Supporting Information

Development of Small Molecules with a Non-Canonical Binding Mode to HIV-1 Trans Activation Response (TAR) RNA

Fardokht A. Abulwerdi,[†,‡] Matthew D. Shortridge,[#] Joanna Sztuba-Solinska,[‡] Robert Wilson,[†] Stuart F. J. Le Grice,[‡] Gabriele Varani,[#] and John S. Schneekloth, Jr.*[,†]

[†]Chemical Biology Laboratory, National Cancer Institute, Frederick, Maryland 21702, USA

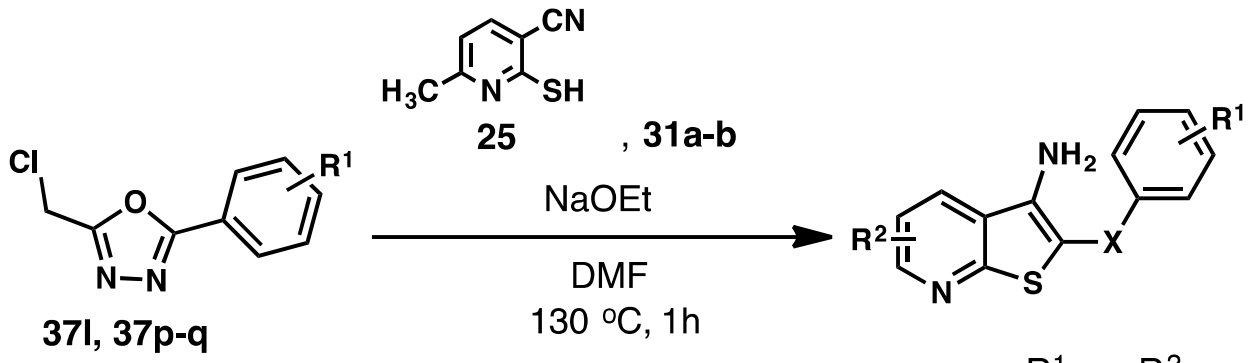
[‡]Basic Research Laboratories, National Cancer Institute, Frederick, Maryland 21702, USA

[#]Department of Chemistry, University of Washington, Seattle, Washington 98195, USA

*E-mail: schneeklothjs@mail.nih.gov

Table of Contents

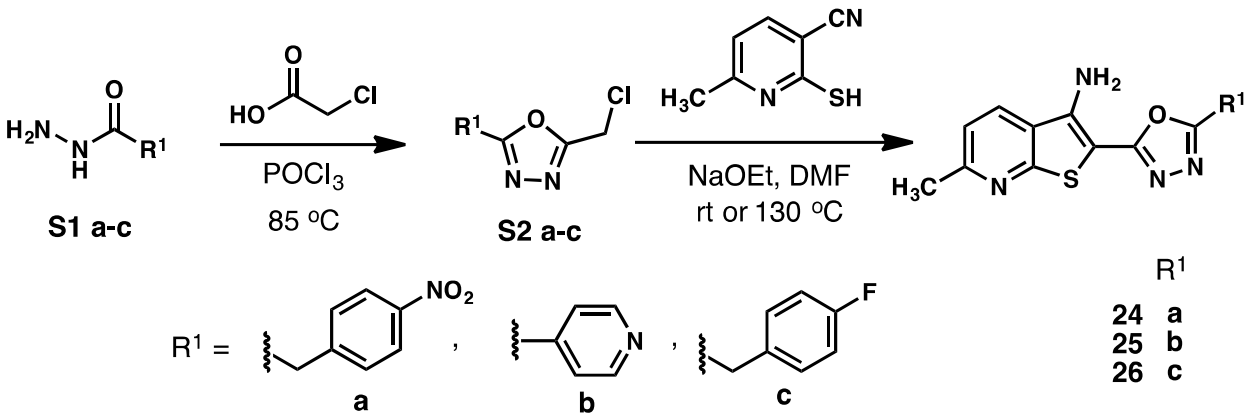
Scheme S1



	R^1
l	3-CF_3
p	4-Cl
q	3-CN

	R^1	R^2
20	3-CF_3	5-CH_3
21	3-CF_3	4-CH_3
22	4-Cl	6-CH_3
23	3-CN	6-CH_3

Scheme S2



	R^1
24	**a**
25	**b**
26	**c**

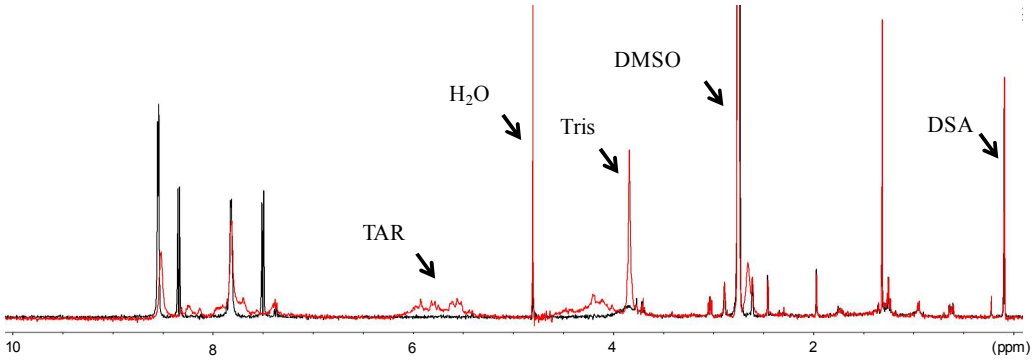
Table S1.
Affinity measurement and Tat/TAR displacement assay for oxadiazole analogs **20**-**26**

Cpd	25-2AP TAR[a] $K_{d\ app}$ ± SD (μM)	23-2AP TAR[a] $K_{d\ app}$ ± SD (μM)	FRET[a] IC_{50} ± SD (μM)
20	>100	NT	NT
21	>100	NT	NT
22	>100	NT	NT
23	>400	>400	>400
24	>400	NT	123.6 ± 49.1
25	>400	NT	>300
26	>400	NT	>400

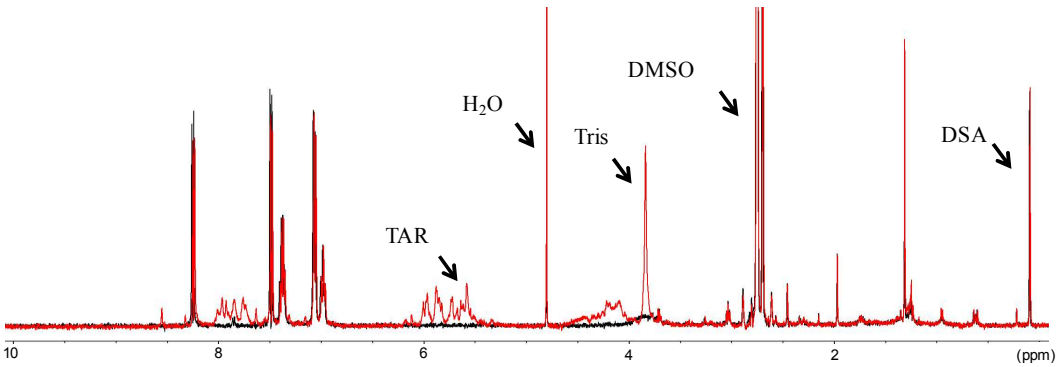
NT: not tested
[a]Highest concentration evaluated was 400 μM unless otherwise indicated. Values represent the average of three replicates, ± standard deviation.

Figure S1

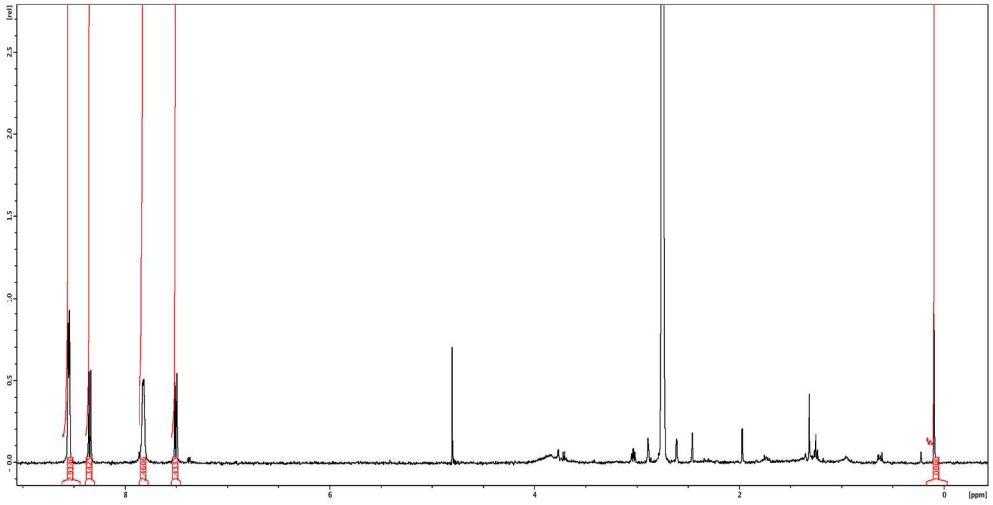
A



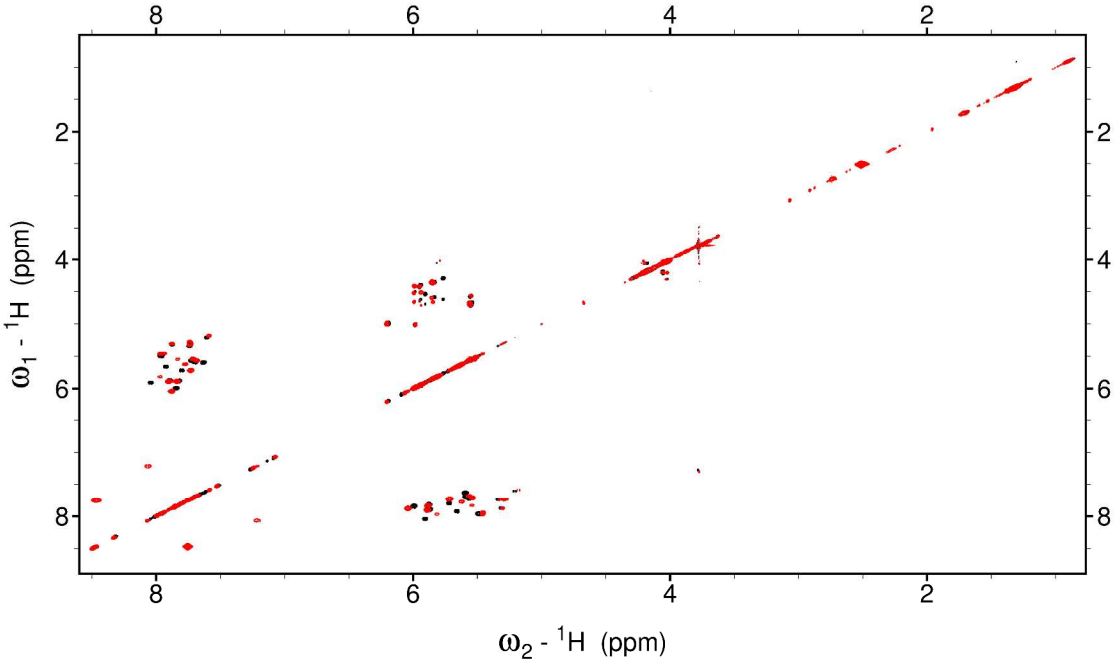
B



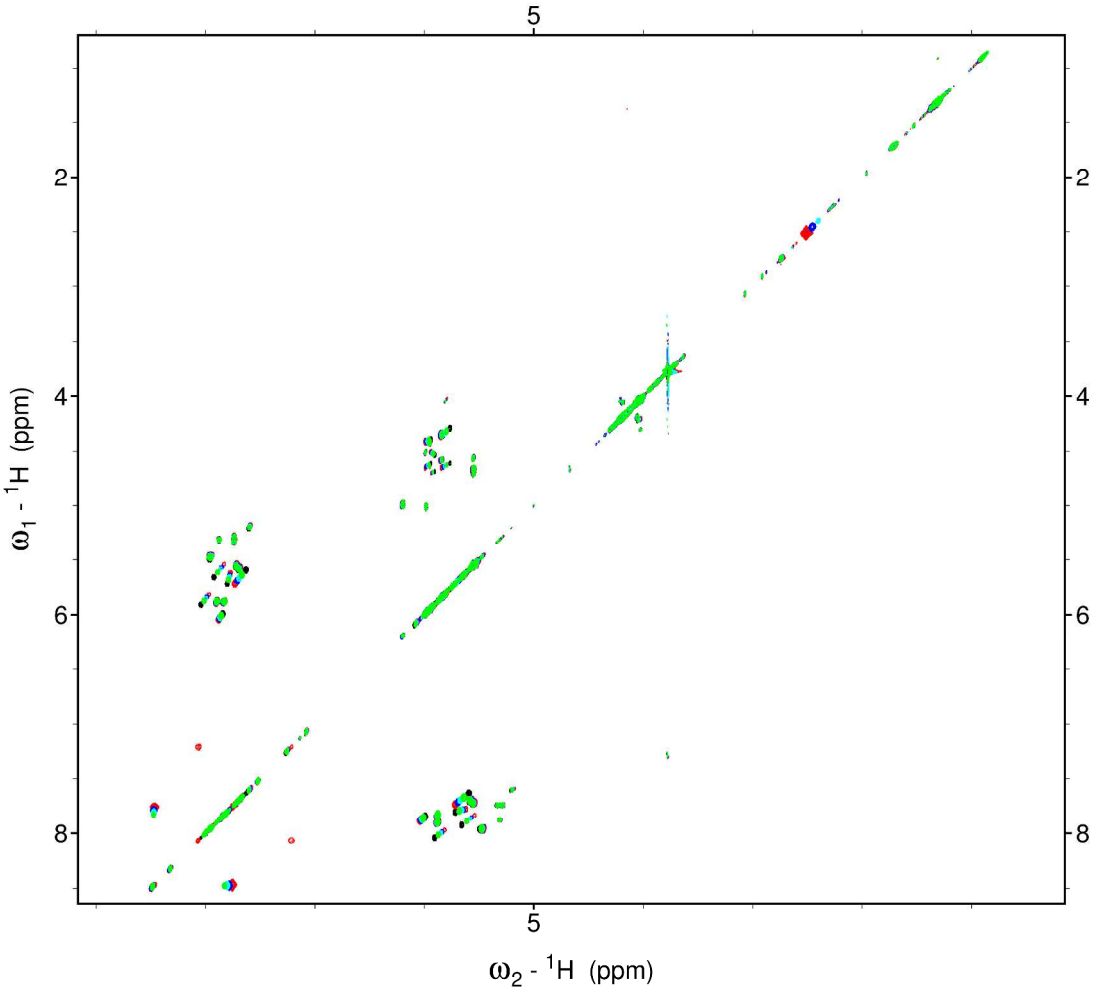
C



D



E



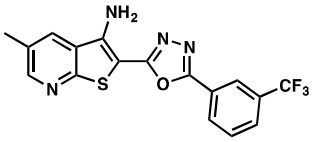
A) Ligand-detected full 1H NMR spectra of **2** (150 μM) and B) **14** (150 μM) in the presence (red spectrum) and absence of TAR hairpin (10 μM) (black spectrum). C) Free ligand **2** in NMR screening buffer showing DSA reference integrating to 100uM while the ligand signal integrates to ~150uM. D) Full TOCSY spectrum showing free RNA (111 uM, black) and RNA bound to 500uM **2** (red). E) Full TOCSY spectrum showing free RNA (111 uM, black) titrated from 100-500uM **2**, with 500uM **2** (red).

Chemistry

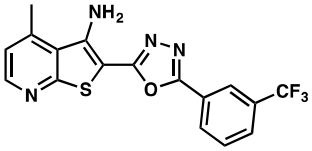
Chemicals were purchased from commercial sources and used without further purification unless otherwise noted. Anhydrous solvents were prepared by passage over activated alumina. Thin-layer chromatography was conducted with E. Merck silica gel 60 F254 precoated plates (0.25 mm) and visualized by exposure to UV light (254 nm). Flash column chromatography was performed using normal phase or reverse phase on a CombiFlash® Rf 200i (Teledyne Isco Inc). ^{1}H NMR spectra were recorded at 400 or 500 MHz, and are reported relative to deuterated solvent signals. Data for ^{1}H NMR spectra are reported as follows: chemical shift (δ ppm), multiplicity, coupling constant (Hz), and integration. ^{13}C NMR spectra were recorded at 100 or 125 MHz. Data for ^{13}C NMR spectra are reported in terms of chemical shift. All NMR spectra were standardized to the NMR solvent signal as reported previously.[1] Analytical LC/MS was performed using a Shimadzu LCMS-2020 Single Quadrupole utilizing a Kinetex 2.6 µm C18 100 Å (2.1 x 50 mm) column obtained from Phenomenex Inc. Runs employed a gradient of 0→90% ACN/0.1% aqueous formic acid over 4 minutes at a flow rate of 0.2 mL/min. Purities of final compounds were assessed by analytical reverse-phase HPLC using Agilent Proshell 120 EC-C18 (4.6 mm x 50 mm; particle size 2.7 µm). Runs employed a gradient of 10% ACN/water (1 min), 10-90% ACN/water (6 min), and 90% ACN/water (2 min) flow = 1 mL/min. High-resolution LC/MS analyses acquired on an Agilent 6520 Accurate-Mass Q-TOF LC/MS System, (Agilent Technologies, Inc., Santa Clara, CA) equipped with a dual electro-spray source, operated in the positive-ion mode. Separation was performed on Zorbax 300SB-C18 Poroshell column (2.1 mm x 150 mm; particle size 5 µm). All final compounds were purified to >95% purity unless otherwise stated.

Representative procedure for oxadiazolyl thienopyridine preparation

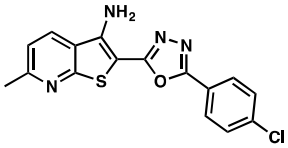
To a stirring solution of desired mercaptonicotinonitrile (0.28 mmol) in anhydrous DMF (2 mL) was added commercially available chloromethyl substituted-1,3,4-oxadiazole (0.24 mmol) and sodium ethoxide (0.63 mmol). The mixture was heated to 130 ^{o}C for 1 h. The mixture was then cooled to room temperature and solid precipitated at the bottom of the flask. The solid was collected by filtration and rinsed with cold MeOH and dried *in vacuo* to give the desired product.



5-Methyl-2-(5-(3-(trifluoromethyl)phenyl)-1,3,4-oxadiazol-2-yl)thieno[2,3-*b*]pyridin-3-amine (20). Synthesized using the representative procedure and with **31b** and **37m**. Precipitated solid was filtered, rinsed with cold MeOH, and dried *in vacuo* to give the title compound (23 mg, 56% yield) as a yellow solid. Purity 85%. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.56 – 8.55 (m, 1H), 8.44 (s, 1H), 8.42 (d, J = 8.0 Hz, 1H), 8.37 (s, 1H), 8.02 (d, J = 7.8 Hz, 1H), 7.90 – 7.86 (m, 1H), 7.22 (s, 2H), 2.46 (s, 3H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 162.28, 160.64, 156.87, 150.93, 143.22, 130.92, 130.81, 130.56, 129.28, 125.56, 124.43, 122.85, 87.38, 17.96. ESI HRMS: 377.06828 $(M+H)^+$.

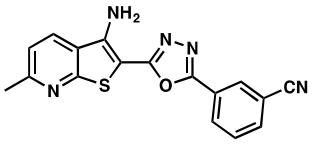


4-Methyl-2-(5-(3-(trifluoromethyl)phenyl)-1,3,4-oxadiazol-2-yl)thieno[2,3-*b*]pyridin-3-amine (21). Synthesized using the representative procedure and with **31a** and commercially available **37m**. Precipitated solid was filtered, rinsed with cold MeOH, and dried *in vacuo* to give the title compound (19 mg, 39% yield) as a yellow solid. Purity 96%. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.50 (d, J = 4.7 Hz, 1H), 8.38 (d, J = 7.9 Hz, 1H), 8.33 (s, 1H), 8.03 (d, J = 7.8 Hz, 1H), 7.89 (t, J = 7.8 Hz, 1H), 7.27 (d, J = 4.7 Hz, 1H), 6.82 (s, 2H), 2.86 (s, 3H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 162.39, 160.42, 160.23, 149.53, 145.43, 145.01, 130.89, 130.52, 130.22, 129.97, 128.24 (q, J = 3.3 Hz), 124.76, 124.58, 124.34, 122.80 (q, J = 3.7 Hz), 122.26, 88.43, 19.87. ESI HRMS: 377.06831 $(M+H)^+$.

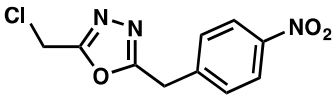


2-(5-(4-Chlorophenyl)-1,3,4-oxadiazol-2-yl)-6-methylthieno[2,3-*b*]pyridin-3-amine (22). Synthesized using the representative procedure and with **25** and commercially available 2-(chloromethyl)-5-(4-chlorophenyl)-1,3,4-oxadiazole, **37p**. Precipitated solid was filtered, rinsed with cold MeOH, and dried *in vacuo* to give the title compound (47 mg, 76% yield) as a yellow solid. Purity 97%. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.47 (d, J = 8.3 Hz, 1H), 8.11 (d, J = 8.6 Hz, 2H), 7.69 (d, J = 8.6 Hz, 2H), 7.40 (d, J = 8.3 Hz, 1H), 7.20 (s, 2H), 2.61 (s, 3H). ^{13}C NMR (125

MHz, DMSO-d_6) δ 162.08, 160.75, 159.26, 159.22, 143.52, 136.33, 131.16, 129.56, 128.31, 123.38, 122.19, 119.89, 86.09, 24.21. ESI HRMS: 343.04218 $(M+H)^+$.

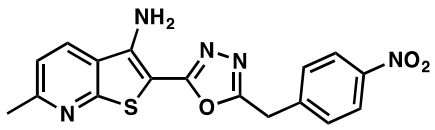


3-(5-(3-Amino-6-methylthieno[2,3-*b*]pyridin-2-yl)-1,3,4-oxadiazol-2-yl)benzonitrile (23). Synthesized using the representative procedure and with **25** and commercially available 3-(5-(chloromethyl)-1,3,4-oxadiazol-2-yl)benzonitrile, **37q**. Precipitated solid was filtered, rinsed with cold MeOH, and dried *in vacuo* to give the title compound (20 mg, 50% yield) as a yellow solid. Purity 94%. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.57 (s, 1H), 8.47 (d, J = 8.3 Hz, 1H), 8.42 – 8.39 (m, 1H), 8.09 (d, J = 7.8 Hz, 1H), 7.82 (t, J = 7.9 Hz, 1H), 7.39 (d, J = 8.3 Hz, 1H), 7.21 (s, 2H), 2.61 (s, 3H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 162.34, 160.20, 159.35, 159.30, 143.61, 134.94, 131.19, 130.89, 130.66, 129.96, 124.58, 123.38, 119.85, 117.95, 112.60, 86.04, 24.21. ESI HRMS: 334.07596 $(M+H)^+$.

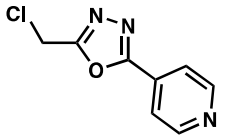


Representative procedure for chloromethyl substituted 1,3,4-oxadiazole preparation

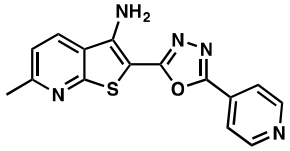
2-(Chloromethyl)-5-(4-nitrobenzyl)-1,3,4-oxadiazole (S2a). Synthesized using reported procedure with modification.[2] A round bottom flask was charged with commercially available 2-(4-nitrophenyl)acetohydrazide, **S1a**, (103 mg, 0.5 mmol), chloroacetic acid (49 mg, 0.52 mmol) and phosphoryl chloride (2 mL). The reaction mixture was heated at 85 ^{o}C overnight. The flask was removed from the oil bath and allowed to cool to room temperature. Excess phosphoryl chloride was removed *in vacuo* and crushed ice (5 mL) was added slowly to the reaction mixture followed by slow addition of solid sodium bicarbonate while keeping the flask on ice. The mixture was diluted with H_2O (10 mL) and extracted with EtOAc (10 mL x 2) and finally washed with brine (10 mL). The organic layer was dried (Na_2SO_4), filtered, and concentrated *in vacuo*. Crude was purified by silica gel column chromatography (hexanes/EtOAc) to give **S2a** (72 mg, 57% yield) as a clear oil which solidified to a white solid upon standing. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (d, J = 8.7 Hz, 2H), 7.51 (d, J = 8.6 Hz, 2H), 4.66 (s, 2H), 4.34 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.57, 163.25, 147.76, 140.46, 130.04, 124.36, 32.88, 31.72. ESI MS: m/z 253.55, 255.55 $(M+H)^+$.



6-Methyl-2-(5-(4-nitrobenzyl)-1,3,4-oxadiazol-2-yl)thieno[2,3-*b*]pyridin-3-amine (24). Synthesized using the representative procedure and with **25** and **S2a**. Reaction was performed at room temperature and was completed in 30 min. The mixture was diluted with H_2O (10 mL) and extracted with EtOAc (10 mL x 2) and finally washed with brine (10 mL). The organic layer was dried (Na_2SO_4), filtered, and concentrated *in vacuo*. Crude was purified by silica gel column chromatography (hexanes/EtOAc) to give **24** (9 mg, 41% yield) as an orange solid. Purity 97%. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.42 (d, J = 8.3 Hz, 1H), 8.25 (d, J = 8.8 Hz, 2H), 7.68 (d, J = 8.8 Hz, 2H), 7.38 (d, J = 8.3 Hz, 1H), 7.10 (s, 2H), 4.54 (s, 2H), 2.59 (s, 3H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 162.15, 161.85, 159.08, 159.00, 146.77, 143.12, 142.52, 131.07, 130.37, 123.82, 123.33, 119.87, 85.89, 30.27, 24.17. ESI HRMS: 368.08196 $(M+H)^+$.

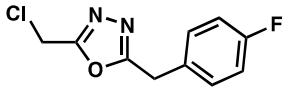


2-(Chloromethyl)-5-(pyridin-4-yl)-1,3,4-oxadiazole (S2b). Synthesized using a similar procedure used to prepare **S2a** except using isoniazid, **S1b**. Crude (112 mg, 79% yield), a dark green solid, was used in the next step without further purification. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.90 – 8.87 (m, 2H), 8.03 – 8.01 (m, 2H), 5.19 (s, 2H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 163.95, 163.34, 150.32, 130.83, 120.68, 33.12. ESI MS: m/z 195.45, 197.45 $(M+H)^+$.

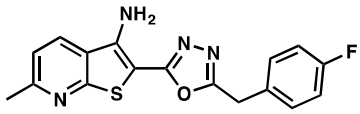


6-Methyl-2-(5-(pyridin-4-yl)-1,3,4-oxadiazol-2-yl)thieno[2,3-*b*]pyridin-3-amine (25). Synthesized using the representative procedure and with **25** and **S2b**. Reaction was heated for 1 hr and was let to cool down to room temperature. The mixture was diluted with H_2O (15 mL) and extracted with EtOAc (10 mL x 3) and MeOH:CH_2Cl_2 3:7 (10 mL x 2). The organic layer was dried (Na_2SO_4), filtered, and concentrated *in vacuo*. Crude was purified by silica gel column chromatography (hexanes/EtOAc) to give **25** (3.2 mg, 10% yield) as a light yellow solid. Purity 99%. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.84 (d, J = 6.0 Hz, 2H), 8.49 (d, J = 8.3 Hz, 1H), 8.04 (d,

J = 6.1 Hz, 2H), 7.40 (d, *J* = 8.3 Hz, 1H), 7.27 (s, 2H), 2.62 (s, 3H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 162.73, 160.00, 159.50, 159.35, 150.86, 144.05, 131.28, 130.37, 123.32, 120.09, 119.94, 85.82, 24.23. ESI HRMS: 310.07548 $(M+H)^+$.



2-(Chloromethyl)-5-(4-fluorobenzyl)-1,3,4-oxadiazole (S2c). Synthesized using a similar procedure used to prepare **S2a** except using 4-fluorophenylacetic acid hydrazide, **S1c**. Crude (132 mg, 96% yield), a brown oil, was used in the next step without further purification. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.29 (dd, *J* = 8.5, 5.3 Hz, 2H), 7.05 (t, *J* = 8.6 Hz, 2H), 4.65 (s, 2H), 4.20 (s, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.86, 162.99, 162.45 (d, *J* = 246.7 Hz), 130.66 (d, *J* = 8.2 Hz), 129.05 (d, *J* = 3.4 Hz), 116.10 (d, *J* = 21.7 Hz), 32.96, 31.21. ESI MS: m/z 226.50 $(M+H)^+$.



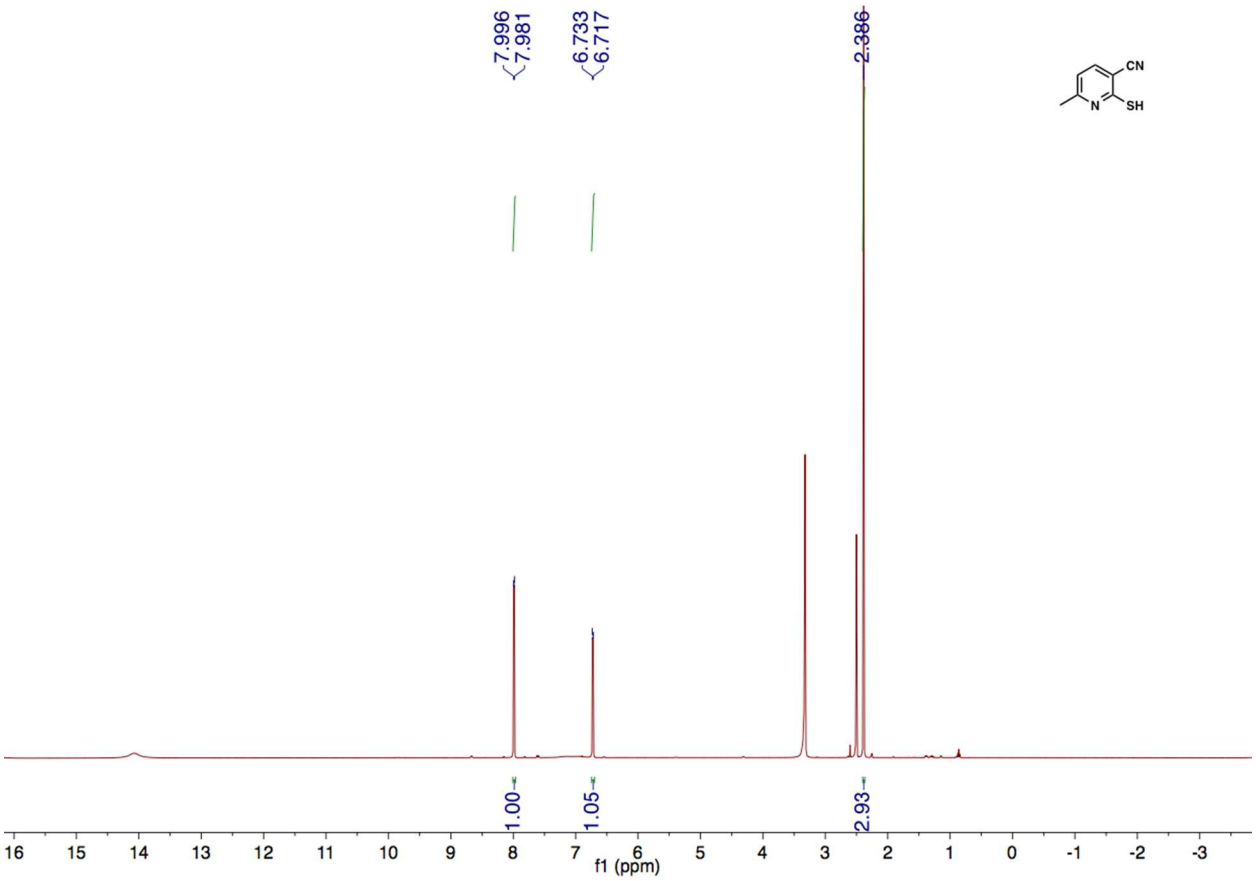
2-(5-(4-Fluorobenzyl)-1,3,4-oxadiazol-2-yl)-6-methylthieno[2,3-*b*]pyridin-3-amine (26). Synthesized using the representative procedure and with **25** and **S2c**. Reaction was heated to 130 ^{o}C and was completed in 40 min. The mixture was diluted with H_2O (10 mL) and extracted with EtOAc (10 mL x 2) and finally washed with brine (10 mL). The organic layer was dried (Na_2SO_4), filtered, and concentrated *in vacuo*. Crude was purified by silica gel column chromatography (hexanes/EtOAc) to give **26** (2 mg, 4% yield) as a yellow solid. Purity 97%. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.41 (d, *J* = 8.3 Hz, 1H), 7.45 – 7.40 (m, 2H), 7.37 (d, *J* = 8.3 Hz, 1H), 7.20 (t, *J* = 8.9 Hz, 2H), 7.08 (s, 2H), 4.34 (s, 2H), 2.59 (s, 3H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 162.68, 162.00, 161.36 (d, *J* = 243.1 Hz), 159.01, 158.97, 143.00, 131.04, 130.89 (d, *J* = 8.2 Hz), 130.82 (d, *J* = 3.2 Hz), 123.34, 119.85, 115.51 (d, *J* = 21.4 Hz), 85.99, 29.70, 24.17. ESI HRMS: 341.08686 $(M+H)^+$.

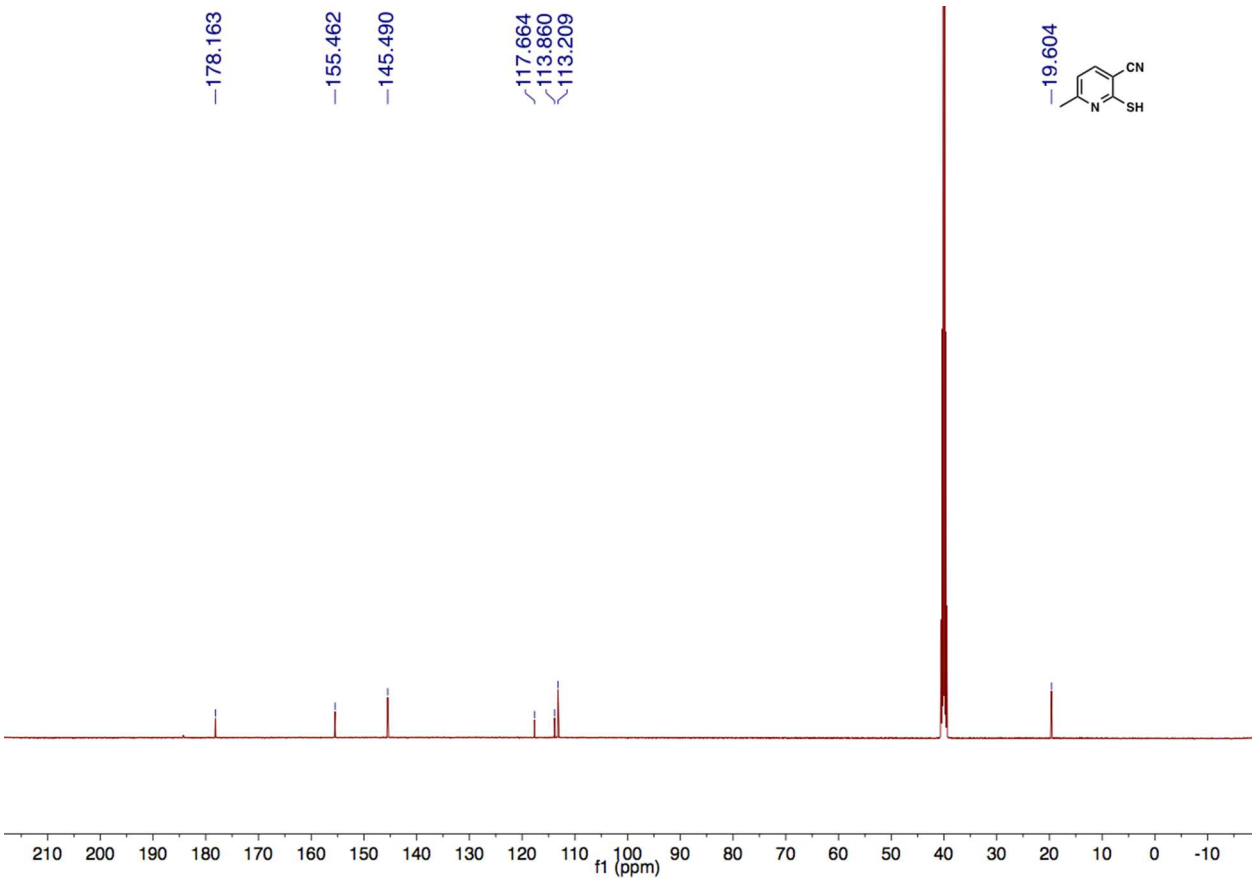
References

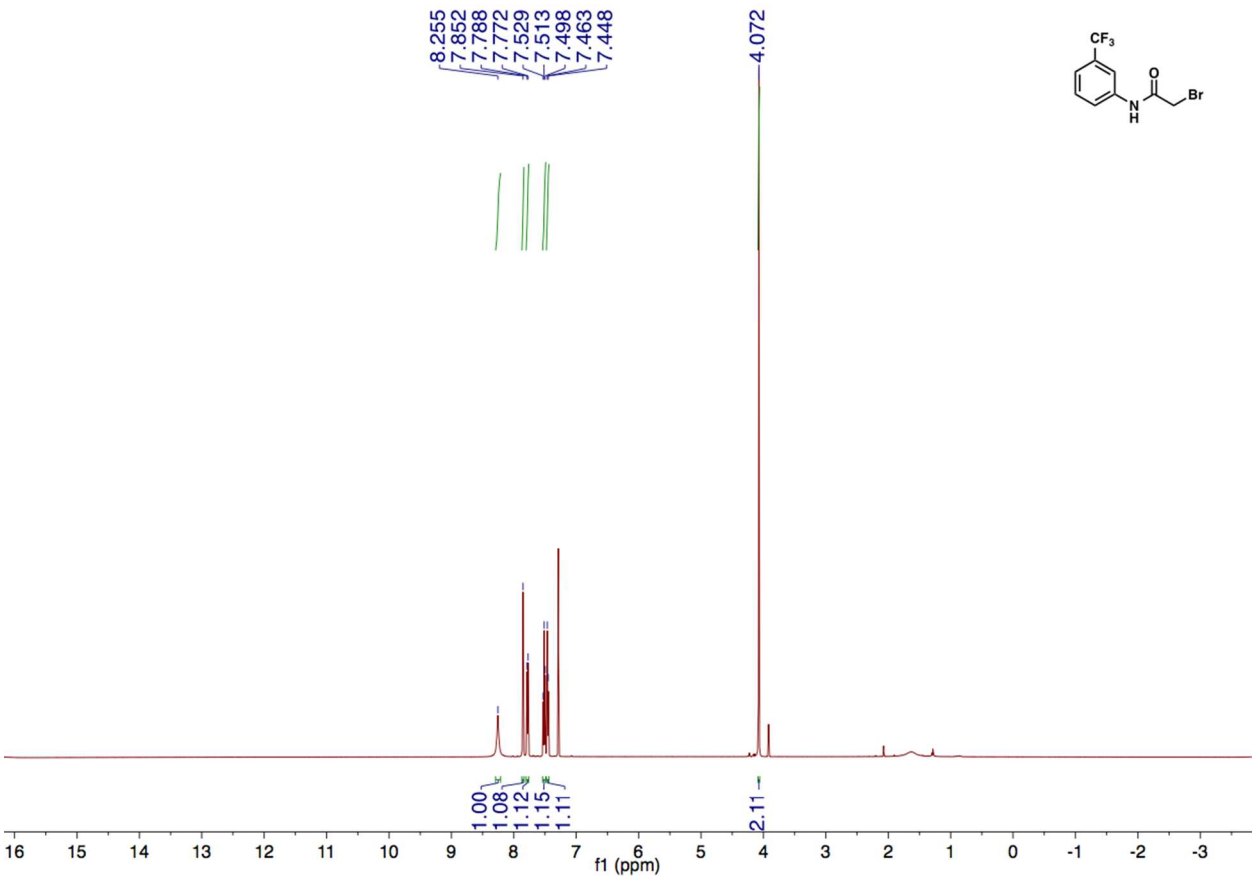
1. Fulmer, G. R.; Miller, A. J. M.; Sherden, N. H.; Gottlieb, H. E.; Nudelman, A.; Stoltz, B. M.; Bercaw, J. E.; Goldberg, K. I. NMR chemical shifts of trace impurities: common laboratory solvents, organics, and gases in deuterated solvents relevant to the organometallic chemist. *Organometallics* **2010**, *29* (9), 2176-2179.

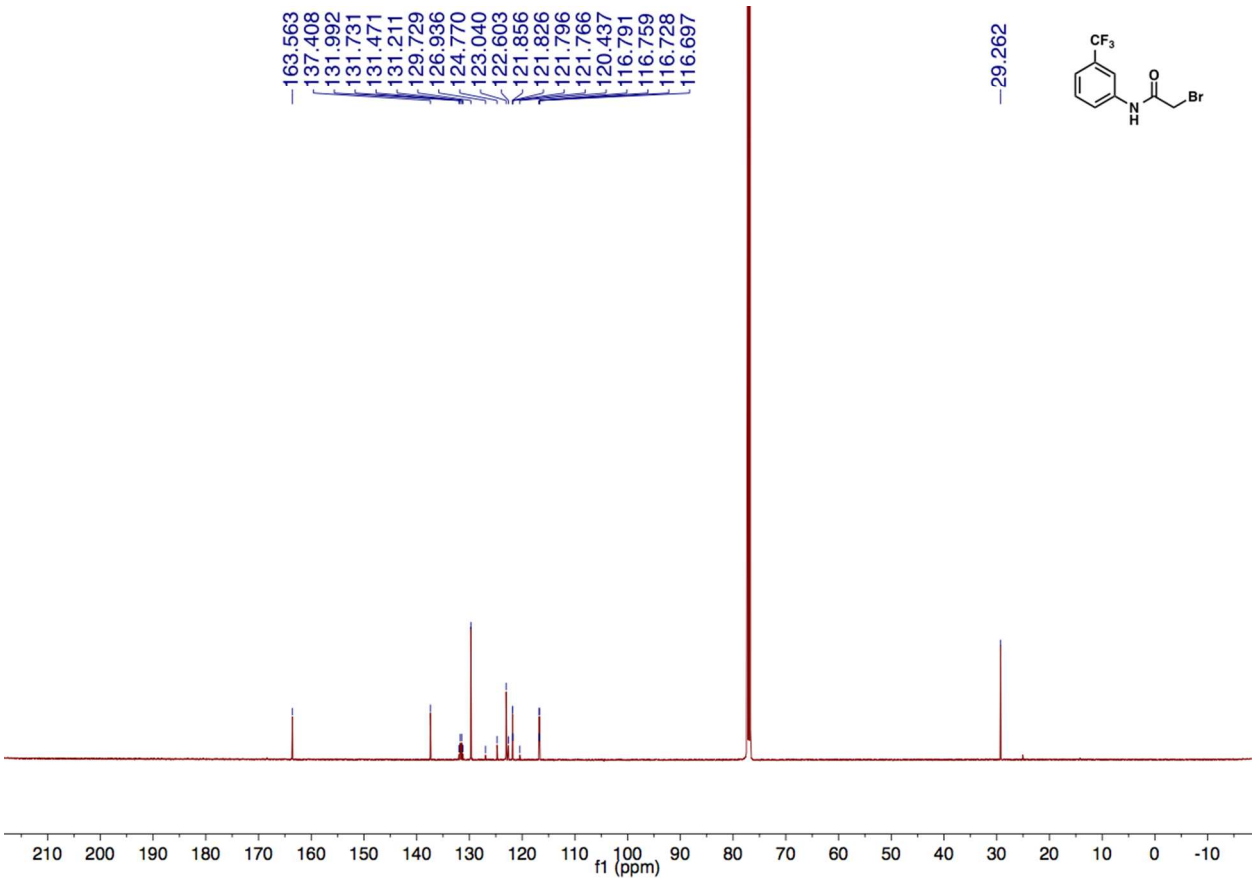
2. Zhang, M. Z.; Mulholland, N.; Beattie, D.; Irwin, D.; Gu, Y. C.; Chen, Q.; Yang, G. F.; Clough, J. Synthesis and antifungal activity of 3-(1,3,4-oxadiazol-5-yl)-indoles and 3-(1,3,4-oxadiazol-5-yl)methyl-indoles. *Eur. J. Med. Chem.* **2013**, *63*, 22-32.

