RSC Advances

Supporting Information

Ruthenium-Catalyzed, 1, 2, 3-Triazole Directed Intermolecular C-H amidation of Arenes with Sulfonyl Azides

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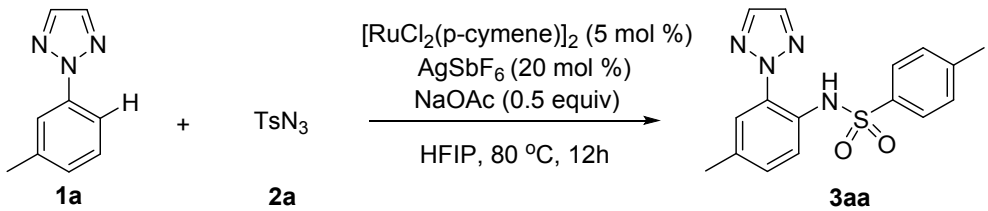
1. General details

All the reactions were monitored by thin-layer chromatography (TLC) and were visualized using UV light. The product purification was done using silica gel column chromatography. Thin layer chromatography (TLC) characterization was performed with precoated silica gel GF254 (0.2mm), while column chromatography characterization was performed with silica gel (100-200mesh).^{1}H and ^{13}C NMR spectra were recorded with tetramethylsilane as the internal standard. ^{1}H NMR spectra were recorded at 400 or 600 MHz (Varian) and ^{13}C NMR spectra were recorded at 100 or 150 MHz (Varian). Chemical shifts are reported in ppm downfield from $CDCl_3$ (δ = 7.26 ppm) for ^{1}H NMR and relative to the central $CDCl_3$ resonance (δ = 77.0 ppm) for ^{13}C NMR spectroscopy. Coupling constants are given in Hz. Melting points were measured with YRT-3 melting point apparatus (Shantou Keyi Instrument & Equipment Co., Ltd., Shantou, China). High resolution mass spectroscopy data of the products were collected on a Waters Micromass GCT or a Bruker Apex IV FTMS instrument. Commercial $[RuCl_2(p\text{-cymene})_2]_2$, $AgSbF_6$, NaOAc, HFIP and other reagents were directly used without further purification.

2. General procedure for the synthesis of 3 (3aa as an example)

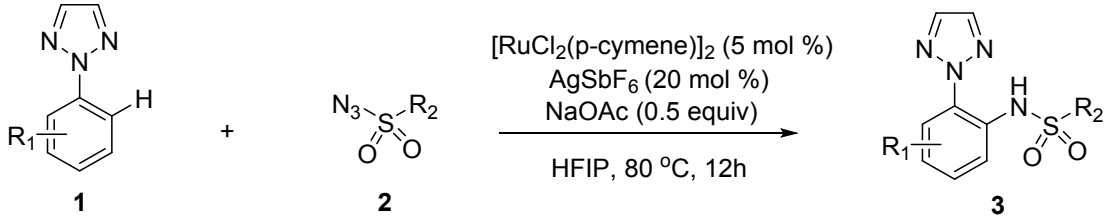


A 15ml sealed tube were charged with 2-(*m*-tolyl)-2*H*-1,2,3-triazole **1a** (31.8 mg, 0.2 mmol), 4-methylbenzenesulfonyl azide **2a** (59.5 mg, 0.3 mmol), $[RuCl_2(p\text{-cymene})_2]_2$ (6.1 mg, 0.01 mmol), $AgSbF_6$ (13.7 mg, 0.04 mmol), NaOAc (8.2 mg, 0.1 mmol), and HFIP (1ml). The mixture was stirred at 80 ^{o}C for 12h, then cooled down to room temperature. The resulting mixture was filtered and washed with DCM. The filtrate was concentrated in vacuum and the resulting residue was purified by flash chromatography on silica (PE/EA=50/1) to afford the desired product **3aa** as a white solid (53.8 mg, 82% yield).

3. Study of substrate scope

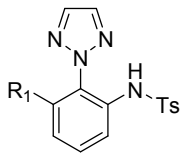
The reaction conditions are optimized as follows: 5 mol % $[RuCl_2(p\text{-cymene})]_2$, 20 mol % $AgSbF_6$, 0.5 equiv NaOAc in HFIP at 80 ^oC for 12h. With the efficient conditions on hand, we then focused on the synthesis of 2-aryl-1,2,3-triazole derivatives. The results were summarized in Table S1. Initially, arenes with *ortho*-halide and *ortho*-amido substituents underwent the C-H amidation smoothly, giving higher yields than those with electron-withdrawing groups (Table S1, compound **3ba**-**3la**). Then the *meta*-substituted substrates were screened. Not surprisingly, the less hindered *ortho*-C-H bond of aryl ring had been exclusively functionalized for all the substrate except *meta*-chloro substituted substrate. (Table S1, compound **3aa**, **3ma**-**3na**). Reactions with *meta*-chloro substituted substrate resulted three separable regioisomeric products (Table S1, Compound **3oa**, **3oa'** and **3oa''**). Continued exploration on substrate scope showed that the reaction of *para*-substituted 2-aryl-1,2,3-triazole with TsN_3 provided mono- and di-amination products under the optimal conditions (Table S1, compound **3pa**-**3ra**, **3pa'**-**3ra'**). For example, the mono- and di-amidation products **3pa** and **3pa'** were obtained in 32% and 20% yields, respectively (Table S1, compound **3pa** and **3pa'**). Interestingly, when the amount of TsN_3 was increased to 3.0 equiv, only diamination product was obtained (Table S1, compound **3pa'**). Thus, the modified conditions were then applied to other *para*-substituted compounds (Table 2, compound **3qa'**and **3ra'**). On the other hand, different sulfonyl azides have also been examined for compatibility in this reaction. Benzenesulfonylazides with functional groups at 4^{th} position were well tolerated during the reaction. The corresponding *ortho*-amidated products were achieved in good to excellent yields (Table 2, compound **3ab**-**3ae**). The results revealed that electron-donating methoxy group could afford a higher yield than the electron-withdrawing groups. In addition, methane sulfonylazide was a suitable substrate for amidation, affording the **3af** in 72% yield (Table 2, compound **3af**).

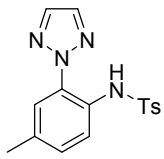
Table S1 Substrate scope[a,b]



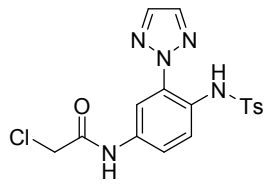
1 + **2** → **3**

3ba, R_1= F, 67% yield
3ca, R_1= Cl, 82% yield
3da, R_1= Br, 71% yield
3ea, R_1= $NHCOCH_3$, 80% yield
3fa, R_1= $NHCOCF_3$, 85% yield
3ga, R_1= $NHCOCH_2Cl$, 87% yield
3ha, R_1= $NHSO_2CH_3$, 87% yield
3ia, R_1= CN, 21% yield (41%)[c]
3ja, R_1= NO_2, 27% yield (66%)[c]
3ka, R_1= COOEt, 81% yield
3la, R_1= COOMe, 73% yield

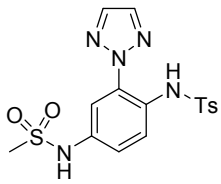




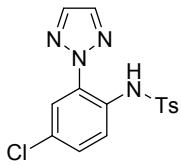
3aa, 82% yield



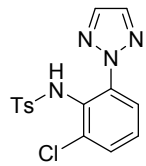
3ma, 84% yield



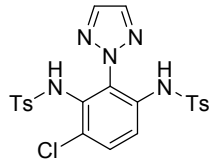
3na, 76% yield



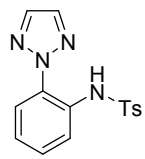
3oa, 35% yield



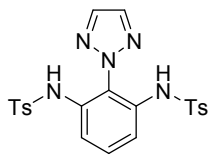
3oa', 27% yield



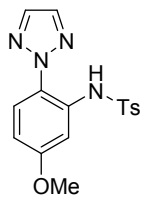
3oa'', 31% yield



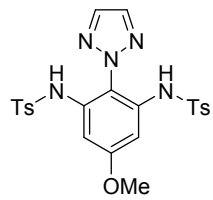
3pa 32% yield[d] (0% yield[e])



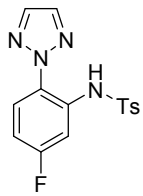
3pa' 20% yield[d] (84% yield[e])



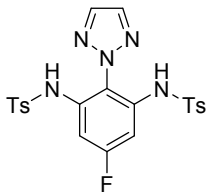
3qa 25% yield[d] (0% yield[e])



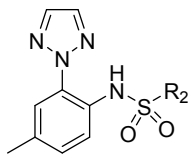
3qa' 31% yield[d] (82% yield[e])



3ra 41% yield[d] (0% yield[e])



3ra' 13% yield[d] (86% yield[e])



3ab, R_2= 4-$OMeC_6H_4$, 96% yield
3ac, R_2= 4-ClC_6H_4, 74% yield
3ad, R_2= 4-$NO_2C_6H_4$, 60% yield
3ae, R_2= C_6H_5, 75% yield
3af, R_2= Me, 72% yield

[a] Reactions were carried out with **1** (0.2 mmol), **2** (0.3 mmol), $[RuCl_2(p\text{-cymene})]_2$ (5 mol %), $AgSbF_6$ (20 mol %) and NaOAc (0.5 equiv.) in HFIP at 80 °C for 12h.

[b] Isolated yield.

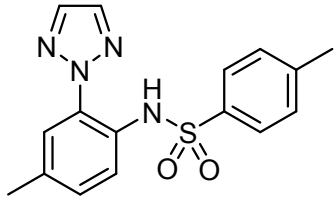
[c] Yields based on the recovered starting material are list in the square brackets.

[d] Reaction was carried out under the optimal conditions.

[e] 0.6mmol TsN_3 is used.

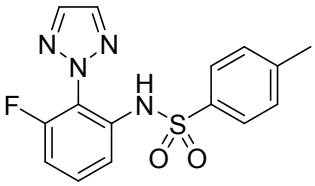
3. Spectroscopic characterization data of products

4-Methyl-N-(4-methyl-2-(2*H*-1,2,3-triazol-2-yl)phenyl)benzenesulfonamide (3aa)



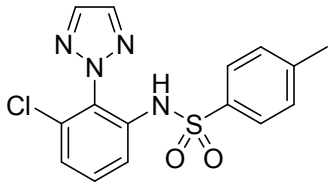
Yield 82%; white solid; m.p.100-102°C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.82 (s, 1H), 7.76 (s, 2H), 7.68 (d, *J* = 8.0 Hz, 1H), 7.65 (s, 1H), 7.34 (d, *J* = 8.0 Hz, 2H), 7.15 (d, *J* = 8.0 Hz, 1H), 7.02 (d, *J* = 8.0 Hz, 2H), 2.36 (s, 3H), 2.29 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 143.45, 135.95, 135.68, 134.75, 130.33, 129.38, 129.20, 126.53, 125.83, 124.71, 122.49, 21.33, 20.76; HRMS (ESI): m/z [M + Na^+] calcd for $C_{16}H_{16}N_4O_2S$+Na^+ 351.0886, found 351.0887.

N-(3-Fluoro-2-(2*H*-1,2,3-triazol-2-yl)phenyl)-4-methylbenzenesulfonamide (3ba)



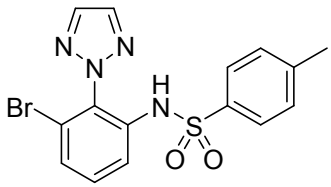
Yield 67%; white solid; m.p. 130-132°C (Lit. [1] 130-132°C); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.42 (s, 1H), 7.84 (s, 2H), 7.60 (d, *J* = 8.4 Hz, 1H), 7.42-7.36 (m, 1H), 7.31 (d, *J* = 8.4 Hz, 2H), 7.10-7.05 (m, 3H), 2.34 (s, 3H).

N-(3-chloro-2-(2*H*-1,2,3-triazol-2-yl)phenyl)-4-methylbenzenesulfonamide (3ca)



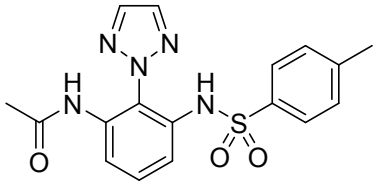
Yield 82%; white solid; m.p. 184-186°C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.85 (s, 2H), 7.71 (d, *J* = 8.0 Hz, 1H), 7.41-7.32 (m, 5H), 7.15 (d, *J* = 8.0 Hz, 2H), 2.37 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 145.20, 136.06, 135.41, 133.99, 131.28, 130.69, 129.71, 127.18, 126.78, 126.71, 122.06, 21.53; HRMS (ESI): m/z [M + Na^+] calcd for $C_{15}H_{13}ClN_4O_2S$+Na^+ 371.0340, found 371.0342.

N-(3-bromo-2-(2*H*-1,2,3-triazol-2-yl)phenyl)-4-methylbenzenesulfonamide (3da)



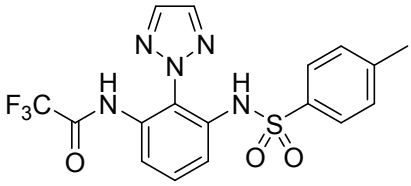
Yield 71%; white solid; m.p. 186-189°C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.85 (s, 2H), 7.76 (dd, J_1 = 8.4 Hz, J_2 = 0.8 Hz, 1H), 7.49 (dd, J_1 = 8.4 Hz, J_2 = 0.8 Hz, 1H), 7.37 (d, J = 8.0 Hz, 2H), 7.32 (t, J = 8.4 Hz, 1H), 7.22 (s, 1H), 7.16 (d, J=8.0 Hz, 2H), 2.37 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 144.24, 136.11, 135.43, 134.24, 131.18, 131.13, 130.24, 129.75, 126.79, 122.44, 120.52, 21.55; HRMS (ESI): m/z [M + Na^+] calcd for $C_{15}H_{13}BrN_4O_2S$+Na^+ 414.9835, found 414.9836.

N-(3-((4-methylphenyl)sulfonamido)-2-(2*H*-1,2,3-triazol-2 yl)phenyl)acetamide (3ea)



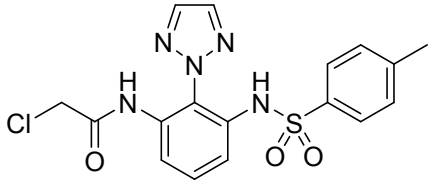
Yield 80%; white solid; m.p. 155-157°C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 9.11 (s, 1H), 8.75 (s, 1H), 8.14 (d, J = 8.4 Hz, 1H), 7.87 (s, 2H), 7.51 (d, J = 8.4 Hz, 1H), 7.40 (t, J = 8.4 Hz, 1H), 7.26 (d, J = 8.4 Hz, 2H), 7.07 (d, J = 8.4 Hz, 2H), 2.34 (s, 3H), 2.04 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 168.02, 143.68, 135.53, 135.20, 131.62, 130.33, 129.54, 129.44, 126.39, 122.25, 121.04, 120.81, 24.75, 21.43; HRMS (ESI): m/z [M + Na^+] calcd for $C_{17}H_{17}N_5O_3S$+Na^+ 394.0944, found 394.0944.

2,2,2-trifluoro-N-(3-((4-methylphenyl)sulfonamido)-2-(2*H*-1,2,3-triazol-2-yl)phenyl)acetamide (3fa)



Yield 85%; white solid; m.p. 112-114°C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 10.61 (s, 1H), 9.16 (s, 1H), 8.16 (d, J = 8.4 Hz, 1H), 7.92 (s, 2H), 7.67 (dd, J_1 = 8.4 Hz, J_2 = 1.2 Hz, 1H), 7.46 (t, J = 8.4 Hz, 1H), 7.29 (d, J = 7.8 Hz, 2H), 7.07 (d, J = 7.8 Hz, 2H), 2.34 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 154.80 (q, J = 37.9 Hz), 143.96, 135.49, 135.36, 130.58, 129.68, 129.55, 128.73, 126.43, 122.85, 122.26, 120.29, 115.49 (q, J = 287.6 Hz), 21.45; HRMS (ESI): m/z [M + Na^+] calcd for $C_{17}H_{14}F_3N_5O_3S$+Na^+ 448.0662, found 448.0662.

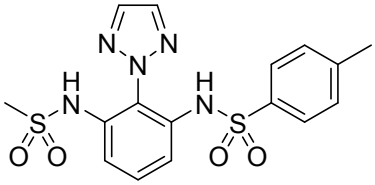
2-chloro-N-(3-((4-methylphenyl)sulfonamido)-2-(2*H*-1,2,3-triazol-2-yl)phenyl)acetamide (3ga)



Yield 87%; white solid; m.p. 90-92°C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.18 (s, 1H), 8.79 (s, 1H), 8.13 (d, J = 8.4 Hz, 1H), 7.87 (s, 2H), 7.58 (d, J = 8.4 Hz, 1H), 7.42 (t, J = 8.4 Hz, 1H), 7.27 (d, J = 8.0 Hz, 2H), 7.07 (d, J = 8.0 Hz, 2H), 4.07 (s, 2H), 2.33 (s, 3H); ^{13}C NMR (150

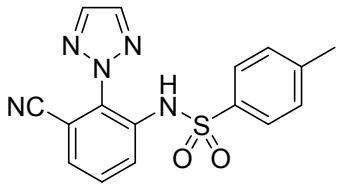
MHz, $CDCl_3$): δ 164.33, 143.80, 135.52, 135.42, 130.74, 130.60, 129.61, 129.50, 126.43, 122.60, 121.65, 120.44, 42.90, 21.45; HRMS (ESI): m/z [M + Na^+] calcd for $C_{17}H_{16}ClN_5O_3S+Na^+$ 428.0555, found 428.0553.

4-methyl-N-(3-(methylsulfonamido)-2-(2*H*-1,2,3-triazol-2-yl)phenyl)benzenesulfonamide (3ha)



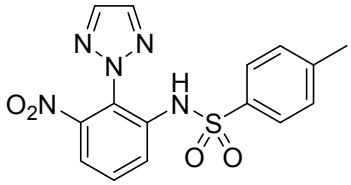
Yield 87%; white solid; m.p. 164-166°C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.83 (s, 1H), 8.38 (s, 1H), 7.90 (s, 2H), 7.63 (d, *J* = 8.4 Hz, 1H), 7.59 (d, *J* = 8.4 Hz, 1H), 7.35 (t, *J* = 8.4 Hz, 1H), 7.26-7.25 (m, 2H), 7.07 (d, *J* = 8.0 Hz, 2H), 2.68 (s, 3H), 2.34 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 143.96, 135.68, 135.37, 131.02, 130.78, 130.05, 129.51, 126.39, 123.34, 122.40, 120.61, 39.47, 21.44; HRMS (ESI): m/z [M + Na^+] calcd for $C_{16}H_{17}N_5O_4S_2+Na^+$ 430.0614, found 430.0618.

N-(3-cyano-2-(2*H*-1,2,3-triazol-2-yl)phenyl)-4-methylbenzenesulfonamide (3ia)



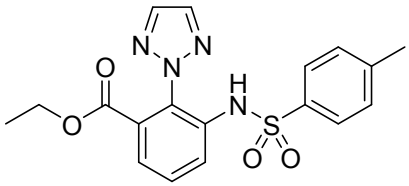
Yield 21%; white solid; m.p. 146-148°C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.05 (s, 1H), 8.08-8.06 (m, 1H), 7.90 (s, 2H), 7.63-7.61 (m, 1H), 7.51 (t, *J* = 8.0 Hz, 1H), 7.29 (d, *J* = 8.0 Hz, 2H), 7.09 (d, *J* = 8.0 Hz, 2H), 2.34 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 144.36, 136.43, 135.21, 131.87, 131.42, 129.72, 129.47, 129.34, 126.34, 115.70, 108.73, 21.49; HRMS (ESI): m/z [M + Na^+] calcd for $C_{16}H_{13}N_5O_2S+Na^+$ 362.0682, found 362.0679.

4-methyl-N-(3-nitro-2-(2*H*-1,2,3-triazol-2-yl)phenyl)benzenesulfonamide (3ja)



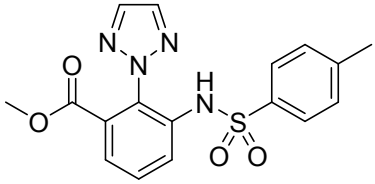
Yield 27%; white solid; m.p. 108-110°C (Lit. [1] 109-110°C); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.71 (s, 1H), 8.06 (d, *J* = 8.0 Hz, 1H), 7.82 (s, 2H), 7.67 (d, *J* = 8.0 Hz, 1H), 7.56 (t, *J* = 8.0 Hz, 1H), 7.31 (d, *J* = 8.0 Hz, 2H), 7.10 (d, *J* = 8.0 Hz, 2H), 2.34 (s, 3H).

