Supporting Information

Humic acid as an efficient and reusable catalyst for one pot three-component green synthesis of 5-substituted 1*H*-tetrazoles in water

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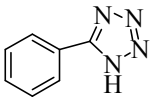
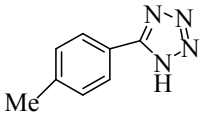
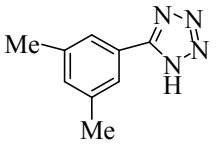
Characterization data of compounds (2a-w)



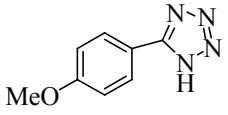
5-phenyl-1*H*-tetrazole (**2a**): white solid; MP: 215-216 °C (lit.[1] 215-217 °C); reaction time 4 h; ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.64-7.65 (3H, m), δ 8.07-8.10 (2H, m); ^{13}C NMR (100 MHz, DMSO-d_6) δ 124.1, 126.9, 129.4, 131.2, 155.2. Anal. Calcd for $C_7H_6N_4$: C, 57.53; H, 4.11; N, 38.36. Found: C, 57.32; H, 4.01; N, 38.58.



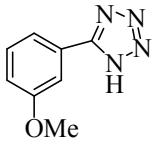
5-(4-methylphenyl)-1*H*-tetrforazole(**2b**): white solid; MP: 248-249 °C (lit.[1] 247-249 °C); reaction time 4 h; ^{1}H-NMR (400 MHz, DMSO-d_6), δ 2.37 (3H, s), 7.40 (2H, d, J = 8.2 Hz), 7.91 (2H, d, J = 8.2 Hz); ^{13}C NMR (100 MHz, DMSO-d_6) δ 21.0, 121.2, 126.9, 129.9, 141.2, 155.1. Anal. Calcd for $C_8H_8N_4$: C, 60.00; H, 5.00; N, 35.00. Found: C, 60.13; H, 5.11; N, 34.86.



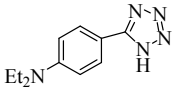
5-(3,5-dimethylphenyl)-1*H*-tetrazole (**2c**): white solid; MP: 204-206 °C (lit.[8] 205-207 °C); reaction time 4 h; ^{1}H NMR (400 MHz, DMSO-d_6) δ 2.30 (6H, m), 7.35 (1H, s), 7.44 (2H, s); ^{13}C NMR (100 MHz, DMSO-d_6) δ 20.9, 21.3, 111.6, 119.5, 129.9, 135.2, 139.5, 139.6. Anal. Calcd for $C_9H_{10}N_4$: C, 62.07; H, 5.75; N, 32.18. Found: C, 62.31; H, 5.94; N, 32.01.



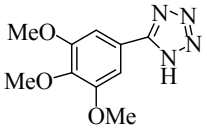
5-(4-methoxyphenyl)-1*H*-tetrazole (**2d**): white solid; MP: 231-232 °C (lit.[2] 230-231 °C); reaction time 5 h; ^{1}H NMR (400 MHz, DMSO-*d6*): δ 3.83 (3H, s), 7.15 (2H, d, J = 8.9 Hz), 7.97 (2H, d, J = 8.8 Hz); ^{13}C NMR (100 MHz, DMSO-d_6) δ 55.4, 114.8, 116.4, 128.6, 154.8, 161.4. Anal. Calcd for $C_8H_8N_4O$: C, 54.55; H, 4.55; N, 31.82. Found: C, 54.40; H, 4.69; N, 31.69.



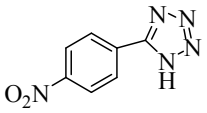
5-(3-methoxyphenyl)-1*H*-tetrazole (**2e**): white solid; MP: 158-159 °C (lit.[8] 157-158 °C); reaction time 5 h; ^{1}H NMR (400 MHz, DMSO-*d6*): δ 3.85 (3H, s), 7.18 (1H, s), 7.52 (1H, t, *J* = 8.0 Hz), 7.58-7.64 (2H, m); ^{13}C NMR (100 MHz, DMSO-d_6) δ 55.4, 112.1, 116.9, 119.2, 125.4, 130.6, 155.3, 159.8. Anal. Calcd for $C_8H_8N_4O$: C, 54.55; H, 4.55; N, 31.82. Found: C, 54.35; H, 4.72; N, 31.61.



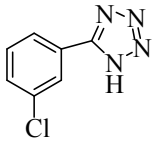
5-(4-*N*,*N*-diethylaminophenyl)-1*H*-tetrazole (**2f**): beige solid; MP: 89-90 °C (lit.[8] 90 °C); reaction time 6 h; ^{1}H NMR (400 MHz, DMSO-*d6*): δ 1.11 (6H, t, *J* = 7.0 Hz), 3.41 (4H, q, *J* = 7.0 Hz), 6.80-6.83 (2H,m), 7.80-7.85 (2H, m); ^{13}C NMR (100 MHz, DMSO-d_6) δ 12.3, 43.7, 109.4, 111.2, 128.3, 149.3, 154.8. Anal. Calcd for $C_{11}H_{15}N_5$: C, 60.83; H, 6.91; N, 32.26. Found: C,60.64; H, 6.70; N, 32.49.



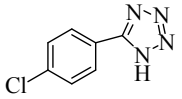
5-(3,4,5-trimethoxyphenyl)-1*H*-tetrazole (**2g**): white solid; MP: 201-202 °C (lit.[7] 201 °C); reaction time 6 h; ^{1}H NMR (400 MHz, DMSO-*d6*): δ 3.74 (3H, s), 3.88 (6H, s), 7.37 (2H, s); ^{13}C NMR (100 MHz, DMSO-d_6) δ 55.7, 60.03, 102.8, 128.4, 136.5, 152.8, 160.5. Anal. Calcd for $C_{10}H_{12}N_4O_3$: C, 50.85; H, 5.08; N, 23.73. Found: C, 50.99; H, 5.29; N, 23.53.



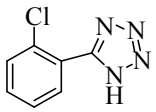
5-(4-nitrophenyl)-1*H*-tetrazole (**2h**): beige solid; MP: 215-216 °C (lit.[1] 214-216 °C); reaction time 3 h; ^{1}H NMR (400 MHz, DMSO-*d6*): δ 8.32 (2H, d, *J* = 8.4 Hz), 8.44 (2H, d, *J* = 8.4 Hz); ^{13}C NMR (100 MHz, DMSO-d_6) δ 124.6, 128.2, 130.7, 148.7, 155.4. Anal. Calcd for $C_7H_5N_5O_2$: C, 43.98; H, 2.62; N, 36.65. Found: C, 43.84; H, 2.78; N, 36.51.



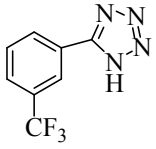
5-(3-chlorophenyl)-1*H*-tetrazole (**2i**): white solid; MP: 130-132 °C (lit.[3] 128-130 °C); reaction time 3 h; ^{1}H NMR (400 MHz, DMSO-*d6*): 7.64 (1H, bt, *J* = 7.5 Hz), 7.67 (1H, dd, *J* = 7.5 Hz, *J* = 2.0 Hz), 8.02 (1H, bdt, *J* = 6.8 Hz, *J* = 1.9 Hz), 8.08 (1H, bt, *J* = 1.9 Hz); ^{13}C NMR (100 MHz, DMSO-d_6) δ 125.9, 126.5, 126.9, 131.3, 131.7, 134.5, 155.3. Anal. Calcd for $C_7H_5ClN_4$: C, 46.54; H, 2.77; N, 31.02. Found: C, 46.49; H, 2.55; N, 31.27.



5-(4-chlorophenyl)-1*H*-tetrazole (**2j**): white solid; MP: 261-262 °C (lit.[1] 260-261 °C); reaction time 3 h; ^{1}H NMR (400 MHz, DMSO-*d6*): δ 7.70 (2H, d, *J* = 8.8 Hz), 8.08 (2H, d, *J* = 8.8 Hz); ^{13}C NMR (100 MHz, DMSO-d_6) δ 123.2, 128.7, 129.5, 135.9, 154.8. Anal. Calcd for $C_7H_5ClN_4$: C, 46.54; H, 2.77; N, 31.02. Found: C, 46.41; H, 2.63; N, 31.16.

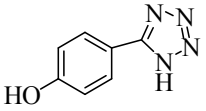


5-(2-chlorophenyl)-1*H*-tetrazole (**2k**): white solid; MP: 180-181 °C (lit.[3] 181-182 °C); reaction time 3 h; ^{1}H NMR (400 MHz, DMSO-*d6*): δ 7.56 (1H, ddd, *J* = 7.6 Hz, *J* = 7.2 Hz, *J* = 1.2 Hz), 7.63 (1H, ddd, *J* = 7.2 Hz, *J* = 8.0 Hz, *J* = 1.6 Hz), 7.71 (1H, dd, *J* = 8.0 Hz, *J* = 1.2 Hz), 7.82 (1H, dd, *J* = 7.6 Hz, *J* = 1.7 Hz); ^{13}C NMR (100 MHz, DMSO-d_6) δ 124.1, 127.7, 130.4, 131.7, 131.9, 132.5, 153.4. Anal. Calcd for $C_7H_5ClN_4$: C, 46.54; H, 2.77; N, 31.02. Found: C, 46.67; H, 2.57; N, 31.23.

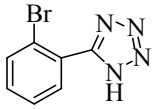


5-(3-trifluoromethylphenyl)-1*H*-tetrazole (**2l**): white solid; MP: 155-156 °C (lit.[4] 156-157

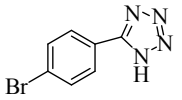
°C); reaction time 4 h;[1]H NMR (400 MHz, DMSO-*d6*): δ 7.87 (1H, ddd, *J* = 7.8 Hz, *J* = 8.2 Hz, *J* = 0.7 Hz), 7.975 (1H, bd, *J* = 7.8 Hz), 8.33-8.42 (2H, m); ^{13}C NMR (100 MHz, DMSO-d_6) δ 123.3, 123.7, 125.5, 127.6, 130.0, 130.7, 130.8, 154.9. Anal. Calcd for $C_8H_5F_3N_4$: C, 44.86; H, 2.34; N, 26.17. Found: C, 44.56; H, 2.15; N, 26.43.



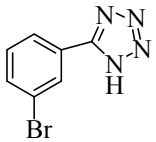
5-(4-hydroxyphenyl)-1*H*-tetrazole (**2m**): white solid; MP: 234-235 °C (lit.[2] 235-236 °C); reaction time 4 h; [1]H NMR (400 MHz, DMSO-*d6*): δ 6.96 (2H, d, *J* = 8.5 Hz), 7.85 (2H, d, *J* = 8.5 Hz); ^{13}C NMR (100 MHz, DMSO-d_6) δ 114.3, 116.1, 128.5, 154.1, 159.9. Anal. Calcd for $C_7H_6N_4O$: C, 51.85; H, 3.70; N, 34.57. Found: C, 51.71; H, 3.58; N, 34.71.



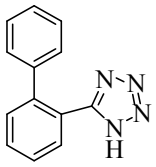
5-(2-bromophenyl)-1*H*-tetrazole (**2n**): brown solid; MP: 178-179 °C (lit.[8] 178-179 °C); reaction time 3 h; [1]H NMR (400 MHz, DMSO-*d6*): δ 7.58-7.61 (2H m,), 7.72 (1H, bd, *J* = 7.2 Hz), 7.88 (1H, bd, *J* = 7.5 Hz); ^{13}C NMR (100 MHz, DMSO-d_6) δ 121.7, 126.4, 128.1, 131.9, 132.6, 133.5, 154.6. Anal. Calcd for $C_7H_5BrN_4$: C, 37.35; H, 2.22; N, 24.90. Found: C, 37.21; H, 2.34; N, 24.99.



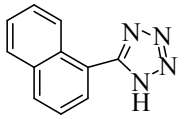
5-(4-bromophenyl)-1*H*-tetrazole (**2o**): brown solid; MP: 265-266 °C (lit.[2] 266-268 °C); reaction time 3 h; [1]H NMR (400 MHz, DMSO-*d6*): δ 7.85 (2H, d, *J* = 8.5 Hz), 8.00 (2H, d, *J* = 8.5 Hz); ^{13}C NMR (100 MHz, DMSO-d_6) δ 132.9, 129.3, 125.2, 123.5. Anal. Calcd for $C_7H_5BrN_4$: C, 37.35; H, 2.22; N, 24.90. Found: C, 37.29; H, 2.37; N, 24.87.



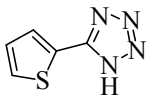
5-(3-bromophenyl)-1*H*-tetrazole (**2p**): brown solid; MP: 154-155 °C (lit.[8] 155-156 °C); reaction time 3 h; ^{1}H NMR (400 MHz, DMSO-*d6*): δ 7.62 (1H, s), 7.85 (1H, s), 8.09 (1H, s), 8.25 (1H, s); ^{13}C NMR (100 MHz, DMSO-d_6) δ 122.5, 126.0, 127.0, 129.3, 132.0, 133.5, 154.6. Anal. Calcd for $C_7H_5BrN_4$: C, 37.35; H, 2.22; N, 24.90. Found: C, 37.55; H, 2.43; N, 24.71.



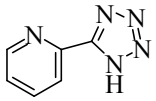
5-(biphenyl-2-yl)-1*H*-tetrazole (**2q**): white solid; MP: 148-149 °C (lit.[5] 149-150 °C); reaction time 6 h; ^{1}H NMR (400 MHz, DMSO-*d6*): δ 7.05-7.17 (2H, m), 7.28-7.36 (3H, m), 7.53-7.62 (2H, m), 7.64-7.74 (2H, m); ^{13}C NMR (100 MHz, DMSO-d_6) δ 123.4, 127.4, 127.7, 128.2, 128.7, 130.5, 130.6, 131.1, 139.2, 141.5, 155.0. Anal. Calcd for $C_{13}H_{10}N_4$: C, 70.27; H, 4.50; N, 25.23. Found: C, 70.38; H, 4.69; N, 25.02.



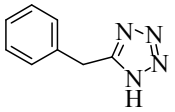
5-(naphthalen-1-yl)-1*H*-tetrazole (**2r**): white solid; MP: 262-263 °C (lit.[2] 261-262 °C); reaction time 4 h; ^{1}H NMR (400 MHz, DMSO-*d6*): δ 7.63-7.70 (3H, m), 7.99 (1H, dd, J = 7.2 Hz, J = 1.0 Hz), 8.08-8.11 (1H, m), 8.19 (1H, bd, J = 8.2 Hz), 8.56 (1H, dd, J = 7.3 Hz, J = 1.8 Hz); ^{13}C NMR (100 MHz, DMSO-d_6) δ 121.4, 125.0, 125.3, 126.7, 127.7, 128.4, 128.6, 129.9, 131.4, 133.4, 155.1. Anal. Calcd for $C_{11}H_8N_4$: C, 67.35; H, 4.08; N, 28.57. Found: C, 67.56; H, 4.31; N, 28.35.



