Electronic Supplementary Material (ESI) for Nanoscale Advances.

Fe_3O_4@SiO_2@SBA-3@CPTMS@Arg-Cu: preparation, characterization, and catalytic performance for the conversion of nitriles to amides and synthesis of 5-substituted 1H-tetrazoles

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Selected Spectral Data

2-Chlorobenzamide (Table 4, entry 1): ^{1}H NMR (400 MHz, DMSO) δ 7.98(s, 2H), 7.48-7.39(m, 4H)). ^{13}C NMR (100 MHz, DMSO-d_6, ppm) δ 168. 6, 162.2, 137.4, 130.9, 130.0, 129.0, 127.4.

4-Chlorobenzamide (Table 4, entry 2): ^{1}H NMR (400 MHz, DMSO) δ 8.0 (s, 2H), 7.89 (d, *J* = 8 Hz, 2H), 7.87 (d, *J* = 8 Hz, 2H). ^{13}C NMR (100 MHz, DMSO-d_6, ppm) δ 167.2, 162.5, 136.4, 133.4, 129.7, 128.6.

4-Bromobenzamide (Table 4, entry 3): ^{1}H NMR (400 MHz, DMSO) δ 8.0 (s, 2H), 7.82 (d, *J* = 6 Hz, 2H), 7.65 (d, *J* = 8 Hz, 2H). ^{13}C NMR (100 MHz, DMSO-d_6, ppm) δ 166.9, 133.4, 131.2, 129.6, 124.9.

4-Nitrobenzamide (Table 4, entry 4): ^{1}H NMR (400 MHz, DMSO) δ 8.3 (d, *J* = 12 Hz, 2H), 8.0 (d, *J* = 8 Hz, 2H), 7.7 (s, 1H).

Benzamide (Table 4, entry 8): ^{1}H NMR (400 MHz, DMSO) δ 7.98(s, 2H), 7.82(d, *J* = 6 Hz, 2H), 7.50-7.45(m, 3H).^{13}C NMR (100 MHz, DMSO-d_6, ppm) δ 168.3, 162.2, 134.6, 131.6, 128.6, 127.8.

5-phenyl-1H-tetrazole (Table 6, entry 1): ^{1}H NMR (400 MHz, DMSO) δ 8.03(d, *J* = 6 Hz, 3H), 7.57(d, *J* = 6 Hz, 2H).^{13}C NMR (100 MHz, DMSO-d_6, ppm) δ 162.2, 155.1, 131.6, 129.7, 127.3, 124.5.

5-(4-Chlorophenyl)-1H-tetrazole (Table 6, entry 2): ^{1}H NMR (400 MHz, DMSO) δ 8.05 (d, *J* = 8.4 Hz, 2H), 7.69 (d, *J* = 8.4 Hz, 2H). ^{13}C NMR (100 MHz, DMSO-d_6, ppm) δ 162.1, 155.3, 148.5, 133.2, 131.4, 126.4, 125.8, 121.7.

5-(4-Bromophenyl)-1H-tetrazole (Table 6, entry 3): ^{1}H NMR (400 MHz, DMSO) δ 7.95(d, *J* = 6, 2H), 7.78(d, *J* = 6, 2H). ^{13}C NMR (100 MHz, DMSO-d_6, ppm) δ 162.2, 155.3, 132.8, 129.2, 125.0, 123.9.

5-(4-nitrophenyl)-1H-tetrazole (Table 6, entry 4): ^{1}H NMR (400 MHz, DMSO) δ 8.35(d, *J* = 6 Hz, 2H), 8.22(d, *J* = 6 Hz, 2H). ^{13}C NMR (100 MHz, DMSO-d_6, ppm) δ 162.2, 155.8, 148.9, 130.9, 128.4, 124.8.

1-(4-(1H-tetrazol-5-yl)phenyl)ethan-1-one(Table 6, entry 5): ^{13}C NMR (100 MHz, DMSO-d_6, ppm) δ 197.3, 138.5, 129.1, 128.4, 127.1, 26.8.

4-(1H-tetrazol-5-yl)benzonitrile (Table 6, entry 6): ^{1}H NMR (400 MHz, DMSO) δ 8.20(d, *J* = 12 Hz, 2H), 8.08(d, *J* = 12 Hz, 2H). ^{13}C NMR (100 MHz, DMSO-d_6, ppm) δ 166.7, 162.2, 155.9, 133.7, 129.1, 127.9, 118.5, 113.7.

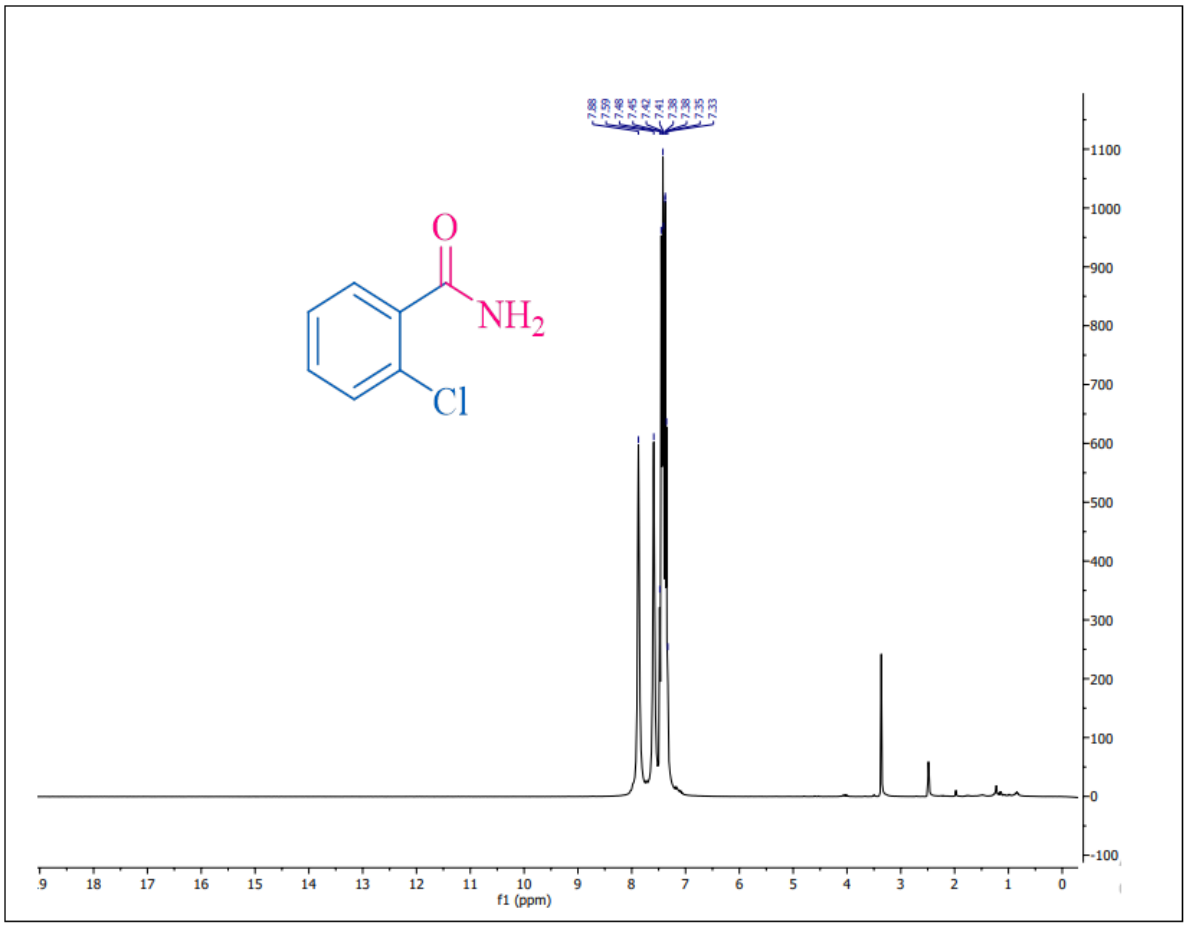
5-(3-nitrophenyl)-1H-tetrazole (Table 6, entry 7): δ 8.74(s, 1H), 8.41(q, *J* = 8, 2H), 7.86(t, *J* = 8, 1H).^{13}C NMR (100 MHz, DMSO-d_6, ppm) δ 162.1, 155.3, 148.5, 133.2, 131.4, 126.4, 125.8, 121.7.

2-(1H-tetrazol-5-yl)benzonitrile (Table 6, entry 8): ^{1}H NMR (400 MHz, DMSO) δ 8.06(s, 2H),

7.92(t, *J*=6, 1H), 7.77(t, J=6, 1H). ^{13}C NMR (100 MHz, DMSO-d_6, ppm) δ 162.2, 135.3, 134.1, 131.7, 130.0, 127.8, 117.6, 110.5.

2-(1H-Tetrazol-5-yl) phenol (Table 6, entry 10): ^{1}H NMR (400 MHz, DMSO) δ 8.00-7.98 (m, 1H), 7.44 (d, *J*=8, 1H), 7.40 (t, *J*=4, 1H), 7.08-6.97 (m, 1H). ^{13}C NMR (100 MHz, DMSO-d_6, ppm) δ 162.5, 155.7, 152.0, 133.0, 129.4, 120.0, 116.7, 110.8.