Ethyl 3-((4-methylphenyl)sulfonamido)-2-(2*H*-1,2,3-triazol-2-yl)benzoate (3ka)



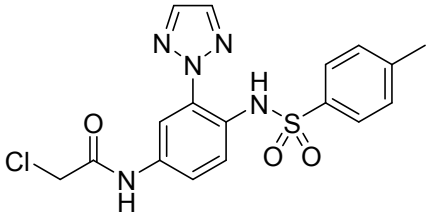
Yield 81%; colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.51 (s, 1H), 7.95 (d, *J* = 8.4 Hz, 1H), 7.77 (s, 2H), 7.61 (d, *J* = 8.4 Hz, 1H), 7.49 (t, *J* = 8.4 Hz, 1H), 7.28-7.26 (m, 2H), 7.07 (d, *J* = 8.0 Hz, 2H), 4.07 (q, *J* = 7.2 Hz, 2H), 2.32 (s, 3H), 1.05 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 165.81, 143.96, 135.58, 135.45, 131.39, 129.86, 129.60, 129.50, 129.37, 127.09, 127.04, 126.39, 61.55, 21.44, 13.83; HRMS (ESI): m/z [M + Na^+] calcd for $C_{18}H_{18}N_4O_4S$+Na^+ 409.0941, found 409.0940.

Methyl 3-((4-methylphenyl)sulfonamido)-2-(2*H*-1,2,3-triazol-2-yl)benzoate (3la)



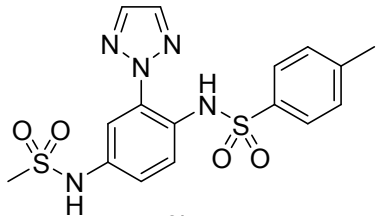
Yield 73%; white solid; m.p. 110-112°C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.56 (s, 1H), 7.96 (d, *J* = 8.0 Hz, 1H), 7.77 (s, 2H), 7.60 (d, *J* = 8.0 Hz, 1H), 7.49 (t, *J* = 8.0 Hz, 1H), 7.27 (d, *J* = 8.0 Hz, 2H), 7.07 (d, *J* = 8.0 Hz, 2H), 3.61 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 166.27, 143.98, 135.67, 135.47, 131.38, 129.83, 129.61, 129.46, 128.90, 127.22, 126.97, 126.41, 52.46, 21.45; HRMS (ESI): m/z [M + Na^+] calcd for $C_{17}H_{16}N_4O_4S$+Na^+ 395.0784, found 395.0784.

2-chloro-N-(4-((4-methylphenyl)sulfonamido)-3-(2*H*-1,2,3-triazol-2-yl)phenyl)acetamide (3ma)



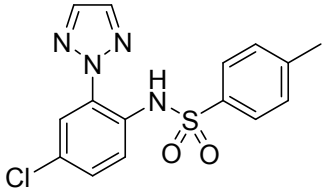
Yield 84%; white solid; m.p. 154-156°C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.99 (s, 1H), 8.29 (s, 1H), 8.16 (d, *J* = 2.4 Hz, 1H), 7.81-7.79 (m, 3H), 7.54 (dd, J_1 = 8.8 Hz, J_2 = 2.4 Hz, 1H), 7.38 (d, *J* = 8.4 Hz, 2H), 7.03 (d, *J* = 8.4 Hz, 2H), 4.19 (s, 2H), 2.29 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 163.98, 143.79, 135.52, 135.09, 134.34, 130.39, 129.37, 126.63, 125.08, 120.00, 113.59, 42.77, 21.40; HRMS (ESI): m/z [M + Na^+] calcd for $C_{17}H_{16}ClN_5O_3S$+Na^+ 428.0555, found 428.0554.

4-methyl-N-(4-(methylsulfonamido)-2-(2*H*-1,2,3-triazol-2-yl)phenyl)benzenesulfonamide (3na)



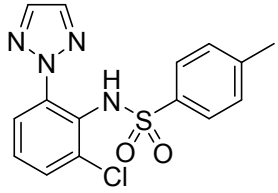
Yield 76%; white solid; m.p. 146-148°C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 10.08 (s, 1H), 7.82 (s, 2H), 7.81 (d, J = 8.8 Hz 1H), 7.78 (d, J = 8.4 Hz, 1H), 7.45 (d, J = 8.4 Hz, 2H), 7.20 (dd, J_1 = 8.8 Hz, J_2 = 2.4 Hz, 1H), 7.08 (d, J = 8.4 Hz, 2H), 6.60 (s, 1H), 3.04 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 143.96, 135.56, 135.25, 134.27, 130.61, 129.45, 126.67, 125.47, 125.29, 120.66, 114.17, 39.56, 21.41; HRMS (ESI): m/z [M + Na^+] calcd for $C_{16}H_{17}N_5O_4S_2$+Na^+ 430.0614, found 430.0614.

N-(4-chloro-2-(2*H*-1,2,3-triazol-2-yl)phenyl)-4-methylbenzenesulfonamide (3oa)



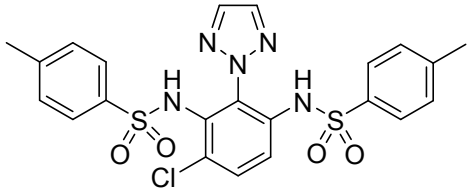
Yield 35%; white solid; m.p. 104-106°C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.11 (s, 1H), 7.93 (d, J = 2.4 Hz, 1H), 7.82 (s, 2H), 7.75(d, J = 8.8 Hz, 1H), 7.43 (d, J = 8.4 Hz, 2H), 7.29 (dd, J_1= 8.8 Hz, J_2 = 2.4 Hz, 1H), 7.08 (d, J = 8.4 Hz, 2H), 2.31 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 143.94, 135.63, 135.24, 130.78, 130.40, 129.47, 128.56, 127.14, 126.71, 125.01, 122.08, 21.44; HRMS (ESI): m/z [M + Na^+] calcd for $C_{15}H_{13}ClN_4O_2S$+Na^+ 371.0340, found 371.0341.

N-(2-chloro-6-(2*H*-1,2,3-triazol-2-yl)phenyl)-4-methylbenzenesulfonamide (3oa')



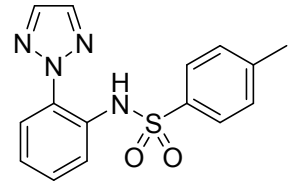
Yield 27%; white solid; mp. 164-166°C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.67 (s, 1H), 7.63 (dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 7.59 (s, 2H), 7.56(dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 7.34 (t, J = 8.0 Hz, 1H), 7.27 (d, J = 8.0 Hz, 2H), 7.02 (d, J = 8.0 Hz, 2H), 2.33 (s, 3H).

N,N'-(4-chloro-2-(2*H*-1,2,3-triazol-2-yl)-1,3-phenylene)bis(4-methylbenzenesulfonamide) (3oa")



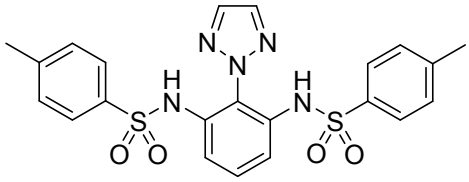
Yield 31%; white solid; m.p. 178-180°C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.65 (s, 1H), 7.71 (d, *J* = 8.8 Hz, 1H), 7.64 (s, 1H), 7.57 (s, 2H), 7.53 (d, *J* = 8.8 Hz, 1H), 7.22 (d, *J* = 8.0 Hz, 2H), 7.13 (d, *J* = 8.0 Hz, 2H), 7.05 (d, *J* = 8.0 Hz, 2H), 7.02 (d, *J* = 8.0 Hz, 2H), 2.36 (s, 3H), 2.32 (s, 3H).

N-(2-(2*H*-1,2,3-triazol-2-yl)phenyl)-4-methylbenzenesulfonamide (3pa)



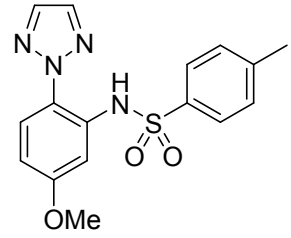
Yield 32% (under optimal conditions); white solid; m.p. 123-124°C (Lit.[1] 123-124°C); ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.11 (s, 1H), 7.88 (dd, J_1 = 8.4 Hz, J_2 = 1.2 Hz, 1H), 7.81-7.79 (m, 3H), 7.42 (d, *J* = 8.4 Hz, 2H), 7.36-7.32 (m, 1H), 7.24-7.20 (m, 1H), 7.05 (d, *J* = 8.4 Hz, 2H), 2.29 (s, 3H).

N,N'-(2-(2*H*-1,2,3-Triazol-2-yl)-1,3-phenylene)bis(4-methylbenzenesulfonamide) (3pa')



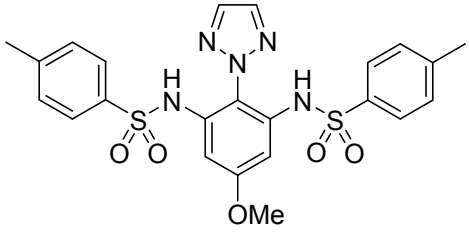
Yield 84% (0.6 equiv TsN_3 was used); white solid; m.p. 153-155°C (Lit.[1] 153-154°C); ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.76 (s, 2H), 7.70 (s, 2H), 7.59 (d, *J* = 8.4 Hz, 2H), 7.39 (t, *J* = 8.4 Hz, 1H), 7.13 (d, *J* = 8.4 Hz, 4H), 7.00 (d, *J* = 8.4 Hz, 4H), 2.32 (s, 6H).

N-(5-methoxy-2-(2H-1,2,3-triazol-2-yl)phenyl)-4-methylbenzenesulfonamide (3qa)



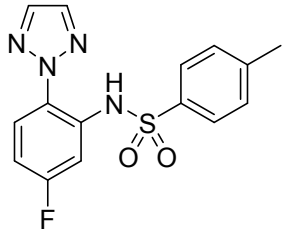
Yield 25% (under optimal conditions); white solid; m.p. 82-84°C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.13 (s, 1H), 7.78 -7.76 (m, 3H), 7.46 (d, *J* = 8.4 Hz, 2H), 7.31 (d, *J* = 2.4 Hz, 1H), 7.08 (d, *J* = 8.4 Hz, 2H), 6.73 (dd, J_1 = 8.8 Hz, *J* = 2.8 Hz, 1H), 3.85 (s, 3H), 2.31 (s, 3H).

N,N'-(5-methoxy-2-(2*H*-1,2,3-triazol-2-yl)-1,3-phenylene)bis(4-methylbenzenesulfonamide) (3qa')



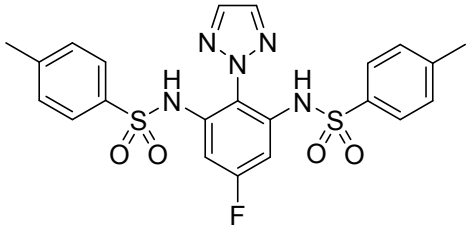
Yield 82% (0.6 equiv TsN_3 was used); white solid; m.p. 160-162°C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.77 (s, 2H), 7.69 (s, 2H), 7.19 (d, *J* = 8.4 Hz, 4H), 7.09 (s, 2H), 7.03 (d, *J* = 8.4 Hz, 4H), 3.86 (s, 3H), 2.33 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 159.54, 143.88, 135.31, 134.62, 131.42, 129.46, 126.36, 117.71, 107.96, 55.85, 21.46; HRMS (ESI): m/z [M + Na^+] calcd for $C_{23}H_{23}N_5O_5S_2$+Na^+ 536.1033, found 536.1035.

N-(5-fluoro-2-(2*H*-1,2,3-triazol-2-yl)phenyl)-4-methylbenzenesulfonamide (3ra)



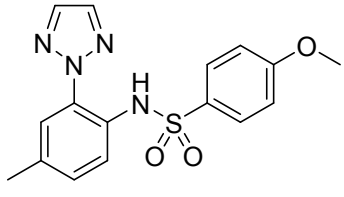
Yield 40% (under optimal conditions); white solid; m.p. 96-98°C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.37 (s, 1H), 7.93-7.89 (m, 1H), 7.82 (s, 2H), 7.55-7.53 (m, 3H), 7.13 (d, *J* = 8.0 Hz, 2H), 6.91-6.86 (m, 1H), 2.33 (s, 3H).

N,N'-(5-fluoro-2-(2*H*-1,2,3-triazol-2-yl)-1,3-phenylene)bis(4-methylbenzenesulfonamide) (3ra')



Yield 86% (0.6 equiv TsN_3 was used); white solid; m.p. 168-170°C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.91 (s, 2H), 7.79 (s, 2H), 7.29-7.27 (m, 6H), 7.08 (d, *J* = 7.8 Hz, 4H), 2.35 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 161.55 (d, *J* = 249.2 Hz), 144.25, 135.22, 135.15, 132.21 (d, *J* = 14.0 Hz), 129.65, 126.47, 126.37, 125.15, 119.41, 108.51 (d, *J* = 27.9 Hz), 21.49; HRMS (ESI): m/z [M + Na^+] calcd for $C_{22}H_{20}FN_5O_4S_2$+Na^+ 524.0833, found 524.0833.

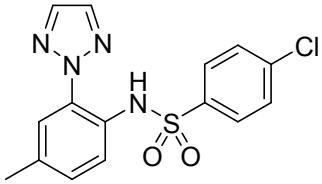
4-methoxy-N-(4-methyl-2-(2*H*-1,2,3-triazol-2-yl)phenyl)benzenesulfonamide (3ab)



Yield 96%; white solid; m.p. 106-108°C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.81 (s, 1H), 7.77 (s,

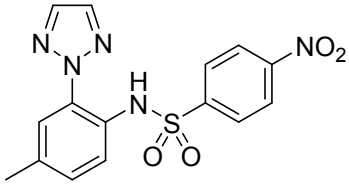
2H), 7.68 (d, *J* = 8.0 Hz, 1H), 7.66 (s, 1H), 7.40 (d, *J* = 8.8 Hz, 2H), 7.16 (d, *J* = 8.0 Hz, 1H), 6.69 (d, *J* = 8.8Hz, 2H), 3.76 (s, 3H), 2.36 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 162.78, 135.92, 134.81, 130.37, 130.33, 129.41, 128.73, 125.96, 124.72, 122.53, 113.80, 55.45, 20.81; HRMS (ESI): m/z [M + Na^+] calcd for $C_{16}H_{16}N_4O_3S+Na^+$ 367.0835, found 367.0832.

4-chloro-N-(4-methyl-2-(2*H*-1,2,3-triazol-2-yl)phenyl)benzenesulfonamide (3ac)



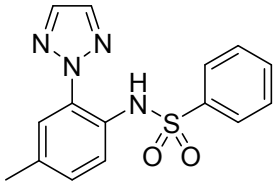
Yield 74%; white solid; m.p. 94-96°C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.78 (s, 1H), 7.77 (s, 2H), 7.68 (d, *J* = 8.0 Hz, 2H), 7.37 (d, *J* = 8.0 Hz, 2H), 7.21-7.18 (m, 3H), 2.38 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 139.21, 137.05, 136.67, 134.92, 130.67, 129.58, 128.92, 127.98, 125.33, 125.29, 122.72, 20.88; HRMS (ESI): m/z [M + Na^+] calcd for $C_{15}H_{13}ClN_4O_2S+Na^+$ 371.0340, found 371.0340.

N-(4-methyl-2-(2*H*-1,2,3-triazol-2-yl)phenyl)-4-nitrobenzenesulfonamide (3ad)



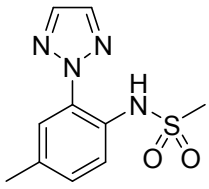
Yield 60%; white solid; m.p. 124-126°C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.82 (s, 1H), 8.06 (d, *J* = 8.8 Hz, 2H), 7.76 (s, 2H), 7.71 (d, *J* = 8.0 Hz, 1H), 7.65 (s, 1H), 7.59 (d, *J* = 8.8 Hz, 2H), 7.22 (d, *J* = 8.0 Hz, 1H), 2.39 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 149.86, 144.05, 137.40, 135.09, 130.88, 129.76, 127.82, 125.68, 124.65, 123.81, 122.88, 20.93; HRMS (ESI): m/z [M + Na^+] calcd for $C_{15}H_{13}N_5O_4S+Na^+$ 382.0580, found 382.0581.

N-(4-methyl-2-(2*H*-1,2,3-triazol-2-yl)phenyl)benzenesulfonamide (3ae)



Yield 75%; white solid; m.p. 98-100°C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.80 (s, 1H), 7.75 (s, 2H), 7.69 (d, *J* = 8.0 Hz, 1H), 7.63 (s, 1H), 7.46-7.43 (m, 2H), 7.38 (t, *J* = 8.0 Hz, 1H), 7.23 (t, *J* = 8.0 Hz, 2H), 7.17(d, *J* = 8.0 Hz, 1H), 2.36 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 138.58, 136.31, 134.84, 132.65, 130.61, 129.48, 128.61, 126.52, 125.68, 125.17, 122.56, 20.84; HRMS (ESI): m/z [M + Na^+] calcd for $C_{15}H_{14}N_4O_2S+Na^+$ 337.0730, found 337.0726.

N-(4-methyl-2-(2*H*-1,2,3-triazol-2-yl)phenyl)methanesulfonamide (3af)

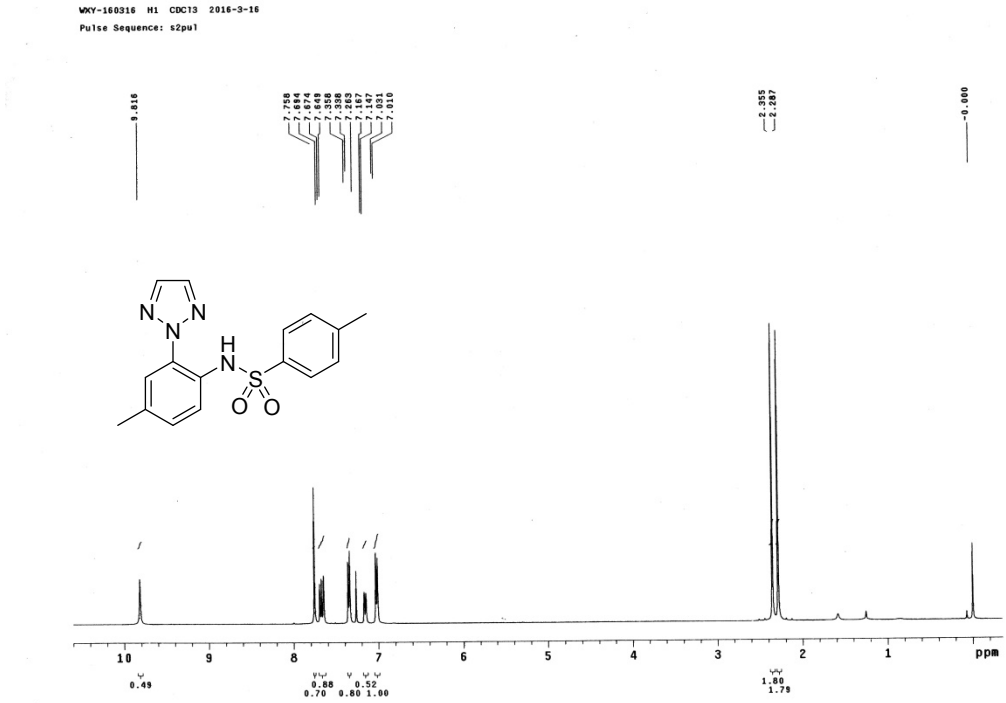


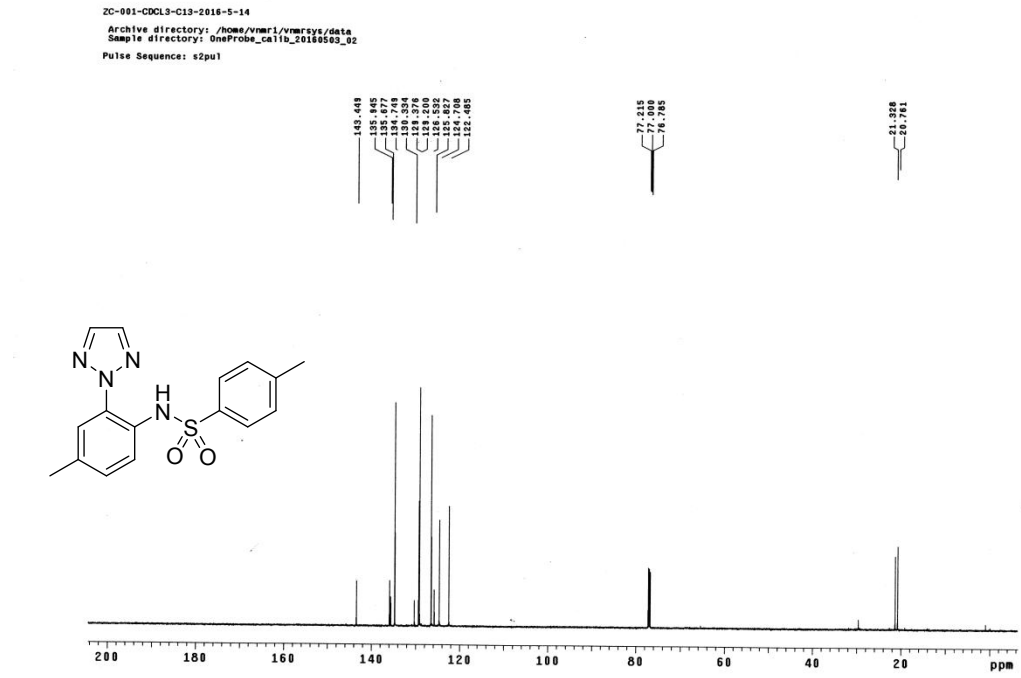
Yield 72%; white solid; m.p. 78-80°C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.69 (s, 1H), 7.91 (s, 2H), 7.70 (d, *J* = 8.4 Hz, 1H), 7.27(s, 1H), 7.22 (d, *J* = 8.4 Hz, 1H), 2.81 (s, 3H), 2.42 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 135.73, 135.21, 129.76, 129.48, 126.13, 123.01, 122.83, 39.13, 20.80; HRMS (ESI): m/z [M + Na^+] calcd for $C_{10}H_{12}N_4O_2S$+Na^+ 275.0573, found 275.0576.

