Supporting Information

Sulfinates and thiocyanates triggered 6-*endo* cyclization of *o*-alkynylisocyanobenzenes

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Experimental section

General information:

^{1}H NMR spectra were recorded with a Bruker AVANCE 400 spectrometer (400 MHz) in $CDCl_3$ by using tetramethylsilane (δ = 0 ppm) or residual non-deuterated solvent peak as an internal standard. ^{13}C NMR spectra were recorded with a Bruker AVANCE 400 (100 MHz) spectrometer. Infrared spectra were recorded with a Bruker ALPHA FT-IR spectrometer and only partial data were listed. High-Resolution Mass Spectra (HRMS) were recorded with a Bruker micro TOF spectrometer in the ESI mode. Melting points were recorded with a Sanyo Gallenkamp apparatus. Reactions were monitored by Thin-Layer Chromatography and visualized by UV and a solution of $KMnO_4$. *N*-(2-Arylethynyl)phenyl)formamides and *N*-(2-alkylethynyl)phenyl)formamides were synthesized according to literature procedures. The structures of known compounds were confirmed by comparing their ^{1}H NMR and ^{13}C NMR data with those in the literature. All reagents and solvents were obtained from commercial sources and used without further purification. Column chromatography was performed by using Merck silica gel 60 (Art 7734).

General procedure for the synthesis of *N*-(2-(arylethynyl)phenyl)formamides and *N*-(2-(alkylethynyl)phenyl)formamides 1

To a round-bottom flask filled with formic acid (1.5 mL) was added Ac_2O (2 mL) at room temperature, and the resulting mixture was stirred for 10 minutes. To this mixture was added the solution of 2-iodoaniline derivatives (10 mmol) in CH_2Cl_2 (8 mL) then the reaction chamber was stirred for 2 hours at room temperature. After completion, the reaction was quenched with H_2O (5 mL) and the resulting mixture was extracted with CH_2Cl_2 (3 × 10 mL). The combined organic layers were washed with brine (20 mL), dried ($MgSO_4$), filtered, and concentrated (aspirator). Crude product was purified by column chromatography on silica gel (hexanes/ethyl acetate) to yield the corresponding *N*-(2-iodoaryl)formamide. The obtained *N*-(2-iodoaryl)formamide was subjected to coupling reaction in the next step. To the two-neck flask containing *N*-(2-iodoaryl)formamide (50 mmol), $PdCl_2(PPh_3)_2$ (0.65 mmol), and CuI (0.5 mmol) was added THF (60 mL) and NEt_3 (60 mL) under argon atmosphere. Then, monosubstituted acetylene (75 mmol) was added dropwise to reaction mixture. The reaction was allowed to stir at room temperature under Ar atmosphere for overnight. After completion, the reaction was quenched with diluted HCl solution (20 mL) and the resulting mixture was extracted with ethyl acetate (3 × 20 mL). The combined organic layers were washed with brine (20 mL), dried over $MgSO_4$, filtered, and concentrated (aspirator). Crude product was purified by column chromatography on silica gel (hexane/ethyl acetate) to provide the corresponding *N*-(2-(arylethynyl)phenyl)formamide or *N*-(2-(alkylethynyl)phenyl)formamide **1**.

General procedure for the synthesis of *o*-alkynylisocyanobenzenes 2

To a solution of *N*-(2-(arylethynyl)phenyl)formamide or *N*-(2-(alkylethynyl)phenyl)formamide **1** (0.5 mmol) and diisopropylethylamine (4.0 mmol) in CH_2Cl_2 (4 mL) was added dropwise $POCl_3$ (0.75 mmol) at 0 ^{o}C under argon atmosphere. The reaction mixture was stirred at 0 °C for 30–60 minutes. After completion, the reaction was quenched with $NaHCO_3$ (5 mL) and the resulting mixture was extracted with CH_2Cl_2 (3 × 10 mL). The combined organic layers were washed with brine (20 mL), dried ($MgSO_4$), filtered, and concentrated (aspirator). Crude product was filtered through a short-

path layer of aluminium oxide 60 PF_{254} (Type E), (eluted with 100% ethyl acetate) to provide the corresponding *o*-alkynylisocyanobenzene **2** which were subsequently used in the next step.

General Procedure for the Synthesis of 2-sulfonyl- and 2-thiocyanato-3-substituted quinolines 4 and 6

To a round-bottomed flask filled with *o*-alkynylisocyanobenzene **2** (freshly prepared from the corresponding *N*-(2-(arylethynyl)phenyl)formamide or *N*-(2-(alkynyl)phenyl)formamide (0.5 mmol) was diluted with DMF (2 mL). To this mixture was added sulfur nucleophiles (1.0 mmol, 2.0 equiv). The reaction mixture was stirred at room temperature for overnight (O/N, 17–18 h). After completion, the reaction mixture was diluted with H_2O (5 mL) and the resulting mixture was extracted with ethyl acetate (3 × 10 mL). The combined organic layers were washed with brine (20 mL), dried ($MgSO_4$), filtered, and concentrated (aspirator). Crude product was purified by column chromatography on silica gel (hexanes/ethyl acetate) to yield the corresponding 2-sulfonyl- and 2-thiocyanato-3-substituted quinolines (**4** and **6**).

Characterization data of compounds 4 and 6

***3-Phenyl-2-tosylquinoline (4aa)*:** white solid (146 mg, 81%); mp = 155.0−156.5 °C (from CH_2Cl_2/hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.10 (d, J = 8.0 Hz, 1H), 8.10 (s, 1H), 7.82 (d, J = 8.2 Hz, 1H), 7.77-7.73 (m, 1H), 7.66-7.62 (m, 1H), 7.60 (d, J = 8.3 Hz, 2H), 7.43−7.38 (m, 5H), 7.18 (d, J = 8.1 Hz, 2H), 2.39 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 155.9, 145.1, 144.0, 140.5, 136.4, 136.3, 133.4, 130.6, 130.0, 129.3, 129.0, 129.0, 128.4, 128.1, 127.7, 127.3, 21.5 ppm; IR (neat): 1310, 1128, 1072 (SO_2) cm^{-1}; HRMS (ESI-TOF) *m/z* [M + H]$^+$ calcd for $C_{22}H_{18}NO_2S$ 360.1058, found 360.1062.

***2-((4-Methoxyphenyl)sulfonyl)-3-phenylquinoline (4ab)*:** pale yellow solid (94 mg, 50%); mp = 122.2−124.5 °C (from CH_2Cl_2/hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.13−8.11 (m, 2H), 7.84 (d, J = 8.2 Hz, 1H), 7.79−7.75 (m, 1H), 7.68−7.63 (m, 3H), 7.44−7.40 (m, 5H), 6.86 (d, J = 8.9 Hz, 2H), 3.84 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 163.4, 156.2, 145.2, 140.5, 136.6, 133.4, 131.3, 130.7, 130.6, 130.1, 129.2, 128.4, 128.2, 127.7, 127.3, 113.6, 55.6 ppm; IR (neat): 1305, 1105, 1074 (SO_2) cm^{-1}; HRMS (ESI-TOF) *m/z* [M + Na]$^+$ calcd for $C_{22}H_{17}NO_3SNa$ 398.0827, found 398.0825.

***2-((4-Chlorophenyl)sulfonyl)-3-phenylquinoline (4ac)*:** pale yellow solid (129 mg, 68%); mp = 124.0−126.0 °C (from CH_2Cl_2/hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.14 (s, 1H), 8.05 (d, J = 8.6 Hz, 1H), 7.84 (d, J = 8.2 Hz, 1H), 7.78−7.74 (m, 1H), 7.70−7.63 (m, 3H), 7.45−7.41 (m, 5H), 7.39−7.36 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 155.5, 145.0, 140.6, 139.8, 137.7, 136.1, 133.2, 130.8, 130.5, 130.0, 129.9, 129.5, 128.6, 128.4, 128.3, 127.8, 127.3 ppm; IR (neat): 1311, 1157, 1076 (SO_2) cm^{-1}; HRMS (ESI-TOF) *m/z* [M + Na]$^+$ calcd for $C_{21}H_{14}ClNO_2S$ Na 402.0331, found 402.0337.

***2-((4-Bromophenyl)sulfonyl)-3-phenylquinoline (4ad)*:** pale yellow solid (138 mg, 65%); mp = 154.8−156.0 °C (from CH_2Cl_2/hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.15 (s, 1H), 8.07 (d, J = 8.5 Hz, 1H), 7.84 (d, J = 8.1 Hz, 1H), 7.78−7.74 (m, 1H), 7.68−7.66 (m, 1H), 7.64−7.61 (m, 2H), 7.56−7.53 (m, 2H), 7.46−7.40 (m, 5H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 155.6, 145.2, 140.7, 138.4, 136.3, 133.4, 131.7, 130.9, 130.8, 130.1, 130.0, 129.6, 128.6, 128.5, 128.0, 127.5 ppm; IR (neat): 1311, 1156, 1067 (SO_2) cm^{-1}; HRMS (ESI-TOF) *m/z* [M + H]$^+$ calcd for $C_{21}H_{15}BrNO_2S$ 424.0007, found 424.0008.

***2-((4-Nitrophenyl)sulfonyl)-3-phenylquinoline (4ae)*:** pale yellow needle (111 mg, 56%); mp = 195.0−196.5 °C (from CH_2Cl_2/hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.28 (d, J = 8.9 Hz, 2H), 8.22 (s, 1H), 8.02−7.96 (m, 3H), 7.89 (d, J = 8.2 Hz, 1H), 7.78 (t, J = 8.4 Hz, 1H), 7.71 (t, J = 4.0 Hz, 1H), 7.51−7.45 (m, 5H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 155.1, 150.4, 145.1, 144.9, 140.8, 135.7, 133.2,

131.0, 130.6, 130.0, 129.8, 129.8, 128.7, 128.6, 128.1, 127.5, 123.4 ppm; IR (neat): 1306, 1158, 1076 (SO_2) cm^{-1}; HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{21}H_{15}N_2O_4S$ 391.0753, found 391.0752.

***3-Phenyl-2-(phenylsulfonyl)quinoline (4af)*:** pale yellow solid (130 mg, 75%); mp = 128.5−131.0 °C (from CH_2Cl_2/hexanes); ^1H NMR ($CDCl_3$, 400 MHz): δ 8.12−8.09 (m, 2H), 7.84 (d, *J* = 8.1 Hz, 1H), 7.76 (t, *J* = 8.4 Hz, 1H), 7.72 (d, *J* = 8.5 Hz, 2H), 7.66 (t, *J* = 8.0 Hz, 1H), 7.53 (t, *J* = 3.7 Hz, 1H), 7.43−7.36 (m, 7H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 155.7, 144.1, 140.5, 139.3, 136.3, 133.4, 133.1, 130.7, 130.0, 129.4, 129.0, 128.5, 128.3, 128.2, 127.7, 127.3 ppm; IR (neat): 1311, 1153, 1075 (SO_2) cm^{-1}; HRMS (ESI-TOF) *m/z* $[M + Na]^+$ calcd for $C_{21}H_{15}NO_2SNa$ 368.0721, found 368.0725.

***2-(Naphthalen-2-ylsulfonyl)-3-phenylquinoline (4ag)*:** white solid (129 mg, 65%); mp = 170.0−171.5 °C (from CH_2Cl_2/hexanes); ^1H NMR ($CDCl_3$, 400 MHz): δ 8.22 (s, 1H), 8.10 (s, 1H), 8.01 (d, *J* = 8.8 Hz, 1H), 7.89−7.82 (m, 4H), 7.78−7.75 (m, 2H), 7.68−7.62 (m, 2H), 7.57 (*t*, *J* = 7.6 Hz, 1H), 7.43−7.33 (m, 5H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 155.9, 145.3, 140.6, 136.4, 135.1, 133.6, 131.9, 130.9, 130.7, 130.2, 130.1, 129.6, 129.4, 129.0, 128.6, 128.4, 127.8, 127.8, 127.3, 127.2, 124.1 ppm; IR (neat): 1306, 1140, 1064 (SO_2) cm^{-1}; HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{25}H_{18}NO_2S$ 396.1058, found 396.1054.

***3-Phenyl-2-(quinolin-8-ylsulfonyl)quinoline (4ah)*:** dark orange viscous liquid (44 mg, 22%); ^1H NMR ($CDCl_3$, 400 MHz): δ 8.56 (dd, *J* = 4.0 Hz, *J* = 1.6 Hz, 1H), 8.26 (d, *J* = 8.4 Hz, 1H), 8.14 (dd, *J* = 7.2 Hz, *J* = 1.2 Hz, 1H), 8.11 (dd, *J* = 8.2 Hz, *J* = 1.8 Hz, 1H), 7.99 (s, 1H), 7.90 (dd, *J* = 8.0 Hz, *J* = 1.2 Hz, 1H), 7.83−7.76 (m, 2H), 7.66 (t, *J* = 7.6 Hz, 1H), 7.40 (t, *J* = 7.6 Hz, 1H), 7.32−7.26 (m, 1H), 7.18 (t, *J* = 7.4 Hz, 1H), 7.07 (t, *J* = 7.6 Hz, 2H), 7.00−6.98 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 156.6 150.9, 145.6, 144.0, 139.8, 137.0, 136.1, 135.8, 133.3, 132.7, 131.5, 130.5, 130.4, 129.8, 128.9, 128.6, 128.1, 127.9, 127.3, 127.3, 125.5, 121.6 ppm; IR (neat): 1305, 1126, 1088 (SO_2) cm^{-1}; HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{24}H_{16}N_2O_2S$ 419.0830, found 419.0831.

***2-(Methylsulfonyl)-3-phenylquinoline (4ai)*:** pale yellow solid (75 mg, 53%); mp = 146.0−148.0 °C (from CH_2Cl_2/hexanes); ^1H NMR ($CDCl_3$, 400 MHz): δ 8.22 (s, 1H), 8.17 (d, *J* = 8.4 Hz, 1H), 7.91(d, *J* = 8.2 Hz, 1H), 7.84−7.82 (m, 1H), 7.73−7.71 (m, 1H), 7.62−7.60 (m, 2H), 7.49−7.46 (m, 3H), 3.45 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 156.0, 144.8, 140.5, 136.0, 132.6, 130.8, 129.8, 129.6, 129.3, 128.7, 128.5, 128.0, 127.6, 40.75 ppm; IR (neat): 1296, 1129, 1073 (SO_2) cm^{-1}; HRMS (ESI-TOF) *m/z* $[M + Na]^+$ calcd for $C_{16}H_{13}NO_2SNa$ 306.0565, found 306.0561.

6-Methyl-3-phenyl-2-tosylquinoline (4ba): pale yellow solid (133 mg, 71%); mp = 143.5−144.5 °C (from CH_2Cl_2/hexanes); ^1H NMR ($CDCl_3$, 400 MHz): δ 8.02−8.00 (m, 2H), 8.61−7.57 (m, 4H), 7.44−7.36 (m, 5H), 7.17 (d, *J* = 8.2 Hz, 2H), 2.55 (s, 3H), 2.39 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 155.1 143.9, 139.8, 139.7, 136.7, 136.5, 133.5, 133.0, 130.0, 129.8, 129.0, 129.0, 128.6, 128.1, 127.7, 126.0, 21.8, 21.6 ppm; IR (neat): 1314, 1146, 1076 (SO_2) cm^{-1}; HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{23}H_{20}NO_2S$ 374.1215, found 374.1211.

***3-Phenyl-2-tosyl-6-(trifluoromethyl)quinoline (4ca)*:** brown solid (68 mg, 32%); mp = 144.5−145.5 °C (from CH_2Cl_2/hexanes); ^1H NMR ($CDCl_3$, 400 MHz): δ 8.23 (s, 1H), 8.20 (d, *J* = 9.2 Hz, 1H), 8.17 (s, 1H), 7.92 (dd, *J* = 9.0 Hz, *J* = 1.8 Hz, 1H), 7.63 (d, *J* = 8.4 Hz, 2H), 7.48−7.43 (m, 5H), 7.23 (d, *J* = 8.0 Hz, 2H), 2.43 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 162.5, 141.8, 140.9, 139.5, 138.3, 133.7, 132.1, 131.6, 129.3, 129.2, 129.0, 128.6, 127.7 (d, $J_{C,F}$ = 3.0 Hz), 127.4, 127.1, 126.1, 125.6 (d, $J_{C,F}$ = 4.0 Hz), 123.6 (d, $J_{C,F}$ = 274.3 Hz), 117.9, 21.4 ppm; IR (neat): 1327, 1104, 1067 (SO_2) cm^{-1}; HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{23}H_{17}F_3NO_2S$ 428.0932, found 428.0934.

***6-Fluoro-3-phenyl-2-tosylquinoline (4da)*:** pale yellow solid (117 mg, 62%); mp = 138.0−139.0 °C (from CH_2Cl_2/hexanes); ^1H NMR ($CDCl_3$, 400 MHz): δ 8.14−8.10 (m, 1H), 8.06 (s, 1H), 7.60 (d, *J* = 8.2

Hz, 2H), 7.56−7.51 (m, 1H), 7.46−7.39 (m, 6H), 7.20 (d, *J* = 8.0 Hz, 2H), 2.41 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): *δ* 162.1 (d, $J_{C,F}$ = 253.2 Hz), 155.7, 144.2, 142.3, 139.8 (d, $J_{C,F}$ = 5.5 Hz), 136.2, 134.4, 132.9 (d, $J_{C,F}$ = 9.5 Hz), 130.0, 129.5, 129.1 (d, $J_{C,F}$ = 8.7 Hz), 128.4, 127.8, 121.2 9 (d, $J_{C,F}$ = 26.2 Hz), 110.4 (d, $J_{C,F}$ = 22.1 Hz), 21.6 ppm; IR (neat): 1315, 1144, 1074 (SO_2) cm^{-1}; HRMS (ESI-TOF) *m/z* [M + H]$^+$ calcd for $C_{22}H_{17}FNO_2S$ 378.0964, found 378.0962.

6-Chloro-3-phenyl-2-tosylquinoline (4ea)**:** yellow viscous liquid (104 mg, 53%); ^{1}H NMR ($CDCl_3$, 400 MHz): *δ* 8.04−8.02 (m, 2H), 7.82 (d, *J* = 2.0 Hz, 1H), 7.69 (dd, *J* = 9.2 Hz, *J* = 2.4 Hz, 1H), 7.61 (d, *J* = 8.4 Hz, 2H), 7.47−7.39 (m, 5H), 7.21 (d, *J* = 8.0 Hz, 2H), 2.42 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): *δ* 156.5, 144.3, 143.6, 139.5, 136.1, 135.4, 134.6, 131.7, 130.0, 129.2, 129.1, 128.4, 127.8, 126.0, 21.6 ppm; IR (neat): 1354, 1121, 1081 (SO_2) cm^{-1}; HRMS (ESI-TOF) *m/z* [M + Na]$^+$ calcd for $C_{22}H_{16}ClNO_2SNa$ 416.0488, found 416.0489.

6-Bromo-3-phenyl-2-tosylquinoline (4fa)**:** pale yellow amorphous solid (127 mg, 58%); ^{1}H NMR ($CDCl_3$, 400 MHz): *δ* 8.03 (s, 1H), 8.01 (d, *J* = 1.6 Hz, 1H), 7.97 (d, *J* = 8.8 Hz, 1H), 7.83 (dd, *J* = 9.0 Hz, *J* = 1.8 Hz, 1H), 7.60 (d, *J* = 8.0 Hz, 2H), 7.47−7.38 (m, 5H), 7.20 (d, *J* = 8.0 Hz, 2H), 2.42 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): *δ* 156.6, 144.3, 143.8, 139.4, 136.1, 134.6, 134.2, 131.7, 123.0, 129.5, 129.4, 129.2, 129.1, 128.5, 127.8, 123.7, 21.6 ppm; IR (neat): 1401, 1140, 1068 (SO_2) cm^{-1}; HRMS (ESI-TOF) *m/z* [M + H]$^+$ calcd for $C_{22}H_{17}BrNO_2S$ 438.0163, found 438.0163.

6-Nitro-3-phenyl-2-tosylquinoline (4ga): pale yellow solid (59 mg, 29%); decomposition at 155.0 °C (from CH_2Cl_2/hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz): *δ* 8.80 (d, *J* = 2.4 Hz 1H), 8.49 (dd, *J* = 7.7 Hz, *J* = 2.4 Hz 1H), 8.34 (s, 1H), 8.20 (d, *J* = 9.2 Hz, 1H), 7.65 (d, *J* = 8.2 Hz, 2H), 7.49−7.46 (m, 5H), 7.25 (d, *J* = 8.2 Hz, 2H), 2.44 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): *δ* 156.6, 147.1, 146.8, 144.7, 142.2, 135.4, 135.3, 132.0, 129.9, 129.4, 129.2, 128.8, 128.6, 128.5, 128.0, 127.4, 124.2, 123.9, 123.8, 21.7 ppm; IR (neat): 1323, 1155, 1074 (SO_2) cm^{-1}; HRMS (ESI-TOF) *m/z* [M + H]$^+$ calcd for $C_{22}H_{17}N_2O_4S$ 405.0909, found 405.0910.

7-Chloro-3-phenyl-2-tosylquinoline (4ha)**:** pale yellow crystal (85 mg, 43%); mp = 193.0−194.0 °C (from CH_2Cl_2/hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz): *δ* 8.12 (s, 1H), 8.05 (d, *J* = 1.6 Hz, 1H), 7.79 (d, *J* = 8.8 Hz, 1H), 7.65 (d, *J* = 8.4 Hz, 2H), 7.60 (dd, *J* = 8.6 Hz, *J* = 1.8 Hz, 1H), 7.44 (s, 5H), 7.24 (d, *J* = 8.4 Hz, 2H), 2.43 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): *δ* 157.3, 145.4, 144.4, 140.4, 136.6, 136.2, 136.0, 133.7, 130.4, 130.0, 129.4, 129.1, 128.9, 128.5, 128.5, 128.0, 126.8, 21.7 ppm; IR (neat): 1312, 1138, 1075 (SO_2) cm^{-1}; HRMS (ESI-TOF) *m/z* [M + H]$^+$ calcd for $C_{22}H_{17}ClNO_2S$ 394.0669, found 394.0670.

3-(p-Tolyl)-2-tosylquinoline (4ia)**:** yellow solid (129 mg, 69%); mp = 125.0−127.0 °C (from CH_2Cl_2/hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz): *δ* 8.11 (s, 1H), 8.07 (d, *J* = 8.4 Hz, 1H), 7.83 (d, *J* = 8.4 Hz, 1H), 7.75 (t, *J* = 7.6 Hz, 1H), 7.66−7.63 (m, 3H), 7.32 (d, *J* = 8.0 Hz, 2H), 7.22 (t, *J* = 7.4 Hz, 4H), 2.44 (s, 3H), 2.41 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): *δ* 156.2, 145.0, 144.0, 140.4, 137.9, 136.3, 133.5, 133.4, 130.4, 129.9, 129.8, 129.1, 129.0, 128.4, 127.2, 21.5, 21.2 ppm; IR (neat): 1309, 1140, 1072 (SO_2) cm^{-1}; HRMS (ESI-TOF) *m/z* [M + Na]$^+$ calcd for $C_{23}H_{19}NO_2SNa$ 396.1034, found 396.1037.

3-(4-Methoxyphenyl)-2-tosylquinoline (4ja)**:** yellow solid (130 mg, 67%); mp = 162.0−163.0 °C (from CH_2Cl_2/hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz): *δ* 8.10 (s, 1H), 8.08 (d, *J* = 8.8 Hz, 1H), 7.83 (d, *J* = 8.0 Hz, 1H), 7.75 (t, *J* = 7.6 Hz, 1H), 7.67−7.62 (m, 3H), 7.35 (d, *J* = 8.4 Hz, 2H), 7.21 (d, *J* = 8.0 Hz, 2H), 6.94 (d, *J* = 8.8 Hz, 2H), 3.89 (s, 3H), 2.41 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): *δ* 153.6, 156.2, 145.0, 144.0, 140.5, 136.3, 133.2, 131.3, 130.4, 130.0, 129.2, 129.1, 128.9, 128.6, 128.5, 121.2, 113.2, 55.2, 21.6 ppm; IR (neat): 1285, 1142, 1072 (SO_2) cm^{-1}; HRMS (ESI-TOF) *m/z* [M + H]$^+$ calcd for $C_{23}H_{20}NO_3S$ 390.1164, found 390.1163.

***3-(4-Fluorophenyl)-2-tosylquinoline (4ka)*:** pale orange solid (119 mg, 63%); mp = 172.5−173.5 °C (from CH_2Cl_2/hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.11−8.09 (m, 2H), 7.85 (d, J = 8.4 Hz, 1H), 7.78 (d, J = 7.6 Hz, 1H), 7.68 (t, J = 7.4 Hz, 1H), 7.63 (d, J = 8.0 Hz, 2H), 7.41−7.37 (m, 2H), 7.23 (d, J = 8.0 Hz, 2H), 7.10 (t, J = 8.8 Hz, 2H), 2.43 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 162.8 (d, $J_{C,F}$ = 247.9 Hz), 156.1, 145.2, 144.3, 140.6, 136.1, 132.4, 131.9 (d, $J_{C,F}$ = 8.3 Hz), 130.8, 130.1, 129.4, 129.1, 129.1, 128.4, 127.3, 114.8 (d, $J_{C,F}$ = 21.7 Hz), 2.42 ppm; IR (neat): 1293, 1153, 1075 (SO_2) cm^{-1}; HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{22}H_{17}FNO_2S$ 378.0964, found 378.0965.

***3-(4-Chlorophenyl)-2-tosylquinoline (4la)*:** pale brown solid (126 mg, 64%); mp = 150.0−151.0 °C (from CH_2Cl_2/hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.10 (s, 1H), 8.08 (d, J = 8.6 Hz, 1H), 7.85 (d, J = 8.0 Hz, 1H), 7.79−7.75 (m, 1H), 7.69−7.63 (m, 3H), 7.39−7.34 (m, 4H), 7.23 (d, J = 8.1 Hz, 2H), 2.42 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 155.9, 145.3, 144.3, 140.5, 136.0, 134.9, 134.5, 132.1, 131.4, 130.8, 130.1, 129.5, 129.2, 129.1, 128.0, 127.3, 21.6 ppm; IR (neat): 1316, 1135, 1073 (SO_2) cm^{-1}; HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{22}H_{17}ClNO_2S$ 394.0669, found 394.0668.

***3-(4-Bromophenyl)-2-tosylquinoline (4ma)*:** white solid (123 mg, 56%); mp = 153.0−154.0 °C (from CH_2Cl_2/hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.10−8.08 (m, 2H), 7.86 (d, J = 8.0 Hz, 1H), 7.78 (t, J = 7.6 Hz, 1H), 7.69 (d, J = 8.0 Hz, 1H), 7.65 (d, J = 8.0 Hz, 2H), 7.55 (d, J = 8.4 Hz, 2H), 7.30 (d, J = 8.4 Hz, 2H), 7.24 (d, J = 8.4 Hz, 2H), 2.43 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 156.0, 145.4, 144.4, 140.4, 136.1, 135.5, 132.2, 131.7, 131.0, 130.9, 130.2, 129.5, 129.3, 129.1, 128.4, 127.4, 122.8, 21.7 ppm; IR (neat): 1315, 1154, 1075 (SO_2) cm^{-1}; HRMS (ESI-TOF) *m/z* $[M + Na]^+$ calcd for $C_{22}H_{16}BrNO_2SNa$ 459.9983, found 459.9984.

***3-(4-Nitrophenyl)-2-tosylquinoline (4na)*:** white solid (69 mg, 34%); mp = 213.0−214.0 °C (from CH_2Cl_2/hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.27 (d, J = 8.8 Hz, 2H), 8.12 (s, 1H), 8.02 (d, J = 8.4 Hz, 1H), 7.85 (d, J = 8.2 Hz, 1H), 7.80−7.75 (m, 1H), 7.69 (d, J = 8.3 Hz, 3H), 7.64 (d, J = 8.8 Hz, 2H), 7.26−7.22 (m, 2H), 2.41 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 155.8, 147.7, 145.6, 144.7, 143.4, 140.2, 135.6, 131.3, 131.0, 131.0, 130.1, 129.8, 129.4, 129.3, 128.0, 127.5, 123.0, 21.7 ppm; IR (neat): 1316, 1154, 1073 (SO_2) cm^{-1}; HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{22}H_{17}N_2O_4S$ 405.0909, found 405.0908.

***3-(m-Tolyl)-2-tosylquinoline (4oa)*:** pale yellow solid (125 mg, 67%); mp = 174.0−176.0 °C (from CH_2Cl_2/hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.14 (d, J = 8.6 Hz, 1H), 8.10 (s, 1H), 7.83 (d, J = 8.1 Hz, 1H), 7.79−7.75 (m, 1H), 7.67−7.63 (m, 1H), 7.58 (d, J = 8.3 Hz, 2H), 7.32−7.29 (m, 1H), 7.28−7.22 (m, 2H), 7.18 (d, J = 8.0 Hz, 2H), 7.06 (s, 1H), 2.40 (s, 3H), 2.35 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 156.0, 145.2, 143.9, 140.4, 137.3, 136.5, 136.3, 133.6, 130.6, 130.1, 129.3, 129.0, 129.0, 128.9, 128.5, 127.6, 127.3, 127.3, 127.2, 21.5, 21.3 ppm; IR (neat): 1289, 1135, 1074 (SO_2) cm^{-1}; HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{23}H_{20}NO_2S$ 374.1215, found 374.1216.

***3-(3-Fluorophenyl)-2-tosylquinoline (4pa)*:** pale yellow solid (102 mg, 54%); mp = 154.0−155.0 °C (from CH_2Cl_2/hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.11−8.10 (m, 2H), 7.85 (d, J = 8.0 Hz, 1H), 7.79−7.76 (m, 1H), 7.68 (d, J = 8.0 Hz, 1H), 7.63 (d, J = 8.2 Hz, 2H), 7.38−7.35 (m, 1H), 7.26−7.21 (m, 3H), 7.15−7.10 (m, 1H), 7.06−7.02 (m, 1H), 2.41 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 162.0 (d, J_{CF} = 246.7 Hz), 155.8, 145.3, 144.3, 140.4, 138.5 (d, J_{CF} = 8.0 Hz), 136.1, 132.0, 130.9, 130.1, 129.5, 129.2 (d, J_{CF} = 8.4 Hz), 129.1, 128.3, 127.4, 126.1 (d, J_{CF} = 2.7 Hz), 117.1 (d, J_{CF} = 22.4Hz), 115.1 (d, J_{CF} = 20.9 Hz), 21.6 ppm; IR (neat): 1288, 1149, 1068 (SO_2) cm^{-1}; HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{22}H_{17}FNO_2S$ 378.0964, found 378.0965.

***3-(3-Chlorophenyl)-2-tosylquinoline (4qa)*:** pale yellow solid (95 mg, 48%); mp = 139.0−140.5 °C (from CH_2Cl_2/hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.17 (d, J = 8.4 Hz, 1H), 8.10 (s, 1H), 7.86 (d, J = 8.0 Hz, 1H), 7.81 (t, J = 7.6 Hz, 1H), 7.69 (t, J = 7.6 Hz, 1H), 7.59 (d, J = 8.0 Hz, 2H), 7.41−7.34 (m, 3H),

7.22 (d, *J* = 8.4 Hz, 2H), 7.14 (s, 1H), 2.43 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): *δ* 155.7, 145.4, 144.4, 140.4, 138.2, 136.2, 133.7, 132.0, 131.0, 130.2, 129.8, 129.5, 129.2, 129.0, 129.0, 128.7, 128.4, 128.3, 127.4, 21.6 ppm; IR (neat): 1292, 1145, 1071 (SO_2) cm^{-1}; HRMS (ESI-TOF) *m/z* [M + Na]$^+$ calcd for $C_{22}H_{16}ClNO_2SNa$ 416.0488, found 416.0489.

***3-(3-Bromophenyl)-2-tosylquinoline (4ra)*:** pale orange solid (110 mg, 50%); mp = 154.8−155.9 °C (from CH_2Cl_2/hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz): *δ* 8.18 (d, *J* = 8.4 Hz, 1H), 8.10 (s, 1H), 7.86 (d, *J* = 8.4 Hz, 1H), 7.87-7.80 (m, 2H), 7.71−7.68 (d, *J* = 7.2 Hz, 1H), 7.59-7.55 (m, 3H), 7.46 (d, *J* = 7.6 Hz, 1H), 7.31 (t, *J* = 8.4 Hz, 1H), 7.22 (d, *J* = 8.0 Hz, 2H), 2.43 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): *δ* 155.7, 145.5, 144.2, 140.4, 138.4, 136.2, 132.5, 131.9, 131.2, 131.0, 130.3, 129.6, 129.3, 129.2, 128.9, 128.4, 127.4, 121.8, 21.7 ppm; IR (neat): 1310, 1135, 1075 (SO_2) cm^{-1}; HRMS (ESI-TOF) *m/z* [M + Na]$^+$ calcd for $C_{22}H_{16}BrNO_2SNa$ 459.9983, found 459.9987.

***3-(2-Fluorophenyl)-2-tosylquinoline (4sa)*:** brown solid (83 mg, 44%); mp = 208.5−209.5 °C (from CH_2Cl_2/hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz): *δ* 8.18−8.16 (m, 2H), 7.85−7.78 (m, 2H), 7.69−7.66 (m, 3H), 7.47−7.39 (m, 2H), 7.26−7.21 (m, 3H), 7.09 (t, *J* = 8.9 Hz, 1H), 2.40 (s, 3H);^{13}C NMR ($CDCl_3$, 100 MHz): *δ* 161.1, 157.4 (d, $J_{C,F}$ = 255.5 Hz), 145.9, 144.3, 141.2, 136.2, 132.4 (d, $J_{C,F}$ = 1.6 Hz), 131.0, 130.5 (d, $J_{C,F}$ = 8.1 Hz), 130.2, 129.4, 129.2, 129.1, 128.3, 127.4, 126.7, 124.2 (d, J_{CF} = 16.3 Hz), 123.5 (d, $J_{C,F}$ = 3.4 Hz), 115.2 (d, $J_{C,F}$ = 21.8 Hz), 21.6 ppm; IR (neat): 1314, 1144, 1074 (SO_2) cm^{-1}; HRMS (ESI-TOF) *m/z* [M + H]$^+$ calcd for $C_{22}H_{17}FNO_2S$ 378.0964, found 378.0967.

***3-(2-Chlorophenyl)-2-tosylquinoline (4ta)*:** brown solid (26 mg, 13%); mp = 132.0−133.0 °C (from CH_2Cl_2/hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz): *δ* 8.21 (d, *J* = 8.8 Hz, 1H), 8.11 (s, 1H), 7.87−7.80 (m, 2H), 7.70 (d, *J* = 8.0 Hz, 1H), 7.66 (d, *J* = 8.0 Hz, 2H), 7.45-8.34 (m, 4H), 7.21 (d, *J* = 8.0 Hz, 2H), 2.40 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): *δ* 155.7, 146.0, 144.3, 141.0, 136.1, 135.2, 134.0, 132.5, 131.0, 130.3, 129.9, 129.4, 129.2, 129.1, 128.4, 127.5, 126.0, 21.6 ppm; IR (neat): 1311, 1182, 1077 (SO_2) cm^{-1}; HRMS (ESI-TOF) *m/z* [M + Na]$^+$ calcd for $C_{22}H_{16}ClNO_2SNa$ 416.0488, found 416.0489.

***3-(Naphthalen-2-yl)-2-tosylquinoline (4ua)*:** pale orange viscous liquid (16 mg, 8%); ^{1}H NMR ($CDCl_3$, 400 MHz): *δ* 8.38 (d, *J* = 8.4 Hz, 1H), 8.16 (s, 1H), 7.93 (d, *J* = 8.0 Hz, 1H), 7.90−7.82 (m, 3H), 7.72 (t, *J* = 7.4 Hz, 1H), 7.58−7.51 (m, 2H), 7.39 (t, *J* = 7.6 Hz, 1H), 7.24 (s, 1H), 7.12 (d, *J* = 7.6 Hz, 1H), 6.92 (d, *J* = 8.4 Hz, 1H), 6.80 (d, *J* = 8.0 Hz, 2H), 2.16 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): *δ* 156.6, 145.9, 143.7, 141.6, 135.8, 133.1, 133.0, 132.3, 131.3, 131.0, 130.5, 129.5, 129.4, 128.9, 128.8, 128.6, 128.0, 127.3, 125.9, 125.5, 125.4, 124.7, 21.3 ppm; IR (neat): 1316, 1155, 1087 (SO_2) cm^{-1}; HRMS (ESI-TOF) *m/z* [M + Na]$^+$ calcd for $C_{26}H_{19}NO_2SNa$ 432.1034, found 432.1036.

