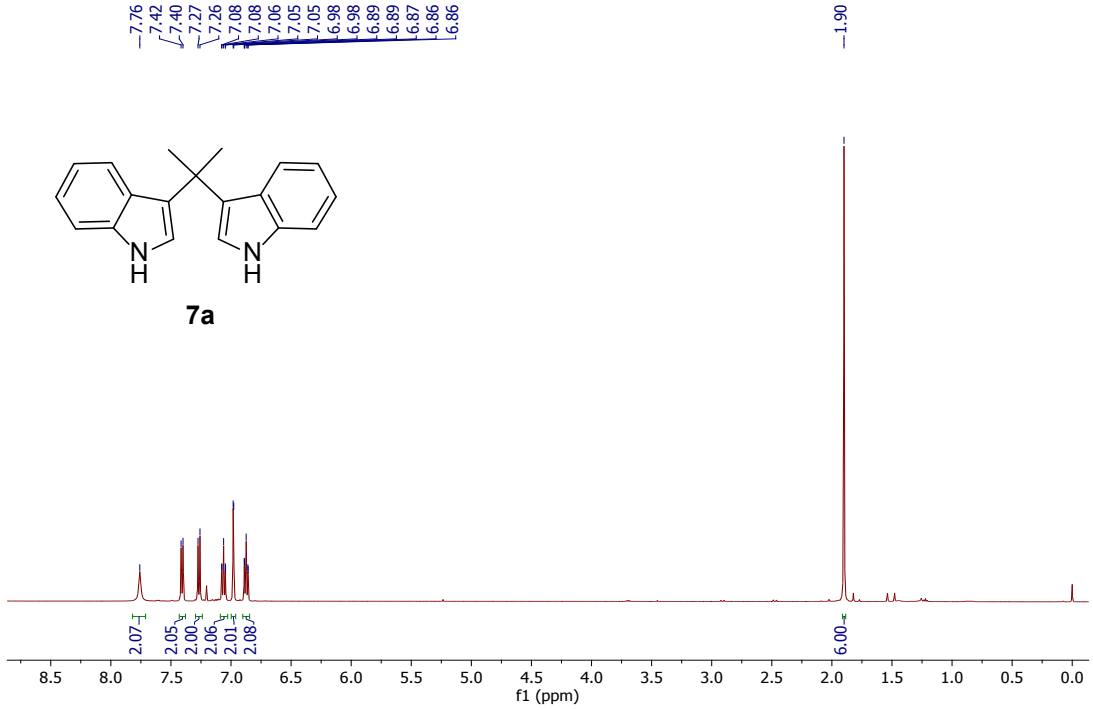
This journal is © The Royal Society of Chemistry 2013

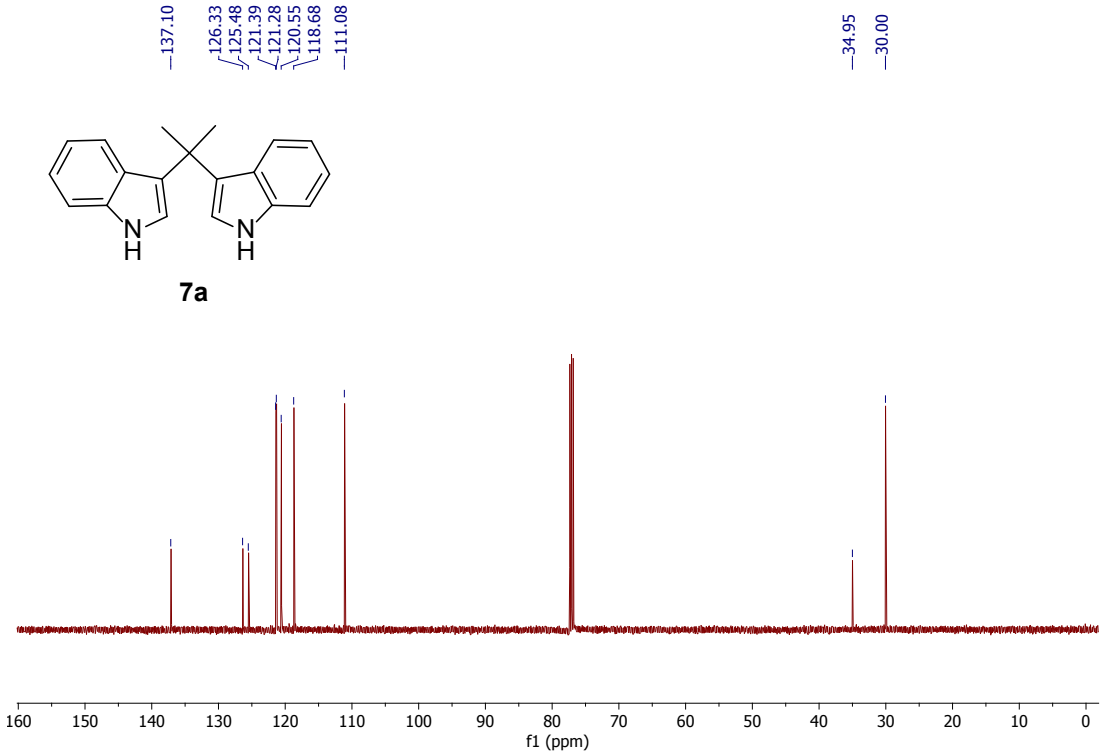
Supplementary information

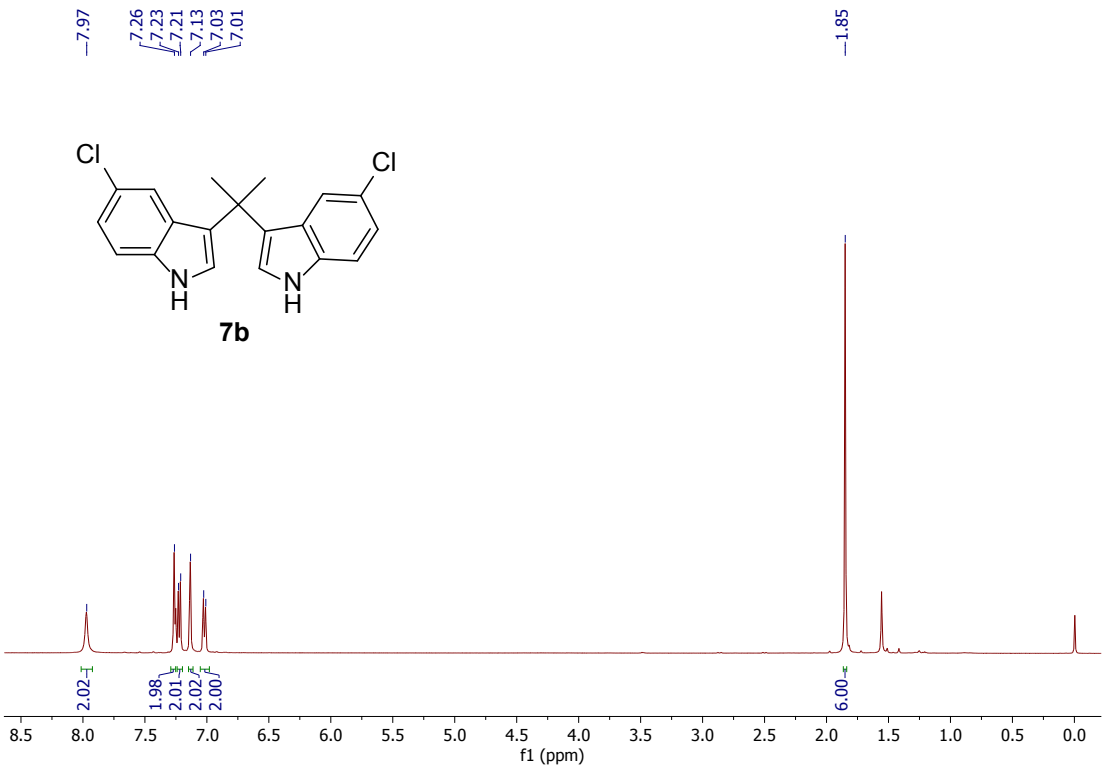
Bismuth Triflate-Catalyzed Condensation of Indoles with Acetone

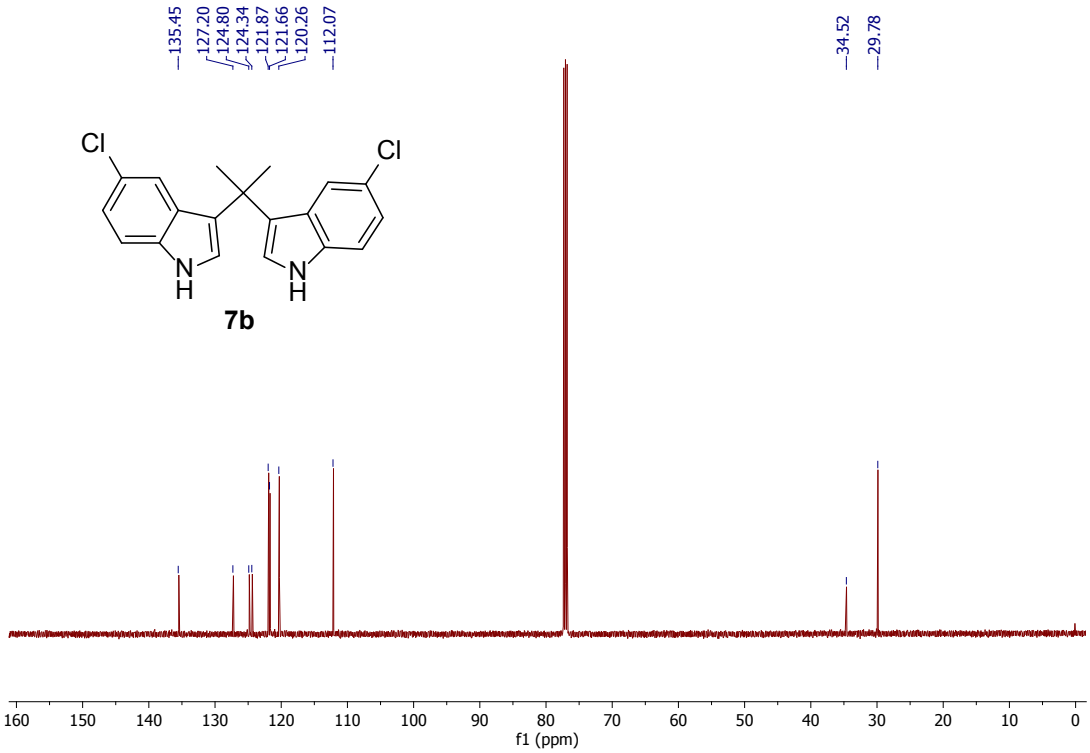
Ganesh M. Shelke,[a] V. Kameshwara Rao,[a] Rakesh Tiwari,[b] Bhupender S Chhikara,[b] Keykavous Parang[b] and Anil Kumar*,[a]

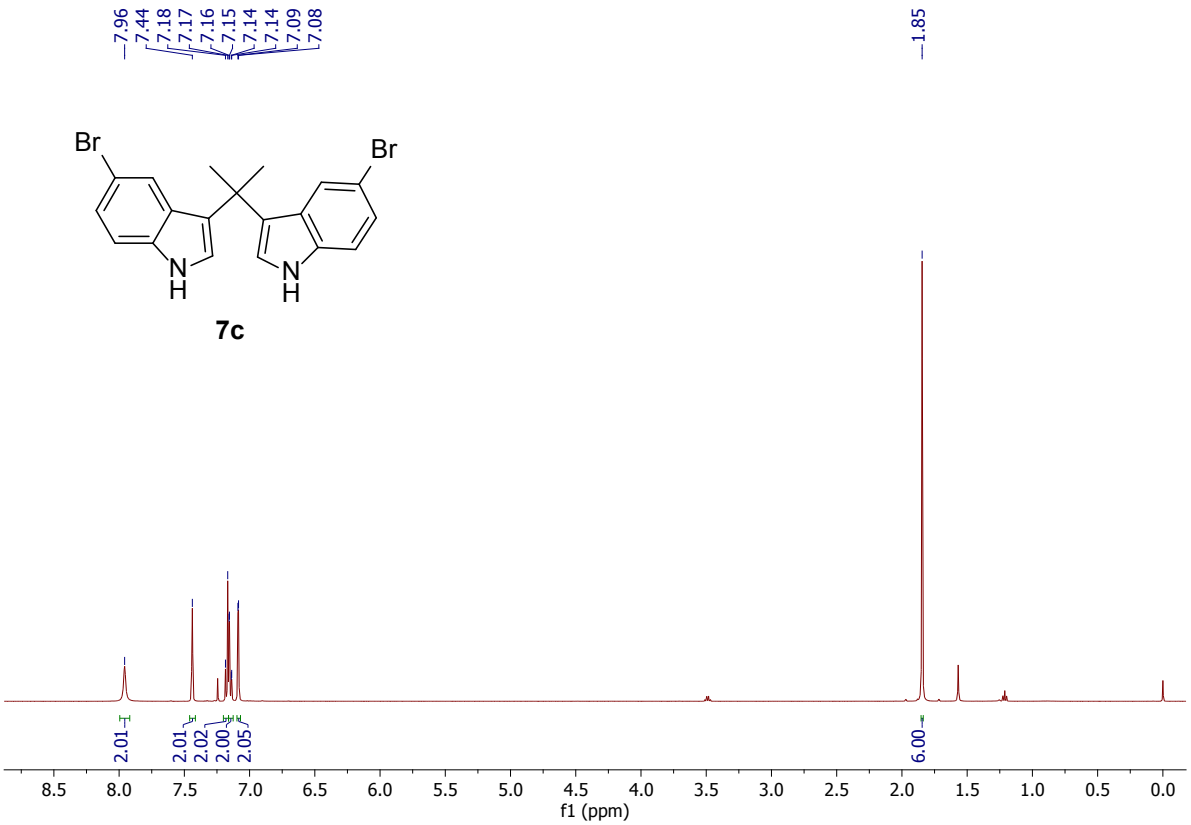
Copies of ^{1}H NMR and ^{13}C NMR for compound **7**, **8** & **9**

