Supporting Information For:

Ruthenium(II)-Catalyzed Intermolecular Annulation of Alkenyl Sulfonamides with Alkynes: Access to Azabicyclic Sultams

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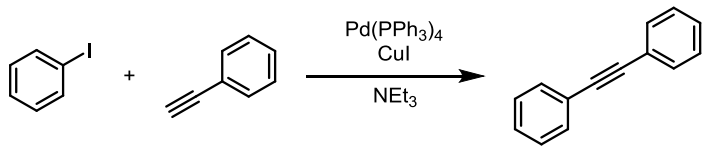
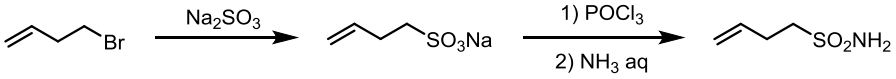
1. General experimental details: Commercially available reagents were used without further purification. Solvents were treated prior to use according to the standard methods. ^{1}H NMR and ^{13}C NMR spectra were recorded at room temperature in $CDCl_3$ on 400 MHz instrument with tetramethylsilane (TMS) as internal standard. Flash column chromatography was performed on silica gel (200-300 mesh). All reactions were monitored by TLC or NMR analysis. HRMS data was obtained with Micromass HPLC-Q-TOF mass spectrometer (ESI) or Agilent 6540 Accurate-MS spectrometer (Q-TOF).

2. General procedure for the preparation of alkynes[1]



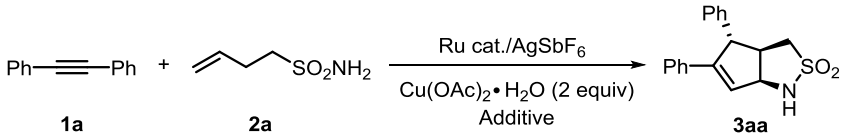
$Pd(PPh_3)_4$ (2 mol%), CuI (4 mol%), Et_3N (2.0 equiv.) and iodobenzene (1.1 equiv.) were dissolved in 10.0 mL DMF and heated to 80 ℃. Subsequently, phenylacetylene (1.0 equiv.) was added to the resulting mixture by syringe, and the reaction was stirred under argon atmosphere for 10 h. After cooling to room temperature, the solvent was removed and extracted with CH_2Cl_2 (4×50 mL). The combined organic layer was washed with brine, dried over Na_2SO_4, concentrated under reduced pressure to give crude alkyne. The residue was purified by silica gel flash chromatography using petroleum ether to afford the desired product.

3. General procedure for the preparation of homoallylic sulfonamides[2]



Homoallylic sulfonamides was prepared by a slightly modified procedure. 4-Bromobutene was refluxed with sodium sulfite (1.1 equiv.) for 12 h in water. After complete evaporation of solvent, $POCl_3$ (10 equiv.) was added and reaction mixture was refluxed at 135 ℃ for 6 h. Then excess $POCl_3$ was removed under vacuum. Residue was dissolved in acetonitrile and aq. NH_3 was added at 0 ℃ after one hour of stirring at same temperature, water was added and reaction mixture was extracted with ethyl acetate. Organic layer was separated, washed with water and brine. After drying over Na_2SO_4, solvent was concentrated and purified using silica gel flash chromatography (30% ethyl acetate/ petroleum ether). Product was obtained as yellow oil (70%).

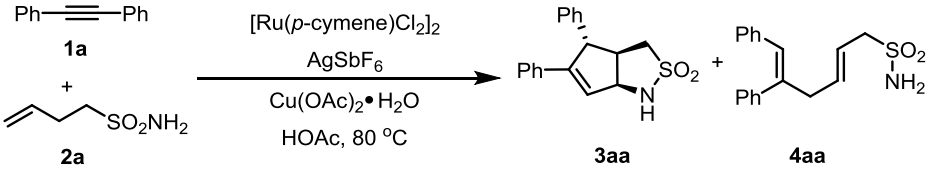
4. General procedure for the generation of the fused sultams from homoallylic sulfonamides with alkynes



Under an argon atmosphere, $[Ru(p\text{-cymene})Cl_2]_2$ (0.03 mmol), $AgSbF_6$ (0.12 mmol), $Cu(OAc)_2 \cdot H_2O$ (0.6 mmol) and AcOH (0.3 mmol) were added to a Schlenk tube in DCE (8.0 ml).

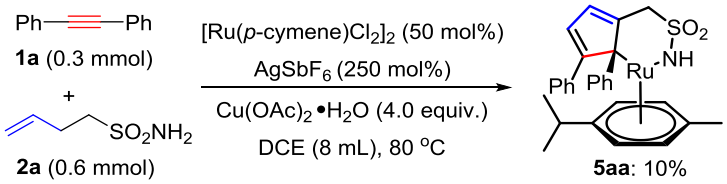
After stirring for 15 min, alkyne **1** (0.30 mmol) and homoallylic sulfonamides **2** (0.60 mmol) was added. The mixture was stirred at 80 °C for 16 h. The solvent was evaporated and the crude product was directly purified by flash column chromatography on silica gel (30% ethyl acetate/ petroleum ether) to give the desired product.

5. General procedure for the generation of 4aa

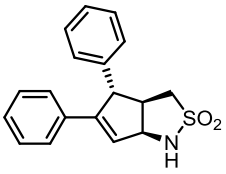


Under an argon atmosphere, [Ru(*p*-cymene)Cl_2]$_2$ (0.03 mmol), $AgSbF_6$ (0.12 mmol) and $Cu(OAc)_2$ H_2O (0.6 mmol) was added to a Schlenk tube in AcOH (2.0 ml). After stirring for 15 min, alkyne **2a** (0.60 mmol) and homoallylic sulfonamides **1a** (0.30 mmol) was added. The mixture was stirred at 80 °C for 16 h. The solvent was evaporated and the crude product was directly purified by flash column chromatography on silica gel (30% ethyl acetate/ petroleum ether) to give the desired product **3aa** (26% yield) and **6aa** (15% yield).

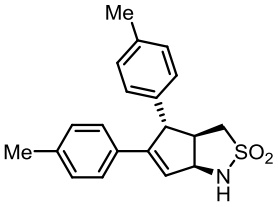
6. General procedure for the generation of 5aa



Under an argon atmosphere, [Ru(*p*-cymene)Cl_2]$_2$ (0.15 mmol), $AgSbF_6$ (0.75 mmol) and $Cu(OAc)_2$ H_2O (1.2 mmol) was added to a Schlenk tube in DCE (8.0 ml). After stirring for 15 min, alkyne **2a** (0.60 mmol) and homoallylic sulfonamides **1a** (0.30 mmol) was added. The mixture was stirred at 80 °C for 0.5 h. The solvent was evaporated and the crude product was directly purified by flash column chromatography on silica gel (5% methanol/ dichloromethane) to give the desired product **5aa** (10% yield).

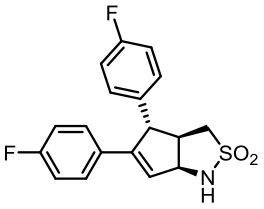


4,5-Diphenyl-3,3a,4,6a-tetrahydro-1H-cyclopenta[c]isothiazole 2,2-dioxide (**3aa**): white solid, 61.2 mg, 66% yield, m.p.164 – 165 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.25 – 7.20 (m, 4H), 7.17 – 7.14 (m, 4H), 7.09 (d, *J* = 7.1 Hz, 2H), 6.25 (s, 1H), 4.82 (dd, *J* = 7.6, 6.0 Hz, 1H), 4.52 (d, *J* = 5.9 Hz, 1H), 4.29 (s, 1H), 3.38 (dd, *J* = 12.4, 8.6 Hz, 1H), 3.29 – 3.24 (m, 1H), 3.09 (dd, *J* = 12.4, 7.2 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 147.8, 142.2, 133.8, 129.3, 128.6, 128.5, 127.34, 127.25, 127.1, 125.6, 63.2, 57.9, 52.6, 49.5; **HRMS** calculated for $C_{18}H_{18}NO_2S^+$ $[M+H]^+$ 312.1053, found 312.1053.

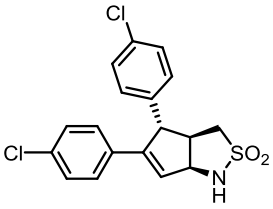


4,5-Di-p-tolyl-3,3a,4,6a-tetrahydro-1H-cyclopenta[c]isothiazole 2,2-dioxide (**3ba**): black solid, 59.2 mg, 58% yield, m.p.87 – 88 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.22 (d, *J* = 7.9 Hz, 2H), 7.09 – 7.02 (m, 6H), 6.24 (s, 1H), 4.85 (t, *J* = 6.6 Hz, 1H), 4.75 (d, *J* = 5.8 Hz,

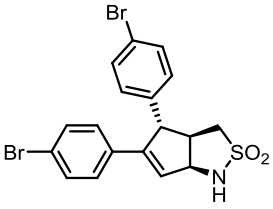
1H), 4.28 (s, 1H), 3.42 (dd, *J* = 12.4, 8.6 Hz, 1H), 3.27 (qd, *J* = 7.8, 2.8 Hz, 1H), 3.11 (dd, *J* = 12.4, 7.5 Hz, 1H), 2.29 (s, 3H), 2.28 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 147.5, 139.4, 138.4, 136.8, 131.0, 129.8, 129.2, 127.1, 127.0, 124.5, 63.2, 57.4, 52.5, 49.4, 21.3, 21.1; **HRMS** calculated for $C_{20}H_{22}NO_2S^+$ $[M+H]^+$ 340.1366, found 340.1375.



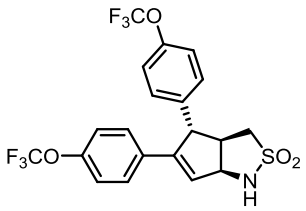
4,5-Bis(4-fluorophenyl)-3,3a,4,6a-tetrahydro-1H-cyclopenta[c]isothiazole 2,2-dioxide (**3ca**): white solid, 84.1 mg, 81% yield, m.p. 166 – 167 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.20 – 7.16 (m, 2H), 7.04 – 7.01 (m, 2H), 6.92 – 6.81 (m, 4H), 6.17 (s, 1H), 4.80 (d, *J* = 4.4 Hz, 1H), 4.61 (s, 1H), 4.27 (s, 1H), 3.36 (dd, *J* = 12.3, 8.7 Hz, 1H), 3.22 (qd, *J* = 7.5, 3.4 Hz, 1H), 3.11 (dd, *J* = 12.4, 6.6 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 162.8 (d, *J* = 249.2 Hz), 162.1 (d, *J* = 246.3 Hz), 146.8, 137.8 (d, *J* = 3.3 Hz), 129.8 (d, *J* = 3.4 Hz), 128.9 (d, *J* = 5.7 Hz), 128.8 (d, *J* = 5.5 Hz), 125.6, 116.3 (d, *J* = 21.5 Hz), 115.7 (d, *J* = 21.6 Hz), 63.1, 57.3, 52.6, 49.4; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -112.38, -115.00; **HRMS** calculated for $C_{18}H_{16}F_2NO_2S^+$ $[M+H]^+$ 348.0864, found 348.0866.



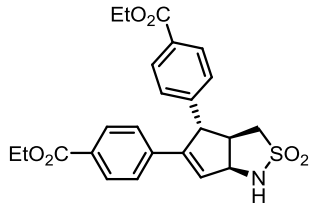
4,5-Bis(4-clorophenyl)-3,3a,4,6a-tetrahydro-1H-cyclopenta[c]isothiazole 2,2-dioxide (**3da**): white solid, 92.4 mg, 81% yield, m.p.161 – 162 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.38 – 7.12 (m, 6H), 7.05 (d, *J* = 7.9 Hz, 2H), 6.27 (s, 1H), 4.84 (s, 2H), 4.32 (s, 1H), 3.40 (dd, *J* = 11.7, 9.0 Hz, 1H), 3.25 (s, 1H), 3.17 (dd, *J* = 12.1, 6.0 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 146.5, 140.6, 134.5, 133.3, 132.1, 129.5, 128.8, 128.6, 128.3, 126.7, 63.1, 57.3, 52.5, 49.2; **HRMS** calculated for $C_{18}H_{16}Cl_2NO_2S^+$ $[M+H]^+$ 380.0273, found 380.0285.



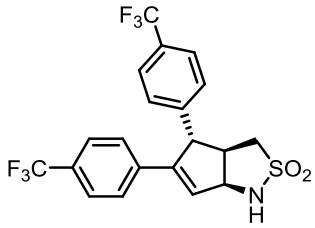
4,5-Bis(4-bromophenyl)-3,3a,4,6a-tetrahydro-1H-cyclopenta[c]isothiazole 2,2-dioxide (**3ea**): white solid, 97.6 mg, 69% yield, m.p.186 – 187 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.41 – 7.34 (m, 4H), 7.13 (d, *J* = 8.2 Hz, 2H), 7.00 (d, *J* = 8.1 Hz, 2H), 6.31 (s, 1H), 4.86 (d, *J* = 6.5 Hz, 1H), 4.56 (d, *J* = 5.8 Hz, 1H), 4.33 (s, 1H), 3.42 (dd, *J* = 12.2, 8.7 Hz, 1H), 3.34 – 3.24 (m, 1H), 3.18 (dd, *J* = 12.3, 6.2 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 146.7, 141.0, 132.5, 132.4, 131.9, 129.0, 128.6, 126.7, 122.9, 121.4, 63.1, 57.3, 52.6, 49.3; **HRMS** calculated for $C_{18}H_{16}Br_2NO_2S^+$ $[M+H]^+$467.9263, found 467.9278.



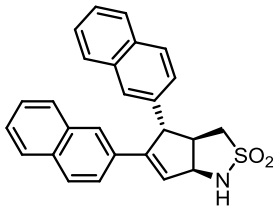
4,5-Bis(4-(trifluoromethoxy)phenyl)-3,3a,4,6a-tetrahydro-1H-cyclopenta[c]isothiazole 2,2-dioxide (**3fa**): white solid, 81.2 mg, 57% yield, m.p. 61 – 62 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.21 (d, *J* = 8.8 Hz, 2H), 7.09 – 7.03 (m, 4H), 6.97 (d, *J* = 8.2 Hz, 2H), 6.22 (s, 1H), 4.94 (s, 1H), 4.79 (d, *J* = 6.2 Hz, 1H), 4.30 (s, 1H), 3.32 (dd, *J* = 12.3, 8.6 Hz, 1H), 3.28 – 3.16 (m, 1H), 3.11 (dd, *J* = 12.3, 6.1 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 149.2 (q, *J* = 1.8 Hz), 148.5 (q, *J* = 1.8 Hz), 146.0, 140.7, 132.3, 128.6, 128.5, 127.2, 121.8, 120.9, 120.5 (q, *J* = 257.6 Hz), 120.4 (q, *J* = 257.6 Hz), 63.1, 57.2, 52.5, 49.3; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -57.83, -57.91; **HRMS** calculated for $C_{20}H_{16}F_6NO_4S^+$ $[M+H]^+$ 480.0699, found 480.0684.



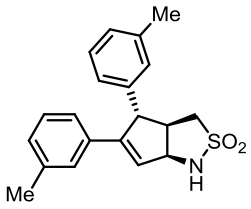
Diethyl 4,4'-2,2-dioxido-3,3a,4,6a-tetrahydro-1H-cyclopenta[c] isothiazole-4,5-diyl)dibenzoate(**3ga**): white solid; 44.0 mg, 32% yield, m.p. 120 – 121 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8.1 Hz, 2H), 7.84 (d, *J* = 8.3 Hz, 2H), 7.30 (d, *J* = 8.3 Hz, 2H), 7.18 (d, *J* = 8.1 Hz, 2H), 6.41 (s, 1H), 5.10 (d, *J* = 6.2 Hz, 1H), 4.90 (t, *J* = 6.9 Hz, 1H), 4.47 (s, 1H), 4.34 – 4.29 (m, 4H), 3.40 (dd, *J* = 12.0, 8.6 Hz, 1H), 3.36 – 3.27 (m, 1H), 3.23 (dd, *J* = 12.1, 5.6 Hz, 1H), 1.35 – 1.30 (m, 6H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 166.2, 166.1, 147.2, 146.6, 137.9, 130.5, 130.2, 129.7, 129.6, 128.6, 127.3, 126.9, 63.2, 61.13, 61.10, 57.8, 52.5, 49.0, 14.34, 14.31; **HRMS** calculated for $C_{24}H_{26}NO_6S^+$ $[M+H]^+$ 456.1475, found 456.1475.



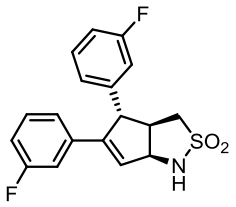
4,5-Bis(4-(trifluoromethyl)phenyl)-3,3a,4,6a-tetrahydro-1H-cycl openta[c]isothiazole 2,2-dioxide (**3ha**): white solid, 24.1 mg, 26% yield, m.p. 182 – 183 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.55 (d, *J* = 7.9 Hz, 2H), 7.49 (d, *J* = 8.1 Hz, 2H), 7.37 (d, *J* = 8.1 Hz, 2H), 7.27 (d, *J* = 6.5 Hz, 2H), 6.44 (s, 1H), 4.93 (s, 1H), 4.73 (s, 1H), 4.51 (s, 1H), 3.43 (dd, *J* = 11.8, 8.7 Hz, 1H), 3.36 – 3.31 (m, 1H), 3.26 (dd, *J* = 12.0, 5.3 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 146.3, 145.9, 136.9, 130.6 (q, *J* = 32.6 Hz), 130.0 (q, *J* = 32.5 Hz), 128.8, 127.7 , 127.3, 126.5 (q, *J* = 3.7 Hz), 125.7 (q, *J* = 3.7 Hz), 124.0 (q, *J* = 271.85 Hz), 123.9 (q, *J* = 271.85 Hz), 63.1, 57.7, 52.6, 49.2; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -62.61, -62.83; **HRMS** calculated for $C_{20}H_{16}F_6NO_2S^+$ $[M+H]^+$ 448.0800, found 448.0806.



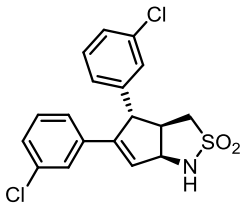
4,5-Di(naphthalen-2-yl)-3,3a,4,6a-tetrahydro-1H-cyclopenta[c]isot hiazole 2,2-dioxide (**3ia**): light yellow solid, 74.5 mg, 60% yield, m.p. 115 – 120 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 – 7.50 (m, 9H), 7.41 – 7.29 (m, 4H), 7.16 (d, *J* = 8.4 Hz, 1H), 6.37 (s, 1H), 4.96 (d, *J* = 4.7 Hz, 1H), 4.86 – 4.85 (m, 1H), 4.51 (s, 1H), 3.36 (dd, *J* = 11.7, 8.8 Hz, 1H), 3.31 – 3.23 (m, 1H), 3.15 (dd, *J* = 12.0, 6.4 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 147.1, 139.8, 133.6, 133.03, 132.99, 132.5, 131.2, 129.2, 128.4, 128.1, 127.72, 127.70, 127.6, 126.7, 126.6, 126.5, 126.4, 126.3, 126.0, 125.9, 125.1, 124.7, 63.3, 57.7, 52.5, 49.2; **HRMS** calculated for $C_{26}H_{22}NO_2S^+$ $[M+H]^+$ 412.1366, found 412.1360.



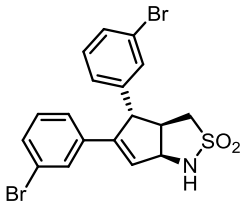
4,5-Di-m-tolyl-3,3a,4,6a-tetrahydro-1H-cyclopenta[c]isothiazole 2,2-dioxide (**3ja**): white solid, 49.0 mg, 43% yield, m.p. 105 – 106 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.20 – 7.08 (m, 4H), 7.03 (t, *J* = 6.4 Hz, 2H), 6.99 – 6.90 (m, 1H), 6.28 (t, *J* = 1.5 Hz, 1H), 4.89 – 4.85 (m, 1H), 4.73 (d, *J* = 5.9 Hz, 1H), 4.28 (s, 1H), 3.43 (dd, *J* = 12.4, 8.6 Hz, 1H), 3.38 – 3.23 (m, 1H), 3.12 (dd, *J* = 12.4, 7.4 Hz, 1H), 2.31 (s, 3H), 2.28 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 147.6, 142.3, 138.8, 138.0, 133.8, 129.3, 129.0, 128.4, 128.0, 127.9, 127.7, 125.4, 124.23, 124.21, 63.2, 57.8, 52.5, 49.4, 21.54, 21.49; **HRMS** calculated for $C_{20}H_{22}NO_2S^+$ $[M+H]^+$ 340.1366, found 340.1368.



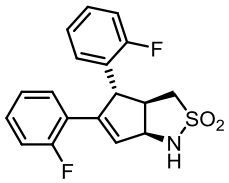
4,5-Bis(3-fluorophenyl)-3,3a,4,6a-tetrahydro-1H-cyclopenta[c]isothiazole 2,2-dioxide (**3ka**): white solid, 50.0 mg, 48% yield, m.p. 131 – 132 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.28 – 7.15 (m, 2H), 7.05 (d, *J* = 7.9 Hz, 1H), 6.99 – 6.88 (m, 4H), 6.82 (d, *J* = 9.6 Hz, 1H), 6.32 (s, 1H), 4.94 (d, *J* = 6.0 Hz, 1H), 4.87 (t, *J* = 6.8 Hz, 1H), 4.34 (s, 1H), 3.41 (dd, *J* = 12.3, 8.7 Hz, 1H), 3.33 – 3.26 (m, 1H), 3.19 (dd, *J* = 12.4, 6.2 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 163.3(d, *J* = 247.2 Hz), 162.7(d, *J* = 245.9 Hz), 146.2 (d, *J* = 2.4 Hz), 144.6 (d, *J* = 6.8 Hz), 135.9 (d, *J* = 7.7 Hz), 130.9 (d, *J* = 8.4 Hz), 130.1 (d, *J* = 8.4 Hz), 127.6, 123.0 (d, *J* = 2.8 Hz), 122.8 (d, *J* = 2.8 Hz), 115.5 (d, *J* = 21.3 Hz), 114.5 (d, *J* = 21.1 Hz), 114.0 (d, *J* = 21.6 Hz), 113.9 (d, *J* = 22.2 Hz), 63.0, 57.5 (d, *J* = 1.4 Hz), 52.5, 49.1; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -111.71, -112.60; **HRMS** calculated for $C_{18}H_{16}F_2NO_2S^+$ $[M+H]^+$ 348.0864, found 348.0864.



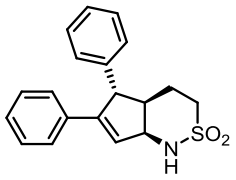
4,5-Bis(3-chlorophenyl)-3,3a,4,6a-tetrahydro-1H-cyclopenta[c]isothiazole 2,2-dioxide (**3la**): white solid, 51.6 mg, 45% yield, m.p. 72 – 73 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.31 (s, 1H), 7.23 – 7.09 (m, 6H), 7.02 (d, *J* = 6.8 Hz, 1H), 6.30 (s, 1H), 4.96 (d, *J* = 6.1 Hz, 1H), 4.87 (t, *J* = 6.9 Hz, 1H), 4.32 (s, 1H), 3.40 (dd, *J* = 12.3, 8.7 Hz, 1H), 3.31 – 3.24 (m, 1H), 3.18 (dd, *J* = 12.3, 6.0 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 145.9, 144.1, 135.4, 135.1, 134.5, 130.6, 129.9, 128.7, 127.8, 127.7, 127.2, 127.0, 125.5, 125.2, 63.0, 57.4, 52.5, 49.0; **HRMS** calculated for $C_{18}H_{16}Cl_2NO_2S^+$ $[M+H]^+$ 380.0273, found 380.0283.



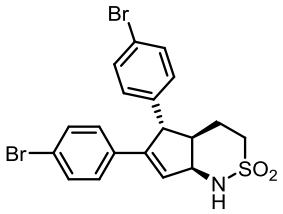
4,5-Bis(3-bromophenyl)-3,3a,4,6a-tetrahydro-1H-cyclopenta[c]isothiazole 2,2-dioxide (**3ma**): white solid, 66.0 mg, 47% yield, m.p. 80 – 81 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.48 (s, 1H), 7.35 – 7.32 (m, 2H), 7.27 (s, 1H), 7.16 – 7.12 (m, 2H), 7.07 (t, *J* = 7.9 Hz, 2H), 6.29 (s, 1H), 4.93 (d, *J* = 6.1 Hz, 1H), 4.87 (t, *J* = 6.9 Hz, 1H), 4.30 (s, 1H), 3.39 (dd, *J* = 12.3, 8.7 Hz, 1H), 3.31 – 3.24 (m, 1H), 3.17 (dd, *J* = 12.4, 6.1 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 145.8, 144.3, 135.7, 131.6, 130.9, 130.7, 130.2, 129.9, 127.9, 126.0, 125.6, 123.4, 122.7, 63.0, 57.4, 52.5, 49.0; **HRMS** calculated for $C_{18}H_{16}Br_2NO_2S^+$ $[M+H]^+$ 467.9263, found 467.9258.



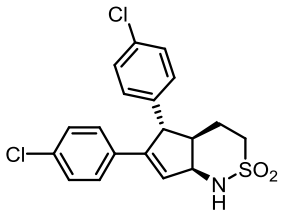
4,5-Bis(2-fluorophenyl)-3,3a,4,6a-tetrahydro-1H-cyclopenta[c]isothiazole 2,2-dioxide (**3na**): white solid, 21.1 mg, 20% yield, m.p. 138 – 139 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.22 – 7.12 (m, 3H), 7.06 – 6.94 (m, 5H), 6.48 (s, 1H), 4.91 (t, *J* = 6.8 Hz, 1H), 4.79 (s, 1H), 4.57 (d, *J* = 6.0 Hz, 1H), 3.49 (dd, *J* = 11.5, 7.6 Hz, 1H), 3.34 – 3.23 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 160.9 (d, *J* = 251.5 Hz), 160.6 (d, *J* = 245.5 Hz), 141.5 (d, *J* = 2.4 Hz), 130.74 (d, *J* = 9.6 Hz), 130.1 (d, *J* = 8.8 Hz), 129.5 (d, *J* = 3.6 Hz), 129.0 (d, *J* = 8.5 Hz), 128.8, 128.3 (d, *J* = 4.0 Hz), 124.7 (d, *J* = 3.6 Hz), 124.3 (d, *J* = 3.5 Hz), 121.8 (d, *J* = 12.5 Hz), 116.3 (d, *J* = 22.8 Hz), 115.8 (d, *J* = 21.9 Hz), 63.6, 52.7, 51.5, 47.5; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -111.09, -118.23; **HRMS** calculated for $C_{18}H_{16}F_2NO_2S^+$ $[M+H]^+$ 348.0864, found 348.0861.



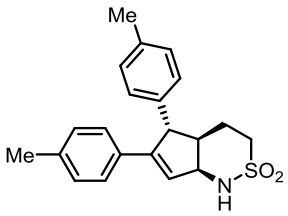
5,6-Diphenyl-1,3,4,4a,5,7a-hexahydrocyclopenta[c][1,2]thiazine 2,2-dioxide (**3ab**): white solid, 52 mg, 53% yield, m.p. 228 – 229 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.26 – 7.18 (m, 8H), 7.08 (d, *J* = 7.1 Hz, 2H), 6.33 (s, 1H), 4.72 – 4.72 (m, 1H), 4.19 (d, *J* = 6.8 Hz, 1H), 4.05 (d, *J* = 8.0 Hz, 1H), 3.30 – 3.23 (m, 1H), 3.13 – 3.07 (m, 1H), 2.49 – 2.43 (m, 1H), 2.27 – 2.20 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 150.7, 141.4, 134.4, 129.0, 128.5, 128.4, 128.0, 127.1, 126.9, 126.6, 62.2, 53.7, 46.1, 45.5, 24.1; **HRMS** calculated for $C_{19}H_{20}NO_2S^+$ $[M+H]^+$ 326.1209, found 326.1217.



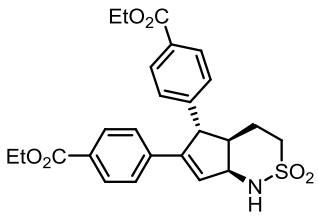
5,6-Bis(4-bromophenyl)-1,3,4,4a,5,7a-hexahydrocyclopenta[c][1,2] thiazine 2,2-dioxide (**3bb**): white solid, 95 mg, 63% yield, m.p. 258 – 259 ℃; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 7.43 (d, *J* = 8.0 Hz, 4H), 7.22 (d, *J* = 8.1 Hz, 2H), 7.10 (d, *J* = 8.0 Hz, 2H), 6.74 (d, *J* = 7.8 Hz, 1H), 6.42 (s, 1H), 4.49 (d, *J* = 7.1 Hz, 1H), 4.32 (d, *J* = 6.5 Hz, 1H), 3.29 – 3.22 (m, 1H), 3.05 – 2.99 (m, 1H), 2.28 – 2.22 (m, 1H), 2.09 – 1.97 (m, 2H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 147.0, 141.6, 134.1, 131.5, 131.2, 130.2, 128.6, 120.9, 119.6, 61.6, 52.3, 45.4, 44.7, 23.9; **HRMS** calculated for $C_{19}H_{18}Br_2NO_2S^+$ $[M+H]^+$ 481.9420, found 481.9392.