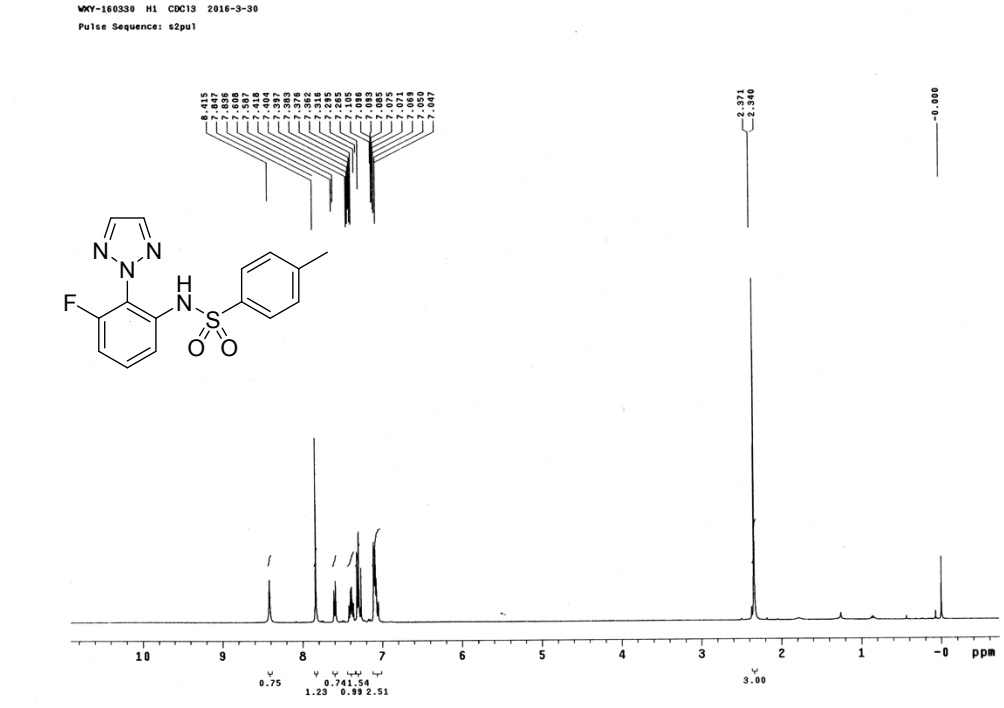
4. References

[1] B. Zhu, X. Cui, C. Pi, D. Chen and Y. Wu, *Adv. Synth. Catal.*, 2016, **358**, 326.

5. ^{1}H NMR and ^{13}C NMR Spectra of Product






WXY-160330 H1 CDC13 2016-3-30
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7.587
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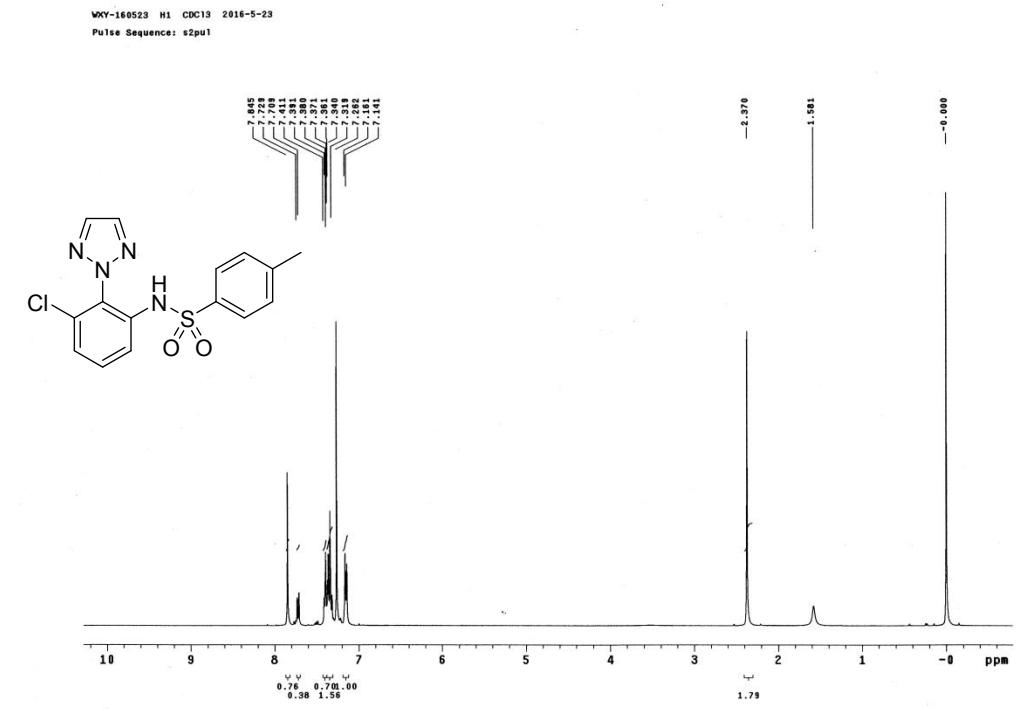
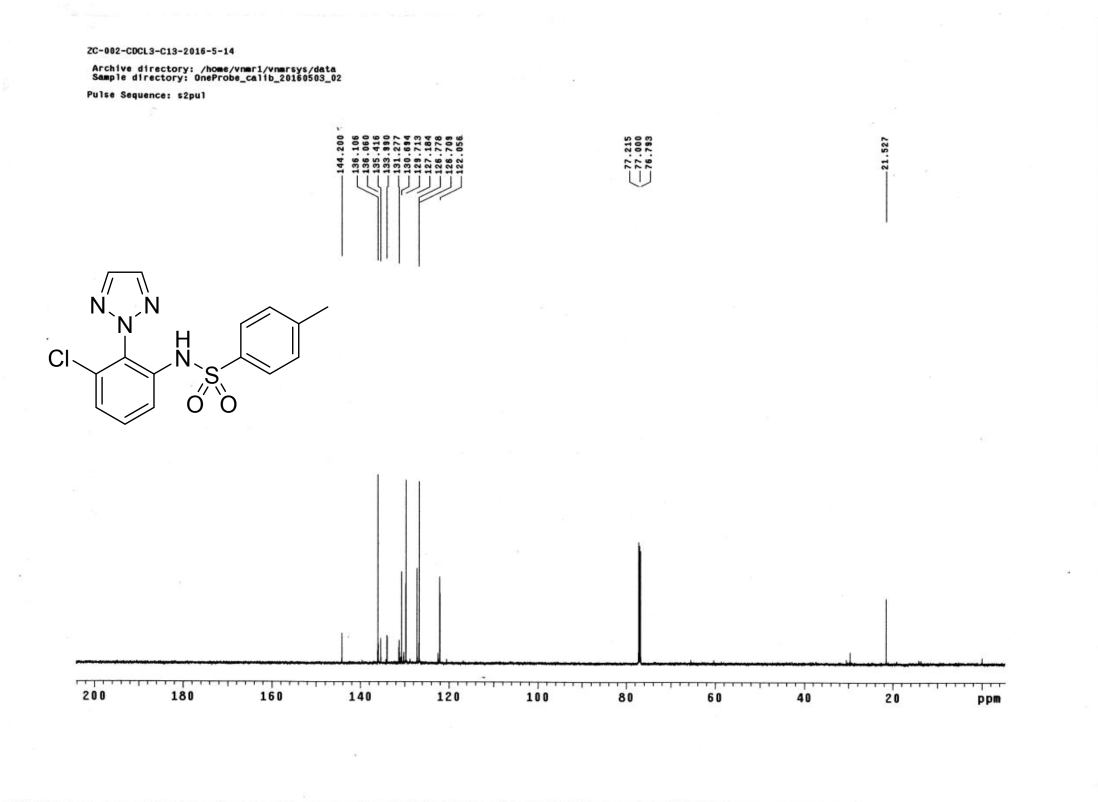
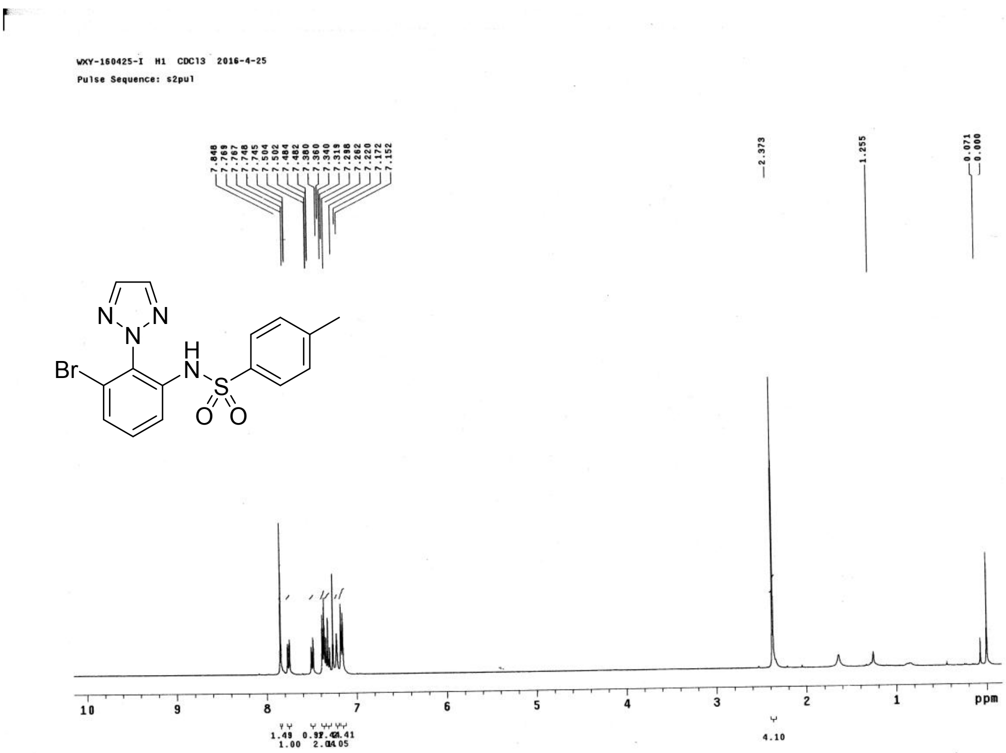
7.362
7.316
7.295
7.265
7.105
7.096
7.083
7.065
7.075
7.071
7.068
7.050
7.047
2.371
2.340
-0.000
F
H
N
S
O
O
10
9
8
7
6
5
4
3
2
1
-0
ppm
0.75
0.74
1.54
1.23
0.99
2.51
3.00

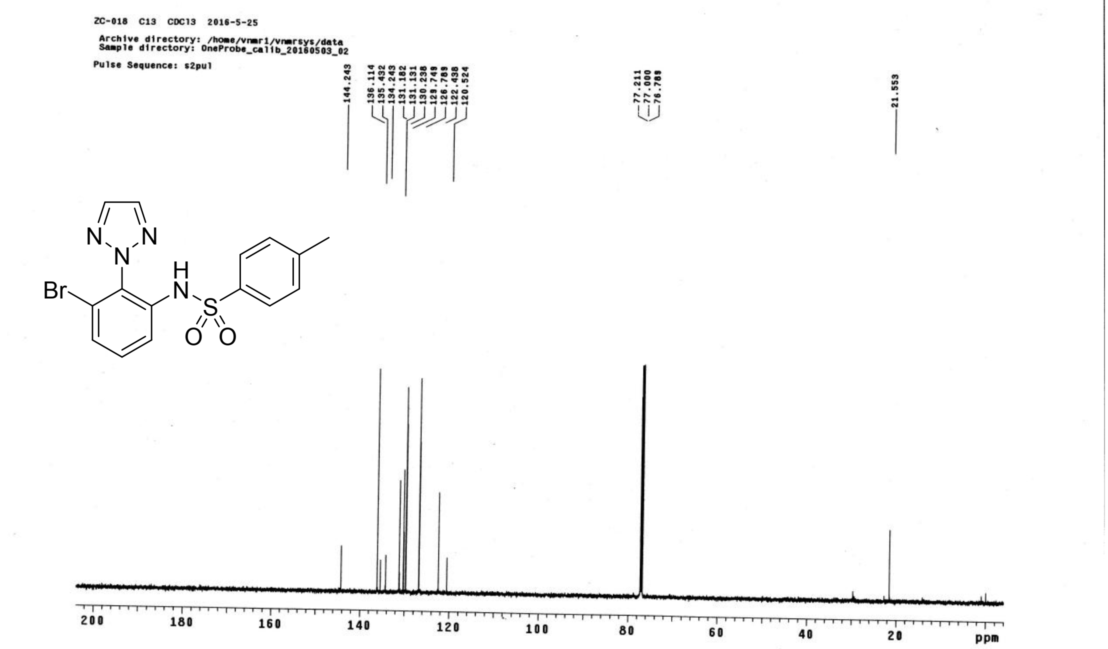

WXY-160523 H1 CDC13 2016-5-23
Pulse Sequence: s2pul
7.845
7.728
7.709
7.441
7.391
7.380
7.371
7.361
7.340
7.318
7.262
7.161
7.141
2.370
1.581
-0.000
Cl
H
N
S
O
O
10
9
8
7
6
5
4
3
2
1
-0
ppm
0.76
0.38
0.70
1.56
1.00
1.79



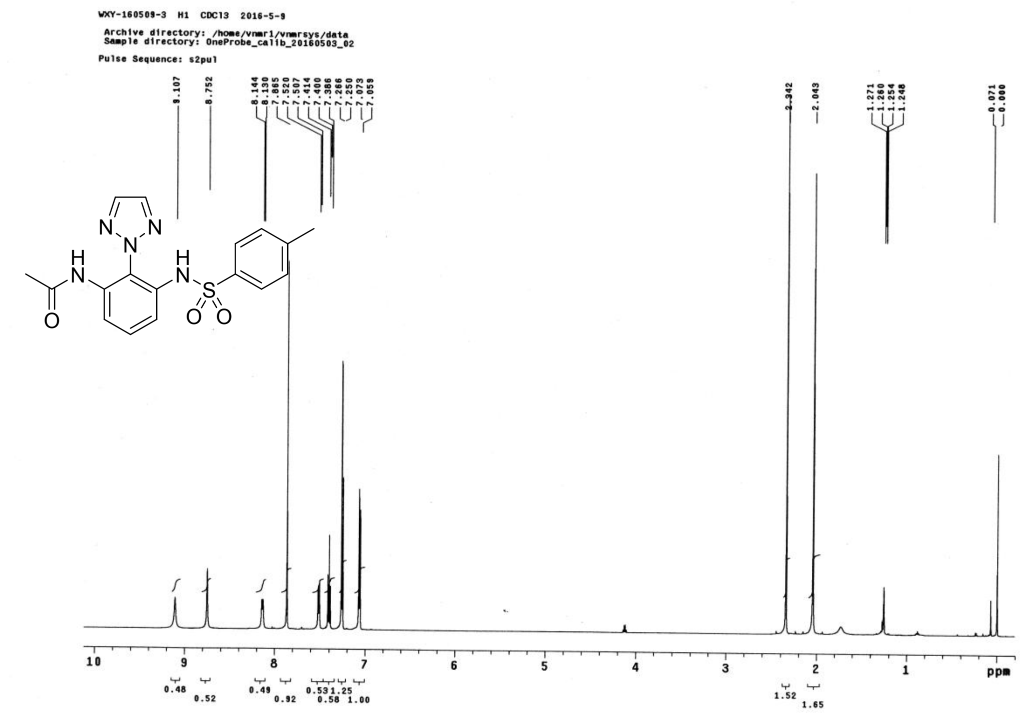
ZC-002-CDCL3-C13-2016-5-14
Archive directory: /home/vnmr1/vnmrsys/data
Sample directory: OneProbe_calib_20160503_02
Pulse Sequence: s2pul
144.200
136.106
136.060
135.416
131.277
77.215
77.000
76.783
21.527
ppm



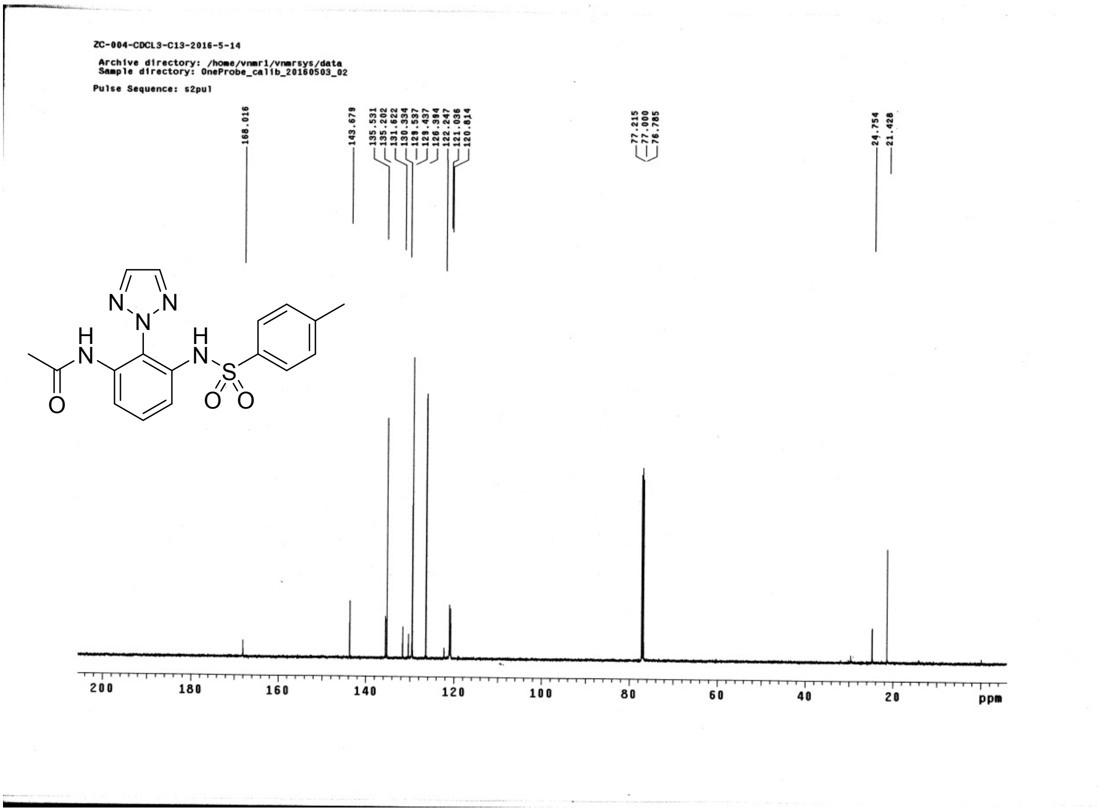
WXY-160425-I H1 CDCl3 2016-4-25
Pulse Sequence: s2pul
7.848
7.769
7.767
7.748
7.745
7.504
7.502
7.484
7.482
7.380
7.360
7.340
7.319
7.298
7.262
7.220
7.172
7.152
2.373
1.255
0.071
0.000
ppm
4.10

