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Supporting Information

In Situ Fabrication of HDA-mediated NiFe-Fe_2O_3 Nanorods: An Efficient and Recyclable Heterogeneous Catalyst for the Synthesis of 2,3-dihydroquinazolin-4(1*H*)-ones in Water

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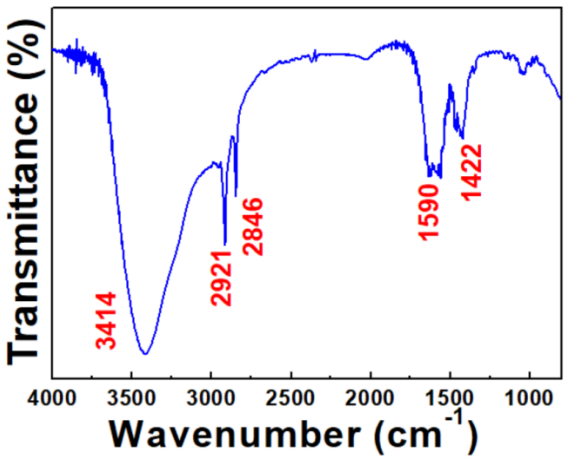


Figure S1: FT-IR spectra of as-synthesized Ni_2Fe_3 sample.

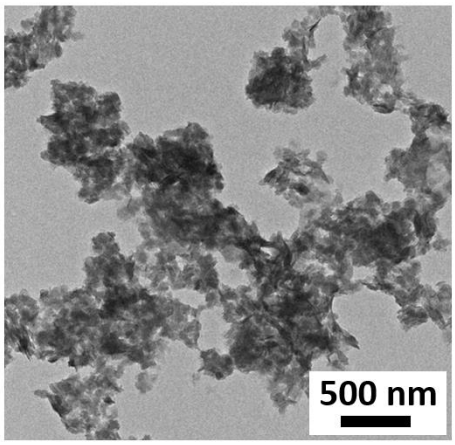


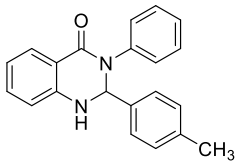
Figure S2: TEM image of the sample prepared without the addition of HDA.

Table S1: A comparison of catalytic activity of present catalyst with various catalysts in the condensation reaction of isatoic anhydride, aldehyde and amine/ammonium acetate

Entry	Catalyst	Conditions	Time	Yield (%)	Ref.
1	ZnO NPs (20 mol%),	Solvent-free, 70 °C	3 h	88	1
2	Pt-MWCNTs nanocomposites (0.04 g)	Irradiated in a ultrasound bath, EtOH, 60 °C	10 mins	90	2
3	Titanium silicon oxide nano powder (10 mol%),	H_2O, 100 °C	3 h	94	3
4	Fe_3O_4 NPs (0.15 or 0.50 mmol)	H_2O, reflux,	5 h	85	4
5	Nano-In_2O_3 (5 mol%)	H_2O/EtOH (2:1), 80 °C	4 h	88	5
6	Nano-Fe_3O_4-DOPA-SnO_2 (10 mg)	H_2O, 80 °C	45-90 mins	86	6
7	NiFe-Fe_2O_3 NPs (15 mg)	H_2O, 70 °C.	3 h	98	**This work**

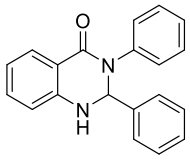
Spectral data of 2,3-dihydroquinazolin-4(1*H*)-ones

2-(4-Chlorophenyl)-3-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 2a)



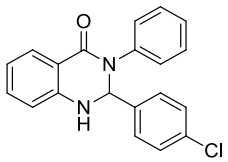
White solid; 98% yield;^{1}H NMR (500 MHz, DMSO-d_6) δ 7.80 (d, J = 7.8 Hz, 1H), 7.68 (d, J = 2.0 Hz, 1H), 7.30 (ddt, J = 39.0, 38.1, 7.8 Hz, 11H), 6.87-6.74 (m, 2H), 6.31 (s, 1H), 2.29 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 165.62, 149.91, 144.22, 141.15, 140.90, 137.05, 132.26, 131.93, 131.28, 129.82, 129.44, 129.27, 120.79, 118.74, 118.14, 75.77, 23.95.

3-Phenyl-2-(*p*-tolyl)-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 2b)



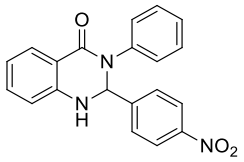
White solid; 92% yield;^{1}H NMR (500 MHz, DMSO-d_6) δ 7.74 (d, J = 7.6 Hz, 1H), 7.65 (d, J = 2.1 Hz, 1H), 7.42-7.18 (m, 11H), 6.82-6.66 (m, 2H), 6.29 (s, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 165.63, 149.91, 144.15, 144.04, 137.12, 131.96, 131.72, 131.65, 129.91, 129.58, 129.36, 120.88, 118.69, 118.15, 75.97.

2,3-Diphenyl-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 2c)



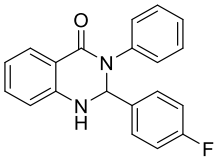
White solid; 96% yield; ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.77-7.63 (m, 2H), 7.46-7.18 (m, 10H), 6.76 (dd, J = 13.8, 7.9 Hz, 2H), 6.33 (s, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 165.54, 149.73, 143.93, 142.97, 137.23, 136.27, 132.04, 131.87, 131.73, 129.61, 129.51, 121.10, 118.62, 118.20, 75.32.

2-(4-Nitrophenyl)-3-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 2d)



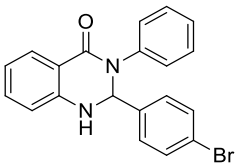
Brown solid;67% yield;^{1}H NMR (500 MHz, DMSO-d_6) δ 8.25-8.13 (m, 2H), 7.81 (d, J = 3.0 Hz, 1H), 7.75 (dd, J = 7.8, 1.4 Hz, 1H), 7.69-7.60 (m, 2H), 7.42-7.26 (m, 5H), 7.26-7.17 (m, 1H), 6.81-6.70 (m, 2H), 6.49 (s, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 165.32, 151.36, 150.72, 149.44, 143.82, 137.35, 132.13, 131.43, 131.26, 129.60, 129.46, 127.01, 121.33, 118.63, 118.31, 75.02.

2-(4-Fluorophenyl)-3-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 2e)



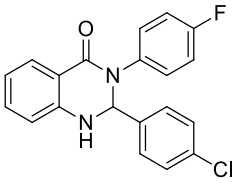
Brown solid; 95% yield;^{1}H NMR (500 MHz, DMSO-d_6) δ 7.76 (dd, J = 23.2, 7.9 Hz, 2H), 7.67-7.58 (m, 1H), 7.49-7.03 (m, 8H), 6.84-6.70 (m, 2H), 6.33 (s, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 162.73, 147.02, 141.09, 137.32, 134.30, 129.33, 129.27, 129.12, 128.47, 126.91, 126.60, 118.13, 115.74, 115.57, 115.29, 72.53.

2-(4-Bromophenyl)-3-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 2f)



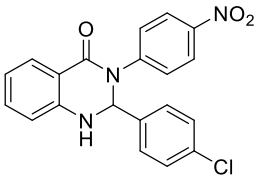
White solid; 96% yield;^{1}H NMR (500 MHz, DMSO-d_6) δ 7.69 (dd, J = 36.2, 4.9 Hz, 2H), 7.51 (d, J = 8.4 Hz, 2H), 7.27 (ddt, J = 43.4, 36.0, 7.1 Hz, 8H), 6.84-6.68 (m, 2H), 6.31 (s, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 162.63, 146.85, 141.09, 140.57, 134.35, 131.80, 129.31, 129.17, 128.49, 126.70, 126.61, 122.01, 118.21, 115.77, 115.34, 72.46.

2-(4-Chlorophenyl)-3-(4-fluorophenyl)-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 2g)



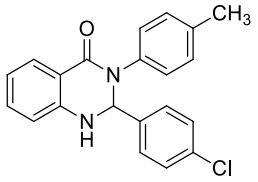
Brown solid;82% yield;^{1}H NMR (500 MHz, DMSO-d_6) δ 7.78-7.57 (m, 2H), 7.44-7.23 (m, 7H), 7.16 (t, J = 8.6 Hz, 2H), 6.75 (dd, J = 15.9, 7.9 Hz, 2H), 6.31 (s, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 162.81, 147.08, 139.81, 137.16, 134.41, 133.50, 131.62, 129.16, 128.92, 128.46, 118.19, 116.00, 115.82, 115.42, 115.25, 72.71.

2-(4-Chlorophenyl)-3-(4-nitrophenyl)-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 2h)



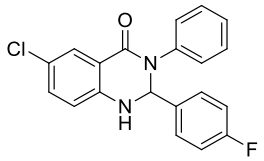
Brown solid; 71% yield; ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.79-7.55 (m, 3H), 7.44-7.14 (m, 7H), 6.87-6.72 (m, 2H), 6.30 (s, 1H), 6.02 (s, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 162.63, 151.95, 146.83, 140.19, 138.48, 135.97, 134.28, 133.38, 131.62, 129.65, 128.97, 128.86, 128.44, 126.70, 125.50, 118.18, 116.80, 115.73, 115.24, 72.58.

2-(4-Chlorophenyl)-3-(*p*-tolyl)-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 2i)



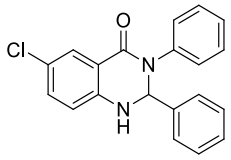
Light brown solid;93% yield;^{1}H NMR (500 MHz, DMSO-d_6) δ 7.79-7.58 (m, 2H), 7.46-7.14 (m, 8H), 6.78 (dd, J = 15.4, 7.8 Hz, 2H), 6.30 (s, 1H), 2.29 (s, 3H); NMR (125 MHz, DMSO-d_6) δ 162.63, 146.83, 140.19, 138.48, 135.97, 134.28, 133.38, 131.62, 129.65, 128.97, 128.86, 128.44, 126.70, 125.50, 118.18, 115.73, 115.24, 72.58, 20.98.

6-Chloro-2-(4-chlorophenyl)-3-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 2j)



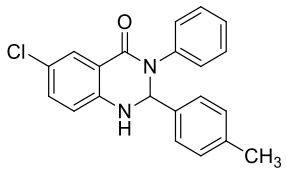
Off white solid; 50% yield;^{1}H NMR (500 MHz, DMSO-d_6) δ 7.95 (d, J = 8.5 Hz, 3H), 7.86 (d, J = 2.4 Hz, 1H), 7.66-7.55 (m, 1H), 7.42-7.21 (m, 6H), 6.80 (dd, J = 15.5, 8.8 Hz, 1H), 6.38 (s, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 164.42, 153.62, 148.58, 143.54, 142.59, 137.02, 136.86, 132.11, 131.84, 130.30, 129.70, 124.69, 121.63, 120.84, 120.26, 119.62, 113.79, 75.27.

6-Chloro-2,3-diphenyl-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 2k)



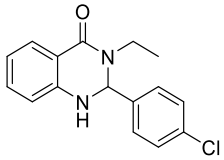
White solid; 72% yield;^{1}H NMR (500 MHz, $CDCl_3$-d_1) δ 7.98 (d, J = 2.4 Hz, 3H), 7.40-7.11 (m, 9H), 6.58 (d, J = 8.6 Hz, 1H), 6.08 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$-d_1) δ 154.95, 136.65, 133.15, 132.36, 126.72, 123.06, 122.07, 121.94, 121.73, 121.43, 119.95, 119.74, 119.61, 117.59, 110.91, 109.34, 67.47.

6-Chloro-3-phenyl-2-(*p*-tolyl)-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 2l)



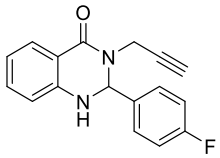
Pale yellow solid; 70% yield; ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.85 (d, J = 2.2 Hz, 1H), 7.68 (d, J = 2.4 Hz, 1H), 7.46-7.19 (m, 8H), 7.14 (d, J = 7.9 Hz, 2H), 6.82 (d, J = 8.7 Hz, 1H), 6.31 (s, 1H), 2.25 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6) δ164.57, 148.73, 143.84, 141.16, 140.74, 136.88, 132.38, 132.04, 129.80, 129.60, 129.55, 124.46, 120.23, 119.77, 75.77, 23.97.

2-(4-Chlorophenyl)-3-ethyl-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 2m)



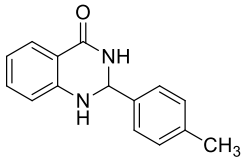
Pale yellow solid; 95% yield; ^{1}H NMR (400 MHz, DMSO) δ 8.35 (s, 1H), 7.69 (d, J = 7.6 Hz, 1H), 7.56-7.28 (m, 5H), 6.80-6.59 (dd, J = 11.7, 7.9 Hz, 2H), 5.95 (s, 1H), 2.93 (dd, J = 13.7, 6.9 Hz, 2H), 1.12 (dt, J = 14.3, 7.3 Hz, 3H); ^{13}C NMR (100 MHz, DMSO) δ 162.32, 146.47, 140.80, 133.68, 133.42, 128.97, 128.48, 127.84, 117.73, 115.36, 114.70, 69.62, 38.69, 13.63.

2-(4-Fluorophenyl)-3-(prop-2-yn-1-yl)-2,3-dihydroquinazolin-4(1*H*)-one (Table 2, entry 2n)



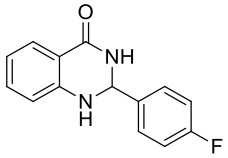
Brown solid; 82% yield; ^{1}H NMR (400 MHz, DMSO) δ 7.69 (dd, J = 7.7, 1.4 Hz, 1H), 7.51-36 (m, 3H), 7.24 (dddd, J = 19.2, 8.9, 7.0, 1.8 Hz, 2H), 6.75-6.66 (m, 2H), 6.00 (s, 1H), 3.61 (s, 2H), 3.17 (t, J = 2.4 Hz, 1H); ^{13}C NMR (100 MHz, DMSO) δ 163.46, 162.09, 146.45, 136.23, 133.79, 128.78, 128.70, 127.67, 117.44, 115.51, 115.30, 114.41, 113.99, 79.00, 74.53, 69.71, 33.13.

2-(4-Methylphenyl)-2,3-dihydroquinazolin-4(1*H*)-one (Table 3, entry 3a)



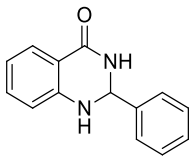
White crystalline solid, 98% yield;^{1}H NMR (500 MHz, DMSO-d_6) δ 8.22 (s, 1H), 7.60 (d, J = 7.3 Hz, 1H), 7.36 (d, J = 7.4 Hz, 2H), 7.30-7.13 (m, 3H), 7.04 (s, 1H), 6.73 (d, J = 7.9 Hz, 1H), 6.66 (t, J = 7.1 Hz, 1H), 5.70 (s, 1H), 2.29 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 164.18, 148.42, 139.19, 138.25, 133.80, 129.34, 127.86, 127.30, 117.60, 115.50, 114.93, 66.86, 21.25.

2-(4-Fluorophenyl)-2,3-dihydroquinazolin-4(1*H*)-one (Table 3, entry 3b)



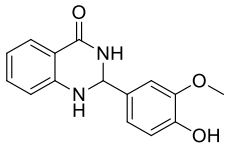
White crystalline solid, 96% yield;^{1}H NMR (500 MHz, DMSO-d_6) δ8.26 (s, 1H), 7.59 (dd, J = 7.7, 1.3 Hz, 1H), 7.55-7.47 (m, 2H), 7.26-7.15 (m, 3H), 7.07 (s, 1H), 6.72 (d, J = 8.0 Hz, 1H), 6.69-6.62 (m, 1H), 5.75 (s, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) δ164.08, 163.60, 161.65, 148.31, 138.30, 138.28, 133.86, 129.58, 129.51, 127.87, 117.76, 115.68, 115.51, 115.46, 114.95, 66.45.

2,3-Dihydro-2-phenylquinazolin-4(1*H*)-one (Table 3, entry 3c)



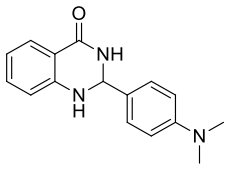
White crystalline solid; 94% yield; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.32 (s, 1H), 7.65 (dd, J = 7.7, 1.1 Hz, 1H), 7.53 (d, J = 7.1 Hz, 2H), 7.47-7.34 (m, 3H), 7.32-7.23 (m, 1H), 7.15 (s, 1H), 6.78 (d, J = 8.0 Hz, 1H), 6.74-6.67 (m, 1H), 5.79 (s, 1H);^{13}C NMR (125 MHz, DMSO-d_6) δ164.09, 148.37, 142.12, 133.81, 128.95, 128.82, 127.84, 127.36, 117.61, 115.45, 114.89, 67.05.

2-(4-Hydroxy-3-methoxyphenyl)-2,3-dihydroquinazolin-4(1*H*)-one (Table 3, entry 3d)



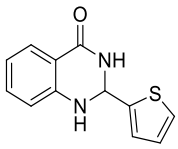
White crystalline solid, 95% yield; ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.16 (s, 1H), 8.18 (s, 1H), 7.65 (d, J = 7.7 Hz, 1H), 7.27 (t, J = 7.6 Hz, 1H), 7.14 (s, 1H), 7.02 (s, 1H), 6.93 (d, J = 8.1 Hz, 1H), 6.80 (t, J = 7.9 Hz, 2H), 6.72 (t, J = 7.5 Hz, 1H), 5.70 (s, 1H), 3.80 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 150.40, 148.69, 147.86, 147.36, 133.69, 132.34, 127.83, 120.11, 117.59, 115.49, 115.35, 114.89, 111.53, 67.30, 56.21.

2-(4-(Dimethylamino)phenyl)-2,3-dihydroquinazolin-4(1*H*)-one (Table 3, entry 3e)



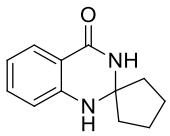
White crystalline solid, 91% yield; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.12 (s, 1H), 7.63 (d, J = 7.7 Hz, 1H), 7.33 (d, J = 8.3 Hz, 2H), 7.25 (t, J = 7.6 Hz, 1H), 6.96 (s, 1H), 6.72 (dt, J = 14.8, 5.7 Hz, 4H), 5.66 (s, 1H), 2.91 (s, 6H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 164.29, 151.16, 148.68, 133.59, 129.08, 128.17, 127.79, 117.39, 115.49, 114.83, 112.39, 67.08.

2-(Thiophen-2-yl)-2,3-dihydroquinazolin-4(1*H*)-one (Table 3, entry 3f)



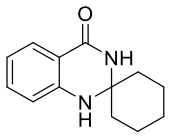
White crystalline solid;98% yield;^{1}H NMR (500 MHz, DMSO-d_6) δ 8.47 (s, 1H), 7.64 (dd, J = 7.7, 1.1 Hz, 1H), 7.48 (dd, J = 5.0, 1.0 Hz, 1H), 7.33-7.22 (m, 2H), 7.15 (d, J = 3.0 Hz, 1H), 7.00 (dd, J = 5.0, 3.5 Hz, 1H), 6.82-6.68 (m, 2H), 6.04 (s, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 163.63, 147.75, 146.93, 133.89, 127.82, 126.97, 126.41, 126.22, 118.03, 115.61, 115.21, 63.06.

1'H-Spiro[cyclopentane-1,2'-quinazolin]-4'(3'*H*)-one (Table 3, entry 3g)



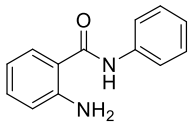
White crystalline solid, 95% yield; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.13 (s, 1H), 7.61 (d, J = 7.5 Hz, 1H), 7.24 (t, J = 7.6 Hz, 1H), 6.82-6.70 (m, 2H), 6.66 (t, J = 7.4 Hz, 1H), 1.83 (d, J = 4.4 Hz, 4H), 1.70 (s, 4H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 163.95, 148.03, 133.51, 127.75, 117.04, 115.08, 114.84, 77.57, 22.48.

1'H-Spiro[cycloheptane-1,2'-quinazolin]-4'(3'*H*)-one (Table 3, entry 3h)



Yellow crystalline solid; 97% yield,^{1}H NMR (500 MHz, DMSO-d_6) δ7.97 (s, 1H), 7.62 (dd, J = 7.7, 1.3 Hz, 1H), 7.30-7.23 (m, 1H), 6.86 (d, J = 8.1 Hz, 1H), 6.71-6.63 (m, 2H), 1.88-1.73 (m, 2H), 1.73-1.60 (m, 5H), 1.60-1.35 (m, 2H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 163.66, 147.23, 133.58, 127.57, 116.94, 115.04, 114.91, 68.27, 37.63, 25.12, 21.35.

