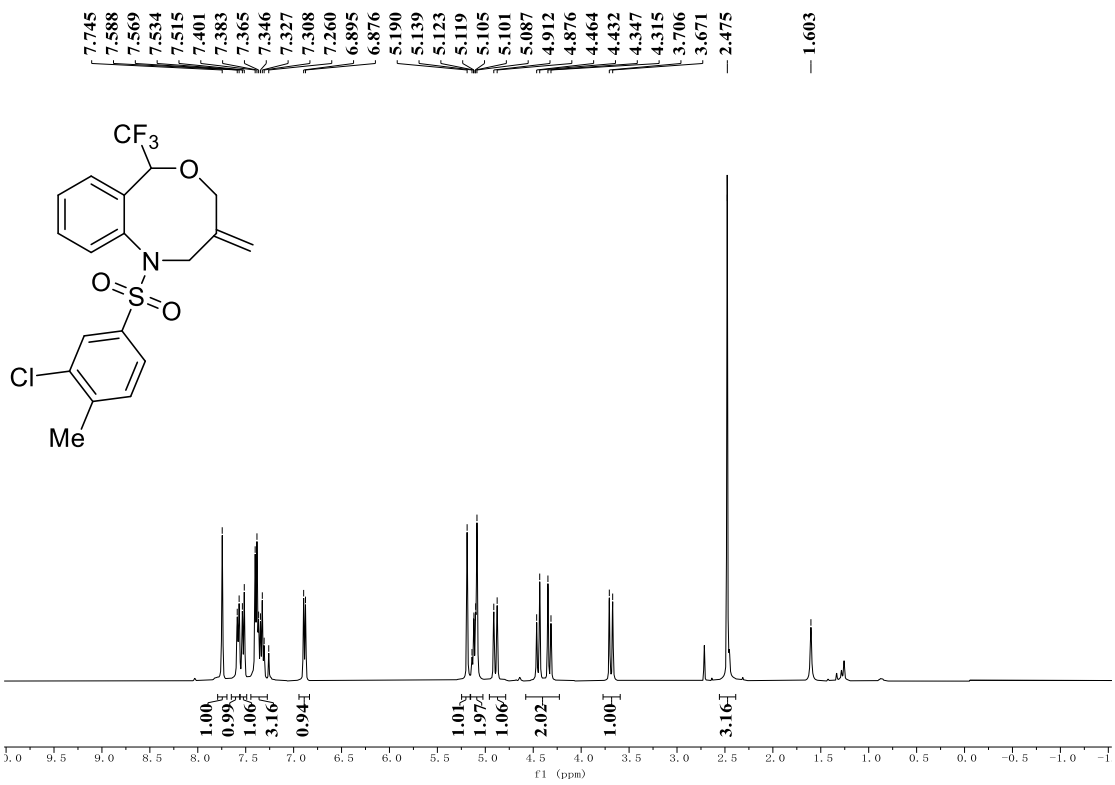
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of Compound **3n**



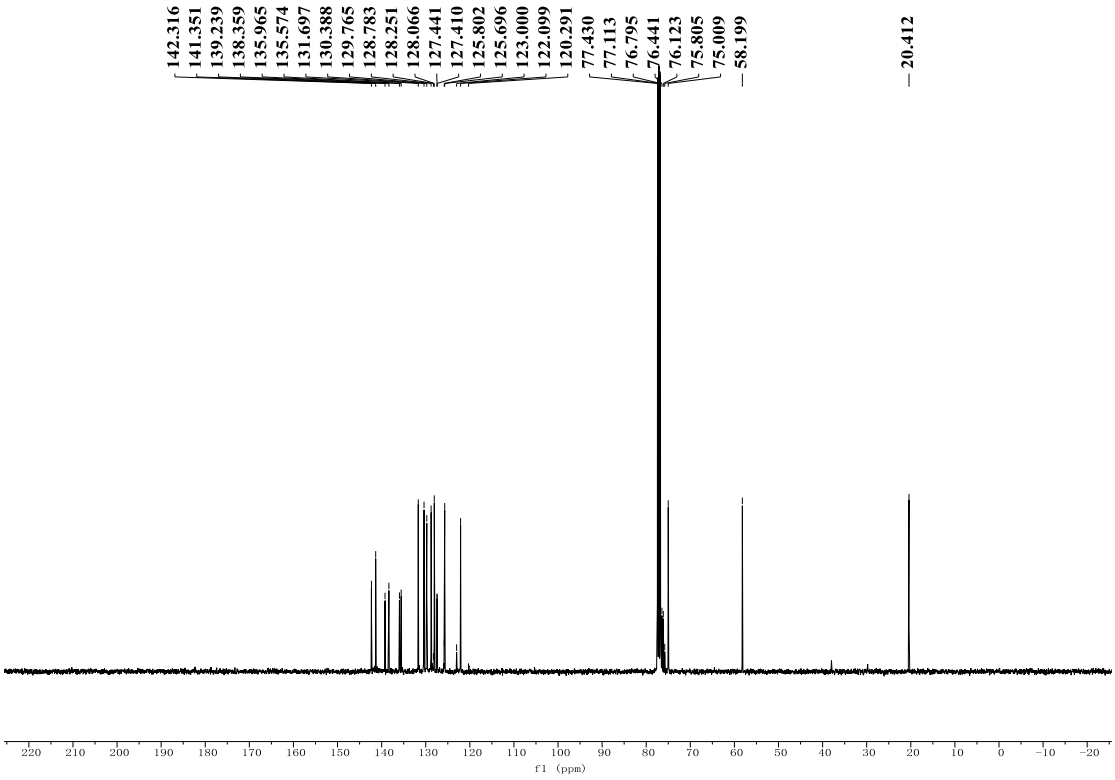
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of Compound **3o**



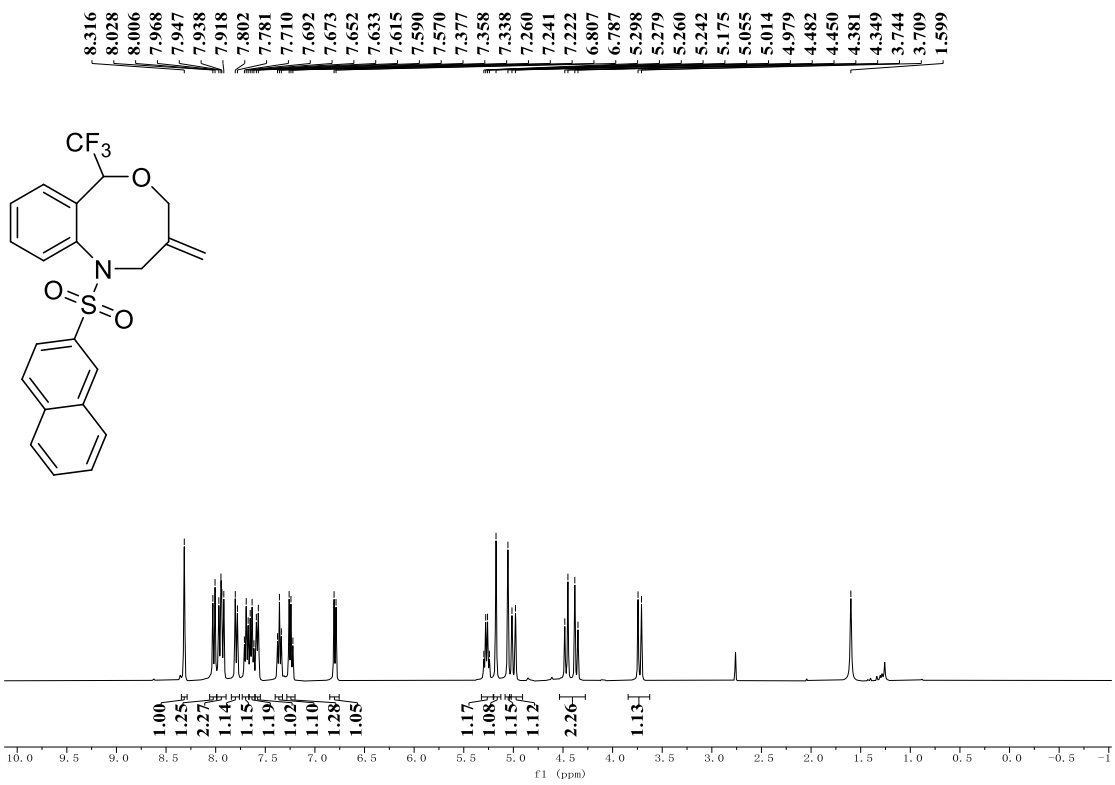
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of Compound **3o**



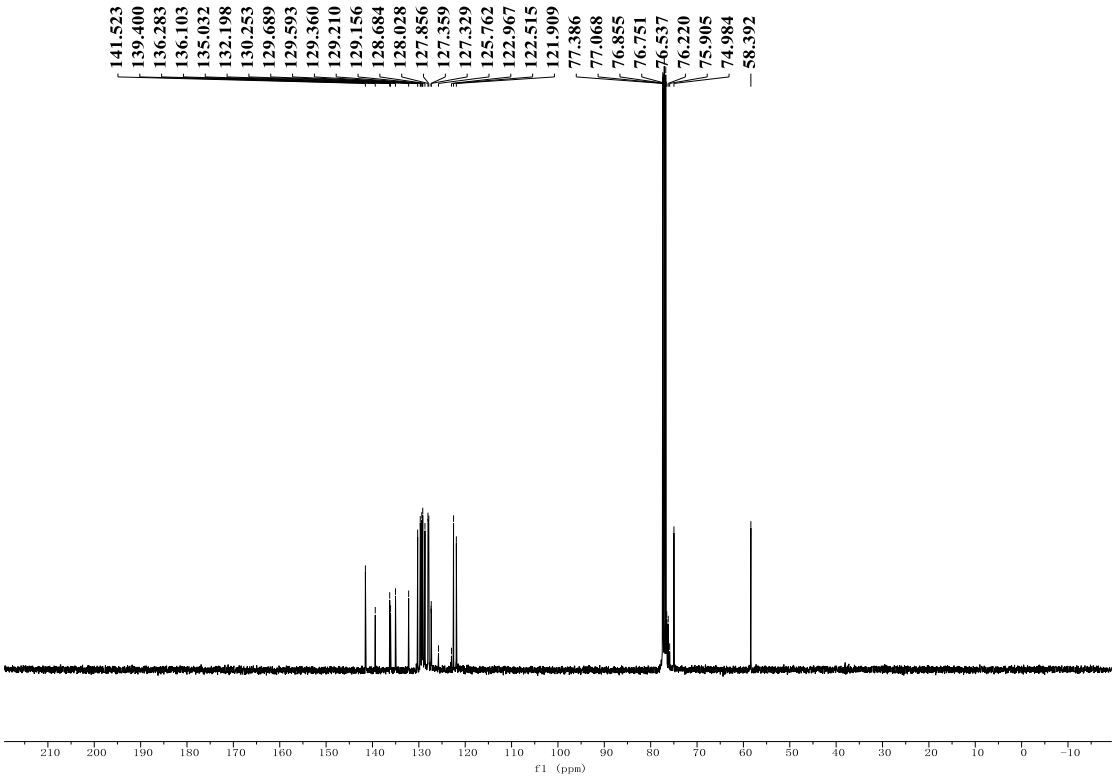
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of Compound **3p**



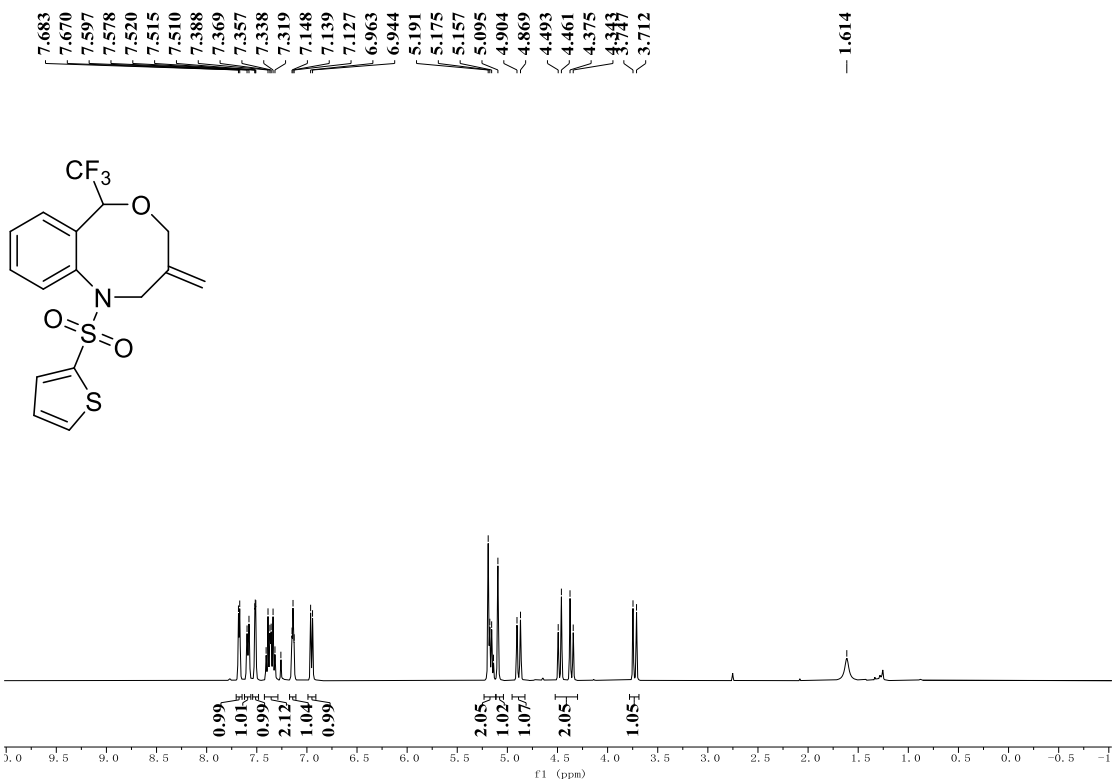
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of Compound **3p**



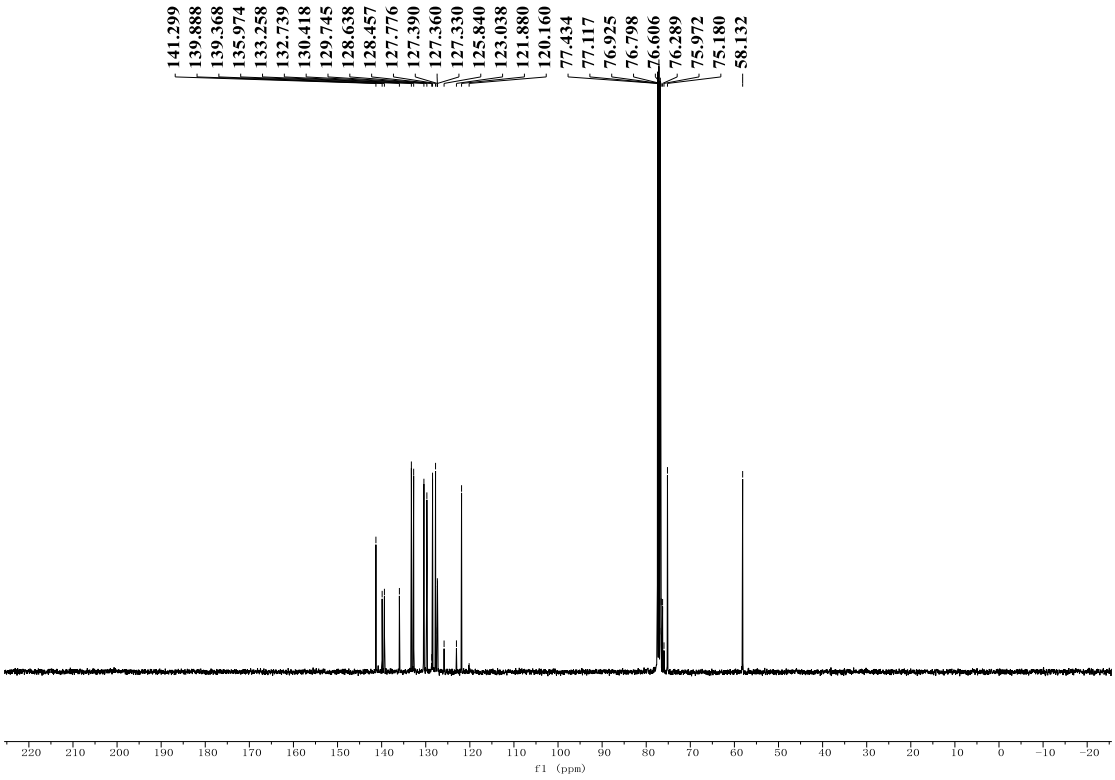
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of Compound **3q**



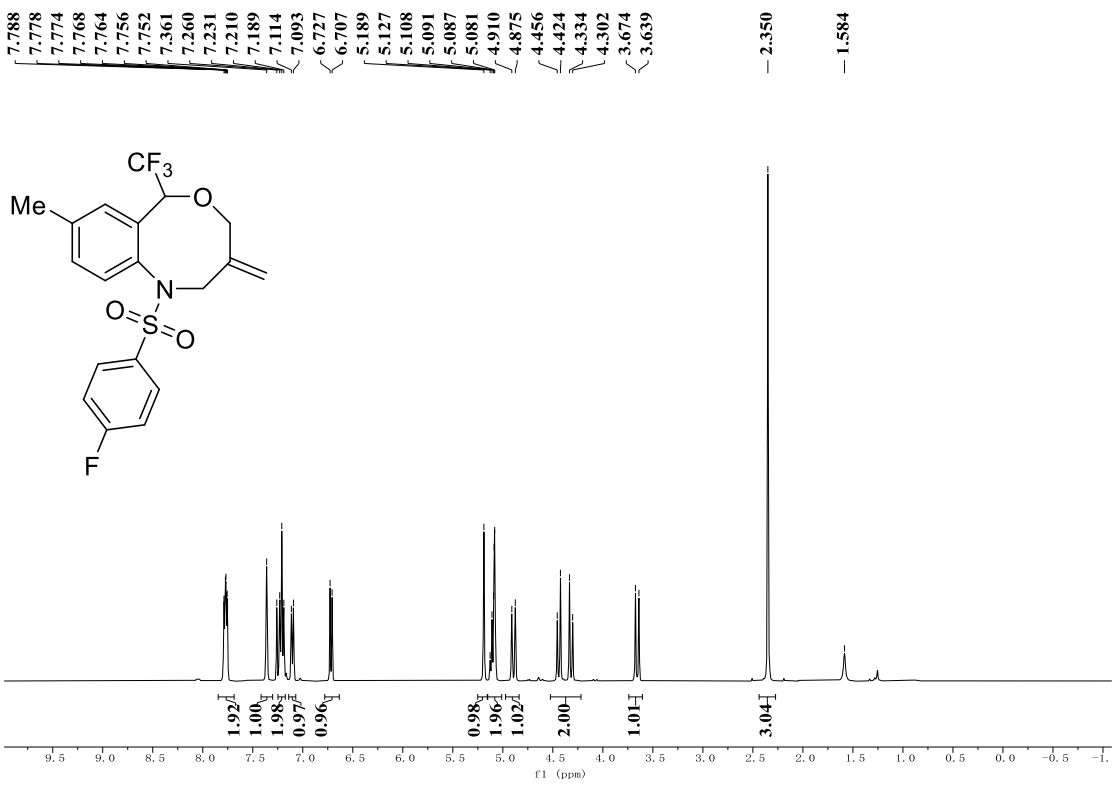
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of Compound **3q**



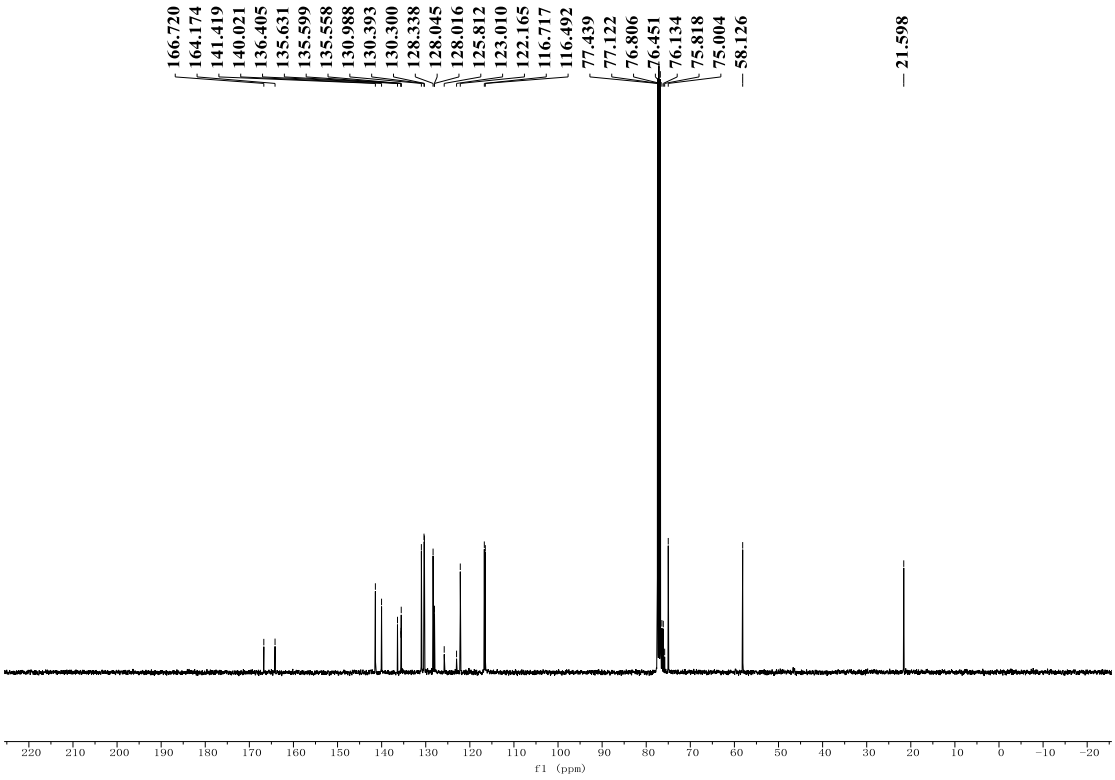
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of Compound **3r**



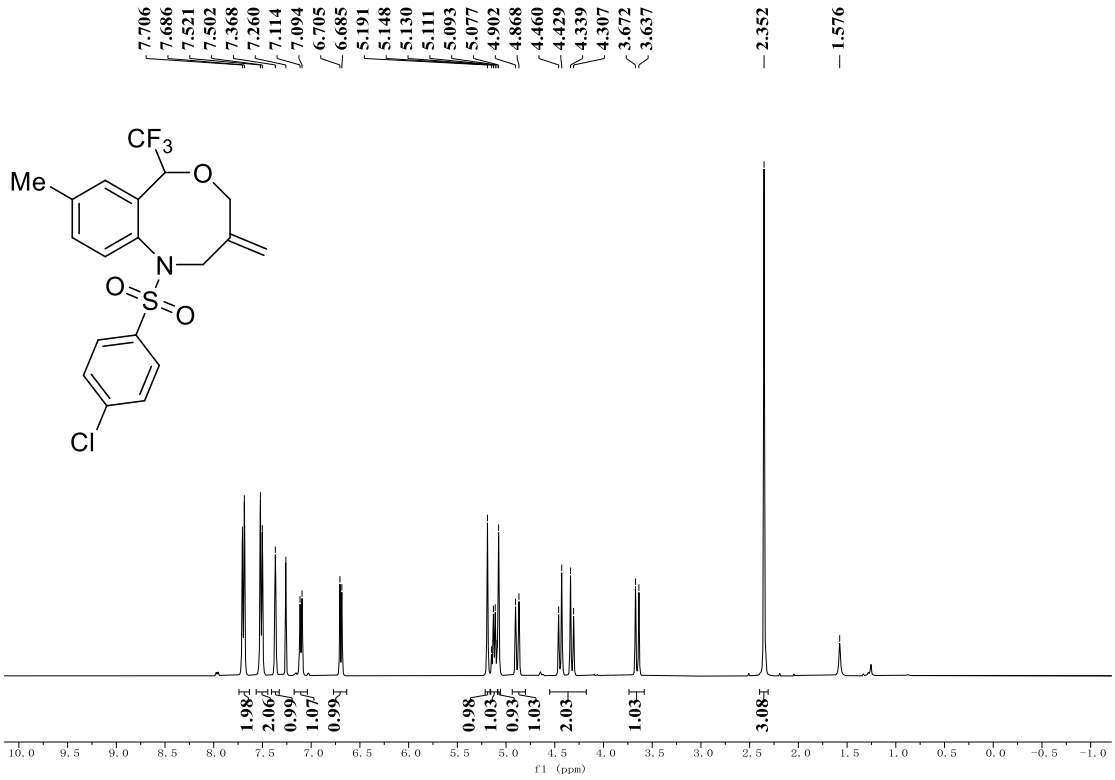
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of Compound **3r**



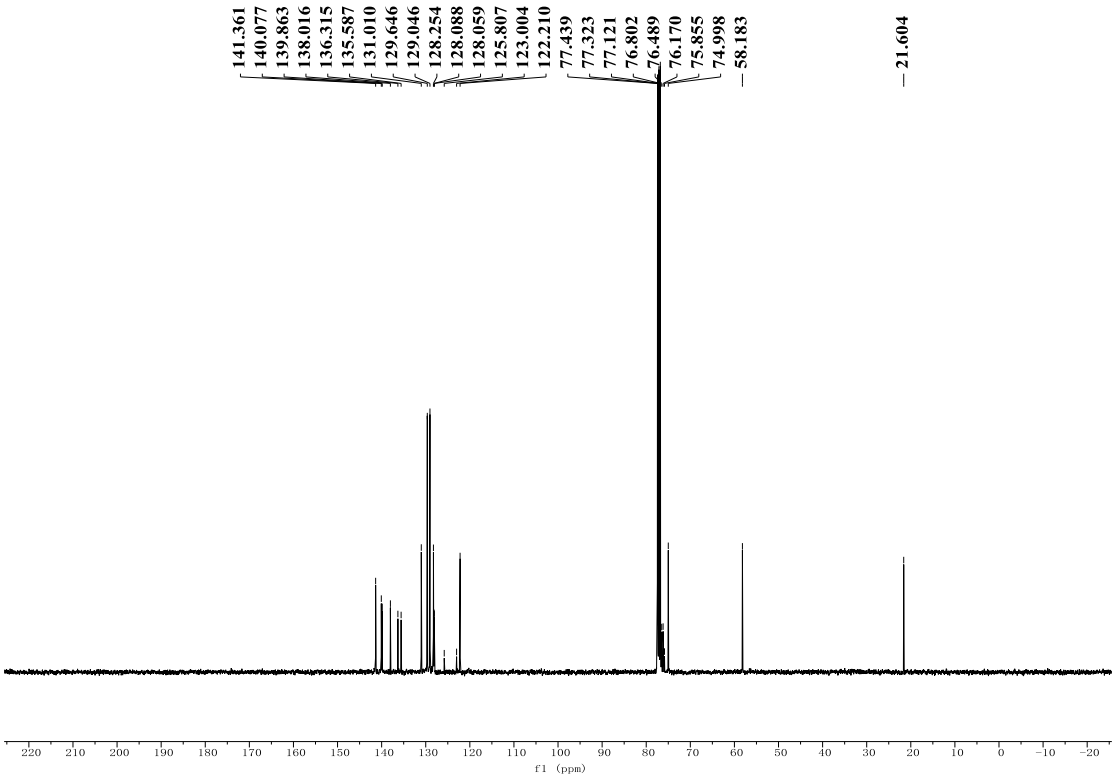
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of Compound **3s**



