Supporting Information

In Situ Generation of Functionality in a Reactive Binicotinic-Acid-Based Ligand for the Design of Multi-Functional Copper (II) Complexes: Syntheses, Structures and Properties

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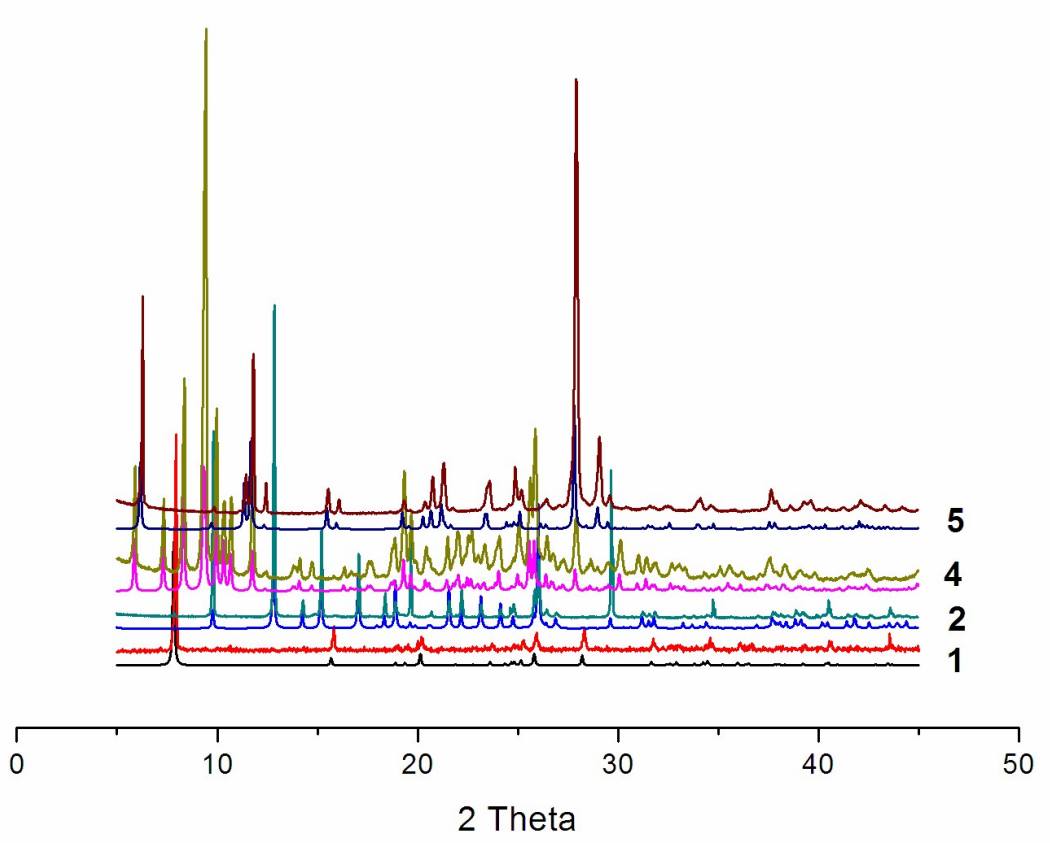


Figure S1. Comparison of the experimental and simulated PXRD patterns of complexes **1**, **2**, **4**, and **5**. The top is the experimental pattern, and the bottom is the simulated one

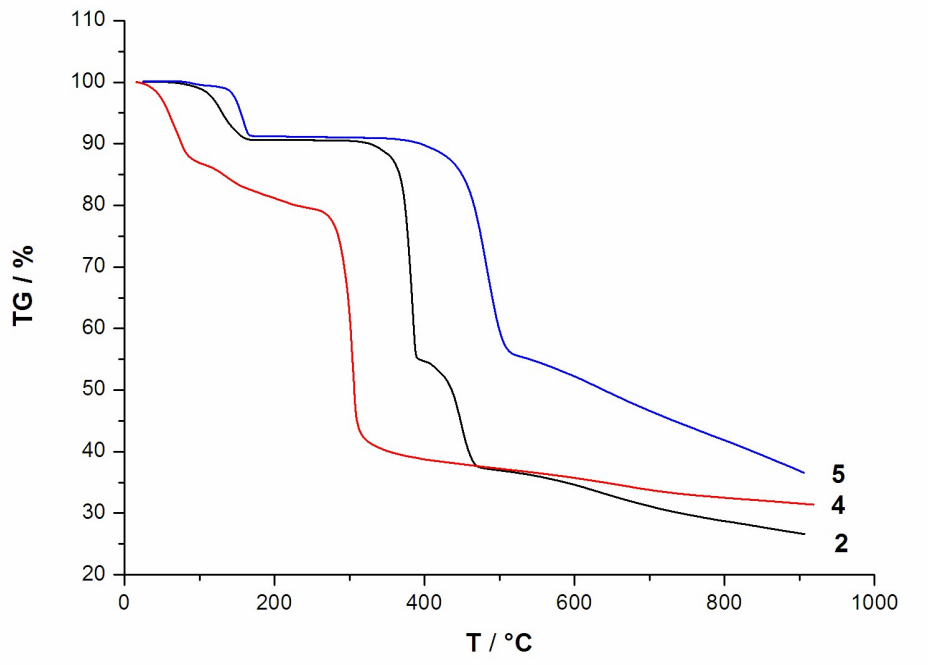


Figure S2. The thermogravimetry curves of **2, 4,** and **5**.

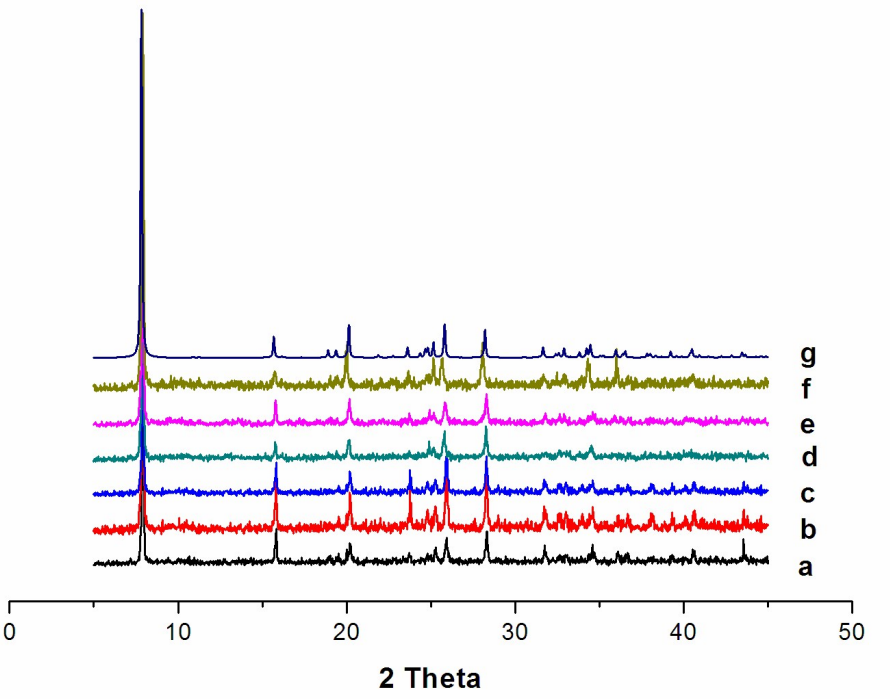


Figure S3. PXRD patterns of **1**: (a) the as-synthesis pattern, (b) dehydrated solid obtained on heating at 120 °C for 8 h under vacuum, (c) after the first recycling, (d) second, (e) third, and (f) after the fourth recycling. (g) the simulated XRD pattern.

