The condensation of salicylaldehydes and malononitrile revisited: synthesis of new dimeric chromene derivatives

Marta Costa, Filipe Areias, Luís Abrunhosa,[#] Armando Venâncio[#] and Fernanda Proença[1]*

Supporting Information

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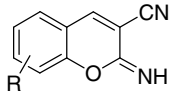


2-imino-2*H*-chromene-3-carbonitrile 1a: yellow solid; yield 86% ($NaHCO_3$) or 90% (Na_2CO_3); ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.15-7.21 (m, 1H), 7.26 (td, J = 7.5 Hz, 0.9 Hz, 1H), 7.51-7.61 (m, 2H), 8.36 (d, J = 1.5 Hz, 1H), 8.84 (s, 1H). Anal. Calcd for $C_{10}H_6N_2O.0.1H_2O$: C, 69.85; H, 3.49; N, 16.30. Found: C, 70.13; H, 3.47; N, 16.08.

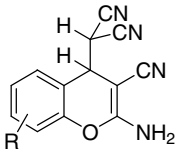
2-imino-8-methoxy-2*H*-chromene-3-carbonitrile 1b: yellow solid; yield 90% ($NaHCO_3$) or 91% (Na_2CO_3); ^{1}H NMR (300 MHz, DMSO-d_6) δ 3.81 (s, 3H), 7.12 (dd, J = 7.6 Hz, 1.5 Hz, 1H), 7.19 (t, J = 7.8 Hz, 1H), 7.30 (dd, J = 8.1 Hz, 1.8 Hz, 1H), 8.33 (s, 1H), 8.90 (s, 1H). Anal. Calcd for $C_{11}H_8N_2O_2.0.1H_2O$: C, 65.41; H, 3.96; N, 13.88. Found: C, 65.51; H, 4.15; N, 13.81.

8-hydroxy-2-imino-2*H*-chromene-3-carbonitrile 1c: yellow solid; yield 89% ($NaHCO_3$) or 70% (Na_2CO_3); ^{1}H NMR (300 MHz, DMSO-d_6) δ 6.94-7.40 (m, 3H), 8.30 (s, 1H), 8.64 (s, 1H), 10.19 (brs, 1H). Anal. Calcd for $C_{10}H_6N_2O_2$: C, 64.52; H, 3.23; N, 15.05. Found: C, 64.40; H, 3.45; N, 15.04.

6-bromo-2-imino-2*H*-chromene-3-carbonitrile 1d: yellow solid; yield 86% (Na_2CO_3); mp 183-185 ºC; ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.13 (d, J = 9.0 Hz, 1H), 7.70 (dd, J = 8.7 Hz, 2.4 Hz, 1H), 7.79 (d, J = 2.4 Hz, 1H), 8.26 (s, 1H), 9.00 (s, 1H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 105.5, 114.9, 115.46, 117.8, 119.3, 131.3, 136.2, 145.6, 150.8, 152.8; IR (Nujol mull) 2233, 1650, 1595, 1558. Anal. Calcd for $C_{10}H_5N_2OBr$: C, 48.19; H, 2.01; N, 11.24. Found: C, 47.94; H, 2.04; N, 11.16.

7,8-dihydroxy-2-imino-2*H*-chromene-3-carbonitrile 1e: red solid; yield 62% (Na_2CO_3); mp > 300 ºC; ^{1}H NMR (300 MHz, DMSO-d_6) δ 6.67 (d, J = 8.4 Hz, 1H), 6.92 (d, J = 8.4 Hz, 1H), 7.20-9.00 (brs, 3H), 8.15 (s, 1H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 109.3, 110.4, 112.5, 116.0, 121.0, 132.3, 142.9, 147.2, 153.6, 153.6; IR (Nujol mull) 2211, 1686, 1639,1580, 1547, 1510. HRMS m/z (FAB) calcd for $C_{10}H_6N_2O_3$ $(M + H)^+$ 202.038, found 203.0460.

7-diethylamino-2-imino-2*H*-chromene-3-carbonitrile 1f: yellow solid; yield 88% ($NaHCO_3$); mp 134-136 ºC; ^{1}H NMR (300 MHz, DMSO-d_6) δ 1.08-1.18 (m, 6H), 3.39-3.44 (m, 4H), 6.29 (d, J = 2.1 Hz, 1H), 6.59 (dd, J = 8.8 Hz, 2.4 Hz, 1H), 7.30 (d, J = 8.7 Hz, 1H), 8.05 (s, 1H), 8.20 (s, 1H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 12.3, 44.2, 96.2, 94.3, 106.0, 108.2, 116.7, 130.6, 146.4, 152.7, 153.2, 156.3; IR (Nujol mull) 2207, 1646, 1629, 1541, 1522. Anal. Calcd for $C_{14}H_{15}N_3O$: C, 69.71; H, 6.22; N, 17.43. Found: C, 69.69; H, 6.27; N, 17.44.

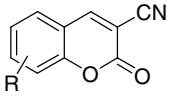


(2-amino-3-cyano-4*H*-chromene-4-yl)malononitrile 2a: white solid; yield 84% (Method A – dichloromethane), 74% (Method A – dichloromethane and triethylamine) or 91% (Method B); ^{1}H NMR (300 MHz, DMSO-d_6) δ 4.58 (d, *J* = 3.9 Hz, 1H), 5.06 (d, *J* = 3.9 Hz, 1H), 7.13 (dd, *J* = 8.1 Hz, 0.9 Hz, 1H), 7.26 (dt, *J* = 7.5 Hz, 0.9 Hz, 1H), 7.42 (dt, *J* = 7.8 Hz, 1.2 Hz, 1H), 7.47 (dd, *J* = 7.7 Hz, 1.2 Hz, 1H), 7.50 (s, 2H). Anal. Calcd for $C_{13}H_8N_4O$: C, 66.10; H, 3.39; N, 23.73. Found: C, 65.98; H, 3.49; N, 23.72.

(2-amino-3-cyano-8-methoxy-4*H*-chromene-4-yl)malononitrile 2b: white solid; yield 82% (Method A – dichloromethane and triethylamine), 94% (Method A – methanol) or 100% (Method B); ^{1}H NMR (300 MHz, DMSO-d_6) δ 3.38 (s, 3H), 4.55 (d, *J* = 3.9 Hz, 1H), 5.03 (d, *J* = 3.9 Hz, 1H), 7.00 (dd, *J* = 8.0 Hz, 1.5 Hz, 1H), 7.11 (dd, *J* = 8.1 Hz, 1.5 Hz, 1H), 7.19 (t, *J* = 8.1 Hz, 1H), 7.50 (s, 2H). Anal. Calcd for $C_{14}H_{10}N_4O_2$: C, 63.16; H, 3.59; N, 21.05. Found: C, 63.05; H, 3.84; N, 20.92.

(2-amino-6-bromo-3-cyano-4*H*-chromene-4-yl)malononitrile 2d: white solid; yield 63% (Method A – dichloromethane), 92% (Method A – dichloromethane and triethylamine) or 73% (Method B); mp 164-166 ºC; ^{1}H NMR (300 MHz, DMSO-d_6) δ 4.61 (d, *J* = 3.6 Hz, 1H), 5.13 (d, *J* = 3.9 Hz, 1H), 7.11 (d, *J* = 9.0 Hz, 1H), 7.50-7.60 (m, 3H), 7.70 (d, *J* = 2.4 Hz, 1H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 32.4, 36.7, 48.4, 112.7, 112.9, 116.4, 118.6, 119.1, 120.3, 131.4, 131.9, 149.0, 163.2; IR (Nujol mull) 2262, 2190, 2140, 1660, 1640, 1595, 1569 cm^{-1}. Anal. Calcd for $C_{13}H_7N_4OBr.0.25H_2O$: C, 48.83; H, 2.35; N, 17.53. Found: C, 49.01; H, 2.29; N, 17.18.

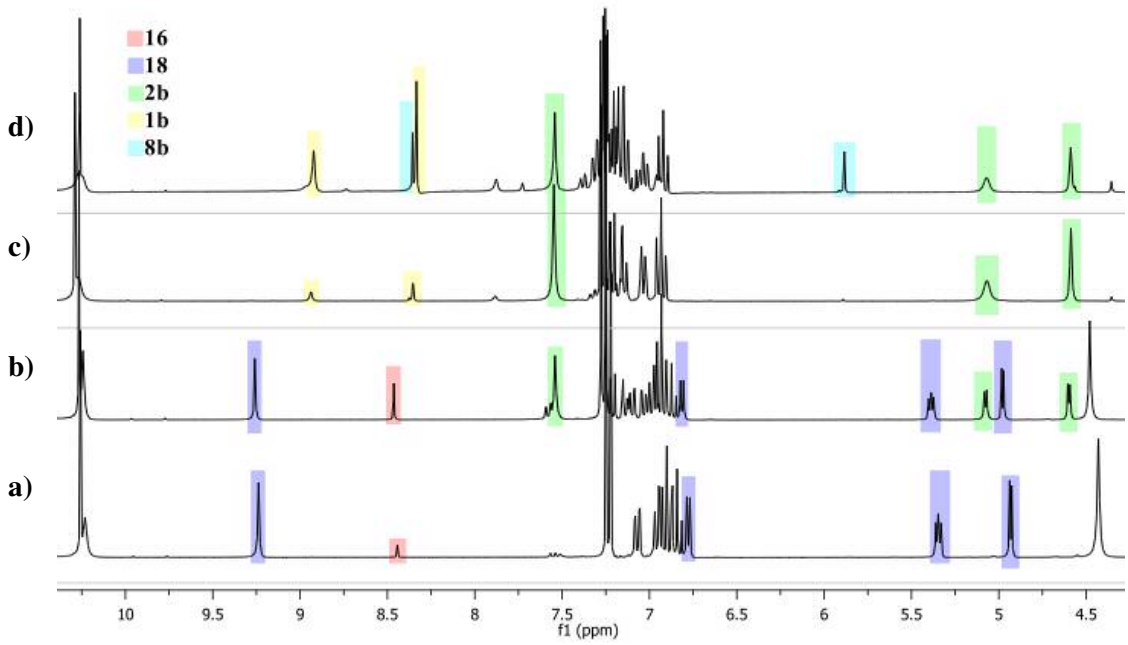
(2-amino-6-bromo-3-cyano-8-methoxy-4*H*-chromene-4-yl)malononitrile 2g: white solid; yield 73% (Method A – dichloromethane and triethylamine); mp 160-162 ºC; ^{1}H NMR (300 MHz, DMSO-d_6) δ 3.86 (s, 3H), 4.57 (d, *J* = 3.9 Hz, 1H), 5.10 (d, *J* = 3.9 Hz, 1H), 7.24 (d, *J* = 2.1 Hz, 1H), 7.31 (d, *J* = 2.1 Hz, 1H), 7.60 (s, 2H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 32.3, 36.8, 48.5, 56.4, 112.7, 112.9, 115.8, 116.3, 119.1, 120.5, 122.0, 138.6, 148.1, 163.12; IR (Nujol mull) 2255, 2192, 2118, 1668, 1649, 1612, 1598, 1576. Anal. Calcd for $C_{14}H_9N_4O_2Br$: C, 48.70; H, 2.61; N, 16.23. Found: C, 48.39; H, 2.67; N, 16.44.



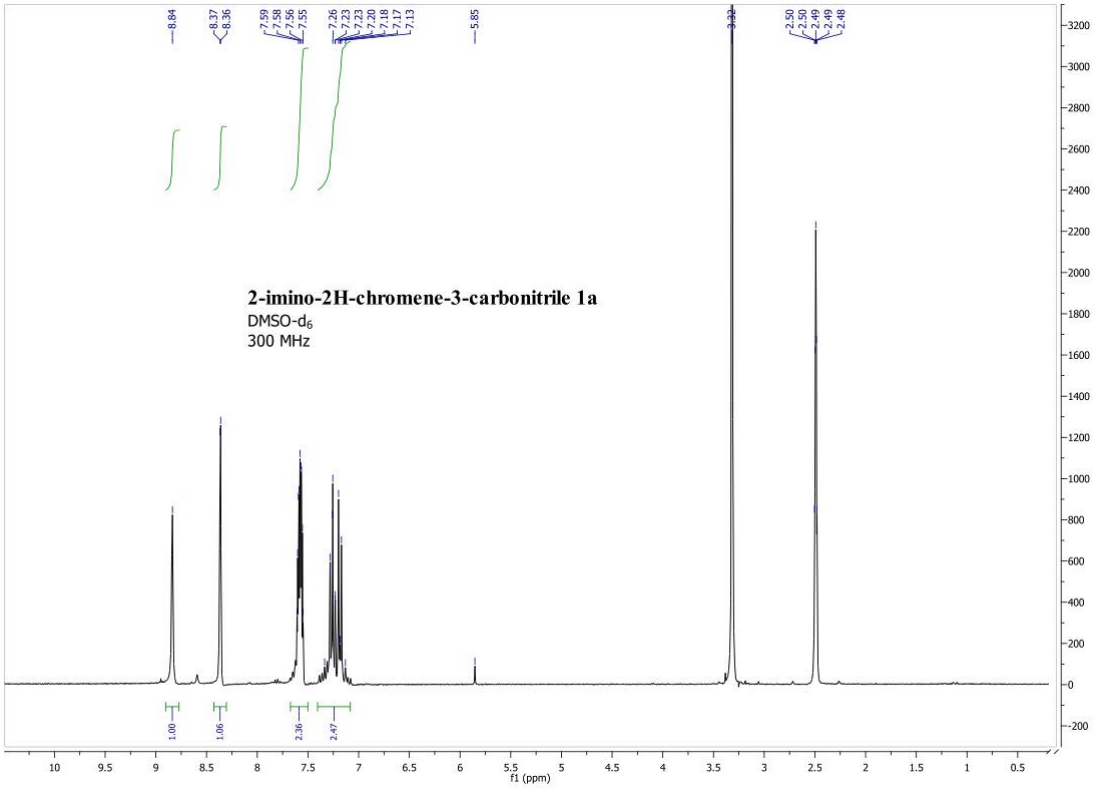
2-oxo-2*H*-chromene-3-carbonitrile 7a: yellow solid; yield 87%; ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.50-7.43 (m, 2H), 7.76-7.81 (m, 2H), 8.94 (s, 1H). Anal. Calcd for $C_{10}H_5NO_2$: C, 70.18; H, 2.92; N, 8.19. Found: C, 69.83; H, 2.86; N, 8.30.

2-oxo-8-hydroxy-2*H*-chromene-3-carbonitrile 7c: yellow solid; yield 84%; ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.15-7.30 (m, 3H), 8.87 (s, 1H), 10.55 (s. 1H). Anal. Calcd for $C_{10}H_5NO_3.0.1H_2O$: C, 63.56; H, 2.65; N, 7.42. Found: C, 63.55; H, 2.74; N, 7.60.

2-oxo-6-bromo-2*H*-chromene-3-carbonitrile 7d: yellow solid; yield 90%; mp 188-190 ºC; ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.47 (d, J = 8.7 Hz, 1H), 7.93 (dd, J = 9.0 Hz, 2.4 Hz, 1H), 8.03 (d, 2.4 Hz, 1H), 8.83 (s, 1H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 103.4, 114.3, 116.9, 119.1, 119.2, 131.7, 137.5, 153.1, 156.4; IR (Nujol mull) 2235, 1735, 1662, 1601, 1556. Anal. Calcd for $C_{10}H_4NO_2Br$: C, 48.00; H, 1.60; N, 5.60. Found: C, 47.75; H, 1.66; N, 5.95.