***3-(Thiophen-2-yl)-2-tosylquinoline (4va)*:** pale yellow solid (93 mg, 51%); mp = 134.0−135.0 °C (from CH_2Cl_2/hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz): *δ* 8.26 (s, 1H), 8.06 (d, *J* = 8.8 Hz, 1H), 7.84 (d, *J* = 8.0 Hz, 1H), 7.76 (t, *J* = 7.6 Hz, 1H), 7.68−7.64 (m, 3H), 7.48 (d, *J* = 3.6 Hz, 1H), 7.43 (d, *J* = 5.2 Hz, 1H), 7.23 (d, *J* = 8.0 Hz, 2H), 7.14 (t, *J* = 4.4 Hz, 1H), 2.42 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): *δ* 156.2, 145.1, 144.1, 141.6, 135.9, 135.8, 130.9, 130.8, 130.1, 129.9, 129.4, 129.2, 129.1, 128.2, 127.4, 127.3, 125.9, 21.6 ppm; IR (neat): 1310, 1153, 1060 (SO_2) cm^{-1}; HRMS (ESI-TOF) *m/z* [M + Na]$^+$ calcd for $C_{20}H_{15}NO_2S_2Na$ 388.0442, found 388.0443.

***3-Butyl-2-tosylquinoline (4wa)*:** pale yellow solid (104 mg, 61%); mp = 65.5−66.5.0 °C (from CH_2Cl_2/hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz): *δ* 8.10 (s, 1H), 7.94 (d, *J* = 8.4 Hz, 2H), 7.87 (d, *J* = 8.4 Hz, 1H), 7.77 (d, *J* = 7.6 Hz, 1H), 7.63 (t, *J* = 7.2 Hz, 1H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.35 (d, *J* = 8.0 Hz, 2H), 3.29 (t, *J* = 8.0 Hz, 2H), 2.46 (s, 3H), 1.81−1.73 (m, 2H), 1.55−1.46 (m, 2H), 0.99 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): *δ* 157.1, 144.4, 144.3, 138.8, 136.2, 133.4, 129.8, 129.6, 129.4, 129.2, 129.0,

128.8, 126.8, 33.1, 30.8, 22.6, 21.6, 13.8 ppm; IR (neat): 1309, 1141, 1087 (SO_2) cm^{-1}; HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{20}H_{22}NO_2S$ 340.1371, found 340.1368.

***3-Hexyl-2-tosylquinoline (4xa)*:** brown viscous liquid (123 mg, 67%); ^1H NMR ($CDCl_3$, 400 MHz): *δ* 8.10 (s, 1H), 7.94 (d, *J* = 8.2 Hz, 2H), 7.88 (d, *J* = 8.4 Hz, 1H), 7.78 (d, *J* = 7.4 Hz, 1H), 7.66−7.62 (m, 1H), 7.60−7.56 (m, 1H), 7.36 (d, *J* = 4.1 Hz, 2H), 3.28 (t, *J* = 8.0 Hz, 2H), 2.65 (s, 3H), 1.79−1.73 (s, 2H), 1.49−1.46 (m, 2H), 1.37−1.33 (m, 4H), 0.92−0.89 (m, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): *δ* 157.1, 144.5, 144.3, 138.8, 136.2, 133.6, 129.9, 129.7, 129.5, 129.2, 129.1, 128.8, 126.8, 31.6, 31.2, 31.0, 29.3, 22.6, 21.7, 14.1 ppm; IR (neat): 1311, 1140, 1086 (SO_2) cm^{-1}; HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{22}H_{26}NO_2S$ 368.1684, found 368.1687.

***3-Isopentyl-2-tosylquinoline (4ya)*:** yellow viscous liquid (112 mg, 66%); ^1H NMR ($CDCl_3$, 400 MHz): *δ* 8.10 (s, 1H), 7.94 (d, *J* = 8.4 Hz, 2H), 7.88 (d, *J* = 8.4 Hz, 1H), 7.77 (d, *J* = 7.6 Hz, 1H), 7.66−7.62 (m, 1H), 7.60−7.56 (m, 1H), 7.36 (d, *J* = 8.0 Hz, 2H), 3.30−3.26 (m, 2H), 2.47 (s, 3H), 1.79−1.71 (m, 1H), 1.69−1.64 (m, 2H), 1.02 (d, *J* = 6.4 Hz, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz): *δ* 157.1, 144.4, 144.3, 138.8, 136.2, 133.8, 129.9, 129.6, 129.4, 129.2, 129.1, 128.8, 126.8, 40.3, 29.1, 28.3, 22.5, 21.7 ppm; IR (neat): 1311, 1140, 1086 (SO_2) cm^{-1}; HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{21}H_{24}NO_2S$ 354.1528, found 354.1529.

***3-Cyclopropyl-2-tosylquinoline (4za)*:** pale brown crystal (100 mg, 62%); mp = 140.5−141.5 °C (from CH_2Cl_2/hexanes); ^1H NMR ($CDCl_3$, 400 MHz): *δ* 7.94 (d, *J* = 8.0 Hz, 2H), 7.89 (d, *J* = 8.4 Hz, 1H), 7.83 (s, 1H), 7.73 (d, *J* = 8.0 Hz, 1H), 7.64−7.60 (m, 1H), 7.56 (t, *J* = 7.4 Hz, 1H), 7.36 (d, *J* = 8.4 Hz, 2H), 2.97−2.90 (m, 1H), 2.46 (s, 3H), 1.18−1.13 (m, 2H), 0.86−0.82 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): *δ* 157.7, 144.3, 144.1, 136.2, 134.5, 134.2, 129.9, 129.6, 129.4, 129.2, 129.1, 128.9, 126.8, 21.7, 11.5, 9.4 ppm; IR (neat): 1308, 1135, 1076 (SO_2) cm^{-1}; HRMS (ESI-TOF) *m/z* $[M + Na]^+$ calcd for $C_{19}H_{17}NO_2SNa$ 346.0878, found 346.0877.

***3-Phenyl-2-thiocyanatoquinoline (6a)*:** pale yellow solid (89 mg, 68%); mp = 102.5−103.5 °C (from CH_2Cl_2/hexanes); ^1H NMR (CD_3OD, 400 MHz): δ 8.19 (s, 1H), 8.08 (d, *J* = 8.4 Hz, 1H), 7.97 (d, *J* = 8.0 Hz, 1H), 7.82 (t, *J* = 7.6 Hz, 1H), 7.65 (t, *J* = 7.6 Hz, 1H), 7.56−7.48 (m, 5H); ^{13}C NMR (CD_3OD, 100 MHz): δ 149.8, 148.8, 138.6, 137.3, 135.2, 132.0, 130.6, 130.4, 130.2, 129.25, 129.21, 128.8, 109.0 ppm; IR (neat): 2160 cm^{-1}; HRMS (ESI-TOF) m/z $[M + H]^+$ calcd for $C_{16}H_{11}N_2S$ 263.0643, found 263.0641.

***6-Methyl-3-phenyl-2-thiocyanatoquinoline (6b)*:** white solid (111 mg, 80%); mp = 102.5−103.5 °C (from CH_2Cl_2/hexanes); ^1H NMR (CD_3OD, 400 MHz): δ 8.10 (s, 1H), 7.97 (d, *J* = 8.4 Hz, 1H), 7.74 (s, 1H), 7.67 (dd, *J* = 8.8 Hz, *J* = 1.6 Hz, 1H), 7.56−7.53 (m, 2H), 7.51−7.49 (m, 2H), 2.55 (s, 3H); ^{13}C NMR (CD_3OD, 100 MHz): δ 148.6, 147.5, 139.3, 138.1, 137.5, 135.2, 134.2, 130.5, 130.4, 130.2, 128.9, 127.9, 109.2, 21.6 ppm; IR (neat): 2160 cm^{-1}; HRMS (ESI-TOF) m/z $[M + Na]^+$ calcd for $C_{17}H_{12}N_2SNa$ 299.0619, found 299.0614.

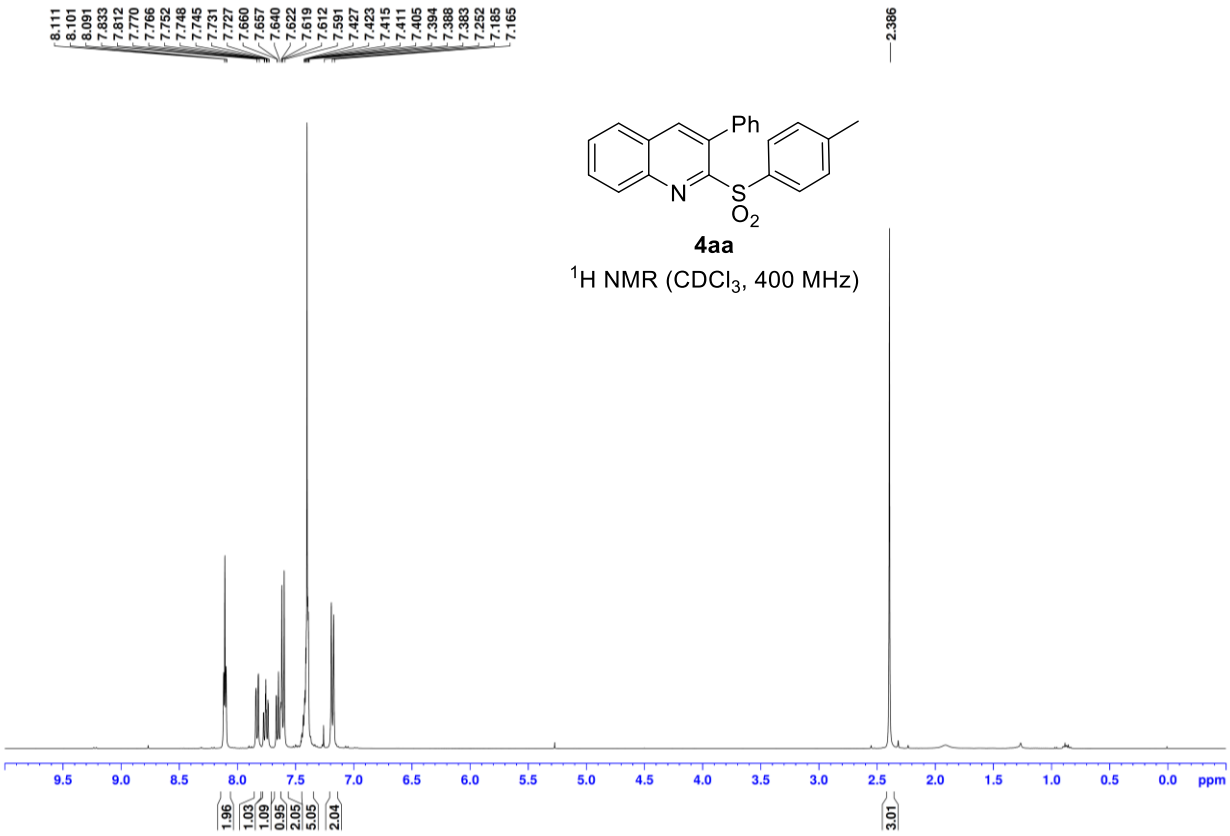
***2-Thiocyanato-3-(p-tolyl)quinoline (6c)*:** white solid (111 mg, 80%); mp = 98.8−100.0 °C (from CH_2Cl_2/hexanes); ^1H NMR (CD_3OD, 400 MHz): δ 8.18 (s, 1H), 8.08 (d, *J* = 8.4 Hz, 1H), 7.97 (d, *J* = 8.4 Hz, 1H), 7.82 (t, *J* = 7.8 Hz, 1H), 7.65 (t, *J* = 7.6 Hz, 1H), 7.39−7.35 (m, 4H), 2.44 (s, 3H); ^{13}C NMR (CD_3OD, 100 MHz): δ 150.2, 148.7, 140.9, 138.5, 135.2, 138.4, 131.9, 130.8, 130.3, 129.2, 128.9, 128.8, 109.1, 21.3 ppm; IR (neat): 2160 cm^{-1}; HRMS (ESI-TOF) m/z $[M + Na]^+$ calcd for $C_{17}H_{12}N_2SNa$ 299.0619, found 299.0614.

***2-Thiocyanato-3-(m-tolyl)quinoline (6d)*:** white solid (111 mg, 80%); mp = 77.3−77.8 °C (from CH_2Cl_2/hexanes); ^1H NMR (CD_3OD, 400 MHz): δ 8.15 (s, 1H), 8.06 (d, *J* = 8.4 Hz, 1H), 7.94 (d, *J* = 8.4 Hz, 1H), 7.80 (t, *J* = 7.6 Hz, 1H), 7.63 (t, *J* = 7.6 Hz, 1H), 7.41 (t, *J* = 7.4 Hz, 1H), 7.34 (d, *J* = 7.6 Hz, 1H),

7.29 (s, 1H), 7.26 (d, *J* = 7.6 Hz, 1H), 2.43 (s, 3H); ^{13}C NMR (CD_3OD, 100 MHz): δ 149.9, 148.8, 140.4, 138.4, 137.3, 135.3, 131.9, 131.2, 130.9, 130.1, 129.22, 129.20, 128.9, 127.4 ppm; IR (neat): 2161 cm^{-1}; HRMS (ESI-TOF) m/z $[M + Na]^+$ calcd for $C_{17}H_{12}N_2SNa$ 299.0619, found 299.0616.

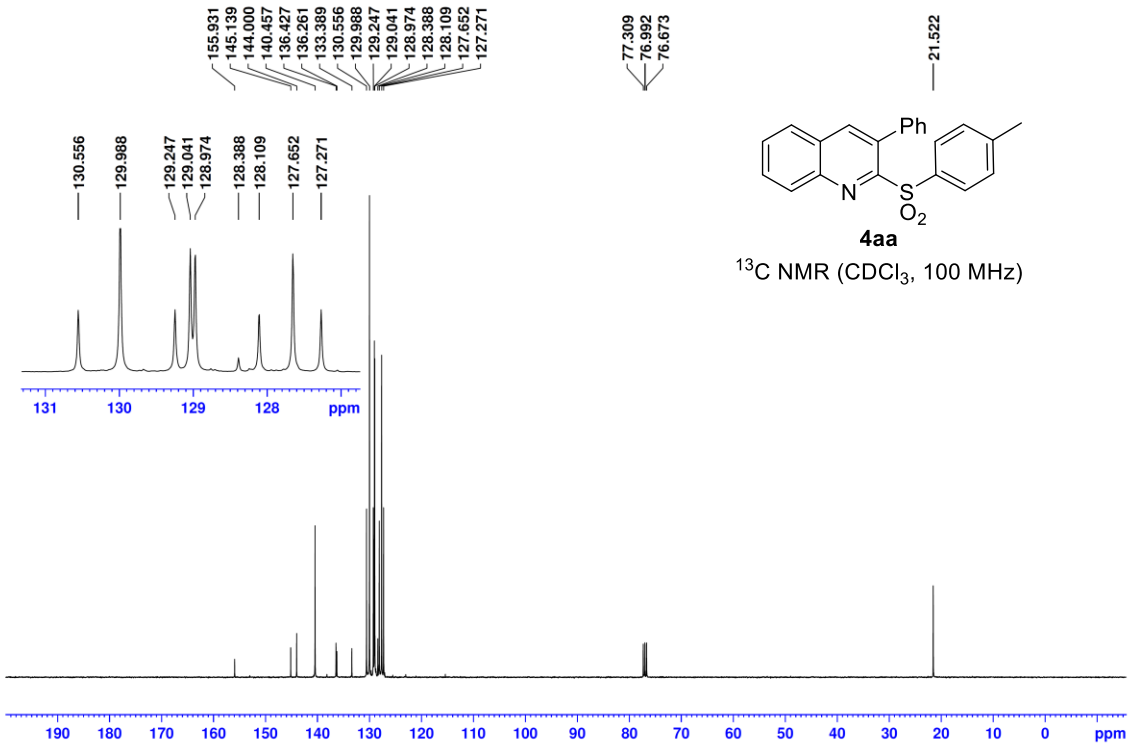
***3-(2-Fluorophenyl)-2-thiocyanatoquinoline (6e)*:** pale yellow oil (108 mg, 77%); ^{1}H NMR (CD_3OD, 400 MHz): δ 8.27 (s, 1H), 8.10 (d, *J* = 8.4 Hz, 1H), 7.99 (d, *J* = 8.4 Hz, 1H), 7.86 (t, *J* = 7.8 Hz, 1H), 7.67 (t, *J* = 7.6 Hz, 1H), 7.62−7.57 (m, 1H) 7.47 (t, *J* = 7.4 Hz, 1H), 7.39−7.35 (m, 2H); ^{13}C NMR (CD_3OD, 100 MHz): ^{13}C NMR (CD_3OD, 100 MHz): δ 161.2 (d, $J_{C,F}$ = 245.5 Hz), 150.1, 149.1, 140.1, 133.3 (d, $J_{C,F}$ = 32.4 Hz), 133.1, 132.4, 129.3, 129.2, 129.0, 128.7 (d, $J_{C,F}$ = 30.4 Hz), 126.2, 124.6 (d, $J_{C,F}$ = 16.2 Hz), 117.2 (d, $J_{C,F}$ = 21.6 Hz), 108.7 ppm; IR (neat): 2165 cm^{-1}; HRMS (ESI-TOF) m/z $[M + Na]^+$ calcd for $C_{16}H_9FN_2SNa$ 303.0368, found 303.0366.

***3-Phenyl-2-tosylquinoline-4-d ([d_1]-4aa)*:** white solid; mp = 155.7−157.0 °C (from CH_2Cl_2/hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.12 (d, *J* = 8.4 Hz, 1H), 8.12 (s, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.80−7.76 (m, 1H), 7.67 (t, *J* = 7.6 Hz, 1H), 7.61 (d, *J* = 8.4 Hz, 2H), 7.45−7.40 (m, 5H), 7.20 (d, *J* = 8.0 Hz, 2H), 2.41 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 156.1, 145.3, 144.1, 140.5, 136.5, 136.4, 133.5, 130.6, 130.2, 130.1, 129.3, 129.2, 129.1, 128.4, 128.2, 127.8, 127.3, 127.3, 21.6 ppm; IR (neat): 1310, 1129, 1072 (SO_2) cm^{-1}; HRMS (ESI-TOF) m/z $[M + H]^+$ calcd for $C_{22}H_{17}DNO_2S$ 361.1121, found 361.1128.



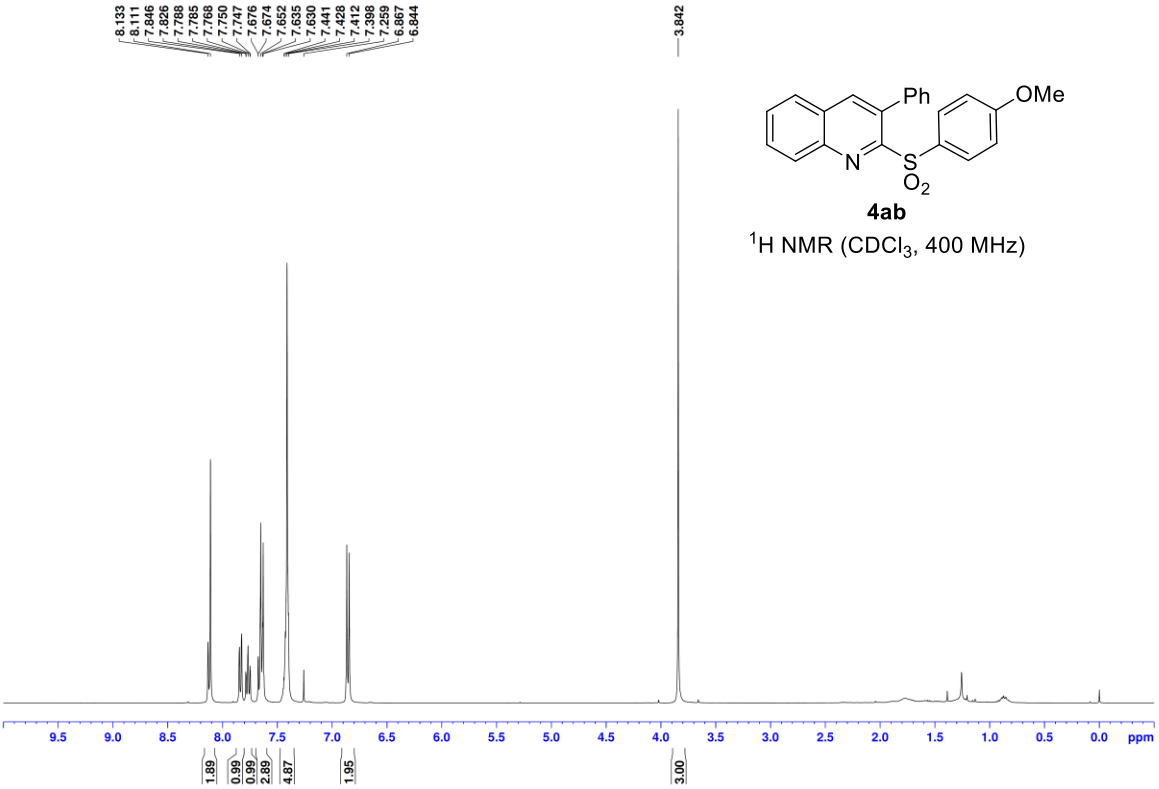
4aa

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



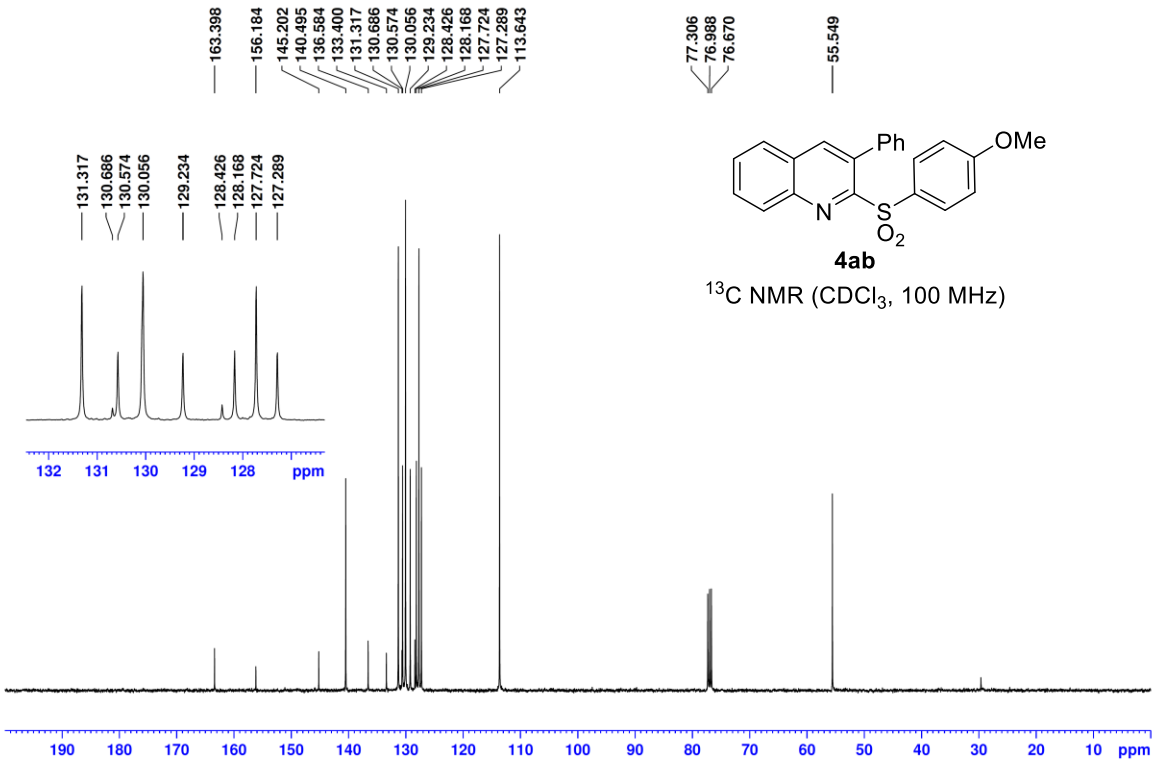
4aa

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



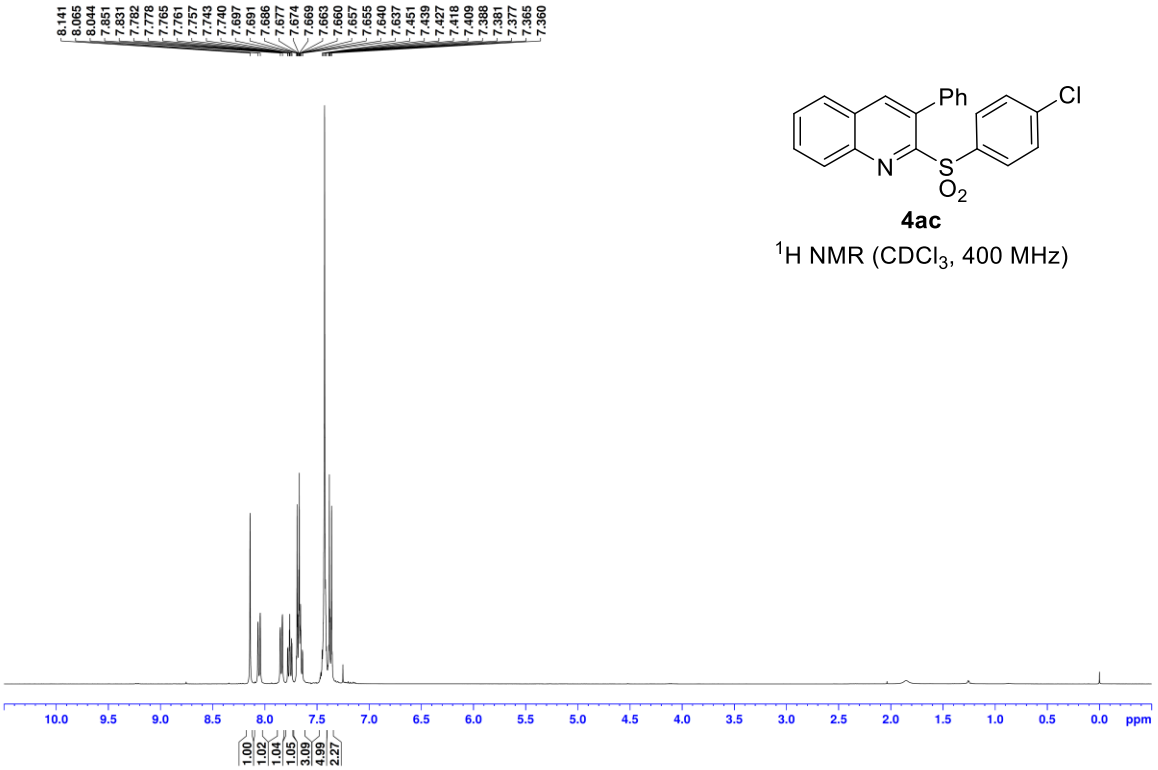
4ab

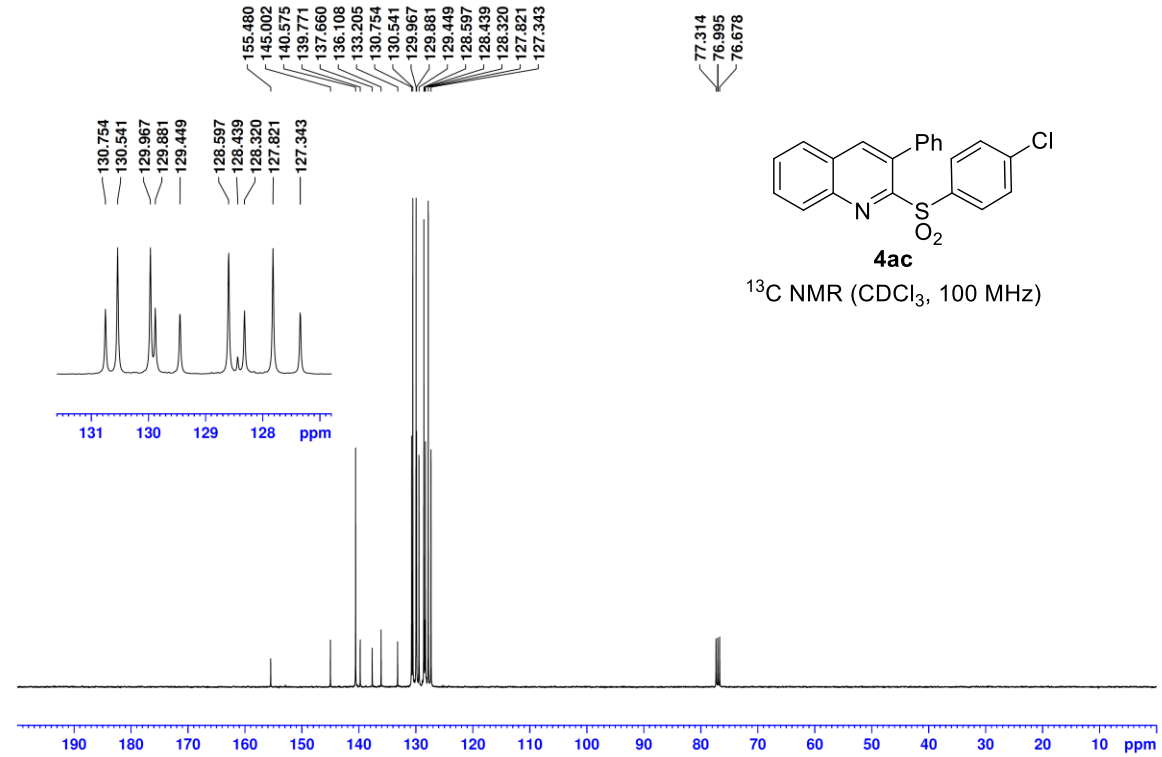
^{1}H NMR ($CDCl_3$, 400 MHz)

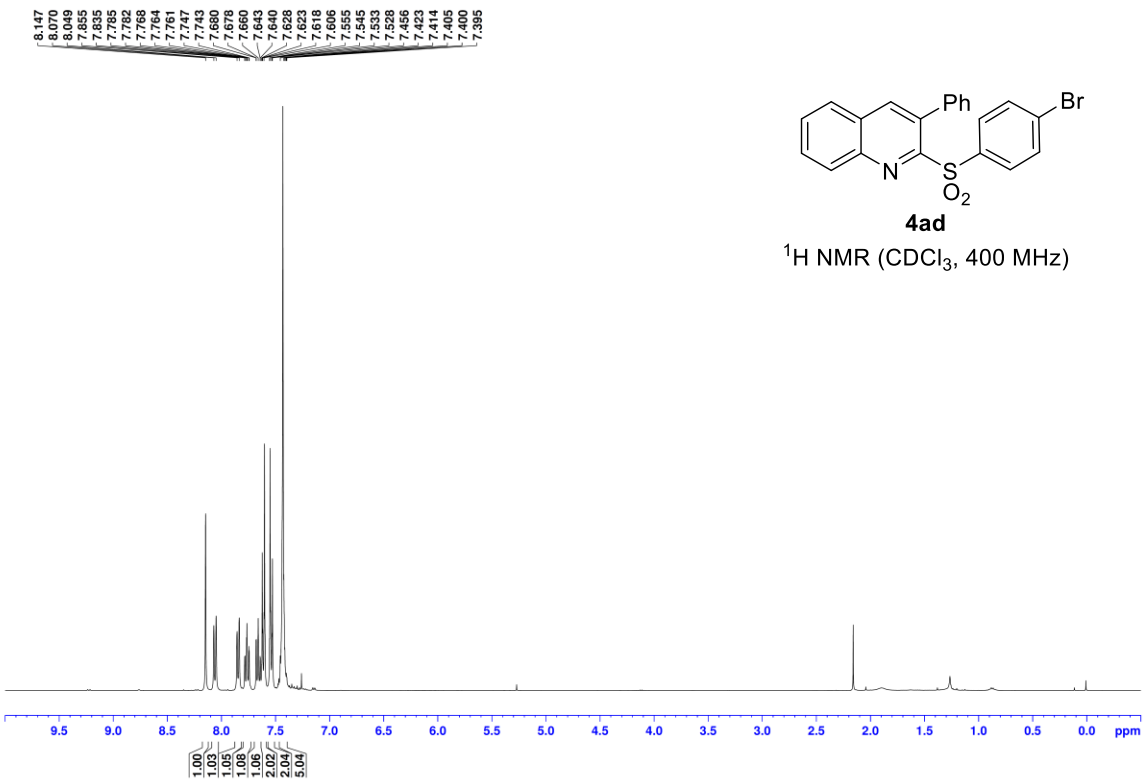


4ab

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

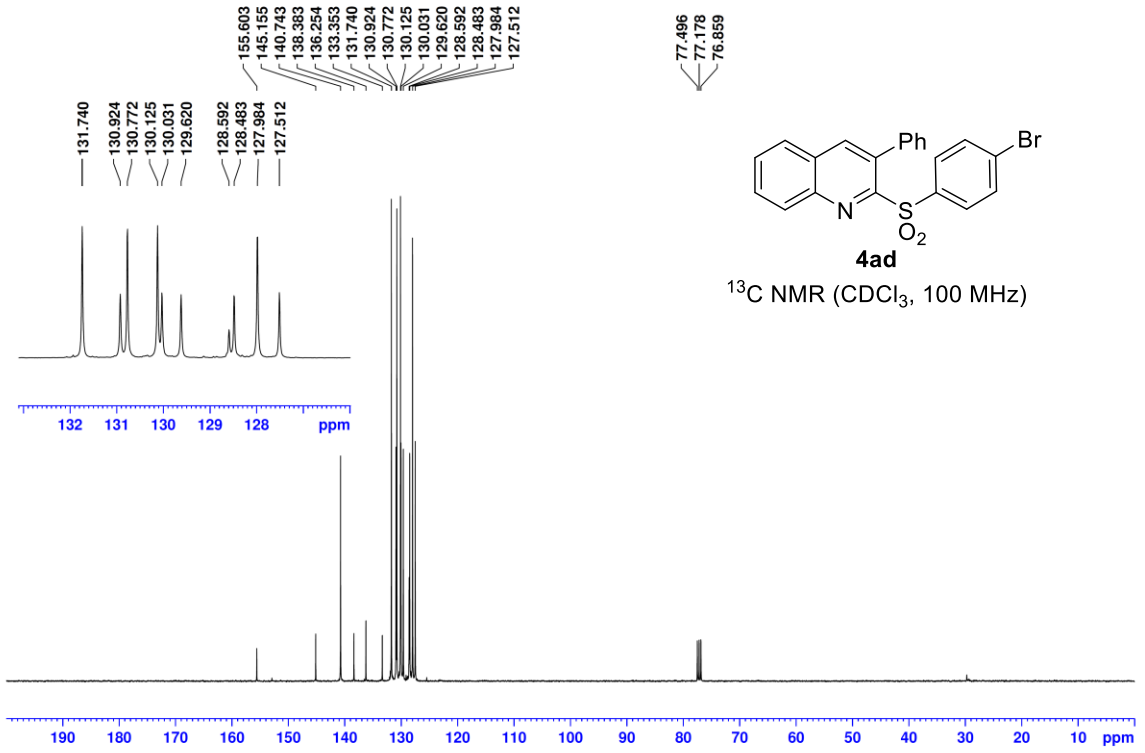

8.141
8.065
8.044
7.851
7.831
7.782
7.778
7.765
7.761
7.757
7.743
7.740
7.697
7.691
7.686
7.677
7.674
7.669
7.663
7.660
7.657
7.655
7.640
7.637
7.451
7.439
7.427
7.418
7.409
7.388
7.381
7.377
7.365
7.360
Ph
Cl
N
S
O2
4ac
1H NMR (CDCl3, 400 MHz)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.00 1.02 1.04 1.05 3.09 4.99 2.27


155.480
145.002
140.575
139.771
137.660
136.108
133.205
130.754
130.541
129.967
129.881
129.449
128.597
128.439
128.320
127.821
127.343
77.314
76.995
76.678
130.754
130.541
129.967
129.881
129.449
128.597
128.439
128.320
127.821
127.343
131 130 129 128 ppm
Ph
Cl
N
S
O2
4ac
13C NMR (CDCl3, 100 MHz)
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm