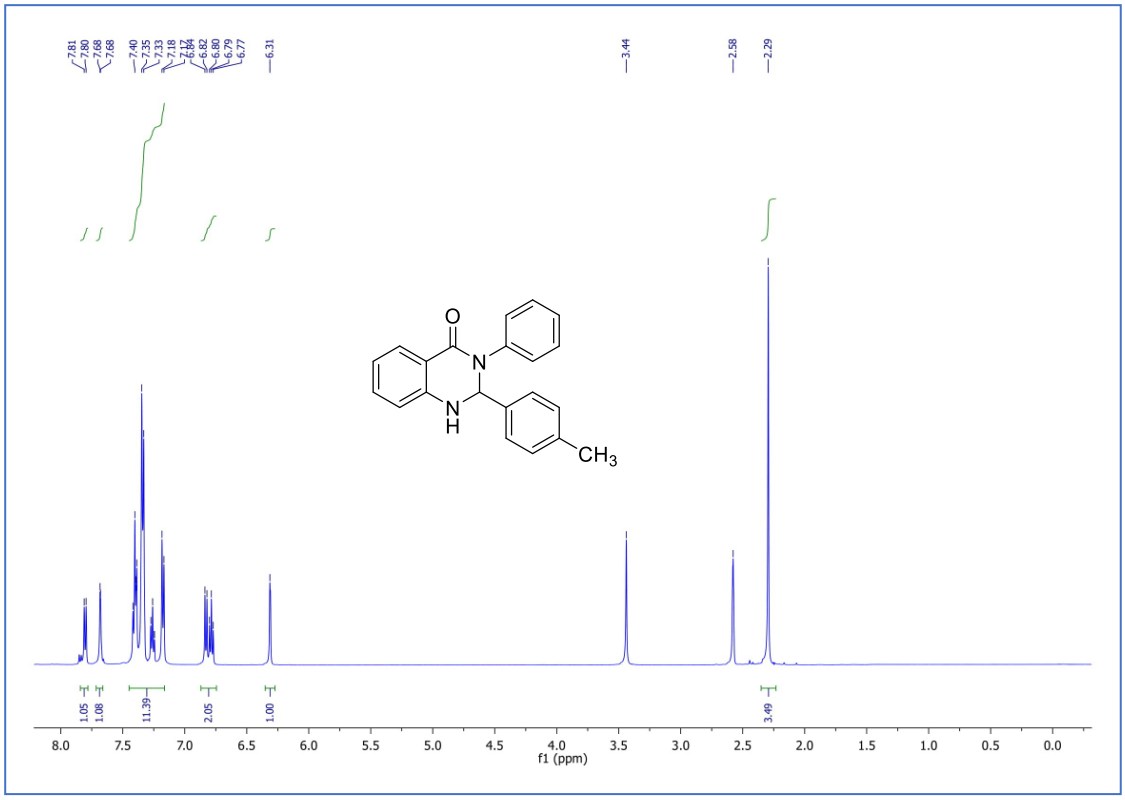
2-Amino-N-phenylbenzamide (III)

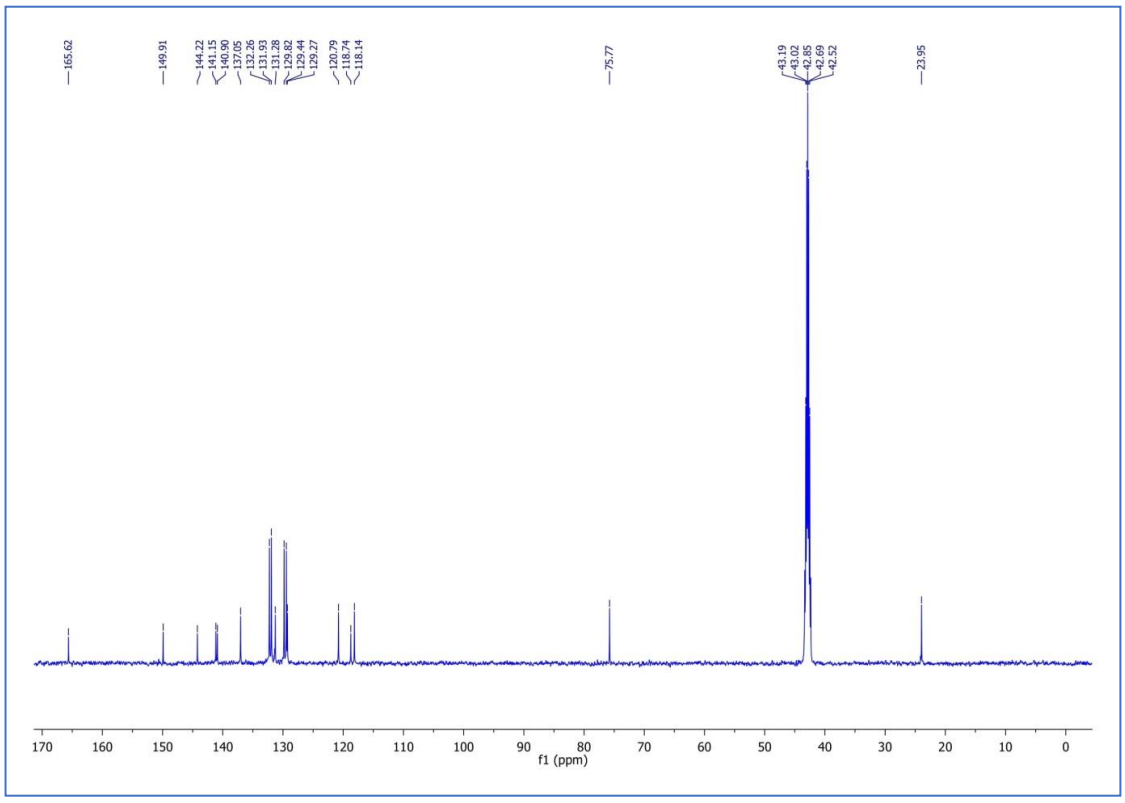


White crystalline solid; 95% yield; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.81 (s, 1H), 7.62-7.55 (m, 2H), 7.49 (dd, J = 8.2, 1.3 Hz, 1H), 7.39 (dd, J = 10.8, 5.1 Hz, 2H), 7.3-7.23 (m, 1H), 7.17 (t, J = 7.4 Hz, 1H), 6.73 (dd, J = 11.0, 4.4 Hz, 2H), 5.52 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 167.47, 148.86, 137.74, 132.65, 128.96, 127.07, 124.40, 120.45, 117.44, 116.73, 116.14.

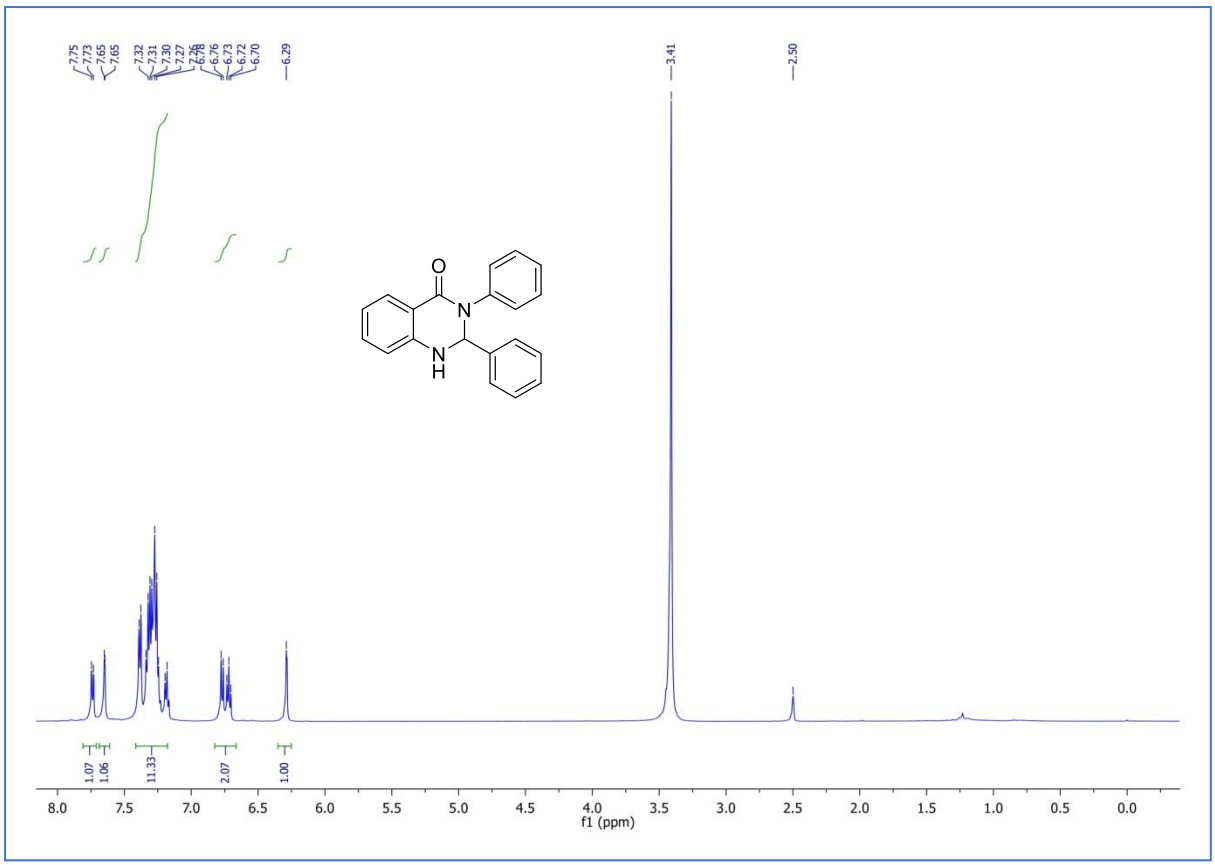
Copies of ^{1}H and ^{13}C NMR spectra of synthesized compounds

(2a, Table 2)





(2b, Table 2)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7.65
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7.31
7.30
7.27
6.76
6.73
6.72
6.70
6.29
3.41
2.50
O
N
N
H
1.07
1.06
11.33
2.07
1.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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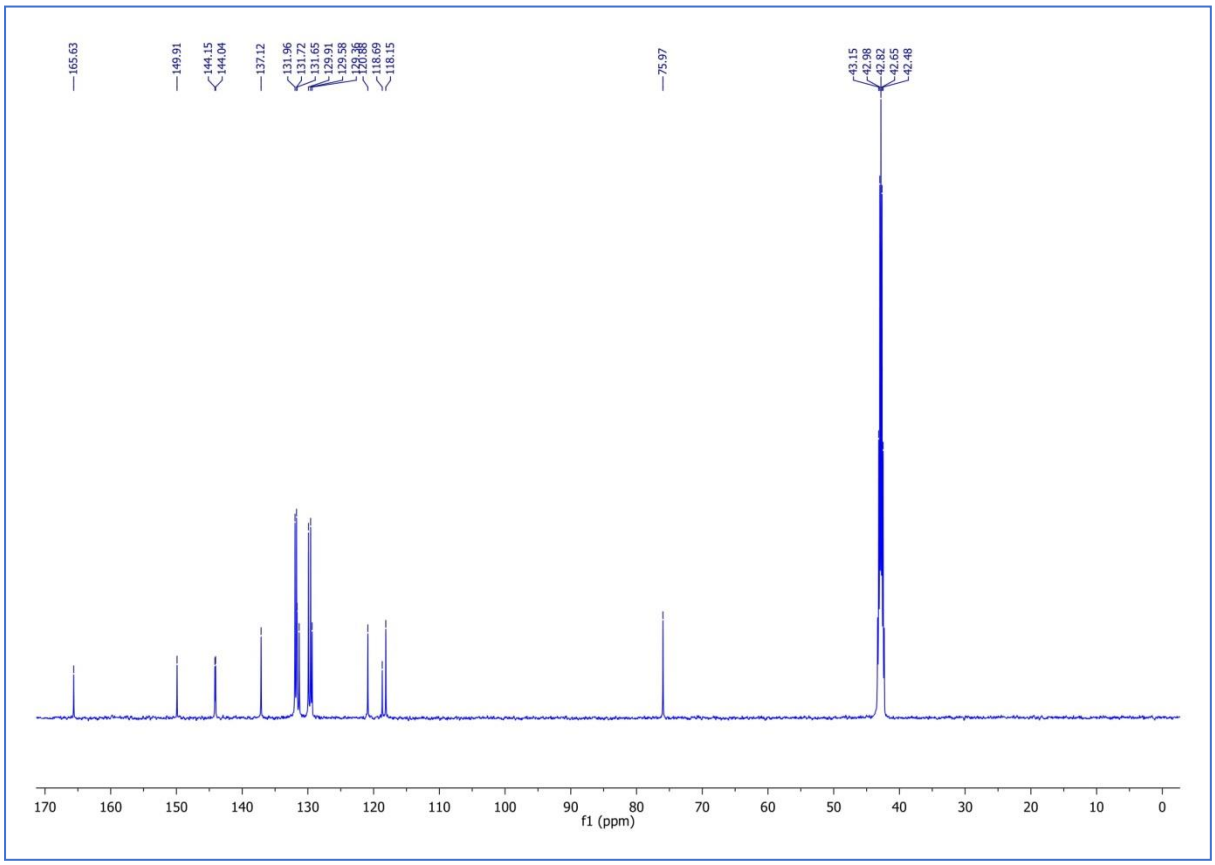
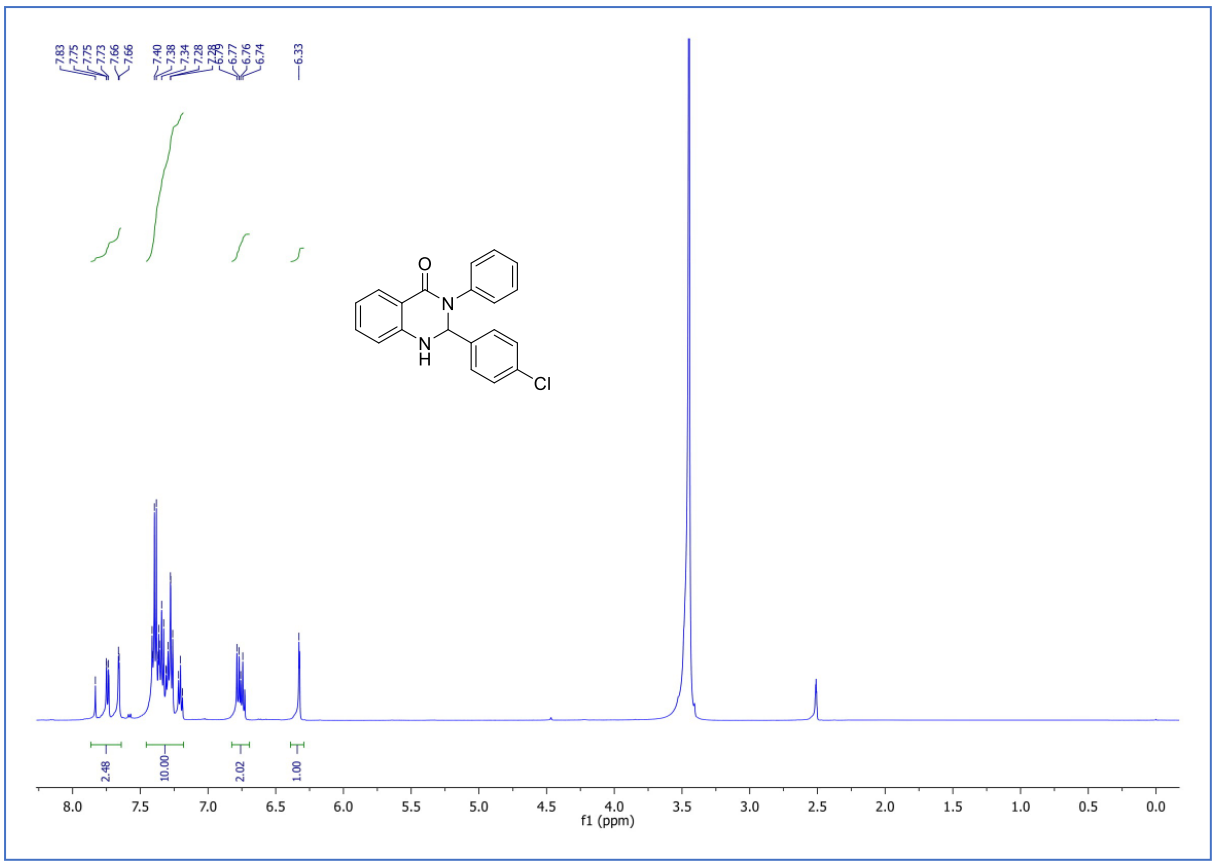
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


165.63
149.91
144.15
144.04
137.12
131.96
131.72
131.65
129.91
129.58
118.69
118.15
75.97
43.15
42.98
42.82
42.65
42.48
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

(2c, Table 2)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7.34
7.28
6.77
6.76
6.74
6.33
O
N
N
H
Cl
2.48
10.00
2.02
1.00
8.0
7.5
7.0
6.5
6.0
5.5
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4.5
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1.0
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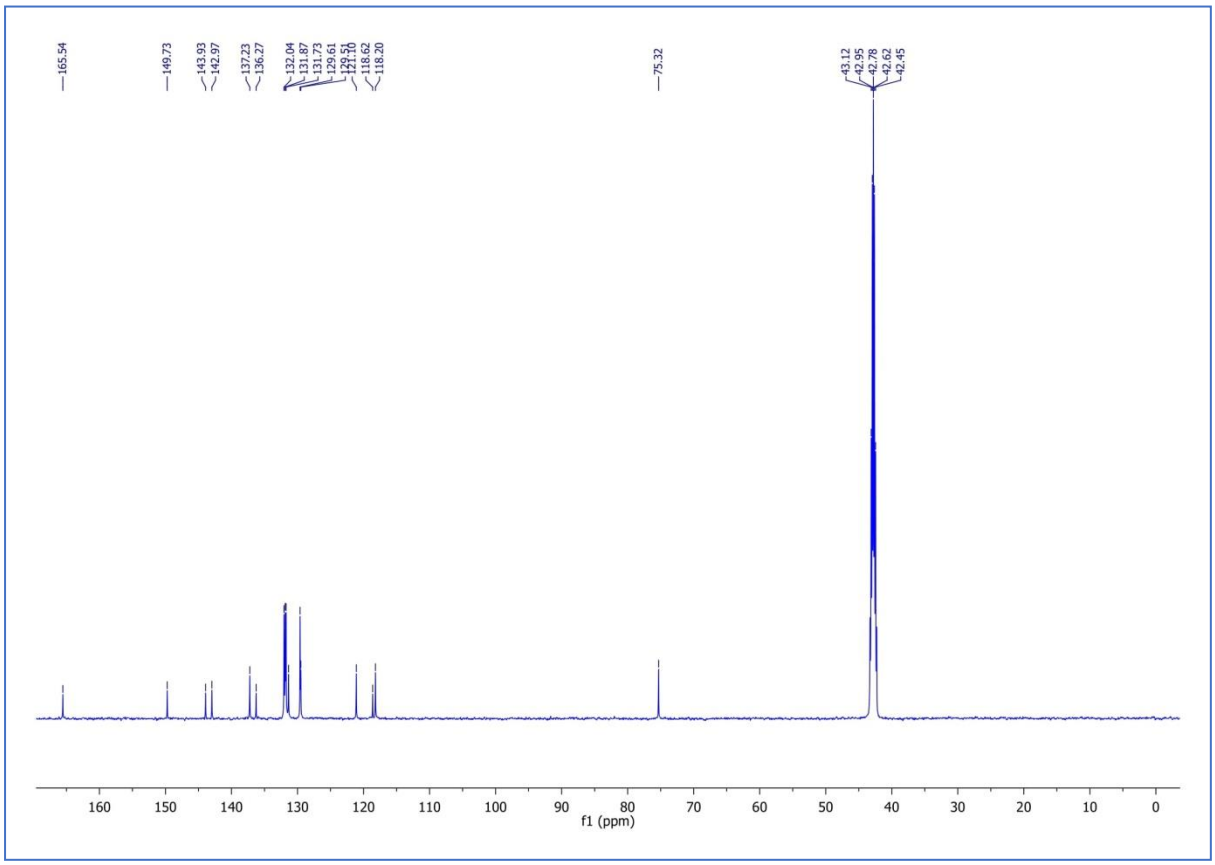
f1 (ppm)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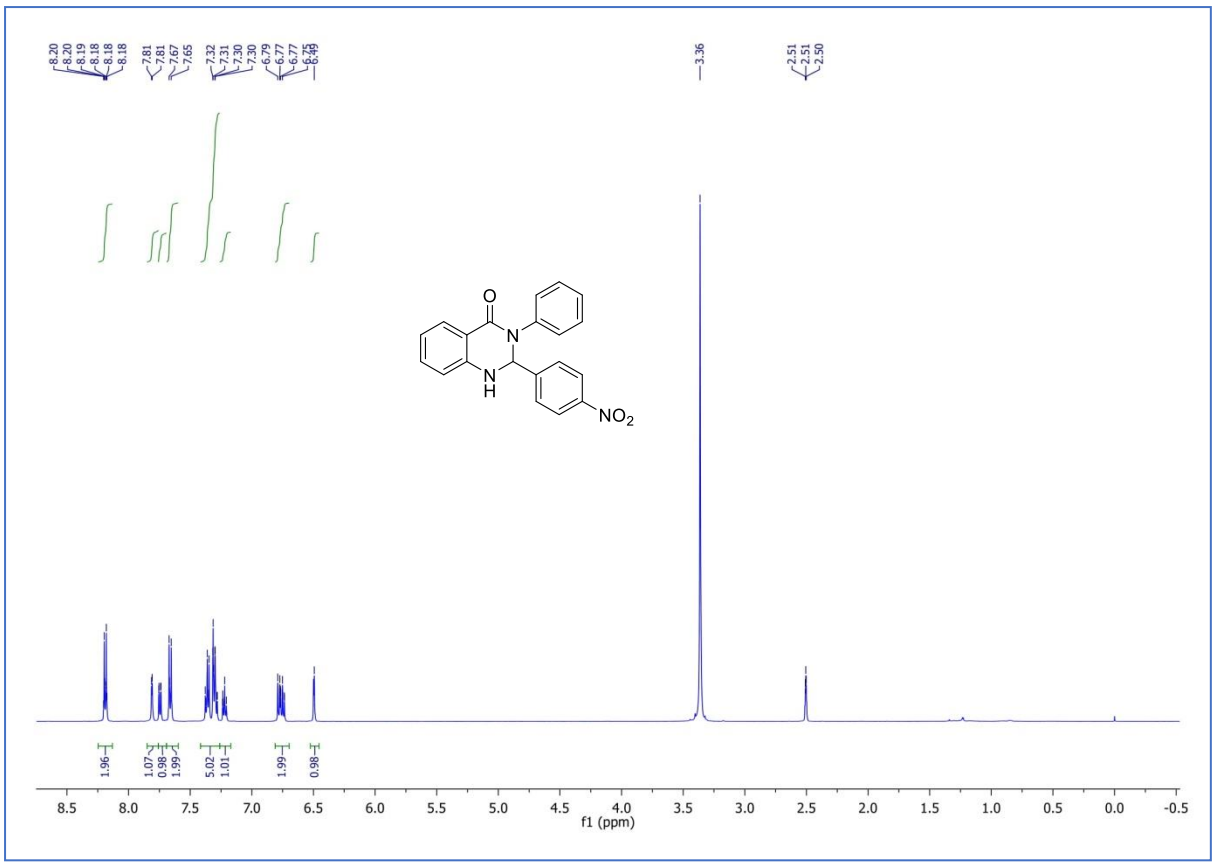
143.93
142.97
137.23
136.27
132.04
131.87
131.73
129.61
118.62
118.20
75.32
43.12
42.95
42.78
42.62
42.45
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