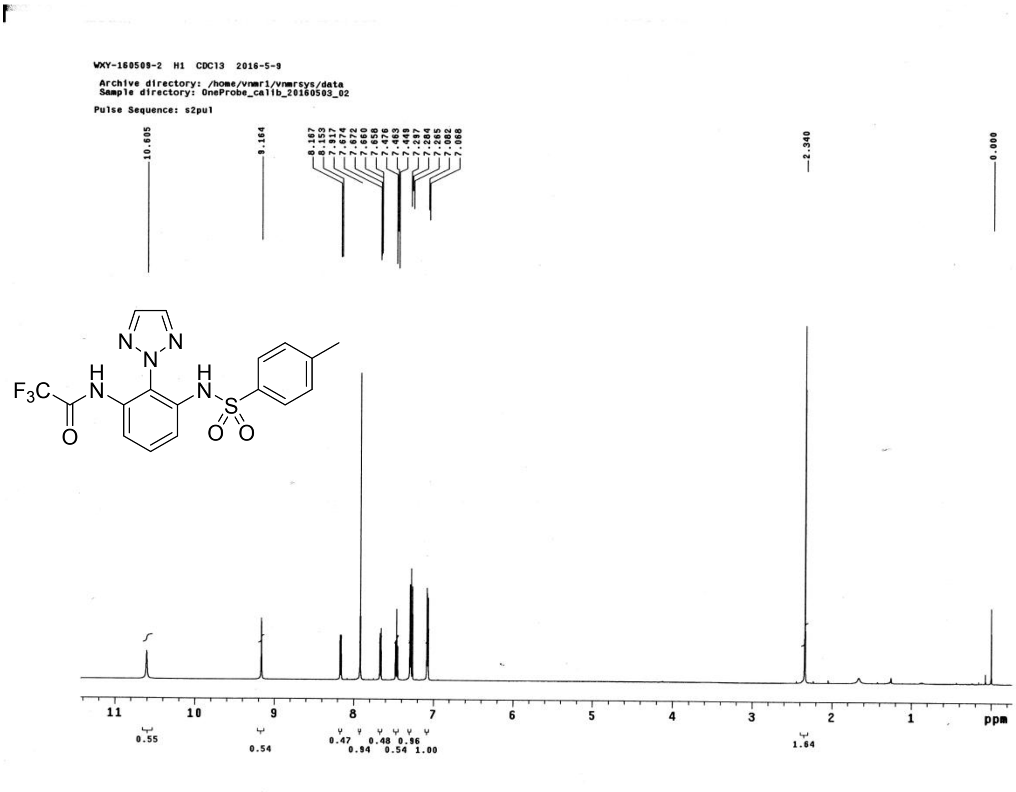


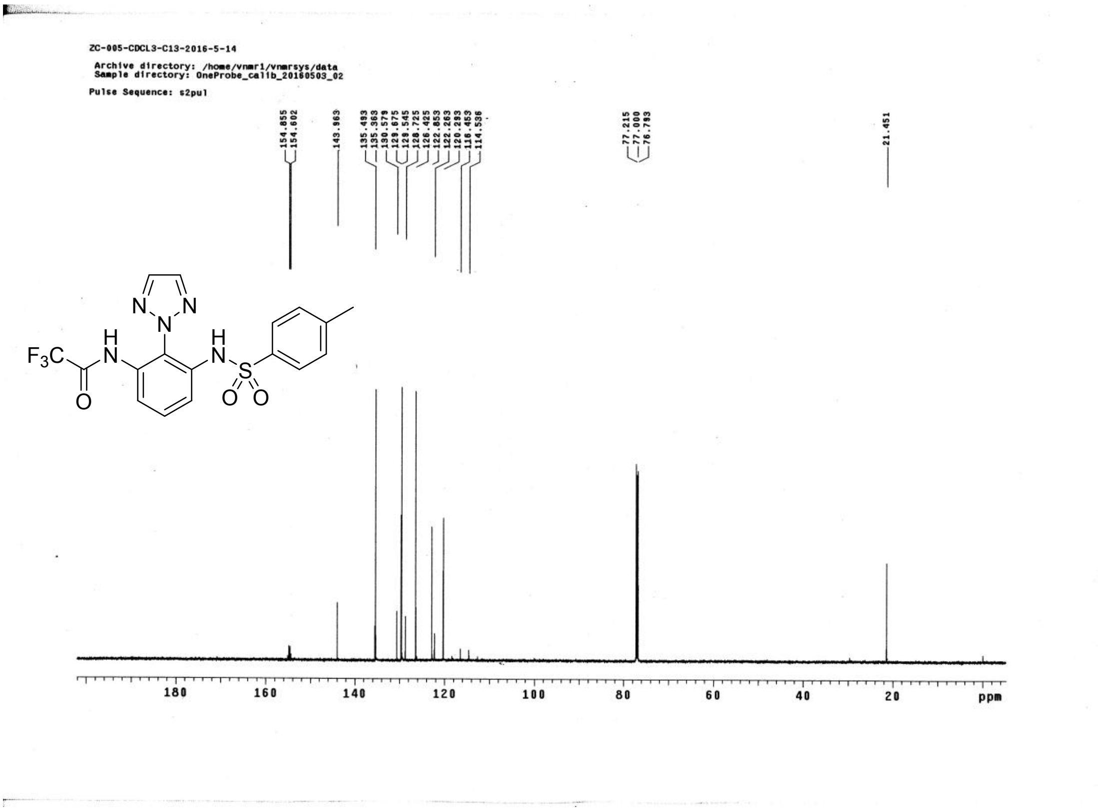
ZC-018 C13 CDCl3 2016-5-25
Archive directory: /home/vnmr1/vnmrsys/data
Sample directory: OneProbe_calib_20160503_02
Pulse Sequence: s2pul
144.243
136.114
135.492
134.243
131.182
131.131
130.236
129.748
126.789
122.438
120.524
77.211
77.000
76.789
21.553
Br
ppm

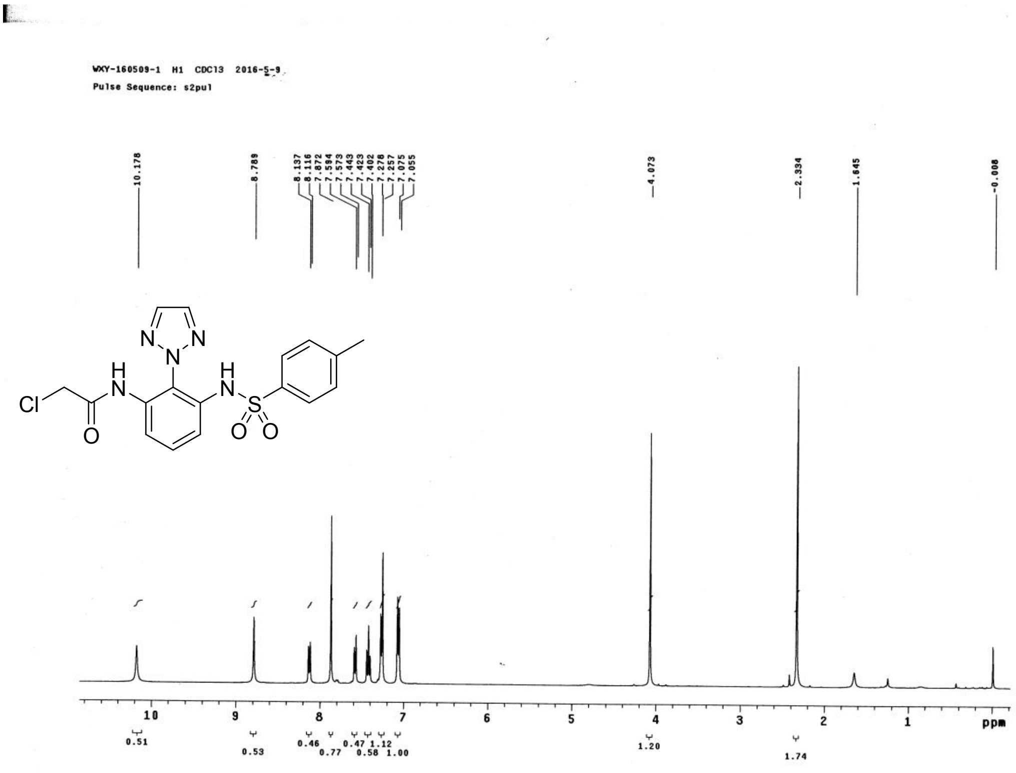


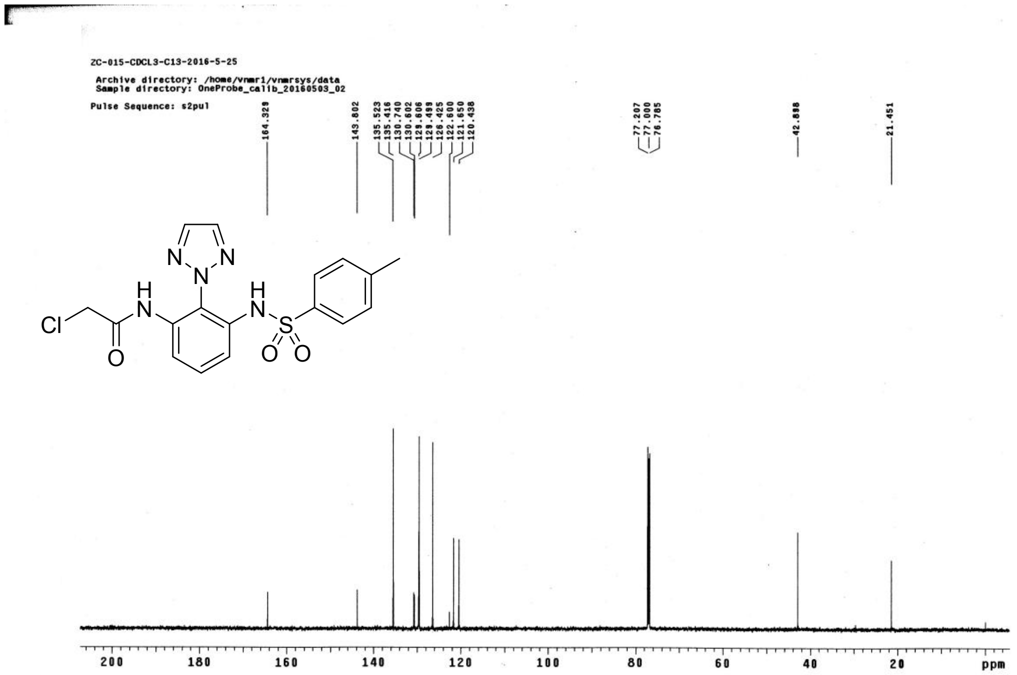
WXY-160509-3 H1 CDCl3 2016-5-9
Archive directory: /home/vnmr1/vnmrsys/data
Sample directory: OneProbe_calib_20160503_02
Pulse Sequence: s2pul
9.107
8.752
8.144
8.130
7.885
7.520
7.507
7.414
7.400
7.386
7.286
7.250
7.073
7.059
2.342
2.043
1.271
1.260
1.254
1.248
0.071
0.000
0.48
0.52
0.49
0.92
0.53
0.58
1.25
1.00
1.52
1.65
ppm

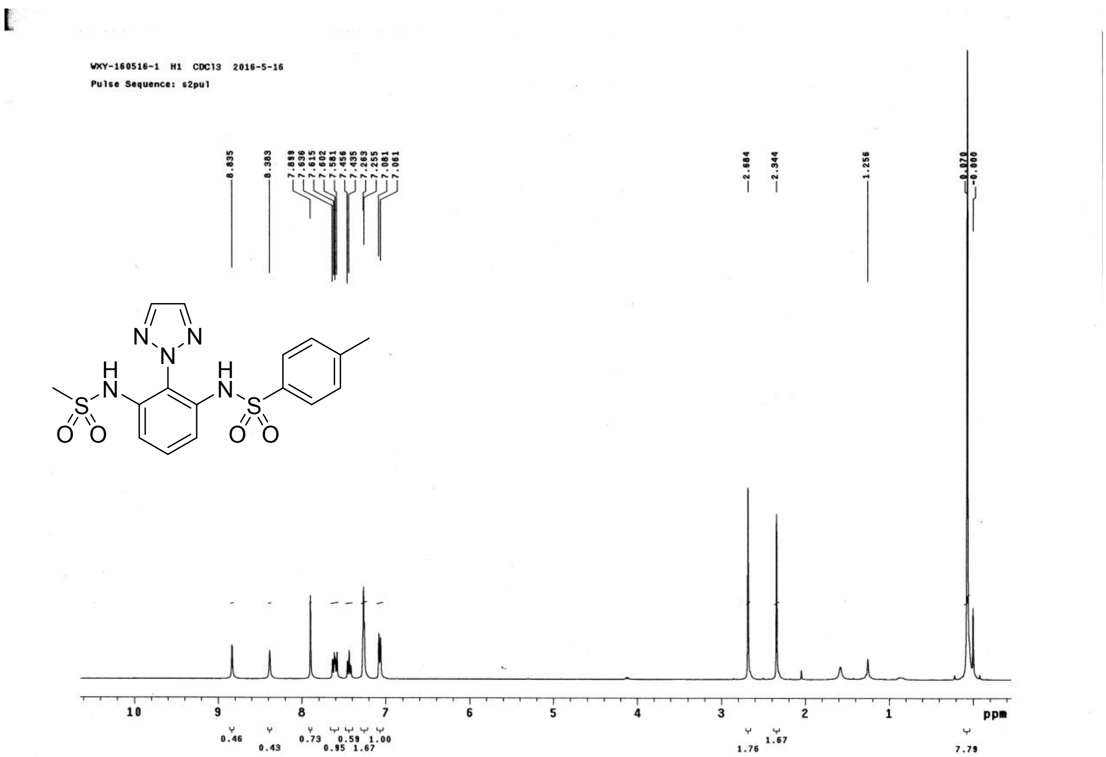

ZC-004-CDCL3-C13-2016-5-14
Archive directory: /home/vnmr1/vnmrsys/data
Sample directory: OneProbe_calib_20160503_02
Pulse Sequence: s2pul
168.016
143.679
135.531
135.202
131.622
130.394
129.537
129.437
126.394
122.247
121.036
120.814
77.215
77.000
76.785
24.754
21.428
200
180
160
140
120
100
80
60
40
20
ppm

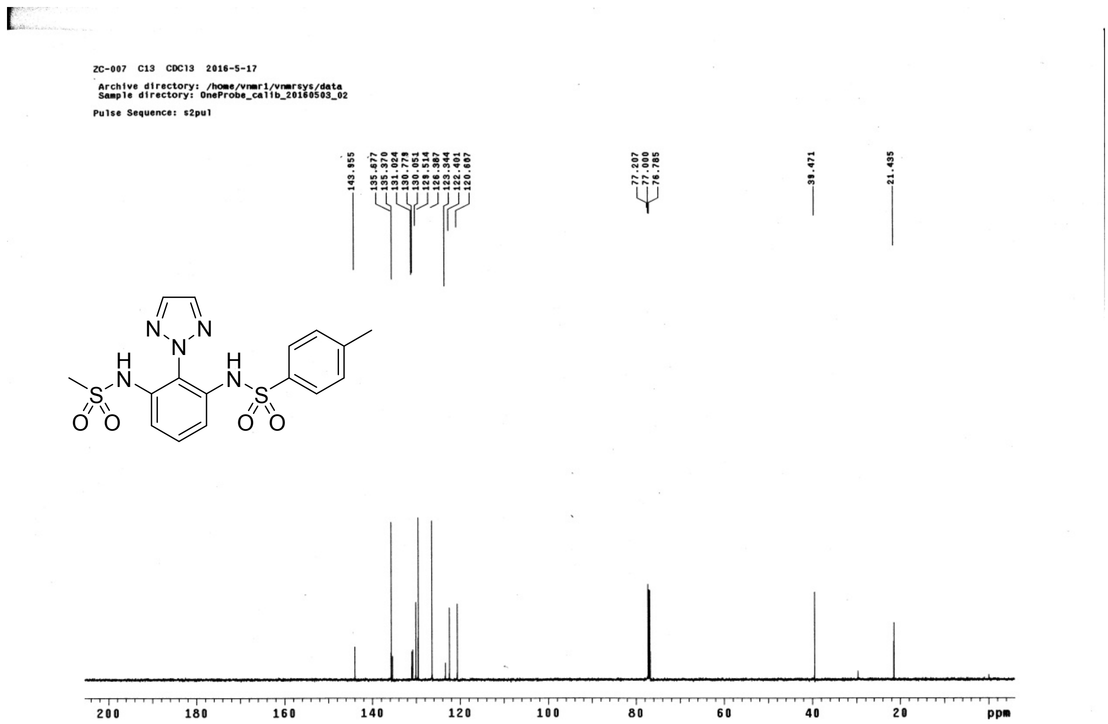

WXY-160509-2 H1 CDCl3 2016-5-9
Archive directory: /home/vnmr1/vnmrsys/data
Sample directory: OneProbe_calib_20160503_02
Pulse Sequence: s2pul
10.605
9.164
8.167
8.153
7.917
7.674
7.672
7.660
7.658
7.476
7.463
7.449
7.297
7.284
7.285
7.082
7.068
2.340
0.000
F3C
11
10
9
8
7
6
5
4
3
2
1
ppm
0.55
0.54
0.47
0.94
0.48
0.54
0.96
1.00
1.64


ZC-005-CDCL3-C13-2016-5-14
Archive directory: /home/vnmr1/vnmrsys/data
Sample directory: OneProbe_calib_20160503_02
Pulse Sequence: s2pul
F3C
ppm

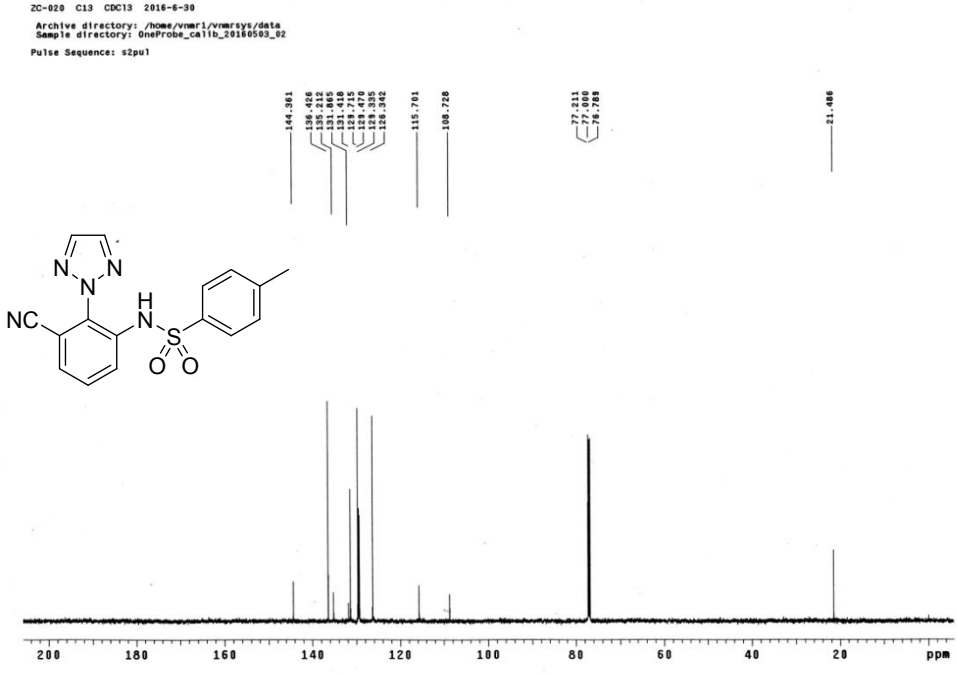

WXY-160509-1 H1 CDCl3 2016-5-9
Pulse Sequence: s2pul
Cl
ppm

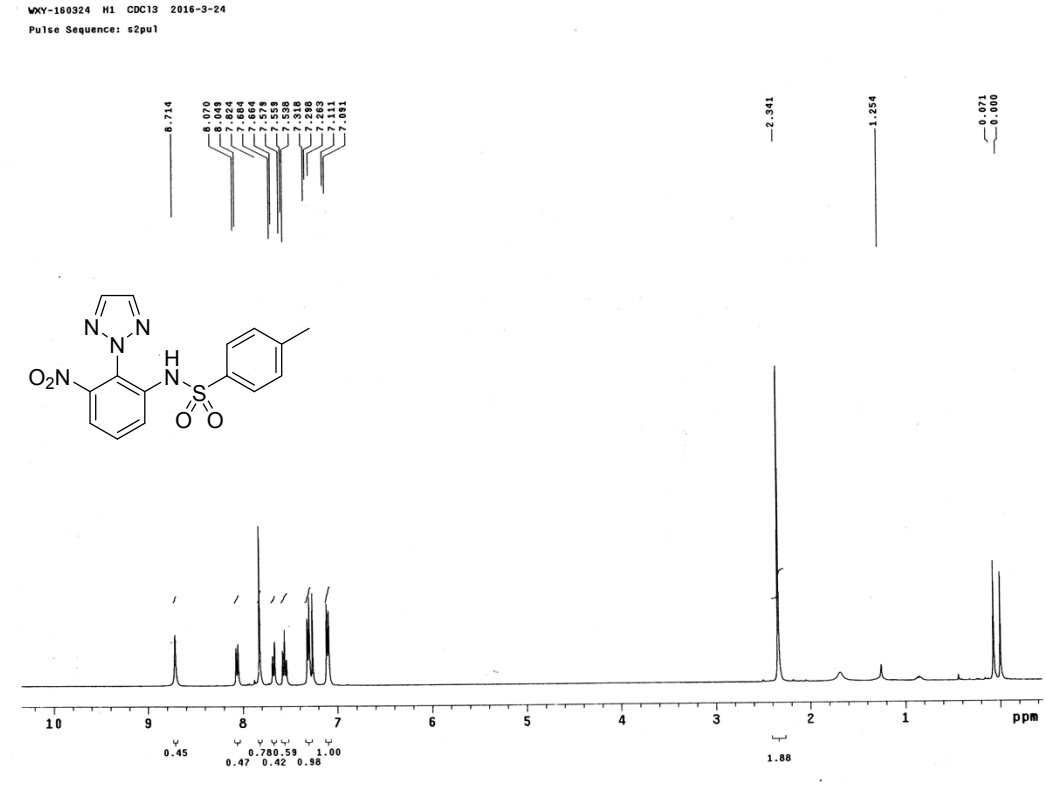

ZC-015-CDCL3-C13-2016-5-25
Archive directory: /home/vnmr1/vnmrsys/data
Sample directory: OneProbe_calib_20160503_02
Pulse Sequence: s2pul
Cl
H
N
N
N
N
N
H
S
O
O
O
ppm