5-benzyl-1H-tetrazole (Table 6, entry 11): ^{1}H NMR (400 MHz, DMSO) δ 8.04(s, 1H), 7.31(m, 5H), 4.28(s, 2H). ^{13}C NMR (100 MHz, DMSO-d_6, ppm) δ 155.7, 136.2, 131.6, 129.7, 129.1, 129.0, 127.3, 29.2.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7.38
7.38
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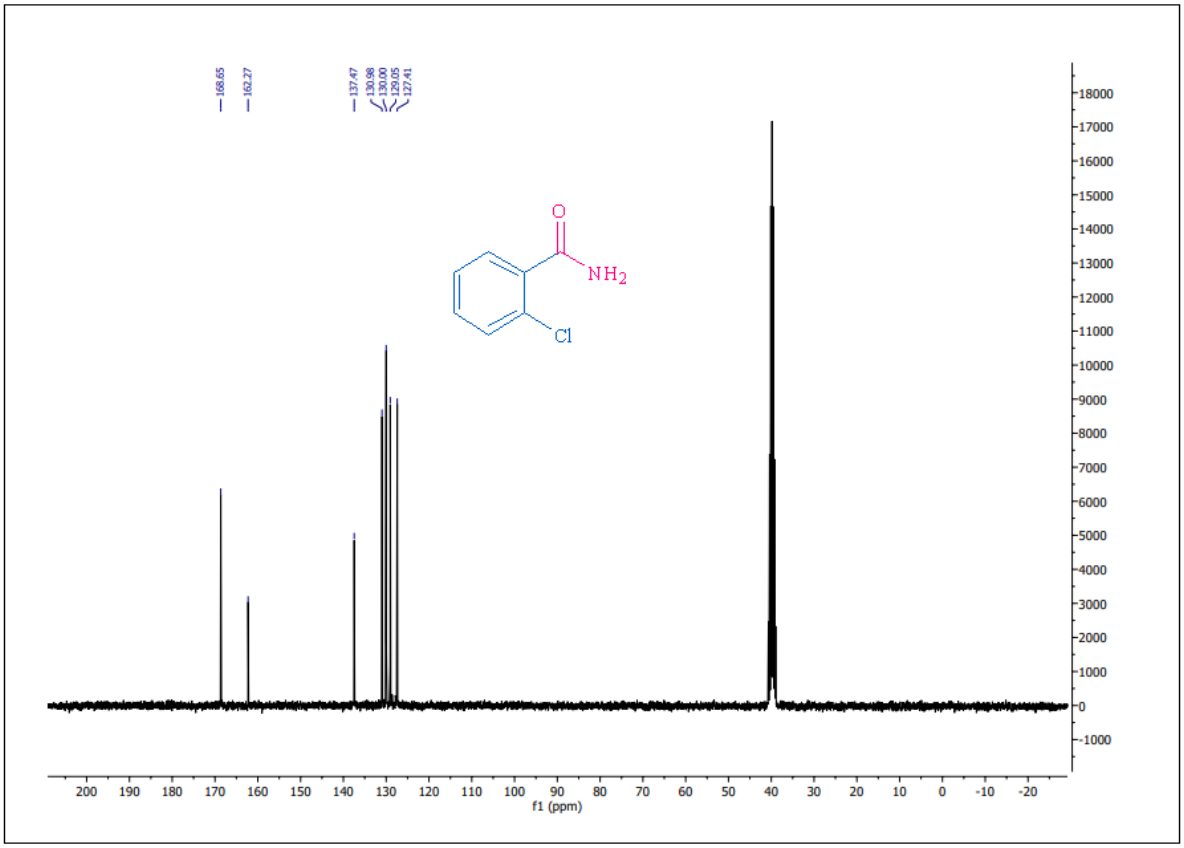
1000
900
800
700
600
500
400
300
200
100
0
-100
f1 (ppm)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162.27
137.47
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130.00
129.05
127.41
O
NH2
Cl
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17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
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1000