(2d, Table 2)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8.19
8.18
8.18
8.18
7.81
7.81
7.67
7.65
7.32
7.31
7.30
7.30
6.79
6.77
6.77
6.75
6.49
3.36
2.51
2.51
2.50
O
N
N
H
NO2
1.96
1.07
0.98
1.99
5.02
1.01
1.99
0.98
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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3.0
2.5
2.0
1.5
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0.5
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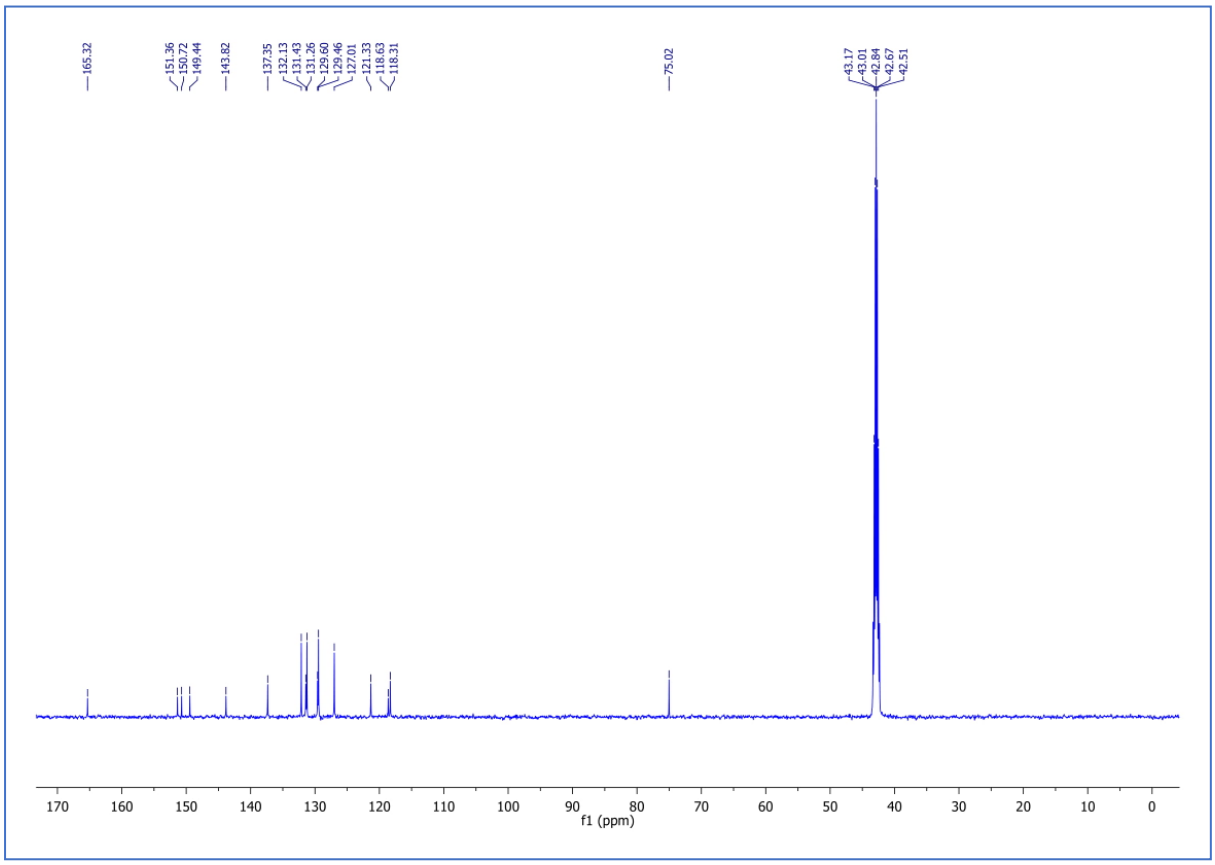
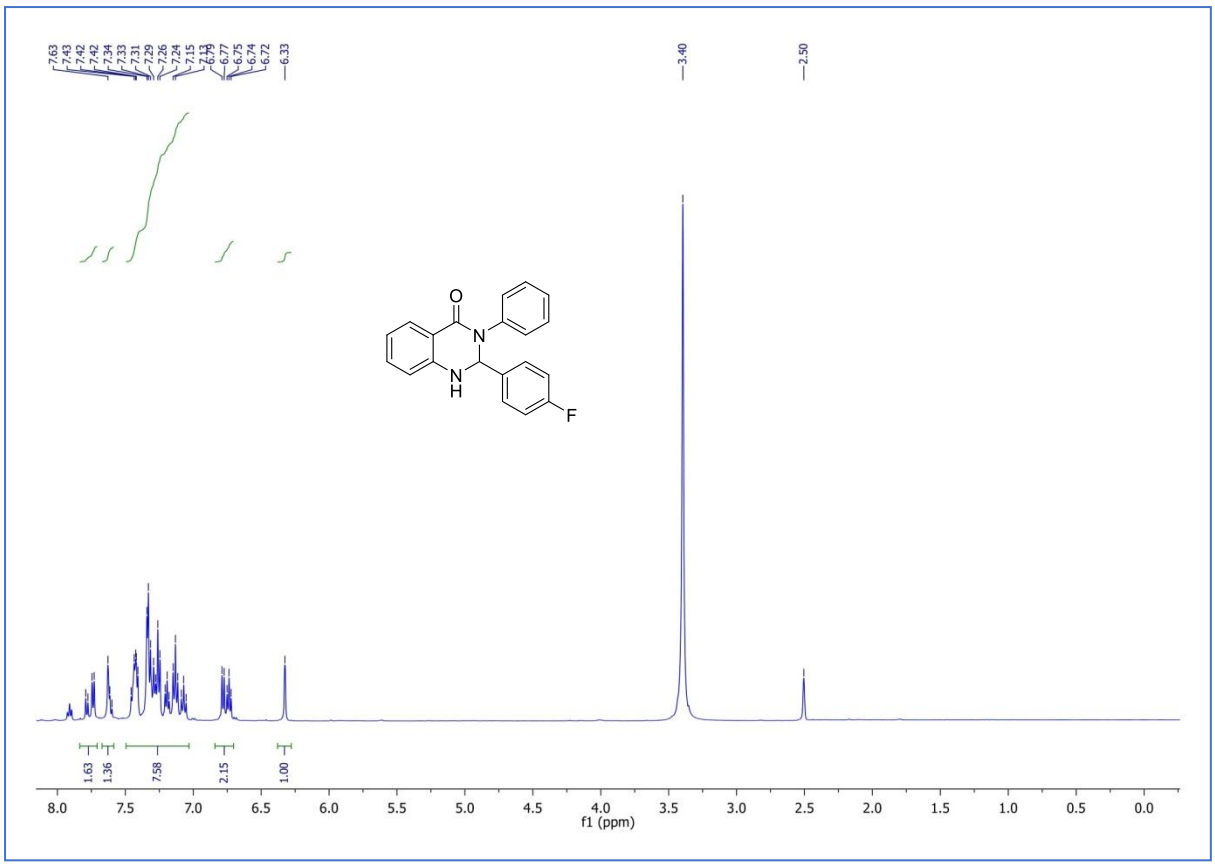
-0.5
f1 (ppm)


165.32
151.36
150.72
149.44
143.82
137.35
132.13
131.43
131.26
129.60
129.46
127.01
121.33
118.63
118.31
75.02
43.17
43.01
42.84
42.67
42.51
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

(2e, Table 2)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7.29
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7.24
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6.77
6.75
6.74
6.72
6.33
3.40
2.50
O
N
N
H
F
1.63
1.36
7.58
2.15
1.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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3.5
3.0
2.5
2.0
1.5
1.0
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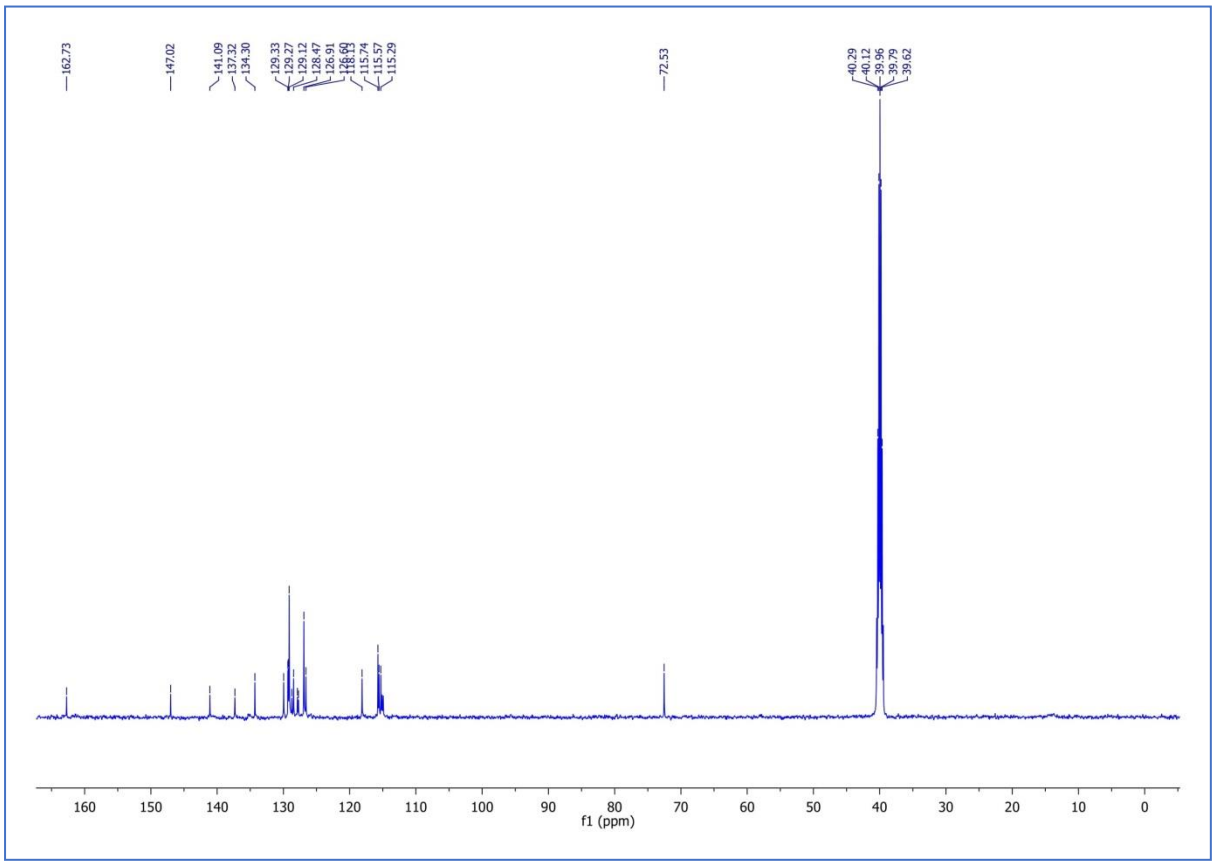
0.0
f1 (ppm)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137.32
134.30
129.33
129.27
129.12
128.47
126.91
115.74
115.57
115.29
72.53
40.29
40.12
39.96
39.79
39.62
160
150
140
130
120
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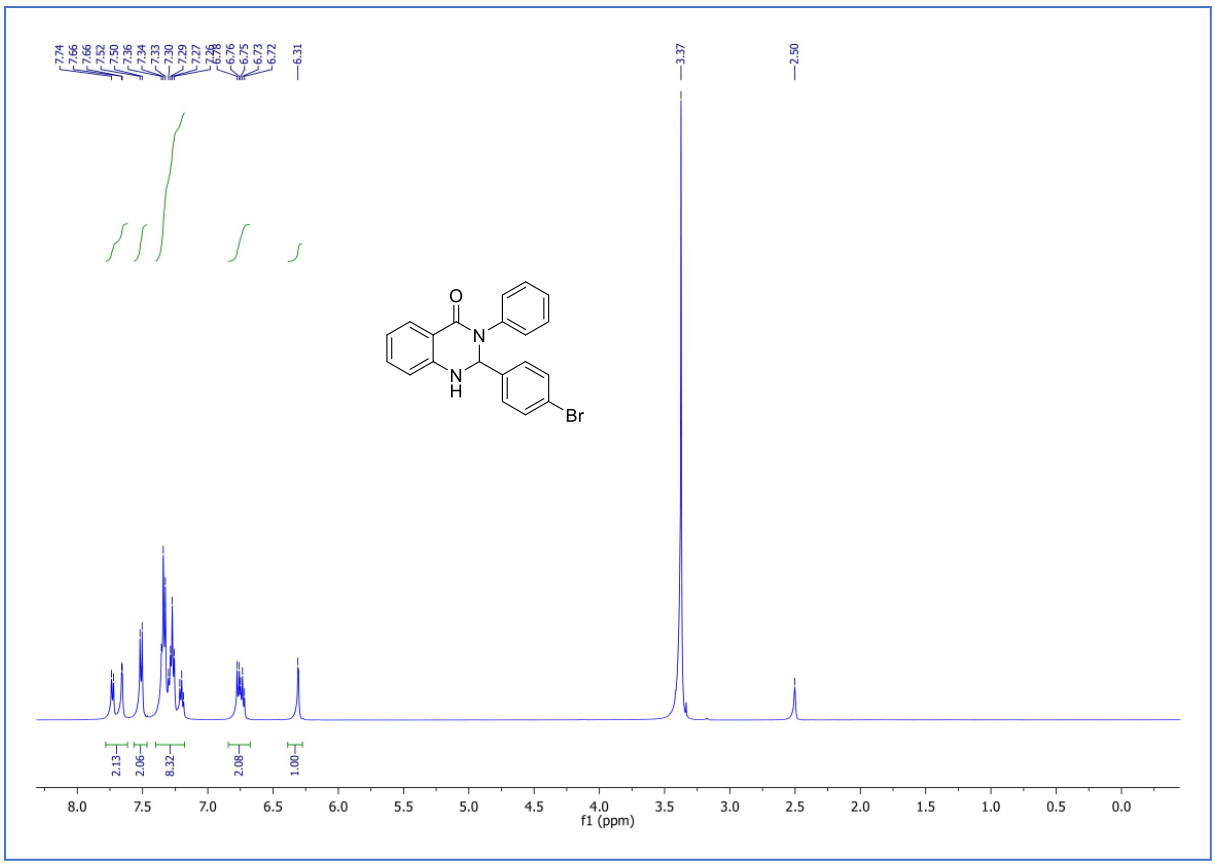
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

(2f, Table 2)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7.34
7.33
7.30
7.29
7.27
6.76
6.75
6.73
6.72
6.31
3.37
2.50
O
N
N
H
Br
2.13
2.06
8.32
2.08
1.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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3.5
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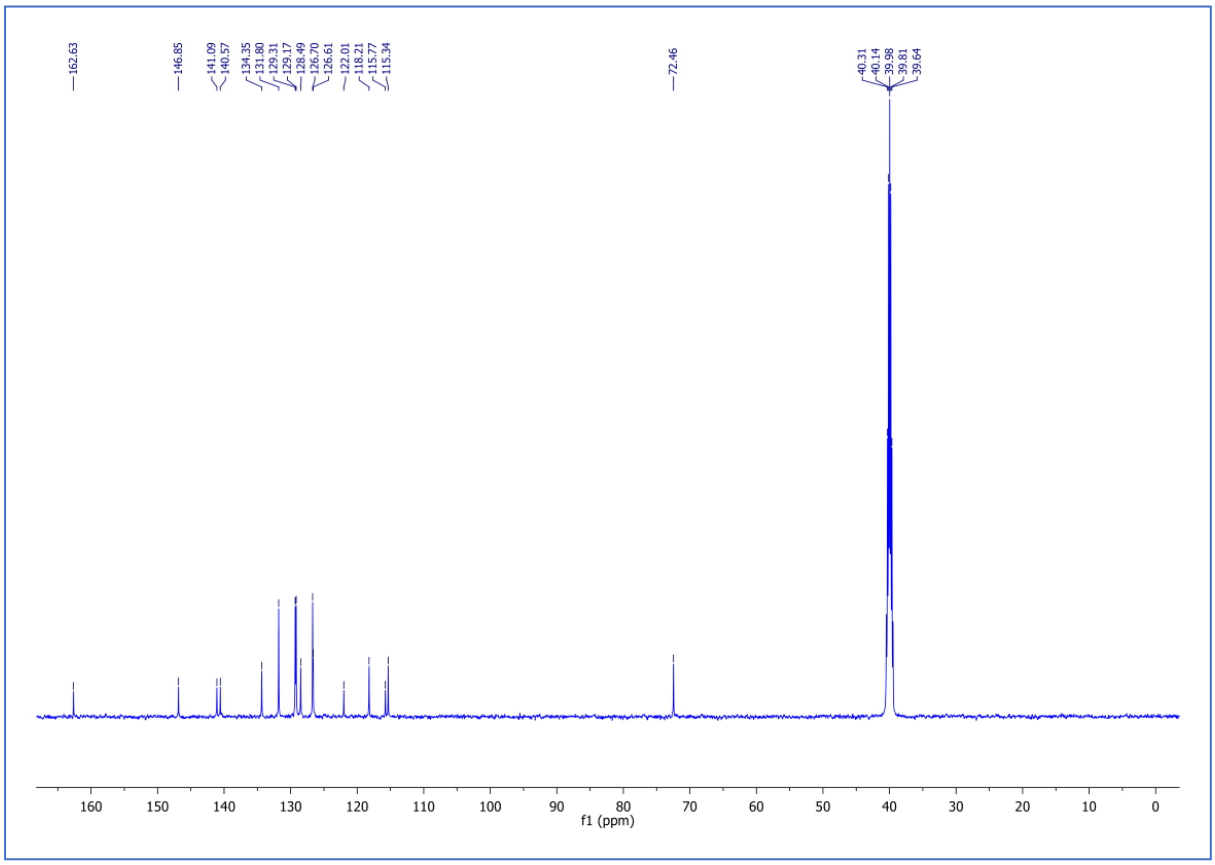
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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129.17
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128.70
126.61
122.01
118.21
115.77
115.34
72.46
40.31
40.14
39.98
39.81
39.64
160
150
140
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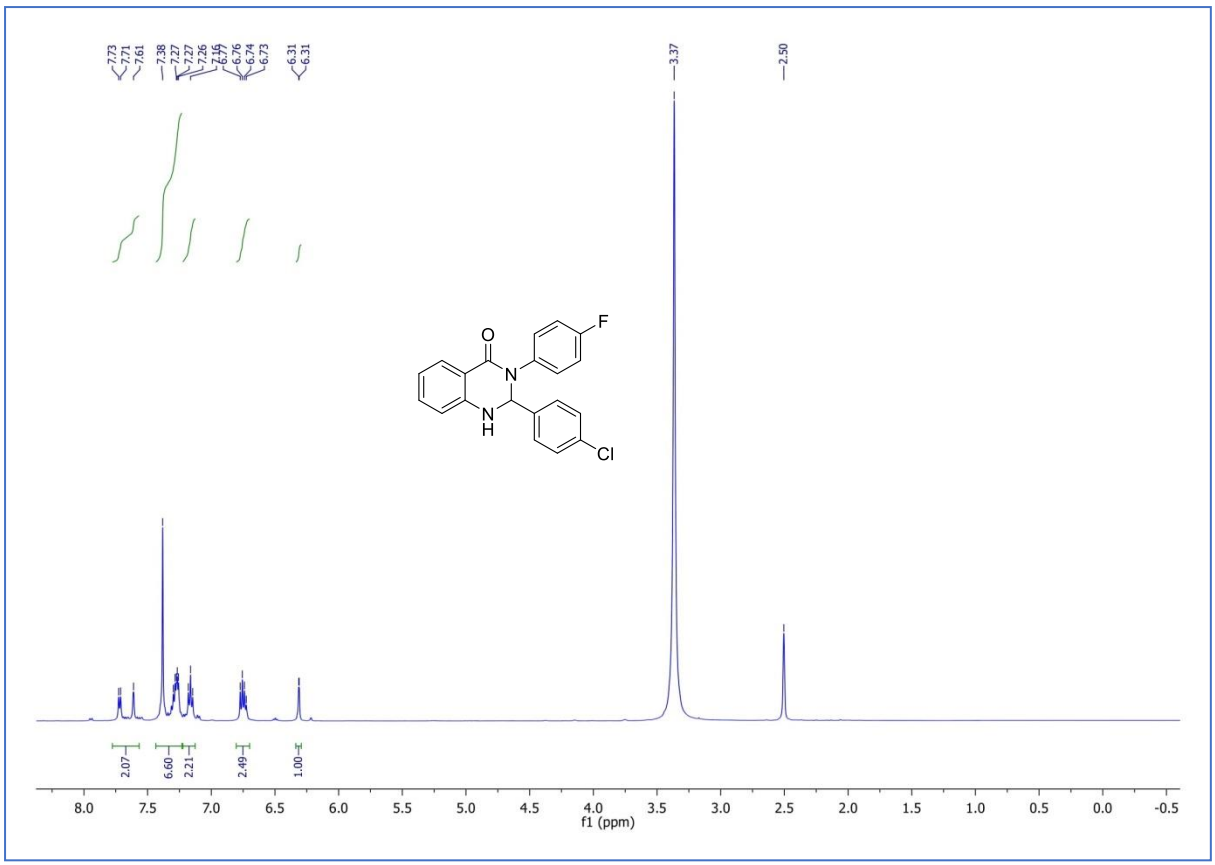
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

