Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Copper catalyzed cyanation through C=C bond cleavage of *gem*-aryl dibromide followed by second cyanation of iodoarene by released CN unit

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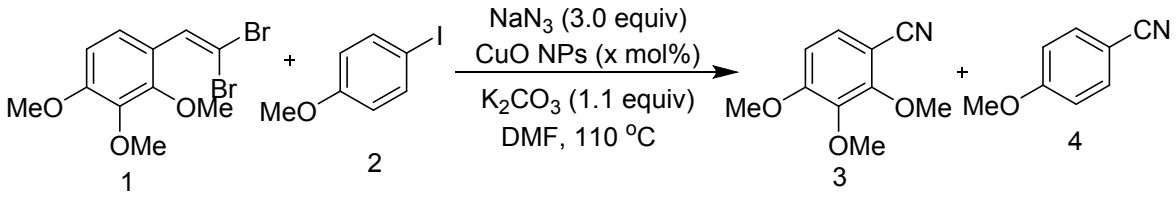
Reaction Optimization

Table 1. Screening of catalyst (CuO NPs) loading[a]

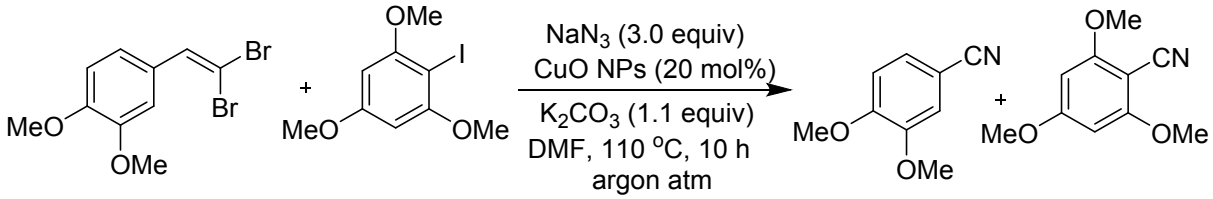


Entry	CuO NPs loading (mol %)	Yield of 3[b]	Yield of 4[b]
1	5	43%	20%
2	10	55%	23%
3	15	73%	57%
4	20	89%	77%
5	25	86%	71%

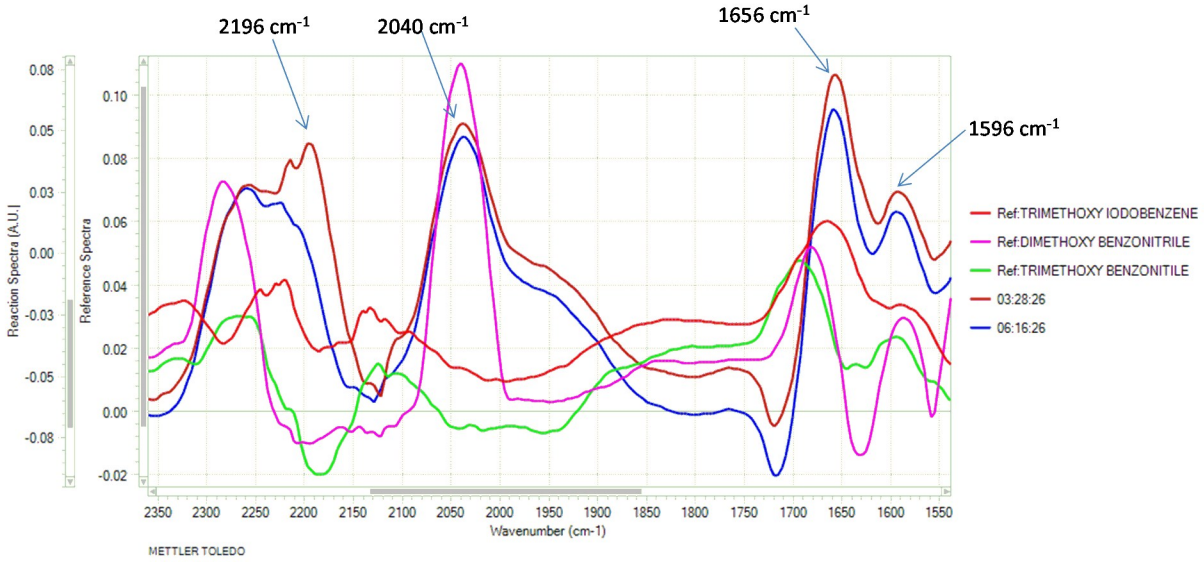
[a]Reaction conditions: A mixture of 1-(2,2-dibromovinyl)-2,3,4-trimethoxybenzene (1) (1.5 mmol), 4-iodoanisole (0.5 mmol), NaN_3 (3 equiv), and K_2CO_3 (1.1 equiv) in dry solvent (2.0 mL) was heated under argon atmosphere. [b]Yield of isolated products with respect to corresponding starting materials.

Mechanistic Studies

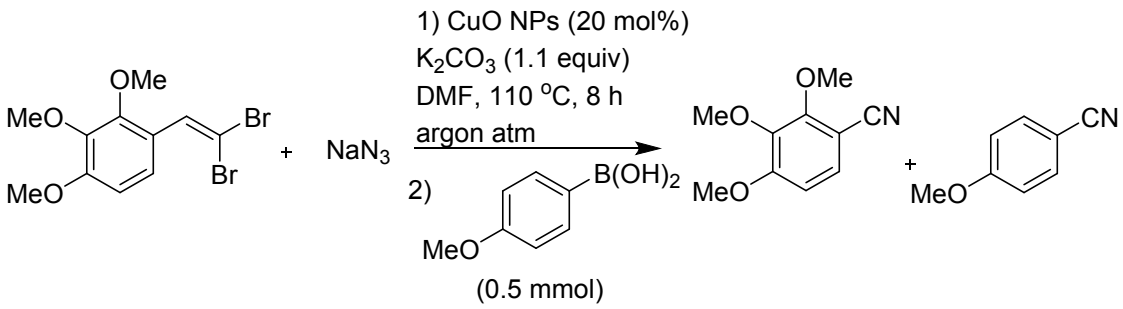
a) IR study of the following reactions



In an oven dried 50 mL round bottom flask, a mixture of 4-(2,2-dibromovinyl)-1,2-dimethoxybenzene (1.93 g, 6.0 mmol, 1.0 equiv), 2-iodo-1,3,5-trimethoxybenzene (588.0 mg, 2.0 mmol, 0.33 equiv), NaN_3 (1.17 g, 18.0 mmol, 3.0 equiv), CuO NPs (96 mg, 20 mol %) and K_2CO_3 (911.0 mg, 1.1 mmol, 1.1 equiv) in dry DMF (10 mL) was heated at 110 °C for 8 h in an oil bath under argon atmosphere in IR machine.



b) Trapping of in situ generated CN moiety by aryl boronic acid



In an oven dried 10 mL round bottom flask, a mixture of 1-(2,2-dibromovinyl)-2,3,4-trimethoxybenzene (352.0 mg, 1.0 mmol, 1.0 equiv), NaN_3 (195.0 mg, 3.0 mmol, 3.0 equiv), CuO NPs (16 mg, 20 mol %) and K_2CO_3 (152.0 mg, 1.1 mmol, 1.1 equiv) in dry DMF (3 mL) was heated at 110 ^oC for 8 h in an oil bath under argon atmosphere. (4-Methoxyphenyl)boronic acid (76.0 mg, 0.5 mmol) was added to the reaction mixture followed by stirring for another 7 h. The reaction mixture was allowed to cool and was extracted with EtOAc (3x20 mL). The extract was washed with water (10 mL) and brine (10 mL). The organic phase was dried (Na_2SO_4) and evaporated to leave the crude product. The crude product was analyzed by GC-MS and showed the presence of 2,3,4-trimethoxy benzonitrile (193) and 4-methoxy benzonitrile (133).

Dept. of Organic Chemistry, IACS, Kolkata
Library Search Report

Data File:	BCR_Lab03	Original Data Path:	C:\Xcalibur\demo\MS\Data\BC Ranu Lab\Pintu\200617
Current Data Path:	C:\Xcalibur\demo\MS\Data\BC Ranu Lab\Pintu\200617	Sample Type:	Unknown
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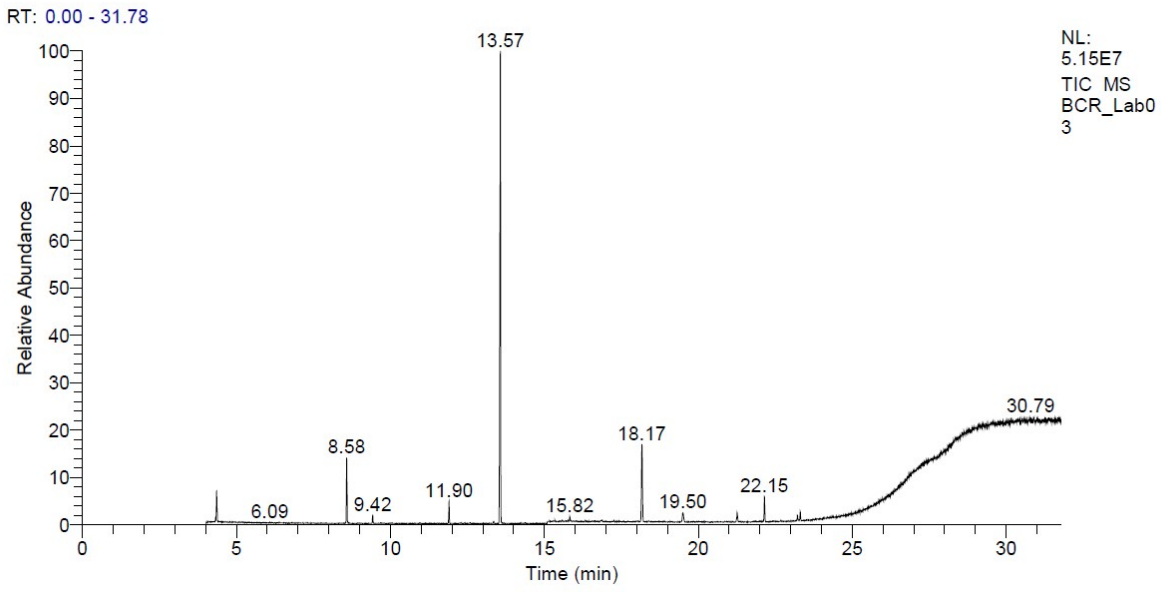
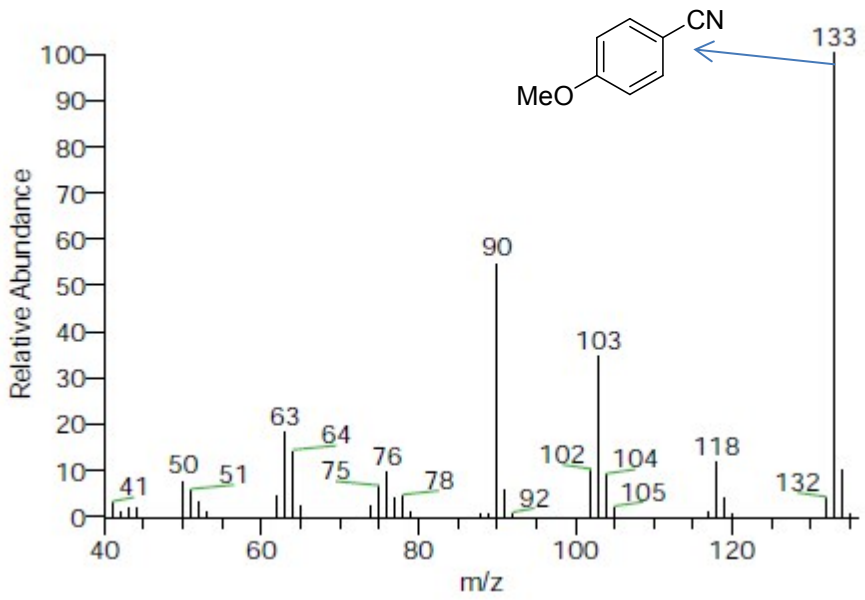
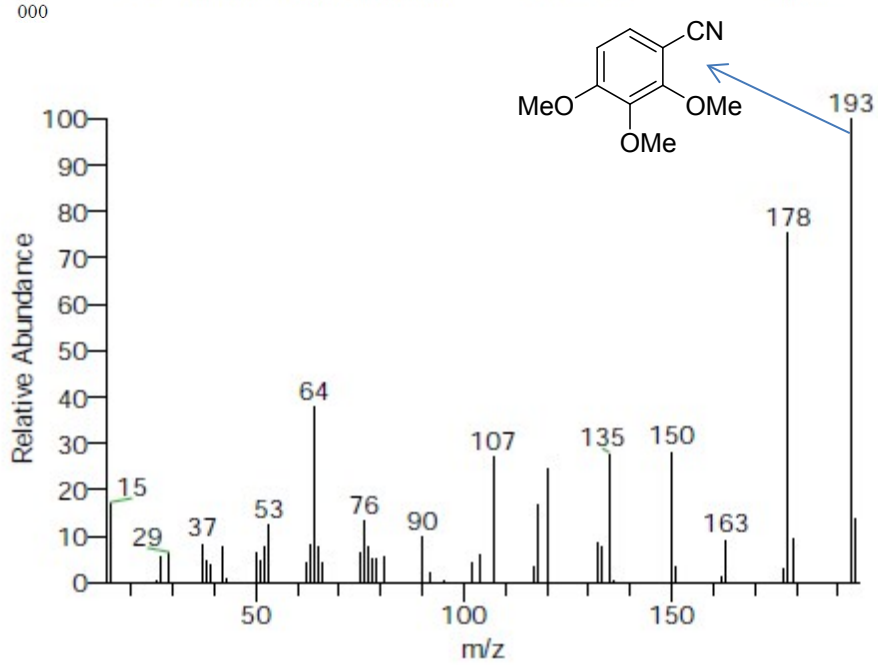
Acquisition Date:	06/20/17 01:44:33 PM	Run Time(min):	27.78
Scans:	8168	Low Mass(m/z):	35.00000
High Mass(m/z):	550		

Instrument Method: C:\Xcalibur\demo\MS\Instrument method\PAU_SB_234_45_SP.meth
Original Processing Method:

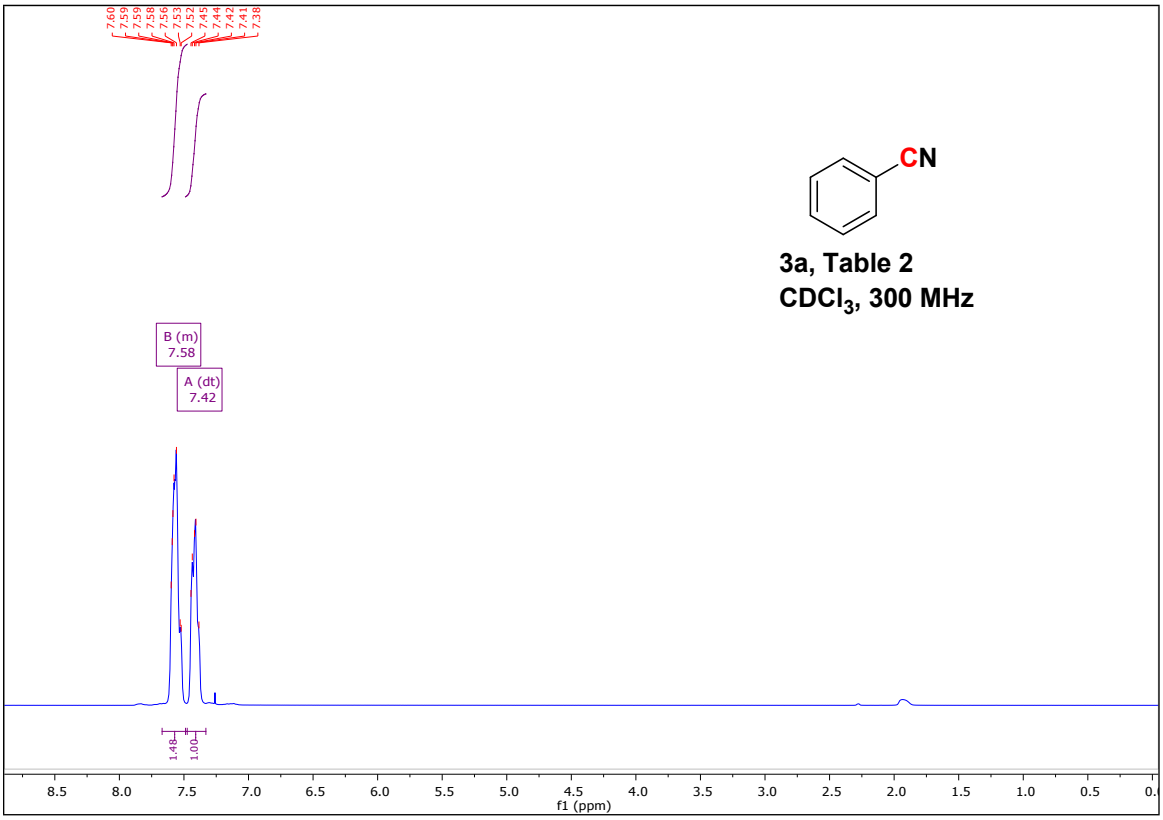


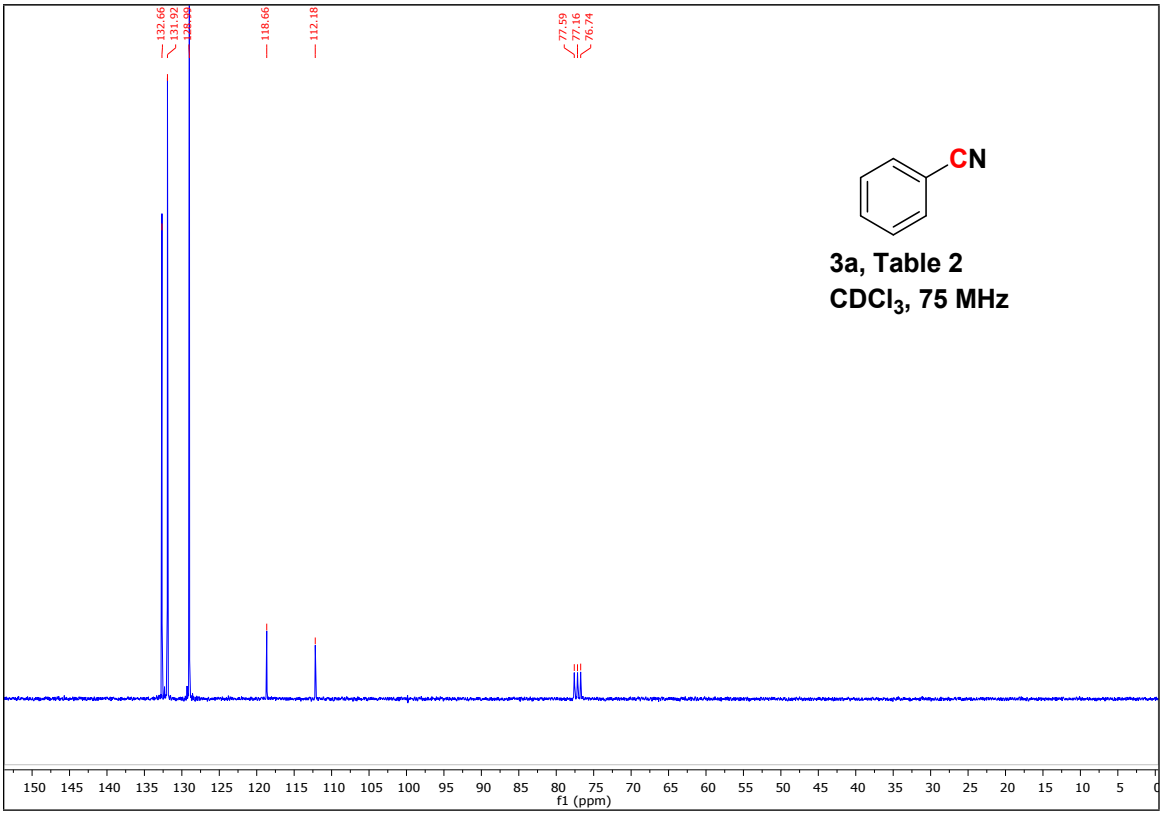


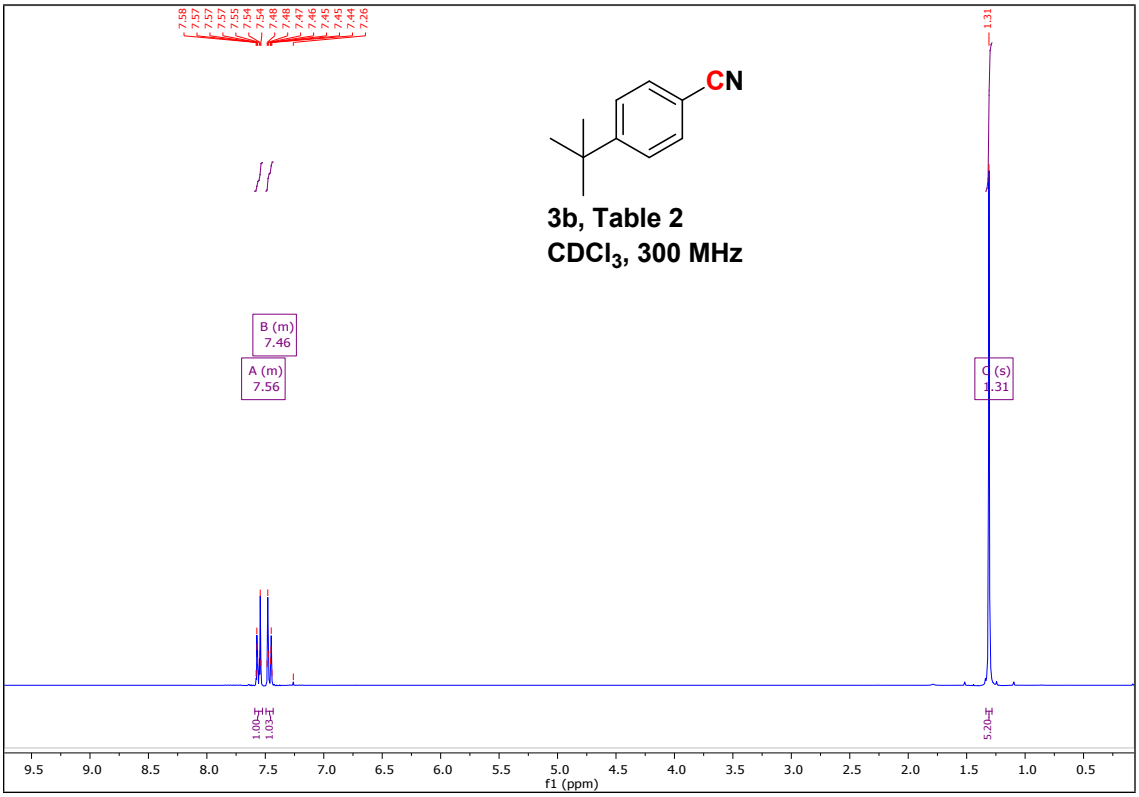
RT	Scan #	RSI	Compound Name	Cas #	Library	Molecular Weight
9.42	1595.000000	902	Benzene, 1-isocyano-4-methoxy-	10349-38-9	mainlib	133



RT	Scan #	RSI	Compound Name	Cas #	Library	Molecular Weight
13.57	2814.000000	943	Benzonitrile, 2,3,4-trimethoxy-	43020-38-8	mainlib	193


7.60
7.59
7.59
7.58
7.56
7.53
7.52
7.45
7.44
7.42
7.41
7.38
CN
3a, Table 2
CDCl3, 300 MHz
B (m)
7.58
A (dt)
7.42
1.48
1.00
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
f1 (ppm)


132.66
131.92
118.66
112.18
77.59
77.16
76.74
CN
3a, Table 2
CDCl3, 75 MHz
150
145
140
135
130
125
120
115
110
105
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
f1 (ppm)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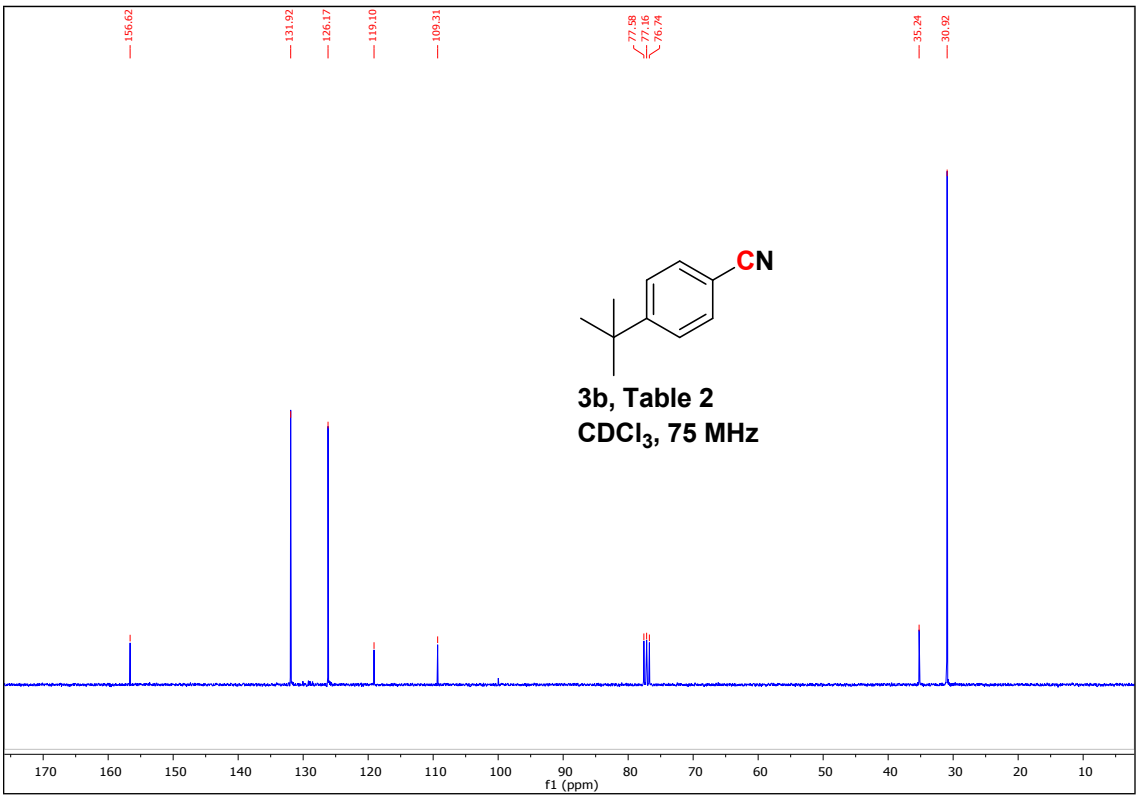
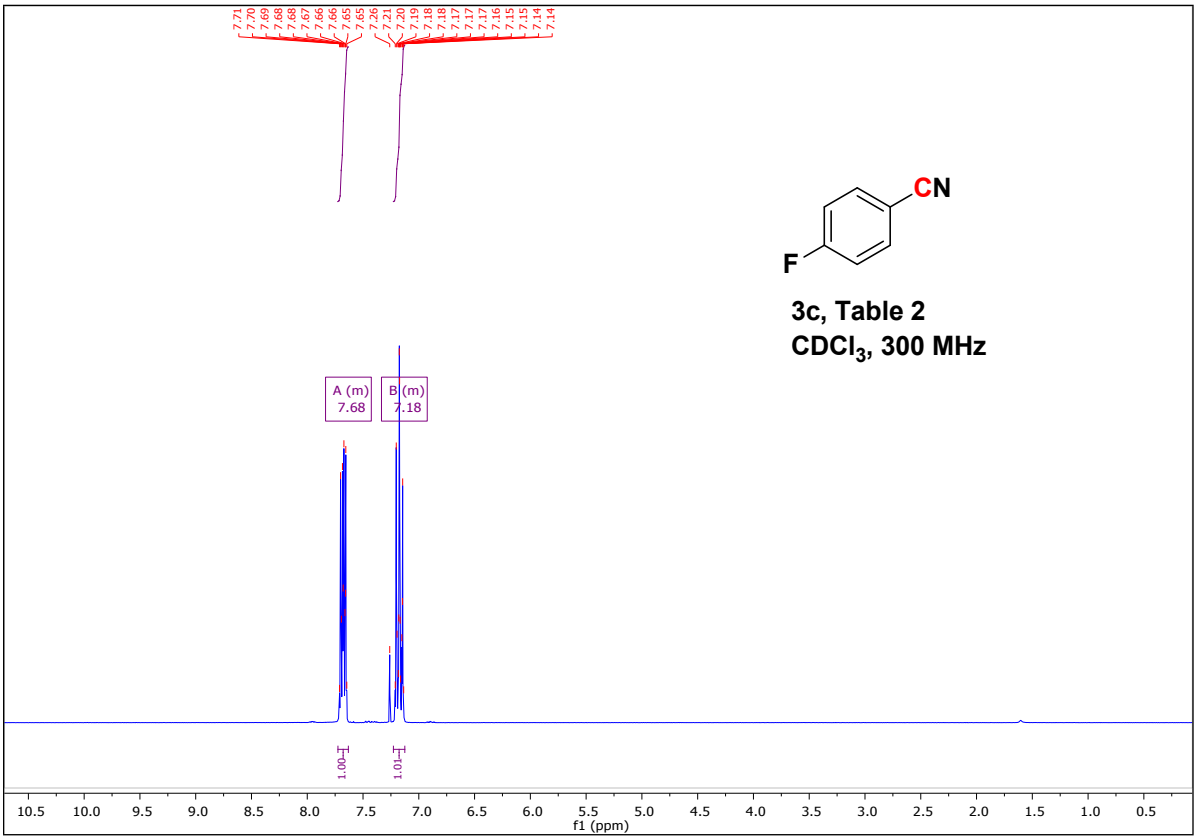
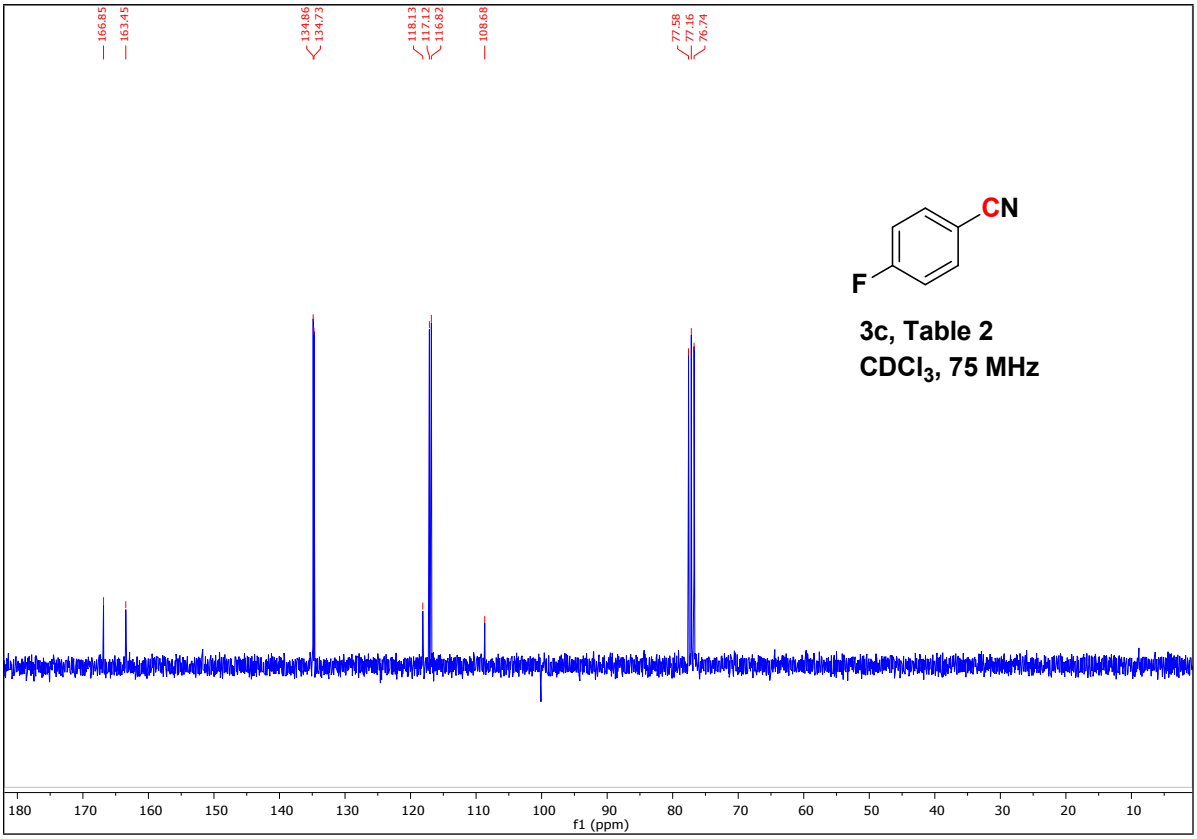
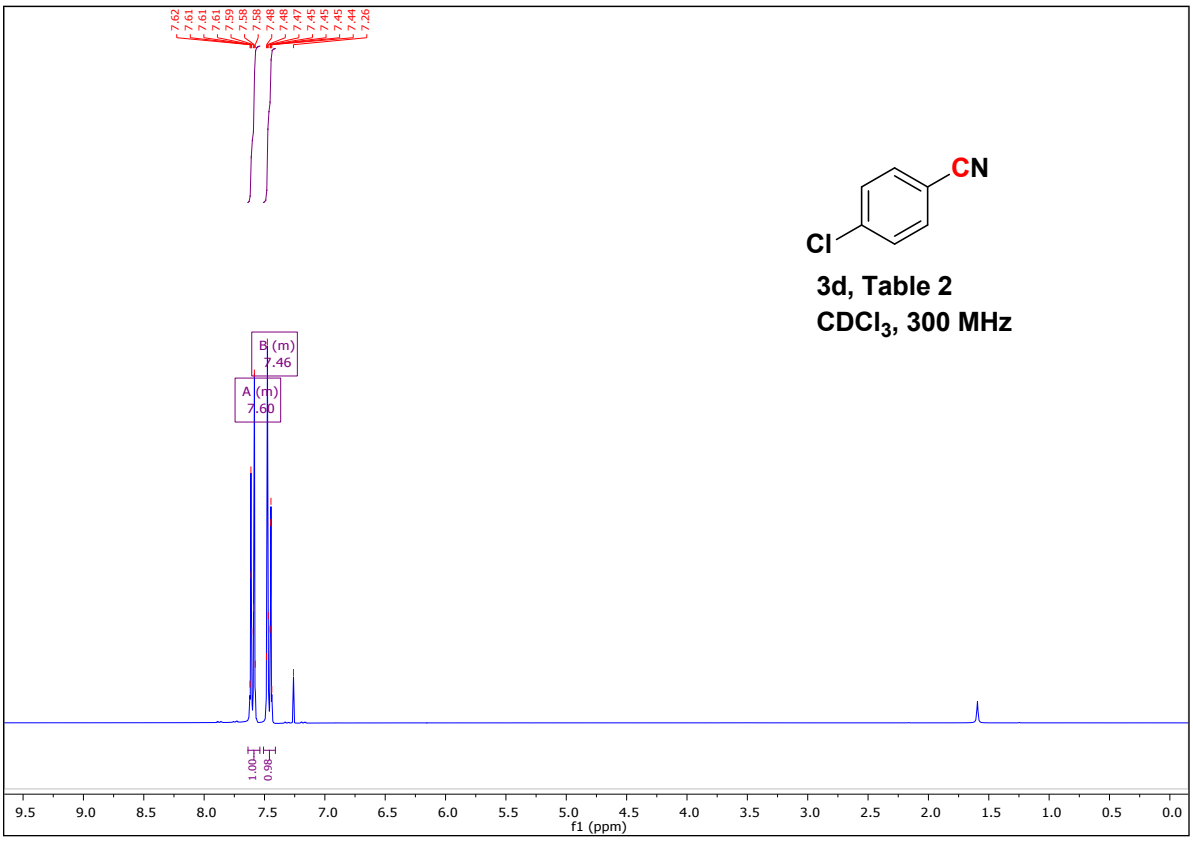
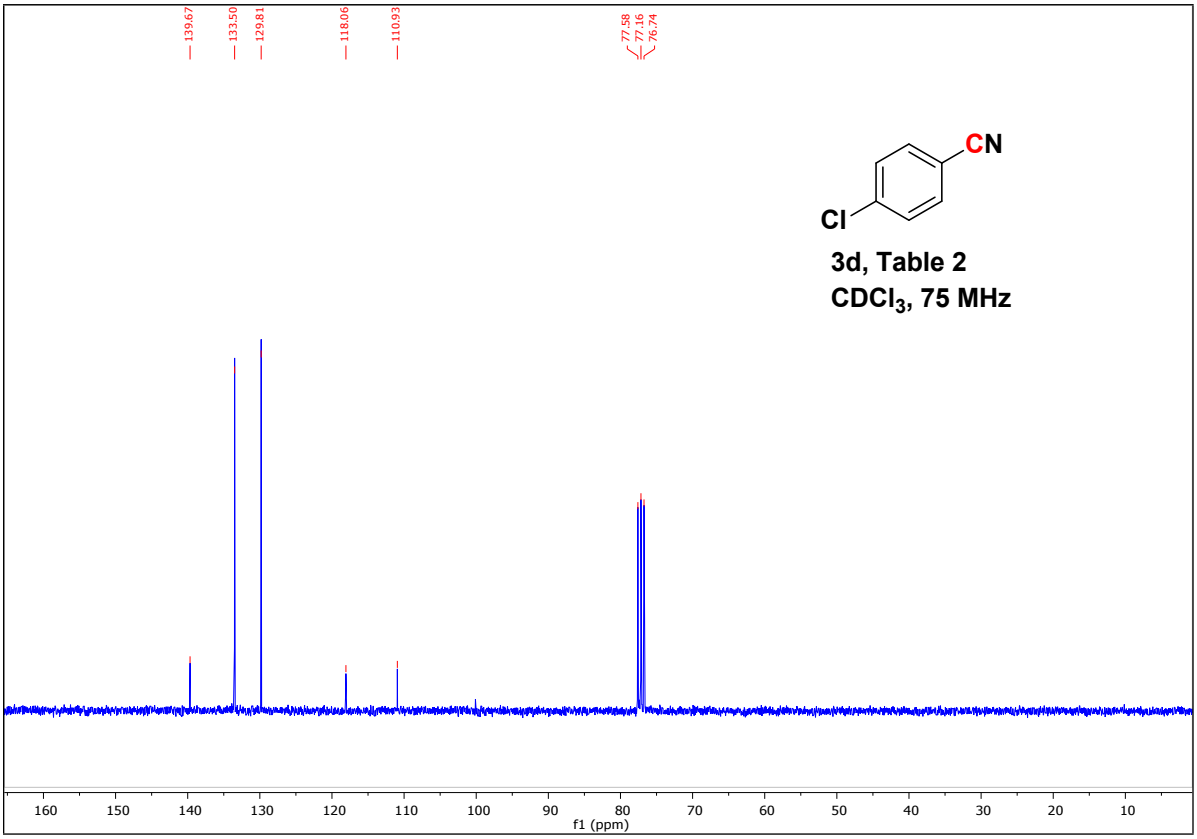
7.57
7.57
7.57
7.55
7.54
7.54
7.48
7.47
7.46
7.45
7.45
7.44
7.26
1.31
CN
3b, Table 2
CDCl3, 300 MHz
B (m)
7.46
A (m)
7.56
C (s)
1.31
1.00
1.03
5.20
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

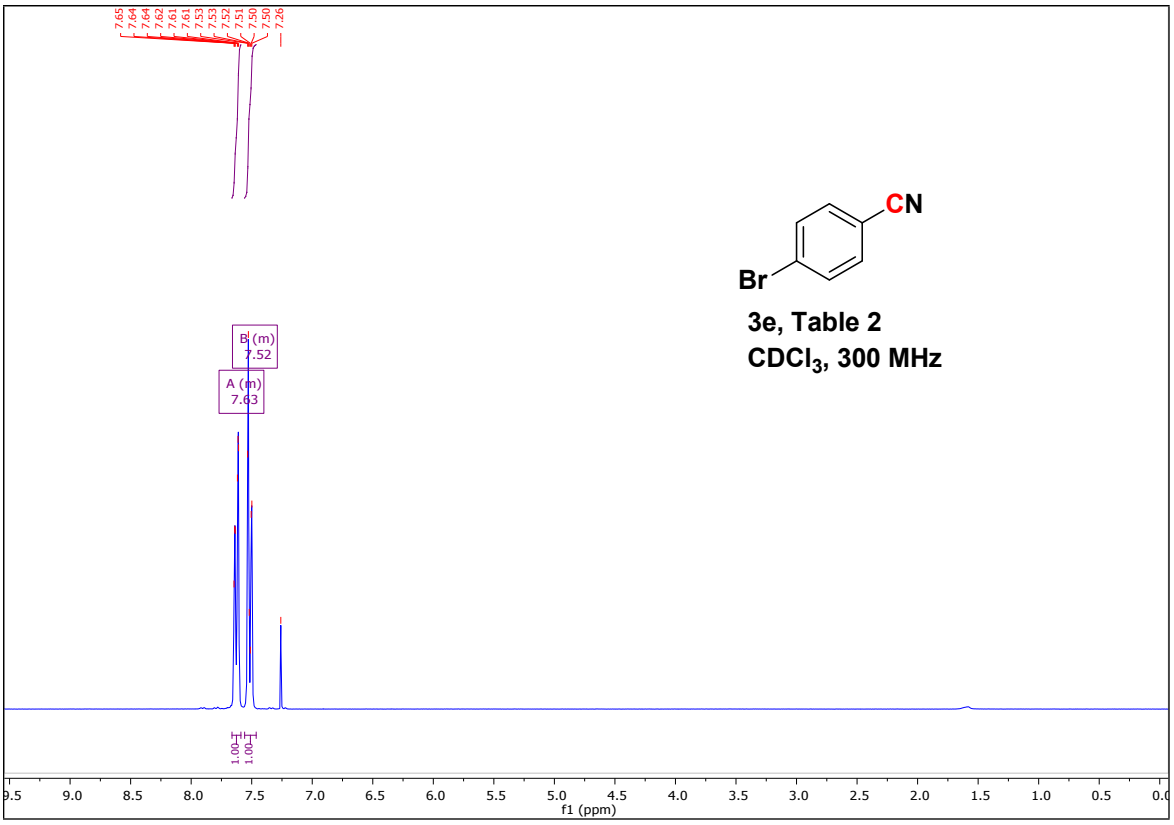

156.62
131.92
126.17
119.10
109.31
77.58
77.16
76.74
35.24
30.92
CN
3b, Table 2
CDCl3, 75 MHz
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

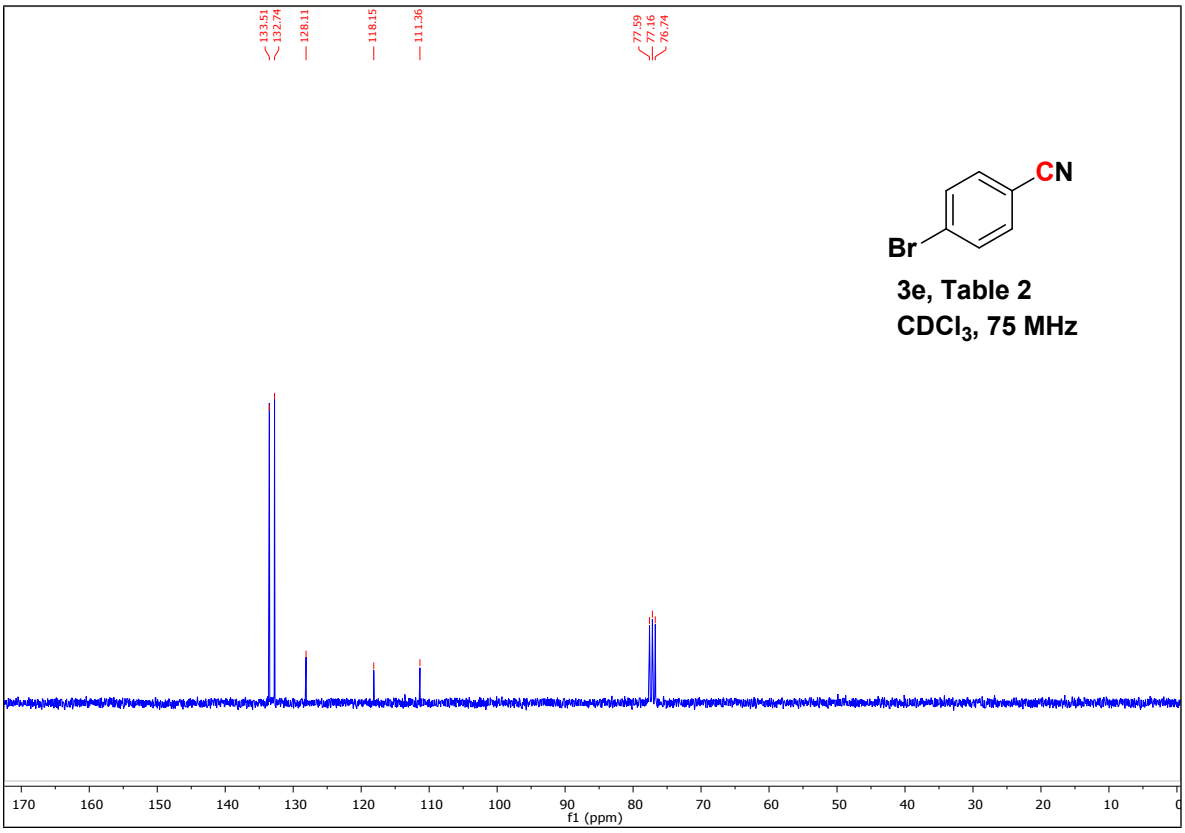

7.71
7.70
7.69
7.68
7.68
7.67
7.66
7.66
7.65
7.65
7.26
7.21
7.20
7.19
7.18
7.18
7.17
7.17
7.17
7.16
7.15
7.15
7.14
7.14
CN
F
3c, Table 2
CDCl3, 300 MHz
A (m)
7.68
B (m)
7.18
1.00
1.01
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

