Electronic Supplementary Material (ESI) for Chemical Communications
This journal is © The Royal Society of Chemistry 2012

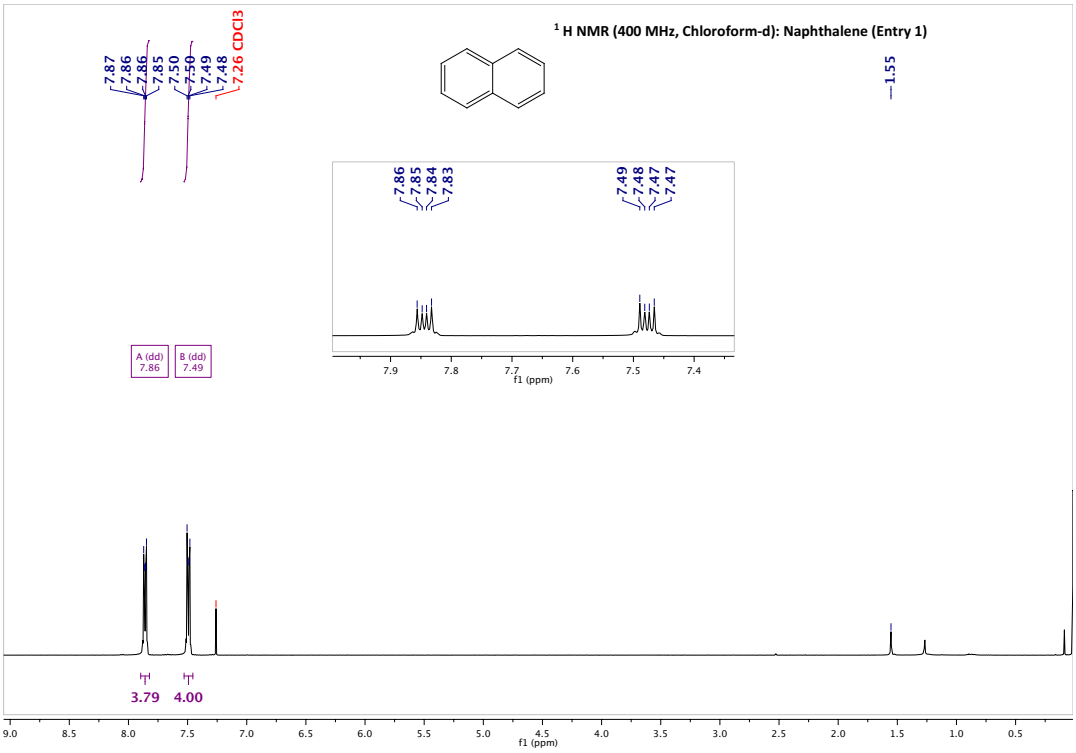
An efficient dehydroxymethylation reaction by a palladium catalyst†

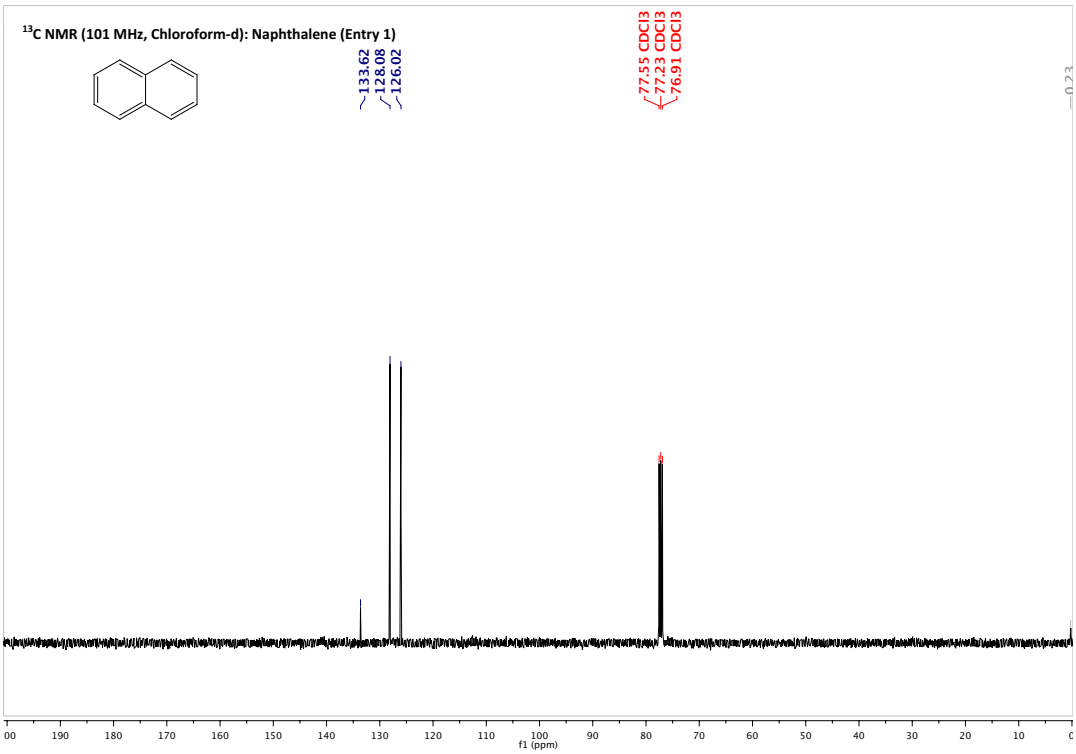
Atanu Modak, Togati Naveen and Debabrata Maiti*

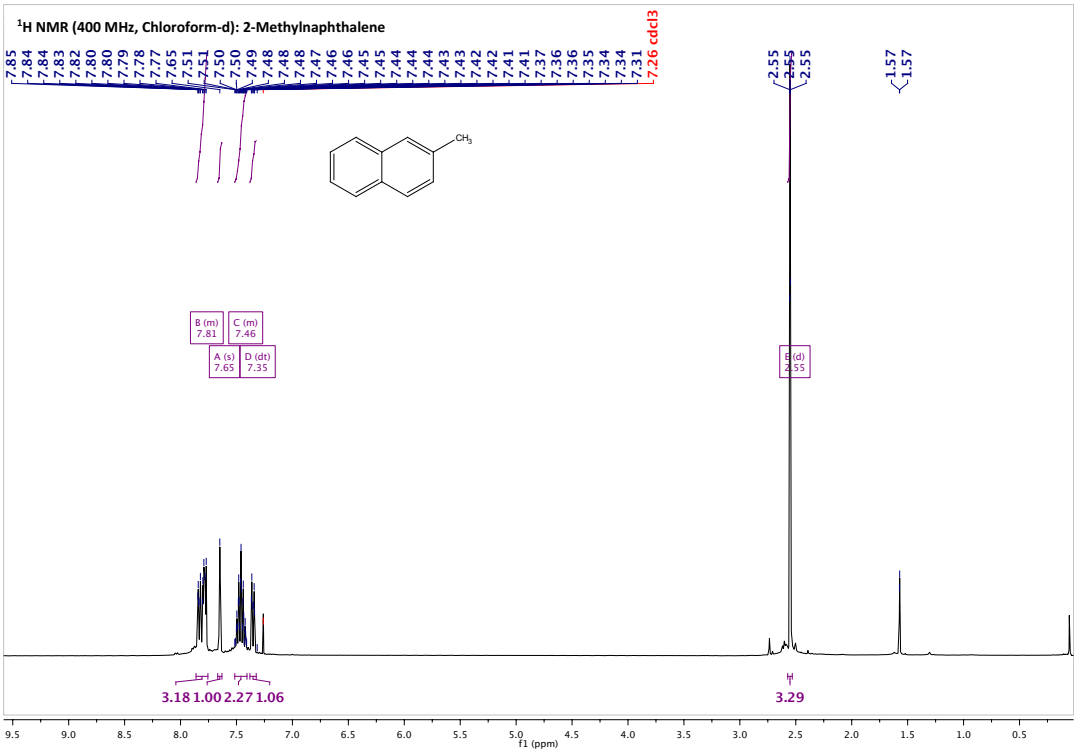
Department of Chemistry, Indian Institute of Technology Bombay, Powai, Mumbai 400076

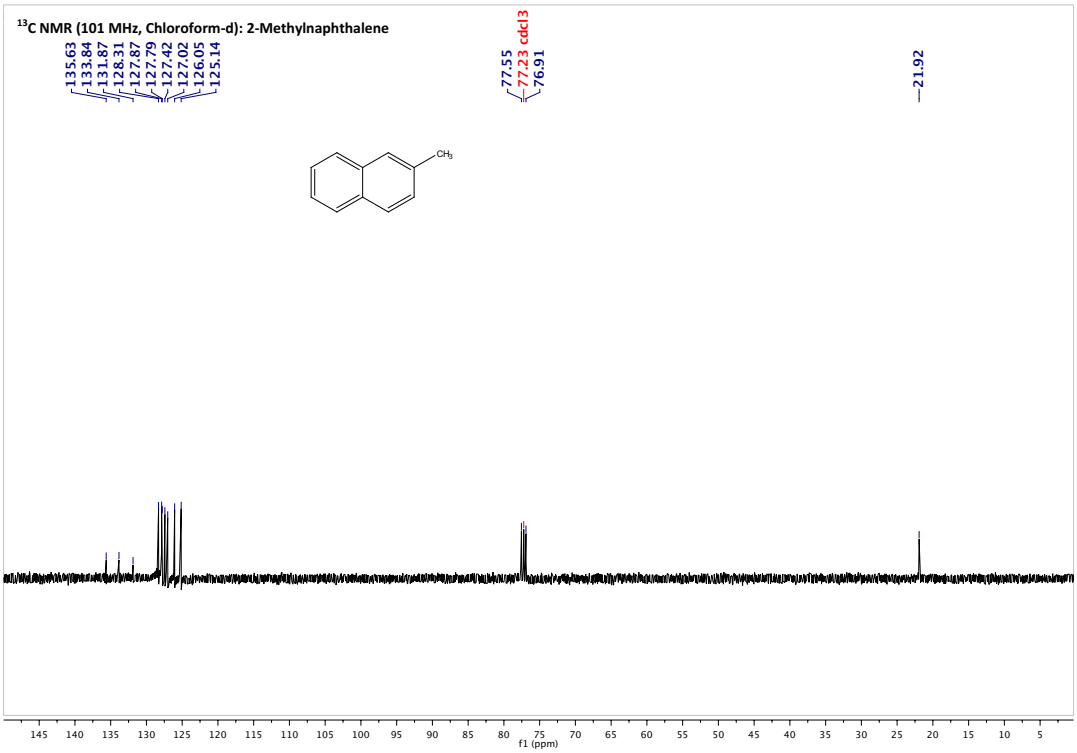
RECEIVED DATE (automatically inserted by publisher); E–mail: dmaiti@chem.iitb.ac.in

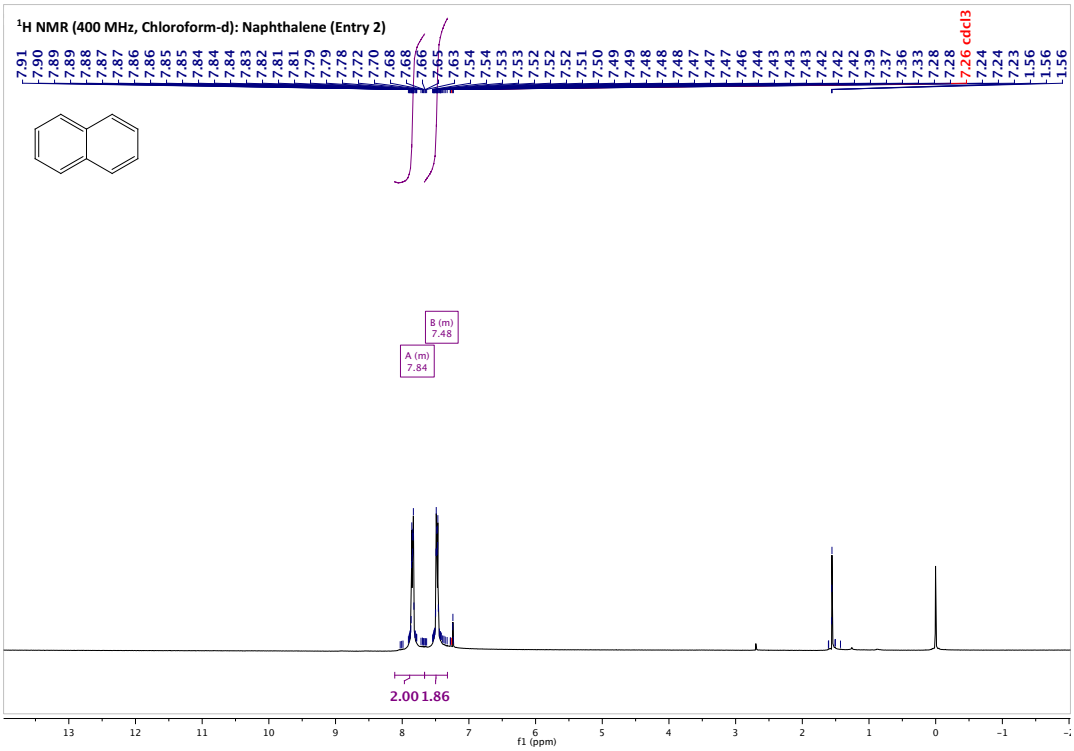
Spectral Data (^{1}H NMR, ^{13}C NMR)

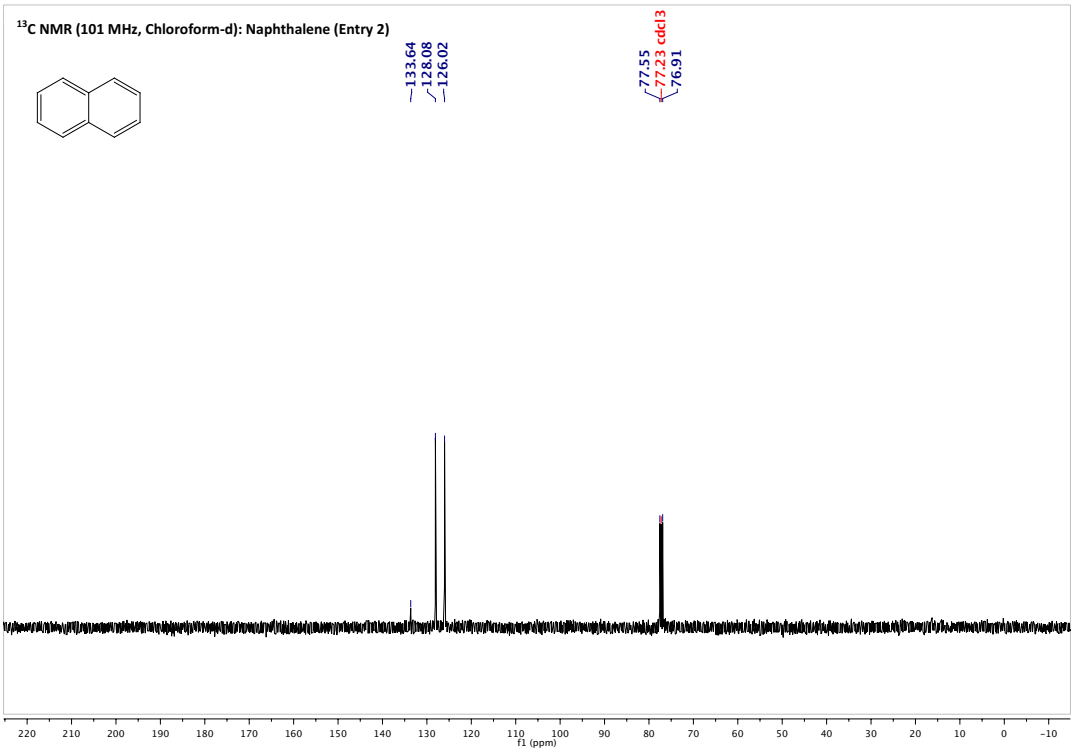

1 H NMR (400 MHz, Chloroform-d): Naphthalene (Entry 1)
7.87
7.86
7.86
7.85
7.50
7.50
7.49
7.48
7.26 CDCl3
1.55
7.86
7.85
7.84
7.83
7.49
7.48
7.47
7.47
A (dd) 7.86
B (dd) 7.49
3.79
4.00
f1 (ppm)

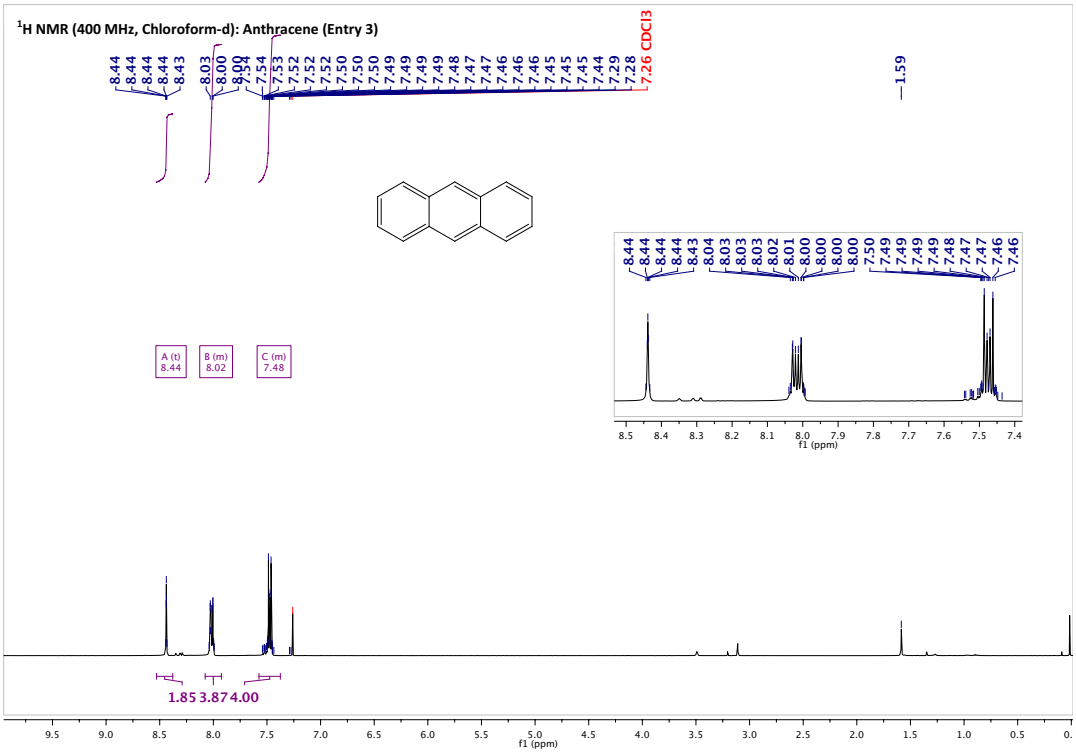

13C NMR (101 MHz, Chloroform-d): Naphthalene (Entry 1)
133.62
128.08
126.02
77.55 CDCl3
77.23 CDCl3
76.91 CDCl3
f1 (ppm)

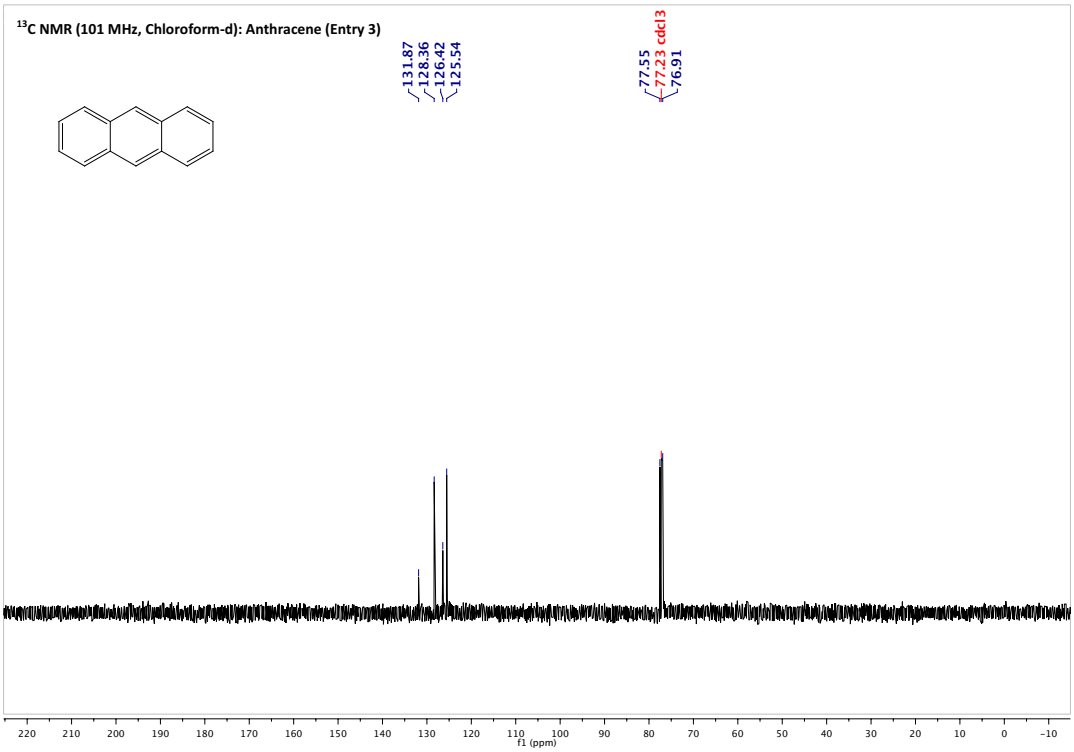

1H NMR (400 MHz, Chloroform-d): 2-Methylnaphthalene
7.85 7.84 7.84 7.83 7.82 7.80 7.80 7.79 7.78 7.77 7.65 7.51 7.51 7.50 7.50 7.49 7.48 7.48 7.48 7.47 7.46 7.46 7.45 7.45 7.44 7.44 7.44 7.43 7.43 7.42 7.42 7.41 7.41 7.37 7.36 7.36 7.35 7.34 7.34 7.31 7.26 cdcl3
2.55 2.55 2.55
1.57 1.57
CH3
B (m) 7.81
C (m) 7.46
A (s) 7.65
D (dt) 7.35
E (d) 2.55
3.18 1.00 2.27 1.06
3.29
f1 (ppm)

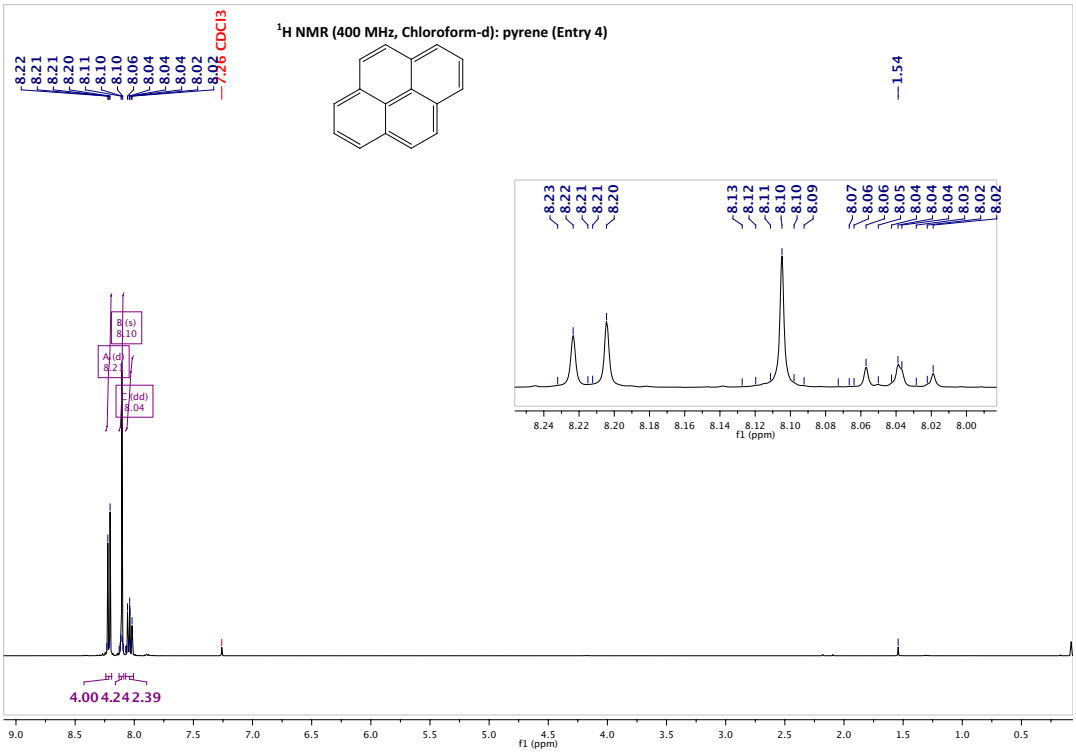

13C NMR (101 MHz, Chloroform-d): 2-Methylnaphthalene
135.63 133.84 131.87 128.31 127.87 127.79 127.42 127.02 126.05 125.14
77.55 77.23 cdcl3 76.91
21.92
CH3
f1 (ppm)

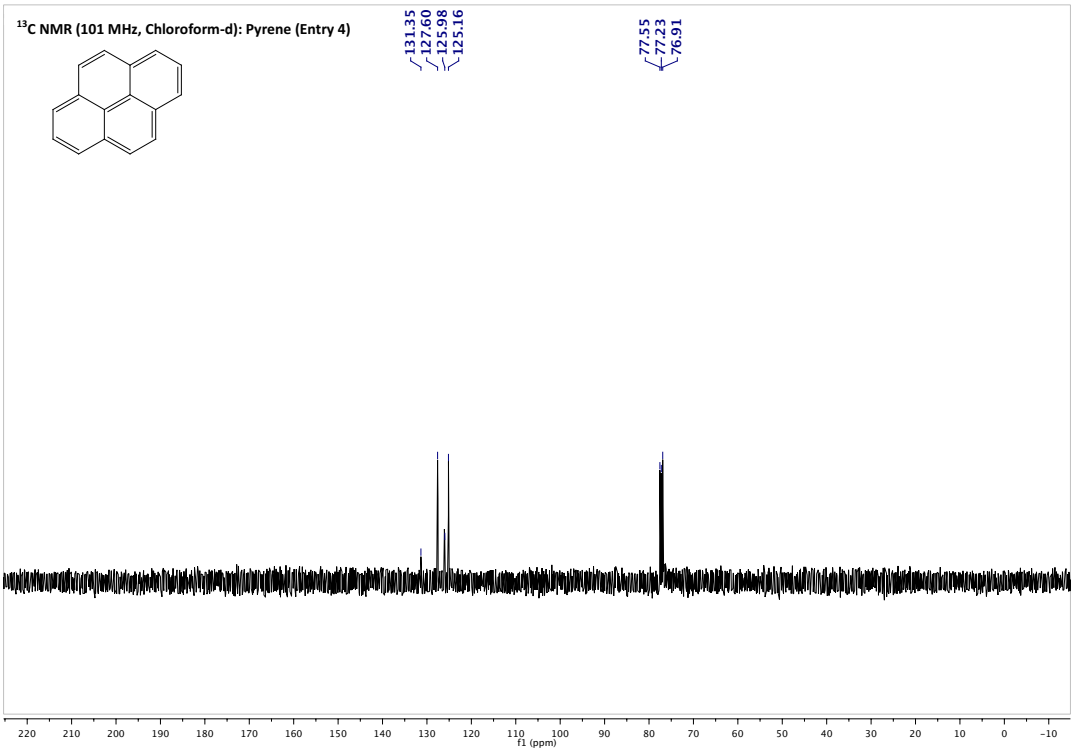

¹H NMR (400 MHz, Chloroform-d): Naphthalene (Entry 2)
7.91 7.90 7.89 7.89 7.88 7.87 7.87 7.86 7.86 7.85 7.85 7.84 7.84 7.84 7.83 7.82 7.81 7.81 7.79 7.79 7.78 7.72 7.70 7.68 7.68 7.66 7.65 7.63 7.54 7.54 7.53 7.53 7.52 7.52 7.52 7.51 7.50 7.49 7.49 7.48 7.48 7.48 7.47 7.47 7.47 7.46 7.44 7.43 7.43 7.42 7.42 7.42 7.39 7.37 7.36 7.33 7.28 7.26 cdcl3 7.24 7.24 7.23 1.56 1.56 1.56
B (m) 7.48
A (m) 7.84
2.00 1.86
13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1
f1 (ppm)

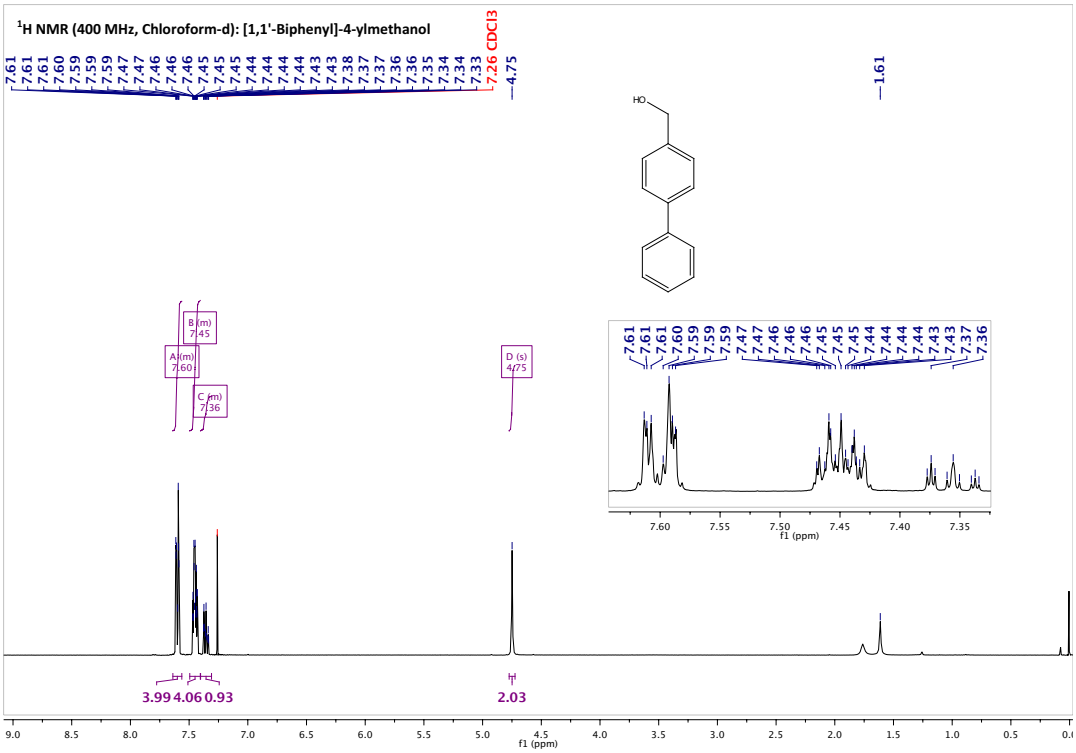

¹³C NMR (101 MHz, Chloroform-d): Naphthalene (Entry 2)
133.64 128.08 126.02
77.55 77.23 cdcl3 76.91
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

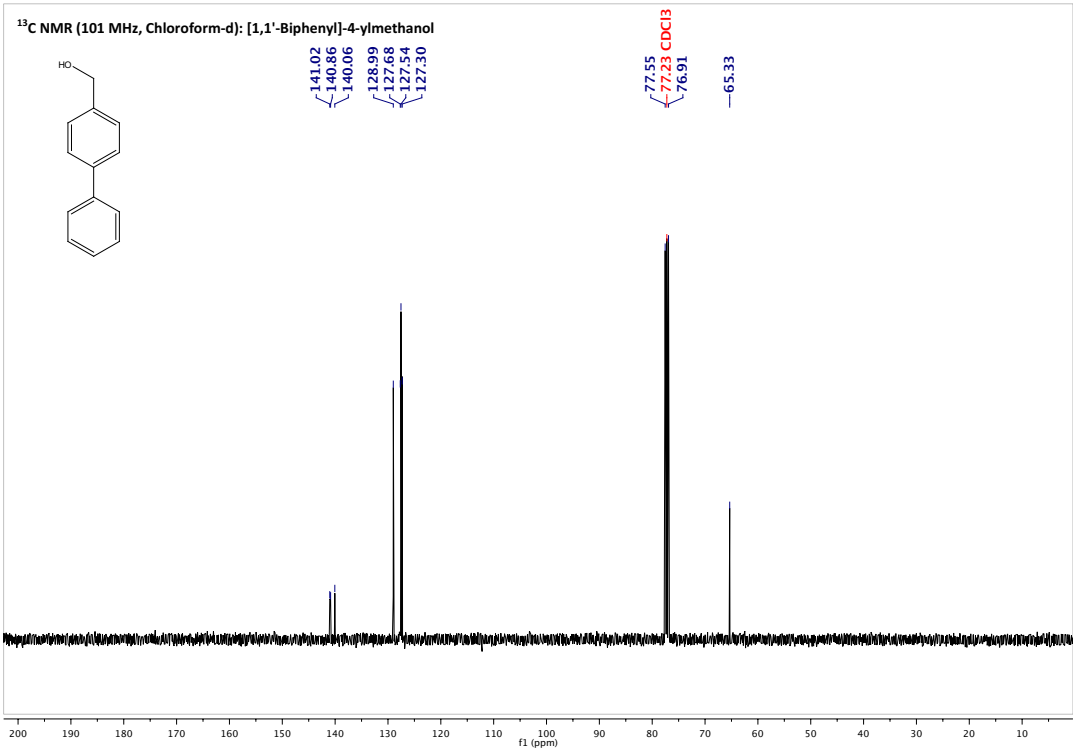

¹H NMR (400 MHz, Chloroform-d): Anthracene (Entry 3)
7.26 CDCl3
1.59
A (t) 8.44
B (m) 8.02
C (m) 7.48
1.85 3.87 4.00
f1 (ppm)

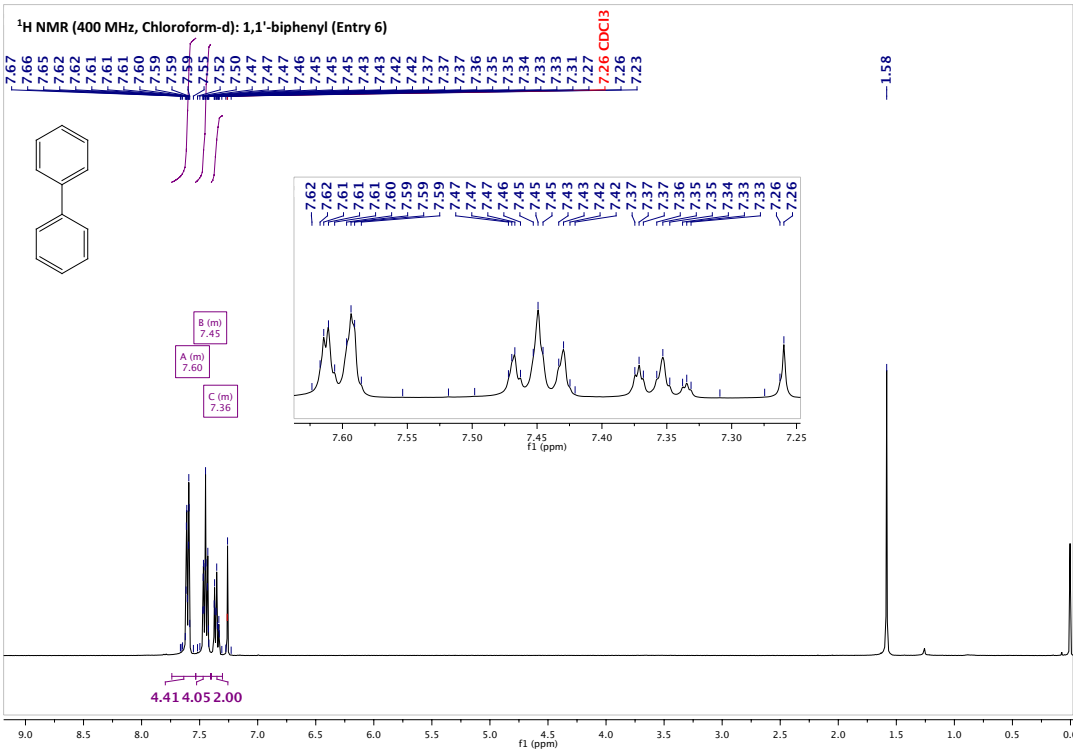

¹³C NMR (101 MHz, Chloroform-d): Anthracene (Entry 3)
131.87
128.36
126.42
125.54
77.55
77.23 cdcl3
76.91
f1 (ppm)

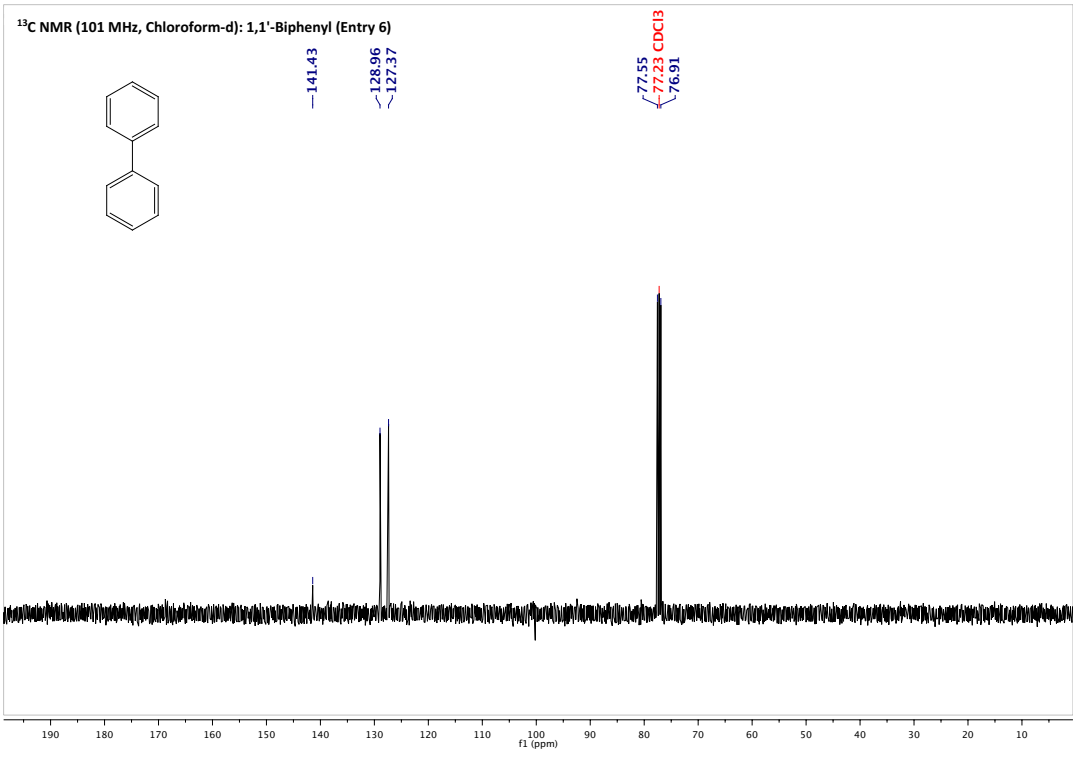

^{1}H NMR (400 MHz, Chloroform-d): pyrene (Entry 4)
8.22
8.21
8.21
8.20
8.11
8.10
8.10
8.06
8.04
8.04
8.04
8.02
8.02
7.26 CDCl3
1.54
B (s) 8.10
A (d) 8.21
C (dd) 8.04
4.00 4.24 2.39
f1 (ppm)