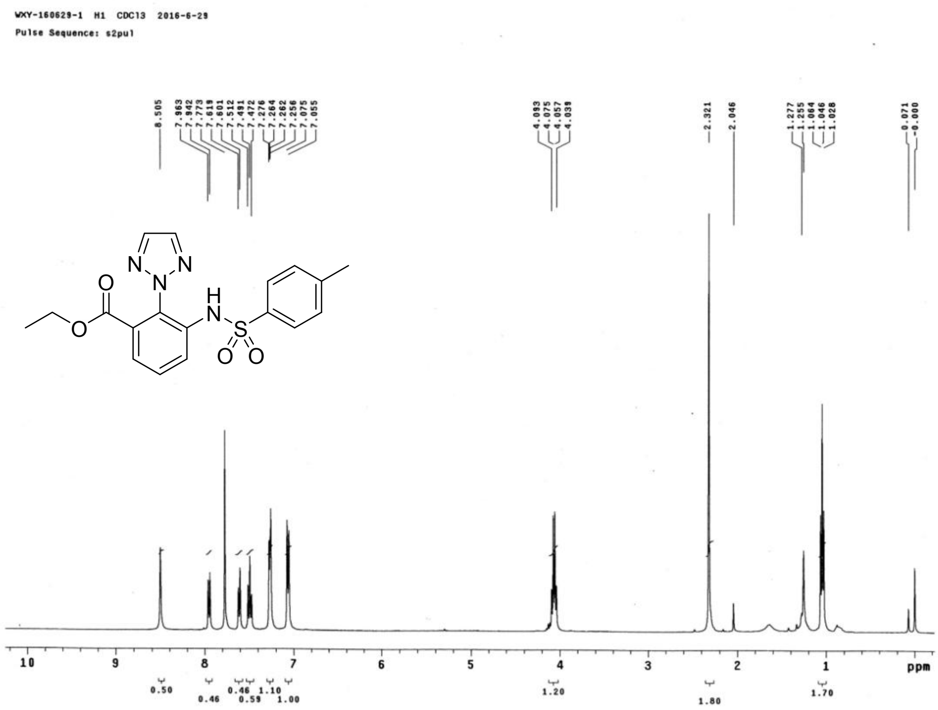

WXY-160516-1 H1 CDCl3 2016-5-16
Pulse Sequence: s2pul
S
H
N
N
N
N
N
H
S
O
O
O
O
ppm

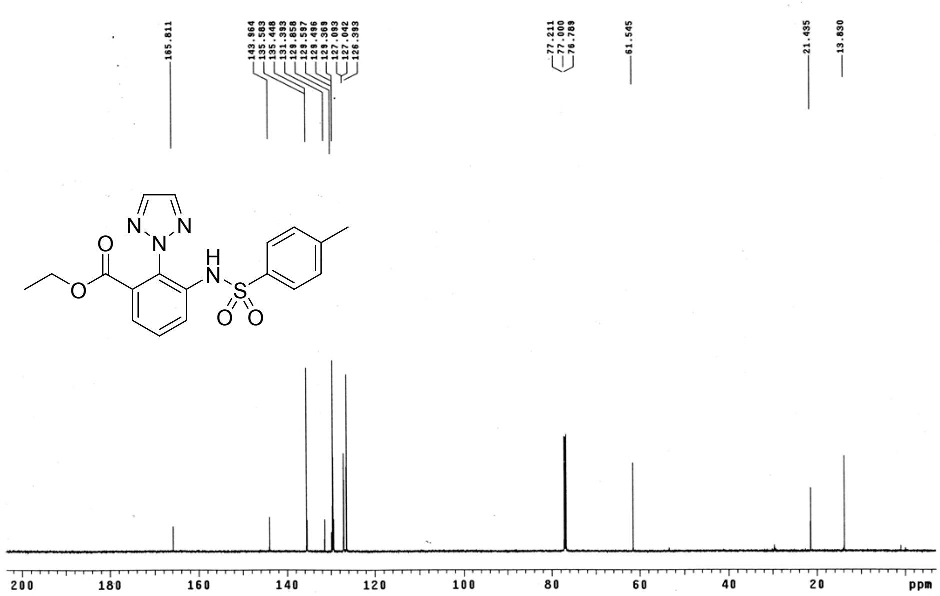

ZC-007 C13 CDCl3 2016-5-17
Archive directory: /home/vnmr1/vnmrsys/data
Sample directory: OneProbe_calib_20160503_02
Pulse Sequence: s2pul
143.955
135.877
135.370
131.024
130.779
130.051
129.514
126.307
123.344
122.401
120.807
77.207
77.000
76.785
39.471
21.435
N
N
N
H
N
S
O
O
H
N
S
O
O
200
180
160
140
120
100
80
60
40
20
ppm

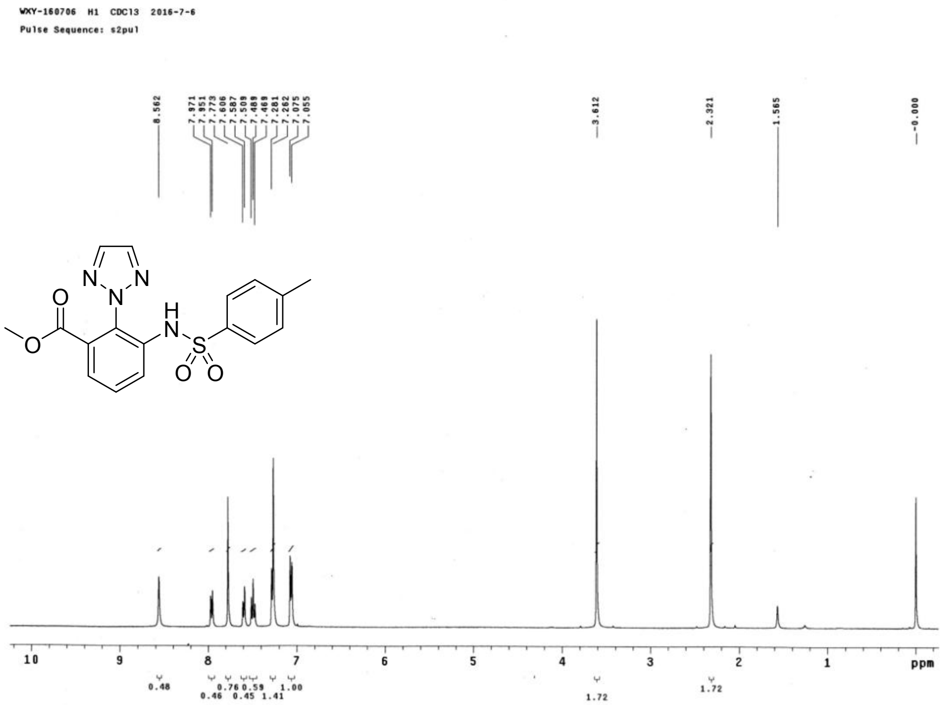

WXY-160630 H1 CDCl3 2016-6-30
Pulse Sequence: s2pul
9.049
8.080
8.062
8.060
7.902
7.632
7.616
7.613
7.534
7.514
7.494
7.297
7.277
7.263
7.095
7.075
2.341
1.579
0.000
N
N
N
NC
H
N
S
O
O
10
9
8
7
6
5
4
3
2
1
ppm
0.80
1.23
0.78
0.91
0.71
1.69
2.35
3.00

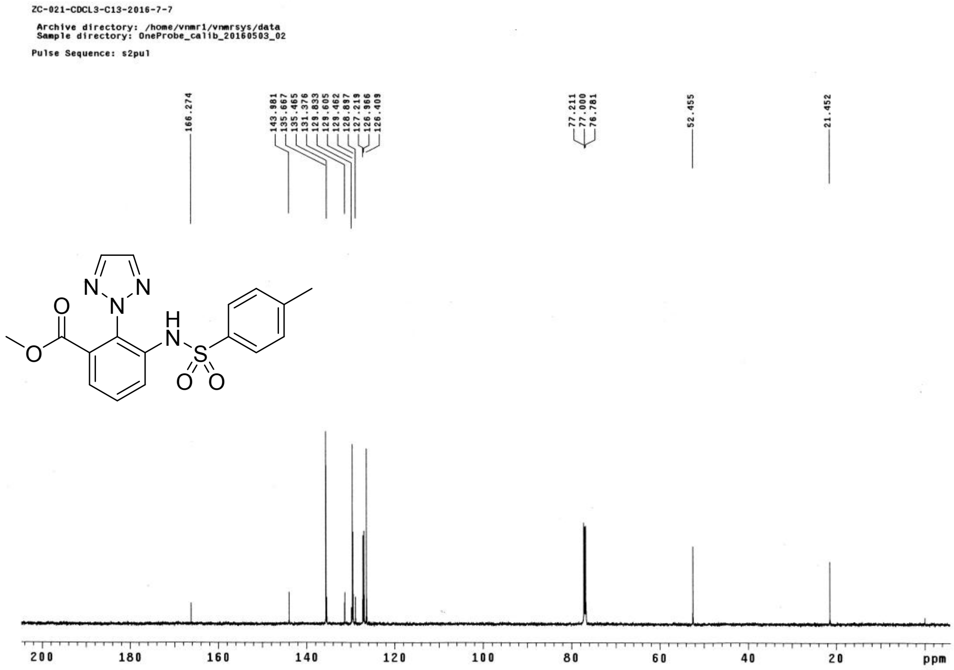

ZC-020 C13 CDCl3 2016-6-30
Archive directory: /home/vnmr1/vnmrsys/data
Sample directory: OneProbe_calib_20160503_02
Pulse Sequence: s2pul
144.361
136.426
135.212
131.865
131.418
130.715
129.470
129.335
128.342
115.761
108.728
77.211
77.000
76.788
21.486
NC
N
N
N
H
N
S
O
O
200
180
160
140
120
100
80
60
40
20
ppm

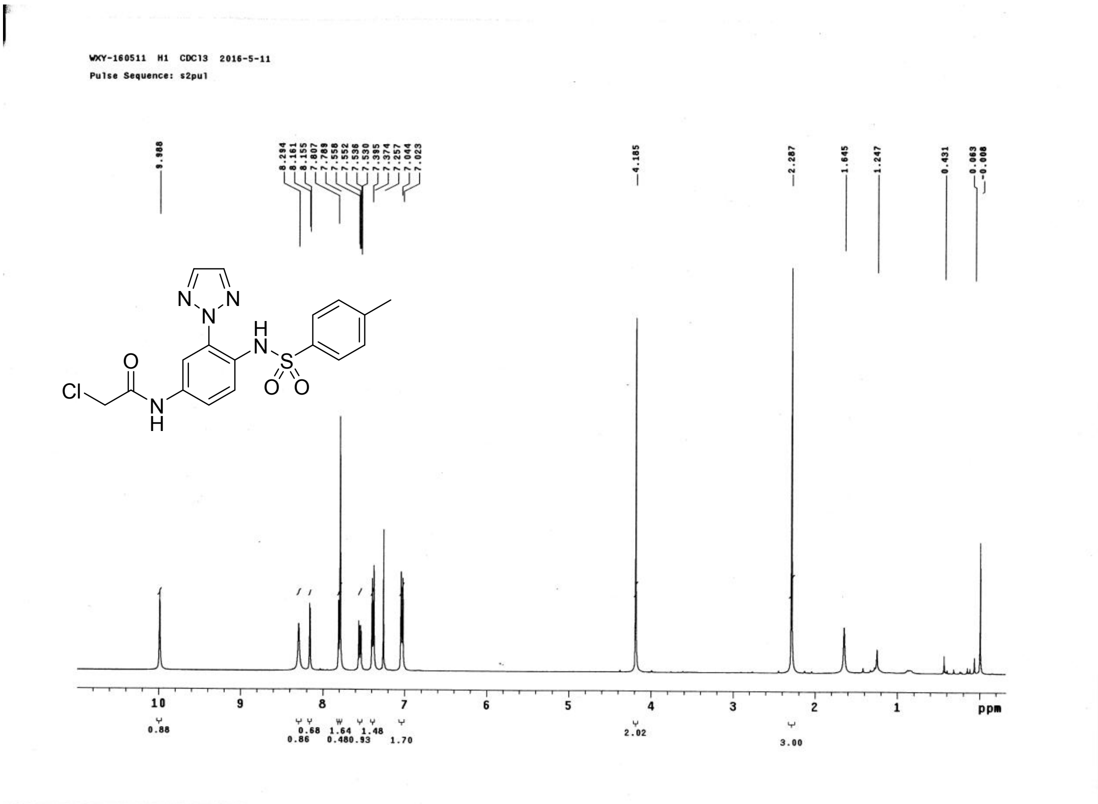

WXY-160324 H1 CDCl3 2016-3-24
Pulse Sequence: s2pul
8.714
8.070
8.049
7.824
7.804
7.664
7.579
7.559
7.538
7.318
7.298
7.263
7.111
7.091
2.341
1.254
0.071
0.000
O2N
N
N
N
H
N
S
O
O
10
9
8
7
6
5
4
3
2
1
ppm
0.45
0.47
0.42
0.78
0.59
0.58
1.00
1.88

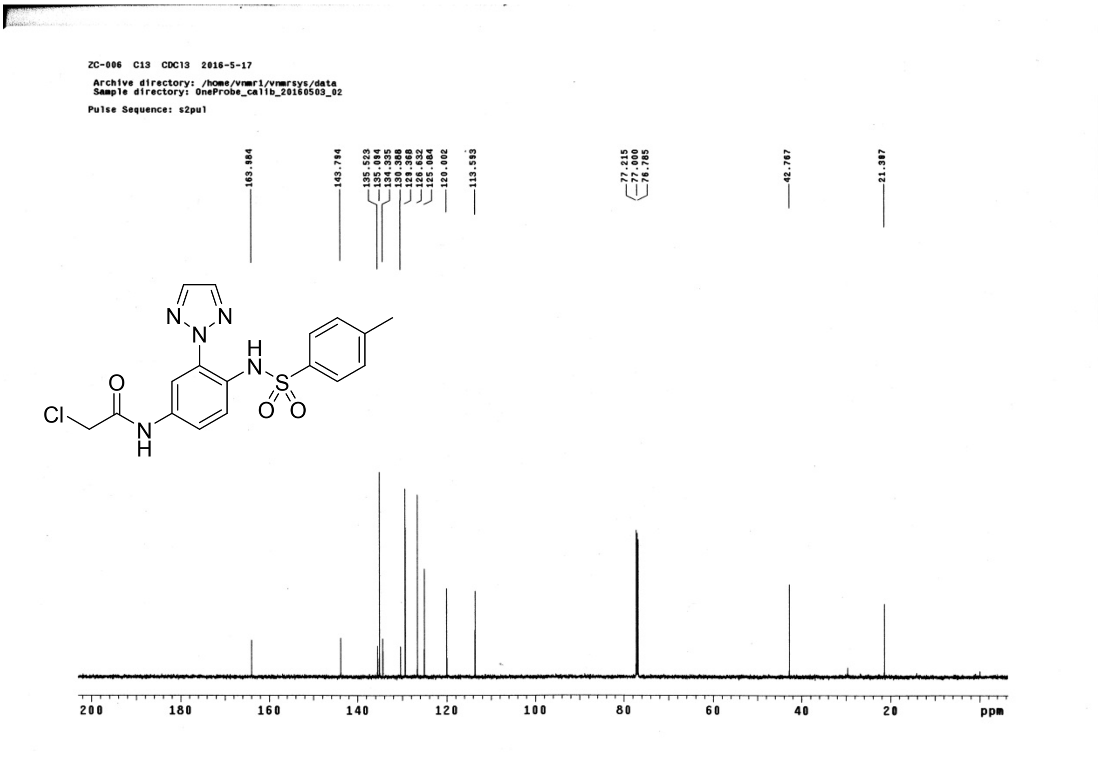


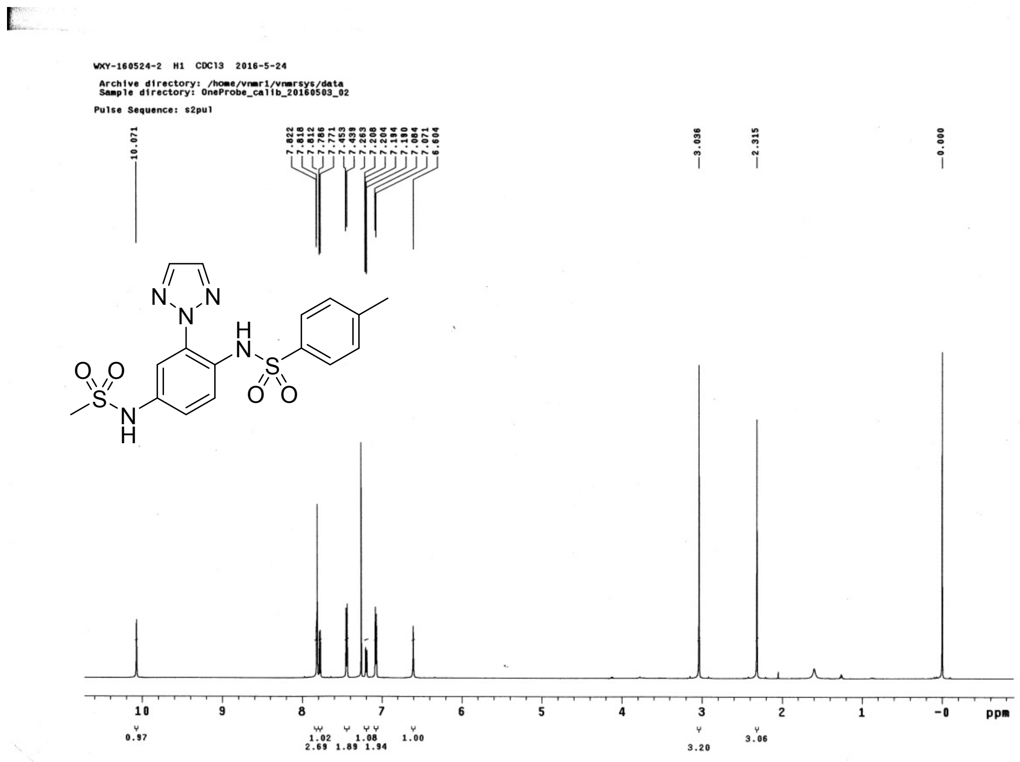


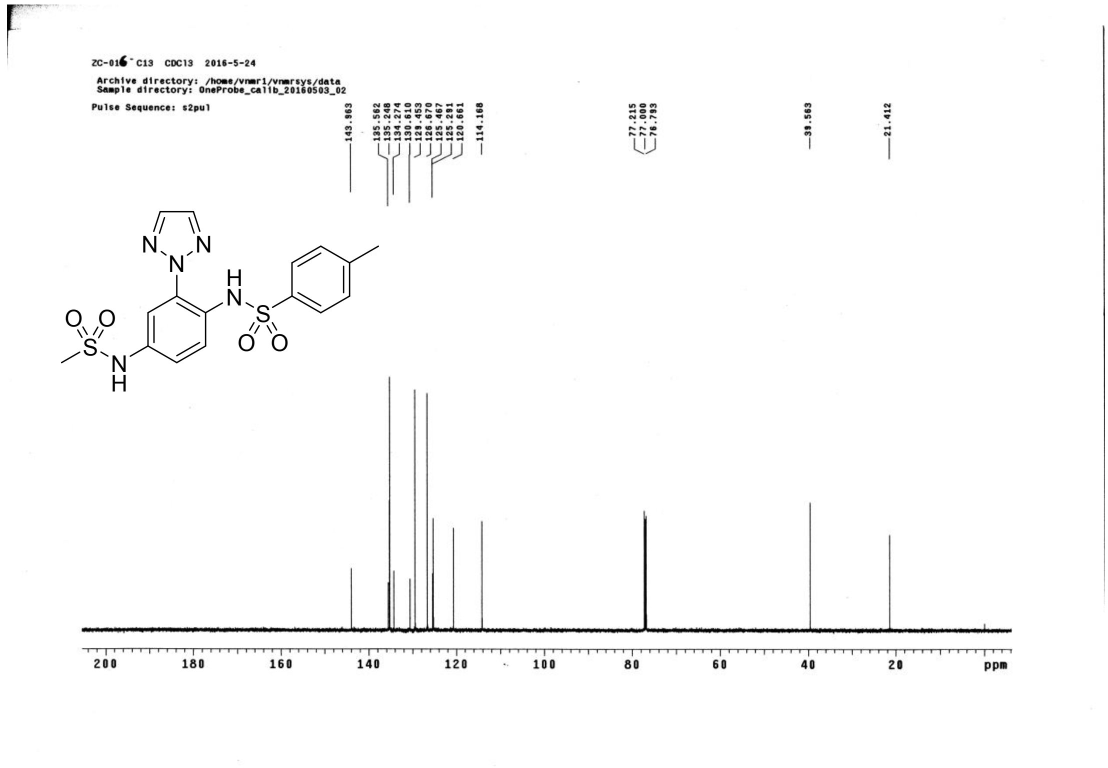

WXY-160706 H1 CDCl3 2016-7-6
Pulse Sequence: s2pul
8.562
7.971
7.951
7.773
7.606
7.587
7.509
7.489
7.469
7.281
7.262
7.075
7.055
3.612
2.321
1.565
-0.000
N
N
N
O
O
N
H
S
O
O
10
9
8
7
6
5
4
3
2
1
ppm
0.48
0.76
0.59
1.00
0.46
0.45
1.41
1.72
1.72

