Supporting Information 3

A new MCM-41 supported HPF_6 catalyst for the library synthesis of highly substituted 1,4-dihydropyridines and oxidation to pyridines: report of one-dimensional packing towards LMSOMs and studies on their photophysical properties

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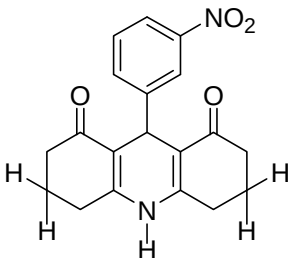
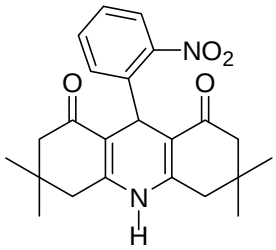


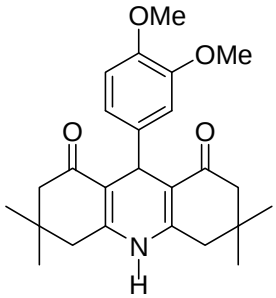
3,4,6,7-tetrahydro-9-(3-nitrophenyl)acridine-1,8(2H,5H,9H,10H)-dione (**7a**):

White solid, mp 224-226 °C (CH_2Cl_2 + EtOAc, equal volumes); IR ν_{max} (KBr) 3282, 3200, 2958, 1628, 1530, 1492, 1365, 1124, and 1146 cm^{-1}; ^1H NMR (300 MHz, DMSO-D_6) δ: 9.61 (1H, s), 7.98-7.93 (2H, m), 7.61 (1H, d, J = 8.1 Hz), 7.49 (1H, d, J = 8.1 Hz), 5.00 (1H, s), 2.56-2.51 (4H, m), 2.25-2.20 (4H, m), 1.97-1.77 (4H, m); ^{13}C NMR (75 MHz, DMSO-D_6) δ: 194.9, 149.4, 147.5, 134.4, 129.4, 122.1, 120.7, 111.6, 36.7, 32.9, 26.3, 20.8; Anal. Calcd for $C_{19}H_{18}N_2O_4$: C, 67.44; H, 5.36; N, 8.28. Found C, 67.70; H, 5.41; N, 8.41.



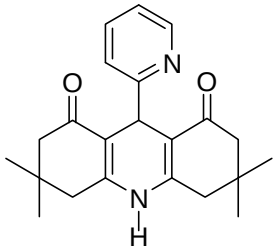
3,4,6,7-tetrahydro-3,3,6,6-tetramethyl-9-(2-nitrophenyl)acridine-1,8(2H,5H,9H,10H)-dione (**7b**):

White solid, mp 194-196 °C (CH_2Cl_2 + EtOAc, equal volumes); IR ν_{max} (KBr) 3280, 3200, 3072, 2958, 1633, 1530, 1490, 1365, and 1146 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$) δ: 8.52 (1H, s), 7.69 (1H, d, J = 8.1 Hz), 7.47-7.46 (2H, m), 7.21-7.15 (1H, m), 5.84 (1H, s), 2.34-2.05 (8H, m), 1.00 (6H, s), 0.90 (6H, s); ^{13}C NMR (75 MHz, $CDCl_3$) δ: 193.5, 149.3, 147.5, 141.1, 131.9, 129.7, 125.9, 123.0, 110.5, 49.6, 31.4, 28.8, 28.2, 26.0; Anal. Calcd for $C_{23}H_{26}N_2O_4$: C, 70.03; H, 6.64; N, 7.10. Found C, 70.33; H, 6.70; N, 7.29.



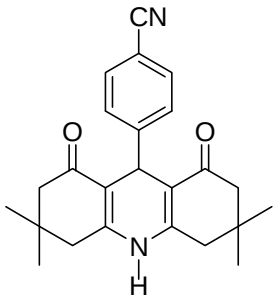
3,4,6,7-tetrahydro-9-(3,4-dimethoxyphenyl)-3,3,6,6-tetramethylacridine-1,8(2H,5H,9H,10H)-dione (**7c**):

White solid, mp 214-216 °C (CH_2Cl_2 + EtOAc, equal volumes); IR ν_{max} (KBr) 3273, 3199, 3068, 2950, 1641, 1610, 1482, 1365, and 1222 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$) δ: 8.13 (1H, s), 6.91 (1H, s), 6.80 (1H, d, J = 8.1 Hz), 6.67-6.64 (1H, m), 5.02 (1H, s), 3.83 (1H, s), 3.74 (1H, s), 2.37-2.12 (8H, m), 1.05 (6H, s), 0.96 (6H, s); ^{13}C NMR (75 MHz, $CDCl_3$) δ: 193.8, 148.5, 147.4, 146.2, 139.4, 118.9, 111.4, 111.0, 110.7, 54.8, 49.7, 31.5, 28.6, 25.8; Anal. Calcd for $C_{25}H_{31}NO_4$: C, 73.32; H, 7.63; N, 3.42. Found C, 73.60; H, 7.69; N, 3.55.



3,4,6,7-tetrahydro-3,3,6,6-tetramethyl-9-(pyridin-2-yl)acridine-1,8(2H,5H,9H,10H)-dione (**7d**):

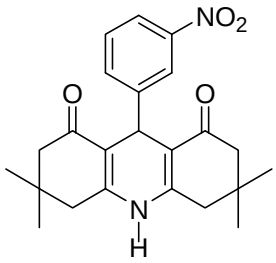
Red solid, mp 284-286 °C (CH_2Cl_2 + EtOAc, equal volumes); IR ν_{max} (KBr) 3288, 3072, 2960, 1634, 1530, 1490, 1365, 1124, and 1145 cm^{-1}; ^1H NMR (300 MHz, DMSO-D_6) δ: 9.20 (1H, s), 8.30 (1H, d, J = 3.9 Hz), 7.55 (1H, d, J = 6.3 Hz), 7.30 (1H, d, J = 7.5 Hz), 7.03 (1H, d, J = 5.1 Hz), 4.96 (1H, s), 2.50-1.92 (8H, m), 1.00 (6H, s), 0.87 (6H, s); ^{13}C NMR (75 MHz, DMSO-D_6) δ: 193.8, 163.3, 149.4, 147.9, 134.5, 122.4, 120.6, 109.8, 49.7, 34.9, 31.6, 28.6, 25.6; Anal. Calcd for $C_{22}H_{26}N_2O_2$: C, 75.40; H, 7.48; N, 7.99. Found C, 75.21; H, 7.51; N, 8.09.



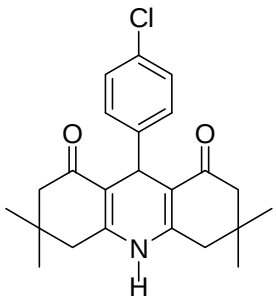
4-(1,2,3,4,5,6,7,8,9,10-decahydro-3,3,6,6-tetramethyl-1,8-dioxoacridin-9-yl)benzonitrile (**7e**):

Yellowish white solid, mp 194-196 °C (CH_2Cl_2 + EtOAc, equal volumes); IR ν_{max} (KBr) 3208, 3072, 2958, 1633, 1530, 1490, 1365, 1124, and 1141cm^{-1}; ^1H NMR (300 MHz, DMSO-D_6) δ: 9.45 (1H, s), 7.65 (2H, d,

J = 8.1 Hz), 7.34 (2H, d, J = 8.1 Hz), 4.86 (1H, s), 2.56-1.96 (8H, m), 1.06 (6H, s), 0.89 (6H, s); ^{13}C NMR (75 MHz, DMSO-D_6) δ: 193.7, 151.8,149.2, 131.3, 128.6, 128.1, 118.4, 109.9, 107.7, 49.5, 33.2, 31.5, 28.4, 25.9; Anal. Calcd for $C_{24}H_{26}N_2O_2$: C, 76.98; H, 7.00; N, 7.48. Found C, 76.70; H, 7.09; N, 7.36.

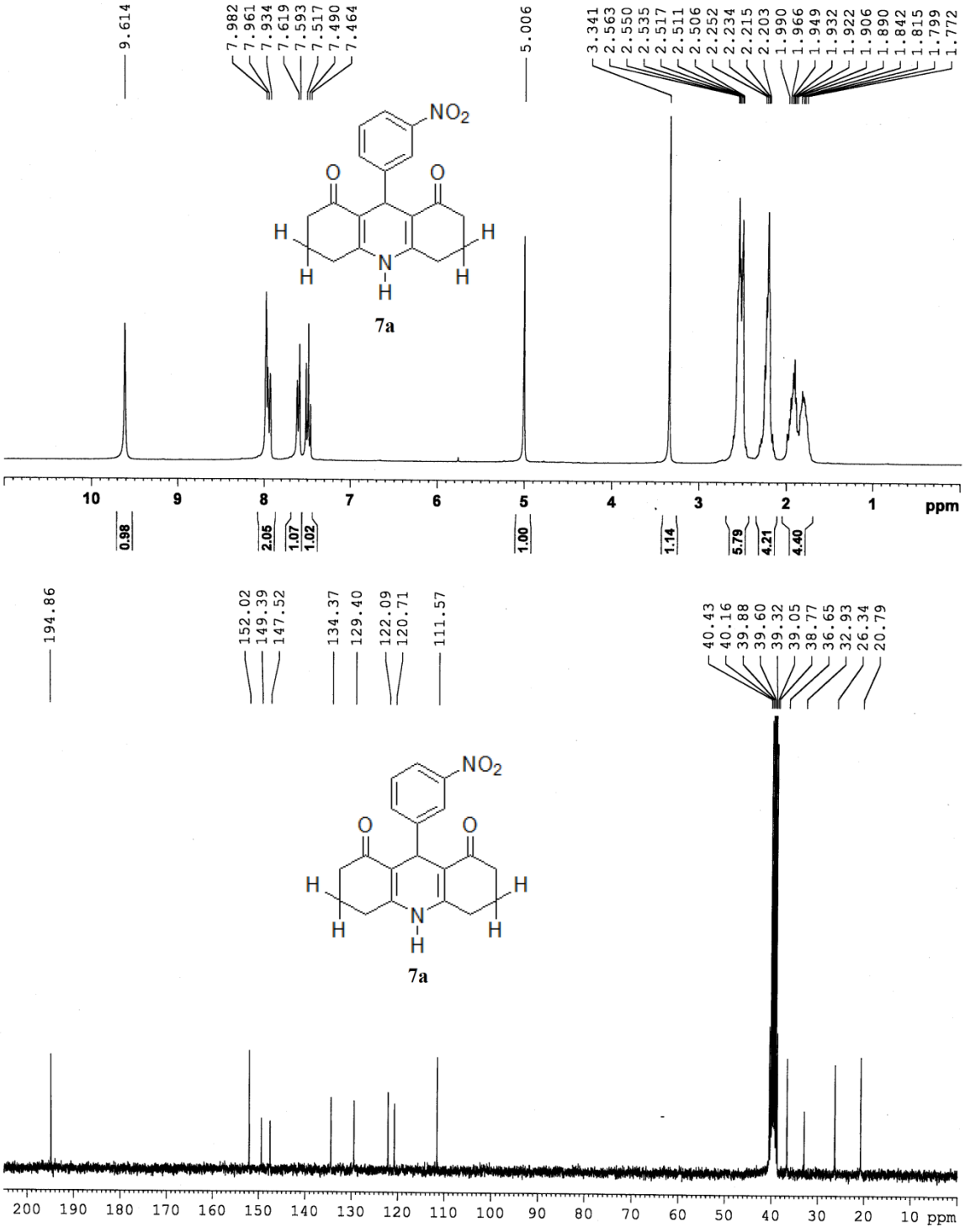


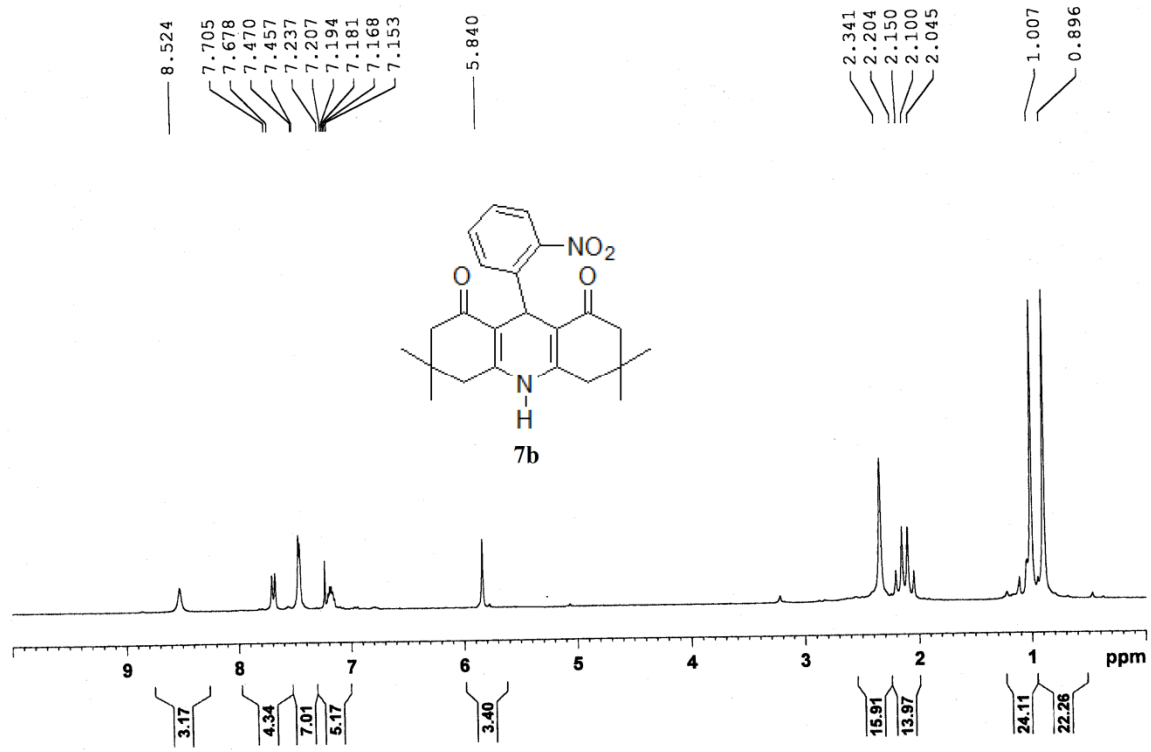
3,4,6,7-tetrahydro-3,3,6,6-tetramethyl-9-(3-nitrophenyl)acridine-1,8(2H,5H,9H,10H)-dione (**7f**): Yellowish white solid, mp 212-214 °C (CH_2Cl_2 + EtOAc, equal volumes); IR ν_{max} (KBr) 3288, 3160, 3078, 2958, 1634, 1530, 1490, 1365, and 1124 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 8.00 (1H, s), 7.89 (1H, d, J = 7.5 Hz), 7.74 (1H, d, J = 7.5 Hz), 7.48 (1H, d, J = 8.1 Hz), 5.09 (1H, s), 2.39-2.09 (8H, m), 1.04 (6H, s), 0.91 (6H, s); Anal. Calcd for $C_{23}H_{26}N_2O_4$: C, 70.03; H, 6.64; N, 7.10. Found C, 70.28; H, 6.55; N, 7.01.