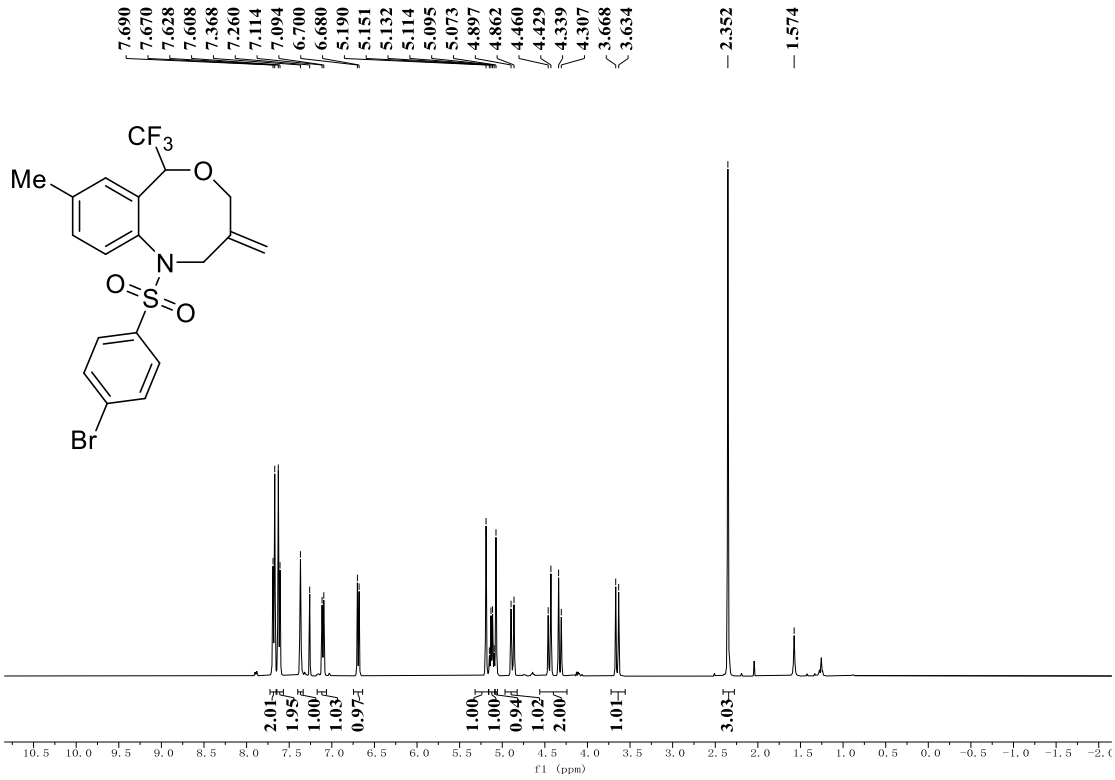
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of Compound **3s**



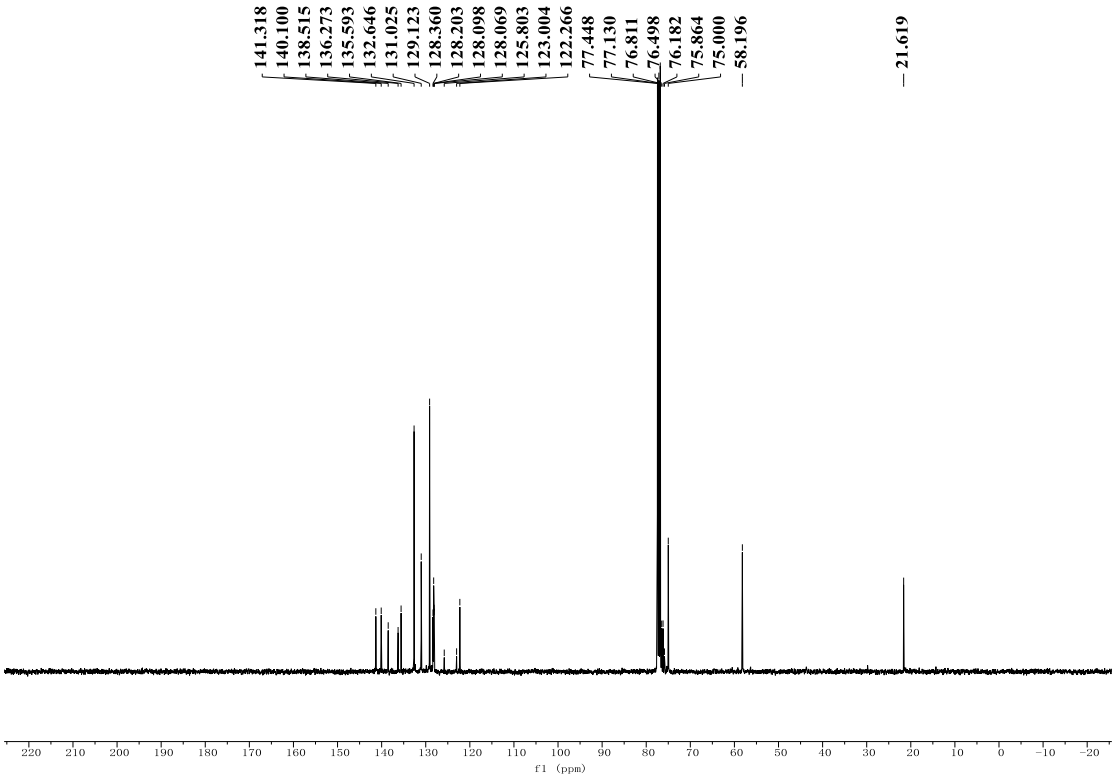
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of Compound **3t**



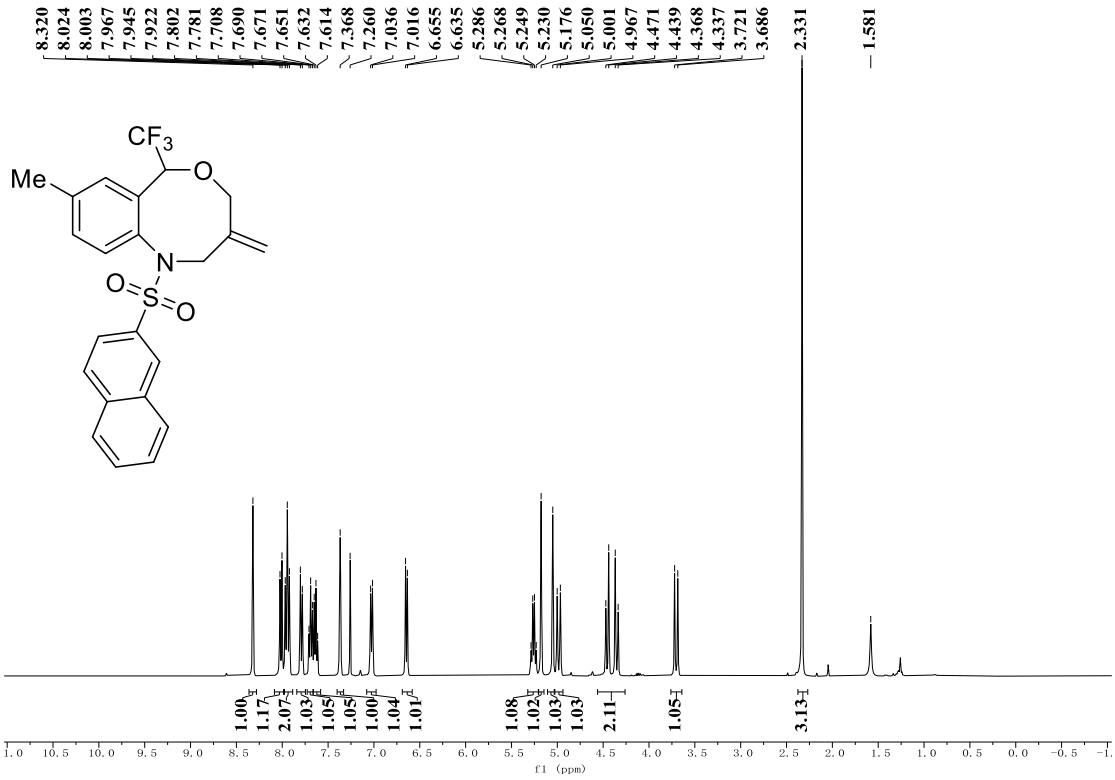
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of Compound **3t**



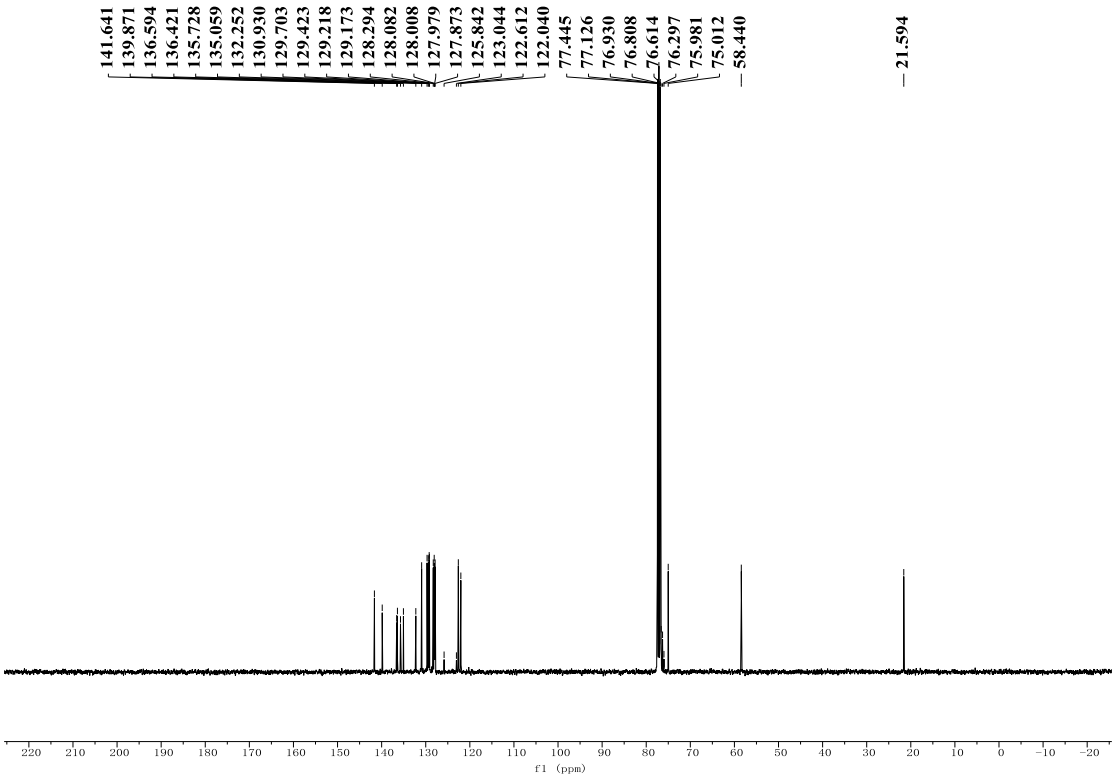
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of Compound **3u**



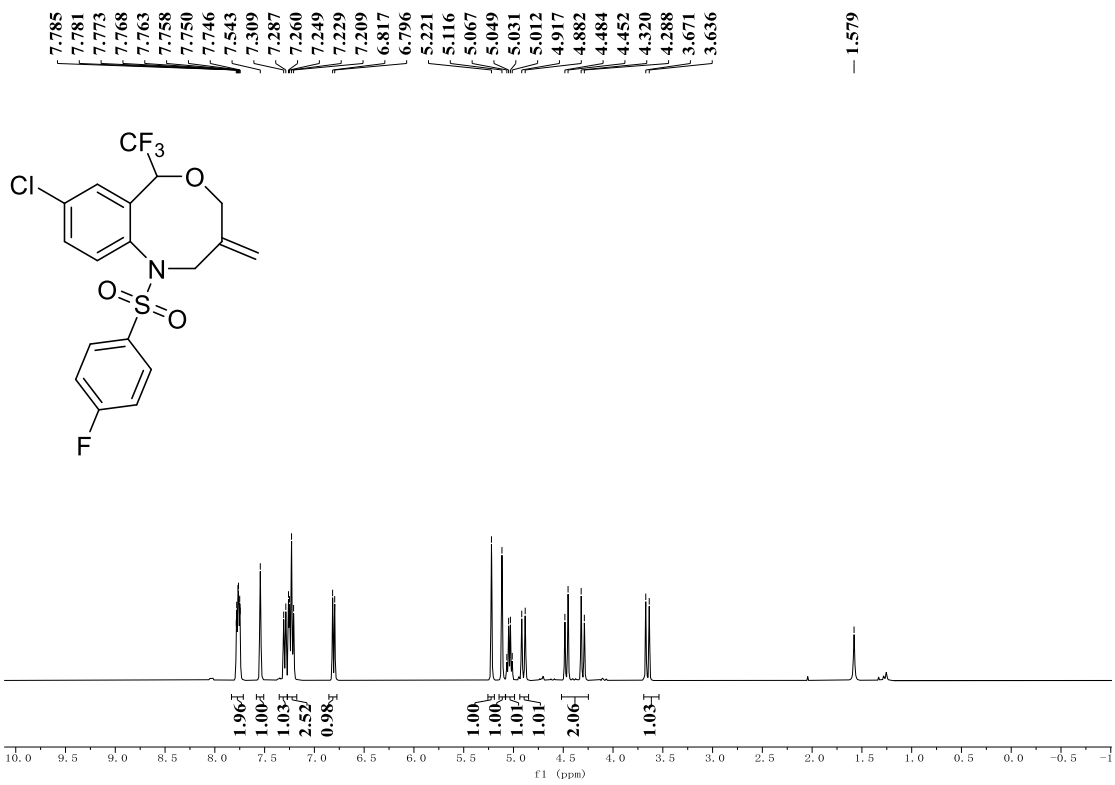
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of Compound **3u**



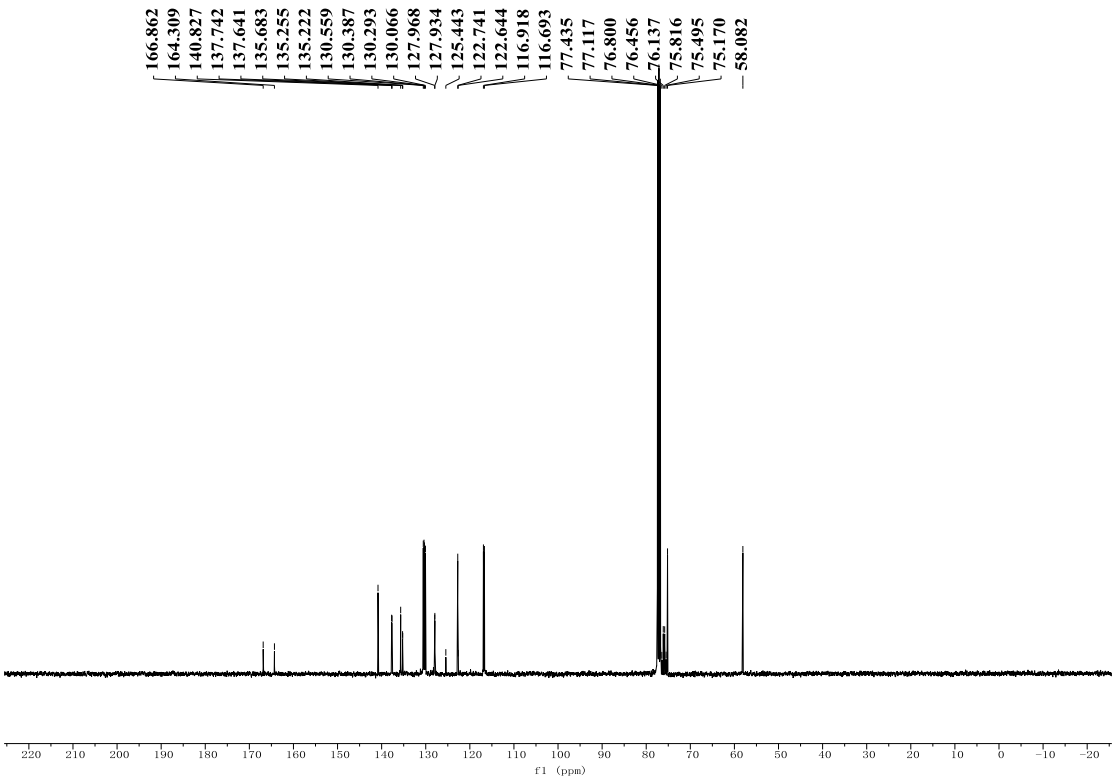
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of Compound **3v**



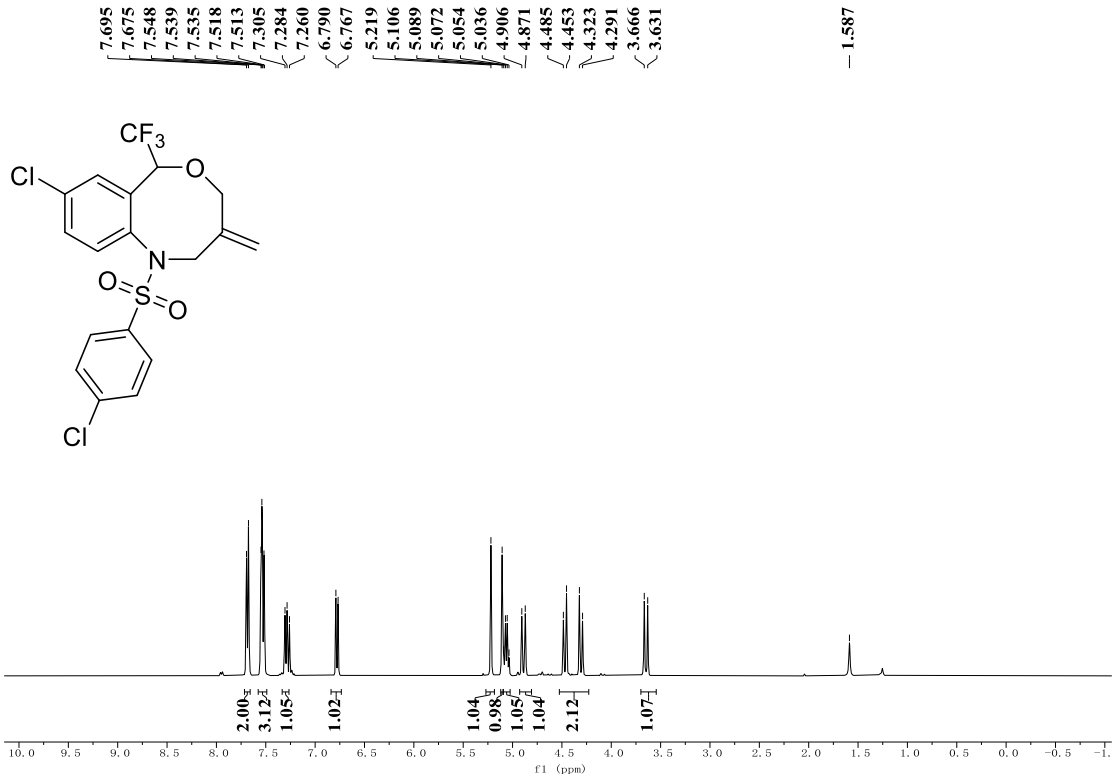
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of Compound **3v**



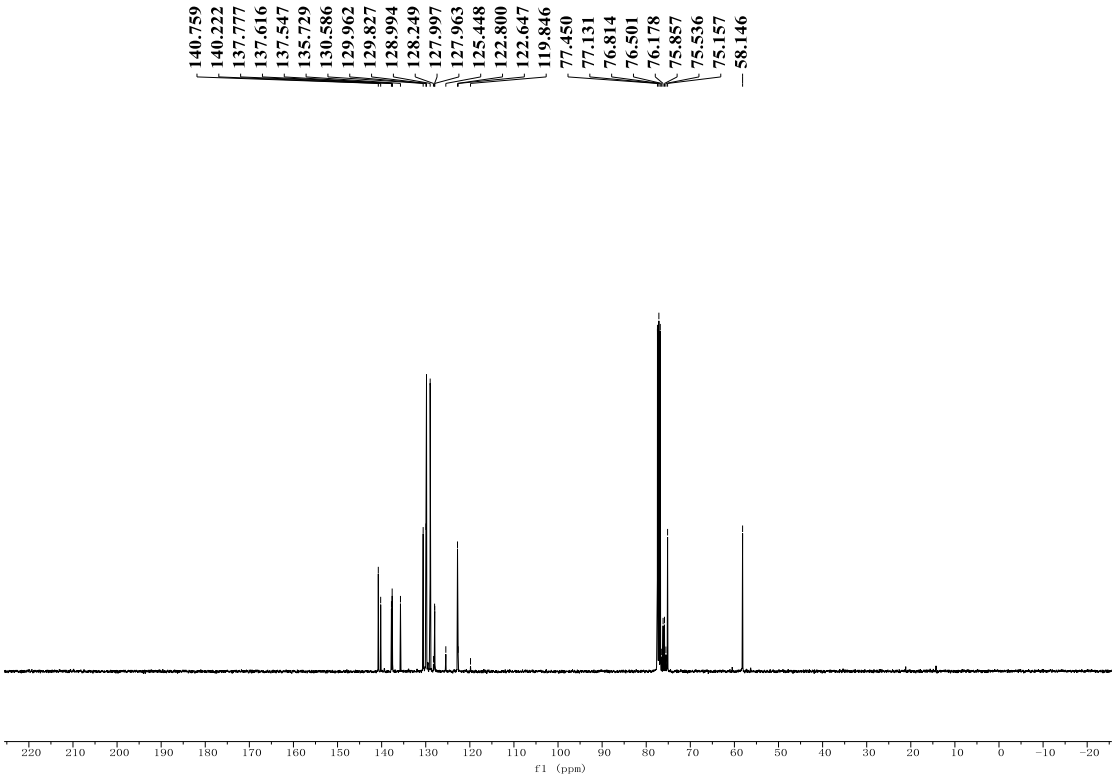
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of Compound **3w**



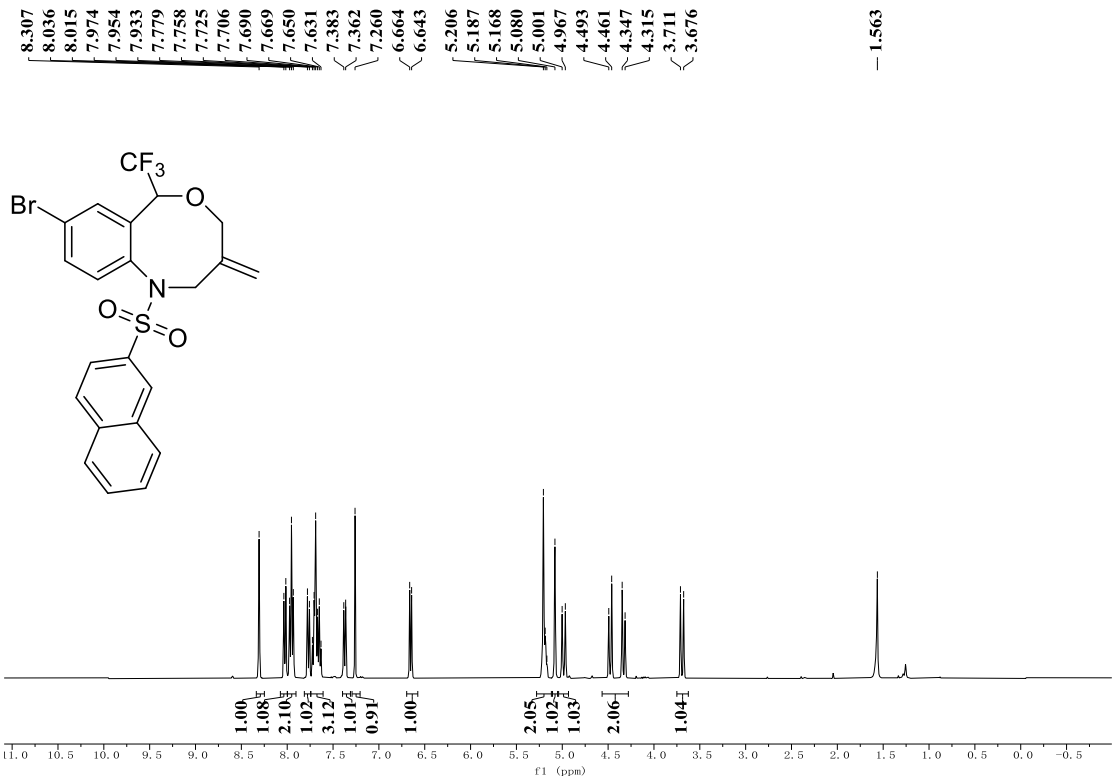
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of Compound **3w**



