And

Electronic Supplementary Information

On-water, Catalyst-Free and Room-temperature Construction of 2-Aryl-1,3,4-oxadiazole Derivatives from 1,1-Dichloro-2-nitroethene and Hydrazides

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1. General information

Melting points (mp) were recorded on Büchi B540 apparatus (Büchi Labortechnik AG, Flawil, Switzerland) and are uncorrected. ^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker AM-400 (^{1}H at 400 MHz, ^{13}C at 100 MHz) spectrometer with DMSO-d_6 as the solvent and TMS as the internal standard. Chemical shifts are reported in δ (parts per million) values. High-resolution electron mass spectra (ESI-TOF) were performed on a Micromass LC-TOF spectrometer. Analytical thin-layer chromatography (TLC) was carried out on precoated plates (silica gel 60 F254), and spots were visualized with ultraviolet (UV) light. Chromatographic analysis was performed using an ACQUITY UPLC-H Class system (Waters Corp., USA), equipped with BEH C18 reversed phase column with 50 mm×2.1 mm i.d. and 1.7 μm particle size, equipped with a quaternary solvent delivery system, a 48-vial autosampler (10 μL loop), and a photodiode array detector (PDA). The UPLC separations were carried out using gradient separation at a flow rate of 0.4 mL min^{-1}. The mobile phase was a mixture of MilliQ ultrapure water (A) and acetonitrile (B). The following elution gradient totally lasted 15 min: initial mobile-phase composition, 90:10 (v/v) phase A:B; 0-3.5 min, linear change from 10 to 45% B; 3.5-7 min, linear change from 45 to 60% B; 7-8 min linear change from 60 to 100% B; 8-10 min 100% B; 10-11 min, 90:10 (v/v) phase A:B. The column and injection chamber were maintained at 40 and 25 °C, respectively. The sample injection volume was 3 μL and the detector was set at 321 nm. The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, coupling constant (Hz) and integration. Gaussian09 calculated the electron cloud density and Multiwfn plotted electron cloud density map.

Reagents: Phthalohydrazide was synthesized according to the reported procedures[1], *N*'-phenyl-4-

(trifluoromethyl)benzohydrazide and *N*'-phenylbenzohydrazide were synthesized according to method reported by Zheng-Ming Li *et. al.*[2], 1,1-dichloro-2-nitroethene (DCNE) synthesis under the following steps: 36% hydrochloric acid (41.7 g, 0.411 mol) and 65% nitric acid (39.8 g, 0.411 mol) were add to round-bottom flask, drop add the 1,1-dichloroethylene (31.0 g, 0.315 mol) with Constant pressure hopper and keep temperature at 20-25 °C , after reaction of 3 h, the mixture was continuously stirred for 1 h, washed with water, and extracted by chloroform, collect the organic phase, then add the chloroform layer to 235 mL 4% sodium hydroxide solution at the conditions of ice bath agitation, after simple separation and chloroform washing, concentrate the organic phase, dried with anhydrous magnesium sulfate, then obtain 29 g pale yellow oil. All other solvents and reagents were purchased directly from commercial suppliers and used as received without further purification.

[1]C.-Y. Zhang, X.-H. Liu, B.-L. Wang, S.-H. Wang and Z.-M. Li, *Chem. Biol. Drug Des.*, 2010, **75**, 489-493.
[2]K. Karthik, K. B. Priyanka, S. Manjula and G. Sammaiah, *Int. J. Pharm. Pharm. Sci.*, 2013, **5**, 224-227.

2. General Procedure for the Synthesis of 2-(nitromethyl)-5-phenyl-1,3,4-oxadiazole

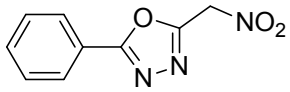
Toluene as the solvent:

Benzohydrazide (136.1 mg, 1 mmol) and 1,1-dichloro-2-nitroethene (169.1 mg, 1.2 mmol) were added to 10 mL of toluene in a 25 mL round-bottom flask. Then stirred for 2 at reflux state, then the mixture was purified by chromatography eluting with petroleum ether / acetic ester (3:1) and afforded the desired product (192.7 mg, 94% yield).

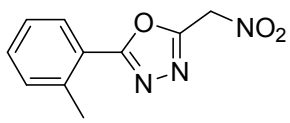
Water as the solvent:

Benzohydrazide (136.1 mg, 1 mmol) and 1,1-dichloro-2-nitroethene (169.1 mg, 1.2 mmol) were added to 10 mL of water in a 25 mL round-bottom flask. Then stirred for 12 h at room temperature, the product precipitated from the reaction mixture and can be easily separated by filtration, then give the product (184.5 mg, 90% yield).

3. Characterization data of products

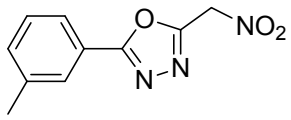


2-(nitromethyl)-5-phenyl-1,3,4-oxadiazole. Isolated as a yellowish powder; m.p. 137.2–137.7 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ_H: 8.07 (d, J = 7.2 Hz, 2H), 7.77–7.56 (m, 3H), 6.52 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ_C: 165.56, 157.50, 132.60, 129.57, 126.78, 122.62, 68.64; HRMS (ESI) calc. for $C_9H_6N_3O_3$ [M - H]$^-$ 204.0409, found 204.0412.

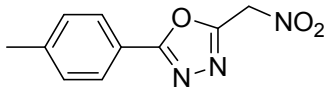


2-(nitromethyl)-5-(o-tolyl)-1,3,4-oxadiazole. Isolated as a yellowish powder; m.p. 67.1–67.7 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ_H 7.92 (d, J = 8.0 Hz, 1H), 7.56 (m, 1H), 7.48 (d, J = 7.6 Hz,

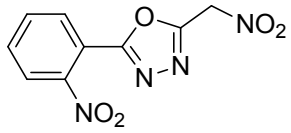
1H), 7.43–7.47 (m, 1H), 6.50 (s, 2H), 2.65 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ_C 165.77, 157.09, 131.98, 131.83, 128.91, 126.59, 121.82, 68.60, 21.26; HRMS (ESI) calc. for $C_{10}H_8N_3O_3$ [M - H]$^-$ 218.0566, found 218.0567.



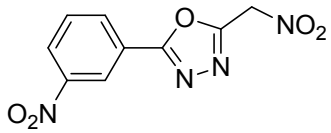
2-(nitromethyl)-5-(m-tolyl)-1,3,4-oxadiazole. Isolated as a yellowish powder; m.p. 128.8–129.3 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ_H 7.86 (m, 2H), 7.58–7.42 (m, 2H), 6.50 (s, 2H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ_C 165.64, 157.41, 139.12, 133.22, 129.45, 127.04, 123.94, 122.53, 68.63, 20.72; HRMS (ESI) calc. for $C_{10}H_8N_3O_3$ [M - H]$^-$ 218.0566, found 218.0563.



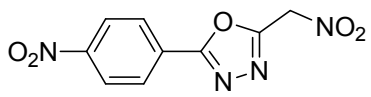
2-(nitromethyl)-5-(p-tolyl)-1,3,4-oxadiazole. Isolated as a yellowish powder; m.p. 134.8–135.3 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ_H 7.94 (d, J = 8.0 Hz, 2H), 7.45 (d, J = 8.0 Hz, 2H), 6.48 (s, 2H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ_C 165.65, 157.24, 142.88, 130.10, 126.72, 119.86, 68.64, 21.11; HRMS (ESI) calc. for $C_{10}H_8N_3O_3$ [M - H]$^-$ 218.0566, found 218.0565.



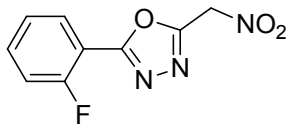
2-(nitromethyl)-5-(2-nitrophenyl)-1,3,4-oxadiazole Isolated as a yellowish powder; m.p. 104.0–104.7 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ_H 8.33–8.21 (m, 1H), 8.13–8.05 (m, 1H), 8.01–7.98 (m, 2H), 6.55 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ_C 162.43, 158.37, 147.77, 133.99, 133.90, 131.57, 125.04, 116.59, 68.36; HRMS (ESI) calc. for $C_9H_5N_4O_5$ [M - H]$^-$ 249.0260, found 249.0256.



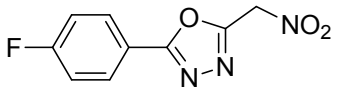
2-(nitromethyl)-5-(3-nitrophenyl)-1,3,4-oxadiazole. Isolated as a yellowish powder; m.p. 123.8–124.5 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ_H 8.71 (s, 1H), 8.50–8.53 (m, 1H), 8.47–8.49 (m, 1H), 7.94–7.98 (m, 1H), 6.54 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ_C 164.03, 158.05, 148.22, 132.77, 131.50, 126.90, 124.06, 121.34, 68.53; HRMS (ESI) calc. for $C_9H_5N_4O_5$ [M - H]$^-$ 249.0260, found 249.0259.



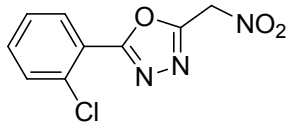
2-(nitromethyl)-5-(4-nitrophenyl)-1,3,4-oxadiazole. Isolated as a yellowish powder; m.p. 132.4–133.1 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ_H 8.47 (d, J = 8.8 Hz, 2H), 8.31 (d, J = 8.8 Hz, 2H), 6.53 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ_C 164.20, 158.32, 149.56, 128.28, 128.11, 124.76, 68.59; HRMS (ESI) calc. for $C_9H_5N_4O_5$ [M - H]$^-$ 249.0260, found 249.0258.



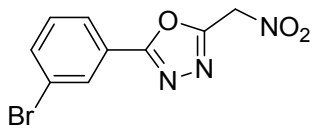
2-(2-fluorophenyl)-5-(nitromethyl)-1,3,4-oxadiazole. Isolated as a yellowish powder; m.p. 120.9–121.6 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ_H 8.08 (m, 1H), 7.83–7.68 (m, 1H), 7.61–7.36 (m, 2H), 6.53 (s, 2H); ^{19}F NMR (376 MHz, DMSO-d_6) δ_F -110.46 (m); HRMS (ESI) calc. for $C_9H_5FN_3O_3$ [M - H]$^-$ 222.0315, found 222.0314.



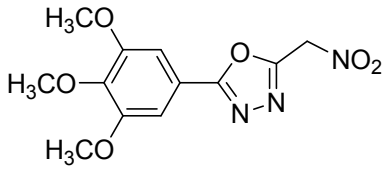
2-(4-fluorophenyl)-5-(nitromethyl)-1,3,4-oxadiazole. Isolated as a yellowish powder; m.p. 92.4–93.0 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ_H 8.13 (dd, J = 8.6, 5.4 Hz, 2H), 7.50 (t, J = 8.8 Hz, 2H), 6.52 (s, 2H); ^{19}F NMR (376 MHz, DMSO-d_6) δ_F -106.36 (m); HRMS (ESI) calc. for $C_9H_5FN_3O_3$ [M - H]$^-$ 222.0315, found 222.0312.



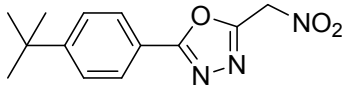
2-(2-chlorophenyl)-5-(nitromethyl)-1,3,4-oxadiazole. Isolated as a yellowish powder; m.p. 74.0–74.8 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ_H 8.02 (dd, J = 7.6, 1.2 Hz, 1H), 7.77 (d, J = 7.2 Hz, 1H), 7.71 (m, 1H), 7.62 (m, 1H), 6.54 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ_C 163.74, 157.90, 133.77, 131.97, 131.46, 131.21, 128.01, 121.86, 68.54; HRMS (ESI) calc. for $C_9H_5ClN_3O_3$ [M - H]$^-$ 238.0019, found 238.0018.



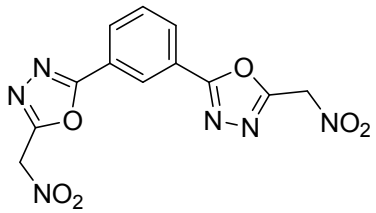
2-(3-bromophenyl)-5-(nitromethyl)-1,3,4-oxadiazole. Isolated as a yellowish powder; m.p. 86.3–86.8 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ_H 8.02–7.86 (m, 2H), 7.73–7.49 (m, 2H), 6.54 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ_C 164.38, 157.93, 134.40, 133.81, 131.89, 128.39, 124.03, 120.98, 68.54; HRMS (ESI) calc. for $C_9H_5BrN_3O_3$ [M - H]$^-$ 281.9514, found 281.9513.



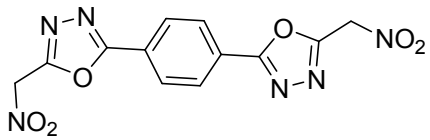
2-(nitromethyl)-5-(3,4,5-trimethoxyphenyl)-1,3,4-oxadiazole. Isolated as a yellowish powder; m.p. 137.5–138.1 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ_H 7.31 (s, 2H), 6.47 (s, 2H), 3.90 (s, 6H), 3.77 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ_C 165.49, 157.39, 153.50, 140.95, 117.71, 104.08, 68.59, 60.22, 56.13. HRMS (ESI) calc. for $C_{12}H_{12}N_3O_6$ [M - H]$^-$ 294.0726, found 294.0724.



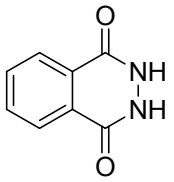
2-(4-(tert-butyl)phenyl)-5-(nitromethyl)-1,3,4-oxadiazole. Isolated as a yellowish powder; m.p. 89.5–91.0 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ_H 7.98 (d, J = 8.4 Hz, 2H), 7.66 (d, J = 8.4 Hz, 2H), 6.49 (s, 2H), 1.33 (s, 9H); ^{13}C NMR (100 MHz, DMSO-d_6) δ_C 165.56, 157.29, 155.62, 126.65, 126.42, 119.90, 68.63, 34.86, 30.72; HRMS (ESI) calc. for $C_{13}H_{14}N_3O_3$ [M - H]$^-$ 260.1035, found 260.1036.



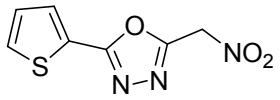
1,3-bis(5-(nitromethyl)-1,3,4-oxadiazol-2-yl)benzene. Isolated as a yellowish powder; m.p. 155.6–156.4 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ_H 8.59 (s, 1H), 8.35 (d, J = 8.0 Hz, 1=2H), 7.93 (m, 1H), 6.53 (s, 4H); ^{13}C NMR (100 MHz, DMSO-d_6) δ_C 164.59, 157.90, 131.22, 130.43, 124.58, 123.93, 68.58; HRMS (ESI) calc. for $C_{12}H_7N_6O_6$ [M - H]$^-$ 331.0427, found 331.0427.



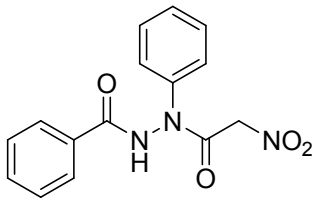
1,4-bis(5-(nitromethyl)-1,3,4-oxadiazol-2-yl)benzene. Isolated as a yellowish powder; m.p. 213.1–213.6 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ_H 8.30 (s, 4H), 6.54 (s, 4H); ^{13}C NMR (100 MHz, DMSO-d_6) δ_C 164.75, 157.97, 127.95, 125.84, 68.63; HRMS (ESI) calc. for $C_{12}H_7N_6O_6$ [M - H]$^-$ 331.0427, found 331.0430.



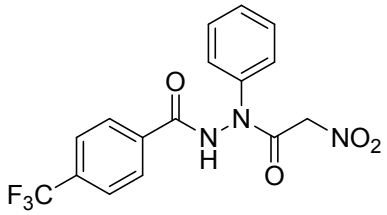
2,3-dihydrophthalazine-1,4-dione. Isolated as a yellowish powder; m.p. 332.8–333.6 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ_H 11.58 (s, 2H), 8.24–7.98 (m, 2H), 7.91 (dd, J = 5.6, 3.2 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ_C 154.62, 132.55, 127.12, 125.09.



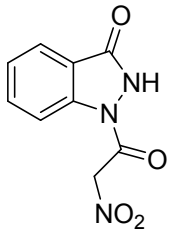
2-(nitromethyl)-5-(thiophen-2-yl)-1,3,4-oxadiazole. Isolated as a yellowish powder; m.p. 133.7–134.2 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ_H 8.04 (d, J = 4.8 Hz, 1H), 7.91 (d, J = 3.6 Hz, 1H), 7.34 (m, 1H), 6.48 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ_C 161.86, 156.84, 132.59, 131.20, 128.97, 123.36, 68.49; HRMS (ESI) calc. for $C_7H_4N_3O_3S$ [M - H]$^-$ 209.9973, found 209.9973.



***N*'-(2-nitroacetyl)-*N*'-phenylbenzohydrazide.** Isolated as a yellowish powder; m.p. 192.1–192.6 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ_H 11.69 (s, 1H), 7.95 (d, J = 7.2 Hz, 2H), 7.65 (m, 1H), 7.55 (m, 4H), 7.44 (m, 2H), 7.31 (m, 1H), 6.00 (d, J = 14.8 Hz, 1H), 5.60 (d, J = 14.8 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ_C 166.07, 163.40, 140.12, 132.83, 131.00, 128.92, 128.69, 127.84, 127.01, 123.53, 78.77; HRMS (ESI) calc. for $C_{15}H_{12}N_3O_4$ [M - H]$^-$ 298.0828, found 298.0831.



