Supporting Information

Protecting Group Controlled Remote Regioselective Electrophilic Aromatic Halogenation Reactions

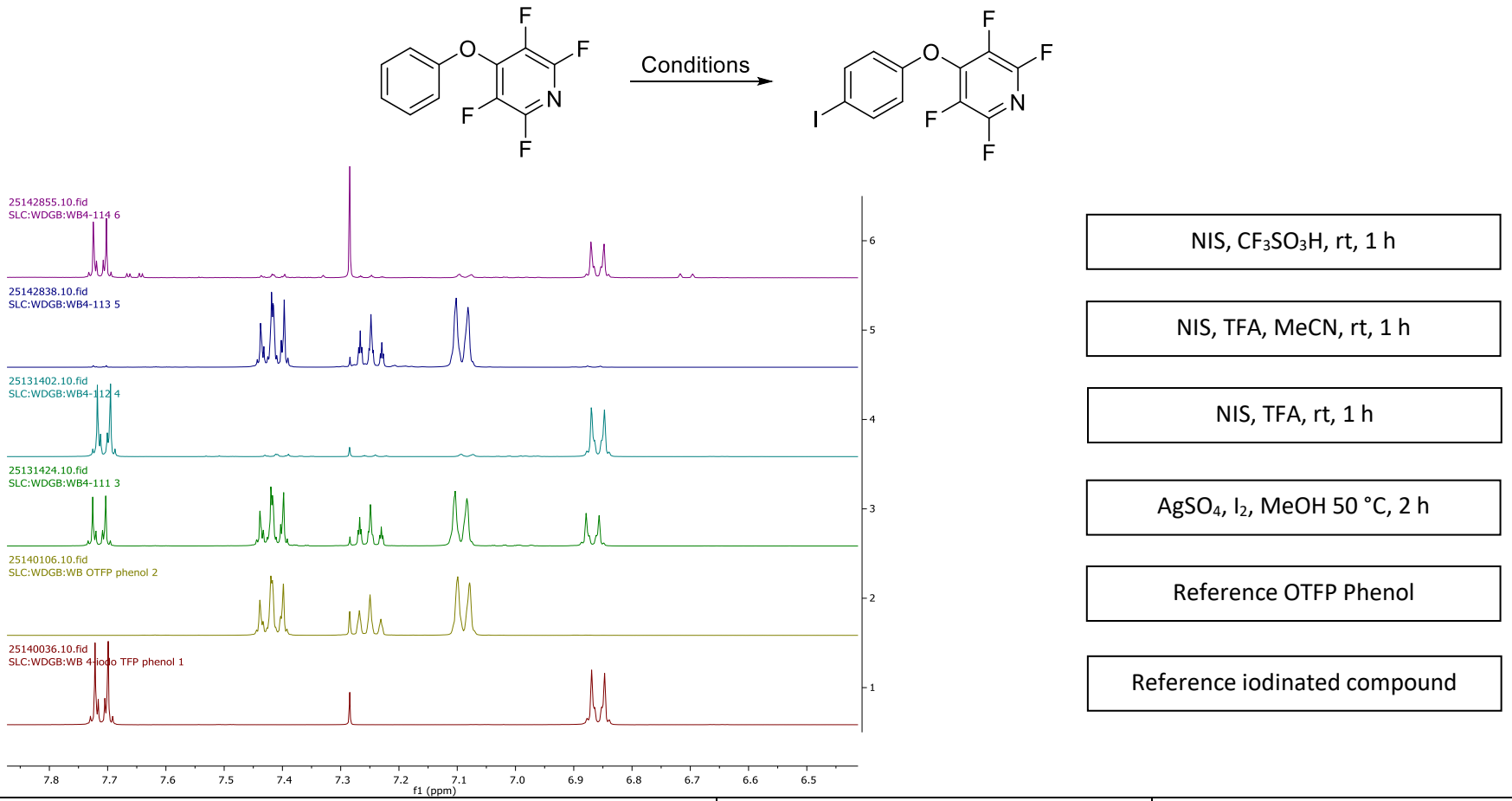
William D. G. Brittain*[,†] and Steven L. Cobb*[,†]

[†]Department of Chemistry, Durham University, South Road, Durham, DH1 3LE, United Kingdom

Email: william.d.brittain@durham.ac.uk, and s.l.cobb@durham.ac.uk

Contents

NMR Data for Reaction Condition Screening

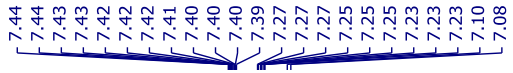


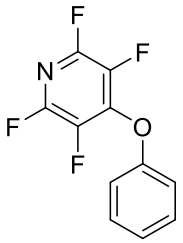
Entry	Conditions	Conversion (%)a	Yield (%)b
1	$AgSO_4$ (1.2 equiv.), I_2 (1.2 equiv.), MeOH, 50 °C, 2 h	31	-
2	NIS (1.1 equiv.), TFA, rt, 1 h	94	80
3	NIS (1.1 equiv.), TFA (0.3 equiv.), MeCN, rt, 1 h	<1	-
4	NIS (1.1. equiv), CF_3SO_3H, rt, 1 h	87	-

a) Conversion determined by integration of ^{1}H NMR spectra
b) Isolated yield following column chromatography
c) Very minor regiosomeric impurities were observed in the ^{1}H NMR spectra's obtained

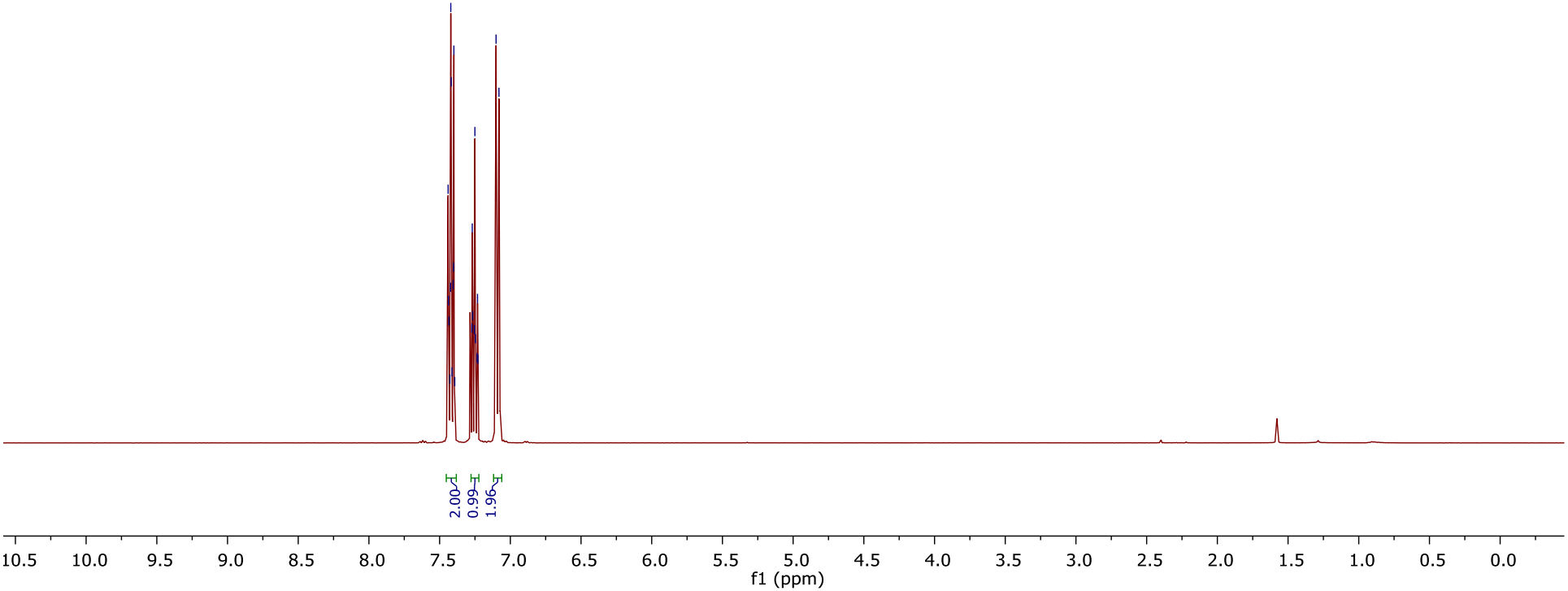
NMR Data for Synthesised Compounds

19131310.10.fid
SLC:WDGB:WB4-36

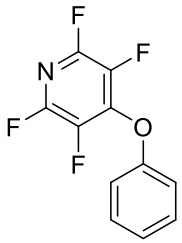




1a



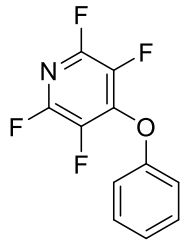
19131310.13.fid
SLC:WDGB:WB4-36



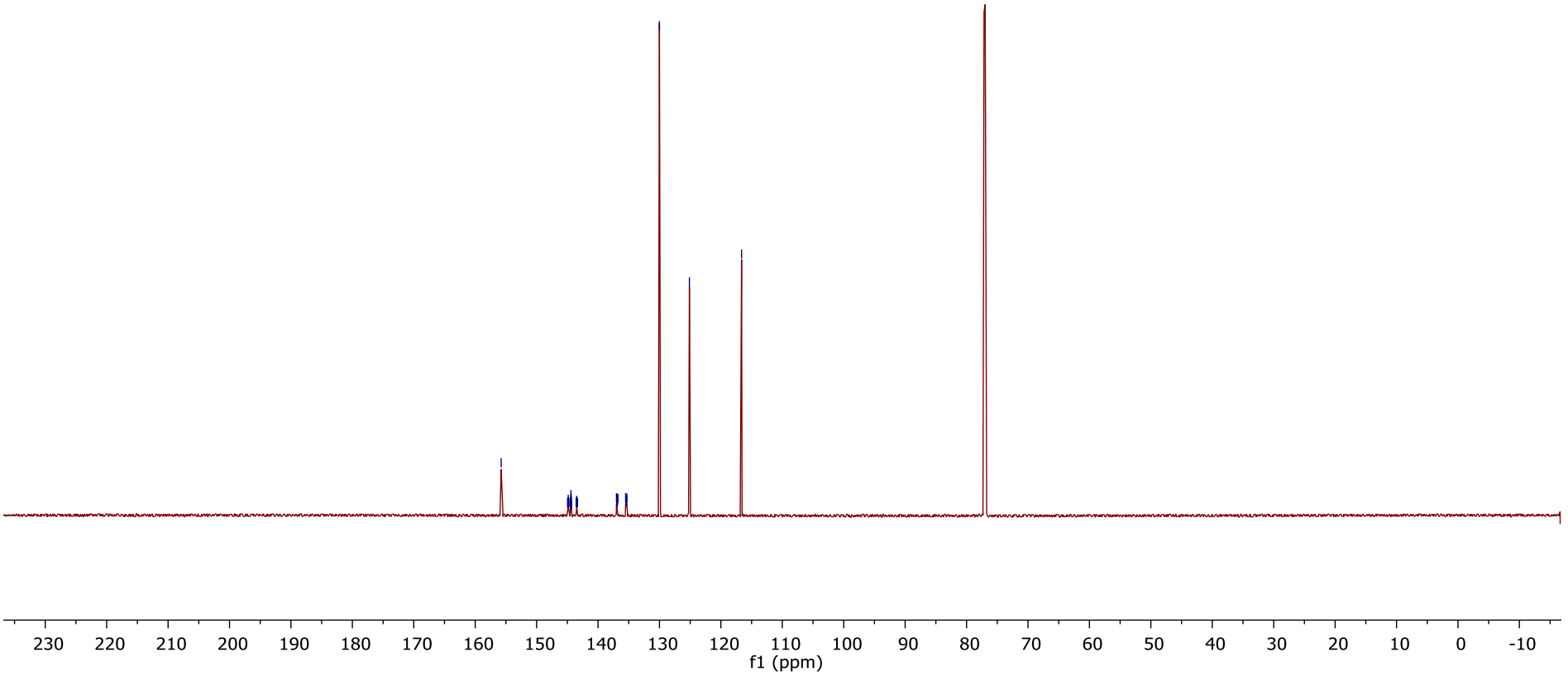
1a

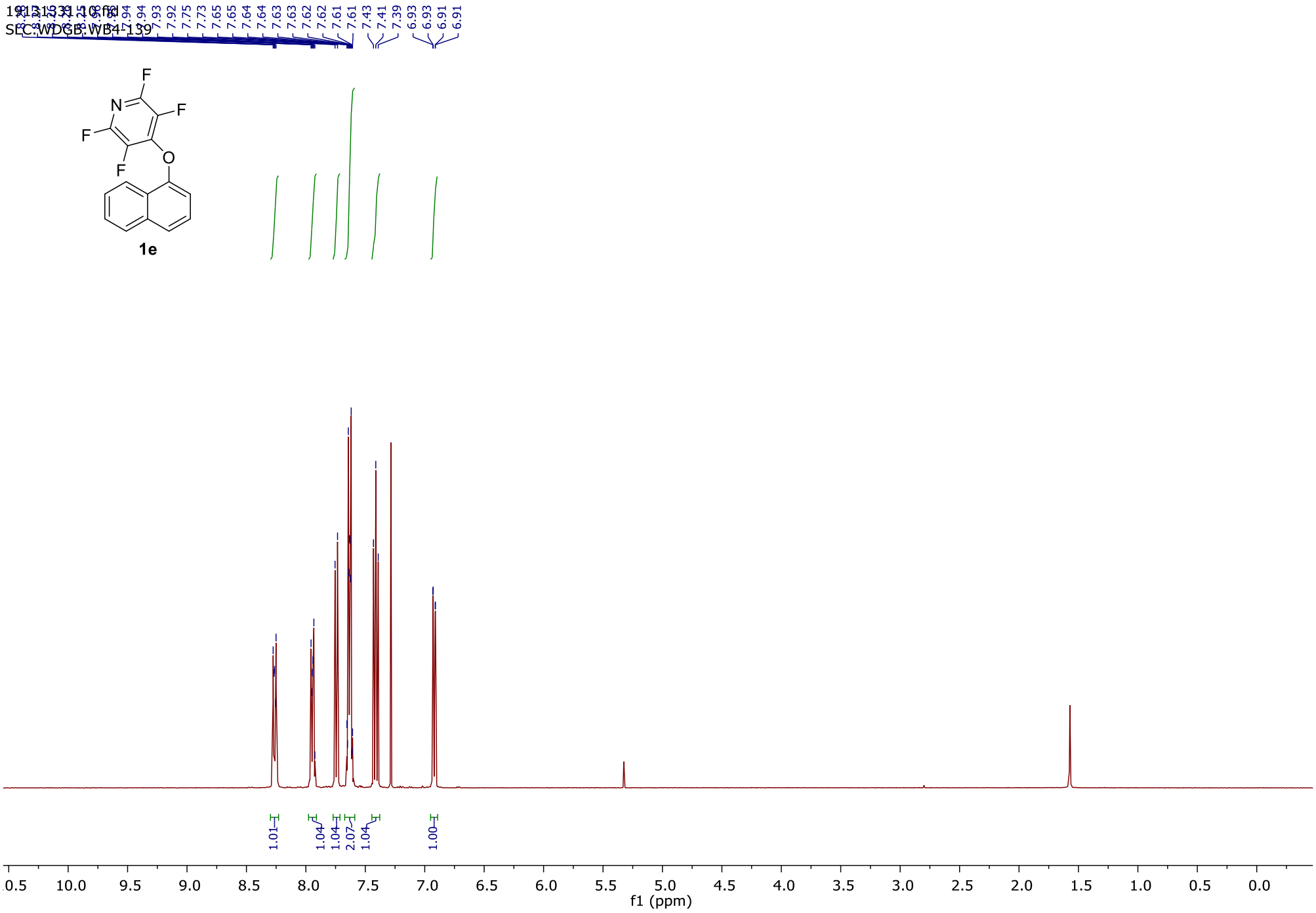
CARBON_01
SLC:WB: WB4-36

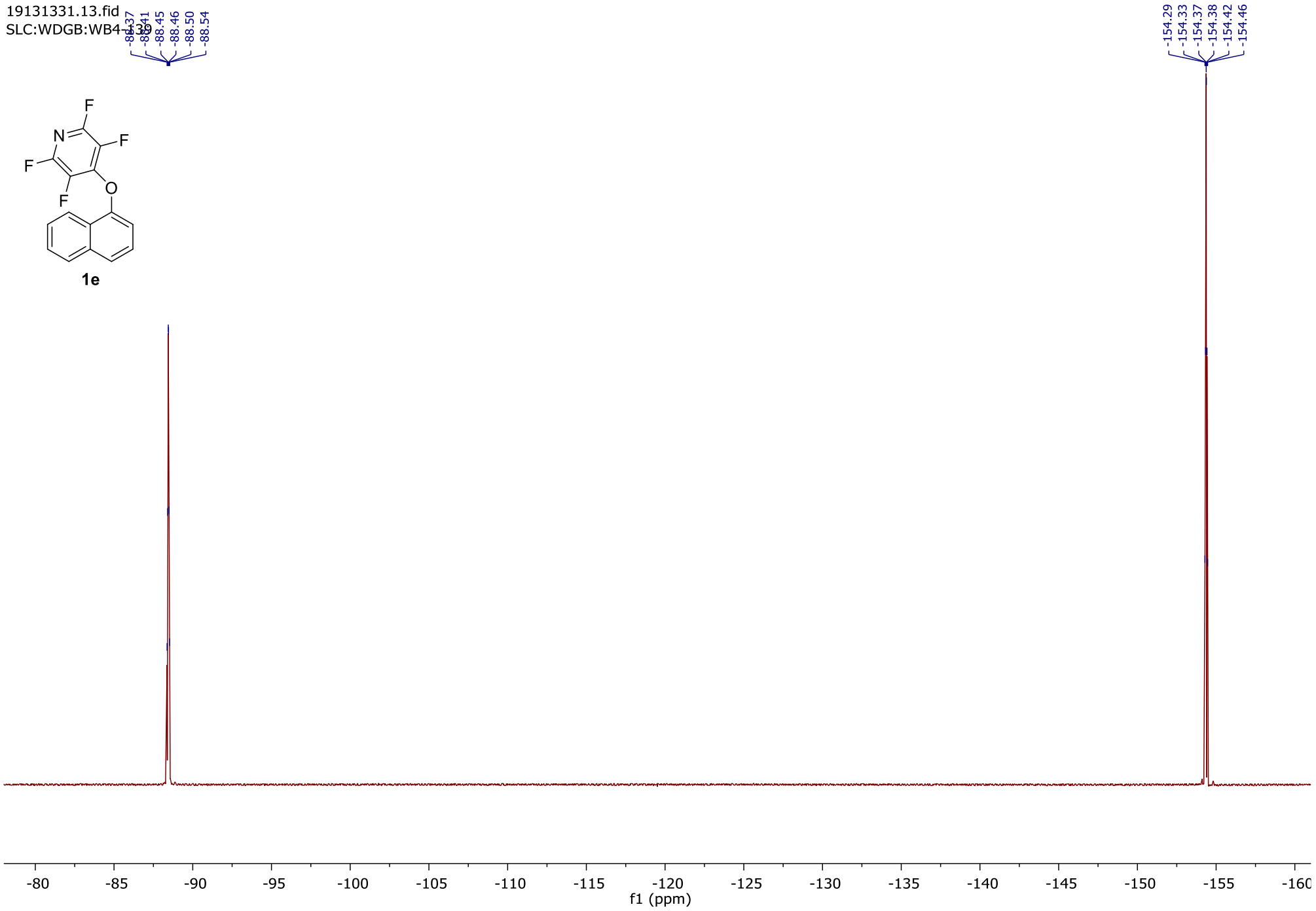
155.77 144.94 144.93 144.86 144.85 144.84 144.77 144.75 144.50 144.47 144.44 144.41 144.38 144.35 144.32 143.56 143.54 143.47 143.47 143.46 143.44 143.39 143.37 137.00 136.95 136.94 136.86 136.84 136.80 136.80 135.51 135.47 135.45 135.37 135.35 135.30 130.01 125.13 116.63



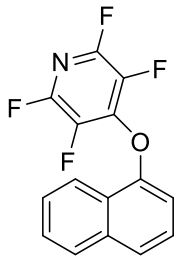
1a



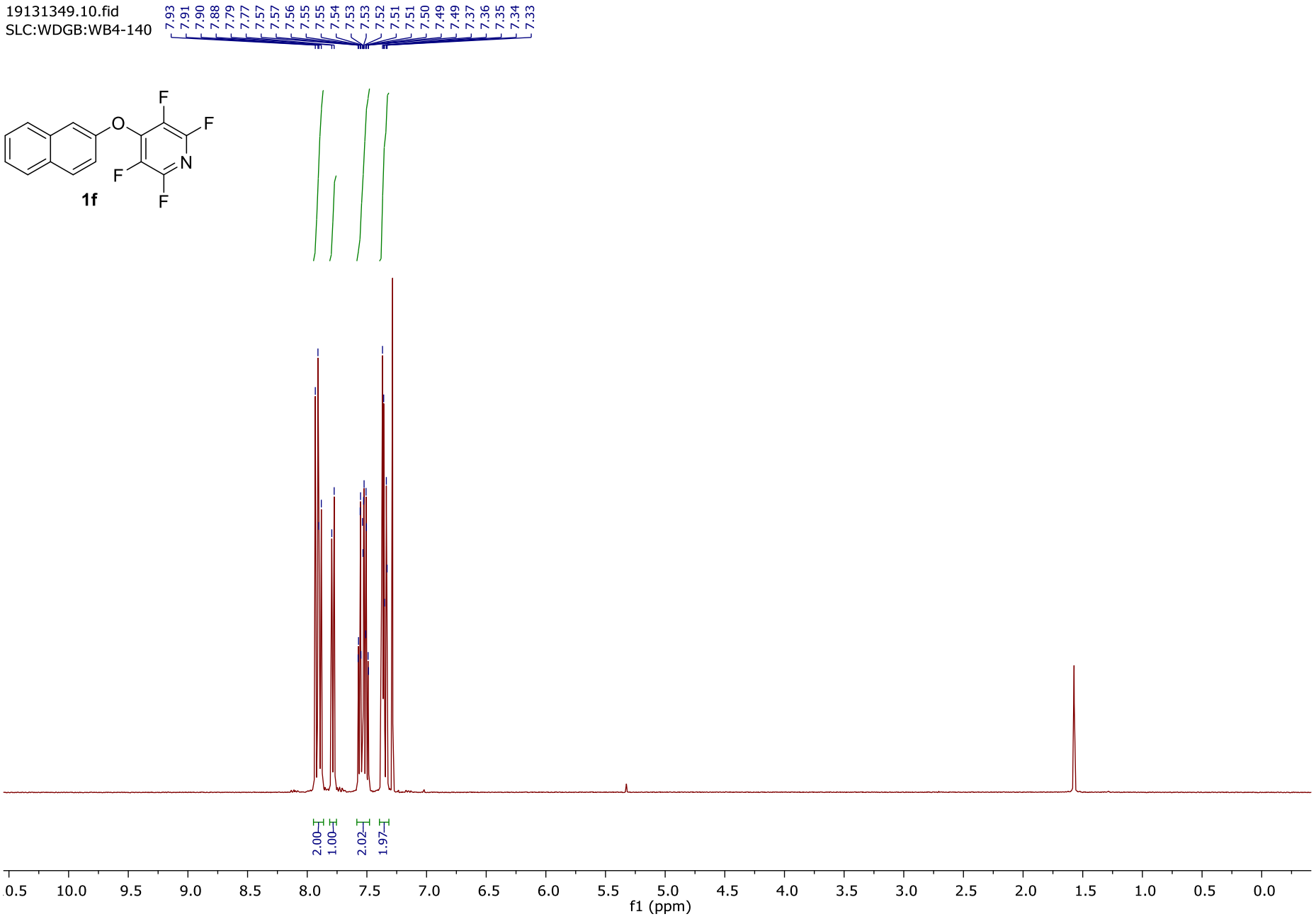

SLC:WDGB:WB4-139
7.94
7.93
7.92
7.75
7.73
7.65
7.65
7.64
7.64
7.63
7.63
7.62
7.62
7.61
7.61
7.43
7.41
7.39
6.93
6.93
6.91
6.91
F
N
F
F
F
O
1e
1.01
1.04
1.04
2.07
1.04
1.00
0.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


19131331.13.fid
SLC:WDGB:WB4-139
-88.37
-88.41
-88.45
-88.46
-88.50
-88.54
-154.29
-154.33
-154.37
-154.38
-154.42
-154.46
F
N
F
F
F
O
1e
-80
-85
-90
-95
-100
-105
-110
-115
-120
-125
-130
-135
-140
-145
-150
-155
-160
f1 (ppm)

CARBON_01
SLC:WB: WB4-139

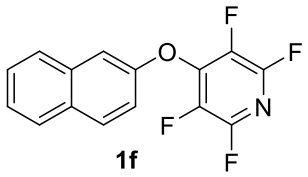


1e


19131349.10.fid
SLC:WDGB:WB4-140
7.93
7.91
7.90
7.88
7.79
7.77
7.57
7.57
7.56
7.55
7.55
7.54
7.53
7.53
7.52
7.51
7.51
7.50
7.49
7.49
7.37
7.36
7.35
7.34
7.33
F
O
F
N
F
F
1f
2.00
1.00
2.02
1.97
0.5
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
0.0
f1 (ppm)

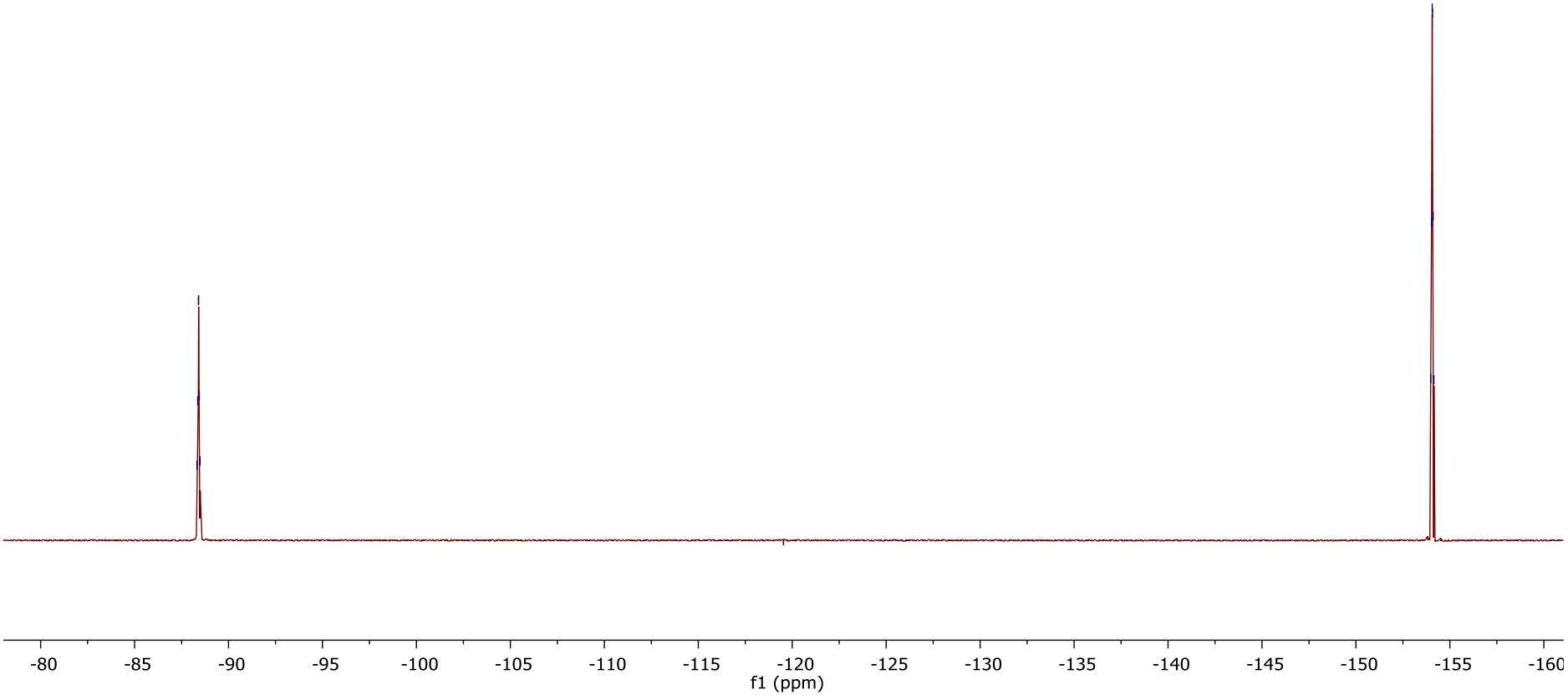
19131349.13.fid
SLC:WDGB:WB4-140

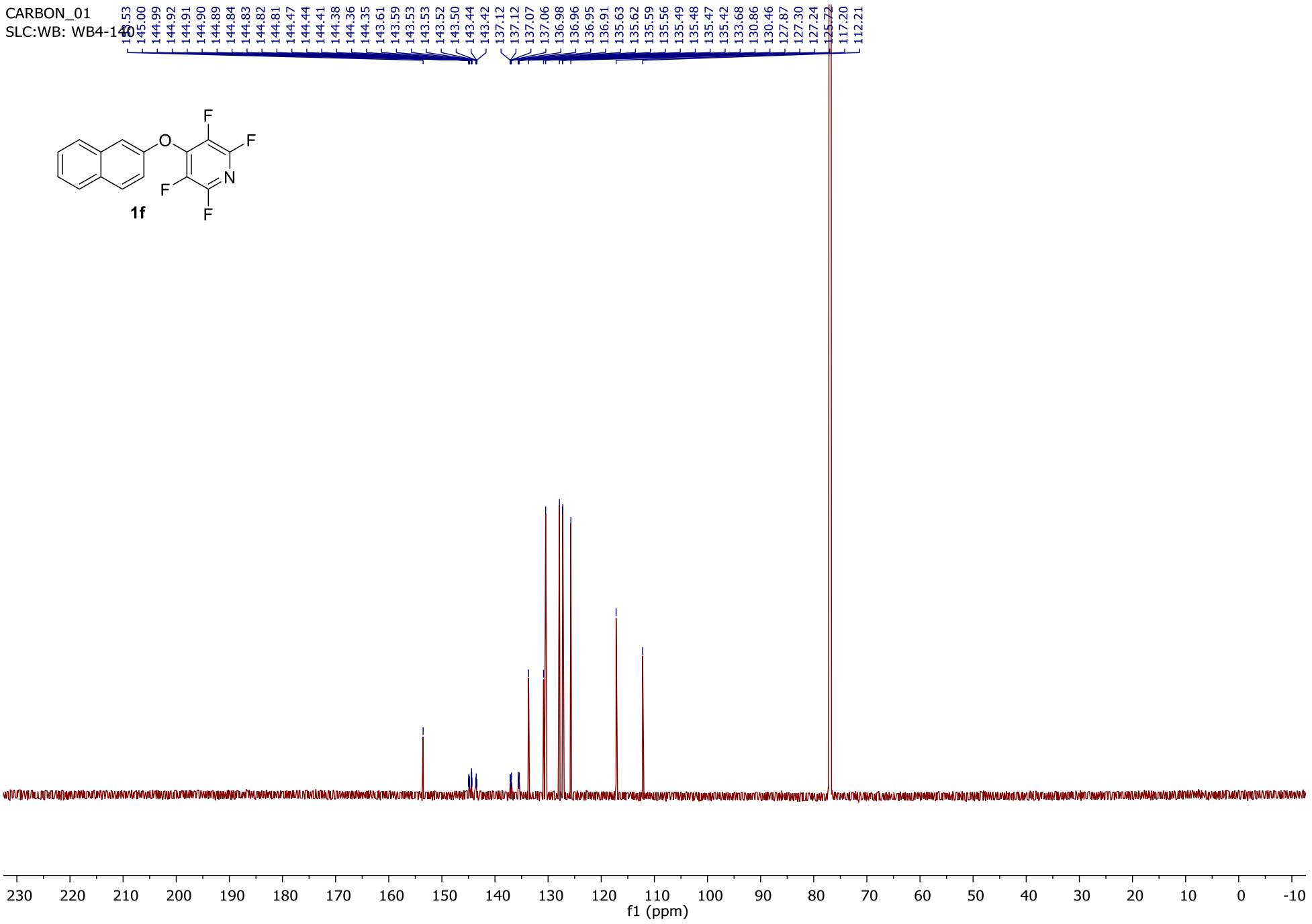
-88.32
-88.36
-88.40
-88.41
-88.45
-88.49



1f

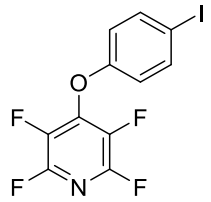
-153.98
-154.02
-154.06
-154.07
-154.11
-154.15




CARBON_01
SLC:WB: WB4-140
145.53
145.00
144.99
144.92
144.91
144.90
144.89
144.84
144.83
144.82
144.81
144.47
144.44
144.41
144.38
144.36
144.35
143.61
143.59
143.53
143.53
143.52
143.50
143.44
143.42
137.12
137.12
137.07
137.06
136.98
136.96
136.95
136.91
135.63
135.62
135.59
135.56
135.49
135.48
135.47
135.42
133.68
130.86
130.46
127.87
127.30
127.24
125.72
117.20
112.21
F
O
F
N
F
F
1f
230
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)

06125523.10.fid
SLC:WDGB:WB4-87 F1-3

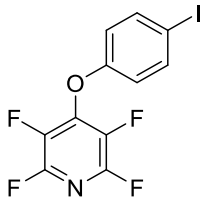
Sample was prepared using the general procedure for iodination A



2,3,5,6-tetrafluoro-4-(4-iodophenoxy)pyridine

06125523.13.fid
SLC:WDGB:WB4-87 F1-19

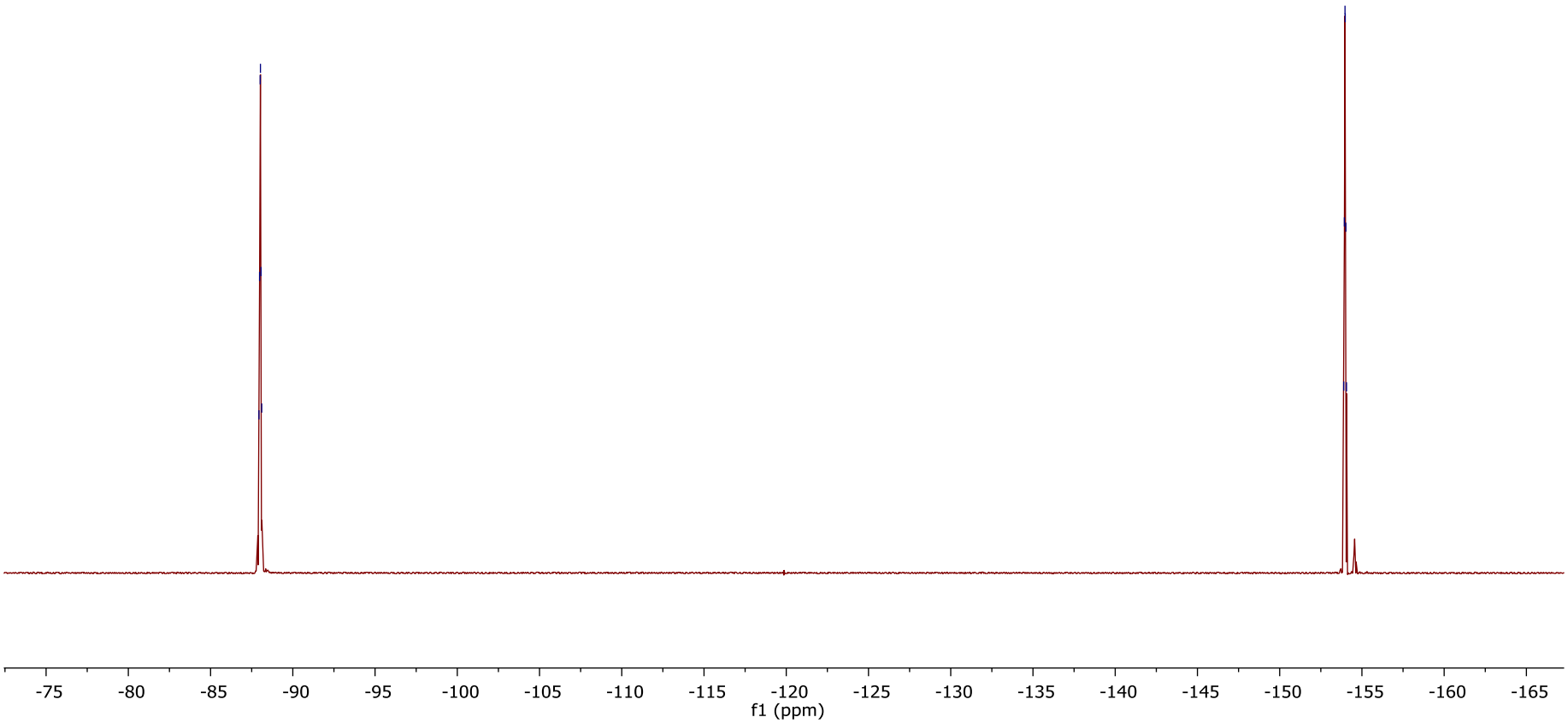
-87.94
-87.98
-88.02
-88.03
-88.07
-88.11



-153.89
-153.93
-153.97
-153.99
-154.02
-154.06

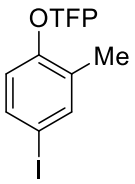
2,3,5,6-tetrafluoro-4-(4-iodophenoxy)pyridine

Sample was prepared using the general procedure for iodination A



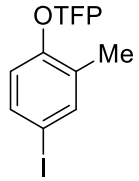
PROTON_01
SLC:WB:WB2MeOTFP

Sample was prepared using the general procedure for iodination A



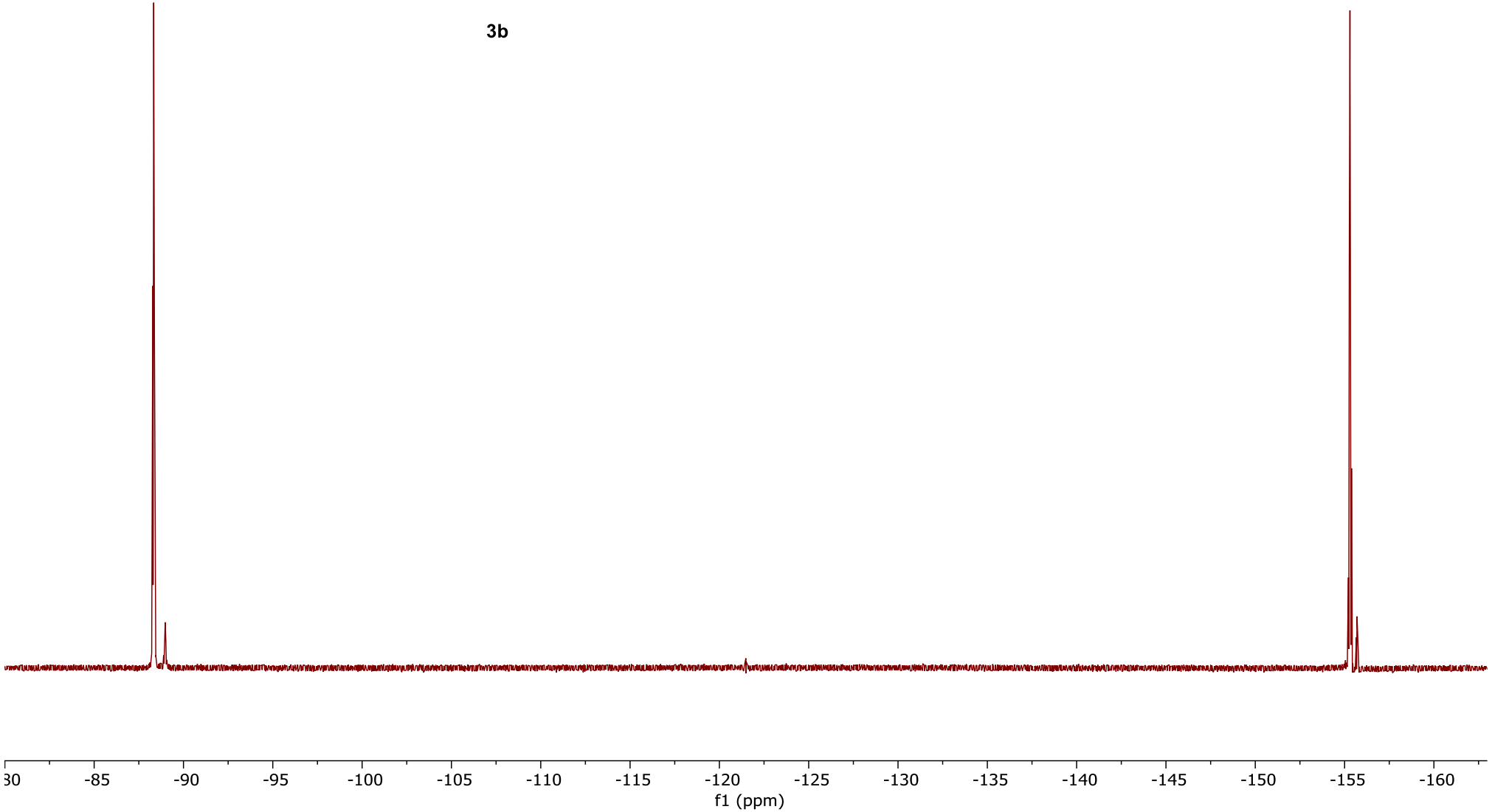
3b

23134625.13.fid
SLC:WDGB:WB 2Me OTFP

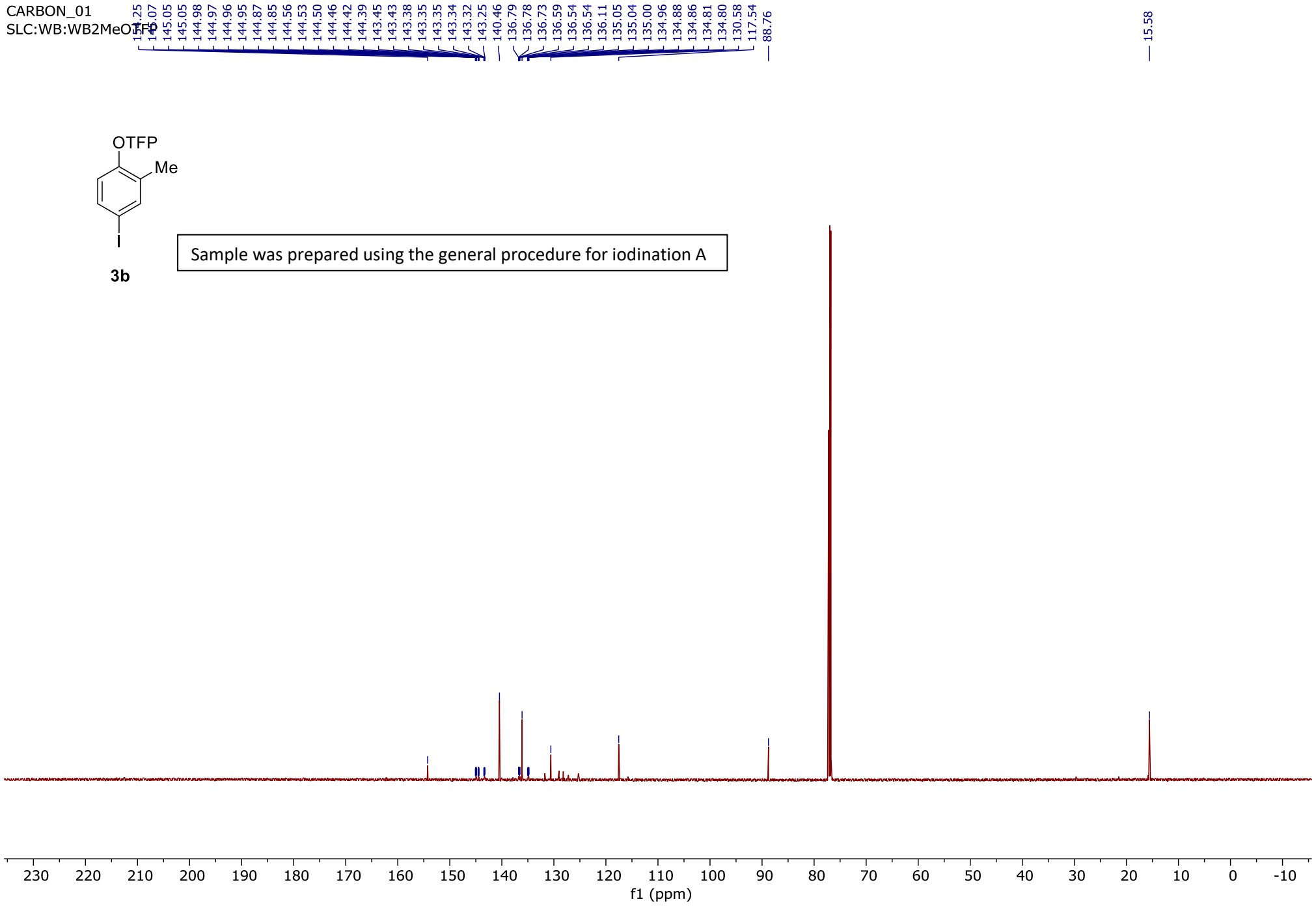


3b

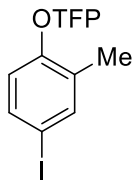
Sample was prepared using the general procedure for iodination A



CARBON_01
SLC:WB:WB2MeOTFP

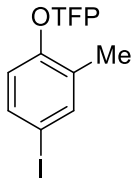


Sample was prepared using the general procedure for iodination A



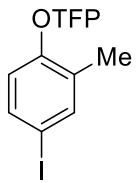
3b

Sample was prepared using the general procedure for iodination A

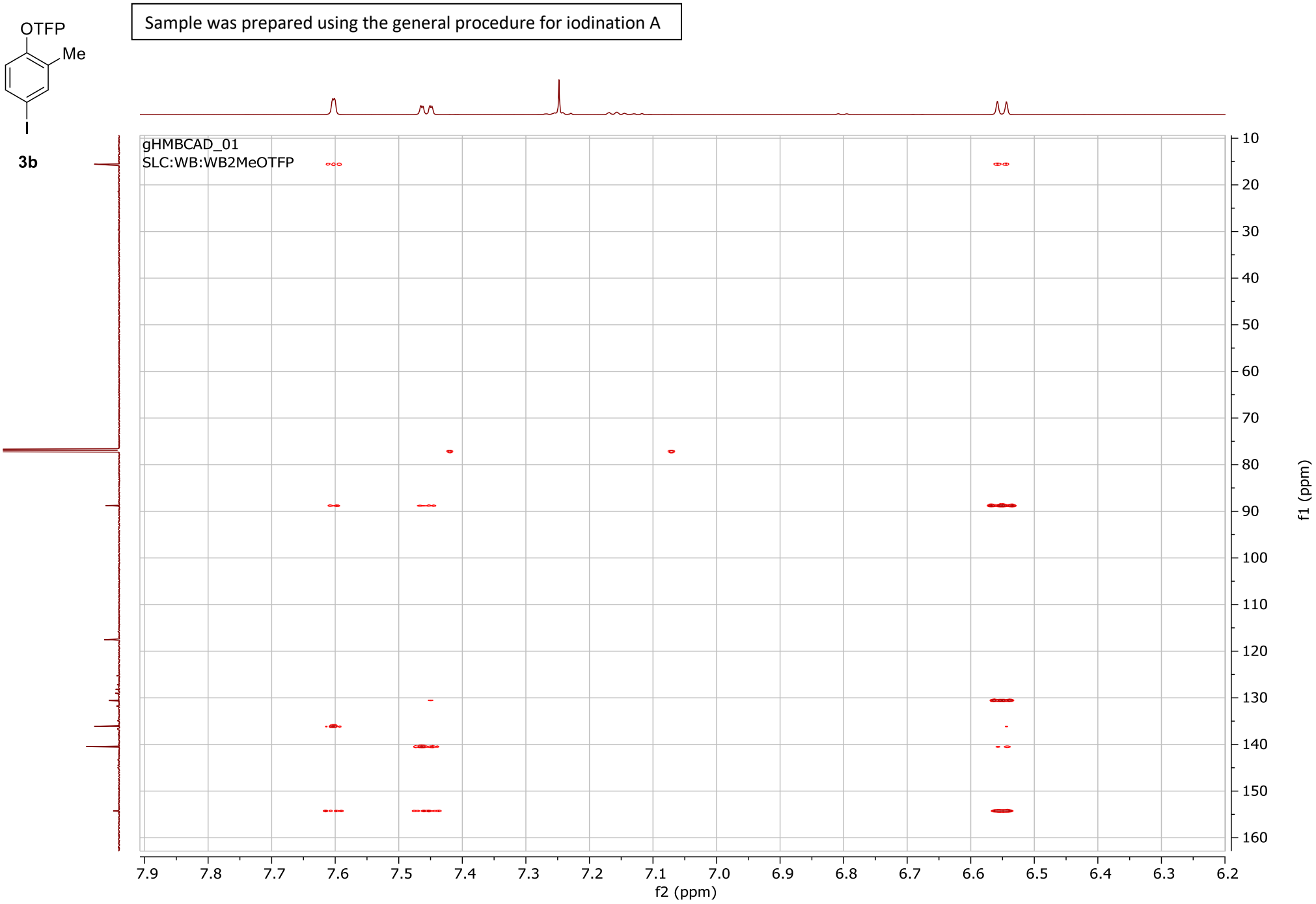


3b

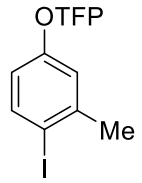
Sample was prepared using the general procedure for iodination A



3b


OTFP
Me
I
3b
Sample was prepared using the general procedure for iodination A
gHMBCAD_01
SLC:WB:WB2MeOTFP
f2 (ppm)
f1 (ppm)

PROTON_01
SLC:WB-3Me_OTFPI



3c

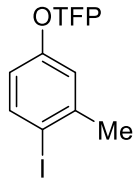
Sample was prepared using the general procedure for iodination A

24092408.13.fid
SLC:WDGB:WB 3Me OTFP

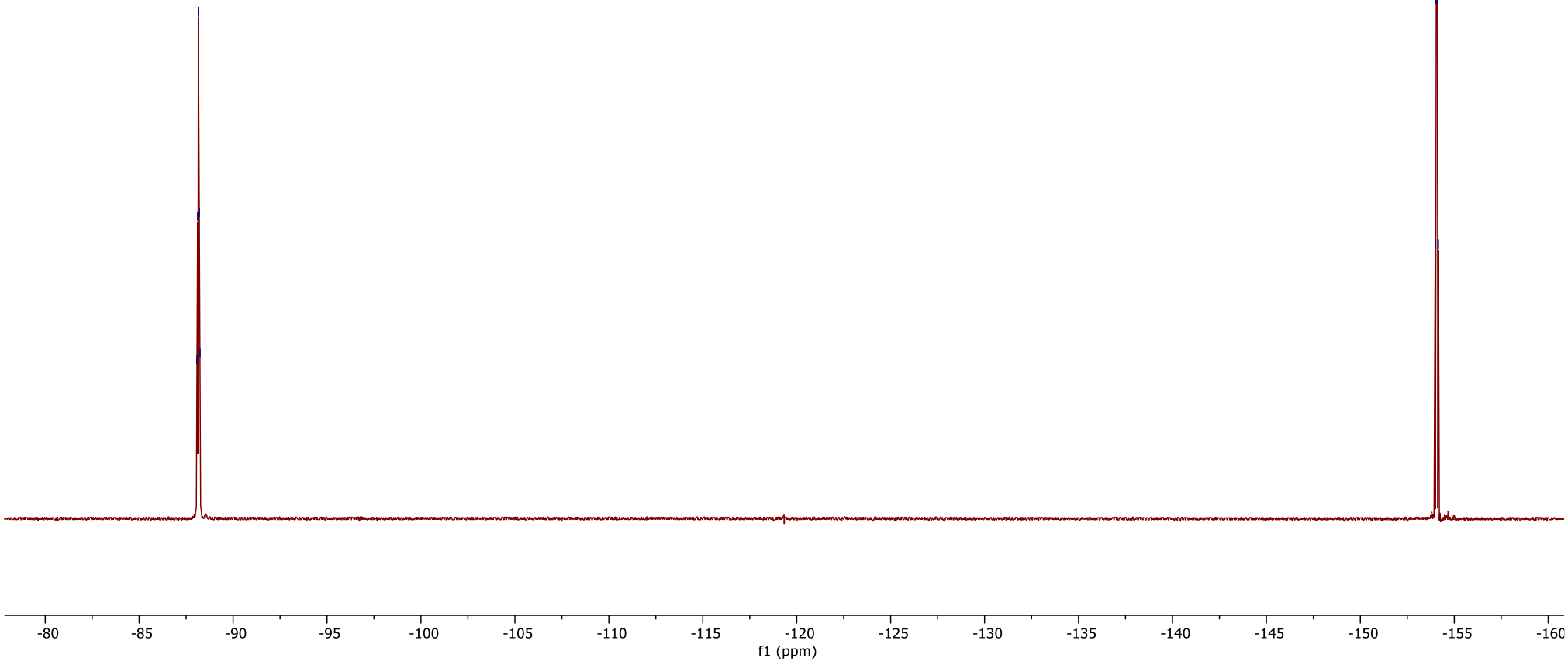
-88.07
-88.11
-88.15
-88.16
-88.20
-88.24

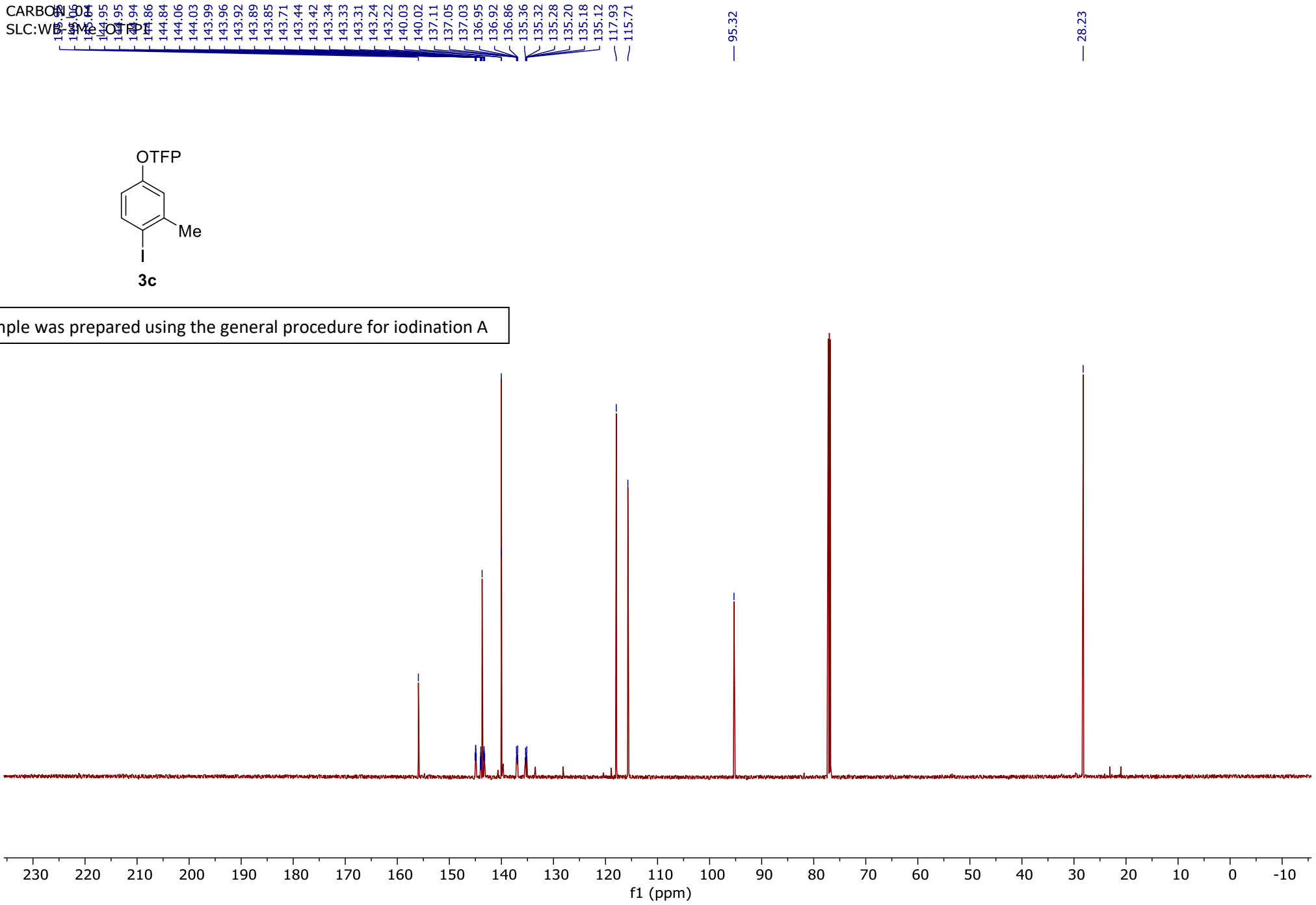
-153.98
-154.02
-154.06
-154.08
-154.11
-154.15

Sample was prepared using the general procedure for iodination A

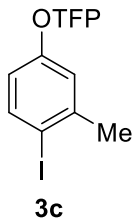


3c



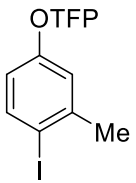

CARBON_01
SLC:WB-3Me-OTFP1
95.32
28.23
OTFP
Me
I
3c
Sample was prepared using the general procedure for iodination A
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

Sample was prepared using the general procedure for iodination A



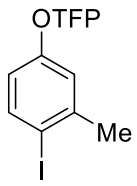
3c

Sample was prepared using the general procedure for iodination A



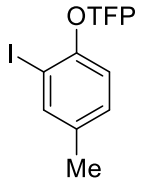
3c

Sample was prepared using the general procedure for iodination A



3c

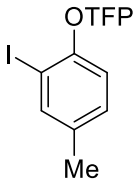
28103545.10.fid
SLC:WDGB:WB4MeOTFP



3d

Sample was prepared using the general procedure for iodination A

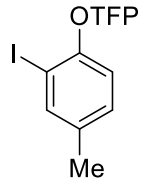
28103545.13.fid
SLC:WDCB:WB4MeOTFP



3d

Sample was prepared using the general procedure for iodination A

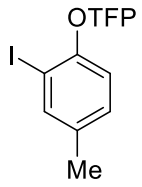
CARBON_01
SLC:WB:WB4MeOTFP



3d

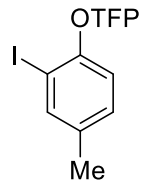
Sample was prepared using the general procedure for iodination A

Sample was prepared using the general procedure for iodination A

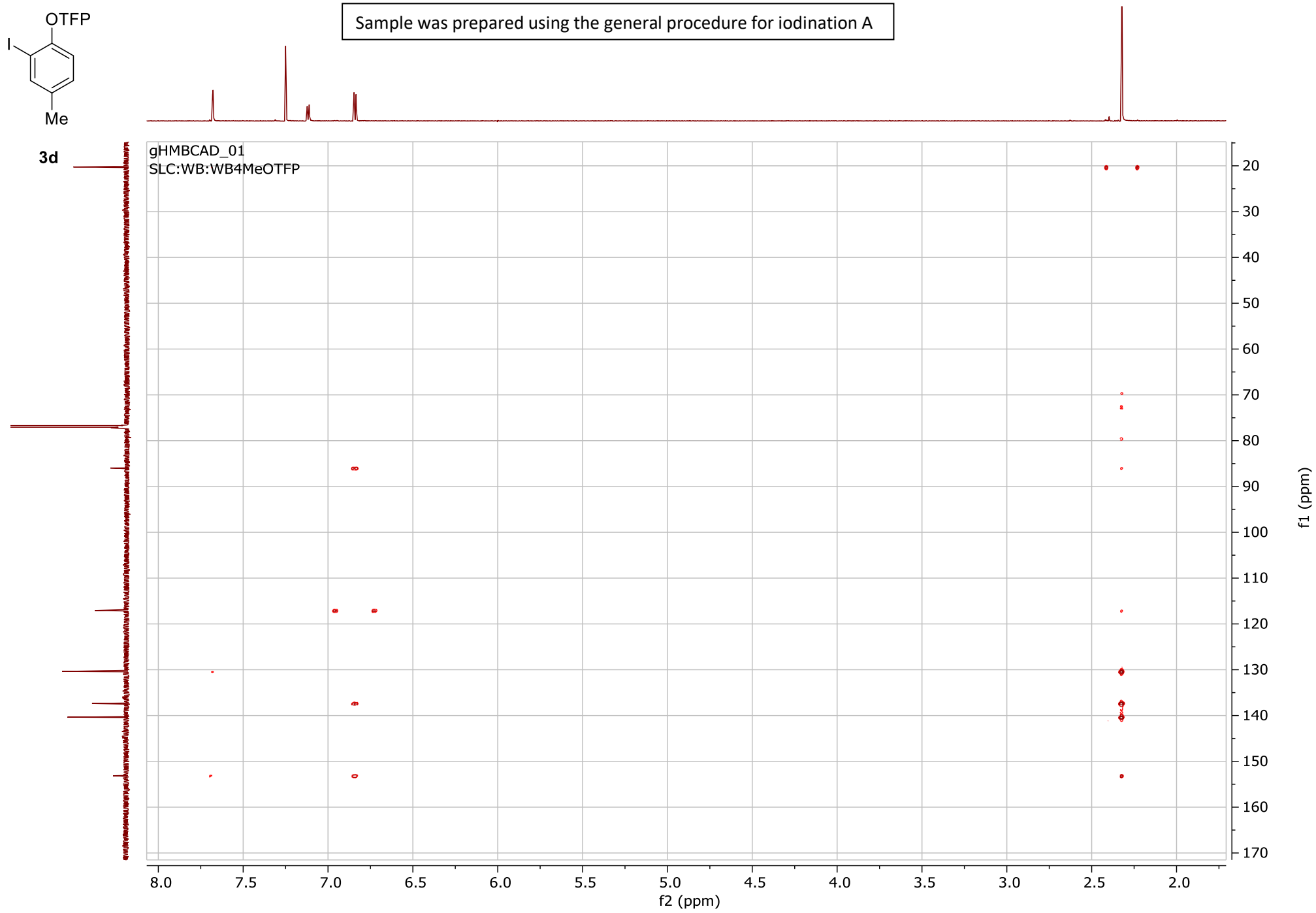


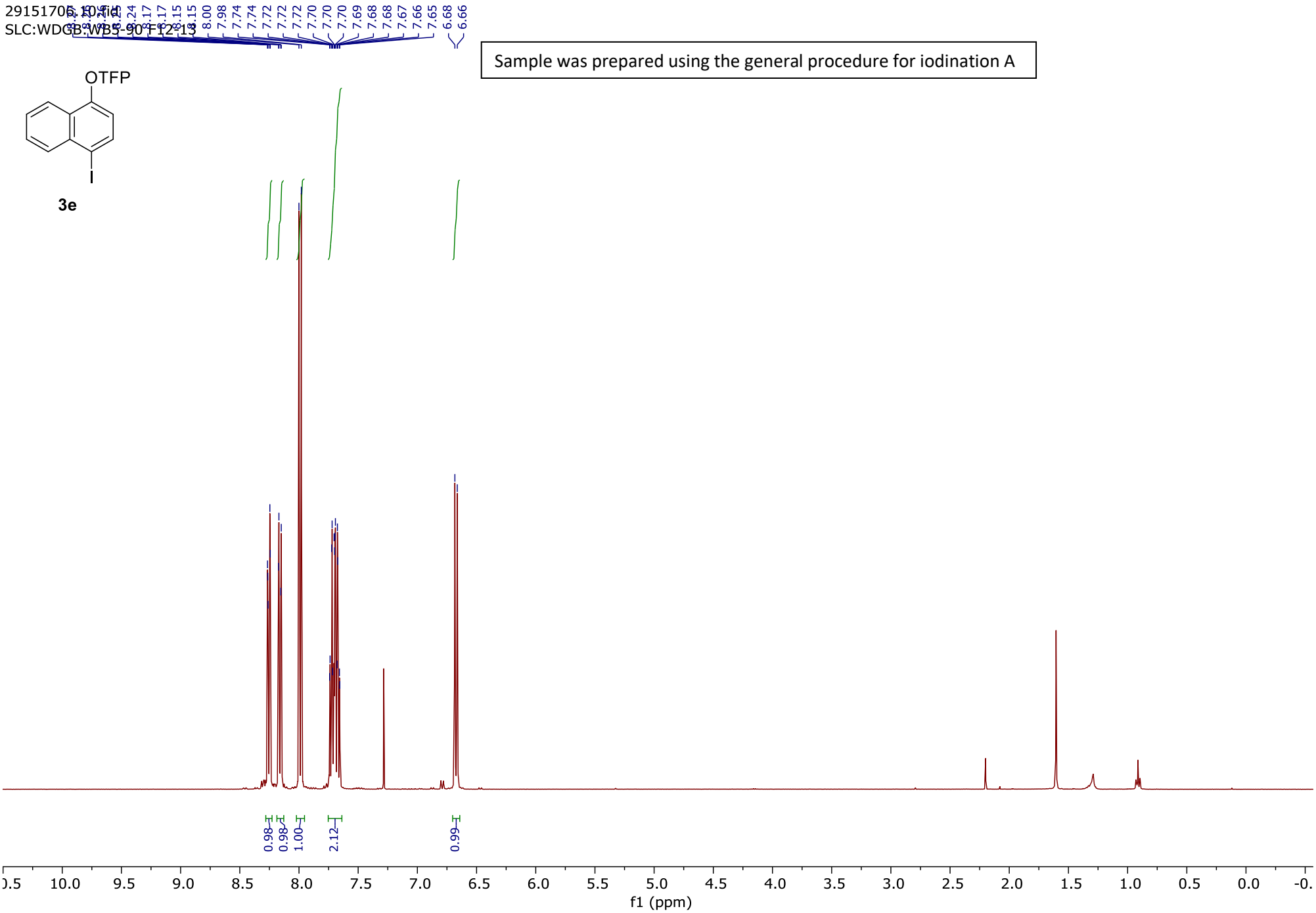
3d

Sample was prepared using the general procedure for iodination A

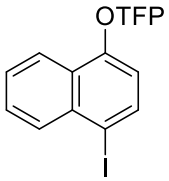


3d


OTFP
I
Me
Sample was prepared using the general procedure for iodination A
3d
gHMBCAD_01
SLC:WB:WB4MeOTFP
f2 (ppm)
f1 (ppm)