5,6-Bis(4-clorophenyl)-1,3,4,4a,5,7a-hexahydrocyclopenta[c][1,2]thi azine 2,2-dioxide 2,2-dioxide(**3cb**): white solid, 75 mg, 61% yield, m.p. 255 – 256 ℃; **^{1}H NMR**(400 MHz, DMSO-d_6) δ 7.30 (d, *J* = 5.9 Hz, 6H), 7.16 (d, *J* = 8.2 Hz, 2H), 6.74 (d, *J* = 7.8 Hz, 1H), 6.41 (t, *J* = 2.1 Hz,1H), 4.49 (t, *J* = 6.9 Hz, 1H), 4.33 (d, *J* = 6.5 Hz, 1H), 3.29 – 3.22 (m, 1H), 3.05 – 2.99 (m, 1H), 2.29 – 2.22 (m, 1H), 2.09 – 1.98 (m, 2H); **^{13}C NMR**(100 MHz, DMSO-d_6) δ 147.0, 141.2, 133.7, 132.2, 131.1, 129.7, 128.6, 128.5, 128.3, 128.3, 61.5, 52.3, 45.4, 44.7, 23.9; **HRMS** calculated for $C_{19}H_{18}Cl_2NO_2S^+$ $[M+H]^+$ 394.0430, found 394.0430.

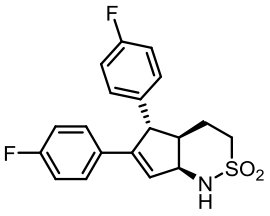


5,6-Bis(4-methyl)-1,3,4,4a,5,7a-hexahydrocyclopenta[c][1,2]thiazi ne 2,2-dioxide 2,2-dioxide (**3db**): light yellow solid, 51 mg, 46% yield, m.p. 258 – 259 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.14 (d, *J* = 8.2 Hz, 2H), 7.05 (d, *J* = 7.8 Hz, 2H), 7.00 (d, *J* = 7.9 Hz, 2H), 6.96 (d, *J* = 7.9 Hz, 2H), 6.28 (t, *J* = 2.3 Hz, 1H), 4.71 (s, 1H), 4.11 (d, *J* = 7.0 Hz, 1H), 3.87 (d, *J* = 8.1 Hz, 1H), 3.25 (ddd, *J* = 13.6, 10.8, 3.9 Hz, 1H), 3.11 (ddd, *J* = 13.7, 6.2, 4.2 Hz, 1H), 2.51 – 2.42 (m, 1H), 2.28 (s, 3H), 2.26 (s, 3H), 2.23 – 2.18 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 150.8, 138.6, 138.3, 136.7, 131.6, 129.7, 129.2, 127.9, 126.8, 125.4, 62.2, 53.3, 46.2, 45.6, 24.1, 21.4, 21.2; **HRMS** calculated for $C_{21}H_{24}NO_2S^+$ $[M+H]^+$ 354.1522, found 354.1500.

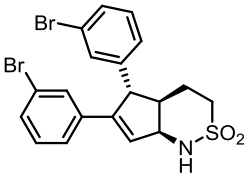


Diethyl 4,4'-(2,2-dioxido-1,3,4,4a,5,7a-hexahydrocyclopenta [c][1,2]thiazine-5,6-diyl)dibenzoate (**3eb**): light yellow solid, 53 mg, 38% yield, m.p. 232 – 233 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 8.1 Hz, 2H), 7.84 (d, *J* = 8.2 Hz, 2H), 7.26 (d, *J* = 8.4

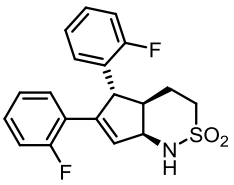
Hz, 2H), 7.14 (d, *J* = 8.2 Hz, 2H), 6.42 (t, *J* = 2.2 Hz, 1H), 4.77 – 4.63 (m, 1H), 4.56 (t, *J* = 7.1 Hz, 1H), 4.35 – 4.28 (m, 5H), 3.30 (ddd, *J* = 14.0, 10.6, 3.7 Hz, 1H), 3.09 (ddd, *J* = 13.8, 6.3, 4.2 Hz, 1H), 2.51 – 2.42 (m, 1H), 2.28 – 2.18 (m, 2H), 1.36 – 1.32 (m, 6H); **^{13}C NMR**(100 MHz, $CDCl_3$) δ 166.3, 166.2, 149.5, 146.3, 138.6, 130.3, 130.1, 129.7, 129.5, 129.1, 128.0, 126.7, 62.2, 61.2, 61.1, 53.5, 45.7, 45.3, 24.0, 14.39, 14.36; **HRMS** calculated for $C_{25}H_{31}N_2O_6S^+$ $[M+NH_4]^+$ 487.1897, found 487.1880.



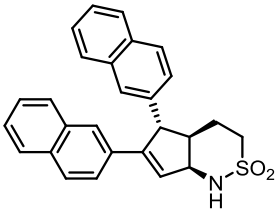
5,6-Bis(4-fluorophenyl)-1,3,4,4a,5,7a-hexahydrocyclopenta[c][1,2]thiazine 2,2-dioxide (**3fb**): light yellow solid, 58 mg, 53% yield, m.p. 248 – 249 ℃; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 7.31 (dd, *J* = 8.6, 5.6 Hz, 2H), 7.17 (dd, *J* = 8.4, 5.6 Hz, 2H), 7.06 (t, *J* = 8.8 Hz, 4H), 6.71 (d, *J* = 7.8 Hz, 1H), 6.33 (s, 1H), 4.48 (t, *J* = 5.6 Hz, 1H), 4.31 (d, *J* = 6.4 Hz, 1H), 3.25 (ddd, *J* = 13.0, 9.4, 3.1 Hz, 1H), 3.01 (ddd, *J* = 13.1, 6.5, 4.0 Hz, 1H), 2.28 – 2.22 (m, 1H), 2.09 – 1.97 (m, 2H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 161.6 (d, *J* = 245.1 Hz), 160.9 (d, *J* = 242.2 Hz), 147.2, 138.4, 131.5 (d, *J* = 3.2 Hz), 129.8 (d, *J* = 8.0 Hz), 128.7 (d, *J* = 8.1 Hz), 127.4, 115.4 (d, *J* = 21.2 Hz), 115.2 (d, *J* = 21.2 Hz), 61.6, 52.4, 45.5, 44.8, 24.1; **^{19}F NMR** (376 MHz, DMSO-d_6) δ -113.81, -116.24; **HRMS** calculated for $C_{19}H_{21}F_2N_2O_2S^+$ $[M+NH_4]^+$ 379.1286, found 379.1309.



5,6-Bis(3-bromophenyl)-1,3,4,4a,5,7a-hexahydrocyclopenta[c][1,2]thiazine 2,2-dioxide (**3gb**): light yellow solid, 75 mg, 52% yield, m.p. 197 – 198 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.45 (q, *J* = 1.3 Hz, 1H), 7.36 – 7.31 (m, 2H), 7.24 (t, *J* = 1.8 Hz, 1H), 7.14 (t, *J* = 7.8 Hz, 1H), 7.10 – 7.05 (m, 2H), 7.00 (dt, *J* = 7.7, 1.3 Hz, 1H), 6.35 (t, *J* = 2.2 Hz, 1H), 4.72 (t, *J* = 6.6 Hz, 1H), 4.19 (d, *J* = 7.9 Hz, 1H), 4.12 (dt, *J* = 6.2, 1.7 Hz, 1H), 3.25 (ddd, *J* = 13.7, 10.0, 3.8 Hz, 1H), 3.10 (ddd, *J* = 13.8, 6.9, 4.1 Hz, 1H), 2.51 – 2.42 (m, 1H), 2.28 – 2.17 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 148.3, 143.4, 136.3, 131.5, 130.9, 130.8, 130.6, 130.2, 129.8, 128.4, 126.5, 125.4, 123.2, 122.8, 62.0, 53.7, 46.2, 45.4, 24.4; **HRMS** calculated for $C_{19}H_{18}Br_2NO_2S^+$ $[M+H]^+$ 481.9420, found 481.9420.

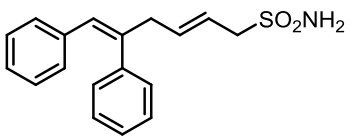


5,6-Bis(2-fluorophenyl)-1,3,4,4a,5,7a-hexahydrocyclopenta[c][1,2]thiazine 2,2-dioxide (**3hb**): yellow solid, 52 mg, 48% yield, m.p. 232 – 233 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.20 – 7.12 (m, 3H), 7.04 – 6.87 (m, 5H), 6.43 (s, 1H), 4.71 – 4.73 (m, 2H), 4.14 (d, *J* = 7.9 Hz, 1H), 3.36 – 3.29 (m, 1H), 3.13 (dt, *J* = 13.5, 4.8 Hz, 1H), 2.56 – 2.46 (m, 1H), 2.29 – 2.18 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 161.1 (d, *J* = 244.7 Hz), 160.3 (d, *J* = 250.6 Hz), 145.7, 130.8 (d, *J* = 6.5 Hz), 129.9 (d, *J* = 8.7 Hz), 129.3 (d, *J* = 3.8 Hz), 129.1 (d, *J* = 4.0 Hz), 128.7 (d, *J* = 8.3 Hz), 127.8 (d, *J* = 14.2 Hz), 124.7 (d, *J* = 3.5 Hz), 124.2 (d, *J* = 3.5 Hz), 122.6 (d, *J* = 13.2 Hz), 116.1 (d, *J* = 22.4 Hz), 115.6 (d, *J* = 22.3 Hz), 62.3, 46.4, 45.7, 44.4, 24.0; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -112.20, -119.83; **HRMS** calculated for $C_{19}H_{18}F_2NO_2S^+$ $[M+H]^+$ 362.1021, found 362.1049.

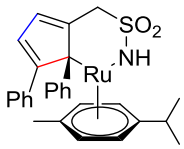


5,6-Di(naphthalen-2-yl)-1,3,4,4a,5,7a-hexahydrocyclopenta[c][1,2]thiazine 2,2-dioxide (**3ib**): light yellow solid, 65 mg, 51% yield, m.p.

226 – 227 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.78 – 7.64 (m, 7H), 7.59 – 7.57 (m, 1H), 7.51 (dd, *J* = 8.6, 1.8 Hz, 1H), 7.48 – 7.33 (m, 4H), 7.19 (dd, *J* = 8.5, 1.8 Hz, 1H), 6.52 (t, *J* = 2.3 Hz, 1H), 4.82 (ddt, *J* = 8.0, 5.7, 2.0 Hz, 1H), 4.47 (dt, *J* = 7.3, 1.7 Hz, 1H), 4.05 (d, *J* = 8.1 Hz, 1H), 3.34 (ddd, *J* = 13.6, 10.4, 4.0 Hz, 1H), 3.15 (ddd, *J* = 13.6, 6.6, 4.1 Hz, 1H), 2.56 – 2.47 (m, 1H), 2.42 – 2.36 (m, 1H), 2.34 – 2.26 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 150.4, 139.0, 133.6, 133.11, 133.10, 132.6, 131.8, 129.1, 128.4, 128.2, 127.8, 127.7, 127.3, 126.9, 126.52, 126.47, 126.42, 126.39, 126.0, 125.6, 124.5, 62.3, 54.1, 46.3, 45.4, 24.3; **HRMS** calculated for $C_{27}H_{24}NO_2S^+$ $[M+H]^+$ 426.1522, found 426.1493.

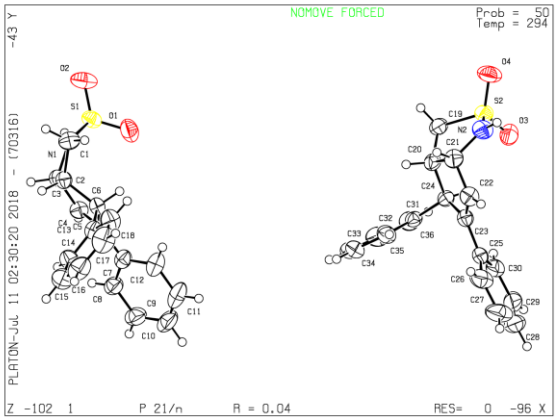


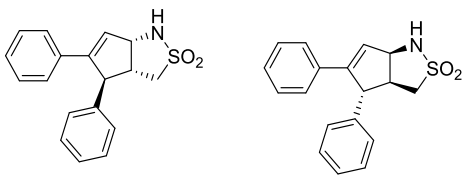
5,6-Di(naphthalen-2-yl)-1,3,4,4a,5,7a-hexahydrocyclopenta[c][1,2]thiazine 2,2-dioxide (**4aa**): light yellow solid, 14% yield, m.p. 115 – 116 ℃; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.31 – 7.21 (m, 3H), 7.16 – 7.05 (m, 5H), 6.97 – 6.92 (m, 2H), 6.51 (s, 1H), 5.83 (dt, *J* = 14.7, 7.0 Hz, 1H), 5.57 (dt, *J* = 14.9, 7.3 Hz, 1H), 4.22 (s, 2H), 3.68 (d, *J* = 7.4 Hz, 2H), 3.32 (d, *J* = 7.0 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 140.5, 140.0, 138.2, 136.9, 129.2, 128.9, 128.8, 128.2, 128.0, 127.4, 126.7, 120.1, 58.5, 43.5; **HRMS** calculated for $C_{18}H_{23}N_2O_2S^+$ $[M+NH_4]^+$ 331.1475, found 331.1464.



(((2,3-diphenylcyclopenta-3,5-dien-2-ide-1-yl)methyl)sulfonyl)amide(*p*-cymene)ruthenium(II) (**5aa**): light yellow solid, 10% yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.37 (s, 5H), 7.25 (d, 1H), 7.19 (t, *J* = 7.4 Hz, 2H), 7.09 (d, *J* = 7.6 Hz, 2H), 6.41 – 6.39 (m, 2H), 6.32 (d, *J* = 6.1 Hz, 1H), 6.02 (d, *J* = 6.0 Hz, 1H), 5.87 (d, *J* = 6.1 Hz, 1H), 5.73 (d, *J* = 2.3 Hz, 1H), 4.74 (d, *J* = 14.3 Hz, 1H), 4.04 (d, *J* = 14.3 Hz, 1H), 2.57 (qq, *J* = 6.9, 6.9 Hz, 1H), 2.23 (s, 3H), 1.07 (d, *J* = 6.8 Hz, 6H); **^{13}C NMR** (176 MHz, $CDCl_3$) δ 131.8, 130.9, 129.4, 129.3, 129.2, 129.1, 128.7, 112.8, 103.3, 102.8, 101.3, 91.4, 89.7, 89.5, 86.9, 85.9, 81.3, 79.8, 51.4, 31.6, 23.3, 22.8, 18.8; **HRMS** calculated for $C_{29}H_{33}NO_2RuS^+$ $[M+H]^+$ 546.1035, found 546.1039.

7. Crystal structure of 3aa





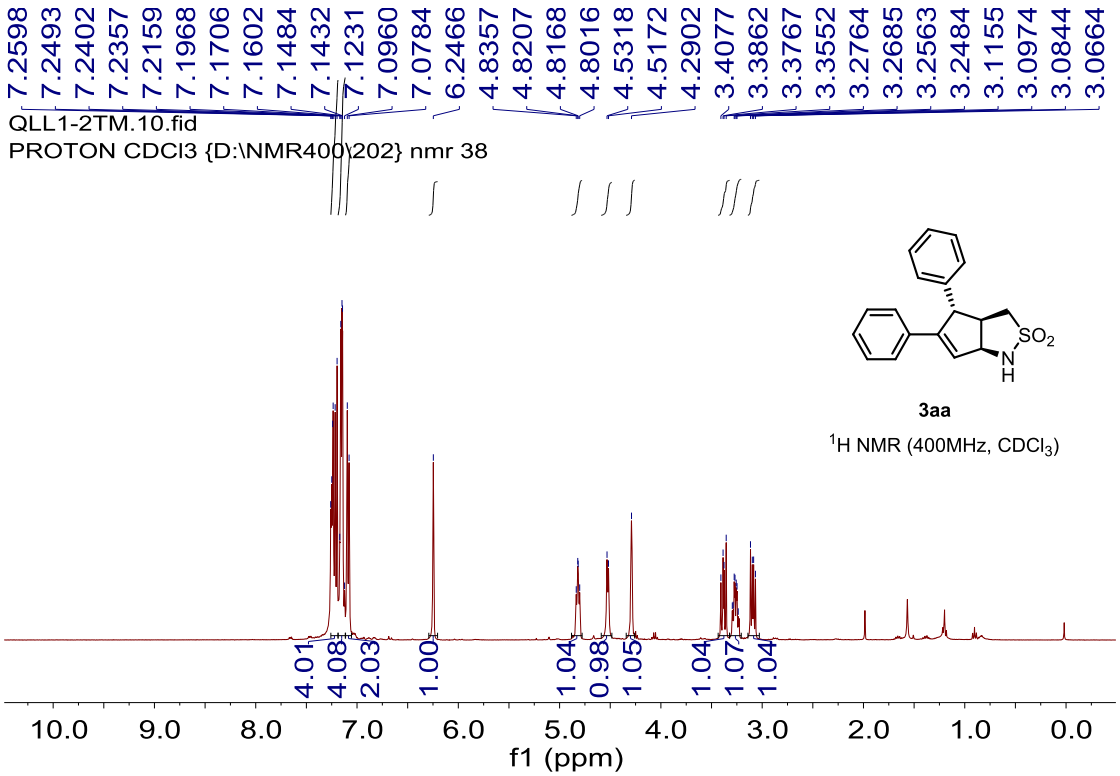
3aa

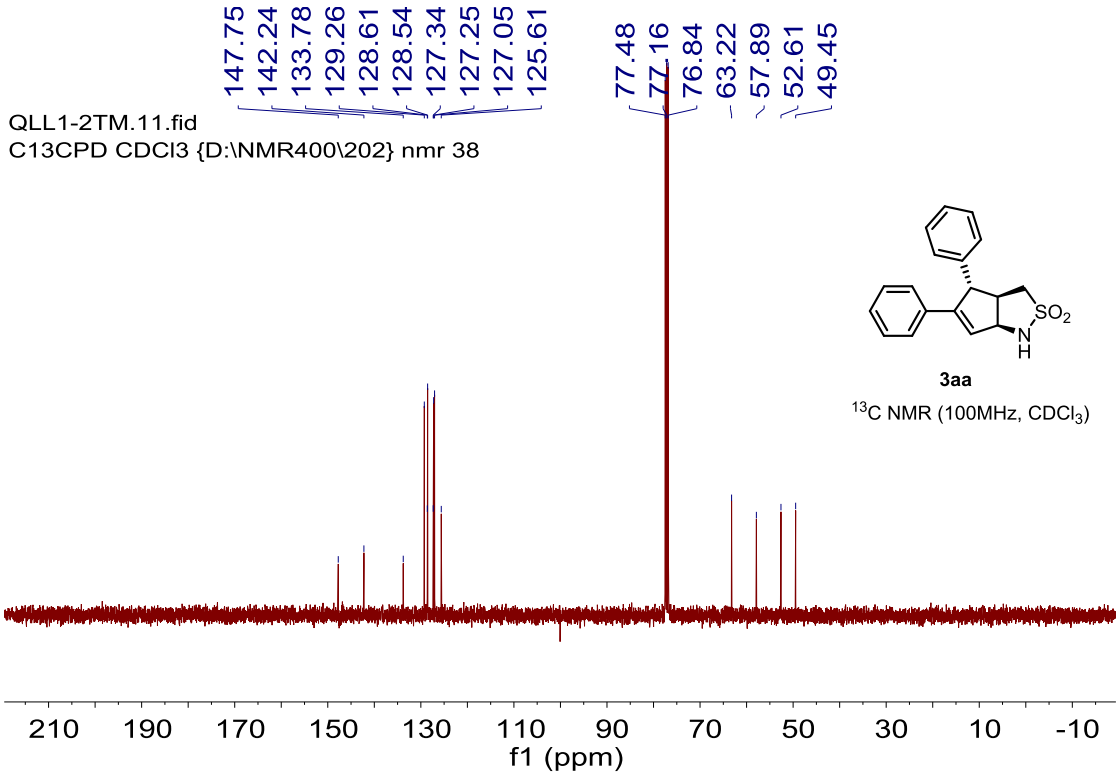
CCDC1854428

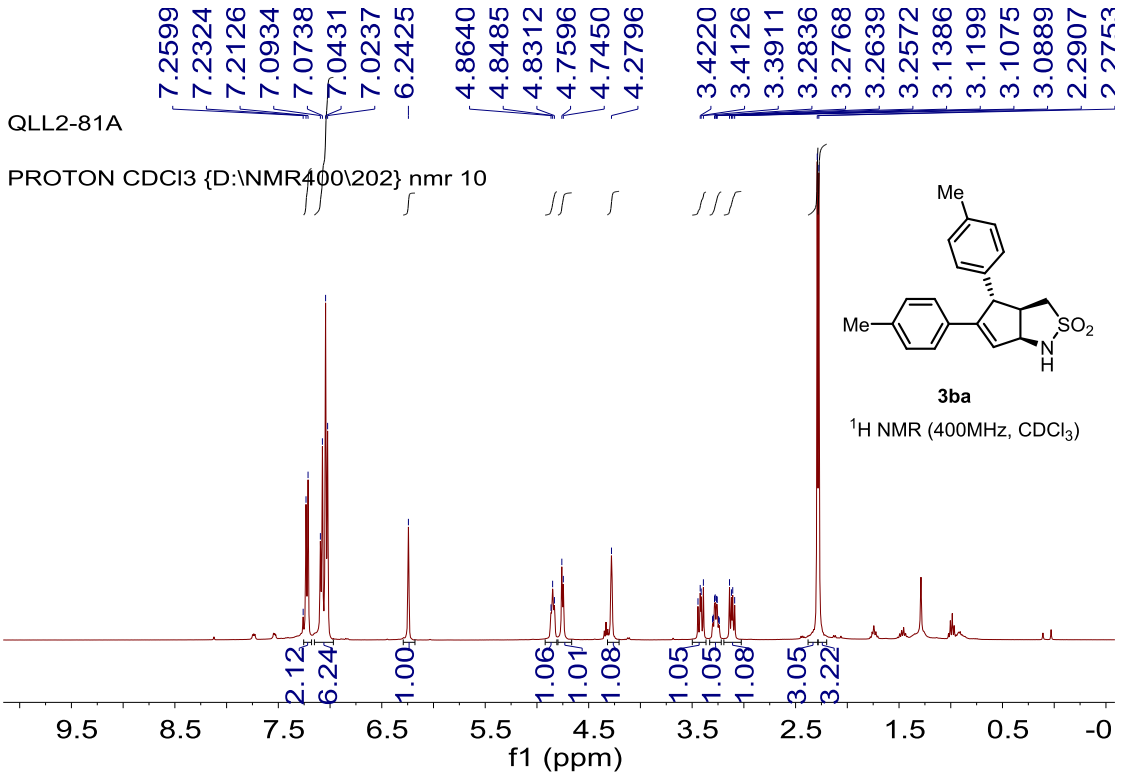
8. References

1. H. Yan, H. Wang, X. Li, X. Xin, C. Wang and B. Wan, *Angew. Chem. Int. Ed.* **2015**, *54*, 10613.
2. A. Padwa, A. C. Flick, C. A. Leverett and T. Stengel, *J. Org. Chem.* **2004**, *69*, 6377.