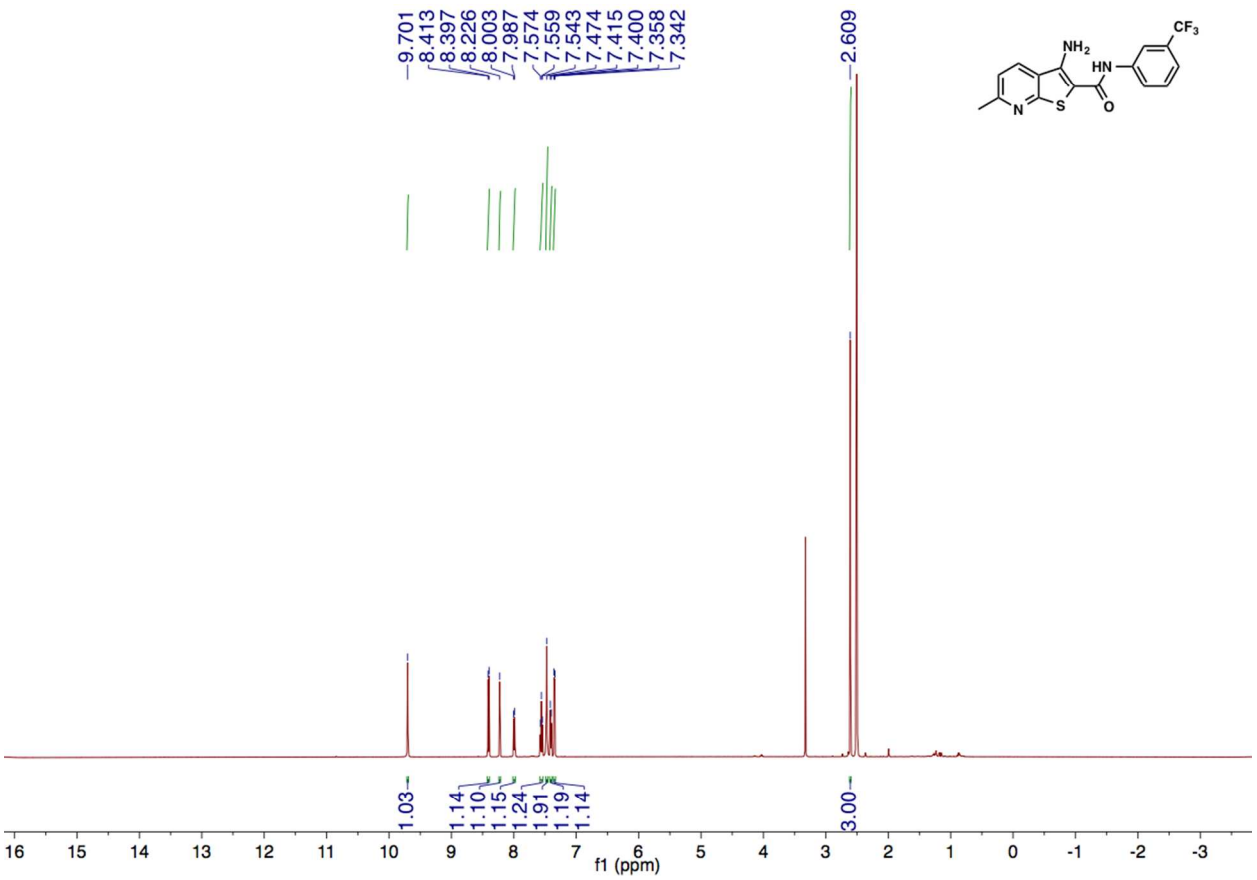
1D 1H and 13C NMR spectra

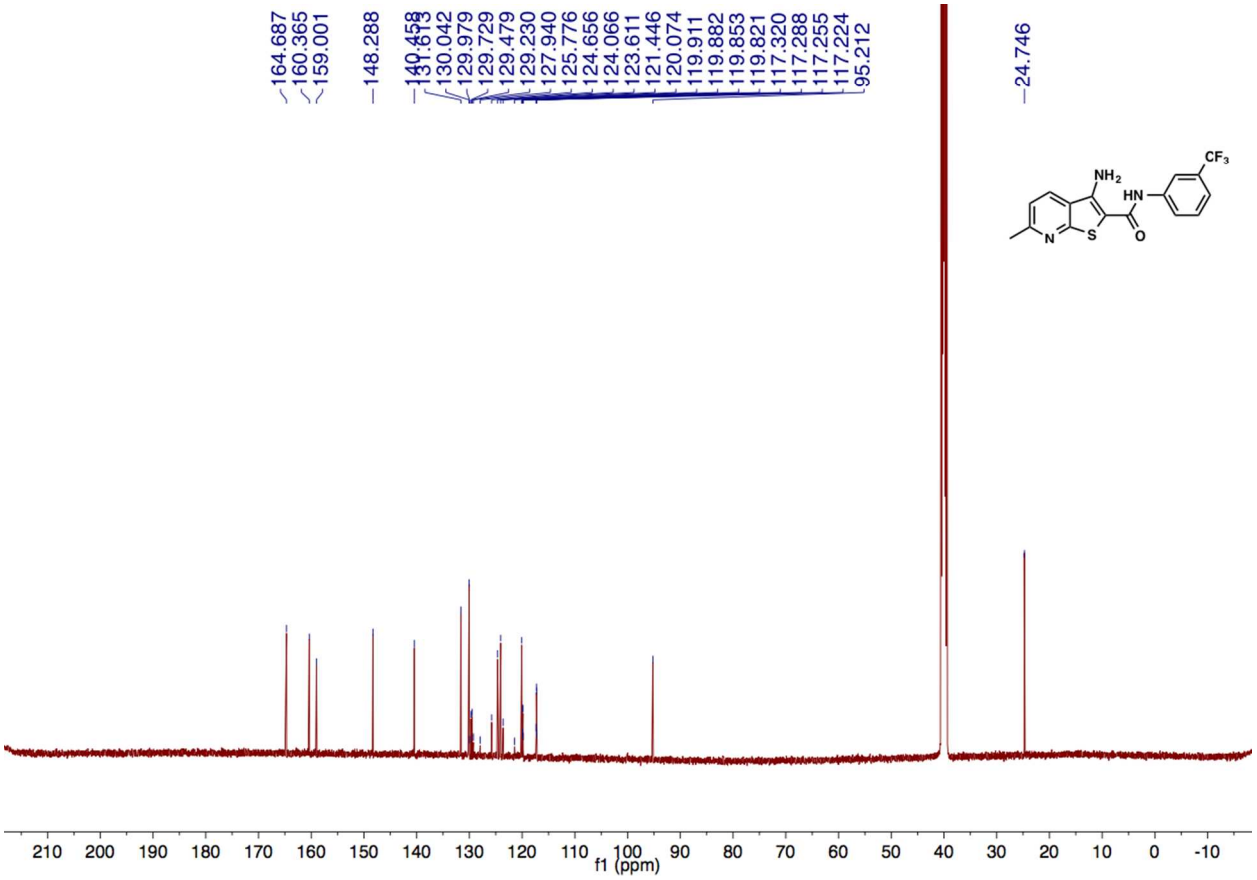


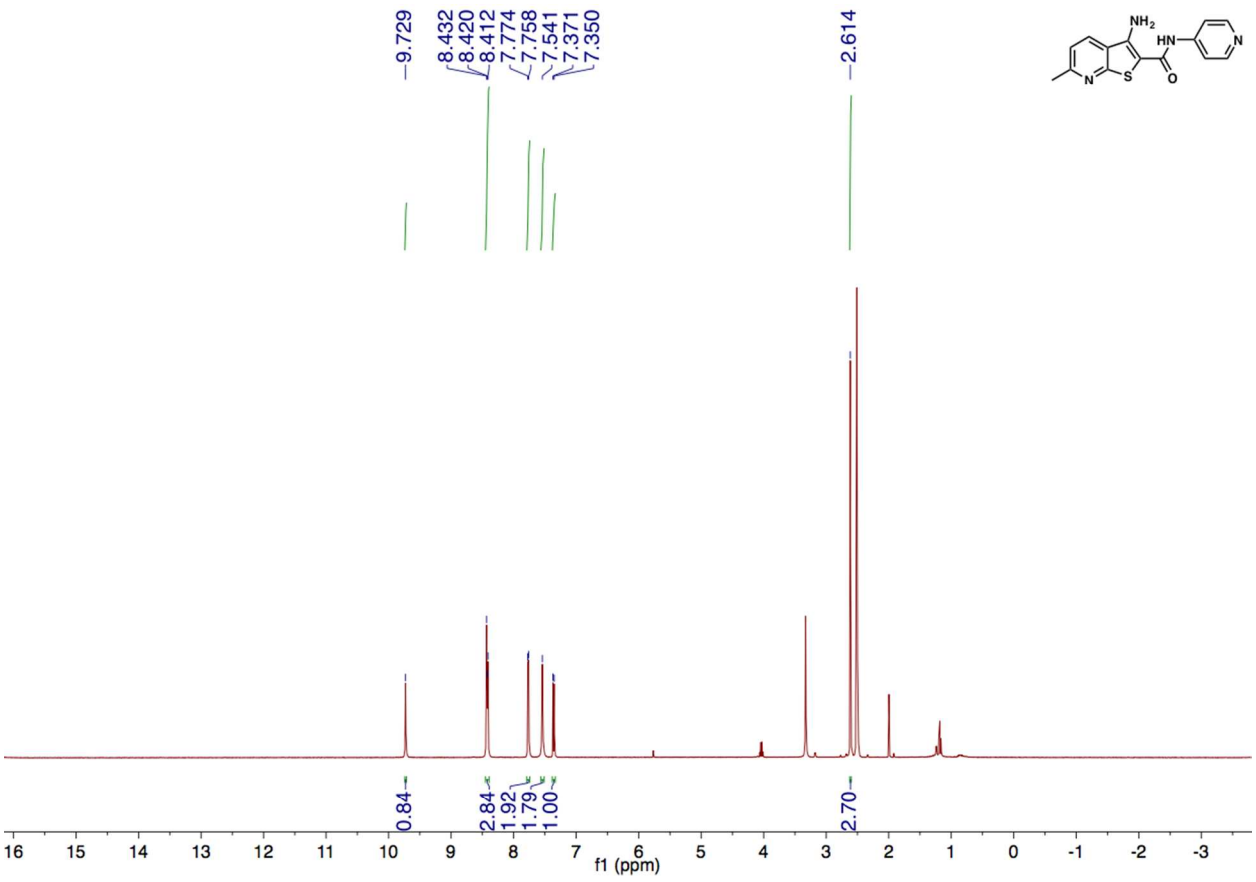

178.163
155.462
145.490
117.664
113.860
113.209
19.604
CN
SH
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

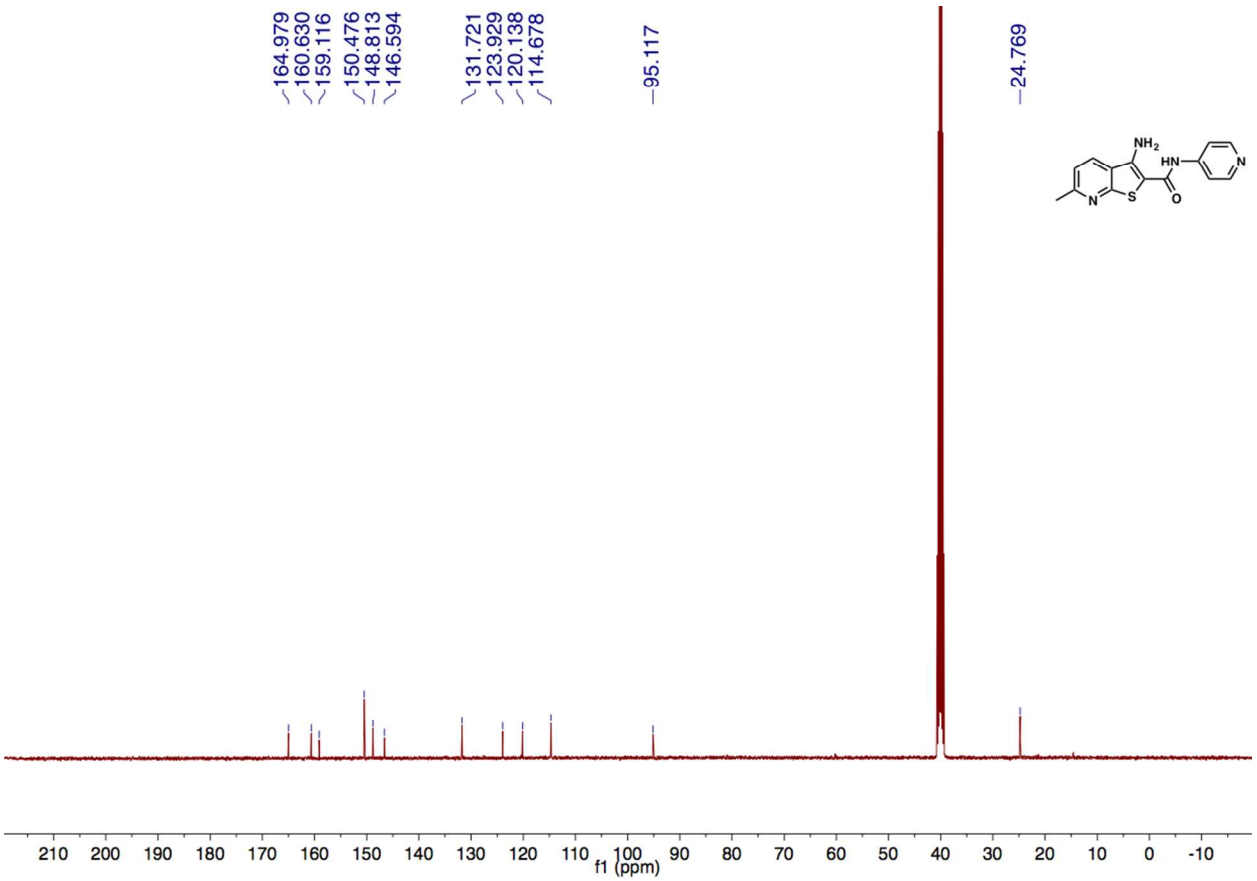

8.255
7.852
7.788
7.772
7.529
7.513
7.498
7.463
7.448
4.072
CF3
O
N
H
Br
1.00
1.08
1.12
1.15
1.11
2.11
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

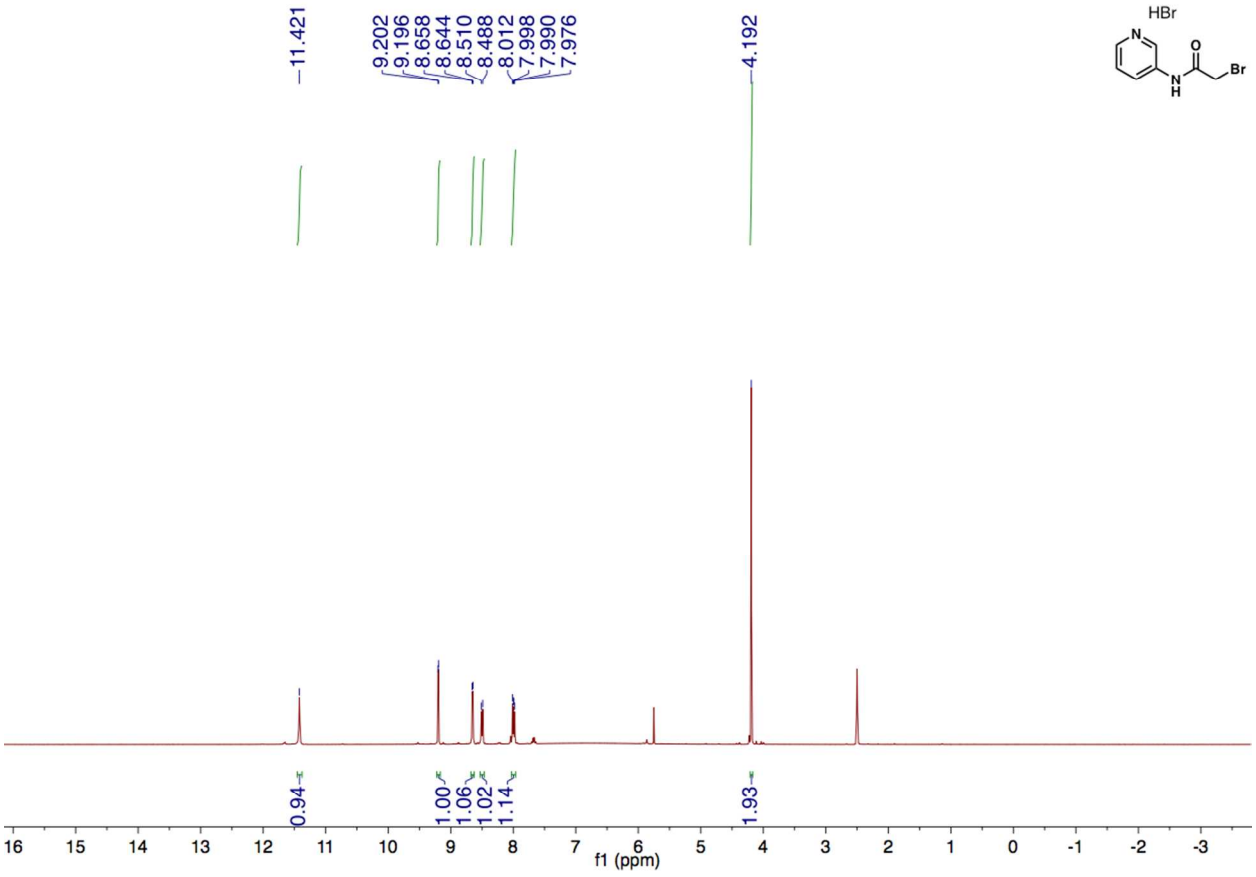

163.563
137.408
131.992
131.731
131.471
131.211
129.729
126.936
124.770
123.040
122.603
121.856
121.826
121.796
121.766
120.437
116.791
116.759
116.728
116.697
29.262
CF3
O
N
H
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

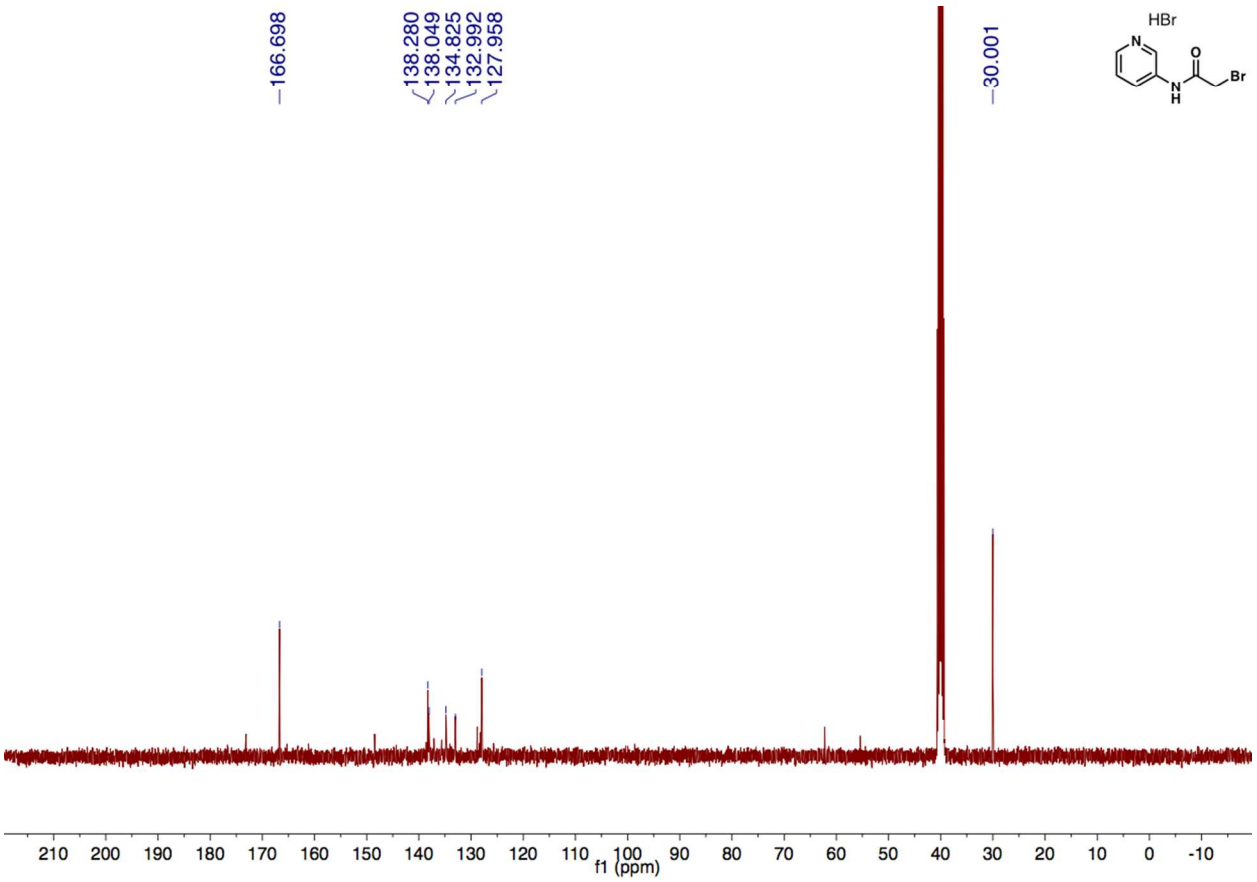

9.701
8.413
8.397
8.226
8.003
7.987
7.574
7.559
7.543
7.474
7.415
7.400
7.358
7.342
2.609
NH2
HN
CF3
N
S
O
1.03
1.14
1.10
1.15
1.24
1.91
1.19
1.14
3.00
f1 (ppm)

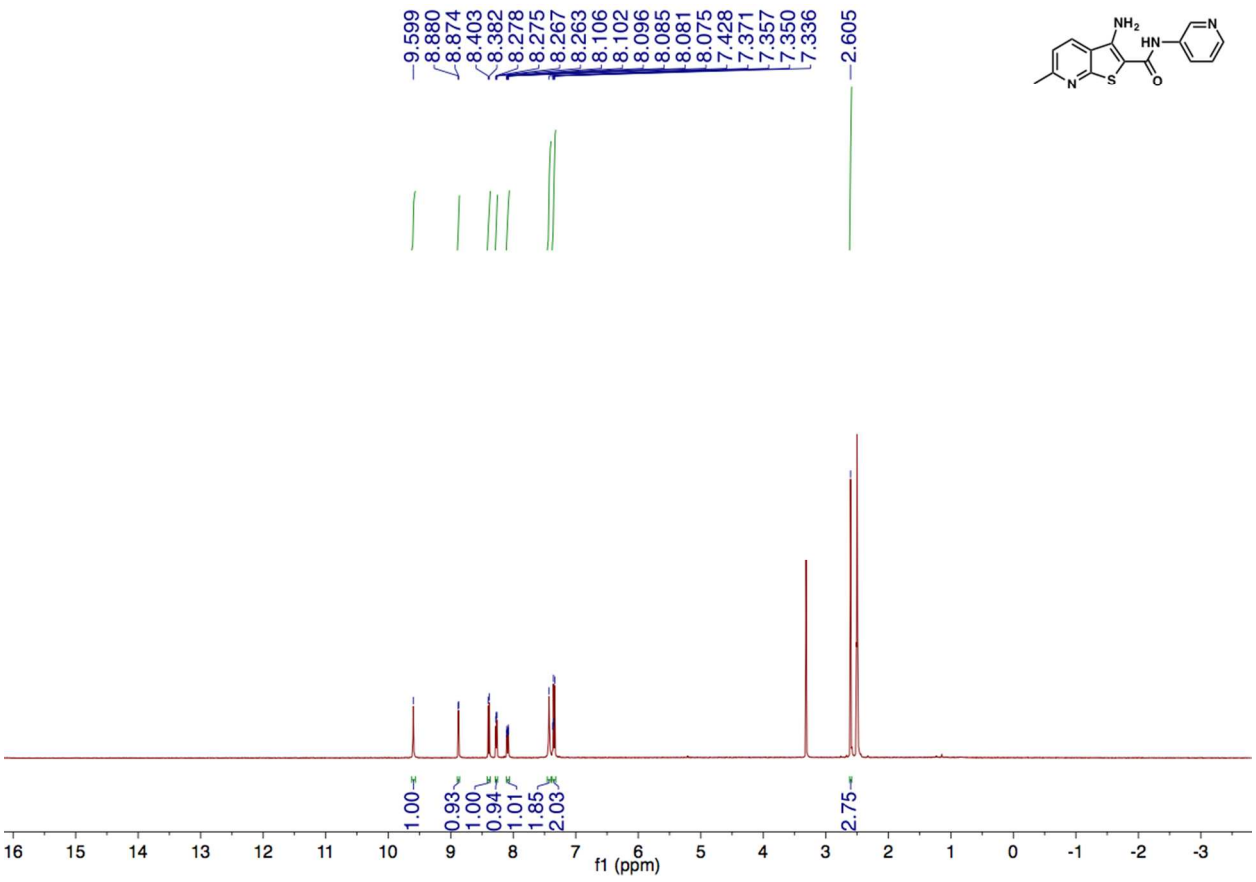

164.687
160.365
159.001
148.288
140.458
131.613
130.042
129.979
129.729
129.479
129.230
127.940
125.776
124.656
124.066
123.611
121.446
120.074
119.911
119.882
119.853
119.821
117.320
117.288
117.255
117.224
95.212
24.746
NH2
HN
CF3
N
S
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

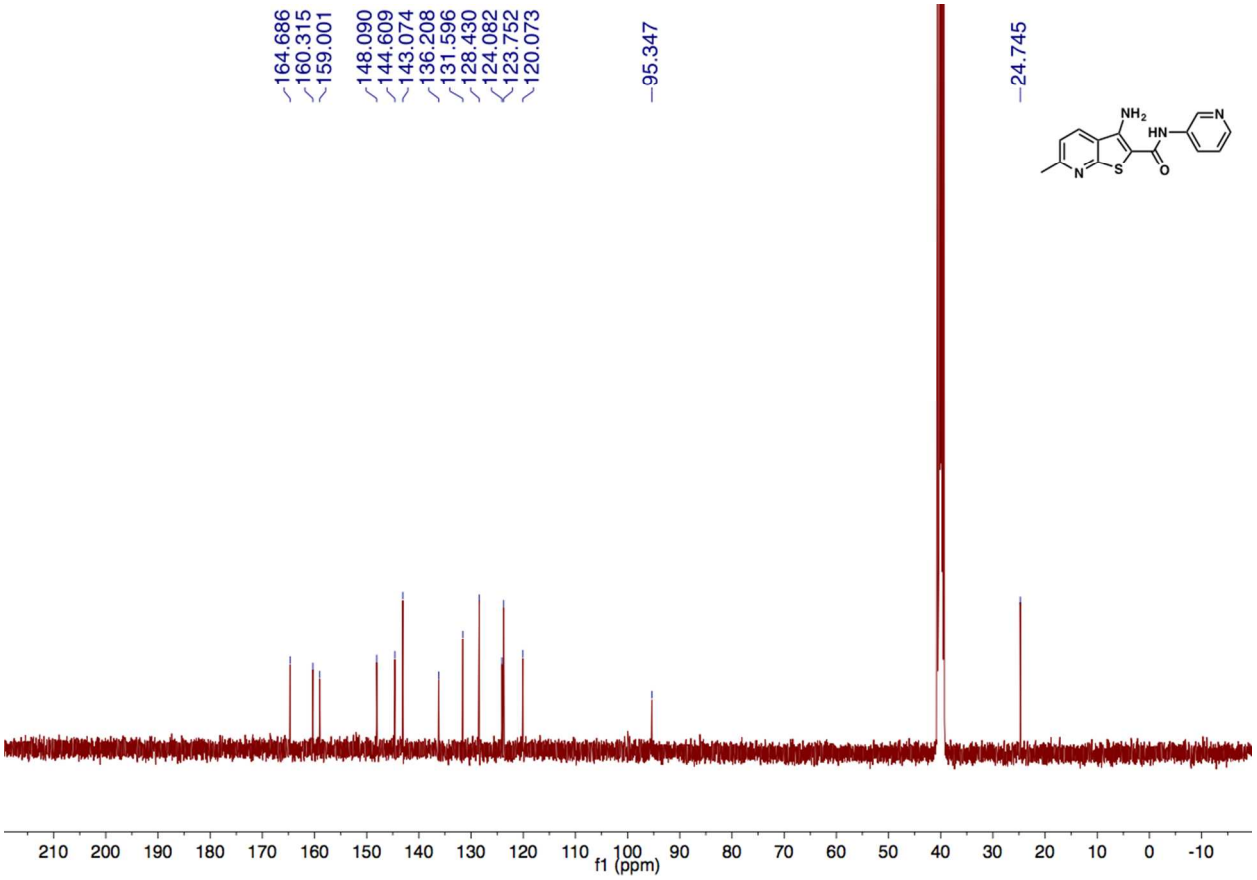

9.729
8.432
8.420
8.412
7.774
7.758
7.541
7.371
7.350
2.614
NH2
HN
N
S
O
N
0.84
2.84
1.92
1.79
1.00
2.70
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

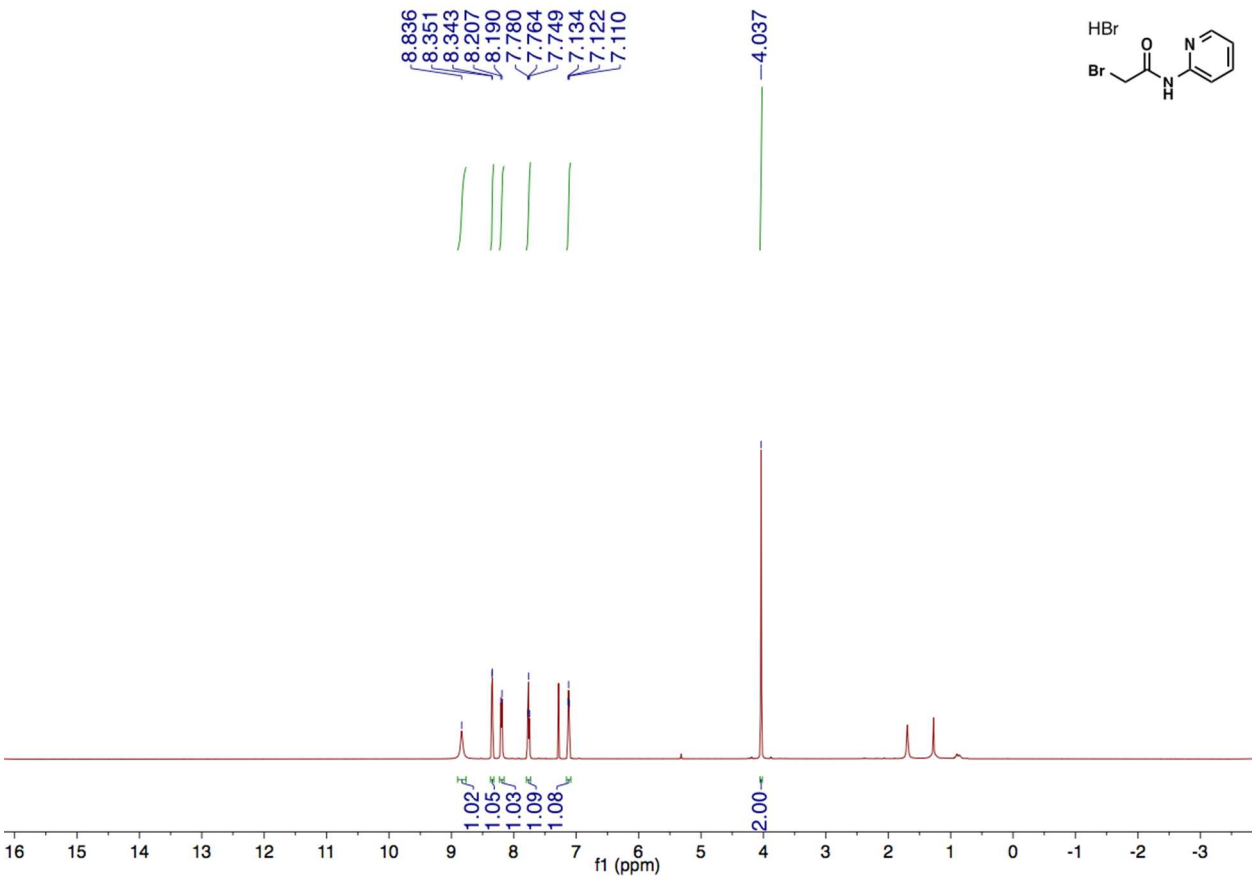

164.979
160.630
159.116
150.476
148.813
146.594
131.721
123.929
120.138
114.678
95.117
24.769
NH2
HN
N
S
O
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

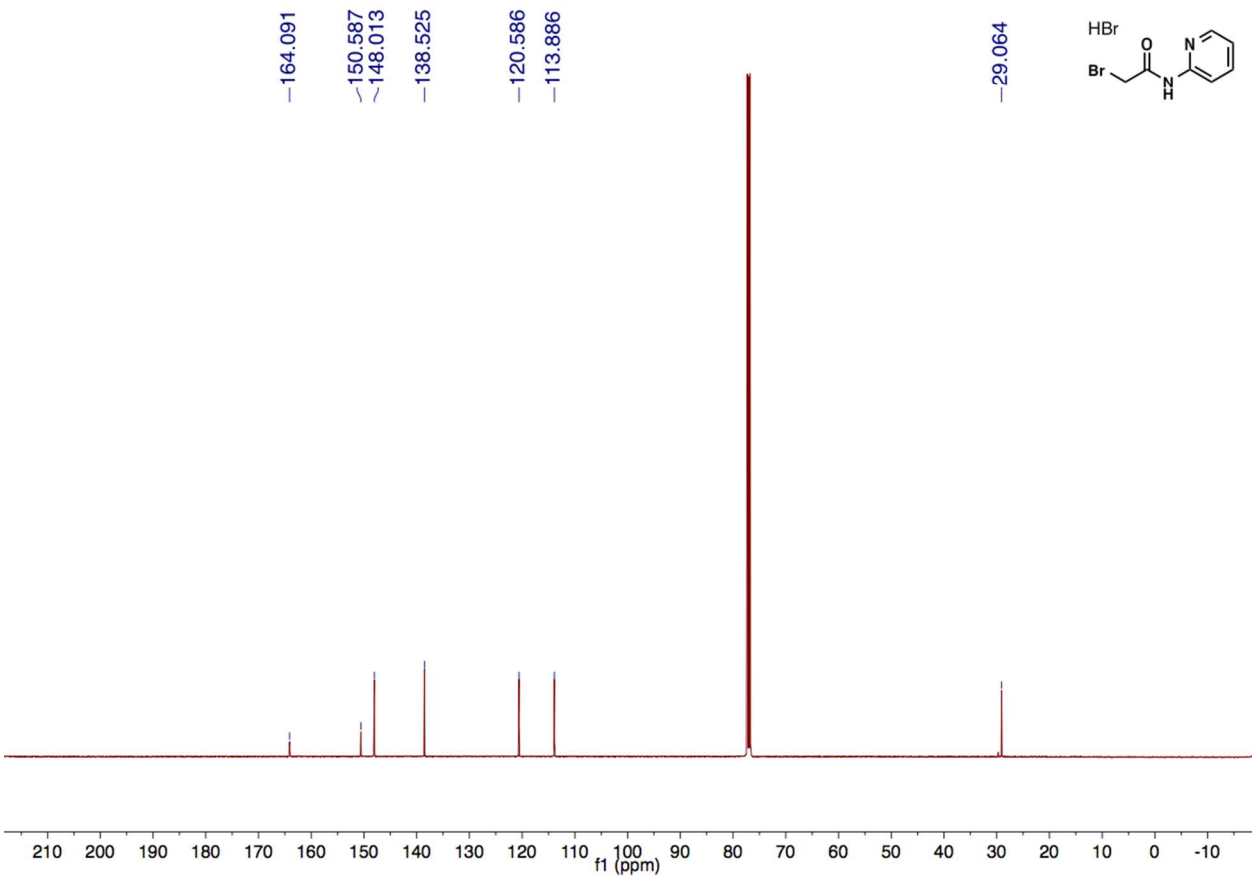

11.421
9.202
9.196
8.658
8.644
8.510
8.488
8.012
7.998
7.990
7.976
4.192
HBr
N
O
N
H
Br
0.94
1.00
1.06
1.02
1.14
1.93
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

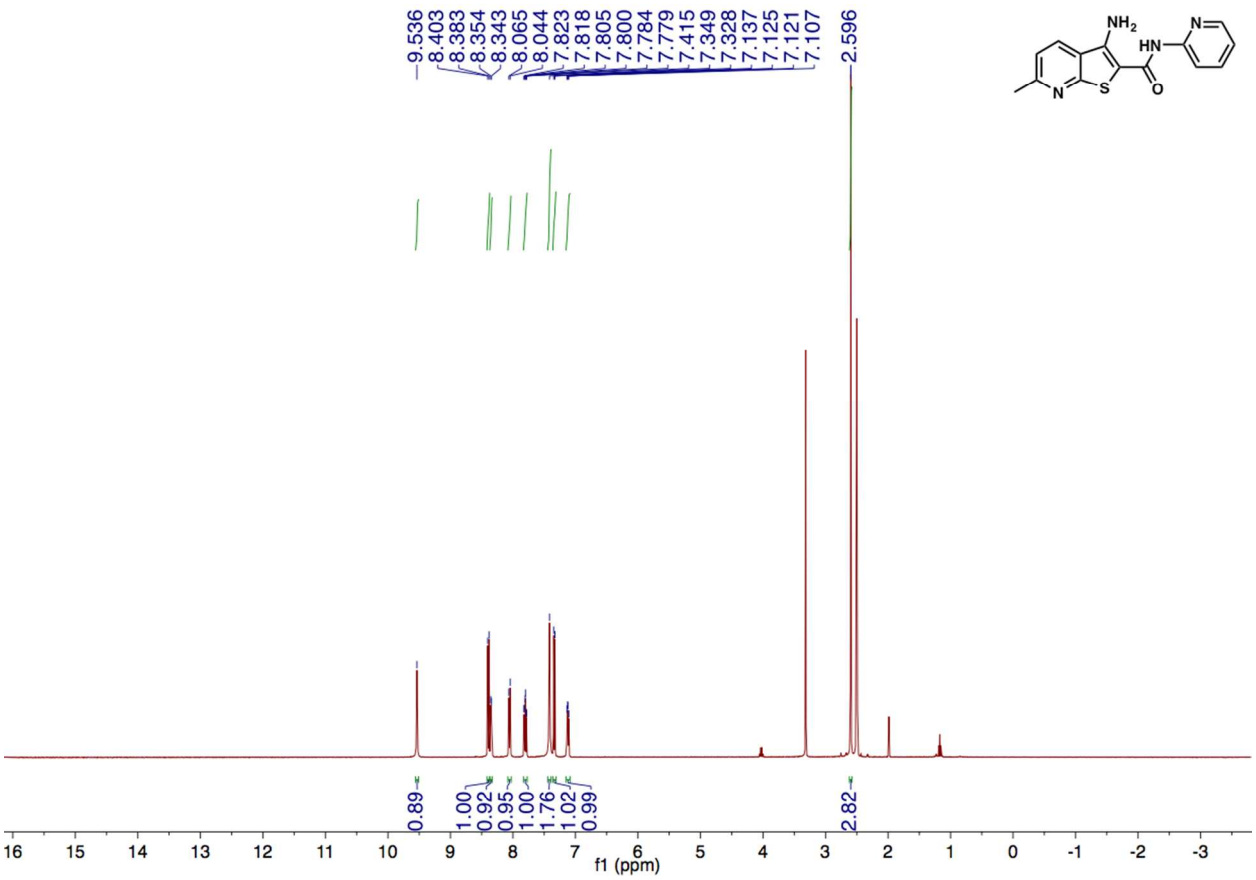

166.698
138.280
138.049
134.825
132.992
127.958
30.001
HBr
N
O
N
H
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