29151706.10.fid
SLC:WDGB:WB5-90-F12-13
8.24 8.17 8.17 8.15 8.15 8.00 7.98 7.74 7.74 7.72 7.72 7.72 7.70 7.70 7.70 7.69 7.68 7.68 7.67 7.66 7.65 6.68 6.66
OTFP
I
3e
Sample was prepared using the general procedure for iodination A
0.98 0.98 1.00 2.12 0.99
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 0.0
f1 (ppm)

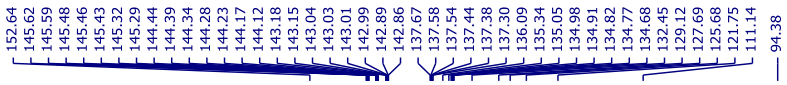
29151706.13.fid
SLC:WDGB:WB5-90 F12-13

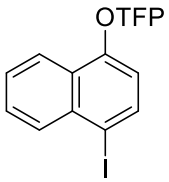


3e

Sample was prepared using the general procedure for iodination A

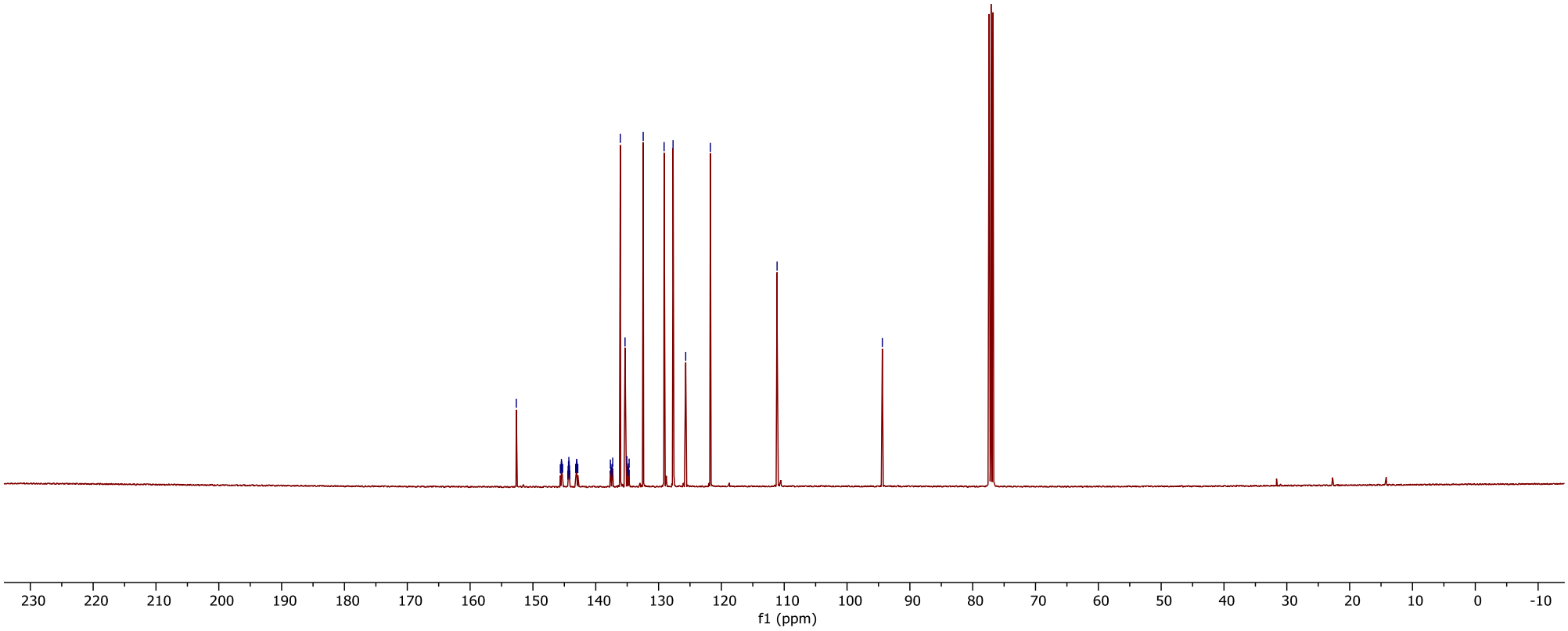
29165119.14.fid
SLC:WB:WB5-90



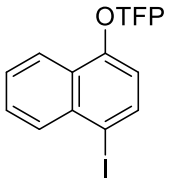


3e

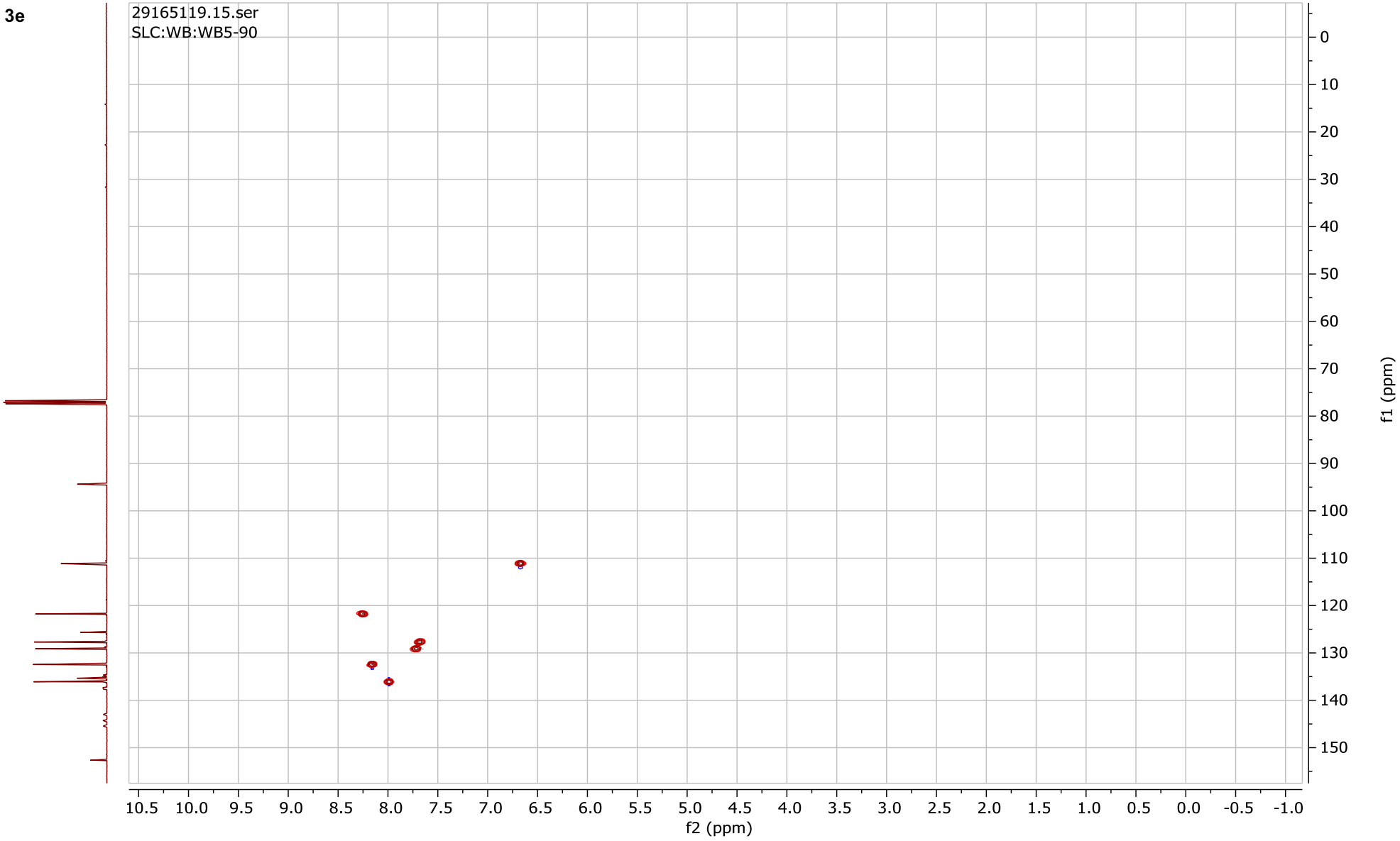
Sample was prepared using the general procedure for iodination A



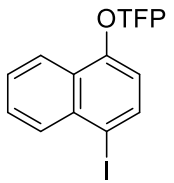
Sample was prepared using the general procedure for iodination A



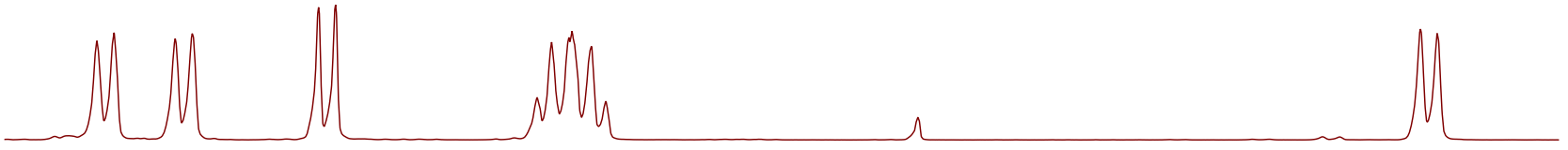
3e

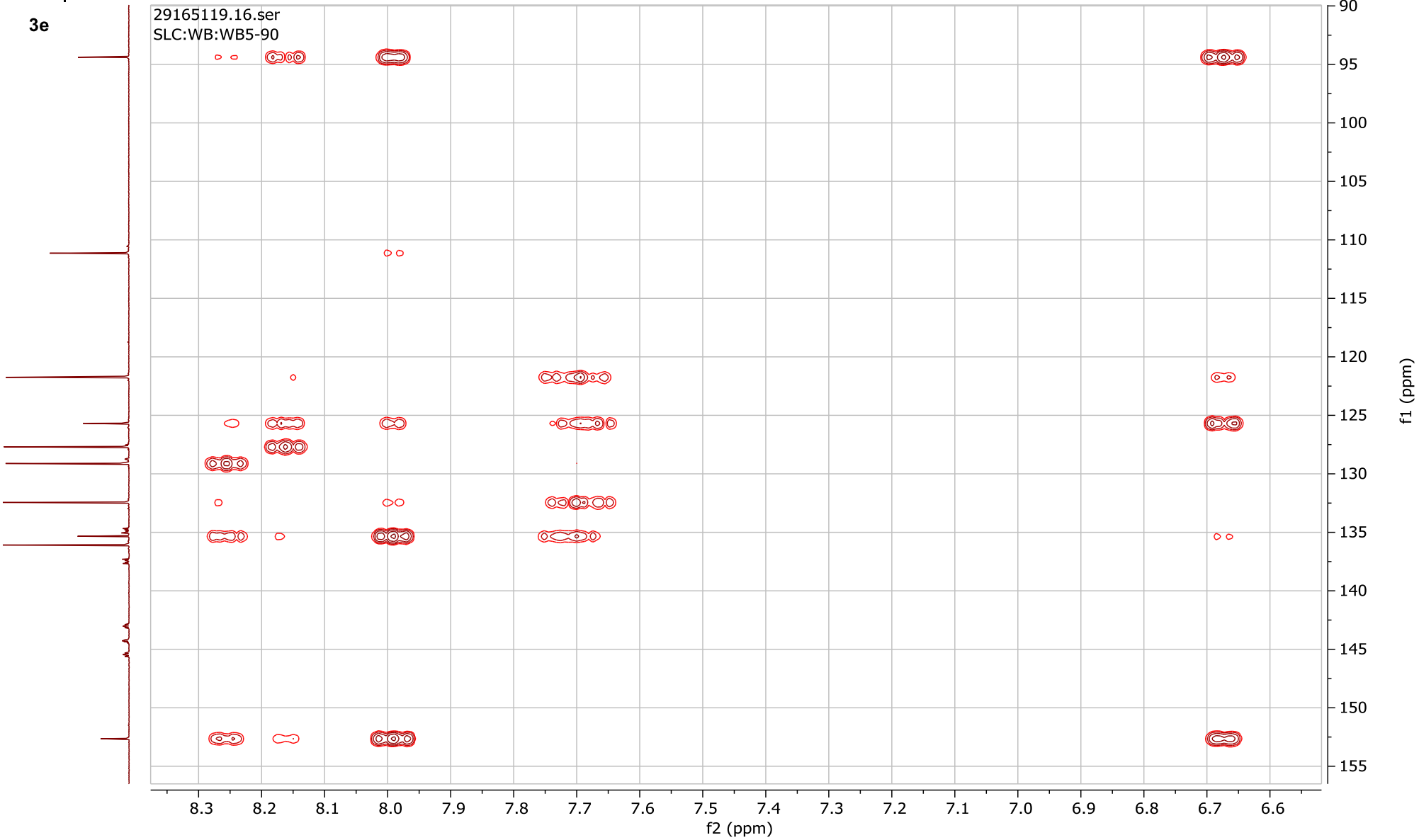


Sample was prepared using the general procedure for iodination A



3e

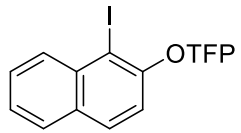




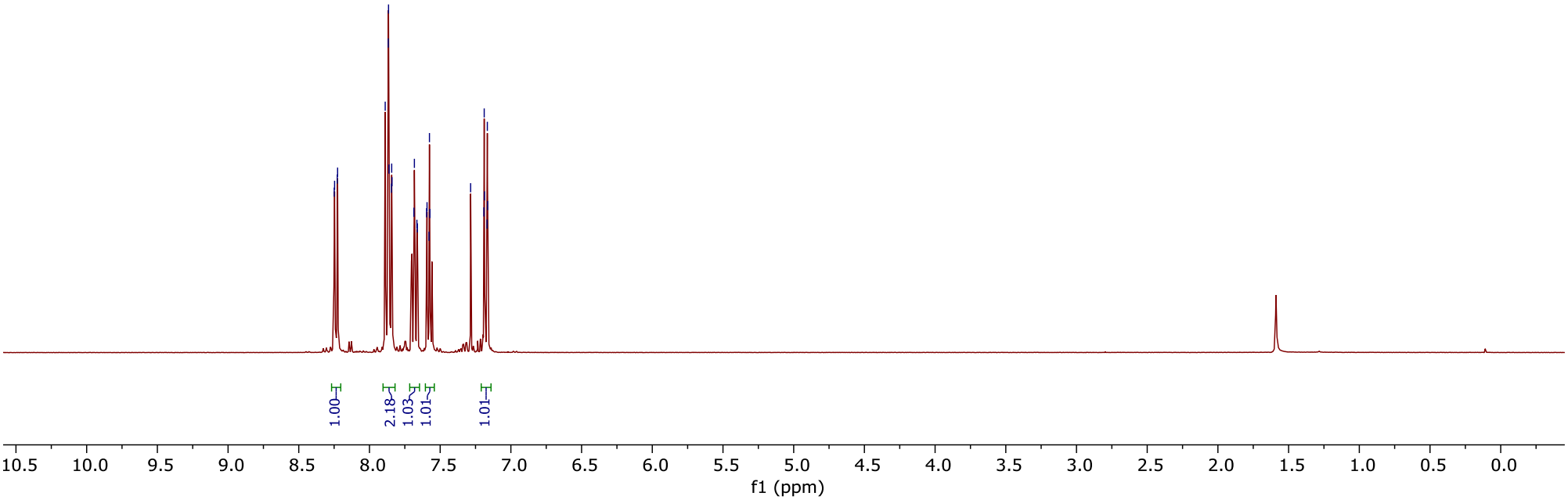
01132411.1r (f2)
SLC:WDGB:WBS-92

8.23 7.89 7.87 7.87 7.86 7.84 7.84 7.84 7.69 7.68 7.66 7.66 7.60 7.59 7.58 7.58 7.57 7.28 7.19 7.19 7.19 7.17 7.17 7.16

Sample was prepared using the general procedure for iodination A



3f

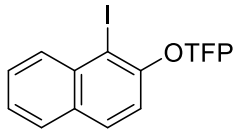


31160118.13.fid
SLC:WDGB:WB5-9

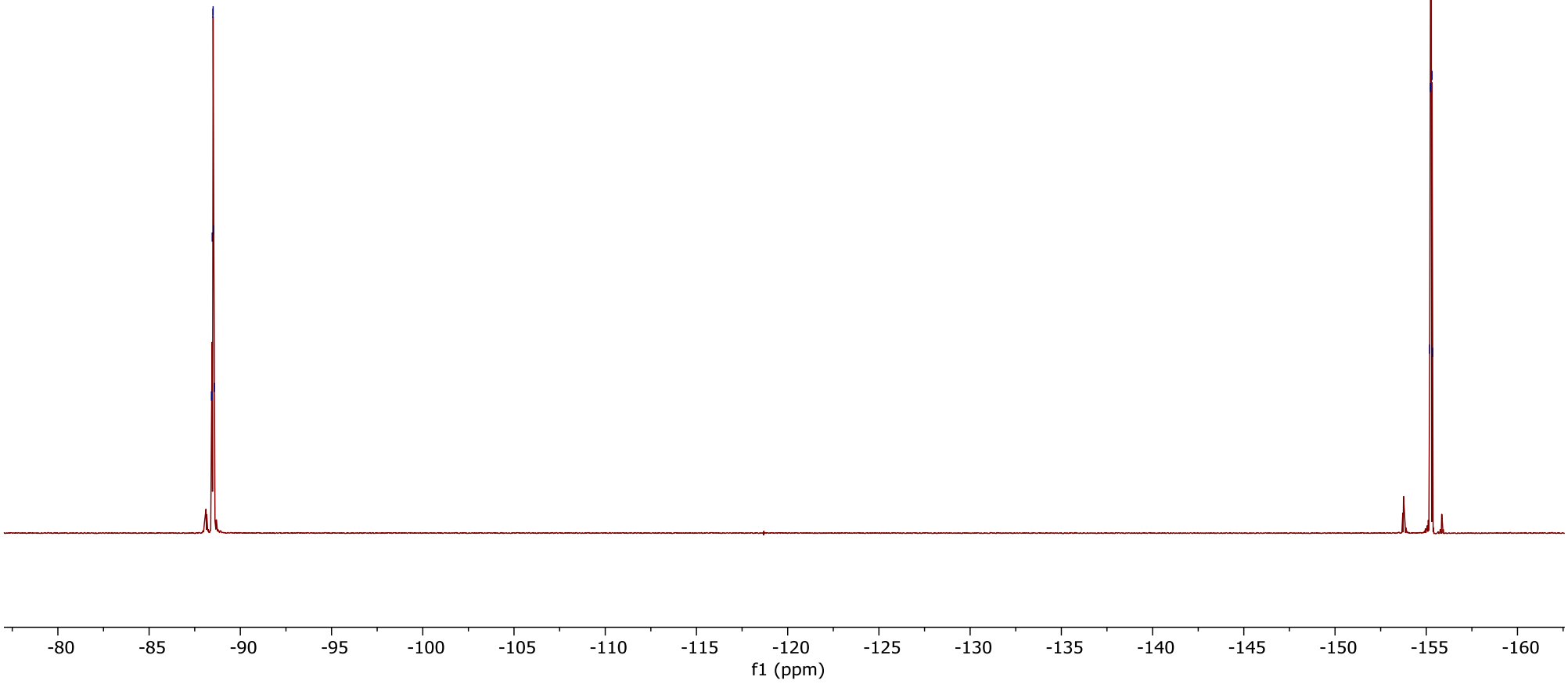
-88.42
-88.46
-88.50
-88.51
-88.55
-88.59

Sample was prepared using the general procedure for iodination A

-155.19
-155.23
-155.27
-155.28
-155.32
-155.35



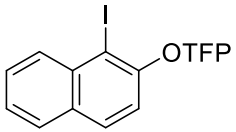
3f



01150945.13.fid
SLC:WB:WB5-92

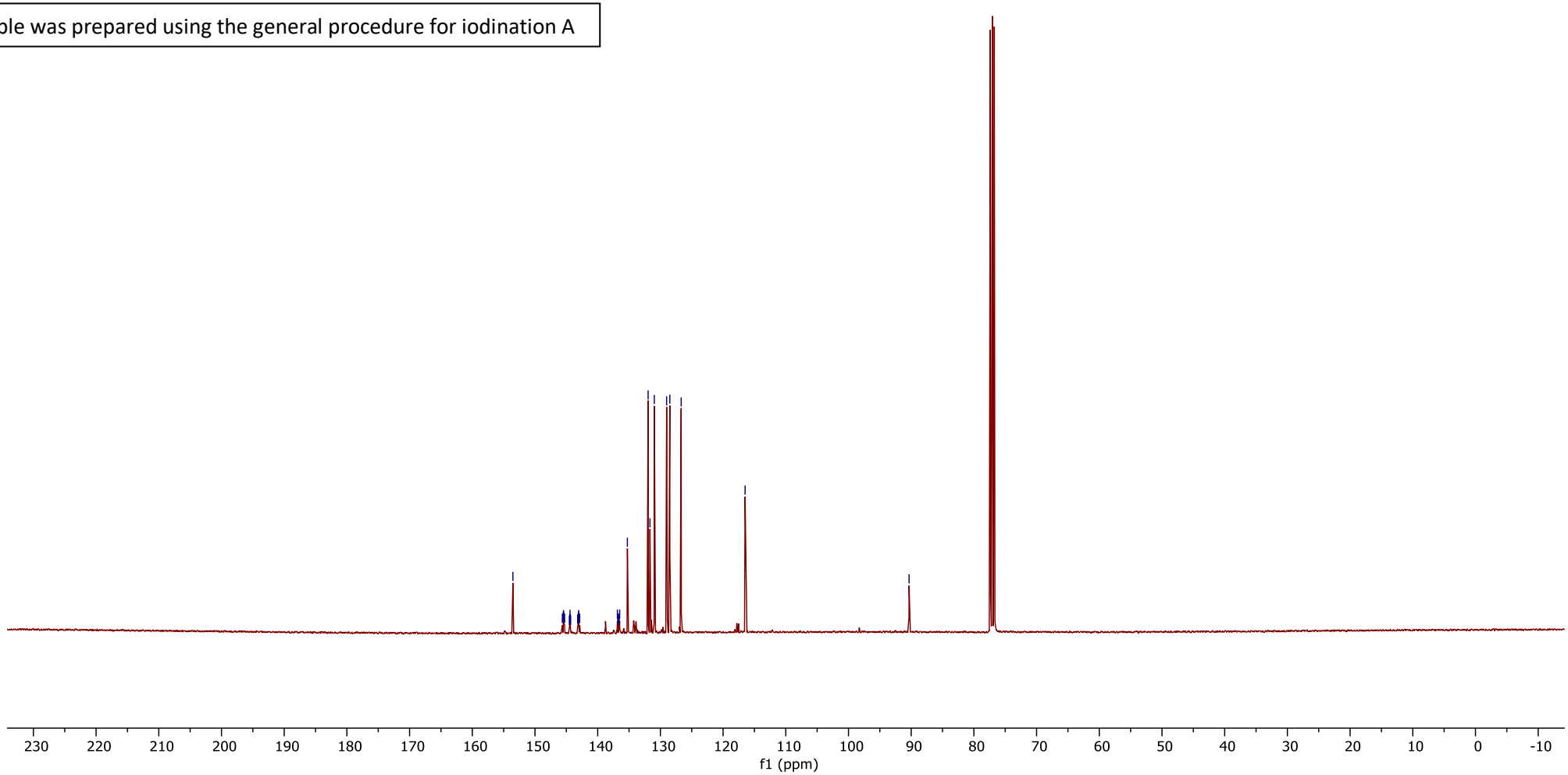
153.52
145.62
145.60
145.48
145.45
145.43
145.32
145.29
144.51
144.47
144.41
144.36
144.32
143.20
143.16
143.06
143.04
143.01
142.90
142.87
136.86
136.78
136.74
136.64
136.57
136.50
135.26
131.96
131.66
130.97
129.01
128.49
126.68
116.49

90.33

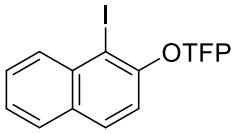


3f

Sample was prepared using the general procedure for iodination A

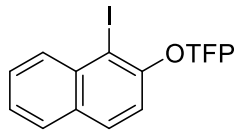


Sample was prepared using the general procedure for iodination A



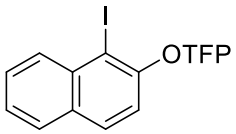
3f

Sample was prepared using the general procedure for iodination A



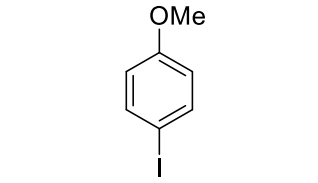
3f

Sample was prepared using the general procedure for iodination A



3f

08174913.10.fid
SLC:WDGB:WB4-121

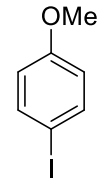


1-iodo-4-methoxybenzene

Sample was prepared using the general procedure for iodination B

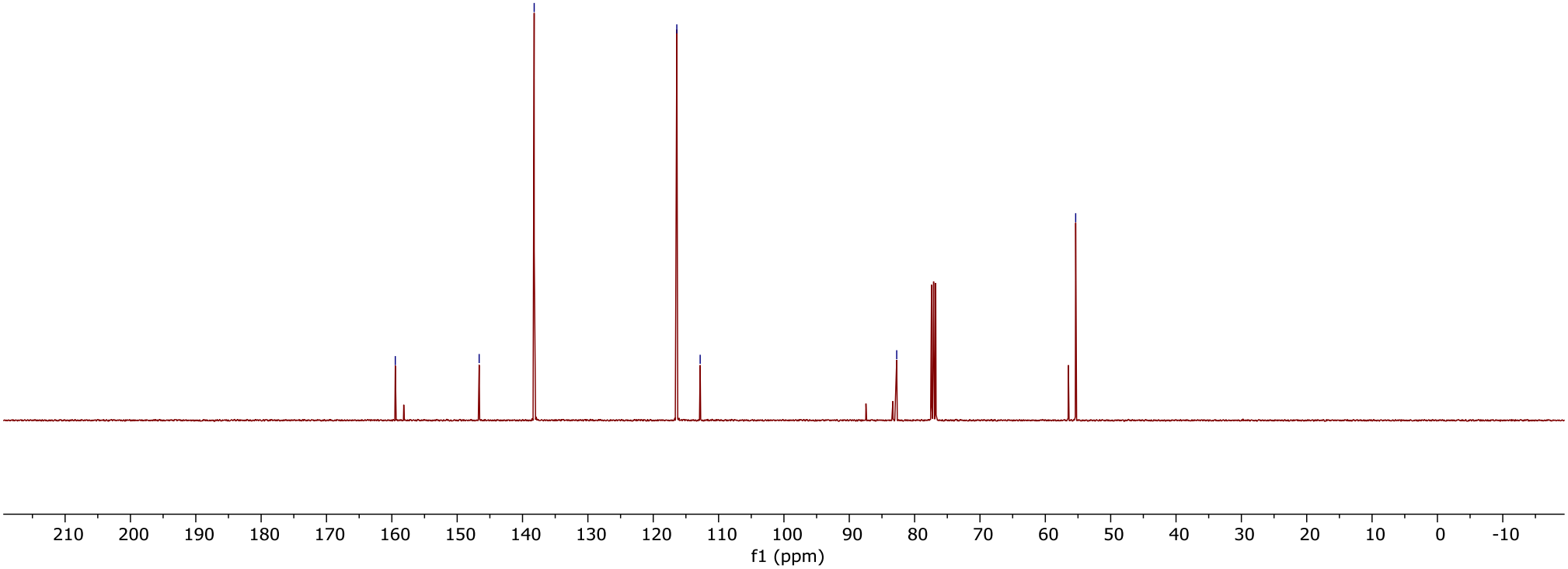
08174913.11.fid
SLC:WDGB:WB4-121

159.47
146.64
138.22
116.39
112.82
82.74
55.36

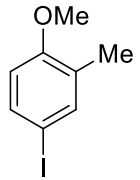


1-iodo-4-methoxybenzene

Sample was prepared using the general procedure for iodination B



08122539.10.fid
SLC:WDGB:WB4-125

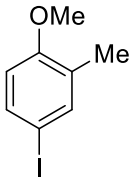


4b

Sample was prepared using the general procedure for iodination B

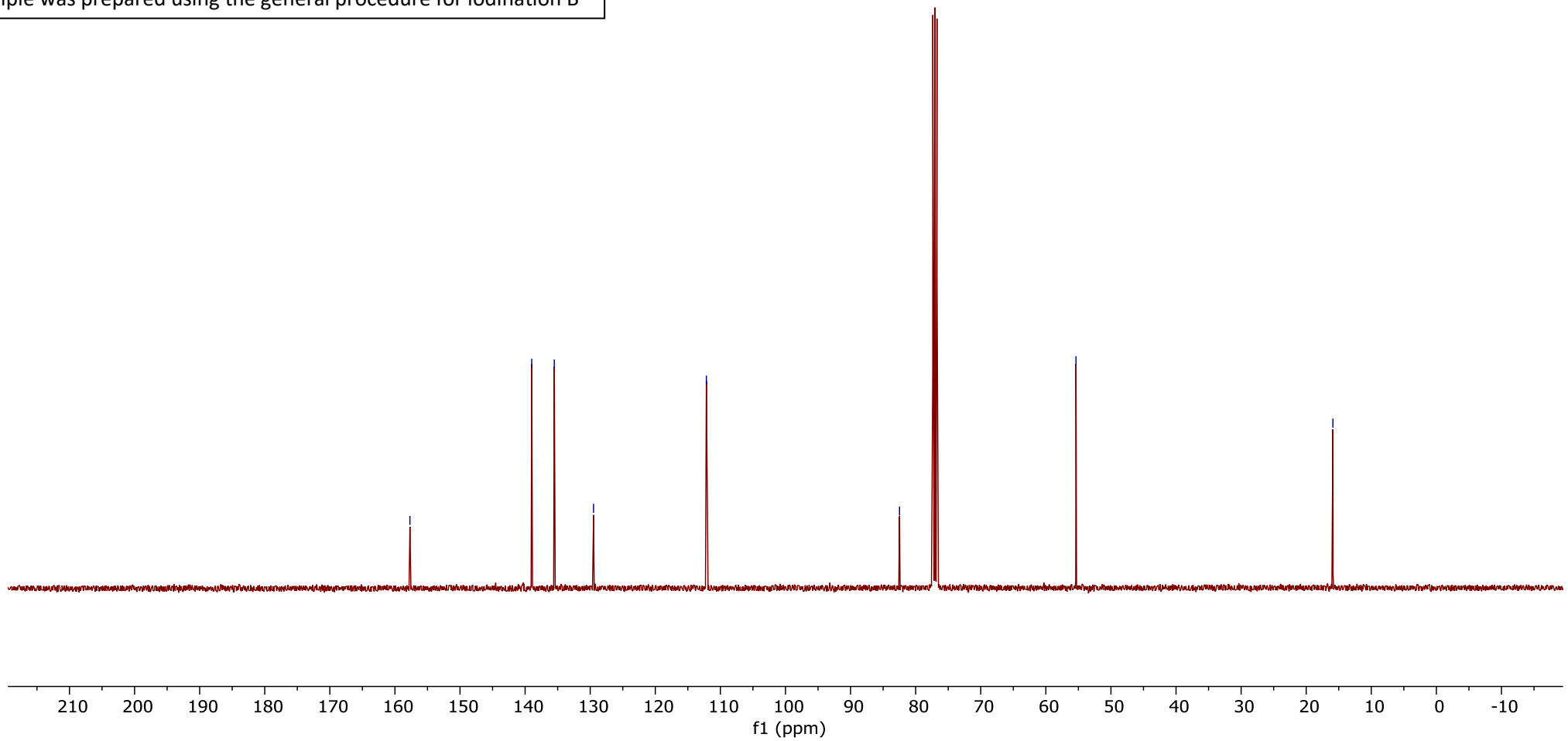
08130831.10.fid
SLC:WDGB:WB4-125

157.70
138.98
135.52
129.49
112.15
82.48
55.37
15.90

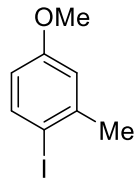


4b

Sample was prepared using the general procedure for iodination B



08122556.10.fid
SLC:WDGB:WB4-126

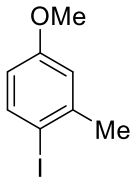


4b

Sample was prepared using the general procedure for iodination B

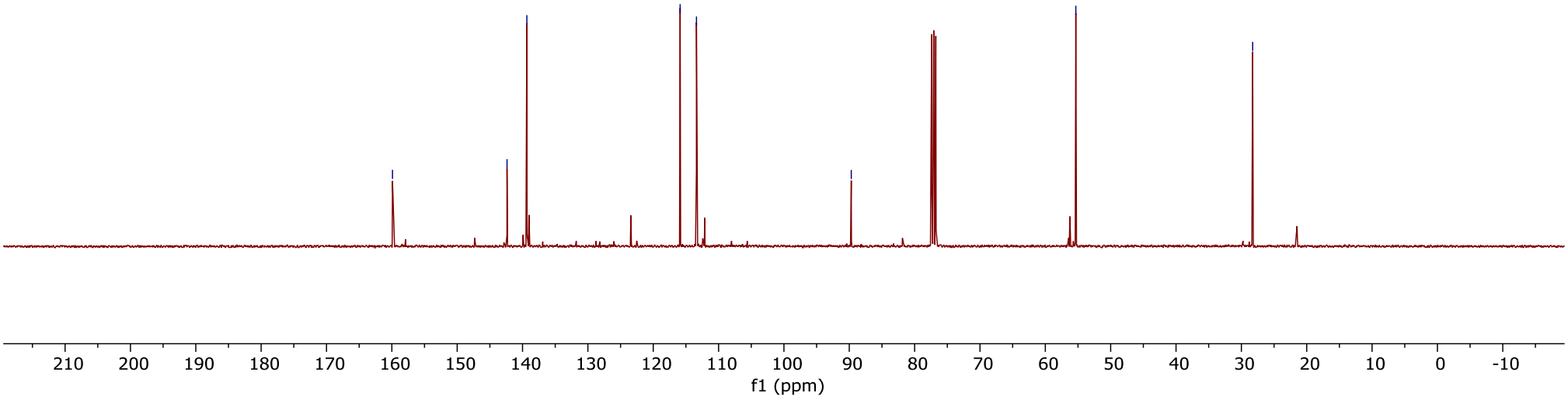
08130901.10.fid
SLC:WDGB:WB4-126

159.90
142.37
139.34
115.88
113.39
89.69
55.33
28.27

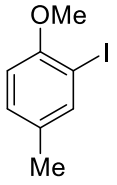


4b

Sample was prepared using the general procedure for iodination B



08122609.10.fid
SLC:WDGB:WB4-127

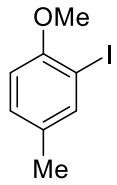


4d

Sample was prepared using the general procedure for iodination B

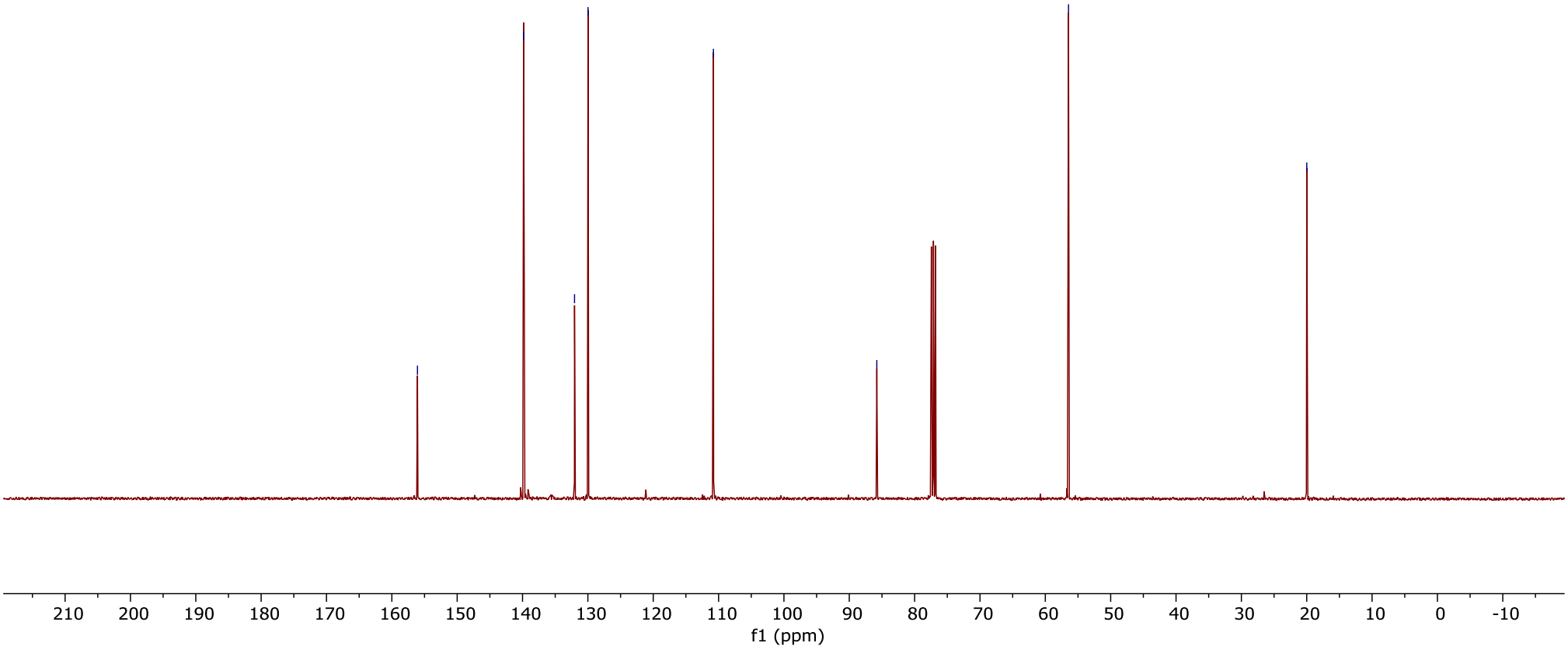
08130917.10.fid
SLC:WDGB:WB4-127

156.08
139.84
132.04
129.98
110.79
85.79
56.45
19.99

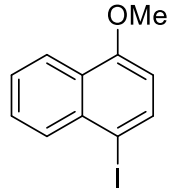


4d

Sample was prepared using the general procedure for iodination B



20150308.10.fid
SLC:WDGB:WB5-1 F2-7

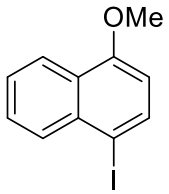


4e

Sample was prepared using the general procedure for iodination B

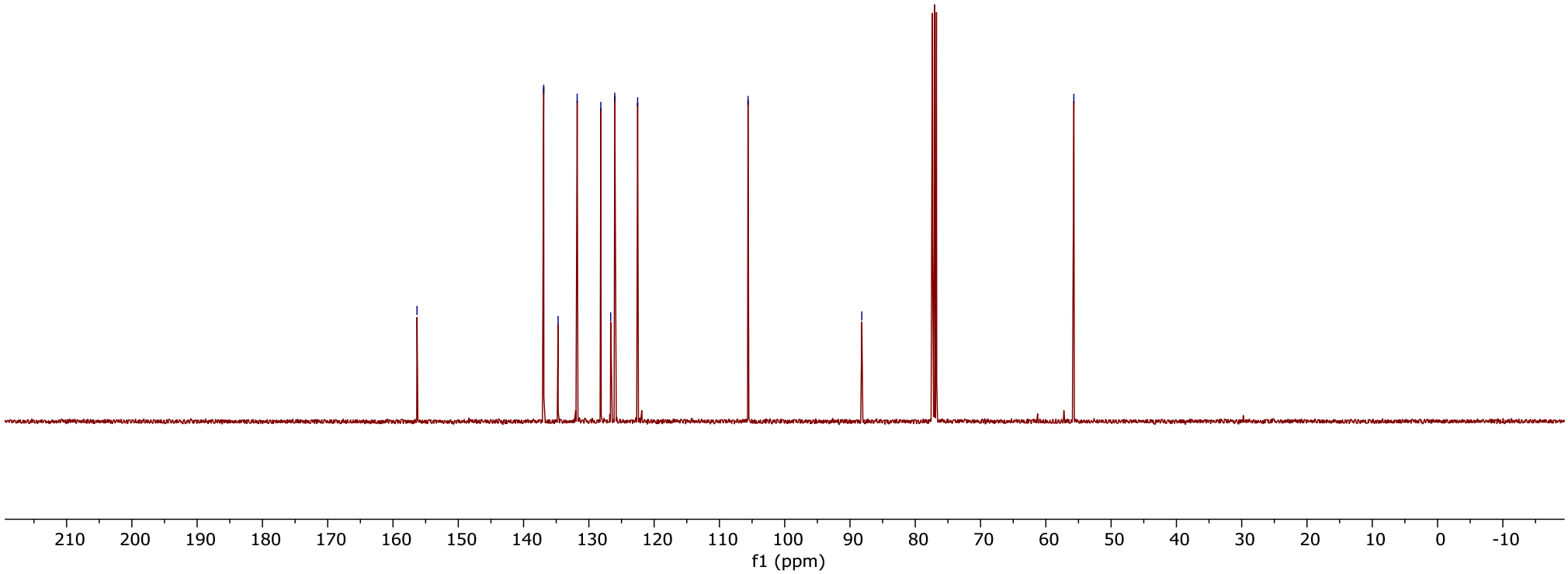
13153117.10.fid
SLC:WDGB:WB5-1

156.32
136.92
134.72
131.79
128.17
126.66
126.03
122.53
105.62
88.19
55.71

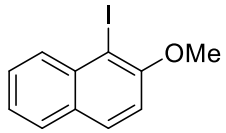


4e

Sample was prepared using the general procedure for iodination B



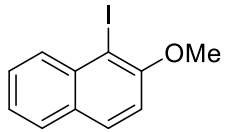
08122625.10.fid
SLC:WDGB:WB5-2



4f

Sample was prepared using the general procedure for iodination B

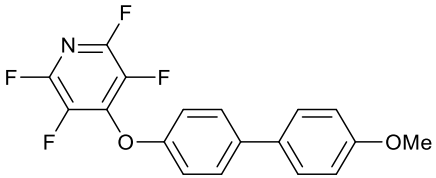
08130935.10.fid
SLC:WDGB:WB5-2



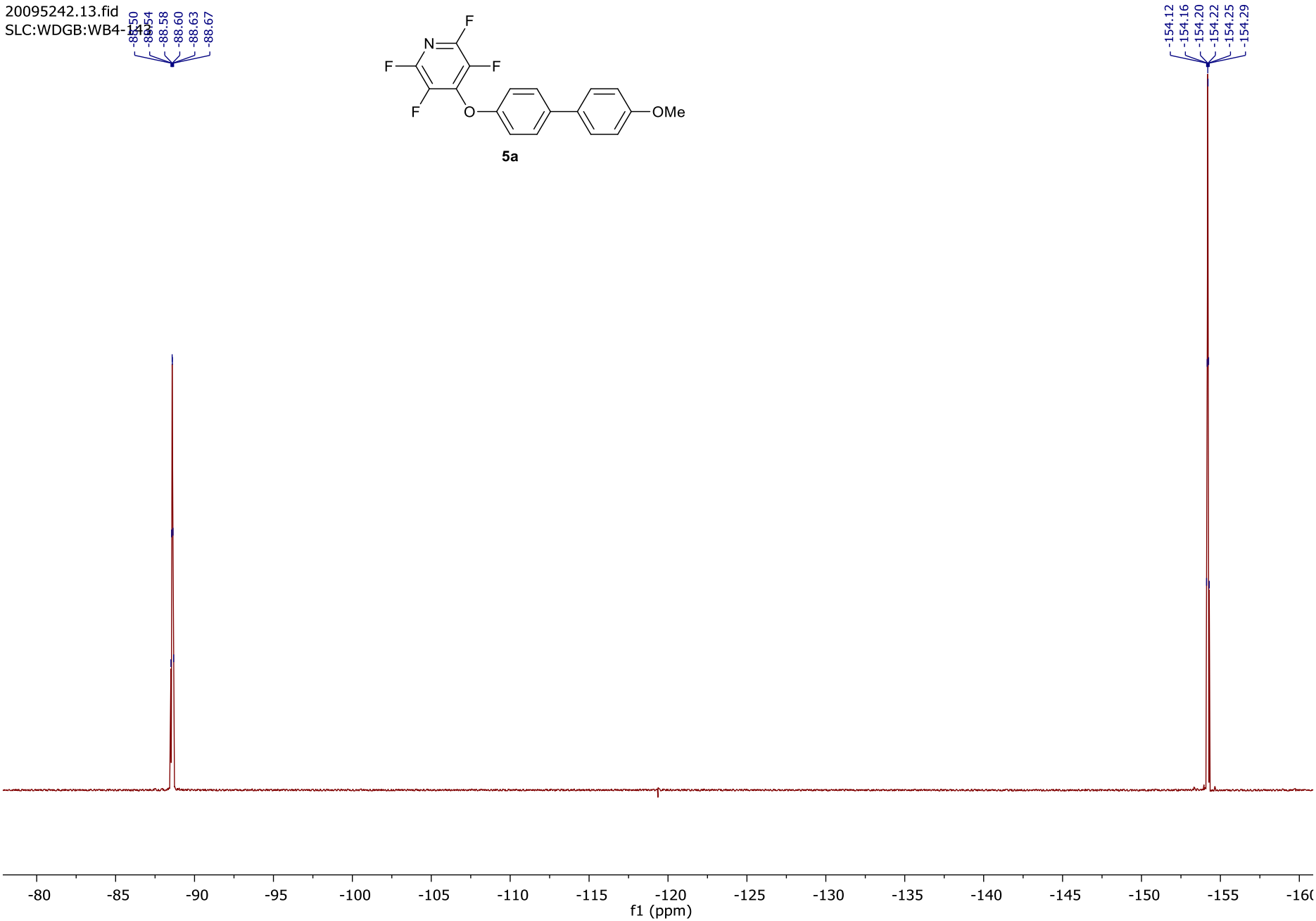
4f

Sample was prepared using the general procedure for iodination B

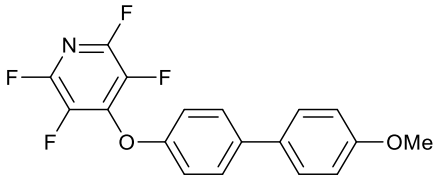
20095242.10.fid
SLC:WDGB:WB4-143



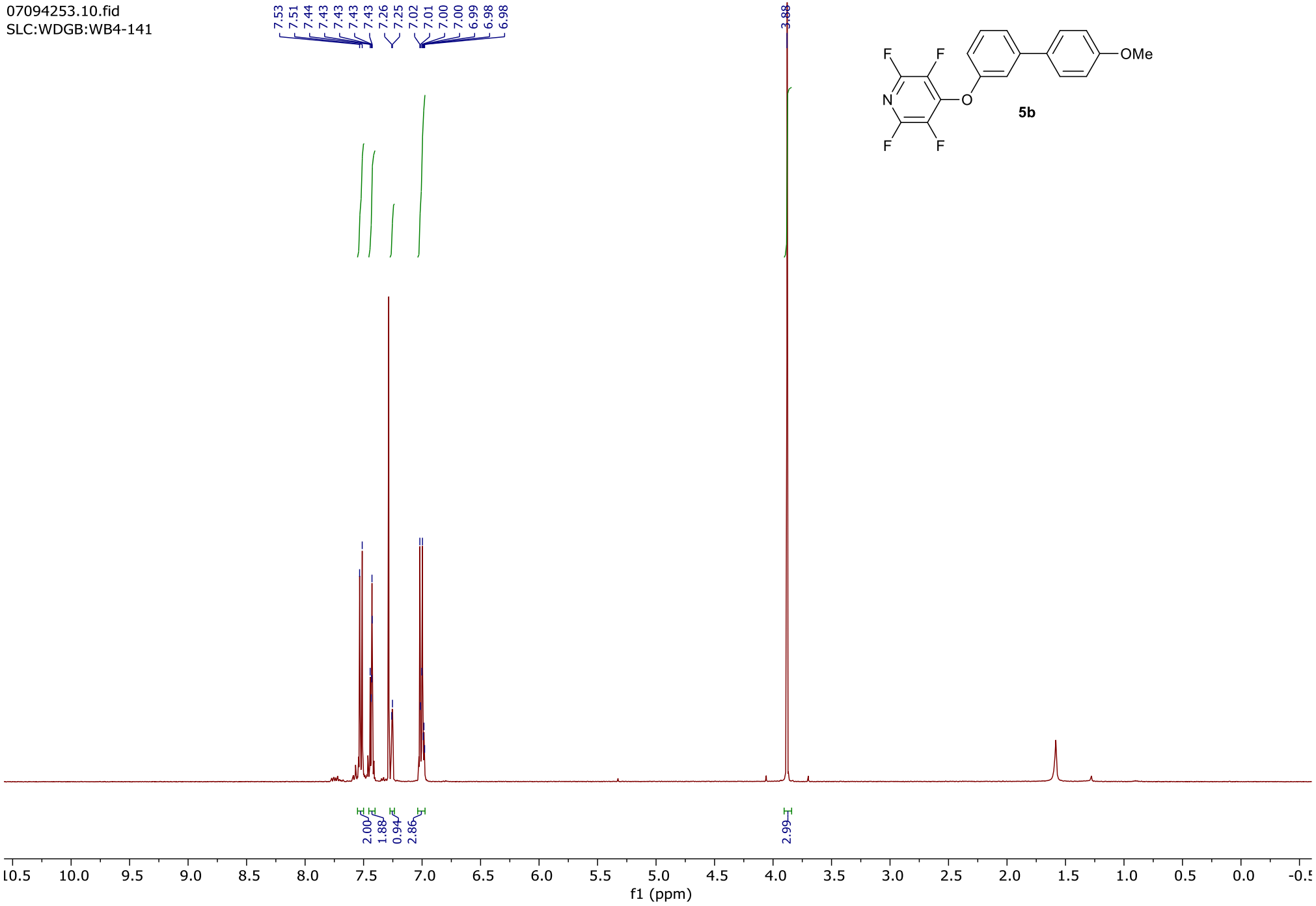
5a


20095242.13.fid
SLC:WDGB:WB4-142
-88.50
-88.54
-88.58
-88.60
-88.63
-88.67
-154.12
-154.16
-154.20
-154.22
-154.25
-154.29
F
N
F
F
F
O
OMe
5a
-80
-85
-90
-95
-100
-105
-110
-115
-120
-125
-130
-135
-140
-145
-150
-155
-160
f1 (ppm)

CARBON_01
SLC:BW:BW4-143

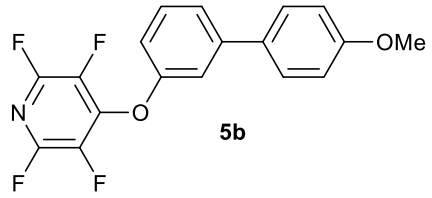


5a


07094253.10.fid
SLC:WDGB:WB4-141
7.53
7.51
7.44
7.43
7.43
7.43
7.43
7.26
7.25
7.02
7.01
7.00
7.00
6.99
6.98
6.98
3.88
F
F
N
O
OMe
F
F
5b
2.00
1.88
0.94
2.86
2.99
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
0.0
-0.5
f1 (ppm)

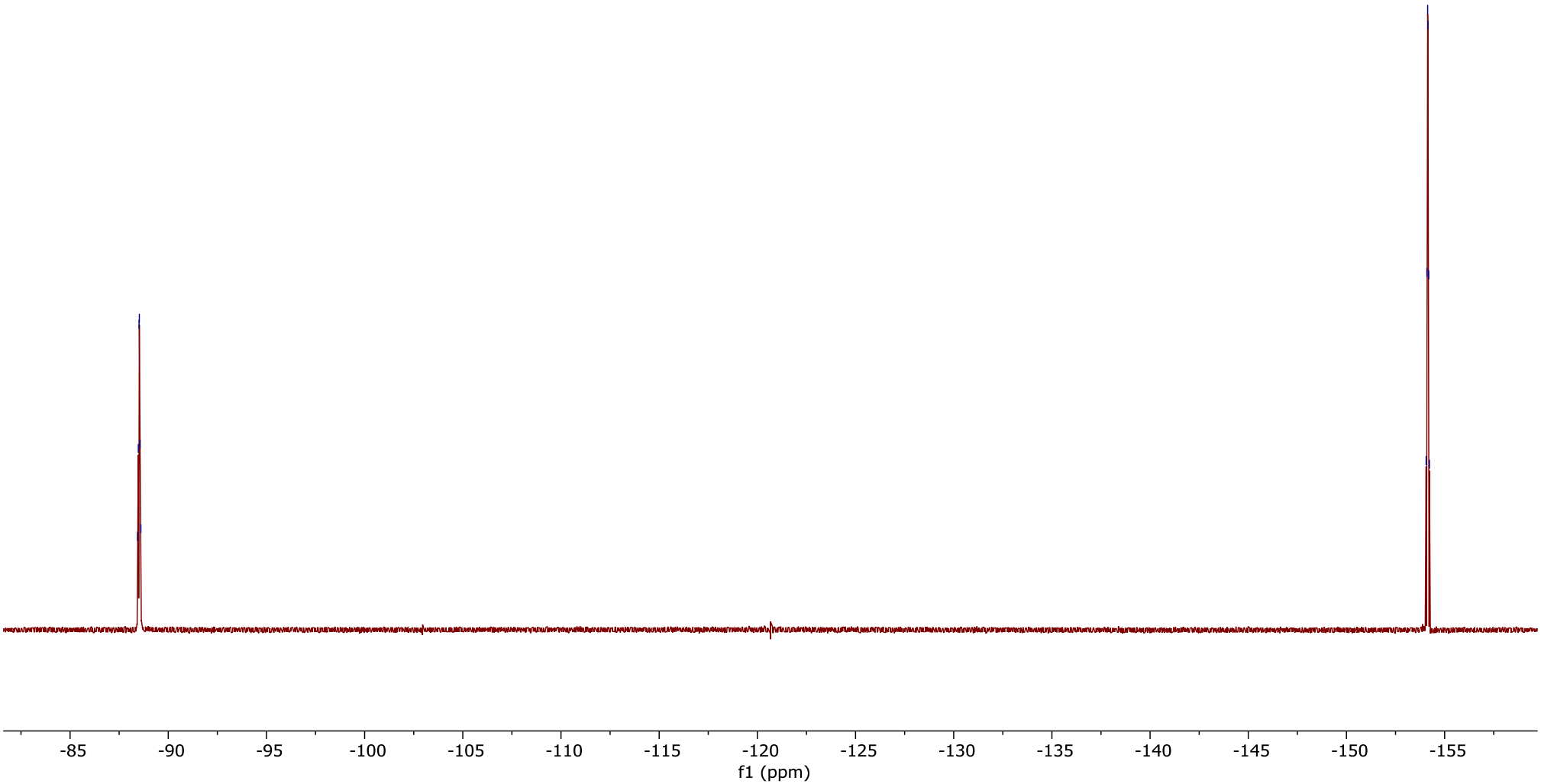
07094253.13.fid
SLC:WDGB:WB1-141

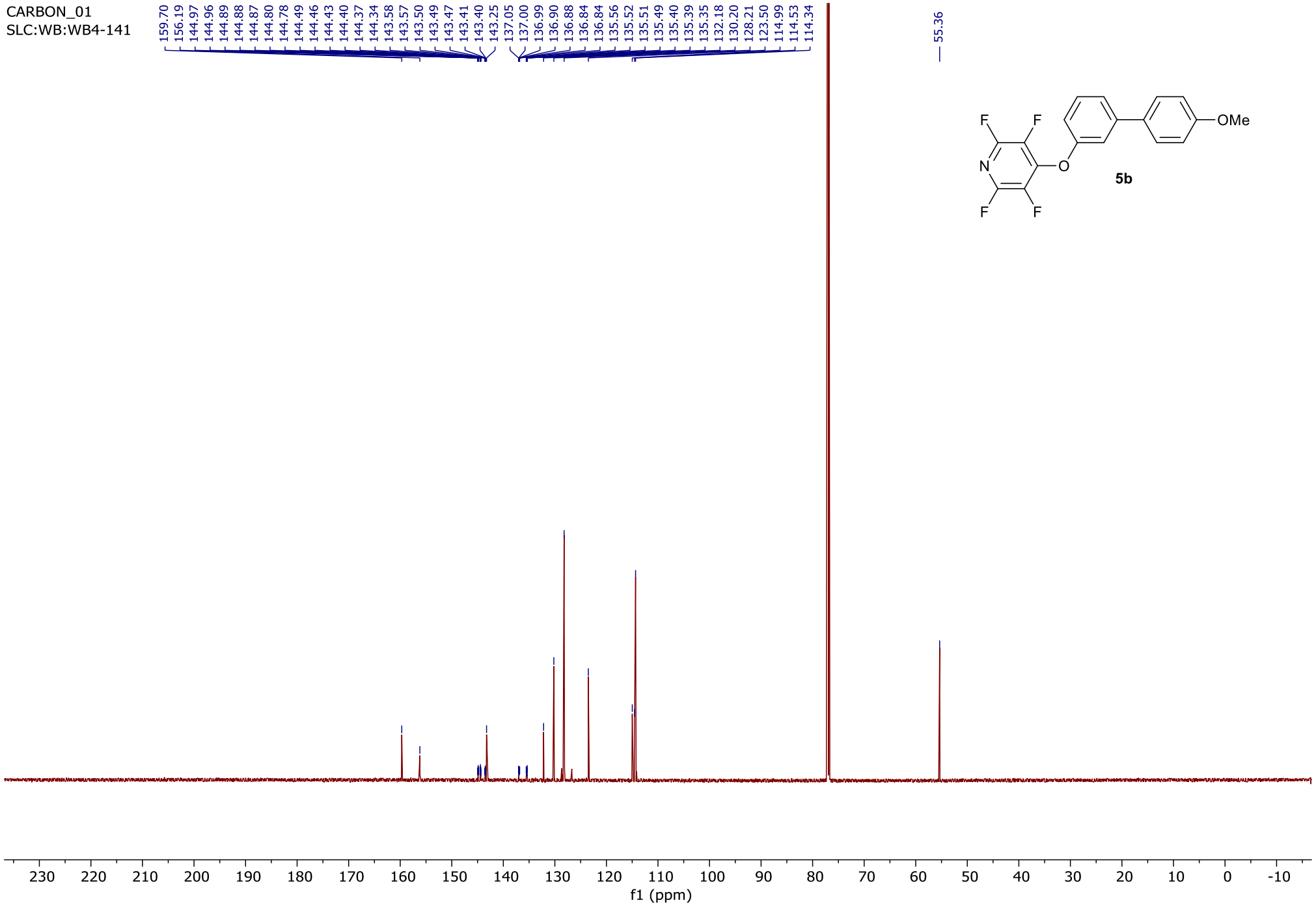
-88.41
-88.48
-88.53
-88.57
-88.61



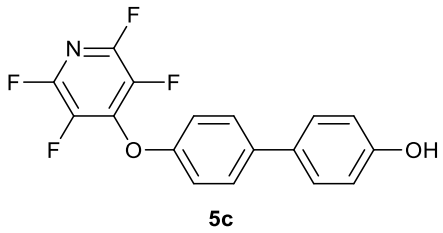
5b

-154.06
-154.10
-154.14
-154.15
-154.19
-154.23

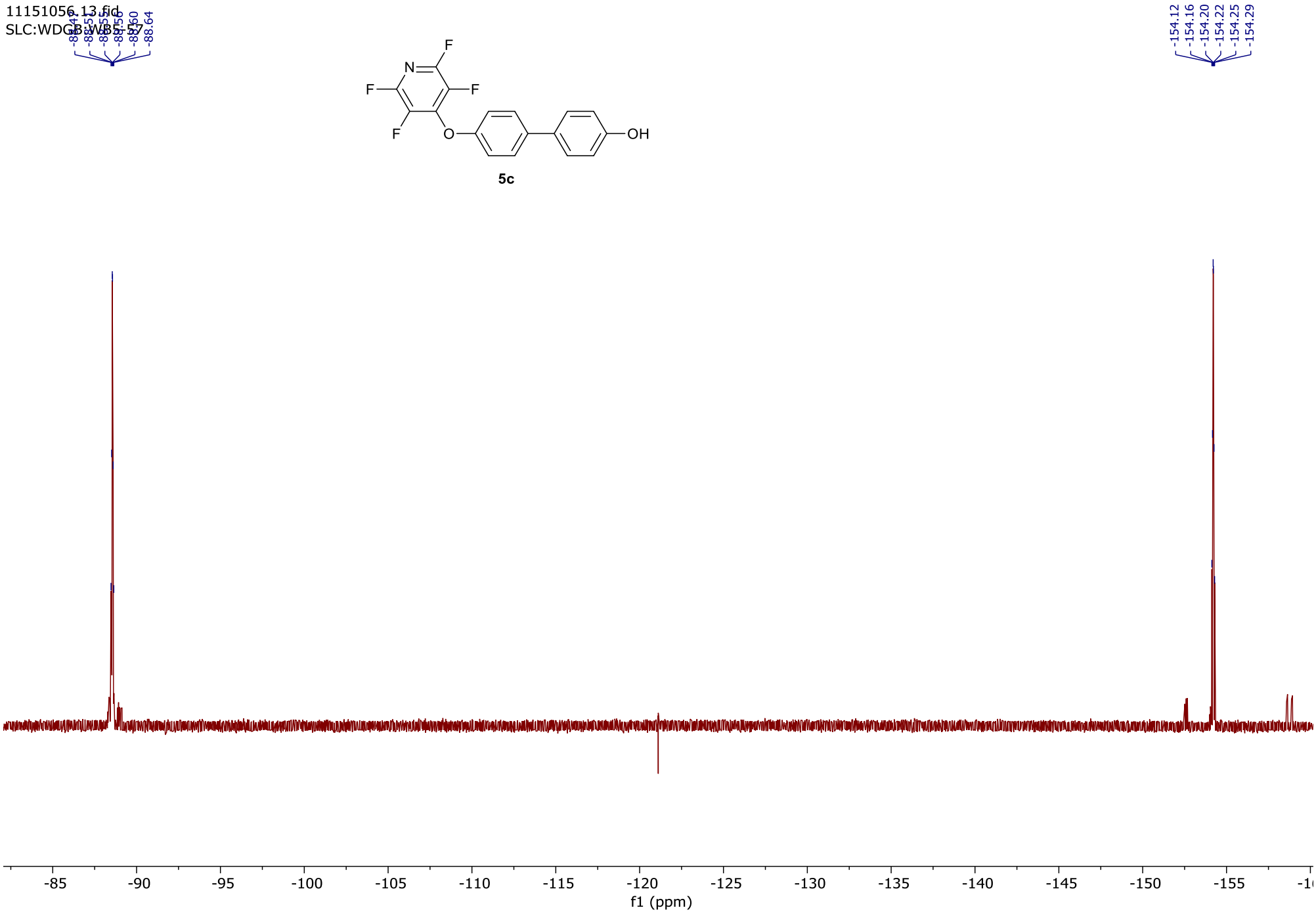



CARBON_01
SLC:WB:WB4-141
159.70
156.19
144.97
144.96
144.89
144.88
144.87
144.80
144.78
144.49
144.46
144.43
144.40
144.37
144.34
143.58
143.57
143.50
143.49
143.47
143.41
143.40
143.25
137.05
137.00
136.99
136.90
136.88
136.84
136.84
135.56
135.52
135.51
135.49
135.40
135.39
135.35
132.18
130.20
128.21
123.50
114.99
114.53
114.34
55.36
F
F
N
O
OMe
F
F
5b
230
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)