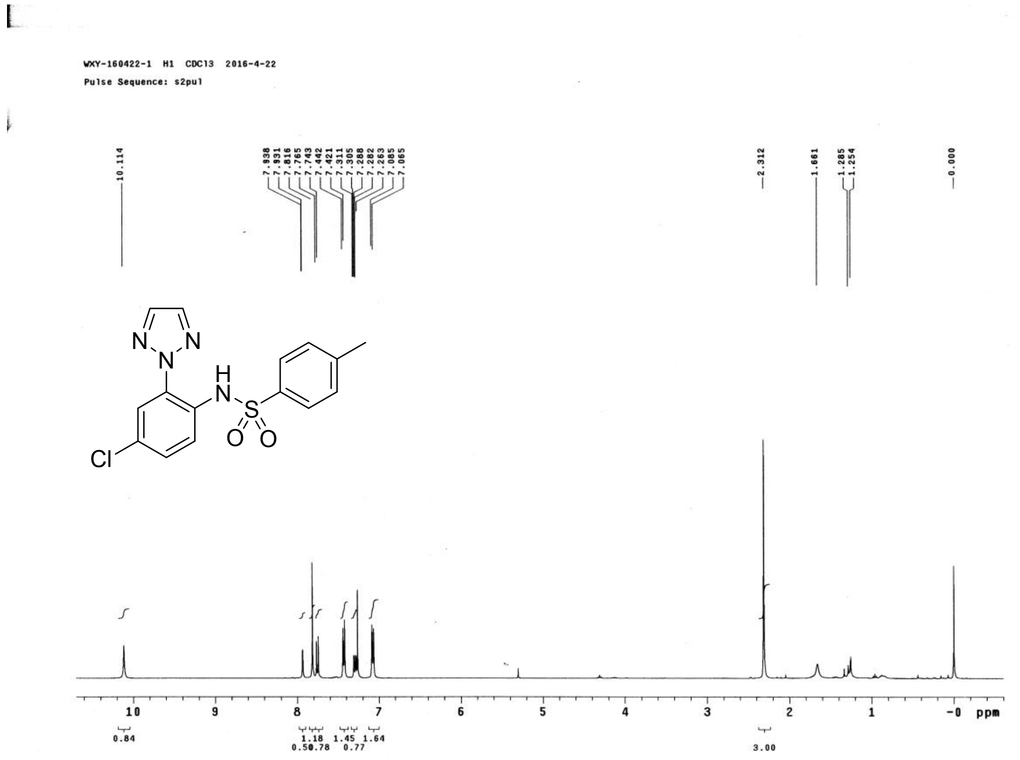

ZC-021-CDCL3-C13-2016-7-7
Archive directory: /home/vnmr1/vnmrsys/data
Sample directory: OneProbe_calib_20160503_02
Pulse Sequence: s2pul
166.274
143.981
135.667
135.465
131.376
129.833
129.605
129.462
128.897
127.218
126.966
126.409
77.211
77.000
76.781
52.455
21.452
N
N
N
O
O
N
H
S
O
O
200
180
160
140
120
100
80
60
40
20
ppm

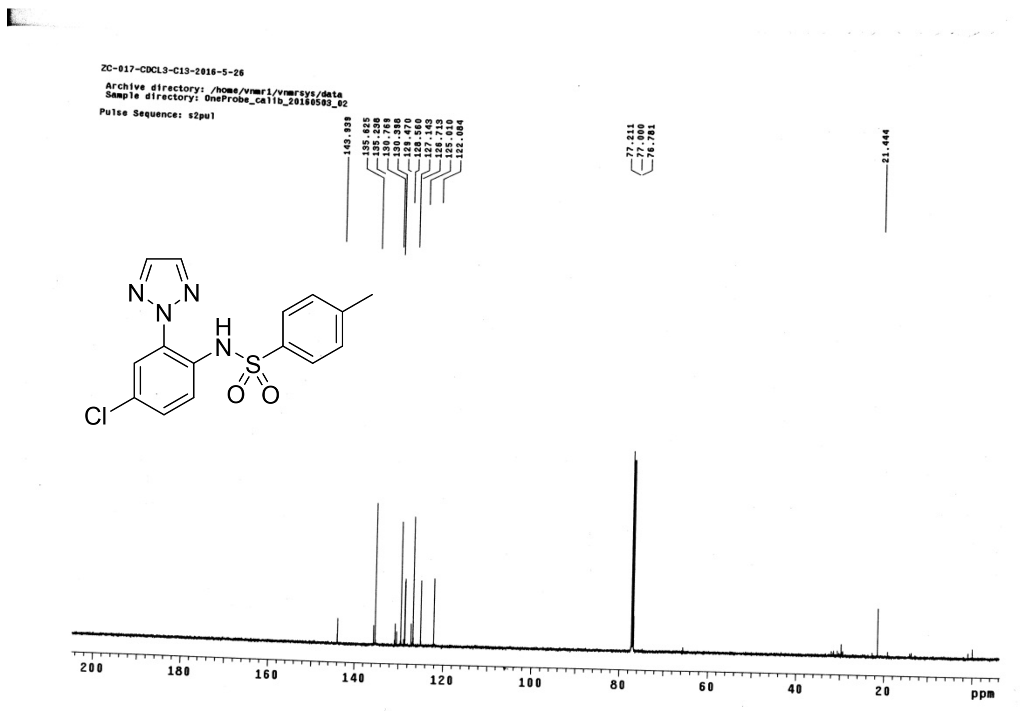

WXY-160511 H1 CDCl3 2016-5-11
Pulse Sequence: s2pul
ppm


ZC-006 C13 CDCl3 2016-5-17
Archive directory: /home/vnmr1/vnmrsys/data
Sample directory: OneProbe_calib_20160503_02
Pulse Sequence: s2pul
ppm


WXY-160524-2 H1 CDCl3 2016-5-24
Archive directory: /home/vnmr1/vnmrsys/data
Sample directory: OneProbe_calib_20160503_02
Pulse Sequence: s2pul
ppm

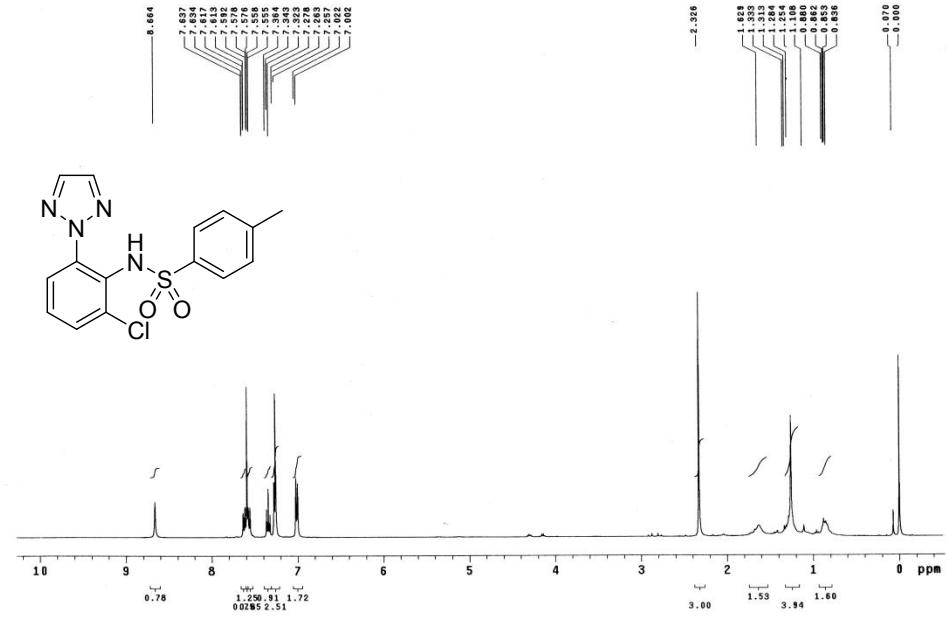

C13 CDCl3 2016-5-24
Archive directory: /home/vnmr1/vnmrsys/data
Sample directory: OneProbe_calib_20160503_02
Pulse Sequence: s2pul
ppm





WXY-160422-2 H1 CDCl3 2016-4-22

Pulse Sequence: s2pul

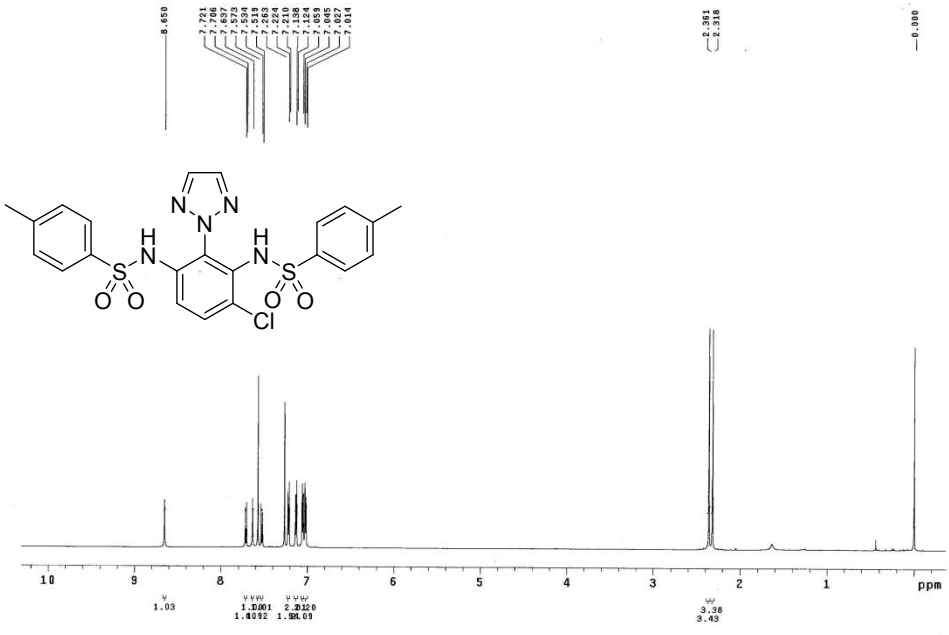


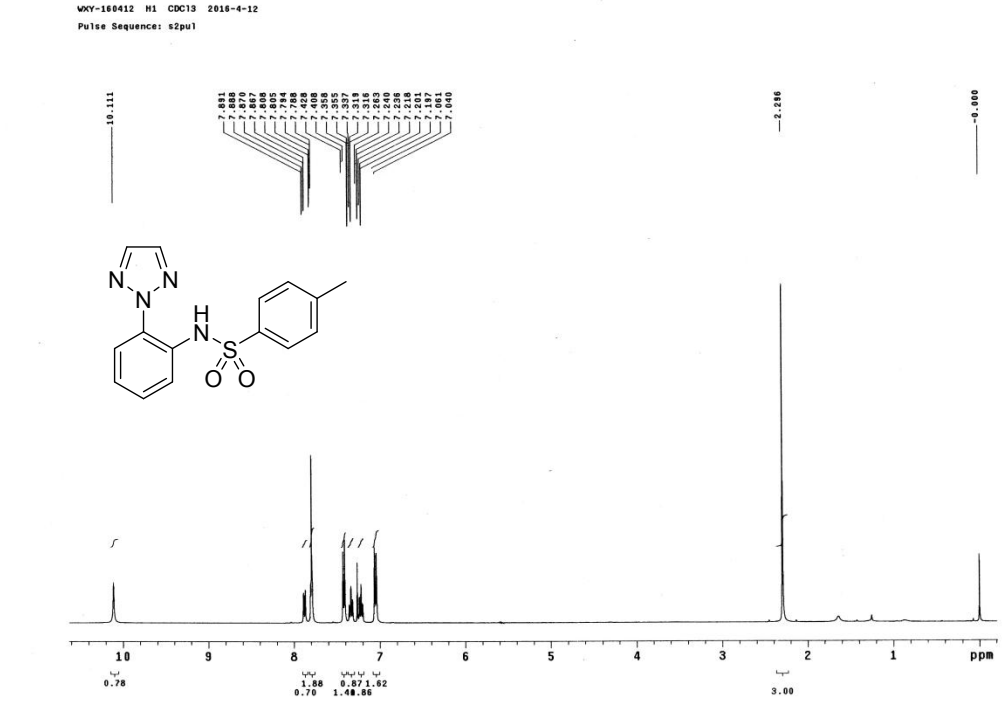
WXY-160524-3 H1 CDCl3 2016-5-24

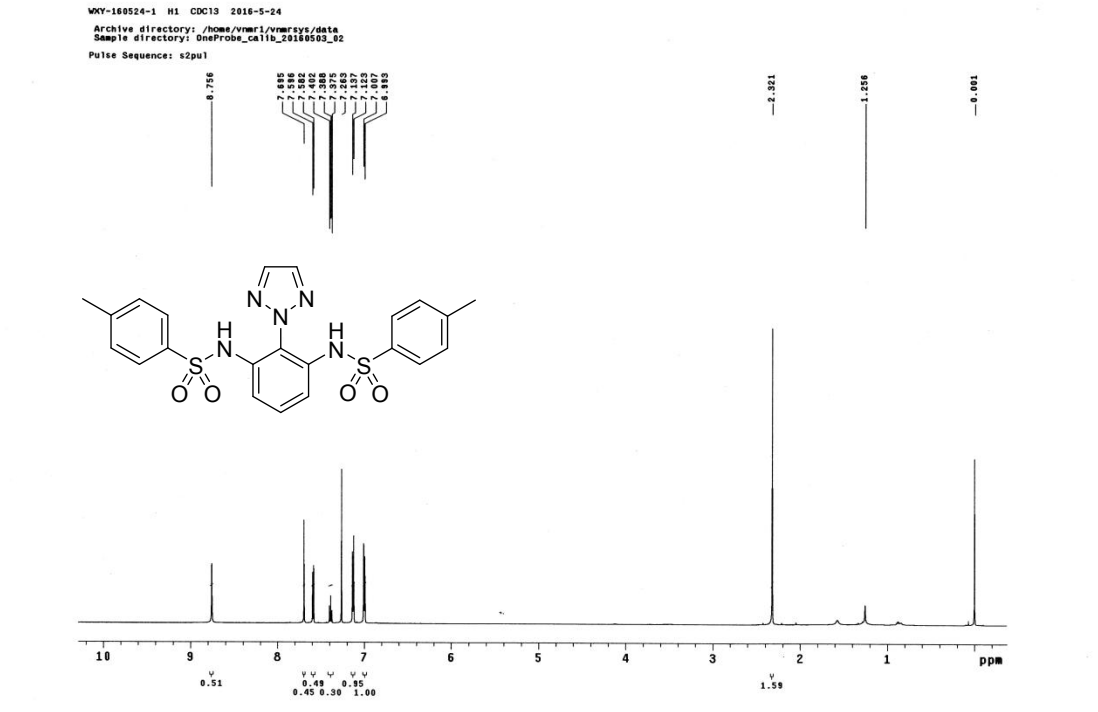
Archive directory: /home/vnmr1/vnmrsys/data

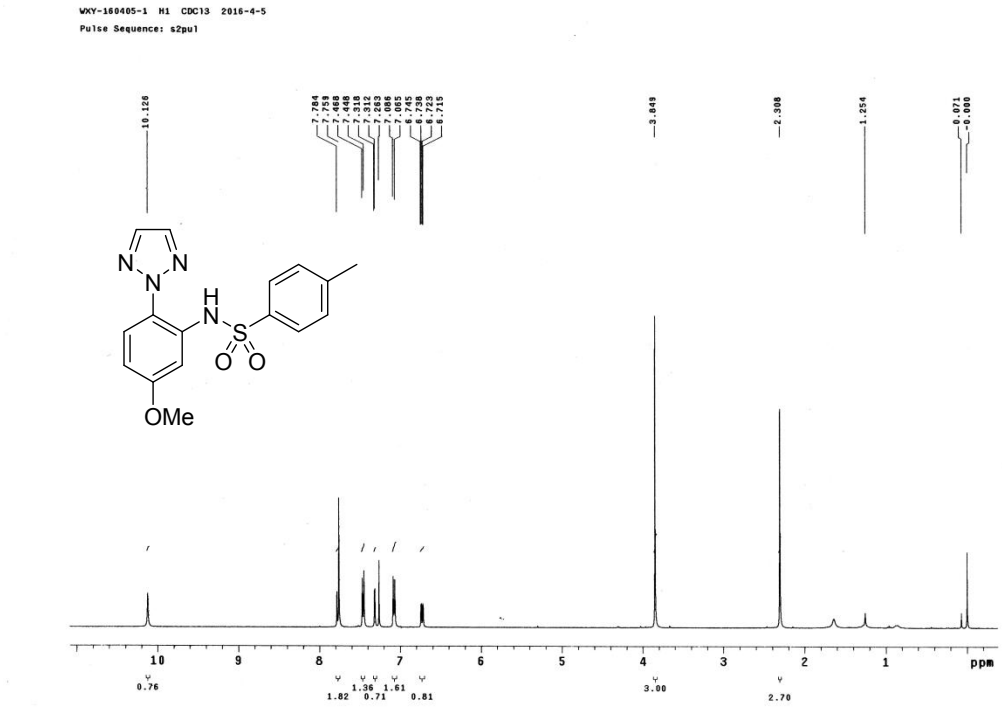
Sample directory: OneProbe_calib_20160503_02