0
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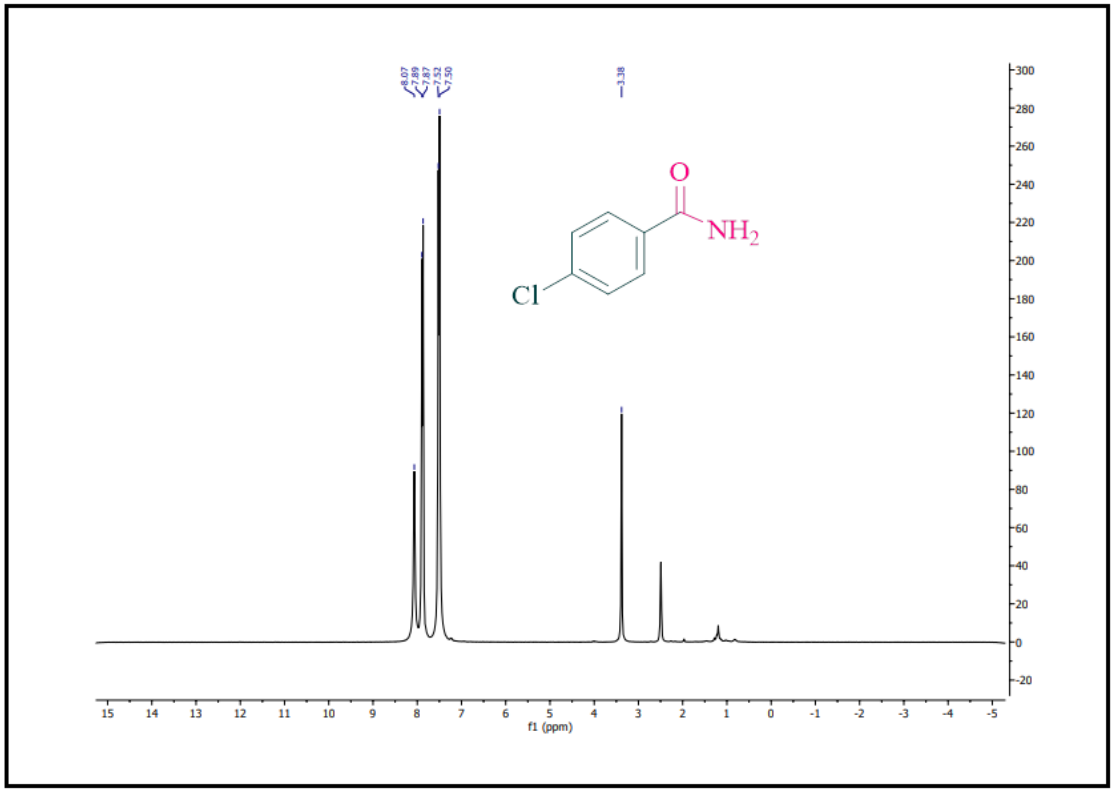
f1 (ppm)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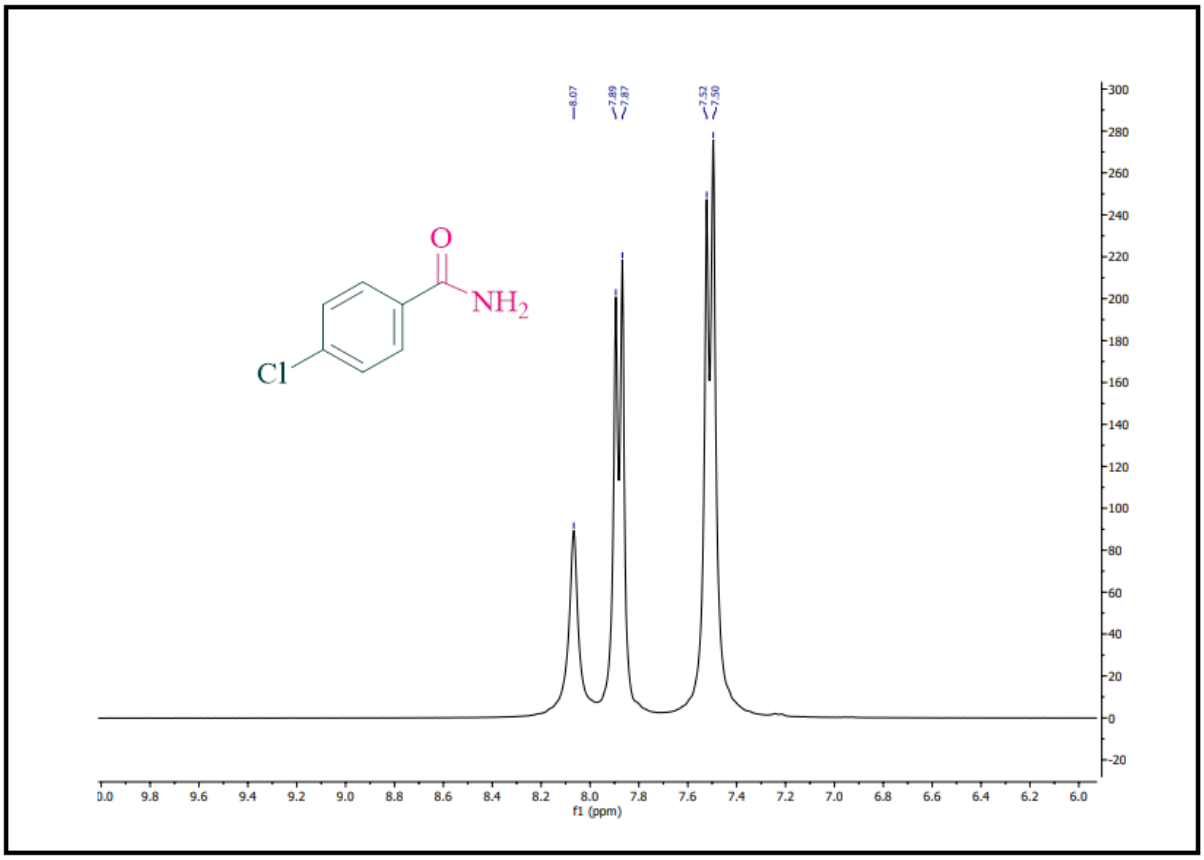
7.87
7.52
7.50
3.38
O
NH2
Cl
f1 (ppm)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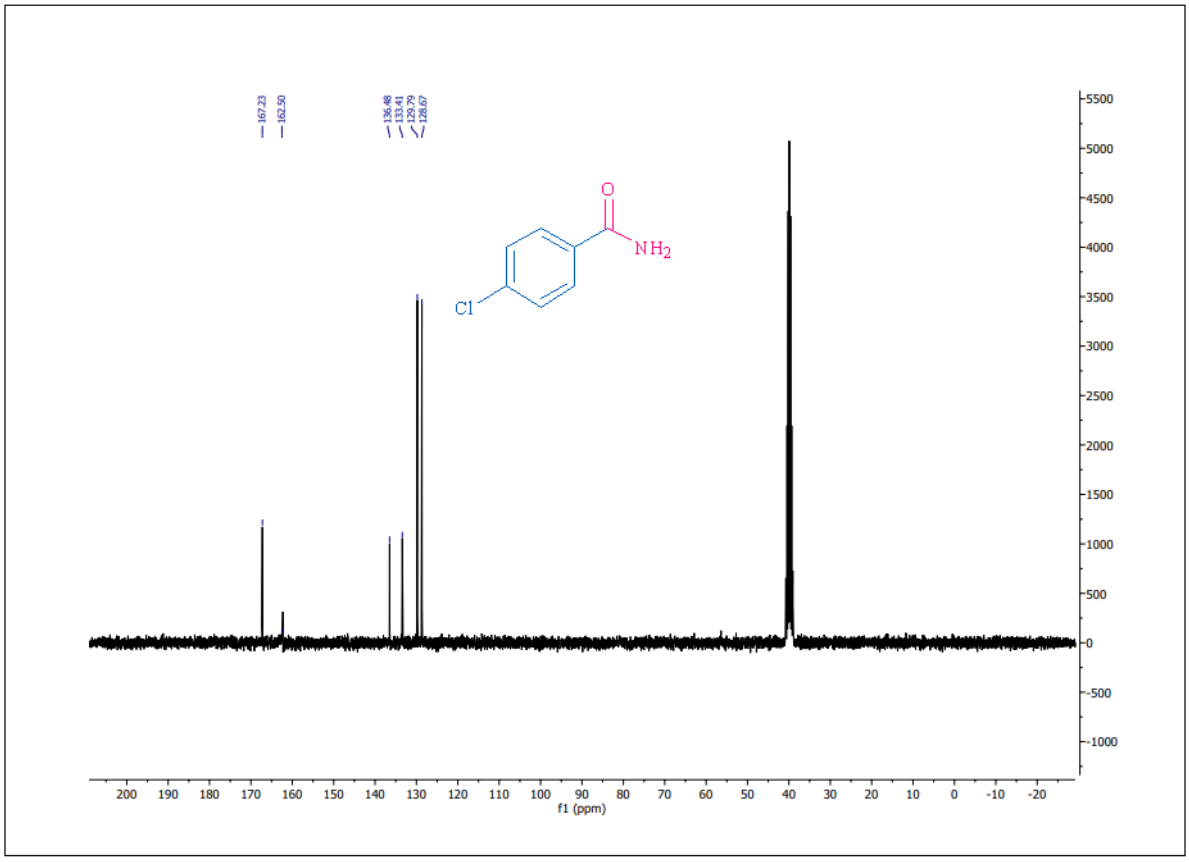
7.50
O
NH2
Cl
f1 (ppm)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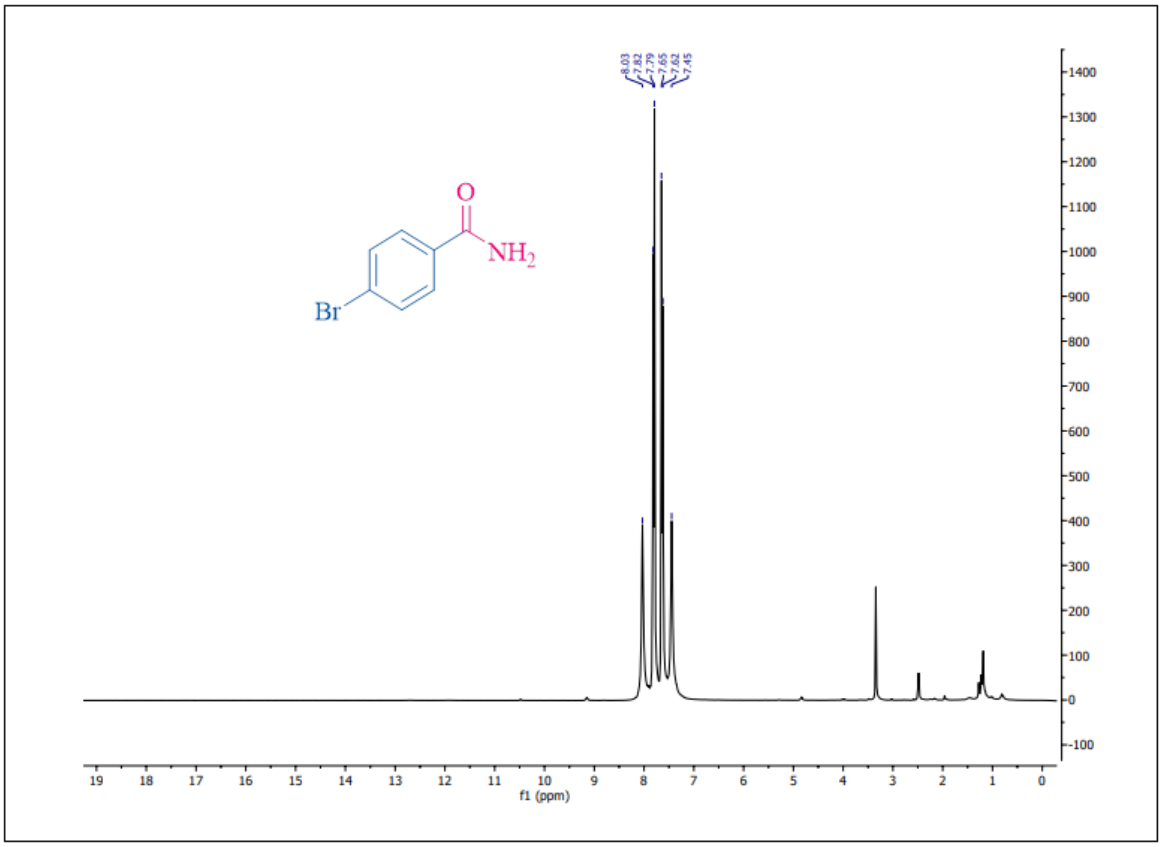
f1 (ppm)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1300
1200
1100
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100
0
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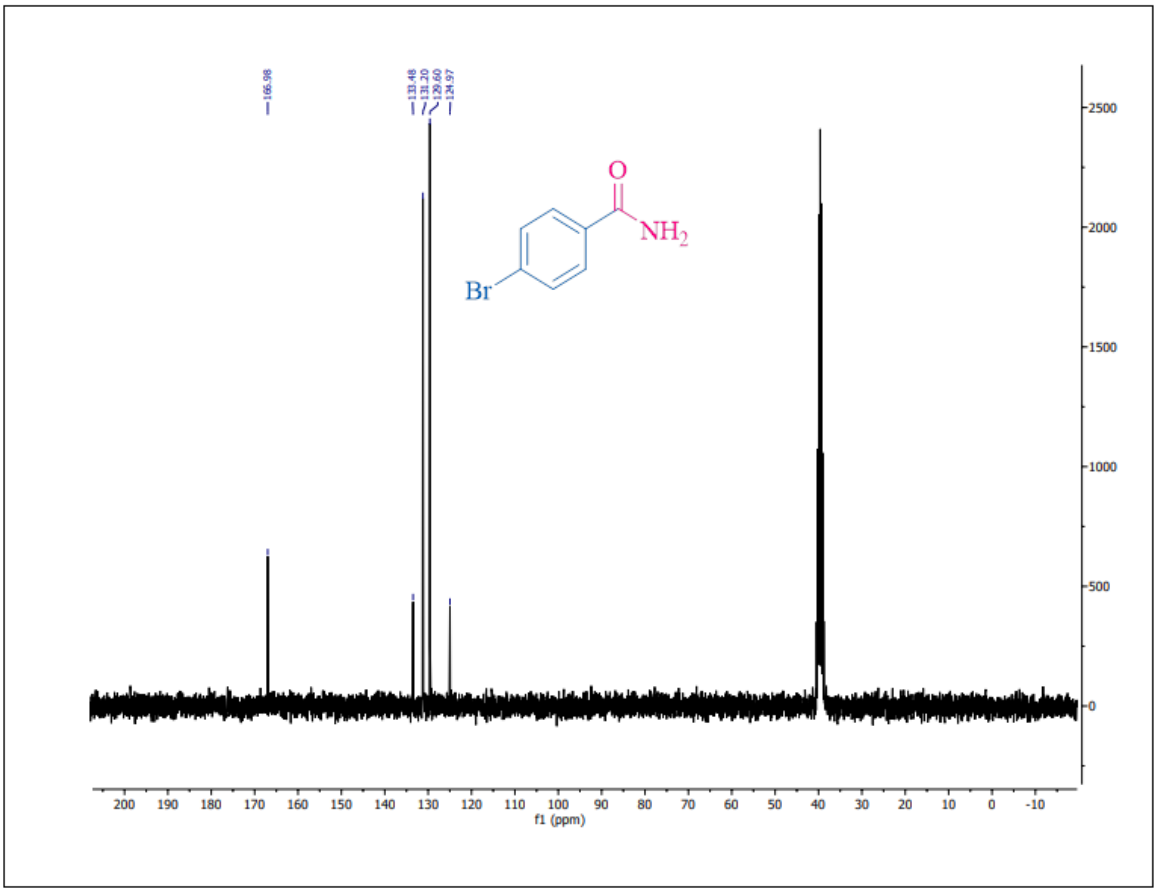