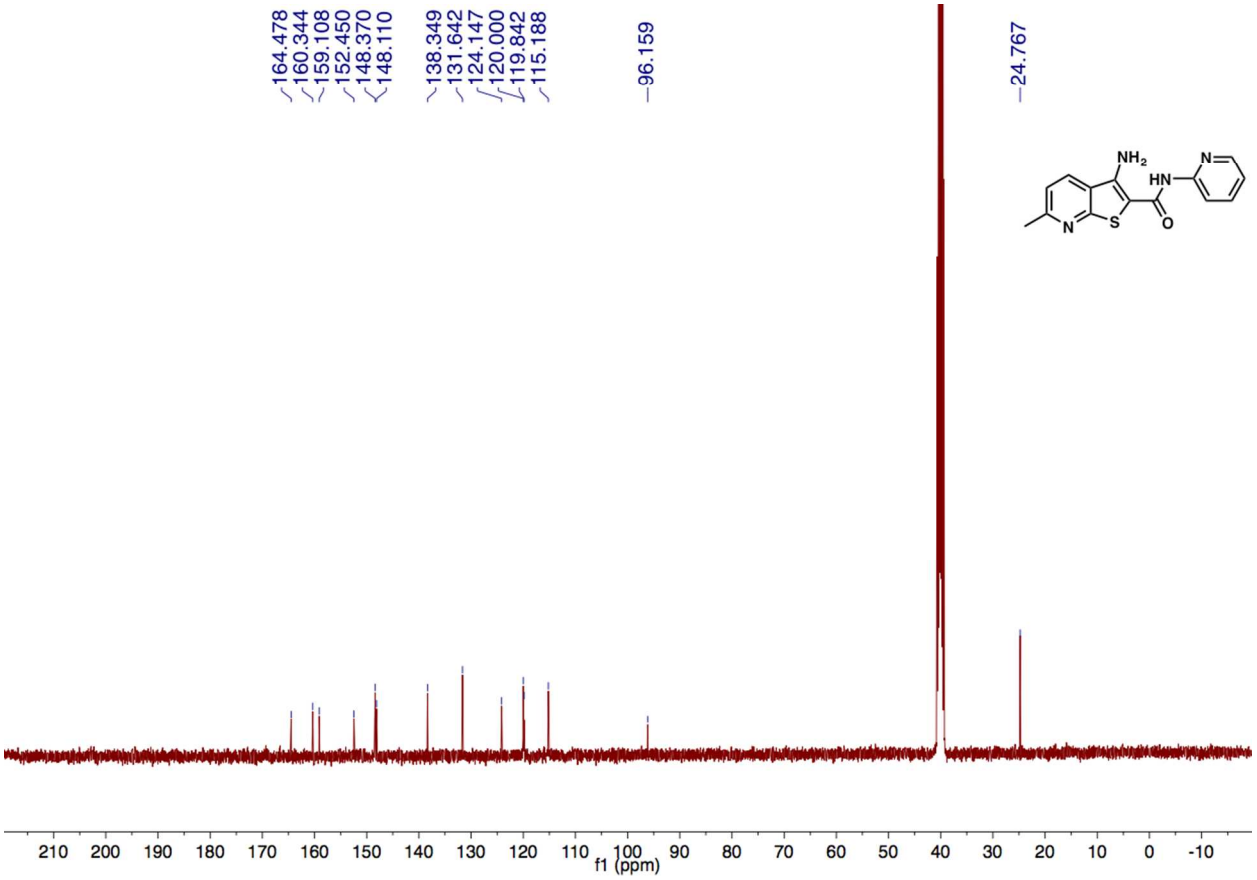

9.599
8.880
8.874
8.403
8.382
8.278
8.275
8.267
8.263
8.106
8.102
8.096
8.085
8.081
8.075
7.428
7.371
7.357
7.350
7.336
2.605
NH2
HN
N
S
O
1.00
0.93
1.00
0.94
1.01
1.85
2.03
2.75
f1 (ppm)

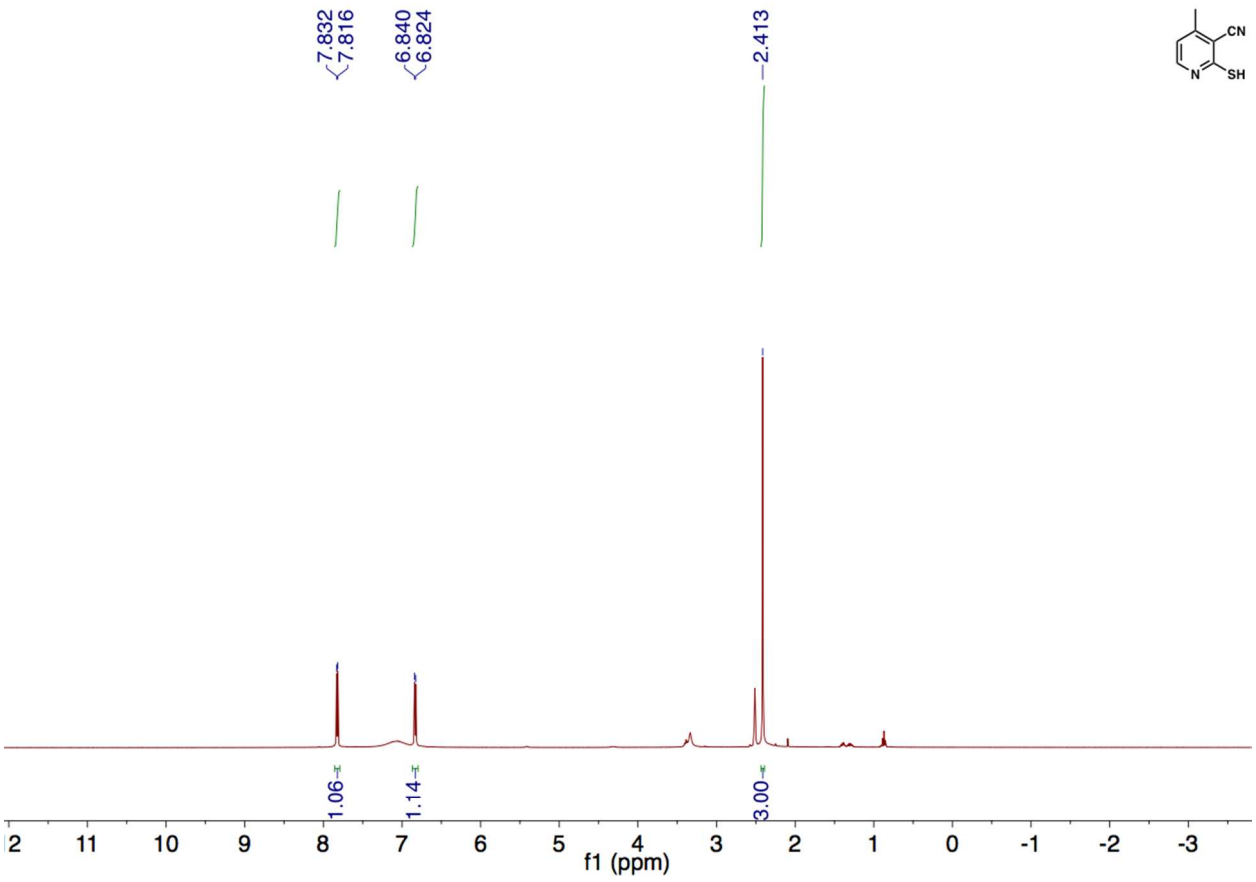

164.686
160.315
159.001
148.090
144.609
143.074
136.208
131.596
128.430
124.082
123.752
120.073
95.347
24.745
NH2
HN
N
S
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

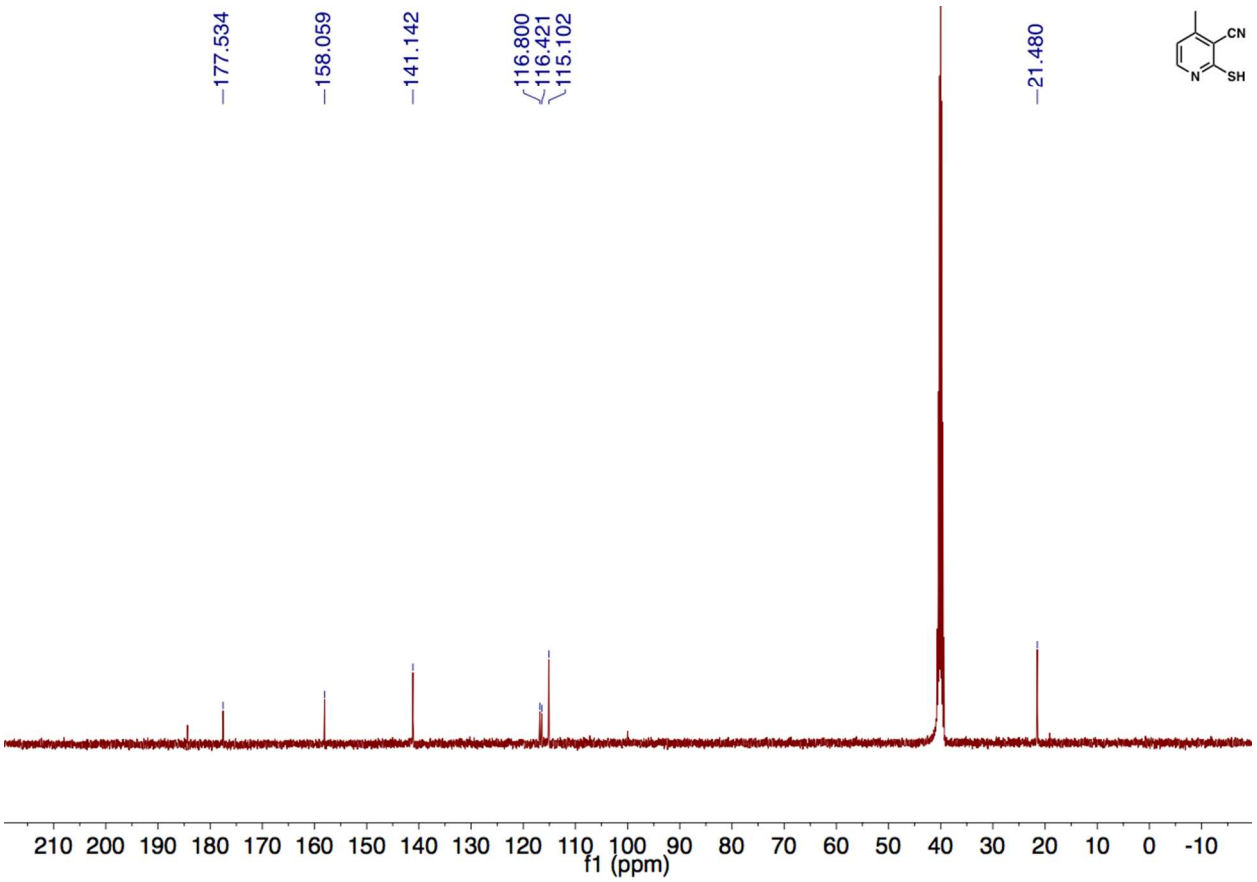

8.836
8.351
8.343
8.207
8.190
7.780
7.764
7.749
7.134
7.122
7.110
4.037
HBr
Br
O
N
H
N
1.02
1.05
1.03
1.09
1.08
2.00
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)

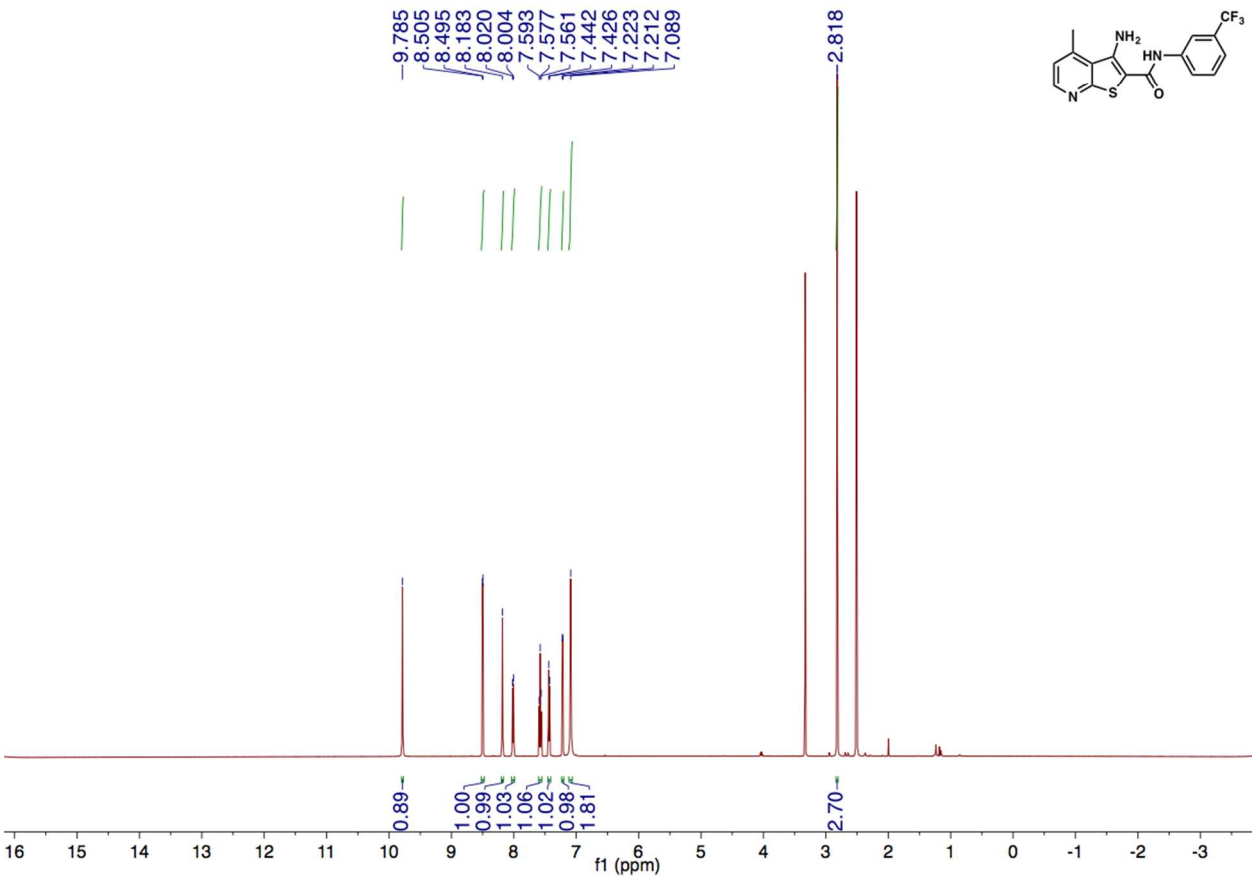

164.091
150.587
148.013
138.525
120.586
113.886
29.064
HBr
Br
O
N
H
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

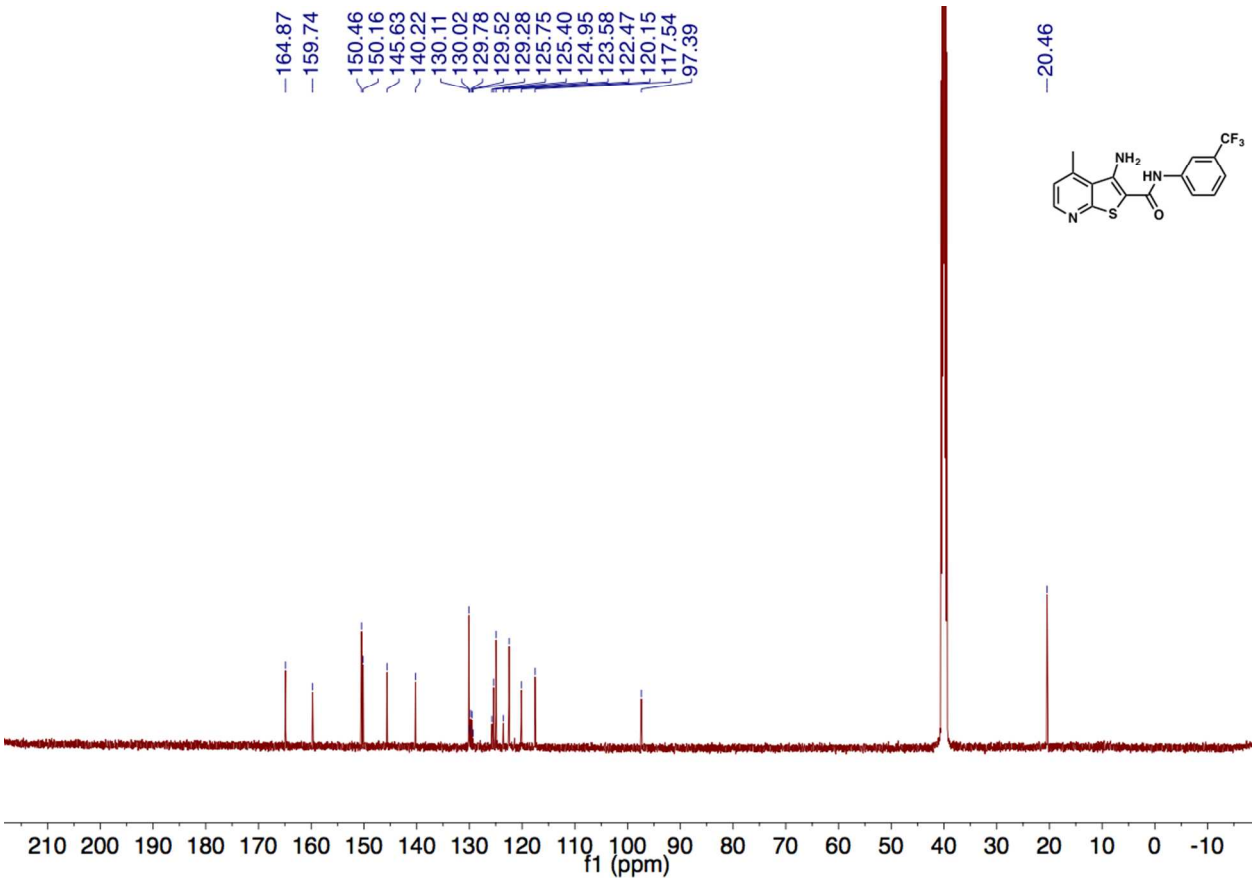

9.536
8.403
8.383
8.354
8.343
8.065
8.044
7.823
7.818
7.805
7.800
7.784
7.779
7.415
7.349
7.328
7.137
7.125
7.121
7.107
2.596
NH2
HN
N
S
O
0.89
1.00
0.92
0.95
1.00
1.76
1.02
0.99
2.82
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

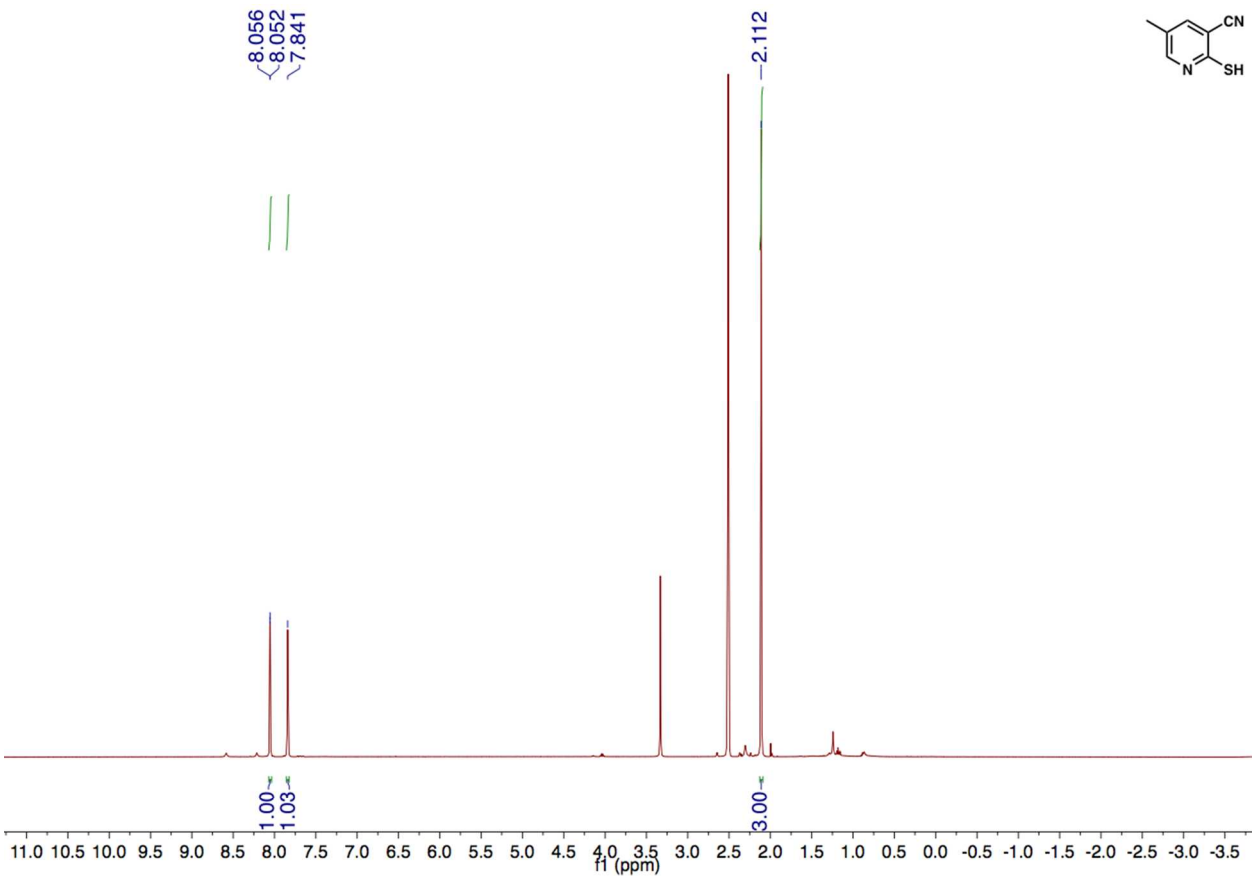

164.478
160.344
159.108
152.450
148.370
148.110
138.349
131.642
124.147
120.000
119.842
115.188
96.159
24.767
NH2
HN
N
S
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

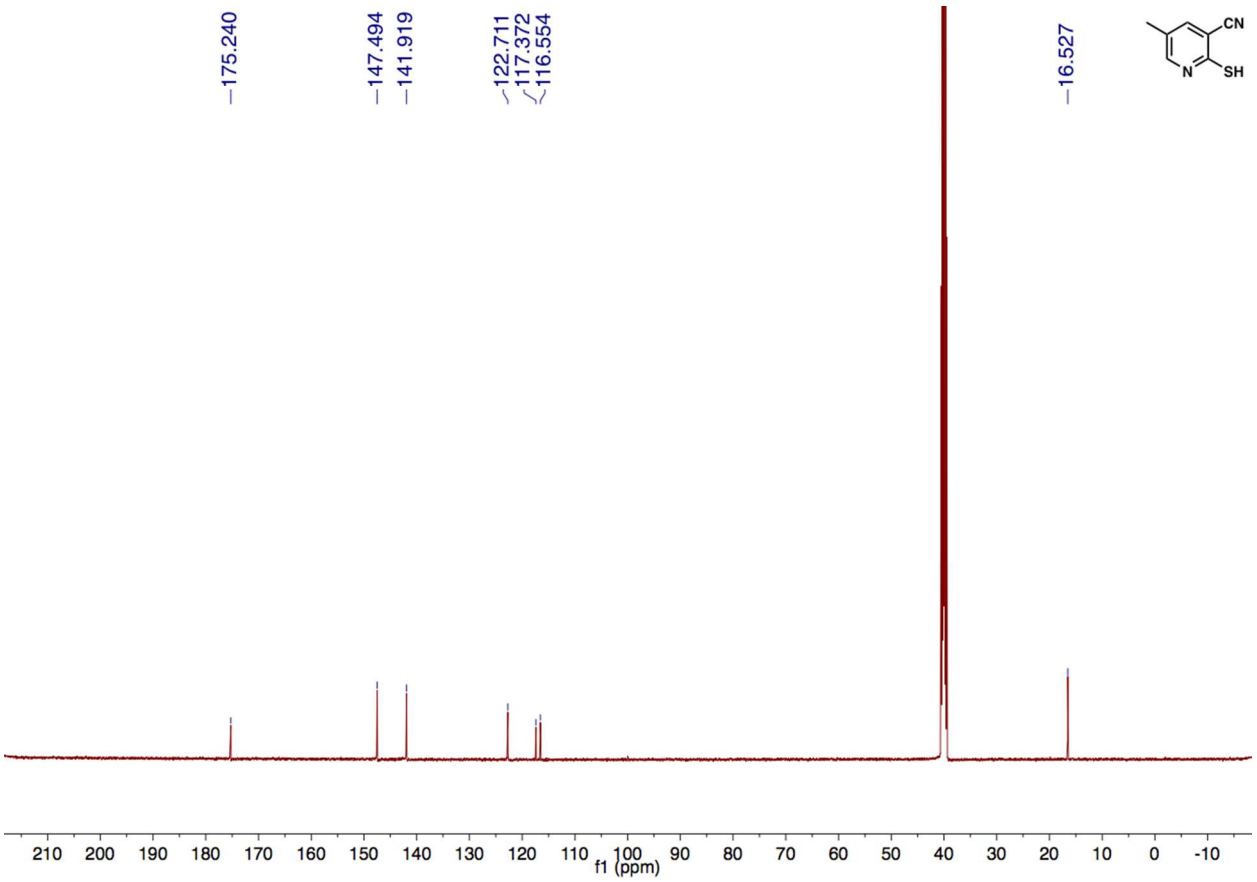

7.832
7.816
6.840
6.824
2.413
CN
SH
N
1.06
1.14
3.00
2
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)

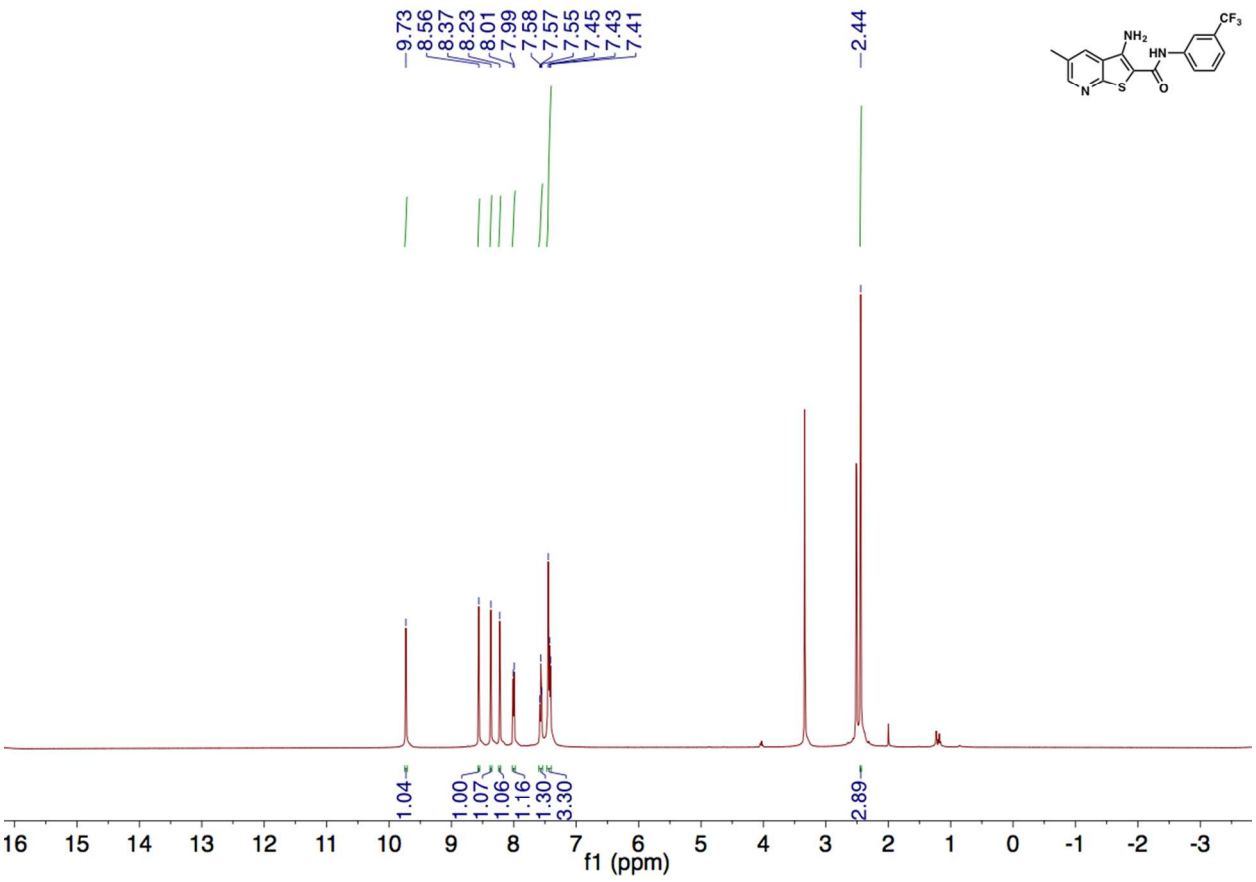

177.534
158.059
141.142
116.800
116.421
115.102
21.480
CN
SH
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

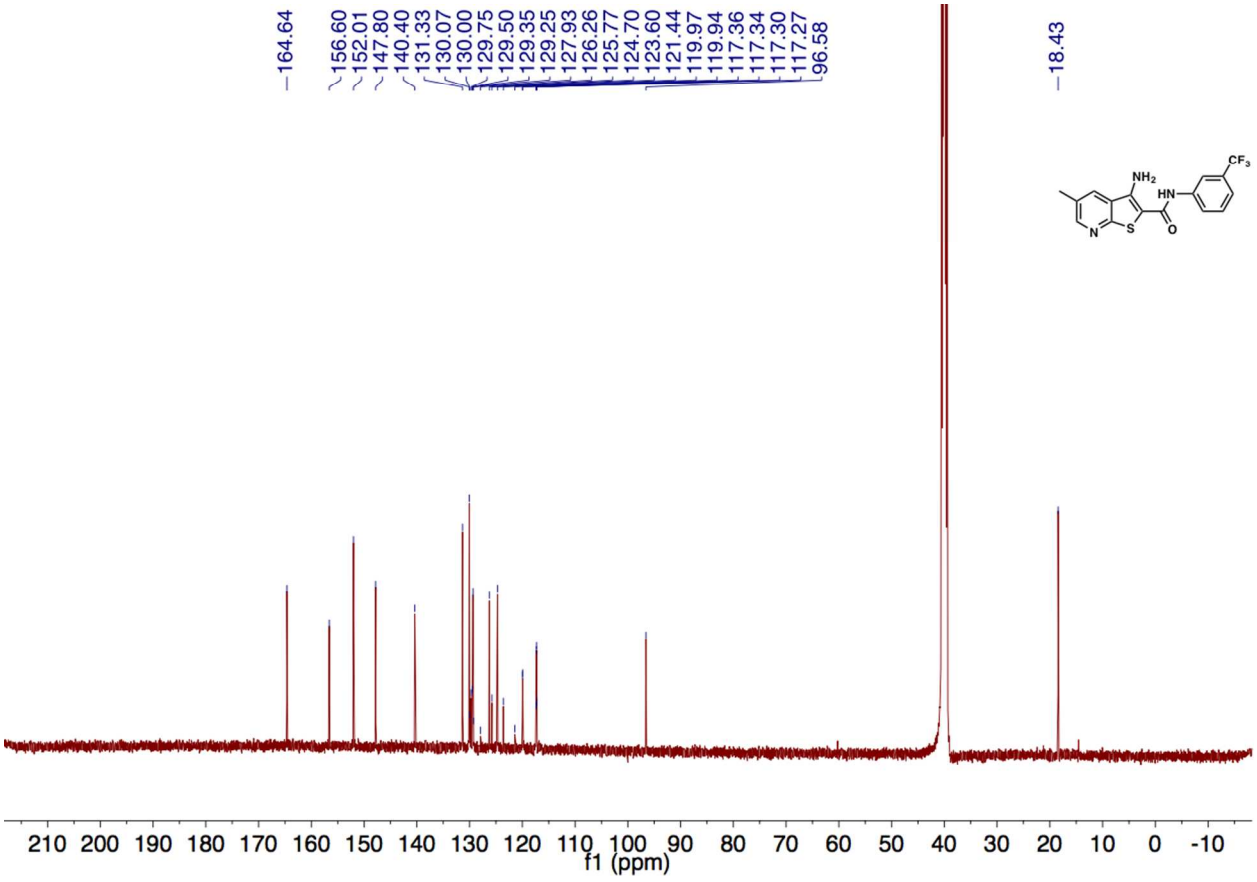

9.785
8.505
8.495
8.183
8.020
8.004
7.593
7.577
7.561
7.442
7.426
7.223
7.212
7.089
2.818
NH2
HN
CF3
N
S
O
0.89
1.00
0.99
1.03
1.06
1.02
0.98
1.81
2.70
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

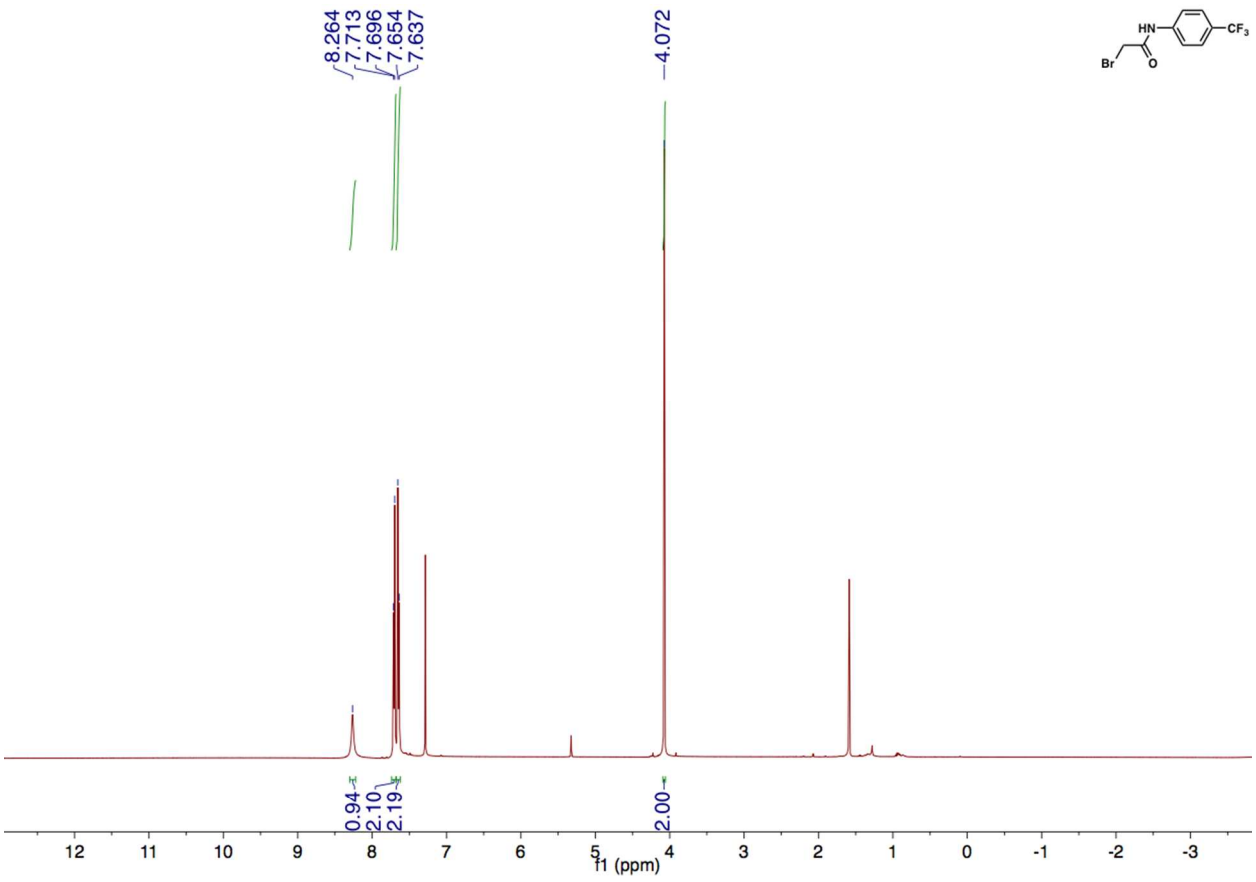

164.87
159.74
150.46
150.16
145.63
140.22
130.11
130.02
129.78
129.52
129.28
125.75
125.40
124.95
123.58
122.47
120.15
117.54
97.39
20.46
NH2
HN
CF3
N
S
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

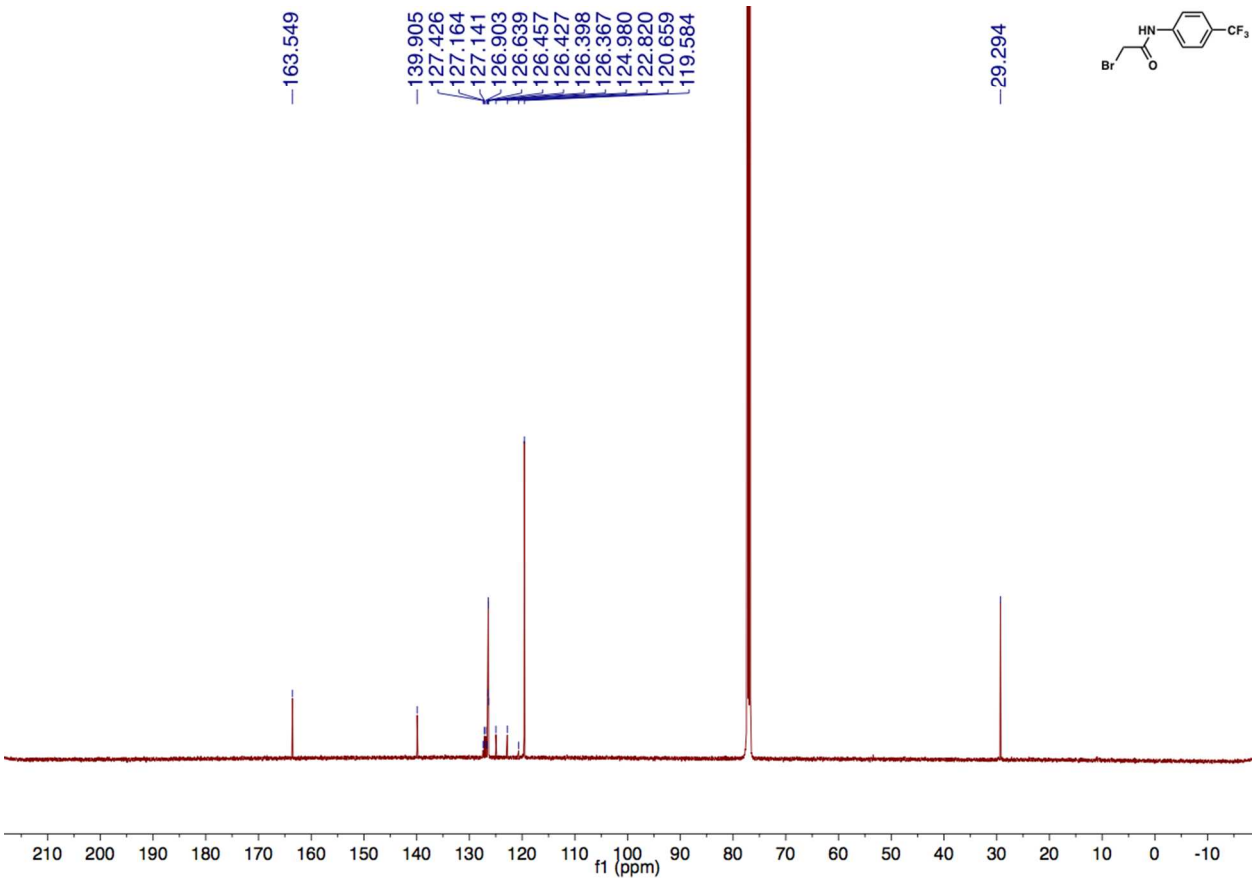

8.056
8.052
7.841
2.112
CN
N
SH
1.00
1.03
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0 -2.5 -3.0 -3.5
f1 (ppm)

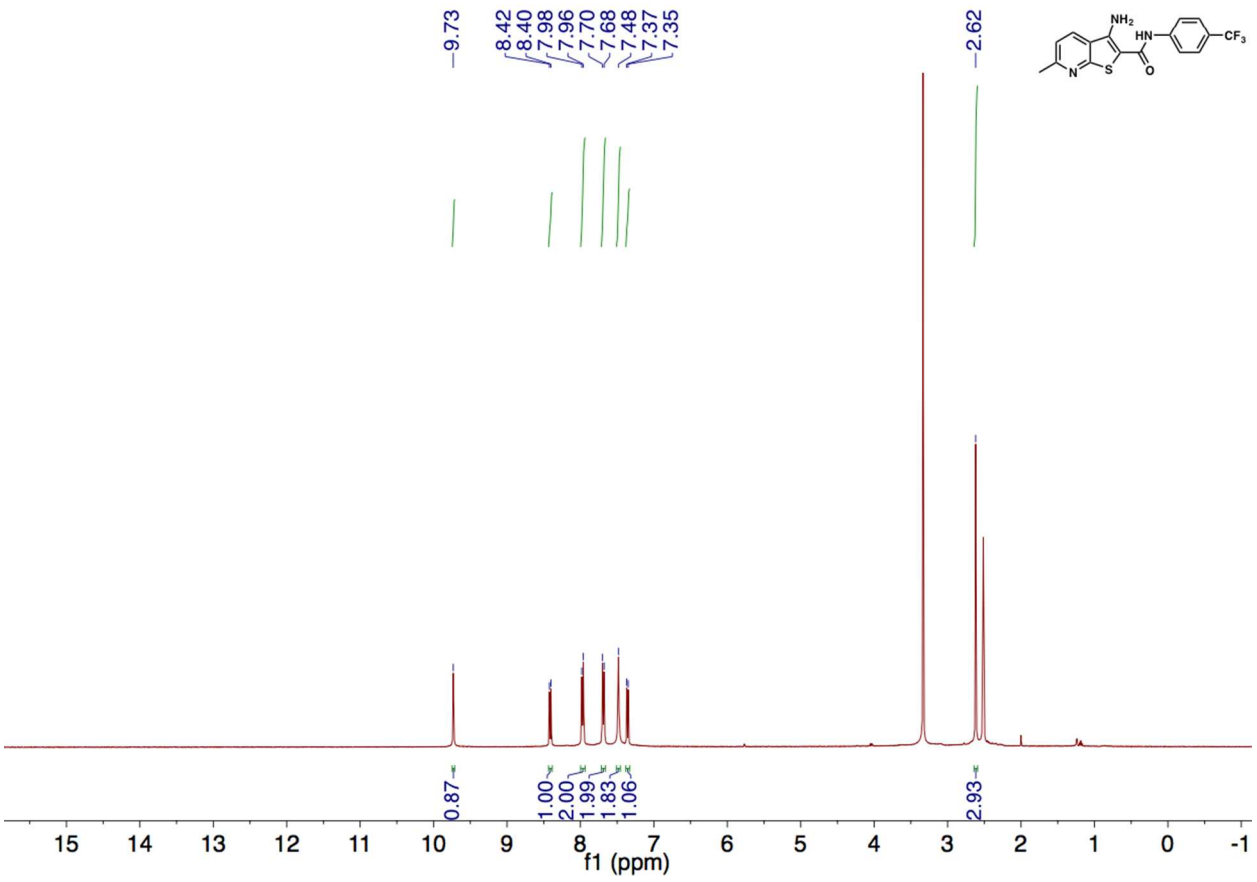

175.240
147.494
141.919
122.711
117.372
116.554
16.527
CN
SH
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