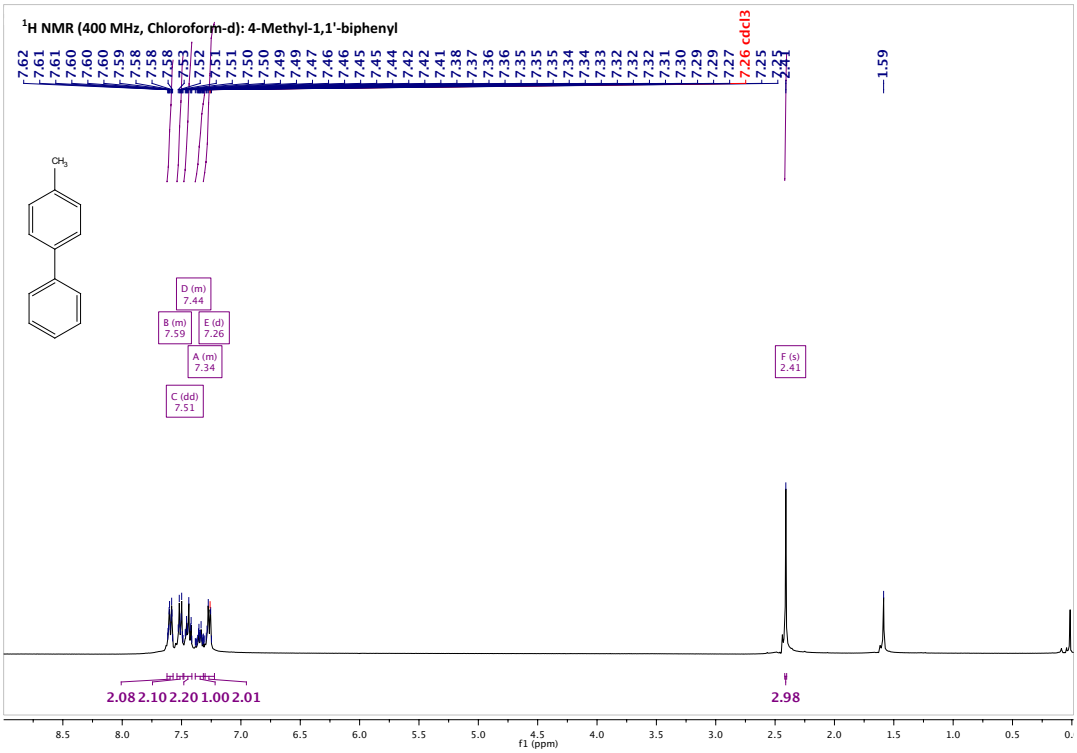

^{13}C NMR (101 MHz, Chloroform-d): Pyrene (Entry 4)
131.35
127.60
125.98
125.16
77.55
77.23
76.91
f1 (ppm)

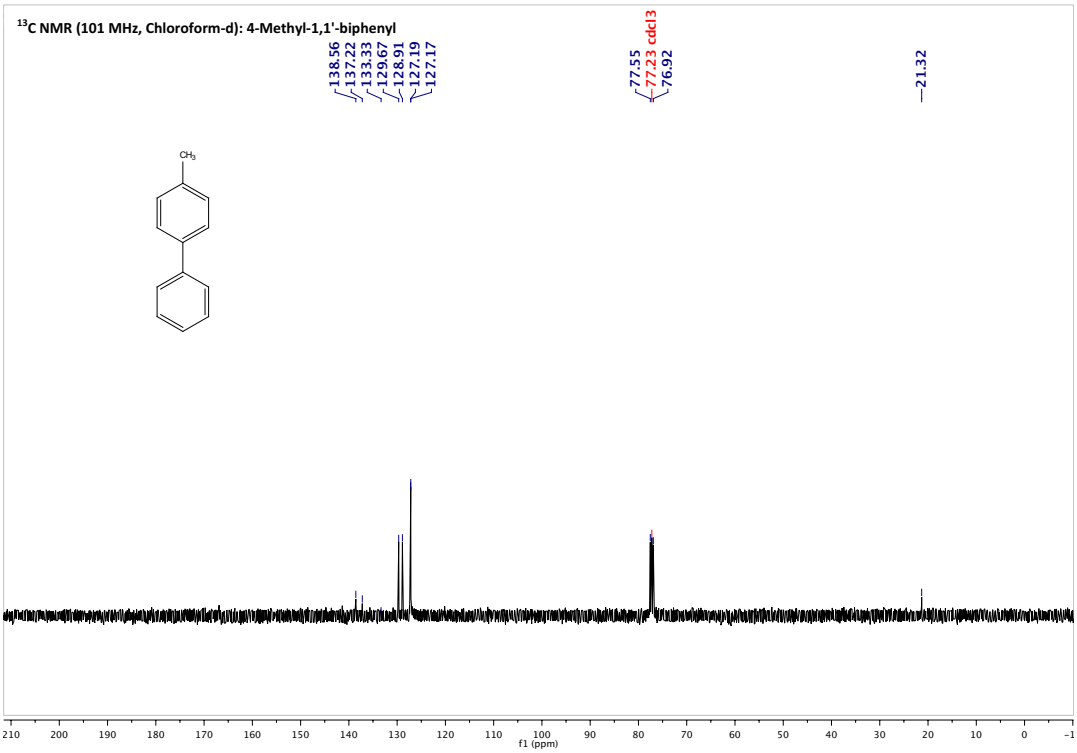

1H NMR (400 MHz, Chloroform-d): [1,1'-Biphenyl]-4-ylmethanol
7.61 7.61 7.61 7.60 7.59 7.59 7.59 7.47 7.47 7.46 7.46 7.46 7.45 7.45 7.45 7.44 7.44 7.44 7.44 7.43 7.43 7.38 7.37 7.37 7.36 7.36 7.35 7.34 7.34 7.33 7.26 CDCl3
4.75
1.61
HO
B (m) 7.45
A (m) 7.60
C (m) 7.36
D (s) 4.75
3.99 4.06 0.93
2.03
f1 (ppm)

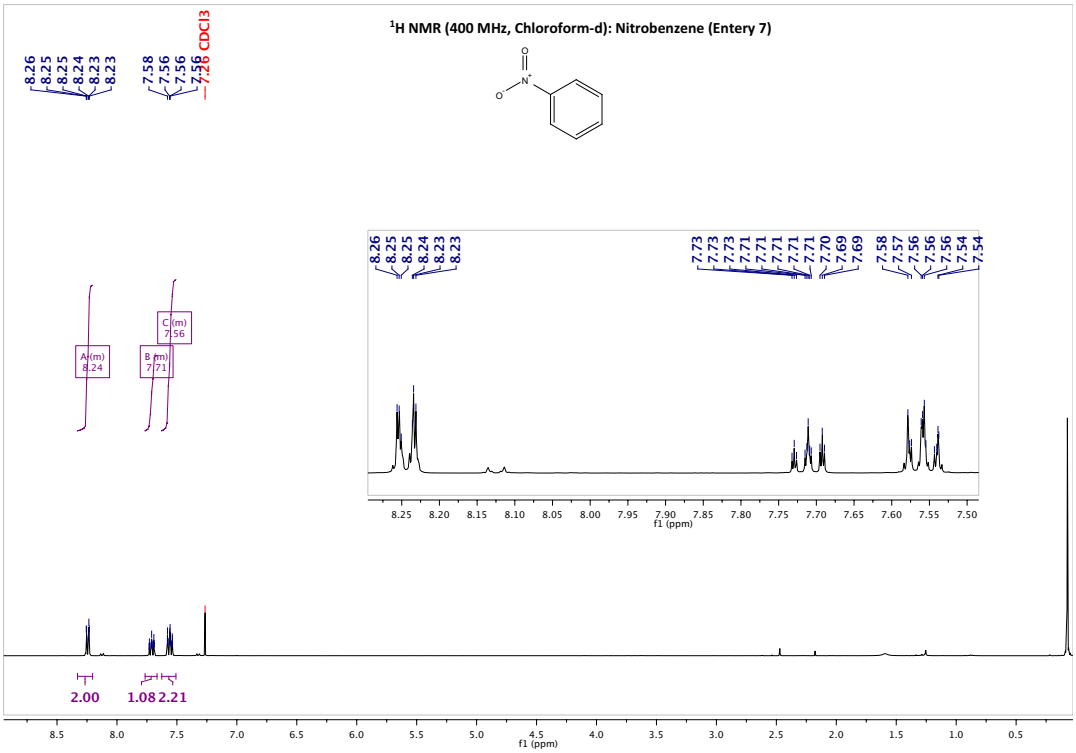

13C NMR (101 MHz, Chloroform-d): [1,1'-Biphenyl]-4-ylmethanol
HO
141.02 140.86 140.06 128.99 127.68 127.54 127.30
77.55 77.23 CDCl3 76.91
65.33
f1 (ppm)

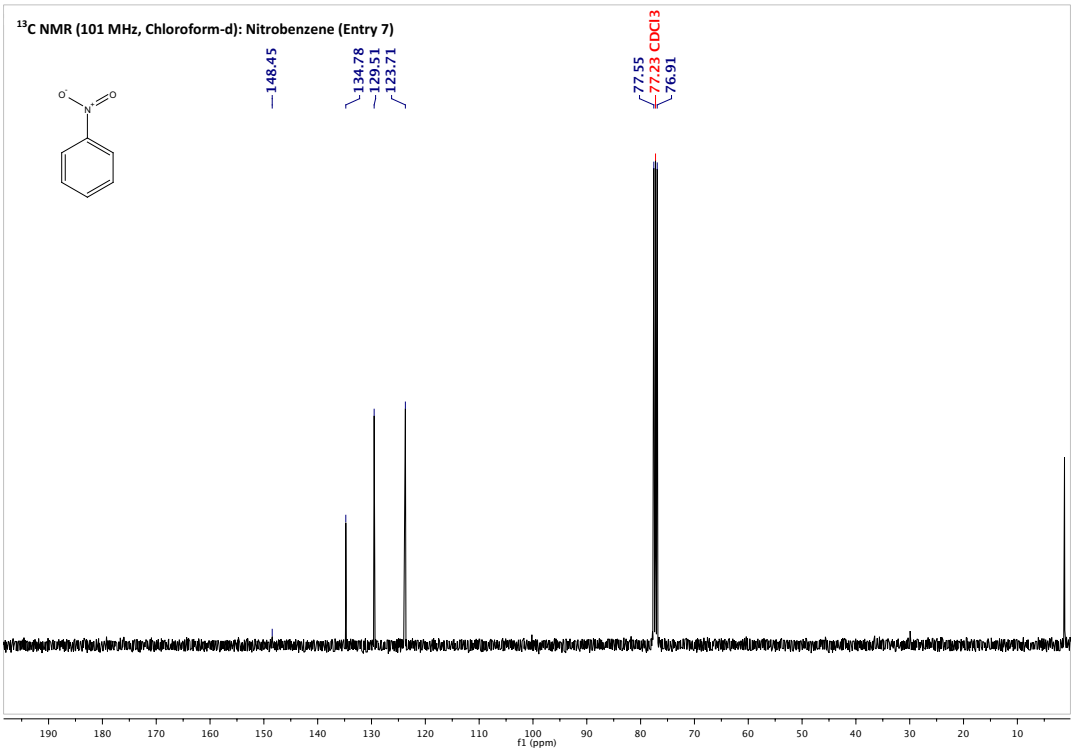

¹H NMR (400 MHz, Chloroform-d): 1,1'-biphenyl (Entry 6)
7.67 7.66 7.65 7.62 7.62 7.61 7.61 7.61 7.60 7.59 7.59 7.59 7.55 7.52 7.50 7.47 7.47 7.47 7.46 7.45 7.45 7.45 7.43 7.43 7.42 7.42 7.37 7.37 7.37 7.36 7.35 7.35 7.34 7.33 7.33 7.31 7.27 7.26 CDCl3 7.26 7.23
1.58
B (m) 7.45
A (m) 7.60
C (m) 7.36
4.41 4.05 2.00
f1 (ppm)

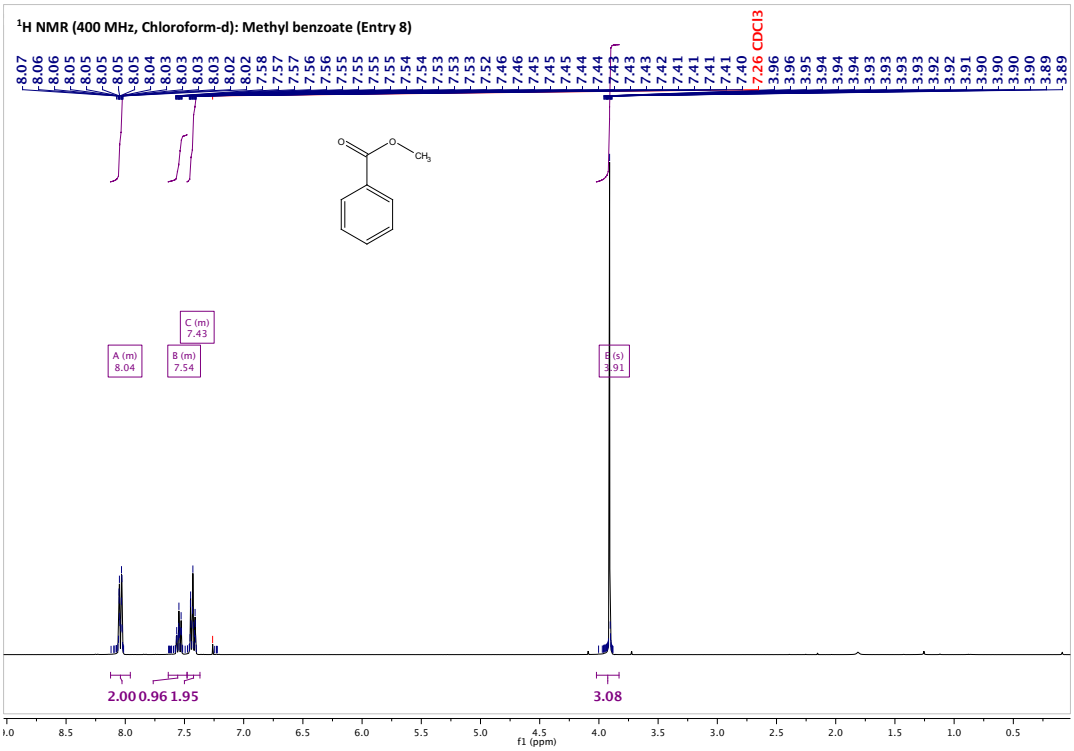

¹³C NMR (101 MHz, Chloroform-d): 1,1'-Biphenyl (Entry 6)
141.43
128.96
127.37
77.55
77.23 CDCl3
76.91
f1 (ppm)

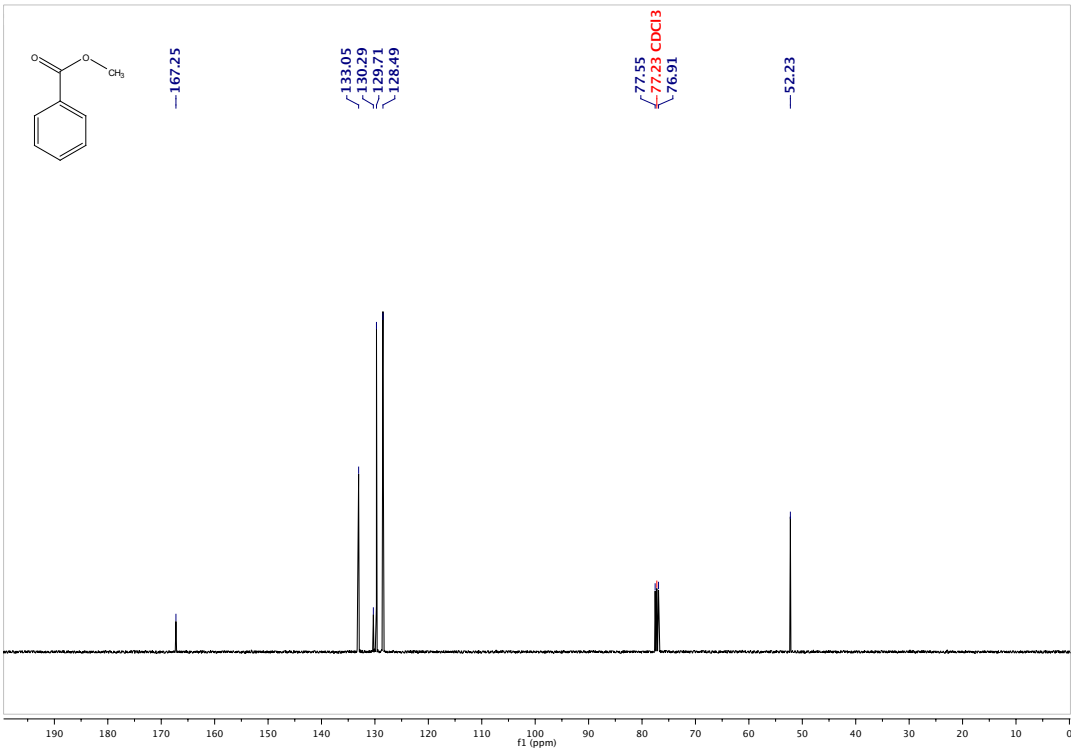

1H NMR (400 MHz, Chloroform-d): 4-Methyl-1,1'-biphenyl
7.62 7.61 7.61 7.60 7.60 7.60 7.59 7.58 7.58 7.58 7.53 7.52 7.51 7.51 7.50 7.50 7.49 7.49 7.47 7.46 7.46 7.45 7.45 7.44 7.42 7.42 7.41 7.38 7.37 7.36 7.36 7.35 7.35 7.35 7.34 7.34 7.33 7.32 7.32 7.32 7.31 7.30 7.29 7.29 7.27 7.26 cdcl3 7.25 7.25 2.41
1.59
CH3
D (m) 7.44
B (m) 7.59
E (d) 7.26
A (m) 7.34
C (dd) 7.51
F (s) 2.41
2.08 2.10 2.20 1.00 2.01
2.98
f1 (ppm)

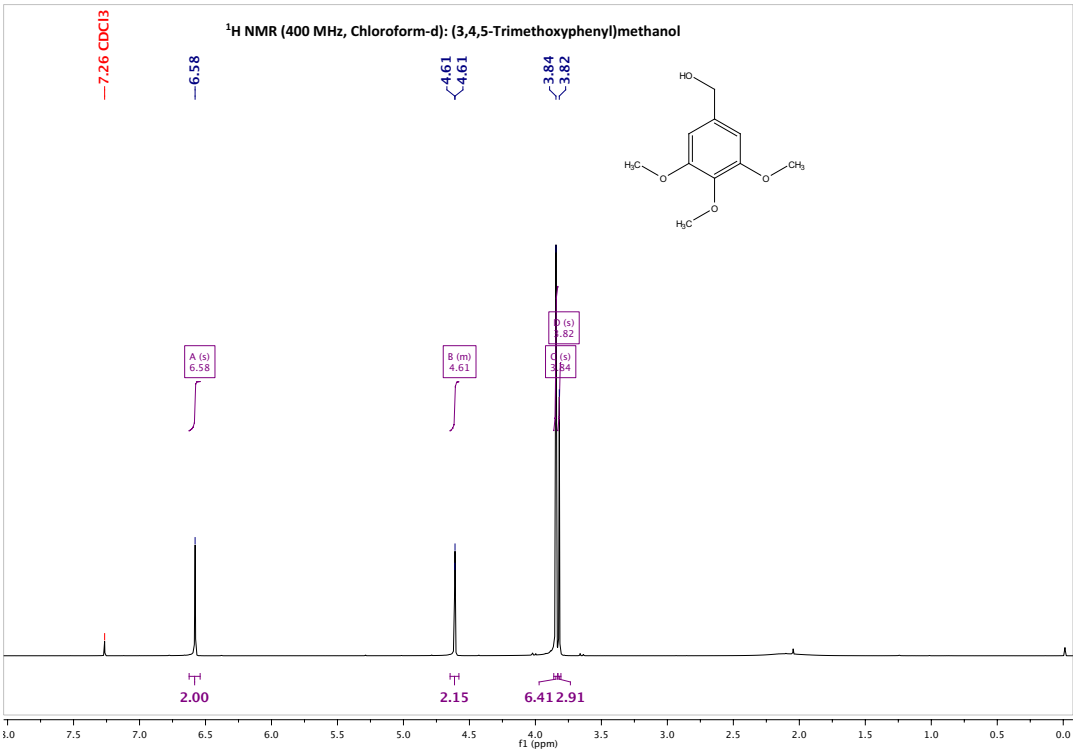

13C NMR (101 MHz, Chloroform-d): 4-Methyl-1,1'-biphenyl
138.56 137.22 133.33 129.67 128.91 127.19 127.17
77.55 77.23 cdcl3 76.92
21.32
CH3
f1 (ppm)

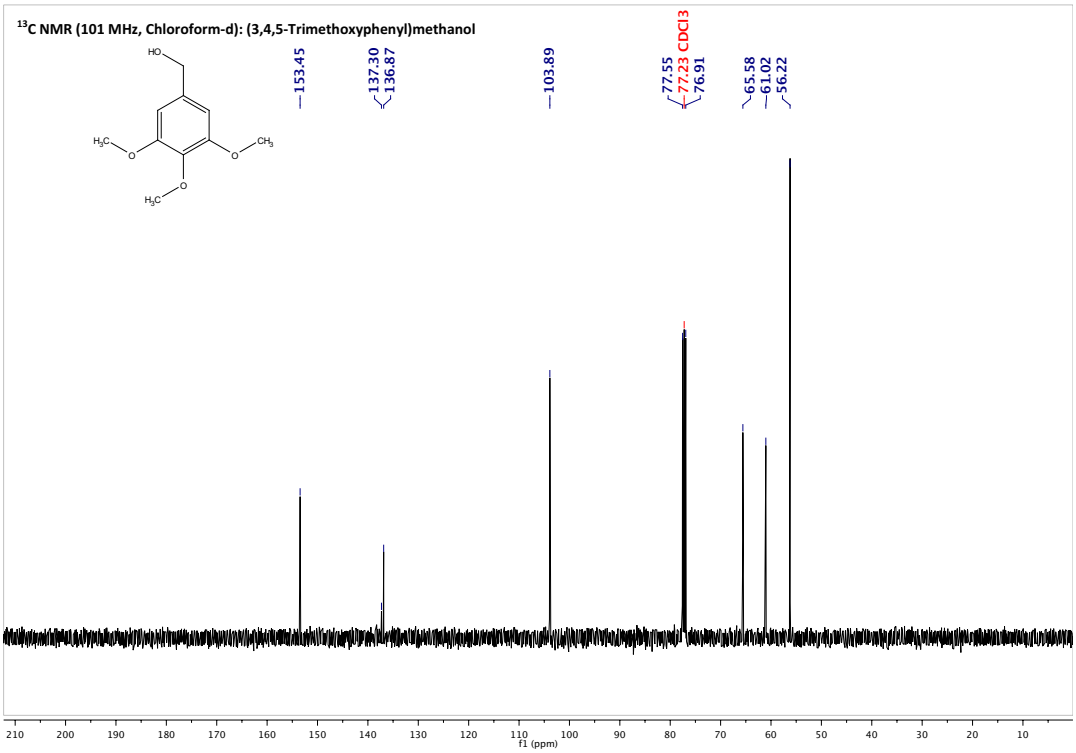

^{1}H NMR (400 MHz, Chloroform-d): Nitrobenzene (Entery 7)
8.26
8.25
8.25
8.24
8.23
8.23
7.58
7.56
7.56
7.56
7.26 CDCl3
A(m) 8.24
B(m) 7.71
C(m) 7.56
2.00
1.08
2.21
f1 (ppm)

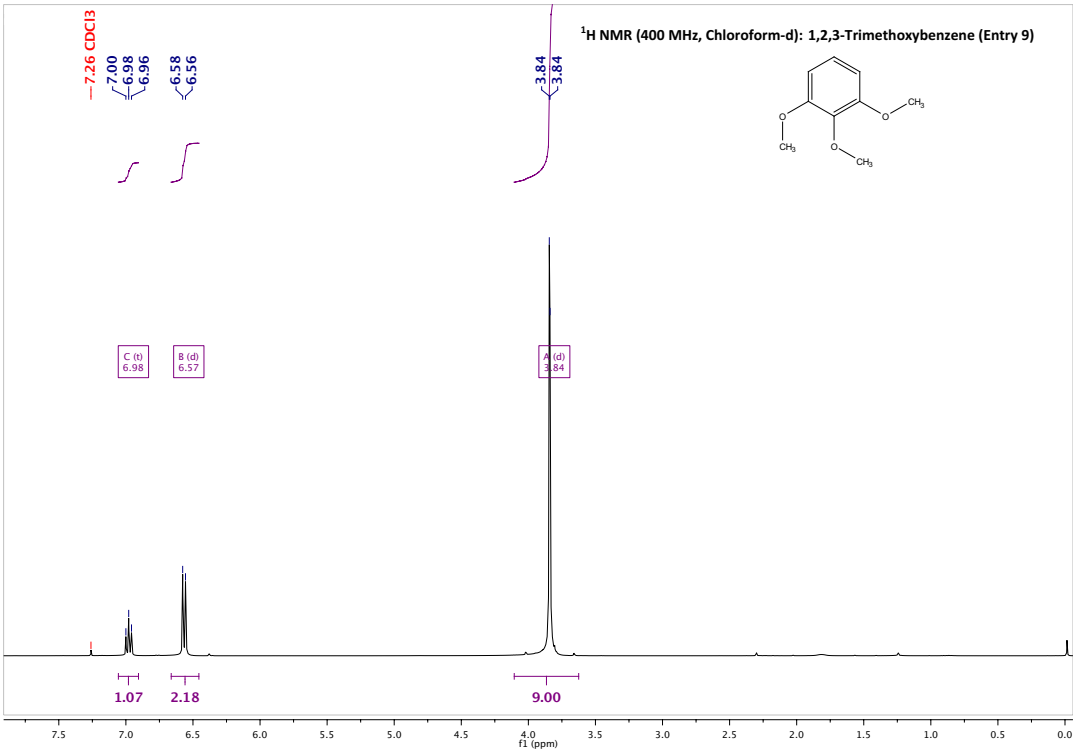

^{13}C NMR (101 MHz, Chloroform-d): Nitrobenzene (Entry 7)
148.45
134.78
129.51
123.71
77.55
77.23 CDCl3
76.91
f1 (ppm)

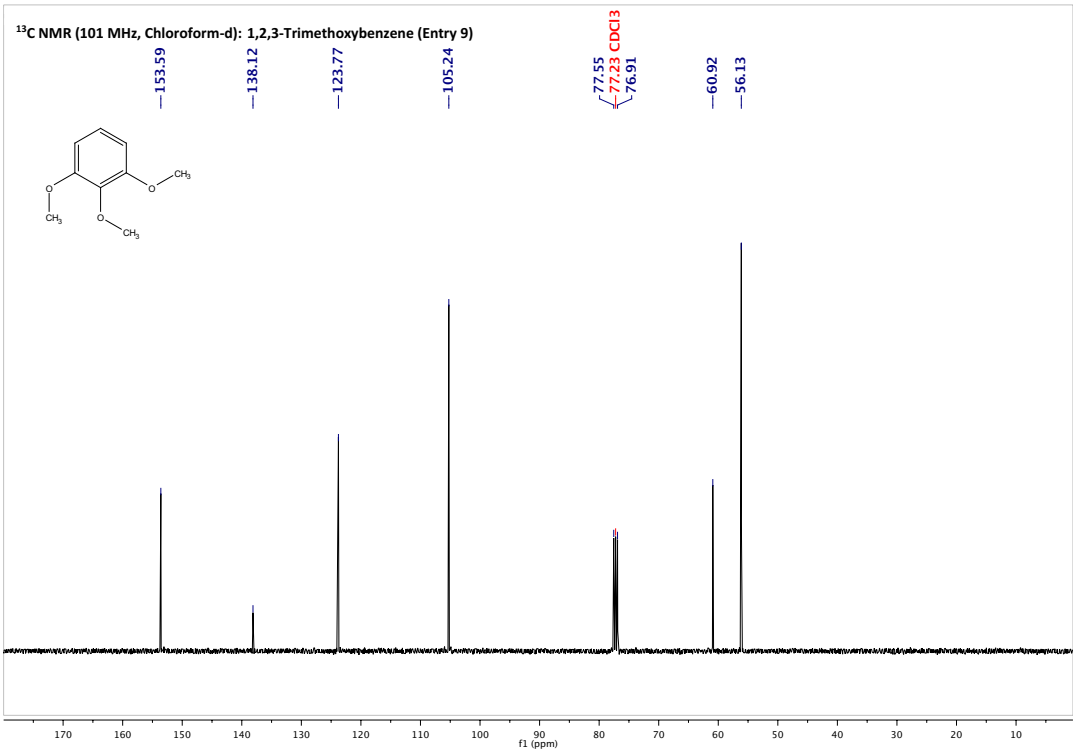

¹H NMR (400 MHz, Chloroform-d): Methyl benzoate (Entry 8)
7.26 CDCl3
A (m) 8.04
B (m) 7.54
C (m) 7.43
D (s) 3.91
2.00 0.96 1.95
3.08
f1 (ppm)

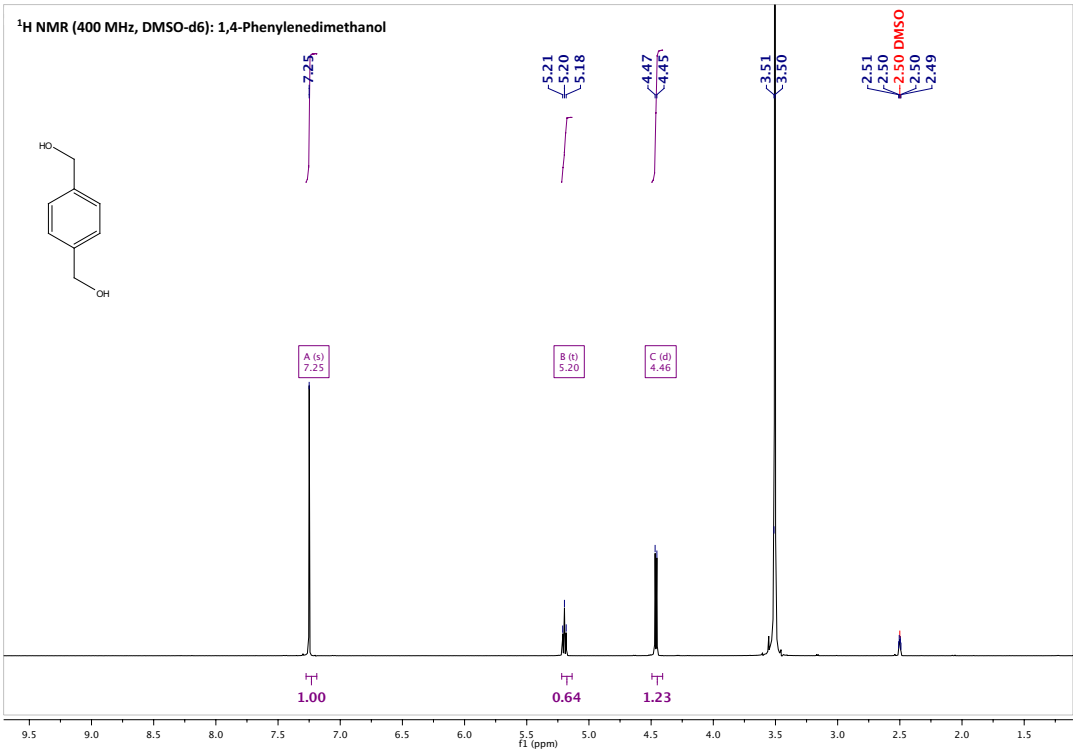

167.25
133.05
130.29
129.71
128.49
77.55
77.23 CDCl3
76.91
52.23
f1 (ppm)

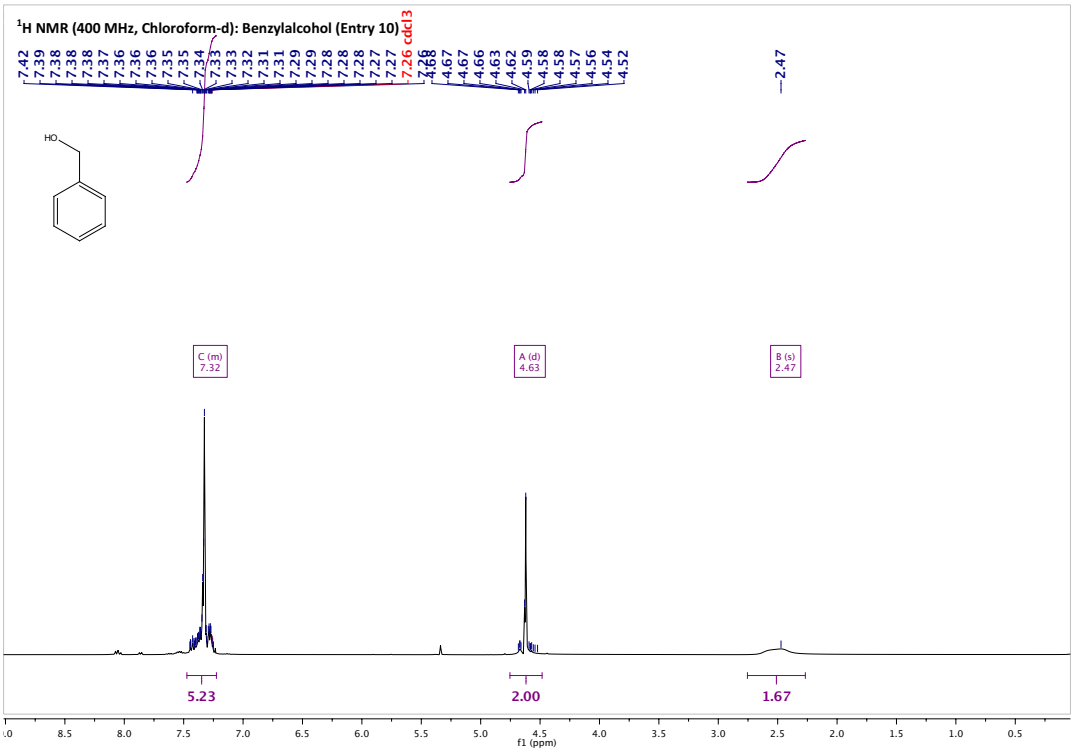

^{1}H NMR (400 MHz, Chloroform-d): (3,4,5-Trimethoxyphenyl)methanol
7.26 CDCl3
6.58
4.61
4.61
3.84
3.82
HO
H3C
O
CH3
O
H3C
O
A (s)
6.58
B (m)
4.61
D (s)
3.82
C (s)
3.84
2.00
2.15
6.41
2.91
f1 (ppm)

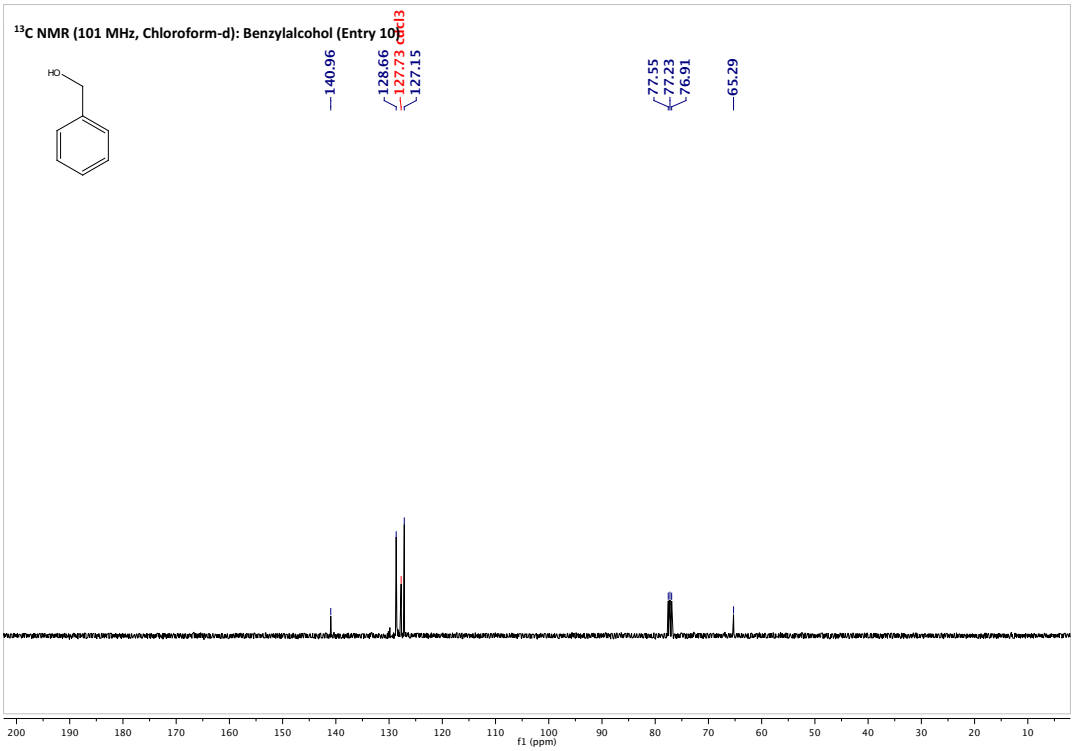

^{13}C NMR (101 MHz, Chloroform-d): (3,4,5-Trimethoxyphenyl)methanol
HO
H3C
O
CH3
O
H3C
O
153.45
137.30
136.87
103.89
77.55
77.23 CDCl3
76.91
65.58
61.02
56.22
f1 (ppm)

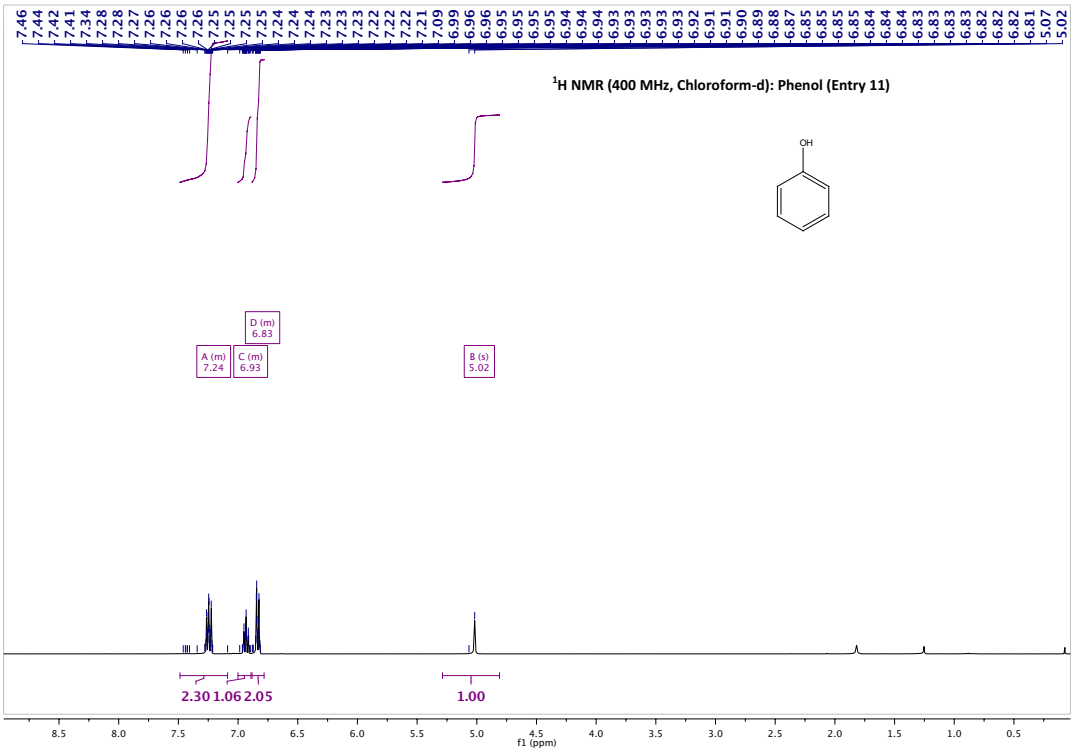

^{1}H NMR (400 MHz, Chloroform-d): 1,2,3-Trimethoxybenzene (Entry 9)
7.26 CDCl3
7.00
6.98
6.96
6.58
6.56
3.84
3.84
C (t) 6.98
B (d) 6.57
A (d) 3.84
1.07
2.18
9.00
f1 (ppm)