(2g, Table 2)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7.27
7.26
7.15
6.76
6.74
6.73
6.31
6.31
3.37
2.50
O
N
N
H
F
Cl
2.07
6.60
2.21
2.49
1.00
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
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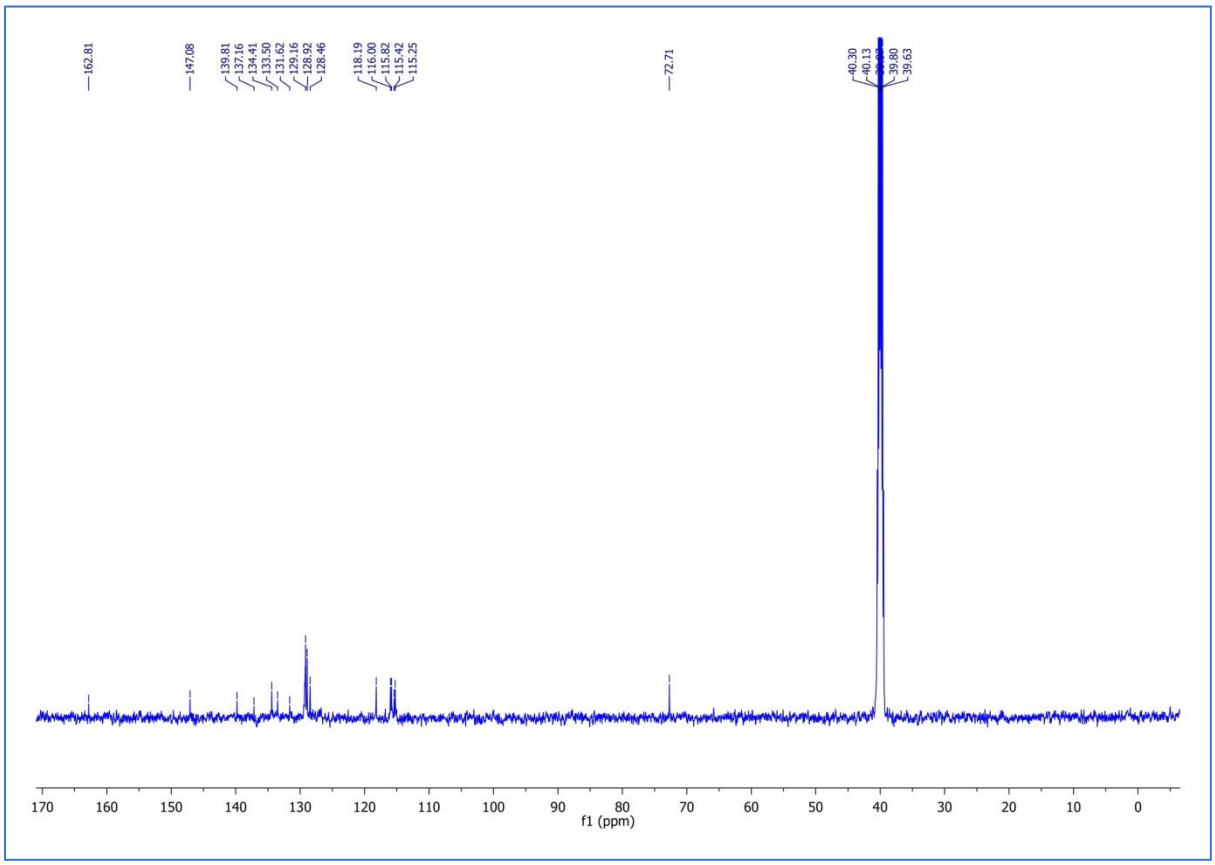
-0.5
f1 (ppm)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129.16
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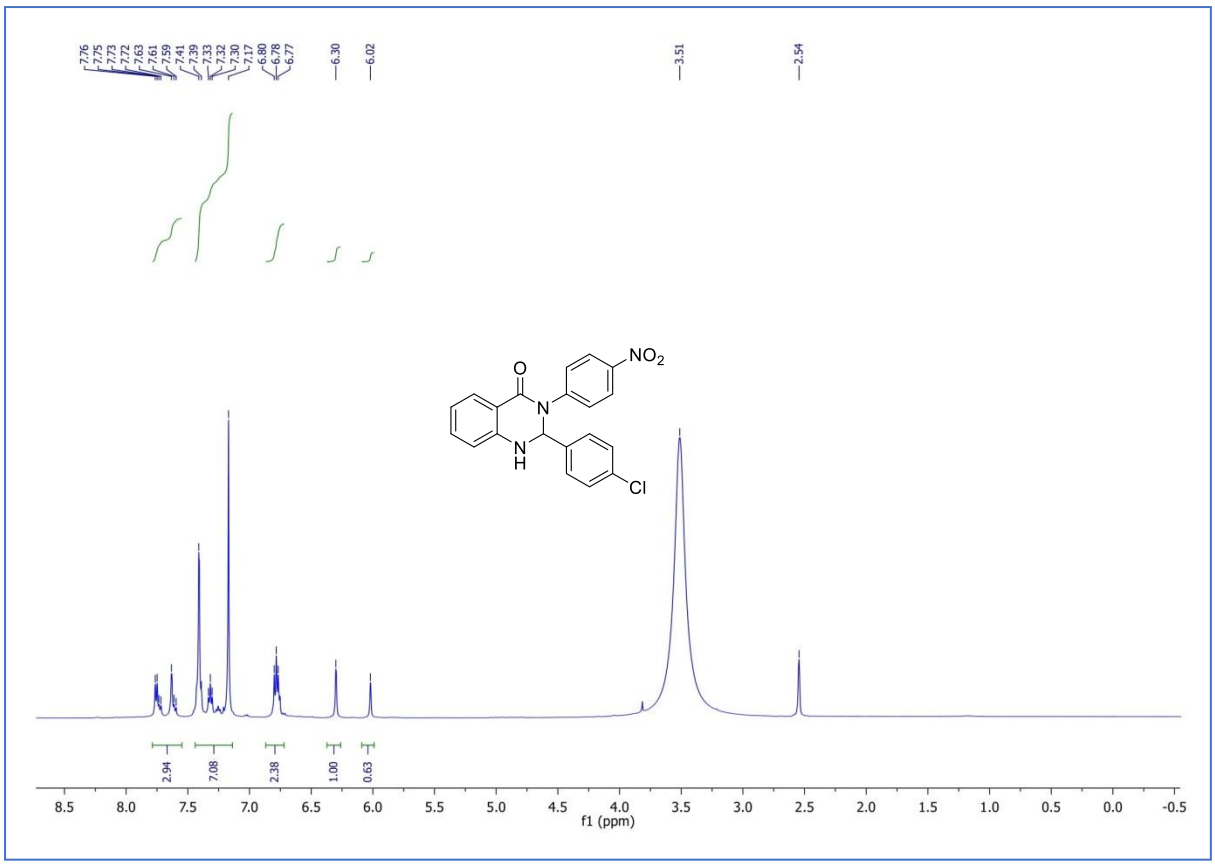
128.46
118.19
116.00
115.82
115.42
115.25
72.71
40.30
40.13
39.80
39.63
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

(2h, Table 2)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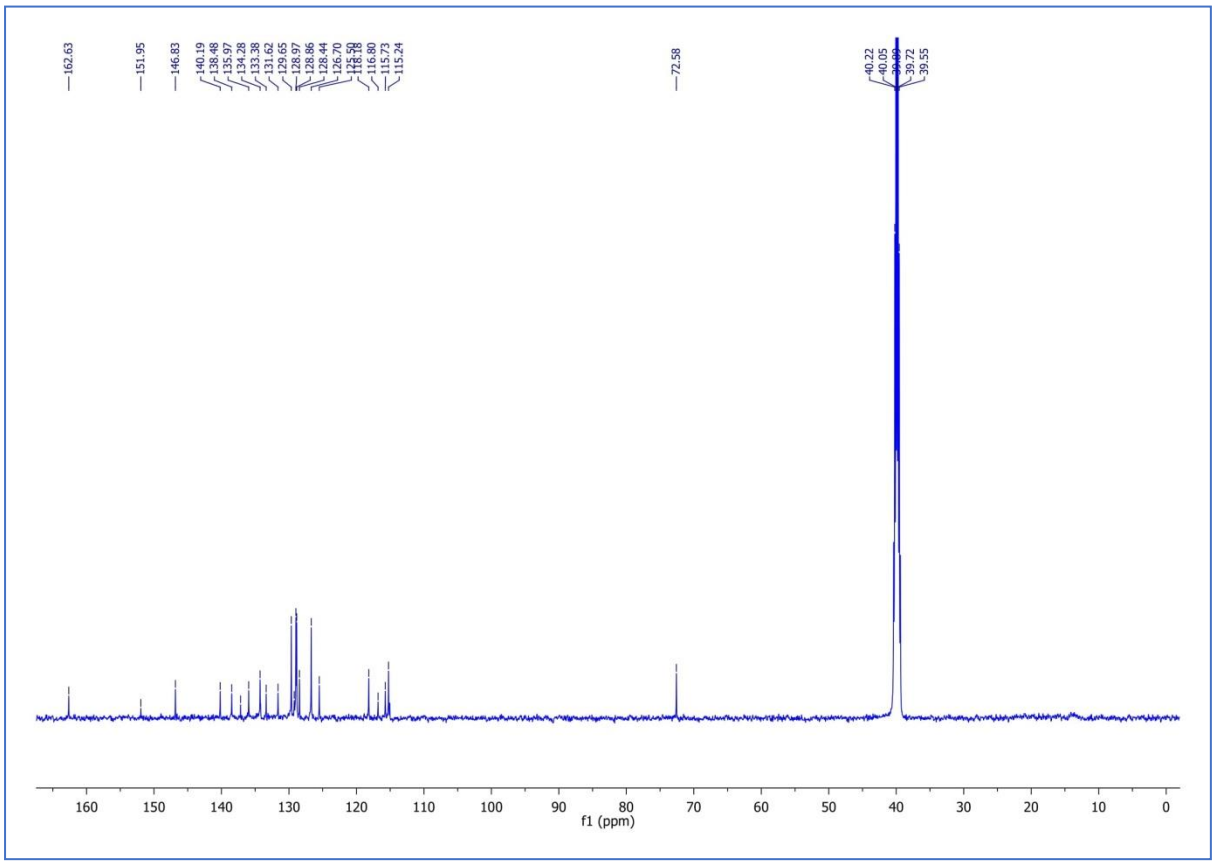
7.61
7.59
7.41
7.39
7.33
7.32
7.30
7.17
6.80
6.78
6.77
6.30
6.02
3.51
2.54
NO2
O
N
N
H
Cl
2.94
7.08
2.38
1.00
0.63
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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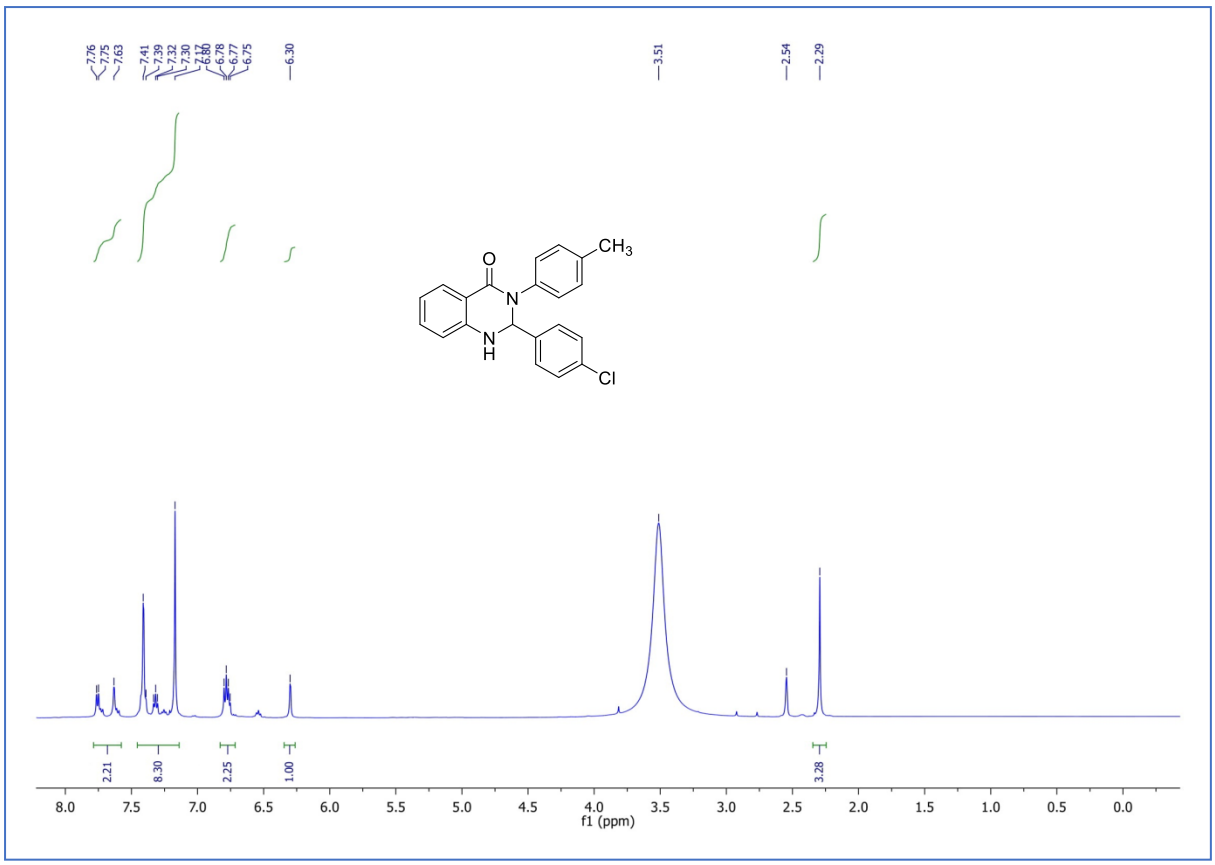
138.48
135.97
134.28
133.38
131.62
129.65
128.97
128.86
128.44
126.70
116.80
115.73
115.24
72.58
40.22
40.05
39.72
39.55
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

(2i, Table 2)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2.54
2.29
O
N
N
H
CH3
Cl
2.21
8.30
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8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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3.5
3.0
2.5
2.0
1.5
1.0
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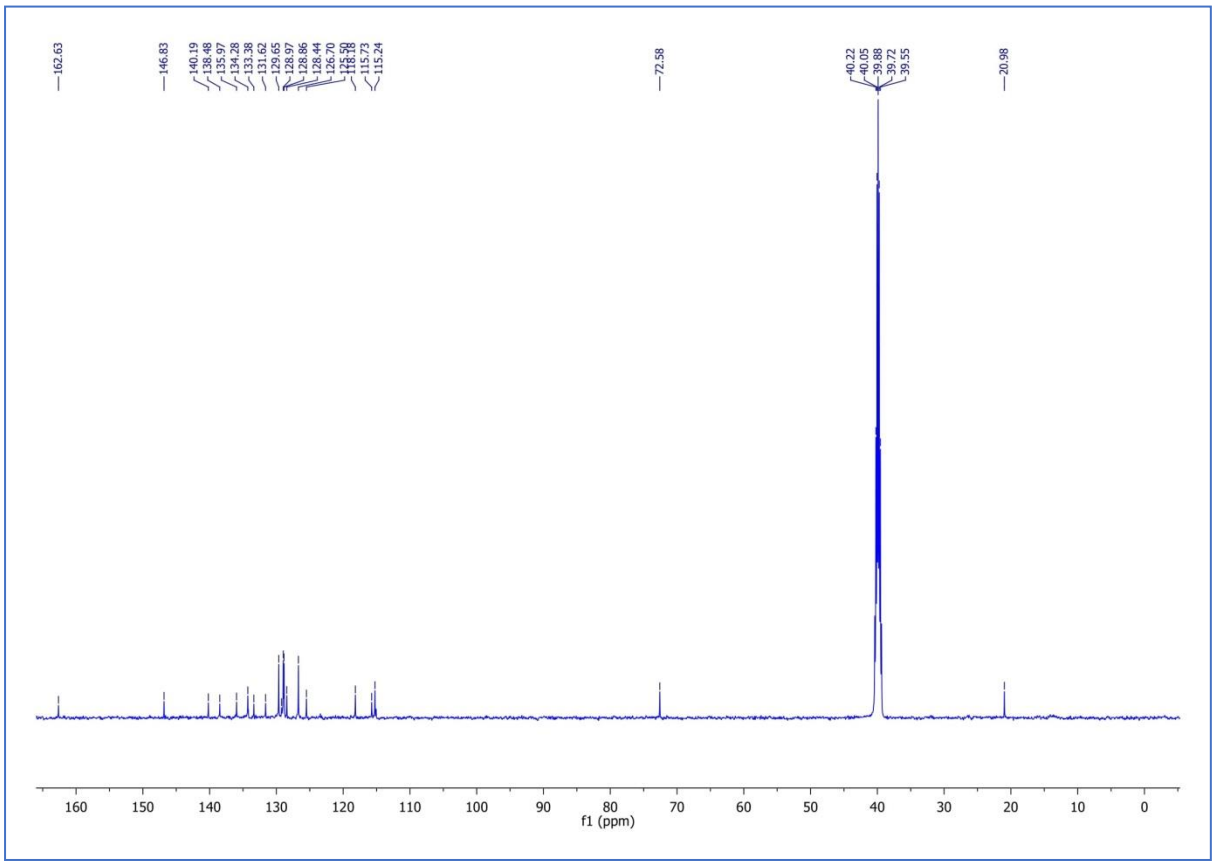
f1 (ppm)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128.86
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126.70
115.73
115.24
72.58
40.22
40.05
39.88
39.72
39.55
20.98
160
150
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90
80
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60
50
40
30
20
10
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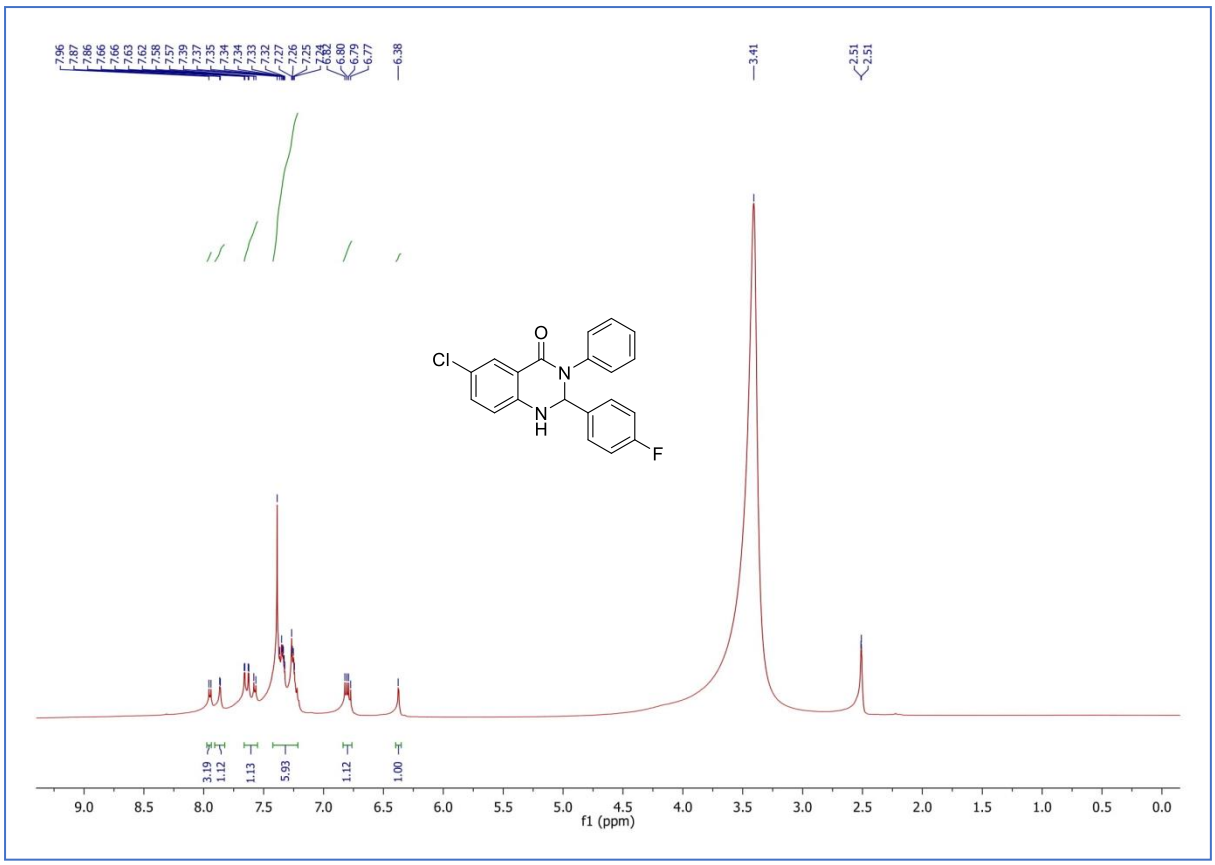
f1 (ppm)