11151056.10.fid
SLC:WDGB:WB5-57

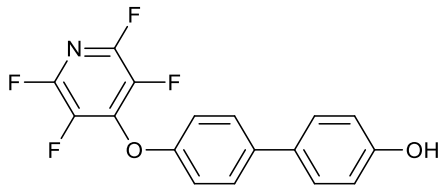


5c

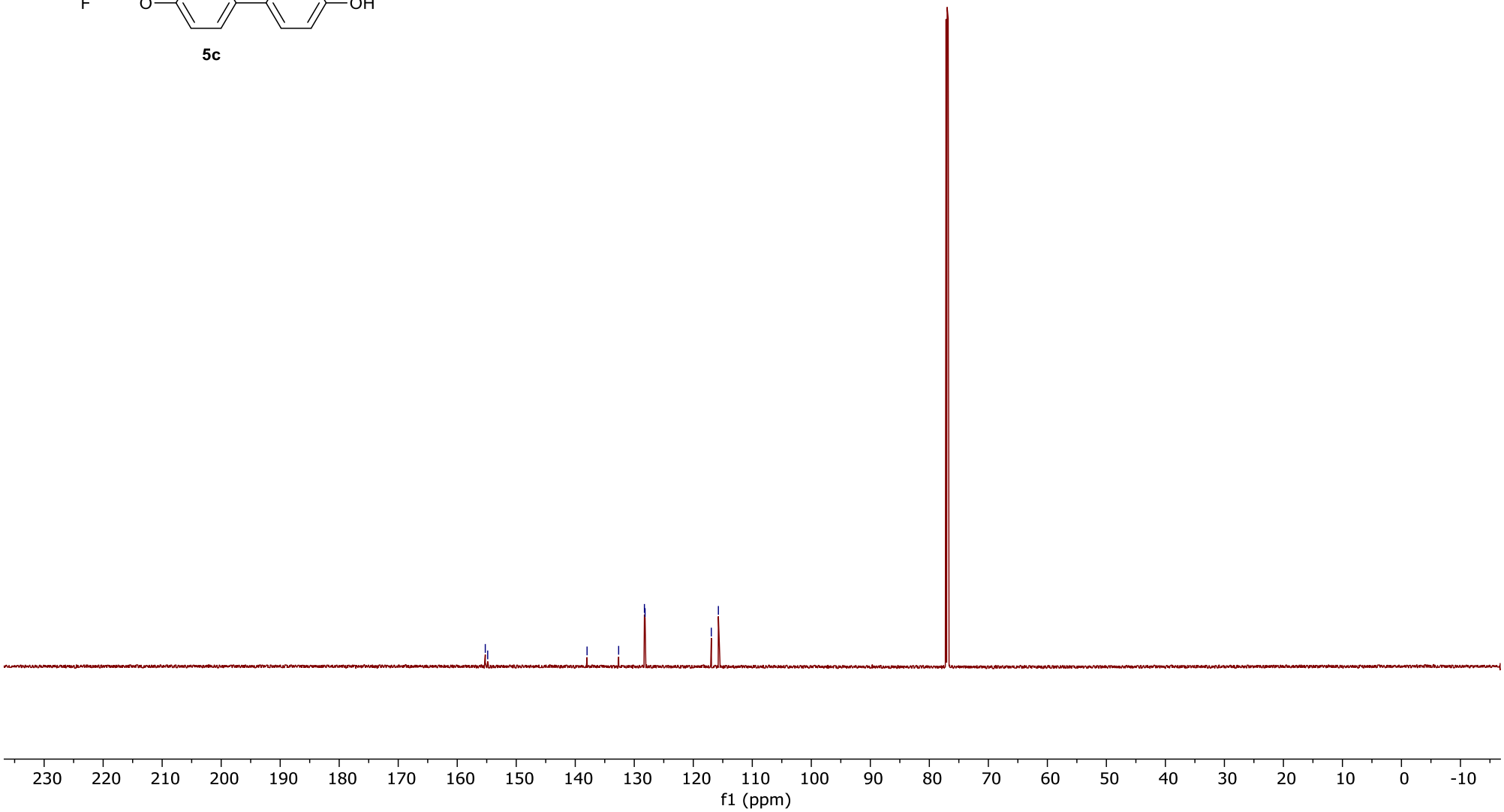

11151056_13.fid
SLC:WDGB:WB1-5
-84.47
-84.51
-87.55
-87.56
-87.60
-88.64
-154.12
-154.16
-154.20
-154.22
-154.25
-154.29
F
N
F
F
F
O
OH
5c
-85
-90
-95
-100
-105
-110
-115
-120
-125
-130
-135
-140
-145
-150
-155
f1 (ppm)

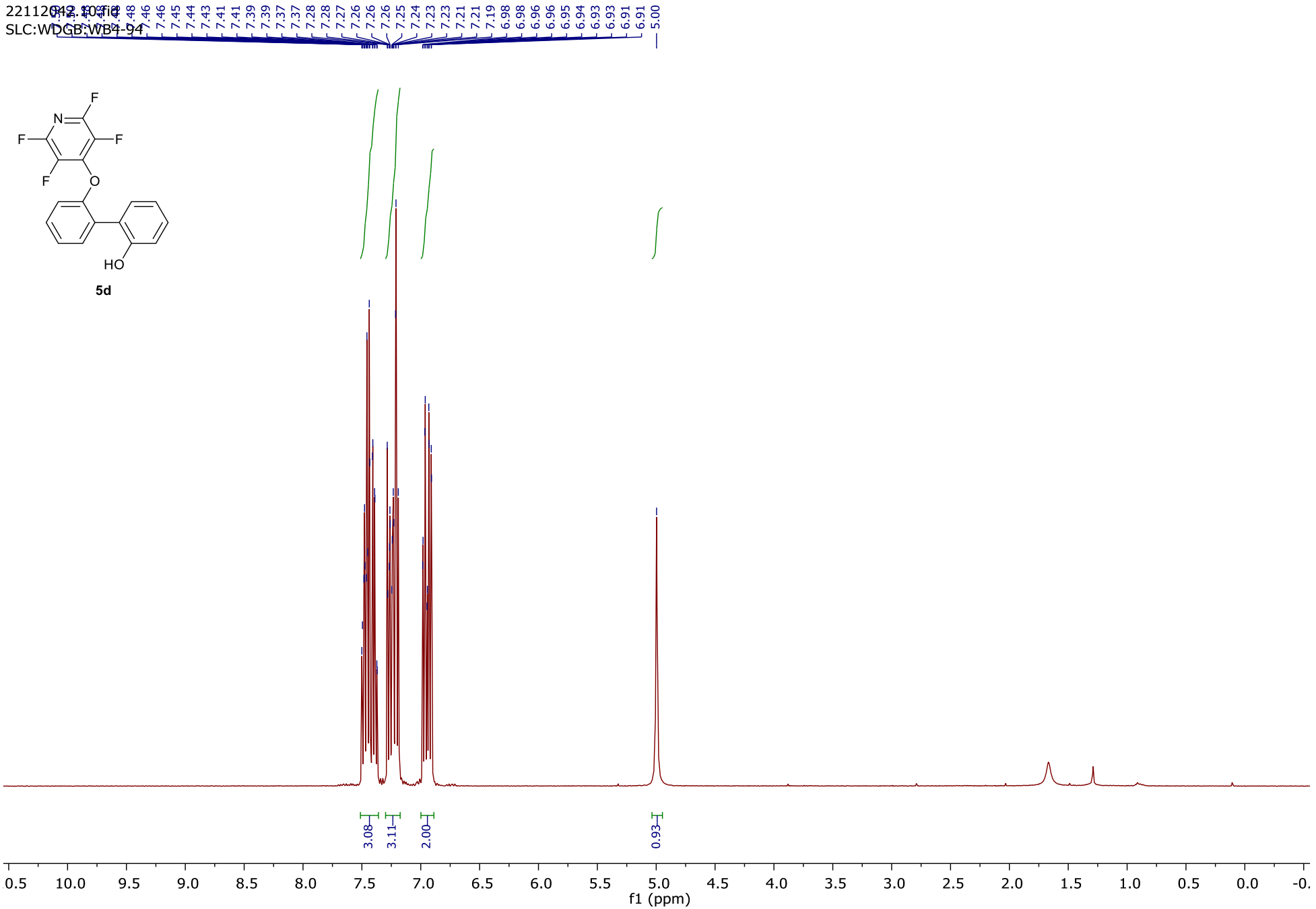
CARBON_01
SLC:WB:WB5-57

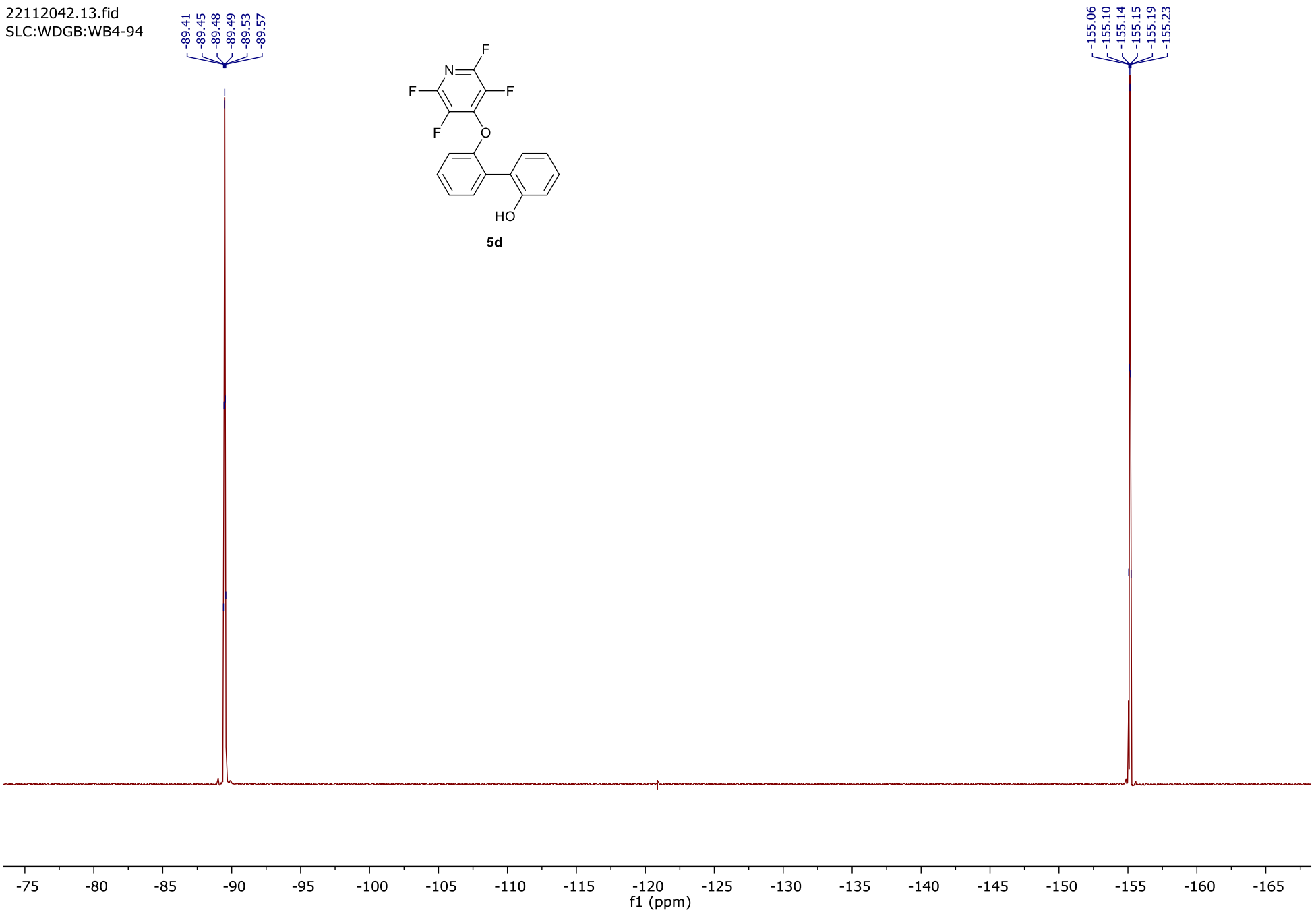
155.25
154.84
138.00
132.65
128.28
128.17
116.94
115.75



5c

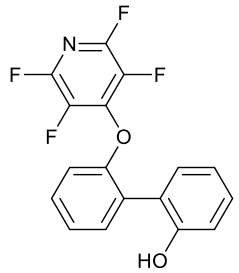



221126H2.10.fid
SLC:WDGB:WB4-94
7.48 7.46 7.46 7.45 7.44 7.43 7.41 7.41 7.39 7.39 7.37 7.37 7.28 7.28 7.27 7.26 7.26 7.26 7.25 7.24 7.23 7.23 7.21 7.21 7.19 6.98 6.98 6.96 6.96 6.95 6.94 6.93 6.93 6.91 6.91 5.00
F
N
F
F
F
O
HO
5d
3.08
3.11
2.00
0.93
0.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)


22112042.13.fid
SLC:WDGB:WB4-94
-89.41
-89.45
-89.48
-89.49
-89.53
-89.57
-155.06
-155.10
-155.14
-155.15
-155.19
-155.23
F
N
F
F
F
O
HO
5d
-75
-80
-85
-90
-95
-100
-105
-110
-115
-120
-125
-130
-135
-140
-145
-150
-155
-160
-165
f1 (ppm)

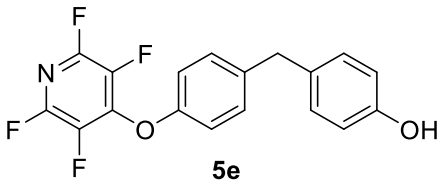
CARBON_01
SLC:WB:WB4-94

153.37
152.79
144.65
144.64
144.58
144.57
144.55
144.52
144.49
144.46
143.26
143.25
143.17
143.17
143.09
143.07
136.08
136.03
136.02
135.94
135.92
135.87
134.60
134.56
134.53
134.45
134.43
134.39
132.36
130.76
130.09
129.96
127.26
126.18
122.59
120.77
118.06
115.85

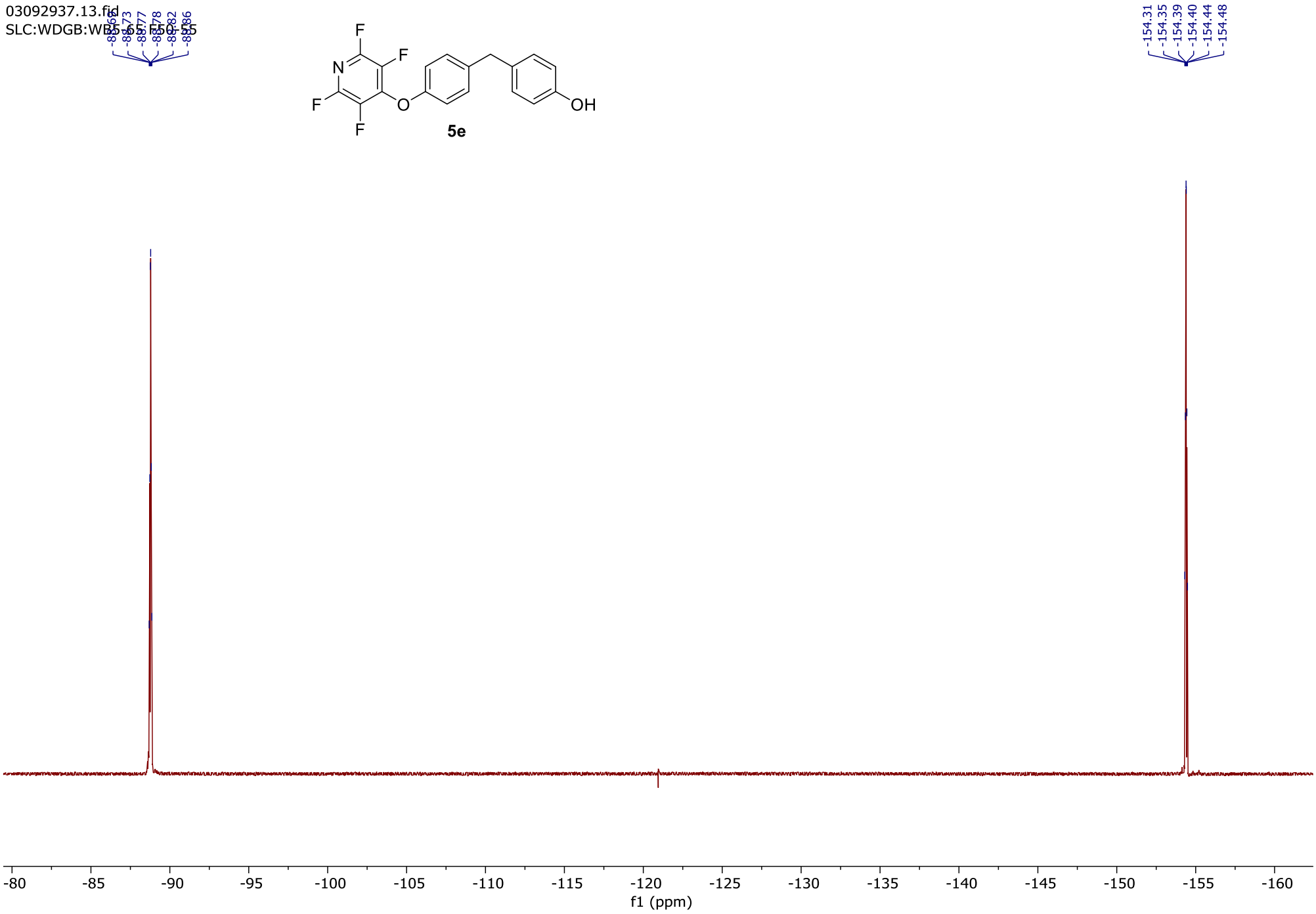


5d

03092937.10.fid
SLC:WDGB:WB5-65 F50-55

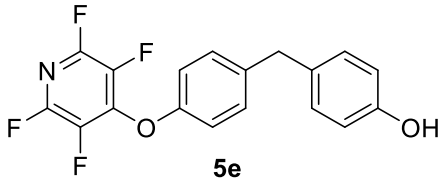


5e

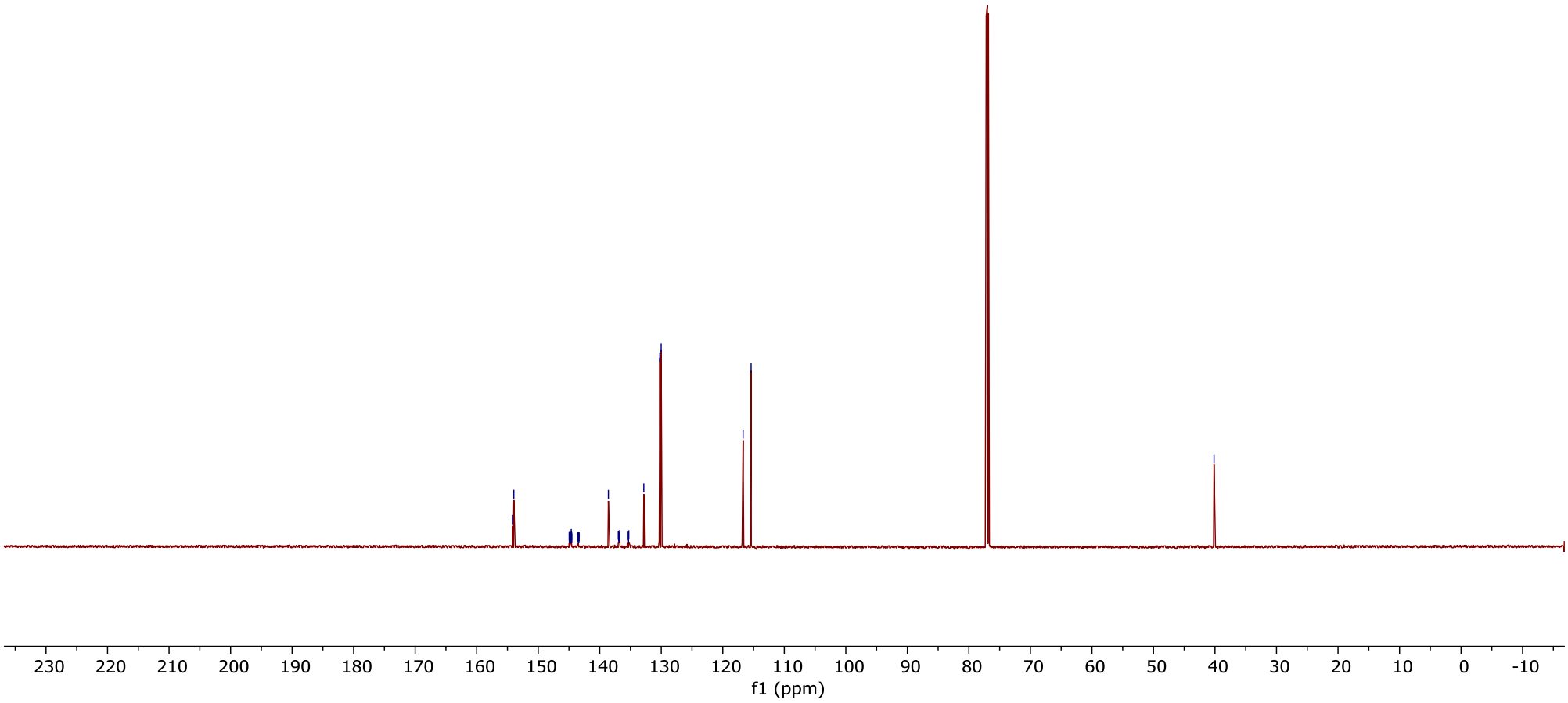

03092937.13.fid
SLC:WDGB:WB5-65-F5-F5
-88.66
-88.73
-88.77
-88.78
-88.82
-88.86
-154.31
-154.35
-154.39
-154.40
-154.44
-154.48
F
F
N
F
O
OH
F
5e
-80
-85
-90
-95
-100
-105
-110
-115
-120
-125
-130
-135
-140
-145
-150
-155
-160
f1 (ppm)

CARBON_01
SLC:WB:WB5-65

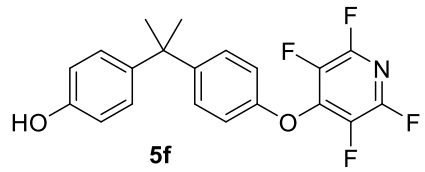
154.17
153.96
144.95
144.94
144.93
144.87
144.86
144.85
144.85
144.84
144.78
144.76
144.74
144.72
144.69
144.66
144.63
144.60
144.57
144.54
143.56
143.55
143.48
143.47
143.46
143.45
143.39
143.38
143.37
138.59
136.97
136.92
136.92
136.83
136.81
136.77
135.48
135.44
135.42
135.34
135.32
135.28
132.84
130.23
130.01
116.70
115.40
40.15



5e



04153550.10.fid
SLC:WDGB:WB5-12

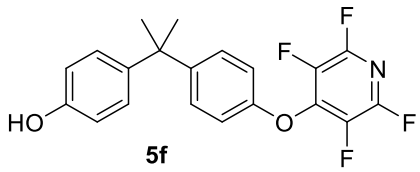


5f

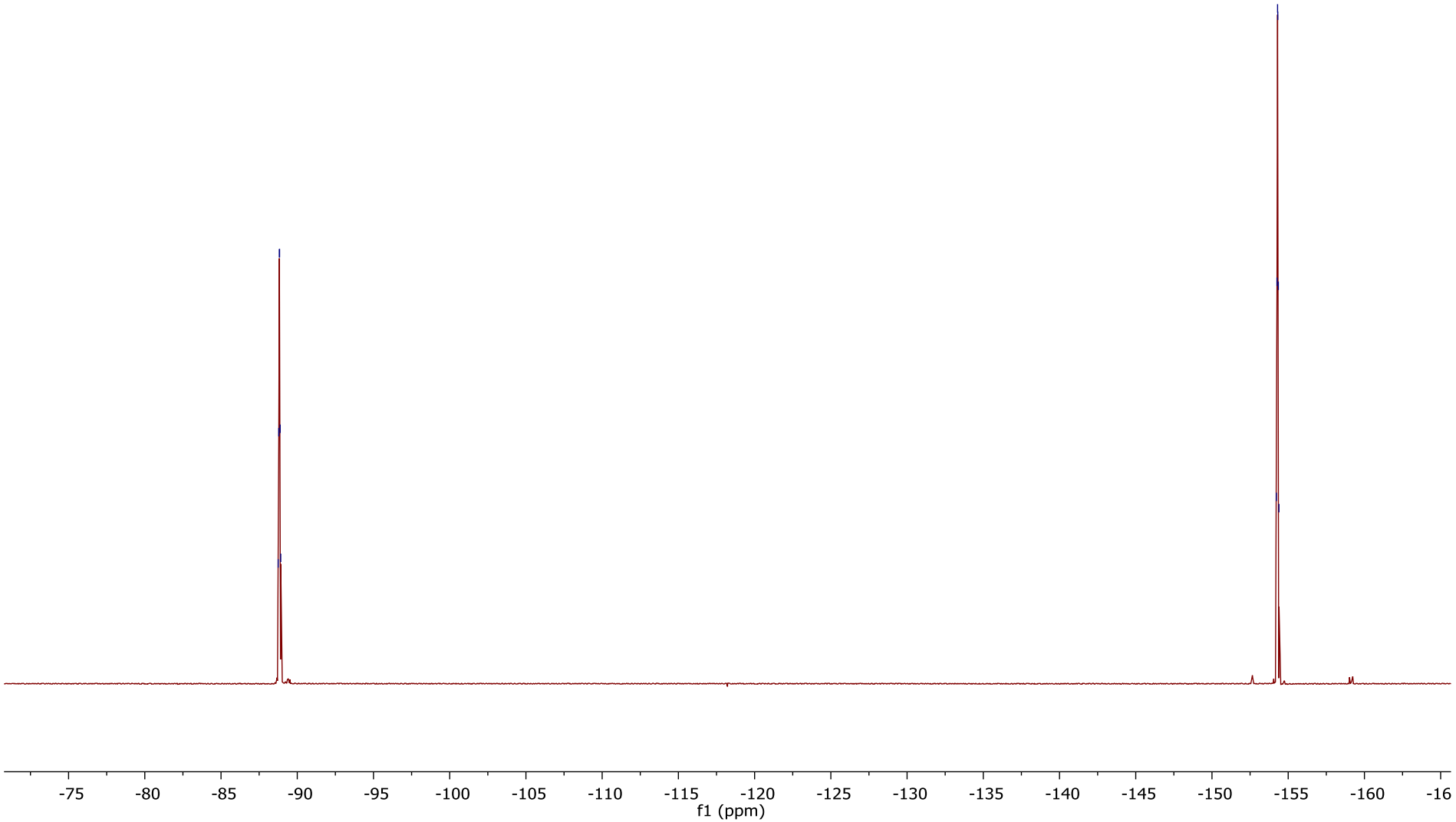
04153550.13.fid
SLC:WDGB:WB5-12

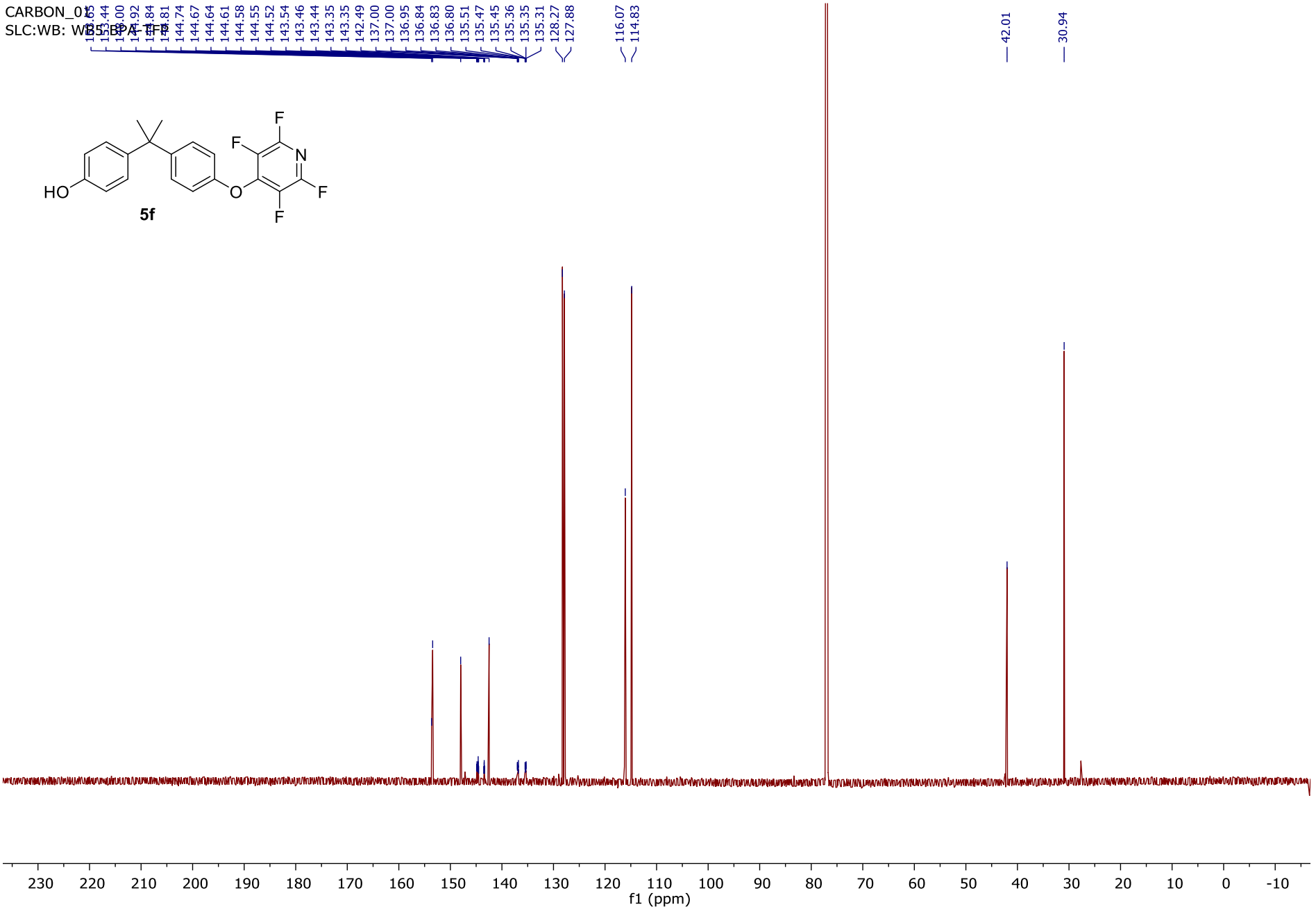
-88.75
-88.79
-88.83
-88.84
-88.88
-88.92

-154.22
-154.26
-154.30
-154.32
-154.35
-154.39

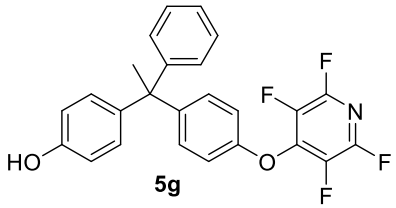


5f

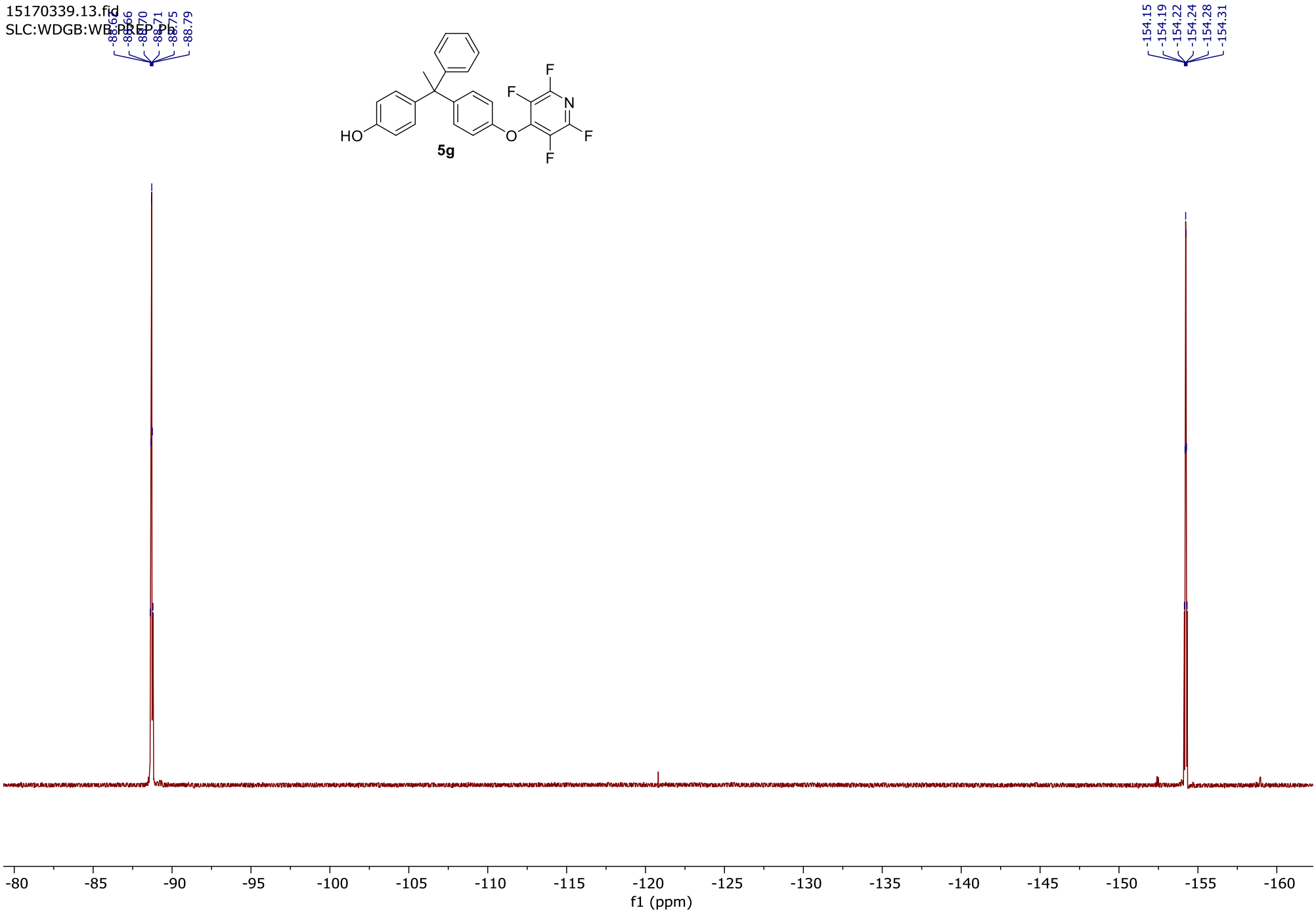



CARBON_01
SLC:WB: WB5BPA-1F5
HO
O
F
F
N
F
F
5f
116.07
114.83
42.01
30.94
f1 (ppm)

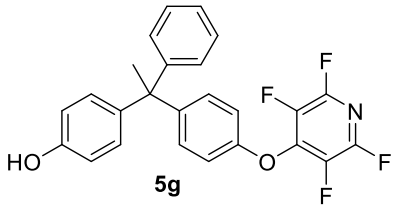
19124533.10.fid
SLC:WB5-26



5g


15170339.13.fid
SLC:WDGB:WB_PRED_01
-88.59
-88.66
-88.70
-88.71
-88.75
-88.79
-154.15
-154.19
-154.22
-154.24
-154.28
-154.31
HO
O
F
F
N
F
F
5g
-80
-85
-90
-95
-100
-105
-110
-115
-120
-125
-130
-135
-140
-145
-150
-155
-160
f1 (ppm)

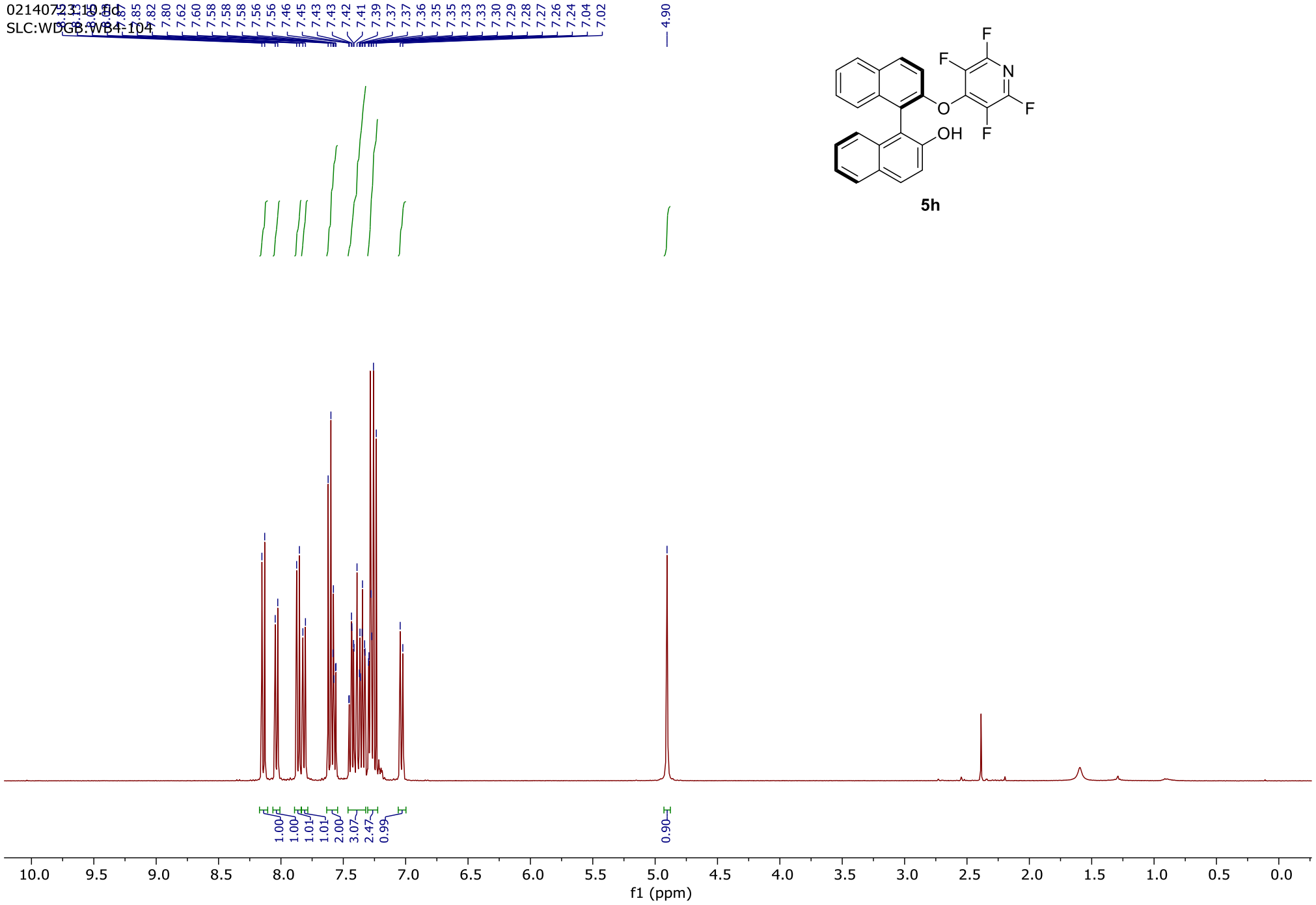
19124533.13.fid
SLC:WB5-26



5g

153.88
153.75
148.86
146.43
142.84
142.83
142.80
142.74
140.96
137.60
137.57
137.46
137.32
135.00
134.84
134.79
134.71
130.26
129.86
128.54
128.02
126.17
115.94
114.75
51.49
30.69

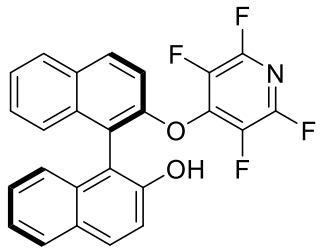
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


F
F
N
O
F
OH
F
5h
f1 (ppm)

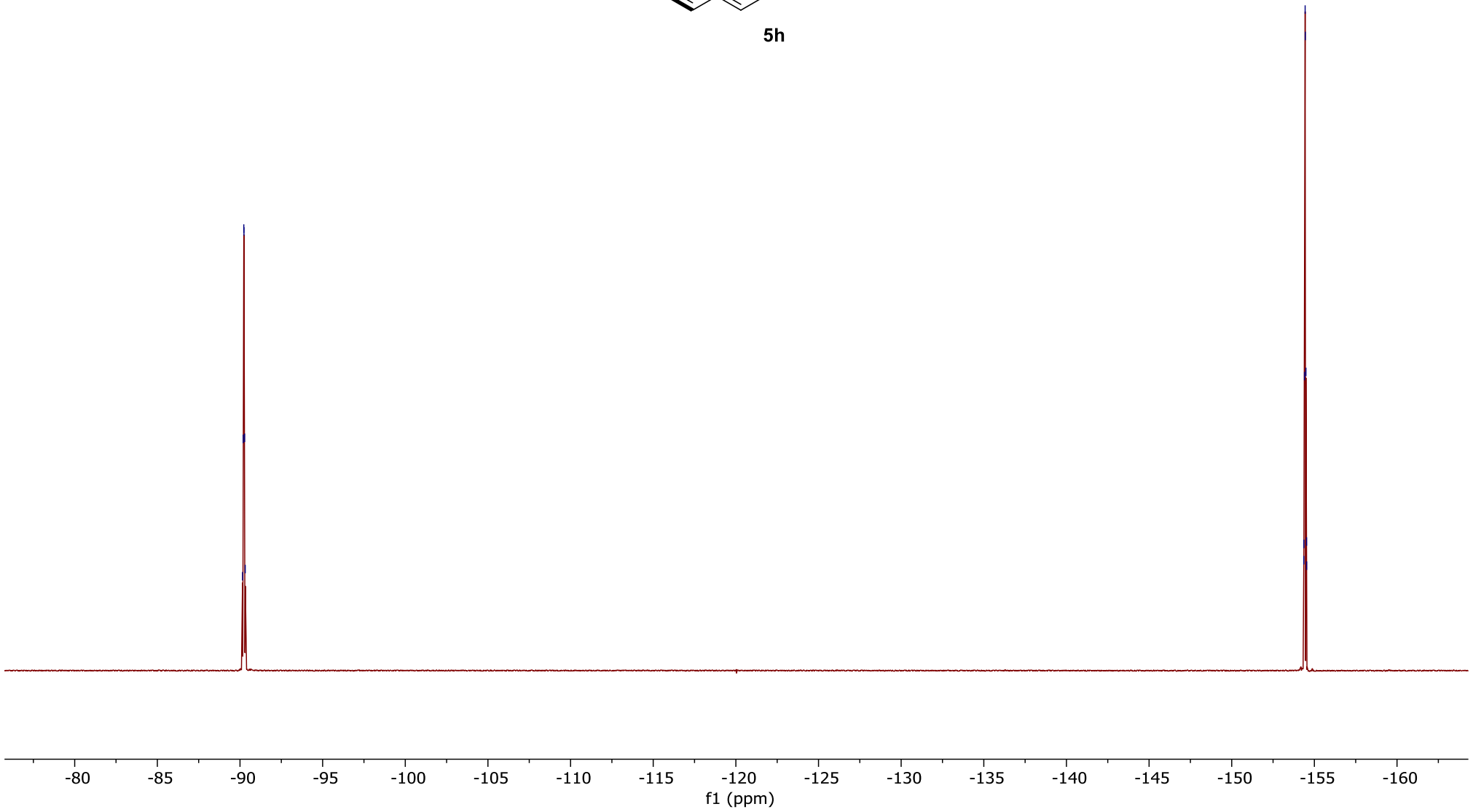
02140723.13.fid
SLC:WDGB:WB4-104

-90.15
-90.19
-90.23
-90.24
-90.28
-90.32

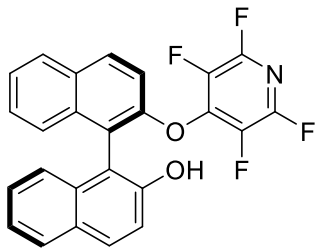
-154.36
-154.36
-154.40
-154.44
-154.45
-154.49
-154.53
-154.53



5h

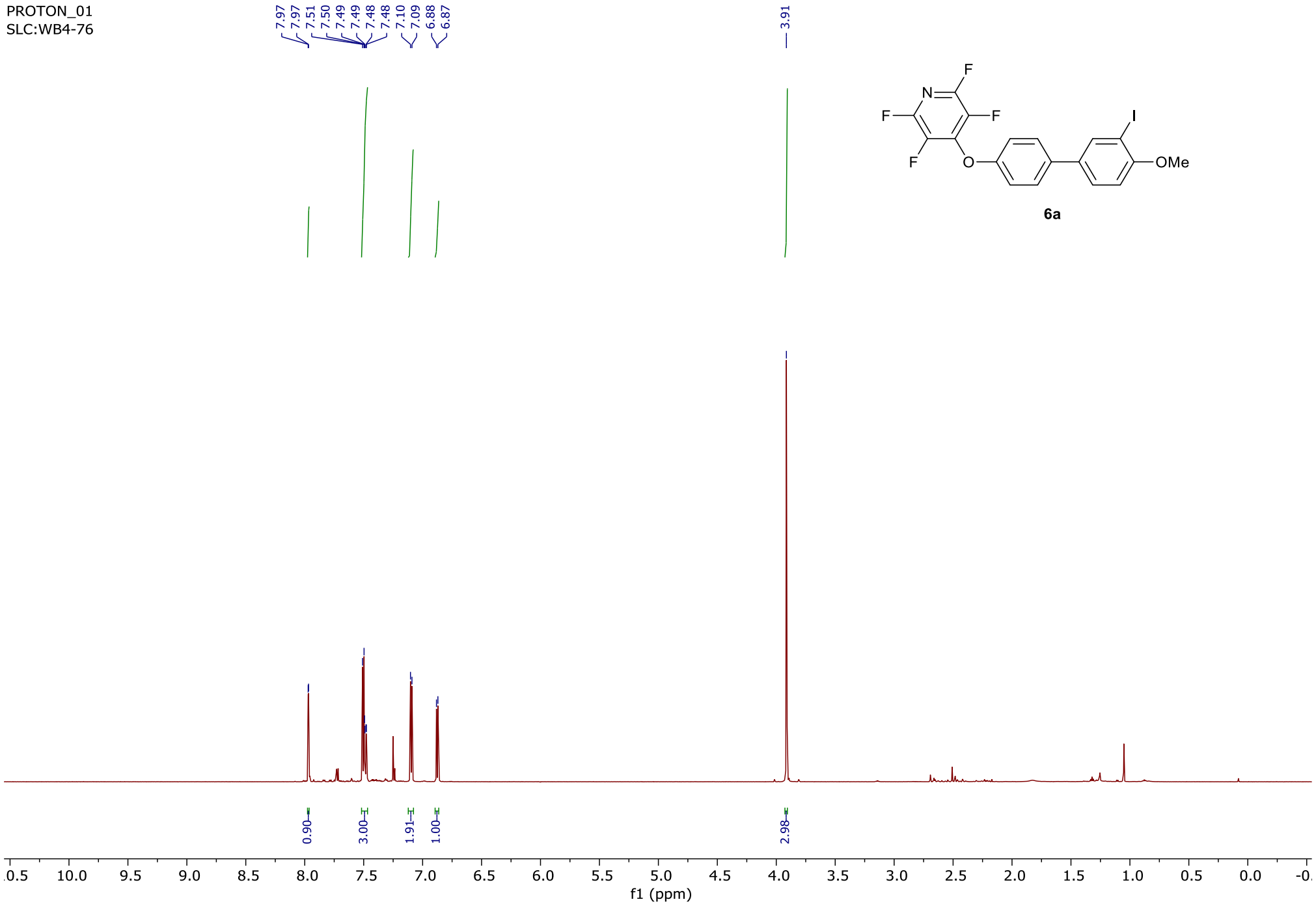


CARBON_01
SLC:WB:WB4-104



5h

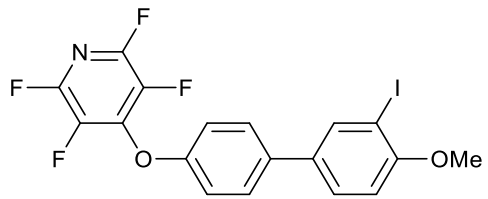
PROTON_01
SLC:WB4-76



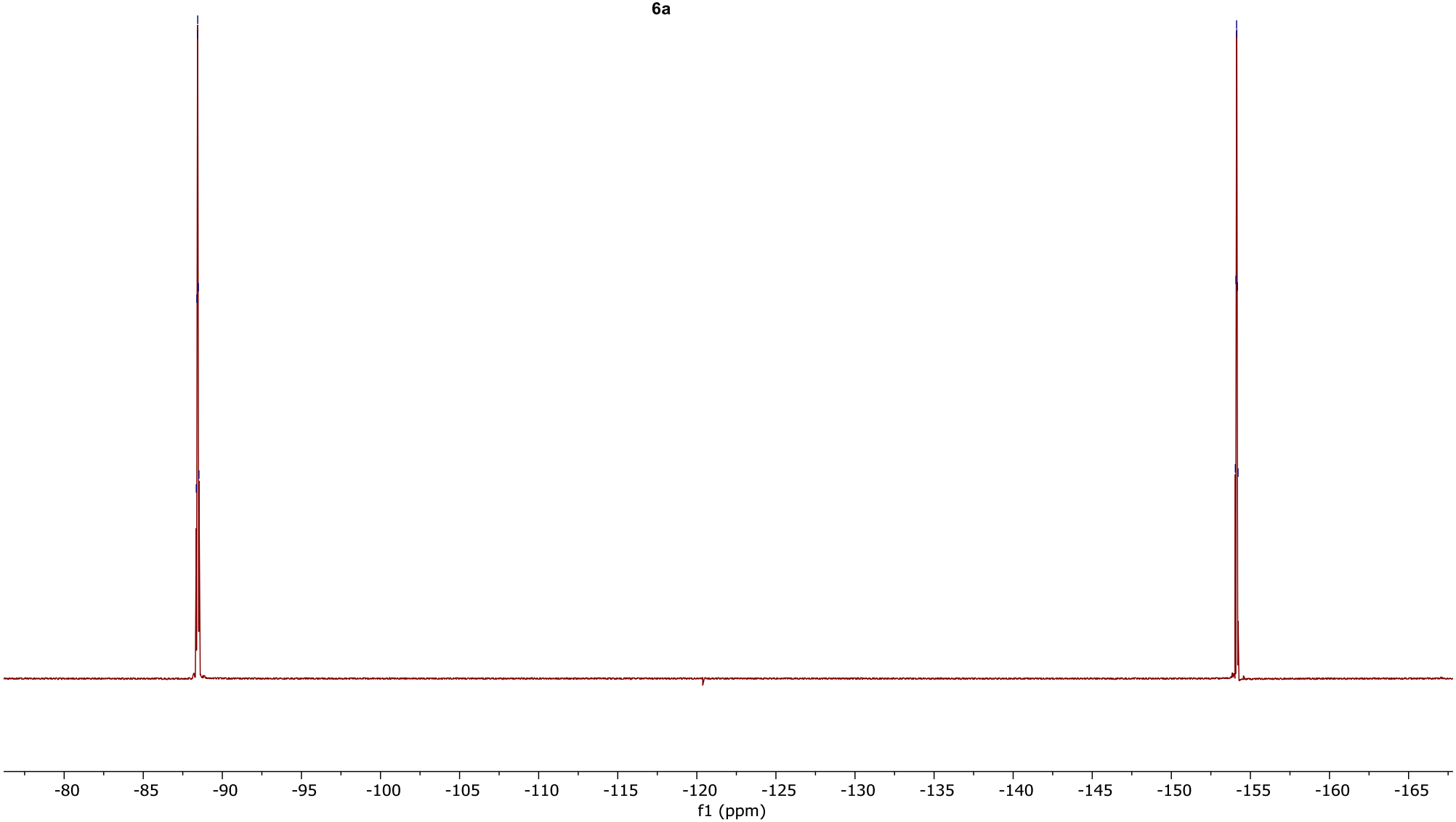
10160349.13.fid
SLC:WDGB:WB4-7

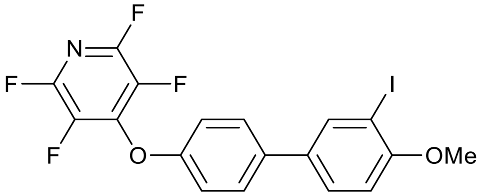
-88.35
-88.39
-88.43
-88.44
-88.48
-88.52

-154.05
-154.09
-154.13
-154.14
-154.18
-154.22

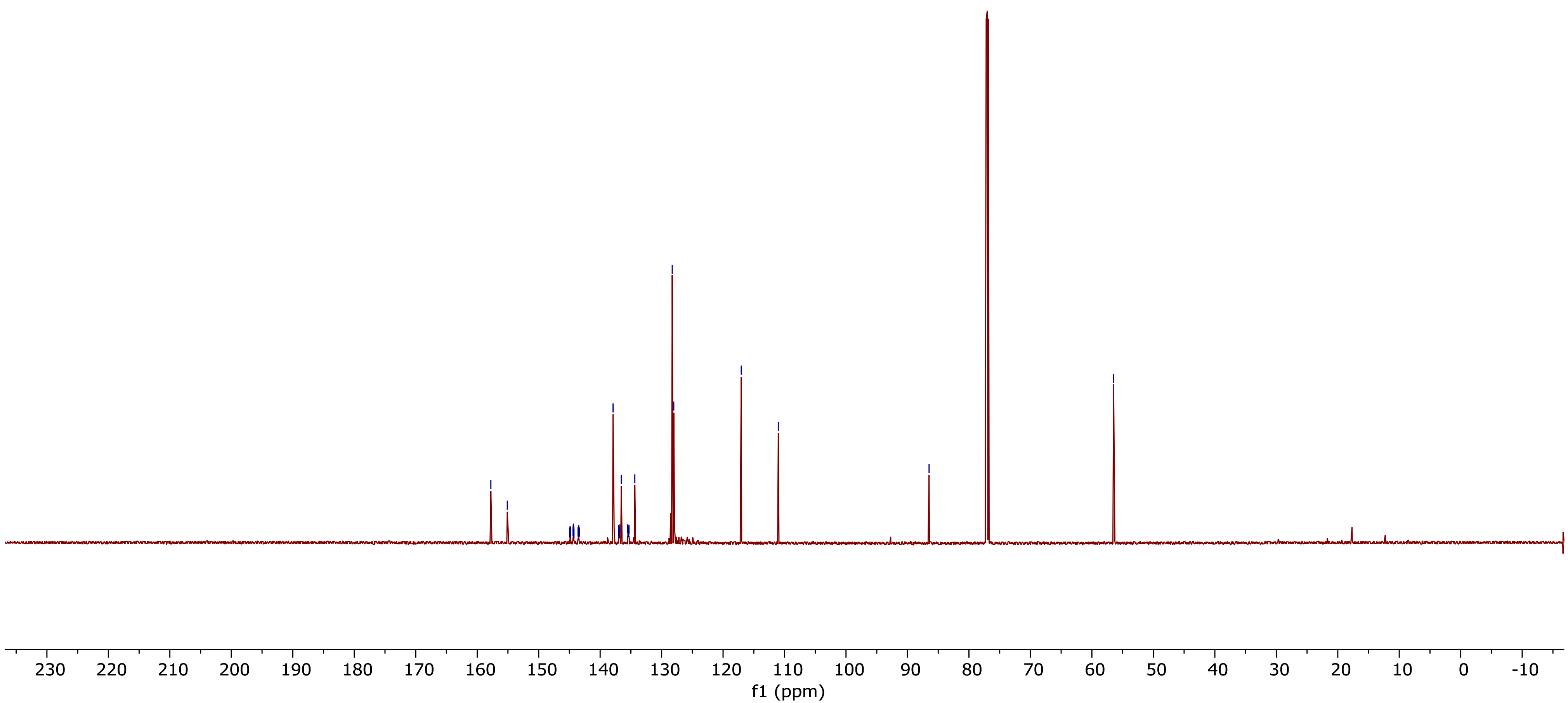


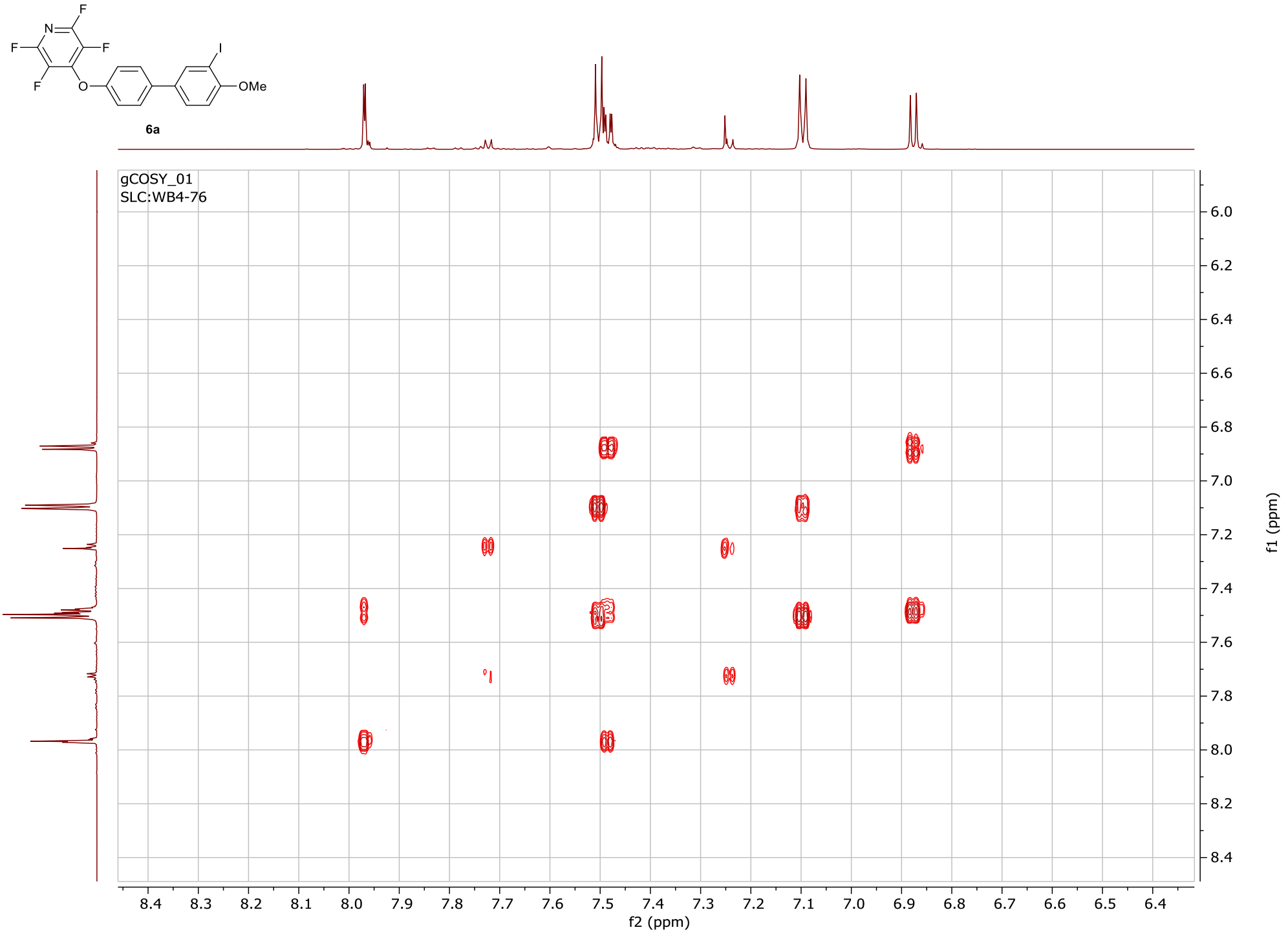
6a

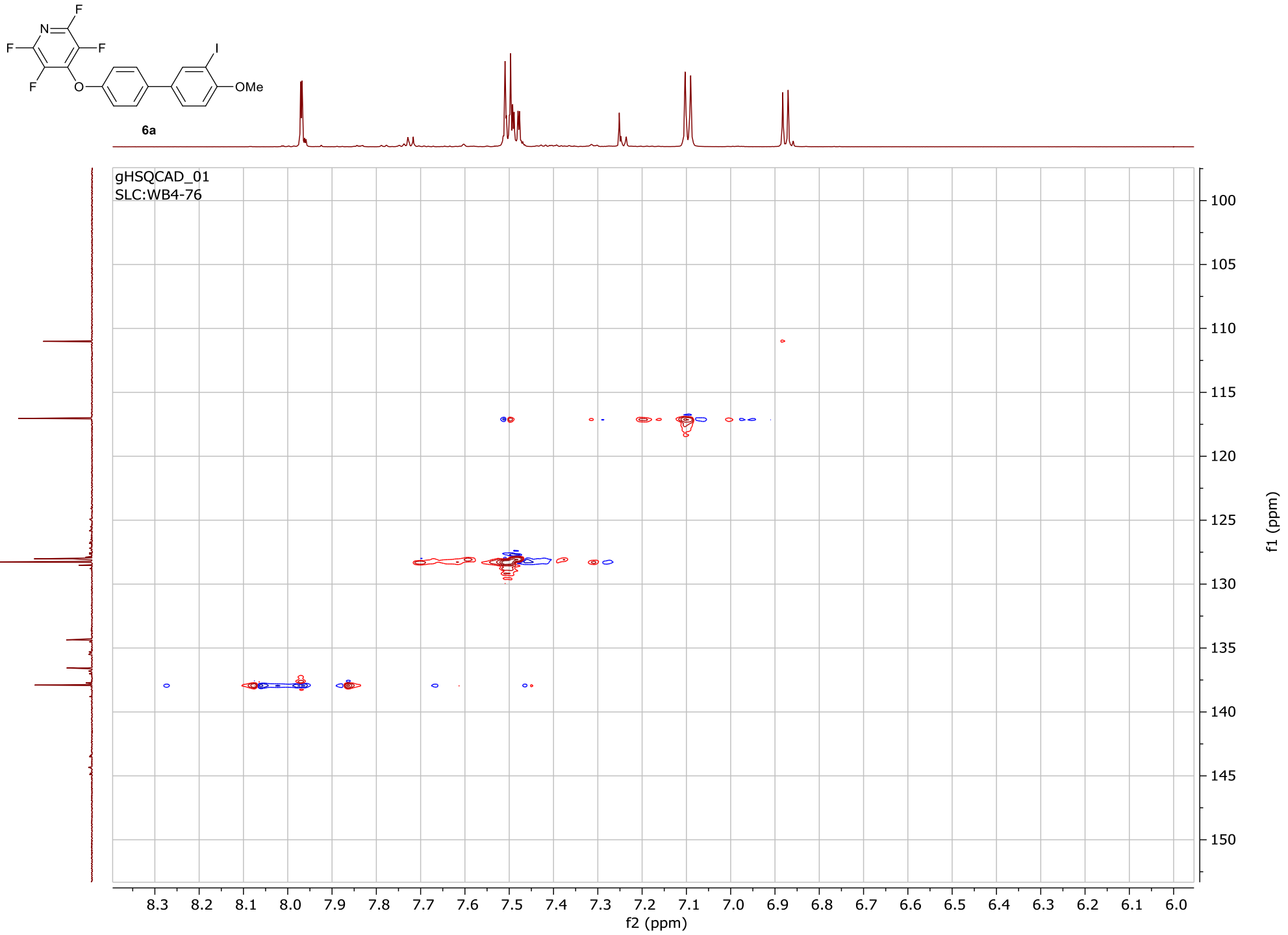


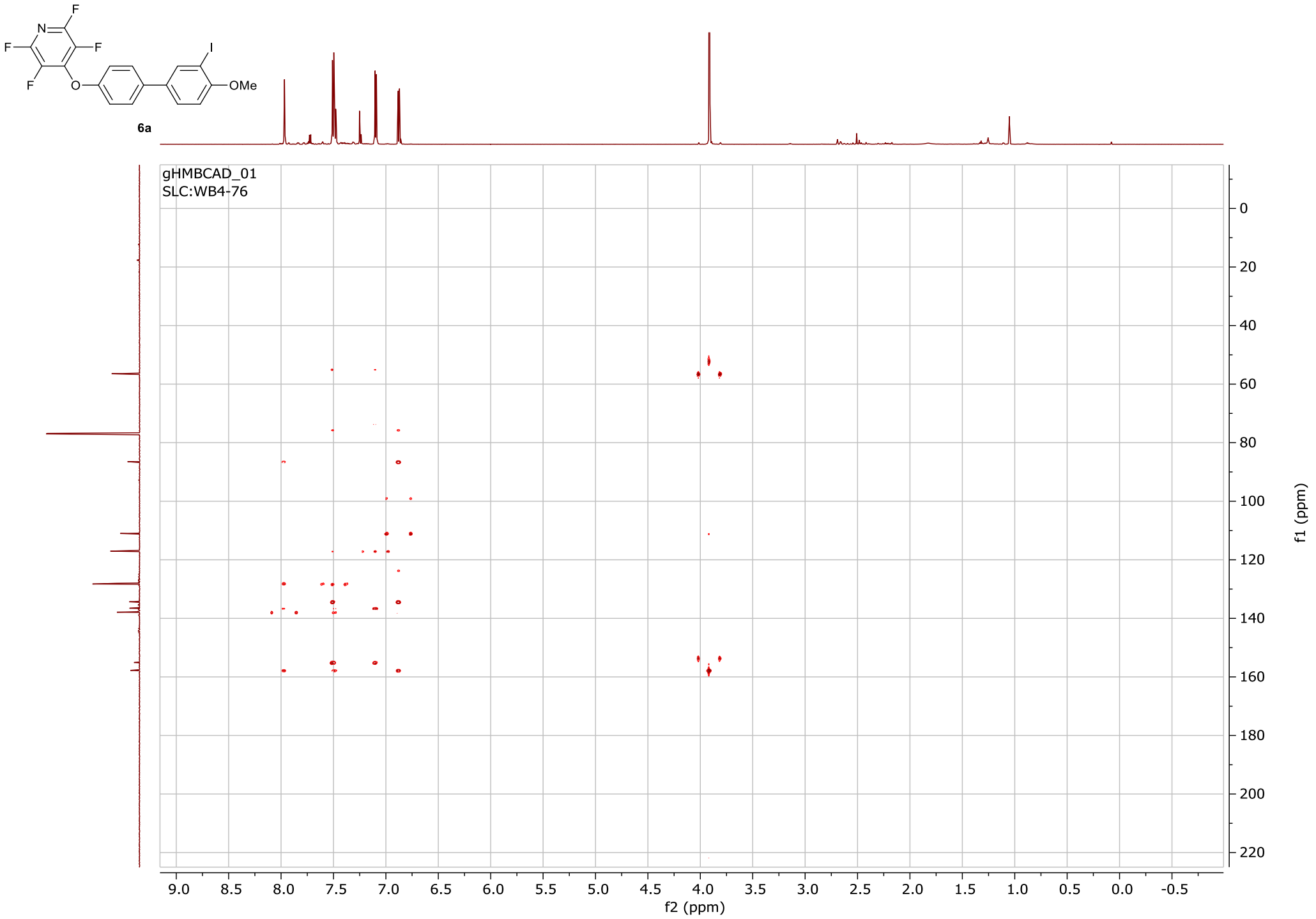

F
N
F
F
F
O
I
OMe

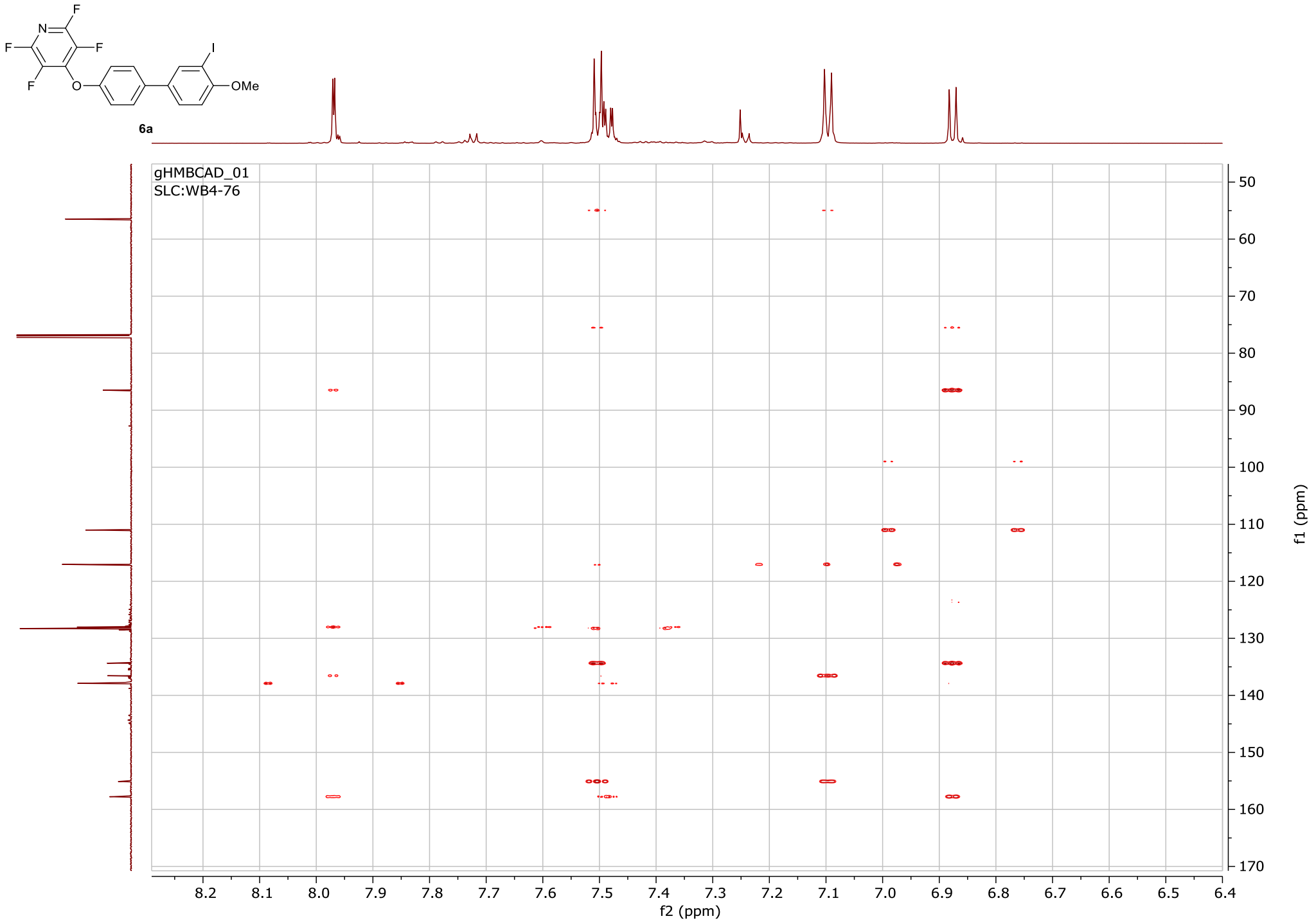
6a


CARBON_01
SLC-WB4-76
144.87
144.81
144.79
144.41
144.38
144.35
144.32
144.29
144.26
143.59
143.57
143.51
143.50
143.49
143.48
143.42
143.40
137.90
137.00
136.95
136.94
136.86
136.84
136.79
136.56
135.51
135.47
135.44
135.41
135.35
135.30
134.36
128.27
128.02
117.04
111.01
86.49
56.47
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