f1 (ppm)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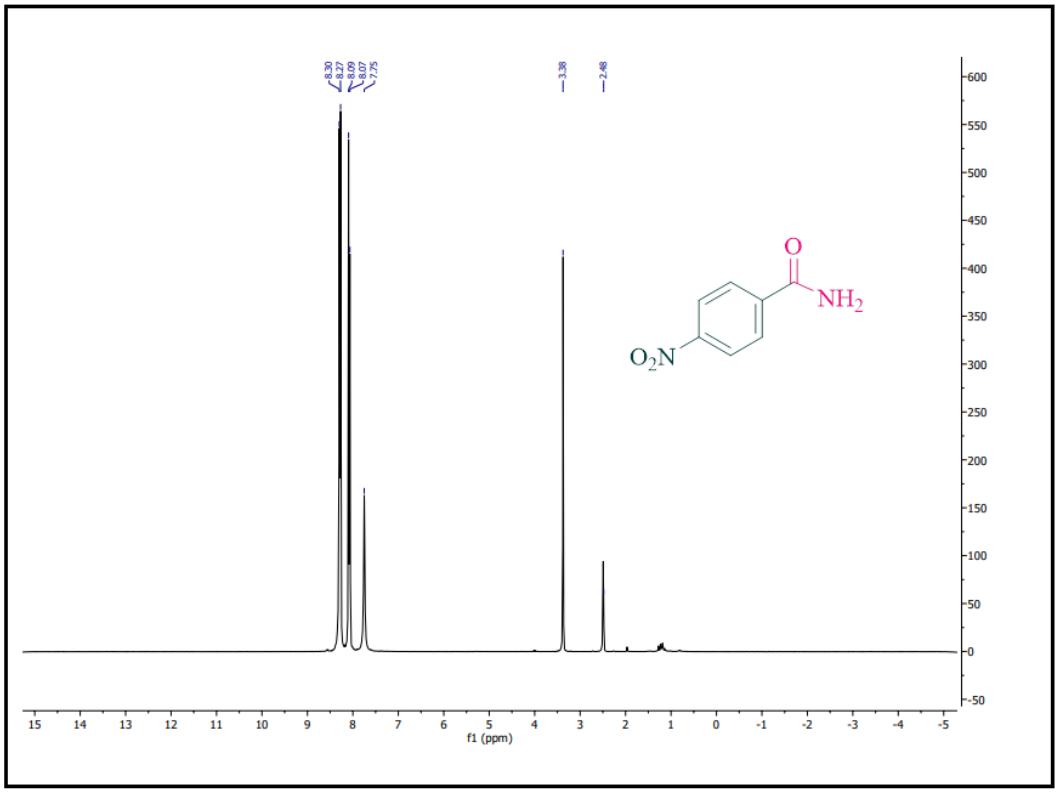
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O2N
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500
450
400
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300
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100
50
0
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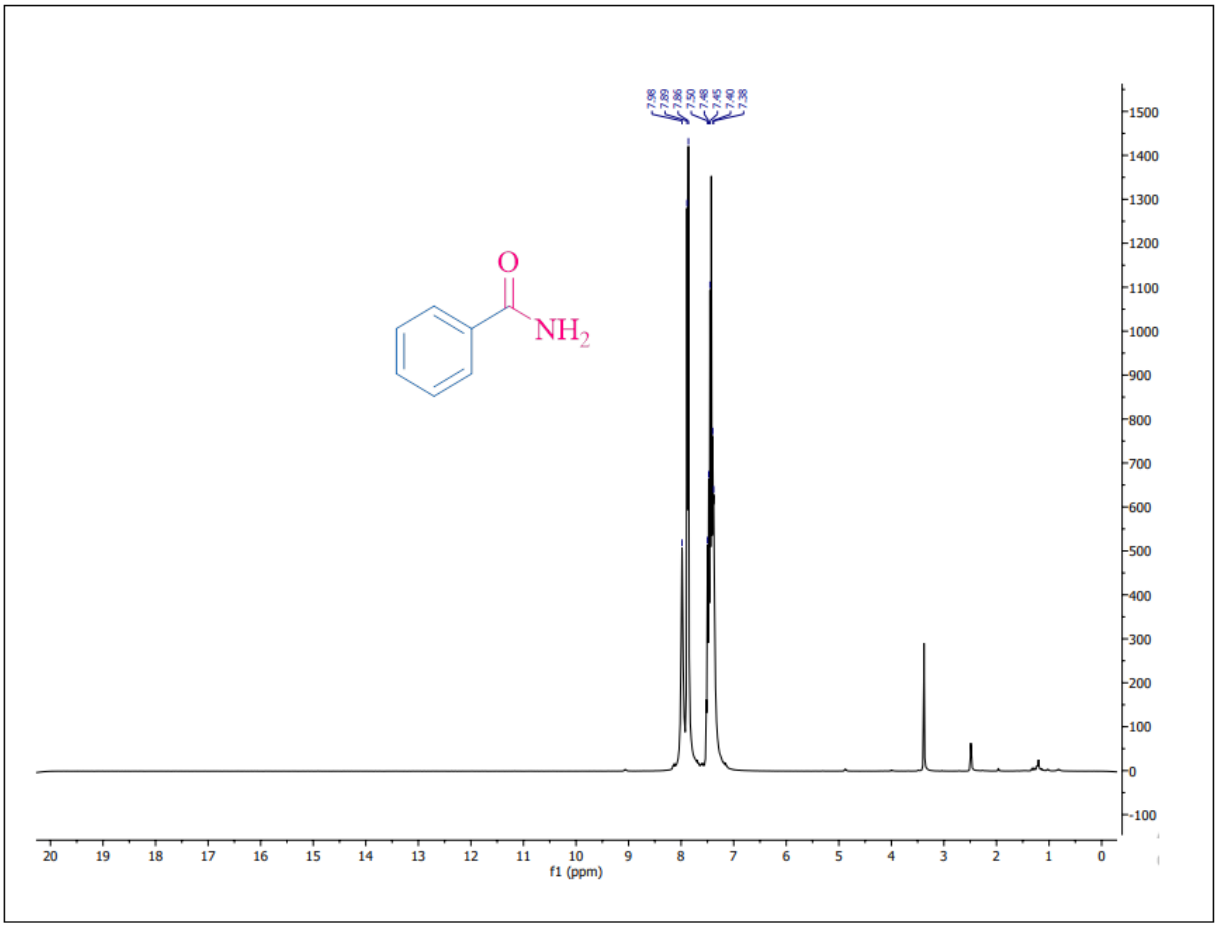
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4 -5
f1 (ppm)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7.38
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NH2
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1300
1200
1100
1000
900