3,4,6,7-tetrahydro-3,3,6,6-tetramethyl-9-(4-chlorophenyl)acridine-1,8(2H,5H,9H,10H)-dione (**7g**): Yellowish white solid, mp 292-294 °C (CH_2Cl_2 + EtOAc, equal volumes); IR ν_{max} (KBr) 3268, 3162, 3072, 2944, 1631, 1528, 1490, and 1120 cm^{-1}; ^{1}H NMR (300 MHz, DMSO-D_6) δ: 9.26 (1H, s), 7.13 (2H, d, J = 8.4 Hz), 7.07 (2H, d, J = 8.4 Hz), 4.70 (1H, s), 2.41-1.87 (8H, m), 0.92 (6H, s), 0.77 (6H, s); ^{13}C NMR (75 MHz, DMSO-D_6) δ: 194.8, 149.9, 146.6, 130.4, 129.9, 128.0, 111.5, 50.6, 33.2, 32.6, 29.5, 26.9; Anal. Calcd for $C_{23}H_{26}ClNO_2$: C, 71.96; H, 6.83; N, 3.65. Found C, 72.14; H, 7.01; N, 3.49.

1H NMR and 13C NMR spectra for 7a-7g

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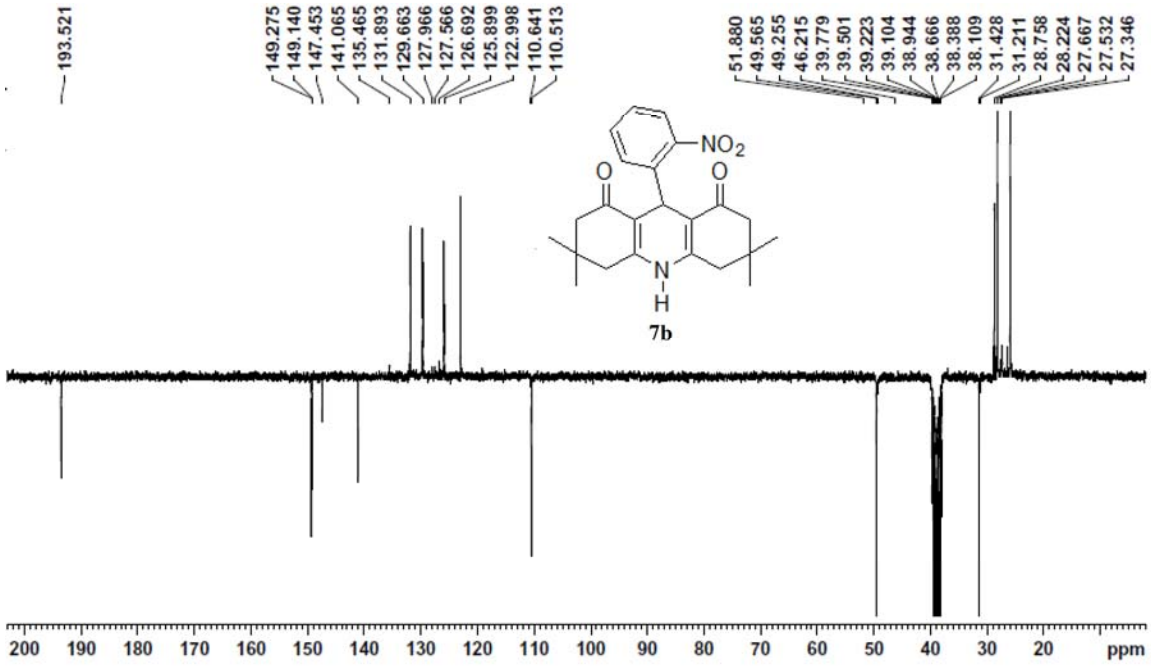
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H
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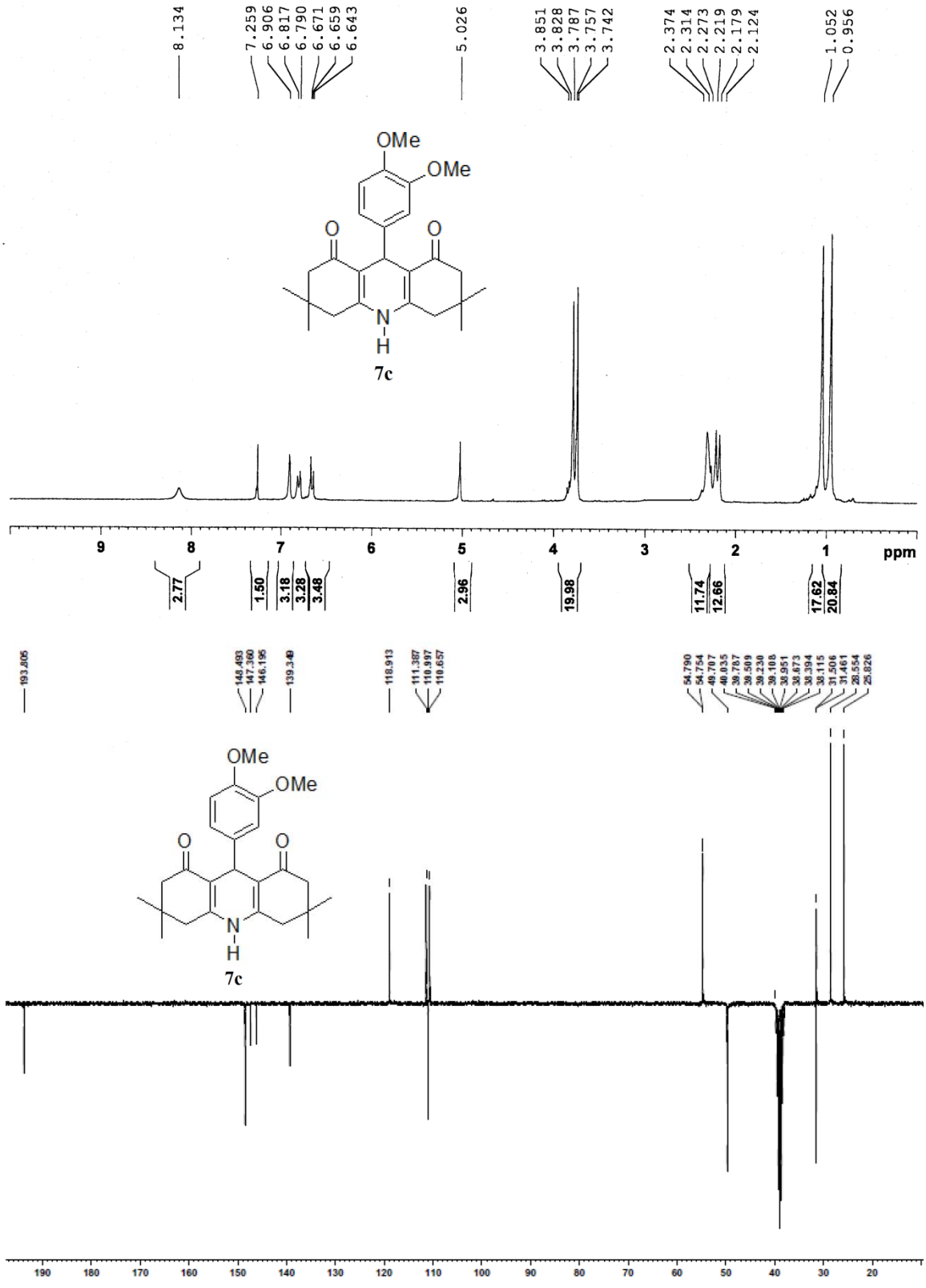
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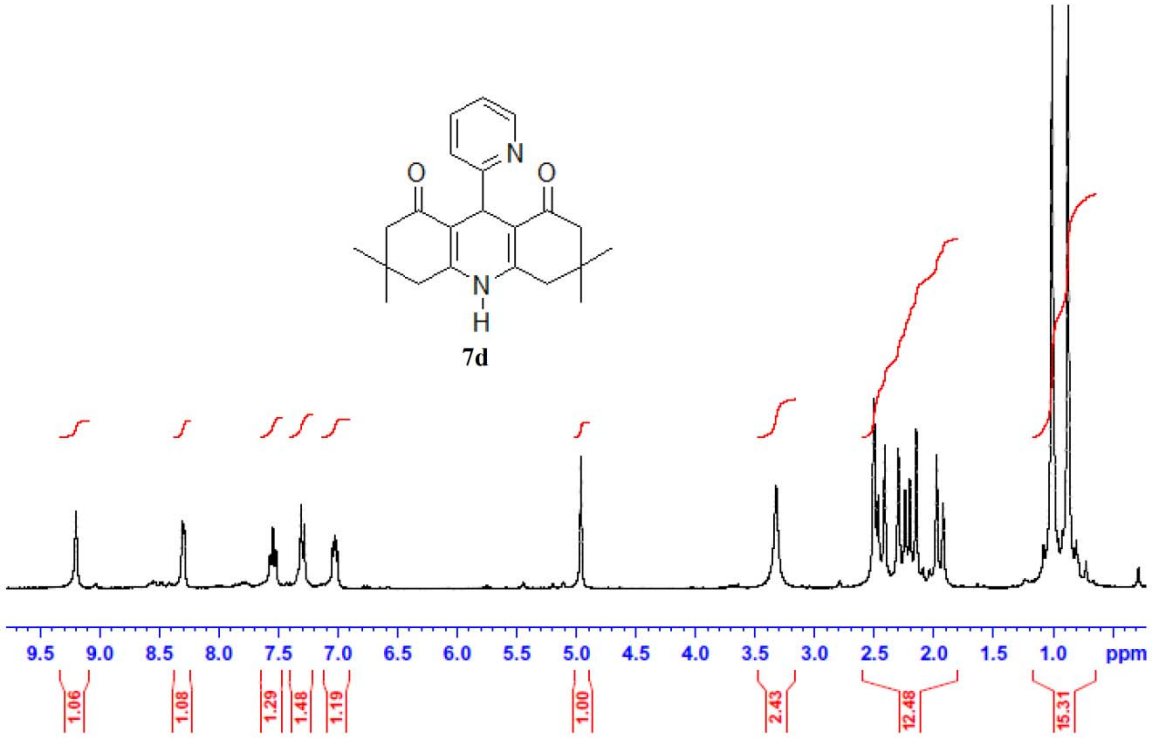
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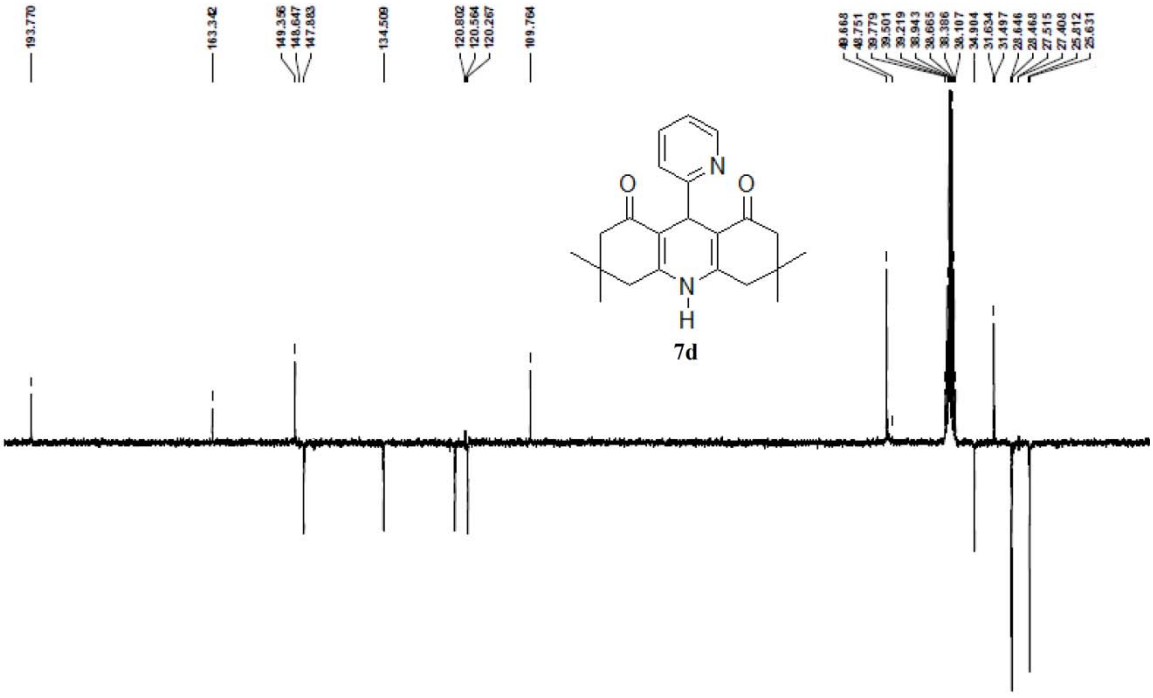
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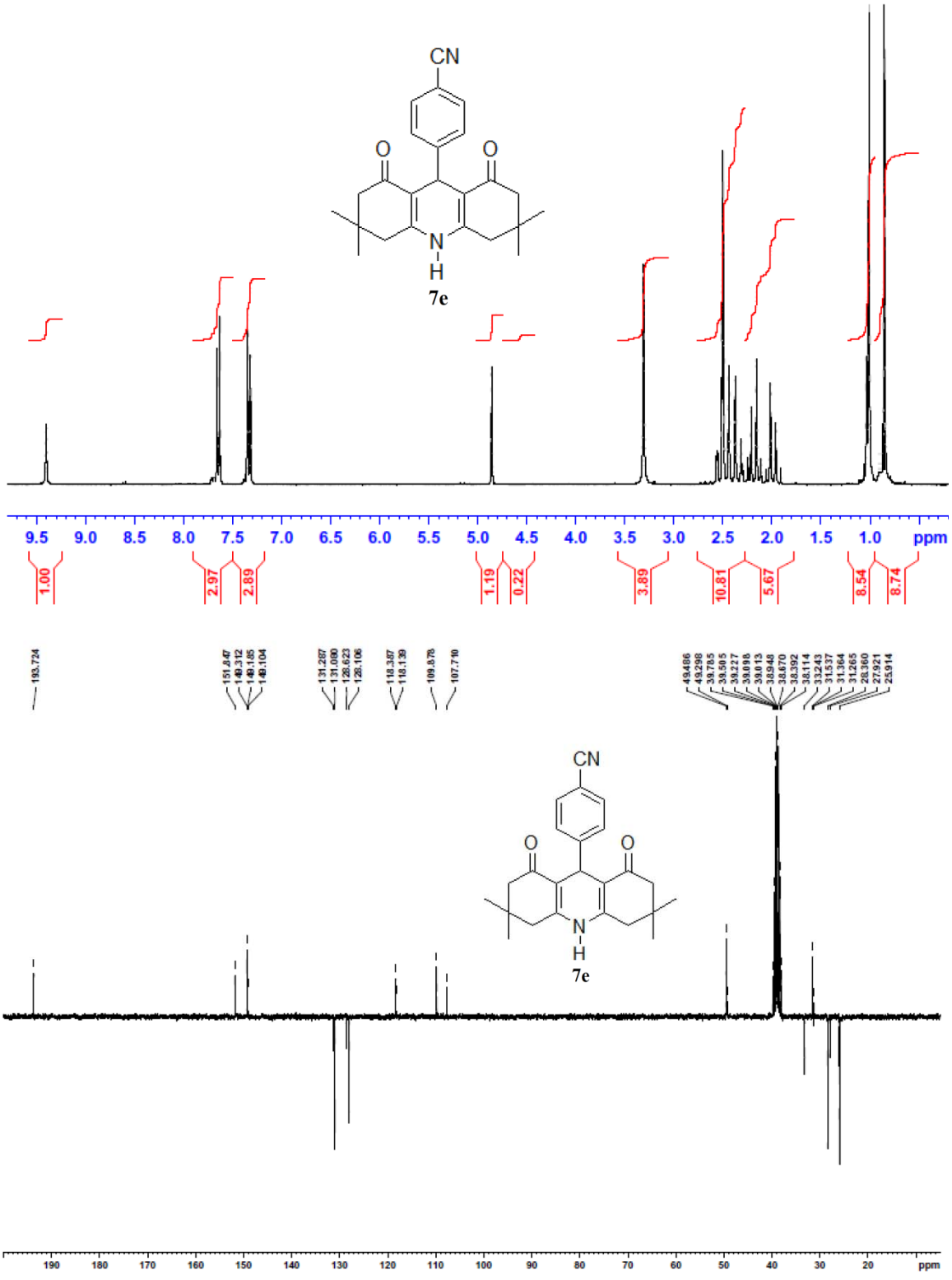