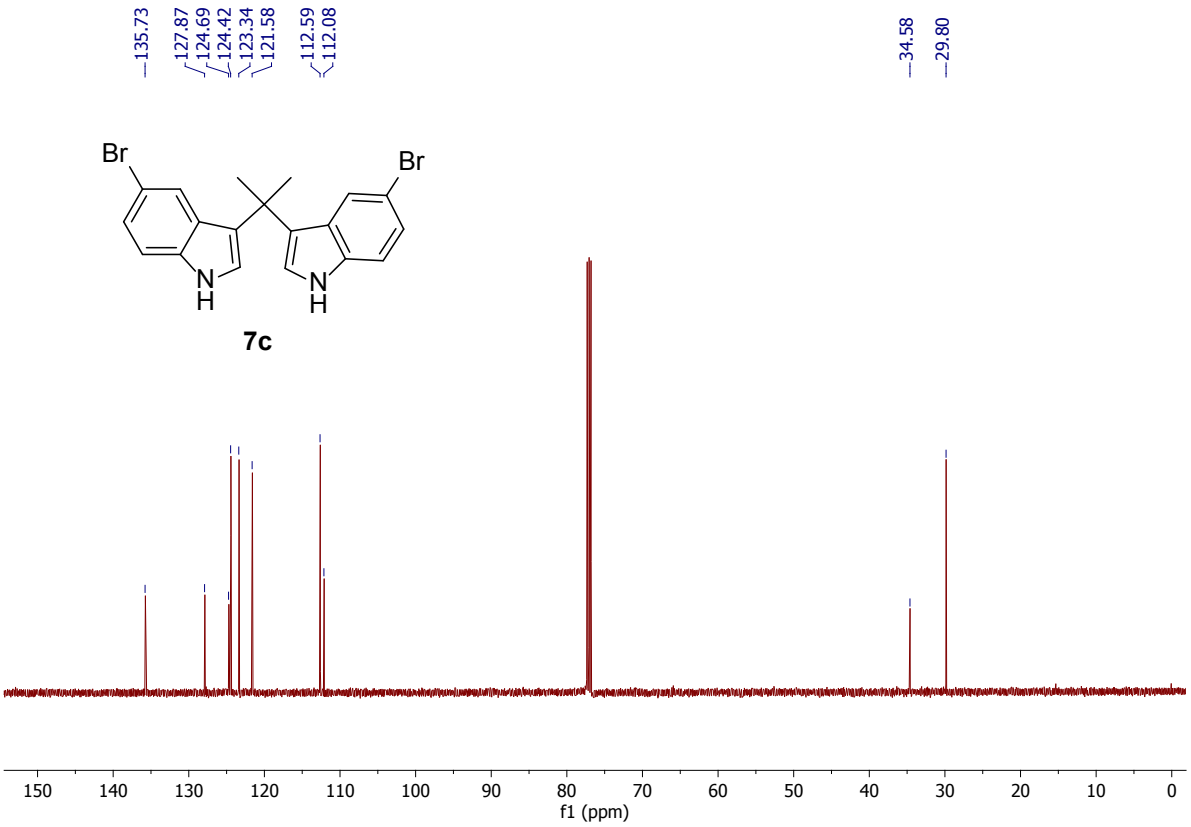


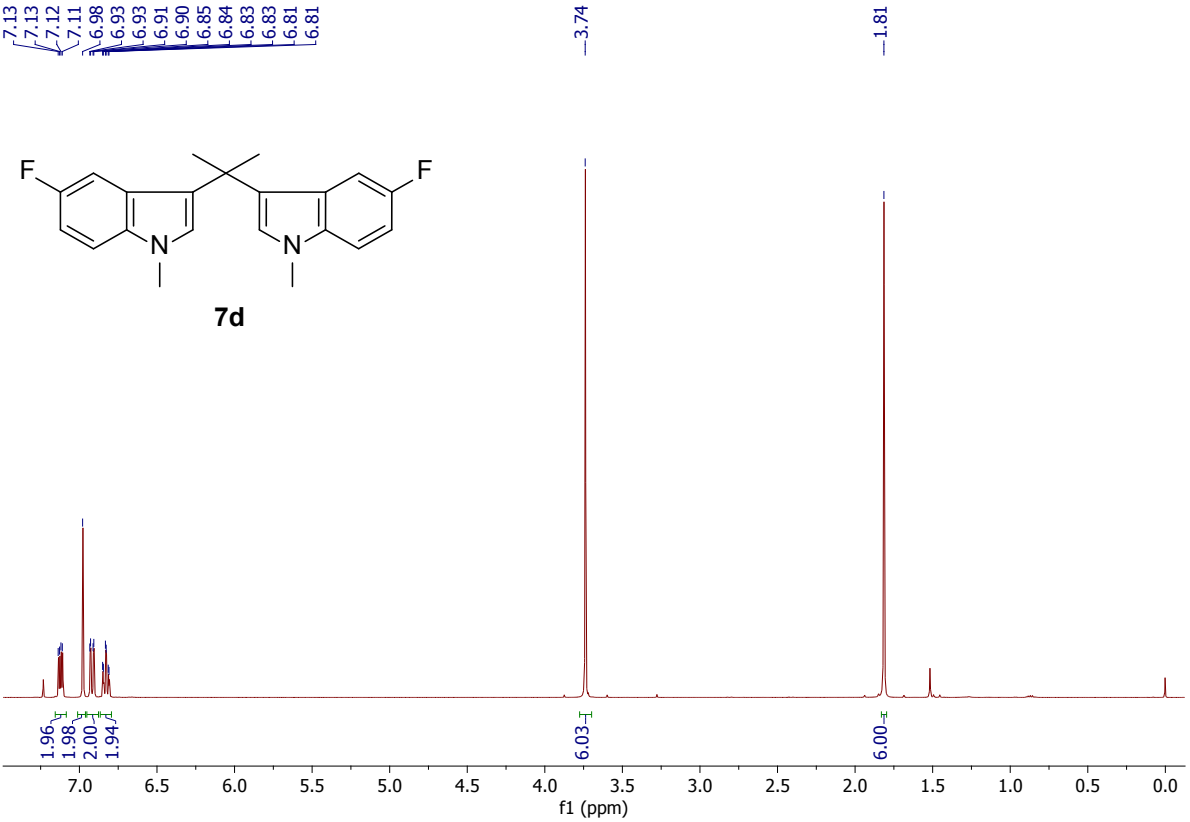


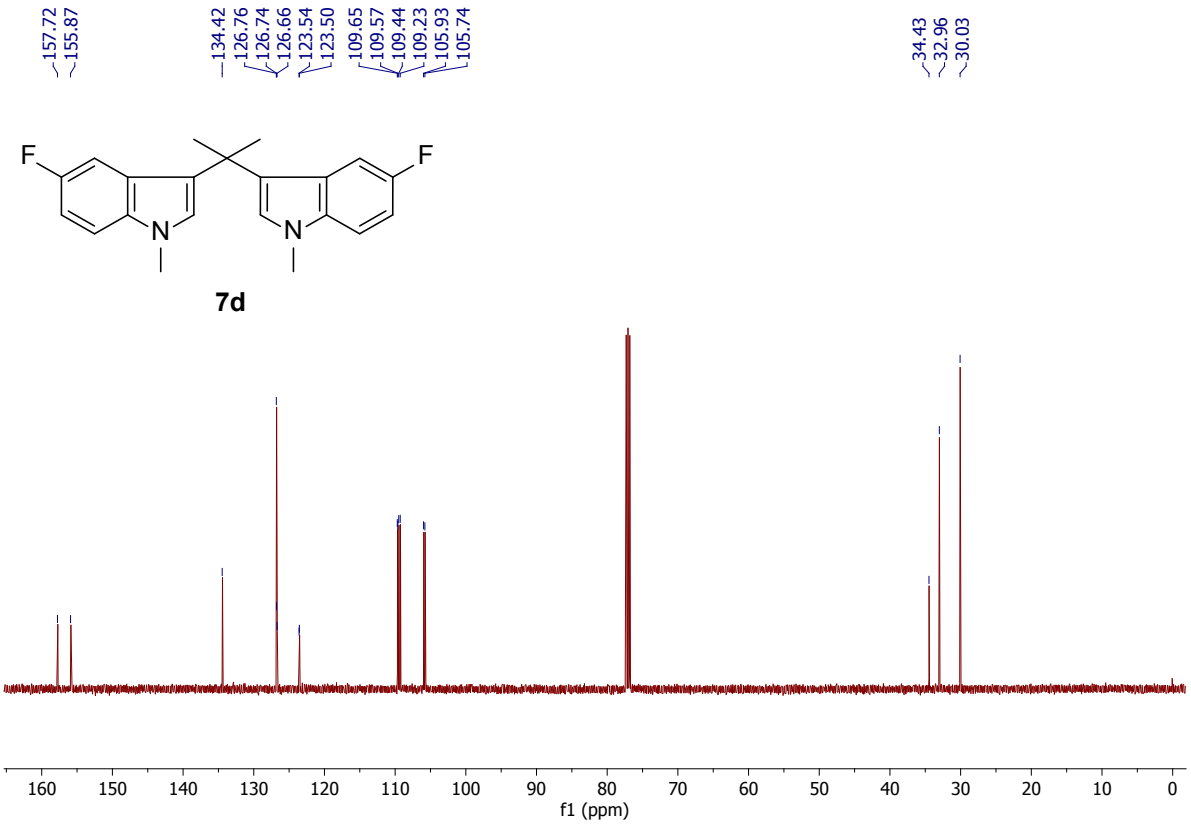

7.97
7.26
7.23
7.21
7.13
7.03
7.01
1.85
Cl
Cl
N
H
N
H
7b
2.02
1.98
2.01
2.02
2.00
6.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

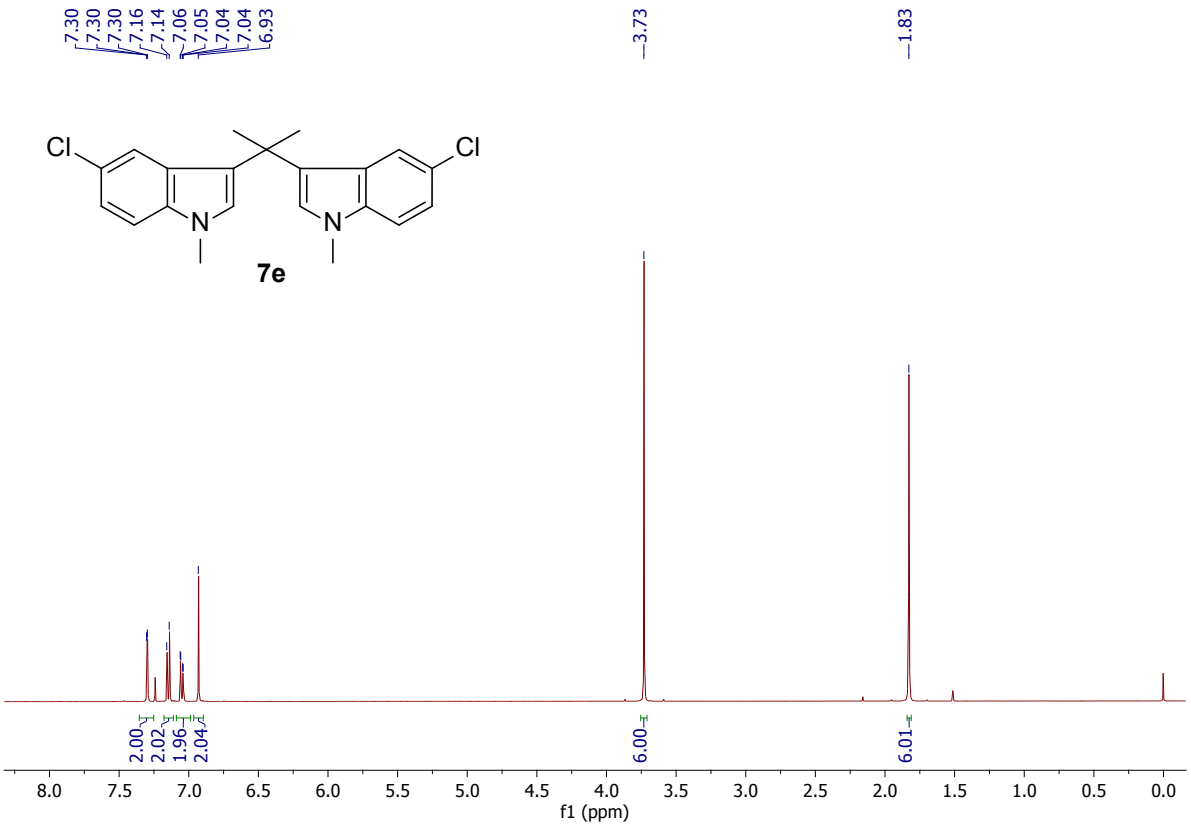

135.45
127.20
124.80
124.34
121.87
121.66
120.26
112.07
34.52
29.78
Cl
Cl
N
H
N
H
7b
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

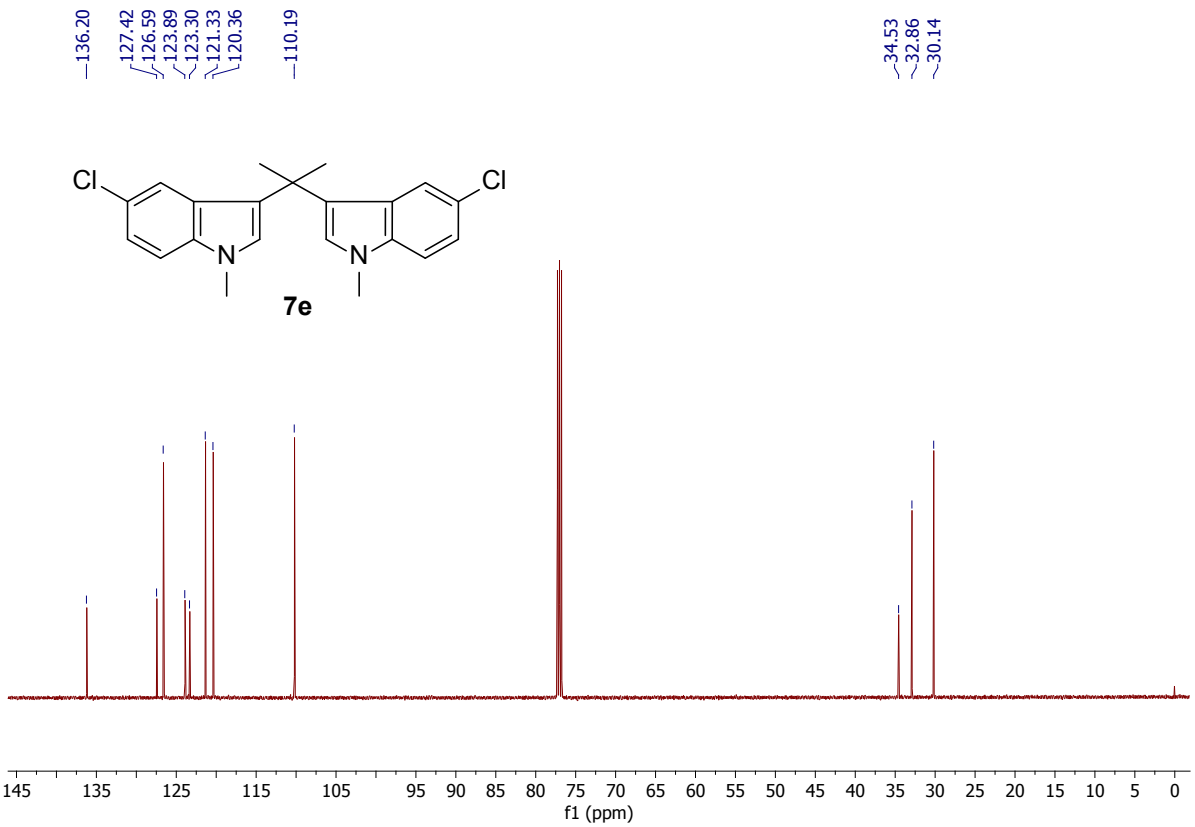

7.96
7.44
7.18
7.17
7.16
7.15
7.14
7.14
7.09
7.08
1.85
Br
Br
N
H
N
H
7c
2.01
2.01
2.02
2.00
2.05
6.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