(2j, Table 2)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2.51
2.51
Cl
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H
F
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1.13
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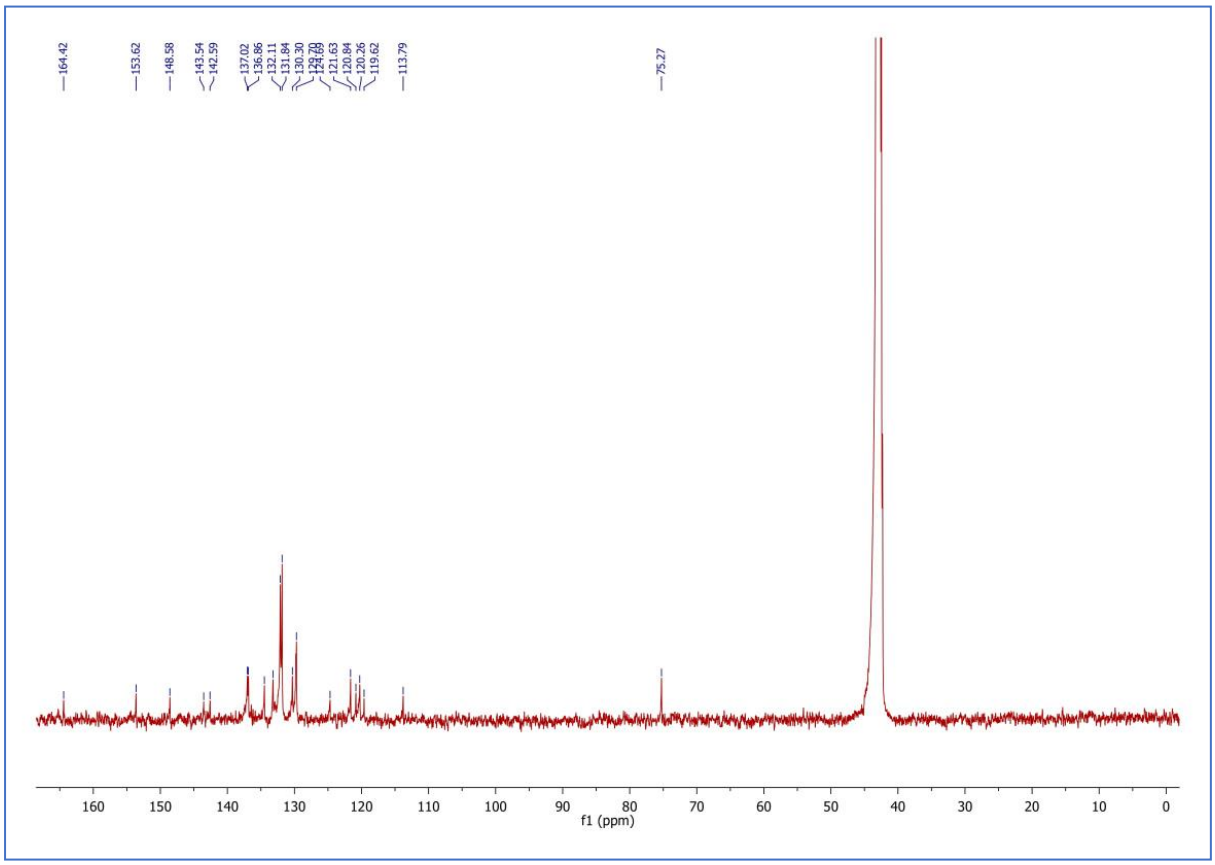
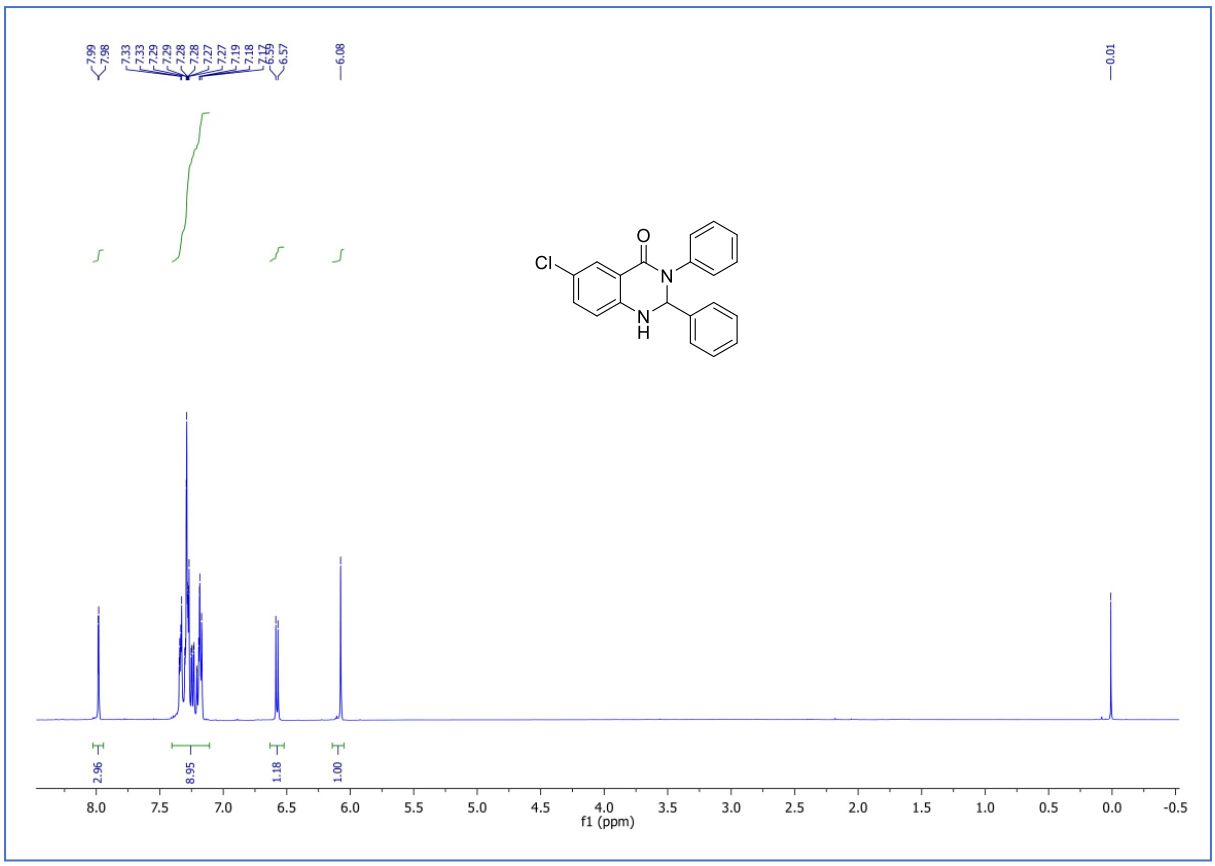
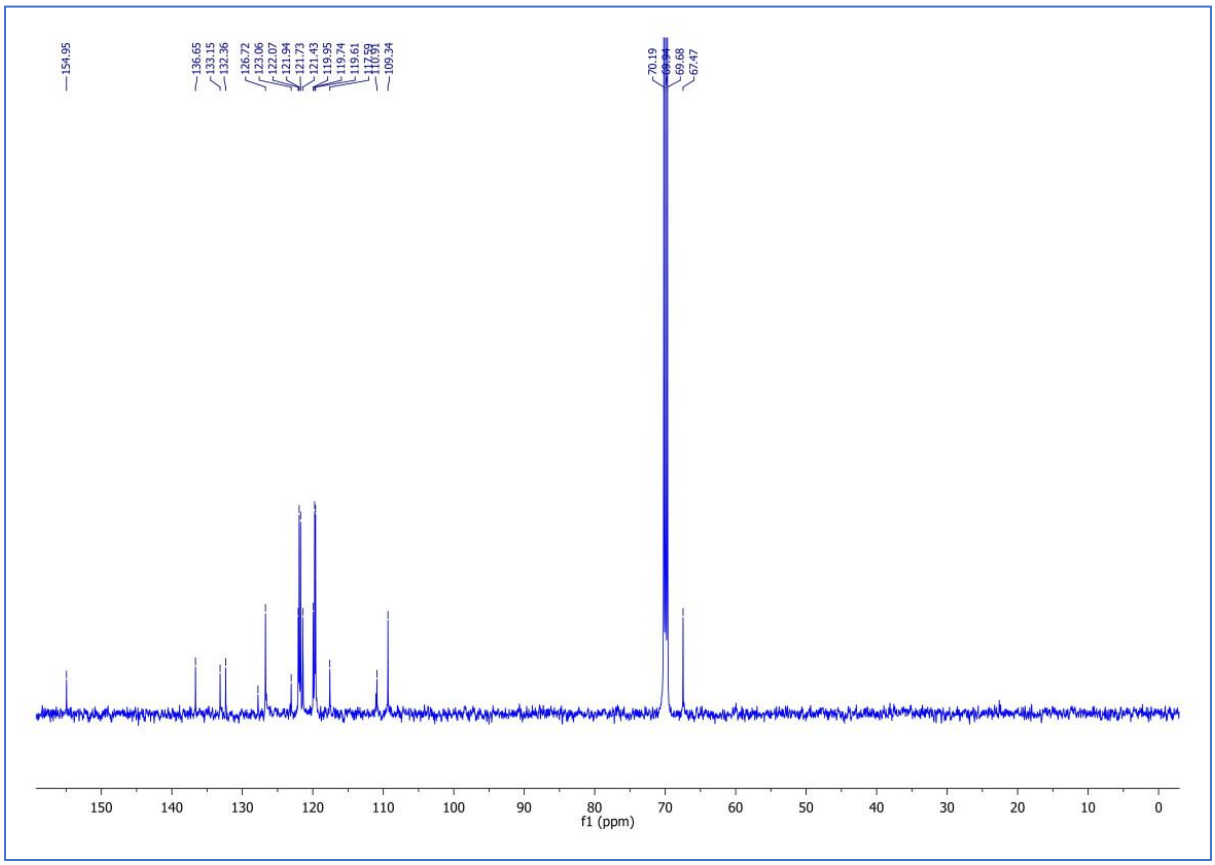
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

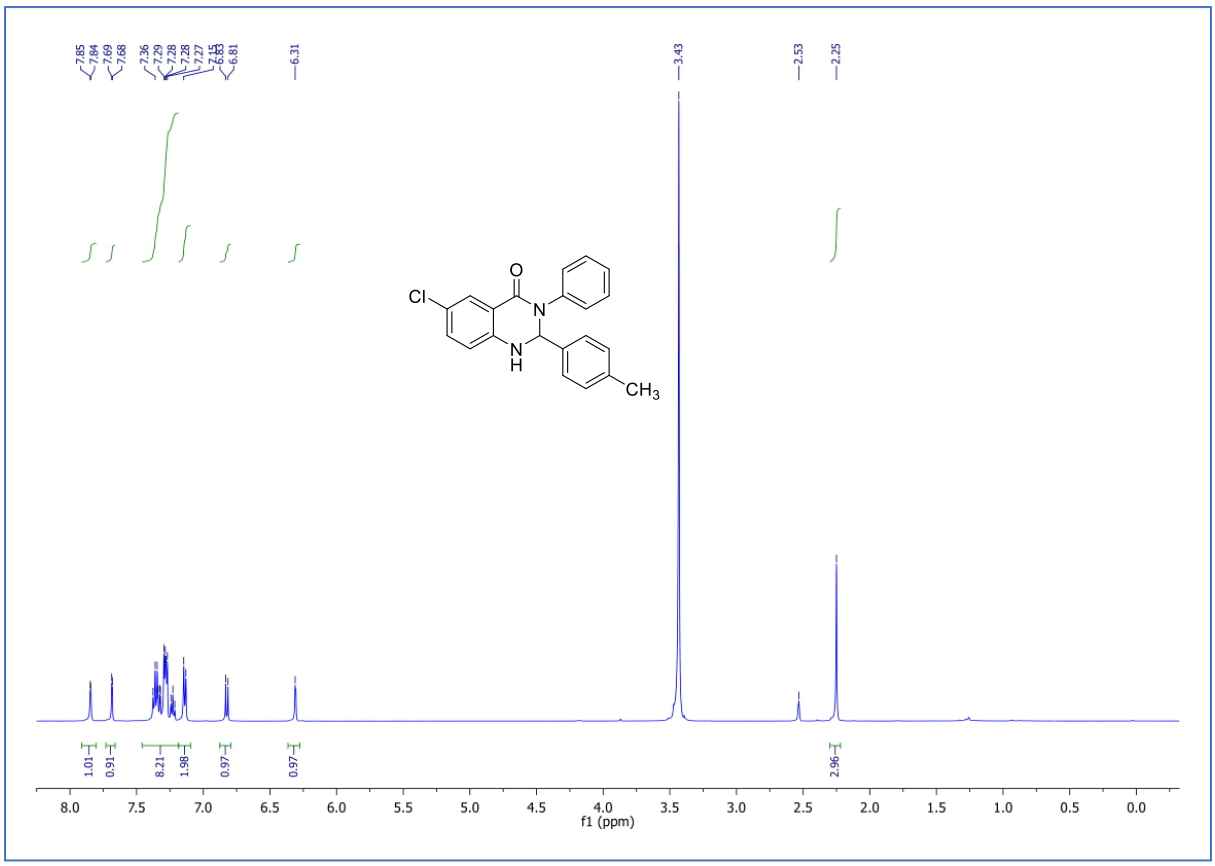

164.42
153.62
148.58
143.54
142.59
137.02
136.86
132.11
131.84
130.30
129.70
124.69
121.63
120.84
120.26
119.62
113.79
75.27
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

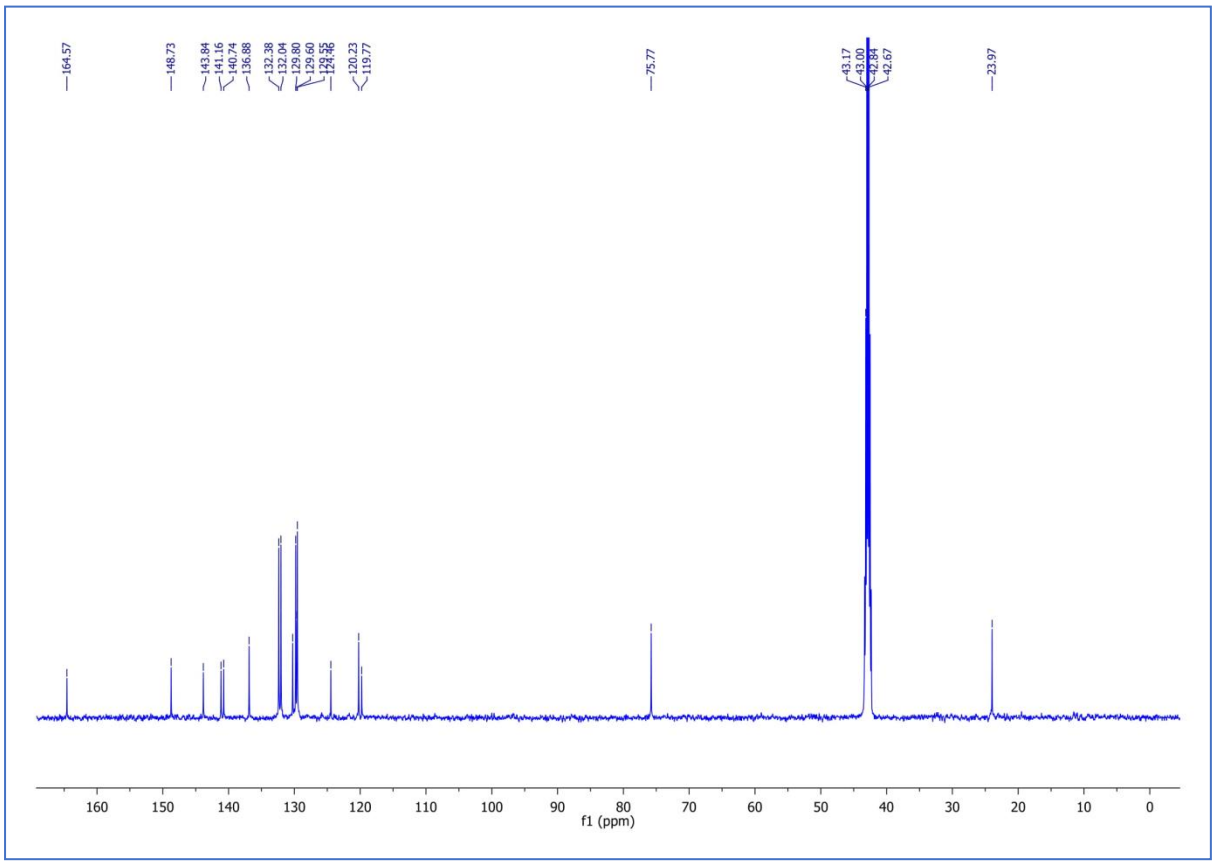
(2k, Table 2)


7.99
7.98
7.33
7.33
7.29
7.29
7.29
7.28
7.28
7.28
7.27
7.27
7.19
7.18
7.17
7.15
6.59
6.57
6.08
0.01
Cl
O
N
N
H
2.96
8.95
1.18
1.00
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)

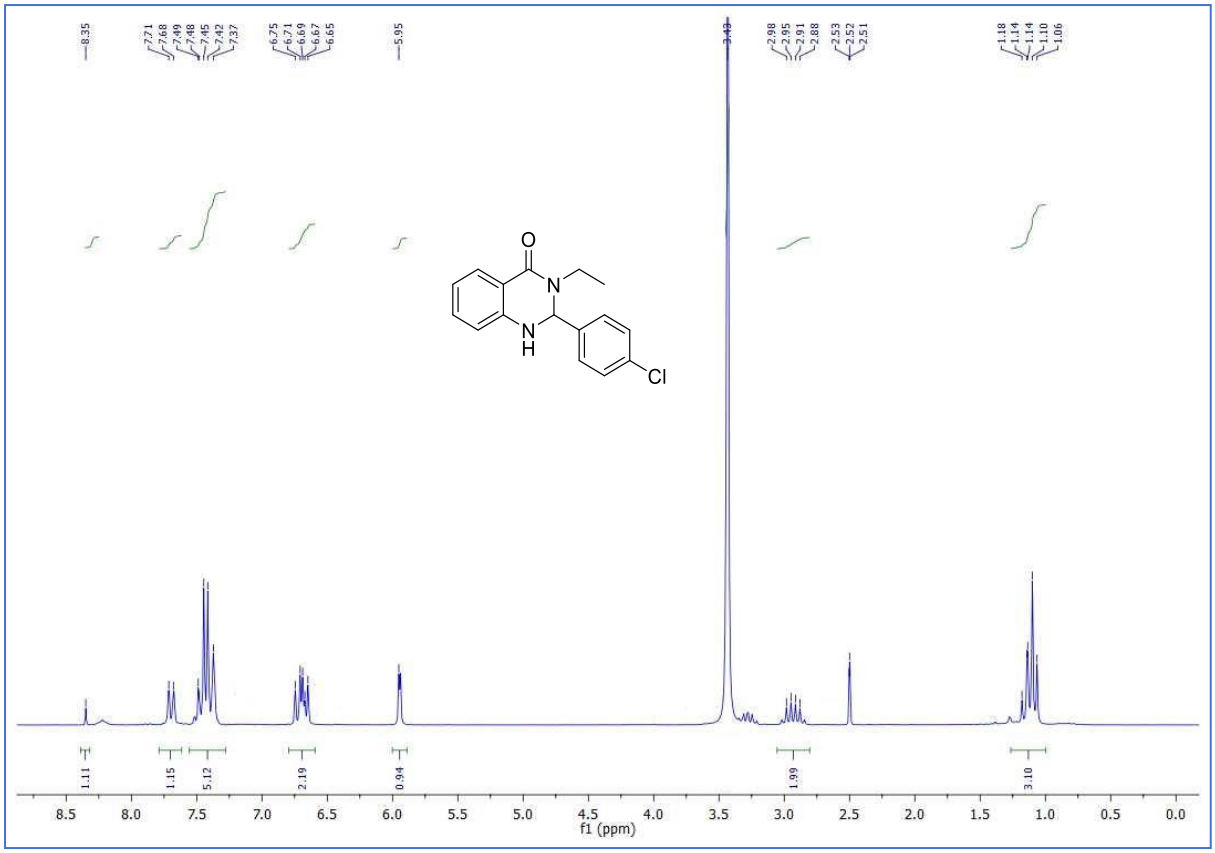

154.95
136.65
133.15
132.36
126.72
123.06
122.07
121.94
121.73
121.43
119.95
119.74
119.61
109.34
70.19
69.68
67.47
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

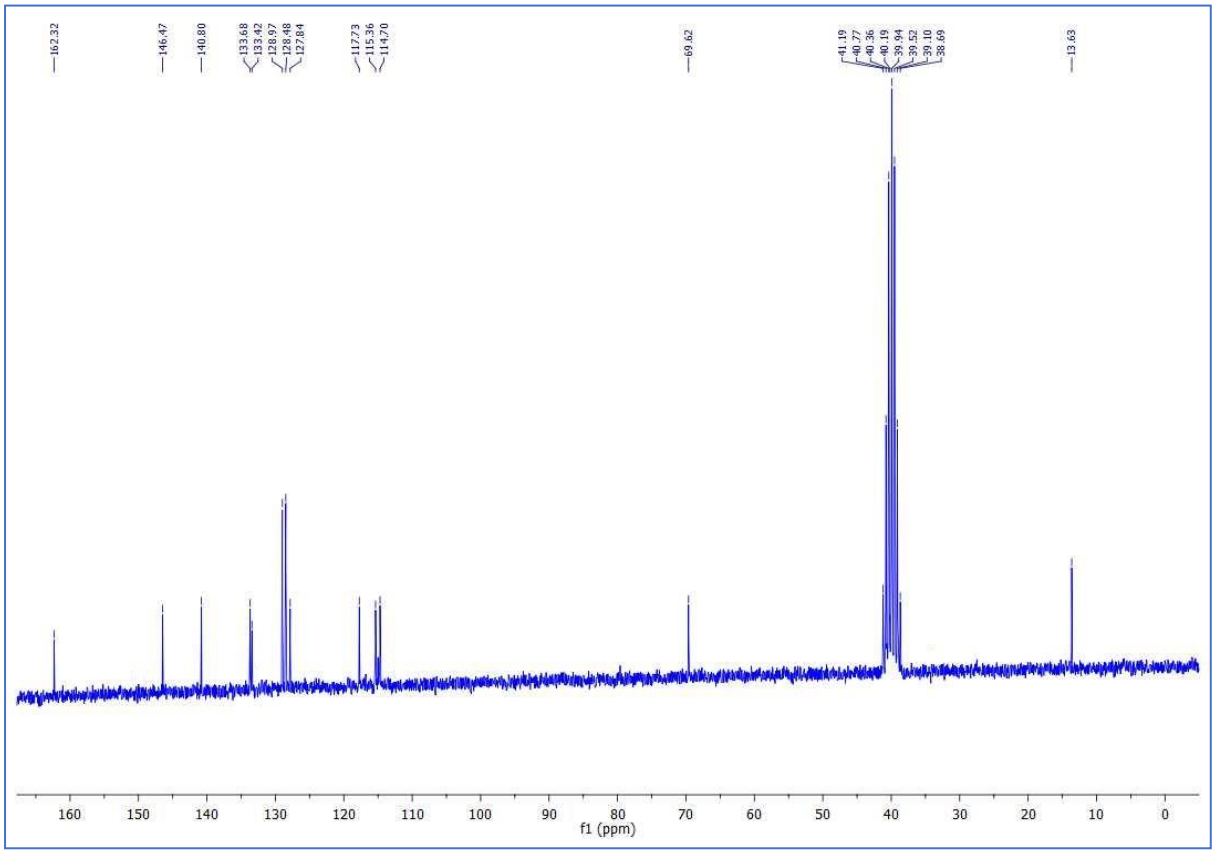
(2l, Table 2)


7.85
7.84
7.69
7.68
7.36
7.29
7.28
7.28
7.27
7.15
6.83
6.81
6.31
3.43
2.53
2.25
Cl
O
N
N
H
CH3
1.01
0.91
8.21
1.98
0.97
0.97
2.96
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
f1 (ppm)

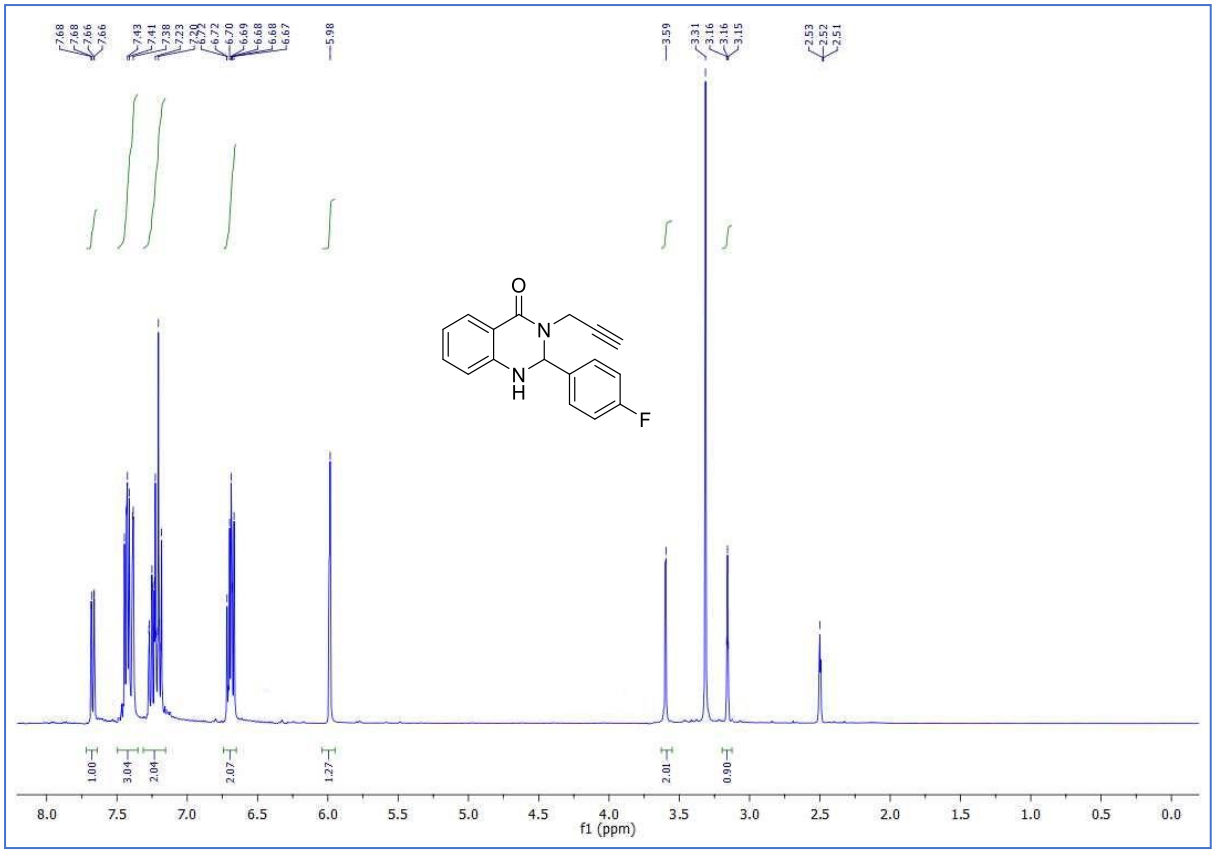

164.57
148.73
143.84
141.16
140.74
136.88
132.38
132.04
129.80
129.60
120.23
119.77
75.77
43.17
43.00
42.84
42.67
23.97
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