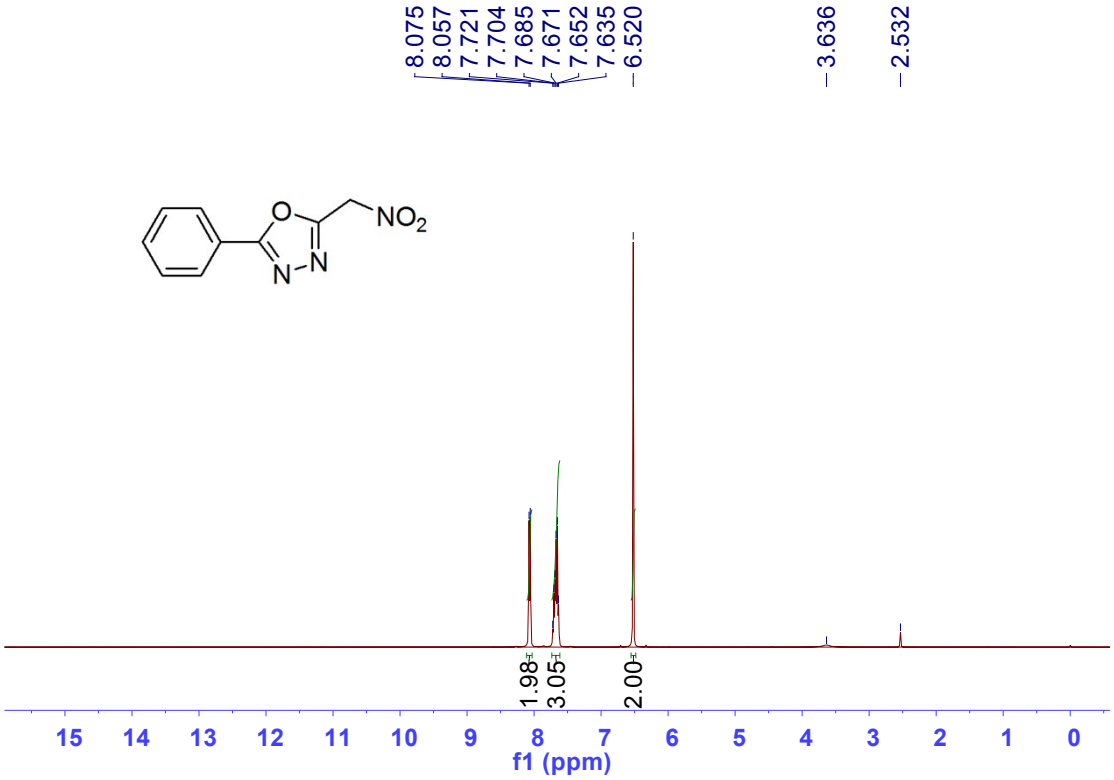
***N*'-(2-nitroacetyl)-*N*'-phenyl-4-(trifluoromethyl)benzohydrazide.** Isolated as a yellowish powder; m.p. 167.3–168.0 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ_H 11.94 (s, 1H), 8.16 (d, J = 7.2 Hz, 2H), 7.96 (d, J = 7.2 Hz, 2H), 7.55 (d, J = 7.2 Hz, 2H), 7.49–7.42 (m, 2H), 7.32 (m, 1H), 6.05 (d, J = 14.8 Hz, 1H), 5.70 (d, J = 14.8 Hz, 1H); ^{19}F NMR (376 MHz, DMSO-d_6) δ_F -61.63 (s); HRMS (ESI) calc. for $C_{16}H_{11}F_3N_3O_4$ [M - H]$^-$ 366.0702, found 366.0700.

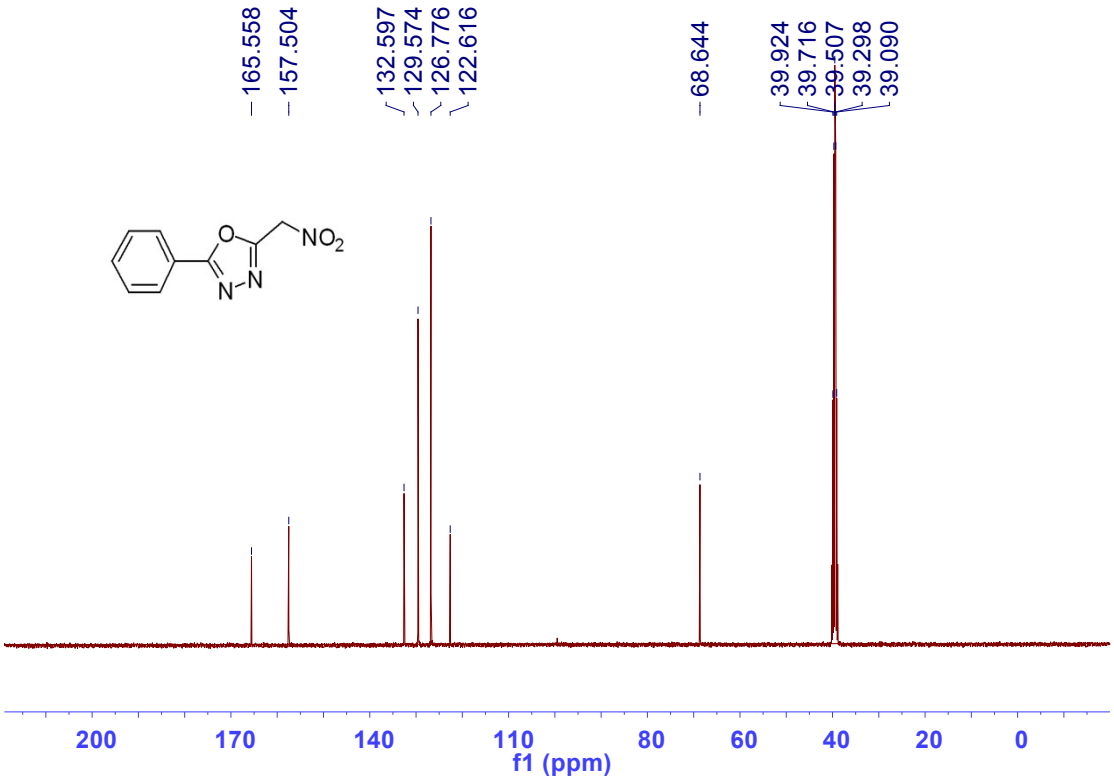


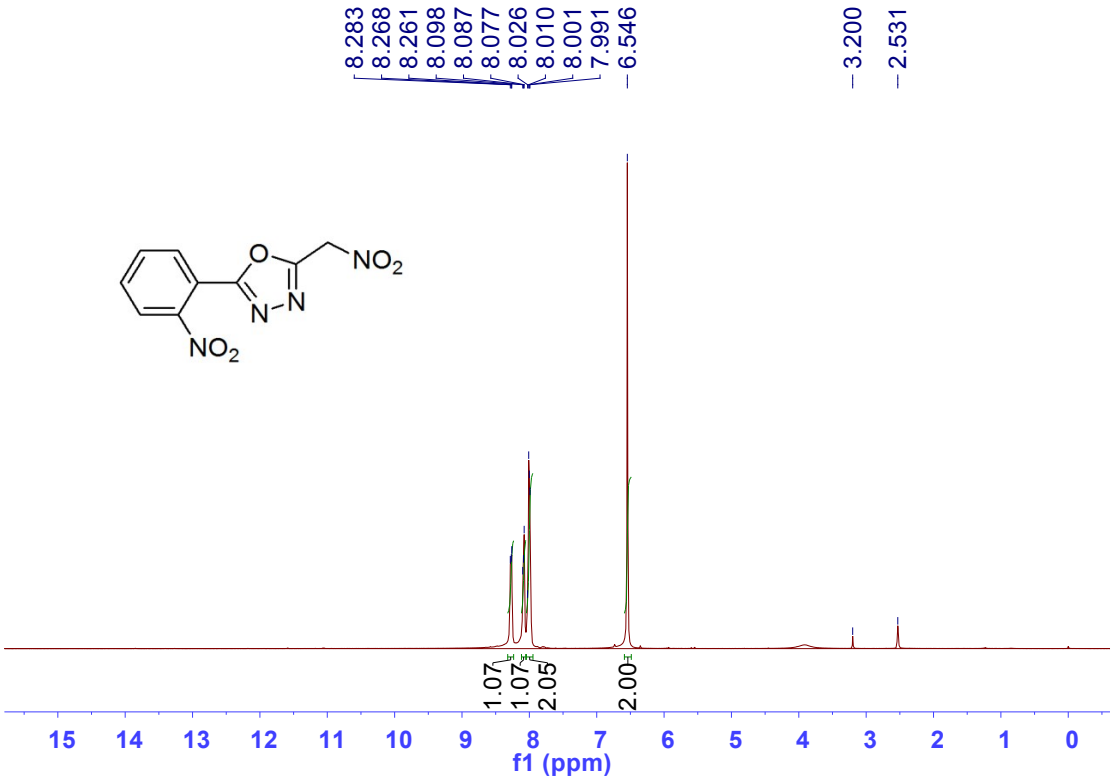
1-(2-nitroacetyl)-1H-indazol-3(2H)-one. Isolated as a yellowish powder; m.p. 191.3–191.6 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ_H 12.57 (s, 1H), 8.23 (d, J = 8.0 Hz, 1H), 7.84 (d, J = 7.6 Hz, 1H), 7.70 (m, 1H), 7.47 (m, 1H), 6.19 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ_C 160.21, 159.46,

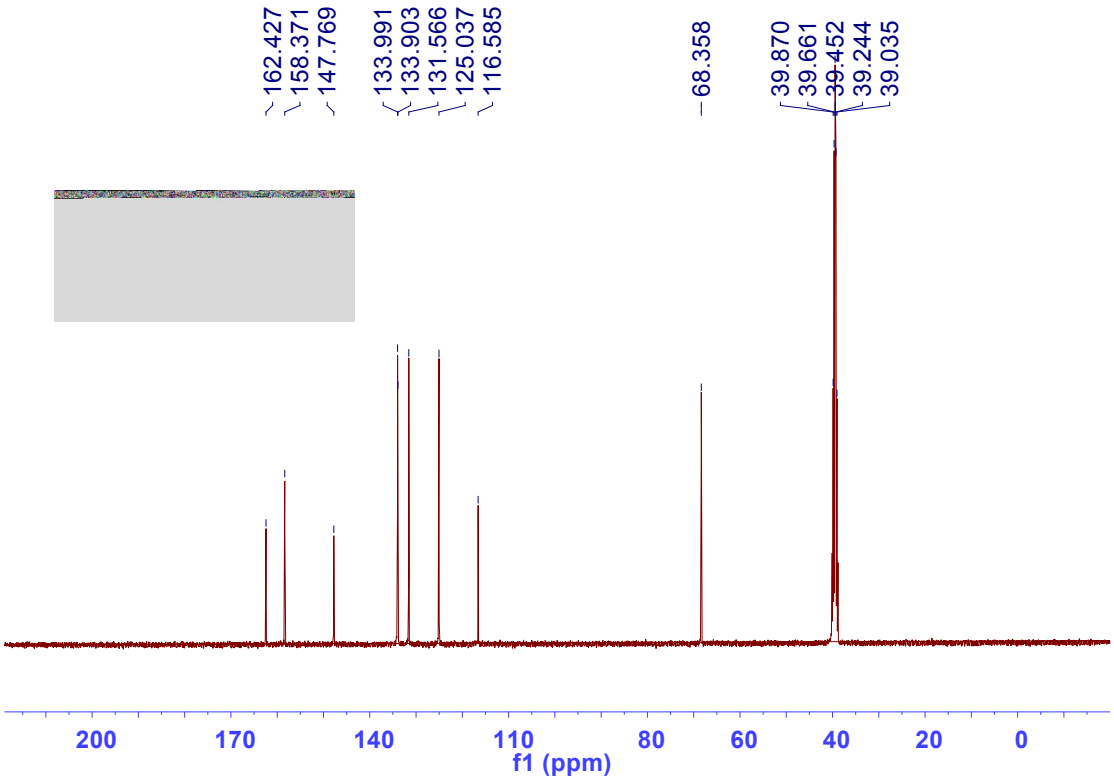
139.43, 130.95, 125.25, 120.84, 118.50, 114.79, 78.42; HRMS (ESI) calc. for $C_9H_7N_3NaO_4$ [M + Na]$^+$ 244.0334, found 244.0331.

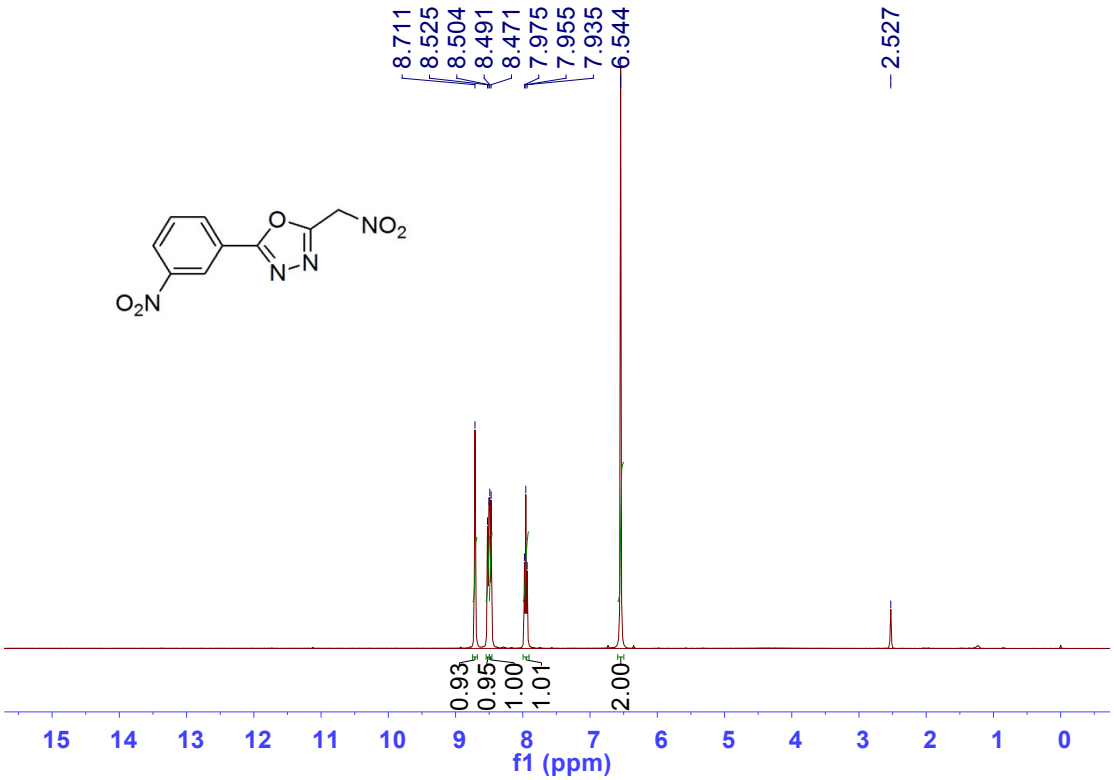
4. Copies of ^{1}H and ^{13}C NMR spectra of products




165.558
157.504
132.597
129.574
126.776
122.616
68.644
39.924
39.716
39.507
39.298
39.090
O
N
N
NO2
200
170
140
110
80
60
40
20
0
f1 (ppm)


8.283
8.268
8.261
8.098
8.087
8.077
8.026
8.010
8.001
7.991
6.546
3.200
2.531
O
N
N
NO2
NO2
1.07
1.07
2.05
2.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)


162.427
158.371
147.769
133.991
133.903
131.566
125.037
116.585
68.358
39.870
39.661
39.452
39.244
39.035
200
170
140
110
80
60
40
20
0
f1 (ppm)


8.711
8.525
8.504
8.491
8.471
7.975
7.955
7.935
6.544
2.527
O
N
N
NO2
O2N
0.93
0.95
1.00
1.01
2.00
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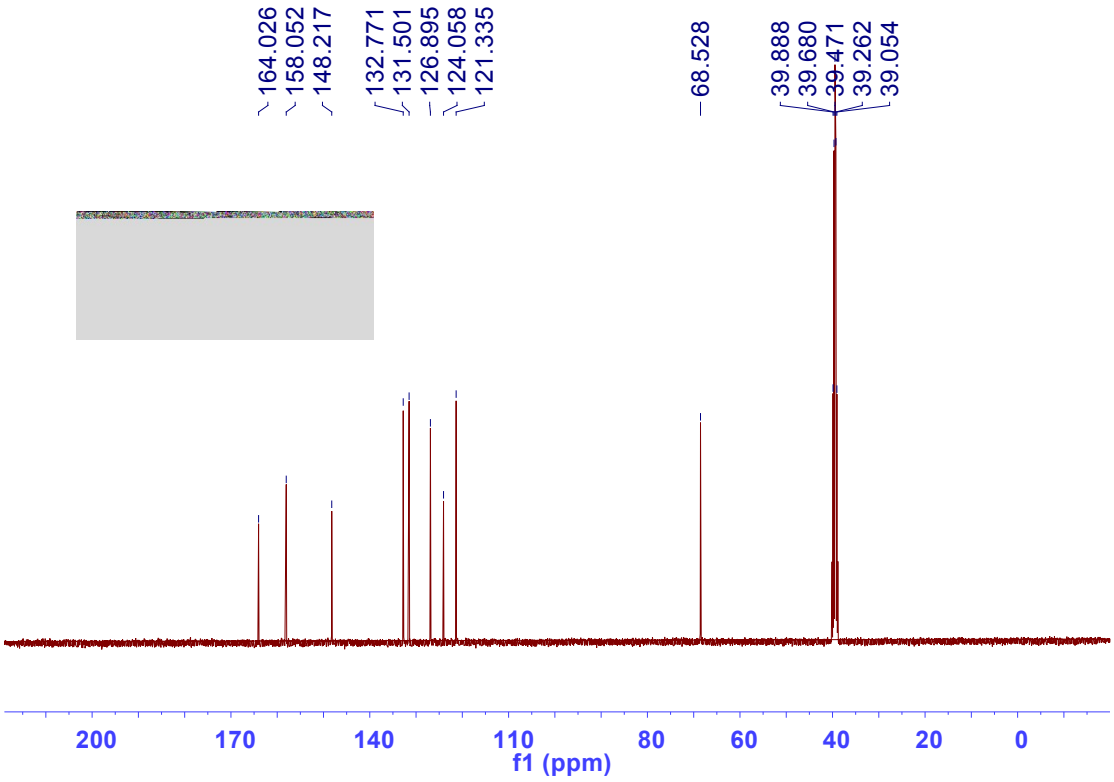
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)