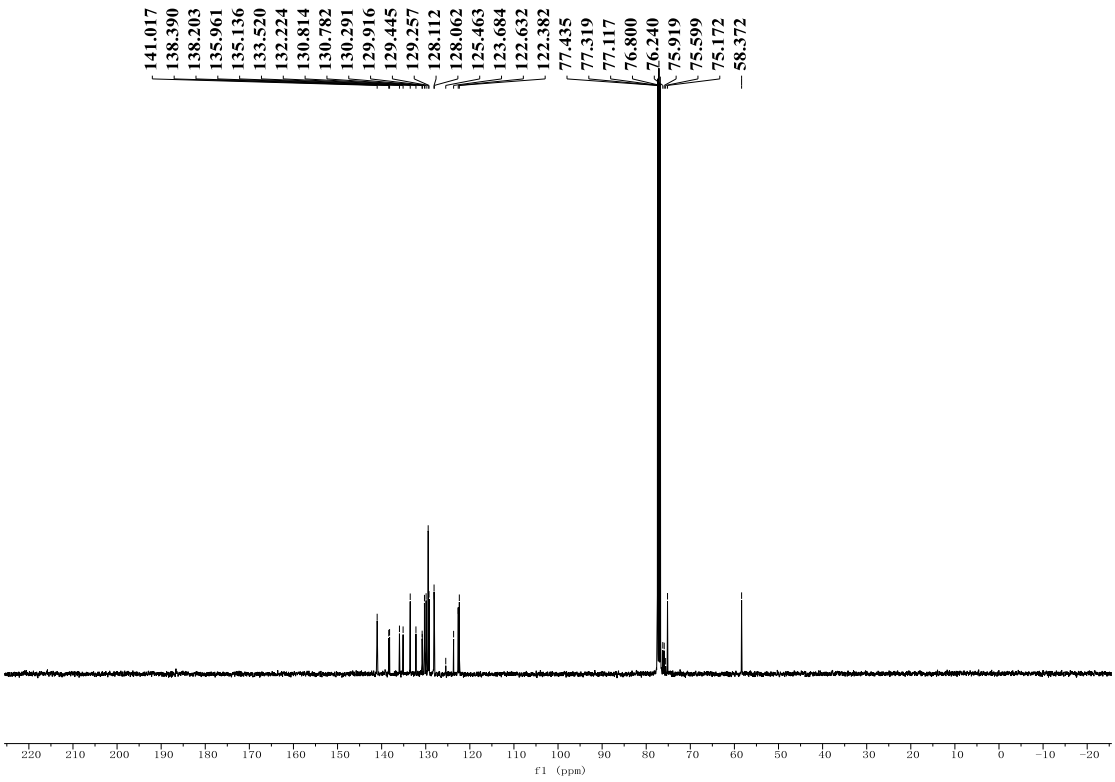
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of Compound **3x**



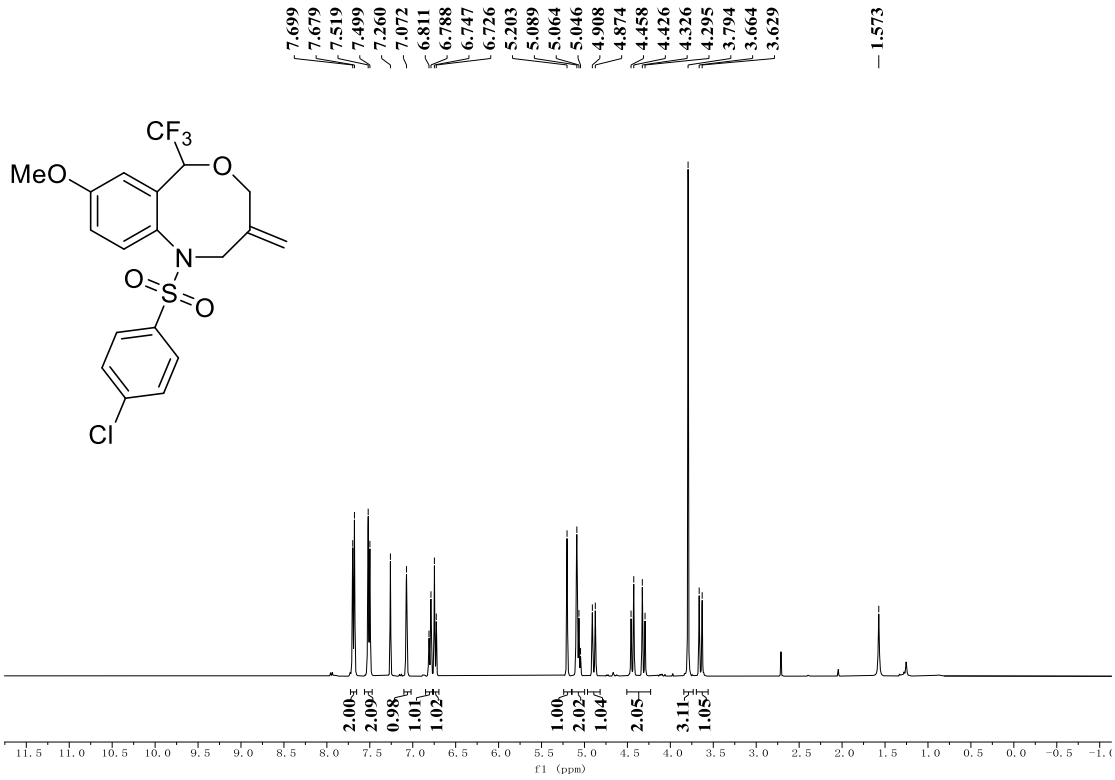
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of Compound **3x**



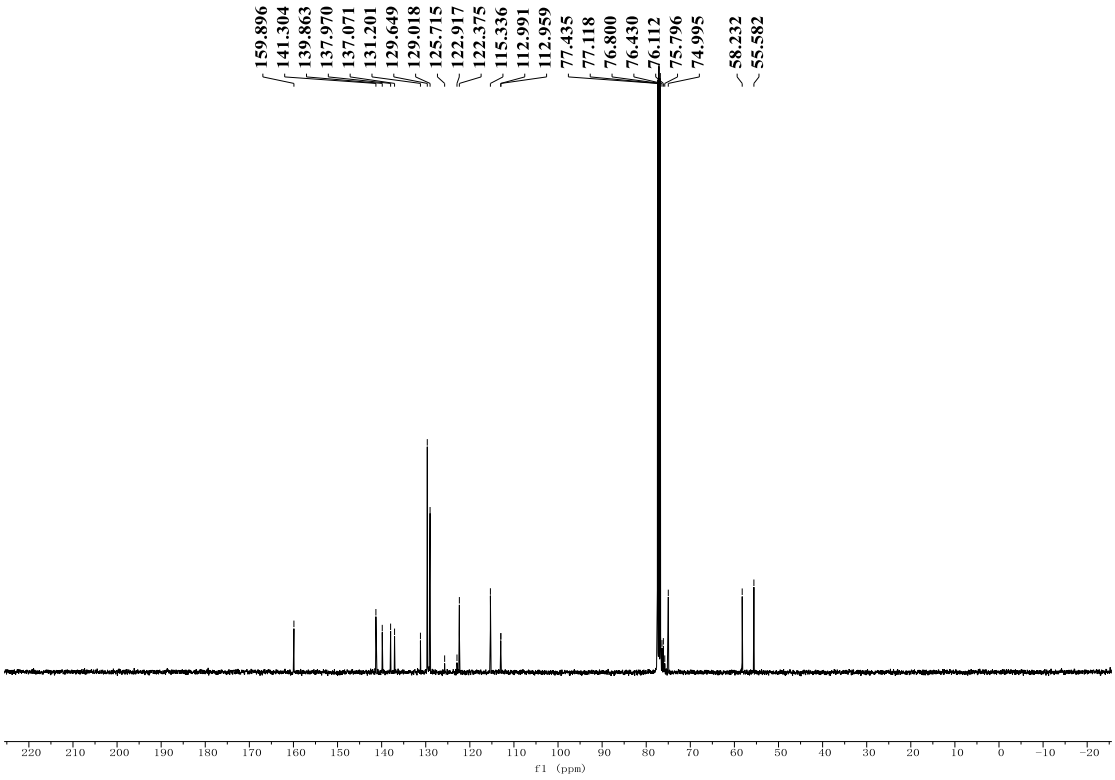
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of Compound **3y**



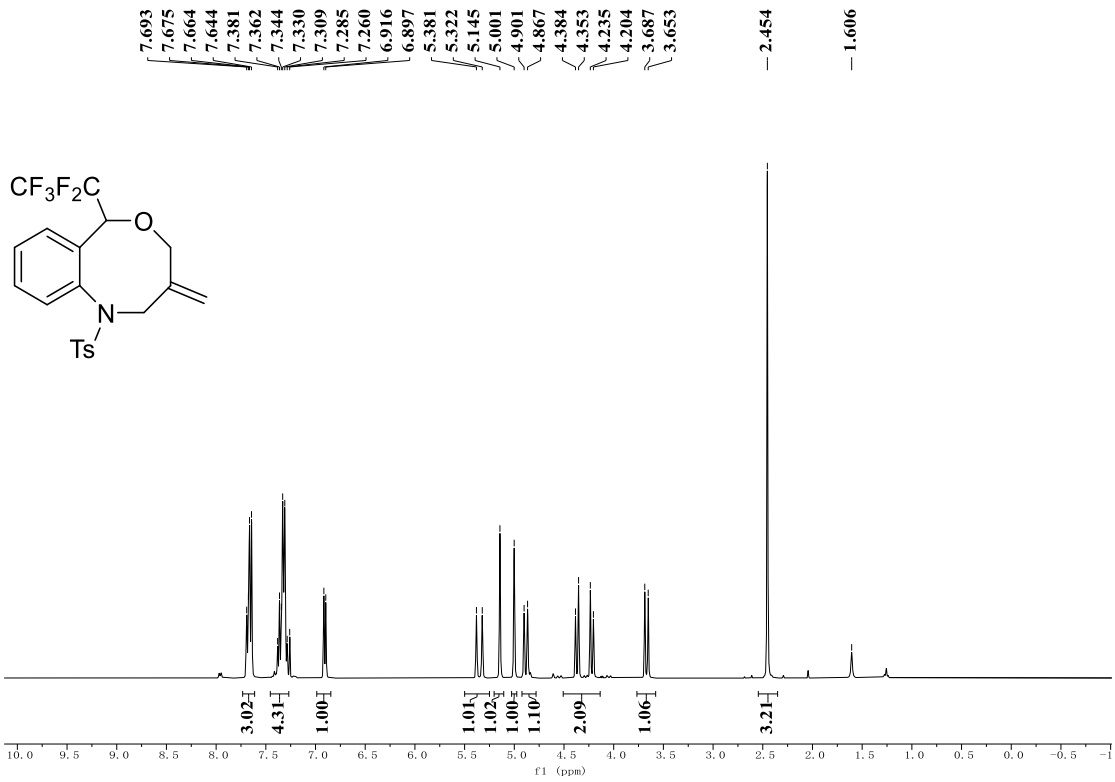
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of Compound **3y**



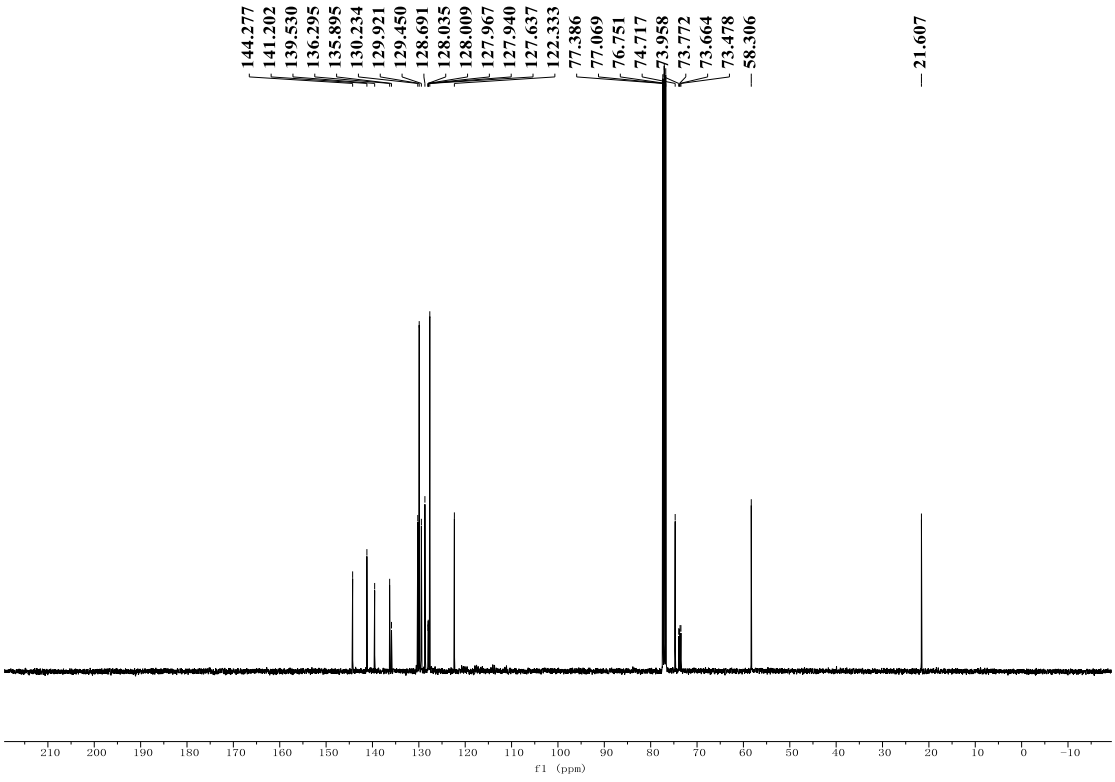
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of Compound **3z**



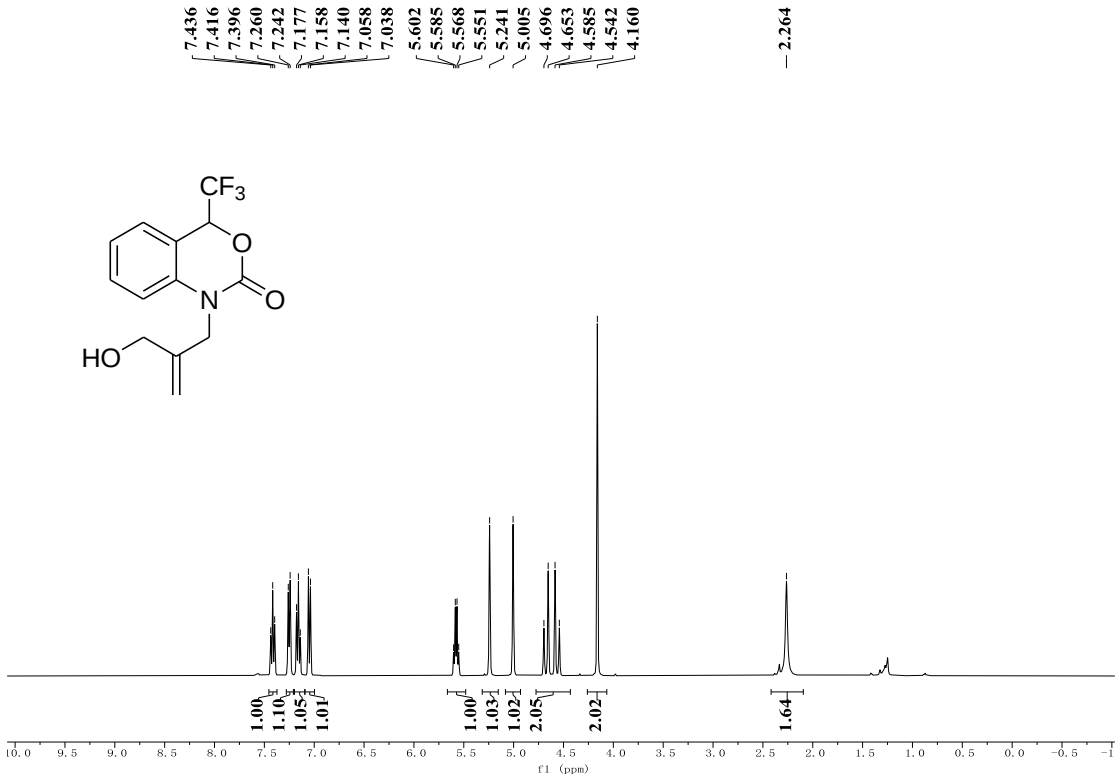
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of Compound **3z**



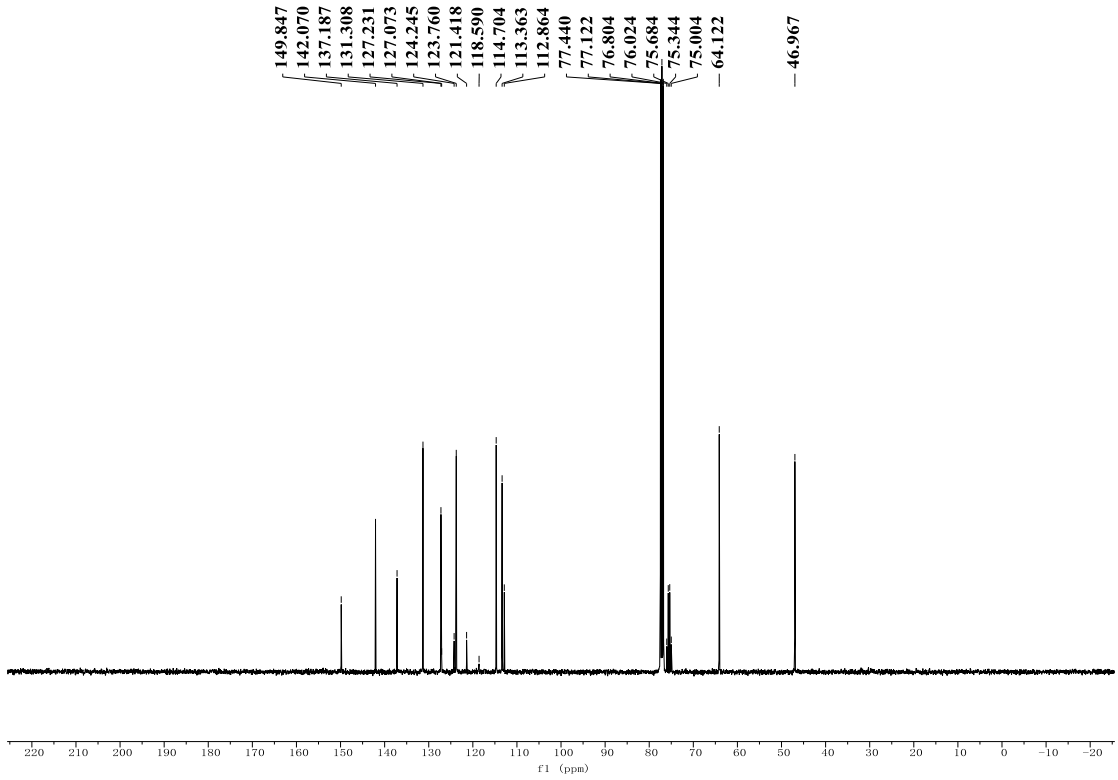
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of Compound **3aa**



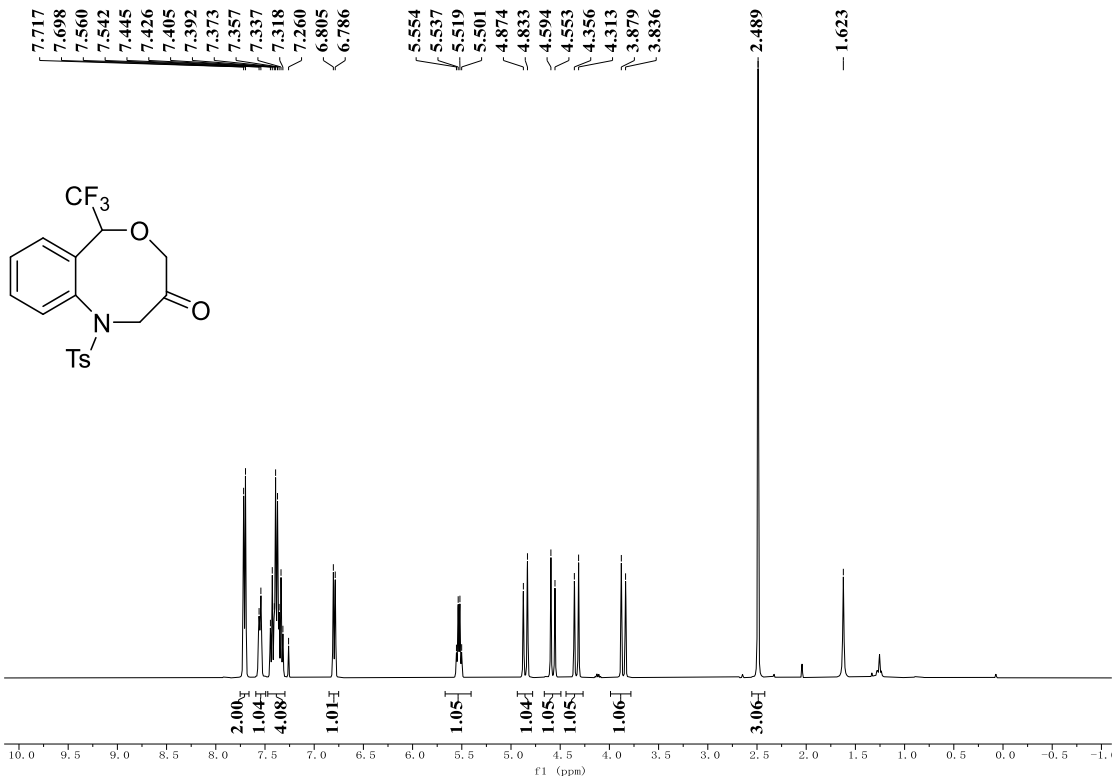
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of Compound **3aa**



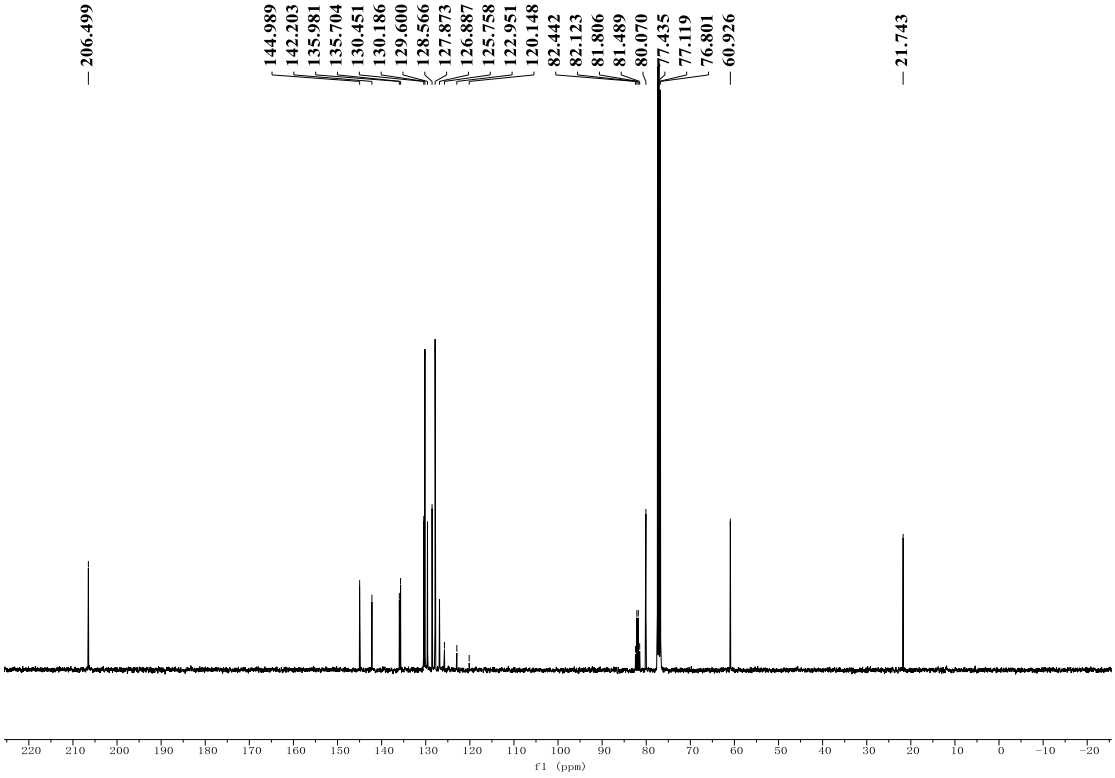
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of Compound **3ad**



^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of Compound **3ad**



^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of Compound **4**



^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of Compound **4**

Crystal Structure of Compound 3a. Single crystal of **3a** suitable for X-ray crystallography was obtained from ethyl acetate/petroleum ether by slow evaporation under room temperature under air. The crystal data was collected on an Agilent Gemini E diffractometer (Mo, 50kV 40Ma) and reducted by CrysAlisPro (Rigaku). The structures were solved by direct methods using SHELXS-97. Refinements were performed with SHELXL-2013 using fullmatrix least-squares calculations on F2, with anisotropic displacement parameters for all the nonhydrogen atoms. Crystallographic data have been deposited in the Cambridge Crystallographic Data Centre as deposition number CCDC 2382735.

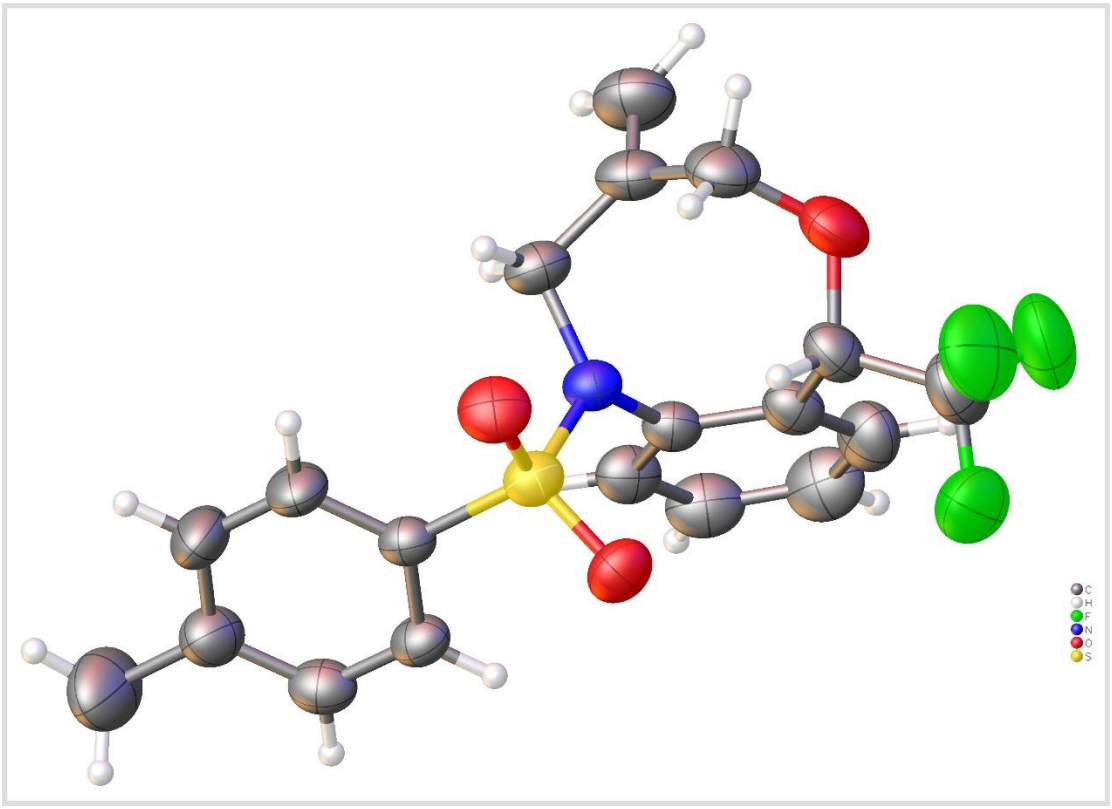


Figure S1. Crystal Structure of **3a** (50% probability level for the thermal ellipsoids).