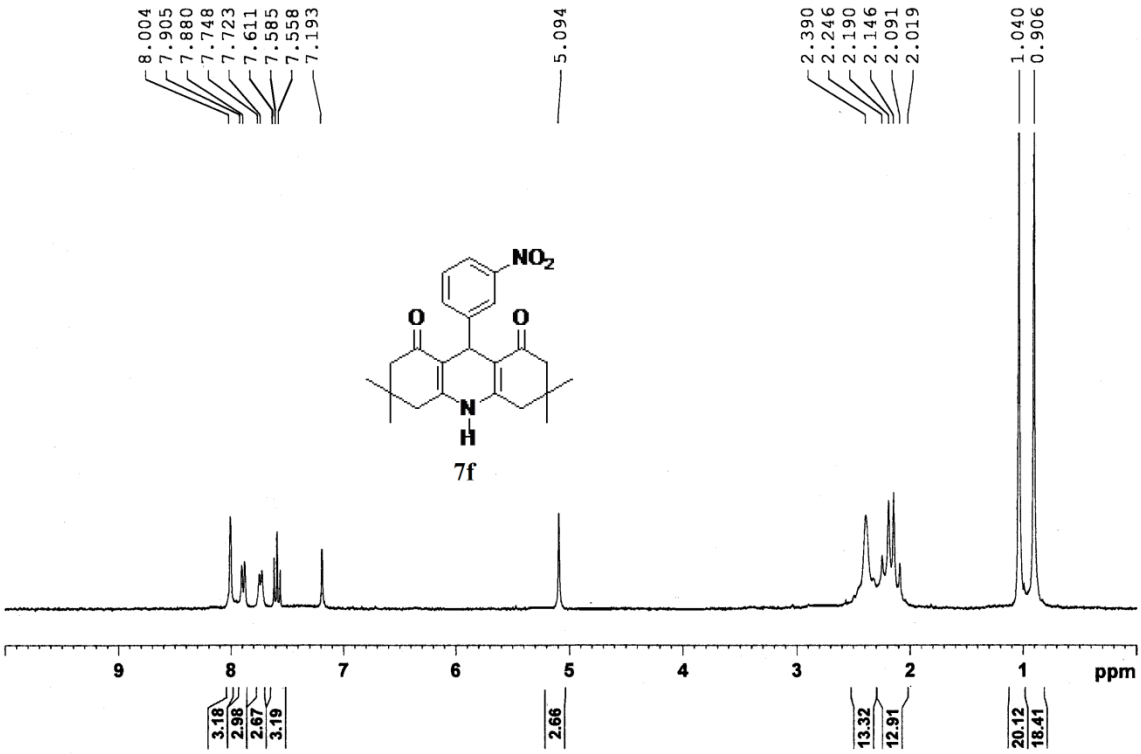

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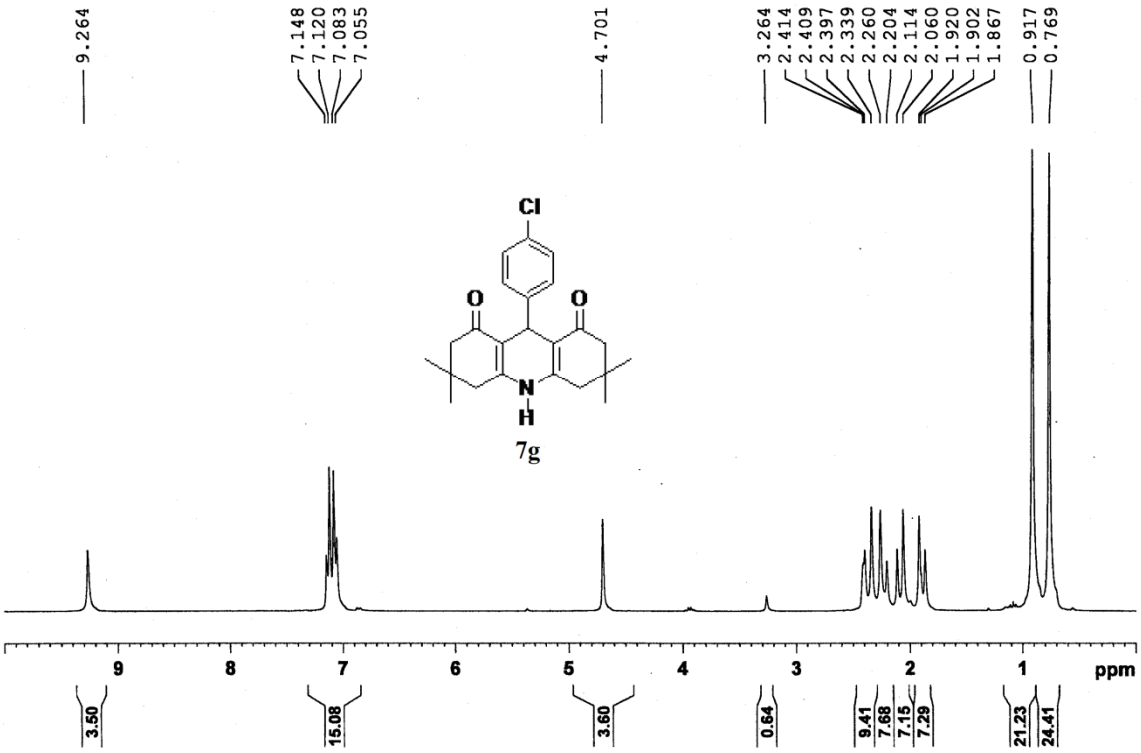
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N
H
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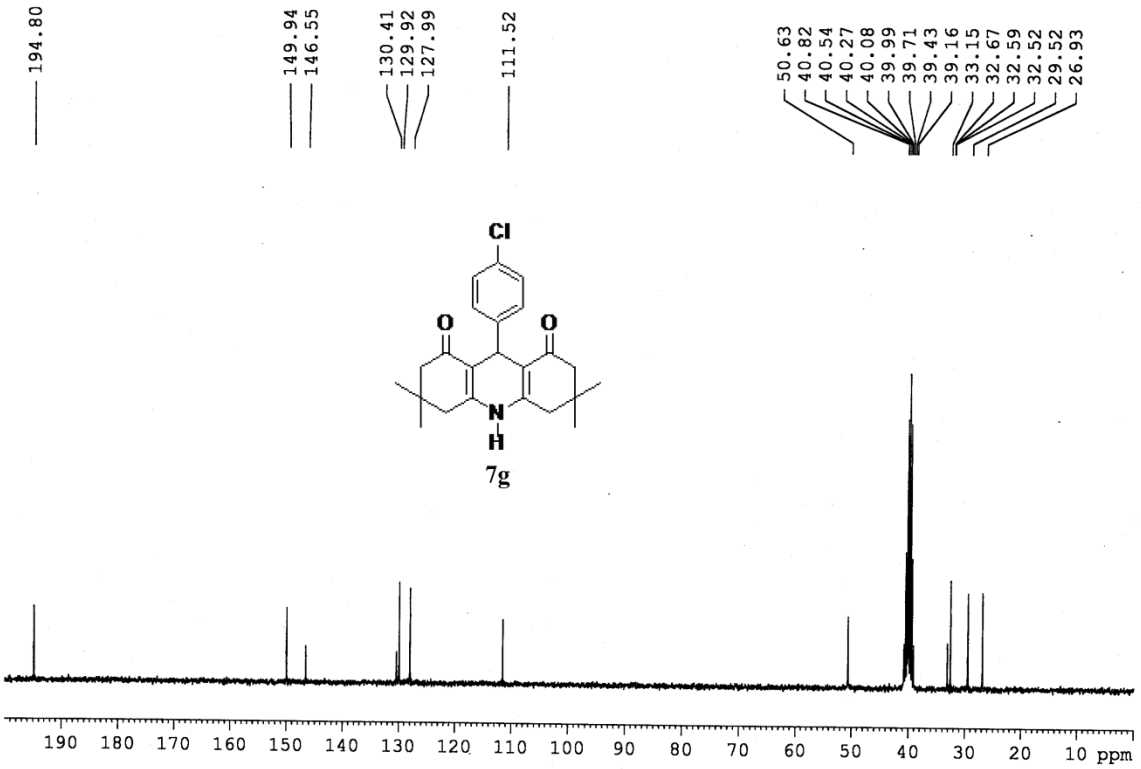
7g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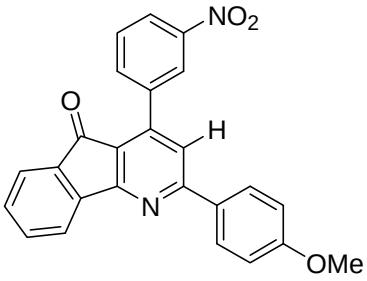
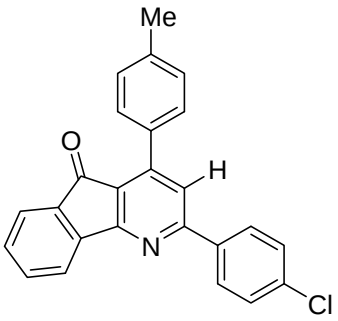
7g

Spectroscopic characterization for 14a-14i



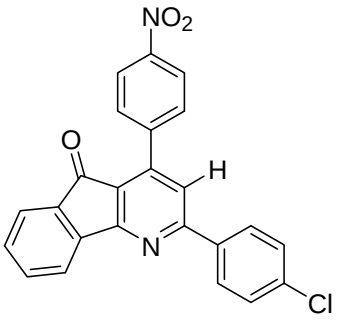
2-(4-methoxyphenyl)-4-(3-nitrophenyl)-5H-indeno[1,2-b]pyridin-5-one (14a):

Yellowish green solid, mp 234-236 °C; IR ν_{max} (KBr) 3432, 2375, 1705, 1551, and 1346 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 8.54 (1H, s, arom), 8.35 (1H, d, J = 7.2 Hz), 8.24-8.19 (2H, m, arom), 8.04 (2H, d, J = 9.0 Hz, arom), 7.79 (1H, s, arom), 7.72-7.66 (4H, m, arom), 7.53 (1H, s, arom), 7.05 (2H, d, J = 9.8 Hz), 3.91 (3H, s, $-OCH_3$); ^{13}C NMR (75 MHz, $CDCl_3$) δ: 190.8, 166.6, 161.8, 161.4, 148.2, 146.5, 137.1, 135.4, 135.3, 135.0, 131.2, 130.4, 129.0, 124.1, 124.0, 123.8, 121.8, 121.1, 119.4, 114.4; Anal. Calcd for $C_{25}H_{16}N_2O_4$: C, 73.52; H, 3.95; N, 6.86. Found C, 73.81; H, 3.87; N, 7.01.