164.026
158.052
148.217
132.771
131.501
126.895
124.058
121.335
68.528
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39.262
39.054
200
170
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110
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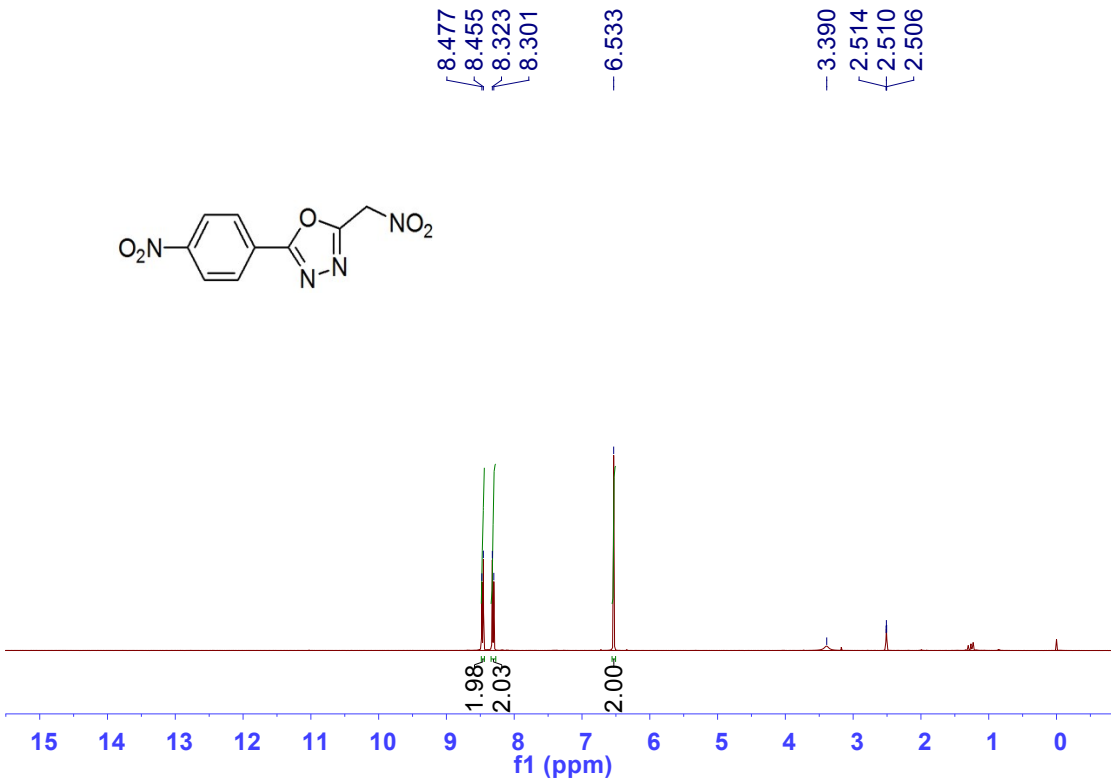
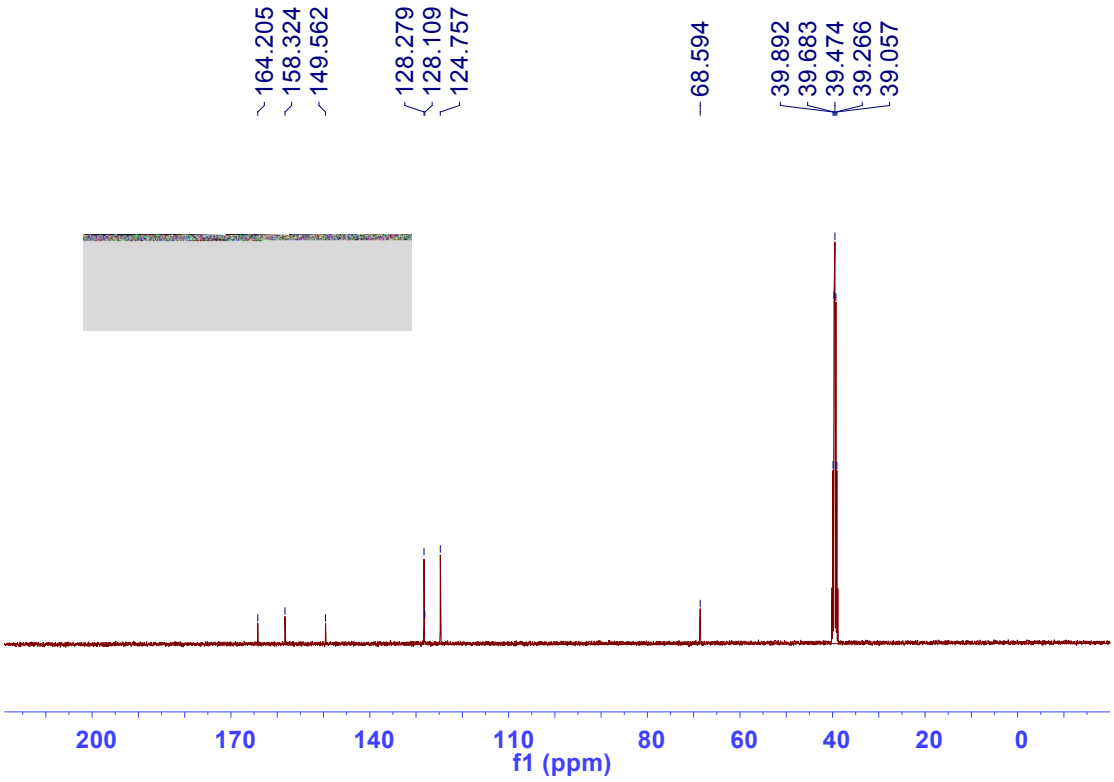
20
0
f1 (ppm)


8.477
8.455
8.323
8.301
6.533
3.390
2.514
2.510
2.506
O2N
O
NO2
N
N
1.98
2.03
2.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)


164.205
158.324
149.562
128.279
128.109
124.757
68.594
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39.474
39.266
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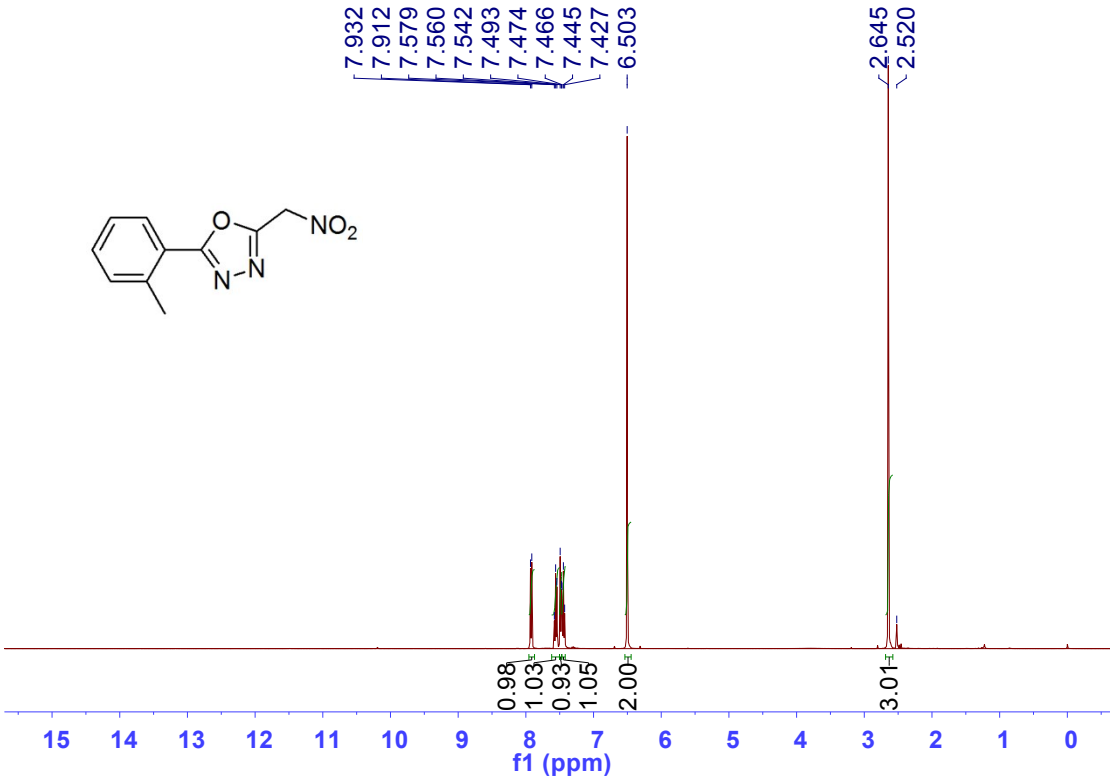
140
110
80
60
40
20
0
f1 (ppm)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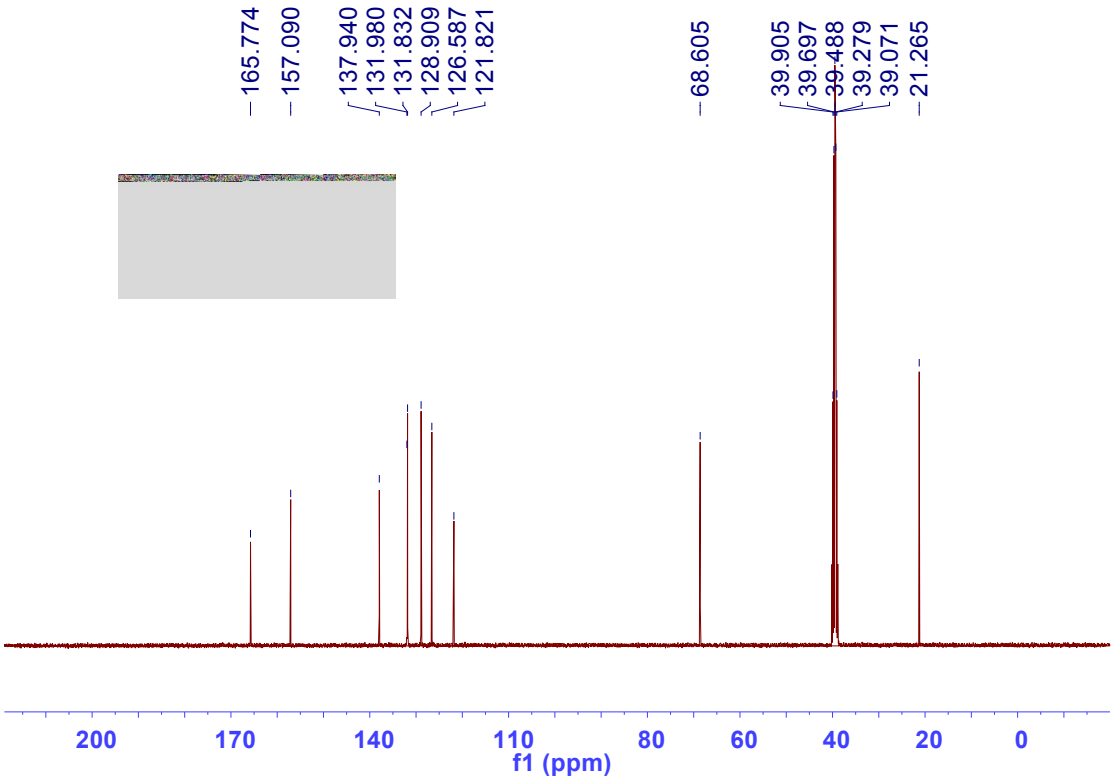
7.912
7.579
7.560
7.542
7.493
7.474
7.466
7.445
7.427
6.503
2.645
2.520
O
N
N
NO2
0.98
1.03
0.93
1.05
2.00
3.01
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)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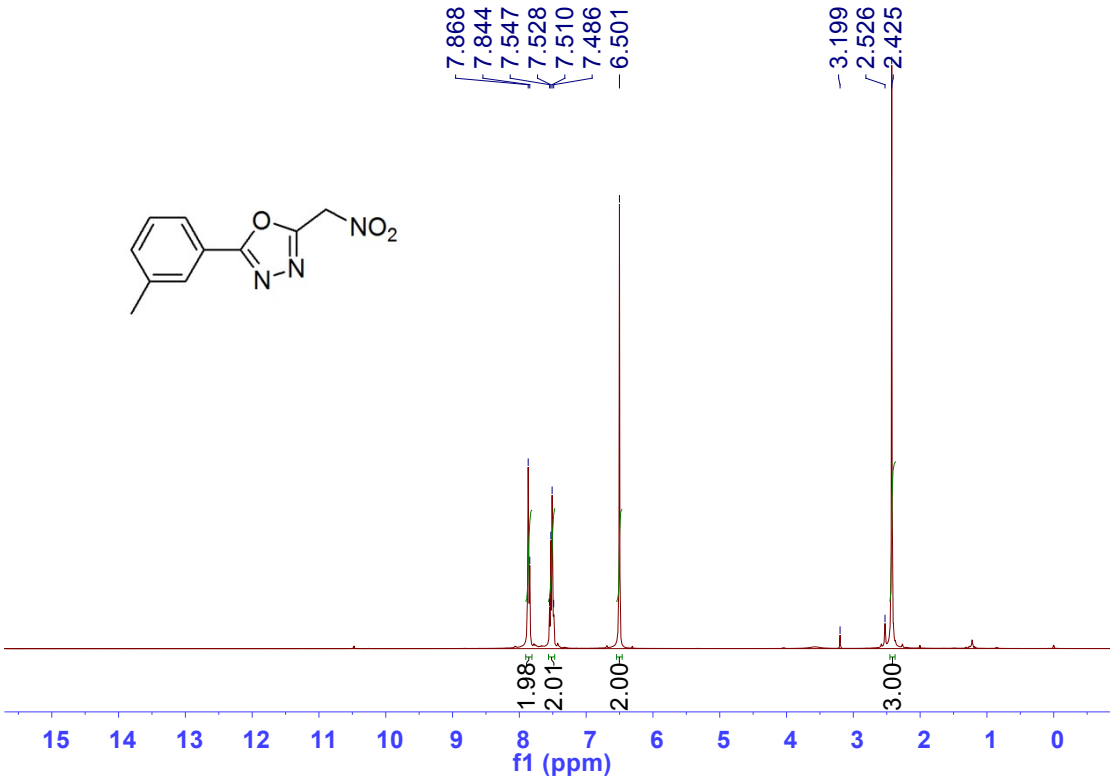
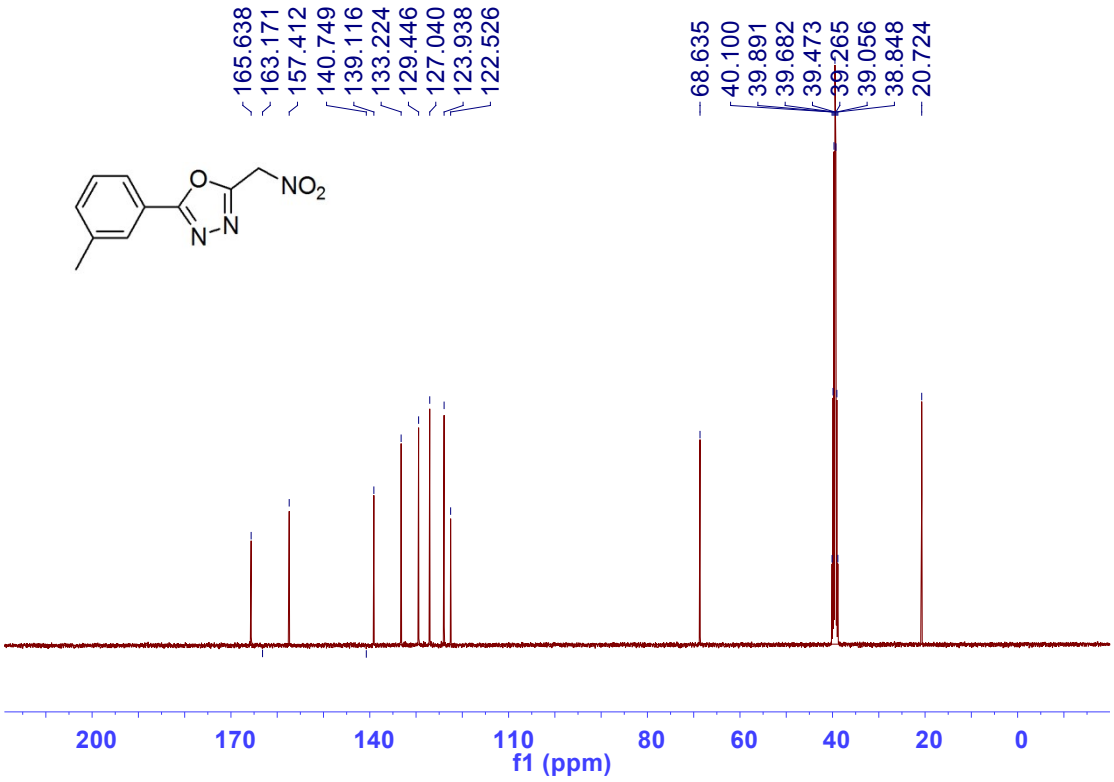
137.940
131.980
131.832
128.909
126.587
121.821
68.605
39.905
39.697
39.488
39.279
39.071
21.265
200
170
140
110
80
60
40
20
0
f1 (ppm)