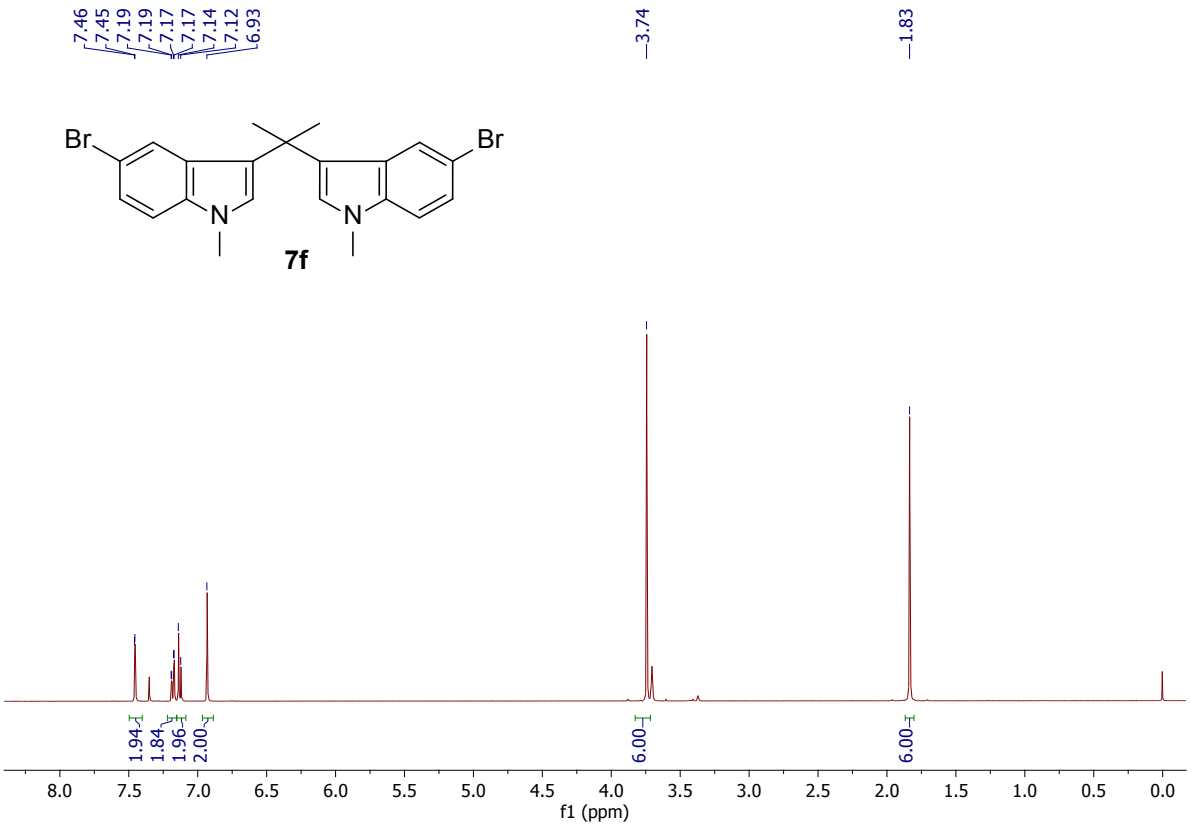

135.73
127.87
124.69
124.42
123.34
121.58
112.59
112.08
34.58
29.80
Br
Br
N
H
N
H
7c
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

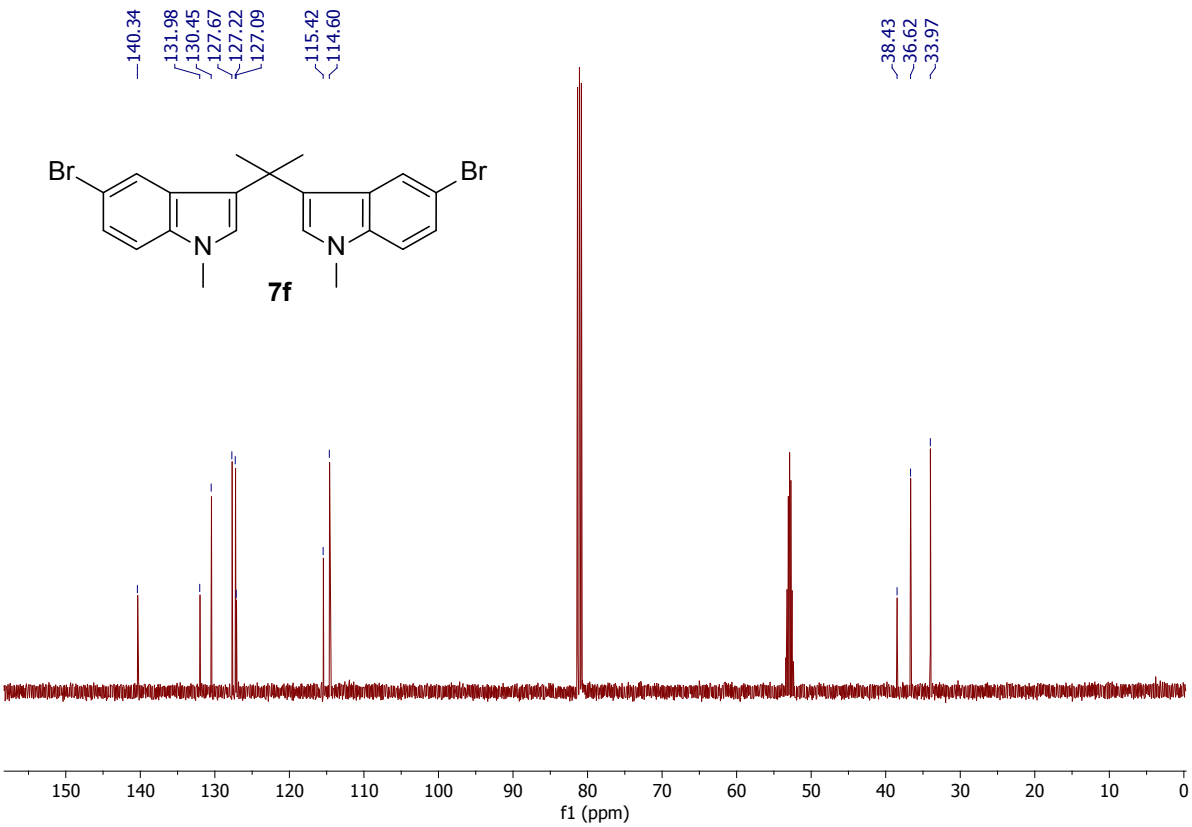

7.13
7.13
7.12
7.11
6.98
6.93
6.93
6.91
6.90
6.85
6.84
6.83
6.83
6.81
6.81
3.74
1.81
F
F
N
N
7d
1.96
1.98
2.00
1.94
6.03
6.00
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

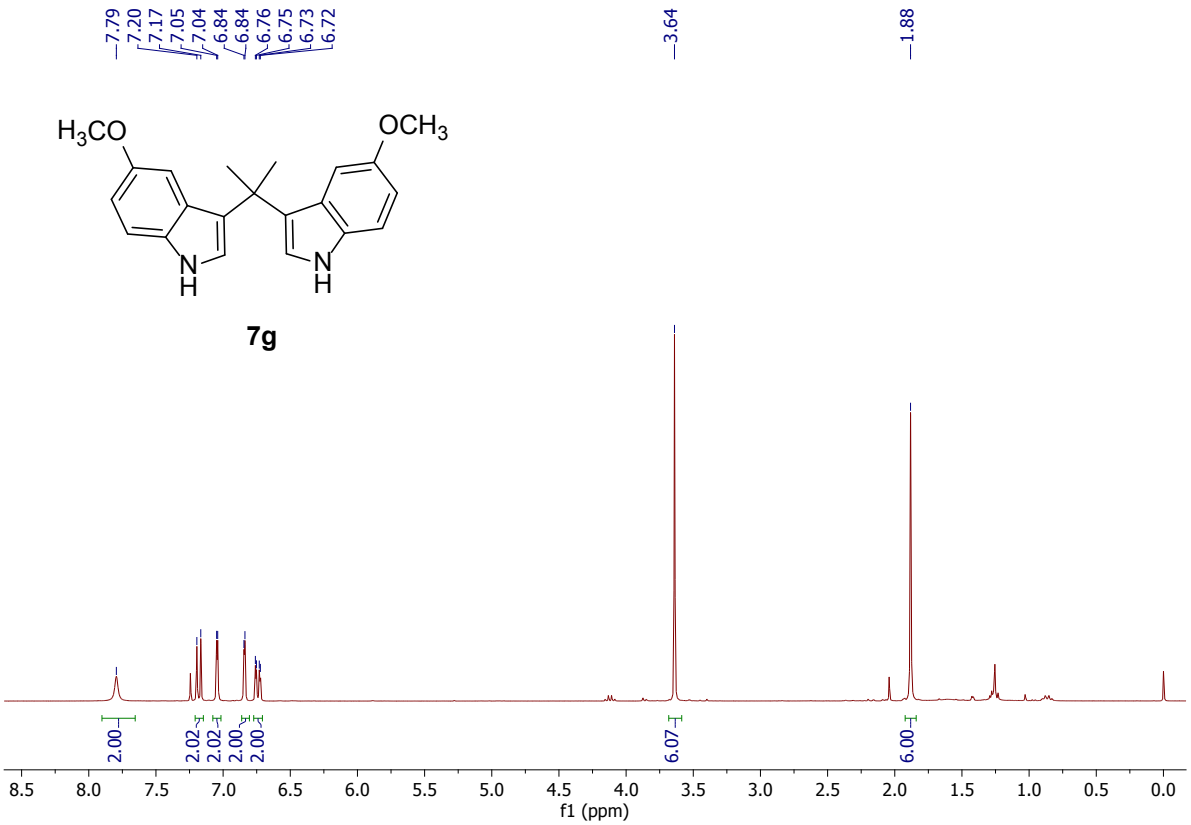

157.72
155.87
134.42
126.76
126.74
126.66
123.54
123.50
109.65
109.57
109.44
109.23
105.93
105.74
34.43
32.96
30.03
F
F
N
N
7d
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

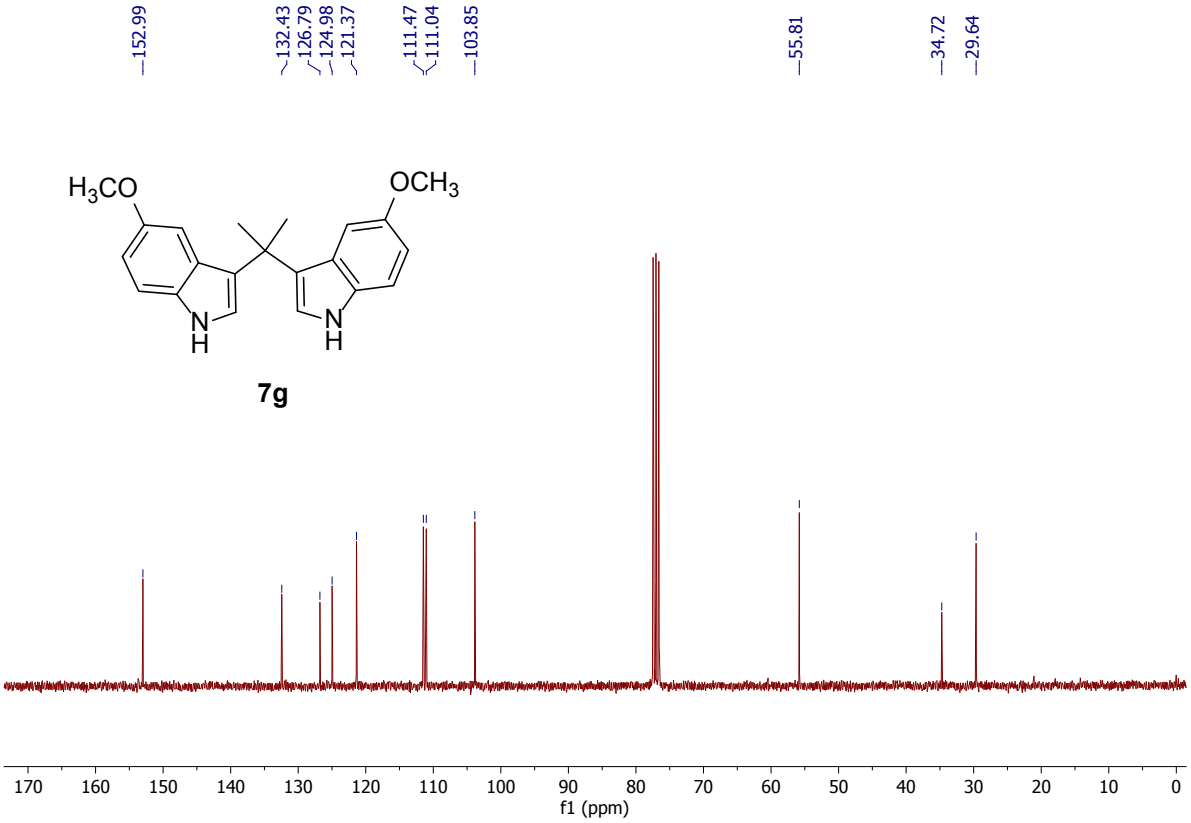

7.30
7.30
7.30
7.16
7.14
7.06
7.05
7.04
7.04
6.93
3.73
1.83
Cl
Cl
N
N
7e
2.00
2.02
1.96
2.04
6.00
6.01
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