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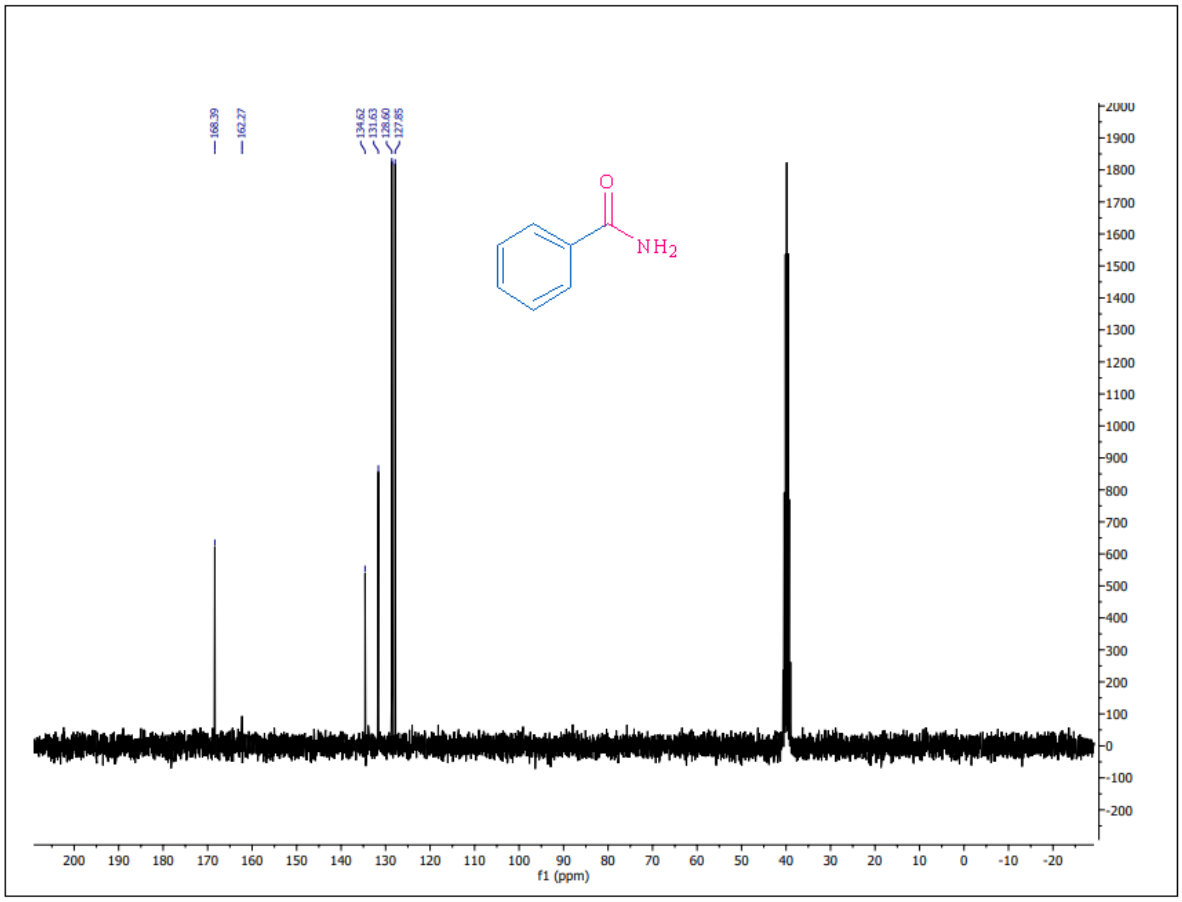
f1 (ppm)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O
NH2
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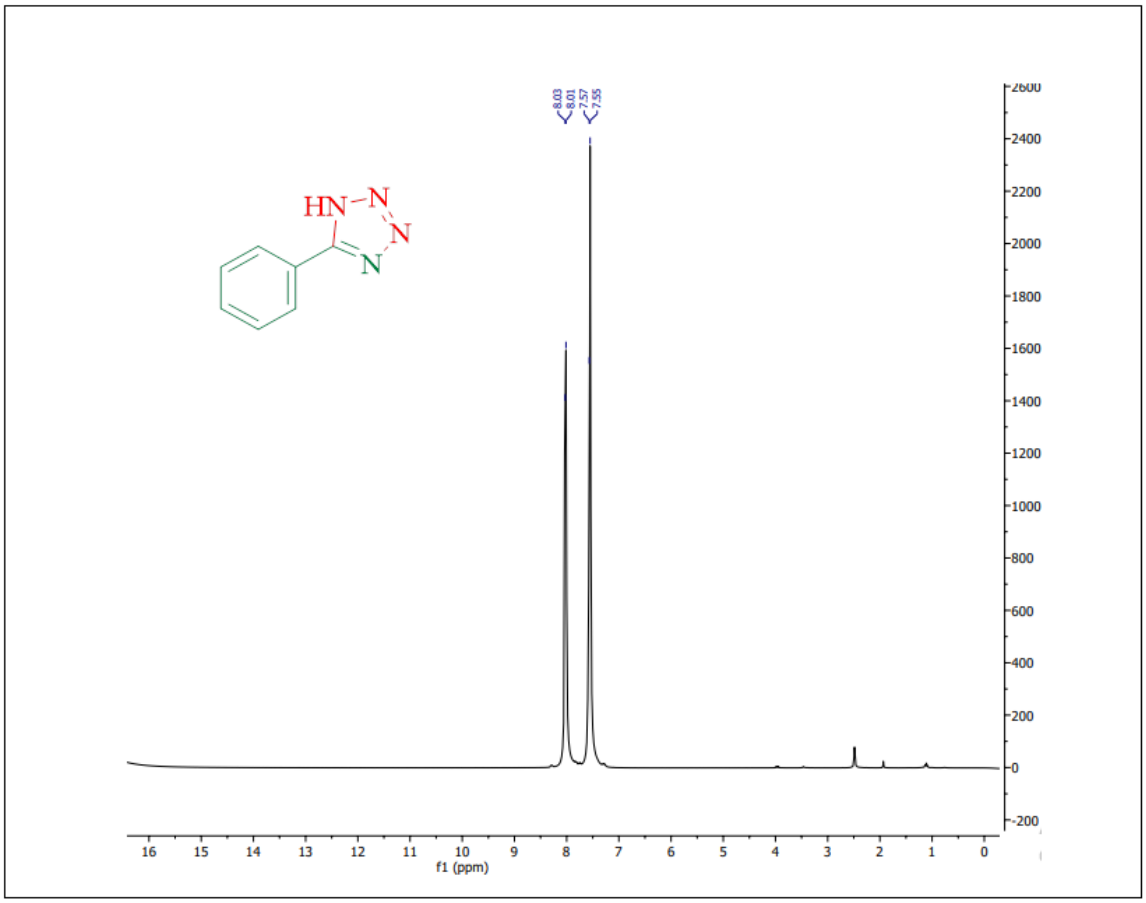
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400
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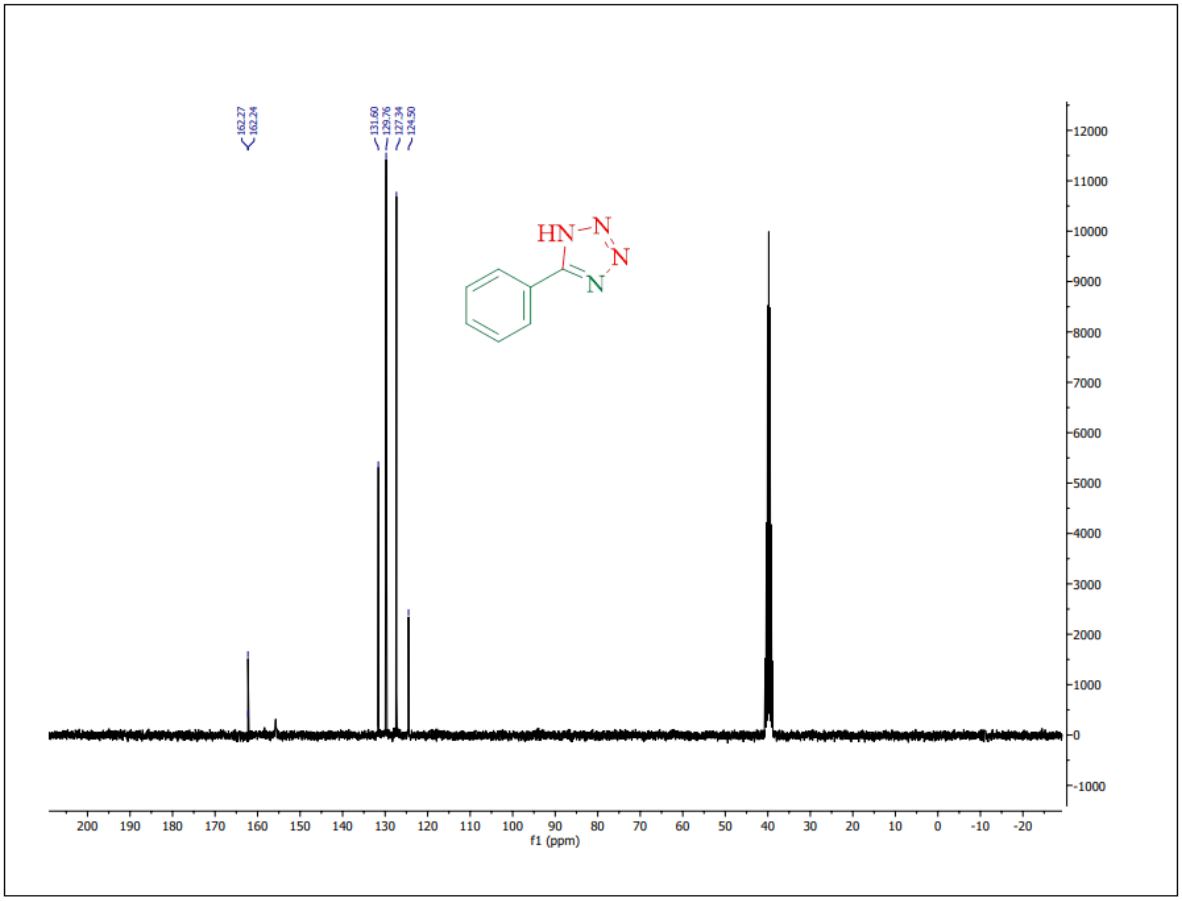
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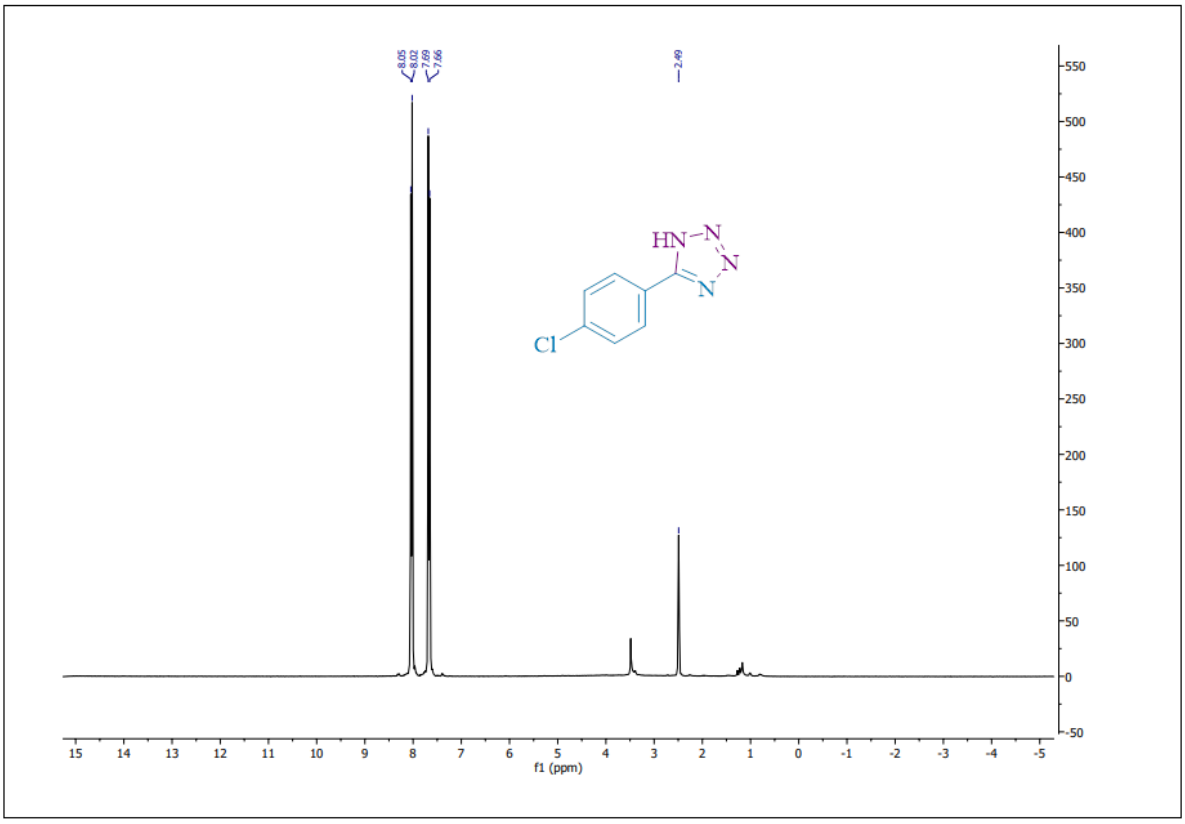
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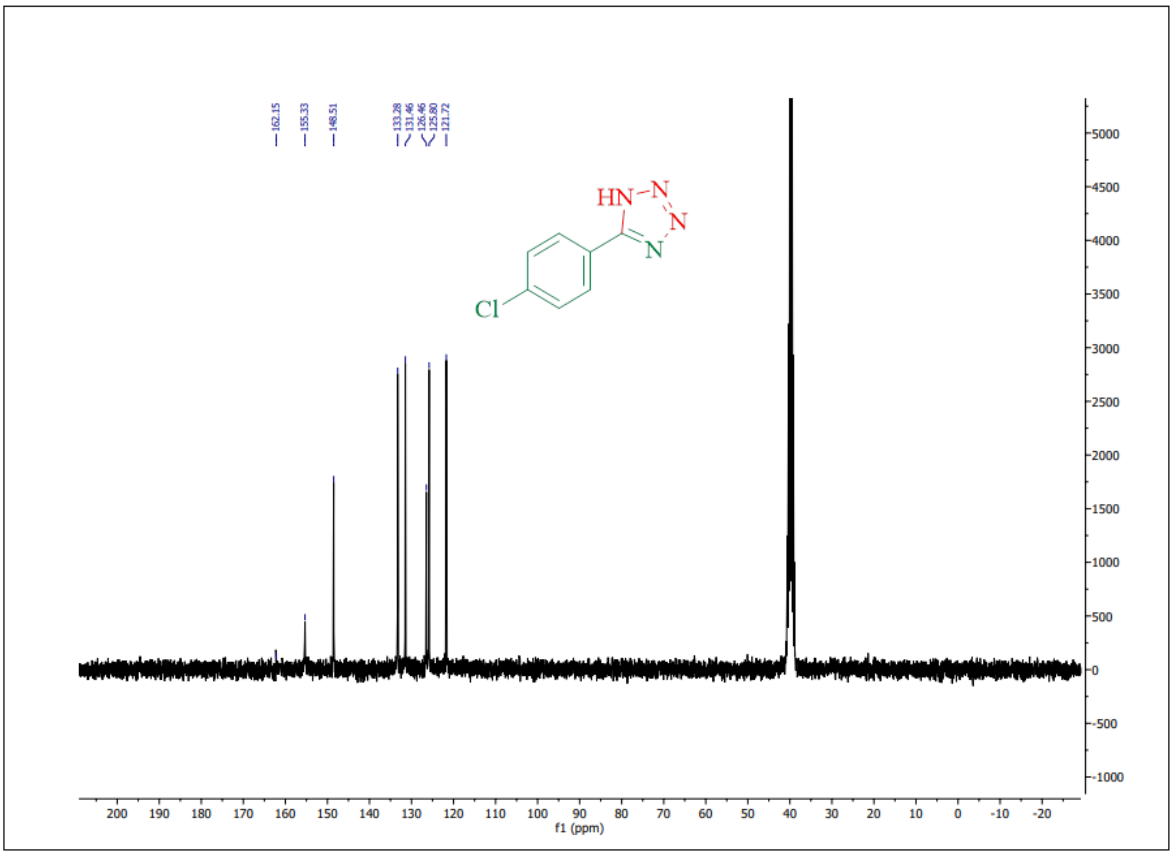
f1 (ppm)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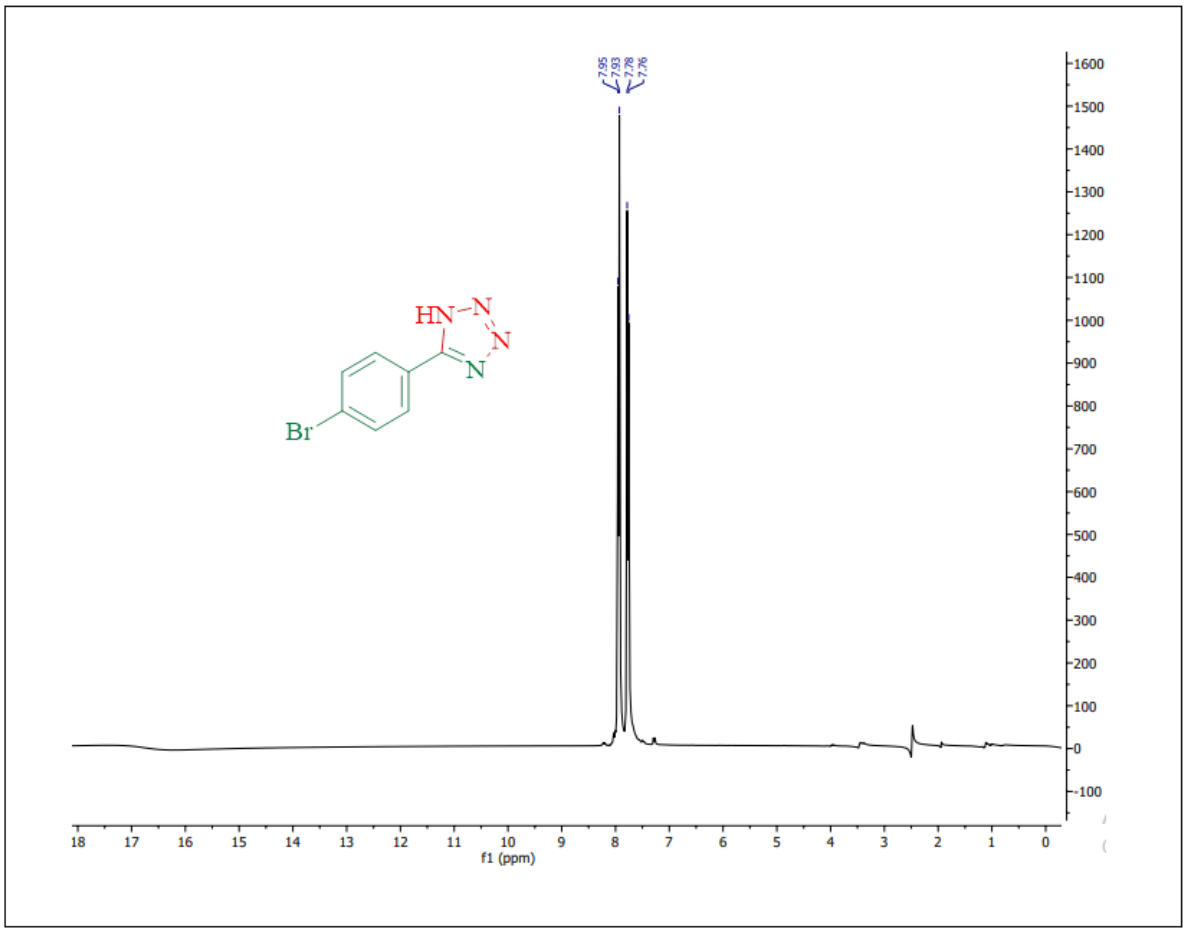