Selection of ^{1}H NMR spectra in the interval from δ 4.3 to 10.3 ppm recorded at (a) t = 2 min, (b) t = 20 min, (c) t = 110 min and (d) t = 22.5 h.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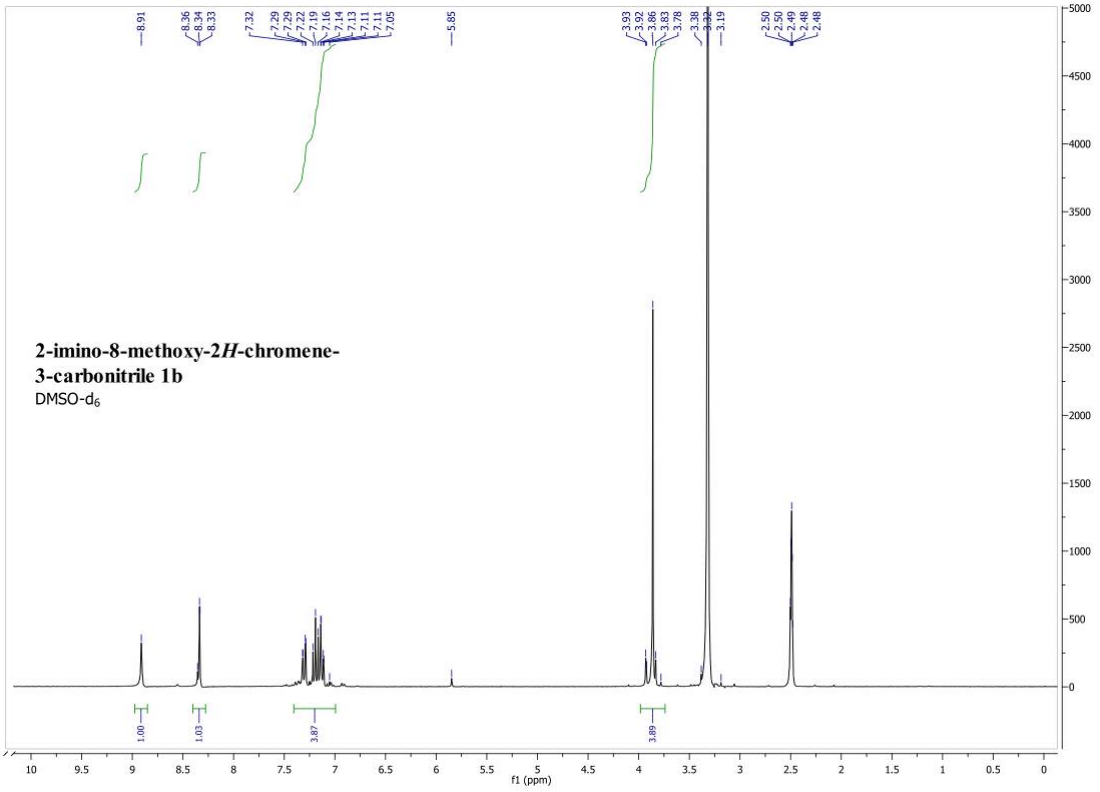
7.58
7.56
7.55
7.26
7.23
7.20
7.18
7.17
7.13
5.85
3.32
2.50
2.50
2.49
2.49
2.48
2-imino-2H-chromene-3-carbonitrile 1a
DMSO-d6
300 MHz
1.00
1.06
2.36
2.47
f1 (ppm)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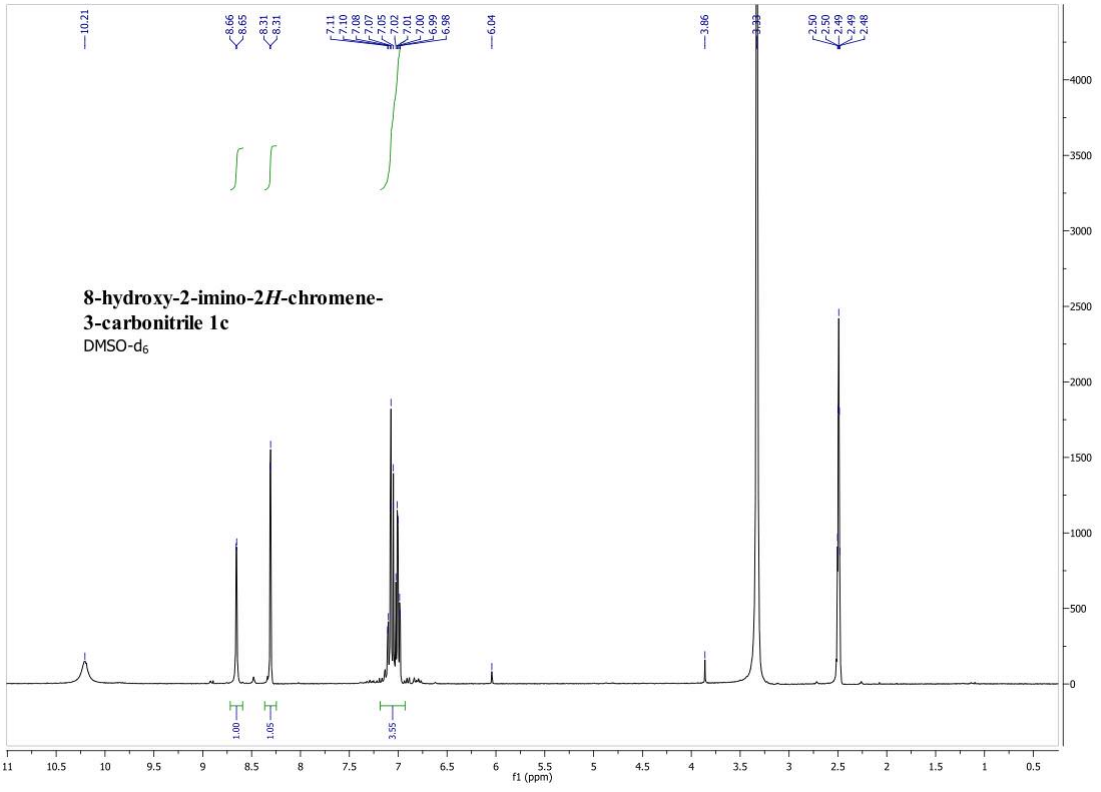
DMSO-d6
f1 (ppm)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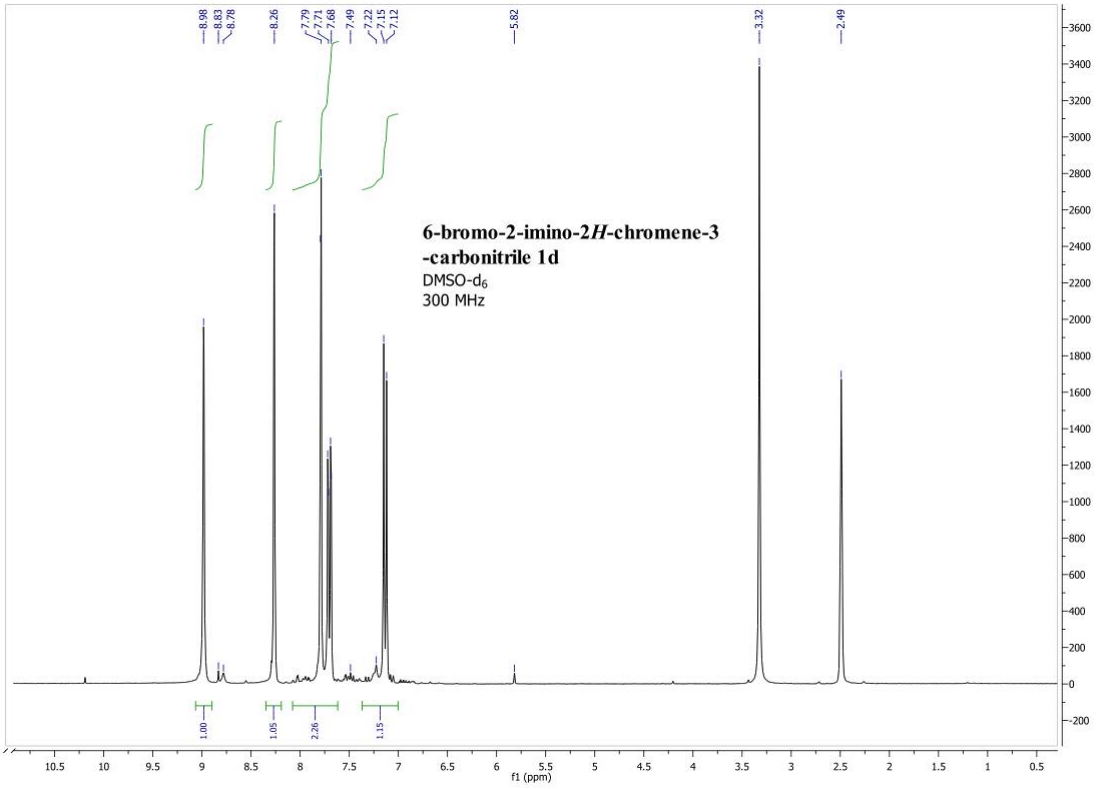
3-carbonitrile 1c
DMSO-d6
f1 (ppm)


8.98
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8.26
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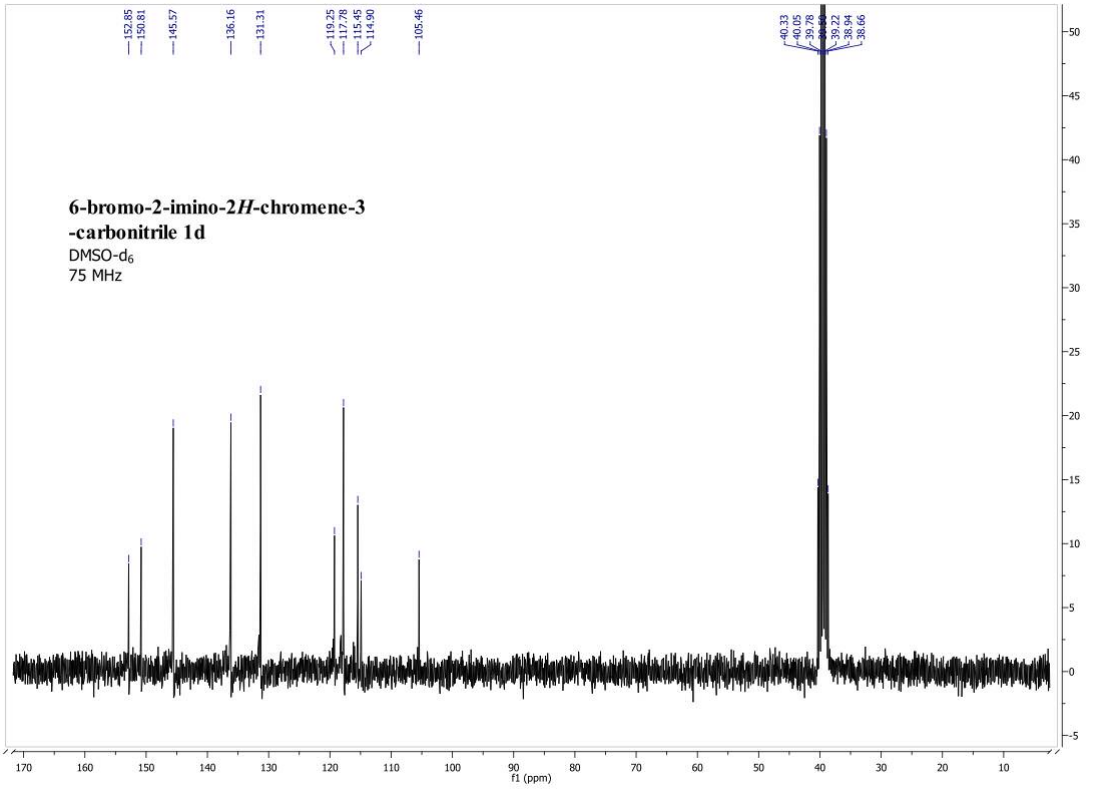
7.71
7.68
7.49
7.22
7.15
7.12
5.82
3.32
2.49
6-bromo-2-imino-2*H*-chromene-3
-carbonitrile 1d
DMSO-d6
300 MHz
1.00
1.05
2.26
1.15
f1 (ppm)


152.85
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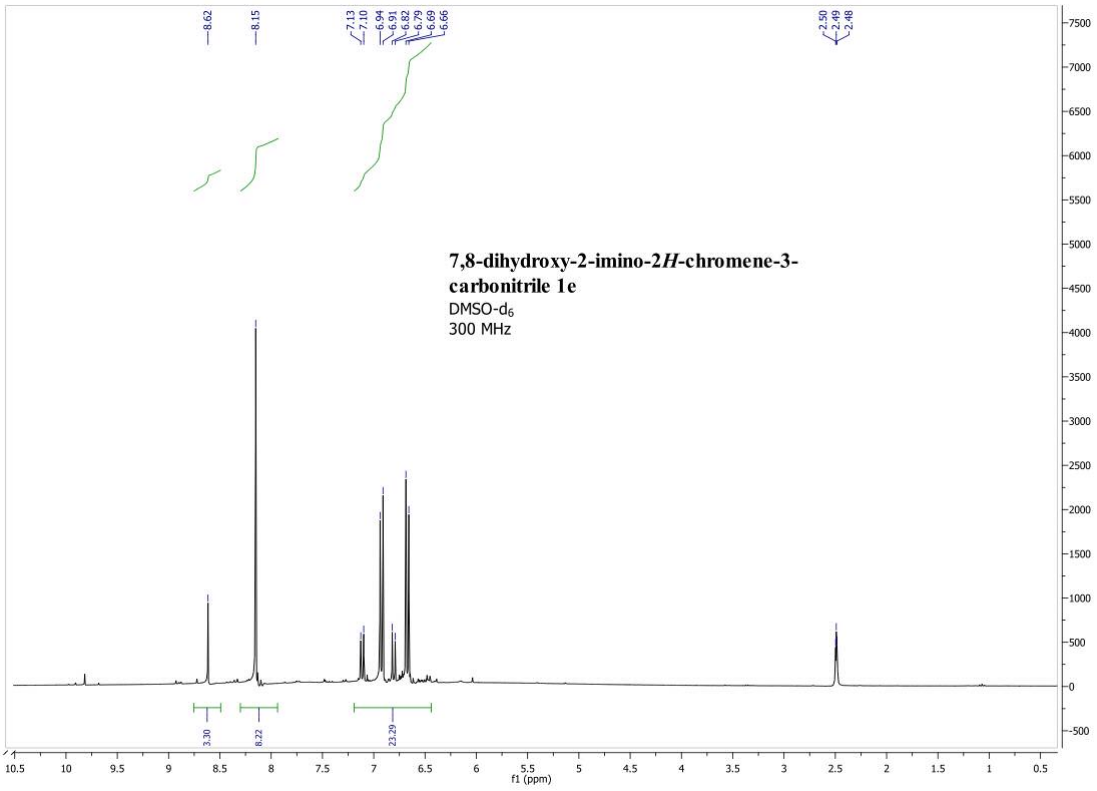
145.57
136.16
131.31
119.25
117.78
115.45
114.90
105.46
40.33
40.05
39.78
39.22
38.94
38.66
6-bromo-2-imino-2*H*-chromene-3
-carbonitrile 1d
DMSO-d6
75 MHz
f1 (ppm)