Table S1 Crystal Data for Compound **3a**

Formula	$C_{19}H_{18}F_3NO_3S$
Formula weight	397.40
Temperature	293 (2) K
Wavelength	0.71073 Å
Crystal system	orthorhombic
Space group	Iba2
Unit cell dimensions	a = 28.744(4) Å, α = 90 °
	b = 11.9871(17) Å, β = 90 °
	c = 11.4197(14) Å, γ = 90 °
Volume	3934.7(9) $Å^3$
Z	8
Density (calculated)	1.342 g / cm^3
Absorption coefficient	0.210 mm^{-1}
F (000)	1648.0
Crystal	0.22 × 0.2 × 0.18
Theta range for data collection	5.444 to 58.596
Limiting indices	$-39 \le h \le 25$, $-15 \le k \le 15$, $-14 \le l \le 14$
Reflections collected	15038
Independent reflections	4618 [R_{int} = 0.0300, R_{sigma} = 0.0362]
Data / restraints / parameters	4618/1/253
Goodness-of-fit on F^2	1.035
Final R indices [$I > 2\sigma(I)$]	R_1 = 0.0409, wR_2 = 0.0868
R indices (all data)	R_1 = 0.0539, wR_2 = 0.0931
Largest diff. peak and hole	0.15/-0.19 e. $Å^{-3}$

Computational Studies

Computational Methods. All density functional theory (DFT) calculations were performed using the Gaussian 09 program.[3] Geometry optimization was conducted at the B3LYP/def2-SVP level of theory, which were dispersion corrected by D3BJ.[4-6] Vibrational frequency analysis was carried out to identify the nature of each stationary points as a minimum or a transition state, and to acquire the Gibbs free energy correction. The solvent effect of THF was evaluated by the IEFPCM solvation model. The single point calculations for the optimized geometries were performed to obtain accurate energies at the B3LYP/def2-TZVP level of theory, which were dispersion corrected by D3BJ. Orbital-weighted dual descriptor was analyzed with MULTIWFN;[7-9] and the result was visualized with VMD software.[10]

Cartesian Coordinates

1a

C	1.79501500	-2.23559600	1.18693700
C	1.02549500	-1.47182800	2.06793900
C	0.75108300	-0.13267200	1.79444700
C	1.23711700	0.45486200	0.61729000
C	2.06301400	-0.28990500	-0.23755300
C	2.32417000	-1.63459300	0.04582800
N	0.90549800	1.79524500	0.26439100
C	1.57751900	2.46904000	-0.76796000
O	2.19449700	1.67783900	-1.68489800
C	2.74200400	0.40237500	-1.38381100

O	1.57160700	3.65591400	-0.91729000
C	4.23856800	0.64303800	-1.10264300
F	4.82677400	1.25432100	-2.13439300
F	4.88316100	-0.51143200	-0.88452800
F	4.39269300	1.41949800	-0.01775800
C	-1.72280000	1.02272200	0.29729700
C	-2.50817800	0.42349400	1.28006700
C	-3.33462600	-0.64208300	0.91973600
C	-3.37796500	-1.11329000	-0.40072600
C	-2.57573300	-0.47848900	-1.36879400
C	-1.75253400	0.59063900	-1.03324000
C	-4.25206500	-2.27541100	-0.78675300
S	-0.69796400	2.41114700	0.72739700
O	-1.00225100	3.52357300	-0.16132100
O	-0.69112700	2.59352500	2.17651700
H	1.99888200	-3.28710100	1.39623700
H	0.63193200	-1.91771100	2.98362000
H	0.16884200	0.45972600	2.49565700
H	2.95867800	-2.20812900	-0.63169500
H	2.68468300	-0.19110000	-2.30803600
H	-2.46892200	0.78306900	2.30855900
H	-3.95402100	-1.11844100	1.68283300

H	-2.60062200	-0.82984000	-2.40299900
H	-1.13619300	1.07355300	-1.79349000
H	-4.87219500	-2.61333400	0.05482600
H	-4.91724100	-2.00666500	-1.62275800
H	-3.63929400	-3.12716200	-1.12523500

2

O	0.88042800	-0.99139700	1.18307200
C	0.36099400	0.35631200	1.17822900
C	-0.08727900	0.74622300	-0.19265500
C	-0.97061500	-0.30170500	-0.78756600
O	-0.37252300	-1.61010100	-0.65860700
C	0.50526700	-1.93264700	0.30363900
O	0.95855200	-3.04425700	0.36871600
C	0.25108800	1.88427900	-0.80320400
H	-0.48176100	0.39005600	1.89082000
H	1.16795600	0.99580500	1.55749500
H	-1.14395400	-0.14967000	-1.86035100
H	-1.94666200	-0.33048600	-0.27242900
H	-0.11879800	2.12316800	-1.80403300
H	0.89190900	2.62252100	-0.31352500

Pd2L

P	-2.28900000	0.96710000	1.63260000
C	-2.07190000	2.74420000	1.19930000
C	-3.81920000	0.50010000	0.72740000
C	-0.96160000	0.14130000	0.66450000
C	-1.30400000	3.19060000	0.11620000
C	-1.17450000	4.55900000	-0.14440000
C	-1.80530000	5.51650000	0.66200000
C	-2.57640000	5.06010000	1.74620000
C	-2.70350000	3.69970000	2.01520000
C	-1.13170000	-0.32550000	-0.64580000
C	-0.06680000	-0.91950000	-1.32960000
C	1.19320000	-1.06230000	-0.73070000
C	1.35530000	-0.59300000	0.58460000
C	0.29520000	-0.00880000	1.27540000
C	-4.49500000	-0.66250000	1.13470000
C	-5.64410000	-1.08600000	0.46920000
C	-6.16660000	-0.35550000	-0.61240000
C	-5.49280000	0.80990000	-1.00620000
C	-4.33460000	1.23480000	-0.34900000
C	-1.65410000	6.99220000	0.39700000
C	2.33610000	-1.72270000	-1.45760000

C	-7.42890000	-0.80230000	-1.30360000
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H	-0.56740000	4.88760000	-0.99230000
H	-3.07330000	5.78440000	2.39790000
H	-3.28290000	3.36420000	2.87920000
H	-2.09970000	-0.22450000	-1.14040000
H	-0.21890000	-1.27780000	-2.35140000
H	2.32700000	-0.69560000	1.07580000
H	0.43260000	0.33580000	2.30460000
H	-4.11290000	-1.23260000	1.98640000
H	-6.15300000	-1.99620000	0.79860000
H	-5.88000000	1.39660000	-1.84380000
H	-3.83000000	2.14490000	-0.67940000
H	-1.11390000	7.18170000	-0.54170000
H	-1.09770000	7.48500000	1.21210000
H	-2.63610000	7.48850000	0.33500000
H	3.27570000	-1.16590000	-1.31610000
H	2.13830000	-1.79980000	-2.53660000
H	2.50710000	-2.74400000	-1.07610000
H	-8.31500000	-0.58510000	-0.68270000
H	-7.42290000	-1.88850000	-1.48530000
H	-7.56500000	-0.29060000	-2.26740000

Pd	-2.28220000	0.71530000	3.91220000
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C	-2.45090000	2.97080000	6.44740000
C	-0.69600000	0.76640000	7.06880000
C	-3.55310000	0.42860000	7.22410000
C	-3.17270000	3.50680000	7.52160000
C	-3.29720000	4.89220000	7.67060000
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C	-1.98290000	5.23210000	5.68350000
C	-1.86070000	3.85380000	5.52580000
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C	-5.68060000	-0.64810000	8.75830000
C	-5.88100000	-0.24510000	7.42610000
C	-4.83470000	0.27590000	6.66760000
C	-0.03010000	-0.42700000	6.74180000
C	1.13250000	-0.79890000	7.41450000
C	1.67870000	0.01450000	8.42270000
C	1.01450000	1.20940000	8.73610000
C	-0.15710000	1.58340000	8.07180000
C	-2.85430000	7.27090000	6.90350000
C	-6.80980000	-1.24260000	9.55950000

C	2.95440000	-0.37970000	9.12100000
H	-3.64630000	2.84260000	8.24720000
H	-3.86770000	5.29140000	8.51370000
H	-1.51930000	5.89870000	4.95080000
H	-1.31780000	3.44630000	4.66910000
H	-2.35790000	0.13470000	9.00480000
H	-4.21470000	-0.80940000	10.33690000
H	-6.87210000	-0.35050000	6.97610000
H	-5.00300000	0.56840000	5.62690000
H	-0.43110000	-1.06210000	5.94660000
H	1.63330000	-1.73400000	7.14820000
H	1.42020000	1.86020000	9.51560000
H	-0.65350000	2.51840000	8.33920000
H	-3.34990000	7.53870000	7.84770000
H	-3.45230000	7.69110000	6.07730000
H	-1.87350000	7.77250000	6.87520000
H	-7.74020000	-0.66830000	9.42740000
H	-6.57160000	-1.27380000	10.63260000
H	-7.02110000	-2.27590000	9.23450000
H	3.82590000	-0.23330000	8.46010000
H	2.94280000	-1.44370000	9.40540000
H	3.12040000	0.21920000	10.02820000

A

O	0.48240000	5.83130000	2.82100000
C	-0.75550000	5.84850000	2.07300000
C	-1.93480000	5.64010000	2.97150000
C	-1.82400000	6.57460000	4.13780000
O	-0.54750000	6.44270000	4.79580000
C	0.56170000	6.08410000	4.13090000
O	1.61500000	6.00780000	4.71170000
C	-3.21220000	5.26460000	2.49130000
H	-0.79980000	6.83290000	1.56860000
H	-0.65370000	5.06840000	1.30860000
H	-2.58270000	6.38350000	4.90760000
H	-1.91160000	7.63020000	3.81510000
H	-4.11000000	5.64970000	2.98520000
H	-3.34820000	5.02760000	1.43000000
P	-0.58220000	2.34380000	4.32850000
C	-0.67040000	0.50100000	4.28970000
C	-0.09990000	2.63240000	6.07730000
C	0.93580000	2.66500000	3.34880000
C	0.18820000	-0.29960000	3.52790000
C	0.03190000	-1.69020000	3.50620000
C	-0.97460000	-2.32030000	4.24730000

C	-1.82520000	-1.51080000	5.01920000
C	-1.68080000	-0.12870000	5.03670000
C	2.20050000	2.87770000	3.90670000
C	3.30400000	3.11840000	3.08340000
C	3.18030000	3.14630000	1.68770000
C	1.90680000	2.92520000	1.13440000
C	0.80160000	2.69850000	1.95030000
C	-0.52980000	3.80350000	6.71410000
C	-0.19460000	4.05300000	8.04760000
C	0.57470000	3.14130000	8.78330000
C	1.00200000	1.96660000	8.13850000
C	0.67020000	1.71190000	6.80950000
C	-1.15140000	-3.81560000	4.23430000
C	4.36410000	3.44030000	0.80300000
C	0.93330000	3.39700000	10.22410000
H	0.98370000	0.15770000	2.93850000
H	0.70780000	-2.29480000	2.89520000
H	-2.62890000	-1.97270000	5.59810000
H	-2.37100000	0.46960000	5.63260000
H	2.32920000	2.87070000	4.98970000
H	4.28260000	3.29280000	3.53880000
H	1.78160000	2.94170000	0.04810000

H	-0.18480000	2.54920000	1.50200000
H	-1.12360000	4.52930000	6.15830000
H	-0.53790000	4.97540000	8.52320000
H	1.60310000	1.23930000	8.69170000
H	1.00640000	0.78730000	6.33600000
H	-0.53290000	-4.29080000	3.45930000
H	-2.20280000	-4.08620000	4.05000000
H	-0.87150000	-4.25660000	5.20610000
H	4.34350000	2.83060000	-0.11370000
H	5.31440000	3.25220000	1.32390000
H	4.36410000	4.49820000	0.48800000
H	0.56870000	4.37700000	10.56360000
H	2.02520000	3.36780000	10.37190000
H	0.50070000	2.62560000	10.88290000
Pd	-2.42330000	3.56770000	3.48710000
P	-4.28320000	2.13220000	3.56990000
C	-4.06610000	0.41540000	2.95500000
C	-5.76560000	2.70280000	2.64190000
C	-4.94540000	1.96760000	5.27860000
C	-4.85260000	-0.67190000	3.35580000
C	-4.61350000	-1.94660000	2.83770000
C	-3.59150000	-2.17160000	1.90390000

C	-2.80730000	-1.07690000	1.50780000
C	-3.03710000	0.19460000	2.02660000
C	-6.26020000	1.55350000	5.55520000
C	-6.70300000	1.43100000	6.87110000
C	-5.85700000	1.72460000	7.95570000
C	-4.55430000	2.15870000	7.67410000
C	-4.10590000	2.28450000	6.35670000
C	-6.42270000	3.87150000	3.06930000
C	-7.50000000	4.38520000	2.35280000
C	-7.95430000	3.76310000	1.17520000
C	-7.29110000	2.60480000	0.75100000
C	-6.21370000	2.07720000	1.47200000
C	-3.33310000	-3.54100000	1.33260000
C	-6.35110000	1.58410000	9.37200000
C	-9.11430000	4.33720000	0.40310000
H	-5.64830000	-0.53530000	4.08940000
H	-5.22970000	-2.78590000	3.17140000
H	-1.98940000	-1.22920000	0.79900000
H	-2.39770000	1.03020000	1.73300000
H	-6.94840000	1.33990000	4.73470000
H	-7.72880000	1.10460000	7.06420000
H	-3.87810000	2.41090000	8.49520000

H	-3.09430000	2.64530000	6.16190000
H	-6.09030000	4.37760000	3.97920000
H	-8.00050000	5.29000000	2.70970000
H	-7.62460000	2.09800000	-0.15880000
H	-5.72430000	1.16810000	1.11810000
H	-3.87330000	-4.32140000	1.88770000
H	-2.25920000	-3.78260000	1.35370000
H	-3.65490000	-3.59510000	0.27860000
H	-5.57920000	1.87230000	10.09960000
H	-6.64970000	0.54430000	9.58500000
H	-7.23890000	2.21370000	9.54700000
H	-8.87770000	5.34490000	0.02250000
H	-10.00720000	4.43880000	1.04160000
H	-9.37970000	3.70510000	-0.45640000

TS1

O	-0.29650000	5.64550000	1.71980000
C	-1.59680000	6.23850000	1.73870000
C	-2.37570000	5.96000000	2.99920000
C	-1.83230000	6.55260000	4.13580000
O	0.20360000	6.00580000	3.94060000
C	0.63560000	5.82200000	2.75350000
O	1.80450000	5.74350000	2.40850000
C	-3.57910000	5.17160000	3.00700000
H	-1.49280000	7.33170000	1.59660000
H	-2.11370000	5.82950000	0.85920000
H	-2.16120000	6.24830000	5.13420000
H	-1.31920000	7.51130000	4.07950000
H	-4.29500000	5.35350000	3.81650000
H	-4.06890000	5.01230000	2.03980000
P	-0.55540000	2.22950000	4.35690000
C	-0.67510000	0.39370000	4.35690000
C	-0.18280000	2.66010000	6.10390000
C	0.99830000	2.51870000	3.44410000
C	0.25130000	-0.41600000	3.68710000
C	0.07860000	-1.80290000	3.63590000
C	-1.01140000	-2.42410000	4.25750000

C	-1.92830000	-1.60820000	4.94040000
C	-1.76980000	-0.22750000	4.98270000
C	2.25250000	2.57760000	4.06470000
C	3.40520000	2.75010000	3.29820000
C	3.33920000	2.85730000	1.90110000
C	2.07990000	2.77750000	1.28900000
C	0.92340000	2.62440000	2.04800000
C	0.07500000	4.01340000	6.39880000
C	0.27930000	4.41590000	7.71660000
C	0.21950000	3.49980000	8.78270000
C	-0.03190000	2.15640000	8.47630000
C	-0.22460000	1.73630000	7.15550000
C	-1.21170000	-3.91540000	4.20460000
C	4.57640000	3.11830000	1.08430000
C	0.42470000	3.96000000	10.20270000
H	1.10940000	0.03380000	3.18690000
H	0.80780000	-2.41210000	3.09500000
H	-2.79640000	-2.06100000	5.42560000
H	-2.51620000	0.37240000	5.50150000
H	2.32850000	2.49240000	5.15050000
H	4.37730000	2.80900000	3.79560000
H	2.00260000	2.87120000	0.20260000

H	-0.05180000	2.60140000	1.55600000
H	0.13410000	4.74580000	5.58790000
H	0.48740000	5.46930000	7.92570000
H	-0.07360000	1.41880000	9.28240000
H	-0.41010000	0.68080000	6.95510000
H	-0.49680000	-4.39710000	3.52220000
H	-2.23070000	-4.16340000	3.86760000
H	-1.08460000	-4.36800000	5.20240000
H	4.51440000	2.64880000	0.09070000
H	5.48310000	2.75250000	1.58890000
H	4.70080000	4.20370000	0.92580000
H	1.40770000	4.44400000	10.32470000
H	0.36690000	3.12220000	10.91240000
H	-0.33510000	4.70490000	10.49210000
Pd	-2.41080000	3.54810000	3.55910000
P	-4.25040000	2.16810000	3.61080000
C	-3.96830000	0.52090000	2.85890000
C	-5.75870000	2.76640000	2.76230000
C	-4.81400000	1.89260000	5.33500000
C	-4.76280000	-0.59900000	3.13670000
C	-4.46790000	-1.83320000	2.55560000
C	-3.38160000	-1.98400000	1.68080000

C	-2.60290000	-0.85230000	1.39350000
C	-2.88870000	0.38020000	1.97400000
C	-6.07040000	1.34150000	5.64310000
C	-6.43820000	1.11720000	6.96830000
C	-5.57460000	1.44090000	8.03030000
C	-4.33230000	2.01030000	7.71770000
C	-3.95950000	2.24110000	6.39180000
C	-6.58810000	3.72050000	3.37740000
C	-7.67080000	4.26600000	2.69020000
C	-7.96010000	3.88790000	1.36780000
C	-7.12290000	2.94170000	0.75890000
C	-6.03780000	2.38690000	1.44160000
C	-3.04330000	-3.31540000	1.06510000
C	-5.99260000	1.20360000	9.45750000
C	-9.14430000	4.47210000	0.64240000
H	-5.60420000	-0.52450000	3.82610000
H	-5.08770000	-2.70080000	2.79630000
H	-1.74400000	-0.94420000	0.72420000
H	-2.25330000	1.24360000	1.76590000
H	-6.77500000	1.10150000	4.84460000
H	-7.41810000	0.68400000	7.18640000
H	-3.64140000	2.28090000	8.52020000

H	-2.99110000	2.69650000	6.17630000
H	-6.39120000	4.03460000	4.40460000
H	-8.30540000	5.00330000	3.18950000
H	-7.32390000	2.62940000	-0.26930000
H	-5.40580000	1.65120000	0.94010000
H	-3.67160000	-4.12180000	1.46940000
H	-1.98870000	-3.57490000	1.24930000
H	-3.18210000	-3.29180000	-0.02860000
H	-5.15250000	1.34240000	10.15270000
H	-6.39020000	0.18530000	9.59190000
H	-6.79360000	1.90240000	9.75260000
H	-9.18430000	5.56660000	0.75900000
H	-10.09010000	4.07150000	1.04560000
H	-9.11450000	4.24020000	-0.43190000

B

O	-0.06060000	1.42630000	-3.42690000
C	-0.21800000	2.79610000	-3.13200000
C	-0.01540000	3.08370000	-1.64740000
C	1.25410000	2.91970000	-1.03210000
O	2.10290000	1.84960000	-4.00610000
C	1.24850000	0.97520000	-3.80820000
O	1.31760000	-0.26330000	-3.85010000
C	-1.13640000	3.16870000	-0.80330000
H	0.50180000	3.38940000	-3.71490000
H	-1.24470000	3.07720000	-3.41040000
H	1.46440000	3.42560000	-0.08450000
H	2.11140000	2.66510000	-1.65720000
H	-1.04890000	3.59470000	0.20210000
H	-2.14080000	3.13100000	-1.22770000
P	1.72060000	-0.06290000	0.44920000
C	1.58990000	-1.88260000	0.30230000
C	1.86730000	0.23370000	2.25230000
C	3.37280000	0.35000000	-0.21600000
C	2.43920000	-2.63970000	-0.51290000
C	2.24330000	-4.01720000	-0.65040000
C	1.20850000	-4.67570000	0.02420000

C	0.37270000	-3.90990000	0.85440000
C	0.55220000	-2.53880000	0.98670000
C	4.42130000	0.78020000	0.60790000
C	5.65320000	1.13320000	0.04900000
C	5.86980000	1.06740000	-1.33470000
C	4.80950000	0.63170000	-2.14790000
C	3.57700000	0.27970000	-1.60470000
C	1.53860000	1.50050000	2.76280000
C	1.61180000	1.75620000	4.13080000
C	2.00870000	0.75600000	5.03430000
C	2.35370000	-0.50100000	4.51440000
C	2.28900000	-0.76190000	3.14440000
C	0.98030000	-6.15590000	-0.12450000
C	7.19070000	1.46060000	-1.94350000
C	2.03230000	1.01990000	6.51670000
H	3.25480000	-2.16170000	-1.05450000
H	2.90970000	-4.58740000	-1.30270000
H	-0.44830000	-4.39480000	1.38770000
H	-0.12560000	-1.97530000	1.62820000
H	4.28300000	0.84610000	1.68800000
H	6.46070000	1.46980000	0.70470000
H	4.93510000	0.58650000	-3.23230000

H	2.78030000	-0.05200000	-2.27550000
H	1.20390000	2.28780000	2.08390000
H	1.34620000	2.74760000	4.50670000
H	2.67790000	-1.29280000	5.19470000
H	2.56020000	-1.75040000	2.77120000
H	1.63800000	-6.59340000	-0.88900000
H	-0.06370000	-6.36360000	-0.40810000
H	1.16590000	-6.68320000	0.82620000
H	7.61460000	0.63500000	-2.53810000
H	7.92470000	1.74070000	-1.17430000
H	7.07000000	2.31670000	-2.62780000
H	2.35100000	2.04990000	6.73680000
H	2.70580000	0.32570000	7.04000000
H	1.02500000	0.89230000	6.94970000
Pd	-0.03910000	1.29430000	-0.34480000
P	-1.95990000	-0.03170000	-0.04590000
C	-1.77130000	-1.62930000	-0.91520000
C	-3.41950000	0.73440000	-0.85030000
C	-2.52750000	-0.38180000	1.65540000
C	-2.51690000	-2.77390000	-0.60430000
C	-2.29950000	-3.96270000	-1.30310000
C	-1.34360000	-4.03960000	-2.32770000

C	-0.61820000	-2.88030000	-2.64190000
C	-0.82110000	-1.69140000	-1.94740000
C	-3.80680000	-0.89840000	1.93220000
C	-4.18500000	-1.17780000	3.24330000
C	-3.31020000	-0.94740000	4.32120000
C	-2.04650000	-0.41130000	4.03970000
C	-1.66160000	-0.12720000	2.72710000
C	-4.22960000	1.64140000	-0.14930000
C	-5.25370000	2.32600000	-0.80410000
C	-5.49690000	2.13520000	-2.17430000
C	-4.67530000	1.23240000	-2.86710000
C	-3.65230000	0.53810000	-2.21900000
C	-1.08430000	-5.32360000	-3.06980000
C	-3.73130000	-1.26950000	5.73060000
C	-6.62080000	2.85650000	-2.87110000
H	-3.25170000	-2.75780000	0.20130000
H	-2.87600000	-4.85300000	-1.03780000
H	0.13380000	-2.89180000	-3.43420000
H	-0.21910000	-0.82460000	-2.22870000
H	-4.51830000	-1.06610000	1.12160000
H	-5.18300000	-1.57930000	3.43860000
H	-1.34900000	-0.20460000	4.85540000

H	-0.67890000	0.30270000	2.54160000
H	-4.05650000	1.82280000	0.91360000
H	-5.87490000	3.02730000	-0.24040000
H	-4.83730000	1.06890000	-3.93580000
H	-3.02420000	-0.15010000	-2.78730000
H	-1.70230000	-6.14850000	-2.68710000
H	-0.02600000	-5.61770000	-2.98170000
H	-1.29500000	-5.20830000	-4.14570000
H	-2.99470000	-0.91210000	6.46400000
H	-3.84420000	-2.35820000	5.86630000
H	-4.70590000	-0.81450000	5.96850000
H	-6.81600000	3.83740000	-2.41240000
H	-7.55700000	2.27480000	-2.80930000
H	-6.40130000	3.00820000	-3.93840000

TS2

O	0.01740000	3.53090000	-3.08970000
C	-0.94090000	4.11840000	-2.30480000
C	-0.84370000	3.79600000	-0.81670000
C	0.40970000	3.59320000	-0.19130000
O	0.49890000	6.00200000	-4.11560000
C	1.28580000	5.13380000	-4.11420000
O	2.26470000	4.50470000	-4.24720000
C	-1.98480000	3.41810000	-0.08060000
H	-0.88040000	5.22960000	-2.35920000
H	-1.97100000	3.86610000	-2.62990000
H	0.50190000	3.75200000	0.88740000
H	1.31840000	3.71610000	-0.77990000
H	-2.00930000	3.52300000	1.00980000
H	-2.95150000	3.36910000	-0.58350000
P	1.28170000	0.33030000	0.00110000
C	1.17660000	-1.41360000	-0.54920000
C	1.79980000	0.19110000	1.76210000
C	2.78850000	0.92550000	-0.86030000
C	1.79370000	-1.84230000	-1.73050000
C	1.64050000	-3.15900000	-2.16990000
C	0.87930000	-4.08350000	-1.44380000

C	0.26260000	-3.64490000	-0.26050000
C	0.39710000	-2.33150000	0.17550000
C	4.05630000	0.44940000	-0.48240000
C	5.19450000	0.83360000	-1.18730000
C	5.10450000	1.70340000	-2.28840000
C	3.83670000	2.17660000	-2.65270000
C	2.68590000	1.79910000	-1.95100000
C	1.58280000	1.28380000	2.61820000
C	1.93750000	1.21810000	3.96410000
C	2.51690000	0.05850000	4.50610000
C	2.74380000	-1.02440000	3.64440000
C	2.39340000	-0.96320000	2.29360000
C	0.71960000	-5.50700000	-1.90620000
C	6.34210000	2.13060000	-3.03370000
C	2.85490000	-0.02160000	5.97160000
H	2.38280000	-1.14430000	-2.32500000
H	2.11150000	-3.46590000	-3.10700000
H	-0.35680000	-4.33820000	0.31340000
H	-0.11560000	-2.01880000	1.08620000
H	4.15710000	-0.23020000	0.36570000
H	6.17180000	0.45190000	-0.87900000
H	3.73170000	2.86850000	-3.48950000