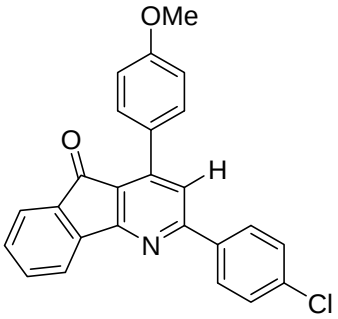
2-(4-chlorophenyl)-4-p-tolyl-5H-indeno[1,2-b]pyridin-5-one (14b):

Yellowish green solid, mp 188-190 °C; IR ν_{max} (KBr) 3423, 3054, 2370, 1712, 1560, and 1363 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 8.12 (2H, d, J = 8.4 Hz), 7.98 (1H, t, J = 8.4 Hz, arom), 7.78-7.45 (6H, m, arom), 7.35-7.31 (2H, m, arom), 7.26 (1H, s, arom), 2.46 (3H, m, $-CH_3$); Anal. Calcd for $C_{25}H_{16}ClNOC$, 78.63; H, 4.22; N, 3.67. Found C, 78.82; H, 4.30; N, 3.87.



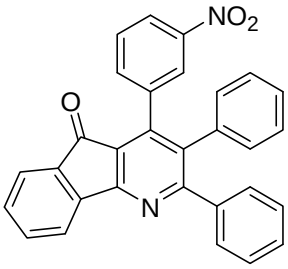
2-(4-chlorophenyl)-4-(4-nitrophenyl)-5H-indeno[1,2-b]pyridin-5-one (14c):

Yellow solid, mp 214-216 °C; IR ν_{max} (KBr) 3434, 1718, 1582, and 1512 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 8.40-8.36 (2H, m, arom), 8.14 (2H, d, J = 8.4 Hz), 7.90-7.80 (3H, m, arom), 7.72-7.60 (2H, m, arom), 7.52-7.48 (4H, m, arom), 7.72-7.66 (4H, m, arom), 7.53 (1H, s, arom), 7.05 (2H, d, J = 9.8 Hz); ^{13}C NMR (75 MHz, $CDCl_3$) δ: 191.1, 160.40, 156.9, 146.9, 142.7, 141.6, 137.2, 136.8, 136.2, 135.8, 135.3, 131.5, 130.1, 129.2, 129.1, 129.0, 128.7, 128.4, 128.2, 124.4, 124.0, 123.5, 121.2, 120.2, 116.9; Anal. Calcd for $C_{24}H_{13}ClN_2O_3$: C, 69.83; H, 3.17; N, 6.79. Found C, 69.61; H, 3.20; N, 6.91.



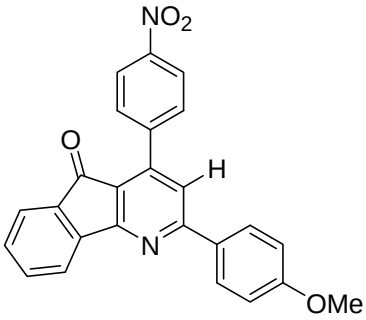
2-(4-chlorophenyl)-4-(4-methoxyphenyl)-5H-indeno[1,2-b]pyridin-5-one (14d):

Yellow solid, mp 204-206 °C; IR ν_{max} (KBr) 3434, 1710, 1581 and 1512 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 8.12 (2H, d, J = 8.7 Hz, arom), 8.02 (2H, d, J = 8.7 Hz), 7.75-7.68 (4H, m, arom), 7.59-7.43 (3H, m, arom), 7.07-7.02 (2H, m, arom), 3.92-3.90 (3H, s, $-OCH_3$); ^{13}C NMR (75 MHz, $CDCl_3$) δ: 189.6, 160.1, 157.8, 154.6, 148.7, 148.3, 141.5, 136.9, 135.8, 134.7, 134.5, 134.4, 133.5, 130.9, 130.6, 128.9, 128.6, 128.3, 128.1, 126.3, 122.9, 121.5, 120.2, 120.0, 115.6, 113.9, 112.9, 54.8; Anal. Calcd for $C_{25}H_{16}ClNO_2$: C, 79.17; H, 5.96; N, 3.18. Found C, 79.40; H, 5.91; N, 3.31.



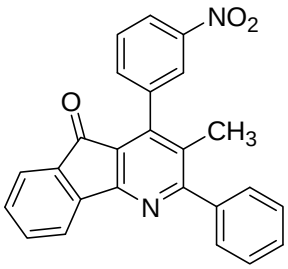
4-(3-nitrophenyl)-2,3-diphenyl-5H-indeno[1,2-b]pyridin-5-one (14e):

Dirty green solid, mp 228-230 °C; IR ν_{max} (KBr) 3421, 1715, 1569, 1518, and 1346 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$) δ: 8.15-8.09 (1H, m, arom), 8.02-8.00 (2H, m, arom), 7.67-7.60 (4H, m, arom), 7.47-7.37 (5H, m, arom), 7.28-7.19 (3H, m, arom), 7.06-7.05 (3H, m, arom), 6.84 (2H, br s, arom); Anal. Calcd for $C_{30}H_{18}N_2O_3$: C, 79.28; H, 3.99; N, 6.16. Found C, 79.40; H, 3.92; N, 6.31.



2-(4-methoxyphenyl)-4-(4-nitrophenyl)-5H-indeno[1,2-b]pyridin-5-one (14f):

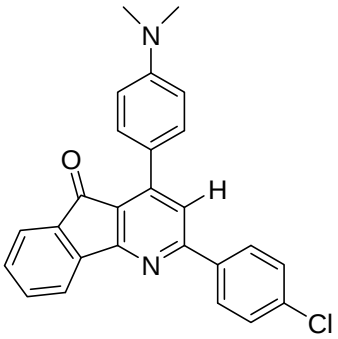
Brown solid, mp 254-256 °C; IR ν_{max} (KBr) 3432, 1712, 1582 and 1502 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$) δ: 8.29-8.27 (4H, m, arom), 7.97-7.52 (7H, m, arom), 7.05 (2H, br s, arom), 3.82-3.80 (3H, s, $-OCH_3$); Anal. Calcd for $C_{25}H_{16}N_2O_4$: C, 73.52; H, 3.95; N, 6.86. Found C, 73.29; H, 3.91; N, 6.98.



3-methyl-4-(3-nitrophenyl)-2-phenyl-5H-indeno[1,2-b]pyridin-5-one (14g):

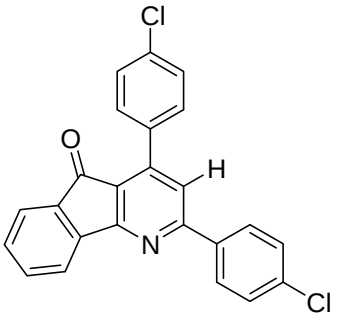
Dirty green solid, mp 214-216 °C; IR ν_{max} (KBr) 3412, 1709, 1571, 1527, and 1365 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$) δ: 8.29 (1H, d, J = 6.3 Hz, arom), 8.15 (1H, br s, arom), 7.86 (1H, d, J = 7.5 Hz, arom), 7.67-7.31 (9H, m, arom), 7.20-7.19 (1H, m, arom), 2.03 (3H, s, $-CH_3$); ^{13}C NMR (75 MHz, $CDCl_3$) δ: 191.1,

164.1, 148.3, 142.9, 140.2, 136.6, 135.2, 135.1, 134.7, 130.9, 129.4, 129.1, 129.0, 128.9, 128.4, 123.9, 123.7, 123.4, 121.1, 17.6; Anal. Calcd for $C_{25}H_{16}N_2O_3$: C, 76.52; H, 4.11; N, 7.14. Found C, 76.55; H, 4.10; N, 7.19.



2-(4-chlorophenyl)-4-(4-(dimethylamino)phenyl)-5H-indeno[1,2-b]pyridin-5-one (14h):

Red solid, mp 264-266 °C; IR ν_{max} (KBr) 3408, 1704, 1571, 1527, and 1366 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$) δ: 8.01 (2H, d, J = 8.7 Hz, arom), 7.86 (1H, d, J = 7.2 Hz, arom), 7.71 (1H, t, J = 6.6 Hz, arom), 7.63-7.50 (3H, m, arom), 7.43-7.34 (4H, m, arom), 6.71 (2H, d, J = 8.7 Hz, arom), 3.01-2.97 (6H, m, -2xNC$\underline{H}_3$); ^{13}C NMR (75 MHz, $CDCl_3$) δ: 191.2, 166.7, 159.0, 152.4, 152.2, 151.5, 150.0, 142.9, 137.1, 135.9, 135.6, 134.8, 134.5, 132.3, 132.2, 131.8, 130.8, 130.5, 128.9, 128.8, 128.6, 128.3, 127.7, 123.6, 123.4, 122.3, 122.1, 121.9, 120.7, 120.2, 111.4, 110.8, 40.2; Anal. Calcd for $C_{26}H_{19}ClN_2O$: C, 76.00; H, 4.66; N, 6.82. Found C, 76.24; H, 4.68; N, 6.91.