9. Copy of NMR Spectra



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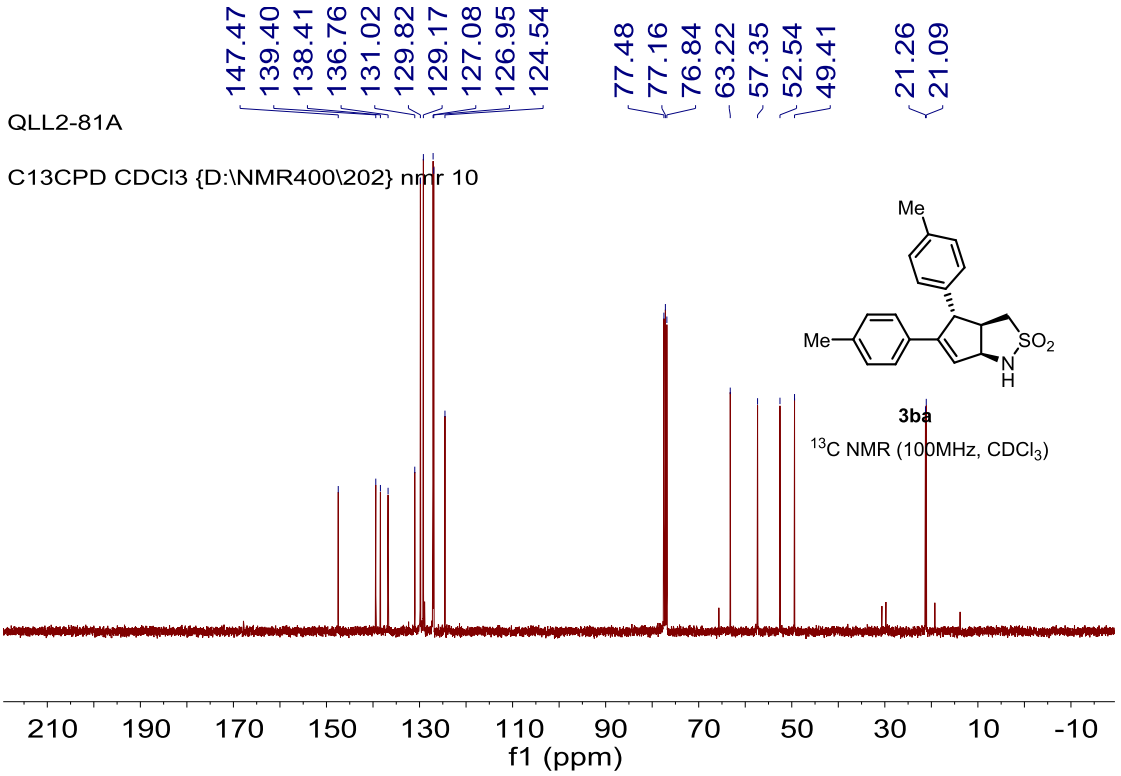
7.2126
7.0934
7.0738
7.0431
7.0237
6.2425
4.8640
4.8485
4.8312
4.7596
4.7450
4.2796
3.4220
3.4126
3.3911
3.2836
3.2768
3.2639
3.2572
3.1386
3.1199
3.1075
3.0889
2.2907
2.12
6.24
1.00
1.06
1.01
1.08
1.05
1.05
1.08
3.05
3.22
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0
f1 (ppm)
Me
Me
SO2
N
H
3ba
1H NMR (400MHz, CDCl3)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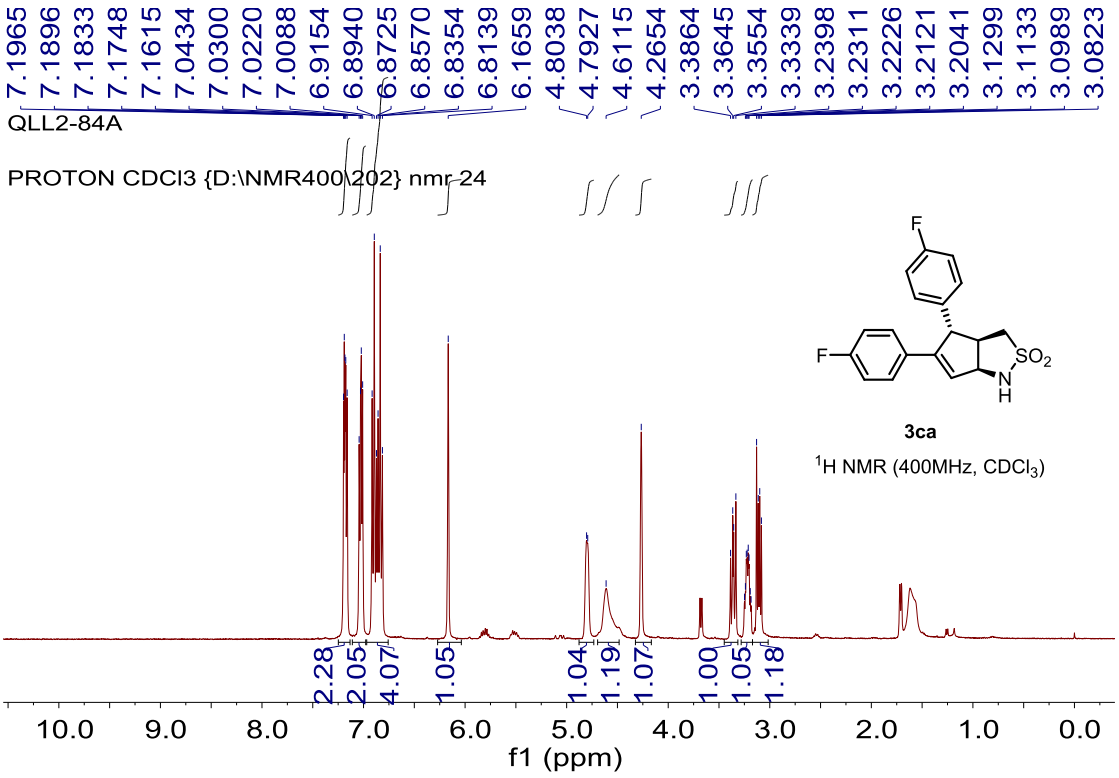
139.40
138.41
136.76
131.02
129.82
129.17
127.08
126.95
124.54
77.48
77.16
76.84
63.22
57.35
52.54
49.41
21.26
21.09
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)
Me
Me
SO2
N
H
3ba
13C NMR (100MHz, CDCl3)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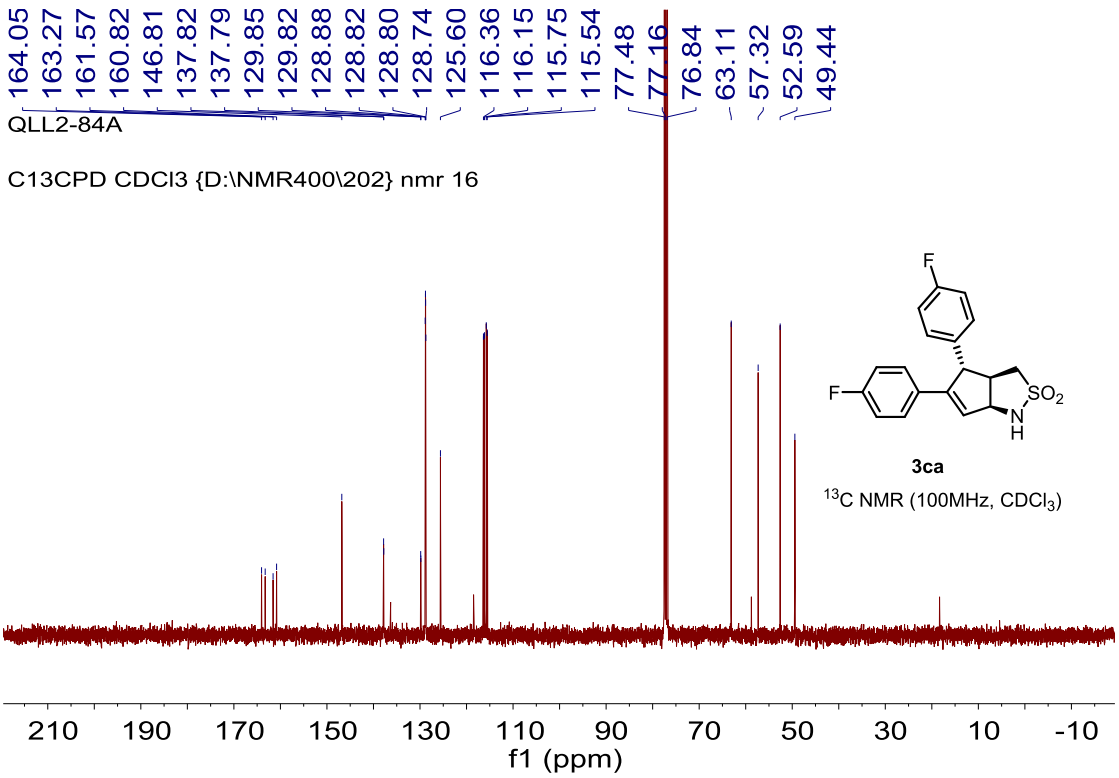
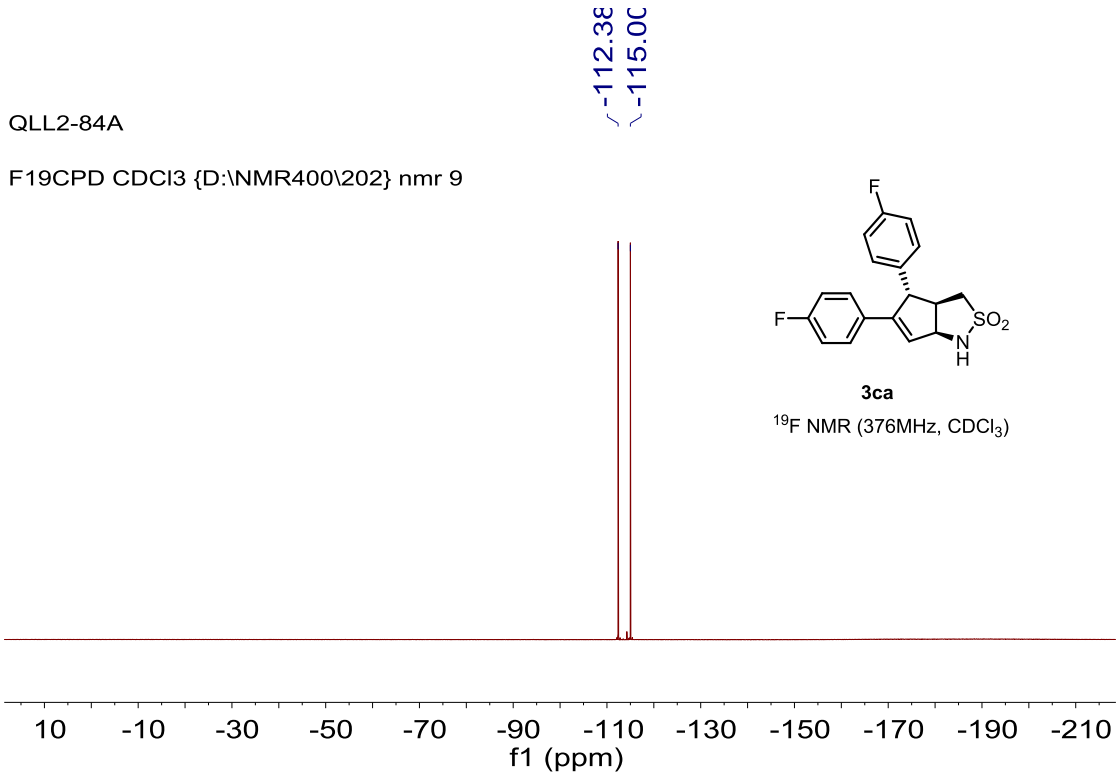
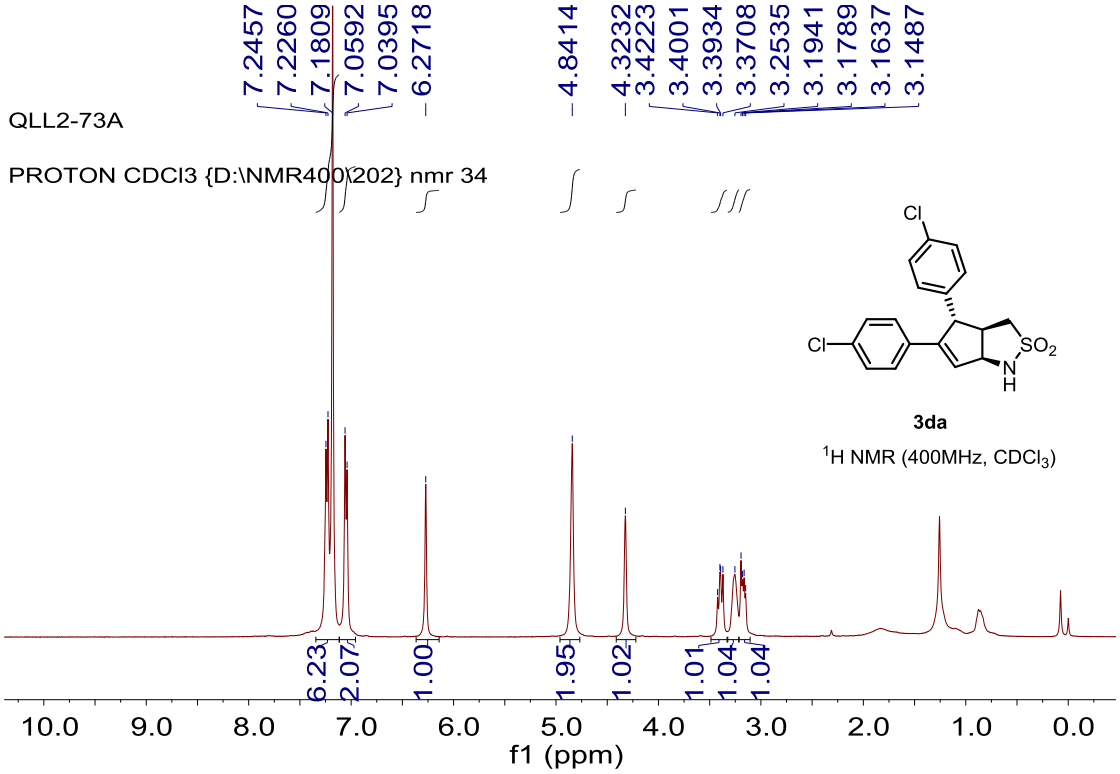
7.1896
7.1833
7.1748
7.1615
7.0434
7.0300
7.0220
7.0088
6.9154
6.8940
6.8725
6.8570
6.8354
6.8139
6.1659
4.8038
4.7927
4.6115
4.2654
3.3864
3.3645
3.3554
3.3339
3.2398
3.2311
3.2226
3.2121
3.2041
3.1299
3.1133
3.0989
3.0823
QLL2-84A
PROTON CDCl3 {D:\NMR400\202} nmr 24
2.28
2.05
4.07
1.05
1.04
1.19
1.07
1.00
1.05
1.18
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)
F
F
SO2
N
H
3ca
1H NMR (400MHz, CDCl3)


164.05
163.27
161.57
160.82
146.81
137.82
137.79
129.85
129.82
128.88
128.82
128.80
128.74
125.60
116.36
116.15
115.75
115.54
77.48
77.16
76.84
63.11
57.32
52.59
49.44
QLL2-84A
C13CPD CDCl3 {D:\NMR400\202} nmr 16
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)
F
F
SO2
N
H
3ca
13C NMR (100MHz, CDCl3)



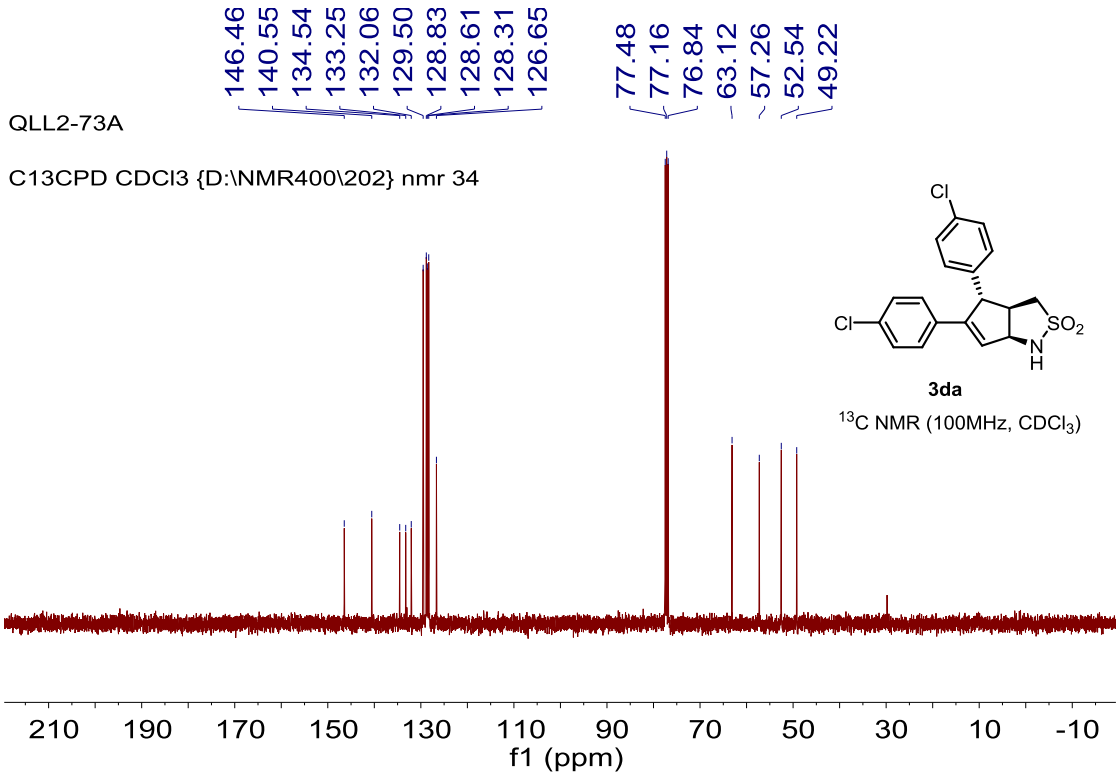
3ca

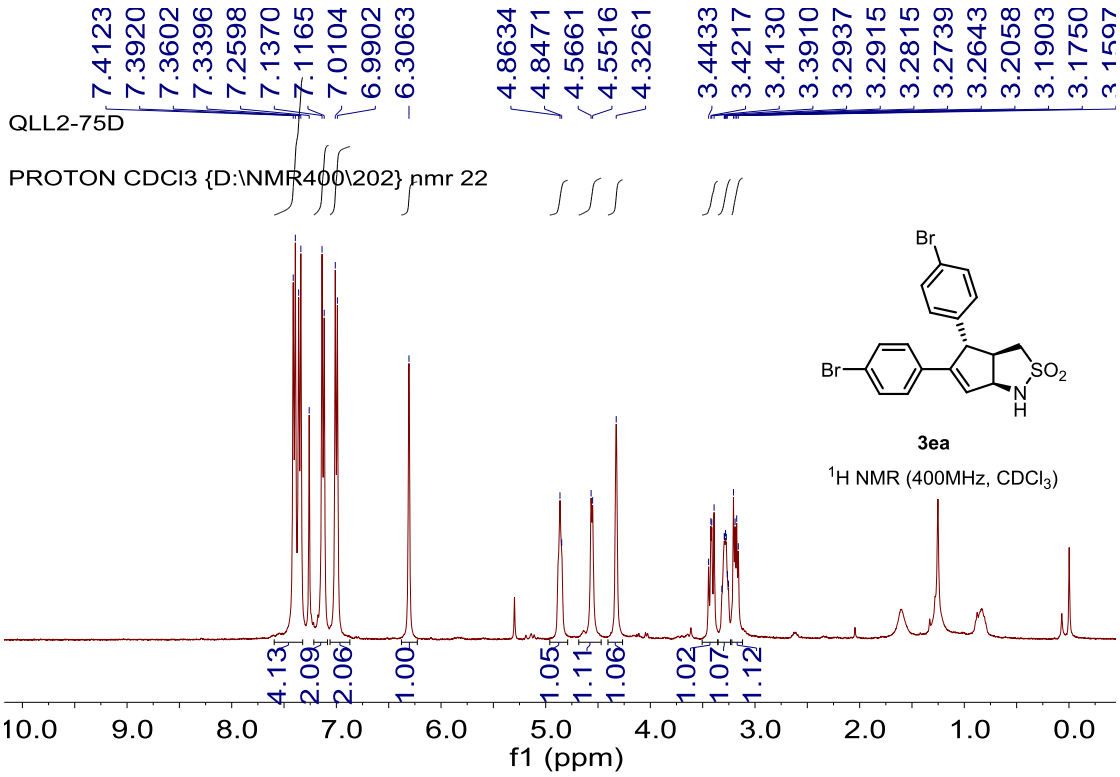
^{19}F NMR (376MHz, $CDCl_3$)



3da

^{1}H NMR (400MHz, $CDCl_3$)


146.46
140.55
134.54
133.25
132.06
129.50
128.83
128.61
128.31
126.65
77.48
77.16
76.84
63.12
57.26
52.54
49.22
QLL2-73A
C13CPD CDCl3 {D:\NMR400\202} nmr 34
Cl
Cl
SO2
N
H
3da
13C NMR (100MHz, CDCl3)
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)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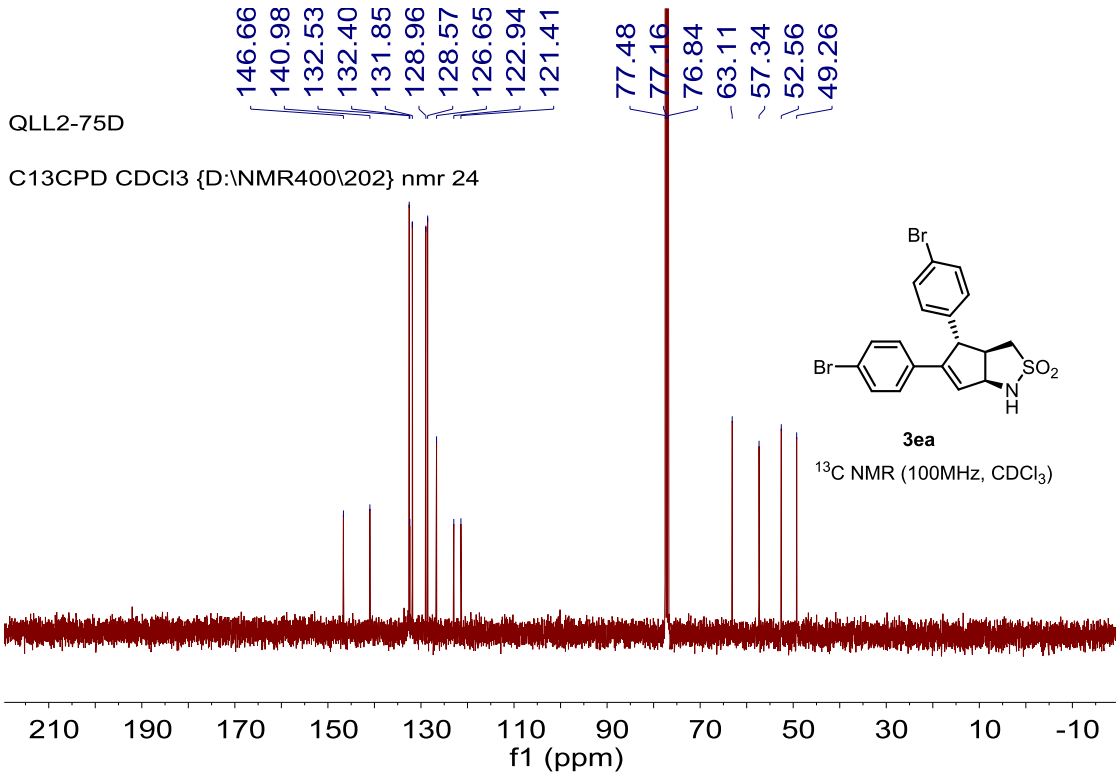
7.3602
7.3396
7.2598
7.1370
7.1165
7.0104
6.9902
6.3063
4.8634
4.8471
4.5661
4.5516
4.3261
3.4433
3.4217
3.4130
3.3910
3.2937
3.2915
3.2815
3.2739
3.2643
3.2058
3.1903
3.1750
QLL2-75D
PROTON CDCl3 {D:\NMR400\202} nmr 22
Br
Br
SO2
N
H
3ea
1H NMR (400MHz, CDCl3)
4.13
2.09
2.06
1.00
1.05
1.11
1.06
1.02
1.07
1.12
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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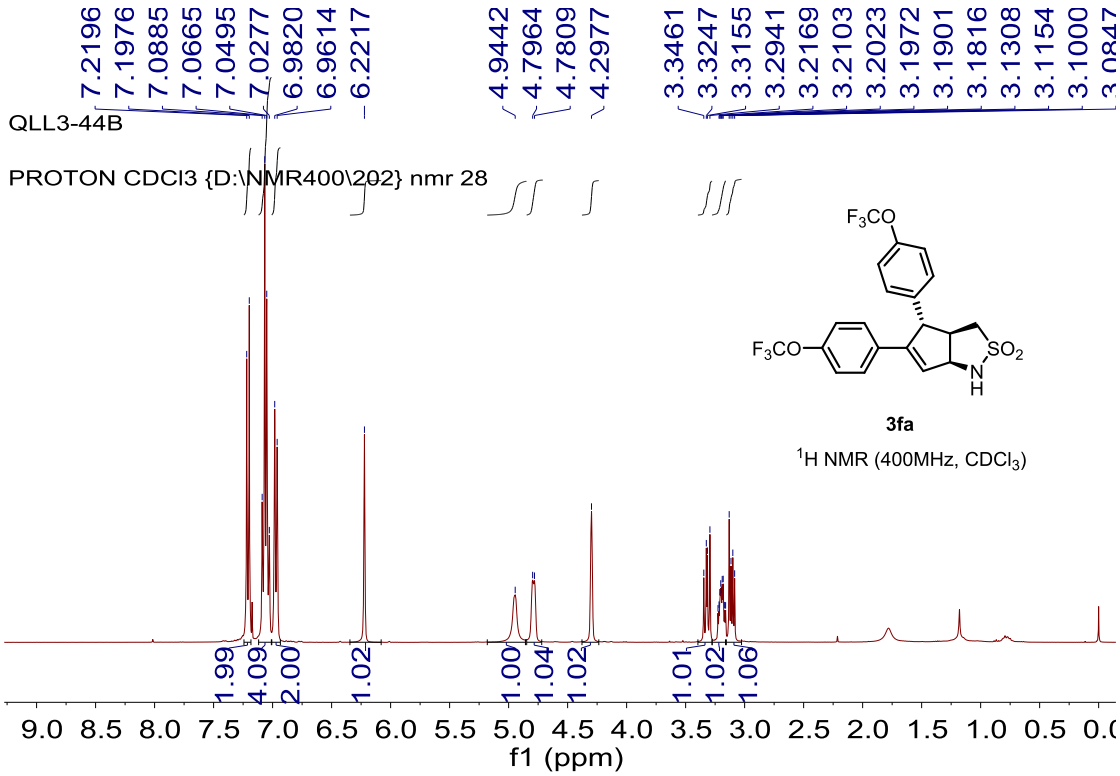
132.53
132.40
131.85
128.96
128.57
126.65
122.94
121.41
77.48
77.16
76.84
63.11
57.34
52.56
49.26
QLL2-75D
C13CPD CDCl3 {D:\NMR400\202} nmr 24
Br
Br
SO2
N
H
3ea
13C NMR (100MHz, CDCl3)
210 190 170 150 130 110 90 70 50 30 10 -10
f1 (ppm)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7.0495
7.0277
6.9820
6.9614
6.2217
4.9442
4.7964
4.7809
4.2977
3.3461
3.3247
3.3155
3.2941
3.2169
3.2103
3.2023
3.1972
3.1901
3.1816
3.1308
3.1154
3.1000
QLL3-44B
PROTON CDCl3 {D:\NMR400\202} nmr 28
F3CO
F3CO
SO2
N
H
3fa
1H NMR (400MHz, CDCl3)
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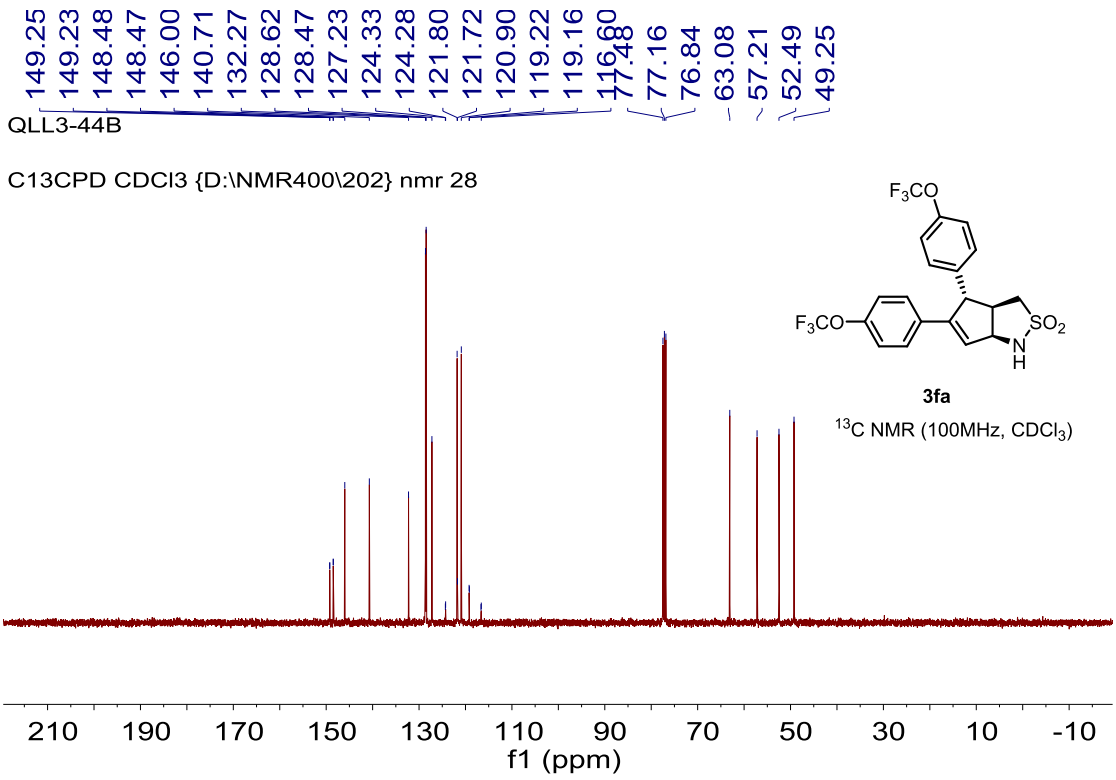
4.09
2.00
1.02
1.00
1.04
1.02
1.01
1.02
1.06
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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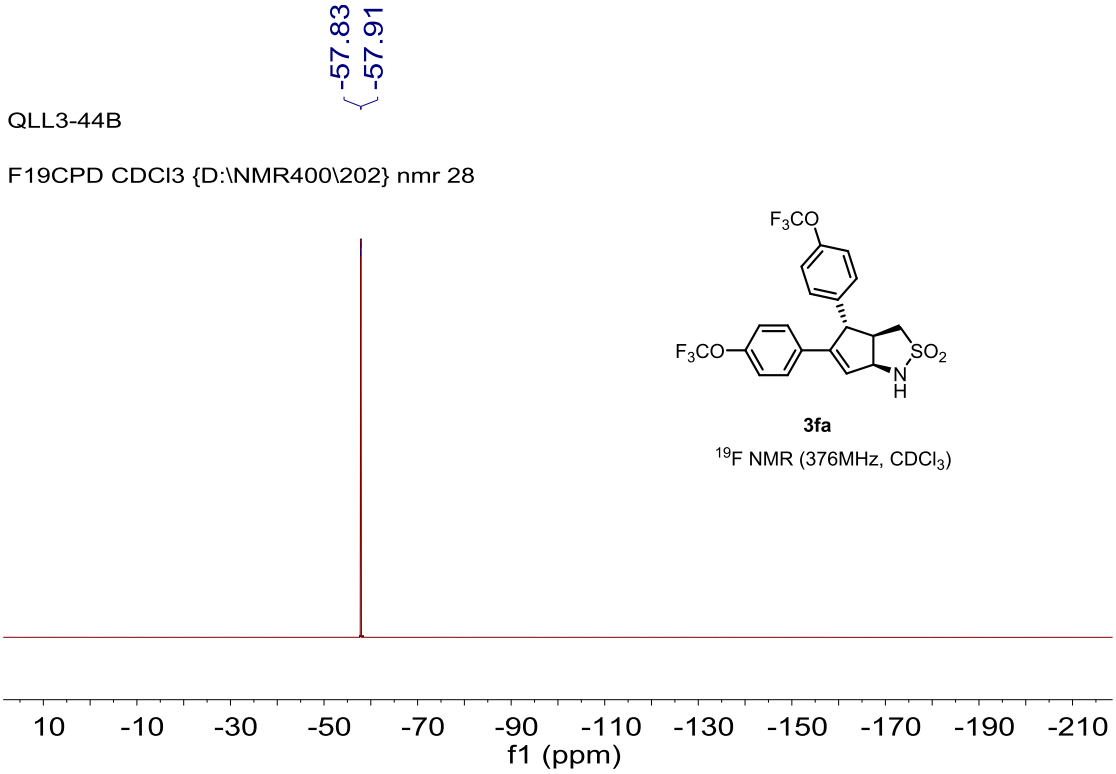
149.23
148.48
148.47
146.00
140.71
132.27
128.62
128.47
127.23
124.33
124.28
121.80
121.72
120.90
119.22
119.16
116.60
77.48
77.16
76.84
63.08
57.21
52.49
49.25
QLL3-44B
C13CPD CDCl3 {D:\NMR400\202} nmr 28
F3CO
F3CO
SO2
N
H
3fa
13C NMR (100MHz, CDCl3)
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)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-57.91
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F3CO
F3CO
SO2
N
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3fa
19F NMR (376MHz, CDCl3)
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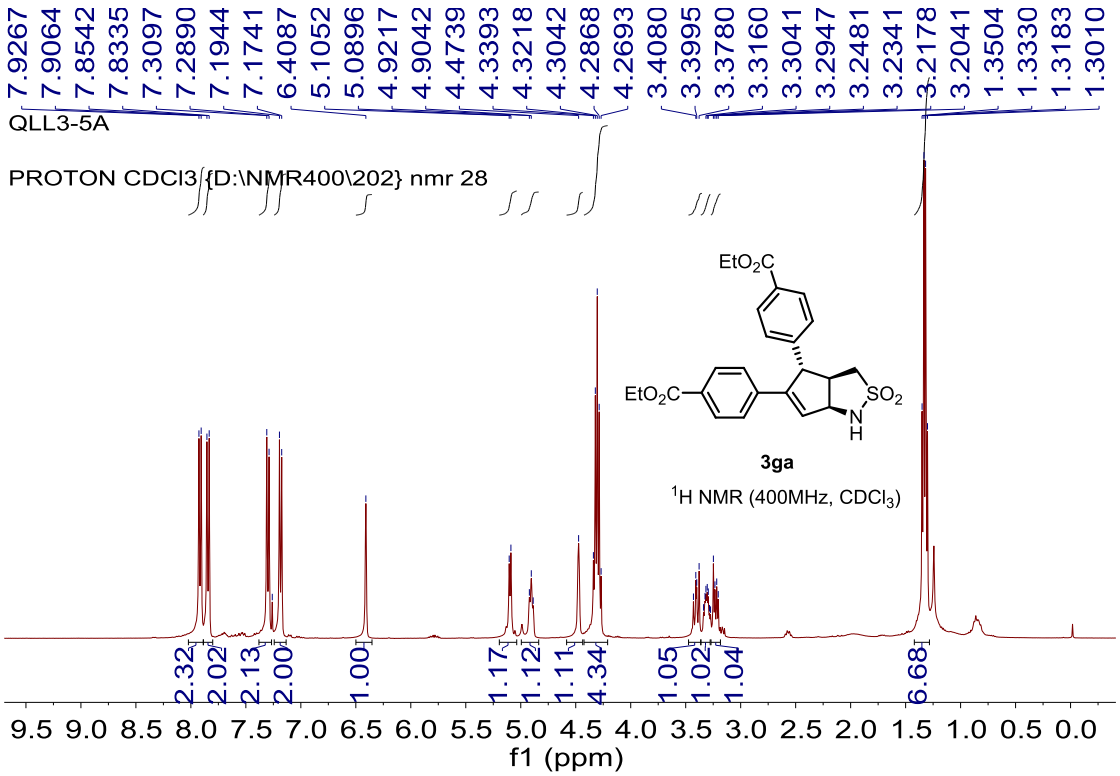
-130
-150
-170
-190
-210
f1 (ppm)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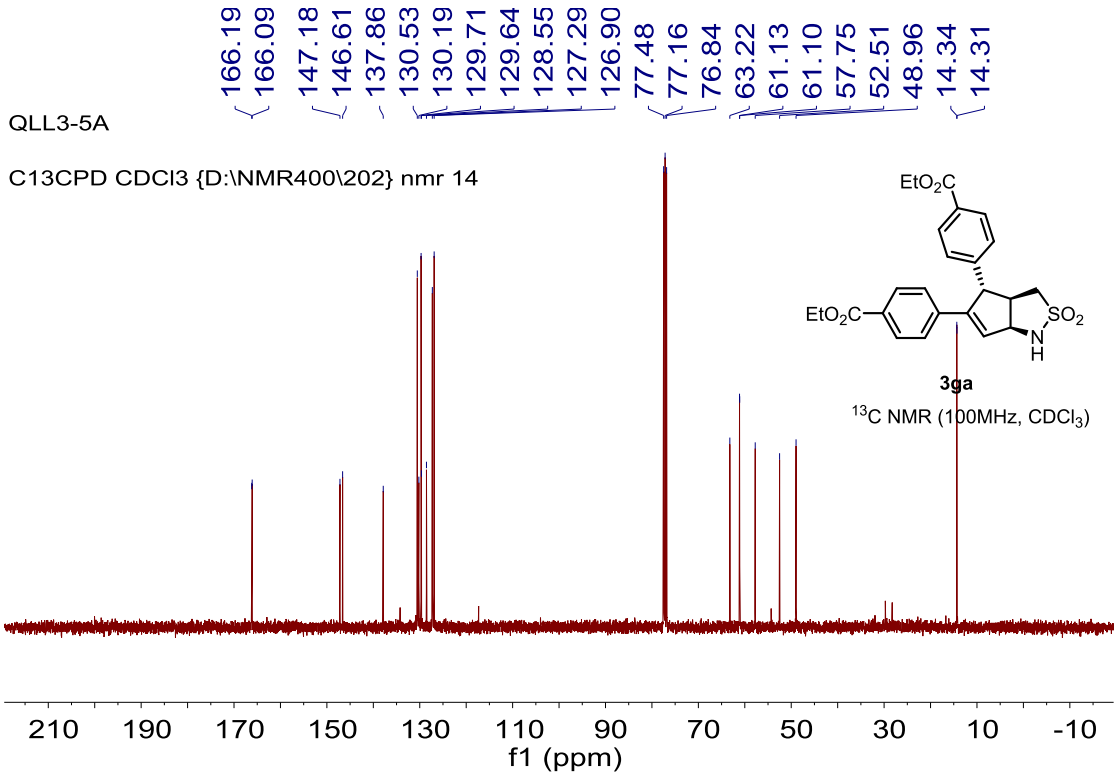
7.3097
7.2890
7.1944
7.1741
6.4087
5.1052
5.0896
4.9217
4.9042
4.4739
4.3393
4.3218
4.3042
4.2868
4.2693
3.4080
3.3995
3.3780
3.3160
3.3041
3.2947
3.2481
3.2341
3.2178
3.2041
1.3504
1.3330
1.3183
1.3010
QLL3-5A
PROTON CDCl3 {D:\NMR400\202} nmr 28
EtO2C
EtO2C
SO2
N
H
3ga
1H NMR (400MHz, CDCl3)
2.32
2.02
2.13
2.00
1.00
1.17
1.12
1.11
4.34
1.05
1.02
1.04
6.68
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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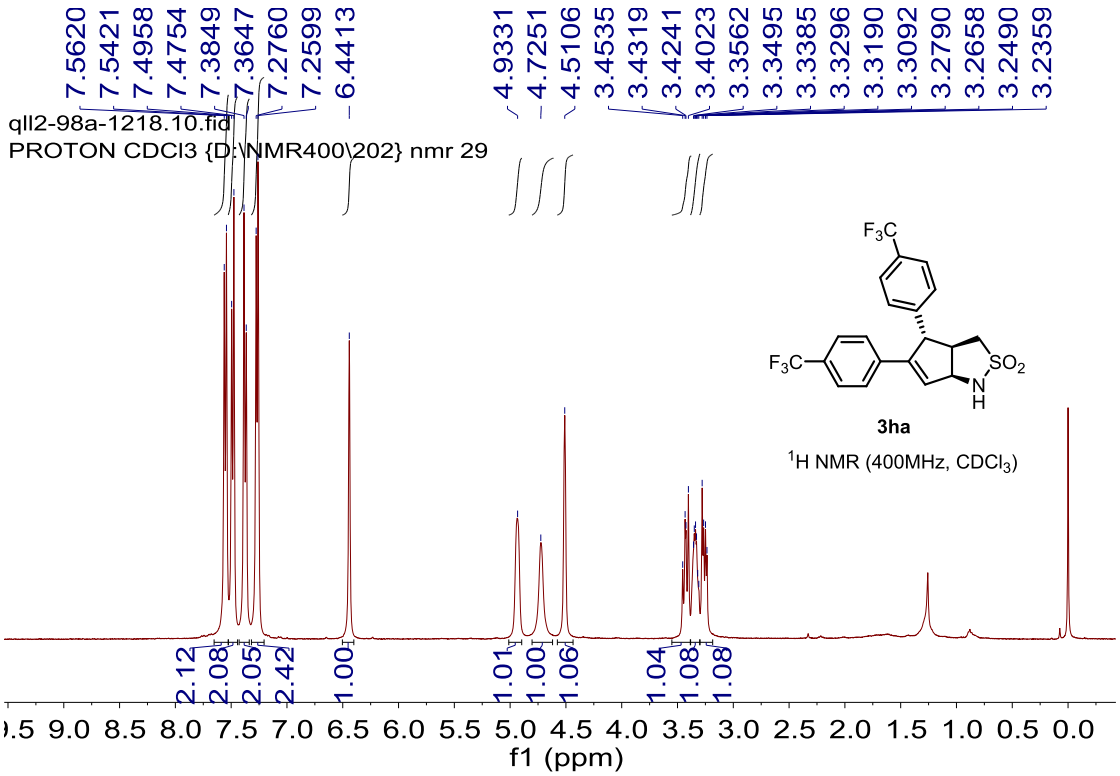
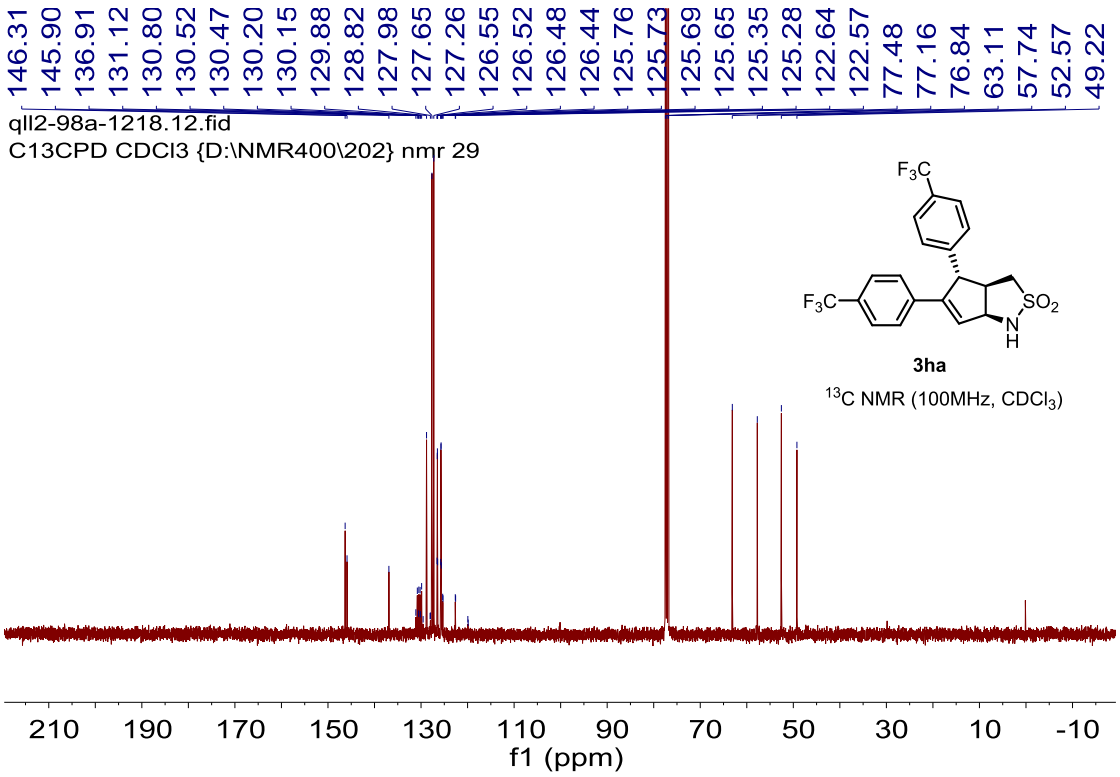
166.09
147.18
146.61
137.86
130.53
130.19
129.71
129.64
128.55
127.29
126.90
77.48
77.16
76.84
63.22
61.13
61.10
57.75
52.51
48.96
14.34
14.31
QLL3-5A
C13CPD CDCl3 {D:\NMR400\202} nmr 14
EtO2C
EtO2C
SO2
N
H
3ga
13C NMR (100MHz, CDCl3)
210 190 170 150 130 110 90 70 50 30 10 -10
f1 (ppm)