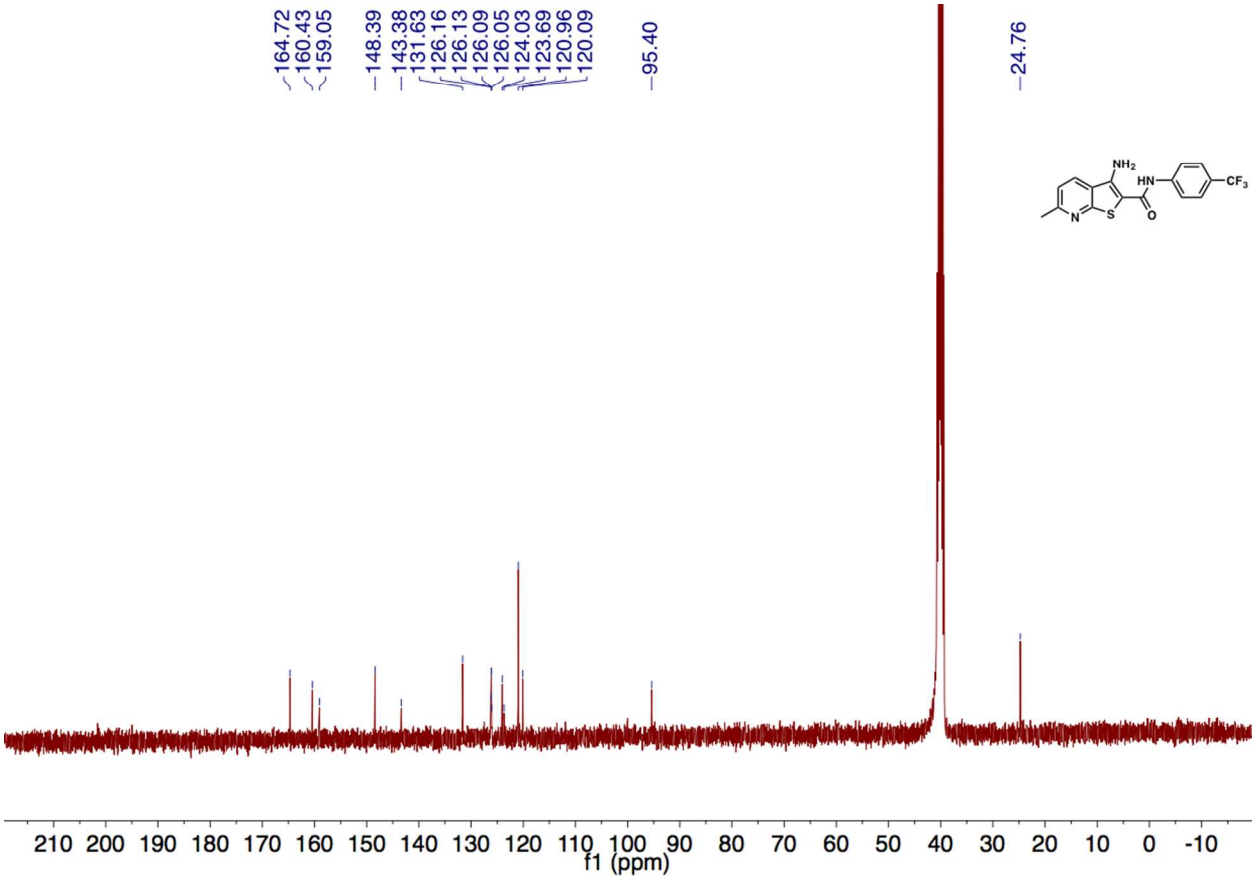

9.73
8.56
8.37
8.23
8.01
7.99
7.58
7.57
7.55
7.45
7.43
7.41
2.44
NH2
HN
CF3
N
S
O
1.04
1.00
1.07
1.06
1.16
1.30
3.30
2.89
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

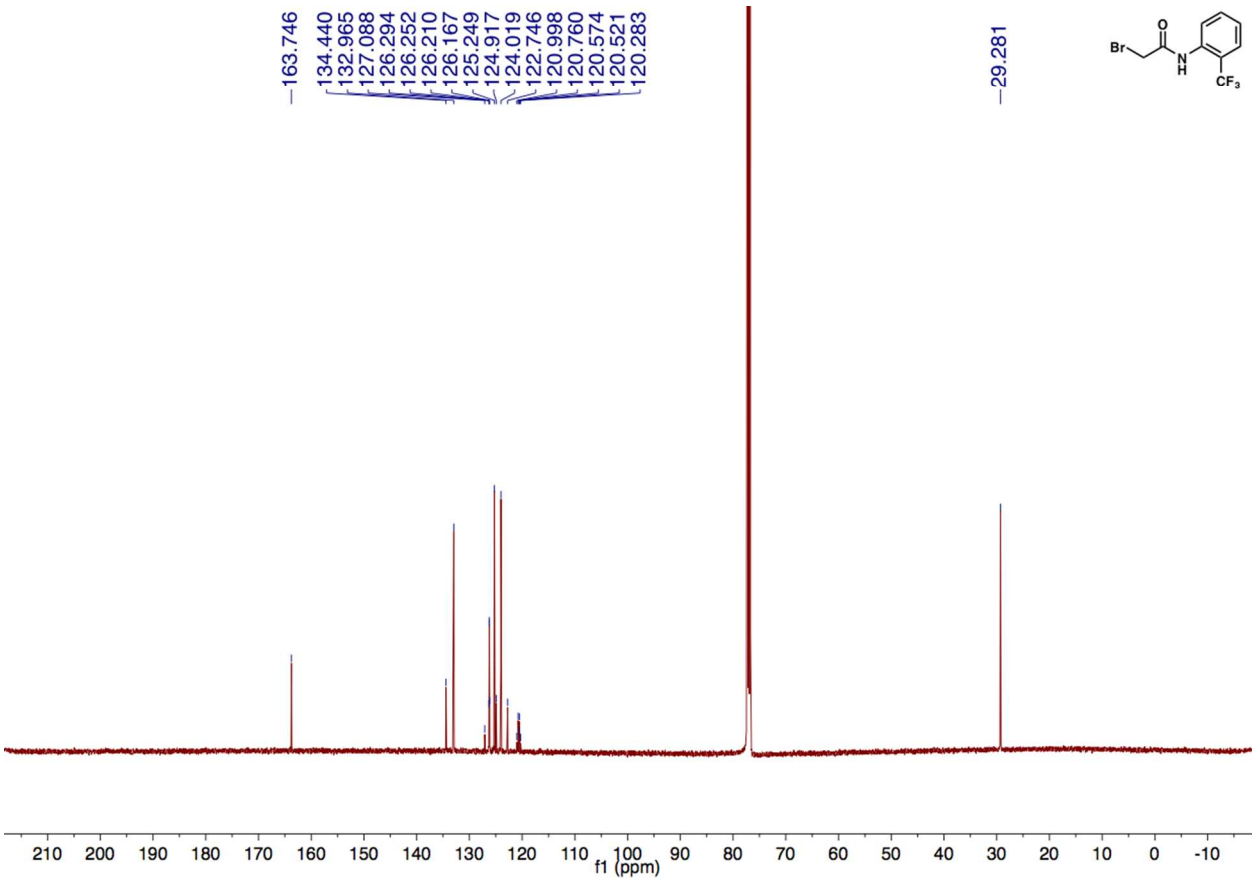

164.64
156.60
152.01
147.80
140.40
131.33
130.07
130.00
129.75
129.50
129.35
129.25
127.93
126.26
125.77
124.70
123.60
121.44
119.97
119.94
117.36
117.34
117.30
117.27
96.58
18.43
NH2
HN
CF3
N
S
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

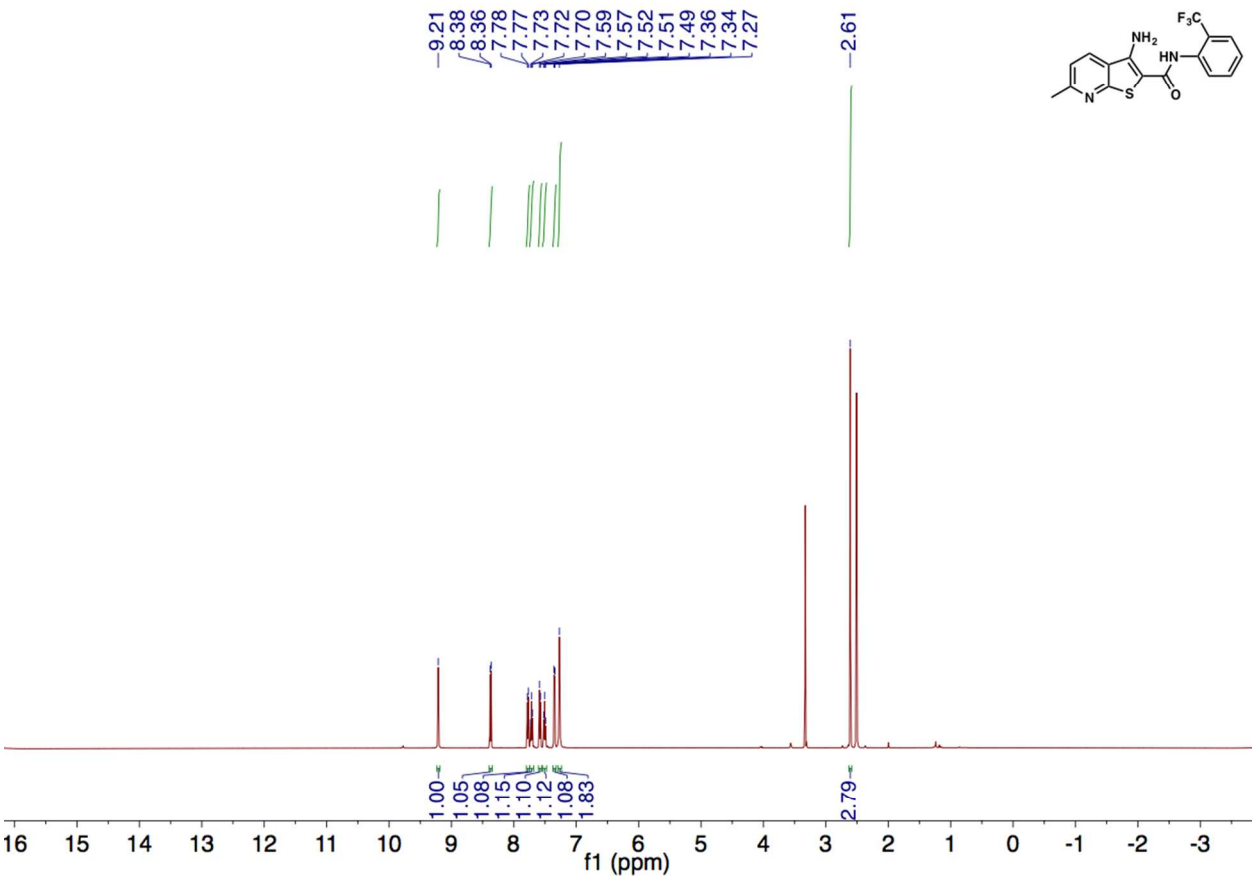

8.264
7.713
7.696
7.654
7.637
4.072
HN
CF3
Br
O
0.94
2.10
2.19
2.00
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)

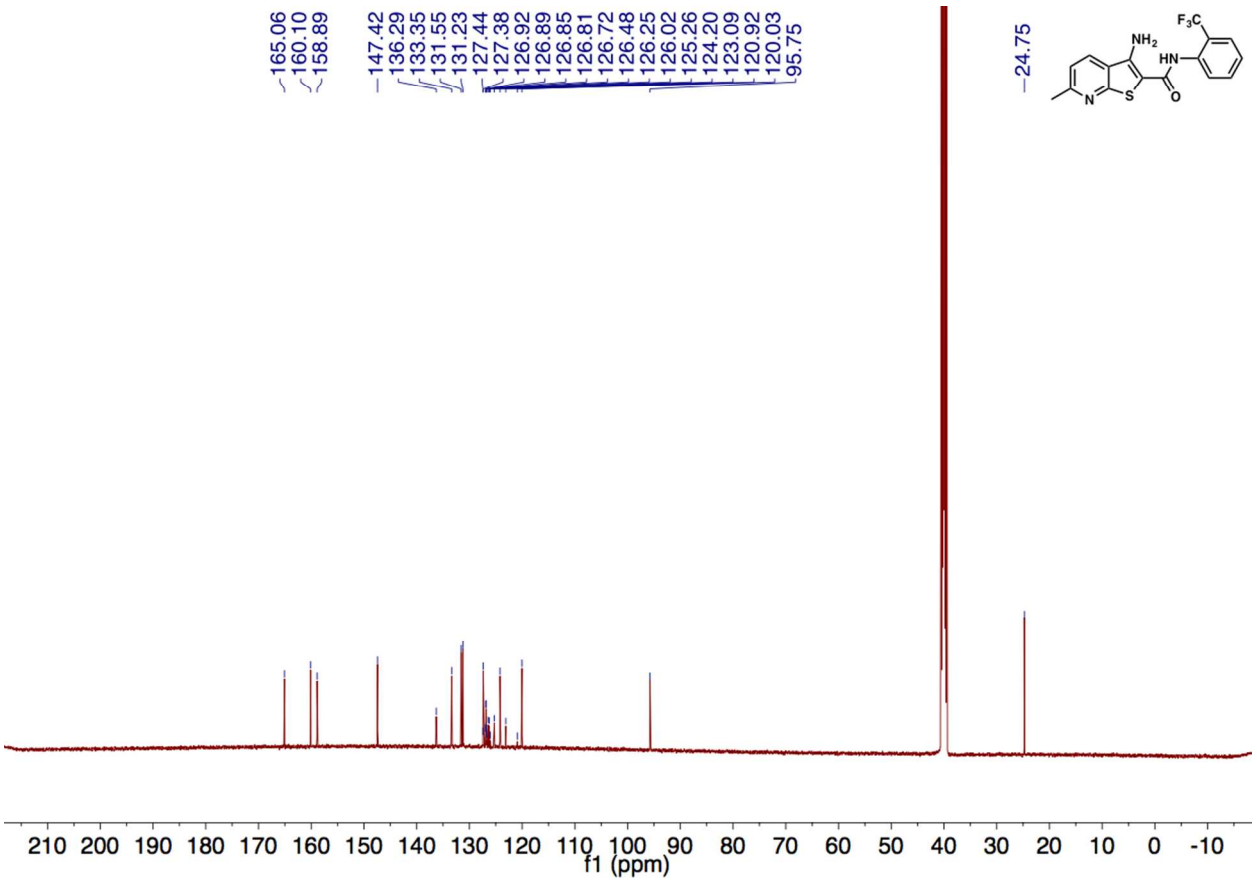

163.549
139.905
127.426
127.164
127.141
126.903
126.639
126.457
126.427
126.398
126.367
124.980
122.820
120.659
119.584
29.294
HN
CF3
Br
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

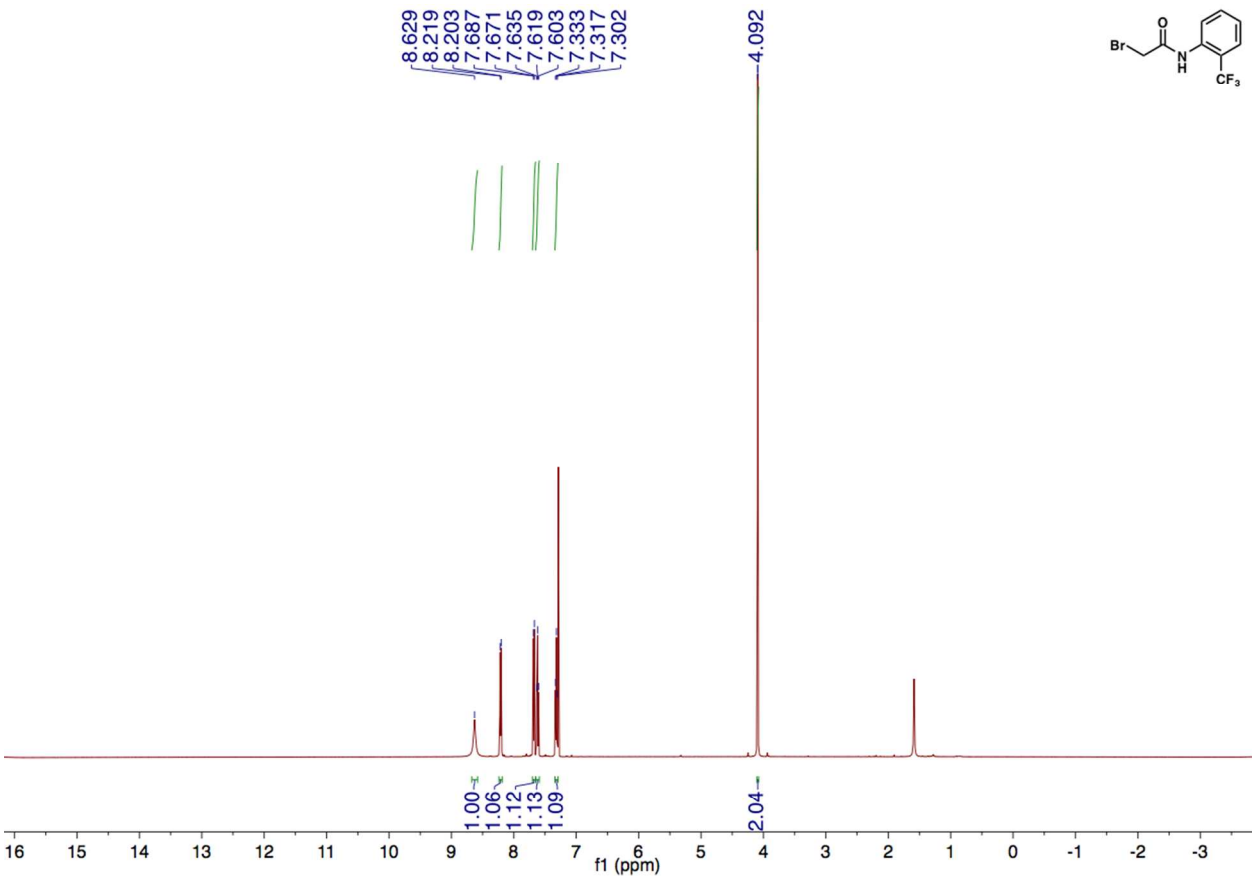

9.73
8.42
8.40
7.98
7.96
7.70
7.68
7.48
7.37
7.35
2.62
NH2
HN
CF3
N
S
O
0.87
1.00
2.00
1.99
1.83
1.06
2.93
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)

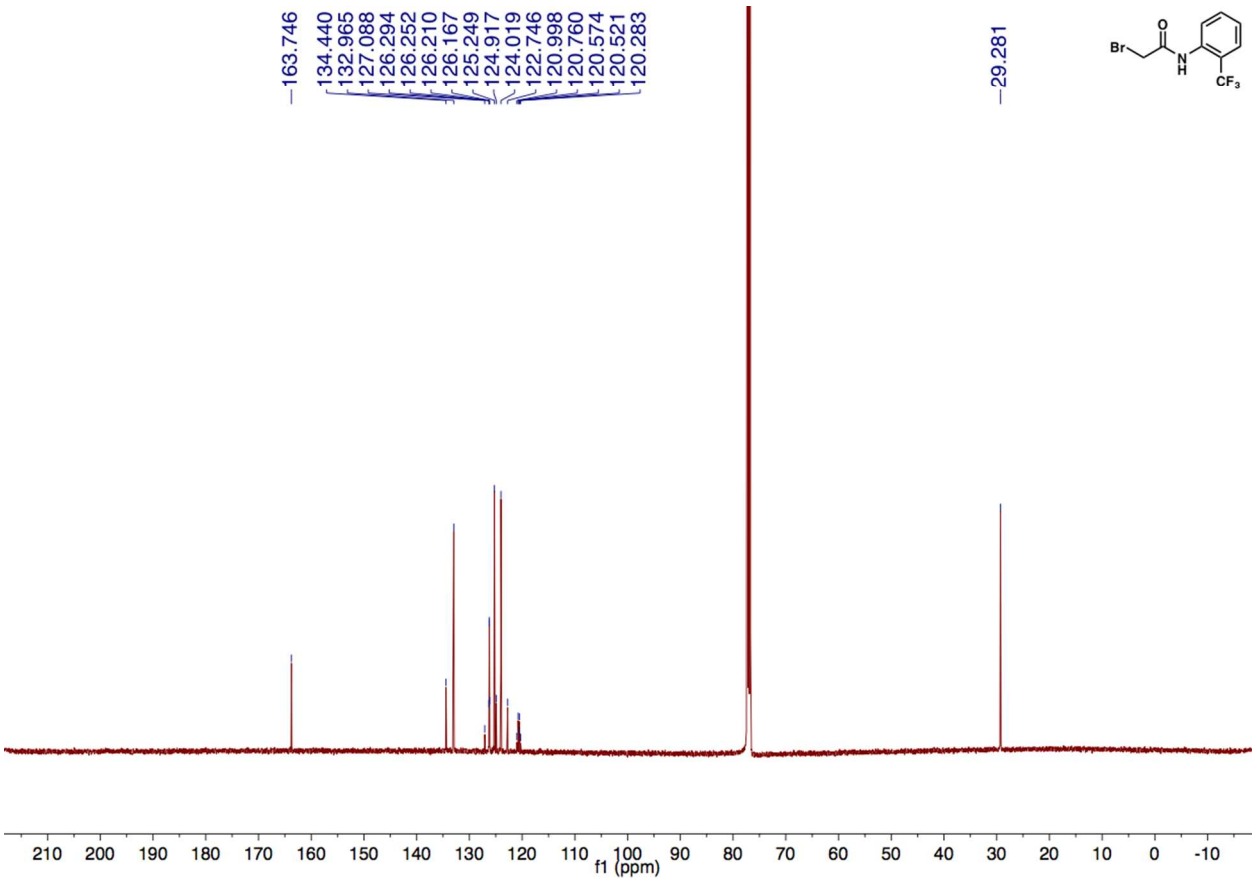

164.72
160.43
159.05
148.39
143.38
131.63
126.16
126.13
126.09
126.05
124.03
123.69
120.96
120.09
95.40
24.76
NH2
HN
CF3
N
S
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

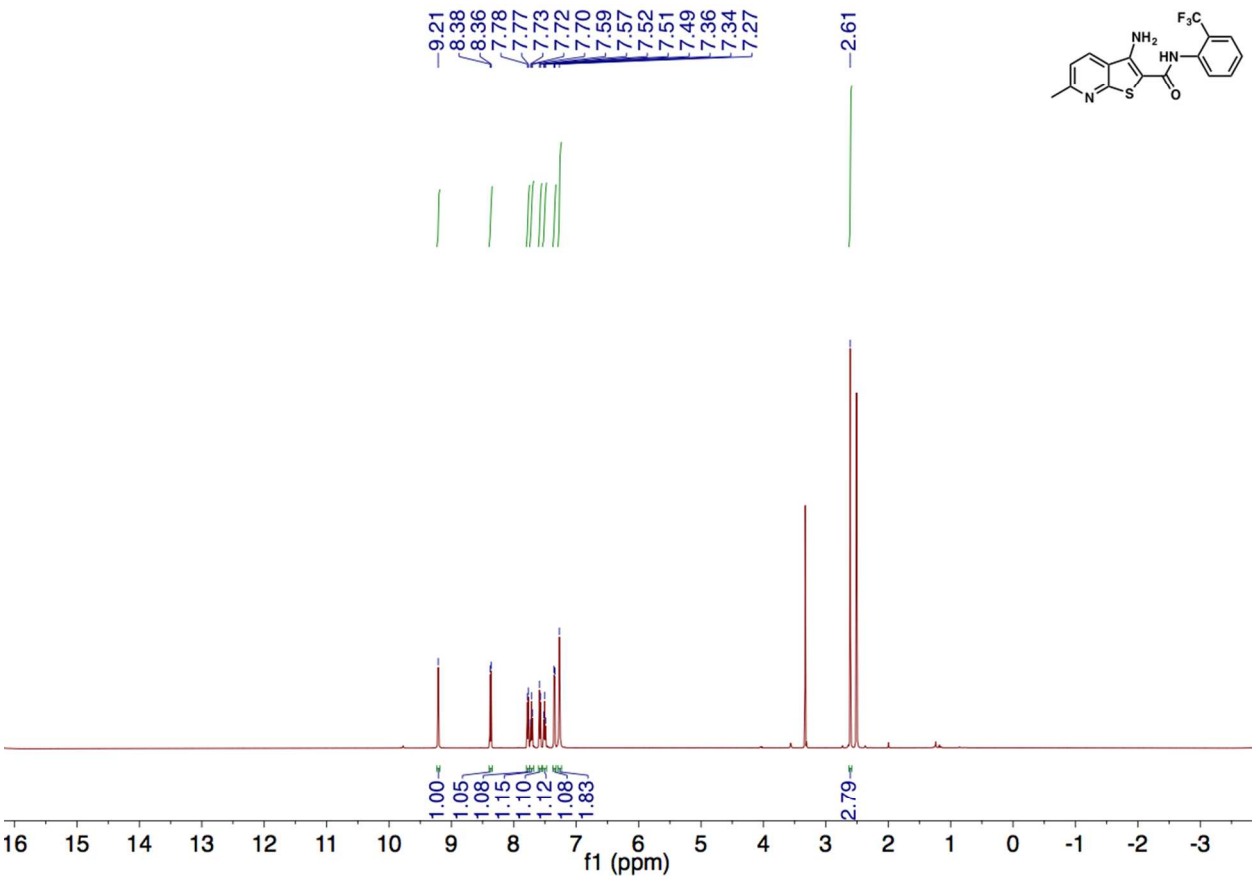

163.746
134.440
132.965
127.088
126.294
126.252
126.210
126.167
125.249
124.917
124.019
122.746
120.998
120.760
120.574
120.521
120.283
29.281
Br
O
N
H
CF3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

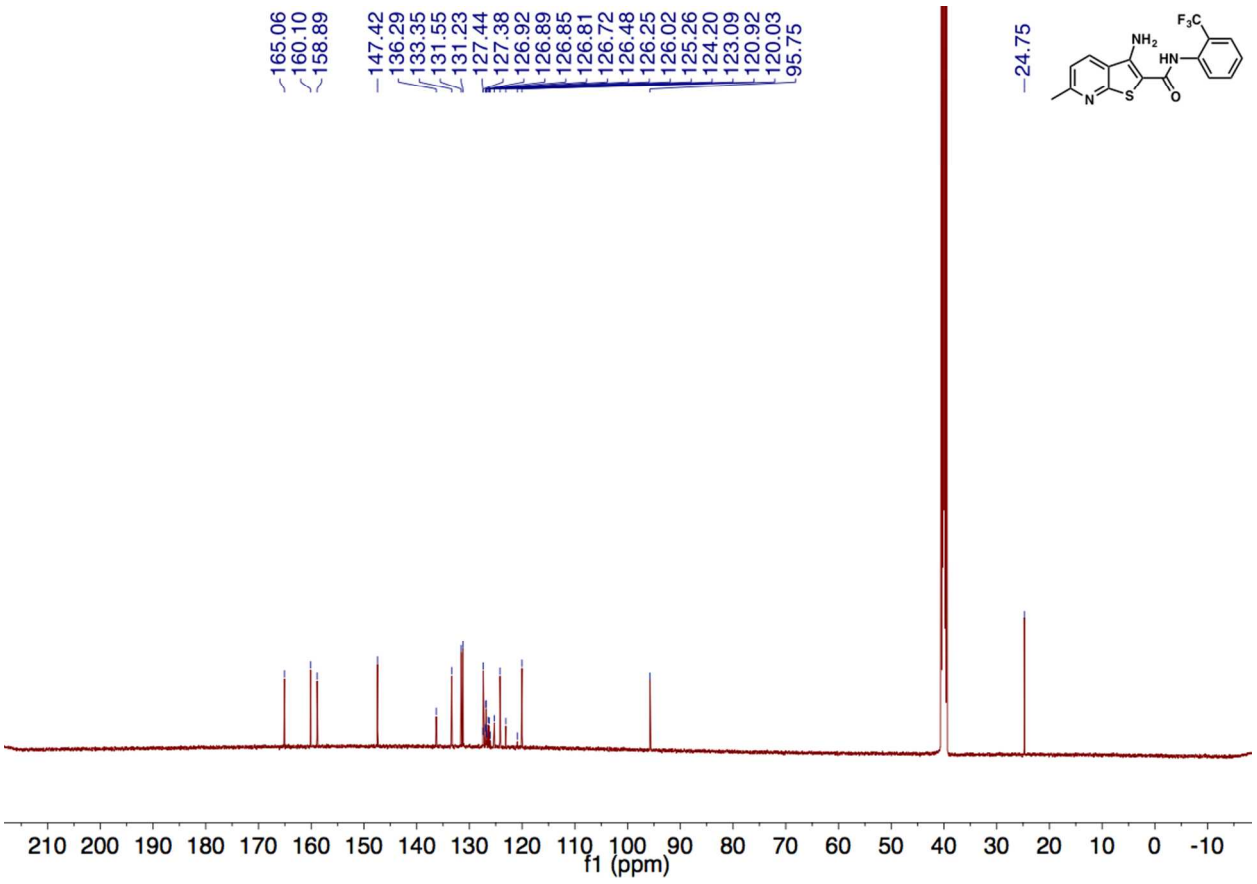

9.21
8.38
8.36
7.78
7.77
7.73
7.72
7.70
7.59
7.57
7.52
7.51
7.49
7.36
7.34
7.27
2.61
NH2
HN
F3C
N
S
O
1.00
1.05
1.08
1.15
1.10
1.12
1.08
1.83
2.79
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

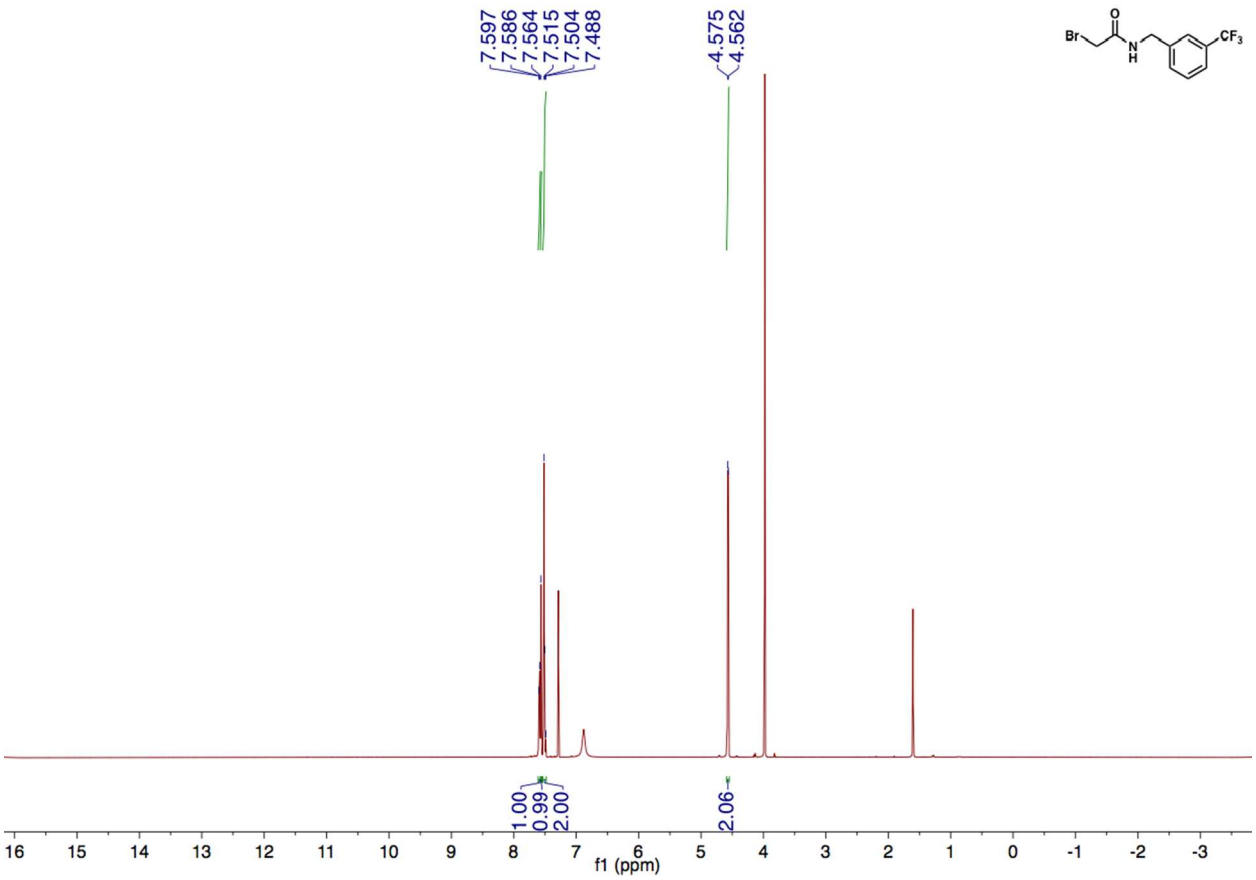

165.06
160.10
158.89
147.42
136.29
133.35
131.55
131.23
127.44
127.38
126.92
126.89
126.85
126.81
126.72
126.48
126.25
126.02
125.26
124.20
123.09
120.92
120.03
95.75
24.75
NH2
HN
F3C
O
N
S
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

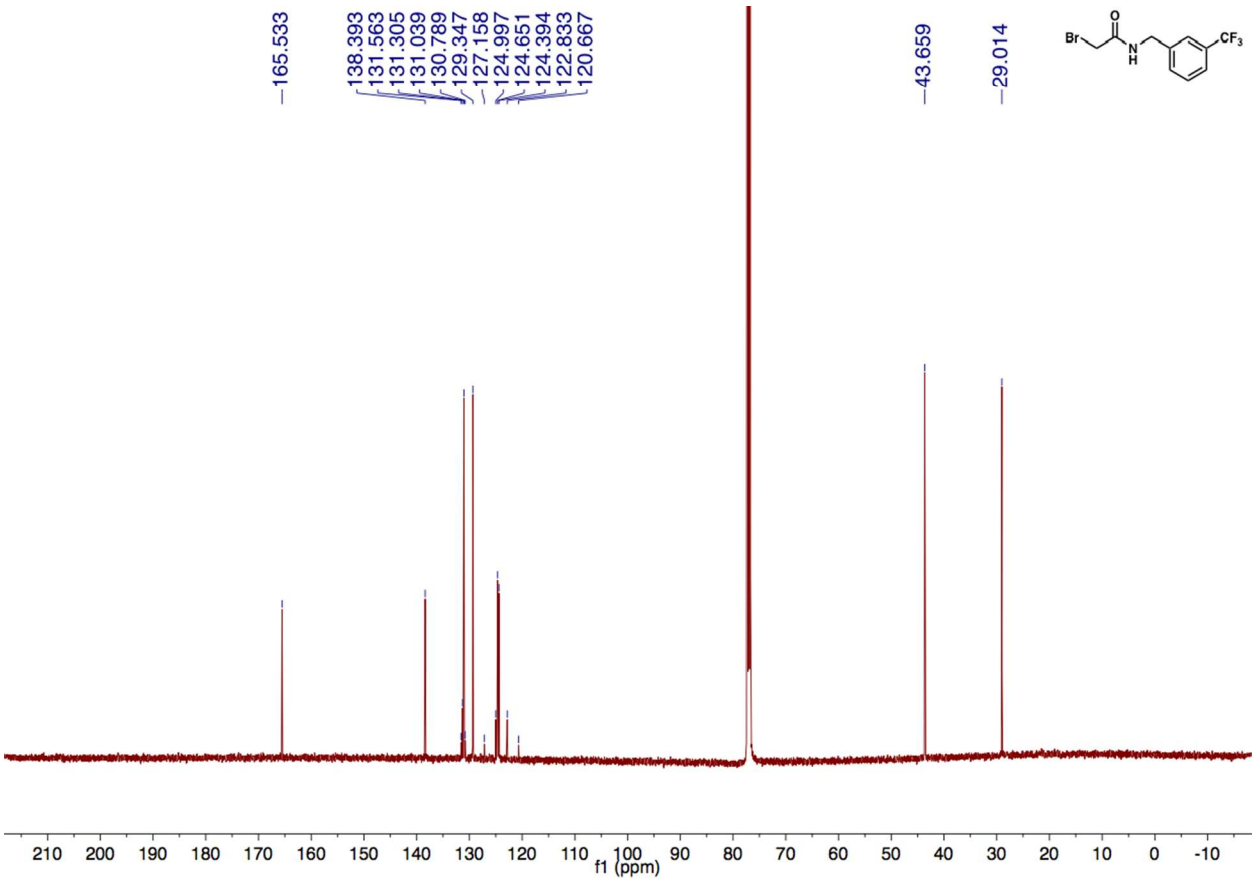

8.629
8.219
8.203
7.687
7.671
7.635
7.619
7.603
7.333
7.317
7.302
4.092
Br
O
N
H
CF3
1.00
1.06
1.12
1.13
1.09
2.04
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

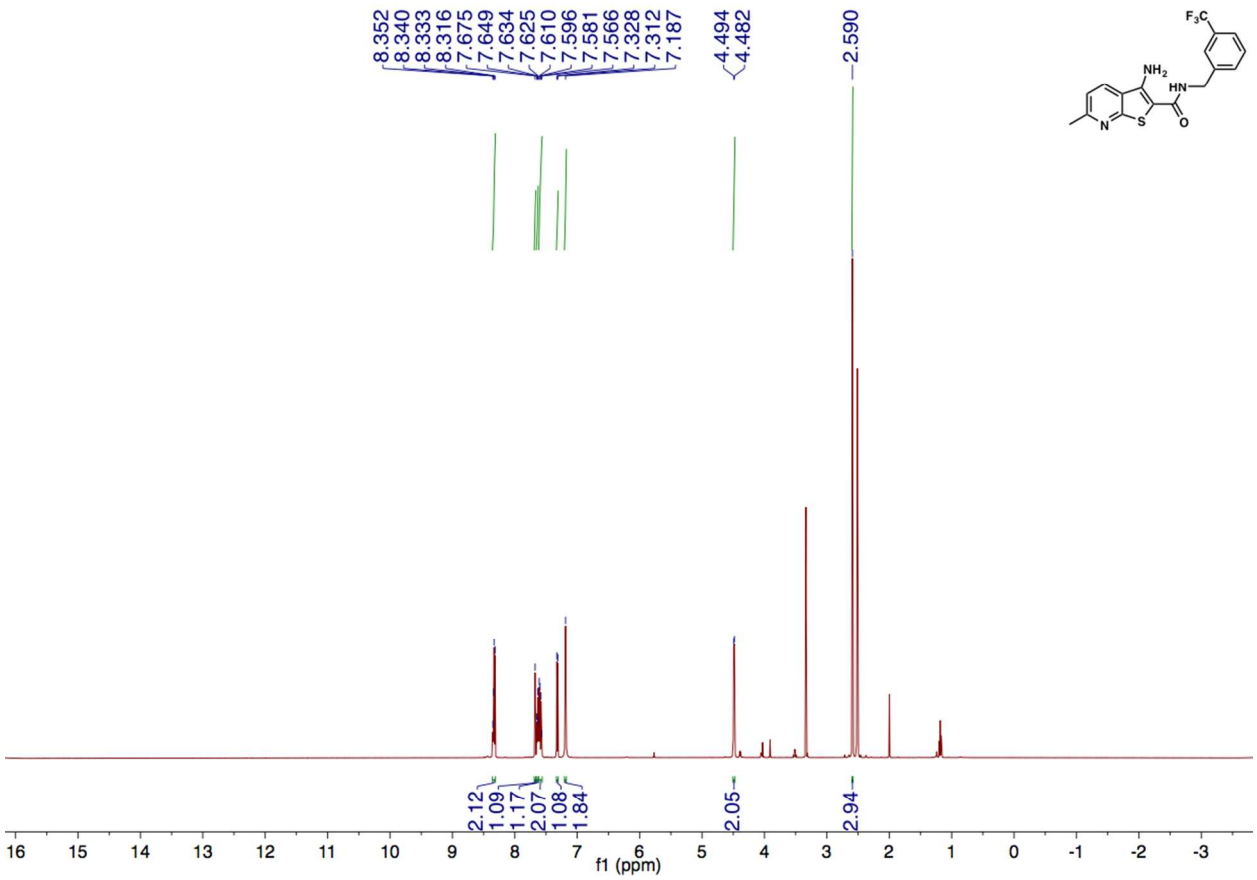

163.746
134.440
132.965
127.088
126.294
126.252
126.210
126.167
125.249
124.917
124.019
122.746
120.998
120.760
120.574
120.521
120.283
29.281
Br
O
N
H
CF3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

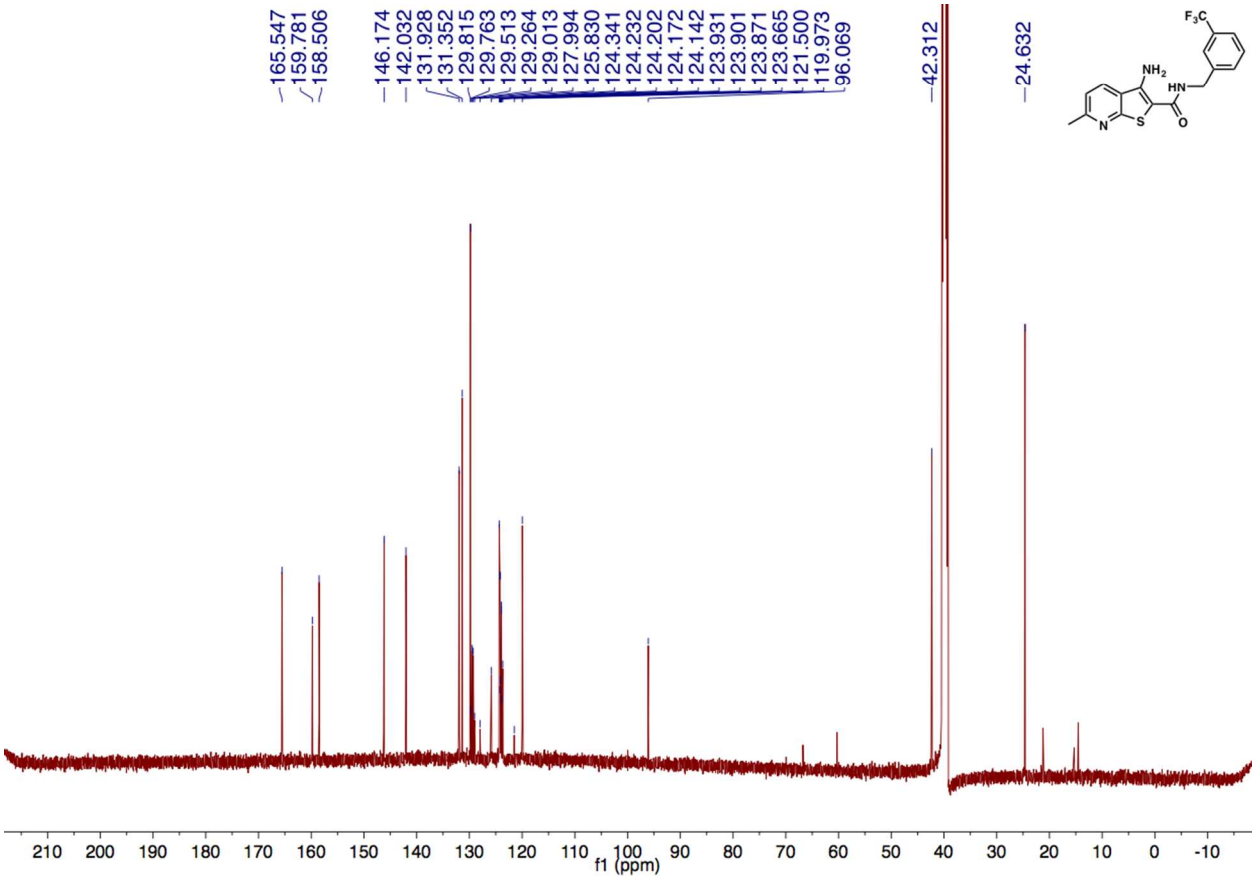

9.21
8.38
8.36
7.78
7.77
7.73
7.72
7.70
7.59
7.57
7.52
7.51
7.49
7.36
7.34
7.27
2.61
NH2
HN
F3C
N
S
O
1.00
1.05
1.08
1.15
1.10
1.12
1.08
1.83
2.79
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