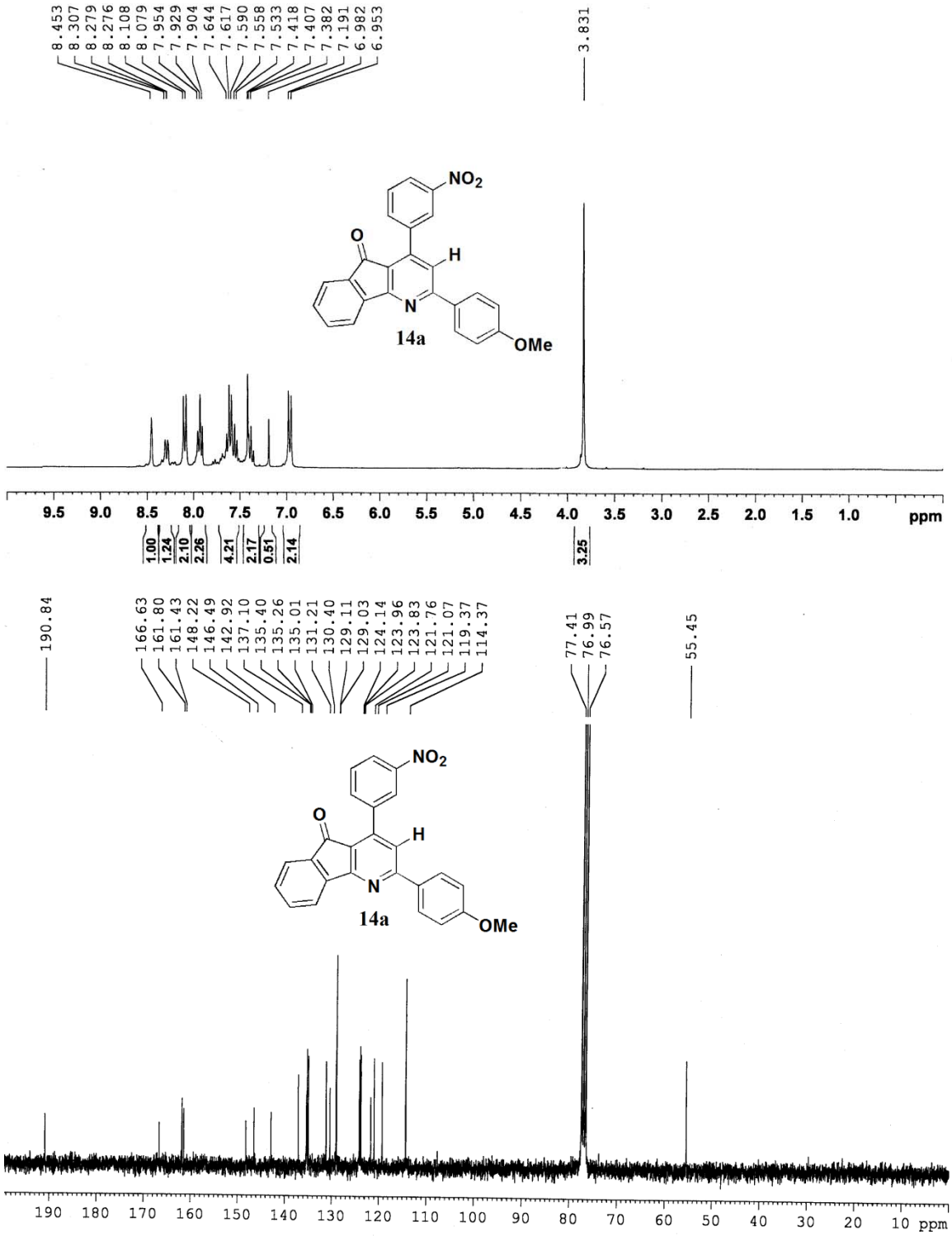


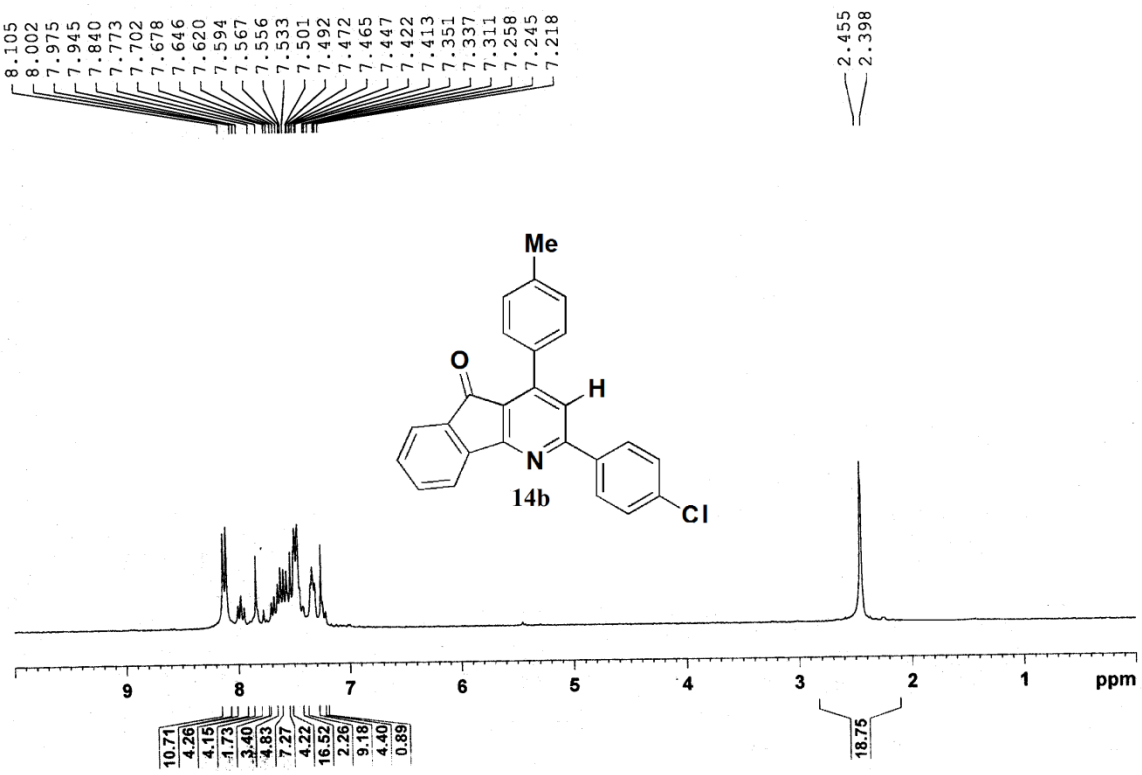
2,4-bis(4-chlorophenyl)-5H-indeno[1,2-b]pyridin-5-one (14i):

Yellowish green solid, mp 180-182 °C; IR ν_{max} (KBr) 3412, 1709, 1572, 1527, and 1365 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$) δ: 8.11 (2H, d, J = 7.8 Hz, arom), 7.97 (1H, d, J = 7.5 Hz, arom), 7.70-7.55 (4H, m, arom), 7.50-7.43 (6H, m, arom); ^{13}C NMR (75 MHz, $CDCl_3$) δ: 190.8, 166.6, 159.9, 148.3, 142.8, 136.5, 135.9, 135.4, 135.0, 133.6, 131.2, 130.4, 129.4, 129.1, 128.9, 128.7, 128.5, 128.4, 128.3, 128.1, 123.8,

122.6, 121.0, 120.5, 116.7; Anal. Calcd for $C_{24}H_{13}Cl_2NO$: C, 71.66; H, 3.26; N, 3.48. Found C, 71.88; H, 3.31; N, 3.61.

1H NMR and 13C NMR spectra for 14a-14i

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7.945
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7.620
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7.556
7.533
7.501
7.492
7.472
7.465
7.447
7.422
7.413
7.351
7.337
7.311
7.258
7.245
7.218
2.455
2.398
Me
O
H
N
14b
Cl
9
8
7
6
5
4
3
2
1
ppm
10.71
4.26
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3.40
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16.52
2.26
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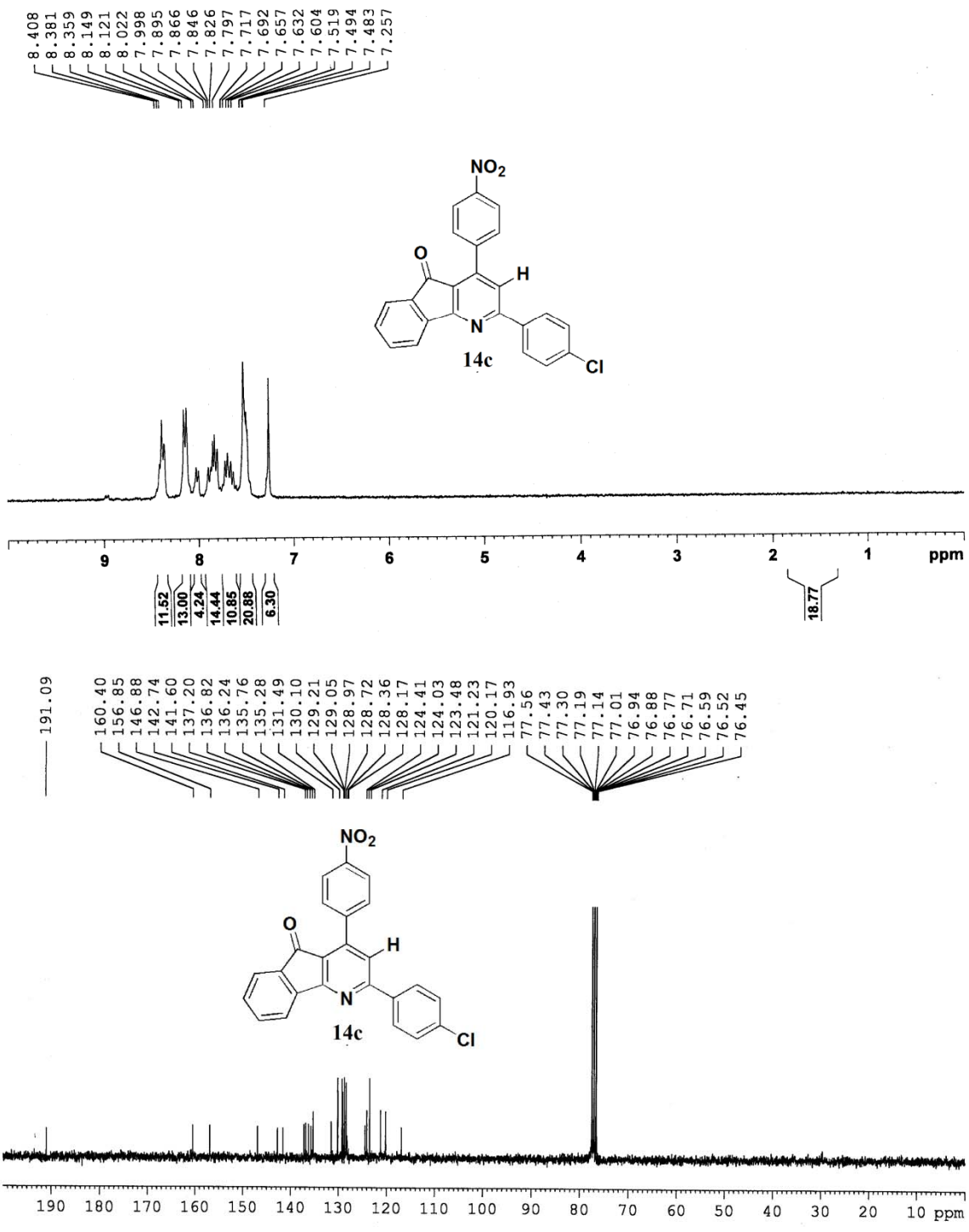
18.75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7.895
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7.846
7.826
7.797
7.717
7.692
7.657
7.632
7.604
7.519
7.494
7.483
7.257
NO2
O
H
N
Cl
14c
9
8
7
6
5
4
3
2
1
ppm
11.52
13.00
4.24
14.44
10.85
20.88
6.30
18.77
191.09
160.40
156.85
146.88
142.74
141.60
137.20
136.82
136.24
135.76
135.28
131.49
130.10
129.21
129.05
128.97
128.72
128.36
128.17
124.41
124.03
123.48
121.23
120.17
116.93
77.56
77.43
77.30
77.19
77.14
77.01
76.94
76.88
76.77
76.71
76.59
76.52
76.45
190
180
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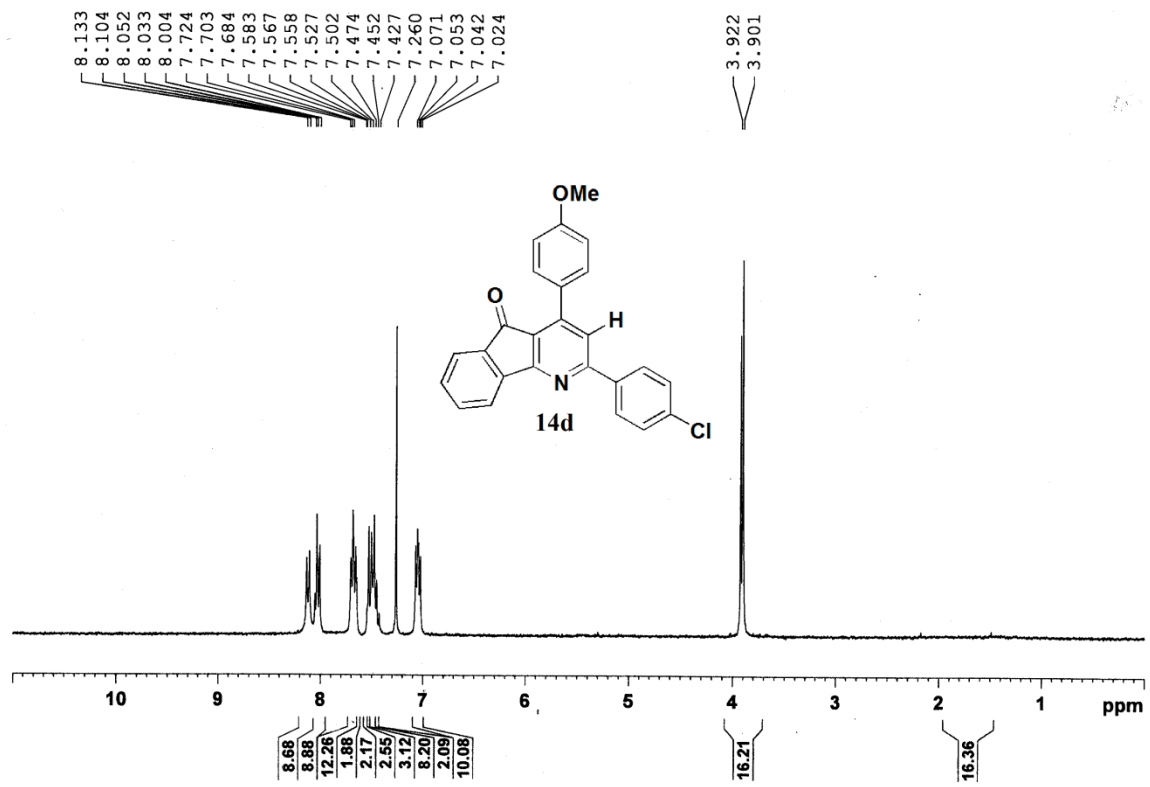
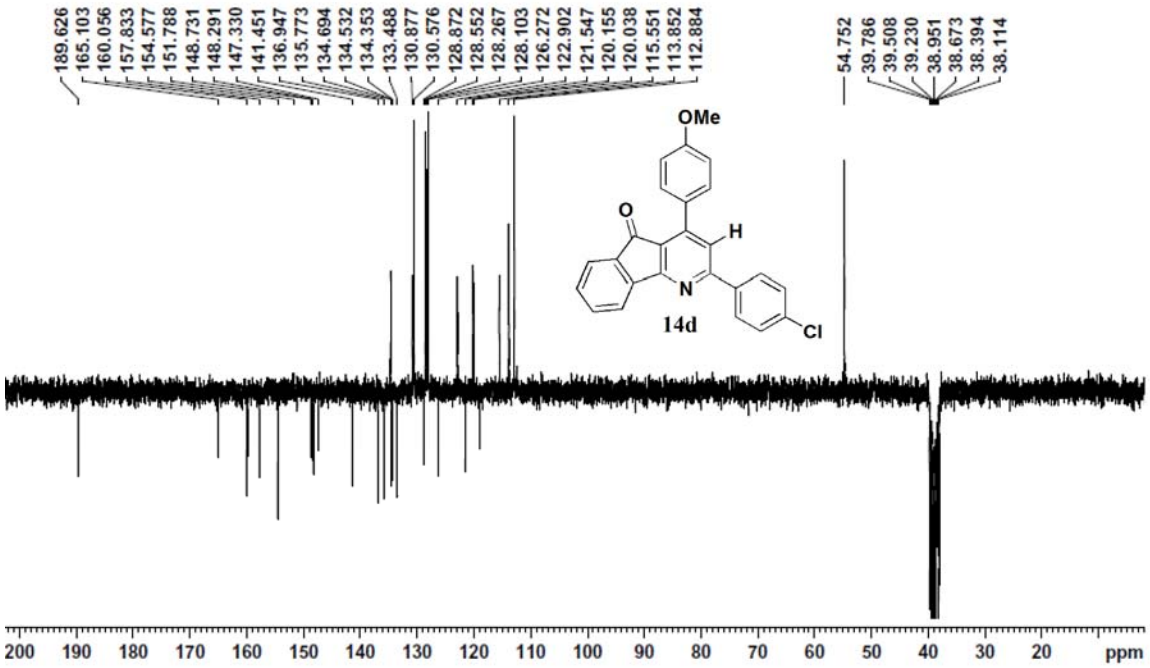
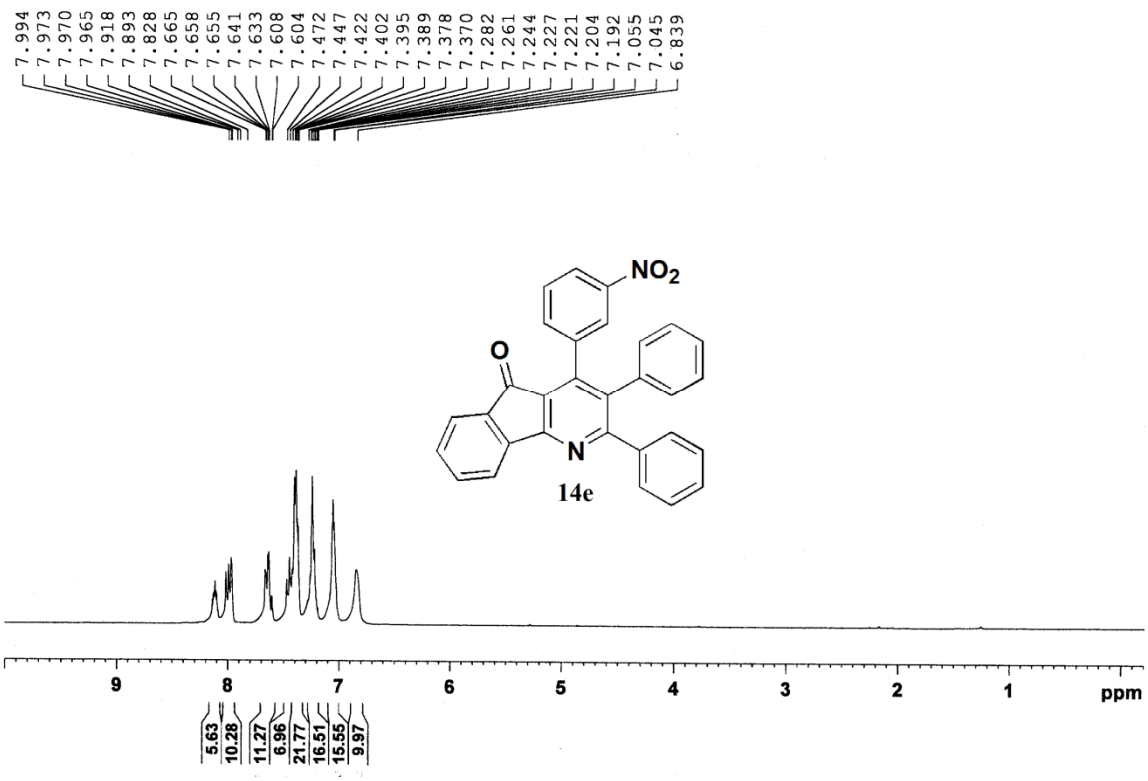
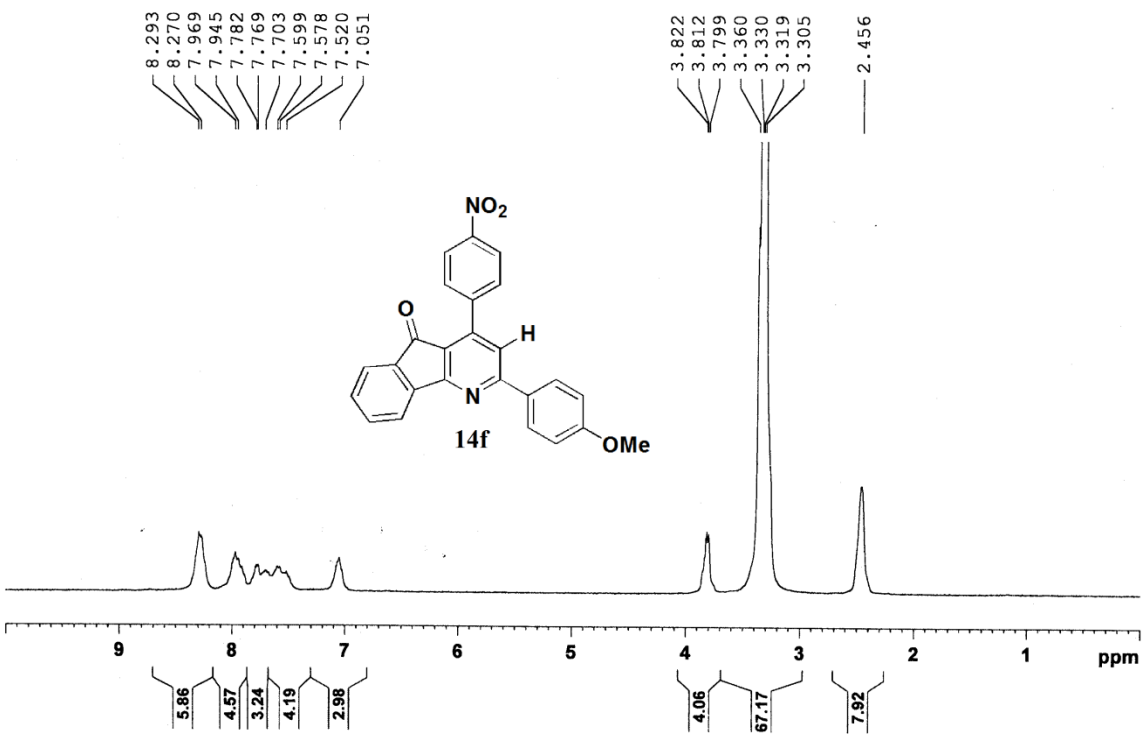
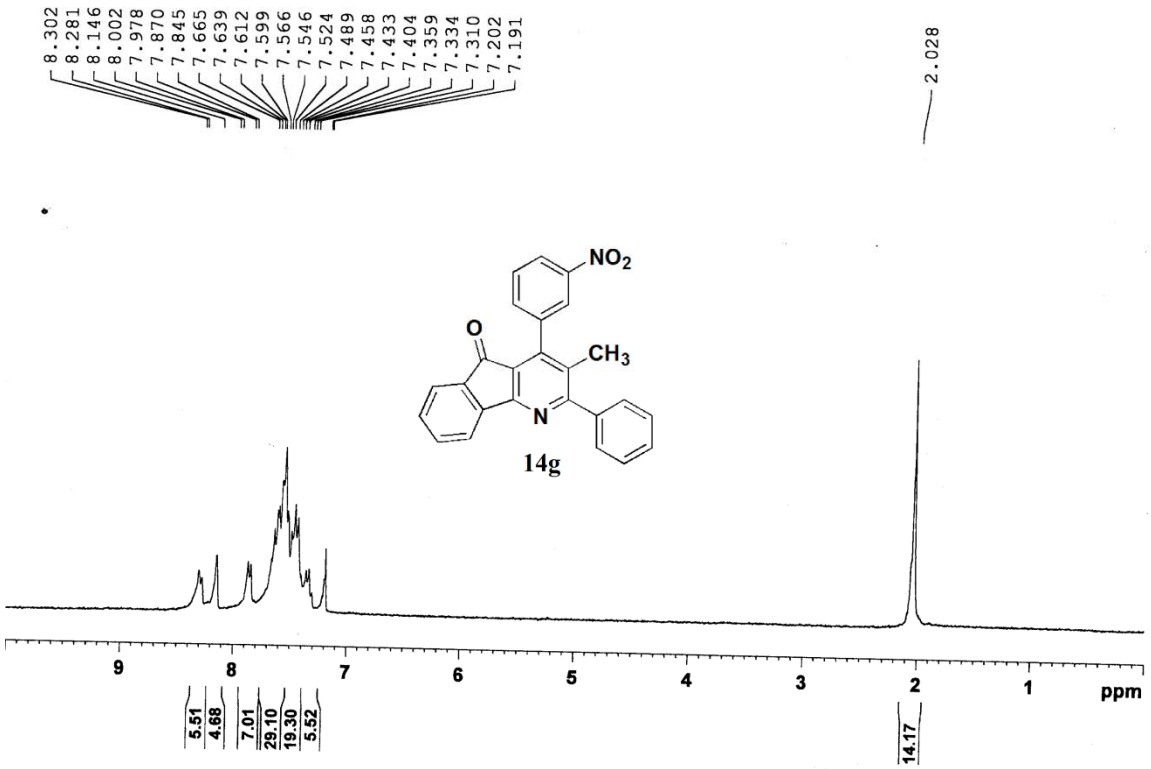
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm







