Supporting Information

Triton B-Promoted Regioselective Intramolecular Addition of Enolates to Tethered Ynamides for the Construction of 8-Membered *O*-Heterocycles.

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Contents

General remarks

All reactions were carried under argon atmosphere. DMF, acetone, THF, toluene, MeCN and acetic acid were used as received from Sigma Aldrich. CH_2Cl_2 was dried using a dry solvent station GT S100 system.

NMR Spectra (^{1}H, ^{13}C) were performed at 298 K. ^{1}H (500 MHz or 300 MHz), ^{13}C (125 MHz) were recorded using a Bruker AV-300 or AV-500 spectrometer with the solvent residual peak as internal standard (chloroform, δ = 7.26 ppm / δ = 77.16 ppm, benzene, δ = 7.16 ppm / δ = 128.06 ppm). ^{19}F NMR (282 MHz) were recorded using a Bruker AV-300 spectrometer without internal standard. Data are presented as follows: chemical shift (ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, sept = septet, m = multiplet, br = broad), coupling constant *J* (Hz) and integration.

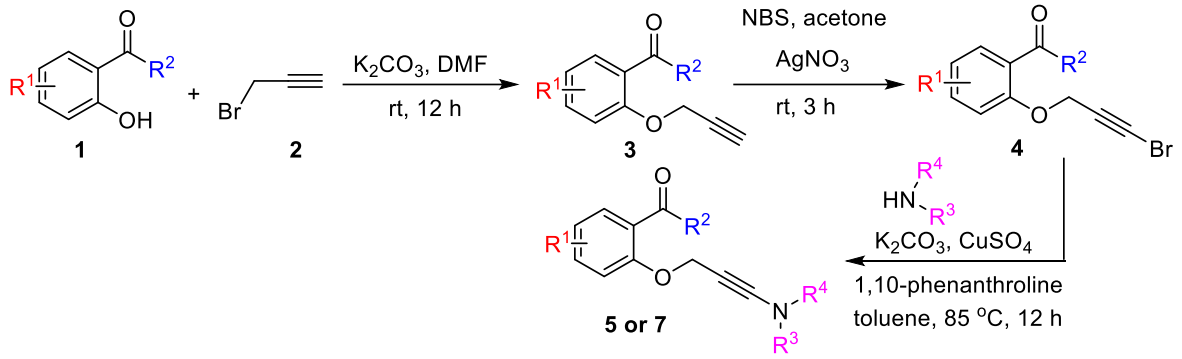
HRMS data were recorded on a micro TOF spectrometer equipped with an orthogonal electrospray (ESI) interface.

Thin layer chromatography was performed using Merck TLC silica gel 60 F_{254} aluminium sheets using petroleum ether/EtOAc or CH_2Cl_2/acetone as eluant and visualized using permanganate stain, ninhydrin stain, vanillin stain and/or UV light. Merck Geduran® 40-63 μm silica gel was used for column chromatography.

Infrared spectra were reported in frequency of absorption using Alpha Bruker Optics spectrometer.

Experimental procedure

1. Experimental procedure for compound **1** and compound **3**



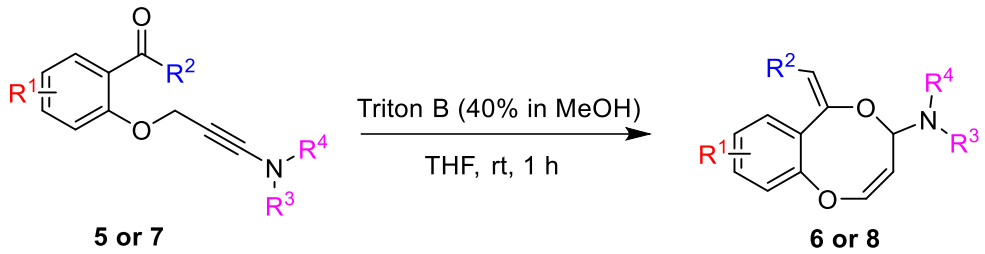
General procedure for compound 5 and compound 7:

Step 1: To a mixture of 2-hydroxy acetophenone (0.2 mmol, 1.0 equiv) and K_2CO_3 (2.0 equiv), in DMF was added a solution of a propargyl bromide (1.1 equiv, 1.0 M) in toluene. The reaction mixture was stirred for 12 h while being monitored with TLC analysis. Upon completion, the reaction mixture was diluted with EtOAc (10 mL) and filtered, and the filtrate was quenched with 1 (N) HCl (10 mL). The aqueous layer was extracted with EtOAc (3 x 10 mL). The organic layer was washed with brine solution (10 mL), dried over Na_2SO_4 and filtered. Solvent was evaporated to get analytically pure product and proceeds for the next step without further purification.

Step 2: Then alkyne acetophenone derivative (0.2 mmol, 1.0 equiv) was treated with NBS (1.2 equiv) and $AgNO_3$ (0.2 equiv) in acetone. The reaction mixture was stirred for 12 h while being monitored with TLC analysis. Upon completion, the reaction mixture was diluted with EtOAc (10 mL) and filtered, and the filtrate was quenched with water. The aqueous layer was extracted with EtOAc (3 x 10 mL). The organic layer was washed with a saturated $NaHCO_3$ solution (10 mL), dried (Na_2SO_4) and filtered. Solvent was evaporated to get analytically pure product and proceeds for the next step without further purification.

Step 3: To a mixture of bromo- alkyne (0.2 mmol, 1.1 equiv) in toluene, K_2CO_3 (2.5 equiv), amine derivative (1 equiv), Copper (II) sulfate ($CuSO_4$) (0.2 equiv) and 1, 10 - Phenanthroline (0.3 equiv) was added successively. The reaction mixture was reacted at 85 °C for 12 h while being monitored with TLC analysis. Upon completion, the reaction mixture was cooled at room temperature and diluted with EtOAc (10 mL) and filtered, and the filtrate was quenched with 1N HCl (1 mL). The aqueous layer was extracted with EtOAc (3 x 10 mL). The organic layer was washed with brine solution (10 mL), dried (Na_2SO_4) and filtered. After evaporation of solvent, the crude product was subjected to column chromatography on silica gel using a petroleum ether/EtOAc mixture to get the desired ynamides **5** and **7**. Ynamides (**5b**, **5d**, **5e**, **5g**, **5j** and **5k**), were not purified and we proceeded directly with the next step without any further purification.

2. Experimental procedure for compound **6** and compound **8**

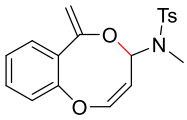


5 or 7 **6 or 8**

General procedure for 6 and 8: To a solution of ynamide **5** or **7** (0.2 mmol, 1.0 equiv) in anhydrous THF (2 mL) was added Triton B (2.5 equiv, 40% in MeOH) *via* syringe over a period of 5 minutes. The resulting solution was stirred at RT. After TLC indicated that the starting material was completely consumed, the solution was concentrated in vacuo, purified by column chromatography on silica gel using a mixture of petroleum ether/EtOAc as eluent to afford the desired product **6** or **8**.

Characterization data

Compound 6a: (Z)-*N*,4-dimethyl-*N*-(6-methylene-4*H*,6H-benzo[b][1,5]dioxocin-4-yl)benzenesulfonamide



$C_{19}H_{19}NO_4S$
MW: 357.42 g. mol^{-1}
Colorless liquid
64% (46 mg, 0.13 mmol)

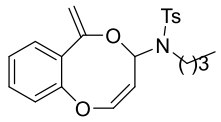
^{1}H NMR (500 MHz, C_6D_6): δ = 7.55 – 7.47 (m, 3H), 7.30 – 7.28 (m,1H), 6.92 – 6.85 (m, 2H), 6.74 – 6.66 (m, 1H), 6.62 (d, *J* = 8.0 Hz, 2H), 5.19 (d, *J* = 6.1 Hz, 1H), 4.78 – 4.74 (m, 2H), 4.70 (d, *J* = 2.0 Hz, 1H), 2.35 (s, 3H), 1.80 (s, 3H) ppm.

^{13}C NMR (126 MHz, C_6D_6): δ = 153.2, 152.7, 143.3, 135.3, 134.0, 129.9, 129.6, 128.0, 127.6 126.9, 124.3, 122.1, 118.6, 117.3, 104.1, 97.8, 87.4, 31.1, 20.7 ppm.

HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{19}H_{20}NO_4S$ 358.1108; Found 358.1103.
IR (neat): ν = 2995, 2940, 1736, 1448, 1372, 1235, 1165, 1043, 970 cm^{-1}

R_f: 0.50 (Petroleum ether / Ethyl acetate 4:1 *v/v*, UV)

Compound 6b: (Z)-*N*-butyl-4-methyl-*N*-(6-methylene-4H,6H-benzo[b][1,5]dioxocin-4-yl)benzenesulfonamide



$C_{22}H_{25}NO_4S$
MW: 399.51 g. mol^{-1}
Colorless liquid
60% (48 mg, 0.12mmol)

^{1}H NMR (500 MHz, C_6D_6): δ = 7.59 (d, *J* = 8.2 Hz, 2H), 7.51 (d, *J* = 14.4 Hz, 1H), 7.30 (d, *J* = 6.9 Hz, 1H), 6.93 – 6.86 (m, 2H), 6.71 (t, *J* = 7.4 Hz, 1H), 6.66 (d, *J* = 8.0 Hz, 2H), 5.22 (d, *J* = 6.2 Hz, 1H), 5.00 (dd, *J* = 14.4, 6.4 Hz, 1H), 4.73 (dd, *J* = 30.4, 1.8 Hz, 2H), 3.08 (d, *J* = 7.5 Hz, 2H), 1.83 (s, 3H), 1.44 – 1.38 (m, 2H), 1.04 – 0.91 (m, 2H), 0.64 (t, *J* = 7.4 Hz, 3H) ppm.

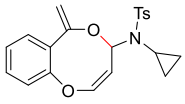
^{13}C NMR (126 MHz, C_6D_6): δ = 153.3, 152.7, 143.2, 136.7, 133.0, 129.9, 129.6 (×2), 126.8 (×2), 124.28, 122.1, 118.6, 117.3, 103.3, 98.2, 87.4, 45.0, 28.5, 20.7, 19.8, 13.3 ppm.

HRMS (ESI/Q-TOF) m/z: $[M+Na]^+$ calcd for $C_{22}H_{25}NNaO_4S$ 422.1396; Found 422.1403.

IR (neat): ν = 2930, 2842, 1736, 1349, 1372, 1235, 1161, 1043, 1055, 982 cm^{-1}

R_f: 0.50 (Petroleum ether / Ethyl acetate 5:1 *v/v*, UV)

Compound 6c: (Z)-*N*-cyclopropyl-4-methyl-*N*-(6-methylene-4H,6H-benzo[b][1,5]dioxocin-4-yl)benzenesulfonamide



$C_{21}H_{21}NO_4S$
MW: 383.46 g. mol^{-1}
Colourless liquid
61% (47 mg, 0.12 mmol)

^{1}H NMR (500 MHz, C_6D_6) δ = 7.65 (d, *J* = 8.0 Hz, 2H), 7.51 (d, *J* = 14.2 Hz, 1H), 7.32 – 7.30 (m, 1H), 6.94 – 6.85 (m, 2H), 6.73 – 6.69 (m, 3H), 5.36 (dd, *J* = 14.2, 6.2 Hz, 1H), 5.25 (d, *J* = 6.2 Hz, 1H), 4.74 (dd, *J* = 29.5, 2.0 Hz, 2H), 1.85 (s, 3H), 1.35 – 1.33 (m, 1H), 0.87 - 0.86 (m, 2H), 0.28 – 0.26 (m, 2H) ppm.

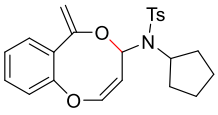
^{13}C NMR (126 MHz, C_6D_6) δ = 153.2, 152.7, 143.4, 135.3, 135.1, 129.9, 129.5, 128.0, 127.6, 127.4, 124.2, 122.1, 118.7, 117.3, 106.6, 97.9, 87.4, 26.7, 20.8, 7.7, 7.7 ppm.

HRMS (ESI/Q-TOF) m/z: $[M+Na]^+$ calcd for $C_{21}H_{21}NNaO_4S$ 406.1083; Found 406.1085.

IR (neat): ν = 2916, 2860, 1662, 1634, 1463, 1365, 1309, 1229, 1169, 1124, 1048, 586 cm^{-1}

R_f: 0.50 (Petroleum ether / Ethyl acetate 6:1 *v/v*, UV)

Compound 6d : (Z)-*N*-cyclopentyl-4-methyl-*N*-(6-methylene-4H,6H-benzo[b][1,5]dioxocin-4-yl)benzenesulfonamide



$C_{23}H_{25}NO_4S$
MW: 411.52 g. mol^{-1}
Colorless liquid
58% (48 mg, 0.17 mmol)

^{1}H NMR (300 MHz, C_6D_6): δ = 7.67 – 7.56 (m, 2H), 7.38 – 7.25 (m, 2H), 6.95 – 6.83 (m, 2H), 6.74 – 6.61 (m, 3H), 5.36 (dd, *J* = 14.7, 6.3 Hz, 1H), 5.23 – 5.21 (m, 1H), 4.74 (dd, *J* = 13.8, 1.9 Hz, 2H), 1.83 (s, 3H), 1.78 – 1.75 (m, 1H), 1.42 – 1.16 (m, 6H), 1.07 – 0.98 (m, 2H) ppm.

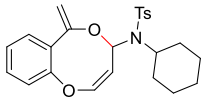
^{13}C NMR (126 MHz, C_6D_6): δ = 153.3, 152.8, 143.1, 137.4, 130.4, 129.9, 129.5, 128.0, 127.6, 127.0, 124.3, 122.1, 118.7, 117.4, 105.3, 98.8, 87.4, 58.2, 26.2, 24.3, 20.8 ppm.

HRMS (ESI/Q-TOF) m/z: $[M+Na]^+$ calcd for $C_{23}H_{25}NNaO_4S$ 434.1397; Found 434.1394.

IR (neat): ν = 2957, 1662, 1462, 1355, 1225, 1160, 985, 760, 666 cm^{-1}

R_f: 0.50 (Petroleum ether / Ethyl acetate 6:1 *v/v*, UV)

Compound 6e : (Z)-*N*-cyclohexyl-4-methyl-*N*-(6-methylene-4H,6H-benzo[b][1,5]dioxocin-4-yl)benzenesulfonamide



$C_{24}H_{27}NO_4S$
MW: 425.54 g. mol^{-1}
Colorless liquid
56% (48 mg, 0.11 mmol)

^{1}H NMR (300 MHz, $CDCl_3$) δ = 7.75 (d, *J* = 8.3 Hz, 2H), 7.37 (t, *J* = 10.7 Hz, 2H), 6.99 (d, *J* = 3.6 Hz, 2H), 6.81 – 6.72 (m, 3H), 5.72 (dd, *J* = 14.7, 6.3 Hz, 1H), 5.35 – 5.33 (m, 1H), 4.83 (dd, *J* = 12.5, 1.9 Hz, 2H), 4.07 – 3.90 (m, 1H), 1.89 (s, 3H), 1.80 – 1.72 (m, 2H), 1.58 – 1.55 (m, 2H), 1.47– 1.38 (m, 2H), 1.07 – 0.90 (m, 3H), 0.80 – 0.66 (m, 1H) ppm.

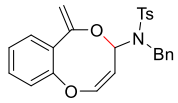
^{13}C NMR (126 MHz, $CDCl_3$) δ = 153.5, 152.9, 143.1, 138.3, 131.5, 123.0, 129.6, 128.1, 127.7, 127.0, 124.4, 122.2, 118.8, 117.4, 105.9, 99.0, 87.5, 58.8, 29.6, 29.5, 26.1, 24.9, 20.8 ppm.

HRMS (ESI/Q-TOF) m/z: $[M+Na]^+$ calcd for $C_{24}H_{27}NNaO_4S$ 448.1553; Found 448.1542.

IR (neat): ν = 2934, 2857, 1668, 1611, 1451, 1339,1303, 1159, 1089, 667 cm^{-1}

R_f: 0.50 (Petroleum ether / Ethyl acetate 7:1 *v/v*, UV)

Compound 6f: (Z)-*N*-benzyl-4-methyl-N-(6-methylene-4*H*,6*H*-benzo[b][1,5]dioxocin-4-yl)benzenesulfonamide



$C_{25}H_{23}NO_4S$
MW: 433.52 g. mol^{-1}
Colorless liquid
68% (59 mg, 0.14 mmol)

^{1}H NMR (500 MHz, C_6D_6): δ = 7.62 (d, *J* = 14.2 Hz, 1H), 7.57 (d, *J* = 8.4 Hz, 2H), 7.24 – 7.22 (m, 1H), 7.15 – 7.14 (m, 2H), 7.04 – 6.94 (m, 3H), 6.86 – 6.82 (m, 1H), 6.75 – 6.73 (m, 1H), 6.68 – 6.60 (m, 3H), 5.08 – 5.07 (m, 1H), 4.95 (dd, *J* = 14.3, 5.6 Hz, 1H), 4.64 (dd, *J* = 47.7, 1.9 Hz, 2H), 4.26 (q, *J* = 16.2 Hz, 2H), 1.84 (s, 3H) ppm.

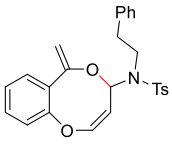
^{13}C NMR (126 MHz, C_6D_6): δ = 153.0, 152.5, 143.4, 136.5, 135.0, 132.5, 129.7, 129.6, 128.5, 128.0, 127.6, 127.5, 127.0, 126.9, 124.1, 122.0, 118.6, 117.3, 105.1, 97.4, 87.4, 49.3, 20.8 ppm.

HRMS (ESI/Q-TOF) m/z: $[M+Na]^+$ calcd for $C_{25}H_{23}NNaO_4S$ 456.1239; Found 456.1240.

IR (neat): ν = 2968, 2925, 1765, 1720, 1468, 1359, 1304, 1162, 1012, 975, 758 cm^{-1}

R_f: 0.50 (Petroleum ether / Ethyl acetate 4:1 *v/v*, UV)

Compound 6g: (Z)-4-methyl-*N*-(6-methylene-4H,6H-benzo[b][1,5]dioxocin-4-yl)-*N*-phenethylbenzenesulfonamide



$C_{26}H_{25}NO_4S$
MW: 447.55 g. mol^{-1}
Colorless liquid
67% (60 mg, 0.13 mmol)

^{1}H NMR (500 MHz, C_6D_6): δ = 7.57 – 7.52 (m, 3H), 7.31 (d, *J* = 7.8 Hz, 1H), 7.05 – 7.00 (m, 3H), 6.93 – 6.89 (m, 2H), 6.87 – 6.84 (m, 2H), 6.74 – 6.69 (m, 1H), 6.61 (d, *J* = 7.5 Hz, 2H), 5.25 (d, *J* = 6.2 Hz, 1H), 5.12 (dd, *J* = 14.4, 6.2 Hz, 1H), 4.82 – 4.70 (m, 2H), 3.35 – 3.32 (m, 2H), 2.84 – 2.76 (m, 2H), 1.80 (s, 3H) ppm.

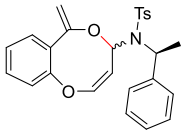
^{13}C NMR (126 MHz, C_6D_6): δ = 153.2, 152.7, 143.3, 137.8, 136.5, 132.6, 129.9, 129.6, 128.6, 128.5, 128.0, 127.6, 126.8, 126.5, 124.3, 122.2, 118.6, 117.4, 103.2, 98.1, 87.5, 46.9, 33.2, 20.7 ppm.

HRMS (ESI/Q-TOF) m/z: $[M+H]^+$ calcd for $C_{26}H_{26}NO_4S$ 448.1577; Found 448.1562.

IR (neat): ν = 3029, 2925, 1739, 1613, 1461, 1359, 1304, 1162, 961, 757 cm^{-1}

R_f: 0.50 (Petroleum ether / Ethyl acetate 5:1 *v/v*, UV)

Compound 6h : 4-methyl-*N*-((Z)-6-methylene-4H,6H-benzo[b][1,5]dioxocin-4-yl)-*N*-((S)-1-phenylethyl)benzenesulfonamide



$C_{26}H_{25}NO_4S$
MW: 447.55 g. mol^{-1}
Colorless liquid
65% (58 mg, 0.13 mmol)

^{1}H NMR (500 MHz, C_6D_6) : δ = 7.60 (d, *J* = 8.2 Hz, 2H), 7.36 – 7.32 (m, 1H), 7.21 – 7.19 (m, 3H), 7.06 – 7.01 (m, 2H), 6.99 – 6.97 (m, 1H), 6.84 – 6.77 (m, 2H), 6.72 – 6.70 (m, 1H), 6.64 (d, *J* = 7.9 Hz, 2H), 5.45 (q, *J* = 7.0 Hz, 1H), 5.12 – 5.05 (m, 1H), 5.05 – 4.99 (m, 1H), 4.68 – 6.66 (m, 1H), 4.62 – 4.55 (m, 1H), 1.83 (s, 3H), 1.20 (t, *J* = 7.0, 3H) ppm.

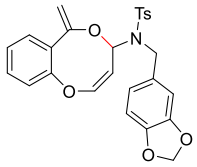
^{13}C NMR (126 MHz, C_6D_6): δ = 153.1, 153.1, 152.6, 152.5, 143.3, 143.3, 138.6, 138.6, 137.2, 137.2, 129.7, 129.6, 129.6, 129.6, 128.5, 128.0, 127.8, 127.6, 127.3, 127.1, 126.7, 126.7, 124.1, 124.1, 121.9, 121.91, 118.6, 118.6, 117.3, 117.3, 106.3, 106.2, 98.1, 98.1, 87.4, 87.3, 55.1, 55.0, 20.8, 14.5, 14.3 ppm.

HRMS (ESI/Q-TOF) m/z: $[M+Na]^+$ calcd for $C_{26}H_{25}NNaO_4S$ 470.1396; Found 470.1400.

IR (neat): ν = 2984, 1735, 1615, 1372, 1235, 1168, 1043, 936, 665 cm^{-1}

R_f: 0.50 (Petroleum ether / Ethyl acetate 5:1 *v/v*, UV)

Compound 6i : (Z)-N-(benzo[d][1,3]dioxol-5-ylmethyl)-4-methyl-N-(6-methylene-4H,6H-benzo[b][1,5]dioxocin-4-yl)benzenesulfonamide



$C_{26}H_{23}NO_6S$
MW: 477.53 g. mol^{-1}
Colorless liquid
62% (59 mg, 0.12 mmol)

^{1}H NMR (500 MHz, C_6D_6): δ = 7.59 – 7.55 (m, 3H), 7.24 – 7.23 (m, 1H), 6.85 – 6.82 (m, 2H), 6.76 - 6.74 (m, 1H), 6.68 – 6.64 (m, 3H), 6.55 – 6.47 (m, 2H), 5.21 (s, 2H), 5.14 – 5.08 (m, 1H), 5.03 (dd, *J* = 14.3, 5.8 Hz, 1H), 4.65 (dd, *J* = 49.5, 1.9 Hz, 2H), 4.23 – 4.09 (m, 2H), 1.85 (s, 3H) ppm.

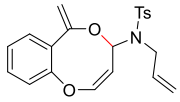
^{13}C NMR (126 MHz, C_6D_6): δ = 153.0, 152.5, 148.3, 147.3, 143.5, 136.4, 132.6, 129.8, 129.7, 128.7, 128.0, 127.8, 127.6, 127.0, 124.2, 122.1, 120.4, 118.5, 117.3, 108.2, 107.5, 105.1, 100.7, 97.6, 87.5, 49.2, 20.8 ppm.

HRMS (ESI/Q-TOF) m/z: $[M+Na]^+$ calcd for $C_{26}H_{23}NNaO_6S$ 500.1138; Found 500.1140.

IR (neat): ν = 3048, 2968, 3028, 2951, 2139, 1679, 1351, 1246, 1030, 886 cm^{-1}

R_f: 0.50 (Petroleum ether / Ethyl acetate 3:1 *v/v*, UV)

Compound 6j: ((Z)-*N*-allyl-4-methyl-*N*-(6-methylene-4H,6H-benzo[b][1,5]dioxocin-4-yl)benzenesulfonamide



$C_{21}H_{21}NO_4S$
MW: 383.46 g. mol^{-1}
Colorless liquid
59% (45 mg, 0.12 mmol)

^{1}H NMR (500 MHz, C_6D_6) δ = 7.56 – 7.51 (m, 3H), 7.29 – 7.27 (m, 1H), 6.91 – 6.85 (m, 2H), 6.71 – 6.67 (m, 1H), 6.63 (d, *J* = 8.0 Hz, 2H), 5.38 – 5.30 (m, 1H), 5.19 (dd, *J* = 6.2, 0.4 Hz, 1H), 5.02 (dd, *J* = 14.3, 6.2 Hz, 1H), 4.86 – 4.78 (m, 2H), 4.72 (dd, *J* = 28.2, 1.9 Hz, 2H), 3.69 (d, *J* = 5.1 Hz, 2H), 1.81 (s, 3H) ppm.

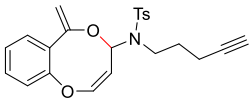
^{13}C NMR (126 MHz, C_6D_6) : δ = 153.2, 152.7, 143.3, 136.7, 132.5, 130.9, 129.8, 129.6, 128.0, 127.6, 126.0, 124.2, 122.1, 118.6, 117.8, 117.3, 104.3, 98.0, 87.4, 47.8, 20.7 ppm.

HRMS (ESI/Q-TOF) m/z: $[M+Na]^+$ calcd for $C_{21}H_{21}NNaO_4S$ 406.1083; Found 406.1061.

IR (neat): ν = 2922, 1745, 1669, 1614, 1449, 1363, 1305, 1163, 1088, 947, 547 cm^{-1}

R_f: 0.50 (Petroleum ether / Ethyl acetate 5:1 *v/v*, UV)

Compound 6k: (Z)-4-methyl-*N*-(6-methylene-4H,6H-benzo[b][1,5]dioxocin-4-yl)-*N*-(pent-4-yn-1-yl)benzenesulfonamide



$C_{23}H_{23}NO_4S$
MW: 409.50 g. mol^{-1}
Colorless liquid
63% (52 mg, 0.13 mmol)

^{1}H NMR (500 MHz, C_6D_6): δ = 7.58 (d, *J* = 8.2 Hz, 2H), 7.49 (d, *J* = 14.4 Hz, 1H), 7.31 – 7.27 (m, 1H), 6.93 – 6.85 (m, 2H), 6.73 – 6.68 (m, 1H), 6.64 (d, *J* = 8.1 Hz, 2H), 5.21 (d, *J* = 6.2 Hz, 1H), 5.08 (dd, *J* = 14.4, 6.2 Hz, 1H), 4.74 (dd, *J* = 27.9, 1.9 Hz, 2H), 3.19 (t, *J* = 7.0 Hz, 2H), 1.82 (s, 3H), 1.74 – 1.71(m, 2H), 1.66 – 1.64 (dd, *J* = 4.9, 2.3 Hz, 1H), 1.58 – 1.51 (m, 2H) ppm.

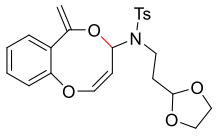
^{13}C NMR (126 MHz, C_6D_6): δ = 153.2, 152.7, 143.3, 136.5, 132.8, 129.9, 129.6, 128.0, 127.8, 127.4, 124.3, 122.1, 118.6, 117.4, 103.3, 98.1, 87.5, 82.5, 69.5, 44.2, 25.2, 20.8, 15.5 ppm.

HRMS (ESI/Q-TOF) m/z: $[M+Na]^+$ calcd for $C_{23}H_{23}NNaO_4S$ 432.1240; Found 432.1219.

IR (neat): ν = 3028, 2926, 1672, 1622, 1452, 1326, 1177, 1128, 1031, 701 cm^{-1}

R_f: 0.50 (Petroleum ether / Ethyl acetate 6:1 *v/v*, UV)

Compound 6l: (Z)-*N*-(2-(1,3-dioxolan-2-yl)ethyl)-4-methyl-*N*-(6-methylene-4H,6H-benzo[b][1,5]dioxocin-4-yl)benzenesulfonamide



$C_{23}H_{25}NO_6S$
MW: 443.51 g. mol^{-1}
Colorless liquid
62% (55 mg, 0.12 mmol)

^{1}H NMR (500 MHz, C_6D_6) δ = 7.60 – 7.57 (m, 2H), 7.55 (d, *J* = 14.1 Hz, 1H), 7.31 – 7.29 (m, 1H), 6.892 - 6.85 (m, 2H), 6.73 – 6.67 (m, 1H), 6.62 (d, *J* = 8.0 Hz, 2H), 5.30 – 5.23 (m, 2H), 4.72 (dd, *J* = 36.2, 1.9 Hz, 2H), 4.57 (t, *J* = 4.0 Hz, 1H), 3.53 (t, *J* = 4.0 Hz, 2H), 3.33 - 3.30 (m, 2H), 3.20 – 3.17 (m, 2H), 2.04 – 1.95 (m, 2H), 1.80 (s, 3H) ppm.

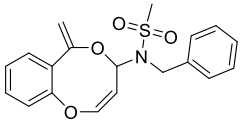
^{13}C NMR (126 MHz, C_6D_6): δ = 153.3, 152.7, 143.3, 136.5, 132.6, 129.8, 129.6, 128.0, 126.9, 124.2, 122.1, 118.6, 117.4, 103.3, 101.8, 98.1, 87.4, 64.5, 40.2, 30.3, 20.8 ppm.

HRMS (ESI/Q-TOF) m/z: $[M+Na]^+$ calcd for $C_{23}H_{25}NNaO_6S$ 466.1295; Found 466.1305.

IR (neat): ν = 2955, 2886, 1734, 1661, 1613, 1486, 1461, 1357, 1303, 1160, 945, 757 cm^{-1}

R_f: 0.50 (Petroleum ether / Ethyl acetate 5:1 *v/v*, UV)

<u>Compound 6m</u>: (Z)-*N*-benzyl-*N*-(6-methylene-4H,6H-benzo[b][1,5]dioxocin-4-yl)methanesulfonamide



$C_{19}H_{19}NO_4S$
MW: 357.42 g. mol^{-1}
Colorless liquid
64% (46 mg, 0.13 mmol)

^{1}H NMR (500 MHz, C_6D_6) δ = 7.28 – 7.20 (m, 2H), 7.13 (d, *J* = 8.5 Hz, 2H), 7.04 – 6.96 (m, 3H), 6.89 – 6.83 (m, 1H), 6.78 (d, *J* = 8.2 Hz, 1H), 6.67 (t, *J* = 8.2 Hz, 1H), 5.03 (d, *J* = 6.1 Hz, 1H), 5.00 – 4.94 (m, 1H), 4.67 (dd, *J* = 39.5, 1.9 Hz, 2H), 4.17 (dd, *J* = 18.2, 4.6 Hz, 2H), 1.98 (s, 3H) ppm.

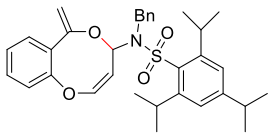
^{13}C NMR (126 MHz, C_6D_6) δ = 153.1, 152.6, 135.1, 132.4, 129.8, 128.6, 128.0, 126.9, 124.2, 122.1, 118.55, 117.3, 104.3, 97.6, 87.4, 48.9, 38.9 ppm.

HRMS (ESI/Q-TOF) m/z: $[M+H]^+$ calcd for $C_{19}H_{19}NNaO_4S$ 380.0927; Found 380.0940.

IR (neat): ν = 3029, 2954, 1666, 1636, 1462, 1354, 1313, 1225, 1155, 1052, 944 cm^{-1}

R_f: 0.50 (Petroleum ether / Ethyl acetate 6:1 *v/v*, UV)

Compound 6n : (Z)-*N*-benzyl-2,4,6-triisopropyl-*N*-(6-methylene-4H,6H-benzo[b][1,5]dioxocin-4-yl)benzenesulfonamide



$C_{33}H_{39}NO_4S$
MW: 545.74 g. mol^{-1}
Colorless liquid
66% (72 mg, 0.13 mmol)

^{1}H NMR (300 MHz, C_6D_6): δ = 7.62 (d, *J* = 13.9 Hz, 1H), 7.23 – 7.19 (m, 5H), 7.06 – 7.00 (m, 2H), 6.96 – 6.93 (m, 1H), 6.87 – 6.81 (m, 1H), 6.74 – 6.71 (m, 1H), 6.67 – 6.60 (m, 1H), 5.02 – 4.89 (m, 2H), 4.61 (dd, *J* = 30.2, 1.9 Hz, 2H), 4.44 – 4.36 (m, 4H), 2.60 – 2.55 (m, 1H), 1.28 (d, *J* = 6.7 Hz, 12H), 1.06 (d, *J* = 6.9 Hz, 6H) ppm.

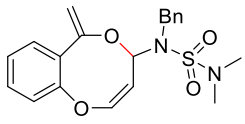
^{13}C NMR (126 MHz, C_6D_6): δ = 153.6, 153.1, 152.5, 151.6, 134.8, 131.8, 131.5, 129.7, 128.5, 128.0, 127.6, 127.4, 127.0, 124.2, 124.1, 121.9, 118.6, 117.3, 103.3, 97.5, 87.3, 48.6, 34.0, 29.6, 24.8, 23.2 ppm.

HRMS (ESI/Q-TOF) m/z: $[M+Na]^+$ calcd for $C_{33}H_{39}NNaO_4S$ 568.2492; Found 568.2486.

IR (neat): ν = 2959, 2929, 2869, 1737, 1662, 1600, 1461, 1369, 1311, 1225, 1154, 1045, 941 cm^{-1}

R_f: 0.50 (Petroleum ether / Ethyl acetate 8:1 *v/v*, UV)

Compound 6o: *(*Z)-*N*-benzyl-N,N-dimethyl-γ^2-azanesulfonamide-*N*-(6-methylene-4*H*,6*H*-benzo[b][1,5]dioxocin-4-yl)benzenesulfonamide



$C_{20}H_{22}N_2O_4S$
MW: 386.47 g.mol^{-1}
White solid
mp: 43-45°C
61% (47 mg, 0.12 mmol)

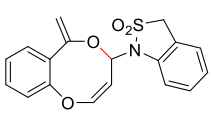
^{1}H NMR (500 MHz, C_6D_6): δ = 7.38 (d, *J* = 14.2 Hz, 1H), 7.26 – 7.23 (m, 1H), 7.19 (d, *J* = 7.4 Hz, 2H), 7.04 (t, *J* = 7.4 Hz, 2H), 6.98 (t, *J* = 7.4 Hz, 1H), 6.85 (t, *J* = 7.6 Hz, 1H), 6.77 (d, *J* = 8.2 Hz, 1H), 6.66 (t, *J* = 7.6 Hz, 1H), 5.05 (d, *J* = 6.0 Hz, 1H), 4.95 (dd, *J* = 14.3, 5.8 Hz, 1H), 4.66 (dd, *J* = 40.7, 1.9 Hz, 2H), 4.37 (d, *J* = 5.4 Hz, 2H), 2.20 (s, 6H) ppm.

^{13}C NMR (126 MHz, C_6D_6) δ = 153.2, 152.6, 135.6, 134.0, 129.8, 128.6, 128.0, 127.6, 127.37, 126.80, 124.2, 122.0, 118.6, 117.3, 102.5, 97.8, 87.3, 50.0, 37.2 ppm.

HRMS (ESI/Q-TOF) m/z: $[M+Na]^+$ calcd for $C_{20}H_{22}N_2NaO_4S$ 409.1192; Found 409.1204.
IR (neat): ν = 3048, 3068, 3028, 2951, 2139, 1679, 1351, 1246, 1020, 840 cm^{-1}

R_f: 0.50 (Petroleum ether / Ethyl acetate 4:1 *v/v*, UV)

Compound 6p: (Z)-1-(6-methylene-4H,6H-benzo[b][1,5]dioxocin-4-yl)-1,3-dihydrobenzo[c]isothiazole 2,2-dioxide



$C_{18}H_{15}NO_4S$
MW: 341.38 g. mol^{-1}

Colorless liquid
73% (50 mg, 0.15 mmol)

^{1}H NMR (300 MHz, C_6D_6) δ = 7.38 – 7.26 (m, 2H), 7.09 (s, 1H), 6.99 – 6.88 (m, 2H), 6.82 – 6.65 (m, 3H), 6.32 (d, *J* = 7.7 Hz, 1H), 5.14 (dd, *J* = 6.6, 0.5 Hz, 1H), 4.91 (dd, *J* = 14.0, 6.6 Hz, 1H), 4.78 (dd, *J* = 18.5, 2.0 Hz, 2H), 3.35 (s, 2H) ppm.

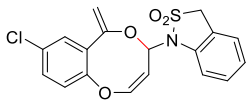
^{13}C NMR (126 MHz, C_6D_6): δ = 153.3, 152.7, 134.6, 132.0, 131.6, 129.9, 128.7, 128.0, 124.3, 124.2, 122.2, 121.0 118.6, 117.4, 104.4, 97.9, 87.5, 46.3 ppm.

HRMS (ESI/Q-TOF) m/z: $[M+Na]^+$ calcd for $C_{18}H_{15}NNaO_4S$ 364.0614; Found 364.0593.

IR (neat): ν = 2984, 1735, 1615, 1372, 1235, 1168, 1043, 936 cm^{-1}

R_f: 0.50 (Petroleum ether / Ethyl acetate 3:1 *v/v*, UV)

<u>Compound 8a</u> : (Z)-1-(8-chloro-6-methylene-4H,6H-benzo[b][1,5]dioxocin-4-yl)-1,3-dihydrobenzo[c]isothiazole 2,2-dioxide



$C_{18}H_{14}ClNO_4S$
MW: 375.82 g. mol^{-1}
Colorless liquid
81% (61 mg, 0.16 mmol)

^{1}H NMR (500 MHz, C_6D_6) δ = 7.44 (d, *J* = 2.4 Hz, 1H), 7.28 (d, *J* = 7.8 Hz, 1H), 7.09 (d, *J* = 14.0 Hz, 1H), 6.89 (dd, *J* = 8.7, 2.4 Hz, 1H), 6.79 (t, *J* = 7.6 Hz, 1H), 6.68 (t, *J* = 7.6 Hz, 1H), 6.60 (d, *J* = 8.7 Hz, 1H), 6.30 (d, *J* = 7.7 Hz, 1H), 4.97 (d, *J* = 6.6 Hz, 1H), 4.84 (dd, *J* = 14.0, 6.6 Hz, 1H), 4.61 (dd, *J* = 40.7, 2.4 Hz, 2H), 3.32 (s, 2H) ppm.

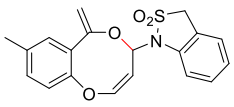
^{13}C NMR (126 MHz, C_6D_6): δ = 151.6, 151.4, 134.5, 132.1, 131.5, 129.9, 128.7, 128.2, 128.0, 124.2, 123.9, 121.0, 119.8, 118.9, 103.8, 98.0, 89.0, 46.2 ppm.

HRMS (ESI/Q-TOF) m/z: $[M+Na]^+$ calcd for $C_{18}H_{14}ClNNaO_4S$ 398.0224; Found 398.0230.

IR (neat): ν = 2927, 2853, 1672, 1625, 1474, 1405, 1314, 1270, 1234, 1174, 971 cm^{-1}

R_f: 0.50 (Petroleum ether / Ethyl acetate 3:1 *v/v*, UV)

Compound 8b : (Z)-1-(8-methyl-6-methylene-4H,6H-benzo[b][1,5]dioxocin-4-yl)-1,3-dihydrobenzo[c]isothiazole 2,2-dioxide



$C_{19}H_{17}NO_4S$
MW: 355.41 g. mol^{-1}
Colorless liquid
72% (51 mg, 0.14 mmol)

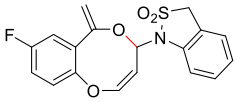
^{1}H NMR (500 MHz, C_6D_6): δ = 7.29 (dd, *J* = 14.6, 6.8 Hz, 2H), 7.13 (d, *J* = 14.2 Hz, 1H), 6.88 (d, *J* = 8.3 Hz, 1H), 6.80 – 6.76 (m, 2H), 6.67 (t, *J* = 7.3 Hz, 1H), 6.29 (d, *J* = 7.7 Hz, 1H), 5.19 (dd, *J* = 6.6, 0.5 Hz, 1H), 4.94 (dd, *J* = 14.0, 6.6 Hz, 1H), 4.81 (dd, *J* = 31.8, 1.9 Hz, 2H), 3.33 (s, 2H), 2.03 (s, 3H) ppm.

^{13}C NMR (126 MHz, C_6D_6): δ = 152.9, 151.3, 134.6, 132.0, 131.7, 131.3, 130.9, 128.7, 128.0, 124.4, 124.1, 121.0, 118.3, 117.3, 104.6, 97.9, 87.2, 46.3, 20.4 ppm

HRMS (ESI/Q-TOF) m/z: $[M+Na]^+$ calcd for $C_{19}H_{17}NNaO_4S$ 378.0770; Found 378.0775.
IR (neat): ν = 2928, 2363, 2323, 2045, 1979, 1671, 1623, 1456, 1326, 1177, 775 cm^{-1}

R_f: 0.50 (Petroleum ether / Ethyl acetate 3:1 *v/v*, UV)

Compound 8c : (Z)-1-(8-fluoro-6-methylene-4H,6H-benzo[b][1,5]dioxocin-4-yl)-1,3-dihydrobenzo[c]isothiazole 2,2-dioxide



$C_{18}H_{14}FNO_4S$
MW: 359.37 g. mol^{-1}
Colorless liquid
69% (50 mg, 0.14 mmol)

^{1}H NMR (500 MHz, C_6D_6): δ = 7.29 (d, *J* = 7.8 Hz, 1H), 7.10 (d, *J* = 14.0 Hz, 1H), 7.06 (dd, *J* = 9.0, 2.7 Hz, 1H), 6.80 - 6.77 (m, 1H), 6.70 – 6.60 (m, 3H), 6.30 (d, *J* = 7.7 Hz, 1H), 4.99 (d, *J* = 6.7 Hz, 1H), 4.87 (dd, *J* = 14.0, 6.7 Hz, 1H), 4.63 (dd, *J* = 47.2, 2.3 Hz, 2H), 3.32 (s, 2H) ppm.

^{13}C NMR (126 MHz, C_6D_6): δ = 158.9, 157.0, 151.7, 149.3, 134.50, 132.1, 131.6, 128.7, 128.2, 128.0, 124.1, 121.0, 119.5, 119.4, 118.8, 118.7, 117.1, 116.9, 110.3, 110.1, 104.0, 98.1, 88.8, 46.2 ppm.

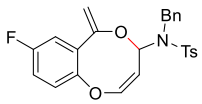
^{19}F NMR (282 MHz, C_6D_6) δ = -120.35 (s) ppm.

HRMS (ESI/Q-TOF) m/z: $[M+Na]^+$ calcd for $C_{18}H_{14}FNNaO_4S$ 382.0520; Found 382.0530.

IR (neat): ν = 2916, 2902, 2856, 1671, 1484, 1312, 1279, 1173, 1131, 1046, 980 cm^{-1}

R_f: 0.50 (Petroleum ether / Ethyl acetate 3:1 *v/v*, UV)

Compound 8d: (Z)-N-benzyl-N-(8-fluoro-6-methylene-4H,6H-benzo[b][1,5]dioxocin-4-yl)-4-methylbenzenesulfonamide



$C_{25}H_{22}FNO_4S$
MW: 451.51 g. mol^{-1}
Colorless liquid
70% (63 mg, 0.14 mmol)

^{1}H NMR (500 MHz, C_6D_6): δ = 7.63 – 7.57 (m, 1H), 7.57 (d, *J* = 8.3 Hz, 2H), 7.14 (d, *J* = 10.7 Hz, 2H), 7.03 – 6.99 (m, 2H), 6.98 – 6.92 (m, 2H), 6.66 (d, *J* = 8.0 Hz, 2H), 6.51 – 6.46 (m, 2H), 4.94 – 4.88 (m, 2H), 4.49 (dd, *J* = 25.5, 2.2 Hz, 2H), 4.25 (q, *J* = 16.2 Hz, 2H), 1.84 (s, 3H) ppm.

^{13}C NMR (126 MHz, C_6D_6): δ = 158.7, 156.8, 151.5, 151.4, 149.0, 143.5, 136.4, 134.9, 132.6, 129.67, 128.6, 128.0, 127.0, 126.9, 119.4, 119.3, 118.7, 118.6, 117.0, 116.8, 110.1, 109.9, 104.7, 97.6, 88.8, 49.3, 20.8ppm.

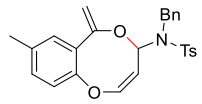
^{19}F NMR (282 MHz, $CDCl_3$) δ = -122.22 (s) ppm.

HRMS (ESI/Q-TOF) m/z: $[M+Na]^+$ calcd for $C_{25}H_{22}FNNaO_4S$ 474.1146; Found 474.1117.

IR (neat): ν = 3034, 2924, 1738, 1662, 1484, 1443, 1358, 1271, 1161, 1088, 1042, 940, 663 cm^{-1}

R_f: 0.50 (Petroleum ether / Ethyl acetate 5:1 *v/v*, UV)

Compound 8e : (Z)-*N*-benzyl-4-methyl-*N*-(8-methyl-6-methylene-4H,6H-benzo[b][1,5]dioxocin-4-yl)benzenesulfonamide



$C_{26}H_{25}NO_4S$
MW: 447.55 g. mol^{-1}
Colourless liquid
67% (60 mg, 0.13 mmol)

^{1}H NMR (300 MHz, C_6D_6) δ = 7.65 (d, *J* = 24.5 Hz, 1H), 7.57 (d, *J* = 12.5 Hz, 1H), 7.17 – 7.15(m, 4H), 7.05 – 6.95 (m, 3H), 6.72 – 6.64 (m, 4H), 5.15 (dd, *J* = 5.5, 0.8 Hz, 1H), 4.97 (dd, *J* = 14.3, 5.5 Hz, 1H), 4.66 (dd, *J* = 30.3, 1.9 Hz, 2H), 4.32 – 4.21 (m, 2H), 1.95 (s, 3H), 1.83 (s, 3H) ppm.

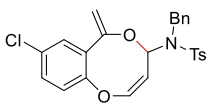
^{13}C NMR (126 MHz, C_6D_6) δ = 152.7, 151.1, 143.4, 136.4, 135.0, 132.5, 131.2, 130.8, 129.7, 128.6, 126.9, 124.3, 118.3, 117.2, 105.3, 97.5, 87.2, 49.4, 20.8, 20.4 ppm.

HRMS (ESI/Q-TOF) m/z: $[M+K]^+$ calcd for $C_{26}H_{25}KNO_4S$ 486.1136; Found 486.1142.

IR (neat): ν = 2948, 2826, 1620, 1420, 1401, 1351, 1246, 1160, 1024, 990, 882 cm^{-1}

R_f: 0.50 (Petroleum ether / Ethyl acetate 5:1 *v/v*, UV)

Compound 8f: (Z)-*N*-benzyl-*N*-(8-chloro-6-methylene-4H,6H-benzo[b][1,5]dioxocin-4-yl)-4-methylbenzenesulfonamide



$C_{25}H_{22}ClNO_4S$
MW: 467.96 g. mol^{-1}
Colorless liquid
66% (62 mg, 0.13 mmol)

^{1}H NMR (500 MHz, C_6D_6): δ = 7.59 (d, *J* = 14.2 Hz, 1H), 7.56 (d, *J* = 8.3 Hz, 2H), 7.30 (d, *J* = 2.4 Hz, 1H), 7.13 (d, *J* = 7.1 Hz, 2H), 7.04 – 6.93 (m, 3H), 6.76 (dd, *J* = 8.8, 2.4 Hz, 1H), 6.66 (d, *J* = 8.0 Hz, 2H), 6.43 (d, *J* = 8.8 Hz, 1H), 4.92 (d, *J* = 5.5 Hz, 1H), 4.86 (dd, *J* = 14.2, 5.5 Hz, 1H), 4.47 (dd, *J* = 23.1, 2.3 Hz, 2H), 4.24 (q, *J* = 16.2 Hz, 2H), 1.84 (s, 3H) ppm.

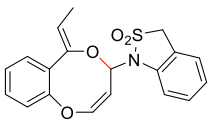
^{13}C NMR (126 MHz, C_6D_6): δ = 151.3, 151.0, 143.5, 136.4, 134.9, 132.7, 129.7, 129.7, 128.6, 128.0, 127.8, 127.6, 127.2, 126.9, 126.8, 123.8, 119.8, 118.8, 104.5, 97.5, 89.0, 49.3, 20.8 ppm.

HRMS (ESI/Q-TOF) m/z: $[M+Na]^+$ calcd for $C_{25}H_{22}ClNNaO_4S$ 490.2850; Found 490.0900.

IR (neat): ν = 3048, 2968, 1728, 1651, 1539, 1479, 1351, 1246, 1220, 1128, 1040, 778cm^{-1}

R_f: 0.50 (Petroleum ether / Ethyl acetate 5:1 *v/v*, UV)

Compound 8g: 1-((2Z,6Z)-6-ethylidene-4H,6H-benzo[b][1,5]dioxocin-4-yl)-1,3-dihydrobenzo[c]isothiazole 2,2-dioxide



$C_{19}H_{17}NO_4S$
MW: 355.41 g. mol^{-1}
Colorless liquid
75% (53 mg, 0.15 mmol)

^{1}H NMR (500 MHz, C_6D_6): δ = 7.34 – 7.29 (m, 2H), 7.13 (d, *J* = 14.2 Hz, 1H), 6.97 – 6.94 (m, 2H), 6.81 – 7.78 (m, 2H), 6.68 (t, *J* = 7.6 Hz, 1H), 6.31 (d, *J* = 7.7 Hz, 1H), 5.23 (q, *J* = 7.0 Hz, 1H), 5.17 (d, *J* = 6.6 Hz, 1H), 4.96 (dd, *J* = 14.0, 6.6 Hz, 1H), 3.38 – 3.24 (m, 2H), 1.85 (d, *J* = 7.0 Hz, 3H) ppm.

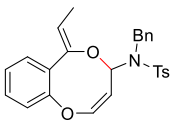
^{13}C NMR (126 MHz, C_6D_6) δ = 152.6, 146.3, 134.6, 132.0, 131.7, 128.7, 128.6, 128.0, 124.1, 123.0, 122.1, 121.0, 119.6, 117.5, 104.8, 98.5, 97.8, 46.2, 9.9 ppm
.

HRMS (ESI/Q-TOF) m/z: $[M+Na]^+$ calcd for $C_{19}H_{17}NNaO_4S$ 378.0770; Found 378.0767.

IR (neat): ν = 2919, 2858, 1732, 1664, 1462, 1309, 1268, 12241173, 1129, 1053, 755 cm^{-1}

R_f: 0.50 (Petroleum ether / Ethyl acetate 4:1 *v/v*, UV)

Compound 8h: *N*-benzyl-*N*-((2Z,6Z)-6-ethylidene-4H,6H-benzo[b][1,5]dioxocin-4-yl)-4-methylbenzenesulfonamide



$C_{26}H_{25}NO_4S$
MW: 447.55 g. mol^{-1}
Colorless liquid
69% (63 mg, 0.14 mmol)

^{1}H NMR (300 MHz, C_6D_6) δ = 7.65 - 5.57 (m, 3H), 7.23 (dd, *J* = 7.9, 1.4 Hz, 1H), 7.16 - 7.13 (m, 2H), 7.06 – 6.96 (m, 3H), 6.88 - 6.82 (m, 1H), 6.79 - 6.75 (m, 1H), 6.74 – 6.67 (m, 3H), 5.17 – 5.08 (m, 2H), 4.95 (dd, *J* = 14.3, 5.3 Hz, 1H), 4.36 – 4.16 (m, 2H), 1.87 (s, 3H), 1.71 (d, *J* = 7.0 Hz, 3H) ppm.

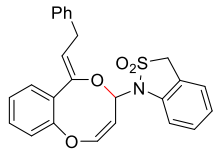
^{13}C NMR (126 MHz, C_6D_6) δ = 152.2, 145.9, 143.6, 136.3, 135.0, 132.2, 129.7, 128.5, 127.4, 127.0, 126.9, 122.9, 122.0, 119.5, 117.3, 105.5, 98.6, 97.0, 49.2, 20.8, 9.8 ppm.

HRMS (ESI/Q-TOF) m/z: $[M+K]^+$ calcd for $C_{26}H_{25}KNO_4S$ 486.1136; Found 486.1166.

IR (neat): ν = 3062, 2917, 1660, 1613, 1455, 1357, 1305, 1222, 1162, 1088, 733 cm^{-1}

R_f: 0.50 (Petroleum ether / Ethyl acetate 5:1 *v/v*, UV)

Compound 8i : (Z)-*N*-benzyl-4-methyl-*N*-(6-methylene-4*H*,6*H*-benzo[b][1,5]dioxocin-4-yl)benzenesulfonamide



$C_{25}H_{21}NO_4S$
MW: 431.51 g. mol^{-1}
Colorless liquid
61% (53 mg, 0.12 mmol)

^{1}H NMR (500 MHz, C_6D_6) δ = 7.30 (t, *J* = 7.1 Hz, 3H), 7.26 (d, *J* = 7.9 Hz, 1H), 7.21 (t, *J* = 7.7 Hz, 2H), 7.12 - 7.08 (m, 2H), 6.95 (d, *J* = 4.3 Hz, 2H), 6.79 (t, *J* = 7.1 Hz, 1H), 6.75 (dd, *J* = 8.4, 3.8 Hz, 1H), 6.68 (t, *J* = 7.6 Hz, 1H), 6.32 (d, *J* = 7.7 Hz, 1H), 5.45 (t, *J* = 7.6 Hz, 1H), 5.15 (d, *J* = 6.7 Hz, 1H), 4.95 (dd, *J* = 14.0, 6.7 Hz, 1H), 3.83 – 3.78 (m, 1H), 3.70 – 3.65 (m, 1H), 3.32 (s, 2H) ppm.

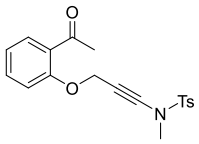
^{13}C NMR (126 MHz, C_6D_6): δ = 152.9, 146.1, 141.3, 134.6, 132.1, 131.7, 129.0, 128.7, 128.6, 128.5, 128.0, 127.8, 127.6, 126.0, 124.1, 123.3, 122.2, 121.0, 119.2, 117.4, 104.6, 103.0, 97.9, 46.3, 30.9 ppm.

HRMS (ESI/Q-TOF) m/z: $[M+Na]^+$ calcd for $C_{25}H_{21}NNaO_4S$ 454.1083; Found 454.1090.

IR (neat): ν = 3028, 2926, 1621, 1453, 1324, 1176, 1128, 1031, 755, 701 cm^{-1}

R_f: 0.50 (Petroleum ether / Ethyl acetate 4:1 *v/v*, UV)

Compound 5a: *N*-(3-(2-acetylphenoxy)prop-1-yn-1-yl)-*N*,4-dimethylbenzenesulfonamide



$C_{19}H_{19}NO_4S$
MW: 357.10 g. mol^{-1}
Colorless gum
64%

^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.78 – 7.76 (m, 1H), 7.63 (d, *J* = 8.3 Hz, 2H), 7.55 – 7.47 (m, 1H), 7.23 (d, *J* = 8.0 Hz, 2H), 7.09 - 7.06 m, 2H), 4.95 (s, 2H), 3.04 (s, 3H), 2.59 (s, 3H), 2.42 (s, 3H) ppm.

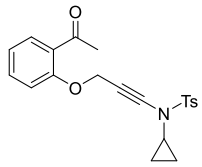
^{13}C NMR (126 MHz, $CDCl_3$) δ = 199.8, 156.7, 145.0, 133.5, 133.0, 130.5, 129.8, 128.9, 127.6, 121.2, 113.2, 82.9, 64.5, 56.5, 38.9, 32.0, 21.7 ppm

HRMS (ESI/Q-TOF) m/z: $[M+k]^+$ calcd for $C_{19}H_{19}KNO_4S$ 396.0666; Found 396.0664

IR (neat): ν = 3002, 2929, 2242, 1666, 1596, 1481, 1451, 1356, 1293, 1266, 1161, 1028, 760 cm^{-1}

R_f: 0.41 (Petroleum ether / Ethyl acetate 4:1 *v/v*, UV)

Compound 5c: *N*-(3-(2-acetylphenoxy)prop-1-yn-1-yl)-*N*-cyclopropyl-4-methylbenzenesulfonamide



$C_{21}H_{21}NO_4S$
MW: 383.46 g. mol^{-1}
Colorless gum
70%

^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.73 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.64 (d, *J* = 8.3 Hz, 2H), 7.49 – 7.44 (m, 1H), 7.21 (d, *J* = 8.1 Hz, 2H), 7.07 – 7.00 (m, 2H), 4. 93 (s, 2H), 2.71 – 2.65 (m, 1H), 2.57 (s, 3H), 2.39 (s, 3H), 0.77 – 0.68 (m, 4H) ppm.

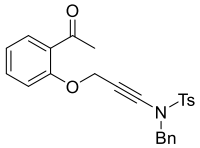
^{13}C NMR (126 MHz, $CDCl_3$) δ = 199.7, 156.7, 145.0, 133.5, 130.4, 129.8, 127.7, 121.2, 113.4, 81.0, 65.9, 56.5, 32.6, 32.0, 21.6, 6.5 ppm.

HRMS (ESI/Q-TOF) m/z: $[M+Na]^+$ calcd for $C_{21}H_{21}NNaO_4S$ 406.1083; Found 406.1067.

IR (neat): ν = 3100, 2950, 2263, 1672, 1490, 1479, 1419, 1298, 1220, 1170, 1020, 870, 806 cm^{-1}

R_f: 0.41 (Petroleum ether / Ethyl acetate 4:1 *v/v*, UV)

Compound 5f: *N*-(3-(2-acetylphenoxy)prop-1-yn-1-yl)-*N*-benzyl-4-methylbenzenesulfonamide



$C_{25}H_{23}NO_4S$
MW: 433.52 g. mol^{-1}
Colorless gum
87%

Colorless gum

^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.78 – 7.76 (m, 1H), 7.62 (d, *J* = 8.4 Hz, 2H), 7.46 – 7.42 (m, 2H), 7.34 – 7.26 (m, 3H), 7.22 (t, *J* = 7.0 Hz, 4H), 7.06 (t, *J* = 7.2 Hz, 1H), 6.92 (d, *J* = 8.4 Hz, 1H), 4.87 (s, 2H), 4.48 (s, 2H), 2.55 (s, 3H), 2.43 (s, 3H) ppm.