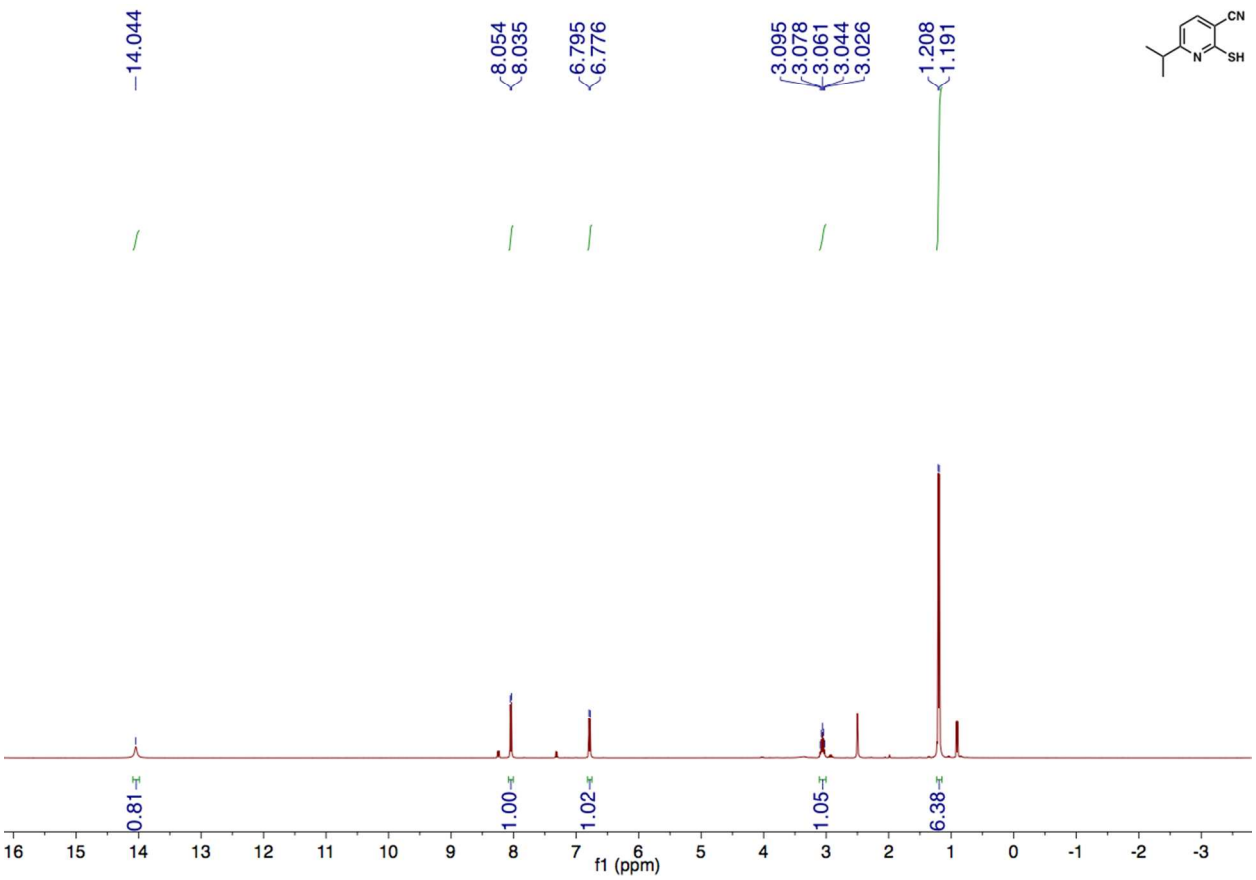

165.06
160.10
158.89
147.42
136.29
133.35
131.55
131.23
127.44
127.38
126.92
126.89
126.85
126.81
126.72
126.48
126.25
126.02
125.26
124.20
123.09
120.92
120.03
95.75
24.75
NH2
HN
O
N
S
F3C
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

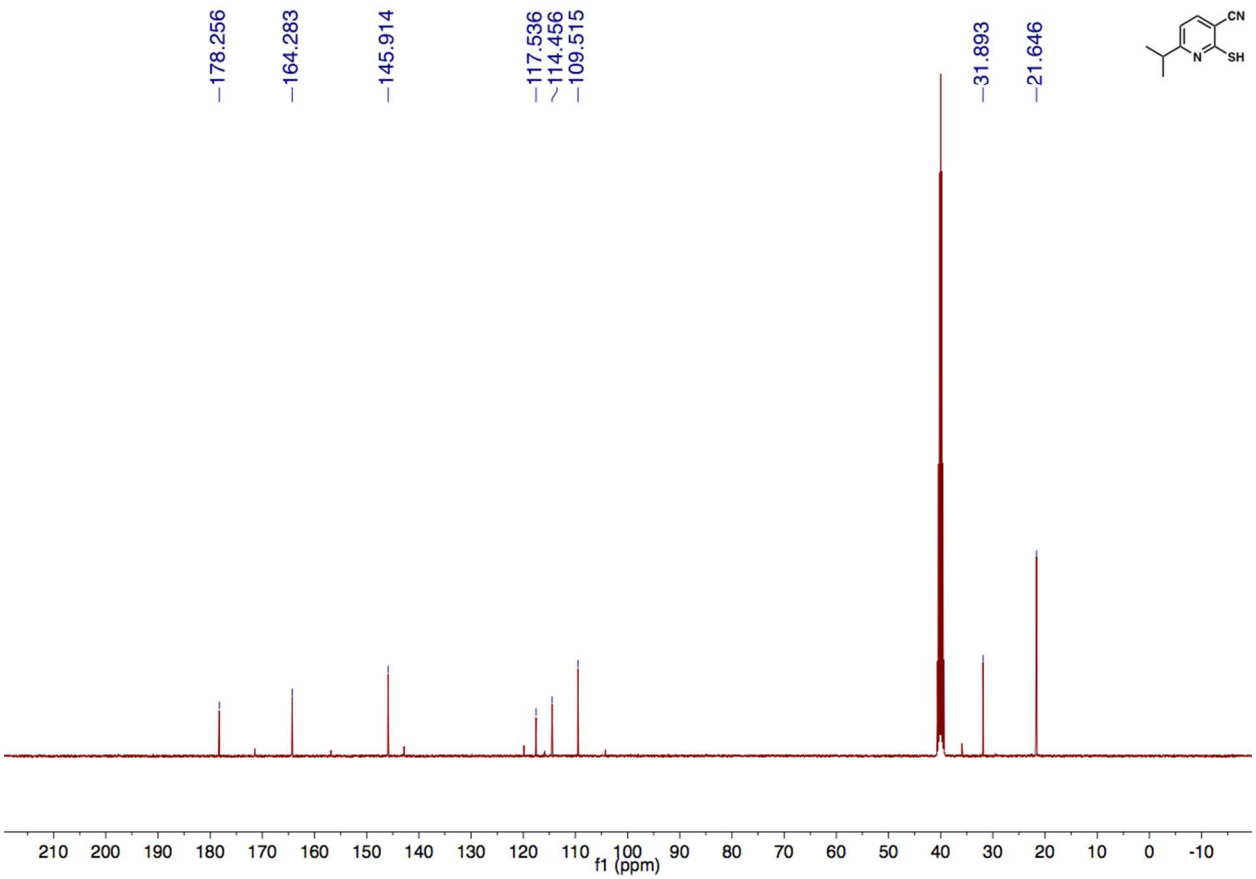

7.597
7.586
7.564
7.515
7.504
7.488
4.575
4.562
Br
O
N
H
CF3
1.00
0.99
2.00
2.06
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

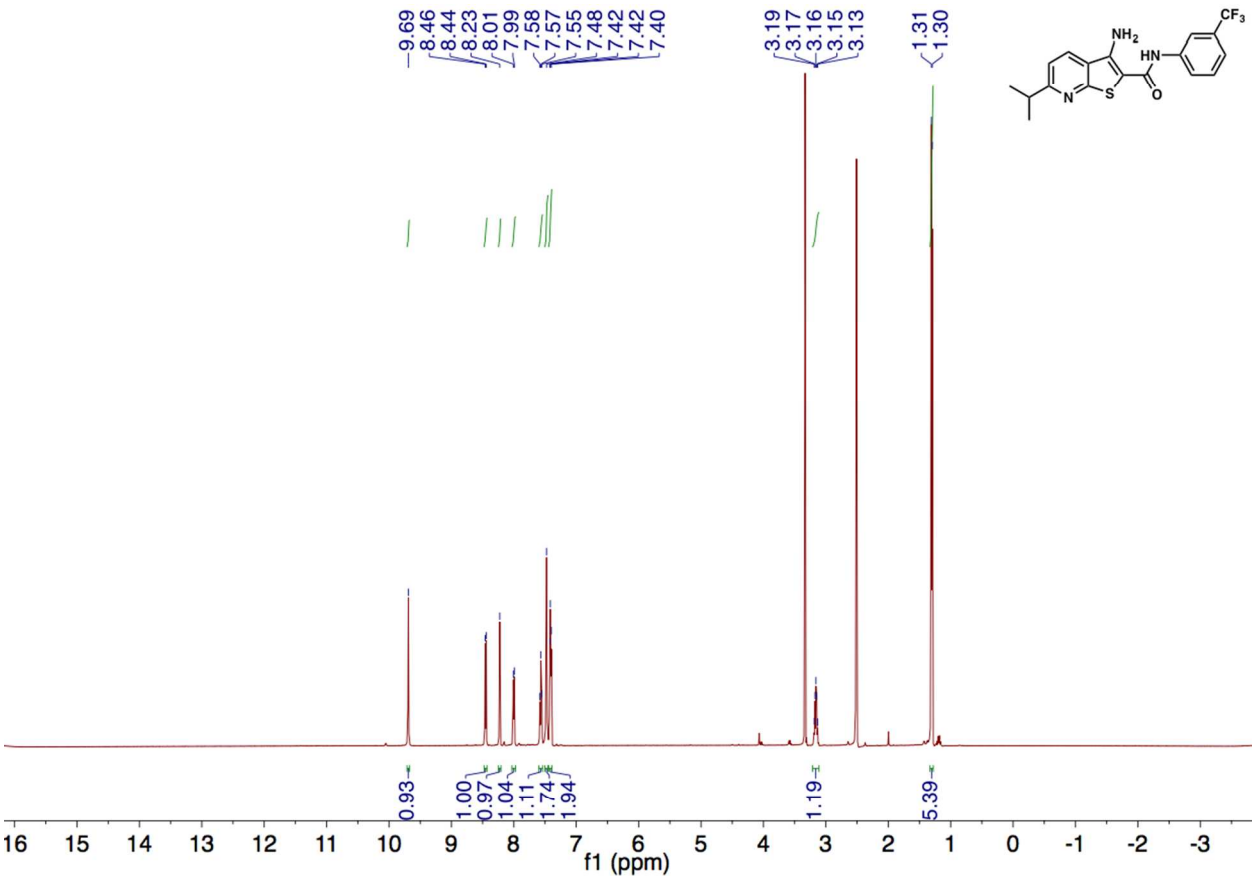

165.533
138.393
131.563
131.305
131.039
130.789
129.347
127.158
124.997
124.651
124.394
122.833
120.667
43.659
29.014
Br
O
N
H
CF3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

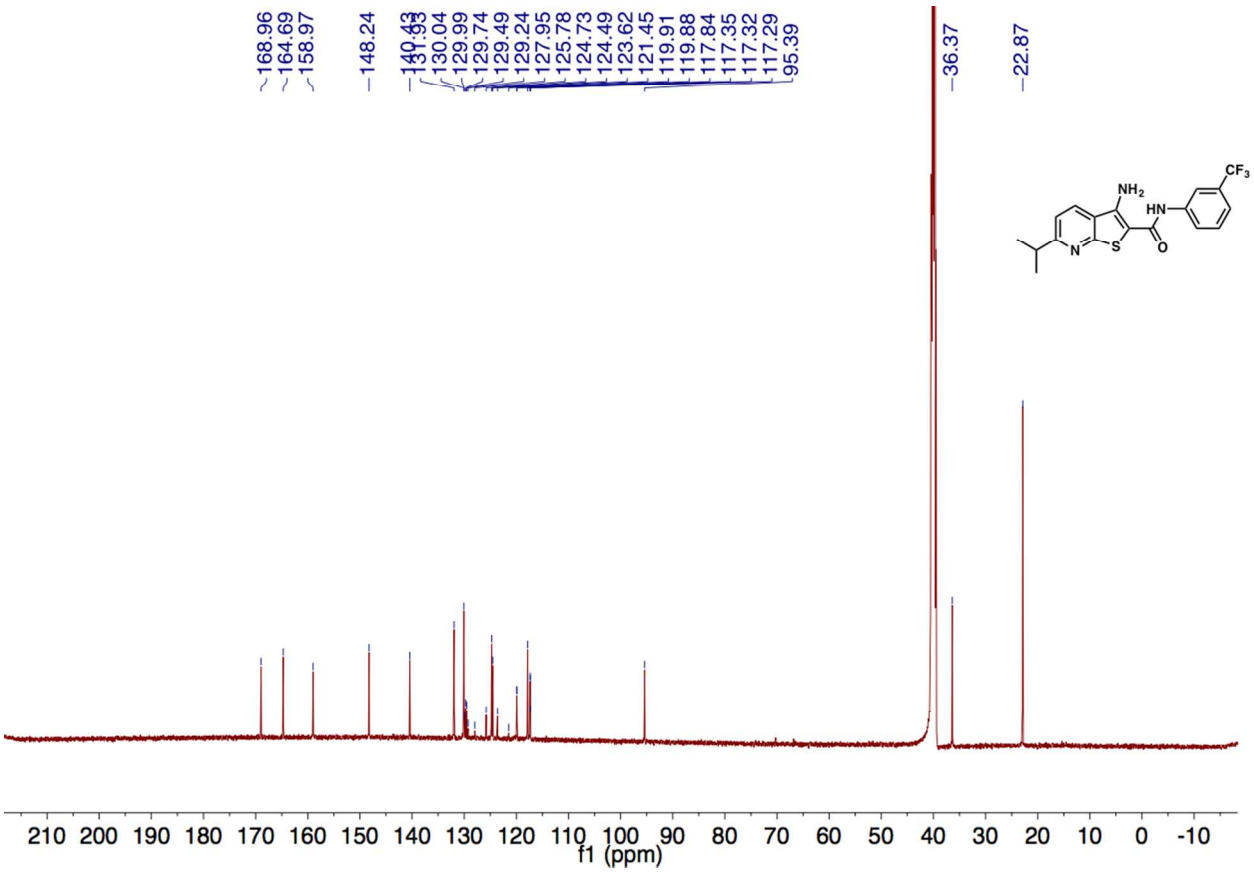

8.352
8.340
8.333
8.316
7.675
7.649
7.634
7.625
7.610
7.596
7.581
7.566
7.328
7.312
7.187
4.494
4.482
2.590
2.12
1.09
1.17
2.07
1.08
1.84
2.05
2.94
f1 (ppm)

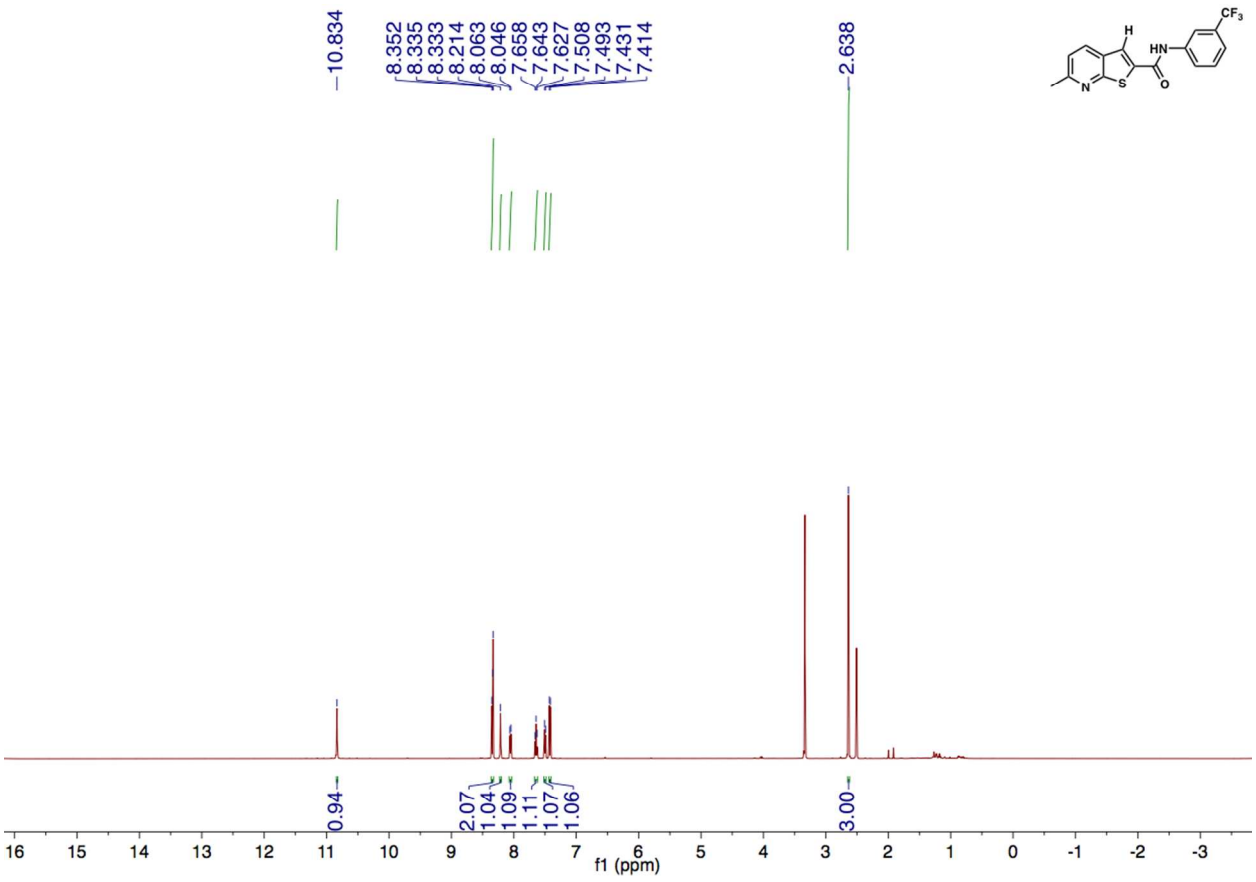

165.547
159.781
158.506
146.174
142.032
131.928
131.352
129.815
129.763
129.513
129.264
129.013
127.994
125.830
124.341
124.232
124.202
124.172
124.142
123.931
123.901
123.871
123.665
121.500
119.973
96.069
42.312
24.632
F3C
NH2
HN
O
N
S
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

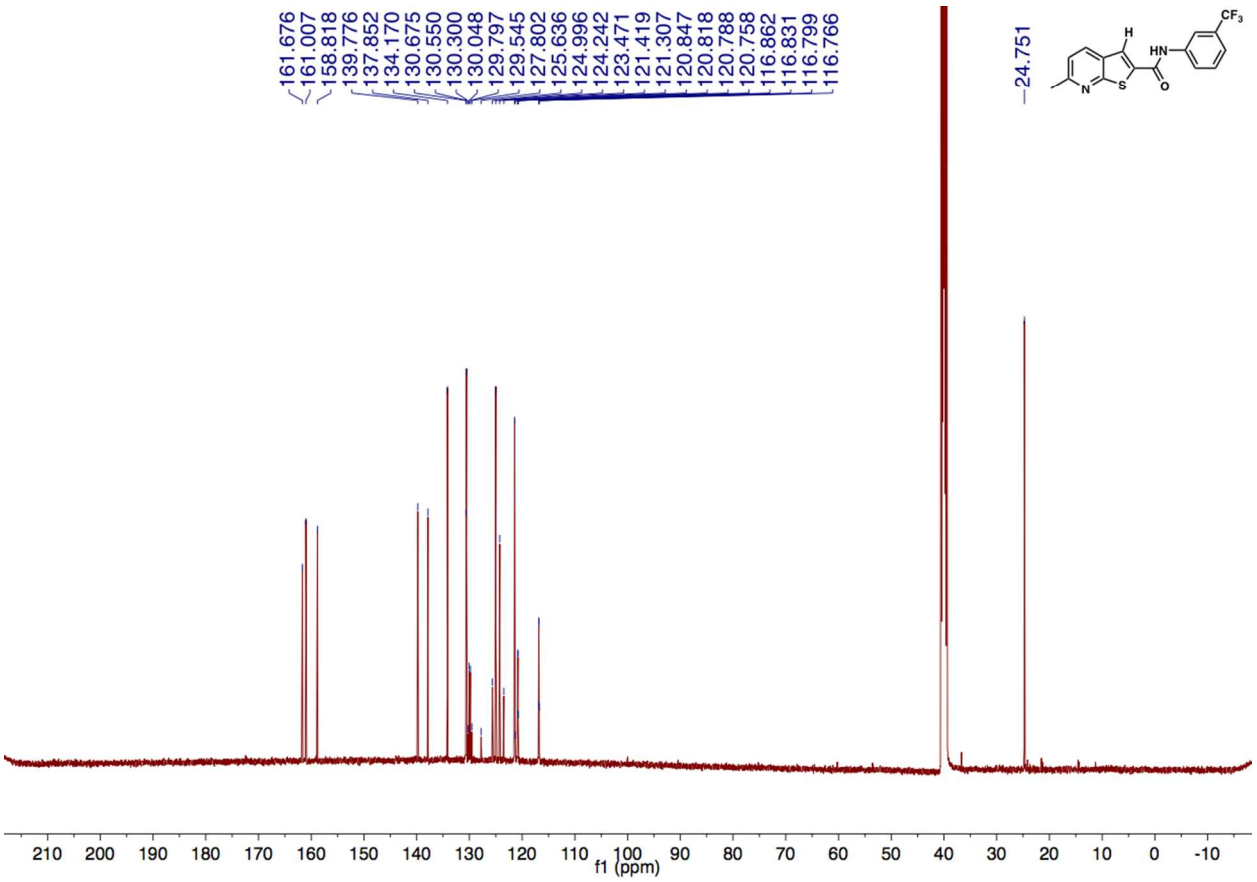

14.044
8.054
8.035
6.795
6.776
3.095
3.078
3.061
3.044
3.026
1.208
1.191
CN
N
SH
0.81
1.00
1.02
1.05
6.38
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)

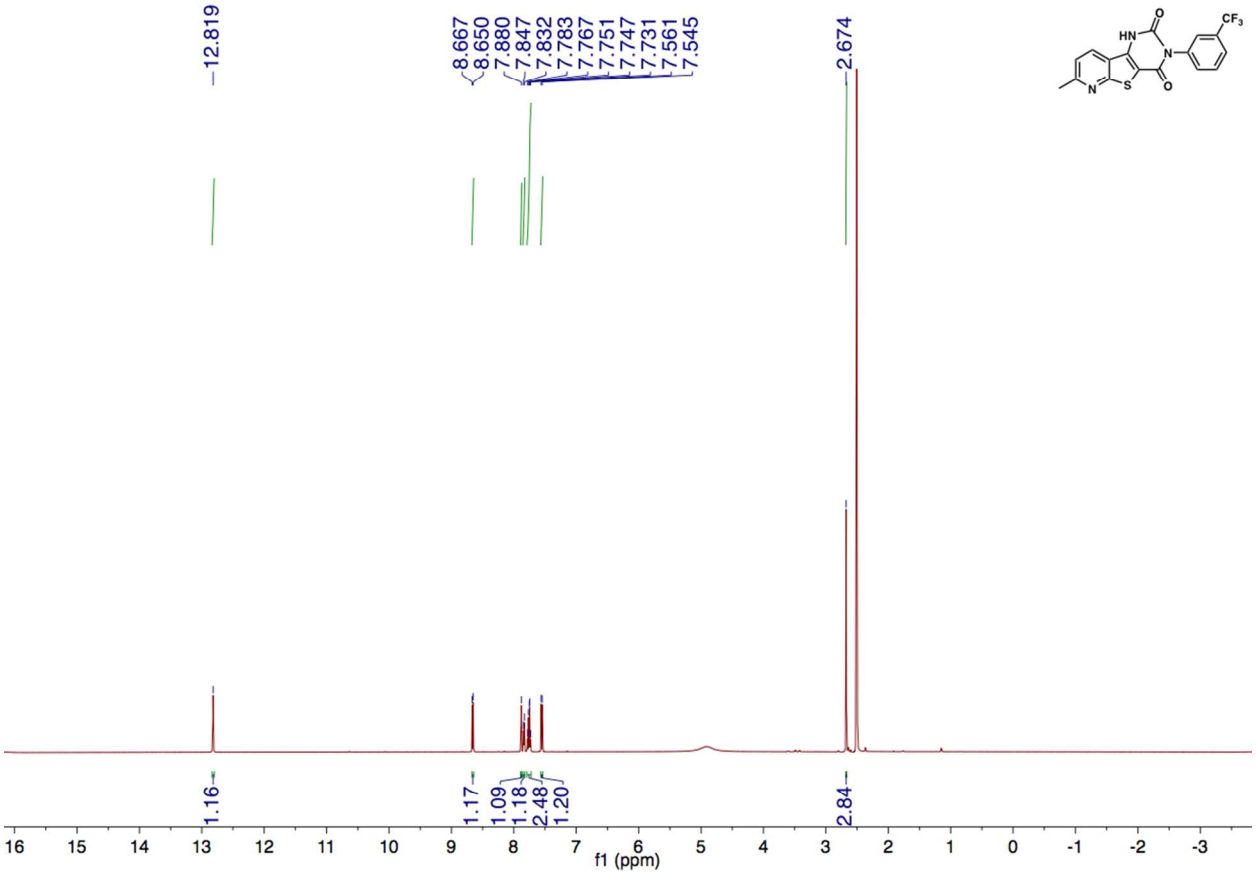

178.256
164.283
145.914
117.536
114.456
109.515
31.893
21.646
CN
N
SH
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

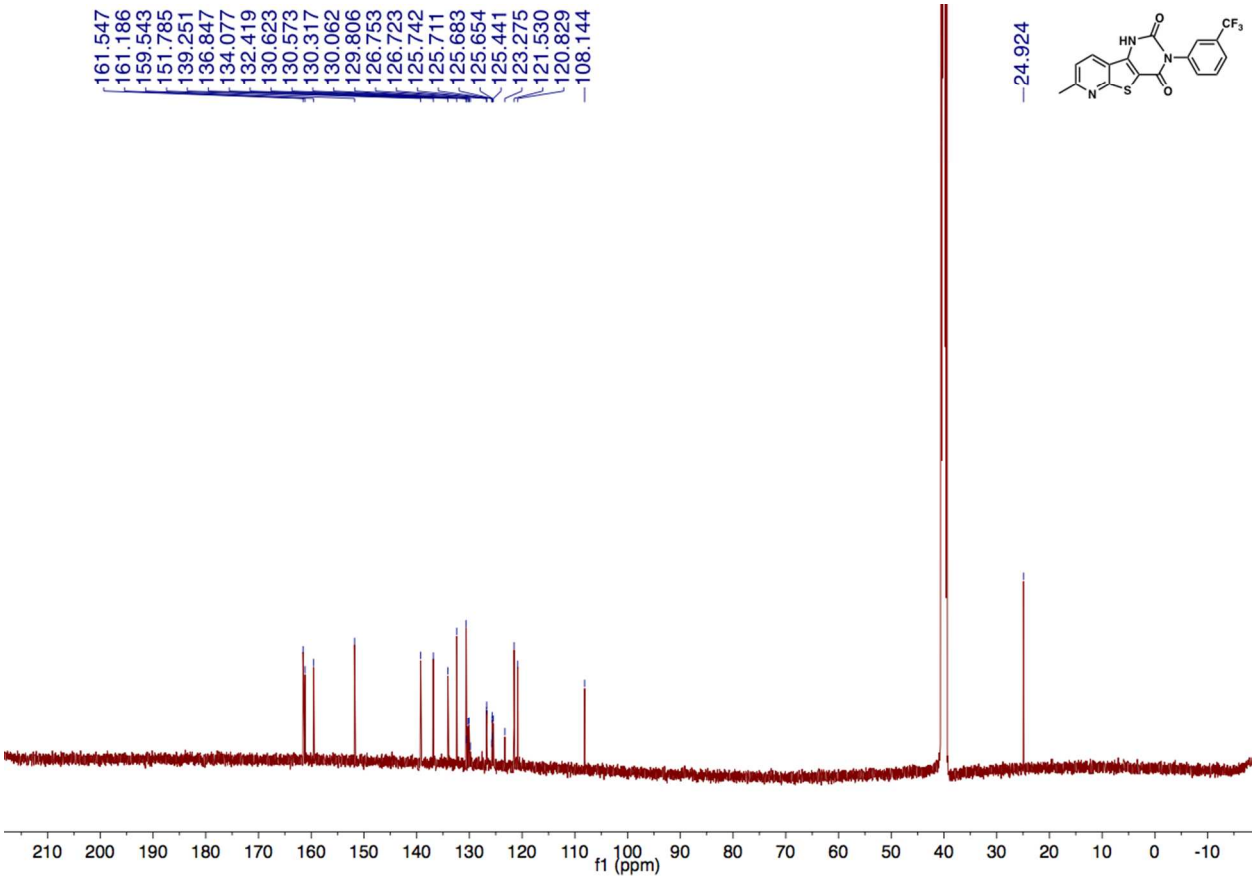

9.69
8.46
8.44
8.23
8.01
7.99
7.58
7.57
7.55
7.48
7.42
7.42
7.40
3.19
3.17
3.16
3.15
3.13
1.31
1.30
NH2
HN
CF3
N
S
O
0.93
1.00
0.97
1.04
1.11
1.74
1.94
1.19
5.39
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

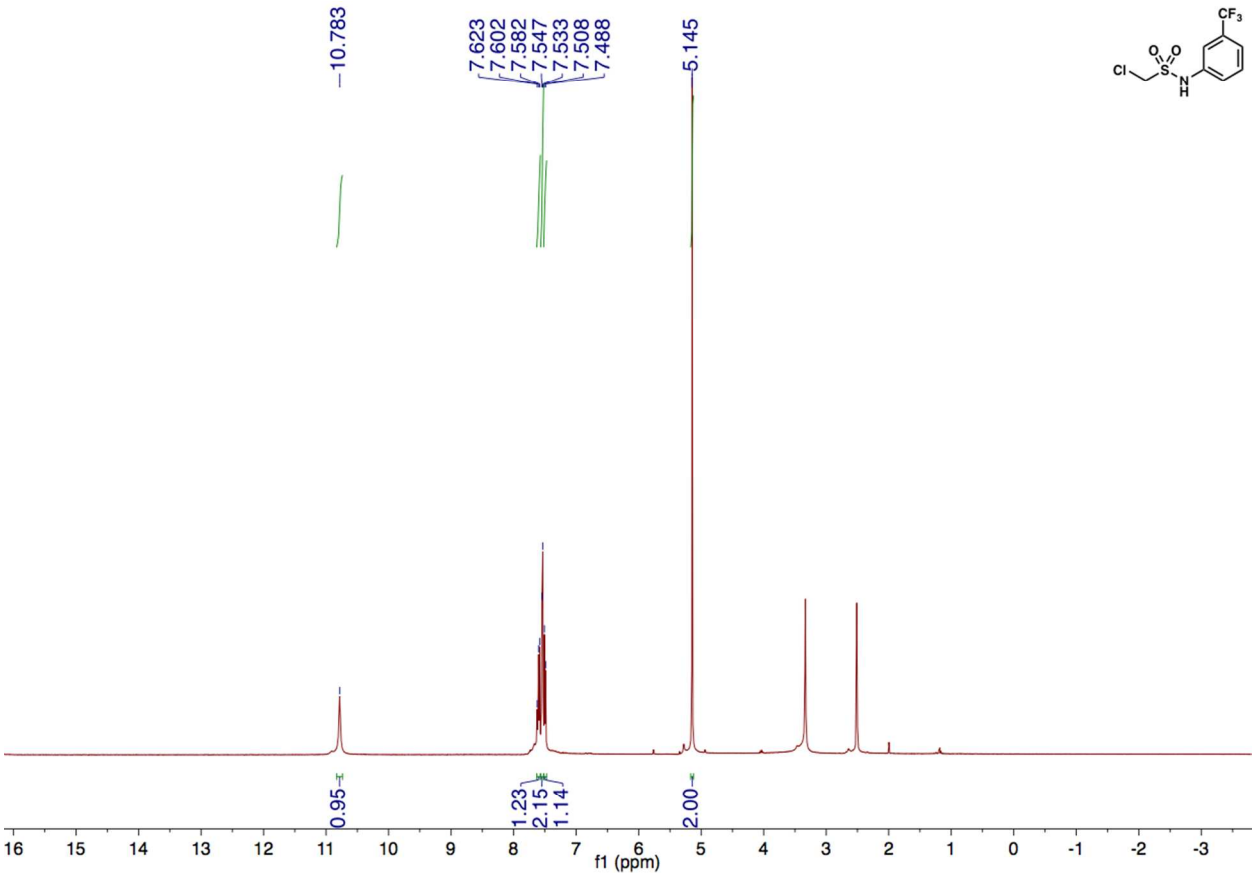

168.96
164.69
158.97
148.24
140.43
131.93
130.04
129.99
129.74
129.49
129.24
127.95
125.78
124.73
124.49
123.62
121.45
119.91
119.88
117.84
117.35
117.32
117.29
95.39
36.37
22.87
NH2
HN
O
N
S
CF3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

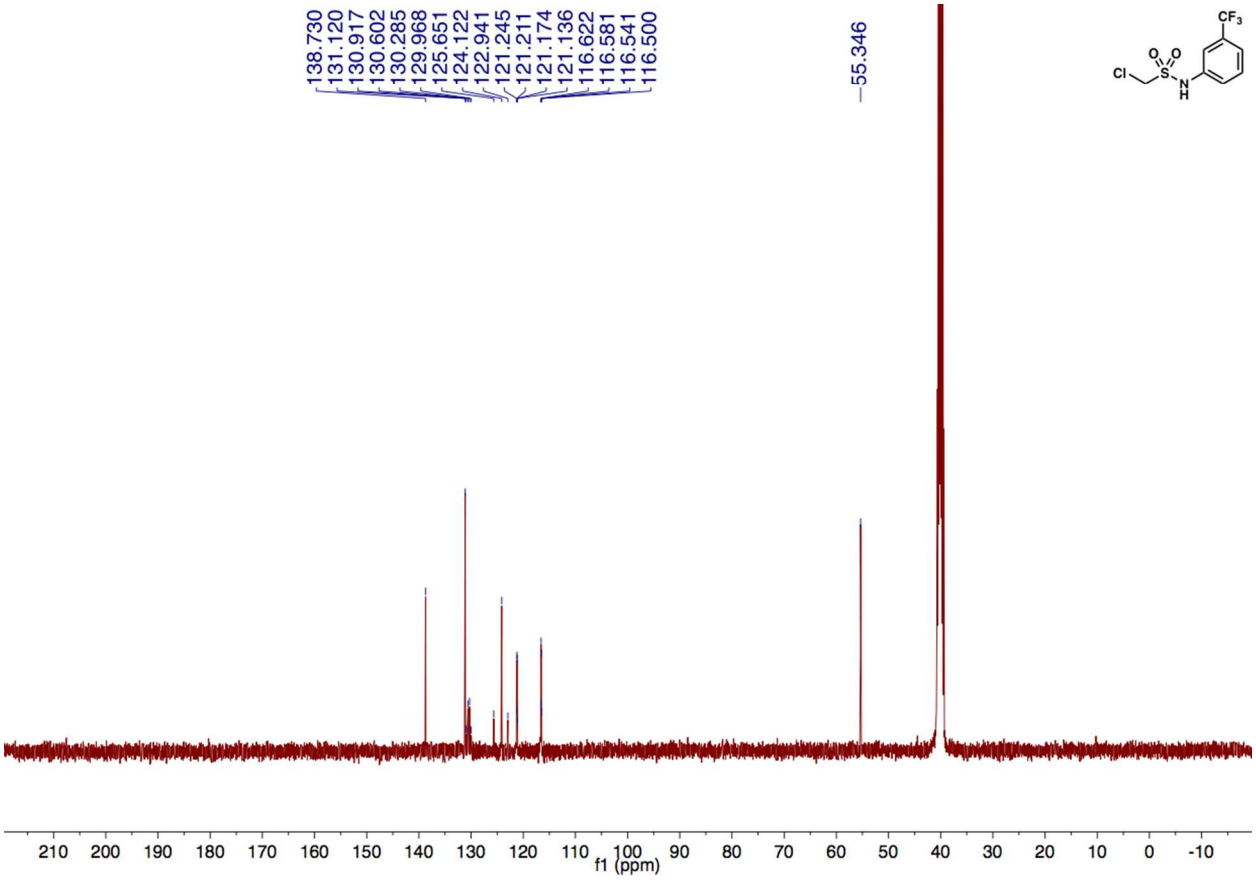

10.834
8.352
8.335
8.333
8.214
8.063
8.046
7.658
7.643
7.627
7.508
7.493
7.431
7.414
2.638
CF3
H
HN
O
S
N
0.94
2.07
1.04
1.09
1.11
1.07
1.06
3.00
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)

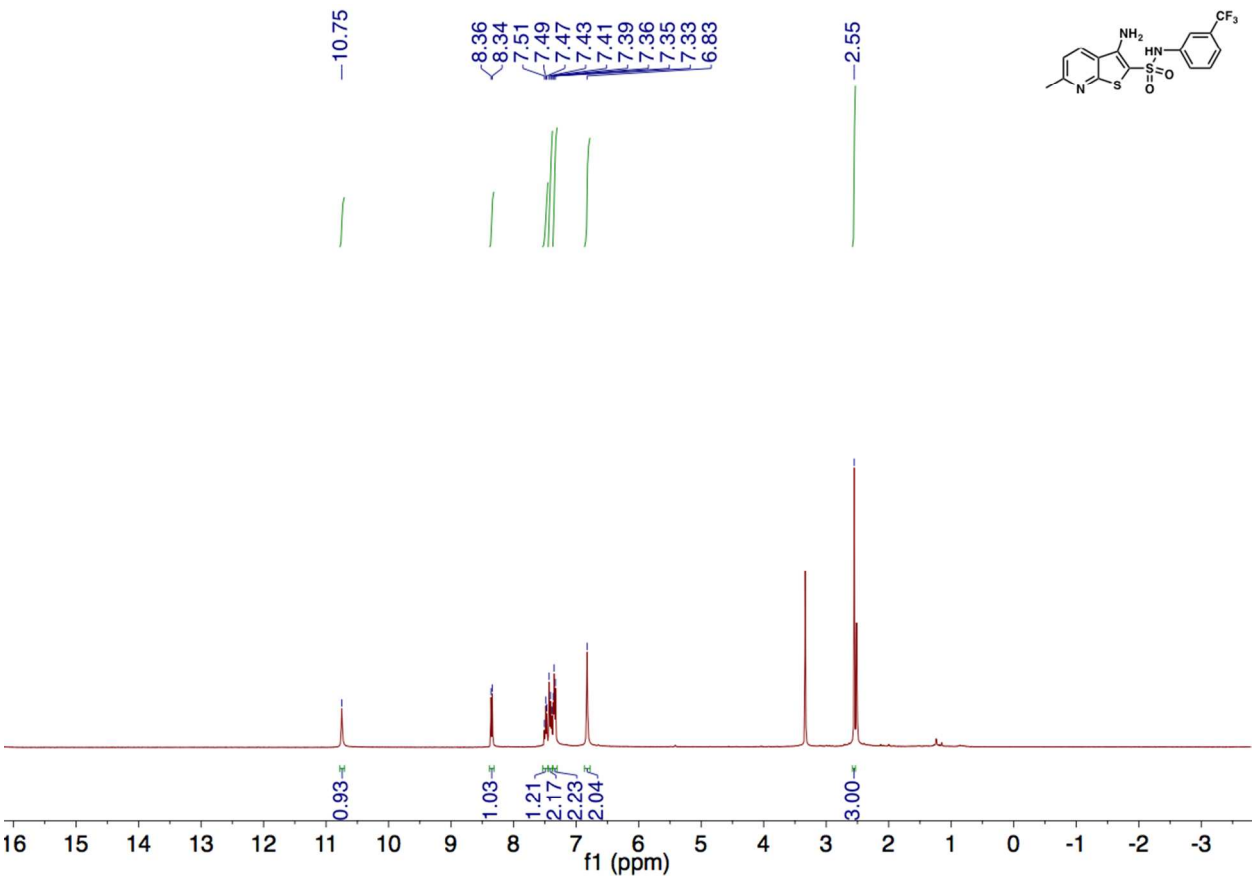

161.676
161.007
158.818
139.776
137.852
134.170
130.675
130.550
130.300
130.048
129.797
129.545
127.802
125.636
124.996
124.242
123.471
121.419
121.307
120.847
120.818
120.788
120.758
116.862
116.831
116.799
116.766
24.751
H
HN
O
S
N
CF3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