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7.665
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7.546
7.524
7.489
7.458
7.433
7.404
7.359
7.334
7.310
7.202
7.191
2.028
NO2
O
CH3
N
14g
9
8
7
6
5
4
3
2
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ppm
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7.01
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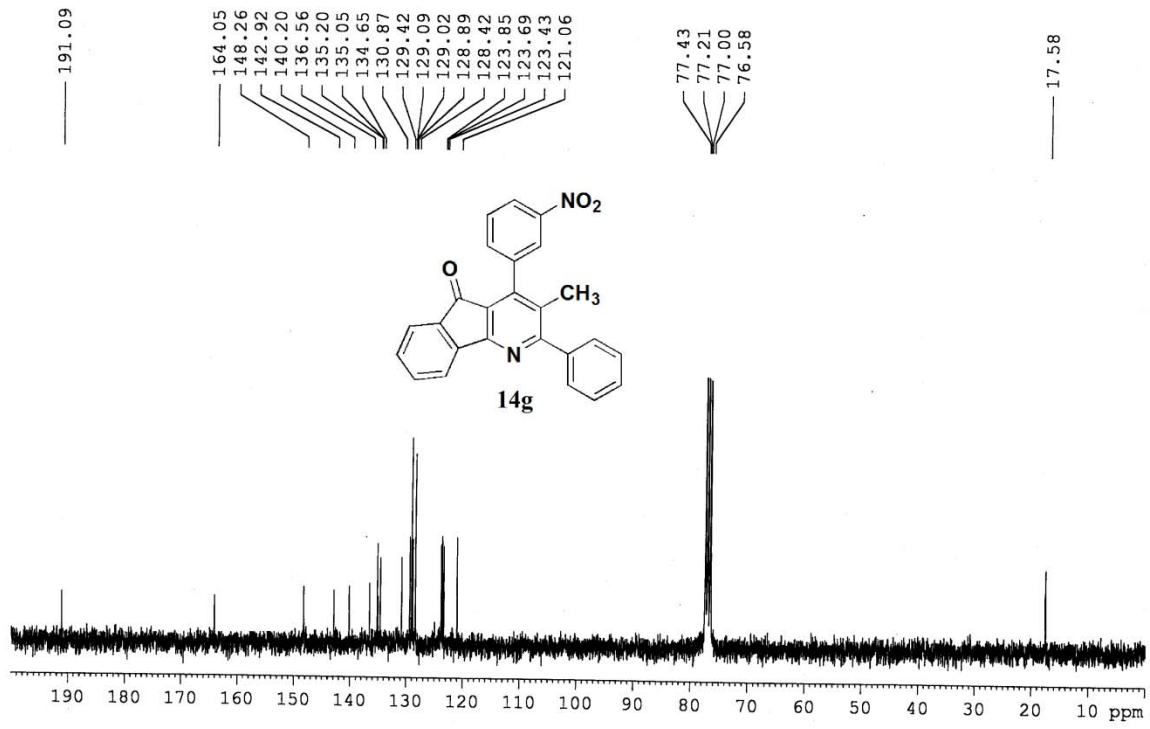
19.30
5.52
14.17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136.56
135.20
135.05
134.65
130.87
129.42
129.09
129.02
128.89
128.42
123.85
123.69
123.43
121.06
77.43
77.21
77.00
76.58
17.58
NO2
O
CH3
N
14g
190
180
170
160
150
140
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120
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100
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80
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60
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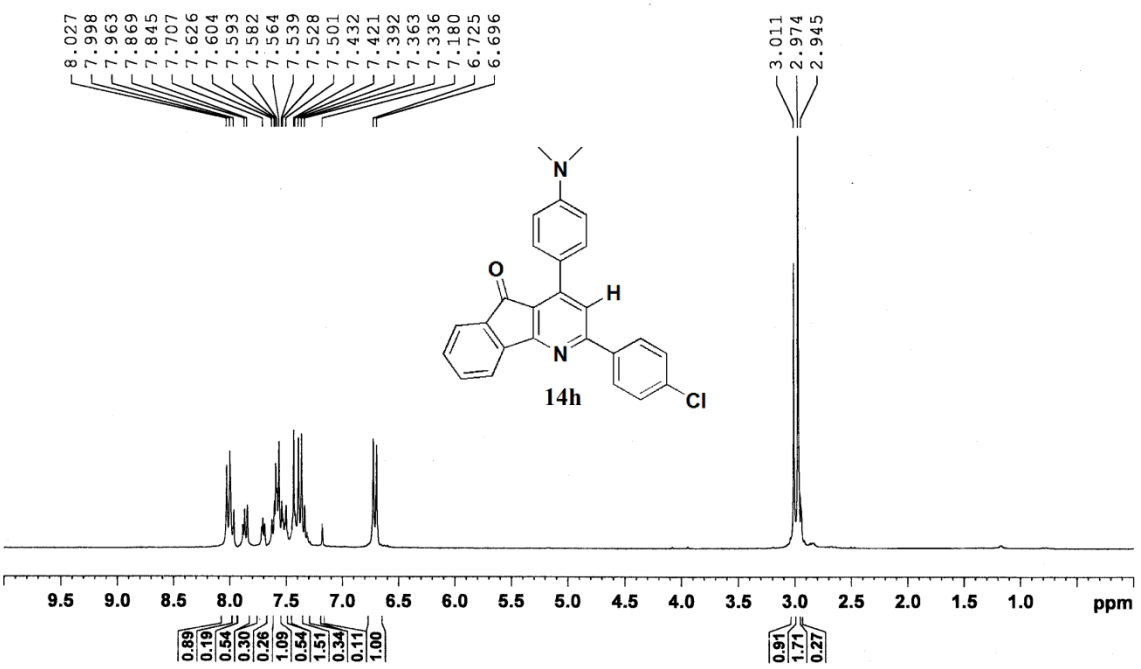
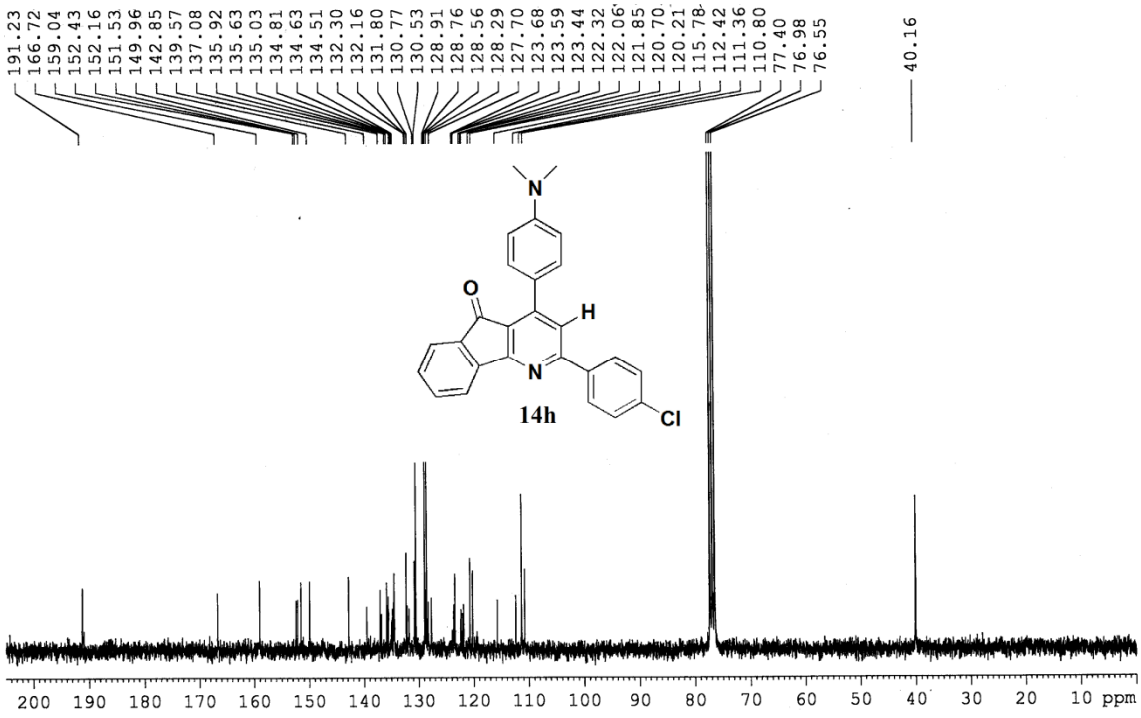
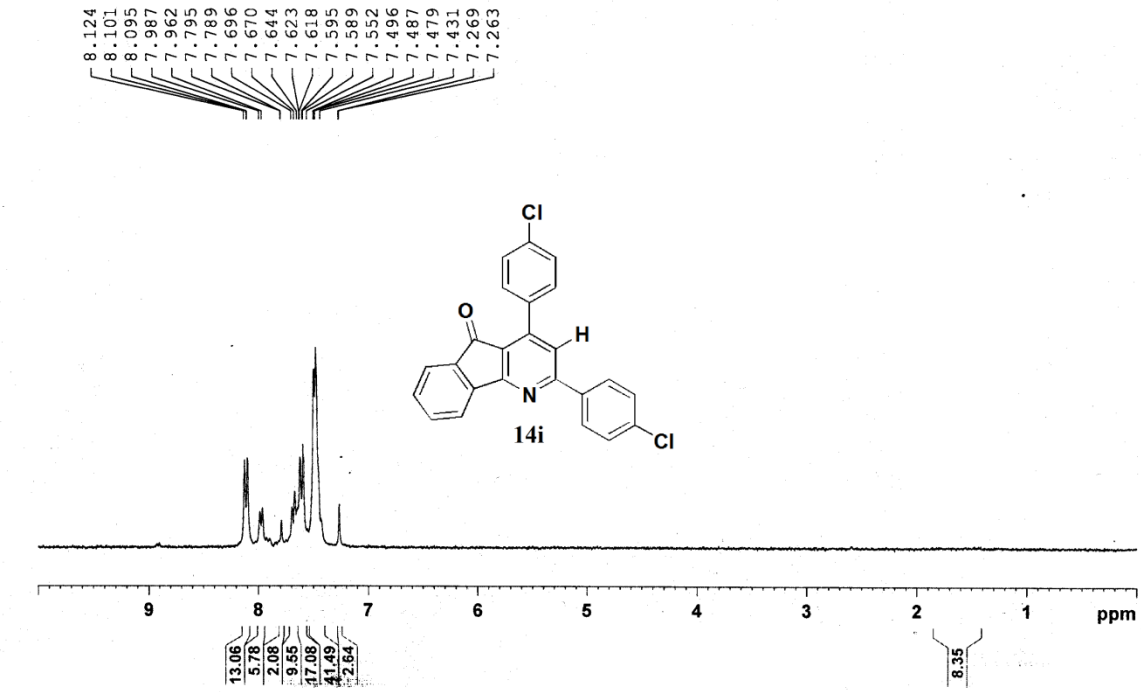
40
30
20
10 ppm