H	1.71720000	2.19270000	-2.26860000
H	1.11310000	2.18770000	2.22900000
H	1.75280000	2.08080000	4.60970000
H	3.20090000	-1.93670000	4.03650000
H	2.57510000	-1.82940000	1.65640000
H	0.98800000	-5.61990000	-2.96650000
H	-0.31690000	-5.85150000	-1.77280000
H	1.36550000	-6.18650000	-1.32390000
H	6.92920000	2.85160000	-2.43940000
H	6.09010000	2.61360000	-3.98880000
H	7.00210000	1.27330000	-3.24030000
H	3.30960000	0.91490000	6.32970000
H	3.54860000	-0.84840000	6.18180000
H	1.94510000	-0.18900000	6.57330000
Pd	-0.64020000	1.66700000	-0.18160000
P	-2.41750000	0.10550000	-0.00060000
C	-2.36010000	-1.40740000	-1.04280000
C	-4.01850000	0.86090000	-0.48020000
C	-2.68870000	-0.47860000	1.71730000
C	-3.10950000	-2.55300000	-0.73890000
C	-3.09370000	-3.65530000	-1.59460000
C	-2.34120000	-3.64410000	-2.77880000

C	-1.58260000	-2.50020000	-3.06430000
C	-1.58370000	-1.39980000	-2.21010000
C	-3.90430000	-1.03500000	2.15660000
C	-4.03980000	-1.49840000	3.46360000
C	-2.97610000	-1.42130000	4.38110000
C	-1.77410000	-0.84920000	3.94430000
C	-1.63500000	-0.37980000	2.63580000
C	-4.78860000	1.58720000	0.44020000
C	-5.91620000	2.29410000	0.01530000
C	-6.29460000	2.31350000	-1.33580000
C	-5.51050000	1.58950000	-2.24830000
C	-4.39520000	0.86620000	-1.83180000
C	-2.35710000	-4.81340000	-3.72810000
C	-3.14100000	-1.92970000	5.78920000
C	-7.50080000	3.08560000	-1.80440000
H	-3.70420000	-2.60180000	0.17320000
H	-3.68040000	-4.54140000	-1.33720000
H	-0.96860000	-2.46880000	-3.96620000
H	-0.98450000	-0.52690000	-2.45260000
H	-4.75740000	-1.09210000	1.47850000
H	-4.99360000	-1.92730000	3.78300000
H	-0.93060000	-0.76000000	4.63390000

H	-0.69360000	0.07510000	2.33330000
H	-4.50280000	1.61960000	1.49360000
H	-6.50520000	2.85340000	0.74740000
H	-5.75200000	1.60900000	-3.31360000
H	-3.79310000	0.35350000	-2.57870000
H	-2.64850000	-5.74520000	-3.22110000
H	-1.37160000	-4.96420000	-4.19370000
H	-3.07910000	-4.64260000	-4.54550000
H	-3.95400000	-1.39720000	6.30960000
H	-2.21970000	-1.80220000	6.37510000
H	-3.40510000	-2.99990000	5.79450000
H	-7.91030000	3.72230000	-1.00670000
H	-8.30280000	2.40500000	-2.13740000
H	-7.24920000	3.72790000	-2.66370000
C	1.64390000	3.80720000	-7.60160000
C	0.42400000	4.48660000	-7.51950000
C	-0.57580000	4.04590000	-6.65180000
C	-0.36650000	2.89030000	-5.89340000
C	0.86980000	2.23270000	-5.93520000
C	1.87140000	2.69460000	-6.78950000
N	-1.32070000	2.34190000	-5.01240000
C	-0.87580000	1.82670000	-3.75170000

O	0.28950000	1.08980000	-3.83460000
C	1.09010000	1.07050000	-5.00020000
O	-1.68060000	1.55590000	-2.88530000
C	0.87100000	-0.29320000	-5.66760000
F	1.22200000	-1.29370000	-4.84140000
F	1.60910000	-0.41100000	-6.78150000
F	-0.41660000	-0.49380000	-6.00240000
C	-3.04780000	2.33860000	-7.11610000
C	-3.69620000	3.40190000	-7.74020000
C	-3.75500000	3.42930000	-9.13470000
C	-3.17210000	2.41210000	-9.90480000
C	-2.53600000	1.34640000	-9.23990000
C	-2.47660000	1.29520000	-7.85120000
C	-3.22450000	2.44350000	-11.40870000
S	-3.01250000	2.27100000	-5.33660000
O	-3.66990000	3.47170000	-4.80690000
O	-3.49240000	0.94470000	-4.93660000
H	2.42750000	4.16230000	-8.27380000
H	0.25440000	5.38340000	-8.11920000
H	-1.50520000	4.60140000	-6.54630000
H	2.83850000	2.18760000	-6.80820000
H	2.13910000	1.06770000	-4.66470000

H	-4.13730000	4.19750000	-7.13880000
H	-4.25920000	4.26070000	-9.63270000
H	-2.08060000	0.54320000	-9.82450000
H	-1.98230000	0.46830000	-7.34340000
H	-2.21170000	2.38370000	-11.83860000
H	-3.78960000	1.58090000	-11.79860000
H	-3.70290000	3.36100000	-11.77860000

C

O	0.22600000	3.82100000	-2.93750000
C	-0.87810000	4.27060000	-2.20180000
C	-0.81830000	3.83410000	-0.75740000
C	0.41280000	3.60470000	-0.10080000
O	0.70730000	5.98600000	-3.50310000
C	1.07590000	4.81010000	-3.58990000
O	2.04830000	4.27800000	-4.13390000
C	-1.98660000	3.40540000	-0.09330000
H	-0.88910000	5.37480000	-2.21730000
H	-1.81570000	3.91630000	-2.65860000
H	0.45840000	3.70600000	0.98710000
H	1.34570000	3.75920000	-0.64270000
H	-2.05990000	3.46660000	0.99740000
H	-2.93150000	3.37920000	-0.63790000
P	1.29000000	0.31710000	0.01490000
C	1.17240000	-1.42760000	-0.53240000
C	1.81300000	0.17640000	1.77330000
C	2.78670000	0.91190000	-0.85690000
C	1.78830000	-1.86070000	-1.71310000
C	1.62680000	-3.17660000	-2.15210000
C	0.85770000	-4.09570000	-1.42720000

C	0.24500000	-3.65360000	-0.24310000
C	0.38850000	-2.34110000	0.19340000
C	4.06190000	0.44270000	-0.49550000
C	5.18760000	0.84520000	-1.21080000
C	5.07850000	1.72850000	-2.30030000
C	3.80380000	2.19430000	-2.65010000
C	2.66780000	1.79190000	-1.93950000
C	1.59760000	1.26470000	2.63590000
C	1.96260000	1.19490000	3.97820000
C	2.55460000	0.03640000	4.51010000
C	2.77630000	-1.04270000	3.64320000
C	2.41420000	-0.97790000	2.29520000
C	0.68330000	-5.51620000	-1.89320000
C	6.30570000	2.18480000	-3.04570000
C	2.93220000	-0.03190000	5.96630000
H	2.38380000	-1.16680000	-2.30650000
H	2.09780000	-3.48730000	-3.08800000
H	-0.37760000	-4.34330000	0.33180000
H	-0.12010000	-2.02640000	1.10550000
H	4.17840000	-0.24240000	0.34620000
H	6.17210000	0.47010000	-0.91690000
H	3.65680000	2.90780000	-3.46390000

H	1.69730000	2.18270000	-2.24620000
H	1.12020000	2.16800000	2.25620000
H	1.77630000	2.05290000	4.62950000
H	3.23760000	-1.95570000	4.02850000
H	2.59150000	-1.84210000	1.65420000
H	0.97580000	-5.63460000	-2.94650000
H	-0.36270000	-5.84070000	-1.78570000
H	1.30080000	-6.20730000	-1.29430000
H	6.84300000	2.96240000	-2.47560000
H	6.04450000	2.61410000	-4.02360000
H	7.01310000	1.35570000	-3.20390000
H	3.67910000	0.73950000	6.21640000
H	3.35340000	-1.01240000	6.22970000
H	2.05680000	0.15000000	6.61080000
Pd	-0.63240000	1.67030000	-0.18390000
P	-2.41470000	0.10820000	-0.02320000
C	-2.37520000	-1.39840000	-1.07420000
C	-4.01560000	0.88000000	-0.47590000
C	-2.67230000	-0.47610000	1.69660000
C	-3.19150000	-2.50830000	-0.81080000
C	-3.18510000	-3.60980000	-1.66710000
C	-2.37770000	-3.63310000	-2.81490000

C	-1.55520000	-2.52520000	-3.06160000
C	-1.54550000	-1.42820000	-2.20290000
C	-3.88620000	-1.03100000	2.14300000
C	-4.01410000	-1.49430000	3.45060000
C	-2.94530000	-1.41720000	4.36230000
C	-1.74610000	-0.84420000	3.91910000
C	-1.61440000	-0.37580000	2.60960000
C	-4.75540000	1.61810000	0.46030000
C	-5.87900000	2.34400000	0.05860000
C	-6.28410000	2.37190000	-1.28470000
C	-5.53120000	1.63550000	-2.21340000
C	-4.42100000	0.89150000	-1.81890000
C	-2.40250000	-4.80150000	-3.76490000
C	-3.10210000	-1.92660000	5.77070000
C	-7.48930000	3.16100000	-1.72630000
H	-3.83370000	-2.52910000	0.06940000
H	-3.82390000	-4.46760000	-1.44010000
H	-0.89680000	-2.52260000	-3.93200000
H	-0.88380000	-0.59270000	-2.40720000
H	-4.74500000	-1.08470000	1.47190000
H	-4.96650000	-1.92200000	3.77550000
H	-0.89890000	-0.75340000	4.60370000

H	-0.67490000	0.07930000	2.30280000
H	-4.44830000	1.64480000	1.50770000
H	-6.44370000	2.91190000	0.80300000
H	-5.79670000	1.65710000	-3.27290000
H	-3.84720000	0.36030000	-2.57530000
H	-2.72640000	-5.72570000	-3.26380000
H	-1.41200000	-4.97600000	-4.21080000
H	-3.10480000	-4.61390000	-4.59560000
H	-3.92040000	-1.40320000	6.29190000
H	-2.18130000	-1.78890000	6.35500000
H	-3.35420000	-2.99970000	5.77640000
H	-7.84880000	3.83090000	-0.93180000
H	-8.32110000	2.49080000	-2.00270000
H	-7.25990000	3.77030000	-2.61490000
C	1.65240000	3.81790000	-7.60780000
C	0.44460000	4.50960000	-7.48120000
C	-0.55560000	4.04040000	-6.62940000
C	-0.35180000	2.84510000	-5.93730000
C	0.87520000	2.18130000	-6.01030000
C	1.87660000	2.67050000	-6.84720000
N	-1.33370000	2.27020000	-5.08660000
C	-0.95680000	1.60320000	-3.92500000

O	0.27270000	1.05510000	-3.92680000
C	1.09390000	1.01200000	-5.09130000
O	-1.67940000	1.47470000	-2.97310000
C	0.87610000	-0.35590000	-5.74750000
F	1.20120000	-1.35020000	-4.90560000
F	1.62920000	-0.48200000	-6.84530000
F	-0.41080000	-0.54130000	-6.09940000
C	-3.07930000	2.38560000	-7.17730000
C	-3.64330000	3.47000000	-7.84630000
C	-3.69590000	3.44180000	-9.24050000
C	-3.18900000	2.35180000	-9.96380000
C	-2.63590000	1.26950000	-9.25230000
C	-2.58400000	1.27140000	-7.86290000
C	-3.22620000	2.32830000	-11.46770000
S	-3.05470000	2.38320000	-5.40310000
O	-3.54310000	3.66720000	-4.89820000
O	-3.64030000	1.12720000	-4.93660000
H	2.43520000	4.19600000	-8.26790000
H	0.28300000	5.43780000	-8.03300000
H	-1.47590000	4.60370000	-6.49050000
H	2.84130000	2.16070000	-6.88680000
H	2.12820000	1.01920000	-4.71910000

H	-4.02570000	4.32210000	-7.28340000
H	-4.13480000	4.28680000	-9.77540000
H	-2.24040000	0.41110000	-9.80050000
H	-2.15320000	0.43130000	-7.31930000
H	-2.20550000	2.28390000	-11.88150000
H	-3.75950000	1.43610000	-11.83340000
H	-3.72300000	3.21940000	-11.87510000

D

O	0.01750000	3.29450000	-3.20770000
C	-0.79360000	4.12540000	-2.40750000
C	-0.71240000	3.80890000	-0.92040000
C	0.54310000	3.56580000	-0.30870000
O	0.92430000	5.83620000	-4.62860000
C	1.80360000	5.09040000	-4.48130000
O	2.72000000	4.38860000	-4.34080000
C	-1.86560000	3.49760000	-0.18030000
H	-0.42940000	5.15690000	-2.54090000
H	-1.84080000	4.08740000	-2.74140000
H	0.65780000	3.73970000	0.76510000
H	1.45150000	3.65060000	-0.90600000
H	-1.87490000	3.60220000	0.90920000
H	-2.83530000	3.46970000	-0.67800000
P	1.32010000	0.32560000	0.02050000
C	1.22080000	-1.39960000	-0.58090000
C	1.74180000	0.15990000	1.80280000
C	2.88770000	0.91830000	-0.72950000
C	1.86880000	-1.79440000	-1.75800000
C	1.72770000	-3.09780000	-2.23770000
C	0.95200000	-4.04330000	-1.55510000

C	0.30080000	-3.63680000	-0.37950000
C	0.41880000	-2.33470000	0.09460000
C	4.12990000	0.58870000	-0.16330000
C	5.31540000	0.97650000	-0.78650000
C	5.29920000	1.70010000	-1.99030000
C	4.05350000	2.02420000	-2.54670000
C	2.85890000	1.64620000	-1.92720000
C	1.52450000	1.26050000	2.64880000
C	1.80560000	1.18020000	4.01070000
C	2.30840000	-0.00270000	4.57910000
C	2.54090000	-1.09170000	3.72690000
C	2.26650000	-1.01510000	2.35910000
C	0.82020000	-5.45770000	-2.05310000
C	6.58330000	2.13870000	-2.64480000
C	2.56020000	-0.09870000	6.06070000
H	2.47400000	-1.08150000	-2.31740000
H	2.22310000	-3.37810000	-3.17060000
H	-0.33290000	-4.34570000	0.15780000
H	-0.12290000	-2.04610000	0.99650000
H	4.17650000	0.02350000	0.76880000
H	6.27290000	0.71070000	-0.32980000
H	4.00880000	2.59830000	-3.47310000

H	1.90440000	1.90710000	-2.38560000
H	1.10770000	2.18120000	2.23850000
H	1.62050000	2.04840000	4.64870000
H	2.94210000	-2.02100000	4.13960000
H	2.45520000	-1.88370000	1.72740000
H	1.04670000	-5.53050000	-3.12670000
H	-0.19600000	-5.84410000	-1.88590000
H	1.51630000	-6.12910000	-1.52090000
H	6.99200000	3.03370000	-2.14480000
H	6.42910000	2.39320000	-3.70350000
H	7.35410000	1.35500000	-2.58300000
H	3.03140000	0.81810000	6.44740000
H	3.20670000	-0.95340000	6.30660000
H	1.61160000	-0.22980000	6.60930000
Pd	-0.56290000	1.68240000	-0.26640000
P	-2.36720000	0.14980000	-0.04980000
C	-2.31190000	-1.36110000	-1.09580000
C	-3.96080000	0.92350000	-0.52350000
C	-2.67140000	-0.44660000	1.65950000
C	-2.97160000	-2.54620000	-0.73930000
C	-2.94870000	-3.65050000	-1.59220000
C	-2.27190000	-3.60500000	-2.82020000

C	-1.60260000	-2.42030000	-3.15770000
C	-1.61620000	-1.31190000	-2.31350000
C	-3.90020000	-1.00010000	2.06620000
C	-4.06870000	-1.47260000	3.36600000
C	-3.02630000	-1.40810000	4.30900000
C	-1.81150000	-0.84020000	3.90430000
C	-1.63970000	-0.36220000	2.60240000
C	-4.71600000	1.65350000	0.40680000
C	-5.86890000	2.33110000	0.00350000
C	-6.29010000	2.31120000	-1.33500000
C	-5.51550000	1.59050000	-2.25730000
C	-4.36810000	0.90390000	-1.86510000
C	-2.27890000	-4.77980000	-3.76300000
C	-3.22690000	-1.92620000	5.70900000
C	-7.52970000	3.04320000	-1.78110000
H	-3.49650000	-2.62610000	0.21250000
H	-3.46510000	-4.56750000	-1.29480000
H	-1.05450000	-2.35660000	-4.10010000
H	-1.11700000	-0.39140000	-2.61110000
H	-4.73610000	-1.04970000	1.36640000
H	-5.03190000	-1.89930000	3.65960000
H	-0.98320000	-0.76070000	4.61330000

H	-0.68990000	0.08860000	2.32520000
H	-4.40410000	1.70360000	1.45210000
H	-6.44760000	2.89240000	0.74250000
H	-5.78850000	1.59120000	-3.31440000
H	-3.76800000	0.40180000	-2.62180000
H	-2.50620000	-5.72060000	-3.24010000
H	-1.30940000	-4.89050000	-4.27150000
H	-3.04260000	-4.64540000	-4.54860000
H	-4.05330000	-1.39800000	6.21220000
H	-2.32080000	-1.80230000	6.31900000
H	-3.49020000	-2.99670000	5.70040000
H	-7.94450000	3.66750000	-0.97610000
H	-8.31560000	2.33710000	-2.09890000
H	-7.31580000	3.69270000	-2.64530000
C	1.45000000	3.76940000	-7.84160000
C	0.20140000	4.39810000	-7.76600000
C	-0.73410000	3.99330000	-6.81640000
C	-0.44890000	2.91630000	-5.96440000
C	0.81080000	2.29850000	-6.02050000
C	1.75550000	2.73670000	-6.95370000
N	-1.32280000	2.46200000	-4.96220000
C	-0.71840000	2.08640000	-3.62300000

O	0.35430000	1.13670000	-3.88430000
C	1.12900000	1.18030000	-5.05260000
O	-1.55850000	1.66320000	-2.79670000
C	0.98250000	-0.19810000	-5.71140000
F	1.34740000	-1.17850000	-4.86680000
F	1.75780000	-0.30740000	-6.80590000
F	-0.28430000	-0.45180000	-6.08590000
C	-3.14960000	2.20140000	-6.96750000
C	-3.95180000	3.21940000	-7.47680000
C	-4.13050000	3.31320000	-8.85890000
C	-3.51430000	2.40470000	-9.73180000
C	-2.72160000	1.37890000	-9.18280000
C	-2.54210000	1.26360000	-7.80810000
C	-3.69400000	2.50860000	-11.22310000
S	-2.95170000	2.05020000	-5.19730000
O	-3.80040000	3.07170000	-4.56070000
O	-3.18830000	0.63330000	-4.88320000
H	2.19070000	4.09900000	-8.57300000
H	-0.03500000	5.23050000	-8.43270000
H	-1.68340000	4.51590000	-6.71790000
H	2.74000000	2.26440000	-6.98130000
H	2.19740000	1.24840000	-4.77590000

H	-4.41880000	3.92970000	-6.79360000
H	-4.75740000	4.11030000	-9.26580000
H	-2.23930000	0.65830000	-9.84830000
H	-1.92840000	0.46760000	-7.38850000
H	-2.72070000	2.60760000	-11.73070000
H	-4.17410000	1.60140000	-11.62540000
H	-4.31410000	3.37350000	-11.49730000

E

O	-0.00880000	3.06860000	-3.19030000
C	-0.79150000	3.99060000	-2.46710000
C	-0.79660000	3.73710000	-0.96330000
C	0.42340000	3.55040000	-0.26790000
C	-1.98370000	3.41360000	-0.28250000
H	-0.34580000	4.98650000	-2.62920000
H	-1.82450000	4.00870000	-2.84470000
H	0.45890000	3.73990000	0.80900000
H	1.36880000	3.65680000	-0.80100000
H	-2.06140000	3.55300000	0.80040000
H	-2.91930000	3.34260000	-0.83720000
P	1.28690000	0.32640000	0.00010000
C	1.20660000	-1.40710000	-0.57860000
C	1.77640000	0.18340000	1.76620000
C	2.80450000	0.95310000	-0.82450000
C	1.82360000	-1.80270000	-1.77200000
C	1.70130000	-3.11660000	-2.22660000
C	0.97290000	-4.07060000	-1.50420000
C	0.34900000	-3.66230000	-0.31460000
C	0.45050000	-2.35060000	0.13670000
C	4.08340000	0.61830000	-0.35060000

C	5.22200000	1.03870000	-1.03690000
C	5.12300000	1.80080000	-2.21390000
C	3.84070000	2.13020000	-2.67610000
C	2.69310000	1.71830000	-1.99280000
C	1.52550000	1.26650000	2.62510000
C	1.86410000	1.19980000	3.97500000
C	2.46020000	0.04870000	4.51730000
C	2.72170000	-1.02380000	3.65230000
C	2.38830000	-0.96140000	2.29730000
C	0.86450000	-5.49540000	-1.97760000
C	6.36010000	2.26740000	-2.93570000
C	2.77940000	-0.03440000	5.98680000
H	2.39010000	-1.08190000	-2.36130000
H	2.17140000	-3.39900000	-3.17170000
H	-0.24990000	-4.37820000	0.25280000
H	-0.06720000	-2.06090000	1.05250000
H	4.19570000	0.02410000	0.55790000
H	6.20950000	0.76840000	-0.65280000
H	3.73130000	2.72530000	-3.58710000
H	1.71170000	1.99140000	-2.37870000
H	1.04030000	2.16210000	2.23500000
H	1.65270000	2.05390000	4.62370000

H	3.19290000	-1.92850000	4.04510000
H	2.59900000	-1.81760000	1.65550000
H	1.00930000	-5.57100000	-3.06510000
H	-0.11690000	-5.92420000	-1.72760000
H	1.63040000	-6.12900000	-1.49740000
H	6.82360000	3.11910000	-2.40890000
H	6.12990000	2.59600000	-3.95950000
H	7.11840000	1.47060000	-2.98780000
H	3.19940000	0.91220000	6.36000000
H	3.49500000	-0.84150000	6.20000000
H	1.86640000	-0.23580000	6.57320000
Pd	-0.63400000	1.63630000	-0.26010000
P	-2.41660000	0.07820000	-0.03910000
C	-2.34900000	-1.46700000	-1.03220000
C	-4.01010000	0.83490000	-0.54060000
C	-2.70520000	-0.46840000	1.68890000
C	-3.00440000	-2.64130000	-0.63320000
C	-2.97850000	-3.77520000	-1.44600000
C	-2.30340000	-3.77140000	-2.67600000
C	-1.63460000	-2.59880000	-3.05400000
C	-1.65030000	-1.46140000	-2.24880000
C	-3.93180000	-1.00040000	2.12860000

C	-4.08400000	-1.43790000	3.44280000
C	-3.02610000	-1.35960000	4.36700000
C	-1.81160000	-0.81610000	3.92810000
C	-1.65630000	-0.37250000	2.61230000
C	-4.77550000	1.58590000	0.36410000
C	-5.89900000	2.29020000	-0.07610000
C	-6.27710000	2.28100000	-1.42750000
C	-5.49640000	1.53380000	-2.32360000
C	-4.38400000	0.81470000	-1.89230000
C	-2.31400000	-4.97860000	-3.57680000
C	-3.21070000	-1.83370000	5.78470000
C	-7.47630000	3.05260000	-1.91500000
H	-3.53040000	-2.68760000	0.32020000
H	-3.49280000	-4.68220000	-1.11590000
H	-1.08100000	-2.56910000	-3.99480000
H	-1.14170000	-0.55680000	-2.57640000
H	-4.77820000	-1.06260000	1.44240000
H	-5.04590000	-1.84830000	3.76220000
H	-0.97100000	-0.72900000	4.62160000
H	-0.70560000	0.06030000	2.30800000
H	-4.49020000	1.63900000	1.41680000
H	-6.48470000	2.86930000	0.64340000

H	-5.73210000	1.53690000	-3.39000000
H	-3.77500000	0.29780000	-2.63040000
H	-2.47170000	-5.90830000	-3.00990000
H	-1.37200000	-5.06890000	-4.13760000
H	-3.12790000	-4.90420000	-4.31890000
H	-3.97930000	-1.23720000	6.30370000
H	-2.27700000	-1.75930000	6.36020000
H	-3.54830000	-2.88250000	5.81110000
H	-7.89360000	3.69620000	-1.12670000
H	-8.27630000	2.37240000	-2.25360000
H	-7.21240000	3.68840000	-2.77560000
C	1.74800000	3.72670000	-7.50450000
C	0.52120000	4.39820000	-7.49390000
C	-0.51880000	3.96240000	-6.67110000
C	-0.35440000	2.81150000	-5.88890000
C	0.88550000	2.14630000	-5.87890000
C	1.93040000	2.61430000	-6.67810000
N	-1.31060000	2.29320000	-5.00120000
C	-0.79060000	1.90190000	-3.61420000
O	0.24070000	0.90090000	-3.84280000
C	1.05720000	0.93770000	-4.98410000
O	-1.68240000	1.52840000	-2.82320000

C	0.81400000	-0.37570000	-5.73910000
F	1.08920000	-1.43660000	-4.95710000
F	1.60200000	-0.46940000	-6.82590000
F	-0.45900000	-0.51030000	-6.14810000
C	-3.09370000	2.39010000	-7.04110000
C	-3.79440000	3.47490000	-7.56190000
C	-3.92840000	3.59210000	-8.94740000
C	-3.36780000	2.64080000	-9.81200000
C	-2.67580000	1.55030000	-9.25170000
C	-2.54250000	1.41150000	-7.87380000
C	-3.50120000	2.76750000	-11.30650000
S	-2.97170000	2.20060000	-5.26760000
O	-3.65520000	3.34710000	-4.64000000
O	-3.45480000	0.84530000	-4.96830000
H	2.56530000	4.07920000	-8.13700000
H	0.37740000	5.28670000	-8.11320000
H	-1.45500000	4.51550000	-6.62730000
H	2.89310000	2.09750000	-6.65800000
H	2.11420000	0.88290000	-4.66620000
H	-4.21810000	4.21790000	-6.88510000
H	-4.47530000	4.44170000	-9.36320000
H	-2.23610000	0.79730000	-9.91070000