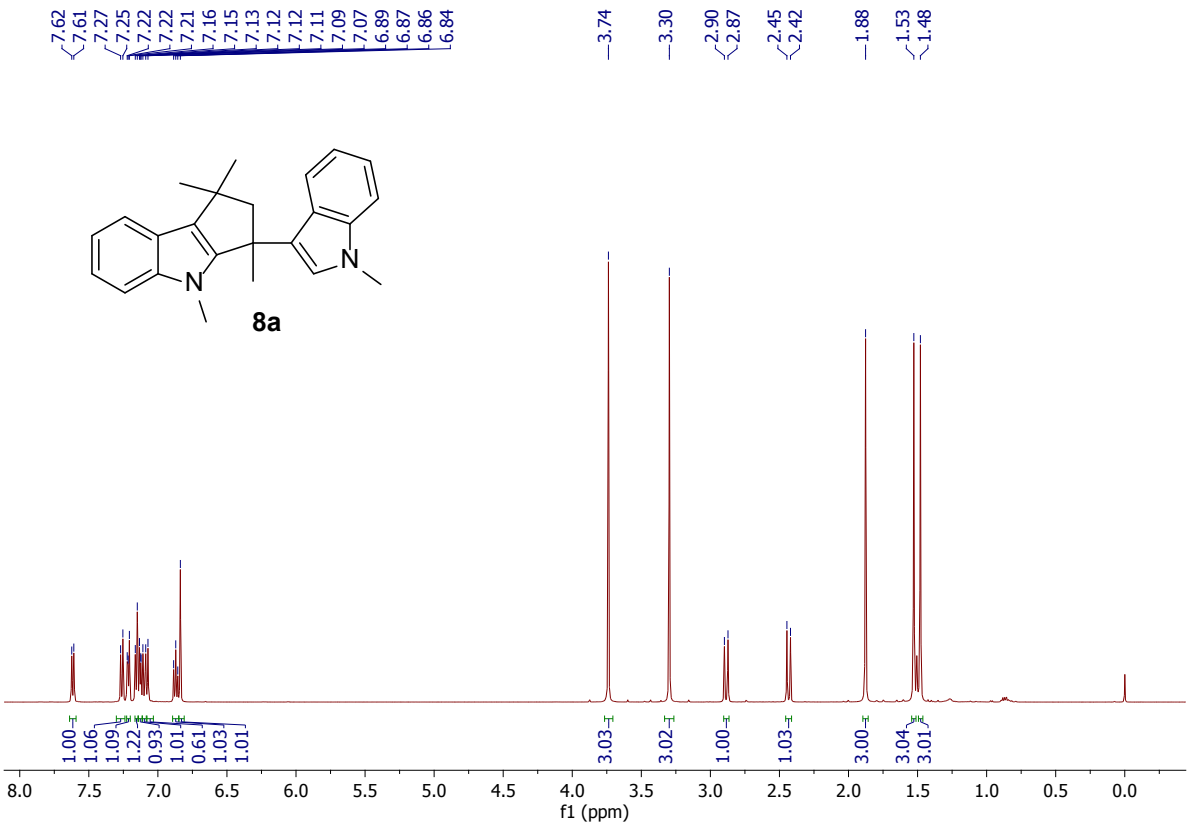

136.20
127.42
126.59
123.89
123.30
121.33
120.36
110.19
34.53
32.86
30.14
Cl
Cl
N
N
7e
145 135 125 115 105 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)

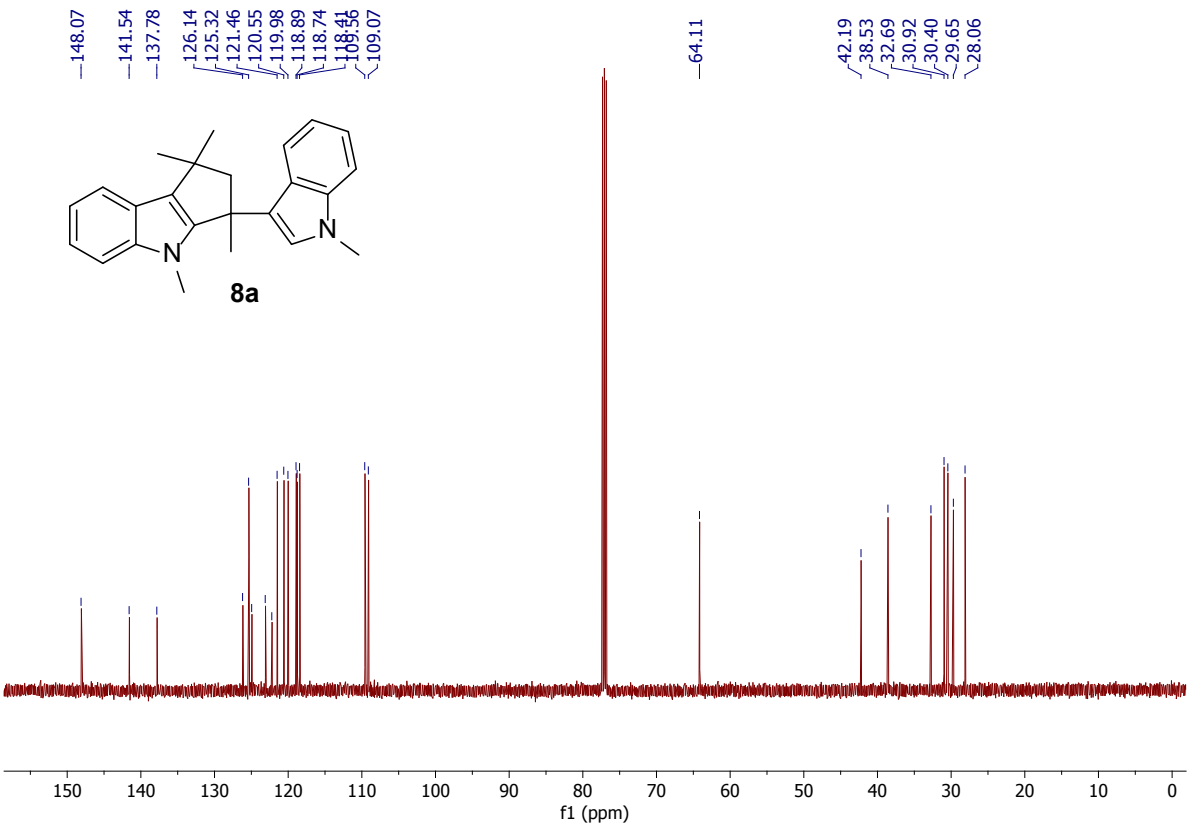

7.46
7.45
7.19
7.19
7.17
7.17
7.14
7.12
6.93
3.74
1.83
Br
Br
N
N
7f
1.94
1.84
1.96
2.00
6.00
6.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

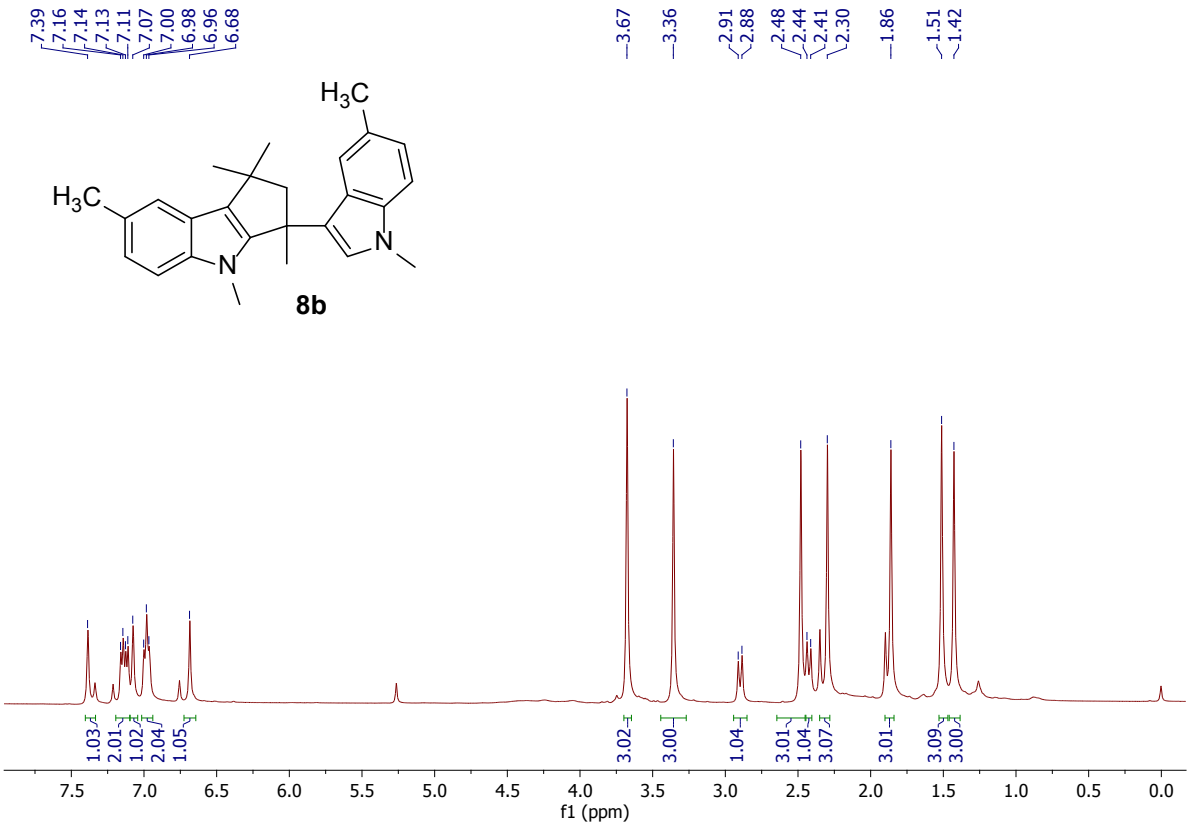

140.34
131.98
130.45
127.67
127.22
127.09
115.42
114.60
38.43
36.62
33.97
Br
Br
N
N
7f
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

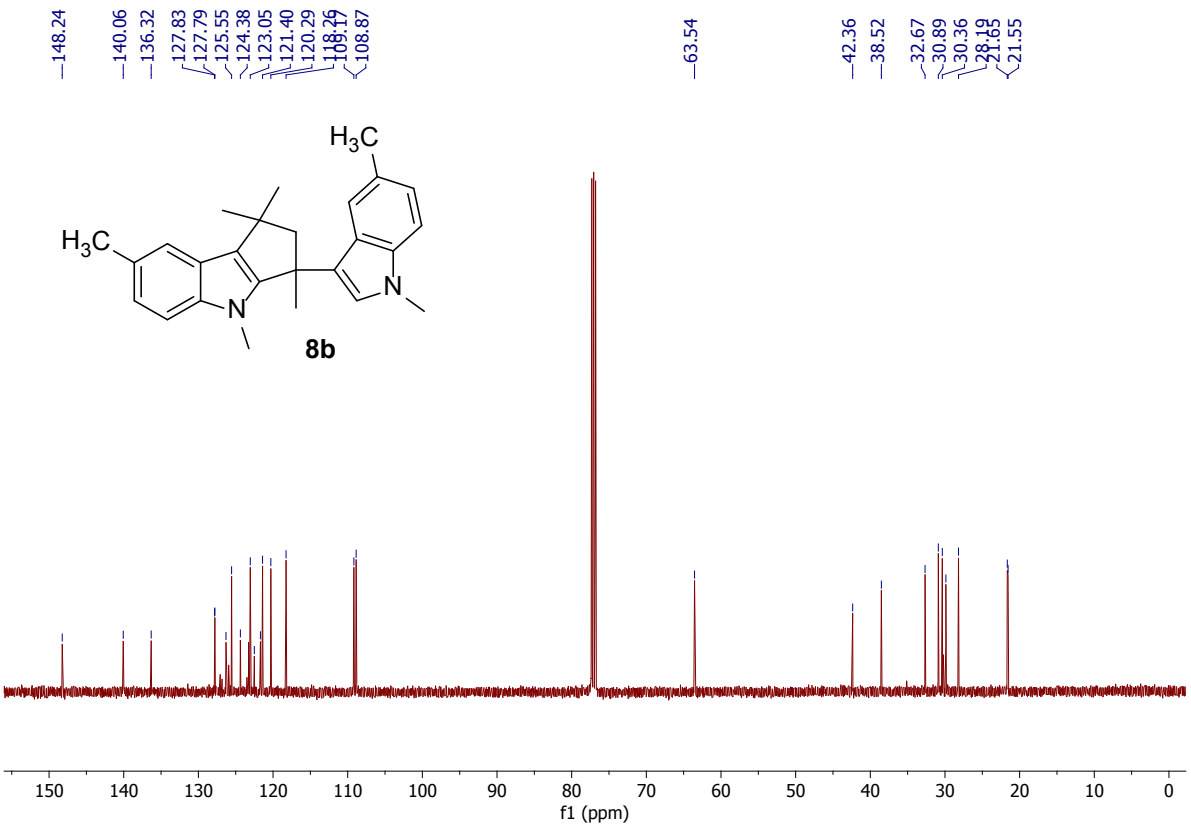

7.79
7.20
7.17
7.05
7.04
6.84
6.84
6.76
6.75
6.73
6.72
3.64
1.88
H3CO
OCH3
N
H
N
H
7g
2.00
2.02
2.02
2.00
2.00
6.07
6.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

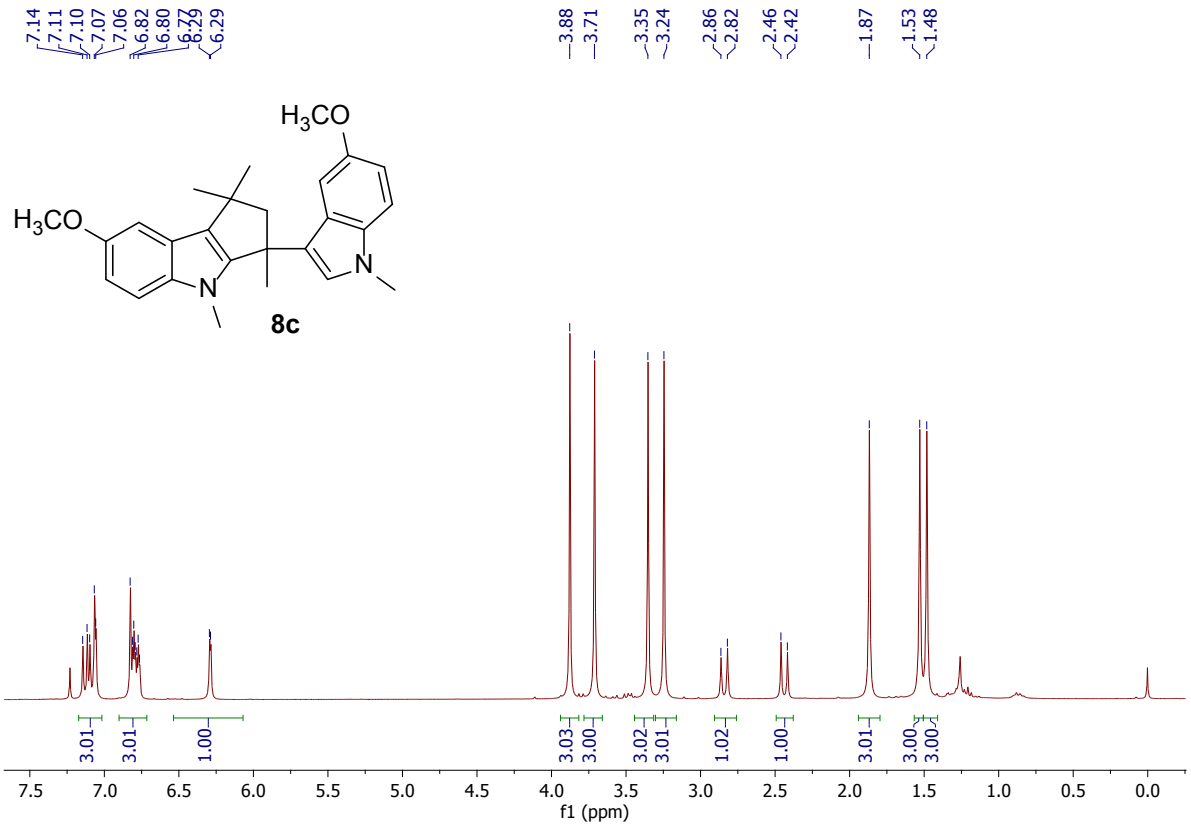

152.99
132.43
126.79
124.98
121.37
111.47
111.04
103.85
55.81
34.72
29.64
H3CO
OCH3
N
H
N
H
7g
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