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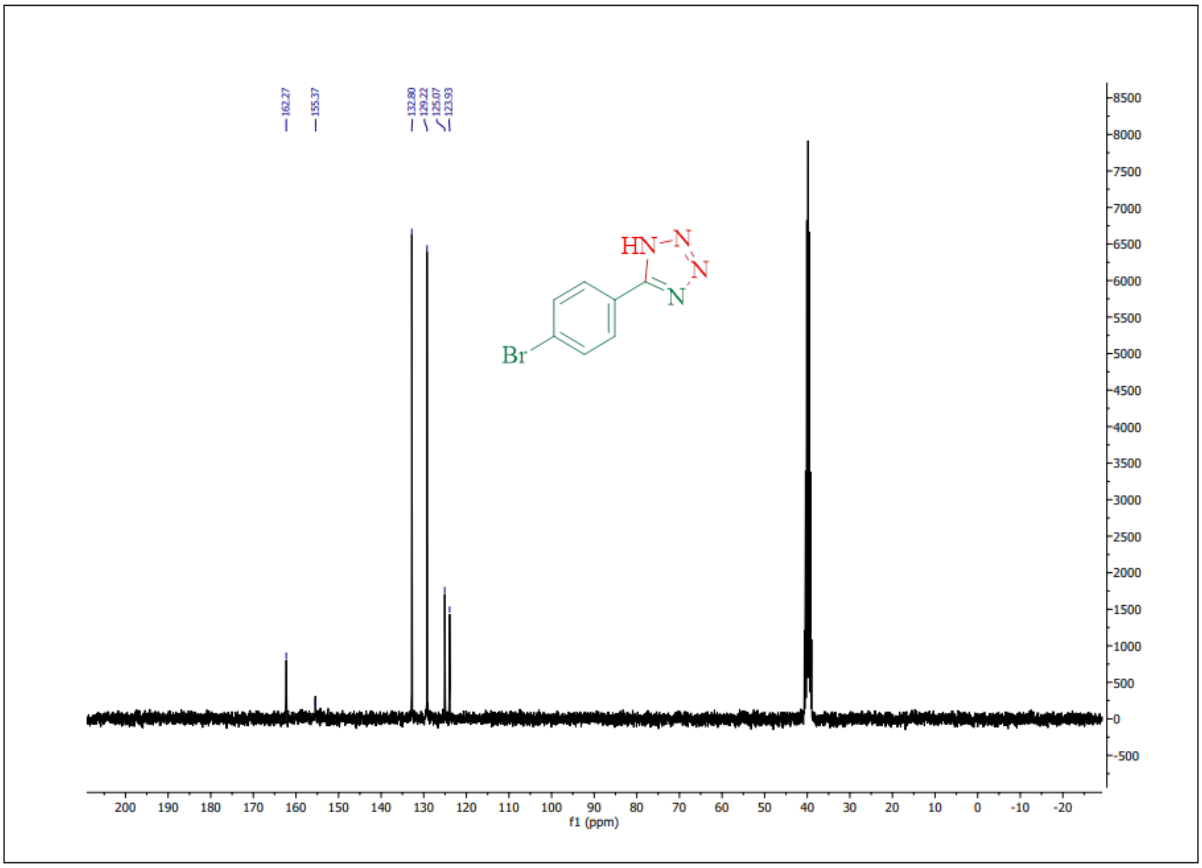
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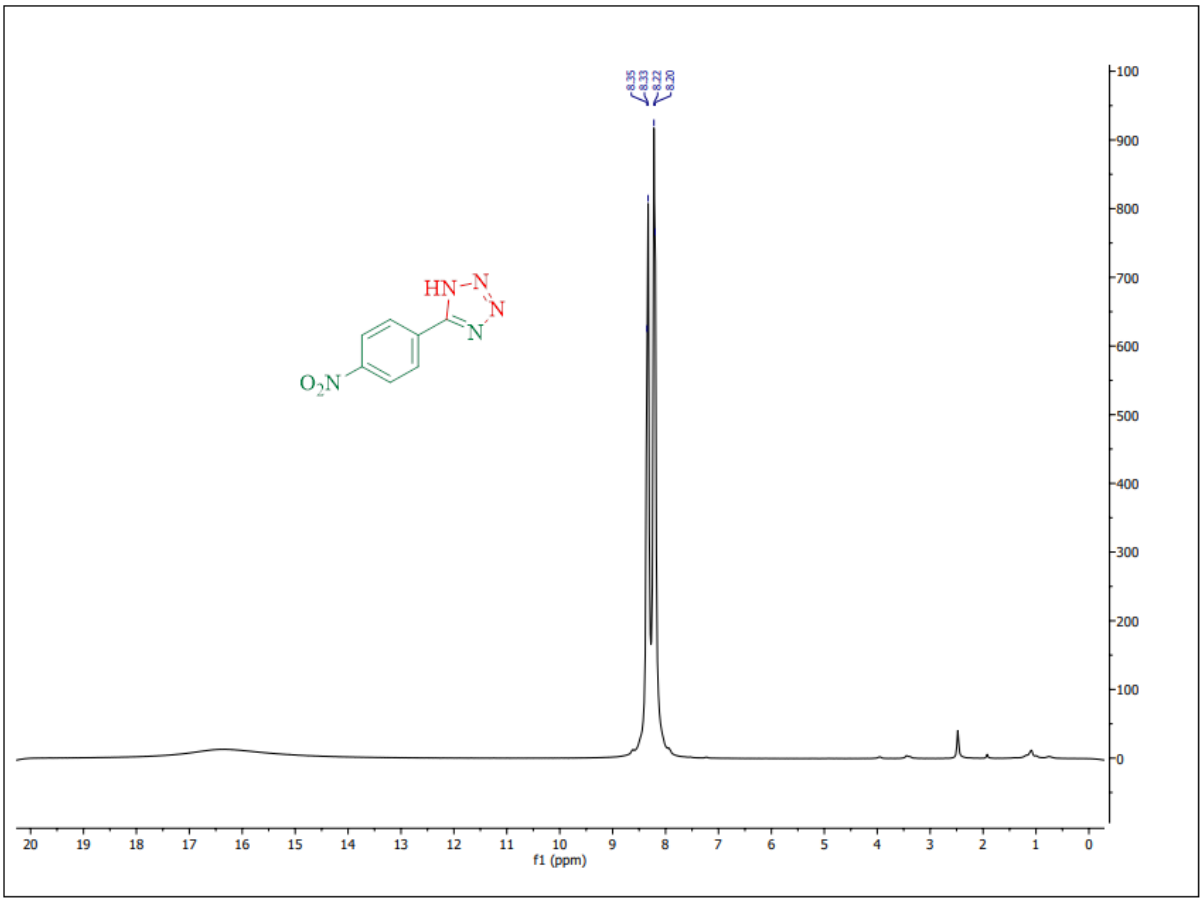
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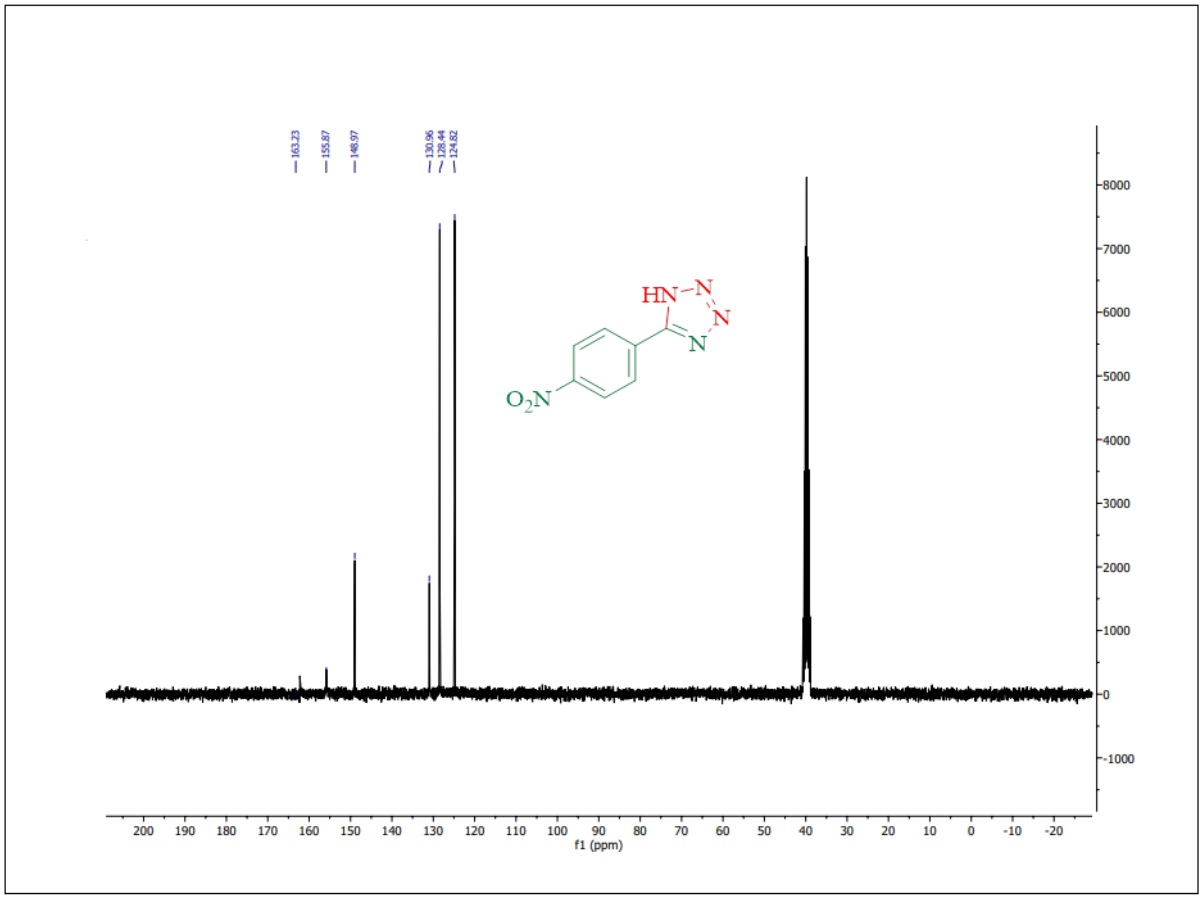
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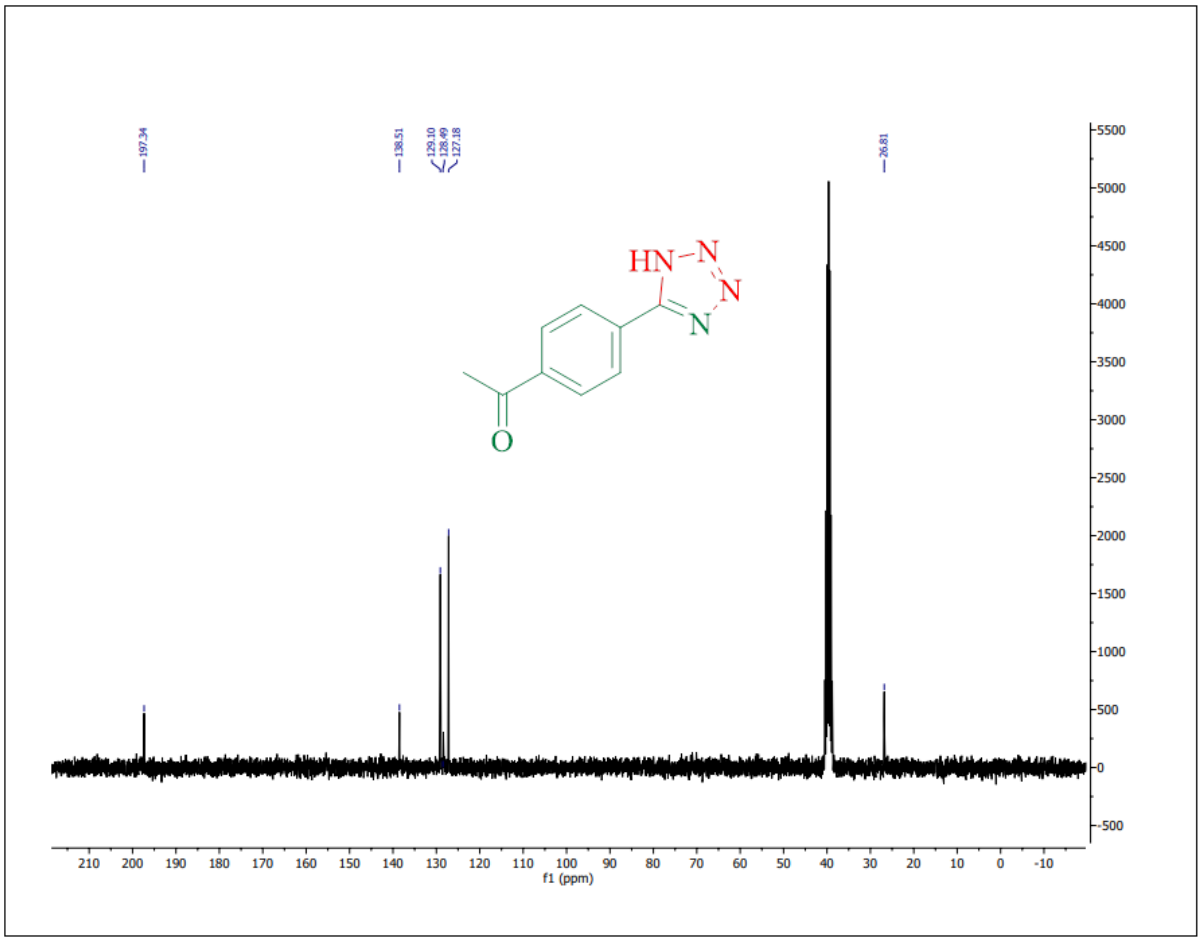
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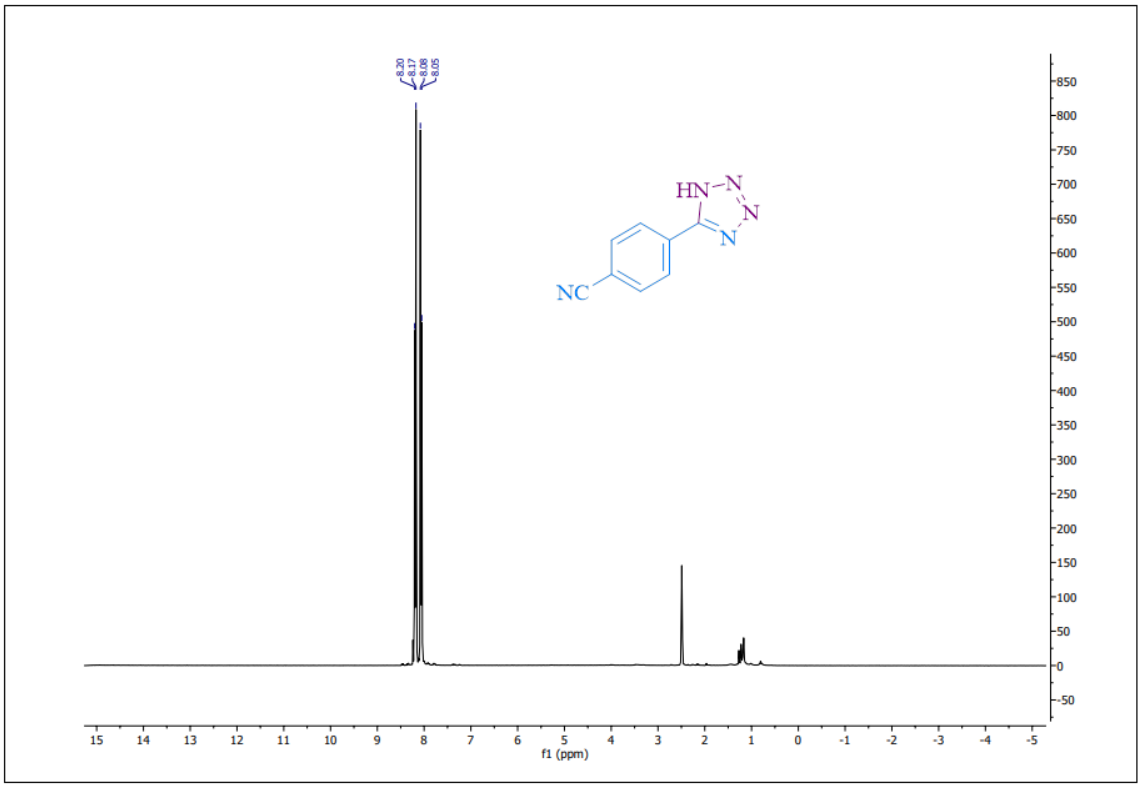
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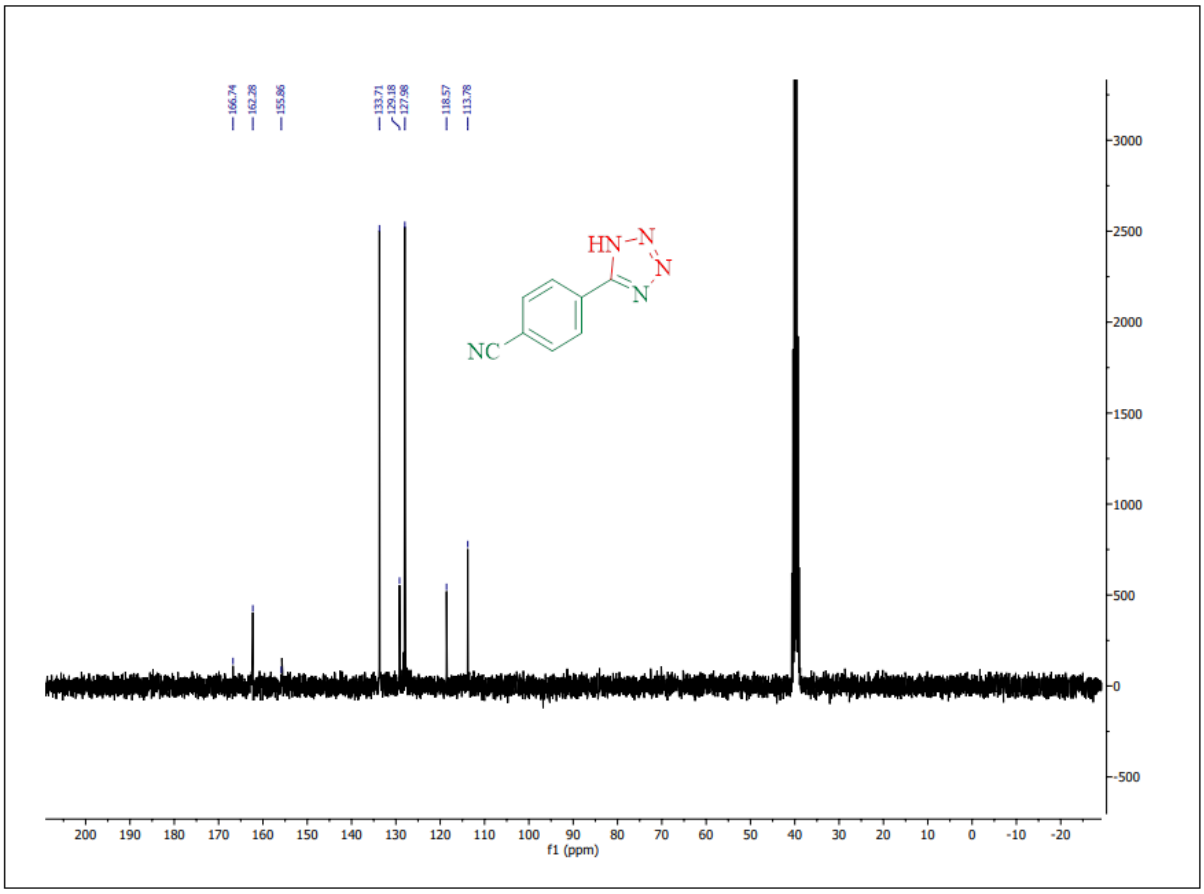
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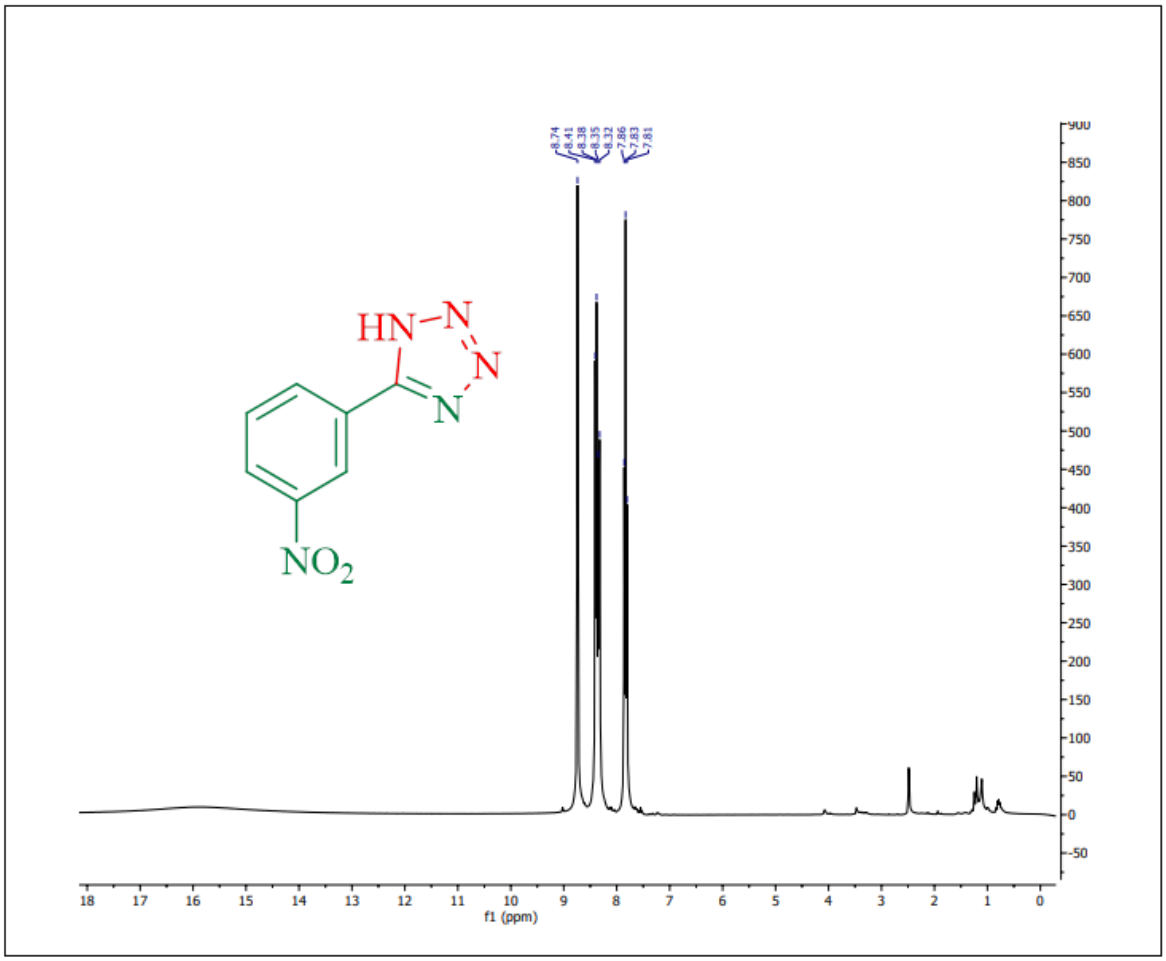
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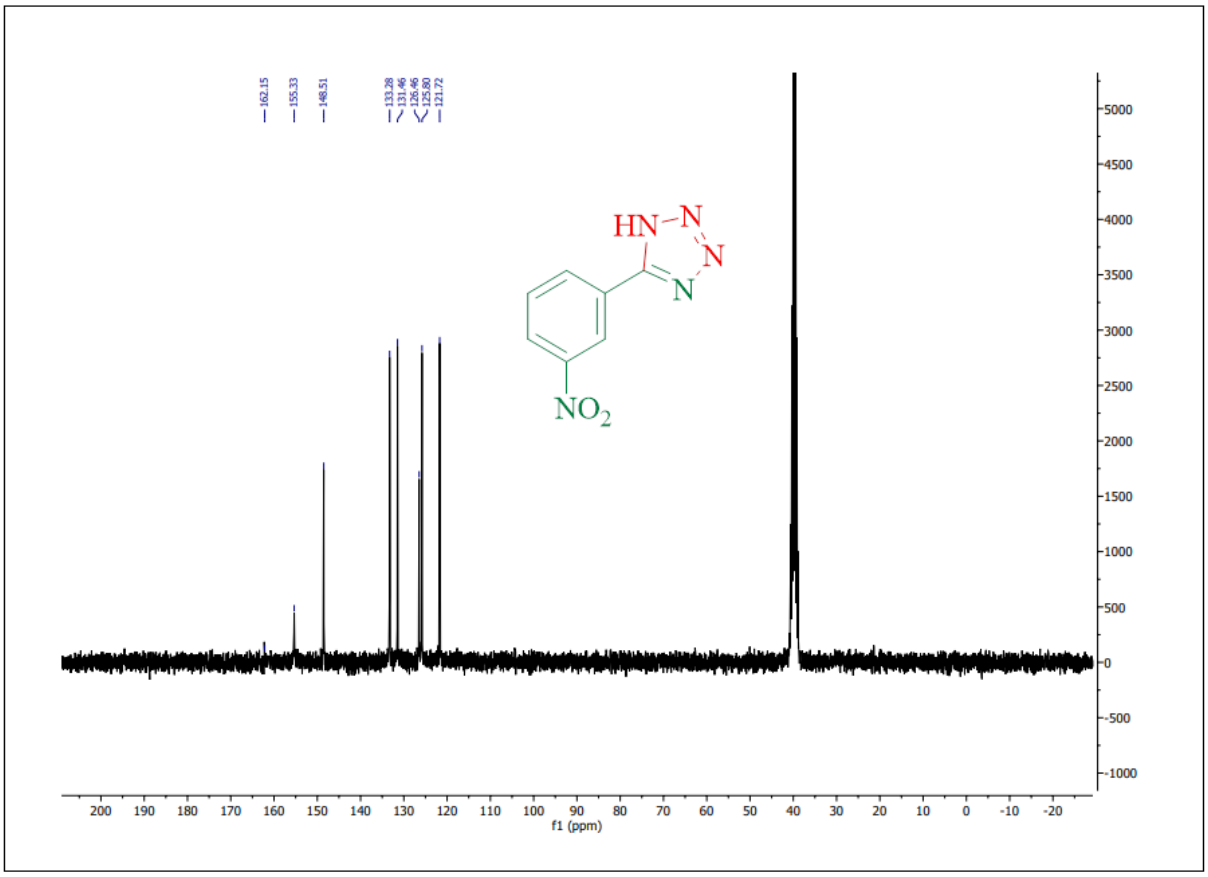