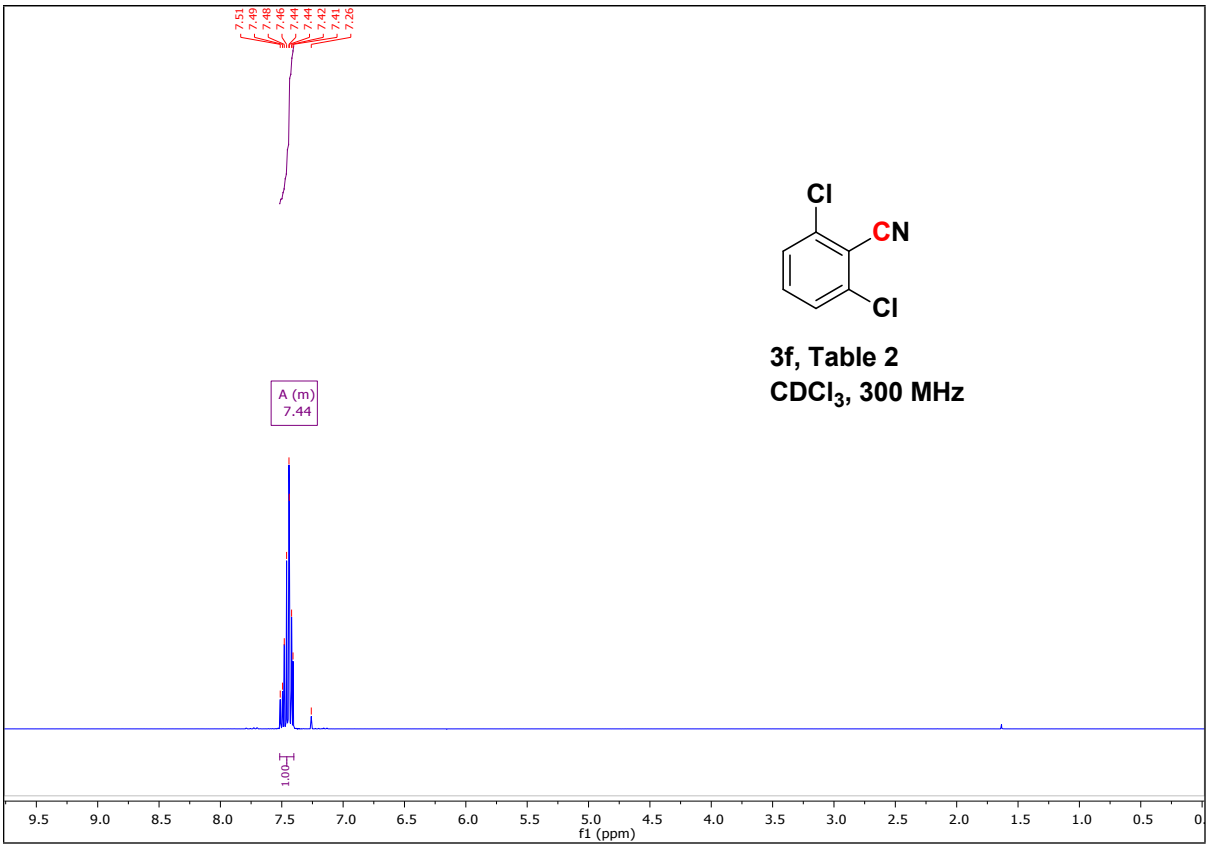

166.85
163.45
134.86
134.73
118.13
117.12
116.82
108.68
77.58
77.16
76.74
CN
F
3c, Table 2
CDCl3, 75 MHz
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

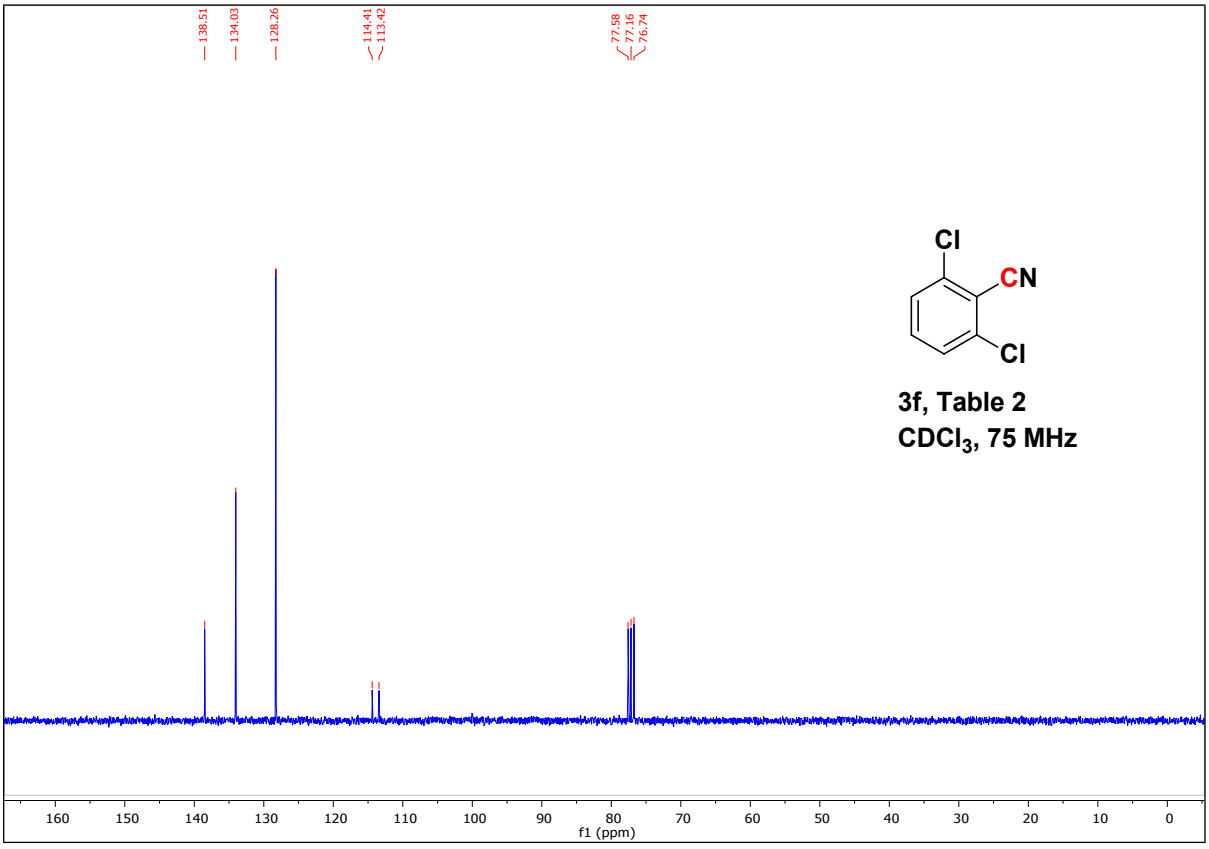

7.62
7.61
7.61
7.61
7.59
7.58
7.58
7.48
7.48
7.47
7.45
7.45
7.45
7.44
7.26
B (m)
7.46
A (m)
7.60
1.00
0.98
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
CN
Cl
3d, Table 2
CDCl3, 300 MHz

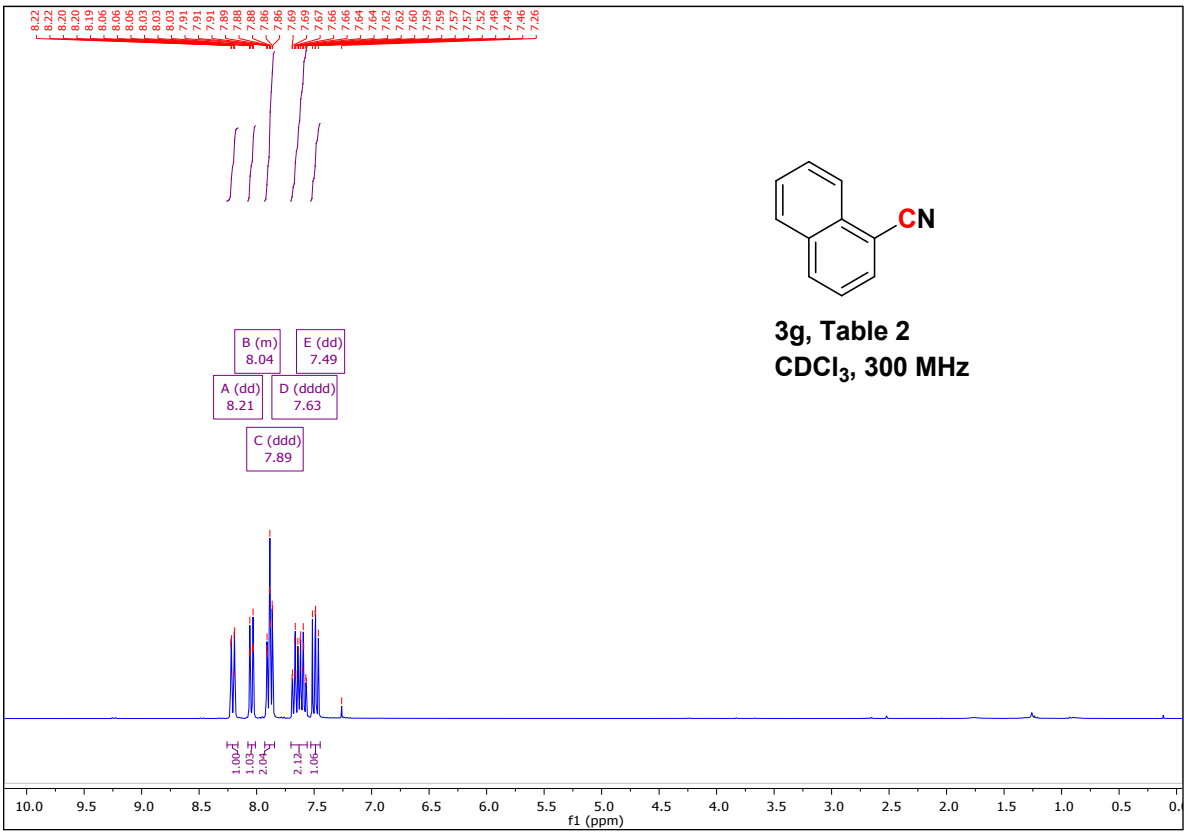

139.67
133.50
129.81
118.06
110.93
77.58
77.16
76.74
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)
CN
Cl
3d, Table 2
CDCl3, 75 MHz


7.65
7.64
7.64
7.62
7.61
7.61
7.53
7.53
7.52
7.51
7.50
7.50
7.26
B (m)
7.52
A (m)
7.63
1.00
1.00
CN
Br
3e, Table 2
CDCl3, 300 MHz
f1 (ppm)

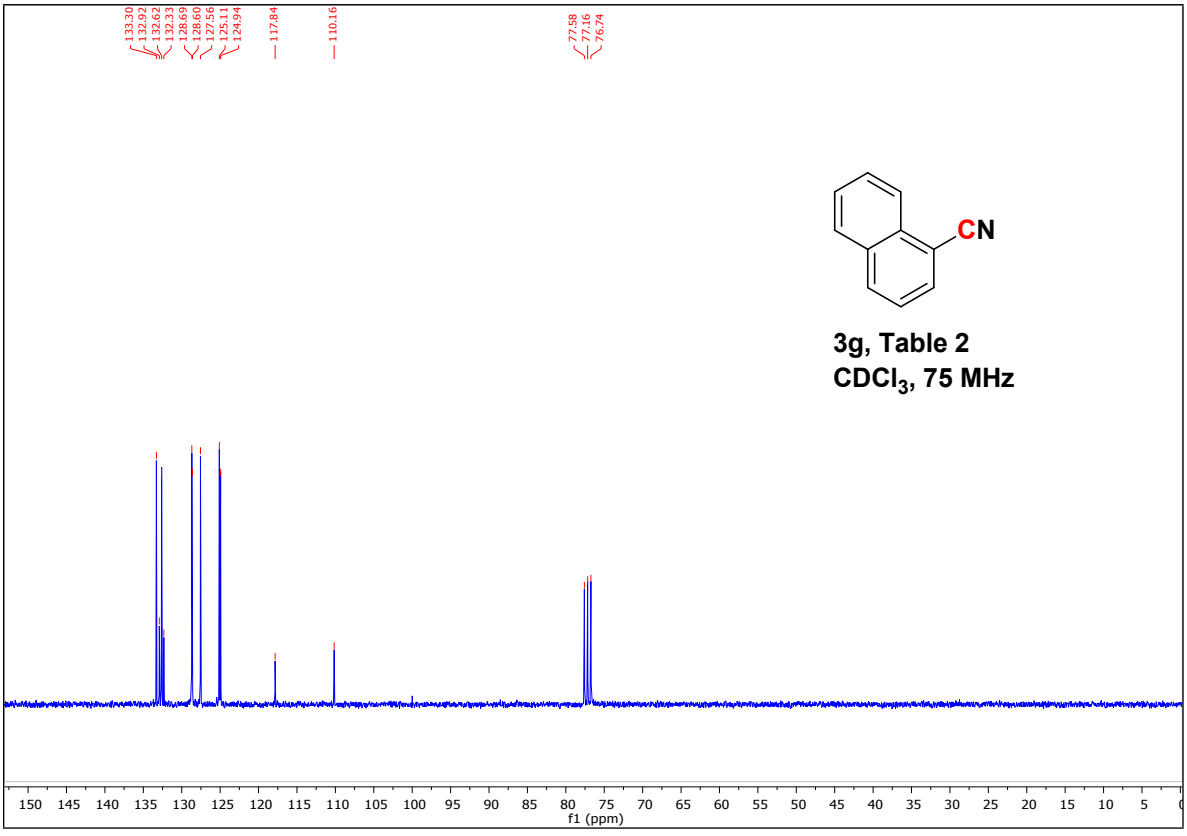

133.51
132.74
128.11
118.15
111.36
77.59
77.16
76.74
CN
Br
3e, Table 2
CDCl3, 75 MHz
f1 (ppm)


7.51
7.49
7.48
7.46
7.44
7.44
7.42
7.41
7.26
A (m)
7.44
1.00
Cl
CN
Cl
3f, Table 2
CDCl3, 300 MHz
f1 (ppm)

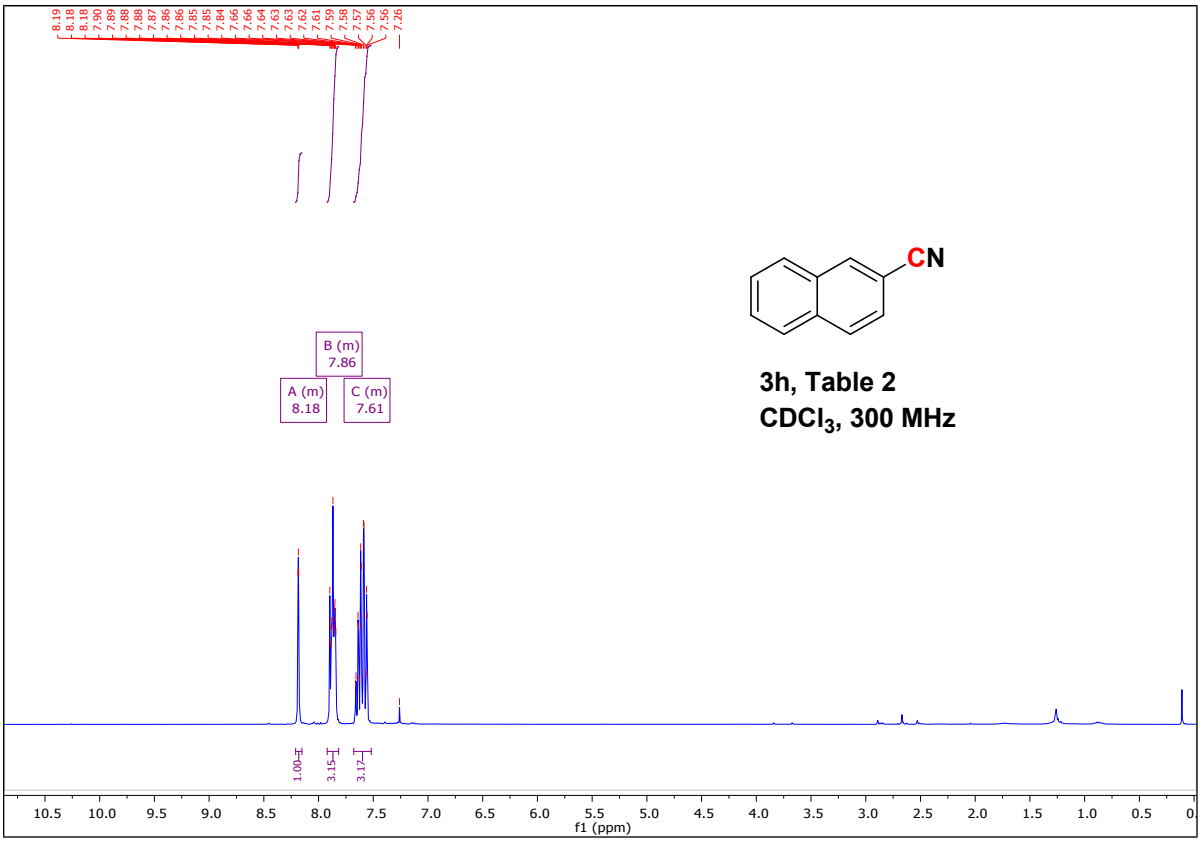

138.51
134.03
128.26
114.41
113.42
77.58
77.16
76.74
Cl
CN
Cl
3f, Table 2
CDCl3, 75 MHz
f1 (ppm)



3g, Table 2
$CDCl_3$, 300 MHz



3g, Table 2
$CDCl_3$, 75 MHz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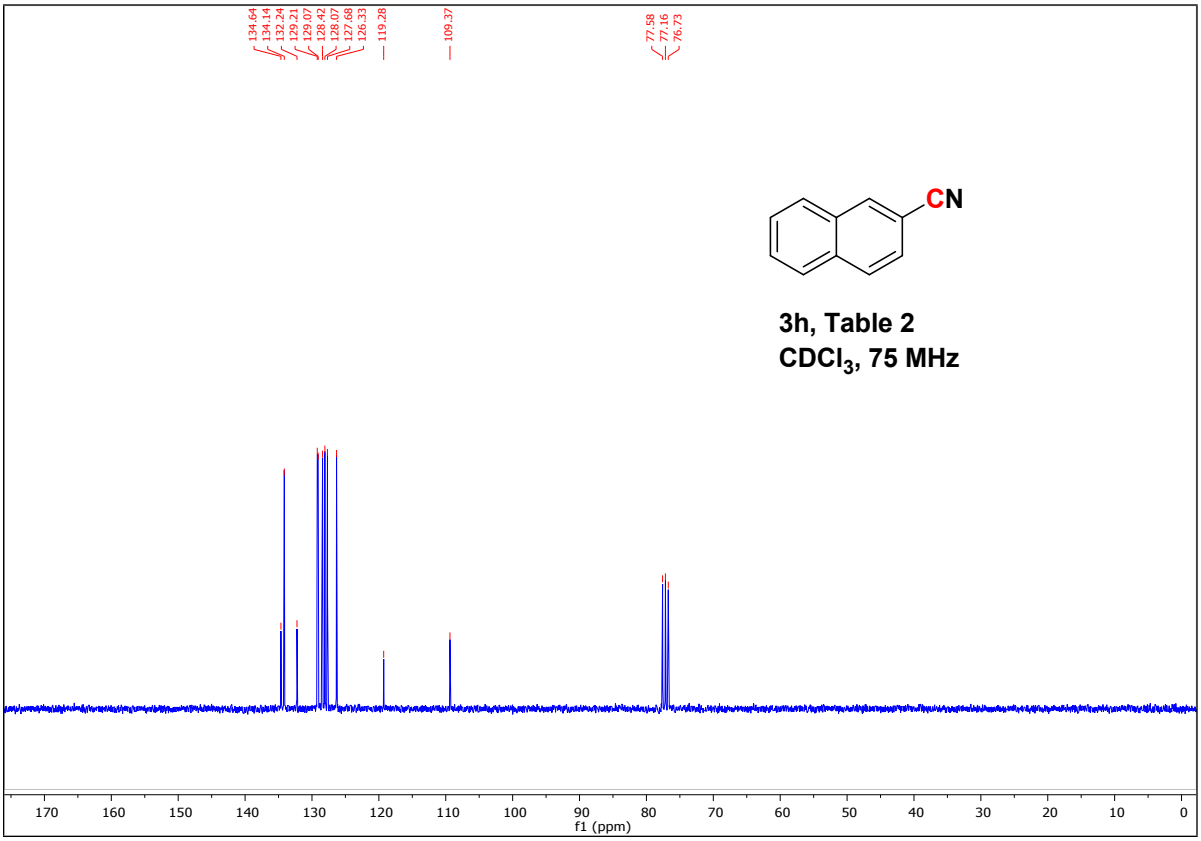
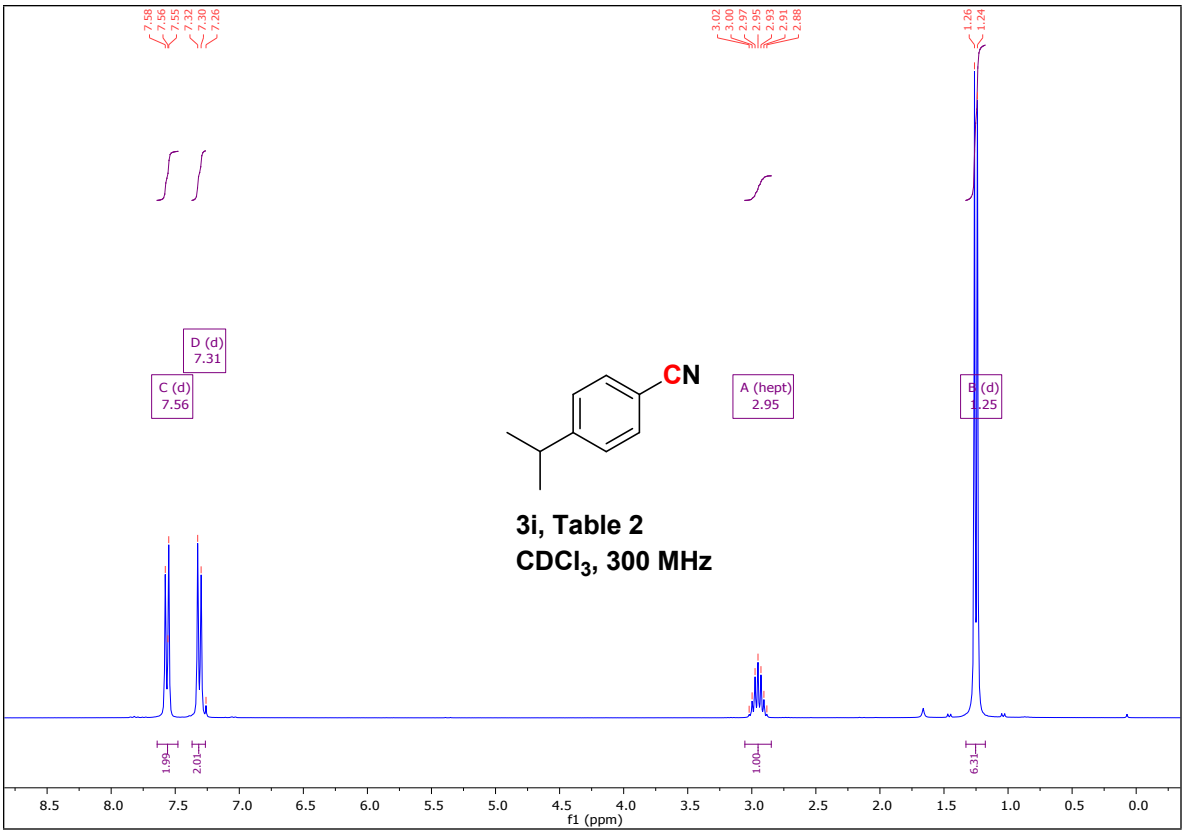
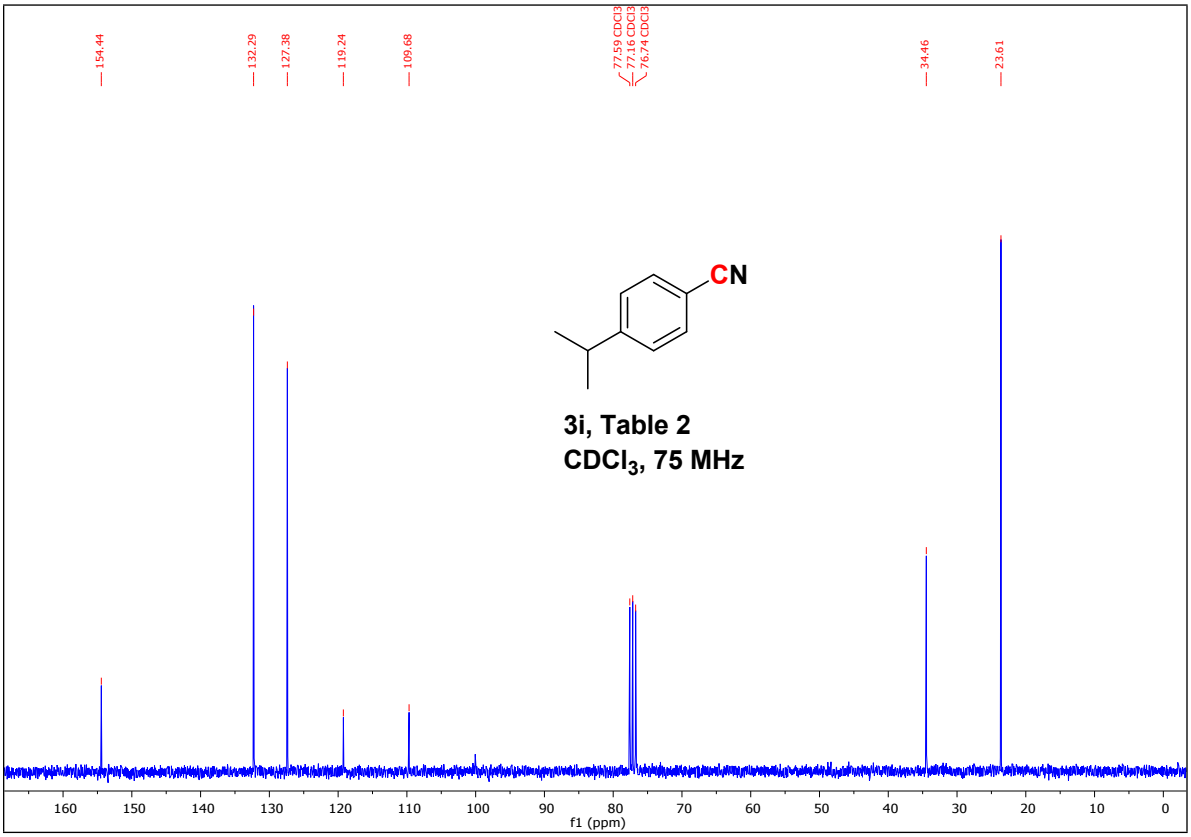
8.18
8.18
7.90
7.89
7.88
7.88
7.87
7.86
7.86
7.85
7.85
7.84
7.66
7.66
7.64
7.63
7.63
7.62
7.61
7.59
7.58
7.57
7.56
7.56
7.26
B (m)
7.86
A (m)
8.18
C (m)
7.61
CN
3h, Table 2
CDCl3, 300 MHz
1.00
3.15
3.17
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
f1 (ppm)

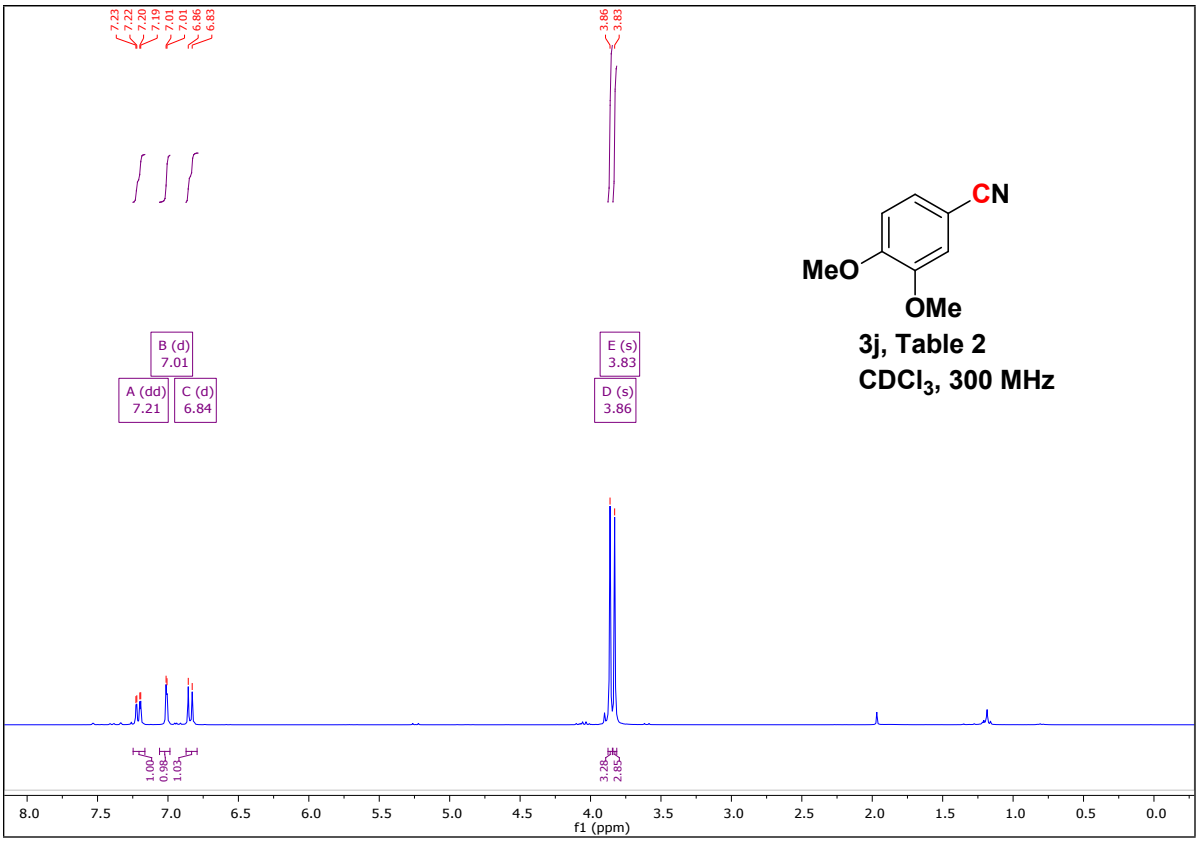

134.64
134.14
132.24
129.21
129.07
128.42
128.07
127.68
126.33
119.28
109.37
77.58
77.16
76.73
CN
3h, Table 2
CDCl3, 75 MHz
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

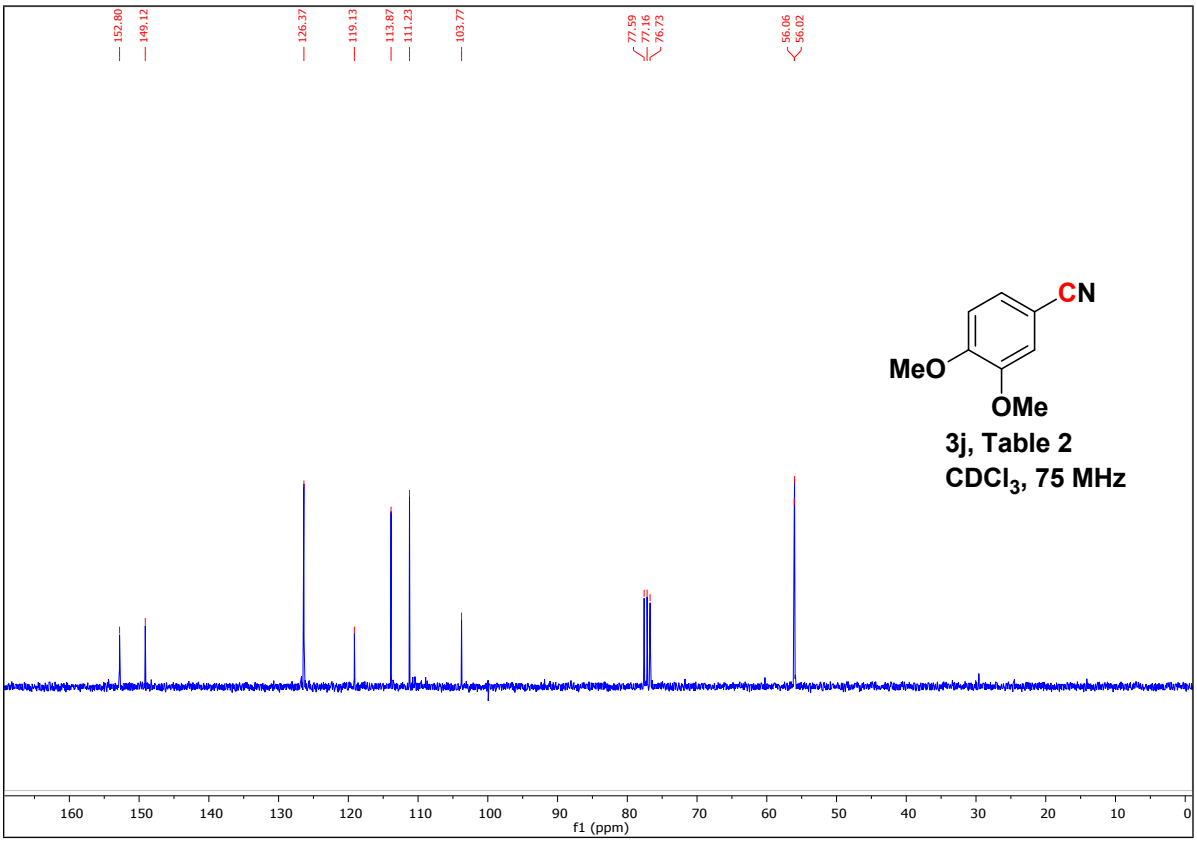


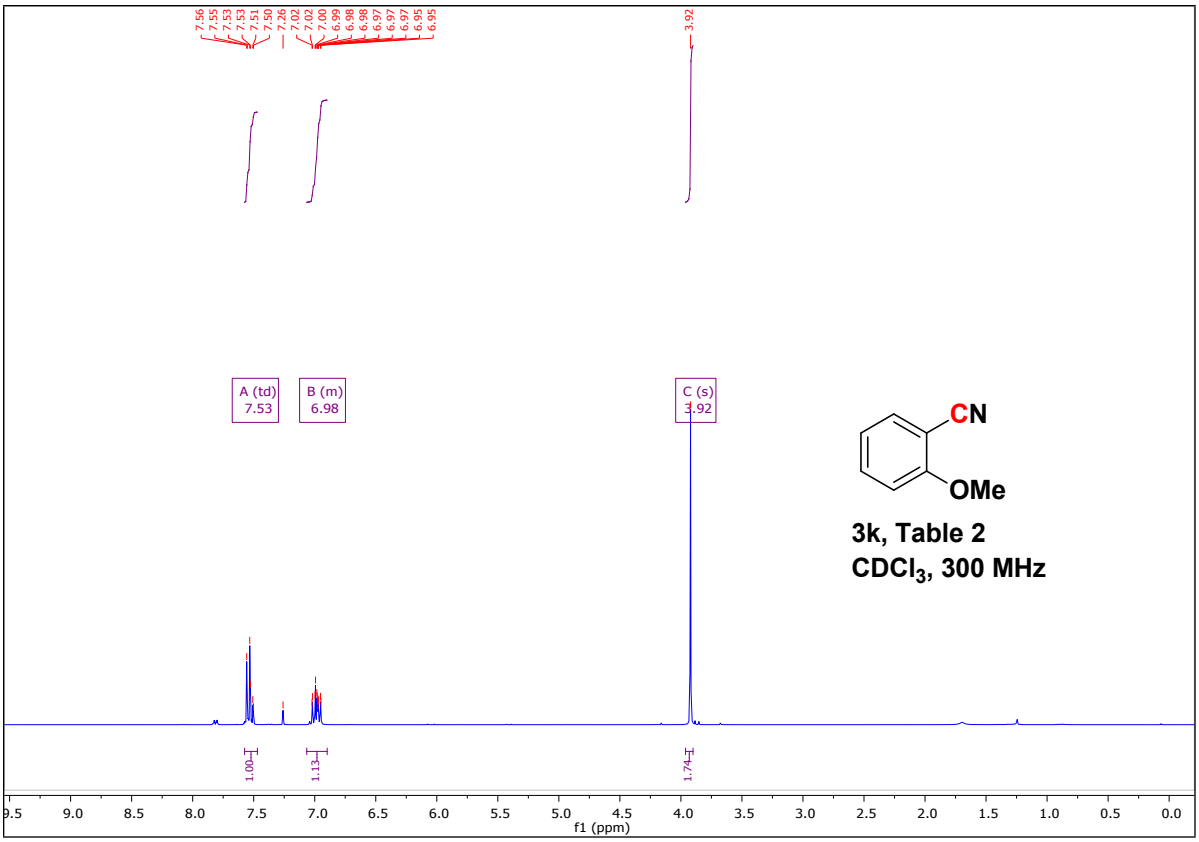
3i, Table 2
$CDCl_3$, 300 MHz

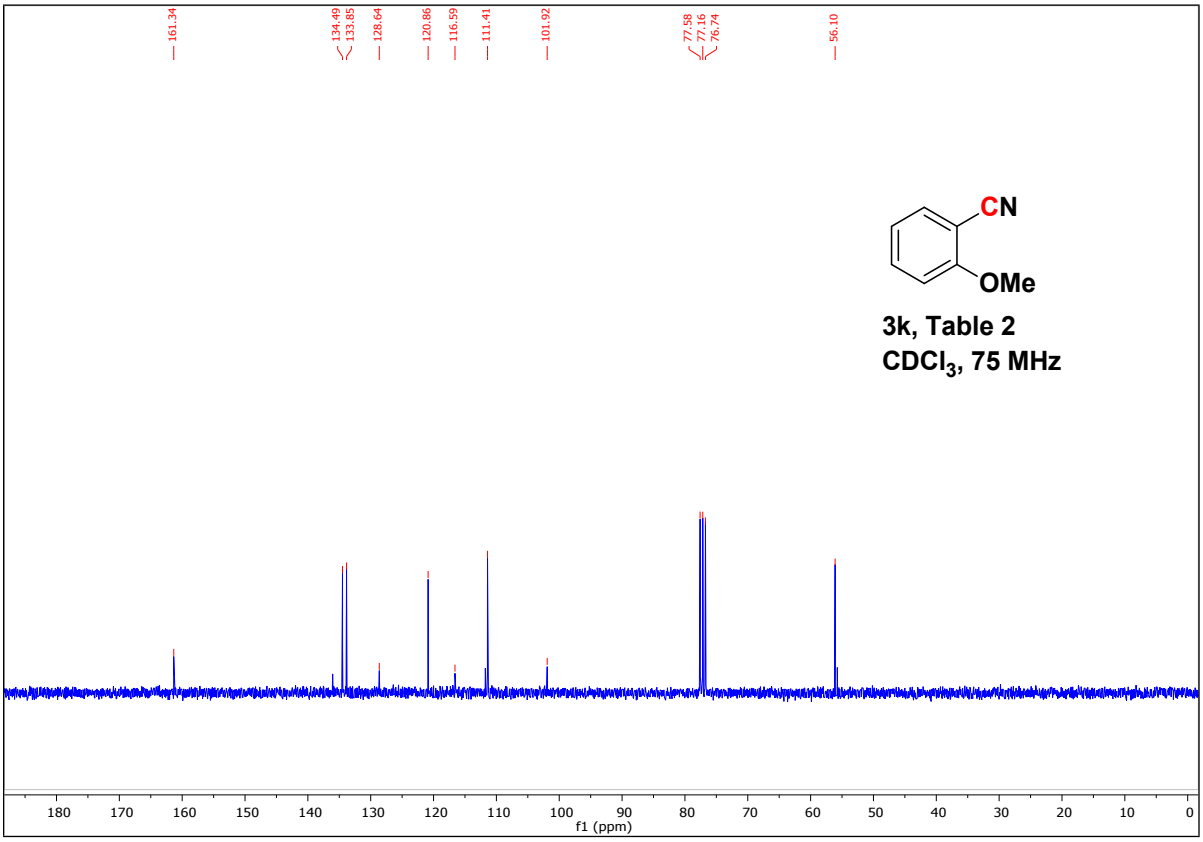


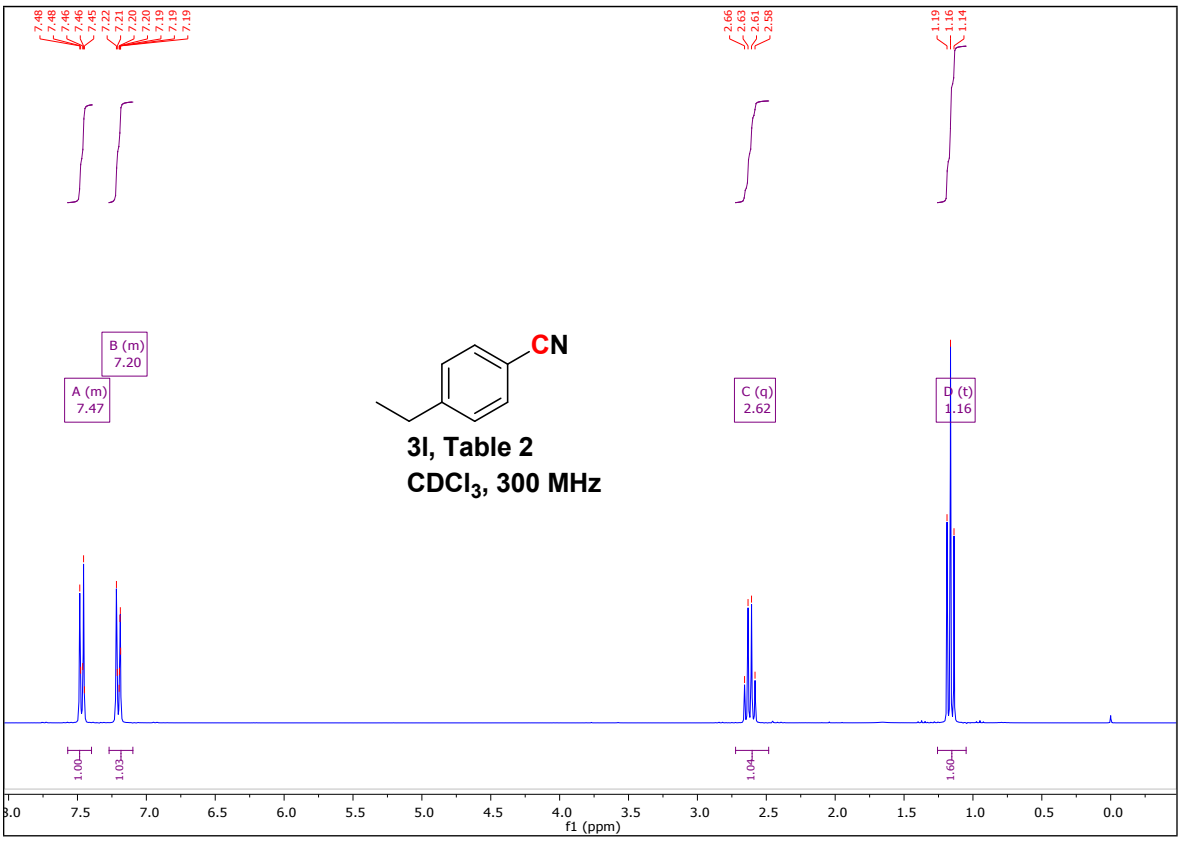
3i, Table 2
$CDCl_3$, 75 MHz

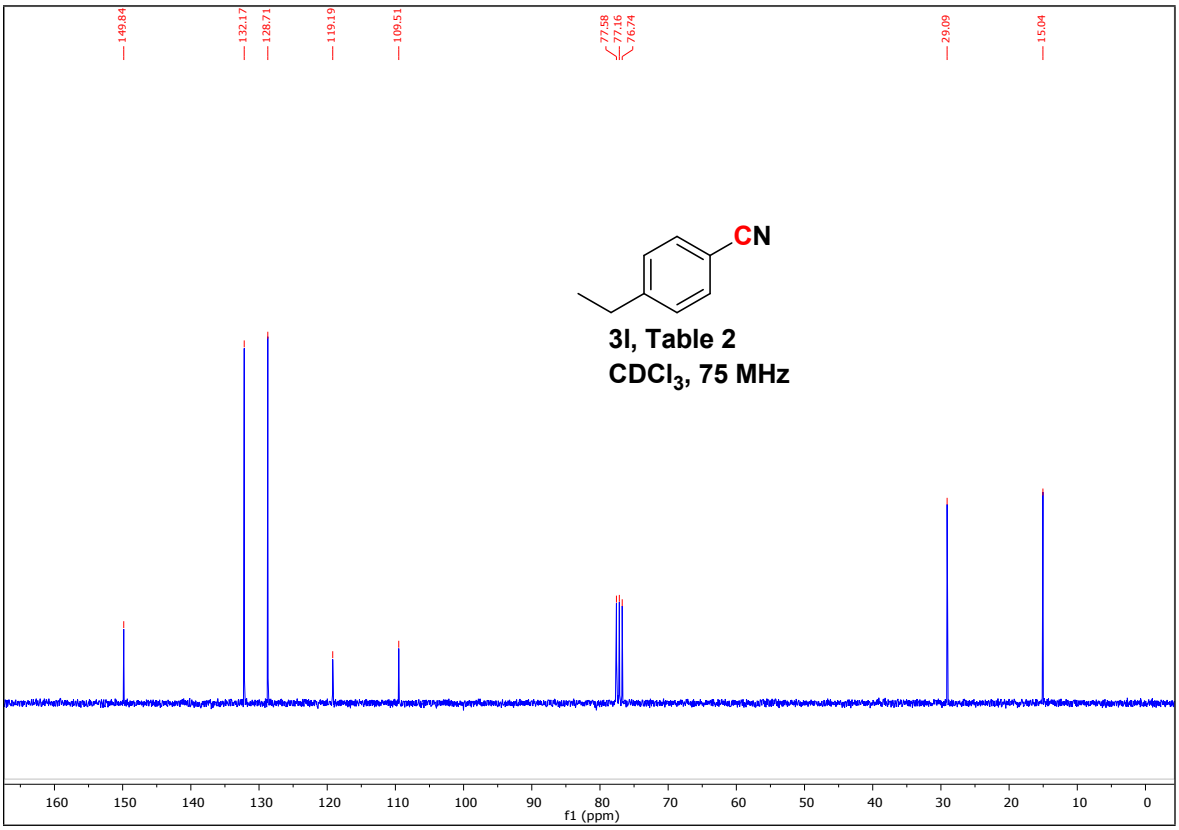

7.23
7.22
7.20
7.19
7.01
7.01
6.86
6.83
3.86
3.83
B (d)
7.01
A (dd)
7.21
C (d)
6.84
E (s)
3.83
D (s)
3.86
CN
MeO
OMe
3j, Table 2
CDCl3, 300 MHz
1.00
0.98
1.03
3.28
2.85
f1 (ppm)