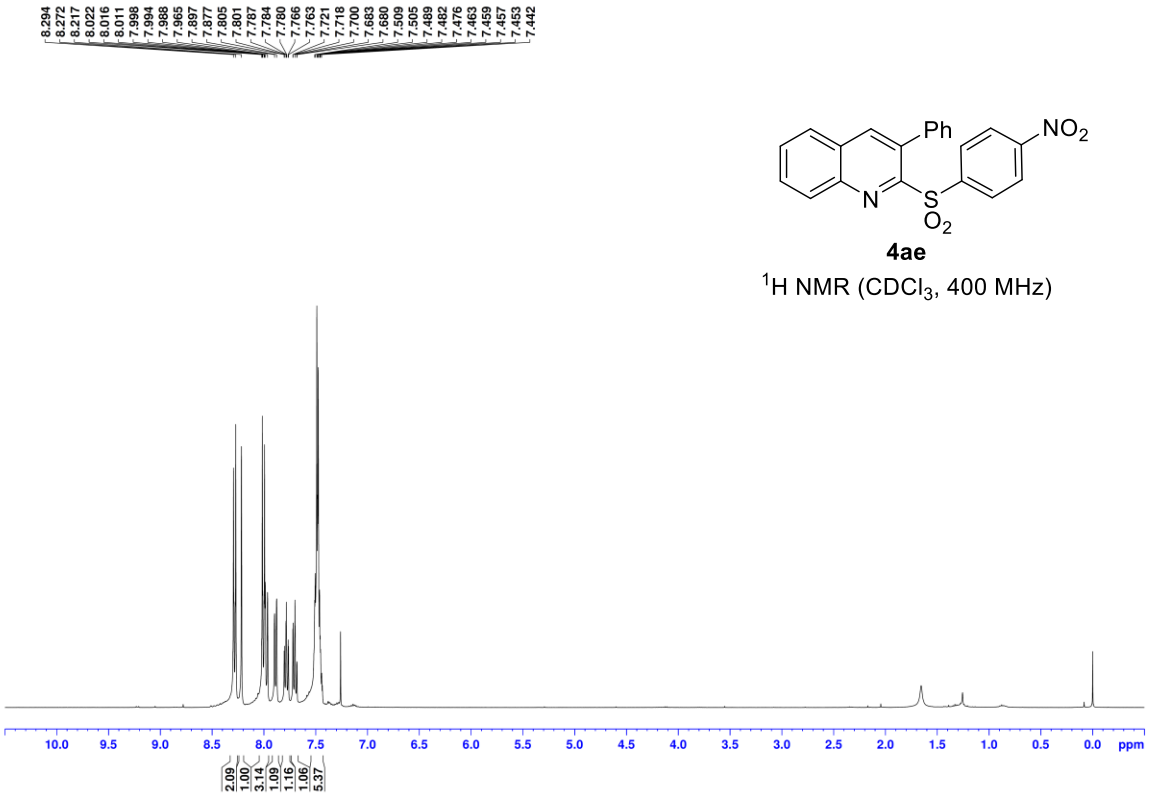
4ad

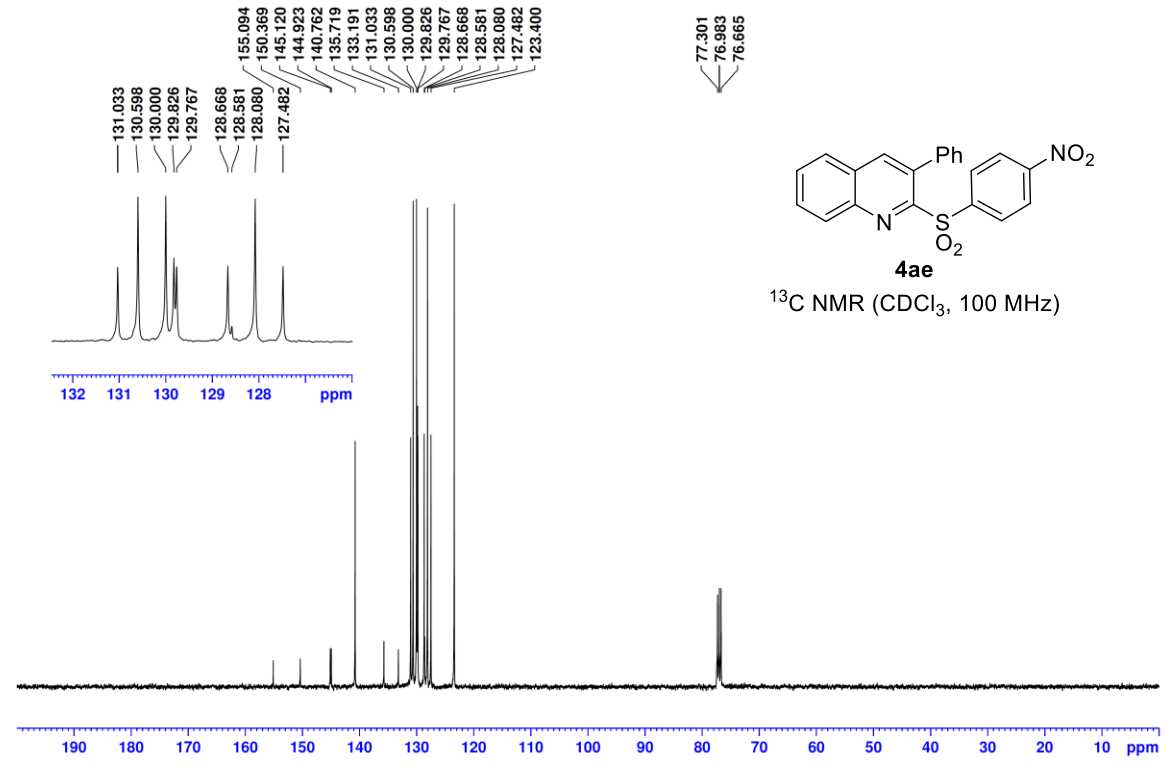
^{1}H NMR ($CDCl_3$, 400 MHz)

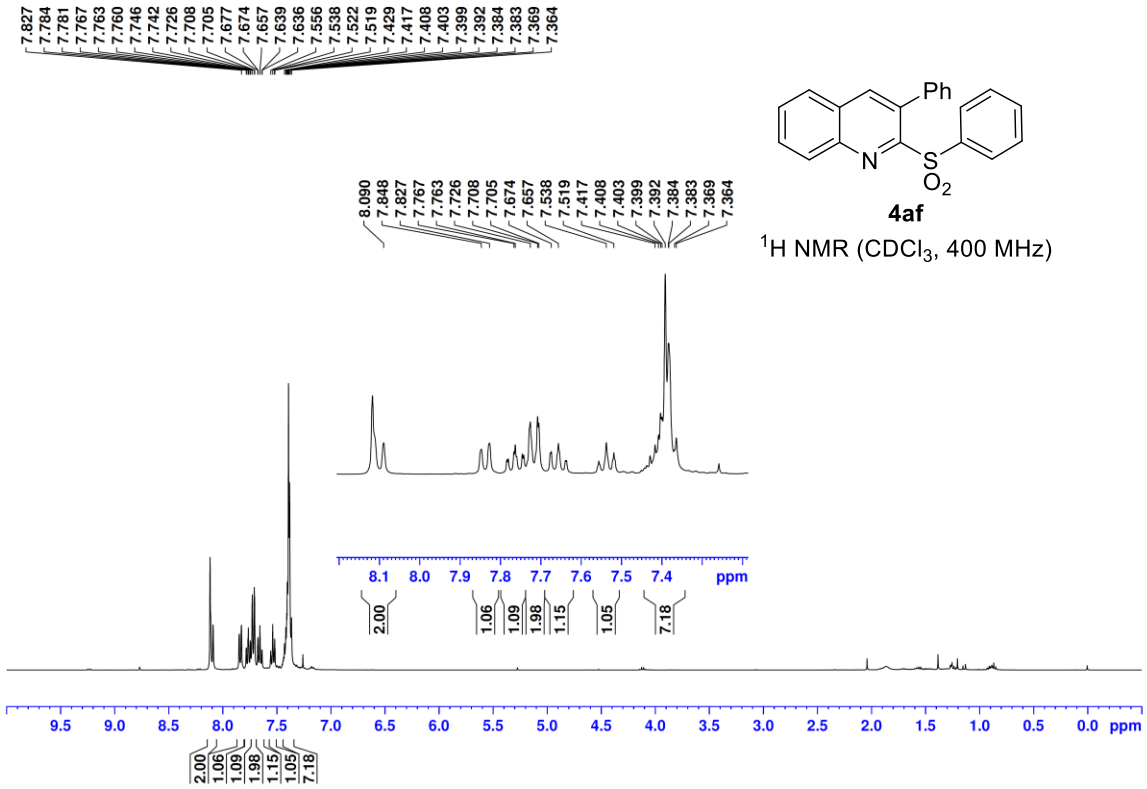


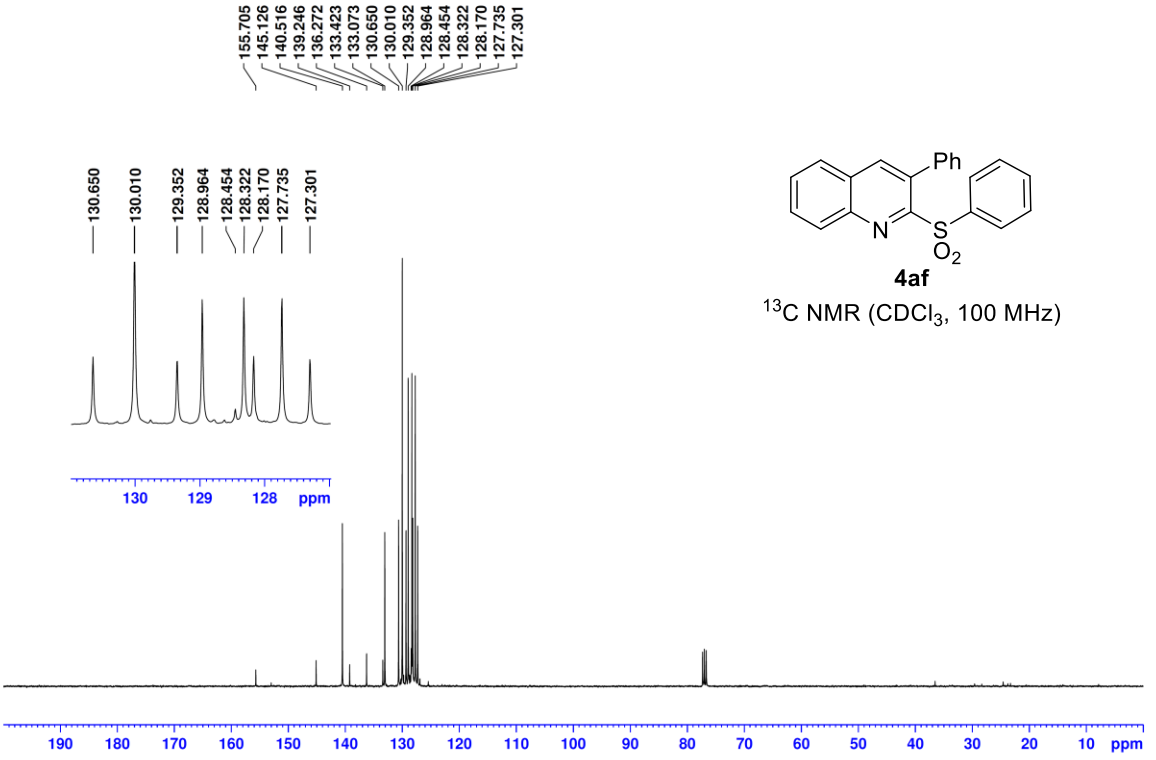
4ad

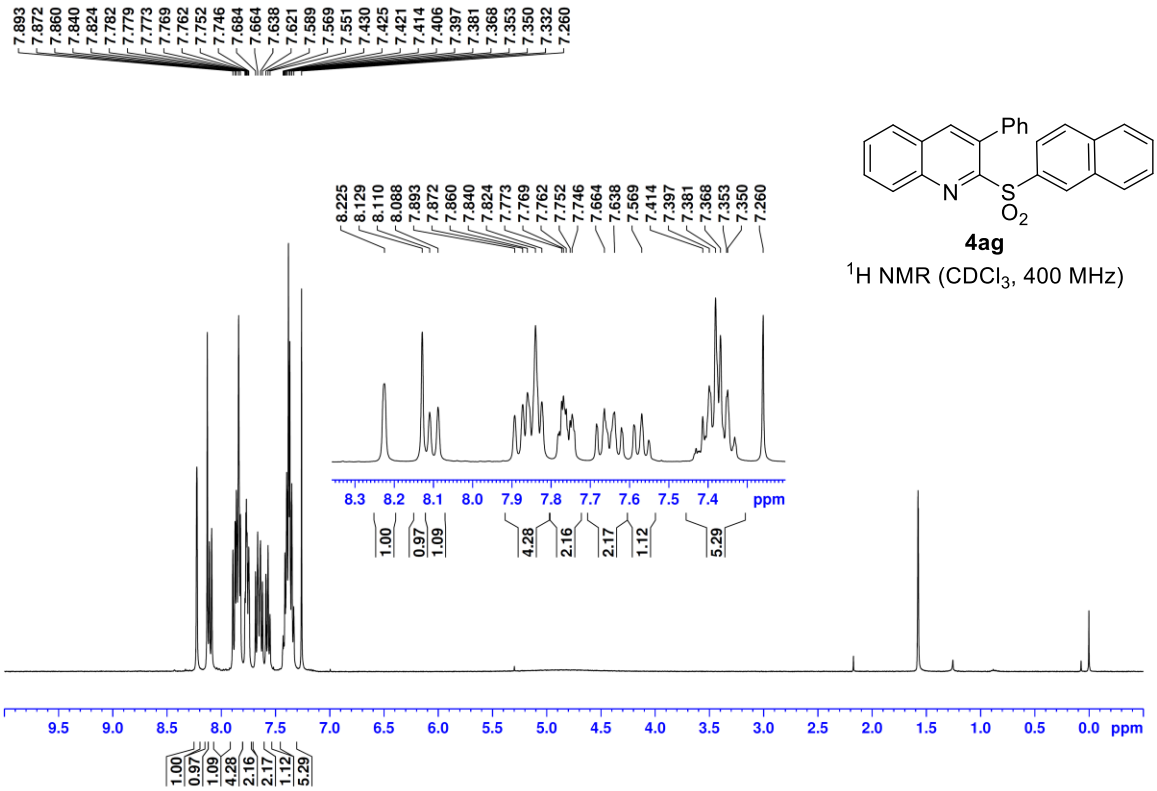
^{13}C NMR ($CDCl_3$, 100 MHz)

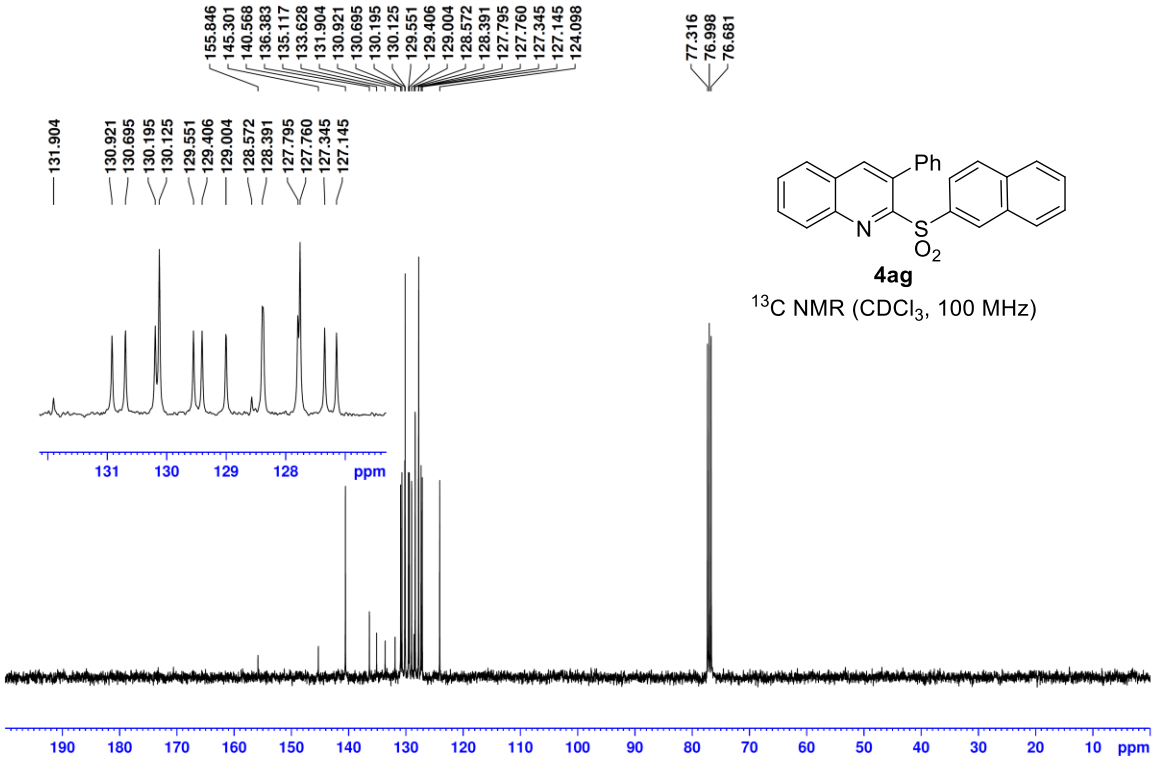

8.294
8.272
8.217
8.022
8.016
8.011
7.998
7.994
7.988
7.965
7.897
7.877
7.805
7.801
7.787
7.784
7.780
7.766
7.763
7.721
7.718
7.700
7.683
7.680
7.509
7.505
7.489
7.482
7.476
7.463
7.459
7.457
7.453
7.442
Ph
NO2
N
S
O2
4ae
1H NMR (CDCl3, 400 MHz)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
2.09
1.00
3.14
1.09
1.16
1.06
5.37


155.094
150.369
145.120
144.923
140.762
135.719
133.191
131.033
130.598
130.000
129.826
129.767
128.668
128.581
128.080
127.482
123.400
77.301
76.983
76.665
131.033
130.598
130.000
129.826
129.767
128.668
128.581
128.080
127.482
132 131 130 129 128 ppm
Ph
NO2
N
S
O2
4ae
13C NMR (CDCl3, 100 MHz)
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.827
7.784
7.781
7.767
7.763
7.760
7.746
7.742
7.726
7.708
7.705
7.677
7.674
7.657
7.639
7.636
7.556
7.538
7.522
7.519
7.429
7.417
7.408
7.403
7.399
7.392
7.384
7.383
7.369
7.364
8.090
7.848
7.827
7.767
7.763
7.726
7.708
7.705
7.674
7.657
7.538
7.519
7.417
7.408
7.403
7.399
7.392
7.384
7.383
7.369
7.364
8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 ppm
2.00
1.06
1.09
1.98
1.15
1.05
7.18
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 ppm
Ph
N
S
O2
4af
1H NMR (CDCl3, 400 MHz)


155.705
145.126
140.516
139.246
136.272
133.423
133.073
130.650
130.010
129.352
128.964
128.454
128.322
128.170
127.735
127.301
130 129 128 ppm
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
Ph
N
S
O2
4af
13C NMR (CDCl3, 100 MHz)


7.893
7.872
7.860
7.840
7.824
7.782
7.779
7.773
7.769
7.762
7.752
7.746
7.684
7.664
7.638
7.621
7.589
7.569
7.551
7.430
7.425
7.421
7.414
7.406
7.397
7.381
7.368
7.353
7.350
7.332
7.260
8.225
8.129
8.110
8.088
7.893
7.872
7.860
7.840
7.824
7.773
7.769
7.762
7.752
7.746
7.664
7.638
7.569
7.414
7.397
7.381
7.368
7.353
7.350
7.260
Ph
N
S
O2
4ag
1H NMR (CDCl3, 400 MHz)
8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 ppm
1.00 0.97 1.09 4.28 2.16 2.17 1.12 5.29
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 ppm
1.00 0.97 1.09 4.28 2.16 2.17 1.12 5.29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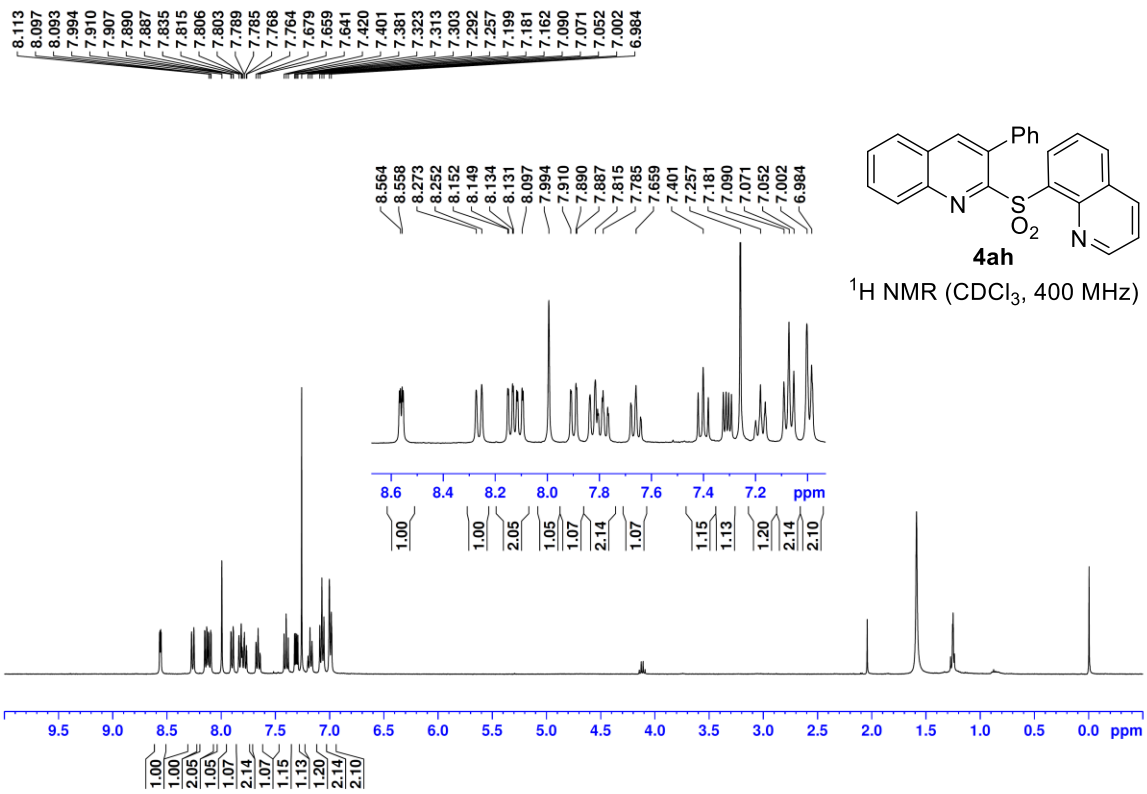
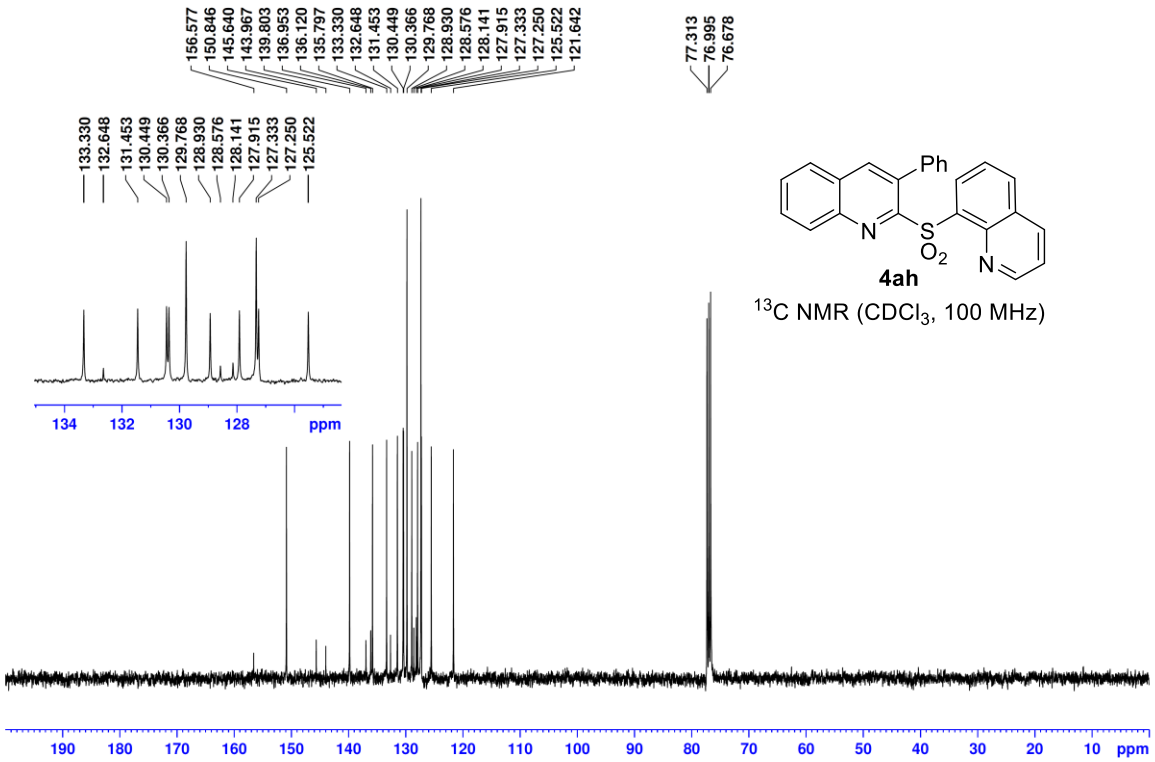
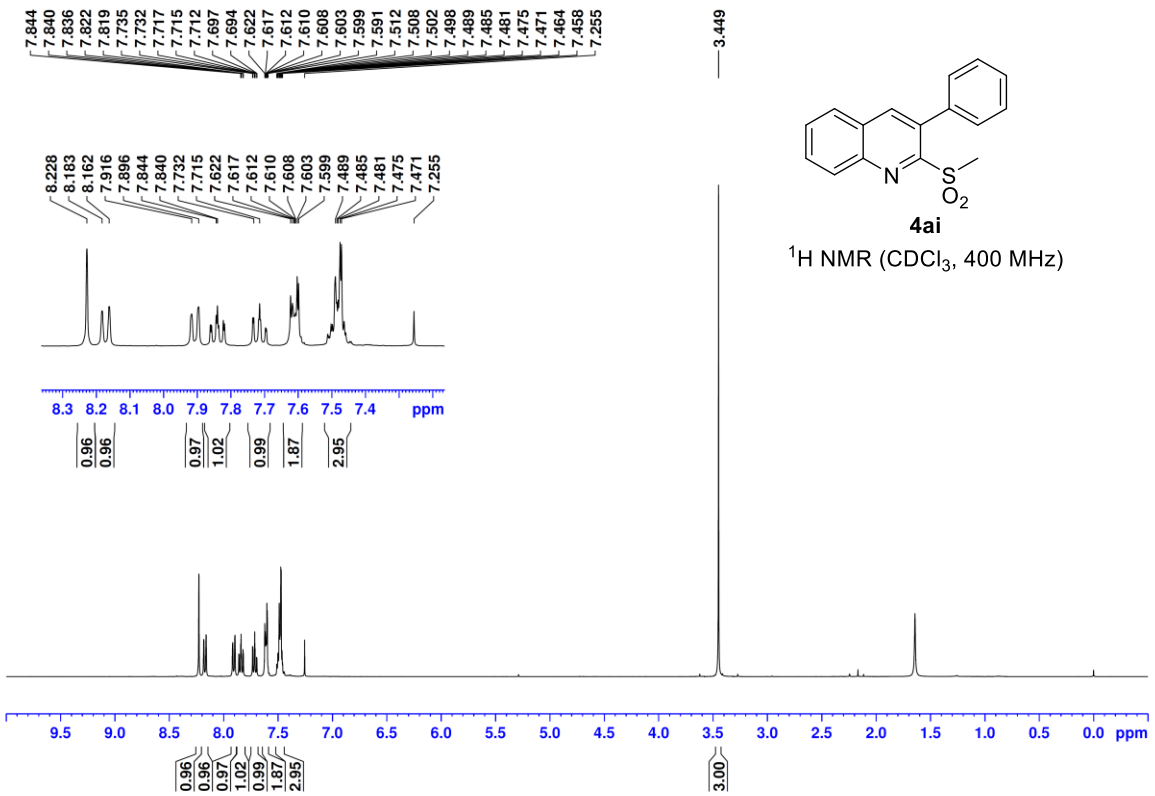
145.301
140.568
136.383
135.117
133.628
131.904
130.921
130.695
130.195
130.125
129.551
129.406
129.004
128.572
128.391
127.795
127.760
127.345
127.145
124.098
77.316
76.998
76.681
131.904
130.921
130.695
130.195
130.125
129.551
129.406
129.004
128.572
128.391
127.795
127.760
127.345
127.145
Ph
N
S
O2
4ag
13C NMR (CDCl3, 100 MHz)
131 130 129 128 ppm
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


8.113
8.097
8.093
7.994
7.910
7.907
7.890
7.887
7.835
7.815
7.806
7.803
7.789
7.785
7.768
7.764
7.679
7.659
7.641
7.420
7.401
7.381
7.323
7.313
7.303
7.292
7.257
7.199
7.181
7.162
7.090
7.071
7.052
7.002
6.984
8.564
8.558
8.273
8.252
8.152
8.149
8.134
8.131
8.097
7.994
7.910
7.890
7.887
7.815
7.785
7.659
7.401
7.257
7.181
7.090
7.071
7.052
7.002
6.984
Ph
N
S
O2
N
4ah
1H NMR (CDCl3, 400 MHz)
8.6
8.4
8.2
8.0
7.8
7.6
7.4
7.2
ppm
1.00
1.00
2.05
1.05
1.07
2.14
1.07
1.15
1.13
1.20
2.14
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
ppm


156.577
150.846
145.640
143.967
139.803
136.953
136.120
135.797
133.330
132.648
131.453
130.449
130.366
129.768
128.930
128.576
128.141
127.915
127.333
127.250
125.522
121.642
77.313
76.995
76.678
133.330
132.648
131.453
130.449
130.366
129.768
128.930
128.576
128.141
127.915
127.333
127.250
125.522
Ph
N
S
O2
N
4ah
13C NMR (CDCl3, 100 MHz)
134
132
130
128
ppm
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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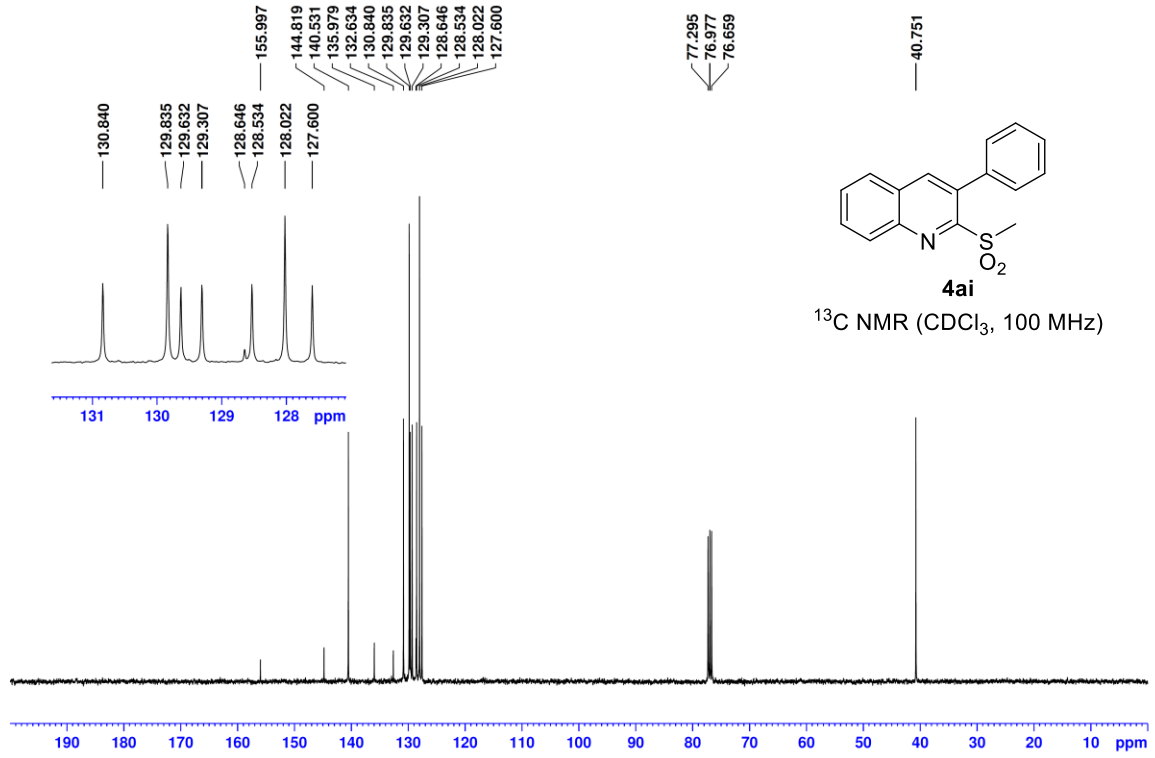
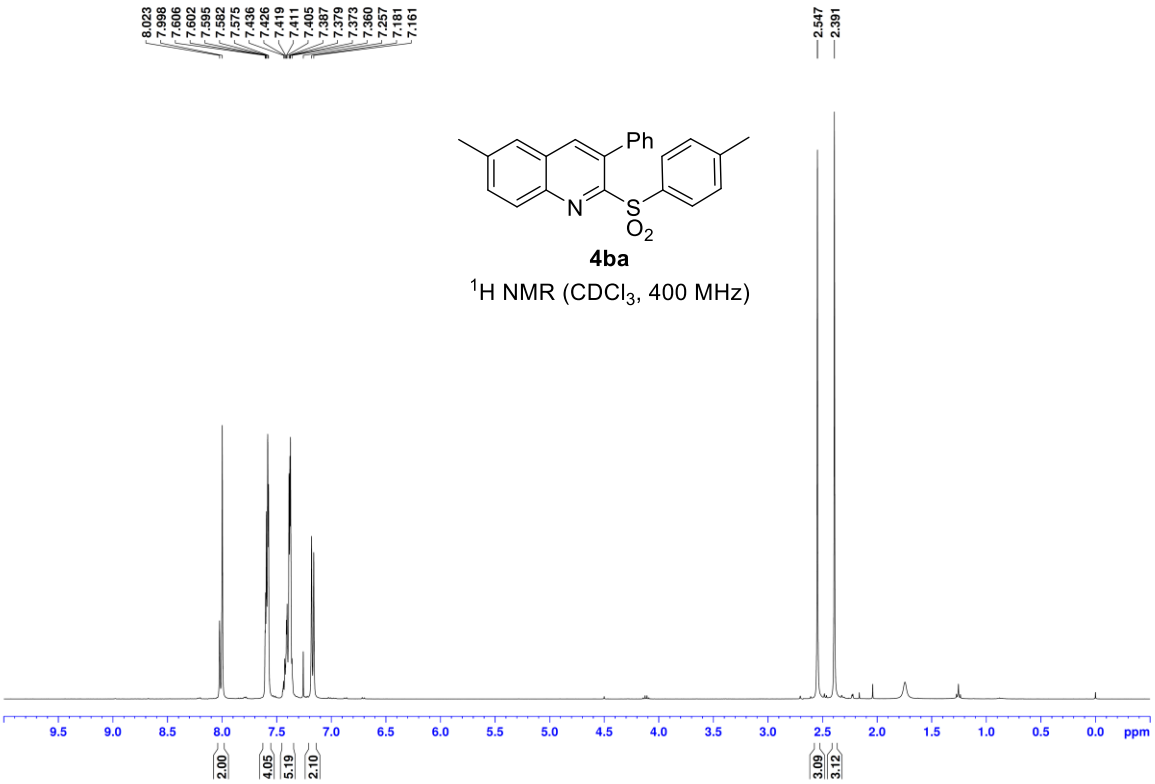
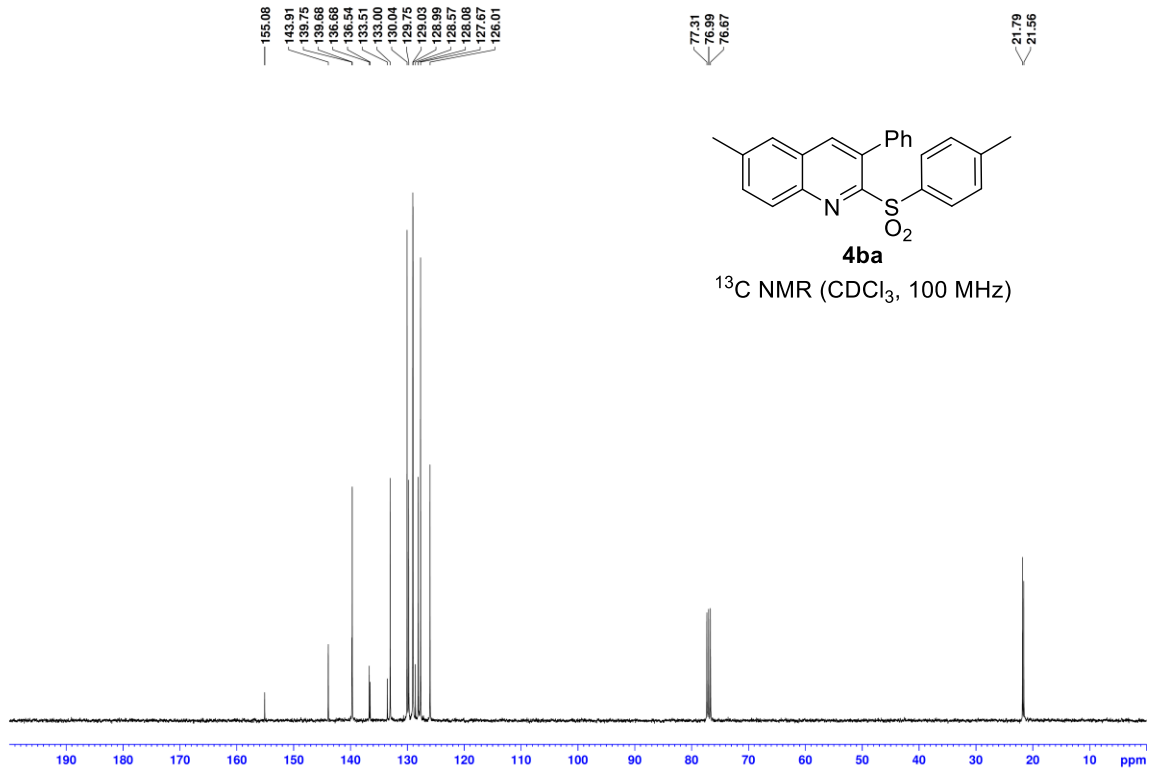
7.840
7.836
7.822
7.819
7.735
7.732
7.717
7.715
7.712
7.697
7.694
7.622
7.617
7.612
7.610
7.608
7.603
7.599
7.591
7.512
7.508
7.502
7.498
7.489
7.485
7.481
7.475
7.471
7.464
7.458
7.255
3.449
8.228
8.183
8.162
7.916
7.896
7.844
7.840
7.732
7.715
7.622
7.617
7.612
7.610
7.608
7.603
7.599
7.489
7.485
7.481
7.475
7.471
7.255
8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 ppm
0.96
0.96
0.97
1.02
0.99
1.87
2.95
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 ppm
0.96
0.96
0.97
1.02
0.99
1.87
2.95
3.00
N
S
O2
4ai
1H NMR (CDCl3, 400 MHz)