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NO2
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4000
3500
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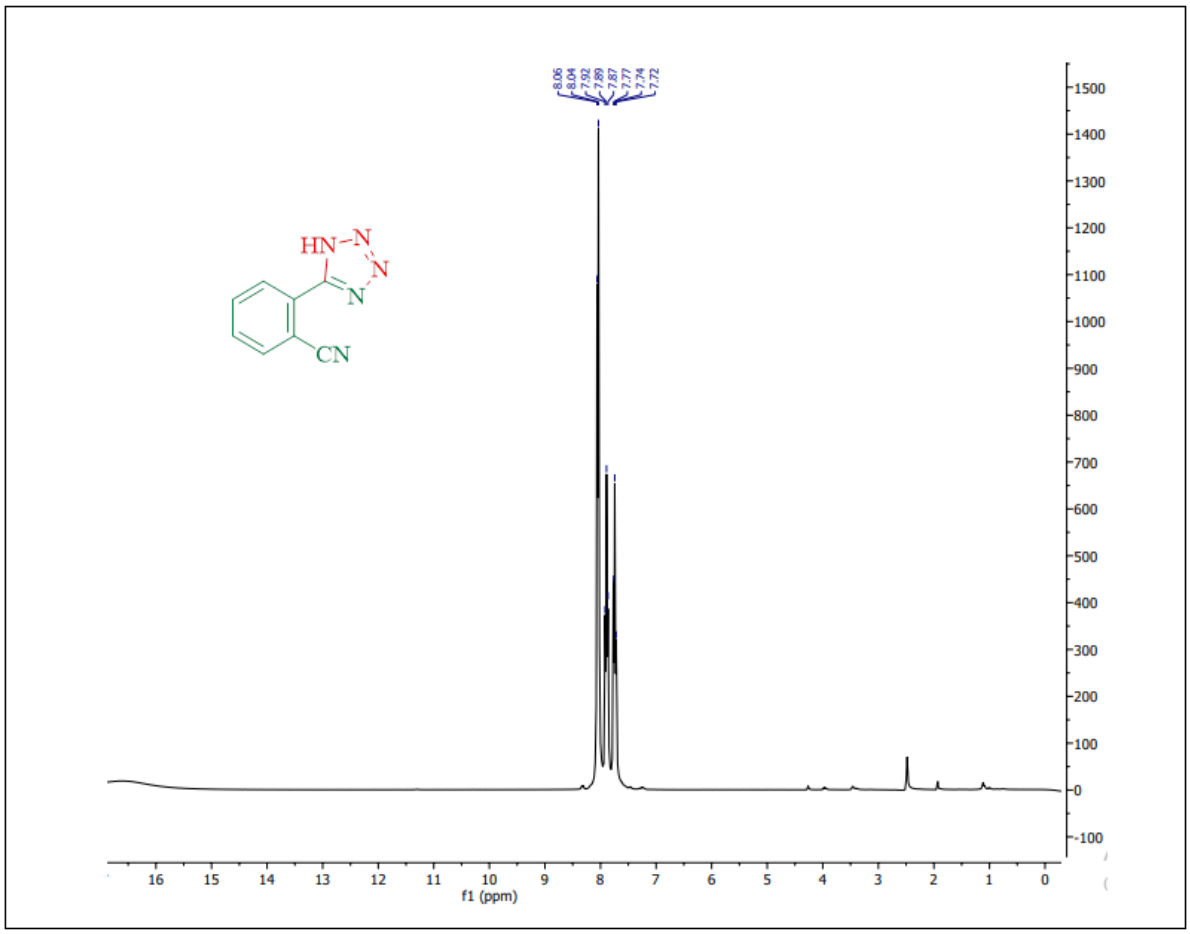
f1 (ppm)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1200
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900
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300
200
100
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9
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5
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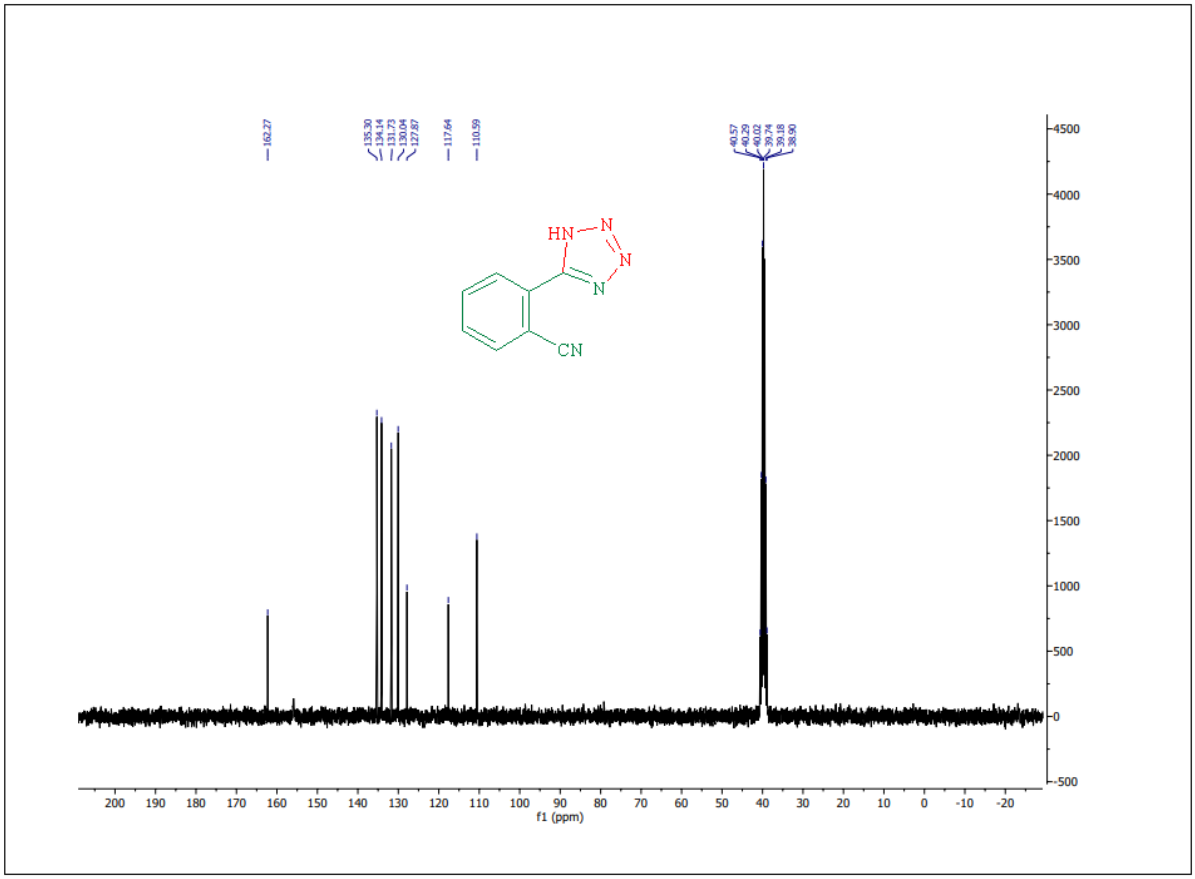
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38.90