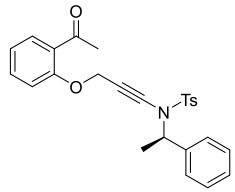
^{13}C NMR (126 MHz, $CDCl_3$) δ = 199.8, 156.7, 144.9, 134.4, 134.1, 133.5, 130.4, 129.8, 128.9, 128.6, 128.57, 128.4, 127.5, 121.2, 113.2, 81.4, 66.7, 56.4, 55.3, 32.0, 21.7 ppm.

HRMS (ESI/Q-TOF) m/z: $[M+Na]^+$ calcd for $C_{25}H_{23}NNaO_4S$ 456.1240; Found 456.1234

IR (neat): ν = 2999, 2929, 2234, 1670, 1595, 1478, 1453, 1357, 1290, 1162, 996, 757 cm^{-1}

R_f: 0.41 (Petroleum ether / Ethyl acetate 5:1 *v/v*, UV)

Compound 5h : *(R)-N*-(3-(2-acetylphenoxy)prop-1-yn-1-yl)-4-methyl-N-(1-phenylethyl)benzenesulfonamide



$C_{26}H_{25}NO_4S$
MW: 447.55 g. mol^{-1}
Colorless gum
70%

^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.78 – 7.77 (m, 1H), 7.63 (d, *J* = 8.2 Hz, 1H), 7.49 (d, *J* = 8.3 Hz, 2H), 7.45 (t, *J* = 9.0 Hz, 1H), 7.20 – 7.15 (m, 5H), 7.11 – 7.09 (m, 1H), 7.06 – 7.01(m, 2H), 5.11 (q, *J* = 7.0 Hz, 1H), 4.97 (s, 2H), 2.56 (s, 3H), 2.37 (s, 3H), 1.45 (d, *J* = 7.0 Hz, 3H) ppm.

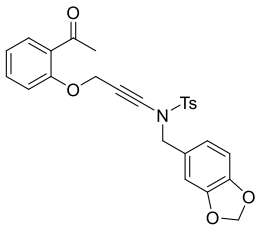
^{13}C NMR (126 MHz, $CDCl_3$) δ = 199.8, 156.8, 144.6, 139.4, 135.1, 133.5, 130.4, 129.5, 129.4, 128.9, 128.5, 128.4, 128.0, 127.4, 127.1, 126.7, 126.1, 121.2, 113.3, 79.3, 68.8, 58.7, 56.6, 32.0, 21.6, 19.5 ppm.

HRMS (ESI/Q-TOF) m/z: $[M+K]^+$ calcd for $C_{26}H_{25}NNaO_4S$ 470.1396; Found 470.1392.

IR (neat): ν = 3030, 2970, 2233, 1542, 1460, 1470, 1400, 1270, 1220, 1169, 975, 850, 772 cm^{-1}

R_f: 0.41 (Petroleum ether / Ethyl acetate 4:1 *v/v*, UV)

Compound 5i : *N*-(3-(2-acetylphenoxy)prop-1-yn-1-yl)-N-(benzo[d][1,3]dioxol-5-ylmethyl)-4-methylbenzenesulfonamide



$C_{26}H_{23}NO_6S$
MW: 477.53 g. mol^{-1}
Colorless gum
73%

^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.78 – 7.75 (m, 1H), 7.63 (d, *J* = 8.3 Hz, 2H), 7.48 – 7.45 (m, 1H), 7.22 (d, *J* = 8.0 Hz, 2H), 7.06 (t, *J* = 7.9 Hz, 1H), 6.95 (d, *J* = 8.3 Hz, 1H), 6.72 – 6.67 (m, 3H), 5.97 (s, 2H), 4.89 (s, 2H), 4.37 (s, 2H), 2.56 (s, 3H), 2.44 (s, 3H) ppm.

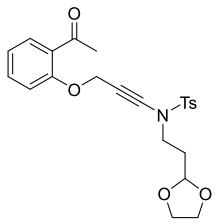
^{13}C NMR (126 MHz, $CDCl_3$) δ = 199.8, 156.7, 147.8, 147.8, 144.9, 134.5, 133.5, 130.5, 129.8, 128.9, 127.7, 127.5, 122.6, 121.2, 113.6, 109.0, 108.1, 101.2, 66.9, 56.5, 55.2, 32.0, 21.7 ppm

HRMS (ESI/Q-TOF) m/z: $[M+K]^+$ calcd for $C_{26}H_{23}KNO_6S$ 516.0878; Found 516.0879.

IR (neat): ν = 2991, 2921, 2246, 1678, 1596, 1496, 1442, 1367, 1292, 1167, 998, 767 cm^{-1}

R_f: 0.5 (Petroleum ether / Ethyl acetate 2:1 *v/v*, UV)

Compound 5l: *N*-(3-(2-acetylphenoxy)prop-1-yn-1-yl)-*N*-benzyl-4-methylbenzenesulfonamide



$C_{23}H_{25}NO_6S$
MW: 433.52 g. mol^{-1}
Colorless gum
65%

^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.78 – 7.76 (m, 1H), 7.64 (d, *J* = 8.3 Hz, 2H), 7.54 – 7.47 (m, 1H), 7.22 (d, *J* = 8.0 Hz, 2H), 7.10 – 7.04 (m, 2H), 4.97 (s, 2H), 4.86 (t, *J* = 4.4 Hz, 1H), 3.95 – 9.92 (m, 2H), 3.85 – 3.81 (m, 2H), 3.51 – 3.38 (m, 2H), 2.60 (s, 3H), 2.42 (s, 3H), 1.99 – 1.92 (m, 2H) ppm.

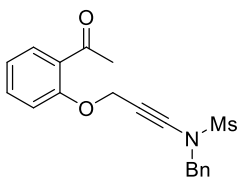
^{13}C NMR (126 MHz, $CDCl_3$) δ = 199.8, 156.7, 144.9, 134.2, 133.5, 130.48, 129.8, 128.9, 127.4, 121.2, 113.2, 101.6, 81.1, 66.4, 65.0, 56.5, 46.6, 32.0, 21.7 ppm

HRMS (ESI/Q-TOF) m/z: $[M+Na]^+$ calcd for $C_{23}H_{25}NNaO_6S$ 466.1294; Found 466.1287.

IR (neat): ν = 2954, 2886, 1672, 1595, 1485, 1450, 1293, 1163, 760 cm^{-1}

R_f: 0.41 (Petroleum ether / Ethyl acetate 3:1 *v/v*, UV)

Compound 5m: *N*-(3-(2-acetylphenoxy)prop-1-yn-1-yl)-*N*-benzylmethanesulfonamide



$C_{19}H_{19}NO_4S$

MW: 357.42 g. mol^{-1}
Colorless gum
68%

^{1}H NMR (300 MHz, $CDCl_3$) δ = 7.76 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.49 – 7.45 (m, 1H), 7.35 – 7.33 (m, 5H), 7.09 – 7.06 (m, 1H), 7.00 (d, *J* = 8.4 Hz, 1H), 4.95 (s, 2H), 4.61 (s, 2H), 2.80 (s, 3H), 2.62 (s, 3H) ppm.

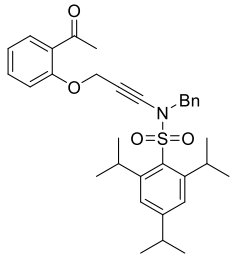
^{13}C NMR (126 MHz, $CDCl_3$) δ = 200.0, 156.8, 134.3, 133.6, 130.7, 129.5, 129.1, 129.0, 128.9, 121.7, 113.7, 81.4, 67.5, 57.0, 55.7, 39.3, 32.2 ppm

HRMS (ESI/Q-TOF) m/z: $[M+Na]^+$ calcd for $C_{19}H_{19}NNaO_4S$ 380.0927; Found 380.0941

IR (neat): ν = 3032, 2929, 2244, 1670, 1598, 1481, 1452, 1354, 1291, 1213, 1160, 956, 826, 757 cm^{-1}

R_f: 0.5 (Petroleum ether / Ethyl acetate 3:1 *v/v*, UV)

Compound 5n: *N*-(3-(2-acetylphenoxy)prop-1-yn-1-yl)-*N*-benzyl-2,4,6-triisopropylbenzenesulfonamide



$C_{33}H_{39}NO_4S$
MW: 545.26 g. mol^{-1}
Colorless gum
74%

^{1}H NMR (300 MHz, $CDCl_3$) δ = 7.71 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.33 – 7.28 (m, 4H), 7.26 – 7.24 (m, 2H), 7.20 (s, 2H), 7.02 – 6.97 (m, 1H), 6.78 (d, *J* = 8.4, 1H), 4.80 (s, 2H), 4.57 (s, 2H), 4.17 – 4.01 (m, 2H), 2.99 – 2.90 (m, 1H), 2.46 (s, 3H), 1.29 (d, *J* = 6.9 Hz, 6H), 1.19 (d, *J* = 6.8 Hz, 12H) ppm.

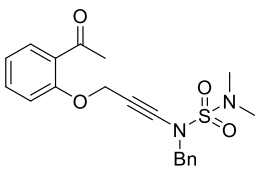
^{13}C NMR (126 MHz, $CDCl_3$) δ = 199.7, 156.8, 154.3, 152.0, 134.3, 133.4, 130.4, 130.2, 128.9, 128.7, 128.6, 128.4, 124.1, 121.0, 113.0, 81.0, 68.6, 56.6, 53.4, 34.2, 31.9, 29.8, 24.7, 23.6 ppm

HRMS (ESI/Q-TOF) m/z: $[M+Na]^+$ calcd for $C_{33}H_{39}NNaO_4S$ 568.2492; Found 568.2200

IR (neat): ν = 2960, 2929, 2241, 1673, 1597, 1482, 1452, 1359, 1291, 1213, 1165, 994, 797 cm^{-1}

R_f: 0.5 (Petroleum ether / Ethyl acetate 6:1 *v/v*, UV)

Compound 5o: *N*-(3-(2-acetylphenoxy)prop-1-yn-1-yl)-*N*- benzyl-*N*,*N*-dimethyl-γ^2-azanesulfonamide



$C_{20}H_{22}N_2O_4S$
MW: 386.47 g. mol^{-1}
Colorless gum
60%

^{1}H NMR (300 MHz, $CDCl_3$) δ = 7.74 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.50 – 7.35 (m, 6H), 7.07 - 7.02 (m, 1H), 6.94 (d, *J* = 7.8 Hz, 1H), 4.90 (s, 2H), 4.57 (s, 2H), 2.81 (s, 6H), 2.60 (s, 3H) ppm.

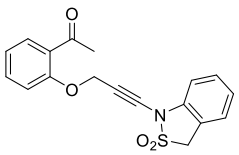
^{13}C NMR (126 MHz, $CDCl_3$) δ = 199.9, 156.8, 135.1, 133.4, 130.4, 128.8, 128.7, 128.6, 128.5, 127.99, 127.96, 121.4, 113.5, 82.5, 66.3, 56.9, 56.5, 38.6, 38.0, 32.0 ppm

HRMS (ESI/Q-TOF) m/z: $[M+Na]^+$ calcd for $C_{20}H_{22}N_2NaO_4S$ 409.1192; Found 409.1176.

IR (neat): ν = 3052, 2942, 2230, 1660, 1483, 1490, 1400, 1270, 1200, 1150, 997, 870, 706 cm^{-1}

R_f: 0.5 (Petroleum ether / Ethyl acetate 2:1 *v/v*, UV)

<u>Compound 5p</u>: 1-(2-((3-(2,2-dioxidobenzo[c]isothiazol-1(3H)-yl)prop-2-yn-1-yl)oxy)phenyl)ethan-1-one



$C_{18}H_{15}NO_4S$
Colorless gum
MW: 341.38 g. mol^{-1}
88%

^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.84 (d, *J* = 7.9 Hz, 1H), 7.74 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.69 (t, *J* = 7.6 Hz, 1H), 7.60 (t, *J* = 7.6 Hz, 1H), 7.53 – 7.47 (m, 1H), 7.42 (d, *J* = 7.8 Hz, 1H), 7.12 (d, *J* = 8.4 Hz, 1H), 7.05 (t, *J* = 7.9 Hz, 1H), 5.03 (s, 2H), 4.79 (s, 2H), 2.67 (s, 3H) ppm.

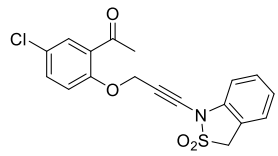
^{13}C NMR (126 MHz, $CDCl_3$) δ = 199.9, 156.8, 133.8, 133.5, 132.6, 131.4, 130.4, 129.8, 129.1, 124.7, 121.9, 121.4, 113.4, 76.9, 68.9, 56.9, 52.3, 32.0 ppm.

HRMS (ESI/Q-TOF) m/z: $[M+Na]^+$ calcd for $C_{18}H_{15}NNaO_4S$ 364.0614; Found 364.0606.

IR (neat): ν = 2924, 2824, 2244, 1673, 1493, 1327, 1217, 1179, 996 cm^{-1}

R_f: 0.5 (Petroleum ether / Ethyl acetate 1:1 *v/v*, UV)

Compound 7a : 1-(5-chloro-2-((3-(2,2-dioxidobenzo[c]isothiazol-1(3H)-yl)prop-2-yn-1-yl)oxy)phenyl)ethan-1-one



$C_{18}H_{14}ClNO_4S$
Colorless gum
MW: 375.82 g. mol^{-1}
86%

^{1}H NMR (300 MHz, $CDCl_3$) δ = 7.85 (d, *J* = 7.8 Hz, 1H), 7.74 – 7.67 (m, 2H), 7.61 (t, *J* = 7.6 Hz, 1H), 7.48 – 7.41 (m, 2H), 7.09 (d, *J* = 8.9 Hz, 1H), 5.03 (s, 2H), 4.80 (s, 2H), 2.65 (s, 3H) ppm.

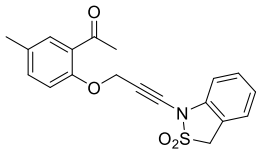
^{13}C NMR (126 MHz, $CDCl_3$): δ = 198.4, 155.3, 133.9, 133.0, 132.5, 131.3, 130.1, 130.1, 129.9, 126.8, 124.7, 121.9, 115.0, 77.4, 68.5, 57.3, 52.3, 31.9 ppm.

HRMS (ESI/Q-TOF) m/z: $[M+Na]^+$ calcd for $C_{18}H_{14}ClNNaO_4S$ 398.0224; Found 398.0245.

IR (neat): ν = 3028, 2970, 2359, 2243, 1738, 1681, 1593, 1480, 1365, 1217, 1169, 811 cm^{-1}

R_f: 0.5 (Petroleum ether / Ethyl acetate 2:1 *v/v*, UV)

Compound 7b: 1-(2-((3-(2,2-dioxidobenzo[c]isothiazol-1(3H)-yl)prop-2-yn-1-yl)oxy)-5-methylphenyl)ethan-1-one



$C_{19}H_{17}NO_4S$
MW: 355.41 g. mol^{-1}
Colorless gum
84%

^{1}H NMR (300 MHz, $CDCl_3$) δ = 7.81 (d, *J* = 7.8 Hz, 1H), 7.70 – 7.65 (m, 1H), 7.58 (t, *J* = 8.0 Hz, 1H), 7.52 (d, *J* = 2.6 Hz, 1H), 7.41 (d, *J* = 6.9 Hz, 1H), 7.30 – 7.27 (m, 1H), 7.01 (d, *J* = 8.4 Hz, 1H), 4.98 (s, 2H), 4.77 (s, 2H), 2.64 (s, 3H), 2.30 (s, 3H) ppm.

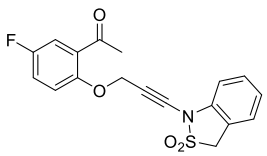
^{13}C NMR (126 MHz, $CDCl_3$) δ = 200.1, 154.8, 134.1, 133.8, 132.5, 131.4, 130.8, 130.6, 129.8, 128.7, 124.7, 121.8, 113.5, 76.7, 69.0, 57.0, 52.3, 32.0, 20.3 ppm

HRMS (ESI/Q-TOF) m/z: $[M+Na]^+$ calcd for $C_{19}H_{17}NNaO_4S$ 378.0770; Found 378.0787.

IR (neat): ν = 2924, 2869, 2245, 1672, 1493, 1326, 1217, 1178, 996, 898, 815, 759 cm^{-1}

R_f: 0.5 (Petroleum ether / Ethyl acetate 2:1 *v/v*, UV)

Compound 7c: 1-(2-((3-(2,2-dioxidobenzo[c]isothiazol-1(3H)-yl)prop-2-yn-1-yl)oxy)-5-fluorophenyl)ethan-1-one



$C_{18}H_{14}FNO_4S$

MW: 359.37 g. mol^{-1}
Colorless gum
75%

^{1}H NMR (300 MHz, $CDCl_3$) δ = 7.86 (d, *J* = 7.7 Hz, 1H), 7.74 – 7.69 (m, 1H), 7.62 (t, *J* = 7.6 Hz, 1H), 7.50 – 7.41 (m, 2H), 7.25 – 7. 18 (m, 1H), 7.13 - 7.09 (m, 1H), 5.03 (s, 2H), 4.80 (s, 2H), 2.68 (s, 3H) ppm.

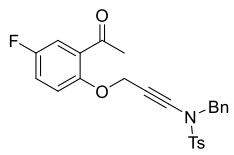
^{13}C NMR (126 MHz, $CDCl_3$): δ = 198.5, 198.4, 158.2, 156.3, 153.0, 153.0, 133.9, 132.6, 131.3, 130.2, 130.1, 129.9, 124.6, 122.0, 120.1, 119.9, 116.7, 116.5, 115.3, 115.3, 77.2, 68.7, 57.7, 52.2, 31.9 ppm.

HRMS (ESI/Q-TOF) m/z: $[M+Na]^+$ calcd for $C_{18}H_{14}FNNaO_4S$ 382.0519; Found 382.0500.

IR (neat): ν = 3050, 2930, 2243, 1655, 1488, 1470, 1417, 1360, 1269, 1169, 995, 861 cm^{-1}

R_f: 0.5 (Petroleum ether / Ethyl acetate 2:1 *v/v*, UV)

Compound 7d : *N*-(3-(2-acetyl-4-fluorophenoxy)prop-1-yn-1-yl)-*N*-benzyl-4-methylbenzenesulfonamide



$C_{25}H_{22}FNO_4S$
MW: 451.51 g. mol^{-1}
Colorless gum
73%

^{1}H NMR (300 MHz, $CDCl_3$) δ = 7.63 (d, *J* = 8.4 Hz, 2H), 7.47 – 7.43 (dd, *J* = 8.9, 3.3 Hz, 1H), 7.33 – 7.17 (m, 7H), 7.11 – 7.05 (m, 1H), 6.86 – 6.82 (m, 1H), 4.84 (s, 2H), 4.48 (s, 2H), 2.53 (s, 3H), 2.44 (s, 3H) ppm.

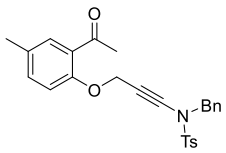
^{13}C NMR (126 MHz, $CDCl_3$): δ = 198.2, 158.0, 156.1, 152.9, 152.9, 145.0, 134.4, 134.0, 129.9, 129.9, 129.8, 128.6, 128.4, 127.5, 119.9, 119.8, 116.6, 116.4, 115.1, 115.0, 81.7, 66.5, 57.2, 55.2, 31.8, 21.7 ppm.

HRMS (ESI/Q-TOF) m/z: $[M+Na]^+$ calcd for $C_{25}H_{22}FNNaO_4S$ 474.1146; Found 474.1136.

IR (neat): ν = 2970, 2938, 2247, 1677, 1489, 1418, 1327, 1269, 1225, 1180, 995 cm^{-1}

R_f: 0.50 (Petroleum ether / Ethyl acetate 5:1 *v/v*, UV)

Compound 7e: *N*-(3-(2-acetyl-4-methylphenoxy)prop-1-yn-1-yl)-*N*-benzyl-4-methylbenzenesulfonamide



$C_{26}H_{25}NO_4S$
MW: 447.55 g. mol^{-1}
Colorless gum

80%

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.63 (d, *J* = 8.3 Hz, 2H), 7.56 (d, *J* = 2.2 Hz, 1H), 7.34 – 7.25 (m, 3H), 7.25 – 7.19 (m, 5H), 6.82 (d, *J* = 8.4 Hz, 1H), 4.83 (s, 2H), 4.48 (s, 2H), 2.53 (s, 3H), 2.43 (s, 3H), 2.34 (s, 3H) ppm.

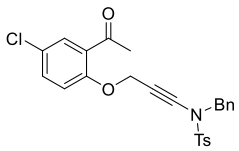
^{13}C NMR (126 MHz, $CDCl_3$): δ = 200.1, 154.8, 144.9, 134.5, 134.2, 134.1, 130.7, 130.6, 129.8, 128.7, 128.6, 128.5, 127.6, 113.3, 81.4, 66.9, 56.6, 55.4, 32.0, 21.8, 20.4 ppm.

HRMS (ESI/Q-TOF) m/z: $[M+Na]^+$ calcd for $C_{26}H_{25}NaNO_4S$ 470.1397; Found 470.1390.

IR (neat): ν = 2923, 2864, 2243, 1672, 1597, 1492, 1455, 1403, 1357, 1286, 1167,999, 811 cm^{-1}

R_f: 0.50 (Petroleum ether / Ethyl acetate 5:1 *v/v*, UV)

<u>Compound 7f</u>: *N*-(3-(2-acetyl-4-chlorophenoxy)prop-1-yn-1-yl)-*N*-benzyl-4-methylbenzenesulfonamide



$C_{25}H_{22}ClNO_4S$
MW: 467.96 g. mol^{-1}
Colorless gum
80%

^{1}H NMR (300 MHz, $CDCl_3$) δ = 7.69 (d, *J* = 2.7 Hz, 1H), 7.63 (d, *J* = 8.3 Hz, 2H), 7.32 – 7.24 (m, 5H), 7.22 – 7.16 (m, 3H), 6.81 (d, *J* = 8.9 Hz, 1H), 4.84 (s, 2H), 4.47 (s, 2H), 2.51 (s, 3H), 2.43 (s, 3H) ppm.

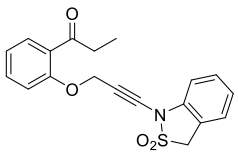
^{13}C NMR (126 MHz, $CDCl_3$): δ = 198.2, 155.2, 145.1, 134.4, 134.1, 133.0, 130.0, 123.0, 129.9, 128.6, 128.5, 127.5, 126.5, 115.0, 81.9, 66.5, 56.9, 55.3, 31.9, 21.7 ppm.

HRMS (ESI/Q-TOF) m/z: $[M+Na]^+$ calcd for $C_{25}H_{22}ClNNaO_4S$ 490.0850; Found 490.0837.

IR (neat): ν = 2922, 2244, 1738, 1676, 1593, 1479, 1401, 1361, 1269, 1216, 1168, 994 cm^{-1}

R_f: 0.5 (Petroleum ether / Ethyl acetate 5:1 *v/v*, UV)

Compound 7g: 1-(2-((3-(2, 2-dioxidobenzo[c]isothiazol-1(3H)-yl)prop-2-yn-1-yl)oxy)phenyl)propan-1-one



$C_{19}H_{17}NO_4S$
MW: 355.41 g. mol^{-1}
Colorless gum
79%

^{1}H NMR (300 MHz, $CDCl_3$) δ = 7.86 (d, *J* = 7.4 Hz, 1H), 7.74 – 7.71 (m, 2H), 7.62 (t, *J* = 7.6 Hz, 1H), 7.53 – 7.41 (m, 2H), 7.15 – 7.04 (m, 2H), 5.03 (s, 2H), 4.80 (s, 2H), 3.06 (q, *J* = 7.3 Hz, 2H), 1.20 (t, *J* = 7.3 Hz, 3H) ppm.

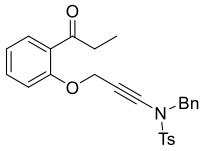
^{13}C NMR (126 MHz, $CDCl_3$): δ = 203.6, 156.3, 133.8, 133.0, 132.6, 131.4, 130.3, 129.8, 129.4, 124.6, 122.0, 121.5, 113.4, 68.9, 56.9, 52.3, 37.2, 8.5 ppm.

HRMS (ESI/Q-TOF) m/z: $[M+ Na]^+$ calcd for $C_{19}H_{17}NNaO_4S$ 378.0770; Found 378.0785.

IR (neat): ν = 3027, 2926, 2244, 1669, 1595, 1480, 1450, 1323, 1282, 1214, 1177, 1133, 1051 cm^{-1}

R_f: 0.5 (Petroleum ether / Ethyl acetate 3:1 *v/v*, UV)

Compound 7h: *N*-benzyl-4-methyl-*N*-(3-(2-propionylphenoxy)prop-1-yn-1-yl)benzenesulfonamide



$C_{26}H_{25}NO_4S$
MW: 447.525g.mol^{-1}
Colorless gum
82%

^{1}H NMR (300 MHz, $CDCl_3$) δ = 7.71 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.61 (d, *J* = 8.3 Hz, 2H), 7.44 – 7.38 (m, 1H), 7.32 – 7.26 (m, 3H), 7.23 – 7.18 (m, 4H), 7.08 – 7.02 (m, 1H), 6.92 (d, *J* = 8.4 Hz, 1H), 4.85 (s, 2H), 4.47 (s, 2H), 2.92 (q, *J* = 7.2 Hz, 2H), 2.42 (s, 3H), 1.13 (t, *J* = 7.2 Hz, 3H) ppm.

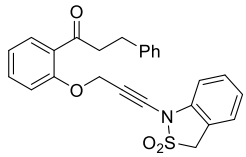
^{13}C NMR (126 MHz, $CDCl_3$) δ = 168.6, 152.7, 145.1, 136.3, 135.9, 130.9, 130.1, 129.5, 128.8, 128.5, 128.5, 128.1, 126.5, 125.1, 124.5, 124.3, 117.8, 117.7, 65.6, 49.8, 21.8, 21.7, 14.4 ppm.

HRMS (ESI/Q-TOF) m/z: $[M+Na]^+$ calcd for $C_{26}H_{25}NNaO_4S$ 470.1396; Found 470.1398.

IR (neat): ν = 2936, 2876, 2244, 1673, 1596, 1482, 1452, 1363, 1213, 1168, 1090 cm^{-1}

R_f: 0.5 (Petroleum ether / Ethyl acetate 5:1 *v/v*, UV)

Compound 7i: 1-(2-((3-(2, 2-dioxidobenzo[c]isothiazol-1(3H)-yl)prop-2-yn-1-yl)oxy)phenyl)-3-phenylpropan-1-one



$C_{25}H_{21}NO_4S$
MW: 431.51 g. mol^{-1}
Colorless gum
77%

^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.85 (d, *J* = 7.8 Hz, 1H), 7.75 – 7.67 (m, 2H), 7.61 (t, *J* = 7.1 Hz, 1H), 7.53 - 7.48 (m, 1H), 7.40 (d, *J* = 7.7 Hz, 1H), 7.30 – 7.23 (m, 4H), 7.21 – 7.15 (m, 1H), 7.14 – 7.03 (m, 2H), 5.00 (s, 2H), 4.67 (s, 2H), 3.45 – 3.34 (m, 2H), 3.10 – 3.00 (m, 2H) ppm.

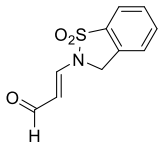
^{13}C NMR (126 MHz, $CDCl_3$) δ = 201.7, 156.5, 141.7, 133.8, 133.4, 132.6, 131.4, 130.5, 129.8, 129.0, 128.5, 128.4, 125.8, 124.6, 121.9, 121.6, 113.3, 77.0, 68.8, 57.0, 52.2, 45.5, 30.5 ppm.

HRMS (ESI/Q-TOF) m/z: $[M+K]^+$ calcd for $C_{25}H_{21}KNO_4S$ 470.0823; Found 470.0818.

IR (neat): ν = 3044, 2929, 2266, 1666, 1480, 1417, 1360, 1269, 1150, 977 cm^{-1}

R_f: 0.5 (Petroleum ether / Ethyl acetate 3:1 *v/v*, UV)

Compound 10: (E)-3-(1,1-dioxidobenzo[d]isothiazol-2(3H)-yl)acrylaldehyde



$C_{10}H_9NO_3S$
MW: 233.25 g. mol^{-1}
Colorless oil
88%

^{1}H NMR (300 MHz, $CDCl_3$) δ = 9.51 (d, *J* = 7.8 Hz, 1H), 7.92 (d, *J* = 7.5 Hz, 1H), 7.82 – 7.71 (m, 2H), 7.67 (dd, *J* = 14.3, 7.1 Hz, 1H), 7.57 (d, *J* = 7.8 Hz, 1H), 5.71 (dd, *J* = 13.8, 7.8 Hz, 1H), 4.76 (s, 2H) ppm.

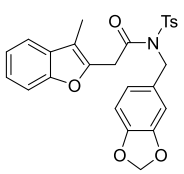
^{13}C NMR (126 MHz, $CDCl_3$) δ = 190.2, 143.7, 134.3, 133.2, 130.7, 130.1, 125.0, 121.9, 111.5, 47.6 ppm.

HRMS (ESI/Q-TOF) m/z: $[M+Na]^+$ calcd for $C_{10}H_9NNaO_3S$ 246.0195; Found 246.0201.

IR (neat): ν = 2955, 2922, 1670, 1625, 1457, 1329, 1290, 1176, 1123, 1032, 1016, 777, 595, 556 cm^{-1}

R_f: 0.5 (Petroleum ether / Ethyl acetate 1:1 *v/v*, UV)

Compound 11: *N*-(benzo[d][1,3]dioxol-5-ylmethyl)-2-(3-methylbenzofuran-2-yl)-*N*-tosylacetamide



$C_{26}H_{23}NO_6S$

MW: 477.53 g. mol^{-1}
Colorless gum
62%

^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.69 (d, *J* = 8.3 Hz, 2H), 7.46 – 7.40 (m, 1H), 7.36 7.29 (m, 3H), 7.27 – 7.19 (m, 2H), 6.98 – 6.90 (m, 2H), 6.78 (d, *J* = 7.9 Hz, 1H), 5.98 (s, 2H), 5.05 (s, 2H), 4.13 (s, 2H), 2.44 (s, 3H), 2.06 (s, 3H) ppm.

^{13}C NMR (126 MHz, $CDCl_3$) δ = 168.8, 154.1, 147.8, 147.2, 145.2, 145.1, 136.3, 130.1, 129.9 (x 2), 129.7, 127.6 (x 2), 124.0, 122.3, 122.0, 119.2, 113.5, 110.9, 108.9, 108.2, 101.1, 49.7, 35.0, 21.7, 7.9 ppm.

HRMS (ESI/Q-TOF) m/z: $[M+Na]^+$ calcd for $C_{26}H_{23}NNaO_6S$ 500.1138; Found 500.1147.

IR (neat): ν = 3248, 3068, 3028, 2951, 2139, 1679, 1351, 1246 cm^{-1}

R_f: 0.5 (Petroleum ether / Ethyl acetate 4:1 *v/v*, UV)


7.532
7.531
7.507
7.503
7.490
7.304
7.301
7.288
7.286
7.155
6.924
6.921
6.907
6.905
6.893
6.891
6.869
6.867
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6.851
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6.717
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6.690
6.687
6.630
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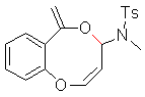
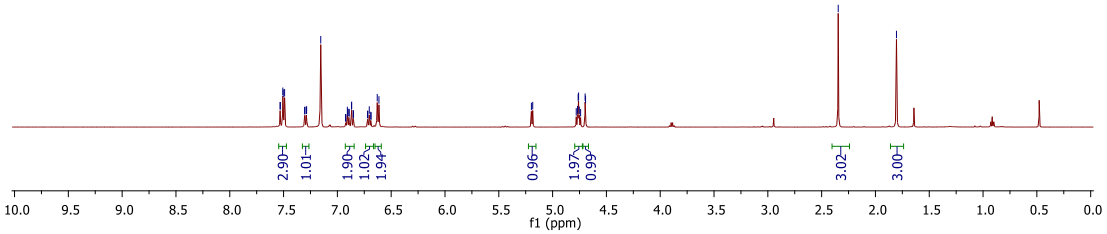

Ts
N
O
O

6a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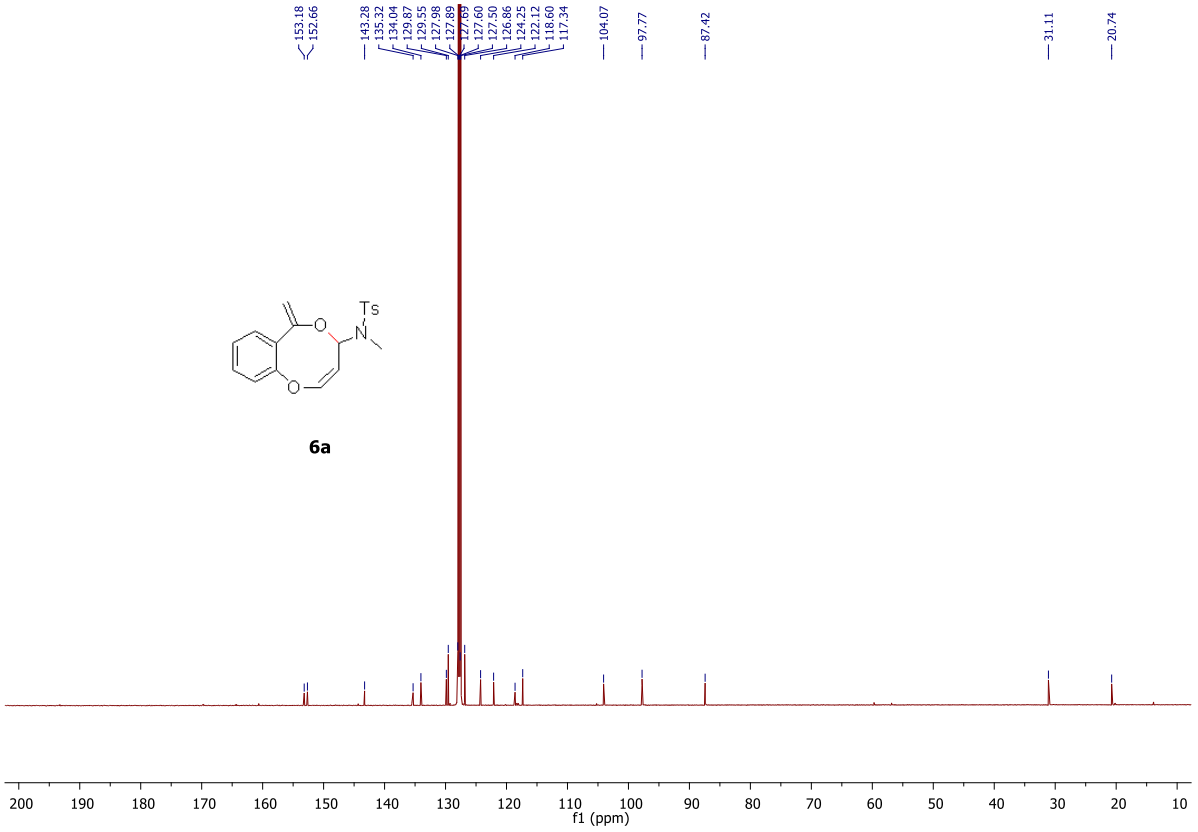
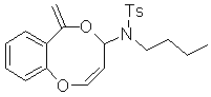
1.90
1.02
1.94
0.96
1.97
0.99
3.02
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


153.18
152.66
143.28
135.32
134.04
129.87
129.55
127.98
127.89
127.69
127.60
127.50
126.86
124.25
122.12
118.60
117.34
104.07
97.77
87.42
31.11
20.74
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

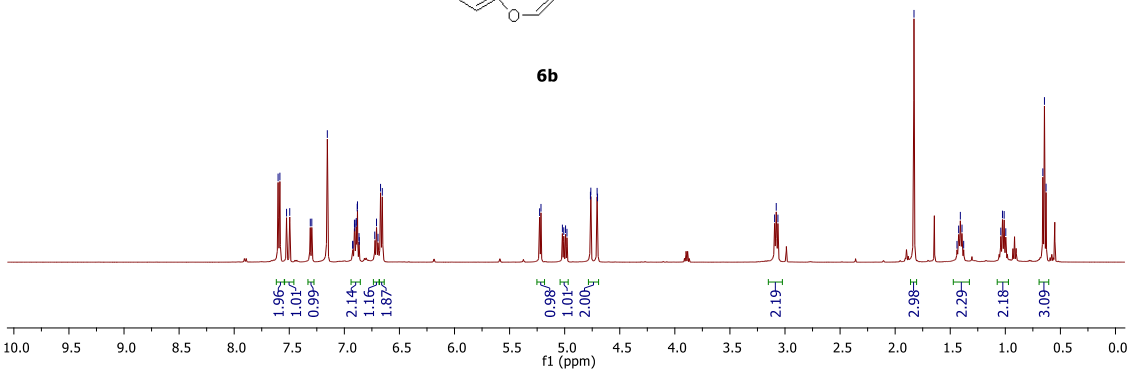
Ts
N
O
O

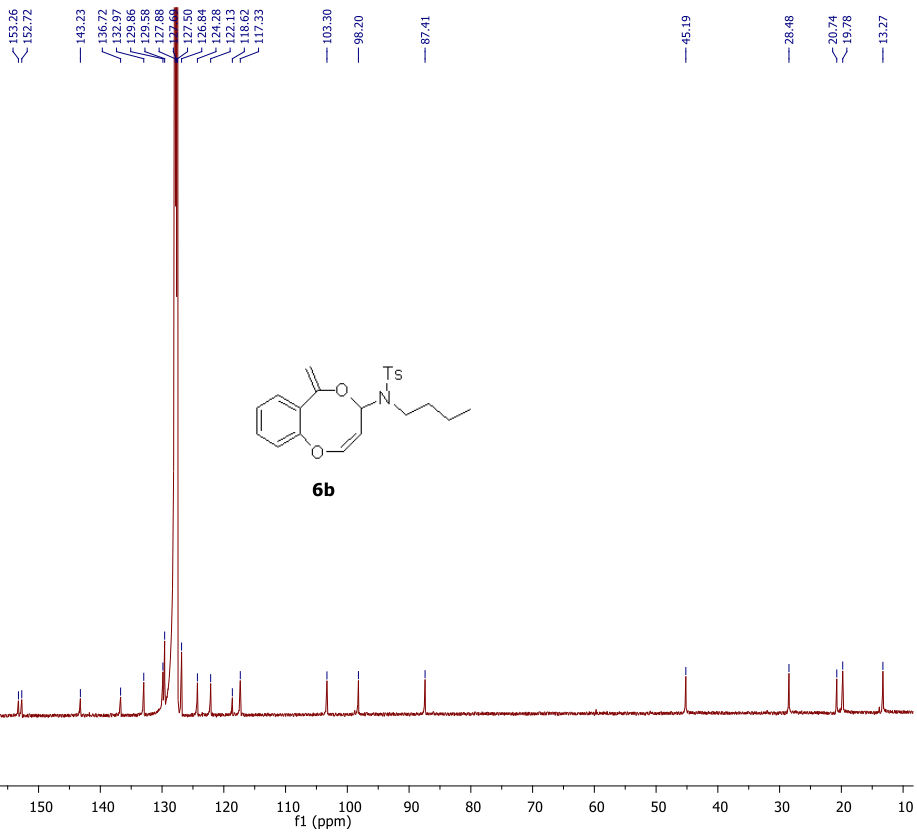
6a


7.602
7.585
7.525
7.496
7.309
7.295
7.154
6.925
6.922
6.908
6.906
6.895
6.892
6.883
6.881
6.867
6.865
6.724
6.708
6.695
6.671
6.655
5.227
5.215
5.211
5.008
4.992
4.979
4.766
4.762
4.705
4.702
3.094
3.079
3.064
1.829
1.424
1.408
1.393
1.378
1.041
1.026
1.011
0.659
0.645
0.630


Ts
N
O
O

6b


1.96
1.01
0.99
2.14
1.16
1.87
0.98
1.01
2.00
2.19
2.98
2.29
2.18
3.09
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

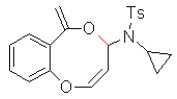

153.26
152.72
143.23
136.72
132.97
129.86
129.58
127.88
127.60
127.50
126.84
124.28
122.13
118.62
117.33
103.30
98.20
87.41
45.19
28.48
20.74
19.78
13.27

Ts
N
O
O

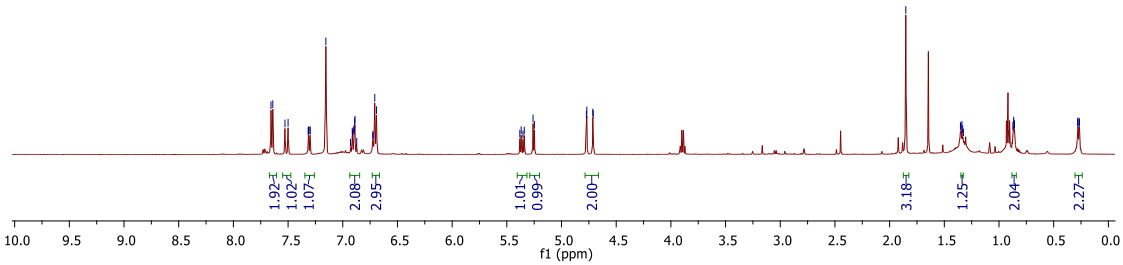
6b

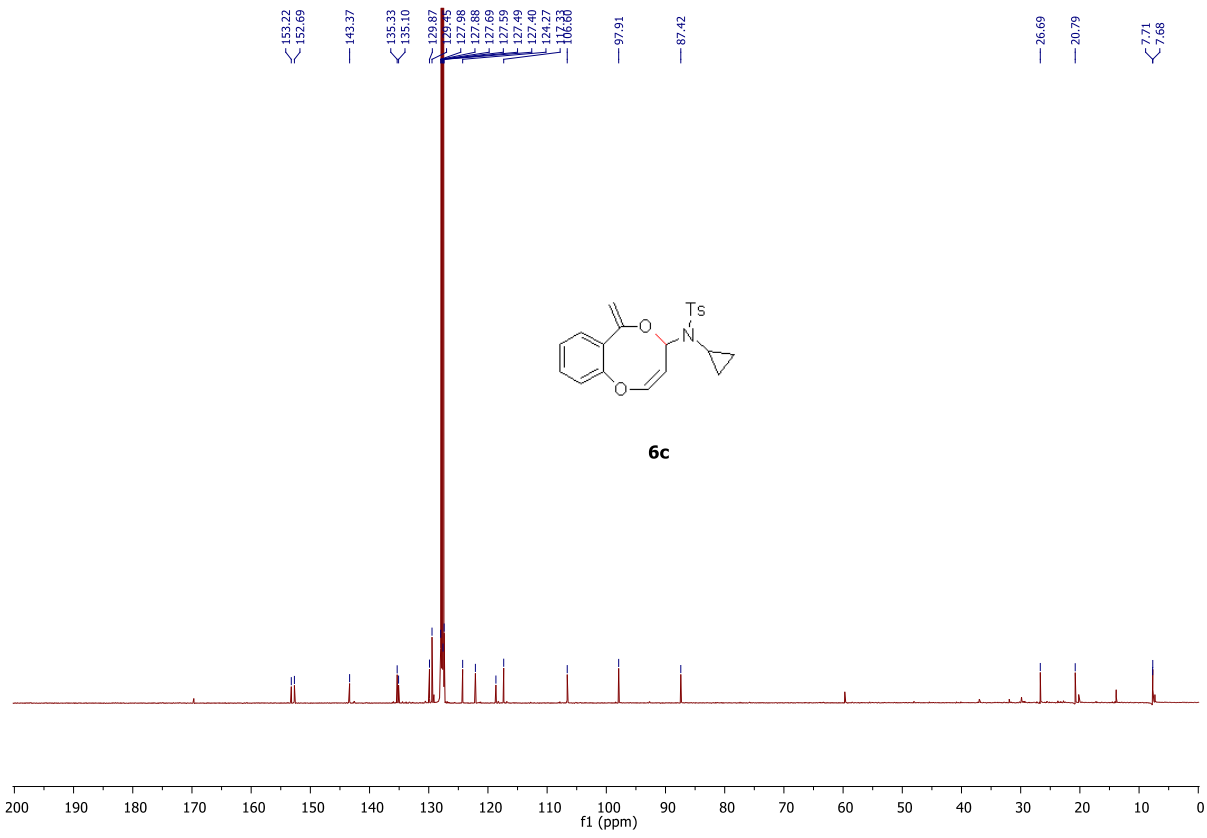
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.656
7.640
7.538
7.500
7.316
7.314
7.300
7.298
7.155
6.930
6.913
6.910
6.899
6.897
6.891
6.888
6.872
6.726
6.723
6.708
6.692
5.381
5.369
5.353
5.340
5.260
5.248
4.773
4.769
4.714
4.710
1.852
1.352
1.346
1.339
1.332
1.326
0.873
0.866
0.862
0.858
0.281
0.278
0.268
0.264


Ts
N
O
O

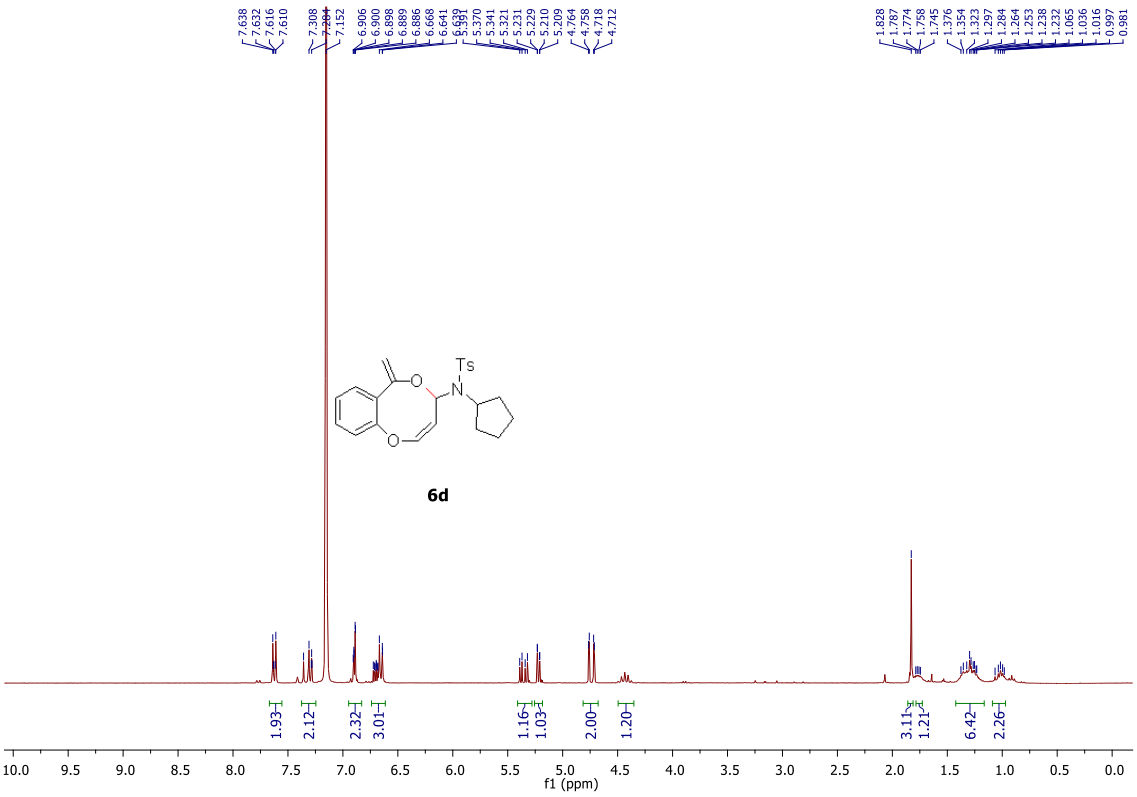
6c

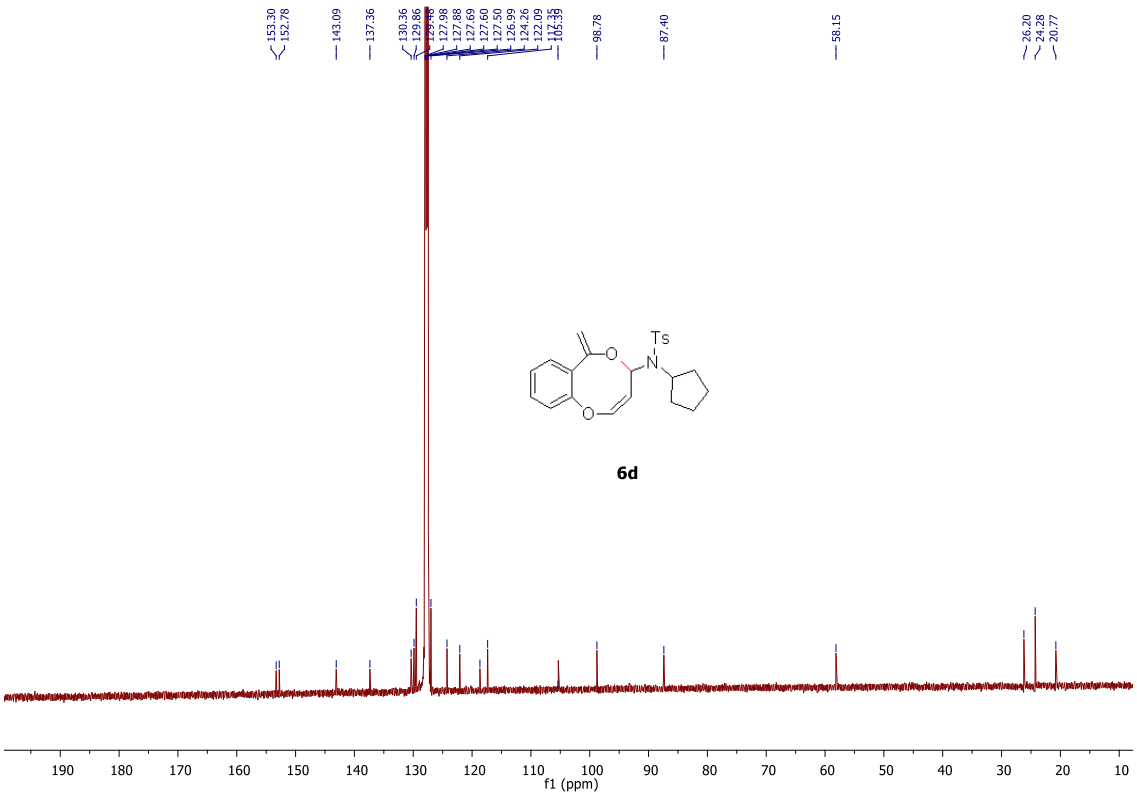

1.92
1.02
1.07
2.08
2.95
1.01
0.99
2.00
3.18
1.25
2.04
2.27
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


153.22
152.69
143.37
135.33
135.10
129.87
129.45
127.98
127.88
127.69
127.59
127.49
127.40
124.27
97.91
87.42
26.69
20.79
7.71
7.68
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

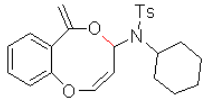
Ts
N
O
O

6c

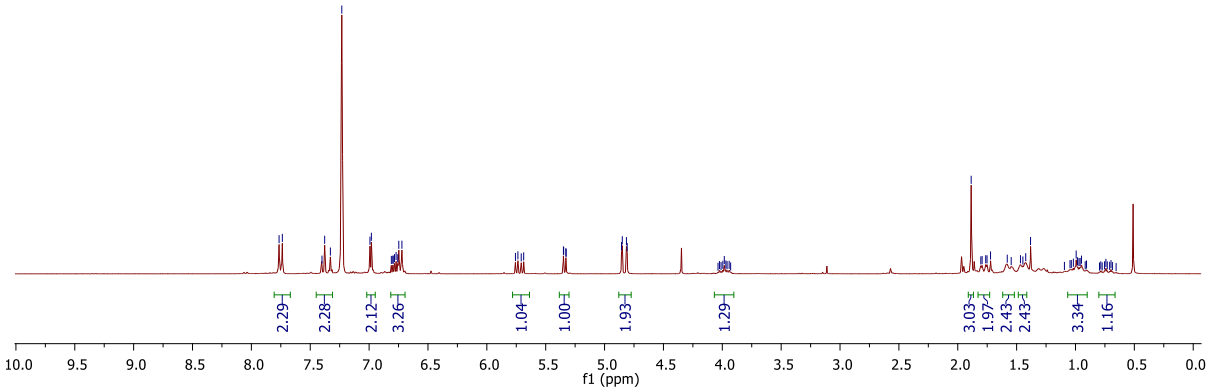

7.638
7.632
7.616
7.610
7.308
7.284
7.152
6.906
6.900
6.898
6.889
6.886
6.668
6.641
5.370
5.341
5.321
5.231
5.229
5.210
5.209
4.764
4.758
4.718
4.712
1.828
1.787
1.774
1.758
1.745
1.376
1.354
1.323
1.297
1.284
1.264
1.253
1.238
1.232
1.065
1.036
1.016
0.997
0.981
Ts
N
O
O
6d
1.93
2.12
2.32
3.01
1.16
1.03
2.00
1.20
3.11
1.21
6.42
2.26
f1 (ppm)

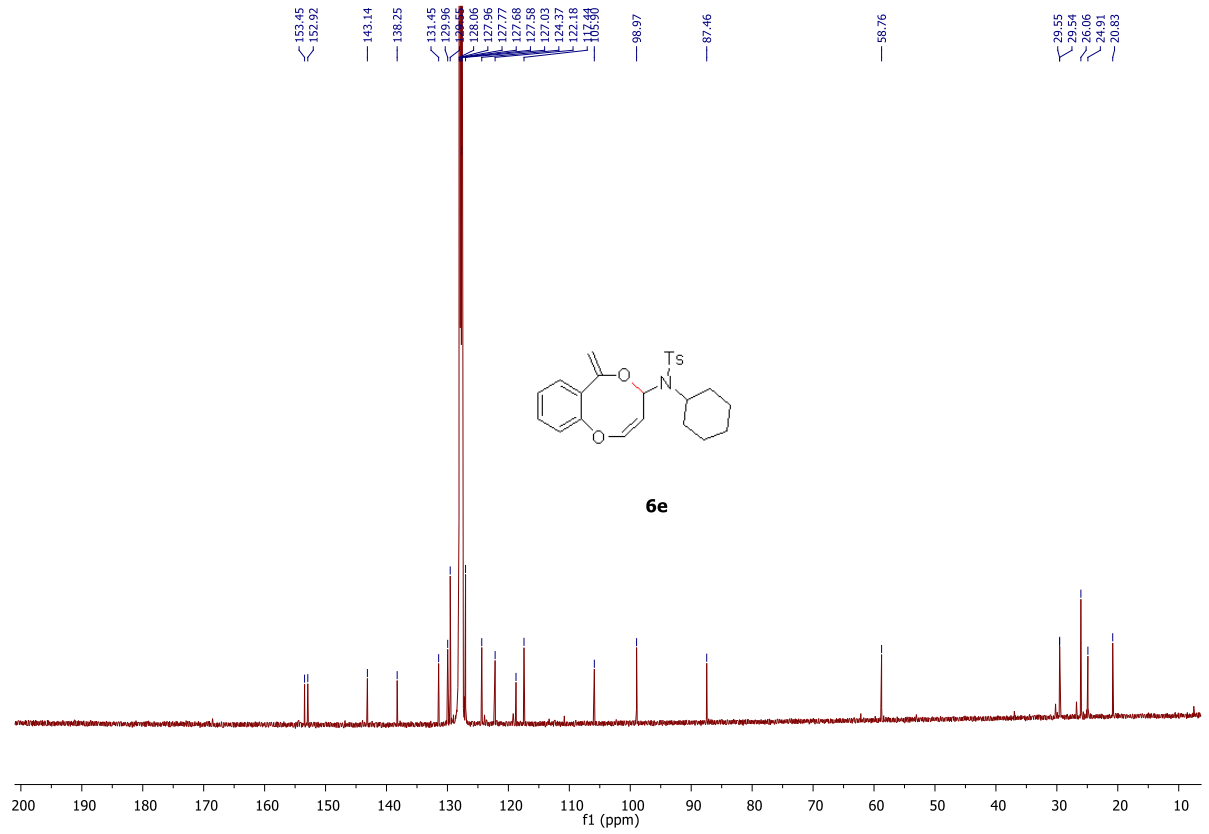

153.30
152.78
143.09
137.36
130.36
129.86
127.98
127.88
127.69
127.60
127.50
126.99
124.26
122.09
98.78
87.40
58.15
26.20
24.28
20.77
Ts
N
O
O
6d
f1 (ppm)


7.765
7.737
7.400
7.377
7.329
7.232
6.993
6.981
6.798
6.796
6.785
6.771
6.756
6.748
5.736
5.708
5.687
5.349
5.347
5.329
4.849
4.814
4.808
4.036
4.023
4.010
3.995
3.983
3.970
3.959
3.942
3.929
1.886
1.804
1.793
1.763
1.751
1.721
1.579
1.546
1.467
1.447
1.423
1.382
1.046
1.036
1.018
0.994
0.983
0.970
0.961
0.949
0.742
0.698