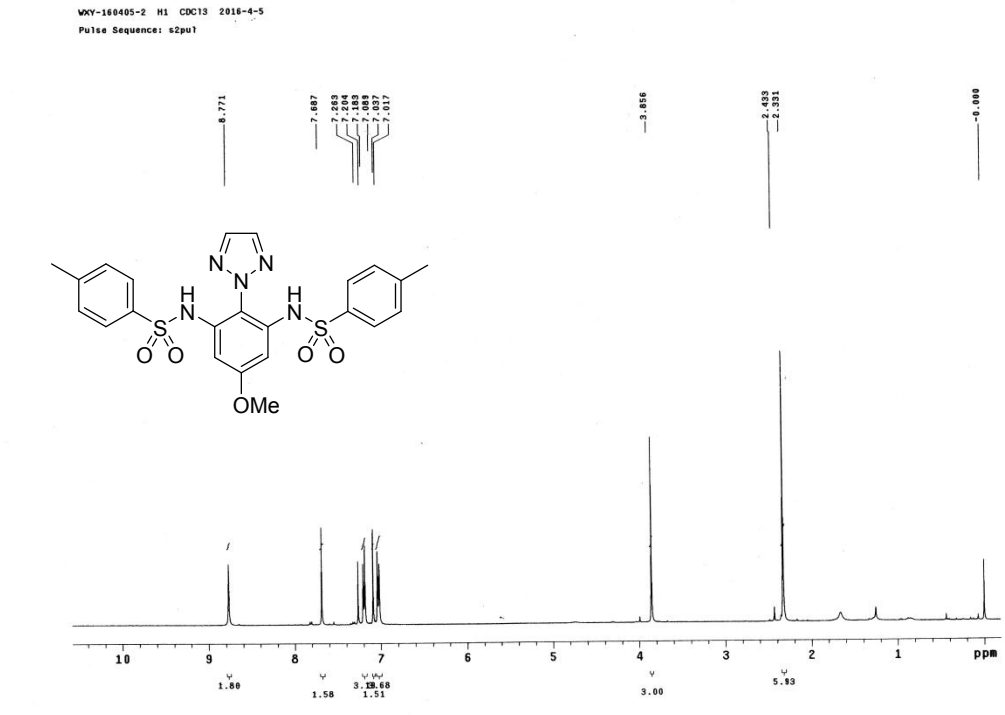
Pulse Sequence: s2pul

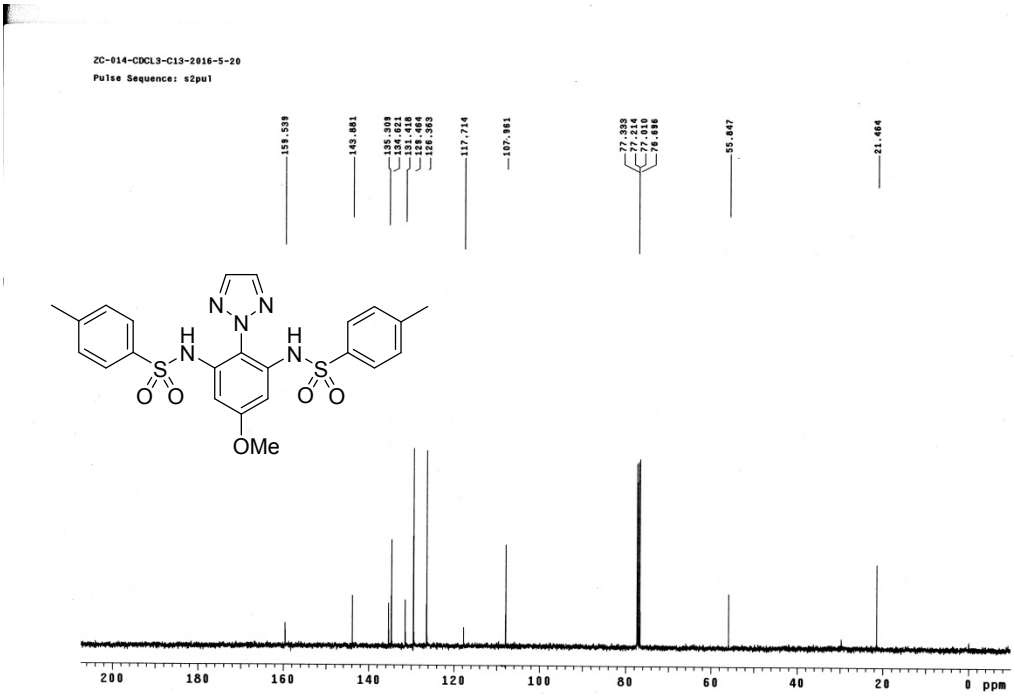


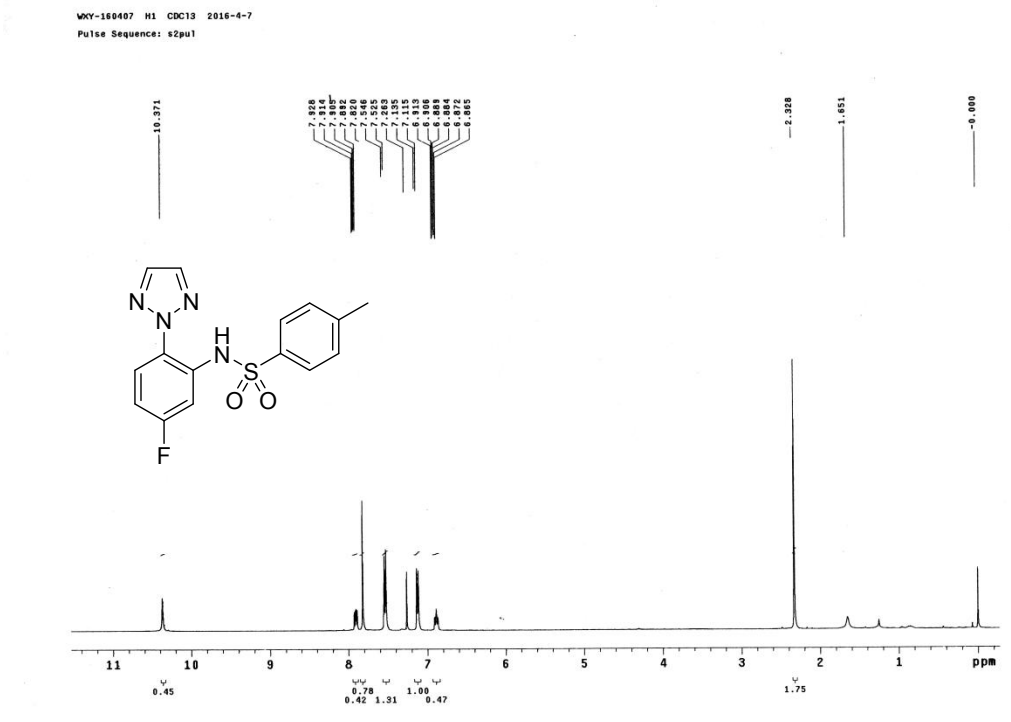

WXY-160412 H1 CDCl3 2016-4-12
Pulse Sequence: s2pul
10.111
7.891
7.888
7.870
7.868
7.806
7.805
7.784
7.782
7.428
7.408
7.358
7.356
7.337
7.319
7.318
7.265
7.240
7.238
7.216
7.201
7.197
7.061
7.040
2.236
-0.000
N
N
N
H
N
S
O
O
10
9
8
7
6
5
4
3
2
1
ppm
0.78
1.88
0.70
0.87
1.48
1.62
0.86
3.00

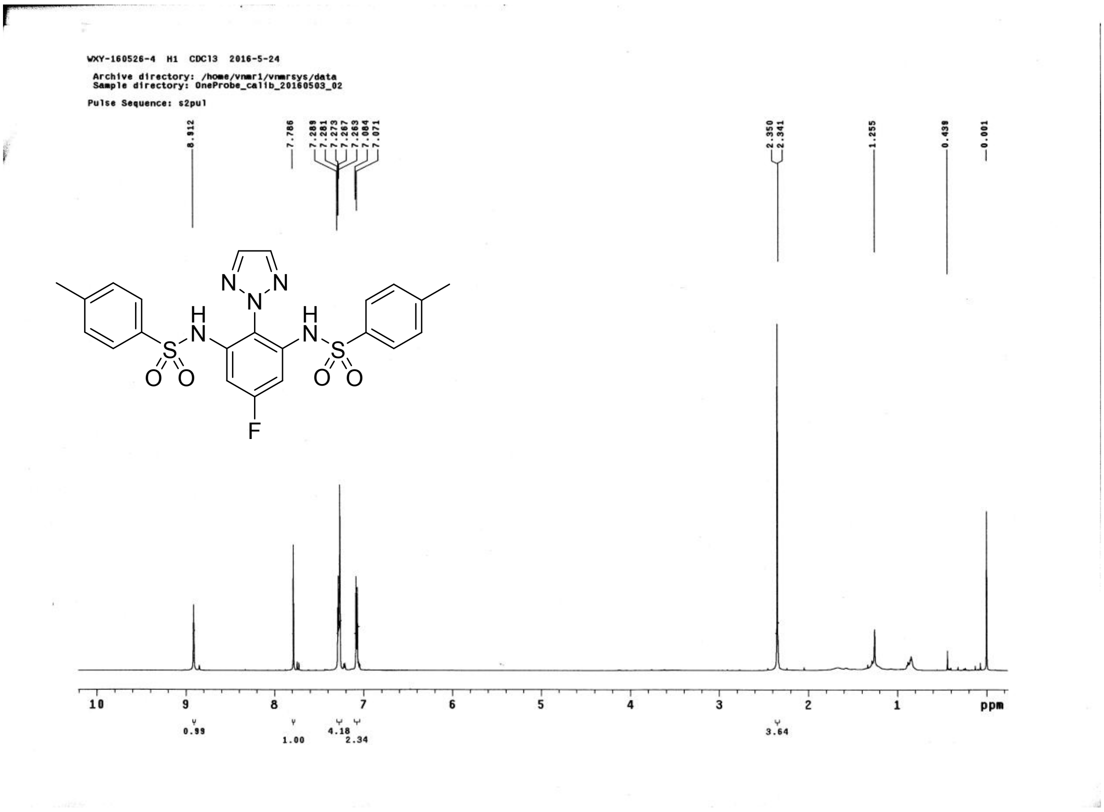

WXY-160524-1 H1 CDCl3 2016-5-24
Archive directory: /home/vnmr1/vnmrsys/data
Sample directory: OneProbe_calib_20160503_02
Pulse Sequence: s2pul
8.756
7.695
7.596
7.582
7.402
7.388
7.375
7.263
7.137
7.135
7.007
6.993
2.321
1.256
-0.001
N
N
N
H
N
S
O
O
H
N
S
O
O
10
9
8
7
6
5
4
3
2
1
ppm
0.51
0.49
0.45
0.30
0.95
1.00
1.59

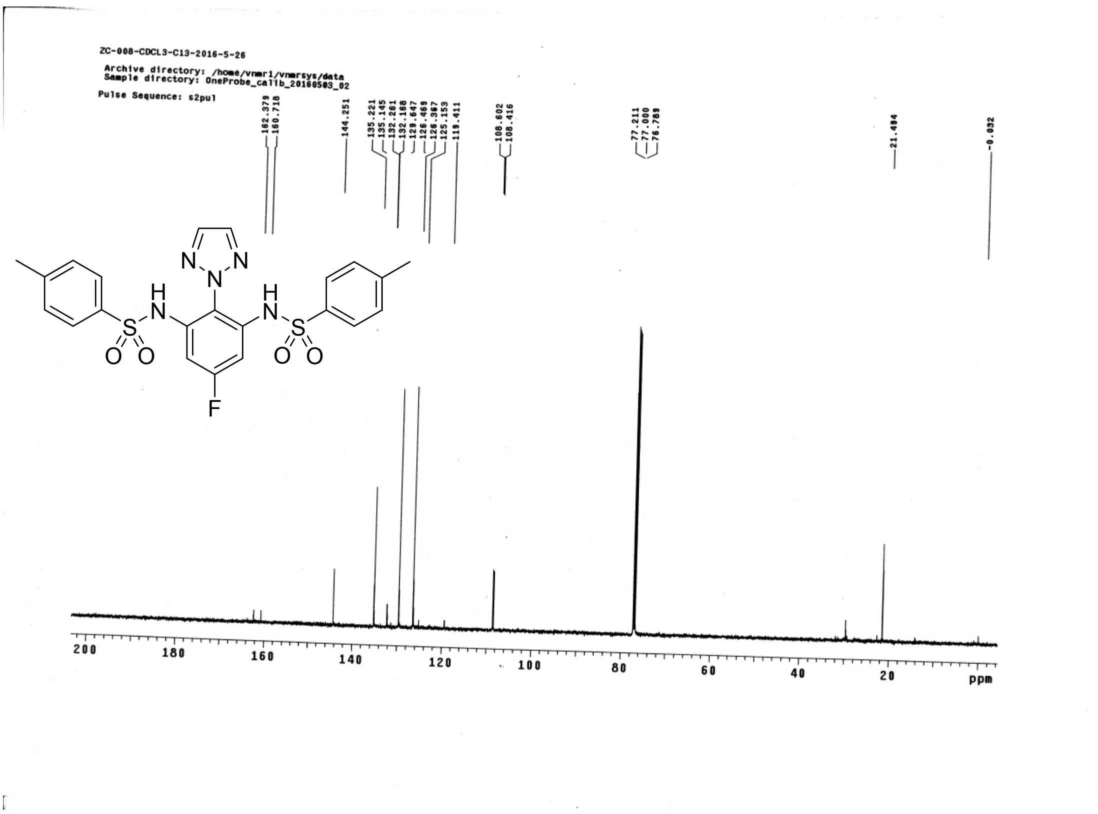

WXY-160405-1 H1 CDCl3 2016-4-5
Pulse Sequence: s2pul
10.126
7.784
7.759
7.468
7.448
7.312
7.288
7.086
7.065
6.745
6.738
6.723
6.715
3.849
2.306
1.254
0.071
0.000
N
N
N
H
N
S
O
O
OMe
10
9
8
7
6
5
4
3
2
1
ppm
0.76
1.82
1.36
0.71
1.61
0.81
3.00
2.70

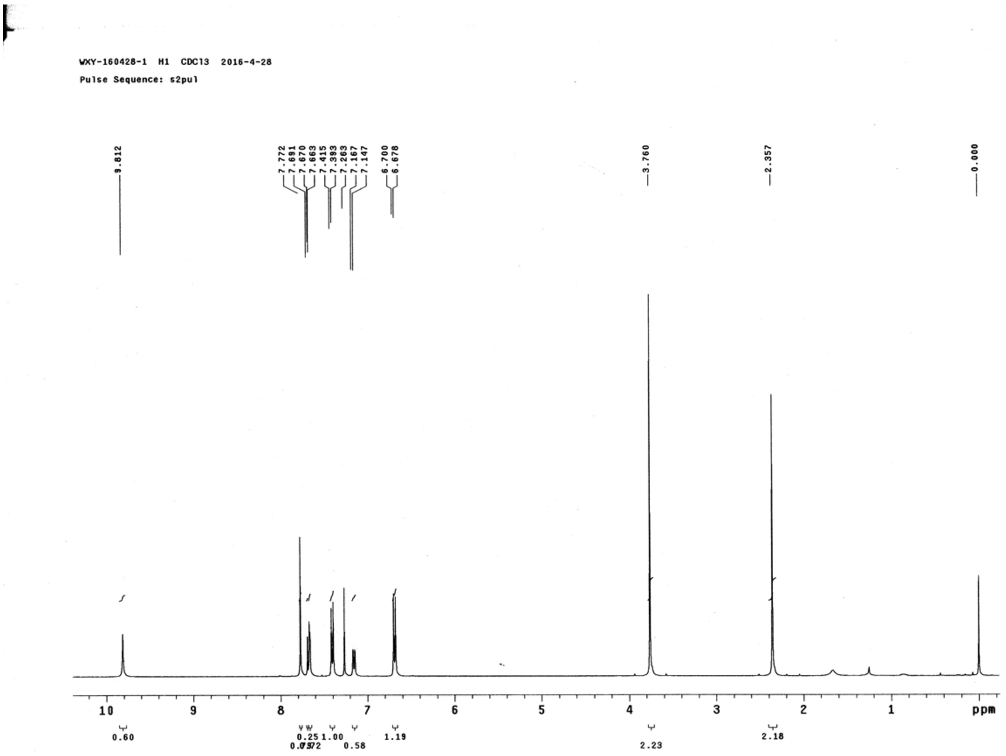

WXY-160405-2 H1 CDCl3 2016-4-5
Pulse Sequence: s2pul
8.771
7.687
7.283
7.204
7.103
7.088
7.037
7.017
3.856
2.433
2.331
0.000
N
N
N
H
N
H
N
S
S
O
O
O
O
OMe
10
9
8
7
6
5
4
3
2
1
ppm
1.80
1.58
3.18
1.68
1.51
3.00
5.83

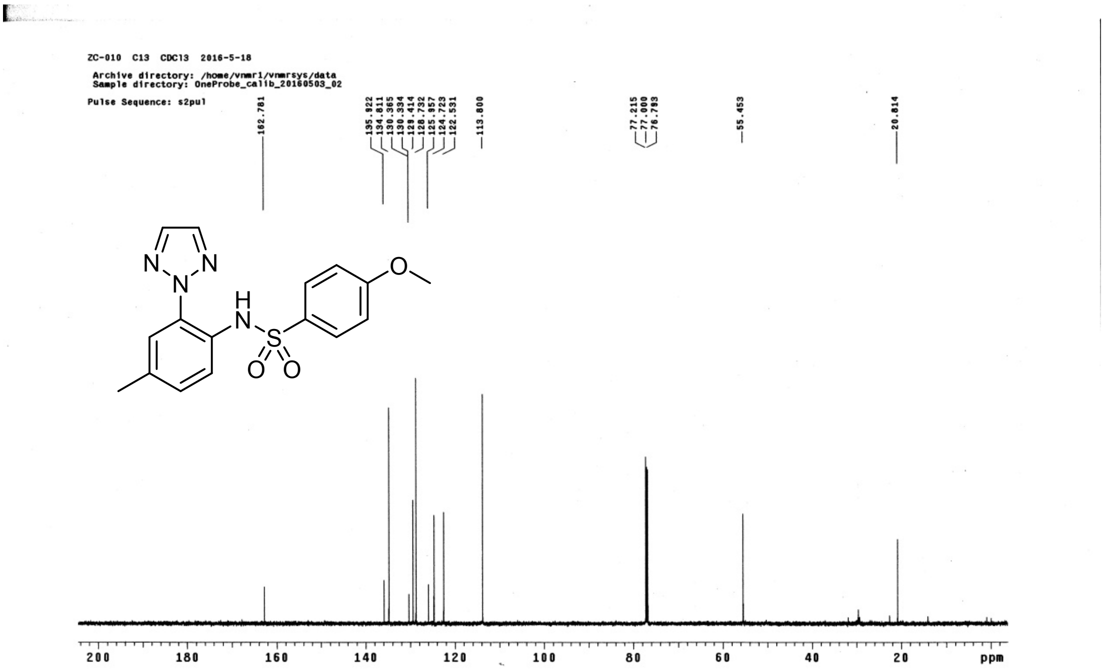

ZC-014-CDCL3-C13-2016-5-20
Pulse Sequence: s2pul
159.539
143.881
135.309
134.621
131.418
131.464
126.363
117.714
107.961
77.333
77.214
77.010
76.698
55.847
21.464
OMe
200
180
160
140
120
100
80
60
40
20
0 ppm

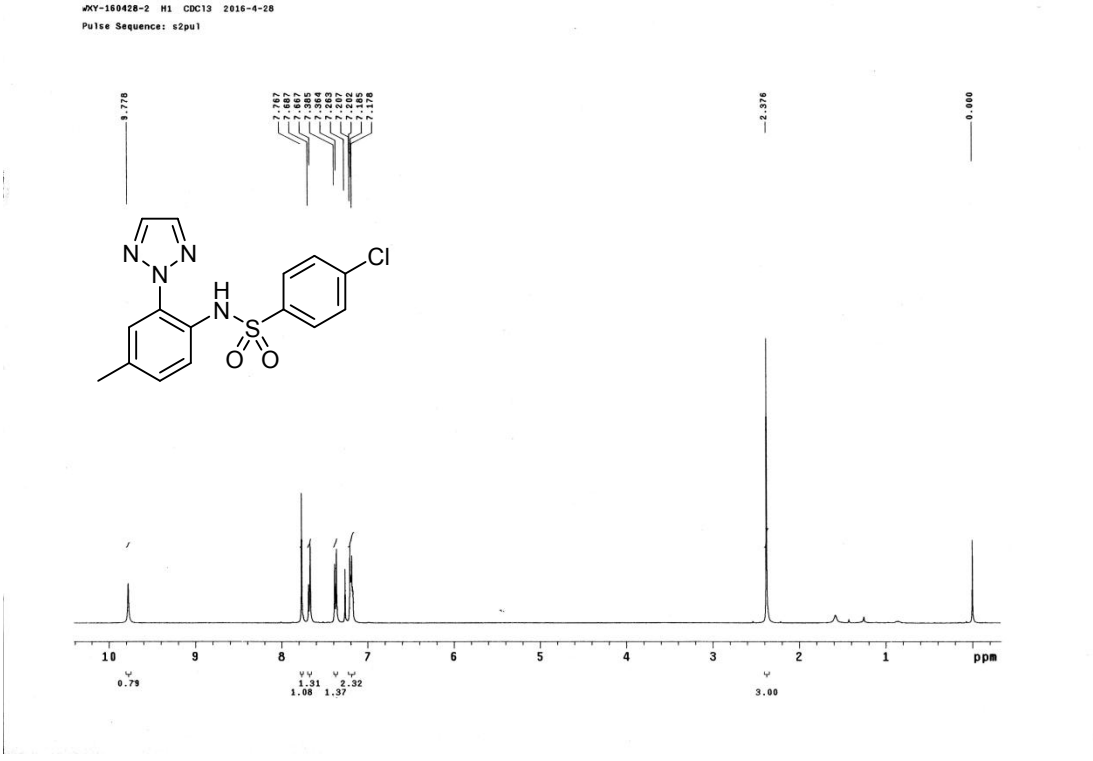

WXY-160407 H1 CDCl3 2016-4-7
Pulse Sequence: s2pul
10.371
7.926
7.907
7.895
7.882
7.820
7.566
7.525
7.263
7.135
7.115
6.913
6.906
6.884
6.884
6.872
6.865
2.328
1.651
-0.000
F
11
10
9
8
7
6
5
4
3
2
1
ppm
0.45
0.78
0.42
1.31
1.00
0.47
1.75