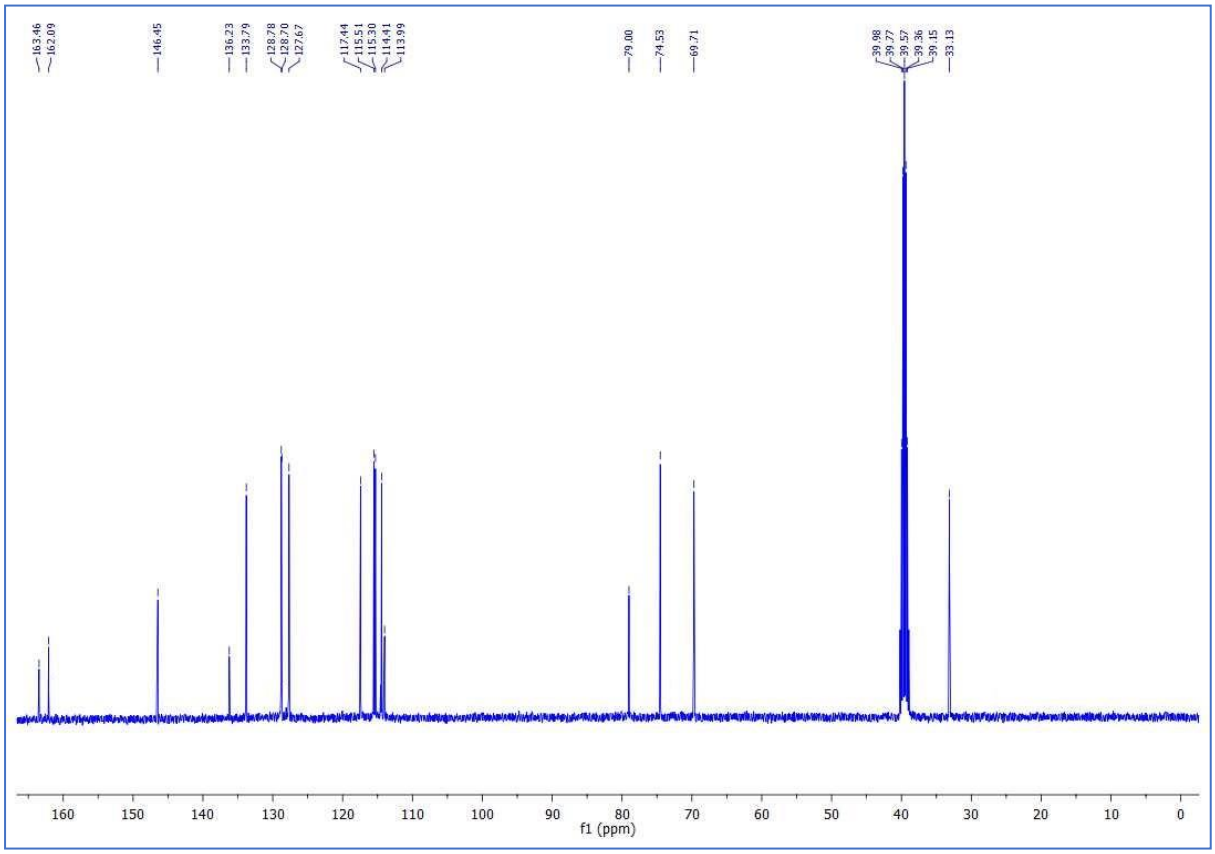
(2m, Table 2)


8.35
7.71
7.68
7.49
7.48
7.45
7.42
7.37
6.75
6.71
6.69
6.67
6.65
5.95
3.43
2.98
2.95
2.91
2.88
2.53
2.52
2.51
1.18
1.14
1.14
1.10
1.06
O
N
N
H
Cl
1.11
1.15
5.12
2.19
0.94
1.99
3.10
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
f1 (ppm)

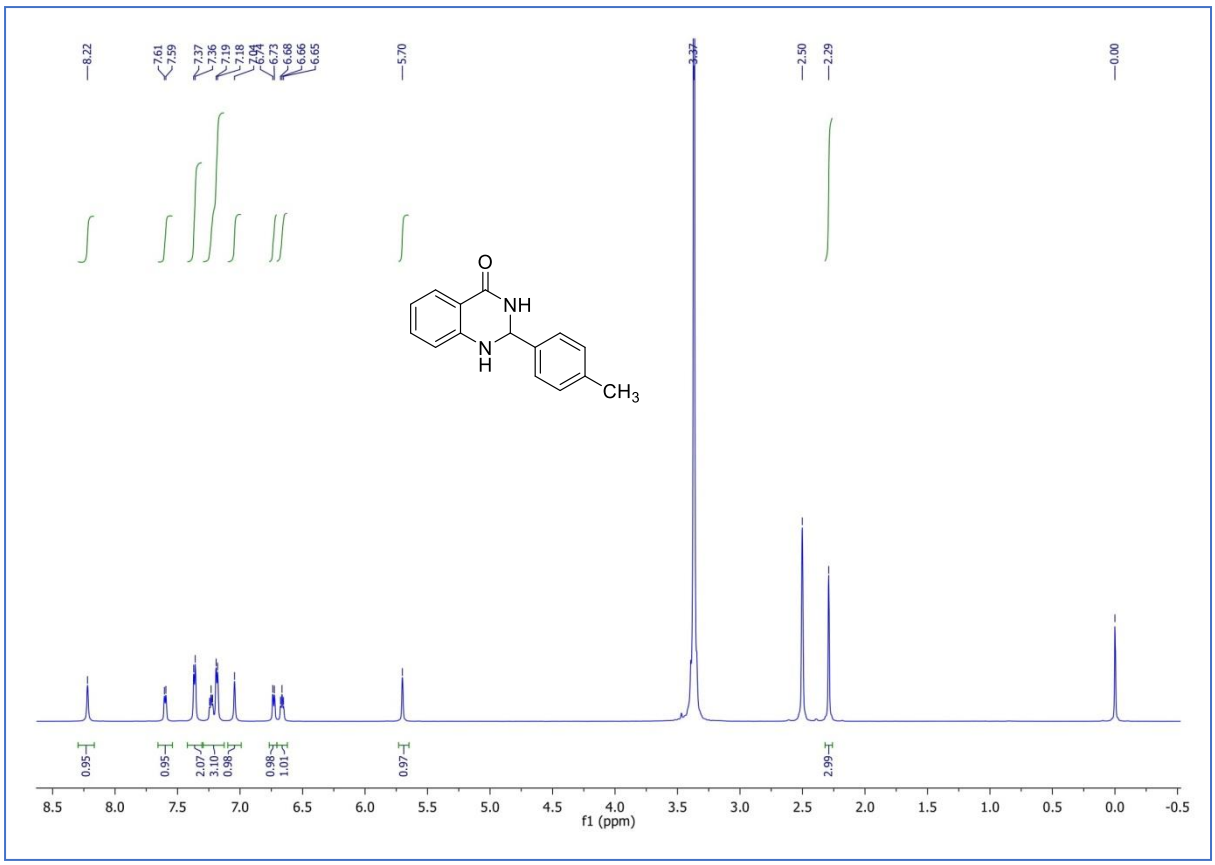

162.32
146.47
140.80
133.68
133.42
128.97
128.48
127.84
117.73
115.36
114.70
69.62
41.19
40.77
40.36
40.19
39.94
39.52
39.10
38.69
13.63
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

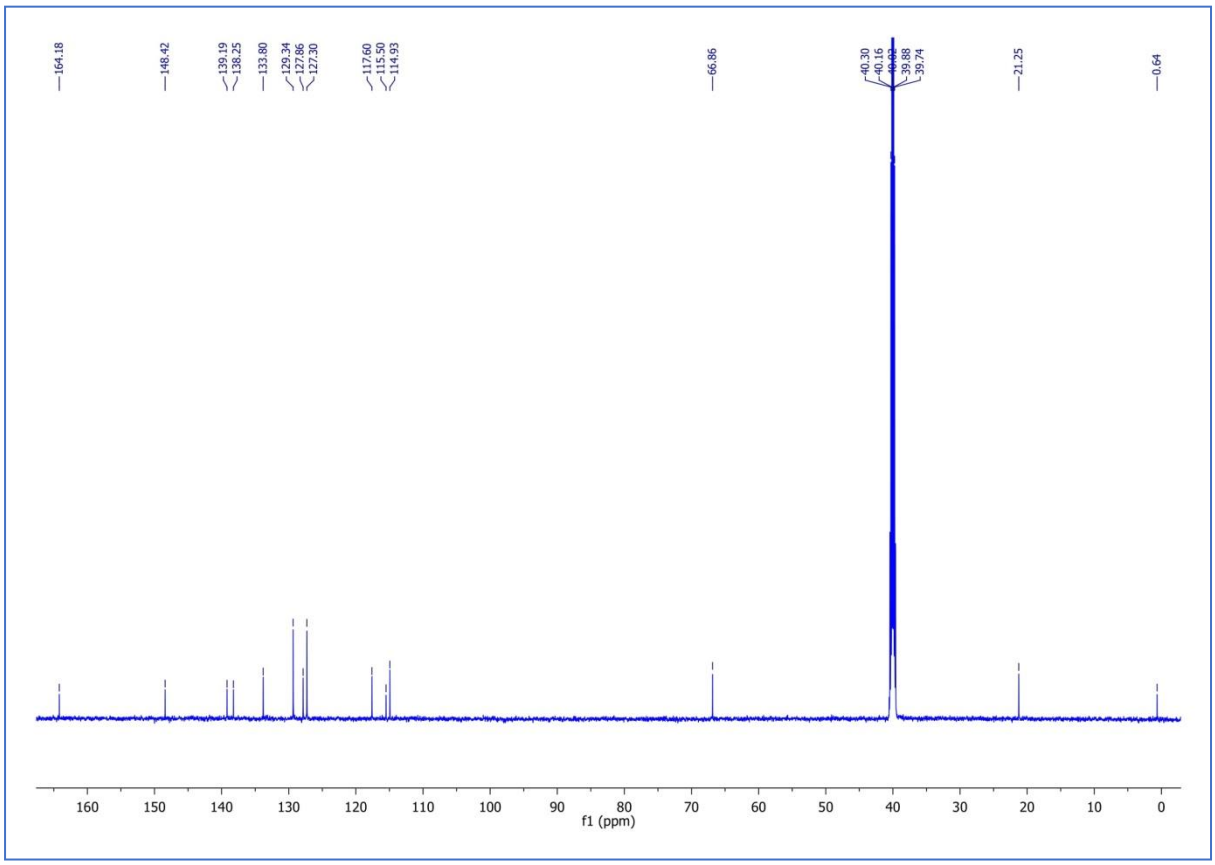
(2n, Table 2)


7.68
7.68
7.66
7.66
7.43
7.41
7.38
7.23
7.20
6.72
6.72
6.70
6.69
6.68
6.68
6.67
5.98
3.59
3.31
3.16
3.16
3.15
2.53
2.52
2.51
O
N
N
H
F
1.00
3.04
2.04
2.07
1.27
2.01
0.90
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
f1 (ppm)

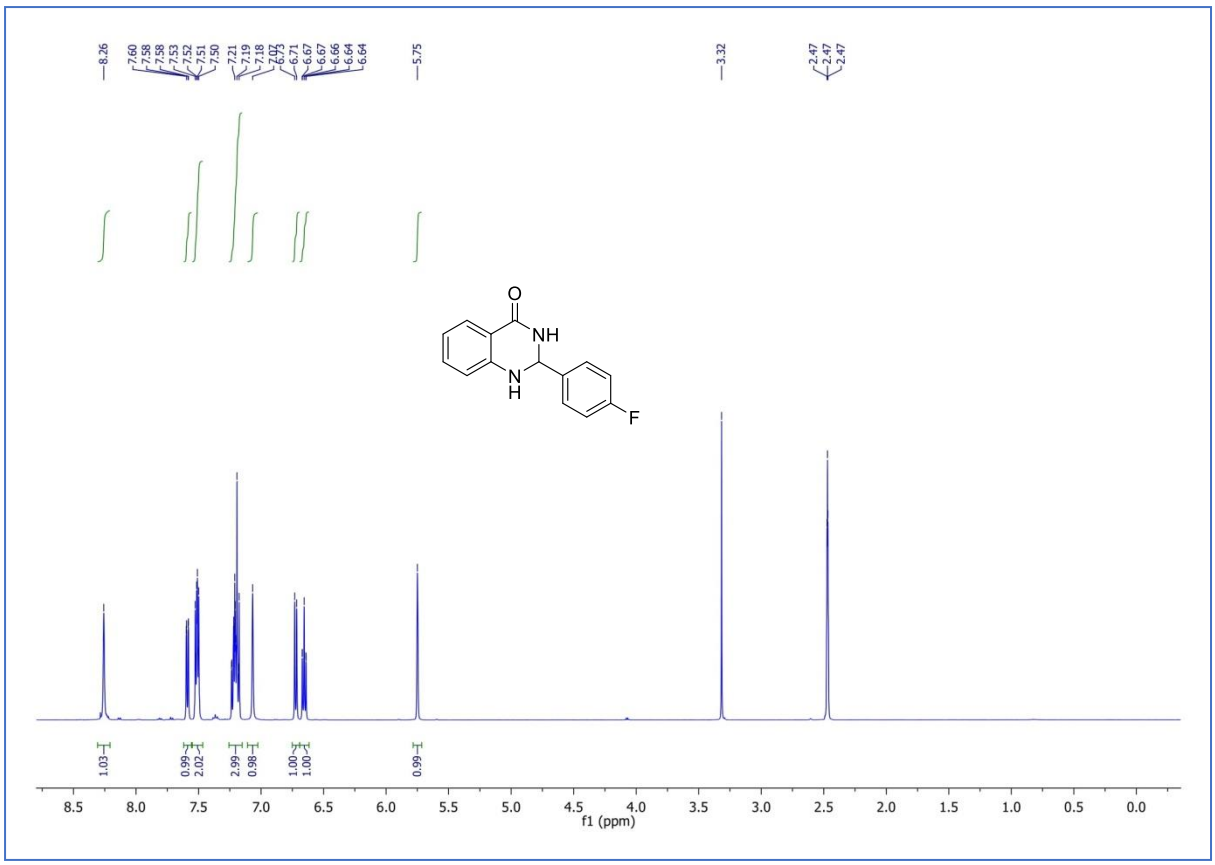

163.46
162.09
146.45
136.23
133.79
128.78
128.70
127.67
117.44
115.51
115.30
114.41
113.99
79.00
74.53
69.71
39.98
39.77
39.57
39.36
39.15
33.13
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

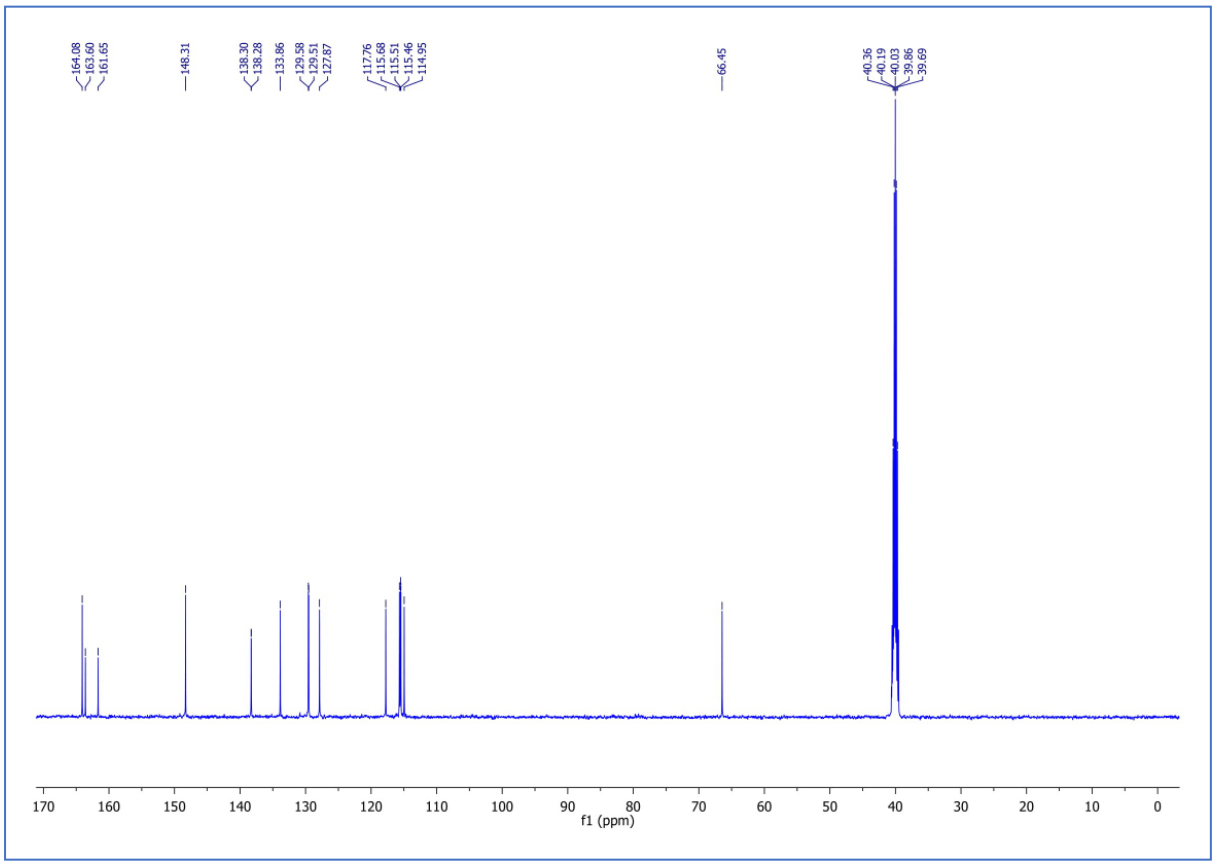
(3a, Table 3)


8.22
7.61
7.59
7.37
7.36
7.19
7.18
6.74
6.73
6.68
6.66
6.65
5.70
3.37
2.50
2.29
0.00
O
NH
N
H
CH3
0.95
0.95
2.07
3.10
0.98
0.98
1.01
0.97
2.99
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)

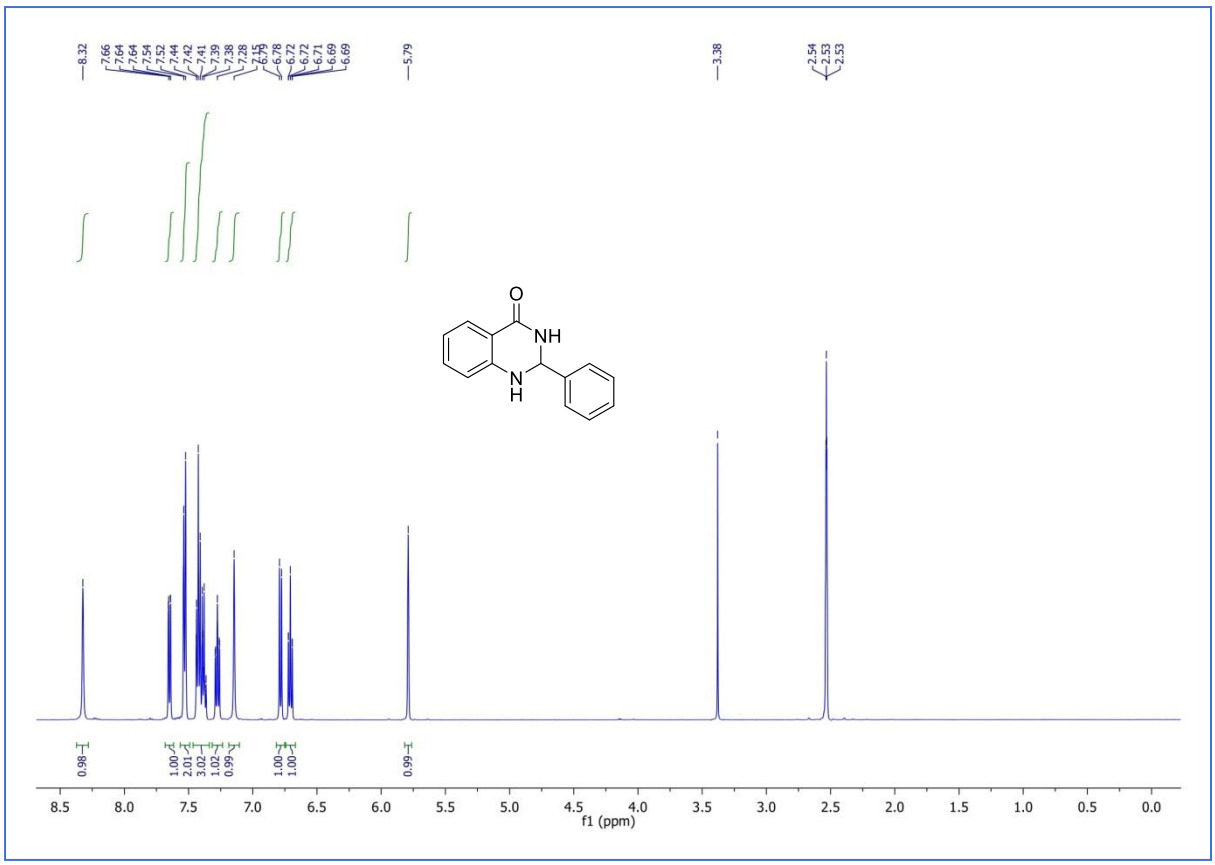

164.18
148.42
139.19
138.25
133.80
129.34
127.86
127.30
117.60
115.50
114.93
66.86
40.30
40.16
39.88
39.74
21.25
0.64
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