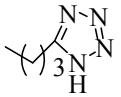
5-(thiophen-2-yl)-1*H*-tetrazole (**2s**): white solid; MP: 203-204 °C (lit.[6] 201-203 °C); reaction time 4 h; ^{1}H NMR (400 MHz, DMSO-*d6*): δ 7.28 (1H, t, J = 4.0 Hz), 7.79 (1H, d, J = 4.0 Hz), 7.86 (1H, d, J = 4.0 Hz); ^{13}C NMR (100 MHz, DMSO-d_6) δ 125.4, 128.6, 129.2, 130.4, 151.3. Anal. Calcd for $C_5H_4N_4S$: C, 39.47; H, 2.63; N, 36.84. Found: C, 39.38; H, 2.41; N, 36.99.



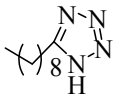
5-(2-pyridyl)-1*H*-tetrazole (**2t**): white solid; MP: 210-211 °C (lit.[2] 211-212 °C); reaction time 4 h; ^{1}H NMR (400 MHz, DMSO-*d6*): δ 7.41 (1H, m), 7.78 (1H, m), 8.02 (1H, d, *J* = 8.0 Hz), 8.50 (1H, d, *J* = 3.2 Hz); ^{13}C NMR (100 MHz, DMSO-d_6) δ 123.0, 126.5,138.6, 144.1, 150.5, 155.2. Anal. Calcd for $C_6H_5N_5$: C, 48.98; H, 3.40; N, 47.62. Found: C, 48.83; H, 3.54; N, 47.73.



5-benzyl-1*H*-tetrazole (**2u**): white solid; MP: 122-123 °C (lit.[1] 123-125 °C); reaction time 6 h; ^{1}H NMR (400 MHz, DMSO-*d6*): δ 4.28 (2H, s), 7.24-7.29 (3H, m), 7.31-7.7.37 (2H, m); ^{13}C NMR (100 MHz, DMSO-d_6) δ 28.8, 126.9, 128.6, 128.6, 135.9, 155.2. Anal. Calcd for $C_8H_8N_4$: C, 60.00; H, 5.00; N, 35.00. Found: C, 60.14; H, 5.12; N, 34.89.



5-butyl-1*H*-tetrazole (**2v**): white solid; MP: 41-42 °C (lit.[5] 41-42 °C); reaction time 8 h; ^{1}H NMR (400 MHz, DMSO-*d6*): δ 0.89 (3H, t, *J* = 7.4 Hz), 1.18-1.30 (2H, m), 1.59-1.67 (2H, m), 2.87 (2H, t, *J* = 7.5 Hz); ^{13}C NMR (100 MHz, DMSO-d_6) δ 13.4, 21.4, 22.3, 29.0, 155.9. Anal. Calcd for $C_5H_{10}N_4$: C, 47.62; H, 7.94; N, 44.44. Found: C, 47.51; H, 8.04; N, 44.31.



5-nonyl-1*H*-tetrazole (**2w**): yellow solid; MP: 28-29 °C; reaction time 8 h; ^{1}H NMR (400 MHz, DMSO-*d6*): δ 0.85 (3H, t, *J* = 6.7 Hz), 1.26 (12H, m), 1.68 (2H, m), 2.85 (2H, t, *J* = 7.5 Hz); ^{13}C NMR (100 MHz, DMSO-d_6) δ 13.9, 22.1, 22.7, 27.0, 28.3, 28.5, 31.2, 156.0. Anal. Calcd for $C_{10}H_{20}N_4$: C, 61.22; H, 10.20; N, 28.57. Found: C, 61.43; H, 10.43; N, 28.38.

[1] F. Abrishamia, M. Ebrahimikia, F. Rafiee, Appl. Organometal. Chem. 2015, 29, 730.

[2] M. Esmaeilpour, J. Javidi, S. Zahmatkesh, Appl. Organometal. Chem. 2016, 30, 897.

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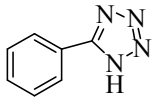
^{1}H and ^{13}C NMR Spectra of all compounds (2a-w)



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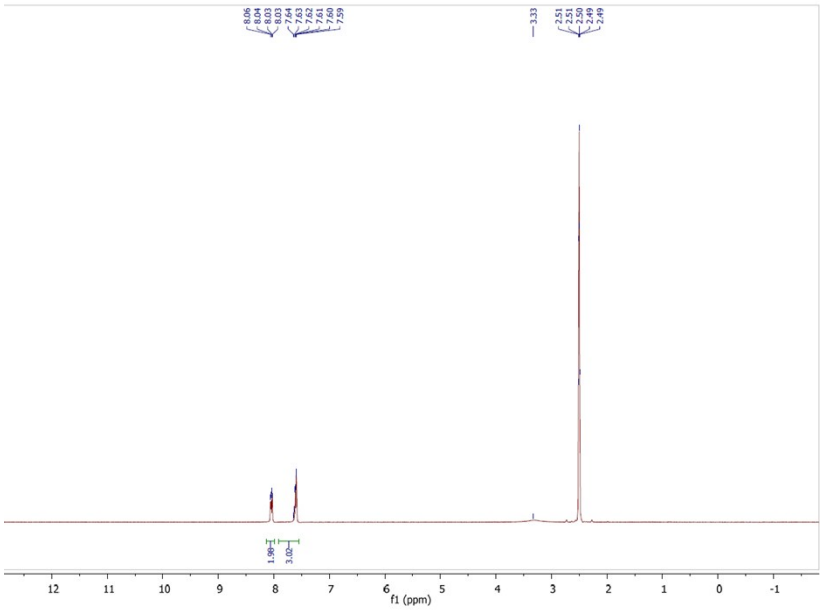

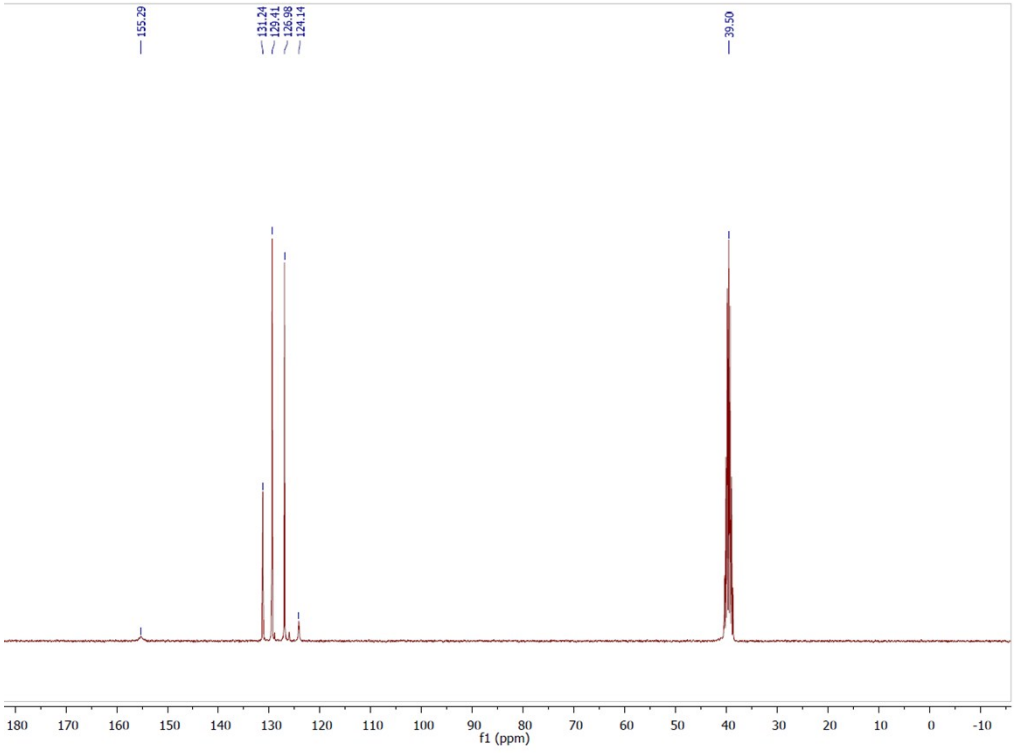

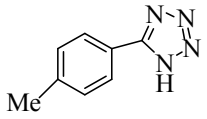
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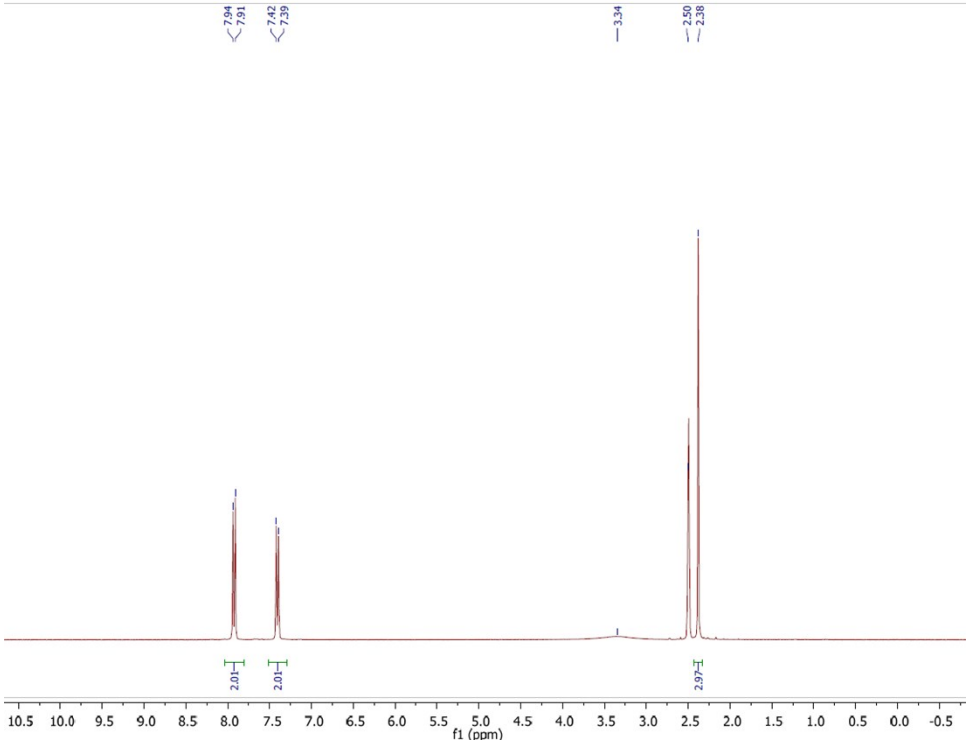
N
N
N
H
Me

2b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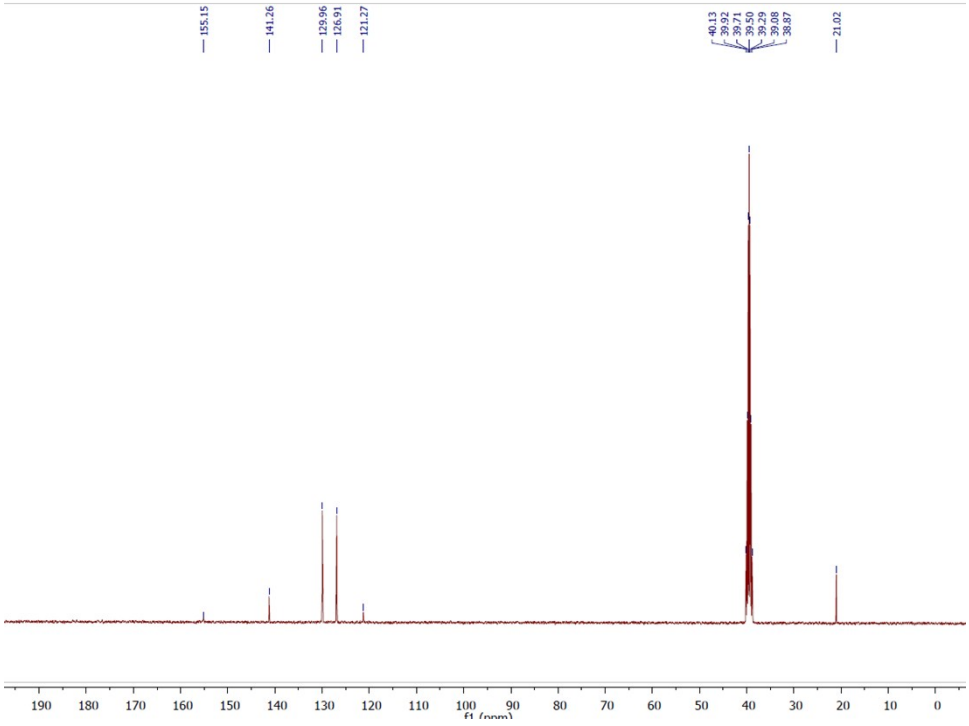
7.91
7.42
7.39
3.34
2.50
2.38
2.01
2.01
2.97
f1 (ppm)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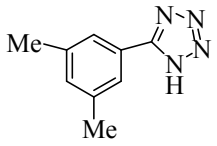
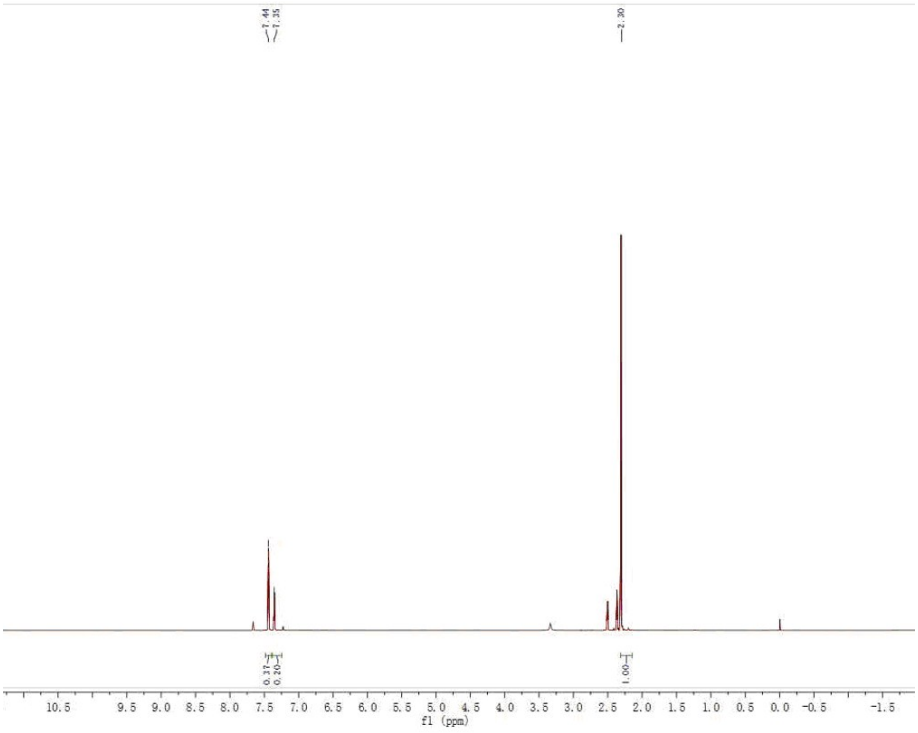
141.26
129.96
126.91
121.27
40.13
39.92
39.71
39.50
39.29
39.08
38.87
21.02
f1 (ppm)