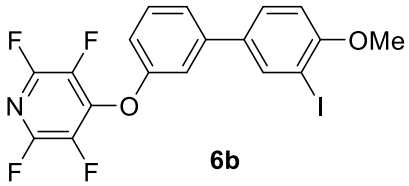

F
N
F
F
F
O
I
OMe
6a
gCOSY_01
SLC:WB4-76
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
6.6
6.5
6.4
f2 (ppm)
6.0
6.2
6.4
6.6
6.8
7.0
7.2
7.4
7.6
7.8
8.0
8.2
8.4
f1 (ppm)


F
N
F
F
F
O
I
OMe
6a
gHSQCAD_01
SLC:WB4-76
100
105
110
115
120
125
130
135
140
145
150
f1 (ppm)
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
6.6
6.5
6.4
6.3
6.2
6.1
6.0
f2 (ppm)


F
N
F
F
F
O
I
OMe
6a
gHMBCAD_01
SLC:WB4-76
f2 (ppm)
f1 (ppm)


F
N
F
F
F
O
I
OMe
6a
gHMBCAD_01
SLC:WB4-76
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
6.6
6.5
6.4
f2 (ppm)
50
60
70
80
90
100
110
120
130
140
150
160
170
f1 (ppm)

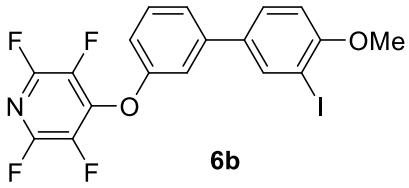
PROTON_01
SLC:WB:WB5-5.1



6b

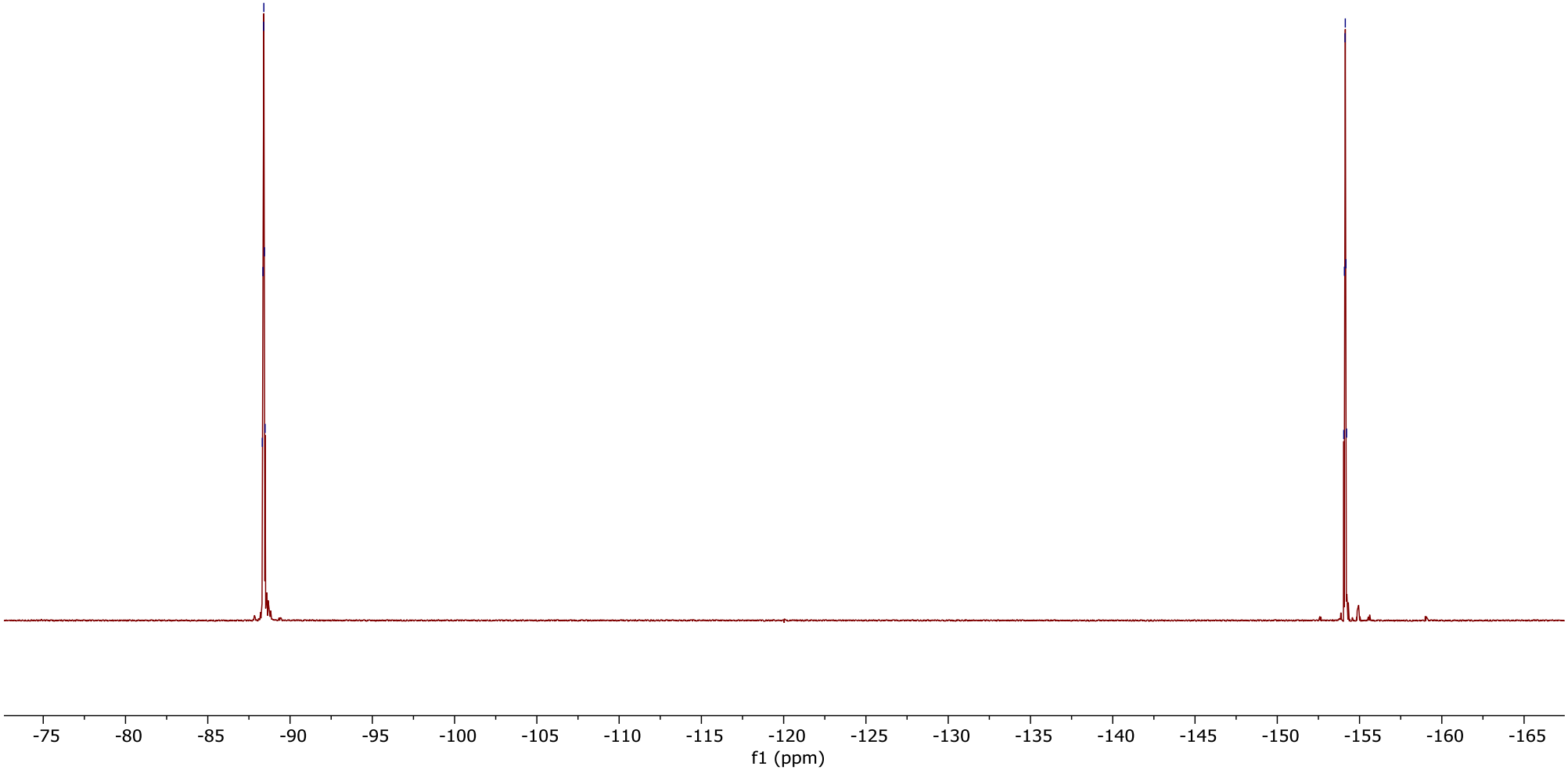
10160329.13.fid
SLC:WDGB:WB5-51

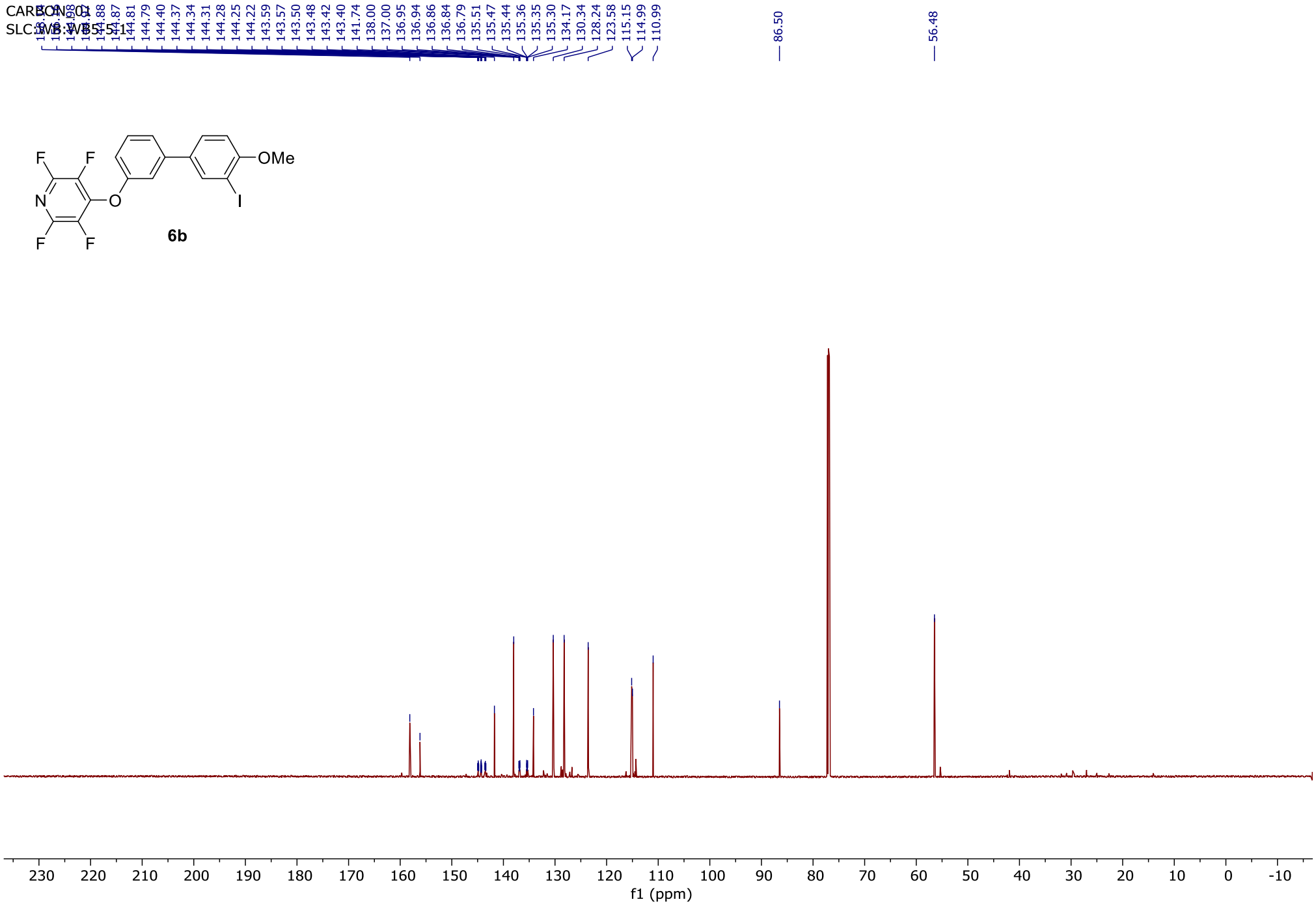
-88.32
-88.36
-88.39
-88.41
-88.44
-88.48

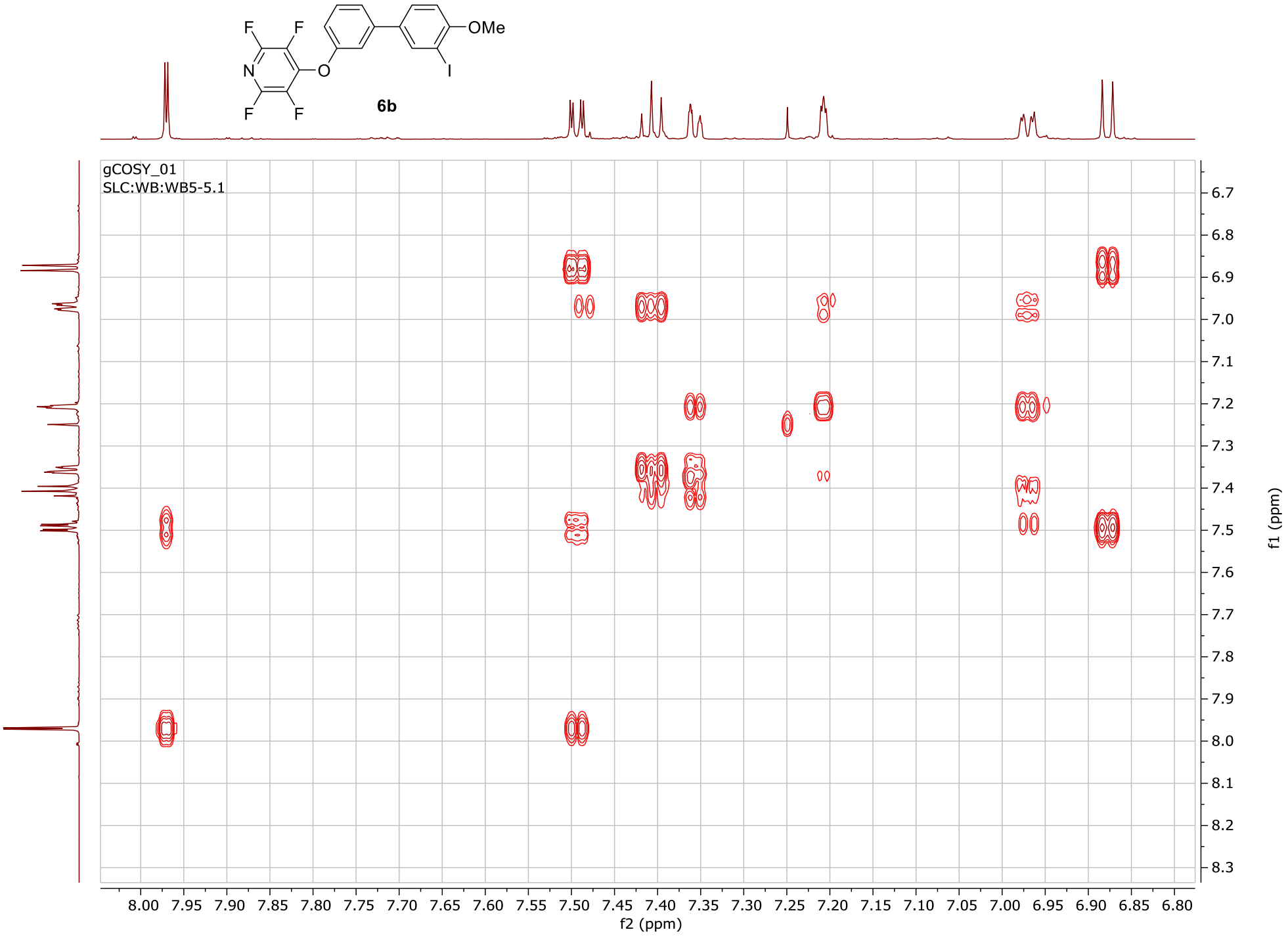


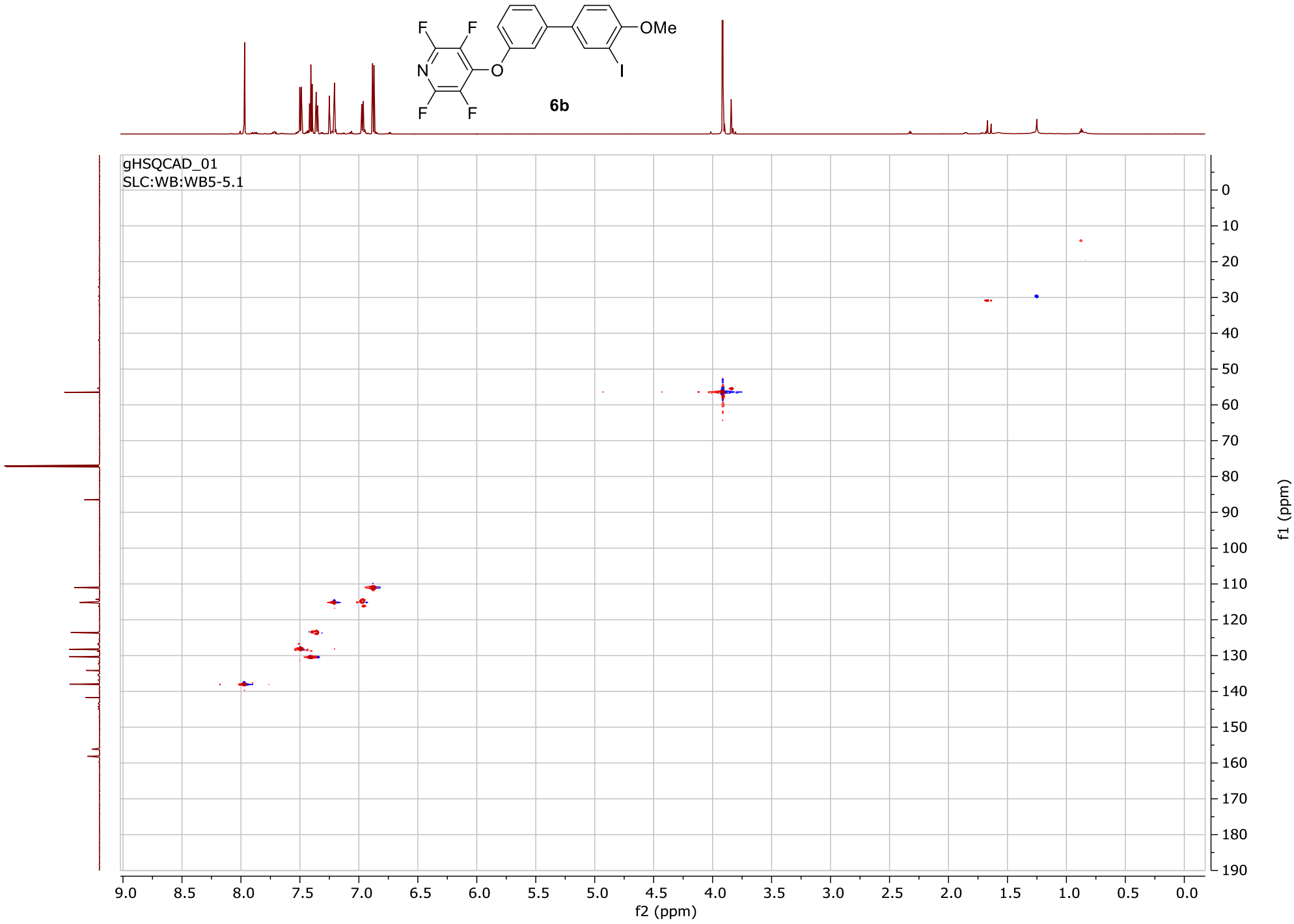
6b

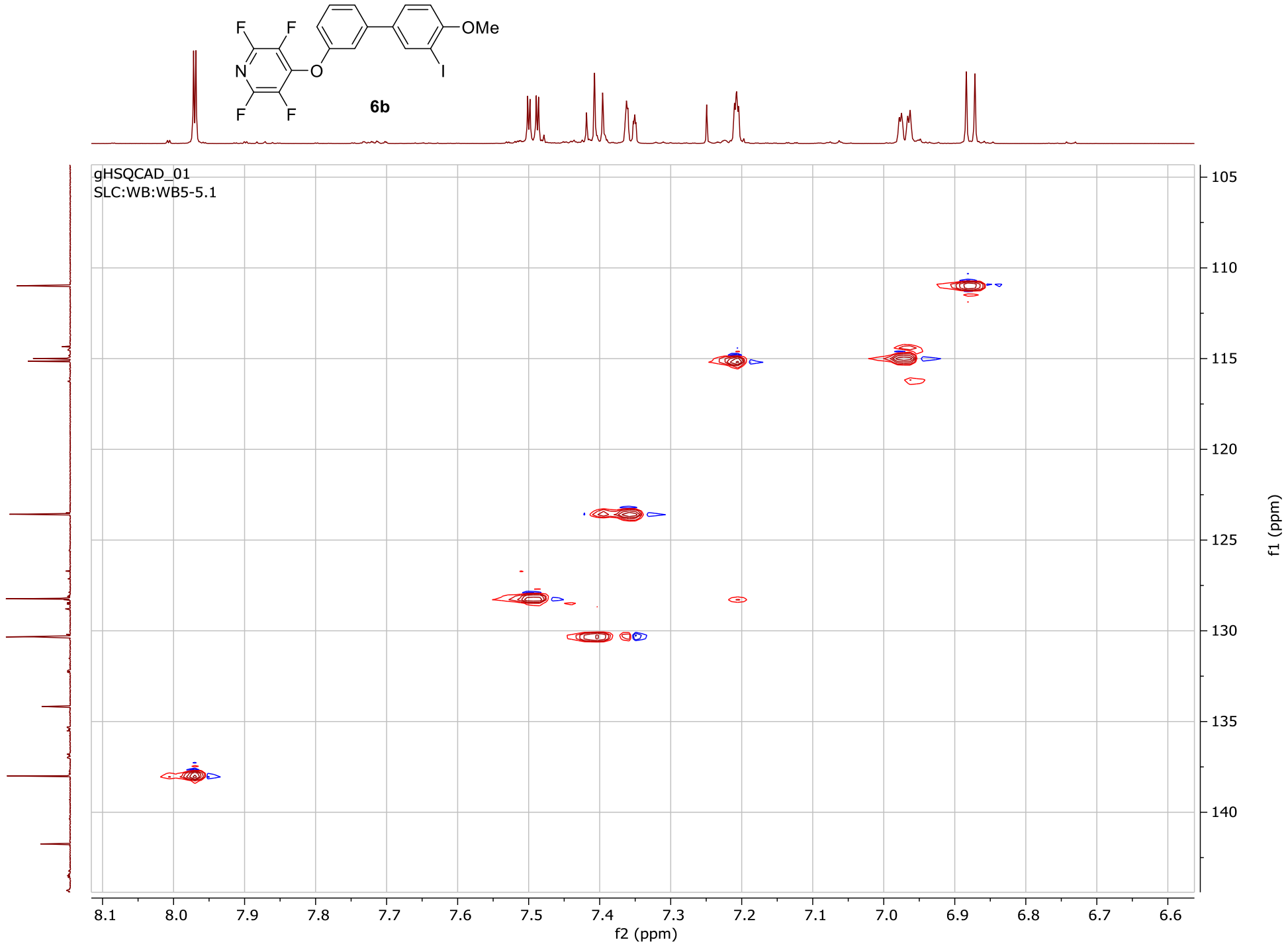
-154.04
-154.08
-154.12
-154.13
-154.17
-154.21

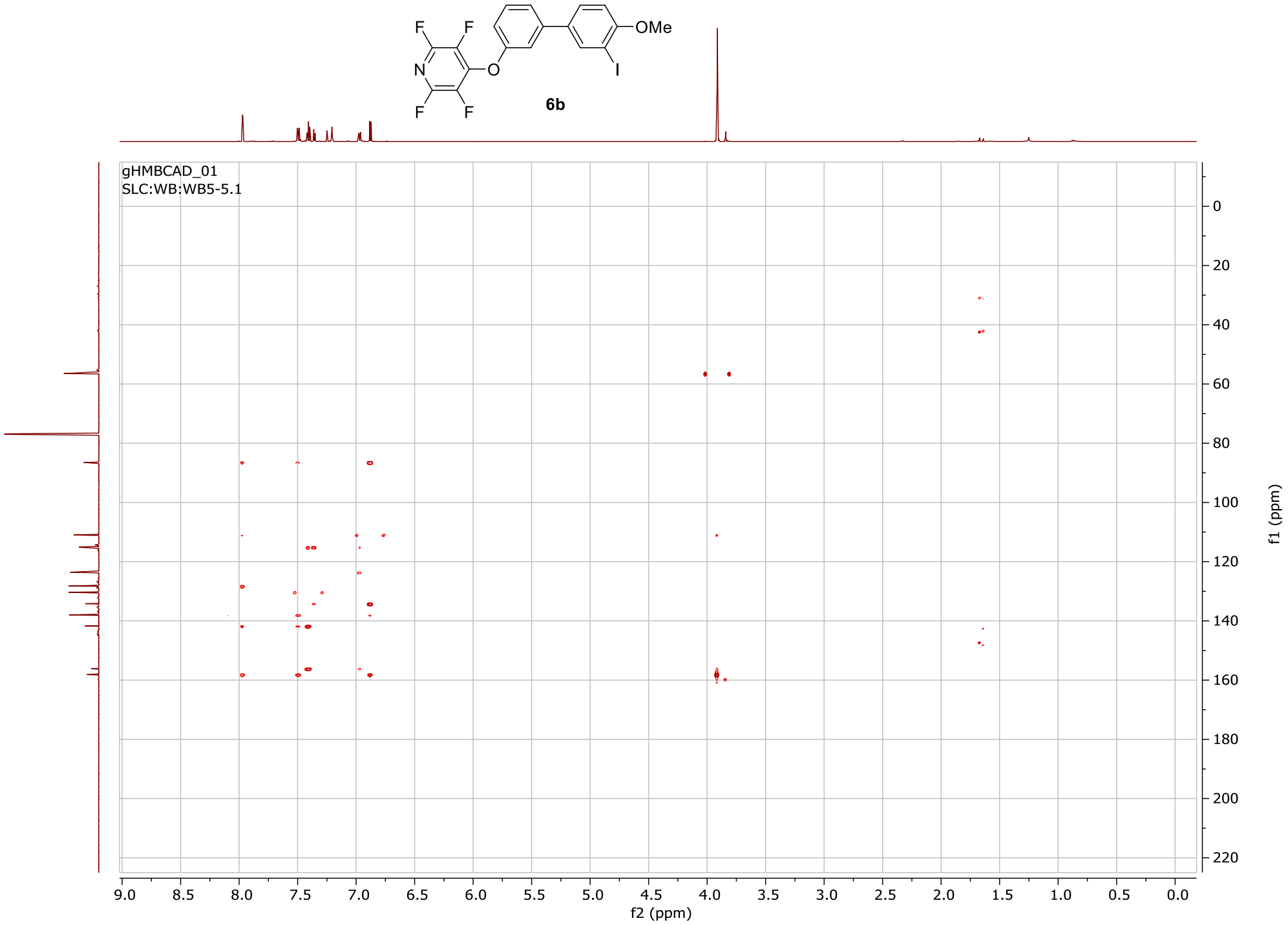


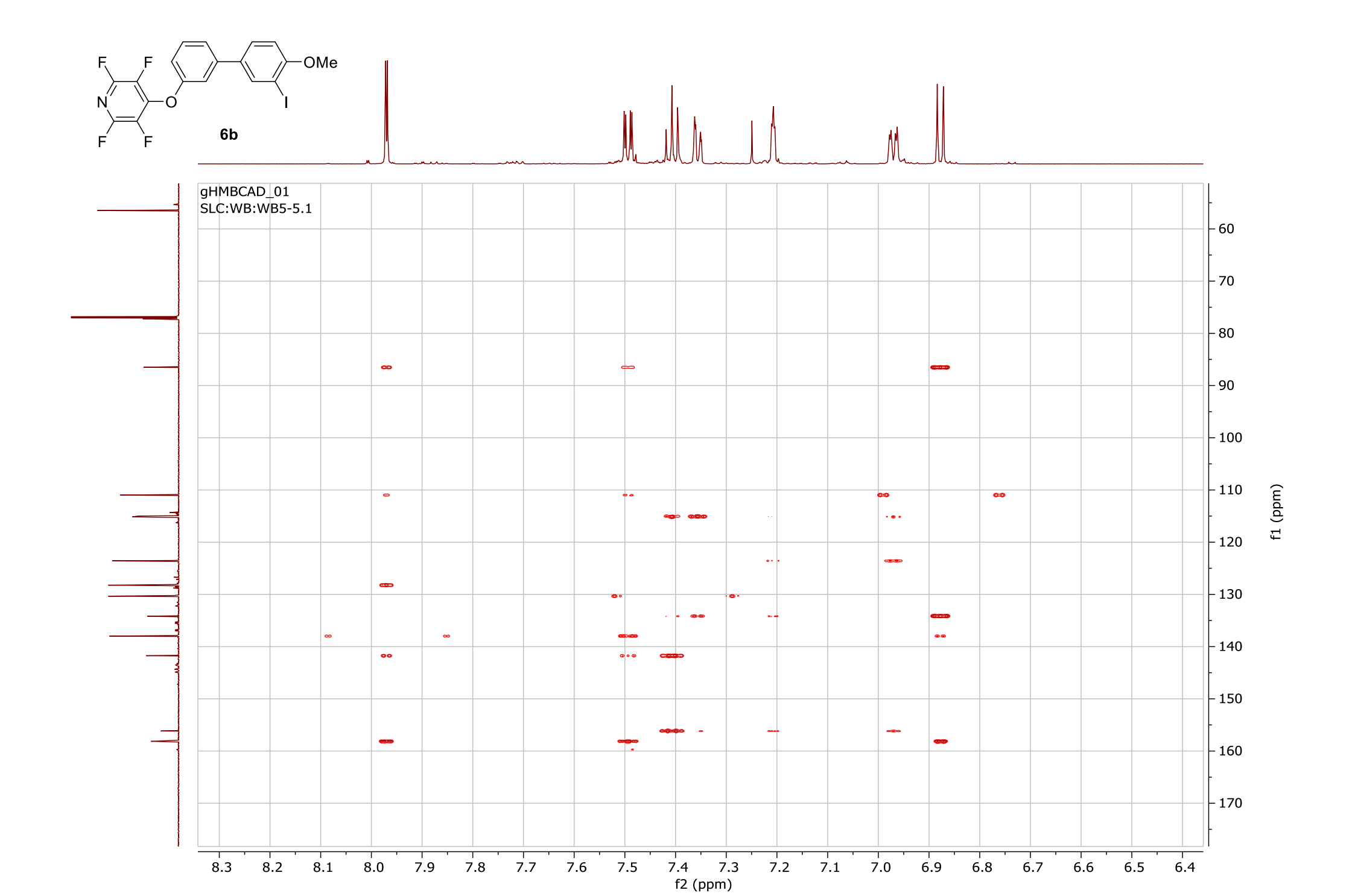

CARBON-01
SLC-WB-WB5-141
144.79
144.40
144.37
144.34
144.31
144.28
144.25
144.22
143.59
143.57
143.50
143.48
143.42
143.40
141.74
138.00
137.00
136.95
136.94
136.86
136.84
136.79
135.51
135.47
135.44
135.36
135.35
135.30
134.17
130.34
128.24
123.58
115.15
114.99
110.99
86.50
56.48
F
F
N
O
OMe
I
F
F
6b
230
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)


F
F
N
O
OMe
I
F
F
6b
gCOSY_01
SLC:WB:WB5-5.1
8.00 7.95 7.90 7.85 7.80 7.75 7.70 7.65 7.60 7.55 7.50 7.45 7.40 7.35 7.30 7.25 7.20 7.15 7.10 7.05 7.00 6.95 6.90 6.85 6.80
f2 (ppm)
6.7 6.8 6.9 7.0 7.1 7.2 7.3 7.4 7.5 7.6 7.7 7.8 7.9 8.0 8.1 8.2 8.3
f1 (ppm)

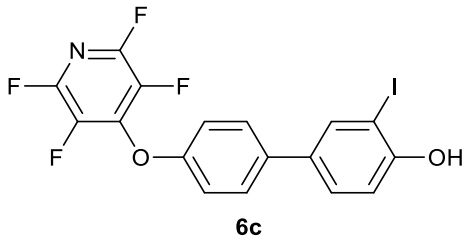

F
F
N
O
OMe
I
F
F
6b
gHSQCAD_01
SLC:WB:WB5-5.1
f2 (ppm)
f1 (ppm)


F
F
N
O
OMe
I
F
F
6b
gHSQCAD_01
SLC:WB:WB5-5.1
105
110
115
120
125
130
135
140
f1 (ppm)
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
6.6
f2 (ppm)

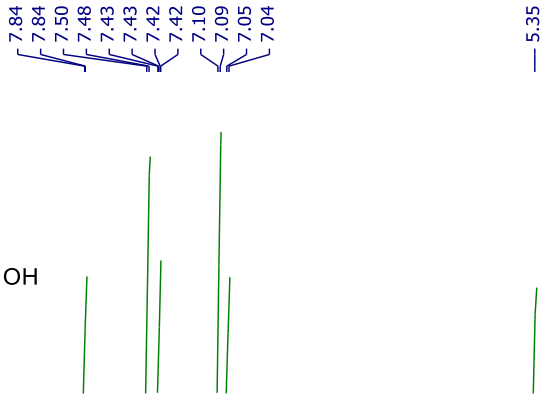

F
F
N
O
OMe
I
F
F
6b
gHMBCAD_01
SLC:WB:WB5-5.1
f1 (ppm)
f2 (ppm)
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
180
200
220

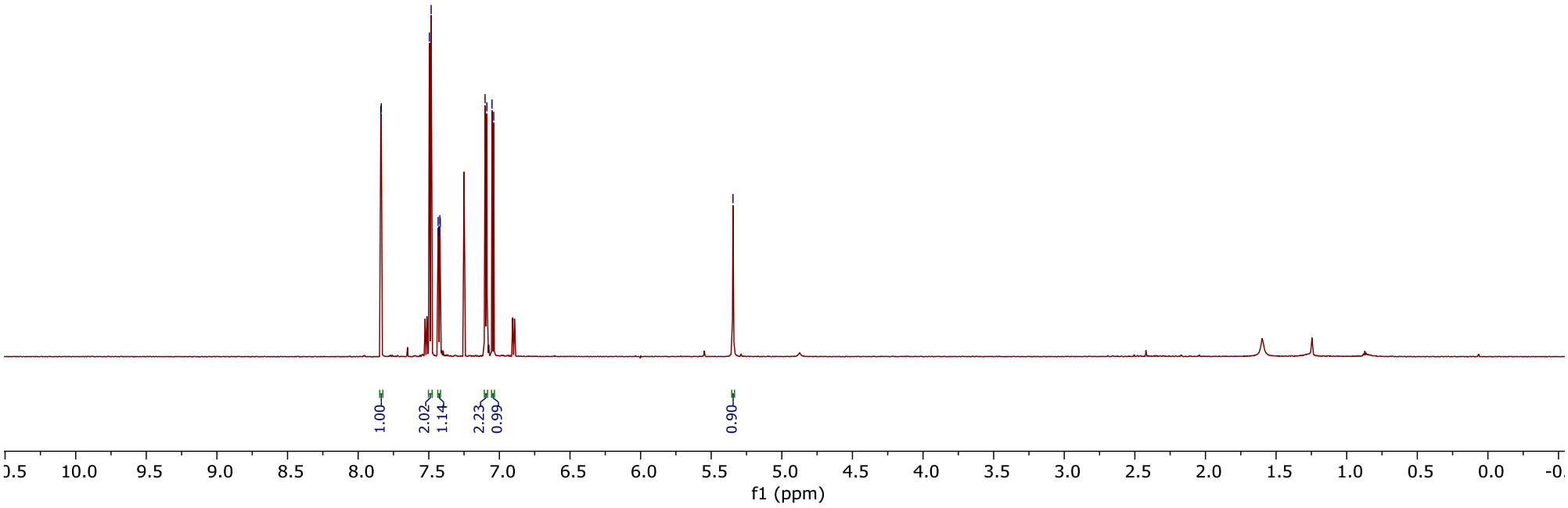

F
F
N
O
OMe
I
F
F
6b
gHMBCAD_01
SLC:WB:WB5-5.1
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
6.6
6.5
6.4
f2 (ppm)
60
70
80
90
100
110
120
130
140
150
160
170
f1 (ppm)

PROTON_01
SLC:WB:WB5-24



6c

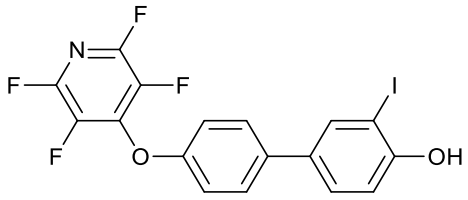




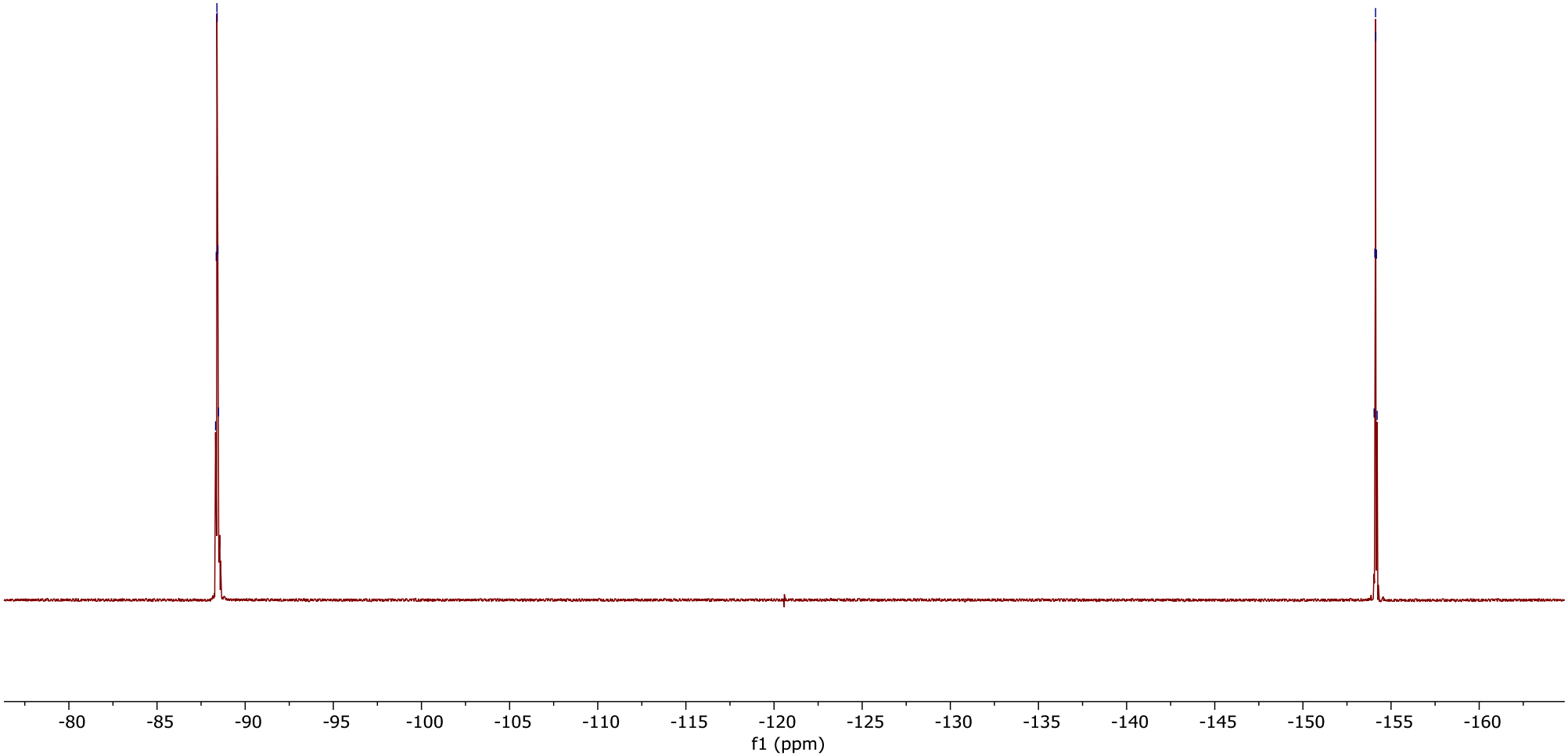
28092839.13.fid
SLC:WDGB:WB5-24

-88.32
-88.36
-88.40
-88.41
-88.45
-88.49

-154.04
-154.08
-154.12
-154.13
-154.17
-154.21

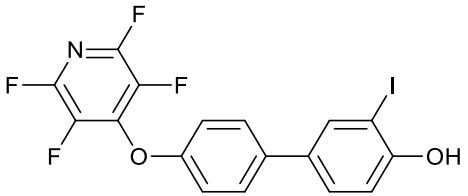


6c

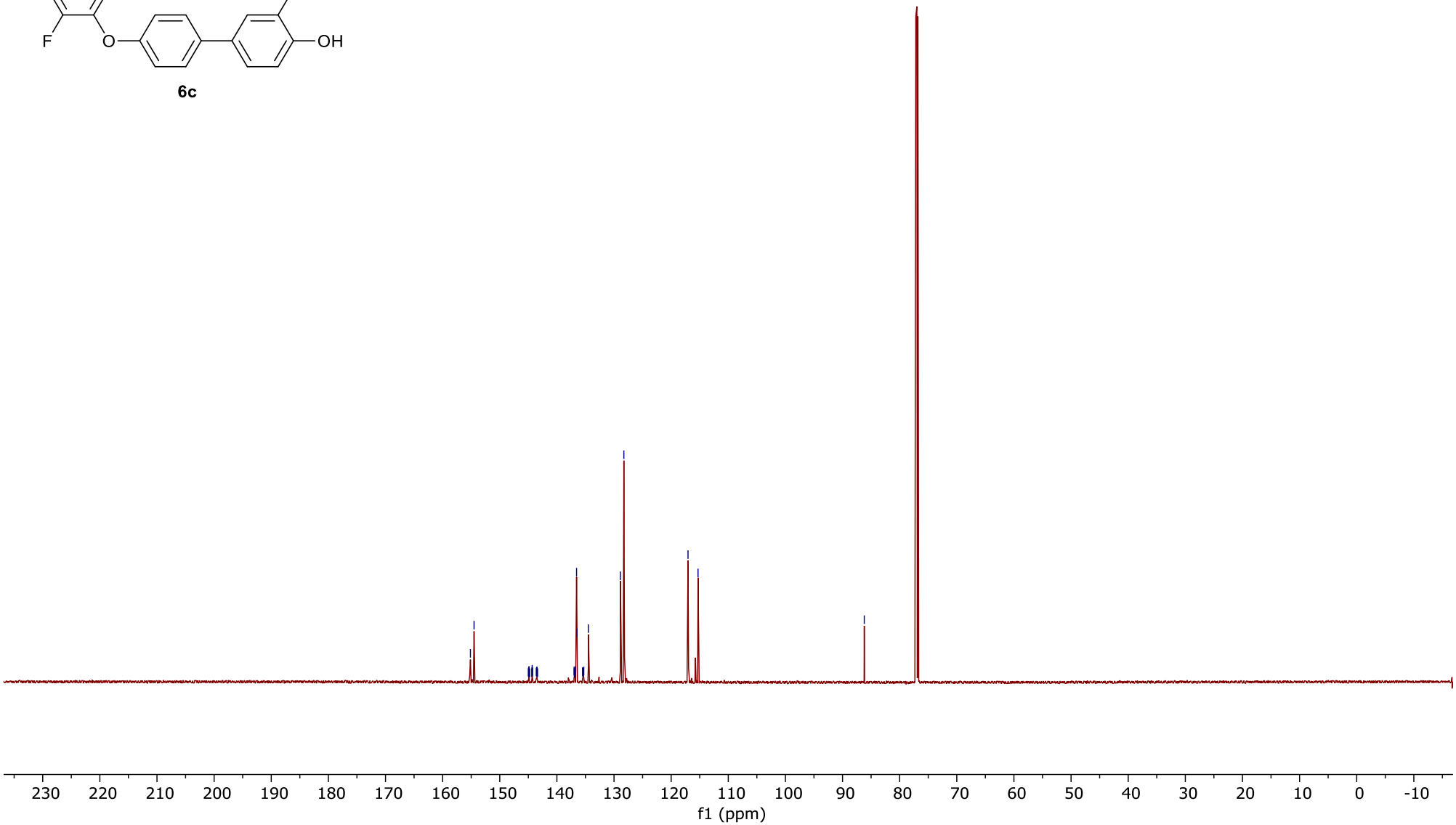


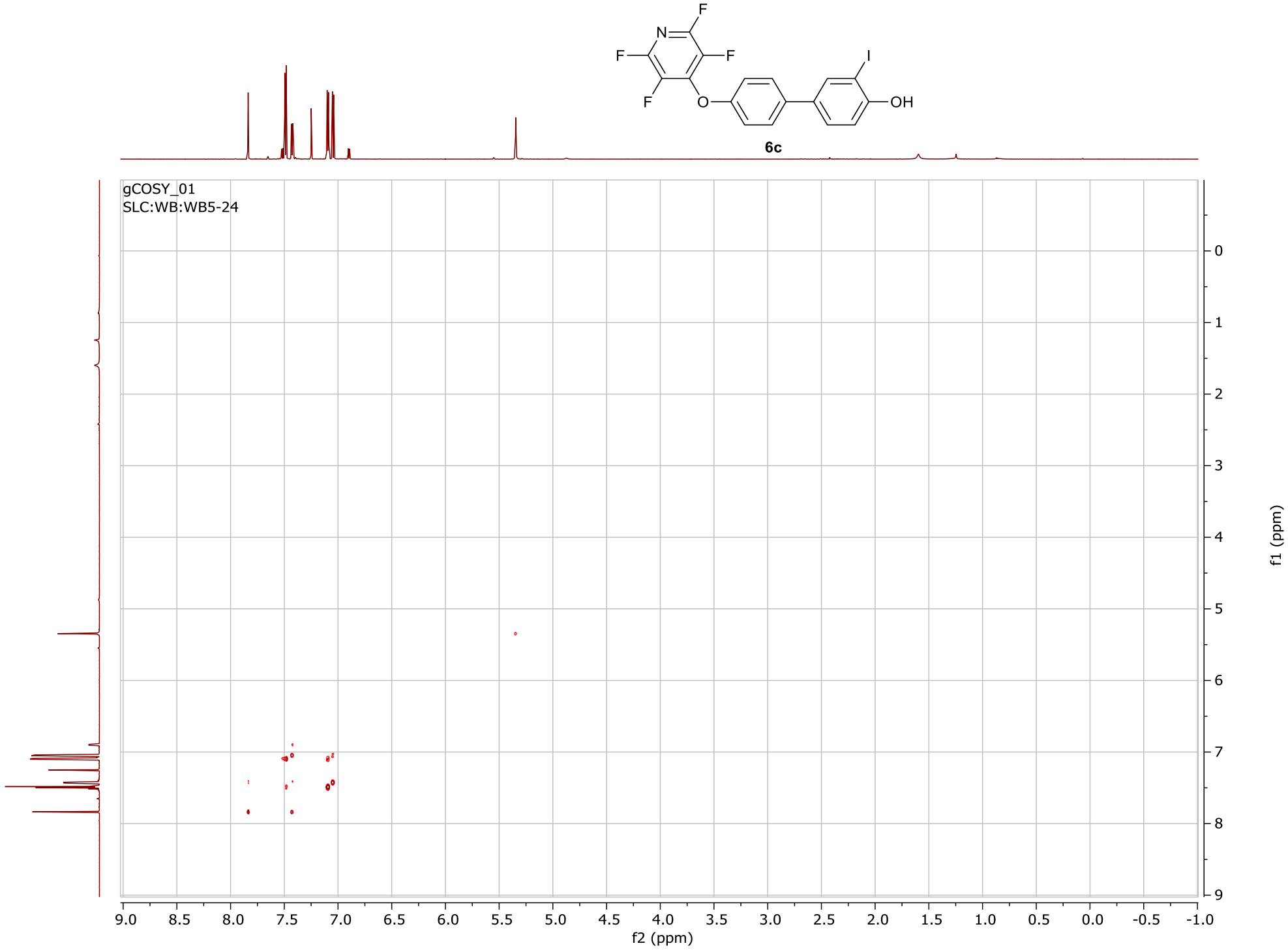
CARBON_01
SLC:WB:WB5-24

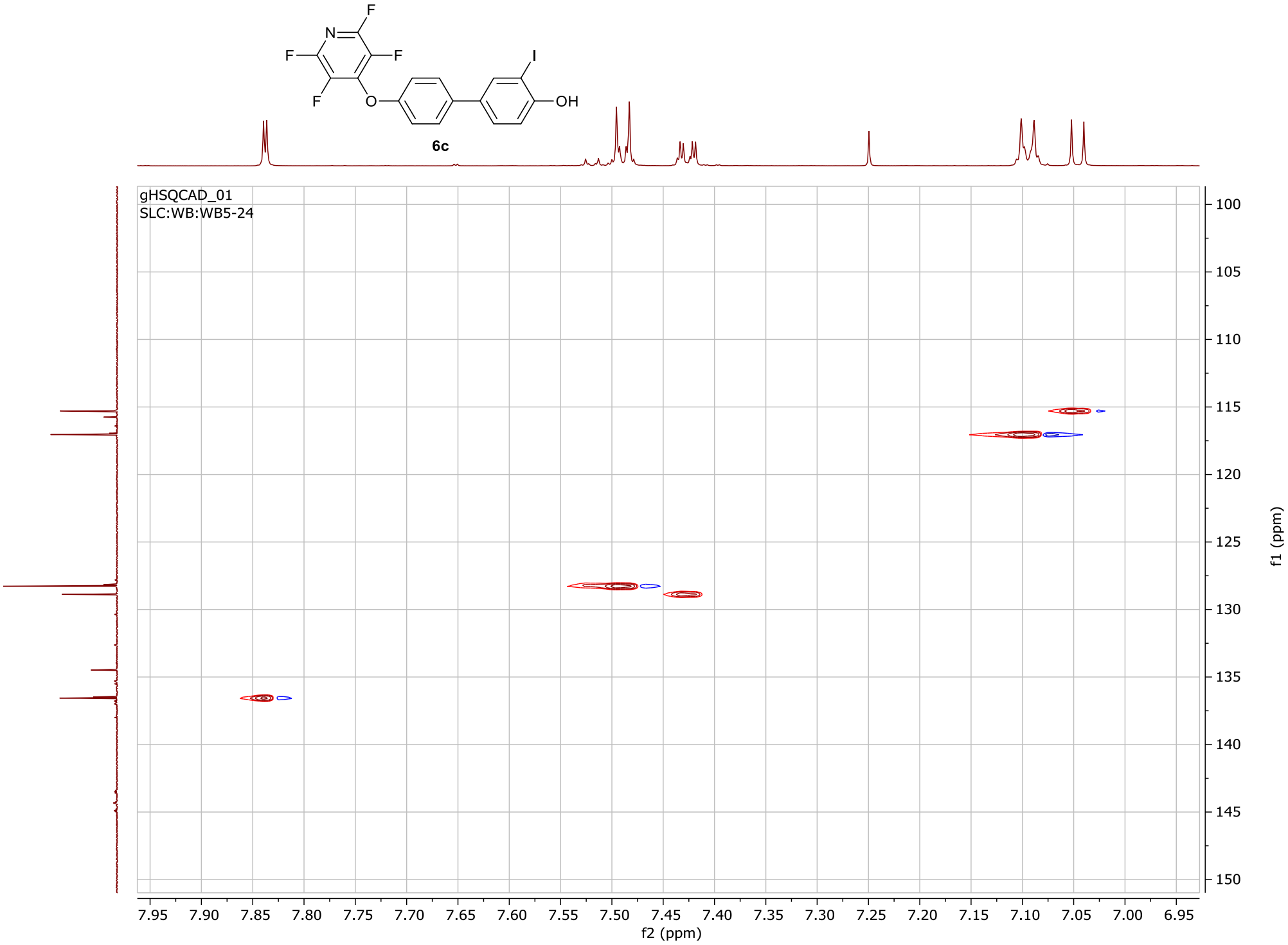
155.14
154.50
144.98
144.97
144.90
144.89
144.88
144.87
144.81
144.79
144.39
144.36
144.33
144.29
144.27
143.59
143.57
143.51
143.50
143.49
143.48
143.42
143.40
136.99
136.95
136.93
136.85
136.83
136.79
136.56
136.47
135.50
135.46
135.44
135.35
135.34
135.29
134.48
128.88
128.28
117.05
115.29
86.19

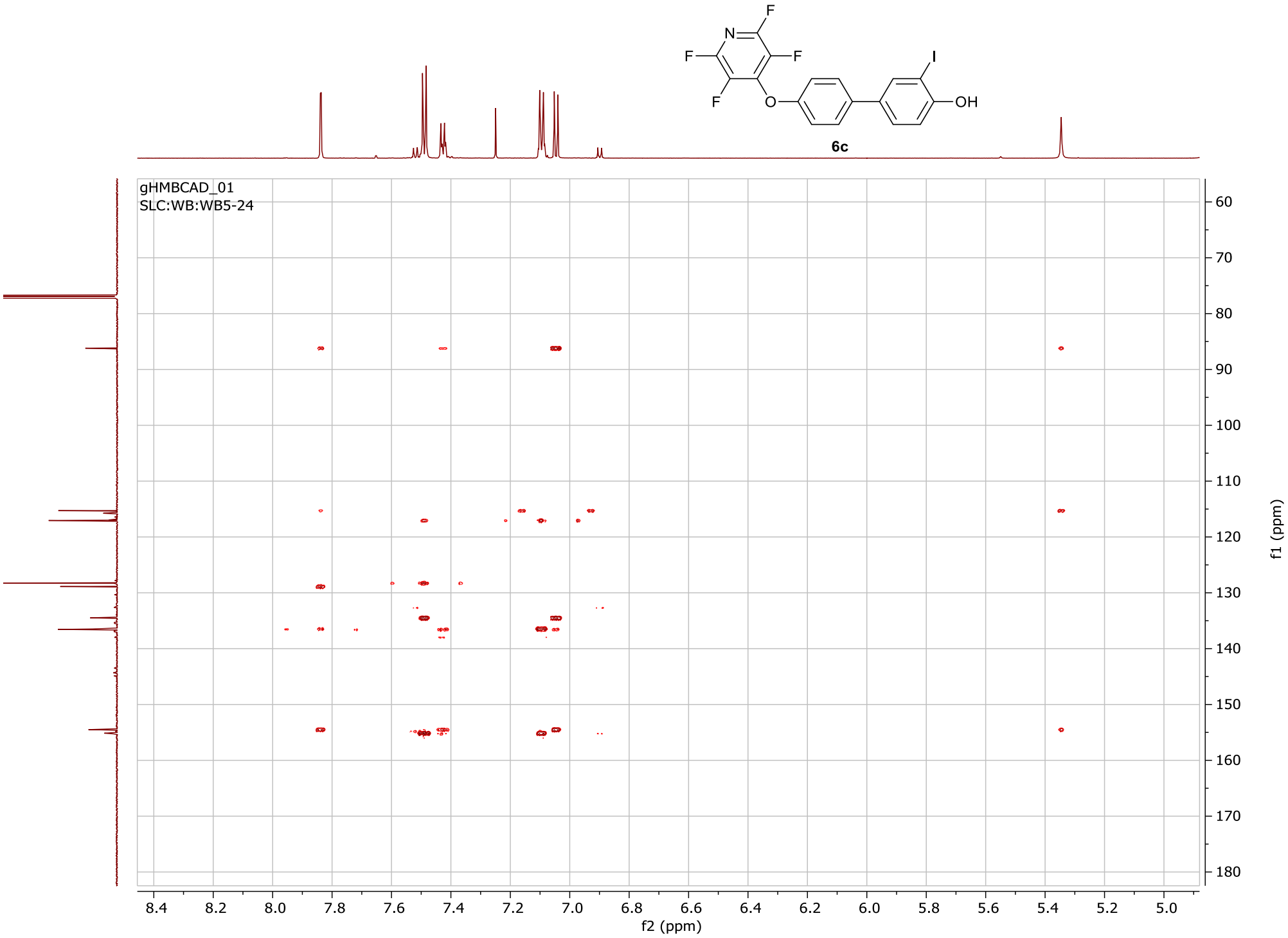


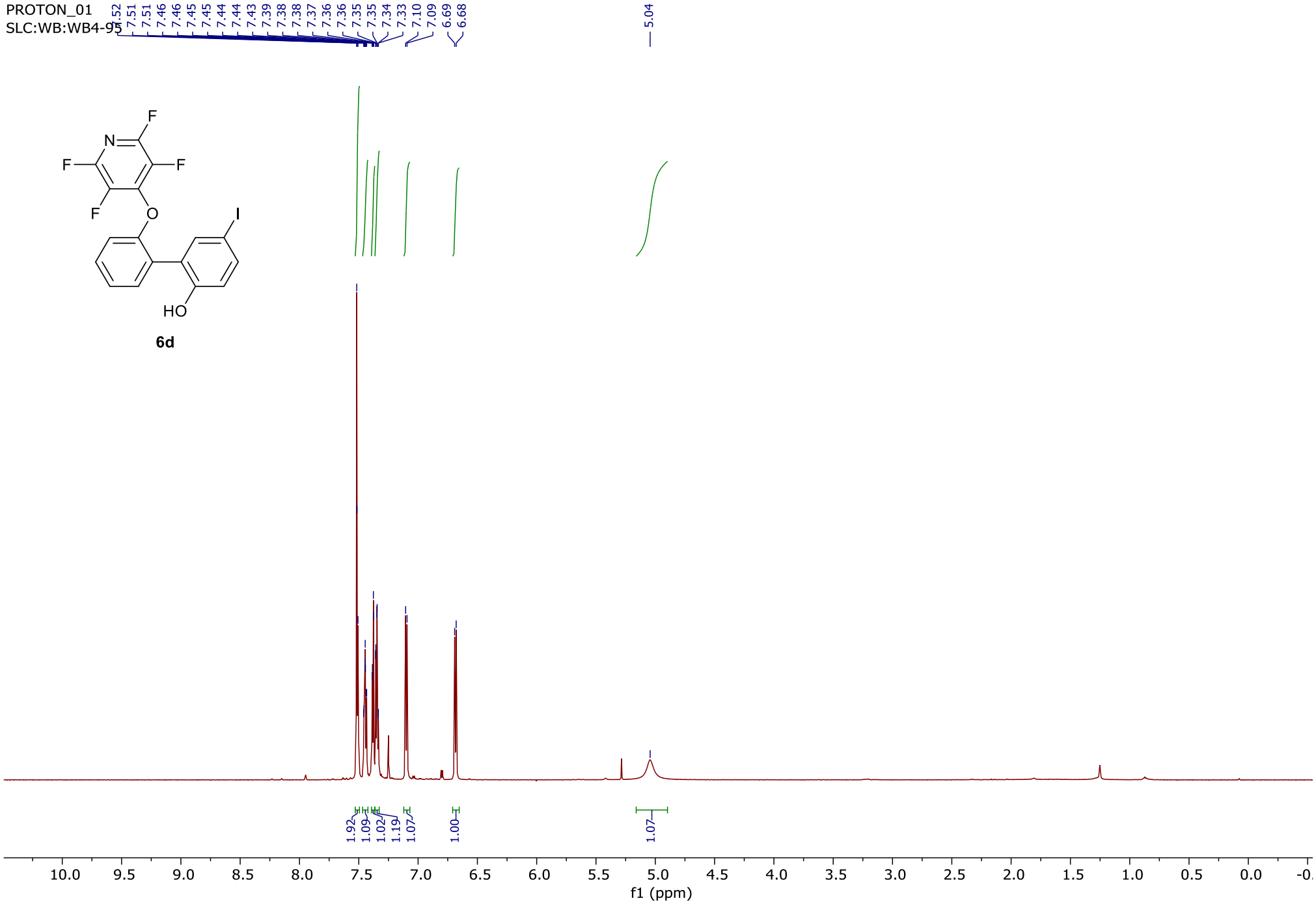
6c

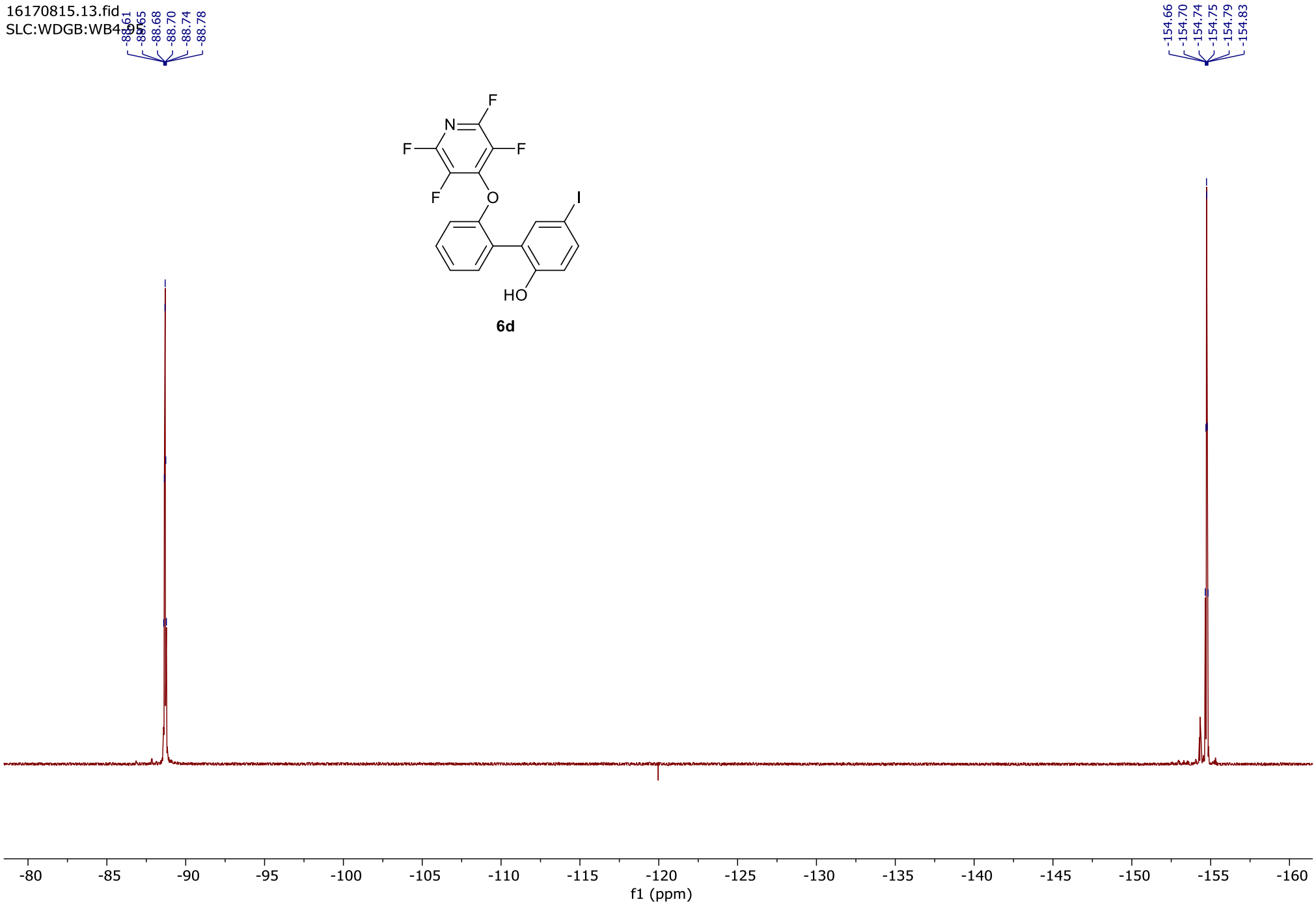



F
N
F
F
F
O
I
OH
6c
gCOSY_01
SLC:WB:WB5-24
f2 (ppm)
f1 (ppm)