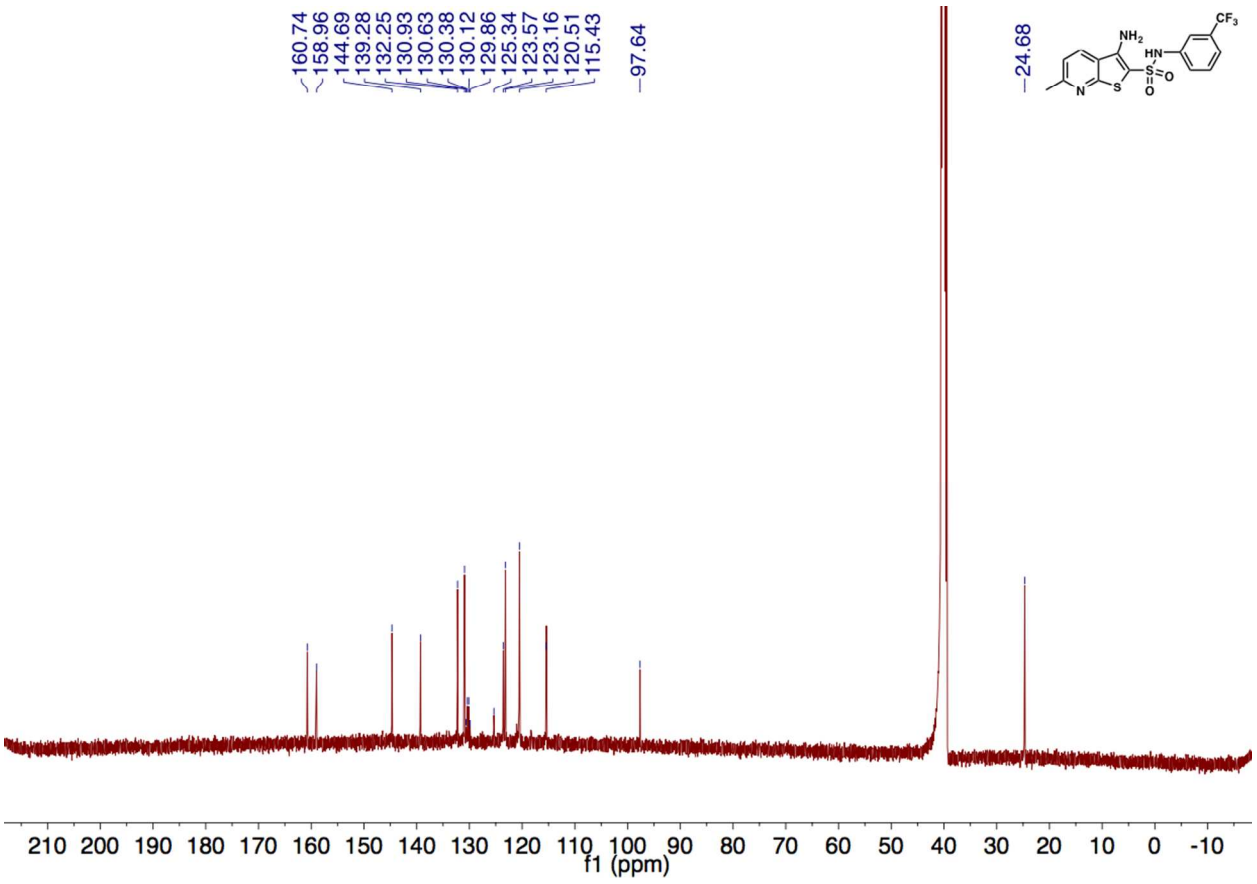

12.819
8.667
8.650
7.880
7.847
7.832
7.783
7.767
7.751
7.747
7.731
7.561
7.545
2.674
1.16
1.17
1.09
1.18
2.48
1.20
2.84
f1 (ppm)

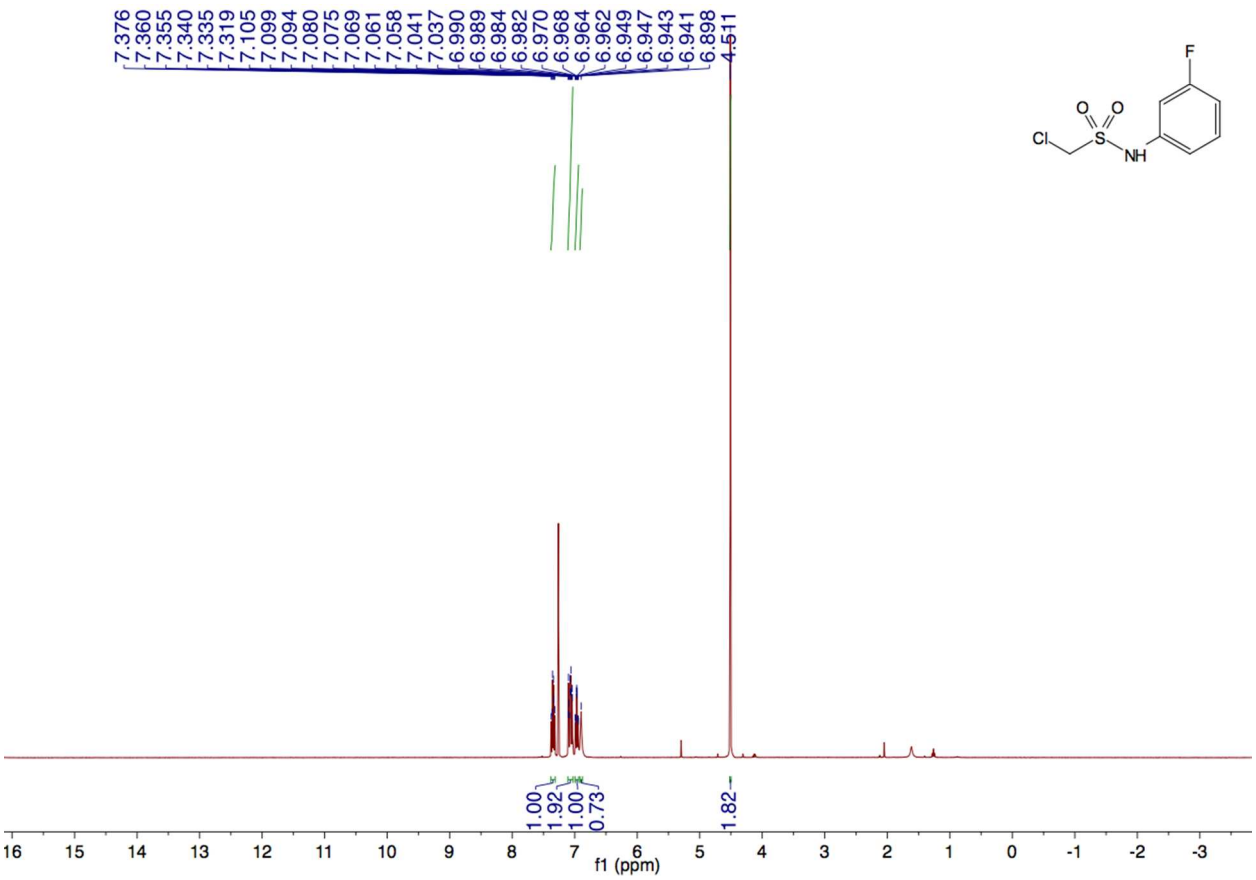

161.547
161.186
159.543
151.785
139.251
136.847
134.077
132.419
130.623
130.573
130.317
130.062
129.806
126.753
126.723
125.742
125.711
125.683
125.654
125.441
123.275
121.530
120.829
108.144
24.924
HN
O
N
S
O
N
CF3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

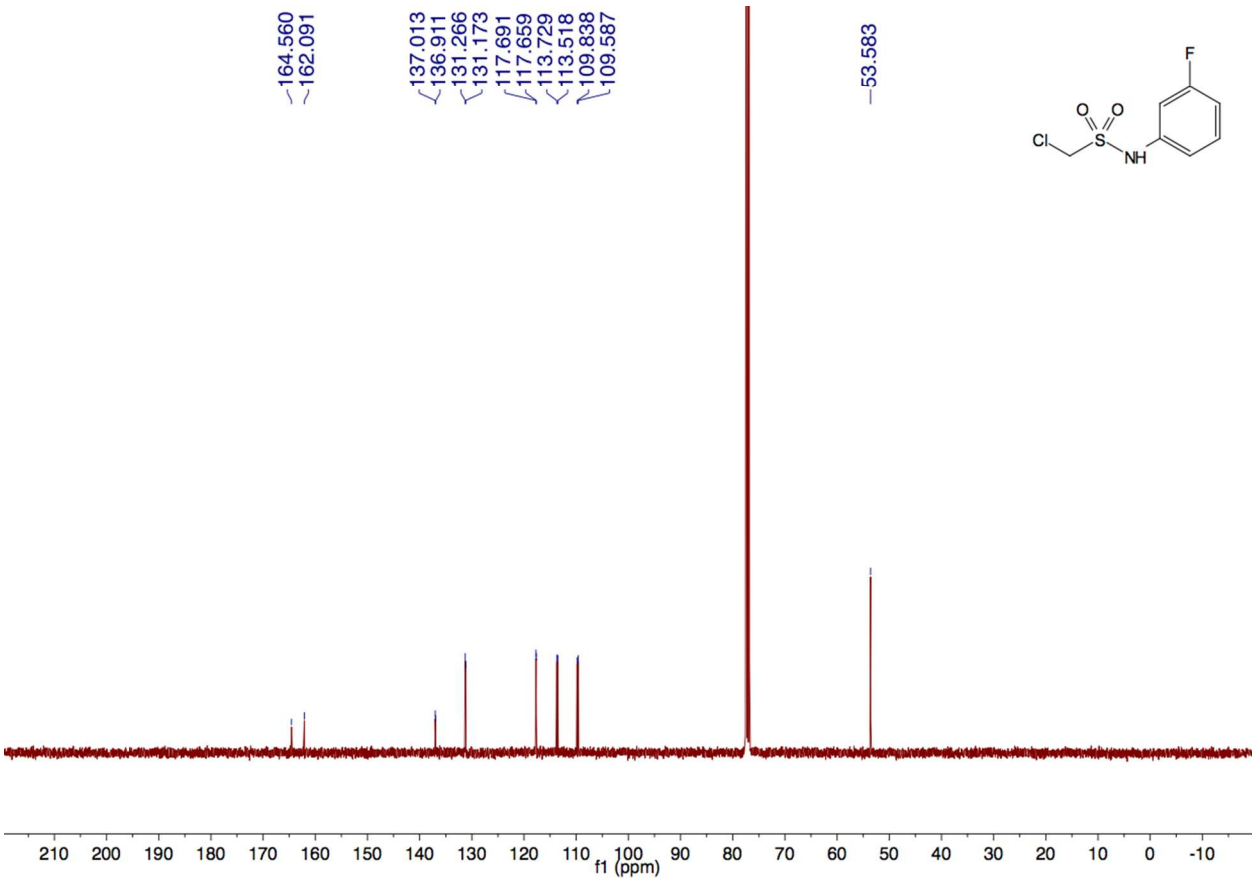

10.783
7.623
7.602
7.582
7.547
7.533
7.508
7.488
5.145
0.95
1.23
2.15
1.14
2.00
f1 (ppm)

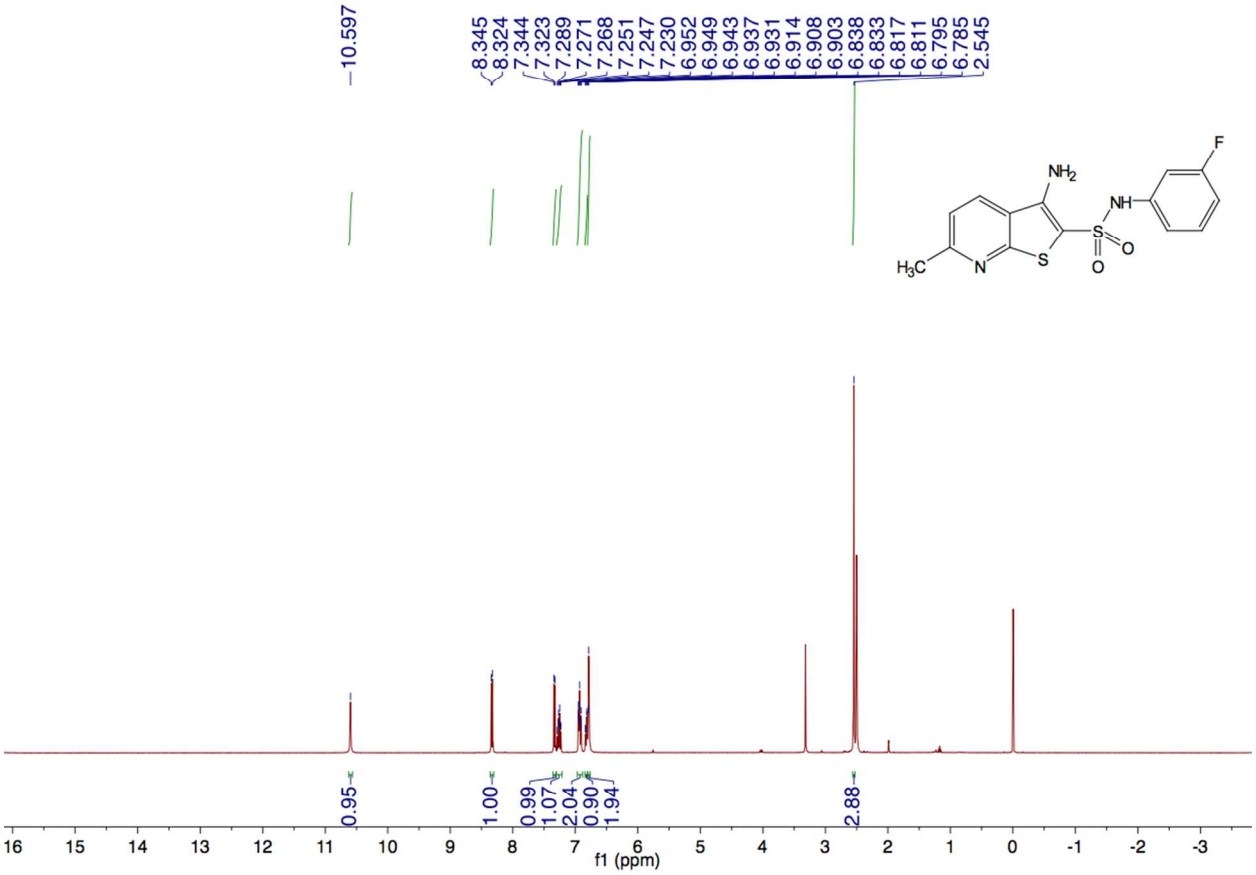

138.730
131.120
130.917
130.602
130.285
129.968
125.651
124.122
122.941
121.245
121.211
121.174
121.136
116.622
116.581
116.541
116.500
55.346
CF3
Cl
S
O
O
N
H
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

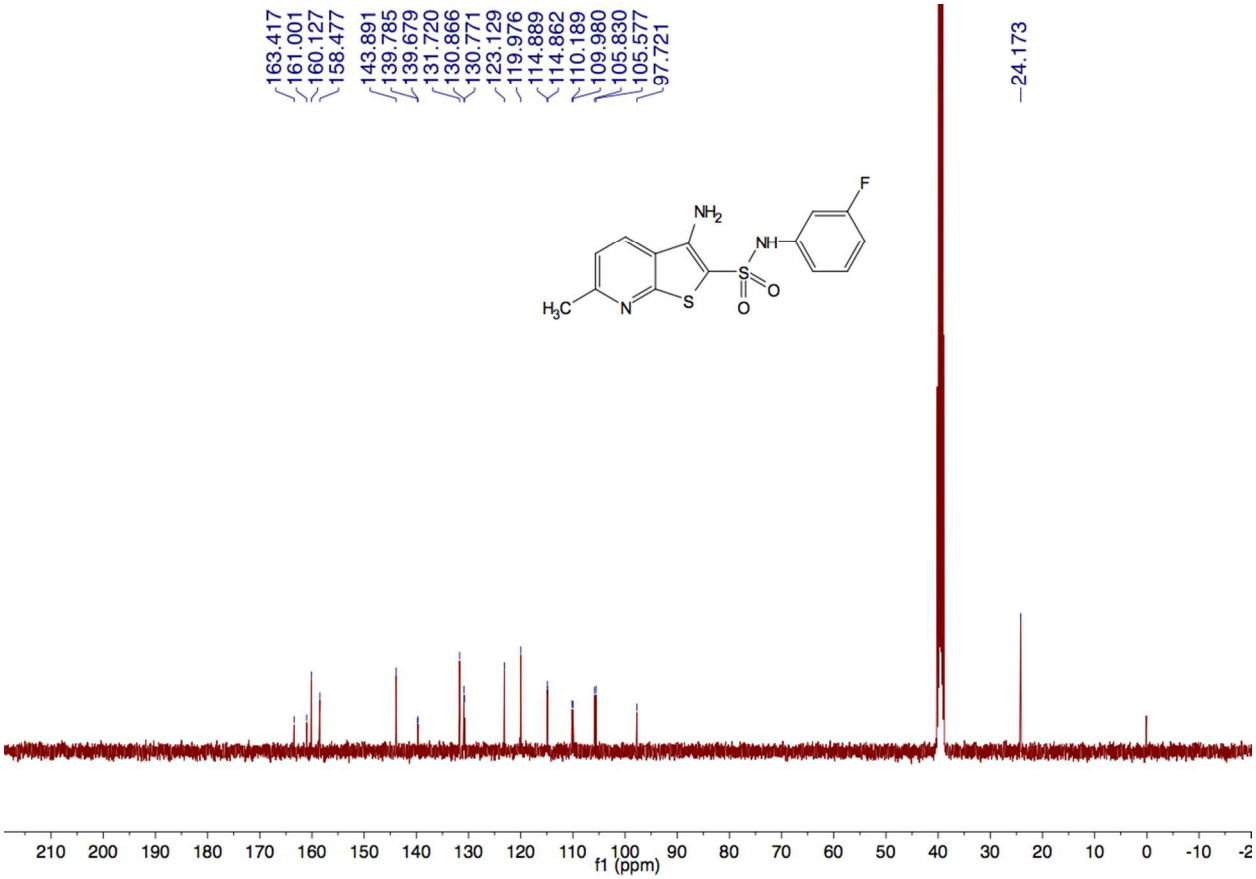

10.75
8.36
8.34
7.51
7.49
7.47
7.43
7.41
7.39
7.36
7.35
7.33
6.83
2.55
NH2
HN
S
O
O
N
S
CF3
0.93
1.03
1.21
2.17
2.23
2.04
3.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

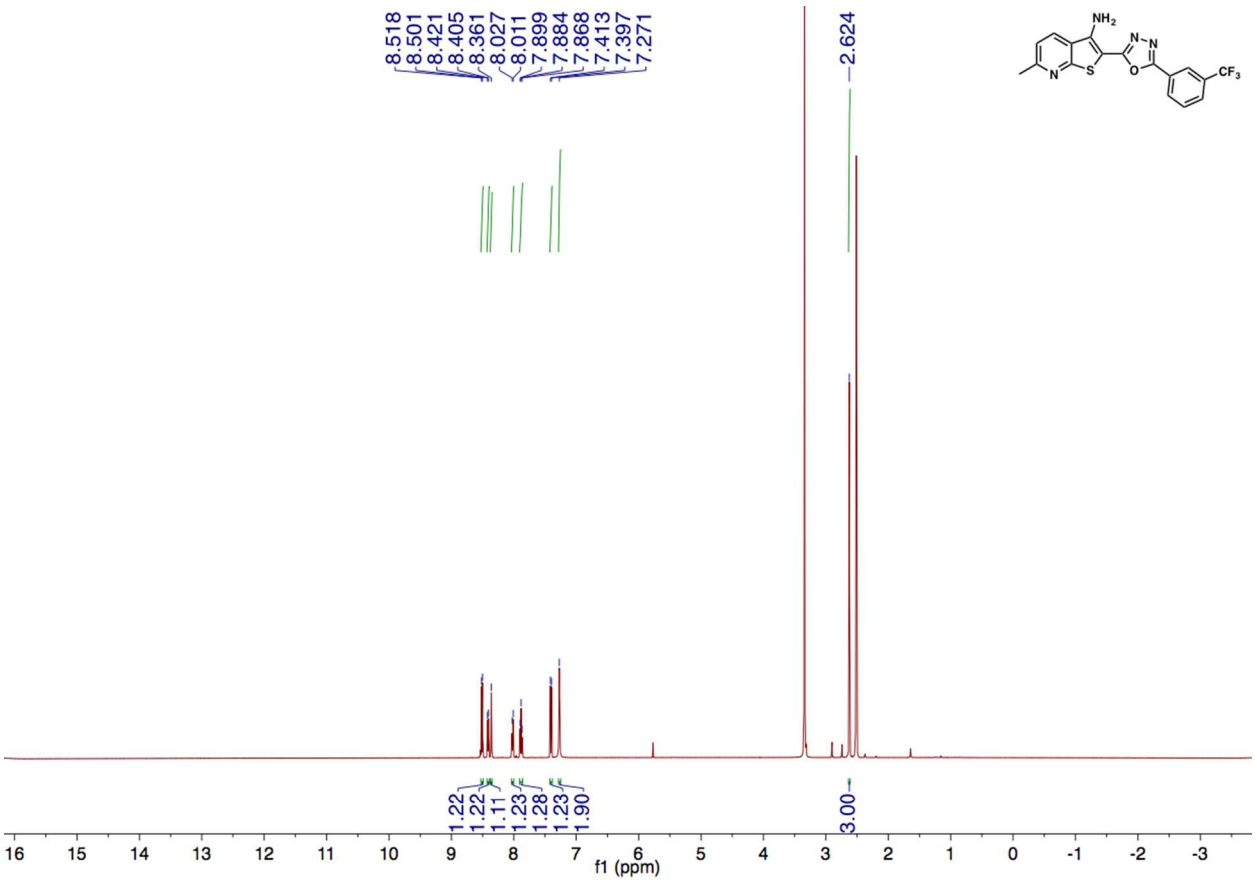

160.74
158.96
144.69
139.28
132.25
130.93
130.63
130.38
130.12
129.86
125.34
123.57
123.16
120.51
115.43
97.64
24.68
NH2
HN
S
O
O
N
S
CF3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

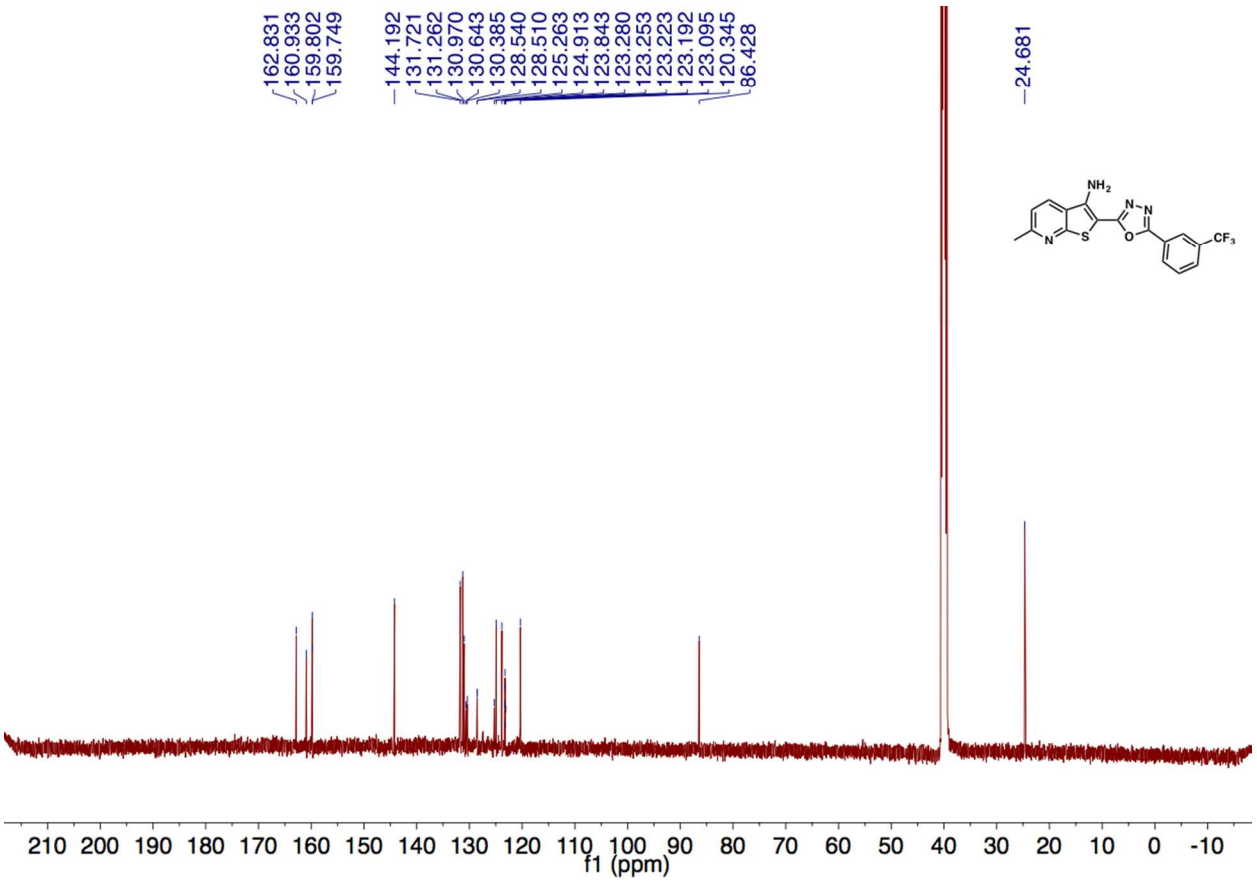

7.376
7.360
7.355
7.340
7.335
7.319
7.105
7.099
7.094
7.080
7.075
7.069
7.061
7.058
7.041
7.037
6.990
6.989
6.984
6.982
6.970
6.968
6.964
6.962
6.949
6.947
6.943
6.941
6.898
4.511
F
O
O
Cl
S
NH
1.00
1.92
1.00
0.73
1.82
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)

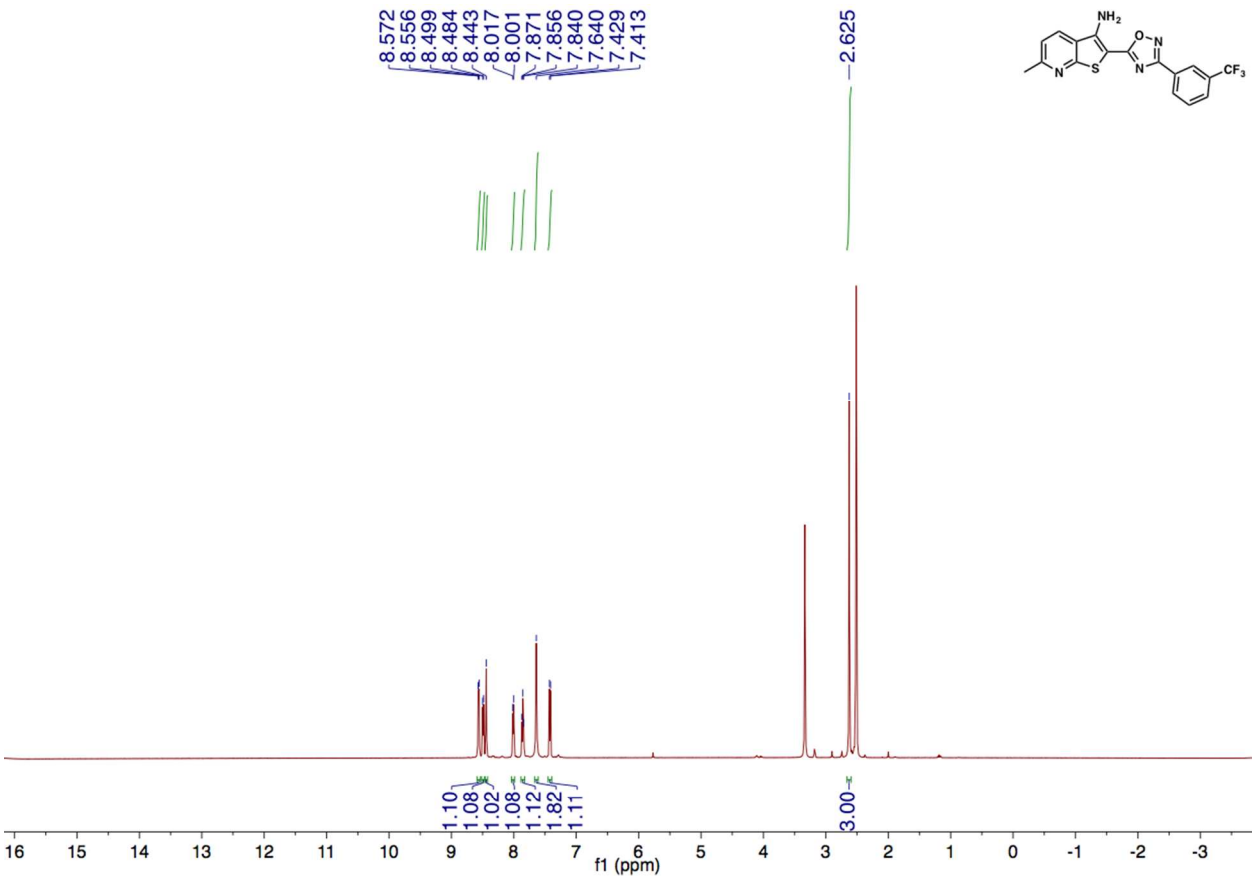

164.560
162.091
137.013
136.911
131.266
131.173
117.691
117.659
113.729
113.518
109.838
109.587
53.583
F
O
O
S
Cl
NH
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

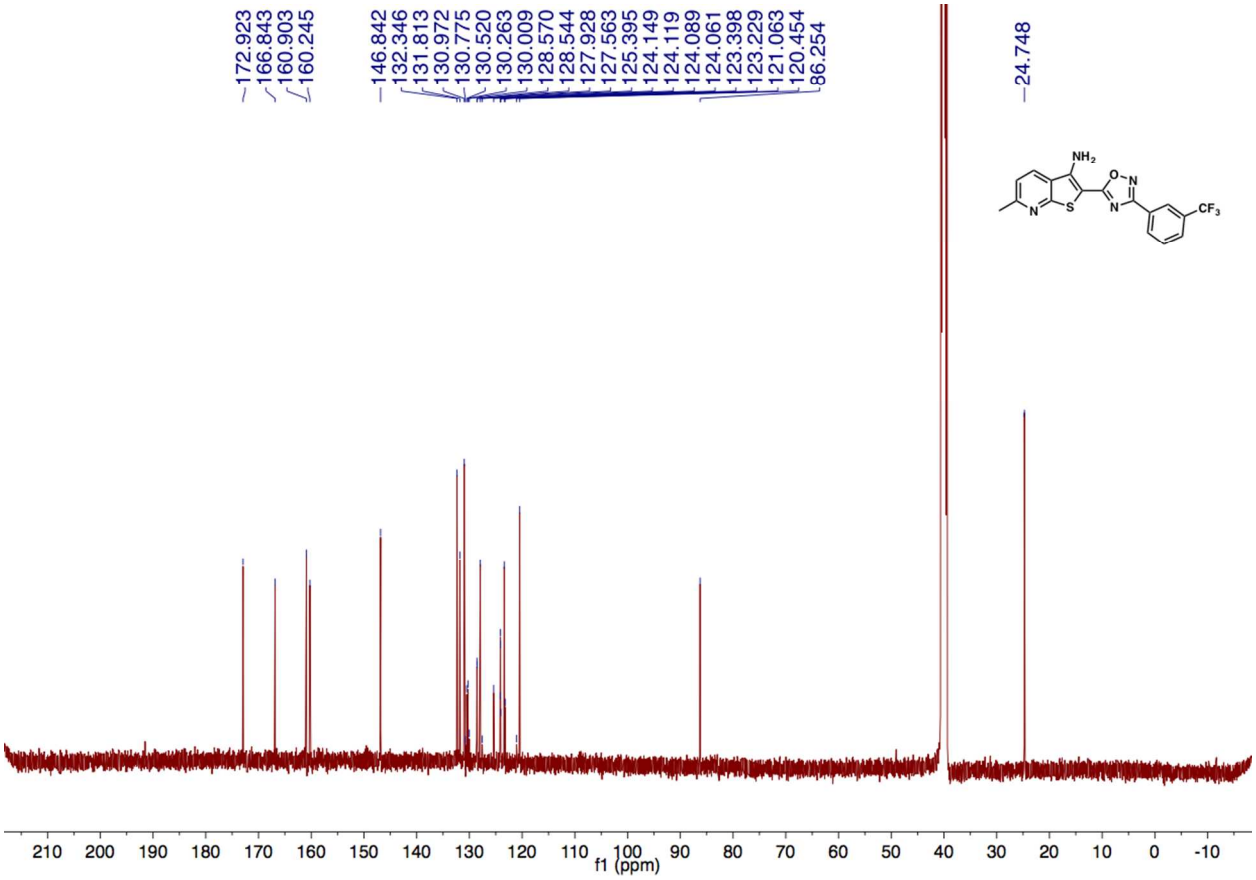

10.597
8.345
8.324
7.344
7.323
7.289
7.271
7.268
7.251
7.247
7.230
6.952
6.949
6.943
6.937
6.931
6.914
6.908
6.903
6.838
6.833
6.817
6.811
6.795
6.785
2.545
NH2
NH
F
S
O
O
H3C
N
S
0.95
1.00
0.99
1.07
2.04
0.90
1.94
2.88
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

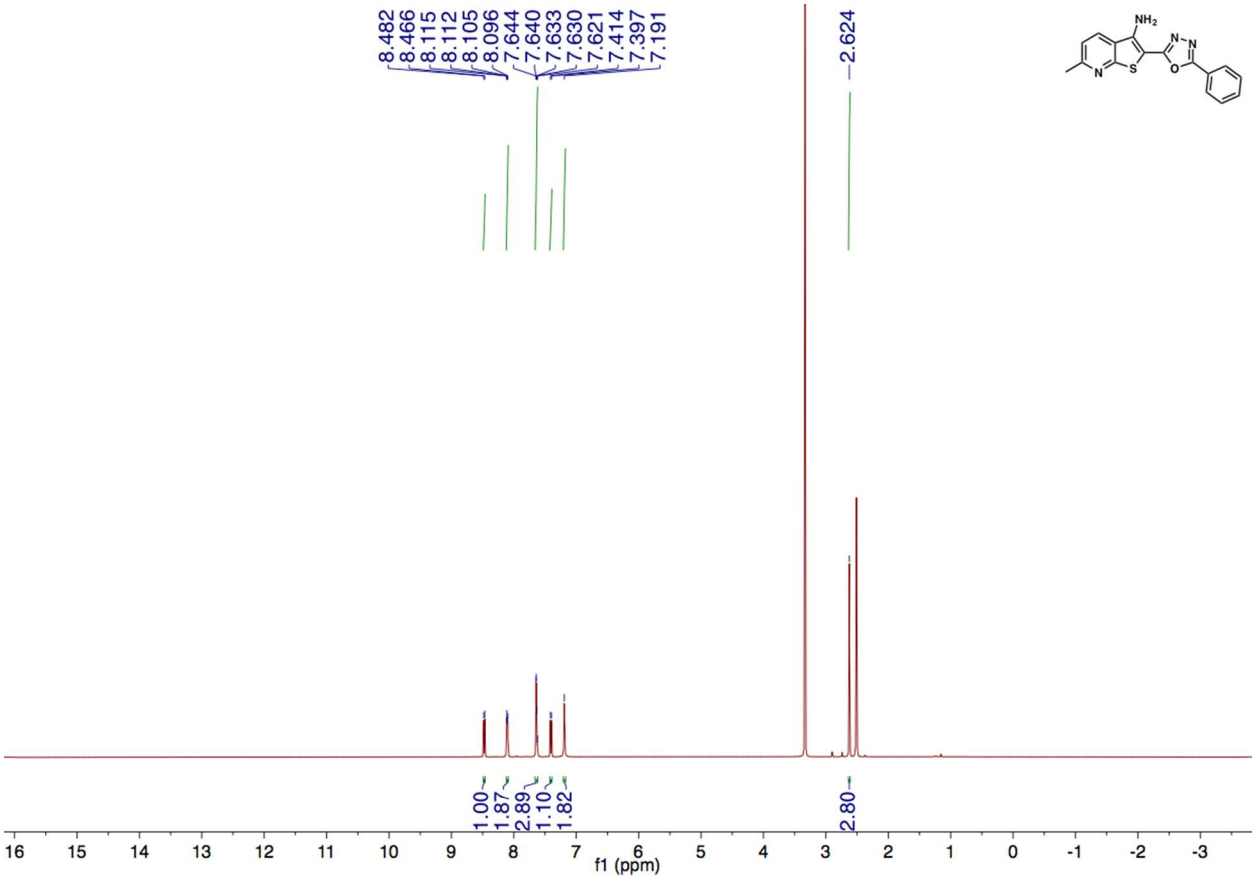

163.417
161.001
160.127
158.477
143.891
139.785
139.679
131.720
130.866
130.771
123.129
119.976
114.889
114.862
110.189
109.980
105.830
105.577
97.721
24.173
NH2
NH
F
S
O
O
H3C
N
S
f1 (ppm)

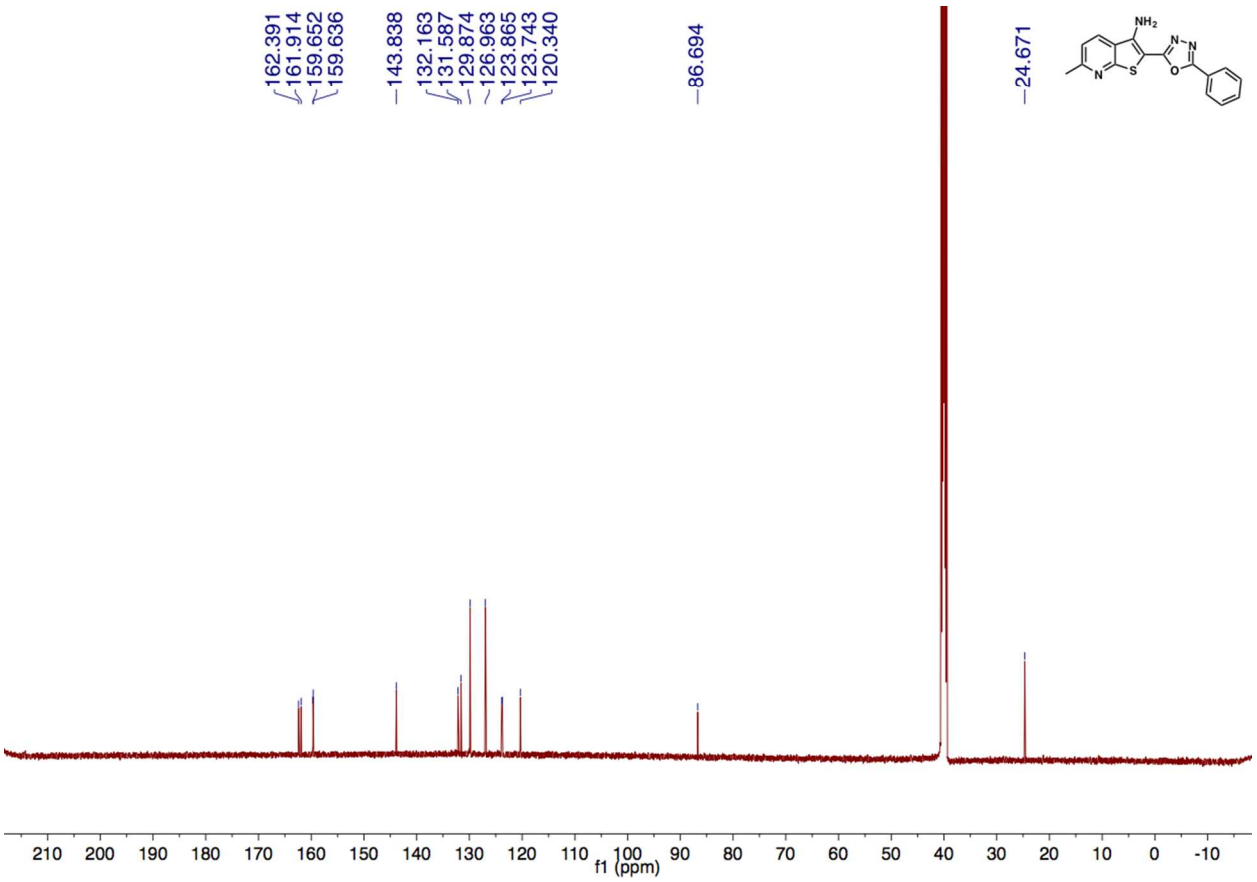

8.518
8.501
8.421
8.405
8.361
8.027
8.011
7.899
7.884
7.868
7.413
7.397
7.271
2.624
NH2
N
S
O
N
N
CF3
1.22
1.22
1.11
1.23
1.28
1.23
1.90
3.00
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)

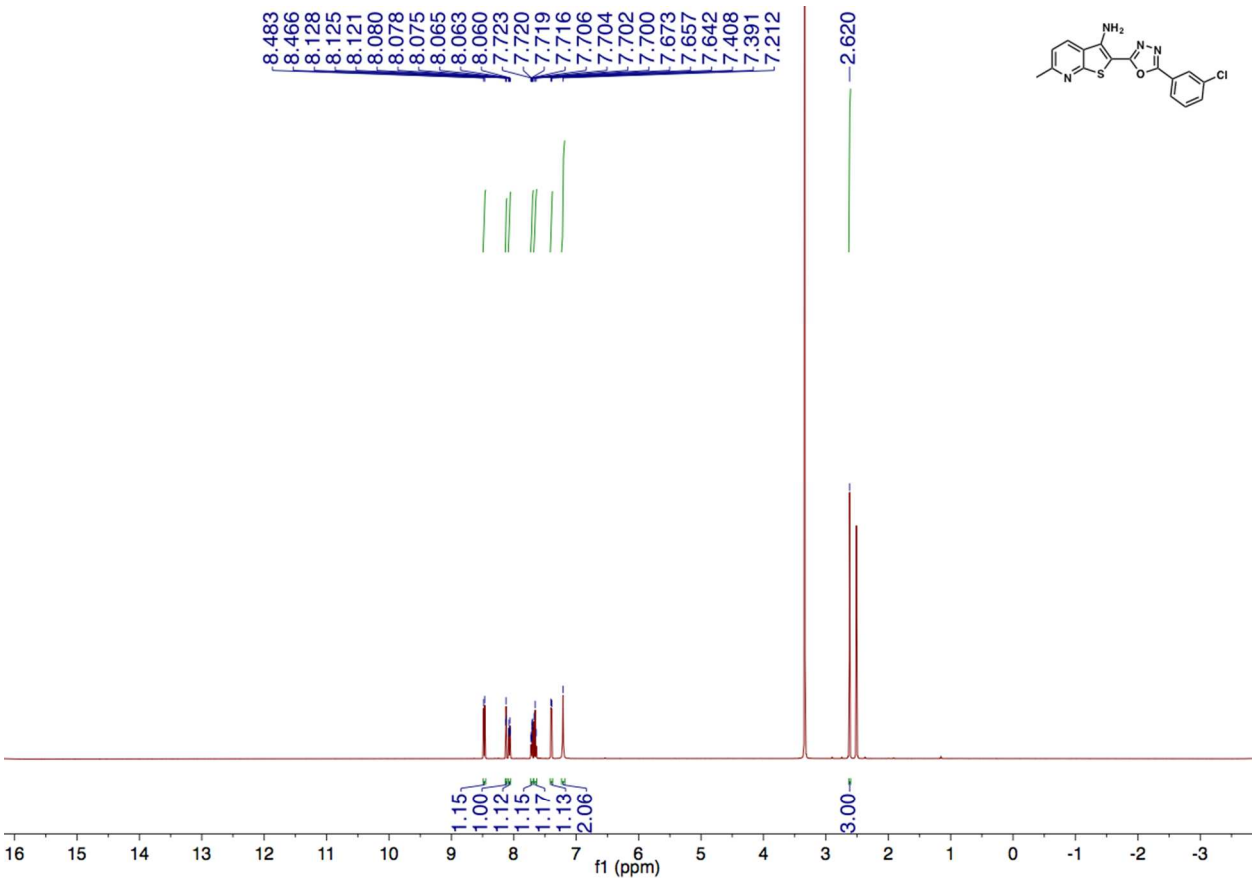

162.831
160.933
159.802
159.749
144.192
131.721
131.262
130.970
130.643
130.385
128.540
128.510
125.263
124.913
123.843
123.280
123.253
123.223
123.192
123.095
120.345
86.428
24.681
NH2
N
S
O
N
N
CF3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