7.868
7.844
7.547
7.528
7.510
7.486
6.501
3.199
2.526
2.425
O
N
N
NO2
1.98
2.01
2.00
3.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)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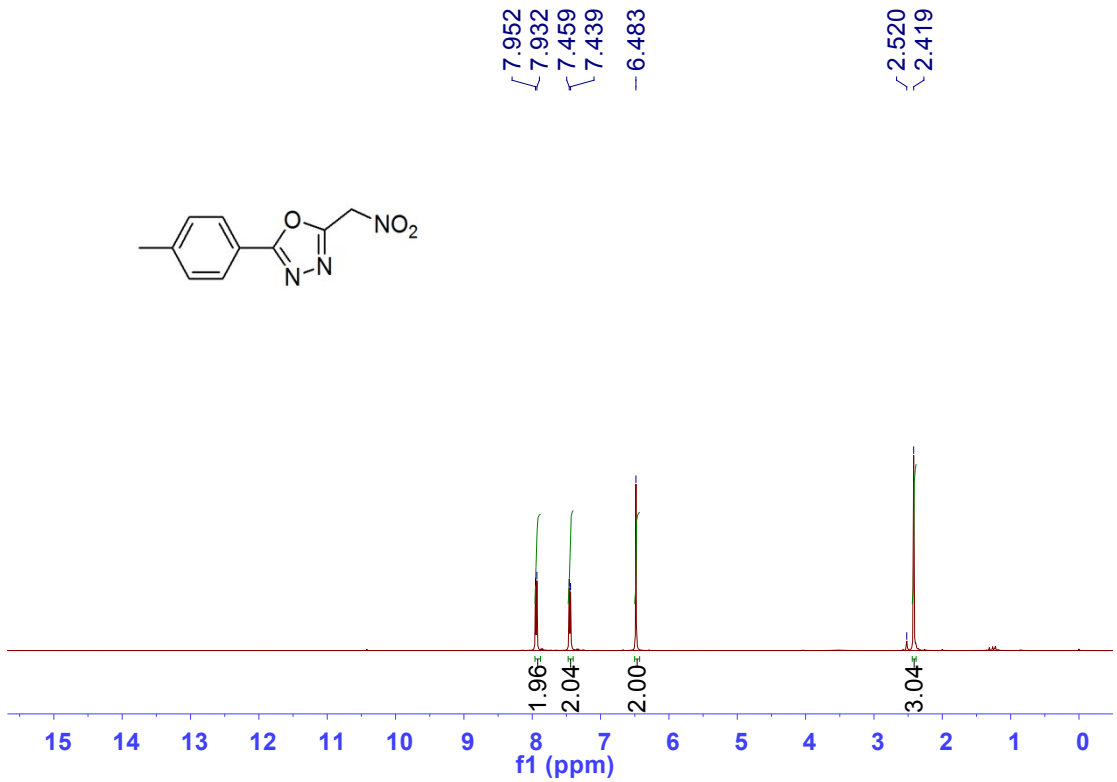
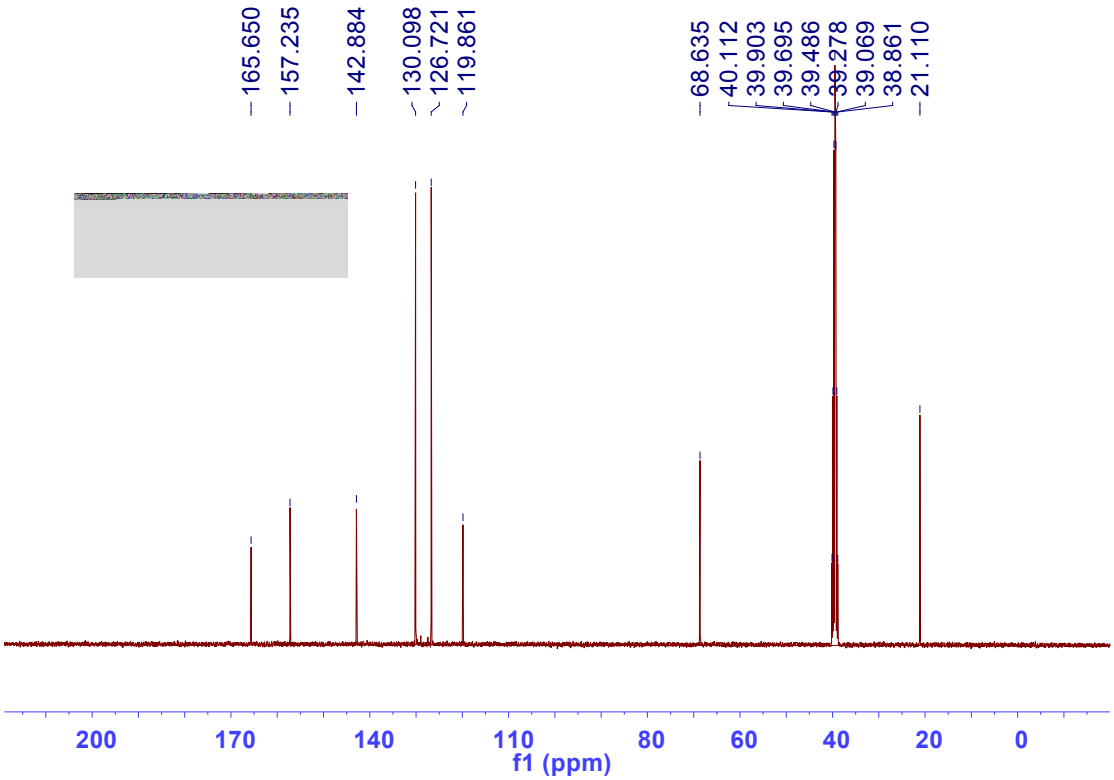
140.749
139.116
133.224
129.446
127.040
123.938
122.526
68.635
40.100
39.891
39.682
39.473
39.265
39.056
38.848
20.724
O
N
N
NO2
200
170
140
110
80
60
40
20
0
f1 (ppm)


7.952
7.932
7.459
7.439
6.483
2.520
2.419
O
N
N
NO2
1.96
2.04
2.00
3.04
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)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142.884
130.098
126.721
119.861
68.635
40.112
39.903
39.695
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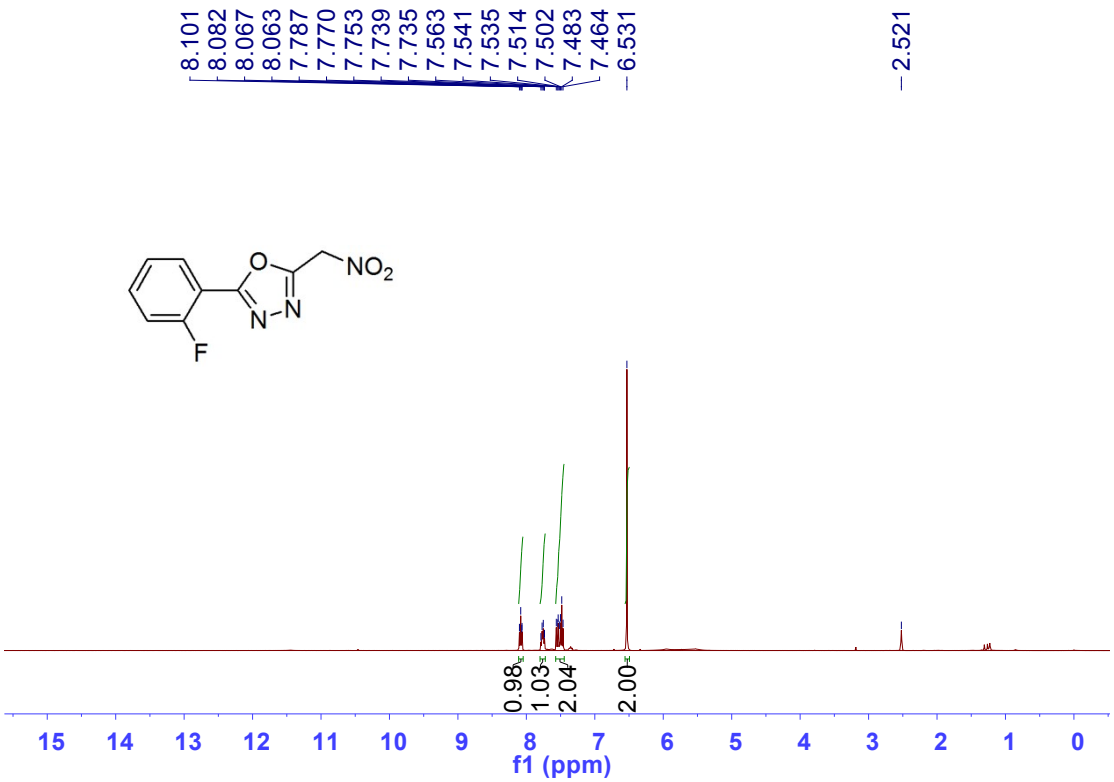
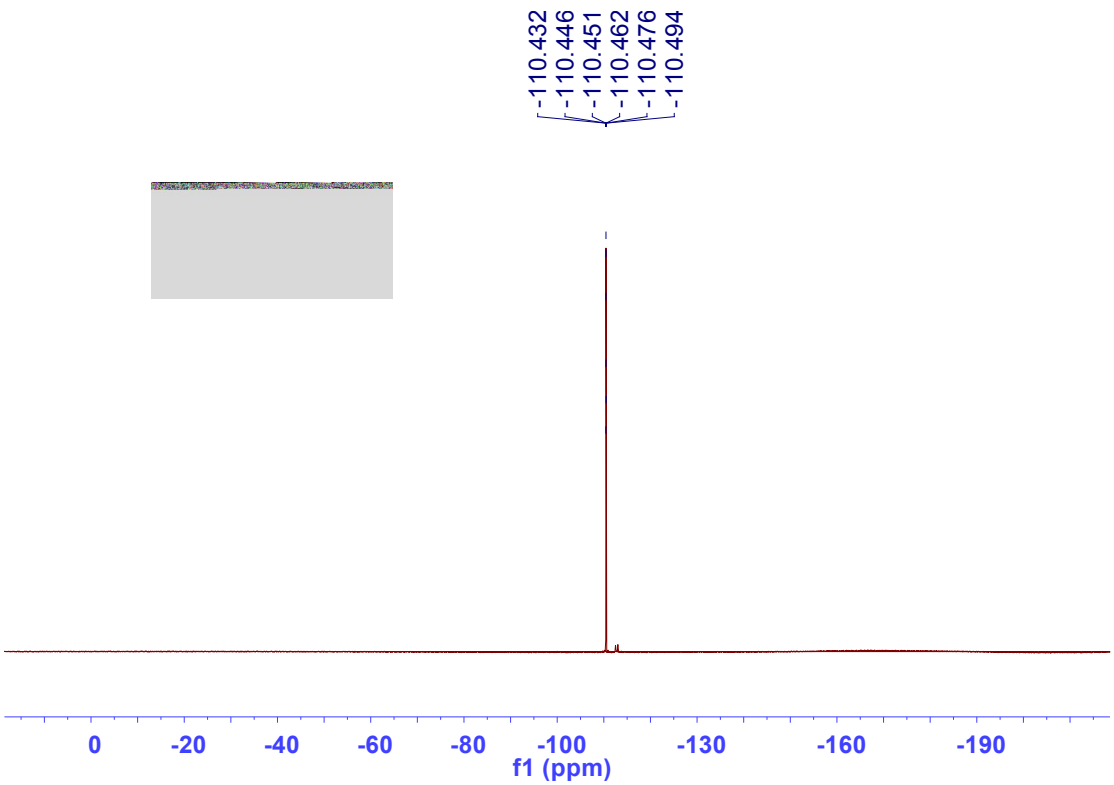
39.069
38.861
21.110
200
170
140
110
80
60
40
20
0
f1 (ppm)


8.101
8.082
8.067
8.063
7.787
7.770
7.753
7.739
7.735
7.563
7.541
7.535
7.514
7.502
7.483
7.464
6.531
2.521
O
N
N
NO2
F
0.98
1.03
2.04
2.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)


-110.432
-110.446
-110.451
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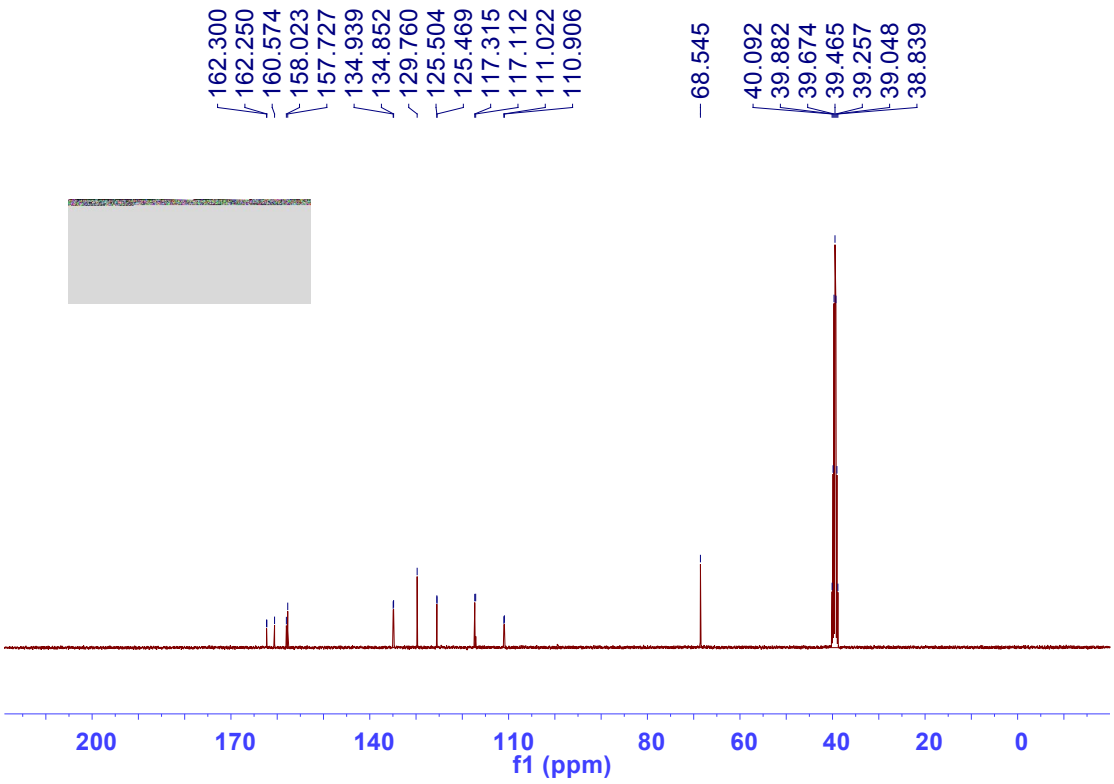
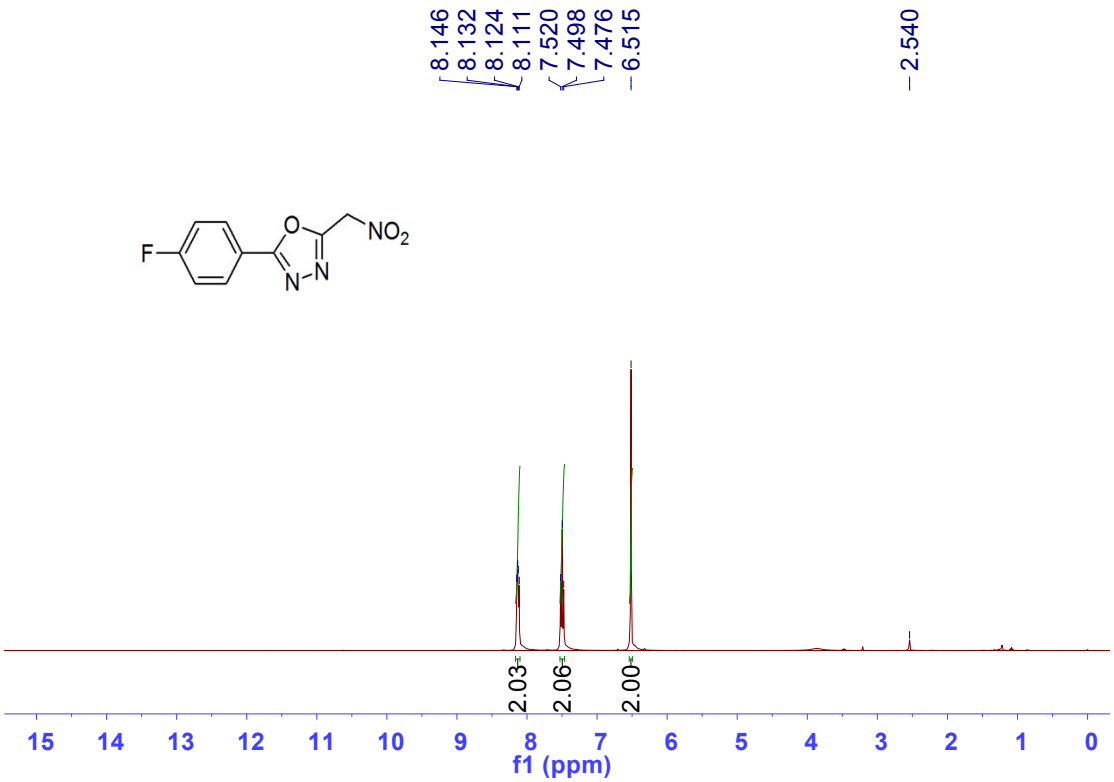
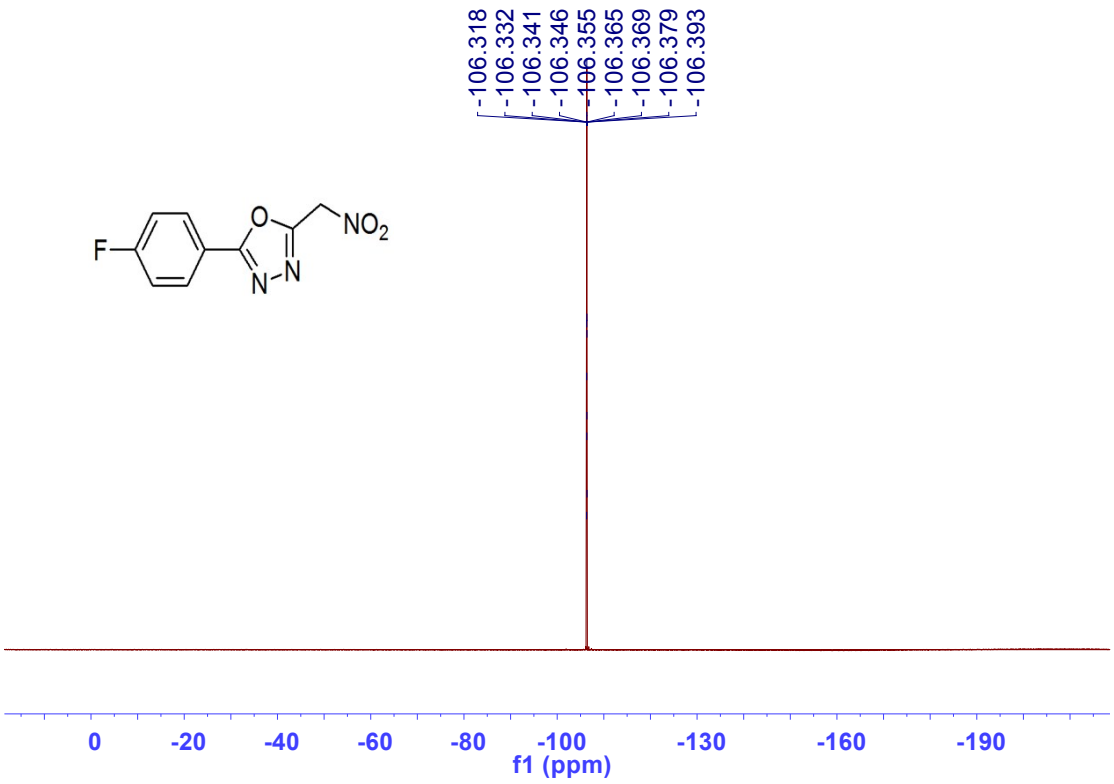
-110.494
0
-20
-40
-60
-80
-100
-130
-160
-190
f1 (ppm)