Ts
O
N
O

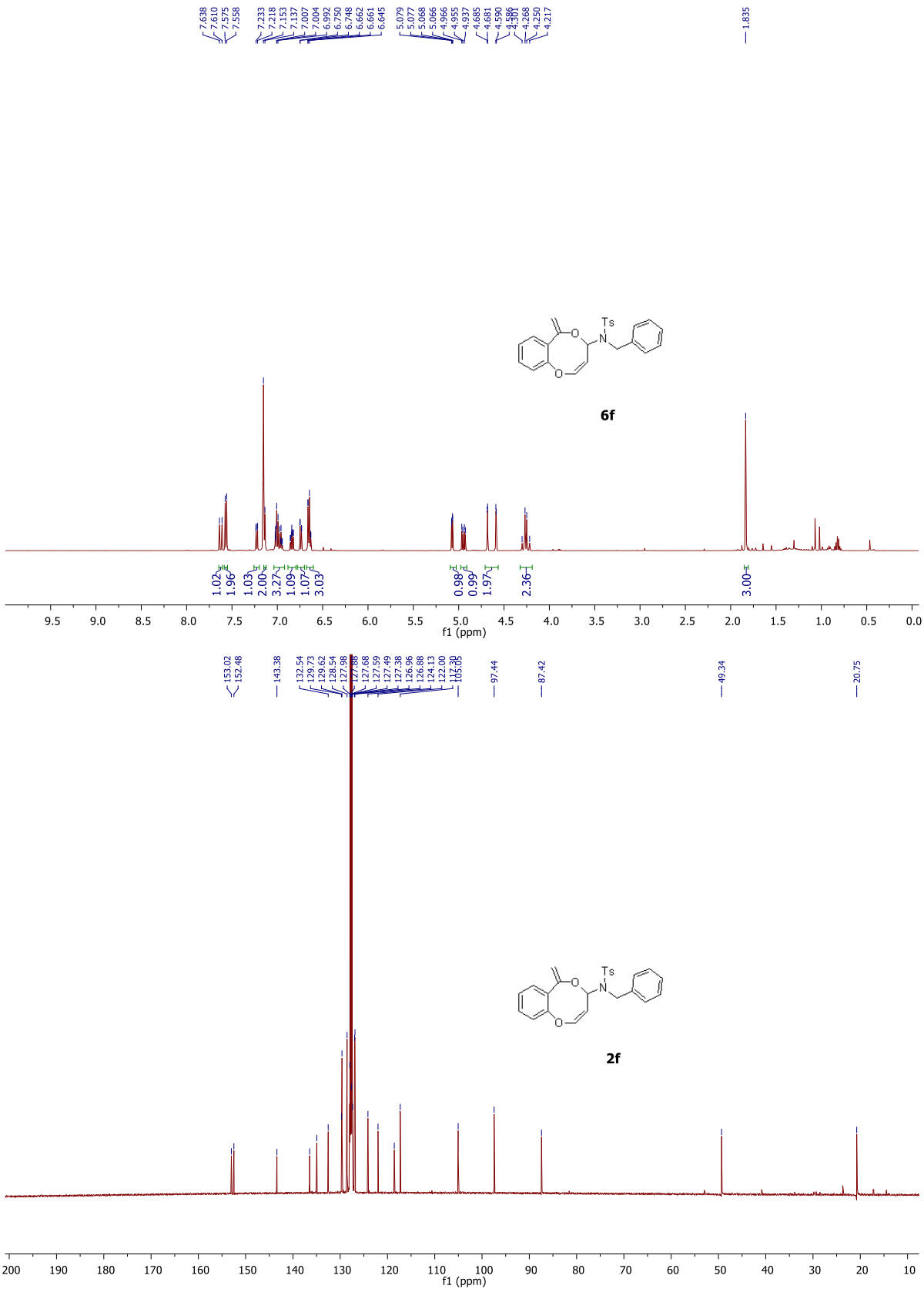
6e


2.29
2.28
2.12
3.26
1.04
1.00
1.93
1.29
3.03
1.97
2.43
2.43
3.34
1.16
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

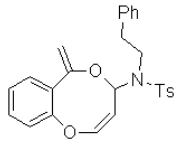

153.45
152.92
143.14
138.25
131.45
129.96
128.66
128.06
127.96
127.77
127.68
127.58
127.03
124.37
122.18
105.94
98.97
87.46
58.76
29.55
29.54
26.06
24.91
20.83
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

Ts
O
N
O

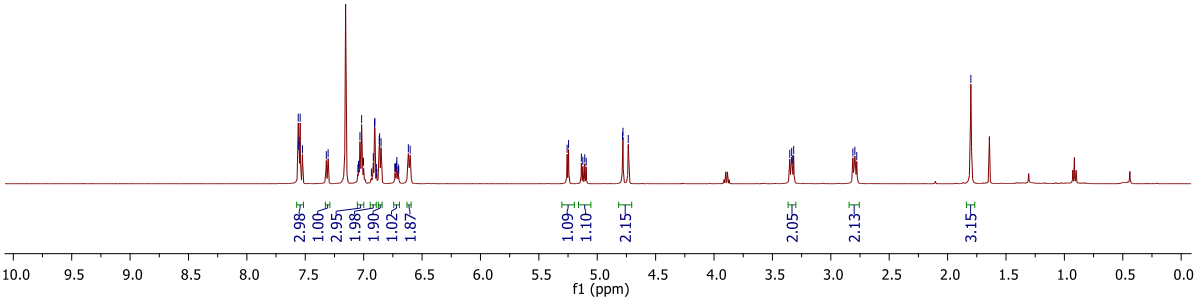
6e

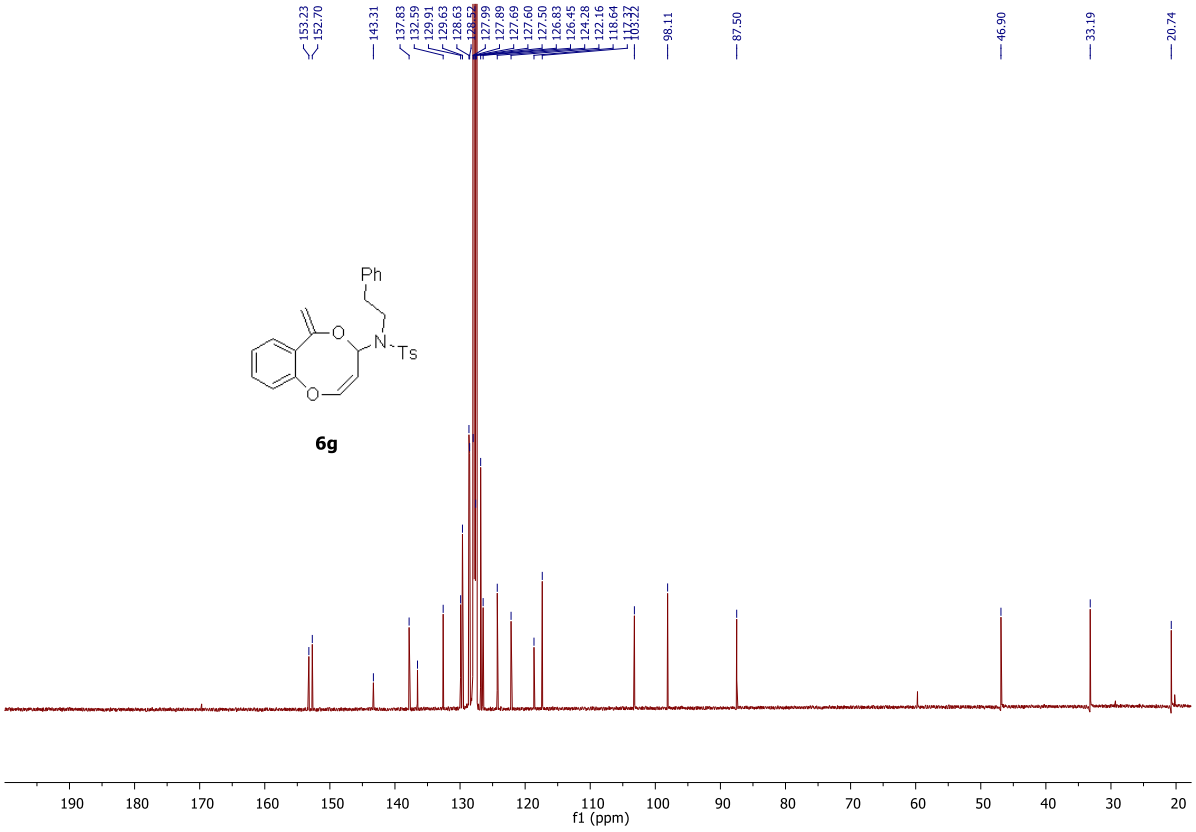

7.638
7.610
7.575
7.558
7.233
7.218
7.153
7.137
7.007
7.004
6.992
6.750
6.748
6.662
6.661
6.645
5.079
5.077
5.068
5.066
4.966
4.955
4.937
4.685
4.681
4.590
4.586
4.268
4.250
4.217
1.835
Ts
N
O
O
6f
1.02
1.96
1.03
2.00
3.27
1.09
1.07
3.03
0.98
0.99
1.97
2.36
3.00
f1 (ppm)
153.02
152.48
143.38
132.54
129.73
129.62
128.54
127.98
127.88
127.68
127.59
127.49
127.38
126.96
126.88
124.13
122.00
117.30
105.05
97.44
87.42
49.34
20.75
Ts
N
O
O
2f
f1 (ppm)


7.560
7.556
7.553
7.544
7.524
7.320
7.304
7.032
7.017
7.002
6.917
6.907
6.904
6.867
6.863
6.851
6.716
6.617
5.598
5.246
5.136
5.123
5.107
5.095
4.784
4.780
4.734
3.351
3.335
3.330
3.318
2.811
2.794
2.778
1.801


Ph
N
Ts
O
O

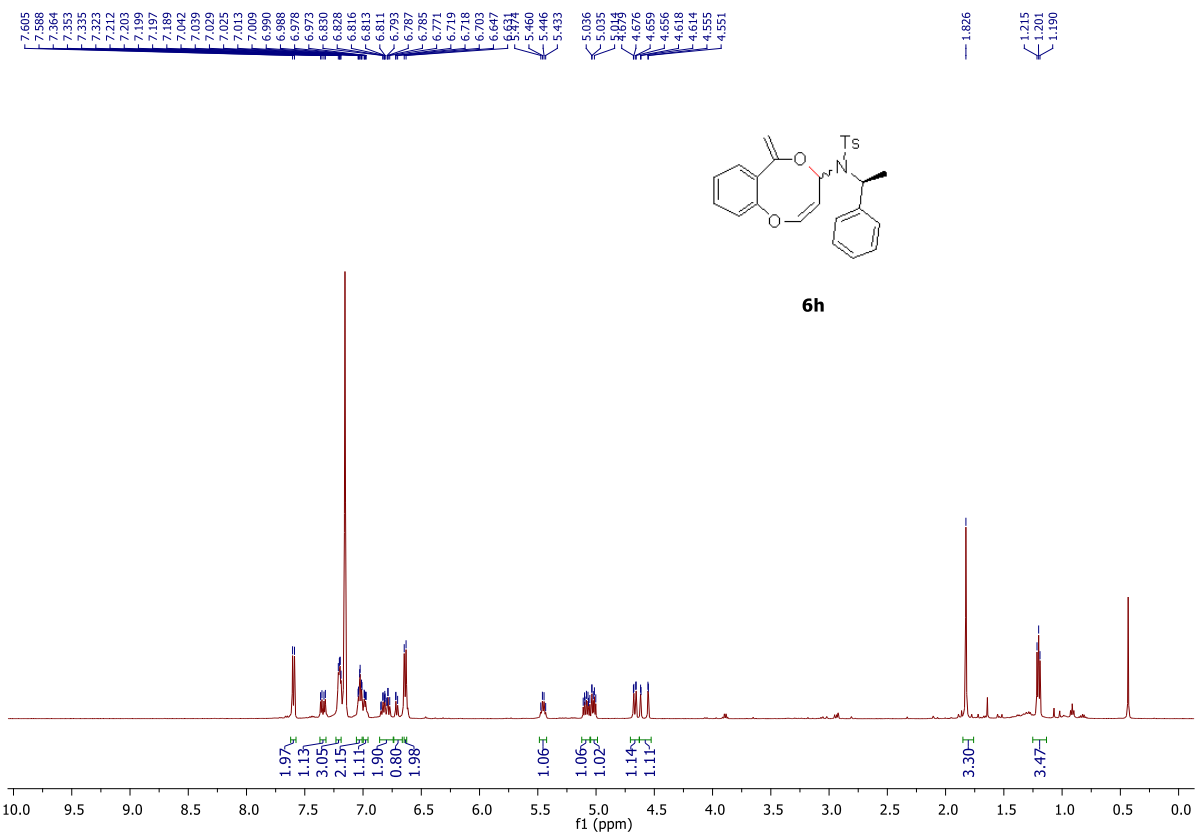
6g


2.98
1.00
2.95
1.98
1.90
1.02
1.87
1.09
1.10
2.15
2.05
2.13
3.15
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


153.23
152.70
143.31
137.83
132.59
129.91
129.63
128.63
128.52
127.99
127.89
127.69
127.60
127.50
126.83
126.45
124.28
122.16
118.64
117.37
103.32
98.11
87.50
46.90
33.19
20.74
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

Ph
N
Ts
O
O

6g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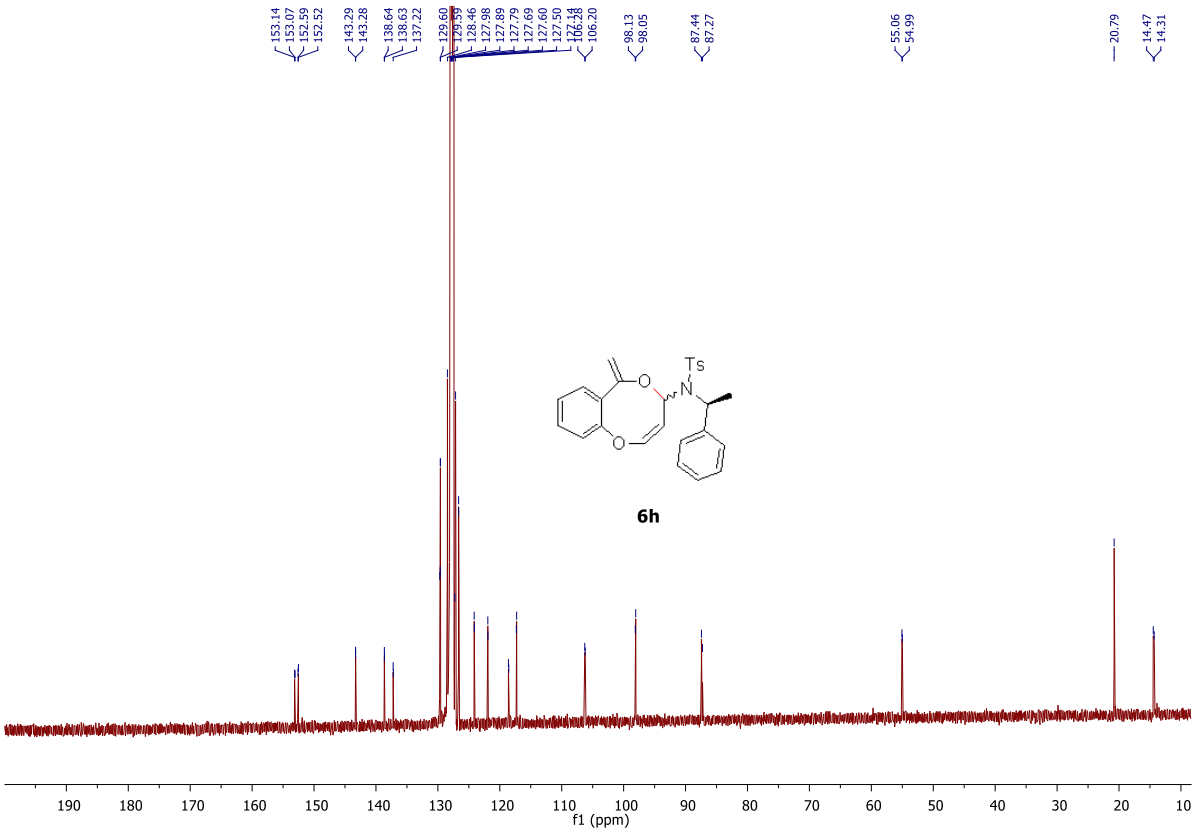
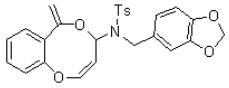
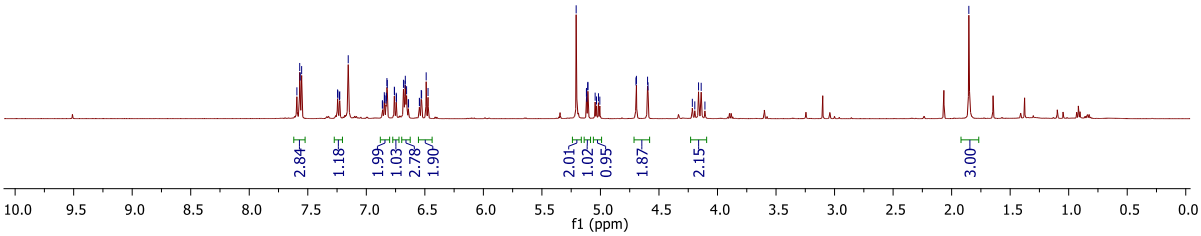
7.588
7.364
7.353
7.335
7.323
7.212
7.203
7.199
7.197
7.189
7.042
7.039
7.029
7.025
7.013
7.009
6.990
6.988
6.978
6.973
6.830
6.828
6.816
6.813
6.811
6.793
6.787
6.785
6.771
6.719
6.718
6.703
6.647
5.474
5.460
5.446
5.433
5.036
5.035
5.014
4.679
4.676
4.659
4.656
4.618
4.614
4.555
4.551
1.826
1.215
1.201
1.190
Ts
N
O
O
6h
1.97
1.13
3.05
2.15
1.11
1.90
0.80
1.98
1.06
1.06
1.02
1.14
1.11
3.30
3.47
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


153.14
153.07
152.59
152.52
143.29
143.28
138.64
138.63
137.22
129.60
129.59
128.46
127.98
127.89
127.79
127.69
127.60
127.50
127.14
106.28
106.20
98.13
98.05
87.44
87.27
55.06
54.99
20.79
14.47
14.31
Ts
N
O
O
6h
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

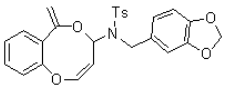

7.593
7.569
7.565
7.552
7.245
7.243
7.155
6.824
6.821
6.761
6.759
6.683
6.669
6.667
6.656
6.489
5.207
5.120
5.119
5.117
5.108
5.107
5.045
5.017
4.696
4.693
4.597
4.215
4.194
4.162
4.139
4.107
1.853


Ts
N
O
O
O
O

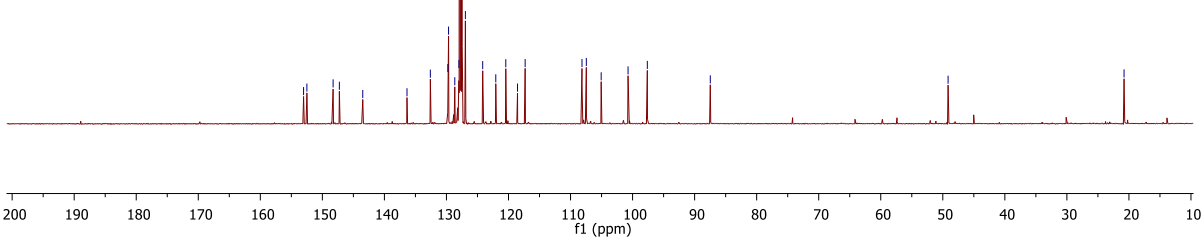
6i

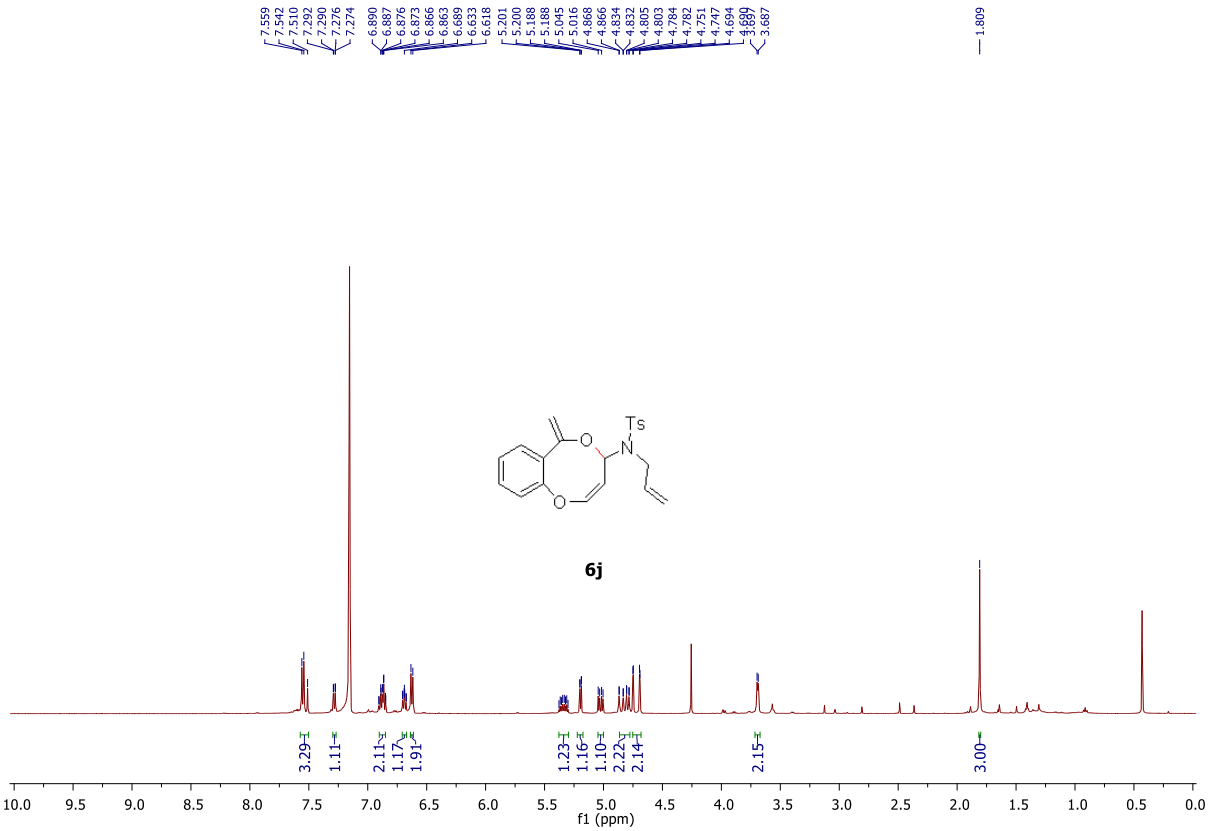

2.84
1.18
1.99
1.03
2.78
1.90
2.01
1.02
0.95
1.87
2.15
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

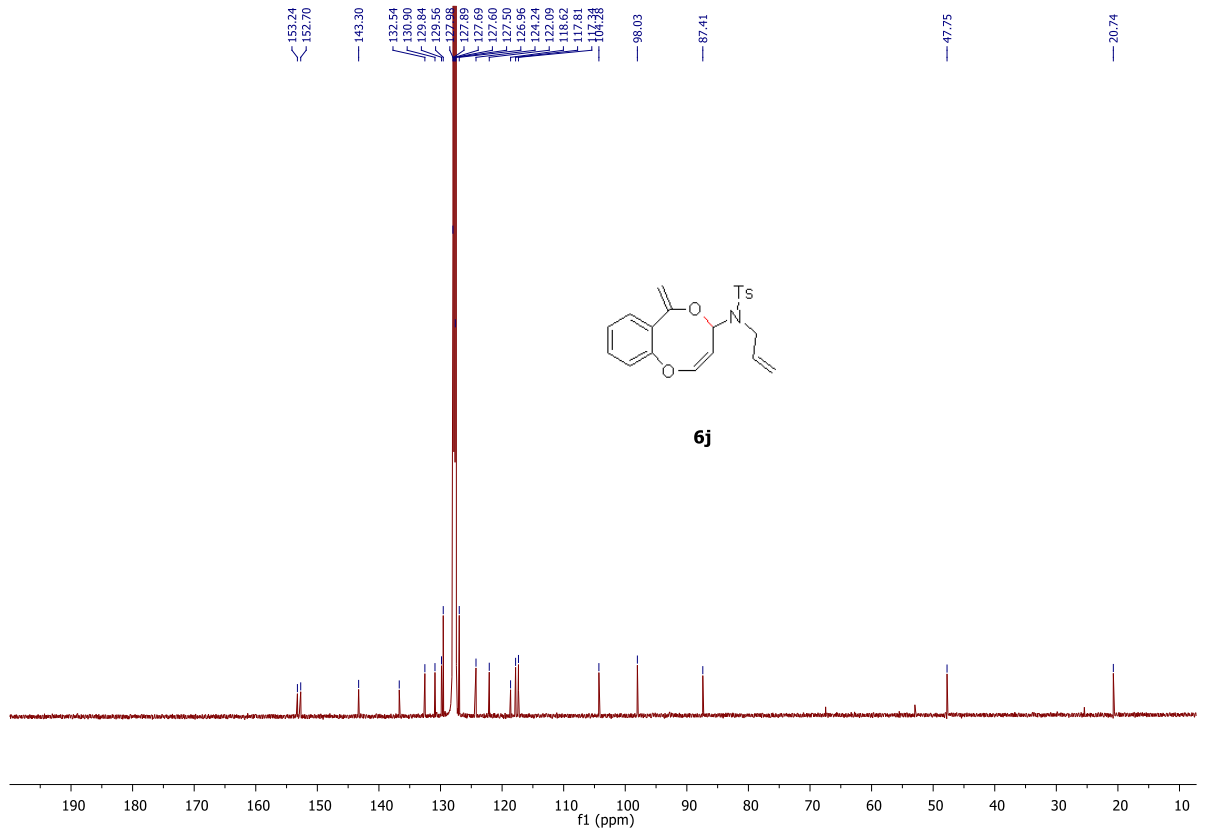

153.03
152.49
148.27
147.26
143.49
132.59
129.77
129.66
128.66
127.99
127.89
127.70
127.50
126.95
124.16
122.05
120.44
118.54
107.45
105.06
100.73
97.62
87.47
49.15
20.79

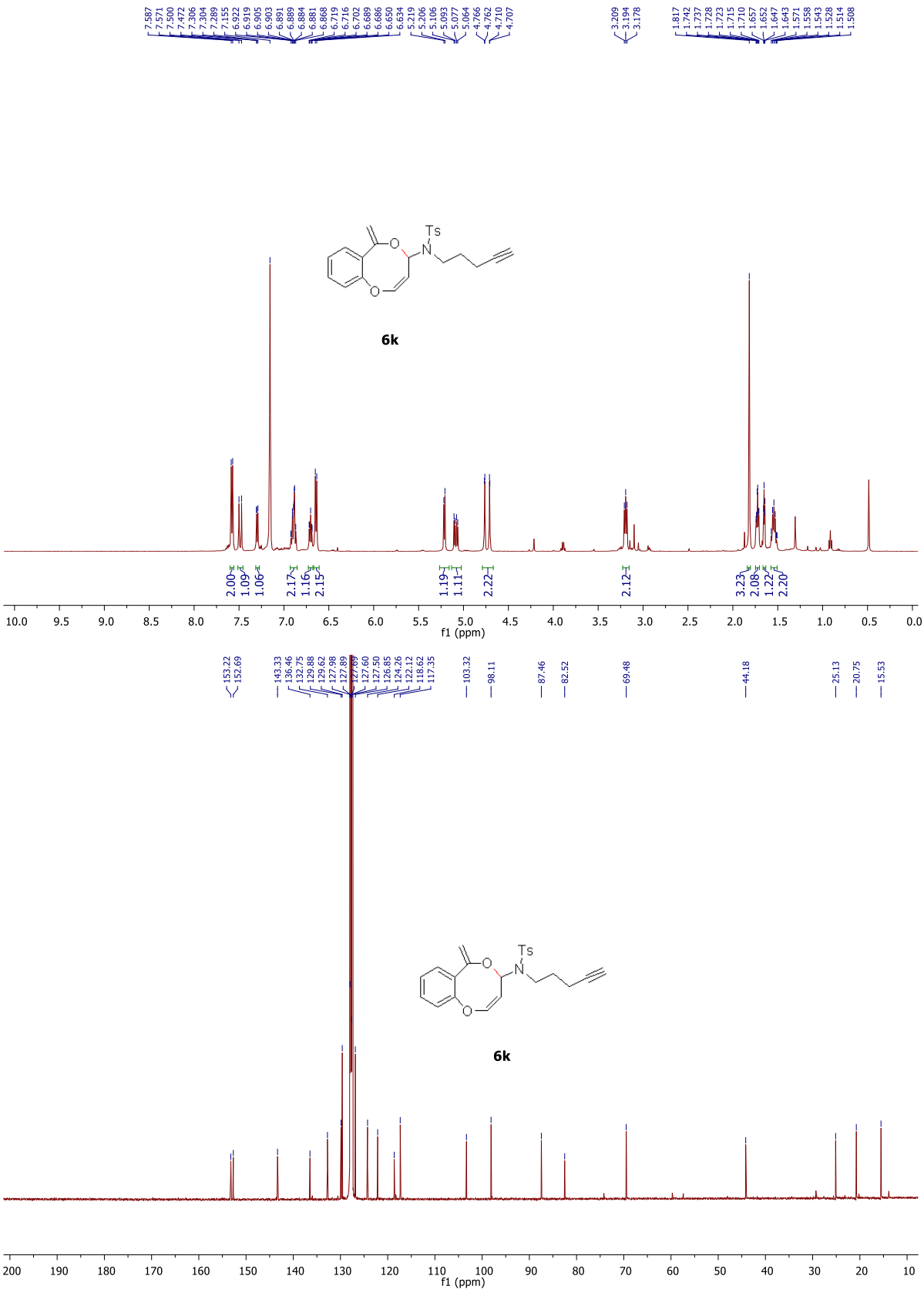

Ts
N
O
O
O
O

6i


200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.559
7.542
7.510
7.292
7.290
7.276
7.274
6.890
6.887
6.876
6.873
6.866
6.863
6.689
6.633
6.618
5.201
5.200
5.188
5.188
5.045
5.016
4.868
4.866
4.834
4.832
4.805
4.803
4.784
4.782
4.751
4.747
4.694
4.690
3.699
3.687
1.809
Ts
N
O
O
6j
3.29
1.11
2.11
1.17
1.91
1.23
1.16
1.10
2.22
2.14
2.15
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


153.24
152.70
143.30
132.54
130.90
129.84
129.56
127.89
127.69
127.60
127.50
126.96
124.24
122.09
118.62
117.81
117.34
104.28
98.03
87.41
47.75
20.74
Ts
N
O
O
6j
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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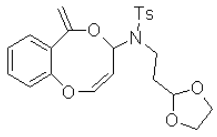
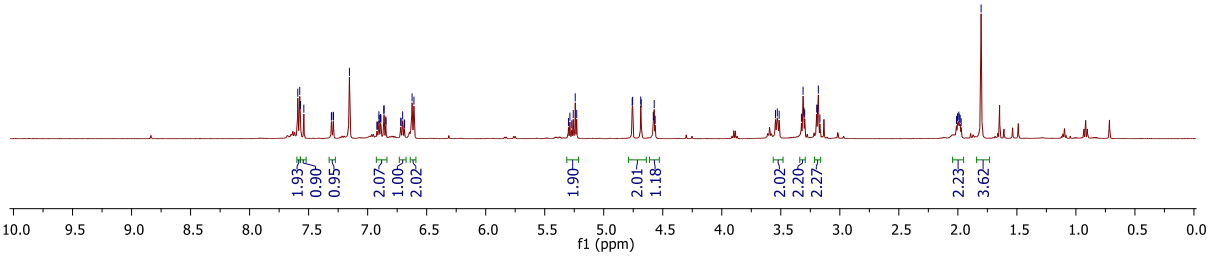
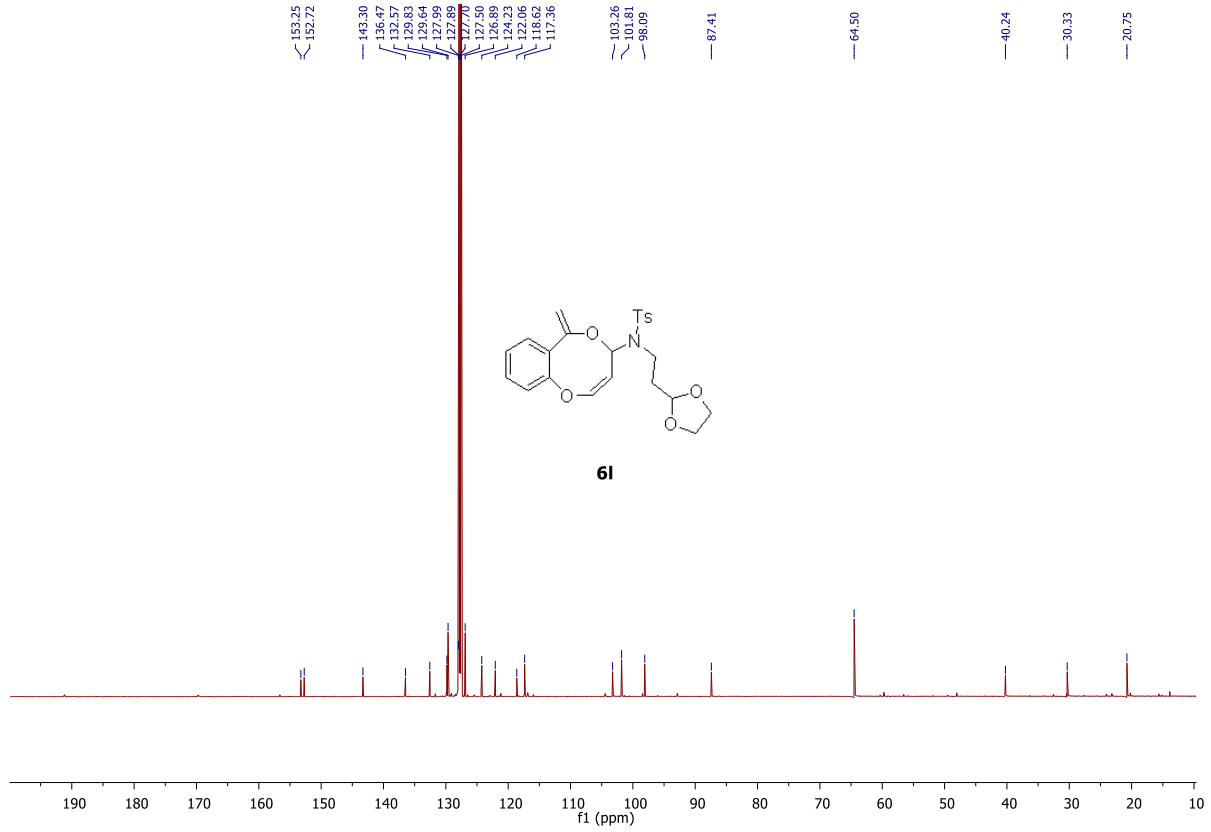
7.571
7.500
7.472
7.306
7.304
7.289
7.155
6.922
6.919
6.905
6.903
6.891
6.889
6.884
6.881
6.868
6.719
6.716
6.702
6.689
6.686
6.650
6.634
5.219
5.206
5.106
5.093
5.077
5.064
4.766
4.762
4.710
4.707
3.209
3.194
3.178
1.817
1.742
1.737
1.728
1.723
1.715
1.710
1.657
1.652
1.647
1.643
1.571
1.558
1.543
1.528
1.514
1.508
Ts
N
O
O
6k
2.00
1.09
1.06
2.17
1.16
2.15
1.19
1.11
2.22
2.12
3.23
2.08
1.22
2.20
f1 (ppm)
153.22
152.69
143.33
136.46
132.75
129.88
129.62
127.98
127.89
127.65
127.60
127.50
126.85
124.26
122.12
118.62
117.35
103.32
98.11
87.46
82.52
69.48
44.18
25.13
20.75
15.53
Ts
N
O
O
6k
f1 (ppm)


7.592
7.575
7.569
7.541
7.307
7.305
7.291
7.289
7.155
6.921
6.918
6.905
6.902
6.891
6.888
6.863
6.861
6.847
6.845
6.719
6.717
6.704
6.690
6.687
6.624
6.608
5.299
5.287
5.271
5.258
5.241
5.229
4.759
4.755
4.686
4.683
4.580
4.572
4.564
3.545
3.530
3.514
3.325
3.311
3.304
3.298
3.196
3.189
3.182
3.169
2.011
2.003
1.992
1.989
1.981
1.972
1.803

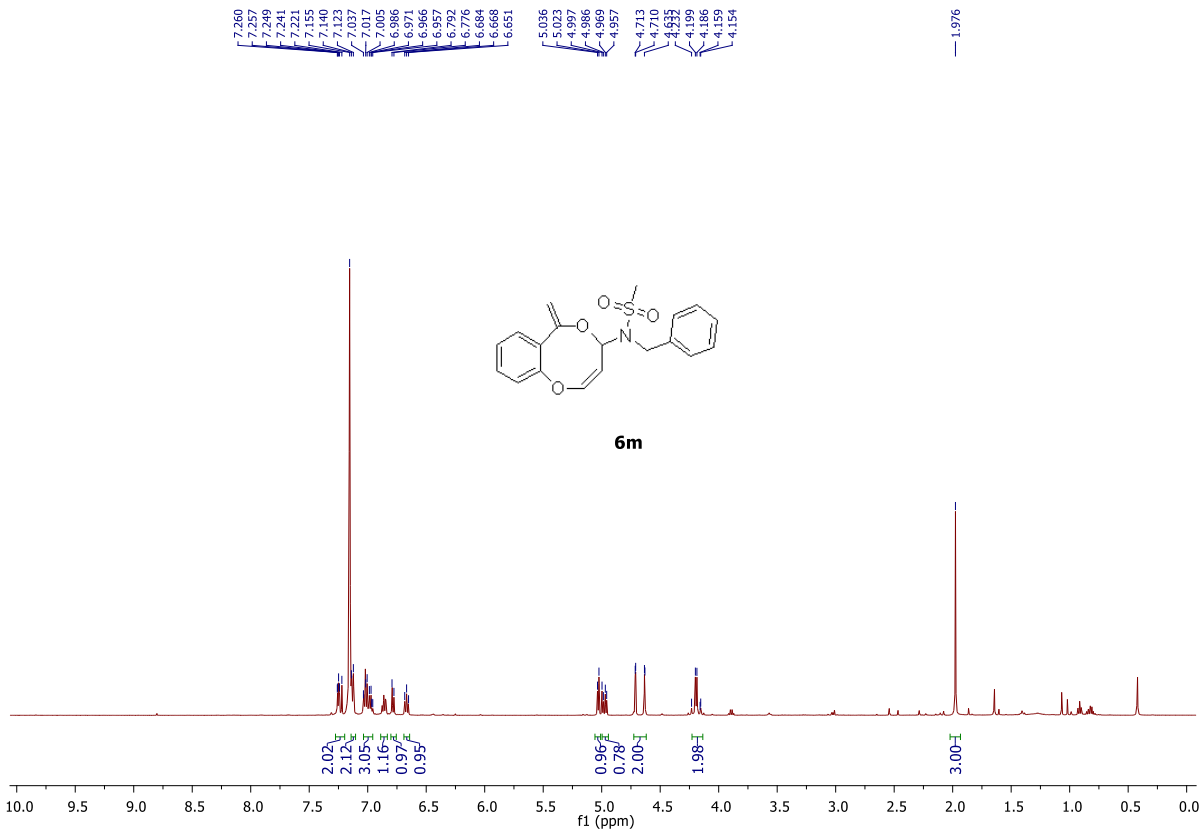

Ts
N
O
O
O
O

6l


1.93
0.90
0.95
2.07
1.00
2.02
1.90
2.01
1.18
2.02
2.20
2.27
2.23
3.62
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


153.25
152.72
143.30
136.47
132.57
129.83
129.64
127.99
127.89
127.70
127.50
126.89
124.23
122.06
118.62
117.36
103.26
101.81
98.09
87.41
64.50
40.24
30.33
20.75
Ts
N
O
O
O
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

6l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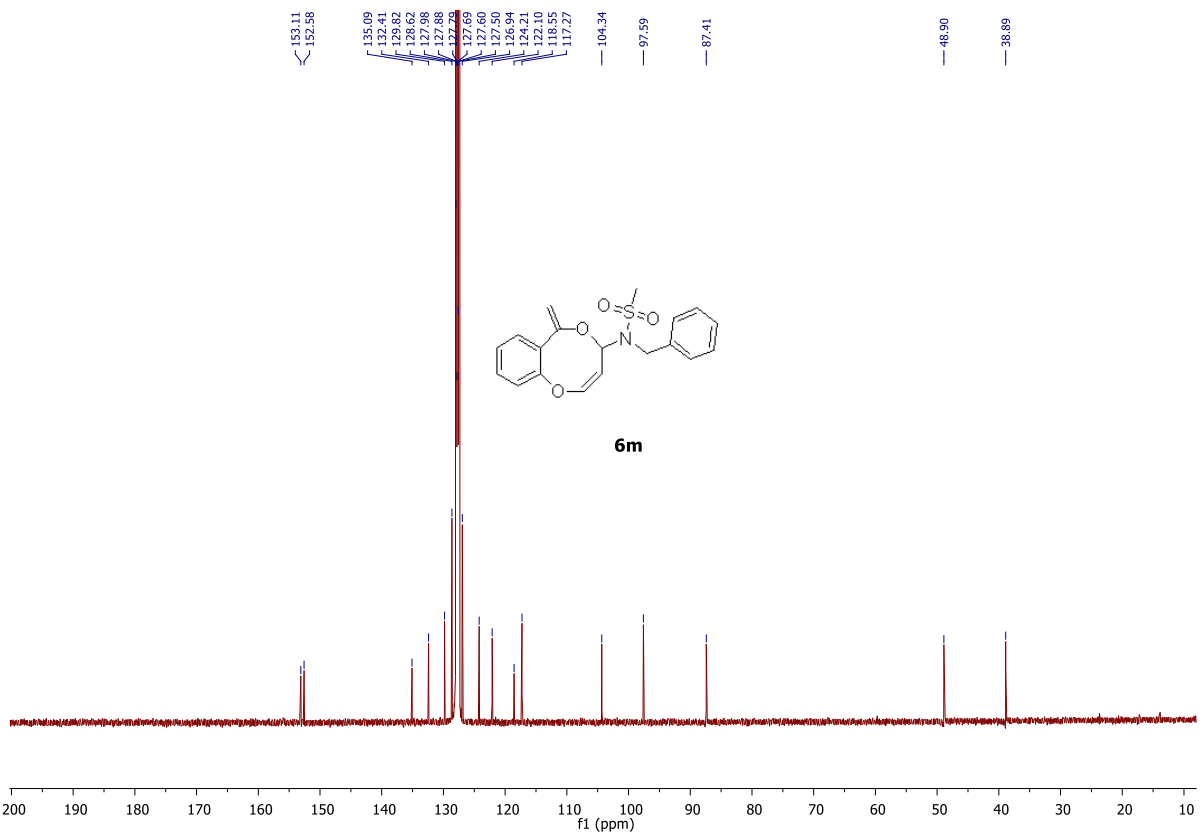
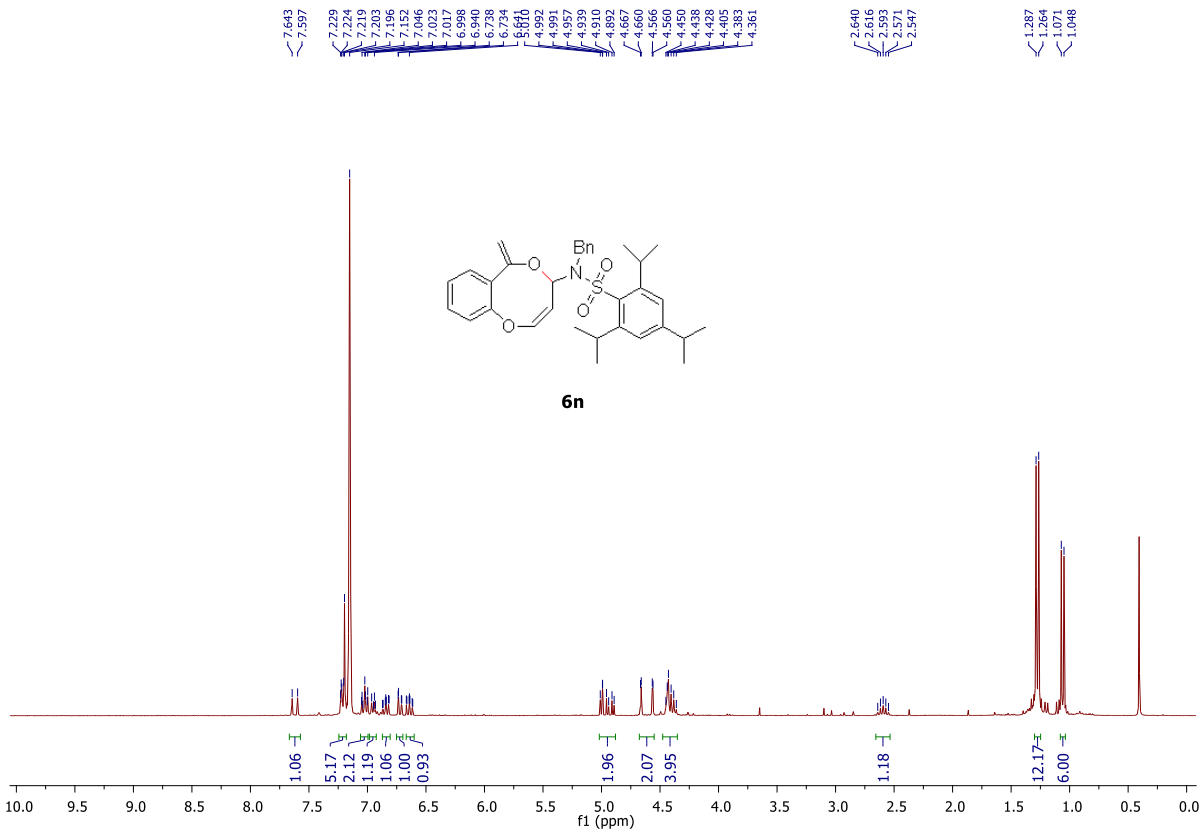
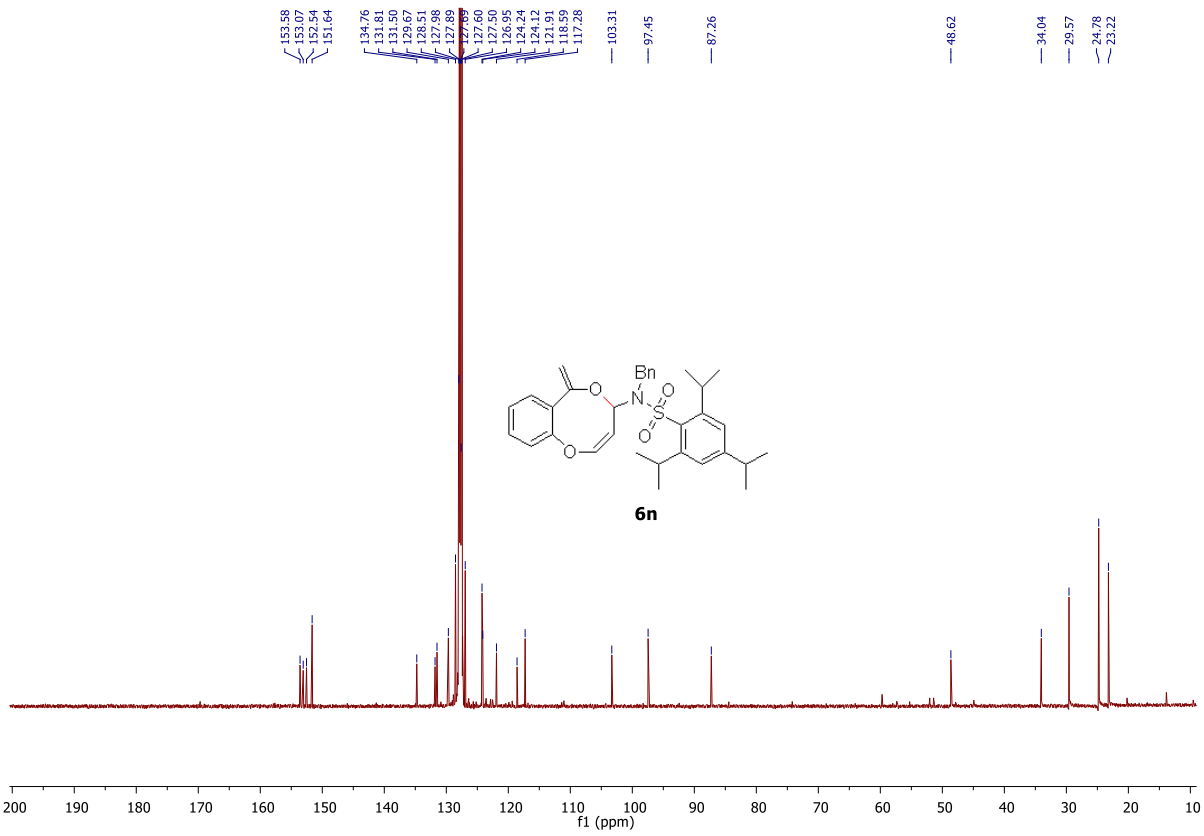
7.257
7.249
7.241
7.221
7.155
7.140
7.123
7.037
7.017
7.005
6.986
6.971
6.966
6.957
6.792
6.776
6.684
6.668
6.651
5.036
5.023
4.997
4.986
4.969
4.957
4.713
4.710
4.633
4.199
4.186
4.159
4.154
1.976
6m
2.02
2.12
3.05
1.16
0.97
0.95
0.96
0.78
2.00
1.98
3.00
f1 (ppm)


153.11
152.58
135.09
132.41
129.82
128.62
127.98
127.88
127.78
127.69
127.60
127.50
126.94
124.21
122.10
118.55
117.27
104.34
97.59
87.41
48.90
38.89
6m
f1 (ppm)


7.643
7.597
7.229
7.224
7.219
7.203
7.196
7.152
7.046
7.023
7.017
6.998
6.940
6.738
6.734
5.010
4.992
4.991
4.957
4.939
4.910
4.892
4.667
4.660
4.566
4.560
4.450
4.438
4.428
4.405
4.383
4.361
2.640
2.616
2.593
2.571
2.547
1.287
1.264
1.071
1.048
Bn
N
S
O
O
O
O
1.06
5.17
2.12
1.19
1.06
1.00
0.93
1.96
2.07
3.95
1.18
12.17
6.00
f1 (ppm)

6n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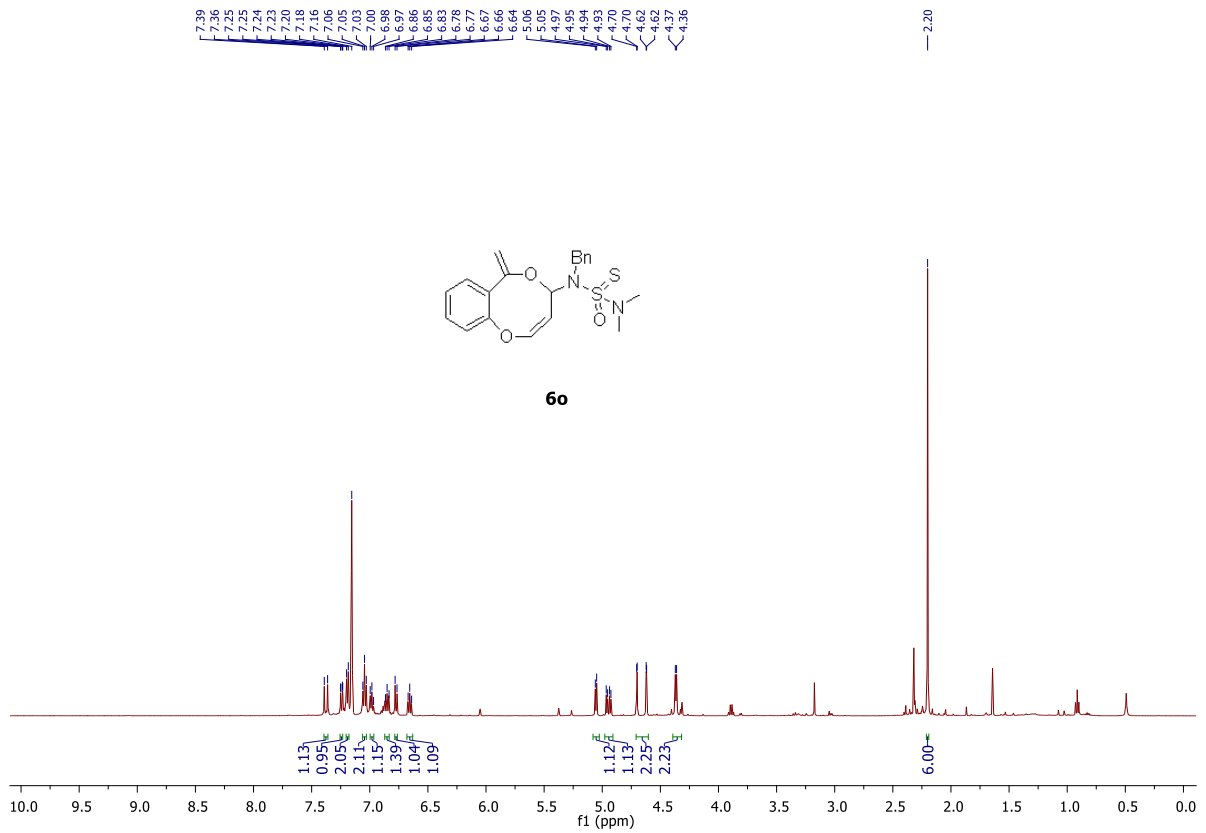
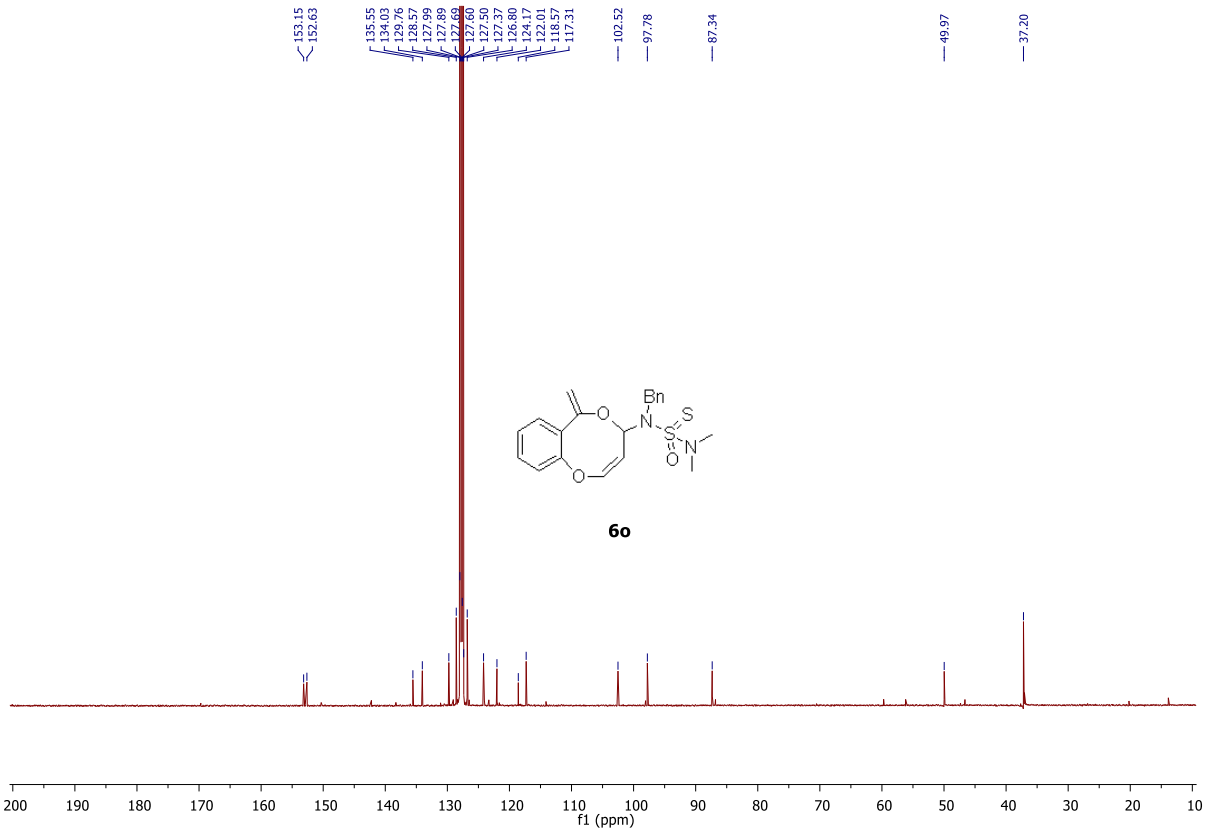
153.07
152.54
151.64
134.76
131.81
131.50
129.67
128.51
127.98
127.89
127.60
127.50
126.95
124.24
124.12
121.91
118.59
117.28
103.31
97.45
87.26
48.62
34.04
29.57
24.78
23.22
Bn
N
S
O
O
O
O
f1 (ppm)