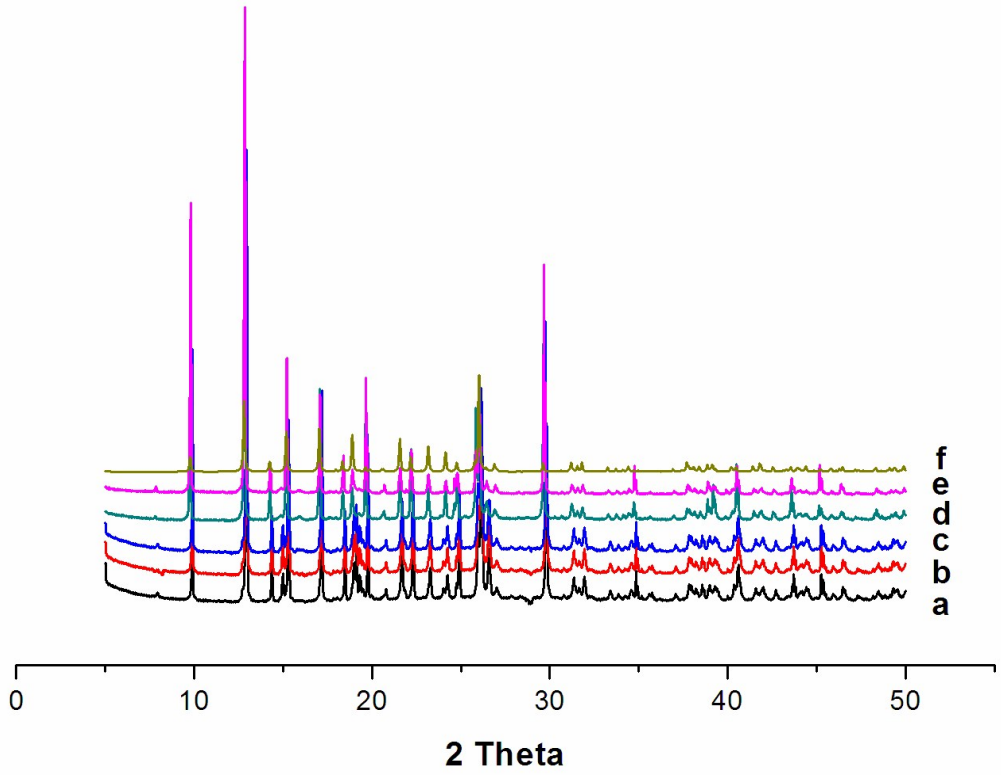


Figure S4. PXRD patterns of **2**: (a) the as-synthesis pattern, (b) dehydrated solid obtained on heating at 120 °C for 8 h under vacuum, (c) after the first recycling, (d) second, (e) third, and (f) after the fourth recycling. (g) the simulated XRD pattern.

NMR data

1. *2-phenyl-2-(phenylamino)acetonitrile* (**Table 2. entry 1**). Little yellow solid, yield, 19 mg, 95%. **^{1}H NMR (400 MHz, $CDCl_3$)** δ = 7.60 (d, J = 4 Hz, 2H), 7.45 (d, J = 8 Hz, 3H), 7.30~7.26 (m, 2H), 6.93 (t, J = 8 Hz, 1H), 6.77 (d, J = 8 Hz, 2H), 5.42 (d, J = 12 Hz, 1H), 4.02 (d, J = 8 Hz, 1H). ^{13}C NMR δ: 50.36, 114.27, 118.32, 120.44, 127.41, 129.49, 129.70, 129.73, 134.05, 144.79.

2. *2-(phenylamino)-2-p-tolylacetonitrile* (**Table 2, entry 2**). Little yellow solid, yield, 22 mg, 95%.. **^{1}H NMR (400 MHz, $CDCl_3$)** δ = 7.46 (d, J = 8 Hz, 2H), 7.29~7.26 (m, 4H), 6.89 (d, J = 8 Hz, 1H), 6.76 (d, J = 8 Hz, 2H), 5.37 (d, J = 8 Hz, 1H), 3.98 (d, J = 8 Hz, 1H), 2.39 (s, 3H). ^{13}C NMR δ: 21.33, 50.05, 114.18, 118.48, 120.29, 127.30, 129.68, 130.10, 131.08, 139.72, 144.63.

3. *2-(p-tolylamino)-2-p-tolylacetonitrile* **(Table 2, entry 3)**. Little yellow solid, yield, 22 mg, 93%. **^{1}H NMR (400 MHz, $CDCl_3$)** δ = 7.46 (d, J = 8 Hz, 2H), 7.27 (d, J = 8 Hz, 2H), 7.07 (d, J = 8 Hz, 2H), 6.69 (d, J = 8 Hz, 2H), 5.34 (d, J = 8 Hz, 1H), 3.84 (d, J = 8 Hz, 1H), 2.39 (s, 3H), 2.28 (s, 3H). ^{13}C NMR δ: 20.63, 21.32, 50.63, 114.60, 116.63, 127.30, 129.83, 130.08, 130.19, 131.39, 139.66, 142.63.

4. *2-(p-tolylamino)-2-(4-methoxyphenyl)acetonitrile* **(Table 2, entry 4)**. Little yellow solid, yield, 23 mg, 92%. **^{1}H NMR (400 MHz, $CDCl_3$)** δ = 7.48 (d, J = 8 Hz, 2H), 7.06 (d, J = 8 Hz, 2H), 6.94 (d, J = 8 Hz, 2H), 6.67 (d, J = 8 Hz, 2H), 5.32 (s, 1H), 3.86 (s, 1H), 3.83 (s, 3H), 2.27 (s, 3H). ^{13}C NMR δ: 20.62, 50.20, 55.63, 114.27, 114.50, 114.68, 118.69, 126.21, 128.72, 129.71, 130.14, 142.55.

5. 2-(4-chlorophenylamino)-2-p-tolylacetonitrile (**Table 2, entry 5**). Little yellow solid, yield, 24 mg, 94%. **^{1}H NMR (400 MHz, $CDCl_3$)** δ = 7.45 (d, J = 8 Hz, 2H), 7.26 (d, J = 8 Hz, 2H), 7.21 (d, J = 8 Hz, 2H), 6.69 (d, J = 8 Hz, 2H), 5.33 (d, J = 8 Hz, 1H), 4.01 (d, J = 8 Hz, 1H), 2.40 (s, 3H). ^{13}C NMR δ: 21.34, 50.17, 115.44, 118.15, 125.19, 127.28, 129.60, 130.19, 130.68, 139.94, 143.38.

6. *2-(p-tolylamino)-2-phenylacetonitrile* **(Table 2, entry 6)**. Little yellow solid, yield, 21 mg, 93%. **^{1}H NMR (400 MHz, $CDCl_3$)** δ = 7.59 (d, J = 4 Hz, 2H), 7.44 (d, J = 4 Hz, 3H), 7.07 (d, J = 8 Hz, 2H), 6.69 (d, J = 8 Hz, 2H), 5.38 (d, J = 8 Hz, 1H), 3.90 (d, J = 8 Hz, 1H), 2.28 (s, 3H). ^{13}C NMR δ: 20.63, 50.78, 114.57, 118.46, 127.38, 129.42, 129.59, 130.18, 134.21, 142.49.

7. 2-(4-methoxyphenylamino)-2-p-tolylacetonitrile (**Table 2, entry 7**). Little yellow solid, yield, 23 mg, 92%. **^{1}H NMR (400 MHz, $CDCl_3$)** δ = 7.47 (d, J = 8 Hz, 2H), 7.26 (s, 2H), 6.84 (d, J = 8 Hz, 2H), 6.75 (d, J = 8 Hz, 2H), 5.31 (s, 1H), 3.78 (s, 3H), 3.76 (s, 1H), 2.39 (s, 3H). ^{13}C NMR δ:

21.33, 51.47, 55.81, 115.14, 116.38, 118.74, 127.31, 130.05, 131.36, 138.60, 139.53, 154.23.

8. 2-(4-methoxyphenylamino)-2-(4-methoxyphenyl)acetonitrile (**Table 2, entry 8**). Little yellow solid, yield, 25 mg, 92%. **^{1}H NMR (400 MHz, CDCl$_3$)** δ = 7.49 (d, J = 8 Hz, 2H), 6.94 (d, J = 8 Hz, 3H), 6.83 (d, J = 12 Hz, 2H), 6.74 (d, J = 8 Hz, 2H), 5.27 (d, J = 8 Hz, 1H), 3.83 (s, 3H), 3.77 (s, 3H), 3.74 (s, 1H). NMR δ: 51.10, 55.54, 55.77, 114.66, 115.09, 116.34, 118.80, 126.26, 128.73, 138.76, 134.16, 160.46.

9. *2-(4-methoxyphenylamino)-2-phenylacetonitrile* (**Table 2, entry 9**). Little yellow solid, yield, 22 mg, 94%. **^{1}H NMR (400 MHz, CDCl$_3$)** δ = 7.59 (d, J = 8 Hz, 2H), 7.44 (d, J = 8 Hz, 2H), 6.84 (d, J = 8 Hz, 1H), 6.75 (d, J = 8 Hz, 1H), 5.34 (d, J = 8 Hz, 1H), 3.79 (d, J = 8 Hz, 1H), 3.77 (s, 3H). ^{13}C NMR δ: 51.64, 55.76, 115.07, 116.36, 118.58, 127.38, 129.38, 129.57, 134.19, 138.65, 154.18.

10. 2-(4-chlorophenylamino)-2-phenylacetonitrile (**Table 2, entry 10**). Little yellow solid, yield, 23 mg, 94%. **^{1}H NMR (400 MHz, CDCl$_3$)** δ = 7.58 (d, J = 4 Hz, 2H), 7.47 (m, J = 8 Hz, 3H), 7.22 (d, J = 8 Hz, 2H), 6.69 (d, J = 8 Hz, 2H), 5.38 (d, J = 8 Hz, 1H), 4.05 (d, J = 8 Hz, 1H). ^{13}C NMR δ: 50.43, 115.50, 117.98, 125.32, 127.37, 129.57, 129.62, 129.86, 133.61, 143.31.