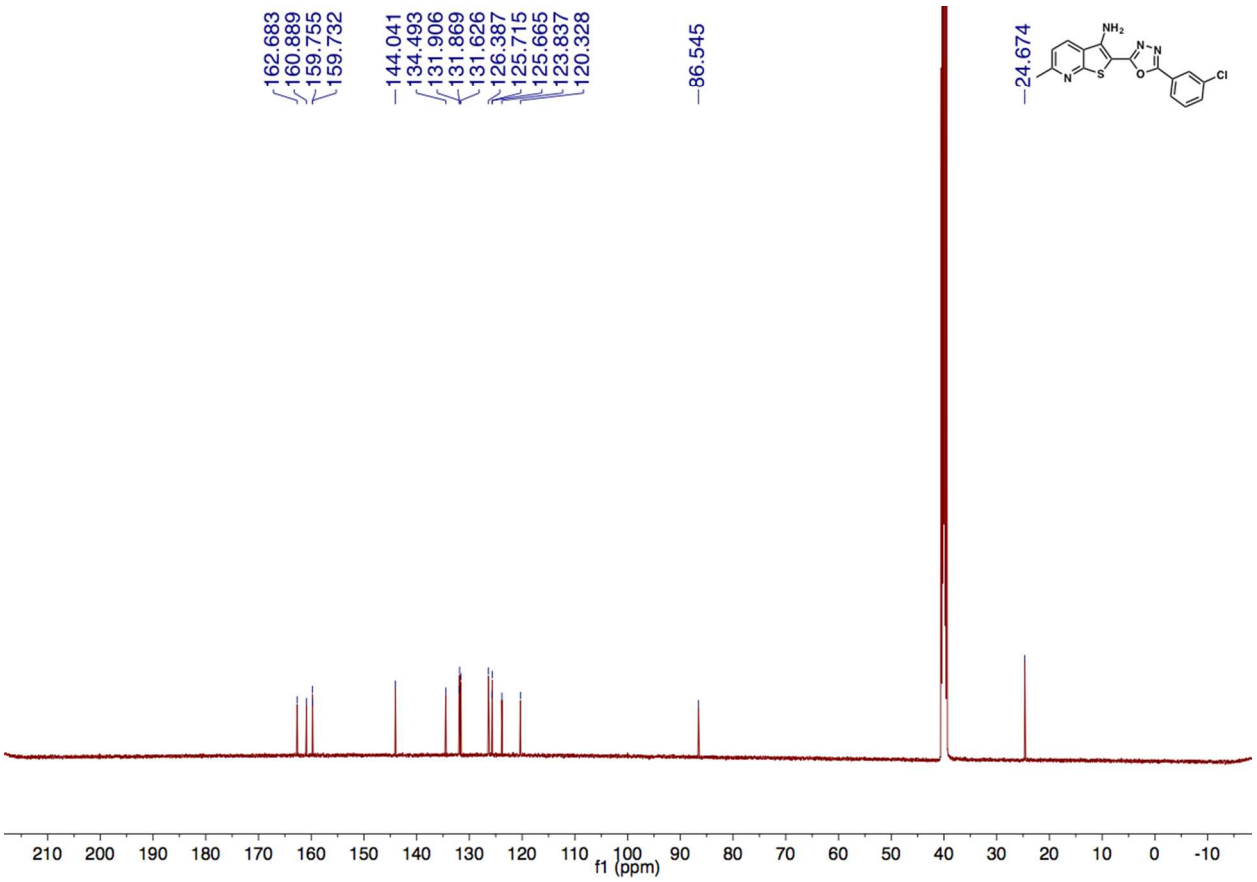

8.572
8.556
8.499
8.484
8.443
8.017
8.001
7.871
7.856
7.840
7.640
7.429
7.413
2.625
NH2
O
N
N
S
N
CF3
1.10
1.08
1.02
1.08
1.12
1.82
1.11
3.00
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)

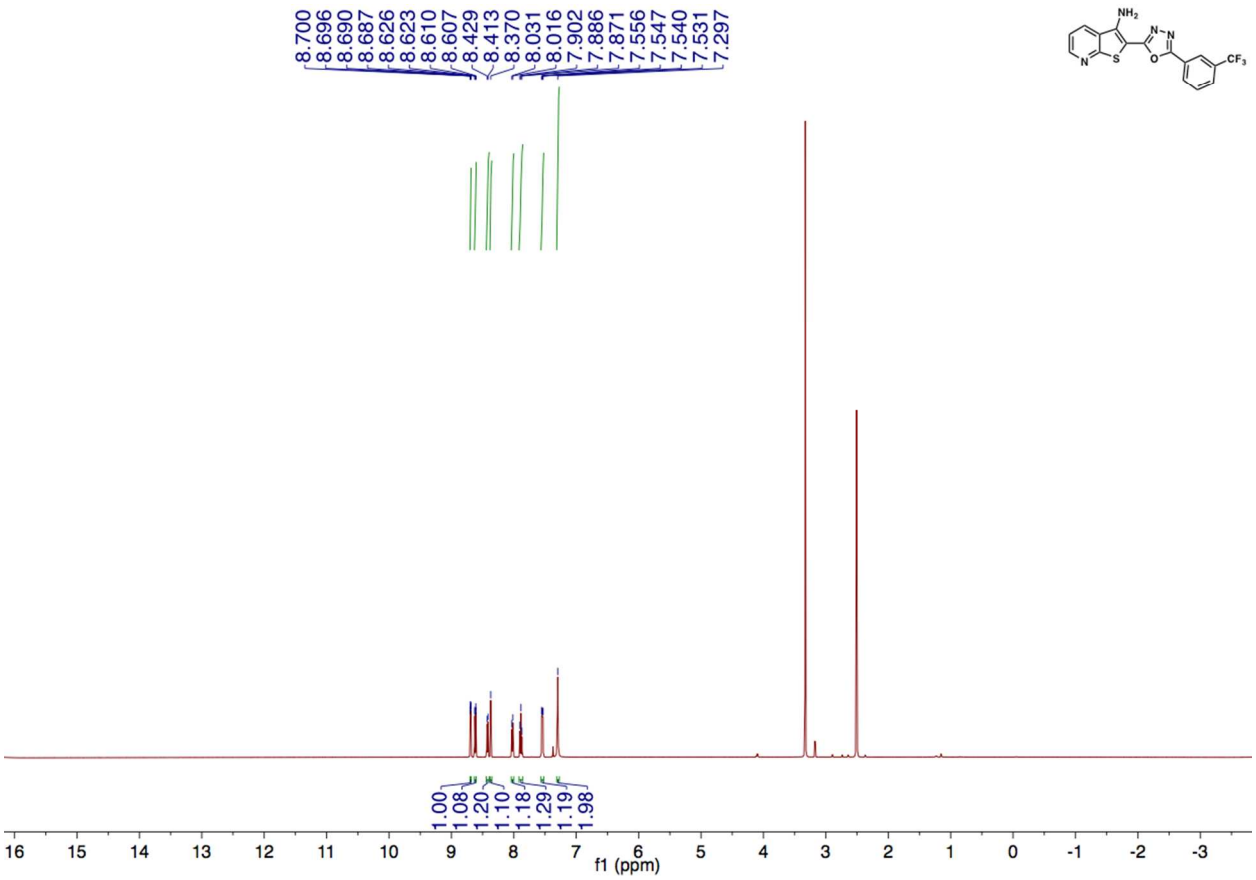

172.923
166.843
160.903
160.245
146.842
132.346
131.813
130.972
130.775
130.520
130.263
130.009
128.570
128.544
127.928
127.563
125.395
124.149
124.119
124.089
124.061
123.398
123.229
121.063
120.454
86.254
24.748
NH2
O
N
N
S
N
CF3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

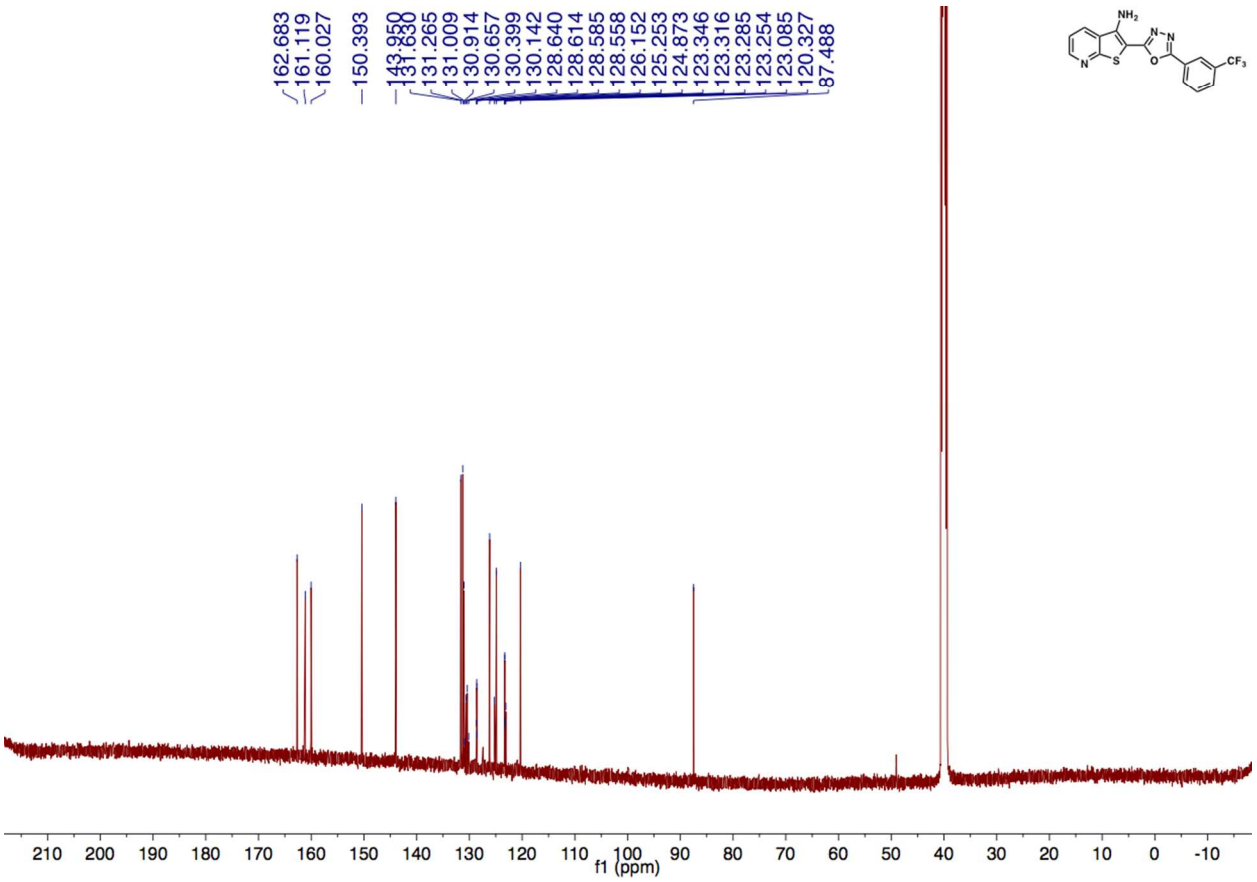

8.482
8.466
8.115
8.112
8.105
8.096
7.644
7.640
7.633
7.630
7.621
7.414
7.397
7.191
2.624
NH2
N
S
O
N
N
1.00
1.87
2.89
1.10
1.82
2.80
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)

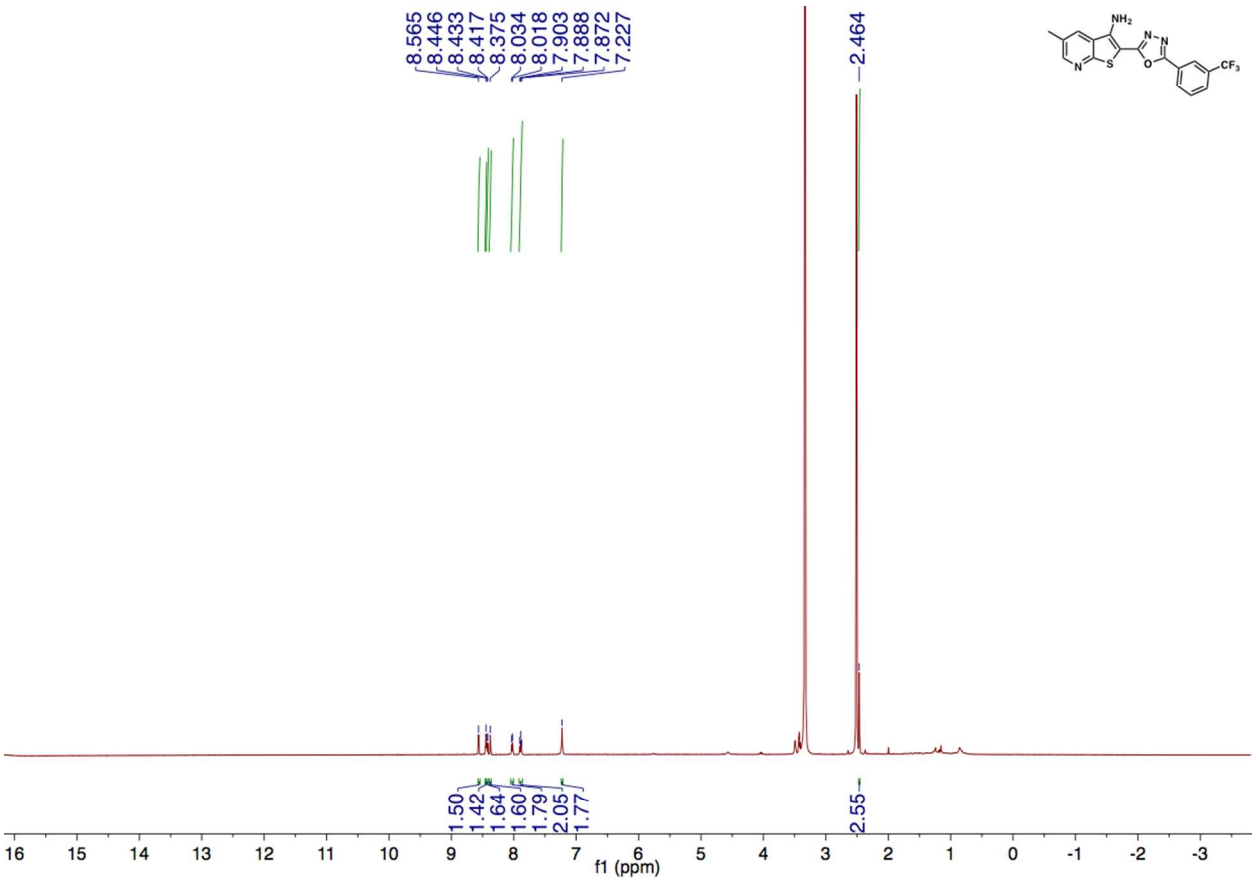

162.391
161.914
159.652
159.636
143.838
132.163
131.587
129.874
126.963
123.865
123.743
120.340
86.694
24.671
NH2
N
S
O
N
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

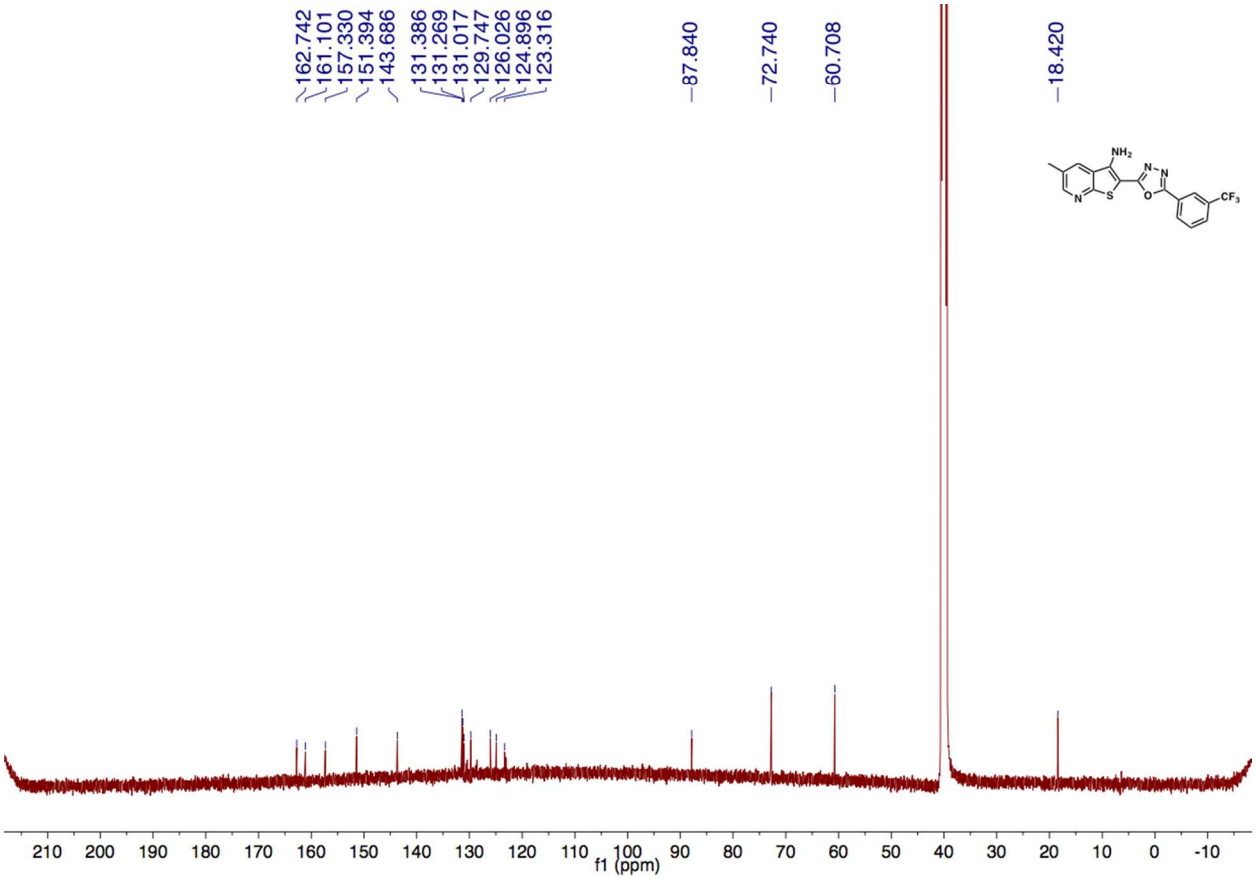

8.483
8.466
8.128
8.125
8.121
8.080
8.078
8.075
8.065
8.063
8.060
7.723
7.720
7.719
7.716
7.706
7.704
7.702
7.700
7.673
7.657
7.642
7.408
7.391
7.212
2.620
NH2
N
S
O
N
N
Cl
1.15
1.00
1.12
1.15
1.17
1.13
2.06
3.00
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)

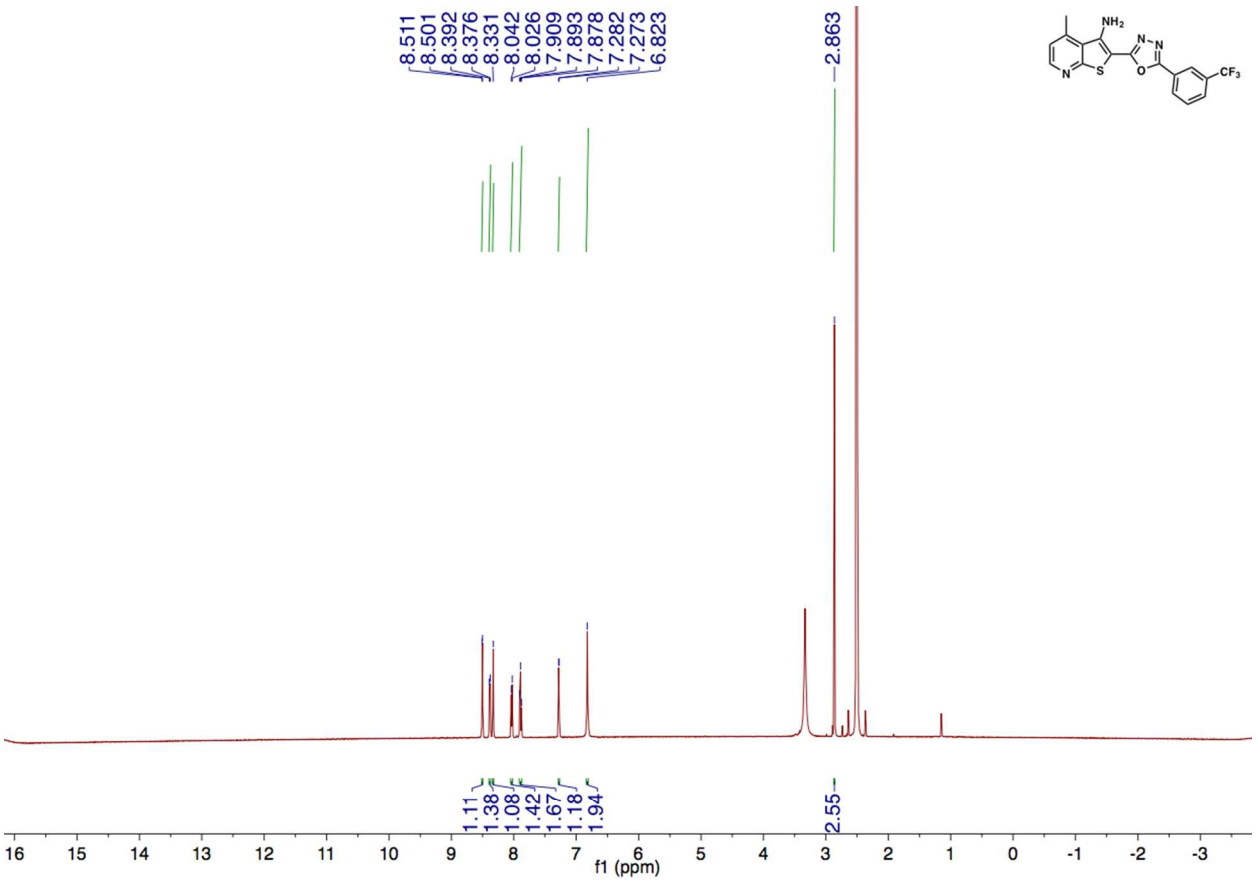

162.683
160.889
159.755
159.732
144.041
134.493
131.906
131.869
131.626
126.387
125.715
125.665
123.837
120.328
86.545
24.674
NH2
N
S
O
N
N
Cl
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

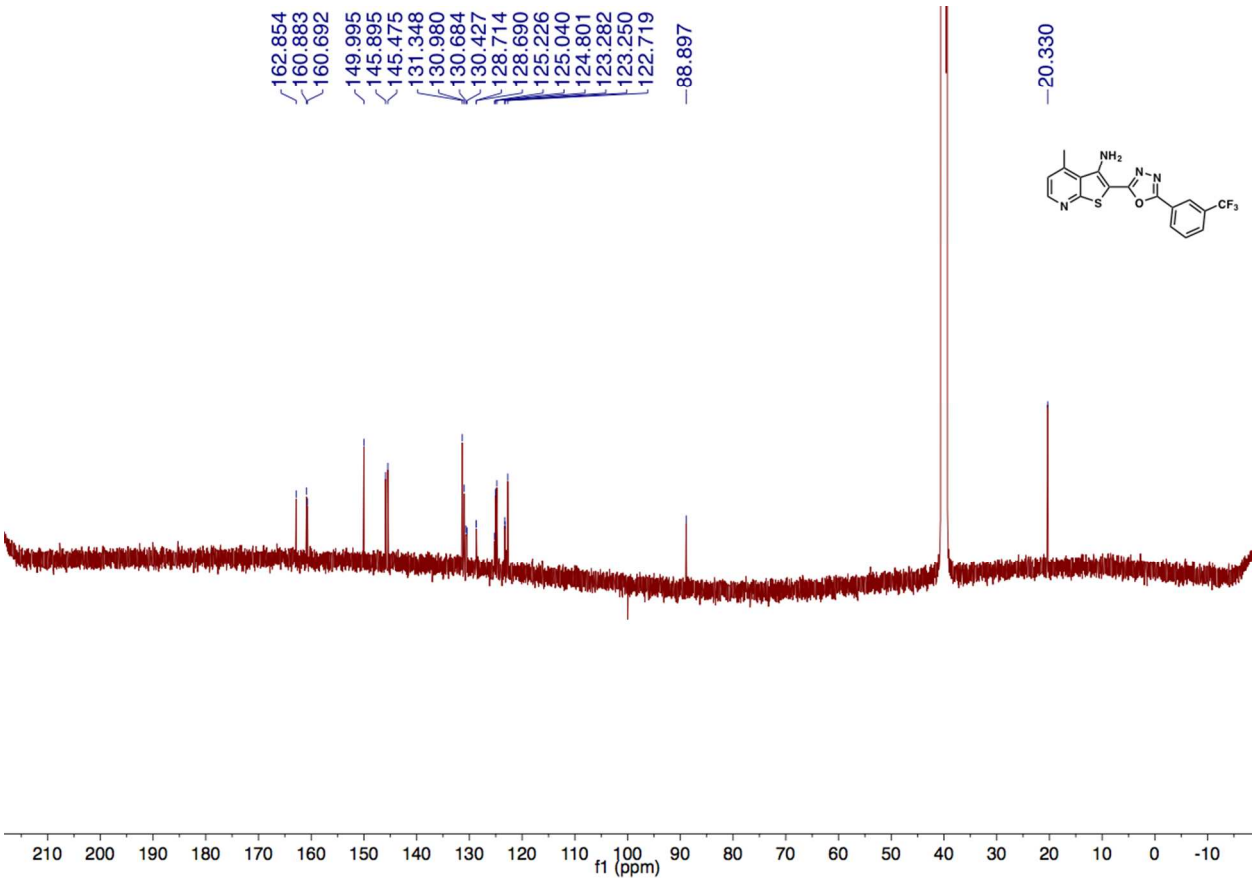

8.700
8.696
8.690
8.687
8.626
8.623
8.610
8.607
8.429
8.413
8.370
8.031
8.016
7.902
7.886
7.871
7.556
7.547
7.540
7.531
7.297
NH2
N
S
O
N
N
CF3
1.00
1.08
1.20
1.10
1.18
1.29
1.19
1.98
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

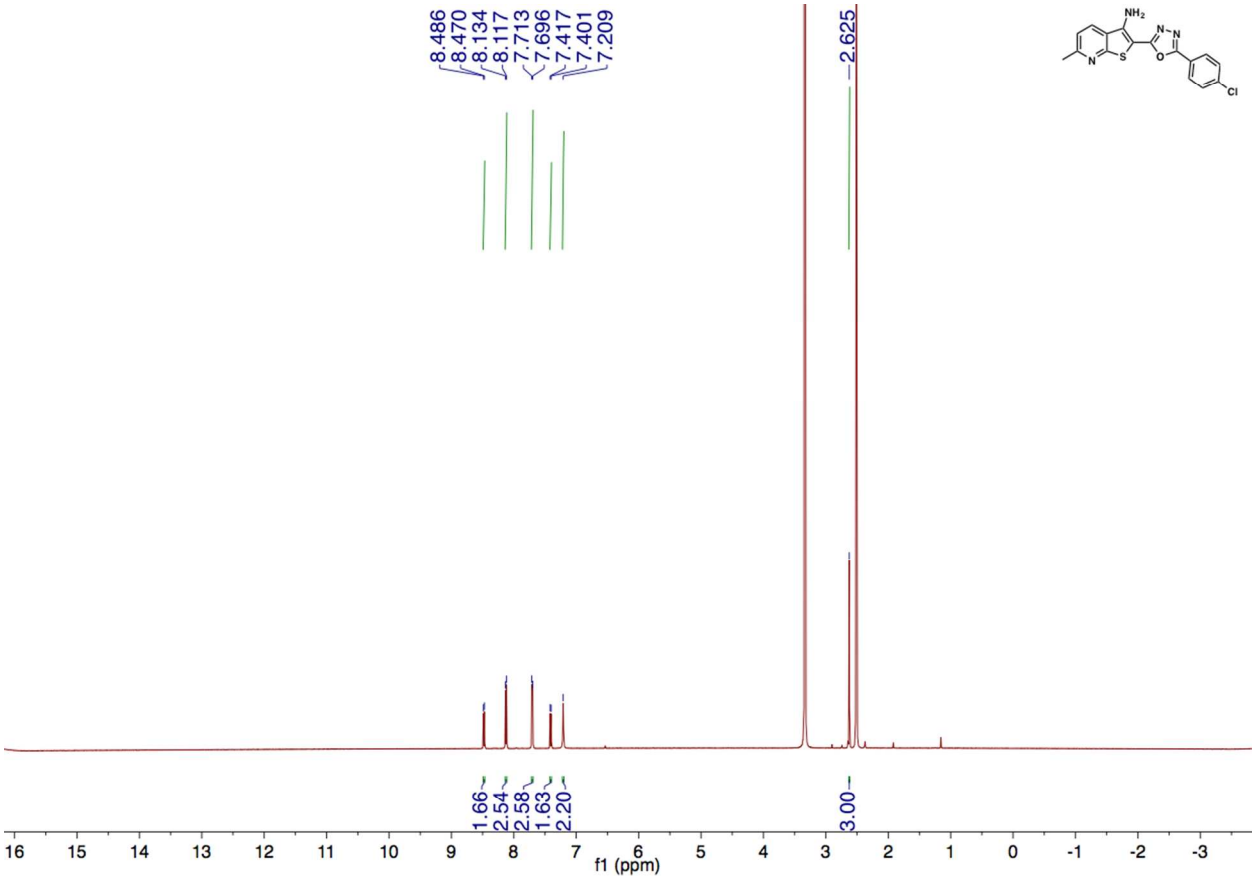

162.683
161.119
160.027
150.393
143.950
131.630
131.265
131.009
130.914
130.657
130.399
130.142
128.640
128.614
128.585
128.558
126.152
125.253
124.873
123.346
123.316
123.285
123.254
123.085
120.327
87.488
NH2
N
S
O
N
N
CF3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

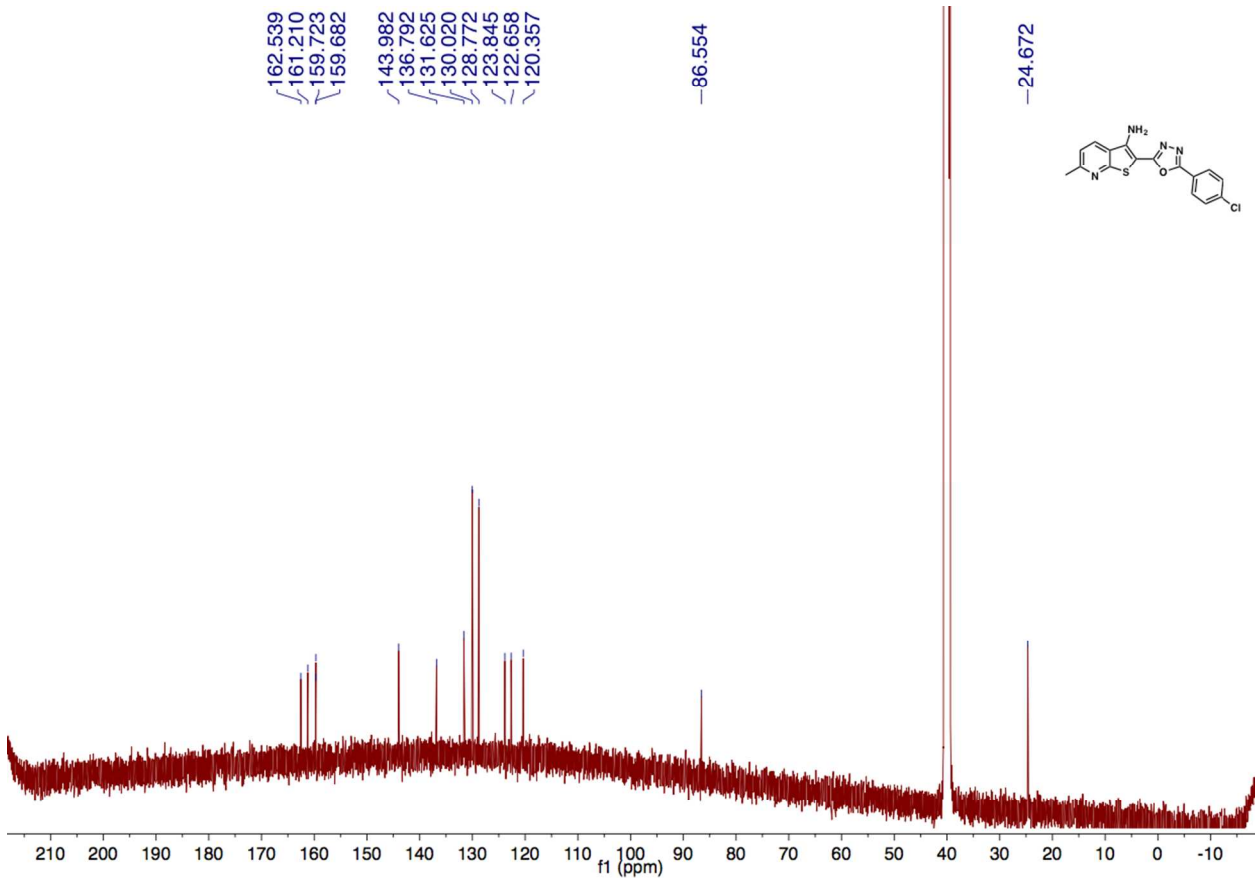

8.565
8.446
8.433
8.417
8.375
8.034
8.018
7.903
7.888
7.872
7.227
2.464
1.50
1.42
1.64
1.60
1.79
2.05
1.77
2.55
f1 (ppm)

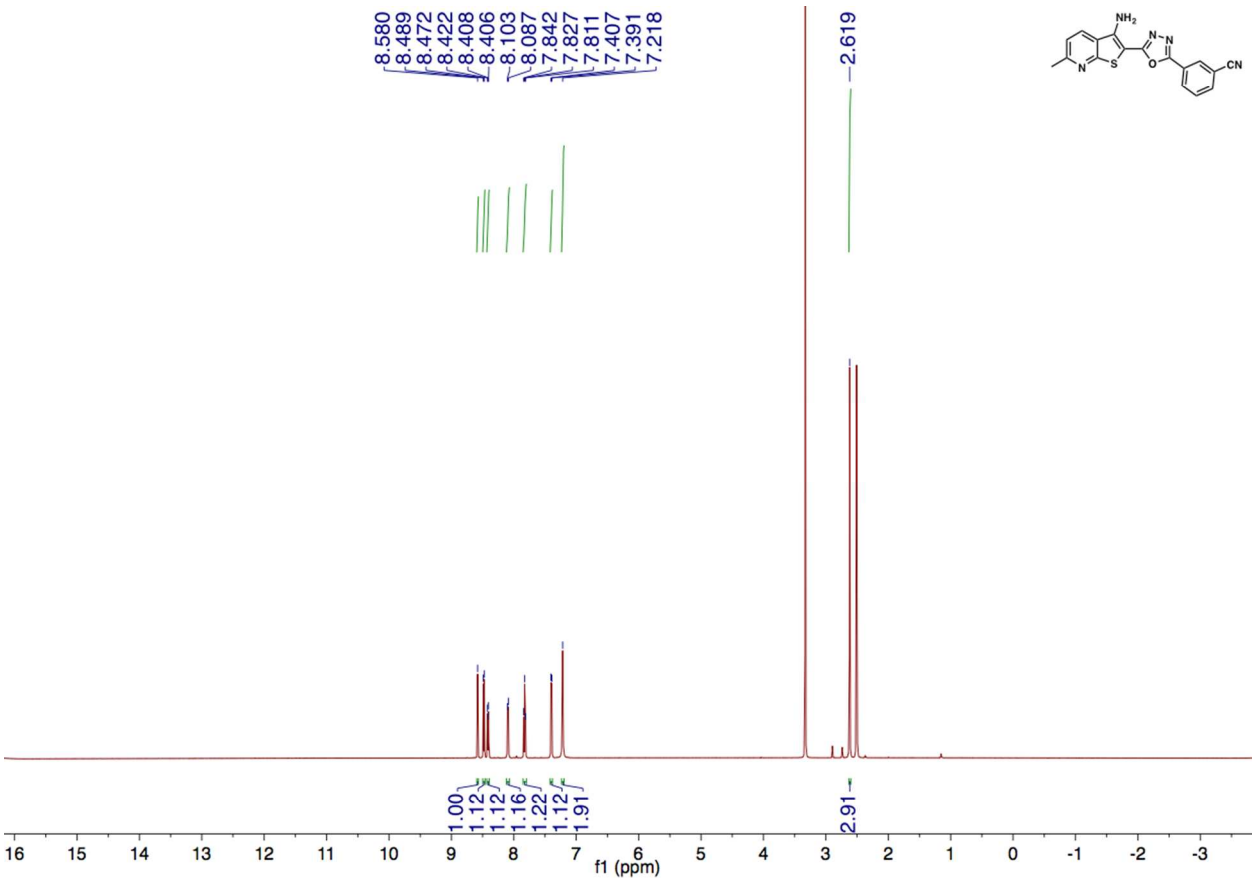

162.742
161.101
157.330
151.394
143.686
131.386
131.269
131.017
129.747
126.026
124.896
123.316
87.840
72.740
60.708
18.420
NH2
N
S
O
N
N
CF3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

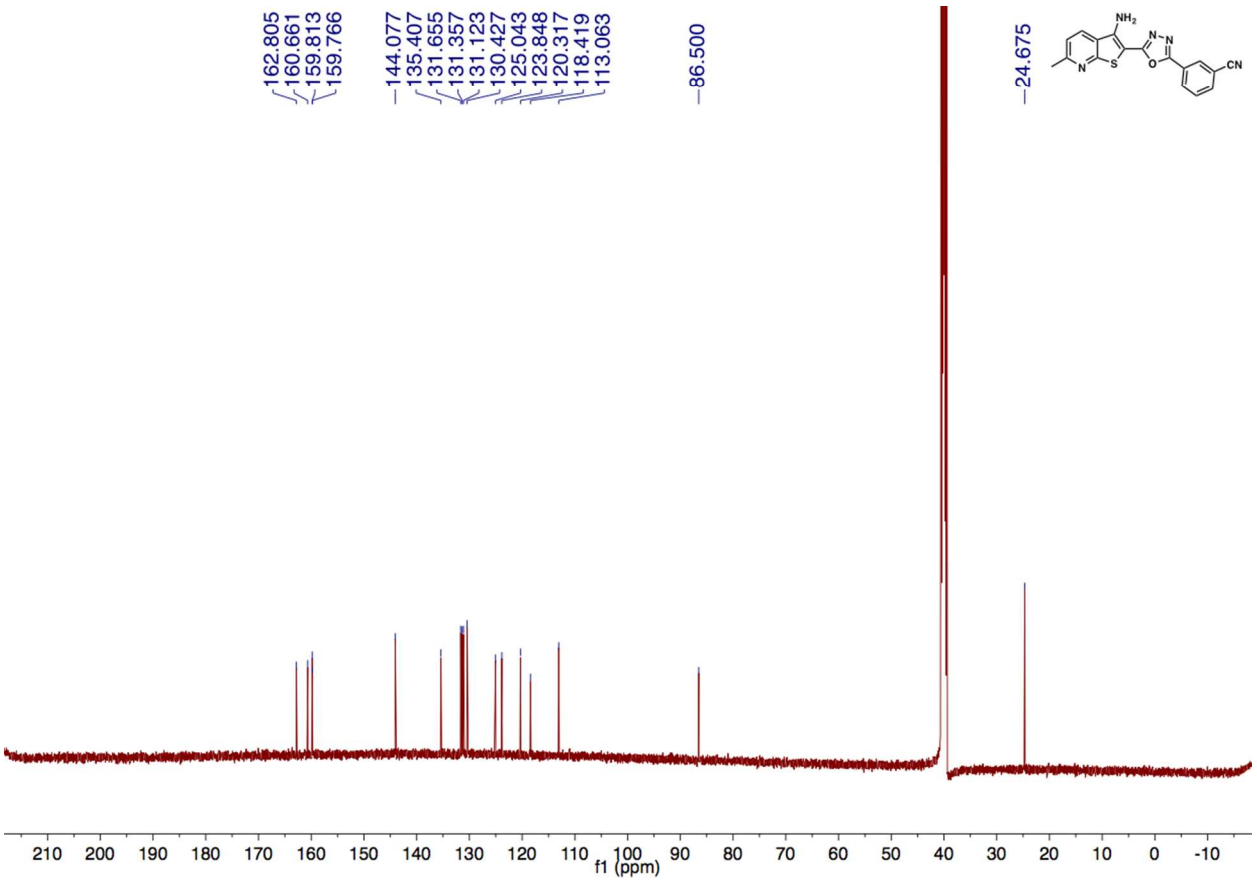

8.511
8.501
8.392
8.376
8.331
8.042
8.026
7.909
7.893
7.878
7.282
7.273
6.823
2.863
NH2
N
S
O
N
N
CF3
1.11
1.38
1.08
1.42
1.67
1.18
1.94
2.55
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)