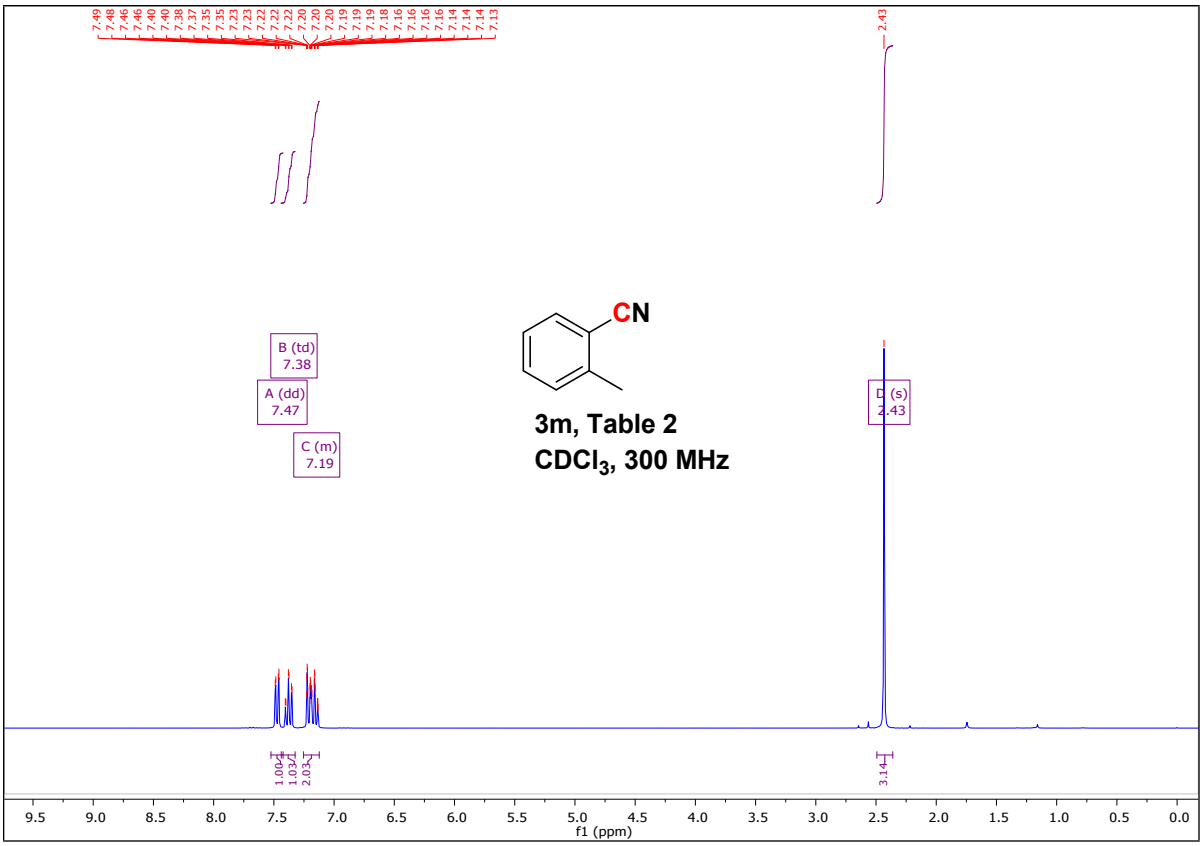

152.80
149.12
126.37
119.13
113.87
111.23
103.77
77.59
77.16
76.73
56.06
56.02
CN
MeO
OMe
3j, Table 2
CDCl3, 75 MHz
f1 (ppm)

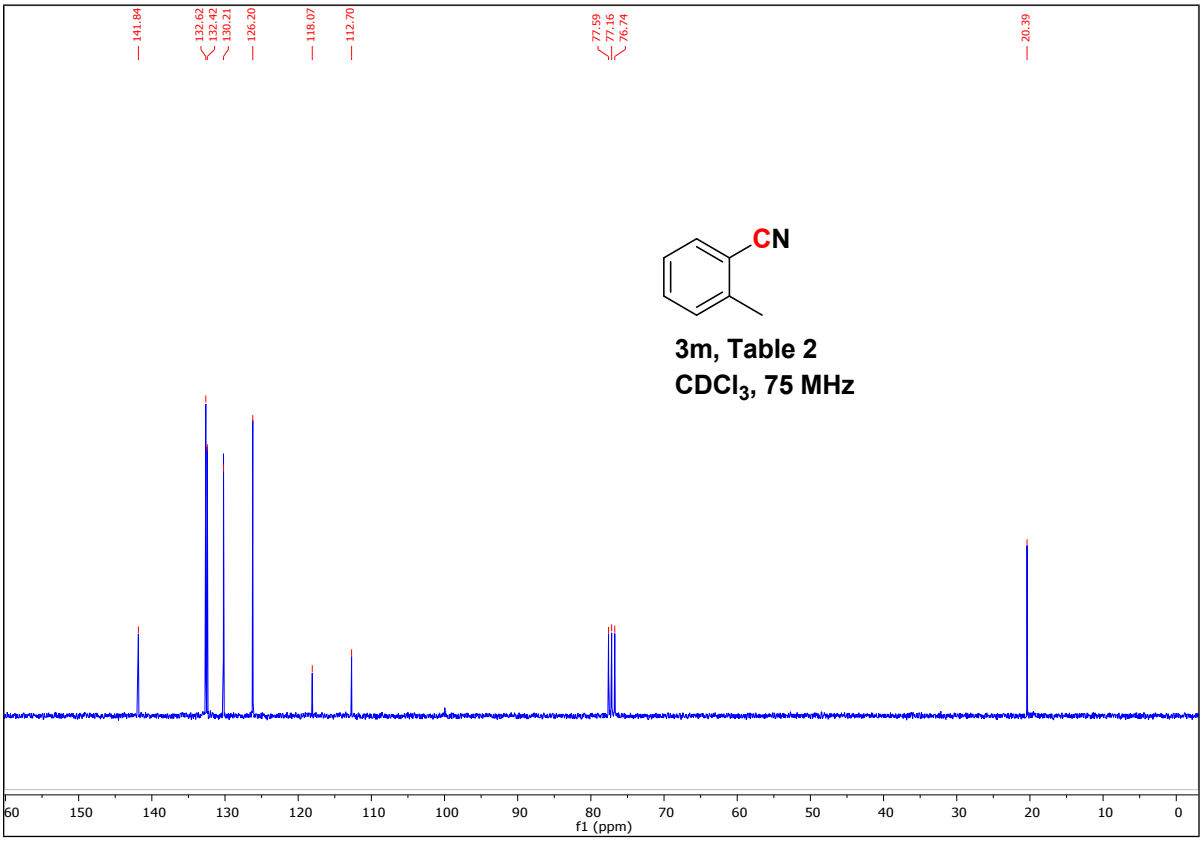

A (td)
7.53
B (m)
6.98
C (s)
3.92
CN
OMe
3k, Table 2
CDCl3, 300 MHz
f1 (ppm)

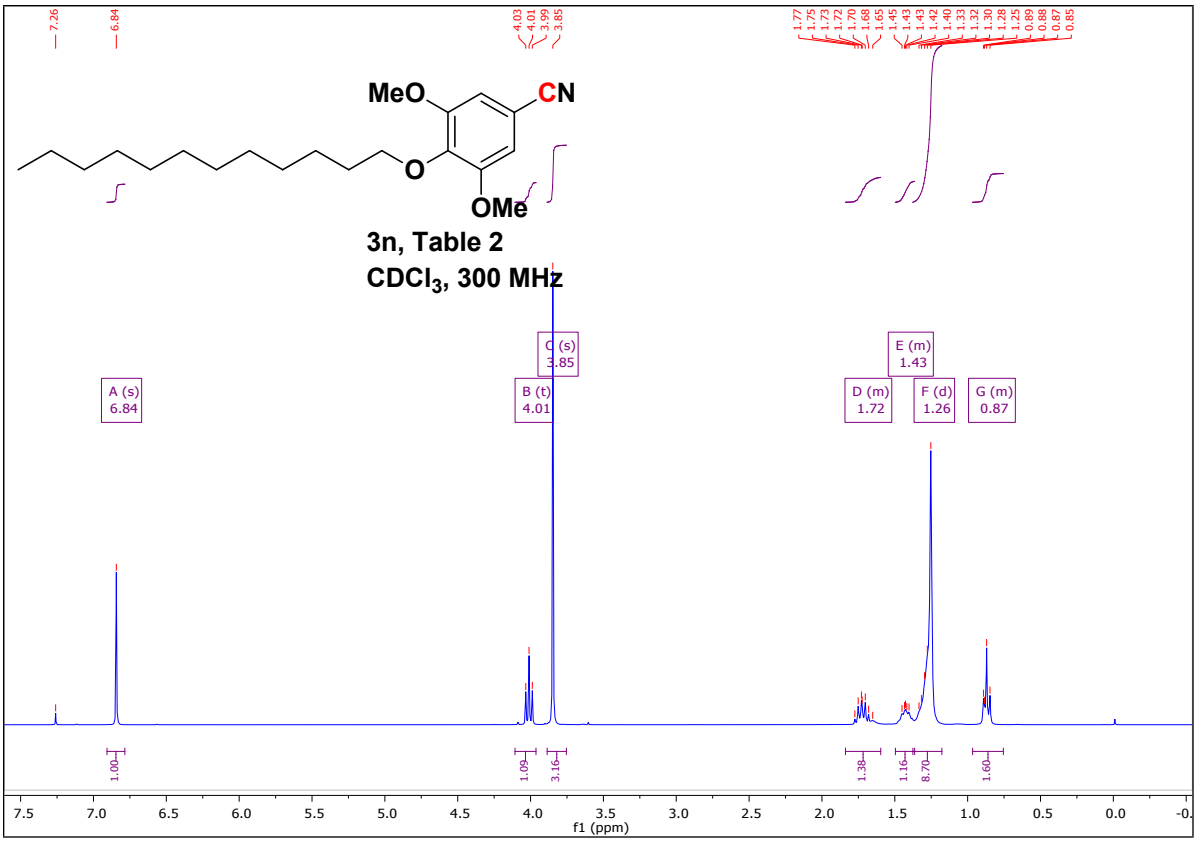

CN
OMe
3k, Table 2
CDCl3, 75 MHz
f1 (ppm)

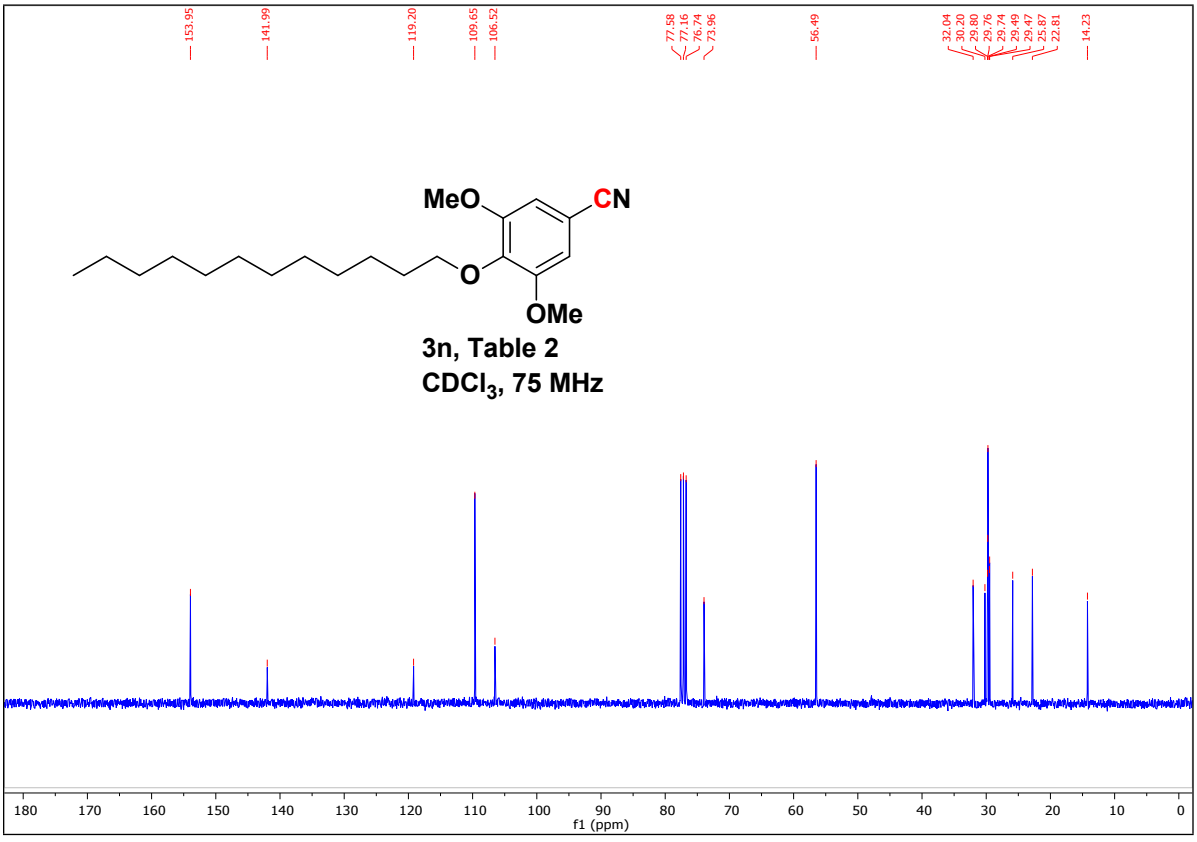

CN
B (m)
7.20
A (m)
7.47
C (q)
2.62
D (t)
1.16
3l, Table 2
CDCl3, 300 MHz
f1 (ppm)

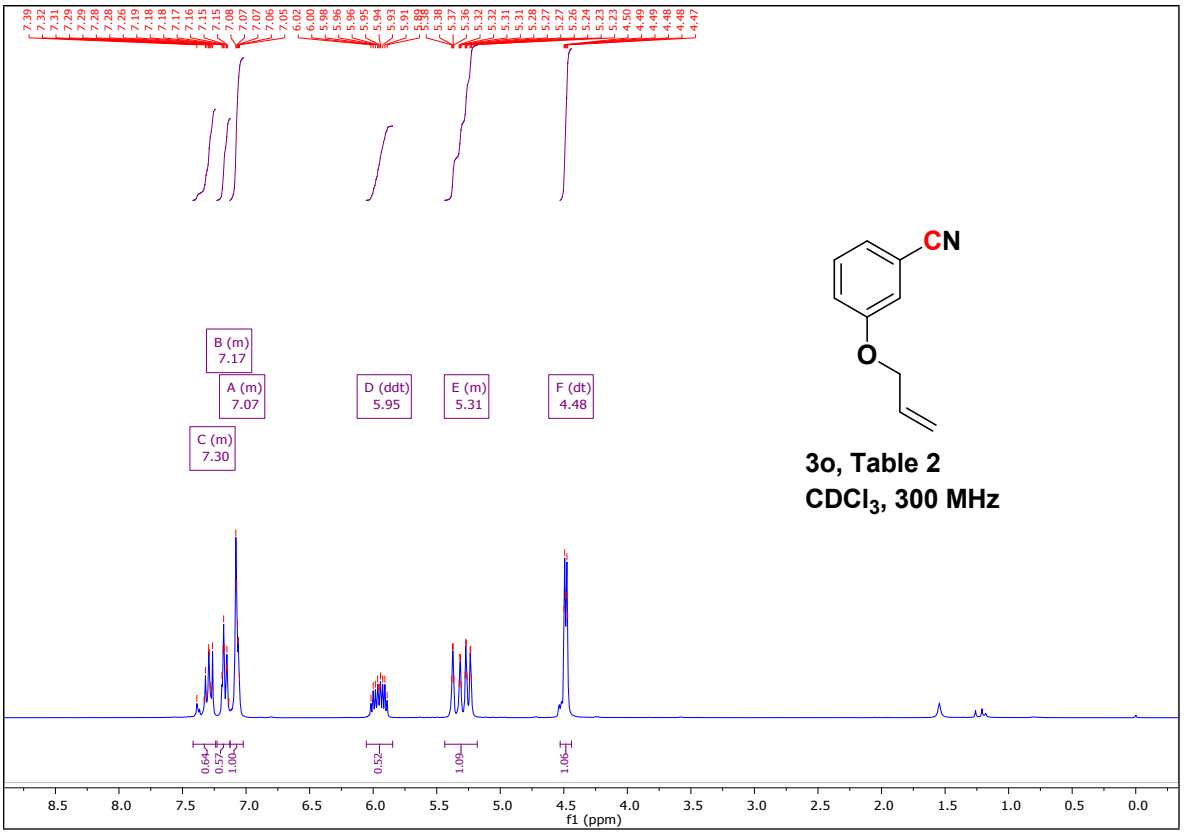

CN
3l, Table 2
CDCl3, 75 MHz
f1 (ppm)

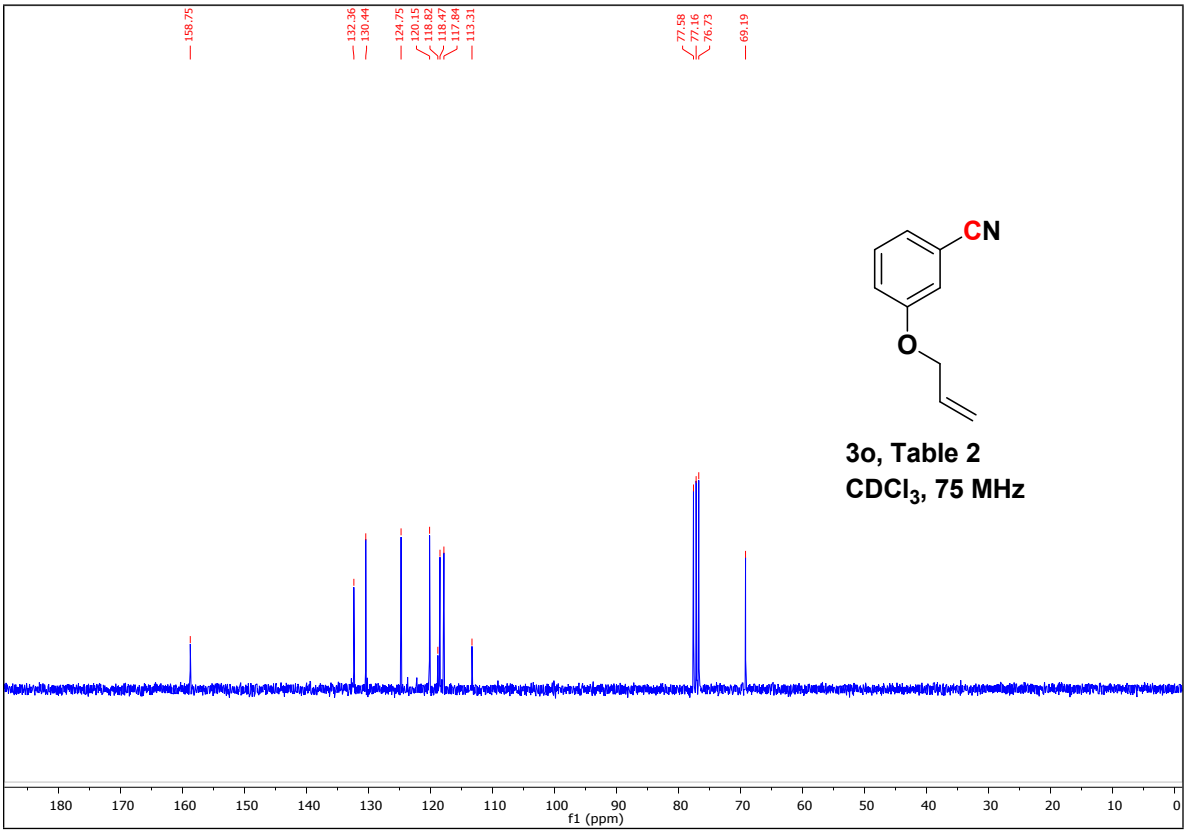

CN
B (td)
7.38
A (dd)
7.47
C (m)
7.19
D (s)
2.43
3m, Table 2
CDCl3, 300 MHz
f1 (ppm)

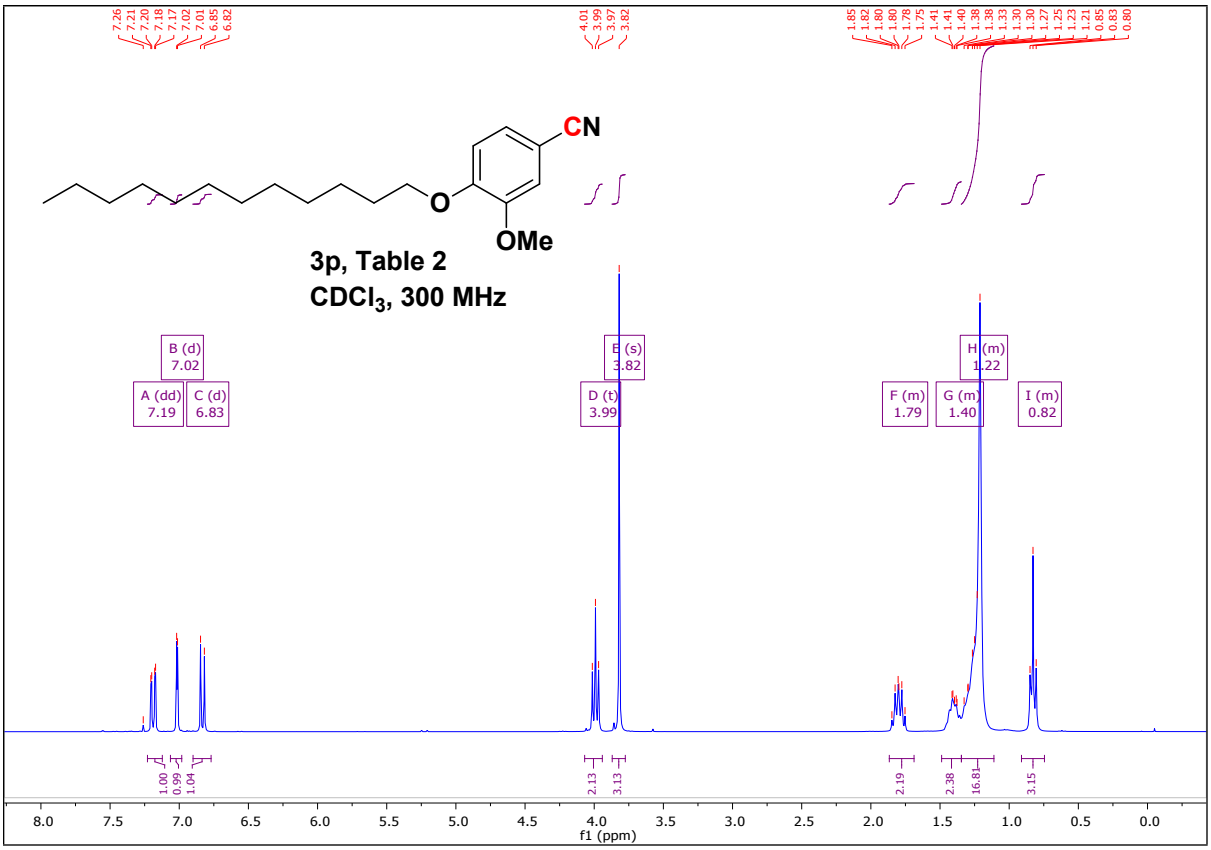

CN
3m, Table 2
CDCl3, 75 MHz
f1 (ppm)

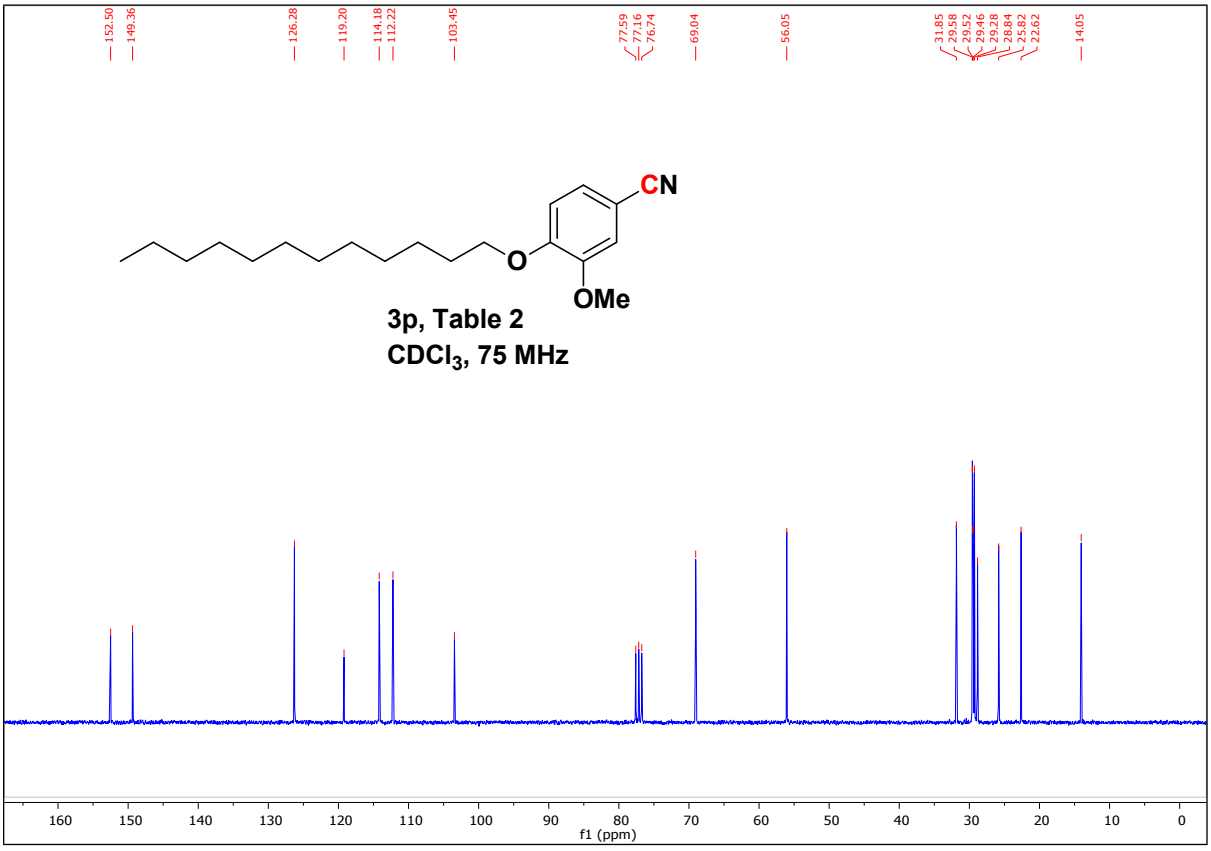

MeO
CN
O
OMe
3n, Table 2
CDCl3, 300 MHz
A (s) 6.84
B (t) 4.01
C (s) 3.85
D (m) 1.72
E (m) 1.43
F (d) 1.26
G (m) 0.87
f1 (ppm)

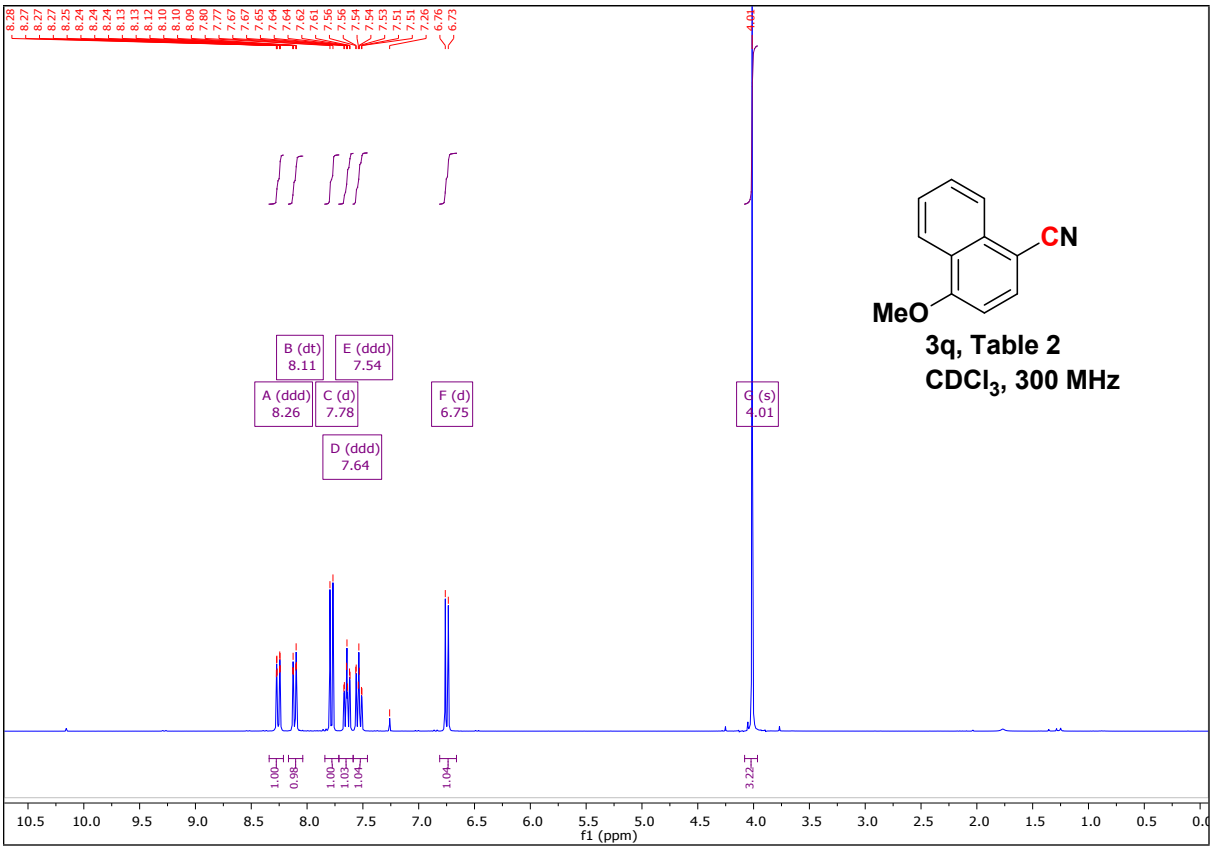

MeO
CN
O
OMe
3n, Table 2
CDCl3, 75 MHz
f1 (ppm)

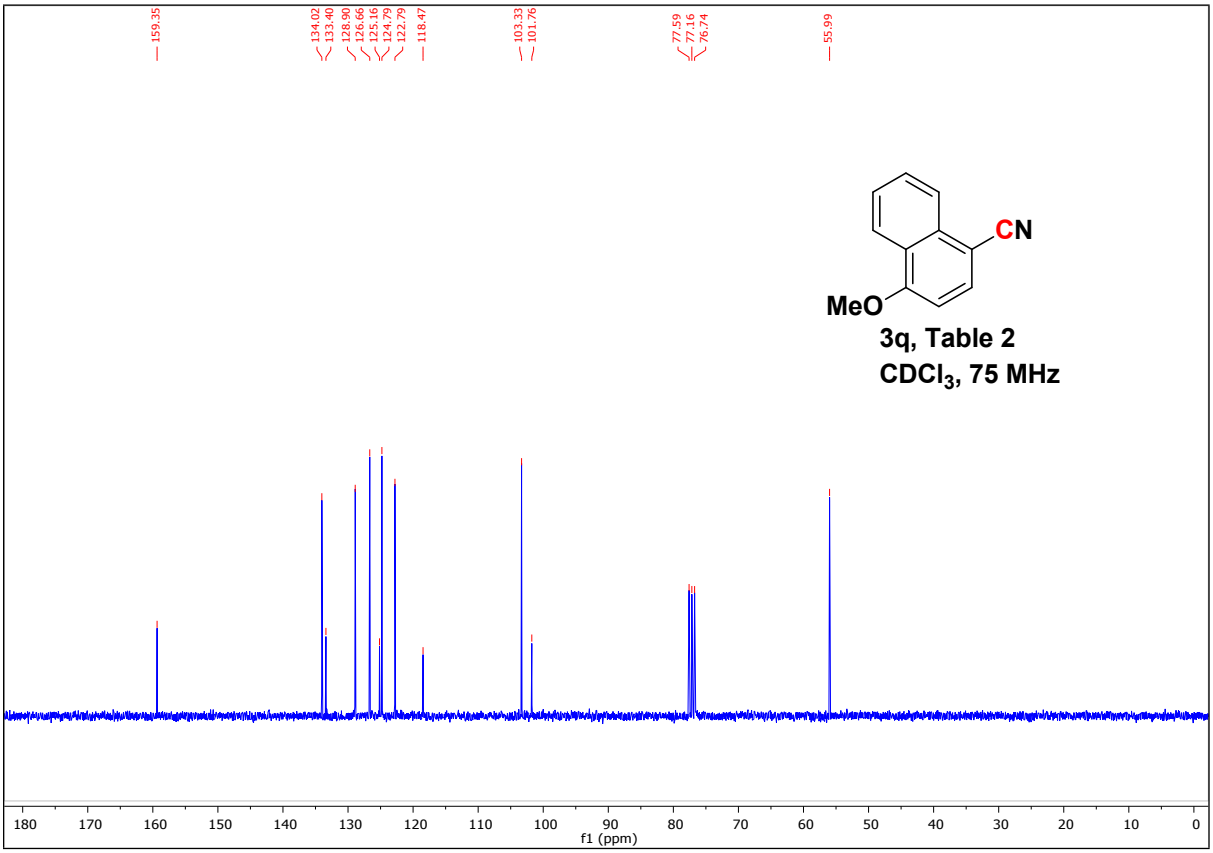

B (m)
7.17
A (m)
7.07
C (m)
7.30
D (ddt)
5.95
E (m)
5.31
F (dt)
4.48
CN
O
3o, Table 2
CDCl3, 300 MHz
f1 (ppm)

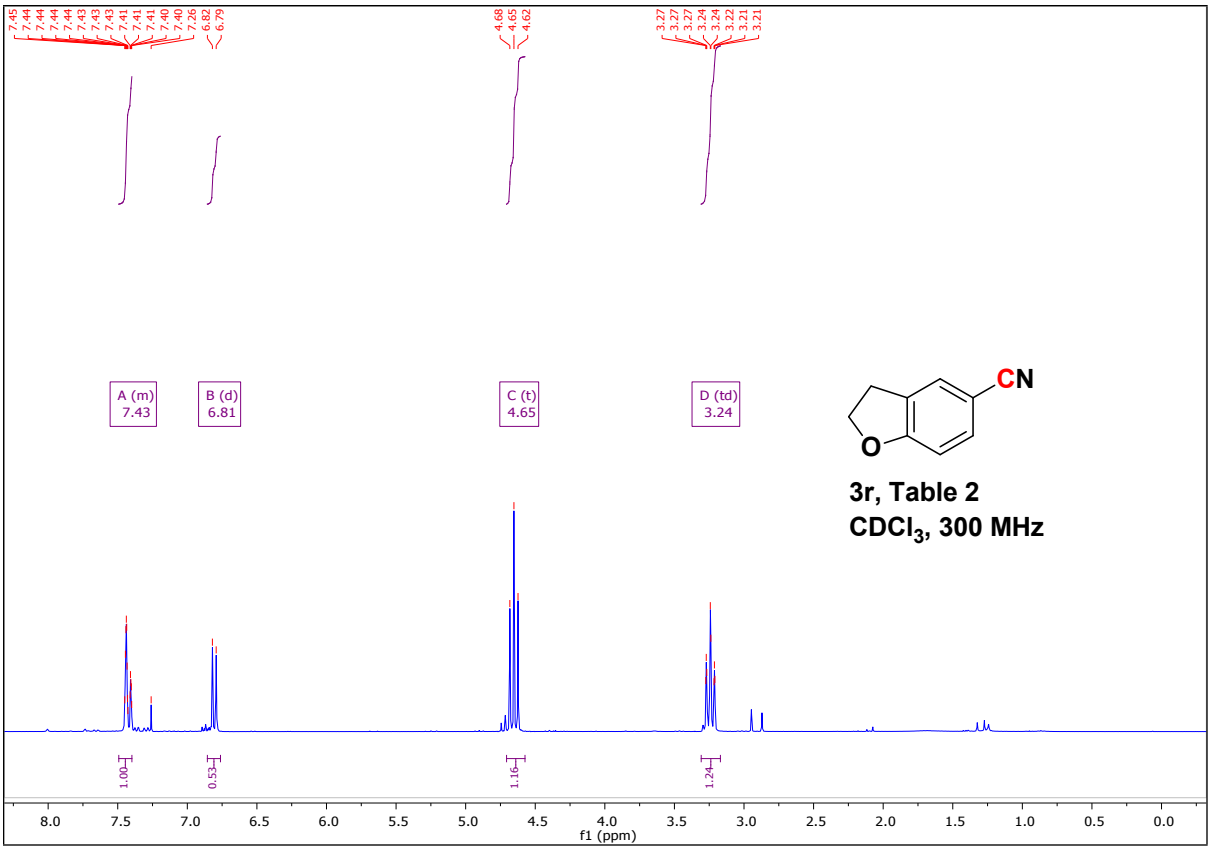

158.75
132.36
130.44
124.75
120.15
118.82
118.47
117.84
113.31
77.58
77.16
76.73
69.19
CN
O
3o, Table 2
CDCl3, 75 MHz
f1 (ppm)

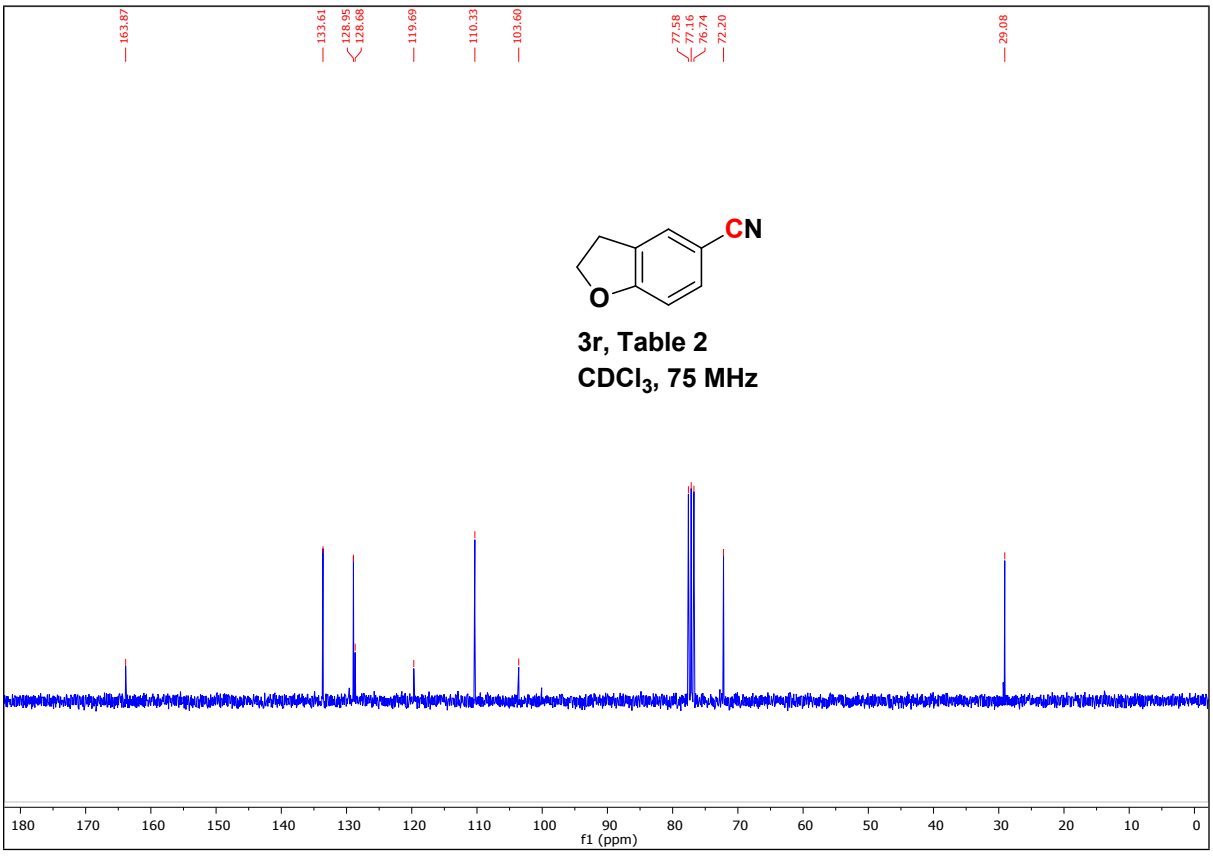

CN
O
OMe
3p, Table 2
CDCl3, 300 MHz
B (d) 7.02
A (dd) 7.19
C (d) 6.83
E (s) 3.82
D (t) 3.99
H (m) 1.22
F (m) 1.79
G (m) 1.40
I (m) 0.82
f1 (ppm)

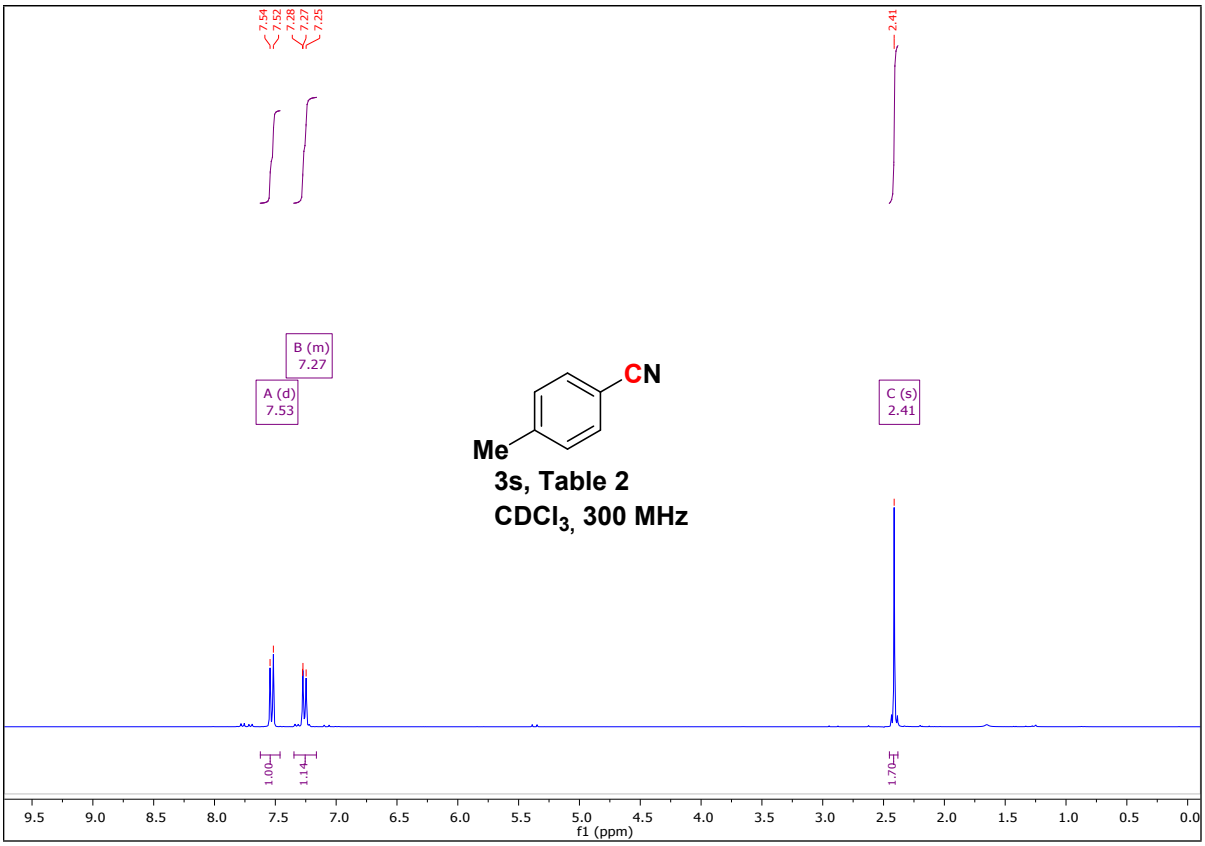

CN
O
OMe
3p, Table 2
CDCl3, 75 MHz
f1 (ppm)