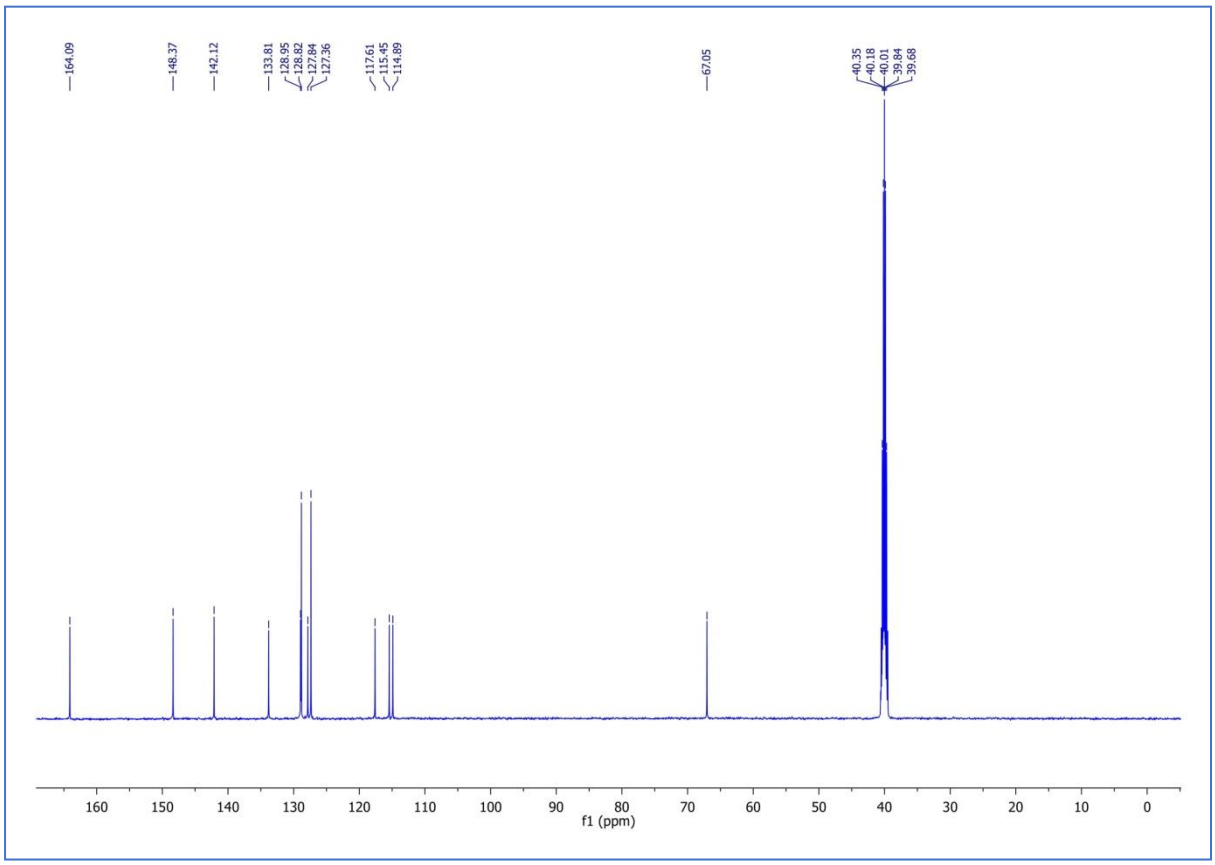
(3b, Table 3)


8.26
7.60
7.58
7.58
7.53
7.52
7.51
7.50
7.21
7.19
7.18
7.07
6.73
6.71
6.67
6.67
6.66
6.64
6.64
5.75
3.32
2.47
2.47
2.47
O
NH
N
H
F
1.03
0.99
2.02
2.99
0.98
1.00
1.00
0.99
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
f1 (ppm)

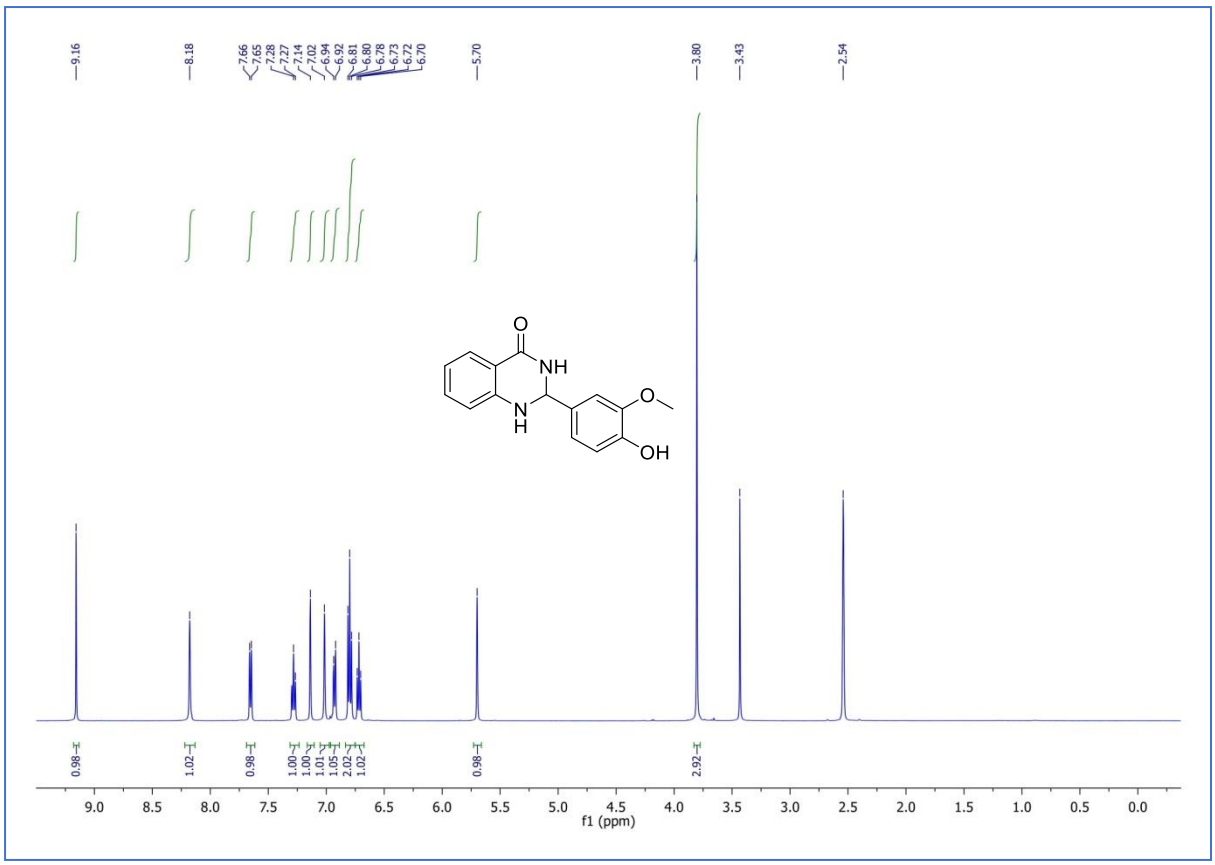

164.08
163.60
161.65
148.31
138.30
138.28
133.86
129.58
129.51
127.87
117.76
115.68
115.51
115.46
114.95
66.45
40.36
40.19
40.03
39.86
39.69
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

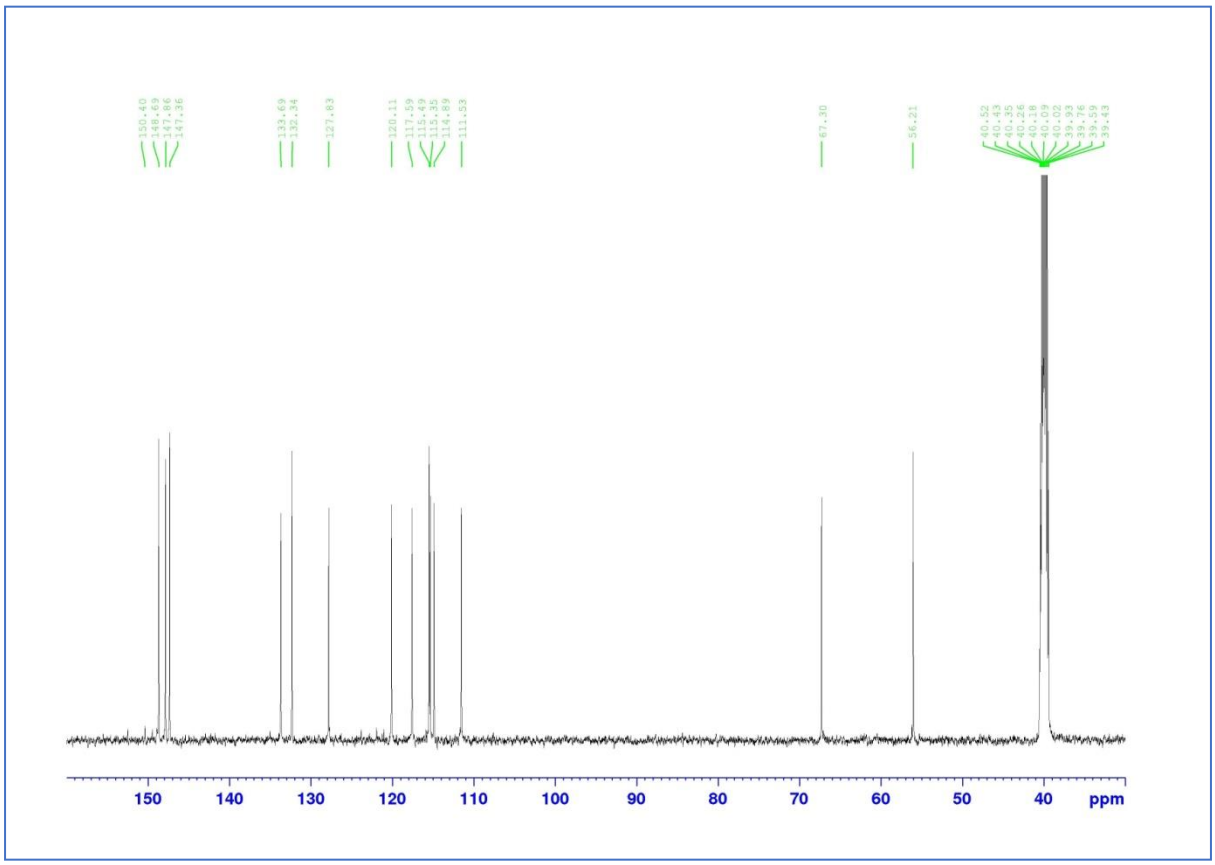
(3c, Table 3)


8.32
7.66
7.64
7.64
7.54
7.54
7.52
7.44
7.42
7.41
7.39
7.38
7.28
6.79
6.78
6.72
6.72
6.71
6.69
6.69
5.79
3.38
2.54
2.53
2.53
O
NH
N
H
0.98
1.00
2.01
3.02
1.02
0.99
1.00
1.00
0.99
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
f1 (ppm)

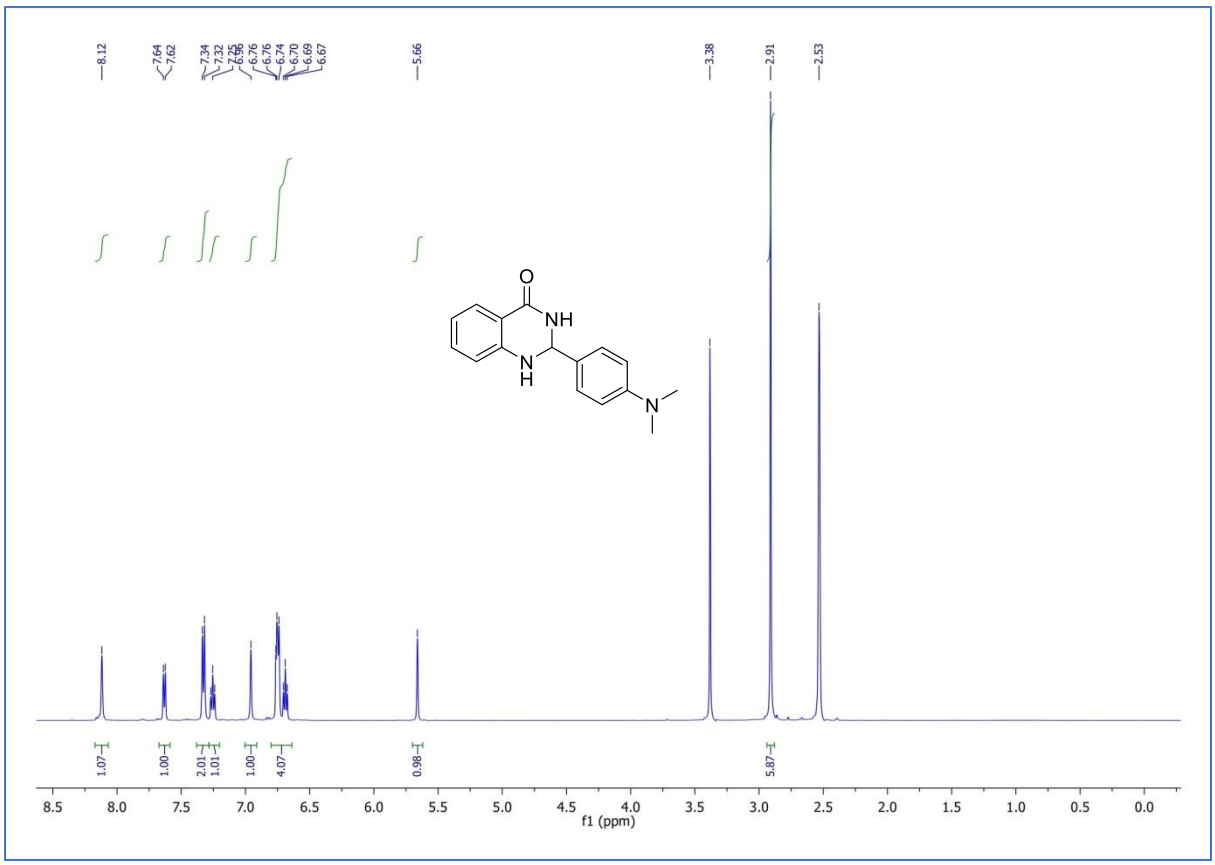

164.09
148.37
142.12
133.81
128.95
128.82
127.84
127.36
117.61
115.45
114.89
67.05
40.35
40.18
40.01
39.84
39.68
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

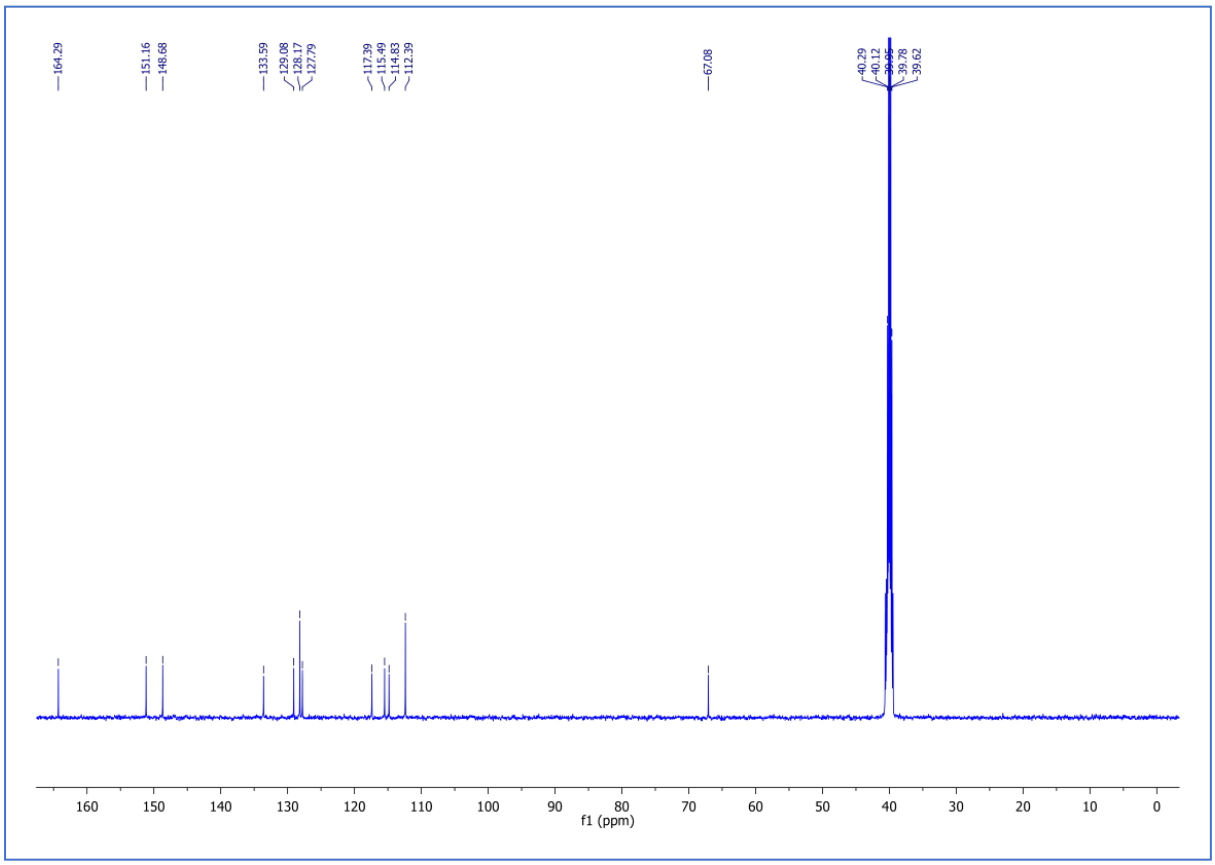
(3d, Table 3)


9.16
8.18
7.66
7.65
7.28
7.27
7.14
7.02
6.94
6.92
6.81
6.80
6.78
6.73
6.72
6.70
5.70
3.80
3.43
2.54
O
NH
N
H
O
OH
0.98
1.02
0.98
1.00
1.00
1.01
1.05
2.02
1.02
0.98
2.92
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
f1 (ppm)

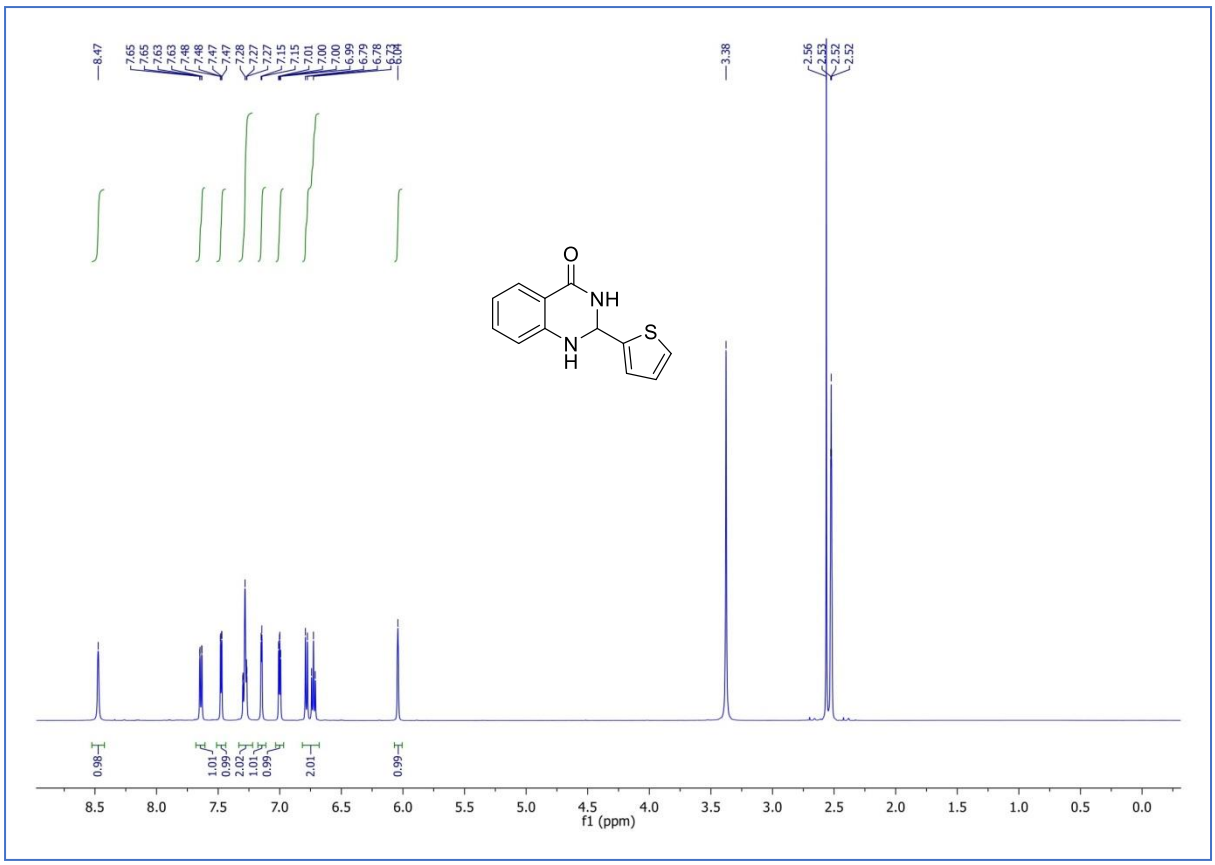

150.40
148.69
147.86
147.36
133.69
132.34
127.83
120.11
117.59
115.49
115.35
114.89
111.53
67.30
56.21
40.52
40.43
40.35
40.26
40.18
40.09
40.00
39.93
39.76
39.59
39.43
150 140 130 120 110 100 90 80 70 60 50 40 ppm

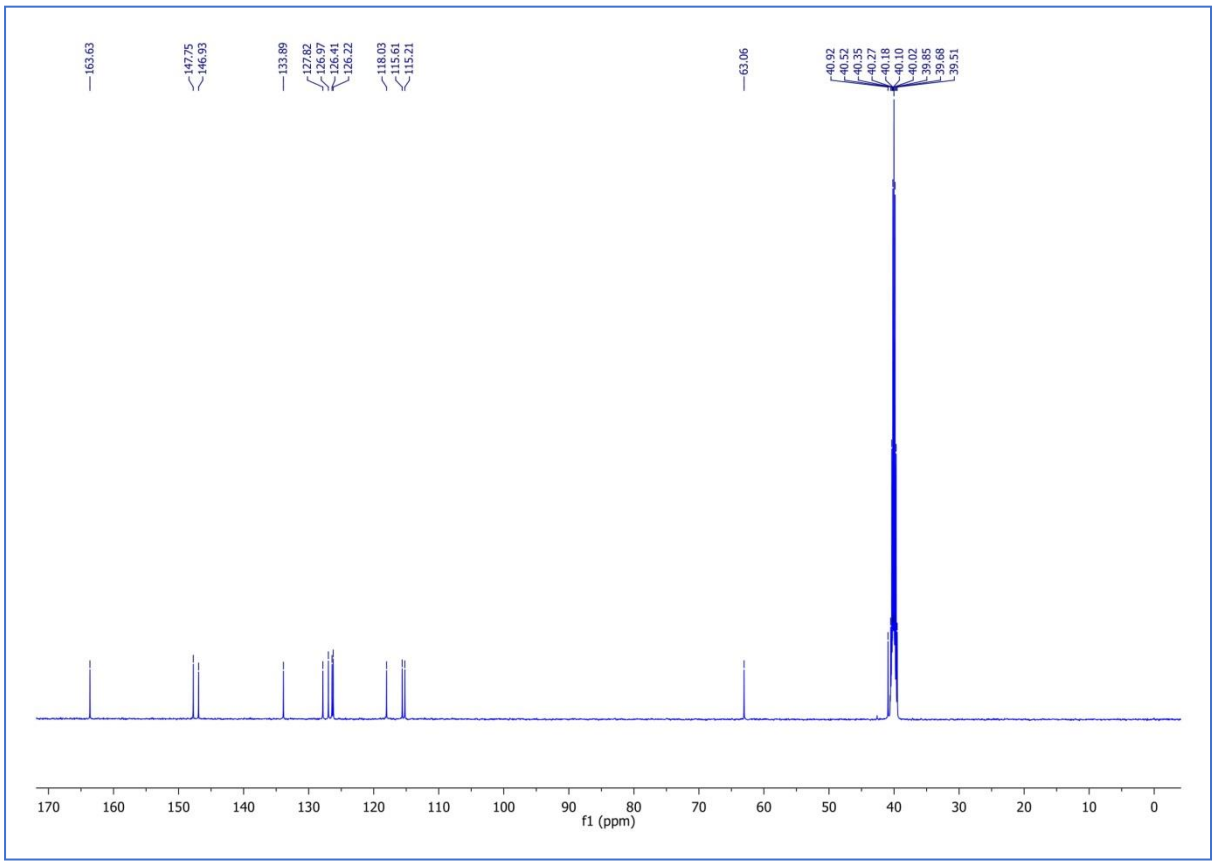
(3e, Table 3)