Table S1. Selected bond distances (Å) and angles (deg) for the complexes **1**−**5**[a]

Complex **1**					
Cu(1)-O(6)^{i}	1.867(2)	Cu(2)-O(1)^{ii}	1.969(2)	Cu(2)-O(2)	2.597(3)
Cu(1)-O(4)	1.910(2)	Cu(2)-O(1)^{iii}	1.9689(19)	Cu(2)-Cu(2)^{v}	2.9427(5)
Cu(1)-N(1)	1.974(3)	Cu(2)-O(1)	1.971(2)	Cu(2)-Cu(2)^{iii}	2.9427(5)
Cu(1)-O(1)	1.997(2)	Cu(2)-O(1)^{iv}	1.971(2)	O(1)-Cu(2)^{iii}	1.9689(19)
Cu(1)-O(2)	2.550(8)				
O(6)^{i}-Cu(1)-O(4)	170.81(11)	O(4)-Cu(1)-O(2)	93.22(8)	O(1)iii-Cu(2)-O(1)^{iv}	97.27(9)
O(6)^{i}-Cu(1)-N(1)	92.90(10)	N(1)-Cu(1)-O(2)	97.94(10)	O(1)-Cu(2)-O(1)^{iv}	160.23(12)
O(4)-Cu(1)-N(1)	86.27(10)	O(1)-Cu(1)-O(2)	80.87(9)	O(1)^{ii}-Cu(2)-O(2)	91.81(6)
O(6)^{i}-Cu(1)-O(1)	93.16(9)	O(1)^{ii}-Cu(2)-O(1)^{iii}	176.37(12)	O(1)^{iii}-Cu(2)-O(2)	91.81(6)
O(4)-Cu(1)-O(1)	87.83(9)	O(1)^{ii}-Cu(2)-O(1)	97.27(9)	O(1)-Cu(2)-O(2)	80.11(6)
N(1)-Cu(1)-O(1)	173.91(9)	O(1)^{iii}-Cu(2)-O(1)	83.36(9)	O(1)^{iv}-Cu(2)-O(2)	80.11(6)
O(6)^{i}-Cu(1)-O(2)	95.95(8)	O(1)^{ii}-Cu(2)-O(1)^{iv}	83.36(9)		
Complex **2**					
Cu(1)-O(3)^{i}	1.865(2)	Cu(1)-N(1)	1.985(3)	Cu(2)-O(4)^{ii}	1.938(2)
Cu(1)-O(1)	1.941(2)	Cu(1)-O(7)	2.273(3)	Cu(2)-O(2)	1.981(2)
Cu(1)-O(8)	1.973(2)	Cu(2)-O(6)	1.871(2)	Cu(2)-N(2)^{ii}	1.982(3)
O(3)^{i}-Cu(1)-O(1)	170.69(11)	N(1)-Cu(1)-O(7)	97.80(10)	O(6)-Cu(2)-O(4)^{ii}	173.41(11)
O(3)^{i}-Cu(1)-O(8)	89.20(10)	O(8)-Cu(1)-N(1)	162.88(11)	O(6)-Cu(2)-O(2)	93.92(10)
O(1)-Cu(1)-O(8)	89.64(9)	O(3)^{i}-Cu(1)-O(7)	96.29(10)	O(4)ii-Cu(2)-O(2)	87.88(10)
O(3)^{i}-Cu(1)-N(1)	92.62(10)	O(1)-Cu(1)-O(7)	93.02(10)	O(6)-Cu(2)-N(2)^{ii}	91.47(10)
O(1)-Cu(1)-N(1)	85.81(10)	O(8)-Cu(1)-O(7)	98.92(10)	O(4)ii-Cu(2)-N(2)^{ii}	85.62(10)
O(2)-Cu(2)-N(2)^{ii}	168.11(10)				
Complex **3**					
Cu(1)-O(5)^{i}	1.861(3)	Cu(1)-N(1)	1.980(3)	Cu(1)-O(2)	2.291(3)
Cu(1)-O(3)	1.917(3)	Cu(1)-O(1)	2.019(3)		
O(5)^{i}-Cu(1)-O(3)	177.36(13)	O(3)-Cu(1)-O(1)	88.75(12)	O(3)-Cu(1)-O(2)	94.61(13)
O(5)^{i}-Cu(1)-N(1)	93.26(11)	N(1)-Cu(1)-O(1)	155.06(13)	N(1)-Cu(1)-O(2)	109.42(12)
O(3)-Cu(1)-N(1)	86.28(11)	O(5)^{i}-Cu(1)-O(2)	87.99(13)	O(1)-Cu(1)-O(2)	95.32(13)
O(5)^{i}-Cu(1)-O(1)	90.60(12)				
Complex **4**					
Cu(1)-O(16)	1.9311(19)	Cu(1)-N(2)	2.292(2)	Cu(2)-N(3)	2.044(2)
Cu(1)-O(14)	1.9635(19)	Cu(2)-O(10)	1.935(2)	Cu(2)-N(1)	2.054(2)
Cu(1)-N(6)	2.041(2)	Cu(2)-O(20)	1.9605(19)	Cu(2)-N(4)	2.266(2)
Cu(1)-N(5)	2.058(2)				
O(16)-Cu(1)-O(14)	168.82(9)	N(6)-Cu(1)-N(5)	165.62(9)	O(10)-Cu(2)-O(20)	173.57(9)
O(16)-Cu(1)-N(6)	88.06(9)	O(16)-Cu(1)-N(2)	113.70(8)	O(10)-Cu(2)-N(3)	88.37(9)
O(14)-Cu(1)-N(6)	90.96(9)	O(14)-Cu(1)-N(2)	77.34(8)	O(20)-Cu(2)-N(3)	88.46(9)
O(16)-Cu(1)-N(5)	82.30(8)	N(6)-Cu(1)-N(2)	86.77(9)	O(10)-Cu(2)-N(1)	82.39(8)
O(14)-Cu(1)-N(5)	96.43(8)	N(5)-Cu(1)-N(2)	106.85(8)	O(20)-Cu(2)-N(1)	98.77(8)
N(3)-Cu(2)-N(1)	159.23(9)				
Complex **5**					
Cu(1)-O(1)	1.893(3)	Cu(1)-N(2)	1.968(3)	Cu(1)-O(8)	2.297(3)
Cu(1)-O(6)	1.938(3)	Cu(1)-O(7)	1.988(2)		
O(1)-Cu(1)-O(6)	172.32(8)	O(6)-Cu(1)-O(7)	89.31(12)	O(6)-Cu(1)-O(8)	95.48(10)
O(1)-Cu(1)-N(2)	94.70(11)	N(2)-Cu(1)-O(7)	161.66(8)	N(2)-Cu(1)-O(8)	106.40(12)
O(6)-Cu(1)-N(2)	83.75(10)	O(1)-Cu(1)-O(8)	92.17(9)	O(7)-Cu(1)-O(8)	91.12(13)
O(1)-Cu(1)-O(7)	89.91(11)				