F
N
F
F
F
O
I
OH
6c
gHSQCAD_01
SLC:WB:WB5-24
100
105
110
115
120
125
130
135
140
145
150
f1 (ppm)
7.95
7.90
7.85
7.80
7.75
7.70
7.65
7.60
7.55
7.50
7.45
7.40
7.35
7.30
7.25
7.20
7.15
7.10
7.05
7.00
6.95
f2 (ppm)


F
N
F
F
F
O
I
OH
6c
gHMBCAD_01
SLC:WB:WB5-24
f2 (ppm)
f1 (ppm)

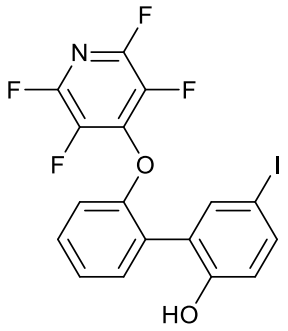

PROTON_01
SLC:WB:WB4-95
7.52
7.51
7.51
7.46
7.46
7.45
7.45
7.44
7.44
7.43
7.39
7.38
7.38
7.37
7.36
7.36
7.35
7.35
7.34
7.33
7.10
7.09
6.69
6.68
5.04
F
N
F
F
F
O
I
HO
6d
1.92
1.09
1.02
1.19
1.07
1.00
1.07
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


16170815.13.fid
SLC:WDGB:WB4_95
-88.61
-88.65
-88.68
-88.70
-88.74
-88.78
-154.66
-154.70
-154.74
-154.75
-154.79
-154.83
F
N
F
F
F
O
I
HO
-80
-85
-90
-95
-100
-105
-110
-115
-120
-125
-130
-135
-140
-145
-150
-155
-160
f1 (ppm)

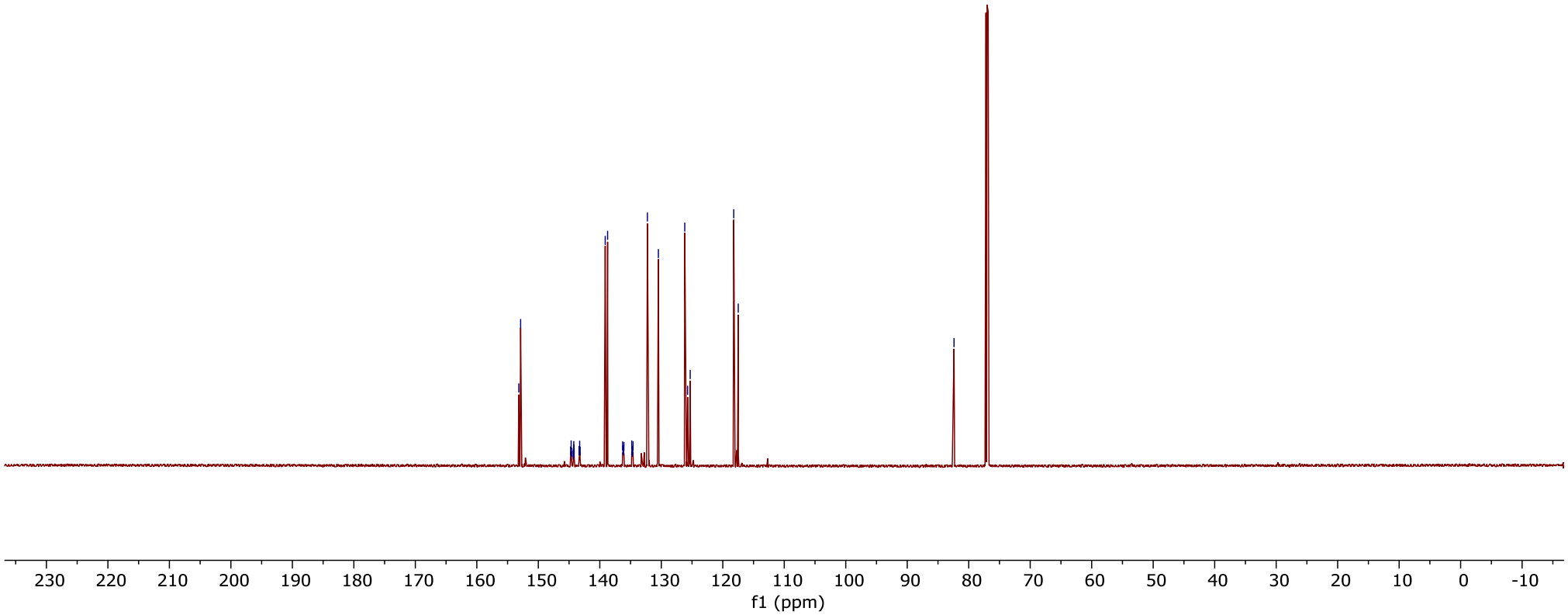
6d

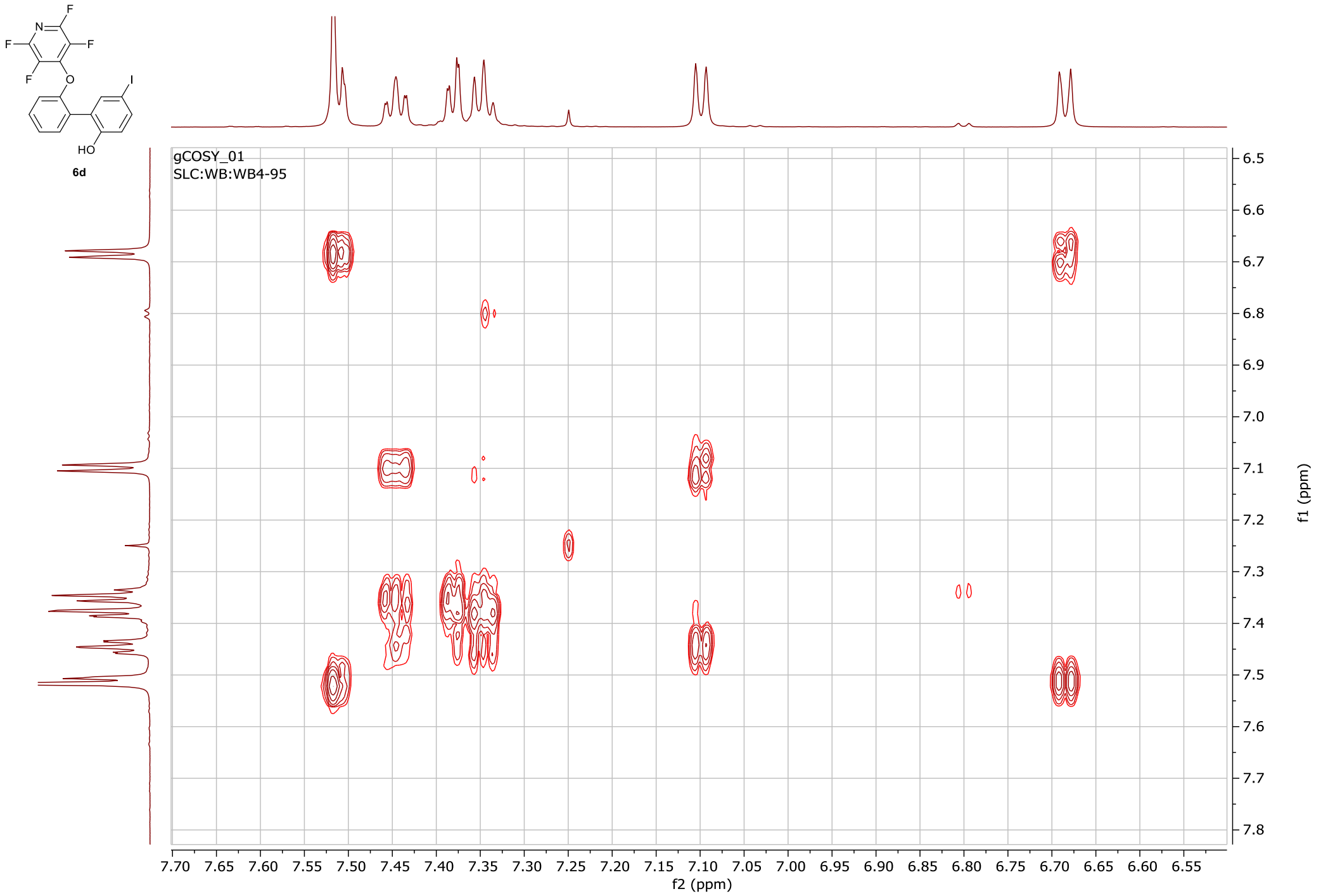
CARBON_01
SLC:WB:WB4-95

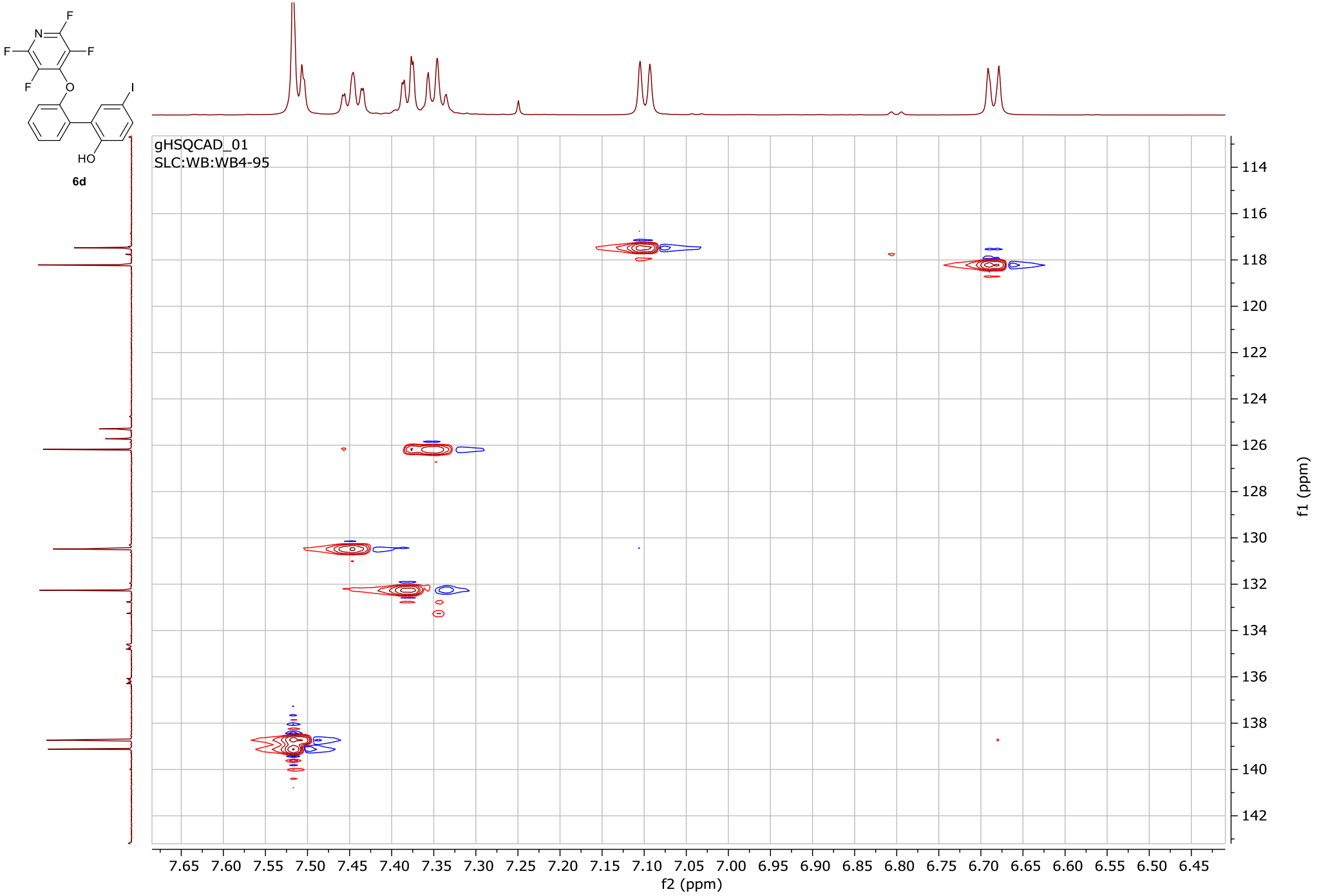
153.18
152.88
144.75
144.66
144.57
144.32
144.29
144.26
144.23
144.20
144.17
143.37
143.35
143.27
143.20
139.12
138.73
136.29
136.23
136.13
136.08
134.80
134.76
134.74
134.64
134.59
132.26
130.48
126.18
125.72
125.30
118.21
117.48
82.39

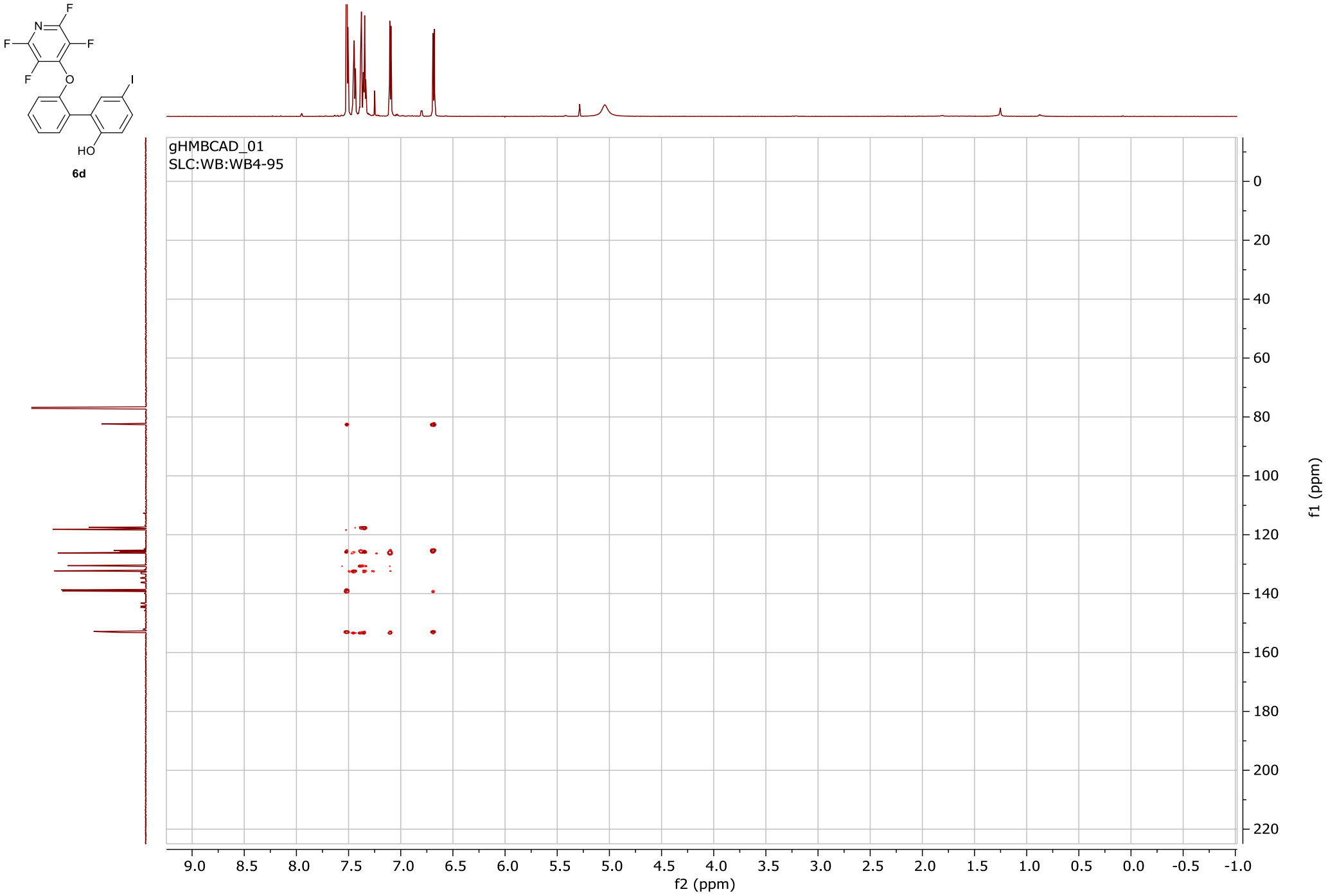


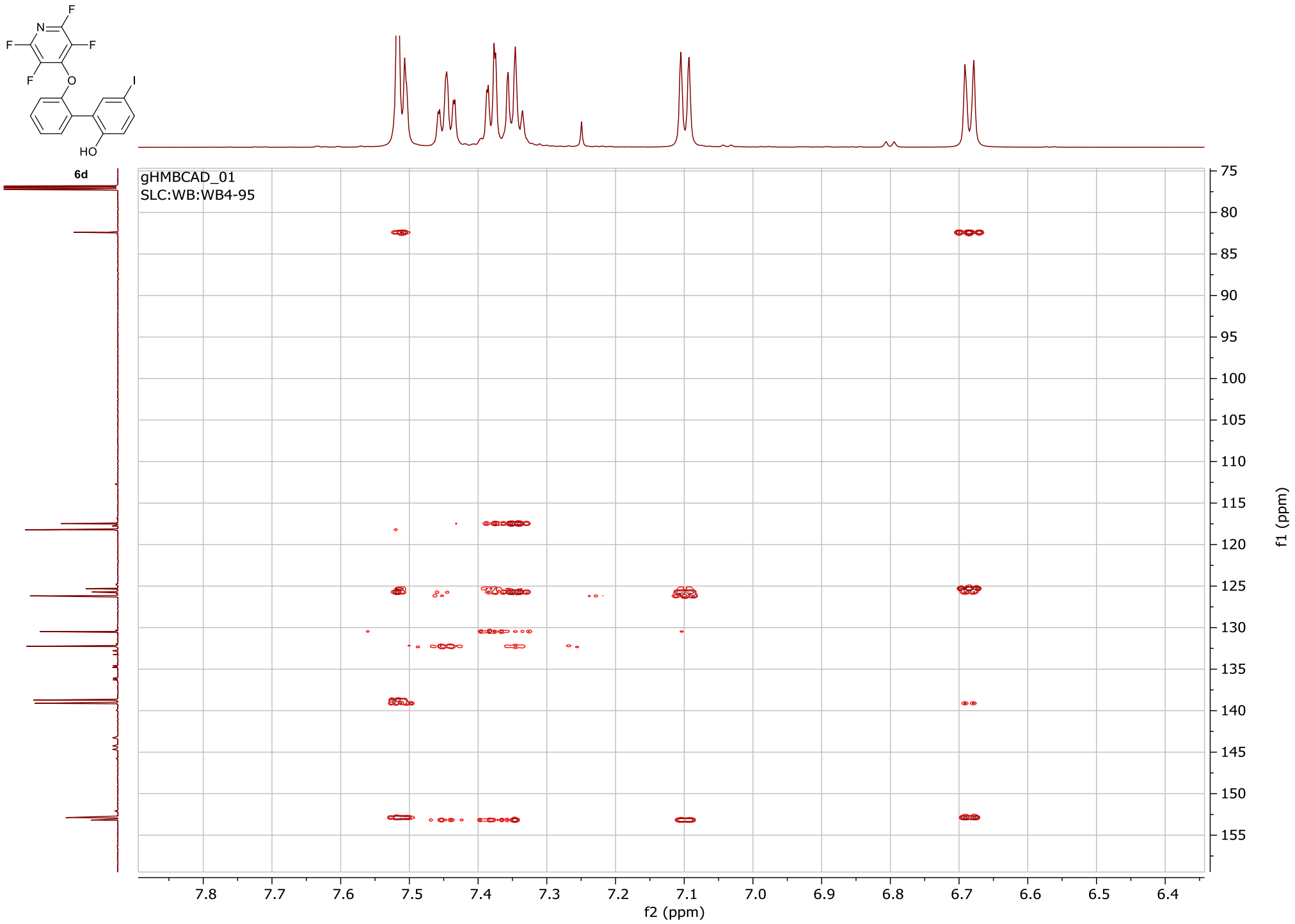
6d



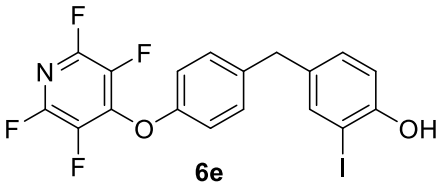

F
N
F
F
F
O
I
HO
6d
gCOSY_01
SLC:WB:WB4-95
7.70 7.65 7.60 7.55 7.50 7.45 7.40 7.35 7.30 7.25 7.20 7.15 7.10 7.05 7.00 6.95 6.90 6.85 6.80 6.75 6.70 6.65 6.60 6.55
f2 (ppm)
6.5 6.6 6.7 6.8 6.9 7.0 7.1 7.2 7.3 7.4 7.5 7.6 7.7 7.8
f1 (ppm)


F
N
F
F
F
O
I
HO
6d
gHSQCAD_01
SLC:WB:WB4-95
114
116
118
120
122
124
126
128
130
132
134
136
138
140
142
f1 (ppm)
7.65 7.60 7.55 7.50 7.45 7.40 7.35 7.30 7.25 7.20 7.15 7.10 7.05 7.00 6.95 6.90 6.85 6.80 6.75 6.70 6.65 6.60 6.55 6.50 6.45
f2 (ppm)


F
N
F
F
F
O
I
HO
6d
gHMBCAD_01
SLC:WB:WB4-95
0
20
40
60
80
100
120
140
160
180
200
220
f1 (ppm)
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
-0.5
-1.0
f2 (ppm)

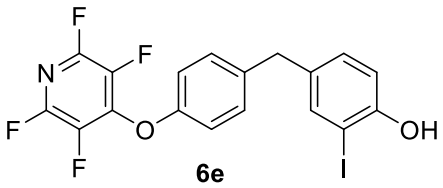

6d
gHMBCAD_01
SLC:WB:WB4-95
F
N
F
F
F
O
I
HO
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
6.6
6.5
6.4
f2 (ppm)
75
80
85
90
95
100
105
110
115
120
125
130
135
140
145
150
155
f1 (ppm)

06094942.10.fid
SLC:WDGB:WB5-71

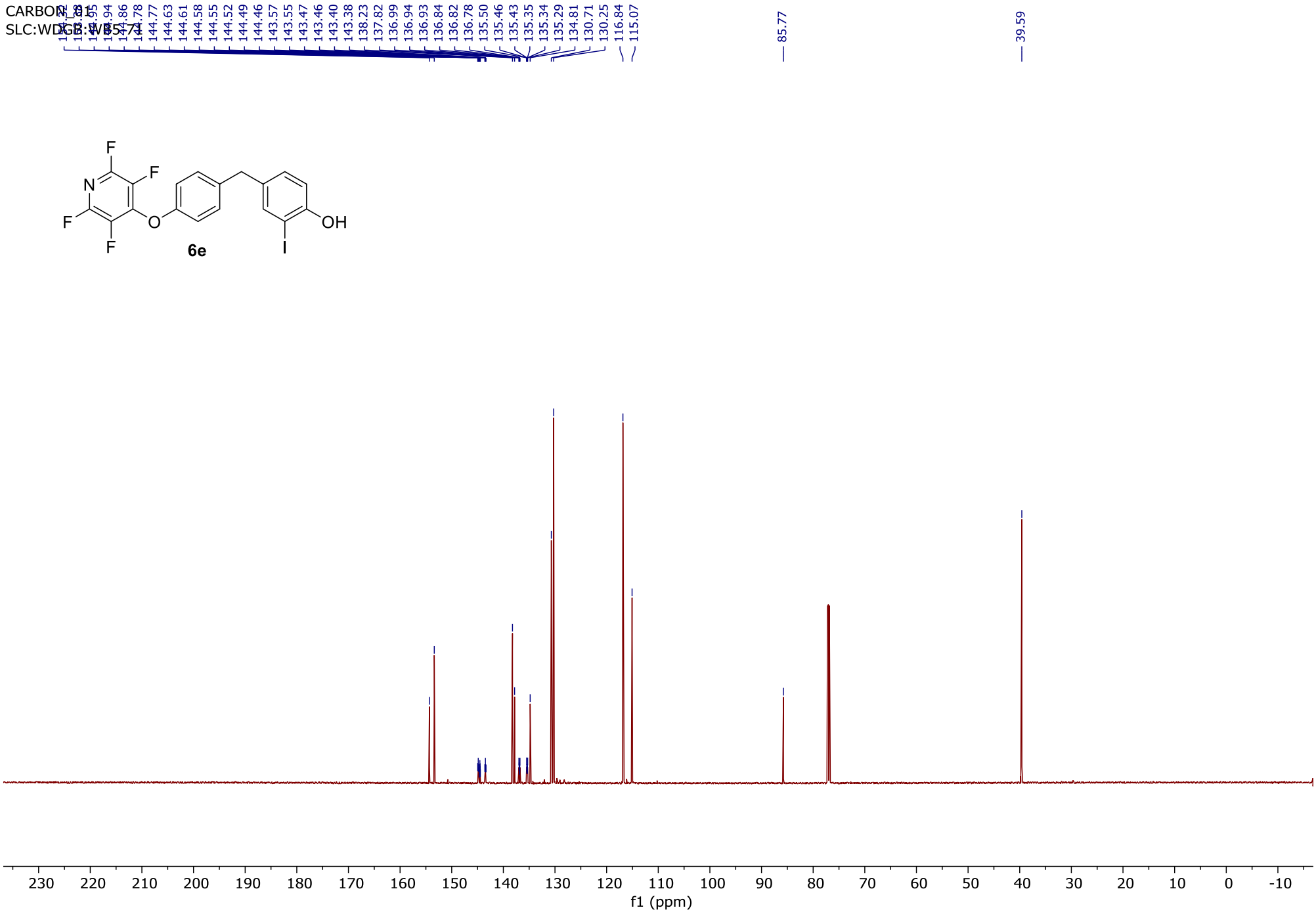


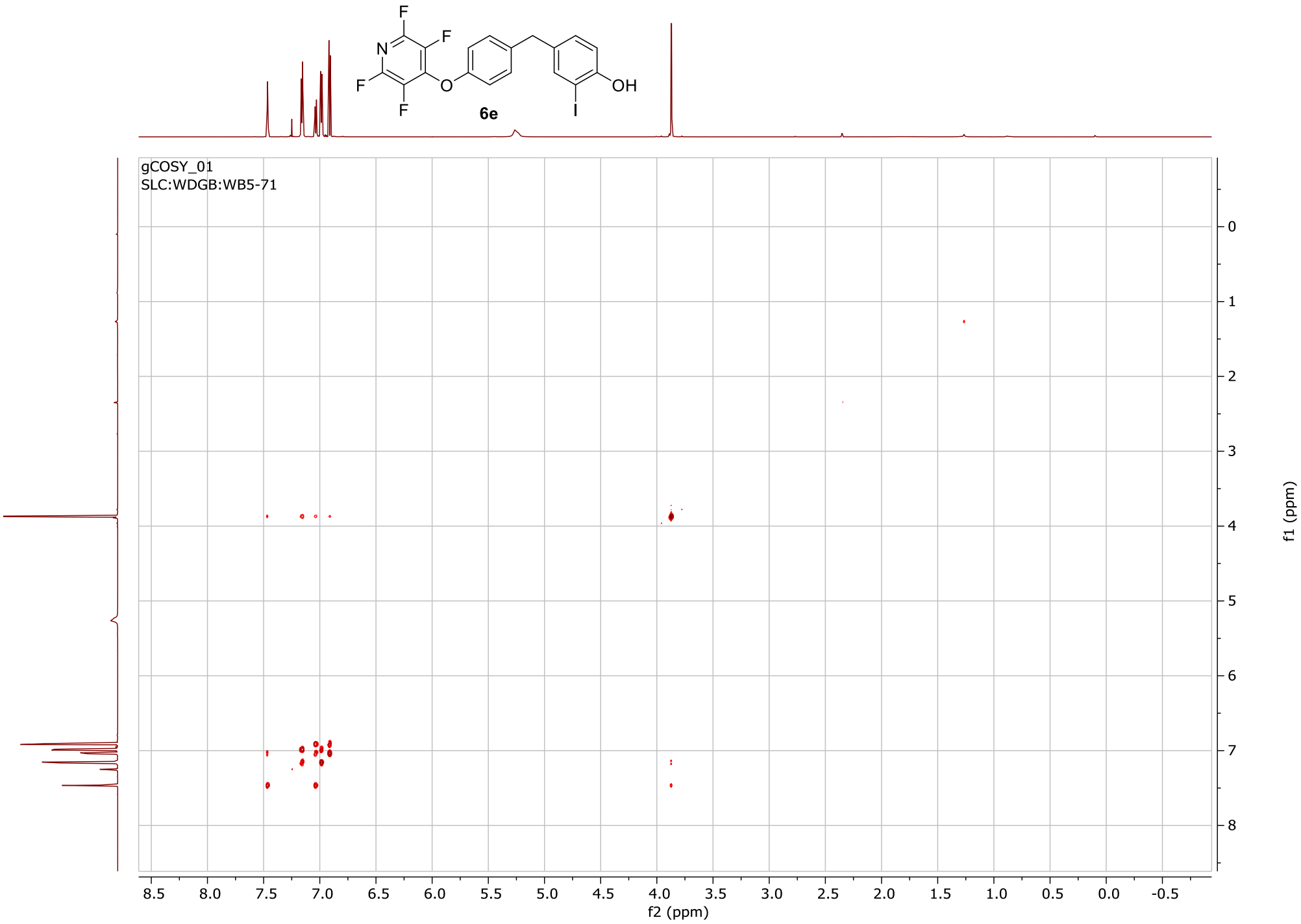
6e

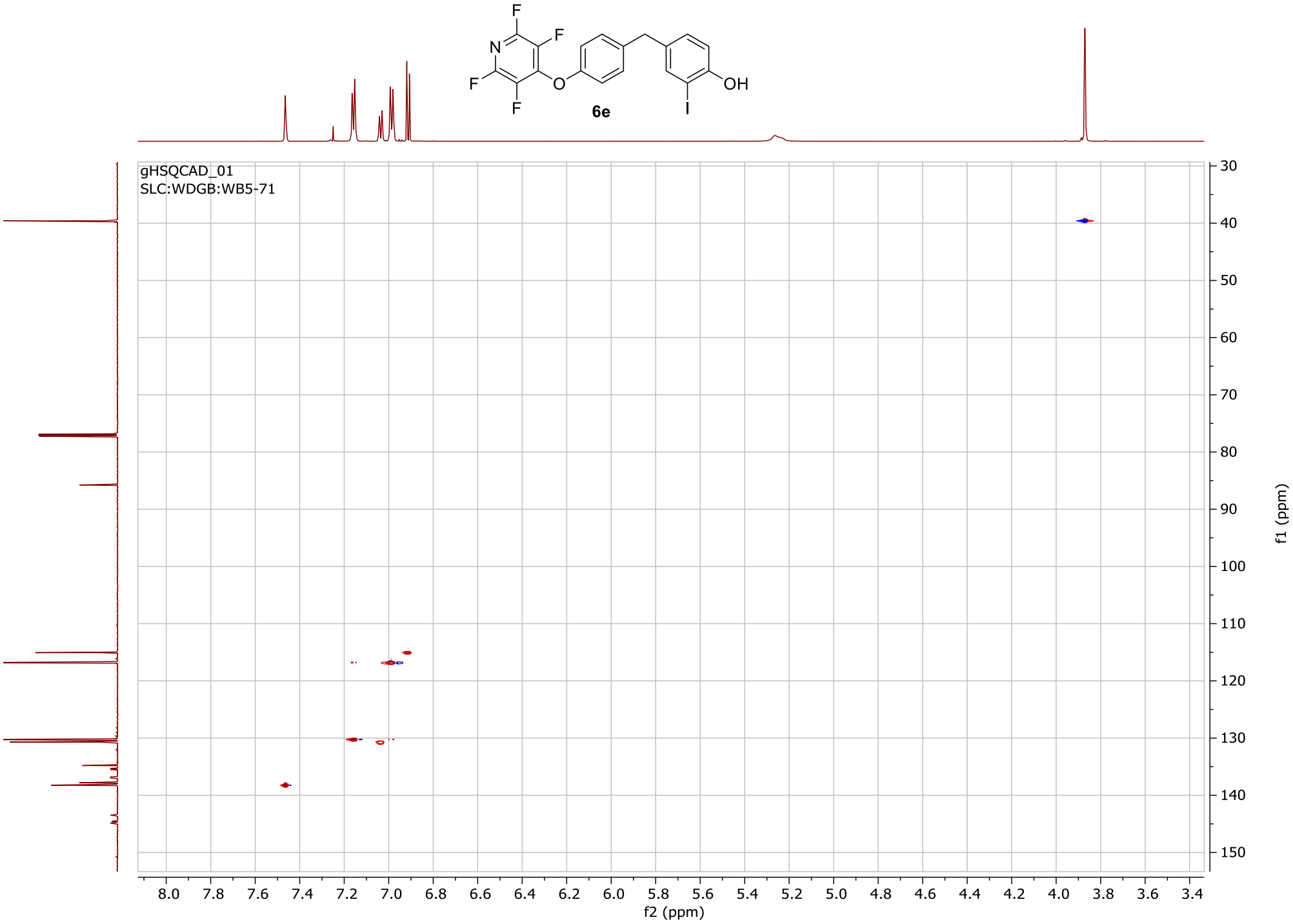
05160212.13.fid
SLC:WDGB:WB5-71

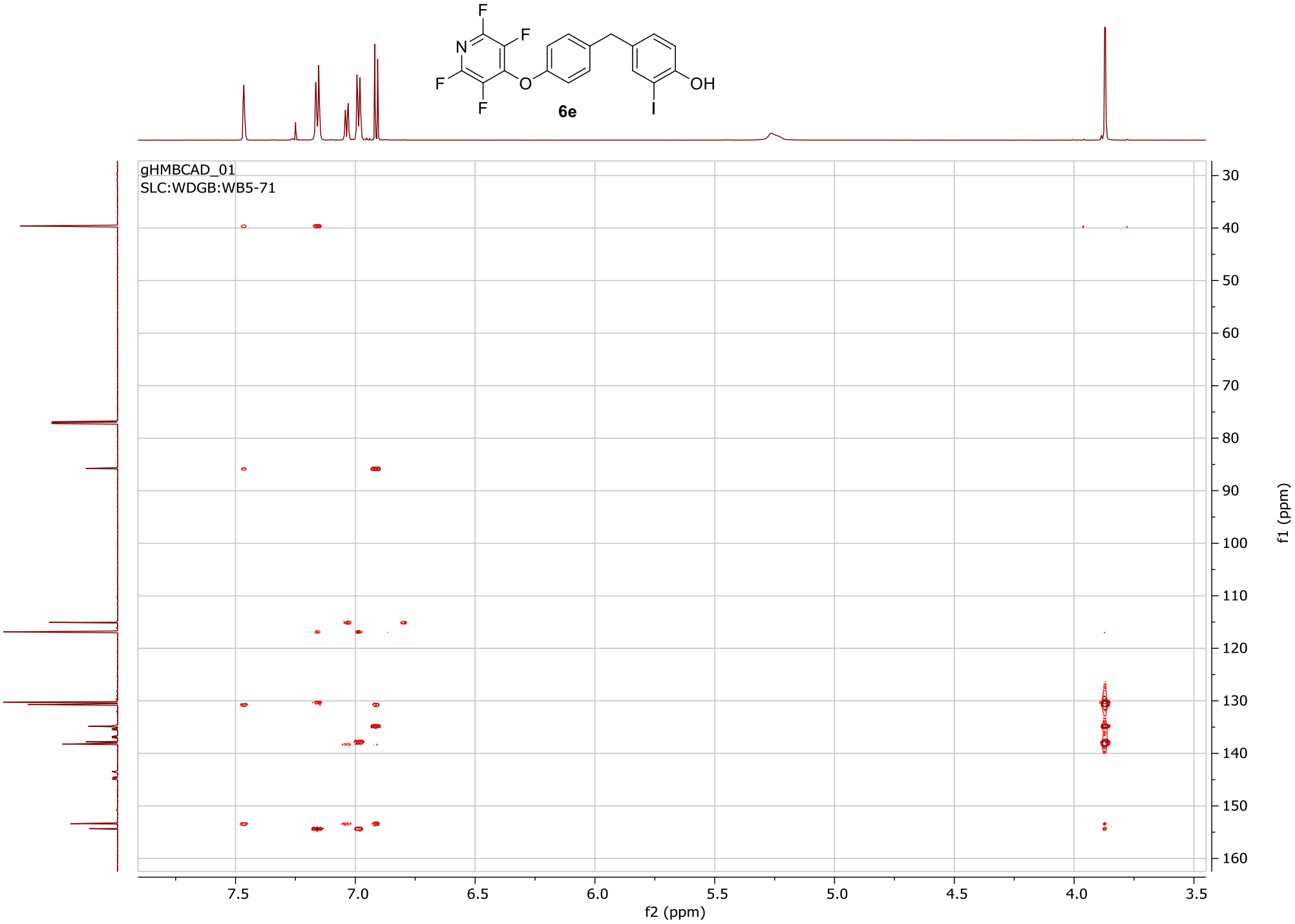


6e

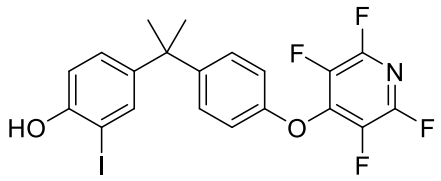

CARBON_01
SLC:WDKG-WB5-174
144.95
144.94
144.86
144.78
144.77
144.63
144.61
144.58
144.55
144.52
144.49
144.46
143.57
143.55
143.47
143.46
143.40
143.38
138.23
137.82
136.99
136.94
136.93
136.84
136.82
136.78
135.50
135.46
135.43
135.35
135.34
135.29
134.81
130.71
130.25
116.84
115.07
85.77
39.59
F
F
N
F
O
OH
F
I
6e
230
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)


F
F
N
F
F
O
OH
I
6e
gCOSY_01
SLC:WDGB:WB5-71
f2 (ppm)
f1 (ppm)


F
F
N
F
F
O
OH
I
6e
gHSQCAD_01
SLC:WDGB:WB5-71
f1 (ppm)
f2 (ppm)
30
40
50
60
70
80
90
100
110
120
130
140
150
8.0
7.8
7.6
7.4
7.2
7.0
6.8
6.6
6.4
6.2
6.0
5.8
5.6
5.4
5.2
5.0
4.8
4.6
4.4
4.2
4.0
3.8
3.6
3.4

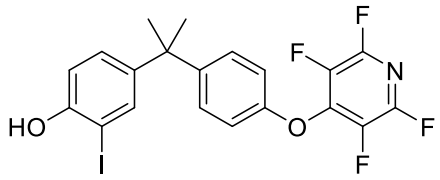

F
F
N
F
F
O
OH
I
6e
gHMBCAD_01
SLC:WDGB:WB5-71
30
40
50
60
70
80
90
100
110
120
130
140
150
160
f1 (ppm)
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
f2 (ppm)

PROTON_01
SLC:WB:WB5-13

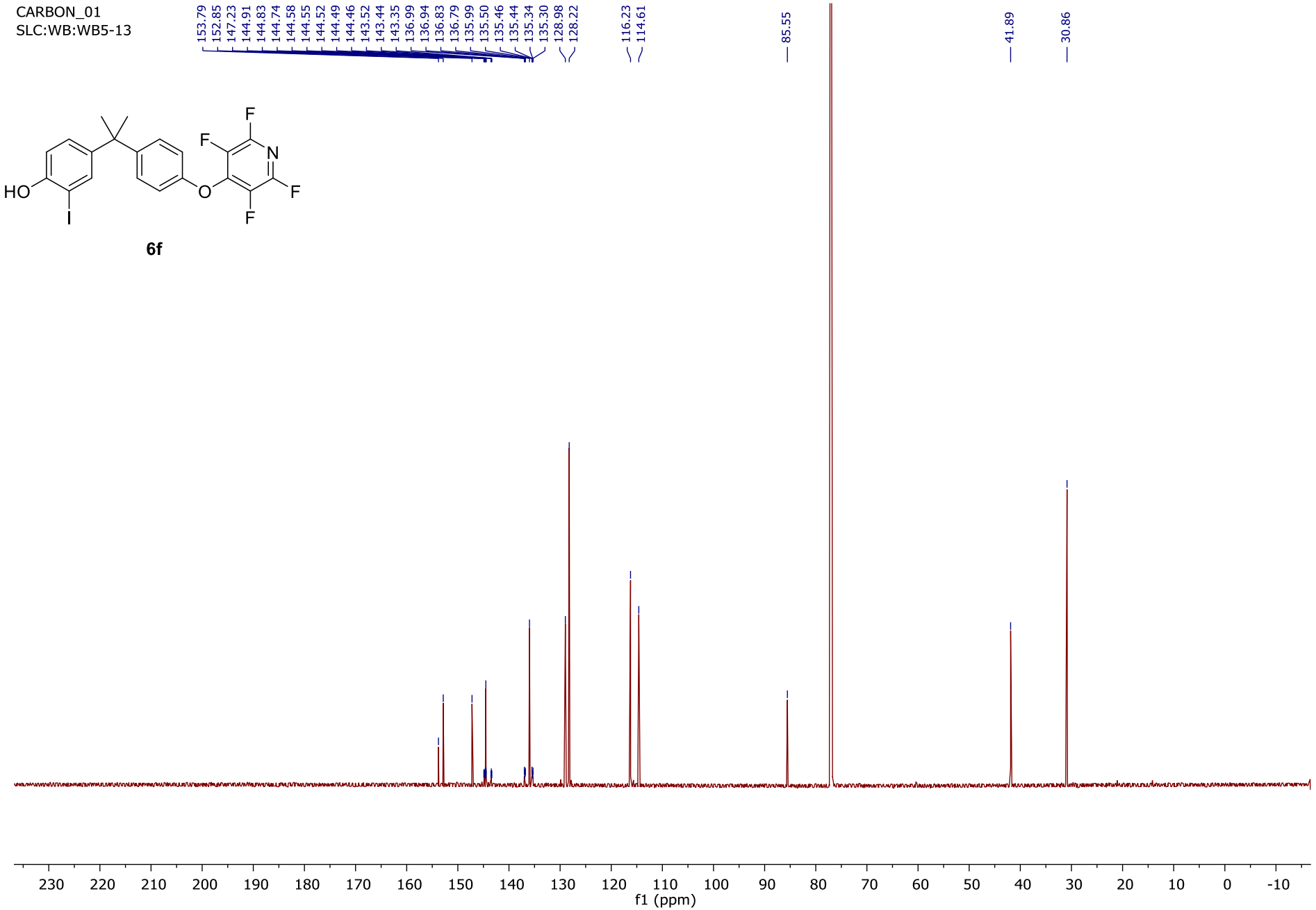


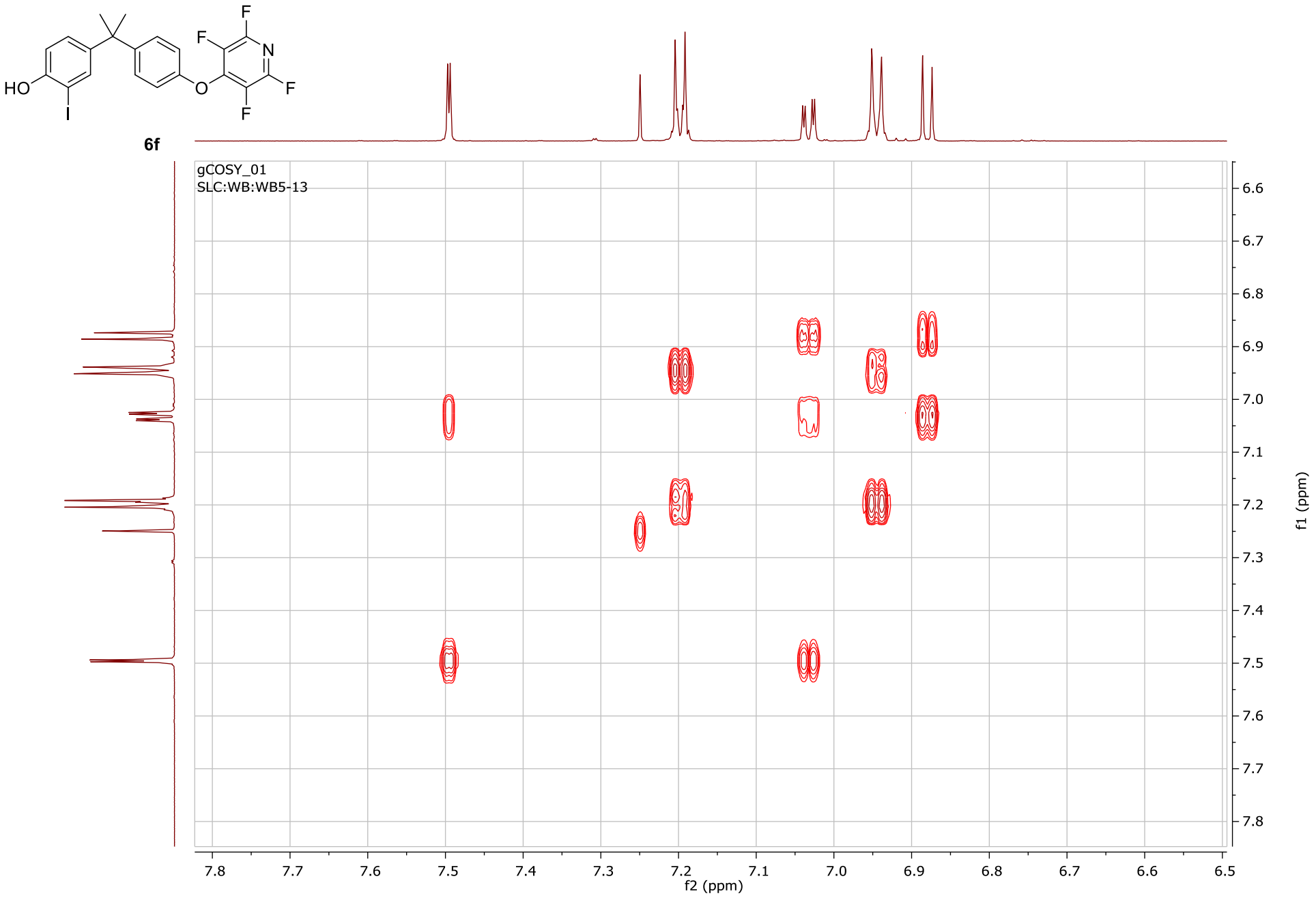
6f

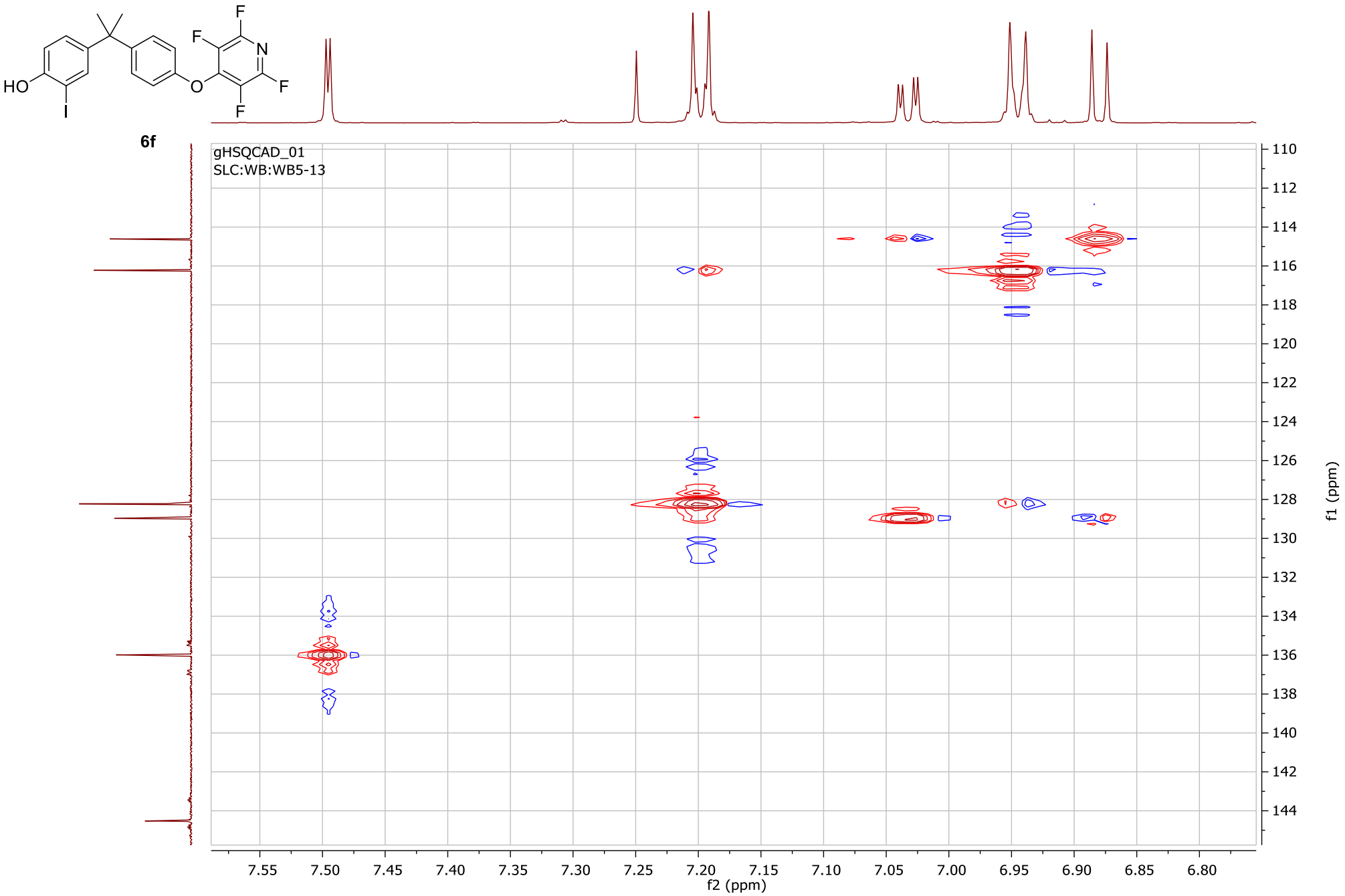
12121631.13.fid
SLC:WDGB:WB5-13 F10-14

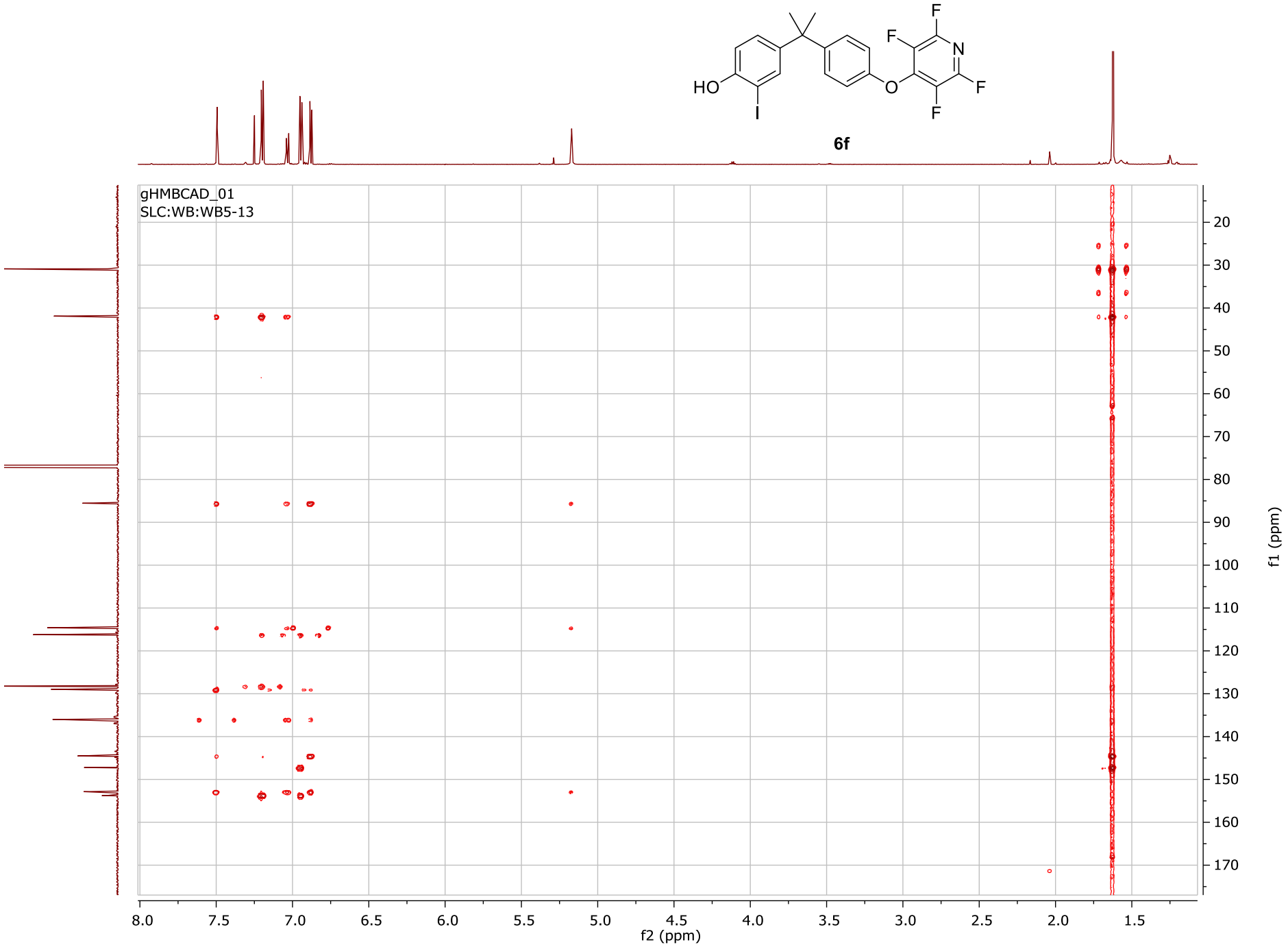


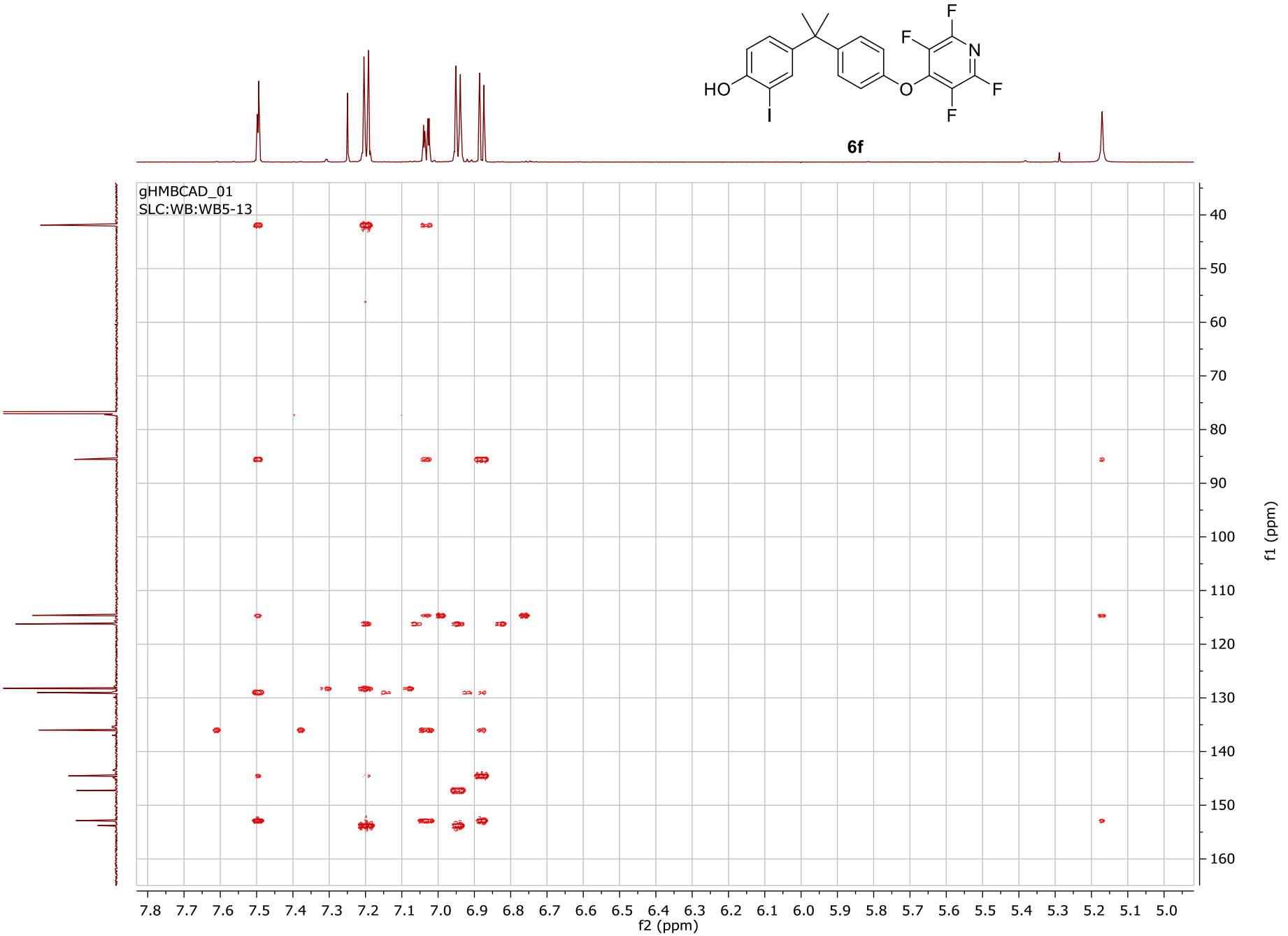
6f


CARBON_01
SLC:WB:WB5-13
153.79
152.85
147.23
144.91
144.83
144.74
144.58
144.55
144.52
144.49
144.46
143.52
143.44
143.35
136.99
136.94
136.83
136.79
135.99
135.50
135.46
135.44
135.34
135.30
128.98
128.22
116.23
114.61
85.55
41.89
30.86
HO
I
O
N
F
F
F
F
6f
230
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)

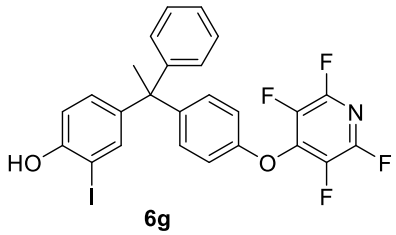

HO
I
O
F
F
F
N
F
6f
gCOSY_01
SLC:WB:WB5-13
f2 (ppm)
f1 (ppm)
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
6.6
6.5


HO
I
O
F
F
F
N
F
6f
gHSQCAD_01
SLC:WB:WB5-13
7.55
7.50
7.45
7.40
7.35
7.30
7.25
7.20
7.15
7.10
7.05
7.00
6.95
6.90
6.85
6.80
f2 (ppm)
110
112
114
116
118
120
122
124
126
128
130
132
134
136
138
140
142
144
f1 (ppm)


HO
I
O
F
F
N
F
F
6f
gHMBCAD_01
SLC:WB:WB5-13
f2 (ppm)
f1 (ppm)

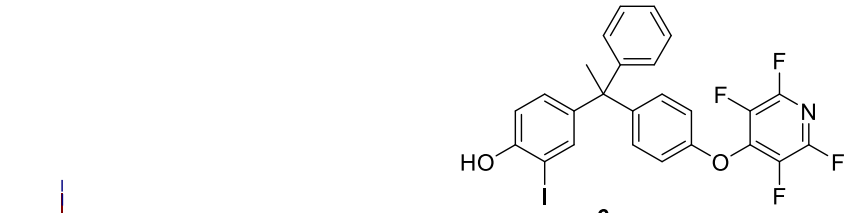

gHMBCAD_01
SLC:WB:WB5-13
HO
I
O
F
F
F
F
N
6f
f2 (ppm)
f1 (ppm)