8.62
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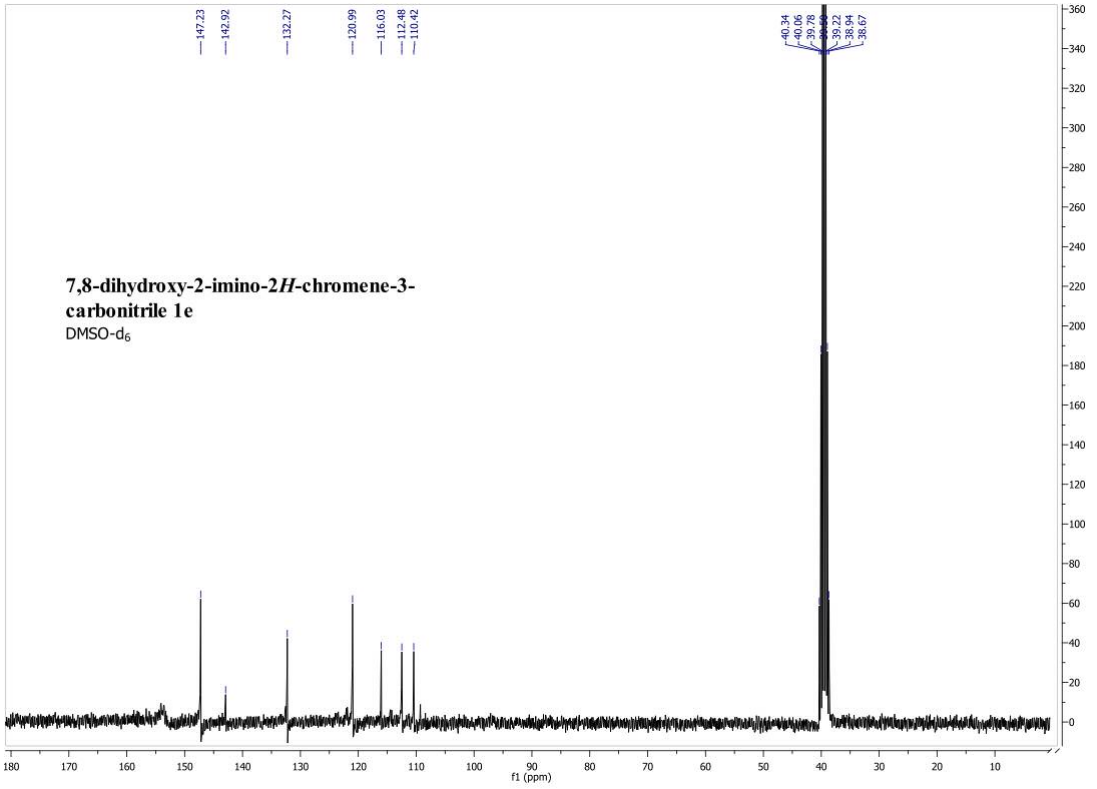
6.91
6.82
6.79
6.69
6.66
2.50
2.49
2.48
7,8-dihydroxy-2-imino-2*H*-chromene-3-carbonitrile 1e
DMSO-d6
300 MHz
3.30
8.22
23.29
f1 (ppm)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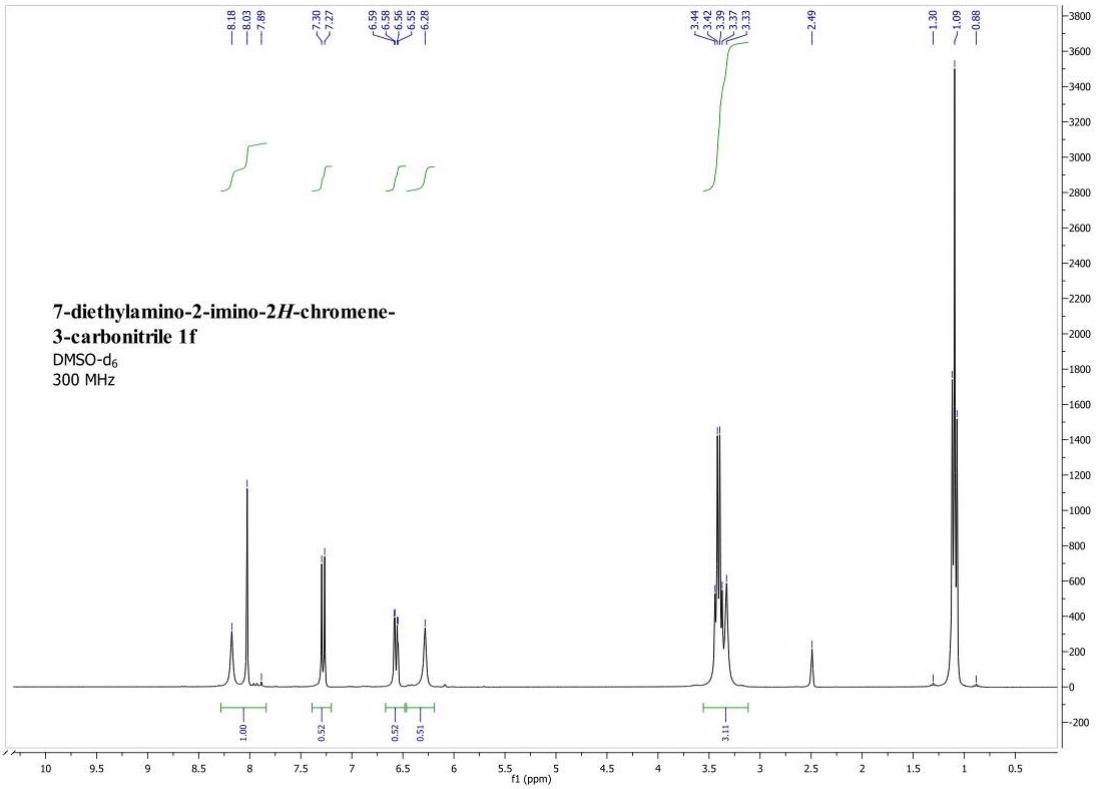
DMSO-d6
f1 (ppm)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6.58
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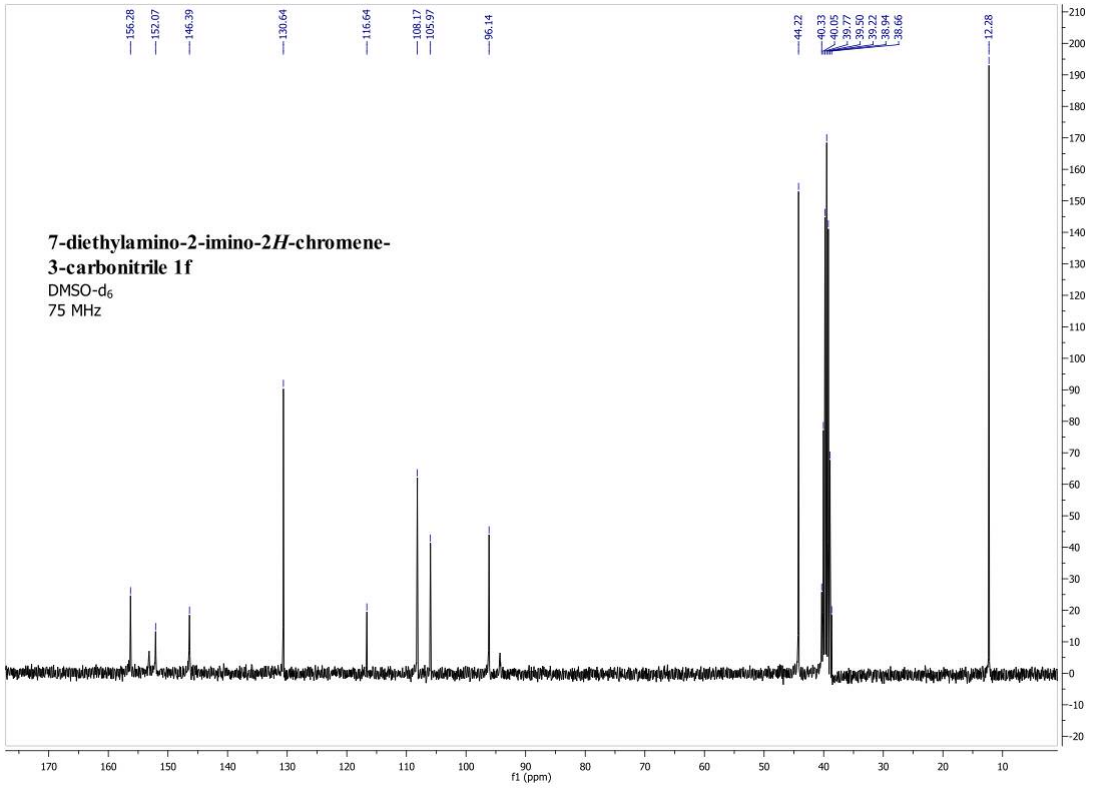
6.55
6.28
3.44
3.42
3.39
3.37
3.33
2.49
1.30
1.09
0.88
7-diethylamino-2-imino-2H-chromene-
3-carbonitrile 1f
DMSO-d6
300 MHz
1.00
0.52
0.52
0.51
3.11
f1 (ppm)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116.64
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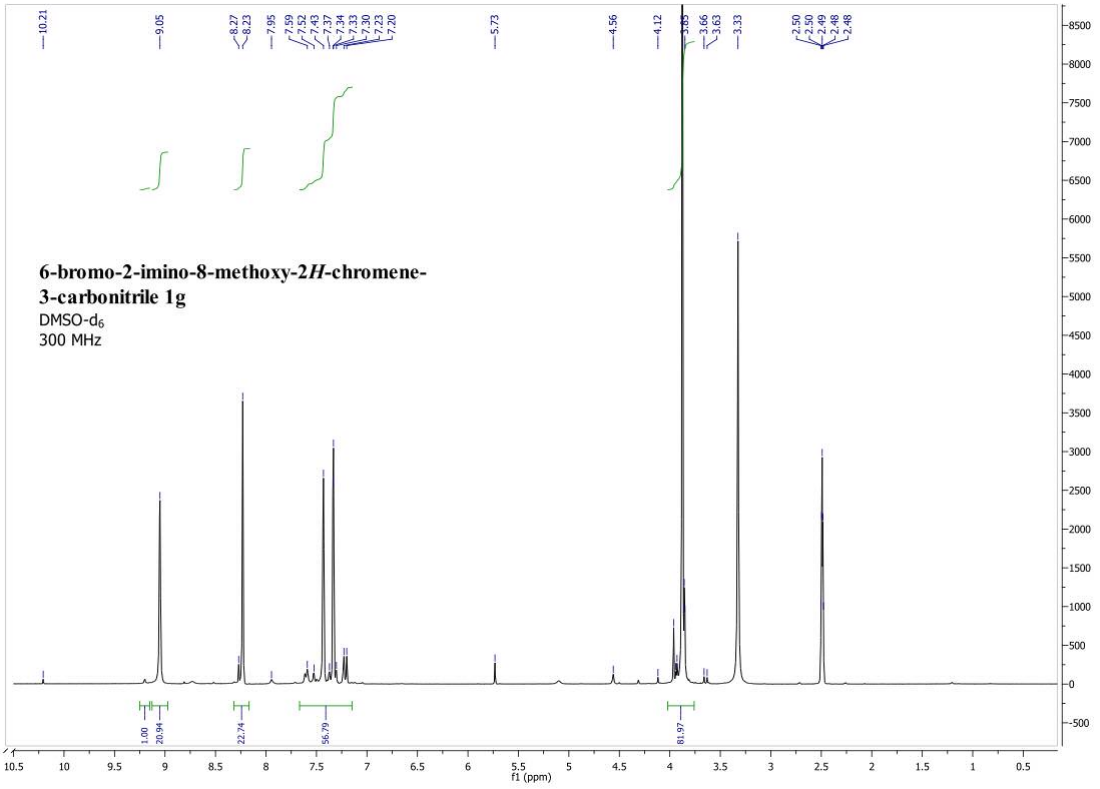
DMSO-d6
75 MHz
f1 (ppm)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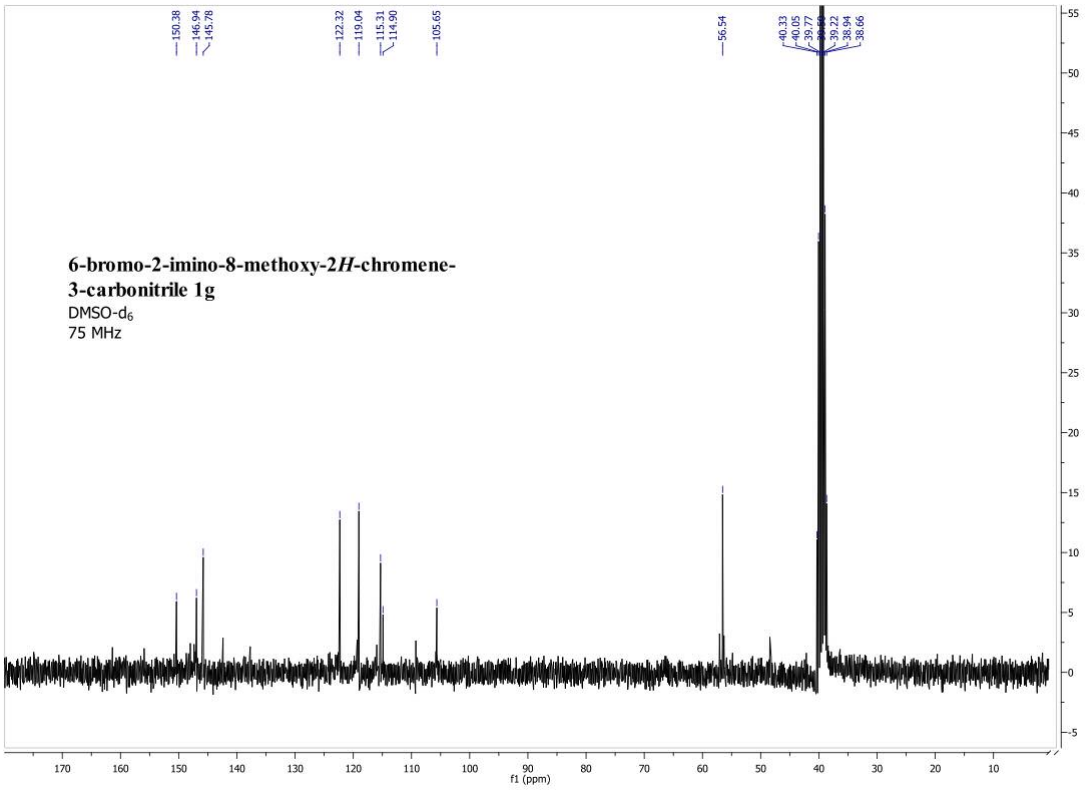
DMSO-d6
300 MHz
f1 (ppm)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39.22
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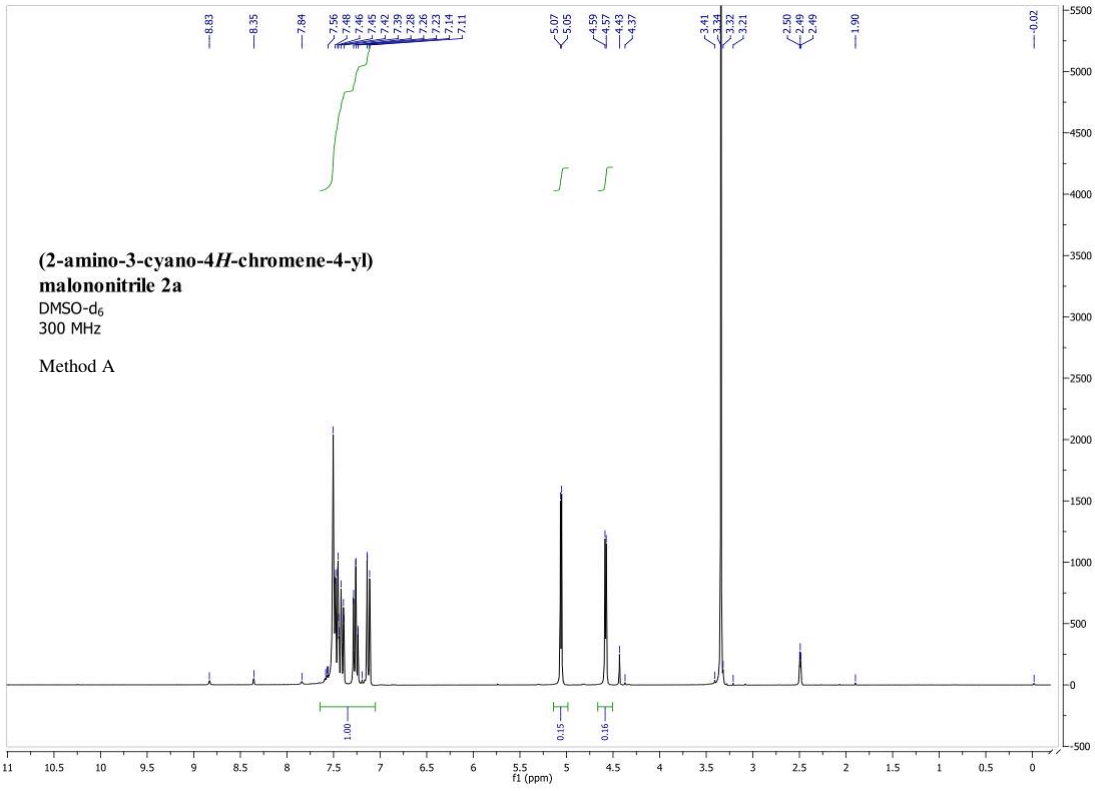
DMSO-d6
75 MHz
f1 (ppm)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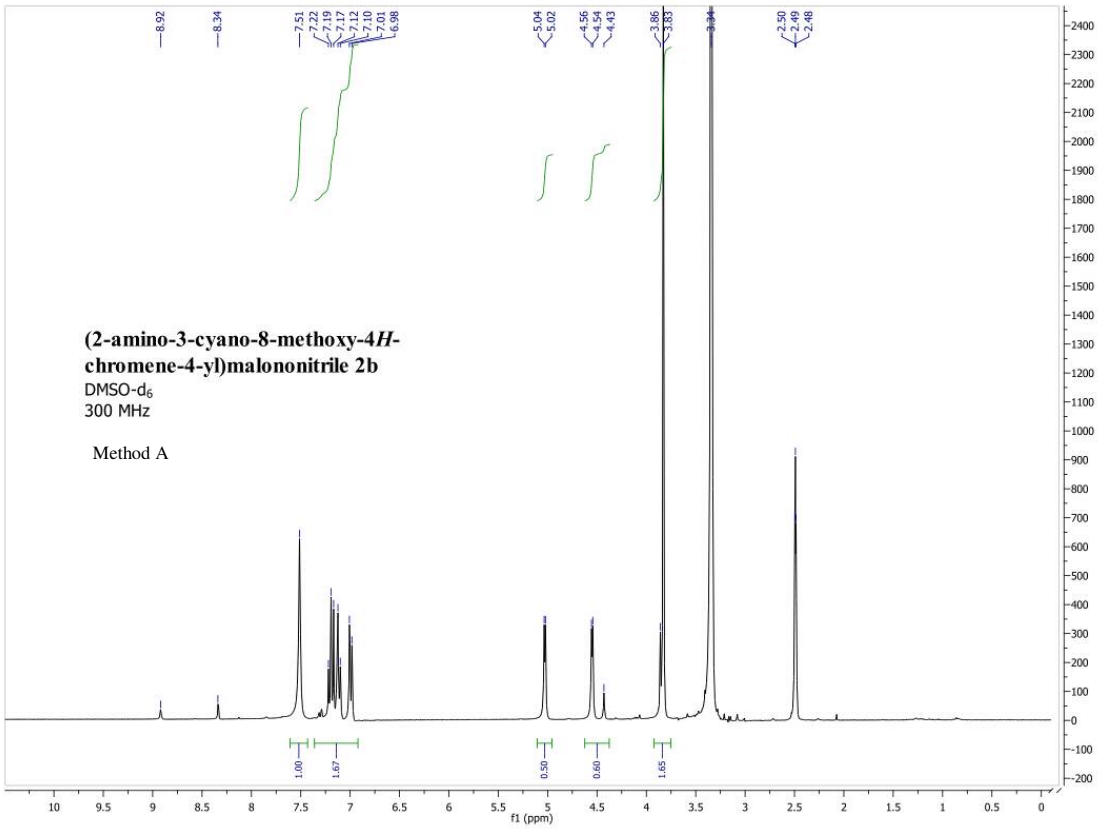
7.14
7.11
5.07
5.05
4.59
4.57
4.43
4.37
3.41
3.34
3.32
3.21
2.50
2.49
2.49
1.90
-0.02
(2-amino-3-cyano-4*H*-chromene-4-yl) malononitrile 2a