155.997
144.819
140.531
135.979
132.634
130.840
129.835
129.632
129.307
128.646
128.534
128.022
127.600
77.295
76.977
76.659
40.751
130.840
129.835
129.632
129.307
128.646
128.534
128.022
127.600
131 130 129 128 ppm
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
N
S
O2
4ai
13C NMR (CDCl3, 100 MHz)



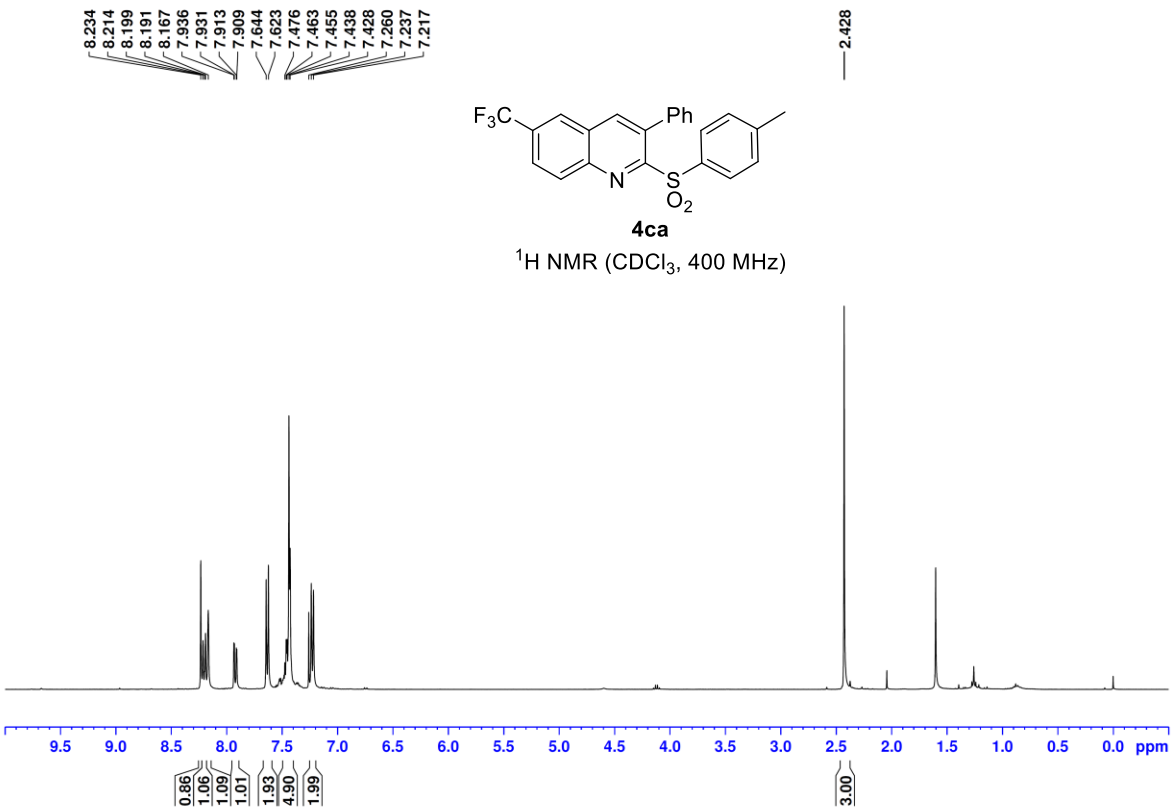
4ba

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



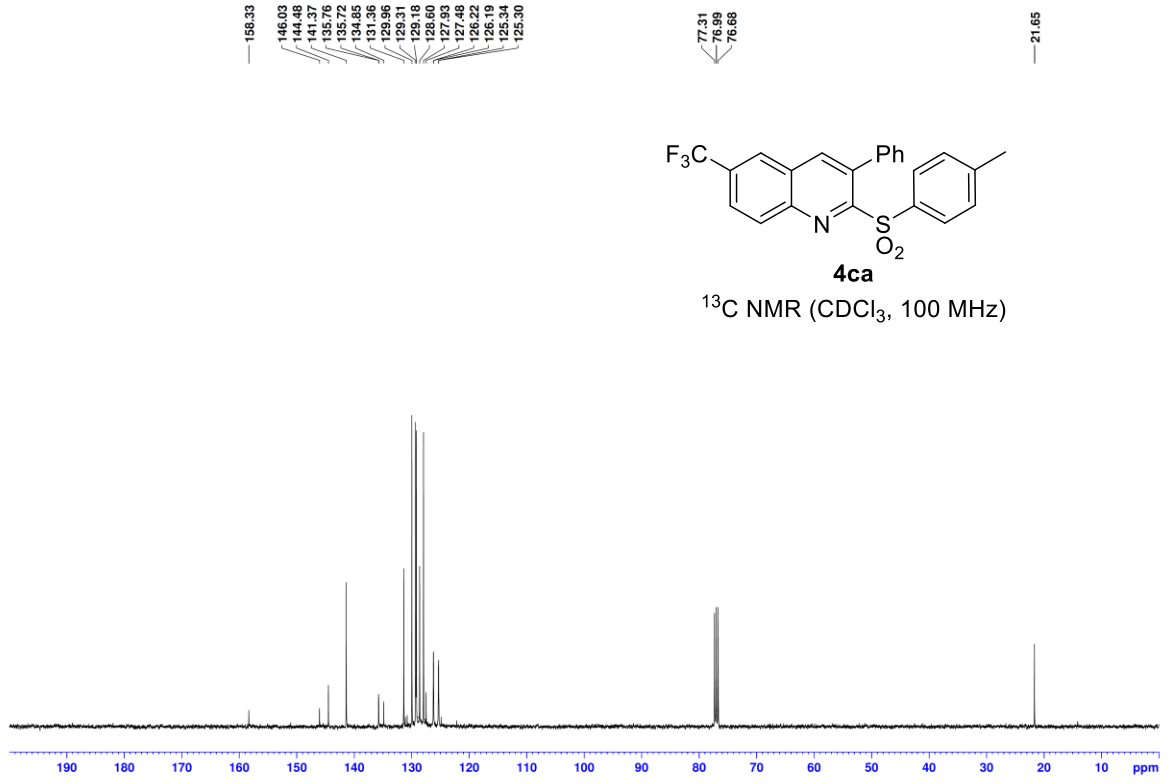
4ba

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



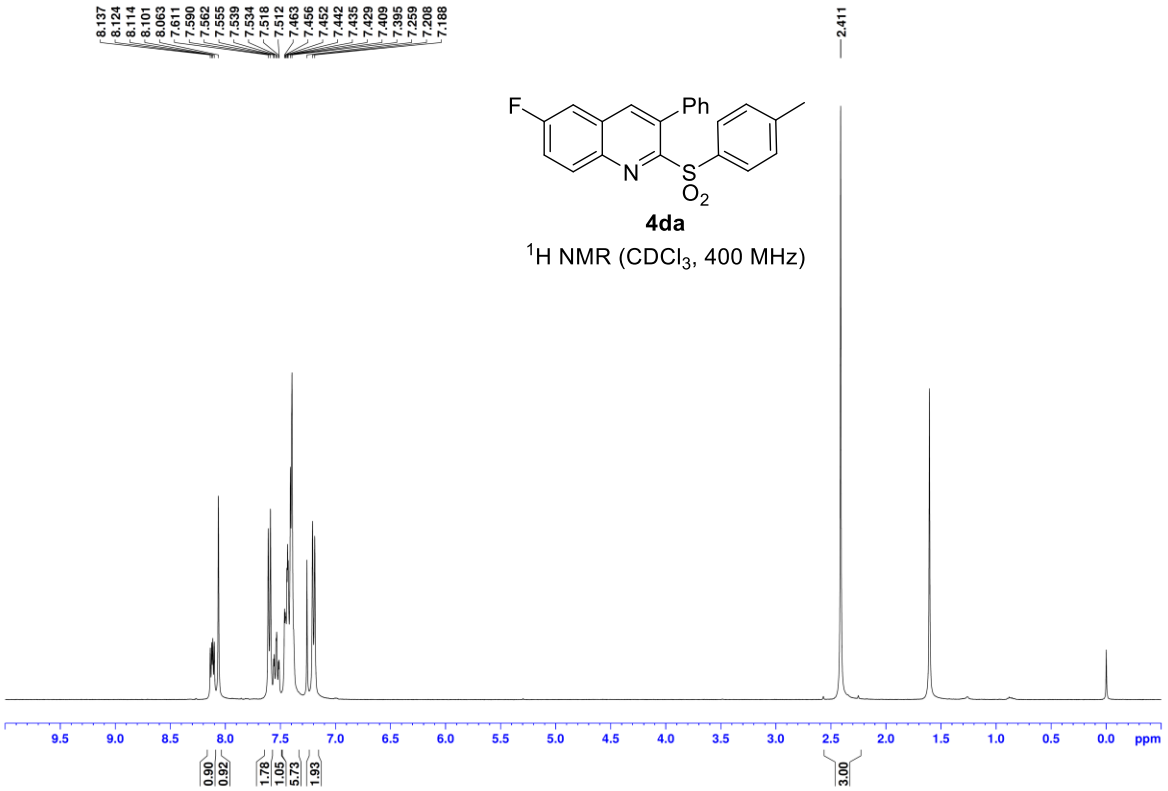
4ca

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



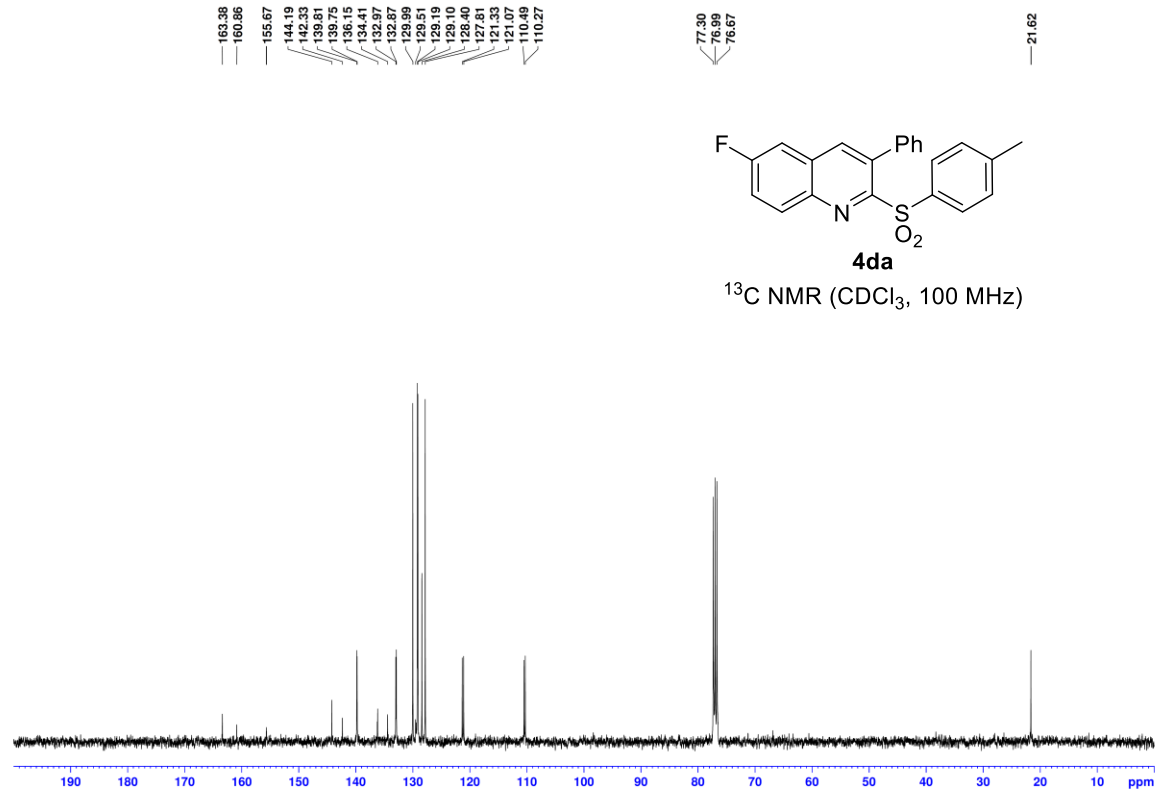
4ca

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



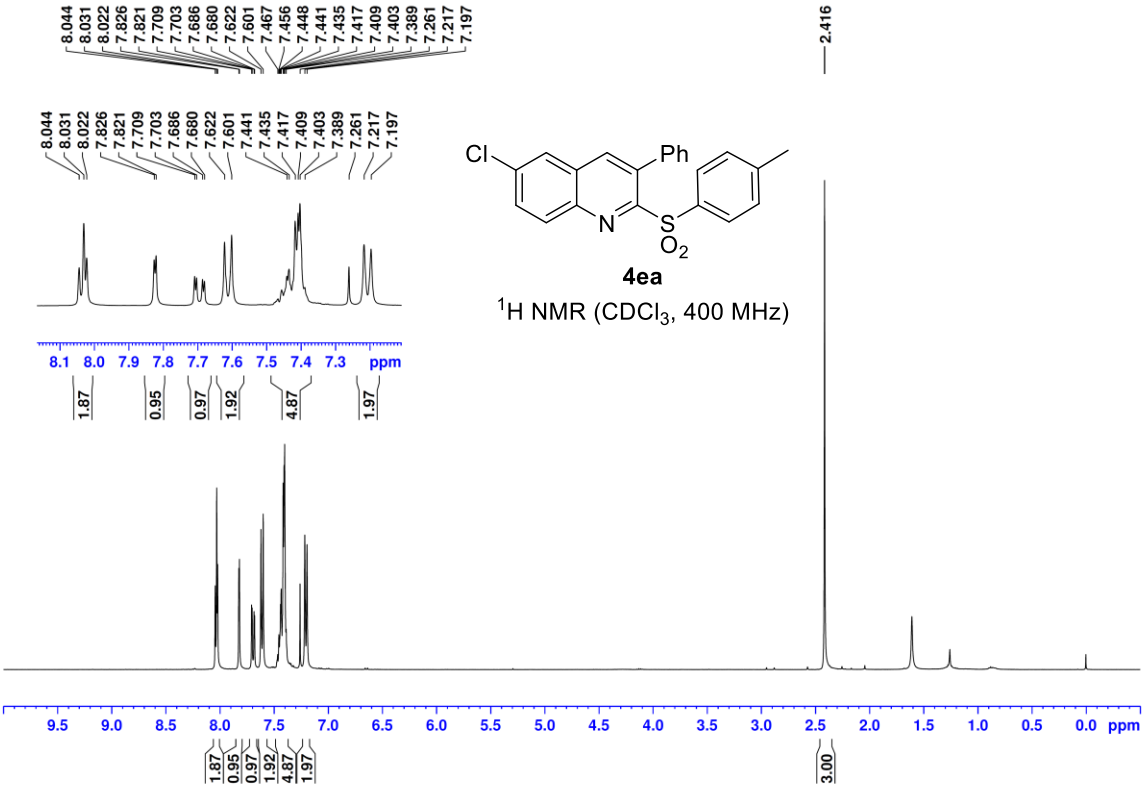
4da

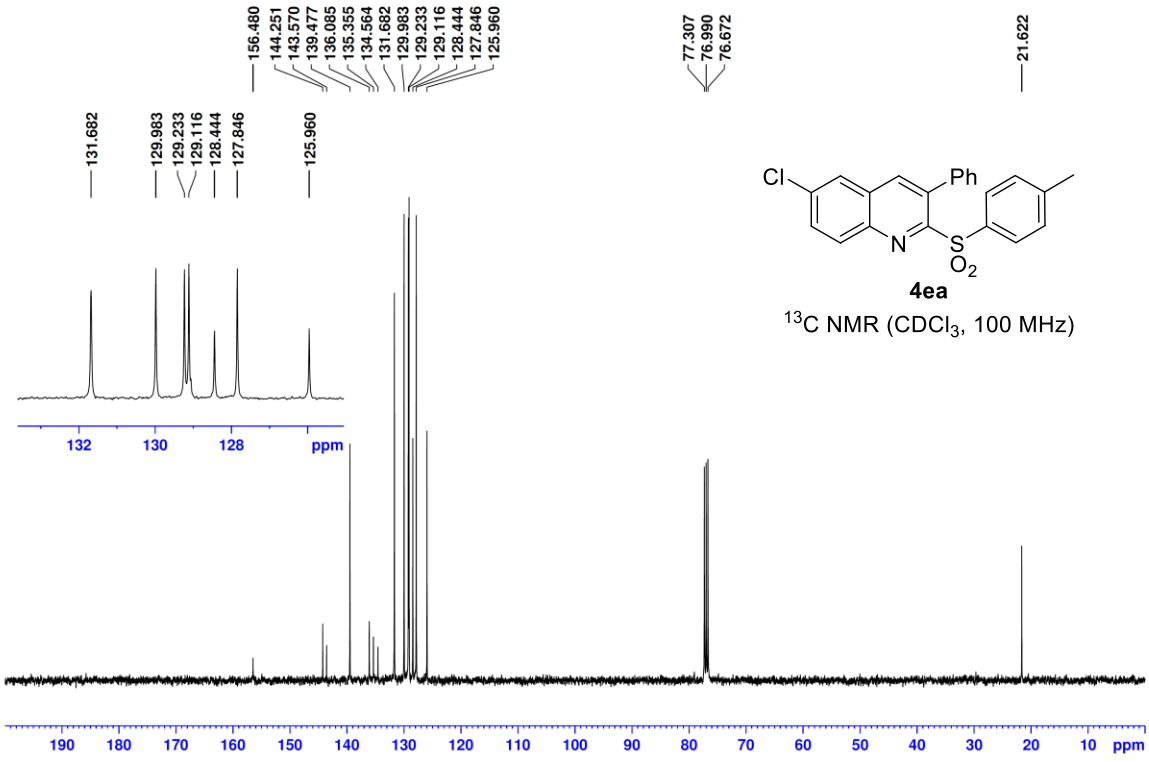
^{1}H NMR ($CDCl_3$, 400 MHz)

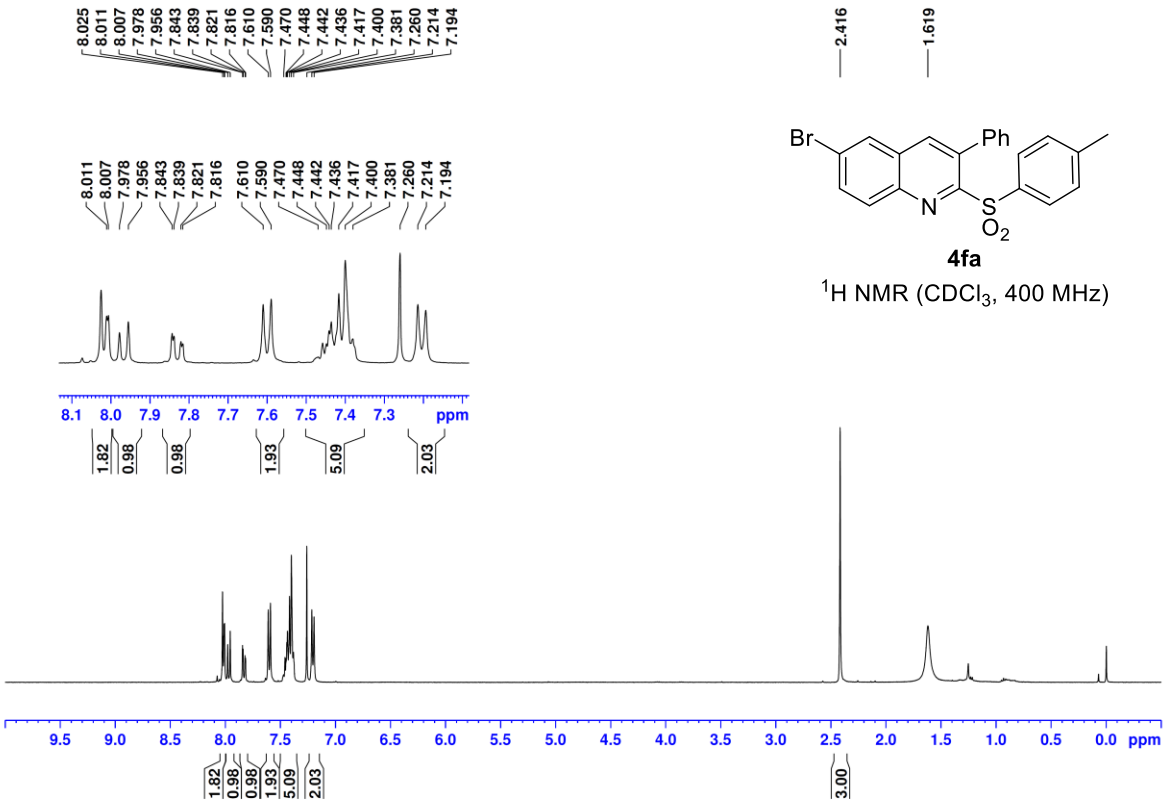


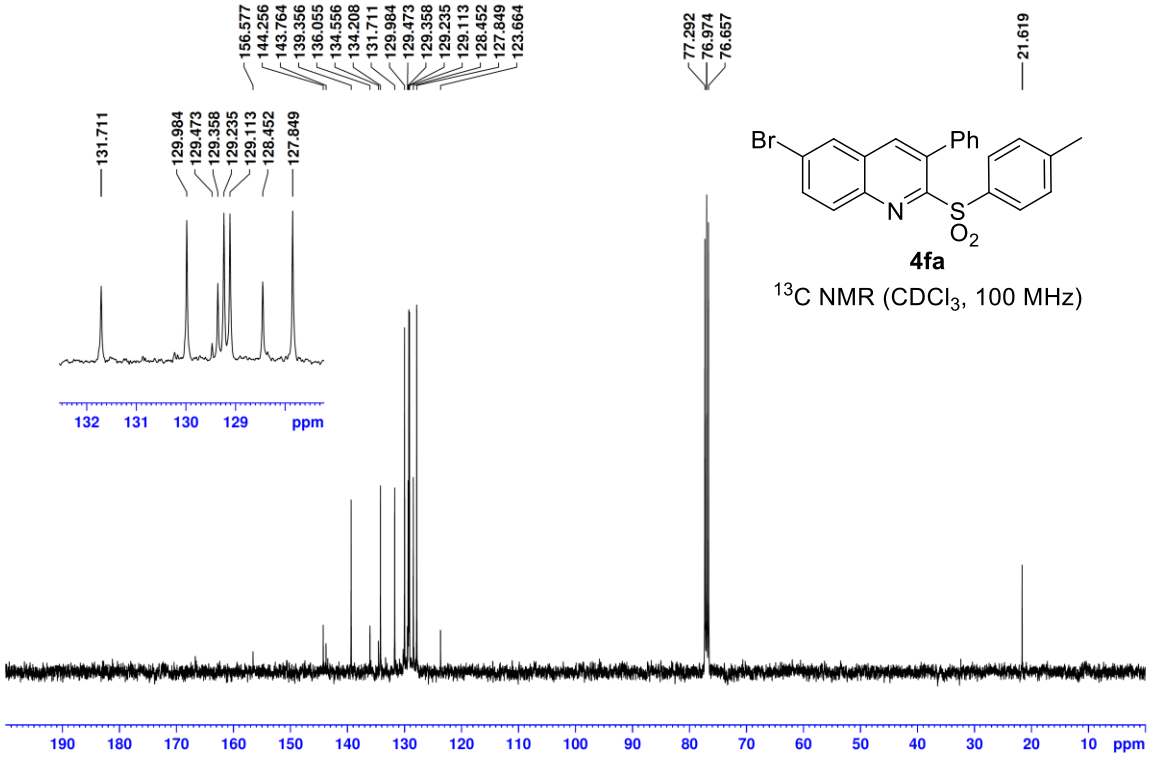
4da

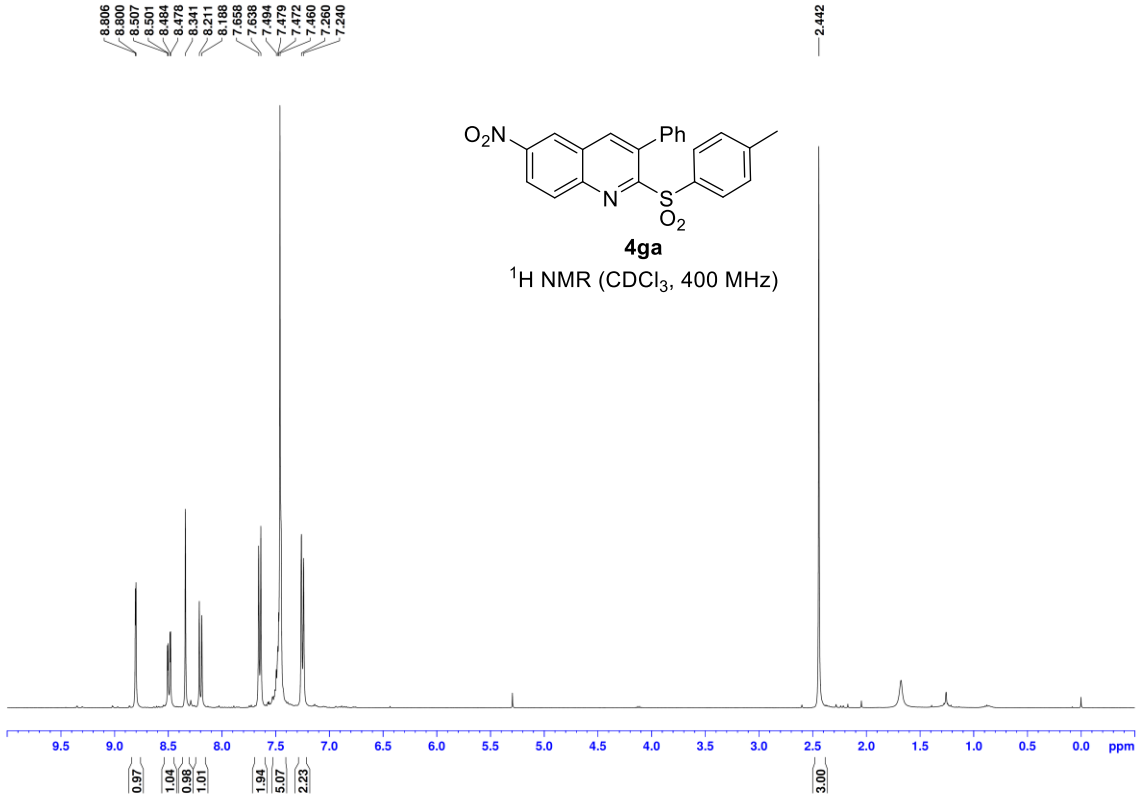
^{13}C NMR ($CDCl_3$, 100 MHz)


8.044
8.031
8.022
7.826
7.821
7.709
7.703
7.686
7.680
7.622
7.601
7.467
7.456
7.448
7.441
7.435
7.417
7.409
7.403
7.389
7.261
7.217
7.197
2.416
Cl
Ph
N
S
O2
4ea
1H NMR (CDCl3, 400 MHz)
8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 ppm
1.87
0.95
0.97
1.92
4.87
1.97
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 ppm
3.00


156.480
144.251
143.570
139.477
136.085
135.355
134.564
131.682
129.983
129.233
129.116
128.444
127.846
125.960
77.307
76.990
76.672
21.622
Cl
Ph
N
S
O2
4ea
13C NMR (CDCl3, 100 MHz)
132 130 128 ppm
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

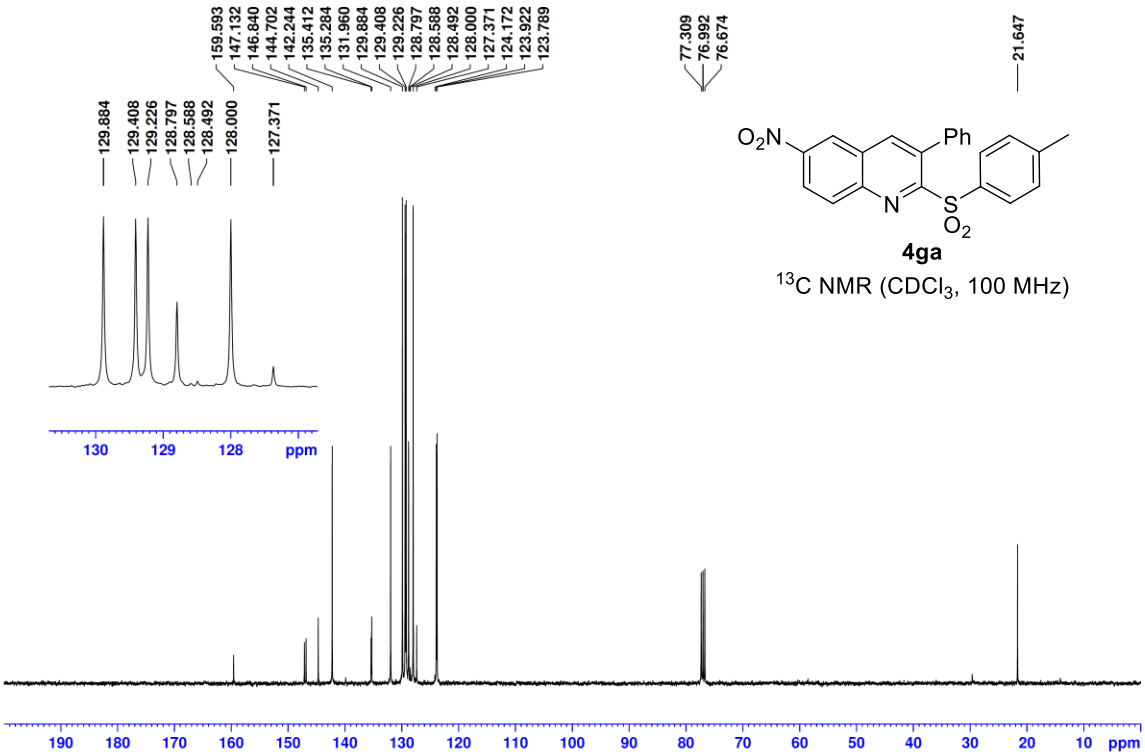

8.025
8.011
8.007
7.978
7.956
7.843
7.839
7.821
7.816
7.610
7.590
7.470
7.448
7.442
7.436
7.417
7.400
7.381
7.260
7.214
7.194
2.416
1.619
Br
Ph
N
S
O2
4fa
1H NMR (CDCl3, 400 MHz)
ppm
1.82
0.98
0.98
1.93
5.09
2.03
3.00


156.577
144.256
143.764
139.356
136.055
134.556
134.208
131.711
129.984
129.473
129.358
129.235
129.113
128.452
127.849
123.664
77.292
76.974
76.657
21.619
Br
Ph
N
S
O2
4fa
13C NMR (CDCl3, 100 MHz)
ppm



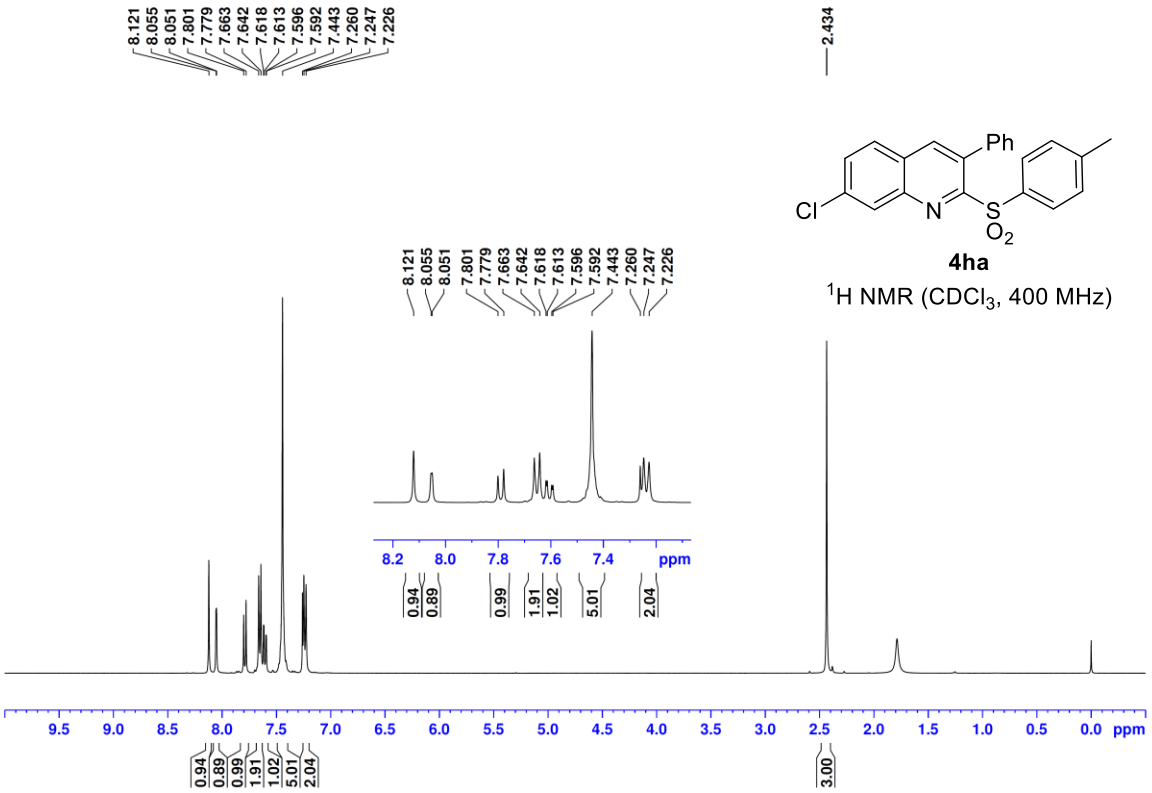
4ga

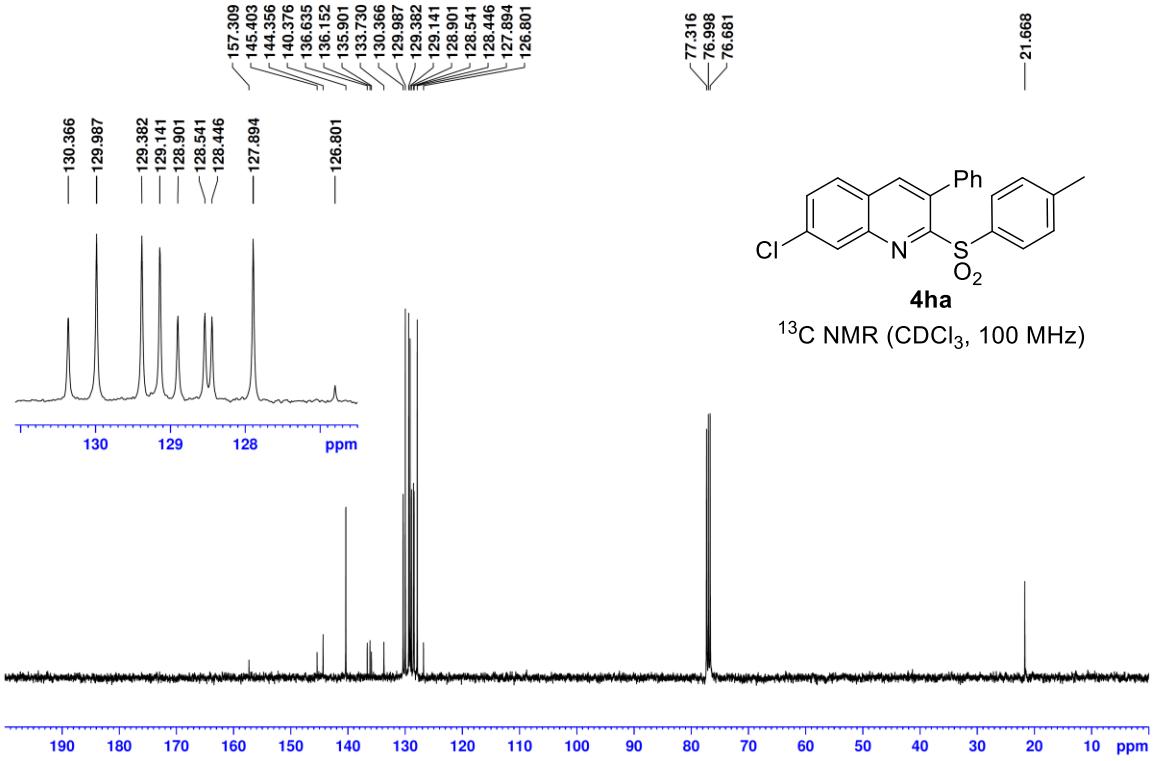
^{1}H NMR ($CDCl_3$, 400 MHz)