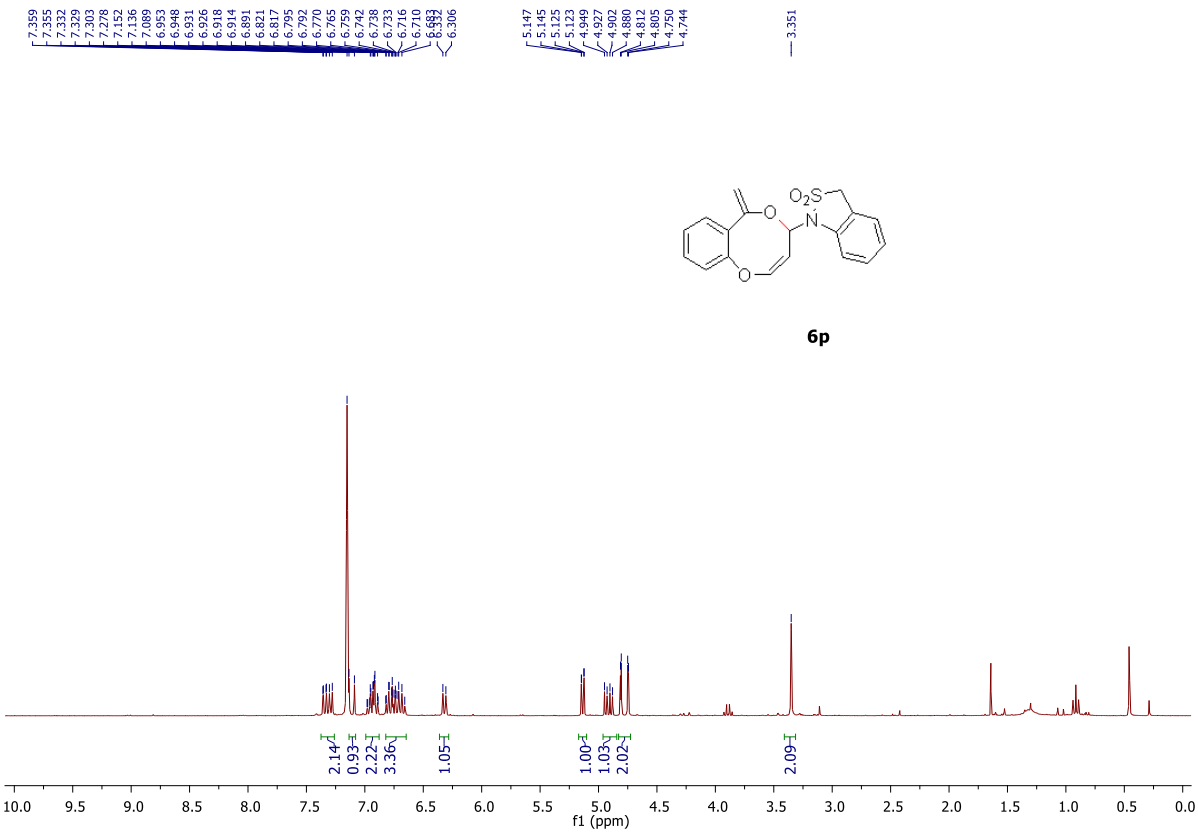
6n

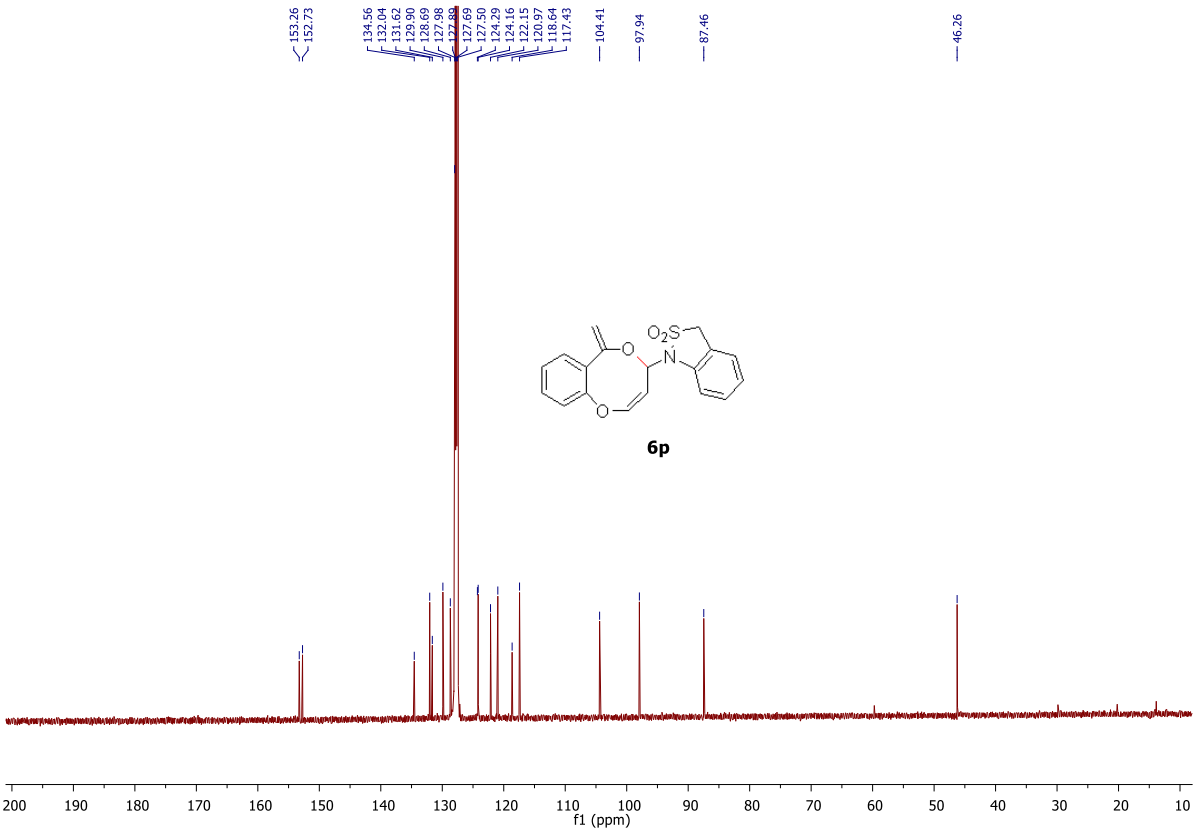

7.39
7.36
7.25
7.25
7.24
7.23
7.20
7.18
7.16
7.06
7.05
7.03
7.00
6.98
6.97
6.86
6.85
6.83
6.78
6.77
6.67
6.66
6.64
5.06
5.05
4.97
4.95
4.94
4.93
4.70
4.70
4.62
4.62
4.37
4.36
2.20
Bn
N
S
O
O
O
S
N
1.13
0.95
2.05
2.11
1.15
1.39
1.04
1.09
1.12
1.13
2.25
2.23
6.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

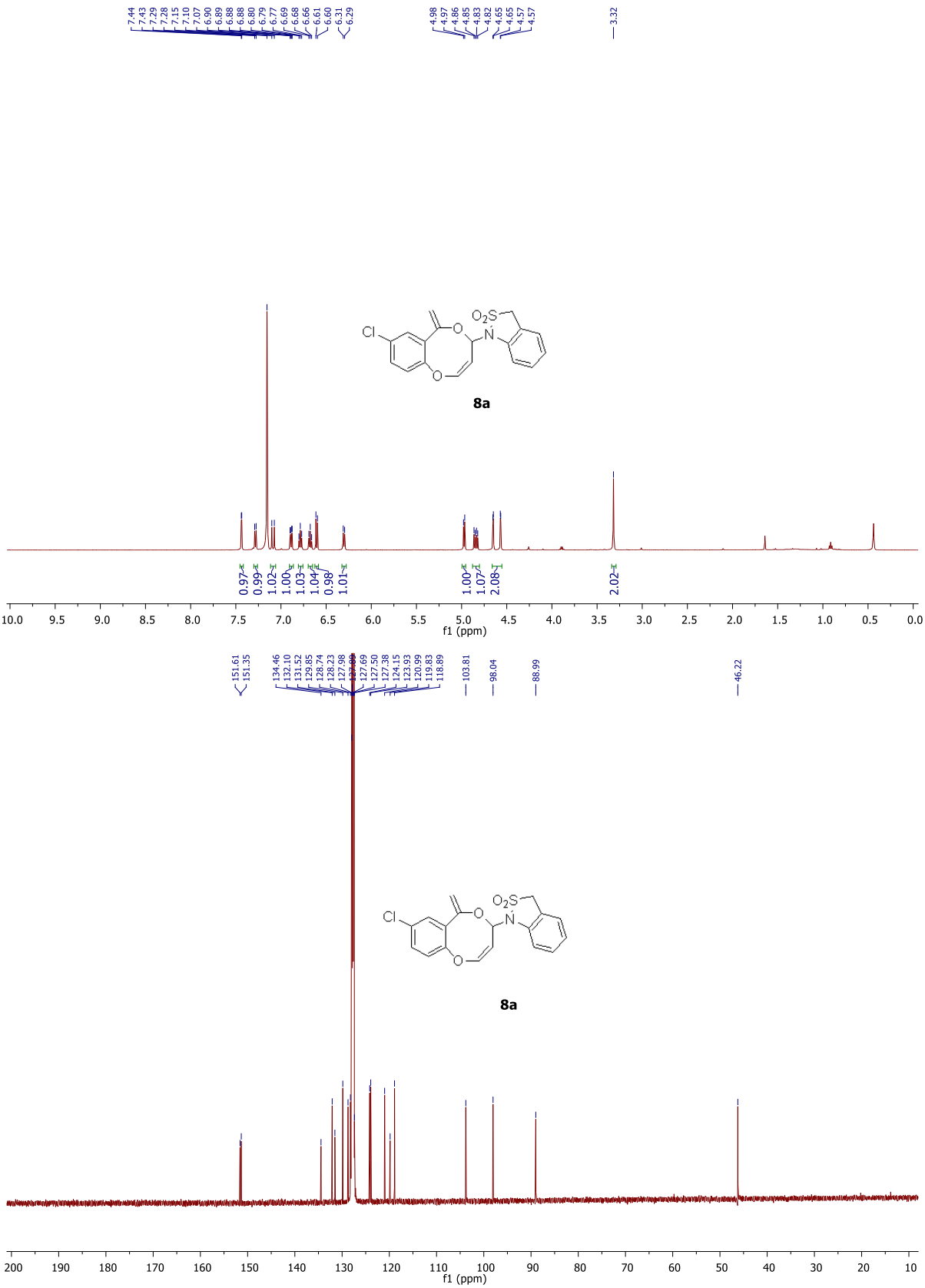
6o

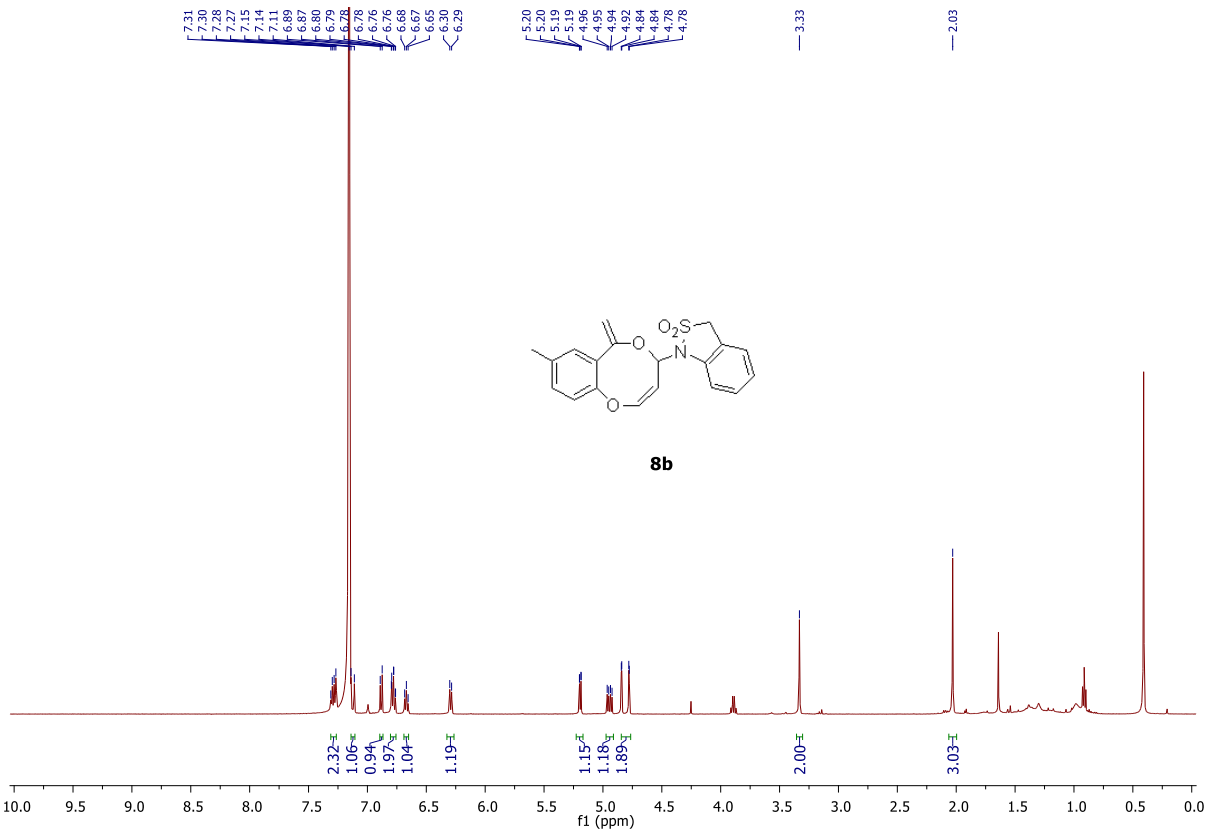

153.15
152.63
135.55
134.03
129.76
128.57
127.99
127.89
127.60
127.50
127.37
126.80
124.17
122.01
118.57
117.31
102.52
97.78
87.34
49.97
37.20
Bn
N
S
O
O
O
S
N
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

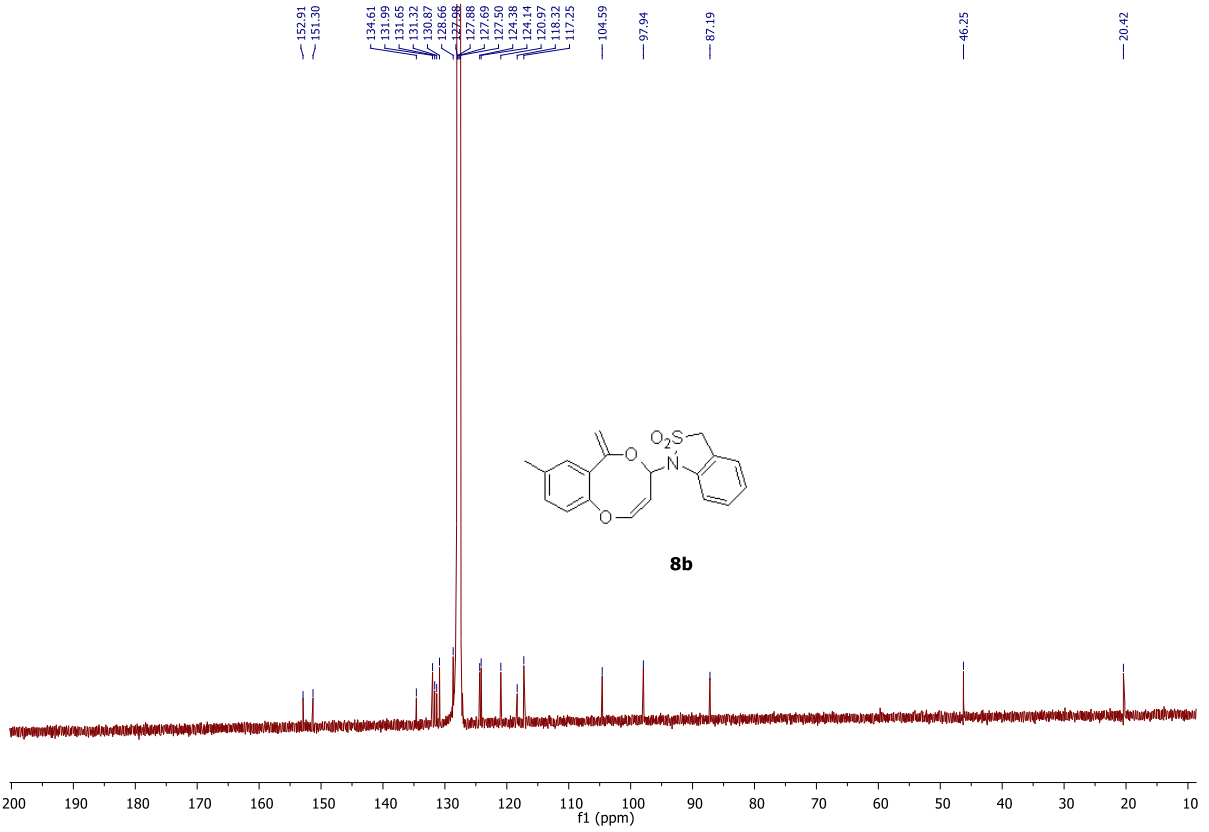
6o

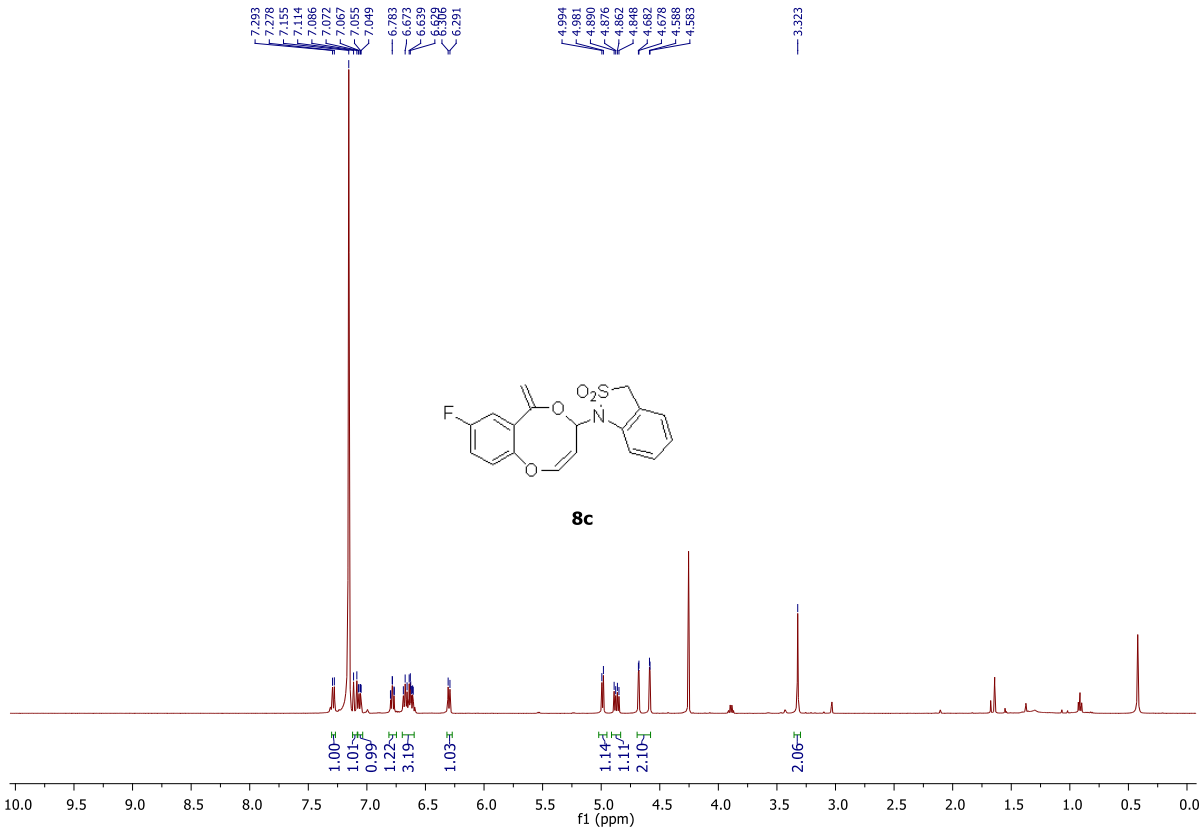

7.359
7.355
7.332
7.329
7.303
7.278
7.152
7.136
7.089
6.953
6.948
6.931
6.926
6.918
6.914
6.891
6.821
6.817
6.795
6.792
6.770
6.765
6.759
6.742
6.738
6.733
6.716
6.710
6.683
6.332
6.306
5.147
5.145
5.125
5.123
4.949
4.927
4.902
4.880
4.812
4.805
4.750
4.744
3.351
O2S
N
O
O
6p
2.14
0.93
2.22
3.36
1.05
1.00
1.03
2.02
2.09
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

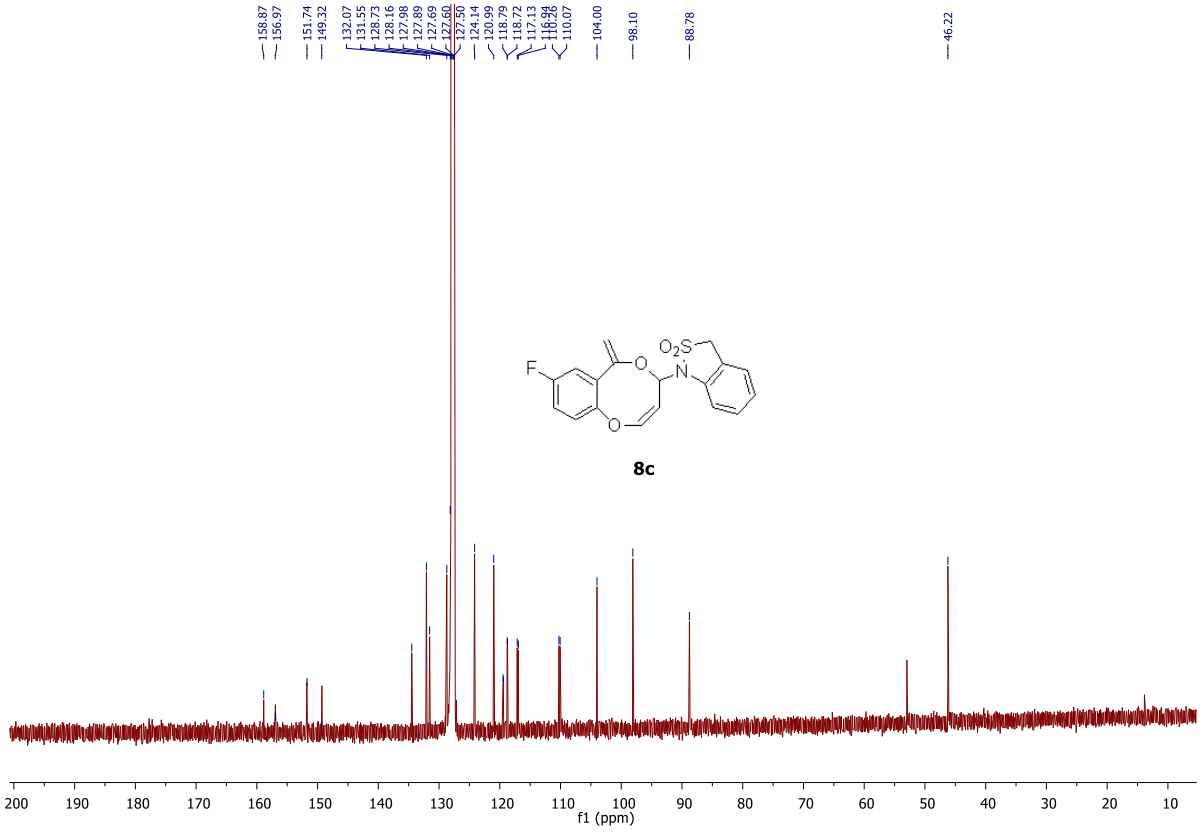

153.26
152.73
134.56
132.04
131.62
129.90
128.69
127.98
127.88
127.69
127.50
124.29
124.16
122.15
120.97
118.64
117.43
104.41
97.94
87.46
46.26
O2S
N
O
O
6p
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

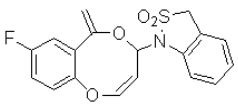

7.44
7.43
7.29
7.28
7.15
7.10
7.07
6.90
6.89
6.88
6.88
6.80
6.79
6.77
6.69
6.68
6.66
6.61
6.60
6.31
6.29
4.98
4.97
4.86
4.85
4.83
4.82
4.65
4.65
4.57
4.57
3.32
Cl
O
O
O2S
N
8a
0.97
0.99
1.02
1.00
1.03
1.04
0.98
1.01
1.00
1.07
2.08
2.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
151.61
151.35
134.46
132.10
131.52
129.85
128.74
128.23
127.98
127.69
127.50
127.38
124.15
123.93
120.99
119.83
118.89
103.81
98.04
88.99
46.22
Cl
O
O
O2S
N
8a
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


7.31
7.30
7.28
7.27
7.15
7.14
7.11
6.89
6.87
6.80
6.79
6.78
6.78
6.76
6.76
6.76
6.68
6.67
6.65
6.30
6.29
5.20
5.20
5.19
5.19
4.96
4.95
4.94
4.92
4.84
4.84
4.78
4.78
3.33
2.03
O2S
N
O
O
8b
2.32
1.06
0.94
1.97
1.04
1.19
1.15
1.18
1.89
2.00
3.03
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


152.91
151.30
134.61
131.99
131.65
131.32
130.87
128.66
127.88
127.69
127.50
124.38
124.14
120.97
118.32
117.25
104.59
97.94
87.19
46.25
20.42
O2S
N
O
O
8b
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

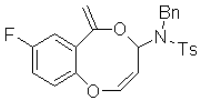

7.293
7.278
7.155
7.114
7.086
7.072
7.067
7.055
7.049
6.783
6.673
6.639
6.629
6.306
6.291
4.994
4.981
4.890
4.876
4.862
4.848
4.682
4.678
4.588
4.583
3.323
F
O
O2S
N
O
8c
1.00
1.01
0.99
1.22
3.19
1.03
1.14
1.11
2.10
2.06
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


158.87
156.97
151.74
149.32
132.07
131.55
128.73
128.16
127.98
127.89
127.69
127.60
127.50
124.14
120.99
118.79
118.72
117.13
116.94
116.28
110.07
104.00
98.10
88.78
46.22
F
O
O2S
N
O
8c
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

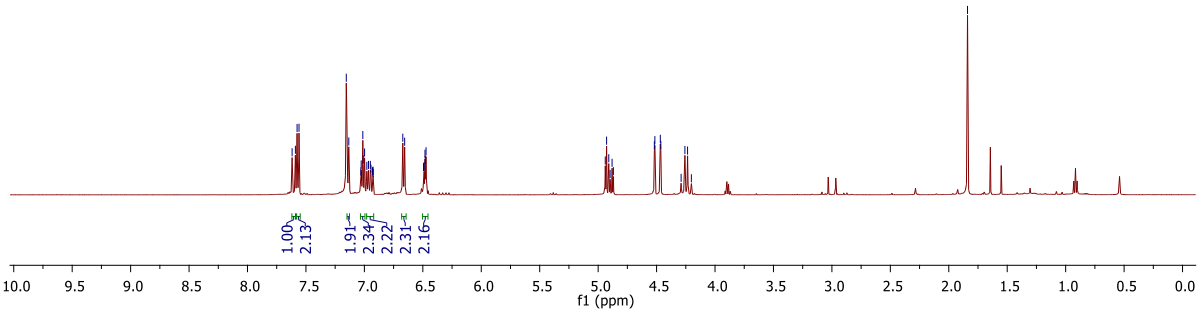

F
O
O2S
N
O

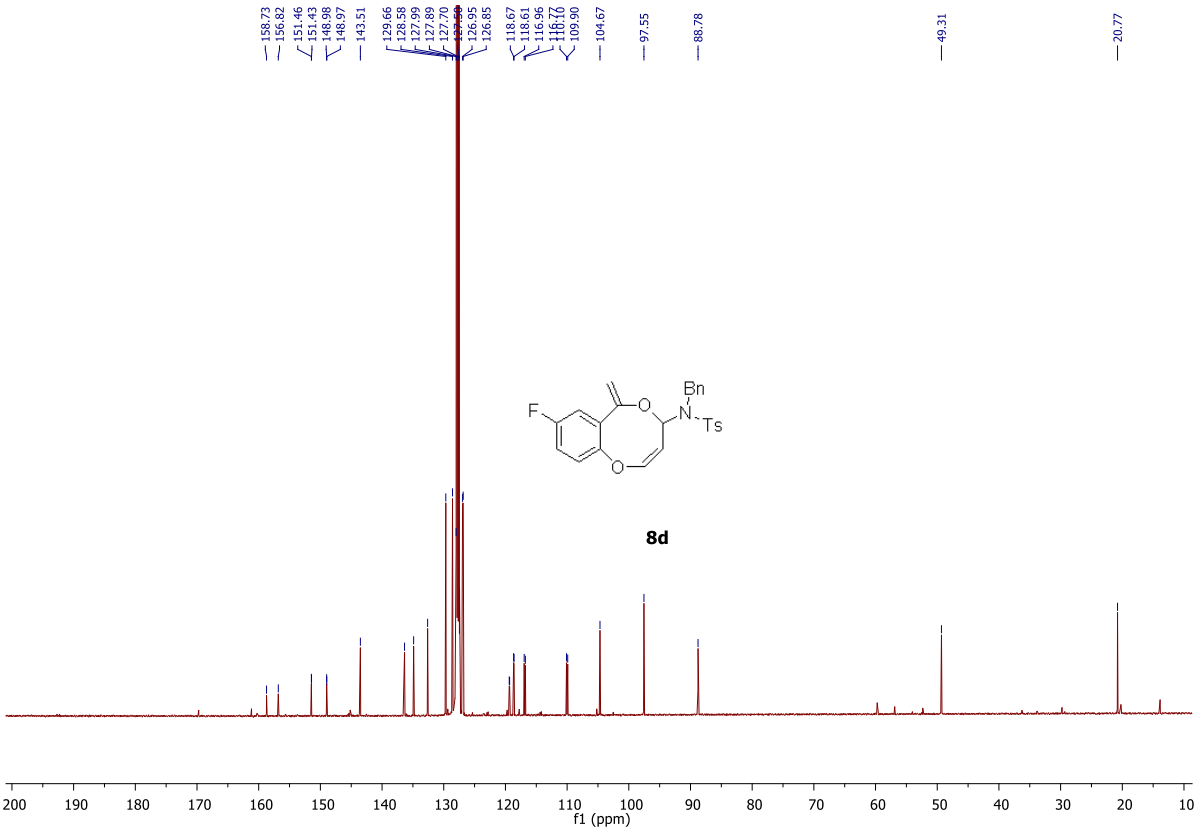
8c

-120.35
-100 -102 -104 -106 -108 -110 -112 -114 -116 -118 -120 -122 -124 -126 -128 -130 -132 -134 -136 -138 -140 -142 -144 -146 -148
f1 (ppm)
7.618
7.590
7.576
7.559
7.155
7.133
7.013
6.655
6.494
6.489
6.482
6.479
6.472
4.939
4.928
4.909
4.898
4.881
4.870
4.519
4.515
4.468
4.464
4.290
4.258
4.235
4.202
1.840

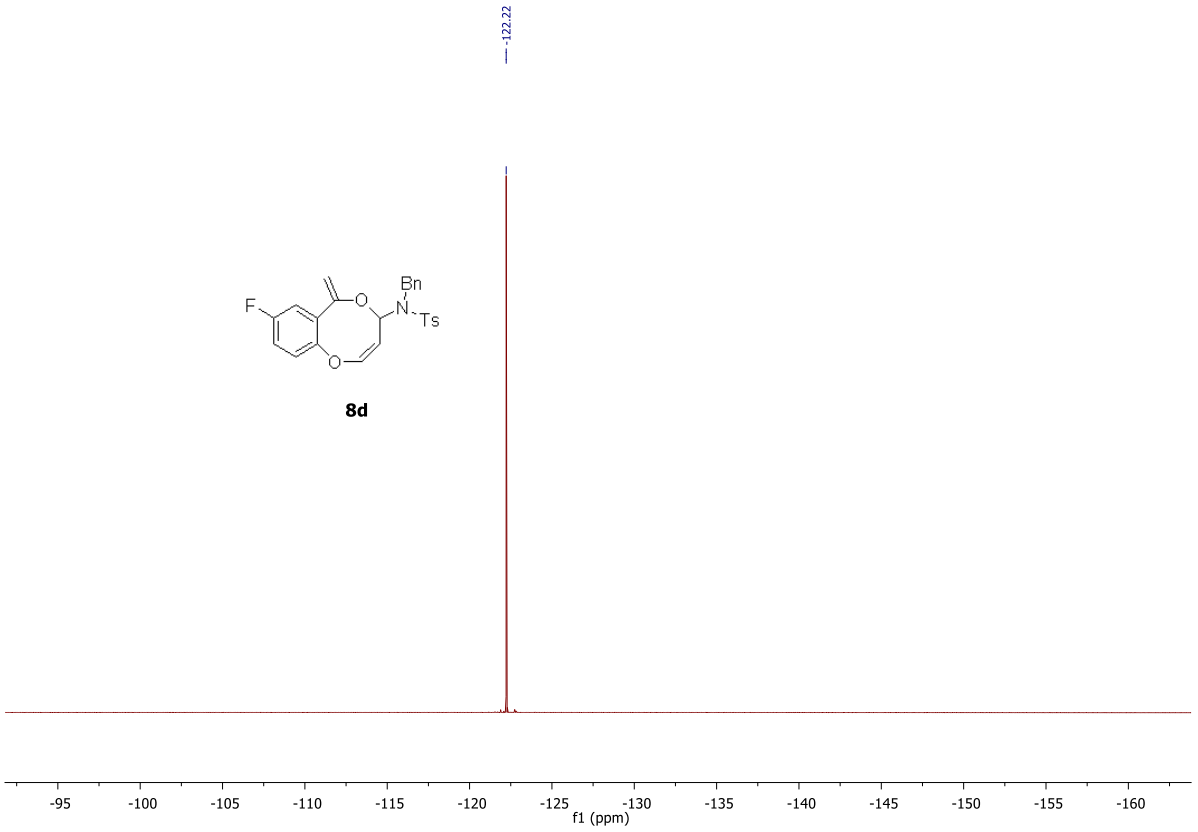

F
O
Bn
N
Ts
O

4d

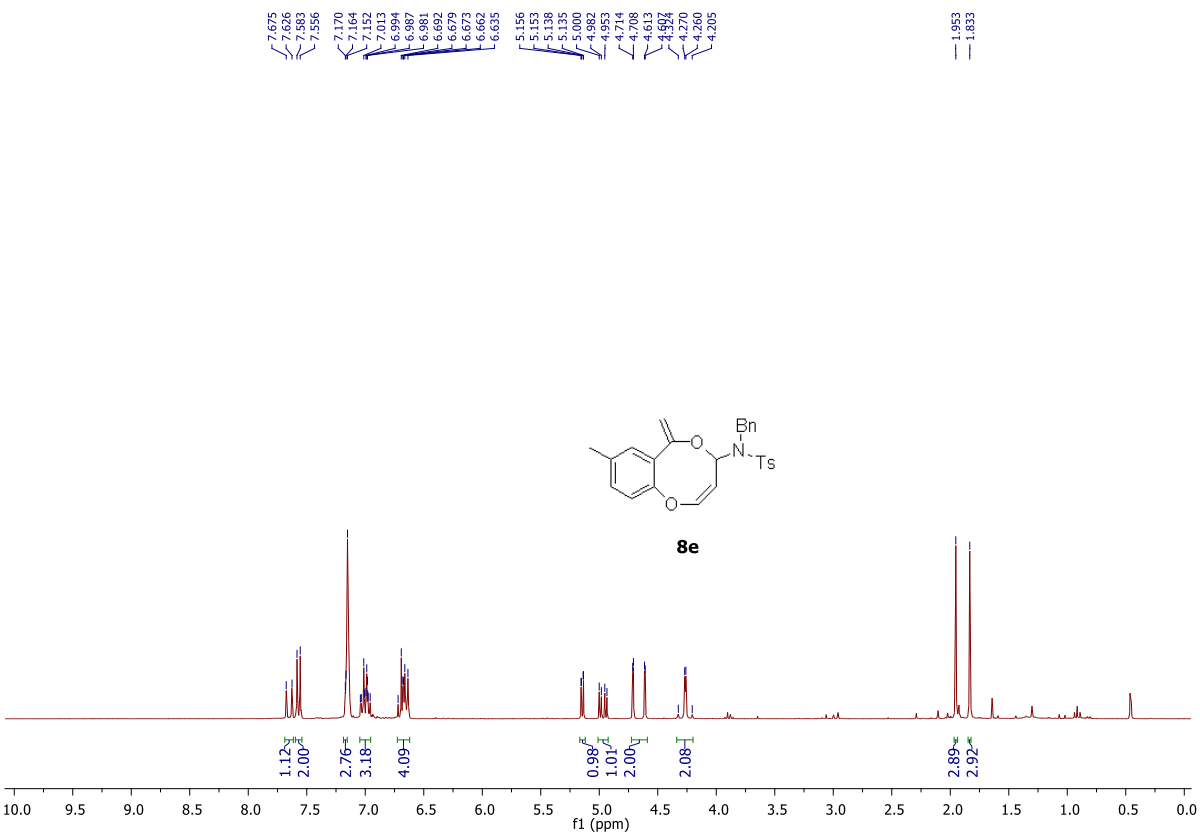

1.00
2.13
1.91
2.34
2.22
2.31
2.16
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

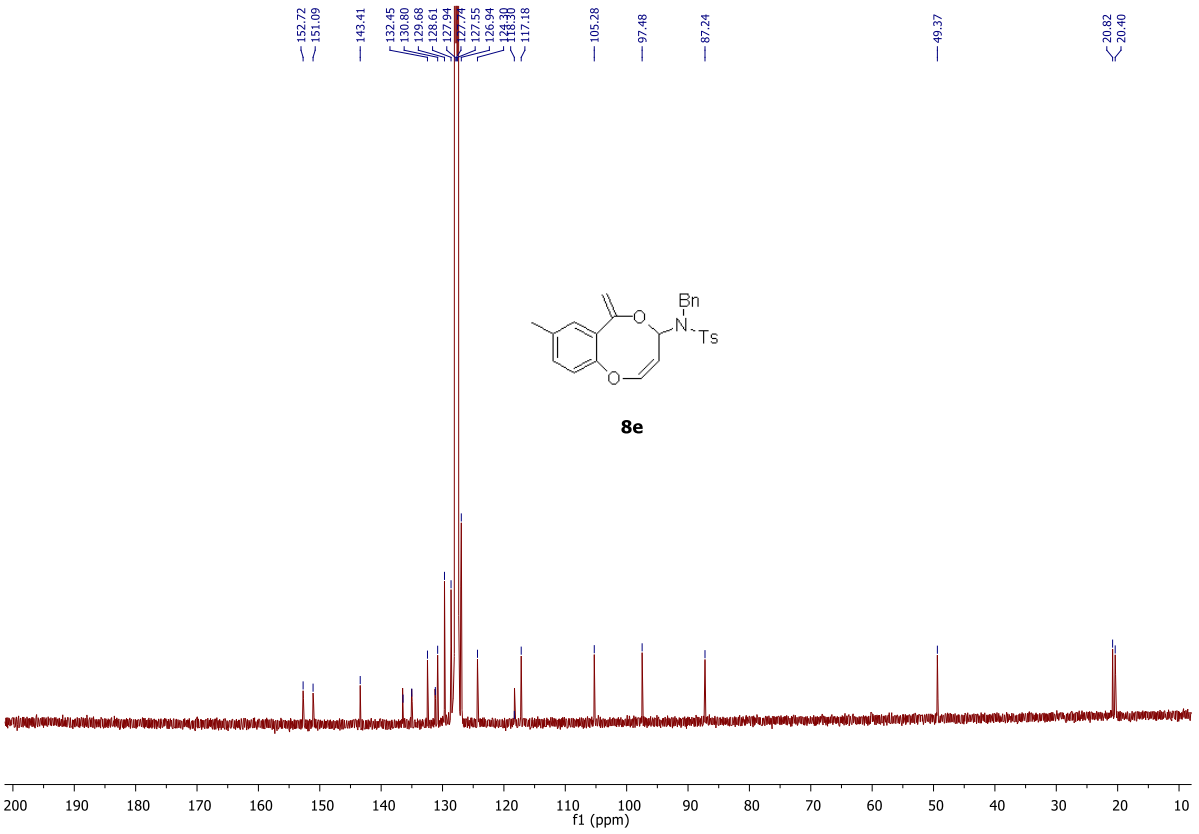

158.73
156.82
151.46
151.43
148.98
148.97
143.51
129.66
128.58
127.99
127.89
127.70
126.95
126.85
118.67
118.61
116.96
109.90
104.67
97.55
88.78
49.31
20.77
F
O
N
Bn
Ts
O
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

8d

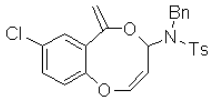

-122.22
F
O
N
Bn
Ts
O
-95
-100
-105
-110
-115
-120
-125
-130
-135
-140
-145
-150
-155
-160
f1 (ppm)

8d

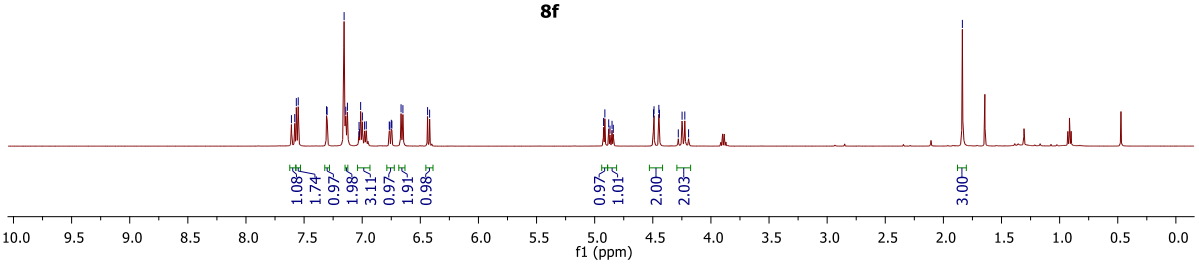

7.675
7.626
7.583
7.556
7.170
7.164
7.152
7.013
6.994
6.987
6.981
6.692
6.679
6.673
6.662
6.635
5.156
5.153
5.138
5.135
5.000
4.982
4.953
4.714
4.708
4.613
4.270
4.260
4.205
1.953
1.833
Bn
N
Ts
O
8e
1.12
2.00
2.76
3.18
4.09
0.98
1.01
2.00
2.08
2.89
2.92
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

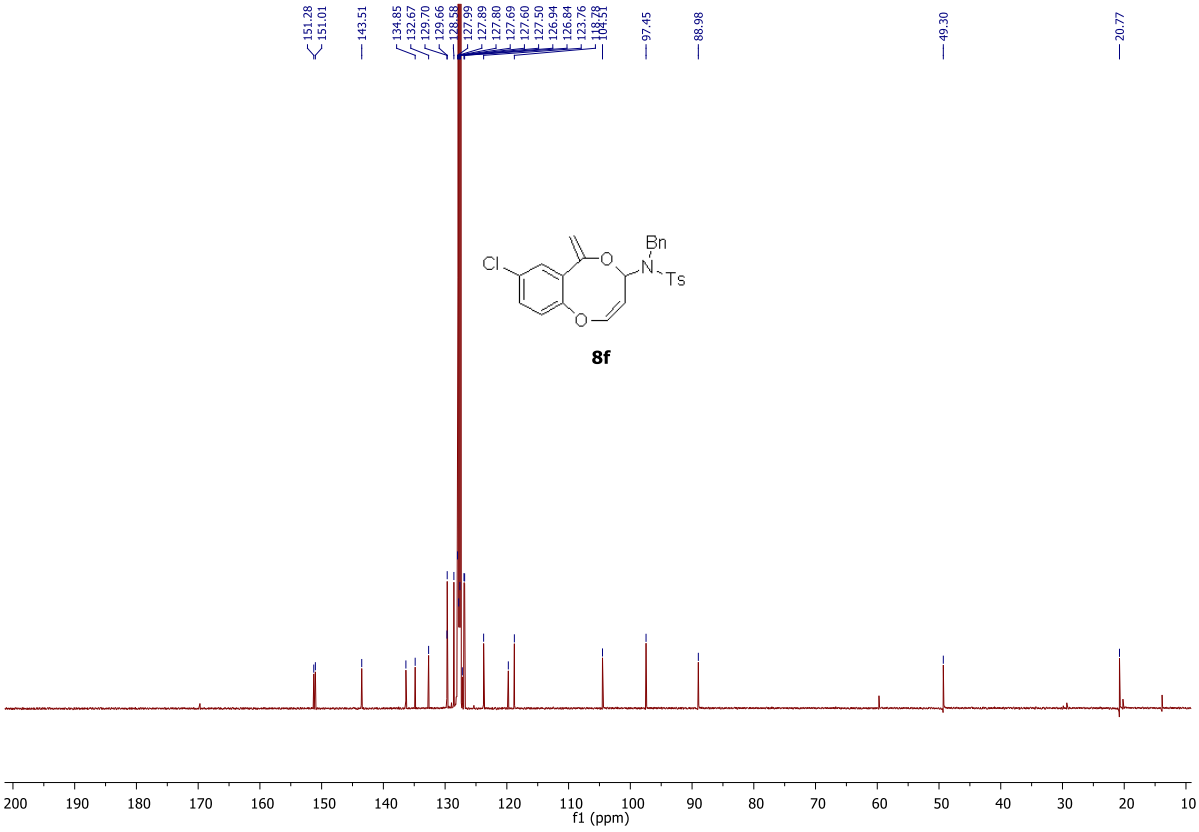

152.72
151.09
143.41
132.45
130.80
129.68
128.61
127.94
127.55
126.94
124.30
118.38
117.18
105.28
97.48
87.24
49.37
20.82
20.40
Bn
N
Ts
O
8e
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.609
7.580
7.567
7.550
7.307
7.302
7.156
7.141
7.127
7.027
7.024
7.013
6.998
6.979
6.965
6.767
6.762
6.750
6.745
6.666
6.650
6.437
6.420
4.923
4.912
4.879
4.868
4.851
4.840
4.494
4.489
4.448
4.443
4.281
4.248
4.225
4.192
1.837


Cl
O
Bn
N
Ts
O

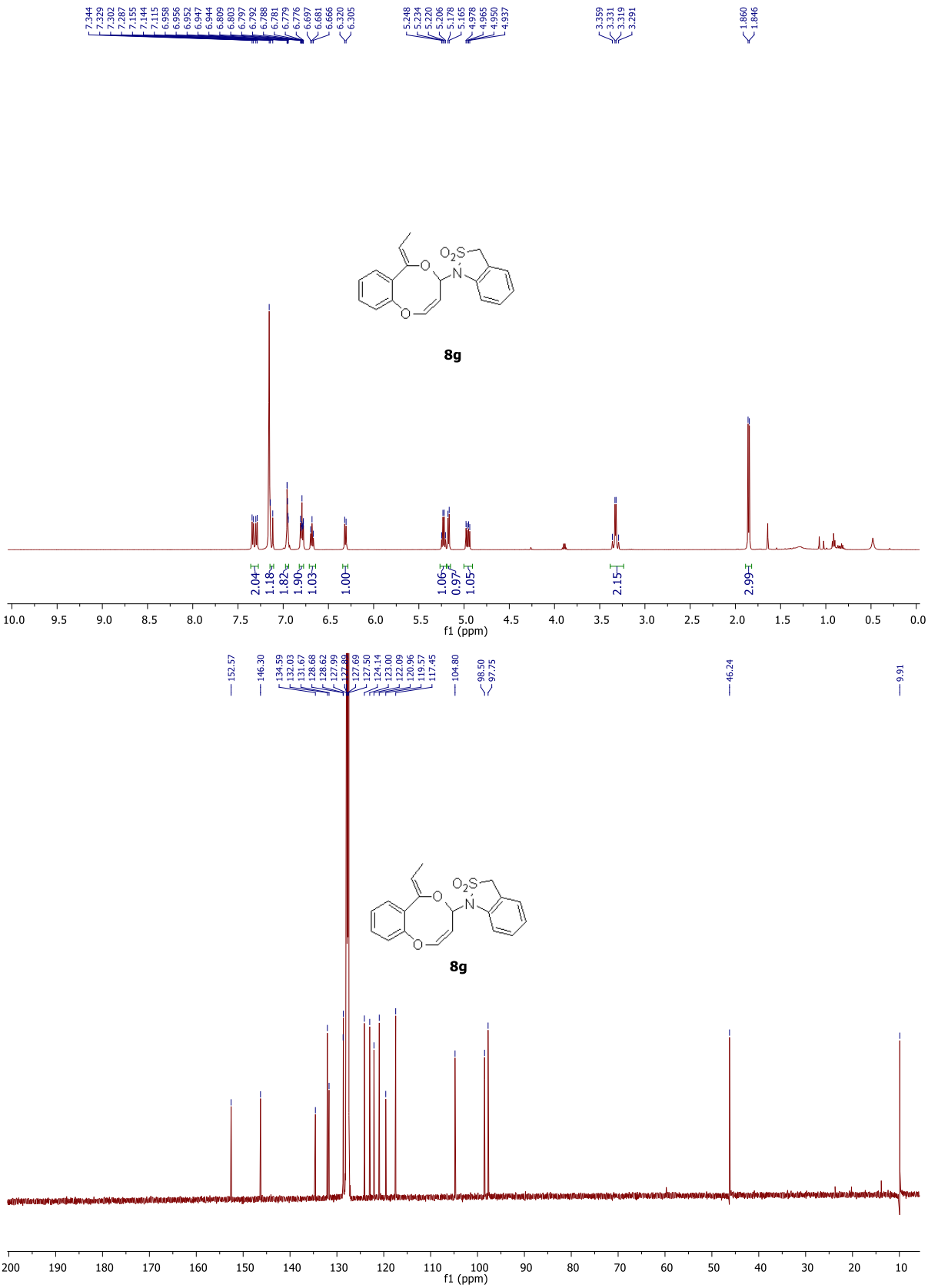
8f

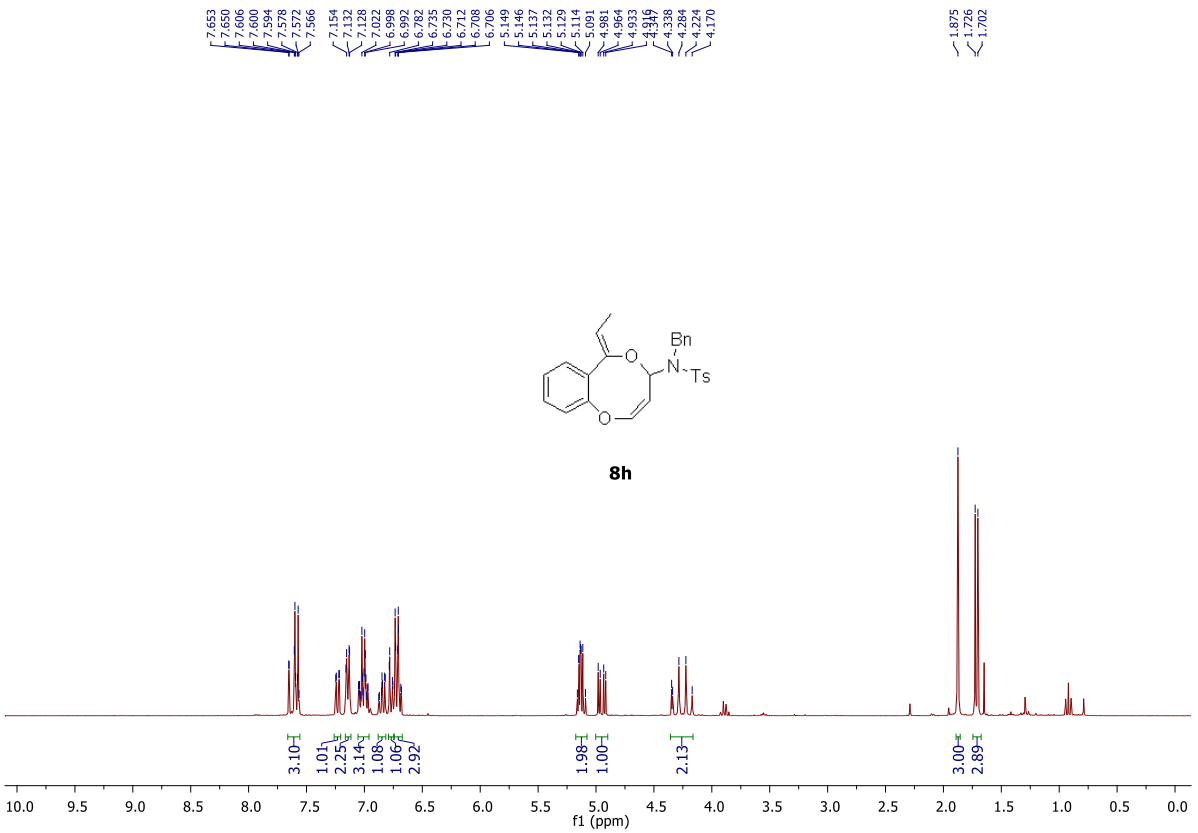

1.08
1.74
0.97
1.98
3.11
0.97
1.91
0.98
0.97
1.01
2.00
2.03
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

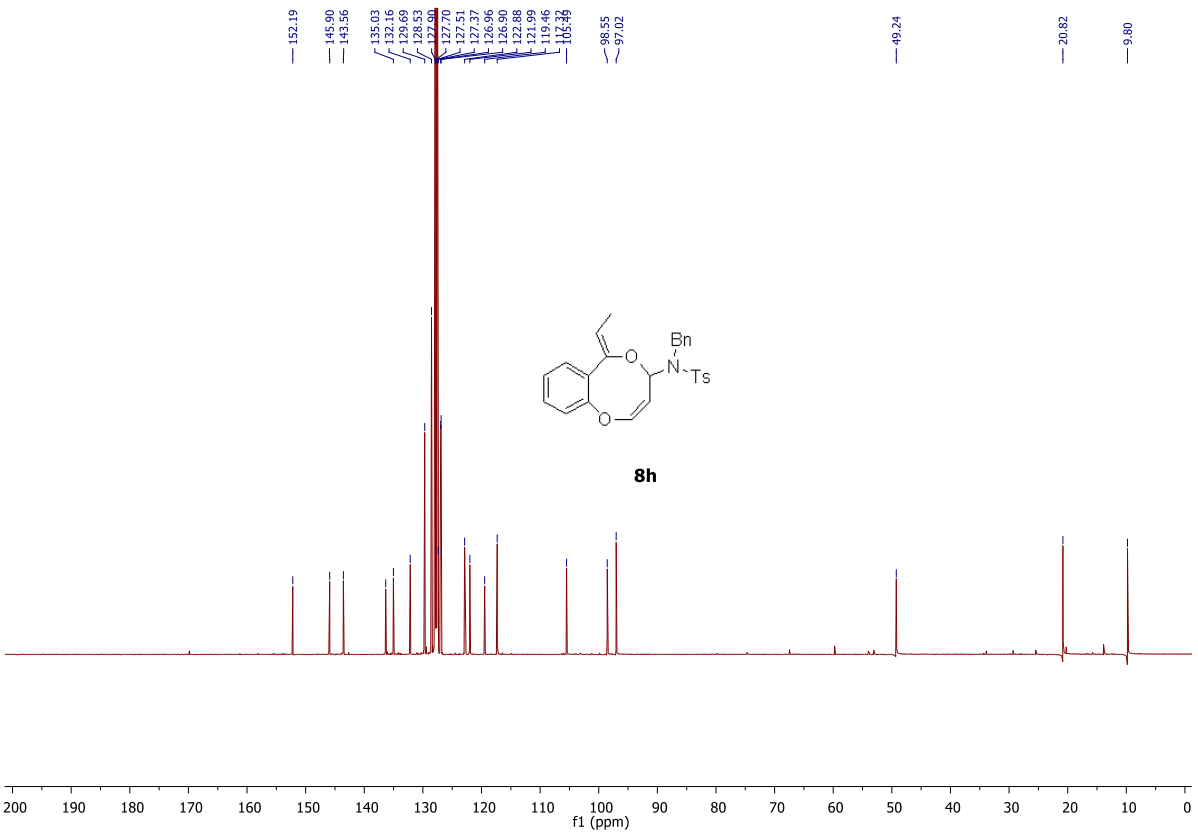

151.28
151.01
143.51
134.85
132.67
129.70
129.66
128.58
127.99
127.89
127.80
127.69
127.60
127.50
126.94
126.84
123.76
118.78
104.51
97.45
88.98
49.30
20.77
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

Cl
O
Bn
N
Ts
O

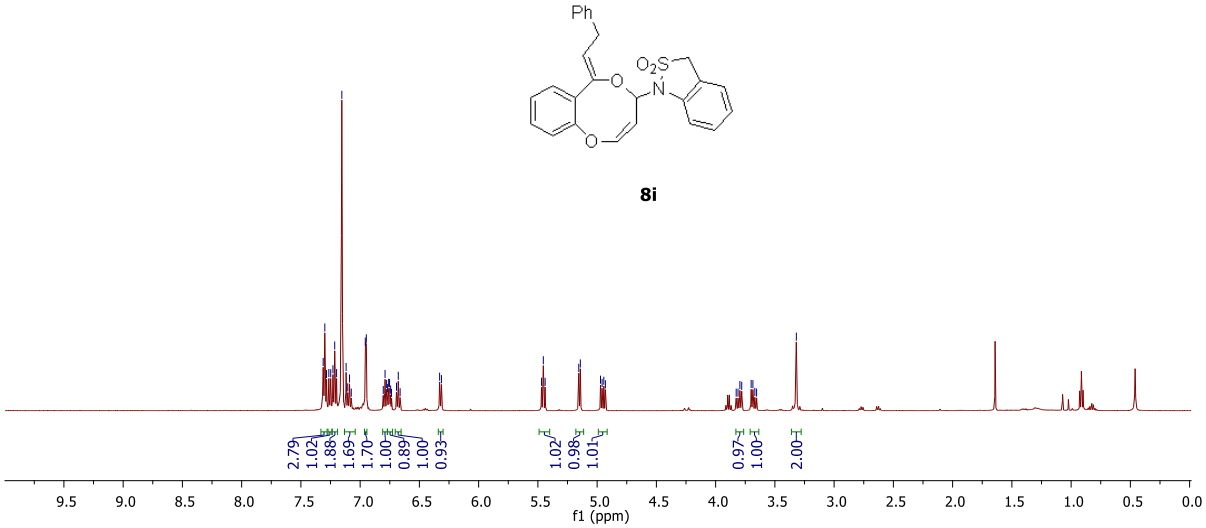
8f


7.344
7.329
7.302
7.287
7.155
7.144
7.115
6.958
6.956
6.952
6.947
6.944
6.809
6.803
6.797
6.792
6.788
6.781
6.779
6.776
6.697
6.681
6.666
6.320
6.305
5.248
5.234
5.220
5.206
5.178
5.165
4.978
4.965
4.950
4.937
3.359
3.331
3.319
3.291
1.860
1.846
8g
2.04
1.18
1.82
1.90
1.03
1.00
1.06
0.97
1.05
2.15
2.99
f1 (ppm)
152.57
146.30
134.59
132.03
131.67
128.68
128.62
127.99
127.80
127.69
127.50
124.14
123.00
122.09
120.96
119.57
117.45
104.80
98.50
97.75
46.24
9.91
8g
f1 (ppm)