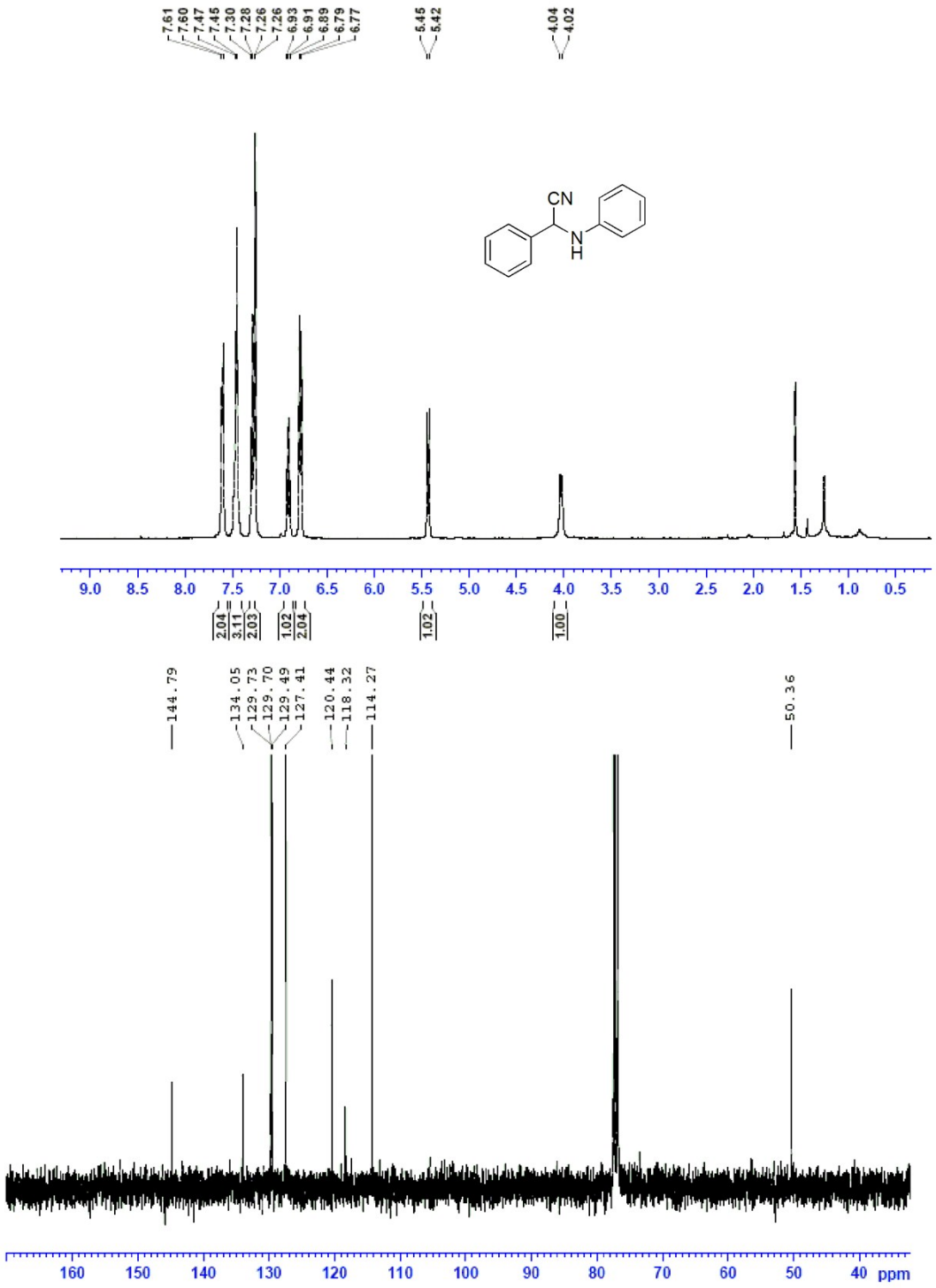
[a] Symmetry transformations used to generate equivalent atoms for **1**: i) $-x+1/2, -y+1/2, -z+1$. ii) $x, -y+1, z+1/2$. iii) $-x, -y, -z$. iv) $-x, y, -z+1/2$. v) $-x, -y, -z+1$. for **2**: i) $-x+1, -y, -z+1$. ii) $-x+2, -y+1, -z+1$. For **3**: i) $-x, -y+1, -z+2$.

Table S2. Geometrical Parameters of Hydrogen Bonds (Å, °) for complexes **1–5**

D-H···A	d(D-H) (Å)	d(H···A) (Å)	d(D···A) (Å)	**<(DHA)**	Symmetry codes

			Complex **1**		
O1-H1W···O6	0.82	1.96	2.732(3)	157.1	$-x+1/2, y-1/2, -z+1/2$
O2-H2W···O5	0.83	1.90	2.723(3)	175.6	$-x, y, -z-1/2$
O3-H4W···O3	0.83	1.47	2.282(19)	172.4	$-x+1, y, -z+3/2$
O3-H3W···O3	0.83	1.88	2.31(2)	110.8	$-x+1, -y, -z+1$
			Complex **2**		
O2-H2w···O4	0.84	2.03	2.861(3)	172.0	$-x+2, y-1/2, -z+3/2$
O8-H4w···O5	0.84	1.88	2.689(3)	162.1	$-x+2, y-3/2, -z+3/2$
O8-H3w···O6	0.82	1.93	2.731(3)	165.9	$x, y-1, z$
O7-H1w···O3	0.82	2.04	2.855(3)	169.3	$-x+1, -y+1, -z+1$
			Complex **3**		
O2-H4w···O4	0.83	1.95	2.749(4)	164.4	$x-1, y, z$
O2-H3w···O3	0.82	1.99	2.800(4)	168.8	$-x, -y, -z+1$
O1-H2w···O5	0.83	2.29	2.828(4)	122.8	$x, y, z-1$
O1-H2w···O2	0.83	2.18	2.950(5)	155.5	$-x, -y+1, -z+1$
O1-H1w···O1	0.83	2.43	3.004(6)	127.5	$-x+1, -y+1, -z+1$
			Complex **4**		
O1-H1w···O21	0.83	1.93	2.759(4)	175.8	
O1-H2w···O17	0.83	2.26	2.890(3)	132.8	$x-1, y, z$
O2-H3w···O3	0.83	2.13	2.811(4)	139.0	
O2-H4w···O9	0.81	2.26	2.905(6)	136.5	$-x+1, -y+1, -z$
O2-H4w···O8	0.81	2.57	3.182(6)	132.6	$-x+1, -y+1, -z$
O3-H5w···O1	0.84	2.13	2.921(4)	156.9	
O3-H6w···O11	0.84	2.02	2.801(3)	154.5	$x-1, y, z$
O4-H7w···O7	0.83	1.95	2.757(4)	164.9	$-x+1, -y+1, -z+1$
O4-H8w···O21	0.83	2.28	3.060(4)	157.0	
O5-H9w···O4	0.83	2.06	2.850(4)	158.6	
O5-H10w···O9	0.85	1.89	2.745(5)	179.7	$x-1, y, z$
O6-H11w···O20	0.83	2.55	3.267(3)	145.4	
O6-H12w···O1	0.83	2.14	2.886(4)	149.4	
O7-H13w···O15	0.84	2.01	2.797(4)	155.9	$-x+1, -y+1, -z+1$
O7-H14w···O4	0.84	2.30	2.757(4)	115.0	$-x+1, -y+1, -z+1$
O8-H15w···O15	0.84	2.02	2.794(4)	152.8	
O8-H16w···O7	0.85	1.87	2.720(5)	179.0	$x, y-1, z-1$
O9-H17w···O14	0.82	2.32	3.014(5)	141.9	
O9-H18w···O8	0.85	2.36	3.212(6)	179.5	
			Complex **5**		
O4-H4···N1	0.82	1.78	2.514(4)	147.6	
O7-H1w···O1	0.83	1.89	2.706(4)	165.2	$-x, -y+2, -z+1$
O7-H2w···O8	0.82	2.03	2.833(4)	164.5	$x-1, y, z$
O8-H4w···O6	0.82	1.98	2.703(4)	145.8	$x+1, y, z$
O8-H3w···O5	0.82	1.91	2.721(4)	172.2	$-x, -y+1, -z+1$
O2-H1'···O3	0.88(6)	1.73(6)	2.607(4)	176(6)	$-x+3, -y+2, -z$