162.300
162.250
160.574
158.023
157.727
134.939
134.852
129.760
125.504
125.469
117.315
117.112
111.022
110.906
68.545
40.092
39.882
39.674
39.465
39.257
39.048
38.839
200
170
140
110
80
60
40
20
0
f1 (ppm)


8.146
8.132
8.124
8.111
7.520
7.498
7.476
6.515
2.540
F
O
N
N
NO2
2.03
2.06
2.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)


-106.318
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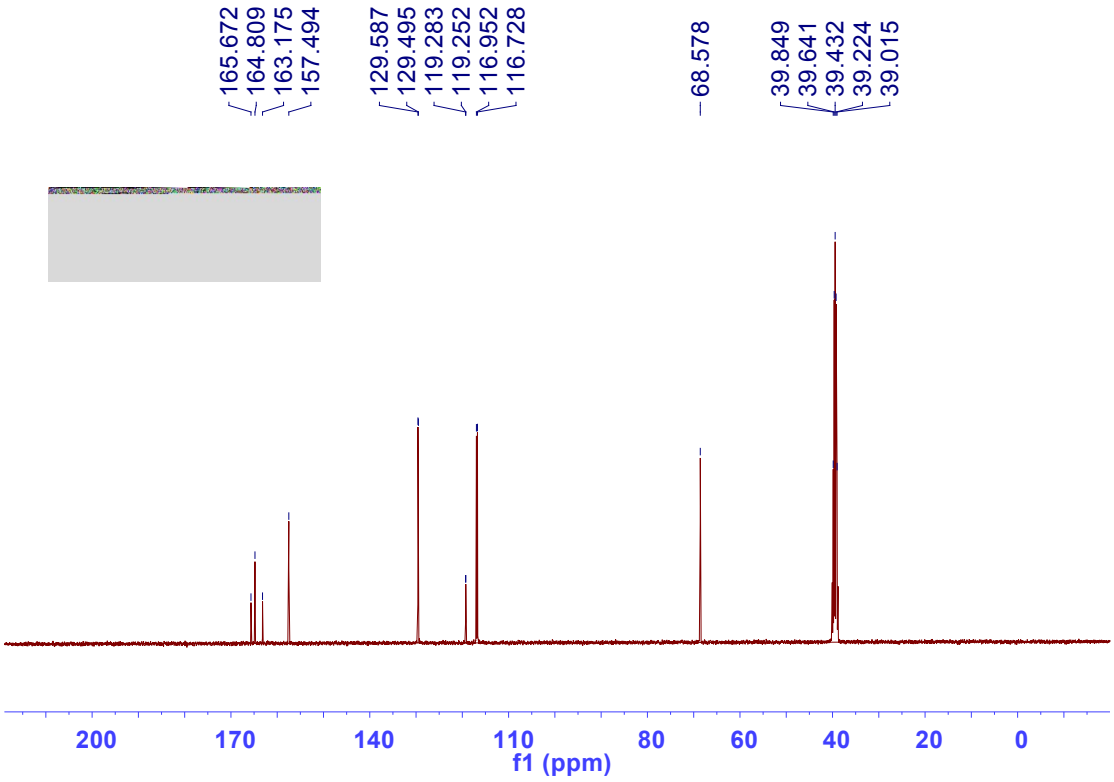
-106.341
-106.346
-106.355
-106.365
-106.369
-106.379
-106.393
F
O
N
N
NO2
0
-20
-40
-60
-80
-100
-130
-160
-190
f1 (ppm)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129.587
129.495
119.283
119.252
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116.728
68.578
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39.432
39.224
39.015
200
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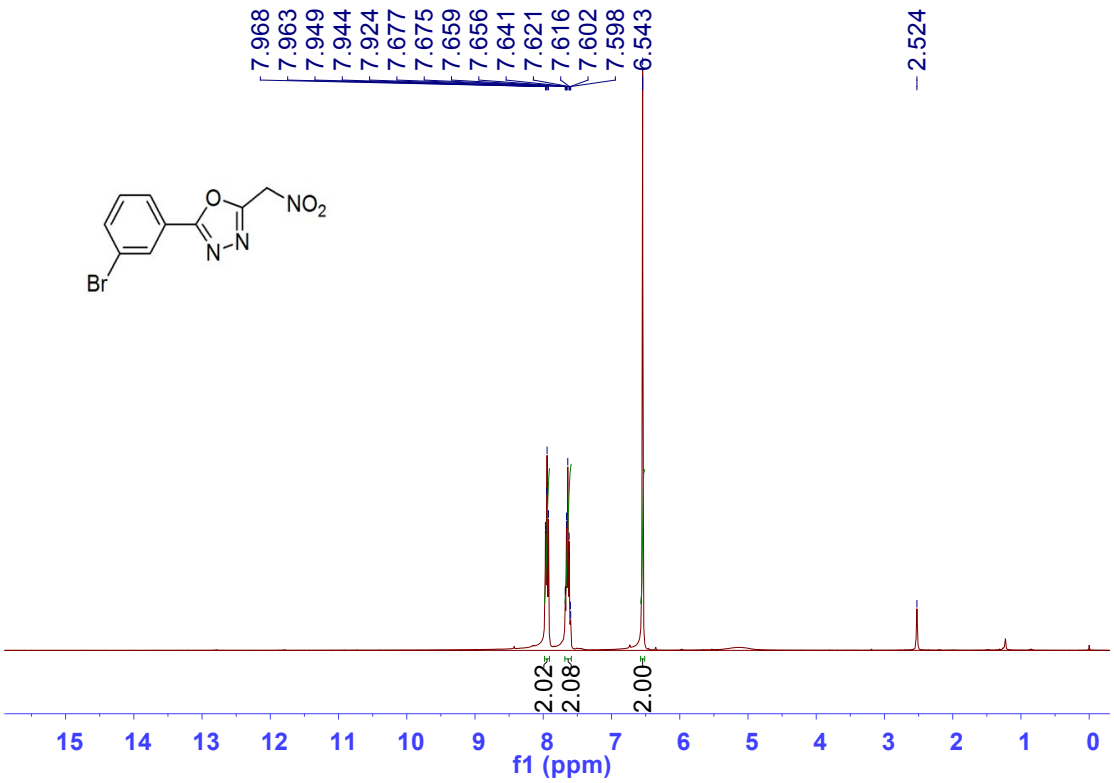
140
110
80
60
40
20
0
f1 (ppm)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7.677
7.675
7.659
7.656
7.641
7.621
7.616
7.602
7.598
6.543
2.524
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N
NO2
Br
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2.08
2.00
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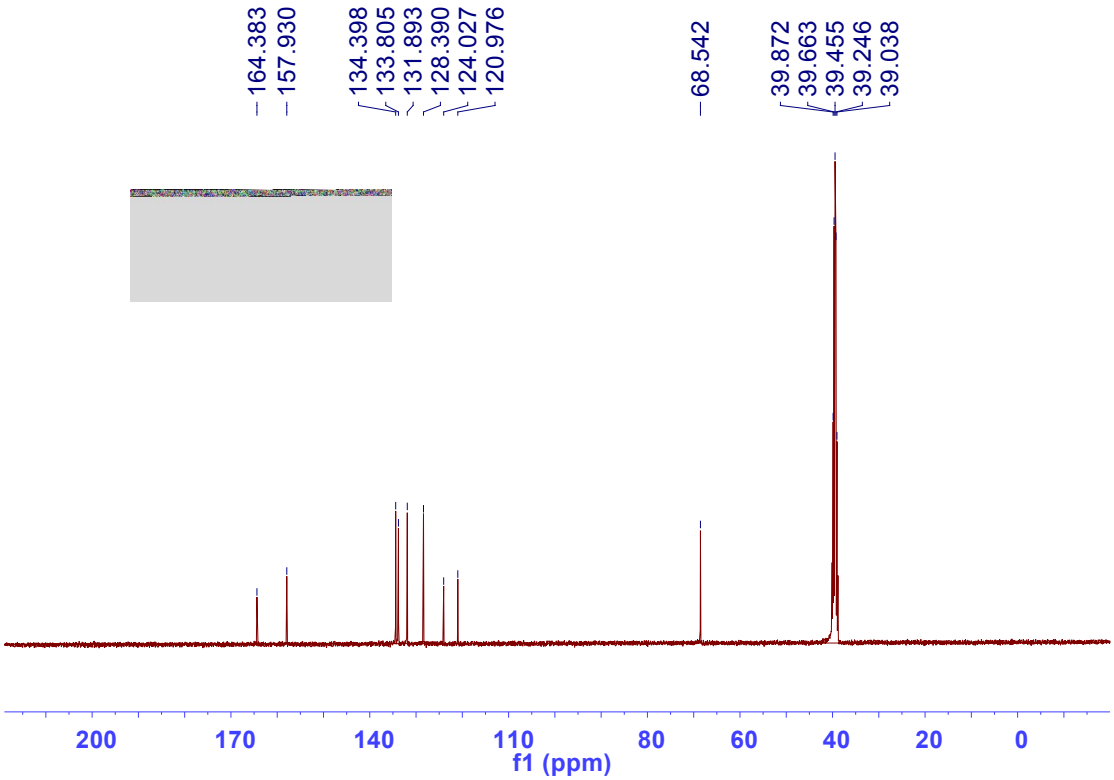
f1 (ppm)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120.976
68.542
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39.246
39.038
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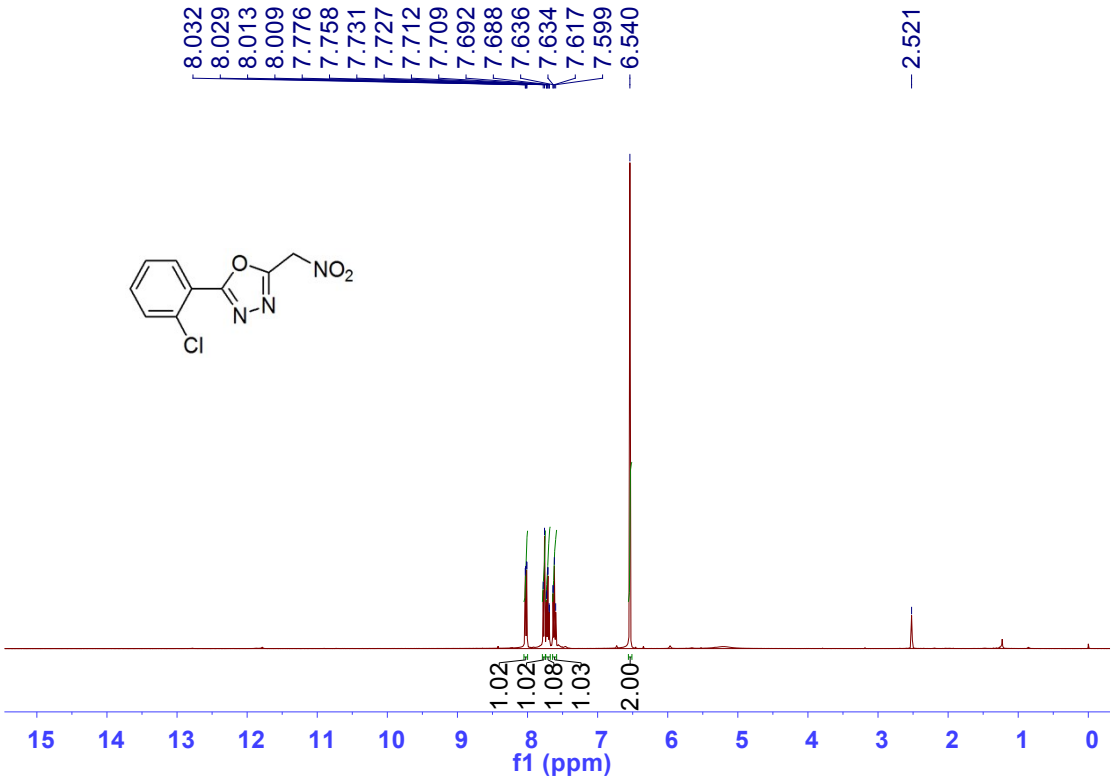
140
110
80
60
40
20
0
f1 (ppm)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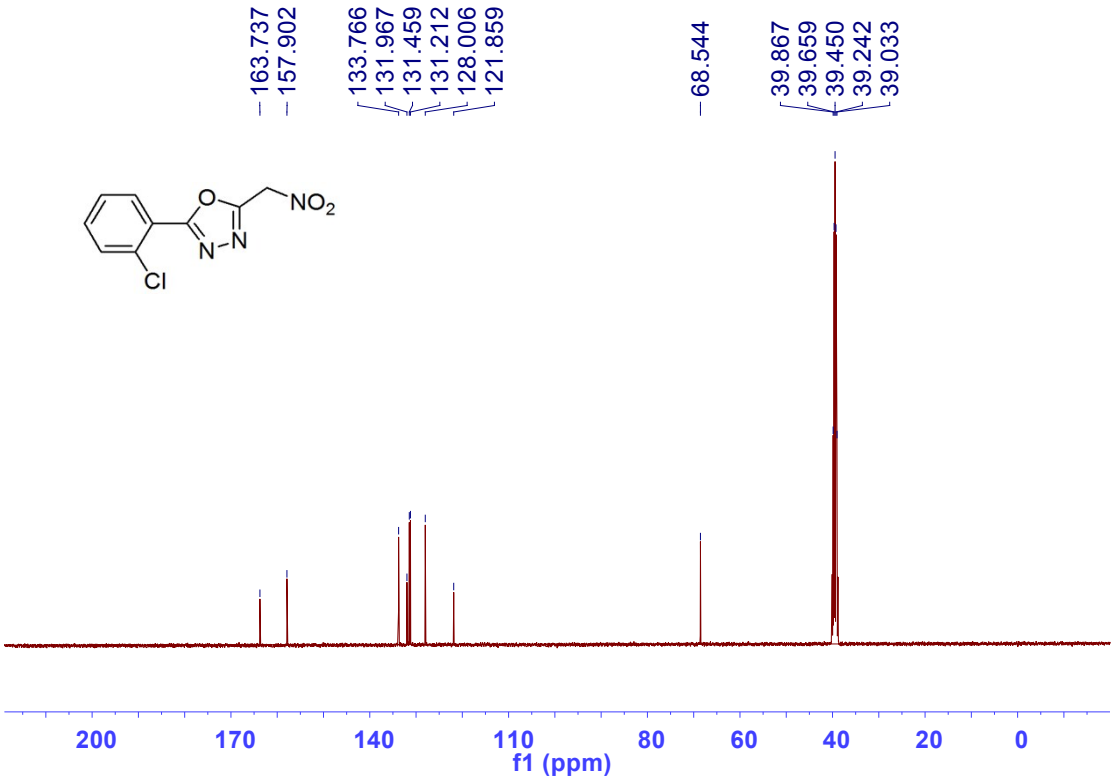
7.758
7.731
7.727
7.712
7.709
7.692
7.688
7.636
7.634
7.617
7.599
6.540
2.521
O
NO2
N
N
Cl
1.02
1.02
1.08
1.03
2.00
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)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131.967
131.459
131.212
128.006
121.859
68.544
39.867
39.659
39.450
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N
NO2
Cl
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110
80
60
40