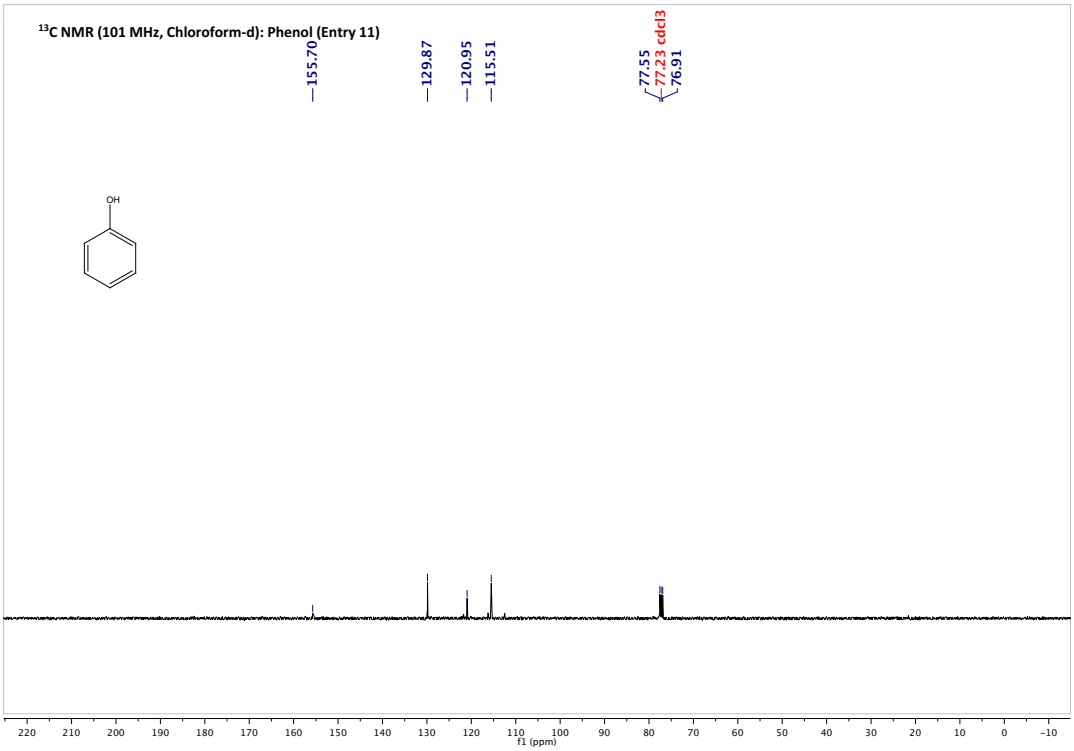

^{13}C NMR (101 MHz, Chloroform-d): 1,2,3-Trimethoxybenzene (Entry 9)
153.59
138.12
123.77
105.24
77.55
77.23 CDCl3
76.91
60.92
56.13
f1 (ppm)


¹H NMR (400 MHz, DMSO-d6): 1,4-Phenylenedimethanol
7.25
5.21
5.20
5.18
4.47
4.45
3.51
3.50
2.51
2.50
2.50 DMSO
2.50
2.49
HO
OH
A (s)
7.25
B (t)
5.20
C (d)
4.46
1.00
0.64
1.23
f1 (ppm)

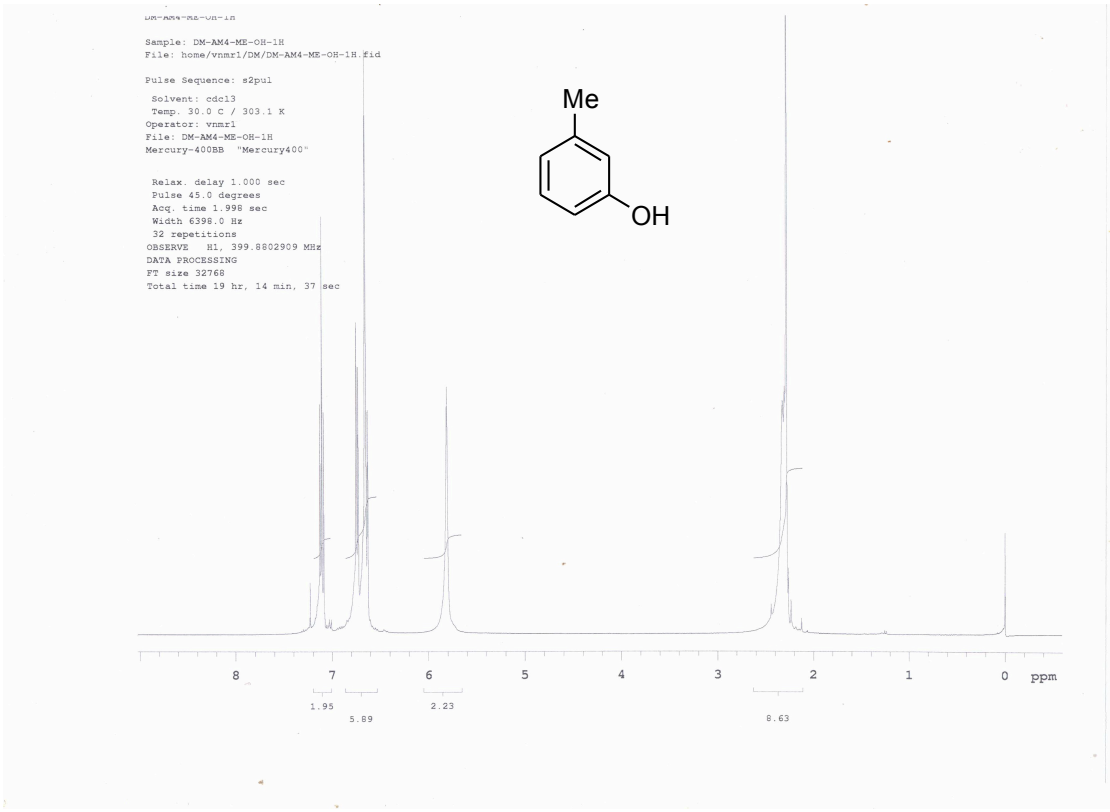

¹H NMR (400 MHz, Chloroform-d): Benzylalcohol (Entry 10)
7.42
7.39
7.38
7.38
7.38
7.37
7.36
7.36
7.36
7.35
7.35
7.34
7.33
7.33
7.32
7.31
7.31
7.29
7.29
7.28
7.28
7.28
7.27
7.27
7.26 cdcl3
4.68
4.67
4.67
4.66
4.63
4.62
4.59
4.58
4.58
4.57
4.56
4.54
4.52
2.47
HO
C (m)
7.32
A (d)
4.63
B (s)
2.47
5.23
2.00
1.67
f1 (ppm)


13C NMR (101 MHz, Chloroform-d): Benzylalcohol (Entry 10)
HO
140.96
128.66
127.73
127.15
CDCl3
77.55
77.23
76.91
65.29
f1 (ppm)

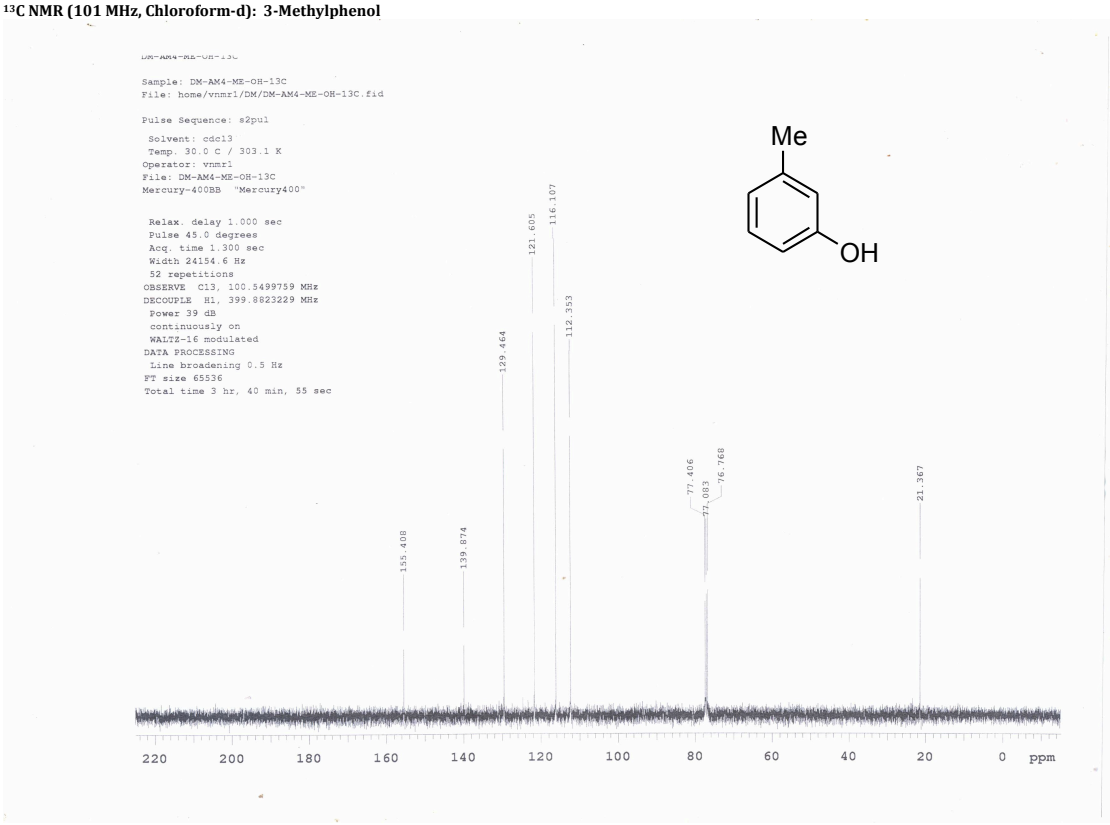

1H NMR (400 MHz, Chloroform-d): Phenol (Entry 11)
OH
D (m) 6.83
A (m) 7.24
C (m) 6.93
B (s) 5.02
2.30 1.06 2.05
1.00
f1 (ppm)

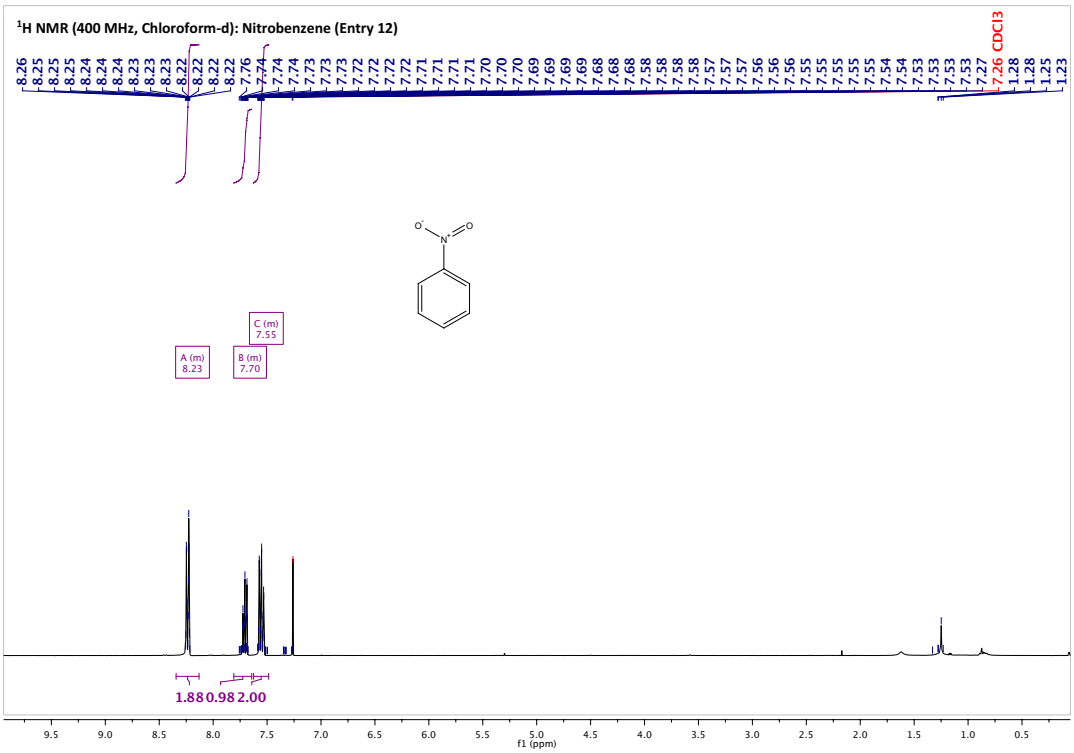


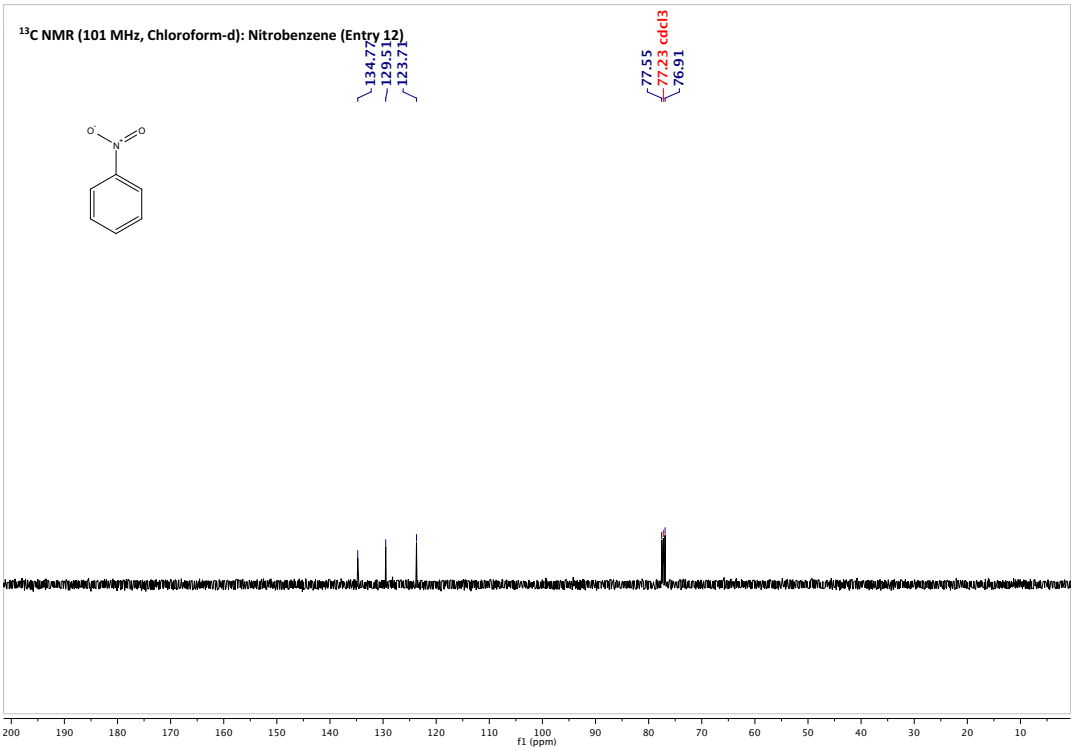
^{1}H NMR (400 MHz, Chloroform-d): 3-Methylphenol

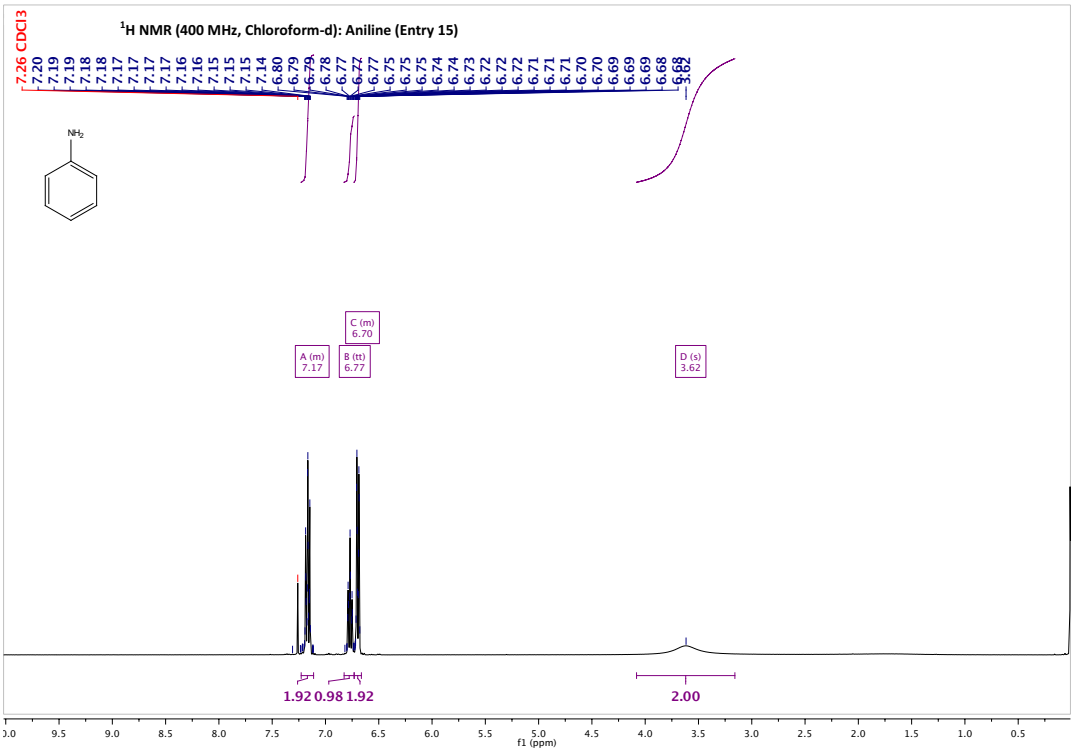


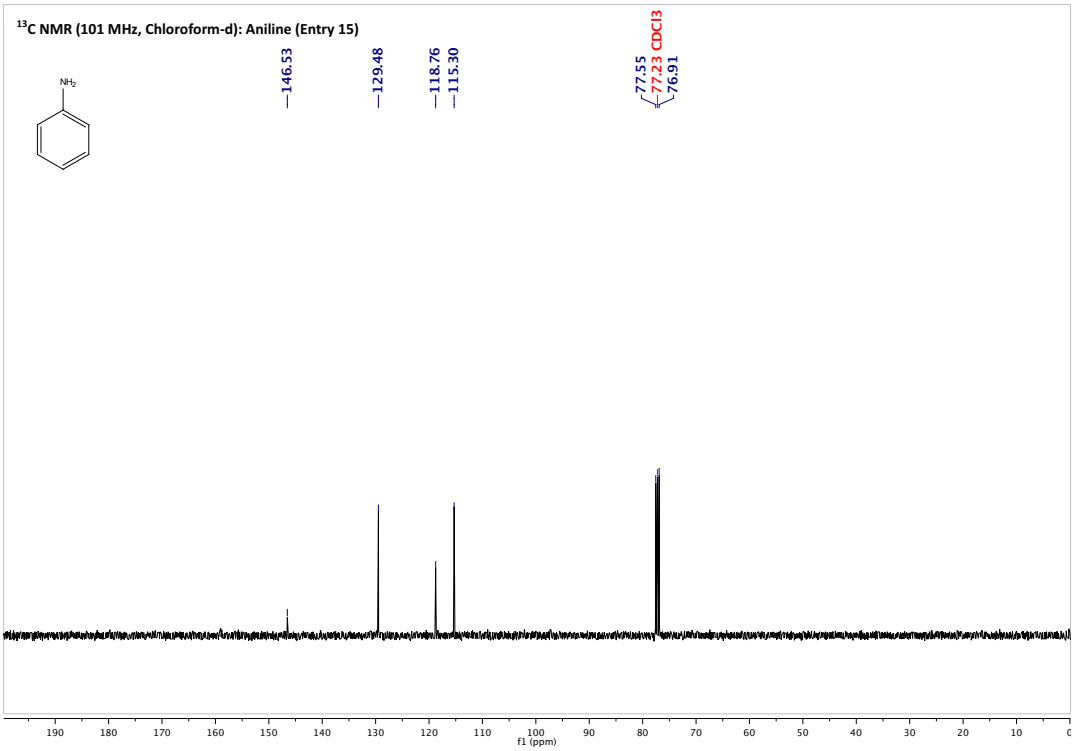
^{13}C NMR (101 MHz, Chloroform-d): 3-Methylphenol

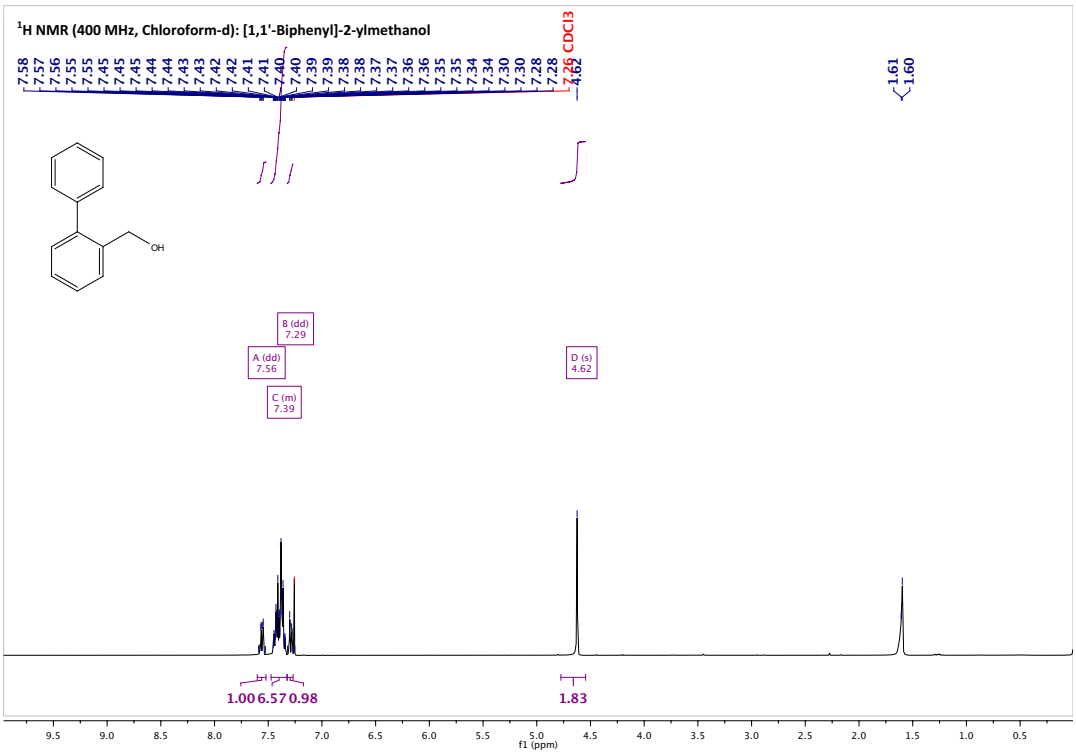


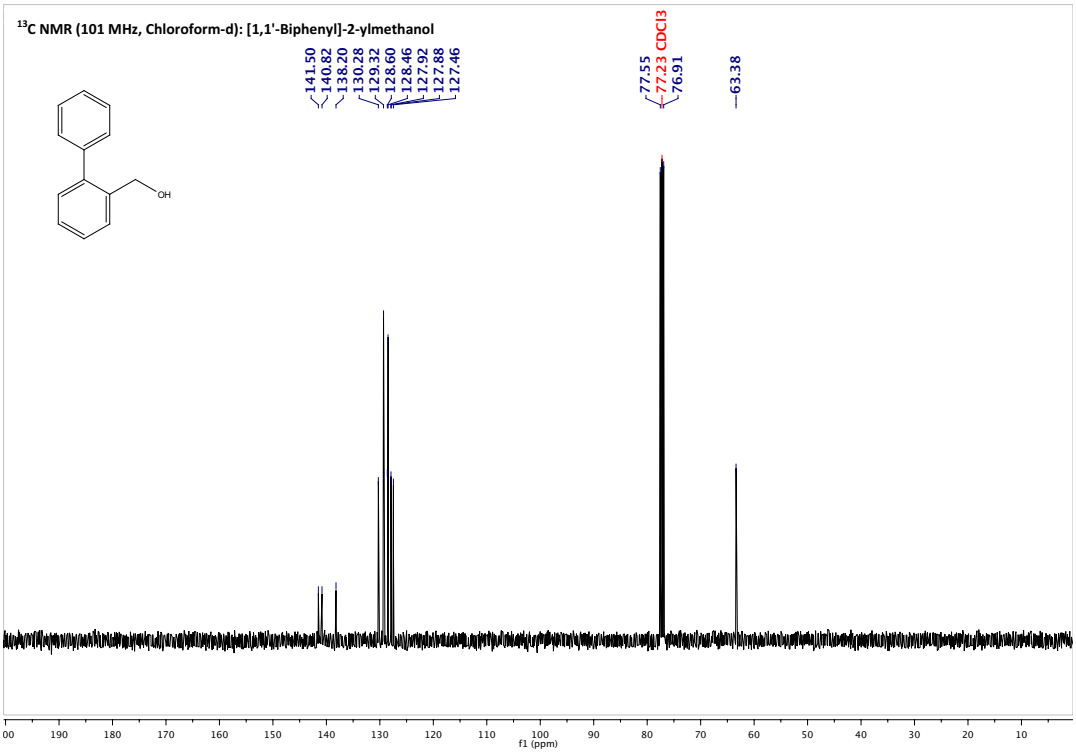


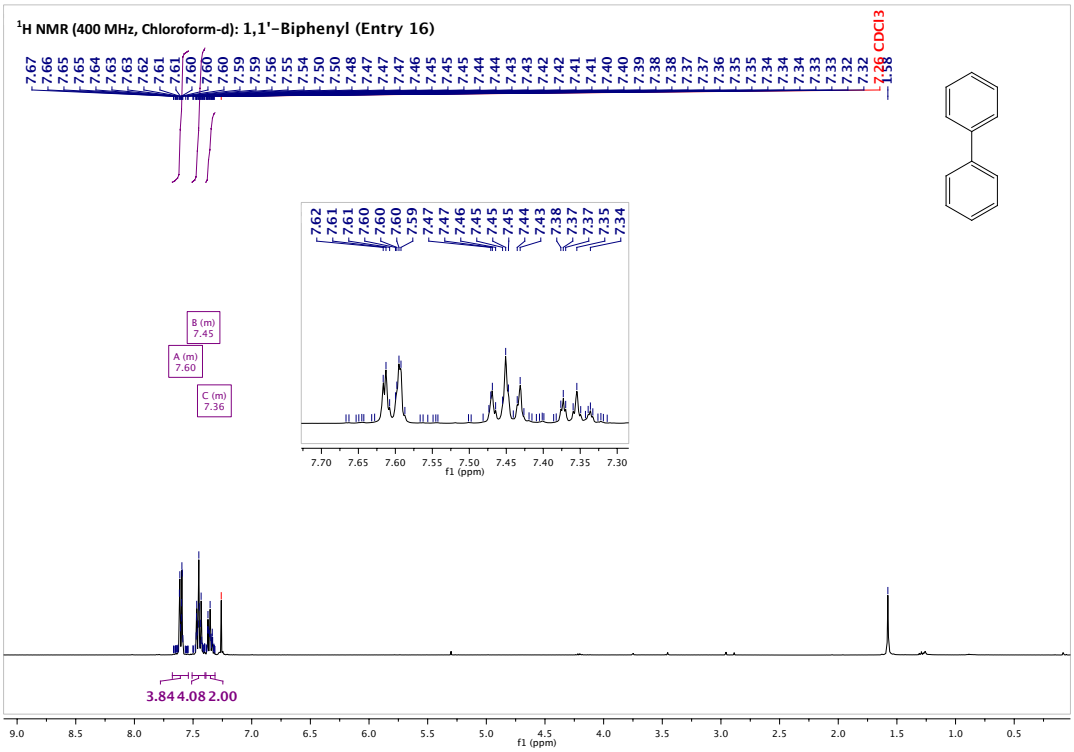

^{13}C NMR (101 MHz, Chloroform-d): Nitrobenzene (Entry 12)
134.77
129.51
123.71
77.55
77.23 cdcl3
76.91
f1 (ppm)

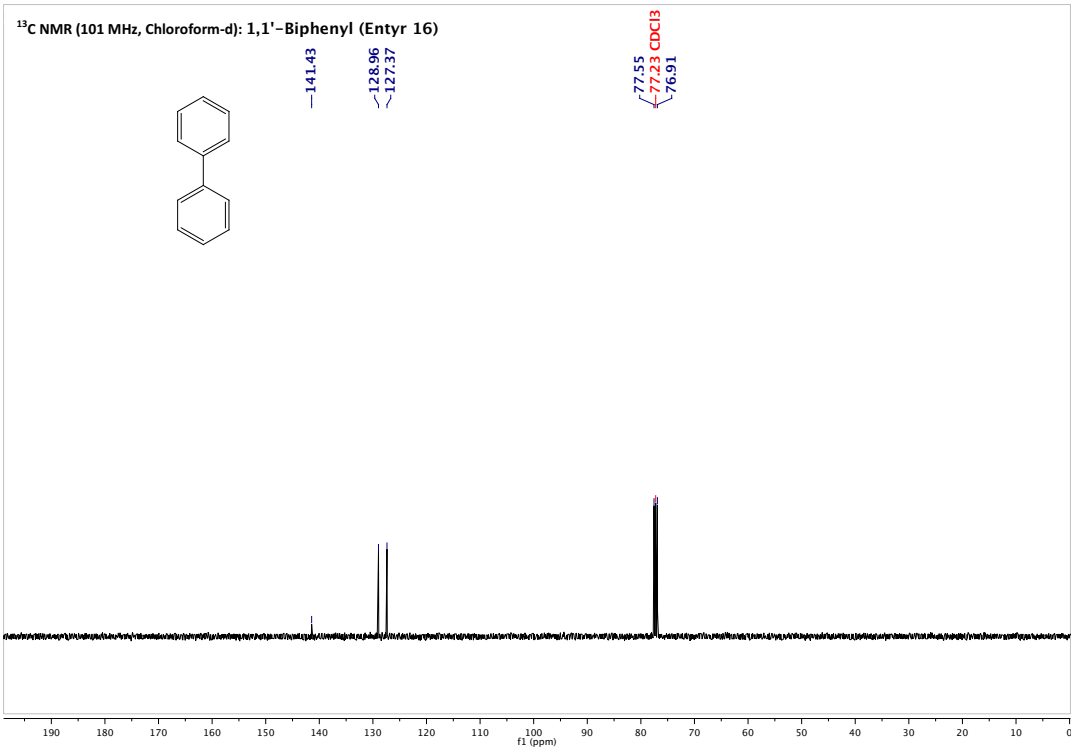

^{1}H NMR (400 MHz, Chloroform-d): Aniline (Entry 15)
7.26 CDCl3
A (m) 7.17
B (tt) 6.77
C (m) 6.70
D (s) 3.62
1.92 0.98 1.92
2.00
f1 (ppm)

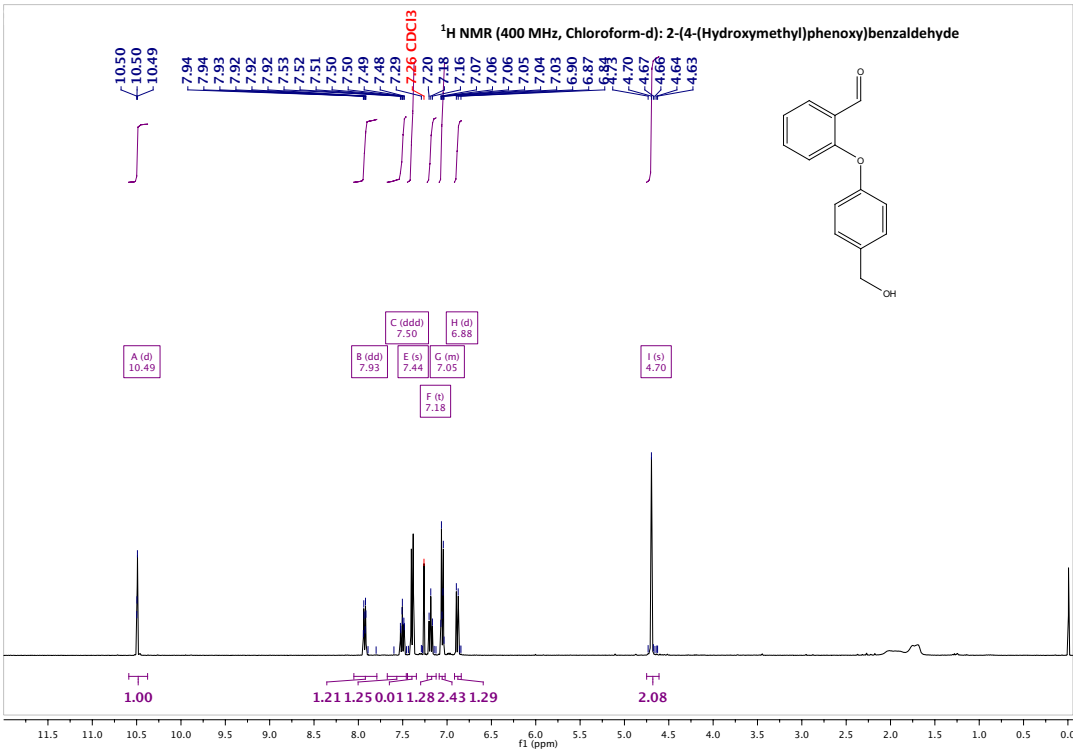

13C NMR (101 MHz, Chloroform-d): Aniline (Entry 15)
NH2
146.53
129.48
118.76
115.30
77.55
77.23 CDCl3
76.91
f1 (ppm)

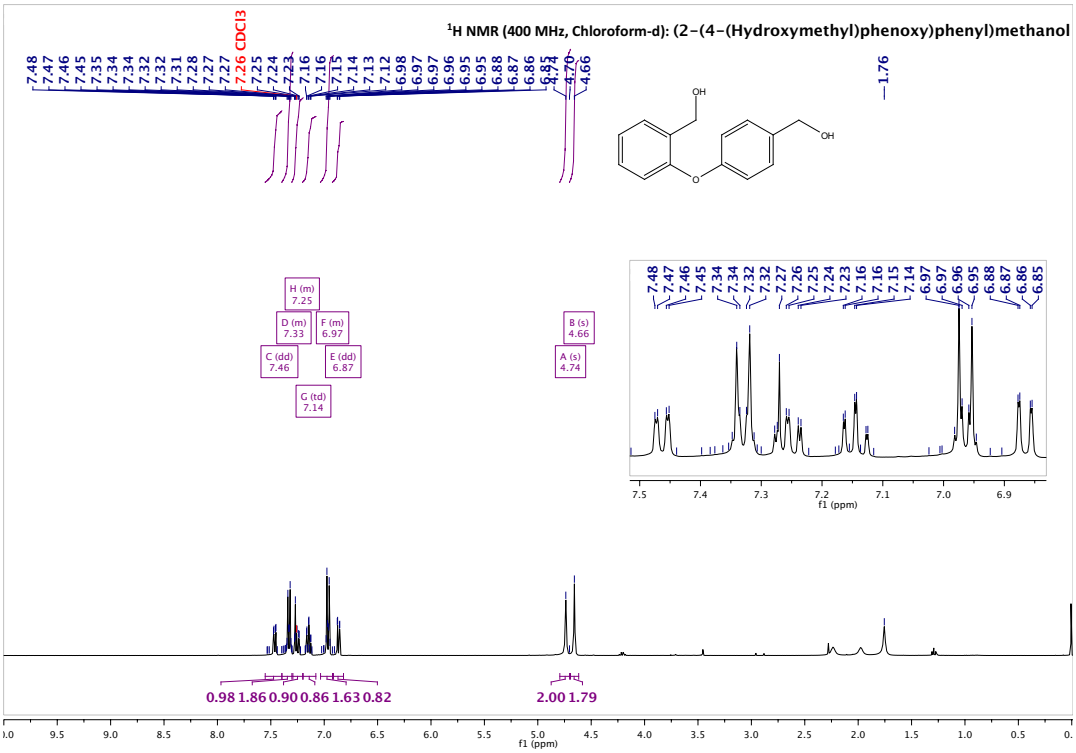

1H NMR (400 MHz, Chloroform-d): [1,1'-Biphenyl]-2-ylmethanol
7.26 CDCl3
4.62
1.61
1.60
OH
B (dd) 7.29
A (dd) 7.56
C (m) 7.39
D (s) 4.62
1.00 6.57 0.98
1.83
f1 (ppm)

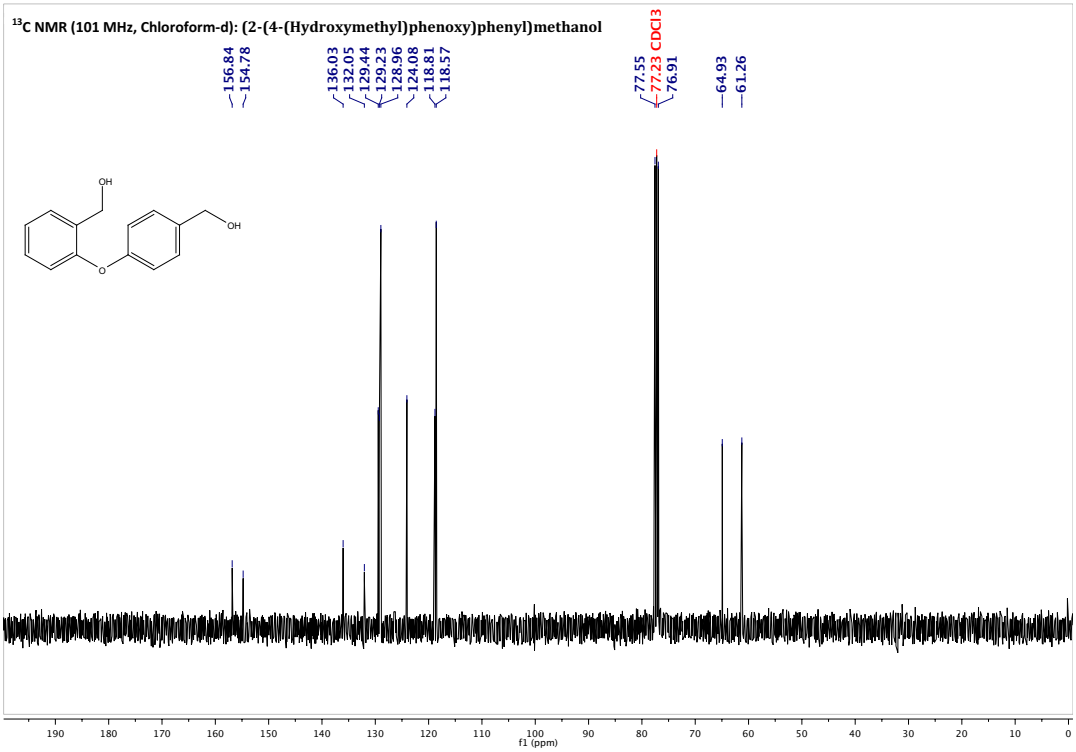

13C NMR (101 MHz, Chloroform-d): [1,1'-Biphenyl]-2-ylmethanol
141.50
140.82
138.20
130.28
129.32
128.60
128.46
127.92
127.88
127.46
77.55
77.23 CDCl3
76.91
63.38
OH
f1 (ppm)