DMSO-d6
300 MHz
Method A
1.00
0.15
0.16
f1 (ppm)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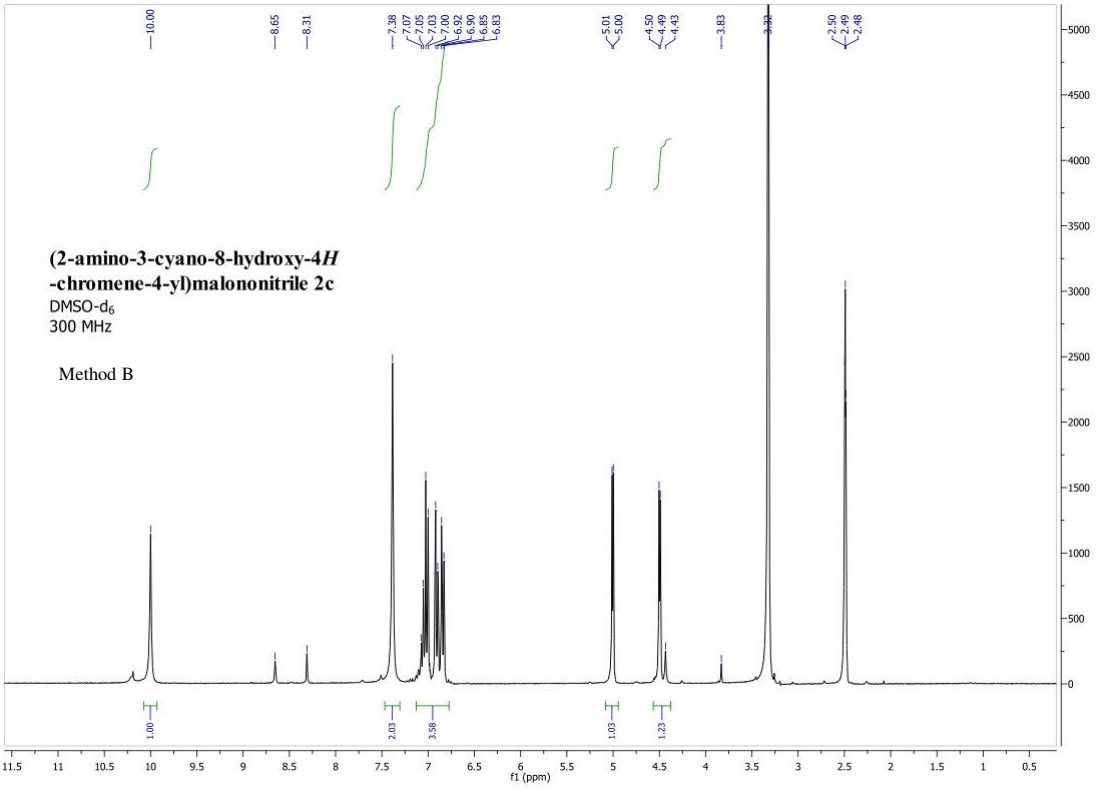
DMSO-d6
300 MHz
Method A
f1 (ppm)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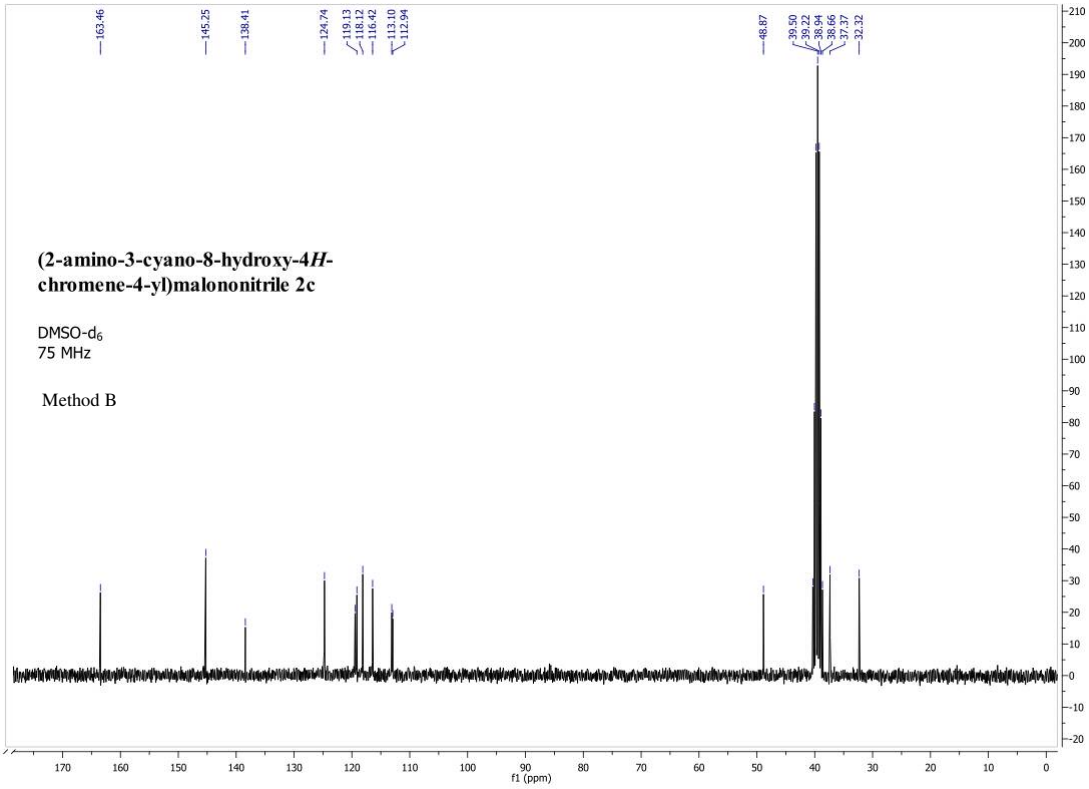
DMSO-d6
300 MHz
Method B
f1 (ppm)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112.94
48.87
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39.22
38.94
38.66
37.37
32.32
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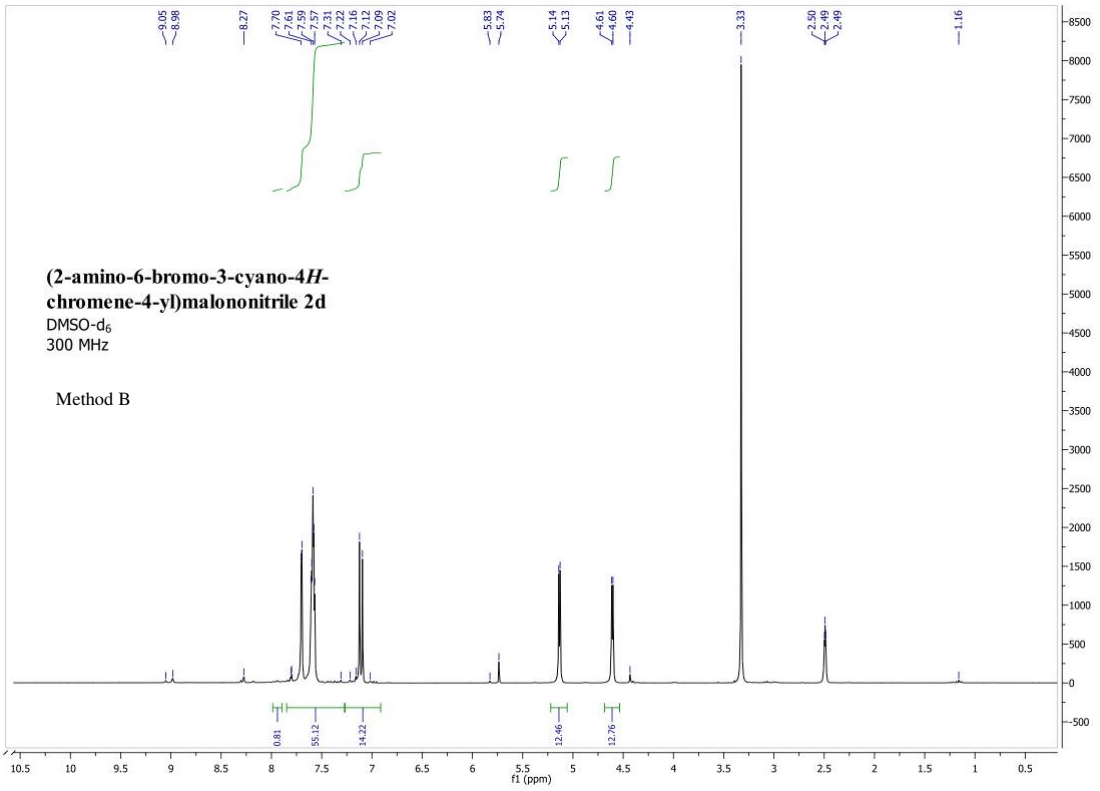
DMSO-d6
75 MHz
Method B
f1 (ppm)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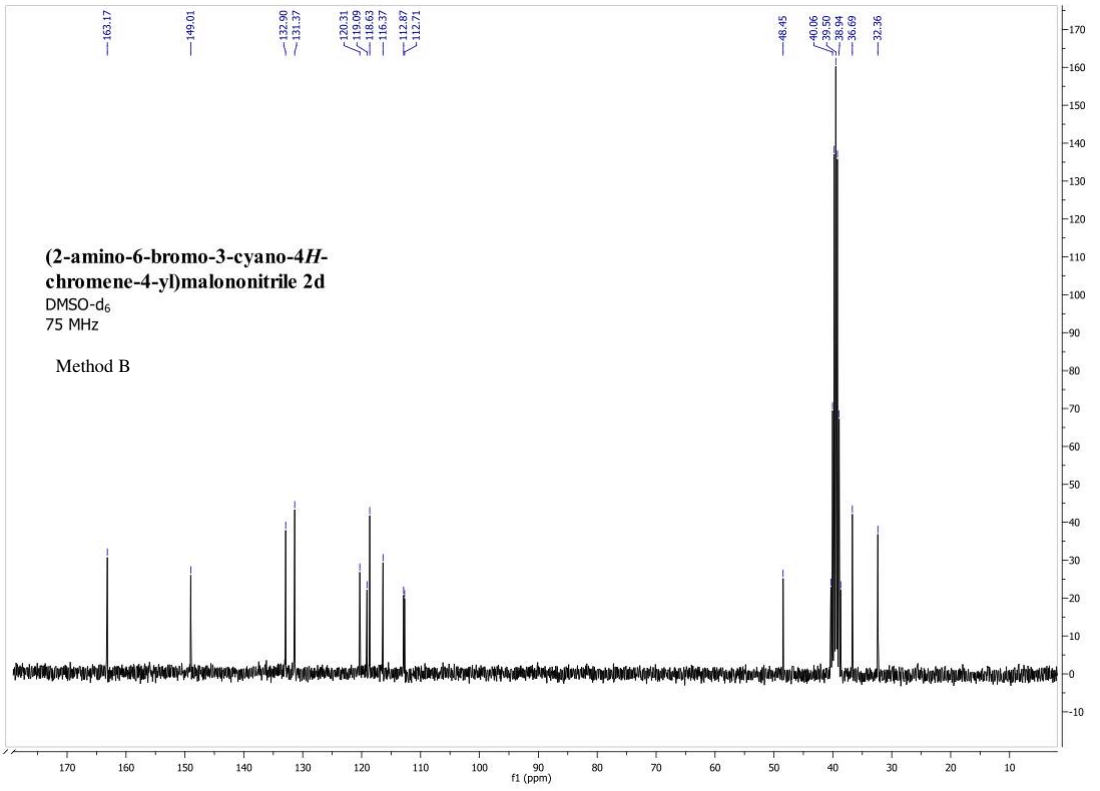
4.61
4.60
4.43
3.33
2.50
2.49
2.49
1.16
(2-amino-6-bromo-3-cyano-4H-chromene-4-yl)malononitrile 2d
DMSO-d6
300 MHz
Method B
0.81
55.12
14.22
12.46
12.76
f1 (ppm)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149.01
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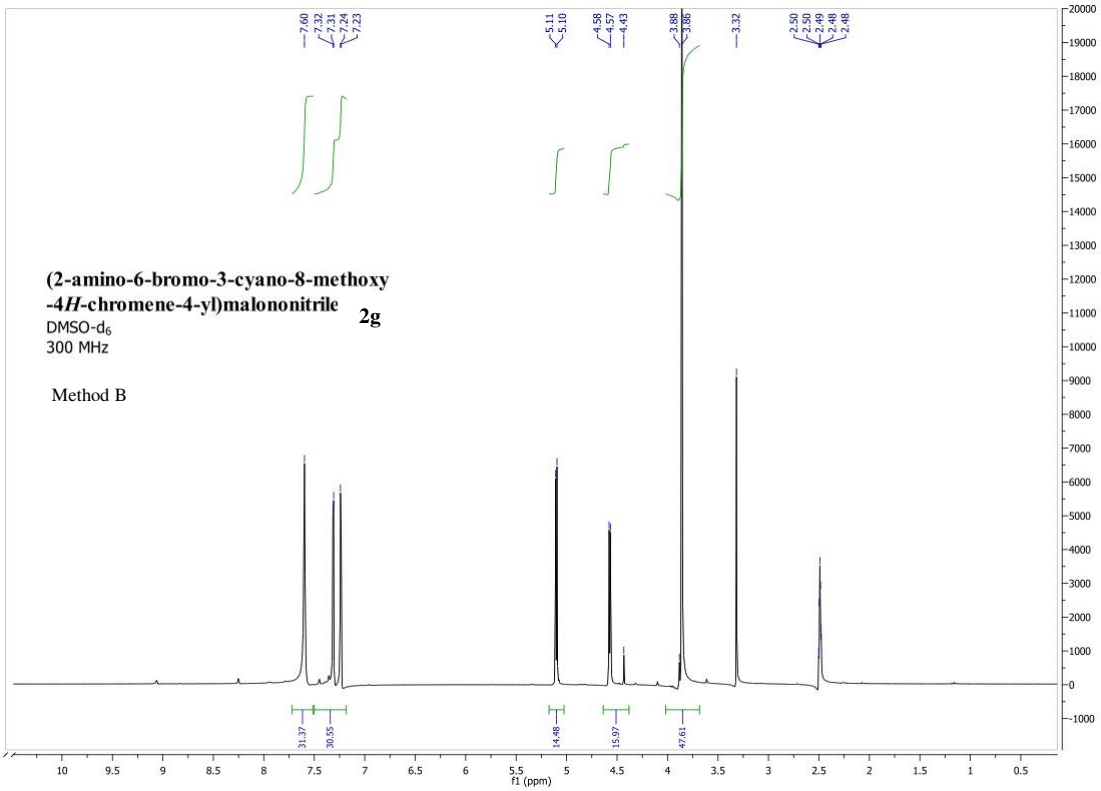
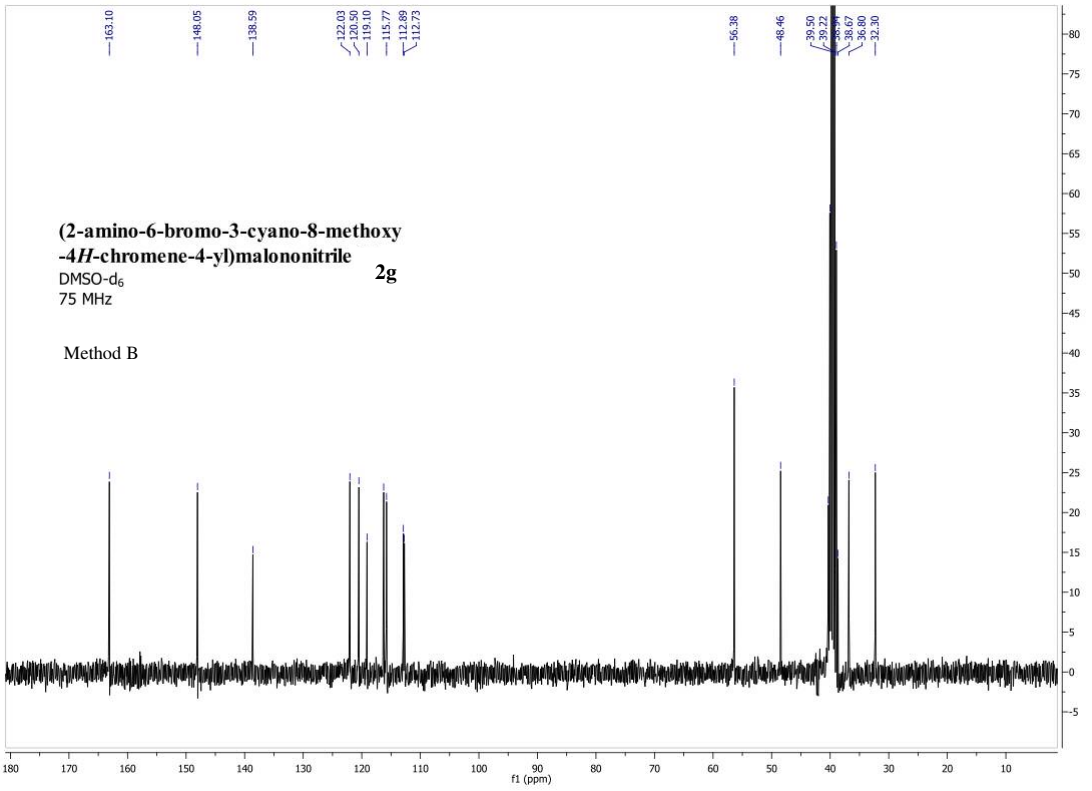
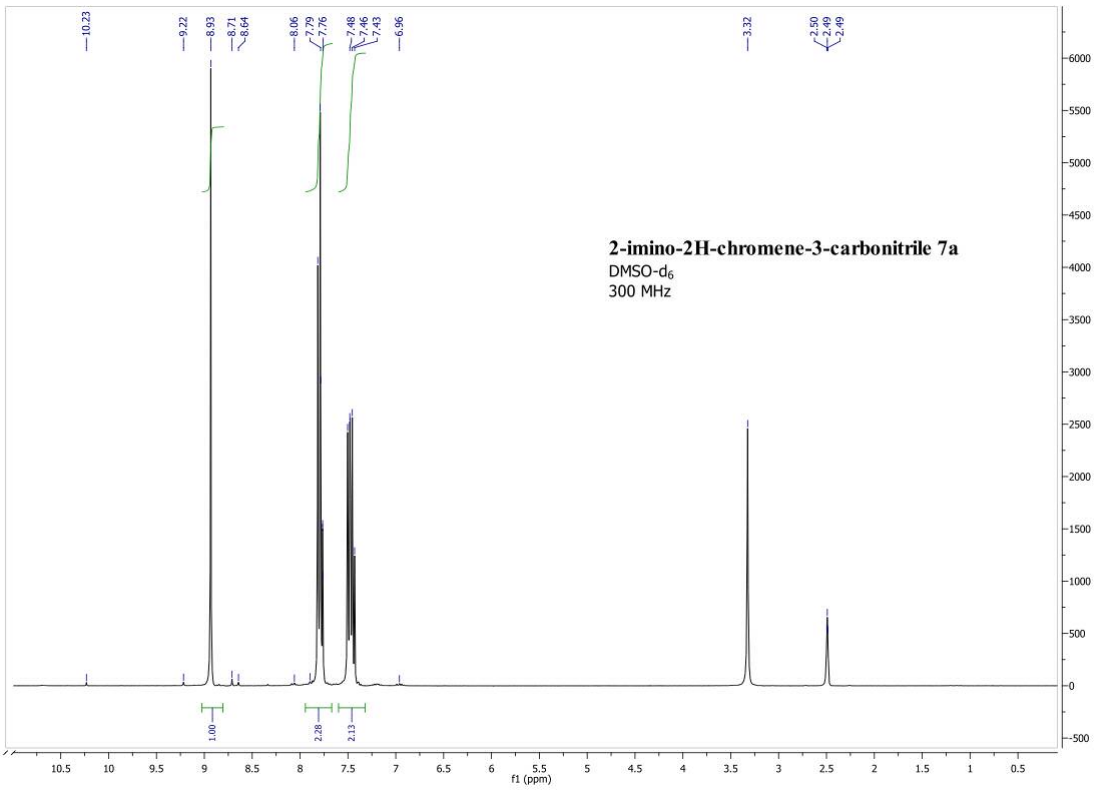
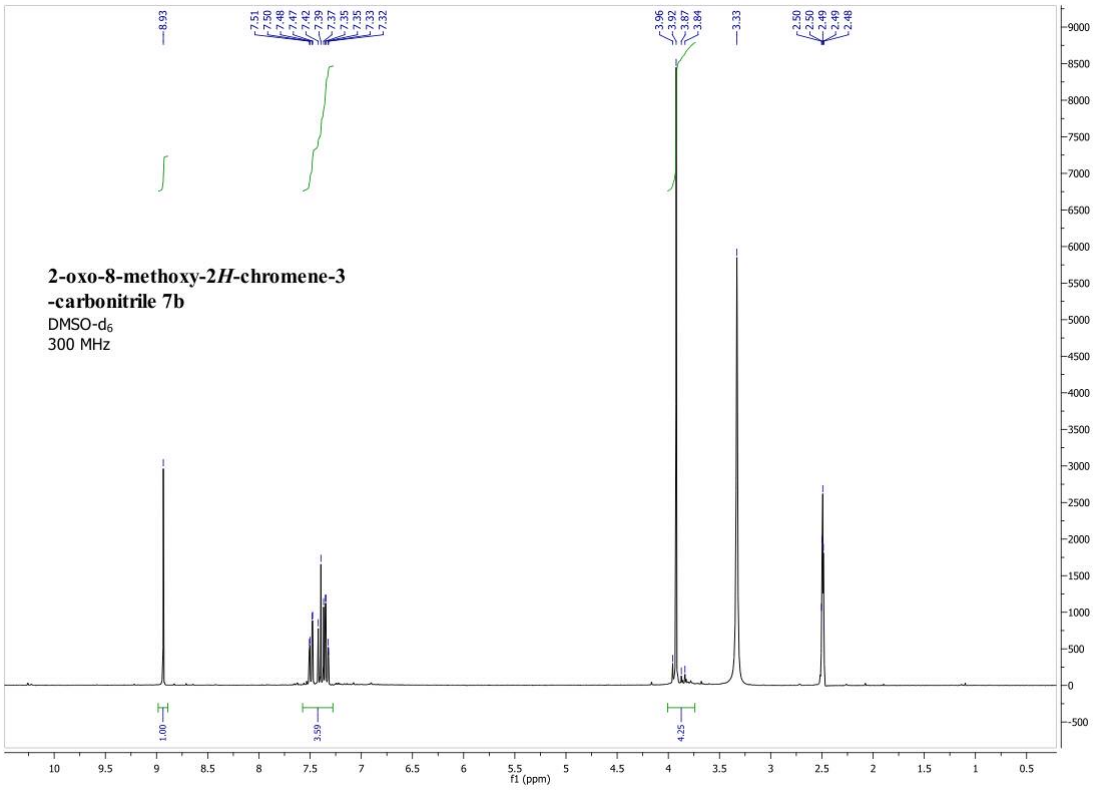
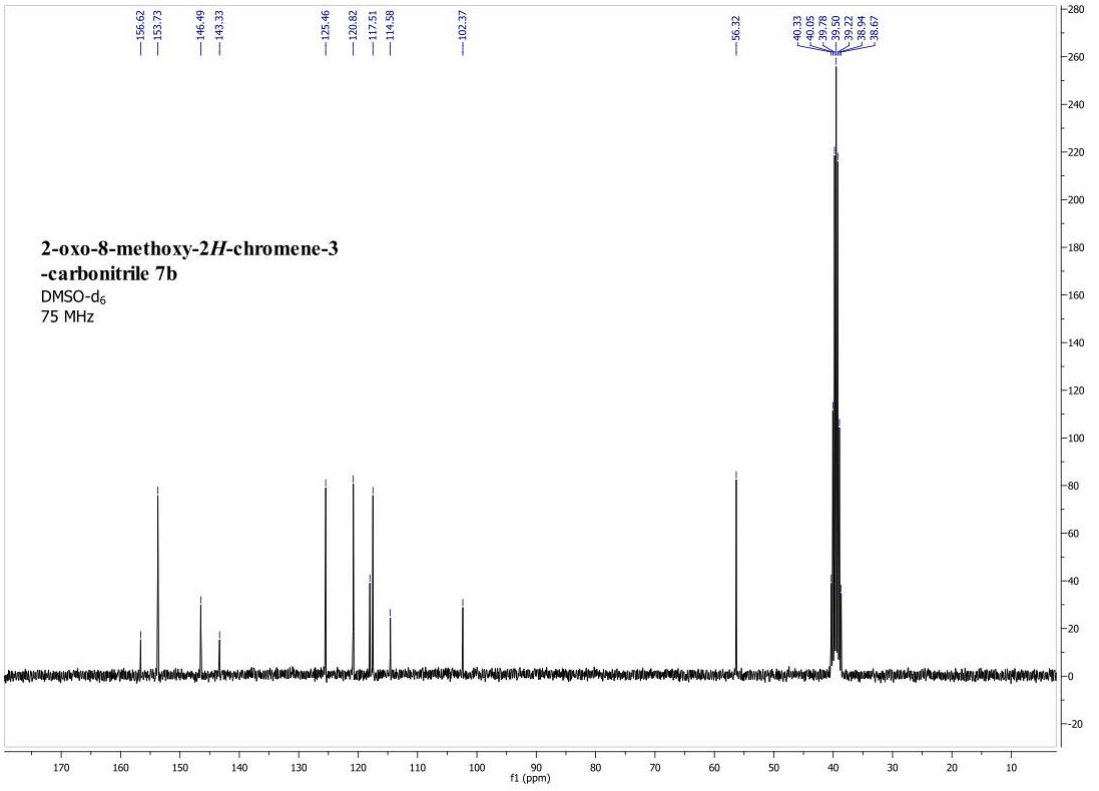
119.09
118.63
116.37
112.87
112.71
48.45
40.06
39.50
38.94
36.69
32.36
(2-amino-6-bromo-3-cyano-4H-chromene-4-yl)malononitrile 2d
DMSO-d6
75 MHz
Method B
f1 (ppm)