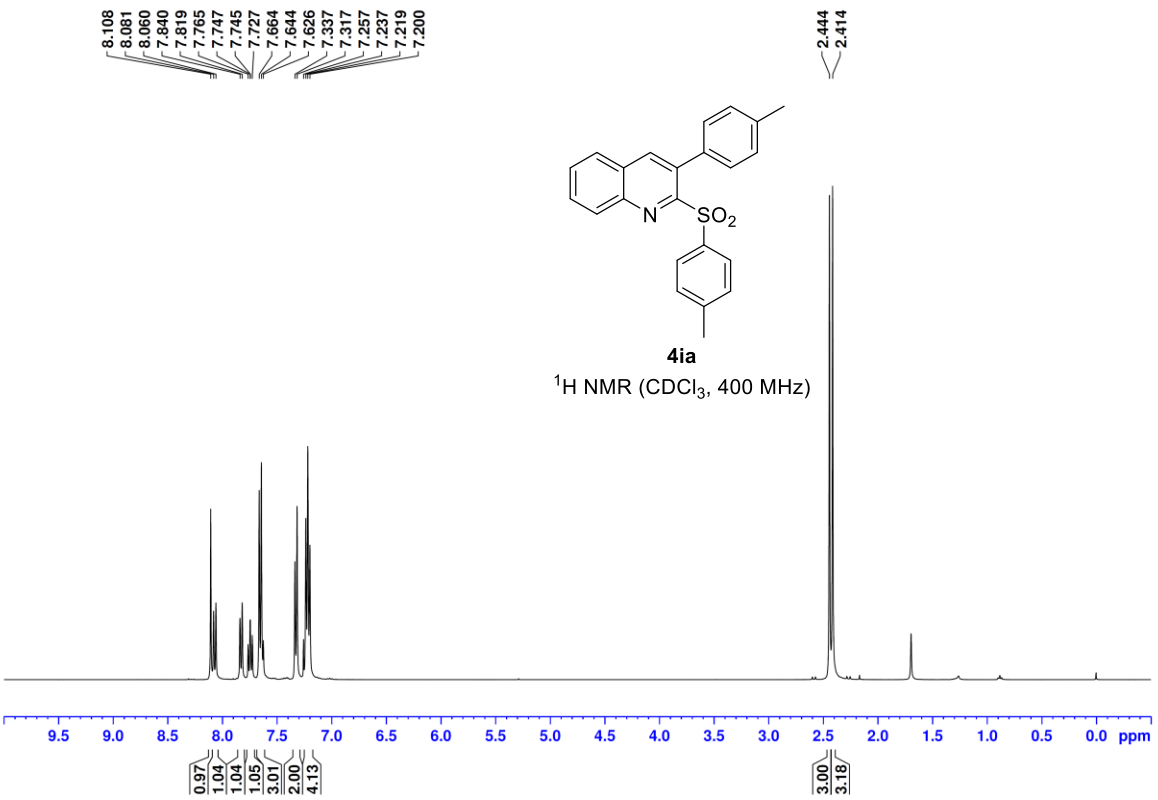


4ga

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

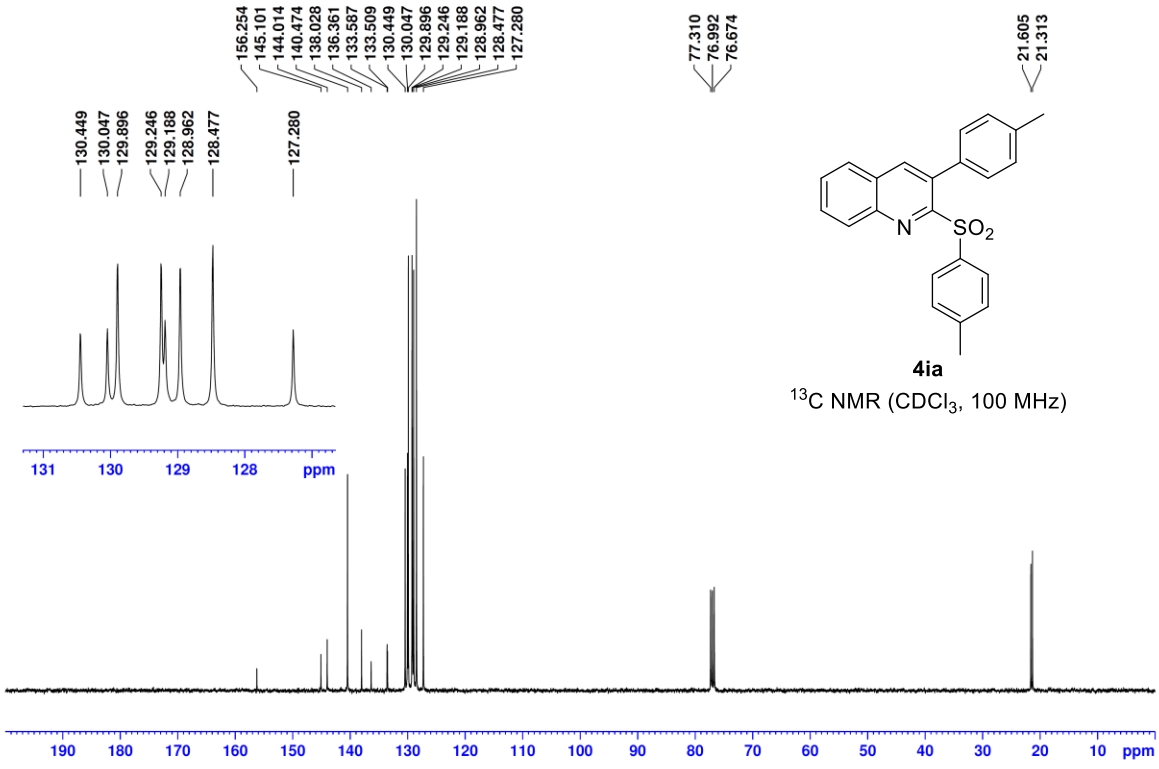

8.121
8.055
8.051
7.801
7.779
7.663
7.642
7.618
7.613
7.596
7.592
7.443
7.260
7.247
7.226
2.434
Ph
Cl
N
S
O2
4ha
1H NMR (CDCl3, 400 MHz)
ppm
0.94
0.89
0.99
1.91
1.02
5.01
2.04
3.00


157.309
145.403
144.356
140.376
136.635
136.152
135.901
133.730
130.366
129.987
129.382
129.141
128.901
128.541
128.446
127.894
126.801
77.316
76.998
76.681
21.668
Ph
Cl
N
S
O2
4ha
13C NMR (CDCl3, 100 MHz)
ppm



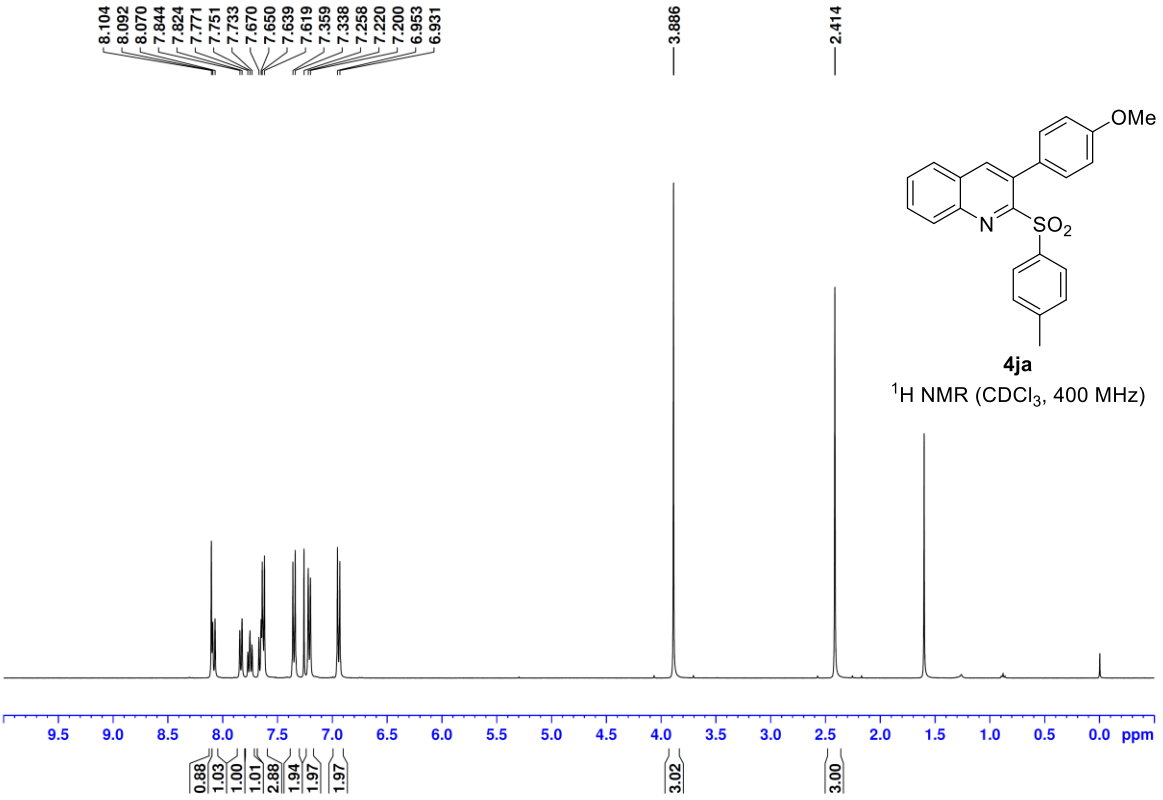
4ia

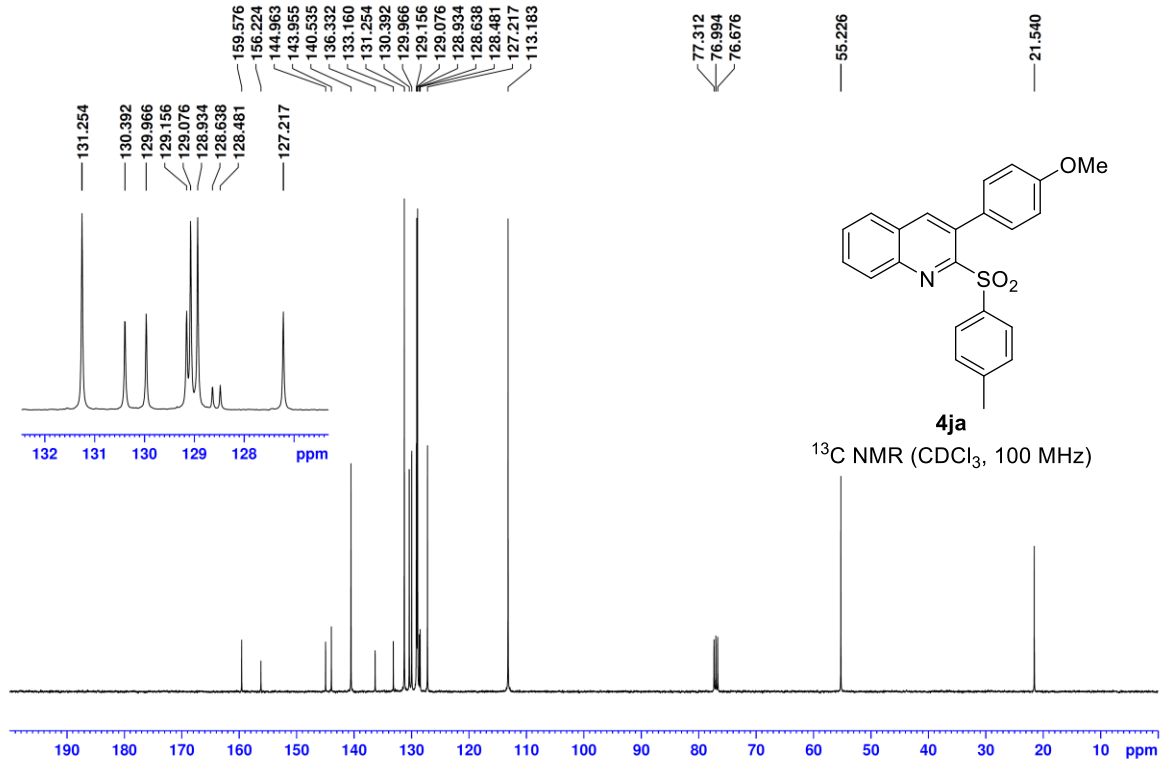
^{1}H NMR ($CDCl_3$, 400 MHz)

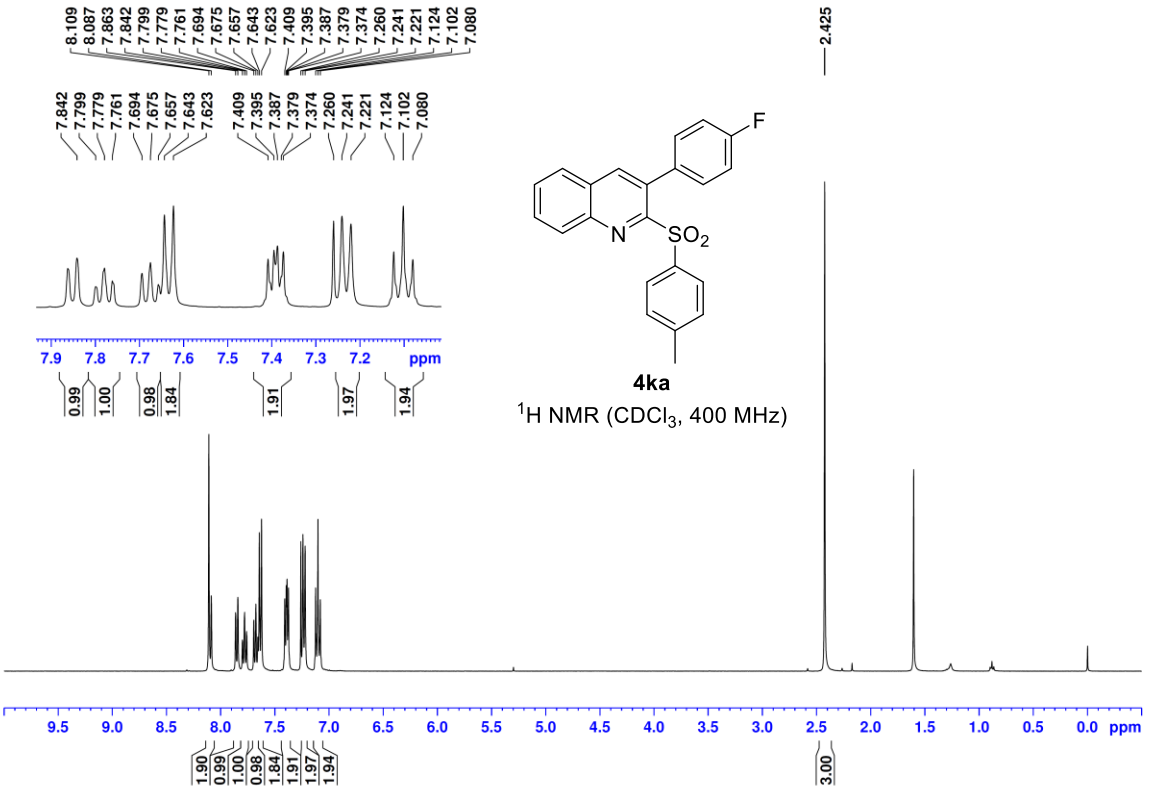


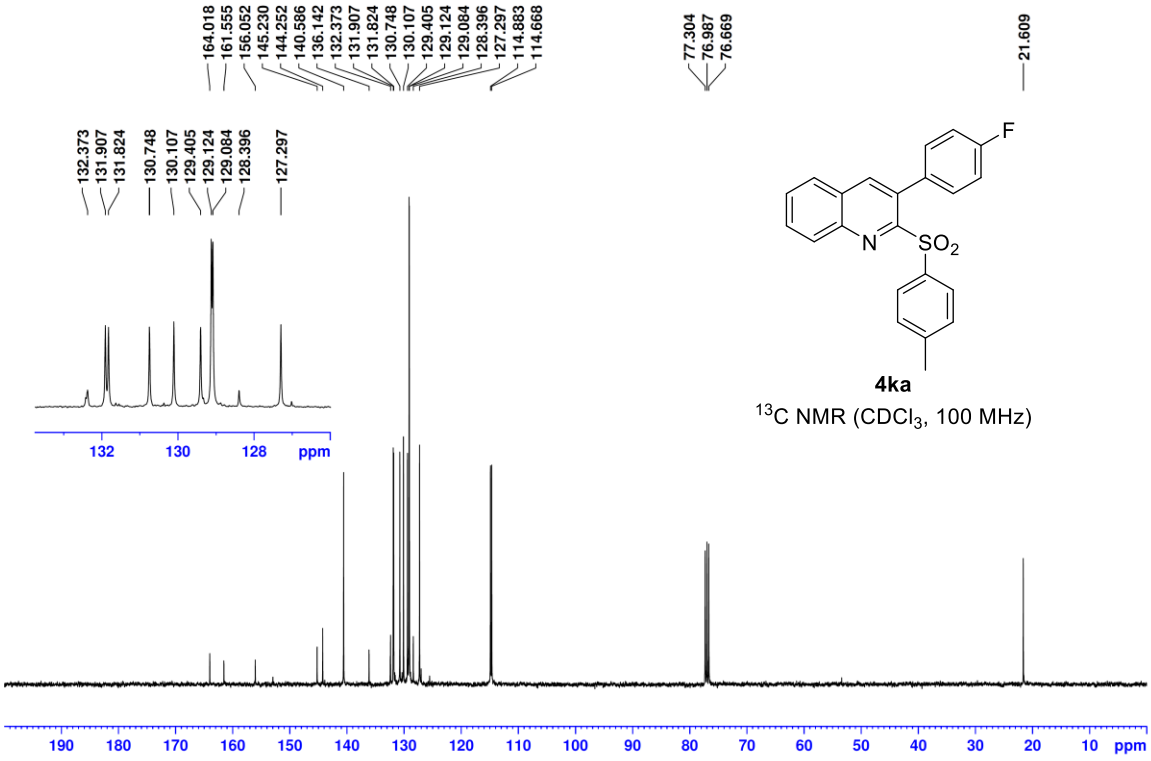
4ia

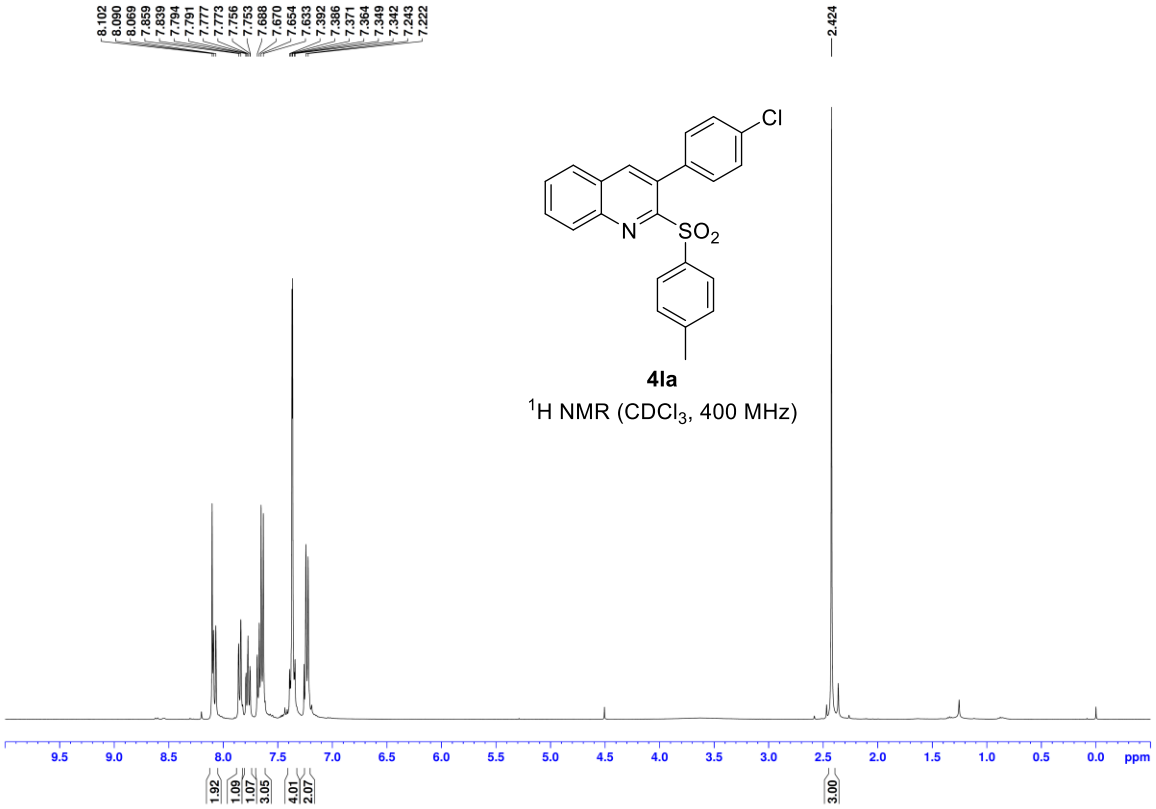
^{13}C NMR ($CDCl_3$, 100 MHz)


8.104
8.092
8.070
7.844
7.824
7.771
7.751
7.733
7.670
7.650
7.639
7.619
7.359
7.338
7.258
7.220
7.200
6.953
6.931
3.886
2.414
OMe
N
SO2
4ja
1H NMR (CDCl3, 400 MHz)
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 ppm
0.88
1.03
1.00
1.01
2.88
1.94
1.97
1.97
3.02
3.00


159.576
156.224
144.963
143.955
140.535
136.332
133.160
131.254
130.392
129.966
129.156
129.076
128.934
128.638
128.481
127.217
113.183
77.312
76.994
76.676
55.226
21.540
131.254
130.392
129.966
129.156
129.076
128.934
128.638
128.481
127.217
132 131 130 129 128 ppm
OMe
N
SO2
4ja
13C NMR (CDCl3, 100 MHz)
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

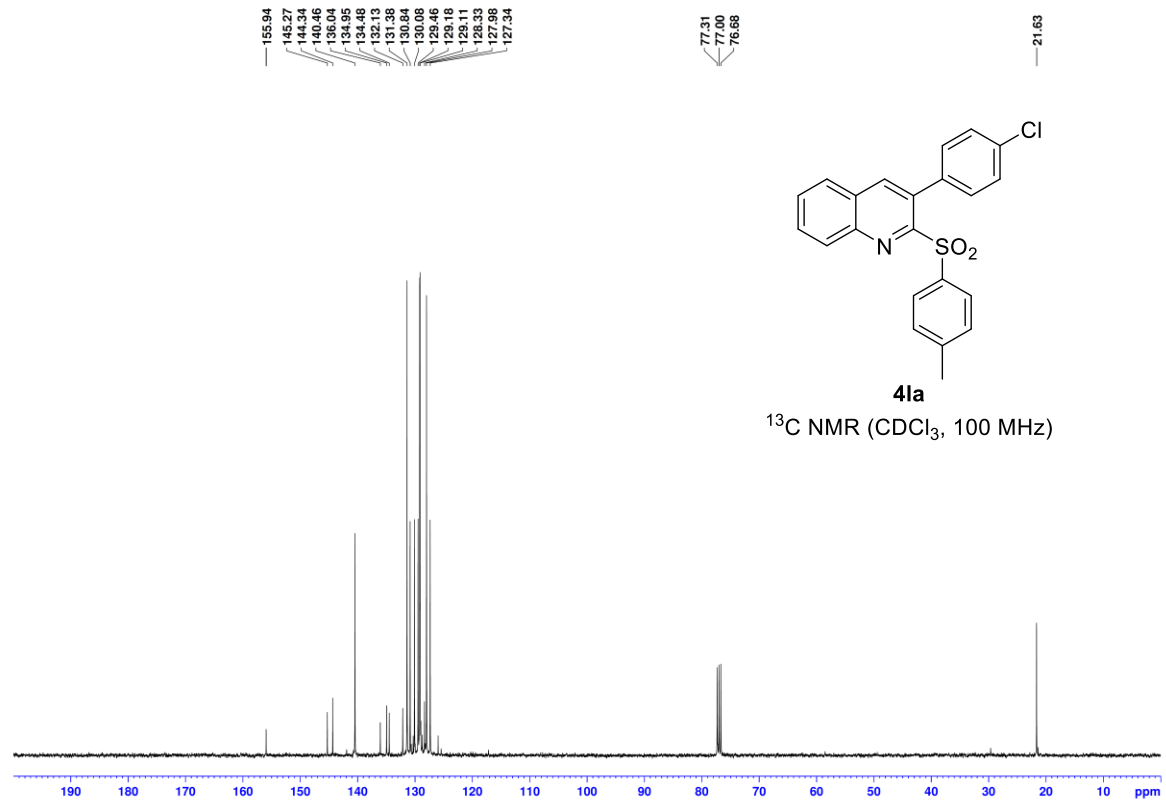

8.109
8.087
7.863
7.842
7.799
7.779
7.761
7.694
7.675
7.657
7.643
7.623
7.409
7.395
7.387
7.379
7.374
7.260
7.241
7.221
7.124
7.102
7.080
2.425
F
N
SO2
4ka
1H NMR (CDCl3, 400 MHz)
ppm
1.90
0.99
1.00
0.98
1.84
1.91
1.97
1.94
3.00


164.018
161.555
156.052
145.230
144.252
140.586
136.142
132.373
131.907
131.824
130.748
130.107
129.405
129.124
129.084
128.396
127.297
114.883
114.668
77.304
76.987
76.669
21.609
F
N
SO2
4ka
13C NMR (CDCl3, 100 MHz)
ppm



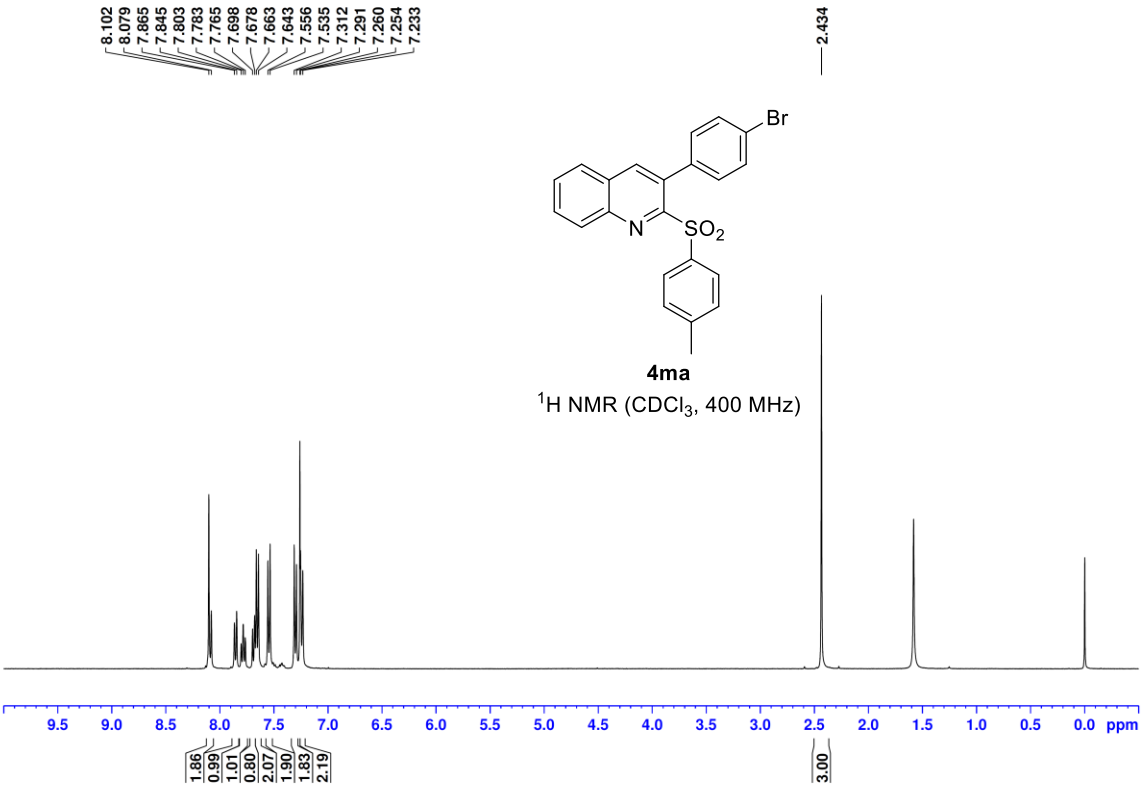
4la

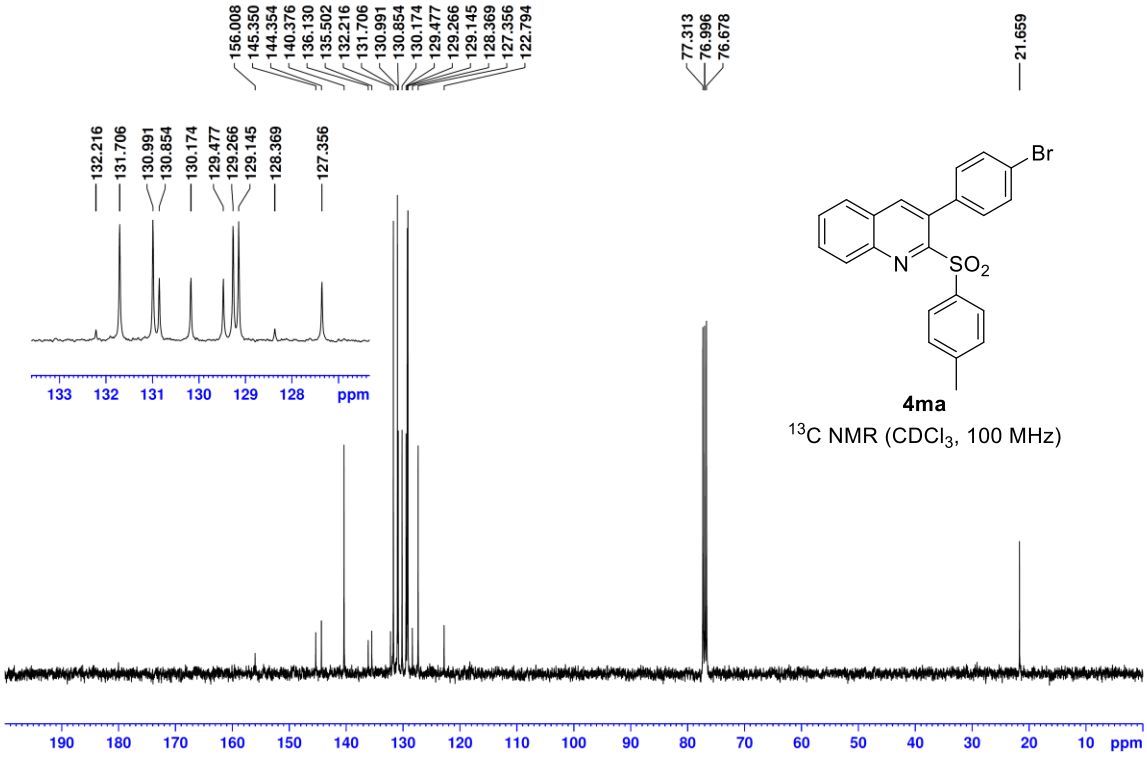
^{1}H NMR ($CDCl_3$, 400 MHz)

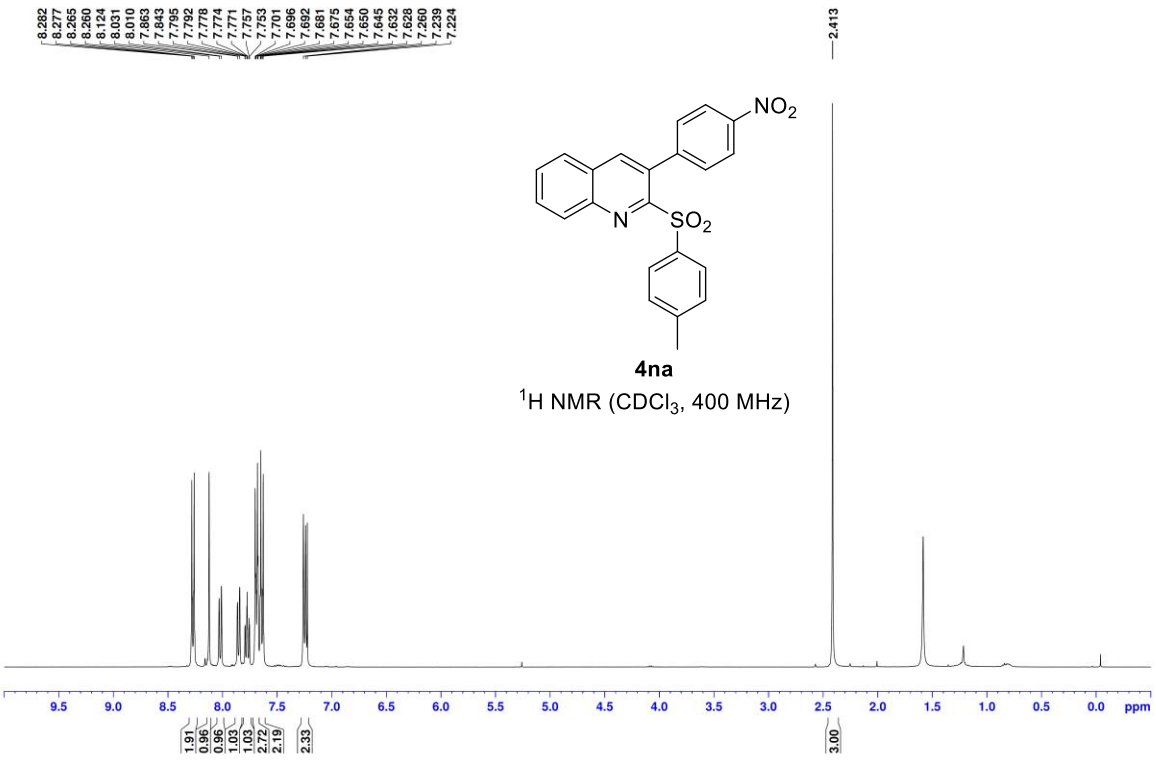


4la

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

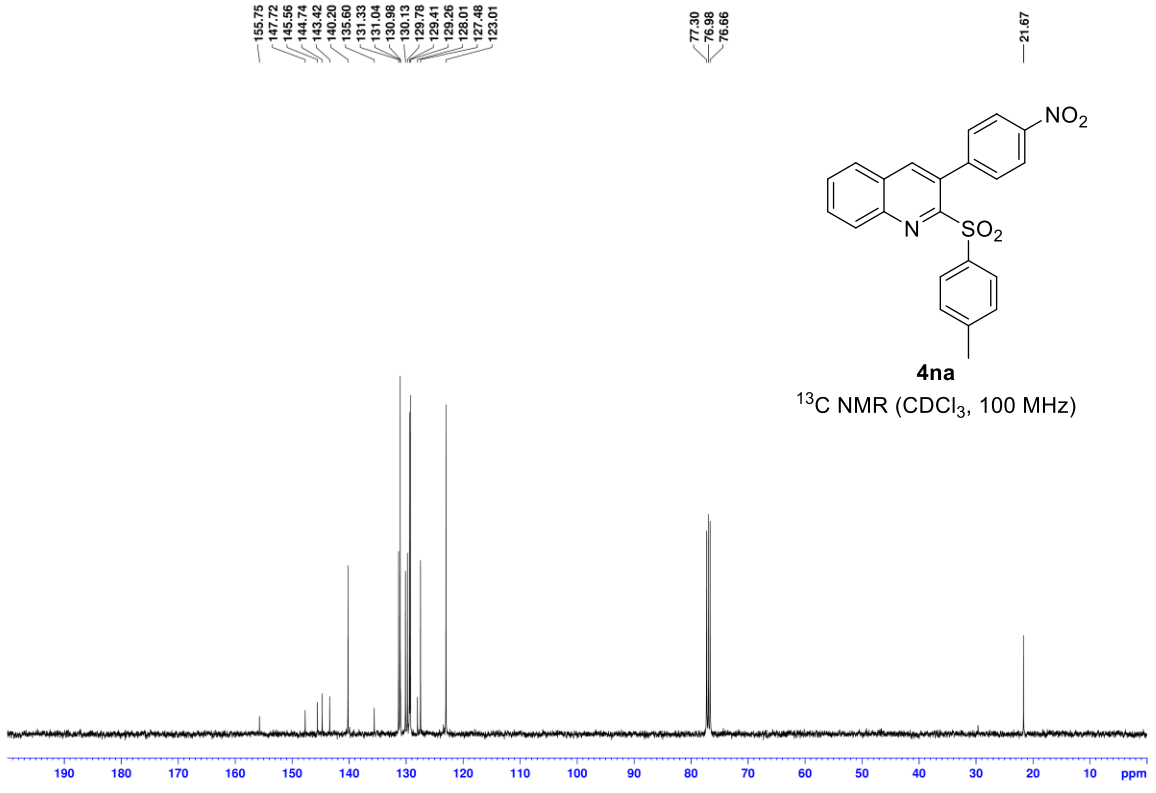

8.102
8.079
7.865
7.845
7.803
7.783
7.765
7.698
7.678
7.663
7.643
7.556
7.535
7.312
7.291
7.260
7.254
7.233
2.434
Br
N
SO2
4ma
1H NMR (CDCl3, 400 MHz)
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.86
0.99
1.01
0.80
2.07
1.90
1.83
2.19
3.00