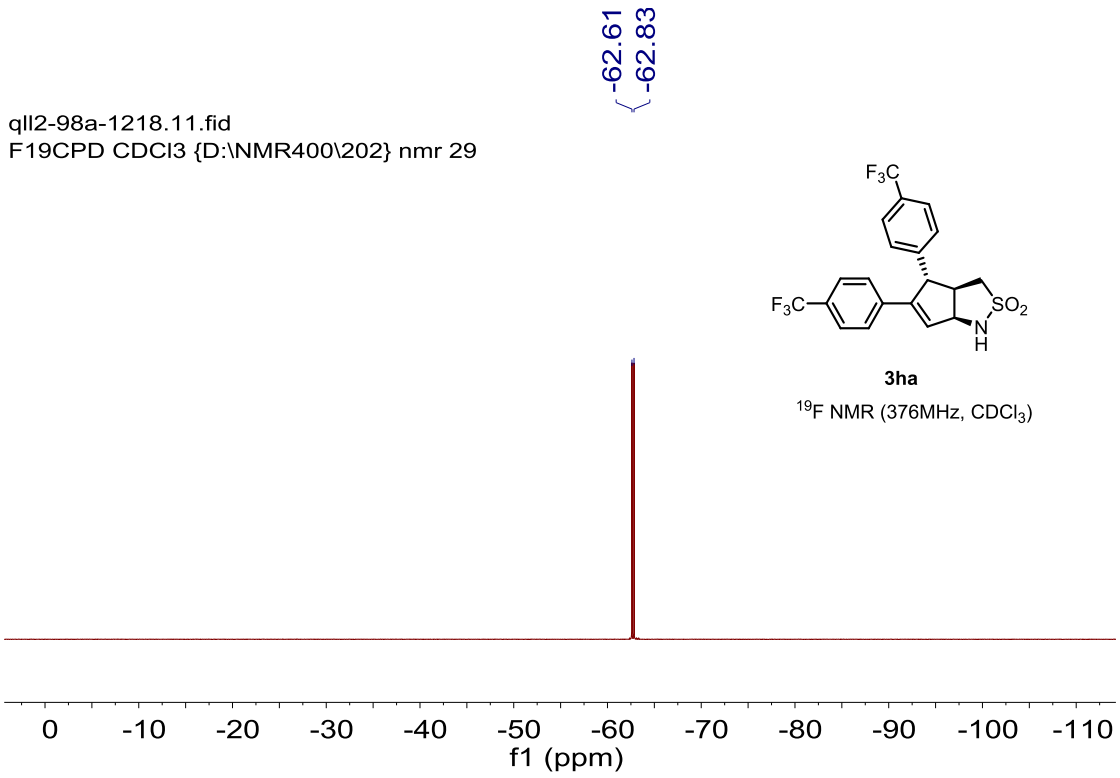
3ha

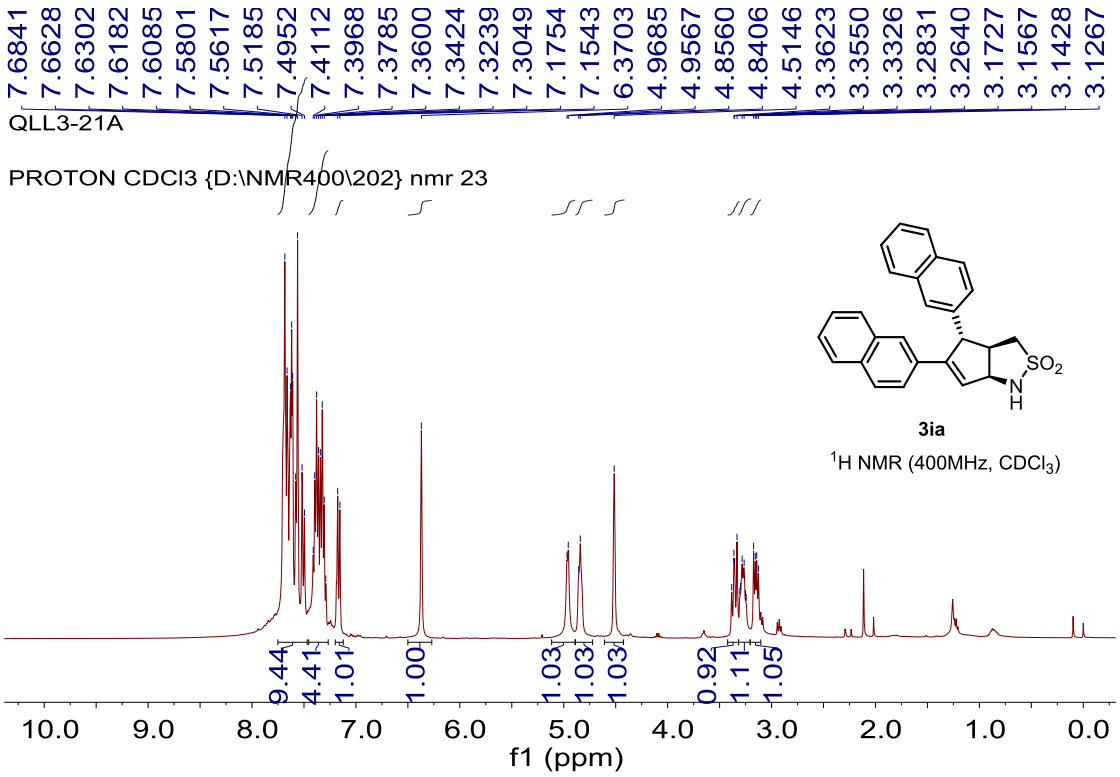
^{1}H NMR (400MHz, $CDCl_3$)

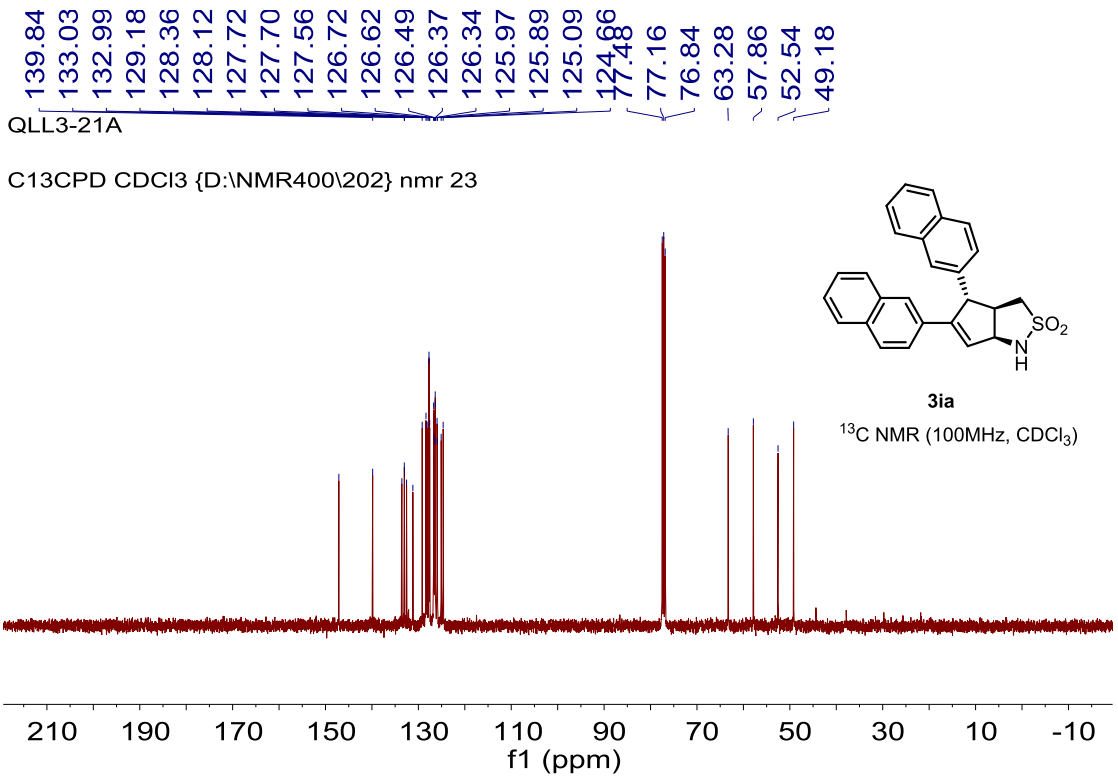


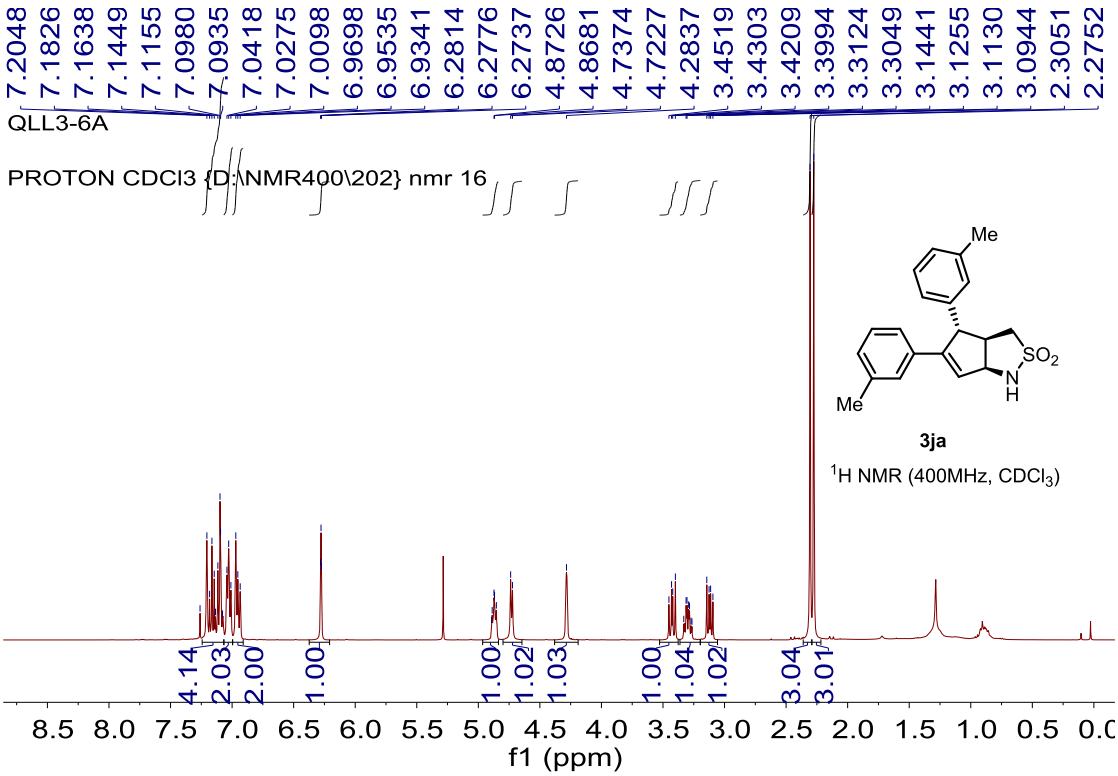
3ha

^{13}C NMR (100MHz, $CDCl_3$)


-62.61
-62.83
qll2-98a-1218.11.fid
F19CPD CDCl3 {D:\NMR400\202} nmr 29
F3C
F3C
SO2
N
H
3ha
19F NMR (376MHz, CDCl3)
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
f1 (ppm)


7.6841
7.6628
7.6302
7.6182
7.6085
7.5801
7.5617
7.5185
7.4952
7.4112
7.3968
7.3785
7.3600
7.3424
7.3239
7.3049
7.1754
7.1543
6.3703
4.9685
4.9567
4.8560
4.8406
4.5146
3.3623
3.3550
3.3326
3.2831
3.2640
3.1727
3.1567
3.1428
3.1267
QLL3-21A
PROTON CDCl3 {D:\NMR400\202} nmr 23
9.44
4.41
1.01
1.00
1.03
1.03
1.03
0.92
1.11
1.05
SO2
N
H
3ia
1H NMR (400MHz, CDCl3)
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