H	-2.00550000	0.56600000	-7.44570000
H	-2.51150000	2.77490000	-11.79110000
H	-4.05650000	1.91200000	-11.72520000
H	-4.02960000	3.68860000	-11.58950000

TS3

O	-2.54090000	-0.75710000	-2.67240000
C	-1.58510000	-0.31010000	-3.59780000
C	-0.20820000	0.22240000	-3.20930000
C	0.92280000	-0.56510000	-3.42120000
C	-0.00780000	1.50480000	-2.61390000
H	-1.40710000	-1.14160000	-4.30000000
H	-2.04130000	0.50900000	-4.18600000
H	1.90020000	-0.10940000	-3.59350000
H	0.81880000	-1.61070000	-3.71910000
H	0.83630000	2.11080000	-2.95770000
H	-0.88350000	2.05620000	-2.26570000
P	2.17180000	-1.71400000	-0.41750000
C	3.43840000	-1.63670000	0.91290000
C	3.14550000	-2.62930000	-1.68750000
C	0.91000000	-2.90080000	0.16060000
C	3.67170000	-2.70080000	1.79540000
C	4.67050000	-2.60750000	2.76730000
C	5.47660000	-1.46500000	2.87360000
C	5.26620000	-0.42530000	1.95480000
C	4.26520000	-0.50800000	0.99130000
C	0.18390000	-3.64240000	-0.78390000

C	-0.90410000	-4.41630000	-0.39480000
C	-1.32720000	-4.45610000	0.94280000
C	-0.59210000	-3.72260000	1.88370000
C	0.50540000	-2.94900000	1.50120000
C	3.88370000	-1.90370000	-2.63270000
C	4.71290000	-2.55560000	-3.54660000
C	4.82780000	-3.95390000	-3.55030000
C	4.09670000	-4.67440000	-2.59180000
C	3.27410000	-4.02690000	-1.66990000
C	6.52630000	-1.33500000	3.94530000
C	-2.57360000	-5.20670000	1.32950000
C	5.68860000	-4.66370000	-4.56230000
H	3.07040000	-3.60870000	1.73580000
H	4.82500000	-3.44090000	3.45770000
H	5.88260000	0.47530000	2.00800000
H	4.12070000	0.32250000	0.30290000
H	0.45450000	-3.59520000	-1.84000000
H	-1.46310000	-4.97340000	-1.15120000
H	-0.89030000	-3.73970000	2.93510000
H	1.03960000	-2.37660000	2.25830000
H	3.82280000	-0.81460000	-2.65070000
H	5.28000000	-1.96610000	-4.27180000

H	4.17770000	-5.76450000	-2.56260000
H	2.72930000	-4.61710000	-0.93140000
H	6.62540000	-2.25990000	4.53140000
H	6.27200000	-0.51810000	4.64130000
H	7.51090000	-1.09280000	3.51380000
H	-2.64610000	-6.17150000	0.80390000
H	-3.46370000	-4.61690000	1.05300000
H	-2.61720000	-5.39640000	2.41210000
H	5.08580000	-4.99180000	-5.42680000
H	6.15490000	-5.56340000	-4.13280000
H	6.48400000	-4.00820000	-4.94630000
Pd	1.00610000	0.18510000	-1.25810000
P	1.57530000	2.00020000	0.13160000
C	2.06010000	1.55060000	1.84390000
C	0.45970000	3.44300000	0.34680000
C	3.06360000	2.82790000	-0.57710000
C	3.07220000	2.21560000	2.54750000
C	3.47760000	1.75950000	3.80310000
C	2.88620000	0.63310000	4.39140000
C	1.84410000	-0.00090000	3.69630000
C	1.43760000	0.44370000	2.44170000
C	3.44030000	4.13030000	-0.20080000

C	4.58420000	4.72120000	-0.73340000
C	5.38980000	4.04340000	-1.66580000
C	5.00040000	2.75410000	-2.05270000
C	3.85330000	2.15920000	-1.52140000
C	0.13850000	4.24420000	-0.75910000
C	-0.73700000	5.32210000	-0.62390000
C	-1.31320000	5.63650000	0.61660000
C	-0.96070000	4.84860000	1.72150000
C	-0.09400000	3.76520000	1.59200000
C	3.36660000	0.08780000	5.70940000
C	6.62140000	4.69820000	-2.23400000
C	-2.30700000	6.75980000	0.75340000
H	3.58020000	3.07390000	2.10740000
H	4.28690000	2.27660000	4.32540000
H	1.35690000	-0.87320000	4.14050000
H	0.63350000	-0.06500000	1.91180000
H	2.82700000	4.69160000	0.50620000
H	4.85770000	5.73360000	-0.42350000
H	5.59840000	2.20680000	-2.78600000
H	3.55480000	1.16280000	-1.85030000
H	0.58730000	4.04400000	-1.73260000
H	-0.97640000	5.93160000	-1.49960000

H	-1.39140000	5.07390000	2.70080000
H	0.13800000	3.15260000	2.46290000
H	4.10080000	0.75530000	6.18280000
H	3.84550000	-0.89530000	5.56490000
H	2.53080000	-0.06190000	6.41140000
H	6.36300000	5.62230000	-2.77700000
H	7.15010000	4.03100000	-2.92940000
H	7.32250000	4.98390000	-1.43290000
H	-3.33790000	6.36700000	0.71530000
H	-2.20360000	7.49560000	-0.05790000
H	-2.19580000	7.28320000	1.71540000
C	-6.58160000	1.78140000	-2.52040000
C	-5.63590000	2.77430000	-2.24280000
C	-4.40460000	2.42580000	-1.69240000
C	-4.11690000	1.08730000	-1.38190000
C	-5.06640000	0.08390000	-1.65460000
C	-6.28630000	0.44640000	-2.24190000
N	-2.83840000	0.73390000	-0.86110000
C	-2.36670000	-0.71460000	-1.24600000
O	-3.46810000	-1.56630000	-0.80180000
C	-4.70970000	-1.37620000	-1.41710000
O	-1.26800000	-1.05390000	-0.76870000

C	-5.72420000	-2.10620000	-0.53120000
F	-5.29960000	-3.34490000	-0.22600000
F	-6.90850000	-2.25150000	-1.16580000
F	-5.96970000	-1.46880000	0.62030000
C	-3.44380000	0.15830000	1.83680000
C	-4.58980000	0.63880000	2.46930000
C	-5.26870000	-0.19200000	3.36250000
C	-4.81970000	-1.49510000	3.61960000
C	-3.65660000	-1.94480000	2.96950000
C	-2.96210000	-1.13150000	2.07940000
C	-5.58430000	-2.41200000	4.53750000
S	-2.54390000	1.23540000	0.73540000
O	-3.12970000	2.57830000	0.87060000
O	-1.12230000	1.04890000	1.03230000
H	-7.54270000	2.04340000	-2.96860000
H	-5.85100000	3.82060000	-2.47270000
H	-3.64650000	3.17910000	-1.48380000
H	-7.01560000	-0.32730000	-2.48460000
H	-4.74450000	-1.89940000	-2.39250000
H	-4.93260000	1.65370000	2.26690000
H	-6.16660000	0.17840000	3.86400000
H	-3.29590000	-2.95770000	3.16040000

H	-2.07690000	-1.48900000	1.55310000
H	-4.90890000	-3.06440000	5.11170000
H	-6.21200000	-1.84930000	5.24390000
H	-6.25150000	-3.06910000	3.95290000

F

O	0.79720000	4.02190000	-3.21710000
C	0.99290000	3.68530000	-1.86350000
C	-0.30650000	3.50820000	-1.08690000
C	-0.35380000	2.42710000	-0.08400000
C	-1.35540000	4.31590000	-1.34750000
H	1.60350000	2.77280000	-1.79890000
H	1.57300000	4.50770000	-1.40960000
H	-1.16670000	2.50700000	0.64740000
H	0.60170000	2.25280000	0.42200000
H	-2.30030000	4.22150000	-0.81520000
H	-1.29070000	5.07640000	-2.12740000
P	1.33470000	-0.33360000	-0.90800000
C	0.59390000	-1.97250000	-0.52230000
C	2.29920000	0.07140000	0.59650000
C	2.58850000	-0.69600000	-2.18820000
C	0.84610000	-2.66180000	0.67110000
C	0.14180000	-3.83180000	0.97360000
C	-0.81750000	-4.35160000	0.09400000
C	-1.03300000	-3.67590000	-1.11900000
C	-0.34930000	-2.50390000	-1.42360000
C	3.41910000	0.34250000	-2.63900000

C	4.36840000	0.10840000	-3.62800000
C	4.50970000	-1.15900000	-4.21730000
C	3.67300000	-2.18970000	-3.76760000
C	2.72740000	-1.96720000	-2.76270000
C	1.60290000	0.43090000	1.76520000
C	2.28800000	0.71320000	2.94480000
C	3.69120000	0.66590000	2.99910000
C	4.37940000	0.30690000	1.83110000
C	3.69910000	0.01020000	0.64740000
C	-1.62090000	-5.57910000	0.43200000
C	5.53220000	-1.39150000	-5.29890000
C	4.42780000	1.01350000	4.26580000
H	1.57790000	-2.27850000	1.38300000
H	0.33970000	-4.34480000	1.91860000
H	-1.77220000	-4.05720000	-1.82590000
H	-0.56160000	-1.98690000	-2.35970000
H	3.30780000	1.34650000	-2.23460000
H	4.99350000	0.93580000	-3.97330000
H	3.75750000	-3.18520000	-4.21120000
H	2.09440000	-2.79160000	-2.43390000
H	0.51350000	0.47030000	1.76220000
H	1.72100000	0.97890000	3.84110000

H	5.47100000	0.25000000	1.84680000
H	4.26710000	-0.28040000	-0.23670000
H	-1.27120000	-6.05310000	1.36030000
H	-1.57060000	-6.32470000	-0.37770000
H	-2.68520000	-5.31930000	0.56070000
H	6.55630000	-1.35300000	-4.89050000
H	5.46980000	-0.61460000	-6.07740000
H	5.39860000	-2.37220000	-5.77800000
H	4.52900000	2.10760000	4.37040000
H	5.44130000	0.58660000	4.27360000
H	3.88960000	0.65240000	5.15550000
Pd	-0.67870000	0.87120000	-1.39630000
P	-2.95280000	0.53200000	-0.66580000
C	-3.57400000	-1.06930000	-1.31920000
C	-4.34270000	1.69610000	-0.93830000
C	-2.95120000	0.23520000	1.14760000
C	-4.13050000	-2.04610000	-0.47800000
C	-4.56670000	-3.26310000	-1.00000000
C	-4.46270000	-3.54750000	-2.37100000
C	-3.92070000	-2.55880000	-3.20580000
C	-3.47650000	-1.33900000	-2.69270000
C	-3.95440000	0.66540000	2.02510000

C	-3.89110000	0.34210000	3.38470000
C	-2.84210000	-0.42840000	3.90510000
C	-1.85400000	-0.87910000	3.01200000
C	-1.90420000	-0.54890000	1.66130000
C	-4.36980000	2.92200000	-0.25030000
C	-5.37080000	3.85870000	-0.49920000
C	-6.37540000	3.61310000	-1.44940000
C	-6.34740000	2.38620000	-2.12790000
C	-5.35030000	1.44020000	-1.88000000
C	-4.88170000	-4.88800000	-2.91440000
C	-2.76070000	-0.75880000	5.37220000
C	-7.42250000	4.65130000	-1.75430000
H	-4.22040000	-1.86250000	0.59280000
H	-4.99410000	-4.01100000	-0.32640000
H	-3.83260000	-2.74620000	-4.27920000
H	-3.05320000	-0.60350000	-3.37430000
H	-4.79960000	1.24670000	1.65600000
H	-4.68230000	0.69260000	4.05270000
H	-1.03020000	-1.49740000	3.37880000
H	-1.13520000	-0.92460000	0.98830000
H	-3.61290000	3.14350000	0.50380000
H	-5.37040000	4.80170000	0.05360000

H	-7.12050000	2.16290000	-2.86760000
H	-5.36190000	0.49740000	-2.42770000
H	-4.08750000	-5.63760000	-2.75220000
H	-5.07690000	-4.84370000	-3.99570000
H	-5.78590000	-5.26230000	-2.41050000
H	-1.95880000	-0.17890000	5.86030000
H	-2.52710000	-1.82360000	5.52910000
H	-3.70220000	-0.52990000	5.89170000
H	-8.32700000	4.19890000	-2.18620000
H	-7.03960000	5.38510000	-2.48520000
H	-7.70840000	5.21330000	-0.85250000
C	-3.54100000	5.46470000	-4.84440000
C	-3.92880000	4.31210000	-4.15310000
C	-3.00790000	3.29230000	-3.93420000
C	-1.70410000	3.38880000	-4.44310000
C	-1.31460000	4.53220000	-5.16300000
C	-2.23760000	5.57440000	-5.33000000
N	-0.72960000	2.41110000	-4.12640000
C	0.78570000	2.90510000	-4.13140000
O	0.91290000	3.53910000	-5.42440000
C	0.11170000	4.66170000	-5.67200000
O	1.58200000	1.97300000	-3.93870000

C	0.17490000	4.86610000	-7.18950000
F	1.44110000	4.85860000	-7.62690000
F	-0.35690000	6.05380000	-7.54850000
F	-0.49240000	3.91570000	-7.86570000
C	0.08650000	0.47180000	-6.01700000
C	-0.31760000	0.91230000	-7.27680000
C	0.50950000	0.66290000	-8.37250000
C	1.72130000	-0.02800000	-8.22170000
C	2.08950000	-0.46760000	-6.93680000
C	1.28950000	-0.21210000	-5.82790000
C	2.62510000	-0.28370000	-9.39890000
S	-0.97220000	0.83220000	-4.63900000
O	-2.36740000	0.72340000	-5.10710000
O	-0.57590000	-0.10050000	-3.54130000
H	-4.24820000	6.28350000	-4.99470000
H	-4.93880000	4.21540000	-3.75260000
H	-3.28180000	2.41650000	-3.35340000
H	-1.93230000	6.48070000	-5.85420000
H	0.56220000	5.57070000	-5.22880000
H	-1.25840000	1.44800000	-7.39820000
H	0.20700000	1.01470000	-9.36160000
H	3.02820000	-1.00870000	-6.80070000

H	1.58870000	-0.52100000	-4.82970000
H	2.92690000	-1.34210000	-9.44670000
H	2.13960000	-0.01850000	-10.34880000
H	3.55070000	0.31050000	-9.31500000

TS4

O	-2.60400000	0.05420000	-2.68430000
C	-1.30840000	-0.27270000	-3.14470000
C	-0.28470000	0.82240000	-2.87990000
C	1.07330000	0.39570000	-2.48940000
C	-0.64630000	2.11740000	-2.99040000
H	-0.98830000	-1.21930000	-2.68720000
H	-1.39170000	-0.43680000	-4.23260000
H	1.84910000	1.16180000	-2.60400000
H	1.39100000	-0.54300000	-2.95580000
H	0.05700000	2.92710000	-2.80470000
H	-1.67260000	2.39040000	-3.24110000
P	1.20410000	-2.30860000	-0.52930000
C	2.41380000	-2.34170000	0.85630000
C	2.14520000	-3.01330000	-1.93500000
C	-0.01810000	-3.59510000	-0.08540000
C	3.69490000	-2.89630000	0.73510000
C	4.62360000	-2.76240000	1.77230000
C	4.29860000	-2.08790000	2.95720000
C	2.99770000	-1.57310000	3.08610000
C	2.07070000	-1.68830000	2.05590000
C	-1.02660000	-3.92610000	-1.00490000

C	-1.98550000	-4.88300000	-0.68840000
C	-1.98860000	-5.52580000	0.56070000
C	-0.98460000	-5.18460000	1.47730000
C	-0.00710000	-4.23730000	1.16080000
C	3.15400000	-2.23010000	-2.52530000
C	3.92780000	-2.73270000	-3.56900000
C	3.71350000	-4.02590000	-4.07470000
C	2.70680000	-4.80170000	-3.48180000
C	1.93480000	-4.30960000	-2.42660000
C	5.30560000	-1.88940000	4.05860000
C	-3.04400000	-6.54770000	0.89450000
C	4.52460000	-4.54820000	-5.23110000
H	3.98470000	-3.41600000	-0.17880000
H	5.62450000	-3.18520000	1.65080000
H	2.71340000	-1.04420000	3.99760000
H	1.07830000	-1.25300000	2.17580000
H	-1.07860000	-3.41740000	-1.96580000
H	-2.76800000	-5.11460000	-1.41550000
H	-0.96530000	-5.66460000	2.45920000
H	0.76120000	-3.99780000	1.89610000
H	3.35470000	-1.22570000	-2.15180000
H	4.71300000	-2.10650000	-4.00110000

H	2.52610000	-5.81650000	-3.84610000
H	1.17250000	-4.94800000	-1.97930000
H	6.24610000	-2.42010000	3.85240000
H	4.91370000	-2.24310000	5.02590000
H	5.53670000	-0.81780000	4.18090000
H	-2.90160000	-7.47040000	0.30670000
H	-4.05130000	-6.17020000	0.65680000
H	-3.01990000	-6.82090000	1.95930000
H	4.11200000	-4.19010000	-6.19010000
H	4.52260000	-5.64750000	-5.26190000
H	5.56810000	-4.20180000	-5.17890000
Pd	0.67030000	0.02800000	-0.50180000
P	1.96730000	1.92150000	0.26000000
C	2.22310000	1.81580000	2.07650000
C	1.53890000	3.68110000	-0.02670000
C	3.68250000	1.76110000	-0.38150000
C	3.50120000	1.90730000	2.65060000
C	3.66550000	1.80060000	4.03110000
C	2.56720000	1.59940000	4.88240000
C	1.29260000	1.52470000	4.30050000
C	1.11770000	1.62510000	2.91930000
C	4.47970000	2.83350000	-0.80170000

C	5.79470000	2.61430000	-1.22530000
C	6.35770000	1.33040000	-1.22840000
C	5.55950000	0.26400000	-0.77900000
C	4.24620000	0.47420000	-0.36950000
C	1.60850000	4.21220000	-1.32680000
C	1.21500000	5.52360000	-1.58480000
C	0.72840000	6.35080000	-0.55940000
C	0.66710000	5.81830000	0.73630000
C	1.06450000	4.50630000	1.00340000
C	2.76090000	1.42800000	6.36590000
C	7.76450000	1.09010000	-1.70940000
C	0.25240000	7.74870000	-0.85370000
H	4.37750000	2.05720000	2.01950000
H	4.67010000	1.87180000	4.45690000
H	0.41580000	1.37560000	4.93610000
H	0.11120000	1.55280000	2.51040000
H	4.08790000	3.85070000	-0.79180000
H	6.39710000	3.46570000	-1.55290000
H	5.97040000	-0.74880000	-0.74920000
H	3.65630000	-0.36750000	-0.01080000
H	1.99190000	3.60360000	-2.14740000
H	1.28370000	5.91210000	-2.60430000

H	0.29990000	6.44050000	1.55660000
H	1.00190000	4.12730000	2.02400000
H	3.02400000	0.38270000	6.60510000
H	1.84540000	1.67170000	6.92440000
H	3.57920000	2.06090000	6.74150000
H	7.76220000	0.66140000	-2.72630000
H	8.29250000	0.37450000	-1.06020000
H	8.34560000	2.02300000	-1.74390000
H	0.27310000	8.38090000	0.04590000
H	-0.78820000	7.73420000	-1.22290000
H	0.86440000	8.22790000	-1.63270000
C	-3.63150000	4.61950000	-1.42950000
C	-2.46390000	4.46370000	-0.67490000
C	-2.05040000	3.19190000	-0.29200000
C	-2.81610000	2.05810000	-0.61300000
C	-4.00990000	2.21450000	-1.34380000
C	-4.38600000	3.49660000	-1.76970000
N	-2.33870000	0.75840000	-0.34240000
C	-2.95870000	-0.47090000	-1.41870000
O	-4.34590000	-0.22570000	-1.28730000
C	-4.84810000	1.00850000	-1.73350000
O	-2.56670000	-1.58240000	-1.07430000

C	-6.26840000	1.07510000	-1.15840000
F	-6.94590000	-0.05380000	-1.40600000
F	-6.97140000	2.08530000	-1.71040000
F	-6.27620000	1.26850000	0.17070000
C	-3.34400000	-0.79360000	1.76600000
C	-4.54980000	-0.23180000	2.19350000
C	-5.58210000	-1.07650000	2.59260000
C	-5.42130000	-2.47330000	2.58050000
C	-4.19180000	-3.00220000	2.15760000
C	-3.15170000	-2.17390000	1.73700000
C	-6.55300000	-3.37390000	3.00120000
S	-2.06180000	0.30980000	1.21970000
O	-2.10790000	1.50120000	2.09400000
O	-0.79420000	-0.48950000	1.26900000
H	-3.94820000	5.61040000	-1.76260000
H	-1.85150000	5.32690000	-0.41070000
H	-1.11570000	3.05570000	0.24420000
H	-5.28880000	3.61700000	-2.37000000
H	-4.96970000	1.00010000	-2.83280000
H	-4.67630000	0.85040000	2.20630000
H	-6.53190000	-0.64460000	2.91800000
H	-4.04630000	-4.08420000	2.14450000

H	-2.21110000	-2.58630000	1.38180000
H	-6.94410000	-3.08800000	3.99080000
H	-7.39390000	-3.30250000	2.29110000
H	-6.23710000	-4.42600000	3.04550000

G

O	2.44010000	2.42230000	-1.83400000
C	1.15400000	2.45670000	-2.47950000
C	0.53420000	1.08290000	-2.64680000
C	-0.91480000	0.94330000	-2.41340000
C	1.29550000	0.00650000	-2.95270000
H	0.48780000	3.12070000	-1.91840000
H	1.34930000	2.90420000	-3.46480000
H	-1.38690000	0.12070000	-2.96190000
H	-1.48240000	1.87380000	-2.51410000
H	0.84650000	-0.97760000	-3.08530000
H	2.37920000	0.08640000	-3.04820000
P	-1.79260000	2.19310000	0.29450000
C	-1.56300000	2.50650000	2.07980000
C	-3.59530000	1.83700000	0.10870000
C	-1.64540000	3.83970000	-0.50210000
C	-1.96090000	3.70670000	2.69290000
C	-1.82050000	3.87630000	4.06970000
C	-1.27970000	2.86120000	4.87670000
C	-0.88170000	1.66820000	4.25540000
C	-1.01400000	1.49070000	2.87720000
C	-2.45670000	4.18020000	-1.59550000

C	-2.26410000	5.38440000	-2.27870000
C	-1.26840000	6.28940000	-1.88850000
C	-0.46930000	5.94790000	-0.78290000
C	-0.64550000	4.74570000	-0.10310000
C	-4.04530000	1.12100000	-1.01370000
C	-5.39840000	0.85440000	-1.19790000
C	-6.35310000	1.26860000	-0.25660000
C	-5.89980000	1.96770000	0.87030000
C	-4.54400000	2.25500000	1.05100000
C	-1.09950000	3.06540000	6.35810000
C	-1.05740000	7.59200000	-2.61480000
C	-7.81200000	0.95980000	-0.46230000
H	-2.38270000	4.51520000	2.09340000
H	-2.13780000	4.81660000	4.52880000
H	-0.44920000	0.86500000	4.85770000
H	-0.65990000	0.56640000	2.41930000
H	-3.25600000	3.51040000	-1.91670000
H	-2.90780000	5.62500000	-3.12880000
H	0.31220000	6.63770000	-0.45180000
H	0.00780000	4.49870000	0.73160000
H	-3.32780000	0.74260000	-1.73870000
H	-5.71640000	0.28450000	-2.07450000

H	-6.61900000	2.28930000	1.62820000
H	-4.23090000	2.79450000	1.94530000
H	-0.14380000	3.57690000	6.56640000
H	-1.08290000	2.10750000	6.89820000
H	-1.90100000	3.69100000	6.77910000
H	-1.73120000	7.68760000	-3.47820000
H	-0.02030000	7.68030000	-2.97750000
H	-1.23590000	8.45080000	-1.94670000
H	-8.22760000	1.55720000	-1.29130000
H	-8.40410000	1.17670000	0.43810000
H	-7.95670000	-0.09970000	-0.72440000
Pd	-0.62110000	0.31180000	-0.46900000
P	-1.52810000	-1.99840000	-0.70410000
C	-0.96290000	-3.38500000	0.36670000
C	-1.46270000	-2.58580000	-2.42670000
C	-3.29950000	-2.01070000	-0.19140000
C	-0.91060000	-4.72040000	-0.04810000
C	-0.53960000	-5.72620000	0.85100000
C	-0.23430000	-5.43270000	2.18690000
C	-0.31420000	-4.09190000	2.59780000
C	-0.66610000	-3.08340000	1.70570000
C	-4.30340000	-2.77900000	-0.79360000

C	-5.60070000	-2.78410000	-0.27130000
C	-5.92500000	-2.05480000	0.88120000
C	-4.90640000	-1.30860000	1.49470000
C	-3.62130000	-1.27840000	0.96370000
C	-2.41920000	-2.17050000	-3.36890000
C	-2.24640000	-2.44190000	-4.72880000
C	-1.11650000	-3.12700000	-5.19640000
C	-0.15270000	-3.51980000	-4.25200000
C	-0.31250000	-3.25040000	-2.89420000
C	0.17900000	-6.50670000	3.15900000
C	-7.31230000	-2.08190000	1.46700000
C	-0.93750000	-3.44190000	-6.65860000
H	-1.15940000	-4.98990000	-1.07550000
H	-0.49330000	-6.76220000	0.50420000
H	-0.07070000	-3.83090000	3.63120000
H	-0.67960000	-2.04800000	2.04340000
H	-4.08120000	-3.38490000	-1.67340000
H	-6.37400000	-3.37820000	-0.76620000
H	-5.13030000	-0.72140000	2.38820000
H	-2.85600000	-0.67030000	1.44870000
H	-3.30640000	-1.62260000	-3.04660000
H	-3.00630000	-2.10820000	-5.44040000