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7.789
7.696
7.670
7.644
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7.618
7.595
7.589
7.552
7.496
7.487
7.479
7.431
7.269
7.263
Cl
O
H
N
Cl
14i
9
8
7
6
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4
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2
1
ppm
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9.55
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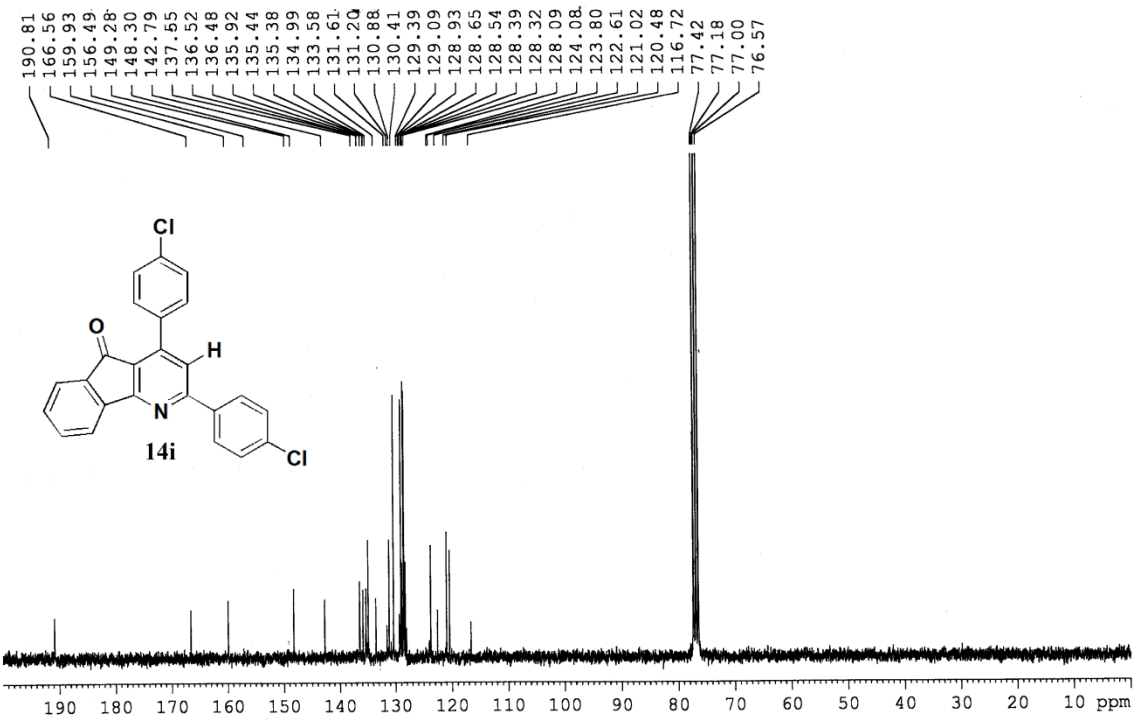
8.35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137.55
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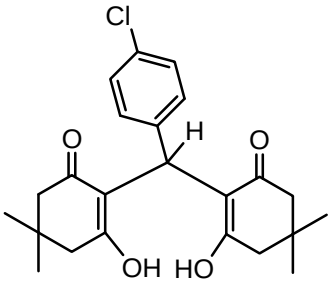
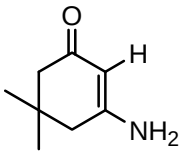
135.92
135.44
135.38
134.99
133.58
131.61
131.20
130.88
130.41
129.39
129.09
128.93
128.65
128.54
128.39
128.32
128.09
124.08
123.80
122.61
121.02
120.48
116.72
77.42
77.18
77.00
76.57
Cl
O
H
N
14i
Cl
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

Spectroscopic characterization for 8b, 9, 10



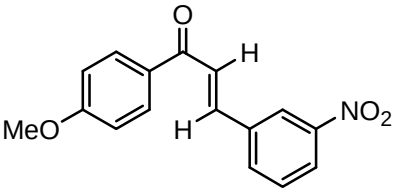
2-((4-chlorophenyl)(2-hydroxy-4,4-dimethyl-6-oxocyclohex-1-enyl)methyl)-3-hydroxy-5,5-dimethylcyclohex-2-enone (**8b**):

White solid, mp 140-142 °C; IR ν_{max} (KBr) 3061, 2950, 2875, 1600, 1490, 1370, 1300, and 1250 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 11.88 (2H, s), 7.23 (2H, d, J = 8.7 Hz), 7.01 (2H, d, J = 8.4 Hz), 5.47 (1H, s), 2.49-2.28 (8H, m), 1.22 (6H, s), 0.99 (6H, s). ^{13}C NMR (75 MHz, $CDCl_3$) δ: 190.6, 189.4, 136.7, 131.6, 128.4, 128.2, 115.3, 47.1, 46.4, 32.4, 31.4, 29.6 and 27.4; Anal. Calcd for $C_{23}H_{27}ClO_4$: C, 68.56; H, 6.75. Found C, 68.70; H, 6.68.



3-amino-5,5-dimethylcyclohex-2-enone (**9**):

White solid, mp 128-130 °C (CH_2Cl_2 + EtOAc, equal volumes); ^{1}H NMR (300 MHz, DMSO-D_6) δ: 6.61 (2H, br s), 4.81 (1H, s), 2.02 (2H, s), 1.81 (2H, s), 0.86 (6H, s); ^{13}C NMR (75 MHz, DMSO-D_6) δ: 194.0, 165.5, 96.0, 50.0, 41.7, 32.3, 28.2; Anal. Calcd for $C_8H_{13}NO$: C, 69.03; H, 9.41; N, 10.06. Found C, 69.31; H, 9.50; N, 10.21.