The ^{1}H and ^{13}C NMR spectra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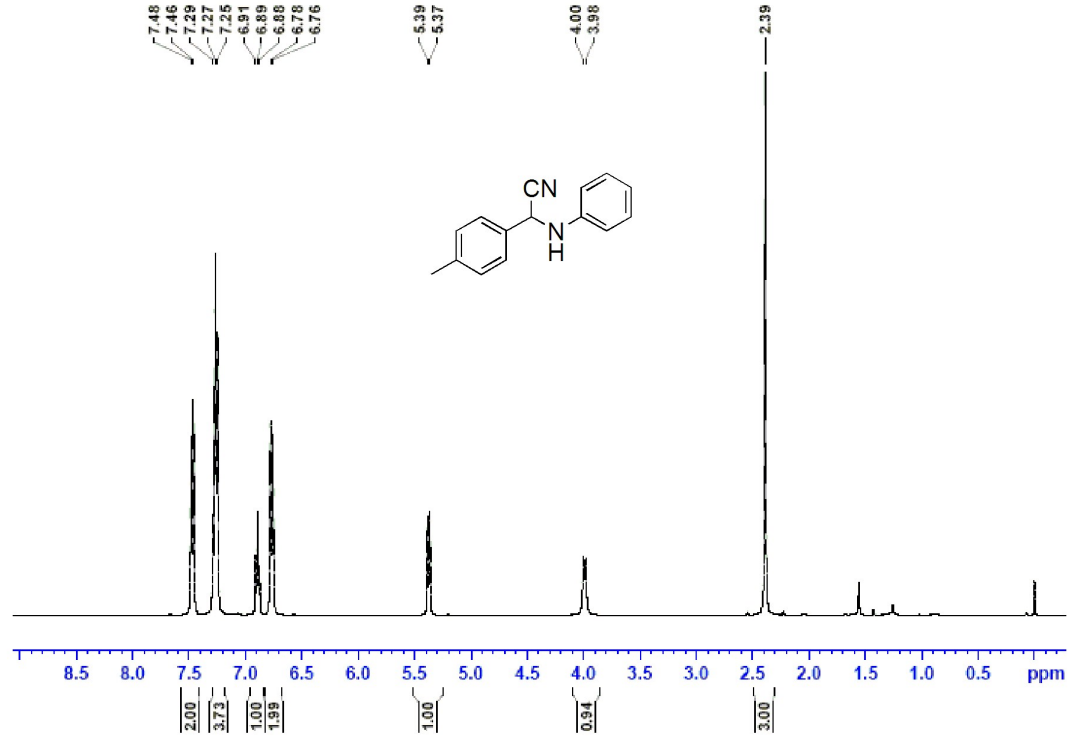
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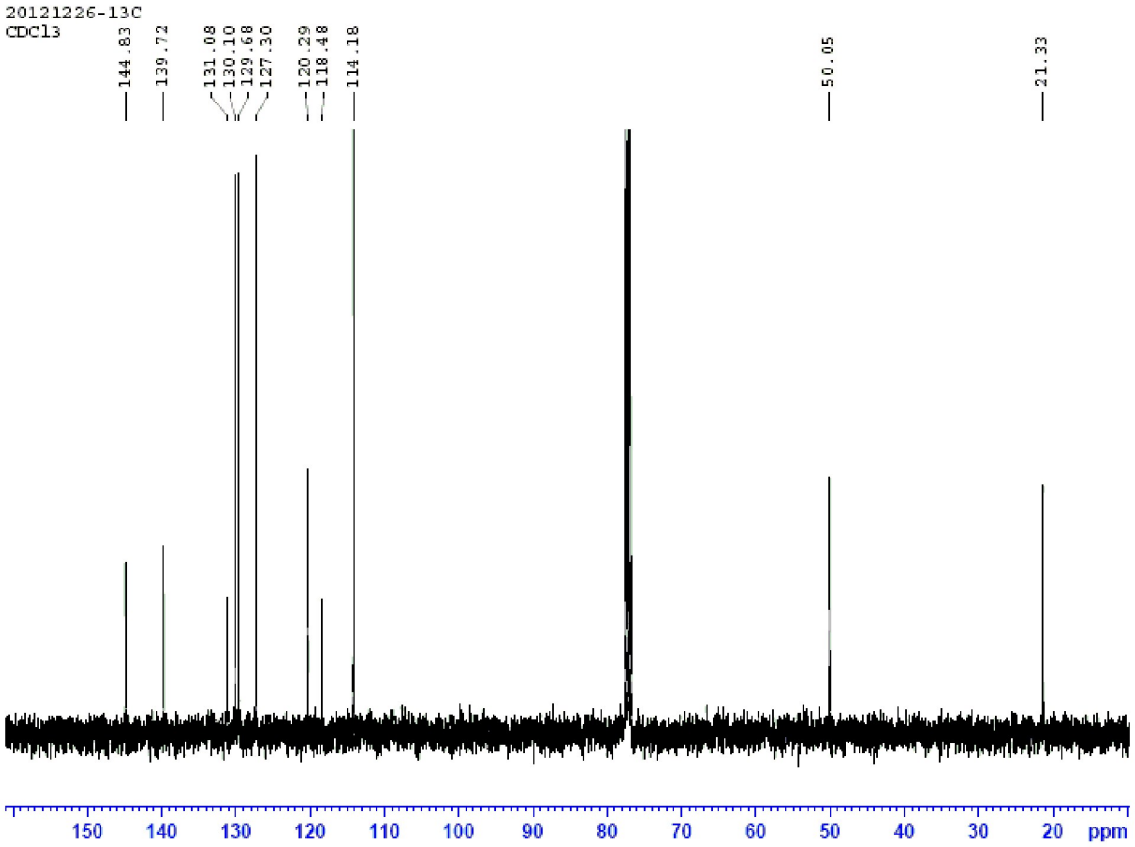
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7.09
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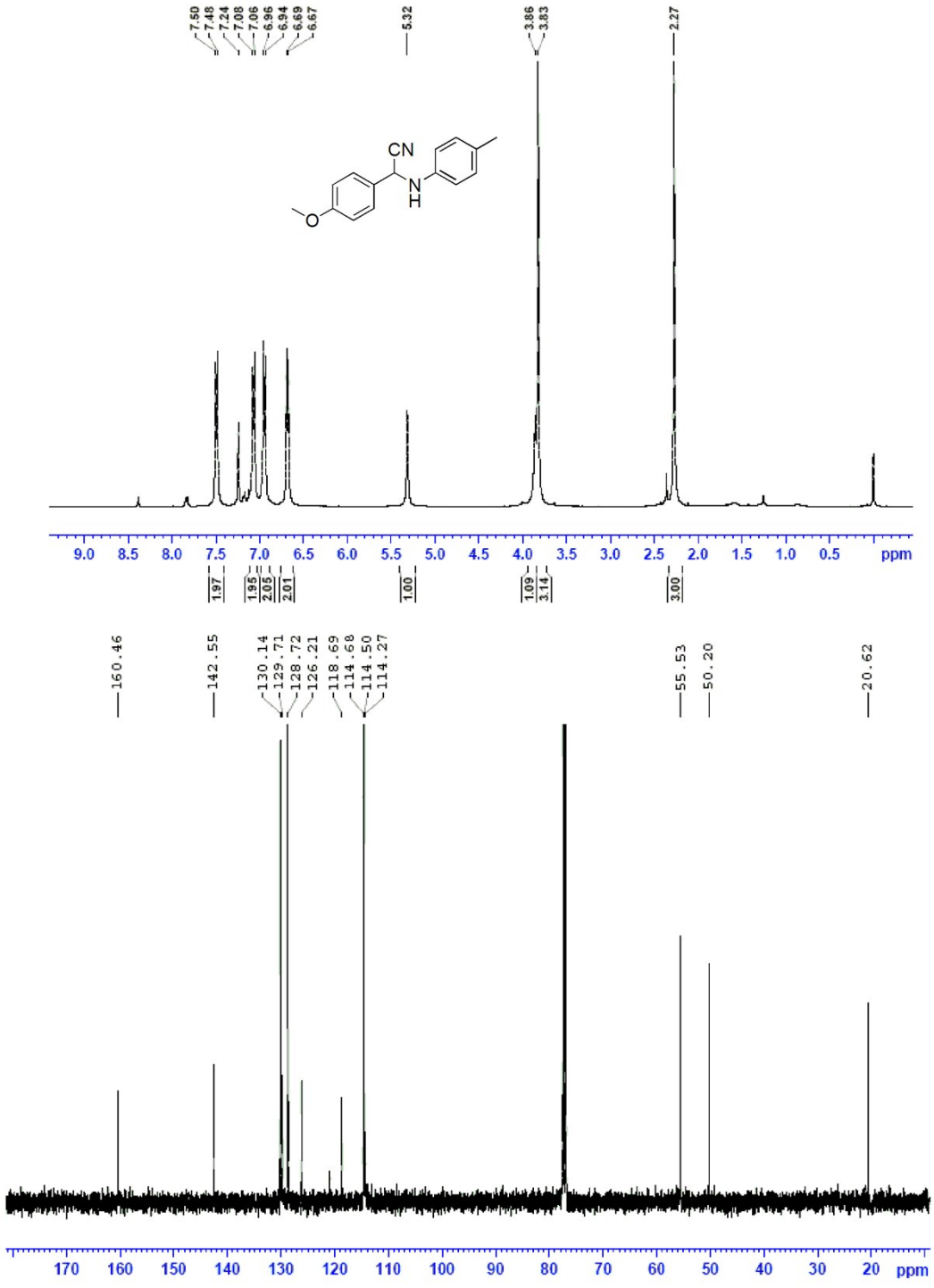
0.5
0.0
ppm
1.96
1.91
1.99
1.99
1.09
1.04
3.02
3.00
142.63
139.66
131.39
130.19
130.08
129.83
127.30
118.63
114.60
50.63
21.32
20.63
140
130
120
110
100
90
80
70
60
50
40
30
ppm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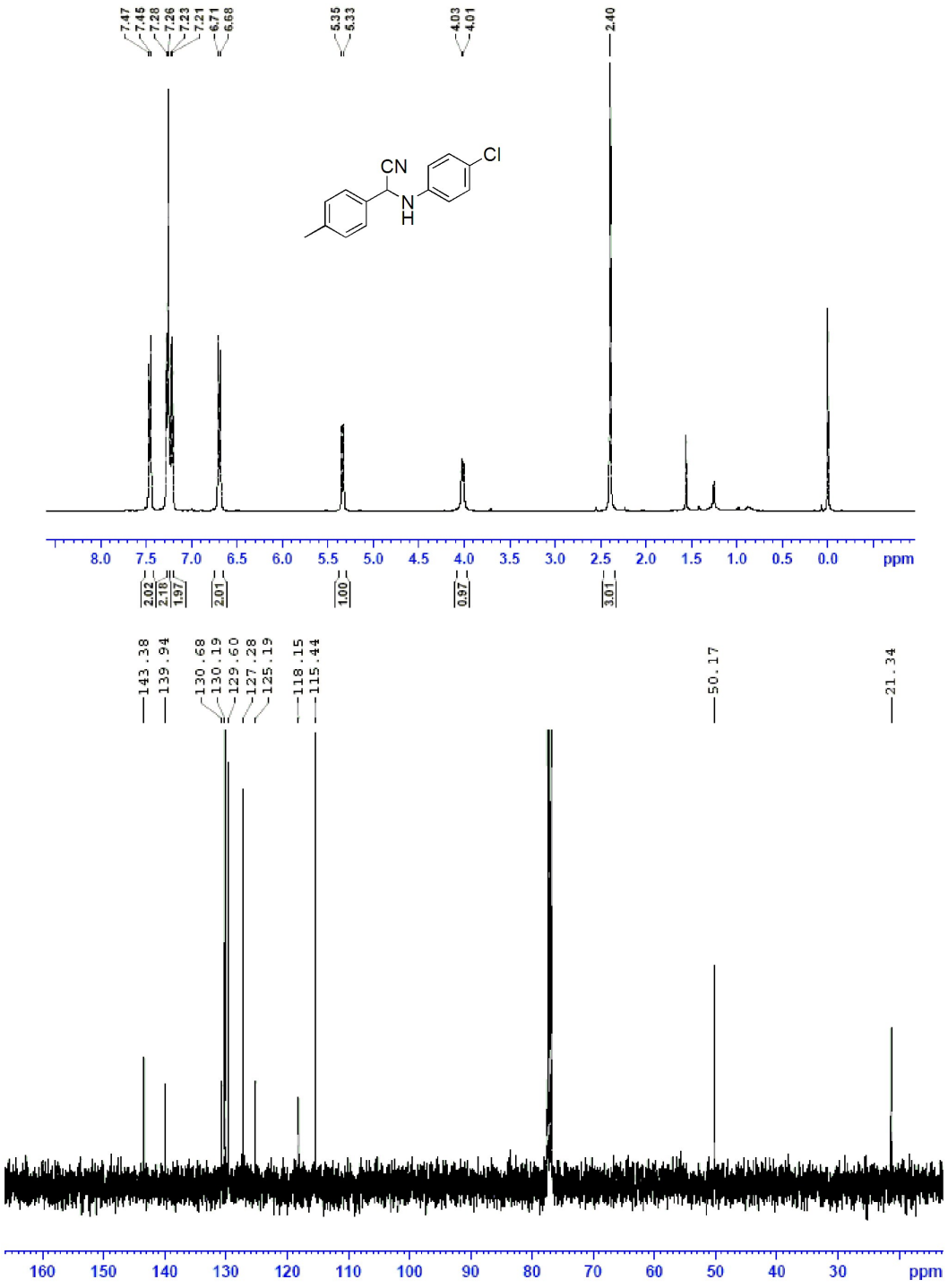