H	0.75030000	-4.03590000	-4.58970000
H	0.47600000	-3.51780000	-2.19090000
H	0.22860000	-7.49350000	2.67660000
H	-0.52790000	-6.57480000	4.00250000
H	1.16920000	-6.28590000	3.59030000
H	-8.05420000	-2.43960000	0.73820000
H	-7.61820000	-1.08210000	1.81100000
H	-7.35590000	-2.75210000	2.34270000
H	0.09460000	-3.24310000	-6.98730000
H	-1.62050000	-2.85080000	-7.28580000
H	-1.13900000	-4.50830000	-6.85910000
C	5.97700000	-0.51560000	-3.11650000
C	5.25490000	-1.63380000	-2.68830000
C	4.31640000	-1.52830000	-1.66600000
C	4.05780000	-0.29460000	-1.01090000
C	4.84110000	0.82460000	-1.41830000
C	5.75840000	0.69990000	-2.46860000
N	3.08560000	-0.08200000	-0.05690000
C	2.44590000	2.54220000	-0.50140000
O	3.67350000	2.55280000	0.01440000
C	4.83750000	2.16060000	-0.70430000
O	1.48020000	2.72120000	0.19380000

C	5.92760000	2.21050000	0.37820000
F	5.94460000	3.40020000	0.99940000
F	7.14170000	2.02920000	-0.16810000
F	5.75770000	1.26600000	1.31300000
C	2.90360000	-2.12820000	1.72310000
C	2.79800000	-3.51740000	1.74060000
C	3.44280000	-4.23660000	2.75090000
C	4.18610000	-3.58510000	3.74510000
C	4.27990000	-2.18100000	3.69770000
C	3.65050000	-1.44980000	2.69350000
C	4.88660000	-4.35900000	4.83170000
S	2.07720000	-1.18590000	0.44200000
O	1.61040000	-2.17630000	-0.56810000
O	0.95800000	-0.46700000	1.16420000
H	6.69860000	-0.58770000	-3.93260000
H	5.41300000	-2.60480000	-3.16610000
H	3.73650000	-2.40240000	-1.37910000
H	6.32730000	1.58150000	-2.77610000
H	5.09660000	2.95070000	-1.42790000
H	2.21310000	-4.02330000	0.97340000
H	3.36470000	-5.32670000	2.76470000
H	4.86350000	-1.65610000	4.45880000

H	3.74830000	-0.36400000	2.64230000
H	4.61450000	-3.97830000	5.82940000
H	4.63590000	-5.42870000	4.79200000
H	5.98160000	-4.26400000	4.74060000

TS5

O	2.68210000	2.34080000	-1.35480000
C	1.41310000	2.34290000	-2.05160000
C	0.86380000	0.94280000	-2.18820000
C	-0.53140000	0.72710000	-2.25240000
C	1.79960000	-0.10250000	-2.36080000
H	0.71020000	3.00710000	-1.53750000
H	1.66430000	2.77860000	-3.03080000
H	-0.88120000	-0.18480000	-2.74410000
H	-1.14750000	1.60800000	-2.46120000
H	1.41740000	-1.11090000	-2.53480000
H	2.73800000	0.13040000	-2.86660000
P	-1.97070000	2.13890000	0.38590000
C	-1.96160000	2.55310000	2.17280000
C	-3.75850000	1.88770000	-0.00820000
C	-1.59110000	3.73970000	-0.42950000
C	-2.35960000	3.79970000	2.68410000
C	-2.35140000	4.03710000	4.05820000
C	-1.94640000	3.04370000	4.96650000
C	-1.54690000	1.80240000	4.44980000
C	-1.54670000	1.56180000	3.07430000
C	-2.22830000	4.12470000	-1.61790000

C	-1.80610000	5.25990000	-2.31860000
C	-0.74730000	6.05000000	-1.85320000
C	-0.11740000	5.66210000	-0.65630000
C	-0.52160000	4.52630000	0.03990000
C	-4.08360000	1.12560000	-1.14440000
C	-5.40660000	0.81800000	-1.44590000
C	-6.45540000	1.23290000	-0.60940000
C	-6.12960000	2.00210000	0.51530000
C	-4.80340000	2.33280000	0.81070000
C	-1.91120000	3.32130000	6.44690000
C	-0.29290000	7.27960000	-2.59620000
C	-7.87440000	0.82590000	-0.90610000
H	-2.67450000	4.59280000	2.00270000
H	-2.66640000	5.01370000	4.43660000
H	-1.22120000	1.01370000	5.13320000
H	-1.21140000	0.59490000	2.69030000
H	-3.06450000	3.53870000	-2.00440000
H	-2.31720000	5.53730000	-3.24460000
H	0.71440000	6.25830000	-0.27020000
H	0.01340000	4.22870000	0.94230000
H	-3.28390000	0.73330000	-1.77380000
H	-5.63020000	0.21230000	-2.32860000

H	-6.92630000	2.33670000	1.18540000
H	-4.58810000	2.91550000	1.70730000
H	-0.99250000	3.86860000	6.72010000
H	-1.92670000	2.39070000	7.03280000
H	-2.76320000	3.94450000	6.75940000
H	-0.82960000	7.39780000	-3.54860000
H	0.78670000	7.23730000	-2.81430000
H	-0.46190000	8.19030000	-1.99730000
H	-8.17710000	1.13560000	-1.91960000
H	-8.58140000	1.26490000	-0.18760000
H	-7.97950000	-0.27060000	-0.85970000
Pd	-0.80370000	0.21040000	-0.19360000
P	-1.84810000	-1.95630000	-0.41170000
C	-1.14930000	-3.40100000	0.48930000
C	-1.90160000	-2.44980000	-2.17150000
C	-3.59690000	-2.01010000	0.16840000
C	-1.07120000	-4.69810000	-0.03030000
C	-0.45240000	-5.71760000	0.69960000
C	0.09050000	-5.47660000	1.96970000
C	-0.03410000	-4.18250000	2.50280000
C	-0.63810000	-3.16100000	1.77510000
C	-4.55150000	-2.91360000	-0.31890000

C	-5.85980000	-2.89680000	0.17260000
C	-6.24610000	-1.99950000	1.17990000
C	-5.27450000	-1.12410000	1.68910000
C	-3.97530000	-1.12460000	1.18850000
C	-2.96320000	-2.07660000	-3.01060000
C	-2.87410000	-2.24820000	-4.39540000
C	-1.72690000	-2.79010000	-4.99050000
C	-0.65920000	-3.14420000	-4.14670000
C	-0.73540000	-2.97220000	-2.76590000
C	0.80790000	-6.55470000	2.74040000
C	-7.65550000	-1.96790000	1.71140000
C	-1.63320000	-2.99480000	-6.48030000
H	-1.47550000	-4.91900000	-1.01980000
H	-0.38450000	-6.72050000	0.26840000
H	0.37500000	-3.96740000	3.49390000
H	-0.68340000	-2.15460000	2.19220000
H	-4.28020000	-3.63240000	-1.09480000
H	-6.59520000	-3.59680000	-0.23360000
H	-5.54650000	-0.41240000	2.47230000
H	-3.24400000	-0.41550000	1.57740000
H	-3.86720000	-1.63850000	-2.58560000
H	-3.71660000	-1.94970000	-5.02560000

H	0.25660000	-3.55300000	-4.58350000
H	0.12410000	-3.21470000	-2.13790000
H	0.73140000	-7.53100000	2.24020000
H	0.40240000	-6.65760000	3.76000000
H	1.87930000	-6.31210000	2.84660000
H	-8.32380000	-2.61880000	1.12920000
H	-8.06390000	-0.94480000	1.68510000
H	-7.69120000	-2.30010000	2.76250000
H	-0.67660000	-2.61860000	-6.87670000
H	-2.45020000	-2.48420000	-7.01050000
H	-1.68650000	-4.06690000	-6.73670000
C	6.73640000	-1.04760000	-2.38720000
C	5.80350000	-2.08680000	-2.38970000
C	4.56000000	-1.88870000	-1.80040000
C	4.22580000	-0.67510000	-1.16090000
C	5.19790000	0.35760000	-1.09680000
C	6.42420000	0.15490000	-1.75520000
N	2.91210000	-0.43750000	-0.71140000
C	2.65000000	2.12430000	-0.04030000
O	3.86380000	1.81650000	0.45210000
C	5.00960000	1.69940000	-0.38020000
O	1.70010000	2.23670000	0.68440000

C	6.14450000	2.02520000	0.61520000
F	5.86490000	3.14580000	1.29150000
F	7.31990000	2.23080000	-0.00340000
F	6.32310000	1.04010000	1.50830000
C	3.37570000	-2.13900000	1.37880000
C	3.53810000	-3.51000000	1.56960000
C	4.44840000	-3.95330000	2.53240000
C	5.19880000	-3.04490000	3.29410000
C	5.01030000	-1.66750000	3.07360000
C	4.09820000	-1.20590000	2.12910000
C	6.19390000	-3.51980000	4.32010000
S	2.15970000	-1.56680000	0.20510000
O	1.71300000	-2.74390000	-0.58020000
O	1.12120000	-0.84960000	0.98230000
H	7.70530000	-1.16600000	-2.87670000
H	6.03250000	-3.03900000	-2.87400000
H	3.80100000	-2.67070000	-1.83480000
H	7.16430000	0.95300000	-1.76770000
H	5.01270000	2.51370000	-1.12090000
H	2.95200000	-4.21030000	0.97390000
H	4.58000000	-5.02670000	2.69090000
H	5.59210000	-0.94440000	3.65070000

H	3.96100000	-0.13810000	1.95810000
H	5.99100000	-3.07100000	5.30570000
H	6.17290000	-4.61340000	4.42910000
H	7.21860000	-3.22510000	4.03880000

H

O	3.01020000	2.82160000	-0.87800000
C	1.58410000	2.72410000	-1.07940000
C	1.27830000	1.73510000	-2.18230000
C	0.06910000	1.71600000	-2.76160000
C	2.36100000	0.78680000	-2.63380000
H	1.11860000	2.41070000	-0.13710000
H	1.22320000	3.72890000	-1.32680000
H	-0.18530000	0.96990000	-3.51760000
H	-0.68560000	2.46580000	-2.52410000
H	1.94730000	0.06940000	-3.36240000
H	3.14260000	1.35740000	-3.15890000
P	-2.49410000	2.08610000	-0.07220000
C	-3.32330000	1.77940000	1.55420000
C	-3.86820000	2.63600000	-1.16590000
C	-1.55460000	3.64750000	0.22970000
C	-4.58700000	2.26640000	1.90930000
C	-5.17800000	1.89470000	3.12180000
C	-4.52650000	1.03750000	4.01800000
C	-3.25370000	0.56180000	3.66280000
C	-2.66930000	0.91760000	2.45190000
C	-1.37560000	4.60820000	-0.77910000

C	-0.48790000	5.67470000	-0.60540000
C	0.26460000	5.81280000	0.56920000
C	0.07710000	4.85350000	1.57940000
C	-0.81490000	3.79550000	1.41710000
C	-4.29830000	1.75260000	-2.16610000
C	-5.36460000	2.08570000	-3.00670000
C	-6.02760000	3.31410000	-2.88090000
C	-5.58600000	4.20290000	-1.88410000
C	-4.52630000	3.87280000	-1.04100000
C	-5.16060000	0.61810000	5.31820000
C	1.26440000	6.92730000	0.73880000
C	-7.17260000	3.68760000	-3.78660000
H	-5.13670000	2.91990000	1.23110000
H	-6.17460000	2.27180000	3.36870000
H	-2.72790000	-0.12470000	4.33180000
H	-1.70590000	0.49280000	2.16270000
H	-1.93170000	4.52920000	-1.71540000
H	-0.37180000	6.40940000	-1.40730000
H	0.64760000	4.93380000	2.50900000
H	-0.92500000	3.06270000	2.21940000
H	-3.77870000	0.79640000	-2.27930000
H	-5.68310000	1.37910000	-3.77790000

H	-6.08400000	5.16990000	-1.76860000
H	-4.20280000	4.58790000	-0.28180000
H	-4.58320000	0.99090000	6.18070000
H	-5.19190000	-0.47990000	5.40310000
H	-6.18860000	0.99740000	5.41000000
H	1.12890000	7.71120000	-0.02070000
H	2.29590000	6.54620000	0.64460000
H	1.18440000	7.39290000	1.73380000
H	-7.42620000	2.86930000	-4.47570000
H	-6.92650000	4.57680000	-4.39050000
H	-8.07460000	3.93700000	-3.20410000
Pd	-1.39620000	0.16770000	-0.64410000
P	-1.87840000	-2.03030000	-0.15380000
C	-0.66970000	-2.94050000	0.90240000
C	-2.26370000	-3.26230000	-1.46850000
C	-3.39300000	-2.08550000	0.90520000
C	-0.33050000	-4.28870000	0.72010000
C	0.57230000	-4.91790000	1.58080000
C	1.15750000	-4.22930000	2.65430000
C	0.82730000	-2.87620000	2.82110000
C	-0.06320000	-2.24000000	1.95740000
C	-3.51500000	-2.88510000	2.04840000

C	-4.66370000	-2.81820000	2.84570000
C	-5.72590000	-1.96580000	2.51900000
C	-5.60380000	-1.17800000	1.36190000
C	-4.45760000	-1.22880000	0.57650000
C	-3.36010000	-4.13380000	-1.42210000
C	-3.59760000	-5.03370000	-2.46620000
C	-2.74810000	-5.09610000	-3.57970000
C	-1.64660000	-4.22240000	-3.61630000
C	-1.41100000	-3.31370000	-2.58610000
C	2.09040000	-4.92720000	3.60920000
C	-6.96510000	-1.87930000	3.37100000
C	-3.01230000	-6.04970000	-4.71680000
H	-0.77700000	-4.85540000	-0.09900000
H	0.82470000	-5.96970000	1.41690000
H	1.29000000	-2.30590000	3.63060000
H	-0.28180000	-1.17990000	2.09210000
H	-2.70360000	-3.55730000	2.33260000
H	-4.73030000	-3.43930000	3.74370000
H	-6.40840000	-0.48890000	1.09280000
H	-4.36220000	-0.57030000	-0.28850000
H	-4.03430000	-4.11370000	-0.56380000
H	-4.46000000	-5.70420000	-2.41110000

H	-0.96640000	-4.25330000	-4.47260000
H	-0.54980000	-2.64330000	-2.62730000
H	1.52370000	-5.47530000	4.38210000
H	2.74630000	-4.21160000	4.12480000
H	2.72480000	-5.66100000	3.08980000
H	-7.84260000	-2.28420000	2.83880000
H	-7.19760000	-0.83230000	3.62220000
H	-6.85290000	-2.44030000	4.31020000
H	-2.08890000	-6.55790000	-5.03690000
H	-3.40570000	-5.51460000	-5.59830000
H	-3.74940000	-6.81700000	-4.43810000
C	6.86880000	-1.54600000	-2.51910000
C	5.71730000	-2.29460000	-2.75630000
C	4.46800000	-1.74950000	-2.45880000
C	4.36140000	-0.46670000	-1.91040000
C	5.52160000	0.31710000	-1.70750000
C	6.76740000	-0.24910000	-2.00930000
N	3.07880000	0.07400000	-1.54600000
C	3.51990000	2.27310000	0.22390000
O	4.78260000	1.83290000	0.05860000
C	5.36910000	1.75480000	-1.24340000
O	2.97570000	2.17360000	1.29080000

C	6.64900000	2.58530000	-1.15650000
F	6.34990000	3.83310000	-0.76750000
F	7.24850000	2.66650000	-2.35530000
F	7.53730000	2.09300000	-0.28100000
C	3.12610000	-1.79550000	0.47060000
C	3.37270000	-3.15430000	0.28020000
C	4.21550000	-3.81360000	1.17210000
C	4.80110000	-3.13580000	2.25170000
C	4.51090000	-1.77060000	2.42610000
C	3.67330000	-1.08990000	1.54690000
C	5.72300000	-3.84670000	3.20530000
S	2.03060000	-0.95250000	-0.63710000
O	1.40390000	-1.92710000	-1.54860000
O	1.17620000	-0.03890000	0.13290000
H	7.85420000	-1.96220000	-2.73780000
H	5.78550000	-3.30190000	-3.17250000
H	3.55790000	-2.32020000	-2.64080000
H	7.68200000	0.31920000	-1.85340000
H	4.73540000	2.29860000	-1.95370000
H	2.89810000	-3.68510000	-0.54390000
H	4.40950000	-4.87960000	1.03520000
H	4.94480000	-1.23260000	3.27250000

H	3.44080000	-0.03520000	1.69860000
H	5.51470000	-3.56150000	4.24790000
H	5.63240000	-4.93850000	3.11730000
H	6.77360000	-3.57860000	3.00110000

TS6

O	2.45400000	2.80770000	1.10020000
C	1.95610000	3.14360000	-0.58930000
C	1.42100000	2.03290000	-1.29530000
C	0.04780000	2.04920000	-1.67220000
C	2.37970000	1.00630000	-1.84770000
H	1.27090000	3.96980000	-0.38800000
H	2.97520000	3.45300000	-0.83580000
H	-0.22680000	1.51590000	-2.59510000
H	-0.46380000	3.00870000	-1.56870000
H	1.81060000	0.22780000	-2.36590000
H	3.04820000	1.47220000	-2.59060000
P	-2.80350000	1.53420000	-0.42810000
C	-3.52270000	1.62390000	1.26280000
C	-4.07810000	0.72740000	-1.47920000
C	-2.89160000	3.28040000	-0.98810000
C	-4.89220000	1.77040000	1.51660000
C	-5.36760000	1.81180000	2.82880000
C	-4.49330000	1.71260000	3.92080000
C	-3.12150000	1.58020000	3.65670000
C	-2.63900000	1.53420000	2.35100000
C	-2.93260000	3.58530000	-2.35850000

C	-2.85130000	4.90800000	-2.79680000
C	-2.71570000	5.96890000	-1.88790000
C	-2.66020000	5.65560000	-0.52010000
C	-2.74590000	4.33600000	-0.07420000
C	-3.82610000	-0.56340000	-1.95940000
C	-4.77030000	-1.24010000	-2.73580000
C	-5.99270000	-0.64120000	-3.06760000
C	-6.23230000	0.66630000	-2.60580000
C	-5.29410000	1.34340000	-1.82900000
C	-4.99540000	1.73560000	5.34020000
C	-2.65640000	7.39910000	-2.35890000
C	-7.02270000	-1.36080000	-3.89860000
H	-5.60420000	1.83000000	0.69300000
H	-6.44170000	1.91070000	3.00770000
H	-2.41920000	1.48950000	4.48940000
H	-1.56940000	1.40750000	2.16810000
H	-3.02640000	2.78200000	-3.09280000
H	-2.88870000	5.12050000	-3.86890000
H	-2.54880000	6.46110000	0.21110000
H	-2.69490000	4.12460000	0.99570000
H	-2.87820000	-1.04540000	-1.72890000
H	-4.54200000	-2.24870000	-3.09040000

H	-7.17170000	1.16260000	-2.86520000
H	-5.50290000	2.36560000	-1.50810000
H	-4.60860000	2.61370000	5.88370000
H	-4.65550000	0.84320000	5.88970000
H	-6.09360000	1.76650000	5.38320000
H	-3.65330000	7.87100000	-2.31140000
H	-2.31080000	7.46690000	-3.40110000
H	-1.98350000	8.00190000	-1.73000000
H	-7.95540000	-1.50880000	-3.32930000
H	-6.66230000	-2.34770000	-4.22220000
H	-7.28580000	-0.77930000	-4.79720000
Pd	-0.67680000	0.62850000	-0.29870000
P	-0.92580000	-1.58100000	0.78660000
C	0.46260000	-2.40600000	1.65770000
C	-1.43040000	-2.80850000	-0.49360000
C	-2.30170000	-1.74360000	2.00870000
C	0.90020000	-3.70140000	1.35560000
C	1.99270000	-4.25180000	2.02950000
C	2.66840000	-3.53340000	3.02480000
C	2.21200000	-2.24330000	3.33100000
C	1.13800000	-1.67920000	2.64990000
C	-2.09700000	-1.98490000	3.37240000

C	-3.17510000	-2.00270000	4.26480000
C	-4.48740000	-1.79330000	3.82590000
C	-4.68810000	-1.56450000	2.45440000
C	-3.61970000	-1.53240000	1.56620000
C	-2.24410000	-3.91400000	-0.20430000
C	-2.65630000	-4.78130000	-1.21800000
C	-2.26880000	-4.57680000	-2.55140000
C	-1.43470000	-3.48260000	-2.83170000
C	-1.02340000	-2.61190000	-1.82250000
C	3.88550000	-4.08930000	3.71660000
C	-5.65670000	-1.81120000	4.77470000
C	-2.76020000	-5.48010000	-3.65280000
H	0.40230000	-4.27900000	0.57550000
H	2.33560000	-5.25650000	1.76490000
H	2.73650000	-1.65150000	4.08290000
H	0.84860000	-0.64780000	2.85110000
H	-1.08980000	-2.15810000	3.75220000
H	-2.98600000	-2.18440000	5.32660000
H	-5.69940000	-1.38660000	2.08010000
H	-3.81540000	-1.33800000	0.51180000
H	-2.56980000	-4.09470000	0.82150000
H	-3.29620000	-5.63250000	-0.96900000

H	-1.11070000	-3.30350000	-3.86080000
H	-0.38690000	-1.75980000	-2.06170000
H	3.76080000	-4.09490000	4.81210000
H	4.76520000	-3.46200000	3.49690000
H	4.10670000	-5.11690000	3.39220000
H	-6.31230000	-2.67760000	4.58320000
H	-6.27580000	-0.90800000	4.65360000
H	-5.32810000	-1.86340000	5.82290000
H	-3.68510000	-5.07930000	-4.10350000
H	-2.99090000	-6.48780000	-3.27650000
H	-2.01880000	-5.57100000	-4.46090000
C	7.10000000	2.05850000	-0.38790000
C	6.64380000	1.61450000	-1.62980000
C	5.37760000	1.04810000	-1.71610000
C	4.54490000	0.89660000	-0.58990000
C	5.01700000	1.30830000	0.67600000
C	6.28910000	1.90980000	0.73360000
N	3.23510000	0.34780000	-0.81880000
C	1.98600000	1.72560000	1.61470000
O	2.93940000	0.81790000	2.00790000
C	4.28040000	1.23490000	2.01360000
O	0.81760000	1.40820000	1.76420000

C	4.97960000	0.33140000	3.05170000
F	4.24510000	0.26180000	4.17410000
F	6.17340000	0.85390000	3.40840000
F	5.20980000	-0.91240000	2.63150000
C	4.11510000	-1.95890000	-2.08530000
C	3.54190000	-2.10800000	-3.35190000
C	4.34880000	-2.50290000	-4.41810000
C	5.71950000	-2.75770000	-4.23830000
C	6.26360000	-2.61150000	-2.95150000
C	5.47250000	-2.21530000	-1.87390000
C	6.57430000	-3.21120000	-5.39190000
S	3.12820000	-1.34150000	-0.73260000
O	1.73020000	-1.67660000	-1.02890000
O	3.78430000	-1.75060000	0.50510000
H	8.08110000	2.52790000	-0.28920000
H	7.26300000	1.71190000	-2.52390000
H	5.01020000	0.70320000	-2.68270000
H	6.65240000	2.27930000	1.69200000
H	4.34090000	2.24430000	2.45050000
H	2.47550000	-1.92940000	-3.49410000
H	3.90580000	-2.62180000	-5.41010000
H	7.32630000	-2.80910000	-2.79110000

H	5.89490000	-2.10180000	-0.87520000
H	7.63090000	-2.94750000	-5.23890000
H	6.52170000	-4.30780000	-5.50490000
H	6.23610000	-2.76960000	-6.34100000

I

O	3.12860000	0.53620000	3.85550000
C	2.80410000	2.97740000	1.51610000
C	1.76250000	2.50020000	0.81000000
C	0.40700000	2.33000000	1.38890000
C	1.94350000	2.12340000	-0.65190000
H	2.70770000	3.20730000	2.57960000
H	3.78630000	3.12770000	1.06060000
H	-0.30010000	2.98500000	0.87140000
H	0.38560000	2.55820000	2.46400000
H	0.96860000	1.98760000	-1.12890000
H	2.48060000	2.91700000	-1.19520000
P	-2.00930000	1.08760000	0.02460000
C	-3.17930000	1.98270000	1.11350000
C	-3.04090000	-0.15860000	-0.84900000
C	-1.65800000	2.32600000	-1.30050000
C	-4.25560000	2.72330000	0.58940000
C	-5.16260000	3.34890000	1.44030000
C	-5.02600000	3.26440000	2.83860000
C	-3.94010000	2.54390000	3.35070000
C	-3.02890000	1.91090000	2.50280000
C	-1.37940000	1.93300000	-2.61780000

C	-1.03050000	2.87610000	-3.58600000
C	-0.93880000	4.24140000	-3.27920000
C	-1.23530000	4.63330000	-1.96470000
C	-1.59640000	3.69820000	-0.99520000
C	-2.42310000	-1.04760000	-1.74550000
C	-3.17540000	-1.99250000	-2.43830000
C	-4.55710000	-2.11700000	-2.23450000
C	-5.16750000	-1.23260000	-1.33380000
C	-4.42660000	-0.26230000	-0.65560000
C	-6.03190000	3.91990000	3.74780000
C	-0.56920000	5.25750000	-4.32750000
C	-5.33820000	-3.20210000	-2.92570000
H	-4.38440000	2.81100000	-0.49120000
H	-5.99480000	3.91610000	1.01470000
H	-3.80340000	2.46590000	4.43170000
H	-2.19520000	1.34920000	2.92590000
H	-1.42200000	0.88420000	-2.90010000
H	-0.82580000	2.54060000	-4.60620000
H	-1.18800000	5.69110000	-1.69280000
H	-1.84400000	4.04980000	0.00660000
H	-1.34520000	-1.00990000	-1.88870000
H	-2.66960000	-2.67080000	-3.12790000

H	-6.24290000	-1.30580000	-1.15100000
H	-4.93640000	0.39480000	0.04710000
H	-6.21720000	4.96500000	3.45330000
H	-5.69680000	3.90960000	4.79470000
H	-7.00170000	3.39630000	3.69900000
H	-0.07730000	4.78540000	-5.19040000
H	0.10520000	6.02610000	-3.91980000
H	-1.46650000	5.78010000	-4.70110000
H	-5.04090000	-3.30160000	-3.98110000
H	-6.42130000	-3.01620000	-2.88400000
H	-5.14490000	-4.17610000	-2.44400000
Pd	-0.26650000	0.33210000	1.32540000
P	-1.11080000	-1.91310000	1.76730000
C	-0.06270000	-3.00270000	2.80950000
C	-1.50810000	-3.12460000	0.44920000
C	-2.60390000	-1.60200000	2.77760000
C	-0.60890000	-3.84550000	3.78750000
C	0.19470000	-4.78090000	4.44210000
C	1.55480000	-4.91330000	4.12620000
C	2.08680000	-4.07340000	3.13480000
C	1.29840000	-3.11970000	2.49120000
C	-2.41770000	-1.14370000	4.09540000