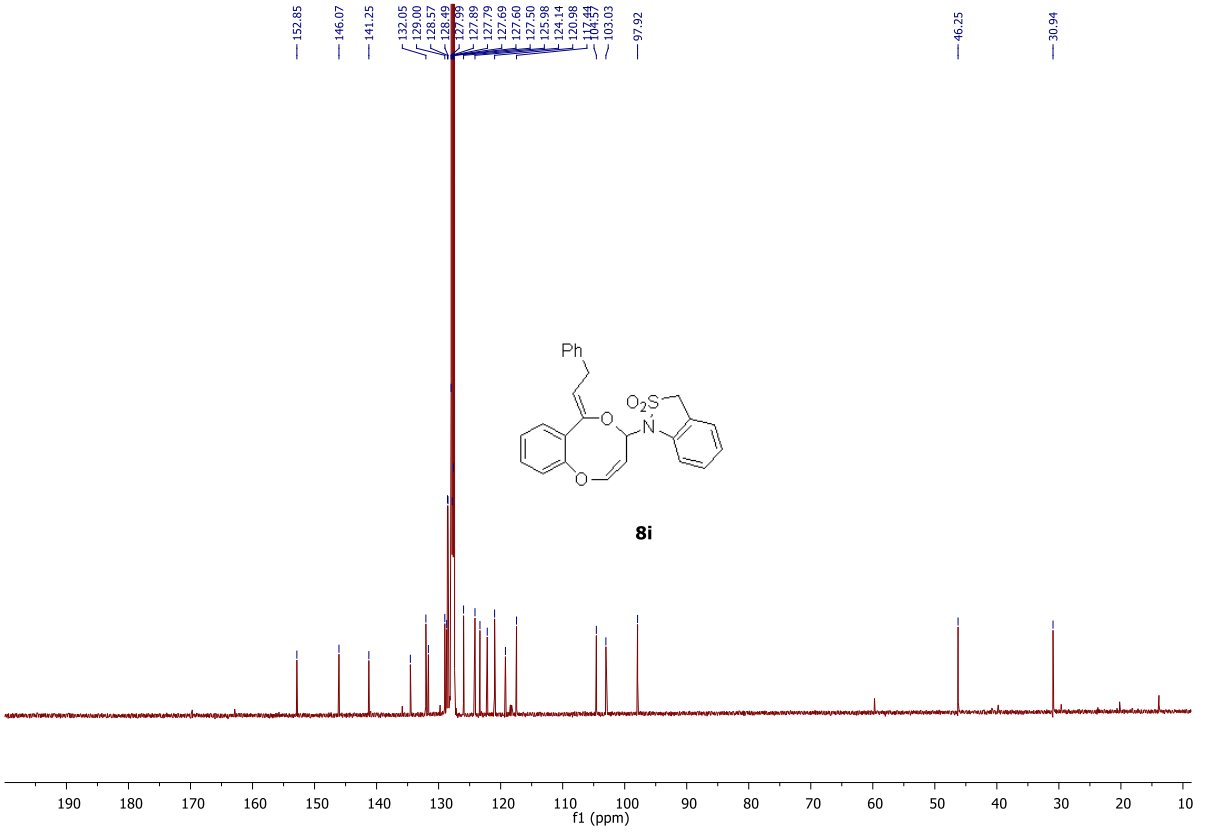

7.653
7.650
7.606
7.600
7.594
7.578
7.572
7.566
7.154
7.132
7.128
7.022
6.998
6.992
6.782
6.735
6.730
6.712
6.708
6.706
5.149
5.146
5.137
5.132
5.129
5.114
5.091
4.981
4.964
4.933
4.338
4.284
4.224
4.170
1.875
1.726
1.702
Bn
N
Ts
O
O
8h
3.10
1.01
2.25
3.14
1.08
1.06
2.92
1.98
1.00
2.13
3.00
2.89
f1 (ppm)


152.19
145.90
143.56
135.03
132.16
129.69
128.53
127.70
127.51
127.37
126.96
126.90
122.88
121.99
119.46
98.55
97.02
49.24
20.82
9.80
Bn
N
Ts
O
O
8h
f1 (ppm)


7.312
7.298
7.284
7.264
7.248
7.230
7.214
7.199
7.155
7.118
7.104
7.090
7.075
6.956
6.948
6.805
6.790
6.777
6.768
6.760
6.752
6.743
6.735
6.693
6.678
6.663
6.329
6.314
5.469
5.454
5.439
5.155
5.142
4.972
4.958
4.944
4.930
3.827
3.811
3.795
3.780
3.700
3.685
3.669
3.654
3.319

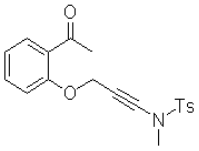

Ph
O2S
N
O
O
2.79
1.02
1.88
1.69
1.70
1.00
0.89
1.00
0.93
1.02
0.98
1.01
0.97
1.00
2.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

8i

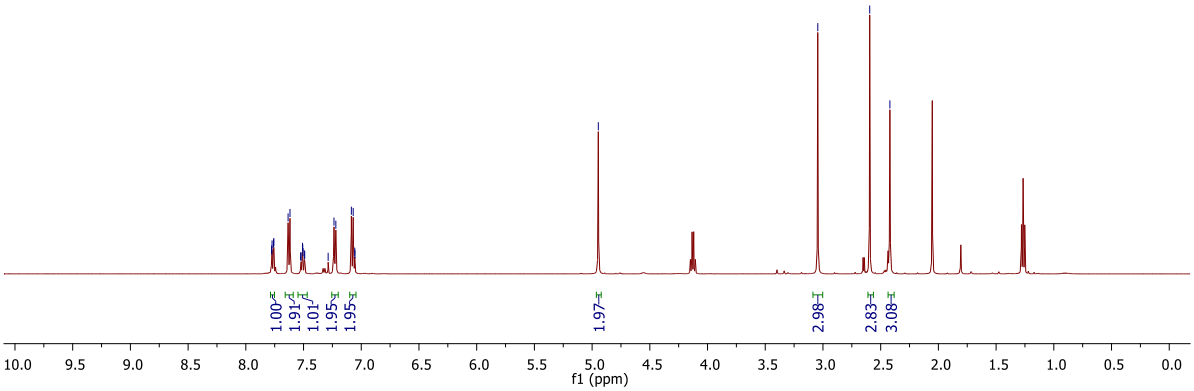

152.85
146.07
141.25
132.05
129.00
128.57
128.49
127.95
127.89
127.79
127.69
127.60
127.50
125.98
124.14
120.98
117.44
104.57
103.03
97.92
46.25
30.94
Ph
O2S
N
O
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

8i

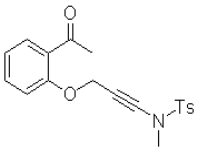

7.777
7.775
7.773
7.760
7.757
7.634
7.617
7.525
7.521
7.509
7.507
7.505
7.494
7.490
7.287
7.236
7.220
7.086
7.070
7.056
7.055
4.946
3.045
2.595
2.420


O
O
N
Ts

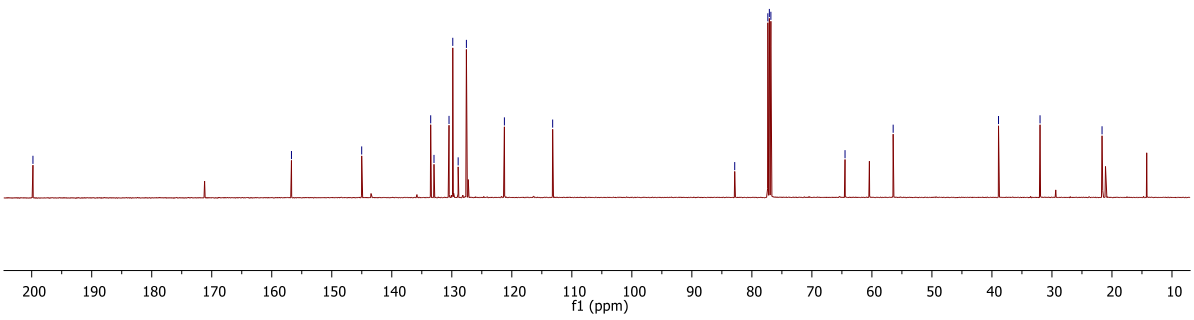
5a


1.00
1.91
1.01
1.95
1.95
1.97
2.98
2.83
3.08
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

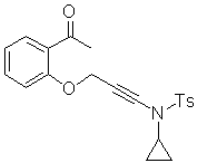

199.79
156.72
145.01
133.52
132.97
130.46
129.84
128.94
127.57
121.24
113.19
82.86
77.34
77.09
76.83
64.48
56.46
38.90
31.98
21.65


O
O
N
Ts

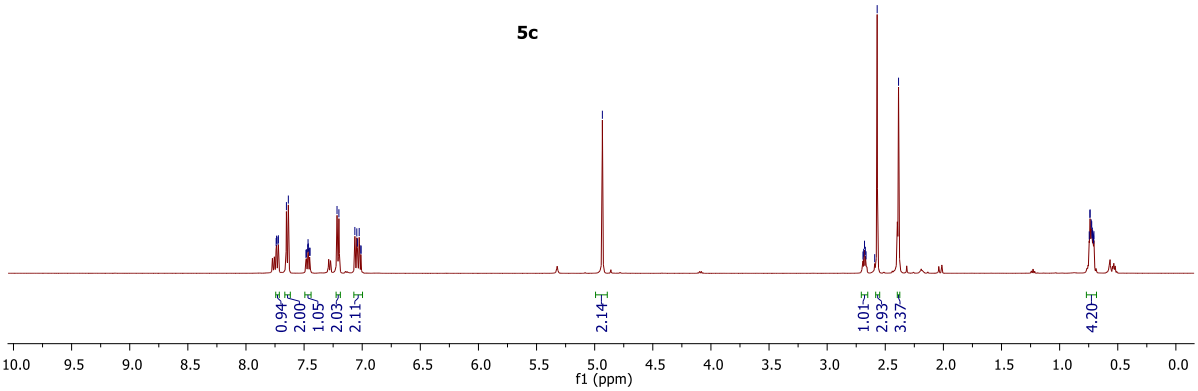
5a


200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

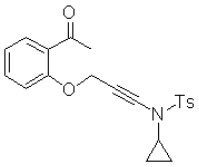

7.740
7.737
7.725
7.721
7.652
7.635
7.484
7.480
7.469
7.466
7.463
7.452
7.449
7.217
7.200
7.063
7.046
7.041
7.026
7.011
7.010
4.934
2.692
2.686
2.679
2.671
2.665
2.591
2.570
2.386
0.745
0.739
0.738
0.728
0.724
0.722
0.719
0.715
0.712
0.710
0.707
0.705


O
O
N
Ts

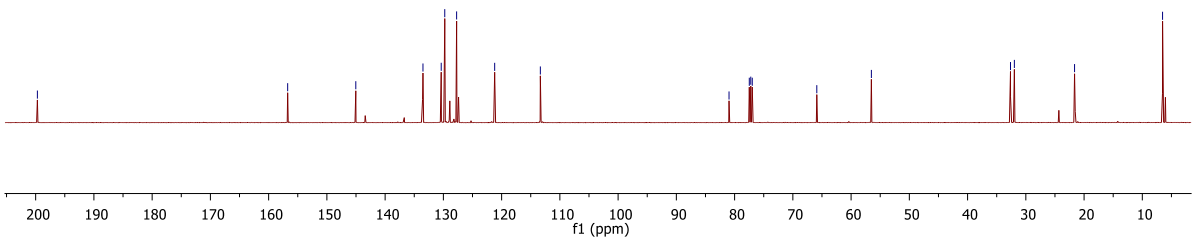
5c

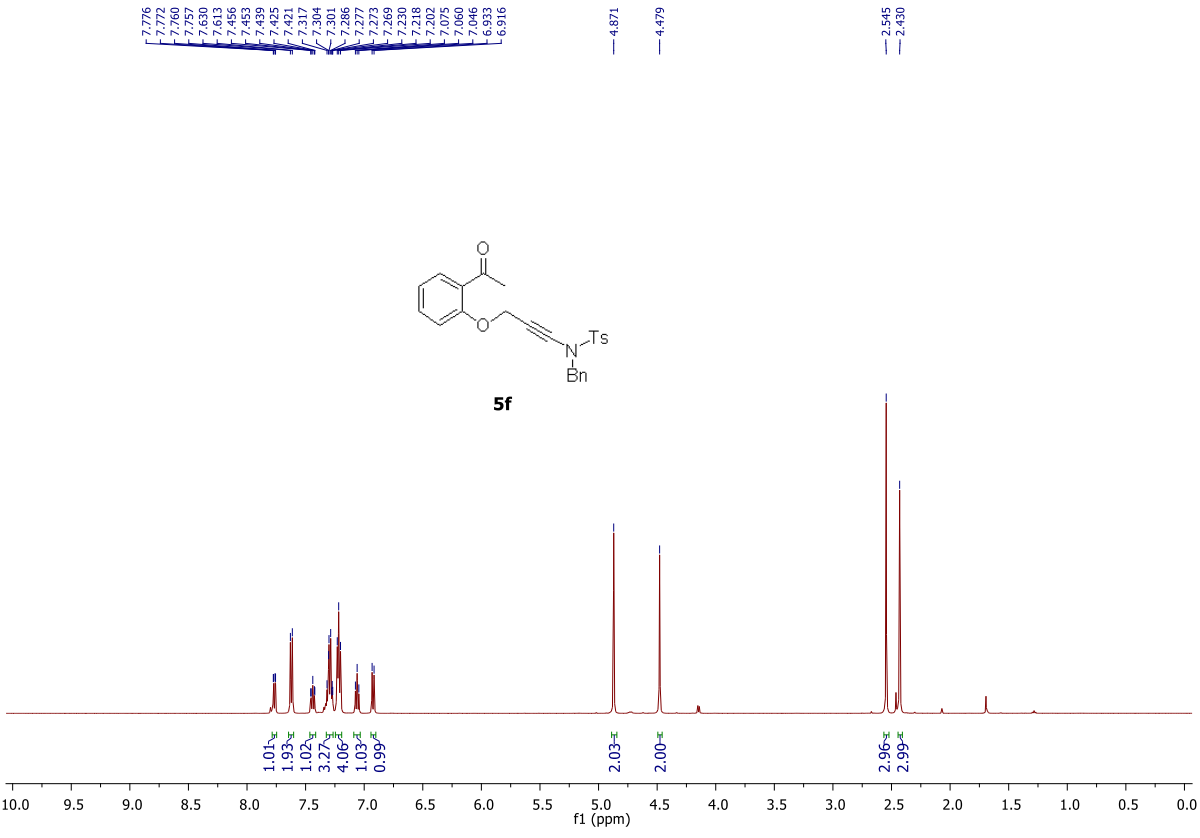

0.94
2.00
1.05
2.03
2.11
2.14
1.01
2.93
3.37
4.20
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

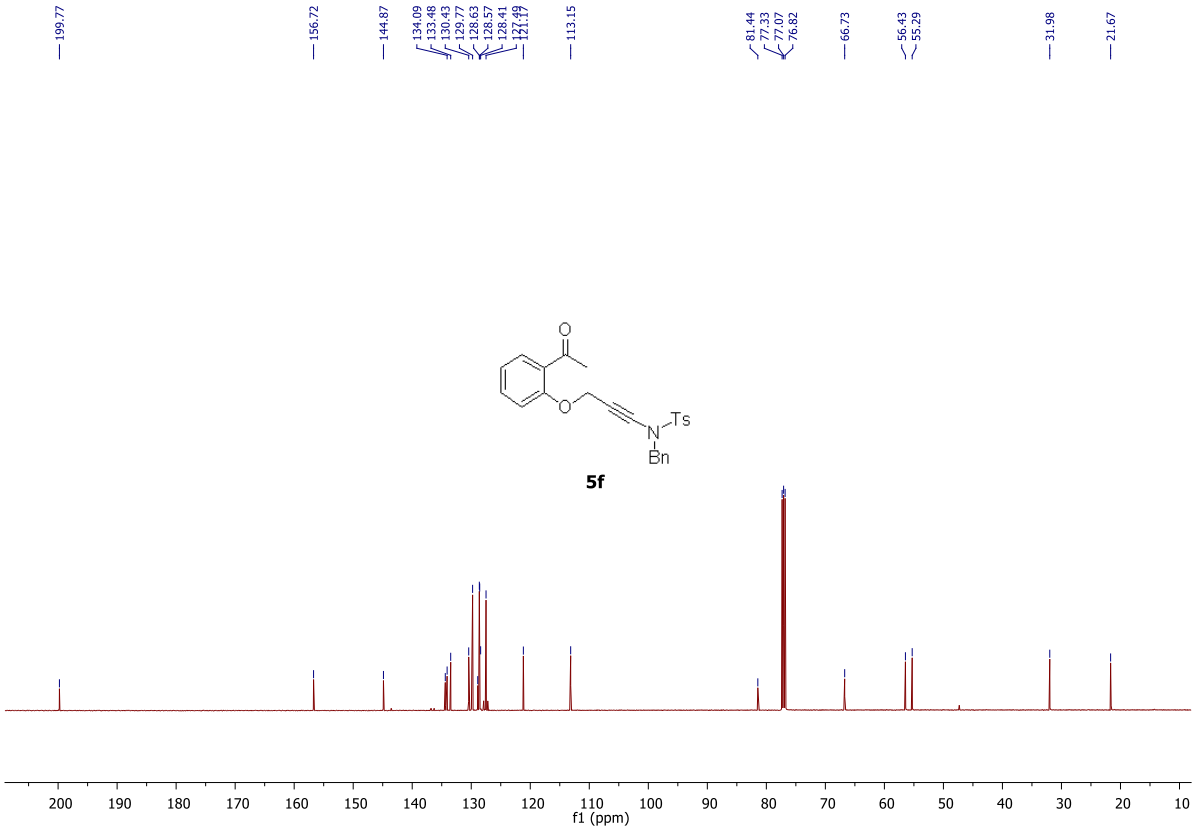

199.70
156.73
145.03
133.50
130.37
129.76
127.73
121.19
113.35
80.96
77.48
77.22
76.97
65.89
56.52
32.63
31.97
21.63
6.52


O
O
N
Ts

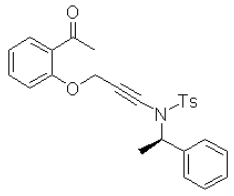
5c


200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

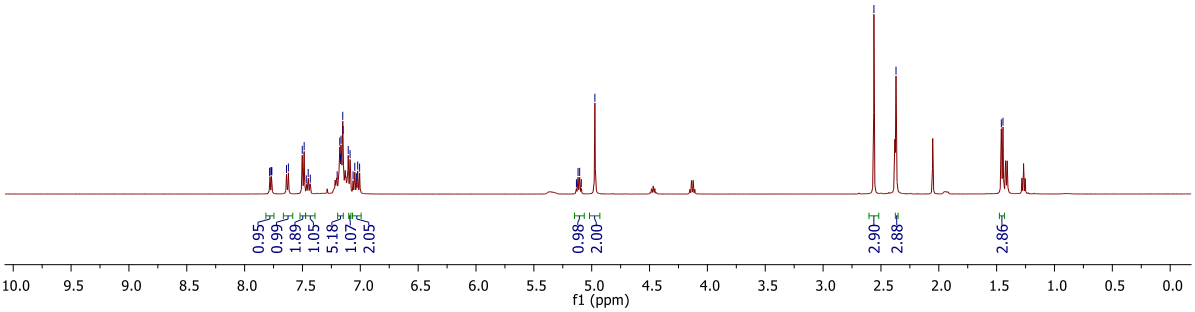

7.776
7.772
7.760
7.757
7.630
7.613
7.456
7.453
7.439
7.425
7.421
7.317
7.304
7.301
7.286
7.277
7.273
7.269
7.230
7.218
7.202
7.075
7.060
7.046
6.933
6.916
4.871
4.479
2.545
2.430
O
O
N
Ts
Bn
5f
1.01
1.93
1.02
3.27
4.06
1.03
0.99
2.03
2.00
2.96
2.99
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


199.77
156.72
144.87
134.09
133.48
130.43
129.77
128.63
128.57
128.41
127.49
121.17
113.15
81.44
77.33
77.07
76.82
66.73
56.43
55.29
31.98
21.67
O
O
N
Ts
Bn
5f
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

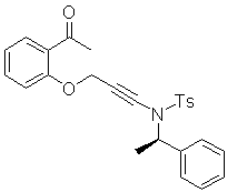

7.783
7.780
7.768
7.765
7.638
7.622
7.502
7.485
7.467
7.450
7.432
7.200
7.177
7.171
7.167
7.152
7.149
7.105
7.089
7.063
7.048
7.034
7.023
7.006
5.132
5.118
5.104
5.090
4.973
2.561
2.370
1.459
1.445


O
O
N
Ts

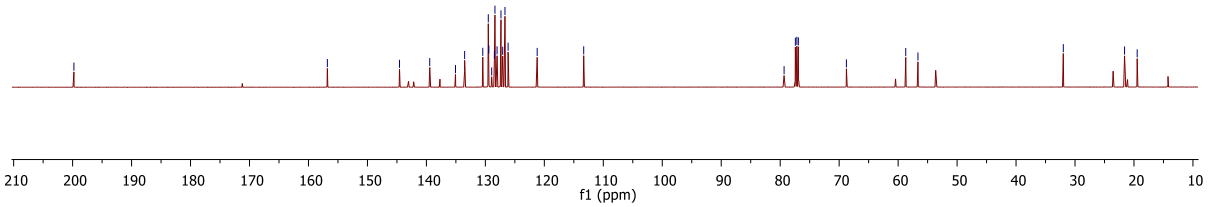
5h

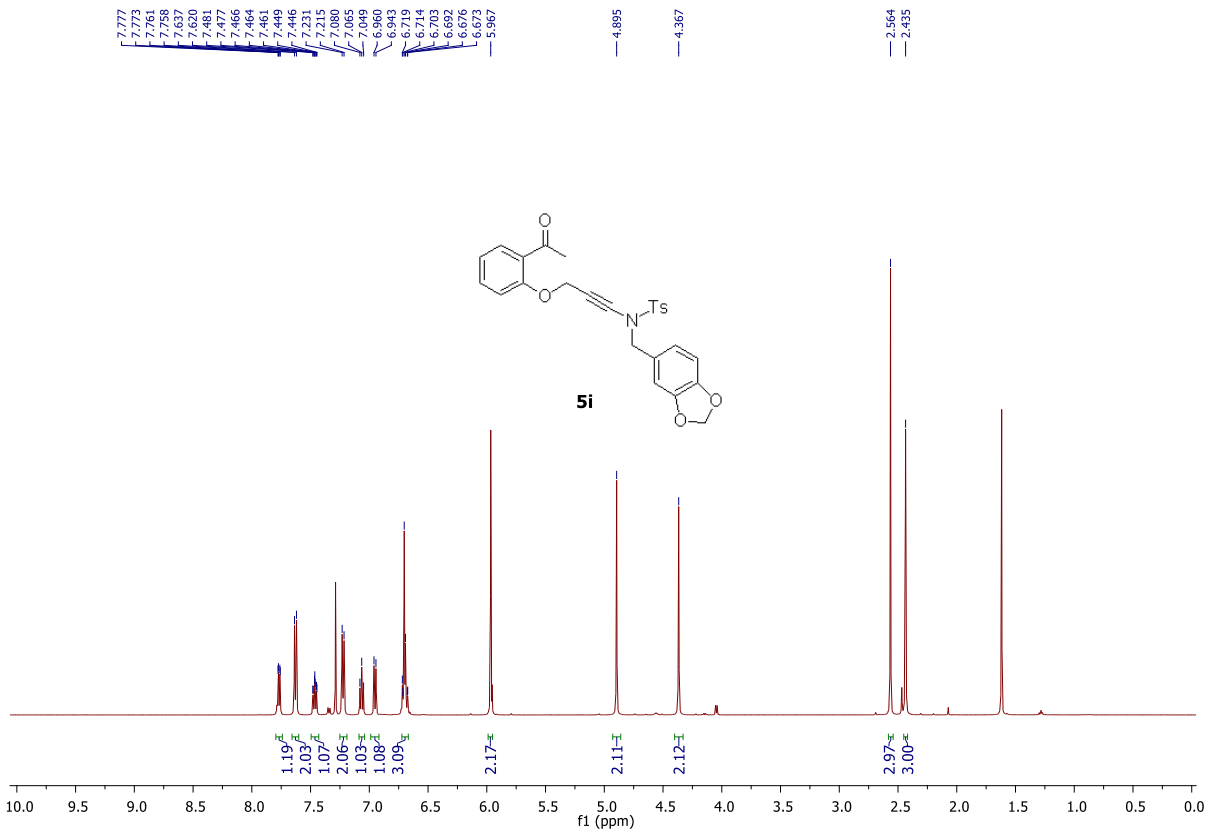

0.95
0.99
1.89
1.05
5.18
1.07
2.05
0.98
2.00
2.90
2.88
2.86
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


199.78
156.80
144.56
129.50
129.41
128.38
128.02
127.35
127.06
126.67
113.32
79.34
77.43
77.17
76.92
68.77
58.71
56.64
31.99
21.60
19.46


O
O
N
Ts

5h


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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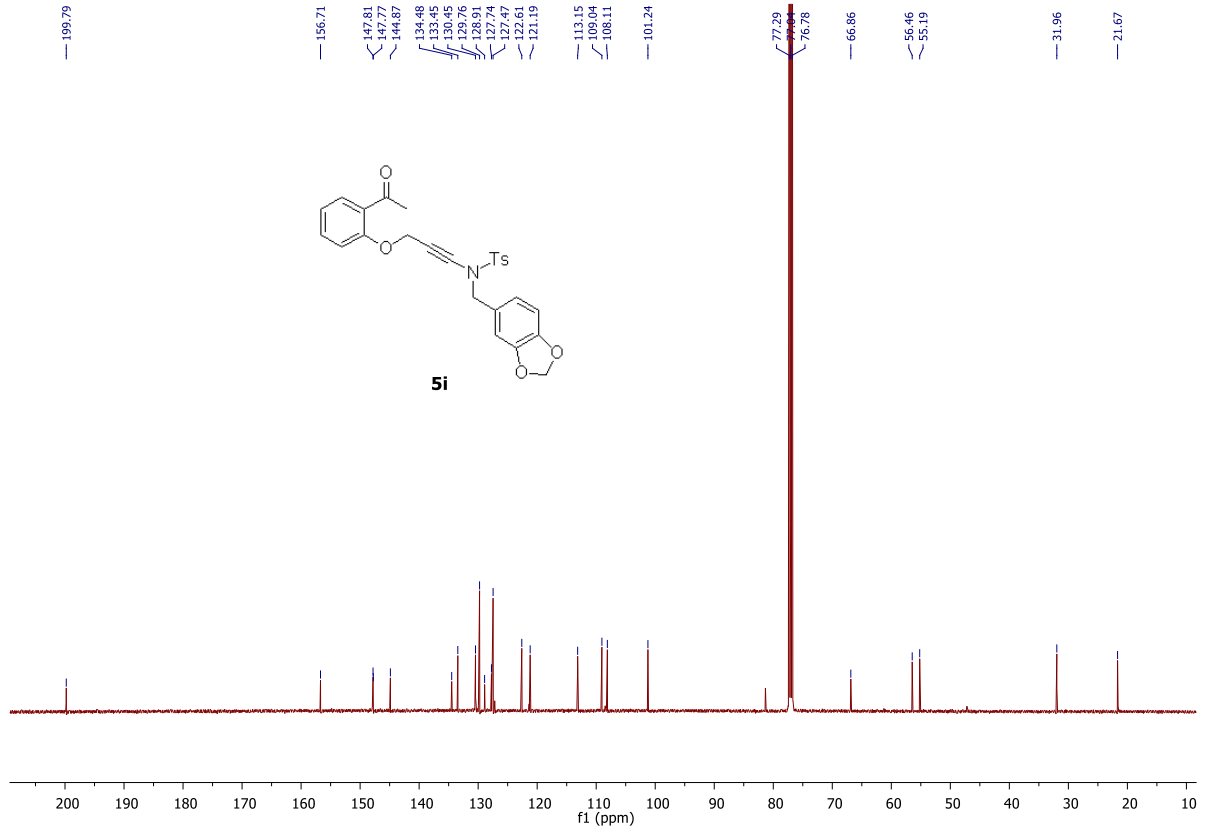
7.773
7.761
7.758
7.637
7.620
7.481
7.477
7.466
7.464
7.461
7.449
7.446
7.231
7.215
7.080
7.065
7.049
6.960
6.943
6.719
6.714
6.703
6.692
6.676
6.673
5.967
4.895
4.367
2.564
2.435
Ts
O
N
5i
1.19
2.03
1.07
2.06
1.03
1.08
3.09
2.17
2.11
2.12
2.97
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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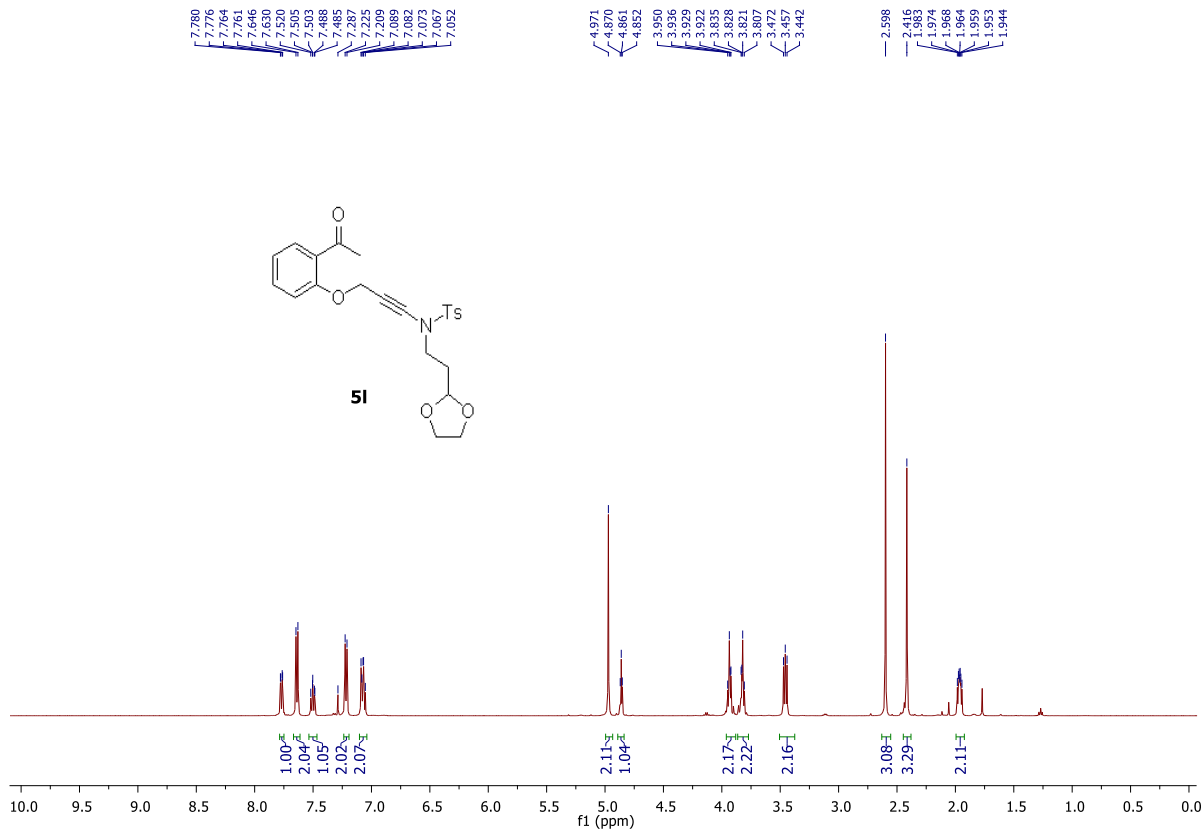
147.81
147.77
144.87
134.48
133.45
130.45
129.76
128.91
127.74
127.47
122.61
121.19
113.15
109.04
108.11
101.24
77.29
77.04
76.78
66.86
56.46
55.19
31.96
21.67
Ts
O
N
5i
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)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7.776
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7.761
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7.505
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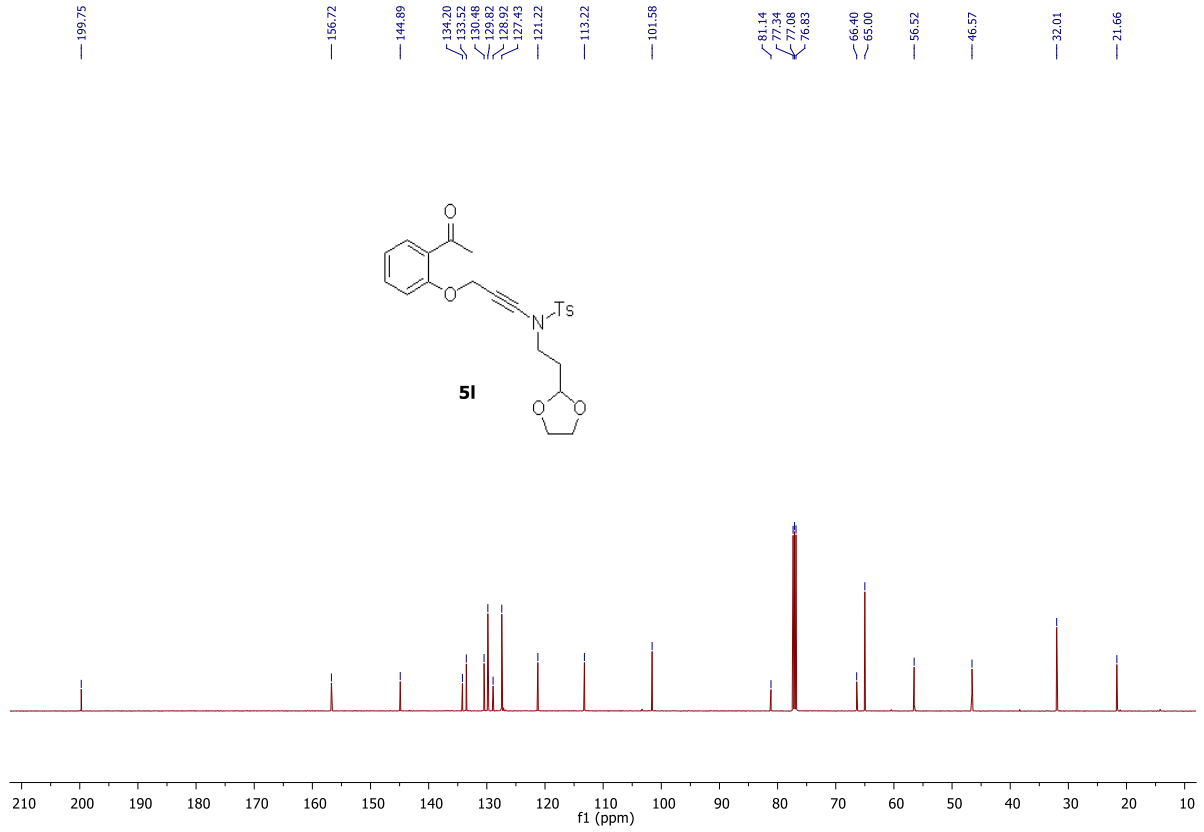
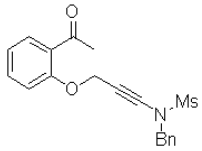
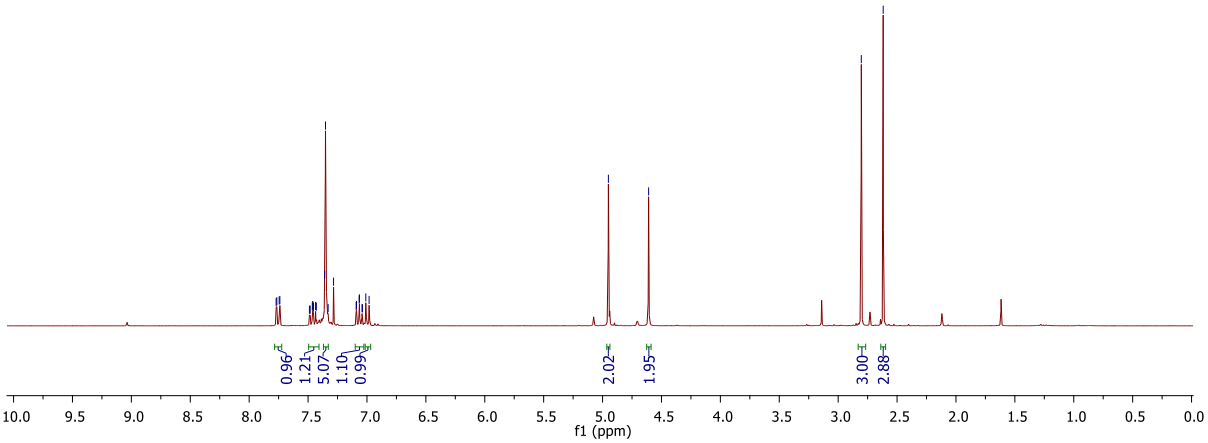
7.485
7.287
7.225
7.209
7.089
7.082
7.073
7.067
7.052
4.971
4.870
4.861
4.852
3.950
3.936
3.929
3.922
3.835
3.828
3.821
3.807
3.472
3.457
3.442
2.598
2.416
1.983
1.974
1.968
1.964
1.959
1.953
1.944
O
O
N
Ts
O
O
5l
1.00
2.04
1.05
2.02
2.07
2.11
1.04
2.17
2.22
2.16
3.08
3.29
2.11
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


199.75
156.72
144.89
134.20
133.52
130.48
129.82
128.92
127.43
121.22
113.22
101.58
81.14
77.34
77.08
76.83
66.40
65.00
56.52
46.57
32.01
21.66
O
O
N
Ts
O
O
5l
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

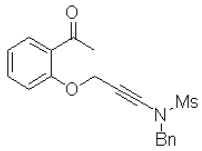

7.771
7.765
7.745
7.739
7.488
7.482
7.464
7.460
7.458
7.454
7.436
7.430
7.359
7.352
7.330
7.284
7.092
7.089
7.066
7.064
7.042
7.038
7.010
6.982
4.950
4.609
2.804
2.618


O
O
N
Ms
Bn

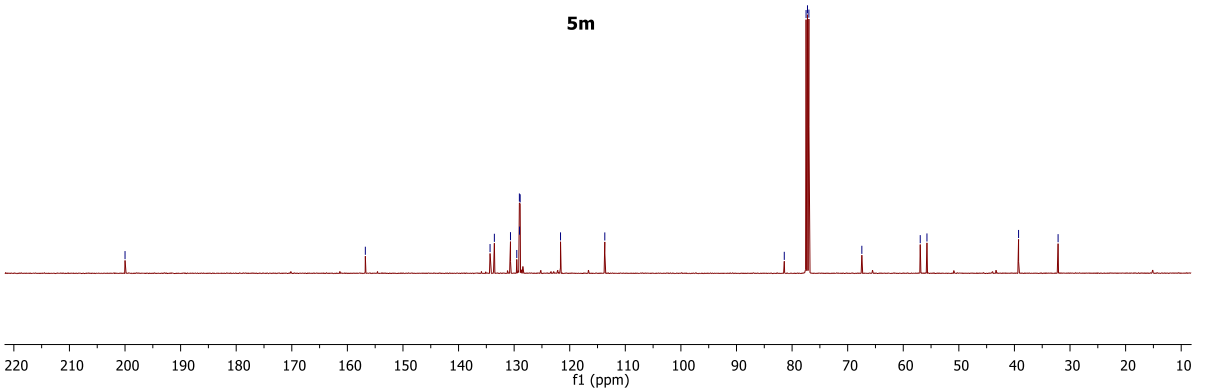
5m

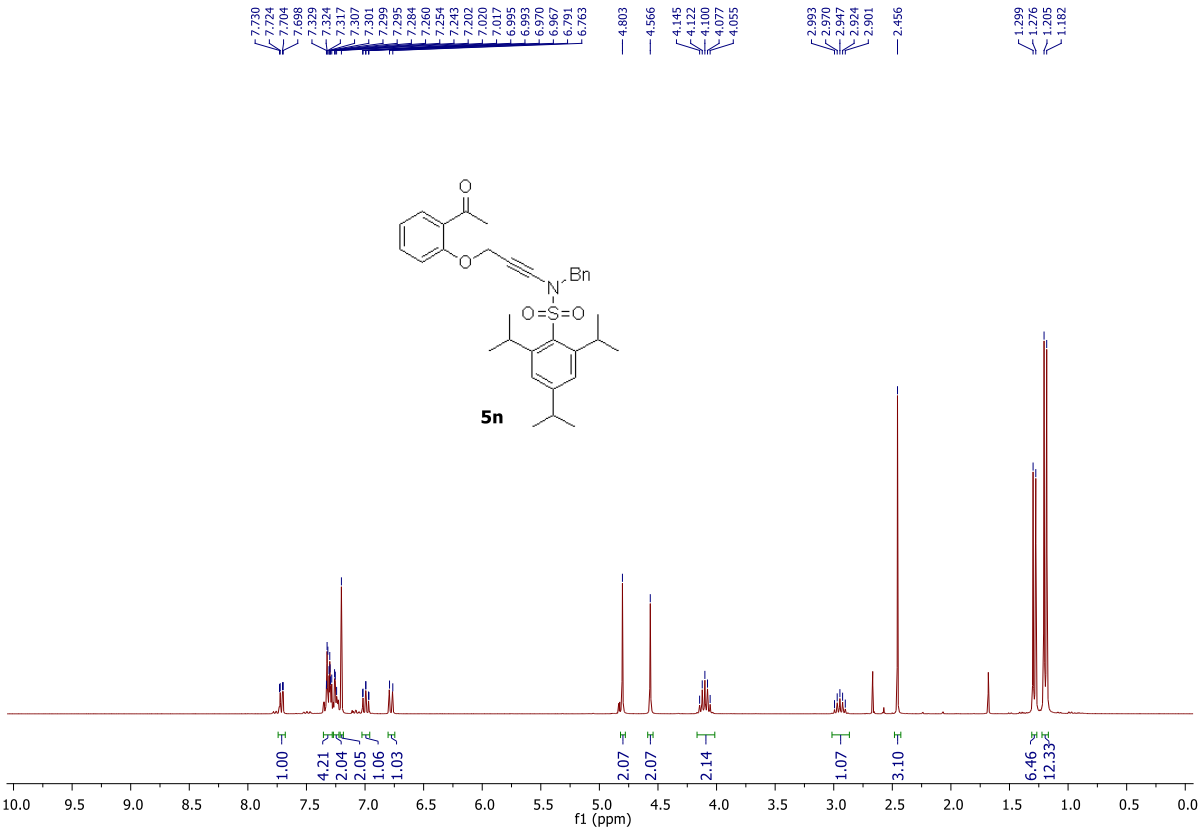

0.96
1.21
5.07
1.10
0.99
2.02
1.95
3.00
2.88
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

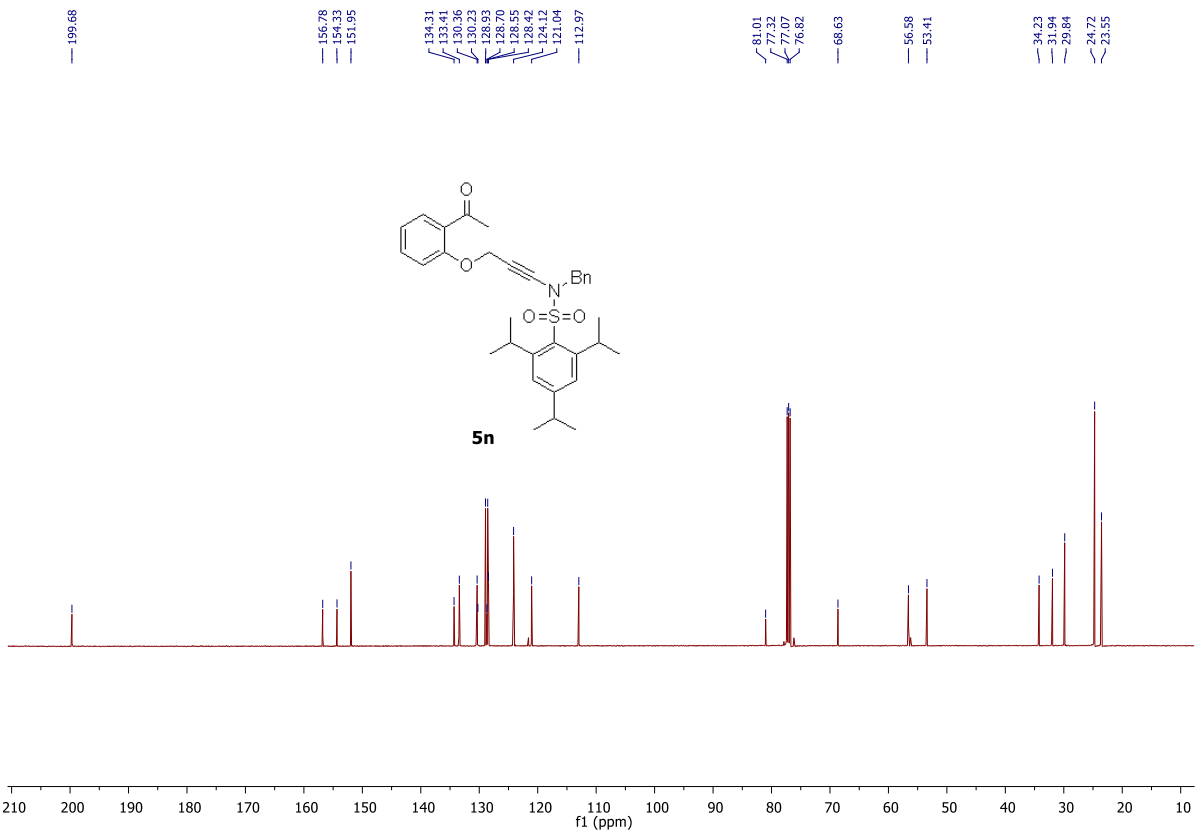

200.00
156.77
134.33
133.56
130.66
129.53
129.06
129.03
128.92
121.66
113.69
81.40
77.48
77.23
76.98
67.45
56.95
55.74
39.26
32.15


O
O
N
Ms
Bn

5m


220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.730
7.724
7.704
7.698
7.329
7.324
7.317
7.307
7.301
7.299
7.295
7.284
7.260
7.254
7.243
7.202
7.020
7.017
6.995
6.993
6.970
6.967
6.791
6.763
4.803
4.566
4.145
4.122
4.100
4.077
4.055
2.993
2.970
2.947
2.924
2.901
2.456
1.299
1.276
1.205
1.182
Bn
N
O=S=O
5n
1.00
4.21
2.04
2.05
1.06
1.03
2.07
2.07
2.14
1.07
3.10
6.46
12.33
f1 (ppm)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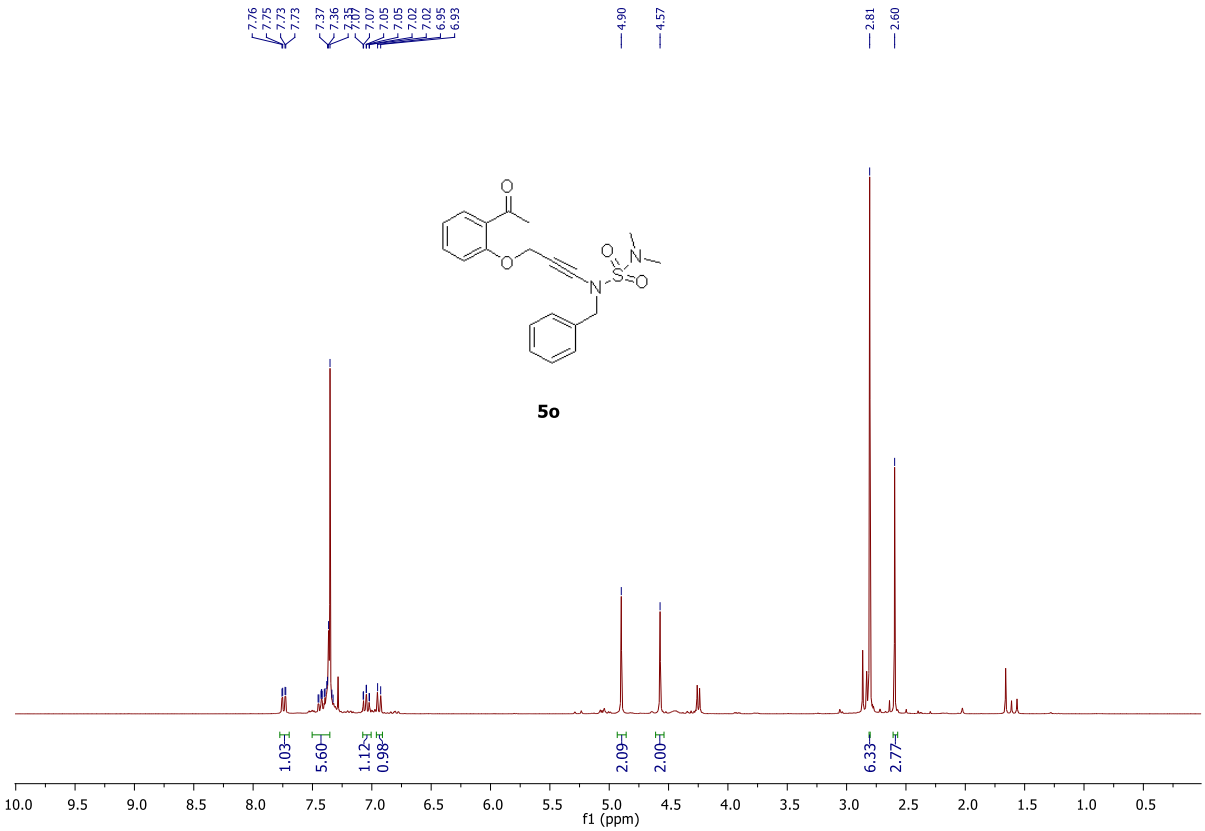
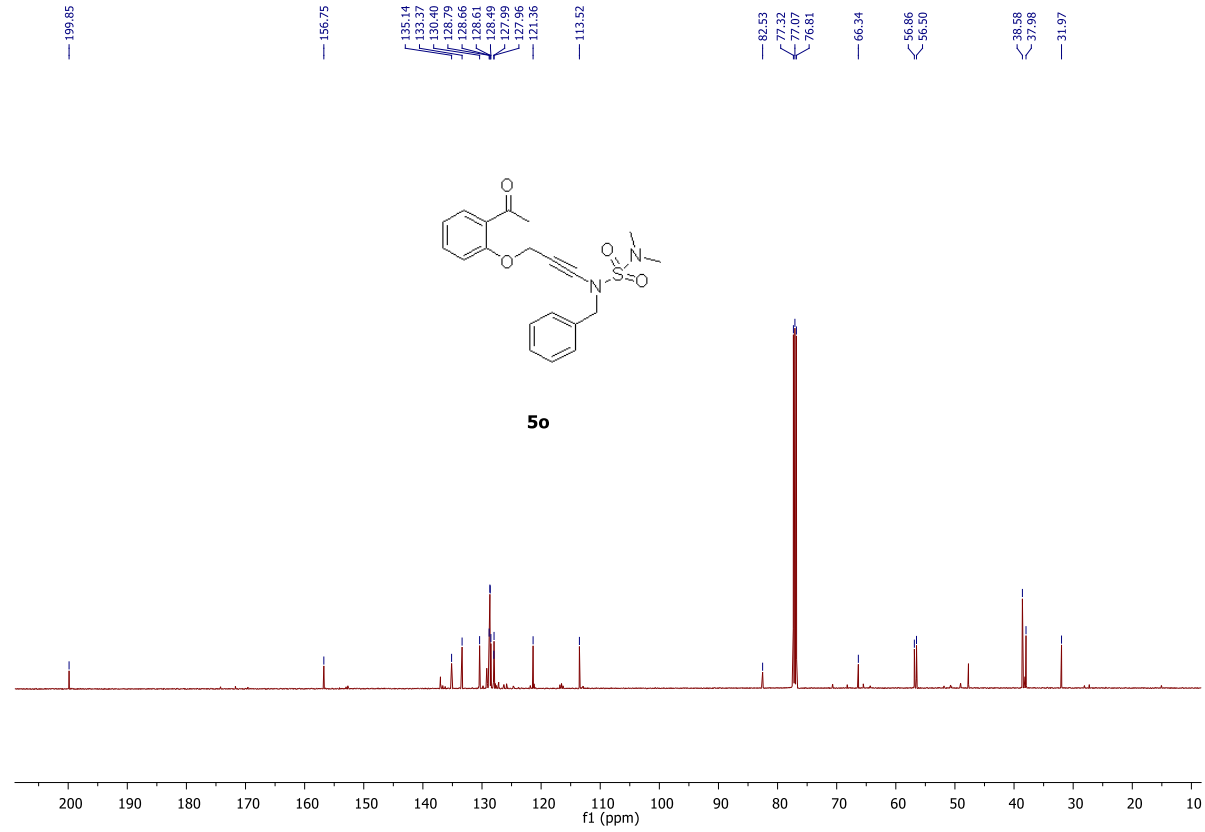
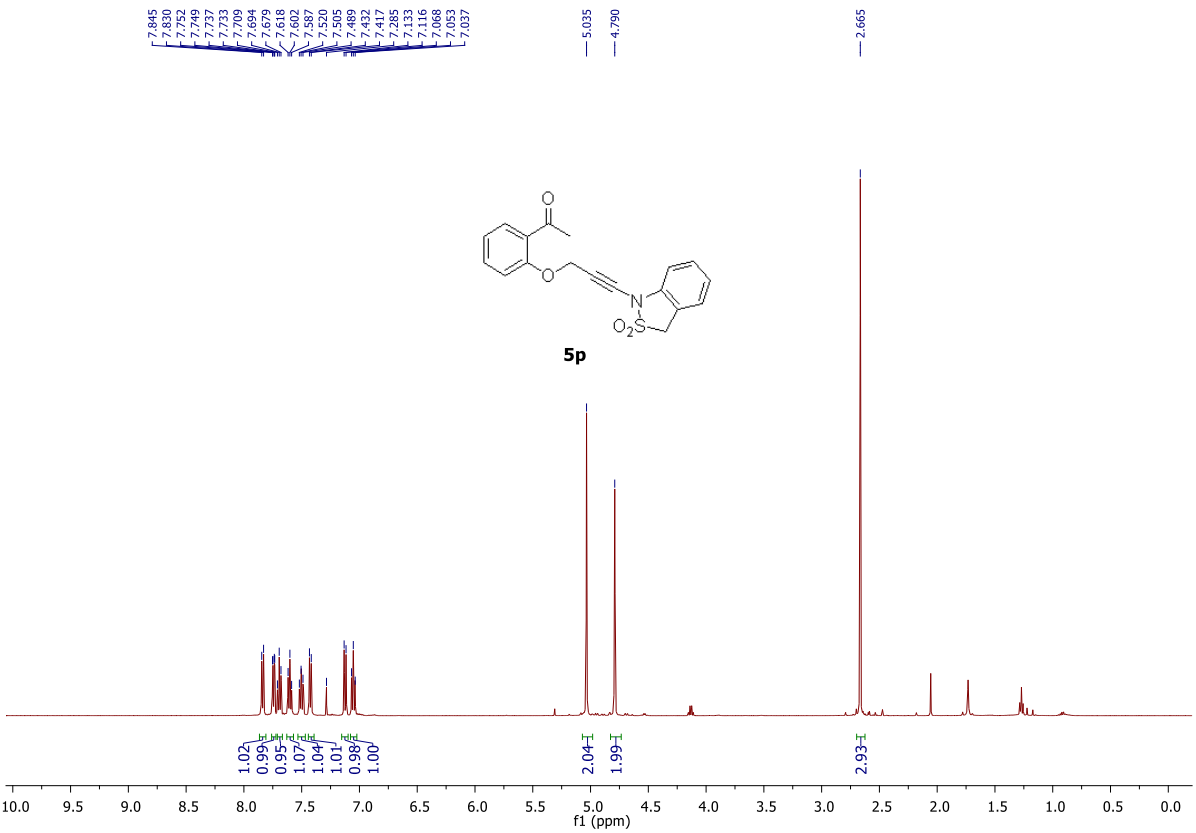
156.78
154.33
151.95
134.31
133.41
130.36
130.23
128.93
128.70
128.55
128.42
124.12
121.04
112.97
81.01
77.32
77.07
76.82
68.63
56.58
53.41
34.23
31.94
29.84
24.72
23.55
Bn
N
O=S=O
5n
f1 (ppm)


7.76
7.75
7.73
7.73
7.37
7.36
7.35
7.07
7.05
7.05
7.02
7.02
6.95
6.93
4.90
4.57
2.81
2.60
1.03
5.60
1.12
0.98
2.09
2.00
6.33
2.77
f1 (ppm)

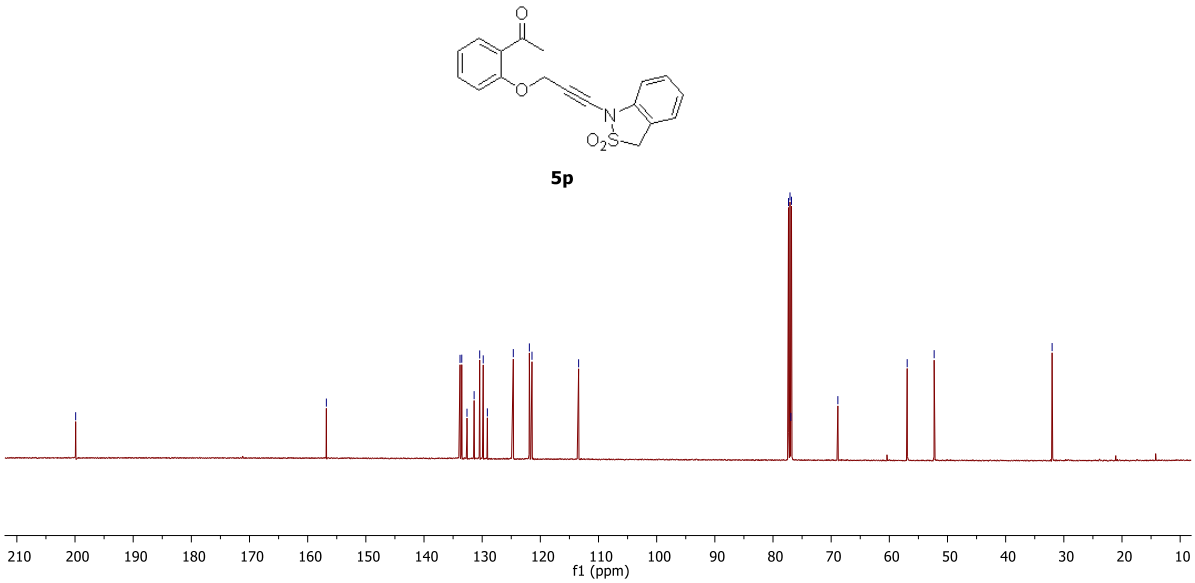
5o


199.85
156.75
135.14
133.37
130.40
128.79
128.66
128.61
128.49
127.99
127.96
121.36
113.52
82.53
77.32
77.07
76.81
66.34
56.86
56.50
38.58
37.98
31.97
f1 (ppm)