Me
N
N
N
N
H
Me

2c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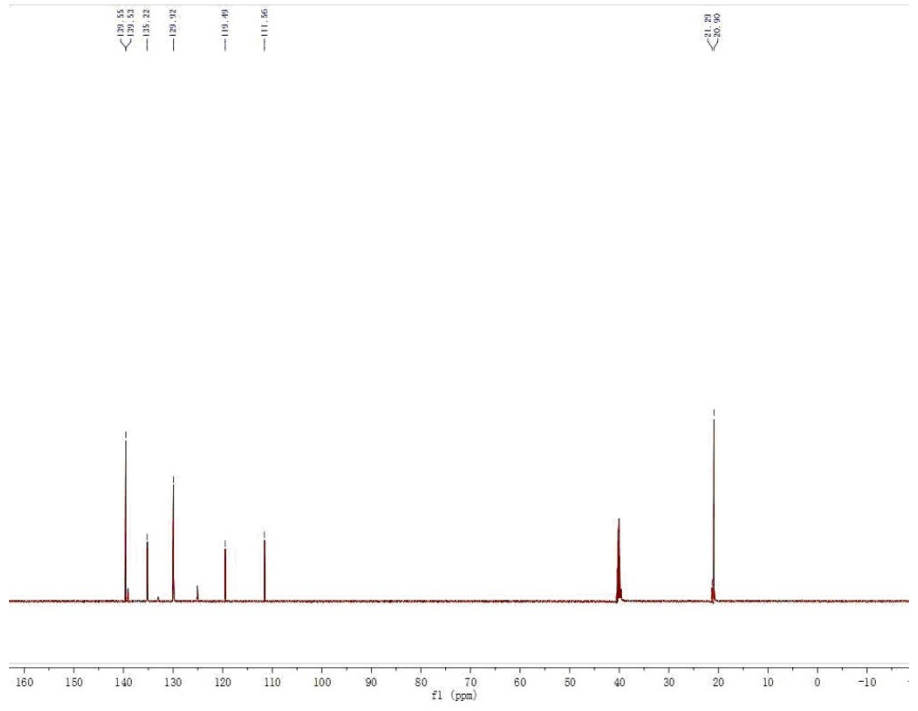
7.35
2.30
0.37
0.20
1.00
10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.5
f1 (ppm)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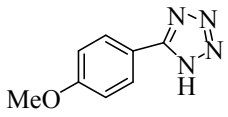
129.53
135.22
129.02
119.49
111.56
21.23
20.90
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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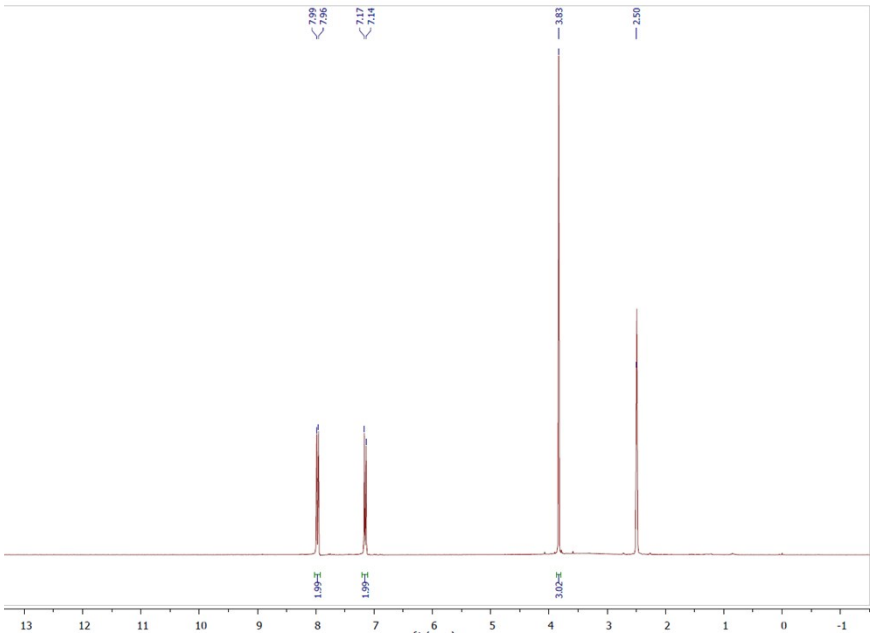
N
N
N
H
MeO

2d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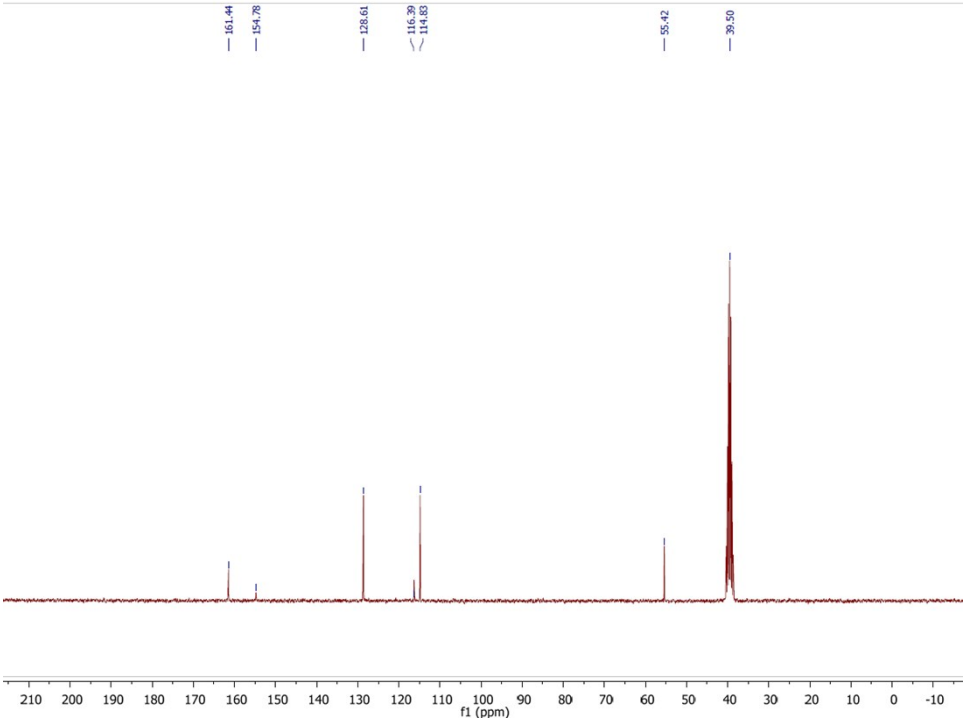
7.17
7.14
3.83
2.50
1.99
1.99
3.02
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1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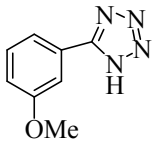
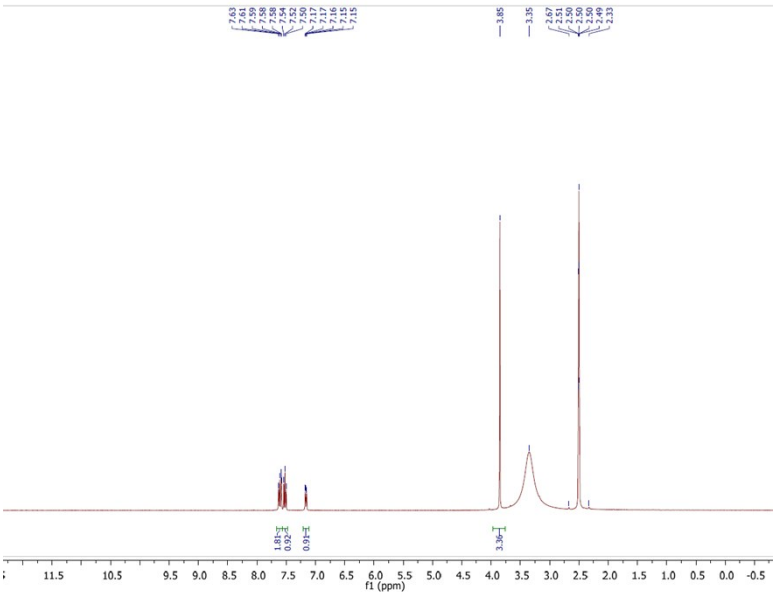
154.78
128.61
116.39
114.83
55.42
39.50
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)



2e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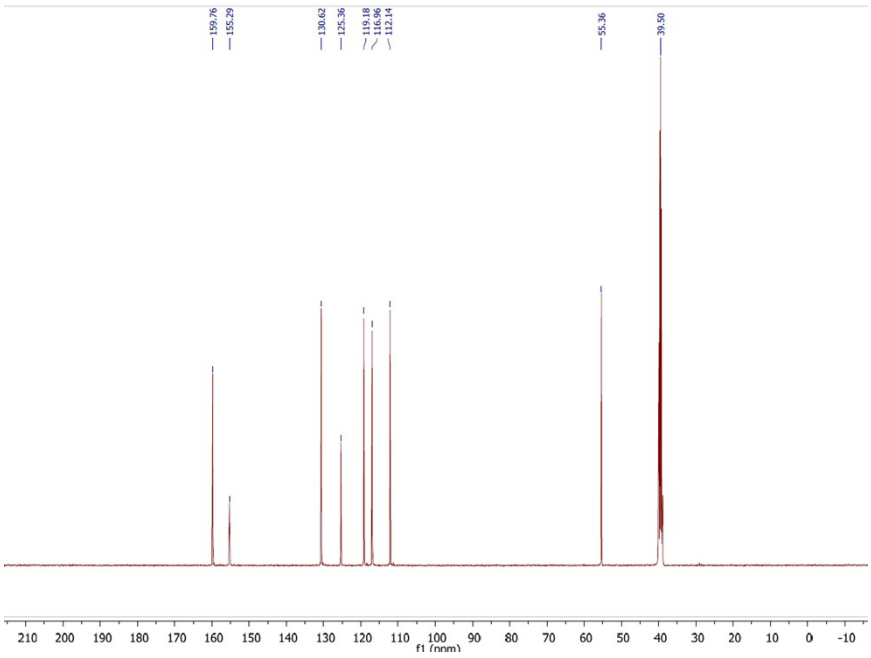
7.61
7.59
7.58
7.58
7.54
7.53
7.50
7.17
7.17
7.16
7.15
7.15
3.85
3.35
2.67
2.51
2.50
2.50
2.50
2.49
2.33
1.81
0.92
0.91
3.36
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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116.96
112.14
55.36
39.50
210
200
190
180
170
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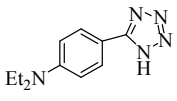
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)



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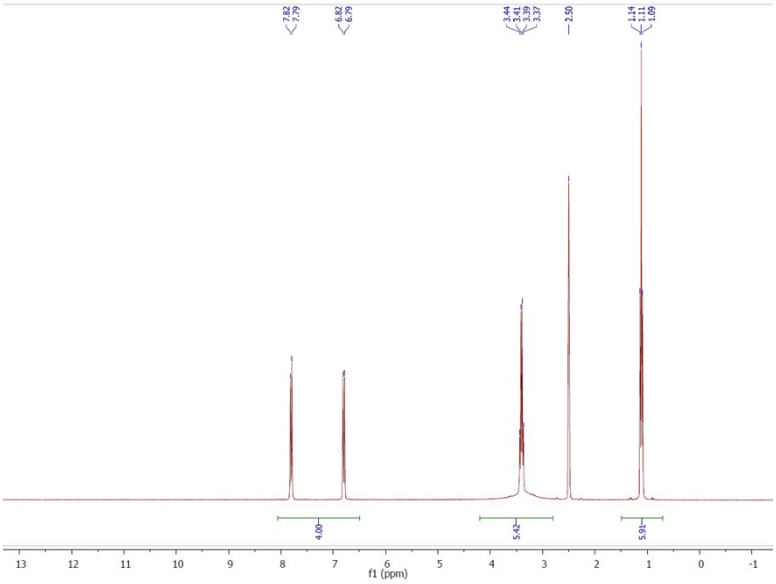
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6.82
6.79
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3.37
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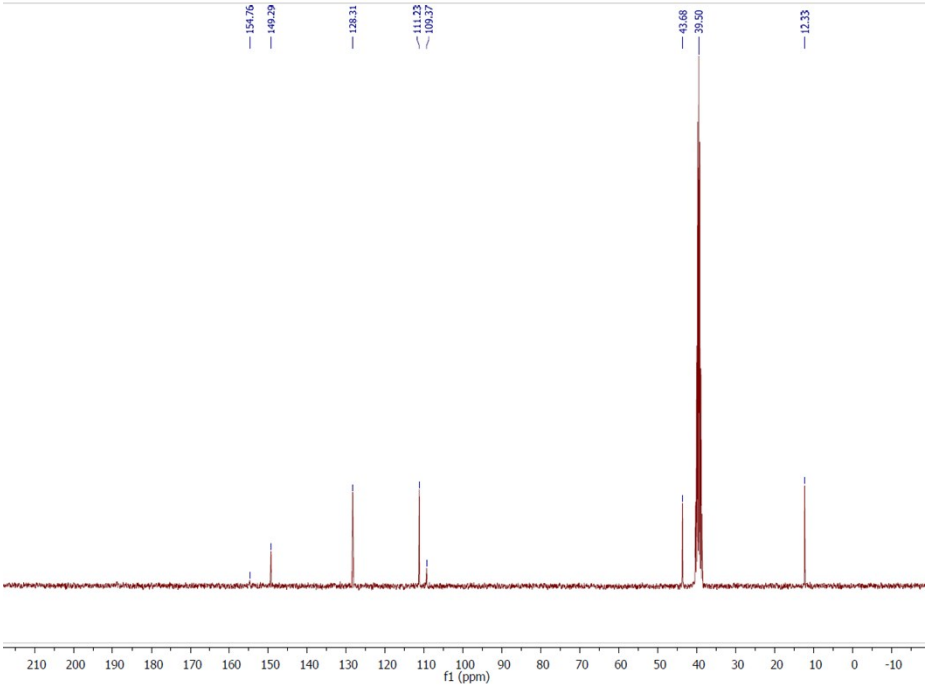
1.14
1.11
1.09
4.00
5.42
5.91
f1 (ppm)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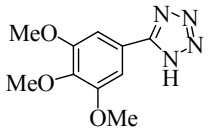
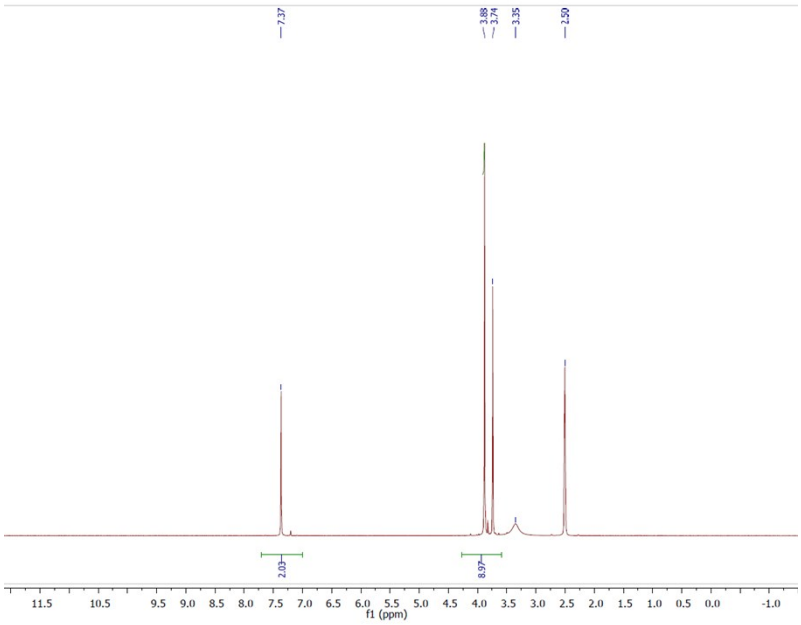
149.29
128.31
111.23
109.37
43.68
39.50
12.33
f1 (ppm)