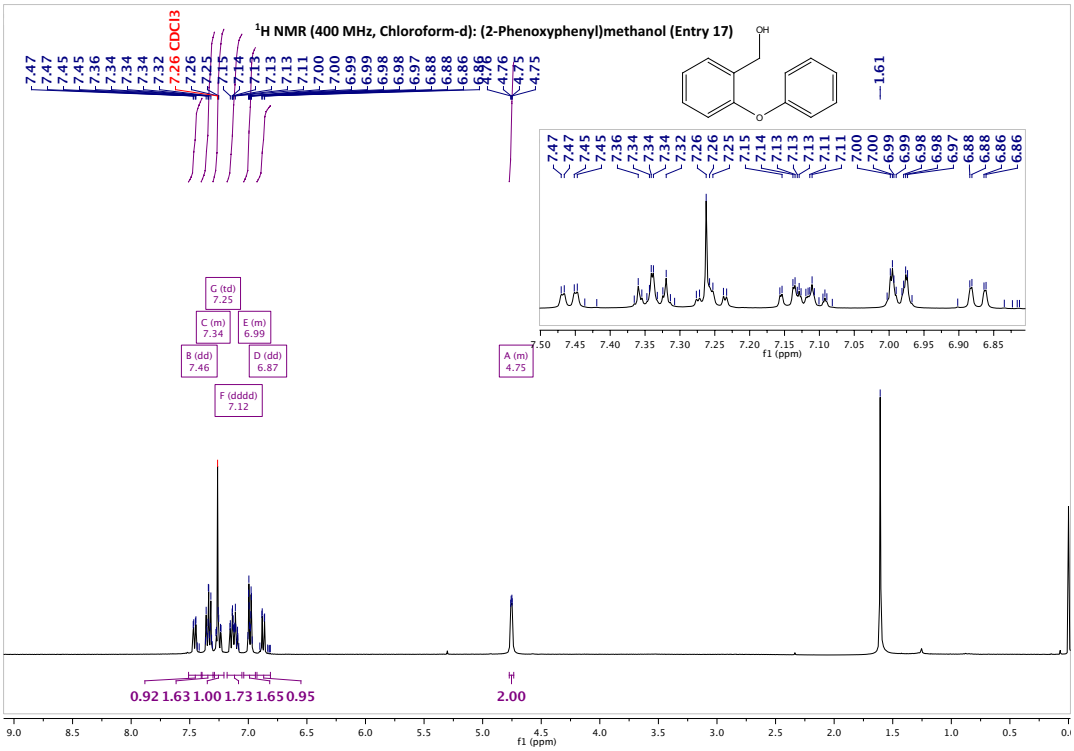

1H NMR (400 MHz, Chloroform-d): 1,1'-Biphenyl (Entry 16)
7.26 CDCl3
1.88
B (m) 7.45
A (m) 7.60
C (m) 7.36
3.84 4.08 2.00
f1 (ppm)

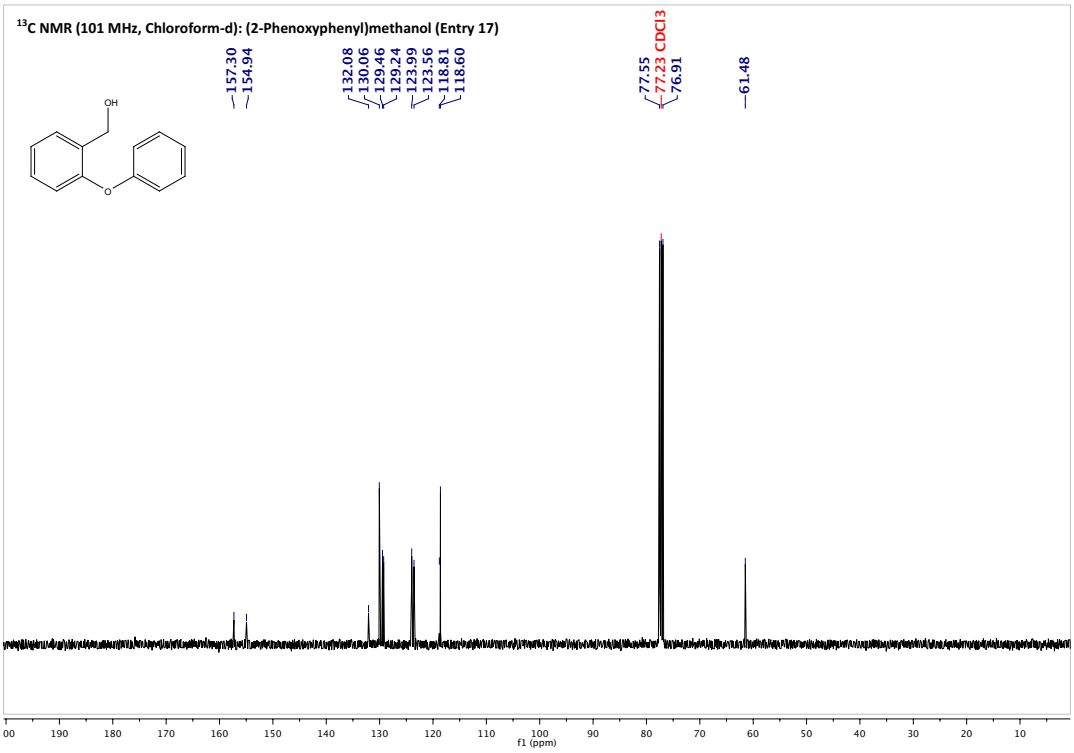

13C NMR (101 MHz, Chloroform-d): 1,1'-Biphenyl (Entyr 16)
141.43
128.96
127.37
77.55
77.23 CDCl3
76.91
f1 (ppm)


1H NMR (400 MHz, Chloroform-d): 2-(4-(Hydroxymethyl)phenoxy)benzaldehyde
10.50
10.50
10.49
7.94
7.94
7.93
7.92
7.92
7.92
7.53
7.52
7.51
7.50
7.50
7.49
7.48
7.29
7.26 CDCl3
7.20
7.18
7.16
7.07
7.06
7.06
7.05
7.04
7.03
6.90
6.87
6.84
6.83
4.70
4.67
4.66
4.64
4.63
OH
A (d) 10.49
B (dd) 7.93
C (ddd) 7.50
E (s) 7.44
F (t) 7.18
G (m) 7.05
H (d) 6.88
I (s) 4.70
1.00
1.21 1.25 0.01 1.28 2.43 1.29
2.08
f1 (ppm)

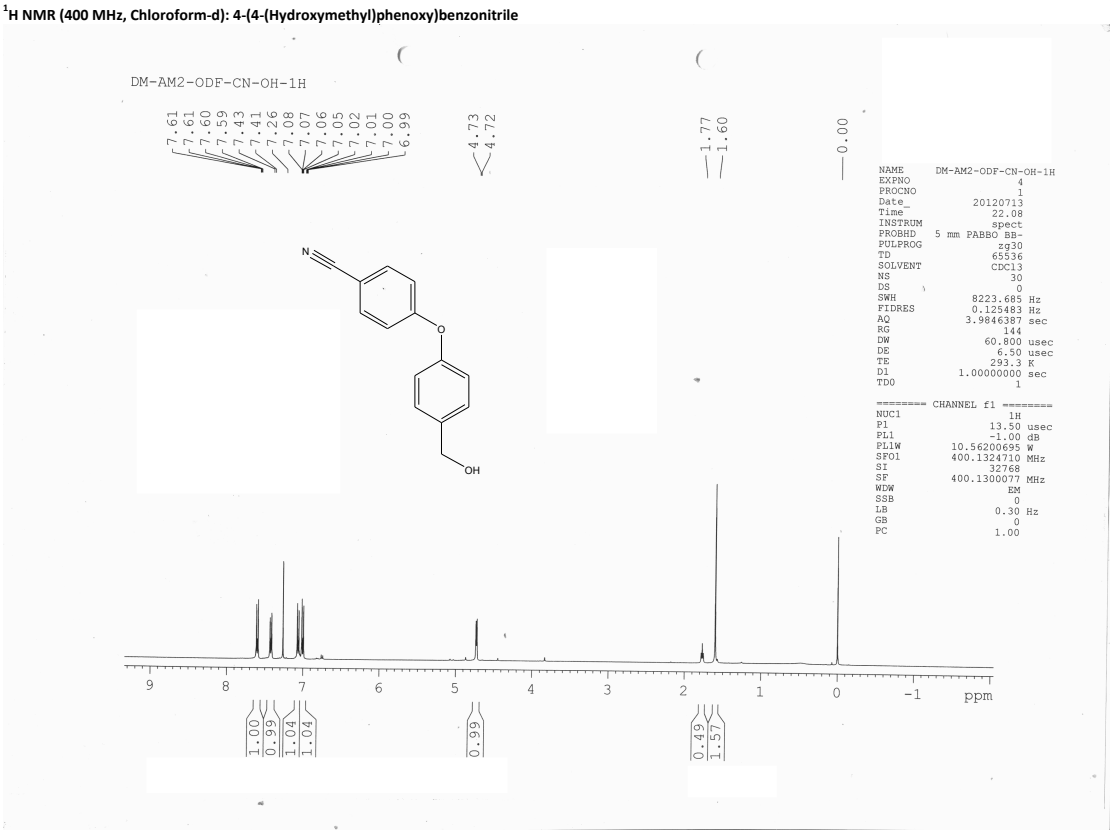

¹H NMR (400 MHz, Chloroform-d): (2-(4-(Hydroxymethyl)phenoxy)phenyl)methanol
7.48 7.47 7.46 7.45 7.35 7.34 7.34 7.32 7.31 7.28 7.27 7.27 7.26 CDCl3 7.25 7.24 7.23 7.16 7.16 7.15 7.14 7.13 7.12 6.98 6.97 6.97 6.96 6.95 6.88 6.87 6.86 4.76 4.66
1.76
OH
OH
O
H (m) 7.25
D (m) 7.33
F (m) 6.97
C (dd) 7.46
E (dd) 6.87
G (td) 7.14
B (s) 4.66
A (s) 4.74
0.98 1.86 0.90 0.86 1.63 0.82
2.00 1.79
f1 (ppm)


¹³C NMR (101 MHz, Chloroform-d): (2-(4-(Hydroxymethyl)phenoxy)phenyl)methanol
156.84 154.78 136.03 132.05 129.44 129.23 128.96 124.08 118.81 118.57 77.55 77.23 CDCl3 76.91 64.93 61.26
OH
OH
O
f1 (ppm)

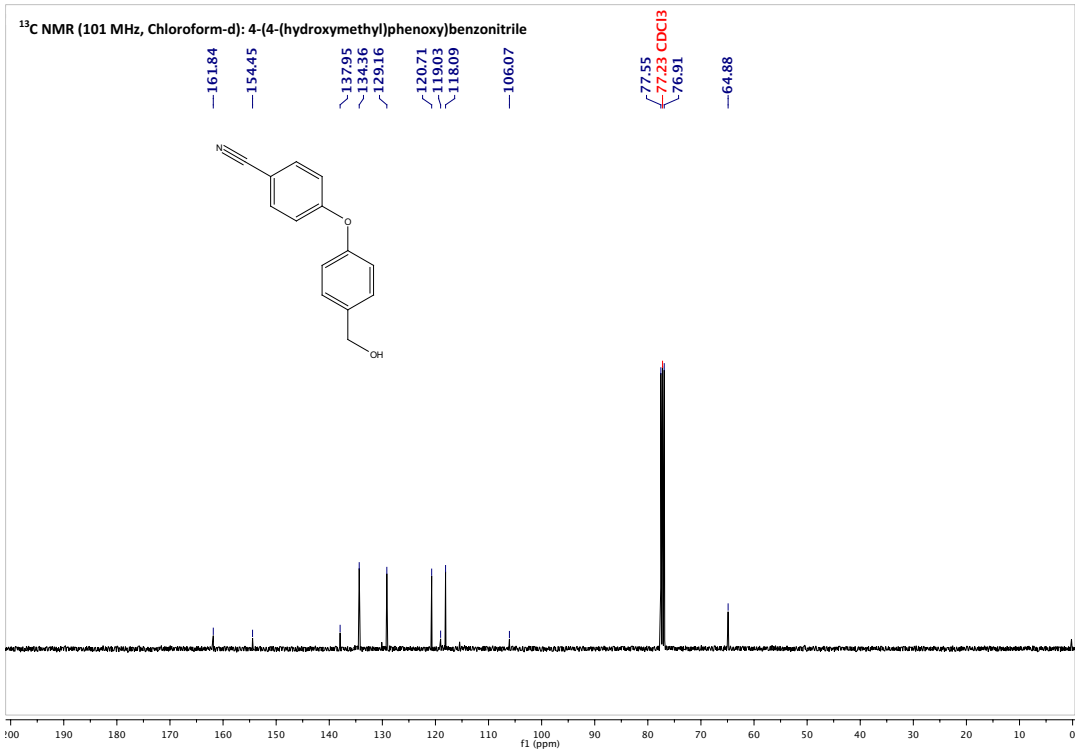

¹H NMR (400 MHz, Chloroform-d): (2-Phenoxyphenyl)methanol (Entry 17)
OH
O
7.26 CDCl3
1.61
G (td) 7.25
C (m) 7.34
E (m) 6.99
B (dd) 7.46
D (dd) 6.87
F (dddd) 7.12
A (m) 4.75
0.92 1.63 1.00 1.73 1.65 0.95
2.00
f1 (ppm)

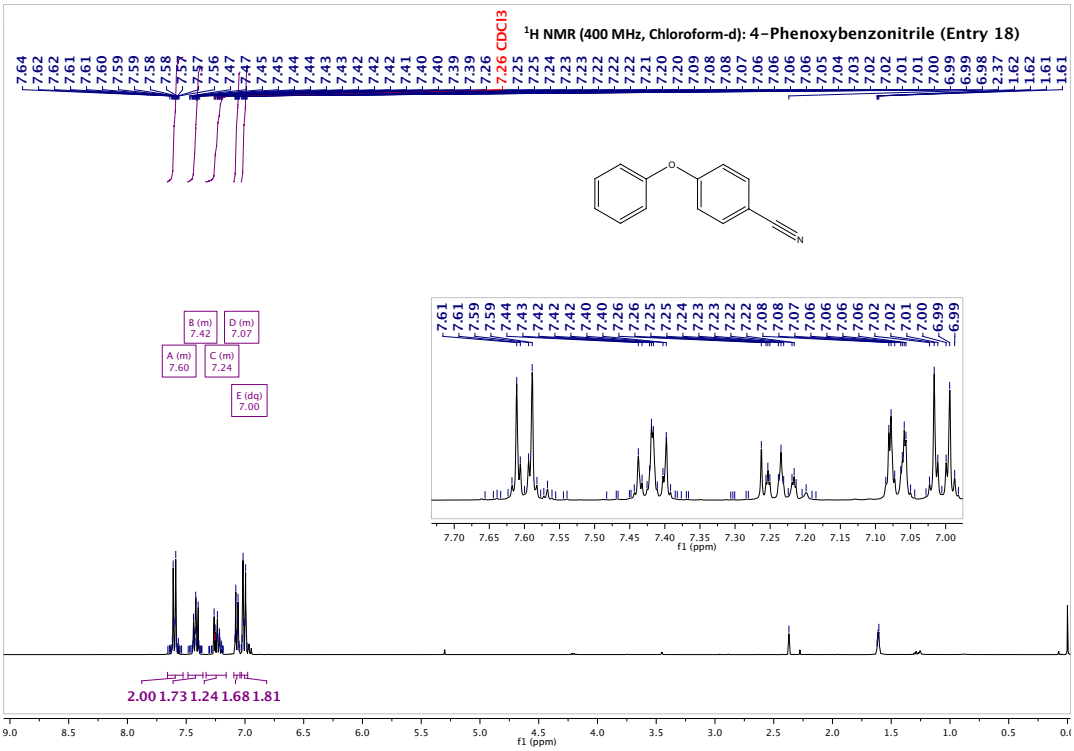

¹³C NMR (101 MHz, Chloroform-d): (2-Phenoxyphenyl)methanol (Entry 17)
OH
O
157.30
154.94
132.08
130.06
129.46
129.24
123.99
123.56
118.81
118.60
77.55
77.23 CDCl3
76.91
61.48
f1 (ppm)

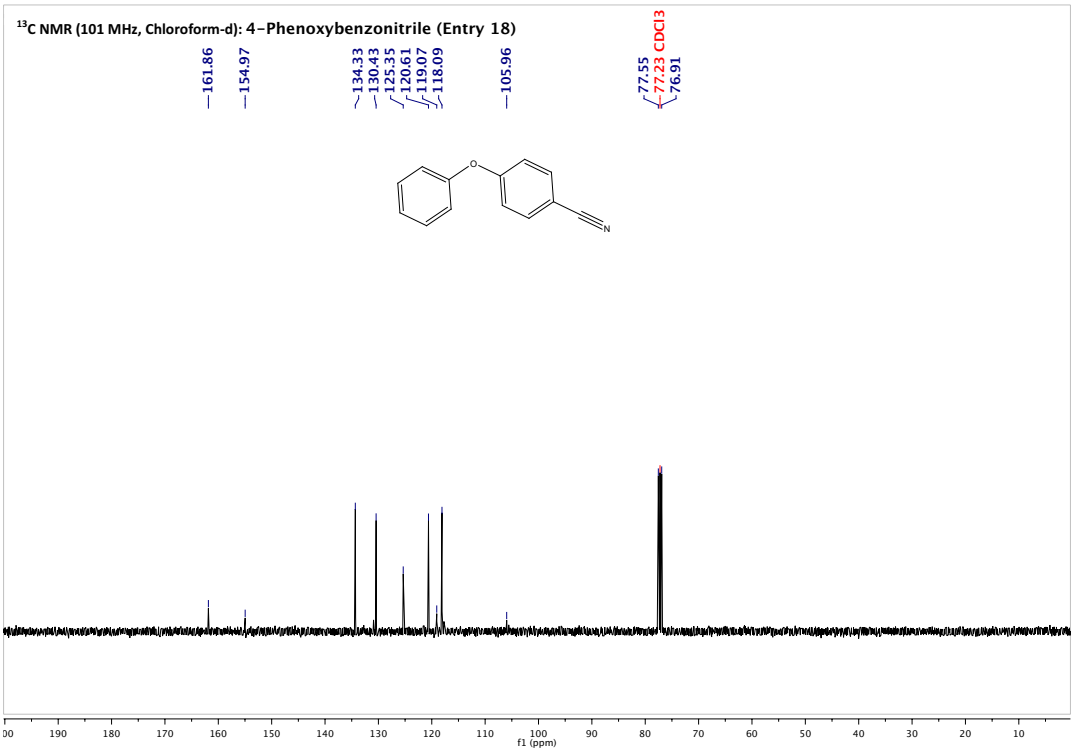
^{1}H NMR (400 MHz, Chloroform-d): 4-(4-(Hydroxymethyl)phenoxy)benzonitrile

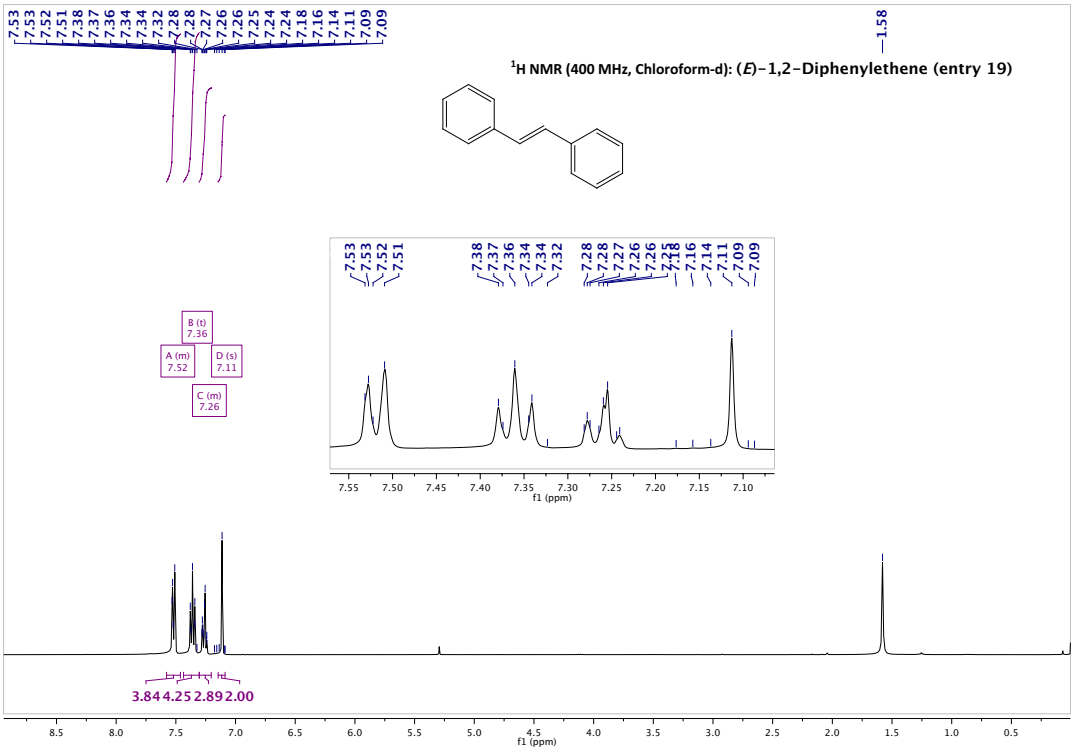


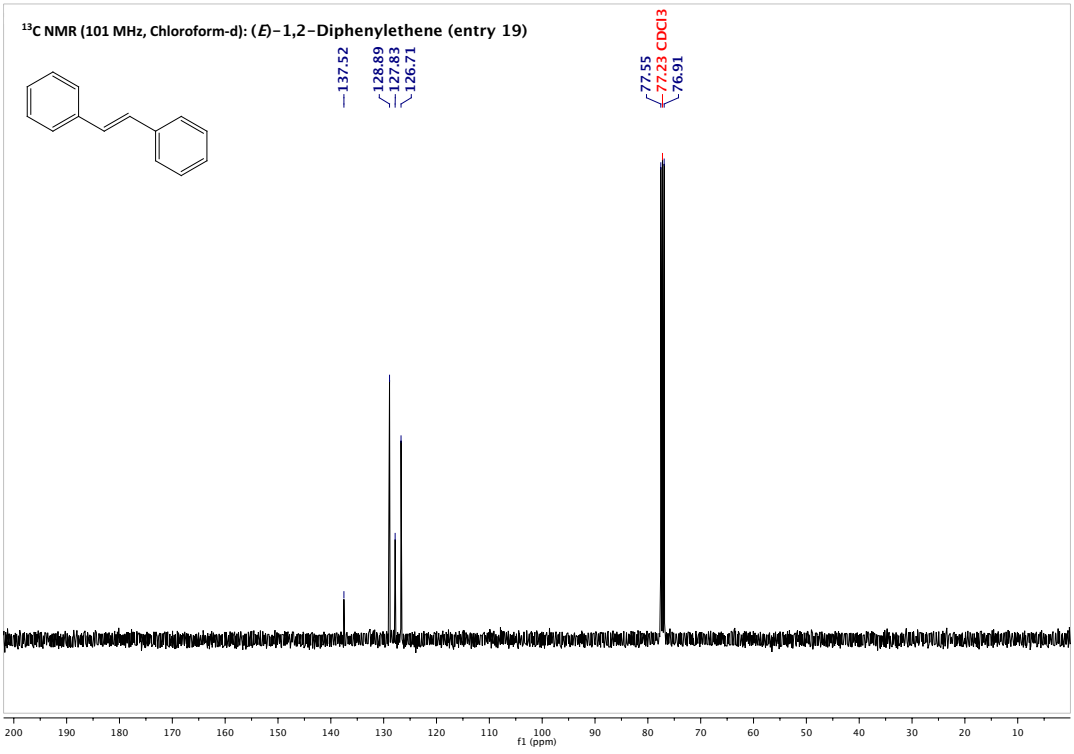
^{13}C NMR (101 MHz, Chloroform-d): 4-(4-(hydroxymethyl)phenoxy)benzonitrile

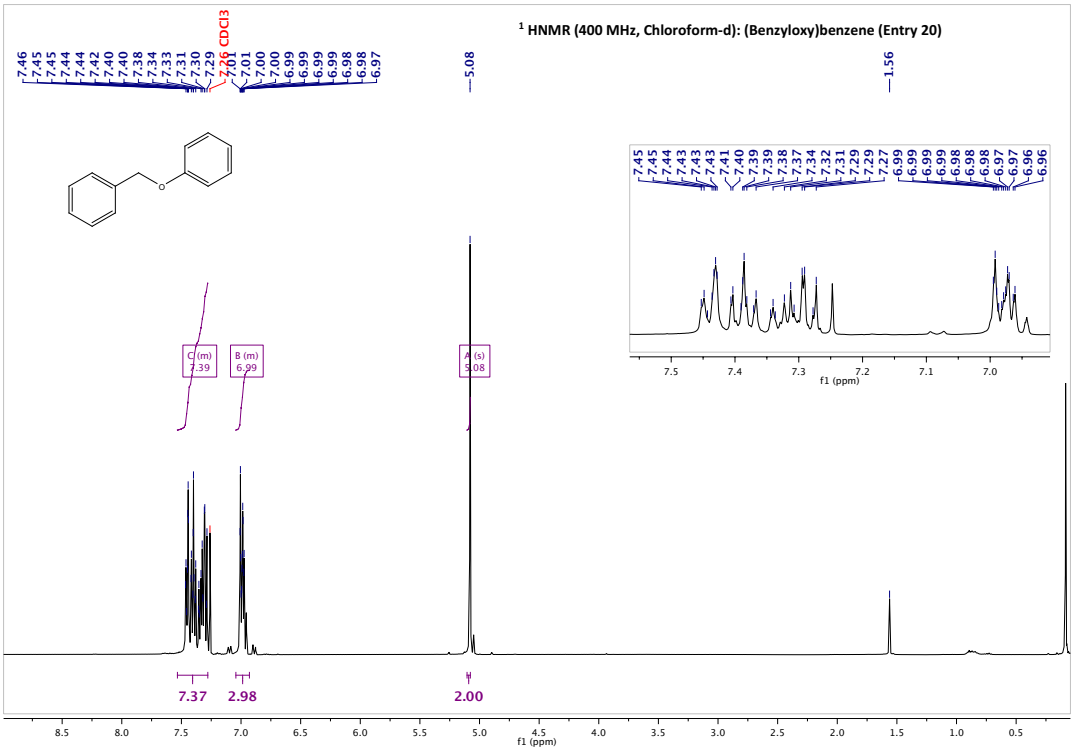


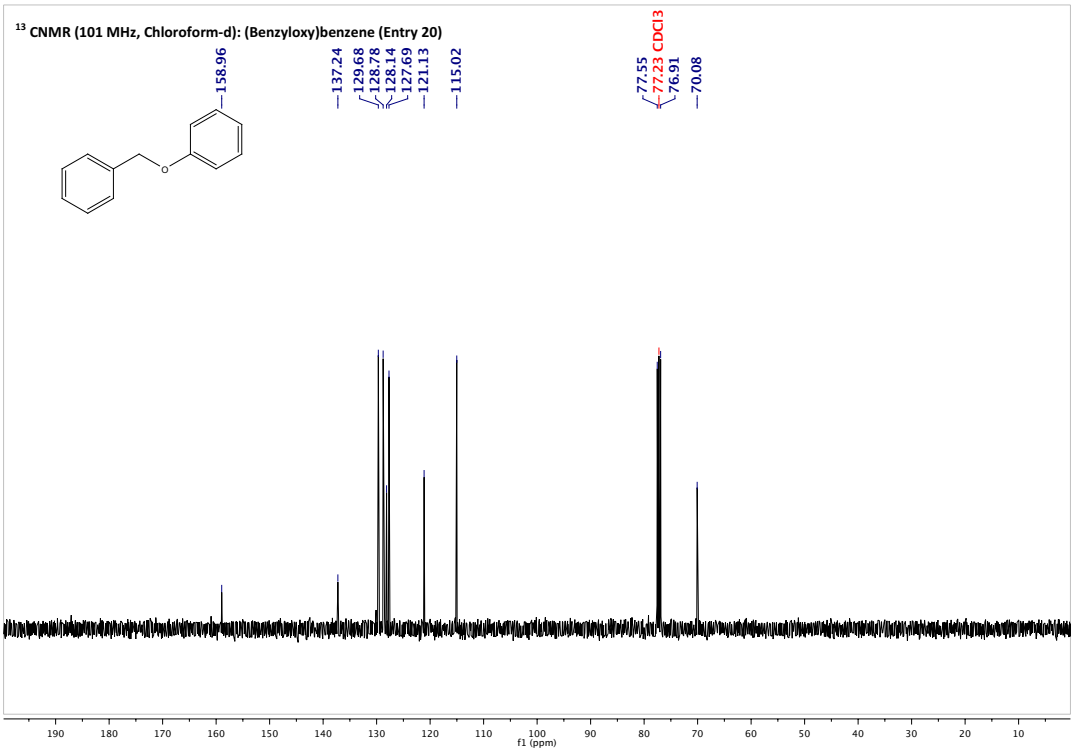

¹H NMR (400 MHz, Chloroform-d): 4-Phenoxybenzonitrile (Entry 18)
7.26 CDCl3
B (m) 7.42
D (m) 7.07
A (m) 7.60
C (m) 7.24
E (dq) 7.00
2.00 1.73 1.24 1.68 1.81
f1 (ppm)

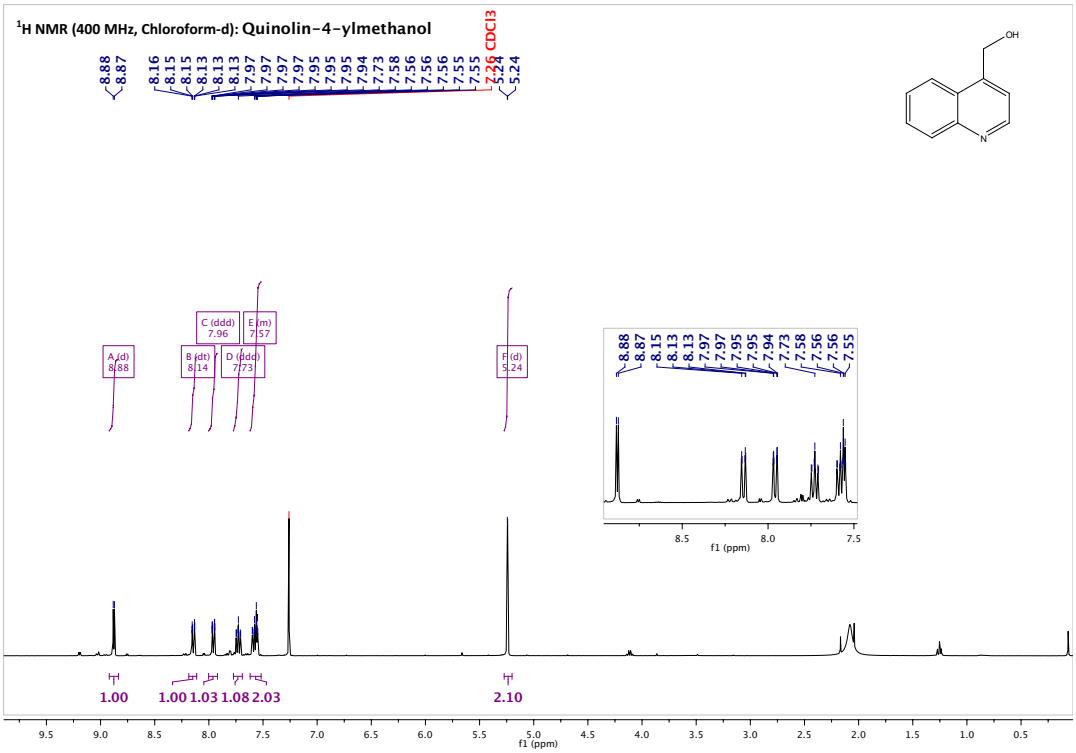

¹³C NMR (101 MHz, Chloroform-d): 4-Phenoxybenzonitrile (Entry 18)
161.86
154.97
134.33
130.43
125.35
120.61
119.07
118.09
105.96
77.55
77.23 CDCl3
76.91
f1 (ppm)

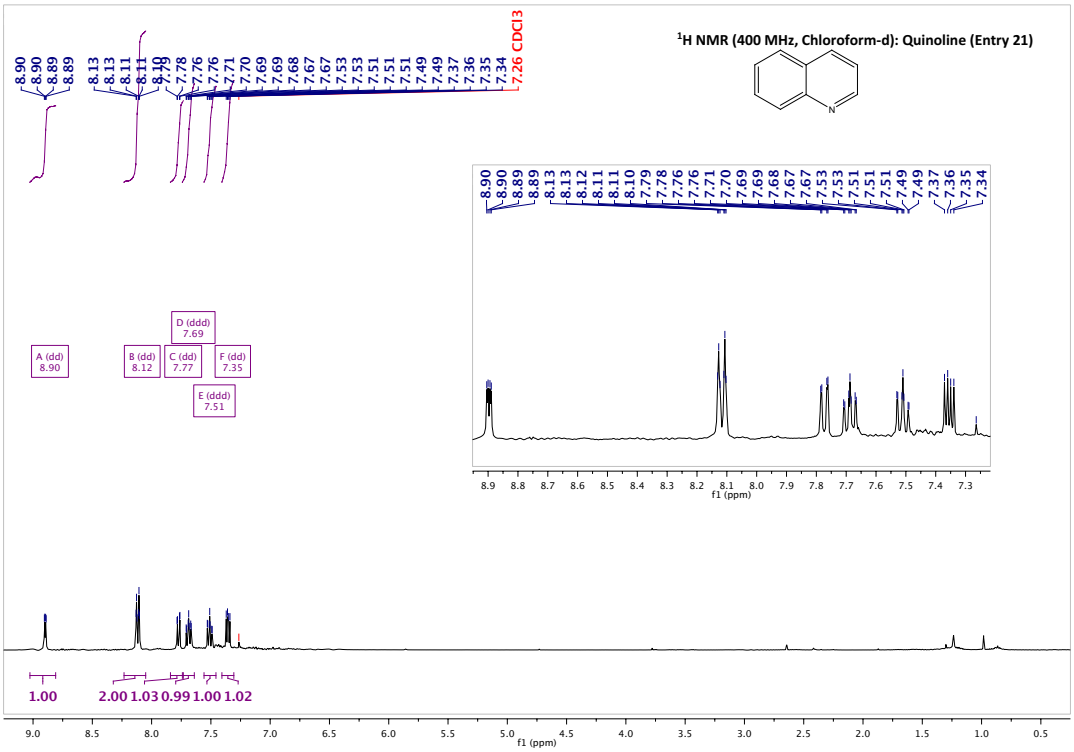

7.53
7.53
7.52
7.51
7.38
7.37
7.36
7.34
7.34
7.32
7.28
7.28
7.27
7.26
7.26
7.25
7.24
7.24
7.18
7.16
7.14
7.11
7.09
7.09
1.58
^{1}H NMR (400 MHz, Chloroform-d): (E)−1,2−Diphenylethene (entry 19)
B (t) 7.36
A (m) 7.52
D (s) 7.11
C (m) 7.26
3.84 4.25 2.89 2.00
f1 (ppm)

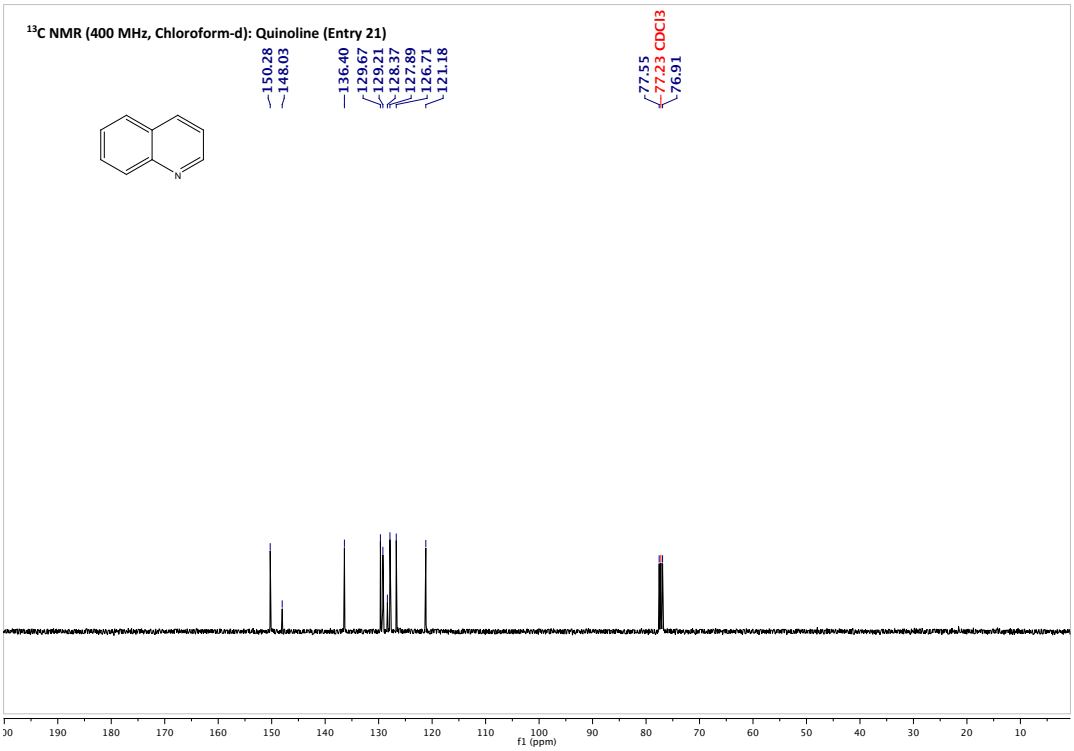

^{13}C NMR (101 MHz, Chloroform-d): (E)−1,2−Diphenylethene (entry 19)
137.52
128.89
127.83
126.71
77.55
77.23 CDCl3
76.91
f1 (ppm)