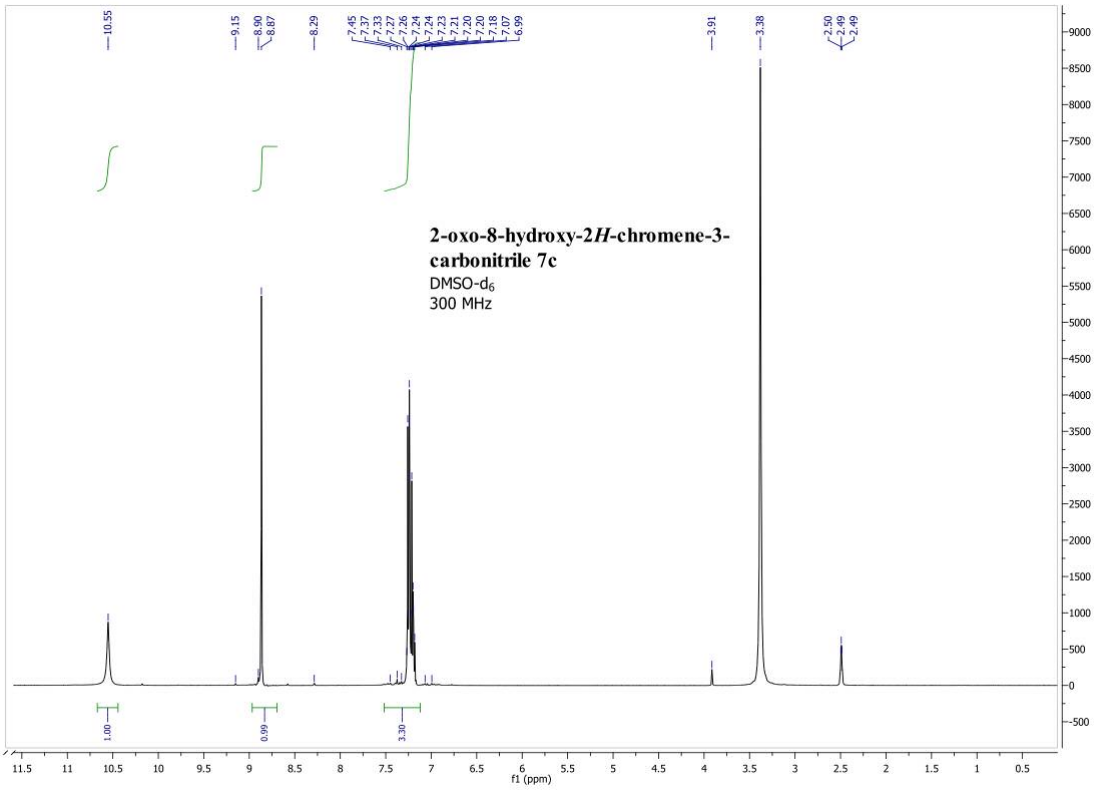

(2-amino-6-bromo-3-cyano-8-methoxy
-4*H*-chromene-4-yl)malononitrile
2g
DMSO-d6
300 MHz
Method B
7.60
7.32
7.31
7.24
7.23
5.11
5.10
4.58
4.57
4.43
3.88
3.86
3.32
2.50
2.50
2.49
2.48
2.48
31.37
30.55
14.48
15.97
47.61
f1 (ppm)

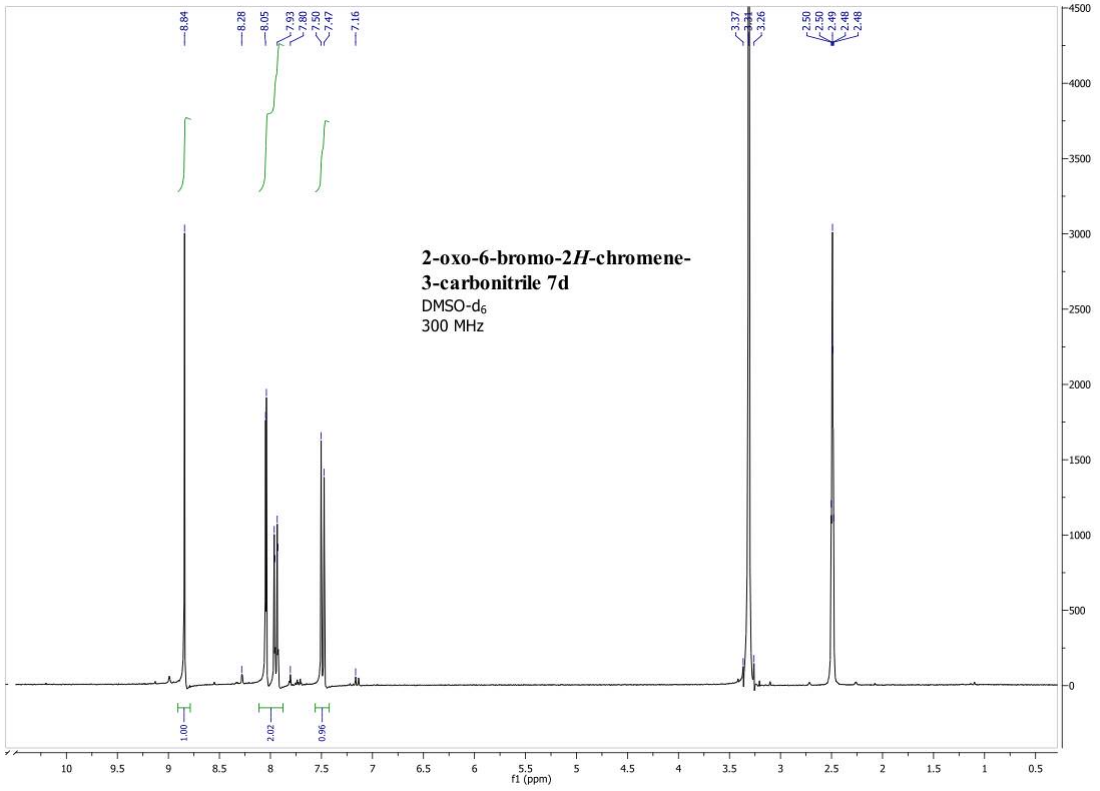

163.10
148.05
138.59
122.03
120.50
119.10
115.77
112.89
112.73
56.38
48.46
39.50
39.22
38.94
38.67
38.39
32.30
(2-amino-6-bromo-3-cyano-8-methoxy
-4*H*-chromene-4-yl)malononitrile
2g
DMSO-d6
75 MHz
Method B
f1 (ppm)