139.84
133.03
132.99
129.18
128.36
128.12
127.72
127.70
127.56
126.72
126.62
126.49
126.37
126.34
125.97
125.89
125.09
124.66
77.48
77.16
76.84
63.28
57.86
52.54
49.18
QLL3-21A
C13CPD CDCl3 {D:\NMR400\202} nmr 23
SO2
N
H
3ia
13C NMR (100MHz, CDCl3)
210 190 170 150 130 110 90 70 50 30 10 -10
f1 (ppm)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7.1638
7.1449
7.1155
7.0980
7.0935
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7.0275
7.0098
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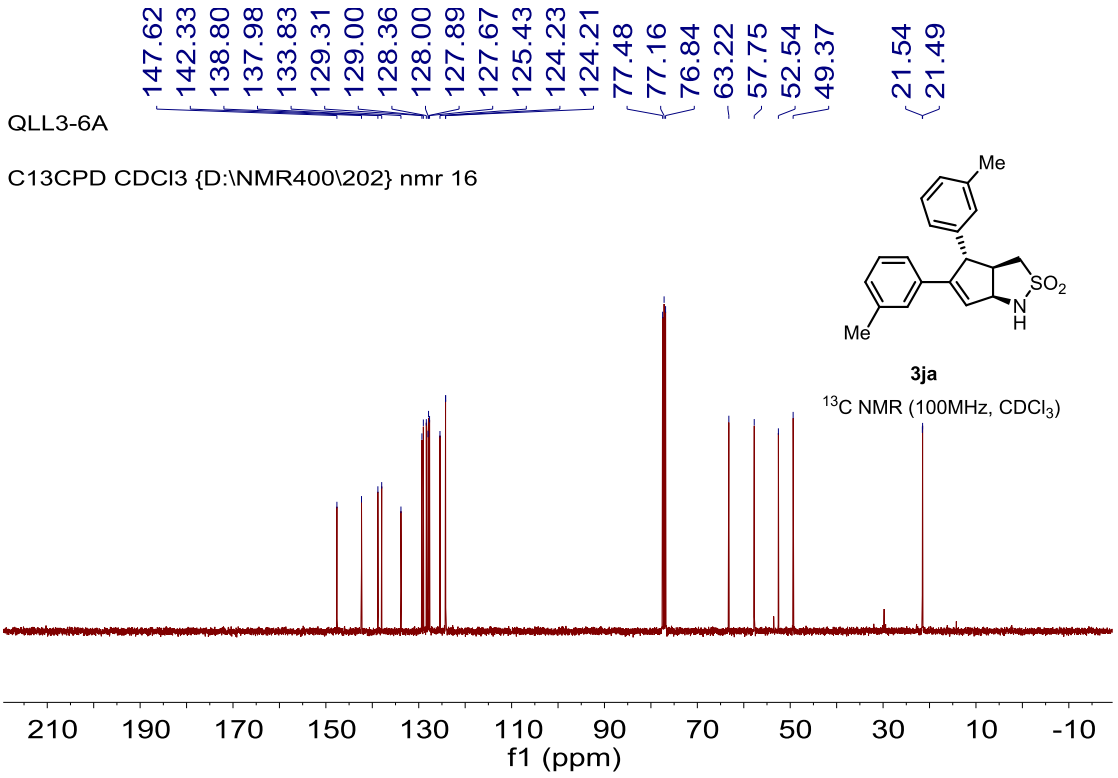
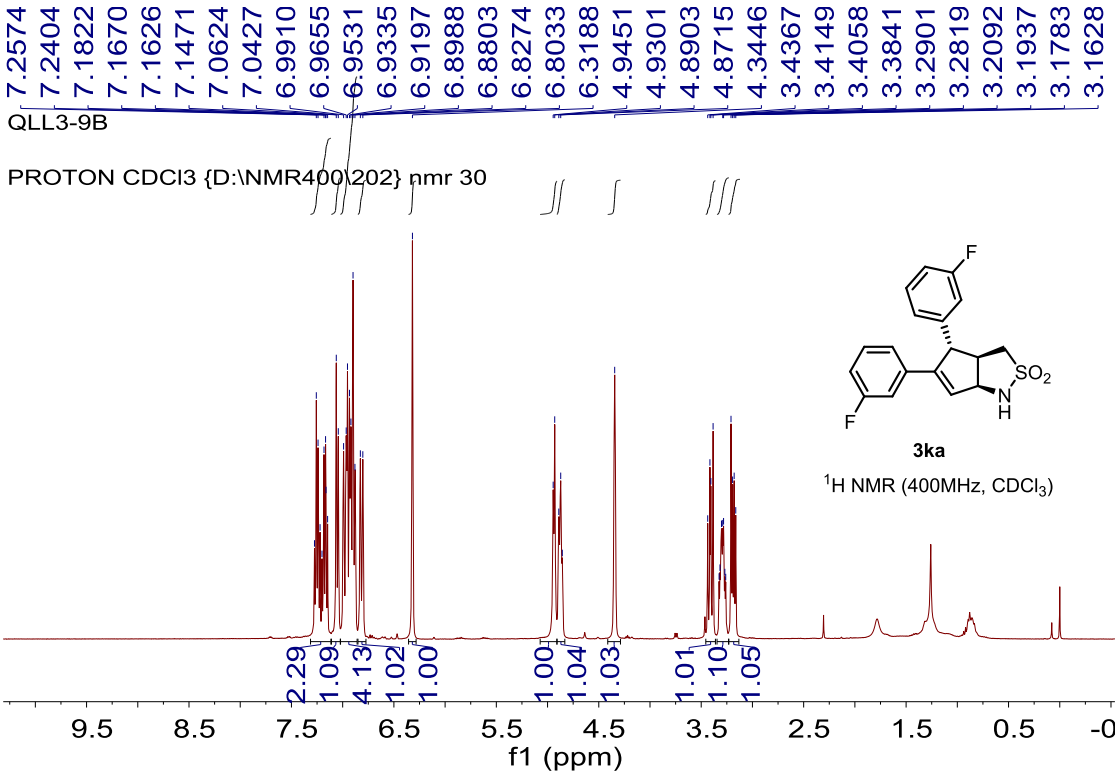
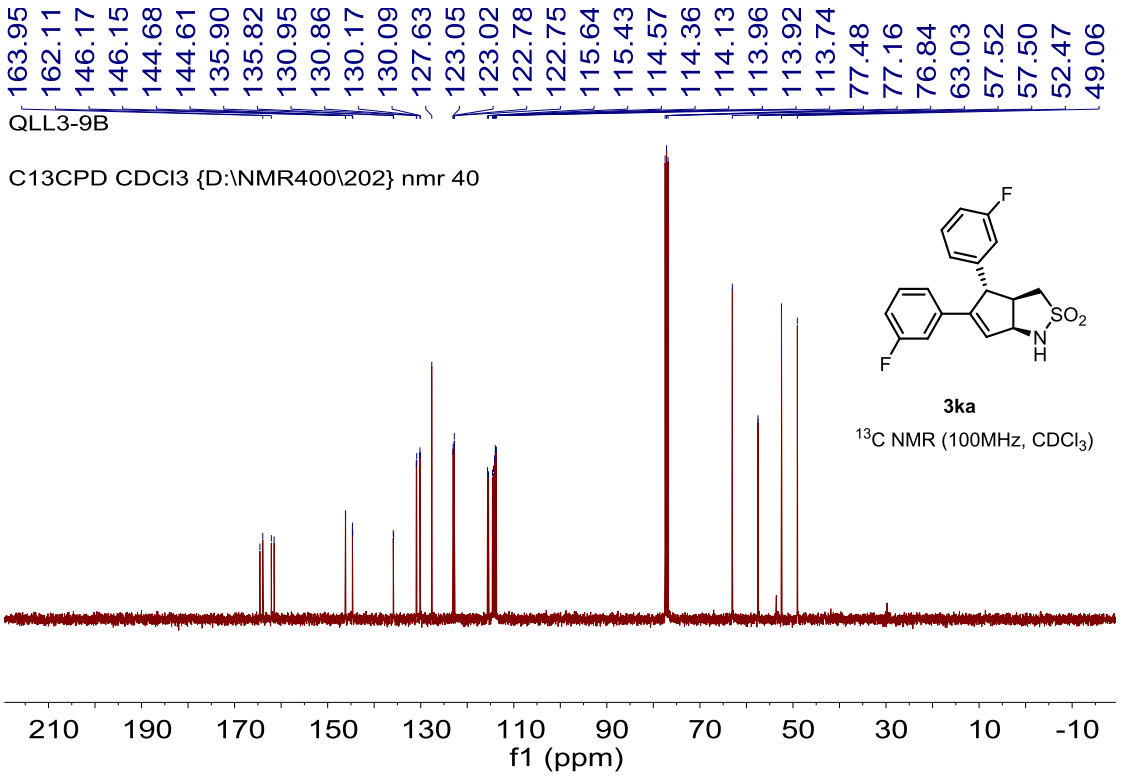
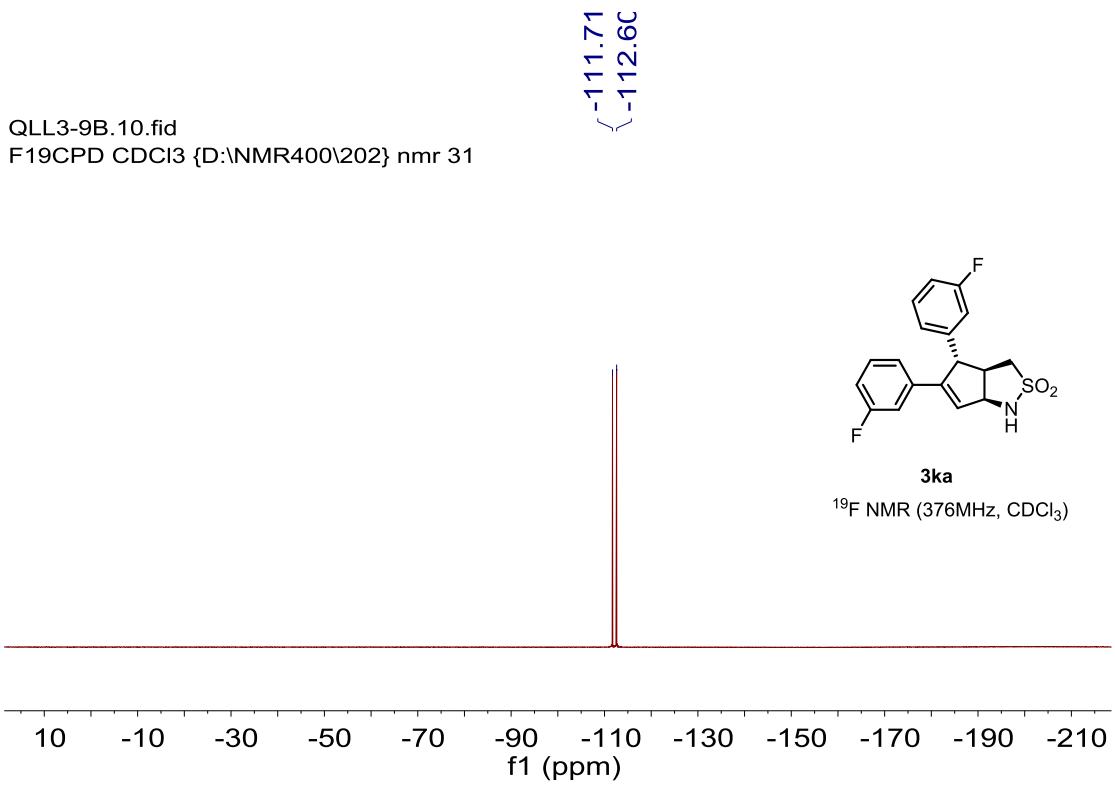
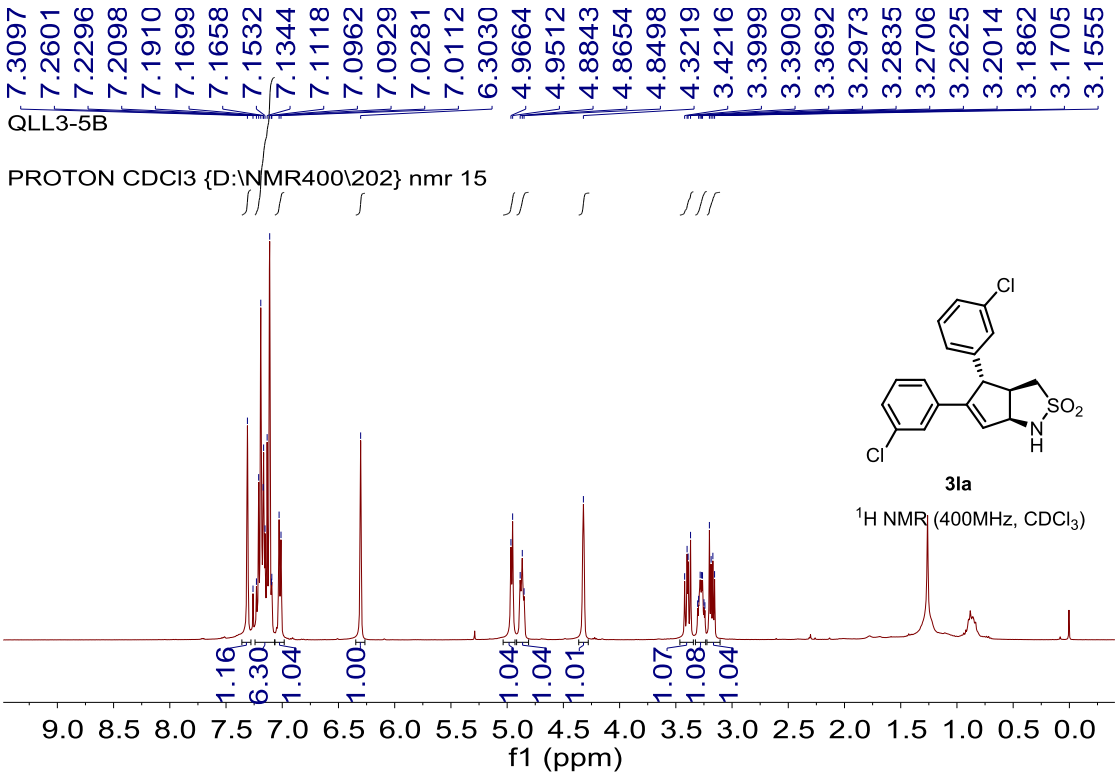
6.9535
6.9341
6.2814
6.2776
6.2737
4.8726
4.8681
4.7374
4.7227
4.2837
3.4519
3.4303
3.4209
3.3994
3.3124
3.3049
3.1441
3.1255
3.1130
3.0944
2.3051
2.2752
QLL3-6A
PROTON CDCl3 {D:\NMR400\202} nmr 16
Me
SO2
N
H
Me
3ja
1H NMR (400MHz, CDCl3)
4.14
2.03
2.00
1.00
1.00
1.02
1.03
1.00
1.04
1.02
3.04
3.01
8.5 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)

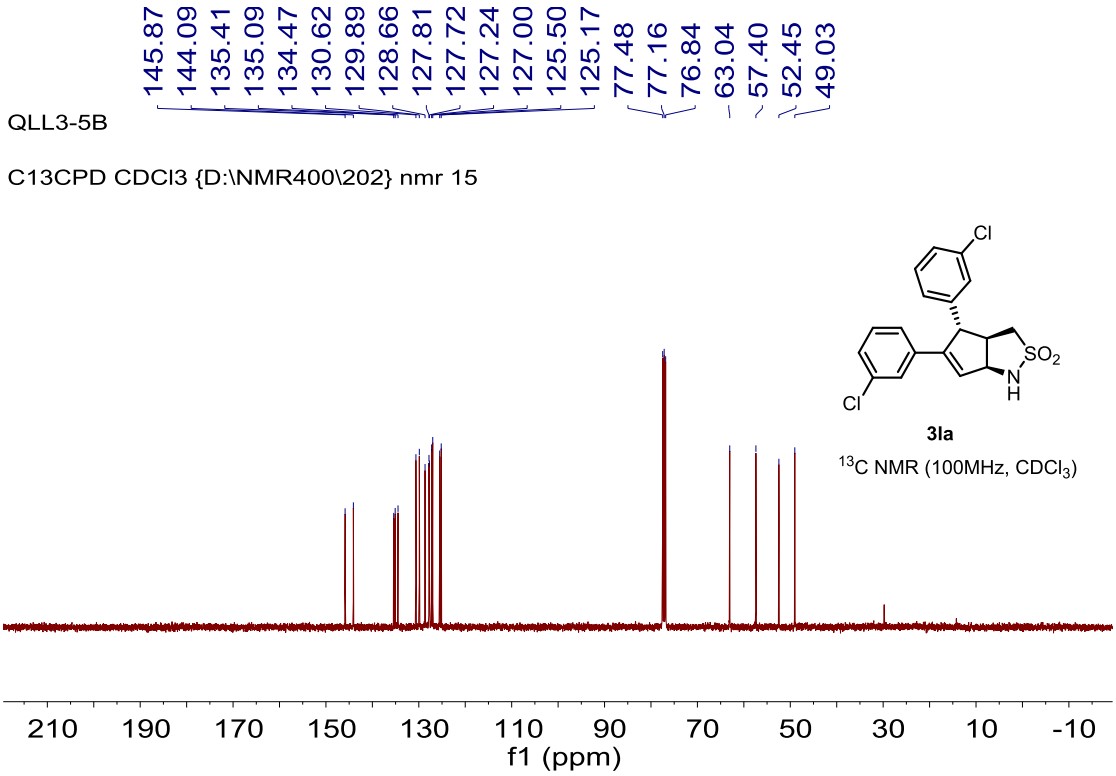

147.62
142.33
138.80
137.98
133.83
129.31
129.00
128.36
128.00
127.89
127.67
125.43
124.23
124.21
77.48
77.16
76.84
63.22
57.75
52.54
49.37
21.54
21.49
QLL3-6A
C13CPD CDCl3 {D:\NMR400\202} nmr 16
Me
SO2
N
H
Me
3ja
13C NMR (100MHz, CDCl3)
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

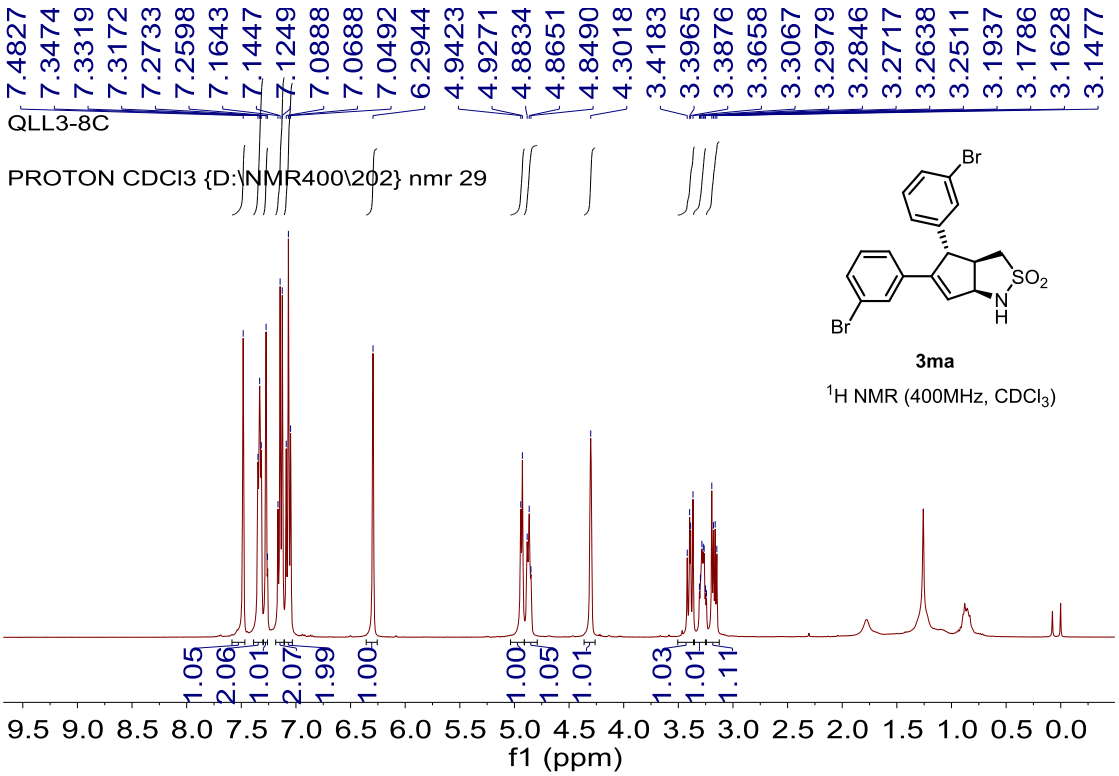

7.2574
7.2404
7.1822
7.1670
7.1626
7.1471
7.0624
7.0427
6.9910
6.9655
6.9531
6.9335
6.9197
6.8988
6.8803
6.8274
6.8033
6.3188
4.9451
4.9301
4.8903
4.8715
4.3446
3.4367
3.4149
3.4058
3.3841
3.2901
3.2819
3.2092
3.1937
3.1783
3.1628
QLL3-9B
PROTON CDCl3 {D:\NMR400\202} nmr 30
F
SO2
N
H
F
3ka
1H NMR (400MHz, CDCl3)
2.29
1.09
4.13
1.02
1.00
1.00
1.04
1.03
1.01
1.10
1.05
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0
f1 (ppm)

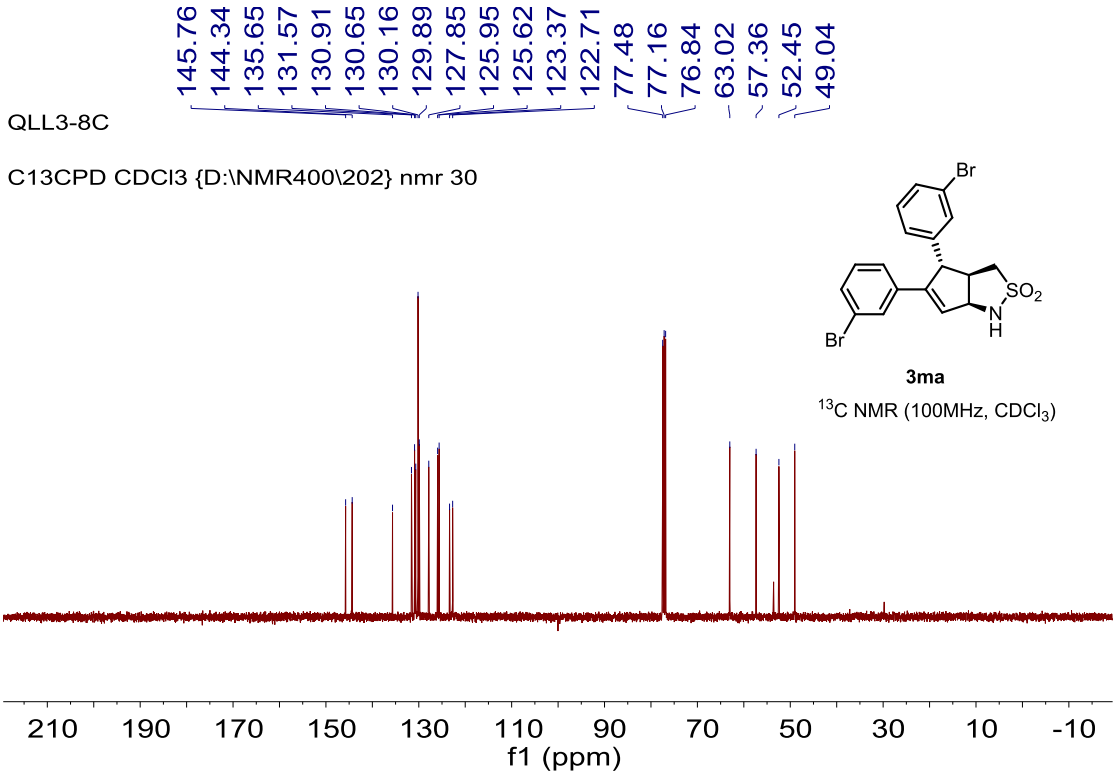

163.95
162.11
146.17
146.15
144.68
144.61
135.90
135.82
130.95
130.86
130.17
130.09
127.63
123.05
123.02
122.78
122.75
115.64
115.43
114.57
114.36
114.13
113.96
113.92
113.74
77.48
77.16
76.84
63.03
57.52
57.50
52.47
49.06
QLL3-9B
C13CPD CDCl3 {D:\NMR400\202} nmr 40
F
SO2
N
H
F
3ka
13C NMR (100MHz, CDCl3)
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

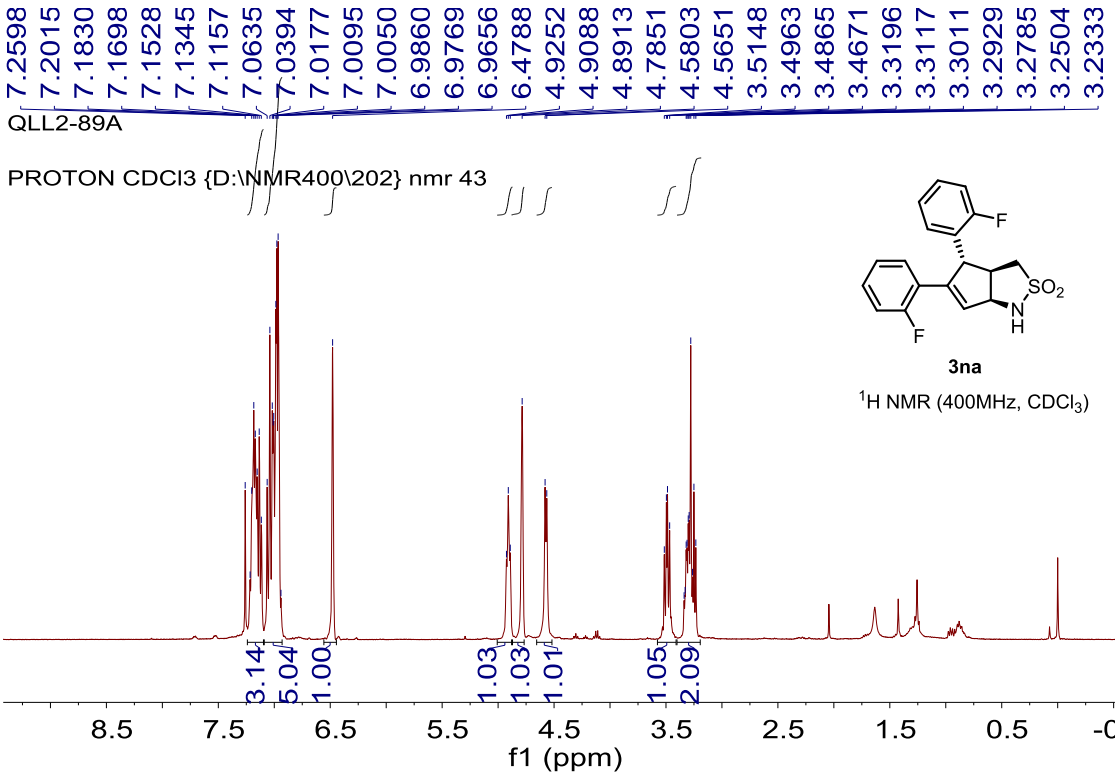

-111.71
-112.60
QLL3-9B.10.fid
F19CPD CDCl3 {D:\NMR400\202} nmr 31
F
SO2
N
H
F
3ka
19F NMR (376MHz, CDCl3)
10
-10
-30
-50
-70
-90
-110
-130
-150
-170
-190
-210
f1 (ppm)

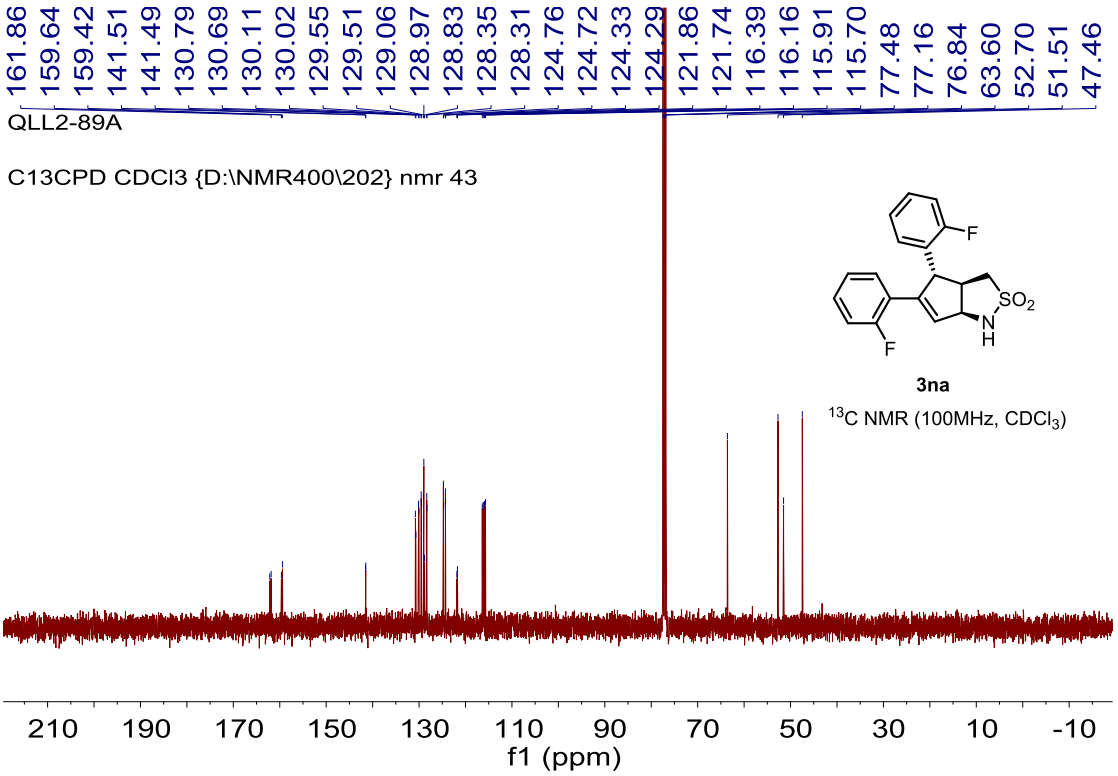

7.3097
7.2601
7.2296
7.2098
7.1910
7.1699
7.1658
7.1532
7.1344
7.1118
7.0962
7.0929
7.0281
7.0112
6.3030
4.9664
4.9512
4.8843
4.8654
4.8498
4.3219
3.4216
3.3999
3.3909
3.3692
3.2973
3.2835
3.2706
3.2625
3.2014
3.1862
3.1705
3.1555
QLL3-5B
PROTON CDCl3 {D:\NMR400\202} nmr 15
1.16
6.30
1.04
1.00
1.04
1.04
1.01
1.07
1.08
1.04
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)
Cl
SO2
N
H
Cl
3la
1H NMR (400MHz, CDCl3)

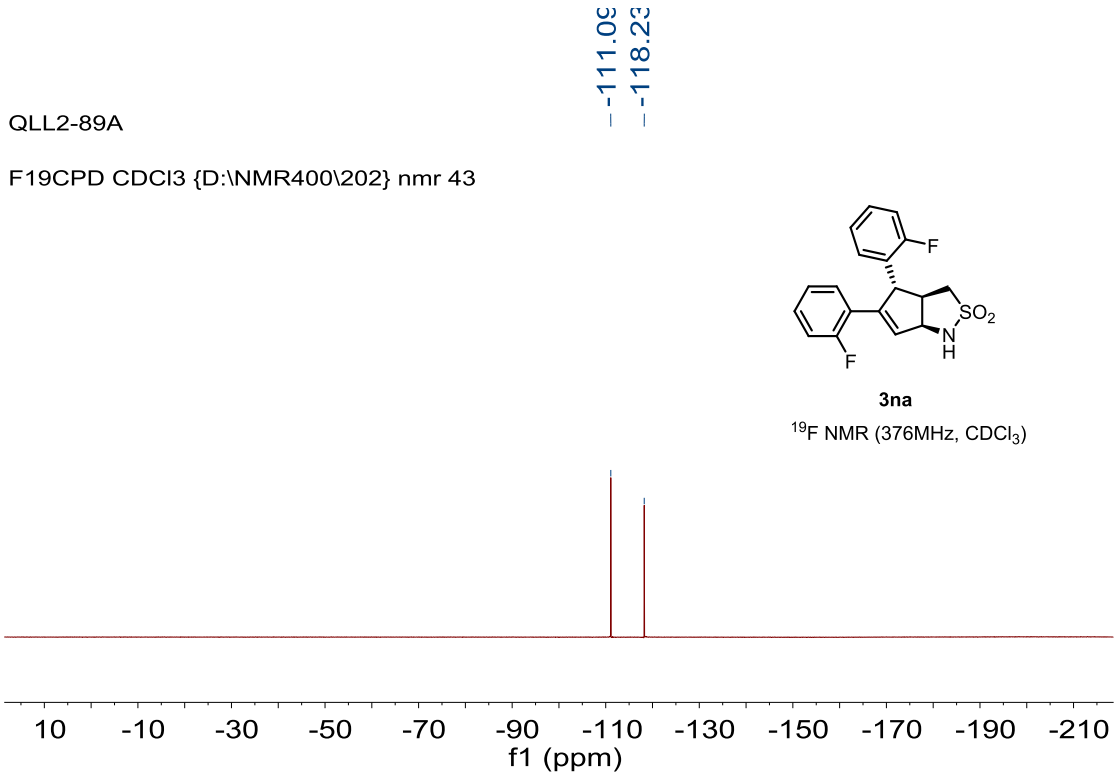

145.87
144.09
135.41
135.09
134.47
130.62
129.89
128.66
127.81
127.72
127.24
127.00
125.50
125.17
77.48
77.16
76.84
63.04
57.40
52.45
49.03
QLL3-5B
C13CPD CDCl3 {D:\NMR400\202} nmr 15
210 190 170 150 130 110 90 70 50 30 10 -10
f1 (ppm)
Cl
SO2
N
H
Cl
3la
13C NMR (100MHz, CDCl3)