PROTON_01
SLC:WB:WB5-29

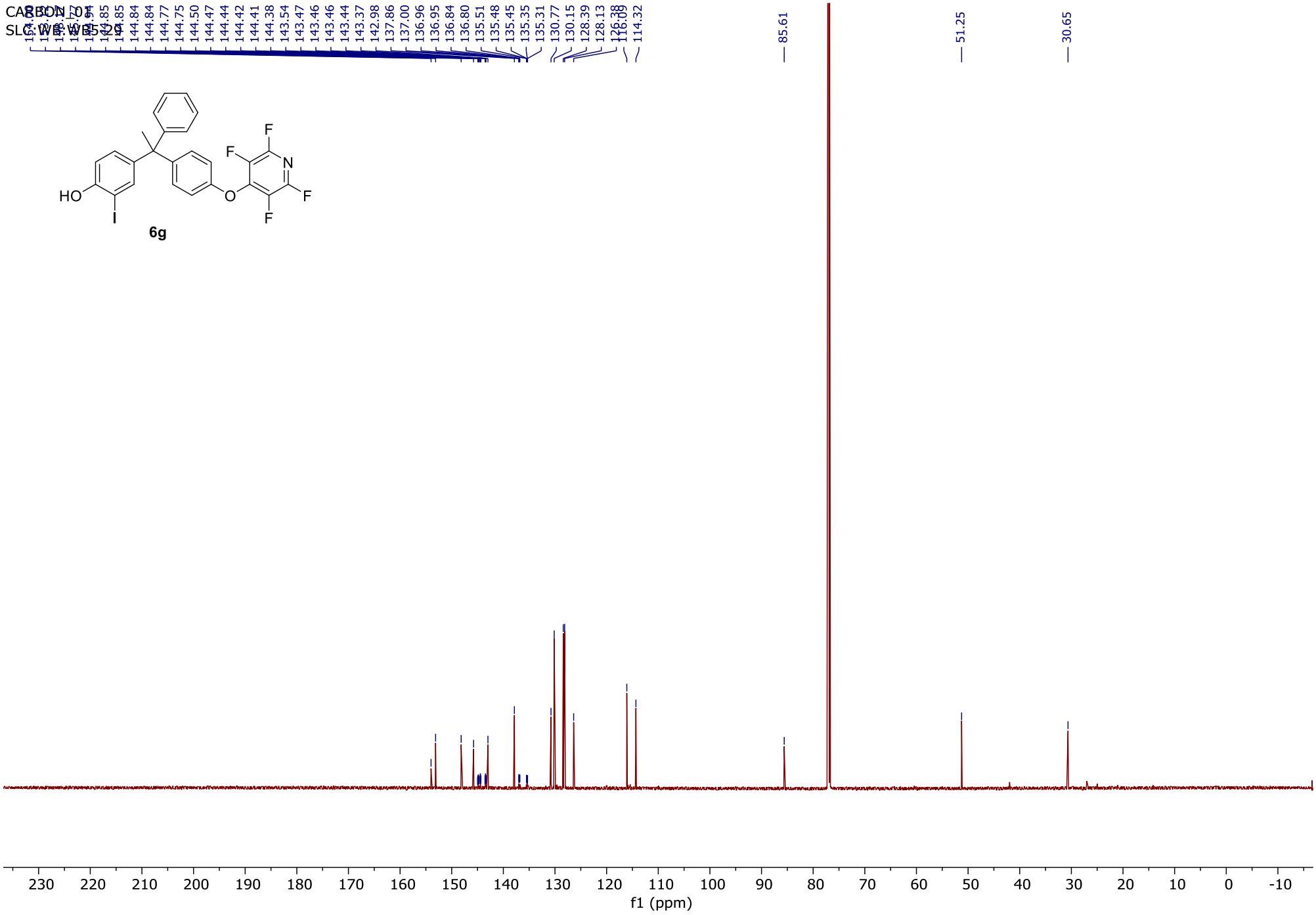


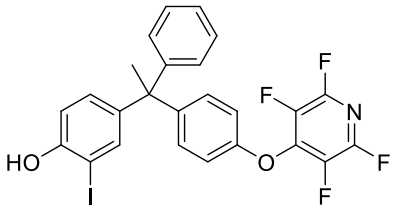
6g

28092913.13.fid
SLC:WDGB:WB-29



6g


CARBON_01
SLC_09_WB_5_20
HO
I
O
F
F
N
F
F
6g
85.61
51.25
30.65
f1 (ppm)

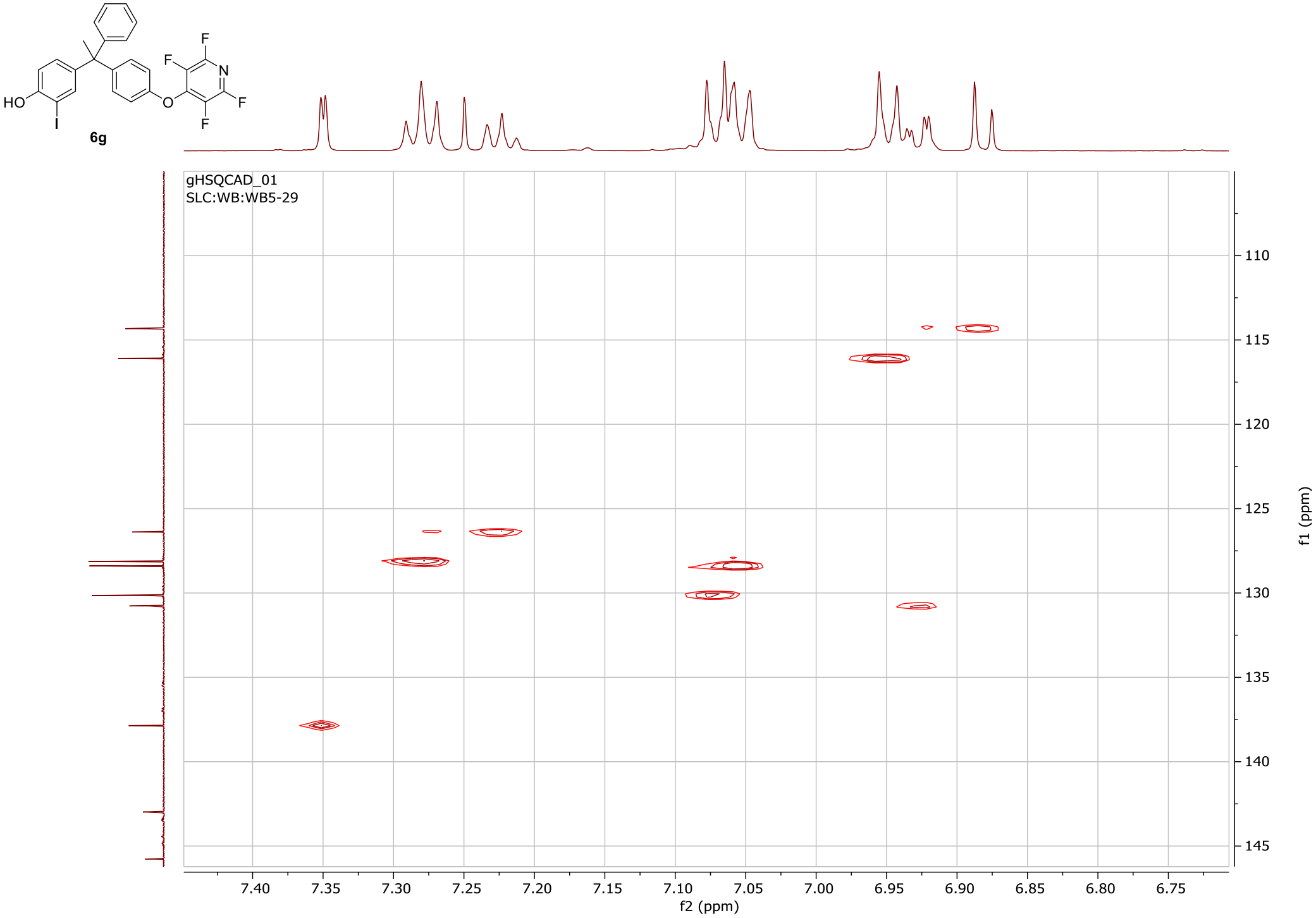


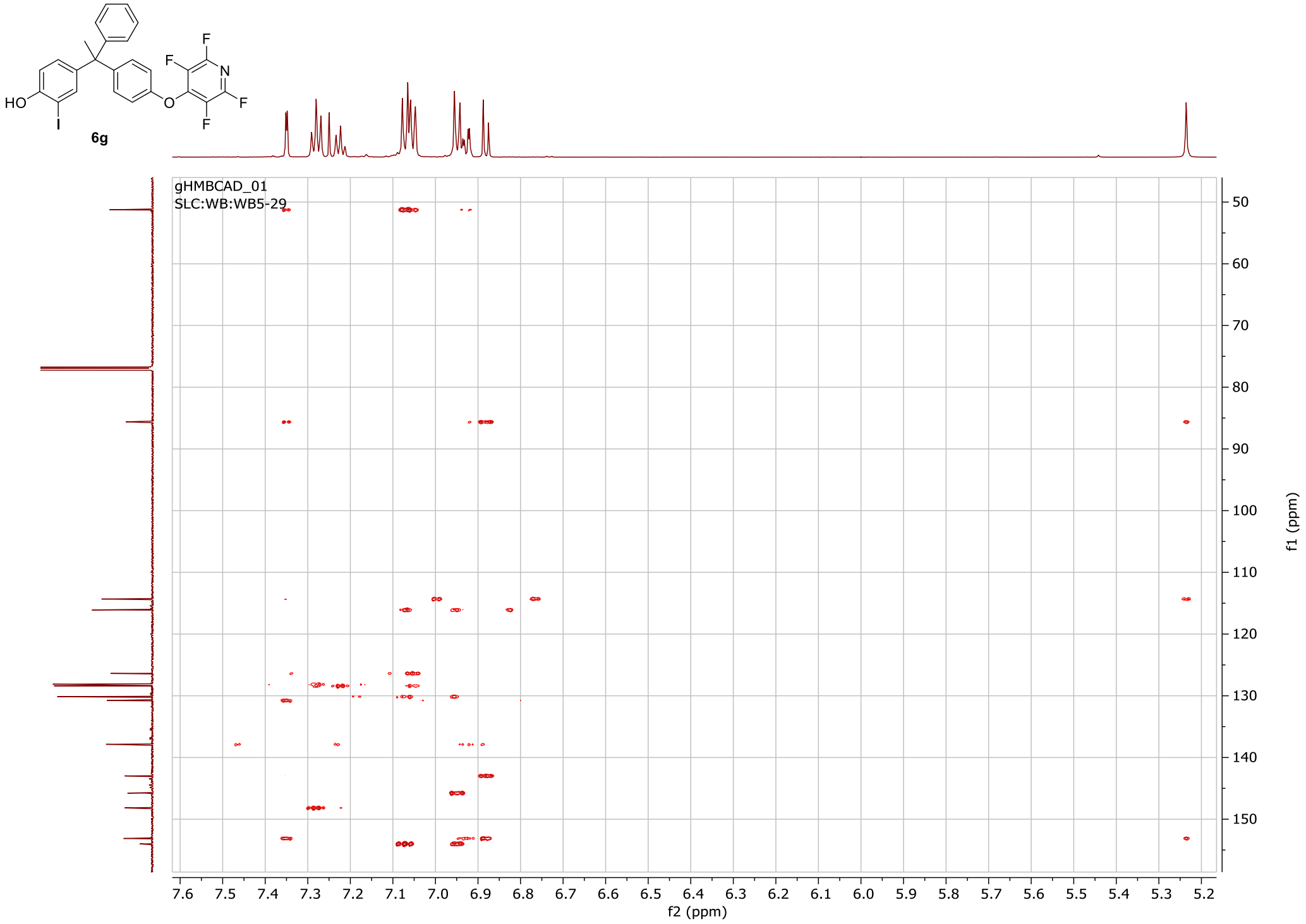
6g

gCOSY_01
SLC:WB:WB5-29

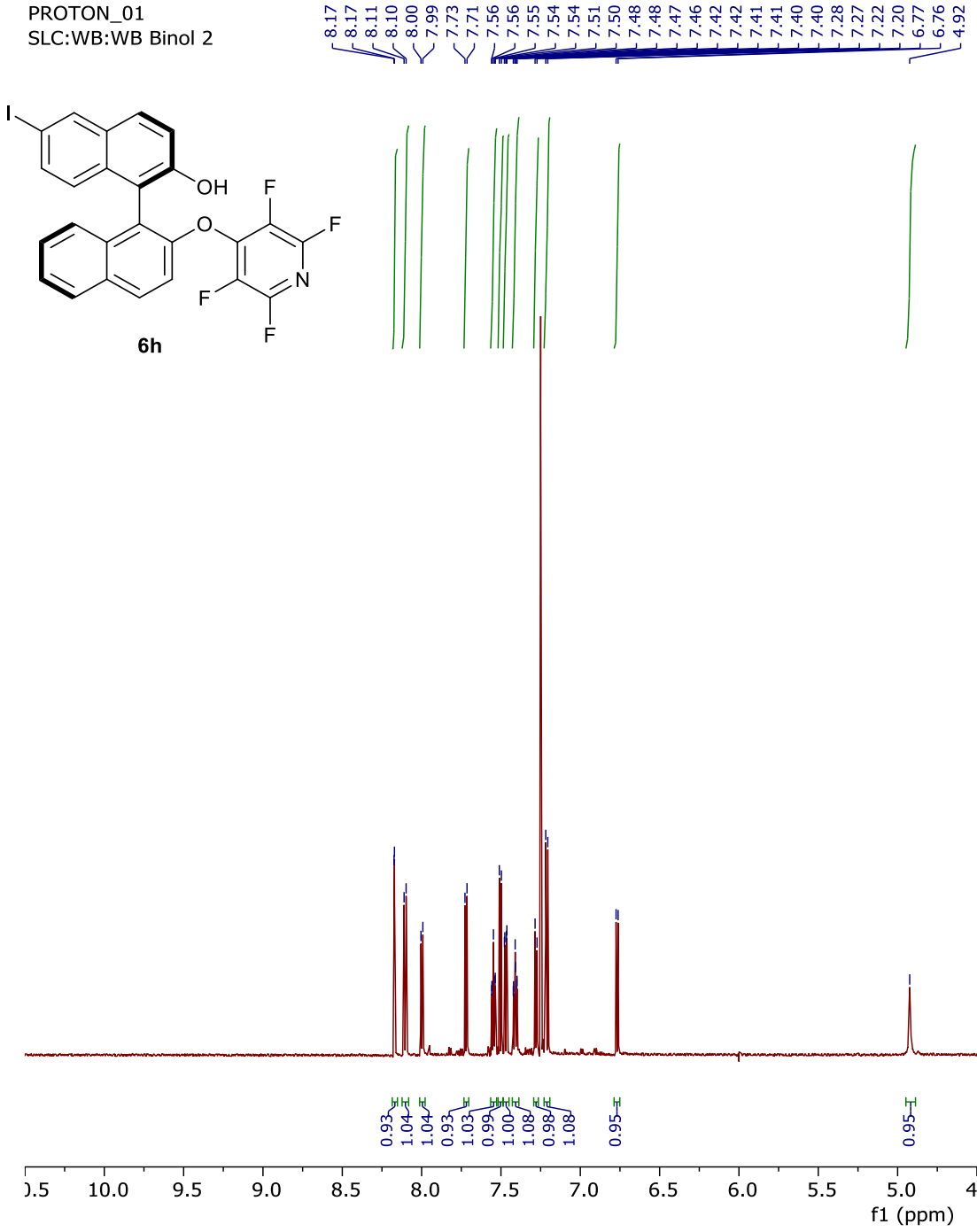
f2 (ppm)

f1 (ppm)


HO
I
O
F
F
N
F
F
6g
gHSQCAD_01
SLC:WB:WB5-29
110
115
120
125
130
135
140
145
f1 (ppm)
7.40
7.35
7.30
7.25
7.20
7.15
7.10
7.05
7.00
6.95
6.90
6.85
6.80
6.75
f2 (ppm)

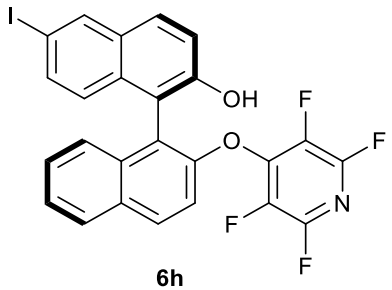

HO
I
F
F
N
O
F
F
6g
gHMBCAD_01
SLC:WB:WB5-29
f2 (ppm)
f1 (ppm)

PROTON_01
SLC:WB:WB Binol 2



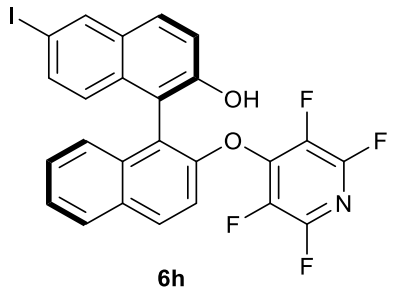
6h

12111058_13.fid
SLC:WDGB-WB-BINOL PREP 2

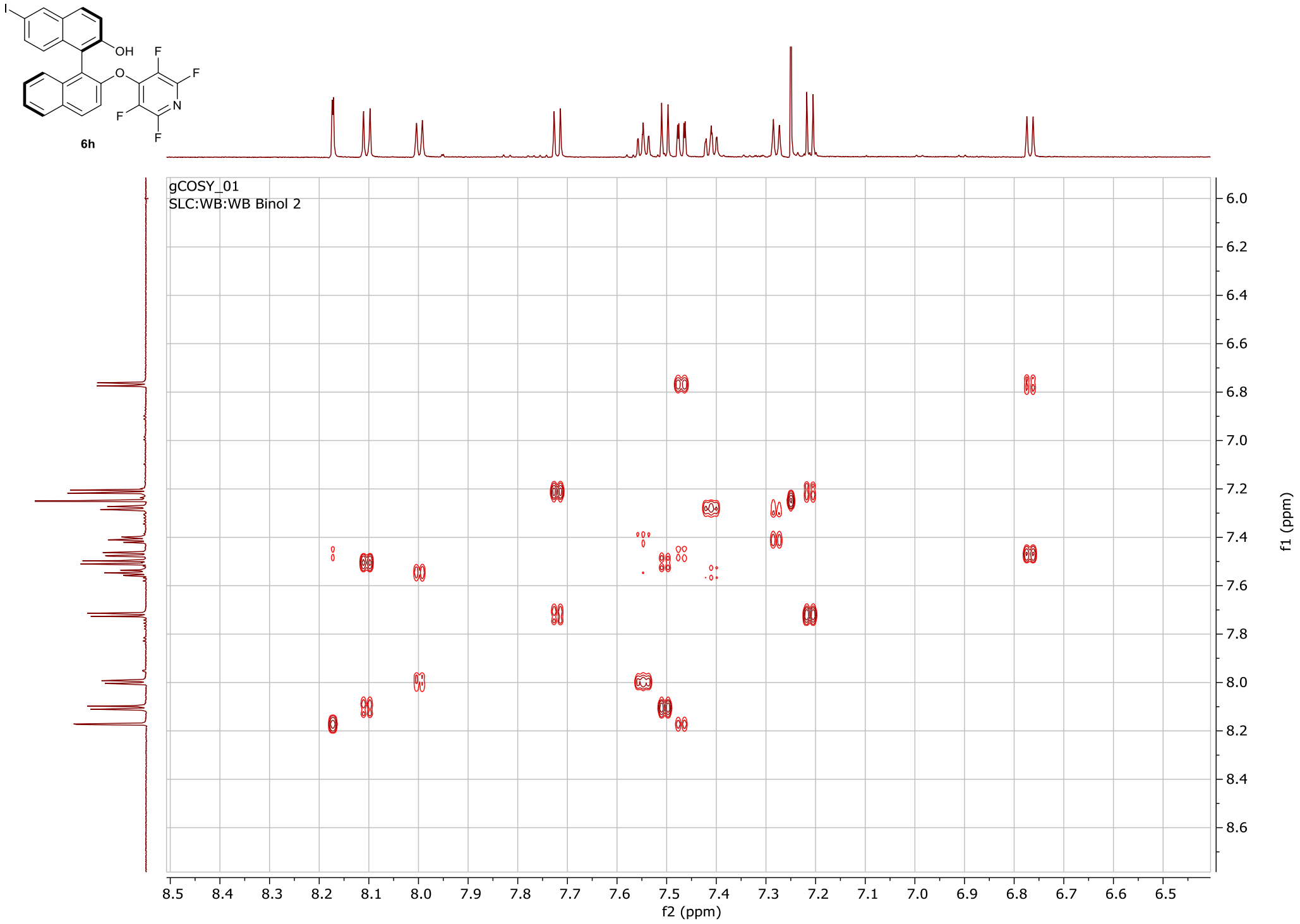


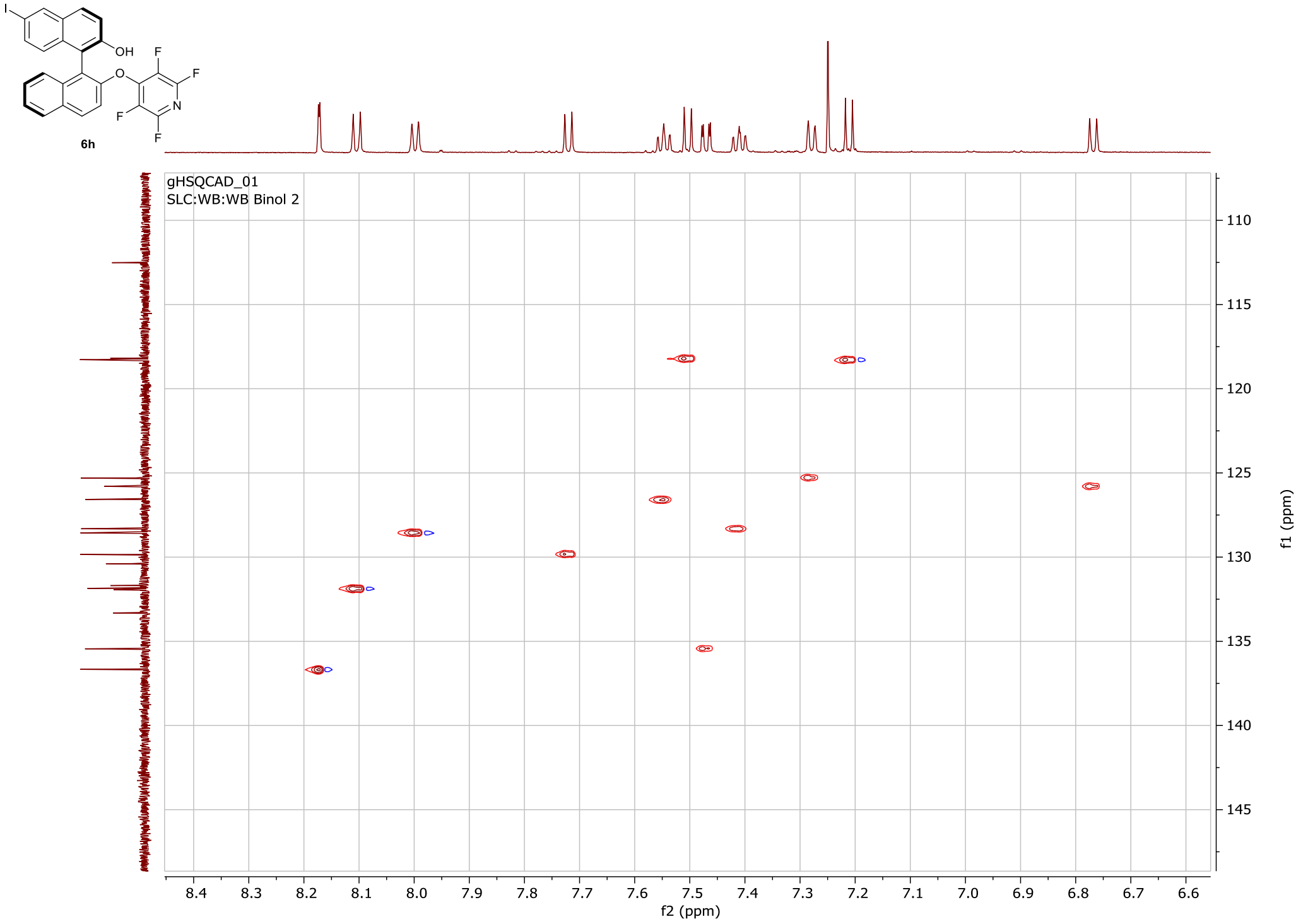
6h

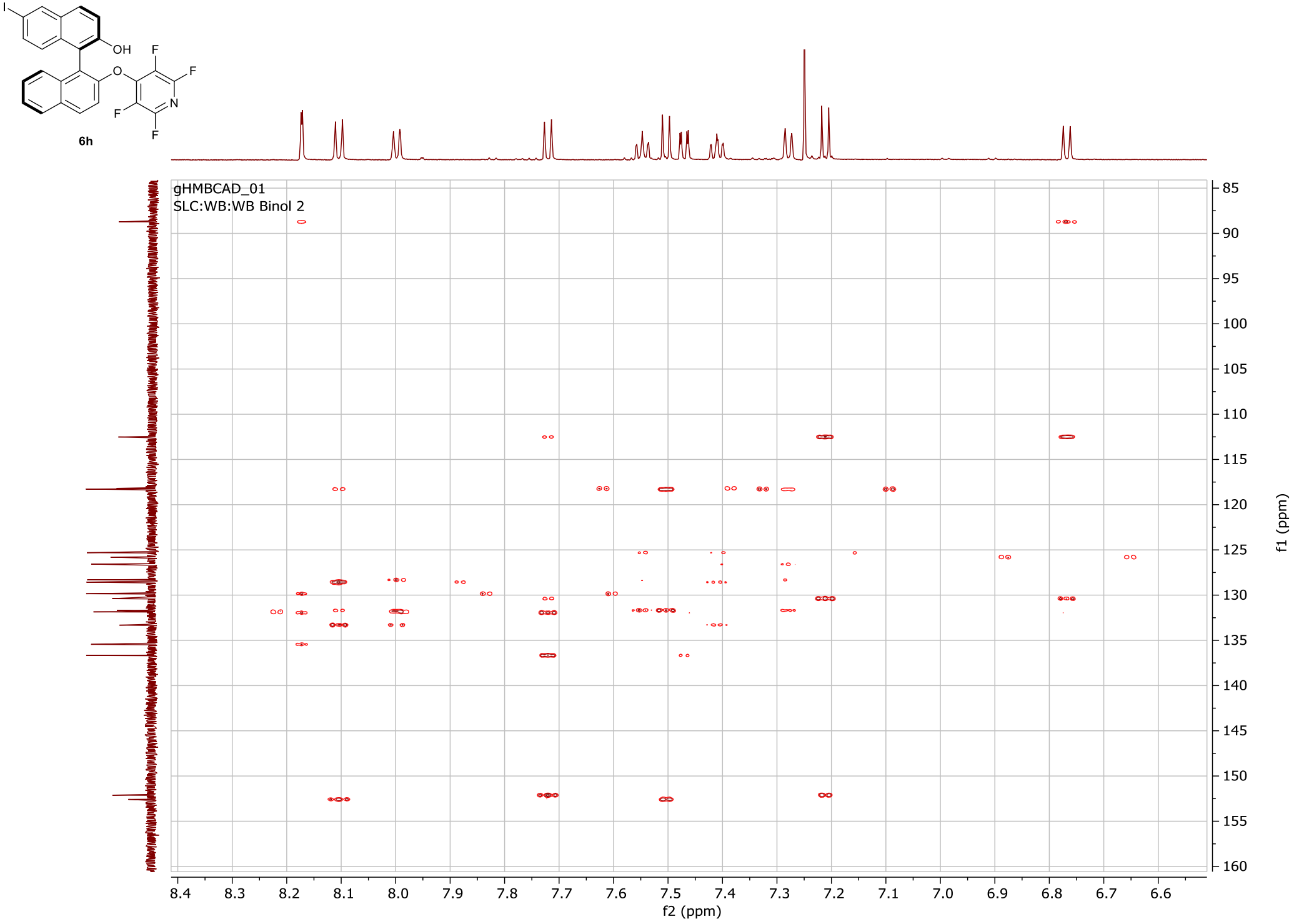
CARBON_01
SLC:WB:WB Binol 2

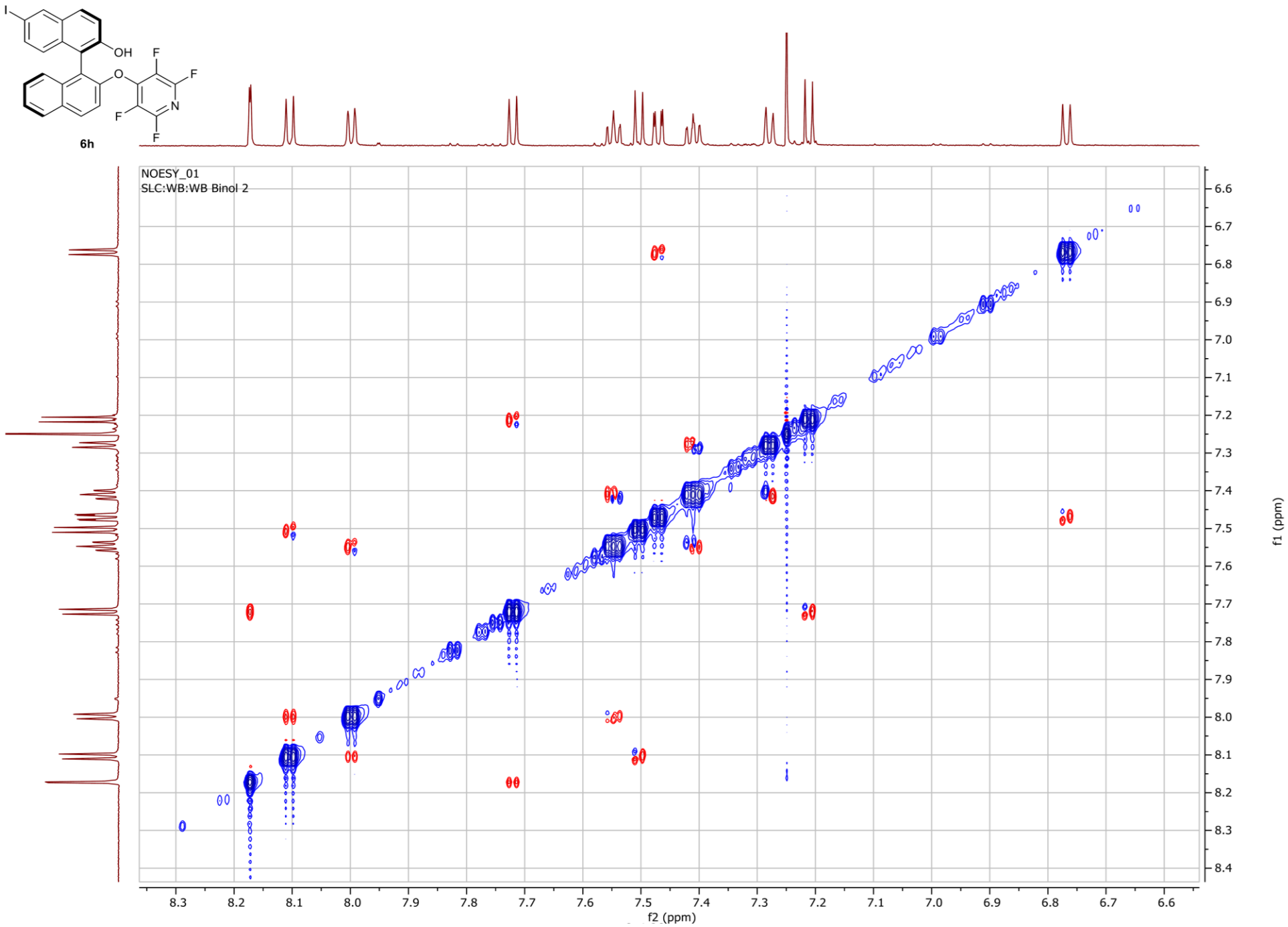


6h

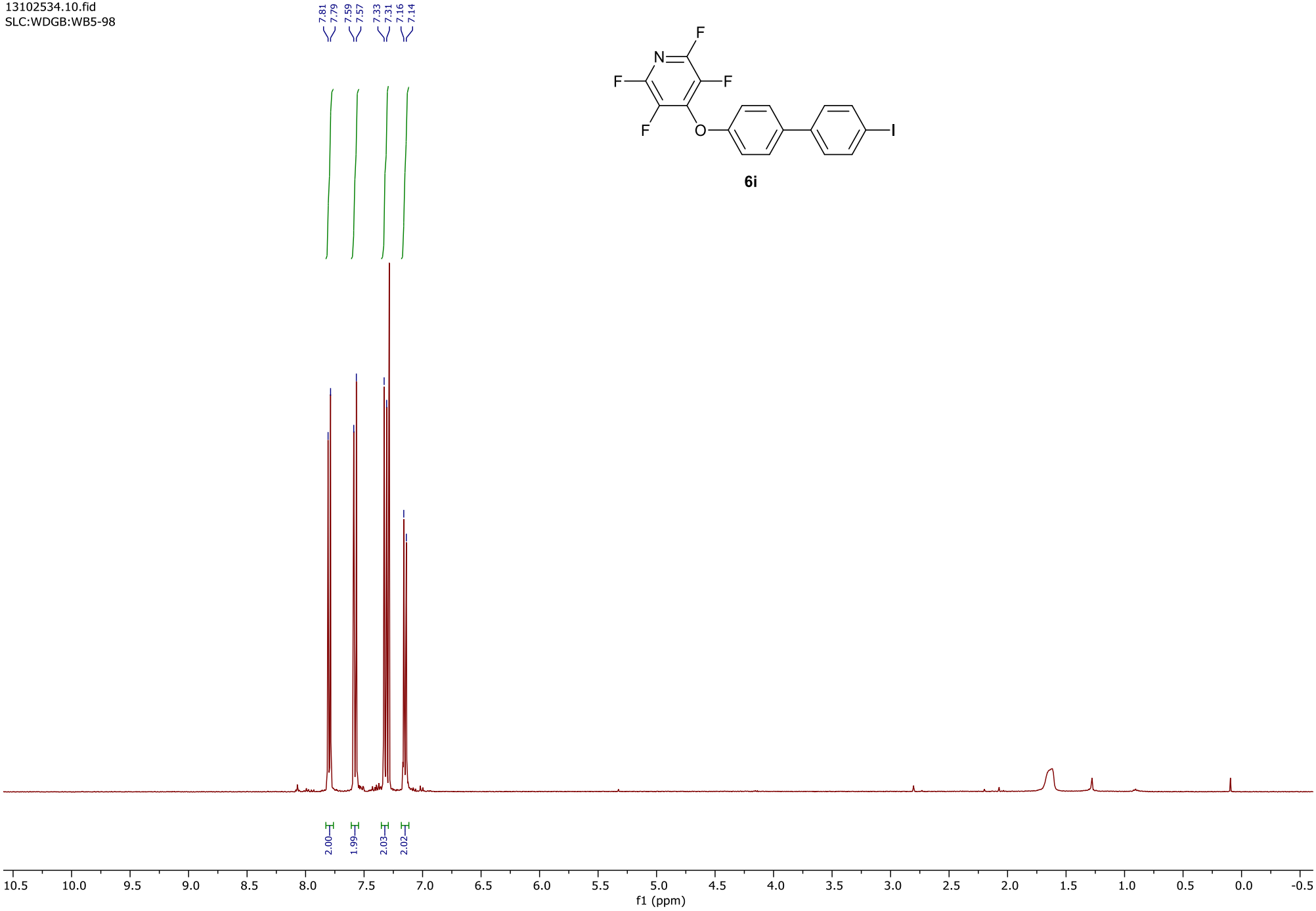

I
OH
O
F
F
F
F
N
6h
gCOSY_01
SLC:WB:WB Binol 2
8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5
f2 (ppm)
6.0 6.2 6.4 6.6 6.8 7.0 7.2 7.4 7.6 7.8 8.0 8.2 8.4 8.6
f1 (ppm)


6h
gHSQCAD_01
SLC:WB:WB Binol 2
f2 (ppm)
f1 (ppm)

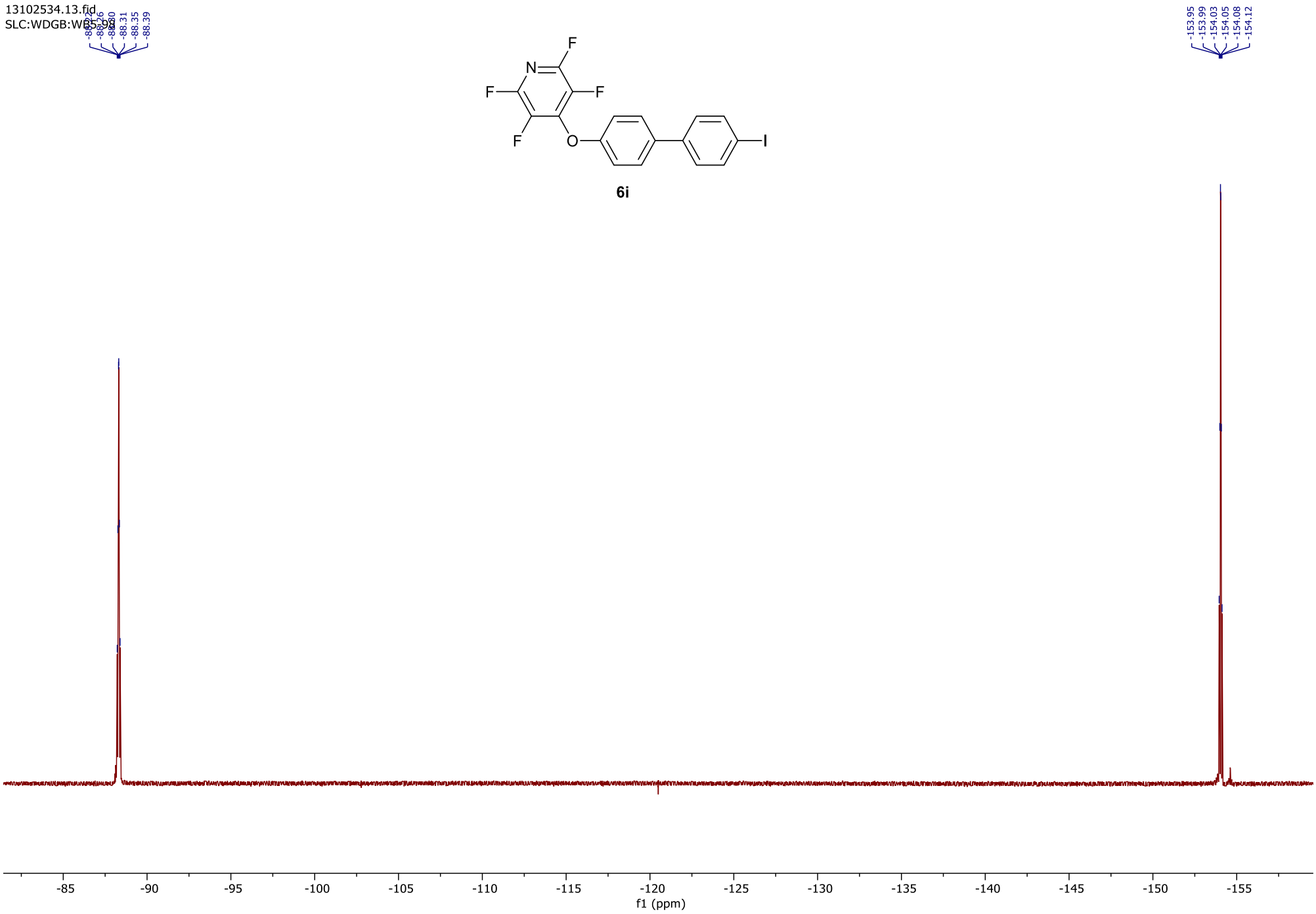

6h
gHMBCAD_01
SLC:WB:WB Binol 2
f2 (ppm)
f1 (ppm)


6h
NOESY_01
SLC:WB:WB Binol 2
f2 (ppm)
f1 (ppm)

13102534.10.fid
SLC:WDGB:WB5-98

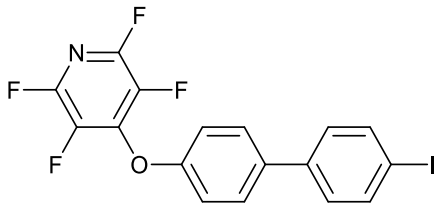


6i

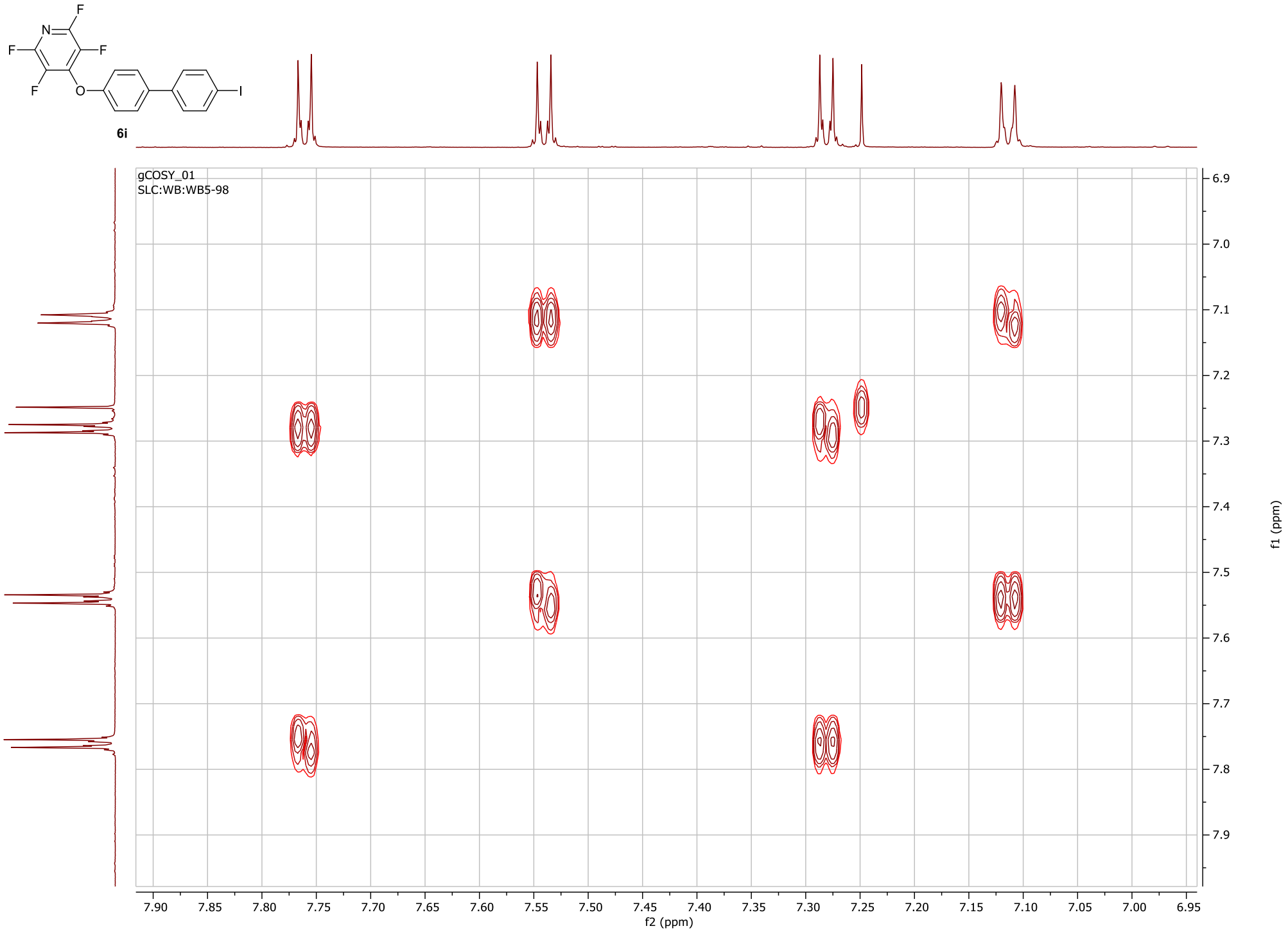

13102534.13.fid
SLC:WDGB:WB5-98
-88.22
-88.26
-88.30
-88.31
-88.35
-88.39
-153.95
-153.99
-154.03
-154.05
-154.08
-154.12
F
N
F
F
F
O
I
-85
-90
-95
-100
-105
-110
-115
-120
-125
-130
-135
-140
-145
-150
-155
f1 (ppm)

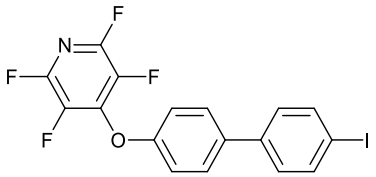
6i

CARBON_01
SLC:WB:WB5-98

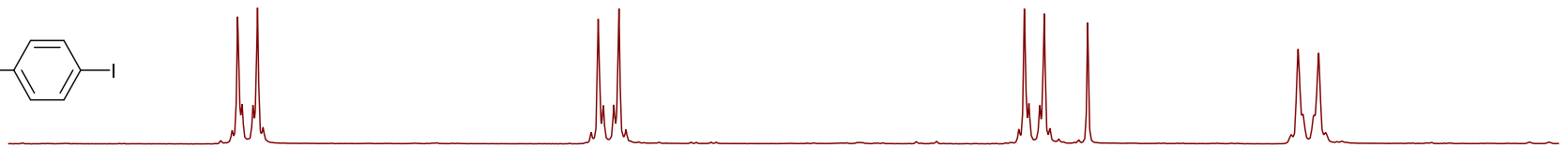


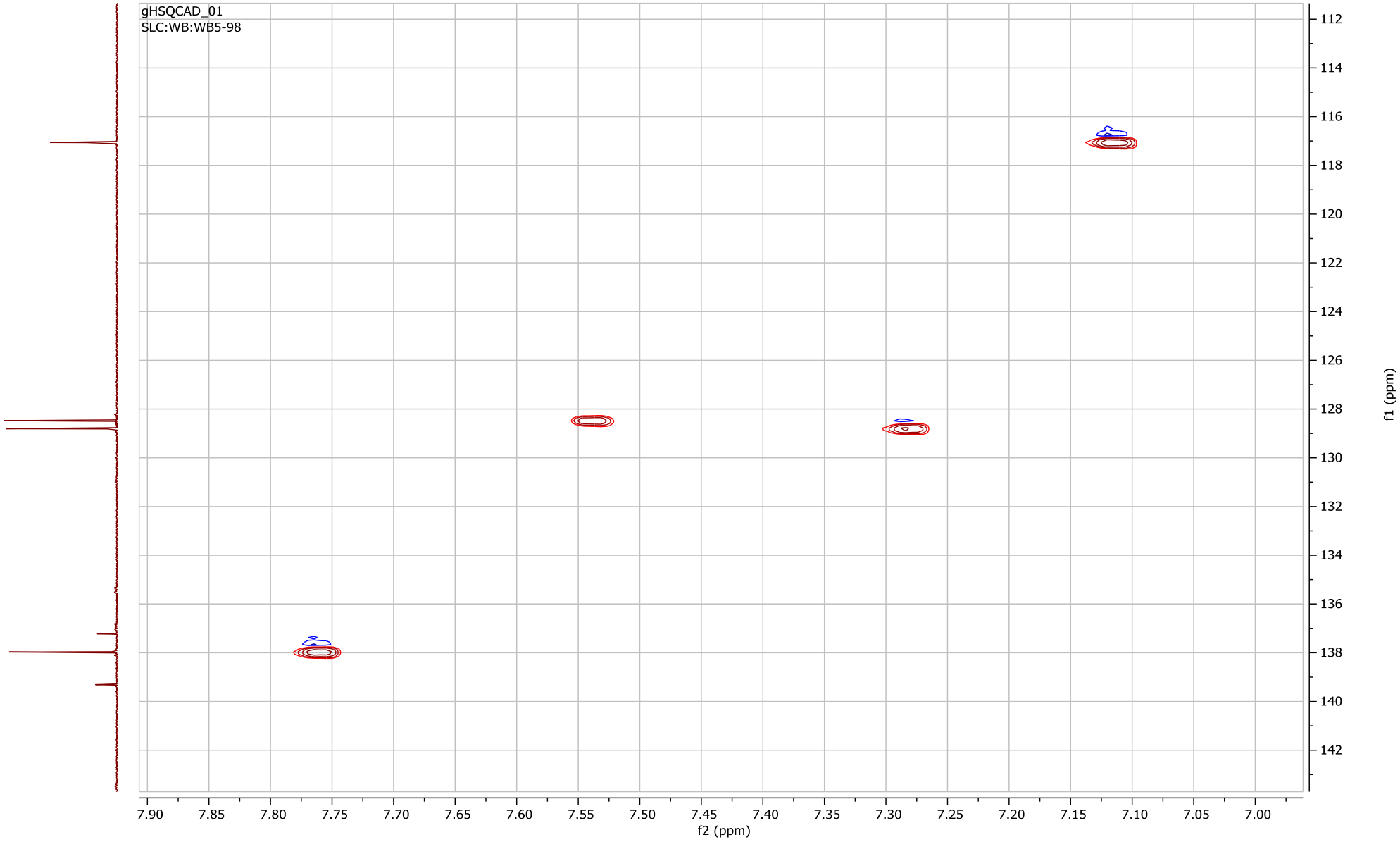
6i

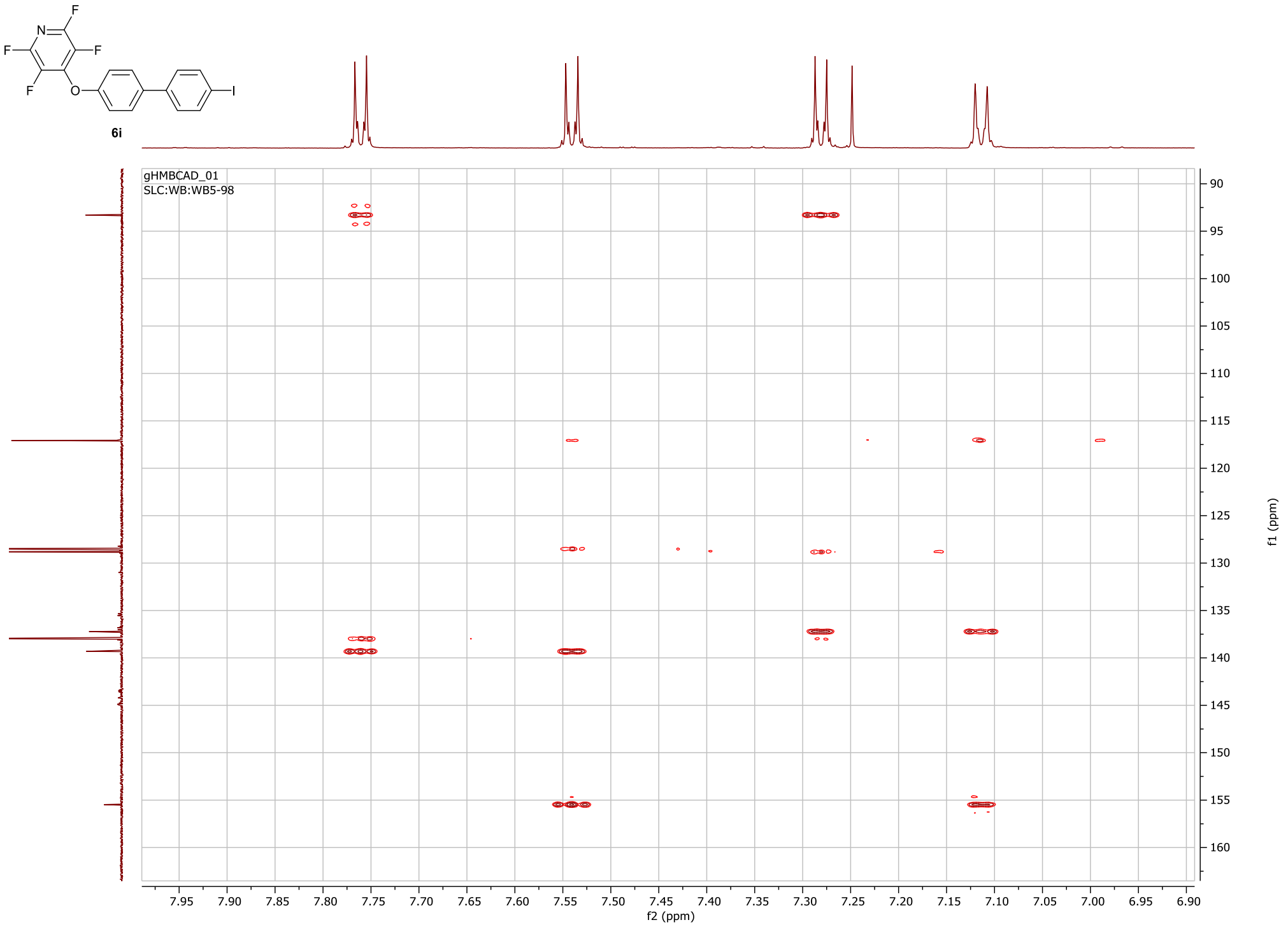

F
N
F
F
F
O
I
6i
gCOSY_01
SLC:WB:WB5-98
7.90
7.85
7.80
7.75
7.70
7.65
7.60
7.55
7.50
7.45
7.40
7.35
7.30
7.25
7.20
7.15
7.10
7.05
7.00
6.95
f2 (ppm)
6.9
7.0
7.1
7.2
7.3
7.4
7.5
7.6
7.7
7.8
7.9
f1 (ppm)


F
N
F
F
F
O
I

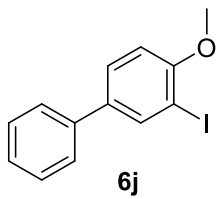
6i




gHSQCAD_01
SLC:WB:WB5-98
112
114
116
118
120
122
124
126
128
130
132
134
136
138
140
142
f1 (ppm)
7.90
7.85
7.80
7.75
7.70
7.65
7.60
7.55
7.50
7.45
7.40
7.35
7.30
7.25
7.20
7.15
7.10
7.05
7.00
f2 (ppm)


F
N
F
F
F
O
I
6i
gHMBCAD_01
SLC:WB:WB5-98
90
95
100
105
110
115
120
125
130
135
140
145
150
155
160
f1 (ppm)
7.95
7.90
7.85
7.80
7.75
7.70
7.65
7.60
7.55
7.50
7.45
7.40
7.35
7.30
7.25
7.20
7.15
7.10
7.05
7.00
6.95
6.90
f2 (ppm)

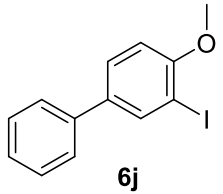
11112615.10.fid
SLC:WDGB:WB6-102 F1-8
Proton.dur CDCl3 /home/nmr/localdata walkup 14



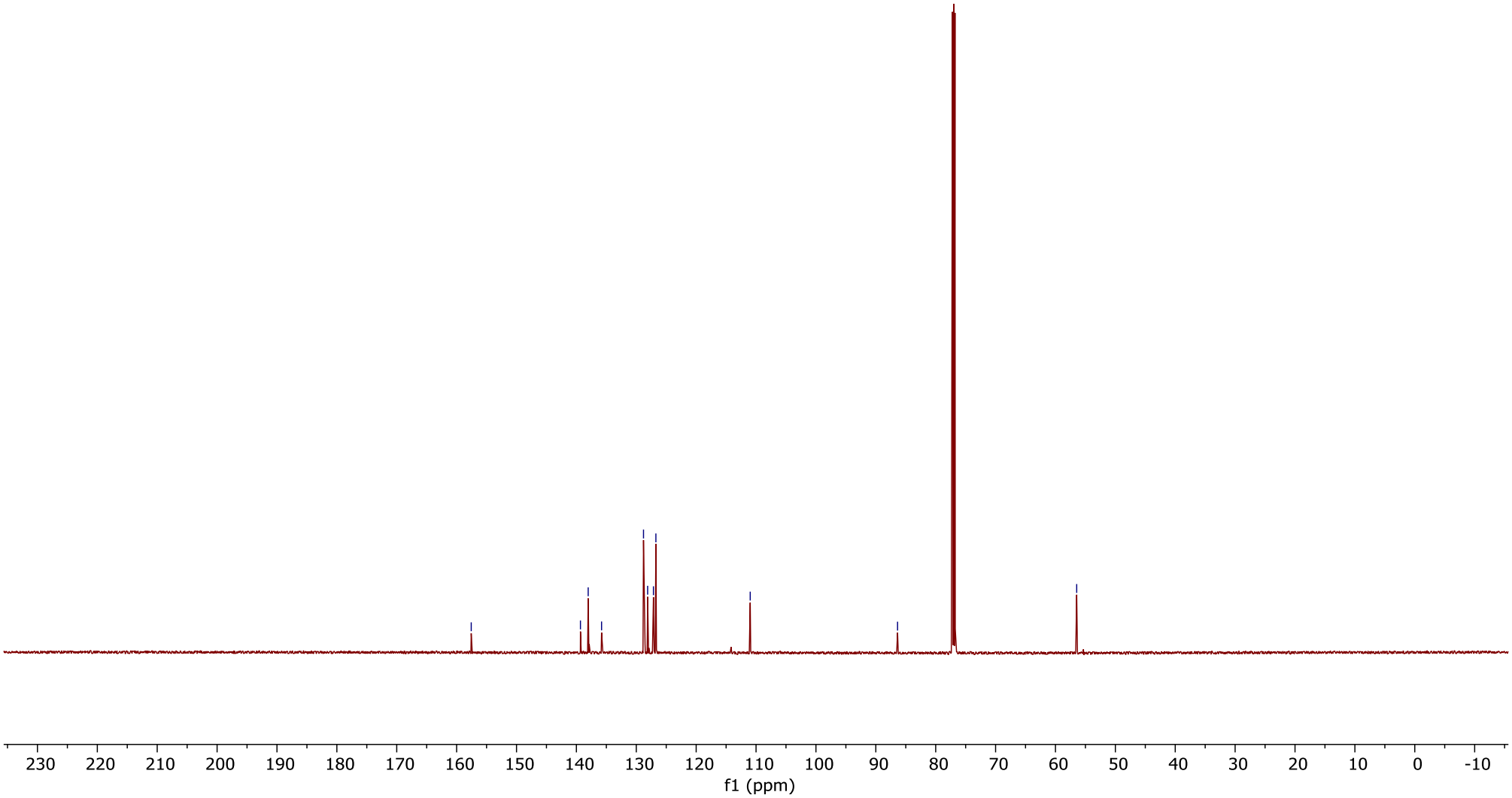
6j

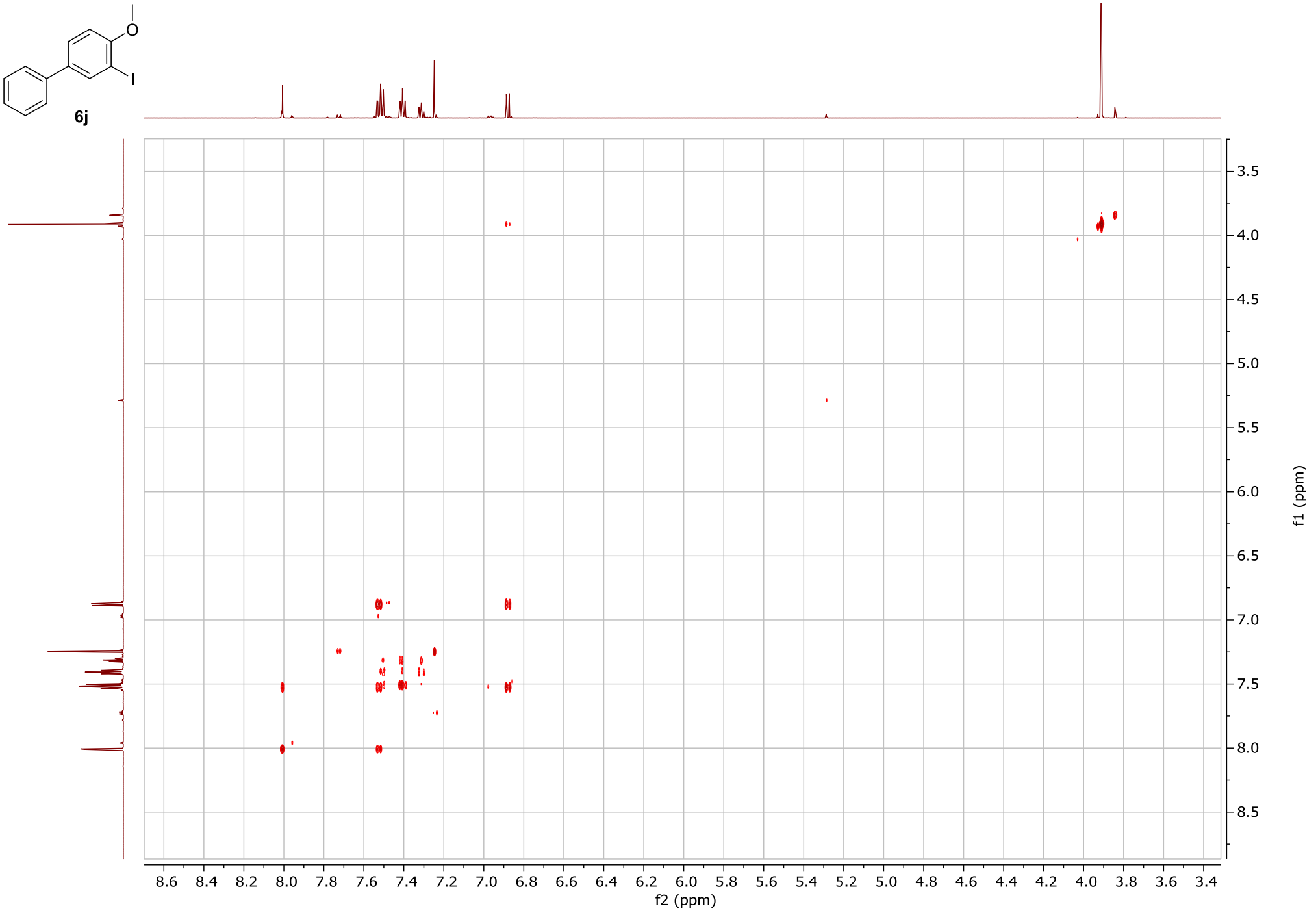
CARBON_01
SLC:WB:WB 6-102

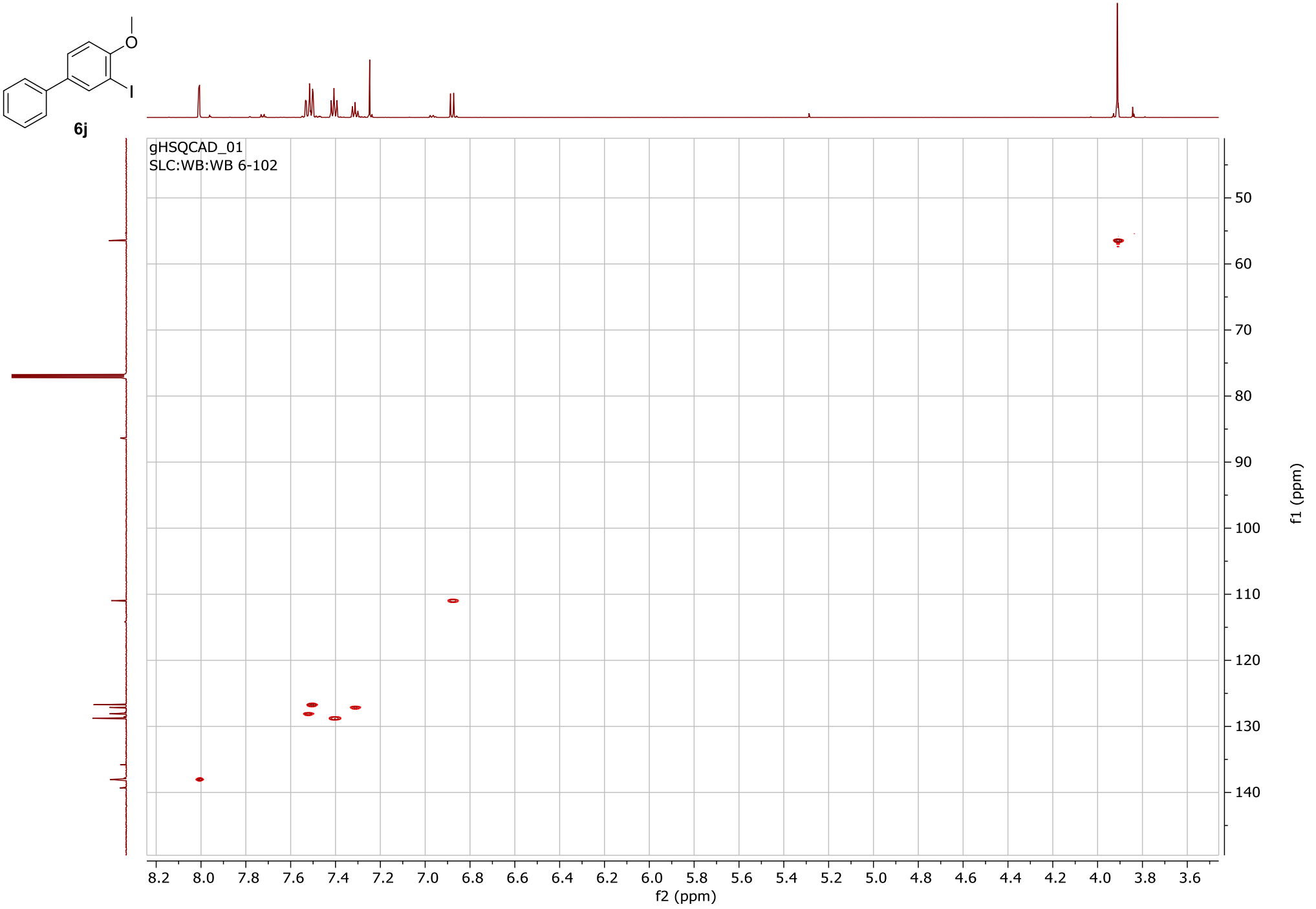
157.56
139.32
138.03
135.80
128.79
128.10
127.13
126.73
110.97
86.37
56.46