156.008
145.350
144.354
140.376
136.130
135.502
132.216
131.706
130.991
130.854
130.174
129.477
129.266
129.145
128.369
127.356
122.794
77.313
76.996
76.678
21.659
132.216
131.706
130.991
130.854
130.174
129.477
129.266
129.145
128.369
127.356
133 132 131 130 129 128 ppm
Br
N
SO2
4ma
13C NMR (CDCl3, 100 MHz)
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm



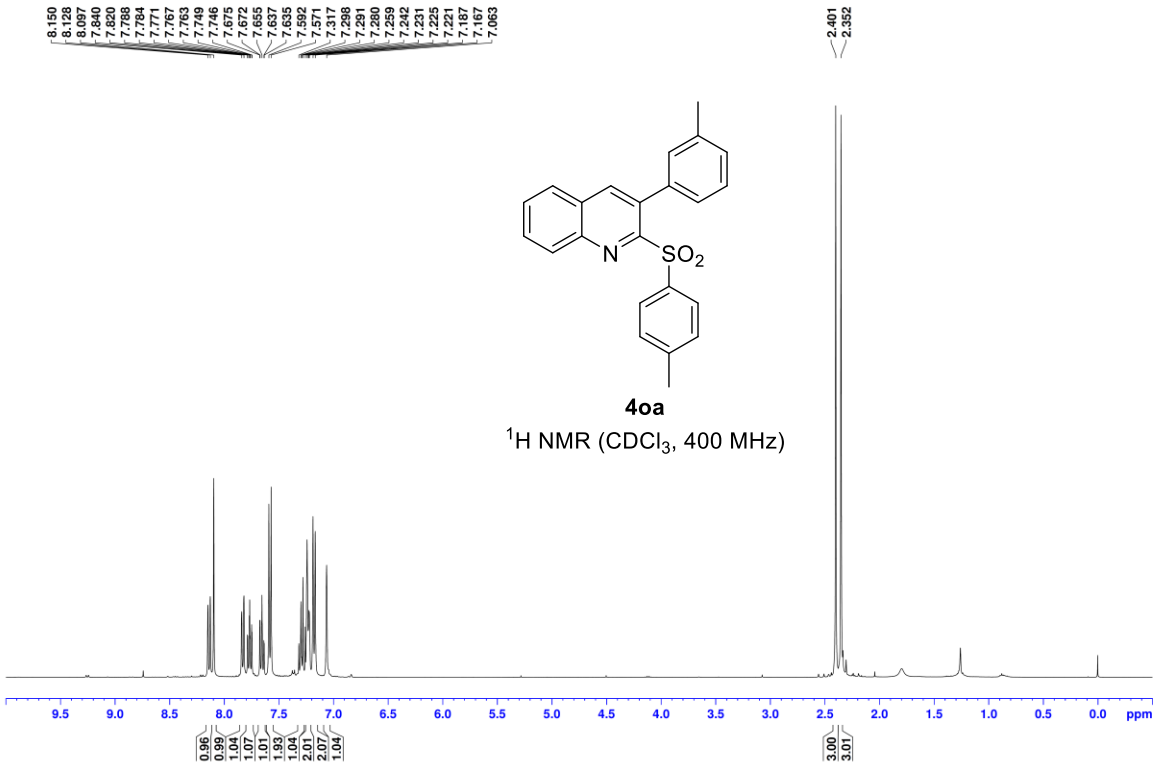
4na

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



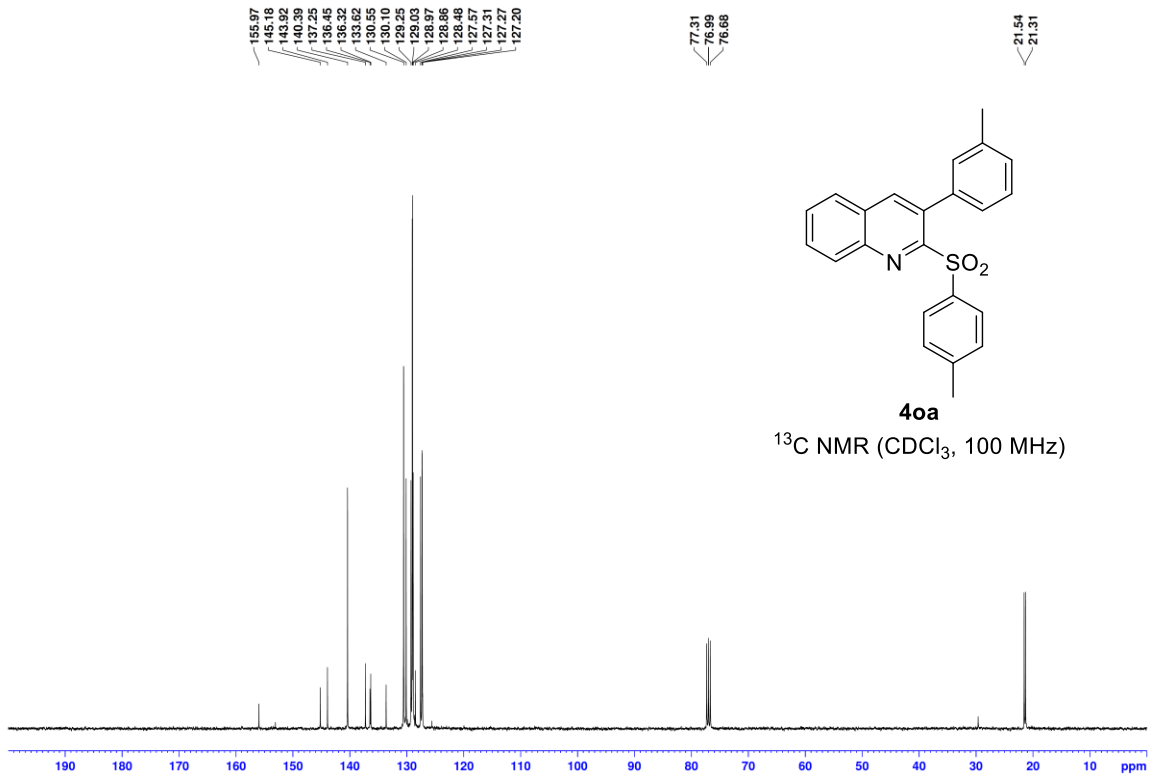
4na

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



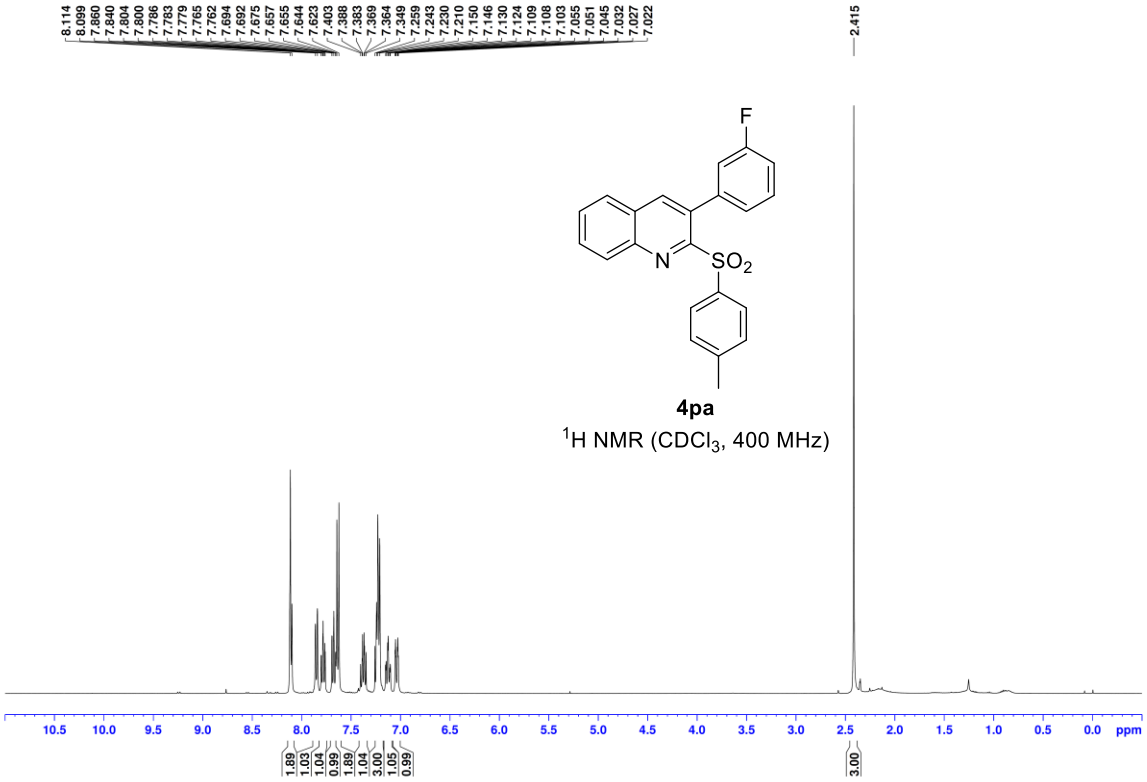
4oa

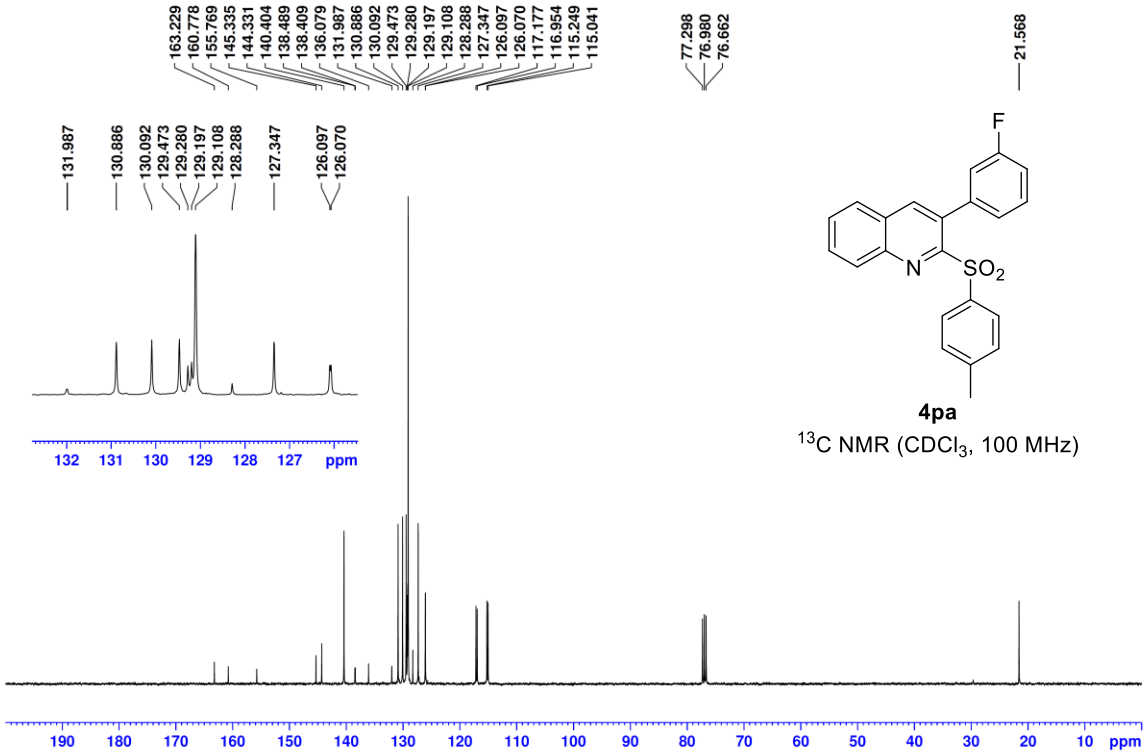
^{1}H NMR ($CDCl_3$, 400 MHz)

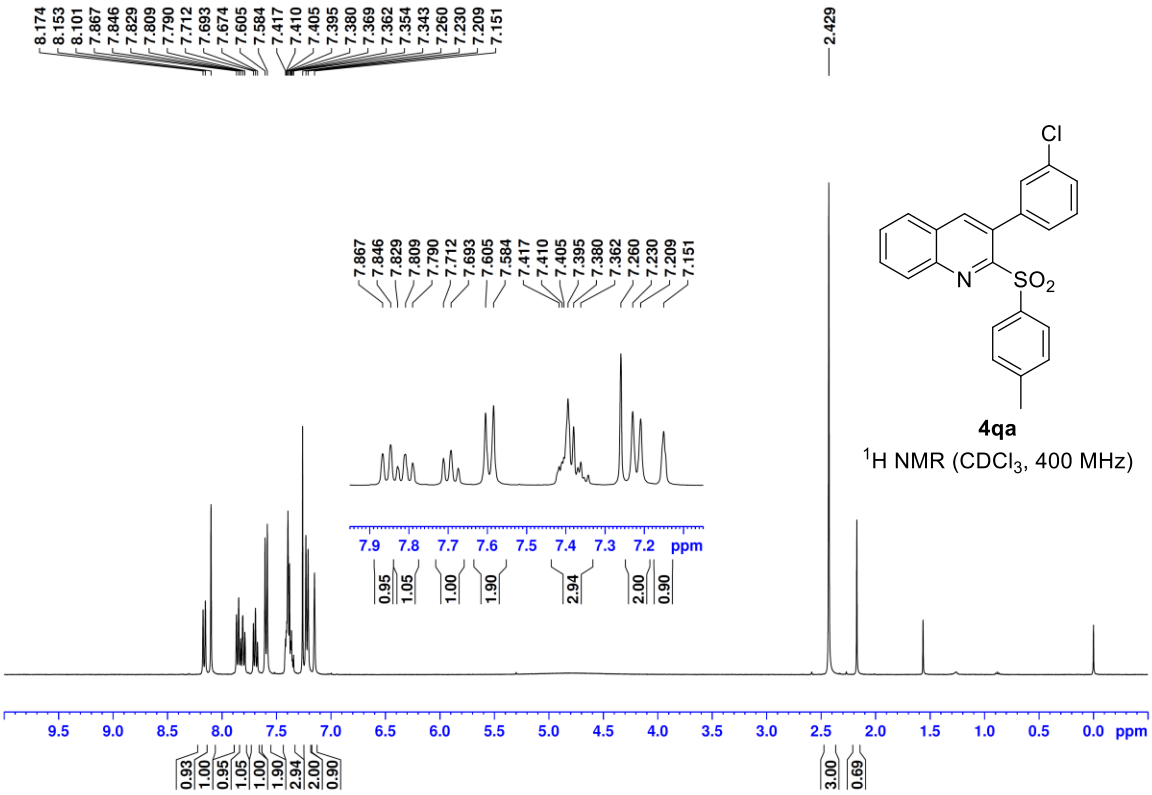


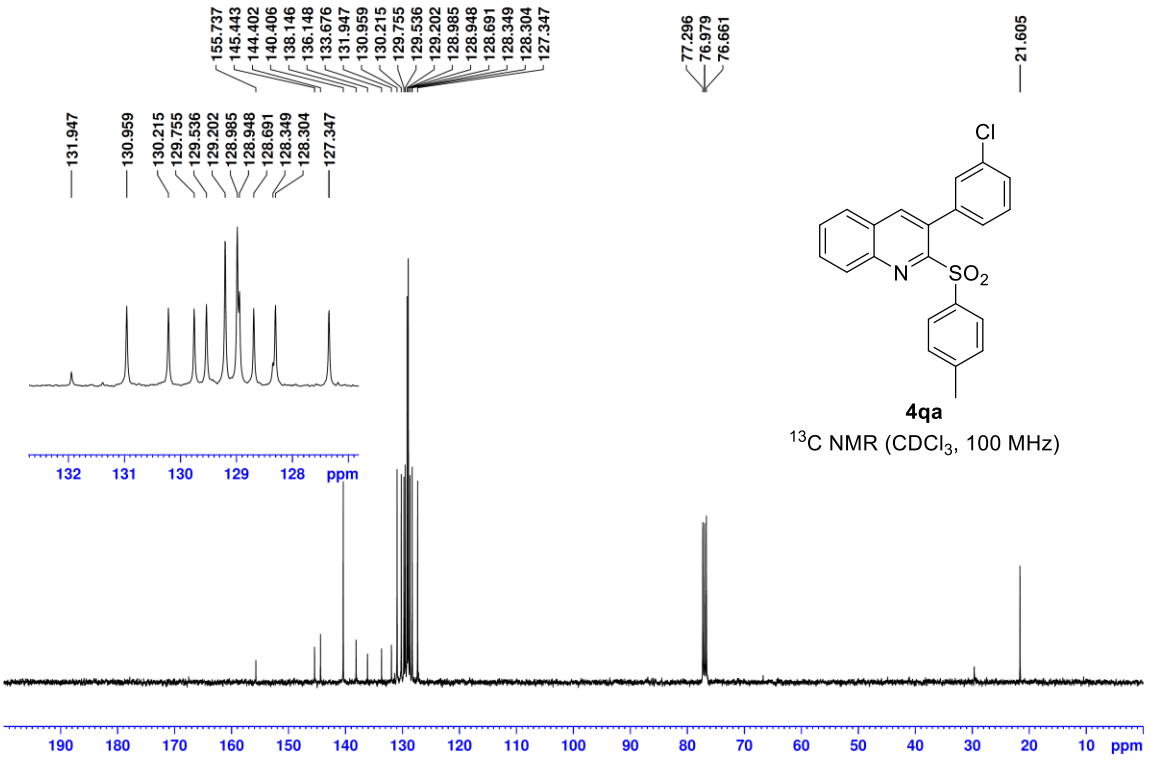
4oa

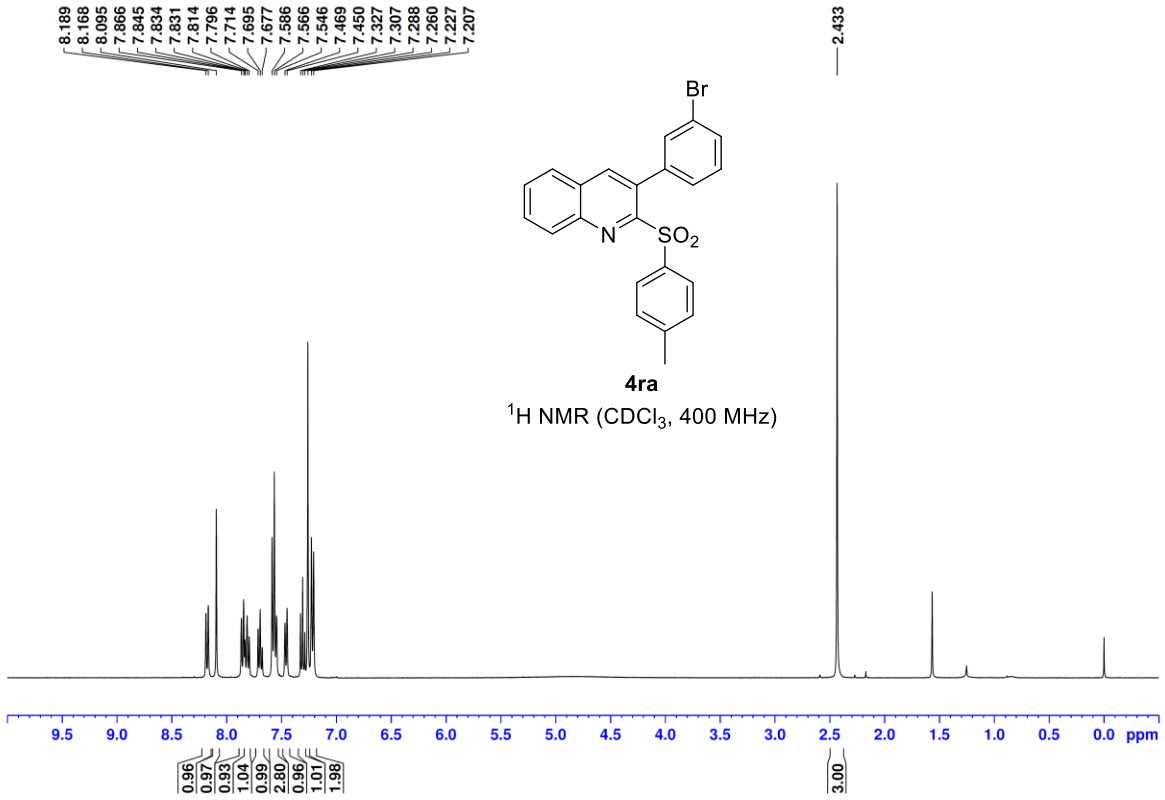
^{13}C NMR ($CDCl_3$, 100 MHz)


8.114
8.099
7.860
7.840
7.804
7.800
7.786
7.783
7.779
7.765
7.762
7.694
7.692
7.675
7.657
7.655
7.644
7.623
7.403
7.388
7.383
7.369
7.364
7.349
7.259
7.243
7.230
7.210
7.150
7.146
7.130
7.124
7.109
7.108
7.103
7.055
7.051
7.045
7.032
7.027
7.022
2.415
F
N
SO2
4pa
1H NMR (CDCl3, 400 MHz)
10.5 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 ppm
1.89 1.03 1.04 0.99 1.89 1.04 3.00 1.05 0.99
3.00


163.229
160.778
155.769
145.335
144.331
140.404
138.489
138.409
136.079
131.987
130.886
130.092
129.473
129.280
129.197
129.108
128.288
127.347
126.097
126.070
117.177
116.954
115.249
115.041
77.298
76.980
76.662
21.568
131.987
130.886
130.092
129.473
129.280
129.197
129.108
128.288
127.347
126.097
126.070
132 131 130 129 128 127 ppm
F
N
SO2
4pa
13C NMR (CDCl3, 100 MHz)
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

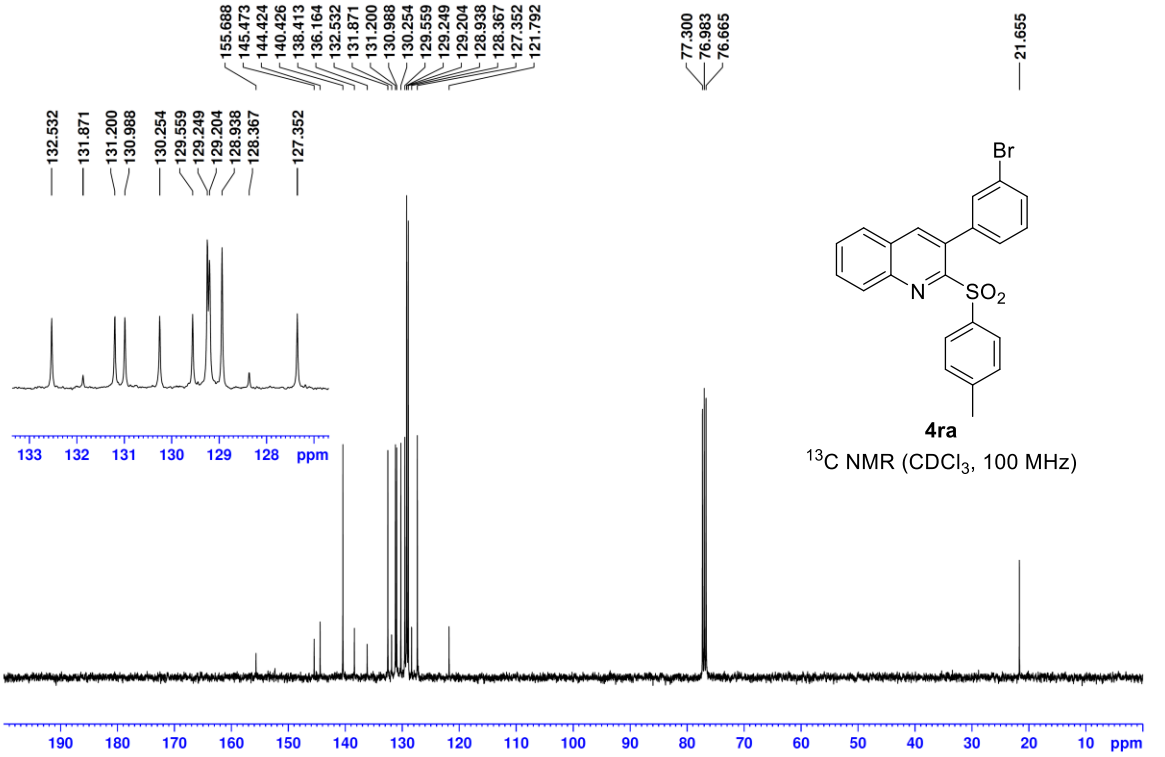

8.174
8.153
8.101
7.867
7.846
7.829
7.809
7.790
7.712
7.693
7.674
7.605
7.584
7.417
7.410
7.405
7.395
7.380
7.369
7.362
7.354
7.343
7.260
7.230
7.209
7.151
2.429
Cl
N
SO2
4qa
1H NMR (CDCl3, 400 MHz)
ppm


155.737
145.443
144.402
140.406
138.146
136.148
133.676
131.947
130.959
130.215
129.755
129.536
129.202
128.985
128.948
128.691
128.349
128.304
127.347
77.296
76.979
76.661
21.605
Cl
N
SO2
4qa
13C NMR (CDCl3, 100 MHz)
ppm