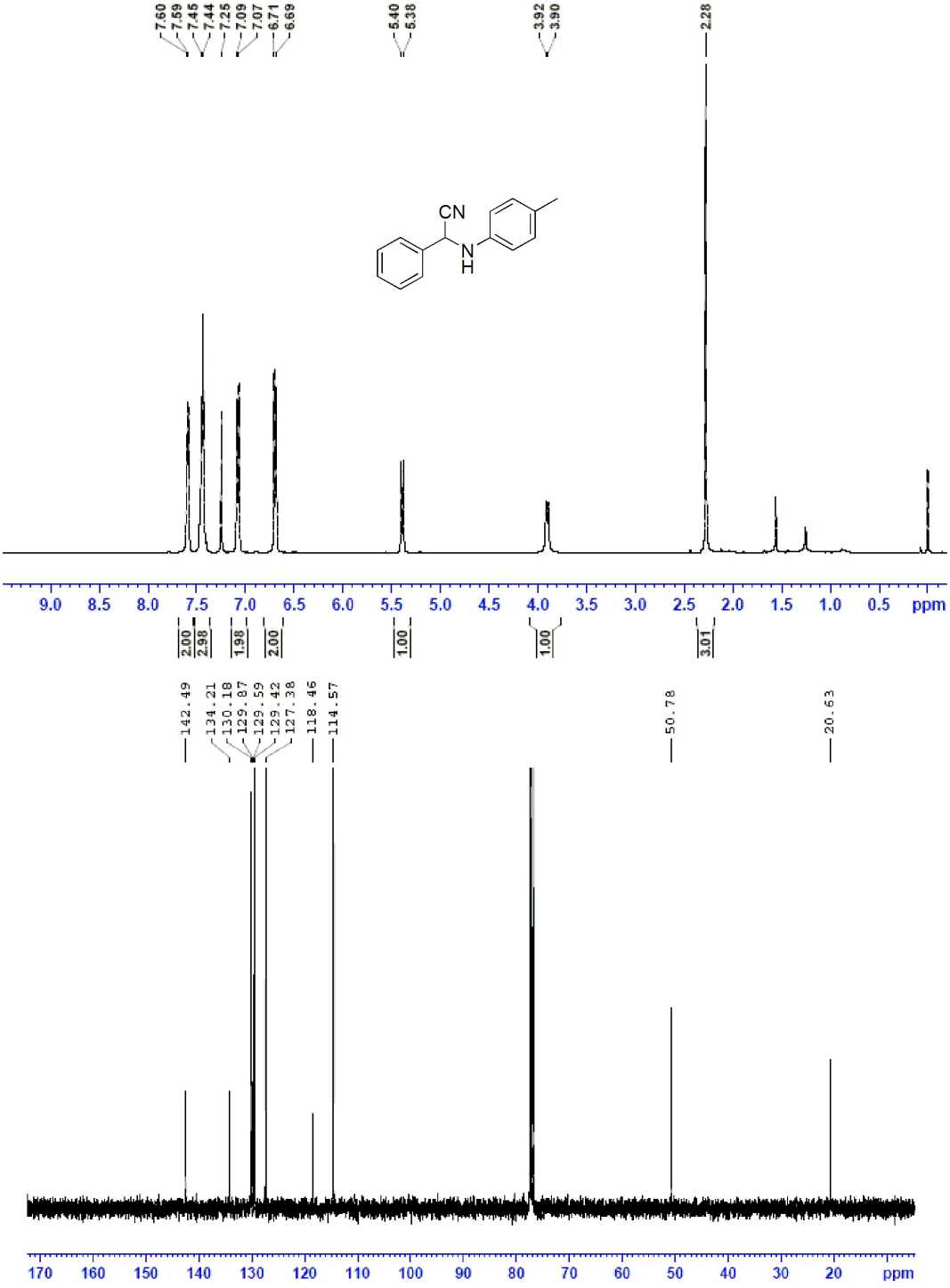
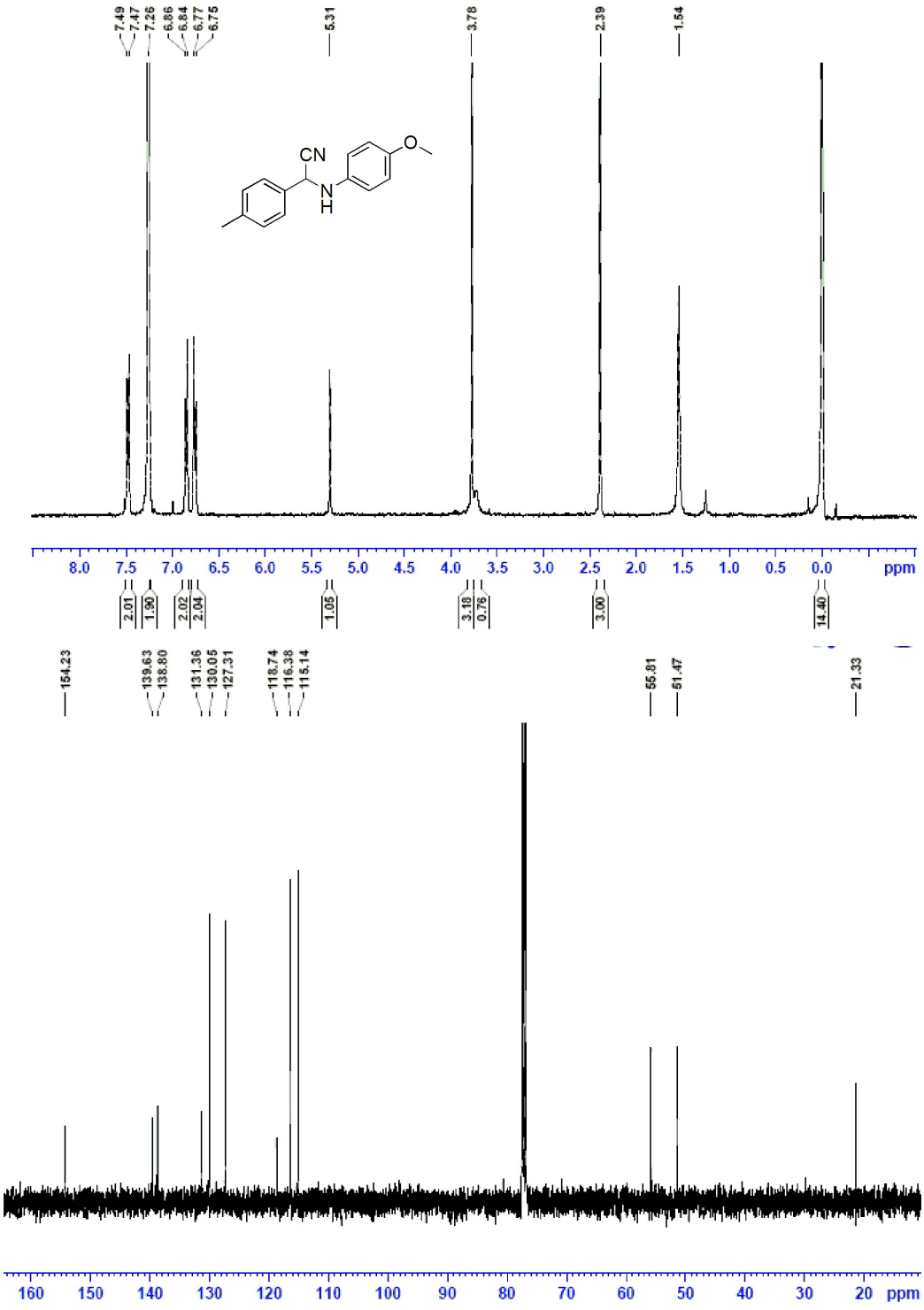
7.48
7.24
7.08
7.06
6.96
6.94
6.69
6.67
5.32
3.86
3.83
2.27
CN
N
H
O
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.97
1.95
2.05
2.01
1.00
1.09
3.14
3.00
160.46
142.55
130.14
129.71
128.72
126.21
118.69
114.68
114.50
114.27
55.53
50.20
20.62
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.47
7.45
7.28
7.26
7.23
7.21
6.71
6.68
5.35
5.33
4.03
4.01
2.40
CN
Cl
N
H
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 ppm
2.02
2.16
1.97
2.01
1.00
0.97
3.01
143.38
139.94
130.68
130.19
129.60
127.28
125.19
118.15
115.44
50.17
21.34
160 150 140 130 120 110 100 90 80 70 60 50 40 30 ppm