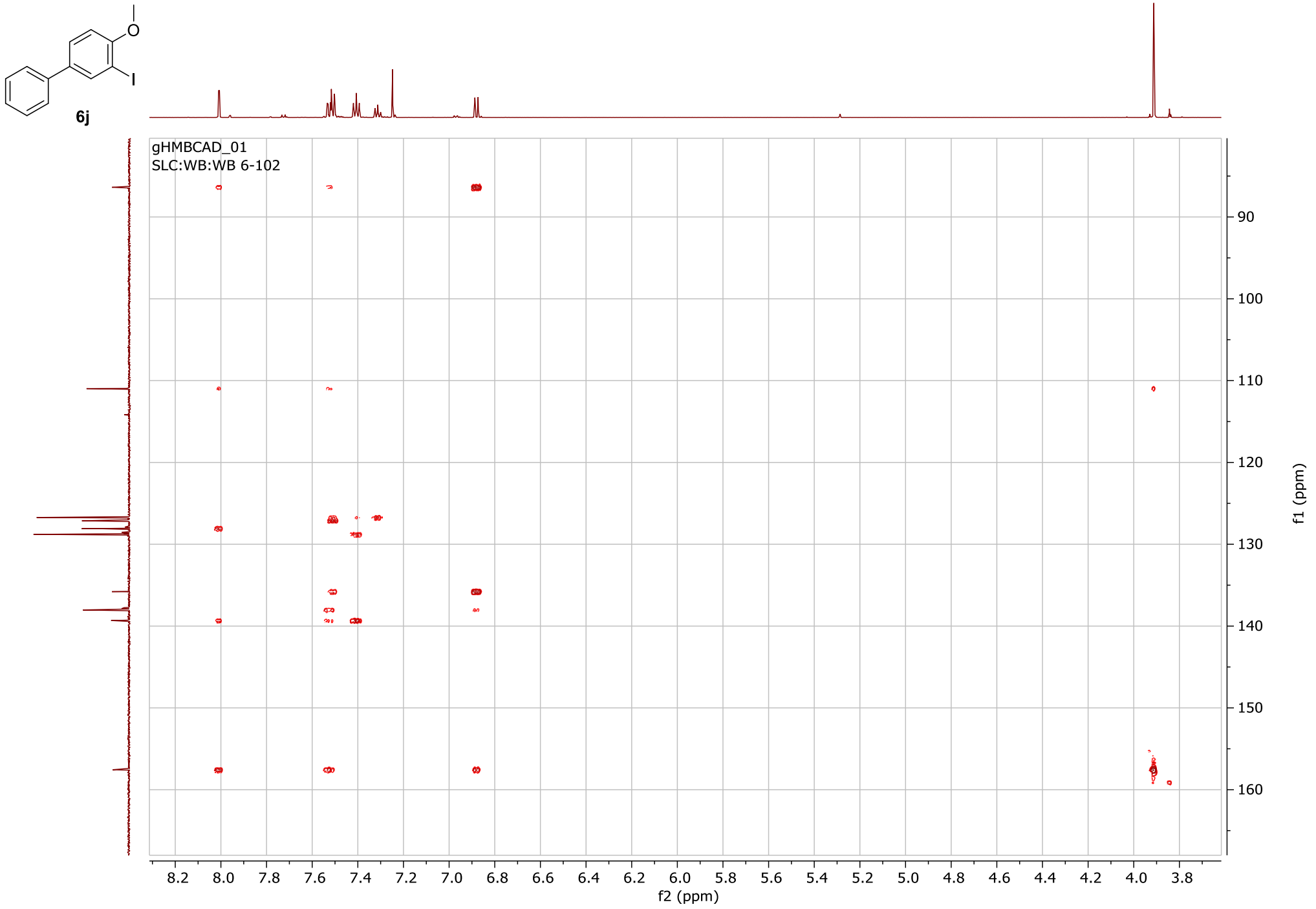


6j

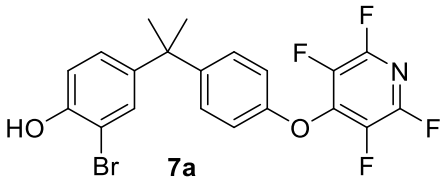



O
I
6j
8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4
f2 (ppm)
3.5 4.0 4.5 5.0 5.5 6.0 6.5 7.0 7.5 8.0 8.5
f1 (ppm)

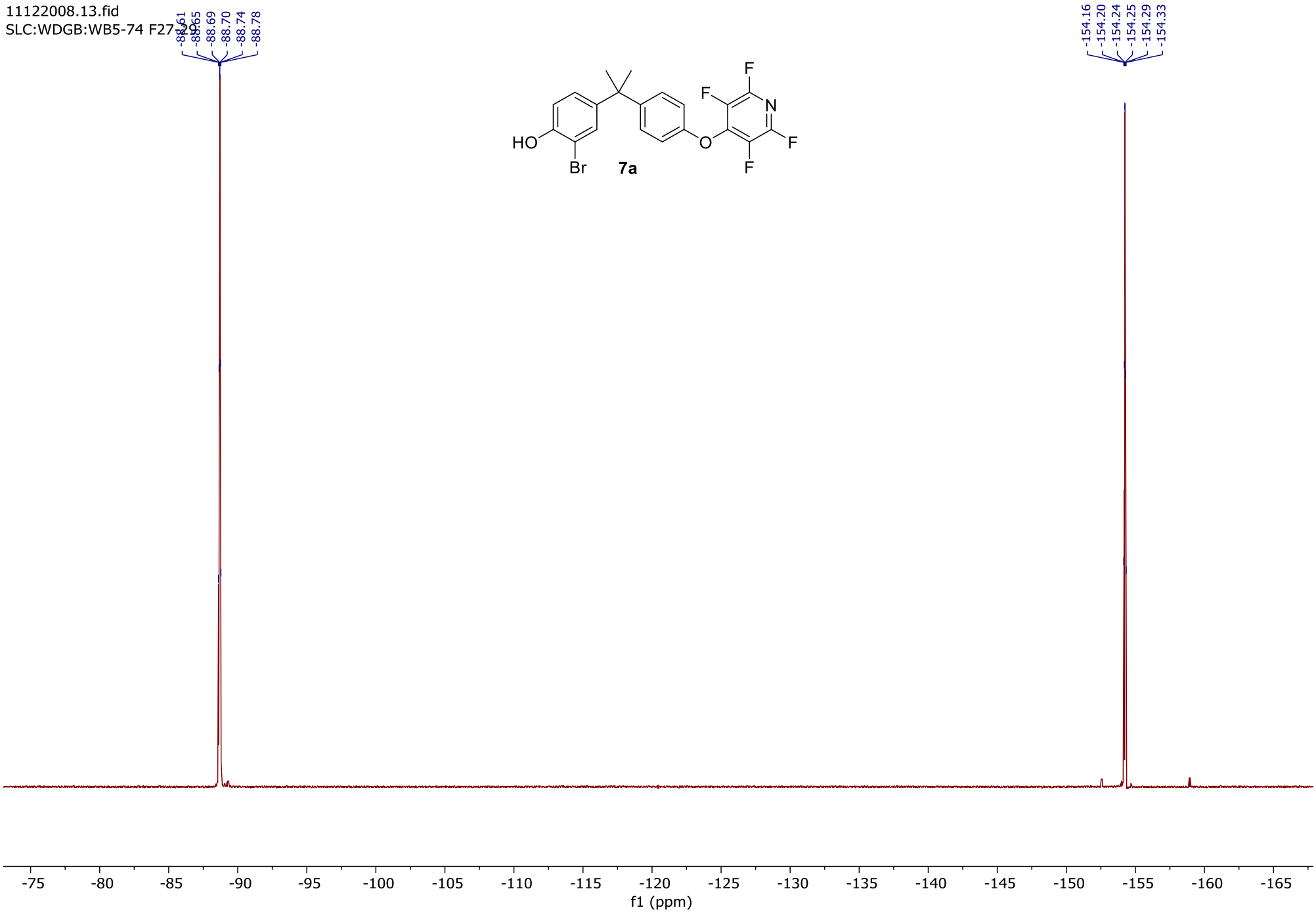

6j
gHSQCAD_01
SLC:WB:WB 6-102
f2 (ppm)
f1 (ppm)

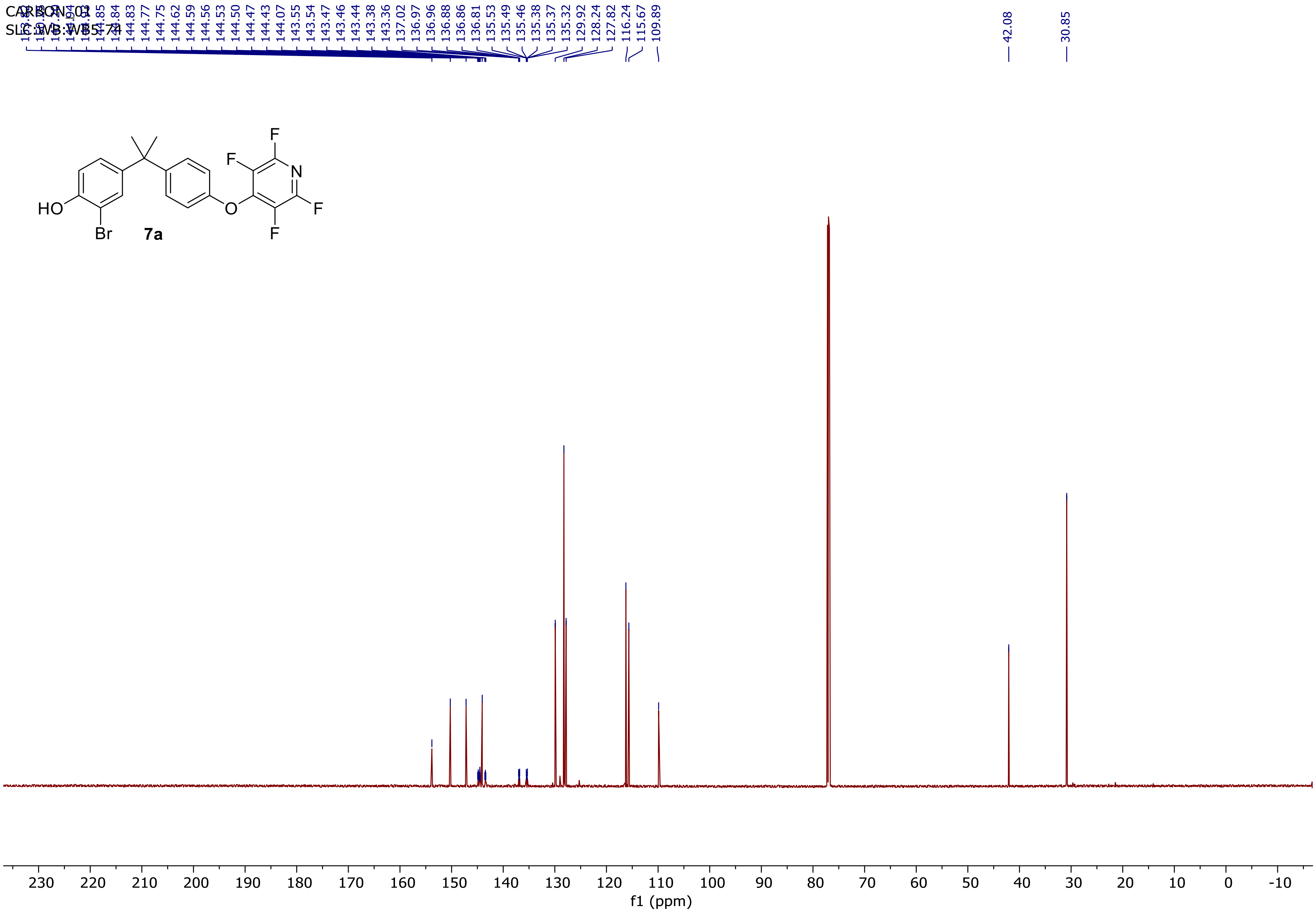

6j
O
I
gHMBCAD_01
SLC:WB:WB 6-102
8.2
8.0
7.8
7.6
7.4
7.2
7.0
6.8
6.6
6.4
6.2
6.0
5.8
5.6
5.4
5.2
5.0
4.8
4.6
4.4
4.2
4.0
3.8
f2 (ppm)
90
100
110
120
130
140
150
160
f1 (ppm)

11122008.10.fid
SLC:WDGB:WB5-74 F27-29

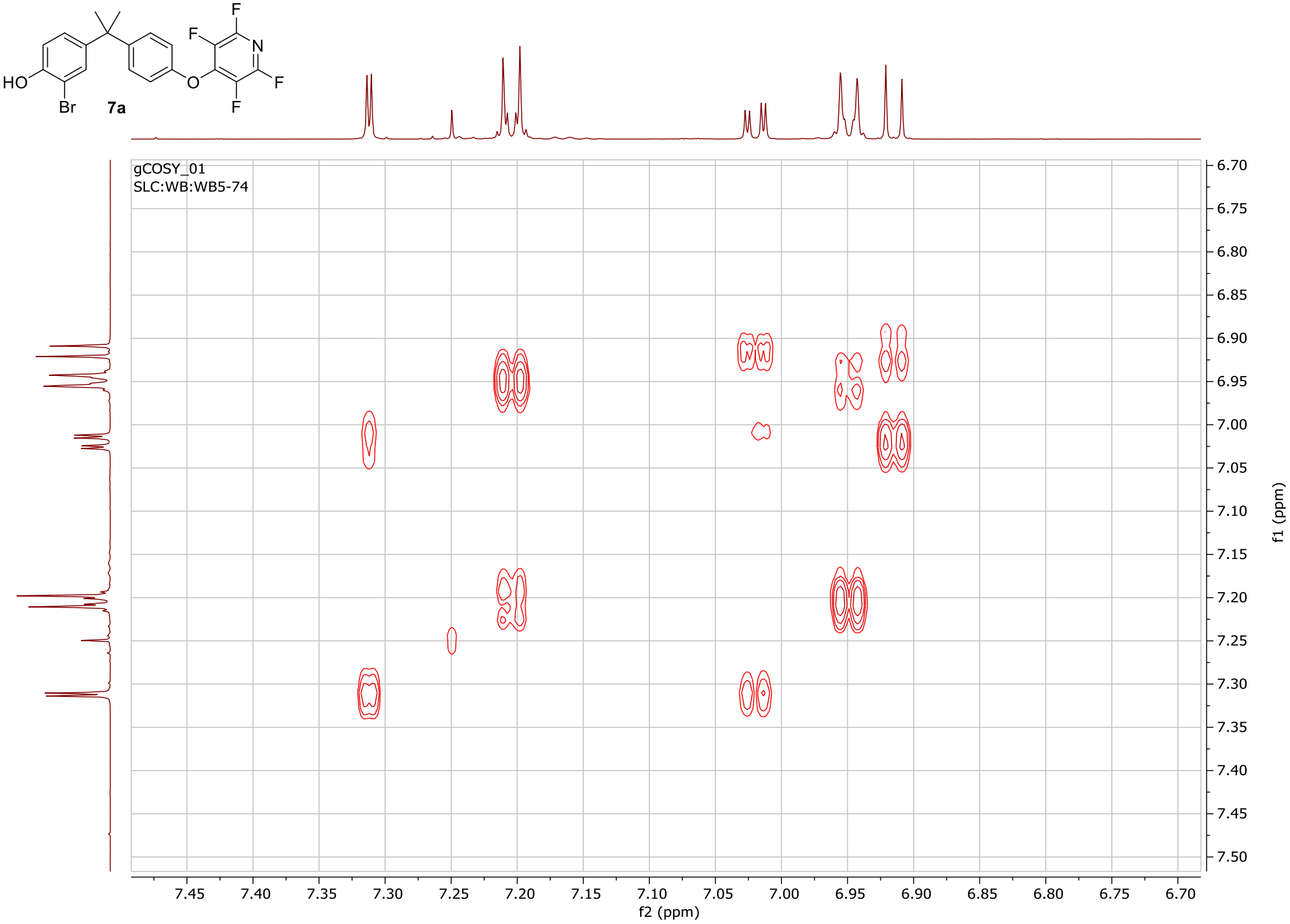


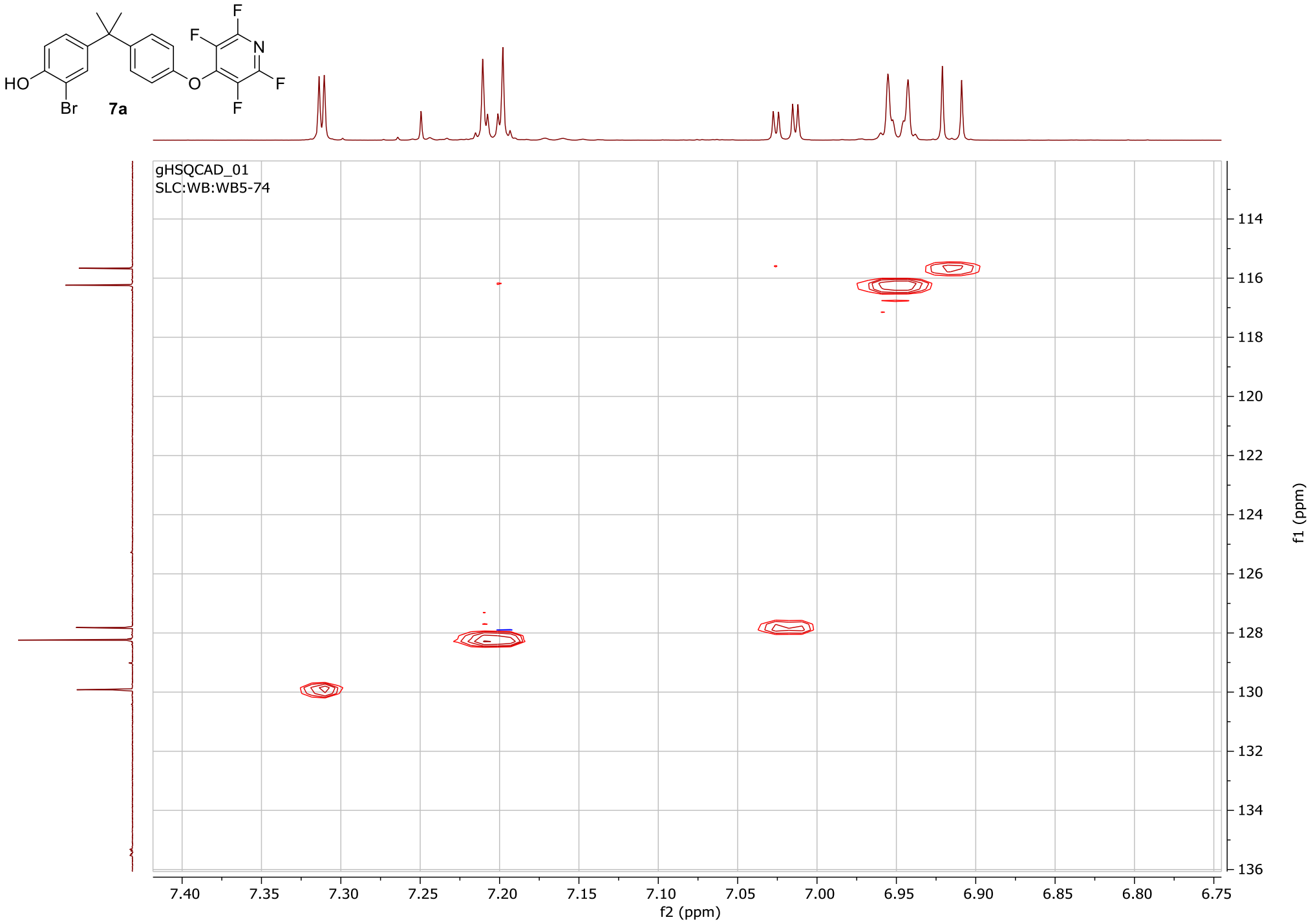
7a

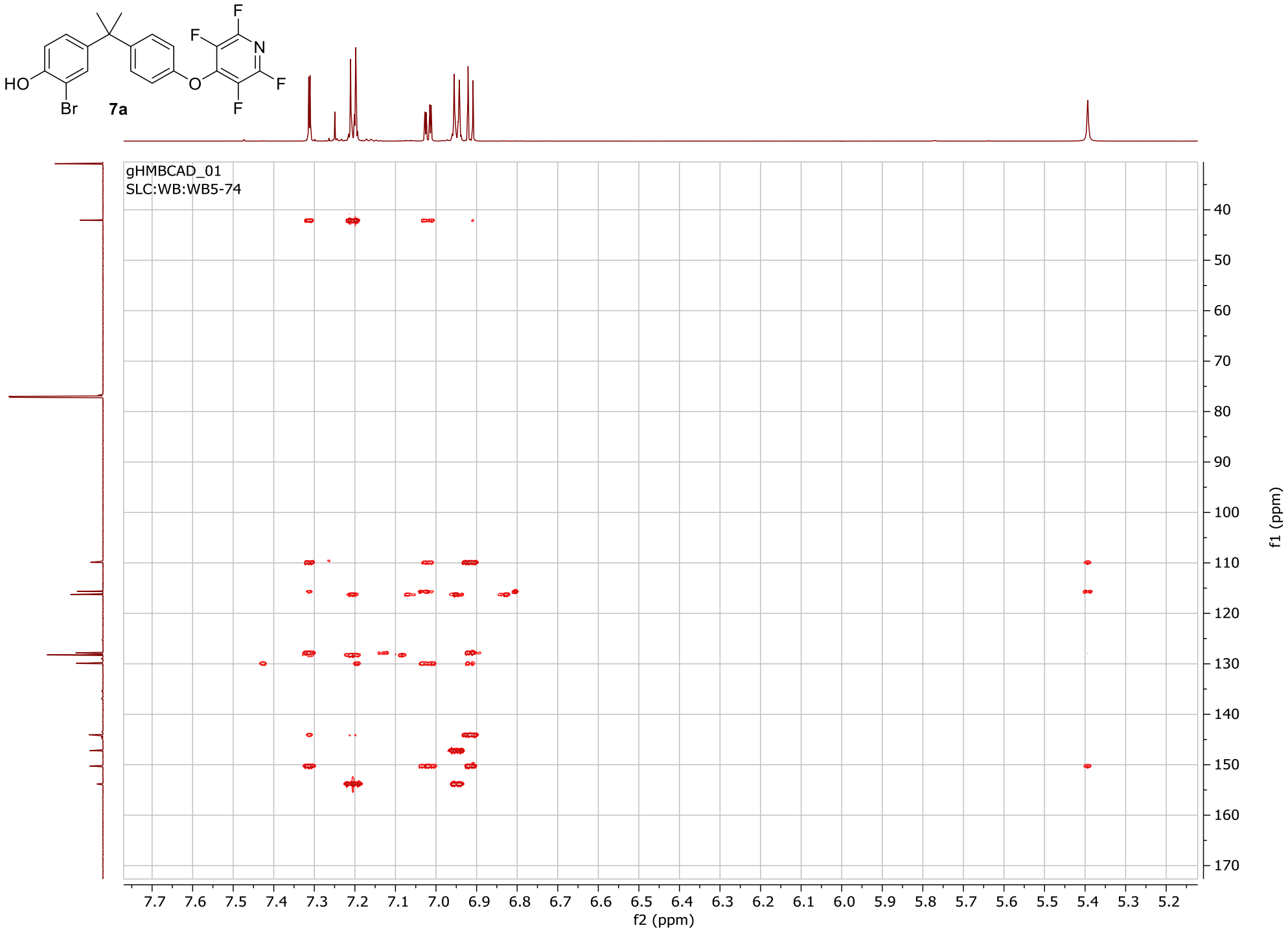

11122008.13.fid
SLC:WDGB:WB5-74 F27 19
-88.61
-88.65
-88.69
-88.70
-88.74
-88.78
-154.16
-154.20
-154.24
-154.25
-154.29
-154.33
HO
Br
7a
F
F
N
O
F
F
-75
-80
-85
-90
-95
-100
-105
-110
-115
-120
-125
-130
-135
-140
-145
-150
-155
-160
-165
f1 (ppm)


CARBON_01
SLC:WB:WB5-74
153.82
150.25
147.20
144.94
144.93
144.85
144.84
144.83
144.77
144.75
144.62
144.59
144.56
144.53
144.50
144.47
144.43
144.07
143.55
143.54
143.47
143.46
143.44
143.38
143.36
137.02
136.97
136.96
136.88
136.86
136.81
135.53
135.49
135.46
135.38
135.37
135.32
129.92
128.24
127.82
116.24
115.67
109.89
42.08
30.85
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)
HO
Br
O
F
F
N
F
F

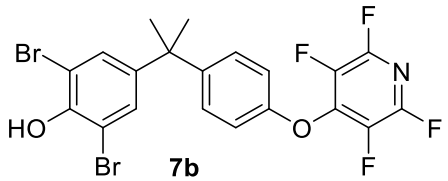
7a


HO
Br
7a
F
F
N
O
F
F
gCOSY_01
SLC:WB:WB5-74
7.45
7.40
7.35
7.30
7.25
7.20
7.15
7.10
7.05
7.00
6.95
6.90
6.85
6.80
6.75
6.70
f2 (ppm)
6.70
6.75
6.80
6.85
6.90
6.95
7.00
7.05
7.10
7.15
7.20
7.25
7.30
7.35
7.40
7.45
7.50
f1 (ppm)


HO
Br
7a
F
F
N
O
F
F
gHSQCAD_01
SLC:WB:WB5-74
114
116
118
120
122
124
126
128
130
132
134
136
f1 (ppm)
7.40
7.35
7.30
7.25
7.20
7.15
7.10
7.05
7.00
6.95
6.90
6.85
6.80
6.75
f2 (ppm)


HO
Br
7a
F
F
N
O
F
F
gHMBCAD_01
SLC:WB:WB5-74
f2 (ppm)
f1 (ppm)

03175634.10.fid
SLC:WDGB:WB6-101
Proton.dur CDCl3 /home/nmr/localdata walkup 46

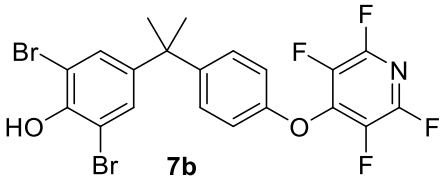


7b

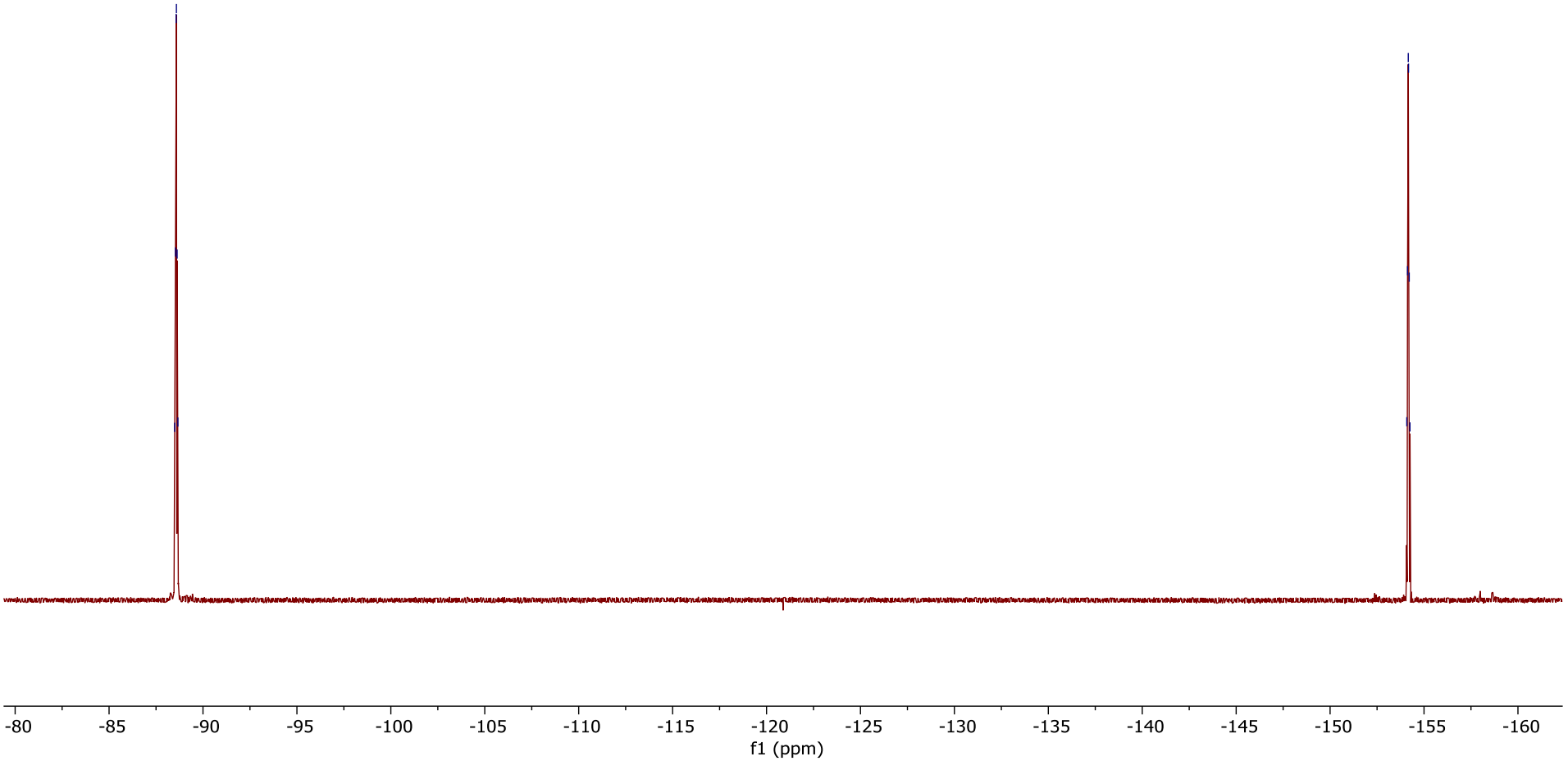
03175634.13.fid
SLC:WDGB:WB6-101
F19_limits_dec.dur CDCl3 /home/nmr/localdata walkup 46

-88.44
-88.53
-88.57
-88.58
-88.62
-88.66

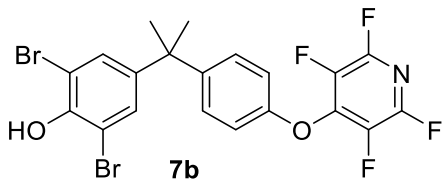
-154.08
-154.12
-154.16
-154.18
-154.21
-154.25



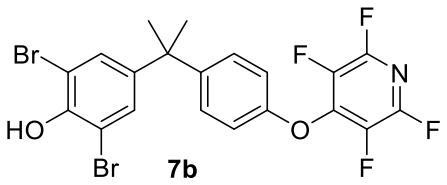
7b



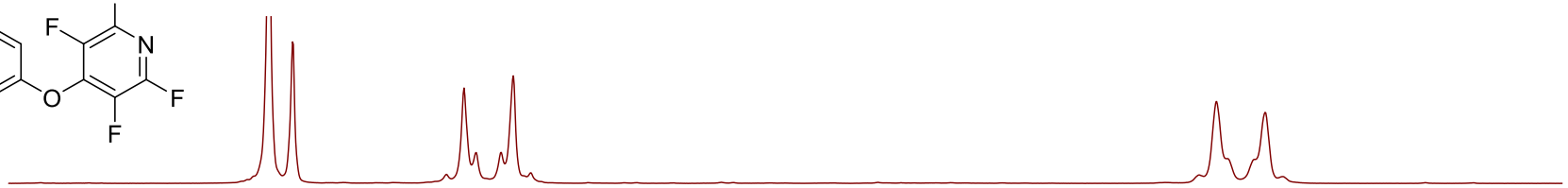
CARBON_01
SLC:WB:WB 6_101

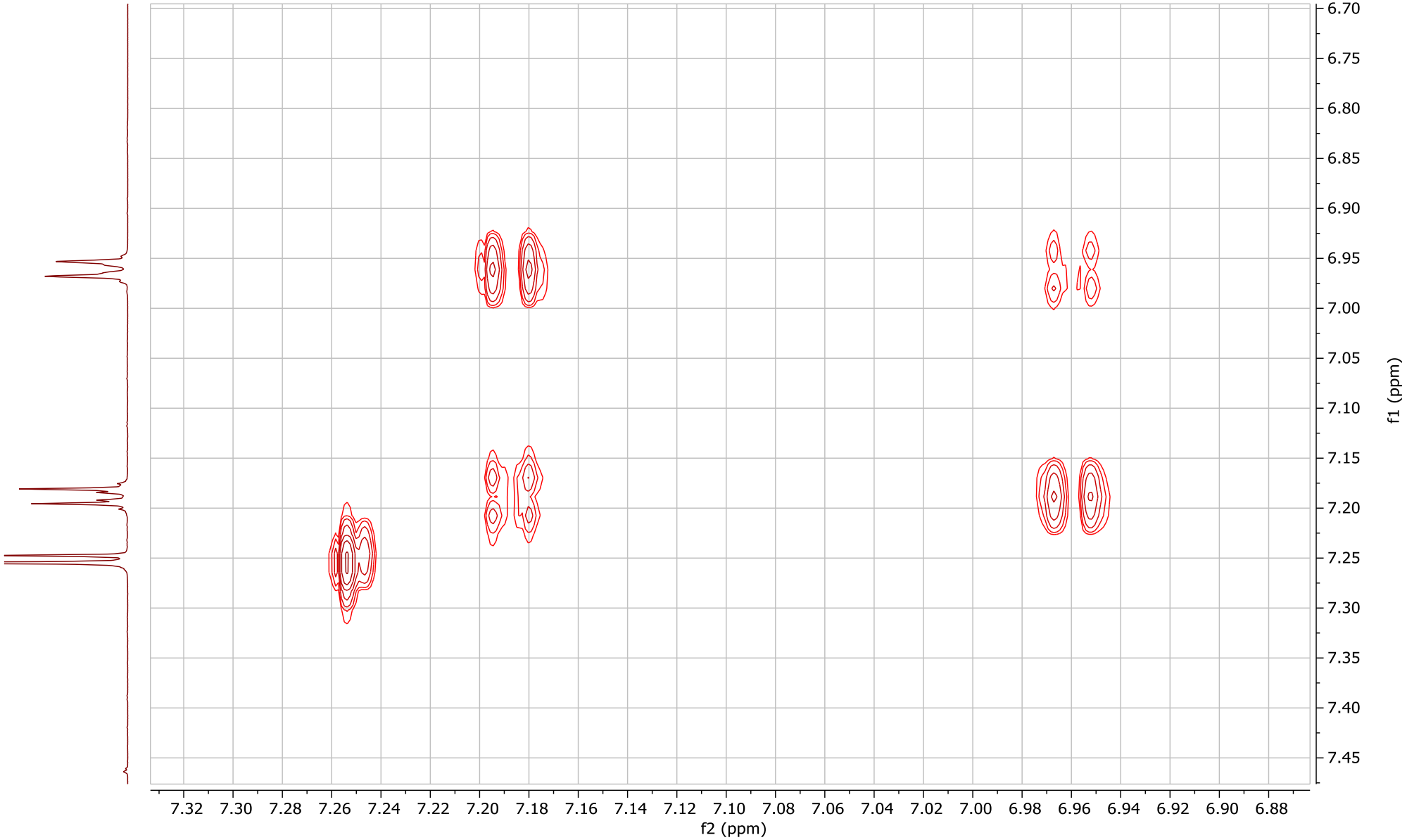


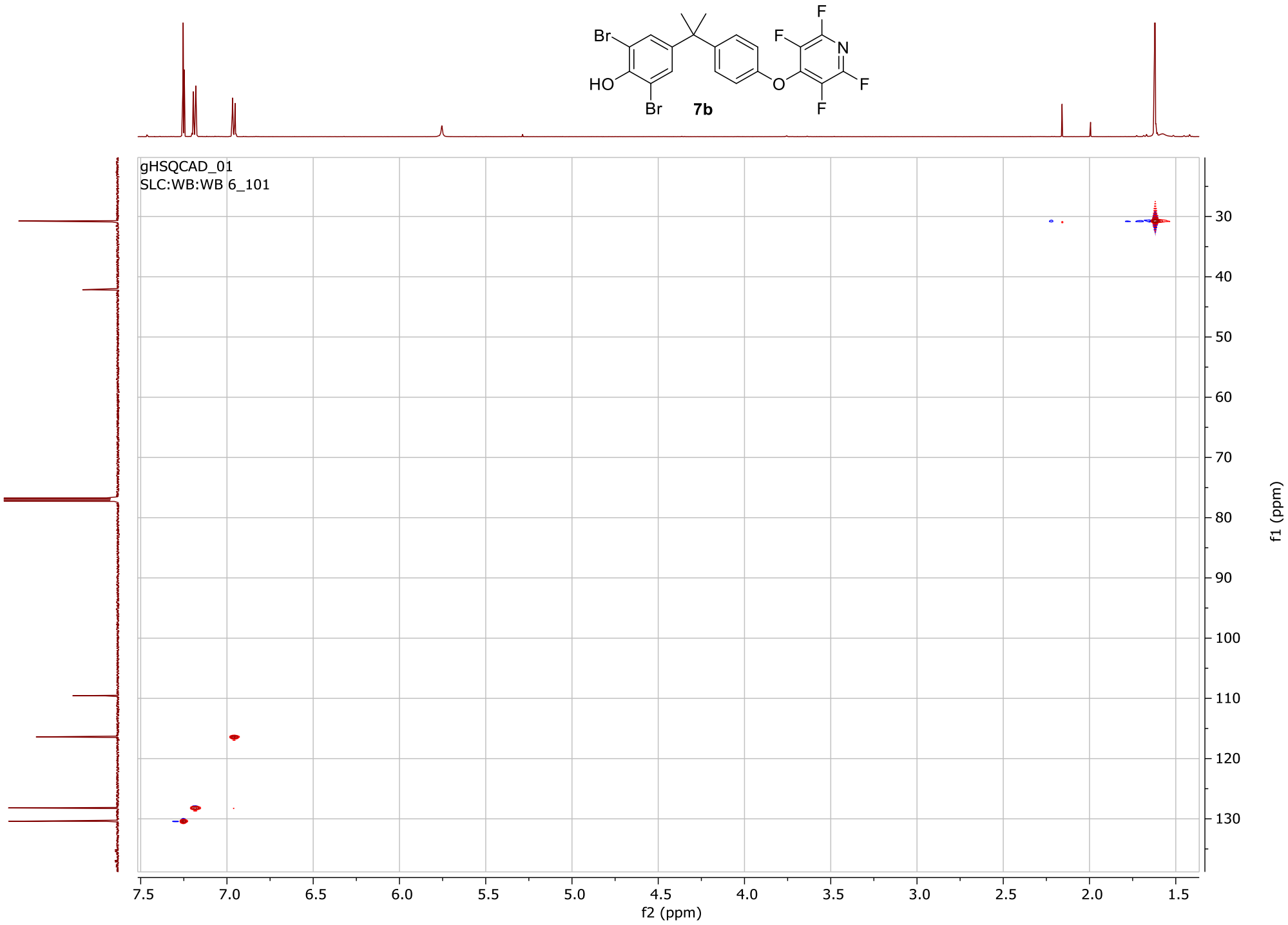
7b

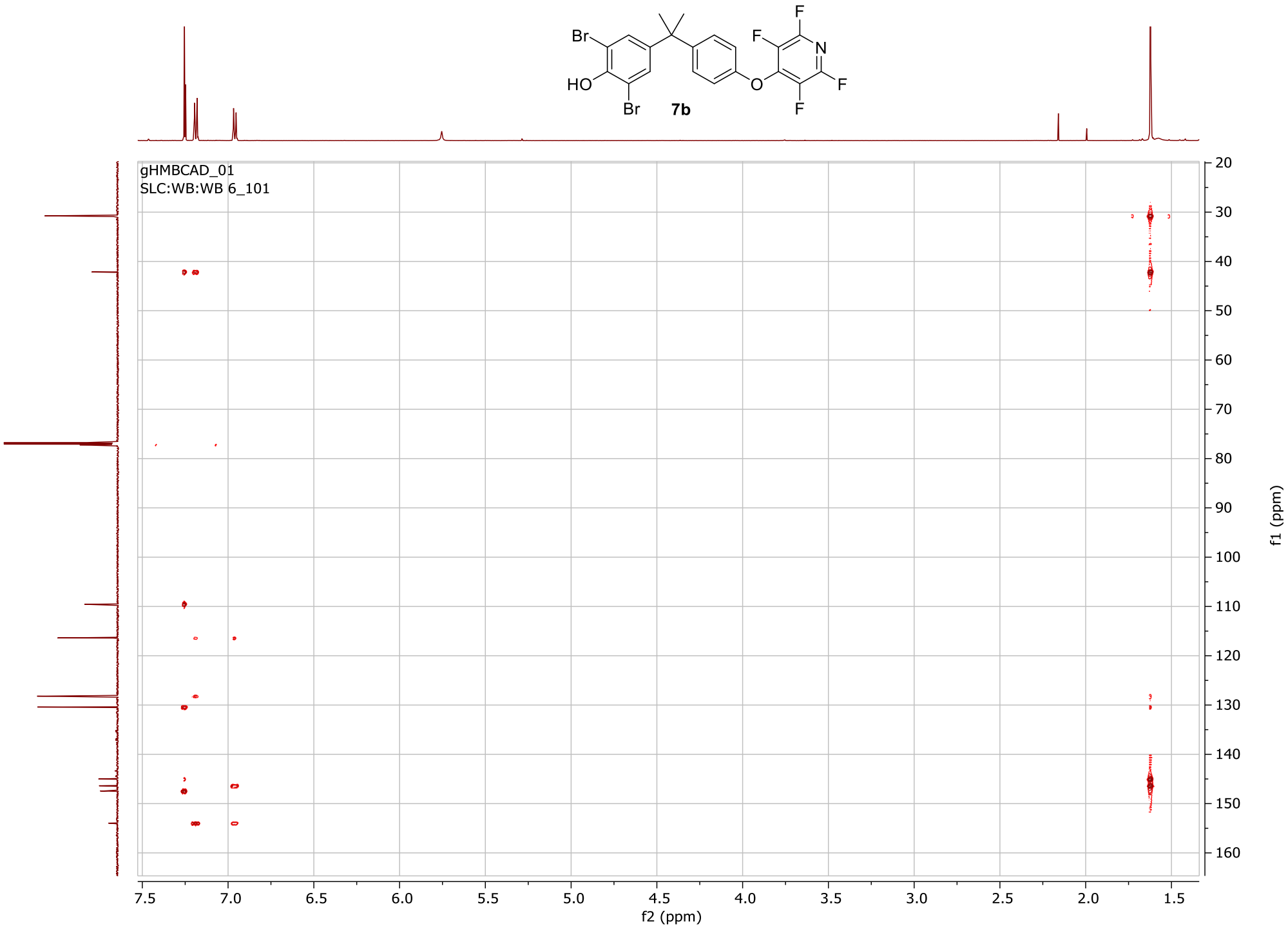

Br
HO
Br
O
F
F
N
F
F

7b

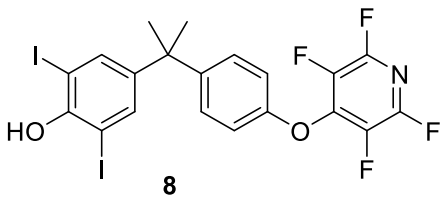



6.70
6.75
6.80
6.85
6.90
6.95
7.00
7.05
7.10
7.15
7.20
7.25
7.30
7.35
7.40
7.45
f1 (ppm)
7.32 7.30 7.28 7.26 7.24 7.22 7.20 7.18 7.16 7.14 7.12 7.10 7.08 7.06 7.04 7.02 7.00 6.98 6.96 6.94 6.92 6.90 6.88
f2 (ppm)

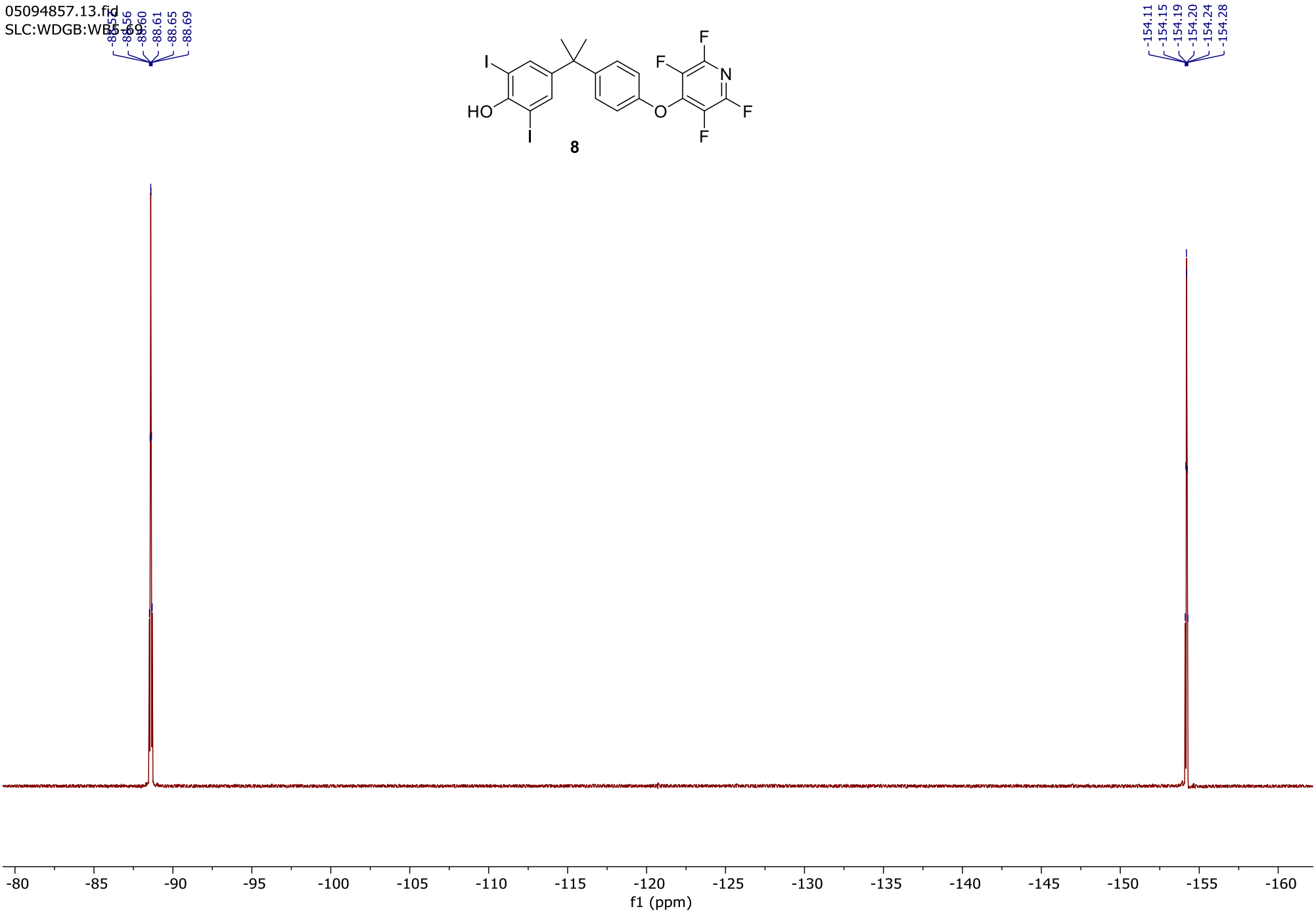

Br
HO
Br
7b
F
F
N
O
F
F
gHSQCAD_01
SLC:WB:WB 6_101
30
40
50
60
70
80
90
100
110
120
130
f1 (ppm)
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
f2 (ppm)

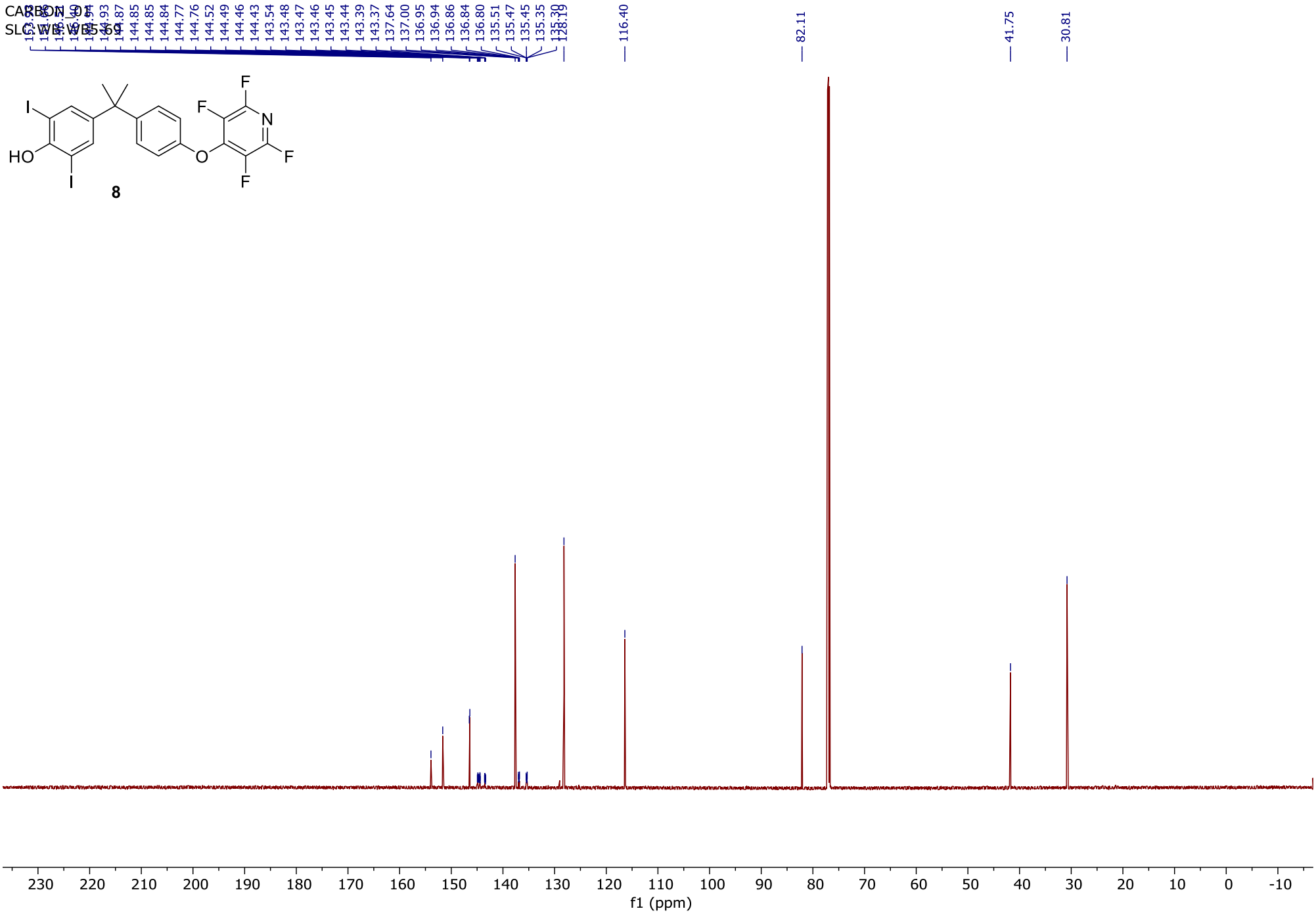

Br
HO
Br
7b
F
F
N
O
F
F
gHMBCAD_01
SLC:WB:WB 6_101
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
f2 (ppm)
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
f1 (ppm)

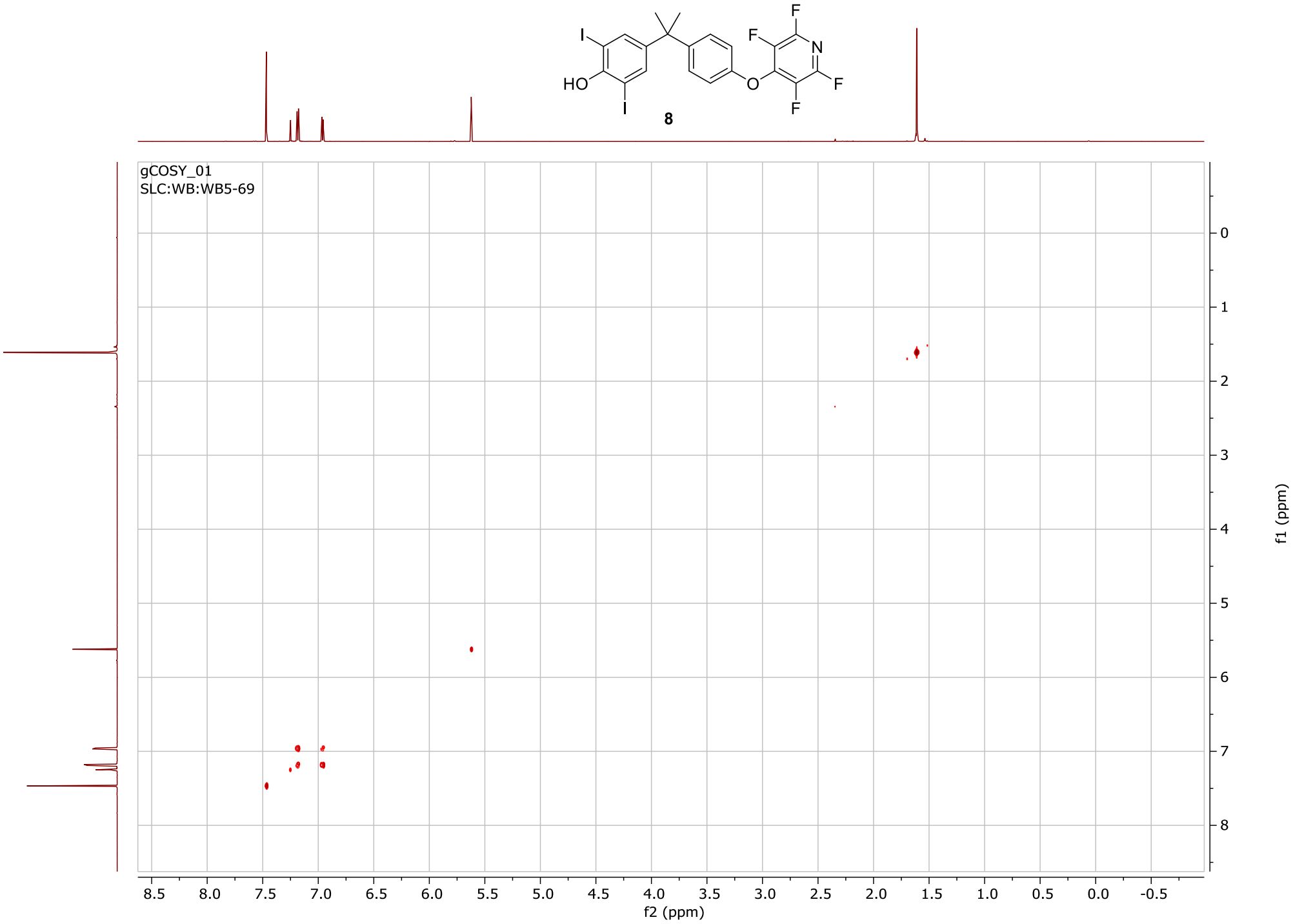
05094857.10.fid
SLC:WDGB:WB5-69

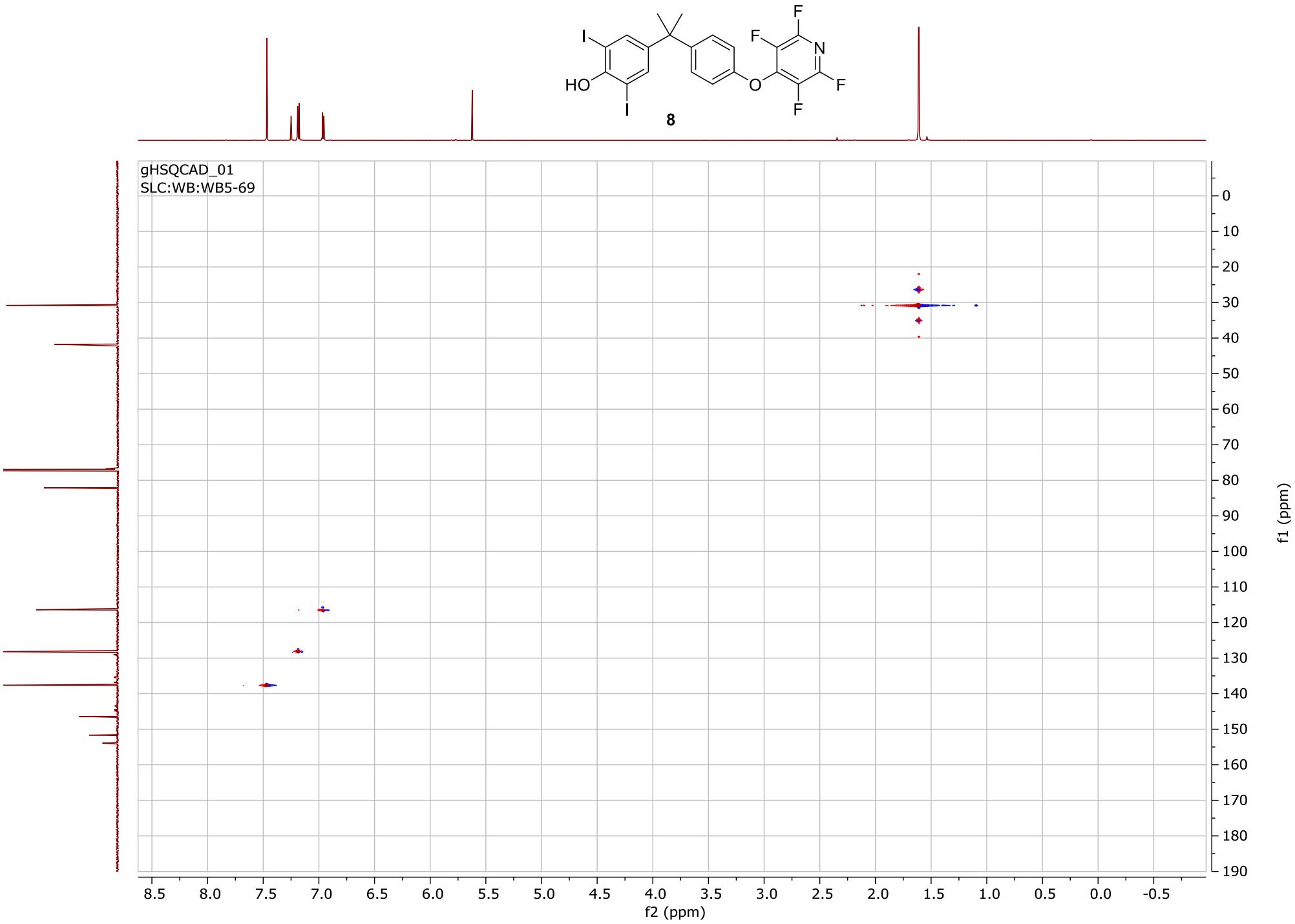


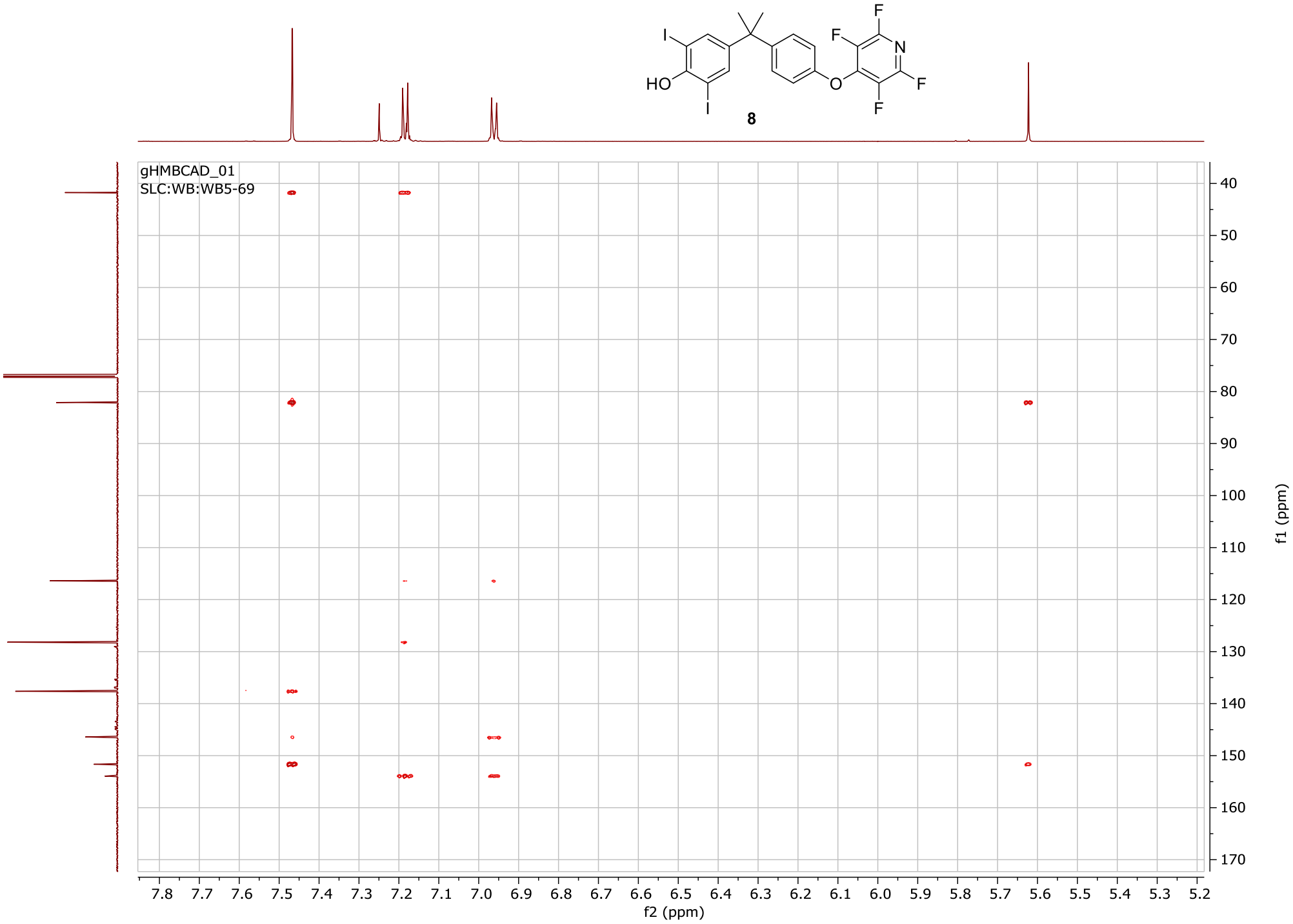
8


05094857.13.fid
SLC:WDGB:WB5-69
-88.52
-88.56
-88.60
-88.61
-88.65
-88.69
-154.11
-154.15
-154.19
-154.20
-154.24
-154.28
I
HO
I
F
F
N
O
F
F
8
-80
-85
-90
-95
-100
-105
-110
-115
-120
-125
-130
-135
-140
-145
-150
-155
-160
f1 (ppm)

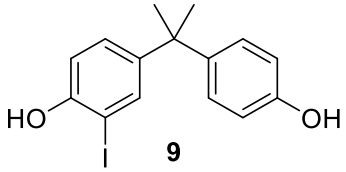

CARBON_01
SLC_WB_WB5360
116.40
82.11
41.75
30.81
I
HO
I
O
F
F
N
F
F
8
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


gCOSY_01
SLC:WB:WB5-69
I
HO
I
F
F
N
O
F
F
8
f2 (ppm)
f1 (ppm)


gHSQCAD_01
SLC:WB:WB5-69
I
HO
I
F
F
N
O
F
F
8
f2 (ppm)
f1 (ppm)


gHMBCAD_01
SLC:WB:WB5-69
I
HO
I
F
F
N
O
F
F
8
f2 (ppm)
f1 (ppm)