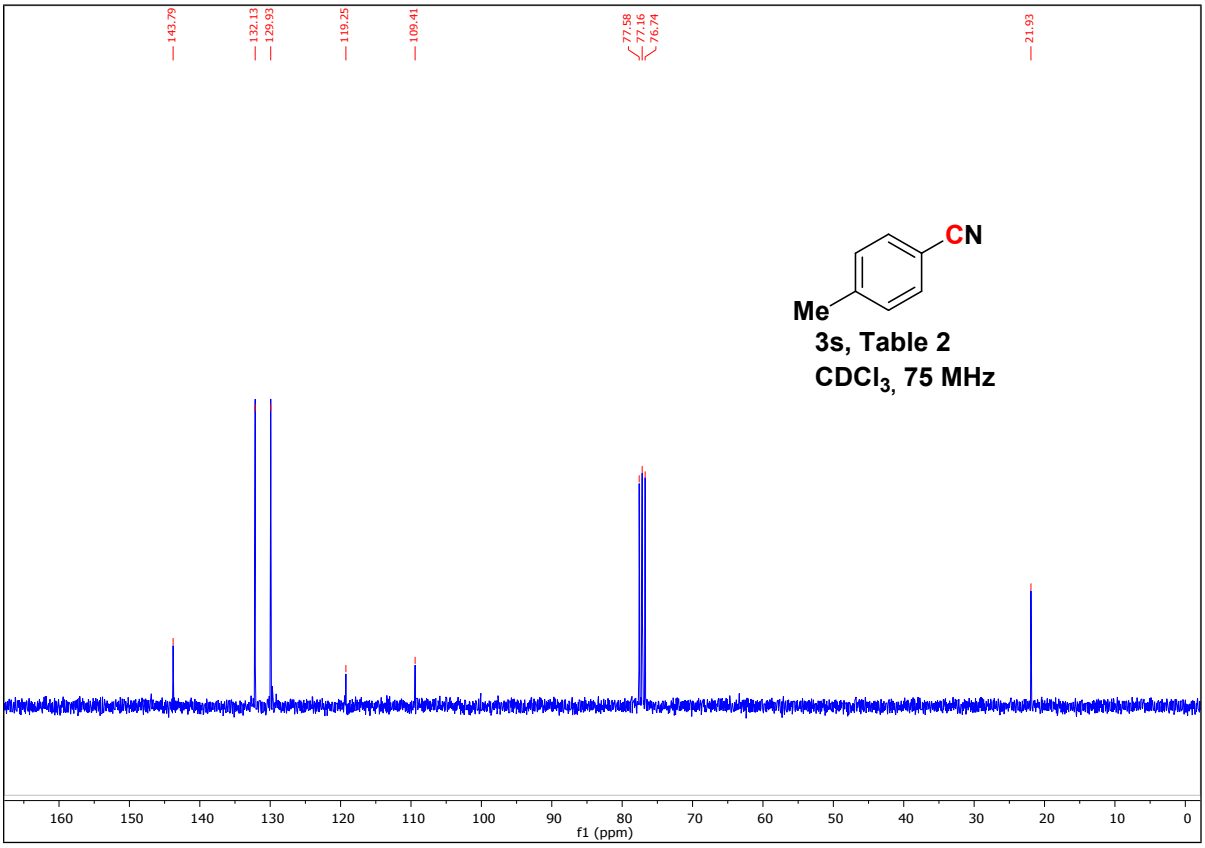

B (dt) 8.11
E (ddd) 7.54
A (ddd) 8.26
C (d) 7.78
F (d) 6.75
D (ddd) 7.64
G (s) 4.01
CN
MeO
3q, Table 2
CDCl3, 300 MHz
f1 (ppm)

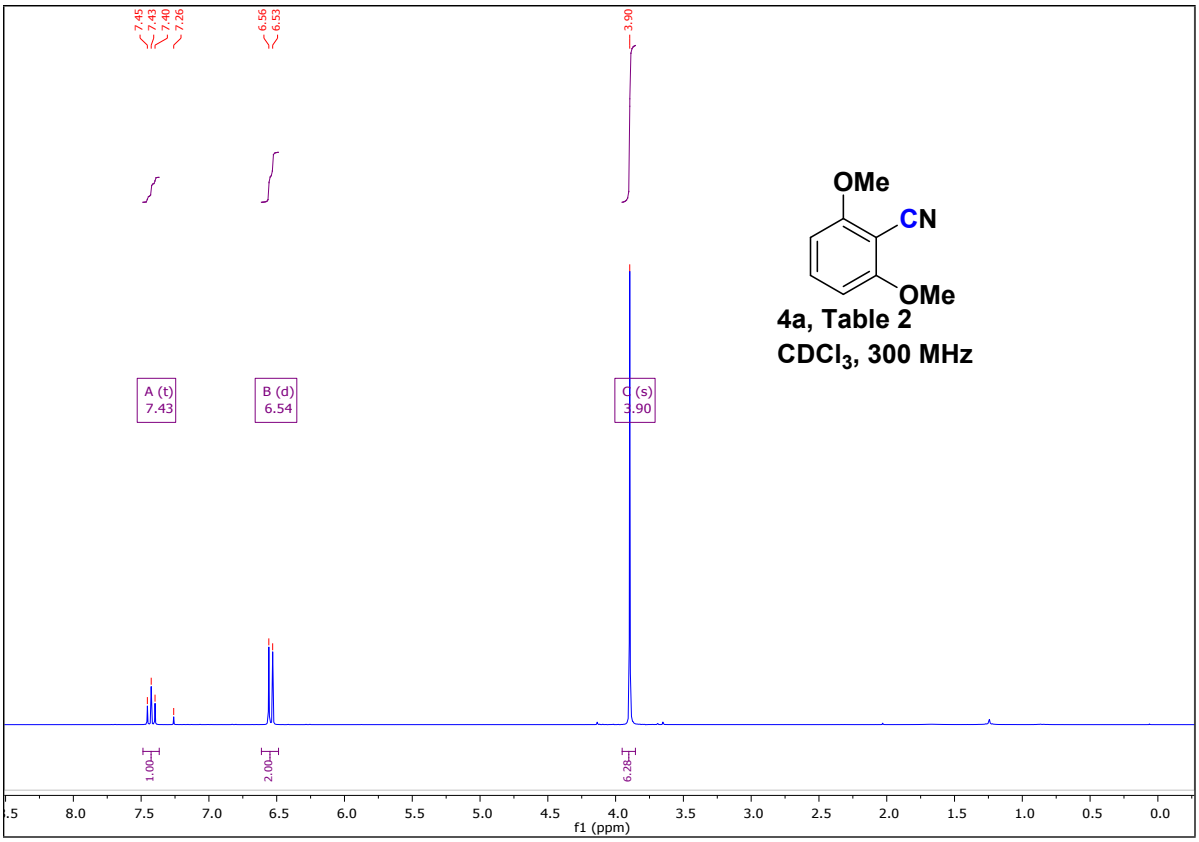

CN
MeO
3q, Table 2
CDCl3, 75 MHz
f1 (ppm)

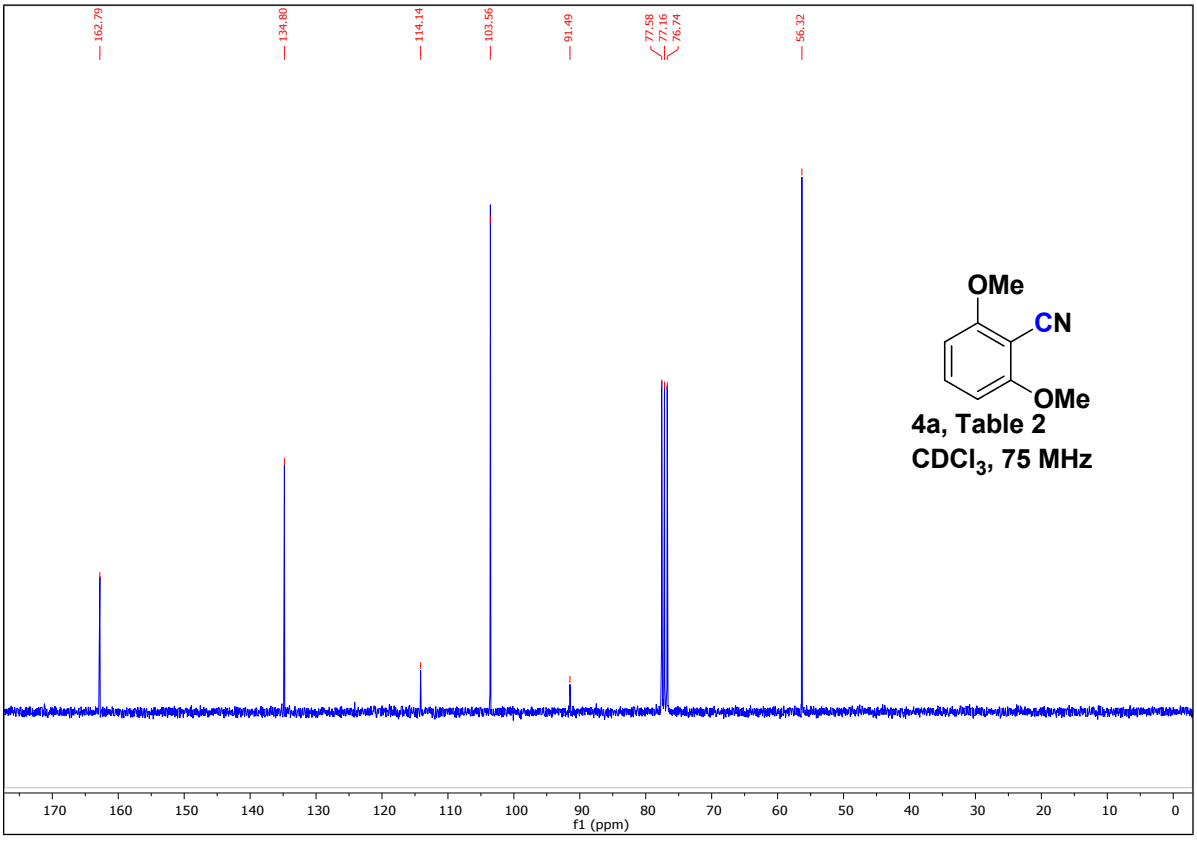

A (m)
7.43
B (d)
6.81
C (t)
4.65
D (td)
3.24
CN
O
3r, Table 2
CDCl3, 300 MHz
f1 (ppm)

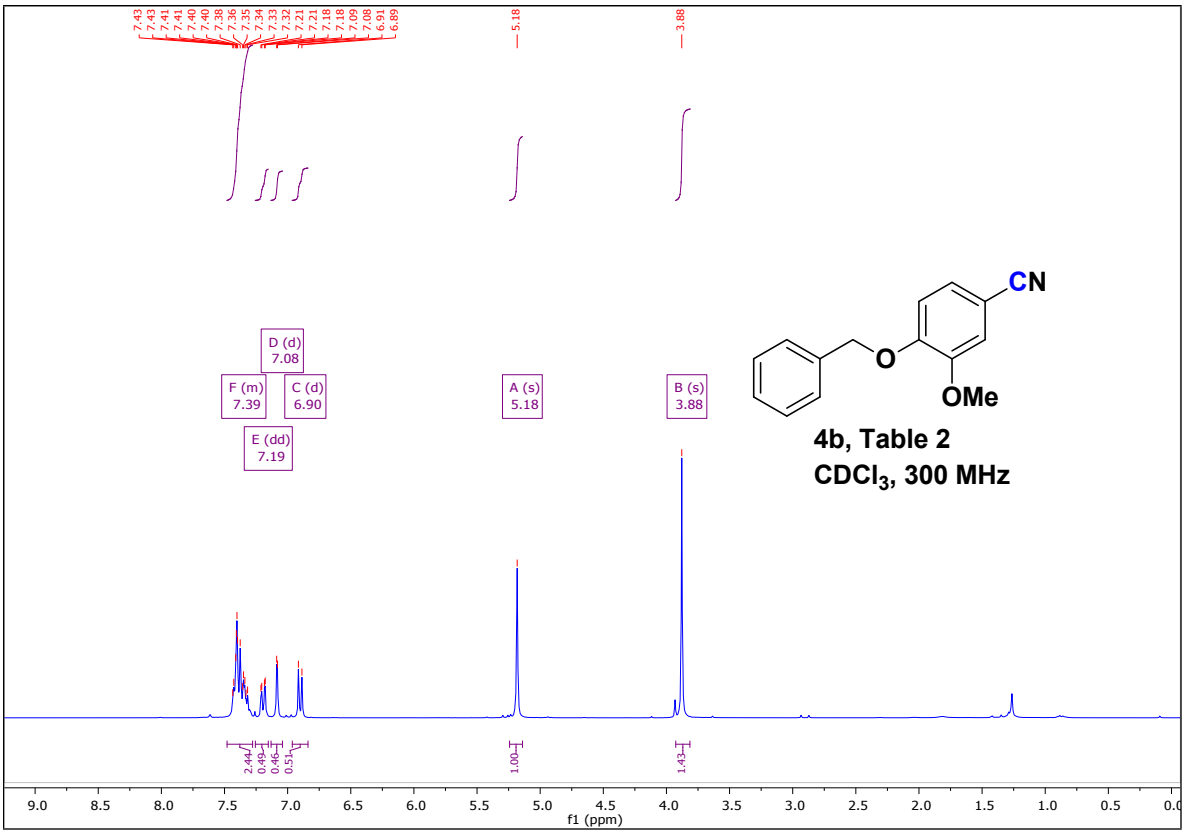

CN
O
3r, Table 2
CDCl3, 75 MHz
f1 (ppm)

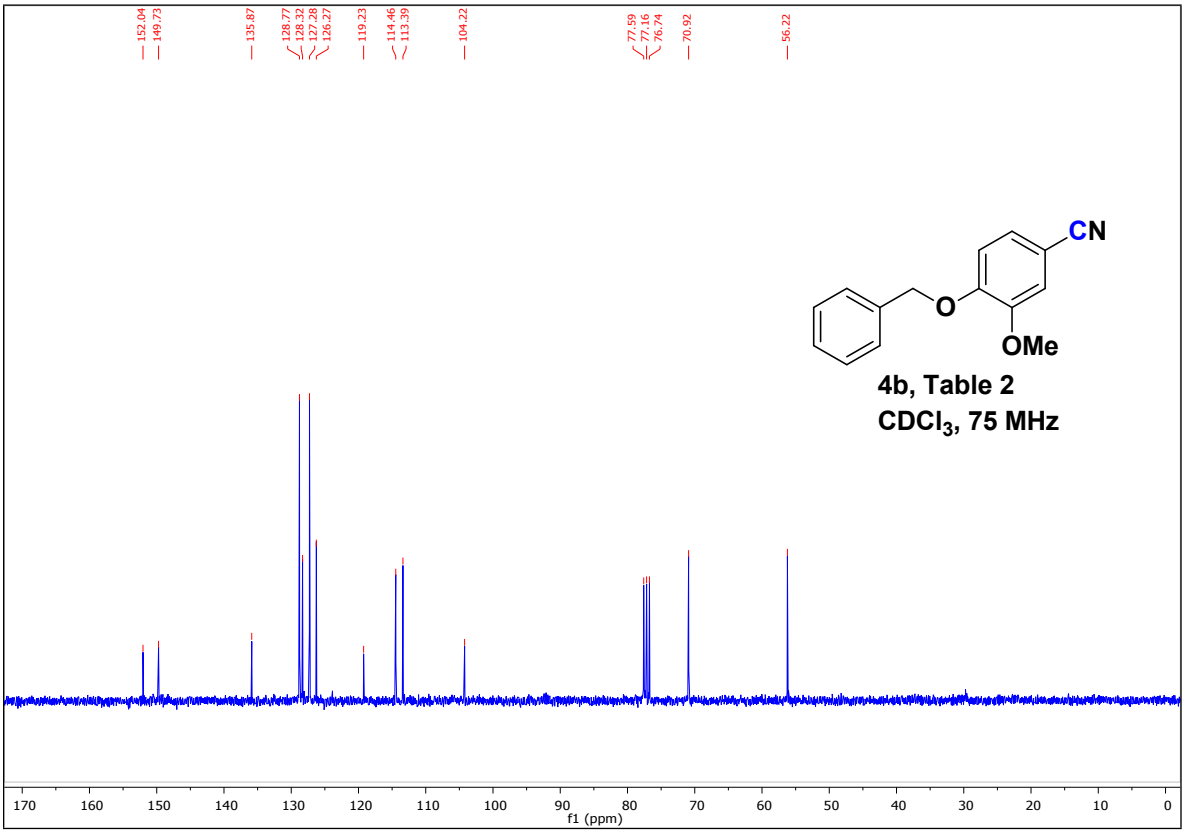

7.54
7.52
7.28
7.27
7.25
2.41
B (m)
7.27
A (d)
7.53
C (s)
2.41
CN
Me
3s, Table 2
CDCl3, 300 MHz
1.00
1.14
1.70
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

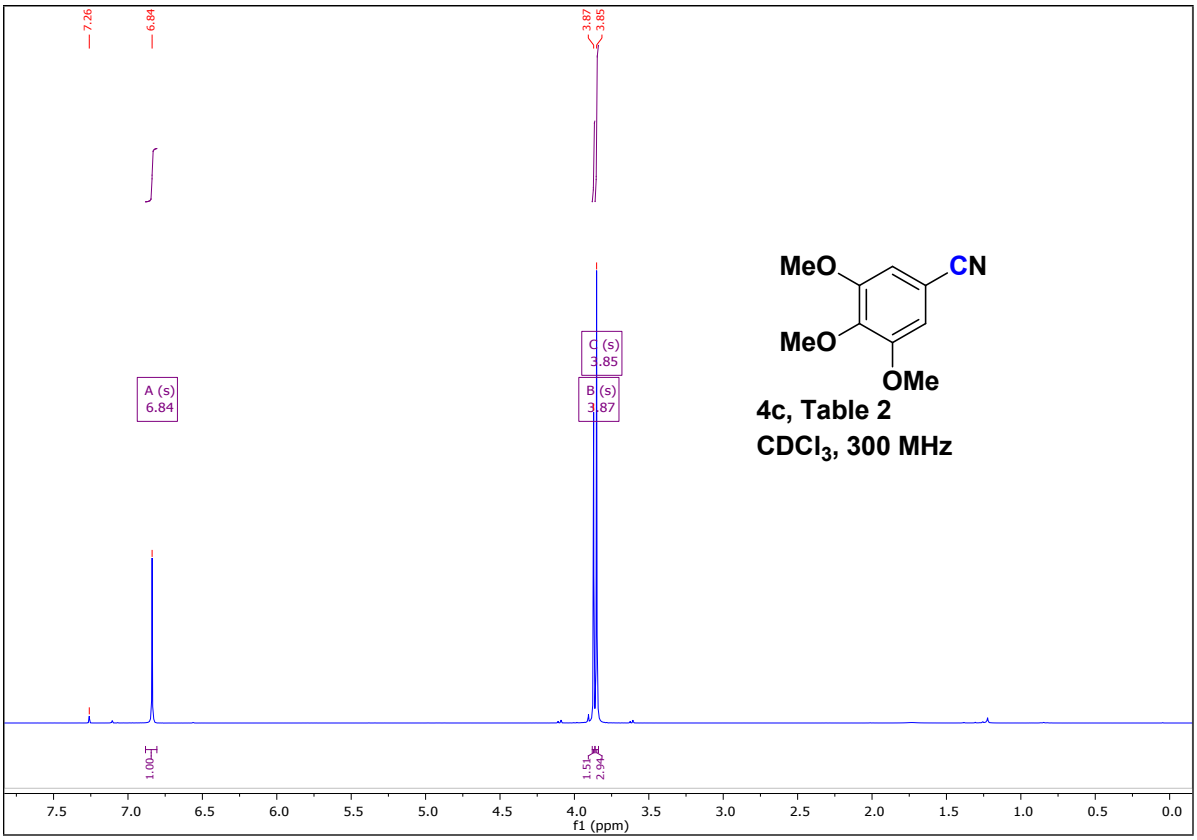

143.79
132.13
129.93
119.25
109.41
77.58
77.16
76.74
21.93
CN
Me
3s, Table 2
CDCl3, 75 MHz
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

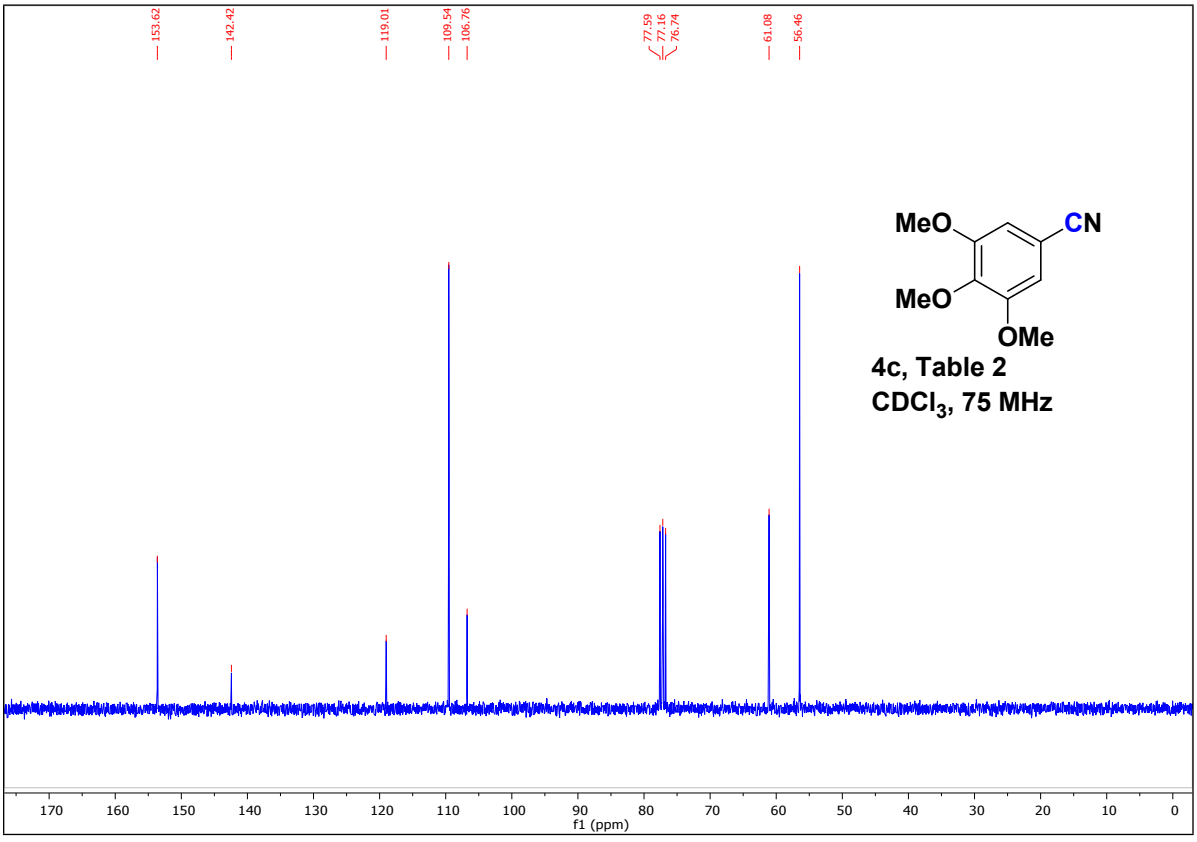

7.45
7.43
7.40
7.26
6.56
6.53
3.90
A (t)
7.43
B (d)
6.54
C (s)
3.90
1.00
2.00
6.28
f1 (ppm)
OMe
CN
OMe
4a, Table 2
CDCl3, 300 MHz

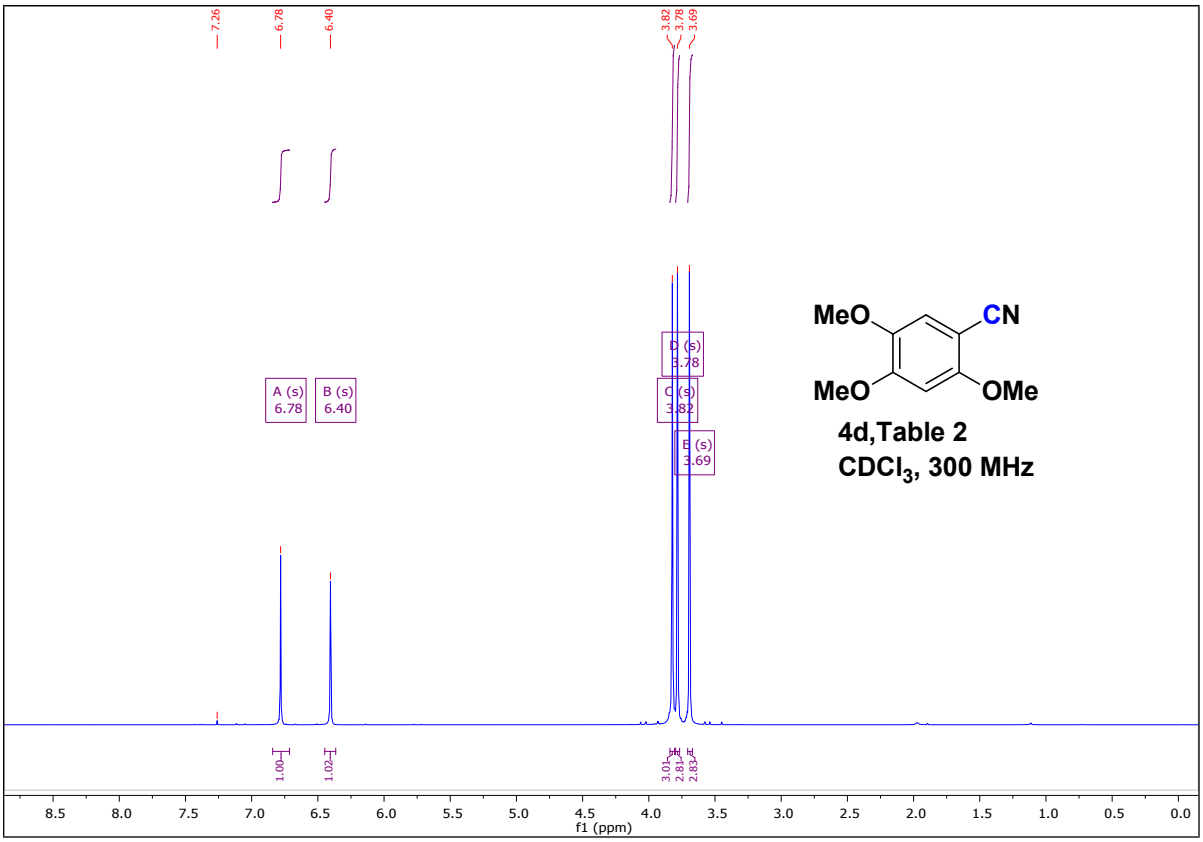

162.79
134.80
114.14
103.56
91.49
77.58
77.16
76.74
56.32
f1 (ppm)
OMe
CN
OMe
4a, Table 2
CDCl3, 75 MHz

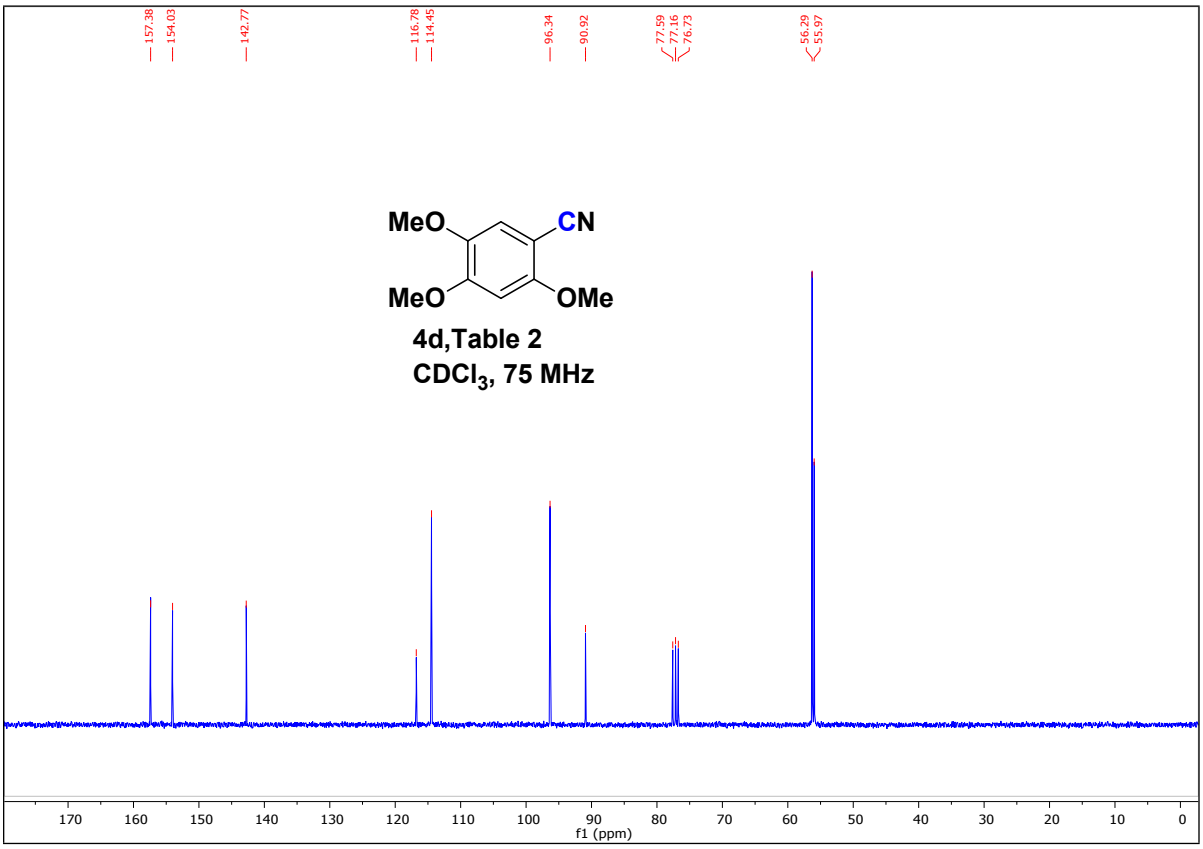

7.43
7.43
7.41
7.41
7.40
7.40
7.38
7.36
7.35
7.34
7.33
7.32
7.21
7.21
7.18
7.18
7.09
7.08
6.91
6.89
5.18
3.88
D (d)
7.08
F (m)
7.39
C (d)
6.90
E (dd)
7.19
A (s)
5.18
B (s)
3.88
CN
O
OMe
4b, Table 2
CDCl3, 300 MHz
2.44
0.49
0.46
0.51
1.00
1.43
f1 (ppm)

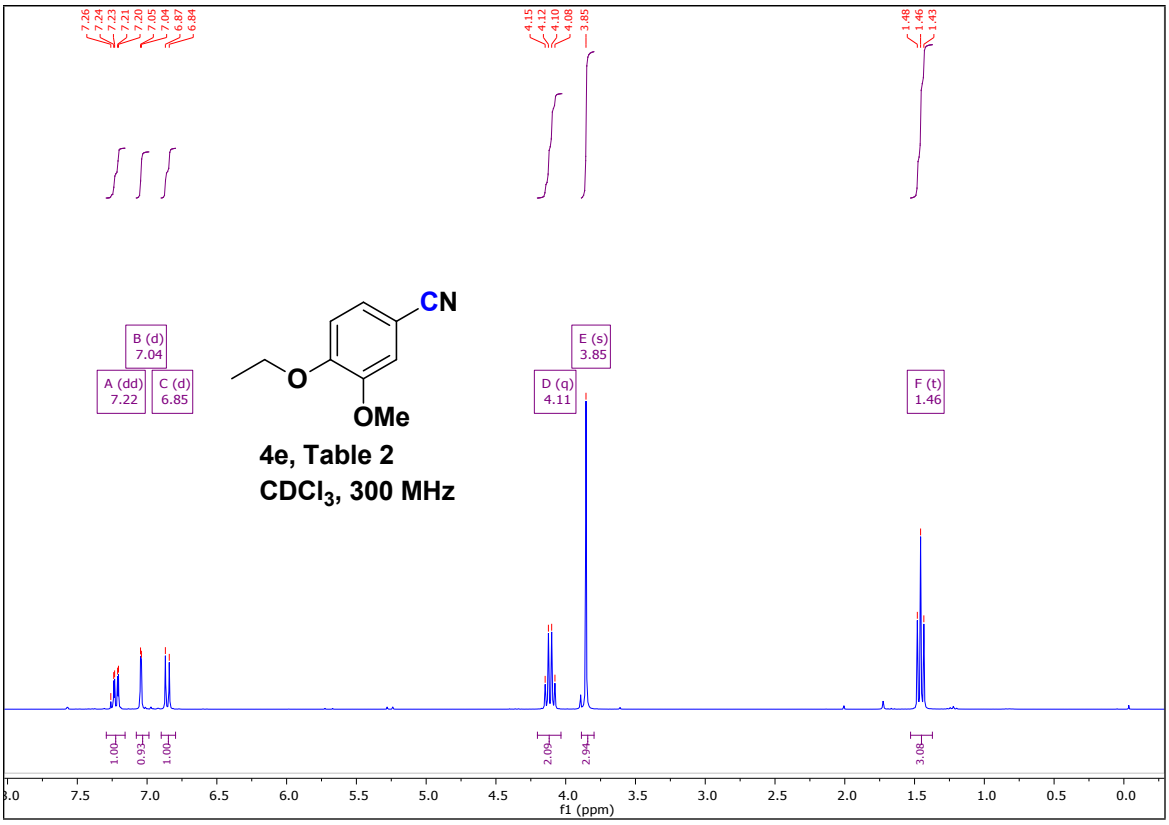

152.04
149.73
135.87
128.77
128.32
127.28
126.27
119.23
114.46
113.39
104.22
77.59
77.16
76.74
70.92
56.22
CN
O
OMe
4b, Table 2
CDCl3, 75 MHz
f1 (ppm)

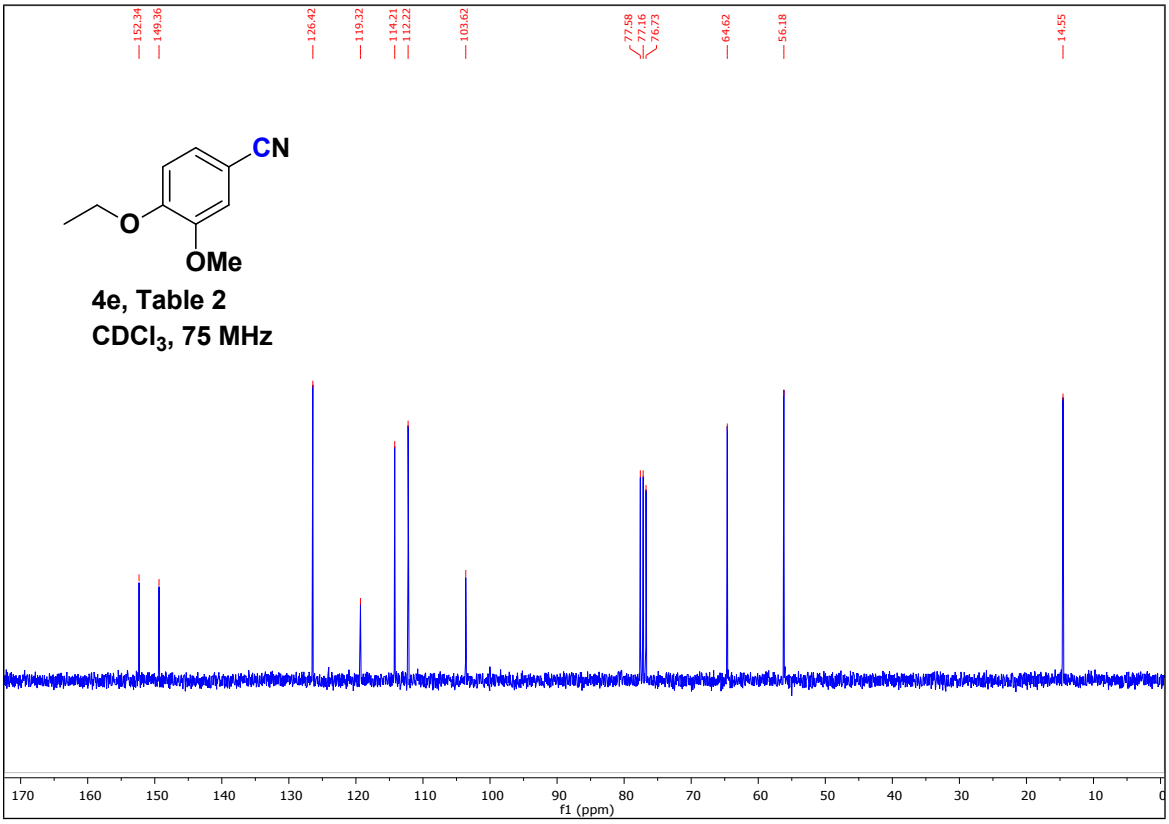

7.26
6.84
3.87
3.85
A (s)
6.84
C (s)
3.85
B (s)
3.87
1.00
1.51
2.94
MeO
CN
MeO
OMe
4c, Table 2
CDCl3, 300 MHz
f1 (ppm)

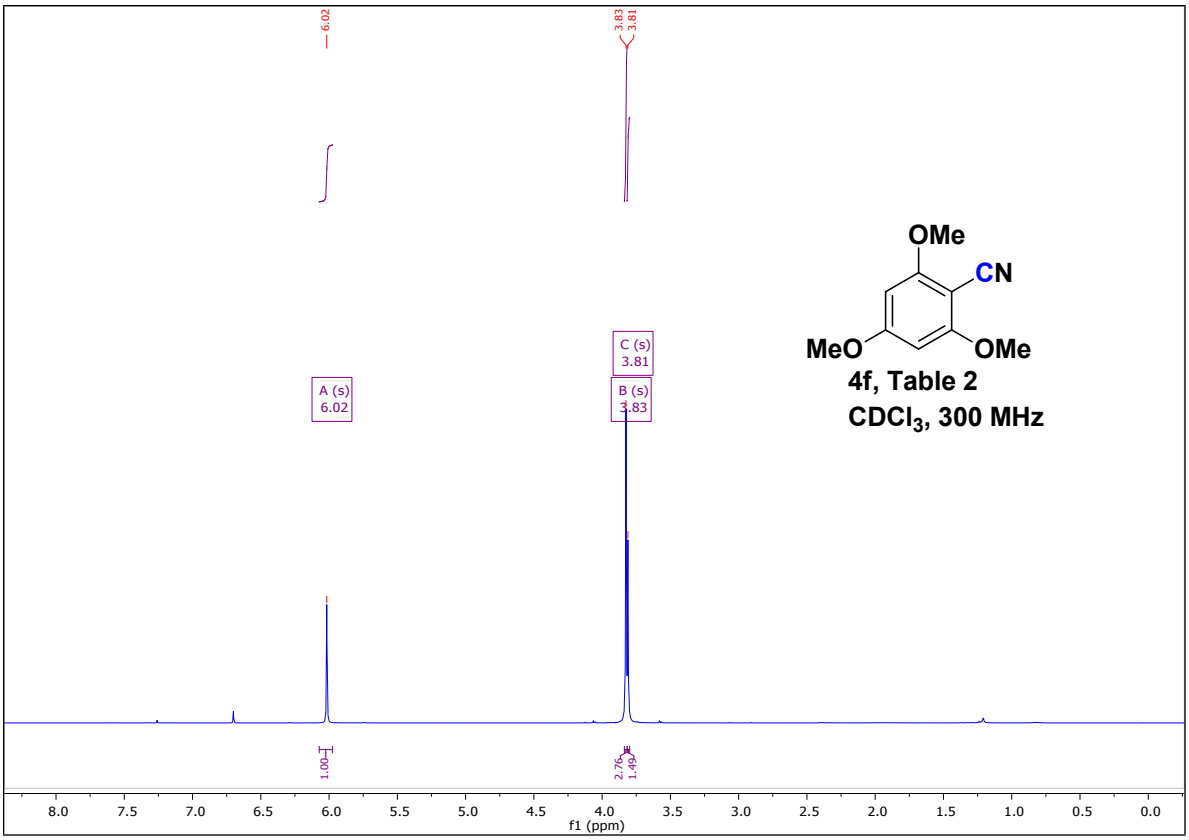

153.62
142.42
119.01
109.54
106.76
77.59
77.16
76.74
61.08
56.46
MeO
CN
MeO
OMe
4c, Table 2
CDCl3, 75 MHz
f1 (ppm)

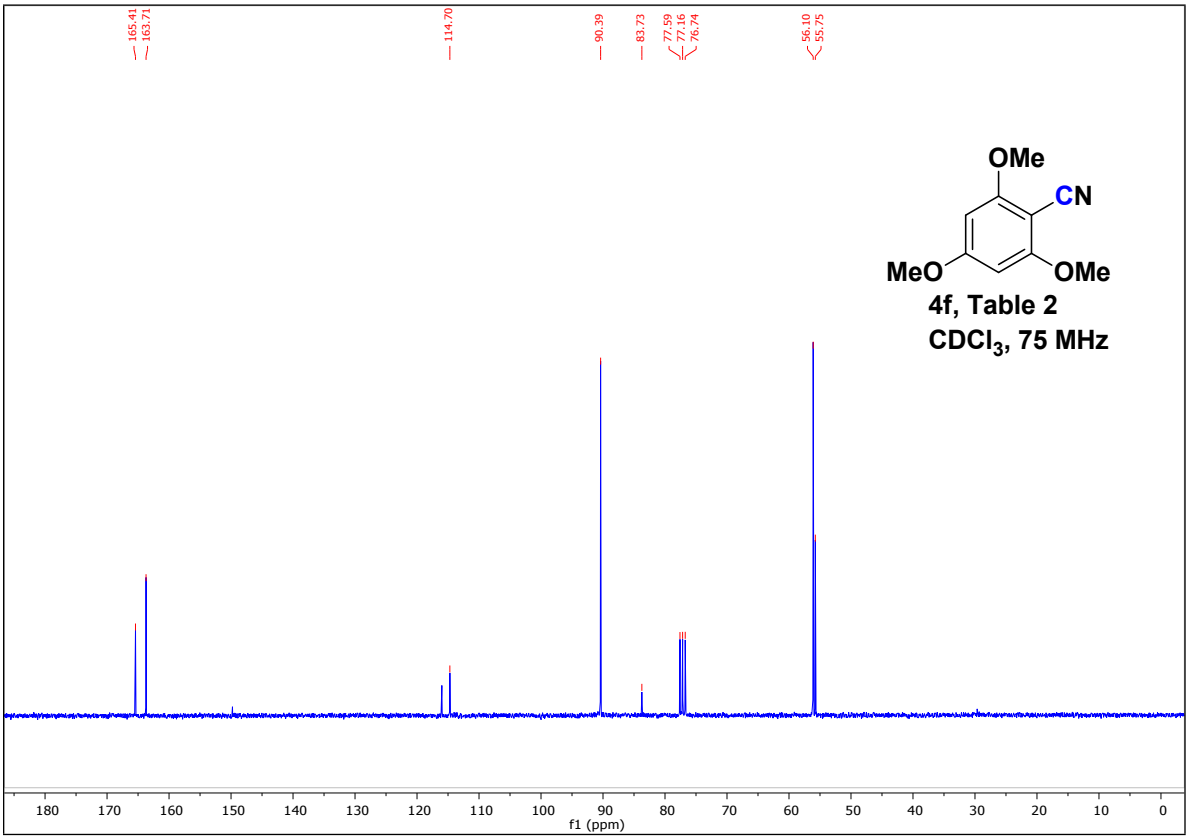

7.26
6.78
6.40
3.82
3.78
3.69
A (s) 6.78
B (s) 6.40
D (s) 3.78
C (s) 3.82
E (s) 3.69
MeO
CN
MeO
OMe
4d,Table 2
CDCl3, 300 MHz
1.00
1.02
3.01
2.81
2.83
f1 (ppm)

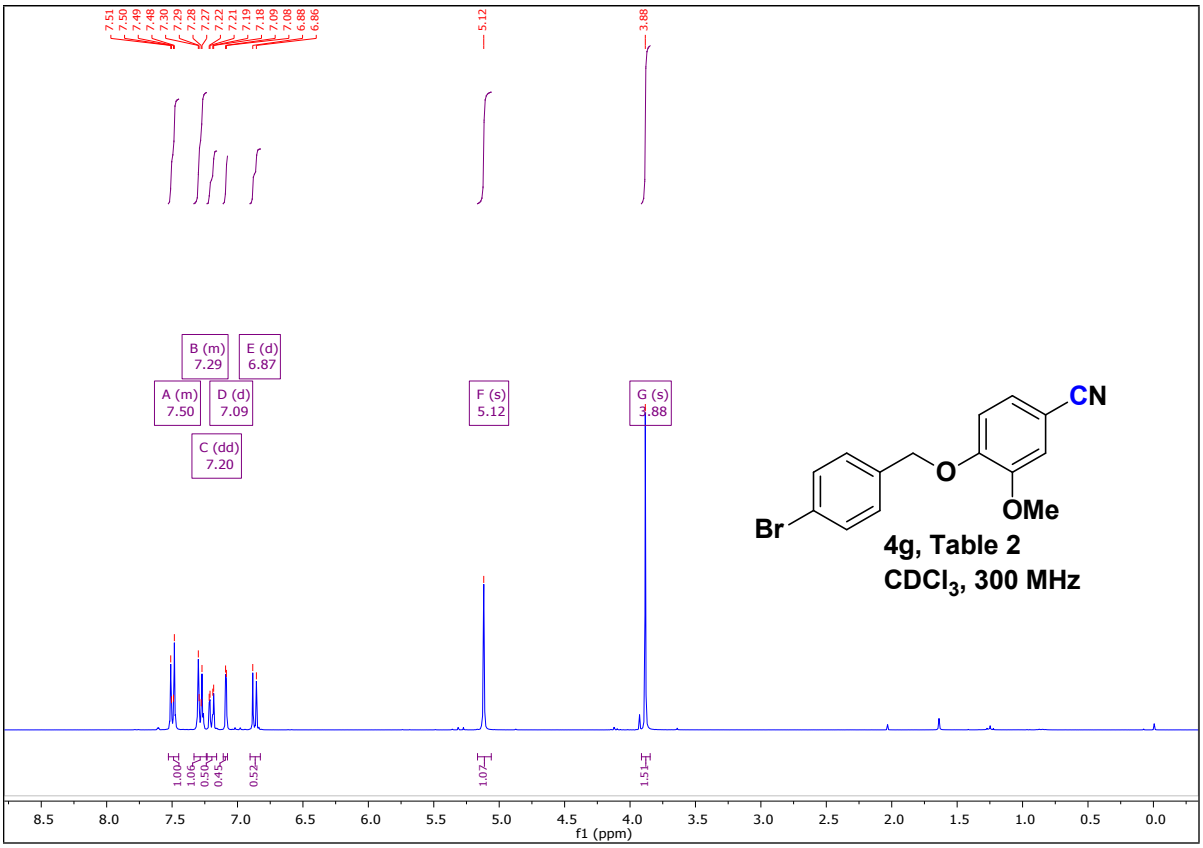

157.38
154.03
142.77
116.78
114.45
96.34
90.92
77.59
77.16
76.73
56.29
55.97
MeO
CN
MeO
OMe
4d,Table 2
CDCl3, 75 MHz
f1 (ppm)