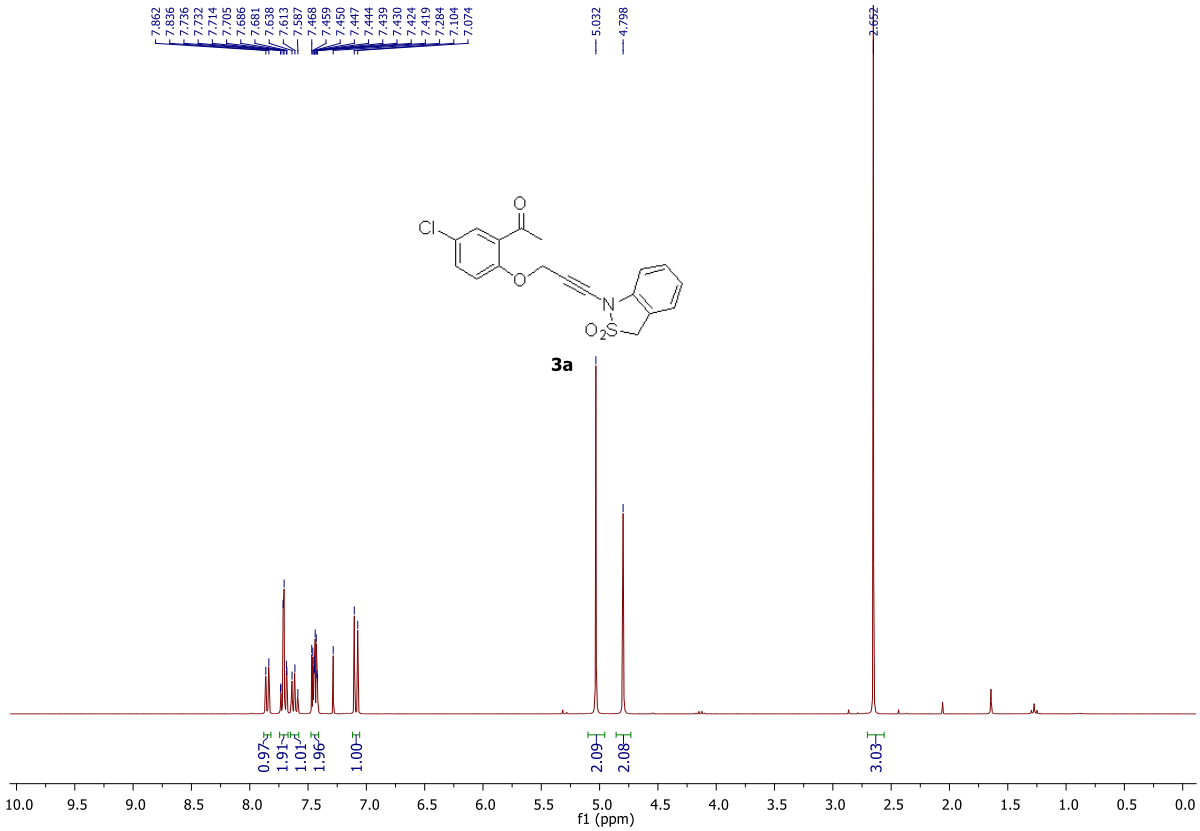
5o

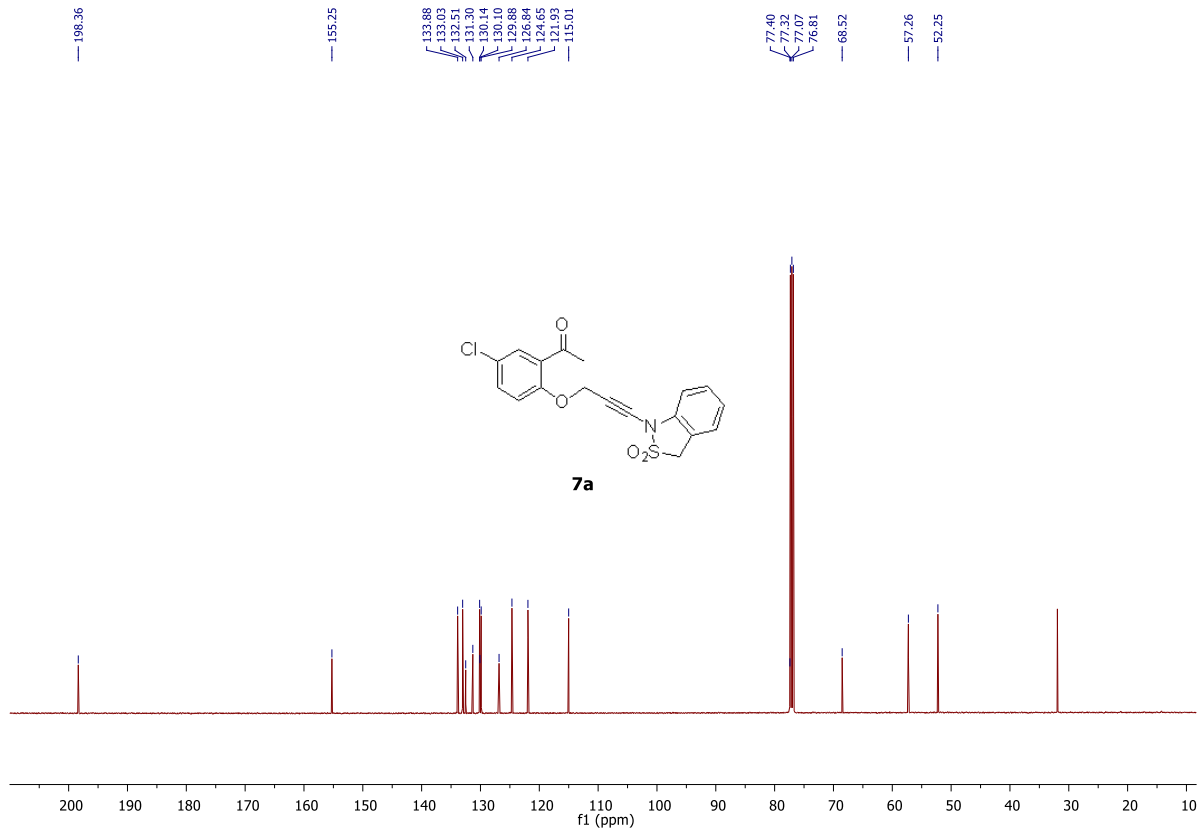

7.845
7.830
7.752
7.749
7.737
7.733
7.709
7.694
7.679
7.618
7.602
7.587
7.520
7.505
7.489
7.432
7.417
7.285
7.133
7.116
7.068
7.053
7.037
5.035
4.790
2.665
1.02
0.99
0.95
1.07
1.04
1.01
0.98
1.00
2.04
1.99
2.93
f1 (ppm)

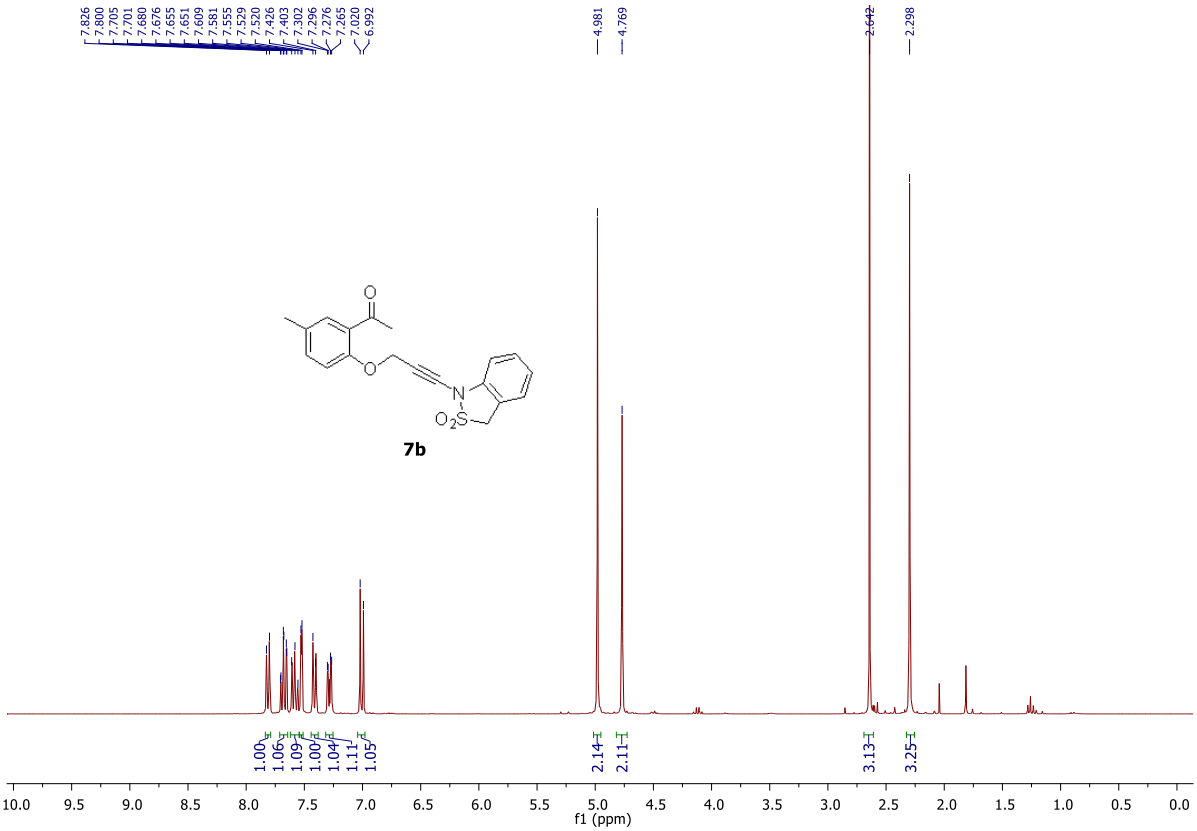
5p


199.89
156.79
133.81
133.51
132.61
131.38
130.42
129.82
129.11
124.65
121.89
121.44
113.42
77.33
77.08
76.93
76.82
68.85
56.93
52.29
32.01
f1 (ppm)

5p


7.862
7.836
7.736
7.732
7.714
7.705
7.686
7.681
7.638
7.613
7.587
7.468
7.459
7.450
7.447
7.444
7.439
7.430
7.424
7.419
7.284
7.104
7.074
5.032
4.798
2.652
Cl
O
O
N
O2S
3a
0.97
1.91
1.01
1.96
1.00
2.09
2.08
3.03
f1 (ppm)


198.36
155.25
133.88
133.03
132.51
131.30
130.14
130.10
129.88
126.84
124.65
121.93
115.01
77.40
77.32
77.07
76.81
68.52
57.26
52.25
Cl
O
O
N
O2S
7a
f1 (ppm)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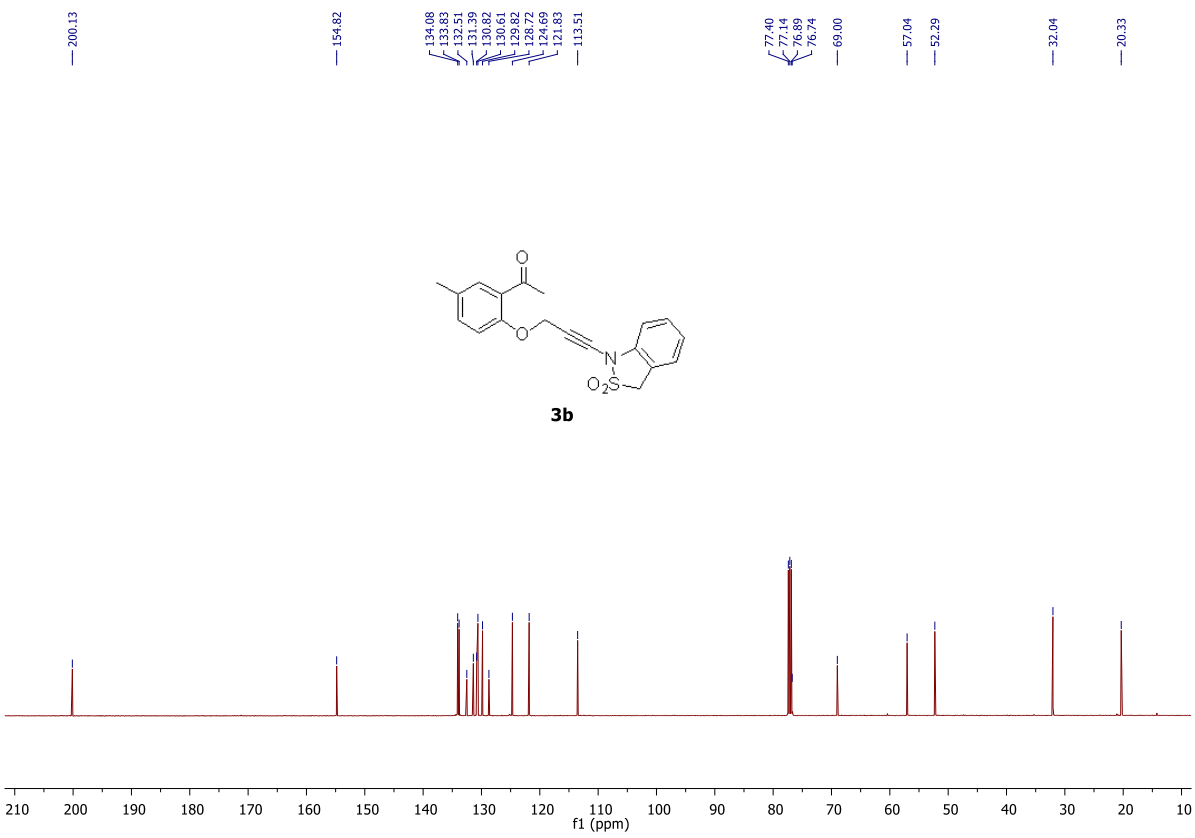
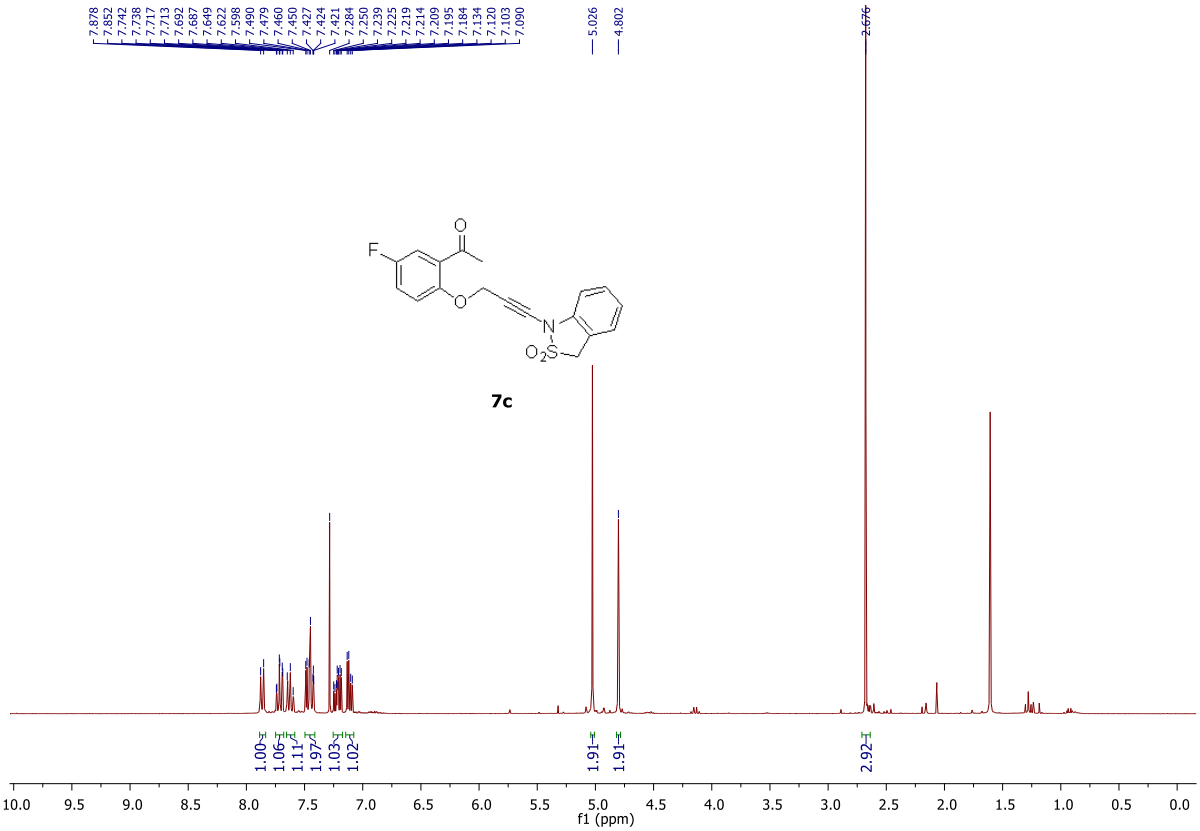
7.680
7.676
7.655
7.651
7.609
7.581
7.555
7.529
7.520
7.426
7.403
7.302
7.296
7.276
7.265
7.020
6.992
4.981
4.769
2.642
2.298
1.00
1.06
1.09
1.00
1.04
1.11
1.05
2.14
2.11
3.13
3.25
f1 (ppm)

7b


200.13
154.82
134.08
133.83
132.51
131.39
130.82
130.61
129.82
128.72
124.69
121.83
113.51
77.40
77.14
76.89
76.74
69.00
57.04
52.29
32.04
20.33
f1 (ppm)

3b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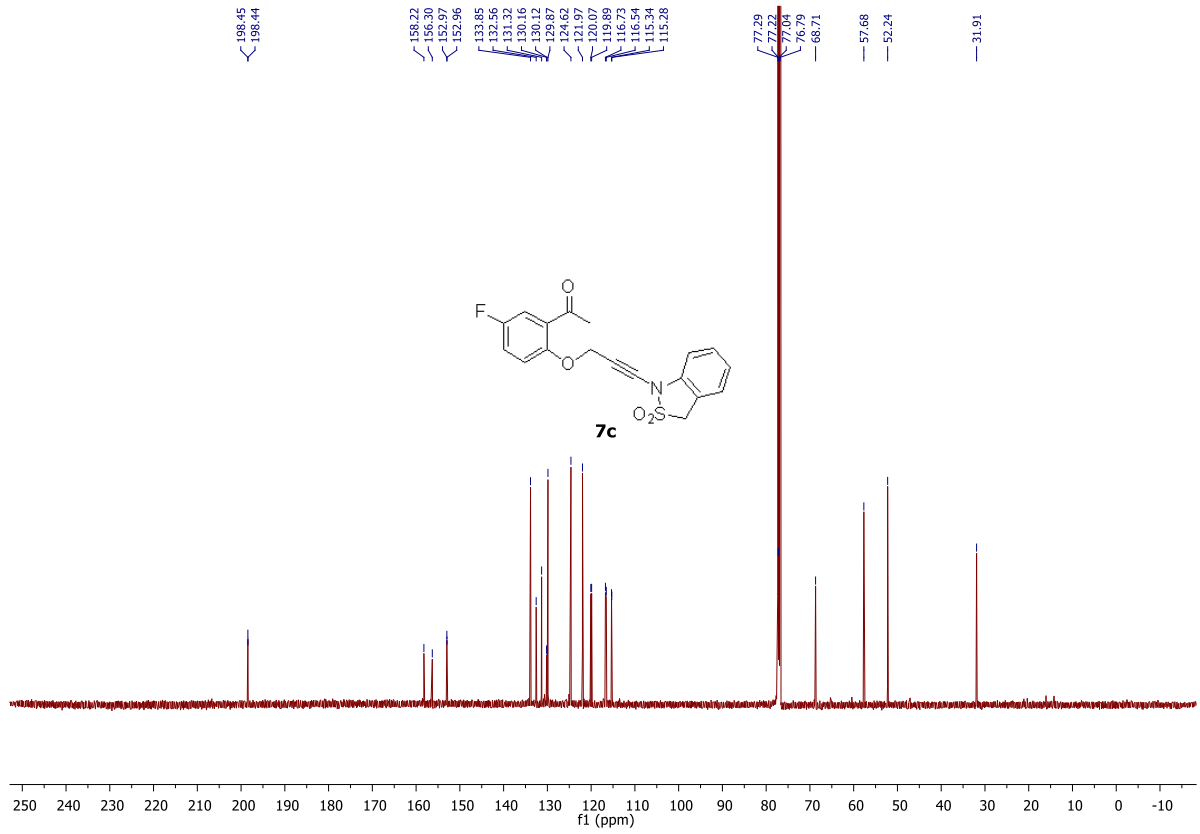
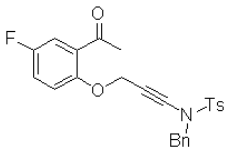
7.852
7.742
7.738
7.717
7.713
7.692
7.687
7.649
7.622
7.598
7.490
7.479
7.460
7.450
7.427
7.424
7.421
7.284
7.250
7.239
7.225
7.219
7.214
7.209
7.195
7.184
7.134
7.120
7.103
7.090
5.026
4.802
2.676
F
O
O
N
O2S
1.00
1.06
1.11
1.97
1.03
1.02
1.91
1.91
2.92
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

7c

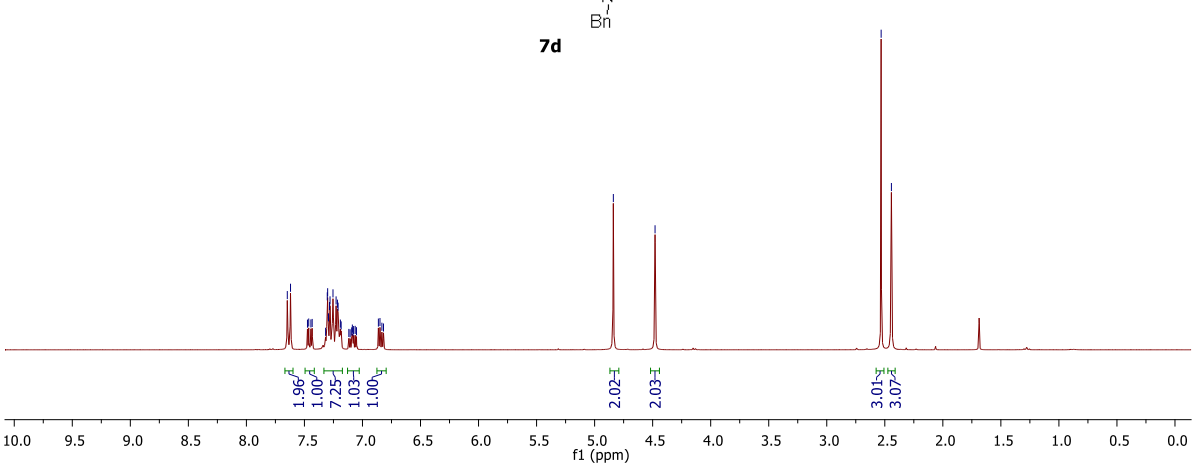

198.45
198.44
158.22
156.30
152.97
152.96
133.85
132.56
131.32
130.16
130.12
129.87
124.62
121.97
120.07
119.89
116.73
116.54
115.34
115.28
77.29
77.22
77.04
76.79
68.71
57.68
52.24
31.91
F
O
O
N
O2S
250 240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

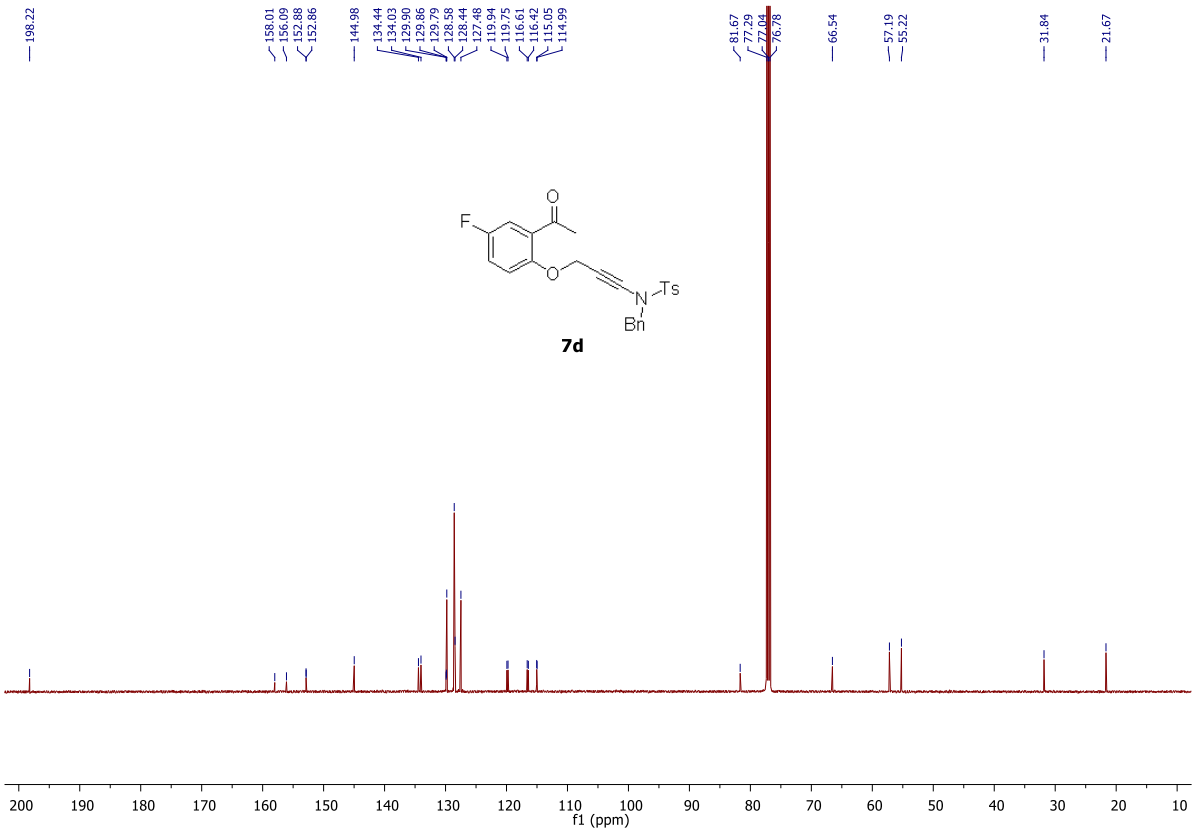
7c


7.648
7.620
7.474
7.463
7.444
7.433
7.318
7.303
7.300
7.293
7.284
7.279
7.254
7.227
7.216
7.210
7.190
7.184
7.117
7.106
7.093
7.087
7.082
7.076
7.063
7.052
6.863
6.849
6.833
6.819
4.839
4.479
2.531
2.443


F
O
O
N
Ts
Bn

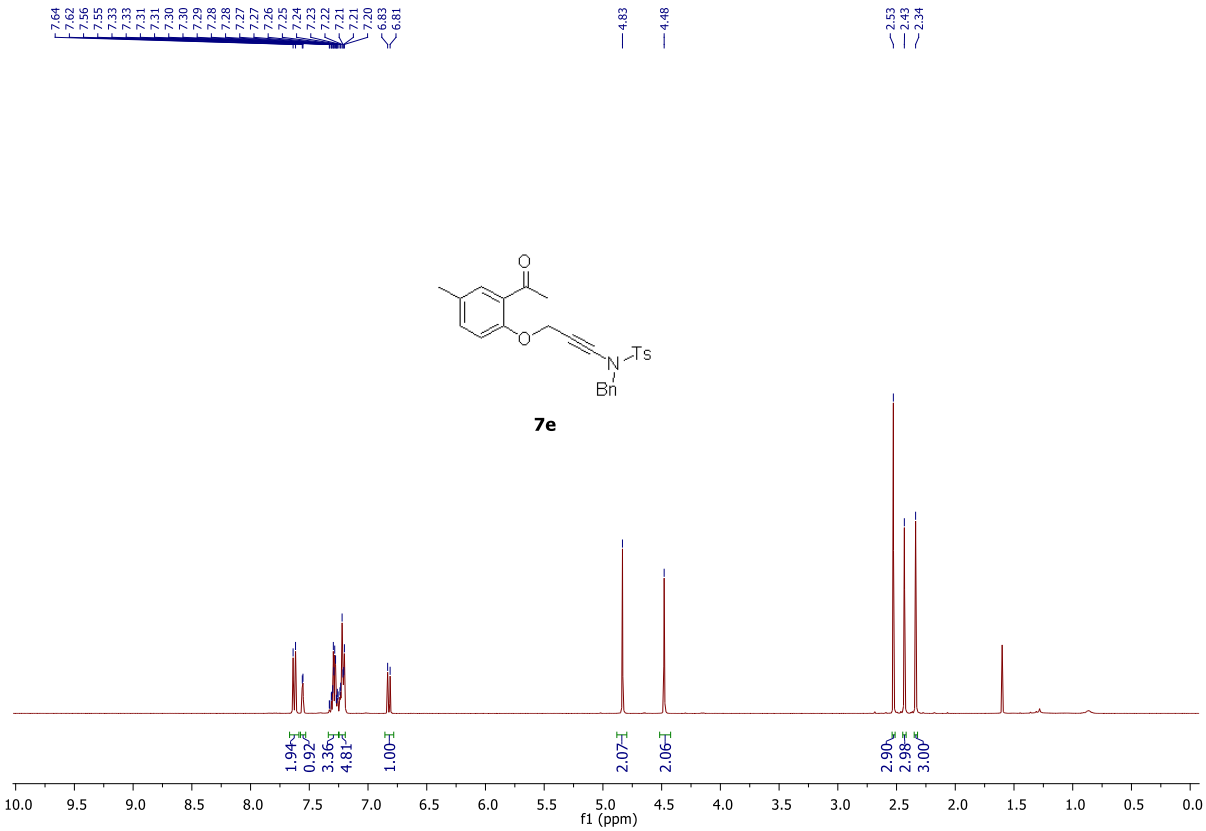
7d


1.96
1.00
7.25
1.03
1.00
2.02
2.03
3.01
3.07
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


198.22
158.01
156.09
152.88
152.86
144.98
134.44
134.03
129.90
129.86
129.79
128.58
128.44
127.48
119.94
119.75
116.61
116.42
115.05
114.99
81.67
77.29
77.04
76.78
66.54
57.19
55.22
31.84
21.67
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

F
O
O
N
Ts
Bn

7d


7.64
7.62
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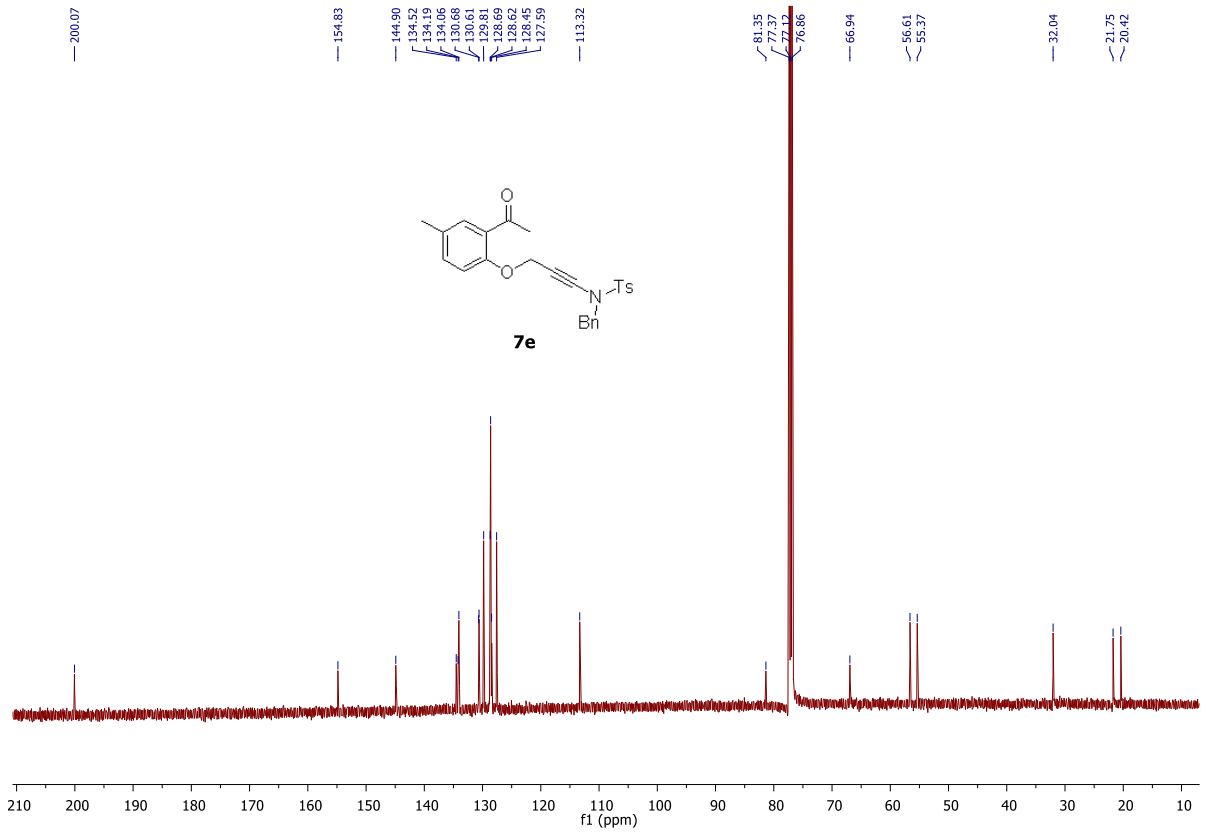
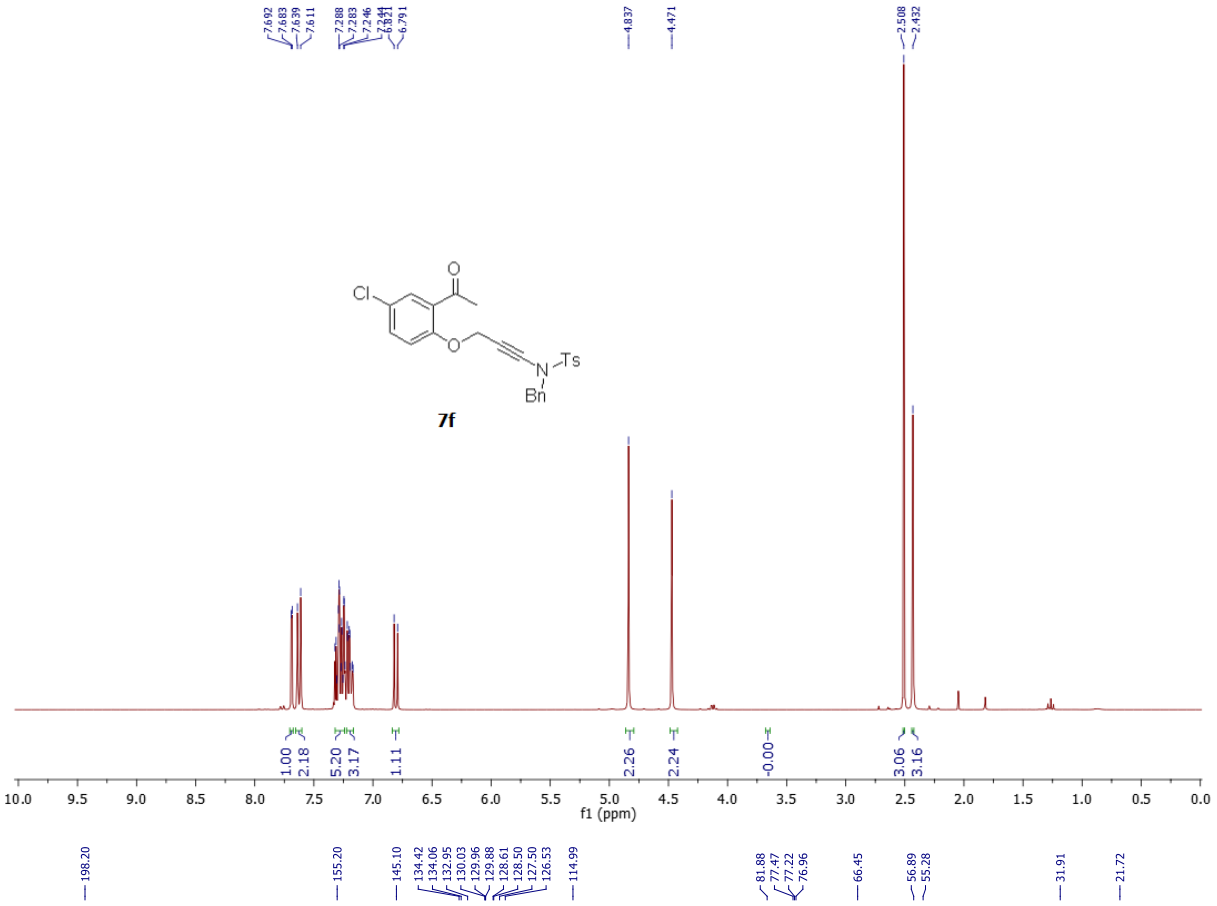
7.33
7.33
7.31
7.31
7.30
7.30
7.29
7.28
7.28
7.27
7.27
7.26
7.25
7.24
7.23
7.22
7.21
7.21
7.20
6.83
6.81
4.83
4.48
2.53
2.43
2.34
O
O
N
Ts
Bn
1.94
0.92
3.36
4.81
1.00
2.07
2.06
2.90
2.98
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

7e


200.07
154.83
144.90
134.52
134.19
134.06
130.68
130.61
129.81
128.69
128.62
128.45
127.59
113.32
81.35
77.37
77.12
76.86
66.94
56.61
55.37
32.04
21.75
20.42
O
O
N
Ts
Bn
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

7e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6.791
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4.471
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2.432
Cl
O
O
N
Ts
Bn
7f
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5.20
3.17
1.11
2.26
2.24
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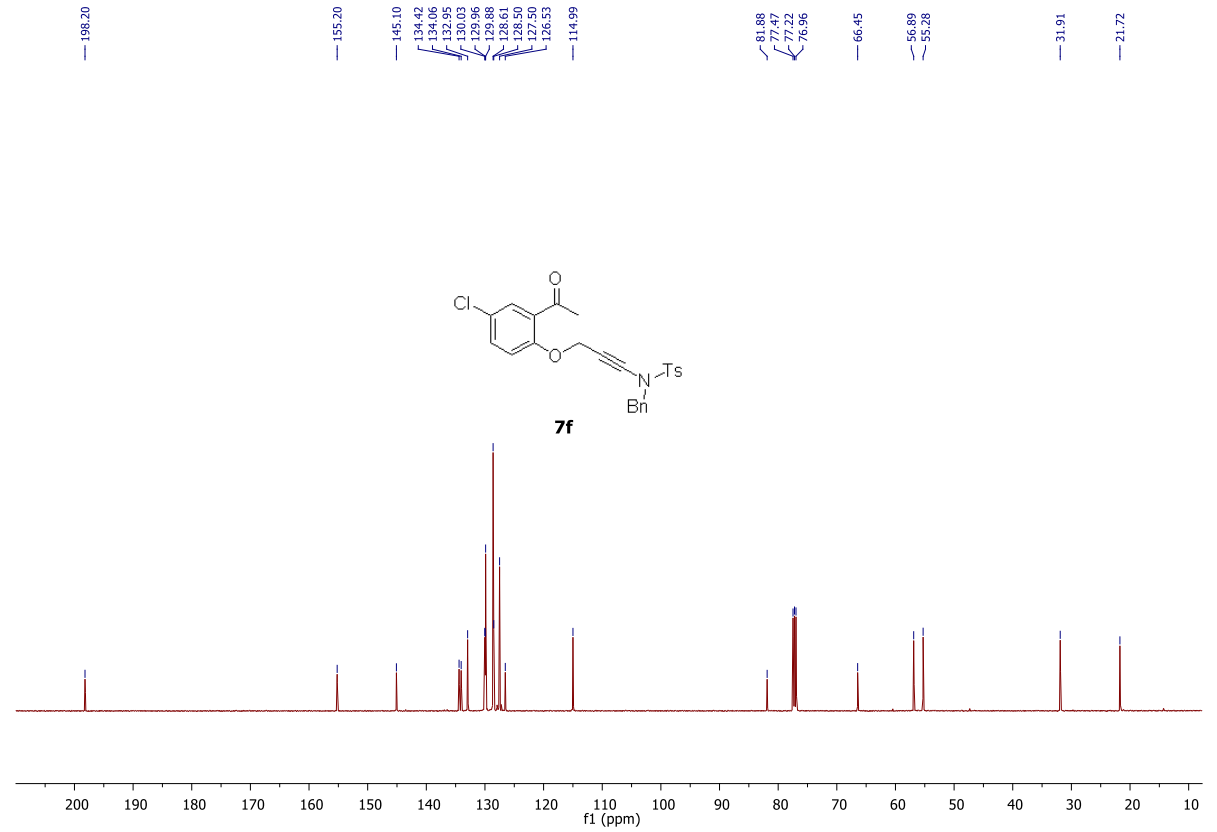
3.06
3.16
f1 (ppm)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145.10
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129.96
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128.50
127.50
126.53
114.99
81.88
77.47
77.22
76.96
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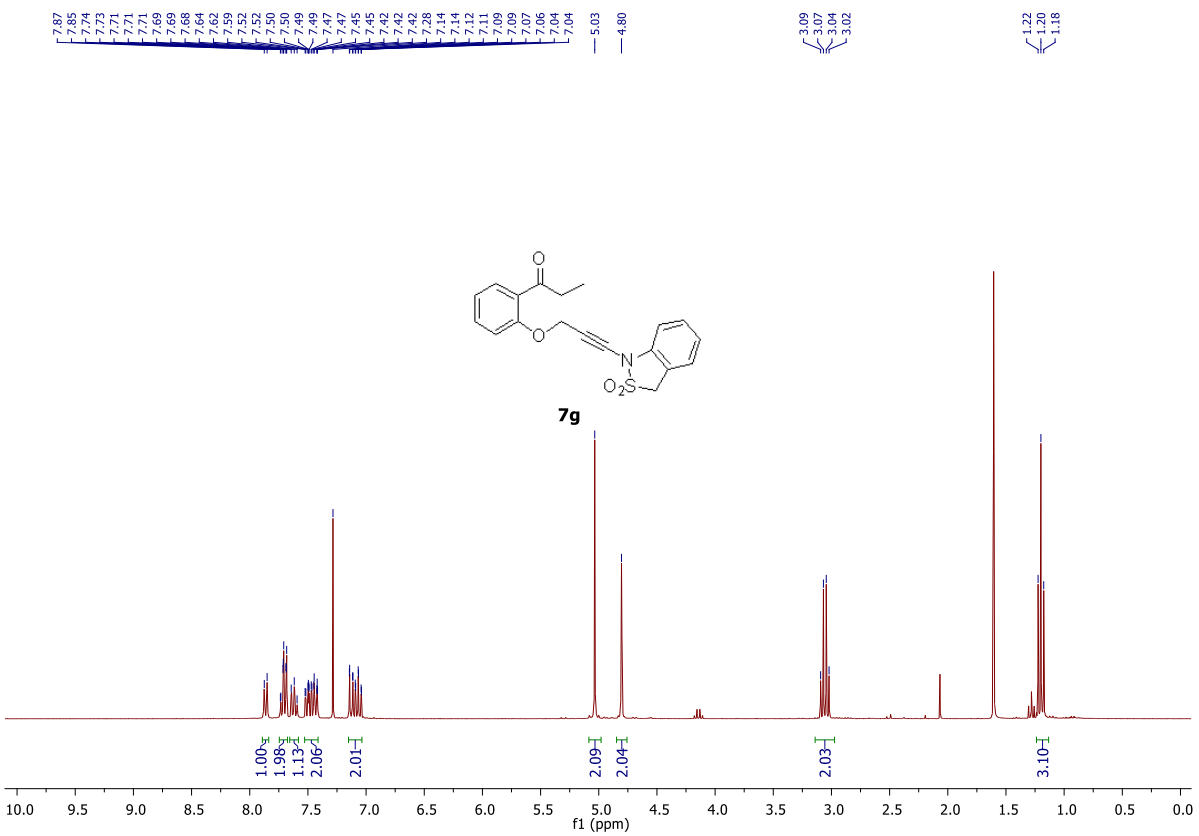
56.89
55.28
31.91
21.72
Cl
O
O
N
Ts
Bn
7f
f1 (ppm)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7.69
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7.50
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7.49
7.47
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7.45
7.45
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7.28
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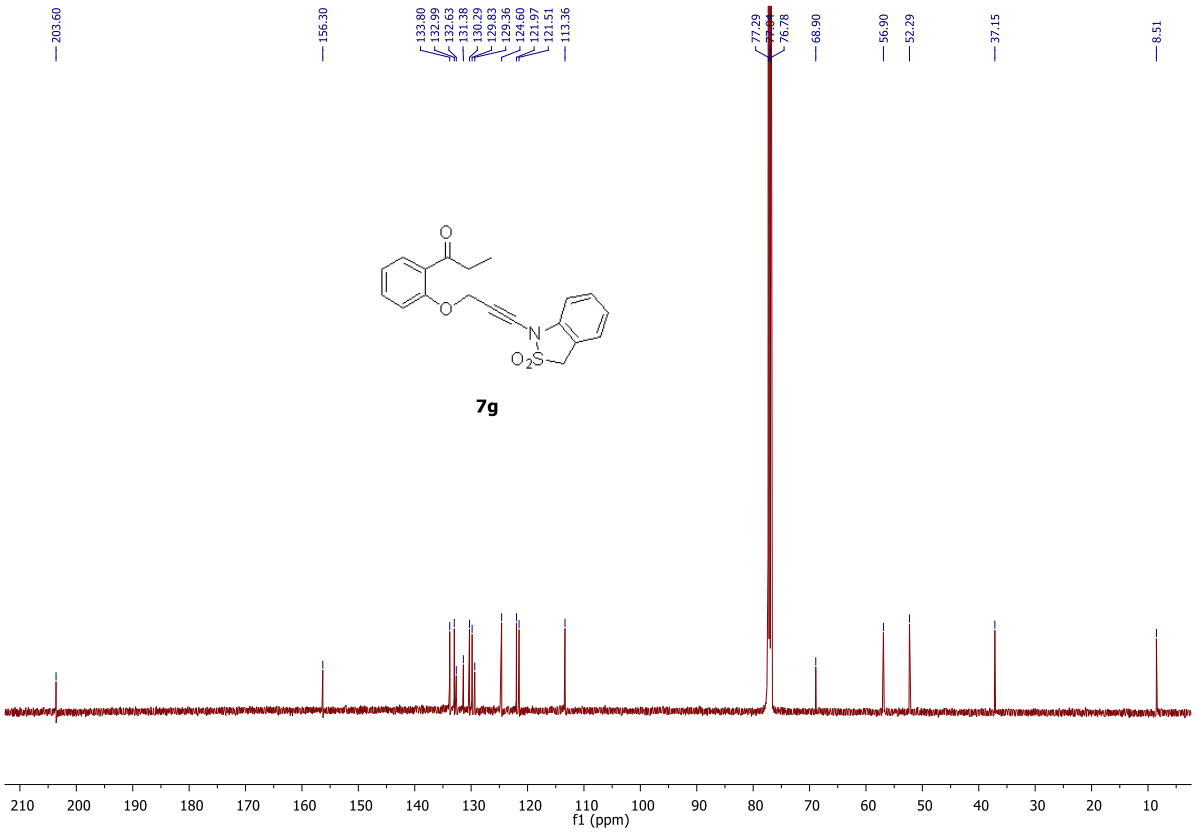
7.14
7.12
7.11
7.09
7.09
7.07
7.06
7.04
7.04
5.03
4.80
3.09
3.07
3.04
3.02
1.22
1.20
1.18
7g
1.00
1.98
1.13
2.06
2.01
2.09
2.04
2.03
3.10
f1 (ppm)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129.83
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113.36
77.29
76.78
68.90
56.90
52.29
37.15
8.51
7g
f1 (ppm)


7.725
7.719
7.699
7.694
7.629
7.601
7.440
7.434
7.416
7.412
7.410
7.406
7.388
7.382
7.309
7.300
7.294
7.282
7.276
7.273
7.265
7.259
7.232
7.226
7.214
7.212
7.187
7.185
7.078
7.074
7.052
7.050
7.028
7.024
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2.933
2.909
2.884
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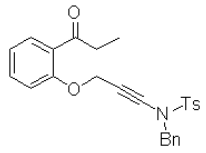
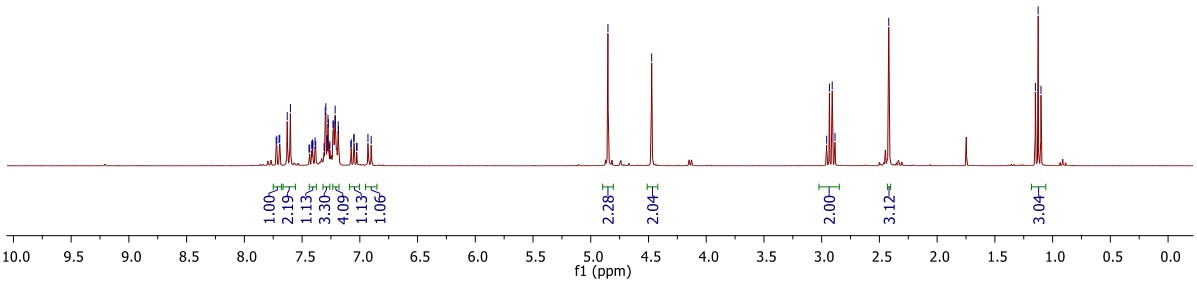
1.149
1.125
1.101


O
O
N
Ts
Bn

7h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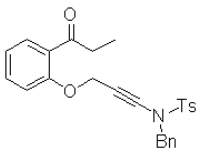
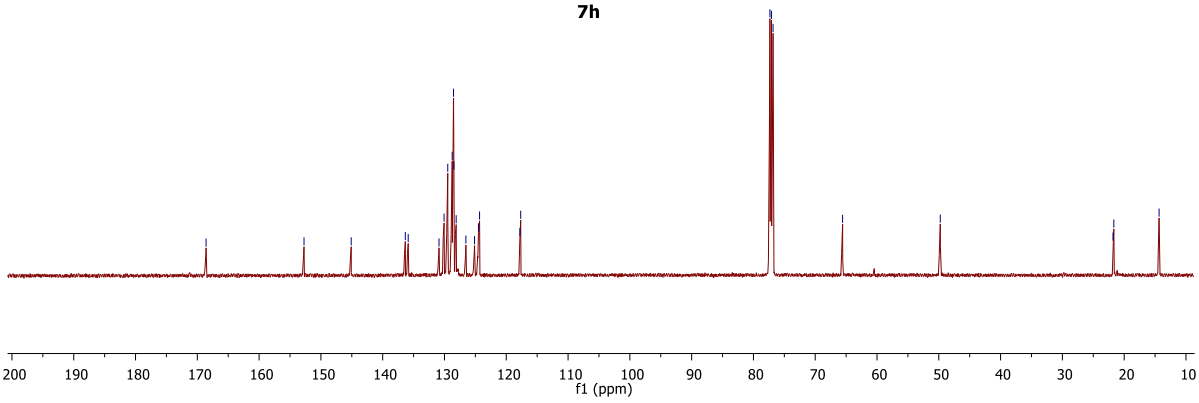
1.13
1.06
2.28
2.04
2.00
3.12
3.04
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

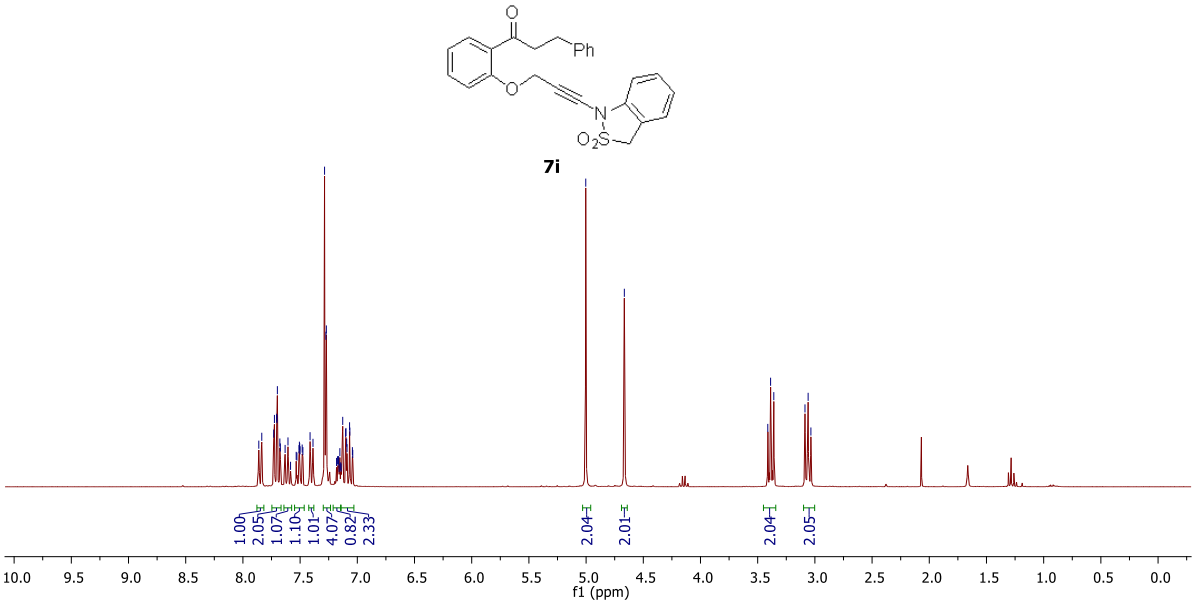

168.59
152.73
145.10
136.34
135.87
129.47
128.75
128.53
128.47
124.32
117.79
117.66
77.33
77.08
76.82
65.57
49.76
21.81
21.68
14.35


O
O
N
Ts
Bn

7h

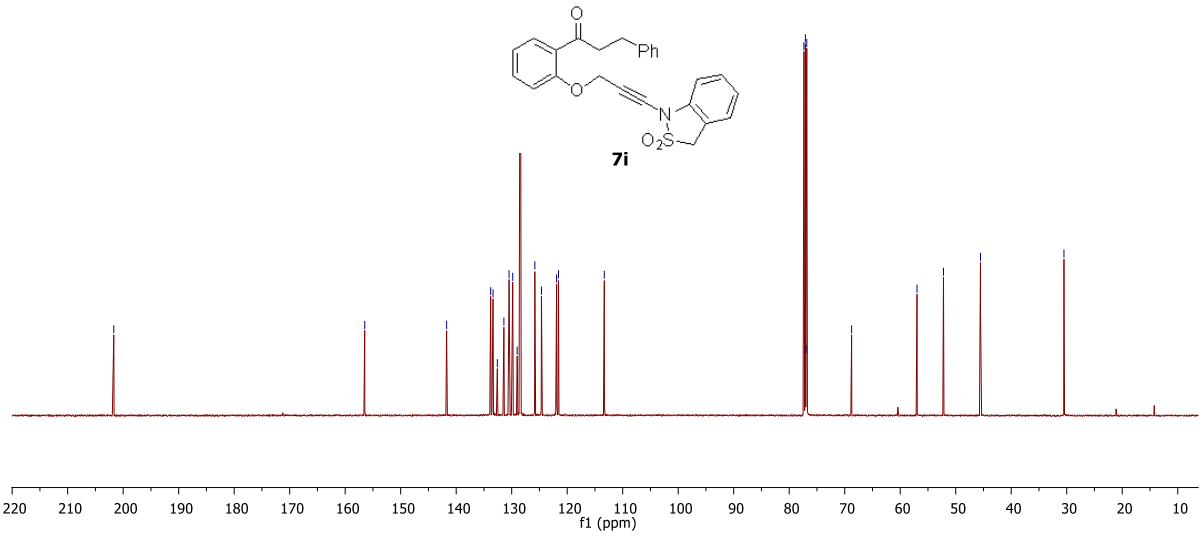

200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.861
7.835
7.731
7.724
7.705
7.703
7.699
7.677
7.673
7.631
7.606
7.583
7.534
7.528
7.510
7.506
7.504
7.500
7.482
7.476
7.413
7.387
7.286
7.275
7.270
7.181
7.171
7.170
7.165
7.162
7.152
7.127
7.102
7.100
7.093
7.090
7.068
7.065
7.043
4.666
3.412
3.387
3.359
3.087
3.059
3.035

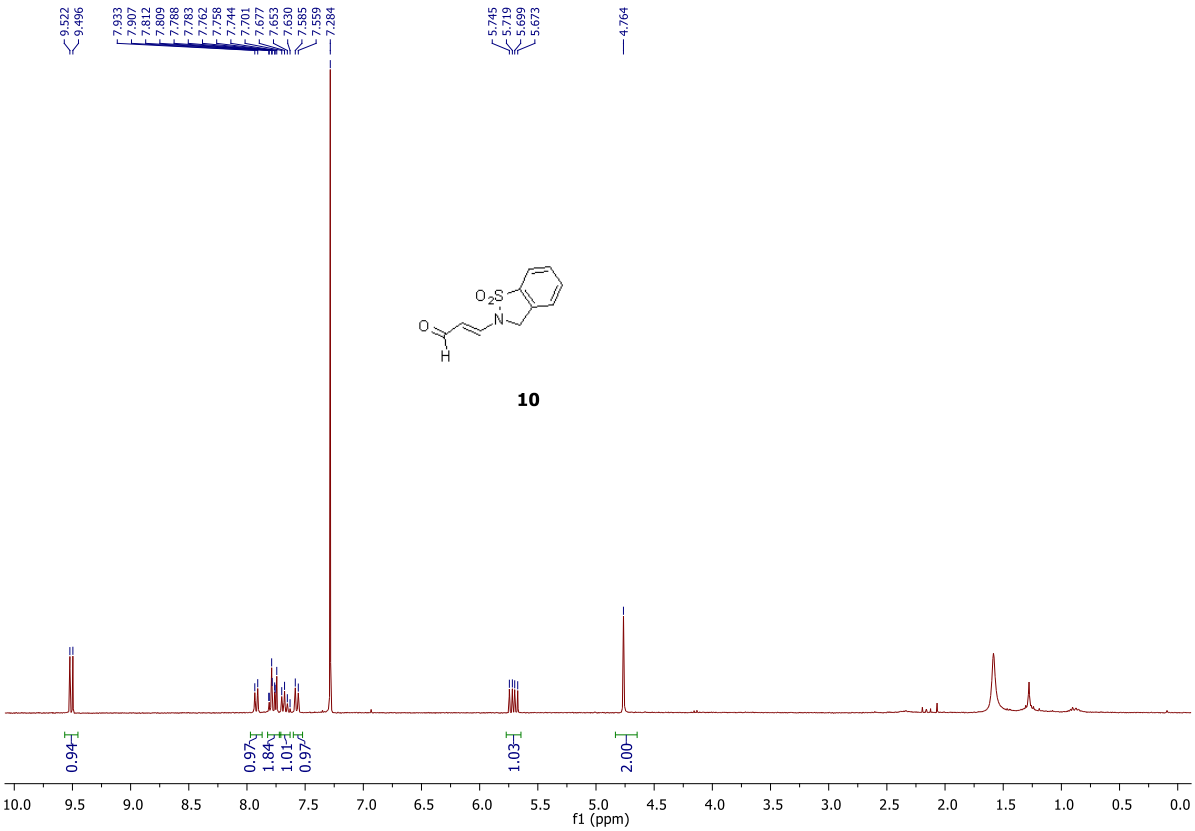

O
Ph
O
N
O2S
1.00
2.05
1.07
1.10
1.01
4.07
0.82
2.33
2.04
2.01
2.04
2.05
f1 (ppm)