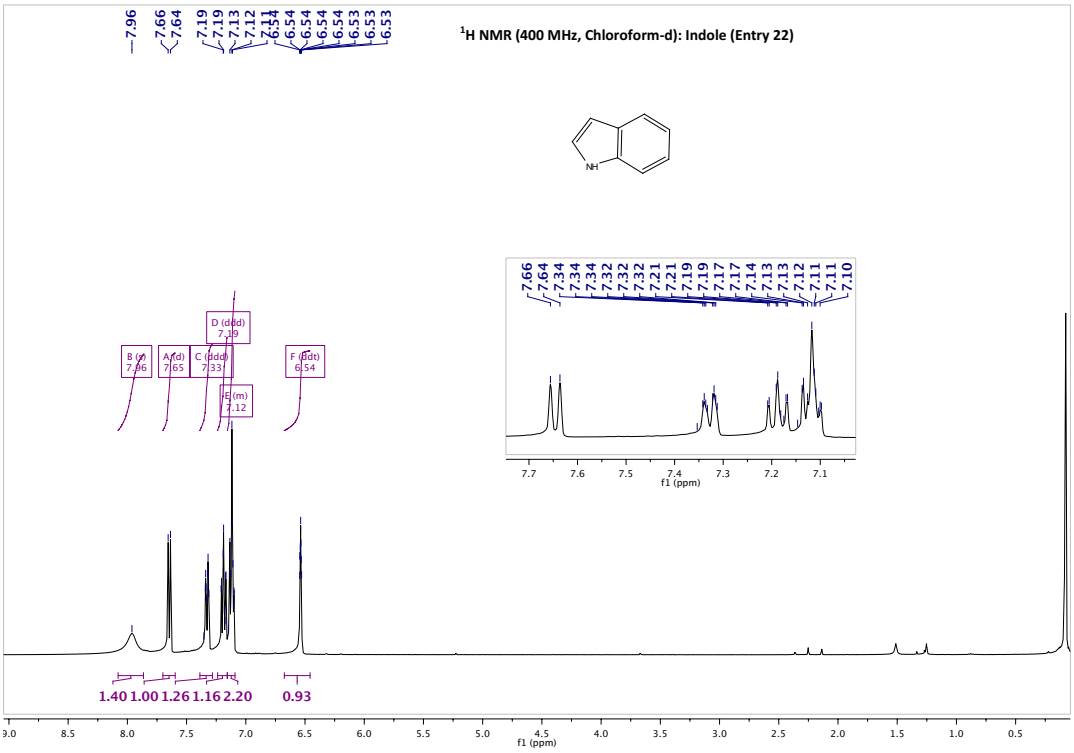

1 HNMR (400 MHz, Chloroform-d): (Benzyloxy)benzene (Entry 20)
7.46 7.45 7.45 7.44 7.44 7.42 7.40 7.40 7.38 7.34 7.33 7.31 7.30 7.29 7.26 CDCl3 7.01 7.00 7.00 6.99 6.99 6.99 6.98 6.98 6.97
5.08
1.56
C (m) 7.39
B (m) 6.99
A (s) 5.08
7.37
2.98
2.00
f1 (ppm)

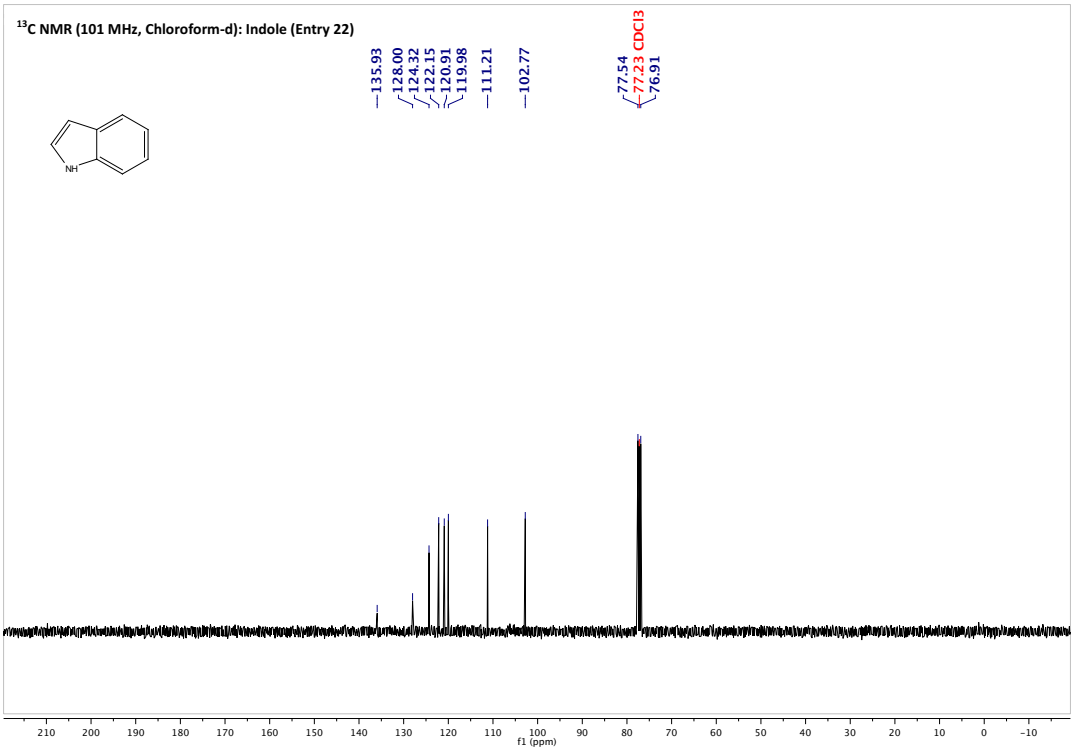

13 CNMR (101 MHz, Chloroform-d): (Benzyloxy)benzene (Entry 20)
158.96
137.24
129.68
128.78
128.14
127.69
121.13
115.02
77.55
77.23 CDCl3
76.91
70.08
f1 (ppm)

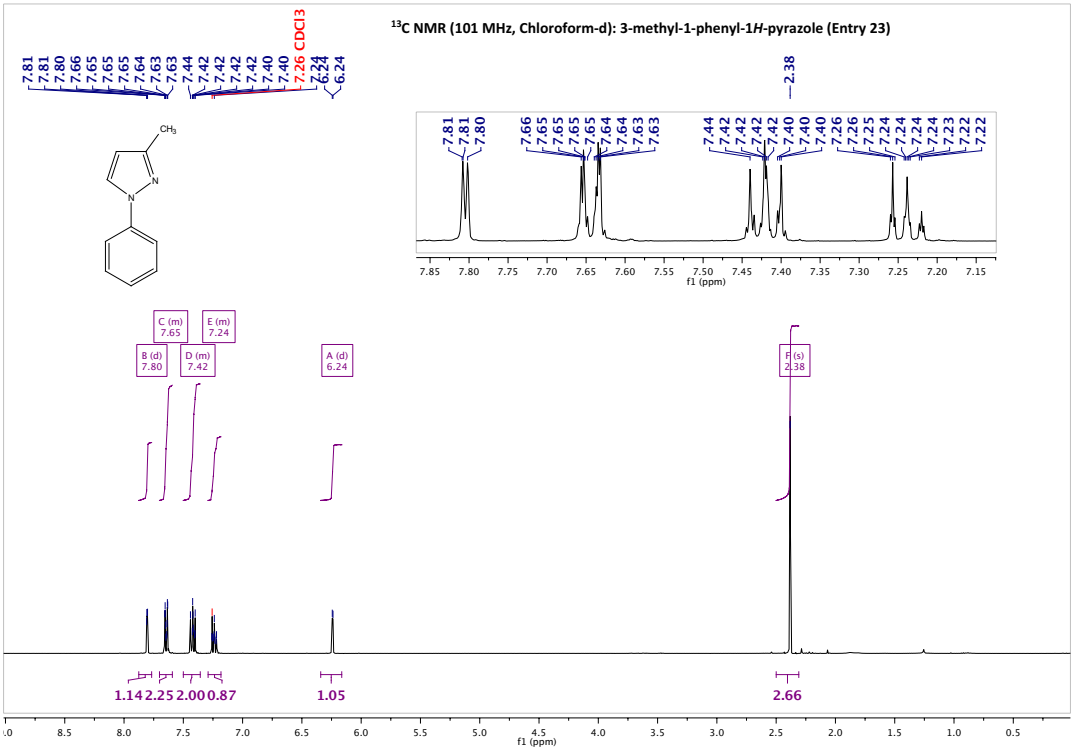

¹H NMR (400 MHz, Chloroform-d): Quinolin-4-ylmethanol
OH
N
A (d) 8.88
B (dt) 8.14
C (ddd) 7.96
D (ddd) 7.73
E (m) 7.57
F (d) 5.24
1.00
1.00 1.03 1.08 2.03
2.10
f1 (ppm)

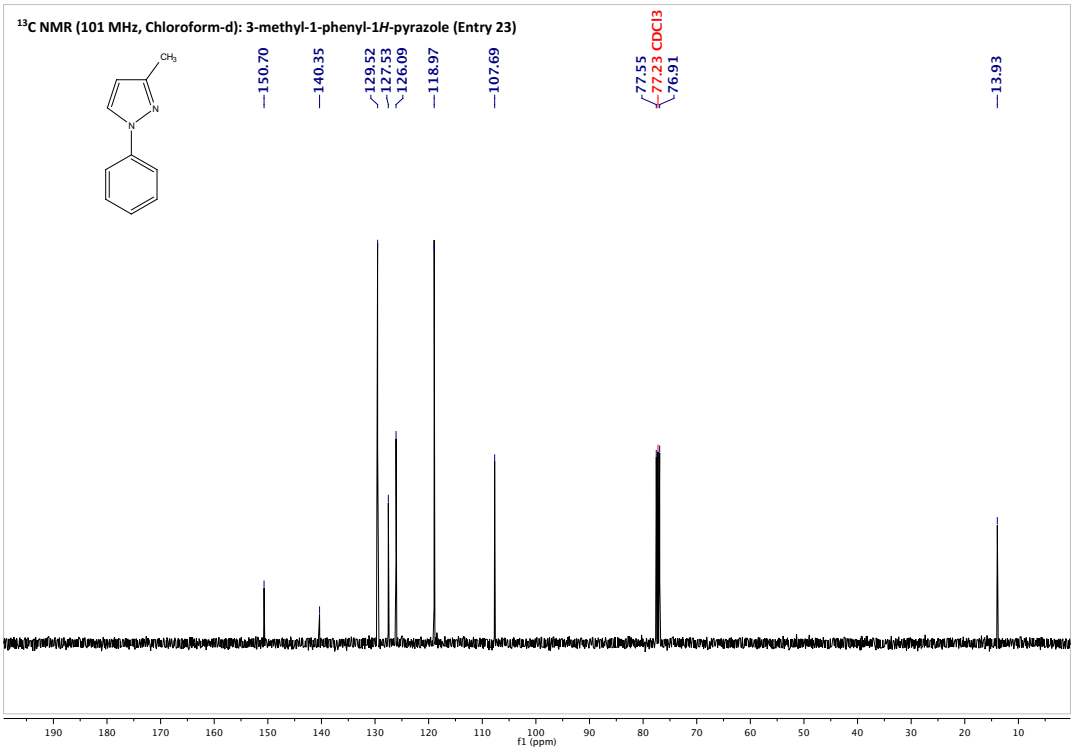

¹H NMR (400 MHz, Chloroform-d): Quinoline (Entry 21)
N
A (dd) 8.90
B (dd) 8.12
C (dd) 7.77
D (ddd) 7.69
E (ddd) 7.51
F (dd) 7.35
1.00
2.00 1.03 0.99 1.00 1.02
f1 (ppm)

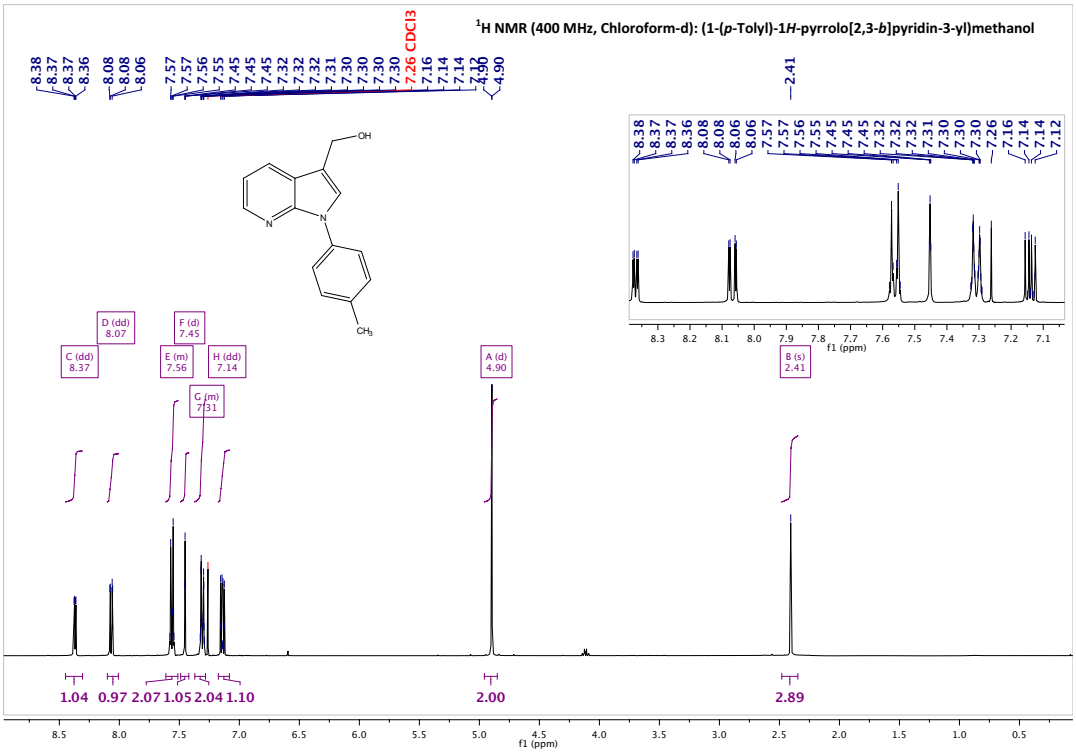

13C NMR (400 MHz, Chloroform-d): Quinoline (Entry 21)
150.28
148.03
136.40
129.67
129.21
128.37
127.89
126.71
121.18
77.55
77.23 CDCl3
76.91
f1 (ppm)

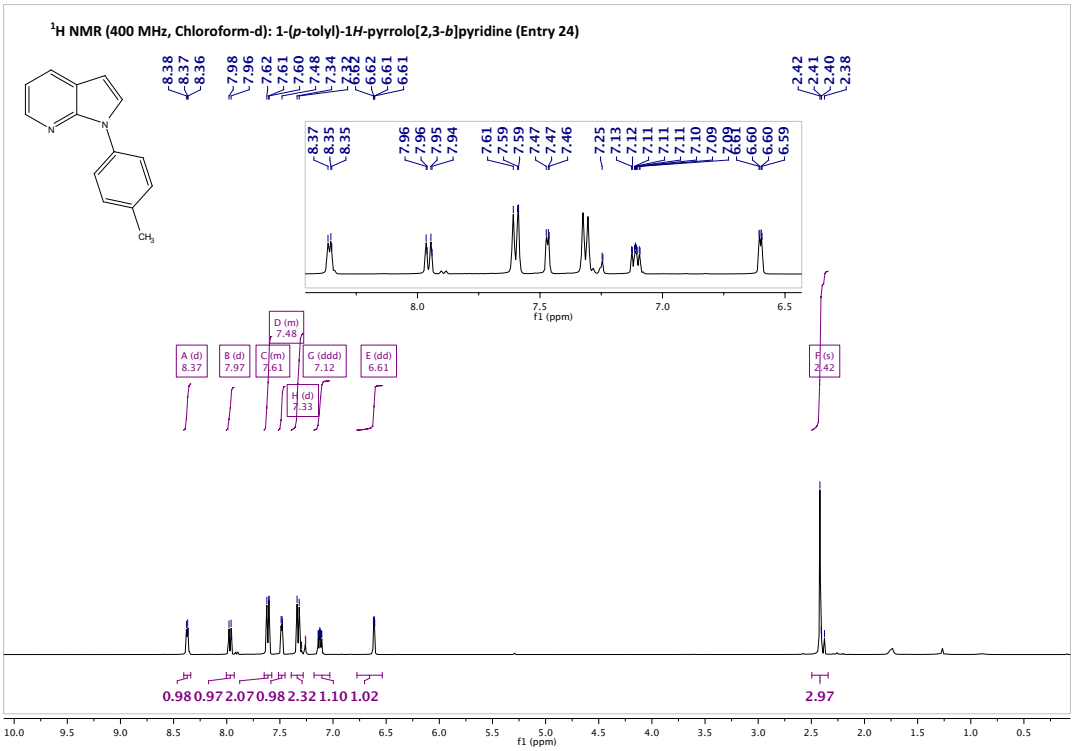

1H NMR (400 MHz, Chloroform-d): Indole (Entry 22)
7.96
7.66
7.64
7.19
7.19
7.13
7.12
6.54
6.54
6.54
6.54
6.53
6.53
6.53
B (d) 7.96
A (d) 7.65
D (ddd) 7.19
C (ddd) 7.33
E (m) 7.12
F (ddd) 6.54
1.40 1.00 1.26 1.16 2.20 0.93
f1 (ppm)

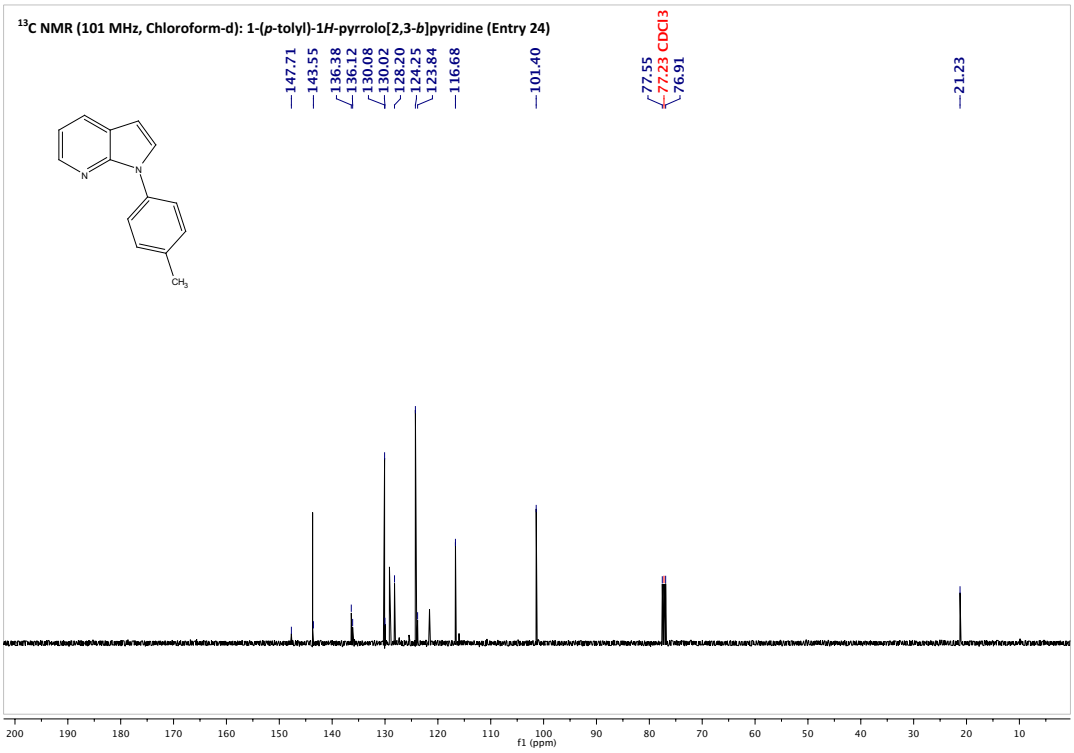

13C NMR (101 MHz, Chloroform-d): Indole (Entry 22)
135.93
128.00
124.32
122.15
120.91
119.98
111.21
102.77
77.54
77.23 CDCl3
76.91
NH
f1 (ppm)

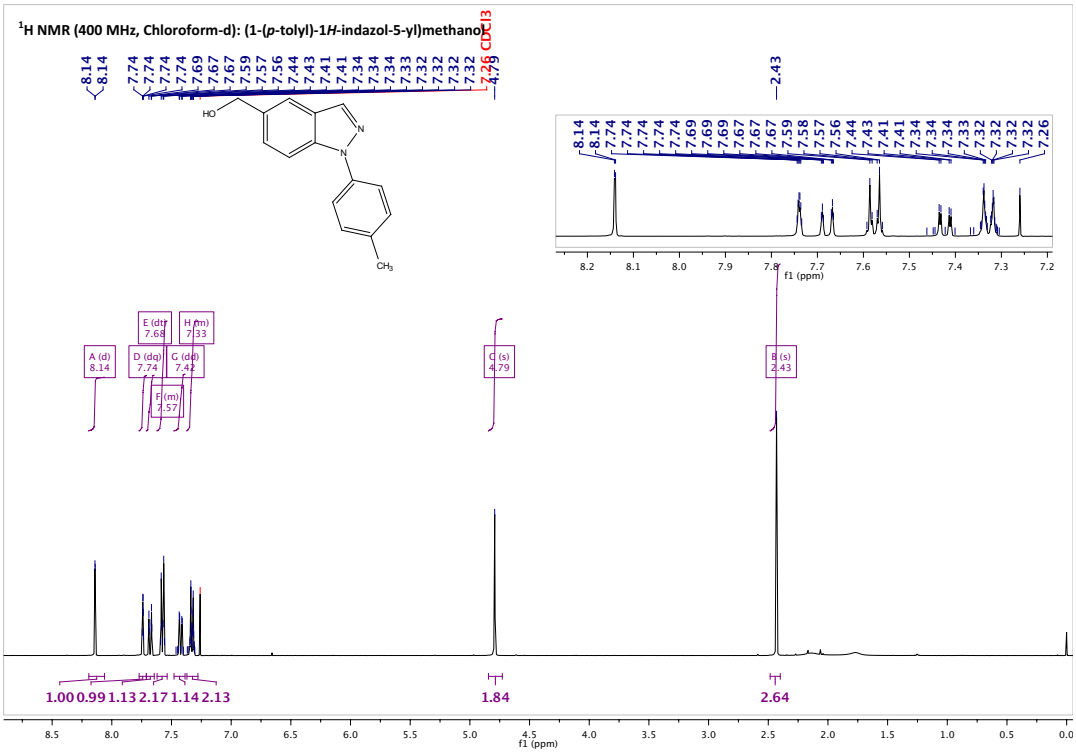

13C NMR (101 MHz, Chloroform-d): 3-methyl-1-phenyl-1H-pyrazole (Entry 23)
7.81
7.81
7.80
7.66
7.65
7.65
7.64
7.63
7.63
7.44
7.42
7.42
7.42
7.40
7.40
7.26 CDCl3
6.24
6.24
2.38
CH3
N
N
C (m) 7.65
E (m) 7.24
B (d) 7.80
D (m) 7.42
A (d) 6.24
F (s) 2.38
1.14 2.25 2.00 0.87
1.05
2.66
f1 (ppm)

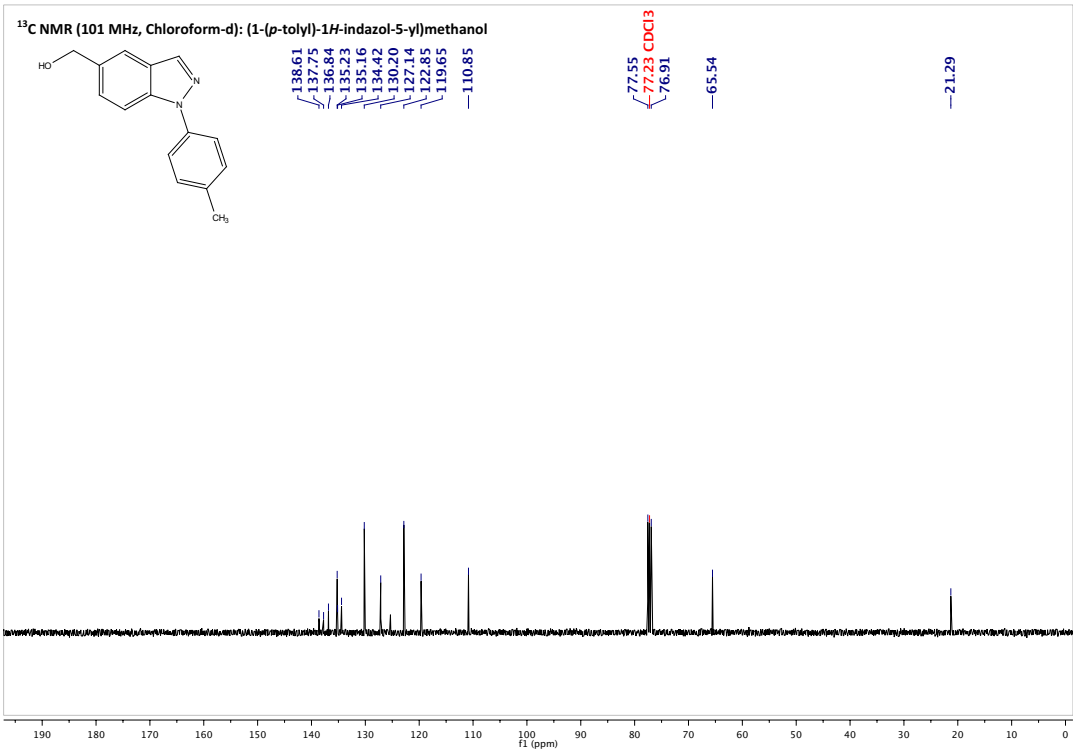

13C NMR (101 MHz, Chloroform-d): 3-methyl-1-phenyl-1H-pyrazole (Entry 23)
150.70
140.35
129.52
127.53
126.09
118.97
107.69
77.55
77.23 CDCl3
76.91
13.93
f1 (ppm)

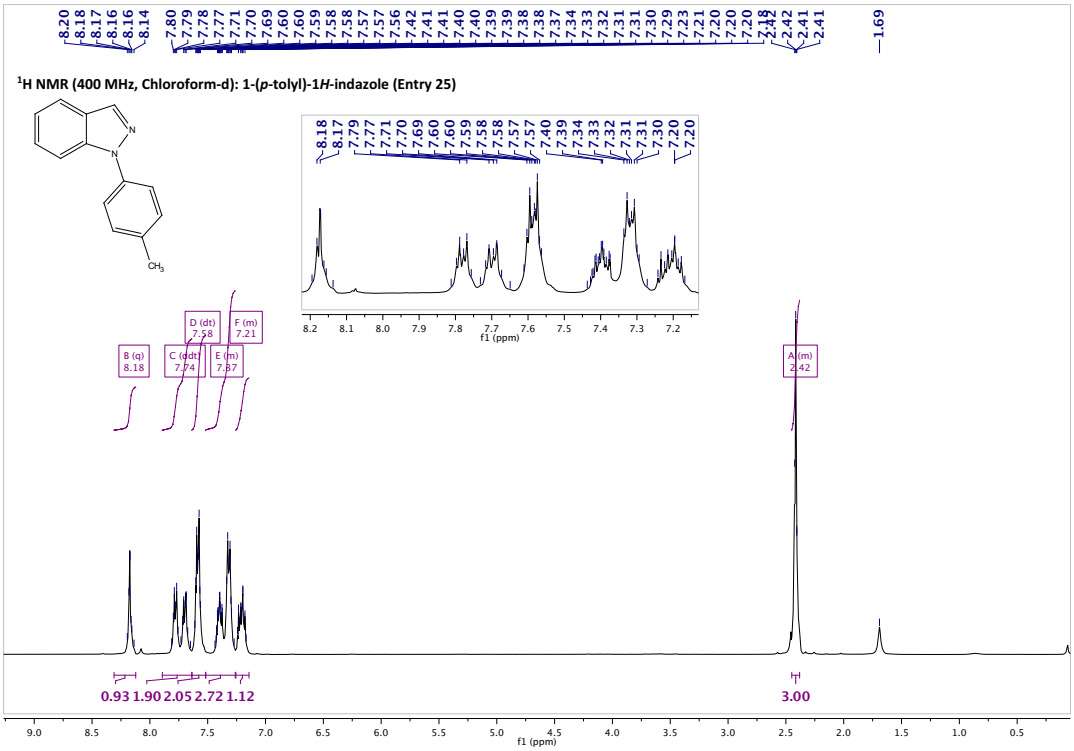

1H NMR (400 MHz, Chloroform-d): (1-(p-Tolyl)-1H-pyrrolo[2,3-b]pyridin-3-yl)methanol
7.26 CDCl3
2.41
D (dd) 8.07
F (d) 7.45
C (dd) 8.37
E (m) 7.56
H (dd) 7.14
G (m) 7.31
A (d) 4.90
B (s) 2.41
1.04 0.97 2.07 1.05 2.04 1.10
2.00
2.89
f1 (ppm)

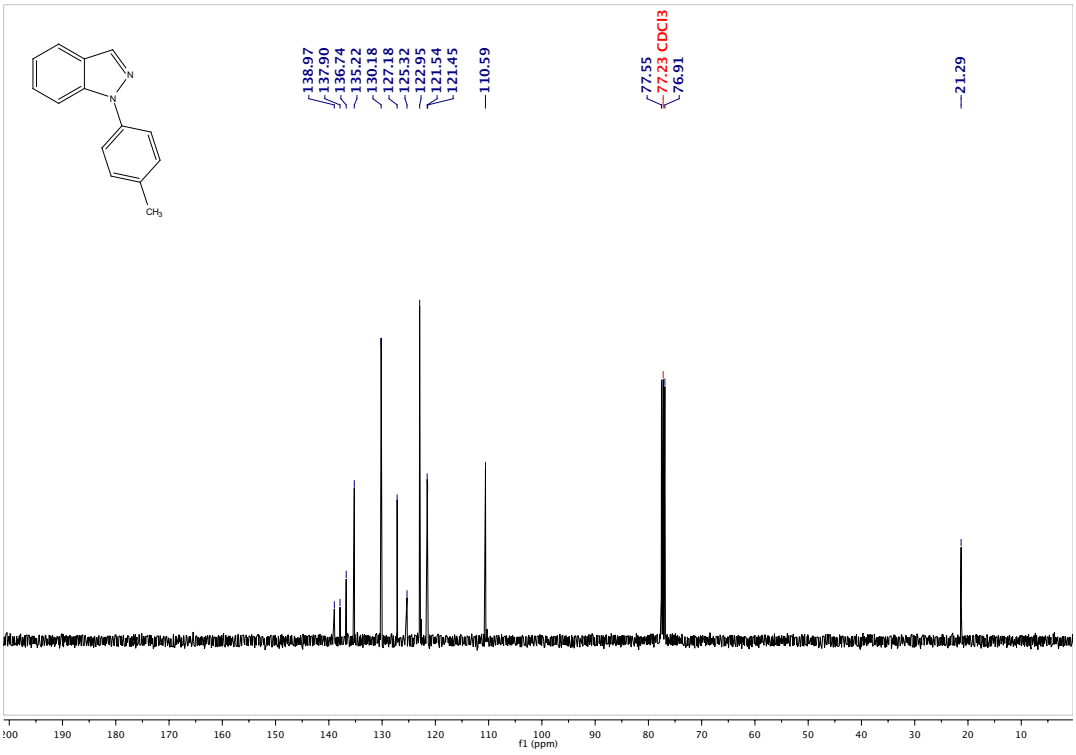

^{1}H NMR (400 MHz, Chloroform-d): 1-(*p*-tolyl)-1*H*-pyrrolo[2,3-*b*]pyridine (Entry 24)
8.38 8.37 8.36 7.98 7.96 7.62 7.61 7.60 7.48 7.34 6.62 6.61 6.61
2.42 2.41 2.40 2.38
8.37 8.35 8.35 7.96 7.96 7.95 7.94 7.61 7.59 7.59 7.47 7.47 7.46 7.25 7.13 7.12 7.11 7.11 7.11 7.10 7.09 6.60 6.60 6.59
f1 (ppm)
A (d) 8.37
B (d) 7.97
C (m) 7.61
D (m) 7.48
E (dd) 6.61
F (s) 2.42
G (ddd) 7.12
H (d) 2.33
0.98 0.97 2.07 0.98 2.32 1.10 1.02
2.97
f1 (ppm)

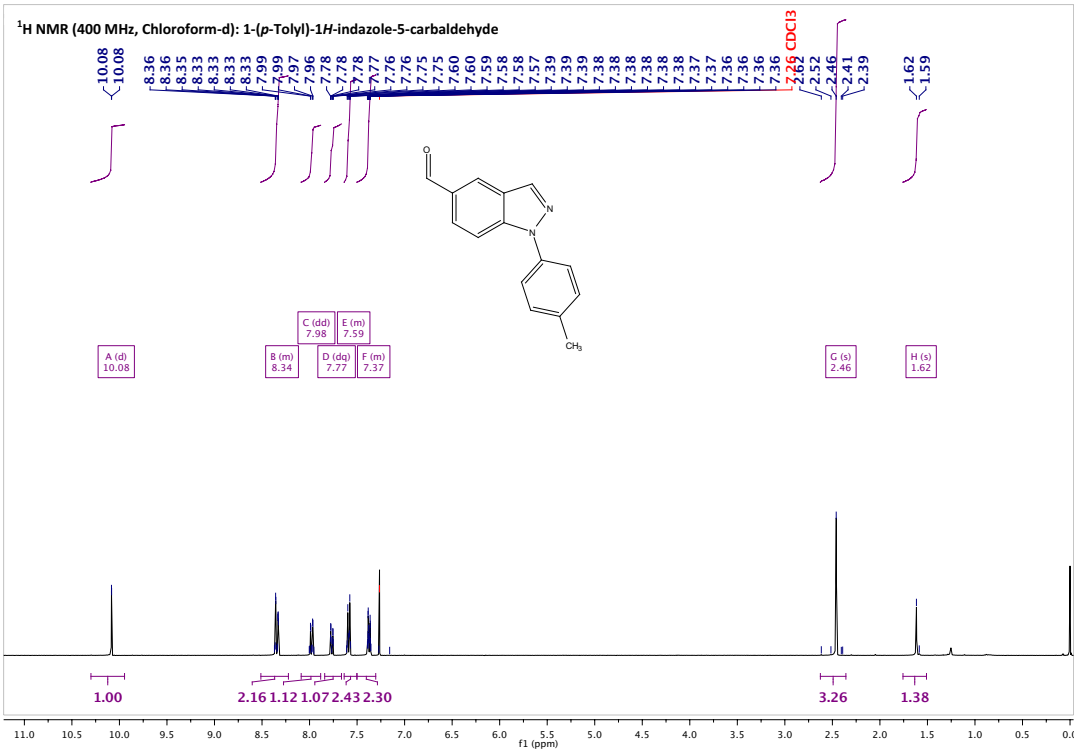

^{13}C NMR (101 MHz, Chloroform-d): 1-(*p*-tolyl)-1*H*-pyrrolo[2,3-*b*]pyridine (Entry 24)
147.71 143.55 136.38 136.12 130.08 130.02 128.20 124.25 123.84 116.68 101.40 77.55 77.23 CDCl3 76.91 21.23
f1 (ppm)

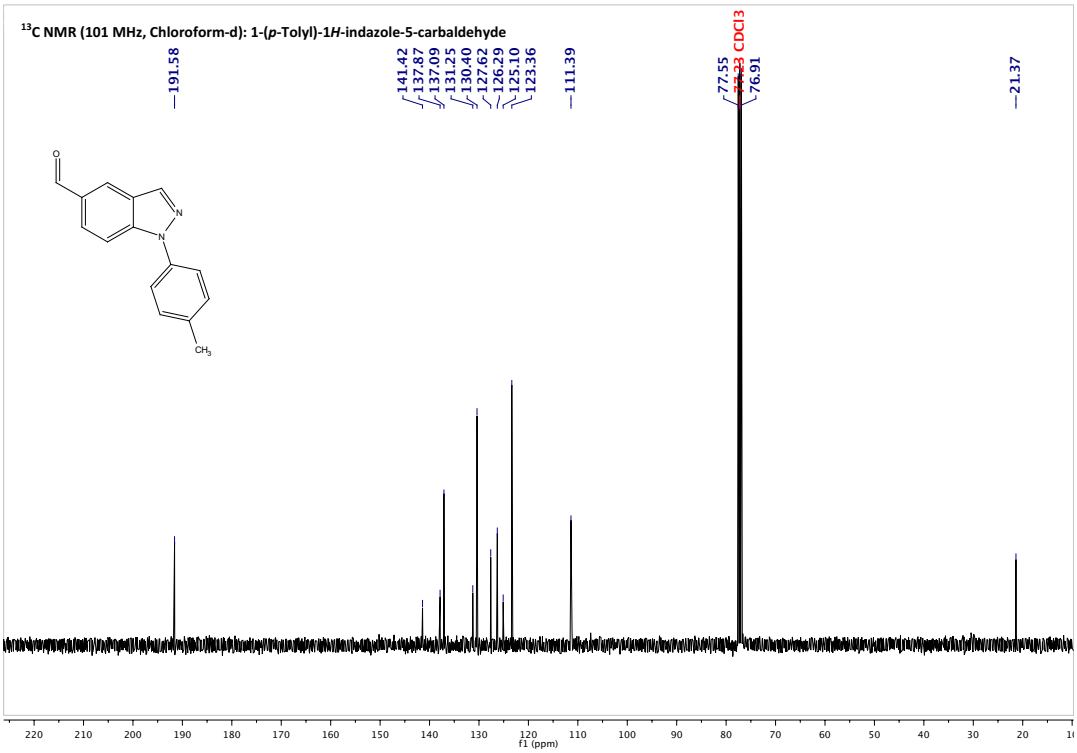

1H NMR (400 MHz, Chloroform-d): (1-(p-tolyl)-1H-indazol-5-yl)methanol
CDCl3
HO
N
CH3
A (d) 8.14
D (dq) 7.74
G (dd) 7.42
E (dt) 7.68
H (m) 7.33
F (m) 7.57
C (s) 4.79
B (s) 2.43
1.00 0.99 1.13 2.17 1.14 2.13
1.84
2.64
f1 (ppm)

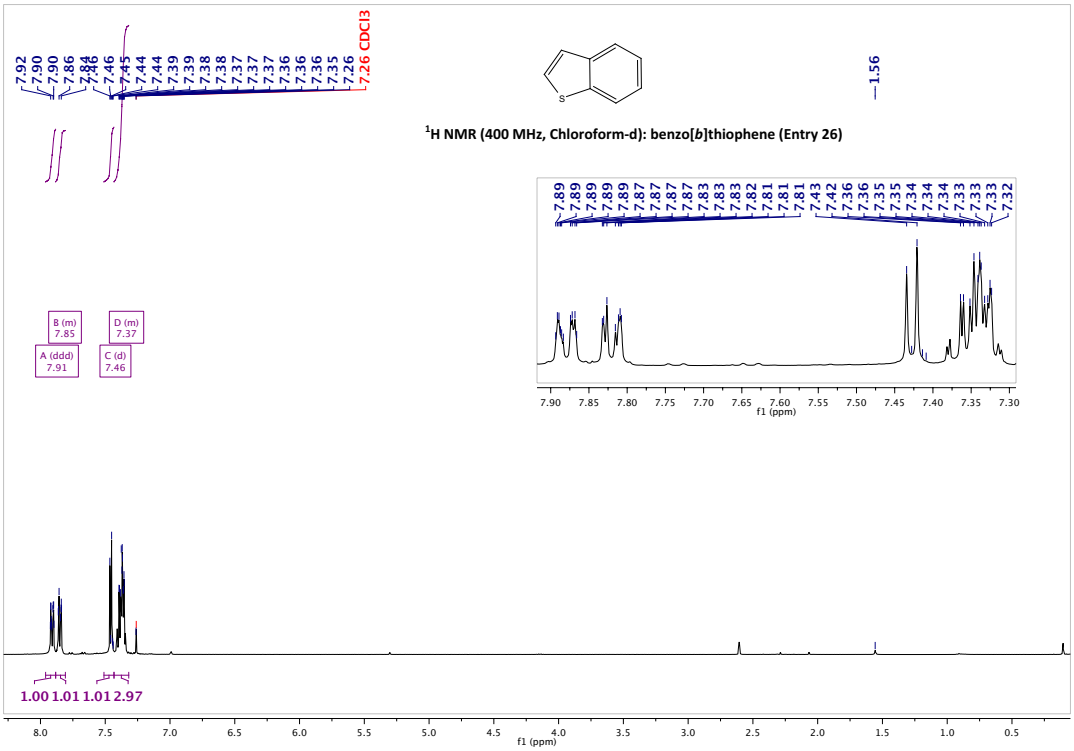

13C NMR (101 MHz, Chloroform-d): (1-(p-tolyl)-1H-indazol-5-yl)methanol
HO
N
CH3
138.61
137.75
136.84
135.23
135.16
134.42
130.20
127.14
122.85
119.65
110.85
77.55
77.23 CDCl3
76.91
65.54
21.29
f1 (ppm)