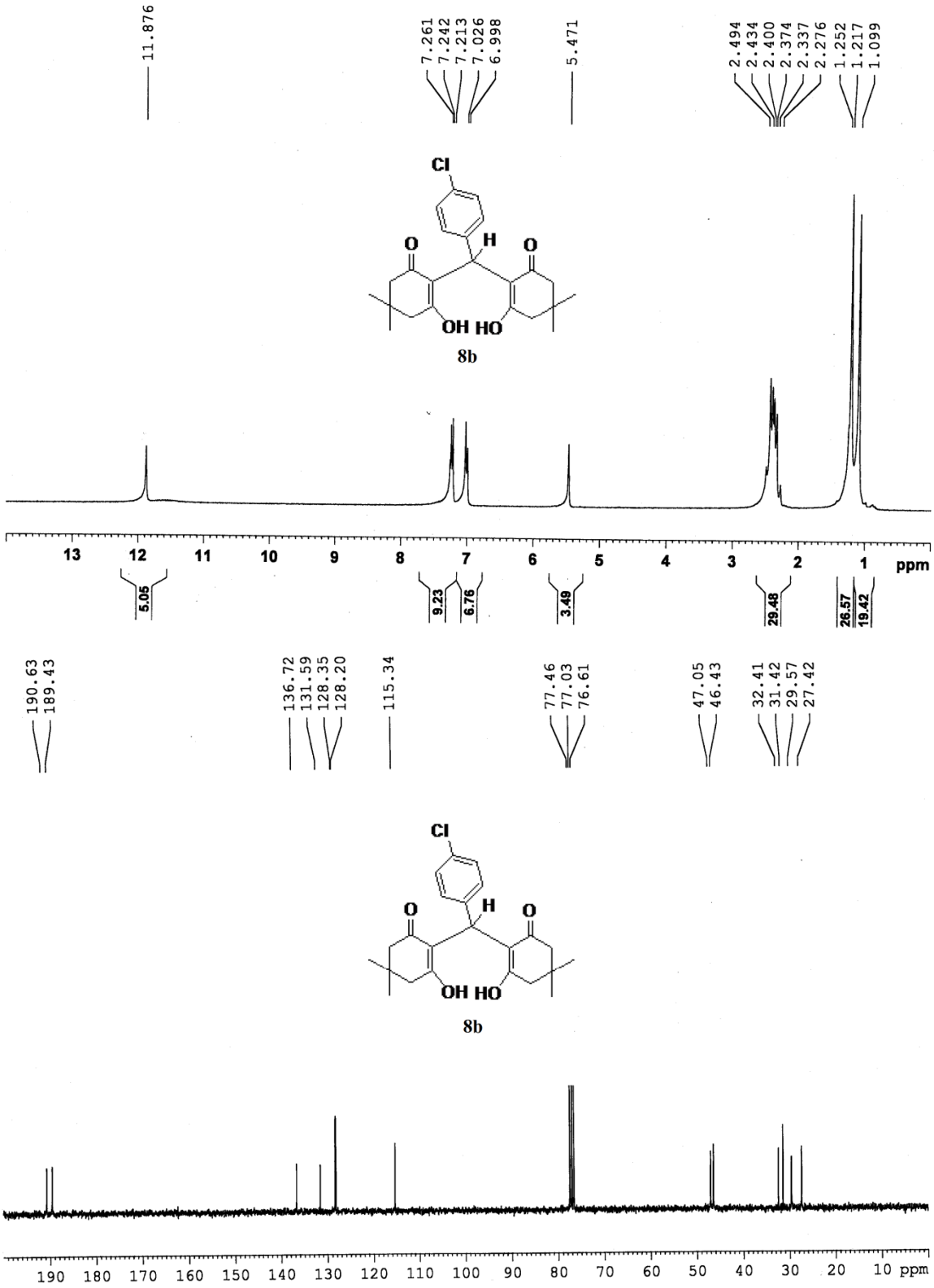


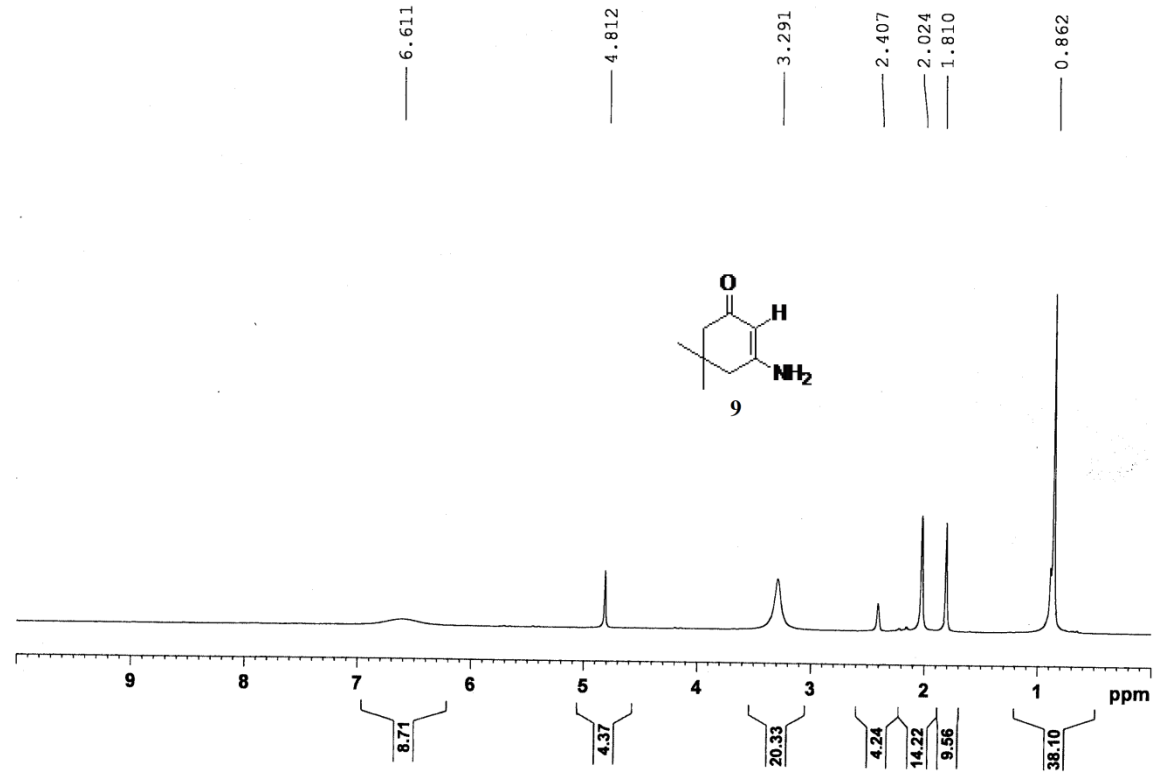
1-(4-methoxyphenyl)-3-(3-nitrophenyl)prop-2-en-1-one (**10**):

White solid, mp 128-130 °C (CH_2Cl_2 + EtOAc, equal volumes); ^{1}H NMR (300 MHz, DMSO-D_6) δ: 8.73 (1H, s), 8.30 (1H, d, J = 7.8 Hz), 8.24-8.11 (4H, m), 7.81-7.69 (2H, m), 7.08 (2H, d, J = 8.7 Hz), 3.86 (3H, s); ^{13}C NMR (75 MHz, DMSO-D_6) δ: 187.2, 163.5, 148.5, 141.7, 136.8, 134.1, 132.2, 131.4, 130.2, 129.3,

125.8, 124.3, 122.4, 121.7, 115.2, 113.1, 55.2; Anal. Calcd for $C_{16}H_{13}NO_4$: C, 67.84; H, 4.63; N, 4.94. Found C, 68.01; H, 4.69; N, 4.78.

1H NMR and 13C NMR spectra for 8b, 9, 10

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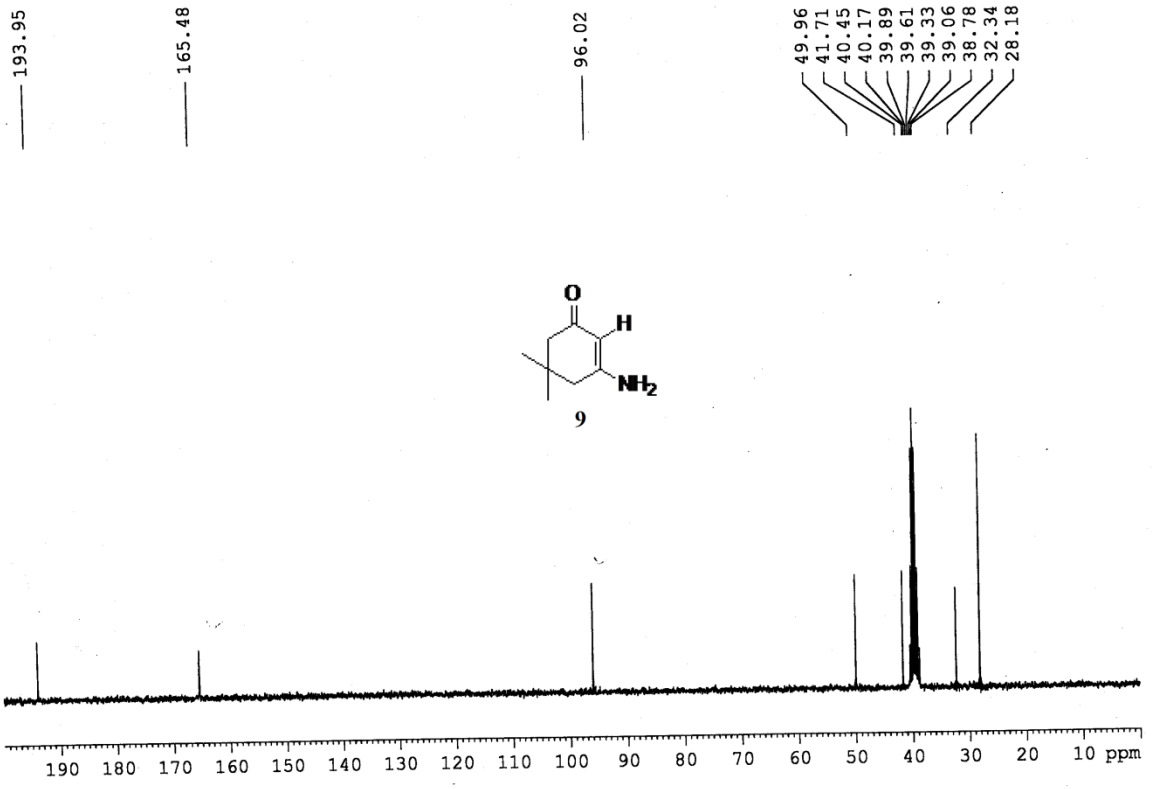
2.407
2.024
1.810
0.862
O
H
NH2
9
9 8 7 6 5 4 3 2 1 ppm
8.71
4.37
20.33
4.24
14.22
9.56
38.10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165.48
96.02
49.96
41.71
40.45
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39.89
39.61
39.33
39.06
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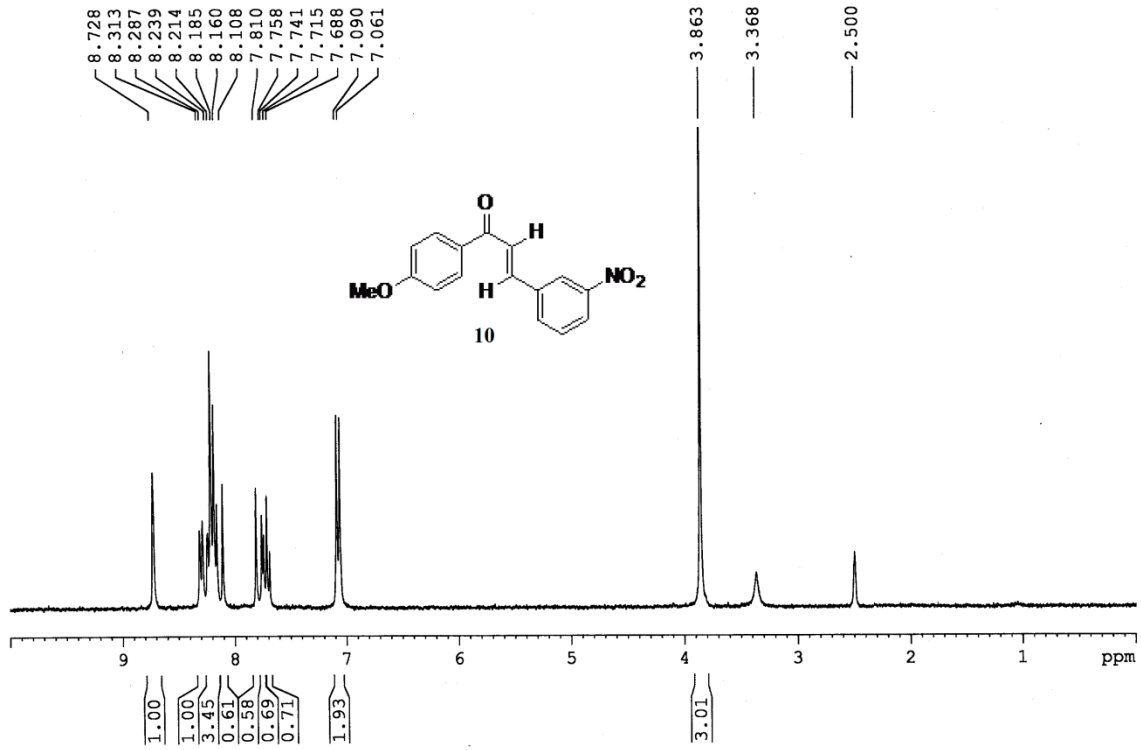
32.34
28.18
O
H
NH2
9
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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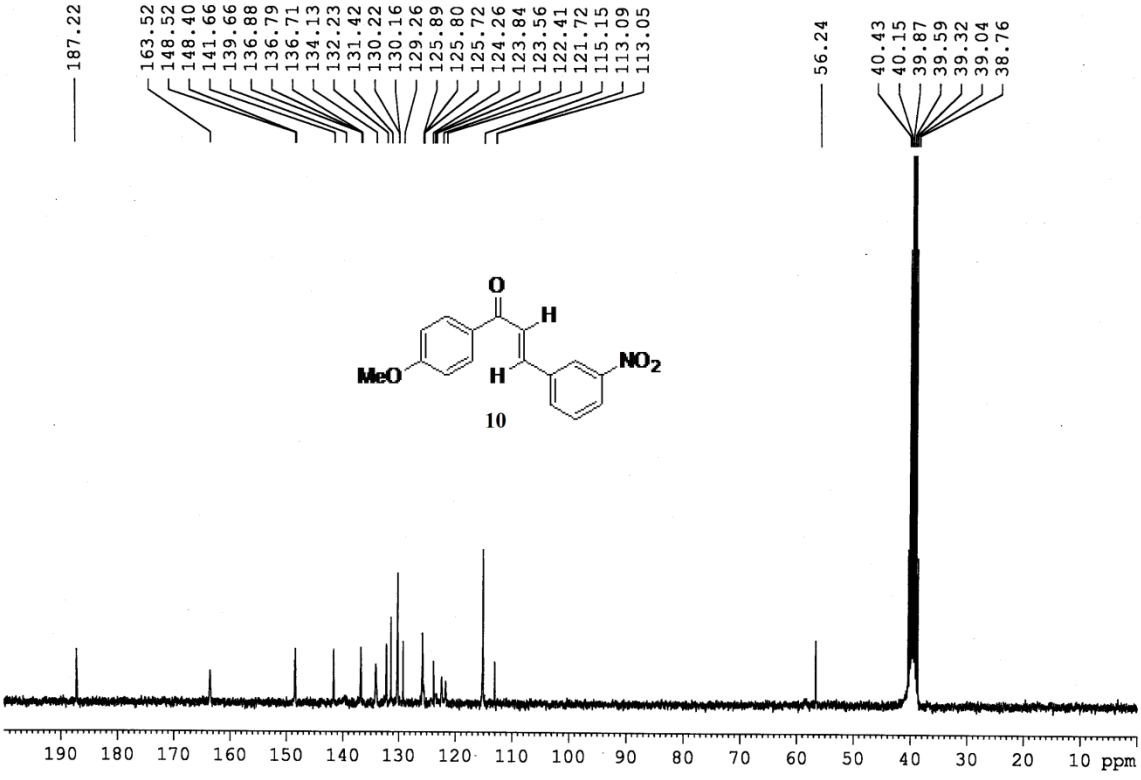
MeO
NO2
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.00
3.45
0.61
0.58
0.69
0.71
1.93
3.01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129.26
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125.80
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124.26
123.84
123.56
122.41
121.72
115.15
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113.05
56.24
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40.15
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39.32
39.04
38.76
MeO
NO2
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190
180
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160
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140
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80
70
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50
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30
20
10 ppm