7i


201.69
156.48
141.73
133.79
133.36
130.48
129.81
128.54
128.38
125.83
124.64
121.91
111.32
77.34
77.09
76.97
76.83
68.76
56.97
52.21
45.54
30.50


O
Ph
O
N
O2S
f1 (ppm)

7i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7.907
7.812
7.809
7.788
7.783
7.762
7.758
7.744
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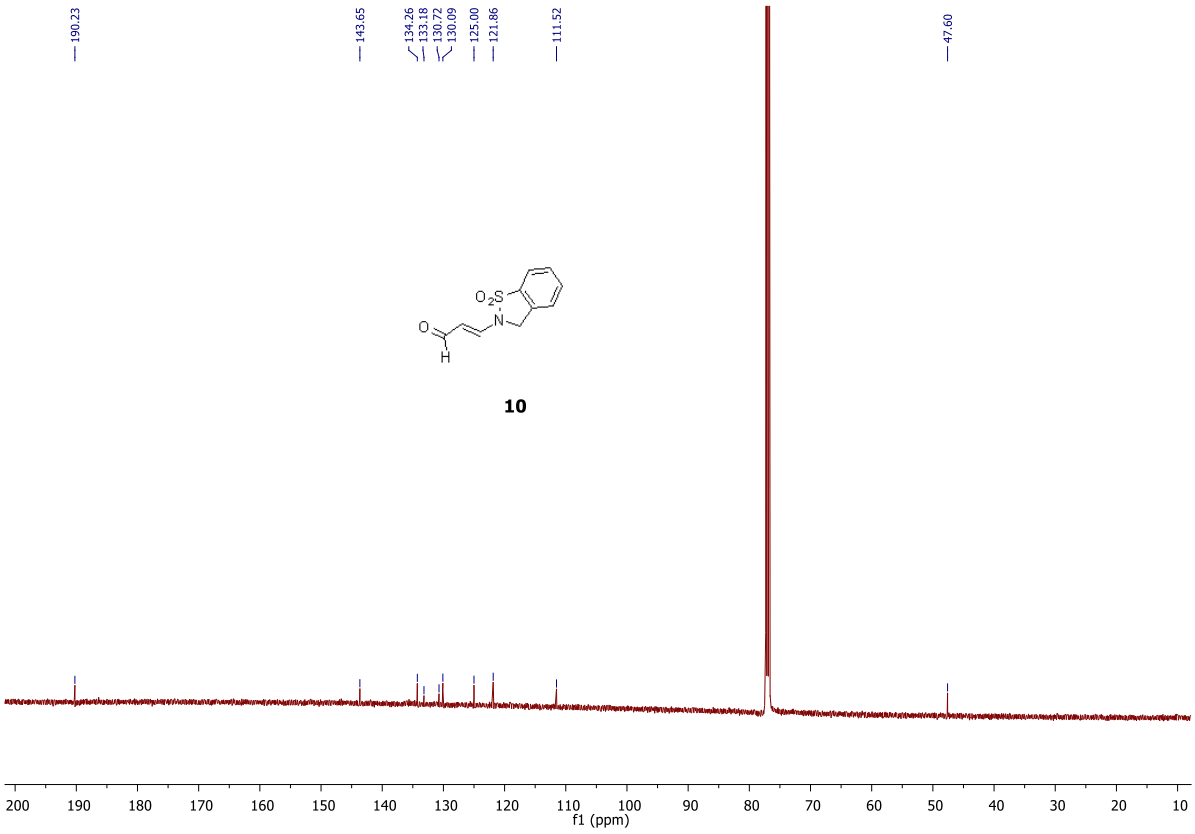
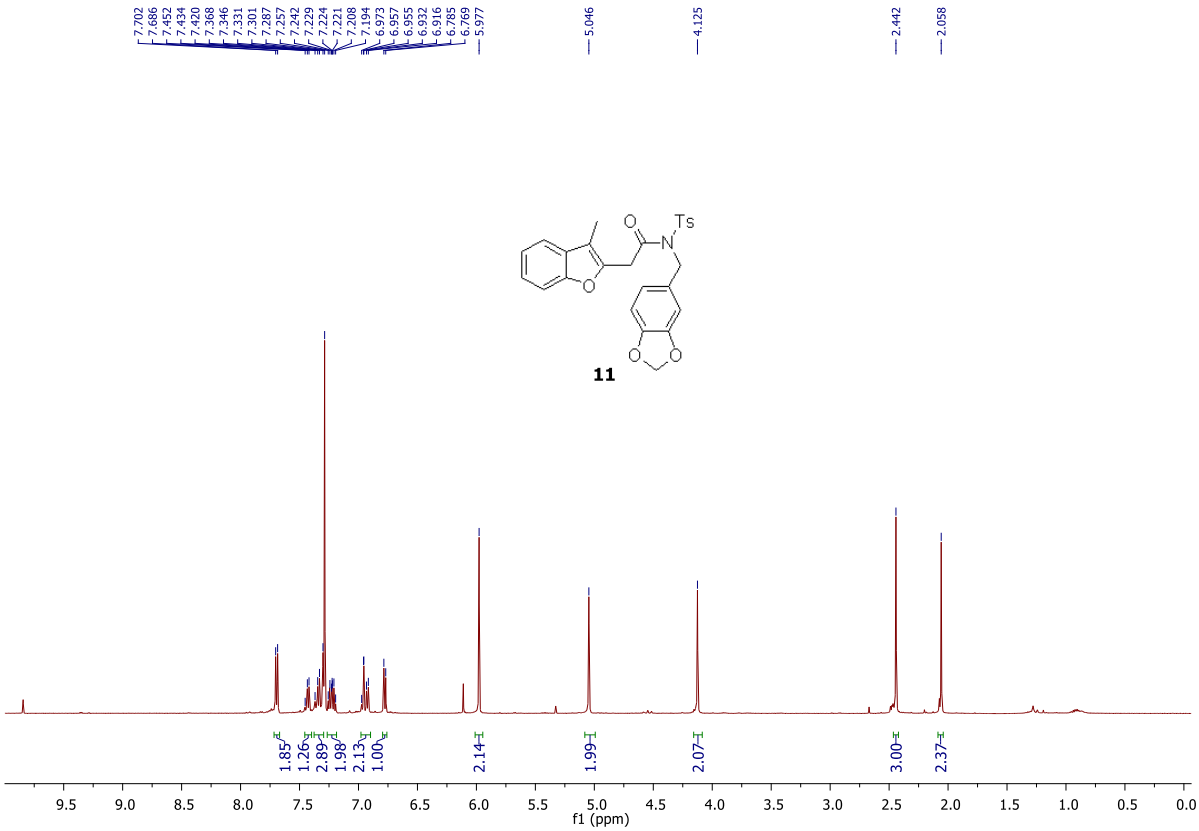
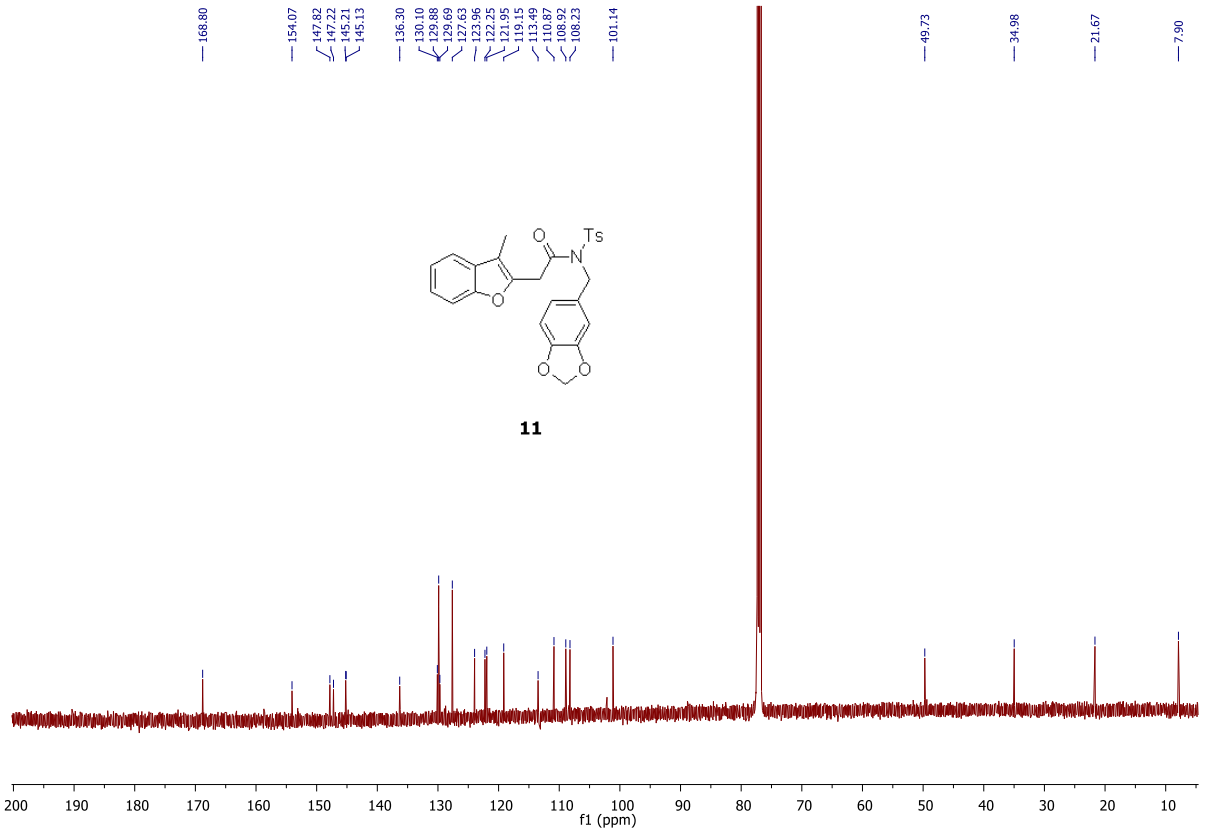
7.677
7.653
7.630
7.585
7.559
7.284
5.745
5.719
5.699
5.673
4.764
0.94
0.97
1.84
1.01
0.97
1.03
2.00
f1 (ppm)

10


190.23
143.65
134.26
133.18
130.72
130.09
125.00
121.86
111.52
47.60
f1 (ppm)

10



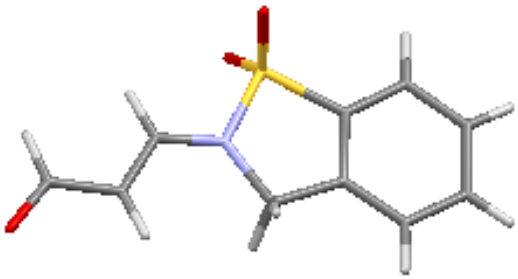


X-Ray Crystallography data

Compound **6** was dissolved in a 0.5 mL acetone and hexane 2 mL were added. The sample was maintained at 4 °C for several days. Crystals were obtained through diffusion.

The X-ray diffraction data were collected at and 173 K on a Bruker SMART CCD diffractometer with MoKα radiation (λ = 0.71073 Å). The diffraction data were corrected for absorption using the SADABS program.[1] The structures were solved using SHELXS97 [2][and refined by full matrix least-squares on F2 using SHELXL-2014 in the anisotropic approximation for all non-hydrogen atoms. The hydrogen atoms were introduced at calculated positions and not refined (riding model).[3]

[1] Bruker. SADABS. Bruker AXS Inc.: Madison, Wisconsin, USA **2001**.
[2] M. Sheldrick, *Acta Crystallogr. Sect. A Found. Crystallogr.* **2008**, *64* (1), 112–122
[3] G. M. Sheldrick, *Acta Crystallogr. Sect. C Struct. Chem.* **2015**, *71* , 3-8



Structure of **6**: ellipsoid contour probability: 50%

Crystal Structure Report for 10

A specimen of $C_{10}H_{10}NO_3S$, approximate dimensions 0.150 mm x 0.160 mm x 0.180 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured (λ = 0.71073 Å).

The integration of the data using a triclinic unit cell yielded a total of 12135 reflections to a maximum θ angle of 28.34° (0.75 Å resolution), of which 2279 were independent (average redundancy 5.325, completeness = 93.9%, R_{int} =5.30%, R_{sig} = 3.00%) and 2072 (90.92%) were greater than 2σ(F^2). The final cell constants of a = 6.4296(4) Å, b = 7.2645(4) Å, c = 11.6117(6) Å, α = 76.869(2)°, β = 79.676(2)°, γ = 67.916(2)°, volume = 486.77(5) $Å^3$, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I). The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.6458 and 0.7545.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P -1, with Z = 2 for the formula unit, $C_{10}H_{10}NO_3S$. The final anisotropic full-matrix least-squares refinement on F^2 with 136variables converged at R1 = 3.44%, for the observed data and wR2 = 9.24% for all data. The goodness-of-fit was 1.017. The largest peak in the final difference electron density synthesis was 0.299 $e^-/Å^3$ and the largest hole was-0.289 $e^-/Å^3$ with an RMS deviation of 0.050 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.530 g/cm^3 and F(000), 234 e^-.

Table 1. Sample and crystal data for 10.

Identification code	e5055
Chemical formula	$C_{10}H_{10}NO_3S$
Formula weight	224.25 g/mol

Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal size	0.150 x 0.160 x 0.180 mm	
Crystal system	triclinic	
Space group	P -1	
Unit cell dimensions	a = 6.4296(4) Å	α = 76.869(2)°
	b = 7.2645(4) Å	β = 79.676(2)°
	c = 11.6117(6) Å	γ = 67.916(2)°
Volume	486.77(5) $Å^3$	
Z	2	
Density (calculated)	1.530 g/cm^3	
Absorption coefficient	0.317 mm^{-1}	
F(000)	234	

Table 2. Data collection and structure refinement for 10.

Theta range for data collection	3.07 to 28.34°
Index ranges	-8<=h<=8, -9<=k<=9, -15<=l<=14
Reflections collected	12135
Independent reflections	2279 [R(int) = 0.0530]
Max. and min. transmission	0.7545 and 0.6458
Structure solution technique	direct methods
Structure solution program	SHELXT 2014/5 (Sheldrick, 2014)
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2018/3 (Sheldrick, 2018)
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	2279 / 0 / 136
Goodness-of-fit on F^2	1.017

Δ/σ_{max}	0.001	
Final R indices	2072 data; I>2σ(I)	R1 = 0.0344, wR2 = 0.0896
	all data	R1 = 0.0378, wR2 = 0.0924
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0346P)^2+0.3297P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.299 and -0.289 eÅ^{-3}	
R.M.S. deviation from mean	0.050 eÅ^{-3}	

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for 10.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
S1	0.66110(6)	0.59483(6)	0.61777(3)	0.02666(13)
O1	0.6661(2)	0.40750(19)	0.59584(12)	0.0378(3)
O2	0.7503(2)	0.7165(2)	0.52273(12)	0.0442(3)
N1	0.7888(2)	0.5516(2)	0.73981(12)	0.0265(3)
C1	0.3998(2)	0.7335(2)	0.68453(13)	0.0235(3)
C2	0.2009(3)	0.8243(2)	0.63078(14)	0.0288(3)
C3	0.0101(3)	0.9263(2)	0.69843(16)	0.0303(3)
C4	0.0189(3)	0.9348(2)	0.81580(16)	0.0300(3)
C5	0.2201(3)	0.8425(2)	0.86789(15)	0.0284(3)
C6	0.4134(2)	0.7408(2)	0.80109(14)	0.0234(3)
C7	0.6444(3)	0.6323(2)	0.84225(14)	0.0268(3)
C8	0.0109(2)	0.4323(2)	0.74296(14)	0.0258(3)
C9	0.1271(3)	0.3844(2)	0.83704(15)	0.0268(3)
C10	0.3627(3)	0.2622(3)	0.82791(16)	0.0315(4)
O3	0.4880(2)	0.2224(2)	0.90428(13)	0.0438(3)

Table 4. Bond lengths (Å) for 10.

S1-O1	1.4282(13)	S1-O2	1.4279(13)
S1-N1	1.6737(13)	S1-C1	1.7474(16)
N1-C8	1.3657(19)	N1-C7	1.460(2)
C1-C6	1.386(2)	C1-C2	1.387(2)
C2-C3	1.381(2)	C2-H2	0.95
C3-C4	1.390(2)	C3-H3	0.95
C4-C5	1.390(2)	C4-H4	0.95
C5-C6	1.384(2)	C5-H5	0.95
C6-C7	1.503(2)	C7-H7A	0.99
C7-H7B	0.99	C8-C9	1.341(2)
C8-H8	0.95	C9-C10	1.438(2)
C9-H9	0.95	C10-O3	1.218(2)
C10-H10	0.95		

Table 5. Bond angles (°) for 10.

O1-S1-O2	117.08(9)	O1-S1-N1	109.04(7)
O2-S1-N1	110.05(8)	O1-S1-C1	112.80(8)
O2-S1-C1	112.50(8)	N1-S1-C1	92.58(7)
C8-N1-C7	123.61(13)	C8-N1-S1	120.11(11)
C7-N1-S1	116.04(10)	C6-C1-C2	123.09(15)
C6-C1-S1	111.29(11)	C2-C1-S1	125.62(13)
C3-C2-C1	117.23(15)	C3-C2-H2	121.4
C1-C2-H2	121.4	C2-C3-C4	120.80(14)
C2-C3-H3	119.6	C4-C3-H3	119.6
C5-C4-C3	120.99(15)	C5-C4-H4	119.5
C3-C4-H4	119.5	C4-C5-C6	118.99(15)
C4-C5-H5	120.5	C6-C5-H5	120.5
C5-C6-C1	118.91(14)	C5-C6-C7	126.42(14)
C1-C6-C7	114.67(13)	N1-C7-C6	105.38(12)

N1-C7-H7A	110.7	C6-C7-H7A	110.7
N1-C7-H7B	110.7	C6-C7-H7B	110.7
H7A-C7-H7B	108.8	C9-C8-N1	124.79(15)
C9-C8-H8	117.6	N1-C8-H8	117.6
C8-C9-C10	119.44(15)	C8-C9-H9	120.3
C10-C9-H9	120.3	O3-C10-C9	124.93(17)
O3-C10-H10	117.5	C9-C10-H10	117.5

Table 6. Torsion angles (°) for 10.

O1-S1-N1-C8	61.22(14)	O2-S1-N1-C8	-68.47(14)
C1-S1-N1-C8	176.43(13)	O1-S1-N1-C7	-113.38(12)
O2-S1-N1-C7	116.93(12)	C1-S1-N1-C7	1.83(12)
O1-S1-C1-C6	110.57(12)	O2-S1-C1-C6	-114.30(12)
N1-S1-C1-C6	-1.34(12)	O1-S1-C1-C2	-68.71(16)
O2-S1-C1-C2	66.42(16)	N1-S1-C1-C2	179.38(14)
C6-C1-C2-C3	0.2(2)	S1-C1-C2-C3	179.42(12)
C1-C2-C3-C4	-0.6(2)	C2-C3-C4-C5	0.6(3)
C3-C4-C5-C6	-0.1(2)	C4-C5-C6-C1	-0.3(2)
C4-C5-C6-C7	-179.89(15)	C2-C1-C6-C5	0.2(2)
S1-C1-C6-C5	-179.05(12)	C2-C1-C6-C7	179.87(14)
S1-C1-C6-C7	0.57(17)	C8-N1-C7-C6	-176.10(13)
S1-N1-C7-C6	-1.72(16)	C5-C6-C7-N1	-179.75(14)
C1-C6-C7-	0.65(18)	C7-N1-C8-	-4.2(2)

N1		C9	
S1-N1-C8-C9	-178.34(13)	N1-C8-C9-C10	-178.09(14)
C8-C9-C10-O3	174.21(17)		

Table 7. Anisotropic atomic displacement parameters (Å^2) for 10.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S1	0.0219(2)	0.0340(2)	0.0193(2)	-0.00758(15)	-0.00075(15)	-0.00340(15)
O1	0.0330(6)	0.0386(7)	0.0392(7)	-0.0205(5)	-0.0117(6)	0.0019(5)
O2	0.0356(7)	0.0579(8)	0.0269(7)	0.0005(6)	0.0066(6)	-0.0116(6)
N1	0.0183(6)	0.0383(7)	0.0212(6)	-0.0118(5)	0.0004(5)	-0.0054(5)
C1	0.0215(7)	0.0237(7)	0.0221(7)	-0.0048(5)	0.0003(6)	-0.0050(5)
C2	0.0293(8)	0.0281(7)	0.0240(8)	-0.0032(6)	-0.0057(7)	-0.0040(6)
C3	0.0239(7)	0.0259(7)	0.0352(9)	-0.0048(6)	-0.0066(7)	-0.0008(6)
C4	0.0228(7)	0.0278(7)	0.0358(9)	-0.0135(7)	0.0019(7)	-0.0027(6)
C5	0.0254(8)	0.0313(8)	0.0287(8)	-0.0131(6)	0.0009(7)	-0.0076(6)
C6	0.0211(7)	0.0254(7)	0.0244(7)	-0.0069(6)	-0.0008(6)	-0.0082(5)
C7	0.0206(7)	0.0375(8)	0.0228(7)	-0.0118(6)	0.0003(6)	-0.0081(6)
C8	0.0205(7)	0.0292(7)	0.0266(8)	-0.0082(6)	0.0023(6)	-0.0077(6)
C9	0.0220(7)	0.0300(7)	0.0276(8)	-0.0096(6)	0.0007(6)	-0.0070(6)
C10	0.0243(8)	0.0332(8)	0.0337(9)	-0.0079(7)	-0.0013(7)	-0.0059(6)
O3	0.0268(6)	0.0544(8)	0.0436(8)	-0.0110(6)	-0.0111(6)	-0.0021(6)

Table 8. Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å^2) for 10.

	x/a	y/b	z/c	U(eq)

	x/a	y/b	z/c	U(eq)
H2	0.1962	0.8166	0.5508	0.035
H3	-0.1288	0.9915	0.6644	0.036
H4	-0.1145	1.0048	0.8611	0.036
H5	0.2248	0.8491	0.9481	0.034
H7A	0.6986	0.7266	0.8672	0.032
H7B	0.6423	0.5220	0.9101	0.032
H8	1.0887	0.3793	0.6734	0.031
H9	1.0544	0.4309	0.9091	0.032
H10	1.4253	0.2084	0.7570	0.038

Computational Details

All calculations have been performed at Density Functional Theory (DFT)[i] level using Gaussian 16[ii] software. All structural optimizations and subsequent harmonic frequency calculations confirming the nature of the stationary points as minima or first order transition states have been performed using the PBE0[iii] global hybrid exchange and correlation functional and the 6-311++G(d,p) Pople basis set. Bulk solvent effects (methanol) were considering using the conductor-like polarizable continuum model (CPCM)[iv]. The above described level of theory applies to all data reported.

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[i] Parr GR, Yang W (1989) Density-Functional Theory of Atoms and Molecules Oxford University Press, USA.

[ii] Frisch MJ, Trucks GW, Schlegel HB, Scuseria GE, Robb MA, Cheeseman JR, Scalmani G, Barone V, Petersson GA, Nakatsuji H, Li X, Caricato M, Marenich AV, Bloino J, Janesko BG, Gomperts R, Mennucci B, Hratchian HP, Ortiz JV, Izmaylov AF, Sonnenberg JL, Williams-Young D, Ding F, Lipparini F, Egidi F, Goings J, Peng B, Petrone A, Henderson T, Ranasinghe D, Zakrzewski VG, Gao J, Rega N, Zheng G, Liang W, Hada M, Ehara M, Toyota K, Fukuda R, Hasegawa J, Ishida M, Nakajima T, Honda Y, Kitao O, Nakai H, Vreven T, Throssell K, Montgomery JA Jr, Peralta JE, Ogliaro F, Bearpark MJ, Heyd JJ, Brothers EN, Kudin KN, Staroverov VN, Keith TA, Kobayashi R, Normand J, Raghavachari K, Rendell AP, Burant JC, Iyengar SS, Tomasi J, Cossi M, Millam JM, Klene M, Adamo C, Cammi R, Ochterski JW, Martin RL, Morokuma K, Farkas O, Foresman JB, Fox DJ Gaussian Inc Wallingford CT 2016.

[iii] Adamo C, Barone V, J. (1999) Chem. Phys. 110, 6158.

[iv] Barone V, Cossi M (1998) J. Phys. Chem. (A) 102, 1995-2001.

1. **Energy profiles**

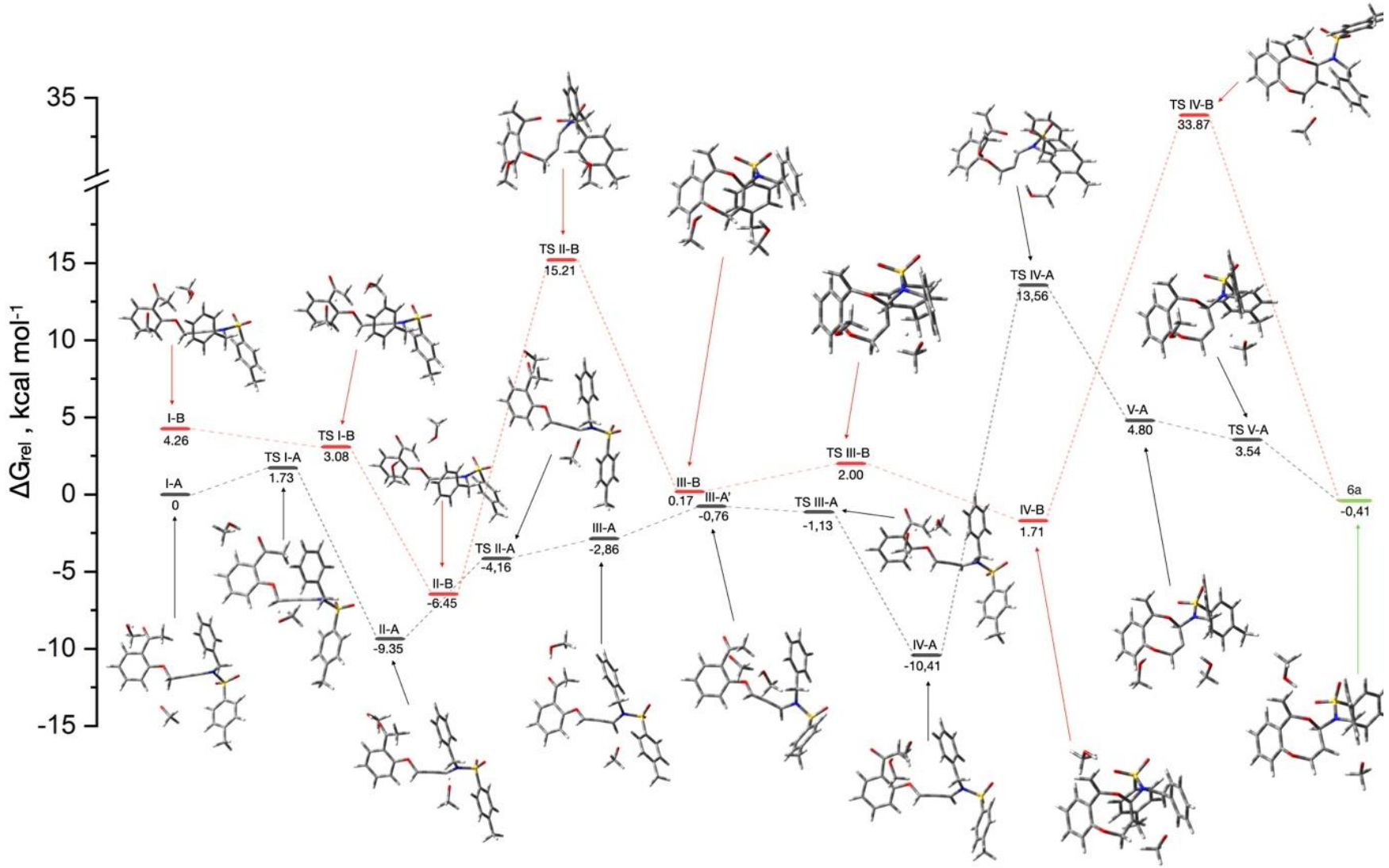


Figure 1. Computed energy profiles (ΔG in kcal/mol) for the reaction pathways A and B.

Figure 2. Computed energy profiles (ΔE, kcal/mol) for the reaction pathways A and B.

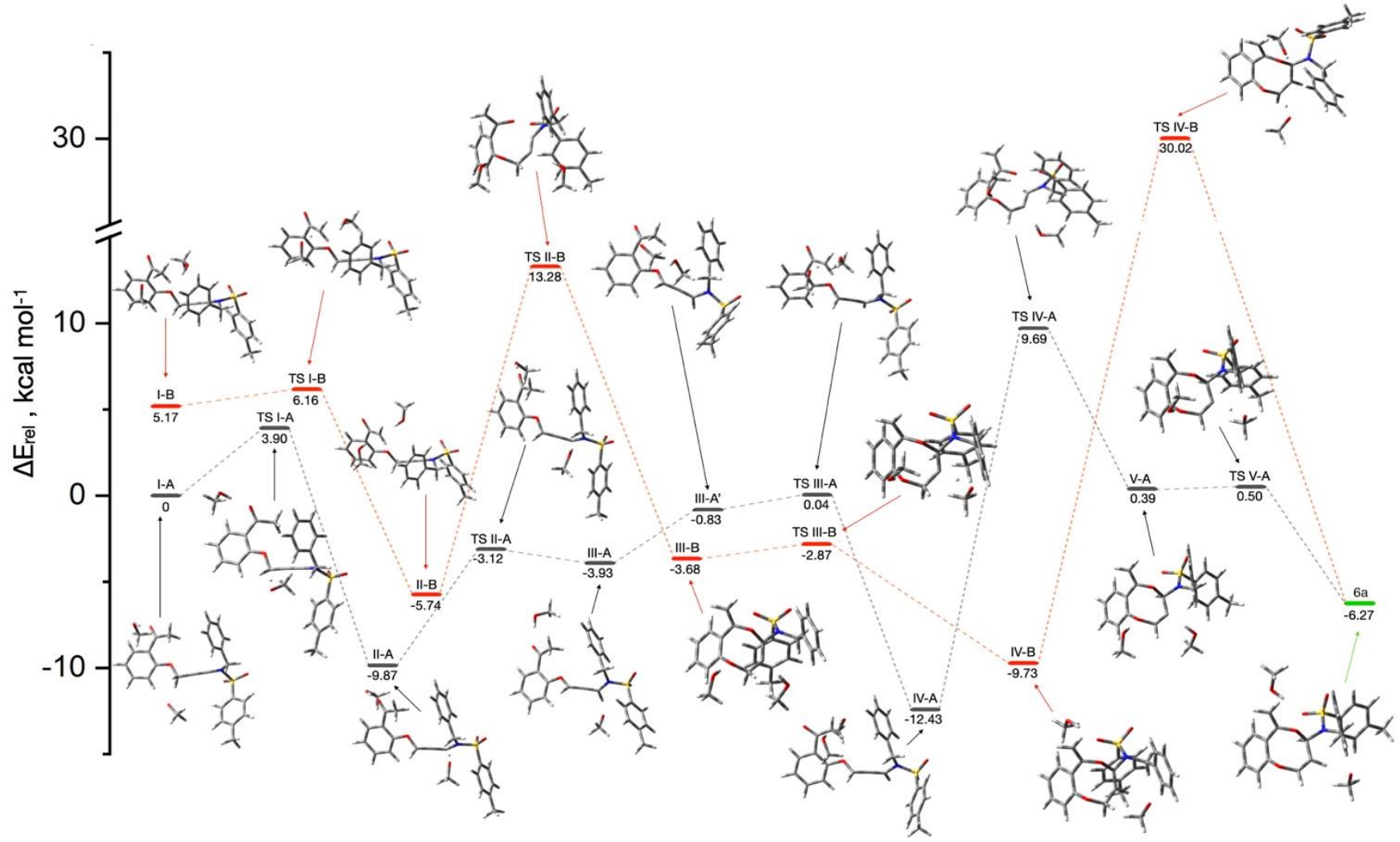
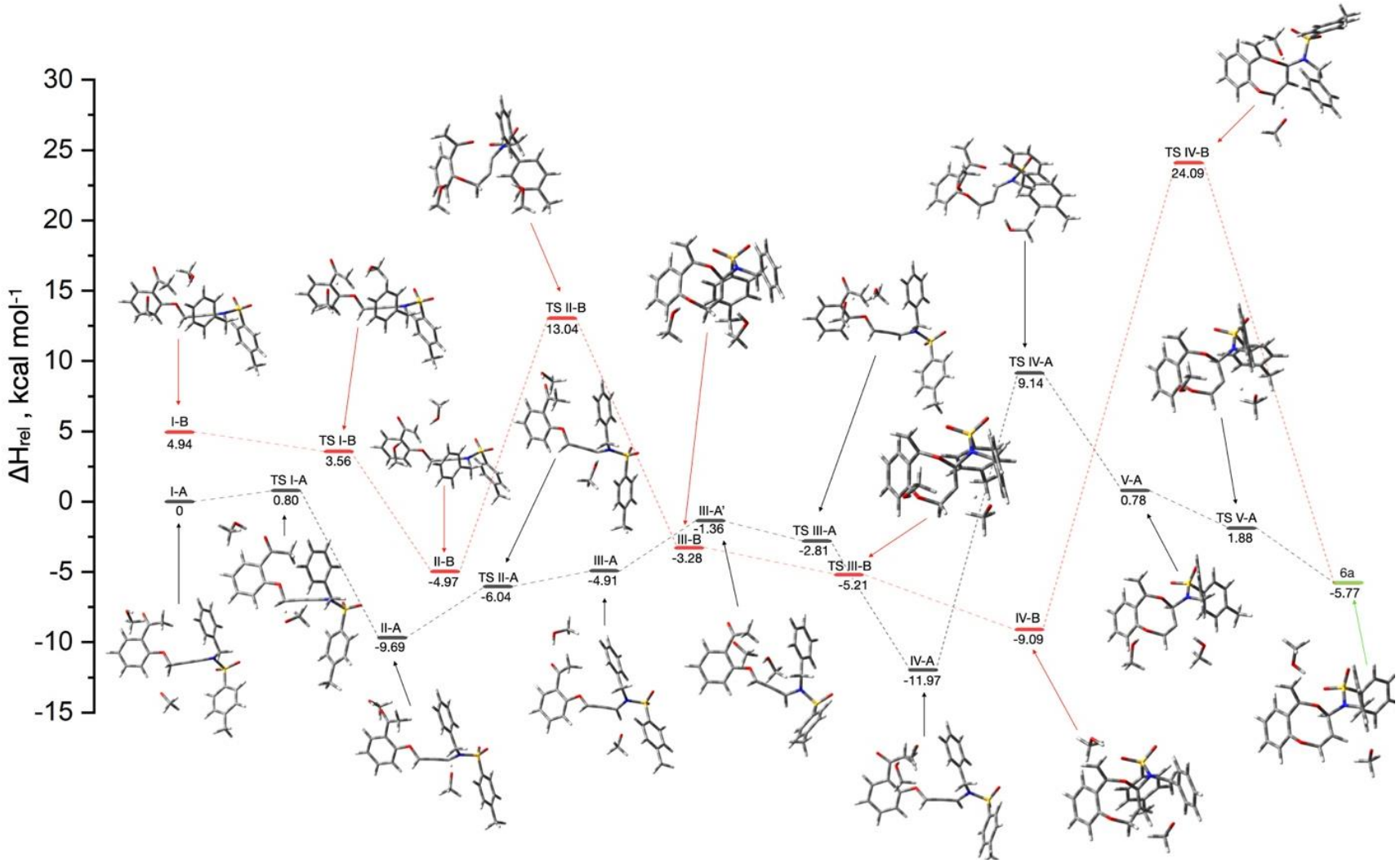


Figure 3. Computed energy profiles (ΔH, kcal/mol) for the reaction pathways A and B.



2. Geometries

Table 1. Optimized geometry and related energy for **I A** compound.

C	4.55183500	0.84615900	-0.26782000
C	3.45022000	1.80643700	-0.60383000
H	3.87519500	2.80724000	-0.68795300
H	2.92513300	1.52513700	-1.51762200
H	2.70936400	1.79839700	0.20089600
O	5.59641400	1.28124400	0.20881000
C	4.41848500	-0.60614200	-0.54709200
C	3.18770200	-1.29353300	-0.61983900
C	5.60108500	-1.32385600	-0.77224900
C	3.16331100	-2.66036200	-0.91715000
C	5.58195300	-2.67040400	-1.08748600
H	6.54161500	-0.78631600	-0.71964000
C	4.35566800	-3.33022000	-1.15357300
H	2.21663000	-3.20707600	-0.90428500
H	6.50738200	-3.20203500	-1.27944600
H	4.32451900	-4.39130800	-1.38315300
O	2.07202200	-0.59163700	-0.33384200
C	-0.24722300	-0.25190200	-0.31887400
C	-1.13703100	0.45189400	0.09567100
N	-2.11171700	1.26470600	0.52972700
C	-2.60642400	2.32103000	-0.38048700
H	-3.41085000	2.83382400	0.14994900
H	-3.01764300	1.86680900	-1.28721000
C	-1.50684000	3.28907100	-0.72541400
C	-1.11172700	3.46187000	-2.04945600
C	-0.88060900	4.03398300	0.27569000
C	-0.10825200	4.37155100	-2.37411100
H	-1.59098200	2.88168900	-2.83276700
C	0.12358500	4.93792200	-0.04543700
H	-1.18012900	3.89955500	1.31113400
C	0.51168300	5.10959500	-1.37283400
H	0.19077300	4.49802300	-3.40962400
H	0.60345100	5.51311200	0.73986600
H	1.29573900	5.81694500	-1.62311200
S	-3.16909500	0.62960400	1.70773100
O	-2.32596500	-0.10716700	2.63131000
O	-3.96183300	1.76095100	2.16098000
C	-4.22388200	-0.50815500	0.86245500
C	-3.79113400	-1.81657800	0.66478000
C	-5.44563900	-0.06448700	0.36489700
C	-4.60429200	-2.68821300	-0.04405800
H	-2.83885800	-2.14835000	1.06193700
C	-6.24421900	-0.95524700	-0.33721800
H	-5.76891200	0.95606900	0.53514200
C	-5.83913000	-2.27566800	-0.55306500

H	-4.27124500	-3.70915100	-0.20343700
H	-7.20086700	-0.61803000	-0.72385700
C	-6.72313400	-3.23674100	-1.28865200
H	-7.39371000	-3.74804800	-0.58918900
H	-7.34639800	-2.72208300	-2.02296100
H	-6.13768500	-4.00324100	-1.80069500
C	0.80563700	-1.12059300	-0.78389900
H	0.81905900	-1.15294600	-1.88114200
H	0.64578400	-2.16499000	-0.41615900
C	-0.81585400	-4.21309700	-0.61621300
H	-1.28064200	-3.30841000	-1.08378600
H	-1.53998800	-4.51659200	0.17794600
H	-0.90559600	-5.00614000	-1.39606300
O	0.45935400	-4.00707200	-0.16772700
C	6.92104400	-0.69341500	2.78558300
H	7.67908500	-1.07924100	3.47082000
H	6.15336400	-0.18006900	3.37893100
H	6.45306400	-1.54594900	2.27638900
O	7.56235200	0.17875300	1.87809900
H	6.89121000	0.52061500	1.26436000

Energy= -1949,67130285 Hartree

Table 2. Optimized geometry and related energy and frequency for transition state **TS I A**.

C	4.39623400	-0.06541600	1.30451200
C	3.21079400	0.44225700	2.06854100
H	3.56584800	1.03486100	2.91209200
H	2.60234600	1.07119700	1.41203000
H	2.56375800	-0.37020100	2.40297400
O	5.49360000	0.45529100	1.49904000
C	4.27169600	-1.19943800	0.35929700
C	3.05596300	-1.60479400	-0.25097300
C	5.44094000	-1.91779400	0.07264900
C	3.06333200	-2.71777000	-1.10751200
C	5.44098900	-3.01368600	-0.77027400
H	6.35980900	-1.59924700	0.55280200
C	4.23811400	-3.40791900	-1.35574800
H	2.13720800	-3.04718000	-1.55798900
H	6.35673300	-3.56124600	-0.96253800
H	4.21196300	-4.27057400	-2.01473400
O	1.96678700	-0.87889100	-0.01505300
C	-0.28316800	-0.29422300	-0.29687300
C	-1.17991600	0.46382500	0.02211400
N	-2.15925700	1.31601700	0.35986400
C	-2.49469300	2.42262100	-0.55863600
H	-3.36286200	2.93278300	-0.13668200
H	-2.77057600	2.02048400	-1.53861700
C	-1.34232800	3.38258800	-0.69022800
C	-0.82746400	3.69422500	-1.94601000

C	-0.79155700	3.98926100	0.44007100
C	0.21783000	4.60557900	-2.07579800
H	-1.24532000	3.22052000	-2.82977400
C	0.25439800	4.89425900	0.31363400
H	-1.18265600	3.74375500	1.42318100
C	0.76115000	5.20641400	-0.94643700
H	0.61007300	4.83972600	-3.06024700
H	0.67493300	5.36022300	1.19908100
H	1.57813300	5.91394700	-1.04466200
S	-3.37326900	0.71329200	1.39471800
O	-2.67755700	-0.00267900	2.45079500
O	-4.22458500	1.85126600	1.71417100
C	-4.30493200	-0.45309300	0.44677700
C	-3.86371800	-1.77091300	0.36717600
C	-5.43800800	-0.02551800	-0.23926500
C	-4.57676500	-2.66809000	-0.41537400
H	-2.98757800	-2.09011300	0.91951800
C	-6.13673200	-0.94025300	-1.01320000
H	-5.77535600	1.00112100	-0.15298900
C	-5.71643500	-2.26959600	-1.11915400
H	-4.24351600	-3.69958900	-0.47518200
H	-7.02961300	-0.61728100	-1.53949500
C	-6.46270800	-3.24075800	-1.98337600
H	-7.52971300	-3.00925800	-2.01198900
H	-6.09049200	-3.19775600	-3.01293300
H	-6.33599400	-4.26648400	-1.63109900
C	0.69985200	-1.26025300	-0.63600500
H	0.84756900	-1.30698300	-1.72214600
H	0.29182600	-2.49318000	-0.22353600
C	-0.35358500	-3.50914400	1.52299300
H	-0.27099100	-2.46472600	1.88396800
H	0.34024300	-4.10549200	2.14508000
H	-1.37228000	-3.84728000	1.78924300
O	-0.09129600	-3.61203400	0.16515800
C	7.40020100	1.08060500	-1.36368700
H	8.29924600	1.27635300	-1.95236000
H	6.74452900	1.95777100	-1.43931800
H	6.88087300	0.22077900	-1.80678800
O	7.80049700	0.82963700	-0.03274800
H	7.00248700	0.64971800	0.49239300

Energy= -1949,66508871 Hartree
Frequency= 1119,82i cm^{-1}

Table 3. Optimized geometry and related energy for **II A** compound.

C	4.90958100	0.25375700	-0.65167600
C	4.20233300	1.38412900	-1.33660500
H	4.91165000	2.19940000	-1.48392700
H	3.75709500	1.07560800	-2.28337100

H	3.38324600	1.73652300	-0.70188400
O	5.94943600	0.48228000	-0.03971000
C	4.40024400	-1.13733600	-0.74510500
C	3.04772500	-1.47328300	-0.97413600
C	5.33529700	-2.17274500	-0.61533500
C	2.67753000	-2.81889600	-1.07251600
C	4.97052500	-3.50247700	-0.72905800
H	6.37198000	-1.90304300	-0.44526500
C	3.63167400	-3.81753200	-0.95584700
H	1.63335200	-3.06815700	-1.21850700
H	5.71577200	-4.28539000	-0.64511700
H	3.32308200	-4.85527600	-1.03565400
O	2.15352800	-0.47147600	-1.03549300
C	-0.21153500	-0.36426600	-0.85070300
C	-1.24978900	-0.11415400	-0.10445200
N	-1.90276700	1.11868600	-0.15203200
C	-1.50464300	2.20913900	-1.03365800
H	-2.34604000	2.89816500	-1.13988300
H	-1.31202200	1.76693900	-2.01737500
C	-0.28420000	2.97265200	-0.57156700
C	0.40415200	3.76616400	-1.49127400
C	0.15713600	2.93842400	0.74874000
C	1.50433700	4.51898000	-1.09718400
H	0.07575600	3.79391800	-2.52720400
C	1.26126300	3.68850600	1.14528900
H	-0.36209700	2.31484800	1.46992700
C	1.93792200	4.48249800	0.22554400
H	2.02776800	5.13088500	-1.82528600
H	1.59473800	3.64865000	2.17770100
H	2.79967500	5.06526400	0.53473600
S	-3.19566600	1.29554400	0.87573900
O	-2.81144200	1.02640700	2.25847700
O	-3.77682500	2.60813700	0.58486100
C	-4.35191200	0.03582700	0.38815200
C	-4.95991400	-0.74123100	1.36303800
C	-4.70294900	-0.08930800	-0.95292400
C	-5.93201600	-1.66054700	0.98443400
H	-4.67020600	-0.63184100	2.40154100
C	-5.67026800	-1.01362500	-1.31311900
H	-4.22042800	0.52204000	-1.70849200
C	-6.30006500	-1.81396200	-0.35239600
H	-6.41007300	-2.27059900	1.74475300
H	-5.94381000	-1.11690800	-2.35889800
C	-7.32879400	-2.82584000	-0.76058700
H	-8.01813800	-2.41253700	-1.50143500
H	-6.84970100	-3.69924800	-1.21603100
H	-7.90800500	-3.17307900	0.09712700
C	0.84908200	-0.75394700	-1.52065100
H	0.85746300	-1.22333100	-2.50059000
C	-2.30100300	-3.42473400	0.53846800
H	-3.28833300	-3.07937500	0.20049700

H	-2.44106400	-4.36818400	1.07458300
H	-1.68983400	-3.63206300	-0.35223400
O	-1.68495900	-2.50542100	1.40634400
H	-1.59599800	-1.63615100	0.91828200
C	6.20039900	-1.20587000	3.01908700
H	6.68940300	-1.63670100	3.89560600
H	5.55008500	-0.38889900	3.35747500
H	5.57292500	-1.98128300	2.56063500
O	7.20924900	-0.75261200	2.14031500
H	6.77721500	-0.37013500	1.35859500

Energy= -1949,68702603 Hartree

Table 4. Optimized geometry and related energy and frequency for transition state **TS II A**.

C	4.93847500	0.34930400	-0.63322800
C	4.11057400	1.43077000	-1.25765200
H	4.74919800	2.29507600	-1.44288700
H	3.62662500	1.09845000	-2.17705000
H	3.31398900	1.72218200	-0.56597300
O	5.99447100	0.64105100	-0.08224600
C	4.52364500	-1.07616800	-0.71723200
C	3.18831500	-1.50742600	-0.84024100
C	5.53657100	-2.04251000	-0.69234100
C	2.90097000	-2.87016100	-0.93615200
C	5.25594000	-3.39297000	-0.80985500
H	6.56260300	-1.70275700	-0.60290900
C	3.92973800	-3.80082700	-0.92928800
H	1.86888900	-3.19602600	-0.98989200
H	6.05874400	-4.12149400	-0.80819600
H	3.68865300	-4.85610200	-1.00728400
O	2.21620600	-0.56779300	-0.79266700
C	-0.13657200	-0.52362500	-0.65890800
C	-1.23442200	-0.26085400	0.00679600
N	-1.92462800	0.94654900	-0.16137300
C	-1.45915900	1.95357200	-1.10508000
H	-2.29830900	2.60879000	-1.34720200
H	-1.17967400	1.42427100	-2.02214500
C	-0.29575200	2.78918700	-0.61951500
C	0.41736200	3.54801600	-1.54951600
C	0.06184600	2.86117500	0.72398400
C	1.46181300	4.36979800	-1.14309600
H	0.15183000	3.49501600	-2.60227200
C	1.11187800	3.67966500	1.13262400
H	-0.47861700	2.27091600	1.45752100
C	1.81365100	4.43832800	0.20247400
H	2.00562700	4.95403600	-1.87882000
H	1.38113400	3.72243500	2.18338500
H	2.63201800	5.07560300	0.52163800
S	-3.25455900	1.25060500	0.80082100

O	-2.91960400	1.05397300	2.20479900
O	-3.73780100	2.56639600	0.38875000
C	-4.45725000	0.03075400	0.33996800
C	-5.14301000	-0.65232200	1.33399200
C	-4.76261000	-0.15324800	-1.00505000
C	-6.15234400	-1.53437400	0.96937600
H	-4.88493600	-0.49863500	2.37501200
C	-5.76862400	-1.04192600	-1.35006600
H	-4.22029000	0.38520300	-1.77529900
C	-6.47882400	-1.74567400	-0.37104400
H	-6.69340500	-2.07013100	1.74324200
H	-6.00910000	-1.19129200	-2.39824900
C	-7.54598000	-2.72472400	-0.75905900
H	-8.11552000	-2.37039800	-1.62158700
H	-7.10015200	-3.68638900	-1.03606400
H	-8.23817000	-2.90676300	0.06541600
C	0.94657400	-0.90522900	-1.27800700
H	0.96949900	-1.42627700	-2.23242000
C	-2.52286700	-3.20562300	0.67451800
H	-2.59127100	-2.81412800	-0.36655400
H	-3.56477100	-3.46944800	0.95454500
H	-1.98240100	-4.17286400	0.58819900
O	-1.92516400	-2.31763200	1.53741500
H	-1.63470700	-1.13327800	0.76966200
C	6.55717900	-1.11166400	2.91001200
H	7.13074100	-1.53479100	3.73760200
H	5.87717000	-0.35273400	3.31787500
H	5.95464900	-1.91399300	2.46467800
O	7.47374700	-0.56210500	1.98594700
H	6.96777300	-0.18859700	1.24603900

Energy= -1949,67628161 Hartree
Frequency= 337,40i cm^{-1}

Table 5. Optimized geometry and related energy for **III A** compound.

C	-4.93818800	0.74517100	-0.23376300
C	-4.24358800	-0.40269200	-0.90053000
H	-4.97932600	-1.17123100	-1.13965800
H	-3.71162800	-0.08585100	-1.79894100
H	-3.49355200	-0.82329500	-0.22400100
O	-6.06677200	0.59599000	0.22359700
C	-4.30490200	2.08851600	-0.15262300
C	-2.92435500	2.33552100	-0.28197900
C	-5.15715400	3.18210000	0.04723900
C	-2.43736800	3.64203200	-0.22326000
C	-4.68017200	4.48020500	0.08787400
H	-6.21703200	2.97889200	0.15187100
C	-3.31223700	4.70407300	-0.04944900
H	-1.36977600	3.81772500	-0.28629200

H	-5.36290800	5.31077900	0.22672400
H	-2.91698700	5.71384200	-0.00738100
O	-2.09469700	1.26981000	-0.39334800
C	0.22279100	0.87979000	-0.42520900
C	1.30249900	0.37282400	0.11906100
N	1.79180600	-0.89481300	-0.22388300
C	1.11047400	-1.70503500	-1.22424300
H	1.81931100	-2.44446400	-1.60151400
H	0.86018800	-1.03758600	-2.05544200
C	-0.13560500	-2.40956500	-0.73478400
C	-0.99572400	-2.97505400	-1.67813400
C	-0.43328900	-2.55024200	0.61766300
C	-2.12631700	-3.67604300	-1.27644800
H	-0.77715800	-2.86694900	-2.73739700
C	-1.56894800	-3.24775800	1.02203500
H	0.22154700	-2.11080900	1.36365200
C	-2.41746800	-3.81499600	0.07816500
H	-2.78393300	-4.11104400	-2.02249400
H	-1.78911800	-3.34635300	2.08041100
H	-3.30195100	-4.35875500	0.39413000
S	3.08666600	-1.52106300	0.62593800
O	2.86306900	-1.37545700	2.05762400
O	3.28574900	-2.86421900	0.09105000
C	4.47177800	-0.50605400	0.17954900
C	5.42680300	-0.22503500	1.14959700
C	4.63793600	-0.09289600	-1.13749800
C	6.56151300	0.48777600	0.78782600
H	5.27839200	-0.55174300	2.17232800
C	5.77675700	0.62203600	-1.47829700
H	3.88672300	-0.31502800	-1.88779100
C	6.75348600	0.92503800	-0.52507800
H	7.31031000	0.71030200	1.54173000
H	5.90871000	0.95206500	-2.50404800
C	7.96408300	1.72697800	-0.89737100
H	8.23628800	1.57413700	-1.94391200
H	7.76918600	2.79652200	-0.76131200
H	8.82059400	1.46814400	-0.27120200
C	-0.82215300	1.47749100	-0.92327700
H	-0.81072500	2.10557600	-1.81151500
H	1.86186600	1.01670000	0.88513000
C	2.98870400	3.16039300	0.94810400
H	4.08577700	3.30555400	1.08885100
H	2.55837600	4.18853700	0.98295800
H	2.88075800	2.84607800	-0.11965700
O	2.41883000	2.28516800	1.83218000
C	-6.96515400	-2.61941400	1.23220700
H	-7.52279000	-3.55858300	1.24109700
H	-7.03823200	-2.16909500	2.23066200
H	-5.91034300	-2.85140000	1.03384700
O	-7.52469100	-1.79267800	0.23330300
H	-7.01898500	-0.96183900	0.21183600

Energy= -1949,67756249 Hartree

Table 6. Optimized geometry and related energy for **III A'** compound.

C	-4.88912200	0.04630500	0.70926800
C	-3.85482100	0.43950600	1.69906800
H	-3.64139700	-0.43842300	2.36849000
H	-2.91151600	0.69781100	1.21652000
H	-4.21999900	1.28395100	2.28608600
O	-5.99823300	0.56067100	0.69008800
C	-4.63072400	-1.11142500	-0.21808300
C	-3.39429100	-1.45361100	-0.78067000
C	-5.72628100	-1.92839500	-0.51600200
C	-3.26214400	-2.57402700	-1.59545100
C	-5.60216500	-3.06100000	-1.30569700
H	-6.68536000	-1.65780000	-0.08815300
C	-4.36148400	-3.38462300	-1.84416300
H	-2.30321800	-2.79451600	-2.05174500
H	-6.46624900	-3.68618300	-1.50157300
H	-4.24672600	-4.25993500	-2.47475400
O	-2.32335200	-0.60904100	-0.58864700
C	0.01103100	-0.57483300	-0.87202100
C	1.11327100	-0.02237700	-1.31487100
N	1.92831100	0.85225500	-0.58546900
C	1.60194700	1.12406000	0.81173800
H	2.52088700	1.42547800	1.32117000
H	1.25724800	0.19684800	1.28211800
C	0.56951900	2.21470900	0.97657400
C	-0.27412100	2.19163600	2.08648300
C	0.48495400	3.27995400	0.08216800
C	-1.18192700	3.22238400	2.30532300
H	-0.22439200	1.35936200	2.78335400
C	-0.42759500	4.30768900	0.29630900
H	1.13366100	3.30183500	-0.78756100
C	-1.26152100	4.28426400	1.40996900
H	-1.83450400	3.18979300	3.17188900
H	-0.48649000	5.12998100	-0.40979500
H	-1.97349900	5.08626400	1.57599600
S	3.53004500	1.01702400	-1.07751000
O	3.51225600	0.87213700	-2.52487400
O	4.01042900	2.24199100	-0.46015400
C	4.42611000	-0.34162700	-0.38188800
C	4.38979600	-1.57887700	-1.02261900
C	5.11946300	-0.16578000	0.80982700
C	5.05932200	-2.64815100	-0.45110000
H	3.86034400	-1.69827100	-1.96123400
C	5.78471900	-1.25172300	1.36500800
H	5.15224800	0.80730700	1.28617700
C	5.76369800	-2.50445100	0.75020900

H	5.04029100	-3.61273800	-0.94897200
H	6.33352100	-1.11891000	2.29189500
C	6.48479400	-3.67353200	1.34995000
H	6.96268400	-3.40605600	2.29375300
H	5.79504600	-4.50210500	1.53628400
H	7.25639400	-4.04441900	0.66832900
C	-1.07342400	-1.19254600	-0.49951800
H	-1.07199600	-2.17933800	-0.04203900
H	1.45141000	-0.19424500	-2.33318400
C	-1.77799600	-1.90830800	3.36255000
H	-1.37160300	-1.08460400	2.72145600
H	-1.35696000	-2.83980000	2.90979700
H	-1.23210900	-1.79850000	4.33148900
O	-3.13824300	-1.89914000	3.47544500
C	-1.82687700	2.01224000	-3.20873300
H	-2.08733400	2.91654600	-3.76220100
H	-0.77374100	2.08104400	-2.91024200
H	-1.94647000	1.15184000	-3.87869400
O	-2.69000000	1.93686200	-2.08979500
H	-2.47670800	1.13699700	-1.59450200

Energy= -1949,67262248 Hartree

Table 7. Optimized geometry and related energy and frequency for transition state **TS III A**.