MeO
MeO
OMe
N
N
N
N
H

2g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3.74
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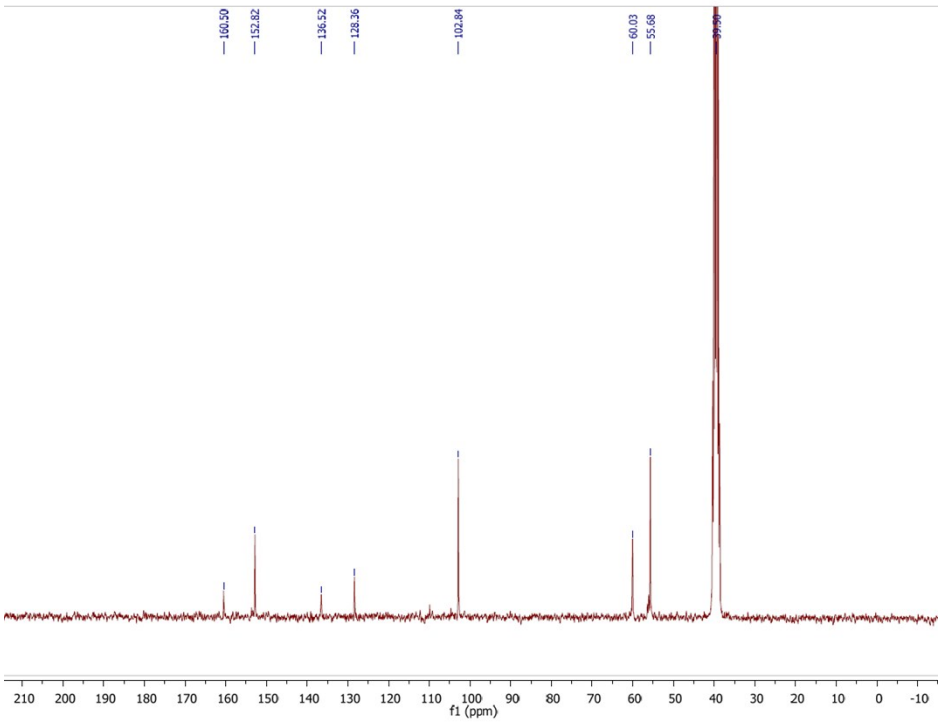
2.50
2.03
8.97
11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -1.0
f1 (ppm)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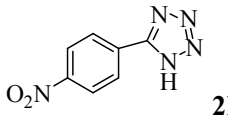

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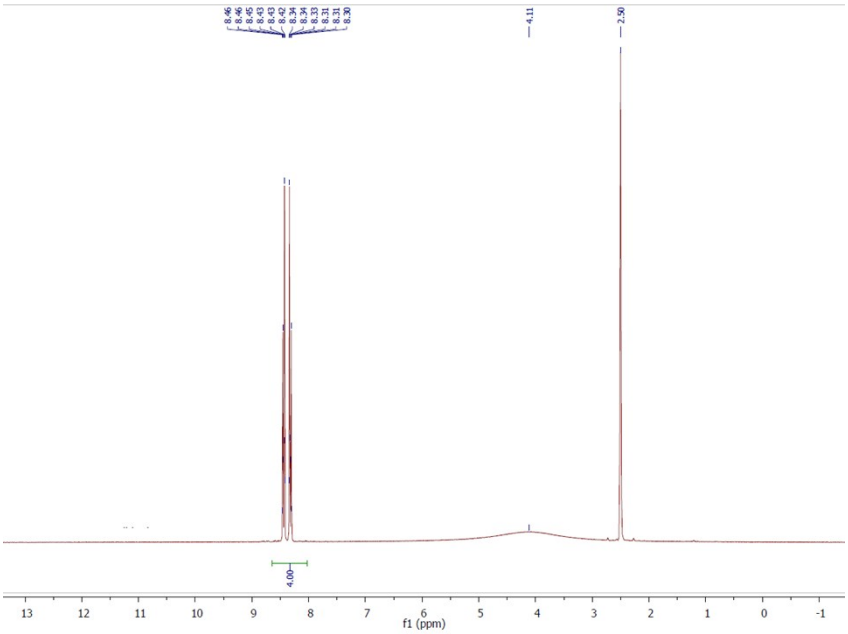
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8.34
8.33
8.31
8.31
8.30
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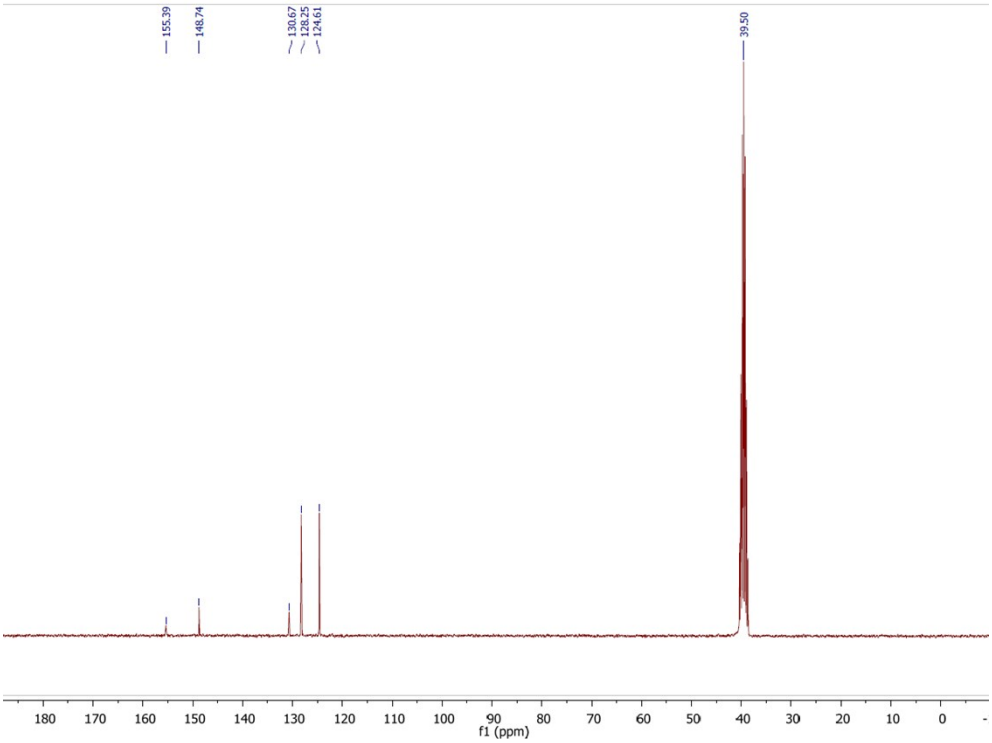
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)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130.67
128.25
124.61
39.50
180
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120
110
100
90
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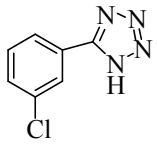
70
60
50
40
30
20
10
0
f1 (ppm)



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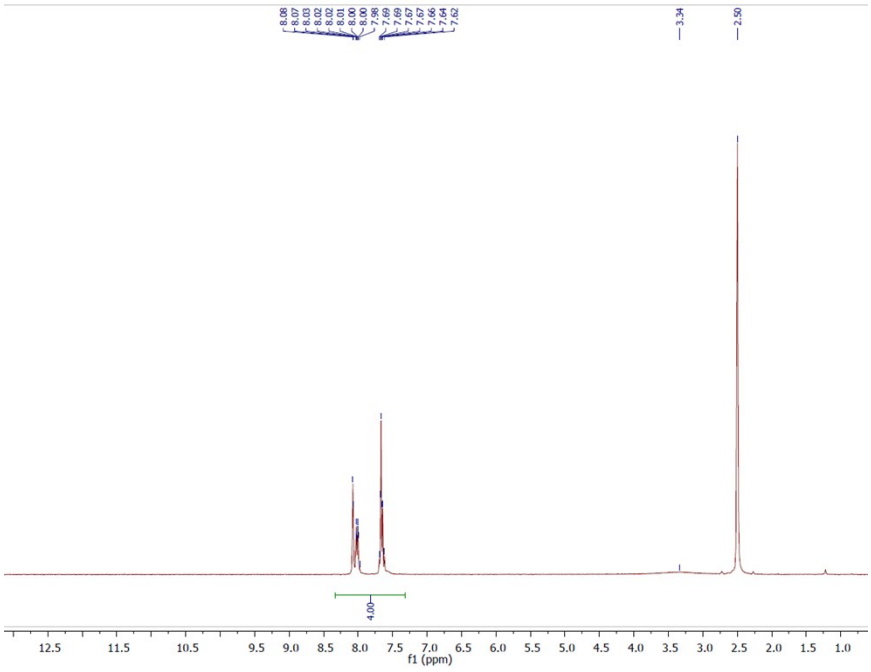
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8.02
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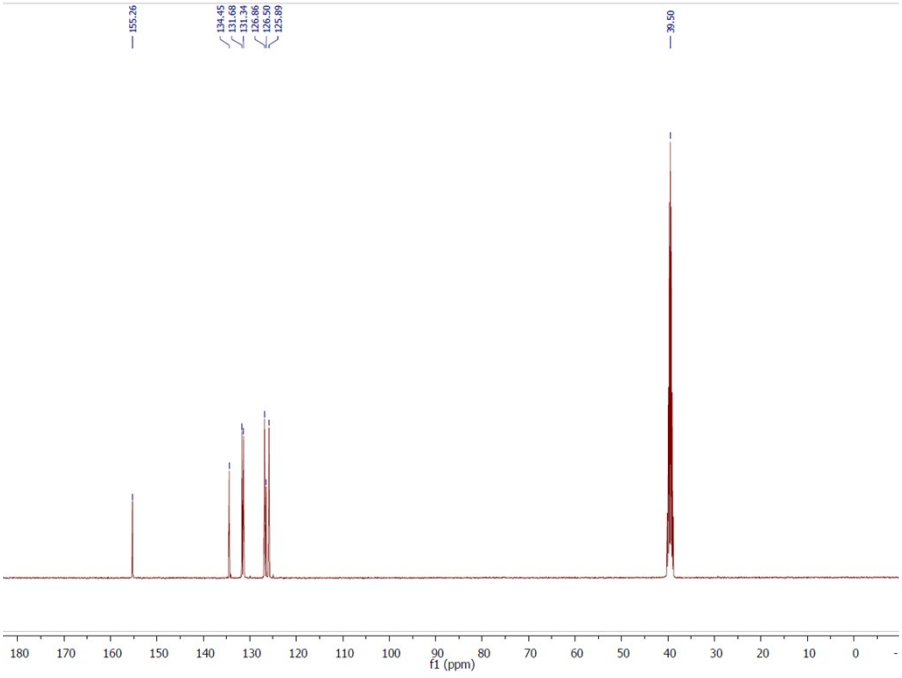
8.01
8.00
8.00
7.98
7.69
7.69
7.67
7.67
7.66
7.64
7.62
3.34
2.50
4.00
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0
f1 (ppm)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39.50
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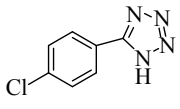
f1 (ppm)