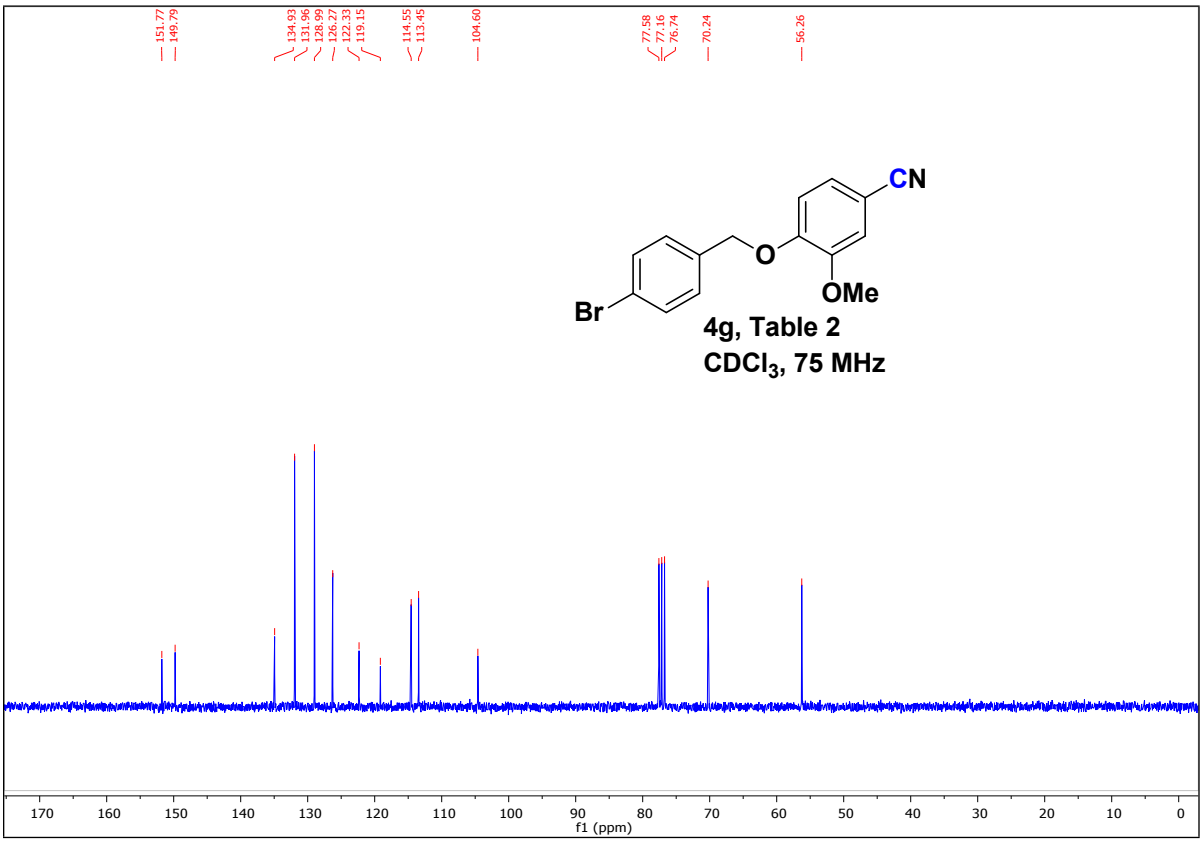

7.26
7.24
7.23
7.21
7.20
7.05
7.04
6.87
6.84
4.15
4.12
4.10
4.08
3.85
1.48
1.46
1.43
B (d)
7.04
A (dd)
7.22
C (d)
6.85
E (s)
3.85
D (q)
4.11
F (t)
1.46
CN
O
OMe
4e, Table 2
CDCl3, 300 MHz
1.00
0.93
1.00
2.09
2.94
3.08
f1 (ppm)

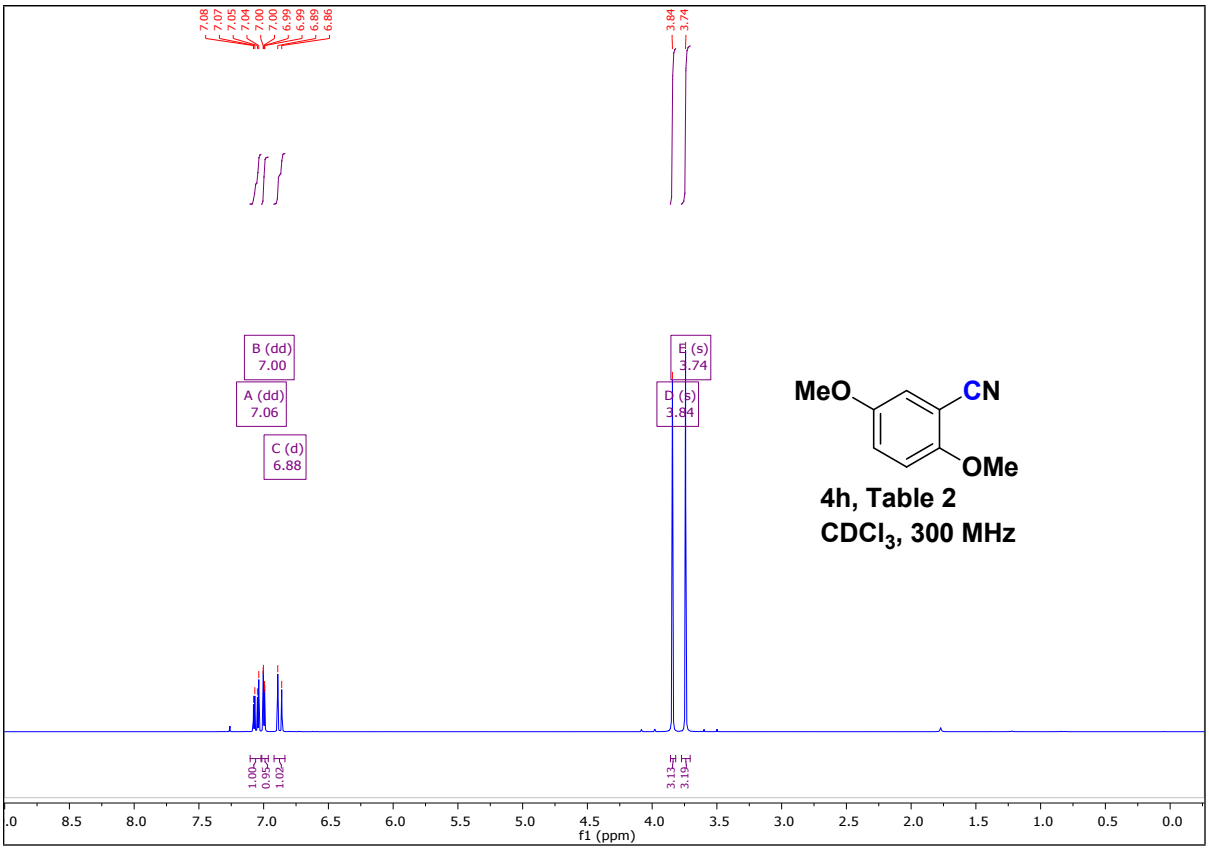

152.34
149.36
126.42
119.32
114.21
112.22
103.62
77.58
77.16
76.73
64.62
56.18
14.55
CN
O
OMe
4e, Table 2
CDCl3, 75 MHz
f1 (ppm)

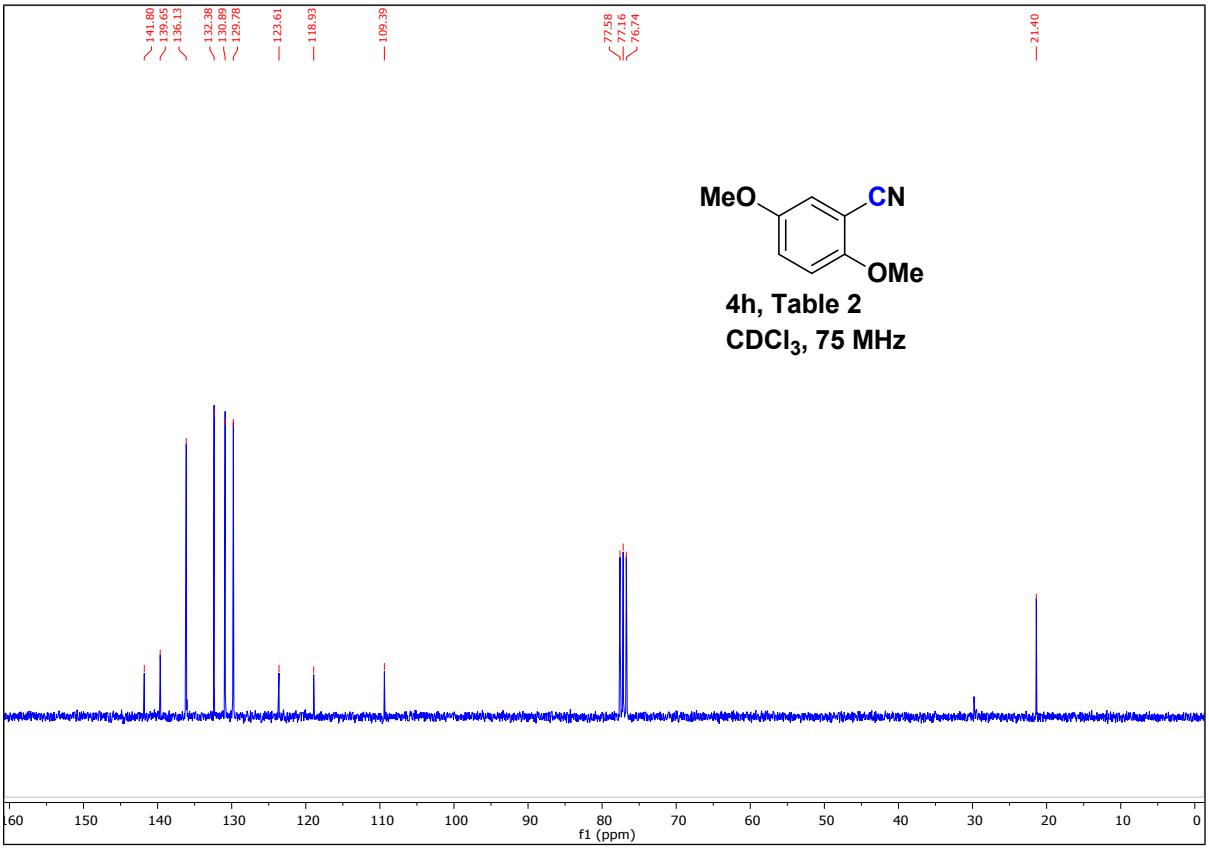

6.02
3.83
3.81
OMe
CN
MeO
OMe
C (s)
3.81
A (s)
6.02
B (s)
3.83
4f, Table 2
CDCl3, 300 MHz
1.00
2.76
1.49
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

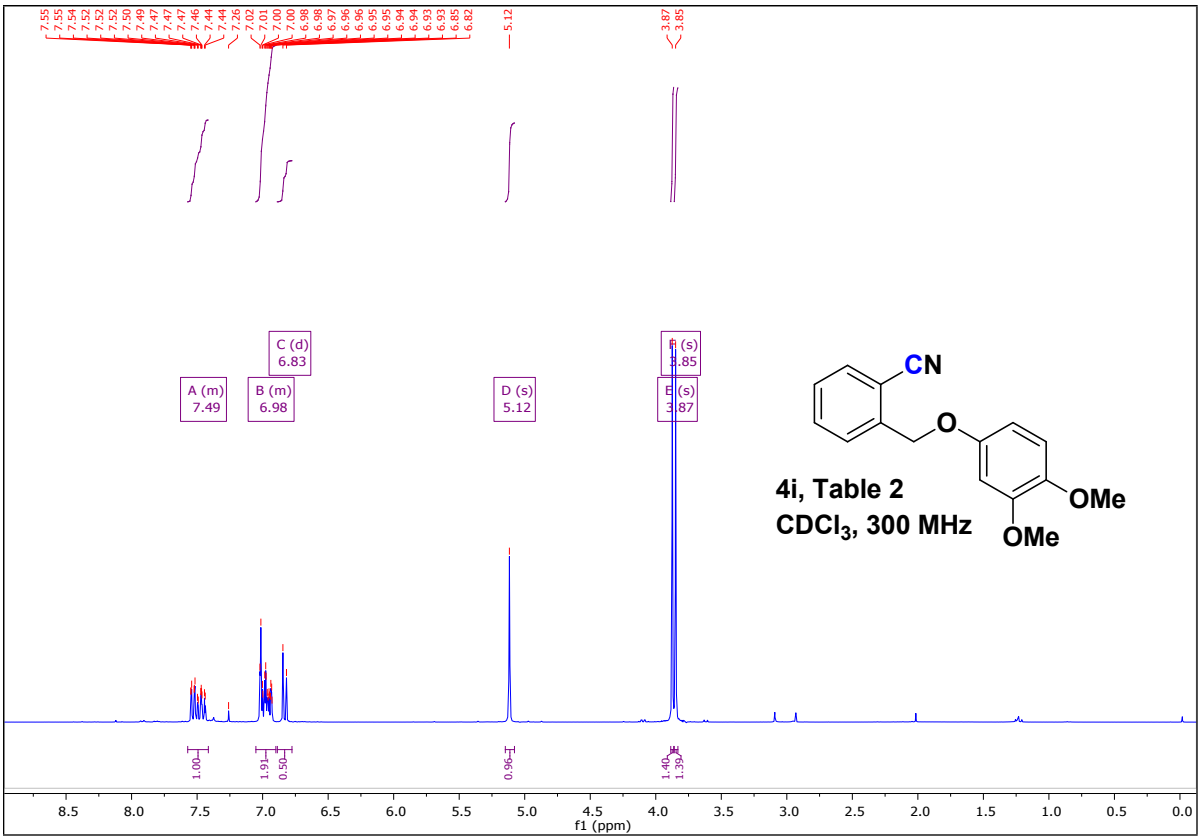

165.41
163.71
114.70
90.39
83.73
77.59
77.16
76.74
56.10
55.75
OMe
CN
MeO
OMe
4f, Table 2
CDCl3, 75 MHz
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

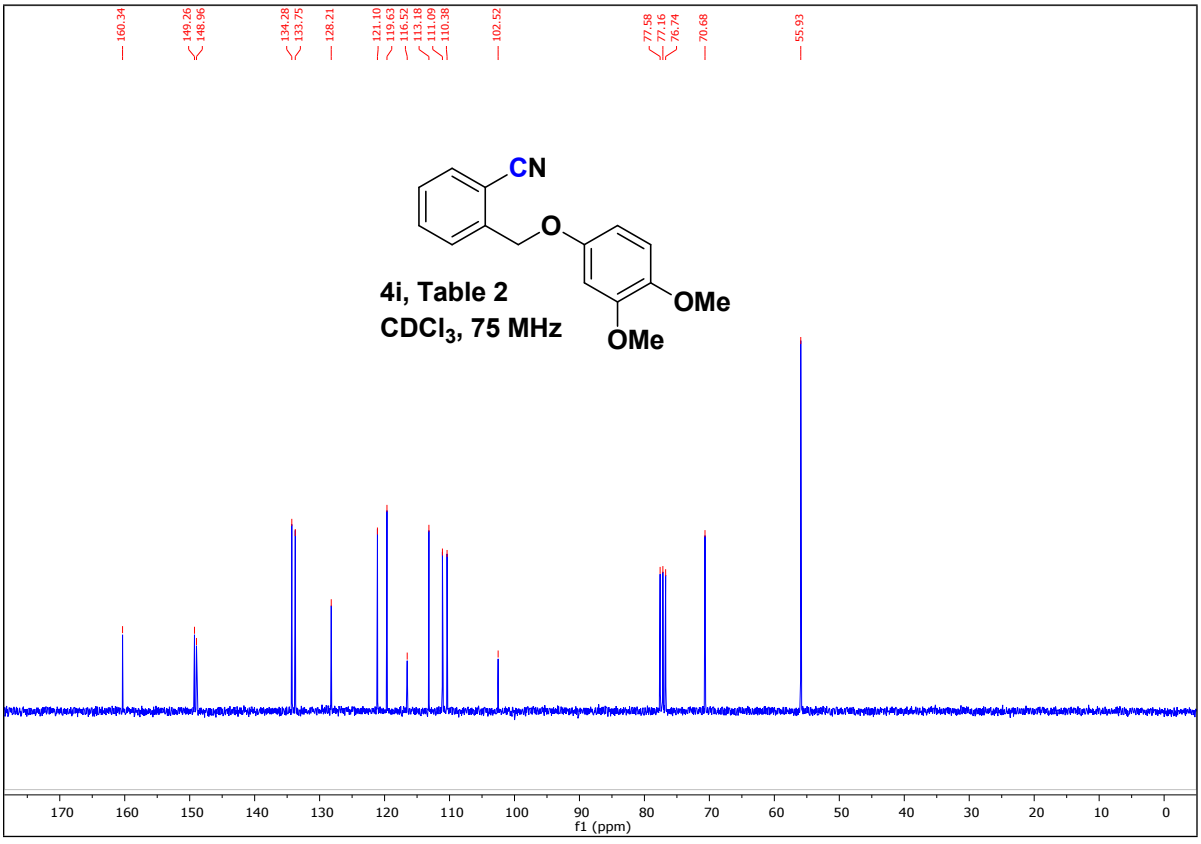

B (m) 7.29
E (d) 6.87
A (m) 7.50
D (d) 7.09
C (dd) 7.20
F (s) 5.12
G (s) 3.88
CN
O
OMe
Br
4g, Table 2
CDCl3, 300 MHz
f1 (ppm)

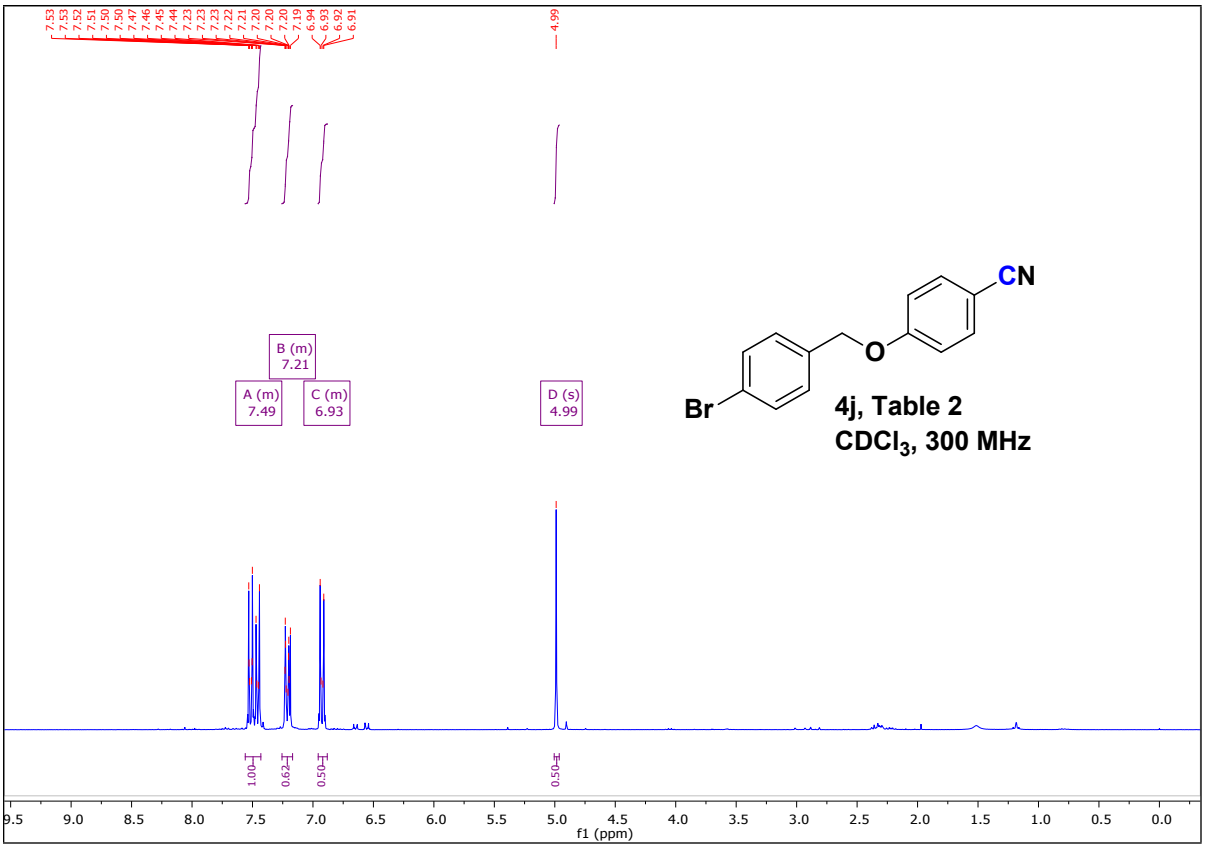

CN
O
OMe
Br
4g, Table 2
CDCl3, 75 MHz
f1 (ppm)

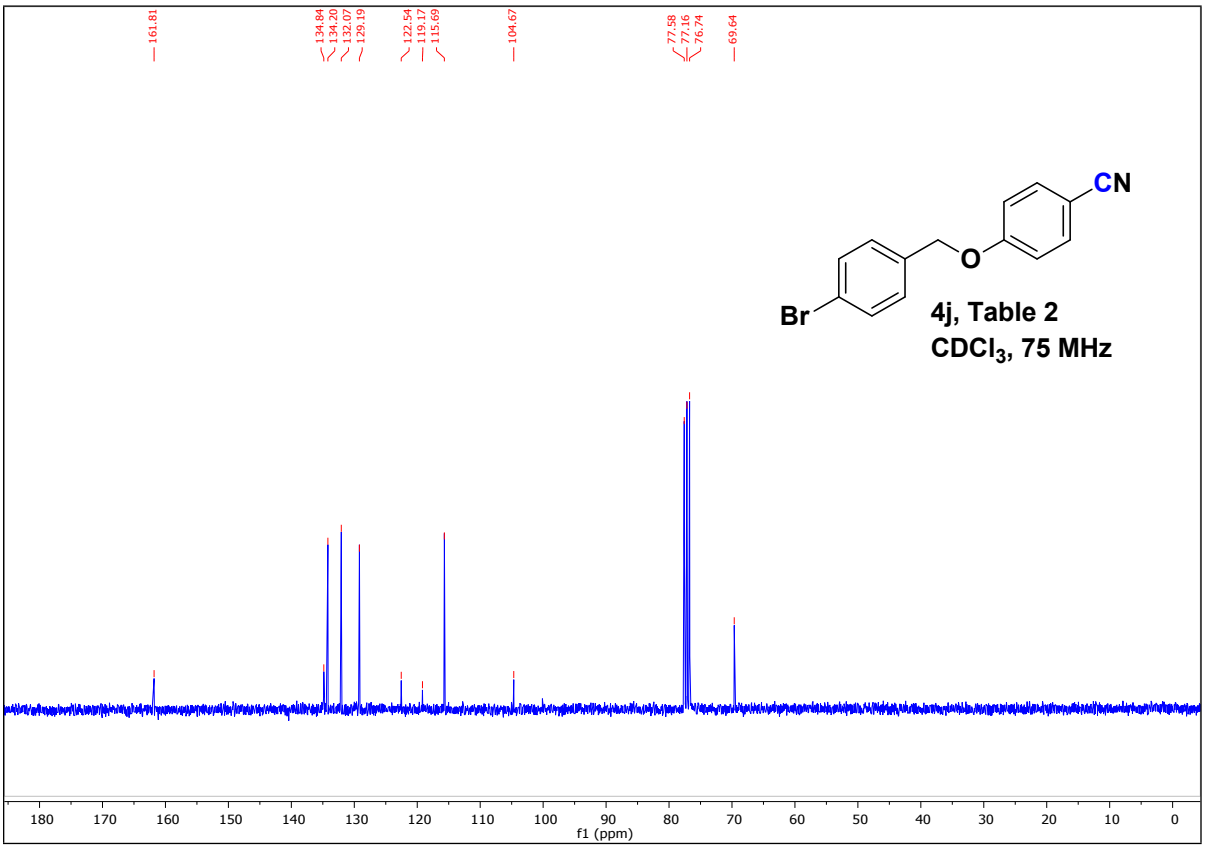

7.08
7.07
7.05
7.04
7.00
7.00
6.99
6.89
6.86
3.84
3.74
B (dd)
7.00
A (dd)
7.06
C (d)
6.88
E (s)
3.74
D (s)
3.84
MeO
CN
OMe
4h, Table 2
CDCl3, 300 MHz
1.00
0.95
1.02
3.13
3.19
f1 (ppm)

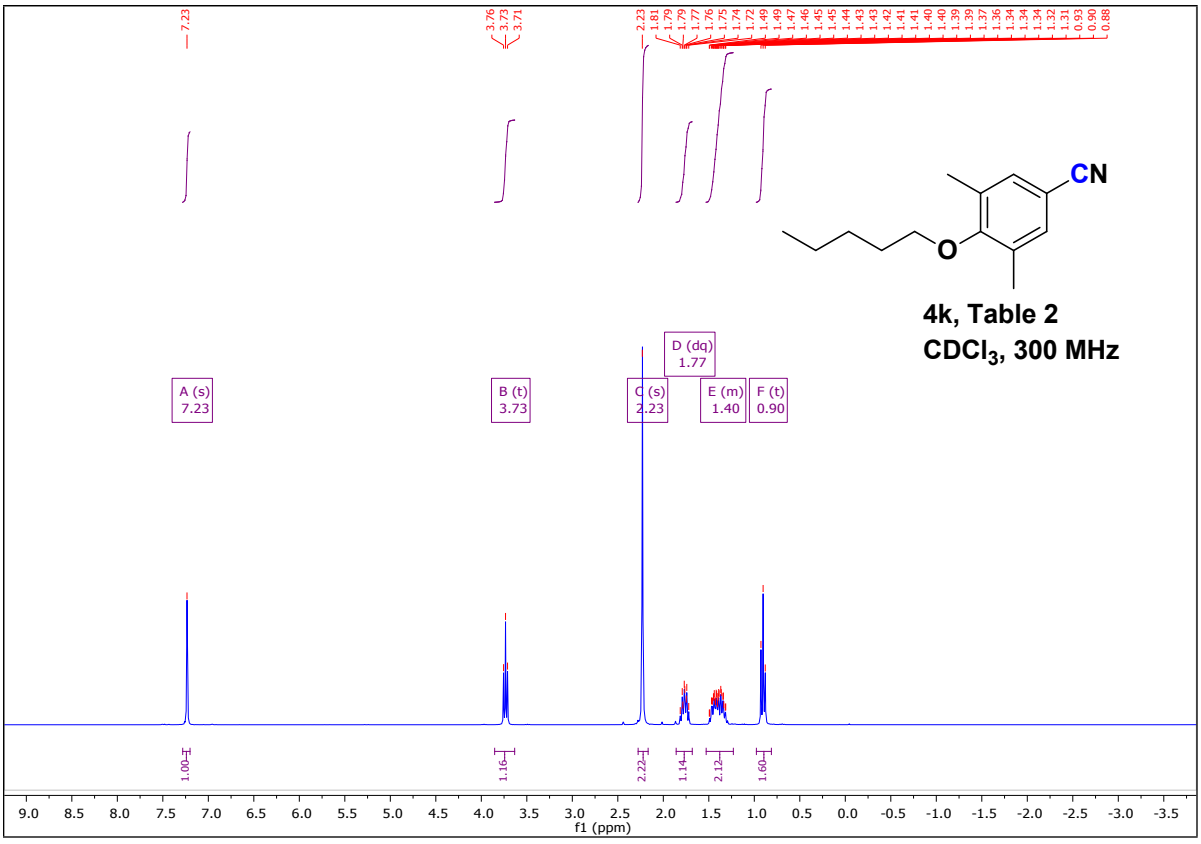

141.80
139.65
136.13
132.38
130.89
129.78
123.61
118.93
109.39
77.58
77.16
76.74
21.40
MeO
CN
OMe
4h, Table 2
CDCl3, 75 MHz
f1 (ppm)

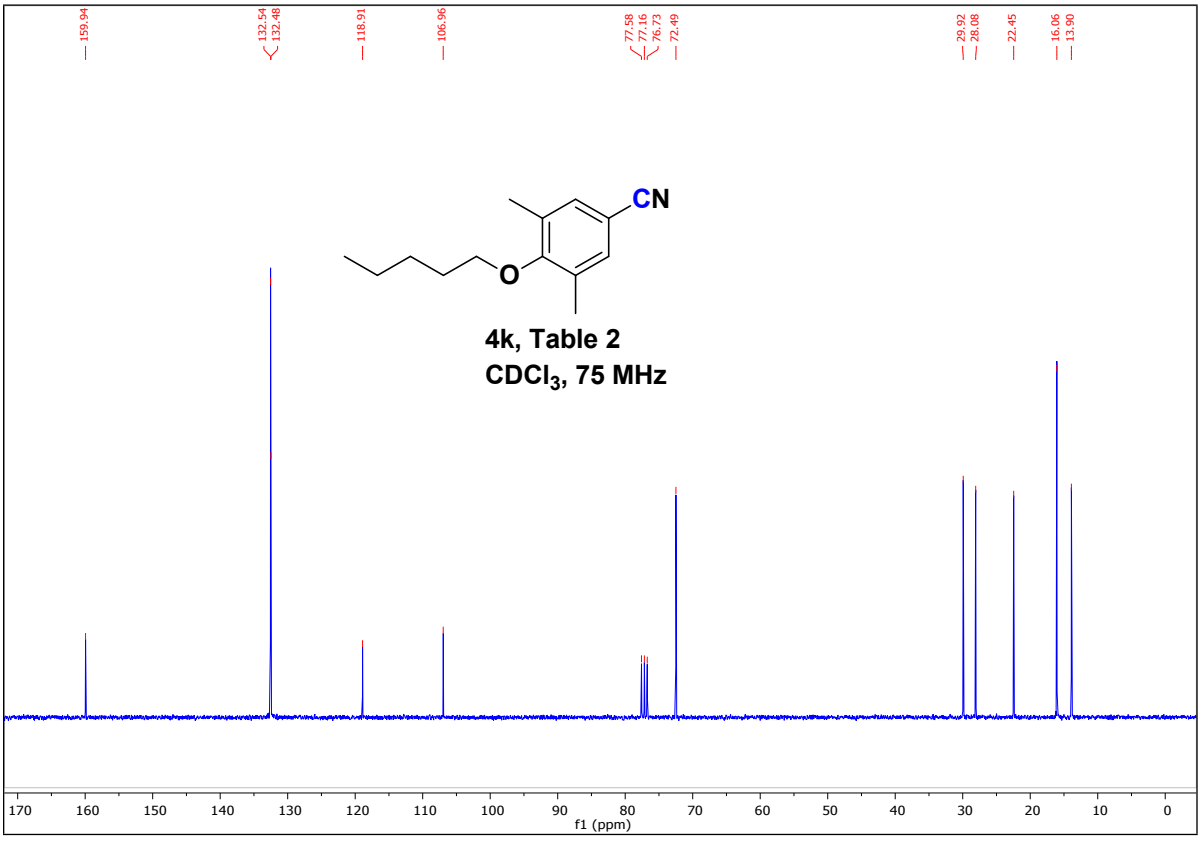

A (m) 7.49
B (m) 6.98
C (d) 6.83
D (s) 5.12
E (s) 3.87
F (s) 3.85
CN
O
OMe
OMe
4i, Table 2
CDCl3, 300 MHz
f1 (ppm)

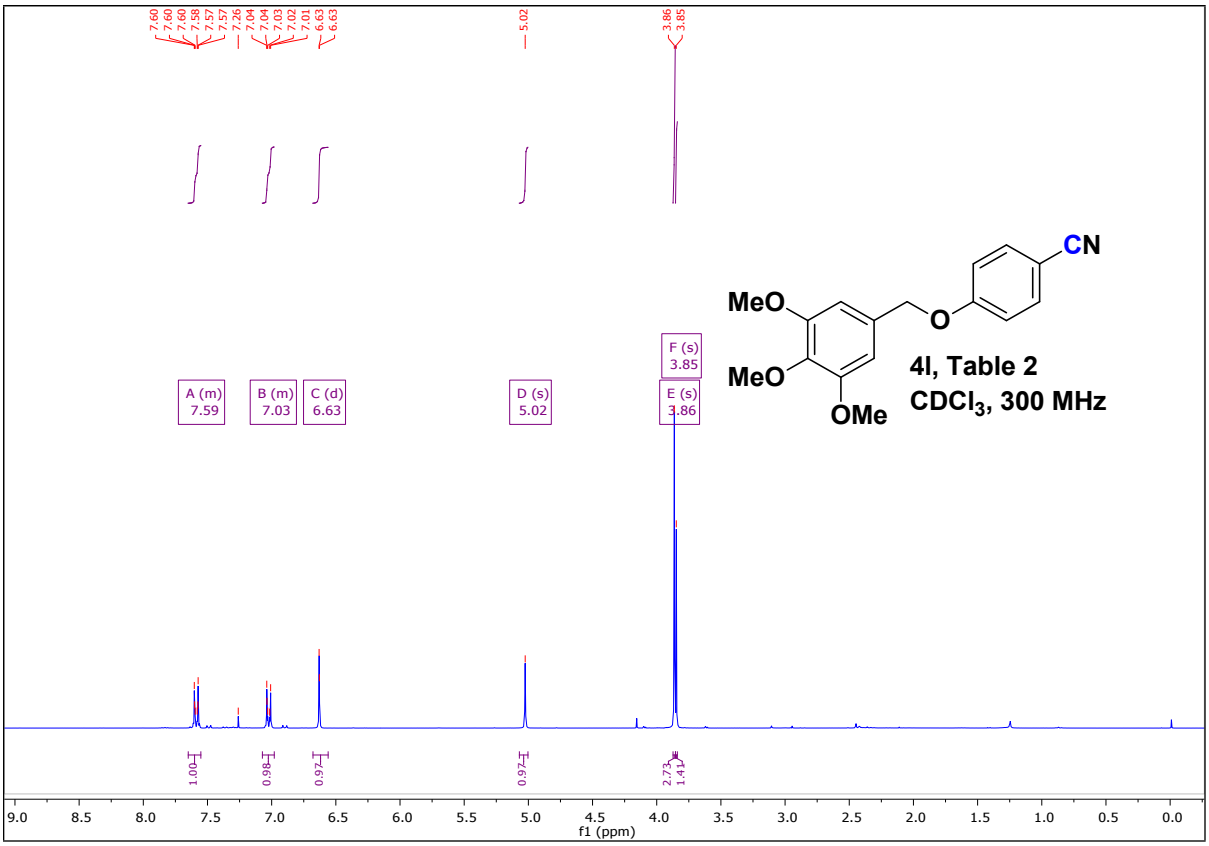

CN
O
OMe
OMe
4i, Table 2
CDCl3, 75 MHz
f1 (ppm)

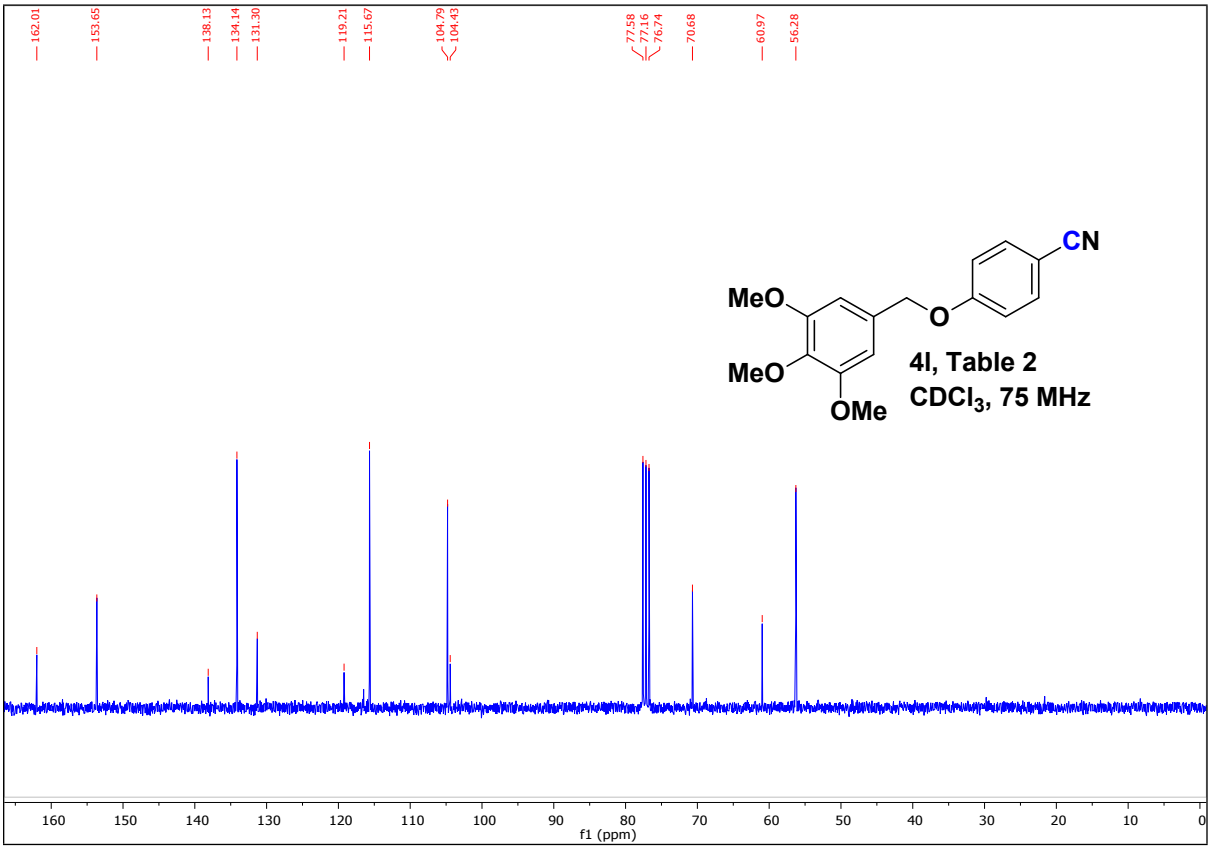

B (m)
7.21
A (m)
7.49
C (m)
6.93
D (s)
4.99
CN
O
Br
4j, Table 2
CDCl3, 300 MHz
f1 (ppm)

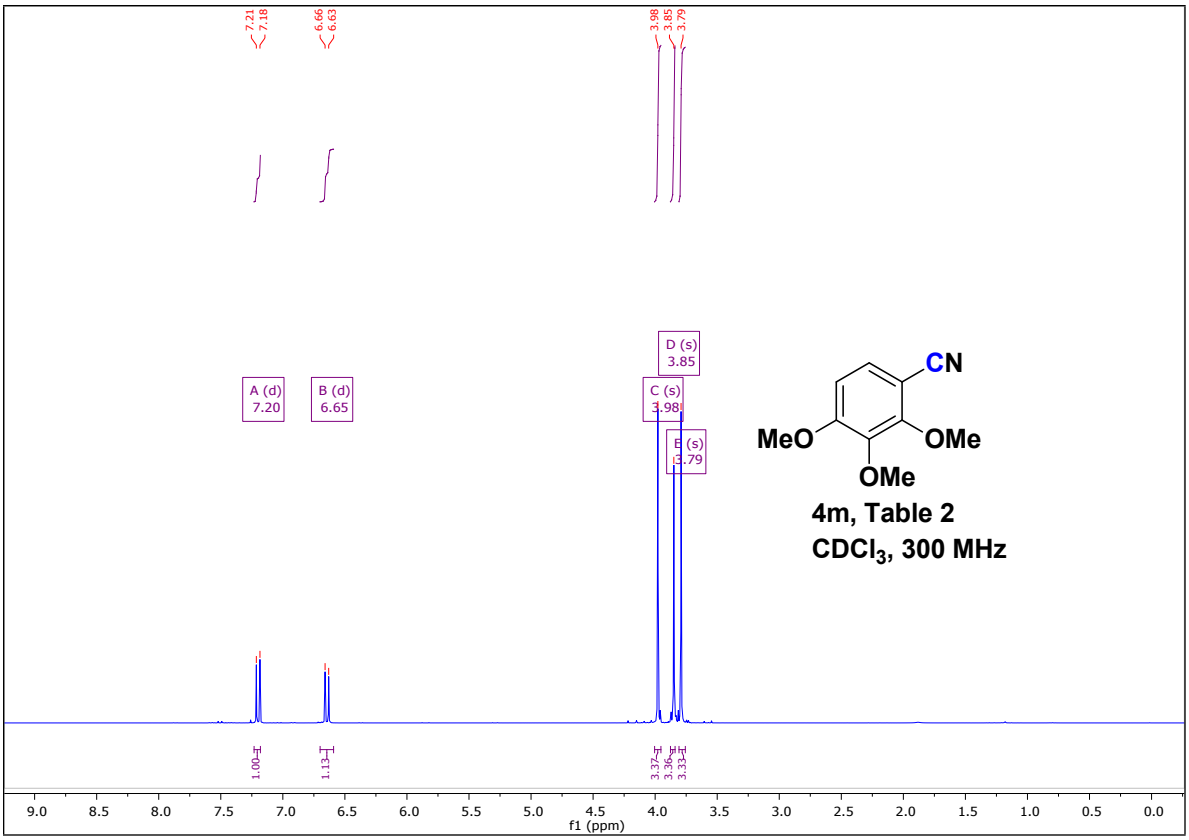

CN
O
Br
4j, Table 2
CDCl3, 75 MHz
f1 (ppm)

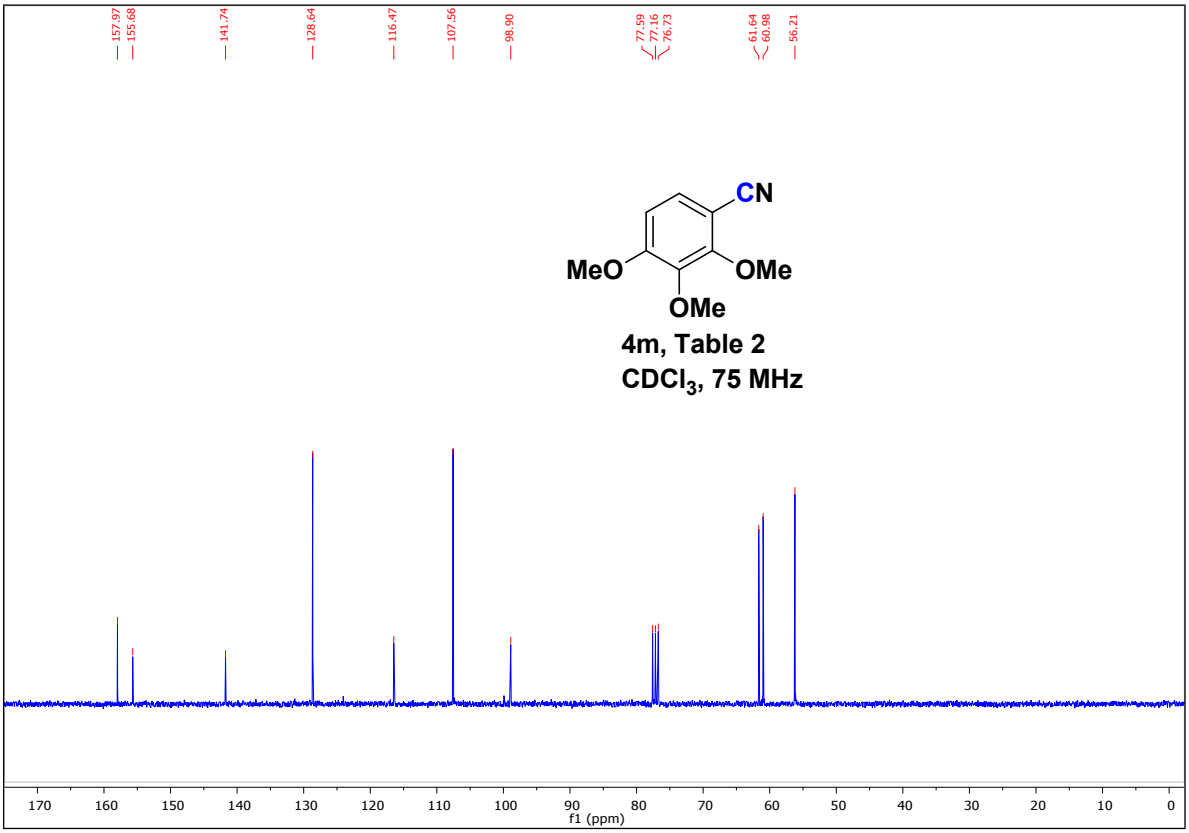

CN
O
4k, Table 2
CDCl3, 300 MHz
A (s) 7.23
B (t) 3.73
C (s) 2.23
D (dq) 1.77
E (m) 1.40
F (t) 0.90
f1 (ppm)

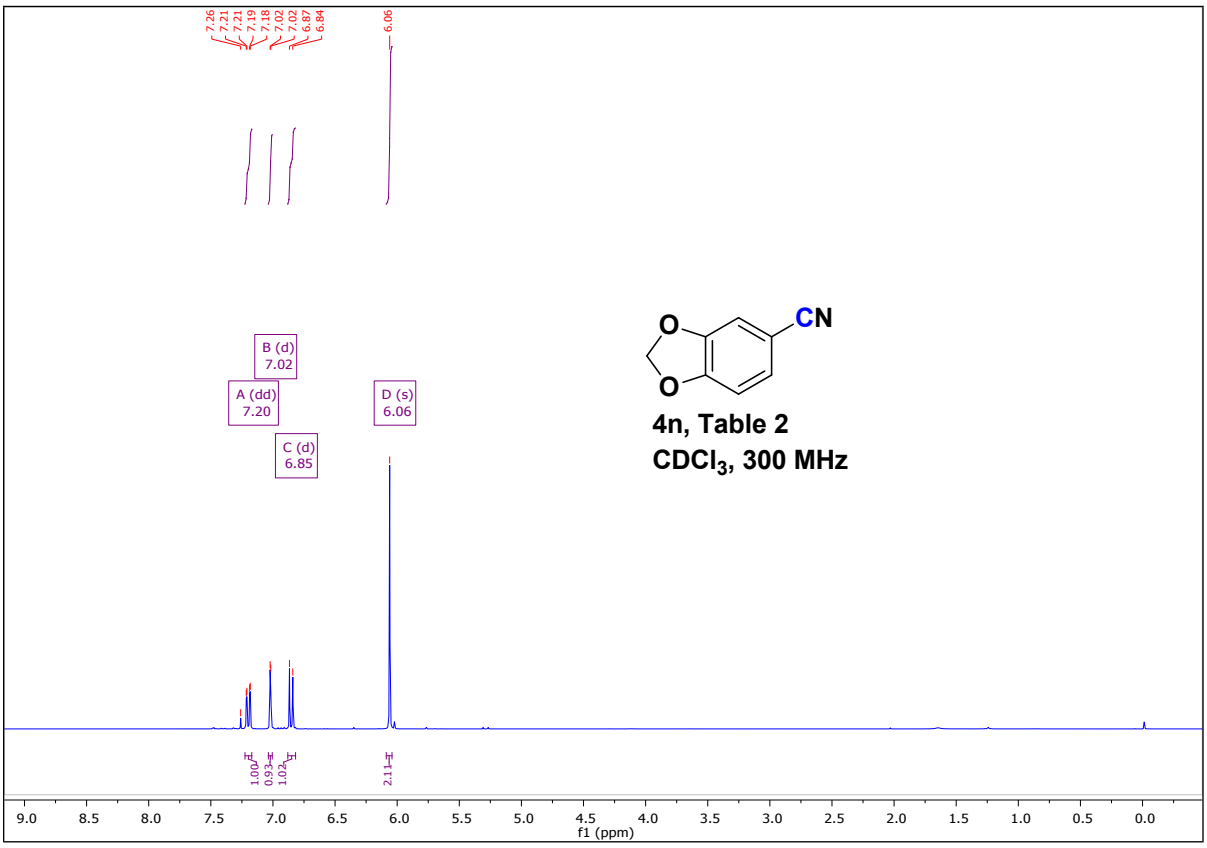

CN
O
4k, Table 2
CDCl3, 75 MHz
f1 (ppm)