7.60
7.59
7.45
7.44
7.25
7.09
7.07
6.71
6.69
5.40
5.38
3.92
3.90
2.28
CN
N
H
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 ppm
2.00
2.98
1.98
2.00
1.00
1.00
3.01
142.49
134.21
130.18
129.87
129.59
129.42
127.38
118.46
114.57
50.78
20.63
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm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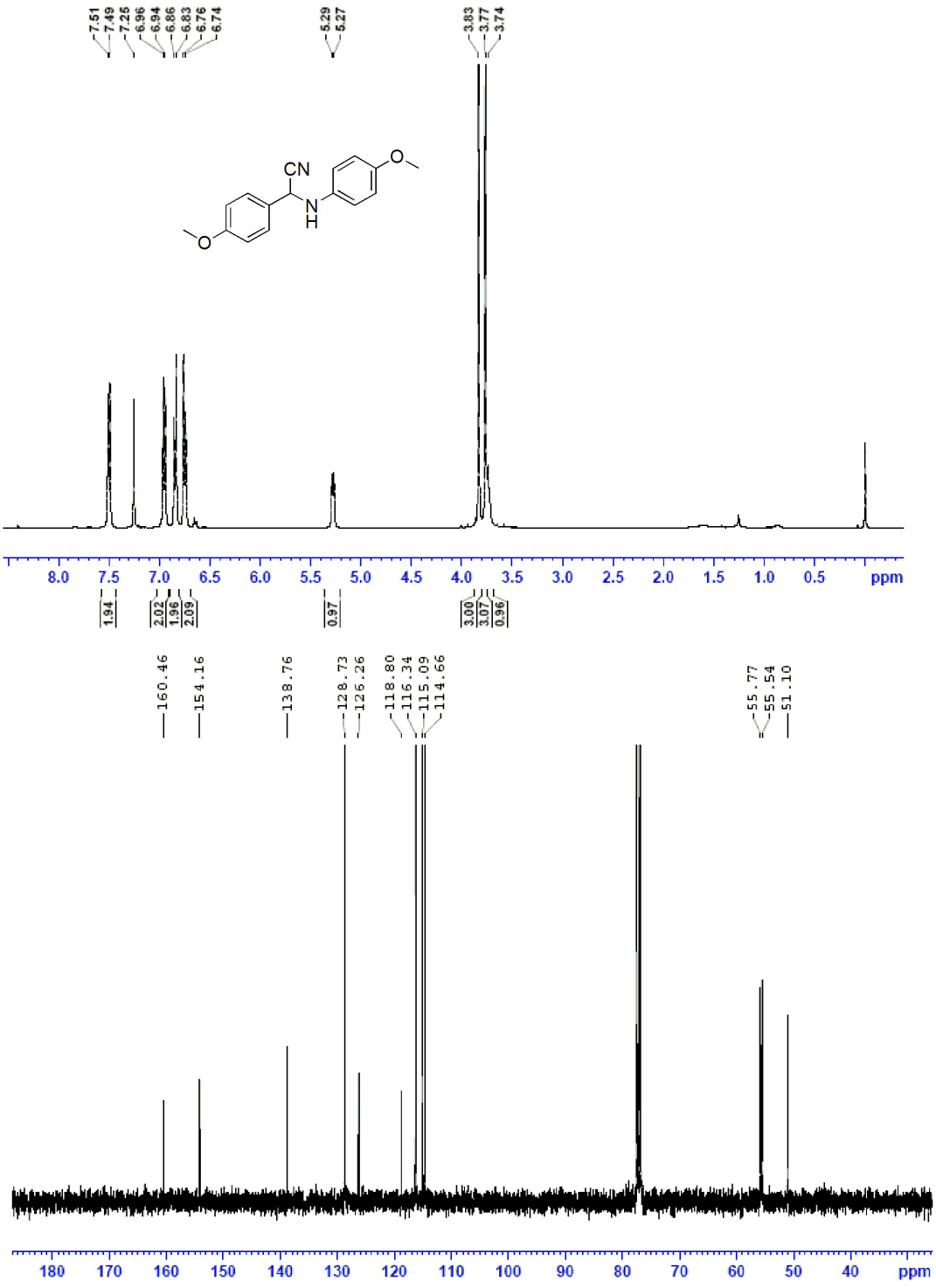
7.47
7.26
6.86
6.84
6.77
6.75
5.31
3.78
2.39
1.54
CN
N
H
O
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
2.01
1.90
2.02
2.04
1.05
3.18
0.76
3.00
14.40
154.23
139.63
138.80
131.36
130.05
127.31
118.74
116.38
115.14
55.81
51.47
21.33
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm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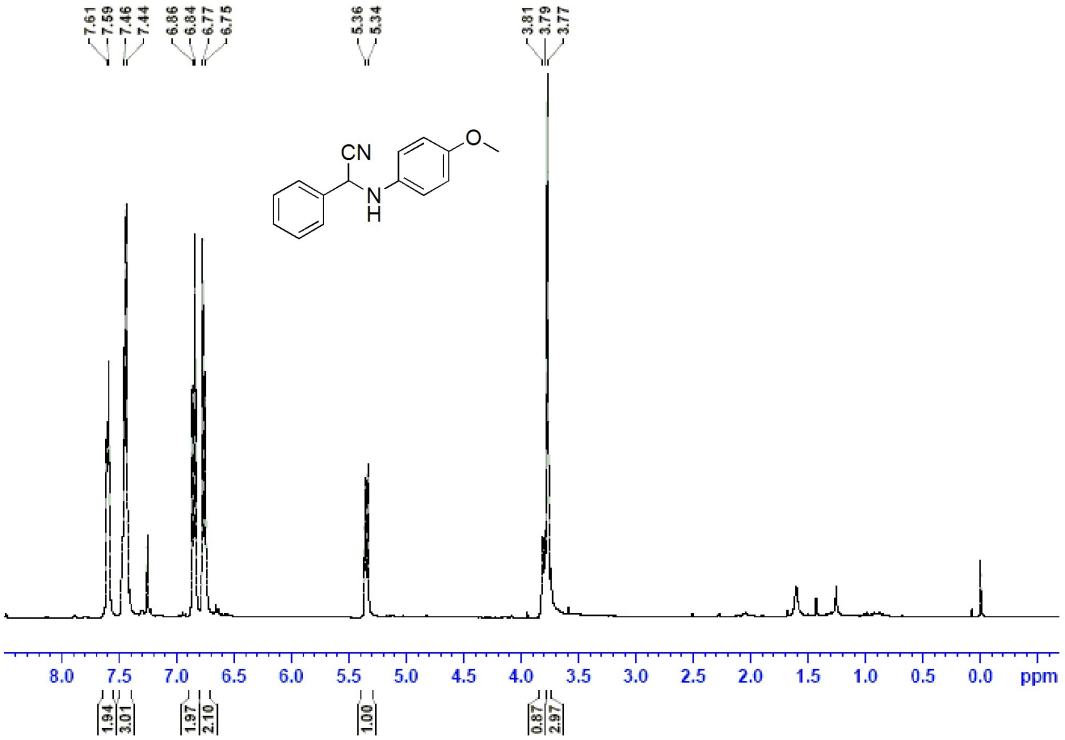
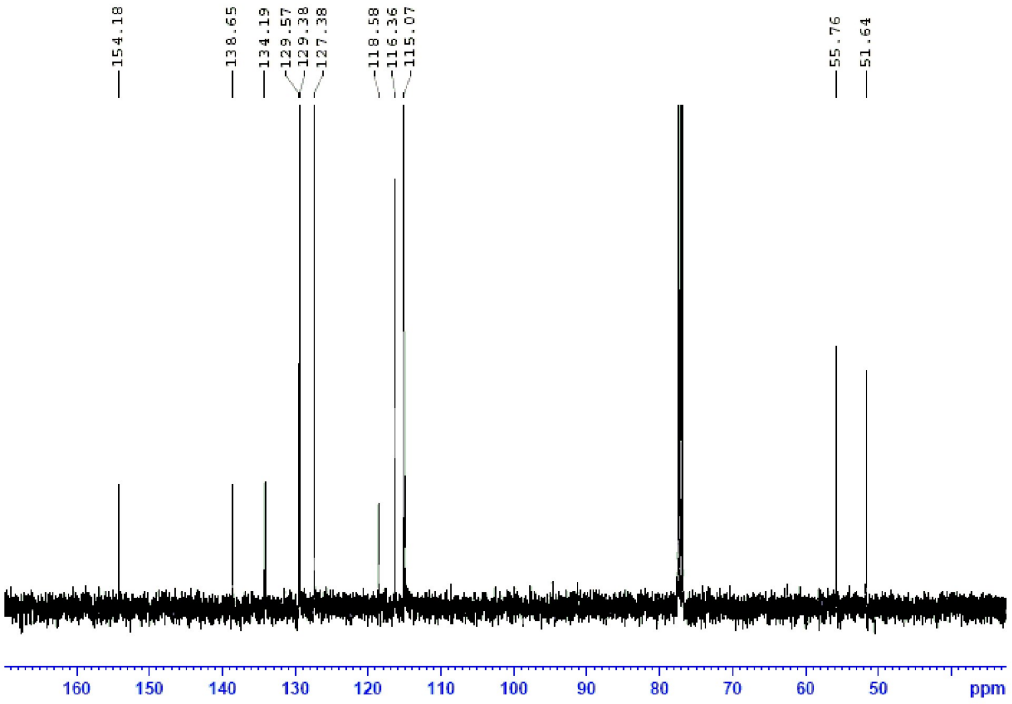
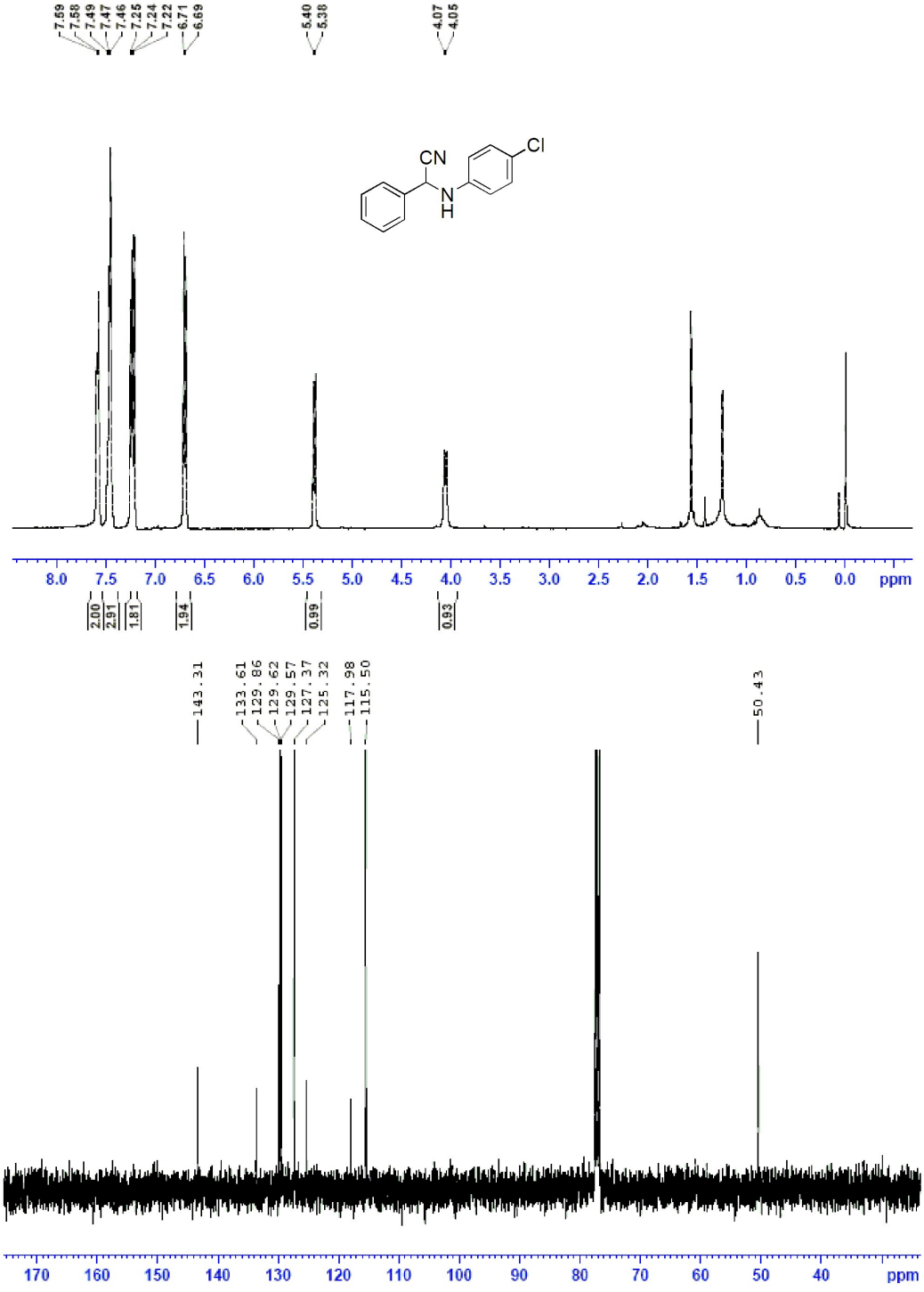
7.49
7.25
6.96
6.94
6.86
6.83
6.76
6.74
5.29
5.27
3.83
3.77
3.74
CN
N
H
O
O
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.94
2.02
1.96
2.09
0.97
3.00
3.07
0.96
160.46
154.16
138.76
128.73
126.26
118.80
116.34
115.09
114.66
55.77
55.54
51.10
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
ppm


7.61
7.59
7.46
7.44
6.86
6.84
6.77
6.75
5.36
5.34
3.81
3.79
3.77
CN
N
H
O
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 ppm
1.94
3.01
1.97
2.10
1.00
0.87
2.97


154.18
138.65
134.19
129.57
129.38
127.38
118.58
116.36
115.07
55.76
51.64
160 150 140 130 120 110 100 90 80 70 60 50 ppm


7.59
7.58
7.49
7.47
7.46
7.25
7.24
7.22
6.71
6.69
5.40
5.38
4.07
4.05
CN
N
H
Cl
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
ppm
2.00
2.91
1.81
1.94
0.99
0.93
143.31
133.61
129.86
129.62
129.57
127.37
125.32
117.98
115.50
50.43
170
160
150
140
130
120
110
100
90
80
70
60
50
40
ppm