C	-4.72042900	0.22016100	0.49436700
C	-3.92461600	0.25552500	1.70387600
H	-4.48002800	-0.51228100	2.50928800
H	-2.91094800	-0.12383600	1.58234800
H	-3.94181700	1.24008100	2.17694000
O	-5.67260700	0.97370500	0.27246100
C	-4.49901900	-0.91803100	-0.47486700
C	-3.25862400	-1.28037200	-1.00758800
C	-5.61603000	-1.65706400	-0.86975000
C	-3.13494700	-2.35248200	-1.88558000
C	-5.50489600	-2.74697000	-1.72279400
H	-6.58370200	-1.36668200	-0.47381200
C	-4.25759300	-3.09605300	-2.22842200
H	-2.16763500	-2.58774400	-2.31655700
H	-6.38636800	-3.31714600	-1.99553600
H	-4.15453100	-3.93552800	-2.90790600
O	-2.16652600	-0.48934500	-0.70778100
C	0.17688300	-0.52638500	-0.91688600
C	1.31326900	-0.00006100	-1.30178900
N	2.14432800	0.80453200	-0.51179100
C	1.77934900	1.04451100	0.88399200
H	2.69409000	1.26925300	1.43828300
H	1.36076900	0.12397400	1.30356900
C	0.80870200	2.18973500	1.04493300
C	-0.23511800	2.08973900	1.96215200

C	0.97947800	3.37906600	0.33632400
C	-1.09277000	3.16482300	2.17645100
H	-0.38119100	1.16431900	2.51223000
C	0.12009400	4.45130500	0.54504100
H	1.79041800	3.46271100	-0.38039400
C	-0.91750700	4.34831300	1.46796600
H	-1.90338800	3.07262000	2.89202900
H	0.26167100	5.37145000	-0.01306100
H	-1.58827800	5.18582600	1.63028900
S	3.77091700	0.89755900	-0.93475600
O	3.80852000	0.77293700	-2.38372300
O	4.28282200	2.09043300	-0.28048900
C	4.57199000	-0.51013100	-0.22058400
C	4.48914400	-1.74081200	-0.86871400
C	5.23380400	-0.37712900	0.99490700
C	5.08076900	-2.84745200	-0.28136700
H	3.98262100	-1.82877800	-1.82336900
C	5.82011300	-1.49936200	1.56548000
H	5.30074800	0.59060700	1.47855200
C	5.75320300	-2.74663500	0.94185000
H	5.02297800	-3.80837700	-0.78316300
H	6.34120500	-1.40086600	2.51251400
C	6.40769500	-3.94962100	1.55063800
H	6.64168100	-3.78607500	2.60406800
H	5.76772300	-4.83161500	1.46771800
H	7.34437800	-4.17884300	1.03127500
C	-0.94323100	-1.12186200	-0.61881200
H	-0.99117300	-2.13604500	-0.22723700
H	1.67234300	-0.13765200	-2.31814500
C	-4.52139800	-2.64682900	3.18738100
H	-3.84754900	-2.63610500	2.30113100
H	-5.29849900	-3.40440600	2.95478600
H	-3.91818900	-3.08034200	4.01218200
O	-5.03590000	-1.40126700	3.47520100
C	-1.72777500	2.22102700	-3.06384500
H	-1.86670500	3.20784400	-3.50986700
H	-0.65103100	2.02618100	-2.98549300
H	-2.17066100	1.47459700	-3.73508500
O	-2.35679600	2.23418100	-1.79682200
H	-2.24325700	1.36330800	-1.39587700

Energy= -1949,67123367 Hartree
Frequency= 494,39i cm^{-1}

Table 8. Optimized geometry and related energy for **IV A** compound.

C	-4.79724800	-0.04416600	0.50271000
C	-3.83607600	0.89054000	0.85980000
H	-3.56883700	0.04059500	2.70733500
H	-2.77919600	0.74324100	0.69718200

H	-4.17299700	1.81661500	1.32026600
O	-6.04587000	0.12207700	0.67016100
C	-4.39179100	-1.38592000	-0.10157700
C	-3.12865100	-1.78082600	-0.57951300
C	-5.41098700	-2.34061800	-0.19393500
C	-2.92384300	-3.04473700	-1.13184900
C	-5.21493500	-3.61351100	-0.71186900
H	-6.38454900	-2.03003200	0.16891500
C	-3.95985500	-3.96760200	-1.18991600
H	-1.95038300	-3.29650800	-1.53927800
H	-6.03853200	-4.31912600	-0.75114800
H	-3.78254800	-4.94802200	-1.62011800
O	-2.08709500	-0.88140600	-0.55627500
C	0.23754900	-0.75756900	-0.84793600
C	1.30684600	-0.20230000	-1.35978500
N	2.07775400	0.79422100	-0.73686400
C	1.75857000	1.17759000	0.63385000
H	2.66598100	1.57501600	1.09606200
H	1.47484500	0.27991900	1.19449200
C	0.66923100	2.22067100	0.72918700
C	-0.00184000	2.37982300	1.94215600
C	0.35775300	3.06455200	-0.33345500
C	-0.96019800	3.37486800	2.09408900
H	0.22800700	1.72059500	2.77506800
C	-0.60847600	4.05556600	-0.18490700
H	0.87128700	2.94267200	-1.28160400
C	-1.26706500	4.21717200	1.02914500
H	-1.47392900	3.48734400	3.04354600
H	-0.84561300	4.70382300	-1.02259700
H	-2.01957300	4.99057500	1.14408500
S	3.66440600	0.98738000	-1.25923800
O	3.64951600	0.68901900	-2.68316300
O	4.08609600	2.29375900	-0.78061400
C	4.63609100	-0.24136300	-0.43343500
C	4.65326700	-1.54189100	-0.93159500
C	5.33116300	0.09807500	0.72258100
C	5.37947200	-2.50909100	-0.25424500
H	4.11900300	-1.79129000	-1.84151700
C	6.05270300	-0.88586400	1.38462200
H	5.31853900	1.11827200	1.08853700
C	6.08856700	-2.19939800	0.91096900
H	5.39878700	-3.52391000	-0.63914000
H	6.59997300	-0.62577100	2.28526400
C	6.89445500	-3.24837100	1.61558700
H	7.01904900	-3.01094300	2.67396000
H	6.42770900	-4.23209400	1.52948900
H	7.89418900	-3.32089100	1.17337400
C	-0.82130600	-1.38208000	-0.40813500
H	-0.75635500	-2.31135300	0.15532000
H	1.65372200	-0.46380600	-2.35579600
C	-2.33264100	-1.28619700	3.41683600

H	-2.64295700	-2.11476400	2.76656100
H	-2.08748800	-1.69667600	4.39925100
H	-1.42142400	-0.84083000	2.99565300
O	-3.35959700	-0.33277200	3.58909700
C	-4.29330800	1.39587300	-2.83565400
H	-5.24666000	0.87210000	-2.68765900
H	-4.34662000	1.94096700	-3.78117300
H	-3.49665900	0.64527900	-2.91706100
O	-4.03782100	2.33299900	-1.81033200
H	-3.97806900	1.84260400	-0.96475900

Energy= -1949,69111279 Hartree

Table 9. Optimized geometry and related energy and frequency for transition state **TS IV A**.

C	-2.80163300	-0.29564700	-1.58720900
C	-3.49391900	0.19109400	-2.65592800
H	0.70379700	-1.54971700	2.42182500
H	-4.42421600	-0.26194900	-2.97638800
H	-3.14364200	1.07740400	-3.17592400
O	-1.72732000	0.27181700	-1.11540200
C	-3.34104600	-1.52639700	-0.92036900
C	-3.48078800	-1.62574300	0.46678200
C	-3.77561700	-2.61390000	-1.68953300
C	-4.05380700	-2.74898600	1.05801700
C	-4.33322500	-3.74544500	-1.10940200
H	-3.65810900	-2.56009000	-2.76695300
C	-4.47917700	-3.81236500	0.27332000
H	-4.16494700	-2.77259900	2.13731500
H	-4.65056100	-4.57401400	-1.73428600
H	-4.92088500	-4.68690100	0.73996600
O	-3.08448300	-0.58653400	1.28845000
C	-0.66933600	-0.79232300	1.30357600
C	-0.30356600	-0.59522200	-0.02694700
N	0.68046700	0.33577500	-0.33781800
C	1.09868300	1.34697800	0.62924700
H	2.18746800	1.30682300	0.74155500
H	0.67908900	1.00521700	1.58427200
C	0.67336300	2.76674600	0.34983000
C	-0.55880100	3.07051900	-0.22865400
C	1.51640400	3.80745800	0.74062700
C	-0.93486700	4.39772400	-0.41214400
H	-1.20557200	2.25765300	-0.55144100
C	1.13617800	5.13396100	0.56232200
H	2.48258700	3.58029200	1.18391000
C	-0.09314600	5.43360100	-0.01596600
H	-1.89397300	4.62466800	-0.86835100
H	1.80471000	5.93254100	0.86847100
H	-0.39076900	6.46721300	-0.16164300
S	1.68844400	0.06390400	-1.65214900

O	1.04177400	-0.94296700	-2.47951100
O	2.03169200	1.36439000	-2.20487200
C	3.16609900	-0.63713800	-0.96592700
C	4.27704700	0.16955700	-0.75266000
C	3.18139200	-1.99043100	-0.63239600
C	5.41862100	-0.39224600	-0.19262000
H	4.25206700	1.21632500	-1.03333100
C	4.32867800	-2.53051800	-0.07599800
H	2.31310800	-2.61328800	-0.81652000
C	5.46302500	-1.74265300	0.15517000
H	6.29013800	0.23308100	-0.02648300
H	4.34740000	-3.58495500	0.18214500
C	6.69798600	-2.34935200	0.74987900
H	6.46446600	-2.88477600	1.67450200
H	7.14176200	-3.07509100	0.06081000
H	7.44919600	-1.58934500	0.97119200
C	-1.83220800	-0.84457800	1.91618500
H	-1.97162000	-1.09975000	2.96402100
H	-0.29912800	-1.45906900	-0.68501200
C	2.38371200	-1.07879200	3.31726600
H	2.96570300	-0.82699300	2.41983700
H	2.01406100	-0.14445900	3.76154800
H	3.06112700	-1.54752500	4.03587300
O	1.34213600	-1.98712000	3.04048400
C	-4.52866100	2.60647300	1.18799000
H	-5.21305200	3.41296500	1.46071500
H	-4.69060000	2.36230300	0.13020200
H	-3.50121000	2.97400200	1.30468500
O	-4.79968100	1.50703400	2.03380100
H	-4.20805200	0.77995700	1.78227200

Energy= -1949,65586583 Hartree
Frequency= 216,02i cm^{-1}

Table 10. Optimized geometry and related energy for **V A** compound.

C	-2.16699000	0.25520000	-1.84335100
C	-2.58007500	1.00396800	-2.87518300
H	-3.30475700	0.61506100	-3.57874500
H	-2.22565200	2.02128600	-2.99681200
O	-1.37255200	0.81039000	-0.89587800
C	-2.60416800	-1.14593000	-1.65544400
C	-3.07346200	-1.58484300	-0.41099100
C	-2.59374300	-2.05131600	-2.72136500
C	-3.51547000	-2.89371700	-0.24266800
C	-3.03734000	-3.35649700	-2.55749200
H	-2.21734700	-1.71808300	-3.68318500
C	-3.49791500	-3.77893300	-1.31310500
H	-3.88526800	-3.19910600	0.73073900

H	-3.01732500	-4.04467600	-3.39586400
H	-3.84757400	-4.79706000	-1.17587800
O	-3.16642700	-0.70497600	0.63777800
C	-0.76718400	-0.37386200	1.20157100
C	-0.40546700	-0.04034800	-0.20174900
N	0.86868200	0.66658600	-0.29293400
C	1.23859100	1.67680000	0.69734300
H	2.31833100	1.83972400	0.62430500
H	1.04041700	1.23985200	1.67981700
C	0.51495800	2.99733000	0.57097700
C	-0.27310500	3.45416100	1.62551600
C	0.64841500	3.79653900	-0.56645900
C	-0.92270400	4.68397700	1.54942600
H	-0.38427000	2.83786900	2.51335200
C	-0.00036900	5.02282300	-0.64650600
H	1.26058000	3.44550200	-1.39141600
C	-0.78873400	5.47114400	0.41159900
H	-1.53488300	5.02392200	2.37893900
H	0.11136100	5.63488700	-1.53630800
H	-1.29468100	6.42930100	0.34743300
S	1.95329900	0.28908900	-1.46479500
O	1.31263100	-0.68396000	-2.34814200
O	2.49783800	1.50341600	-2.06943400
C	3.29983200	-0.49908800	-0.60658100
C	4.58937100	-0.36088100	-1.10939400
C	3.04378700	-1.28758600	0.50891800
C	5.63122200	-1.03129500	-0.48408800
H	4.77412700	0.26704300	-1.97364500
C	4.09982900	-1.94739100	1.12287000
H	2.03713100	-1.36313700	0.91014700
C	5.40570300	-1.83184400	0.63932900
H	6.63920000	-0.92769800	-0.87424000
H	3.90533700	-2.55927900	1.99862600
C	6.54417700	-2.52275400	1.32865900
H	7.00330400	-1.85819300	2.06885700
H	6.20623900	-3.41750800	1.85571600
H	7.32372100	-2.80868200	0.61888500
C	-2.01411000	-0.67968300	1.51972400
H	-2.35491100	-0.95296200	2.51633700
H	-0.29032300	-0.95538200	-0.78897900
C	0.81634900	-2.15742300	3.70832700
H	-0.15794600	-2.49655500	4.09366400
H	1.04997600	-2.76913400	2.82306900
H	1.56963500	-2.38117800	4.47124500
O	0.83715600	-0.78319800	3.42920000
H	0.26882100	-0.61618400	2.58746000
C	-6.03028400	-0.84115800	2.62749300
H	-6.99834200	-0.53307300	3.02886300
H	-5.30825800	-0.86003700	3.45412100
H	-6.13287600	-1.86074800	2.23378300
O	-5.66521600	0.08257500	1.62330600

H	-4.80146200	-0.18563700	1.26807200

Energy= -1949,67068685 Hartree

Table 11. Optimized geometry and related energy and frequency for transition state **TS V A**.

C	-2.12299500	-1.11045700	-1.32301800
C	-2.98763700	-0.84894100	-2.31115000
H	-3.45749000	-1.65787000	-2.85543100
H	-3.25688700	0.17253000	-2.55430300
O	-1.65821300	-0.08961800	-0.55773800
C	-1.70143500	-2.48373100	-0.97099200
C	-1.70321100	-2.90933200	0.36246700
C	-1.31360800	-3.39445000	-1.95896200
C	-1.32309300	-4.20420600	0.69691200
C	-0.93787200	-4.68971200	-1.63058400
H	-1.29639100	-3.06469700	-2.99264800
C	-0.93912500	-5.09426700	-0.29825800
H	-1.35022900	-4.50477000	1.73900600
H	-0.63679300	-5.38016900	-2.41120400
H	-0.64692400	-6.10504500	-0.03297400
O	-2.15786400	-2.07113600	1.35508700
C	-0.31236100	-0.43734800	1.47371500
C	-0.31906100	-0.18654900	0.00209700
N	0.35990000	1.04838700	-0.36894700
C	0.21830300	2.25125700	0.45510600
H	1.05256200	2.91607800	0.22116000
H	0.32166600	1.95336500	1.50081600
C	-1.08138800	2.99059200	0.23996600
C	-1.96228100	3.17492400	1.30336900
C	-1.40648400	3.52883000	-1.00683700
C	-3.15163300	3.87902900	1.12853200
H	-1.71835200	2.75867100	2.27694000
C	-2.59264600	4.22982600	-1.18550600
H	-0.72181900	3.39122400	-1.83855500
C	-3.47047000	4.40654800	-0.11735500
H	-3.82909400	4.01168800	1.96633300
H	-2.83382600	4.64392300	-2.15973500
H	-4.39711600	4.95401200	-0.25783200
S	1.48900400	1.00723400	-1.56970900
O	1.09617900	-0.05009300	-2.49577400
O	1.65117600	2.37482700	-2.05248400
C	3.03954600	0.51846500	-0.84929900
C	3.87966700	1.48575800	-0.30576200
C	3.38618000	-0.82839900	-0.82012400
C	5.07311000	1.09004800	0.28122000
H	3.61305100	2.53522000	-0.35896000
C	4.58533700	-1.20425700	-0.23033800
H	2.73573900	-1.56960100	-1.27045000
C	5.44256100	-0.25685300	0.33463100

H	5.73455400	1.84360200	0.69781700
H	4.86305000	-2.25381300	-0.21588100
C	6.72030800	-0.67576400	0.99775300
H	6.55459100	-0.85349500	2.06619600
H	7.10739800	-1.60189600	0.56747800
H	7.48655700	0.09765600	0.91020800
C	-1.15388000	-1.30221500	2.02122600
H	-1.18722900	-1.52316700	3.08554300
H	0.19947200	-0.99906000	-0.51619800
C	2.42379500	-0.32640400	3.32299600
H	2.48674900	-0.76681800	4.33426400
H	2.33099500	-1.17362500	2.61706500
H	3.40321600	0.14154200	3.12174900
O	1.36806500	0.56775100	3.19242200
H	0.61596600	0.13344500	2.39068900
C	-5.14066200	-0.11431700	1.15679700
H	-6.21098300	0.07907300	1.25777800
H	-4.86452200	0.01134400	0.10252000
H	-4.59977500	0.63451000	1.74962600
O	-4.89717700	-1.42991600	1.61361300
H	-3.95263100	-1.62127900	1.50434800

Energy= -1949,67050486 Hartree
Frequency= 900,80i cm^{-1}

Table 12. Optimized geometry and related energy for **I B** compound.

C	4.40008500	-0.37927200	1.10827500
C	3.68686900	0.90534400	0.91655600
H	2.70956900	0.78150400	0.45253000
H	3.60303300	1.43246300	1.86944400
O	5.16656700	-0.56258100	2.04457700
C	4.31415100	-1.43937900	0.04345500
C	3.12726200	-1.85753300	-0.58236600
C	5.51378900	-2.03832900	-0.34388100
C	3.16561300	-2.82336100	-1.58680600
C	5.56222100	-2.98969400	-1.35347200
H	6.42277400	-1.72114400	0.15634100
C	4.38162000	-3.37538500	-1.97490700
H	2.25508400	-3.16501100	-2.06281700
H	6.51009300	-3.42391300	-1.65140700
H	4.39470300	-4.12128000	-2.76285400
O	1.95964700	-1.32072400	-0.12349600
C	-0.26226500	-0.62994900	-0.41060100
C	-1.11426200	0.10044800	0.03167800
N	-2.02972300	0.95436000	0.50206700
C	-2.26511800	2.21910000	-0.23339000
H	-3.02784700	2.76098600	0.32812200
H	-2.65284800	1.99789600	-1.23238400
C	-0.99942400	3.02778600	-0.32128300

C	-0.41443400	3.28671300	-1.55824800
C	-0.40002600	3.52957800	0.83553400
C	0.75339000	4.04066000	-1.64280400
H	-0.87351300	2.89589000	-2.46173000
C	0.76702700	4.27777900	0.75344900
H	-0.84879600	3.32737100	1.80388300
C	1.34684900	4.53496000	-0.48735200
H	1.20139100	4.23496900	-2.61189400
H	1.22582500	4.66350600	1.65812800
H	2.26001300	5.11784500	-0.55055500
S	-3.28025100	0.29922100	1.46219400
O	-2.64314800	-0.69737600	2.30231300
O	-3.95357600	1.44951100	2.04016000
C	-4.38419300	-0.51333700	0.34835500
C	-4.15064700	-1.84354100	0.01085700
C	-5.44401500	0.20101100	-0.20276600
C	-4.99955100	-2.46031000	-0.89621600
H	-3.32654000	-2.38639200	0.45891400
C	-6.28079500	-0.43698700	-1.10621500
H	-5.61716800	1.23295900	0.08041300
C	-6.07393000	-1.77170300	-1.46681900
H	-4.82592400	-3.49791800	-1.16353800
H	-7.11208400	0.11177900	-1.53747200
C	-7.00330800	-2.45880900	-2.42064100
H	-7.83673000	-2.91586000	-1.87580400
H	-7.42859900	-1.75434300	-3.13852200
H	-6.49418700	-3.25442300	-2.96846300
C	0.77658400	-1.49592400	-0.91709500
H	1.00012000	-1.24789000	-1.96098800
H	0.44806700	-2.54109200	-0.87537200
C	4.71288000	2.16232400	-2.17957300
H	5.47804700	1.75635400	-2.88432200
H	3.96150500	1.33752800	-2.08129300
H	4.18245000	2.95160700	-2.76549200
O	5.21776300	2.58951600	-0.98426900
H	4.31638900	1.53724600	0.21766500
C	1.71166900	-2.83244200	3.10396300
H	1.50639500	-2.95863300	4.16877900
H	2.76710200	-3.07385000	2.92608300
H	1.09048200	-3.54501200	2.54732800
O	1.41075800	-1.49127200	2.76806800
H	1.57095800	-1.37627300	1.82274600

Energy= -1949,66305092 Hartree

Table 13. Optimized geometry and related energy and frequency for transition state **TS I B**.

C	4.46646600	-0.34663800	1.08654600
C	3.80678900	0.90430200	0.78017100
H	2.85258100	0.79781500	0.26777800

H	3.74017200	1.55655100	1.65426300
O	5.26603000	-0.48635200	2.01954000
C	4.32784100	-1.50428400	0.12259300
C	3.11728300	-1.95829400	-0.42849500
C	5.50070200	-2.17006100	-0.23485200
C	3.10665100	-3.02651600	-1.32523400
C	5.50271200	-3.22410800	-1.13938300
H	6.42903800	-1.82671700	0.20974000
C	4.29818400	-3.64739300	-1.68495700
H	2.17597600	-3.39352100	-1.73957300
H	6.43343400	-3.70884000	-1.41348400
H	4.27255600	-4.47301000	-2.38871700
O	1.97047800	-1.34345700	-0.01147900
C	-0.24996200	-0.65633800	-0.32087500
C	-1.09521800	0.11660600	0.05726500
N	-2.00422800	1.01524100	0.45285600
C	-2.19873000	2.23293500	-0.36934700
H	-2.96921900	2.82019700	0.13255900
H	-2.55971200	1.95319100	-1.36369300
C	-0.91830500	3.01647900	-0.46982500
C	-0.28538600	3.17584900	-1.70002700
C	-0.35283600	3.59413400	0.66852600
C	0.89646700	3.90613700	-1.79634800
H	-0.71782900	2.72514800	-2.58866800
C	0.82800000	4.31900900	0.57508400
H	-0.83937000	3.46983400	1.63175700
C	1.45570400	4.47657400	-0.65903100
H	1.38190200	4.02278800	-2.75987300
H	1.26000100	4.76447200	1.46539900
H	2.37932100	5.04175500	-0.73107800
S	-3.29253700	0.43902700	1.41374400
O	-2.69394100	-0.49172900	2.35205800
O	-3.98081900	1.63220900	1.87588500
C	-4.35710500	-0.45561300	0.32459600
C	-4.12176400	-1.81027000	0.10685000
C	-5.38528500	0.21761300	-0.32864400
C	-4.93683000	-2.49409200	-0.78295100
H	-3.32238600	-2.31914500	0.63278900
C	-6.18855300	-0.48710300	-1.21284500
H	-5.56046500	1.27039500	-0.13857200
C	-5.97903700	-1.84803300	-1.45417500
H	-4.76152400	-3.55101600	-0.95741200
H	-6.99516500	0.02966300	-1.72326800
C	-6.87249200	-2.60605800	-2.38845500
H	-7.72294100	-3.02818600	-1.84176300
H	-7.27432400	-1.95698100	-3.16920900
H	-6.34197900	-3.43585800	-2.86011200
C	0.77159300	-1.57952700	-0.75921000
H	0.97545000	-1.43976100	-1.82728300
H	0.42792000	-2.61042600	-0.61006200
C	4.78965000	1.96287800	-2.20222100

H	5.52388100	1.49686300	-2.89120400
H	3.93363500	1.25324100	-2.15763300
H	4.40422100	2.85727400	-2.73401400
O	5.30834100	2.24457800	-0.95607000
H	4.55326600	1.50840500	-0.02862500
C	0.63587700	-2.23854500	3.09314000
H	0.43879100	-2.30919300	4.16489600
H	-0.32415200	-2.13155300	2.57368300
H	1.11258300	-3.17253300	2.76997600
O	1.47474100	-1.11720200	2.88766200
H	1.67138400	-1.06420300	1.94337500

Energy= -1949,66148217 Hartree
Frequency= 607,74i cm^{-1}

Table 14. Optimized geometry and related energy for **II B** compound.

C	4.45467500	-0.49319700	1.14635500
C	3.67433100	0.64906800	1.04392200
H	2.86603900	0.73419400	0.33036800
H	3.86523800	1.47486900	1.72596300
O	5.38982400	-0.65794400	1.99195500
C	4.27244700	-1.62251300	0.14215800
C	3.07589800	-1.99144600	-0.50921000
C	5.41221200	-2.37435200	-0.14752500
C	3.05967400	-3.06020900	-1.40937000
C	5.41105100	-3.42737300	-1.05508000
H	6.31983500	-2.09889400	0.37889100
C	4.22429800	-3.76918200	-1.68714300
H	2.14031400	-3.35604300	-1.89901900
H	6.32485700	-3.97552600	-1.26005600
H	4.18899500	-4.59172700	-2.39457900
O	1.95310300	-1.28483900	-0.20635000
C	-0.29638500	-0.70474700	-0.45589700
C	-1.14433200	0.06798300	-0.08408500
N	-2.06058000	0.96553700	0.30334100
C	-2.37546700	2.09030800	-0.60569800
H	-3.13201300	2.69166500	-0.09859400
H	-2.79858100	1.70634400	-1.53902500
C	-1.14595600	2.91355900	-0.88091800
C	-0.67305600	3.05591800	-2.18285900
C	-0.47205100	3.54995200	0.16313400
C	0.45580500	3.82886300	-2.44340400
H	-1.18932300	2.55862700	-2.99895000
C	0.65713800	4.31635300	-0.09405200
H	-0.83214500	3.43790600	1.18178500
C	1.12347100	4.45834100	-1.39954800
H	0.81499700	3.93282000	-3.46214700
H	1.17439500	4.80686100	0.72424600
H	2.00575900	5.05766300	-1.59971100

S	-3.23946700	0.43544800	1.41547000
O	-2.52912900	-0.39247500	2.37222900
O	-3.93217800	1.64161200	1.83638100
C	-4.35851000	-0.58096300	0.50113100
C	-4.09057500	-1.94124100	0.37314100
C	-5.46893600	0.00042900	-0.10332300
C	-4.95433800	-2.72352000	-0.37861200
H	-3.23125400	-2.37929200	0.86736100
C	-6.32013700	-0.80206300	-0.84900500
H	-5.67284300	1.05754200	0.02340200
C	-6.07521600	-2.16932600	-1.00431200
H	-4.75779700	-3.78676200	-0.47474800
H	-7.19543300	-0.35843500	-1.31290700
C	-6.98470000	-3.02120600	-1.83685400
H	-7.99107900	-2.60064900	-1.88487300
H	-6.60633700	-3.09032800	-2.86270200
H	-7.04767800	-4.03803000	-1.44321700
C	0.74374700	-1.61887400	-0.87692800
H	0.87993000	-1.54929700	-1.96382300
H	0.44587600	-2.64964900	-0.64343000
C	4.75627900	1.55259800	-2.32397700
H	5.33630600	1.99060000	-3.13985300
H	4.67763200	0.47172300	-2.50075600
H	3.74560300	1.98152900	-2.35551400
O	5.42049200	1.84425900	-1.11300700
H	4.90651200	1.42981400	-0.38711500
C	2.10497700	0.34468700	4.28856100
H	1.38437700	0.13314900	5.08223200
H	2.16449000	1.43397800	4.16439000
H	3.08873400	-0.01874800	4.61388400
O	1.65928600	-0.30161500	3.11583600
H	2.29087300	-0.09088300	2.39762000

Energy= -1949,68044590 Hartree

Table 15. Optimized geometry and related energy and frequency for transition state **TS II B**.

C	-2.71777900	0.30636100	-1.51217500
C	-3.89074400	0.89529500	-1.87842300
H	-4.75215300	0.29558300	-2.14994300
H	-3.97554500	1.97755800	-1.92453900
O	-1.62400100	0.94559100	-1.22335400
C	-2.68074200	-1.19752900	-1.49341100
C	-2.61667600	-1.89720700	-0.28953900
C	-2.72180100	-1.93638100	-2.67773900
C	-2.59684200	-3.28858600	-0.25900400
C	-2.68653900	-3.32736300	-2.66307700
H	-2.77654300	-1.40422100	-3.62263900
C	-2.62532200	-4.00584600	-1.44987600
H	-2.57561700	-3.80134300	0.69785700

H	-2.71305400	-3.88016300	-3.59673300
H	-2.61061100	-5.09078800	-1.42722300
O	-2.63325900	-1.18756400	0.89231600
C	-0.30804900	-0.38422900	0.93052400
C	-0.09106200	0.38111600	-0.04236800
N	0.81539000	1.21003700	-0.62448100
C	1.31907800	2.34535900	0.18220700
H	2.14770300	2.78471900	-0.37446800
H	1.69731400	1.96145000	1.13535300
C	0.25922500	3.38606700	0.41624200
C	-0.42781100	3.43436600	1.62747200
C	-0.03966400	4.32570300	-0.57148500
C	-1.40501500	4.40123700	1.84854500
H	-0.19475100	2.71008700	2.40267800
C	-1.01331200	5.29254100	-0.35389300
H	0.49472900	4.29734500	-1.51692800
C	-1.70006600	5.33101100	0.85768400
H	-1.93329900	4.42888100	2.79624800
H	-1.23494600	6.02055000	-1.12779900
H	-2.45928000	6.08746100	1.02895800
S	1.86073200	0.53870300	-1.77135800
O	1.07298800	-0.36341300	-2.59291300
O	2.55310700	1.66718700	-2.38087000
C	3.05182700	-0.42770300	-0.88542300
C	2.78593800	-1.77089100	-0.63364200
C	4.22368600	0.17222500	-0.43548500
C	3.71300400	-2.51533200	0.08085500
H	1.87625200	-2.22531700	-1.00749300
C	5.13708800	-0.59023900	0.27916000
H	4.42705400	1.21353200	-0.65839500
C	4.89587000	-1.93910600	0.55313300
H	3.51655900	-3.56619300	0.27051800
H	6.05867200	-0.13030200	0.62222900
C	5.87371600	-2.74845900	1.35071600
H	5.91326100	-3.78234000	1.00001900
H	6.87820900	-2.32350400	1.30071500
H	5.57665900	-2.77284700	2.40512500
C	-1.35978400	-1.15263100	1.58172900
H	-1.58397500	-0.72124800	2.56186800
H	-1.03185000	-2.18547800	1.75054300
C	2.05142400	-1.30670200	3.58259800
H	1.11530500	-1.63346900	4.05479100
H	2.41077100	-2.11365100	2.93055900
H	2.79177300	-1.15241400	4.37126500
O	1.89937400	-0.08837000	2.88565700
H	1.22786300	-0.21948300	2.17977900
C	-5.12059100	-2.24181200	3.07153500
H	-4.27379600	-2.41095600	3.74921700
H	-6.03317700	-2.20362200	3.67047800
H	-5.19477500	-3.09829000	2.38909700
O	-5.00876300	-1.01697300	2.37637800

H	-4.19807300	-1.05030100	1.84309300

Energy= -1949,65014713 Hartree
Frequency= 230,62i cm^{-1}

Table 16. Optimized geometry and related energy for **III B** compound.

C	-1.31646300	-1.42560000	-1.99681800
C	-1.96935500	-1.60337400	-3.15276000
H	-1.82247200	-2.50681300	-3.72989400
H	-2.67056000	-0.85914000	-3.51353000
O	-1.62627800	-0.34269500	-1.23708500
C	-0.35441500	-2.42562900	-1.48748200
C	-0.50089900	-2.95644600	-0.20178500
C	0.65637700	-2.93261000	-2.30769900
C	0.34165500	-3.96741300	0.25073600
C	1.50282800	-3.93935600	-1.85950000
H	0.77903400	-2.51483400	-3.30112100
C	1.34392800	-4.45904000	-0.57779000
H	0.19414000	-4.36856300	1.24853700
H	2.28649200	-4.31628300	-2.50840400
H	1.99752700	-5.24943600	-0.22291000
O	-1.50853000	-2.49421800	0.59997100
C	-0.50529200	-0.19167700	0.95683800
C	-0.74874600	0.22346600	-0.27792200
N	-0.33958800	1.52337800	-0.76197400
C	-0.55978800	2.66022800	0.13886400
H	-0.05586400	3.52601500	-0.29882800
H	-0.11877000	2.46116200	1.11961000
C	-2.02835800	2.96788700	0.28479600
C	-2.58862500	3.13038100	1.55024300
C	-2.83922800	3.13900000	-0.83860900
C	-3.93283700	3.46538900	1.69492600
H	-1.96738600	2.99018200	2.43041700
C	-4.18168800	3.46905600	-0.69808500
H	-2.41117100	3.00387600	-1.82730800
C	-4.73314500	3.63494400	0.57075700
H	-4.35484000	3.58716300	2.68762500
H	-4.80070800	3.59957600	-1.58033000
H	-5.78182500	3.89233500	0.68040400
S	1.03420000	1.57875800	-1.70222400
O	0.93721200	0.47400100	-2.64857000
O	1.14922100	2.94538600	-2.21099800
C	2.45288600	1.27230400	-0.67868500
C	2.87012300	-0.03886700	-0.46714800
C	3.11484600	2.34037300	-0.08256900
C	3.96707800	-0.27239300	0.34995800
H	2.35050900	-0.85826300	-0.95105600
C	4.20831800	2.08594700	0.73490000
H	2.79000400	3.35738300	-0.27150400

C	4.64816400	0.78057900	0.96780000
H	4.30313100	-1.29284000	0.50897500
H	4.73486200	2.91803800	1.19250800
C	5.81169000	0.51113300	1.87478400
H	6.39632000	-0.34443400	1.52847500
H	6.47119300	1.37856400	1.94615500
H	5.46123700	0.27836800	2.88660300
C	-1.04589100	-1.43705300	1.52457700
H	-1.92603800	-1.22241200	2.14198900
C	1.57839700	0.16615500	3.72900900
H	0.95490600	-0.59674600	4.22070100
H	2.28577300	-0.35521900	3.06699800
H	2.16262600	0.66594000	4.50867600
O	0.81493100	1.12543600	3.04437200
H	0.35250900	0.66500900	2.25334200
H	-0.30711400	-1.92338600	2.17473500
C	-3.23269400	-4.83112300	2.53042900
H	-4.07347400	-5.44953700	2.85264200
H	-2.37669000	-5.49155300	2.34010700
H	-2.97146600	-4.15404700	3.35401200
O	-3.63119100	-4.12941000	1.37134300
H	-2.88808200	-3.56943900	1.08892000

Energy= -1949,67716735 Hartree

Table 17. Optimized geometry and related energy and frequency for transition state **TS III B**.

C	1.13334600	2.04970400	-1.35850900
C	1.80842100	2.52472200	-2.41123500
H	1.59009200	3.51082900	-2.79948300
H	2.59595100	1.94099800	-2.87416000
O	1.53006400	0.86404700	-0.81590000
C	0.05080100	2.81591200	-0.70839900
C	0.08196100	3.05309200	0.66880700
C	-0.97670100	3.39039100	-1.46061400
C	-0.88637000	3.84178500	1.28010900
C	-1.94918500	4.17704600	-0.85581700
H	-1.01076400	3.19824900	-2.52752100
C	-1.90410500	4.40291200	0.51725300
H	-0.82415000	4.01895700	2.34904200
H	-2.74347300	4.61054500	-1.45441500
H	-2.65784100	5.02042000	0.99497900
O	1.10968300	2.53370200	1.41294700
C	0.34874500	0.14142200	1.20491500
C	0.68048400	0.02193400	-0.07524800
N	0.42794500	-1.17516800	-0.83373800
C	0.73254300	-2.45844300	-0.17822400
H	0.38502300	-3.24909400	-0.84733800
H	0.19688700	-2.53881000	0.77193100
C	2.21567900	-2.60858400	0.04116100

C	2.72554300	-2.75743800	1.32920200
C	3.09774300	-2.62523300	-1.04116900
C	4.09294400	-2.92593400	1.53586100
H	2.04349800	-2.73543300	2.17422100
C	4.46243900	-2.78983400	-0.83876100
H	2.70789400	-2.50441400	-2.04787400
C	4.96426300	-2.94149900	0.45258200
H	4.47663700	-3.04036400	2.54488900
H	5.13741900	-2.80370200	-1.68888700
H	6.03019600	-3.07113100	0.61105600
S	-0.85822200	-1.15512100	-1.89157600
O	-0.81955300	0.13631500	-2.56631700
O	-0.77347700	-2.38093500	-2.68347400
C	-2.37621900	-1.22206800	-0.97157600
C	-2.98390200	-0.03591300	-0.57194000
C	-2.93567400	-2.45669400	-0.65646100
C	-4.16864200	-0.09612900	0.14910100
H	-2.54194600	0.91768900	-0.83867400
C	-4.11895600	-2.49585400	0.06770900
H	-2.46238500	-3.37244800	-0.99251000
C	-4.75093700	-1.32095400	0.48468600
H	-4.65211500	0.82727700	0.45381600
H	-4.56473800	-3.45705400	0.30541100
C	-6.01275200	-1.37518500	1.29290900
H	-6.62357800	-0.48297100	1.13895800
H	-6.60955900	-2.25496100	1.04195100
H	-5.77797200	-1.43250400	2.36180300
C	0.75733200	1.27730600	2.06330100
H	1.64721600	1.00918600	2.64469100
C	-1.84341800	-1.12647900	3.33481900
H	-1.70548200	-1.00307600	4.42401900
H	-2.07451700	-0.12318600	2.93020100
H	-2.75680200	-1.73096300	3.19907200
O	-0.73489500	-1.69175500	2.71367500
H	-0.27184700	-0.88341600	1.98228100
H	-0.03578400	1.51044100	2.78491100
C	4.57556600	2.23382900	0.56800800
H	5.61271000	2.57300400	0.51621200
H	4.54824000	1.30435200	1.15173900
H	4.22995800	2.01444100	-0.44929000
O	3.81739900	3.26216100	1.17270000
H	2.88772400	2.98408000	1.19648800

Energy= -1949,67587507 Hartree
Frequency= 945,77i cm^{-1}

Table 18. Optimized geometry and related energy for **IV B** compound.

C	-0.27091400	2.92361600	-0.32540100
C	-0.34766500	3.96734300	-1.15202800

H	-1.18411400	4.65022400	-1.08666900
H	0.43055200	4.15625500	-1.88233400
O	0.87192100	2.15788100	-0.37329900
C	-1.30872700	2.61058500	0.67588600
C	-0.96516800	2.44255700	2.02047100
C	-2.65786200	2.55046000	0.31693600
C	-1.94038800	2.21439600	2.98382500
C	-3.63732600	2.32296500	1.27600700
H	-2.92922500	2.66625800	-0.72718500
C	-3.27810800	2.15245400	2.61007600
H	-1.64273300	2.10304600	4.02152600
H	-4.68029300	2.27405800	0.98143500
H	-4.03976500	1.97751400	3.36292700
O	0.35065300	2.57165100	2.38388500
C	1.02928500	0.45314000	1.31521800
C	0.93788000	0.84999100	0.04693500
N	1.15389200	-0.04927000	-1.04082400
C	2.18011300	-1.10286000	-0.85347000
H	2.17663400	-1.69820200	-1.76963500
H	1.93155800	-1.74669800	0.00090300
C	3.54281500	-0.49718600	-0.64937300
C	4.23609600	-0.76464300	0.53059700
C	4.13536600	0.30166400	-1.62867900
C	5.51362500	-0.24353200	0.72440100
H	3.74502800	-1.37348900	1.28941700
C	5.40794300	0.82516900	-1.43203500
H	3.59557300	0.51427500	-2.54726800
C	6.10090100	0.55183000	-0.25420400
H	6.04944700	-0.45451600	1.64503900
H	5.86320400	1.44375000	-2.19927100
H	7.09547800	0.95947500	-0.10211600
S	-0.19971300	-0.53067700	-1.90359000
O	-1.04598000	0.65765300	-1.99856300
O	0.27700200	-1.17121000	-3.12137800
C	-1.06123100	-1.74228000	-0.94073900
C	-1.95024600	-1.32420100	0.04620500
C	-0.81467900	-3.09316300	-1.16607300
C	-2.59918100	-2.28258200	0.81124300
H	-2.14444800	-0.26831400	0.19940800
C	-1.47329600	-4.03435700	-0.38806400
H	-0.13205600	-3.40043800	-1.95006500
C	-2.36875700	-3.64683600	0.61260300
H	-3.30202800	-1.96396600	1.57497400
H	-1.29369000	-5.09002200	-0.56686600
C	-3.04954200	-4.67114300	1.46936900
H	-4.02238000	-4.31707700	1.81718900
H	-3.19015700	-5.61103000	0.93126700
H	-2.44218700	-4.88729700	2.35553200
C	1.02413200	1.32208300	2.52854600
H	2.04931500	1.57581100	2.81839400
C	0.93812200	-2.65905100	3.07589600

H	1.37555800	-2.78348300	4.09614100
H	0.16059000	-1.86228000	3.20290500
H	0.34728300	-3.59258100	2.90977200
O	1.85311600	-2.38645700	2.09813400
H	1.21671100	-0.61567000	1.51839100
H	0.58046200	0.76232200	3.36163900
C	-4.53067800	0.37967300	-2.63888200
H	-5.50040600	0.67151700	-3.04768500
H	-4.60689400	0.37546900	-1.54400000
H	-4.30937900	-0.64090000	-2.97601300
O	-3.57240300	1.31085300	-3.09990000
H	-2.70898900	1.05219800	-2.74716400

Energy= -1949,68681544 Hartree

Table 19. Optimized geometry and related energy and frequency for transition state **TS IV B**.

C	1.70807600	-1.10623500	1.59051800
C	1.29943400	-1.69699100	2.72134900
H	2.00086800	-2.22845000	3.35086500
H	0.26775100	-1.61689200	3.04347800
O	0.82792900	-0.30059500	0.93635700
C	3.11073200	-1.20234400	1.12838800
C	3.81375700	-0.08079100	0.67211400
C	3.80356900	-2.41469300	1.22488300
C	5.15611600	-0.17032300	0.32101800
C	5.14320100	-2.51099000	0.87565500
H	3.26997400	-3.29327900	1.57167200
C	5.82264500	-1.38515500	0.41888000
H	5.66955700	0.72579400	-0.01241000
H	5.65499400	-3.46430900	0.95456300
H	6.87071400	-1.45010800	0.14522000
O	3.19252800	1.14597700	0.63567700
C	1.54611300	0.78073300	-1.10454700
C	0.76266800	-0.22934500	-0.49115700
N	-0.63971400	-0.22820900	-0.85965600
C	-1.27841900	0.89154500	-1.54352400
H	-2.28697500	0.56801600	-1.82504200
H	-0.77797700	1.11673200	-2.49238300
C	-1.40847800	2.14595600	-0.71424400
C	-1.65822800	3.35373200	-1.36935400
C	-1.36087400	2.12969800	0.67775700
C	-1.87213200	4.52110800	-0.64650100
H	-1.68761100	3.37936300	-2.45562200
C	-1.56819900	3.30029900	1.40243700
H	-1.14469300	1.19945400	1.19044600
C	-1.82869600	4.49774800	0.74511600
H	-2.06741900	5.45159900	-1.17023600
H	-1.52377400	3.27488400	2.48689500
H	-1.99065900	5.40900000	1.31191800

S	-1.43080800	-1.68776900	-1.03252100
O	-1.73231200	-1.98646600	-2.43382800
O	-0.69188500	-2.66862800	-0.25093900
C	-2.99092300	-1.38124400	-0.23225700
C	-4.16544400	-1.40069500	-0.97076000
C	-3.01103800	-1.17390200	1.14505200
C	-5.37743200	-1.20197800	-0.31751400
H	-4.12891500	-1.57274100	-2.04047000
C	-4.22639100	-0.97938100	1.77935600
H	-2.08473900	-1.16773100	1.70926000
C	-5.42818500	-0.98893900	1.05980800
H	-6.29838300	-1.21487100	-0.89211800
H	-4.24688700	-0.81787200	2.85296300
C	-6.73461500	-0.77846400	1.76489500
H	-6.90633100	-1.56392200	2.50742200
H	-6.73991100	0.17603100	2.29967700
H	-7.57129800	-0.78319300	1.06418200
C	2.64988100	1.46095000	-0.62860200
H	3.41014000	1.74798900	-1.36209500
H	1.32325000	-1.24051200	-1.15153200
H	1.31450800	0.99001900	-2.14652800
C	1.91382200	-3.30896600	-1.75025700
H	2.70447300	-3.73639800	-2.38840900
H	2.18652800	-3.54694300	-0.70987800
H	0.98541100	-3.86139000	-1.96905100
O	1.80166800	-1.94149000	-1.97990000
C	3.40502500	4.52820800	-0.15808700
H	3.32895600	5.61127100	-0.32702500
H	4.05308000	4.12796500	-0.95664600
H	3.93981100	4.38354400	0.79582000
O	2.13190300	3.95438100	-0.16136500
H	2.25192300	2.77605800	-0.41757100

Energy= -1949,62346158 Hartree
Frequency= 1378,98i cm^{-1}

Table 20. Optimized geometry and related energy of the product **6a**.

C	-2.84901000	-0.11595000	-0.72605100
C	-3.45193900	-0.00776100	-1.91426700
H	-4.34223300	-0.58448500	-2.12785800
H	-3.07912700	0.68048500	-2.66406400
O	-1.80703200	0.71235700	-0.43159000
C	-3.29367300	-1.05826500	0.32321200
C	-3.47036300	-0.63469300	1.64479300
C	-3.54347700	-2.39999100	0.01824000
C	-3.88227600	-1.52116500	2.63100800
C	-3.96311300	-3.28925400	0.99858700
H	-3.37306300	-2.74167800	-0.99776100
C	-4.12827100	-2.85045100	2.30870400

H	-4.02448500	-1.15203400	3.64111300
H	-4.14915200	-4.32684900	0.74263800
H	-4.45353600	-3.53961700	3.08094500
O	-3.33861300	0.70017000	1.98031000
C	-0.93664000	0.95829200	1.80907600
C	-0.79926700	0.24839100	0.49626600
N	0.50616900	0.45234400	-0.07798300
C	1.21180100	1.74537500	-0.00159400
H	2.18833200	1.59521000	-0.47335800
H	1.40433800	1.95314100	1.06240100
C	0.50857200	2.91056100	-0.65528400
C	0.12768600	3.99635600	0.13199500
C	0.26876200	2.95677400	-2.03057000
C	-0.48768700	5.10820200	-0.43860100
H	0.31559500	3.96224000	1.20150500
C	-0.34719200	4.06353100	-2.60192900
H	0.56114700	2.11439900	-2.64973900
C	-0.72829000	5.14331100	-1.80732700
H	-0.77965500	5.94549100	0.18772500
H	-0.52837800	4.08763000	-3.67220100
H	-1.20854500	6.00740900	-2.25566500
S	1.11707400	-0.69195200	-1.10162700
O	0.25651400	-1.87174600	-0.95390600
O	1.32193300	-0.16541000	-2.44670800
C	2.71810300	-1.05169800	-0.42593000
C	2.83111000	-1.40342200	0.91726300
C	3.82766800	-1.01903700	-1.25880400
C	4.07879000	-1.72720100	1.42194700
H	1.95831200	-1.41262400	1.56149500
C	5.07221600	-1.34753600	-0.73294000
H	3.71745800	-0.73672600	-2.29928300
C	5.21829800	-1.70475900	0.60733800
H	4.17395400	-1.99877100	2.46883400
H	5.94404900	-1.32202100	-1.37897700
C	6.56185700	-2.04807900	1.17648400
H	6.54242200	-3.02974200	1.65869300
H	7.33186400	-2.05940500	0.40322500
H	6.85581700	-1.32051800	1.93960100
C	-2.10384400	1.13323100	2.42088700
H	-2.18548300	1.70145100	3.34256600
H	-0.92743500	-0.82927900	0.61763600
C	1.83507000	1.18343600	4.06847800
H	1.81917800	1.56797500	5.11685500
H	1.12674200	0.31577100	4.07999100
H	2.84341000	0.71493600	3.95894500
O	1.54150300	2.12067000	3.11816900
H	-0.03856000	1.37628000	2.29910800
C	-1.42104500	-2.77687600	-3.99961600
H	-2.01034600	-3.41665900	-4.66006500
H	-0.42713300	-2.64627800	-4.44616300
H	-1.91087400	-1.79653600	-3.94240200

O -1.35687200 -3.40842400 -2.73649100
H -0.82353300 -2.85324400 -2.15026500
Energy= -1949,68128687 Hartree

3. Mulliken charges of the starting geometries and the main transition state geometries for the reaction mechanism A and B. The H atoms are omitted for legibility.

Figure 4. Computed Mulliken charges for **I A** compound.

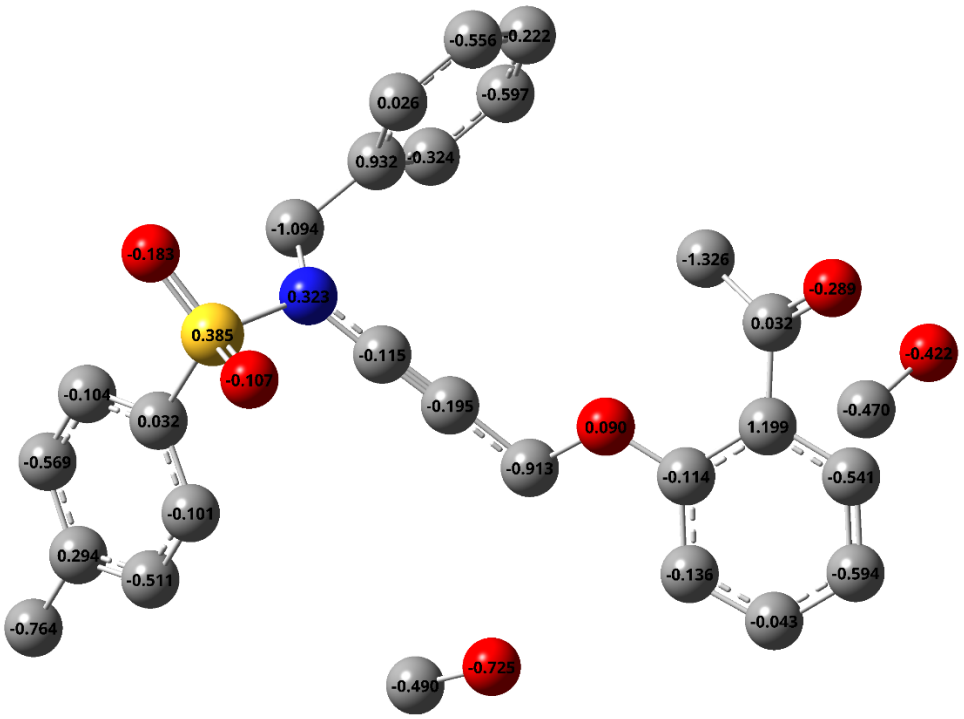


Figure 5. Computed Mulliken charges for transition state **TS IV A**.

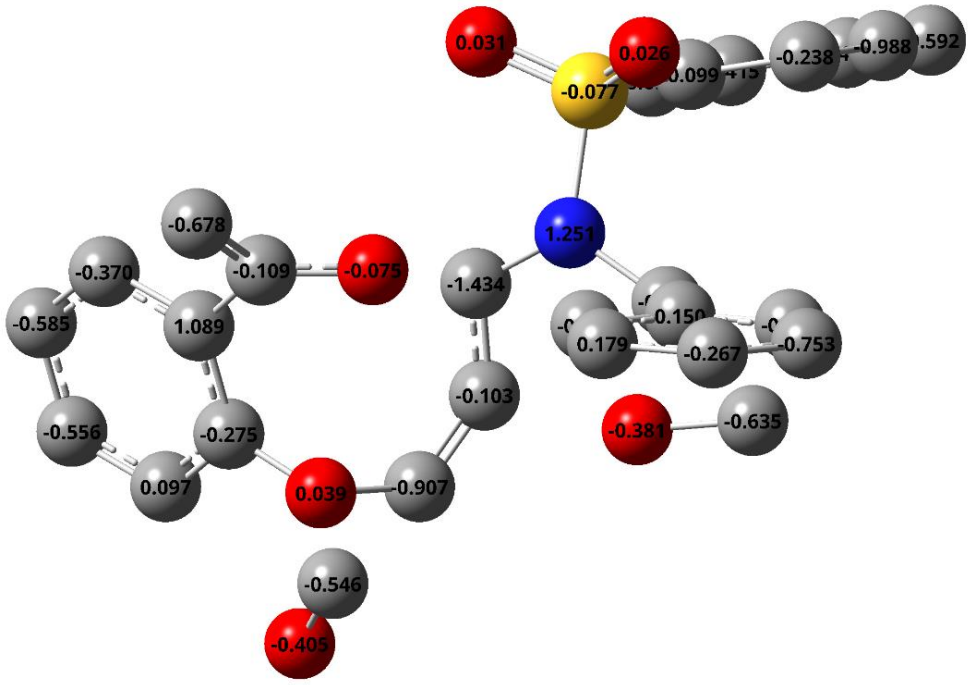


Figure 6. Computed Mulliken charges for **I B** compound.

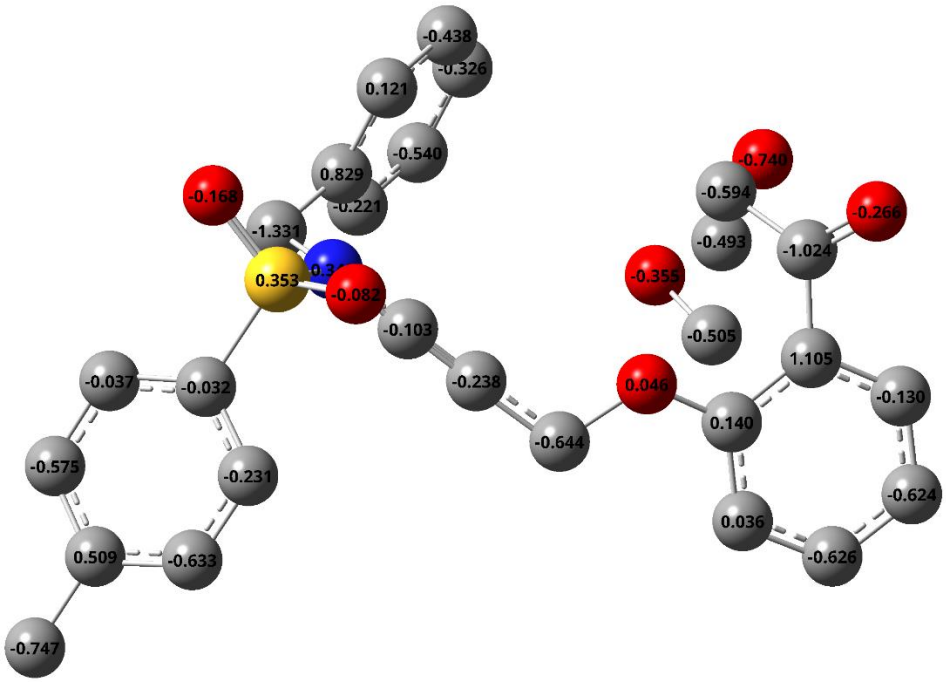


Figure 7. Computed Mulliken charges for transition state **TS II B**.

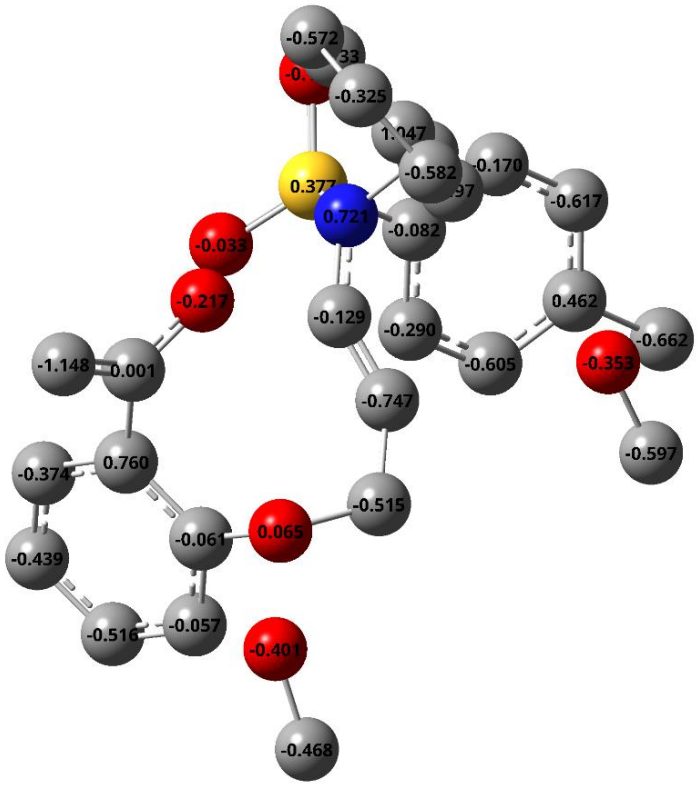
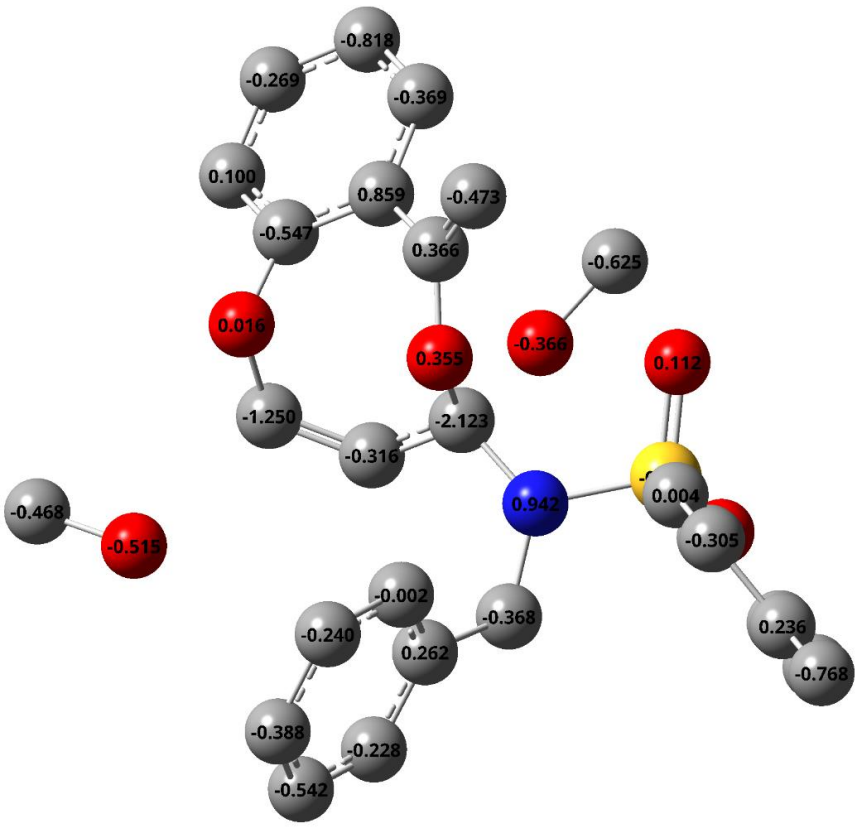


Figure 8. Computed Mulliken charges for transition state **TS IV B**.


-0.818
-0.269
-0.369
0.100
0.859
-0.473
-0.547
0.366
-0.625
0.016
-0.366
0.355
0.112
-1.250
-2.123
-0.316
0.942
0.004
-0.468
-0.515
-0.305
-0.002
-0.368
-0.240
0.262
0.236
-0.768
-0.388
-0.228
-0.542