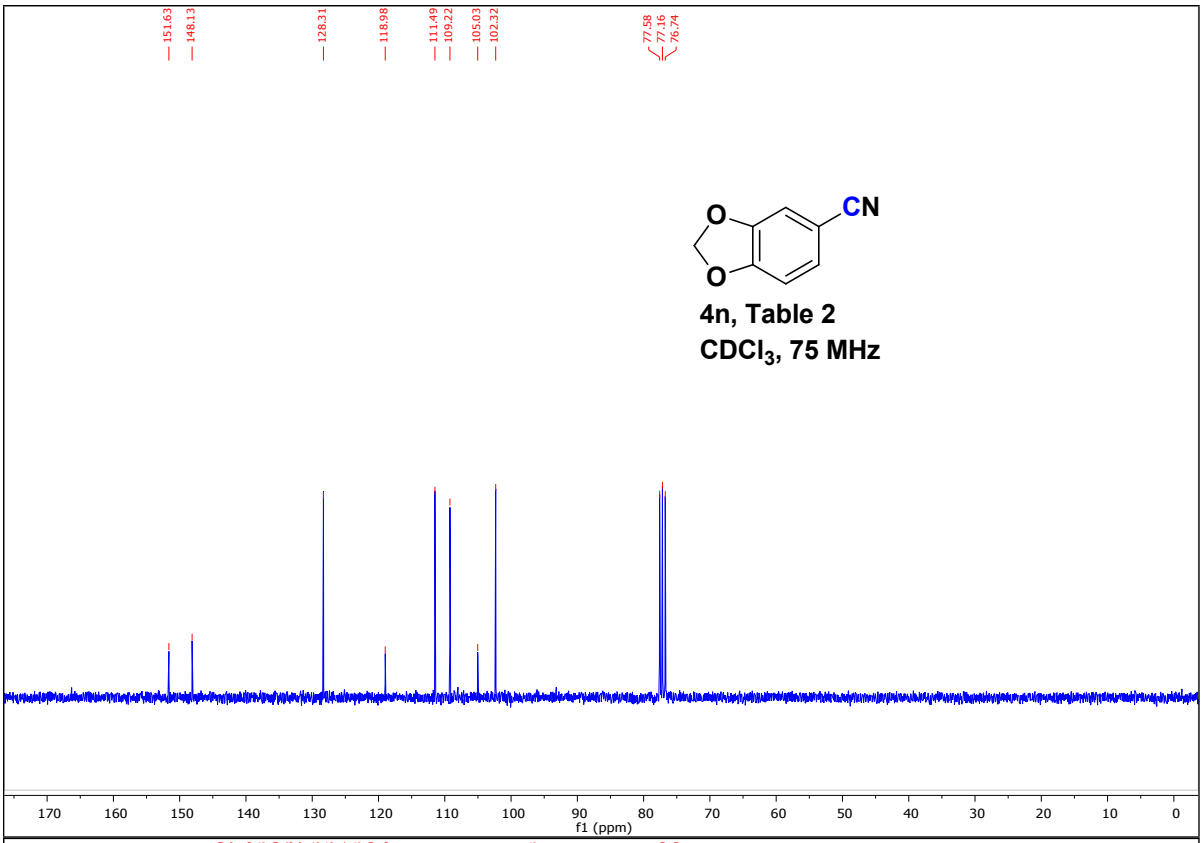

7.60
7.60
7.60
7.58
7.57
7.57
7.26
7.04
7.04
7.03
7.02
7.01
6.63
6.63
5.02
3.86
3.85
A (m)
7.59
B (m)
7.03
C (d)
6.63
D (s)
5.02
F (s)
3.85
E (s)
3.86
1.00
0.98
0.97
0.97
2.73
1.41
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
CN
MeO
MeO
OMe
O
4l, Table 2
CDCl3, 300 MHz

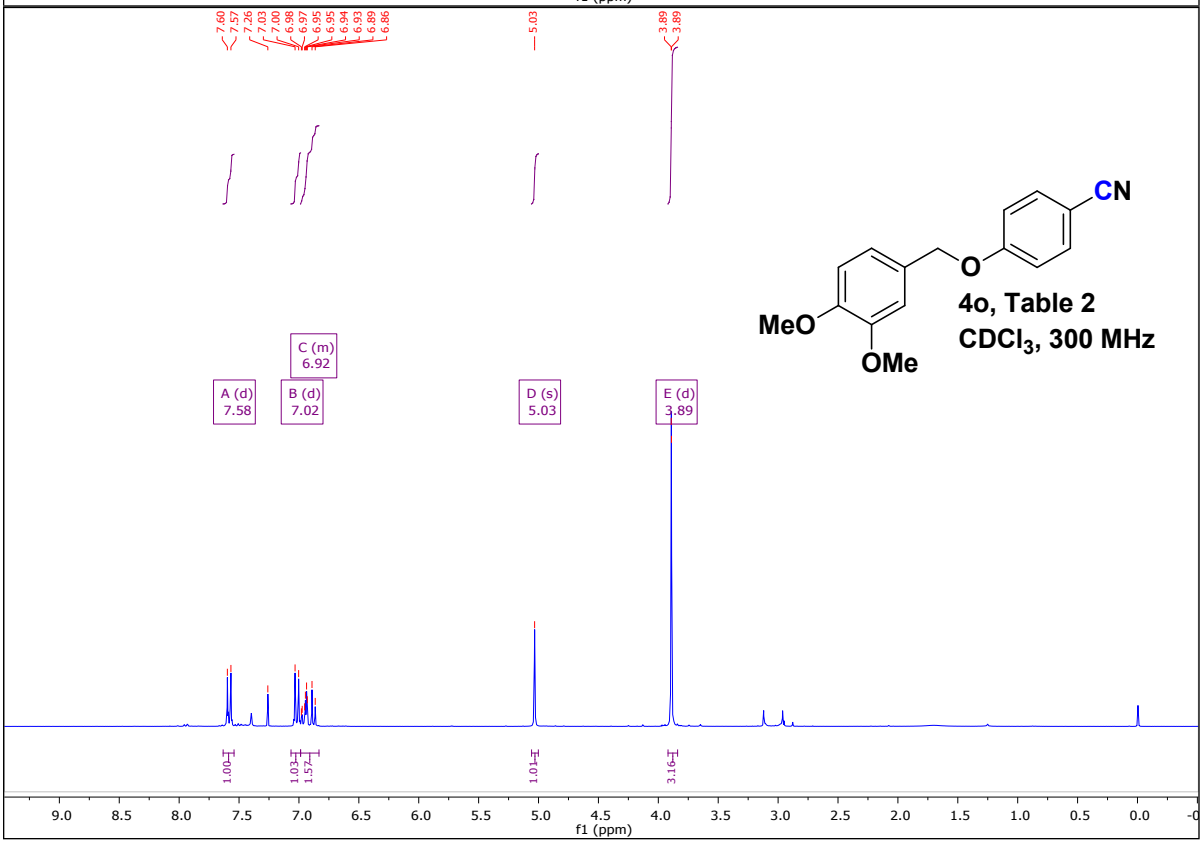

162.01
153.65
138.13
134.14
131.30
119.21
115.67
104.79
104.43
77.58
77.16
76.74
70.68
60.97
56.28
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
CN
MeO
MeO
OMe
O
4l, Table 2
CDCl3, 75 MHz

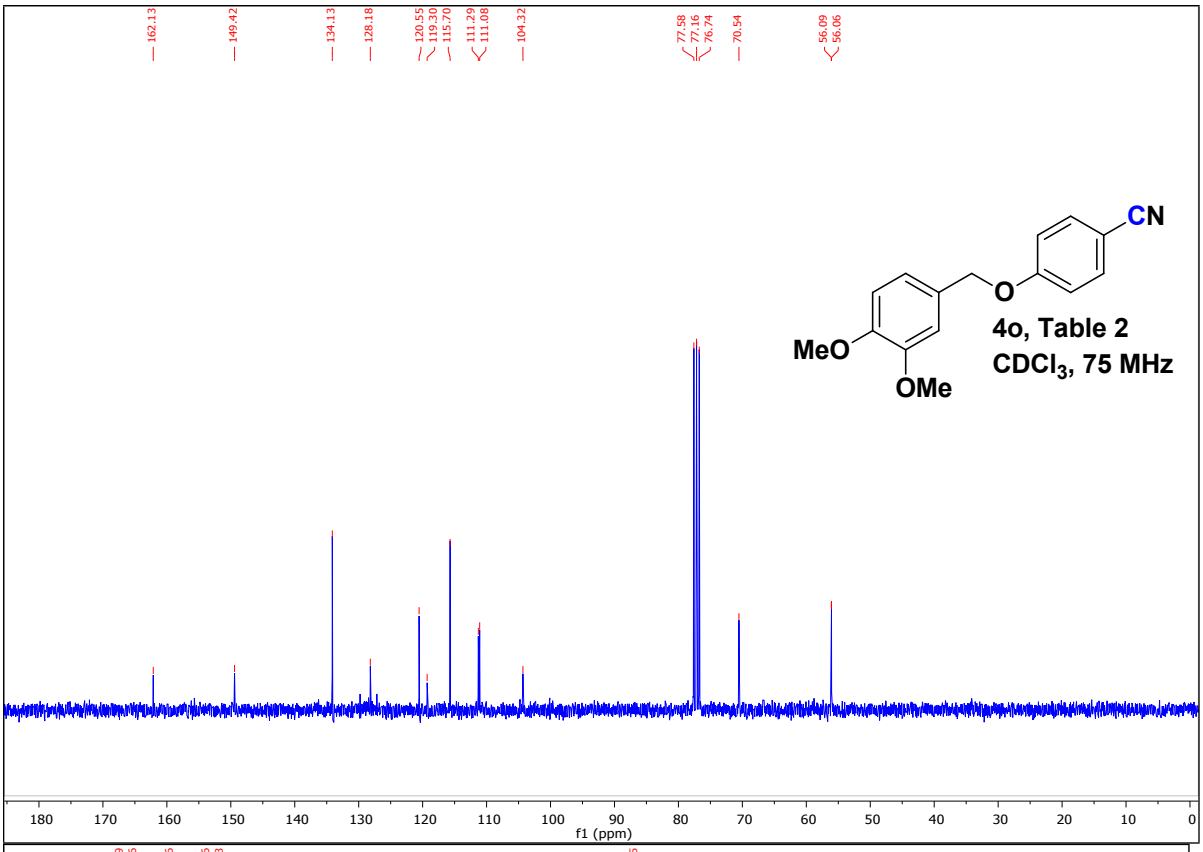

7.21
7.18
6.66
6.63
3.98
3.85
3.79
A (d)
7.20
B (d)
6.65
D (s)
3.85
C (s)
3.98
E (s)
3.79
CN
MeO
OMe
OMe
4m, Table 2
CDCl3, 300 MHz
1.00
1.13
3.37
3.36
3.33
f1 (ppm)

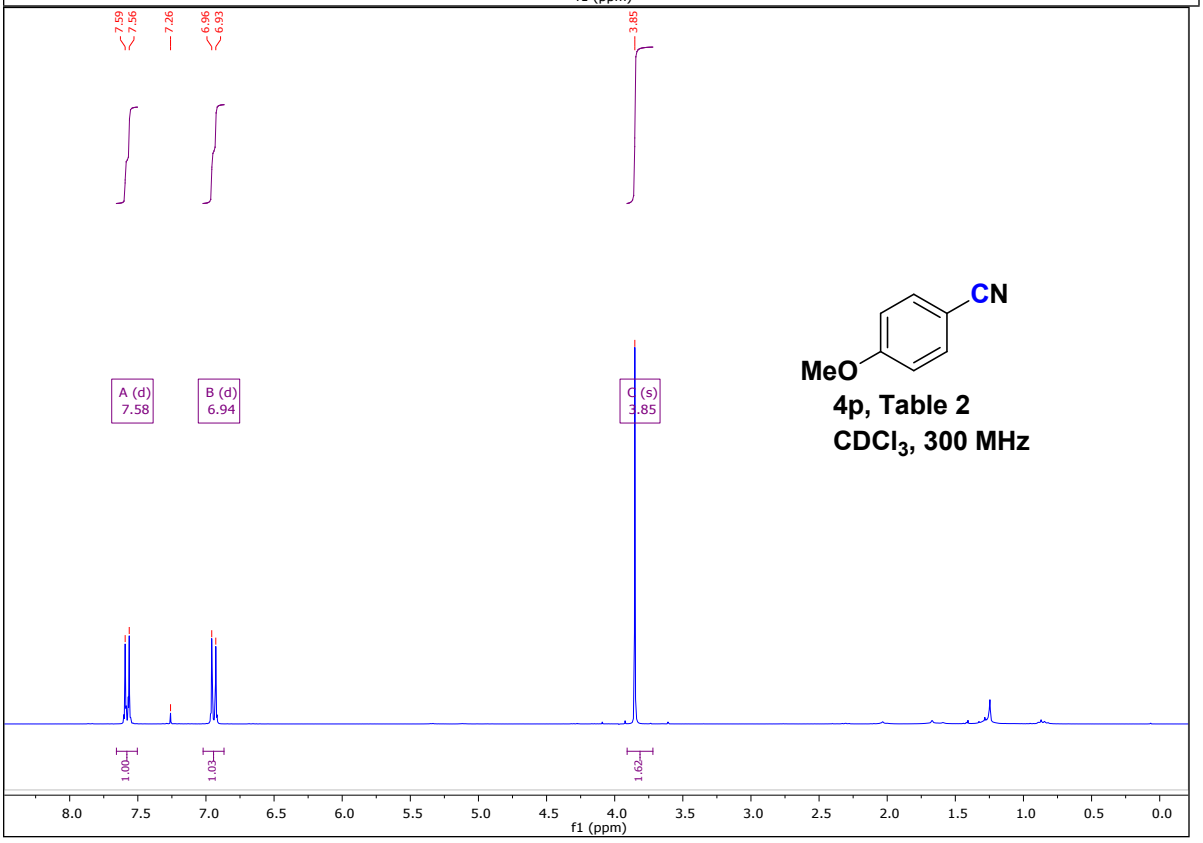

157.97
155.68
141.74
128.64
116.47
107.56
98.90
77.59
77.16
76.73
61.64
60.98
56.21
CN
MeO
OMe
OMe
4m, Table 2
CDCl3, 75 MHz
f1 (ppm)

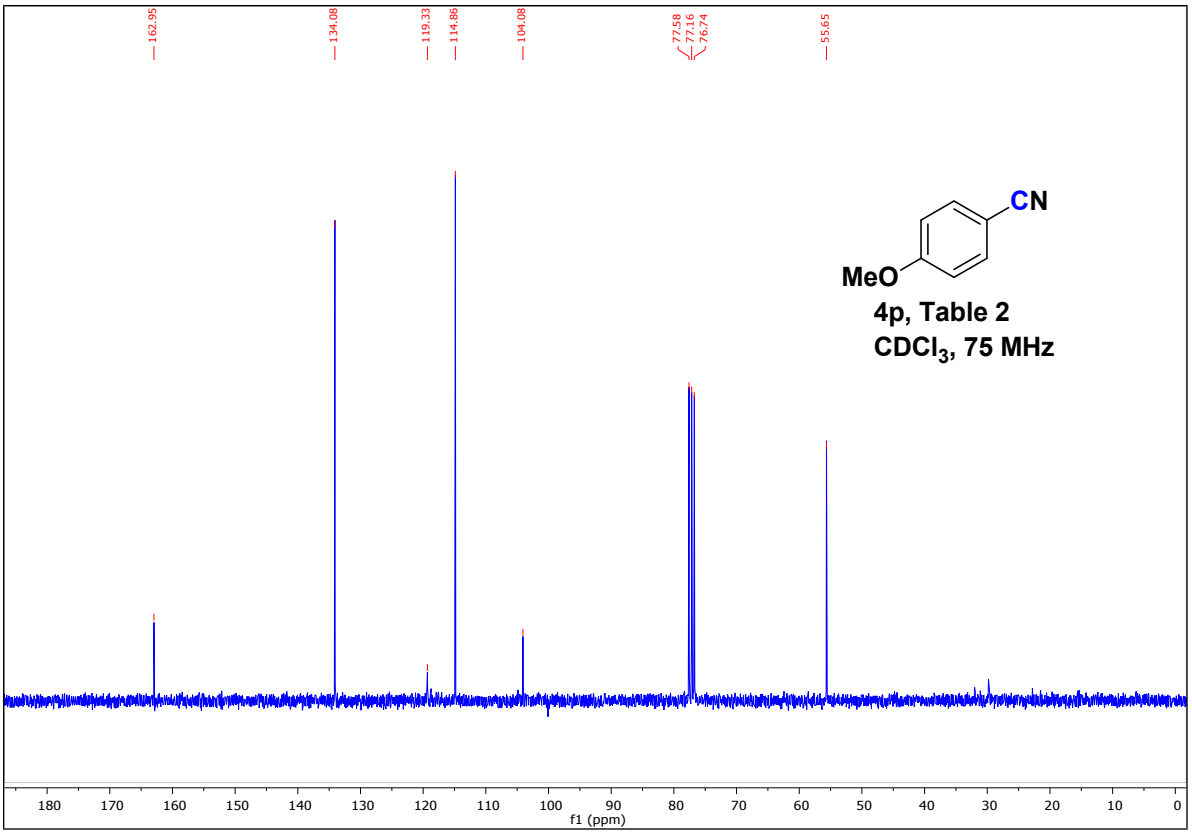

7.26
7.21
7.21
7.19
7.18
7.02
7.02
6.87
6.84
6.06
B (d)
7.02
A (dd)
7.20
C (d)
6.85
D (s)
6.06
1.00
0.93
1.02
2.11
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
O
O
CN
4n, Table 2
CDCl3, 300 MHz

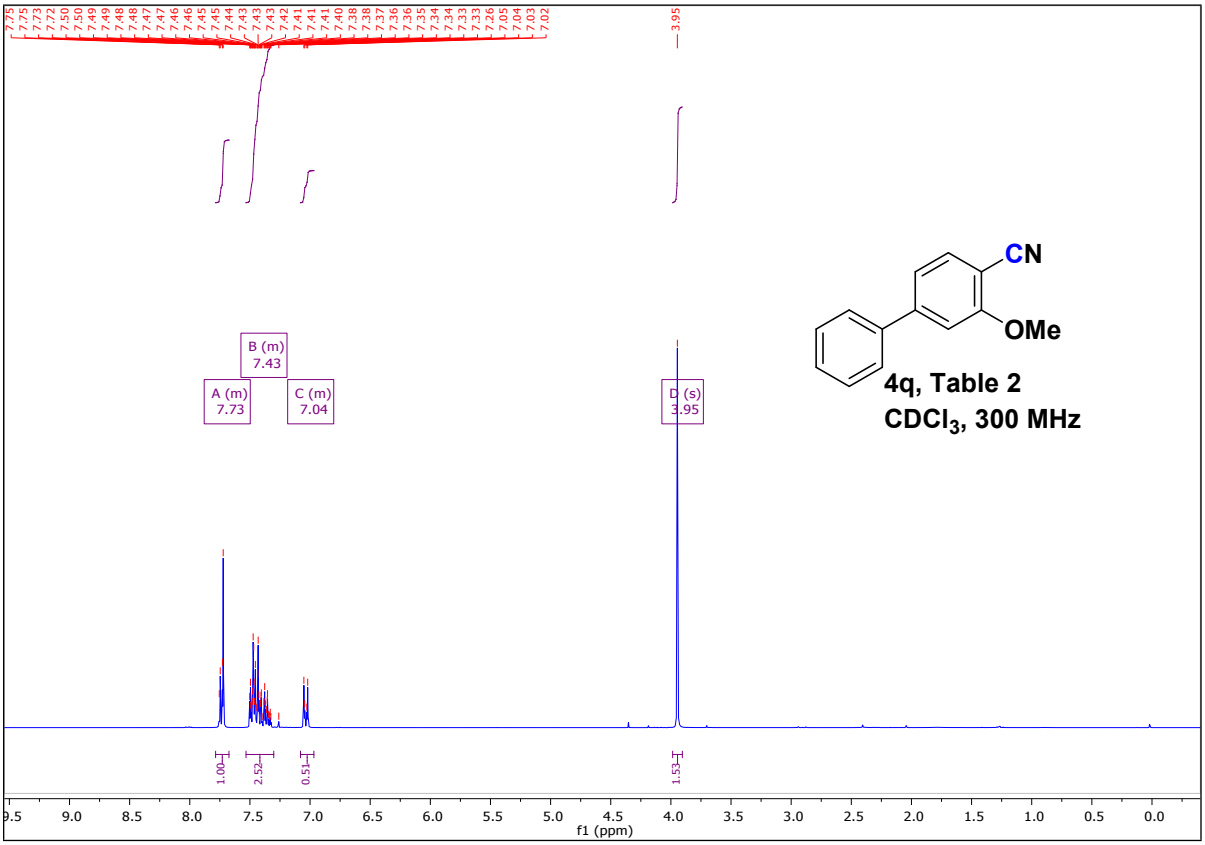

151.63
148.13
128.31
118.98
111.49
109.22
105.03
102.32
77.58
77.16
76.74
O
O
CN
4n, Table 2
CDCl3, 75 MHz
f1 (ppm)

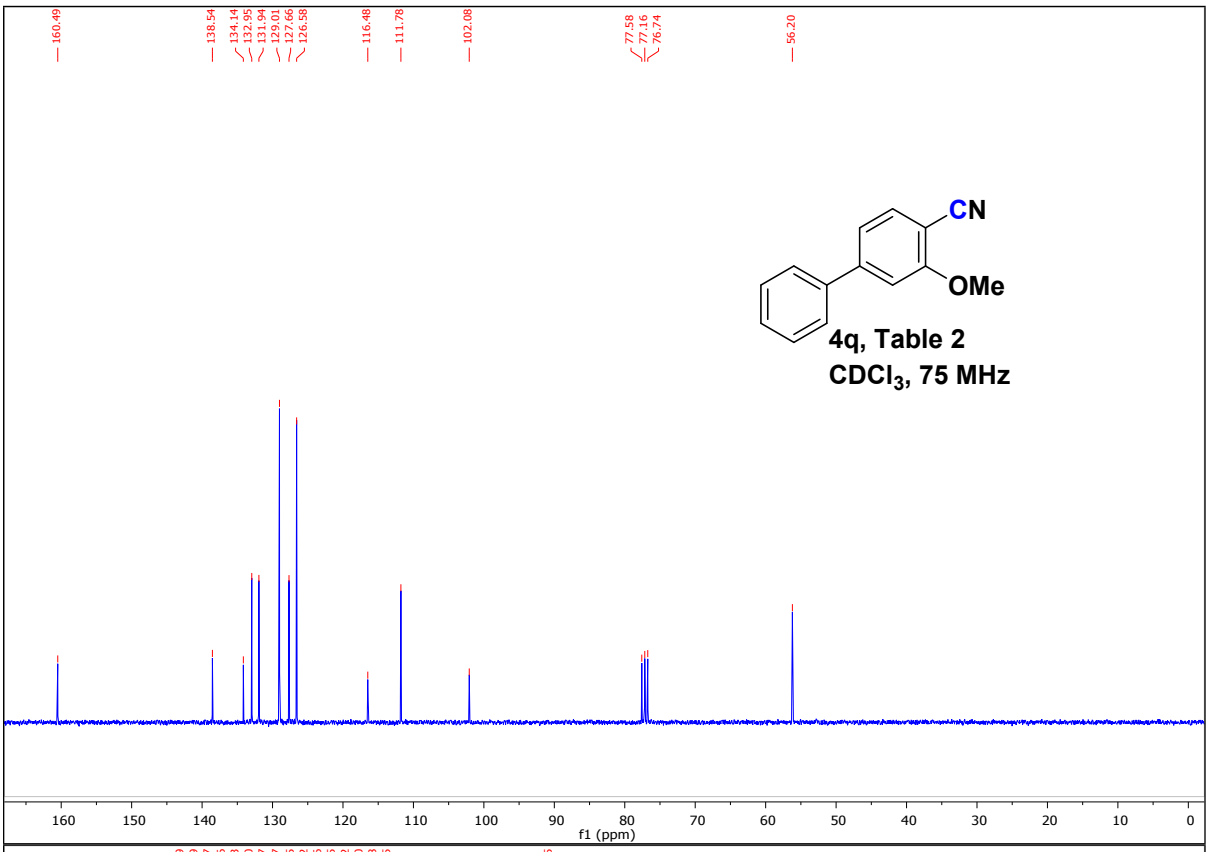

7.60
7.57
7.26
7.03
7.00
6.98
6.97
6.95
6.95
6.94
6.93
6.89
6.86
5.03
3.89
3.89
CN
O
MeO
OMe
4o, Table 2
CDCl3, 300 MHz
C (m)
6.92
A (d)
7.58
B (d)
7.02
D (s)
5.03
E (d)
3.89
1.00
1.03
1.57
1.01
3.16
f1 (ppm)

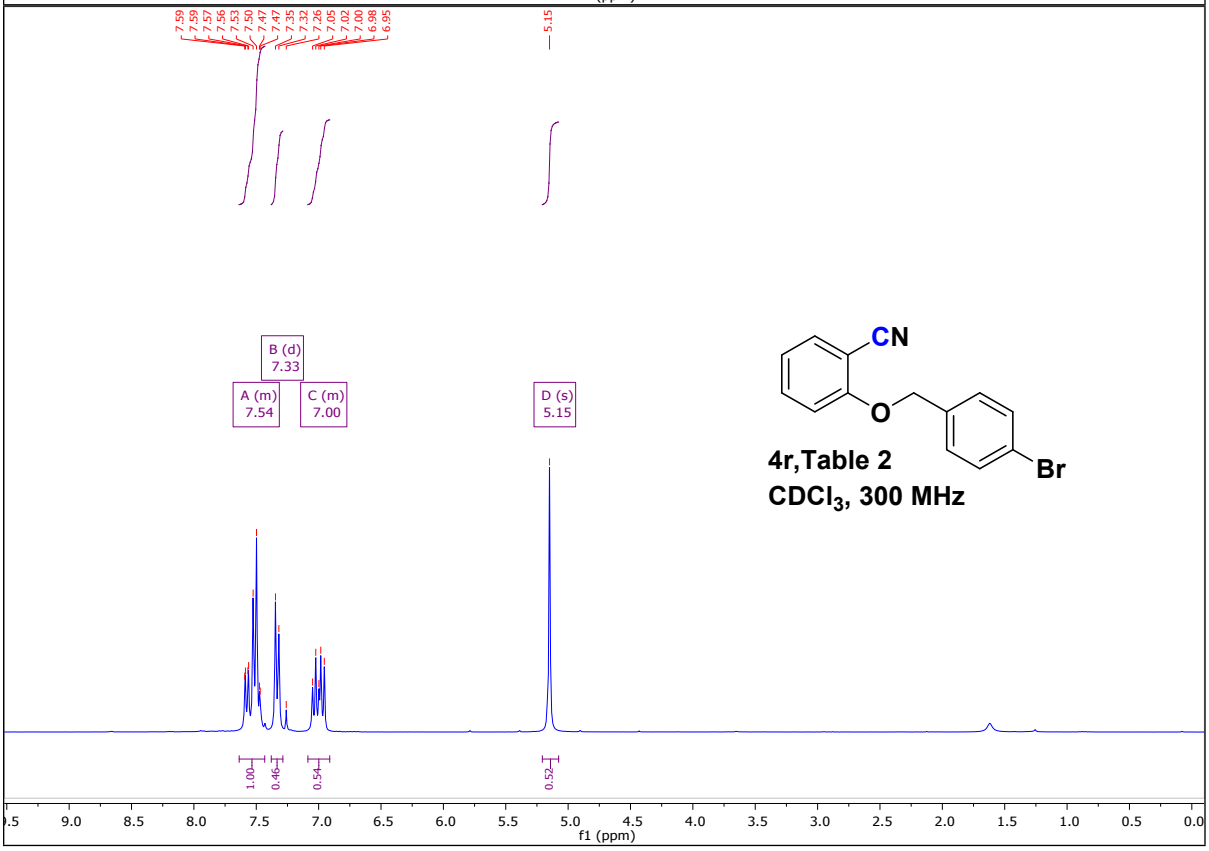

162.13
149.42
134.13
128.18
120.55
119.30
115.70
111.29
111.08
104.32
77.58
77.16
76.74
70.54
56.09
56.06
CN
O
MeO
OMe
4o, Table 2
CDCl3, 75 MHz
f1 (ppm)

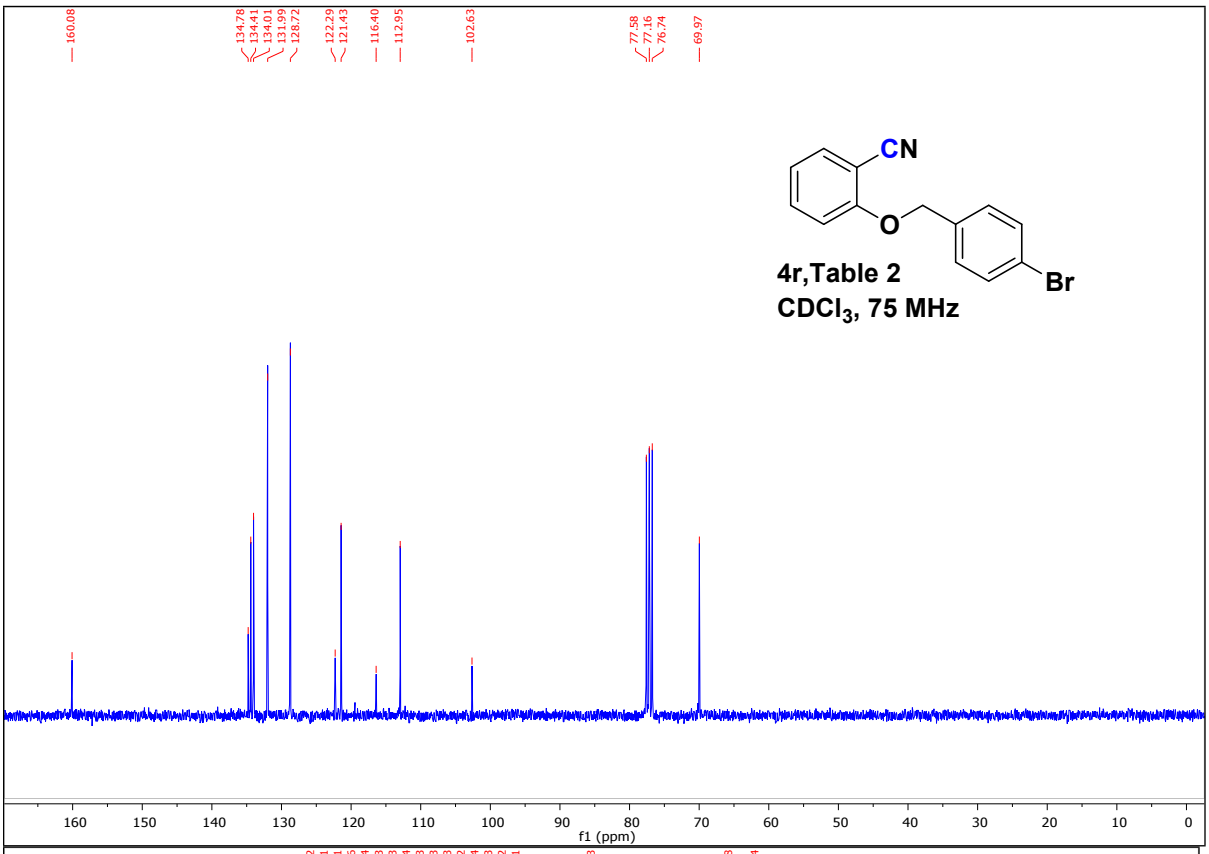

7.59
7.56
7.26
6.96
6.93
3.85
A (d)
7.58
B (d)
6.94
C (s)
3.85
1.00
1.03
1.62
CN
MeO
4p, Table 2
CDCl3, 300 MHz
f1 (ppm)

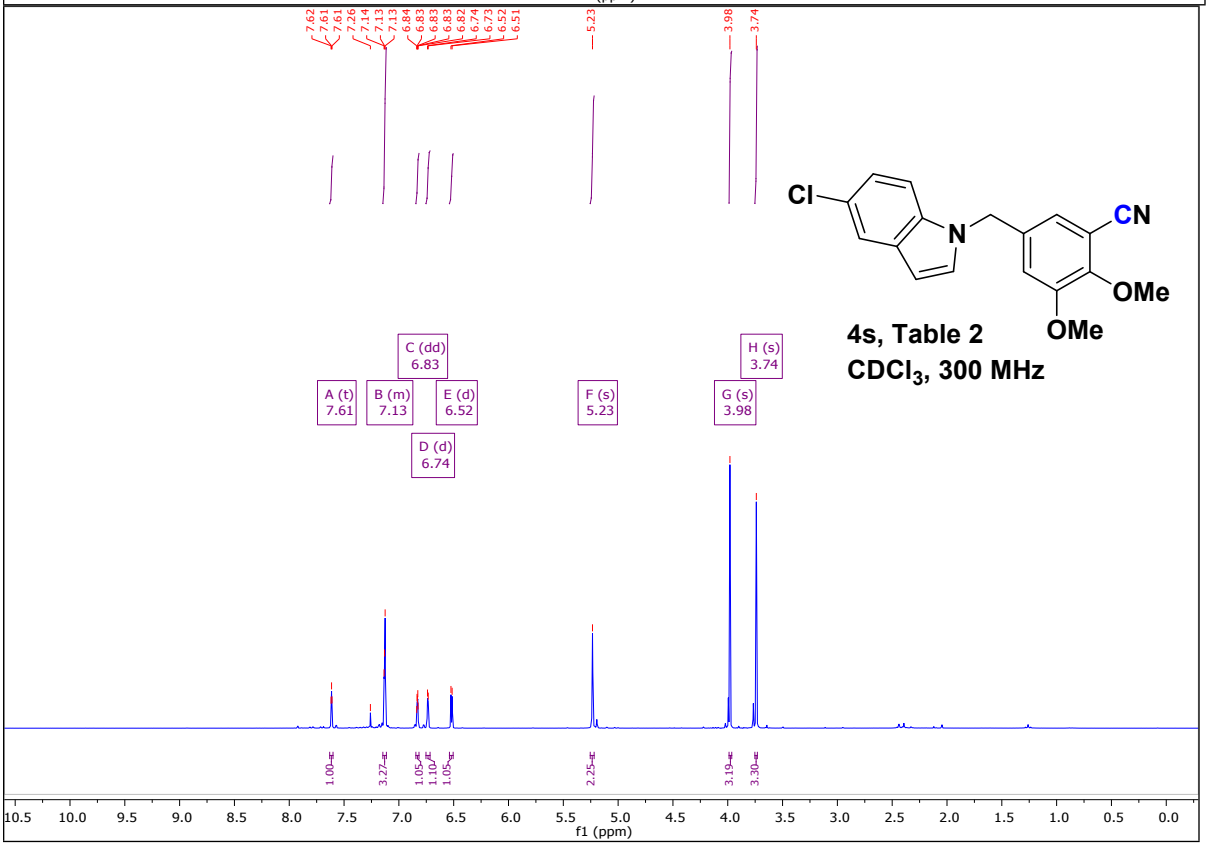

162.95
134.08
119.33
114.86
104.08
77.58
77.16
76.74
55.65
CN
MeO
4p, Table 2
CDCl3, 75 MHz
f1 (ppm)

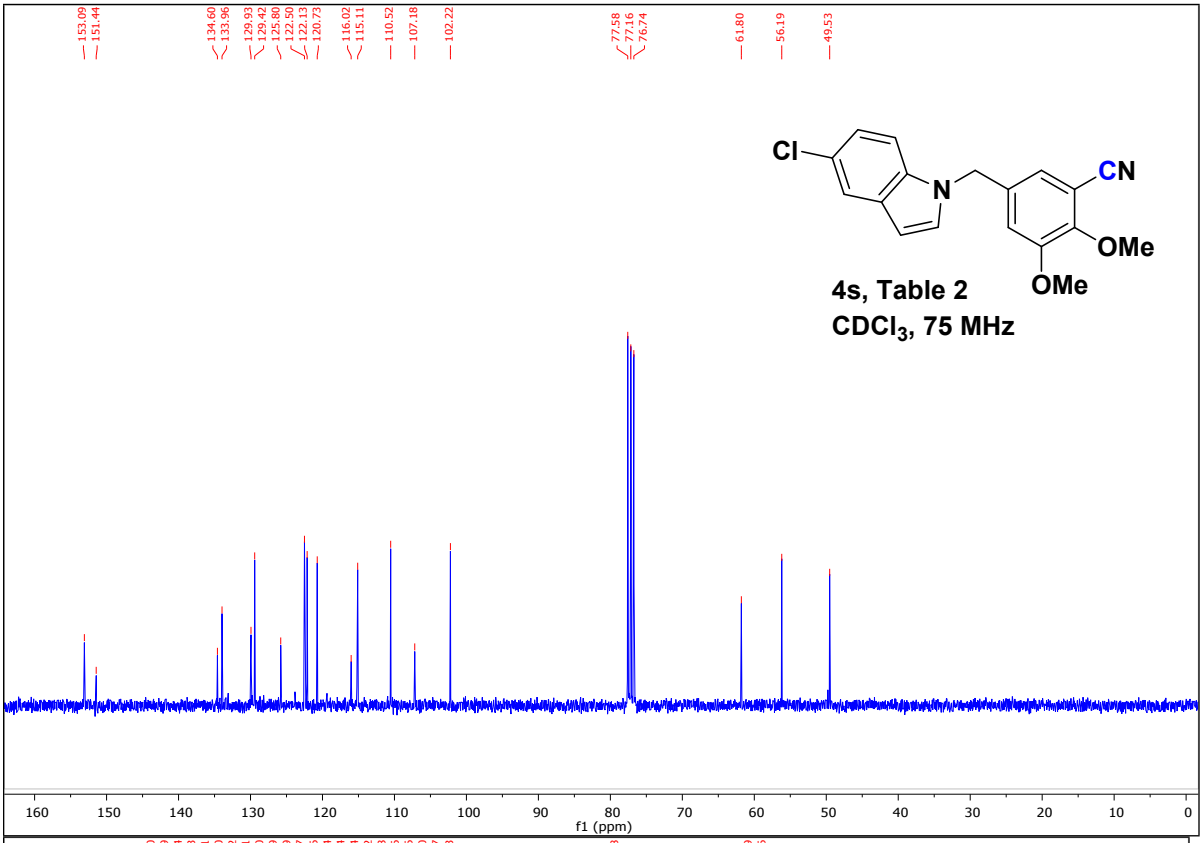

3.95
CN
OMe
4q, Table 2
CDCl3, 300 MHz
B (m)
7.43
A (m)
7.73
C (m)
7.04
D (s)
3.95
1.00
2.52
0.51
1.53
f1 (ppm)

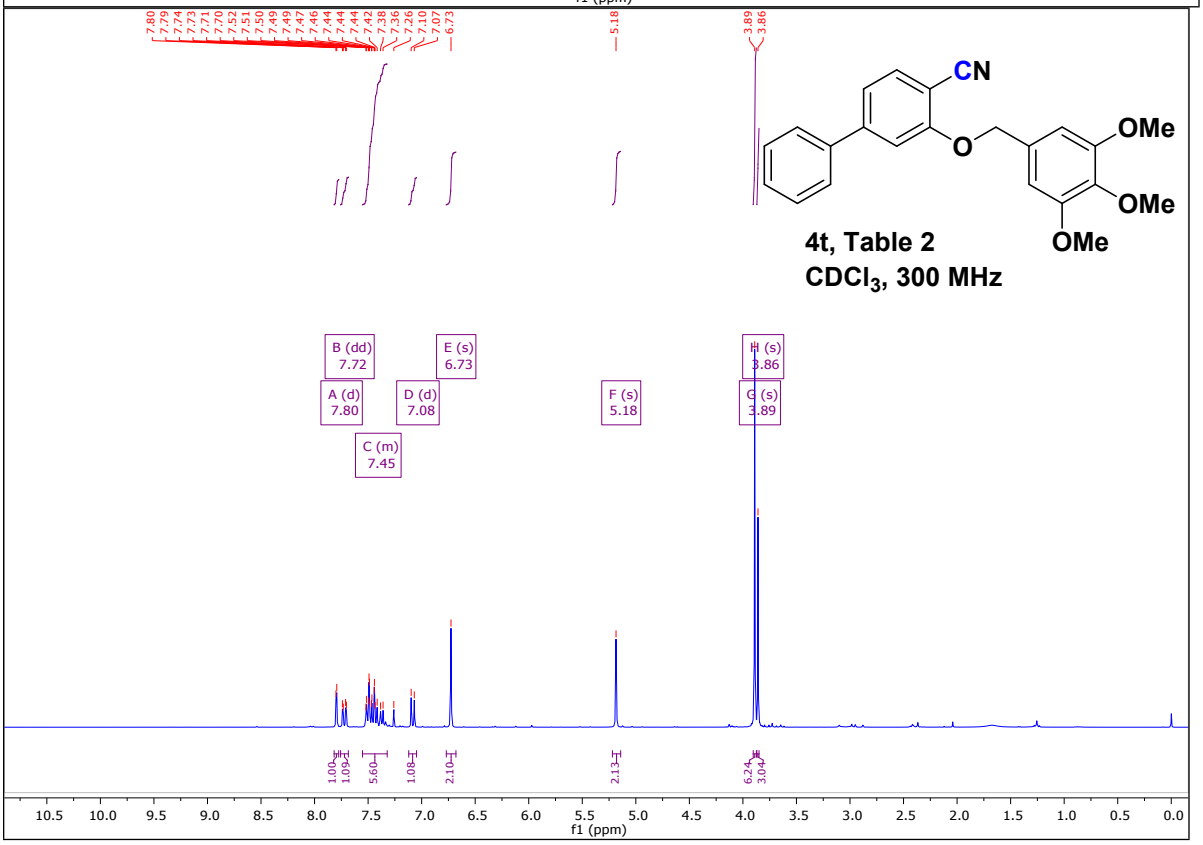

160.49
138.54
134.14
132.95
131.94
129.01
127.66
126.58
116.48
111.78
102.08
77.58
77.16
76.74
56.20
CN
OMe
4q, Table 2
CDCl3, 75 MHz
f1 (ppm)

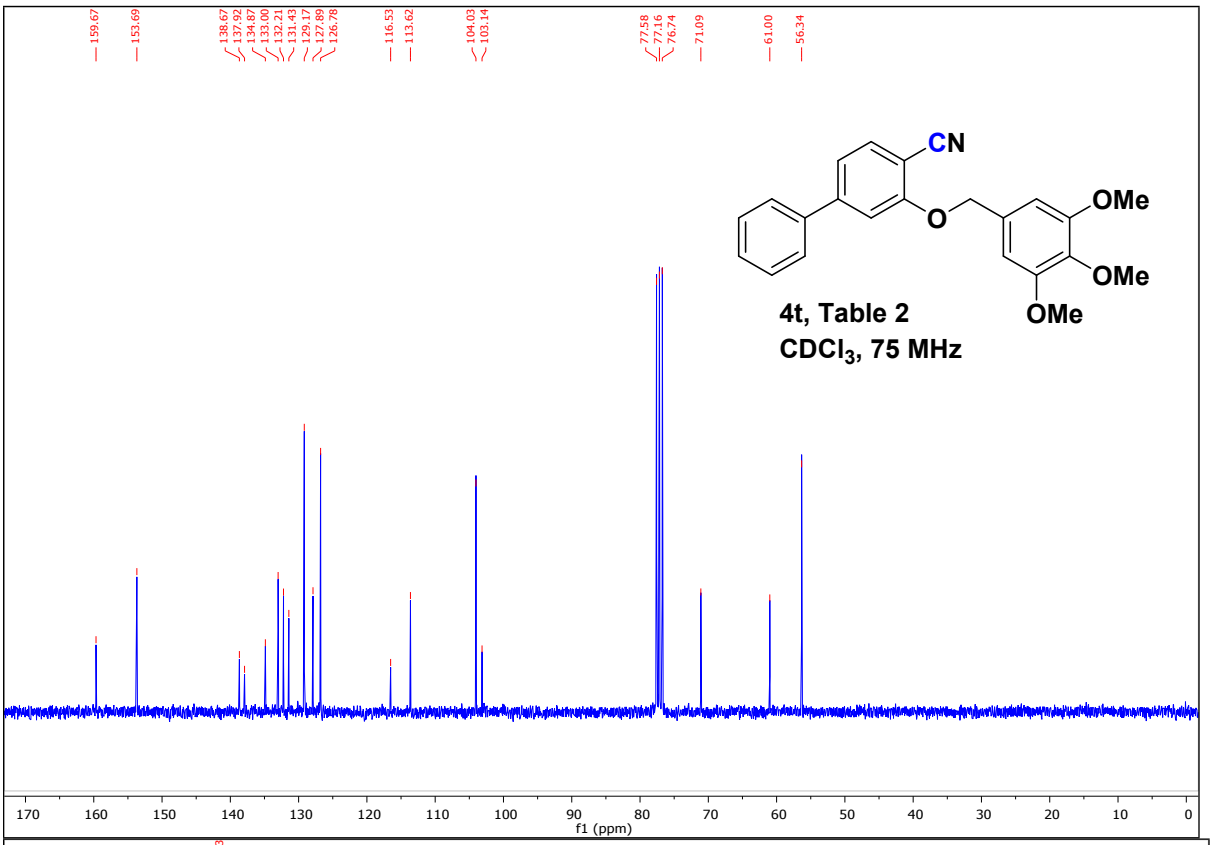

7.59
7.59
7.57
7.56
7.53
7.50
7.47
7.47
7.35
7.32
7.26
7.05
7.02
7.00
6.98
6.95
5.15
B (d)
7.33
A (m)
7.54
C (m)
7.00
D (s)
5.15
1.00
0.46
0.54
0.52
CN
O
Br
4r,Table 2
CDCl3, 300 MHz
f1 (ppm)