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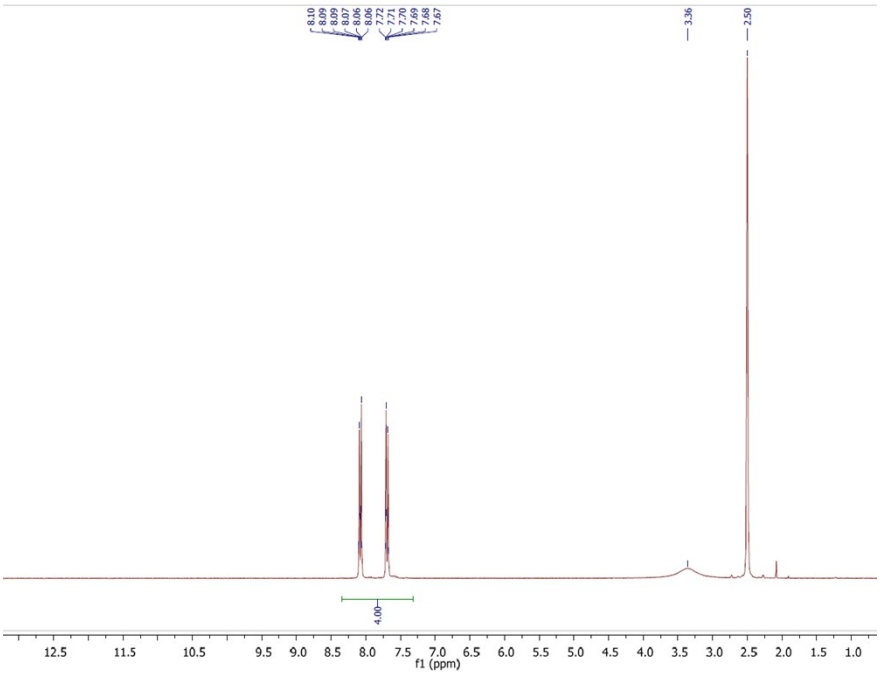
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8.09
8.07
8.07
8.06
8.06
7.72
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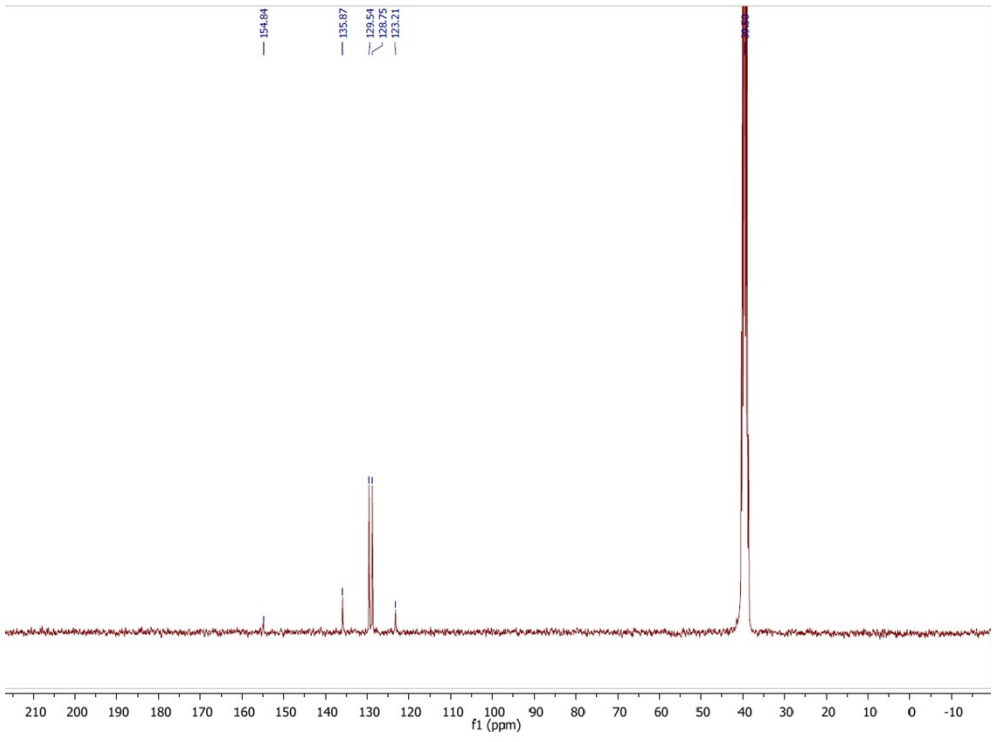
7.70
7.69
7.68
7.67
3.36
2.50
4.00
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0
f1 (ppm)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39.93
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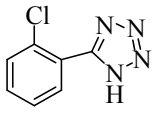
f1 (ppm)



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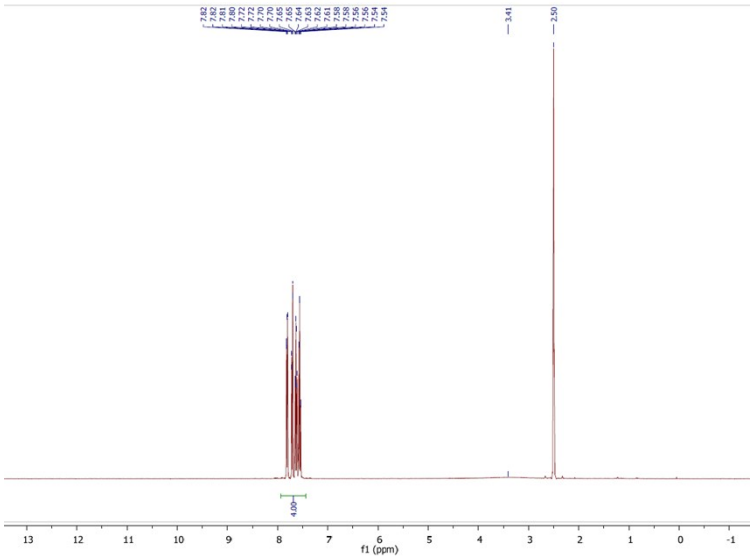
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7.54
3.41
2.50
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12
11
10
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8
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4
3
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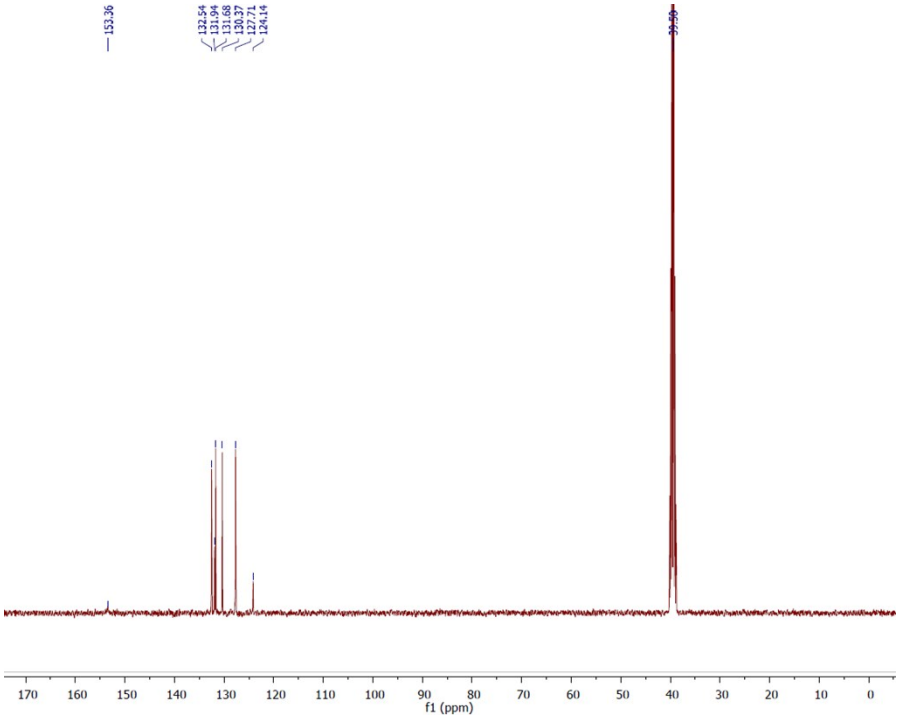
f1 (ppm)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90
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70
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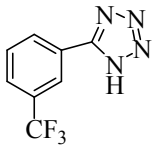
50
40
30
20
10
0
f1 (ppm)



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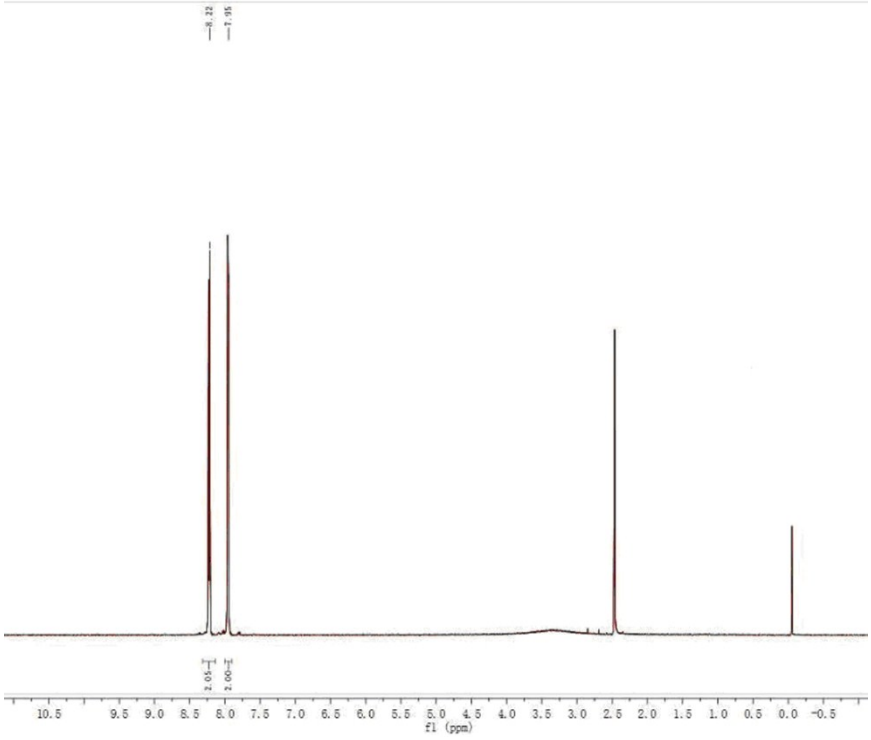
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2.00
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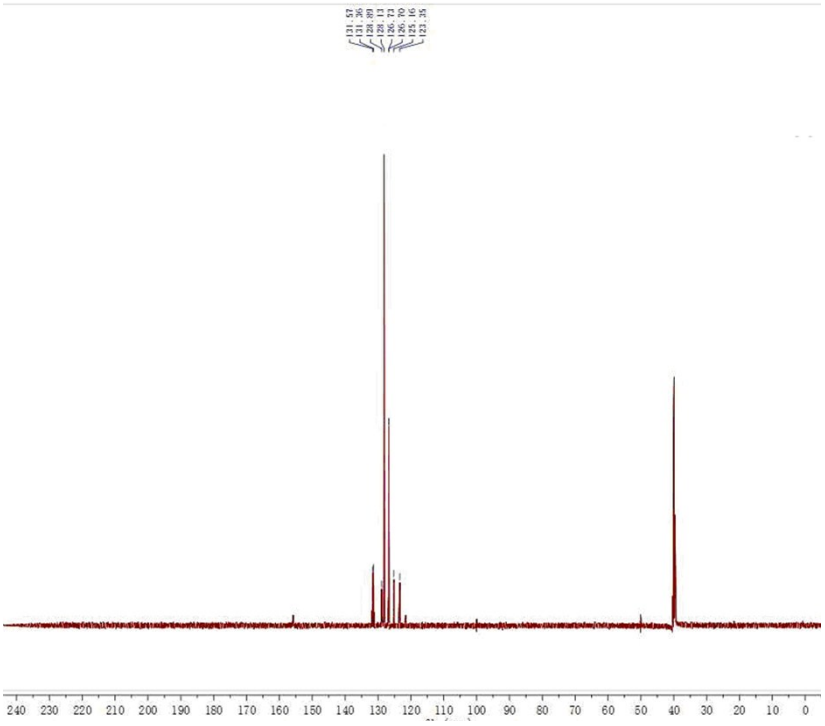
f1 (ppm)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126.70
125.16
123.35
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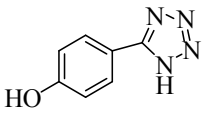
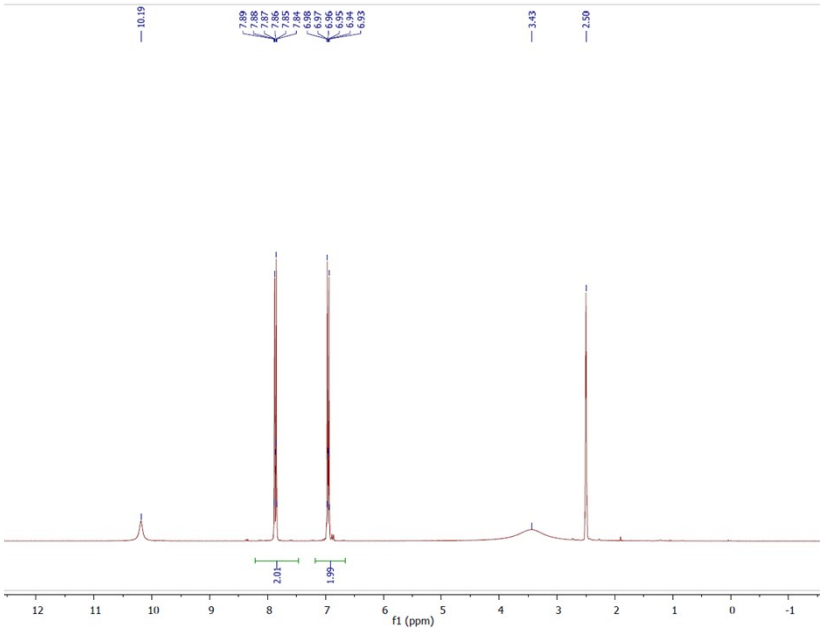