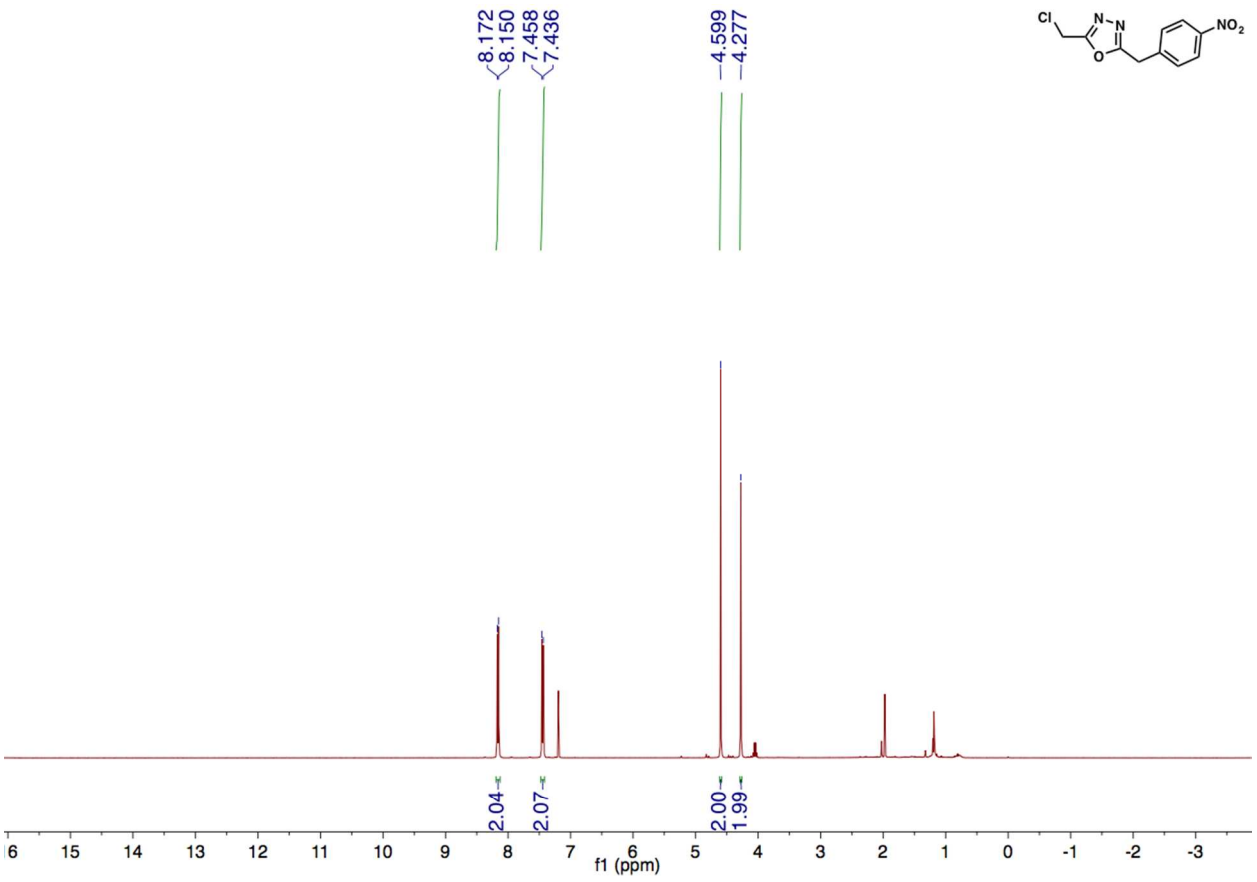

162.854
160.883
160.692
149.995
145.895
145.475
131.348
130.980
130.684
130.427
128.714
128.690
125.226
125.040
124.801
123.282
123.250
122.719
88.897
20.330
NH2
N
S
O
N
N
CF3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

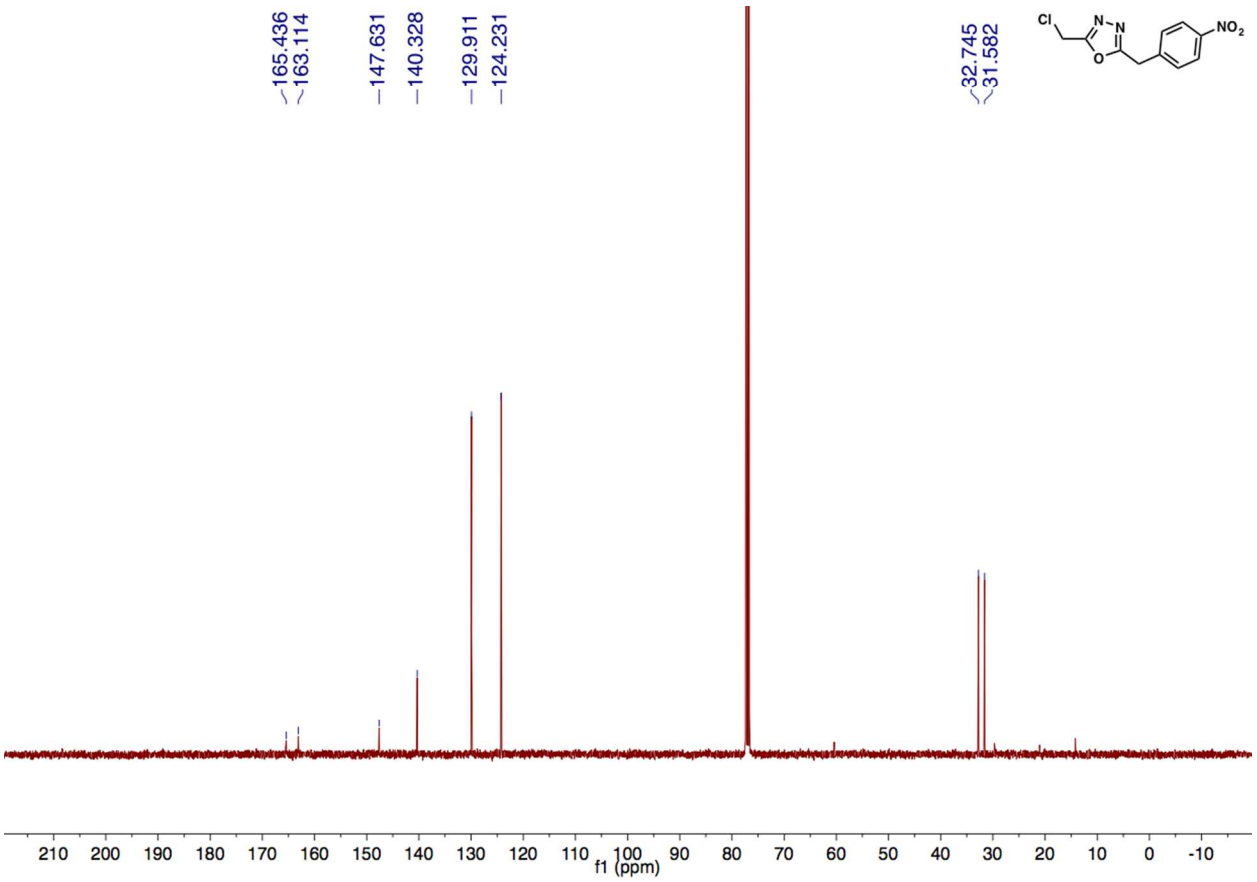

8.486
8.470
8.134
8.117
7.713
7.696
7.417
7.401
7.209
2.625
1.66
2.54
2.58
1.63
2.20
3.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

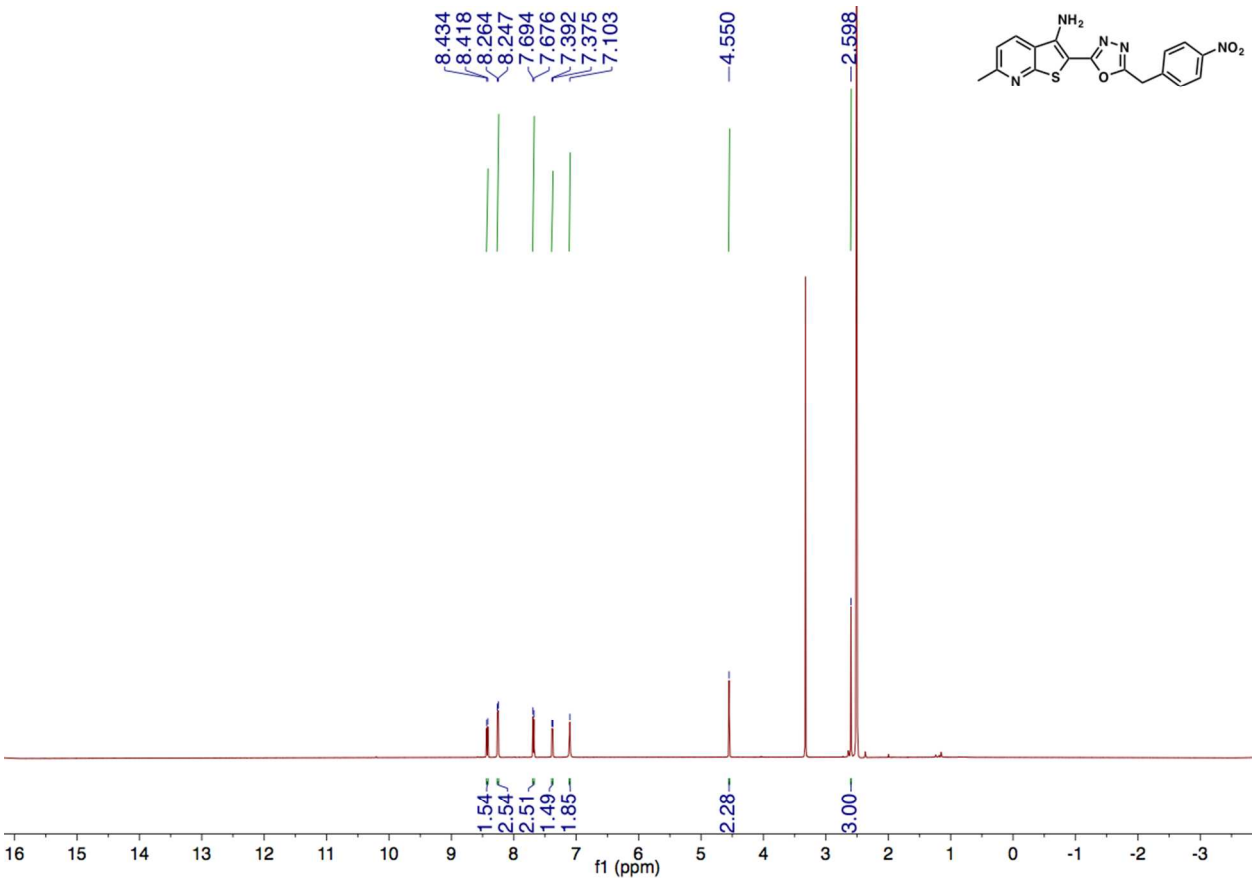

162.539
161.210
159.723
159.682
143.982
136.792
131.625
130.020
128.772
123.845
122.658
120.357
86.554
24.672
NH2
N
S
O
N
N
Cl
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

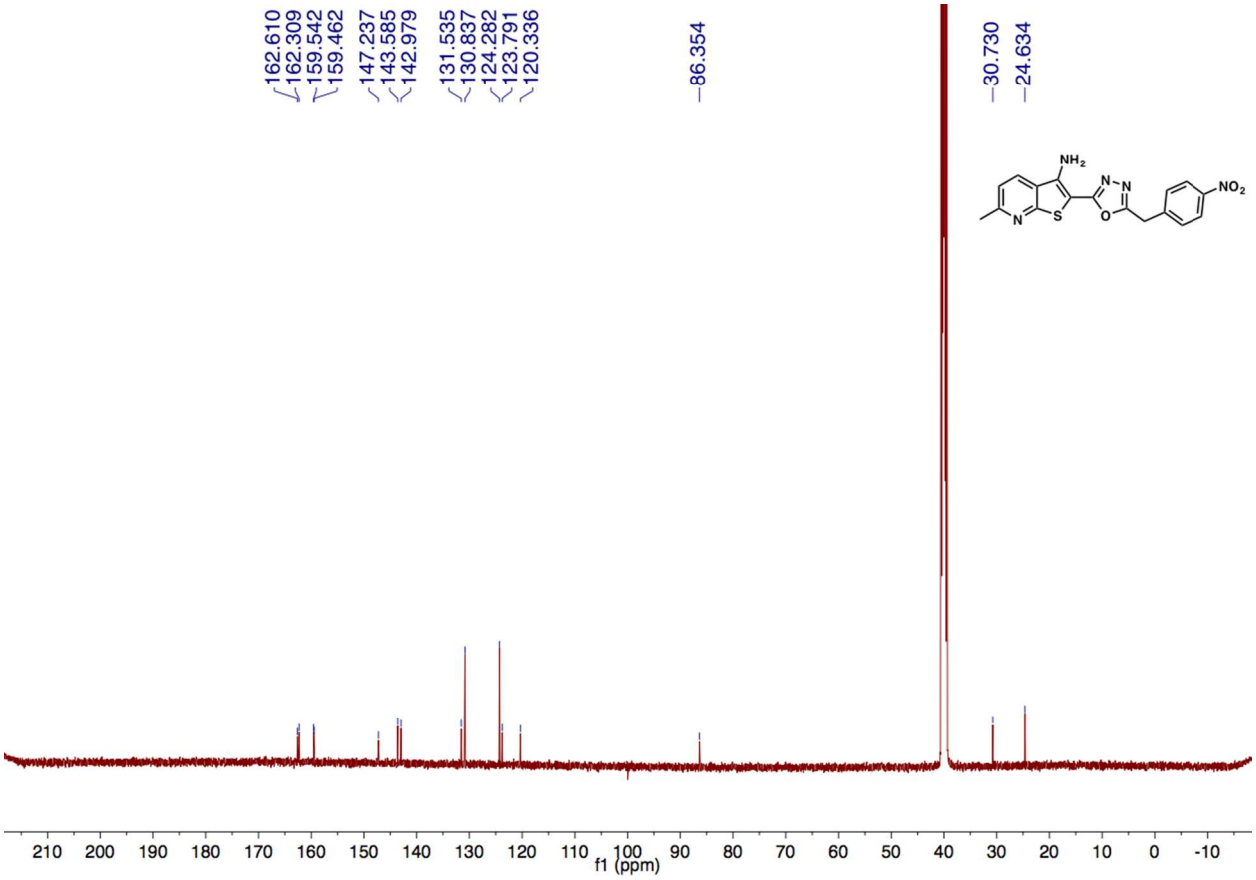

8.580
8.489
8.472
8.422
8.408
8.406
8.103
8.087
7.842
7.827
7.811
7.407
7.391
7.218
2.619
NH2
N
N
O
S
N
CN
1.00
1.12
1.12
1.16
1.22
1.12
1.91
2.91
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)

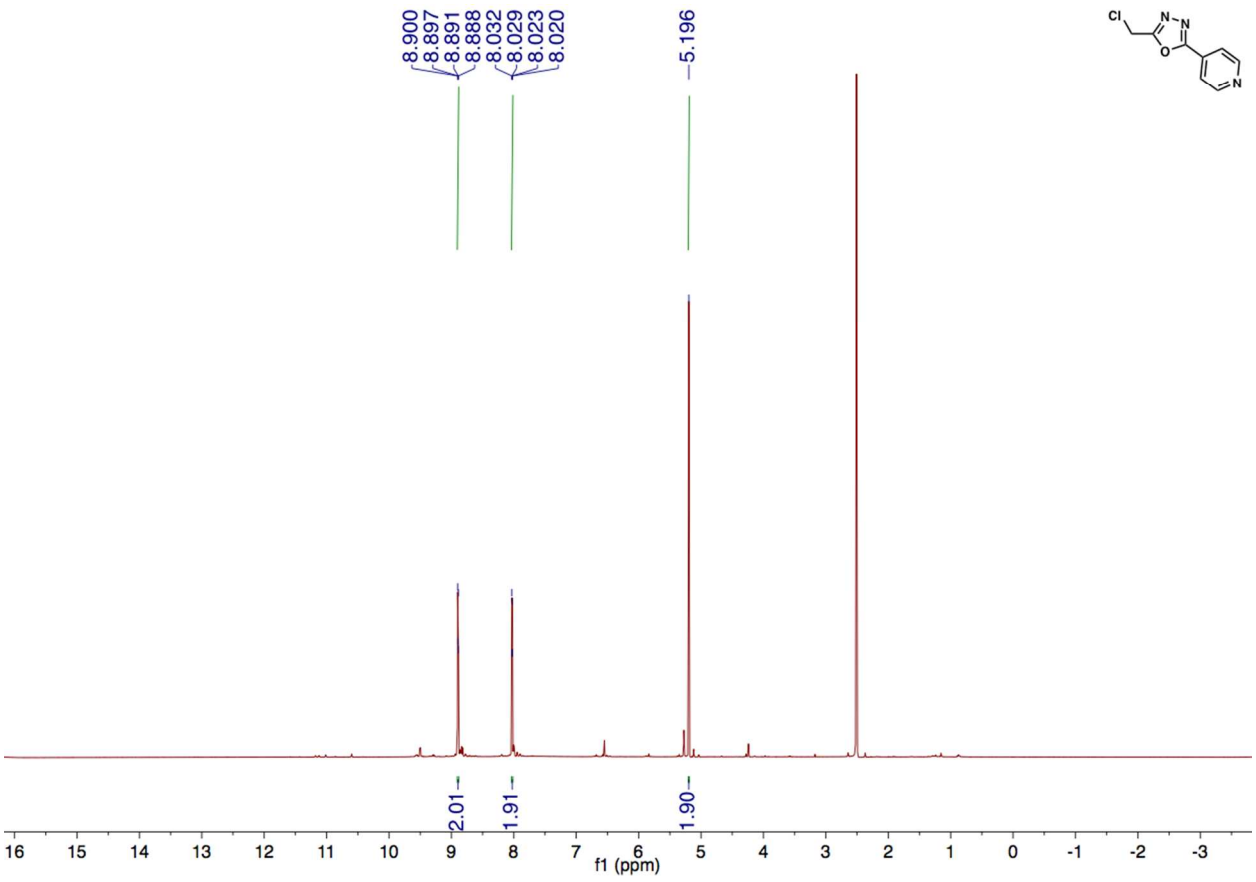

162.805
160.661
159.813
159.766
144.077
135.407
131.655
131.357
131.123
130.427
125.043
123.848
120.317
118.419
113.063
86.500
24.675
NH2
N
N
O
S
N
CN
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

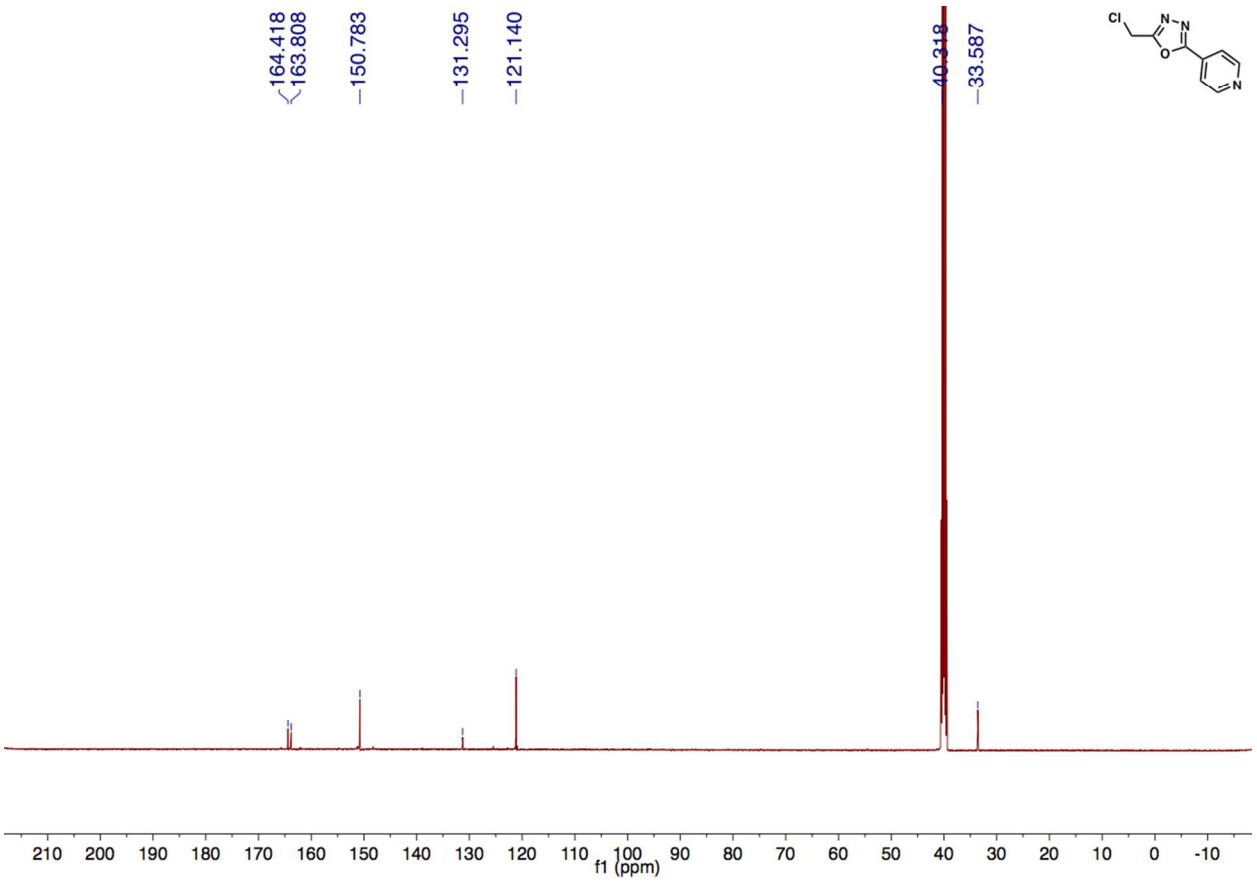

8.172
8.150
7.458
7.436
4.599
4.277
Cl
N
N
O
NO2
2.04
2.07
2.00
1.99
6
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)

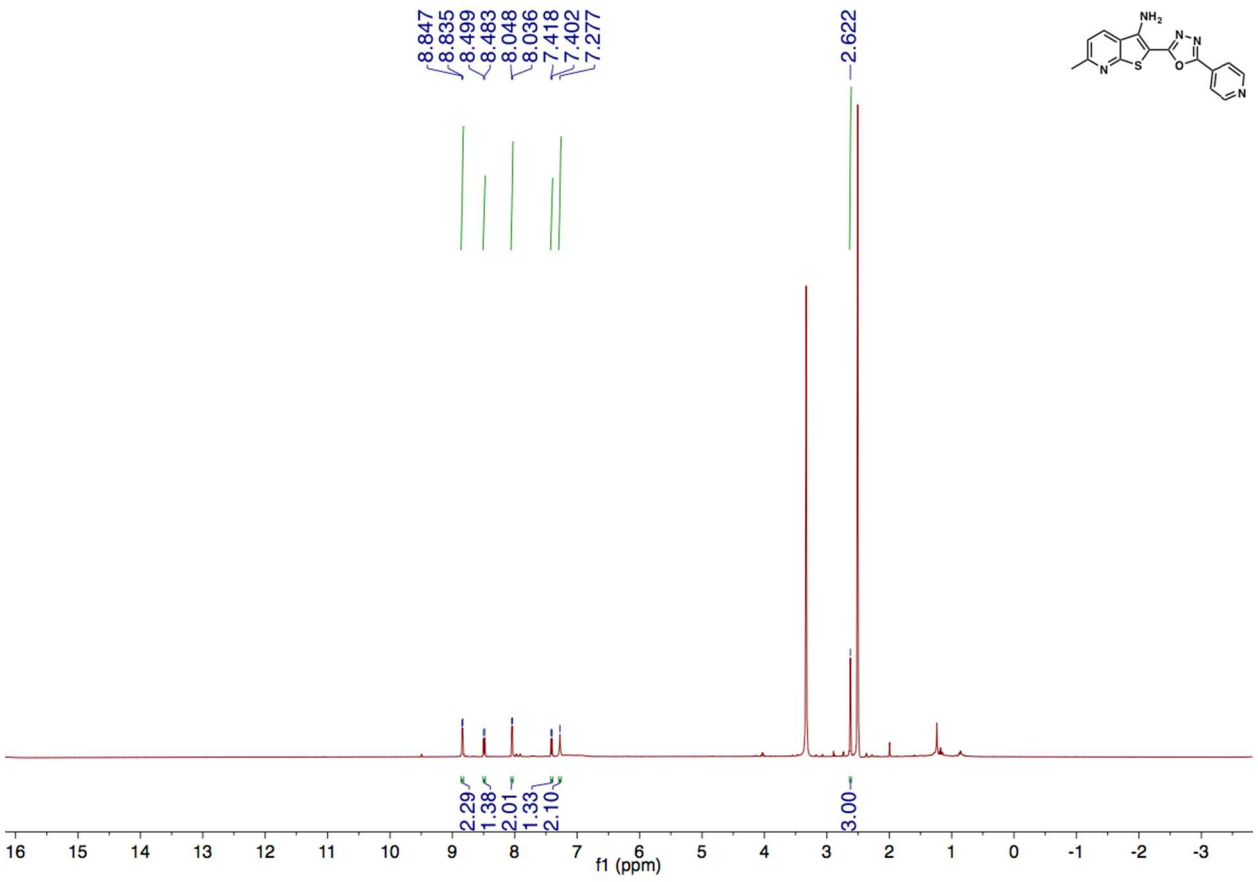

165.436
163.114
147.631
140.328
129.911
124.231
32.745
31.582
Cl
N
N
O
NO2
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

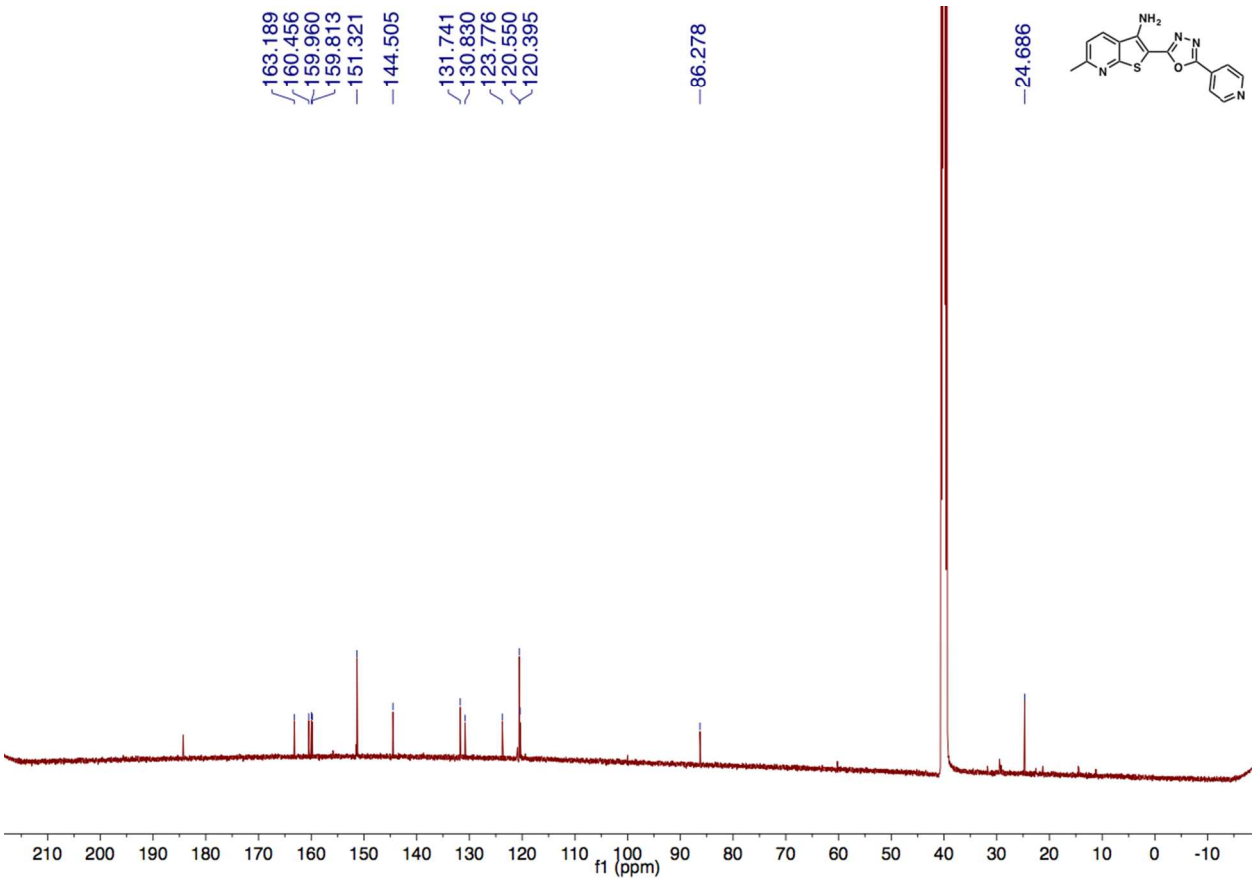

8.434
8.418
8.264
8.247
7.694
7.676
7.392
7.375
7.103
4.550
2.598
NH2
N
S
N
N
O
NO2
1.54
2.54
2.51
1.49
1.85
2.28
3.00
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)

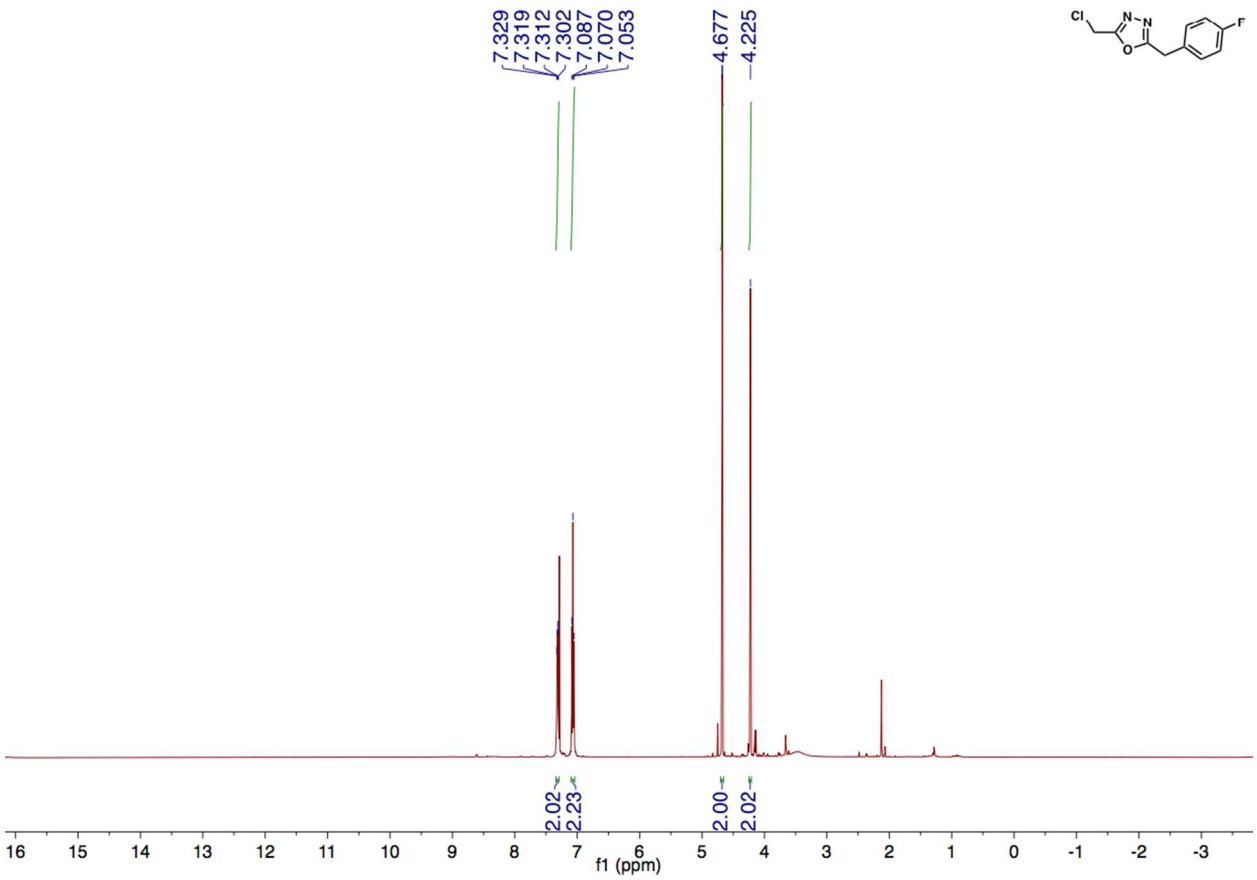

162.610
162.309
159.542
159.462
147.237
143.585
142.979
131.535
130.837
124.282
123.791
120.336
86.354
30.730
24.634
NH2
N
N
O
S
N
NO2
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

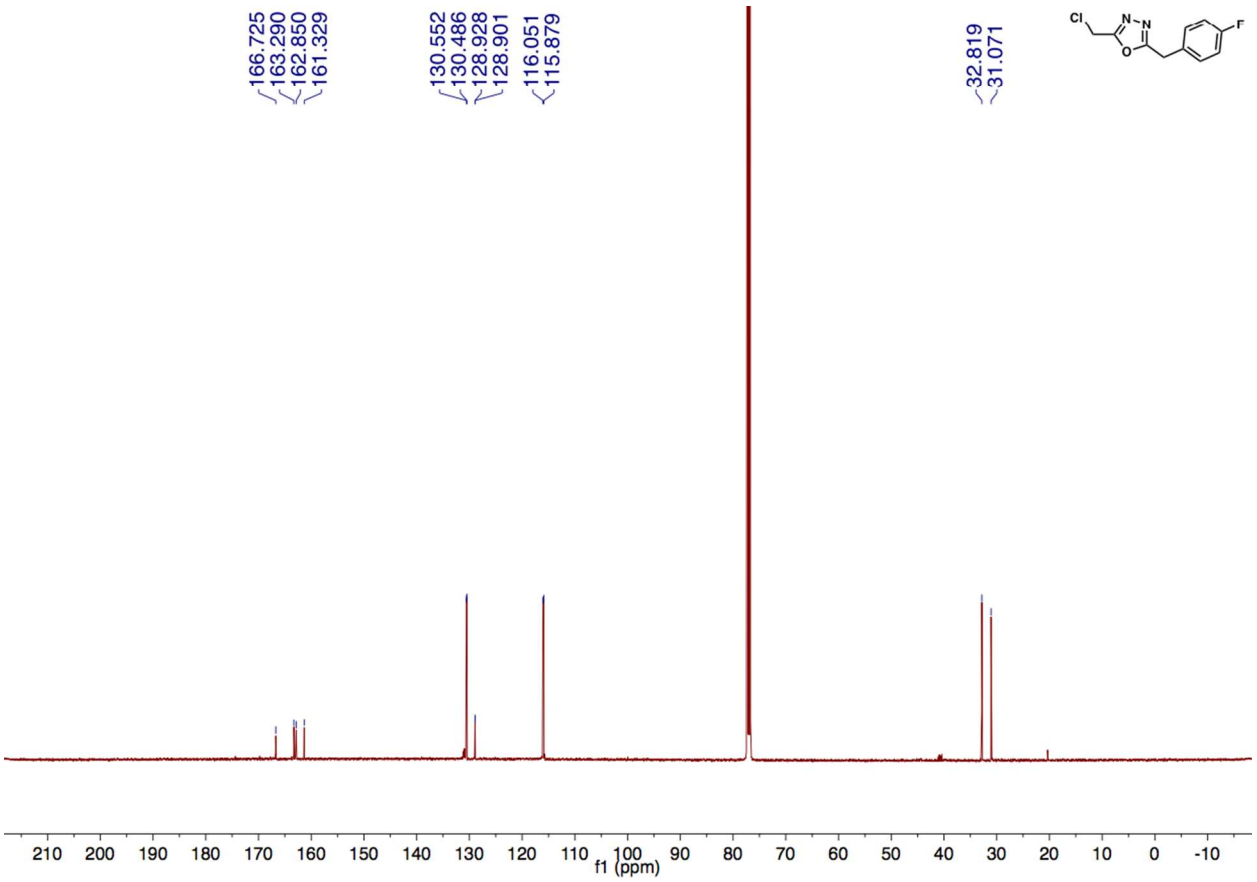

8.900
8.897
8.891
8.888
8.032
8.029
8.023
8.020
5.196
2.01
1.91
1.90
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)
Cl
N
N
O
N

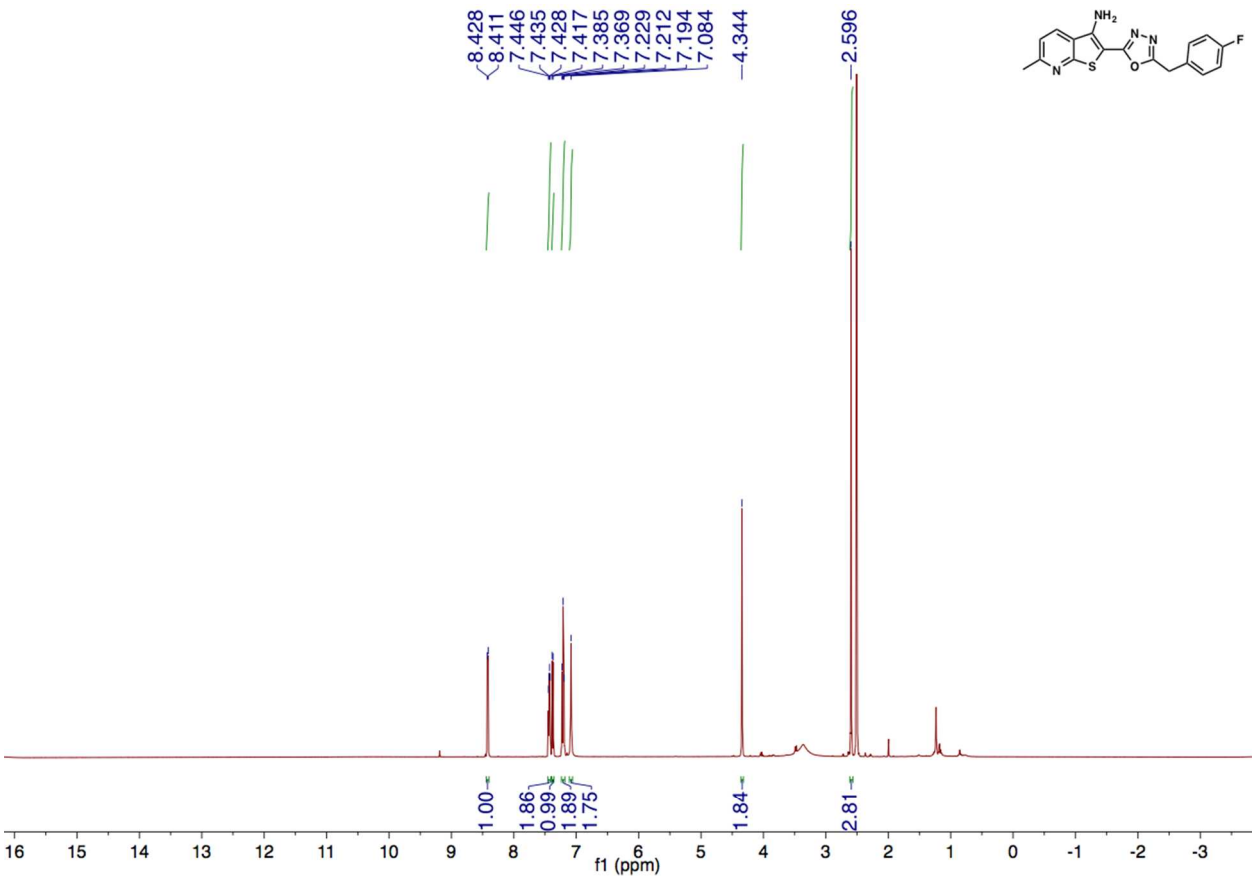

164.418
163.808
150.783
131.295
121.140
40.318
33.587
Cl
N
N
O
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

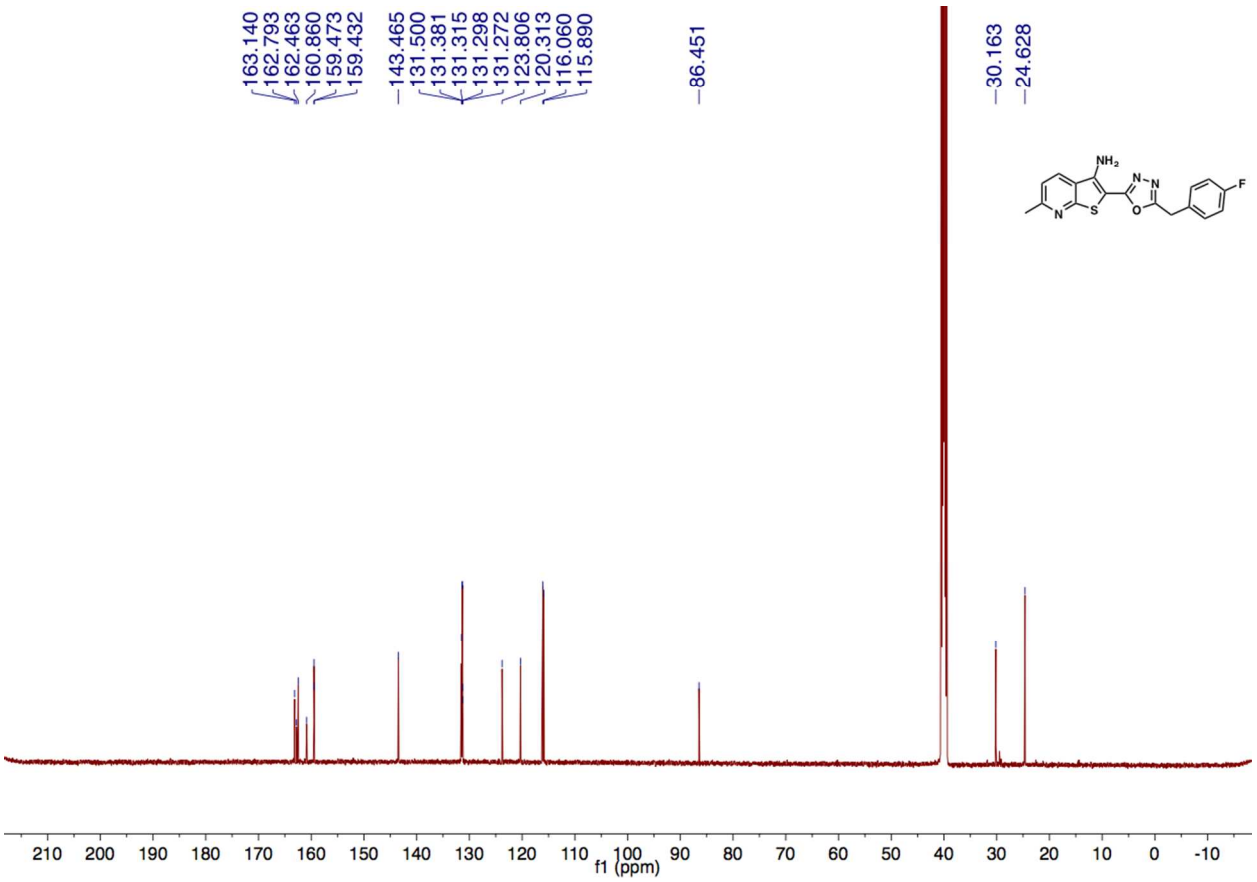

8.847
8.835
8.499
8.483
8.048
8.036
7.418
7.402
7.277
2.622
2.29
1.38
2.01
1.33
2.10
3.00
f1 (ppm)


163.189
160.456
159.960
159.813
151.321
144.505
131.741
130.830
123.776
120.550
120.395
86.278
24.686
NH2
N
S
O
N
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.329
7.319
7.312
7.302
7.087
7.070
7.053
4.677
4.225
Cl
N
N
O
F
2.02
2.23
2.00
2.02
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)


166.725
163.290
162.850
161.329
130.552
130.486
128.928
128.901
116.051
115.879
32.819
31.071
Cl
N
N
O
F
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.428
8.411
7.446
7.435
7.428
7.417
7.385
7.369
7.229
7.212
7.194
7.084
4.344
2.596
NH2
N
S
O
N
F
1.00
1.86
0.99
1.89
1.75
1.84
2.81
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)


163.140
162.793
162.463
160.860
159.473
159.432
143.465
131.500
131.381
131.315
131.298
131.272
123.806
120.313
116.060
115.890
86.451
30.163
24.628
NH2
N
S
O
N
N
F
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)