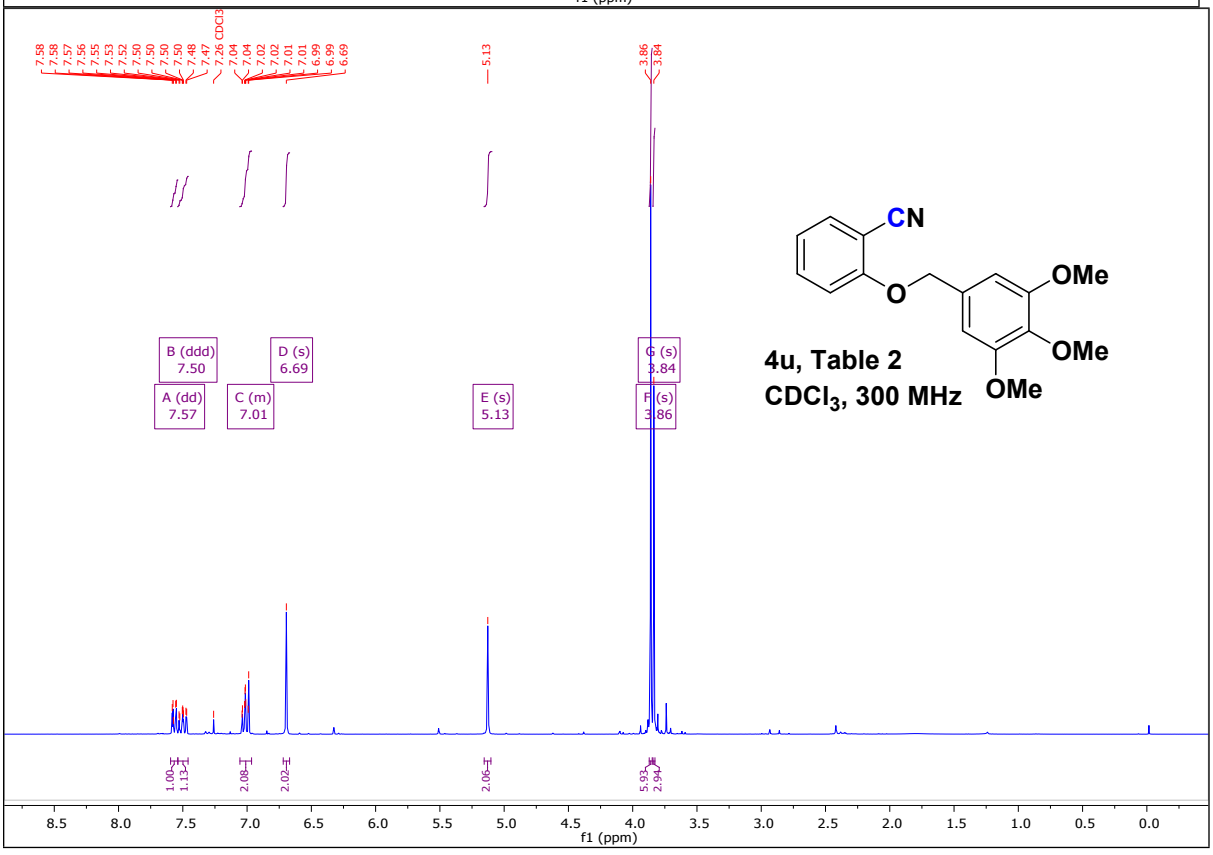

160.08
134.78
134.41
134.01
131.99
128.72
122.29
121.43
116.40
112.95
102.63
77.58
77.16
76.74
69.97
CN
O
Br
4r,Table 2
CDCl3, 75 MHz
f1 (ppm)

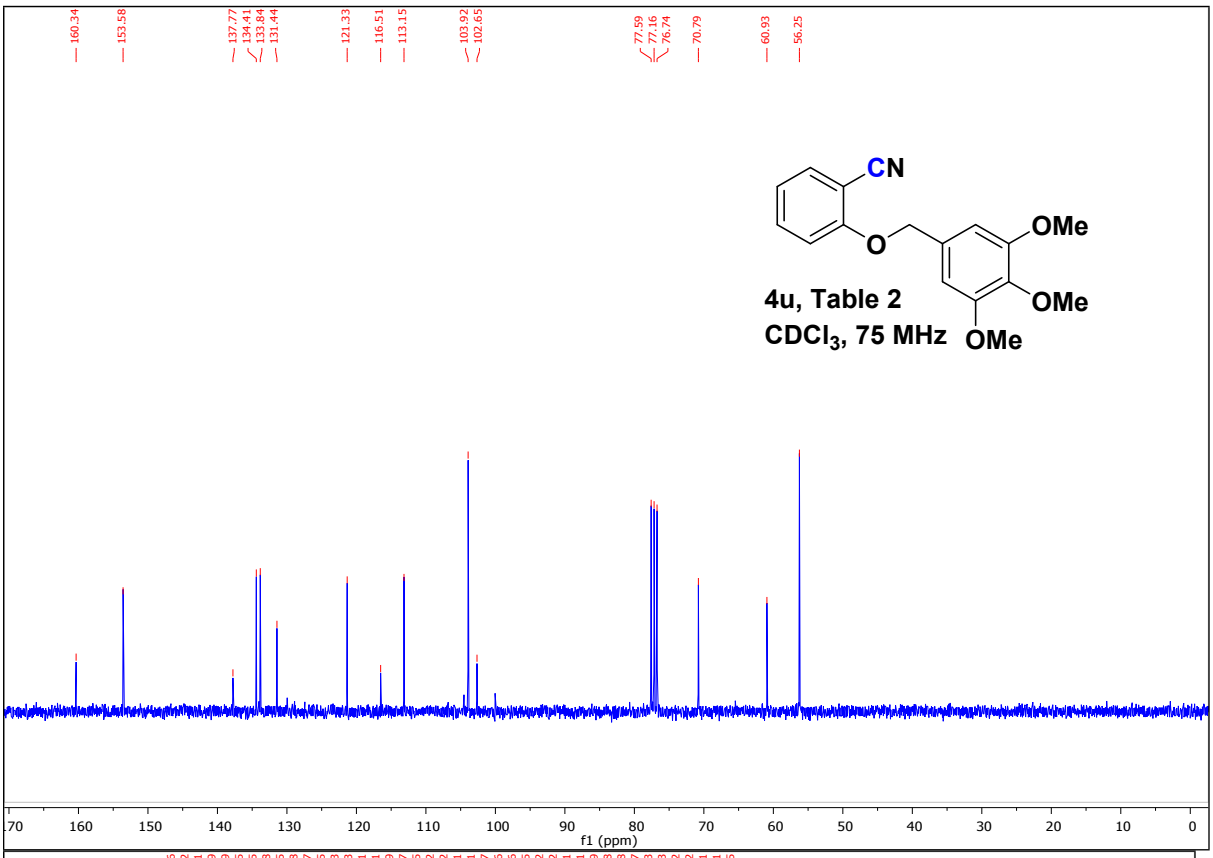

7.62
7.61
7.61
7.26
7.14
7.13
6.84
6.83
6.83
6.83
6.82
6.74
6.73
6.52
6.51
5.23
3.98
3.74
Cl
N
CN
OMe
OMe
4s, Table 2
CDCl3, 300 MHz
C (dd) 6.83
A (t) 7.61
B (m) 7.13
E (d) 6.52
D (d) 6.74
F (s) 5.23
G (s) 3.98
H (s) 3.74
1.00
3.27
1.05
1.10
1.05
2.25
3.19
3.30
f1 (ppm)

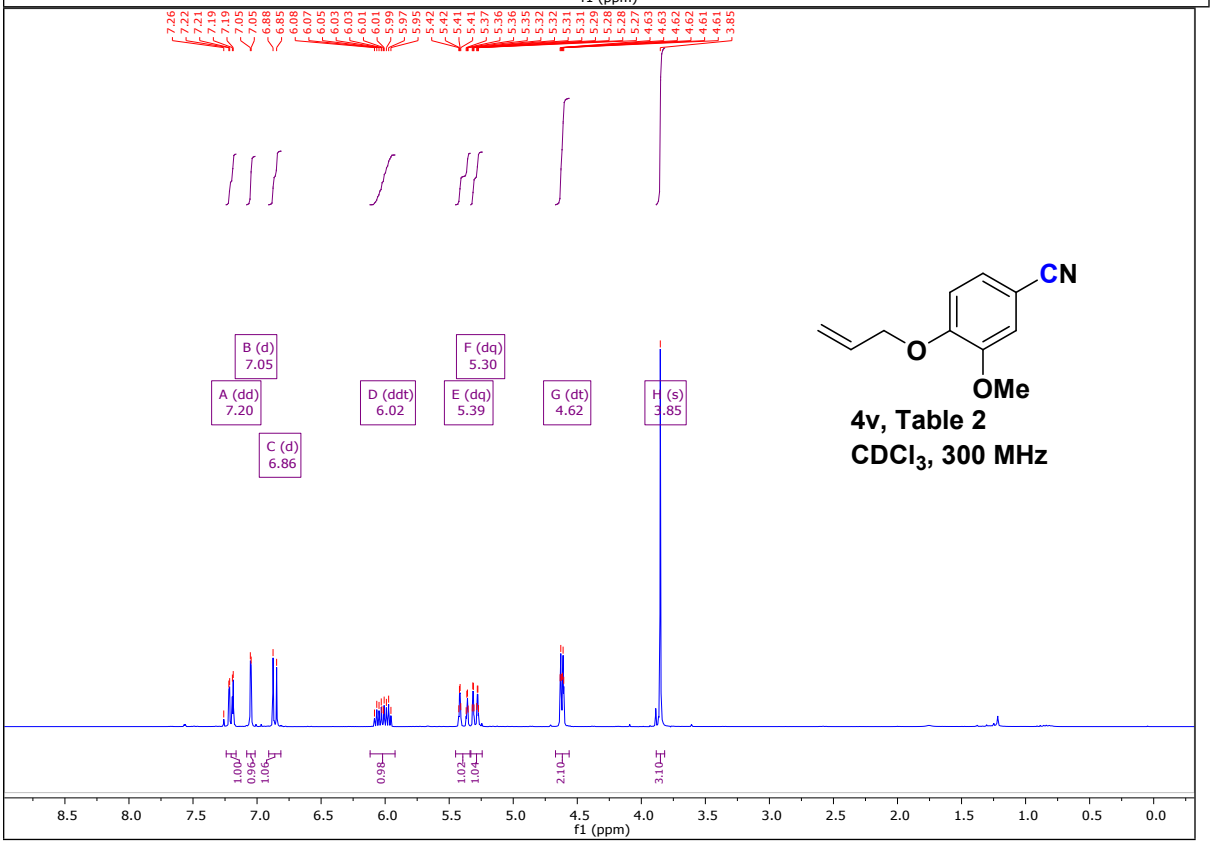

153.09
151.44
134.60
133.96
129.93
129.42
125.80
122.50
122.13
120.73
116.02
115.11
110.52
107.18
102.22
77.58
77.16
76.74
61.80
56.19
49.53
Cl
N
CN
OMe
OMe
4s, Table 2
CDCl3, 75 MHz
f1 (ppm)

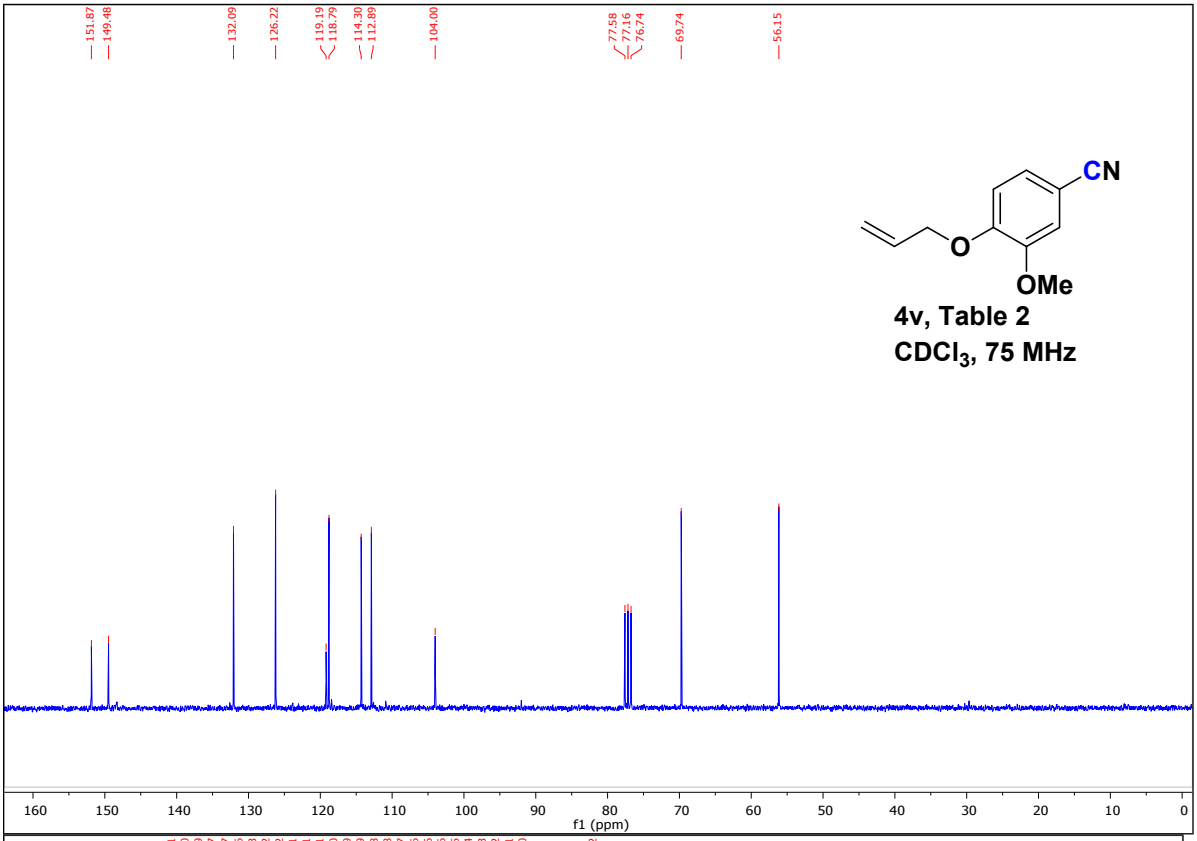

7.80
7.79
7.74
7.73
7.71
7.70
7.52
7.51
7.50
7.49
7.47
7.46
7.44
7.44
7.42
7.38
7.36
7.26
7.10
7.07
6.73
5.18
3.89
3.86
CN
O
OMe
OMe
OMe
4t, Table 2
CDCl3, 300 MHz
B (dd) 7.72
E (s) 6.73
H (s) 3.86
A (d) 7.80
D (d) 7.08
F (s) 5.18
G (s) 3.89
C (m) 7.45
1.00
1.09
5.60
1.08
2.10
2.13
6.24
3.04
f1 (ppm)

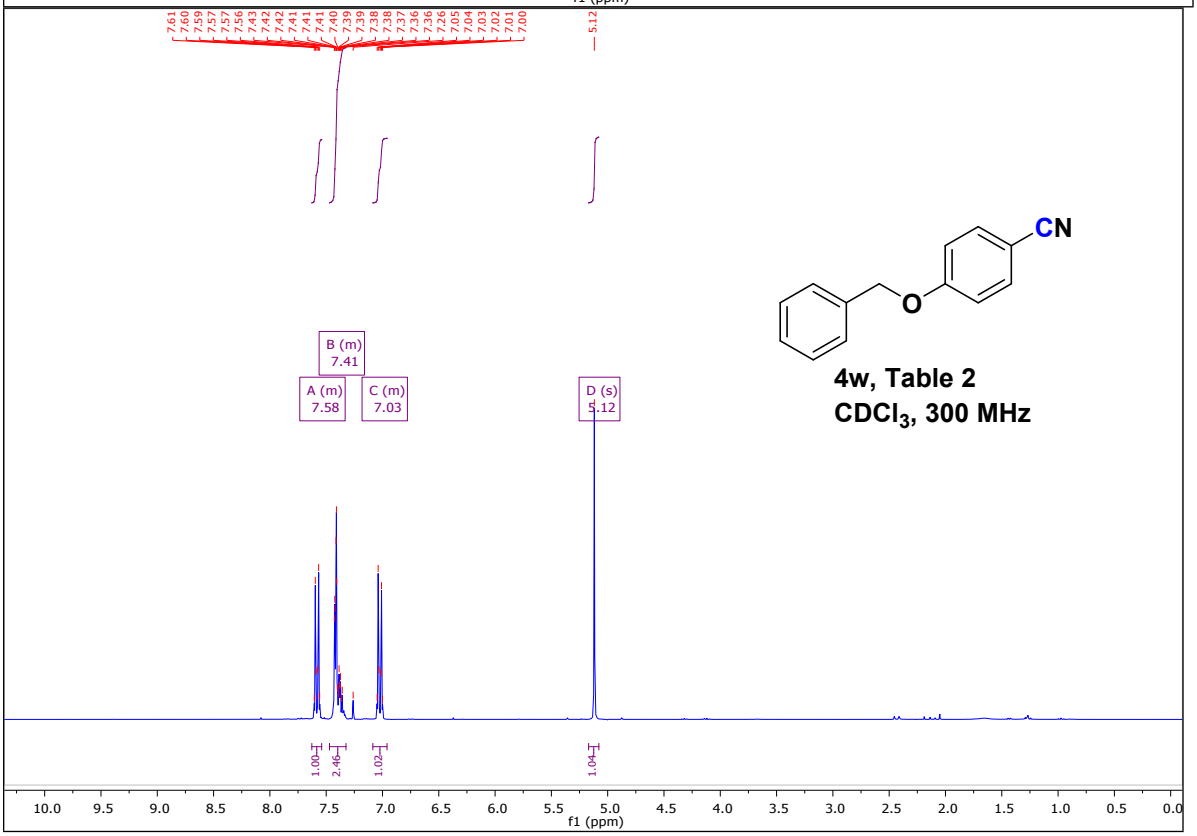

159.67
153.69
138.67
137.92
134.87
133.00
132.21
131.43
129.17
127.89
126.78
116.53
113.62
104.03
103.14
77.58
77.16
76.74
71.09
61.00
56.34
CN
O
OMe
OMe
OMe
4t, Table 2
CDCl3, 75 MHz
f1 (ppm)

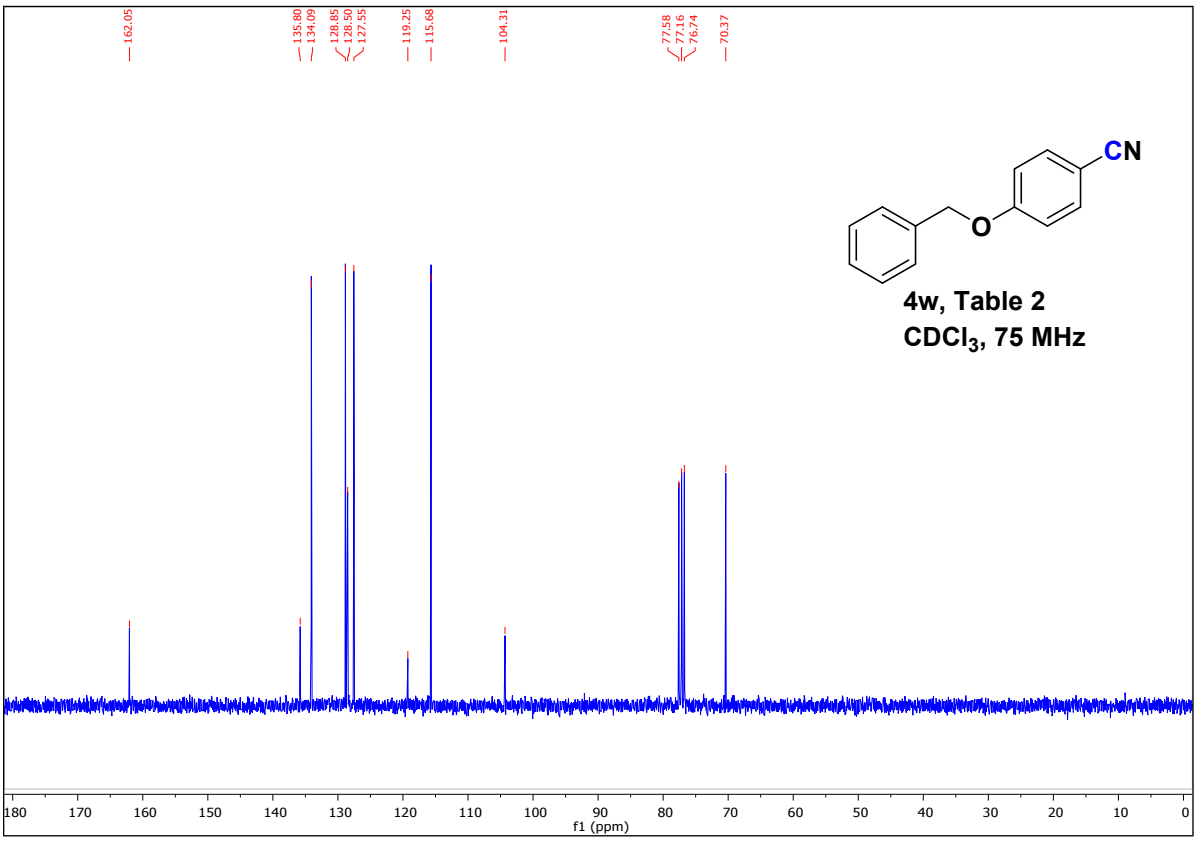

7.58
7.58
7.57
7.56
7.55
7.53
7.52
7.50
7.50
7.50
7.50
7.48
7.47
7.26 CDCl3
7.04
7.04
7.02
7.02
7.01
7.01
6.99
6.99
6.69
5.13
3.86
3.84
B (ddd) 7.50
D (s) 6.69
G (s) 3.84
A (dd) 7.57
C (m) 7.01
E (s) 5.13
F (s) 3.86
CN
O
OMe
OMe
OMe
4u, Table 2
CDCl3, 300 MHz
f1 (ppm)

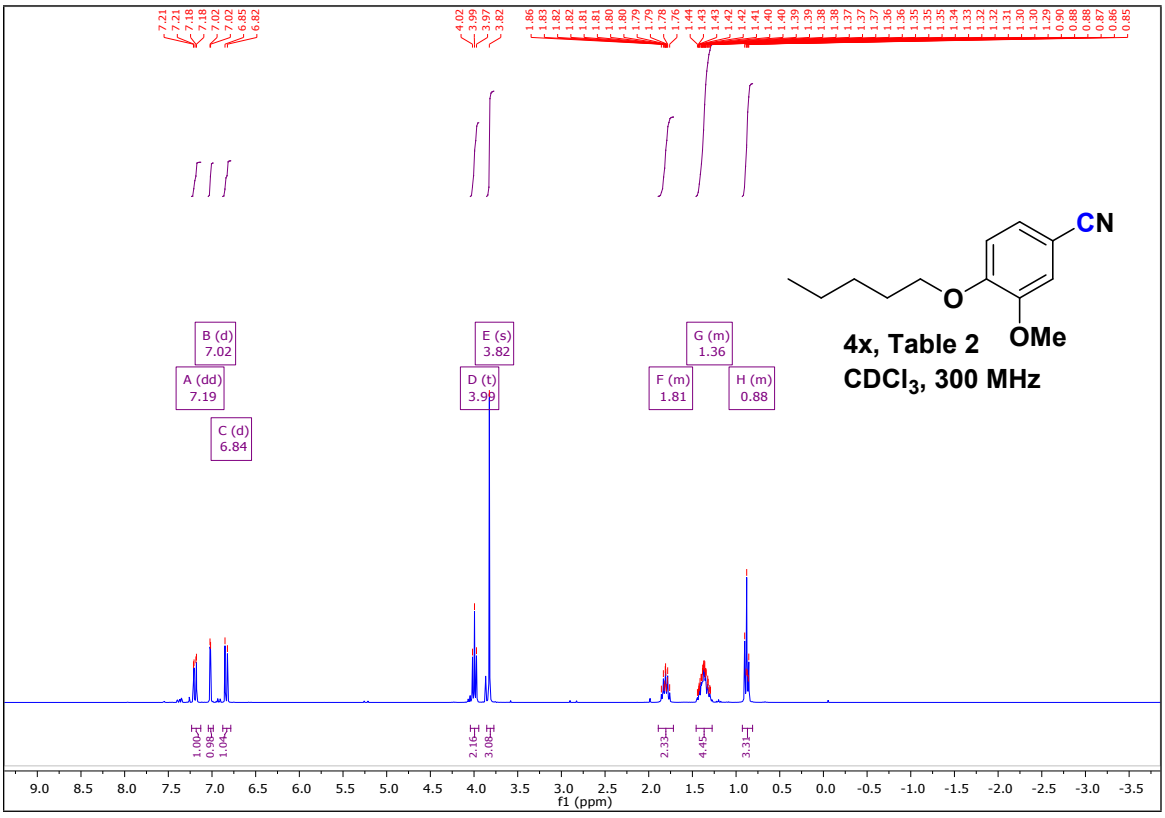

160.34
153.58
137.77
134.41
133.84
131.44
121.33
116.51
113.15
103.92
102.65
77.59
77.16
76.74
70.79
60.93
56.25
CN
O
OMe
OMe
OMe
4u, Table 2
CDCl3, 75 MHz
f1 (ppm)

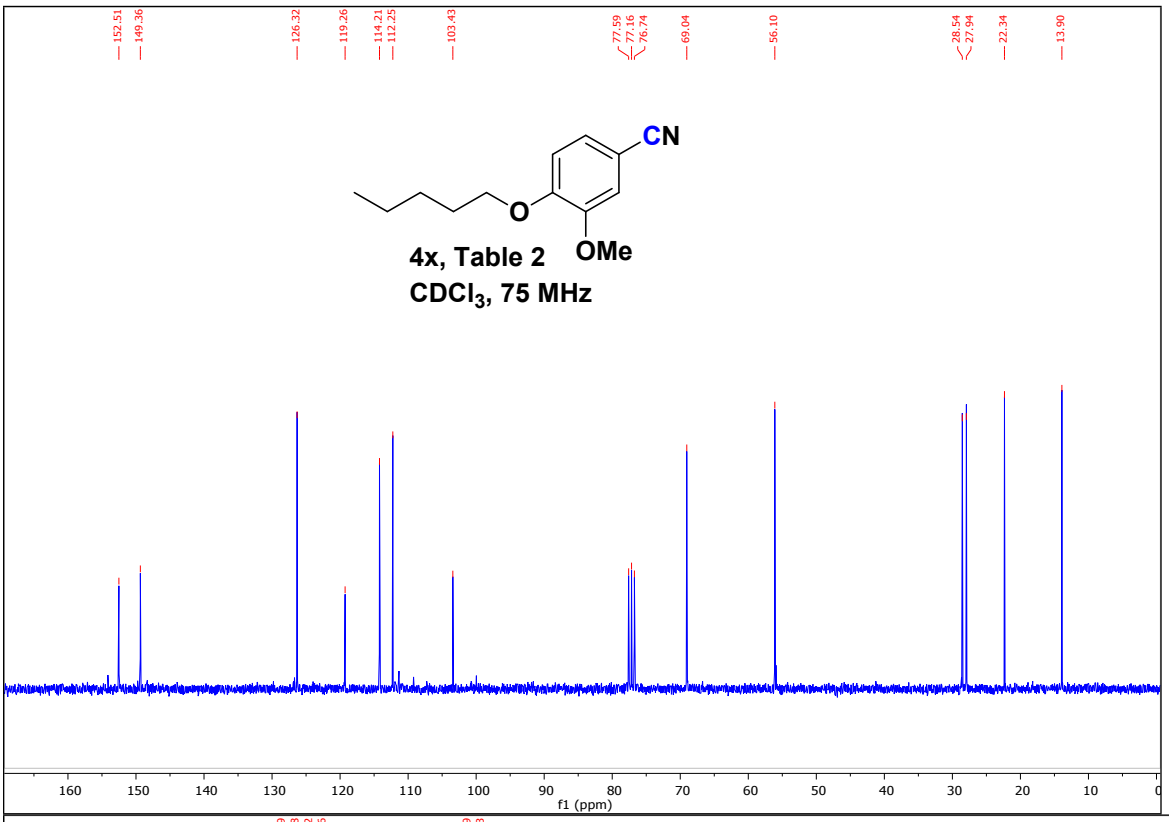

B (d) 7.05
A (dd) 7.20
C (d) 6.86
D (ddt) 6.02
F (dq) 5.30
E (dq) 5.39
G (dt) 4.62
H (s) 3.85
CN
O
OMe
4v, Table 2
CDCl3, 300 MHz
f1 (ppm)

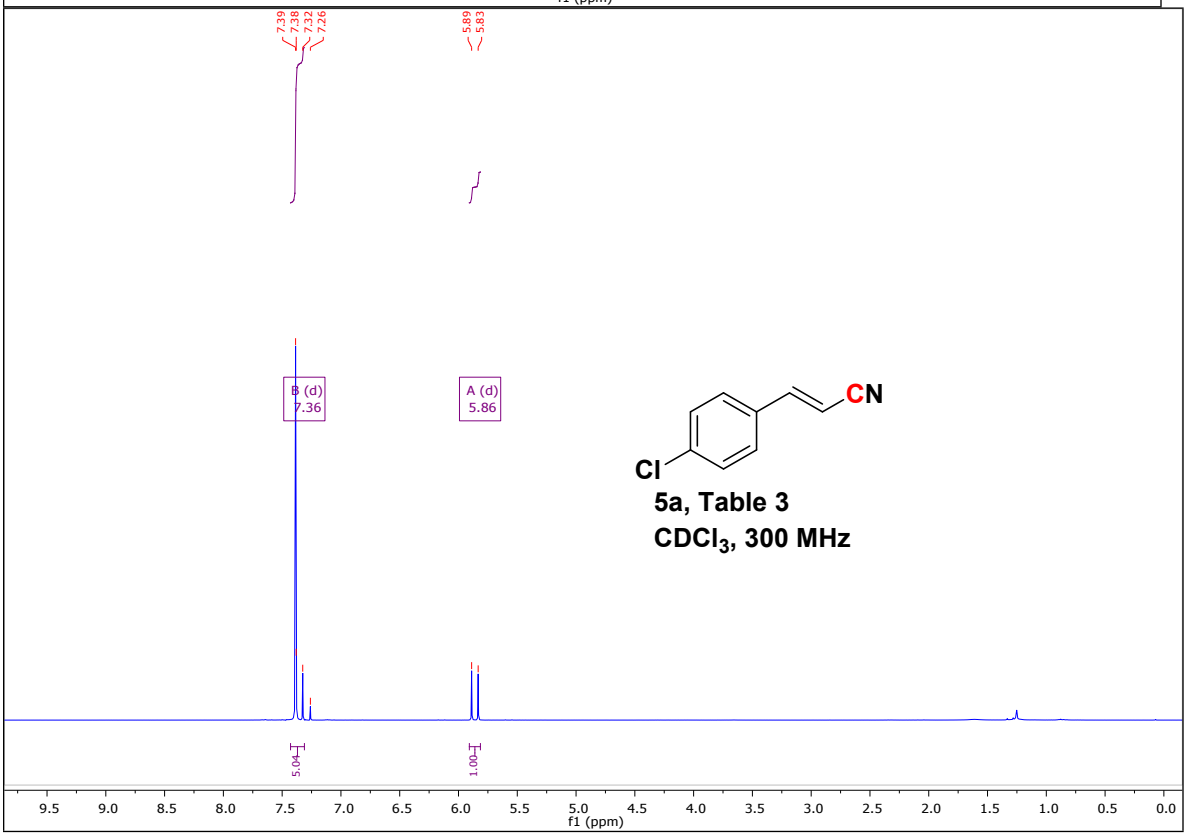

151.87
149.48
132.09
126.22
119.19
118.79
114.30
112.89
104.00
77.58
77.16
76.74
69.74
56.15
CN
O
OMe
4v, Table 2
CDCl3, 75 MHz
f1 (ppm)

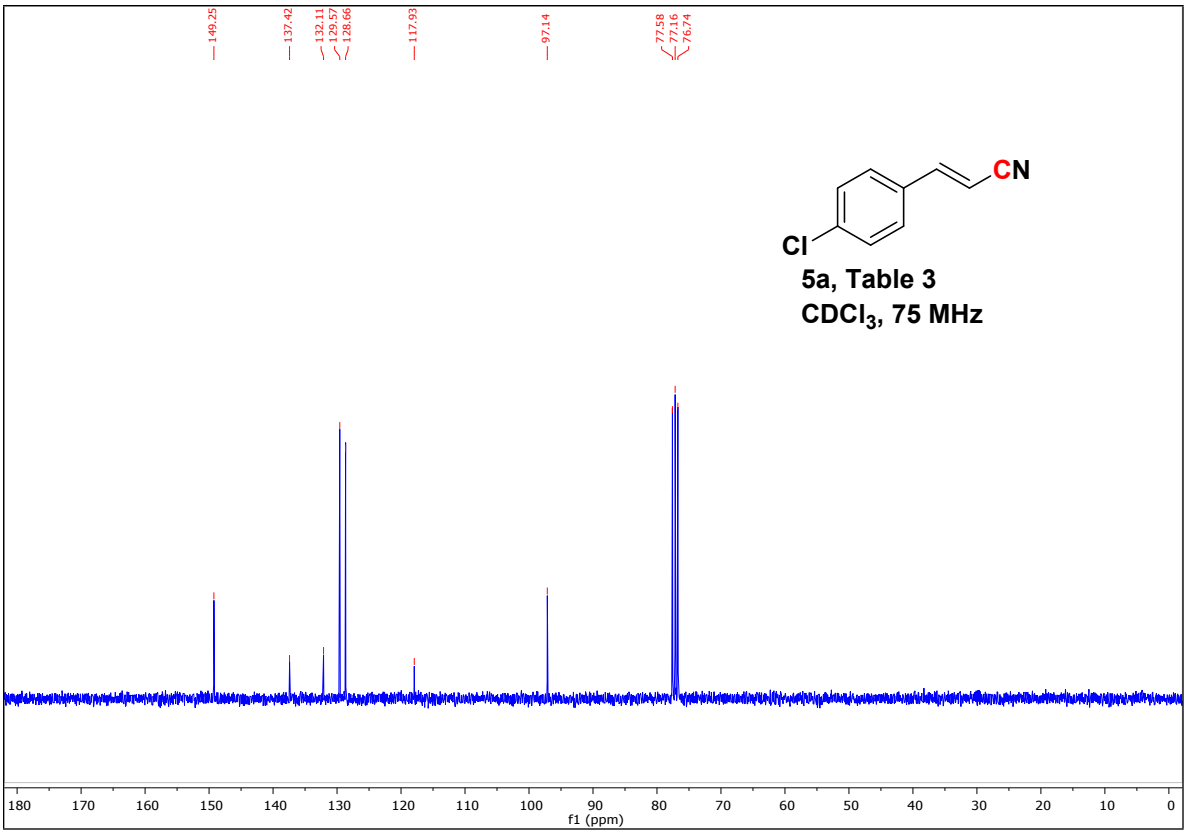

5.12
CN
O
B (m)
7.41
A (m)
7.58
C (m)
7.03
D (s)
5.12
4w, Table 2
CDCl3, 300 MHz
1.00
2.46
1.02
1.04
f1 (ppm)

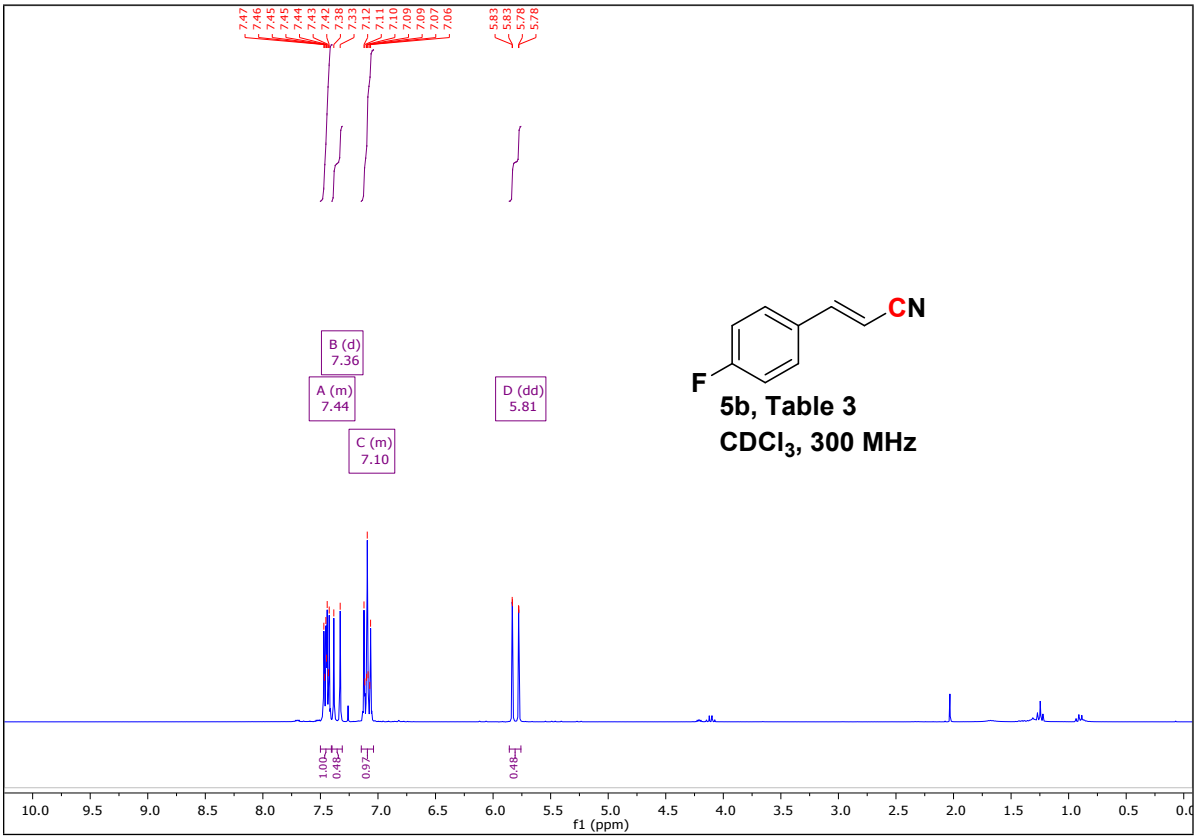

162.05
135.80
134.09
128.85
128.50
127.55
119.25
115.68
104.31
77.58
77.16
76.74
70.37
CN
O
4w, Table 2
CDCl3, 75 MHz
f1 (ppm)

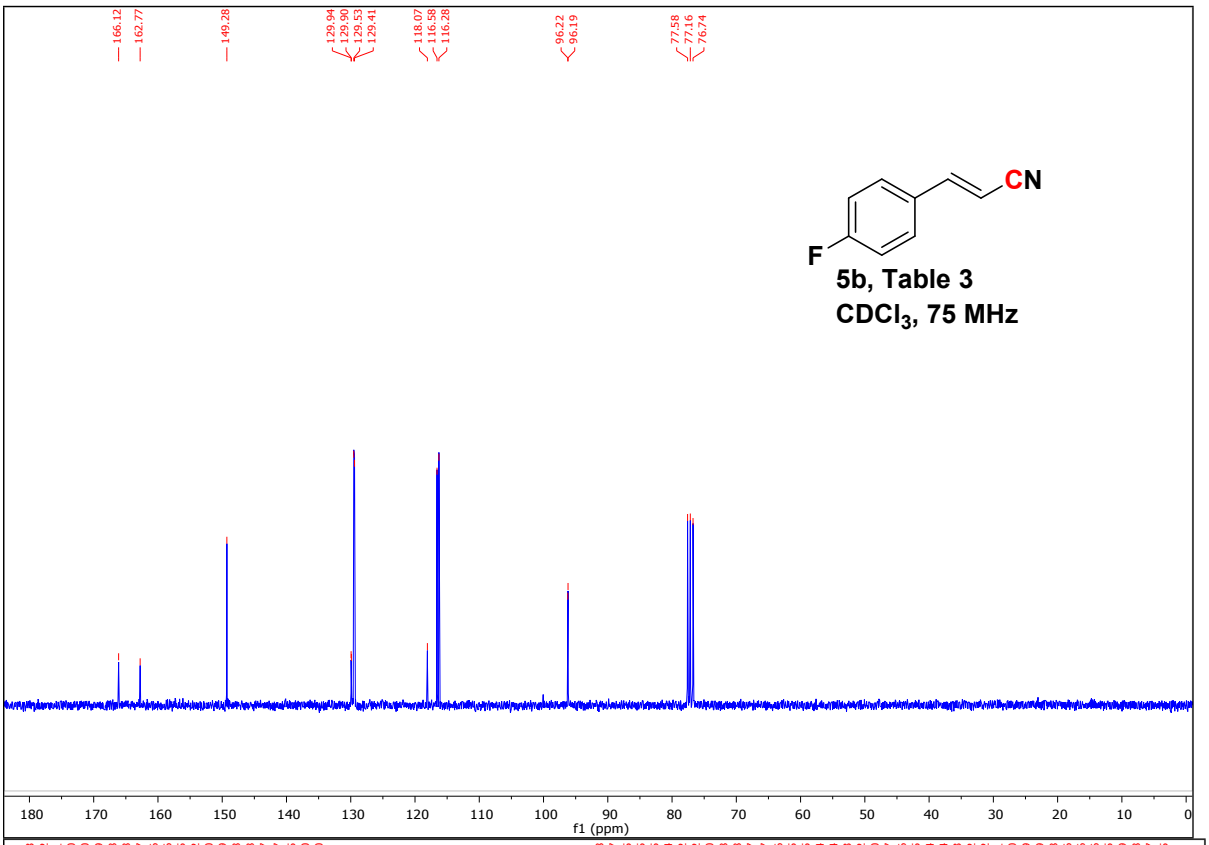

CN
O
OMe
4x, Table 2
CDCl3, 300 MHz
B (d) 7.02
A (dd) 7.19
C (d) 6.84
E (s) 3.82
D (t) 3.99
G (m) 1.36
F (m) 1.81
H (m) 0.88
f1 (ppm)

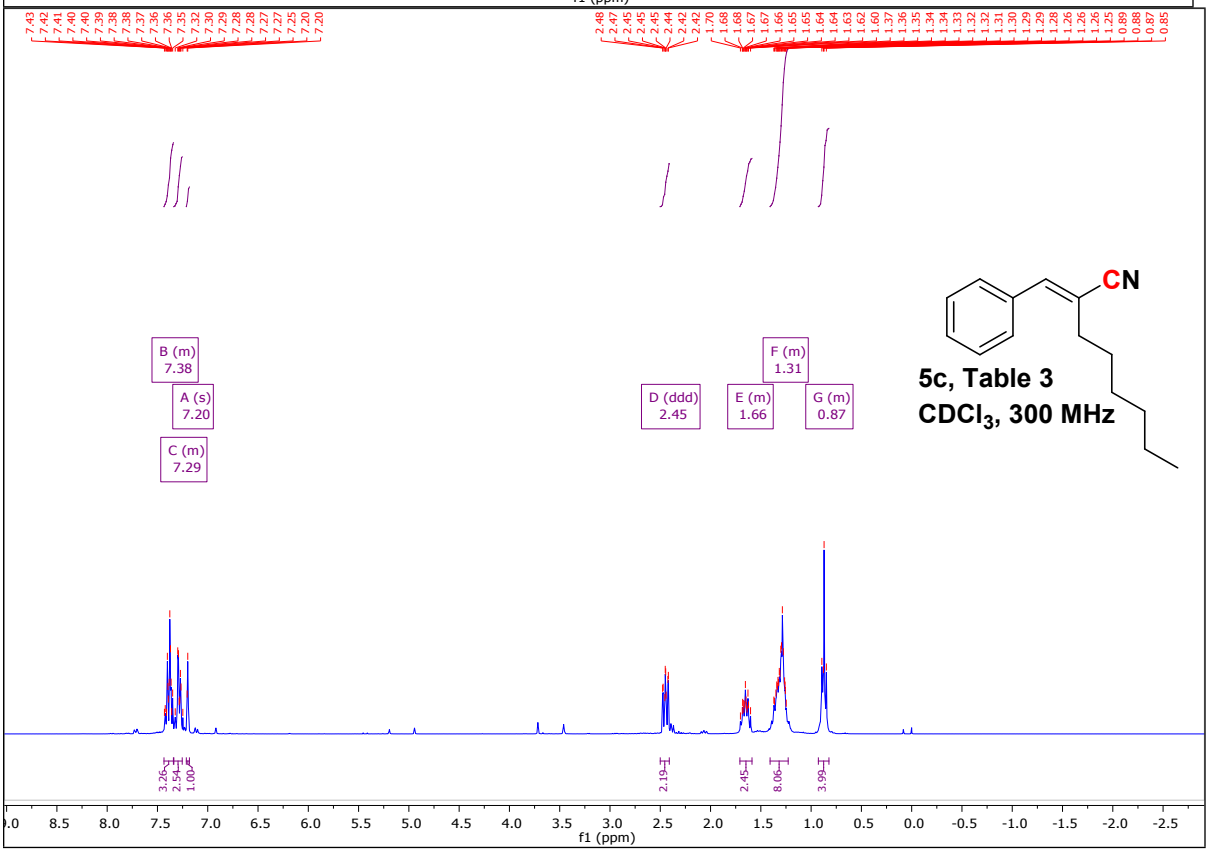

152.51
149.36
126.32
119.26
114.21
112.25
103.43
77.59
77.16
76.74
69.04
56.10
28.54
27.94
22.34
13.90
CN
O
OMe
4x, Table 2
CDCl3, 75 MHz
f1 (ppm)