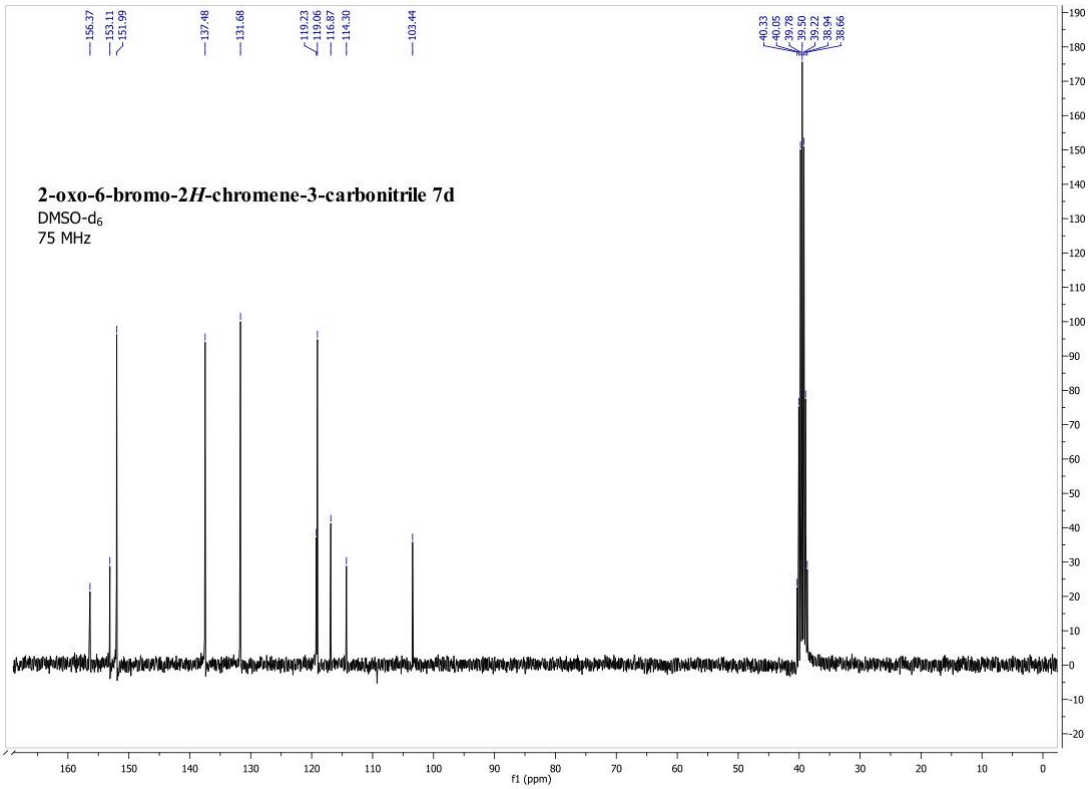

10.23
9.22
8.93
8.71
8.64
8.06
7.79
7.76
7.48
7.46
7.43
6.96
3.32
2.50
2.49
2.49
2-imino-2H-chromene-3-carbonitrile 7a
DMSO-d6
300 MHz
1.00
2.28
2.13
f1 (ppm)

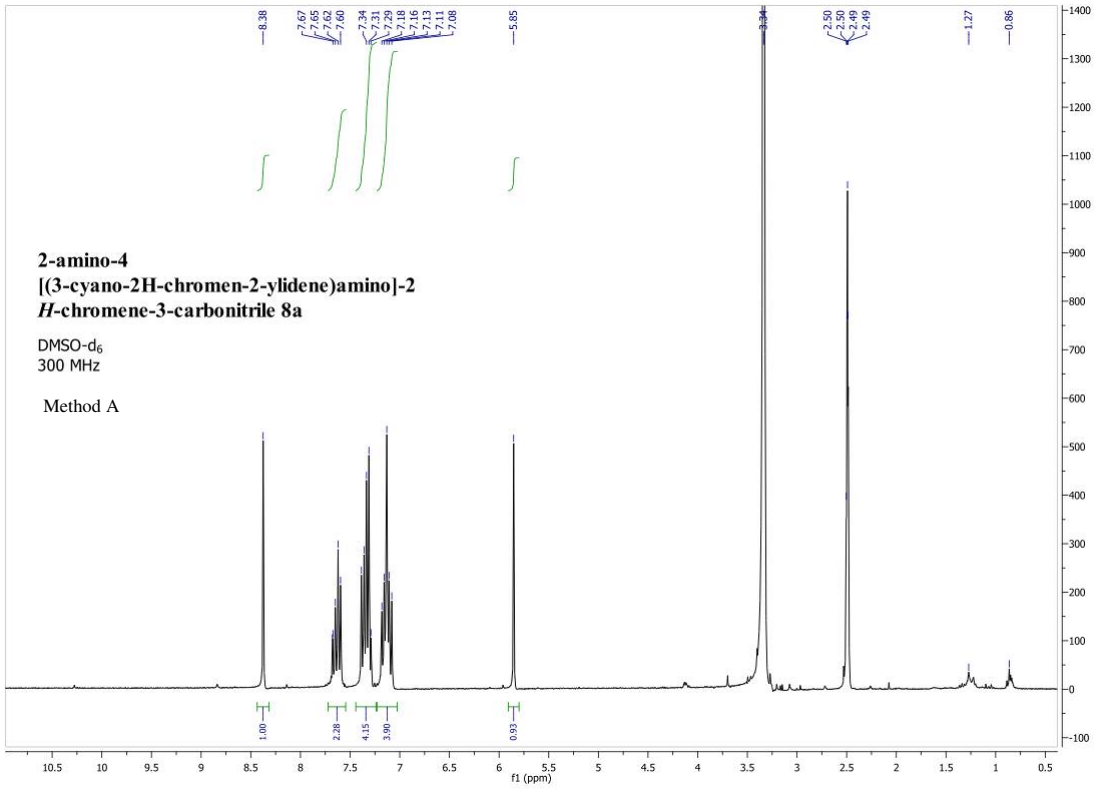

8.93
7.51
7.50
7.48
7.47
7.42
7.39
7.37
7.35
7.35
7.33
7.32
3.96
3.92
3.87
3.84
3.33
2.50
2.50
2.49
2.49
2.48
2-oxo-8-methoxy-2H-chromene-3
-carbonitrile 7b
DMSO-d6
300 MHz
1.00
3.59
4.25
f1 (ppm)

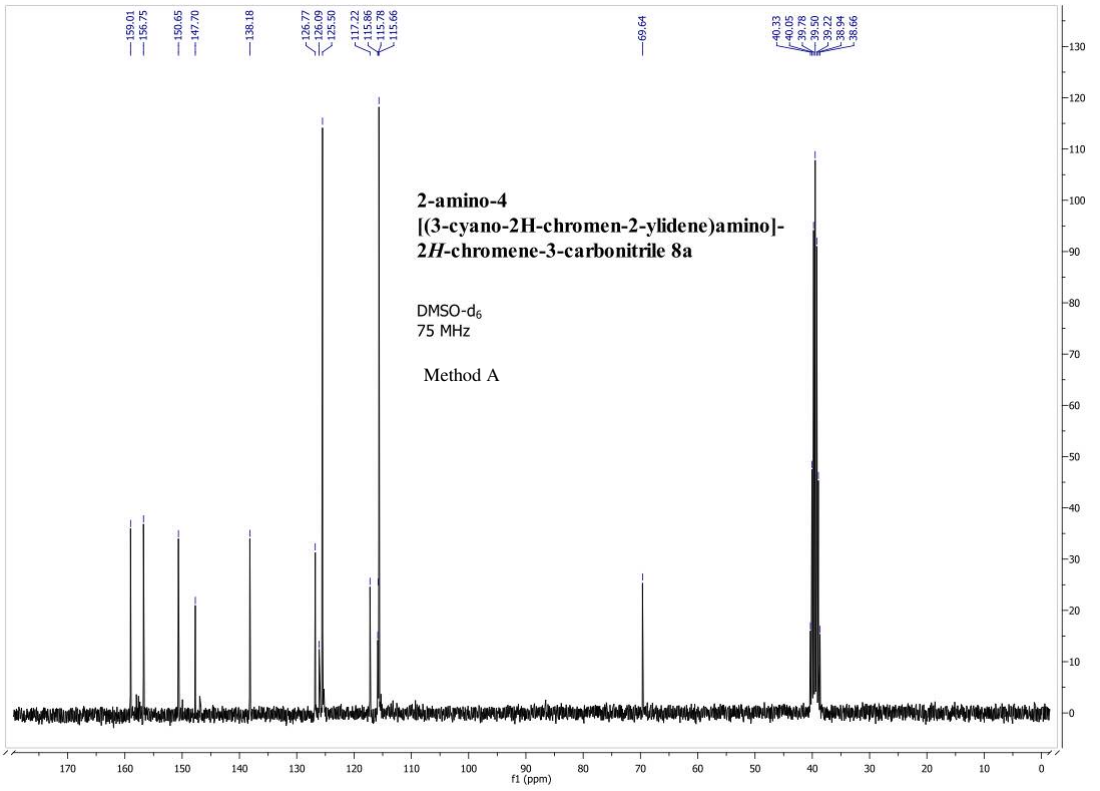

156.62
153.73
146.49
143.33
125.46
120.82
117.51
114.58
102.37
56.32
40.33
40.05
39.78
39.50
39.22
38.94
38.67
2-oxo-8-methoxy-2H-chromene-3
-carbonitrile 7b
DMSO-d6
75 MHz
f1 (ppm)

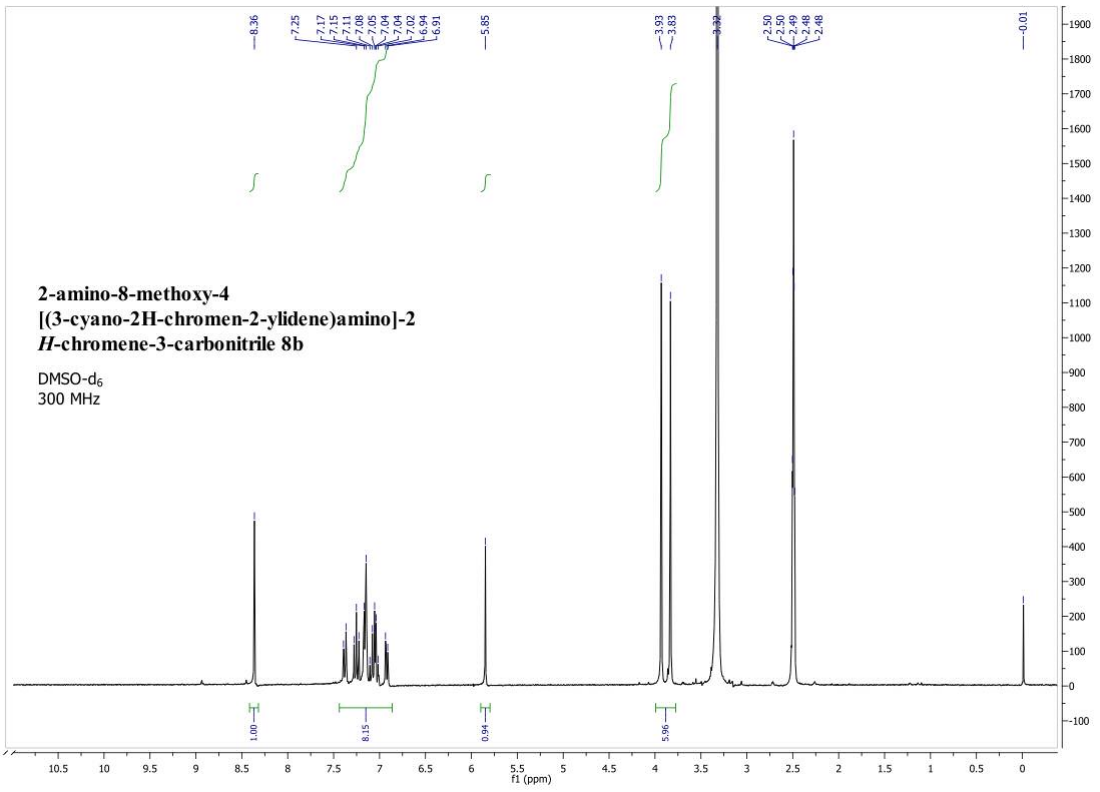

10.55
9.15
8.90
8.87
8.29
7.45
7.37
7.33
7.27
7.26
7.24
7.23
7.21
7.20
7.18
7.07
6.99
3.91
3.38
2.50
2.49
2.49
2-oxo-8-hydroxy-2H-chromene-3-carbonitrile 7c
DMSO-d6
300 MHz
1.00
0.99
3.30
f1 (ppm)

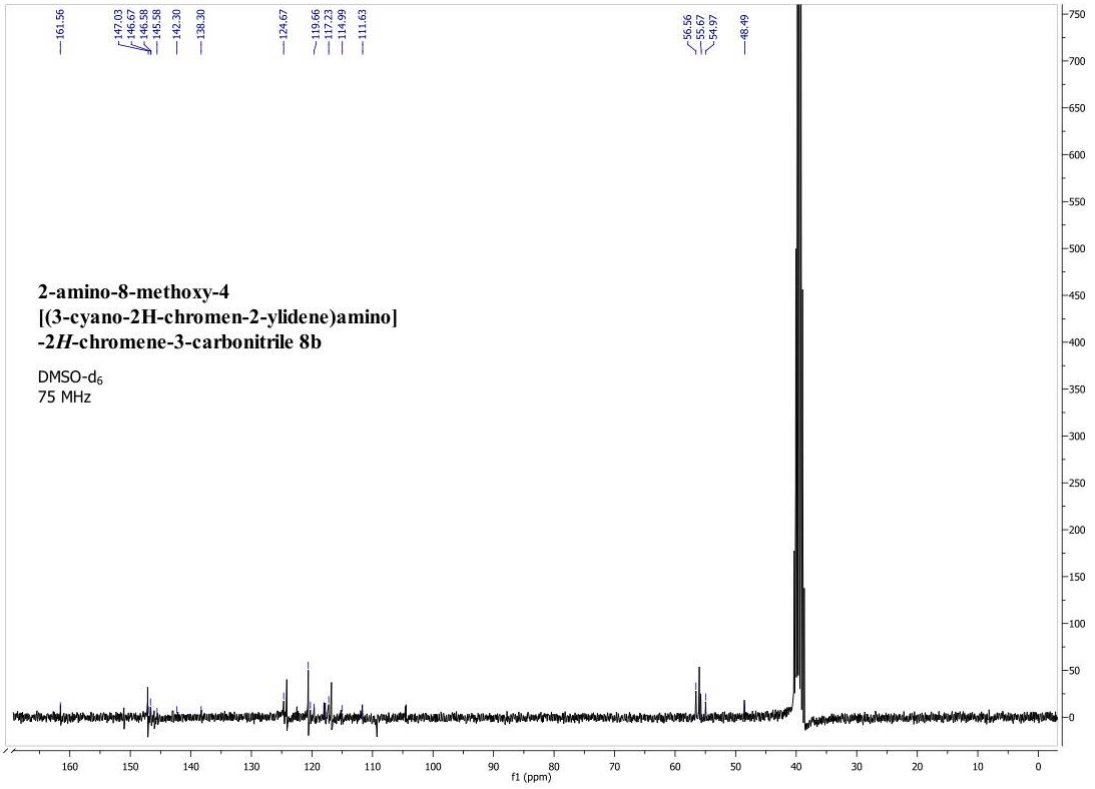

8.84
8.28
8.05
7.93
7.80
7.50
7.47
7.16
3.37
3.31
3.26
2.50
2.50
2.49
2.48
2.48
2-oxo-6-bromo-2H-chromene-3-carbonitrile 7d
DMSO-d6
300 MHz
1.00
2.02
0.96
f1 (ppm)