20
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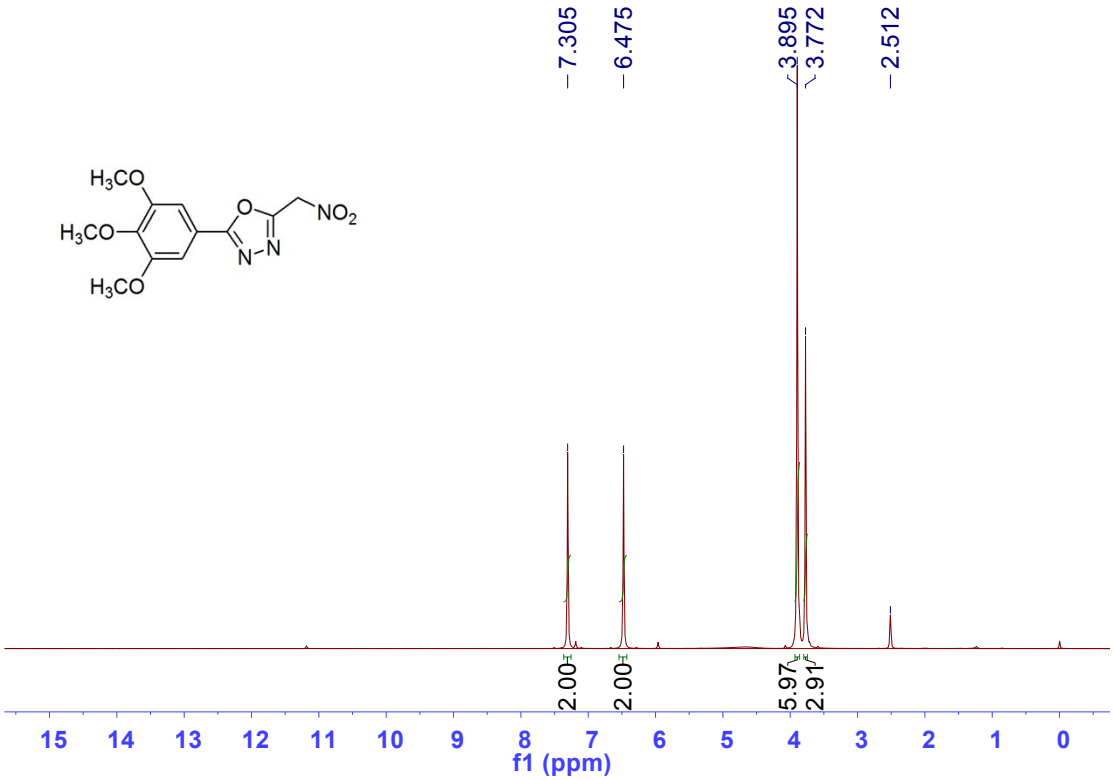
f1 (ppm)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6.475
3.895
3.772
2.512
2.00
2.00
5.97
2.91
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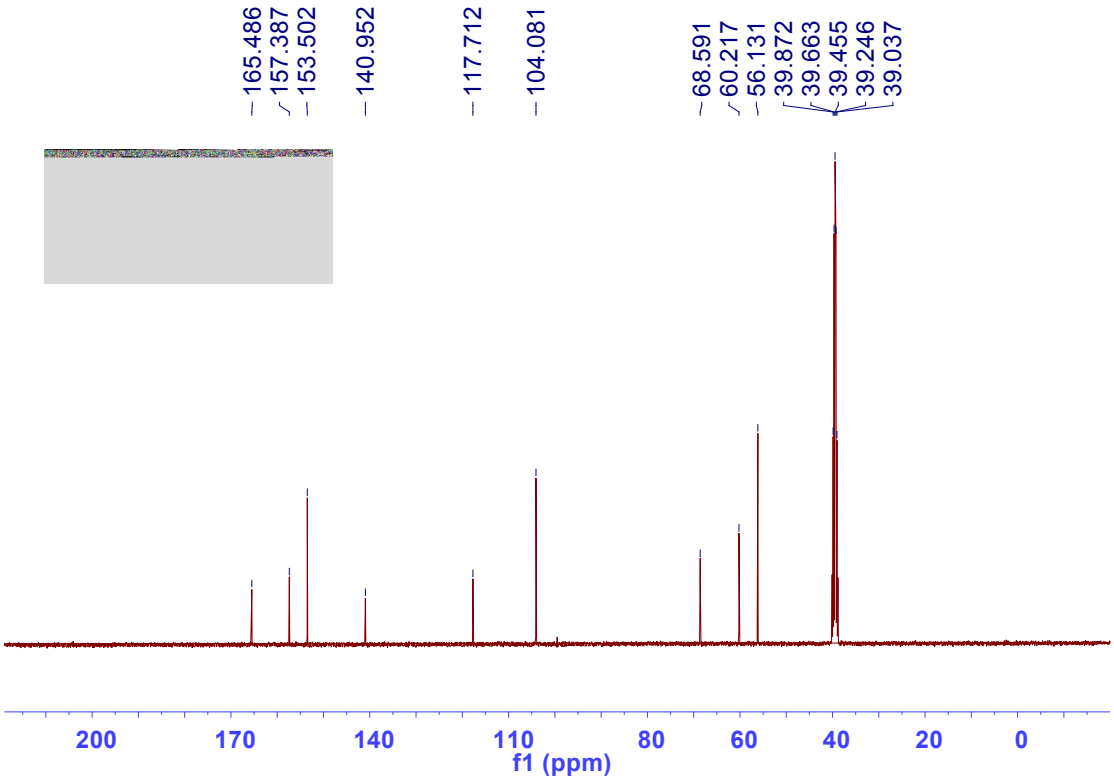
f1 (ppm)
H3CO
H3CO
H3CO
O
N
N
NO2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153.502
140.952
117.712
104.081
68.591
60.217
56.131
39.872
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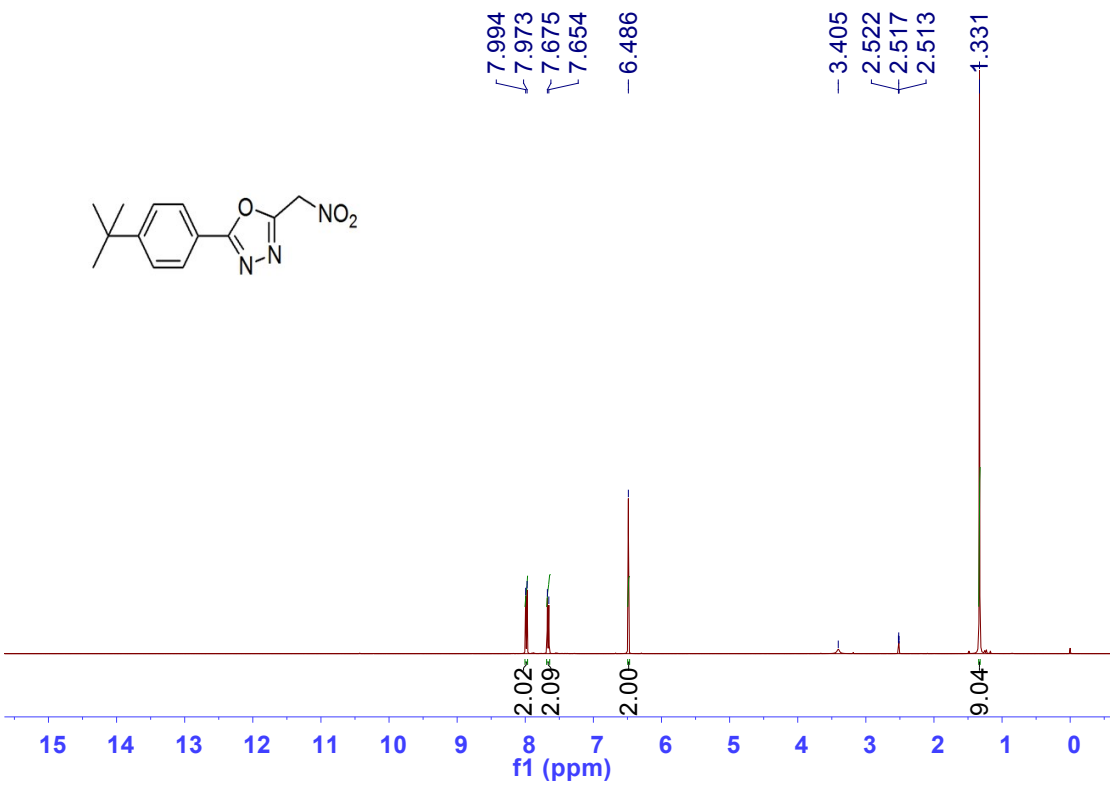
39.455
39.246
39.037
200
170
140
110
80
60
40
20
0
f1 (ppm)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7.675
7.654
6.486
3.405
2.522
2.517
2.513
1.331
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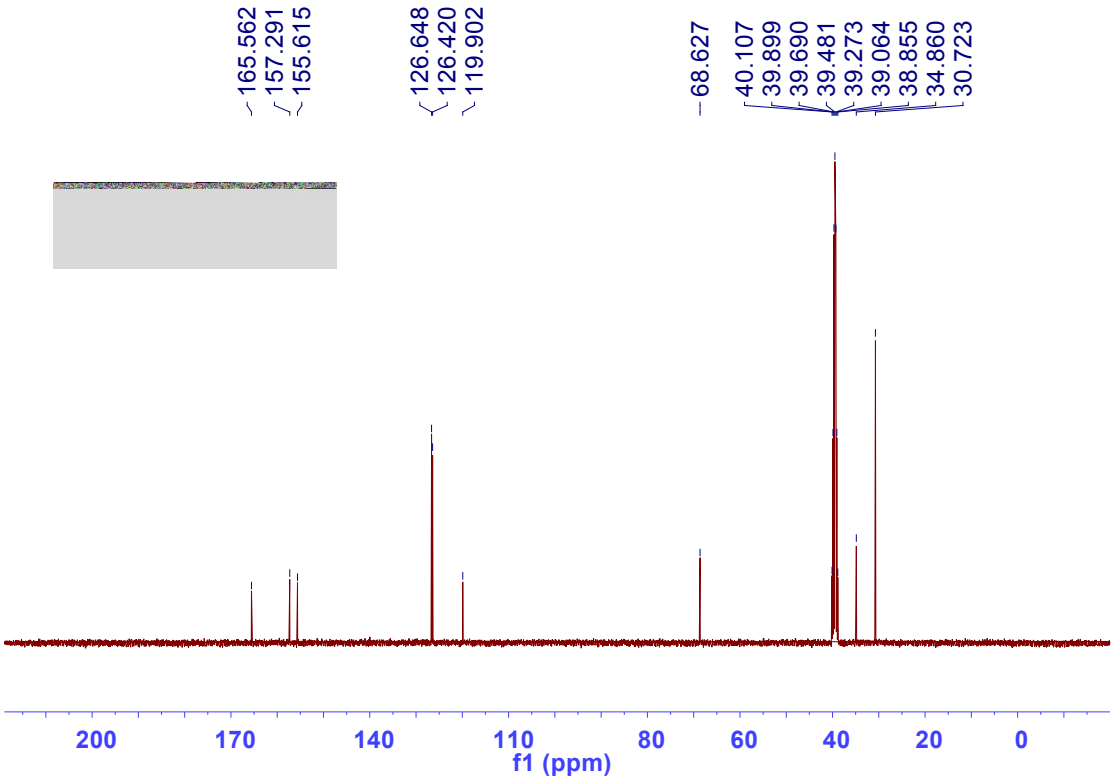
O
N
N
2.02
2.09
2.00
9.04
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)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126.648
126.420
119.902
68.627
40.107
39.899
39.690
39.481
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110
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60
40
20
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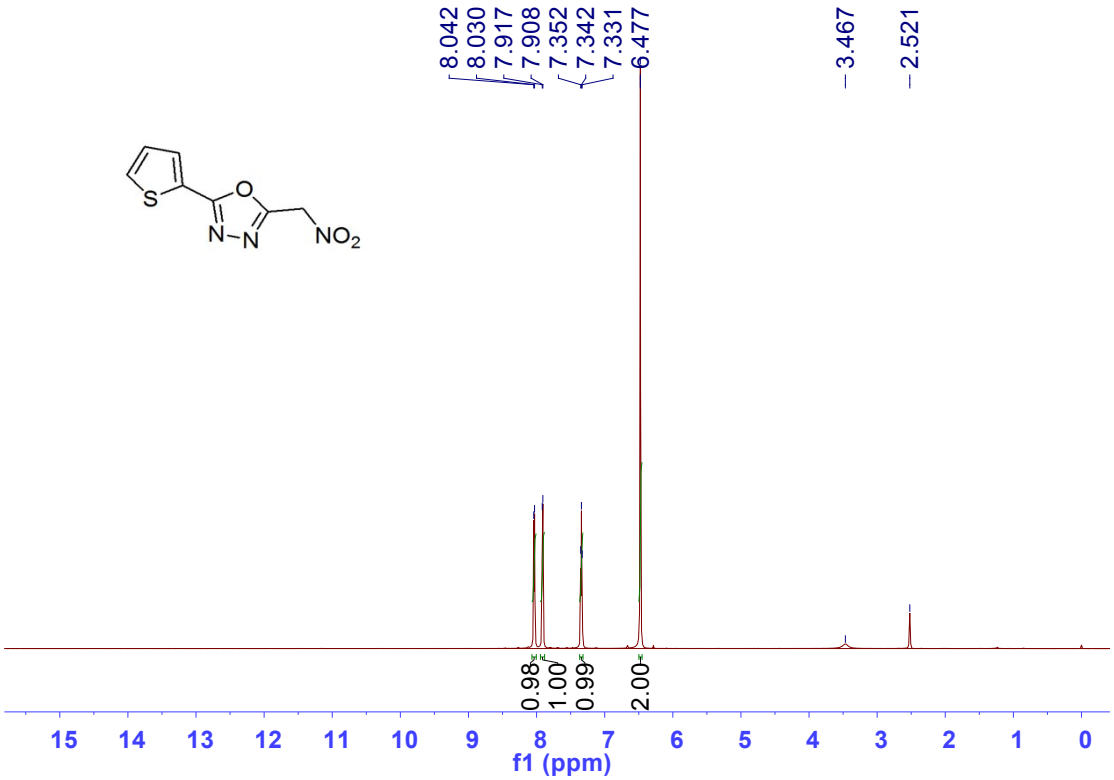
f1 (ppm)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7.342
7.331
6.477
3.467
2.521
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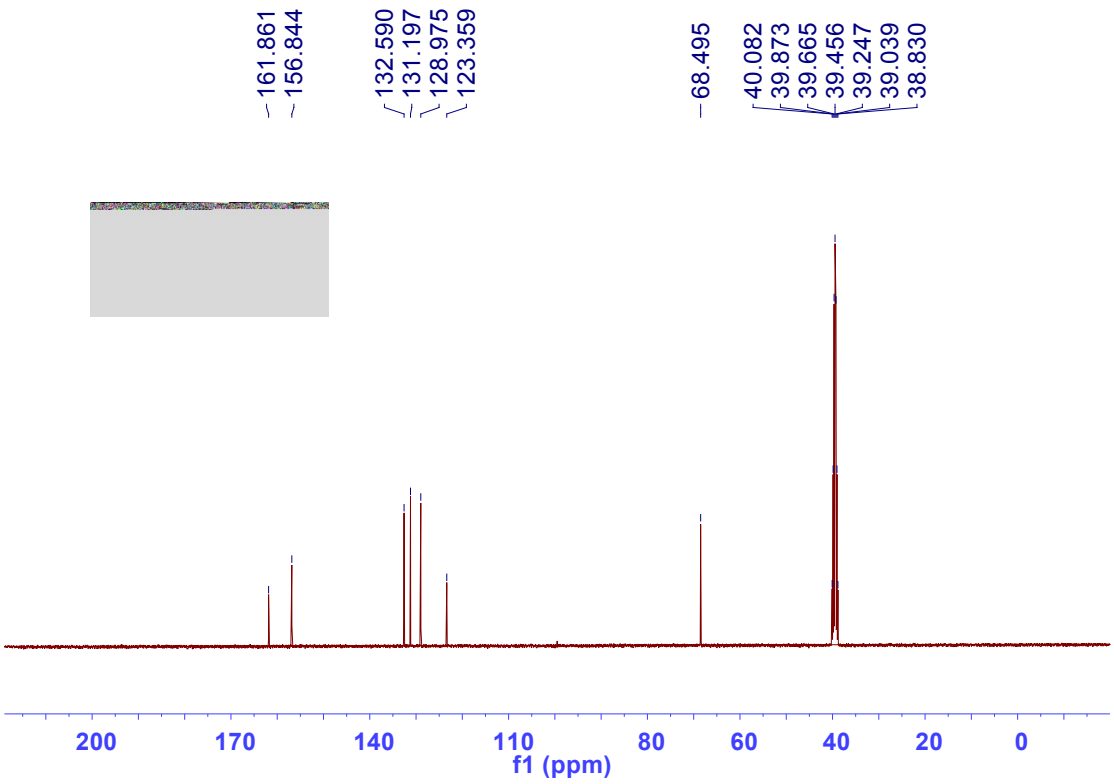
0.99
2.00
S
O
N
N
NO2
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)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132.590
131.197
128.975
123.359
68.495
40.082
39.873
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39.247
39.039
38.830
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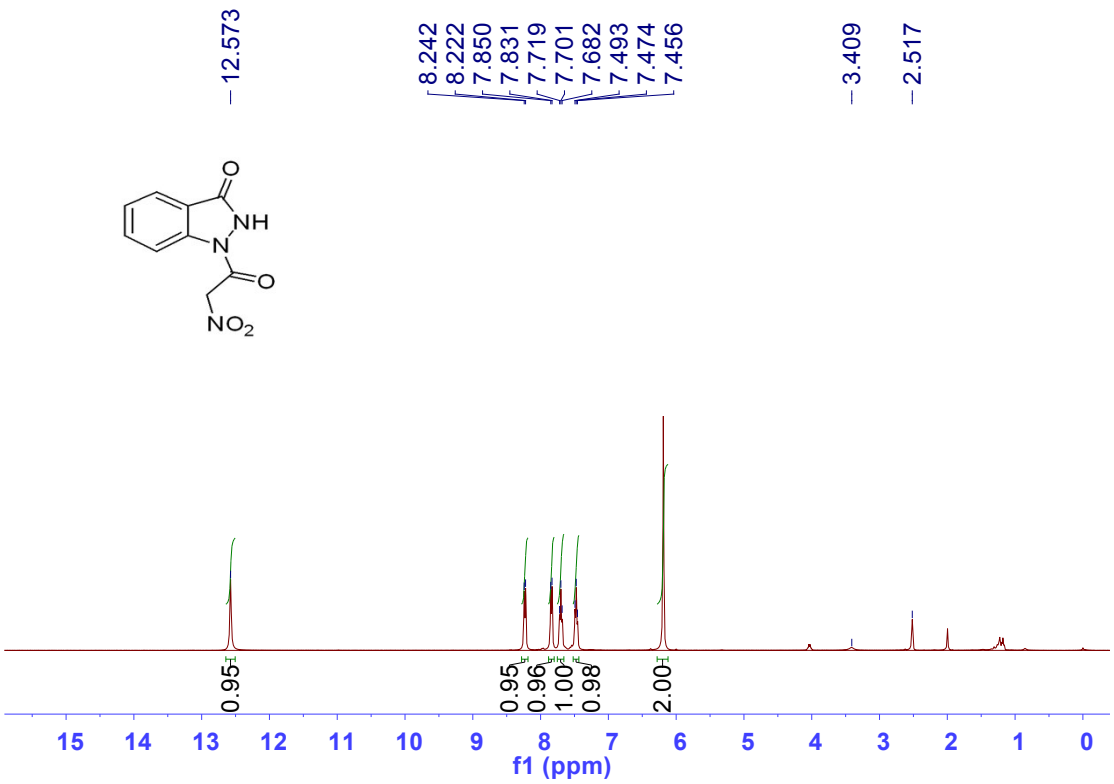
110
80
60
40
20
0
f1 (ppm)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7.719
7.701
7.682
7.493
7.474
7.456
3.409
2.517
O
NH
N
O
NO2
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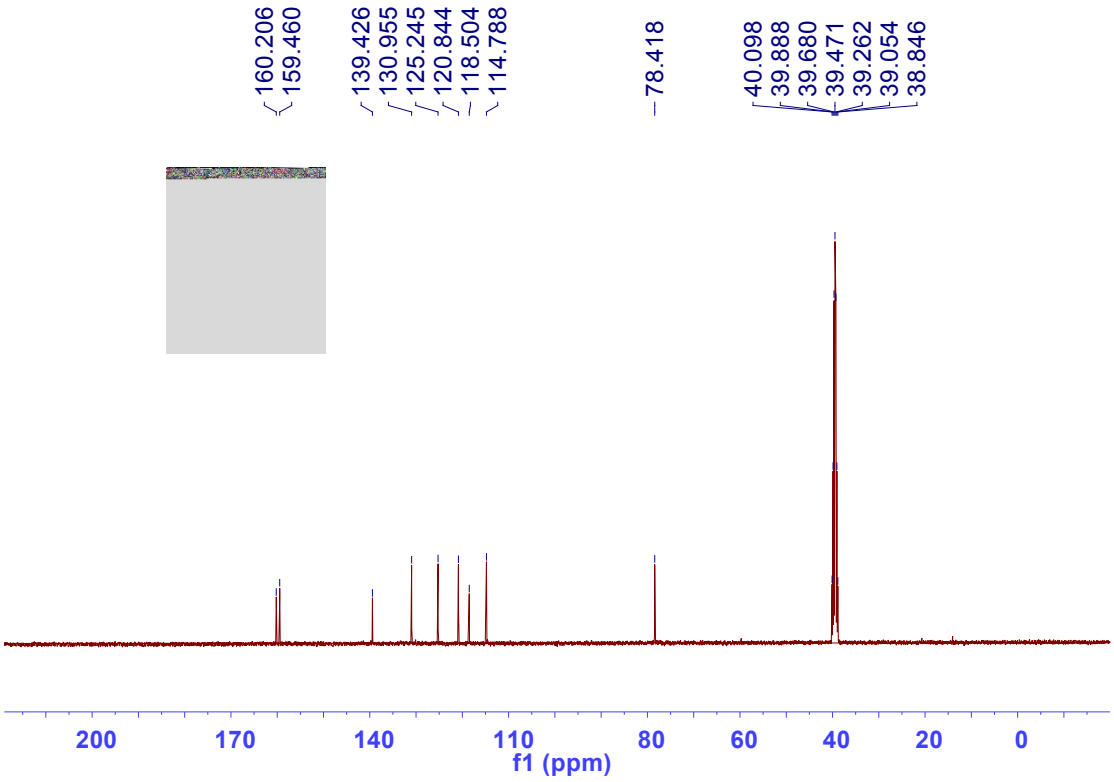
0.95
0.96
1.00
0.98
2.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)