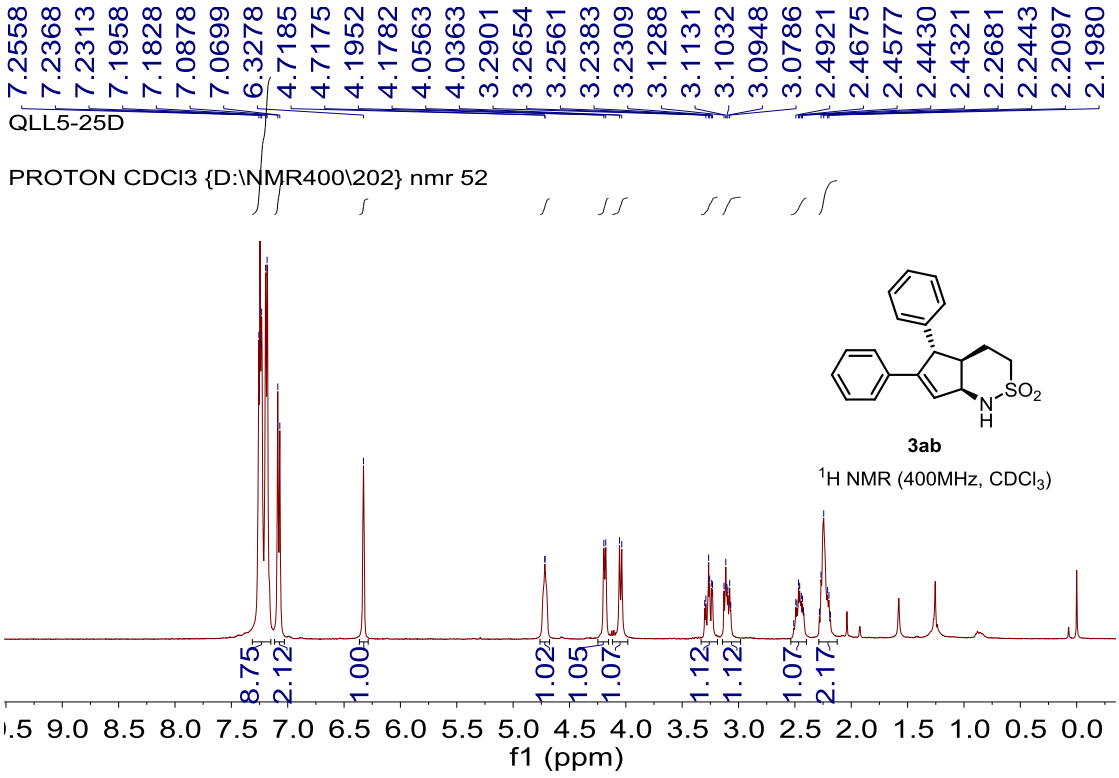

7.4827
7.3474
7.3319
7.3172
7.2733
7.2598
7.1643
7.1447
7.1249
7.0888
7.0688
7.0492
6.2944
4.9423
4.9271
4.8834
4.8651
4.8490
4.3018
3.4183
3.3965
3.3876
3.3658
3.3067
3.2979
3.2846
3.2717
3.2638
3.2511
3.1937
3.1786
3.1628
3.1477
QLL3-8C
PROTON CDCl3 {D:\NMR400\202} nmr 29
Br
SO2
N
H
Br
3ma
1H NMR (400MHz, CDCl3)
1.05
2.06
1.01
2.07
1.99
1.00
1.00
1.05
1.01
1.03
1.01
1.11
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)

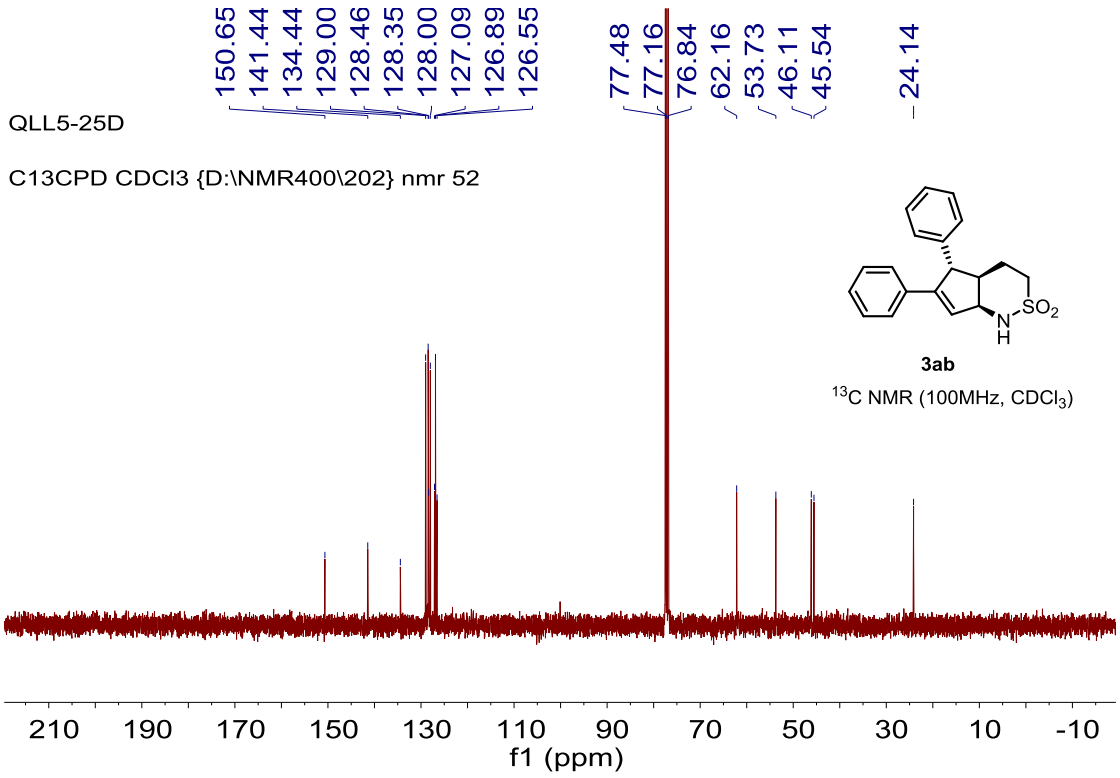

145.76
144.34
135.65
131.57
130.91
130.65
130.16
129.89
127.85
125.95
125.62
123.37
122.71
77.48
77.16
76.84
63.02
57.36
52.45
49.04
QLL3-8C
C13CPD CDCl3 {D:\NMR400\202} nmr 30
Br
SO2
N
H
Br
3ma
13C NMR (100MHz, CDCl3)
210 190 170 150 130 110 90 70 50 30 10 -10
f1 (ppm)

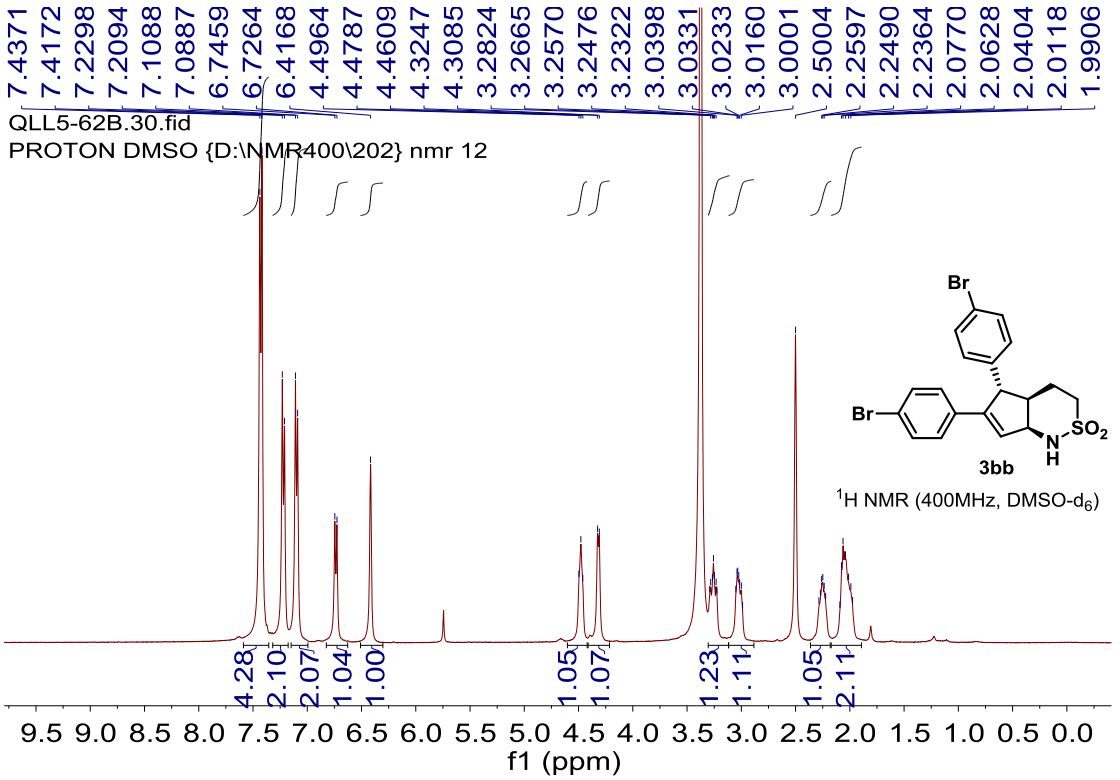

7.2598
7.2015
7.1830
7.1698
7.1528
7.1345
7.1157
7.0635
7.0394
7.0177
7.0095
7.0050
6.9860
6.9769
6.9656
6.4788
4.9252
4.9088
4.8913
4.7851
4.5803
4.5651
3.5148
3.4963
3.4865
3.4671
3.3196
3.3117
3.3011
3.2929
3.2785
3.2504
3.2333
QLL2-89A
PROTON CDCl3 {D:\NMR400\202} nmr 43
3.14
5.04
1.00
1.03
1.03
1.01
1.05
2.09
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)
F
F
SO2
N
H
3na
1H NMR (400MHz, CDCl3)

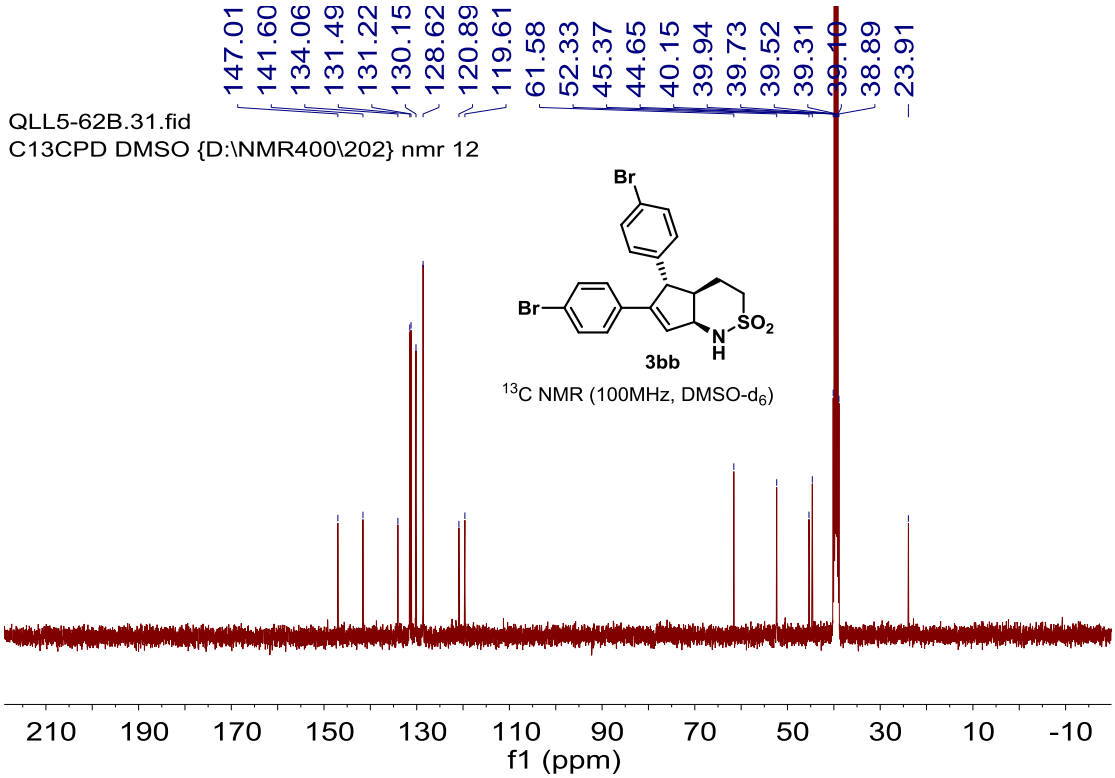

161.86
159.64
159.42
141.51
141.49
130.79
130.69
130.11
130.02
129.55
129.51
129.06
128.97
128.83
128.35
128.31
124.76
124.72
124.33
124.29
121.86
121.74
116.39
116.16
115.91
115.70
77.48
77.16
76.84
63.60
52.70
51.51
47.46
QLL2-89A
C13CPD CDCl3 {D:\NMR400\202} nmr 43
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)
F
F
SO2
N
H
3na
13C NMR (100MHz, CDCl3)

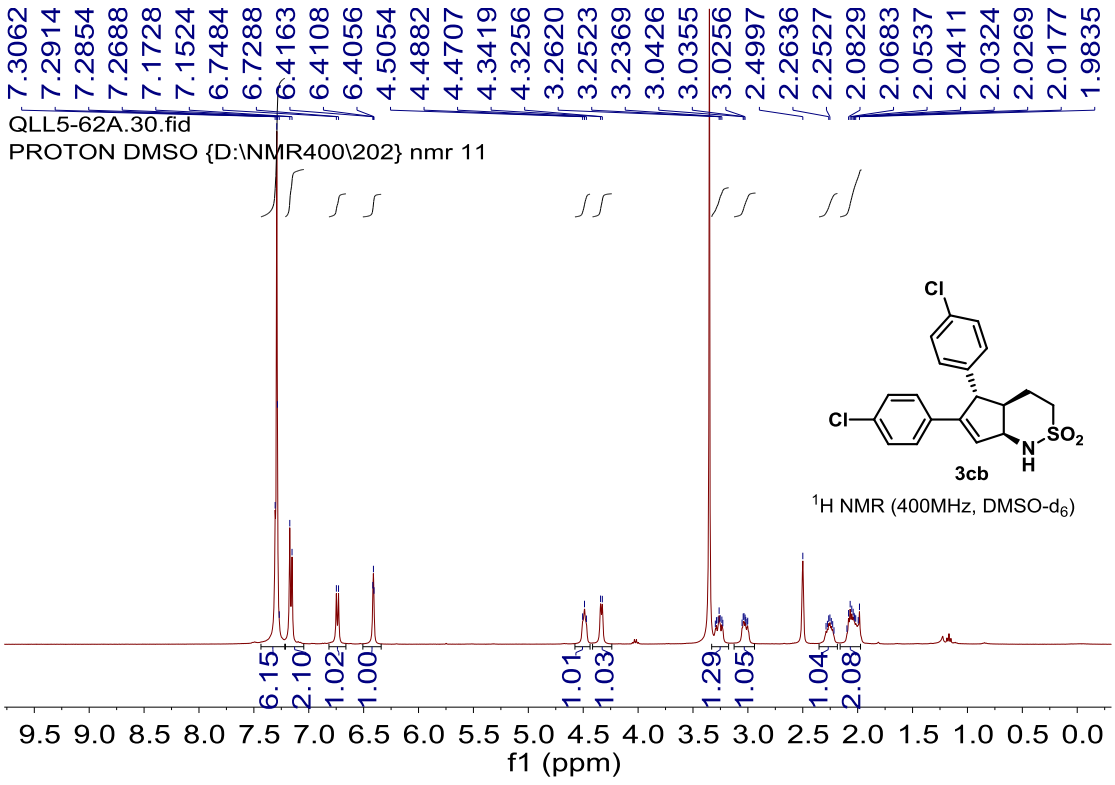

-111.09
-118.23
QLL2-89A
F19CPD CDCl3 {D:\NMR400\202} nmr 43
F
SO2
N
H
F
3na
19F NMR (376MHz, CDCl3)
10 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210
f1 (ppm)

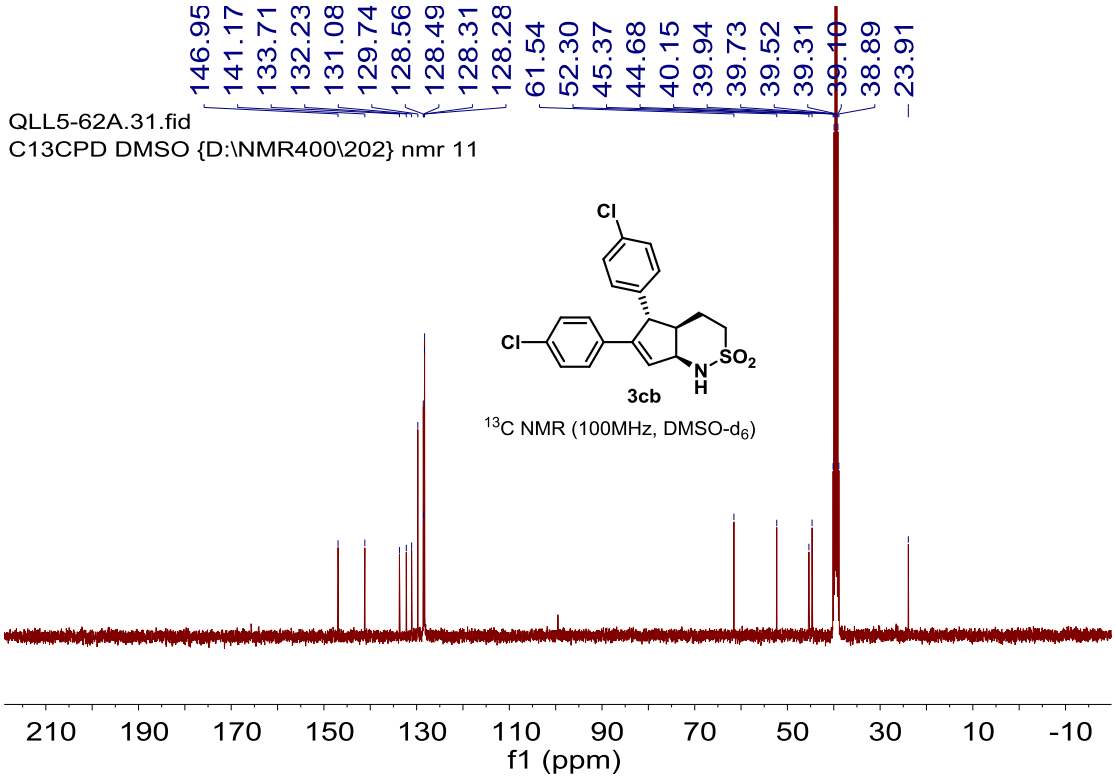

7.2558 7.2368 7.2313 7.1958 7.1828 7.0878 7.0699 6.3278 4.7185 4.7175 4.1952 4.1782 4.0563 4.0363 3.2901 3.2654 3.2561 3.2383 3.2309 3.1288 3.1131 3.1032 3.0948 3.0786 2.4921 2.4675 2.4577 2.4430 2.4321 2.2681 2.2443 2.2097 2.1980
QLL5-25D
PROTON CDCl3 {D:\NMR400\202} nmr 52
8.75 2.12 1.00 1.02 1.05 1.07 1.12 1.12 1.07 2.17
SO2
N
H
3ab
1H NMR (400MHz, CDCl3)
.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)

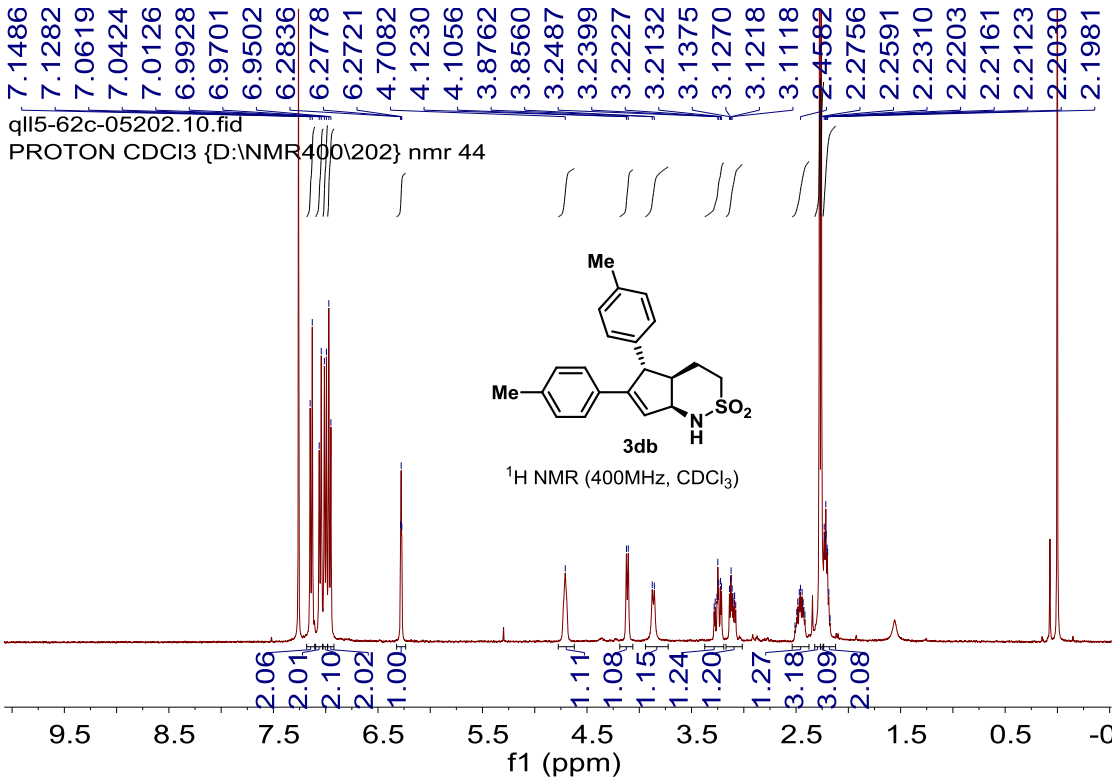

150.65
141.44
134.44
129.00
128.46
128.35
128.00
127.09
126.89
126.55
77.48
77.16
76.84
62.16
53.73
46.11
45.54
24.14
QLL5-25D
C13CPD CDCl3 {D:\NMR400\202} nmr 52
SO2
N
H
3ab
13C NMR (100MHz, CDCl3)
210 190 170 150 130 110 90 70 50 30 10 -10
f1 (ppm)

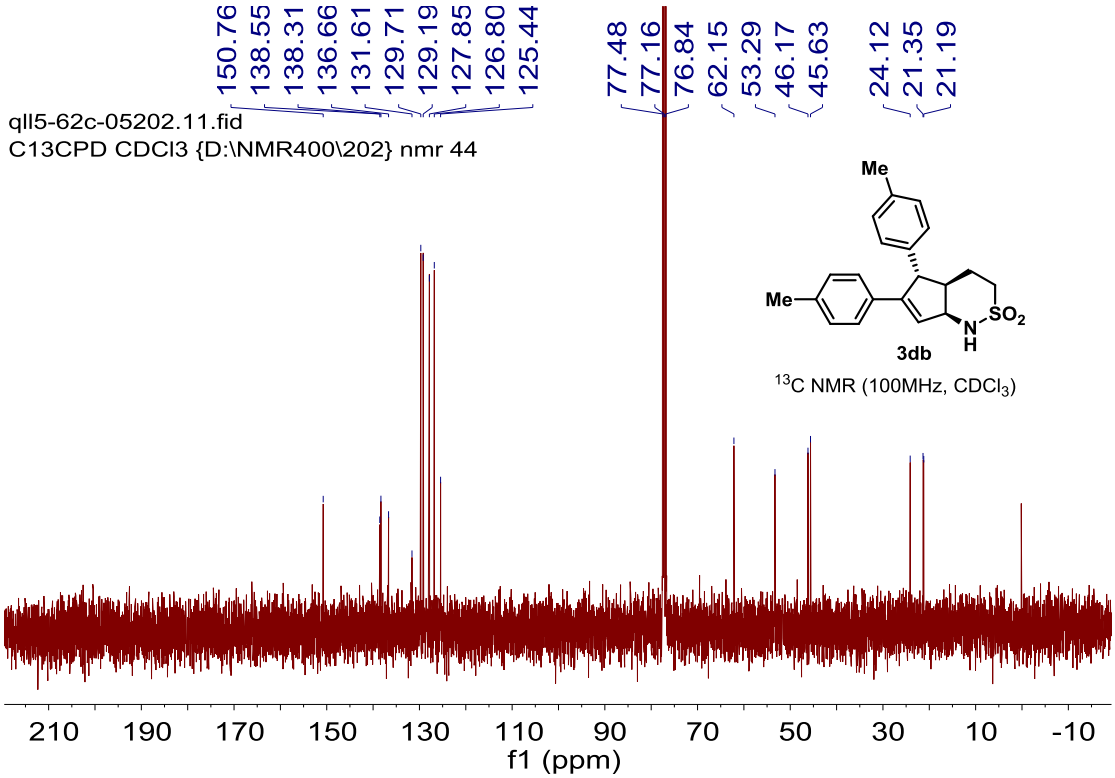

7.4371
7.4172
7.2298
7.2094
7.1088
7.0887
6.7459
6.7264
6.4168
4.4964
4.4787
4.4609
4.3247
4.3085
3.2824
3.2665
3.2570
3.2476
3.2322
3.0398
3.0331
3.0233
3.0160
3.0001
2.5004
2.2597
2.2490
2.2364
2.0770
2.0628
2.0404
2.0118
1.9906
QLL5-62B.30.fid
PROTON DMSO {D:\NMR400\202} nmr 12
Br
Br
SO2
N
H
3bb
1H NMR (400MHz, DMSO-d6)
4.28
2.10
2.07
1.04
1.00
1.05
1.07
1.23
1.11
1.05
2.11
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)

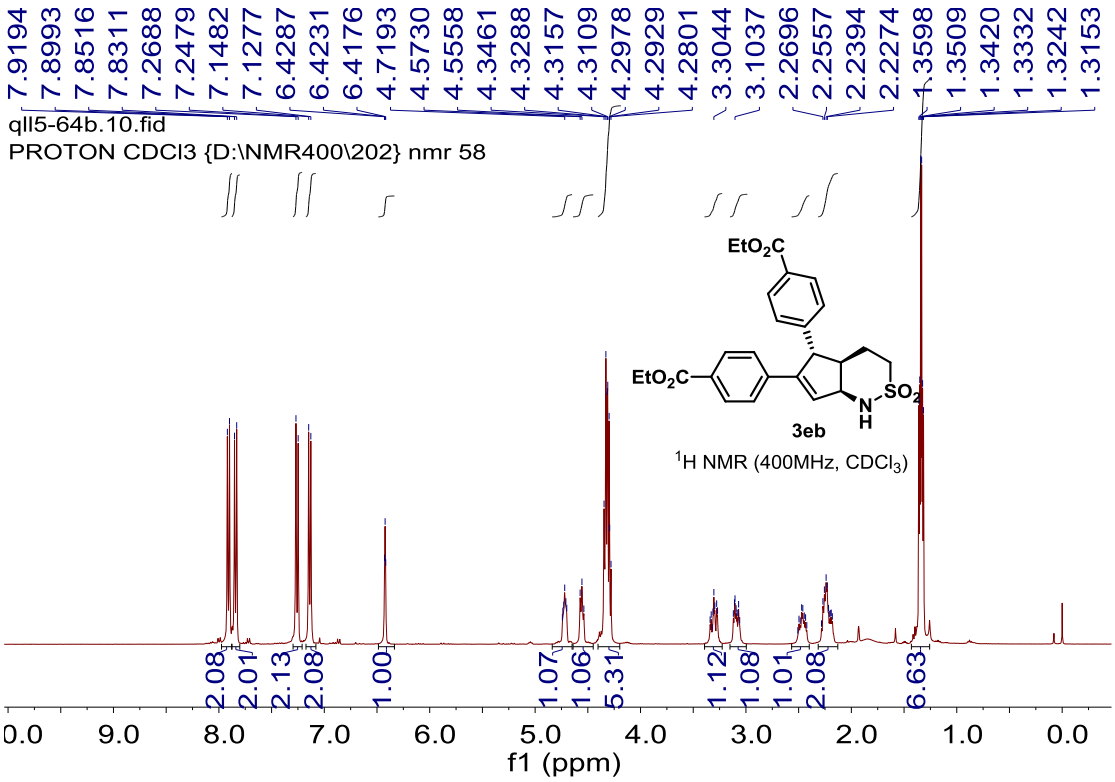

147.01
141.60
134.06
131.49
131.22
130.15
128.62
120.89
119.61
61.58
52.33
45.37
44.65
40.15
39.94
39.73
39.52
39.31
39.10
38.89
23.91
QLL5-62B.31.fid
C13CPD DMSO {D:\NMR400\202} nmr 12
Br
Br
SO2
N
H
3bb
13C NMR (100MHz, DMSO-d6)
210 190 170 150 130 110 90 70 50 30 10 -10
f1 (ppm)