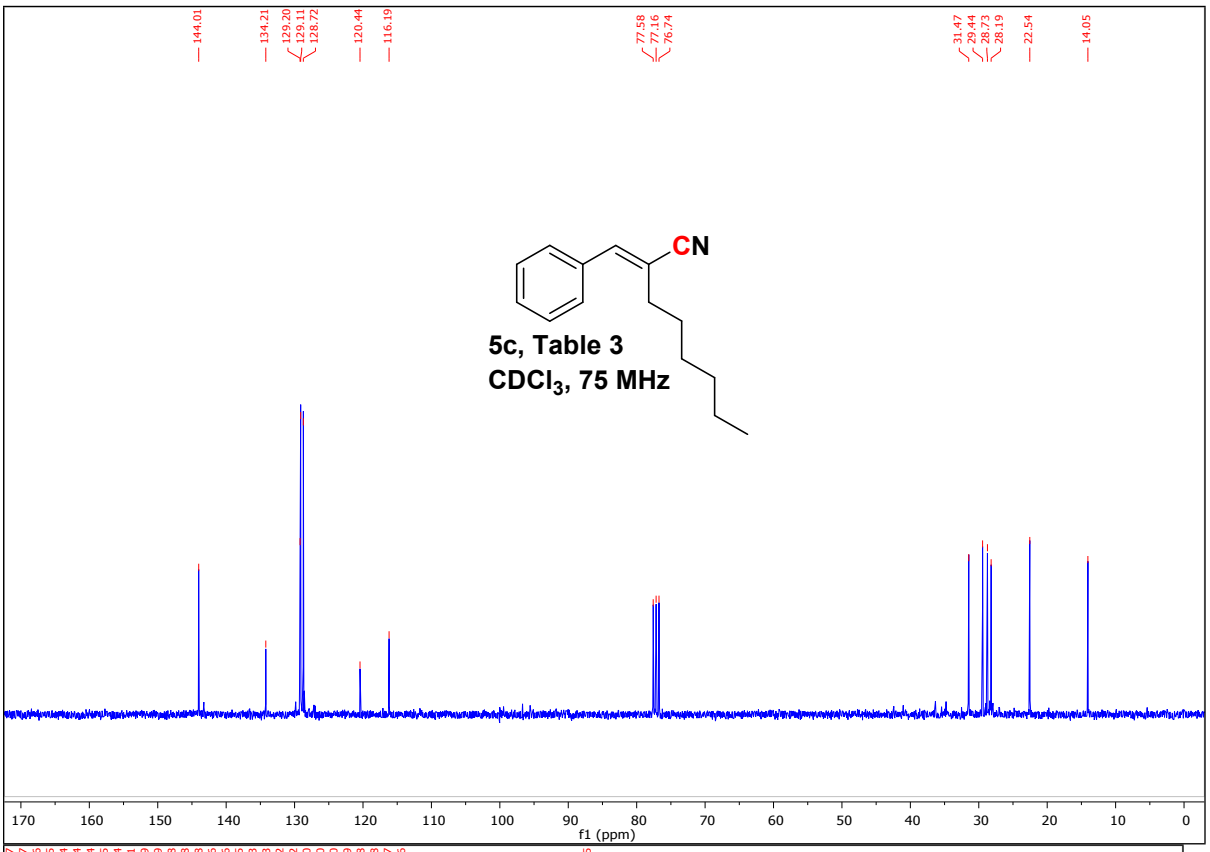

7.39
7.38
7.32
7.26
5.89
5.83
B (d)
7.36
A (d)
5.86
5.04
1.00
CN
Cl
5a, Table 3
CDCl3, 300 MHz
f1 (ppm)

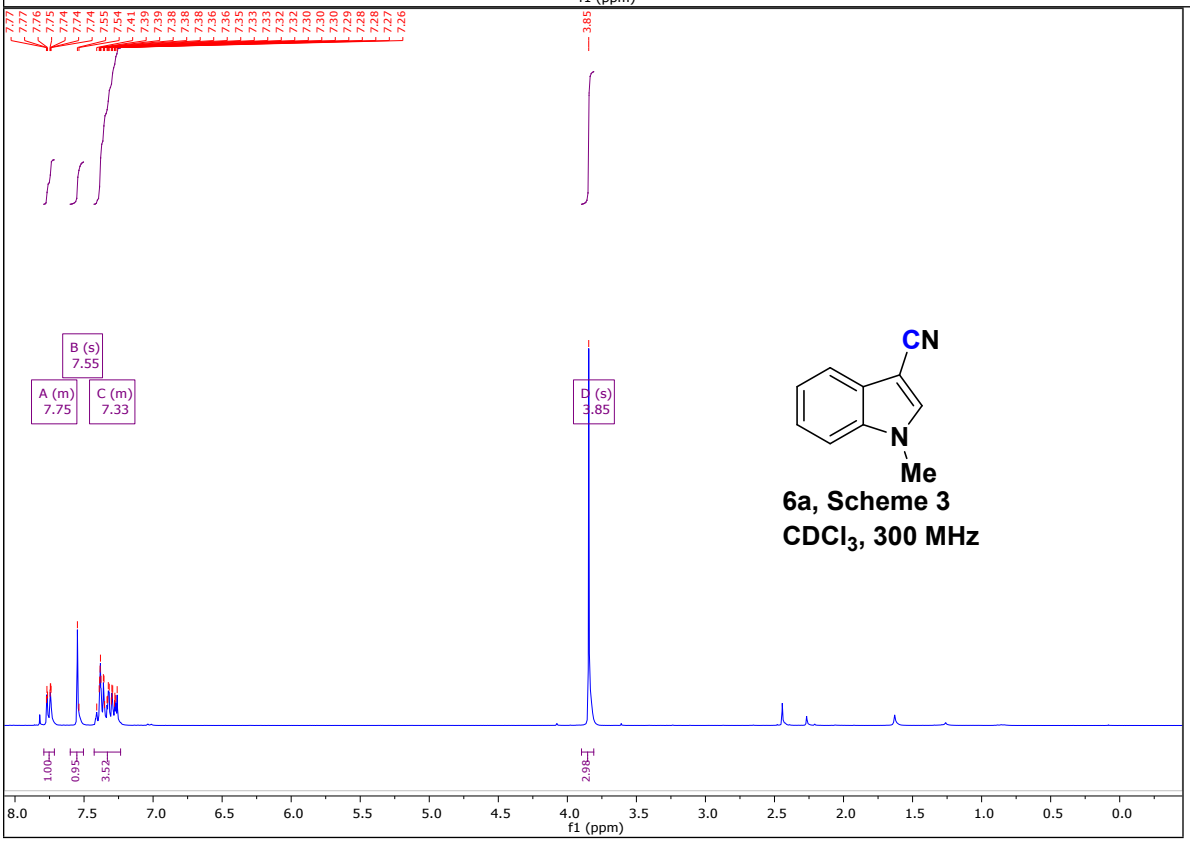

149.25
137.42
132.11
129.57
128.66
117.93
97.14
77.58
77.16
76.74
CN
Cl
5a, Table 3
CDCl3, 75 MHz
f1 (ppm)

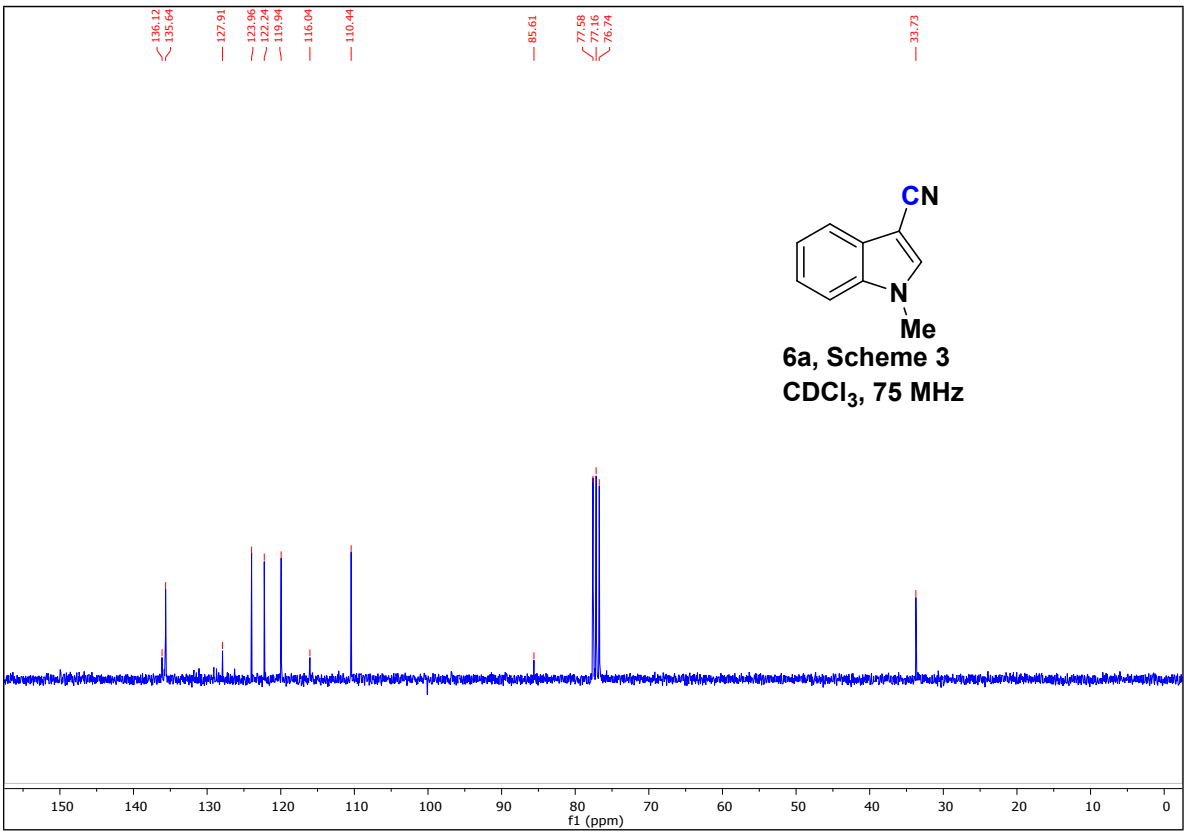

7.47
7.46
7.45
7.45
7.44
7.43
7.42
7.38
7.33
7.12
7.11
7.10
7.09
7.09
7.07
7.06
5.83
5.83
5.78
5.78
B (d)
7.36
A (m)
7.44
C (m)
7.10
D (dd)
5.81
CN
F
5b, Table 3
CDCl3, 300 MHz
1.00
0.48
0.97
0.48
f1 (ppm)

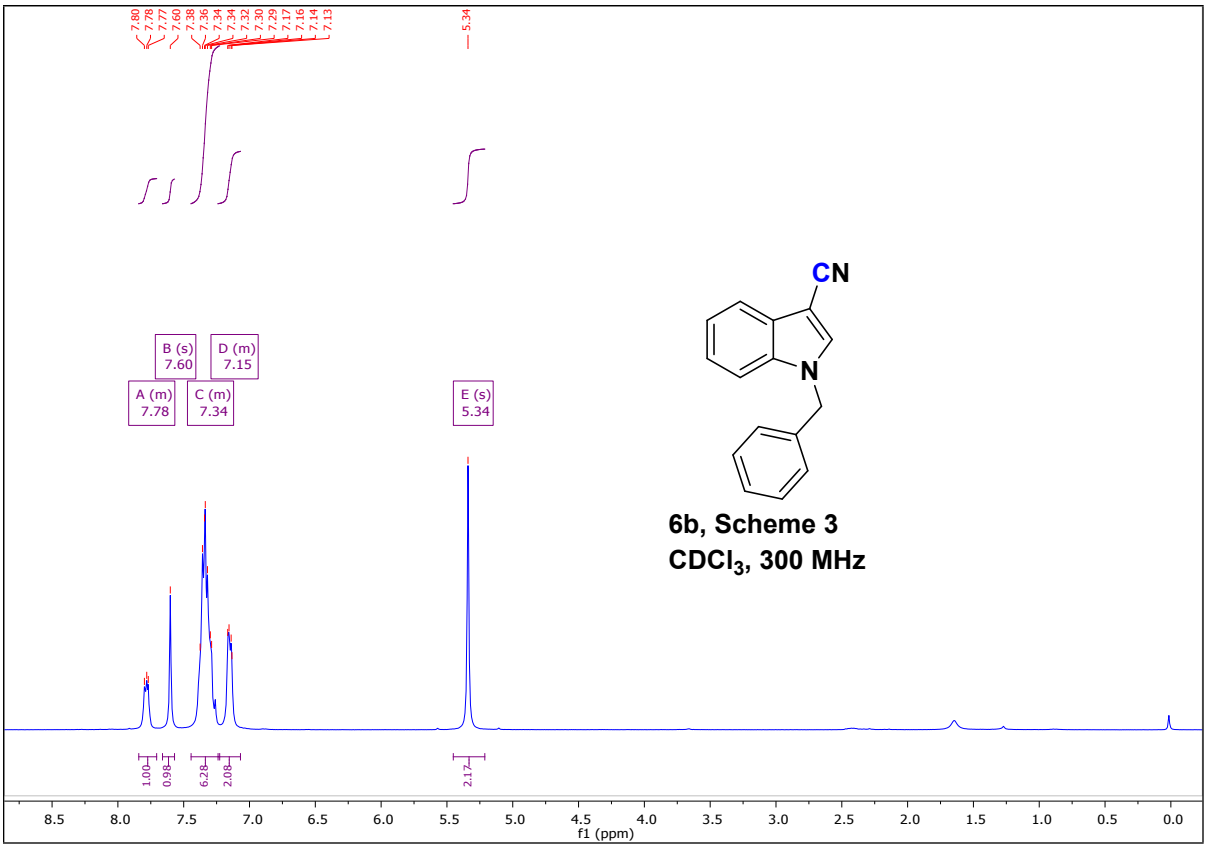

166.12
162.77
149.28
129.94
129.90
129.53
129.41
118.07
116.58
116.28
96.22
96.19
77.58
77.16
76.74
CN
F
5b, Table 3
CDCl3, 75 MHz
f1 (ppm)

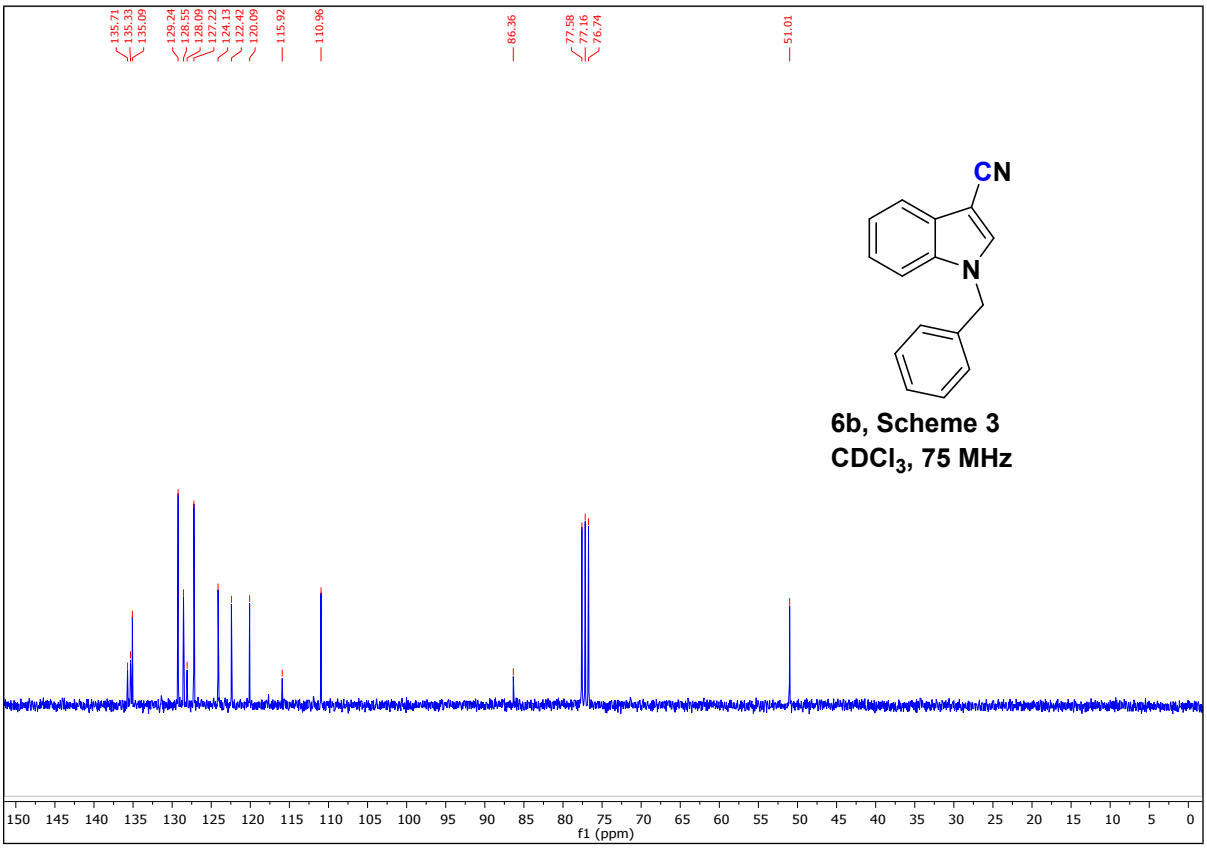

B (m)
7.38
A (s)
7.20
C (m)
7.29
D (ddd)
2.45
E (m)
1.66
F (m)
1.31
G (m)
0.87
CN
5c, Table 3
CDCl3, 300 MHz
f1 (ppm)

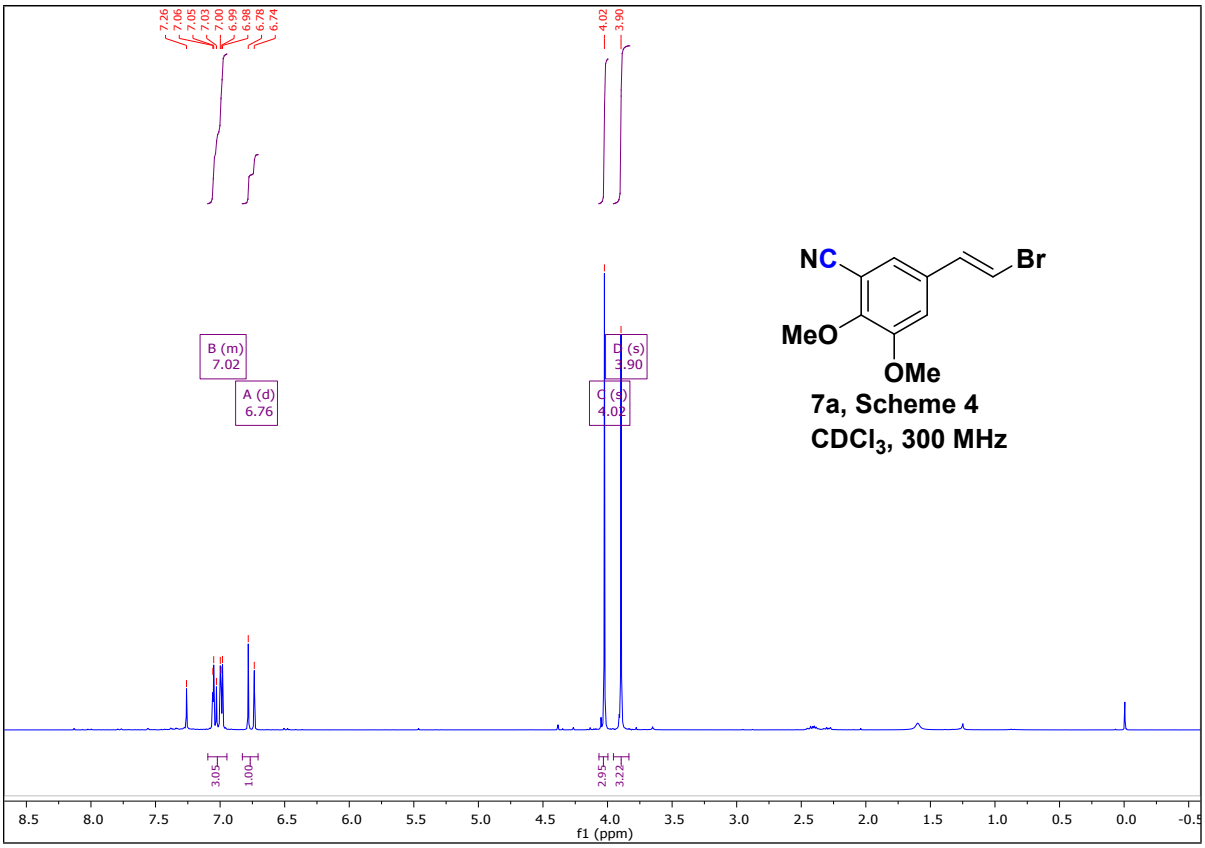

144.01
134.21
129.20
129.11
128.72
120.44
116.19
77.58
77.16
76.74
31.47
29.44
28.73
28.19
22.54
14.05
CN
5c, Table 3
CDCl3, 75 MHz
f1 (ppm)

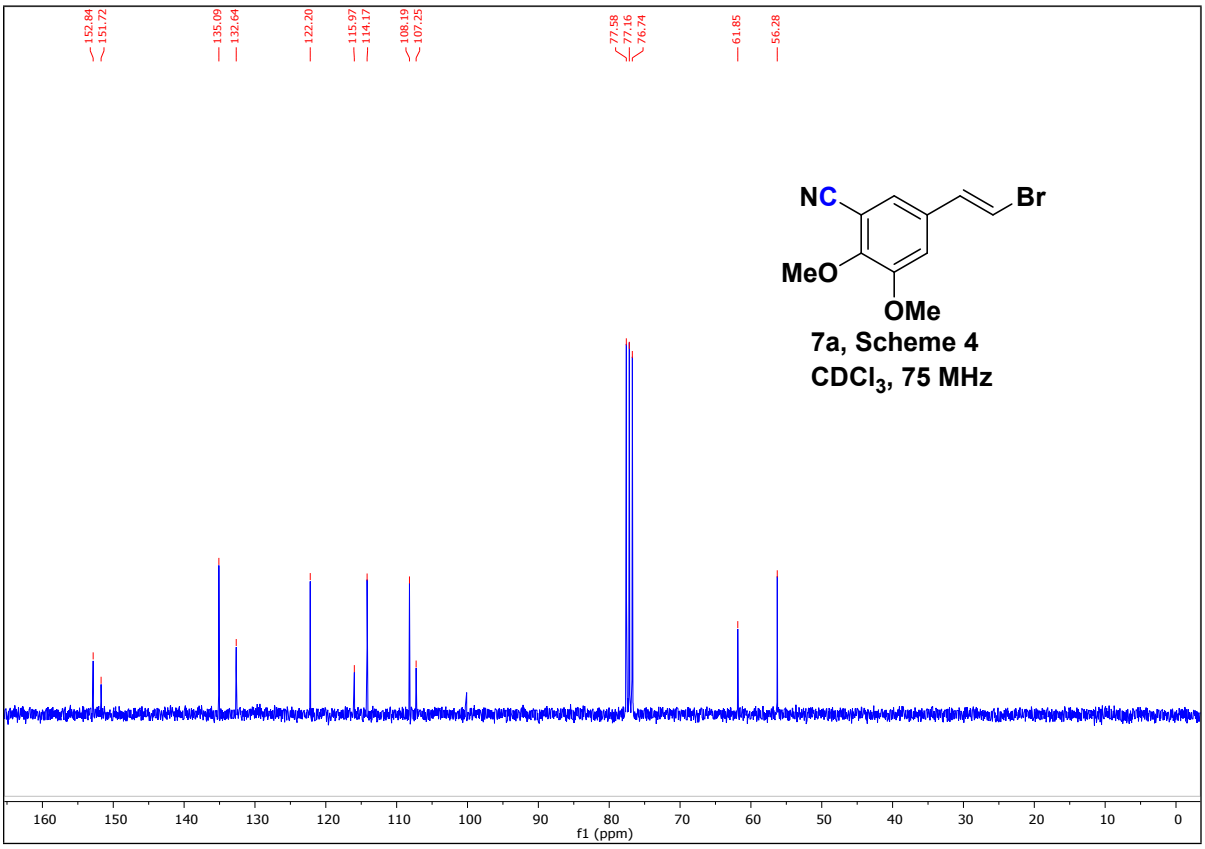

3.85
B (s)
7.55
A (m)
7.75
C (m)
7.33
D (s)
3.85
1.00
0.95
3.52
2.98
CN
N
Me
6a, Scheme 3
CDCl3, 300 MHz
f1 (ppm)

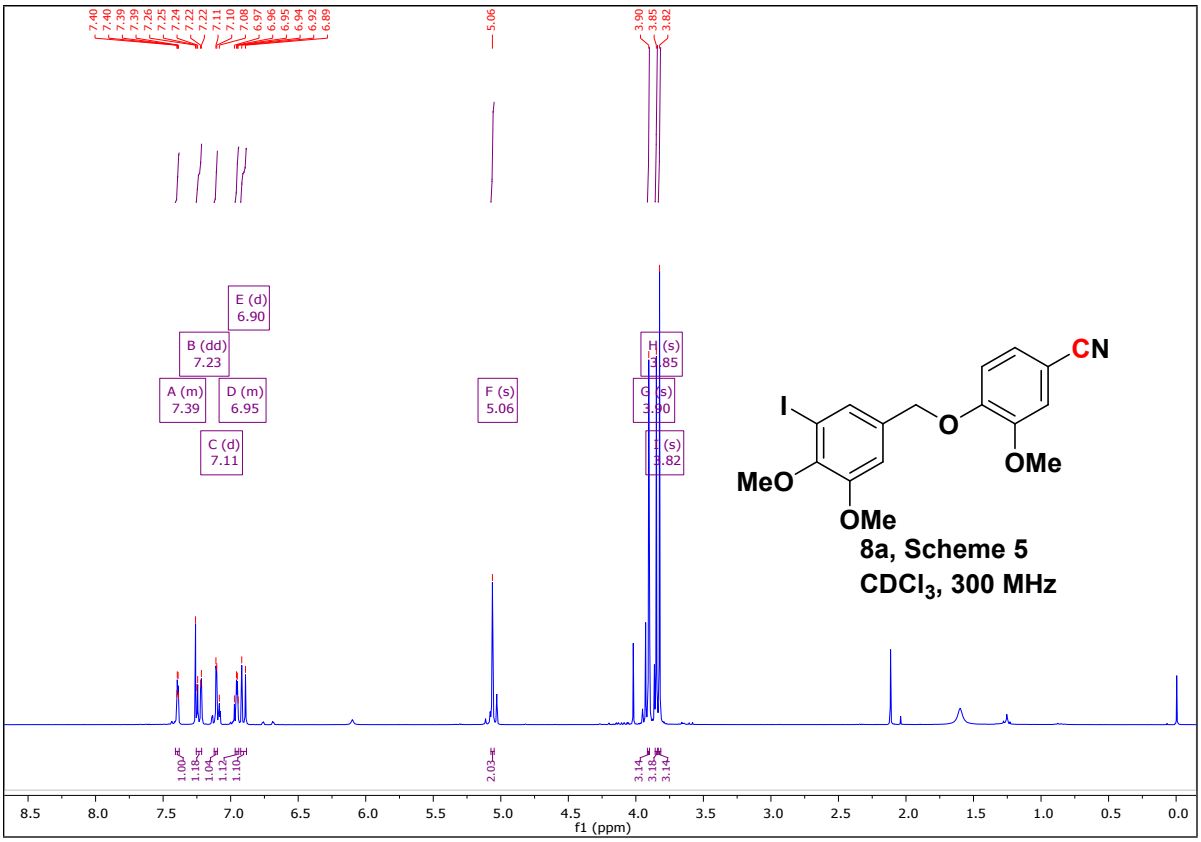

136.12
135.64
127.91
123.96
122.24
119.94
116.04
110.44
85.61
77.58
77.16
76.74
33.73
CN
N
Me
6a, Scheme 3
CDCl3, 75 MHz
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

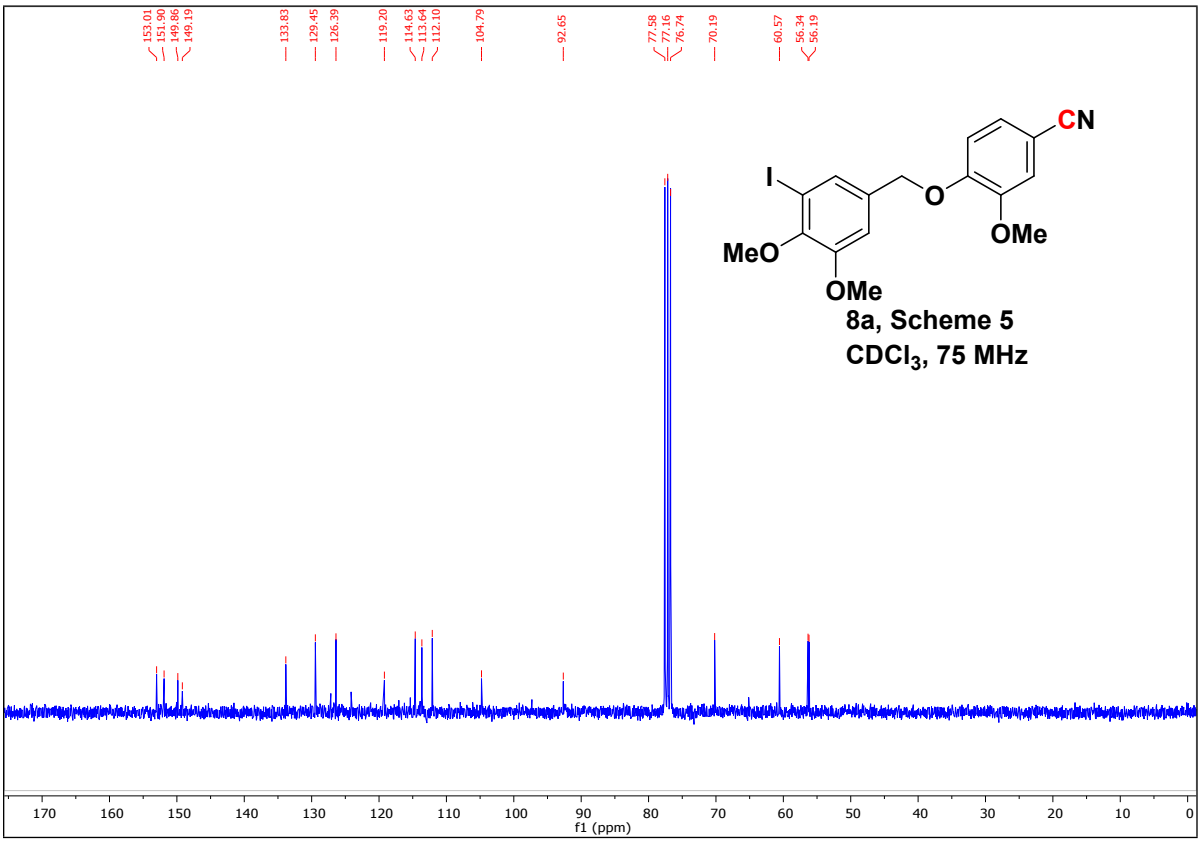

7.80
7.78
7.77
7.60
7.38
7.36
7.34
7.34
7.32
7.30
7.19
7.17
7.16
7.14
7.13
5.34
B (s)
7.60
D (m)
7.15
A (m)
7.78
C (m)
7.34
E (s)
5.34
1.00
0.98
6.28
2.08
2.17
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
CN
N
6b, Scheme 3
CDCl3, 300 MHz

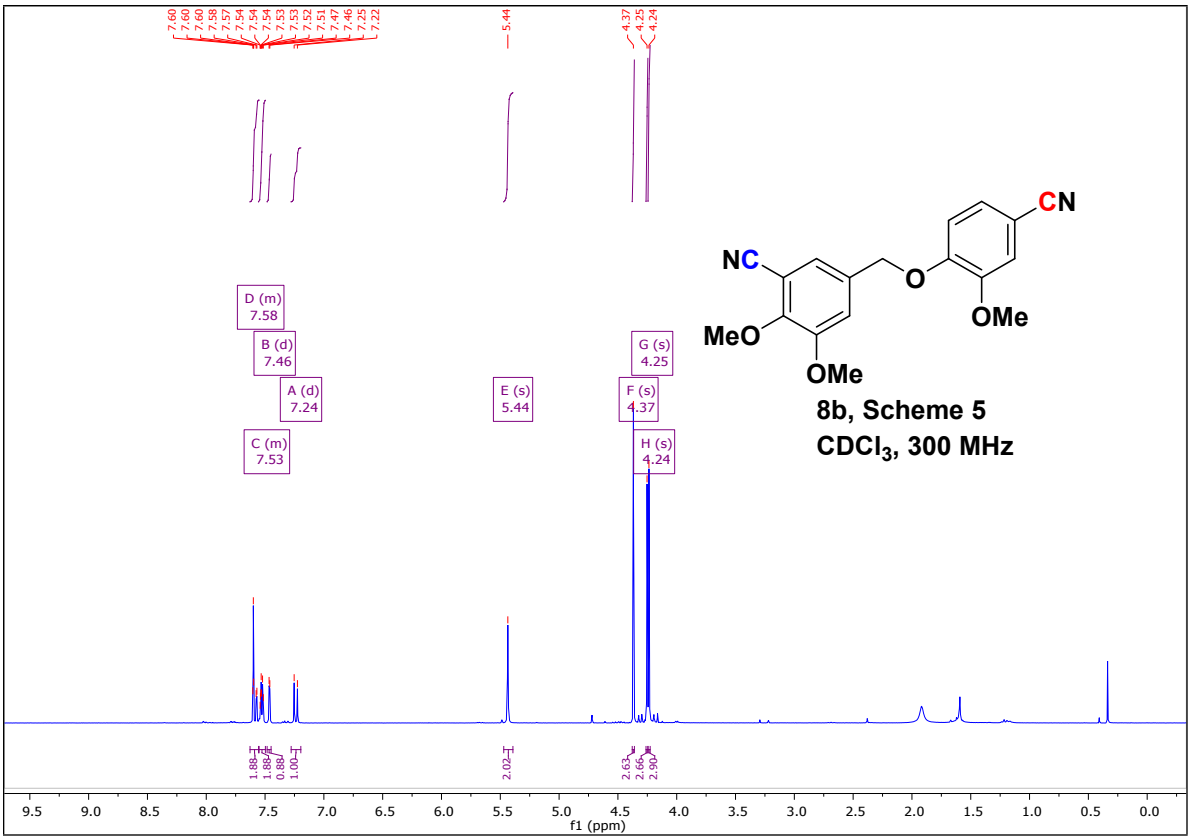

135.71
135.33
135.09
129.24
128.55
128.09
127.22
124.13
122.42
120.09
115.92
110.96
86.36
77.58
77.16
76.74
51.01
150
145
140
135
130
125
120
115
110
105
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
f1 (ppm)
CN
N
6b, Scheme 3
CDCl3, 75 MHz

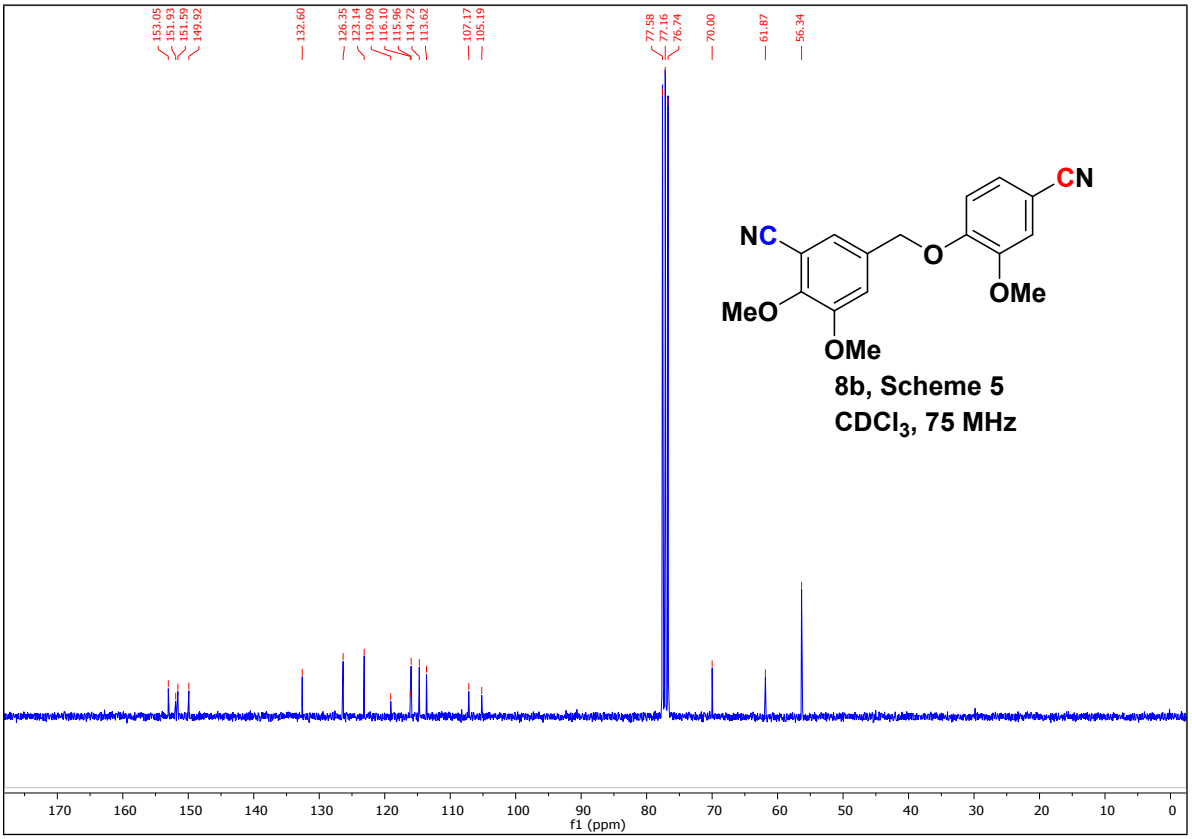

7.26
7.06
7.05
7.03
7.00
6.99
6.98
6.78
6.74
4.02
3.90
B (m)
7.02
A (d)
6.76
D (s)
3.90
C (s)
4.02
NC
Br
MeO
OMe
7a, Scheme 4
CDCl3, 300 MHz
3.05
1.00
2.95
3.22
f1 (ppm)

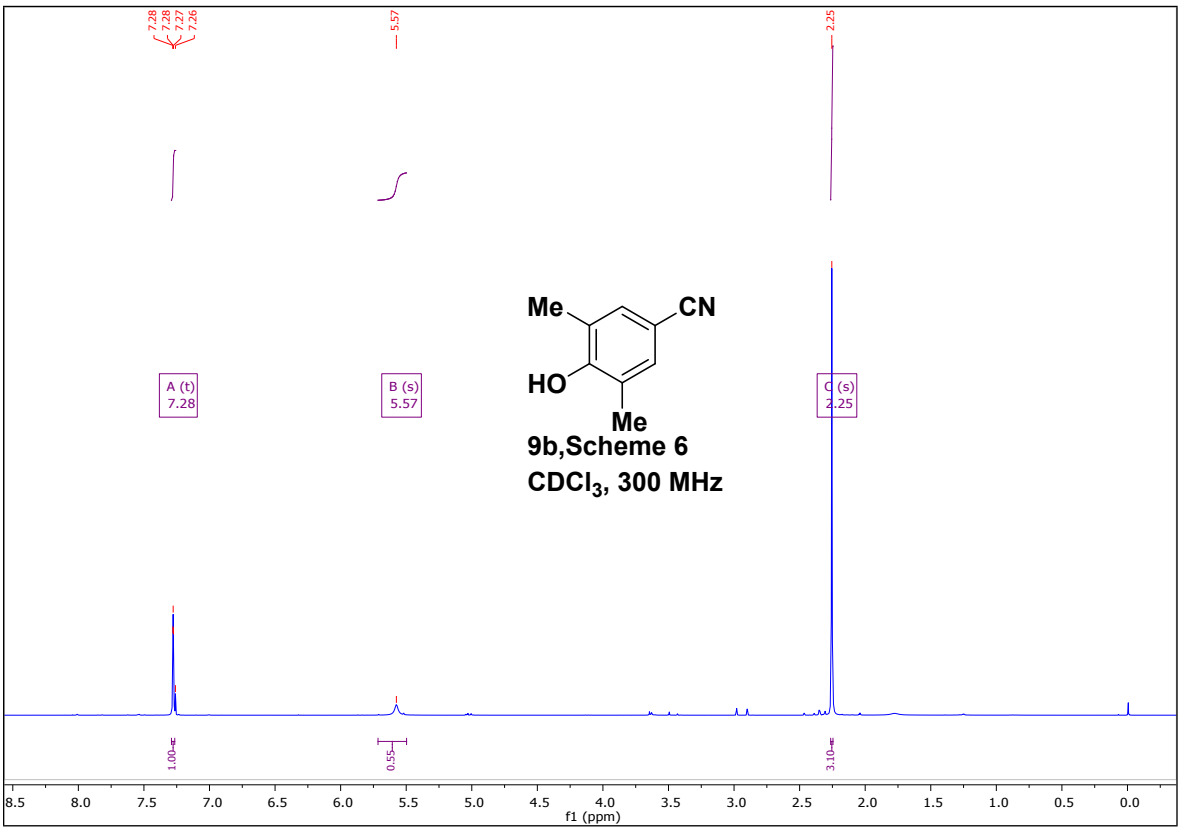

152.84
151.72
135.09
132.64
122.20
115.97
114.17
108.19
107.25
77.58
77.16
76.74
61.85
56.28
NC
Br
MeO
OMe
7a, Scheme 4
CDCl3, 75 MHz
f1 (ppm)

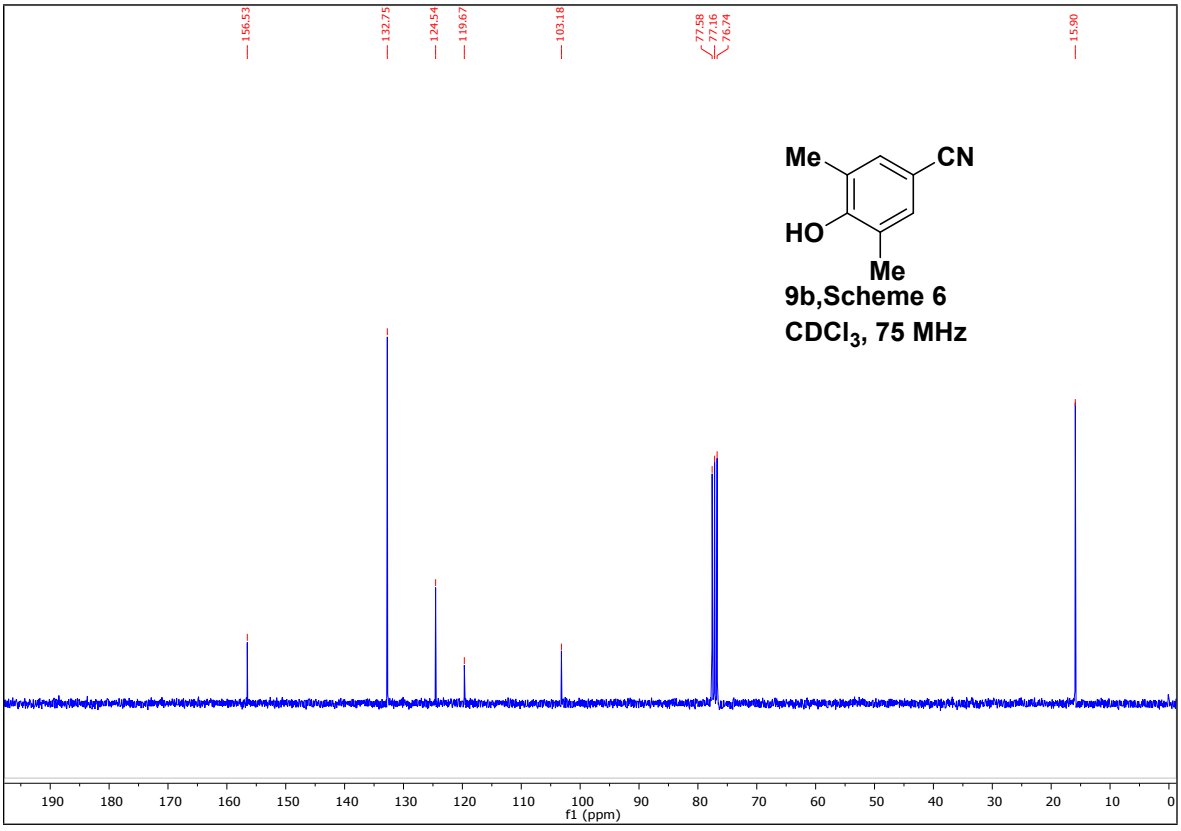

E (d) 6.90
B (dd) 7.23
A (m) 7.39
D (m) 6.95
C (d) 7.11
F (s) 5.06
H (s) 3.85
G (s) 3.90
I (s) 3.82
CN
I
O
MeO
OMe
OMe
8a, Scheme 5
CDCl3, 300 MHz
f1 (ppm)


CN
I
O
MeO
OMe
OMe
8a, Scheme 5
CDCl3, 75 MHz
f1 (ppm)


D (m)
7.58
B (d)
7.46
A (d)
7.24
C (m)
7.53
E (s)
5.44
G (s)
4.25
F (s)
4.37
H (s)
4.24
CN
NC
O
MeO
OMe
OMe
8b, Scheme 5
CDCl3, 300 MHz
f1 (ppm)


CN
NC
O
MeO
OMe
OMe
8b, Scheme 5
CDCl3, 75 MHz
f1 (ppm)


7.28
7.28
7.27
7.26
5.57
2.25
Me
CN
HO
Me
A (t)
7.28
B (s)
5.57
C (s)
2.25
9b,Scheme 6
CDCl3, 300 MHz
1.00
0.55
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)


156.53
132.75
124.54
119.67
103.18
77.58
77.16
76.74
15.90
Me
CN
HO
Me
9b,Scheme 6
CDCl3, 75 MHz
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)