160.206
159.460
139.426
130.955
125.245
120.844
118.504
114.788
78.418
40.098
39.888
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39.471
39.262
39.054
38.846
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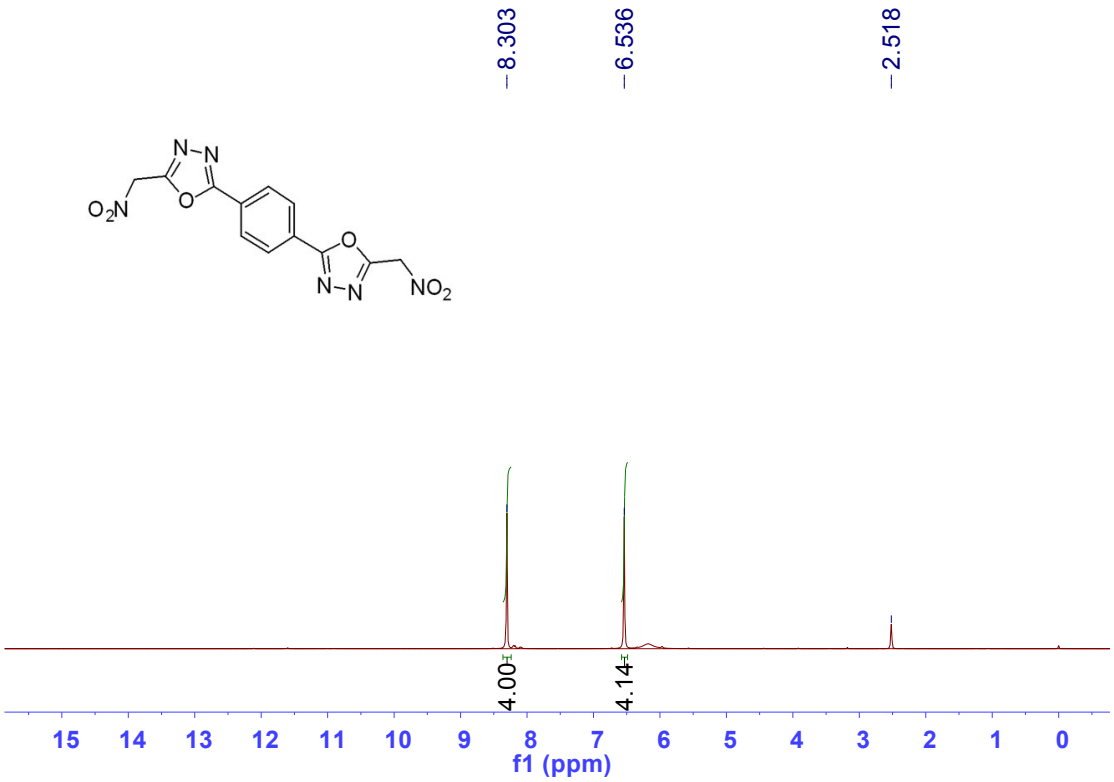
140
110
80
60
40
20
0
f1 (ppm)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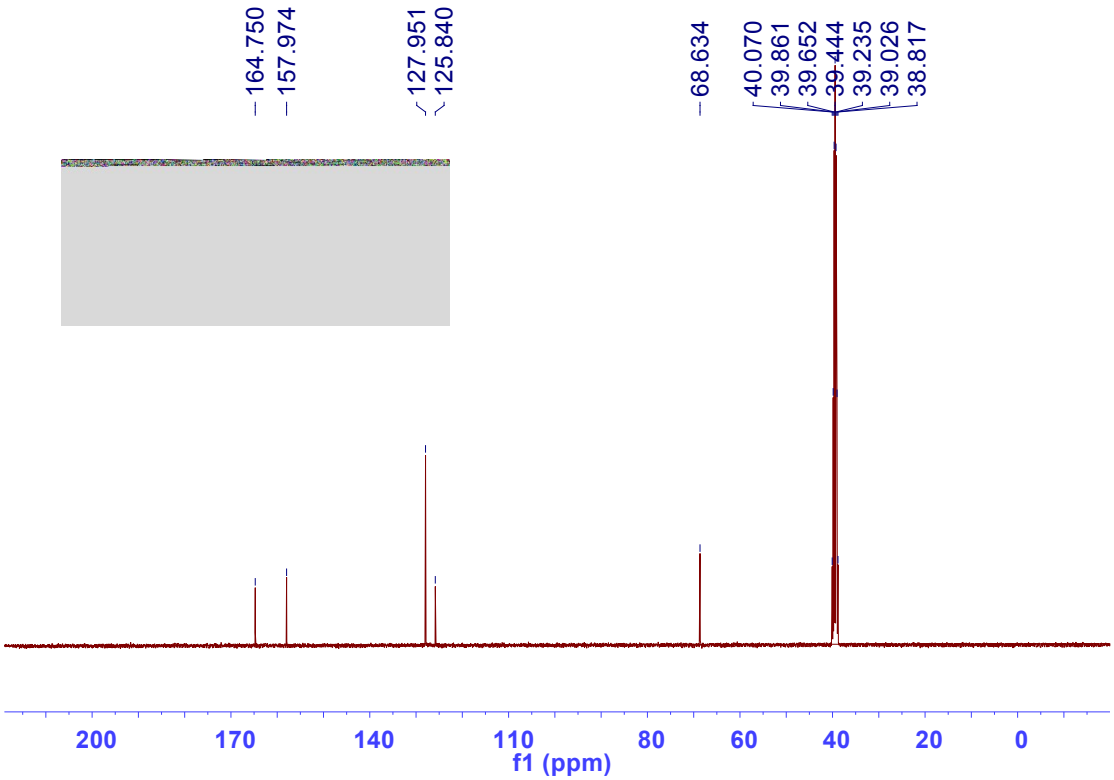
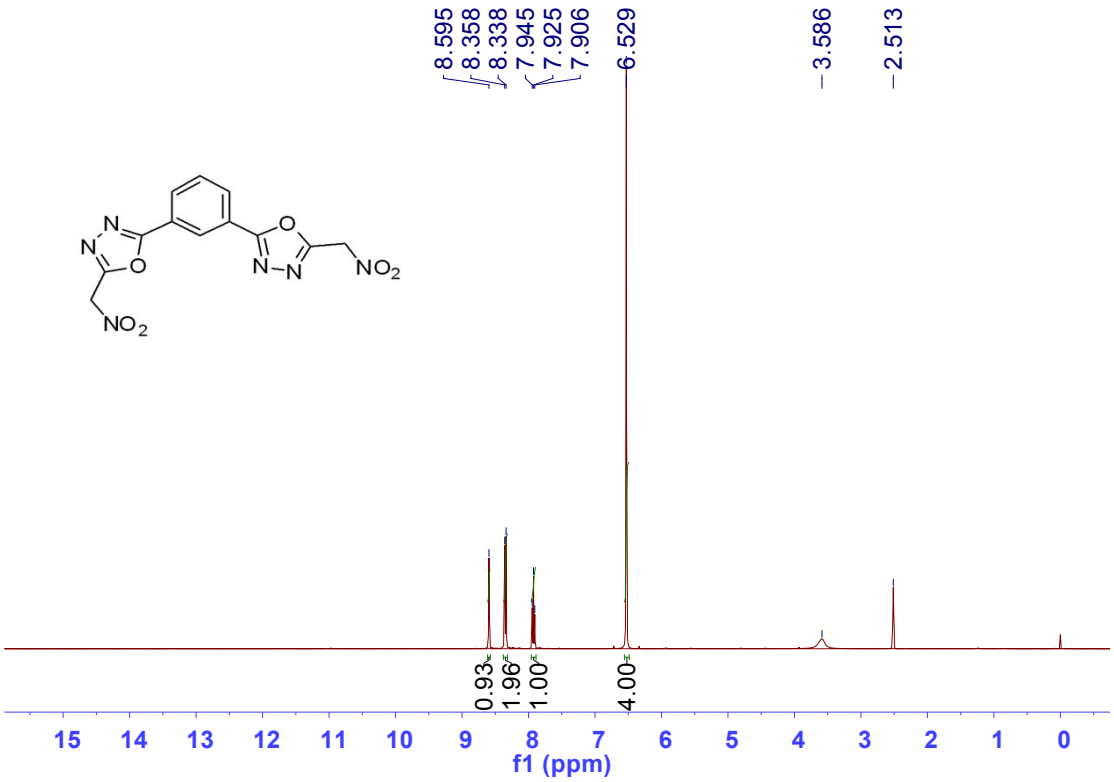
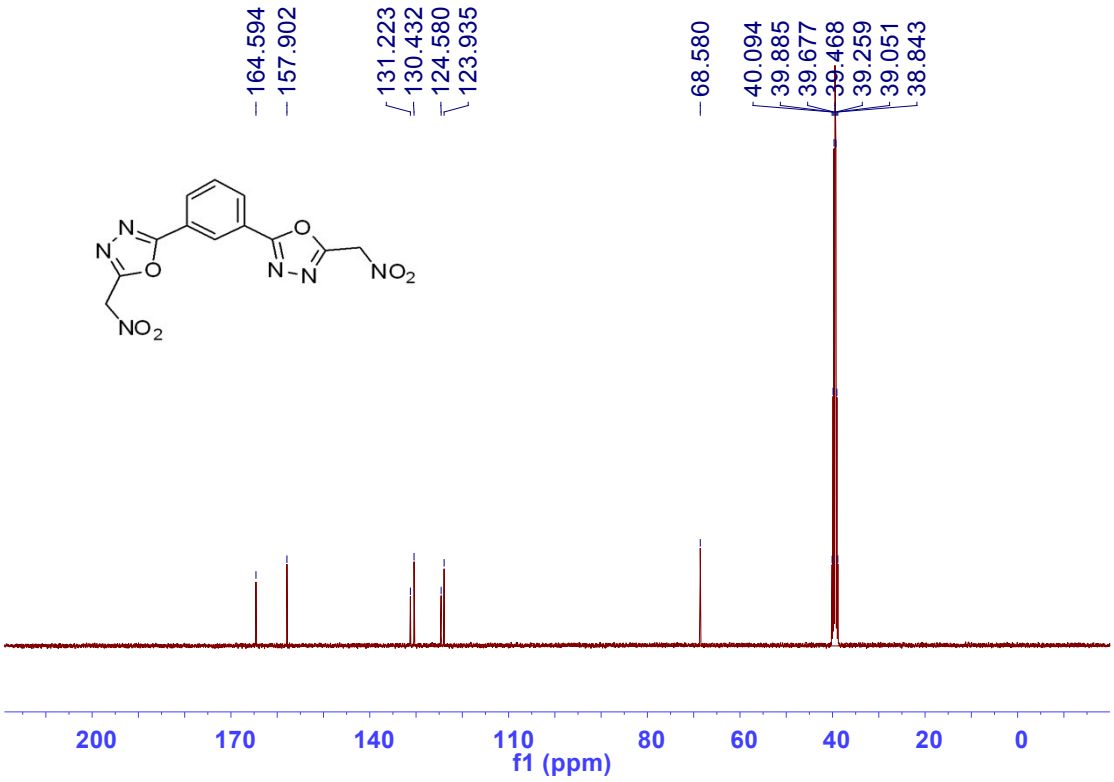
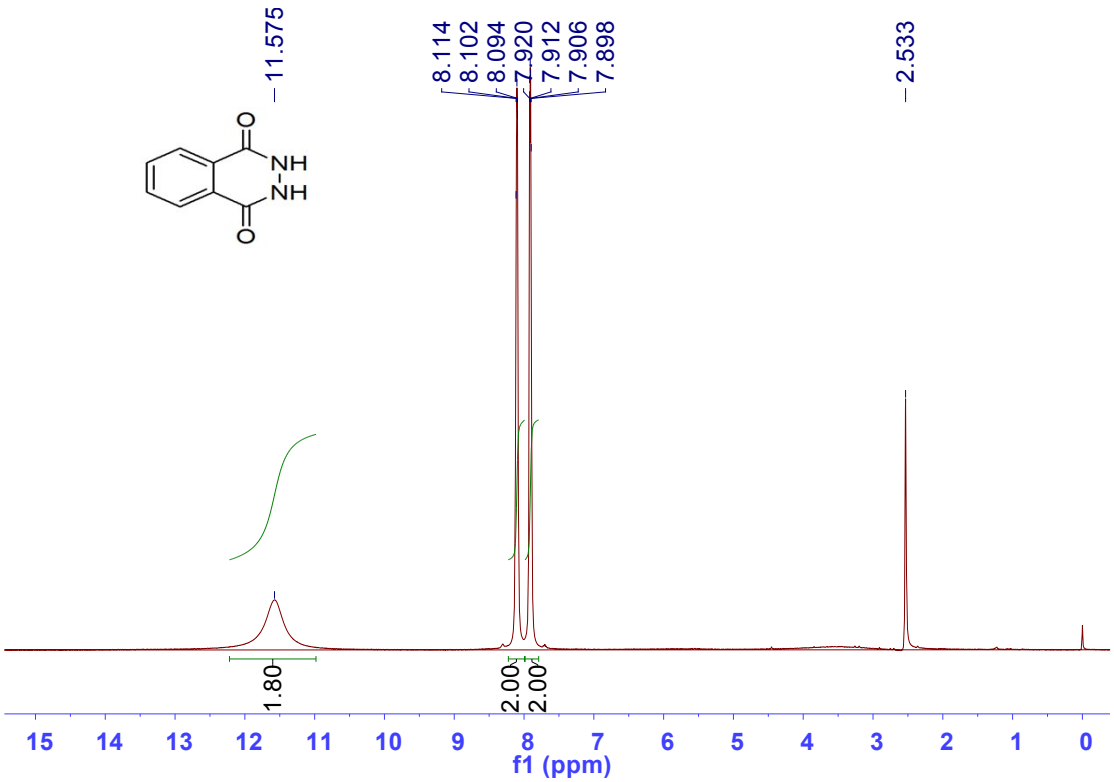
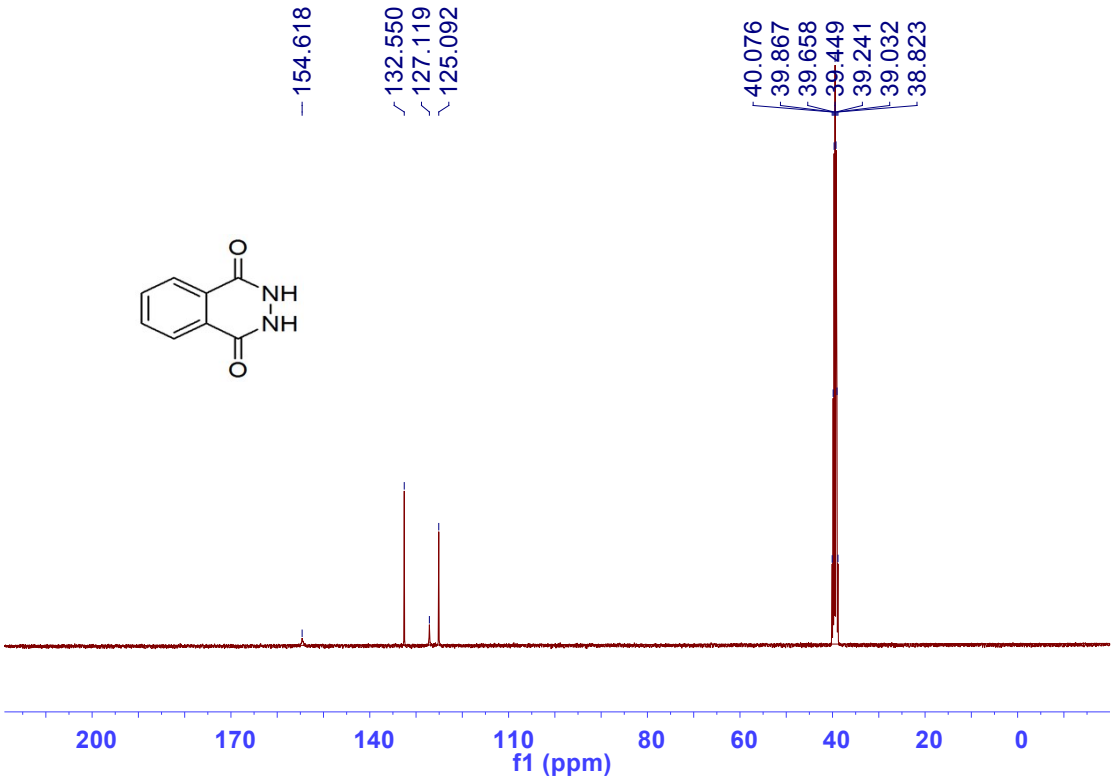
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)