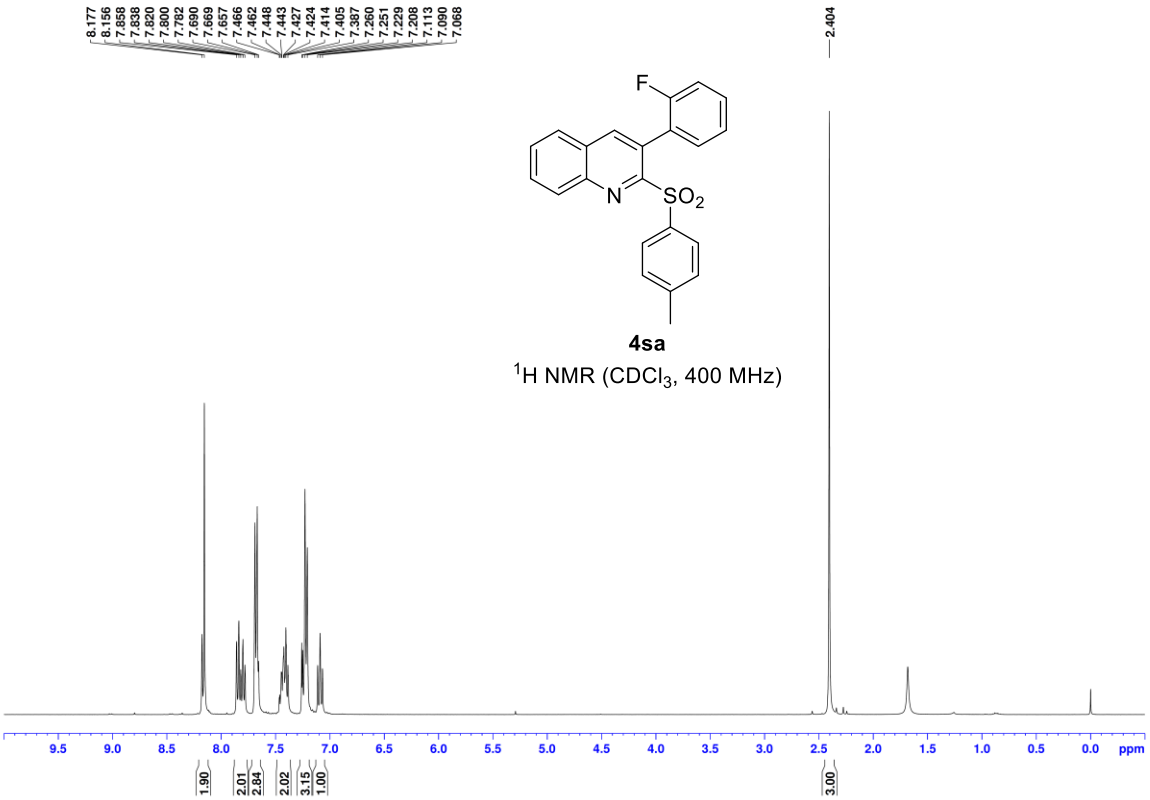
4ra

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



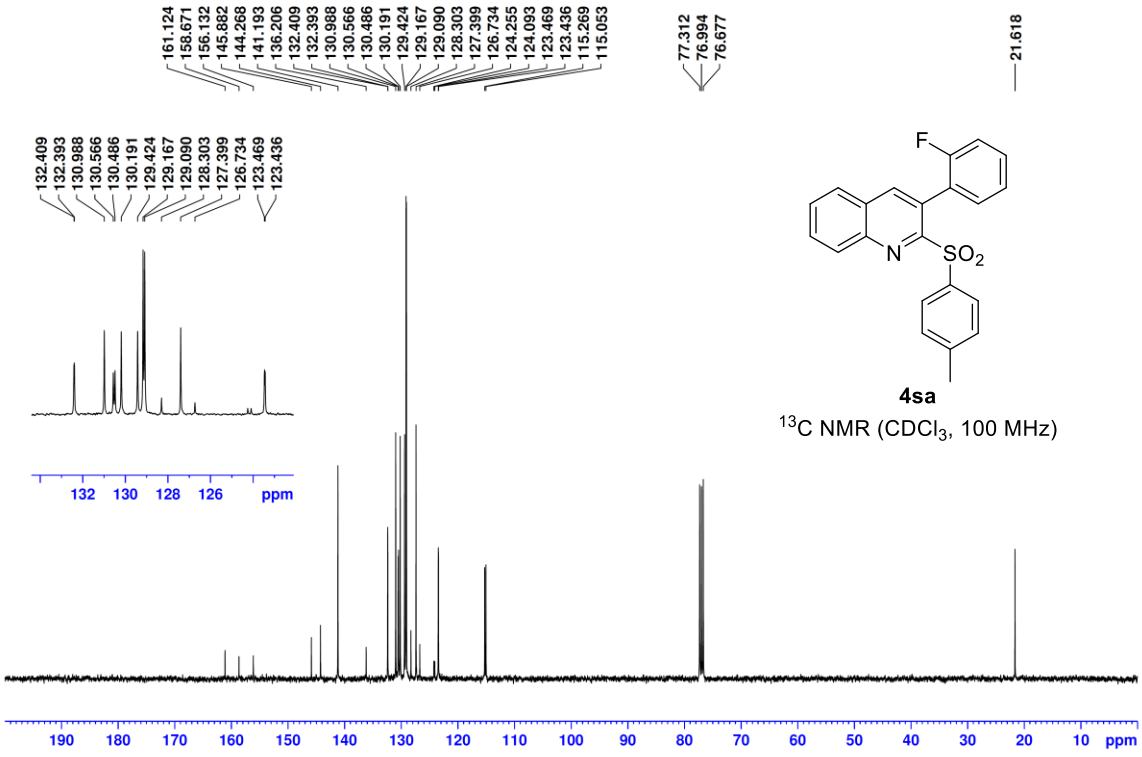
4ra

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



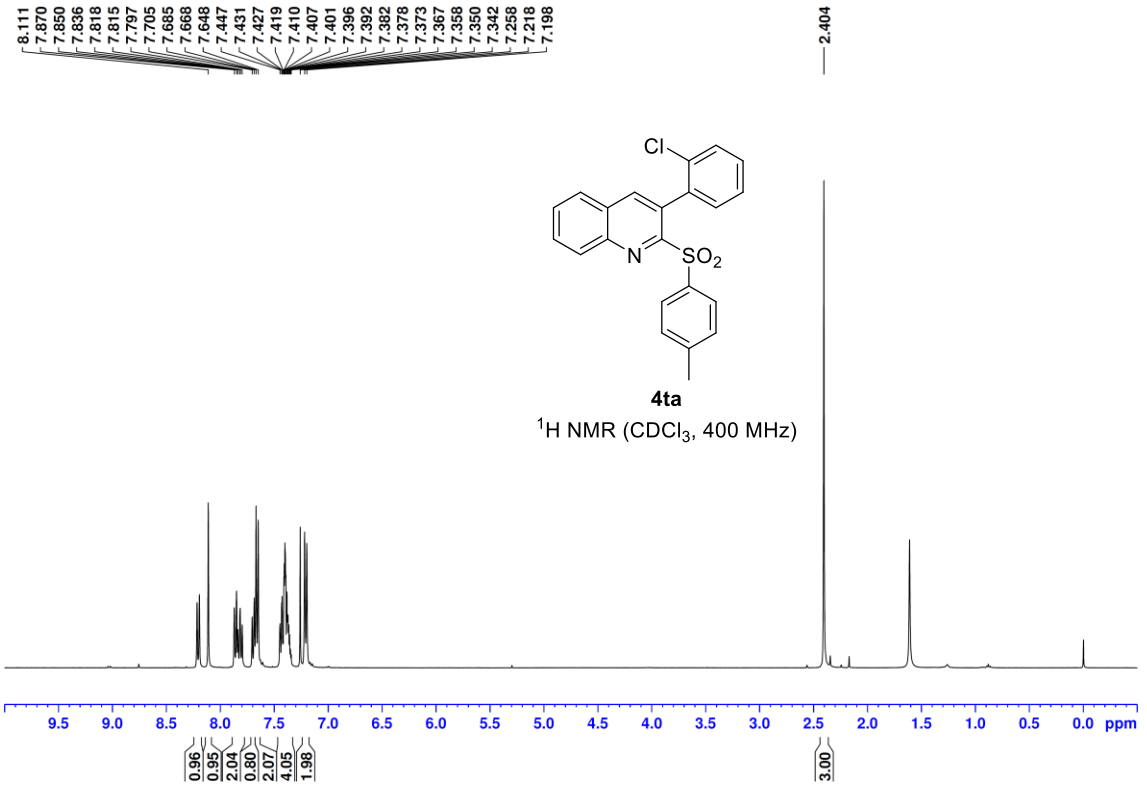
4sa

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



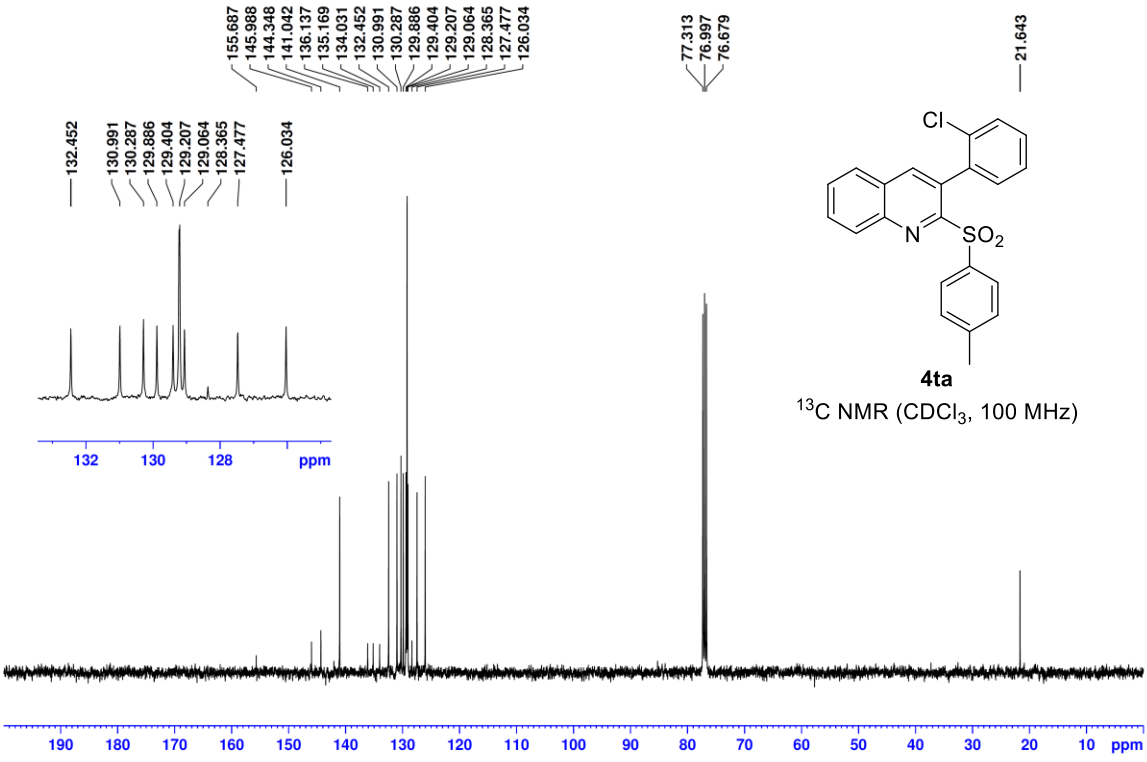
4sa

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



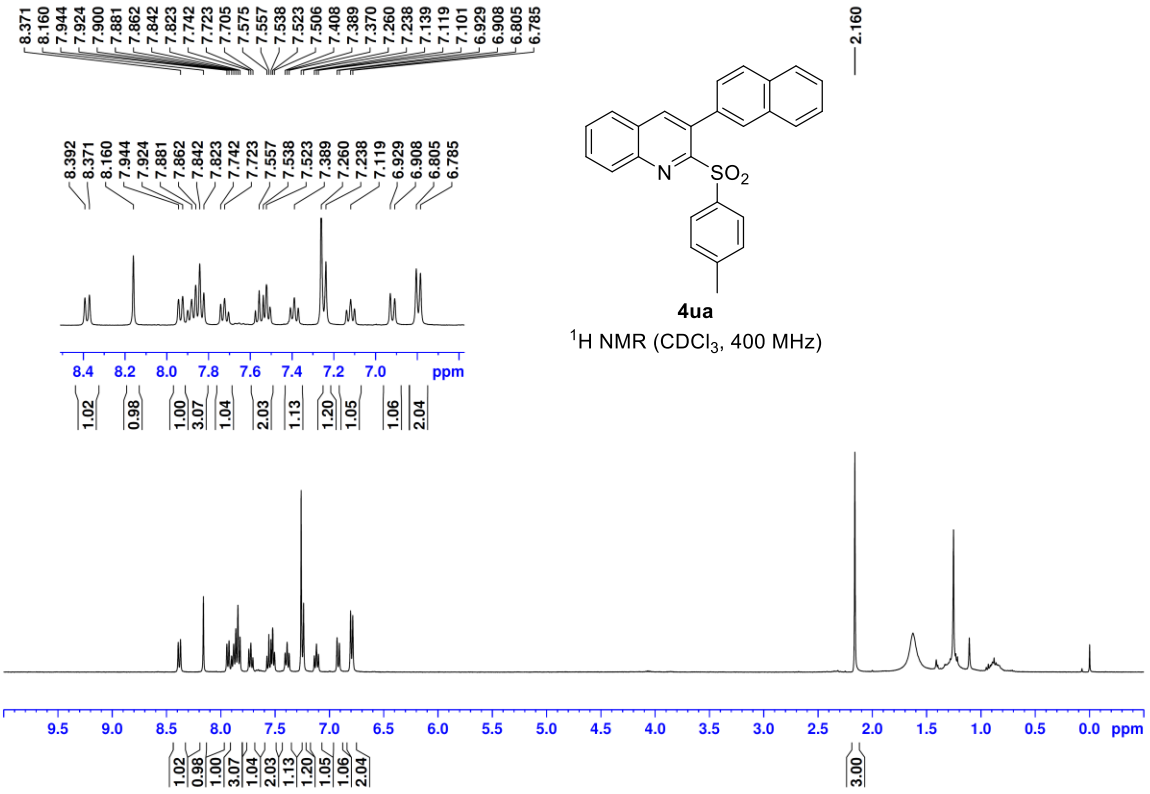
4ta

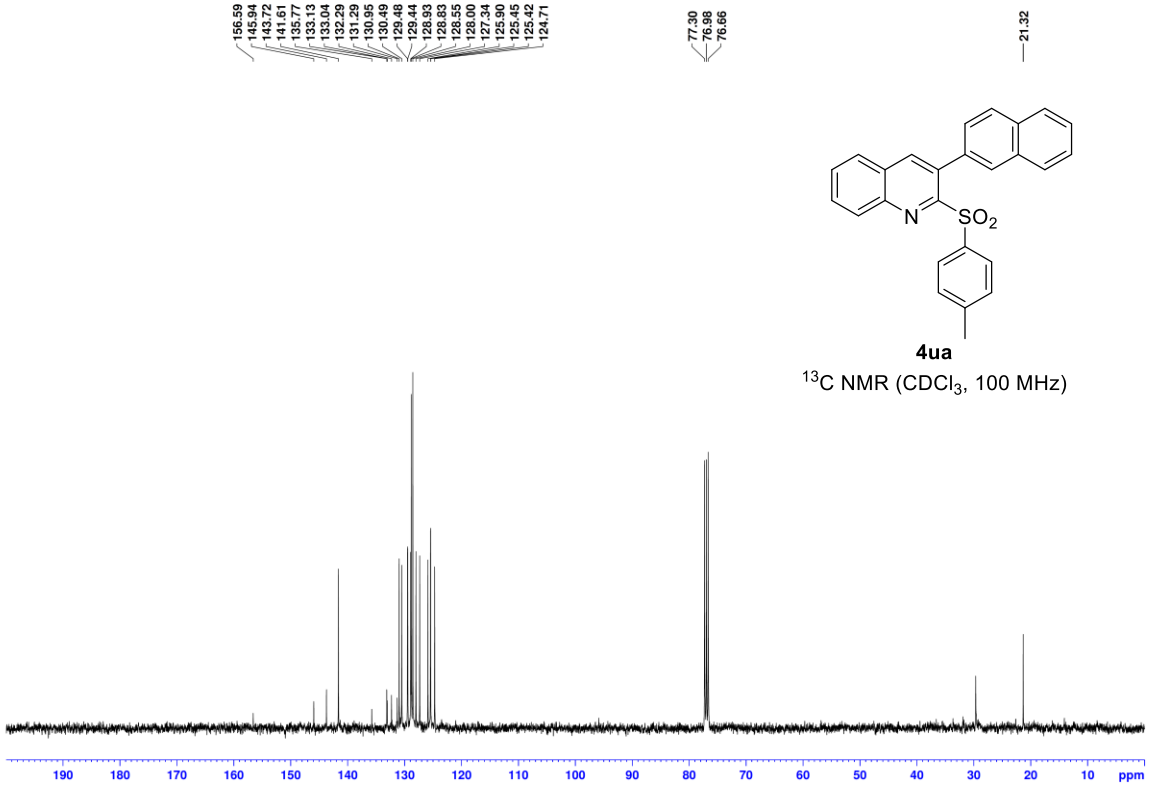
^{1}H NMR ($CDCl_3$, 400 MHz)

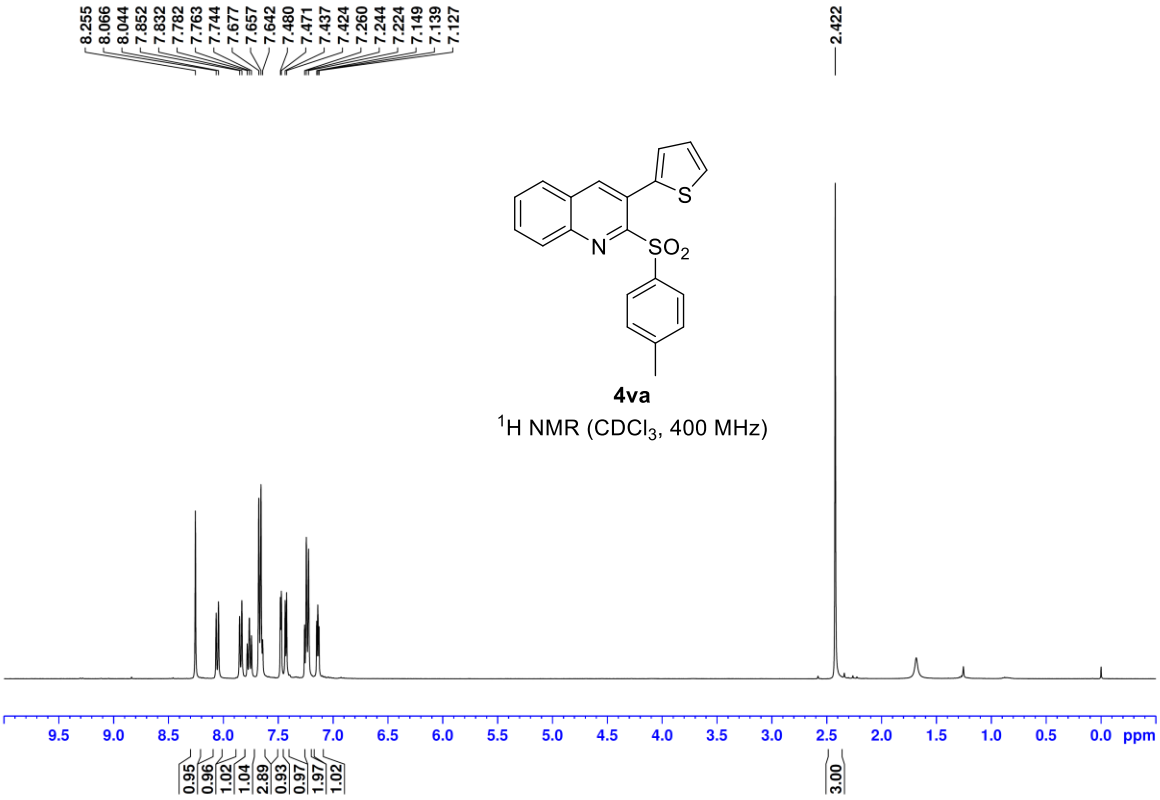


4ta

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

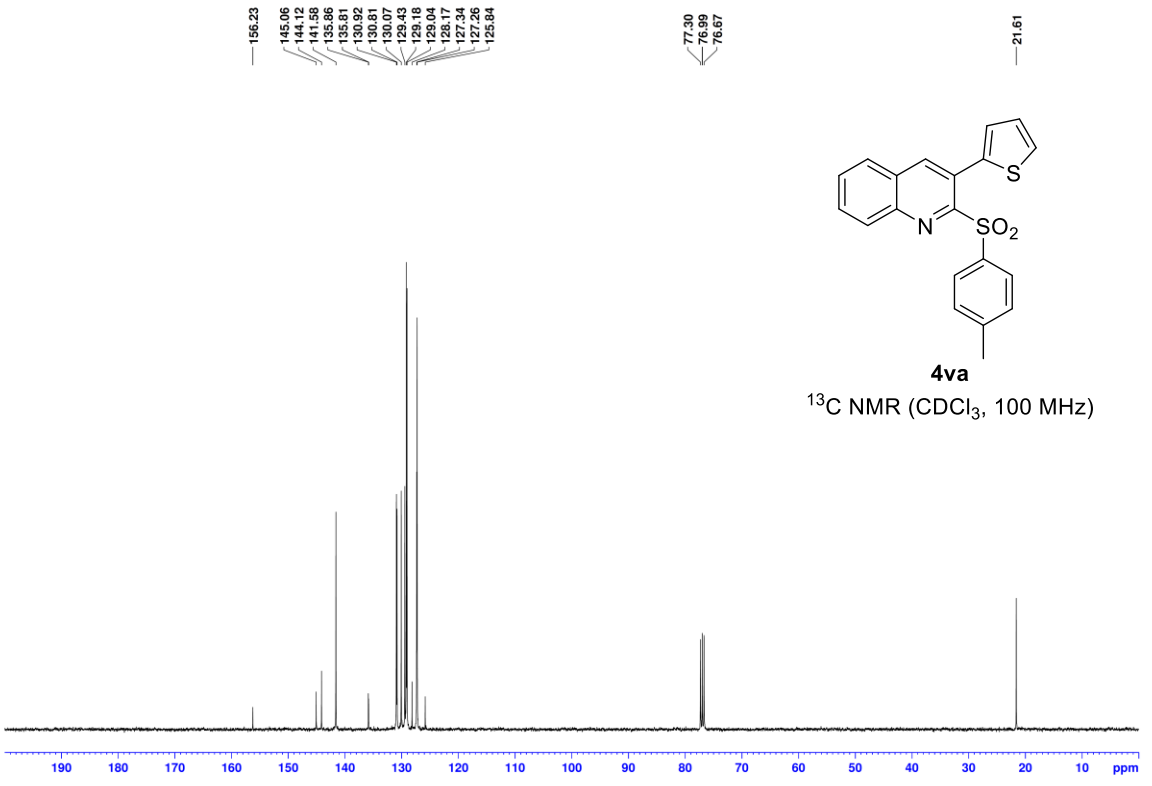

8.371
8.160
7.944
7.924
7.900
7.881
7.862
7.842
7.823
7.742
7.723
7.705
7.575
7.557
7.538
7.523
7.506
7.408
7.389
7.370
7.260
7.238
7.139
7.119
7.101
6.929
6.908
6.805
6.785
2.160
N
SO2
4ua
1H NMR (CDCl3, 400 MHz)
ppm
1.02
0.98
1.00
3.07
1.04
2.03
1.13
1.20
1.05
1.06
2.04
3.00


156.59
145.94
143.72
141.61
135.77
133.13
133.04
132.29
131.29
130.95
130.49
129.48
129.44
128.93
128.83
128.55
128.00
127.34
125.90
125.45
125.42
124.71
77.30
76.98
76.66
21.32
N
SO2
4ua
13C NMR (CDCl3, 100 MHz)
ppm



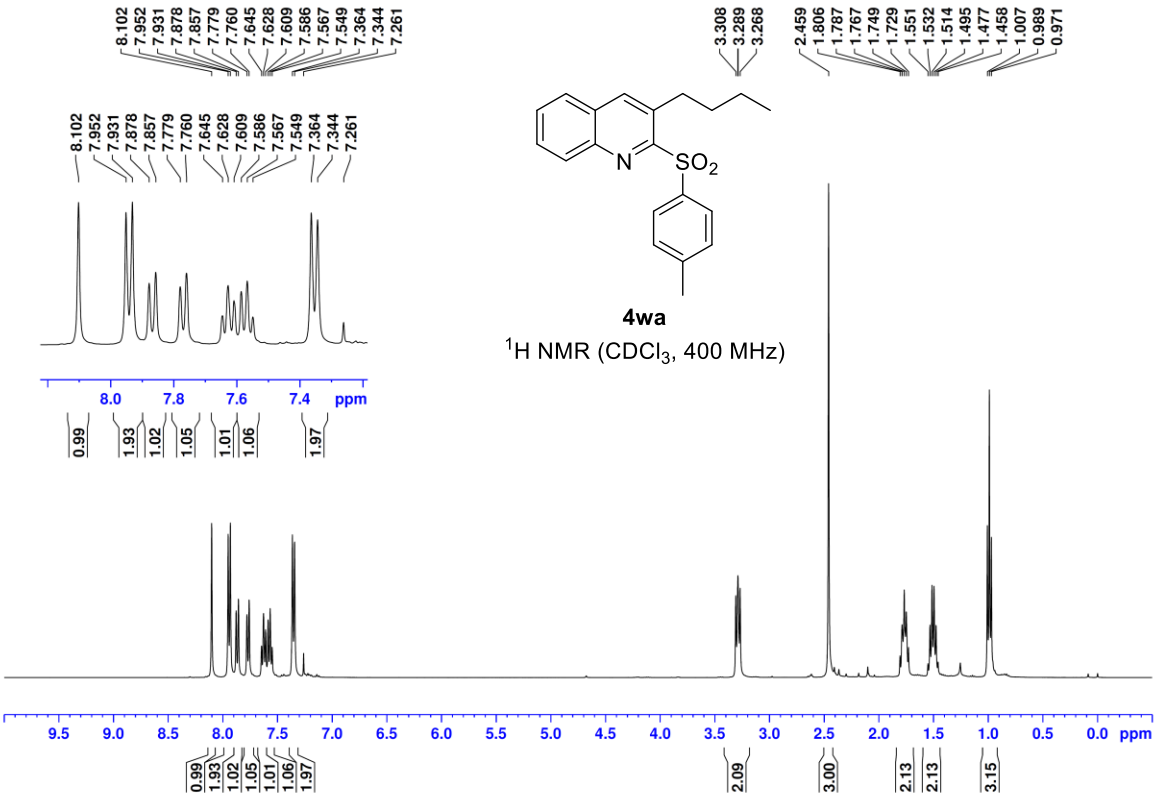
4va

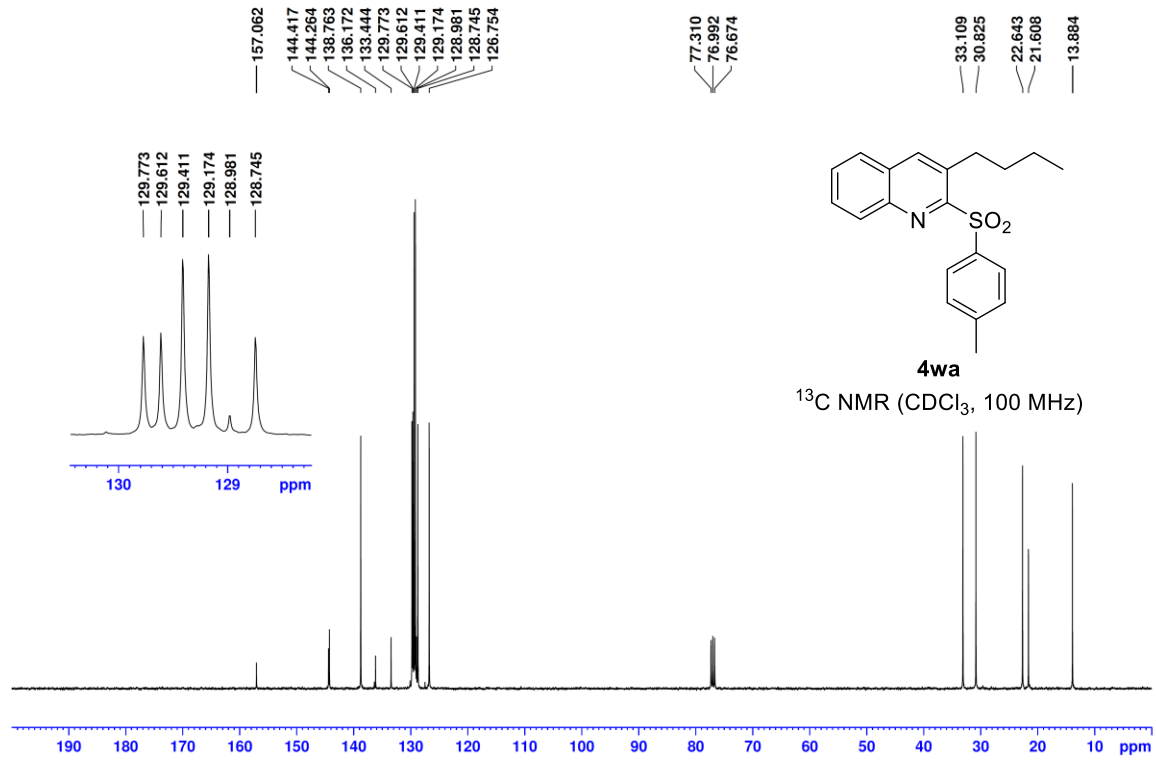
^{1}H NMR ($CDCl_3$, 400 MHz)

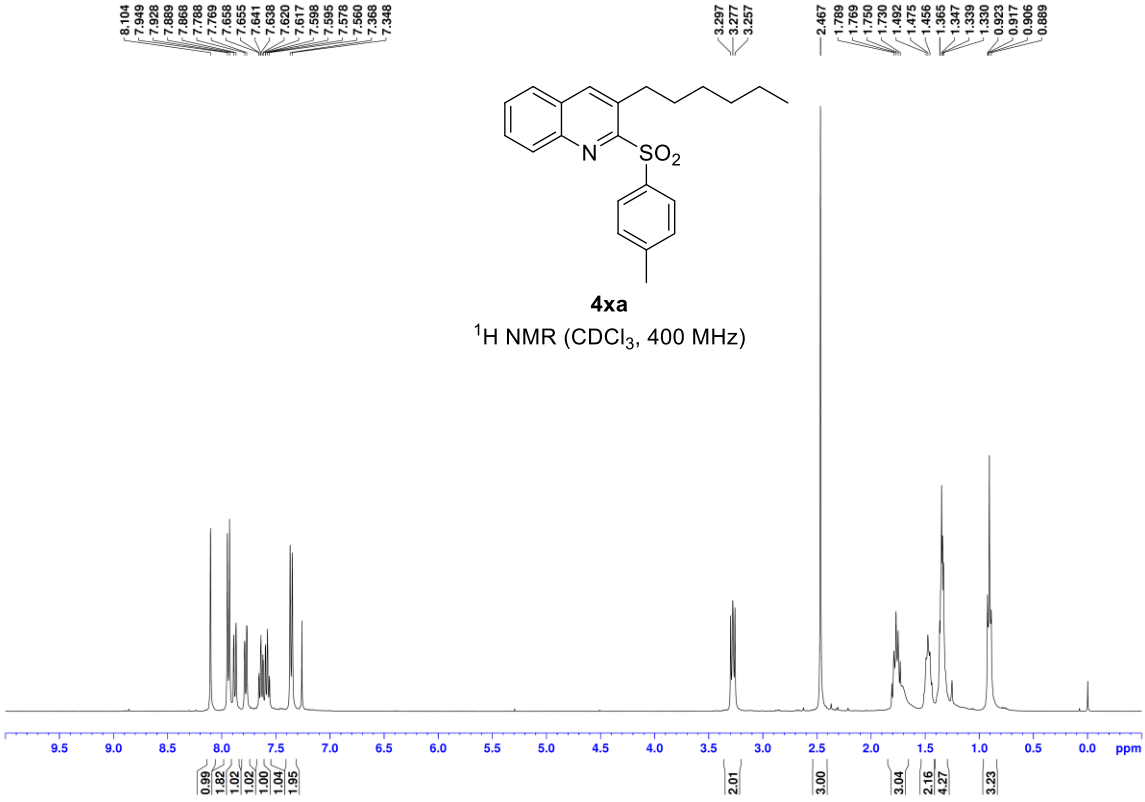


4va

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

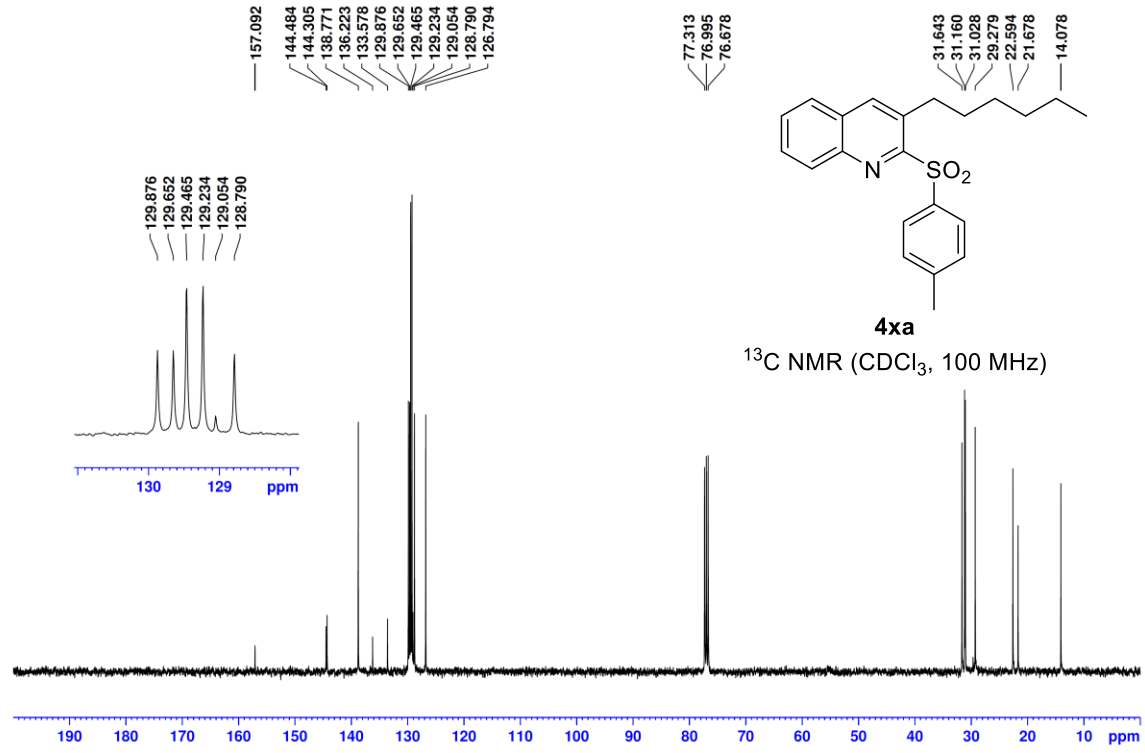

8.102
7.952
7.931
7.878
7.857
7.779
7.760
7.645
7.628
7.609
7.586
7.567
7.549
7.364
7.344
7.261
3.308
3.289
3.268
2.459
1.806
1.787
1.767
1.749
1.729
1.551
1.532
1.514
1.495
1.477
1.458
1.007
0.989
0.971
N
SO2
4wa
1H NMR (CDCl3, 400 MHz)
8.0
7.8
7.6
7.4
ppm
0.99
1.93
1.02
1.05
1.01
1.06
1.97
9.5
9.0
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
ppm
0.99
1.93
1.02
1.05
1.01
1.06
1.97
2.09
3.00
2.13
2.13
3.15


157.062
144.417
144.264
138.763
136.172
133.444
129.773
129.612
129.411
129.174
128.981
128.745
126.754
77.310
76.992
76.674
33.109
30.825
22.643
21.608
13.884
129.773
129.612
129.411
129.174
128.981
128.745
N
SO2
4wa
13C NMR (CDCl3, 100 MHz)
130
129
ppm
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm



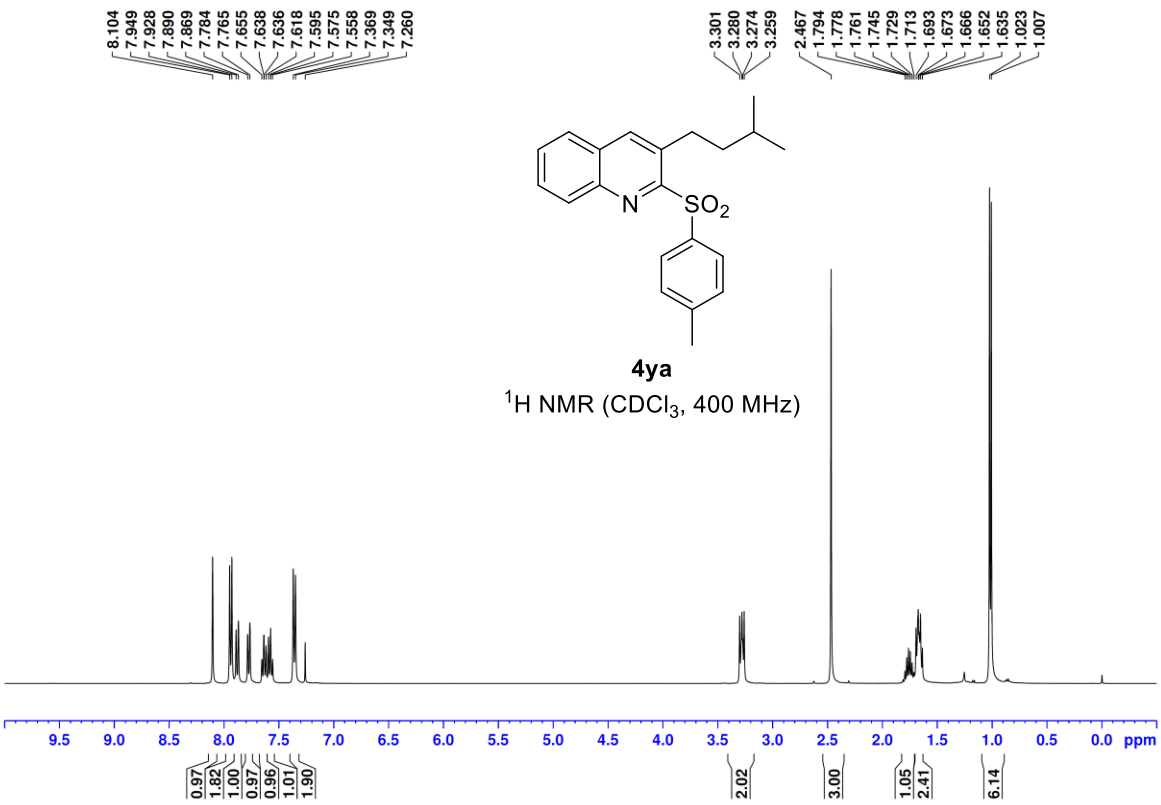
4xa

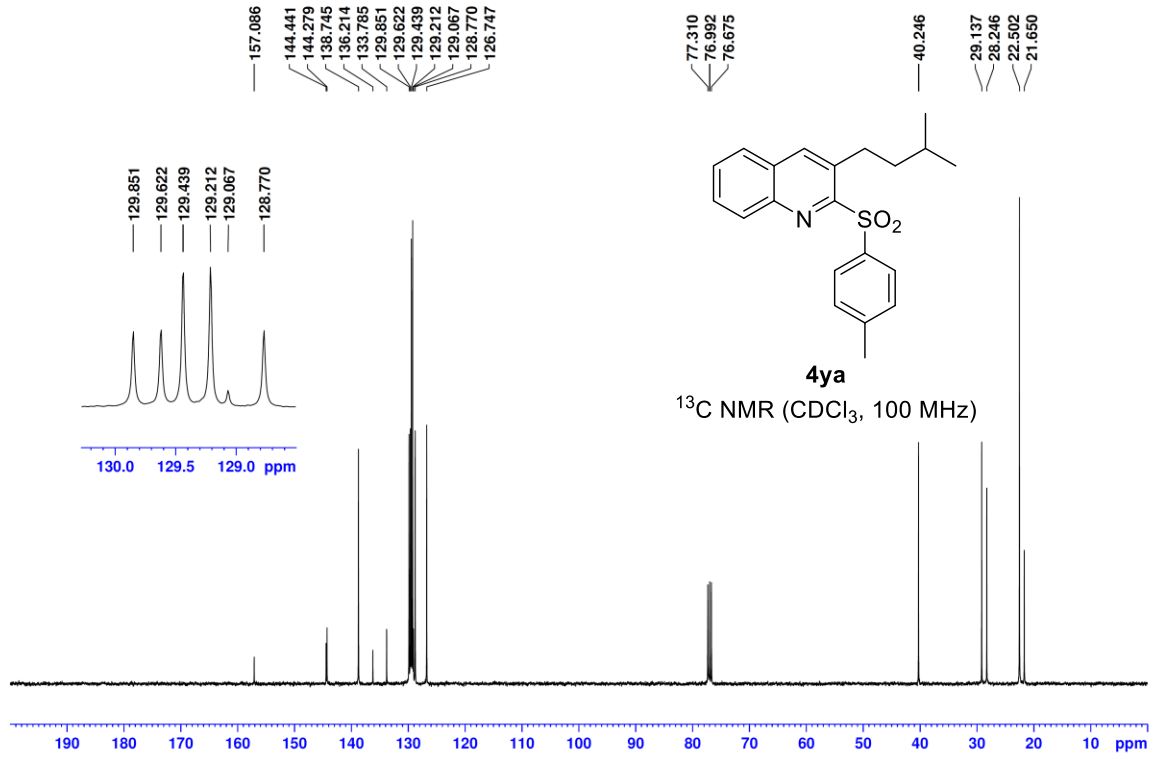
^{1}H NMR ($CDCl_3$, 400 MHz)

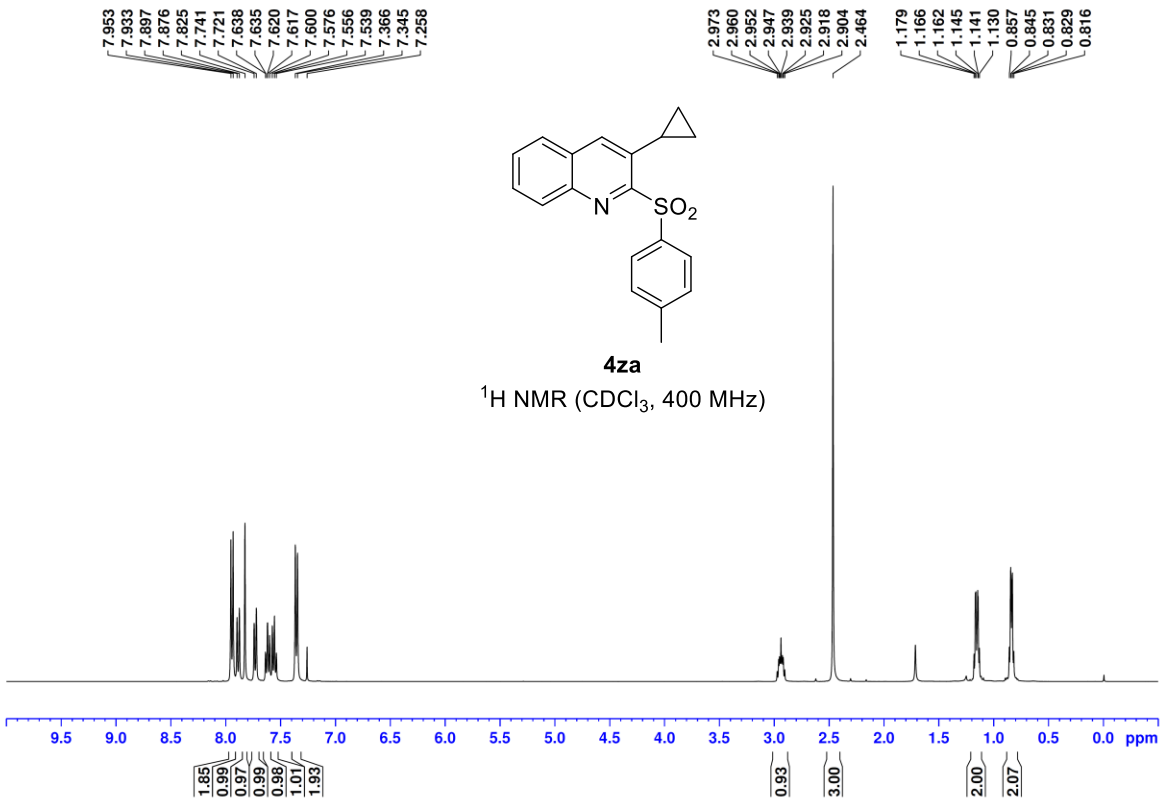


4xa

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

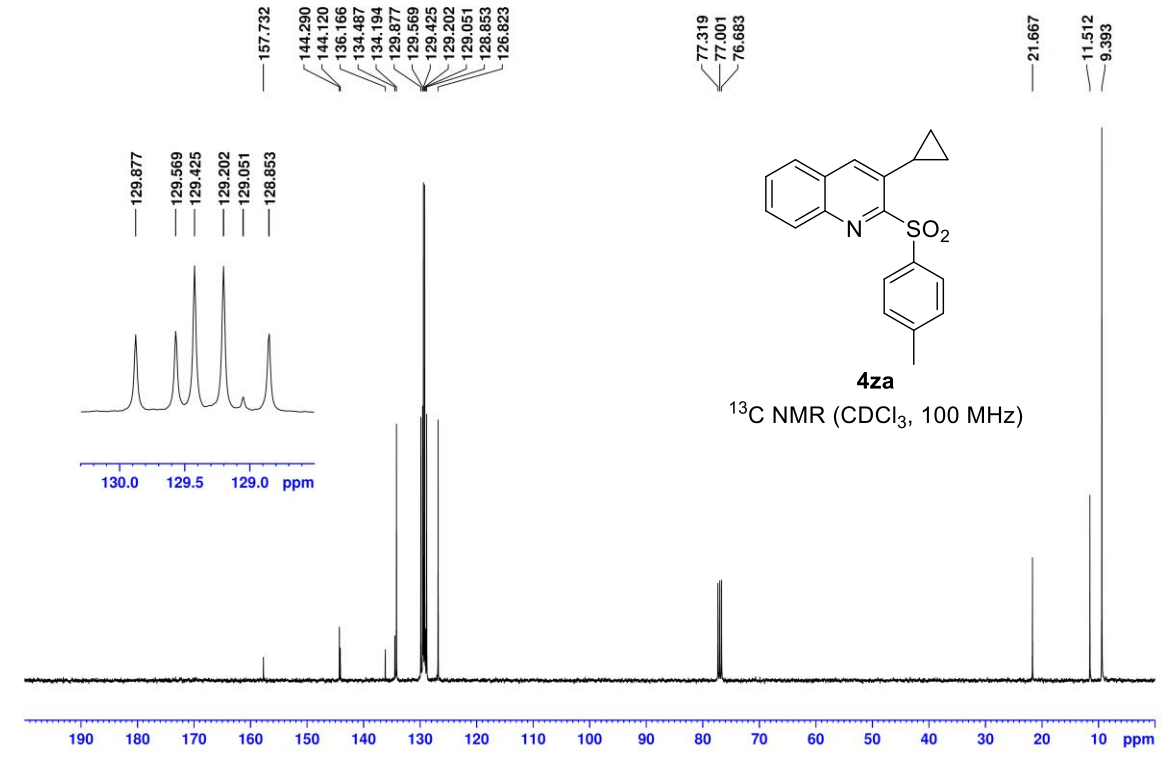

8.104
7.949
7.928
7.890
7.869
7.784
7.765
7.655
7.638
7.636
7.618
7.595
7.575
7.558
7.369
7.349
7.260
3.301
3.280
3.274
3.259
2.467
1.794
1.778
1.761
1.745
1.729
1.713
1.693
1.673
1.666
1.652
1.635
1.023
1.007
N
SO2
4ya
1H NMR (CDCl3, 400 MHz)
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
0.97
1.82
1.00
0.97
0.96
1.01
1.90
2.02
3.00
1.05
2.41
6.14