N
N
N
N
H
HO

2m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6.98
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6.96
6.95
6.94
6.93
3.43
2.50
2.01
1.99
12
11
10
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8
7
6
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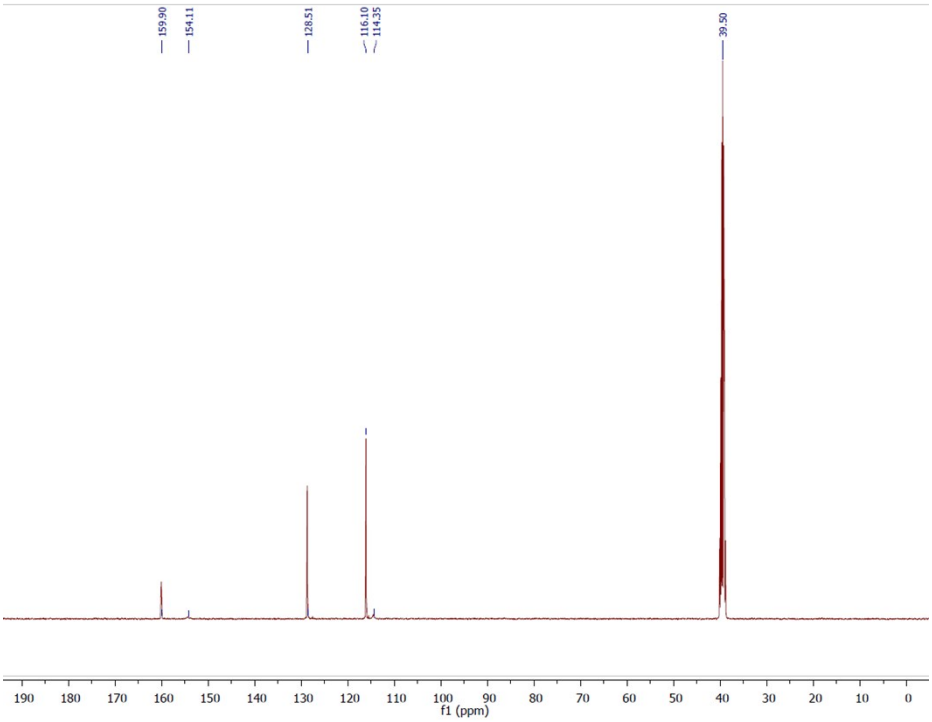
f1 (ppm)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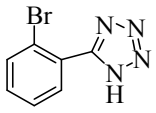
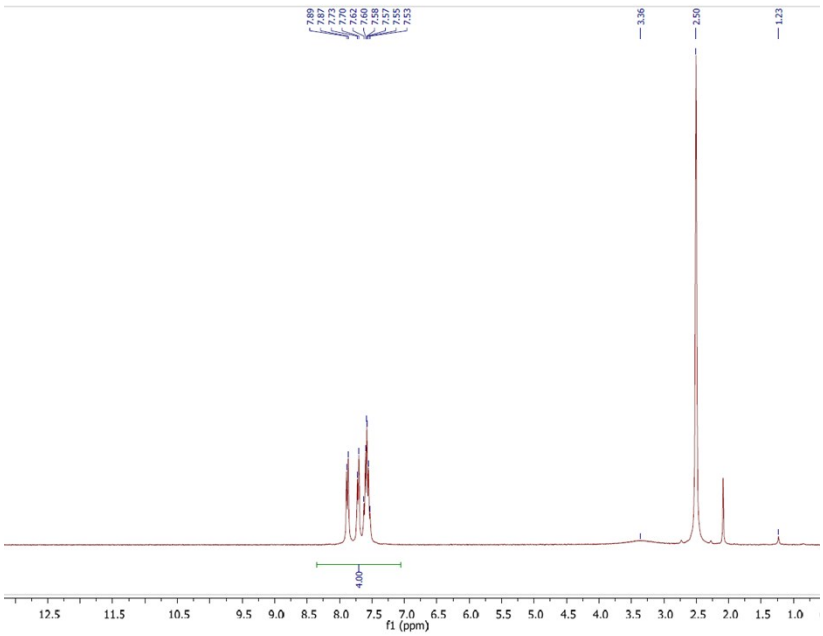
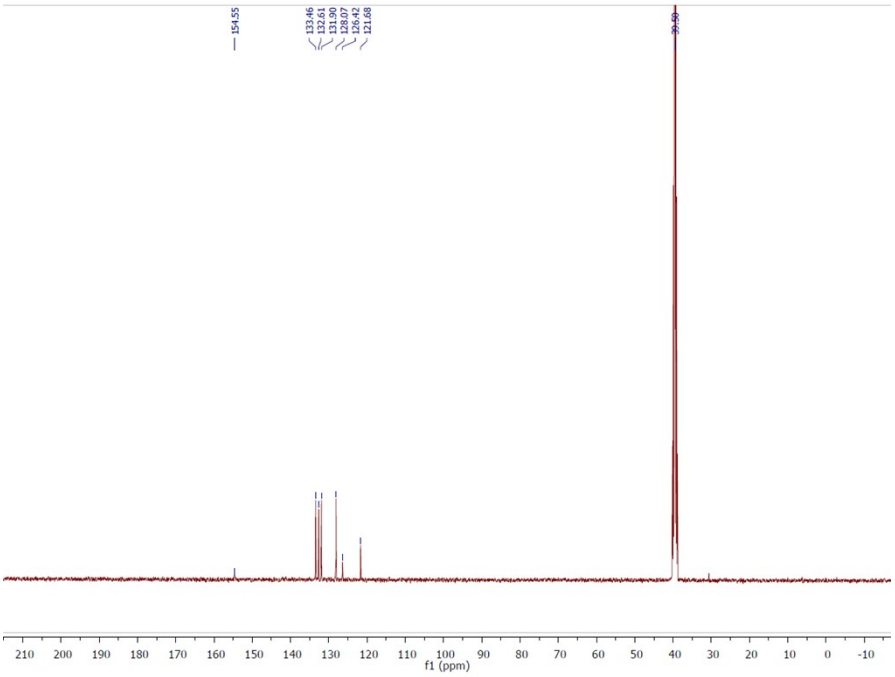
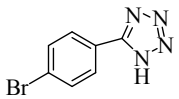
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Br
N
N
N
N
H

2n


7.89
7.87
7.73
7.70
7.62
7.60
7.58
7.57
7.55
7.53
3.36
2.50
1.23
4.00
12.5 11.5 10.5 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
f1 (ppm)


154.55
133.46
132.61
131.90
128.07
126.42
121.68
39.50
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)



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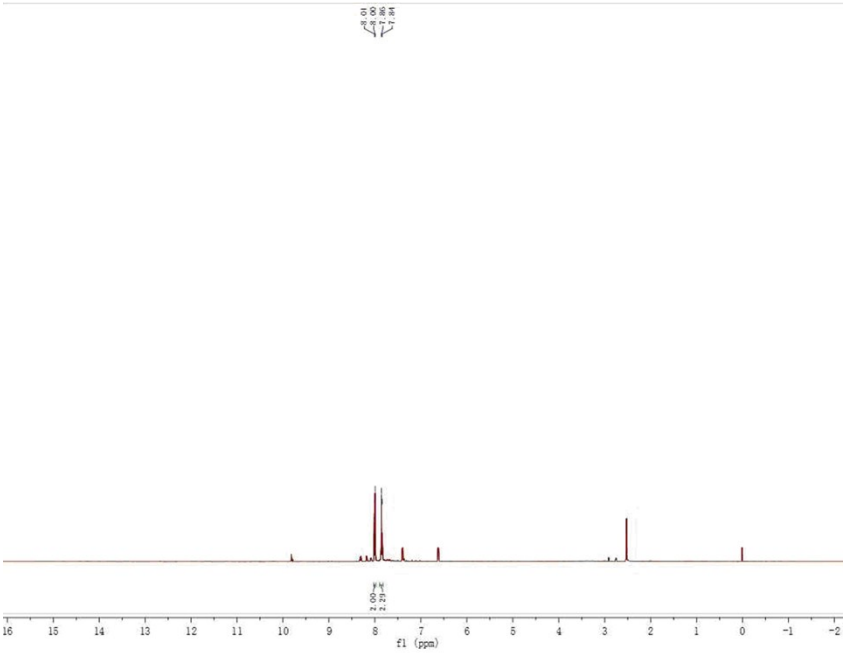
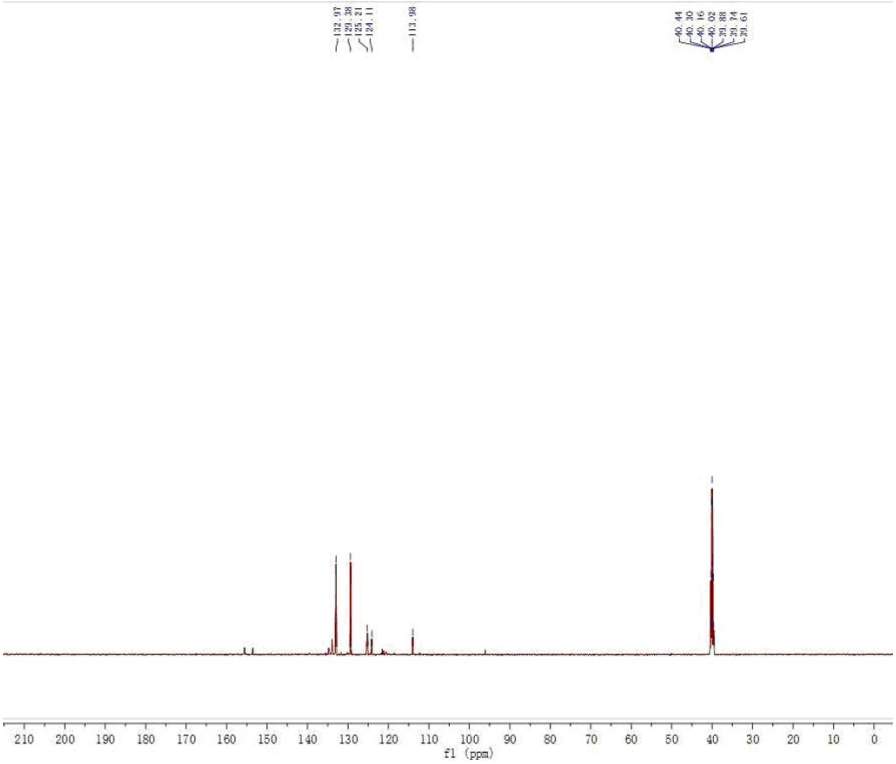
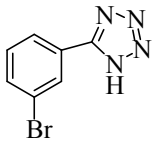
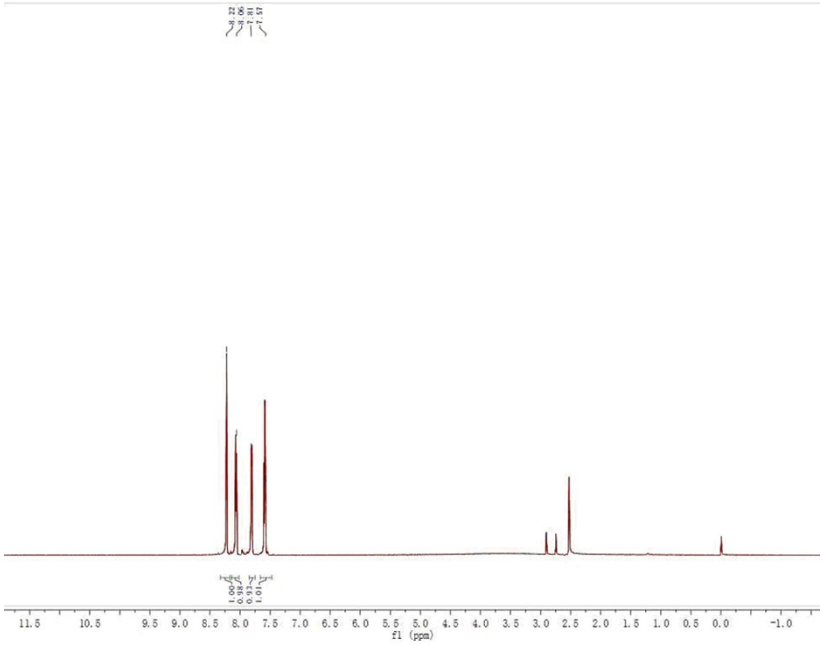
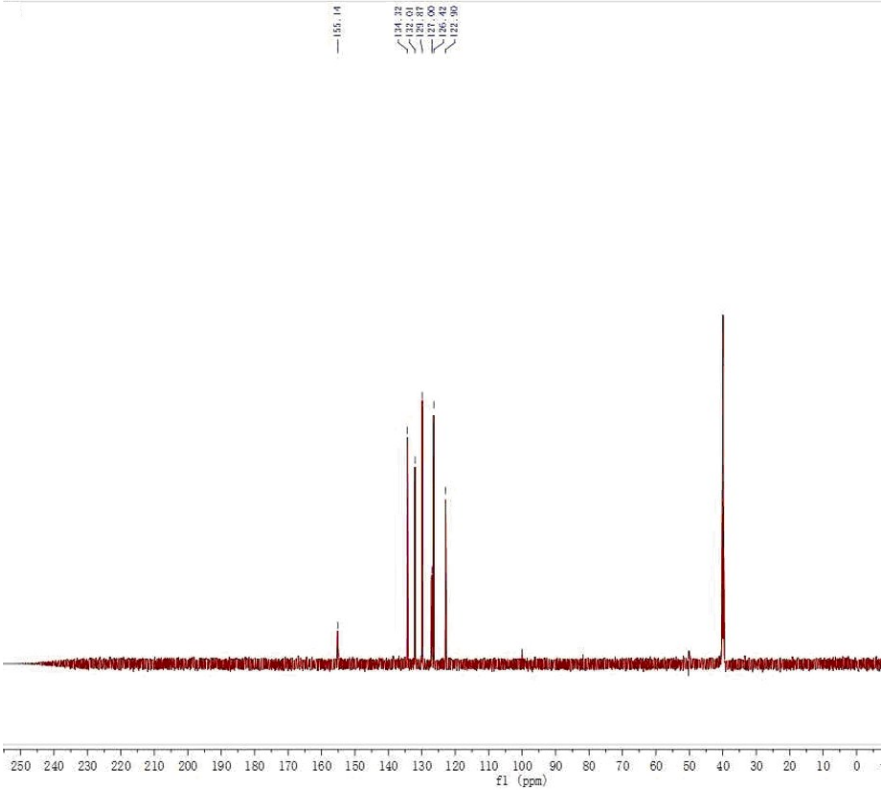

8.01
8.00
7.86
7.84
2.09
2.00
f1 (ppm)

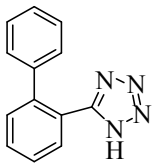

132.97
129.38
125.21
124.11
113.98
40.44
40.30
40.16
40.02
39.88
39.74
39.60
f1 (ppm)


N
N
N
N
H
Br

2p


11.5
10.5
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
-1.0
f1 (ppm)