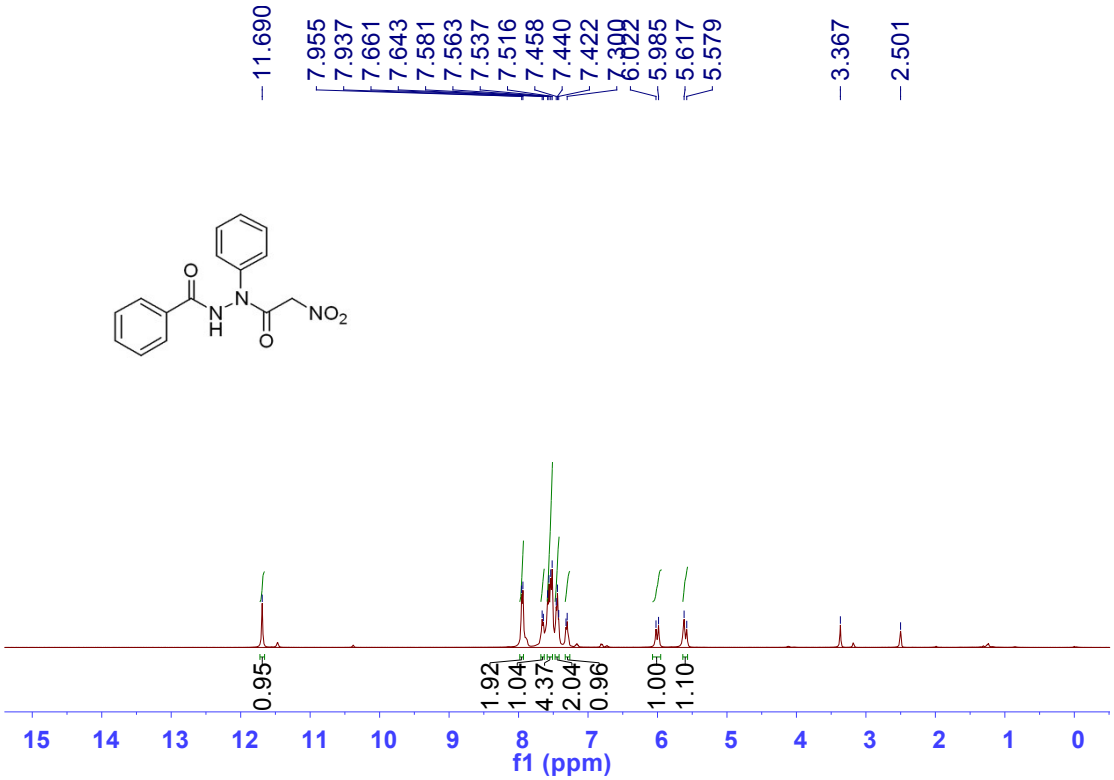

164.750
157.974
127.951
125.840
68.634
40.070
39.861
39.652
39.444
39.235
39.026
38.817
200
170
140
110
80
60
40
20
0
f1 (ppm)

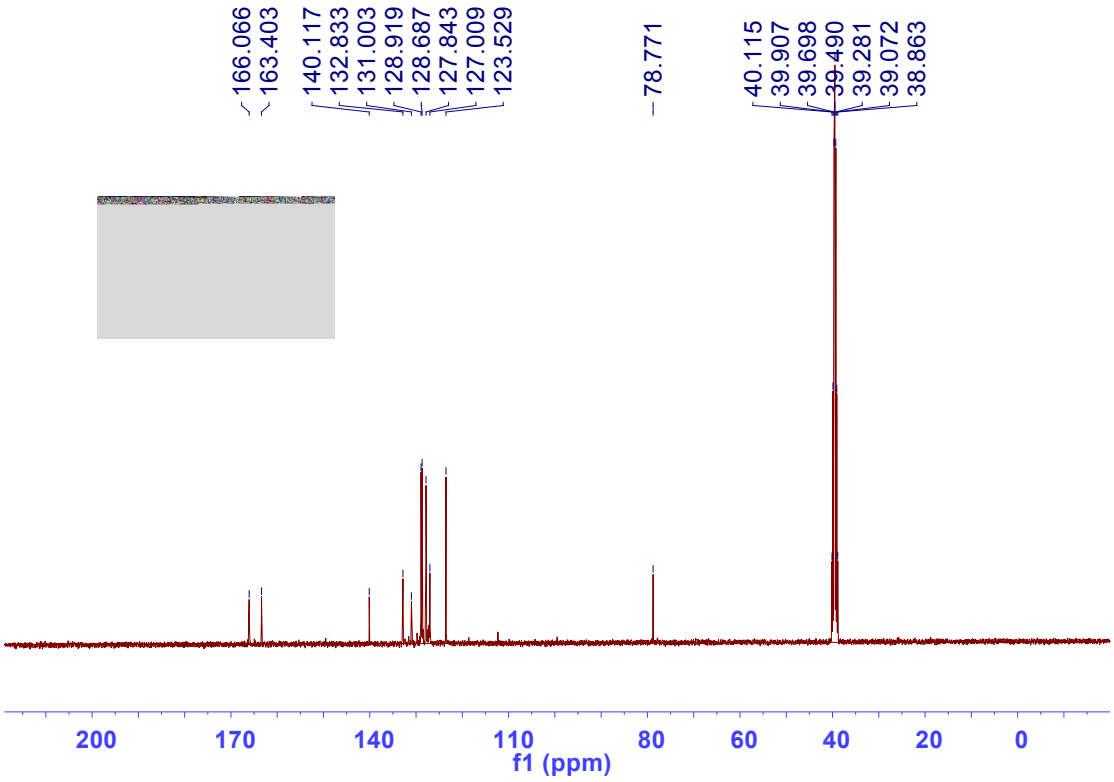

8.595
8.358
8.338
7.945
7.925
7.906
6.529
3.586
2.513
0.93
1.96
1.00
4.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)
N
N
O
O
N
N
NO2
NO2

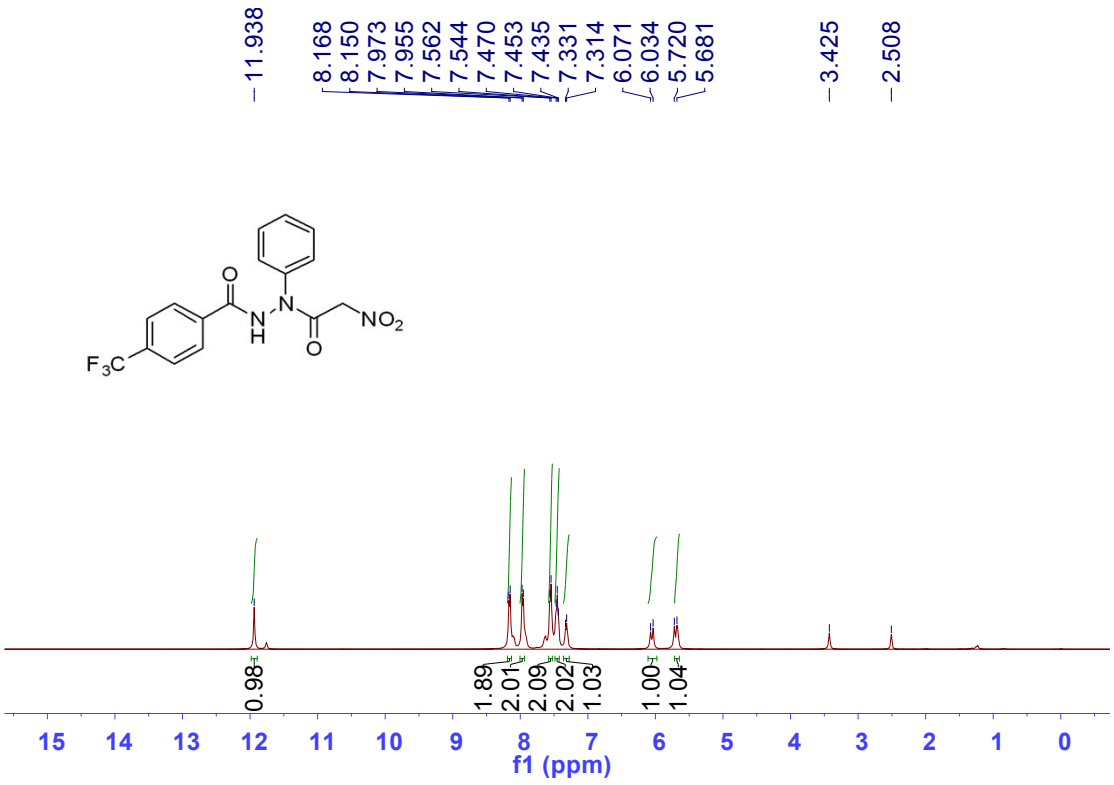

164.594
157.902
131.223
130.432
124.580
123.935
68.580
40.094
39.885
39.677
39.468
39.259
39.051
38.843
N
N
O
O
N
N
NO2
NO2
200
170
140
110
80
60
40
20
0
f1 (ppm)

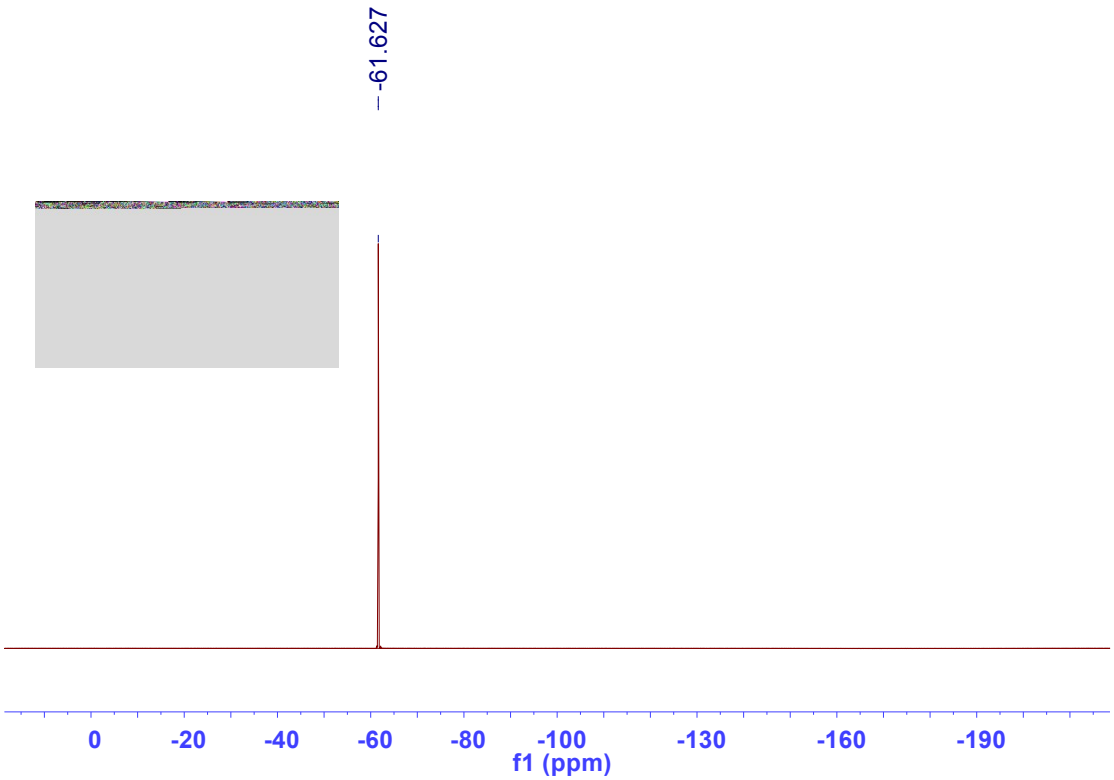

11.575
8.114
8.102
8.094
7.920
7.912
7.906
7.898
2.533
NH
NH
O
O
1.80
2.00
2.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)


154.618
132.550
127.119
125.092
40.076
39.867
39.658
39.449
39.241
39.032
38.823
NH
NH
O
O
200
170
140
110
80
60
40
20
0
f1 (ppm)


11.690
7.955
7.937
7.661
7.643
7.581
7.563
7.537
7.516
7.458
7.440
7.422
7.309
6.022
5.985
5.617
5.579
3.367
2.501
O
N
H
N
O
NO2
0.95
1.92
1.04
4.37
2.04
0.96
1.00
1.10
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)


166.066
163.403
140.117
132.833
131.003
128.919
128.687
127.843
127.009
123.529
78.771
40.115
39.907
39.698
39.490
39.281
39.072
38.863
200
170
140
110
80
60
40
20
0
f1 (ppm)


11.938
8.168
8.150
7.973
7.955
7.562
7.544
7.470
7.453
7.435
7.331
7.314
6.071
6.034
5.720
5.681
3.425
2.508
O
N
N
H
O
NO2
F3C
0.98
1.89
2.01
2.09
2.02
1.03
1.00
1.04
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)


-61.627
0
-20
-40
-60
-80
-100
-130
-160
-190
f1 (ppm)