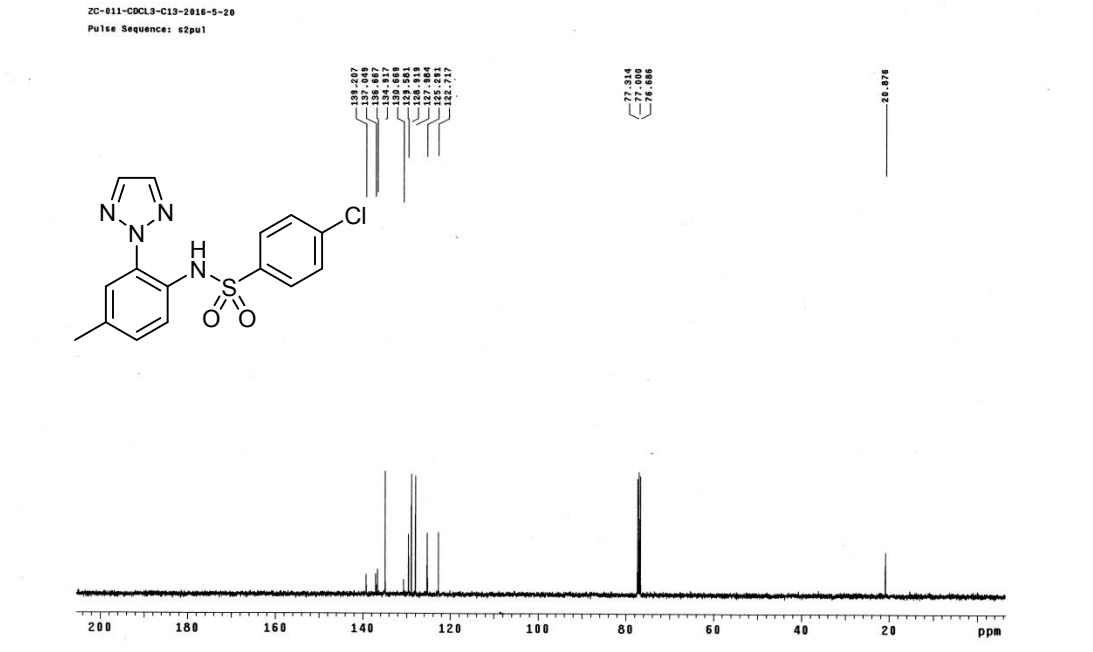

WXY-160526-4 H1 CDCl3 2016-5-24
Archive directory: /home/vnmr1/vnmrsys/data
Sample directory: OneProbe_calib_20160503_02
Pulse Sequence: s2pul
8.912
7.786
7.289 7.281 7.273 7.267 7.263 7.084 7.071
2.350 2.341
1.255
0.439
0.001
N N N
H N S O O
F
10 9 8 7 6 5 4 3 2 1 ppm
0.99 1.00 4.18 2.34 3.64

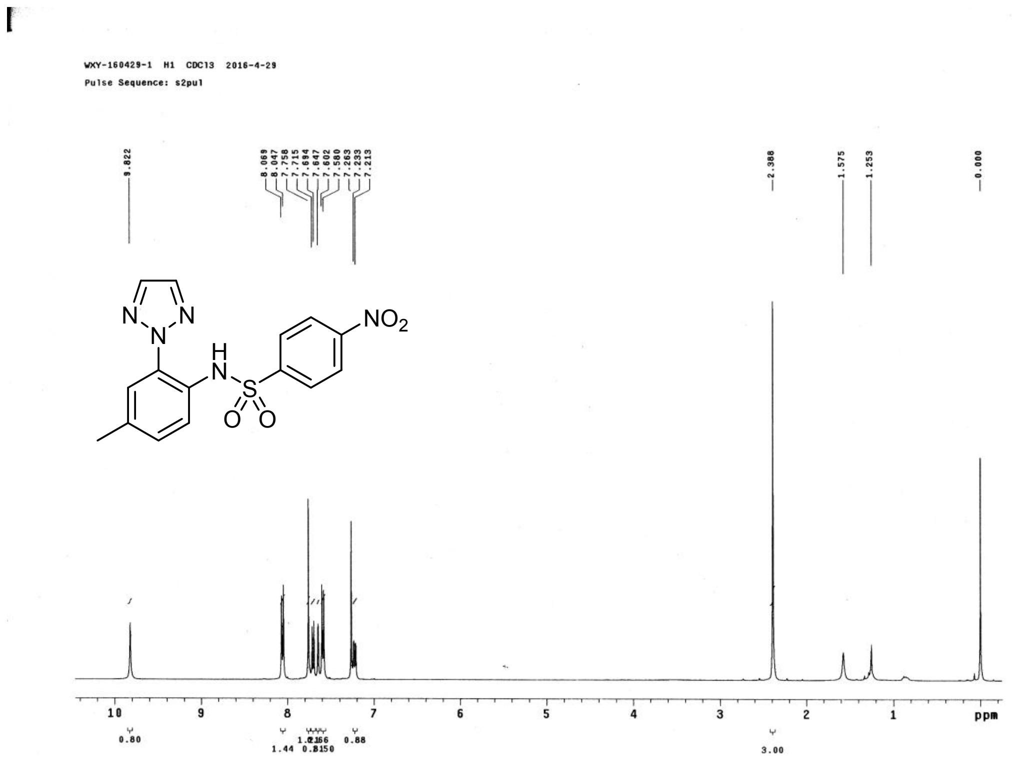

ZC-008-CDCL3-C13-2016-5-26
Archive directory: /home/vnmr1/vnmrsys/data
Sample directory: OneProbe_calib_20160503_02
Pulse Sequence: s2pul
162.379 160.718
144.251
135.221 135.145 132.261 132.168 129.647 126.469 126.367 125.153 119.411
108.602 108.416
77.211 77.000 76.789
21.494
-0.032
F
200 180 160 140 120 100 80 60 40 20 ppm

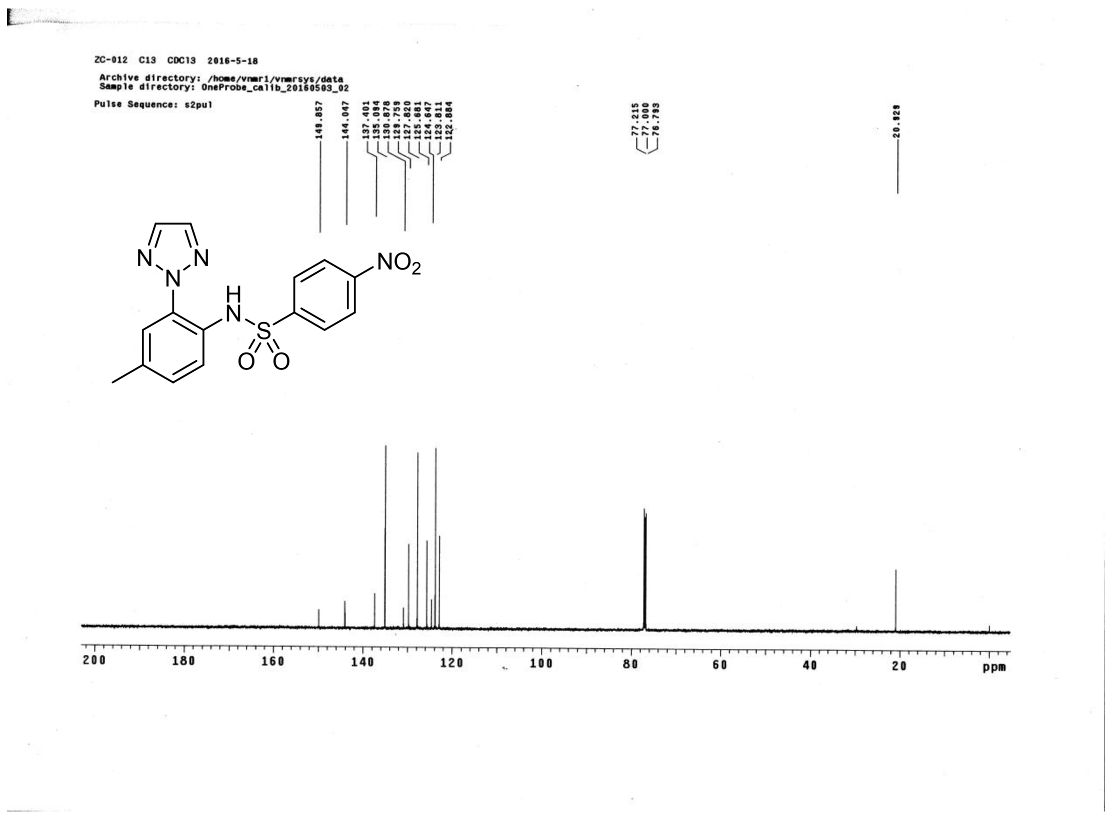

WXY-160428-1 H1 CDCl3 2016-4-28
Pulse Sequence: s2pul
9.812
7.772 7.691 7.670 7.663 7.415 7.393 7.263 7.167 7.147
6.700 6.678
3.760
2.357
0.000
ppm
0.60 0.25 1.00 0.58 1.19 2.23 2.18

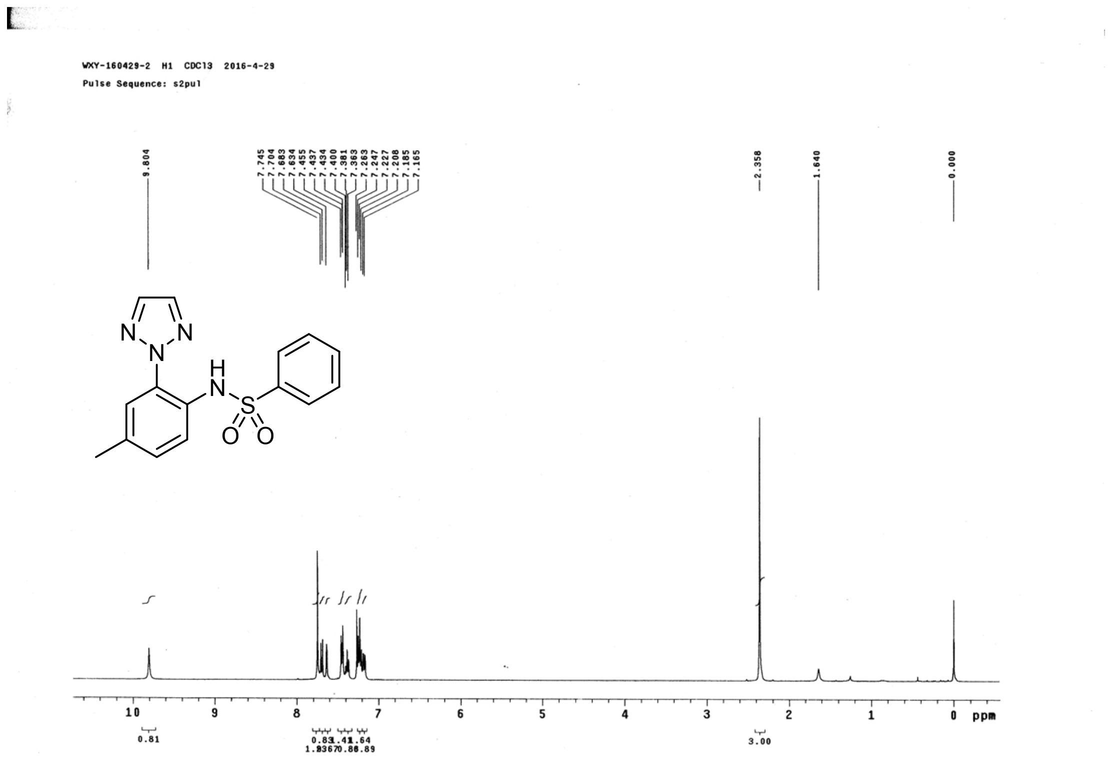

ZC-010 C13 CDCl3 2016-5-18
Archive directory: /home/vnmr1/vnmrsys/data
Sample directory: OneProbe_calib_20160503_02
Pulse Sequence: s2pul
162.781
135.922 134.811 130.965 130.394 129.414 128.792 125.957 124.723 122.531
113.800
77.215 77.000 76.783
55.453
20.814
ppm

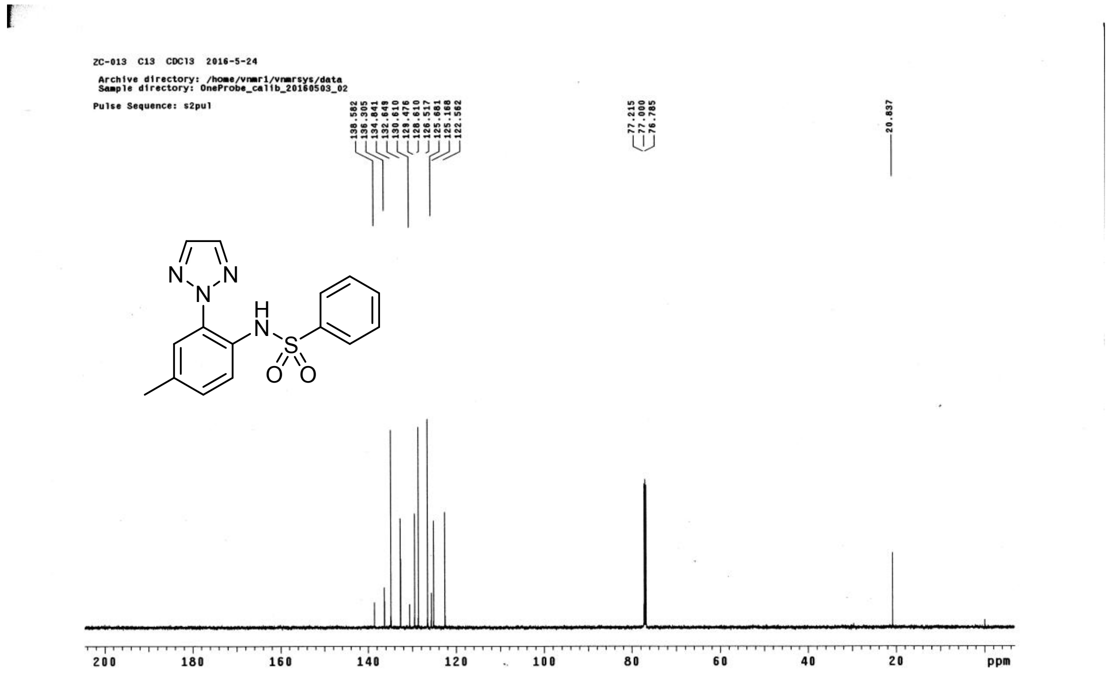

WXY-160428-2 H1 CDCl3 2016-4-28
Pulse Sequence: s2pul
9.778
7.767
7.687
7.667
7.385
7.364
7.263
7.207
7.202
7.185
7.178
2.376
0.000
Cl
H
N
S
O
O
10
9
8
7
6
5
4
3
2
1
ppm
0.79
1.31
1.08
2.32
1.37
3.00

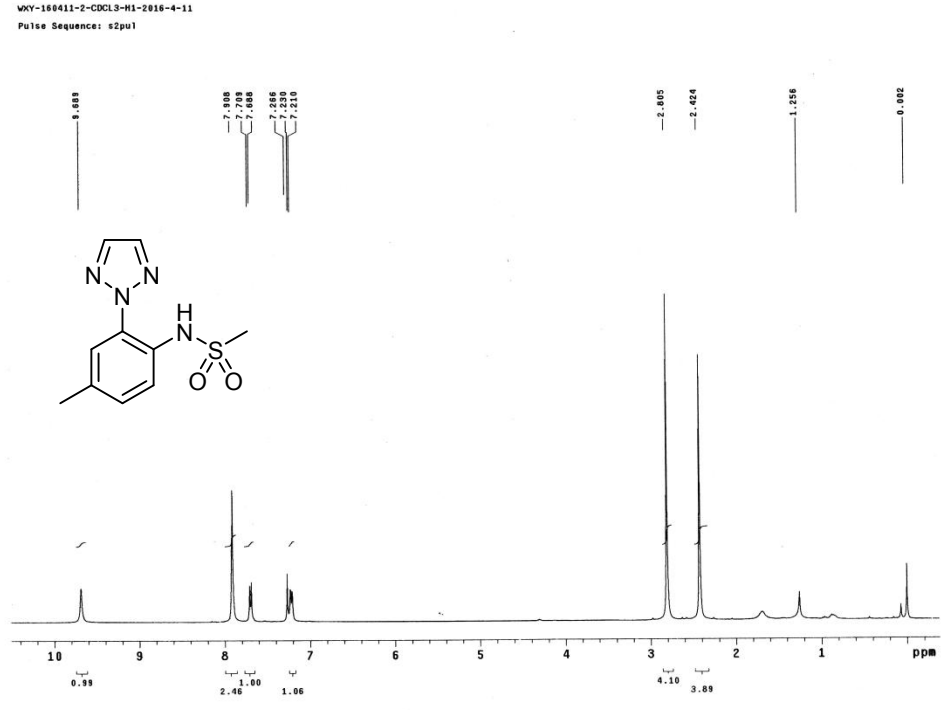

ZC-011-CDCL3-C13-2016-5-20
Pulse Sequence: s2pul
139.207
137.646
136.667
134.917
130.668
128.555
128.018
127.384
125.291
122.737
77.314
77.000
76.686
20.876
Cl
H
N
S
O
O
200
180
160
140
120
100
80
60
40
20
ppm

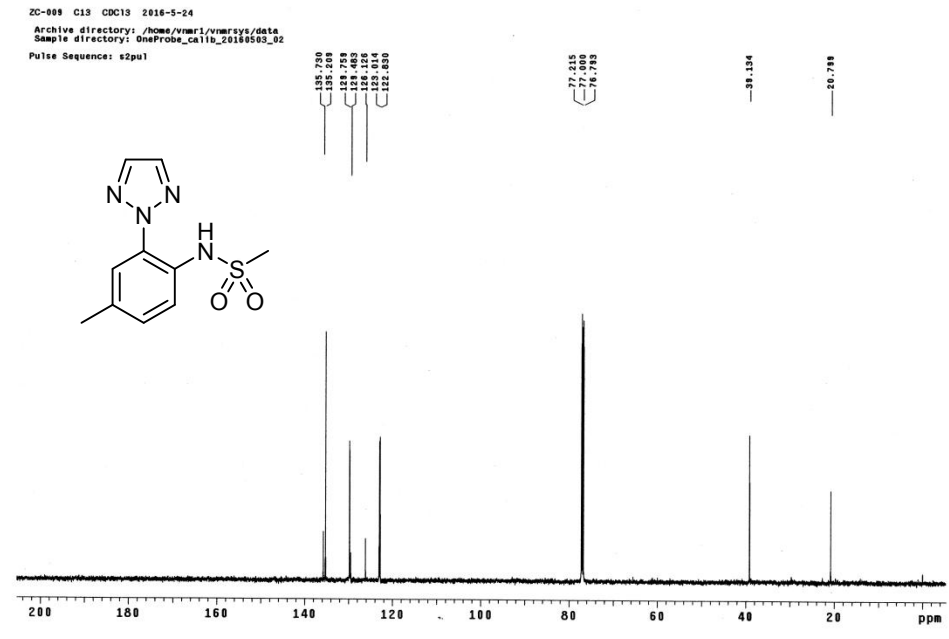

WXY-160429-1 H1 CDCl3 2016-4-29
Pulse Sequence: s2pul
NO2
ppm


ZC-012 C13 CDCl3 2016-5-18
Archive directory: /home/vnmr1/vnmrsys/data
Sample directory: OneProbe_calib_20160503_02
Pulse Sequence: s2pul
NO2
ppm


WXY-160429-2 H1 CDCl3 2016-4-29
Pulse Sequence: s2pul
9.804
7.745
7.704
7.683
7.634
7.455
7.437
7.434
7.400
7.381
7.363
7.263
7.247
7.227
7.208
7.185
7.165
2.358
1.640
0.000
N
N
N
N
H
S
O
O
ppm
0.81
3.00


ZC-013 C13 CDCl3 2016-5-24
Archive directory: /home/vnmr1/vnmrsys/data
Sample directory: OneProbe_calib_20160503_02
Pulse Sequence: s2pul
138.582
136.305
134.841
132.648
130.610
129.476
128.610
126.517
125.661
125.168
122.562
77.215
77.000
76.785
20.837
N
N
N
N
H
S
O
O
200
180
160
140
120
100
80
60
40
20
ppm


WXY-160411-2-CDCL3-H1-2016-4-11
Pulse Sequence: s2pul
9.689
7.906
7.709
7.688
7.266
7.230
7.210
2.605
2.424
1.256
0.002
N
N
N
H
N
S
O
O
10
9
8
7
6
5
4
3
2
1
ppm
0.99
1.00
2.46
1.06
4.10
3.89


ZC-009 C13 CDCl3 2016-5-24
Archive directory: /home/vnmri/vnmrsys/data
Sample directory: OneProbe_calib_20160503_02
Pulse Sequence: s2pul
135.700
135.201
129.759
129.463
126.126
123.814
122.830
77.415
77.000
76.793
39.134
20.799
N
N
N
H
N
S
O
O
200
180
160
140
120
100
80
60
40
20
ppm