250
240
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



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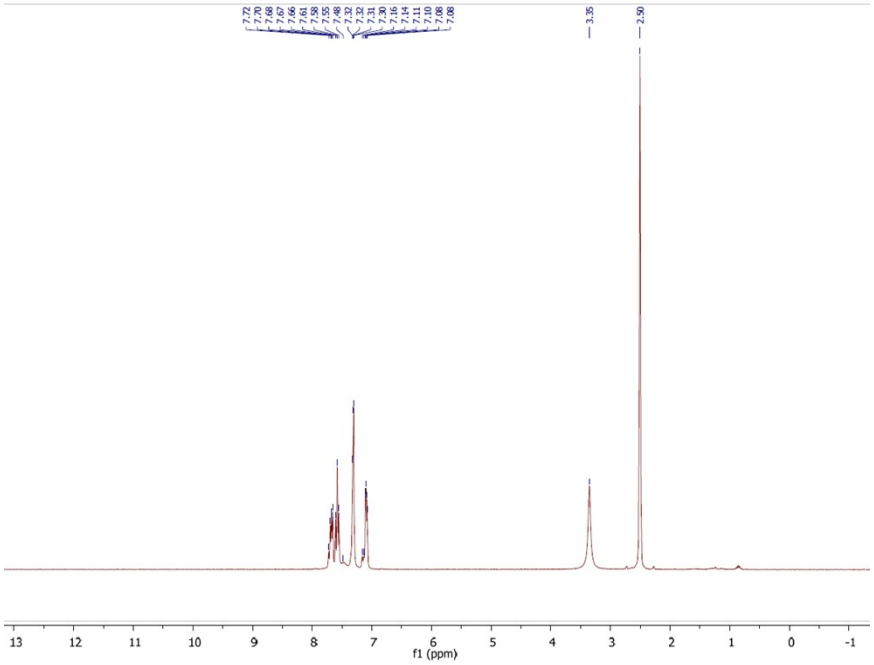
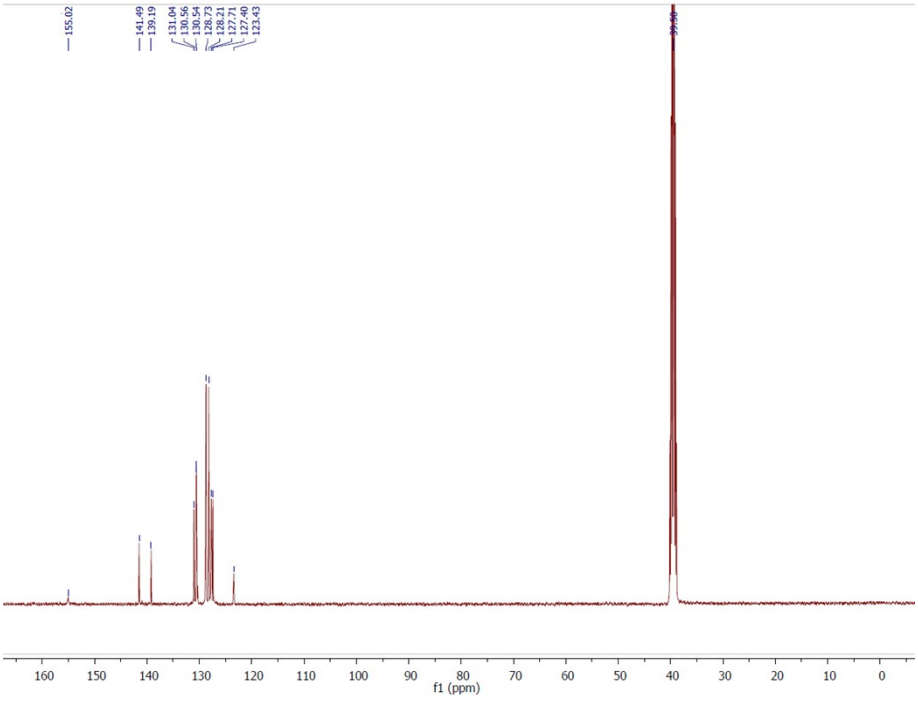
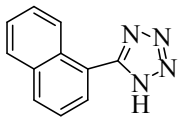
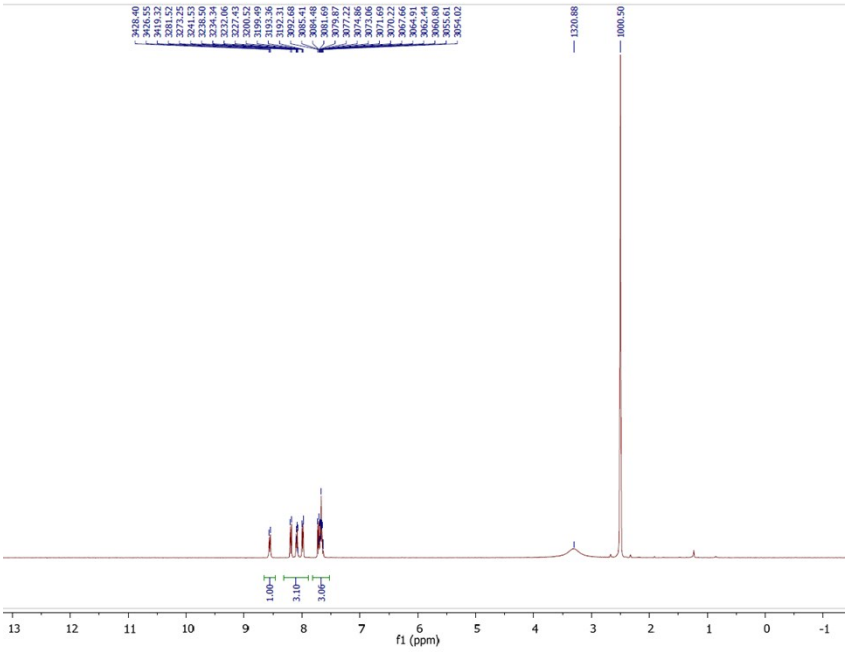
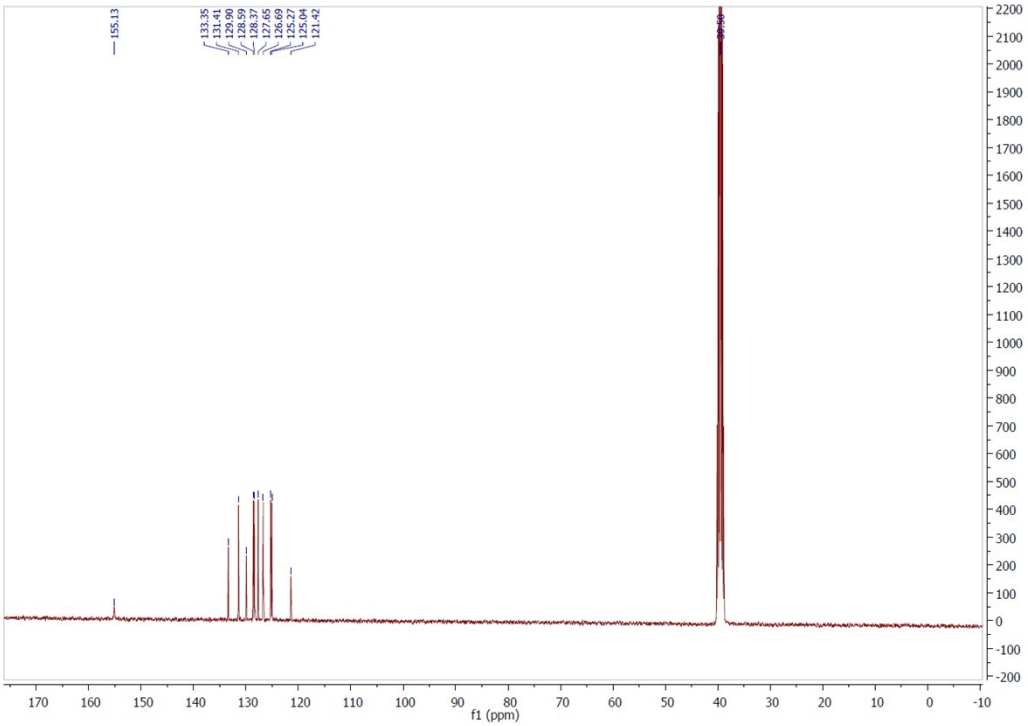

7.72
7.70
7.68
7.67
7.66
7.61
7.58
7.55
7.48
7.32
7.32
7.31
7.30
7.16
7.14
7.11
7.10
7.08
7.08
3.35
2.50
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)

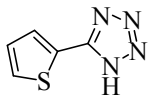

155.02
141.49
139.19
131.04
130.56
130.54
128.73
128.21
127.71
127.40
123.43
39.50
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



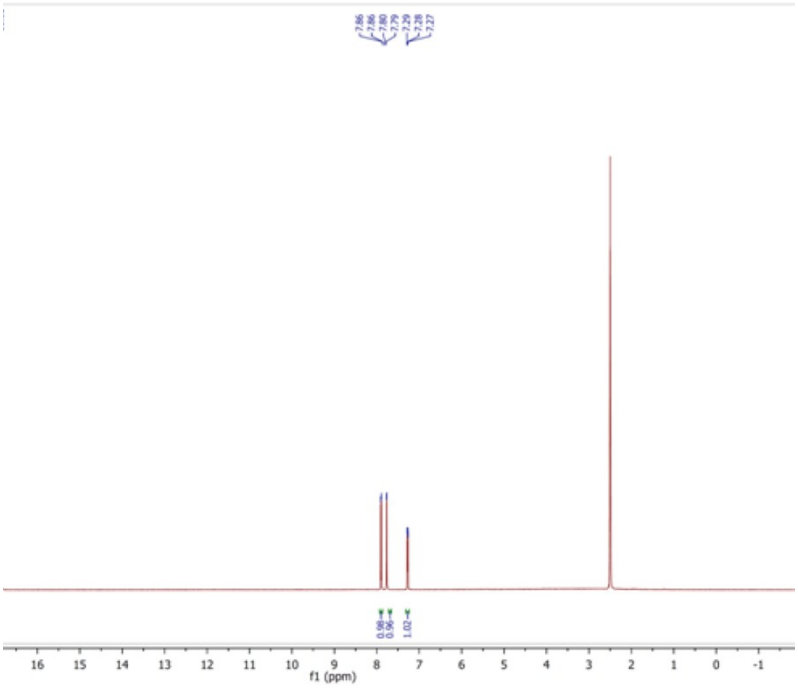
2r

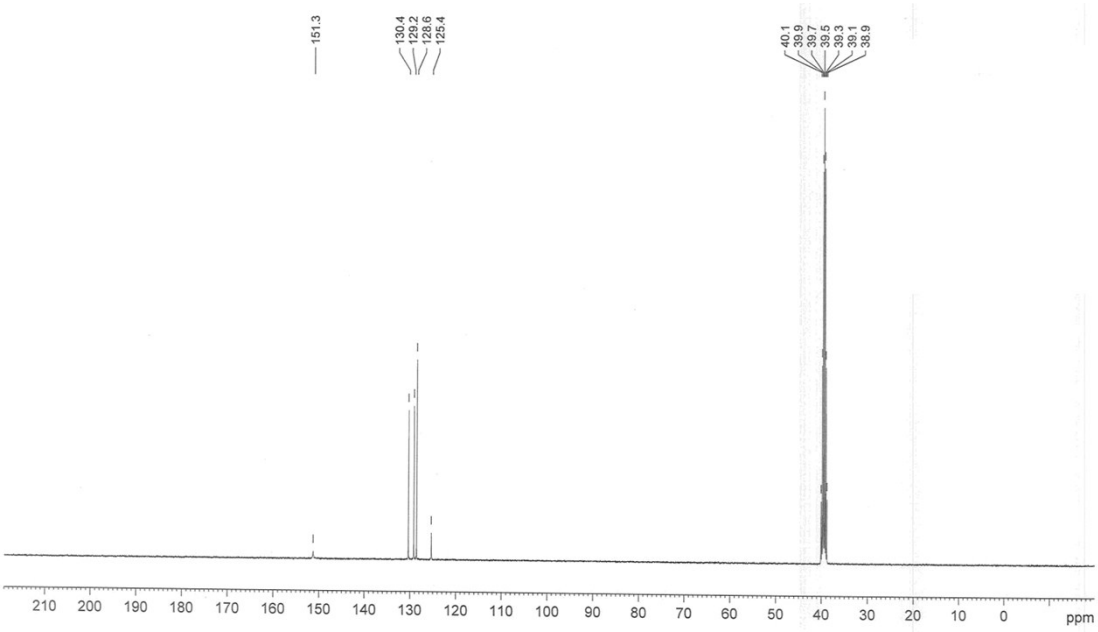

3428.40
3419.32
3281.52
3273.25
3241.53
3234.34
3232.06
3227.43
3199.49
3193.36
3192.31
3092.68
3085.41
3084.48
3081.69
3079.87
3077.22
3074.66
3073.06
3071.69
3070.22
3067.66
3062.44
3060.80
3055.61
3054.02
1320.88
1000.50
1.00
3.10
3.06
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)

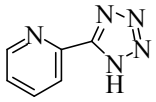

155.13
133.35
131.41
129.90
128.59
128.37
127.65
126.69
125.27
125.04
121.42
39.50
2200
2100
2000
1900
1800
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
-200
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)



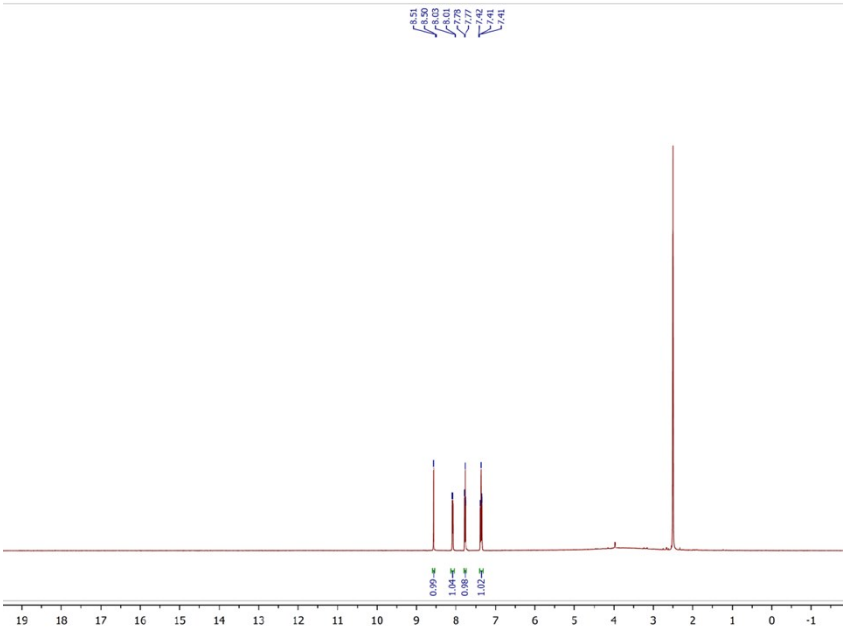
2s

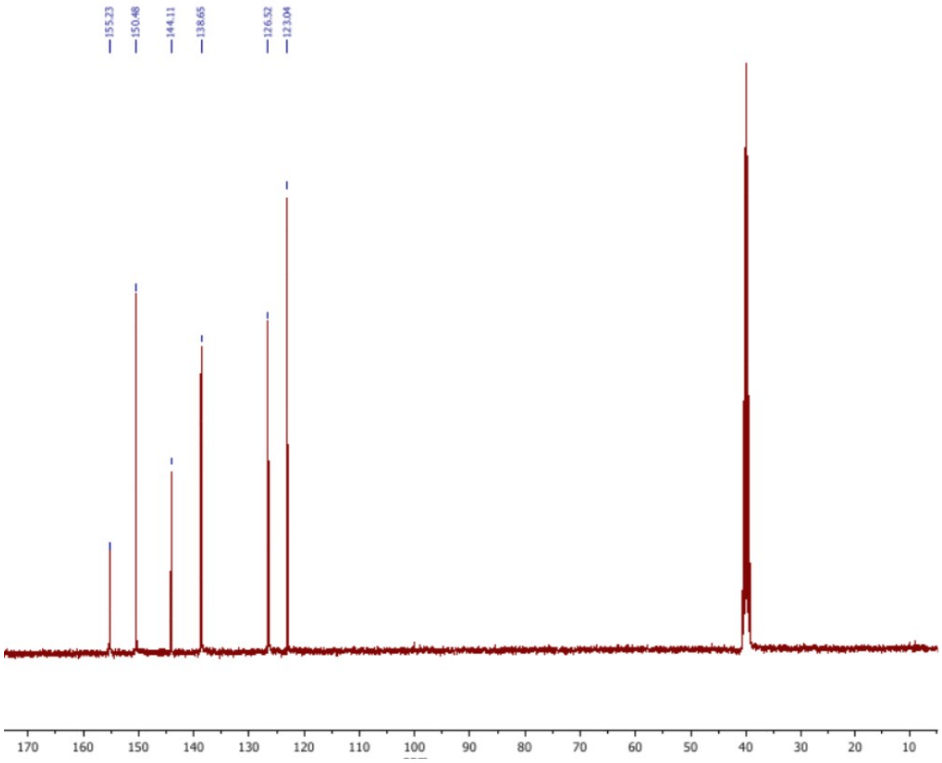

7.86
7.86
7.80
7.79
7.29
7.28
7.27
0.98
0.96
1.02
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