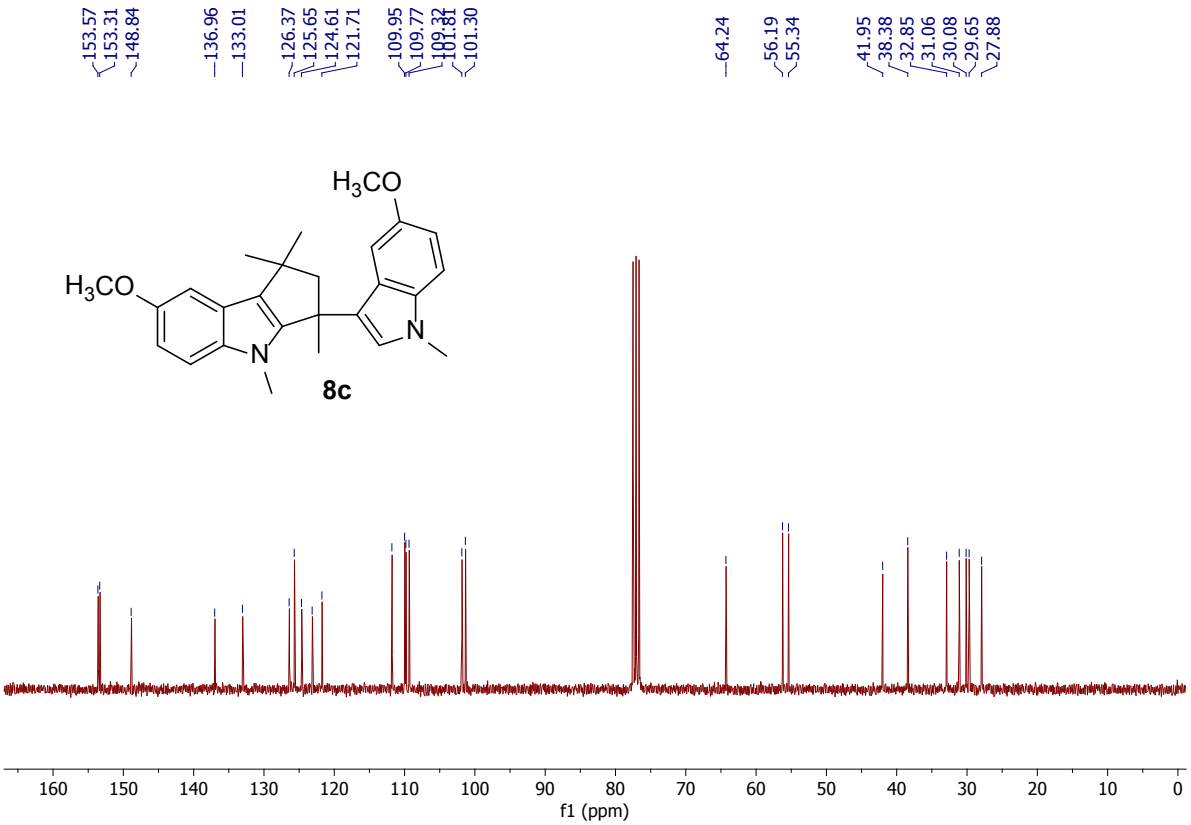

7.62
7.61
7.27
7.25
7.22
7.22
7.21
7.16
7.15
7.13
7.12
7.12
7.11
7.09
7.07
6.89
6.87
6.86
6.84
3.74
3.30
2.90
2.87
2.45
2.42
1.88
1.53
1.48
N
N
8a
1.00
1.06
1.09
1.22
0.93
1.01
0.61
1.03
1.01
3.03
3.02
1.00
1.03
3.00
3.04
3.01
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

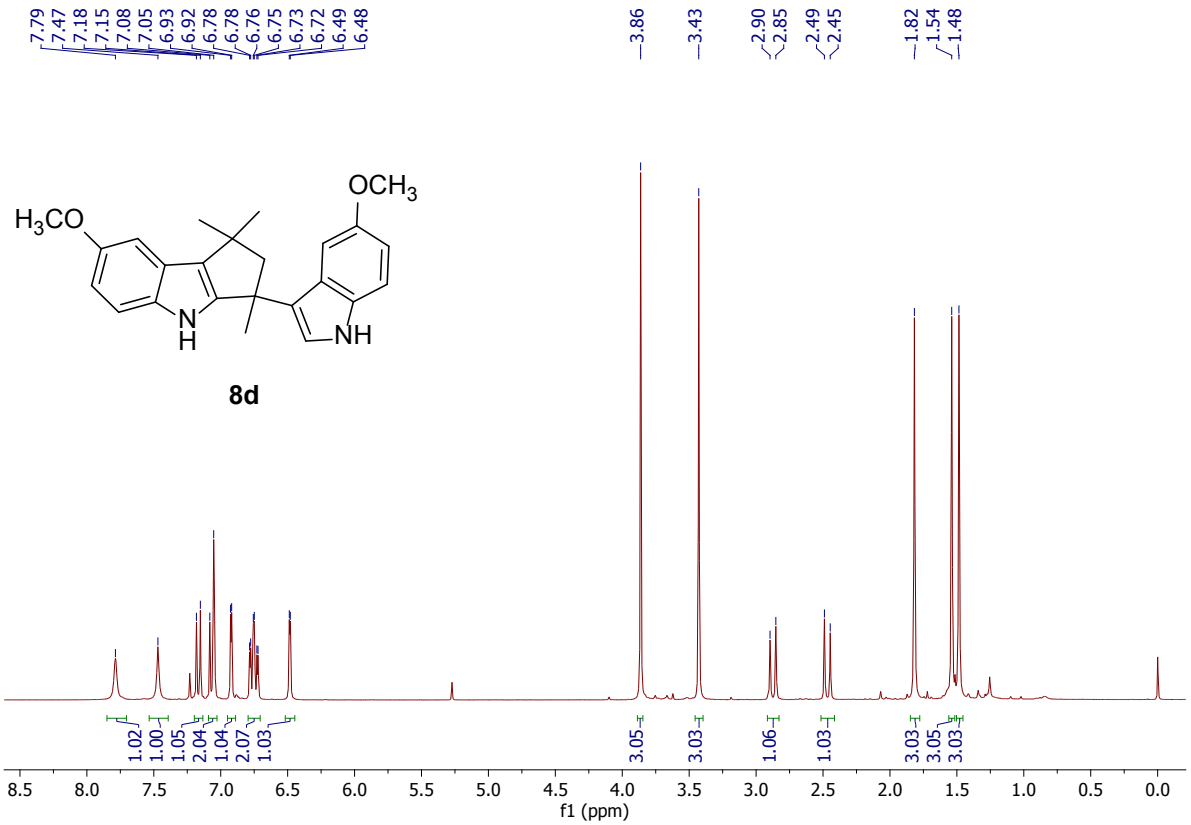

148.07
141.54
137.78
126.14
125.32
121.46
120.55
119.98
118.89
118.74
118.41
109.56
109.07
64.11
42.19
38.53
32.69
30.92
30.40
29.65
28.06
N
N
8a
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

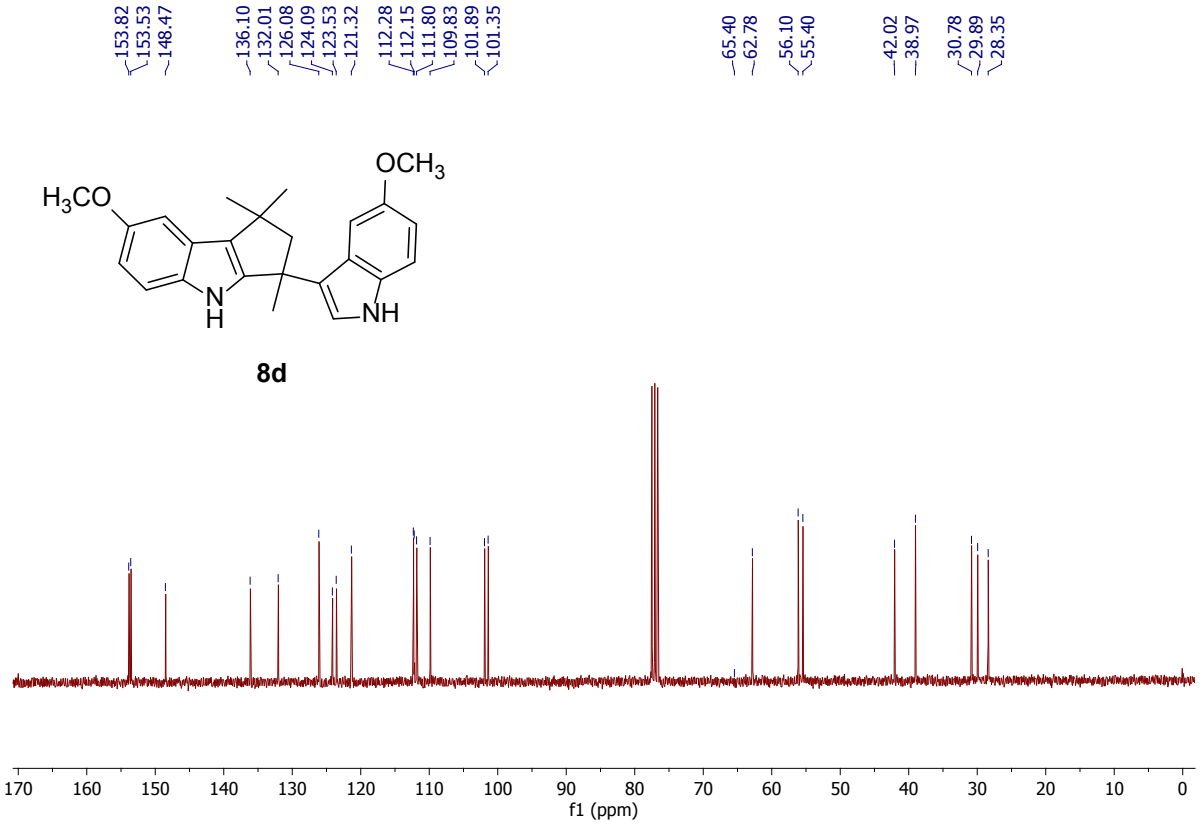

7.39
7.16
7.14
7.13
7.11
7.07
7.00
6.98
6.96
6.68
3.67
3.36
2.91
2.88
2.48
2.44
2.41
2.30
1.86
1.51
1.42
H3C
H3C
N
N
8b
1.03
2.01
1.02
2.04
1.05
3.02
3.00
1.04
3.01
1.04
3.07
3.01
3.09
3.00
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

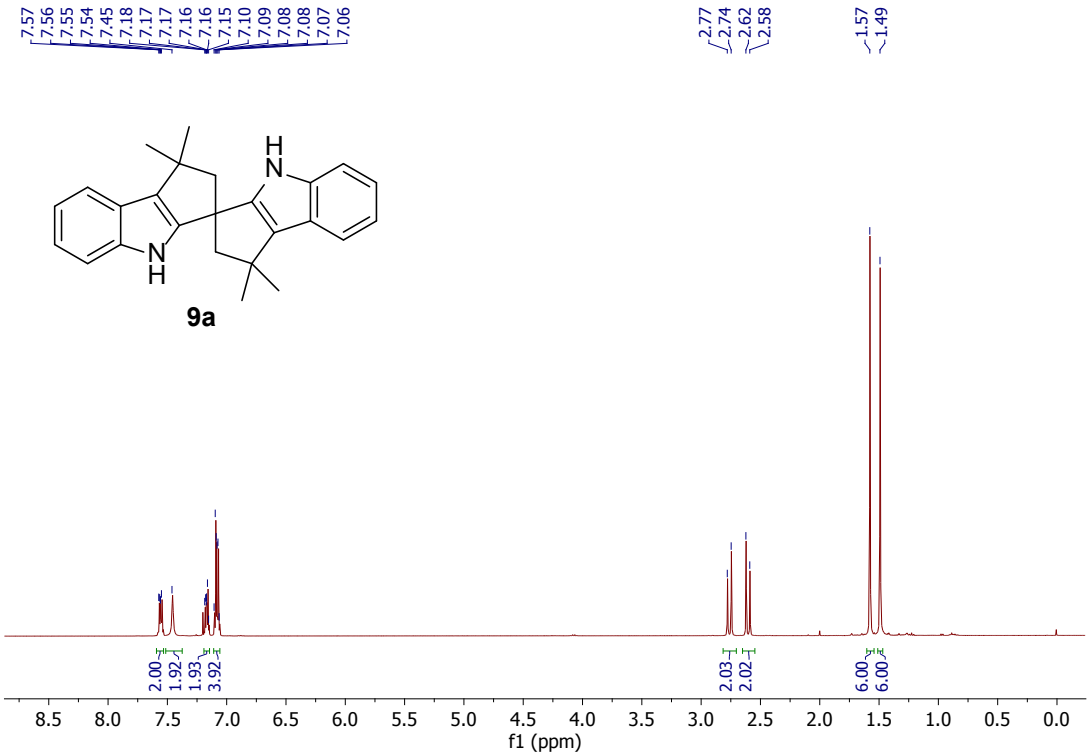

148.24
140.06
136.32
127.83
127.79
125.55
124.38
123.05
121.40
120.29
118.26
109.17
108.87
63.54
42.36
38.52
32.67
30.89
30.36
28.19
21.65
21.55
H3C
H3C
N
N
8b
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