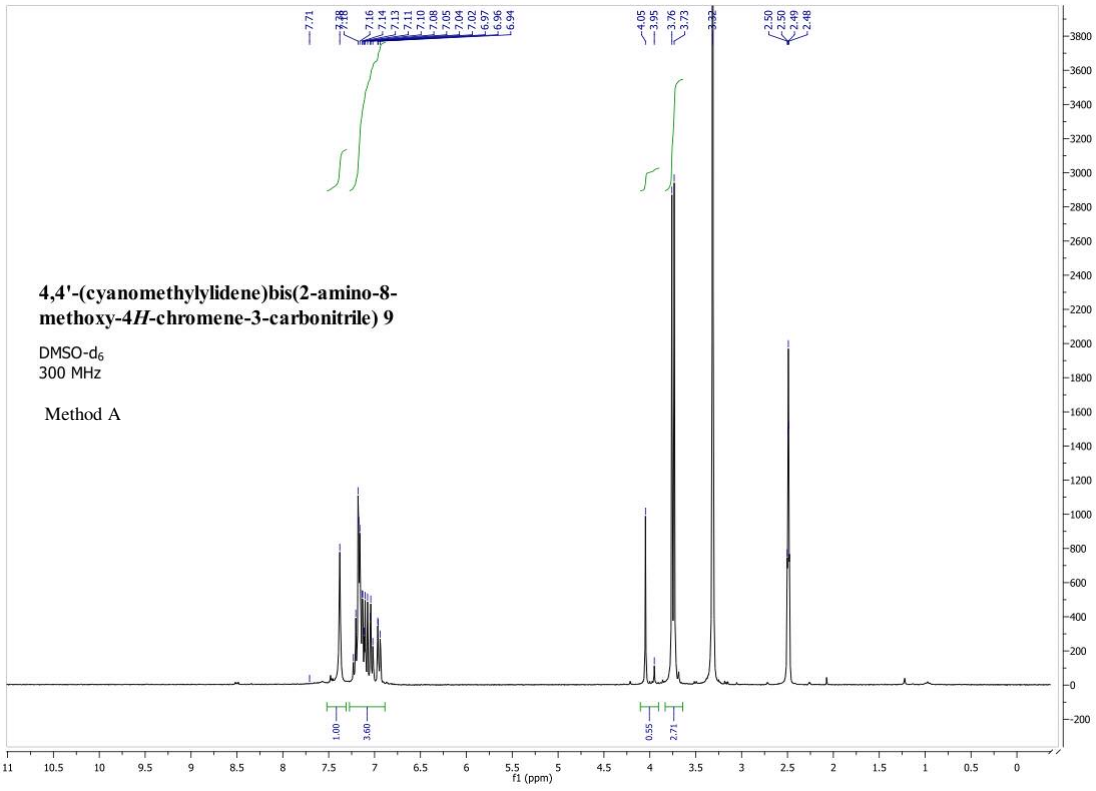

156.37
153.11
151.99
137.48
131.68
119.23
119.06
116.87
114.30
103.44
40.33
40.05
39.78
39.50
39.22
38.94
38.66
2-oxo-6-bromo-2H-chromene-3-carbonitrile 7d
DMSO-d6
75 MHz
f1 (ppm)

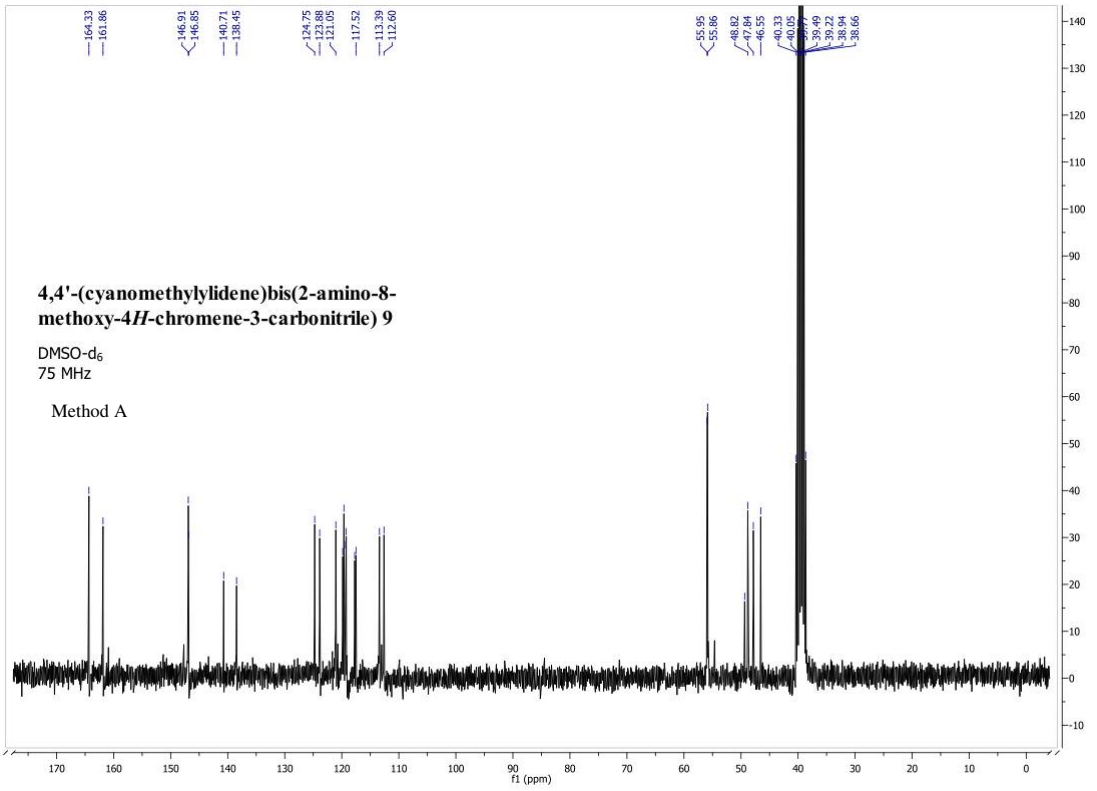

8.38
7.67
7.65
7.62
7.60
7.34
7.31
7.29
7.18
7.16
7.13
7.11
7.08
5.85
3.34
2.50
2.50
2.49
2.49
1.27
0.86
2-amino-4
[(3-cyano-2H-chromen-2-ylidene)amino]-2
H-chromene-3-carbonitrile 8a
DMSO-d6
300 MHz
Method A
1.00
2.28
4.15
3.90
0.93
f1 (ppm)

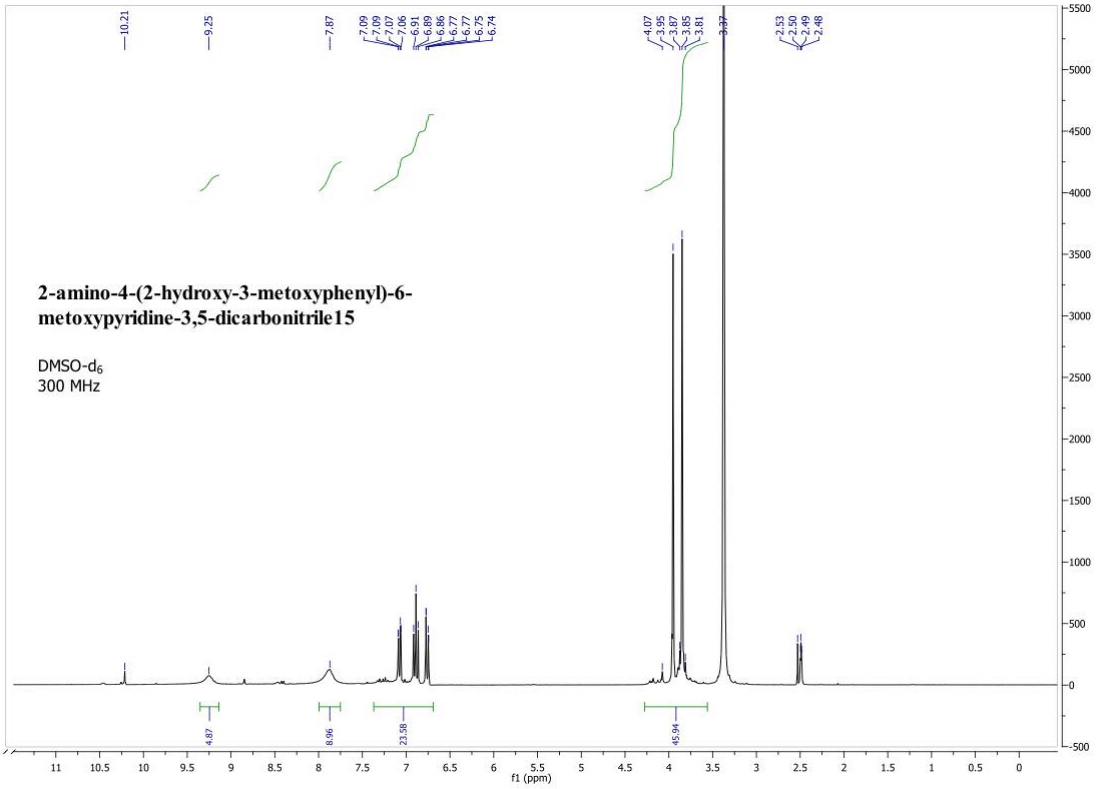

159.01
156.75
150.65
147.70
138.18
126.77
126.09
125.50
117.22
115.86
115.78
115.66
69.64
40.33
40.05
39.78
39.50
39.22
38.94
38.66
2-amino-4
[(3-cyano-2H-chromen-2-ylidene)amino]-
2H-chromene-3-carbonitrile 8a
DMSO-d6
75 MHz
Method A
f1 (ppm)

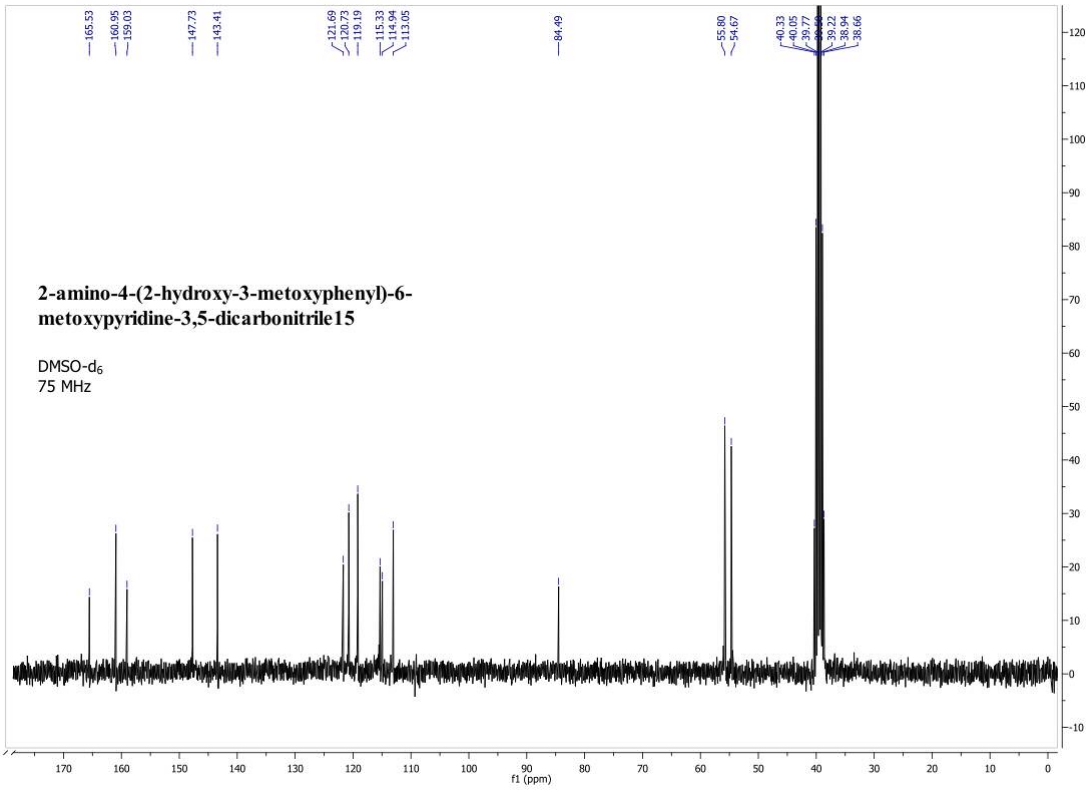

8.36
7.25
7.17
7.15
7.11
7.08
7.05
7.04
7.04
7.02
6.94
6.91
5.85
3.93
3.83
3.32
2.50
2.50
2.49
2.48
2.48
-0.01
2-amino-8-methoxy-4
[(3-cyano-2H-chromen-2-ylidene)amino]-2
H-chromene-3-carbonitrile 8b
DMSO-d6
300 MHz
1.00
8.15
0.94
5.96
f1 (ppm)

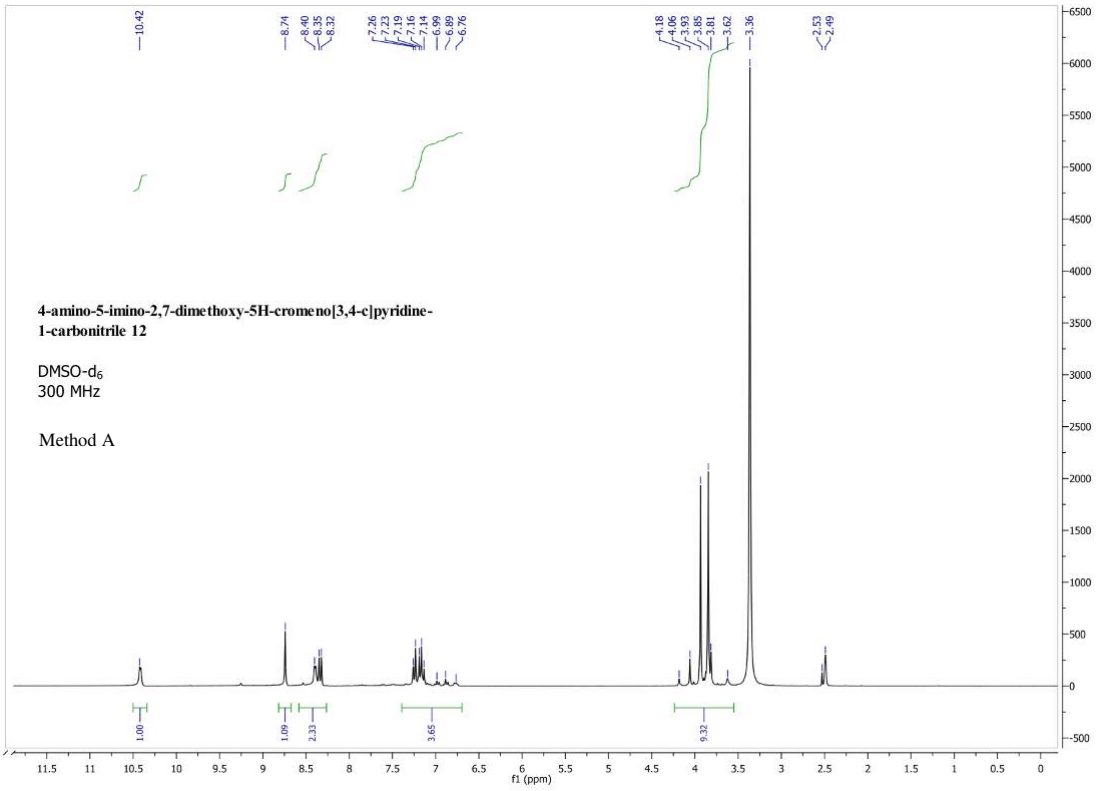

161.56
147.03
146.67
146.58
145.58
142.30
138.30
124.67
119.66
117.23
114.99
111.63
56.56
55.67
54.97
48.49
2-amino-8-methoxy-4
[(3-cyano-2H-chromen-2-ylidene)amino]
-2H-chromene-3-carbonitrile 8b
DMSO-d6
75 MHz
f1 (ppm)