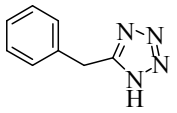

151.3
130.4
129.2
128.6
125.4
40.1
39.9
39.7
39.5
39.3
39.1
38.9
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm



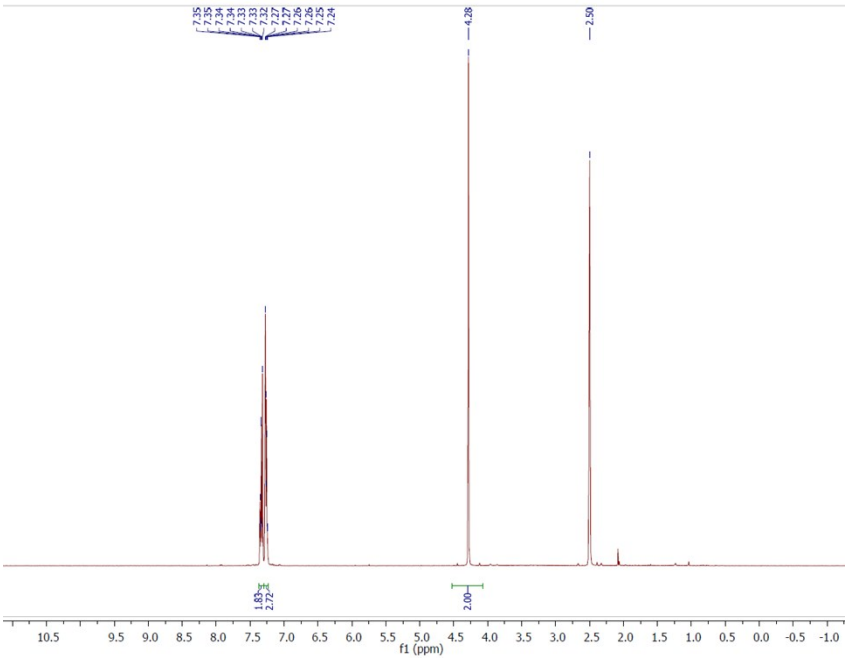
2t

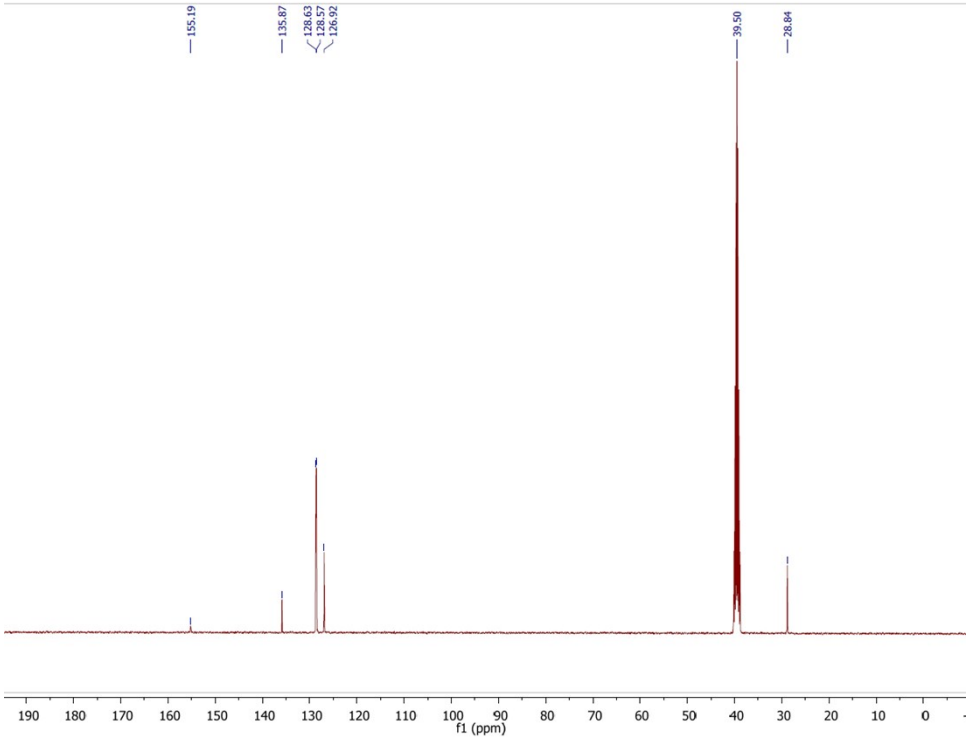

8.51
8.50
8.03
8.01
7.78
7.77
7.42
7.41
7.41
0.99
1.04
0.98
1.02

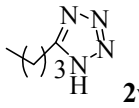

155.23
150.48
144.11
138.65
126.52
123.04



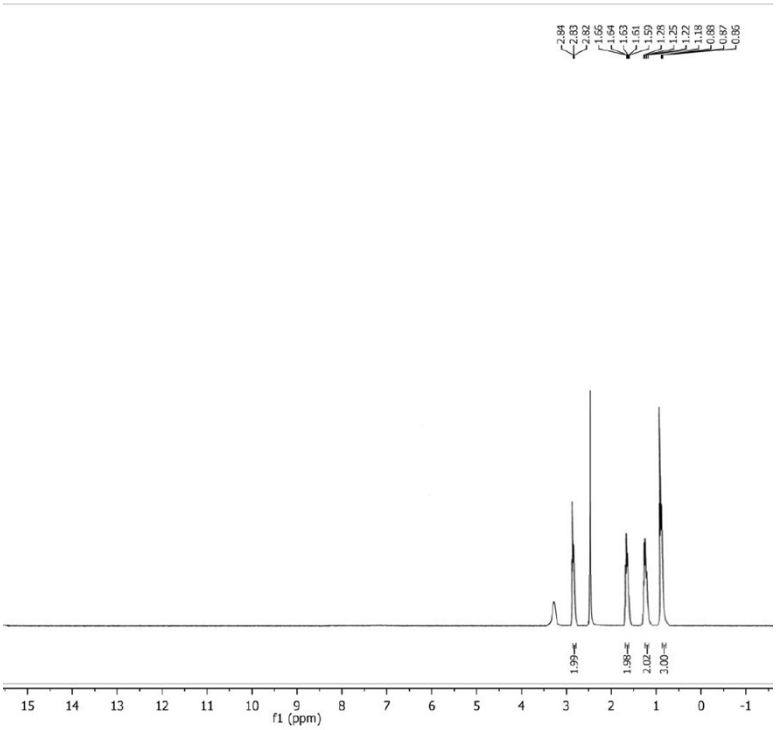
2u

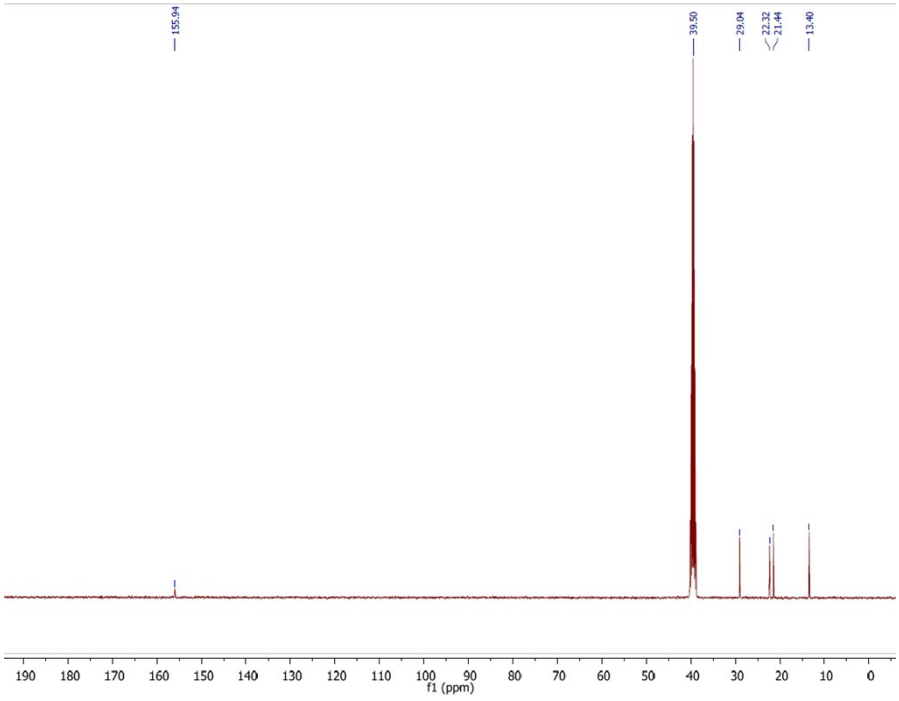

7.35
7.35
7.34
7.34
7.33
7.33
7.32
7.27
7.27
7.26
7.26
7.25
7.24
4.28
2.50
1.83
2.72
2.00
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

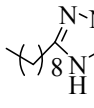

155.19
135.87
128.63
128.57
126.92
39.50
28.84
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



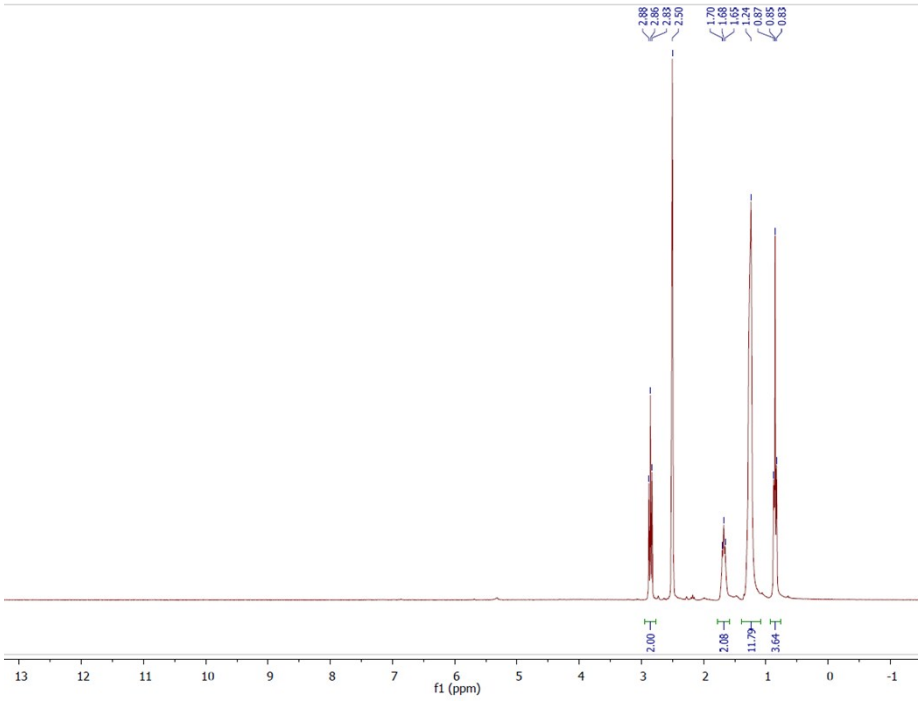
2v

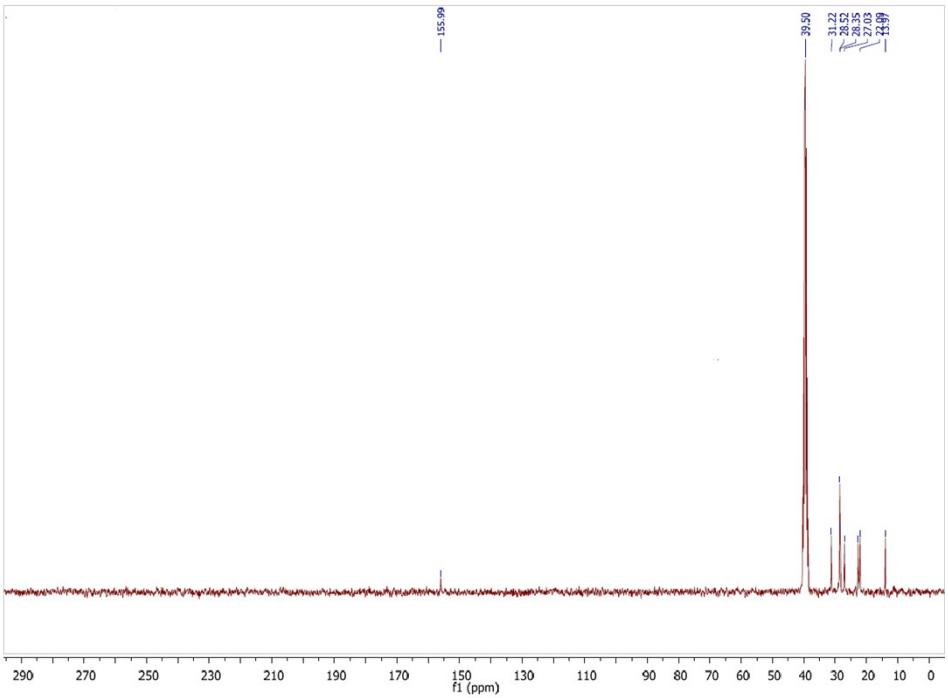

2.84
2.83
2.82
1.66
1.64
1.63
1.61
1.59
1.28
1.25
1.22
1.18
0.88
0.87
0.86
1.99
1.98
2.02
3.00
f1 (ppm)


155.94
39.50
29.04
22.32
21.44
13.40
f1 (ppm)



2w


2.88
2.86
2.83
2.50
1.70
1.68
1.65
1.24
0.87
0.85
0.83
2.00
2.08
11.79
3.64
f1 (ppm)


155.99
39.50
31.22
28.52
28.35
27.03
f1 (ppm)