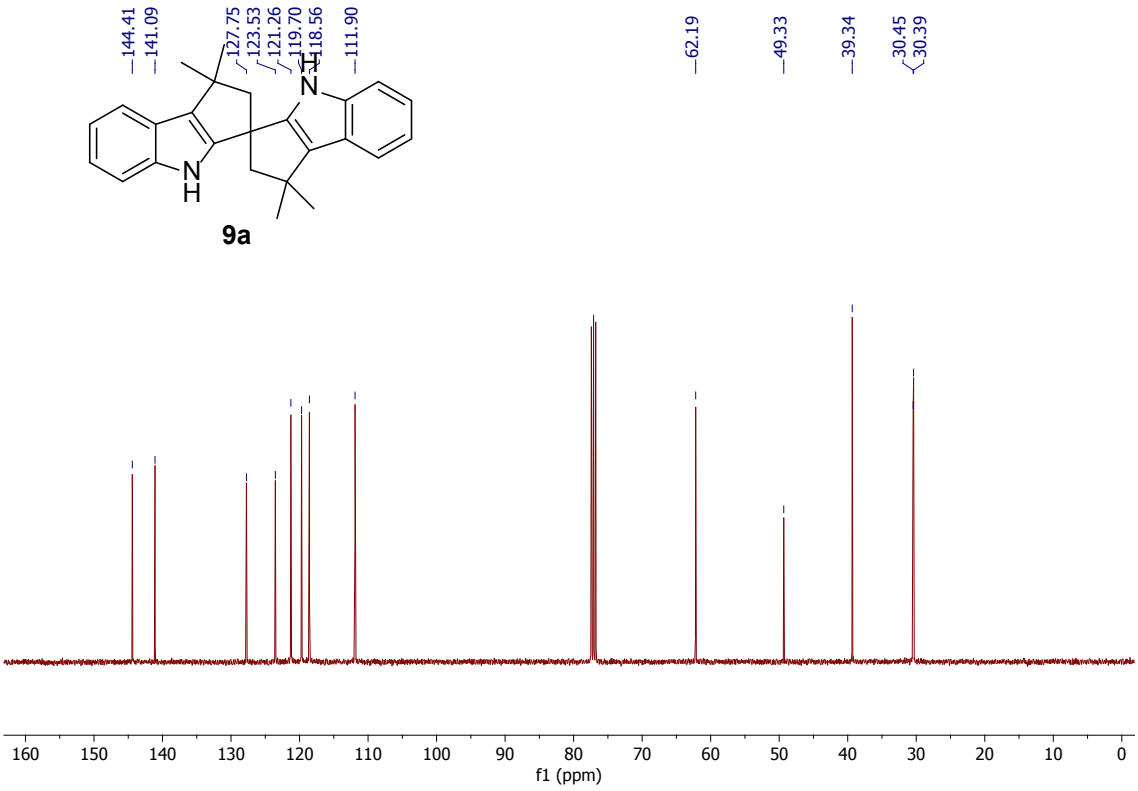

7.14
7.11
7.10
7.07
7.06
6.82
6.80
6.77
6.29
6.29
3.88
3.71
3.35
3.24
2.86
2.82
2.46
2.42
1.87
1.53
1.48
H3CO
H3CO
N
N
8c
3.01
3.01
1.00
3.03
3.00
3.02
3.01
1.02
1.00
3.01
3.00
3.00
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

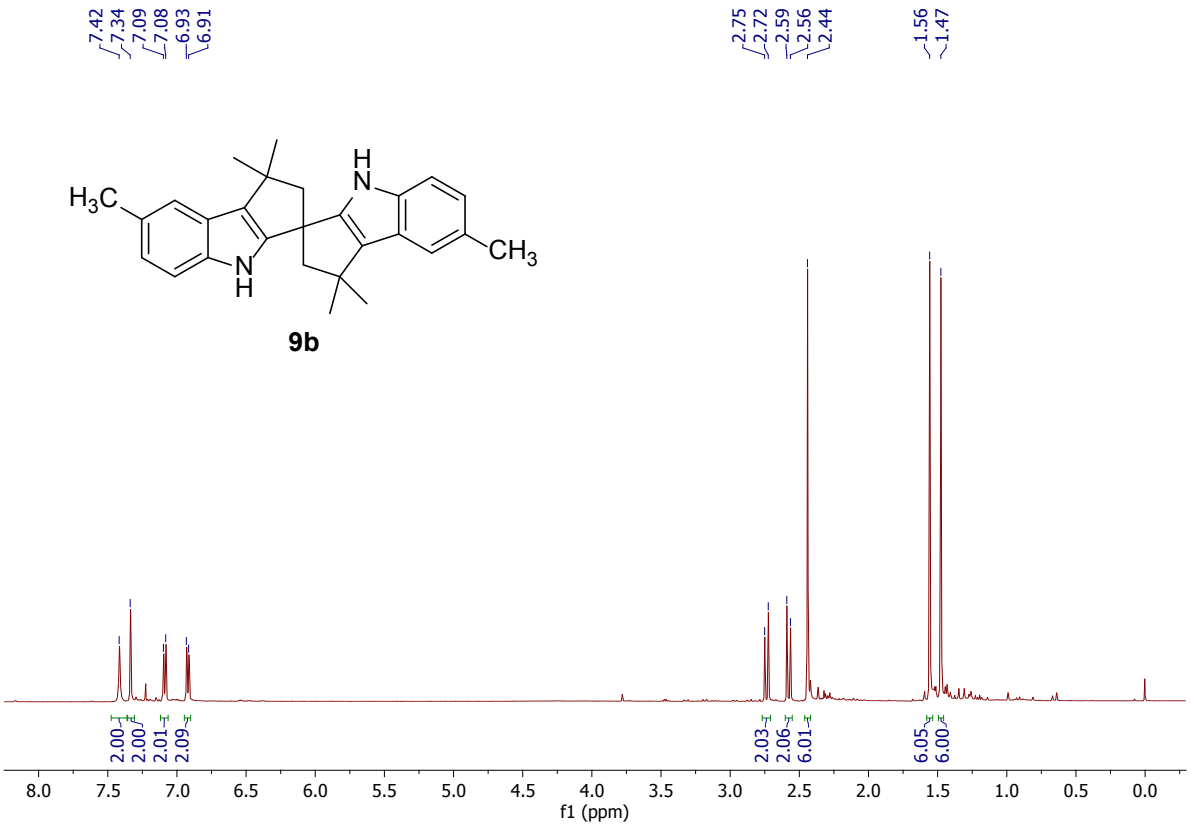

153.57
153.31
148.84
136.96
133.01
126.37
125.65
124.61
121.71
109.95
109.77
109.32
101.81
101.30
64.24
56.19
55.34
41.95
38.38
32.85
31.06
30.08
29.65
27.88
H3CO
H3CO
N
N
8c
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

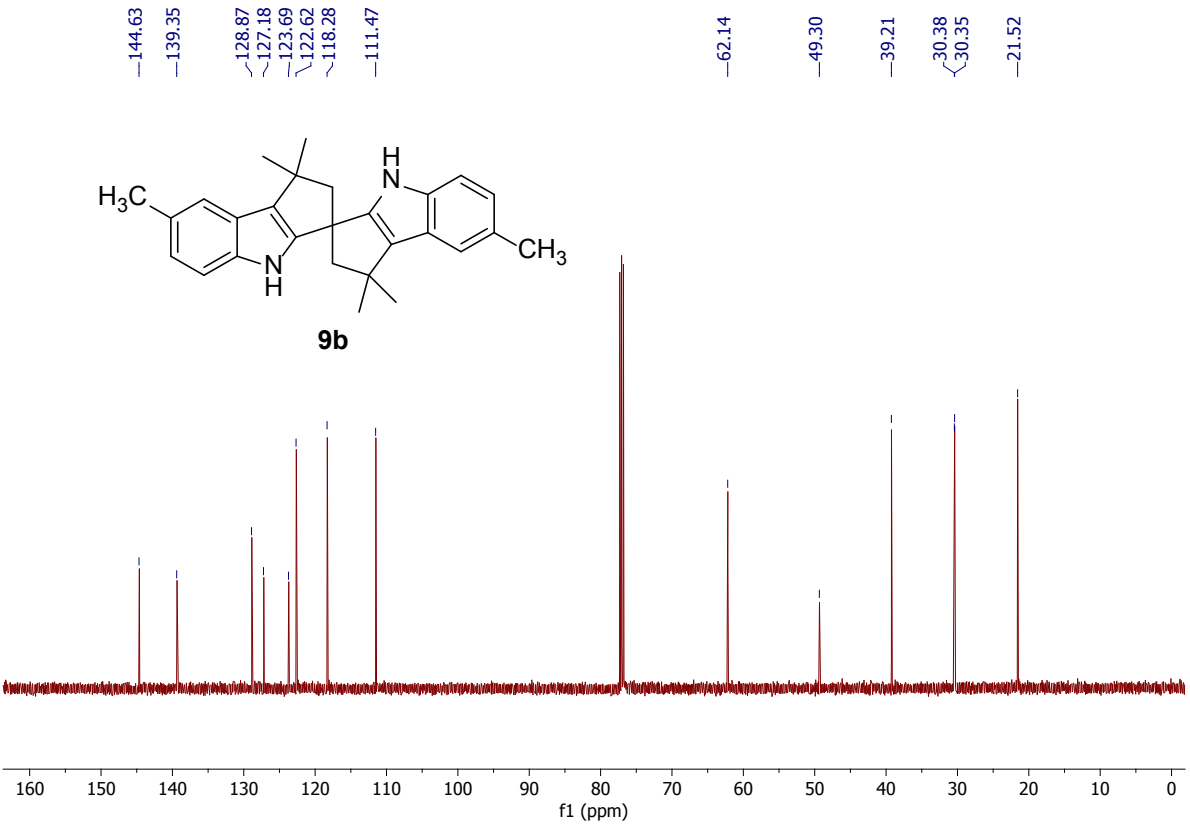

7.79
7.47
7.18
7.15
7.08
7.05
6.93
6.92
6.78
6.78
6.76
6.75
6.73
6.72
6.49
6.48
3.86
3.43
2.90
2.85
2.49
2.45
1.82
1.54
1.48
OCH3
H3CO
N
H
NH
8d
1.02
1.00
1.05
2.04
1.04
2.07
1.03
3.05
3.03
1.06
1.03
3.03
3.05
3.03
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

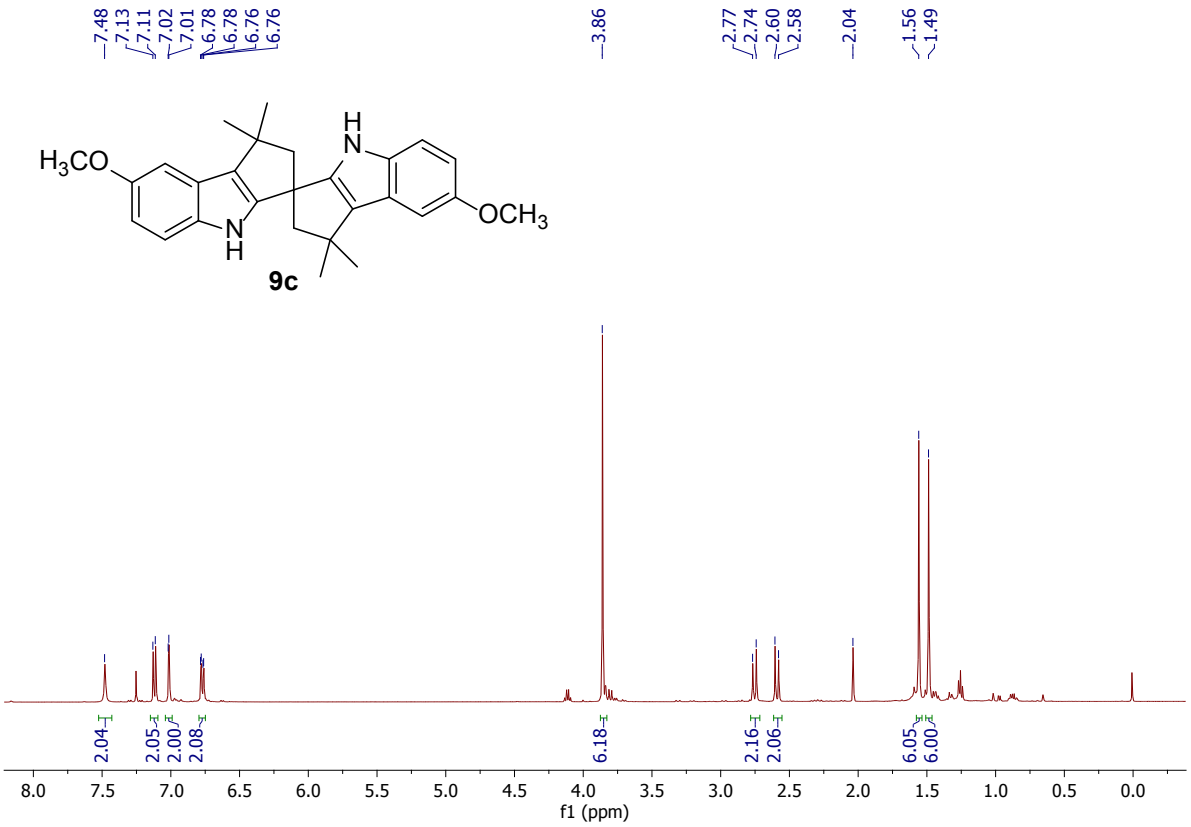

153.82
153.53
148.47
136.10
132.01
126.08
124.09
123.53
121.32
112.28
112.15
111.80
109.83
101.89
101.35
65.40
62.78
56.10
55.40
42.02
38.97
30.78
29.89
28.35
OCH3
H3CO
N
H
NH
8d
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

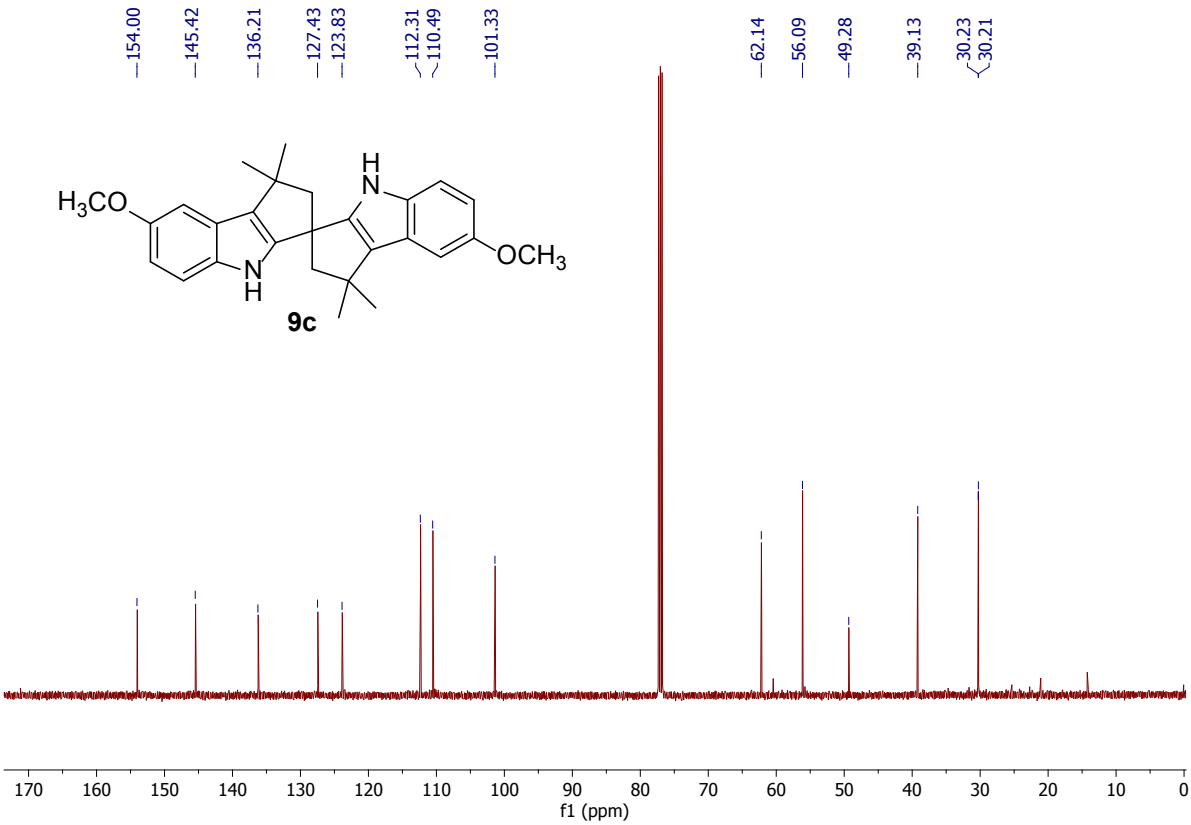

7.57
7.56
7.55
7.54
7.45
7.18
7.17
7.17
7.16
7.16
7.15
7.10
7.09
7.08
7.08
7.07
7.06
2.77
2.74
2.62
2.58
1.57
1.49
H
N
N
H
9a
2.00
1.92
1.93
3.92
2.03
2.02
6.00
6.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