157.086
144.441
144.279
138.745
136.214
133.785
129.851
129.622
129.439
129.212
129.067
128.770
126.747
77.310
76.992
76.675
40.246
29.137
28.246
22.502
21.650
129.851
129.622
129.439
129.212
129.067
128.770
130.0 129.5 129.0 ppm
N
SO2
4ya
13C NMR (CDCl3, 100 MHz)
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm



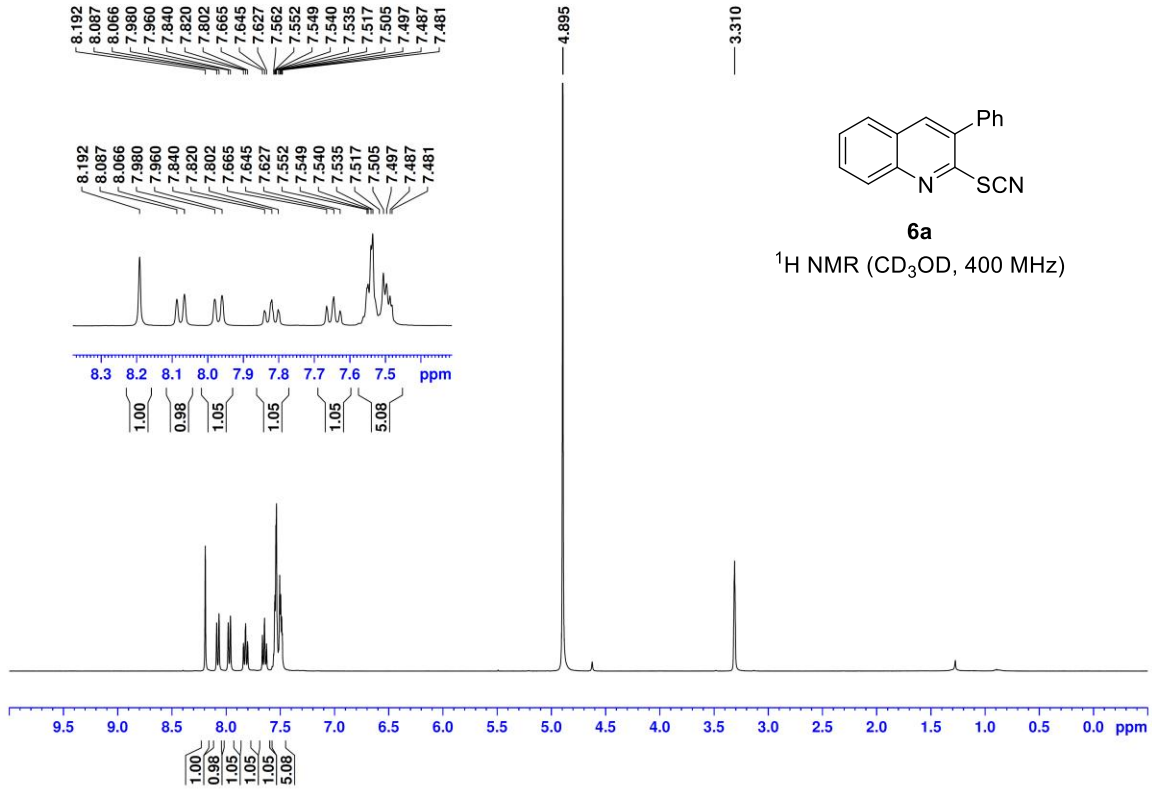
4za

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



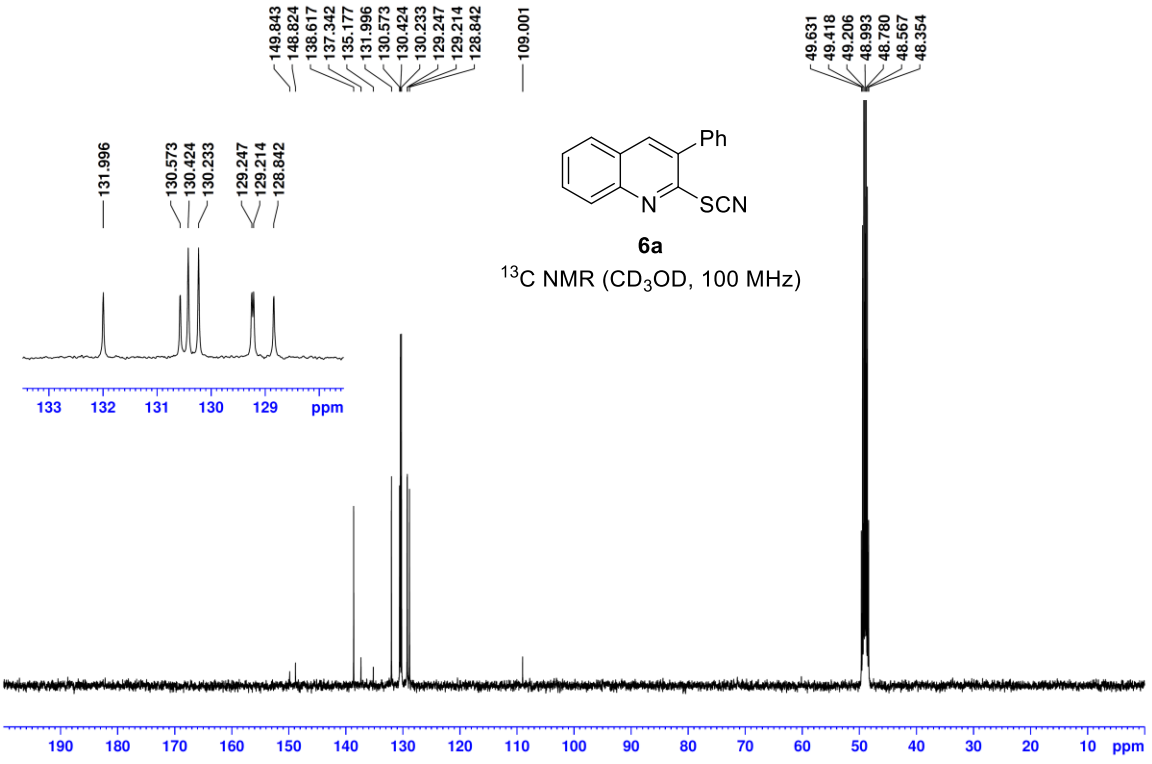
4za

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



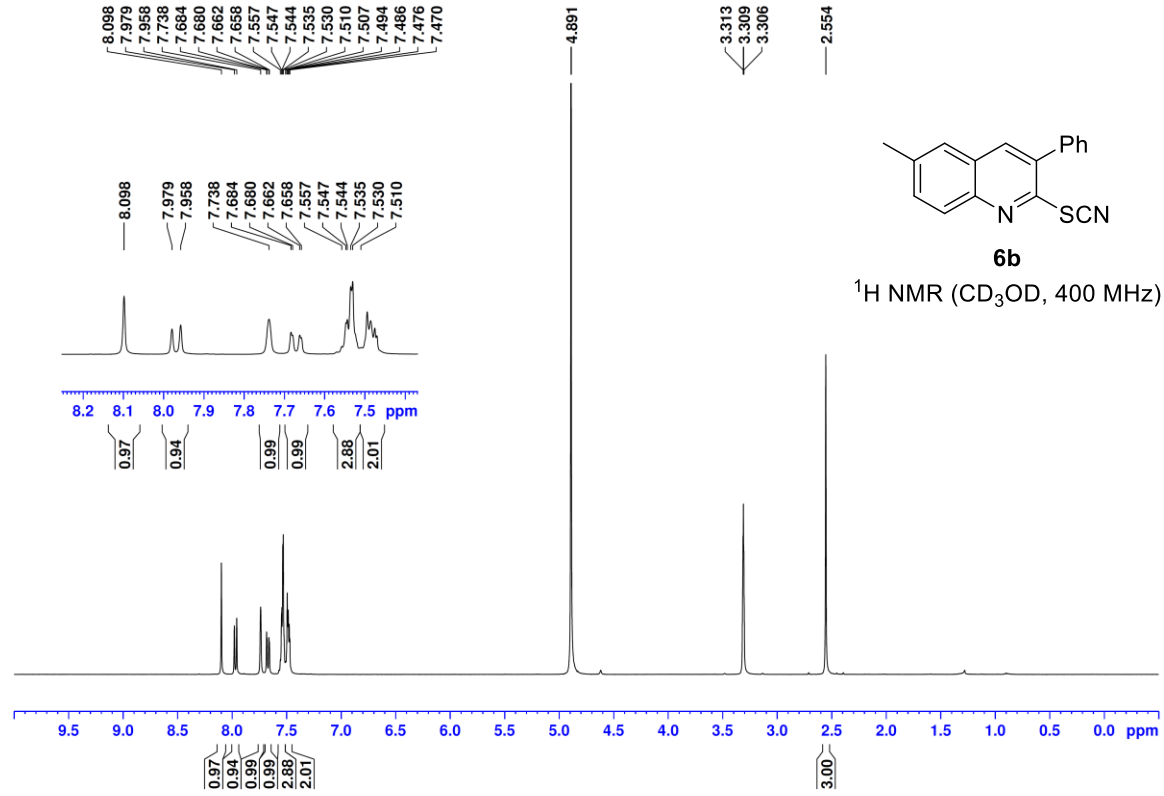
6a

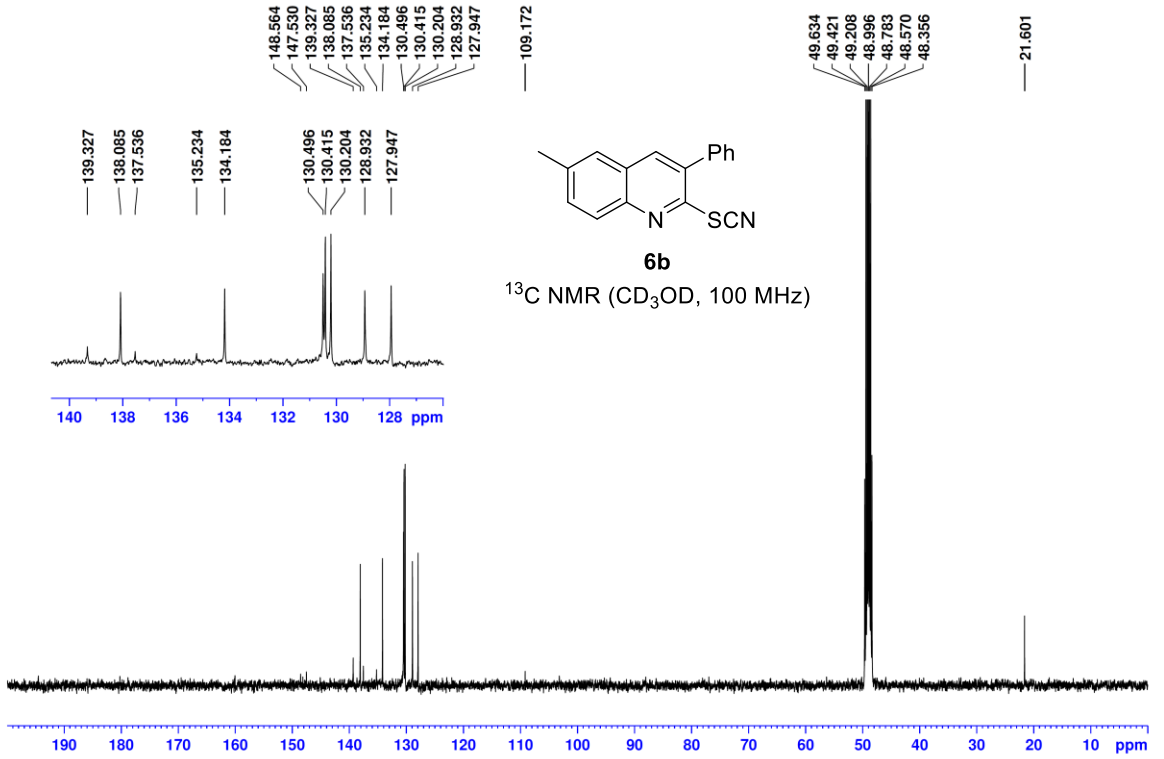
^{1}H NMR (CD_3OD, 400 MHz)

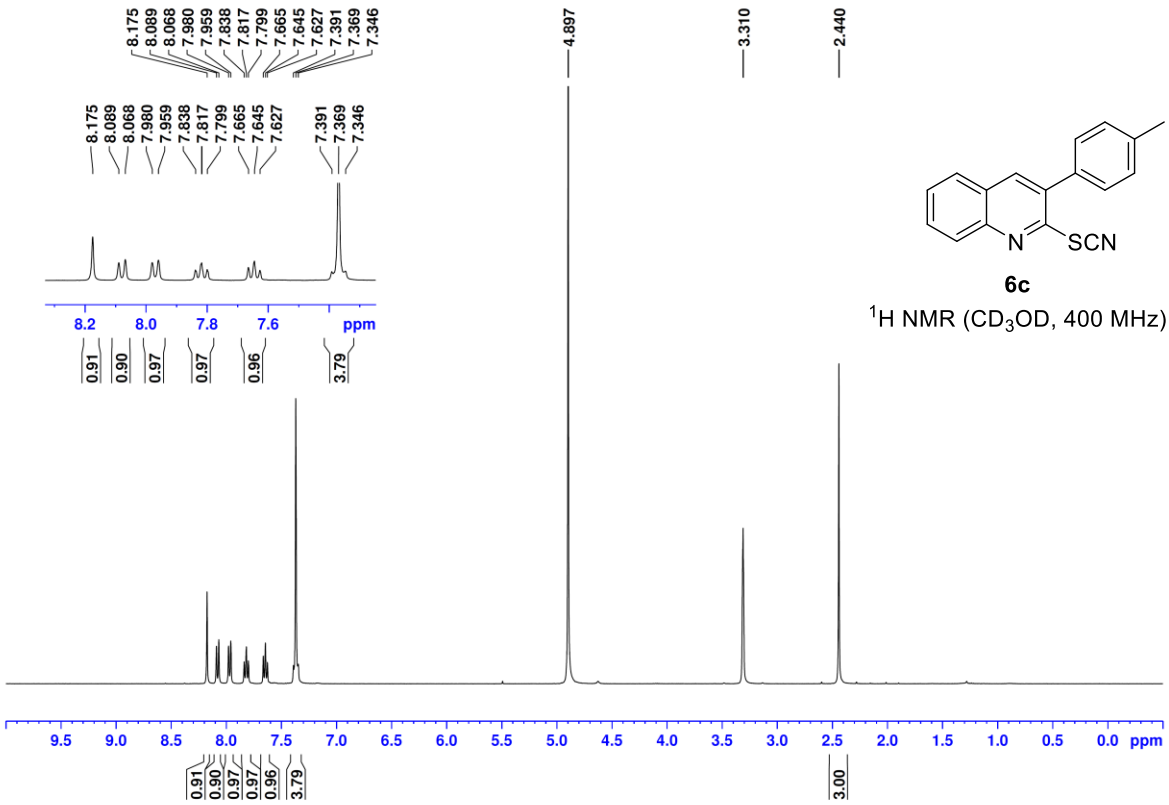


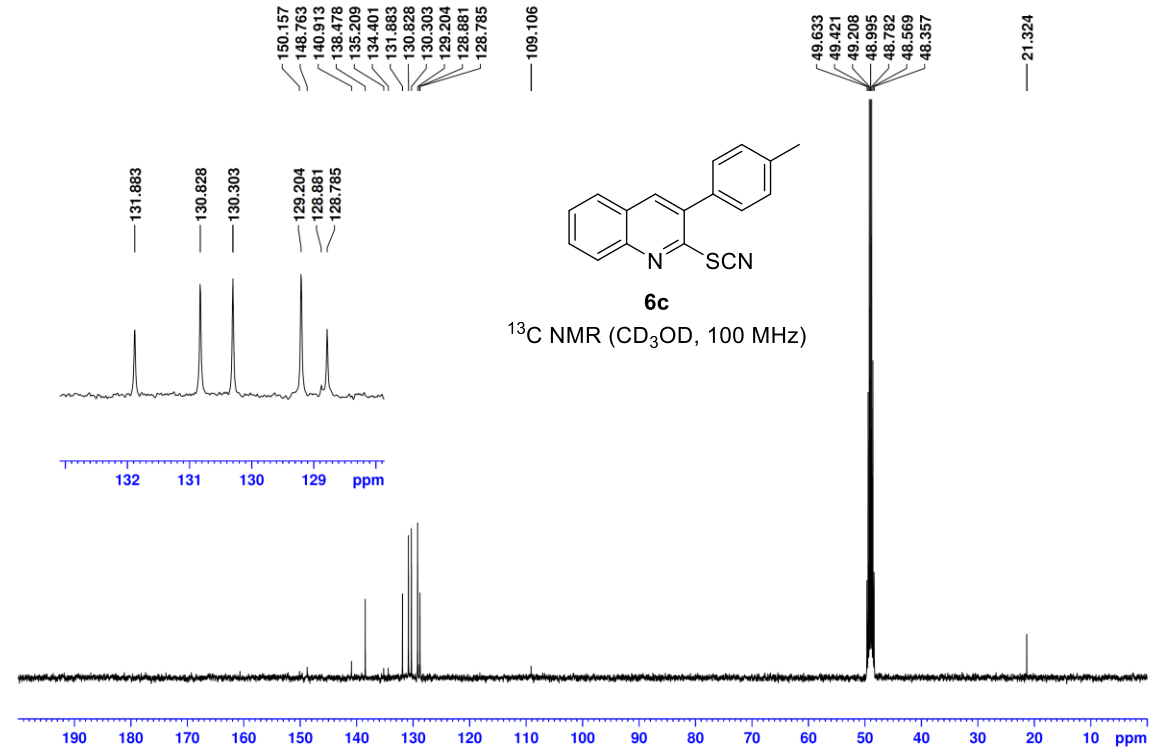
6a

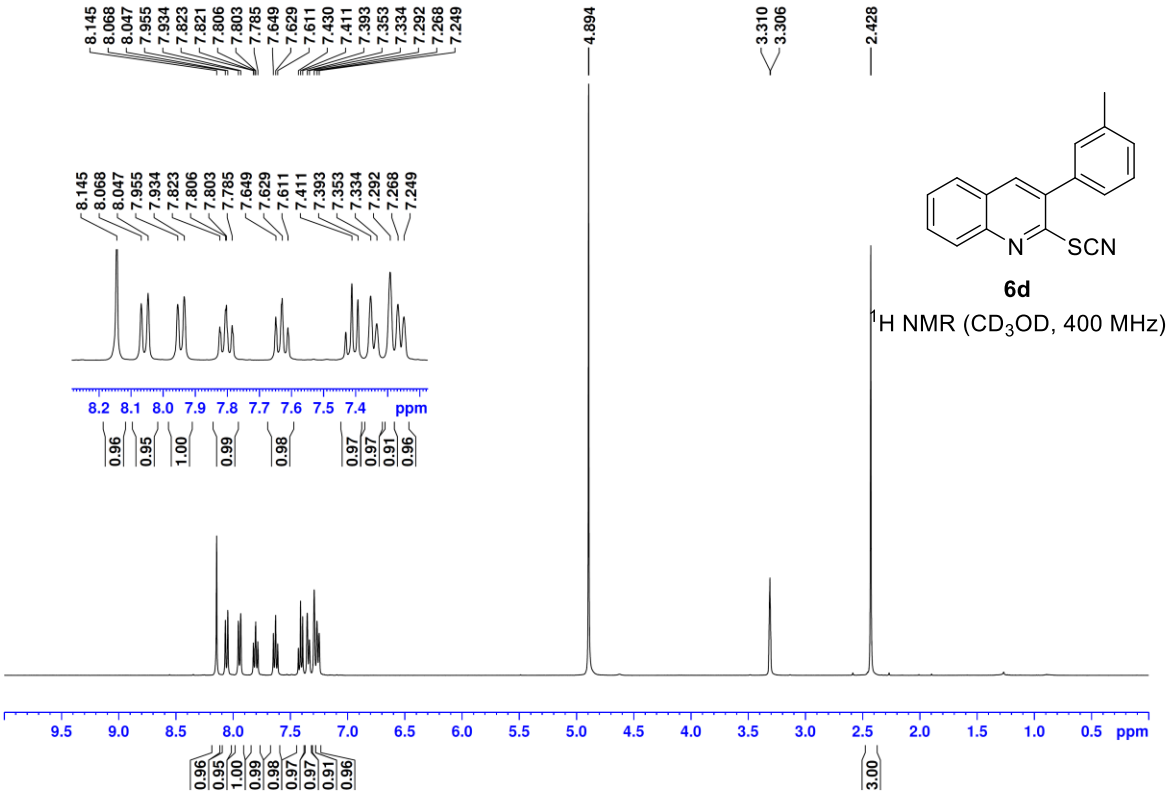
^{13}C NMR (CD_3OD, 100 MHz)

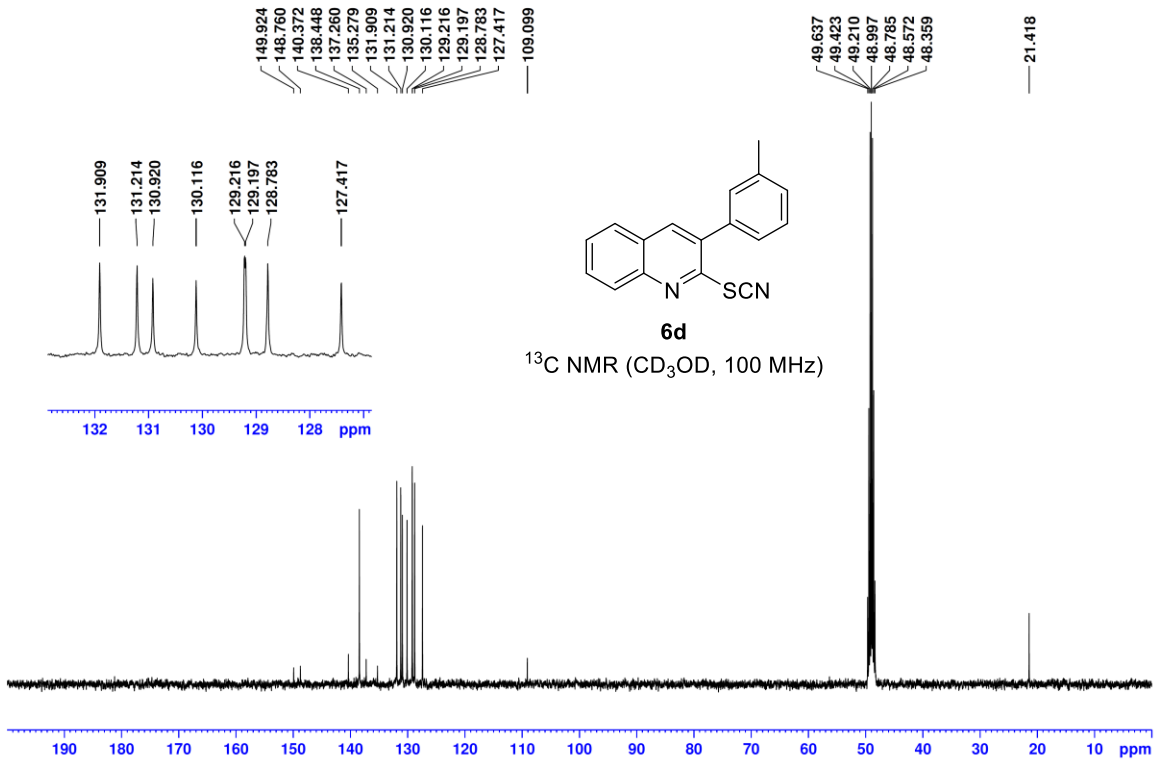

8.098
7.979
7.958
7.738
7.684
7.680
7.662
7.658
7.557
7.547
7.544
7.535
7.530
7.510
7.507
7.494
7.486
7.476
7.470
4.891
3.313
3.309
3.306
2.554
Ph
N
SCN
6b
1H NMR (CD3OD, 400 MHz)
8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 ppm
0.97 0.94 0.99 0.99 2.88 2.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
3.00

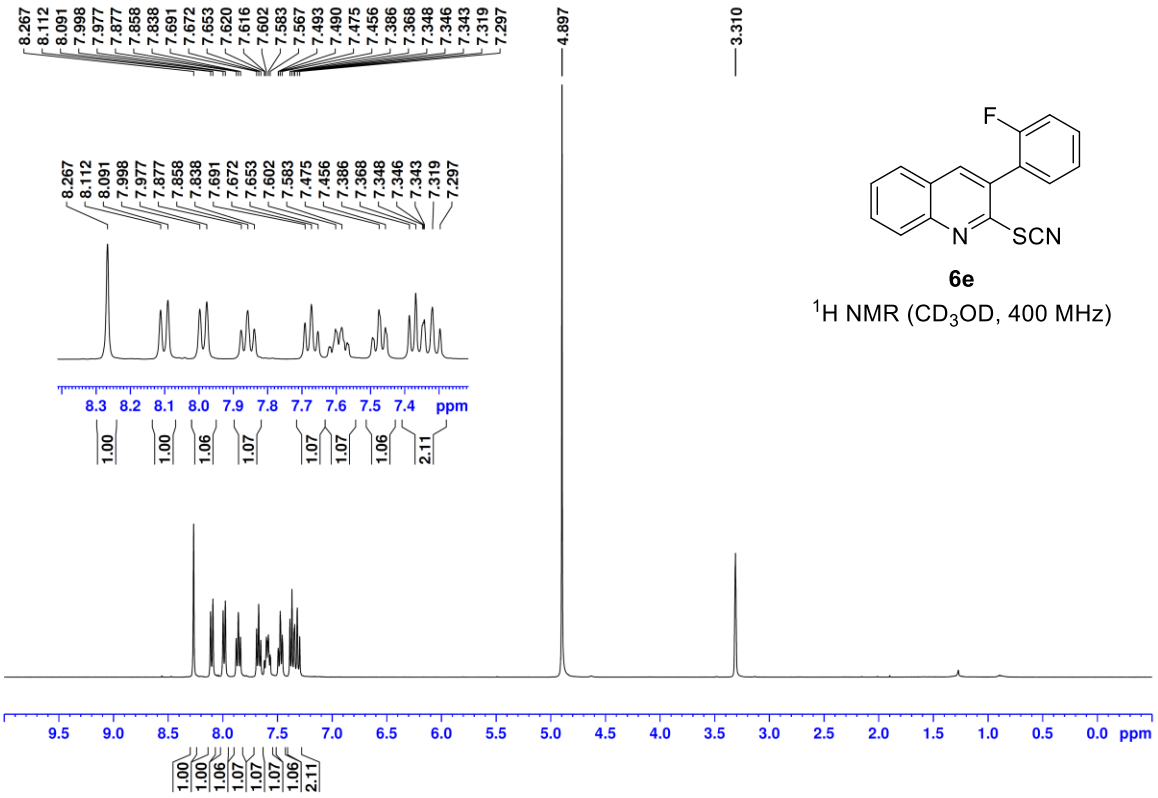

148.564
147.530
139.327
138.085
137.536
135.234
134.184
130.496
130.415
130.204
128.932
127.947
109.172
49.634
49.421
49.208
48.996
48.783
48.570
48.356
21.601
Ph
N
SCN
6b
13C NMR (CD3OD, 100 MHz)
140 138 136 134 132 130 128 ppm
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

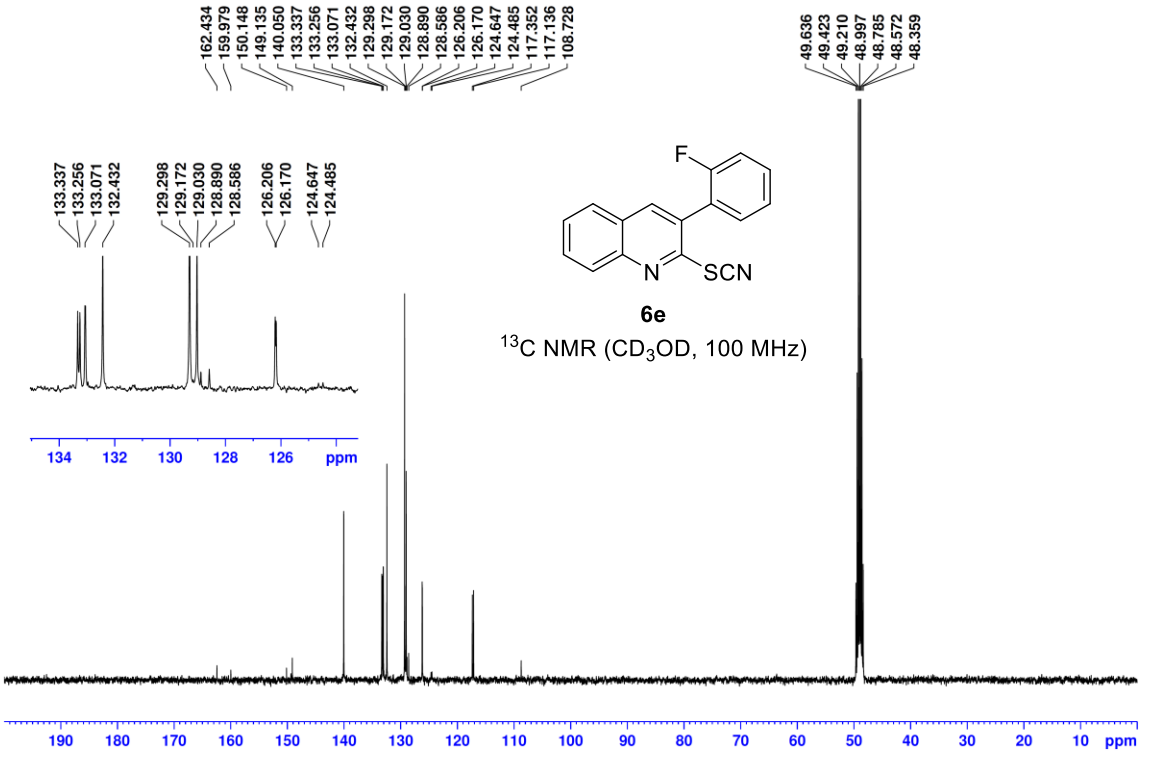

8.175
8.089
8.068
7.980
7.959
7.838
7.817
7.799
7.665
7.645
7.627
7.391
7.369
7.346
4.897
3.310
2.440
N
SCN
6c
1H NMR (CD3OD, 400 MHz)
ppm
0.91
0.90
0.97
0.97
0.96
3.79
3.00

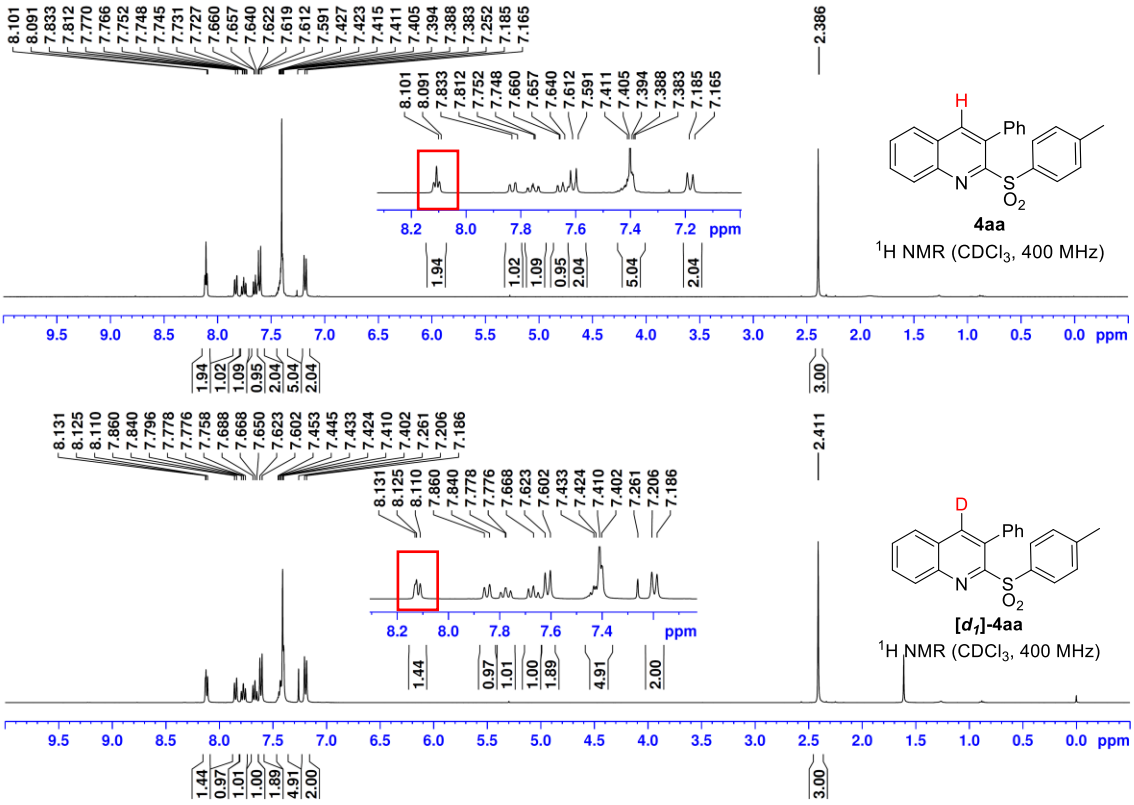

150.157
148.763
140.913
138.478
135.209
134.401
131.883
130.828
130.303
129.204
128.881
128.785
109.106
49.633
49.421
49.208
48.995
48.782
48.569
48.357
21.324
N
SCN
6c
13C NMR (CD3OD, 100 MHz)
ppm


8.145
8.068
8.047
7.955
7.934
7.823
7.821
7.806
7.803
7.785
7.649
7.629
7.611
7.430
7.411
7.393
7.353
7.334
7.292
7.268
7.249
4.894
3.310
3.306
2.428
N
SCN
6d
1H NMR (CD3OD, 400 MHz)
ppm


149.924
148.760
140.372
138.448
137.260
135.279
131.909
131.214
130.920
130.116
129.216
129.197
128.783
127.417
109.099
49.637
49.423
49.210
48.997
48.785
48.572
48.359
21.418
N
SCN
6d
13C NMR (CD3OD, 100 MHz)
ppm


8.267
8.112
8.091
7.998
7.977
7.877
7.858
7.838
7.691
7.672
7.653
7.620
7.616
7.602
7.583
7.567
7.493
7.490
7.475
7.456
7.386
7.368
7.348
7.346
7.343
7.319
7.297
4.897
3.310
F
N
SCN
6e
1H NMR (CD3OD, 400 MHz)
ppm


162.434
159.979
150.148
149.135
140.050
133.337
133.256
133.071
132.432
129.298
129.172
129.030
128.890
128.586
126.206
126.170
124.647
124.485
117.352
117.136
108.728
49.636
49.423
49.210
48.997
48.785
48.572
48.359
F
N
SCN
6e
13C NMR (CD3OD, 100 MHz)
ppm


4aa
^{1}H NMR (CDCl$_3$, 400 MHz)
[d_1]-4aa
^{1}H NMR (CDCl$_3$, 400 MHz)
ppm