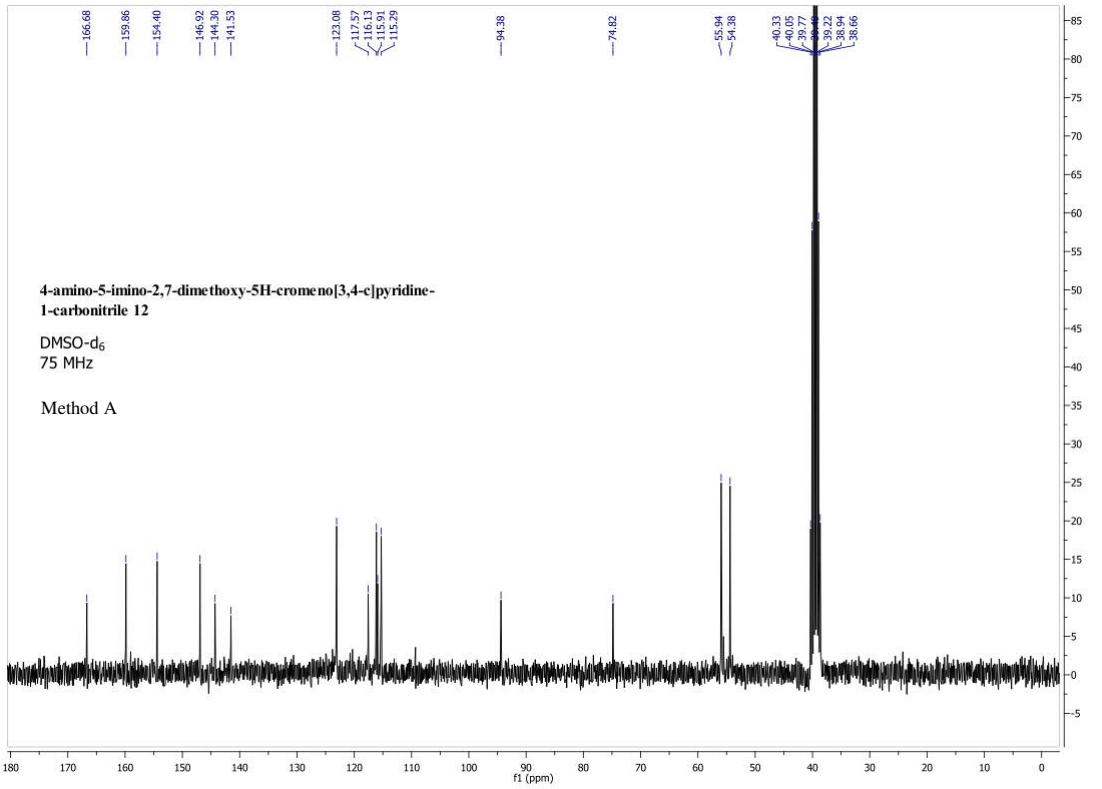

7.71
7.16
7.14
7.13
7.11
7.10
7.08
7.05
7.04
7.02
6.97
6.96
6.94
4.05
3.95
3.76
3.73
2.50
2.50
2.49
2.48
4,4'-(cyanomethylylidene)bis(2-amino-8-
methoxy-4H-chromene-3-carbonitrile) 9
DMSO-d6
300 MHz
Method A
1.00
3.60
0.55
2.71
f1 (ppm)

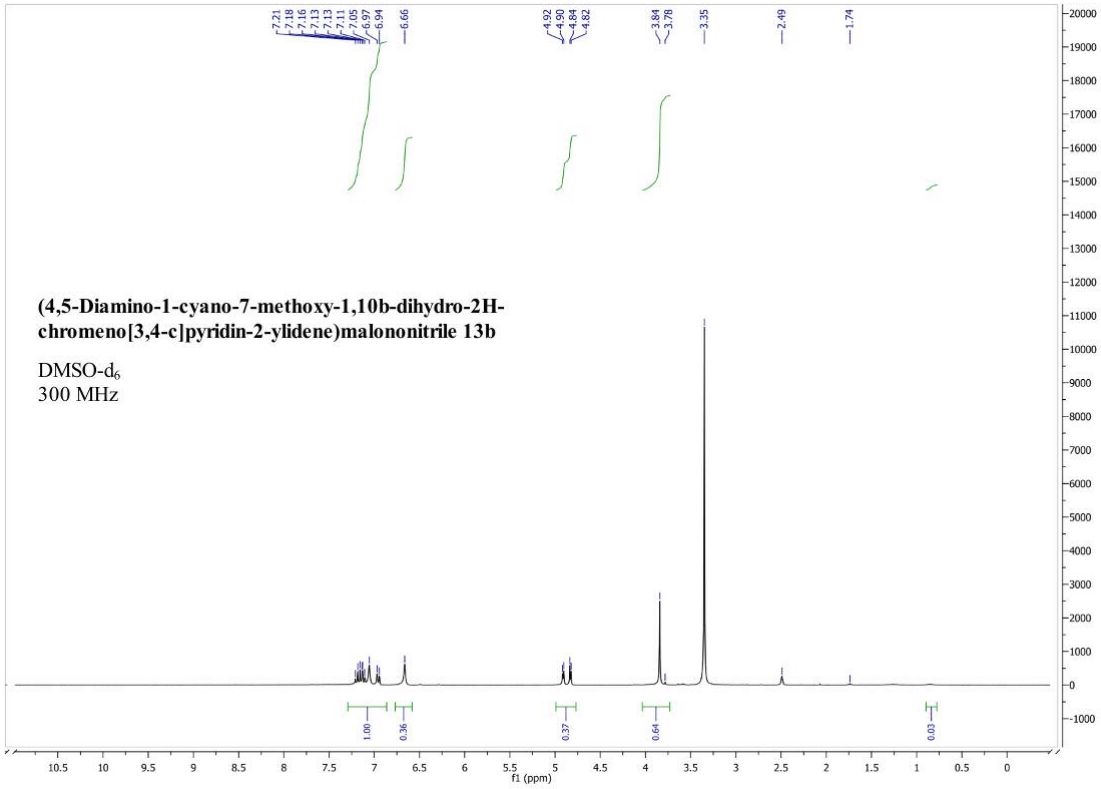

164.33
161.86
146.91
146.85
140.71
138.45
124.75
123.88
121.05
117.52
113.39
112.60
55.95
55.86
48.82
47.84
46.55
40.33
40.05
39.67
39.49
39.22
38.94
38.66
4,4'-(cyanomethylylidene)bis(2-amino-8-methoxy-4H-chromene-3-carbonitrile) 9
DMSO-d6
75 MHz
Method A
f1 (ppm)

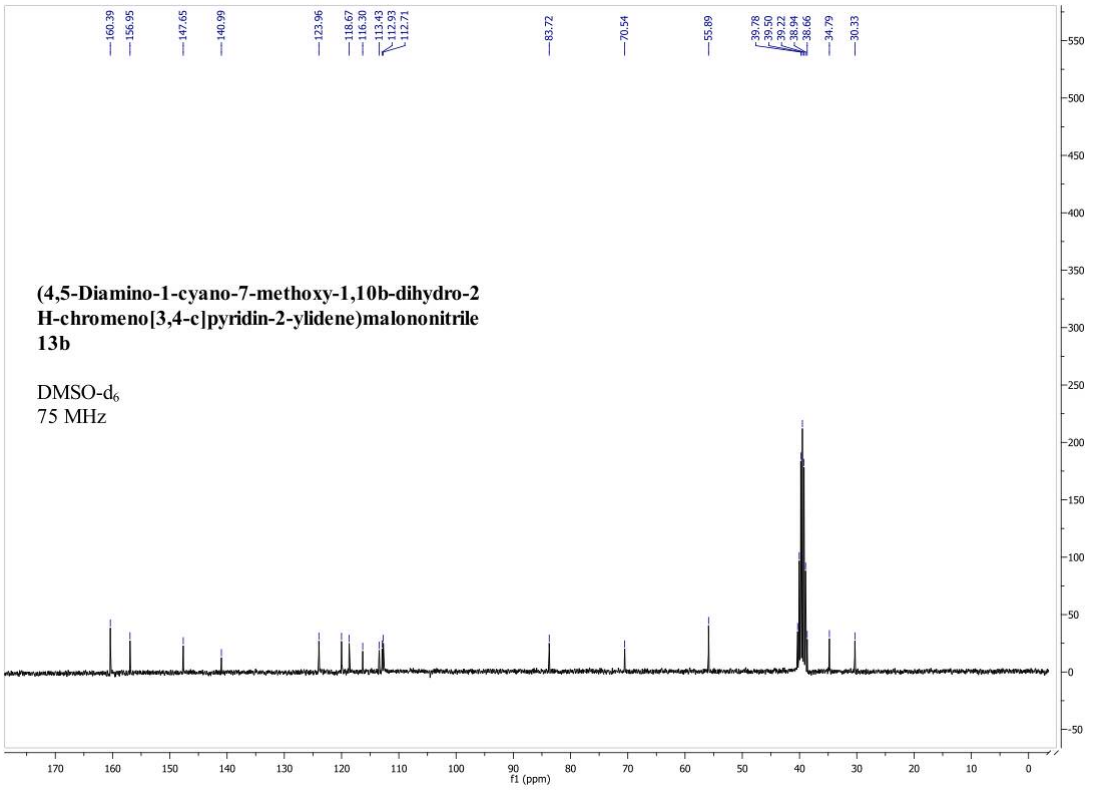

10.21
9.25
7.87
7.09
7.09
7.07
7.06
6.91
6.89
6.86
6.77
6.77
6.75
6.74
4.07
3.95
3.87
3.85
3.81
3.37
2.53
2.50
2.49
2.48
2-amino-4-(2-hydroxy-3-metoxyphenyl)-6-metoxypyridine-3,5-dicarbonitrile15
DMSO-d6
300 MHz
4.87
8.66
23.58
45.94
f1 (ppm)

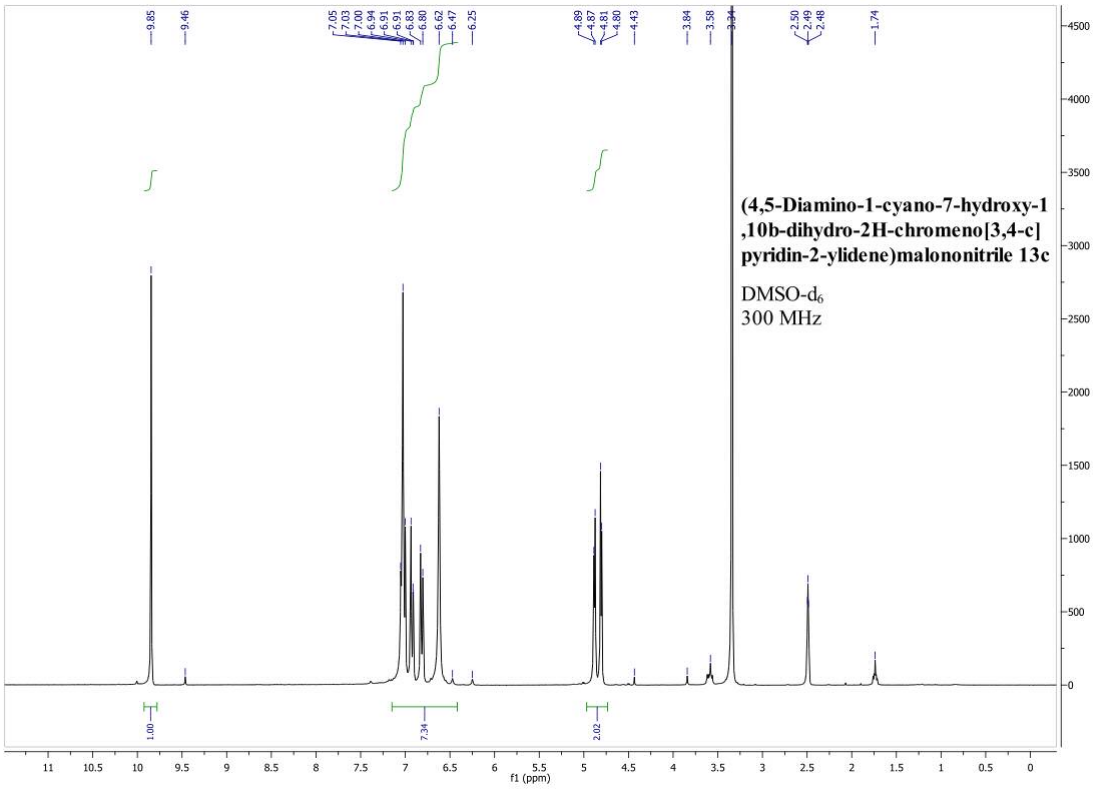

165.53
160.95
159.03
147.73
143.41
121.69
120.73
119.19
115.33
114.94
113.05
84.49
55.80
54.67
40.33
40.05
39.77
39.49
39.22
38.94
38.66
2-amino-4-(2-hydroxy-3-metoxyphenyl)-6-metoxypyridine-3,5-dicarbonitrile15
DMSO-d6
75 MHz
f1 (ppm)

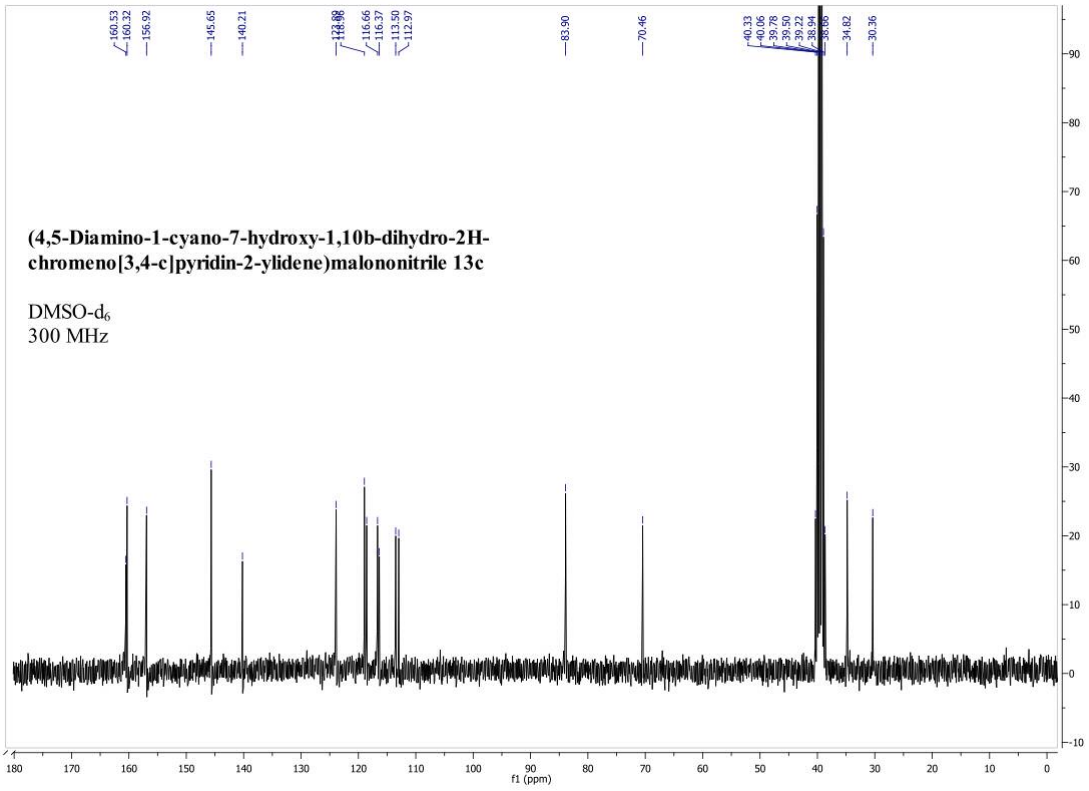

10.42
8.74
8.40
8.35
8.32
7.26
7.23
7.19
7.16
7.14
6.99
6.89
6.76
4.18
4.06
3.93
3.85
3.81
3.62
3.36
2.53
2.49
4-amino-5-imino-2,7-dimethoxy-5H-cromeno[3,4-c]pyridine-1-carbonitrile 12
DMSO-d6
300 MHz
Method A
1.00
1.09
2.33
3.65
9.32
f1 (ppm)


166.68
159.86
154.40
146.92
144.30
141.53
123.08
117.57
116.13
115.91
115.29
94.38
74.82
55.94
54.38
40.33
40.05
39.77
39.22
38.94
38.66
4-amino-5-imino-2,7-dimethoxy-5H-cromeno[3,4-c]pyridine-1-carbonitrile 12
DMSO-d6
75 MHz
Method A
f1 (ppm)


7.21
7.18
7.16
7.13
7.11
7.05
6.97
6.94
6.66
4.92
4.90
4.84
4.82
3.84
3.78
3.35
2.49
1.74
(4,5-Diamino-1-cyano-7-methoxy-1,10b-dihydro-2H-chromeno[3,4-c]pyridin-2-ylidene)malononitrile 13b
DMSO-d6
300 MHz
1.00
0.36
0.37
0.64
0.03
f1 (ppm)


160.39
156.95
147.65
140.99
123.96
118.67
116.30
113.43
112.93
112.71
83.72
70.54
55.89
39.78
39.50
39.22
38.94
38.66
34.79
30.33
(4,5-Diamino-1-cyano-7-methoxy-1,10b-dihydro-2H-chromeno[3,4-c]pyridin-2-ylidene)malononitrile 13b
DMSO-d6
75 MHz
f1 (ppm)


9.85
9.46
7.05
7.03
7.00
6.94
6.91
6.83
6.80
6.62
6.47
6.25
4.89
4.87
4.81
4.80
4.43
3.84
3.58
3.24
2.50
2.49
2.48
1.74
(4,5-Diamino-1-cyano-7-hydroxy-1,10b-dihydro-2H-chromeno[3,4-c]pyridin-2-ylidene)malononitrile 13c
DMSO-d6
300 MHz
1.00
7.34
2.02
f1 (ppm)


160.53
160.32
156.92
145.65
140.21
116.66
116.37
113.50
112.97
83.90
70.46
40.33
40.06
39.78
39.50
39.22
38.94
38.66
34.82
30.36
(4,5-Diamino-1-cyano-7-hydroxy-1,10b-dihydro-2H-chromeno[3,4-c]pyridin-2-ylidene)malononitrile 13c
DMSO-d6
300 MHz
f1 (ppm)