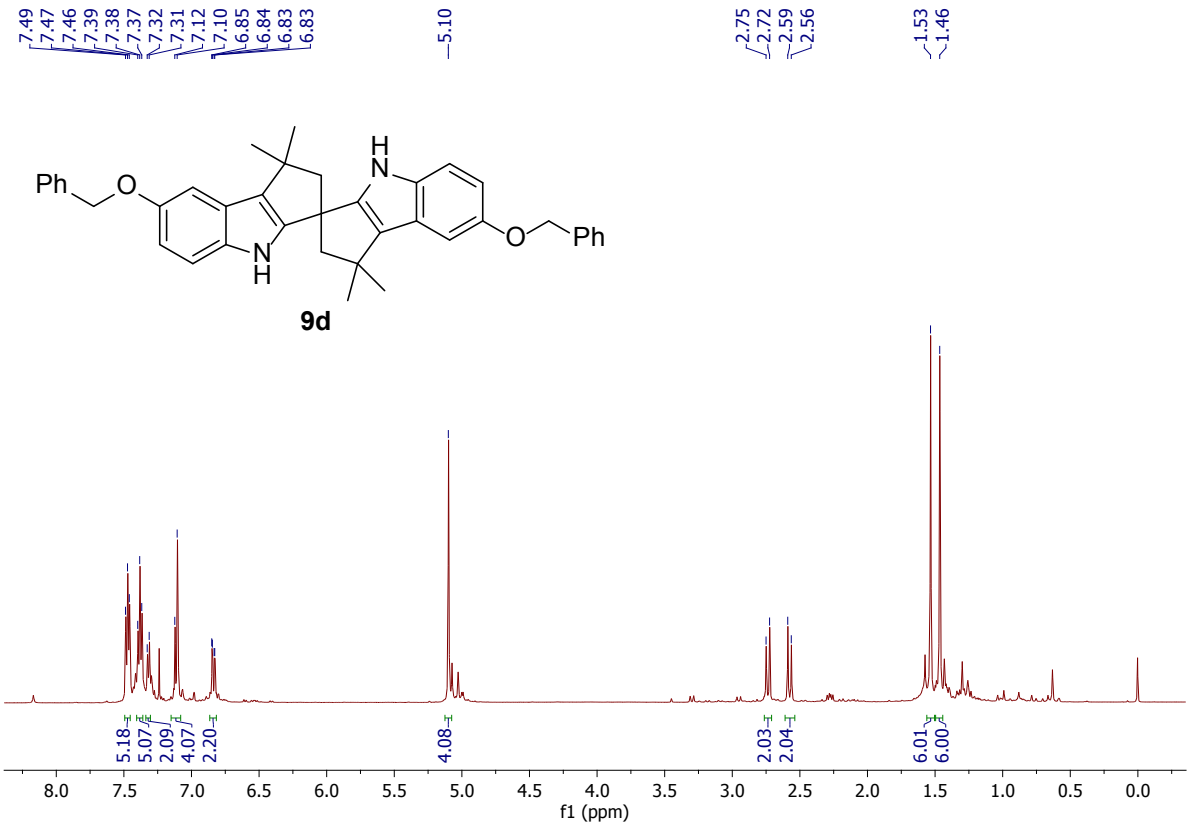

144.41
141.09
127.75
123.53
121.26
119.70
118.56
111.90
62.19
49.33
39.34
30.45
30.39
H
N
N
H
9a
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

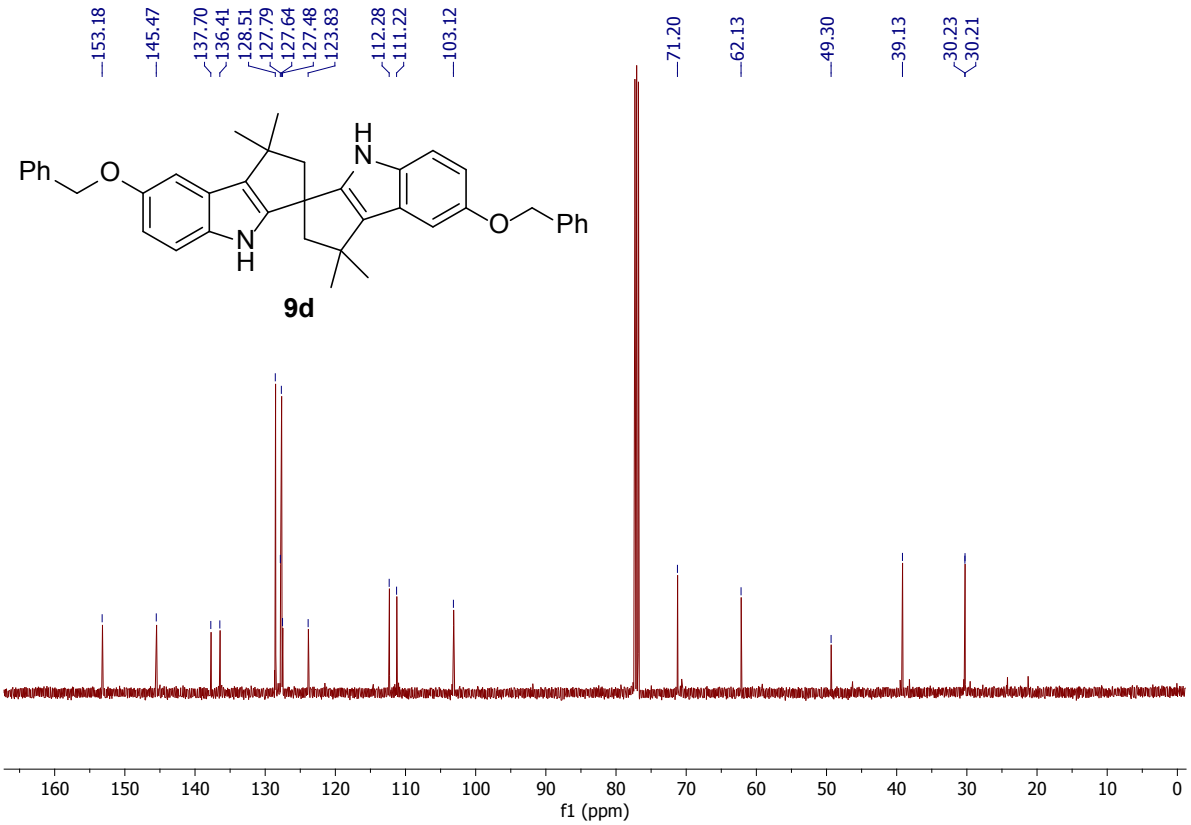

7.42
7.34
7.09
7.08
6.93
6.91
2.75
2.72
2.59
2.56
2.44
1.56
1.47
H3C
H
N
CH3
N
H
9b
2.00
2.00
2.01
2.09
2.03
2.06
6.01
6.05
6.00
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

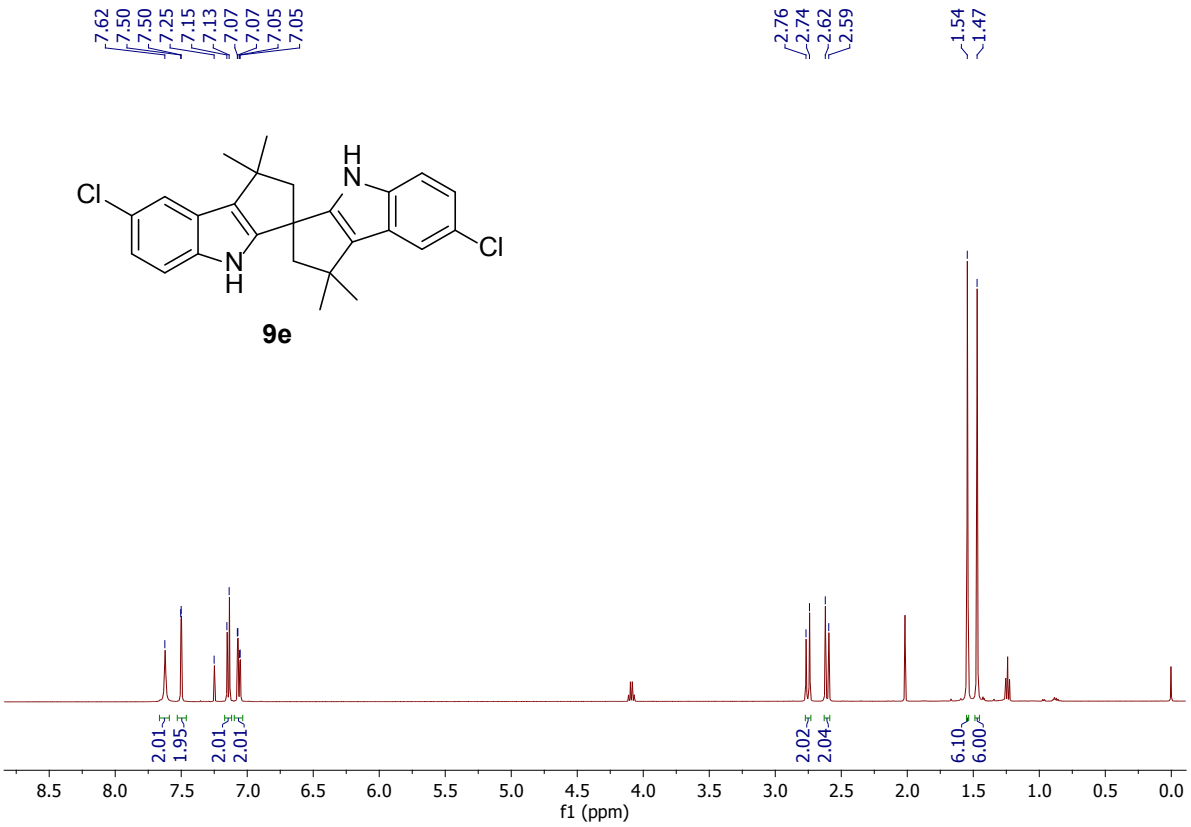

144.63
139.35
128.87
127.18
123.69
122.62
118.28
111.47
62.14
49.30
39.21
30.38
30.35
21.52
H3C
H
N
CH3
N
H
9b
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

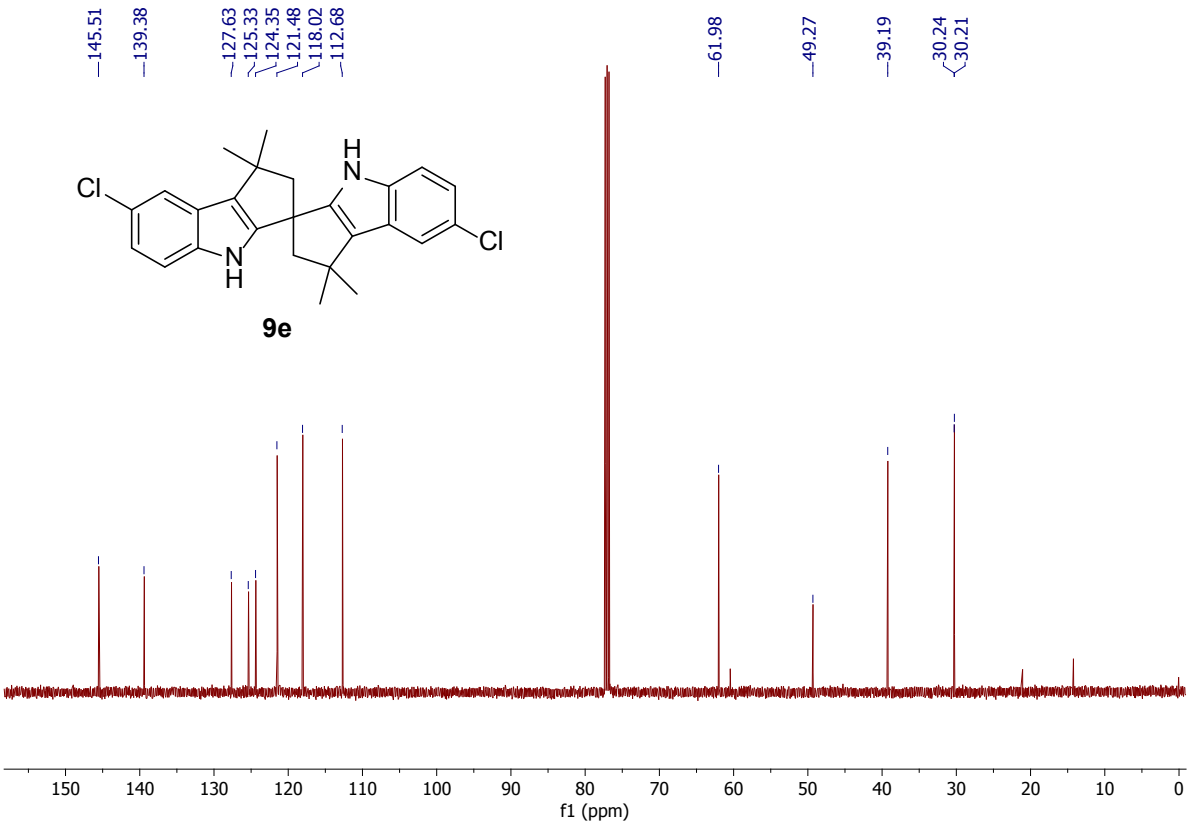

7.48
7.13
7.11
7.02
7.01
6.78
6.78
6.76
6.76
3.86
2.77
2.74
2.60
2.58
2.04
1.56
1.49
H3CO
H
N
N
H
OCH3
9c
2.04
2.05
2.00
2.08
6.18
2.16
2.06
6.05
6.00
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