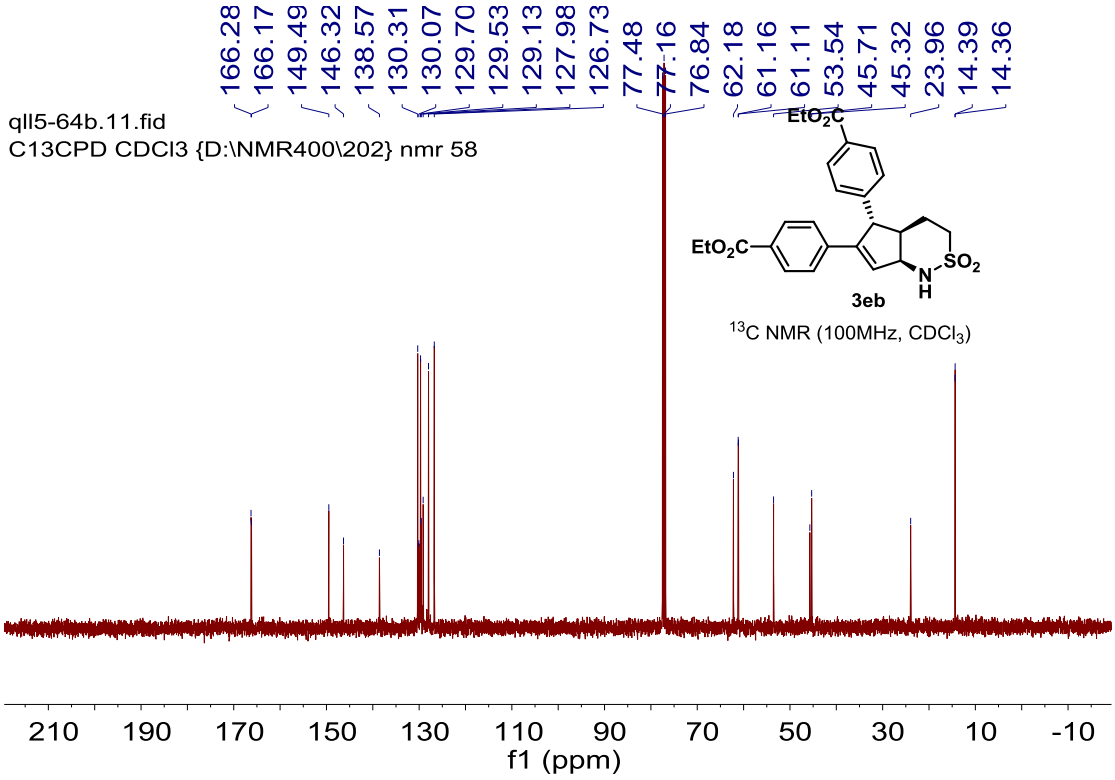

7.3062
7.2914
7.2854
7.2688
7.1728
7.1524
6.7484
6.7288
6.4163
6.4108
6.4056
4.5054
4.4882
4.4707
4.3419
4.3256
3.2620
3.2523
3.2369
3.0426
3.0355
3.0256
2.4997
2.2636
2.2527
2.0829
2.0683
2.0537
2.0411
2.0324
2.0269
2.0177
1.9835
QLL5-62A.30.fid
PROTON DMSO {D:\NMR400\202} nmr 11
Cl
Cl
SO2
N
H
3cb
1H NMR (400MHz, DMSO-d6)
6.15
2.10
1.02
1.00
1.01
1.03
1.29
1.05
1.04
2.08
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)

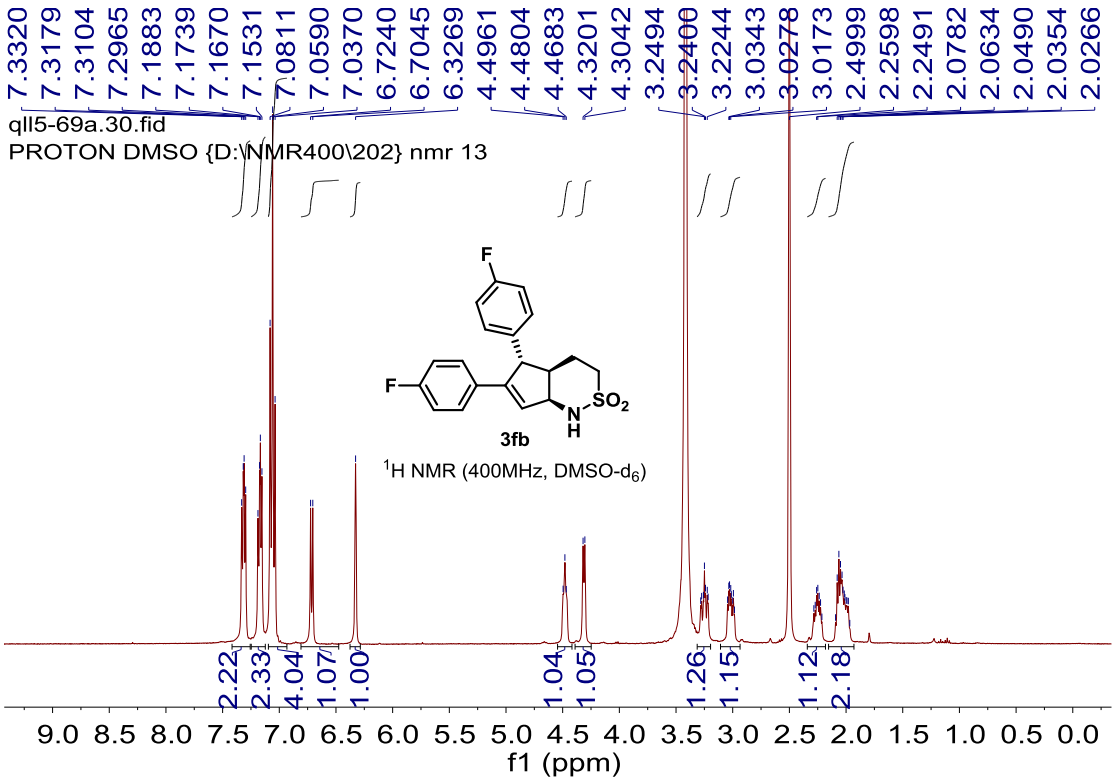

146.95
141.17
133.71
132.23
131.08
129.74
128.56
128.49
128.31
128.28
61.54
52.30
45.37
44.68
40.15
39.94
39.73
39.52
39.31
39.10
38.89
23.91
QLL5-62A.31.fid
C13CPD DMSO {D:\NMR400\202} nmr 11
Cl
Cl
SO2
N
H
3cb
13C NMR (100MHz, DMSO-d6)
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

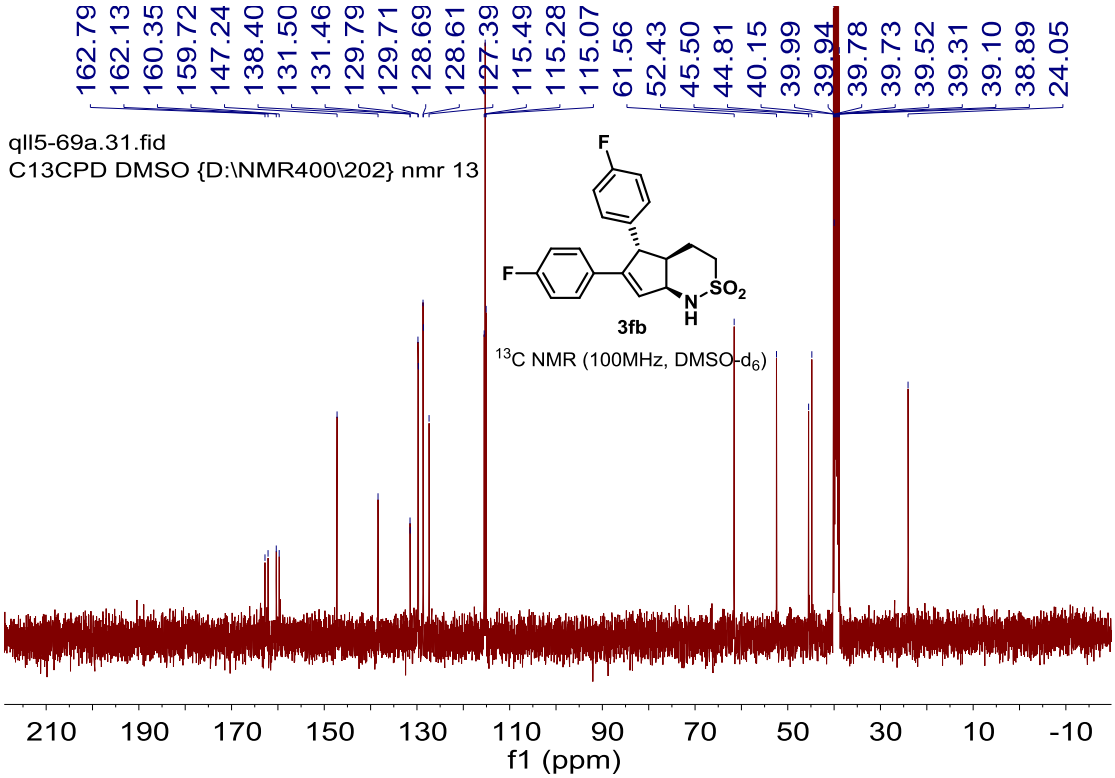

7.1486
7.1282
7.0619
7.0424
7.0126
6.9928
6.9701
6.9502
6.2836
6.2778
6.2721
4.7082
4.1230
4.1056
3.8762
3.8560
3.2487
3.2399
3.2227
3.2132
3.1375
3.1270
3.1218
3.1118
2.4582
2.2756
2.2591
2.2310
2.2203
2.2161
2.2123
2.2030
2.1981
qll5-62c-05202.10.fid
PROTON CDCl3 {D:\NMR400\202} nmr 44
Me
Me
SO2
N
H
3db
1H NMR (400MHz, CDCl3)
2.06
2.01
2.10
2.02
1.00
1.11
1.08
1.15
1.24
1.20
1.27
3.18
3.09
2.08
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

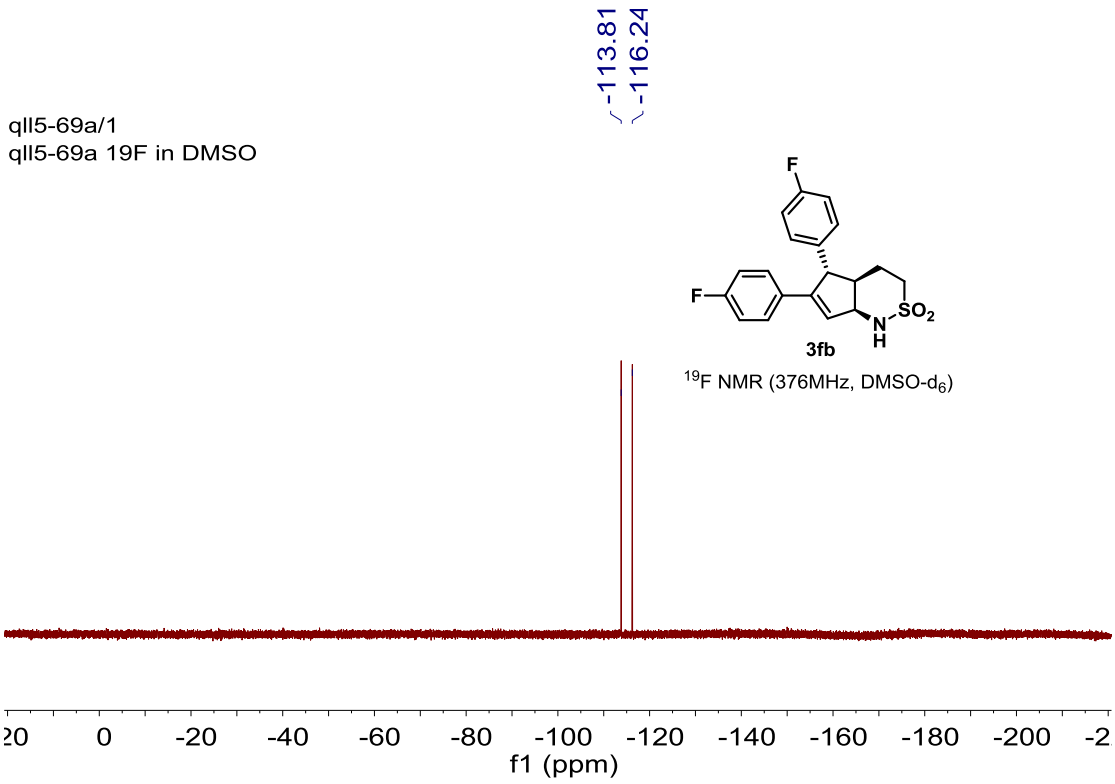

150.76
138.55
138.31
136.66
131.61
129.71
129.19
127.85
126.80
125.44
77.48
77.16
76.84
62.15
53.29
46.17
45.63
24.12
21.35
21.19
qll5-62c-05202.11.fid
C13CPD CDCl3 {D:\NMR400\202} nmr 44
Me
Me
SO2
N
H
3db
13C NMR (100MHz, CDCl3)
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

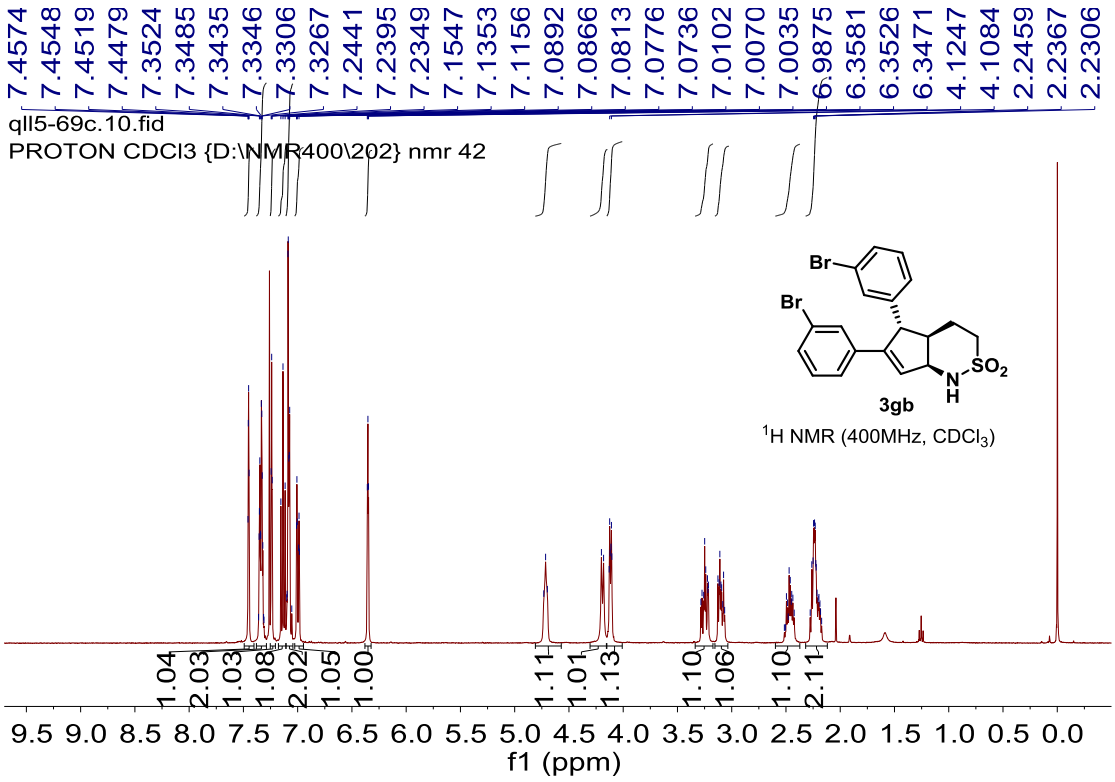

7.9194
7.8993
7.8516
7.8311
7.2688
7.2479
7.1482
7.1277
6.4287
6.4231
6.4176
4.7193
4.5730
4.5558
4.3461
4.3288
4.3157
4.3109
4.2978
4.2929
4.2801
3.3044
3.1037
2.2696
2.2557
2.2394
2.2274
1.3598
1.3509
1.3420
1.3332
1.3242
1.3153
qll5-64b.10.fid
PROTON CDCl3 {D:\NMR400\202} nmr 58
EtO2C
EtO2C
SO2
N
H
3eb
1H NMR (400MHz, CDCl3)
2.08
2.01
2.13
2.08
1.00
1.07
1.06
5.31
1.12
1.08
1.01
2.08
6.63
0.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

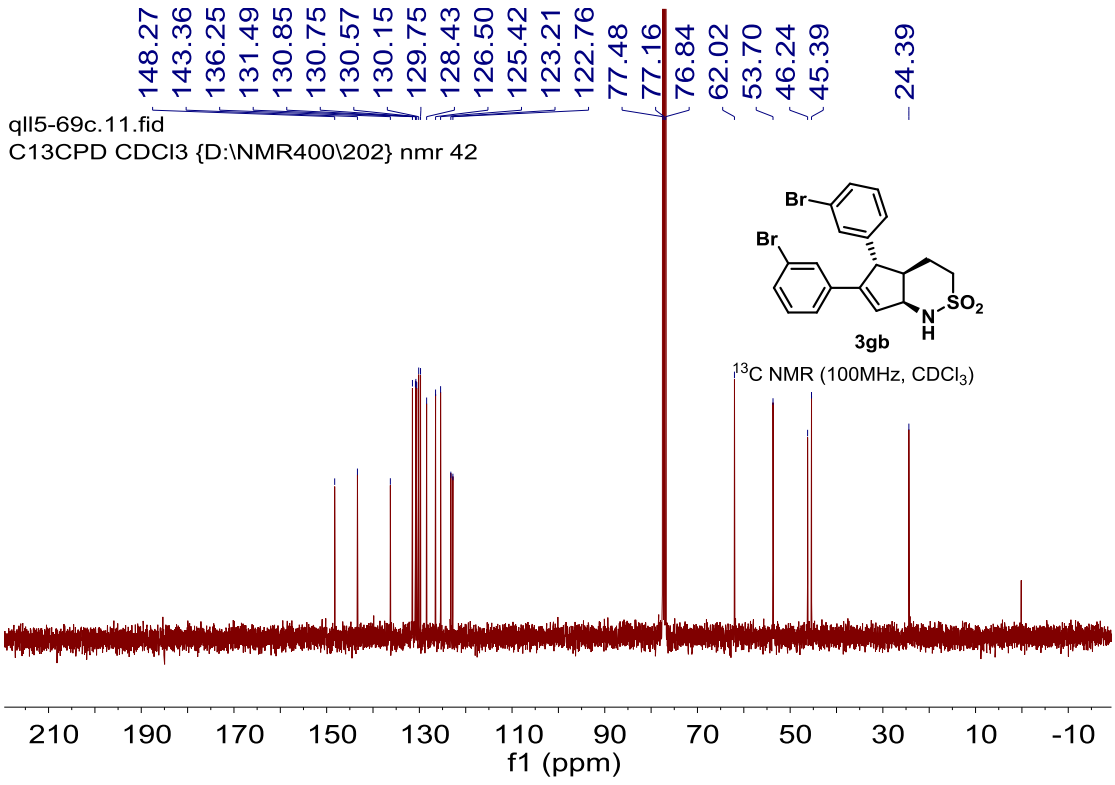

166.28
166.17
149.49
146.32
138.57
130.31
130.07
129.70
129.53
129.13
127.98
126.73
77.48
77.16
76.84
62.18
61.16
61.11
53.54
45.71
45.32
23.96
14.39
14.36
qll5-64b.11.fid
C13CPD CDCl3 {D:\NMR400\202} nmr 58
EtO2C
EtO2C
SO2
N
H
3eb
13C NMR (100MHz, CDCl3)
210 190 170 150 130 110 90 70 50 30 10 -10
f1 (ppm)

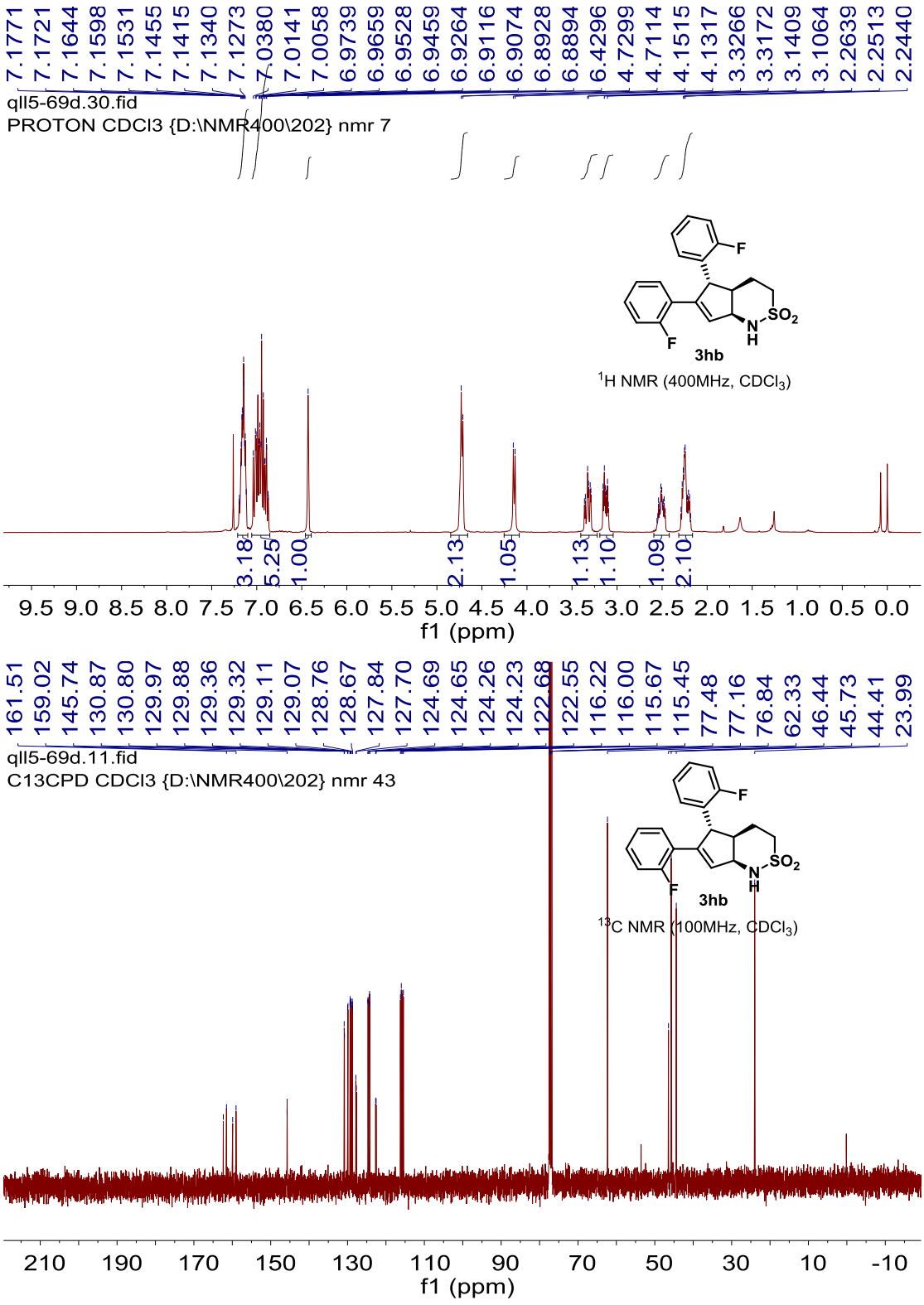

7.3320
7.3179
7.3104
7.2965
7.1883
7.1739
7.1670
7.1531
7.0811
7.0590
7.0370
6.7240
6.7045
6.3269
4.4961
4.4804
4.4683
4.3201
4.3042
3.2494
3.2400
3.2244
3.0343
3.0278
3.0173
2.4999
2.2598
2.2491
2.0782
2.0634
2.0490
2.0354
2.0266
qll5-69a.30.fid
PROTON DMSO {D:\NMR400\202} nmr 13
F
F
SO2
N
H
3fb
1H NMR (400MHz, DMSO-d6)
2.22
2.33
4.04
1.07
1.00
1.04
1.05
1.26
1.15
1.12
2.18
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)

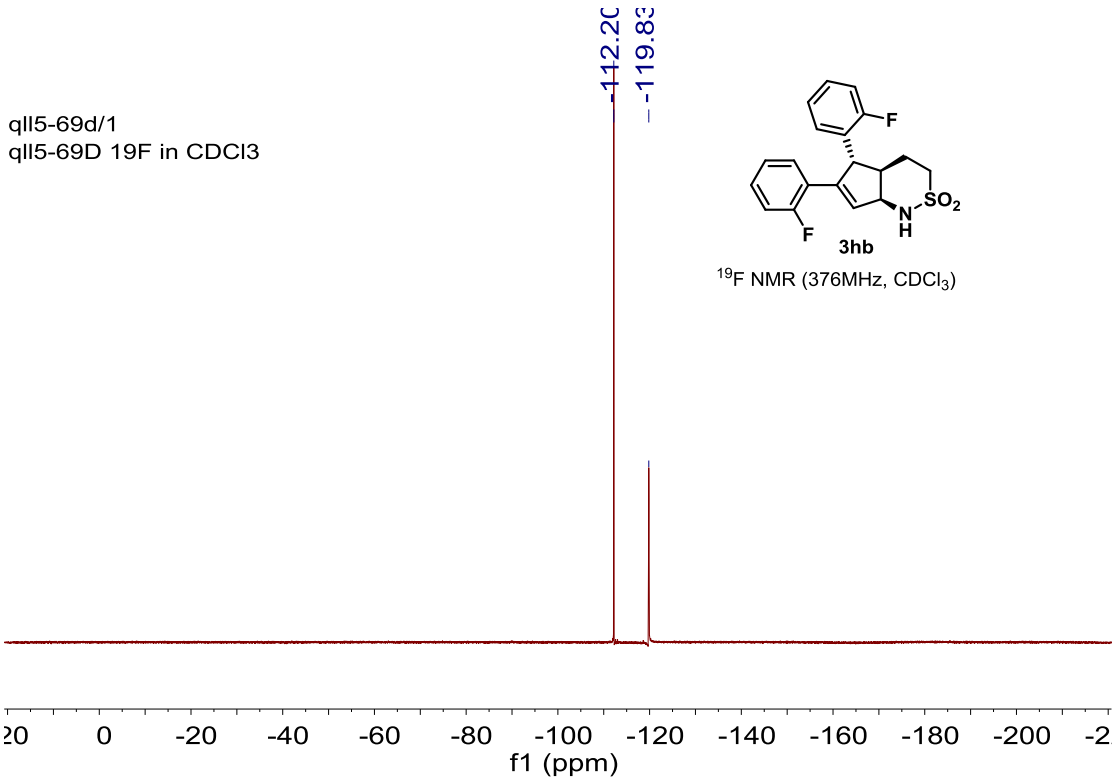

162.79
162.13
160.35
159.72
147.24
138.40
131.50
131.46
129.79
129.71
128.69
128.61
127.39
115.49
115.28
115.07
61.56
52.43
45.50
44.81
40.15
39.99
39.94
39.78
39.73
39.52
39.31
39.10
38.89
24.05
qll5-69a.31.fid
C13CPD DMSO {D:\NMR400\202} nmr 13
F
F
SO2
N
H
3fb
13C NMR (100MHz, DMSO-d6)
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

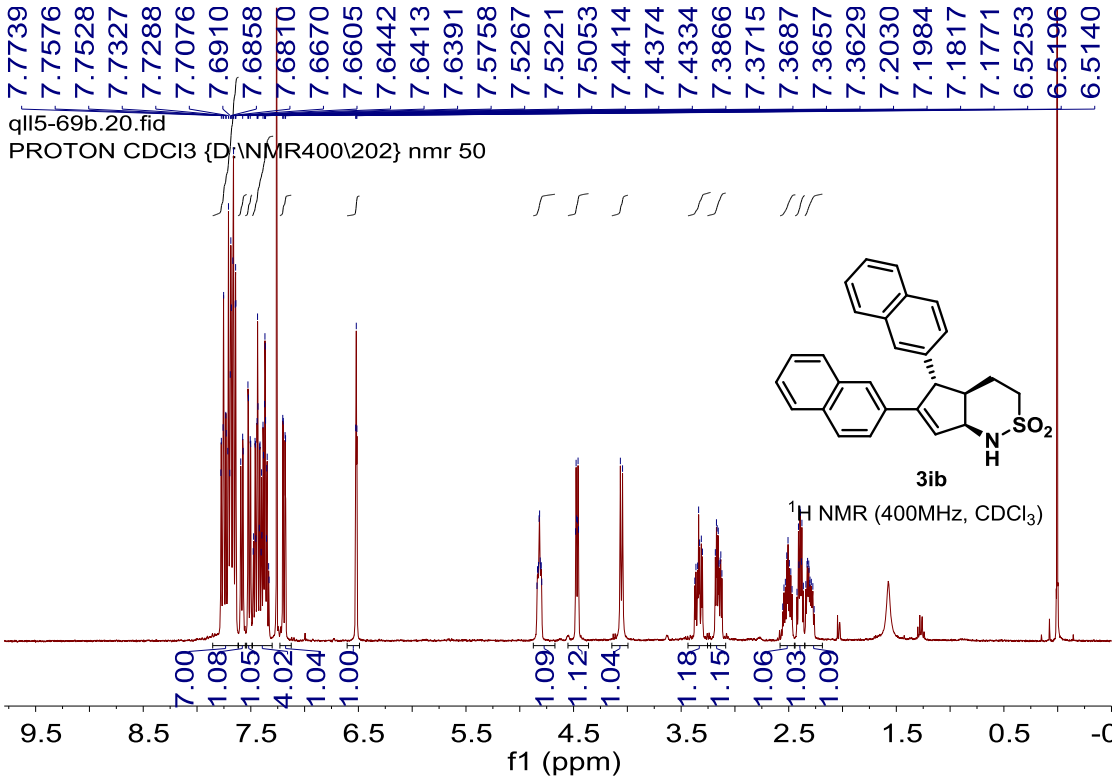

-113.81
-116.24
qll5-69a/1
qll5-69a 19F in DMSO
F
F
SO2
N
H
3fb
19F NMR (376MHz, DMSO-d6)
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-2
f1 (ppm)