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N
CN
4500
4000
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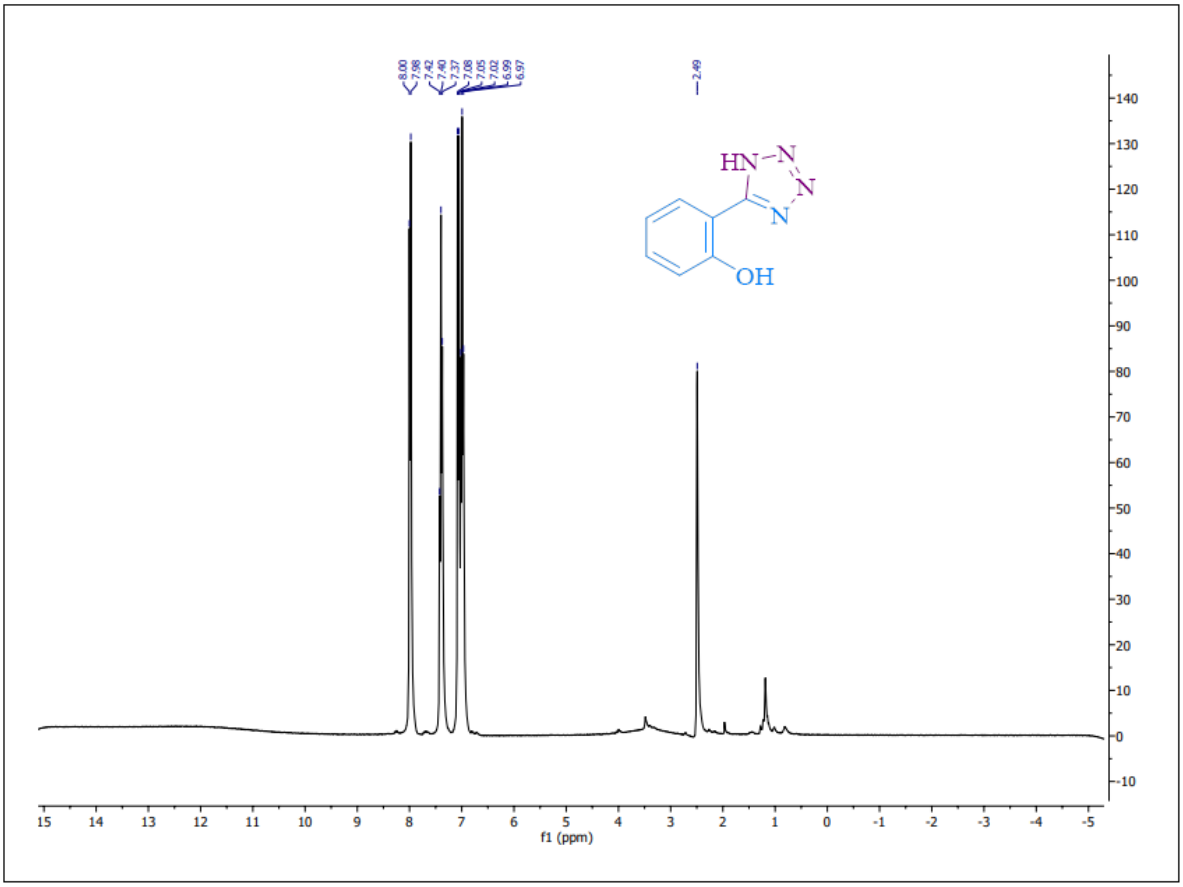
f1 (ppm)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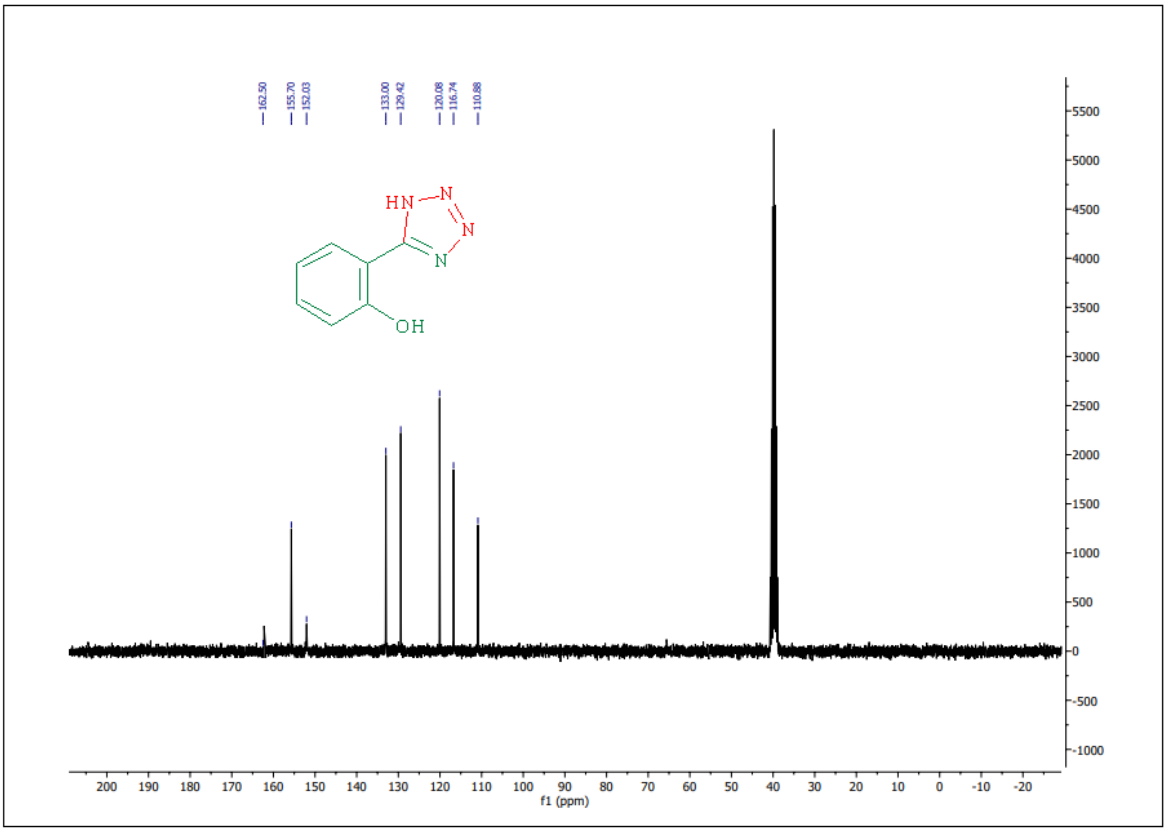
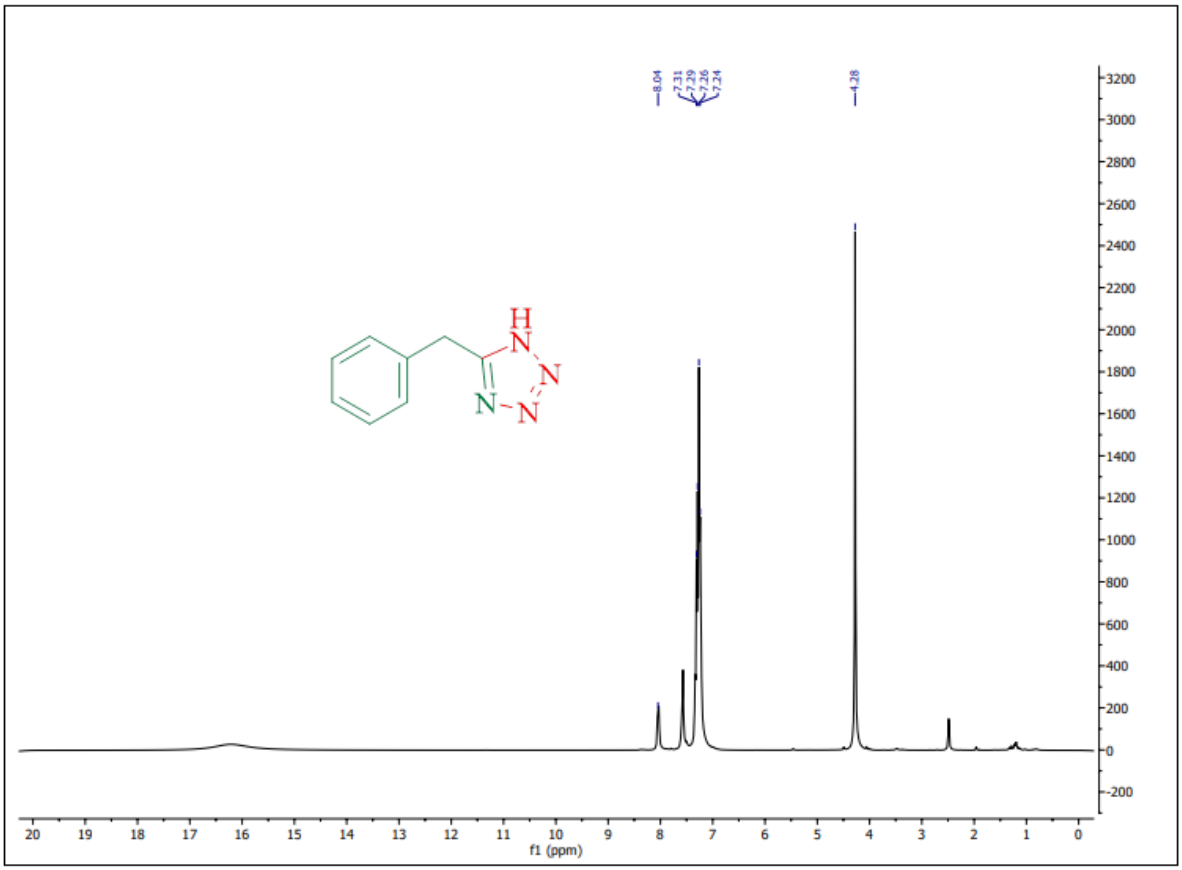
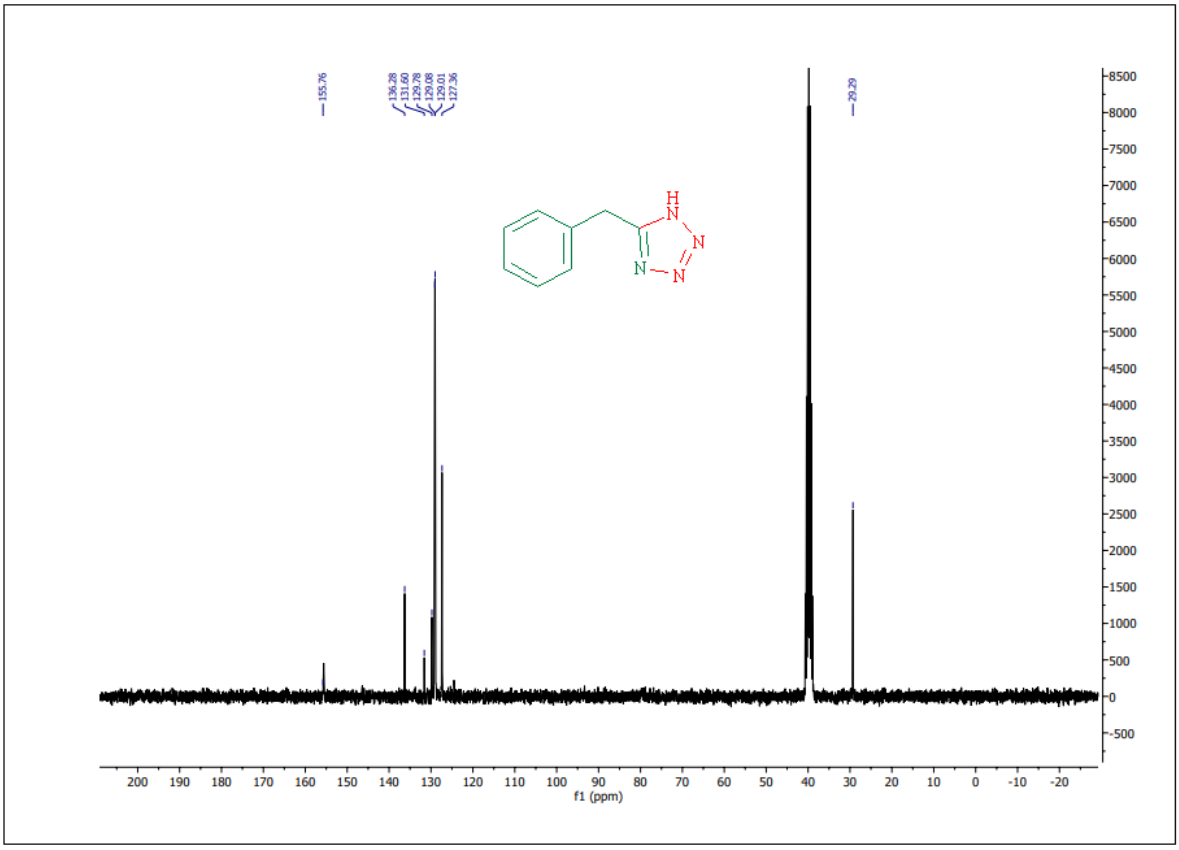
N
OH
f1 (ppm)


162.50
155.70
152.03
133.00
129.42
120.08
116.74
110.88
HN
N
N
N
OH
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
-1000
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


8.04
7.31
7.29
7.26
7.24
4.28
f1 (ppm)


155.76
136.28
131.60
129.78
129.08
129.01
127.36
29.29
H
N
N
N
N
8500
8000
7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)