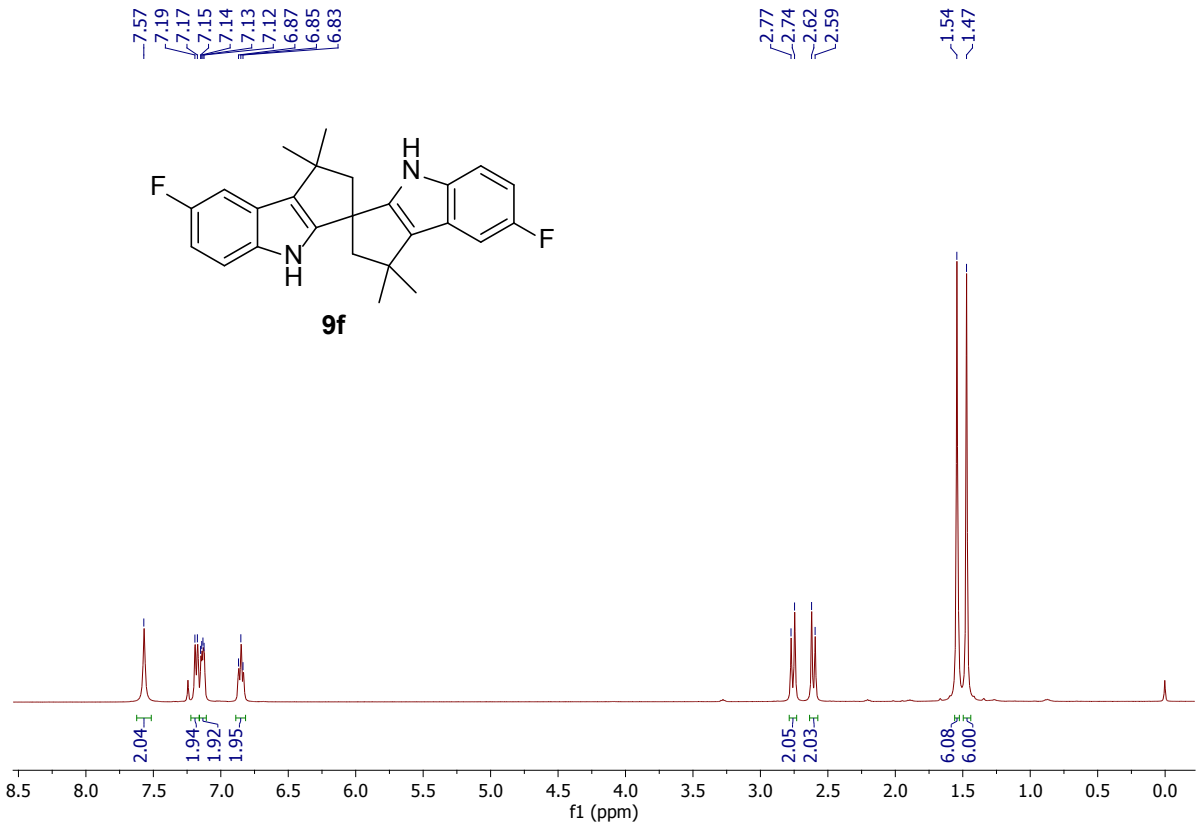

154.00
145.42
136.21
127.43
123.83
112.31
110.49
101.33
62.14
56.09
49.28
39.13
30.23
30.21
H3CO
H
N
N
H
OCH3
9c
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

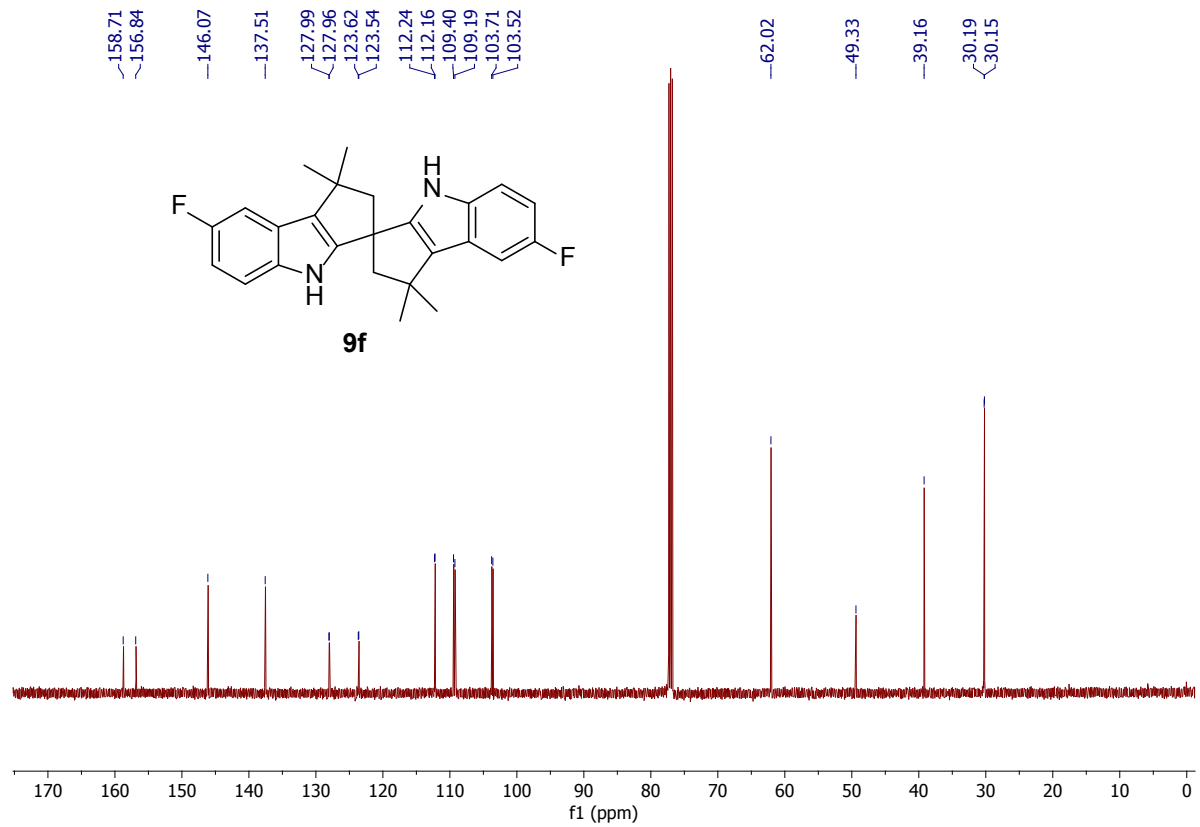

7.49
7.47
7.46
7.39
7.38
7.37
7.32
7.31
7.12
7.10
6.85
6.84
6.83
6.83
5.10
2.75
2.72
2.59
2.56
1.53
1.46
Ph
O
H
N
N
H
O
Ph
9d
5.18
5.07
2.09
4.07
2.20
4.08
2.03
2.04
6.01
6.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

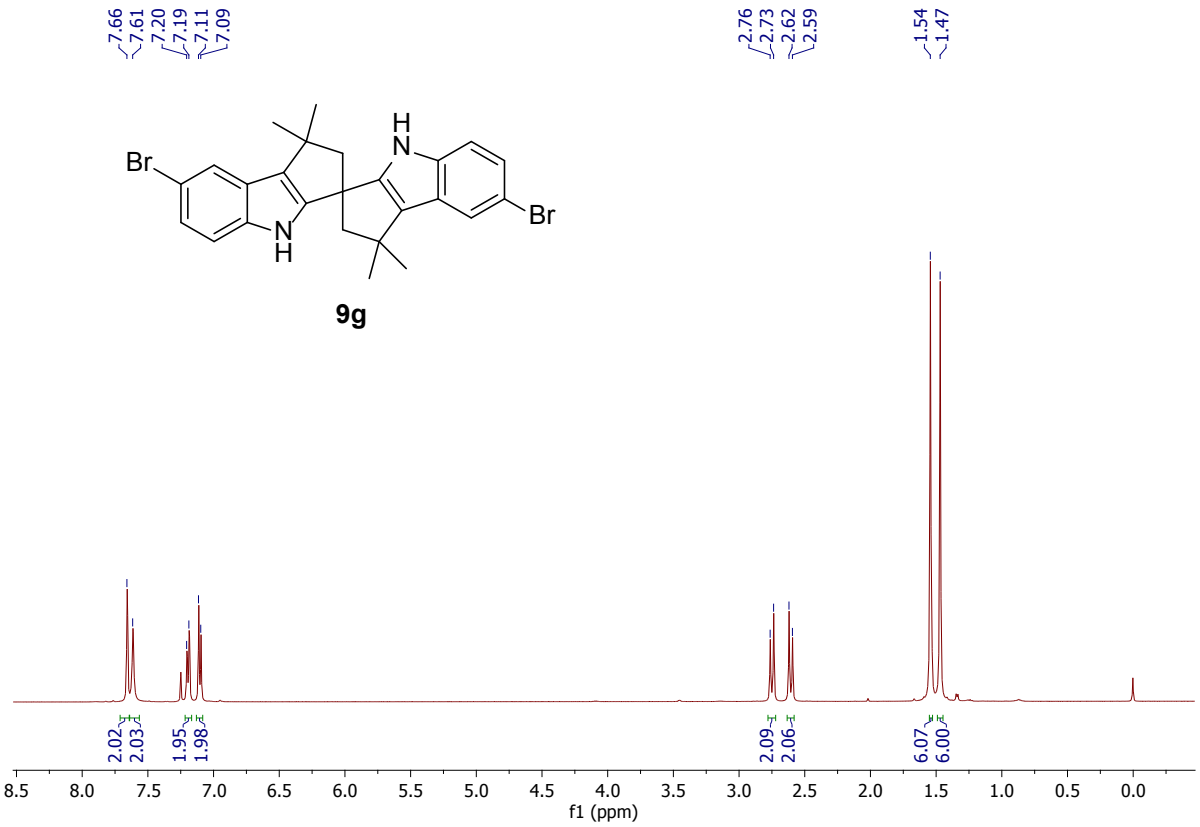

153.18
145.47
137.70
136.41
128.51
127.79
127.64
127.48
123.83
112.28
111.22
103.12
71.20
62.13
49.30
39.13
30.23
30.21
Ph
O
H
N
N
H
O
Ph
9d
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

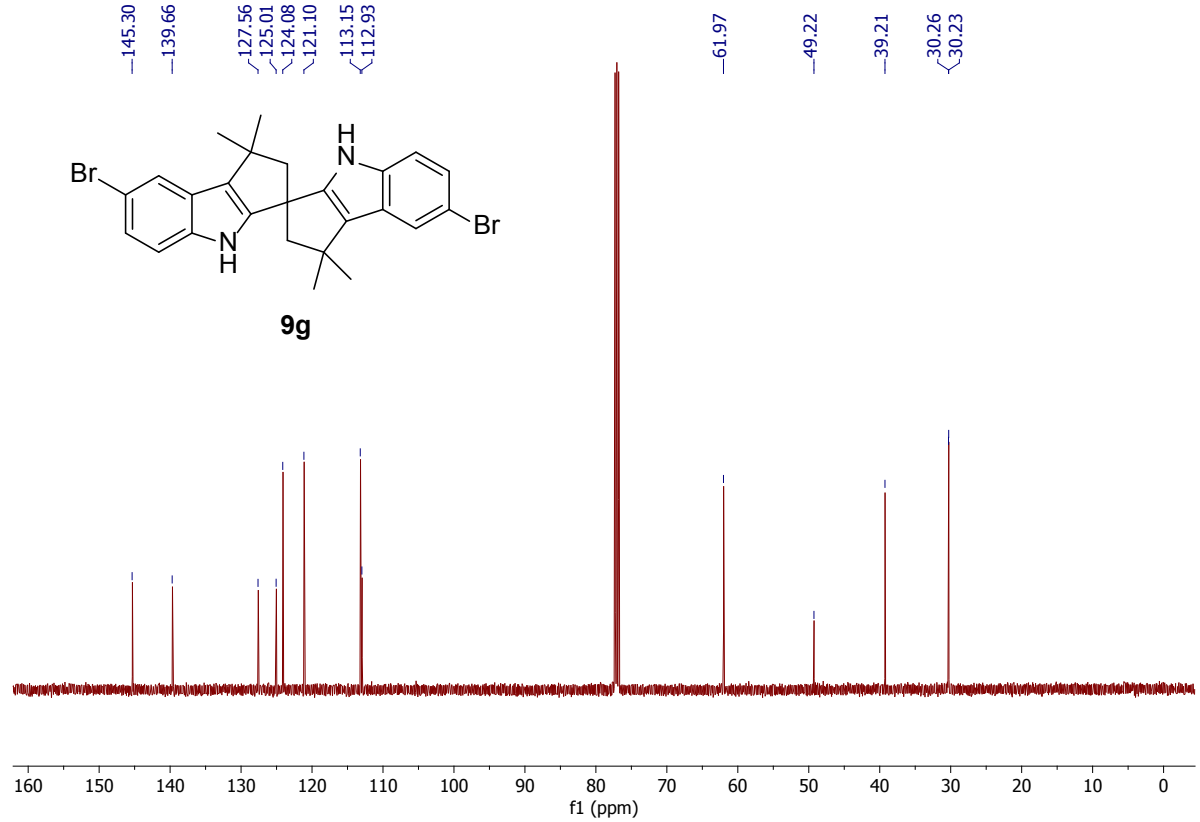

7.62
7.50
7.50
7.25
7.15
7.13
7.07
7.07
7.05
7.05
2.76
2.74
2.62
2.59
1.54
1.47
Cl
H
N
N
H
Cl
9e
2.01
1.95
2.01
2.01
2.02
2.04
6.10
6.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


145.51
139.38
127.63
125.33
124.35
121.48
118.02
112.68
61.98
49.27
39.19
30.24
30.21
Cl
H
N
N
H
Cl
9e
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.57
7.19
7.17
7.15
7.14
7.13
7.12
6.87
6.85
6.83
2.77
2.74
2.62
2.59
1.54
1.47
F
H
N
N
H
F
9f
2.04
1.94
1.92
1.95
2.05
2.03
6.08
6.00
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 0.0
f1 (ppm)


158.71
156.84
146.07
137.51
127.99
127.96
123.62
123.54
112.24
112.16
109.40
109.19
103.71
103.52
62.02
49.33
39.16
30.19
30.15
F
H
N
N
H
F
9f
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.66
7.61
7.20
7.19
7.11
7.09
2.76
2.73
2.62
2.59
1.54
1.47
Br
H
N
N
H
Br
9g
2.02
2.03
1.95
1.98
2.09
2.06
6.07
6.00
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 0.0
f1 (ppm)


145.30
139.66
127.56
125.01
124.08
121.10
113.15
112.93
61.97
49.22
39.21
30.26
30.23
Br
H
N
N
H
Br
9g
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)