8.20 8.18 8.17 8.16 8.16 8.14 7.80 7.79 7.78 7.77 7.71 7.70 7.69 7.60 7.60 7.59 7.58 7.58 7.57 7.57 7.56 7.42 7.41 7.41 7.40 7.40 7.39 7.39 7.38 7.38 7.37 7.34 7.33 7.32 7.31 7.31 7.30 7.29 7.23 7.21 7.20 7.20 7.20 7.18 2.42 2.42 2.41 2.41 1.69
1H NMR (400 MHz, Chloroform-d): 1-(p-tolyl)-1H-indazole (Entry 25)
B (q) 8.18
C (ddt) 7.74
D (dt) 7.58
E (m) 7.37
F (m) 7.21
A (m) 2.42
0.93 1.90 2.05 2.72 1.12
3.00
f1 (ppm)

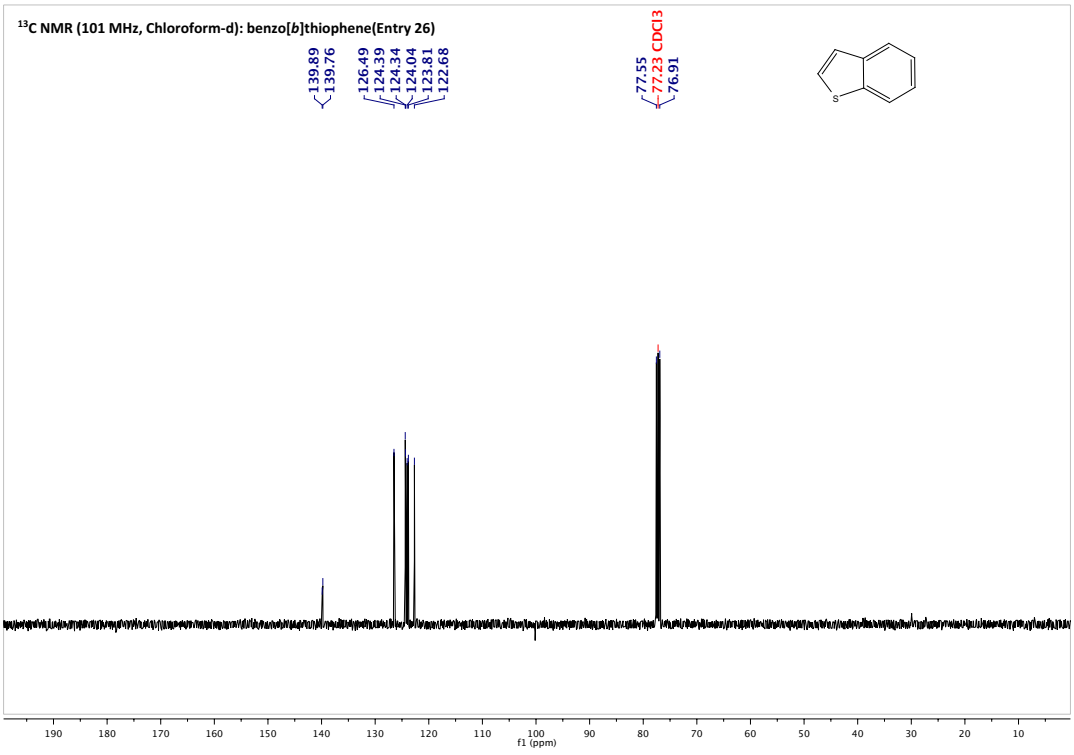

138.97 137.90 136.74 135.22 130.18 127.18 125.32 122.95 121.54 121.45 110.59 77.55 77.23 CDCl3 76.91 21.29
f1 (ppm)


^{1}H NMR (400 MHz, Chloroform-d): 1-(*p*-Tolyl)-1*H*-indazole-5-carbaldehyde
10.08
8.36
8.35
8.33
8.33
8.33
7.99
7.97
7.96
7.78
7.78
7.77
7.76
7.76
7.75
7.60
7.59
7.58
7.57
7.39
7.39
7.38
7.38
7.38
7.38
7.37
7.37
7.36
7.36
7.36
7.26 CDCl3
2.62
2.52
2.46
2.41
2.39
1.62
1.59
A (d) 10.08
B (m) 8.34
C (dd) 7.98
D (dq) 7.77
E (m) 7.59
F (m) 7.37
G (s) 2.46
H (s) 1.62
1.00
2.16 1.12 1.07 2.43 2.30
3.26
1.38
f1 (ppm)

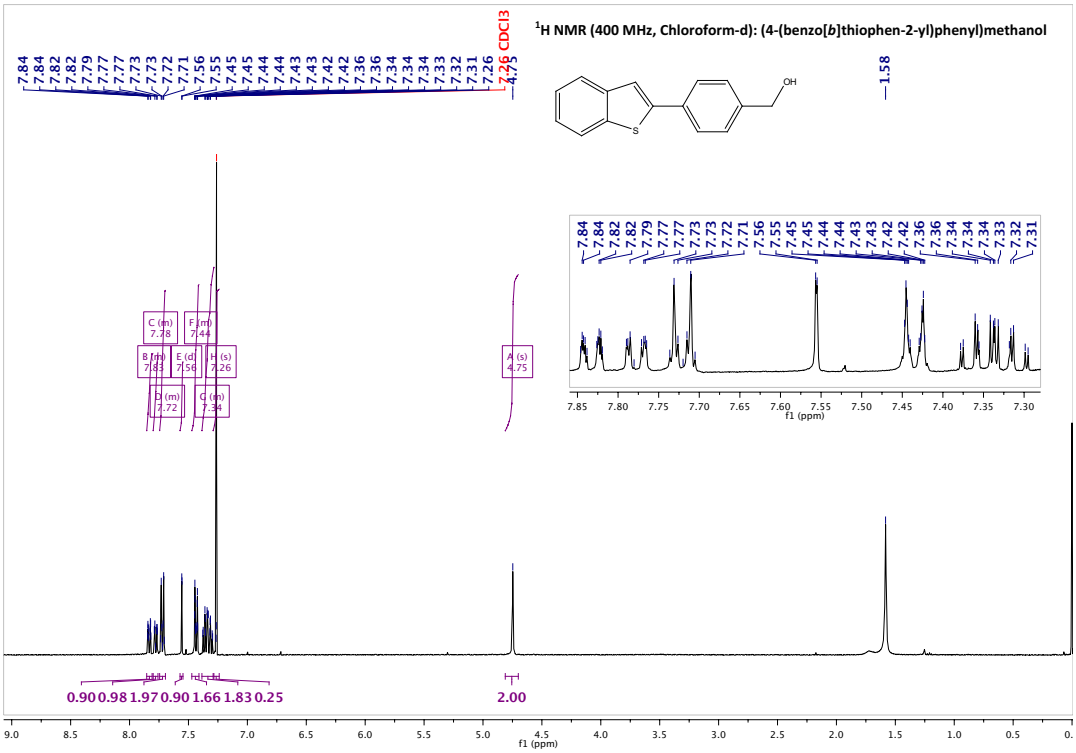

^{13}C NMR (101 MHz, Chloroform-d): 1-(*p*-Tolyl)-1*H*-indazole-5-carbaldehyde
191.58
141.42
137.87
137.09
131.25
130.40
127.62
126.29
125.10
123.36
111.39
77.55
77.23 CDCl3
76.91
21.37
f1 (ppm)

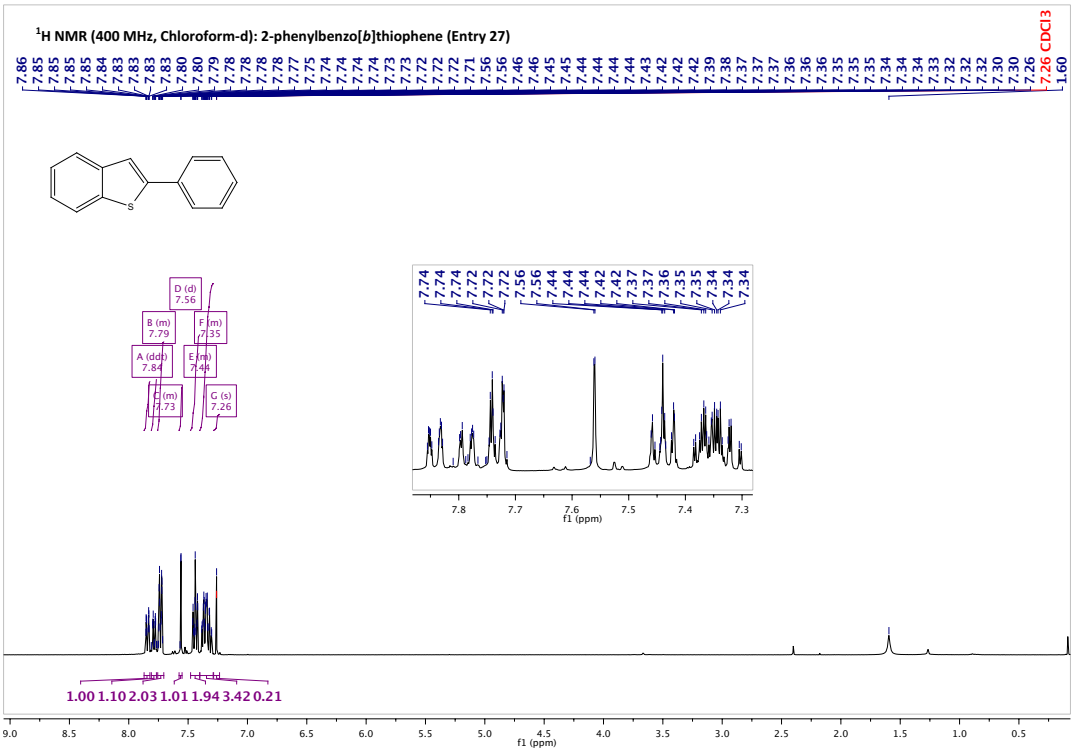


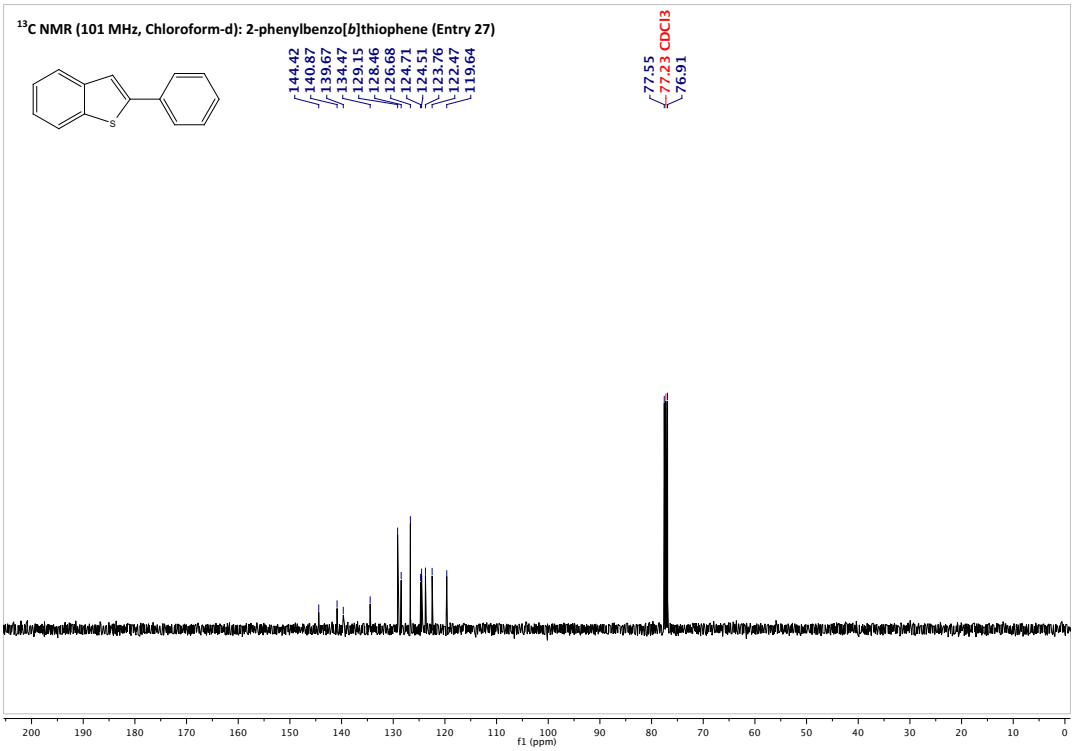
^{1}H NMR (400 MHz, Chloroform-d): benzo[*b*]thiophene (Entry 26)

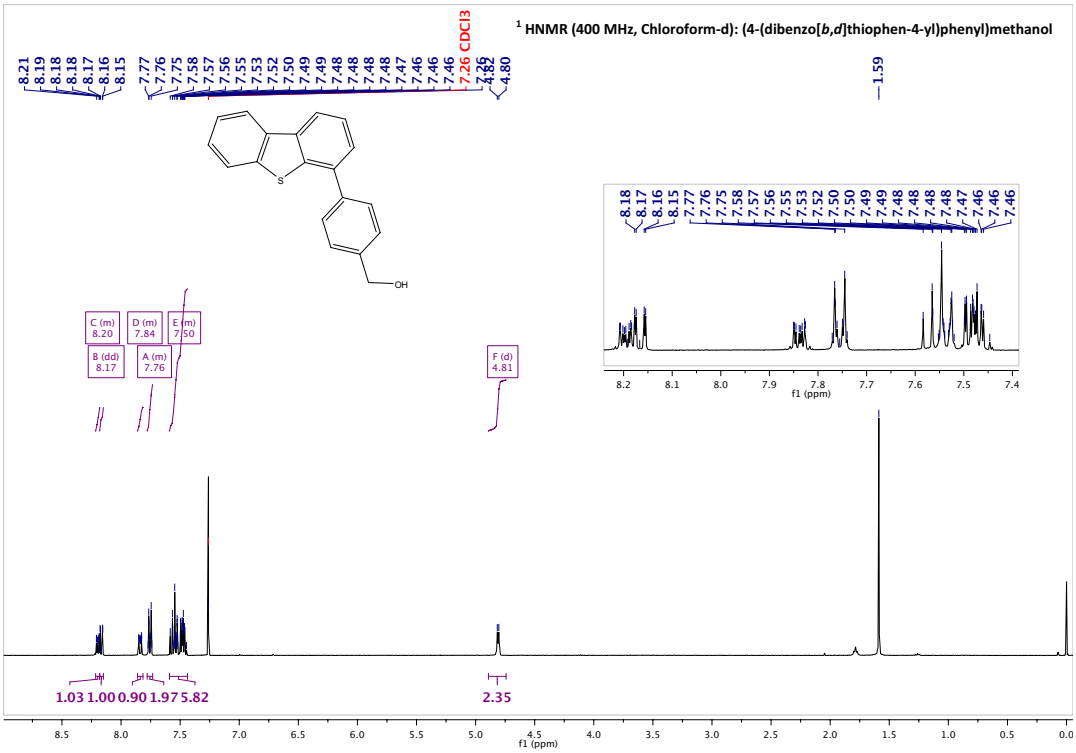


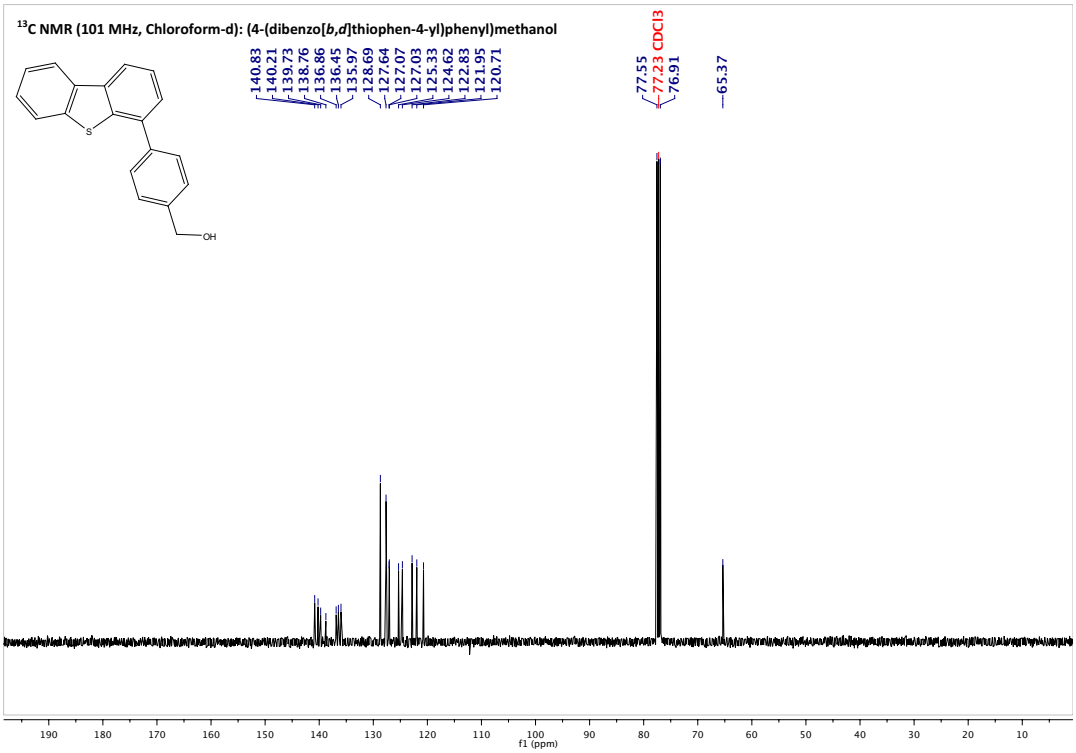
^{13}C NMR (101 MHz, Chloroform-d): benzo[*b*]thiophene(Entry 26)

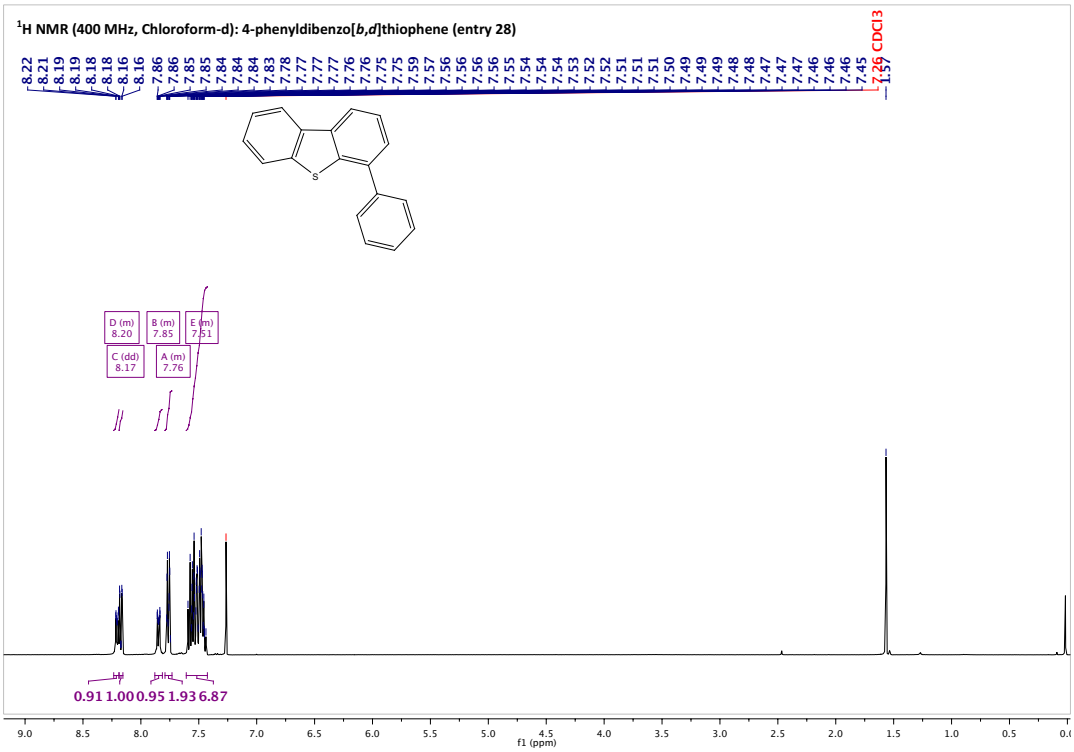

^{1}H NMR (400 MHz, Chloroform-d): (4-(benzo[b]thiophen-2-yl)phenyl)methanol
CDCl3
OH
S
1.58
C (m) 7.78
F (m) 7.44
B (m) 7.83
E (d) 7.56
H (s) 7.26
D (m) 7.72
G (m) 7.34
A (s) 4.75
0.90 0.98 1.97 0.90 1.66 1.83 0.25
2.00
f1 (ppm)

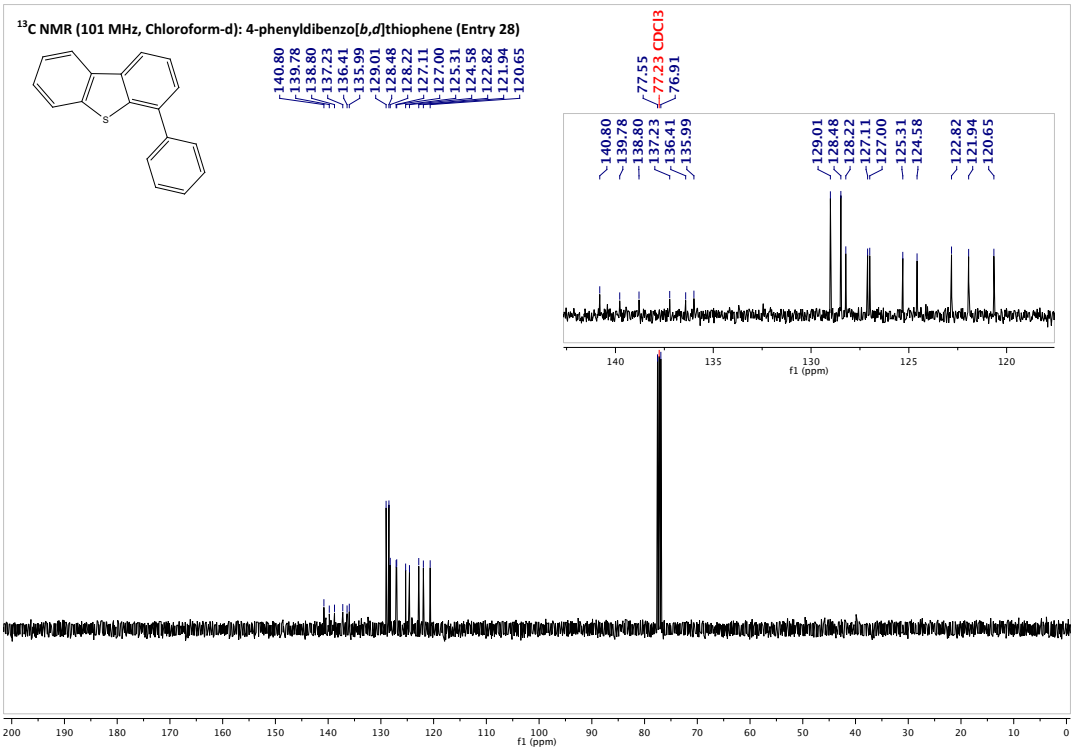

^{1}H NMR (400 MHz, Chloroform-d): 2-phenylbenzo[b]thiophene (Entry 27)
CDCl3
1.60
S
D (d) 7.56
B (m) 7.79
F (m) 7.35
A (ddd) 7.84
E (m) 7.44
C (m) 7.73
G (s) 7.26
1.00 1.10 2.03 1.01 1.94 3.42 0.21
f1 (ppm)

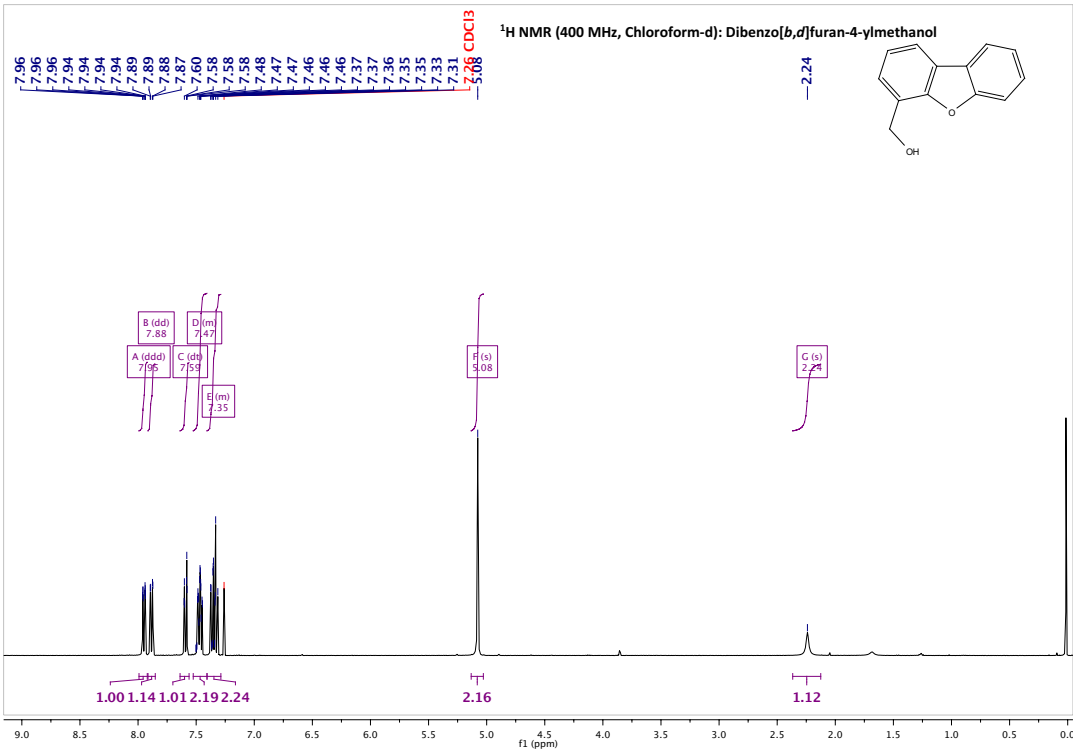

13C NMR (101 MHz, Chloroform-d): 2-phenylbenzo[b]thiophene (Entry 27)
144.42
140.87
139.67
134.47
129.15
128.46
126.68
124.71
124.51
123.76
122.47
119.64
77.55
77.23 CDCl3
76.91
f1 (ppm)

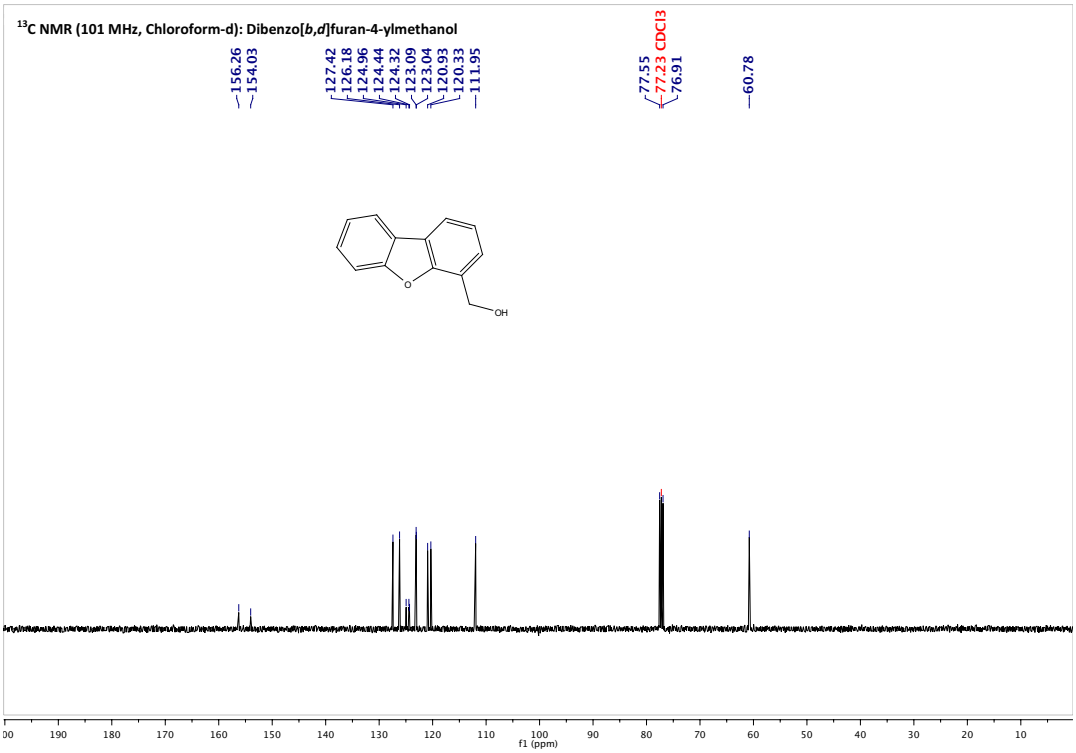

1 HNMR (400 MHz, Chloroform-d): (4-(dibenzo[b,d]thiophen-4-yl)phenyl)methanol
8.21
8.19
8.18
8.18
8.17
8.16
8.15
7.77
7.76
7.75
7.58
7.57
7.56
7.55
7.53
7.52
7.50
7.49
7.49
7.48
7.48
7.48
7.47
7.46
7.46
7.46
7.26 CDCl3
4.82
4.80
1.59
OH
C (m) 8.20
D (m) 7.84
E (m) 7.50
B (dd) 8.17
A (m) 7.76
F (d) 4.81
1.03 1.00 0.90 1.97 5.82
2.35
f1 (ppm)

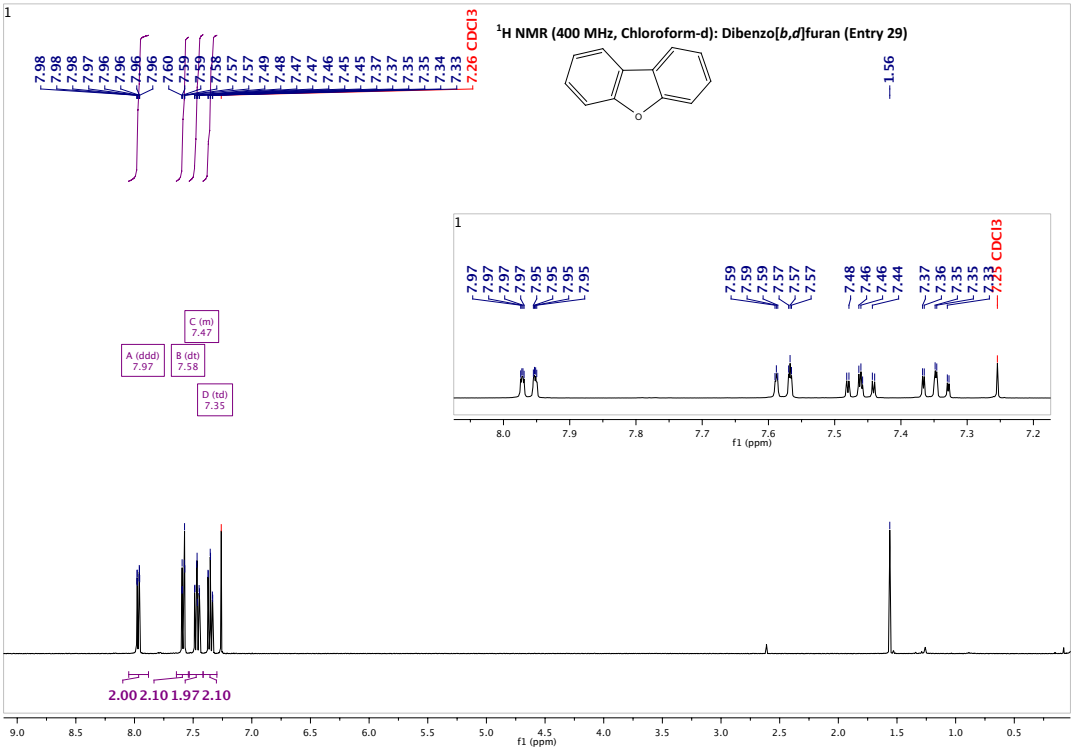

13C NMR (101 MHz, Chloroform-d): (4-(dibenzo[b,d]thiophen-4-yl)phenyl)methanol
140.83
140.21
139.73
138.76
136.86
136.45
135.97
128.69
127.64
127.07
127.03
125.33
124.62
122.83
121.95
120.71
77.55
77.23 CDCl3
76.91
65.37
S
OH
f1 (ppm)

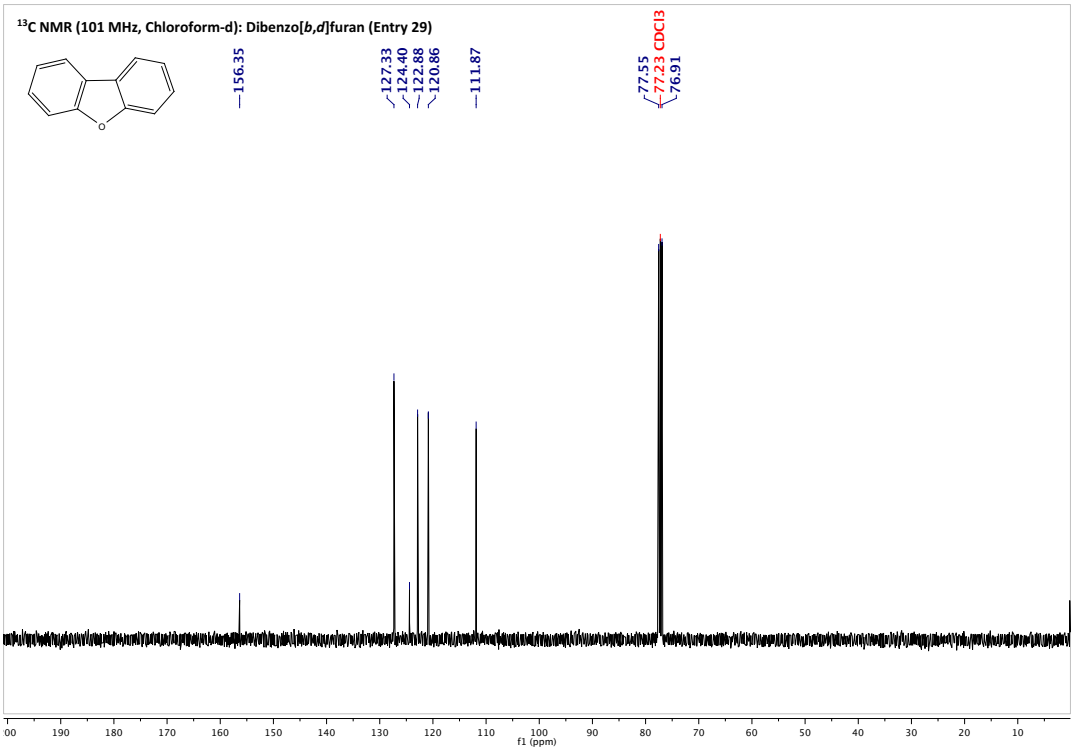

1H NMR (400 MHz, Chloroform-d): 4-phenyldibenzo[b,d]thiophene (entry 28)
7.26 CDCl3
S
D (m) 8.20
B (m) 7.85
E (m) 7.51
C (dd) 8.17
A (m) 7.76
0.91 1.00 0.95 1.93 6.87
f1 (ppm)

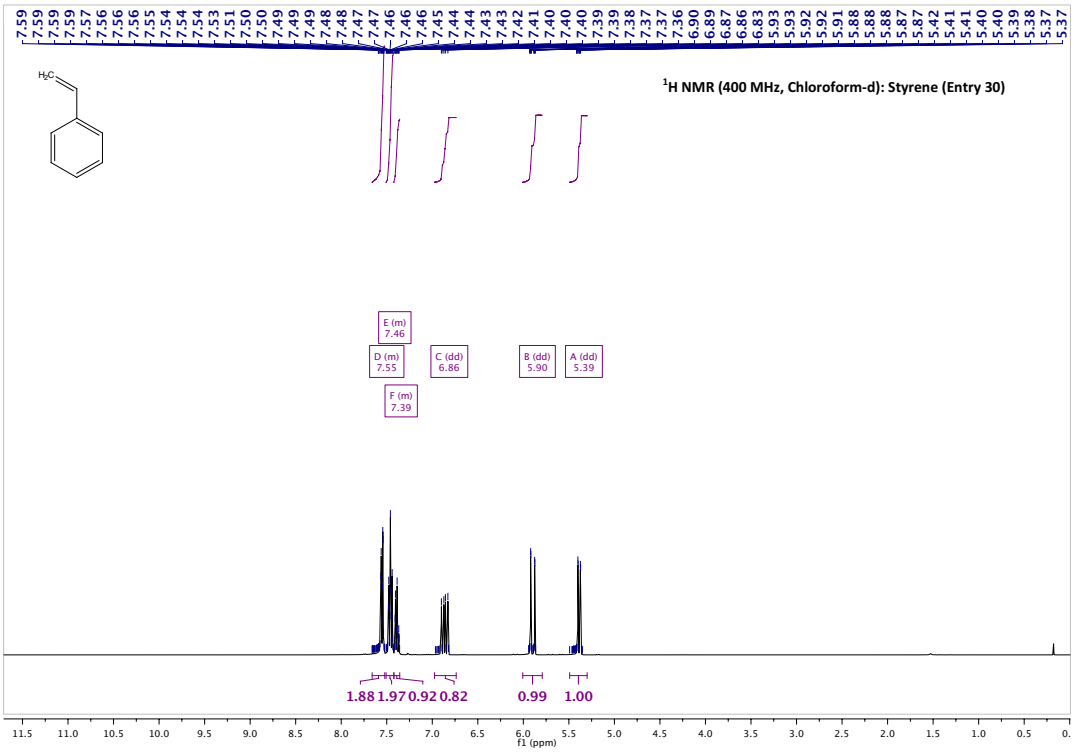

13C NMR (101 MHz, Chloroform-d): 4-phenyldibenzo[b,d]thiophene (Entry 28)
140.80
139.78
138.80
137.23
136.41
135.99
129.01
128.48
128.22
127.11
127.00
125.31
124.58
122.82
121.94
120.65
77.55
77.23 CDCl3
76.91
f1 (ppm)