C	-3.49850000	-0.69240000	4.85030000
C	-4.79790000	-0.66240000	4.31750000
C	-4.97670000	-1.12520000	3.00740000
C	-3.90090000	-1.58690000	2.24670000
C	-2.60150000	-3.99970000	0.46830000
C	-2.77020000	-4.93760000	-0.55200000
C	-1.84410000	-5.04950000	-1.59970000
C	-0.72390000	-4.20350000	-1.58000000
C	-0.55940000	-3.24910000	-0.57860000
C	2.43130000	-5.90830000	4.84190000
C	-5.94990000	-0.10030000	5.10670000
C	-2.06720000	-6.01970000	-2.72950000
H	-1.66970000	-3.78350000	4.03640000
H	-0.24730000	-5.42750000	5.20530000
H	3.14110000	-4.15810000	2.86920000
H	1.74220000	-2.47270000	1.73320000
H	-1.41550000	-1.12460000	4.52870000
H	-3.32690000	-0.33890000	5.87050000
H	-5.97550000	-1.11410000	2.56260000
H	-4.08000000	-1.91530000	1.22630000
H	-3.32630000	-3.96400000	1.28180000
H	-3.63810000	-5.60240000	-0.52870000

H	0.02490000	-4.27820000	-2.37310000
H	0.30880000	-2.58950000	-0.60580000
H	3.02990000	-5.41110000	5.62470000
H	3.14150000	-6.38740000	4.15020000
H	1.83700000	-6.69490000	5.32990000
H	-6.89960000	-0.58860000	4.84170000
H	-6.06710000	0.97720000	4.89730000
H	-5.79140000	-0.20830000	6.18990000
H	-1.11780000	-6.32940000	-3.19110000
H	-2.68160000	-5.55630000	-3.52160000
H	-2.60130000	-6.92010000	-2.39060000
C	6.89490000	1.39850000	-0.62710000
C	6.15700000	1.83020000	-1.73170000
C	4.78500000	1.60790000	-1.75010000
C	4.12770000	0.93820000	-0.70080000
C	4.86850000	0.47300000	0.40330000
C	6.25090000	0.74460000	0.41920000
N	2.69760000	0.85810000	-0.79290000
C	2.38830000	0.14260000	2.96420000
O	2.93810000	-0.29230000	1.74550000
C	4.33130000	-0.24790000	1.63080000
O	1.12760000	0.04120000	2.98160000

C	4.84210000	-1.69430000	1.76560000
F	4.49690000	-2.18060000	2.97260000
F	6.18560000	-1.77610000	1.68740000
F	4.34320000	-2.52310000	0.84290000
C	2.63150000	-0.18390000	-3.34680000
C	2.01940000	0.78540000	-4.14900000
C	2.53120000	1.03070000	-5.42020000
C	3.64540000	0.32090000	-5.90640000
C	4.23290000	-0.64820000	-5.07900000
C	3.73570000	-0.90550000	-3.79980000
C	4.17440000	0.58990000	-7.29010000
S	2.05720000	-0.40670000	-1.67450000
O	0.59860000	-0.21640000	-1.68400000
O	2.63430000	-1.65780000	-1.17590000
H	7.96990000	1.58300000	-0.57060000
H	6.64110000	2.34850000	-2.56190000
H	4.18800000	1.96540000	-2.58970000
H	6.83540000	0.43800000	1.28650000
H	4.72990000	0.26530000	2.52080000
H	1.15740000	1.34050000	-3.77900000
H	2.05750000	1.78730000	-6.05110000
H	5.09880000	-1.20910000	-5.43860000

H	4.19710000	-1.65190000	-3.15270000
H	3.48140000	0.19970000	-8.05460000
H	4.27880000	1.67080000	-7.47280000
H	5.15230000	0.11410000	-7.44910000

TS7

O	0.73890000	-5.13320000	0.94030000
C	-0.58790000	-3.62790000	-1.79530000
C	-0.63180000	-2.34700000	-2.30650000
C	0.52650000	-1.48330000	-2.31630000
C	-1.99500000	-1.82190000	-2.65820000
H	0.36230000	-4.06440000	-1.48320000
H	-1.37850000	-4.34060000	-2.04210000
H	0.50140000	-0.68650000	-3.07930000
H	1.46570000	-2.03780000	-2.34240000
H	-1.93990000	-0.84980000	-3.16670000
H	-2.52900000	-2.51750000	-3.32270000
P	2.81560000	-0.48910000	-0.40060000
C	3.30790000	-0.16730000	1.33790000
C	3.87370000	0.59050000	-1.44460000
C	3.49000000	-2.16100000	-0.72040000
C	4.63180000	0.08400000	1.72210000
C	4.93750000	0.37240000	3.05250000
C	3.93620000	0.41580000	4.03420000
C	2.61840000	0.13170000	3.64570000
C	2.30620000	-0.15530000	2.31980000
C	3.79440000	-2.57520000	-2.02780000

C	4.17330000	-3.89450000	-2.28450000
C	4.25520000	-4.84120000	-1.25290000
C	3.96630000	-4.41470000	0.05410000
C	3.59290000	-3.09890000	0.32010000
C	3.28950000	1.68930000	-2.08920000
C	4.06370000	2.57280000	-2.84520000
C	5.44310000	2.37680000	-2.99440000
C	6.02090000	1.25560000	-2.37080000
C	5.25370000	0.37420000	-1.61180000
C	4.24640000	0.77240000	5.46310000
C	4.62960000	-6.27430000	-1.52710000
C	6.28920000	3.32130000	-3.80720000
H	5.43300000	0.08280000	0.98270000
H	5.97270000	0.58630000	3.33120000
H	1.81920000	0.15640000	4.39070000
H	1.27430000	-0.36000000	2.03200000
H	3.74590000	-1.86280000	-2.85380000
H	4.40680000	-4.19440000	-3.30950000
H	4.03120000	-5.12910000	0.87900000
H	3.37190000	-2.79690000	1.34400000
H	2.21690000	1.85700000	-1.99930000
H	3.57900000	3.42630000	-3.32600000

H	7.09240000	1.07040000	-2.48610000
H	5.73080000	-0.49780000	-1.16080000
H	3.94030000	-0.03310000	6.15040000
H	3.69440000	1.67800000	5.76310000
H	5.31910000	0.96130000	5.61230000
H	4.96310000	-6.41440000	-2.56530000
H	3.76870000	-6.94240000	-1.35580000
H	5.43570000	-6.61270000	-0.85660000
H	5.69430000	4.15570000	-4.20500000
H	6.75810000	2.79990000	-4.65800000
H	7.10730000	3.74190000	-3.20000000
Pd	0.59940000	-0.05550000	-0.71490000
P	0.30250000	2.19300000	0.44480000
C	-1.34980000	2.49370000	1.18130000
C	0.37680000	3.38730000	-0.95760000
C	1.45700000	2.92750000	1.66990000
C	-2.23620000	3.46770000	0.70230000
C	-3.49700000	3.62430000	1.28120000
C	-3.90650000	2.82710000	2.35910000
C	-3.01410000	1.85170000	2.83140000
C	-1.76130000	1.67820000	2.24740000
C	1.06100000	3.36430000	2.93990000

C	2.00780000	3.82480000	3.86150000
C	3.36990000	3.87360000	3.54240000
C	3.75800000	3.44790000	2.26050000
C	2.82470000	2.97820000	1.34420000
C	1.01810000	4.63020000	-0.86960000
C	1.12200000	5.45980000	-1.98970000
C	0.58490000	5.08210000	-3.22830000
C	-0.08130000	3.84670000	-3.30380000
C	-0.18190000	3.01030000	-2.19350000
C	-5.25370000	3.02110000	3.00370000
C	4.40030000	4.35670000	4.52860000
C	0.73500000	5.95440000	-4.44730000
H	-1.94720000	4.10240000	-0.13670000
H	-4.18030000	4.37750000	0.88050000
H	-3.31630000	1.19700000	3.65280000
H	-1.10420000	0.88550000	2.60980000
H	0.00830000	3.34200000	3.22340000
H	1.67510000	4.15230000	4.85030000
H	4.81520000	3.46580000	1.98410000
H	3.16470000	2.64330000	0.36390000
H	1.45180000	4.95450000	0.07700000
H	1.63390000	6.42160000	-1.89680000

H	-0.52120000	3.53040000	-4.25370000
H	-0.69590000	2.05250000	-2.28310000
H	-5.17950000	3.69610000	3.87420000
H	-5.66710000	2.06750000	3.36330000
H	-5.97400000	3.46470000	2.30150000
H	4.89690000	5.27350000	4.16900000
H	5.18960000	3.60160000	4.67460000
H	3.95240000	4.57620000	5.50860000
H	-0.18780000	5.96880000	-5.04760000
H	1.53930000	5.57680000	-5.10210000
H	0.98870000	6.98930000	-4.17500000
C	-5.98560000	-4.56740000	-1.16160000
C	-6.18580000	-3.36250000	-1.84110000
C	-5.14830000	-2.43680000	-1.88180000
C	-3.91830000	-2.67760000	-1.24060000
C	-3.71920000	-3.87200000	-0.51470000
C	-4.77120000	-4.80770000	-0.52260000
N	-2.90780000	-1.69060000	-1.48180000
C	0.65530000	-4.02320000	1.29570000
O	-1.35090000	-3.48240000	0.11170000
C	-2.44800000	-4.23970000	0.29230000
O	0.77560000	-2.95550000	1.74920000

C	-2.83130000	-4.26300000	1.79960000
F	-1.74630000	-4.45140000	2.57540000
F	-3.67880000	-5.28180000	2.10230000
F	-3.42900000	-3.14000000	2.22590000
C	-4.16850000	0.46780000	-0.38820000
C	-4.38170000	1.46070000	-1.34540000
C	-5.58250000	2.16740000	-1.32410000
C	-6.57360000	1.88830000	-0.36760000
C	-6.33090000	0.87470000	0.57300000
C	-5.12950000	0.16850000	0.57840000
C	-7.84990000	2.68570000	-0.32550000
S	-2.65610000	-0.46480000	-0.40900000
O	-1.63570000	0.38790000	-1.09410000
O	-2.41210000	-0.92140000	0.95510000
H	-6.77330000	-5.32420000	-1.13300000
H	-7.13180000	-3.15360000	-2.34550000
H	-5.26160000	-1.49750000	-2.42610000
H	-4.62730000	-5.75570000	-0.00250000
H	-2.27900000	-5.32880000	0.07660000
H	-3.60880000	1.68650000	-2.08060000
H	-5.75300000	2.95660000	-2.06050000
H	-7.09080000	0.64370000	1.32310000

H	-4.93050000	-0.60530000	1.32000000
H	-8.68910000	2.08400000	0.05340000
H	-7.74050000	3.55350000	0.34830000
H	-8.11710000	3.07520000	-1.31870000

J

O	1.06430000	-4.45070000	0.13020000
C	-0.77500000	-3.10400000	-2.20180000
C	-0.78860000	-1.70140000	-2.74450000
C	0.33170000	-0.97590000	-2.86710000
C	-2.13970000	-1.13800000	-3.09980000
H	0.25710000	-3.45720000	-2.06050000
H	-1.28320000	-3.79300000	-2.90040000
H	0.30470000	0.04830000	-3.24910000
H	1.30880000	-1.39120000	-2.61990000
H	-2.03910000	-0.11600000	-3.48860000
H	-2.61720000	-1.75060000	-3.88100000
P	2.99330000	-0.58800000	-0.03100000
C	3.74640000	-0.07240000	1.57750000
C	4.02800000	0.27550000	-1.29690000
C	3.62750000	-2.31850000	-0.18620000
C	5.08360000	0.31680000	1.72520000
C	5.57200000	0.72520000	2.96950000
C	4.74700000	0.74690000	4.10300000
C	3.40930000	0.34930000	3.94980000
C	2.91450000	-0.04500000	2.70890000
C	3.59530000	-2.95540000	-1.44020000

C	3.95310000	-4.29450000	-1.57430000
C	4.34080000	-5.05870000	-0.46040000
C	4.37540000	-4.42150000	0.78700000
C	4.02870000	-3.07430000	0.92550000
C	3.49470000	1.41950000	-1.90700000
C	4.22740000	2.14170000	-2.85150000
C	5.51620000	1.73720000	-3.22700000
C	6.04500000	0.58260000	-2.62260000
C	5.31700000	-0.13830000	-1.67560000
C	5.27220000	1.17230000	5.44960000
C	4.67170000	-6.52170000	-0.60270000
C	6.31210000	2.49870000	-4.25560000
H	5.75220000	0.32100000	0.86270000
H	6.61500000	1.04210000	3.05870000
H	2.73830000	0.37480000	4.81280000
H	1.86140000	-0.31330000	2.59540000
H	3.30030000	-2.39080000	-2.32840000
H	3.92640000	-4.76150000	-2.56310000
H	4.68340000	-4.98800000	1.67060000
H	4.07110000	-2.60780000	1.91140000
H	2.48830000	1.73440000	-1.63150000
H	3.78170000	3.03090000	-3.30610000

H	7.04700000	0.24320000	-2.90100000
H	5.75380000	-1.03570000	-1.23300000
H	5.45620000	0.29700000	6.09630000
H	4.54870000	1.81460000	5.97450000
H	6.22010000	1.72290000	5.35950000
H	3.75190000	-7.13250000	-0.59770000
H	5.30490000	-6.87580000	0.22440000
H	5.19170000	-6.72850000	-1.55090000
H	5.79770000	3.42130000	-4.56110000
H	6.47870000	1.88900000	-5.15970000
H	7.30670000	2.77270000	-3.86770000
Pd	0.84310000	0.18420000	-0.03590000
P	0.13530000	2.32220000	0.48260000
C	-1.53590000	2.76120000	1.12110000
C	0.38850000	3.48900000	-0.92450000
C	1.25320000	3.05880000	1.75790000
C	-2.30670000	3.82330000	0.62800000
C	-3.59340000	4.05470000	1.11820000
C	-4.14810000	3.24520000	2.12130000
C	-3.37220000	2.18320000	2.60890000
C	-2.09280000	1.93690000	2.11120000
C	0.81930000	3.53810000	3.00010000

C	1.73920000	4.01450000	3.94230000
C	3.11230000	4.04650000	3.66800000
C	3.54060000	3.56970000	2.41750000
C	2.63380000	3.07400000	1.48740000
C	0.84630000	4.80400000	-0.76110000
C	1.09790000	5.61470000	-1.87160000
C	0.90050000	5.14050000	-3.17690000
C	0.42420000	3.82760000	-3.33380000
C	0.17490000	3.01430000	-2.22930000
C	-5.52620000	3.51610000	2.66600000
C	4.10060000	4.59420000	4.66520000
C	1.21340000	5.99630000	-4.37740000
H	-1.90510000	4.46750000	-0.15630000
H	-4.18320000	4.87990000	0.70850000
H	-3.78790000	1.52130000	3.37330000
H	-1.52520000	1.07810000	2.47490000
H	-0.24430000	3.53900000	3.24380000
H	1.37570000	4.37310000	4.90980000
H	4.60720000	3.56040000	2.18130000
H	3.00210000	2.68210000	0.53850000
H	1.02040000	5.19780000	0.24210000
H	1.46010000	6.63560000	-1.72050000

H	0.25460000	3.43440000	-4.34050000
H	-0.19170000	1.99710000	-2.36250000
H	-5.49300000	4.27300000	3.46920000
H	-5.97490000	2.60520000	3.08770000
H	-6.19880000	3.89820000	1.88370000
H	4.28450000	5.66920000	4.49210000
H	5.07140000	4.08260000	4.58820000
H	3.73540000	4.48790000	5.69790000
H	0.44280000	5.89230000	-5.15720000
H	2.17390000	5.69910000	-4.83300000
H	1.29120000	7.05960000	-4.10700000
C	-6.14300000	-4.05460000	-2.03800000
C	-6.39480000	-2.73580000	-2.42500000
C	-5.36580000	-1.80210000	-2.35790000
C	-4.08960000	-2.14470000	-1.87740000
C	-3.84320000	-3.46440000	-1.44340000
C	-4.88080000	-4.40580000	-1.56570000
N	-3.09060000	-1.12840000	-1.97450000
C	0.87960000	-3.62340000	0.92590000
O	-1.42720000	-3.14430000	-0.92700000
C	-2.54670000	-3.96090000	-0.80380000
O	0.70340000	-2.81290000	1.74080000

C	-2.74800000	-4.18360000	0.70900000
F	-1.62530000	-4.64290000	1.28380000
F	-3.70180000	-5.10630000	0.93610000
F	-3.11040000	-3.07040000	1.35500000
C	-4.41650000	0.42350000	-0.19290000
C	-5.07310000	1.48500000	-0.81490000
C	-6.36240000	1.81380000	-0.39970000
C	-6.99900000	1.09780000	0.62710000
C	-6.30420000	0.04030000	1.23830000
C	-5.01310000	-0.30030000	0.84040000
C	-8.37820000	1.47960000	1.09300000
S	-2.78760000	-0.01500000	-0.74720000
O	-2.18870000	1.13150000	-1.44990000
O	-2.07800000	-0.62550000	0.38230000
H	-6.92590000	-4.81270000	-2.10940000
H	-7.37840000	-2.44240000	-2.79790000
H	-5.52380000	-0.77490000	-2.68790000
H	-4.69360000	-5.43930000	-1.27040000
H	-2.33980000	-4.97360000	-1.20220000
H	-4.57240000	2.04350000	-1.60580000
H	-6.88390000	2.64670000	-0.87760000
H	-6.78330000	-0.52460000	2.04170000

H	-4.47350000	-1.11810000	1.31590000
H	-8.95250000	0.59870000	1.41650000
H	-8.31600000	2.16390000	1.95670000
H	-8.94280000	1.99710000	0.30400000

K

C	-0.32930000	-3.47480000	-1.67450000
C	-1.03970000	-2.42630000	-2.48270000
C	-0.39120000	-1.64820000	-3.35490000
C	-2.51500000	-2.27390000	-2.21920000
H	0.71630000	-3.57280000	-1.99480000
H	-0.82280000	-4.45570000	-1.79840000
H	-0.91120000	-0.86400000	-3.91130000
H	0.67790000	-1.77140000	-3.53360000
H	-2.93060000	-1.46040000	-2.82820000
H	-3.04940000	-3.19880000	-2.49000000
P	2.47880000	-0.26860000	-0.90500000
C	2.79880000	-0.33390000	0.91450000
C	3.92120000	0.67850000	-1.57320000
C	2.93510000	-1.98310000	-1.42570000
C	4.06520000	-0.20180000	1.49650000
C	4.21130000	-0.20120000	2.88710000
C	3.10320000	-0.34310000	3.73370000
C	1.83910000	-0.49770000	3.14230000
C	1.68470000	-0.48280000	1.75870000
C	3.13140000	-2.25830000	-2.79250000
C	3.35110000	-3.55980000	-3.23760000

C	3.37080000	-4.64190000	-2.33810000
C	3.17870000	-4.36230000	-0.97870000
C	2.96840000	-3.05550000	-0.52610000
C	3.72280000	2.01300000	-1.95360000
C	4.77980000	2.79160000	-2.43140000
C	6.07020000	2.25830000	-2.55650000
C	6.26460000	0.91520000	-2.18730000
C	5.21180000	0.13650000	-1.70640000
C	3.24830000	-0.32440000	5.23340000
C	3.59090000	-6.04860000	-2.83280000
C	7.21420000	3.08220000	-3.08920000
H	4.94810000	-0.07500000	0.86800000
H	5.20700000	-0.07610000	3.32230000
H	0.95600000	-0.61870000	3.77500000
H	0.68650000	-0.57220000	1.32390000
H	3.11700000	-1.43860000	-3.51630000
H	3.50390000	-3.74540000	-4.30490000
H	3.18900000	-5.18180000	-0.25440000
H	2.81240000	-2.87630000	0.53630000
H	2.72170000	2.43820000	-1.87850000
H	4.58980000	3.83010000	-2.71710000
H	7.26090000	0.47290000	-2.27990000

H	5.39460000	-0.90600000	-1.43760000
H	2.92840000	-1.28210000	5.67730000
H	2.61820000	0.46150000	5.68020000
H	4.28890000	-0.14060000	5.53820000
H	2.81280000	-6.34350000	-3.55640000
H	3.57630000	-6.77340000	-2.00590000
H	4.55990000	-6.14350000	-3.35050000
H	6.93380000	4.14010000	-3.19590000
H	7.53720000	2.71810000	-4.07930000
H	8.09200000	3.02400000	-2.42550000
Pd	0.49580000	0.85060000	-1.07230000
P	0.05980000	2.97070000	-0.27050000
C	-1.63730000	3.61450000	0.03810000
C	0.81890000	4.29340000	-1.30470000
C	0.90550000	3.21940000	1.35340000
C	-2.15650000	4.76010000	-0.58220000
C	-3.49140000	5.13180000	-0.39020000
C	-4.34400000	4.38390000	0.43380000
C	-3.81330000	3.24730000	1.06560000
C	-2.49260000	2.85740000	0.85960000
C	0.26100000	3.62070000	2.53000000
C	0.96700000	3.70770000	3.73620000

C	2.33570000	3.41930000	3.80160000
C	2.98010000	3.03380000	2.61340000
C	2.27950000	2.92290000	1.41800000
C	1.41700000	5.44360000	-0.77170000
C	2.03040000	6.37870000	-1.60920000
C	2.06100000	6.19950000	-3.00080000
C	1.44380000	5.05380000	-3.53080000
C	0.83970000	4.11310000	-2.69730000
C	-5.79560000	4.74960000	0.60660000
C	3.10700000	3.52900000	5.09150000
C	2.76250000	7.18400000	-3.90080000
H	-1.51720000	5.36850000	-1.22460000
H	-3.87560000	6.02500000	-0.89150000
H	-4.45650000	2.64280000	1.70880000
H	-2.12010000	1.94720000	1.33380000
H	-0.80200000	3.86400000	2.51770000
H	0.43700000	4.00940000	4.64420000
H	4.04410000	2.78760000	2.63270000
H	2.80160000	2.58930000	0.52150000
H	1.41340000	5.60630000	0.30800000
H	2.49820000	7.26560000	-1.17250000
H	1.45100000	4.89030000	-4.61210000

H	0.39430000	3.20850000	-3.12130000
H	-5.98450000	5.80160000	0.34620000
H	-6.13300000	4.58170000	1.64120000
H	-6.43370000	4.12610000	-0.04350000
H	3.71100000	4.45280000	5.11580000
H	3.80480000	2.68590000	5.21040000
H	2.43720000	3.54790000	5.96390000
H	2.21090000	7.33260000	-4.84200000
H	3.76910000	6.82020000	-4.17080000
H	2.88580000	8.16180000	-3.41240000
C	-4.41160000	-5.25120000	1.45660000
C	-5.25210000	-4.30130000	0.87210000
C	-4.68940000	-3.25160000	0.15140000
C	-3.29620000	-3.10960000	0.02780000
C	-2.44040000	-4.05270000	0.63670000
C	-3.03010000	-5.12880000	1.32260000
N	-2.83270000	-2.03990000	-0.79990000
O	-0.33900000	-3.10640000	-0.28950000
C	-0.91080000	-4.01840000	0.59050000
C	-0.29990000	-3.73190000	1.97700000
F	1.03930000	-3.71010000	1.90990000
F	-0.62690000	-4.70830000	2.85090000

F	-0.70770000	-2.57770000	2.50560000
C	-4.31950000	0.04870000	0.19470000
C	-5.07220000	0.67130000	-0.80350000
C	-6.35740000	1.11520000	-0.50060000
C	-6.90130000	0.94900000	0.78530000
C	-6.12260000	0.30890000	1.76310000
C	-4.83270000	-0.14000000	1.47870000
C	-8.26790000	1.48750000	1.11370000
S	-2.66540000	-0.49970000	-0.17850000
O	-2.16230000	0.31490000	-1.29640000
O	-1.94940000	-0.56270000	1.10040000
H	-4.82980000	-6.09710000	2.00640000
H	-6.33720000	-4.38780000	0.95850000
H	-5.32480000	-2.51780000	-0.34530000
H	-2.38580000	-5.88800000	1.76760000
H	-0.56660000	-5.04590000	0.36070000
H	-4.64330000	0.83000000	-1.79340000
H	-6.94750000	1.61420000	-1.27320000
H	-6.52870000	0.16870000	2.76770000
H	-4.22120000	-0.61730000	2.24460000
H	-8.70810000	0.97460000	1.98080000
H	-8.20590000	2.56160000	1.36000000

H	-8.95540000	1.38960000	0.26020000

3a

C	-1.30680800	-2.61872000	-2.52347000
C	-0.79665500	-1.21085900	-2.67142900
C	0.46836100	-0.94910800	-3.01291000
C	-1.80681500	-0.11323600	-2.44067900
H	-0.53878000	-3.34502800	-2.83500700
H	-2.19664700	-2.77162600	-3.16037900
H	0.83368500	0.07790600	-3.10608800
H	1.18155500	-1.75334500	-3.21499900
H	-1.30720900	0.86744700	-2.42283700
H	-2.51587800	-0.08397300	-3.28483300
C	-6.45516800	-2.02579900	-1.55692100
C	-6.29091800	-0.64299900	-1.67630500
C	-5.01626900	-0.09529800	-1.55544300
C	-3.89929300	-0.90332300	-1.29258300
C	-4.05793700	-2.29790200	-1.16812600
C	-5.34672300	-2.83562000	-1.31800100
N	-2.62063100	-0.26998400	-1.23116000
O	-1.63271600	-2.85664400	-1.15577600
C	-2.93017300	-3.28579400	-0.88058400
C	-2.88447900	-3.72346800	0.59112700
F	-4.08952000	-4.15432700	1.00640600

F	-2.49985100	-2.73860800	1.40456800
F	-2.02323800	-4.74238200	0.74571200
C	-2.14009900	2.15284000	-0.06065100
C	-3.35194900	2.81709800	0.14641200
C	-3.42356300	4.18830100	-0.09919400
C	-2.30274300	4.90731400	-0.54699300
C	-1.09412100	4.21431400	-0.73121400
C	-1.00281400	2.84424600	-0.48844800
C	-2.38323800	6.38524000	-0.82438600
S	-2.06150300	0.38690700	0.20326100
O	-0.64514500	0.03990000	0.35156400
O	-3.04832800	0.03613800	1.22805700
H	-7.44468700	-2.47589000	-1.66111100
H	-7.14886400	0.00323400	-1.87341500
H	-4.85961200	0.97919400	-1.66383100
H	-5.48076100	-3.91670200	-1.24068800
H	-3.16440900	-4.21582800	-1.43522900
H	-4.22069900	2.26682500	0.51000100
H	-4.36735100	4.71316900	0.06712000
H	-0.20702100	4.75902300	-1.06435700
H	-0.05942500	2.31123400	-0.61191300
H	-1.60310800	6.93436800	-0.27351100

H	-2.22452100	6.59120200	-1.89598300
H	-3.36138000	6.79806100	-0.54059000

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