8.12
7.64
7.62
7.34
7.32
6.76
6.74
6.70
6.69
6.67
5.66
3.38
2.91
2.53
O
NH
N
H
N
1.07
1.00
2.01
1.01
1.00
4.07
0.98
5.87
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
f1 (ppm)

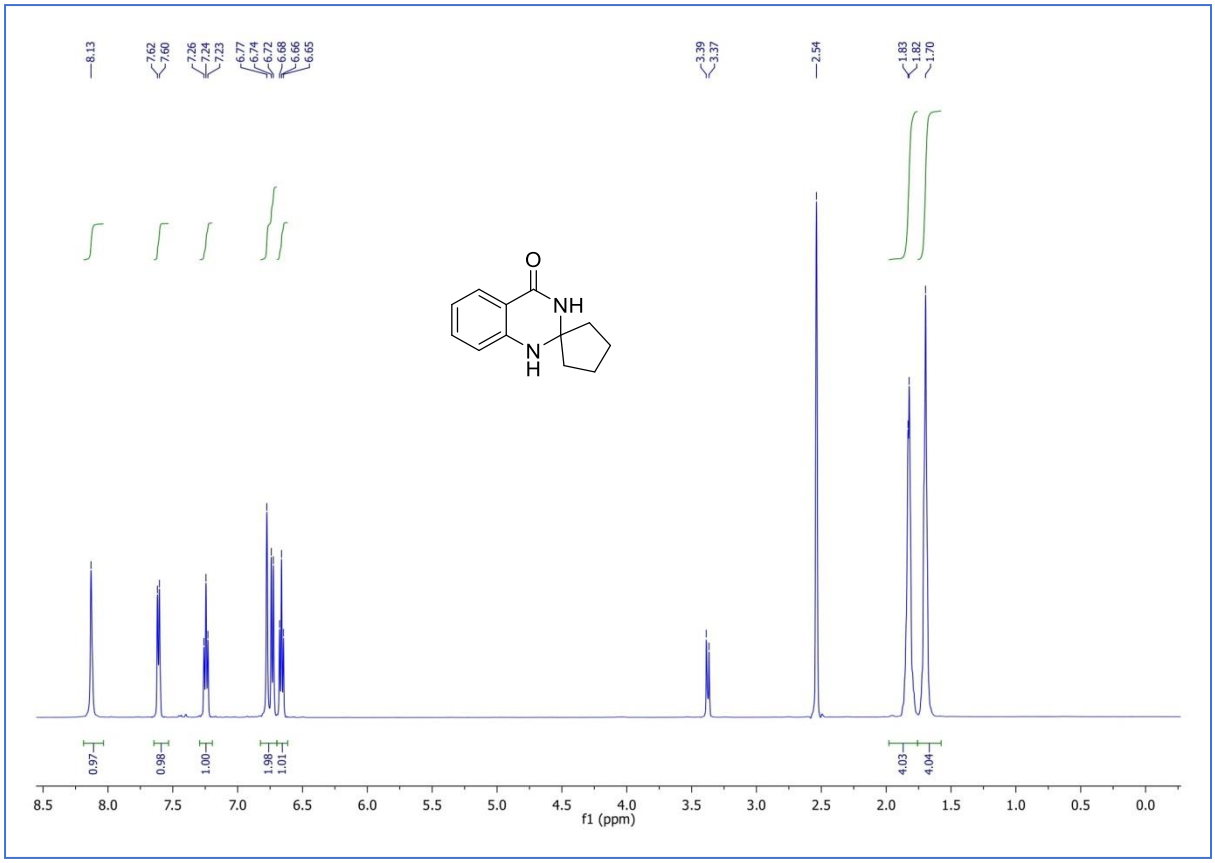

164.29
151.16
148.68
133.59
129.08
128.17
127.79
117.39
115.49
114.83
112.39
67.08
40.29
40.12
39.78
39.62
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

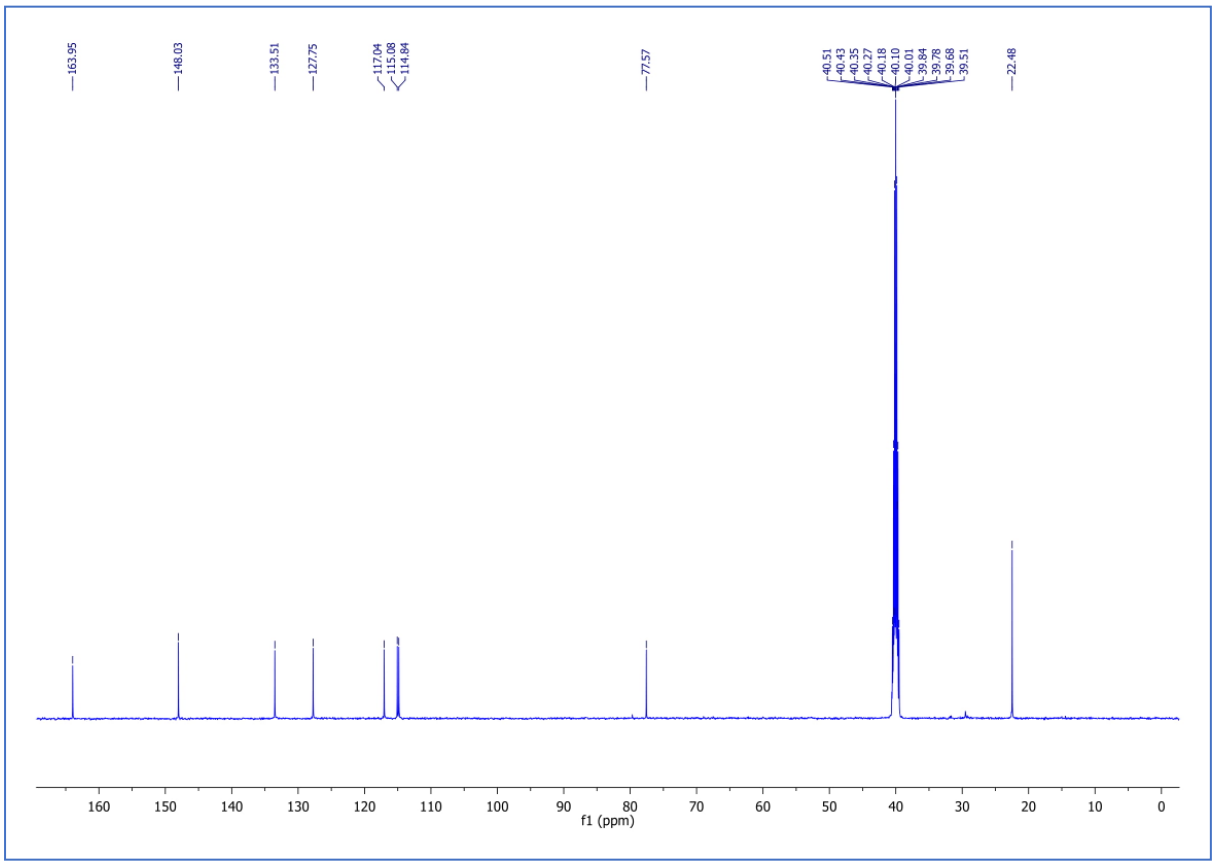
(3f, Table 3)


8.47
7.65
7.65
7.63
7.63
7.48
7.48
7.47
7.47
7.28
7.27
7.27
7.15
7.15
7.01
7.00
7.00
6.99
6.79
6.78
6.73
6.04
3.38
2.56
2.53
2.52
2.52
2.52
O
NH
N
H
S
0.98
1.01
0.99
2.02
1.01
0.99
2.01
0.99
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
f1 (ppm)

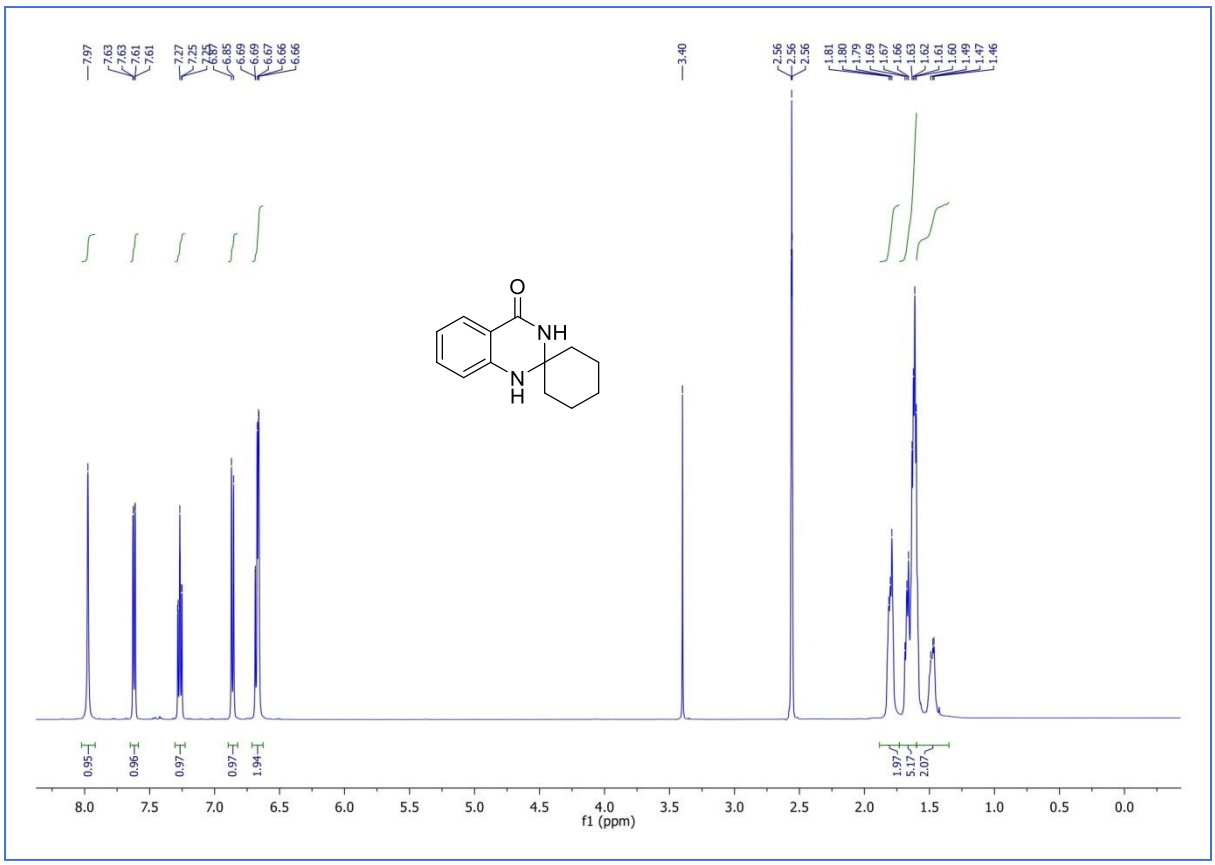

163.63
147.75
146.93
133.89
127.82
126.97
126.41
126.22
118.03
115.61
115.21
63.06
40.92
40.52
40.35
40.27
40.18
40.10
40.02
39.85
39.68
39.51
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

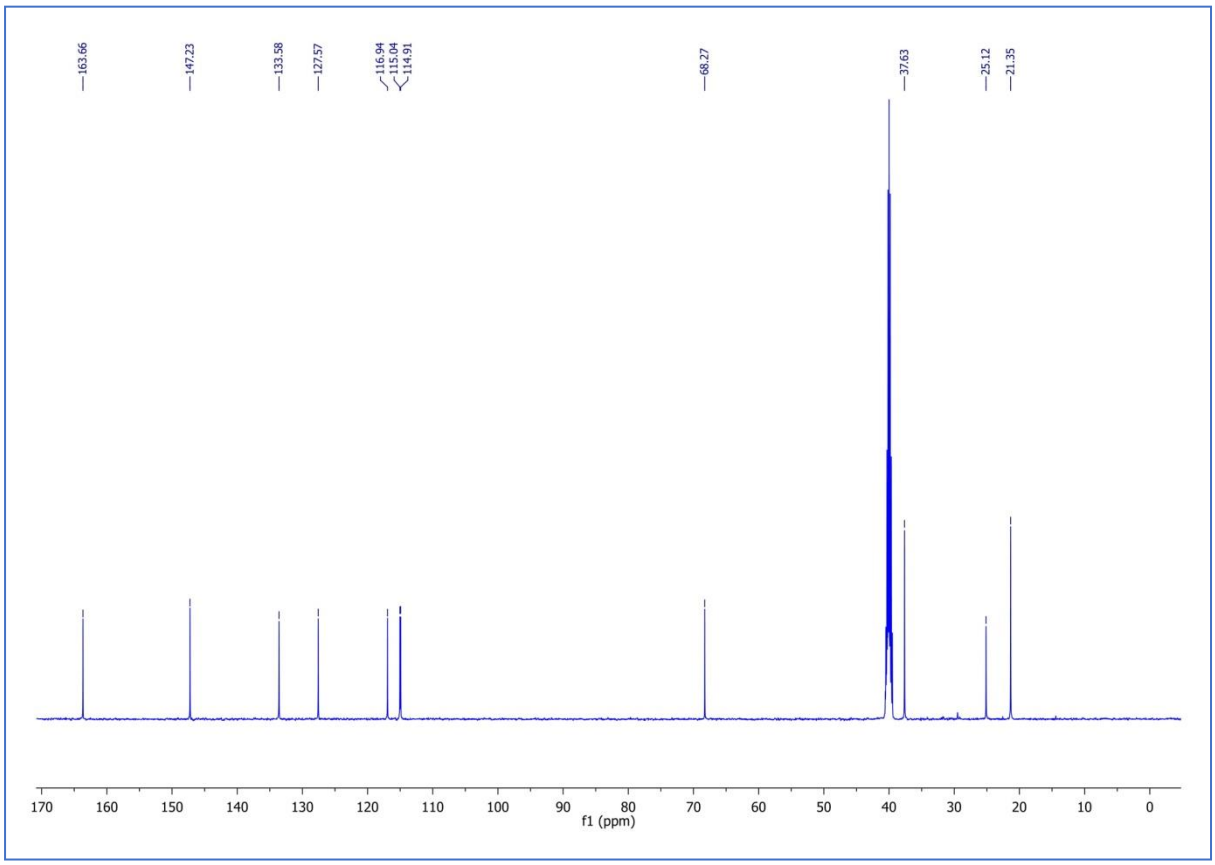
(3g, Table 3)


8.13
7.62
7.60
7.26
7.24
7.23
6.77
6.74
6.72
6.68
6.66
6.65
3.39
3.37
2.54
1.83
1.82
1.70
O
NH
N
H
0.97
0.98
1.00
1.98
1.01
4.03
4.04
f1 (ppm)

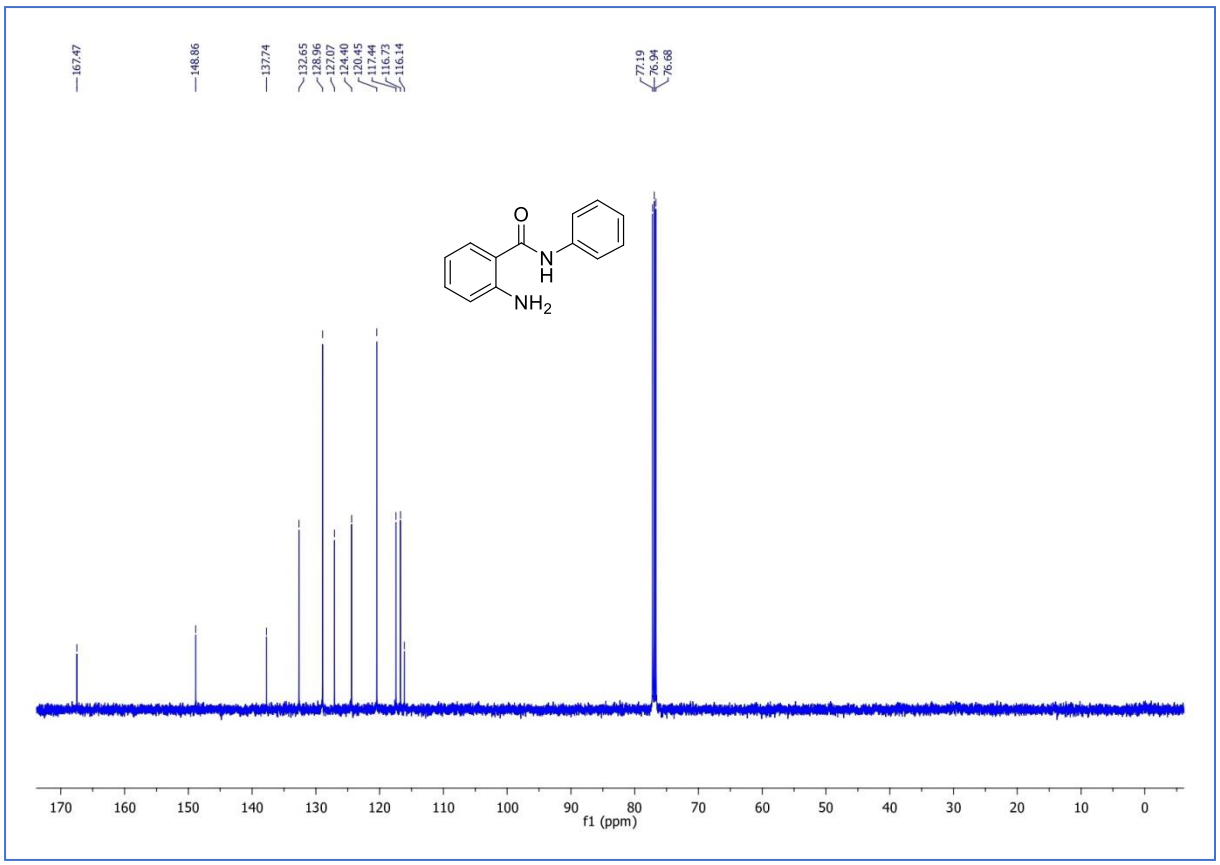

163.95
148.03
133.51
127.75
117.04
115.08
114.84
77.57
40.51
40.43
40.35
40.27
40.18
40.10
40.01
39.84
39.78
39.68
39.51
22.48
f1 (ppm)

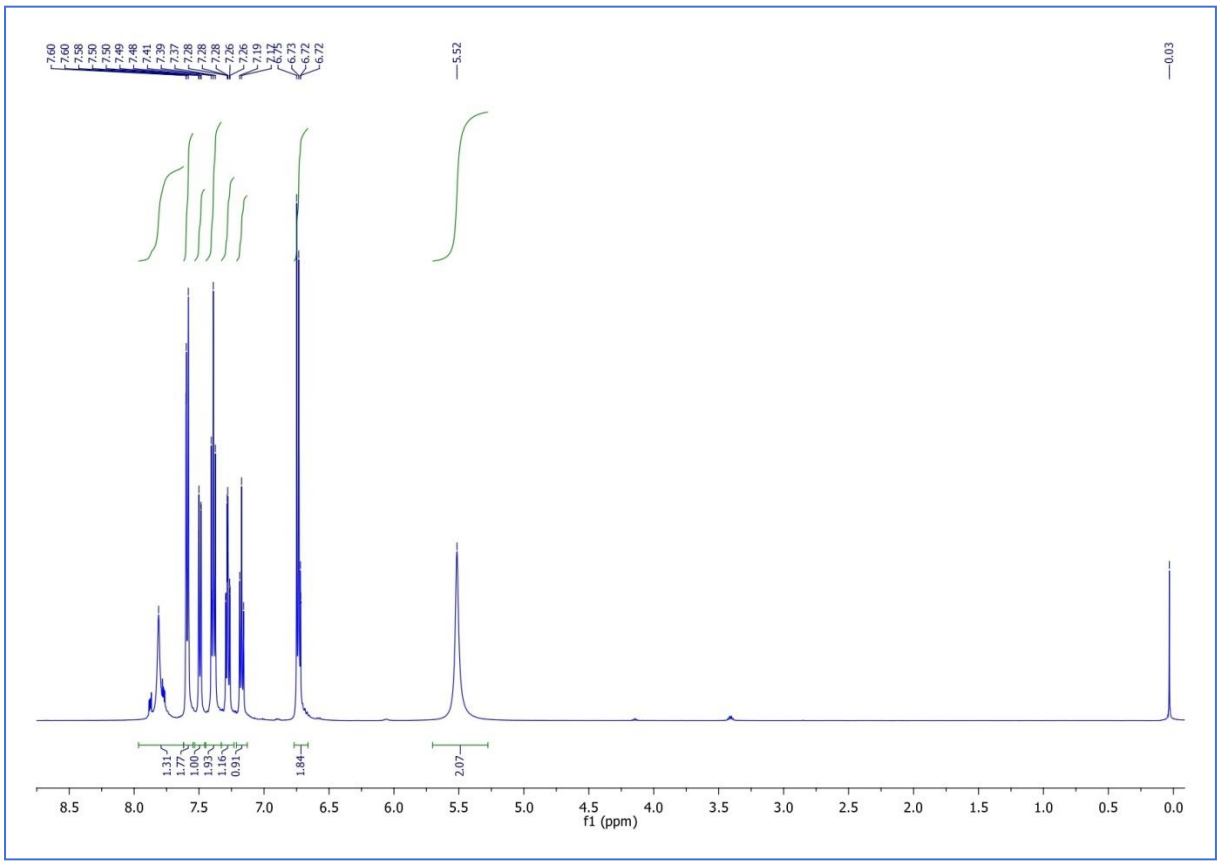
(3h, Table 3)





2-Amino-N-phenylbenzamide (III)


167.47
148.86
137.74
132.65
128.96
127.07
124.40
120.45
117.44
116.73
116.14
77.19
76.94
76.68
O
N
H
NH2
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.60
7.60
7.58
7.50
7.50
7.49
7.48
7.41
7.39
7.37
7.28
7.28
7.28
7.26
7.26
7.19
7.17
6.75
6.73
6.72
6.72
5.52
0.03
1.31
1.77
1.00
1.93
1.16
0.91
1.84
2.07
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
f1 (ppm)

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