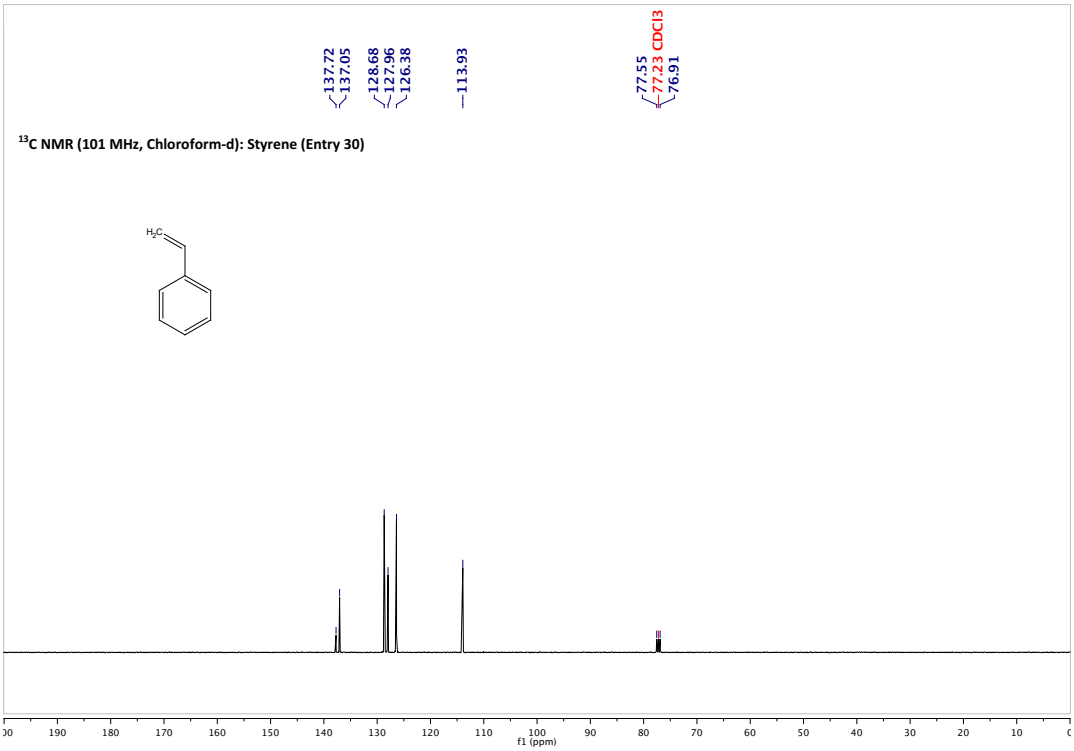

1H NMR (400 MHz, Chloroform-d): Dibenzo[b,d]furan-4-ylmethanol
7.96
7.96
7.94
7.94
7.94
7.94
7.89
7.89
7.88
7.87
7.60
7.58
7.58
7.58
7.48
7.47
7.47
7.46
7.46
7.46
7.37
7.37
7.36
7.35
7.33
7.31
7.26 CDCl3
5.08
2.24
B (dd) 7.88
D (m) 7.47
A (ddd) 7.95
C (dt) 7.59
E (m) 7.35
F (s) 5.08
G (s) 2.24
1.00 1.14 1.01 2.19 2.24
2.16
1.12
f1 (ppm)

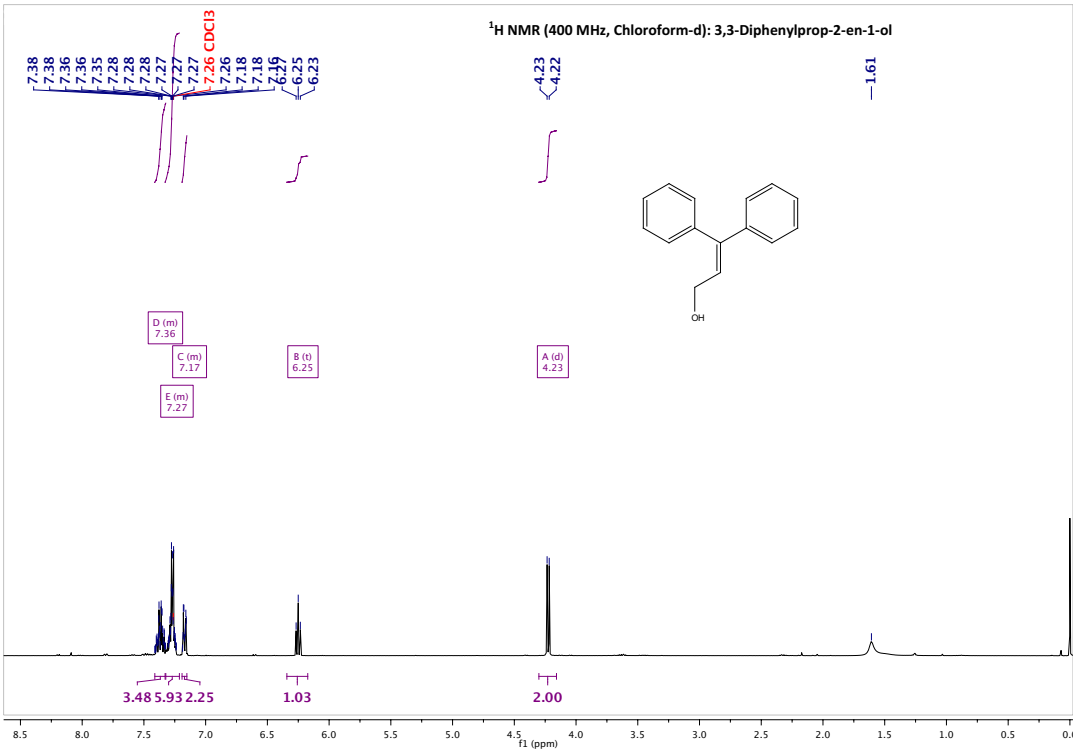

13C NMR (101 MHz, Chloroform-d): Dibenzo[b,d]furan-4-ylmethanol
156.26
154.03
127.42
126.18
124.96
124.44
124.32
123.09
123.04
120.93
120.33
111.95
77.55
77.23 CDCl3
76.91
60.78
OH
f1 (ppm)

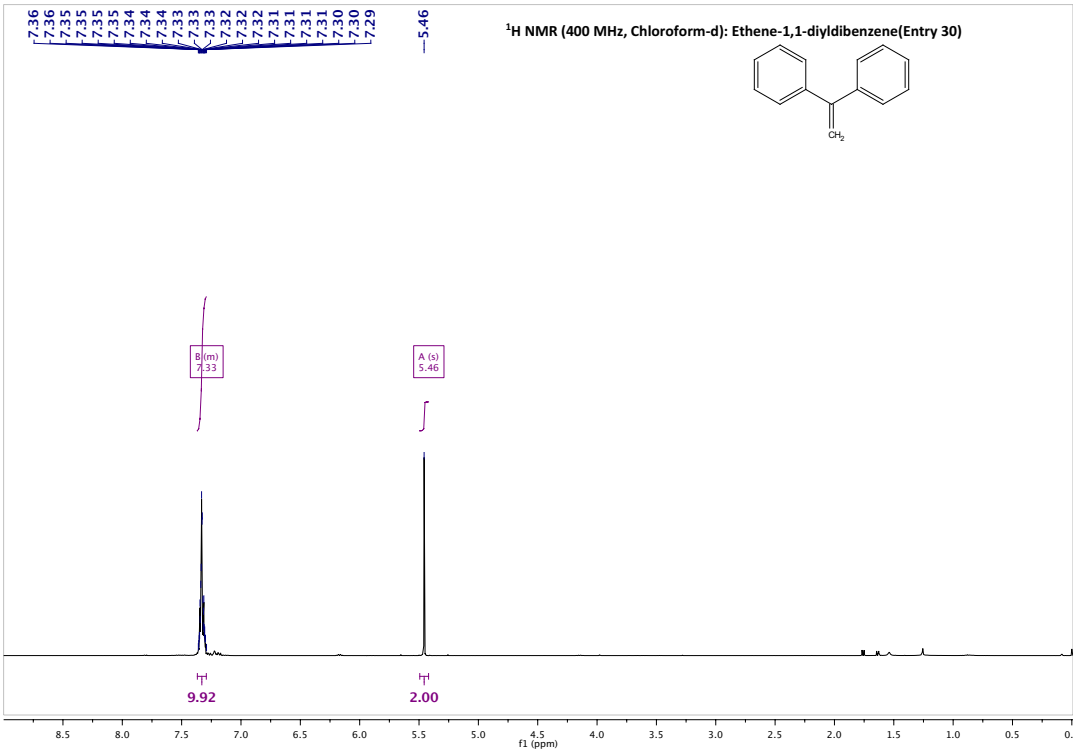

1H NMR (400 MHz, Chloroform-d): Dibenzo[b,d]furan (Entry 29)
7.98
7.98
7.98
7.97
7.96
7.96
7.96
7.96
7.60
7.59
7.59
7.58
7.57
7.57
7.49
7.48
7.47
7.47
7.46
7.45
7.45
7.37
7.37
7.35
7.35
7.34
7.33
7.26 CDCl3
1.56
C (m) 7.47
A (ddd) 7.97
B (dt) 7.58
D (td) 7.35
2.00 2.10 1.97 2.10
f1 (ppm)

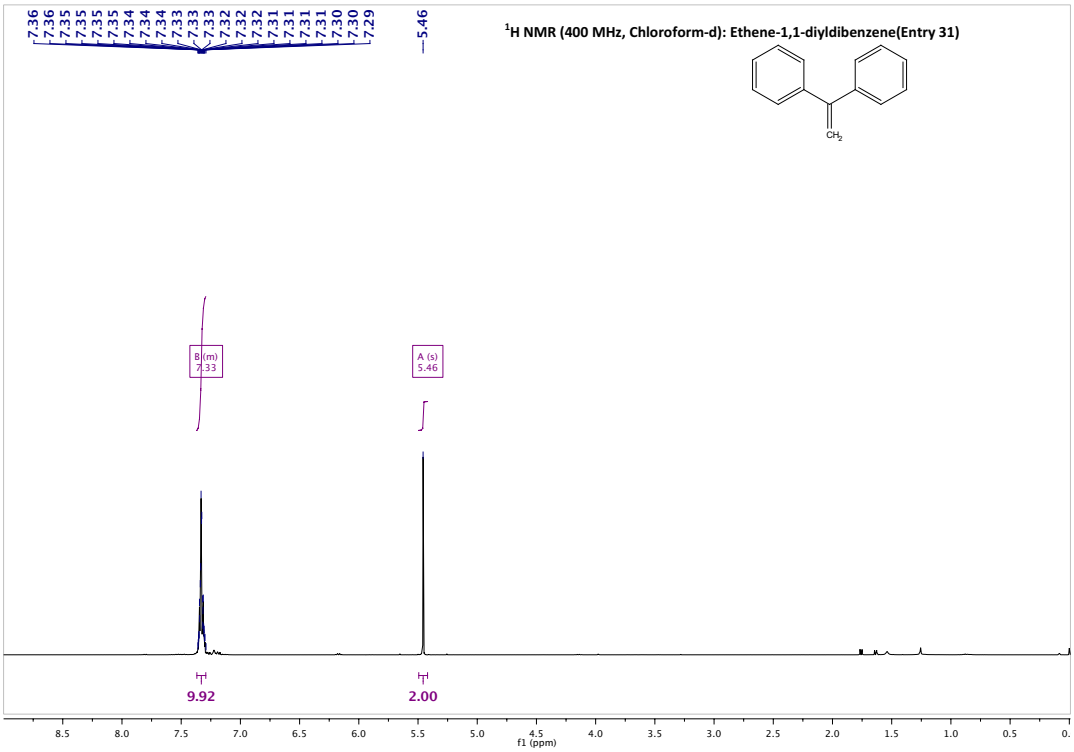

13C NMR (101 MHz, Chloroform-d): Dibenzo[b,d]furan (Entry 29)
156.35
127.33
124.40
122.88
120.86
111.87
77.55
77.23 CDCl3
76.91
f1 (ppm)

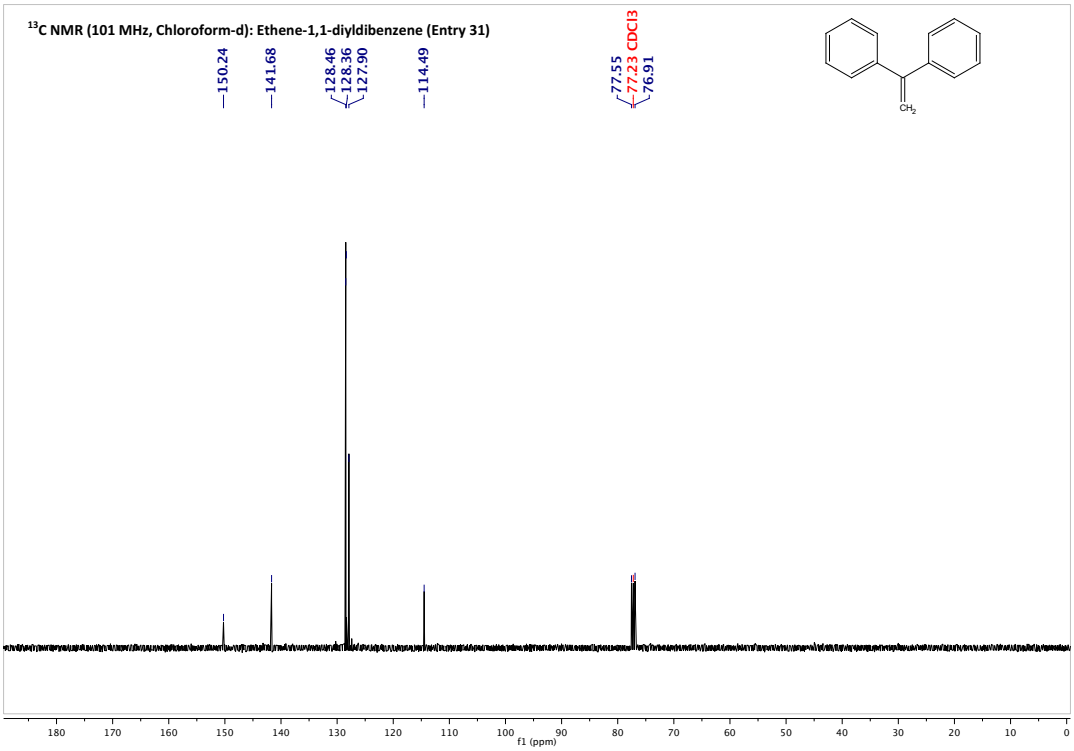

1H NMR (400 MHz, Chloroform-d): Styrene (Entry 30)
E (m) 7.46
D (m) 7.55
C (dd) 6.86
B (dd) 5.90
A (dd) 5.39
F (m) 7.39
1.88 1.97 0.92 0.82 0.99 1.00
f1 (ppm)

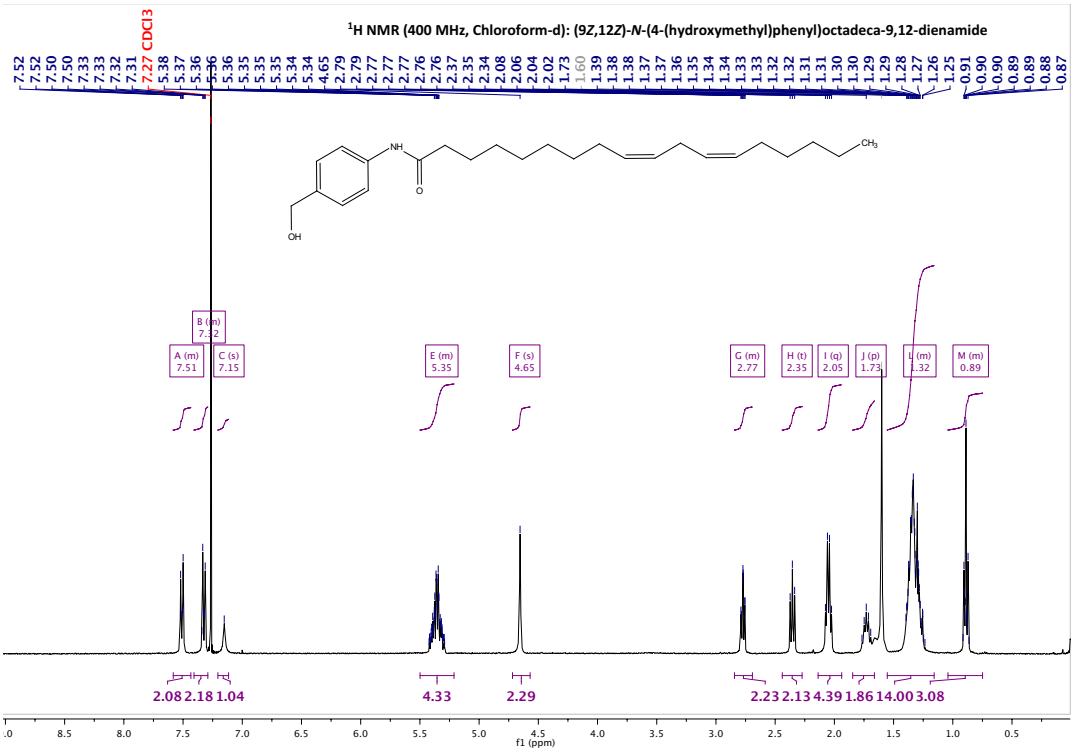

137.72
137.05
128.68
127.96
126.38
113.93
77.55
77.23 CDCl3
76.91
13C NMR (101 MHz, Chloroform-d): Styrene (Entry 30)
H2C
f1 (ppm)

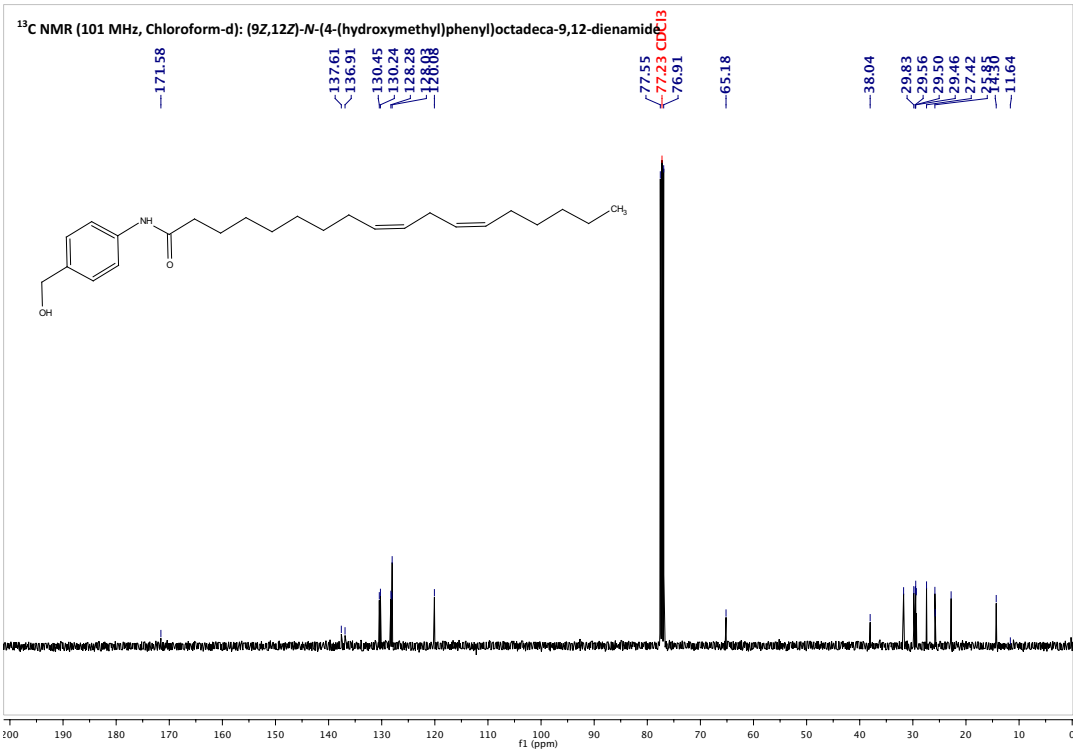

1H NMR (400 MHz, Chloroform-d): 3,3-Diphenylprop-2-en-1-ol
7.38
7.38
7.36
7.36
7.35
7.28
7.28
7.28
7.27
7.27
7.27
7.26 CDCl3
7.26
7.18
7.18
7.16
6.25
6.23
4.23
4.22
1.61
OH
D (m) 7.36
C (m) 7.17
E (m) 7.27
B (t) 6.25
A (d) 4.23
3.48 5.93 2.25
1.03
2.00
f1 (ppm)


7.36 7.36 7.35 7.35 7.35 7.34 7.34 7.34 7.33 7.33 7.33 7.32 7.32 7.31 7.31 7.31 7.30 7.30 7.29
5.46
^{1}H NMR (400 MHz, Chloroform-d): Ethene-1,1-diyldibenzene(Entry 30)
CH2
B (m) 7.33
A (s) 5.46
9.92
2.00
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 0.
f1 (ppm)

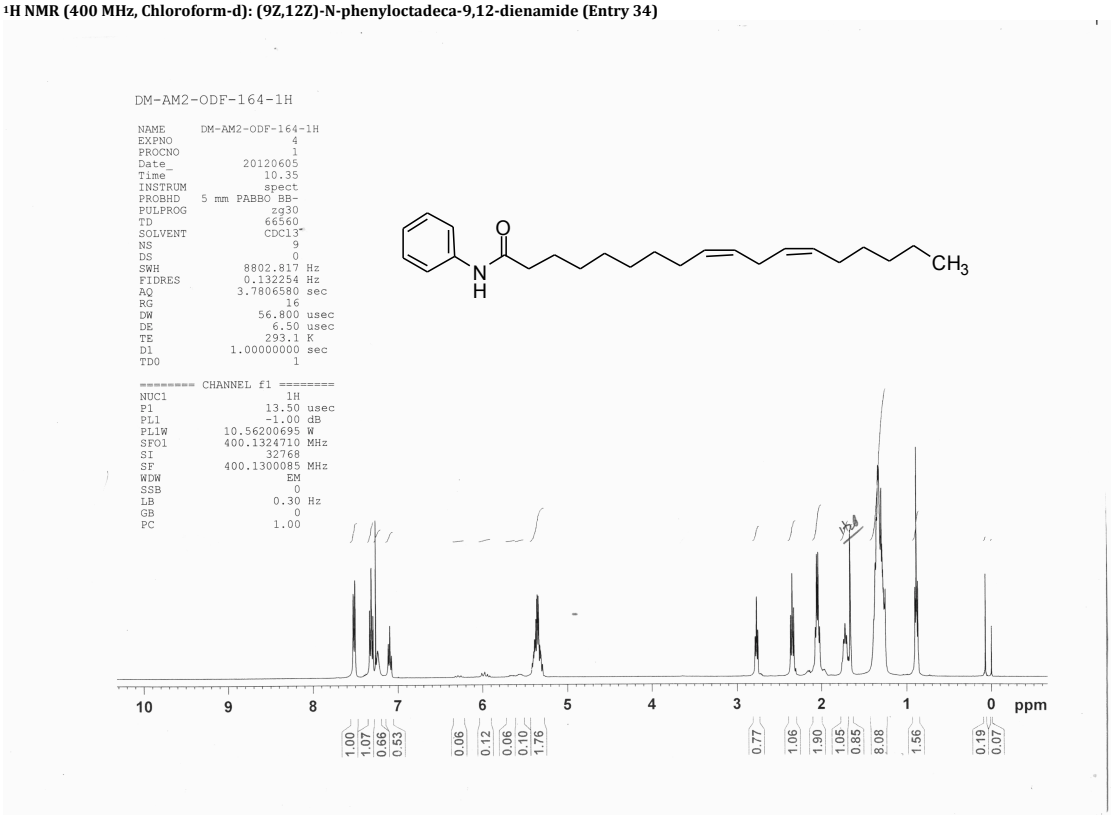

7.36 7.36 7.35 7.35 7.35 7.34 7.34 7.34 7.33 7.33 7.33 7.32 7.32 7.31 7.31 7.31 7.30 7.30 7.29
5.46
^{1}H NMR (400 MHz, Chloroform-d): Ethene-1,1-diyldibenzene(Entry 31)
CH2
B (m) 7.33
A (s) 5.46
9.92
2.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.
f1 (ppm)


13C NMR (101 MHz, Chloroform-d): Ethene-1,1-diyldibenzene (Entry 31)
150.24
141.68
128.46
128.36
127.90
114.49
77.55
77.23 CDCl3
76.91
CH2
f1 (ppm)


1H NMR (400 MHz, Chloroform-d): (9Z,12Z)-N-(4-(hydroxymethyl)phenyl)octadeca-9,12-dienamide
7.27 CDCl3
NH
O
OH
CH3
B (m) 7.32
A (m) 7.51
C (s) 7.15
E (m) 5.35
F (s) 4.65
G (m) 2.77
H (t) 2.35
I (q) 2.05
J (p) 1.73
L (m) 1.32
M (m) 0.89
2.08 2.18 1.04
4.33
2.29
2.23 2.13 4.39 1.86 14.00 3.08
f1 (ppm)

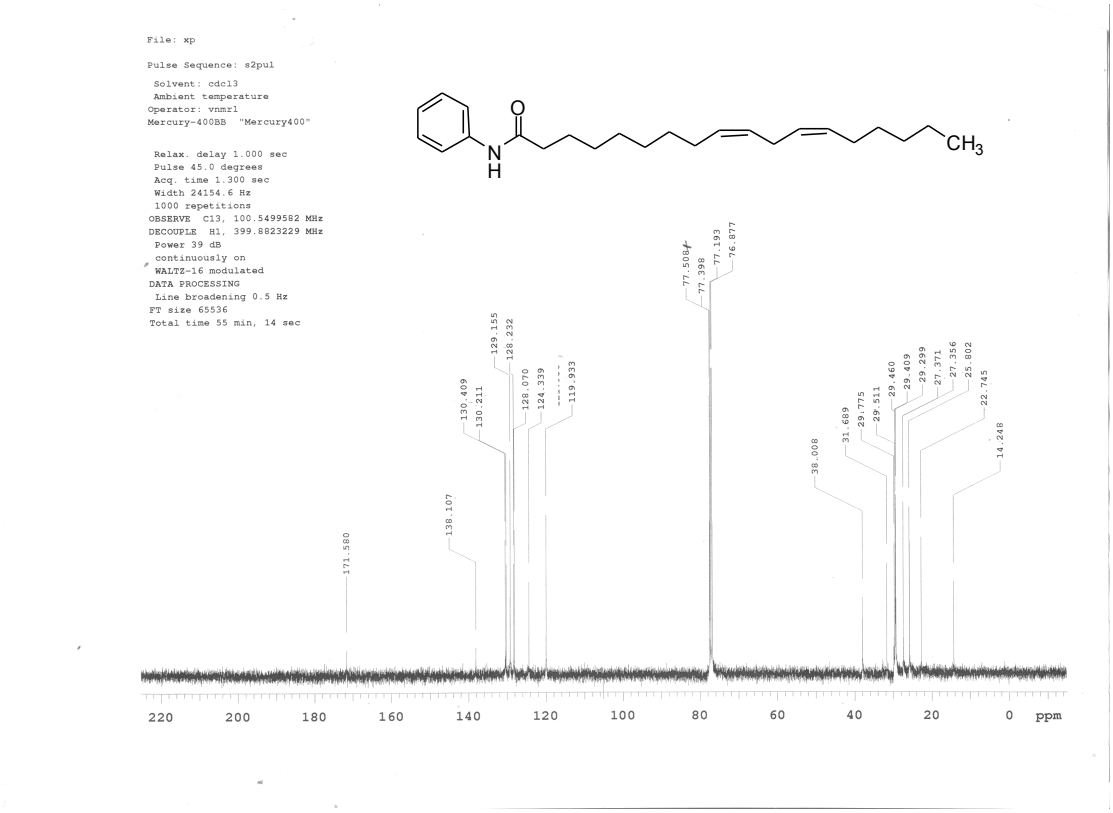


^{13}C NMR (101 MHz, Chloroform-d): (9*Z*,12*Z*)-*N*-(4-(hydroxymethyl)phenyl)octadeca-9,12-dienamide

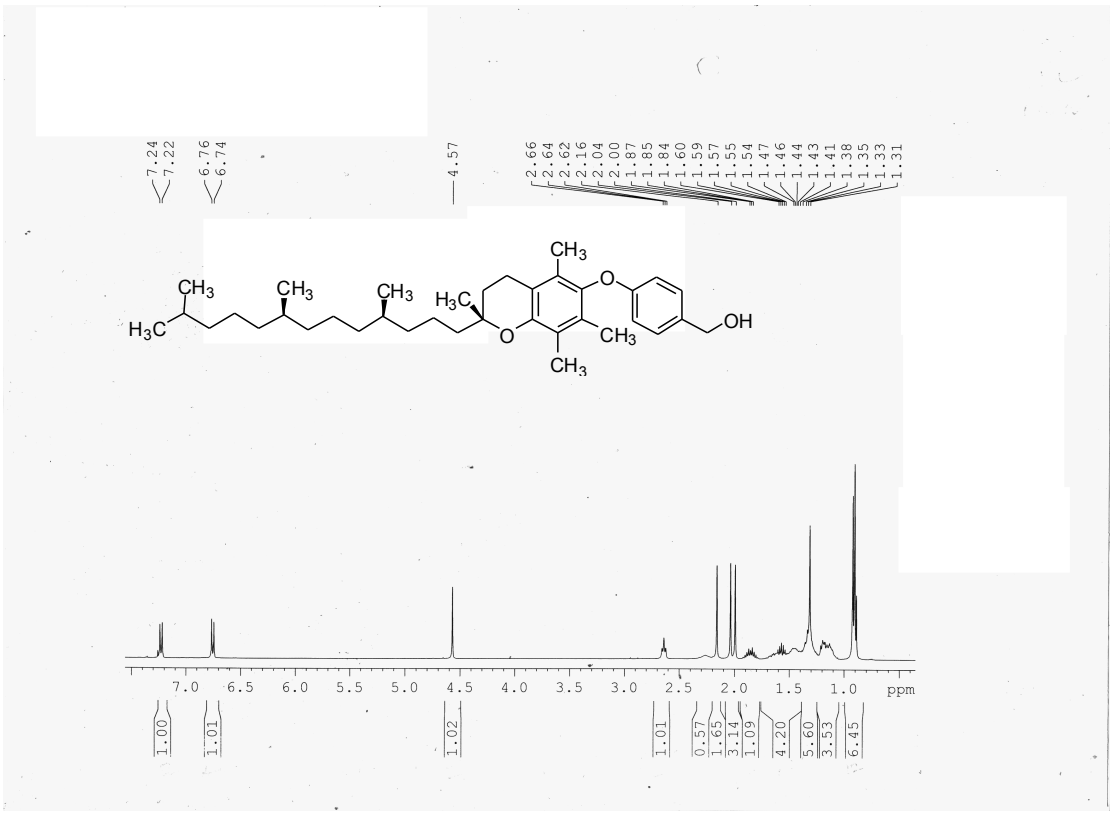


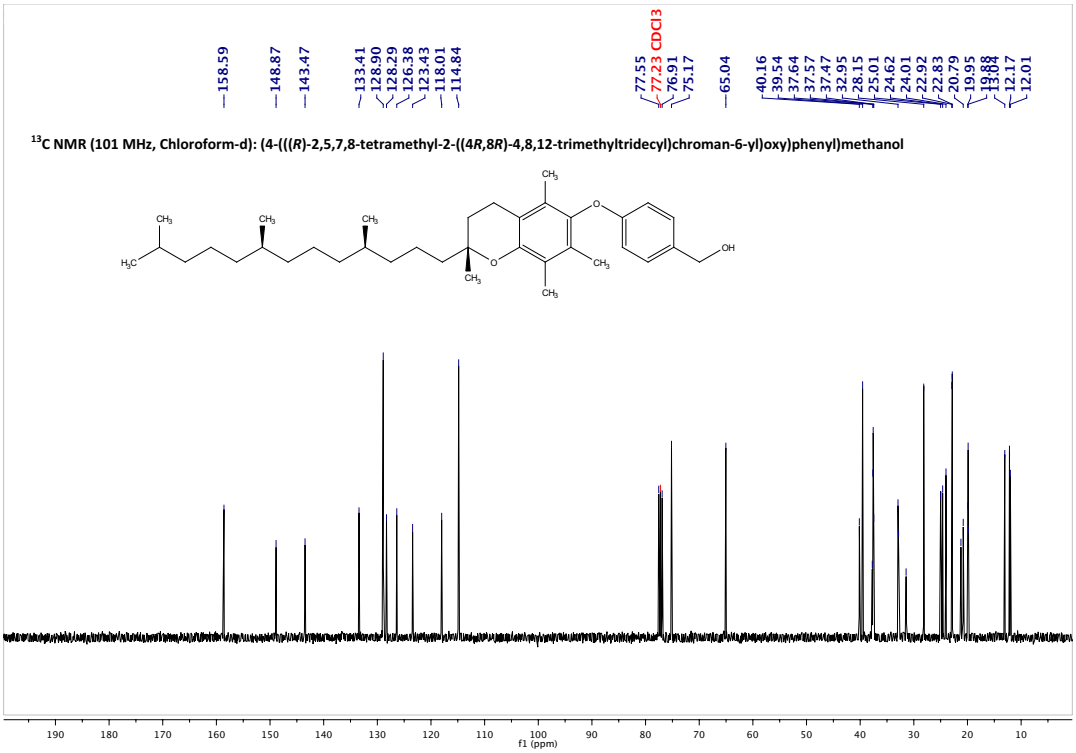
^{1}H NMR (400 MHz, Chloroform-d): (9Z,12Z)-N-phenyloctadeca-9,12-dienamide (Entry 34)

^{13}C NMR (101 MHz, Chloroform-d): (9Z,12Z)-N-phenyloctadeca-9,12-dienamide (Entry 33)



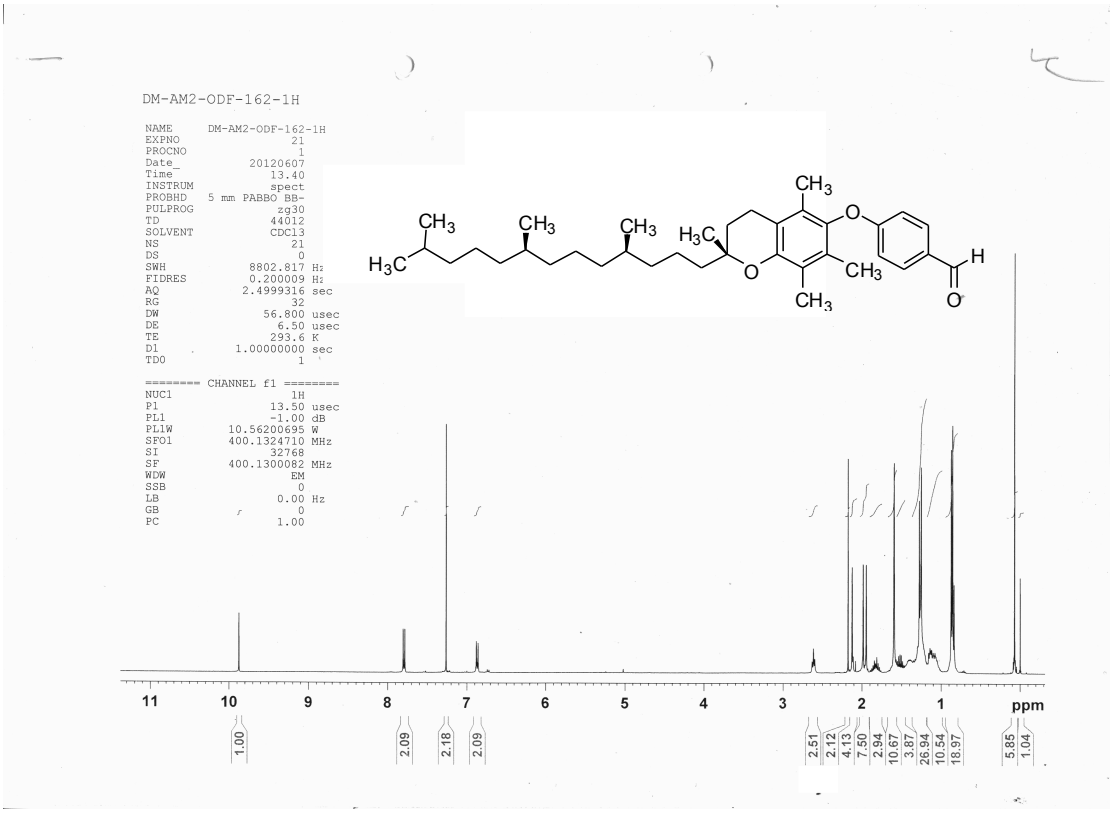
^{1}H NMR (400 MHz, Chloroform-d): (4-((R)-2,5,7,8-tetramethyl-2-((4R,8R)-4,8,12-trimethyltridecyl)chroman-6-yloxy)phenyl)methanol

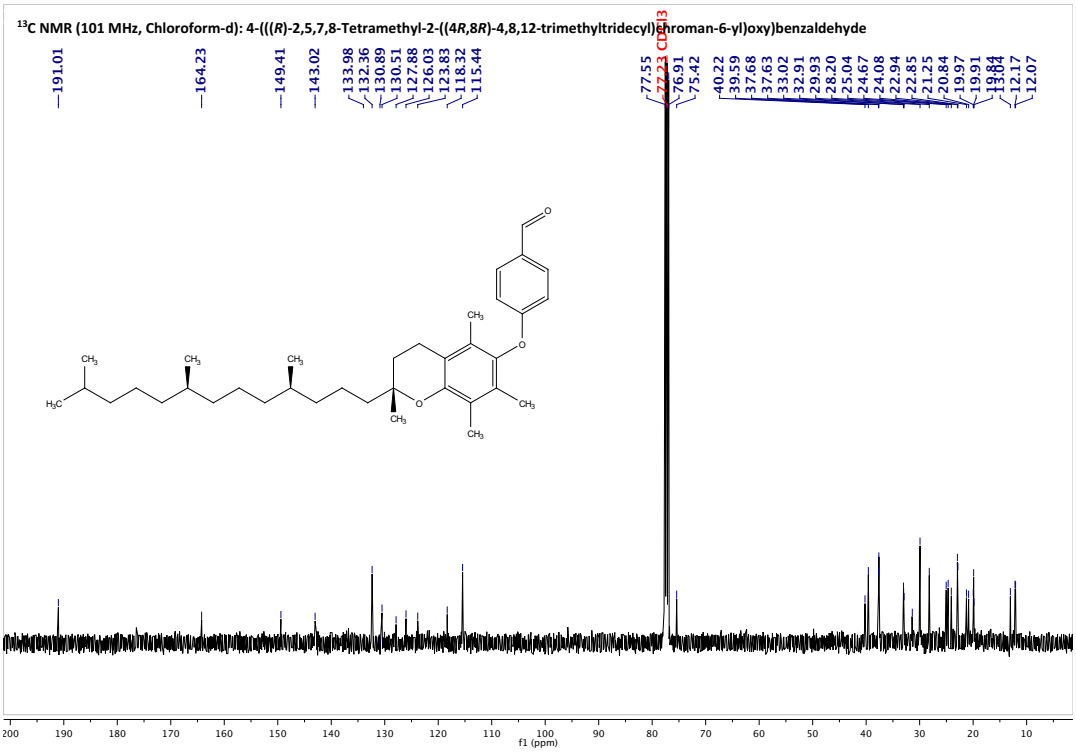




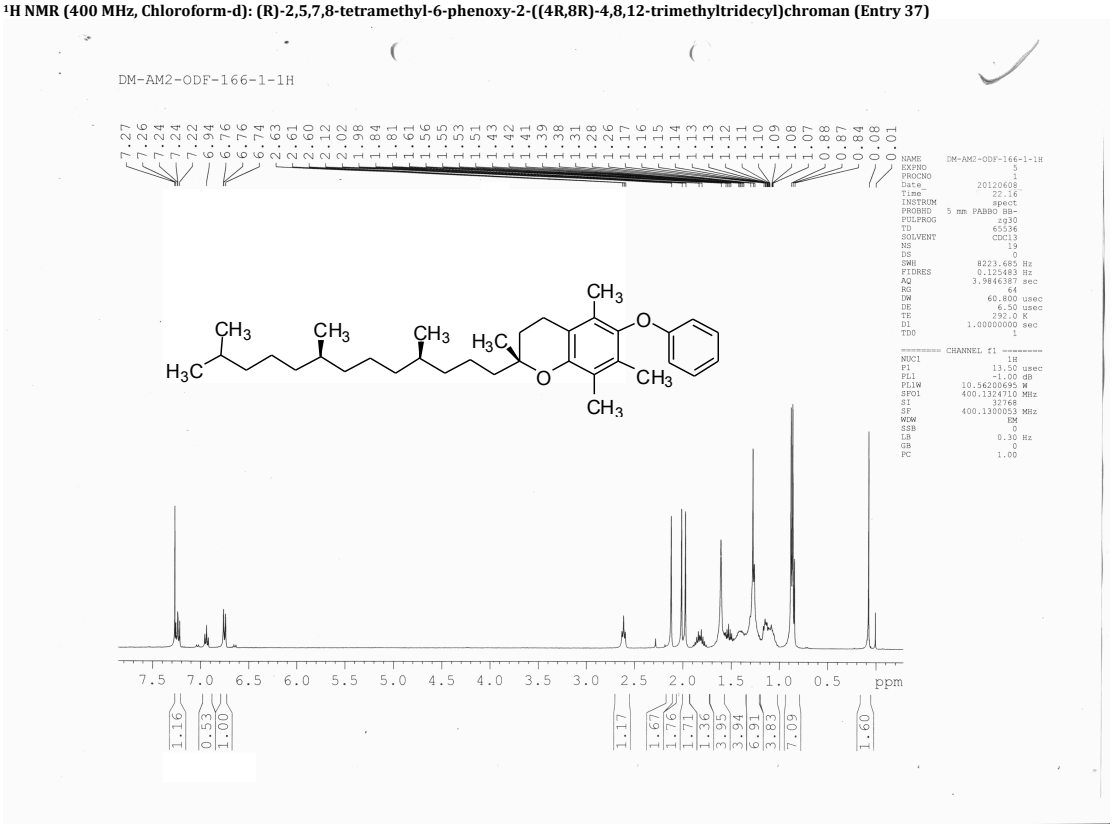
^{13}C NMR (101 MHz, Chloroform-d): (4-(((*R*)-2,5,7,8-tetramethyl-2-((4*R*,8*R*)-4,8,12-trimethyltridecyl)chroman-6-yl)oxy)phenyl)methanol