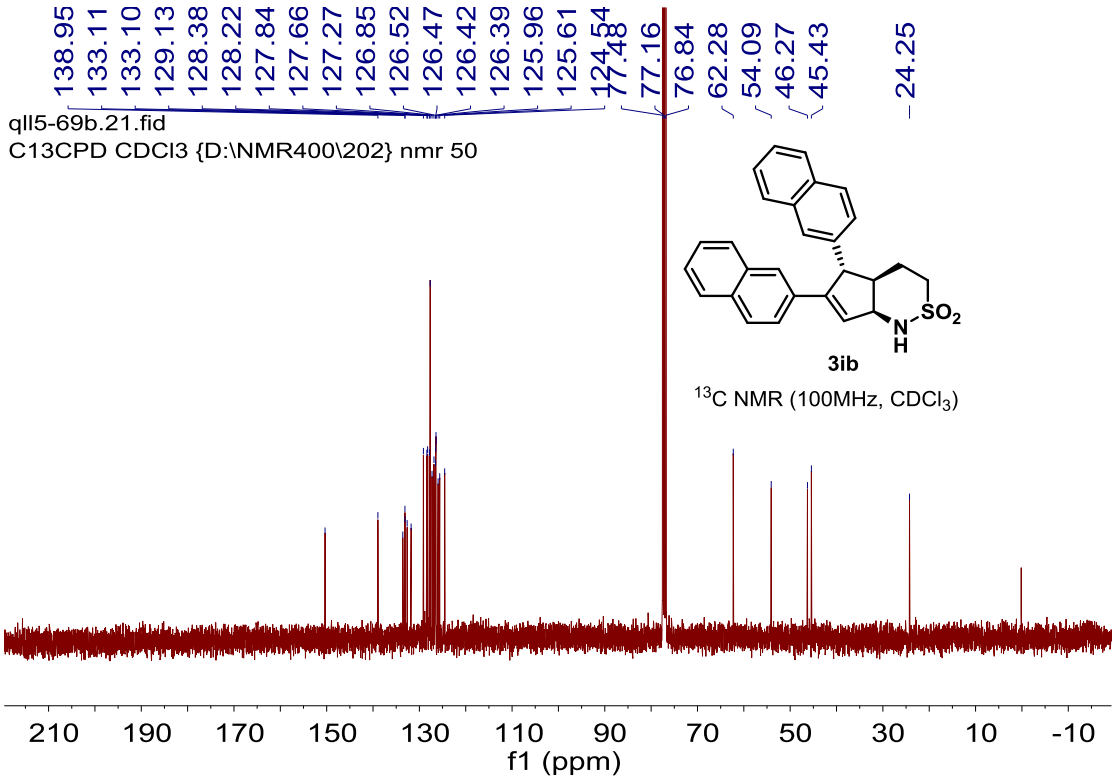

7.4574
7.4548
7.4519
7.4479
7.3524
7.3485
7.3435
7.3346
7.3306
7.3267
7.2441
7.2395
7.2349
7.1547
7.1353
7.1156
7.0892
7.0866
7.0813
7.0776
7.0736
7.0102
7.0070
7.0035
6.9875
6.3581
6.3526
6.3471
4.1247
4.1084
2.2459
2.2367
2.2306
qll5-69c.10.fid
PROTON CDCl3 {D:\NMR400\202} nmr 42
Br
Br
SO2
N
H
3gb
1H NMR (400MHz, CDCl3)
1.04
2.03
1.03
1.08
2.02
1.05
1.00
1.11
1.01
1.13
1.10
1.06
1.10
2.11
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)

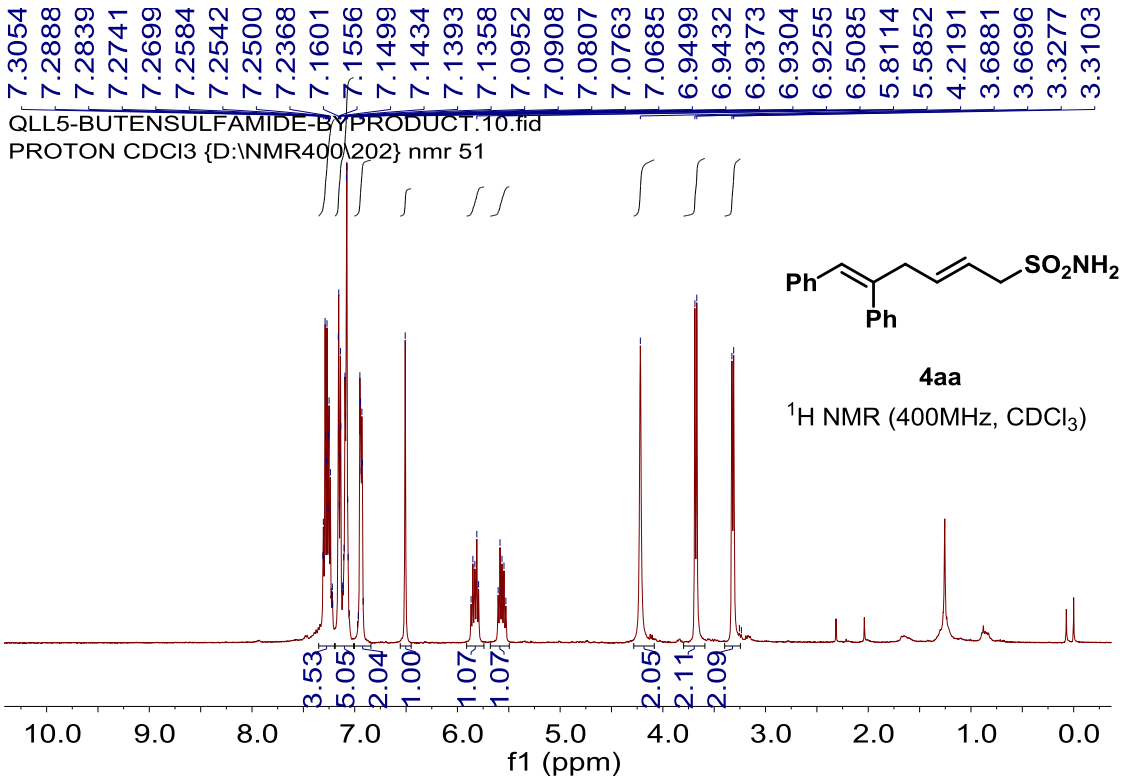

148.27
143.36
136.25
131.49
130.85
130.75
130.57
130.15
129.75
128.43
126.50
125.42
123.21
122.76
77.48
77.16
76.84
62.02
53.70
46.24
45.39
24.39
qll5-69c.11.fid
C13CPD CDCl3 {D:\NMR400\202} nmr 42
Br
Br
SO2
N
H
3gb
13C NMR (100MHz, CDCl3)
210 190 170 150 130 110 90 70 50 30 10 -10
f1 (ppm)

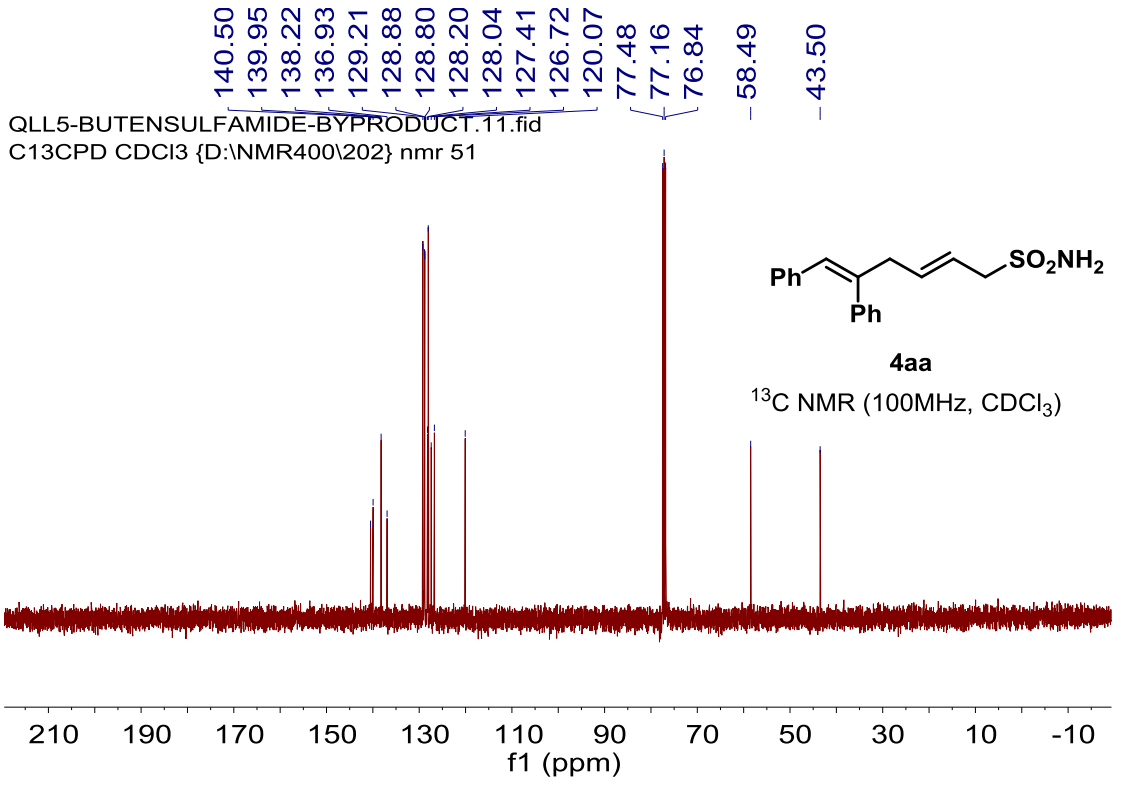

7.1771 7.1721 7.1644 7.1598 7.1531 7.1455 7.1415 7.1340 7.1273 7.0380 7.0141 7.0058 6.9739 6.9659 6.9528 6.9459 6.9264 6.9116 6.9074 6.8928 6.8894 6.4296 4.7299 4.7114 4.1515 4.1317 3.3266 3.3172 3.1409 3.1064 2.2639 2.2513 2.2440
qll5-69d.30.fid
PROTON CDCl3 {D:\NMR400\202} nmr 7
3hb
1H NMR (400MHz, CDCl3)
3.18 5.25 1.00 2.13 1.05 1.13 1.10 1.09 2.10
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)
161.51 159.02 145.74 130.87 130.80 129.97 129.88 129.36 129.32 129.11 129.07 128.76 128.67 127.84 127.70 124.69 124.65 124.26 124.23 122.68 122.55 116.22 116.00 115.67 115.45 77.48 77.16 76.84 62.33 46.44 45.73 44.41 23.99
qll5-69d.11.fid
C13CPD CDCl3 {D:\NMR400\202} nmr 43
3hb
13C NMR (100MHz, CDCl3)
210 190 170 150 130 110 90 70 50 30 10 -10
f1 (ppm)

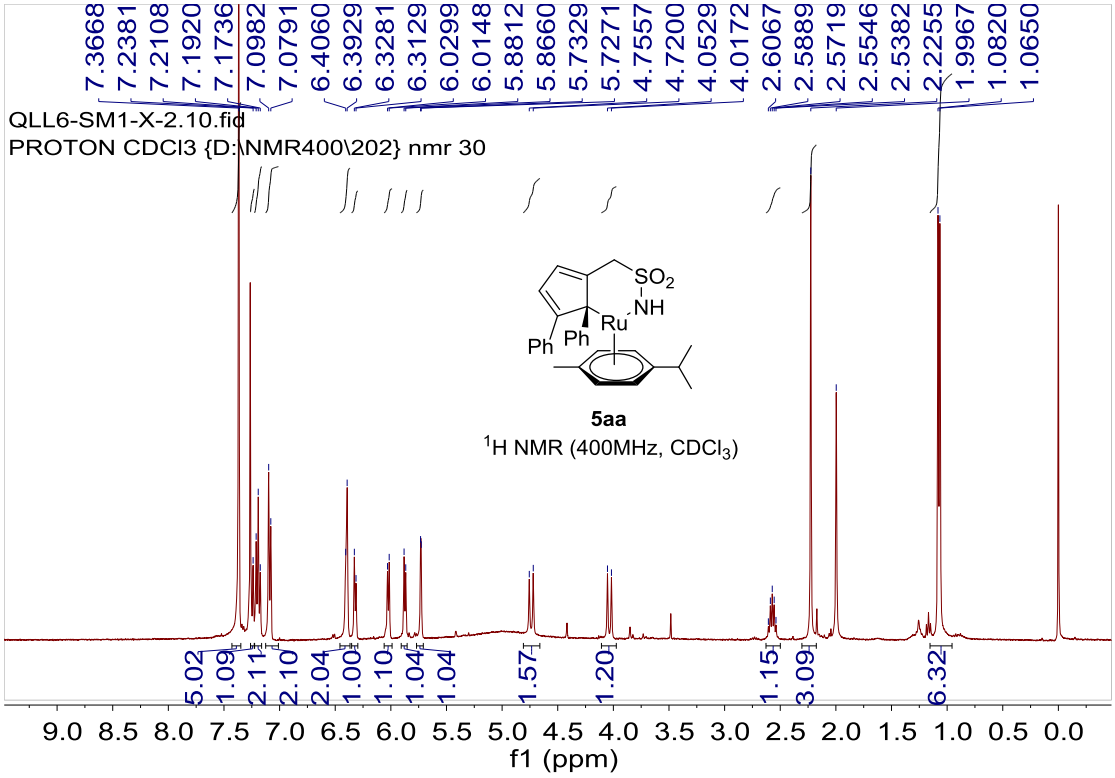

qll5-69d/1
qll5-69D 19F in CDCl3
-112.20
-119.83
F
F
N
H
SO2
3hb
19F NMR (376MHz, CDCl3)
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-2
f1 (ppm)

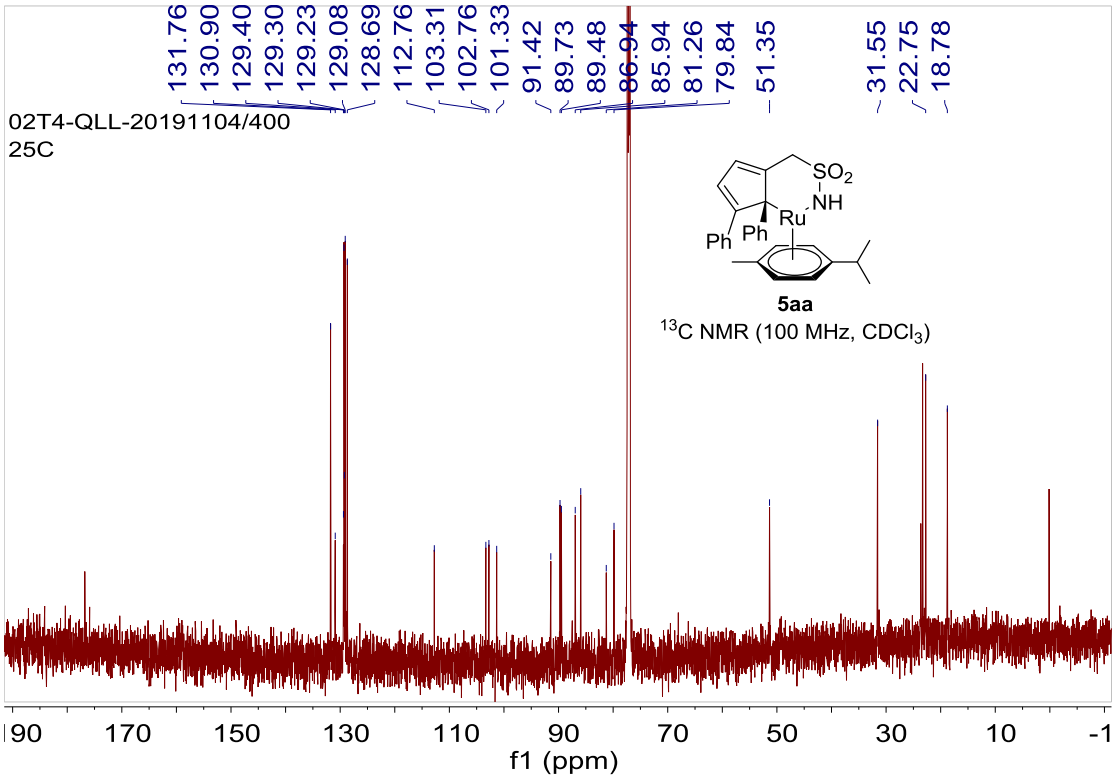

7.7739
7.7576
7.7528
7.7327
7.7288
7.7076
7.6910
7.6858
7.6810
7.6670
7.6605
7.6442
7.6413
7.6391
7.5758
7.5267
7.5221
7.5053
7.4414
7.4374
7.4334
7.3866
7.3715
7.3687
7.3657
7.3629
7.2030
7.1984
7.1817
7.1771
6.5253
6.5196
6.5140
qll5-69b.20.fid
PROTON CDCl3 {D:\NMR400\202} nmr 50
7.00
1.08
1.05
4.02
1.04
1.00
1.09
1.12
1.04
1.18
1.15
1.06
1.03
1.09
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)
SO2
N
H
3ib
1H NMR (400MHz, CDCl3)

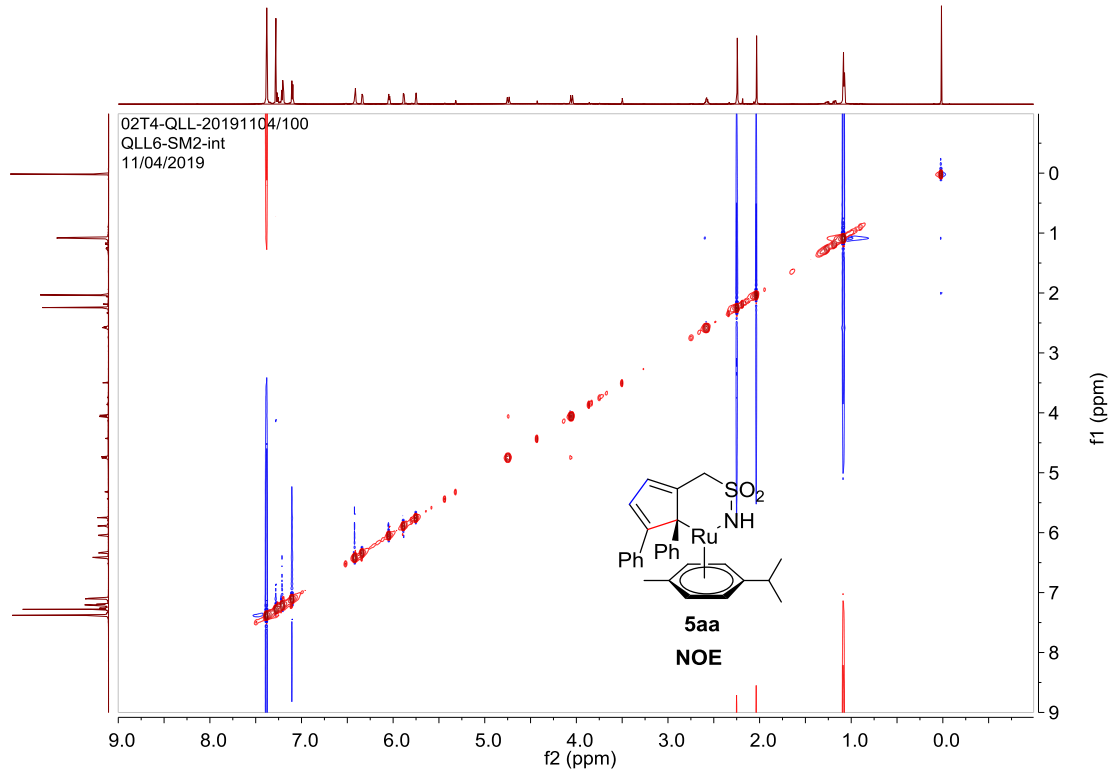

138.95
133.11
133.10
129.13
128.38
128.22
127.84
127.66
127.27
126.85
126.52
126.47
126.42
126.39
125.96
125.61
124.54
77.48
77.16
76.84
62.28
54.09
46.27
45.43
24.25
qll5-69b.21.fid
C13CPD CDCl3 {D:\NMR400\202} nmr 50
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)
SO2
N
H
3ib
13C NMR (100MHz, CDCl3)

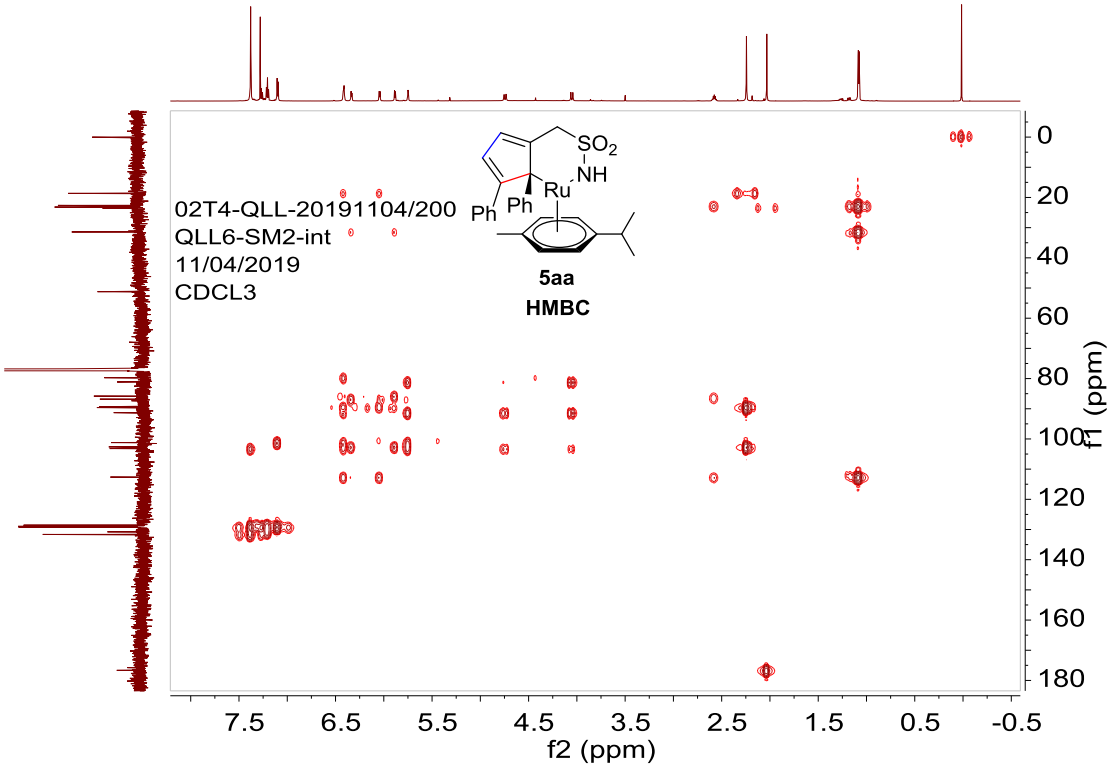

7.3054
7.2888
7.2839
7.2741
7.2699
7.2584
7.2542
7.2500
7.2368
7.1601
7.1556
7.1499
7.1434
7.1393
7.1358
7.0952
7.0908
7.0807
7.0763
7.0685
6.9499
6.9432
6.9373
6.9304
6.9255
6.5085
5.8114
5.5852
4.2191
3.6881
3.6696
3.3277
3.3103
QLL5-BUTENSULFAMIDE-BYPRODUCT.10.fid
PROTON CDCl3 {D:\NMR400\202} nmr 51
Ph
Ph
SO2NH2
4aa
1H NMR (400MHz, CDCl3)
3.53
5.05
2.04
1.00
1.07
1.07
2.05
2.11
2.09
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

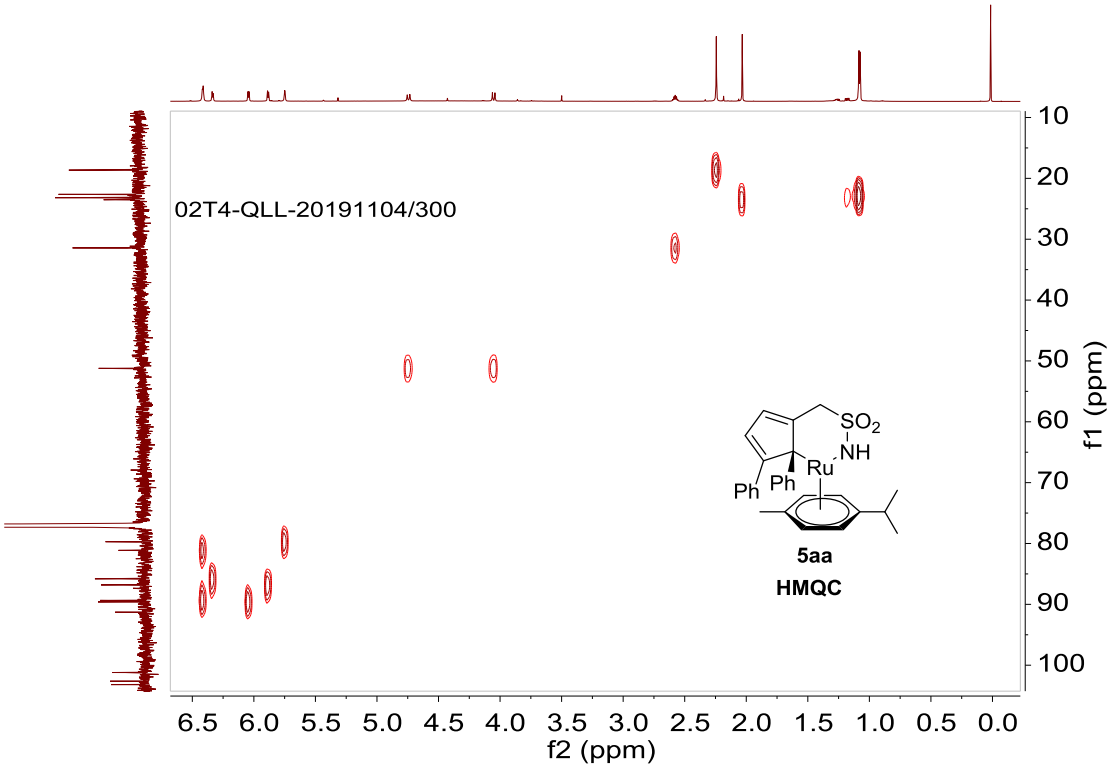

140.50
139.95
138.22
136.93
129.21
128.88
128.80
128.20
128.04
127.41
126.72
120.07
77.48
77.16
76.84
58.49
43.50
QLL5-BUTENSULFAMIDE-BYPRODUCT.11.fid
C13CPD CDCl3 {D:\NMR400\202} nmr 51
Ph
Ph
SO2NH2
4aa
13C NMR (100MHz, CDCl3)
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

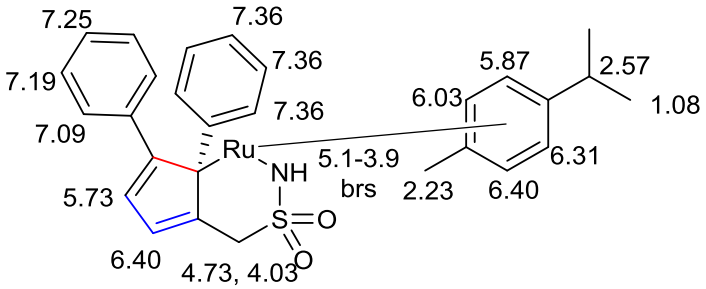

7.3668
7.2381
7.2108
7.1920
7.1736
7.0982
7.0791
6.4060
6.3929
6.3281
6.3129
6.0299
6.0148
5.8812
5.8660
5.7329
5.7271
4.7557
4.7200
4.0529
4.0172
2.6067
2.5889
2.5719
2.5546
2.5382
2.2255
1.9967
1.0820
1.0650
QLL6-SM1-X-2.10.fid
PROTON CDCl3 {D:\NMR400\202} nmr 30
SO2
NH
Ru
Ph
Ph
5aa
1H NMR (400MHz, CDCl3)
5.02
1.09
2.11
2.10
2.04
1.00
1.10
1.04
1.04
1.57
1.20
1.15
3.09
6.32
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)


131.76
130.90
129.40
129.30
129.23
129.08
128.69
112.76
103.31
102.76
101.33
91.42
89.73
89.48
86.94
85.94
81.26
79.84
51.35
31.55
22.75
18.78
02T4-QLL-20191104/400
25C
SO2
NH
Ru
Ph
Ph
5aa
13C NMR (100 MHz, CDCl3)
90 170 150 130 110 90 70 50 30 10 -1
f1 (ppm)


02T4-QLL-20191104/100
QLL6-SM2-int
11/04/2019
SO2
NH
Ru
Ph
Ph
5aa
NOE
f2 (ppm)
f1 (ppm)

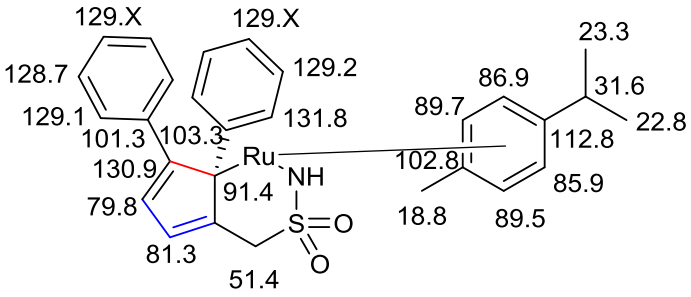

02T4-QLL-20191104/200
QLL6-SM2-int
11/04/2019
CDCL3
SO2
NH
Ru
Ph
Ph
5aa
HMBC
f2 (ppm)
f1 (ppm)





5aa

^{1}H NMR (400MHz, $CDCl_3$)



5aa

^{13}C NMR (100 MHz, $CDCl_3$)