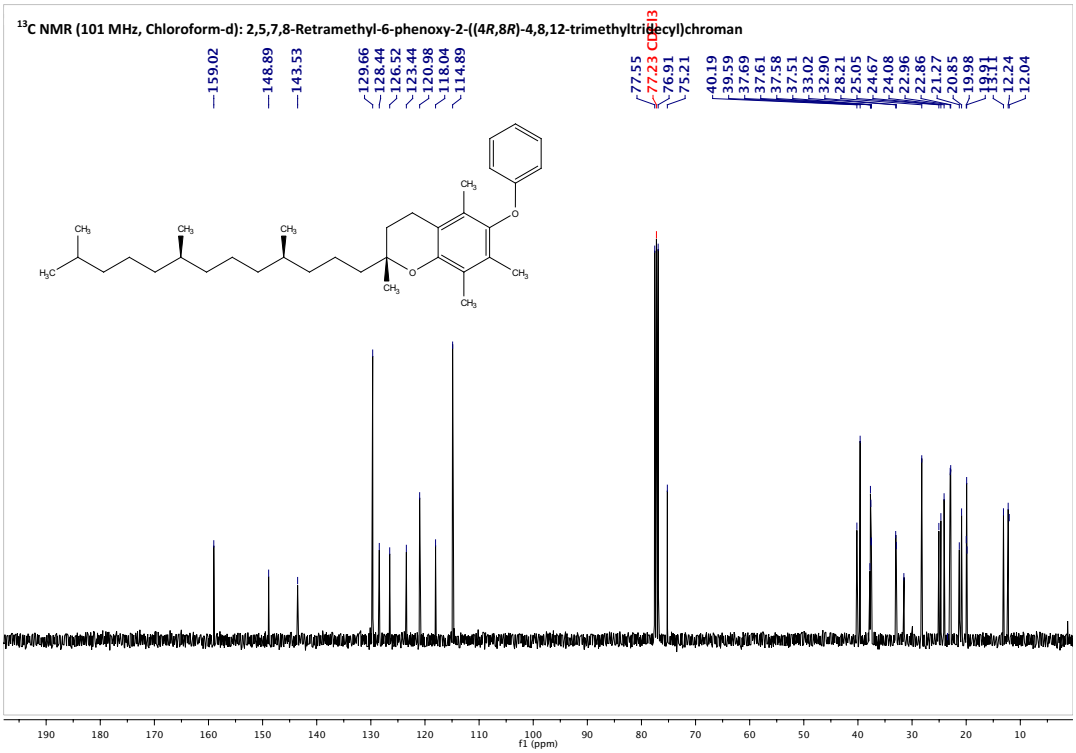
^{1}H NMR (400 MHz, Chloroform-d): 4-((R)-2,5,7,8-Tetramethyl-2-((4R,8R)-4,8,12-trimethyltridecyl)chroman-6-yloxy)benzaldehyde

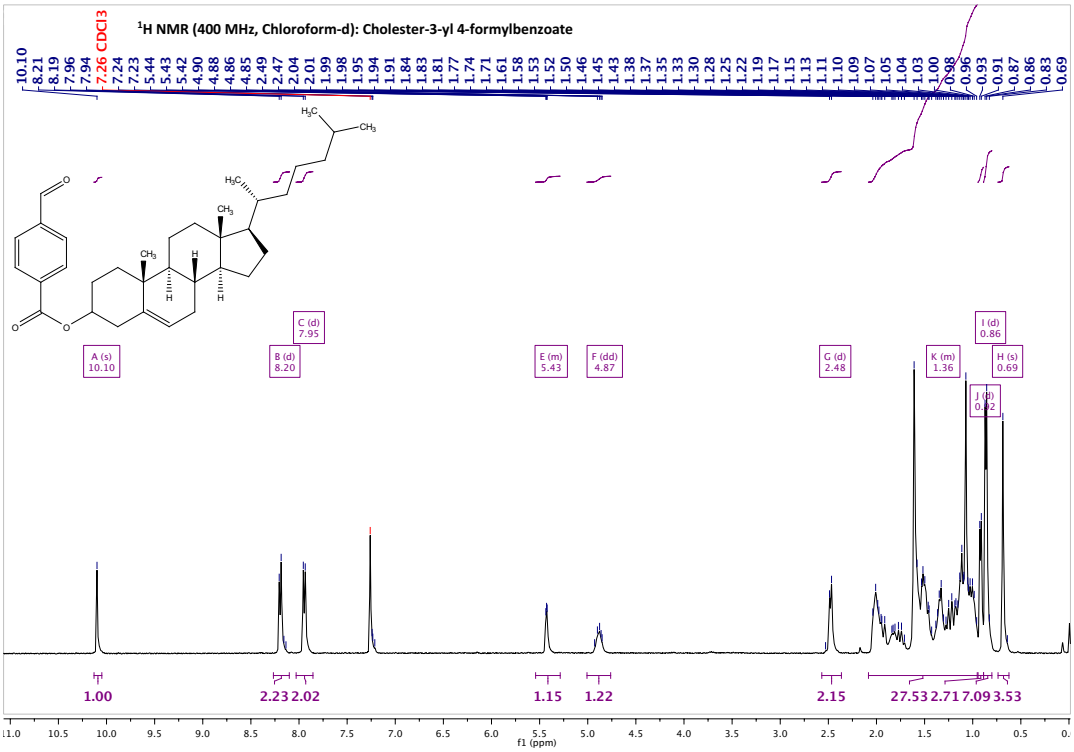




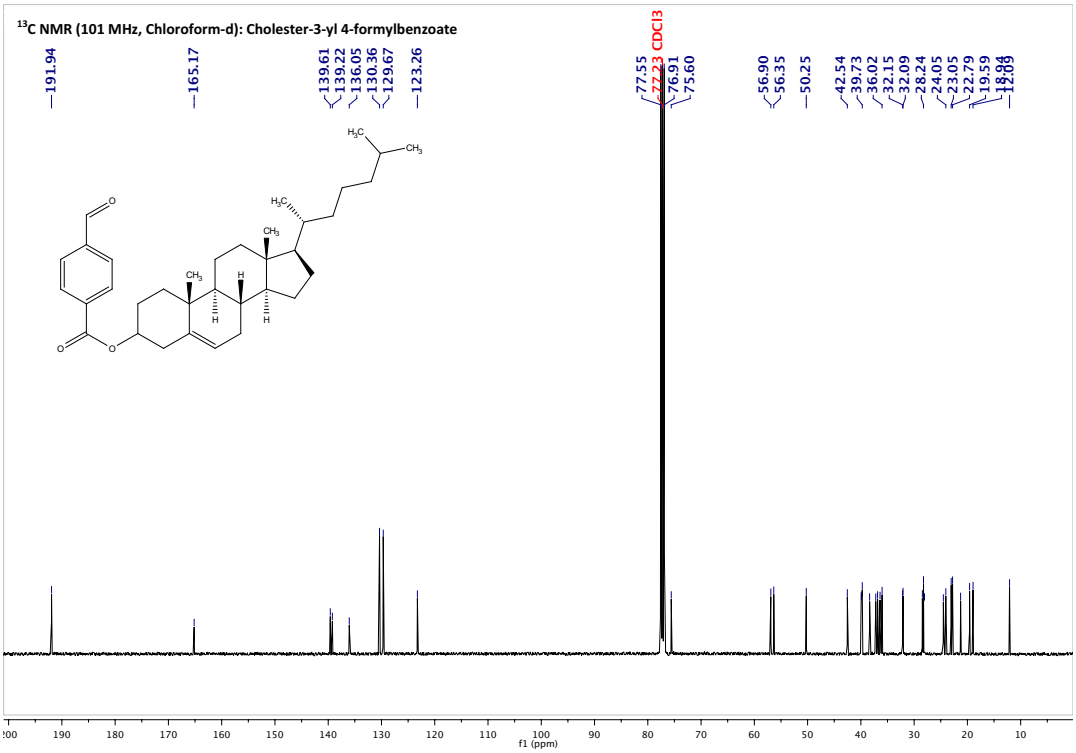
1H NMR (400 MHz, Chloroform-d): (R)-2,5,7,8-tetramethyl-6-phenoxy-2-((4R,8R)-4,8,12-trimethyltridecyl)chroman (Entry 37)



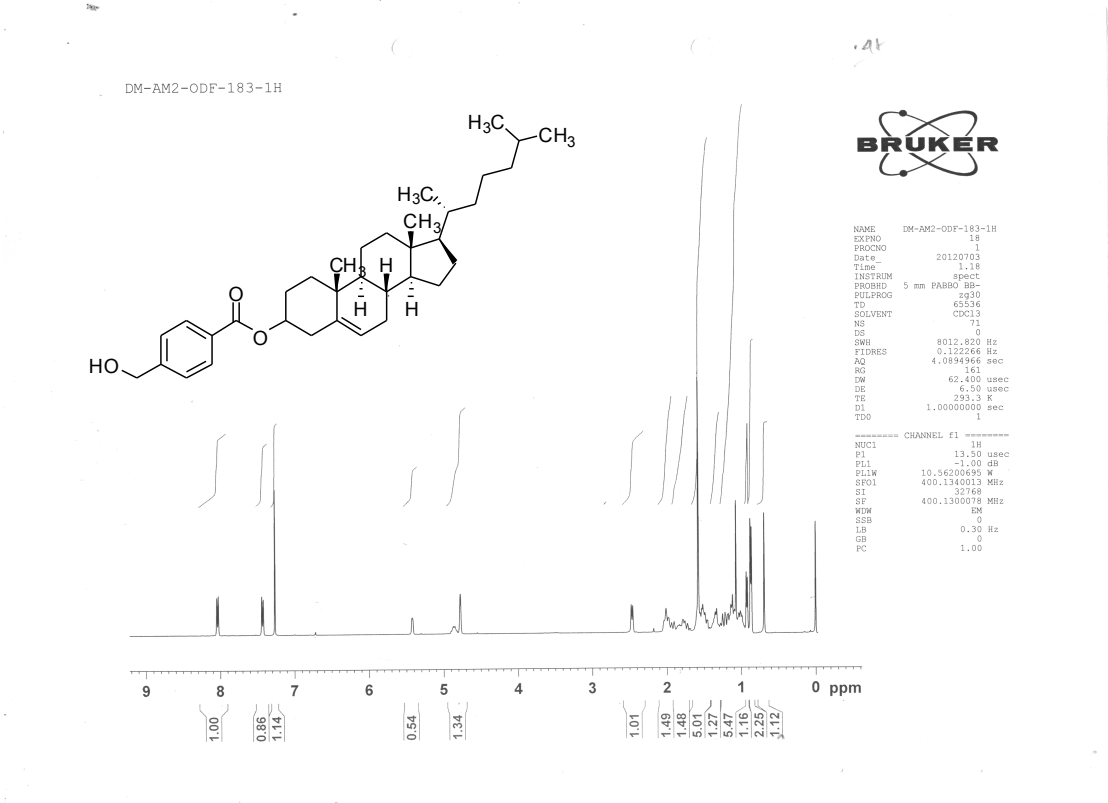

13C NMR (101 MHz, Chloroform-d): 2,5,7,8-Retramethyl-6-phenoxy-2-((4R,8R)-4,8,12-trimethyltridecyl)chroman
159.02
148.89
143.53
129.66
128.44
126.52
123.44
120.98
118.04
114.89
77.55
77.23
CDCl3
76.91
75.21
40.19
39.59
37.69
37.61
37.58
37.51
33.02
32.90
28.21
25.05
24.67
24.08
22.96
22.86
21.27
20.85
19.98
19.91
13.11
12.24
12.04
f1 (ppm)

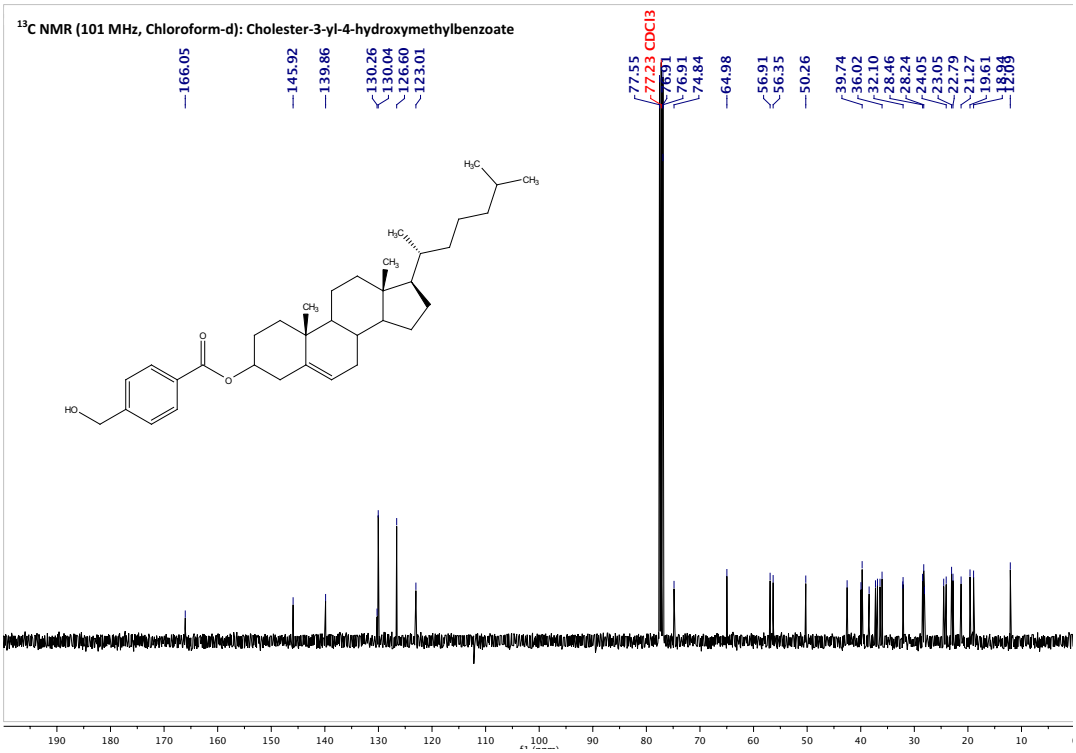

1H NMR (400 MHz, Chloroform-d): Cholester-3-yl 4-formylbenzoate
10.10
8.21
8.19
7.96
7.94
7.26
CDCl3
7.24
7.23
5.44
5.43
5.42
4.90
4.88
4.86
4.85
2.49
2.47
2.04
2.01
1.99
1.98
1.95
1.94
1.91
1.84
1.83
1.81
1.77
1.74
1.71
1.61
1.58
1.53
1.52
1.50
1.46
1.45
1.43
1.38
1.37
1.35
1.33
1.30
1.28
1.25
1.22
1.19
1.17
1.15
1.13
1.11
1.10
1.09
1.07
1.05
1.04
1.03
1.00
0.98
0.96
0.93
0.91
0.87
0.86
0.83
0.69
A (s) 10.10
B (d) 8.20
C (d) 7.95
E (m) 5.43
F (dd) 4.87
G (d) 2.48
K (m) 1.36
I (d) 0.86
H (s) 0.69
J (d) 0.82
1.00
2.23
2.02
1.15
1.22
2.15
27.53
2.71
7.09
3.53
f1 (ppm)

^{13}C NMR (101 MHz, Chloroform-d): Cholester-3-yl 4-formylbenzoate

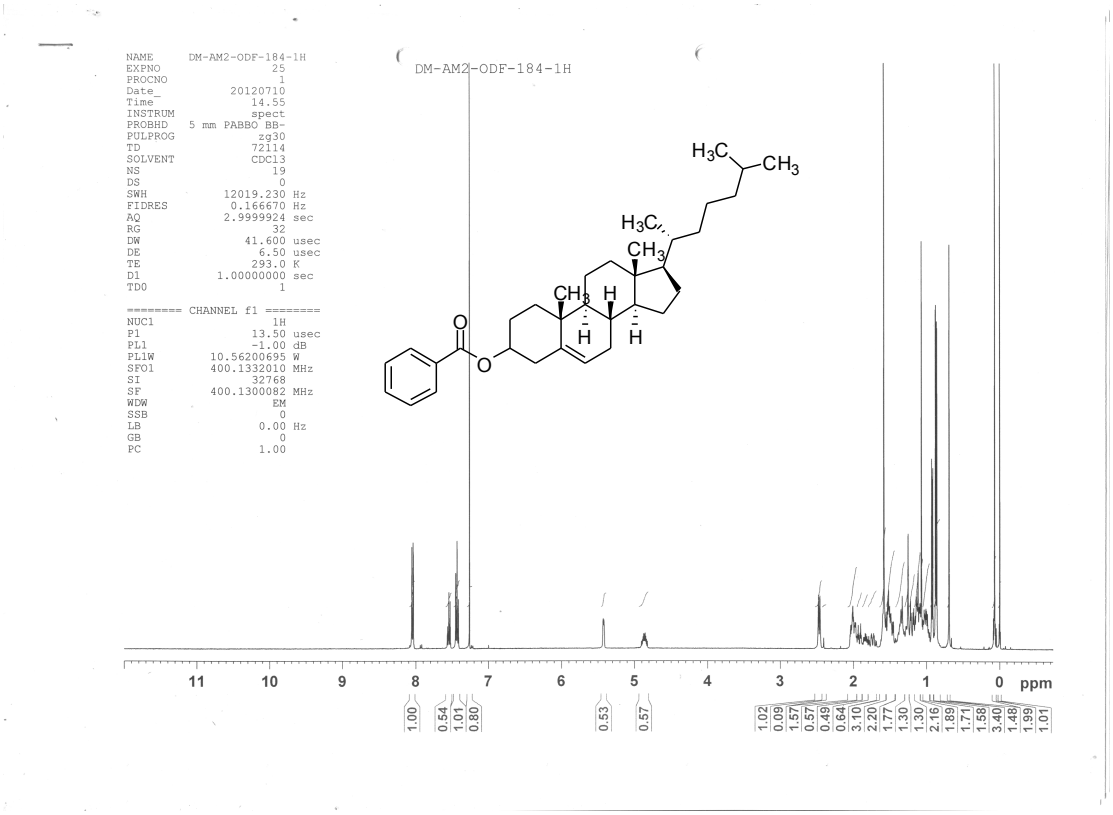


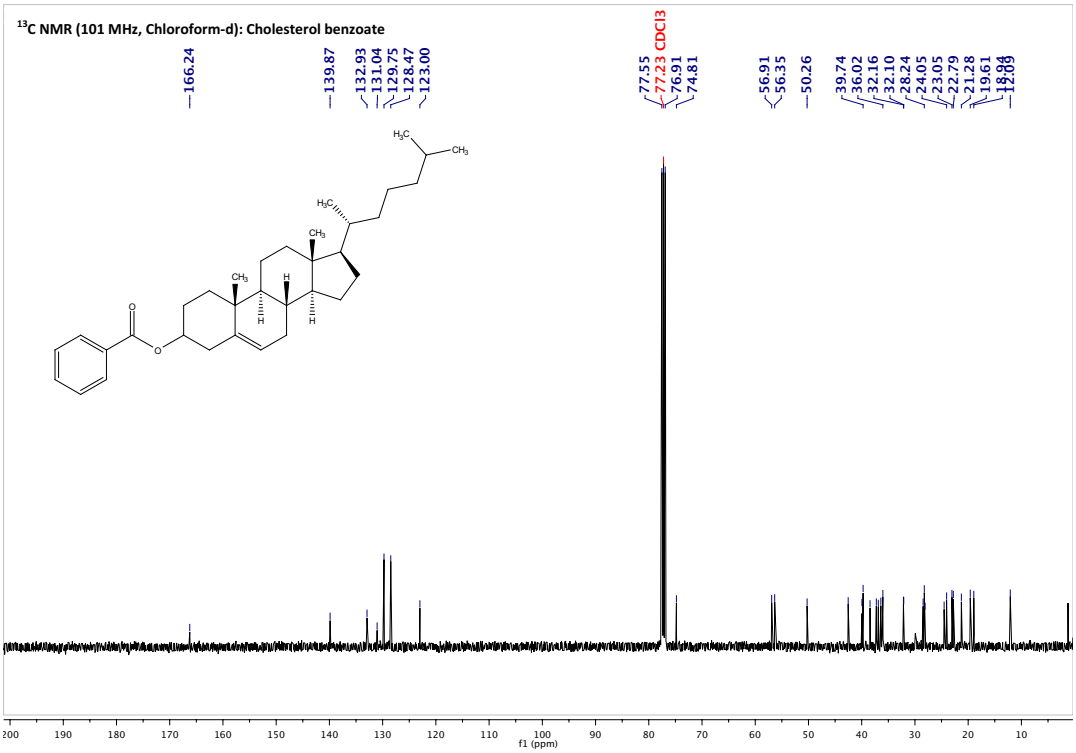
^{1}H NMR (400 MHz, Chloroform-d): Cholester-3-yl-4 hydroxymethyl benzoate



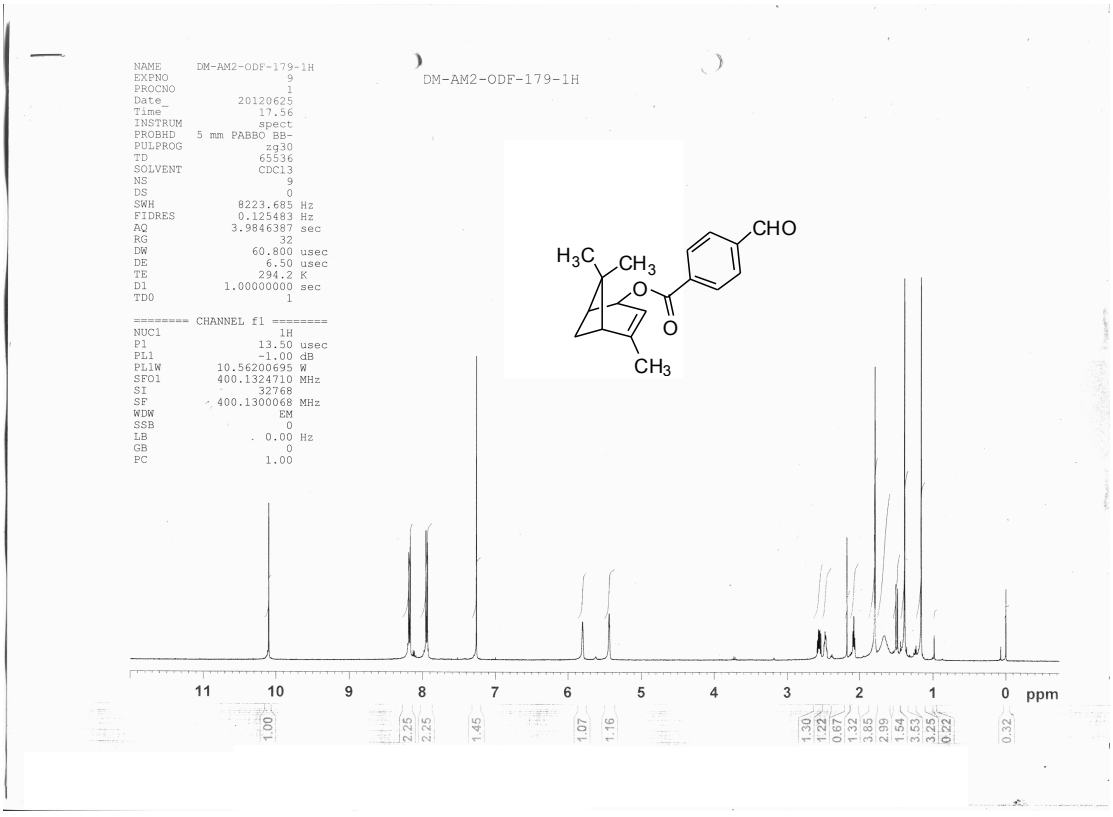


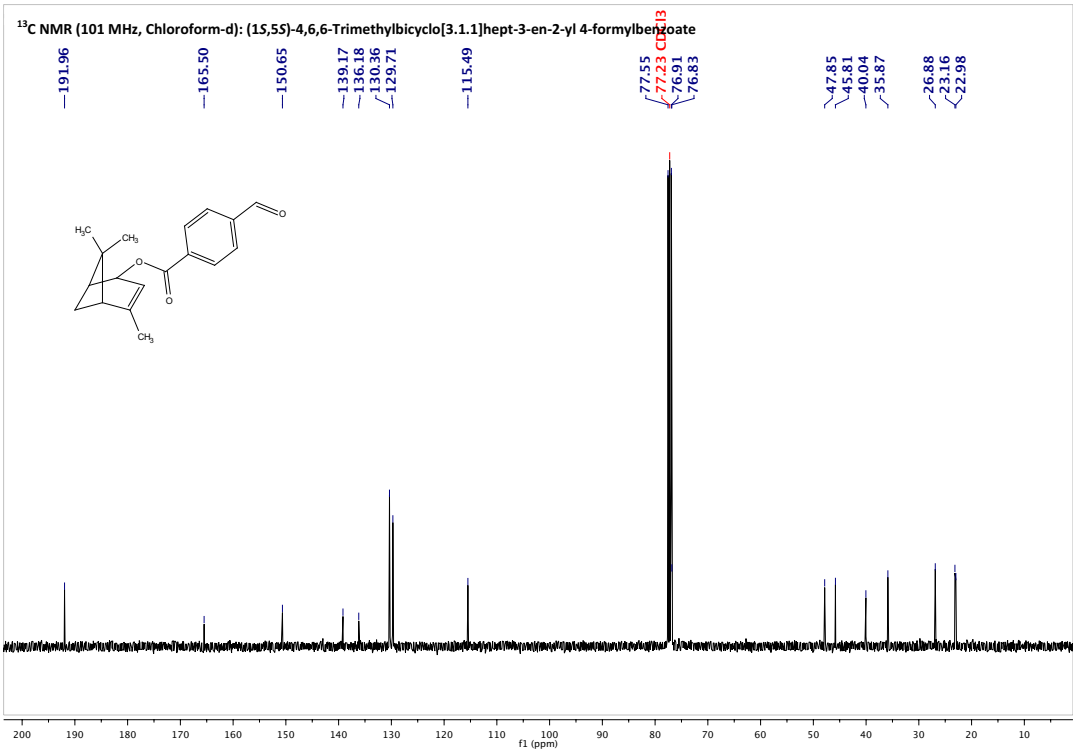
^{1}H NMR (400 MHz, Chloroform-d): Cholester-3-yl-benzoate (Entry 36)



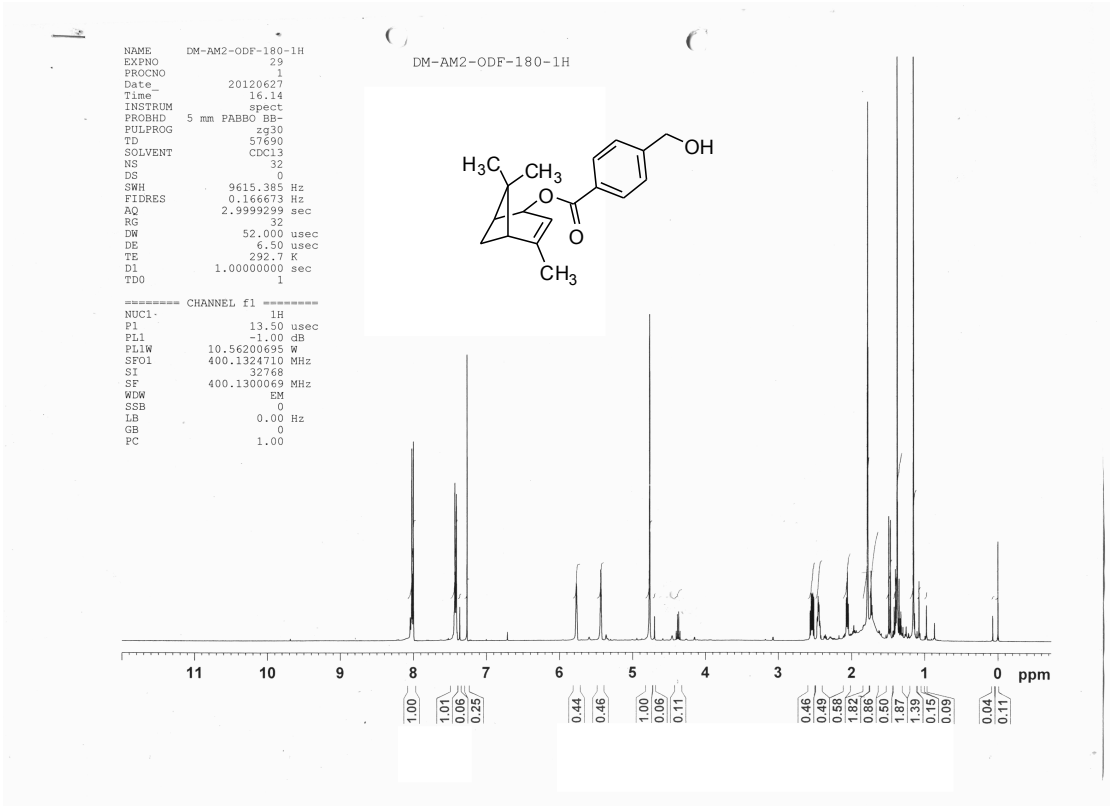


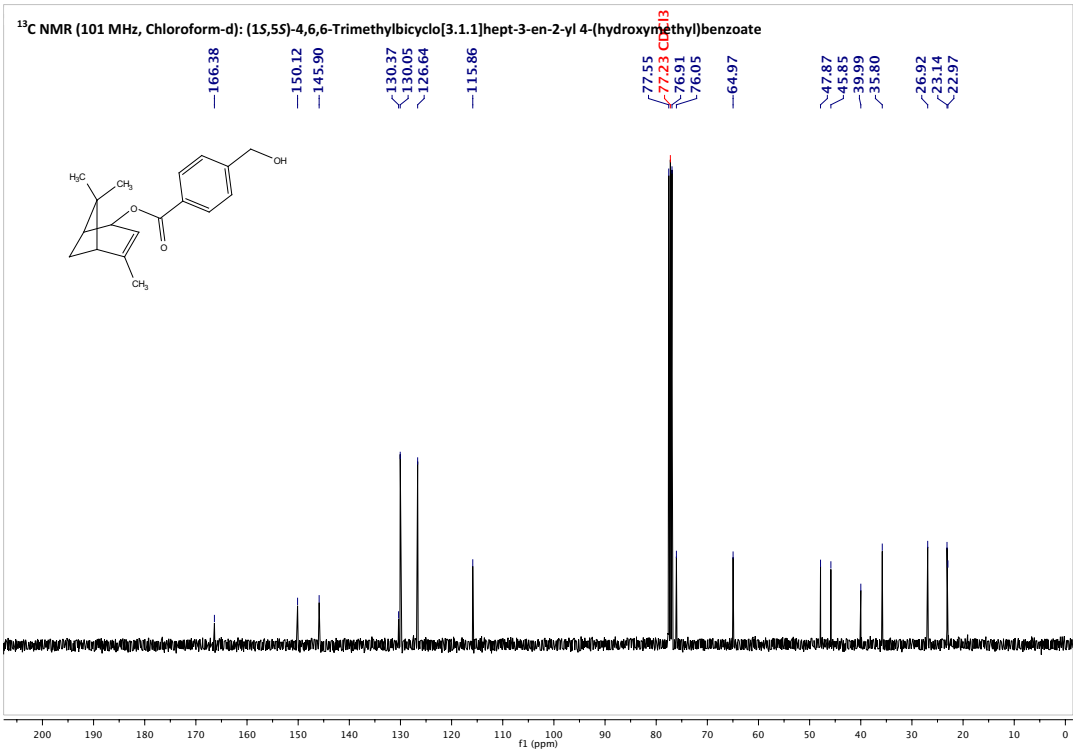
^{1}H NMR (400 MHz, Chloroform-d): 4,6,6-trimethylbicyclo[3.1.1]hept-3-en-2-yl 4-formylbenzoate



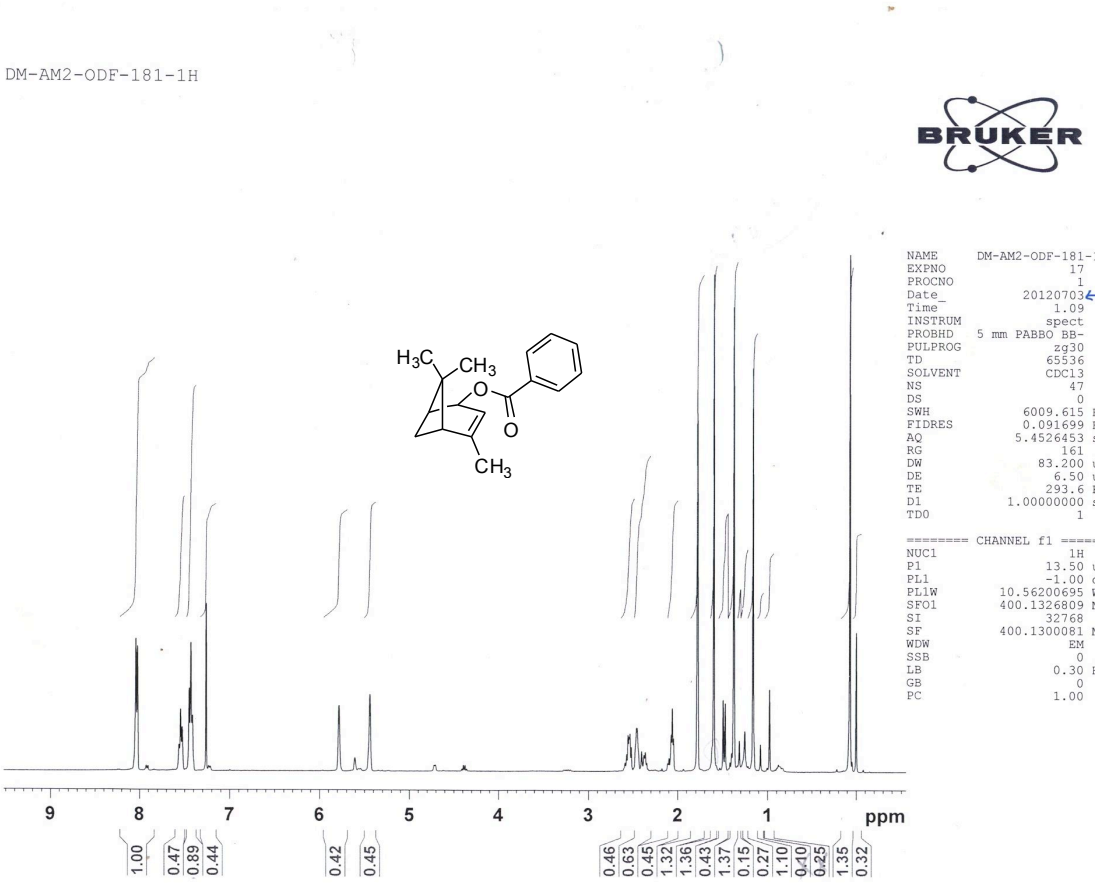


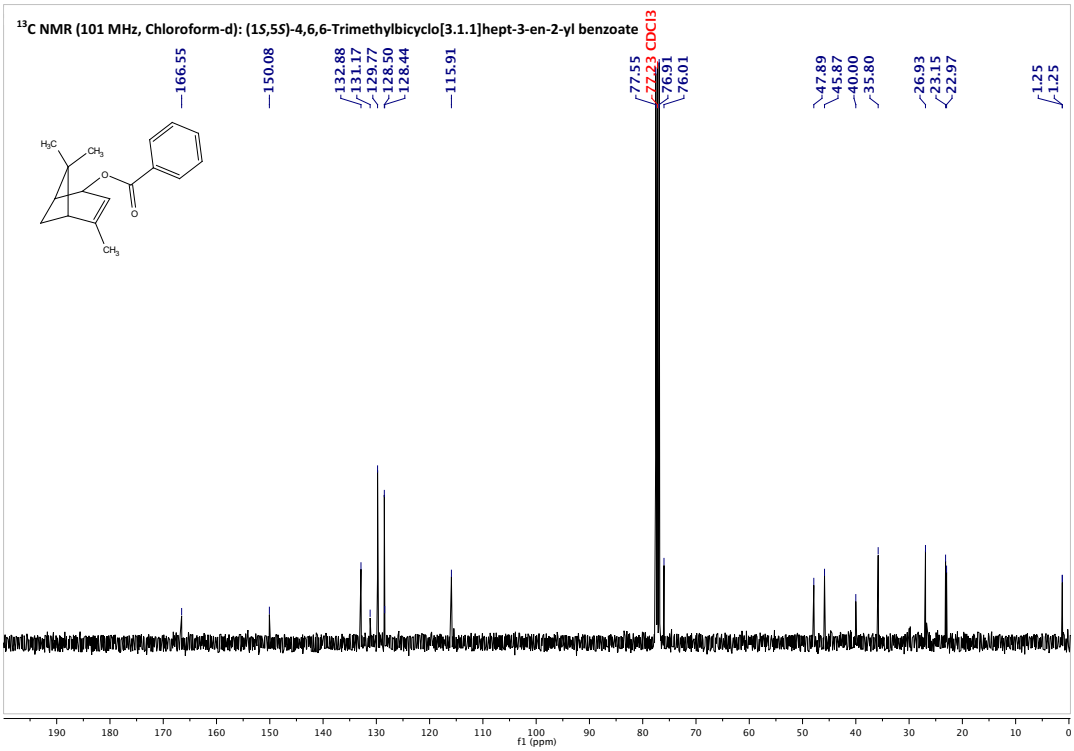
^{1}H NMR (400 MHz, Chloroform-d): 4,6,6-Trimethylbicyclo[3.1.1]hept-3-en-2-yl 4-(hydroxymethyl)benzoate





^{1}H NMR (400 MHz, Chloroform-d): Verbenol benzoate (Entry 35)




13C NMR (101 MHz, Chloroform-d): (1S,5S)-4,6,6-Trimethylbicyclo[3.1.1]hept-3-en-2-yl benzoate
166.55
150.08
132.88
131.17
129.77
128.50
128.44
115.91
77.55
77.23 CDCl3
76.91
76.01
47.89
45.87
40.00
35.80
26.93
23.15
22.97
1.25
1.25
H3C
CH3
O
O
CH3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)