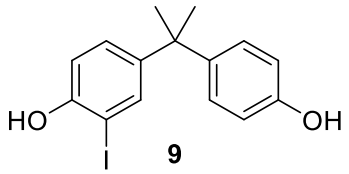
30170139.10.fid
SLC:WDGB:WB5-55



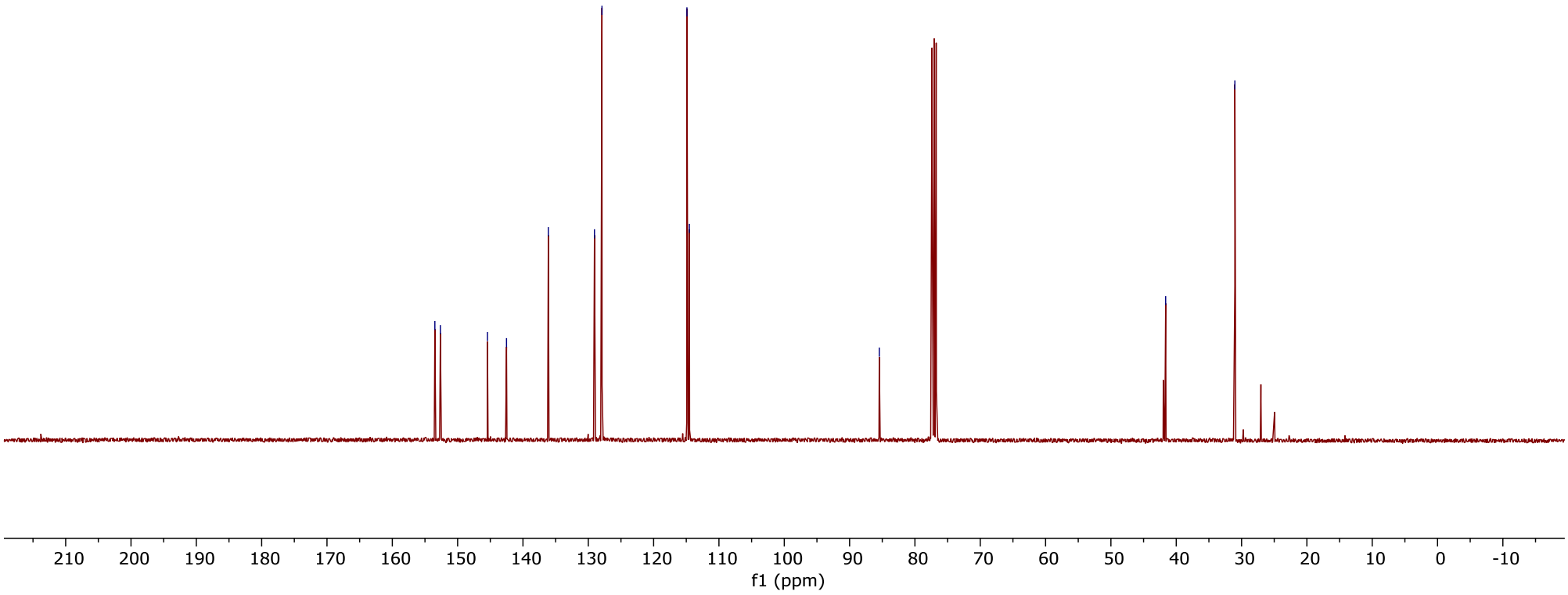
9

05154913.10.fid
SLC:WDGB:WB5-55

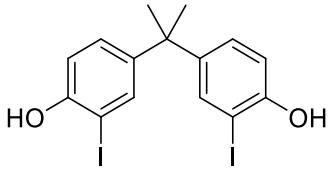
153.49
152.64
145.43
142.52
136.11
129.06
127.91
114.90
114.52
85.46
41.62
31.02



9

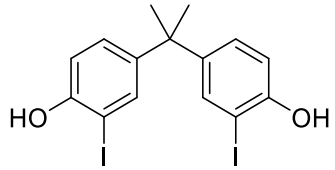


08135629.10.fid
SLC:WDGB:WB5-82

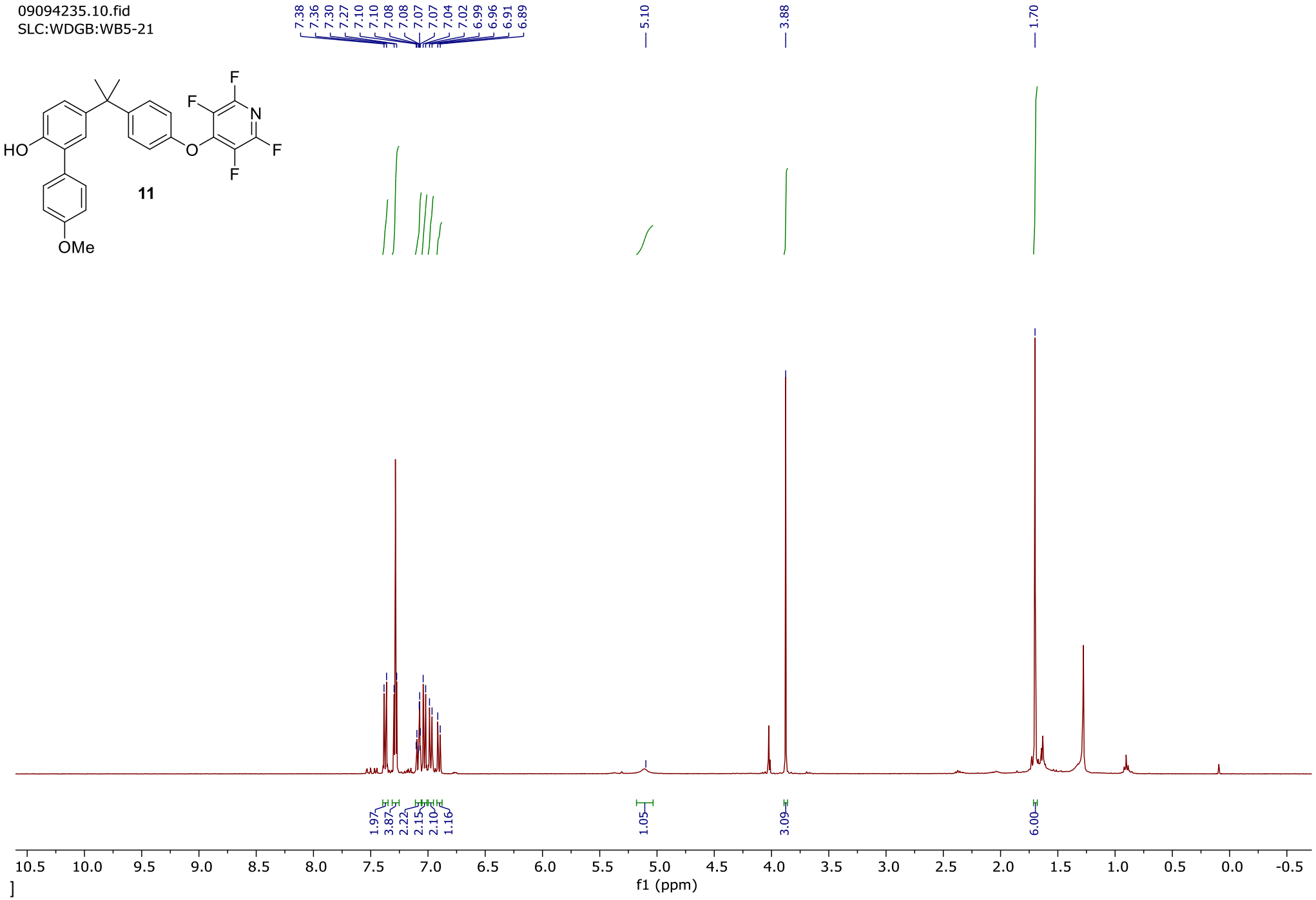


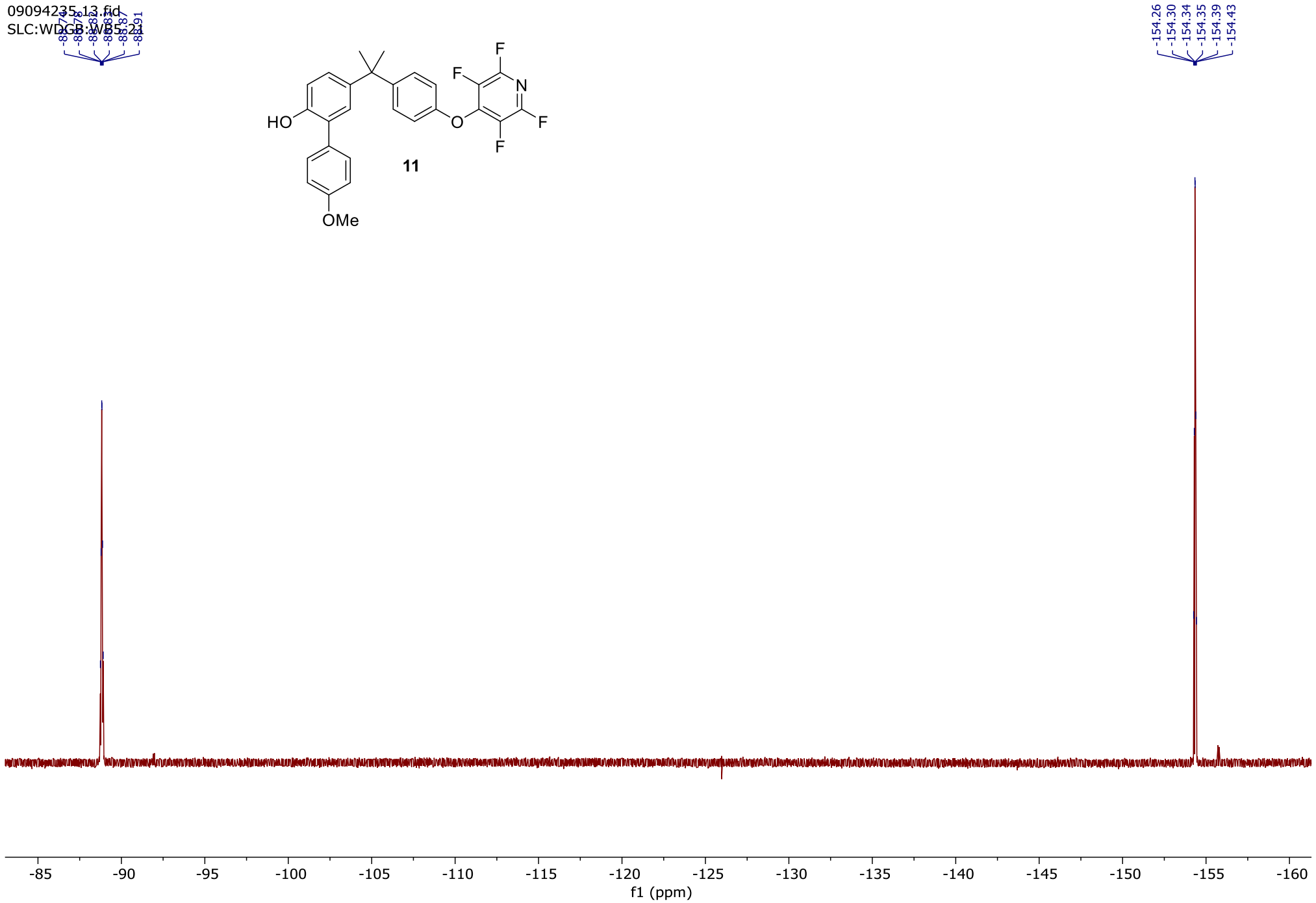
10

08151109.10.fid
SLC:WDGB:WB5-82

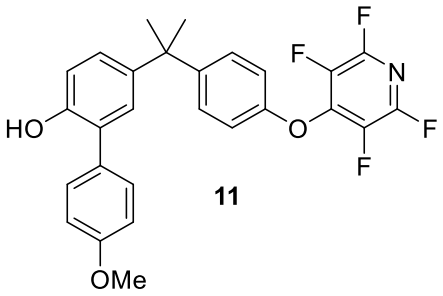


10


09094235.10.fid
SLC:WDGB:WB5-21
7.38
7.36
7.30
7.27
7.10
7.10
7.08
7.08
7.07
7.07
7.04
7.02
6.99
6.96
6.91
6.89
5.10
3.88
1.70
HO
O
N
F
F
F
F
OMe
11
1.97
3.87
2.22
2.15
2.10
1.16
1.05
3.09
6.00
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
0.0
-0.5
f1 (ppm)


09094235_13.fid
SLC:WDGB:WB5_21
-87.78
-88.03
-88.11
-88.22
-88.87
-88.91
-154.26
-154.30
-154.34
-154.35
-154.39
-154.43
HO
O
N
F
F
F
F
OMe
11
-85
-90
-95
-100
-105
-110
-115
-120
-125
-130
-135
-140
-145
-150
-155
-160
f1 (ppm)

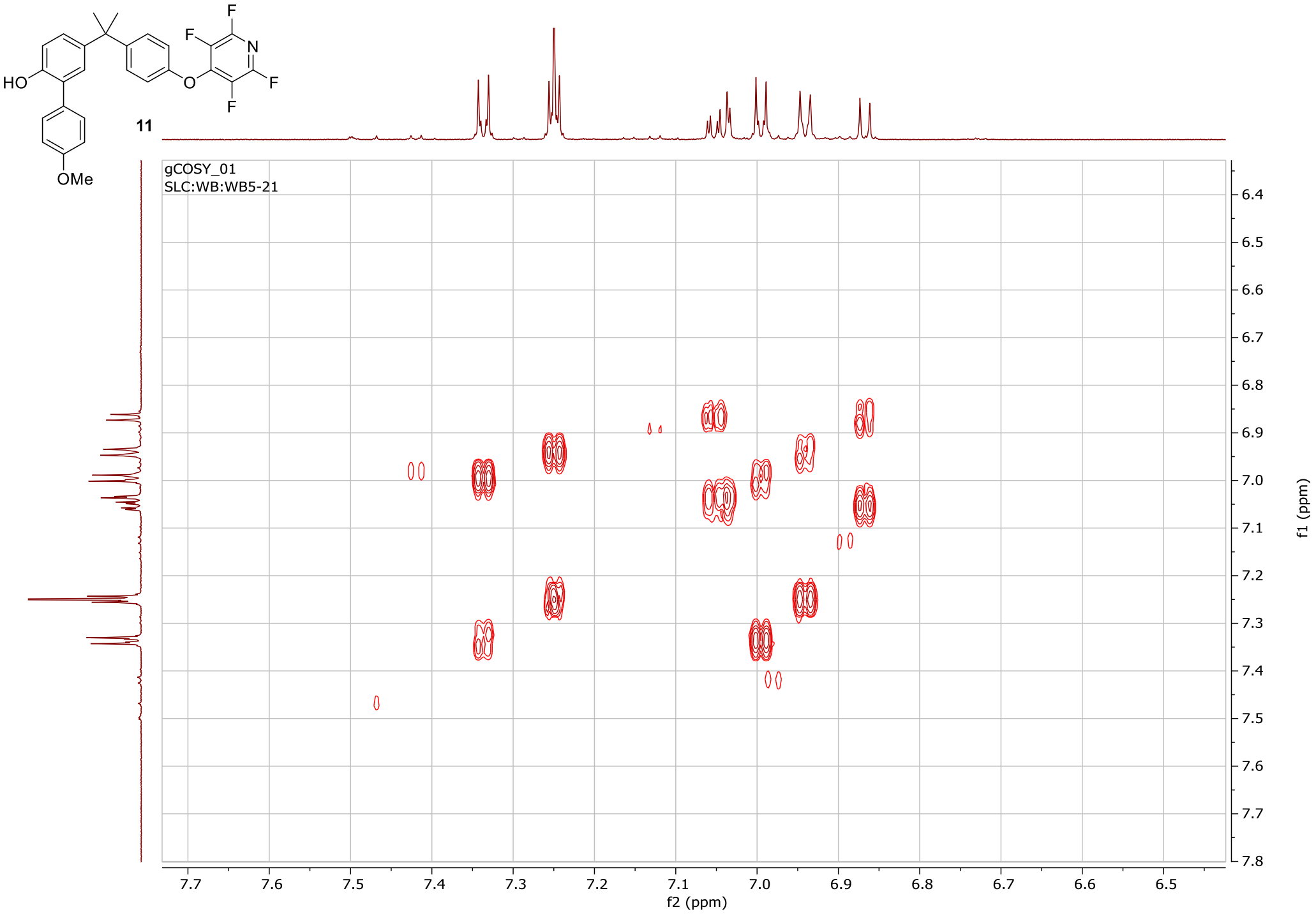
CARBON_01
SLC:WB:WB5-21

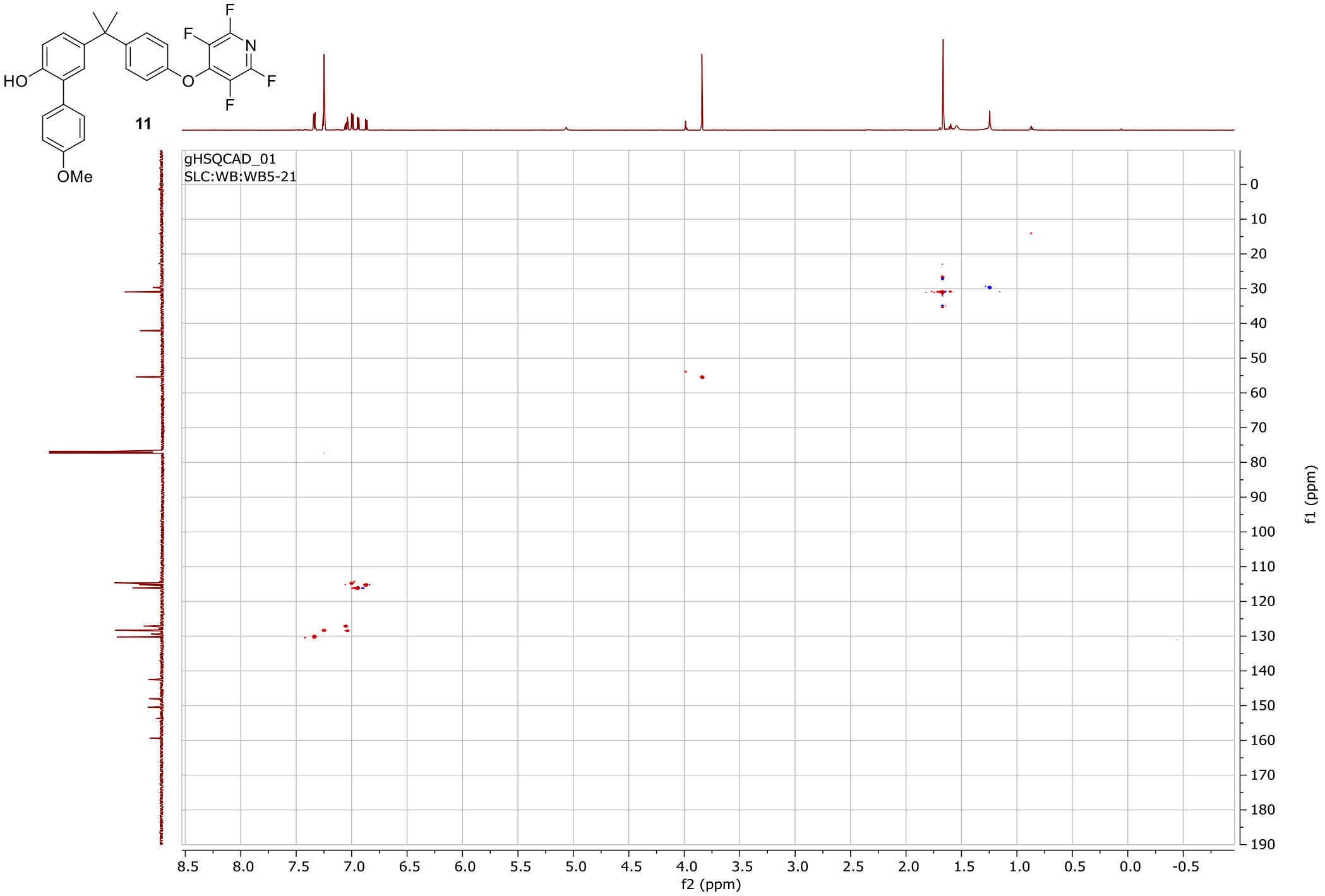


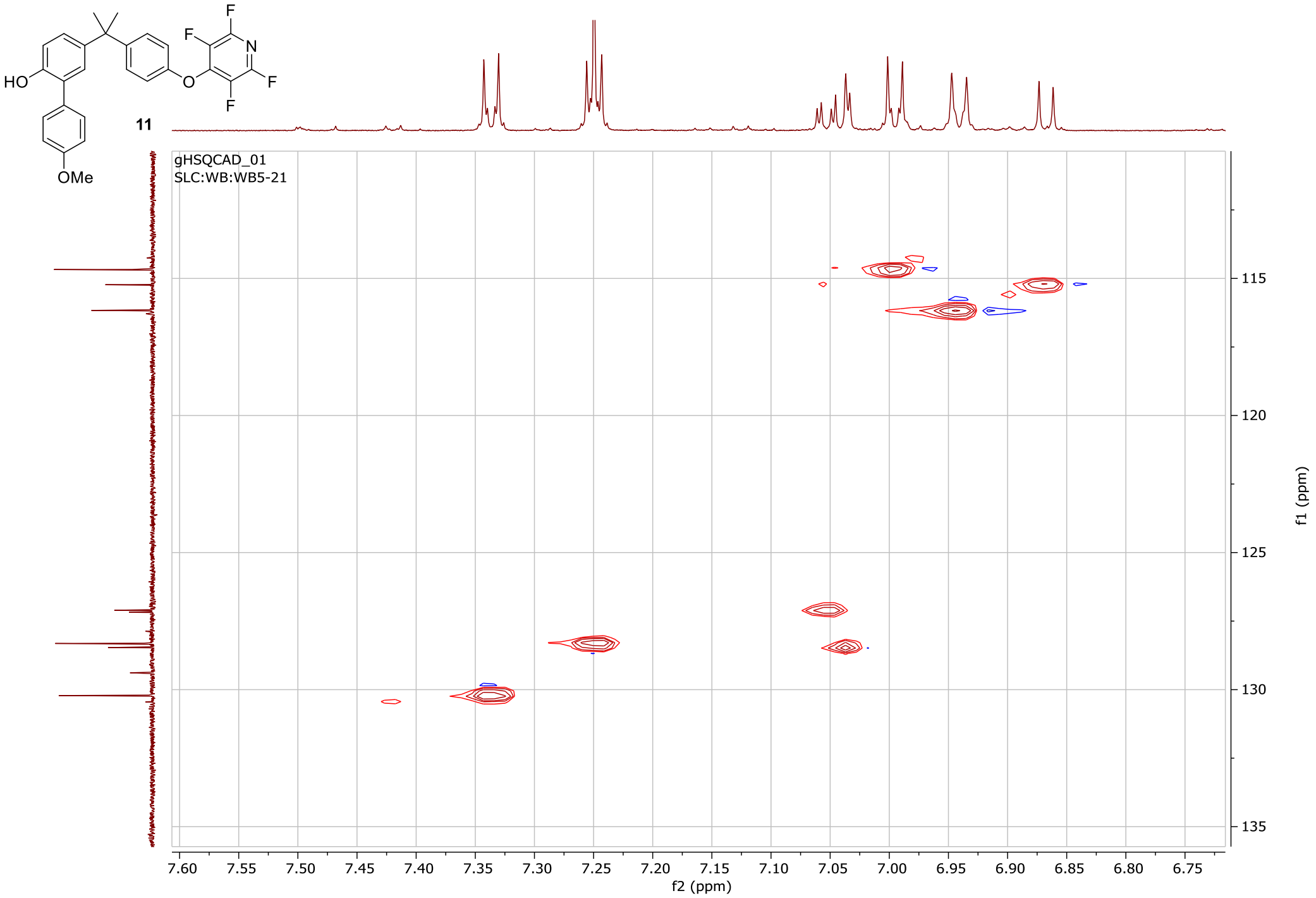
11

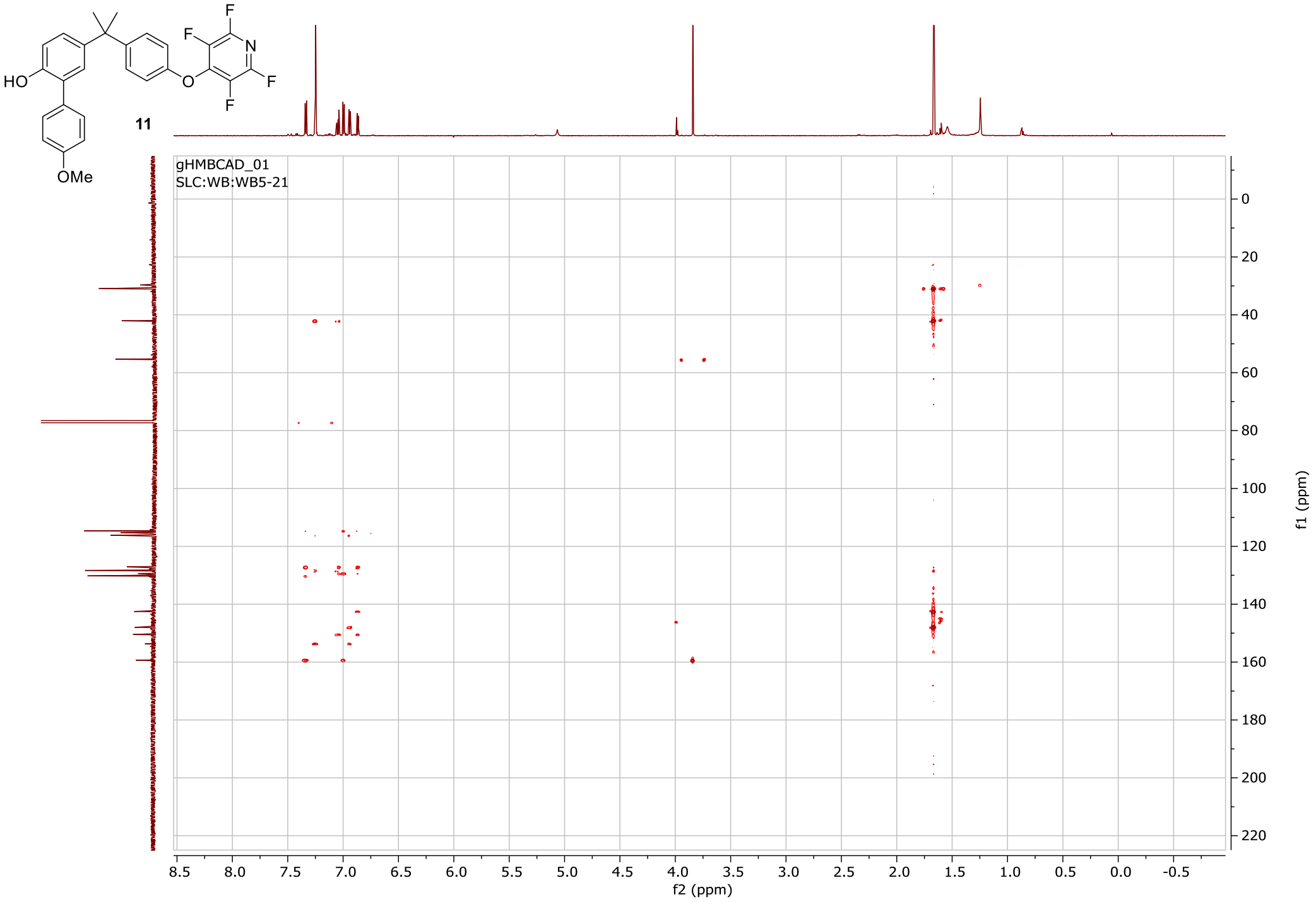
159.31
153.67
150.48
147.99
142.50
130.22
129.38
128.47
128.31
127.18
127.10
116.17
115.23
114.68
55.35
42.08
30.96

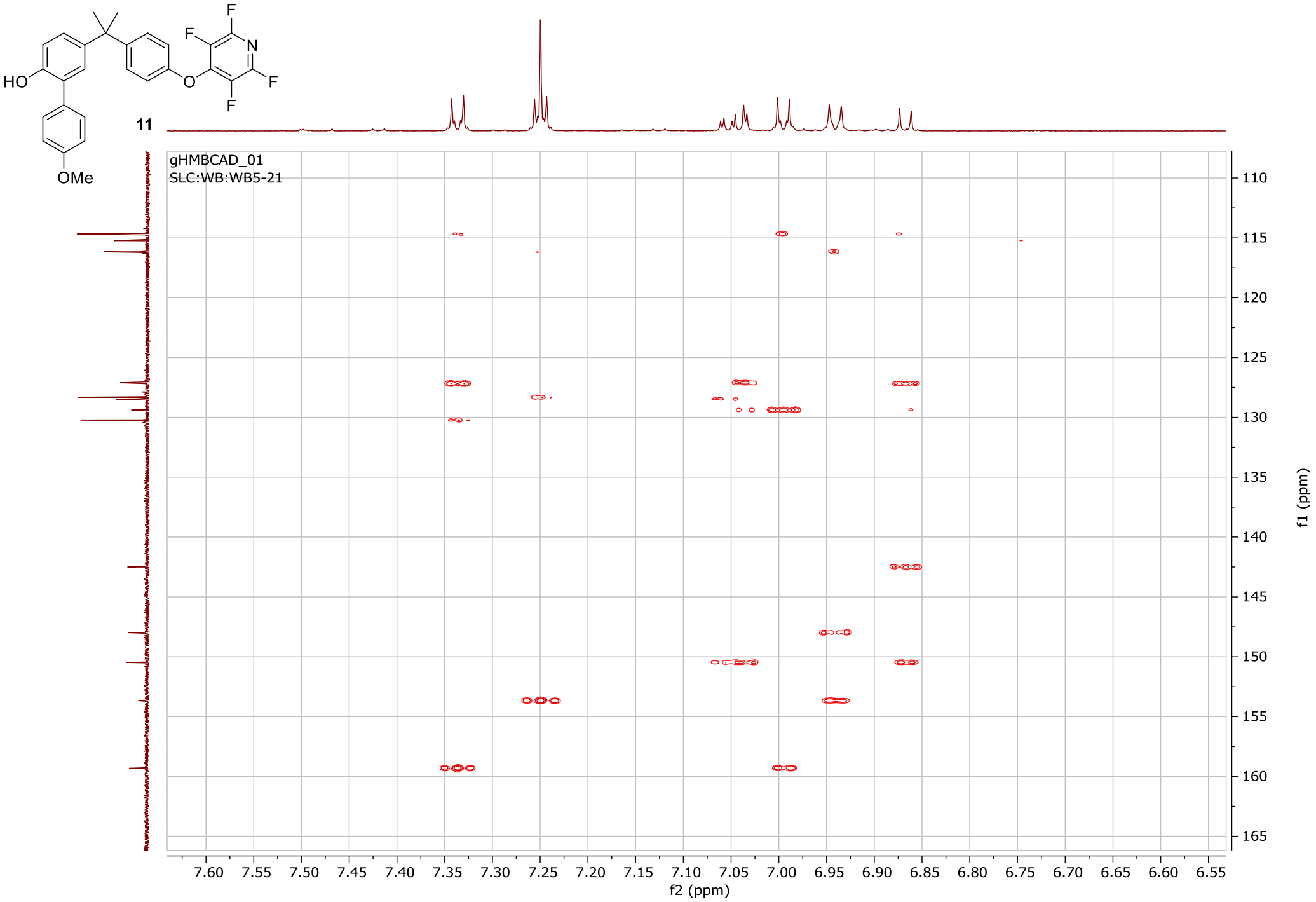
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


HO
OMe
O
F
F
N
F
F
11
gCOSY_01
SLC:WB:WB5-21
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
6.6
6.5
f2 (ppm)
6.4
6.5
6.6
6.7
6.8
6.9
7.0
7.1
7.2
7.3
7.4
7.5
7.6
7.7
7.8
f1 (ppm)

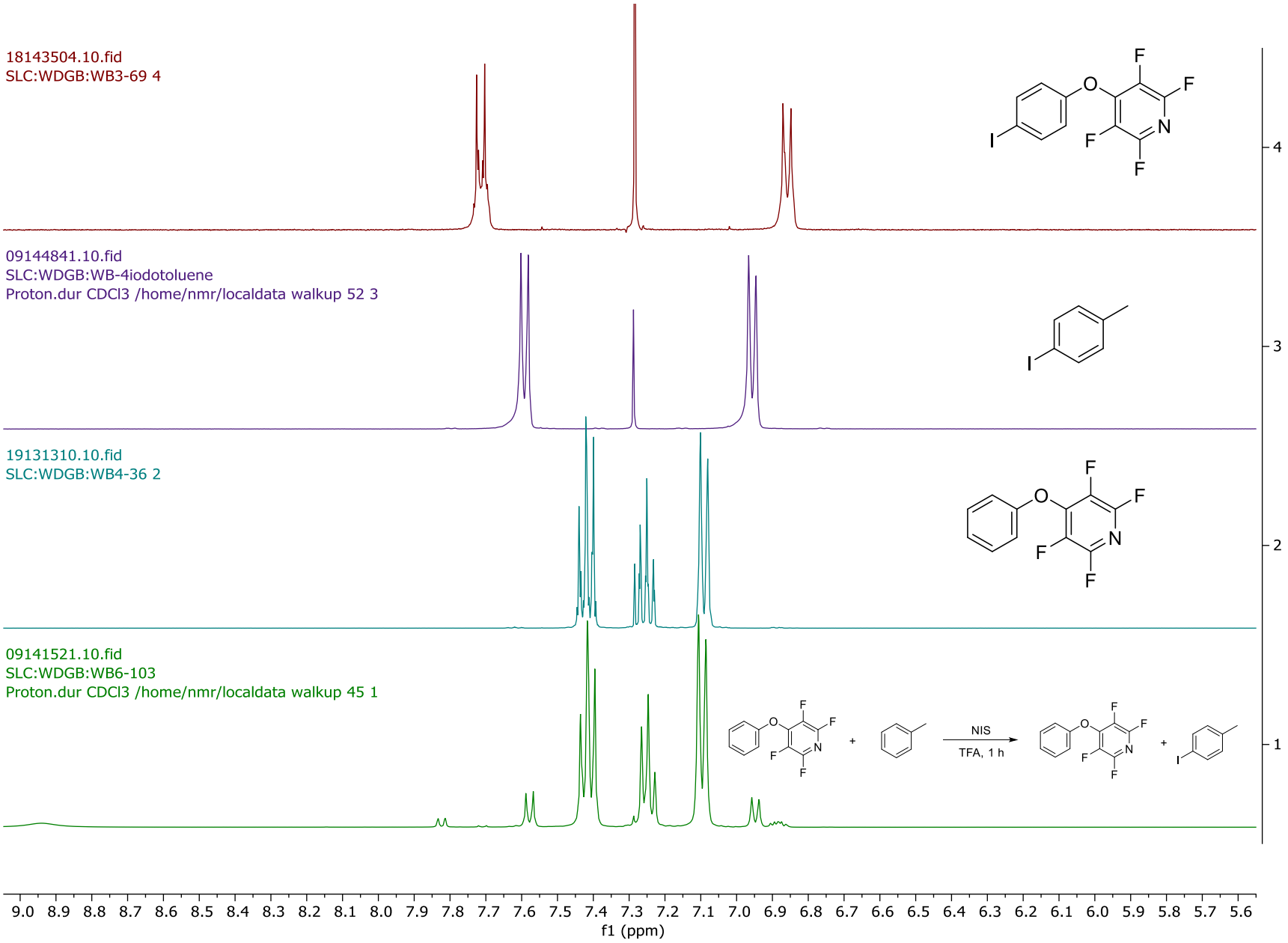

HO
F
F
N
F
O
F
OMe
11
gHSQCAD_01
SLC:WB:WB5-21
f2 (ppm)
f1 (ppm)


HO
F
F
N
F
O
F
OMe
11
gHSQCAD_01
SLC:WB:WB5-21
115
120
125
130
135
f1 (ppm)
7.60
7.55
7.50
7.45
7.40
7.35
7.30
7.25
7.20
7.15
7.10
7.05
7.00
6.95
6.90
6.85
6.80
6.75
f2 (ppm)

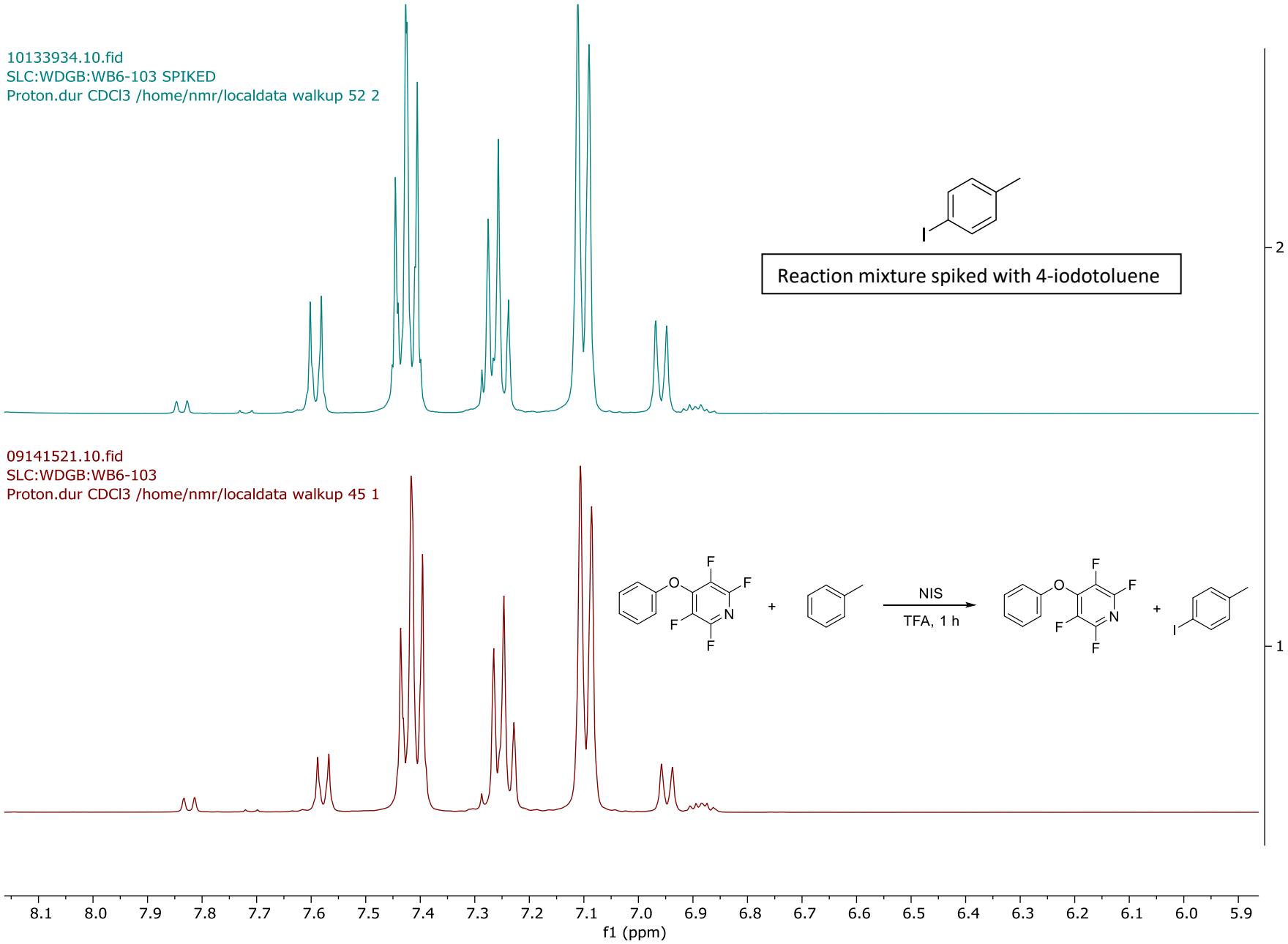

HO
OMe
O
F
F
N
F
F
11
gHMBCAD_01
SLC:WB:WB5-21
f2 (ppm)
f1 (ppm)
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
0
20
40
60
80
100
120
140
160
180
200
220


HO
OMe
O
N
F
F
F
F
11
gHMBCAD_01
SLC:WB:WB5-21
f2 (ppm)
f1 (ppm)
7.60
7.55
7.50
7.45
7.40
7.35
7.30
7.25
7.20
7.15
7.10
7.05
7.00
6.95
6.90
6.85
6.80
6.75
6.70
6.65
6.60
6.55
110
115
120
125
130
135
140
145
150
155
160
165

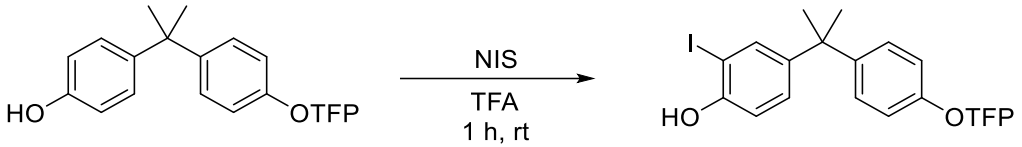
Iodination Competition Experiment

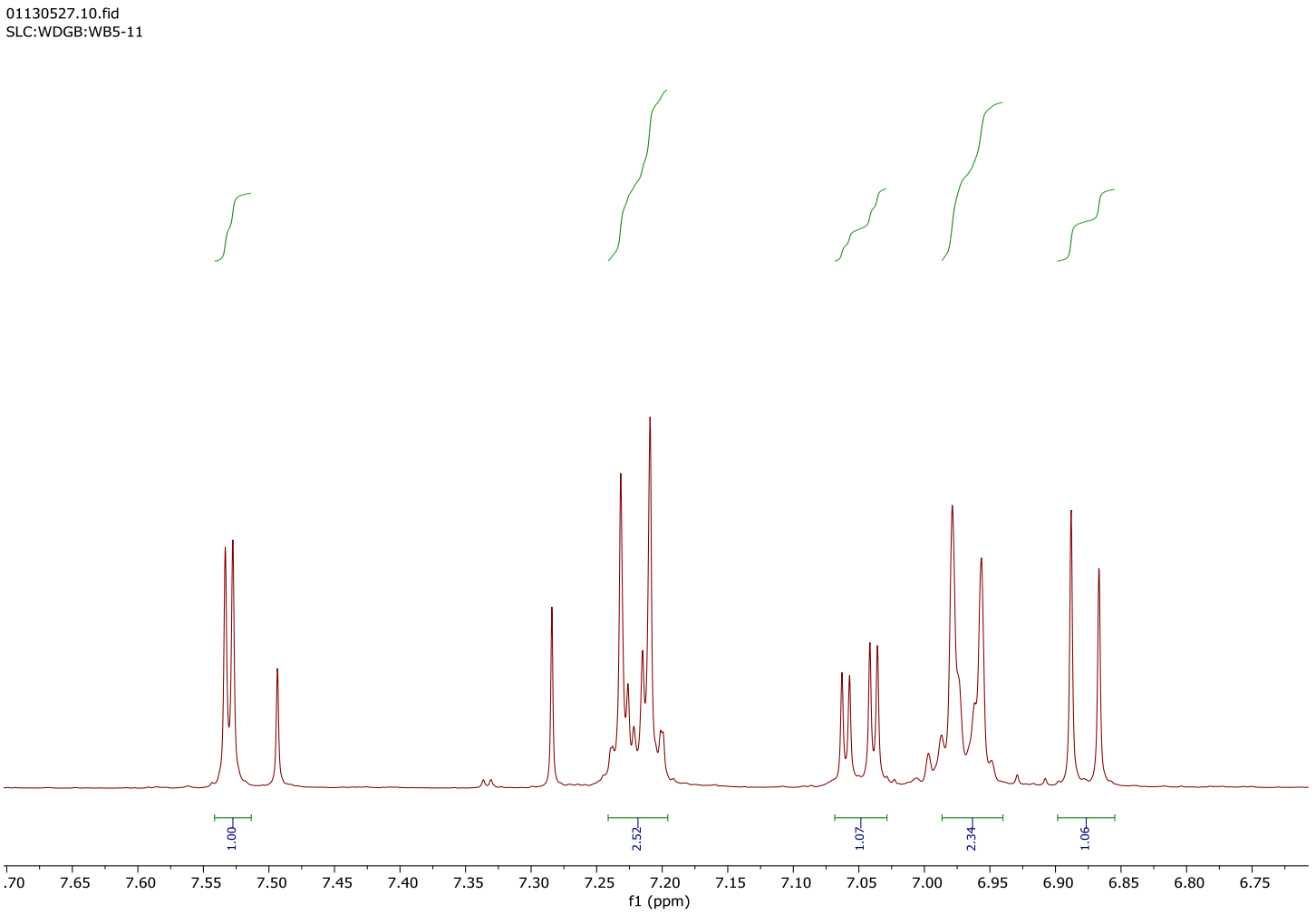


NMR Spiking Experiment

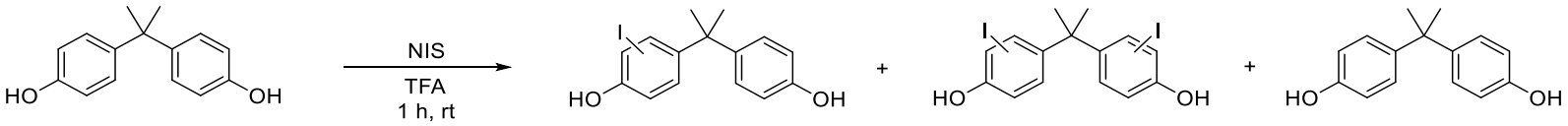


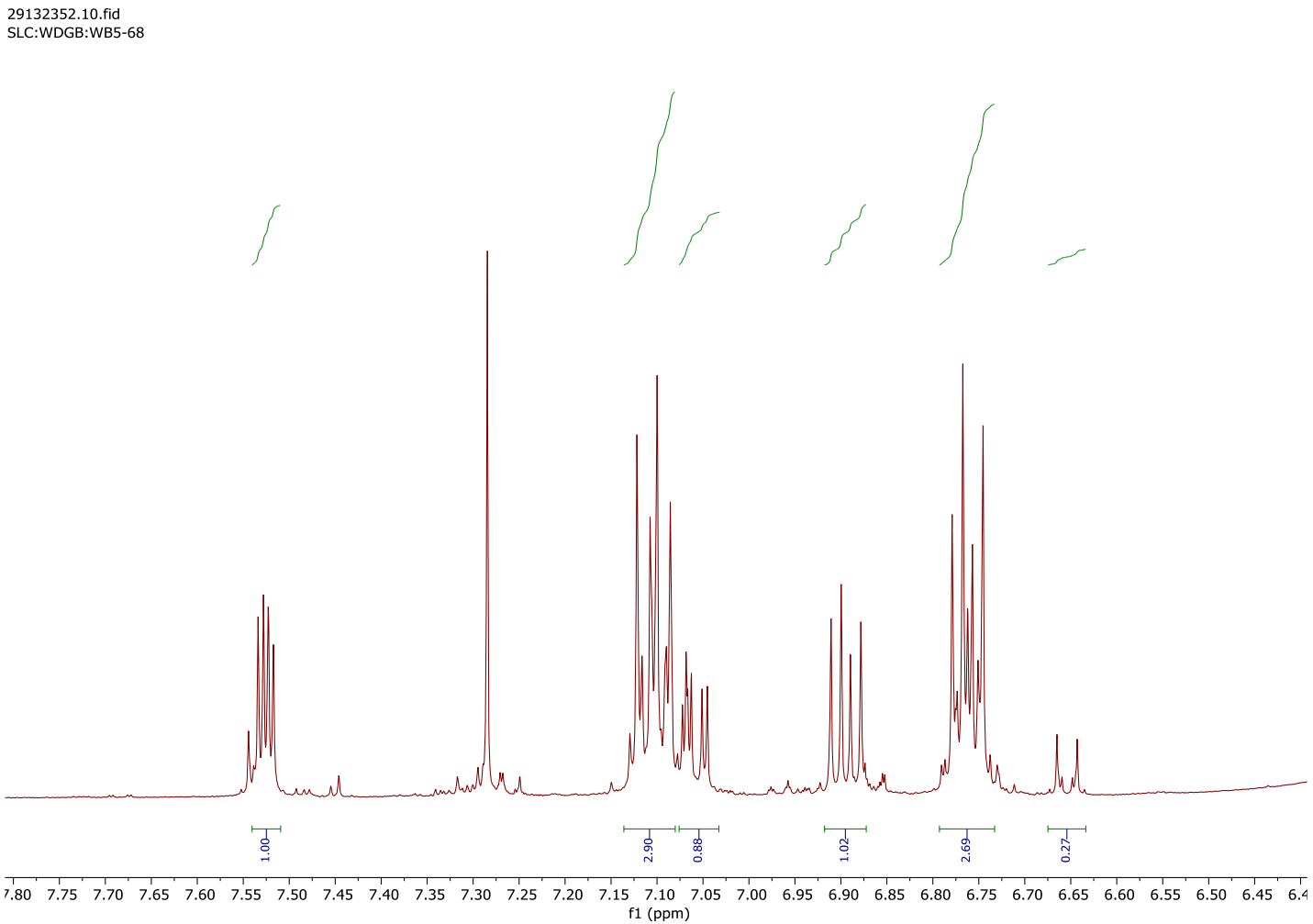
^{1}H NMR of Crude Reaction Mixture of Iodination of TFP-BPA



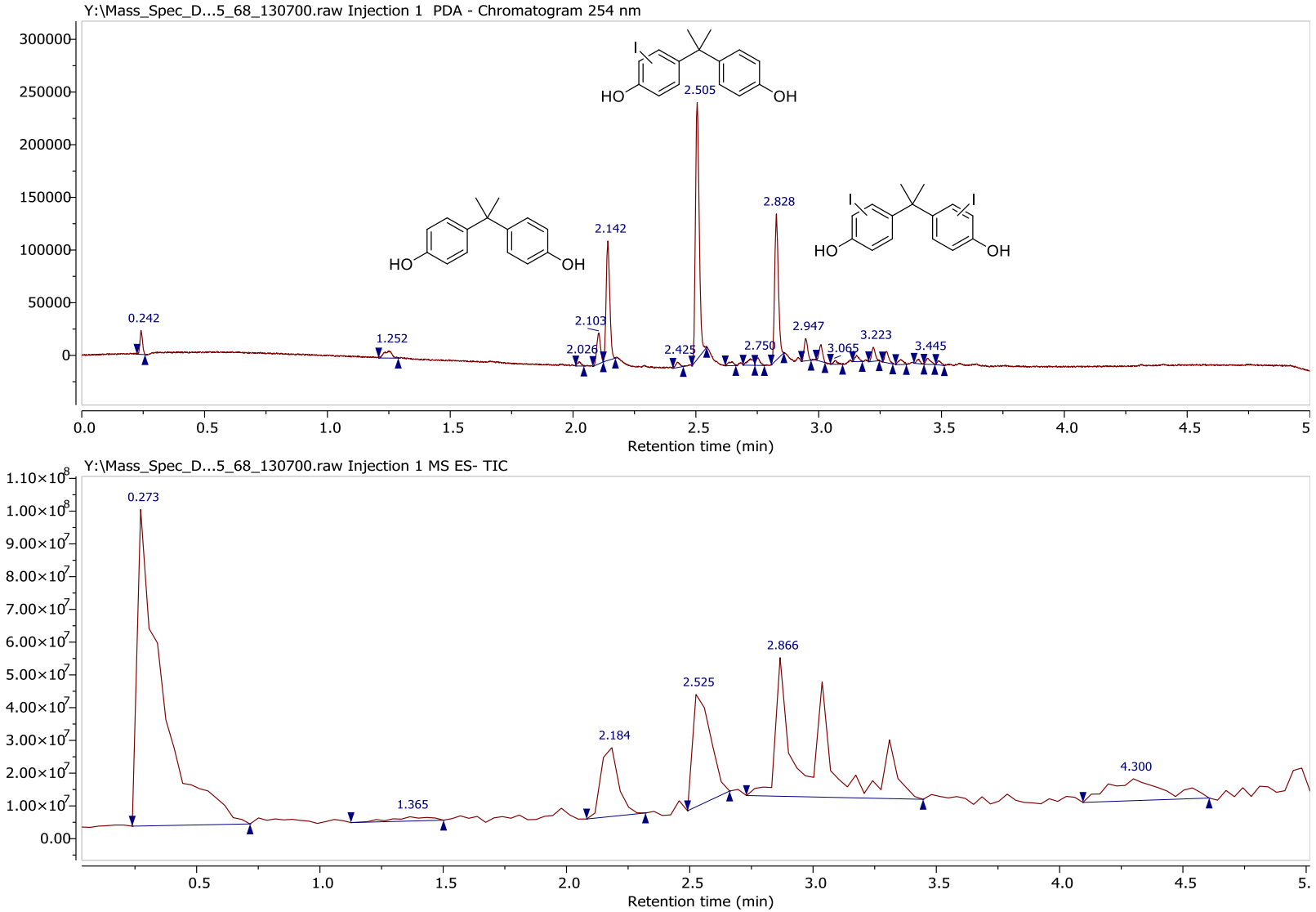


^{1}H NMR of Crude Reaction Mixture of Iodination of BPA

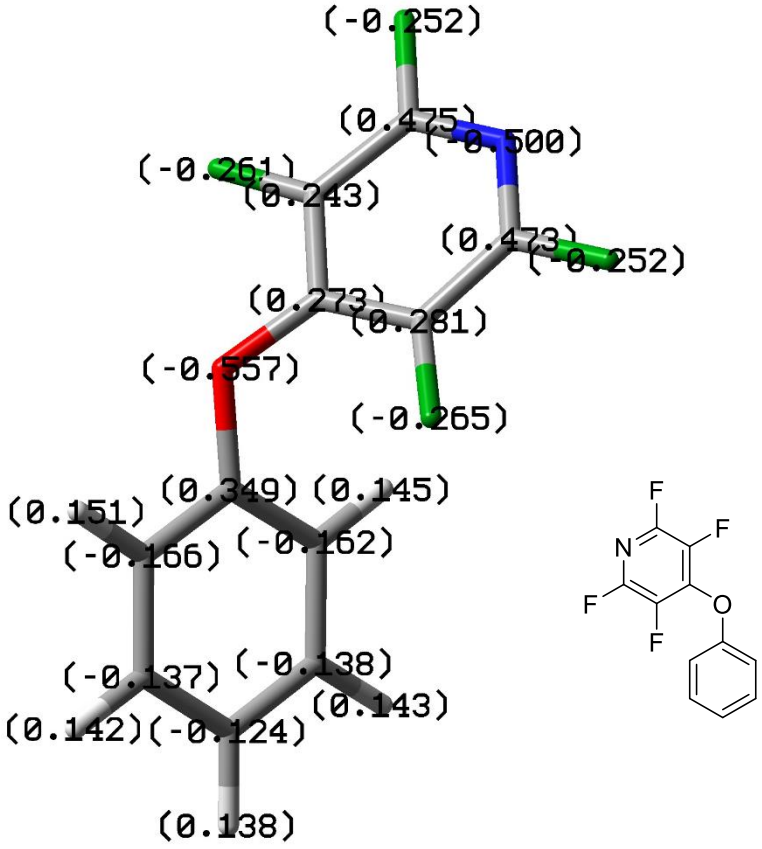


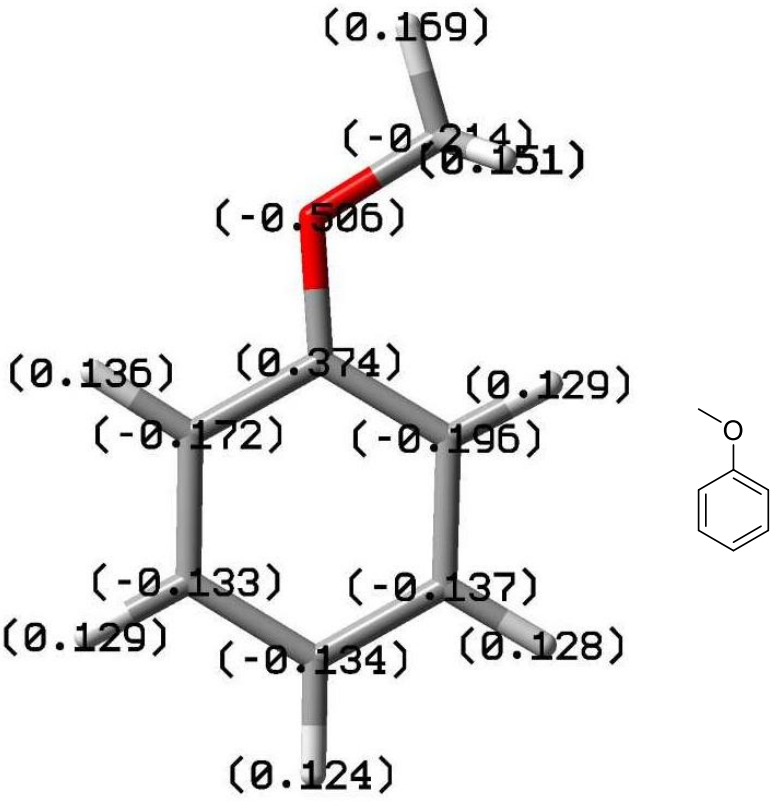


LCMS of Crude Reaction Mixture of Iodination of BPA



Mulliken Atomic Charge Values on Static Optimised Geometries of Anisole and TFP-Phenol





Computations

Optimized geometries of PhOTFP and PhOMe and their Mulliken charges were performed with the Gaussian 09 package[1] using the popular B3LYP[2,3] functional with the 6-31(d) basis set.[4,5] The optimized S_0 geometries were true minima based on no imaginary frequencies found from frequency calculations.

Cartesian Coordinates

PhOTFP

B3LYP 6-31G(d)
Total Energy = -951.466658 au
Imaginary Frequency = 0
Gibbs Free Energy = -951.367192 au

C	-4.374618	0.241140	0.678900
C	-4.222420	-0.333231	-0.585216
C	-2.959932	-0.707014	-1.043691
C	-1.854432	-0.500872	-0.221922
C	-1.984947	0.058442	1.047333
C	-3.254748	0.433841	1.489007
H	-5.359235	0.534127	1.030803
H	-5.088342	-0.489592	-1.222229
H	-2.817141	-1.152945	-2.022549
H	-1.115993	0.193499	1.683595
H	-3.364058	0.873371	2.476425
O	-0.632931	-0.963348	-0.719150
C	0.534646	-0.379437	-0.360958
C	0.769011	1.002743	-0.391631
C	1.616861	-1.208035	-0.036978
C	2.042123	1.465437	-0.072959
C	2.845671	-0.618448	0.243207
N	3.054396	0.681403	0.231724
F	1.461072	-2.534372	0.000712
F	-0.210253	1.855286	-0.717295
F	2.261309	2.781691	-0.091242
F	3.875001	-1.408037	0.553884

PhOMe

B3LYP 6-31G(d)
Total Energy = -346.771321 au
Imaginary Frequency = 0
Gibbs Free Energy = -346.668736 au

C	2.283558	0.330606	-0.000029
C	1.336290	1.351641	-0.000079
C	-0.032584	1.063643	0.000104
C	-0.454700	-0.271095	0.000072
C	0.495022	-1.303614	0.000161
C	1.851813	-1.000474	-0.000167
H	3.344114	0.564725	0.000503
H	1.656099	2.390637	0.000210
H	-0.750287	1.876188	-0.000341
H	0.142631	-2.330484	-0.000108
H	2.578130	-1.809153	-0.000365
O	-1.761457	-0.672070	0.000041
C	-2.768811	0.325067	-0.000119
H	-3.720549	-0.209731	-0.000671
H	-2.711281	0.959260	0.894885
H	-2.710726	0.960471	-0.894111

Crystal Structure Data

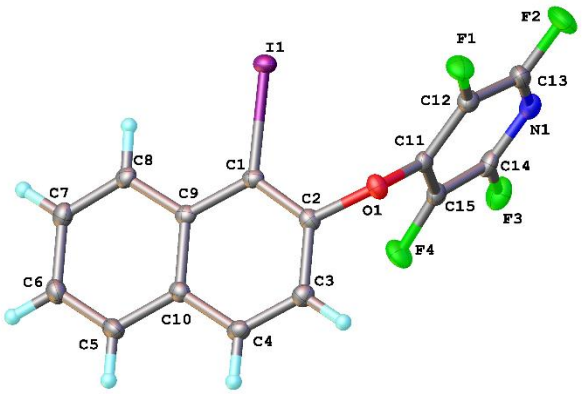


Figure S-1) Crystal structure of compound 3f, ellipsoids are drawn at the 50% probability level. Sample was prepared by slow evaporation from DCM.

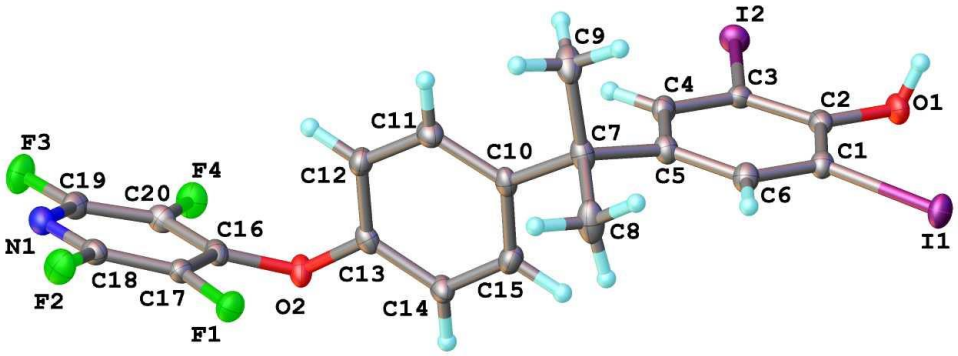


Figure S-2) Crystal structure of compound 8, ellipsoids are drawn at the 50% probability level. Sample was prepared by slow evaporation from toluene.The X-ray single crystal data have been collected using λMoKα radiation (λ =0.71073Å) on an Agilent XCalibur (compound **8,** Sapphire-3 CCD detector, fine-focus sealed tube, graphite monochromator, ω-scan, 1.0°/frame) and on a Bruker D8Venture (compound **3f**, Photon100 CMOS detector, IμS-microsource, focusing mirrors) diffractometers equipped with a Cryostream (Oxford Cryosystems) open-flow nitrogen cryostat at the temperature 120.0(2)K. The structures were solved by direct method and refined by full-matrix least squares on F^2 for all data using Olex2[6] and SHELXTL[7] software. All non-hydrogen atoms were refined anisotropically, hydrogen atoms were placed in the calculated positions and refined in riding mode. Crystal data and parameters of refinement are listed in Table S2. Crystallographic data for the structure have been deposited with the Cambridge Crystallographic Data Centre as supplementary publications CCDC-1948713 and 1947954.

Table S2. Crystal data and structure refinement for compounds **3f** and **8**.

Compound	**3f**	**8**
Empirical formula	$C_{15}H_6F_4INO$	$C_{20}H_{13}F_4I_2NO_2$
Formula weight	419.1	629.11
Crystal system	monoclinic	monoclinic
Space group	$P2_1$	$P2_1/c$

a/Å	4.6677(3)	12.3523(3)
b/Å	11.0185(7)	12.7890(3)
c/Å	13.0170(8)	12.8327(3)
β/°	90.865(2)	94.170(2)
Volume/Å^3	669.40(7)	2021.86(9)
Z	2	4
ρ_{calc}g/cm^3	2.079	2.067
μ/mm^{-1}	2.439	3.163
F(000)	400.0	1192.0
Crystal size/mm^3	0.23 × 0.1 × 0.06	0.38 × 0.17 × 0.15
2Θ range for data collection/°	6.26 to 59.99	4.59 to 58.994
Reflections collected	14627	20412
Independent reflections, R_{int}	3908, 0.0261	5635, 0.0394
Data/restraints/parameters	3908/1/199	5635/0/264
Goodness-of-fit on F^2	1.048	1.024
Final R indexes [I>=2σ (I)]	R_1 = 0.0163, wR_2 = 0.0397	R_1 = 0.0294, wR_2 = 0.0642
Final R indexes [all data]	R_1 = 0.0176, wR_2 = 0.0401	R_1 = 0.0426, wR_2 = 0.0711
Largest diff. peak/hole / e Å^{-3}	0.58/-0.53	0.81/-0.90
Flack parameter	-0.044(7)	n/a

References

1. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr. ; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09, Revision A.02. *Gaussian, Inc Wallingford CT* **2009**.

2. Becke, A. D. Density-Functional Thermochemistry .3. The Role of Exact Exchange. *J. Chem. Phys.* **1993**, *98*, 5648-5652.

3. Lee, C. T.; Yang, W. T.; Parr, R. G. Development of the Colle-Salvetti Correlation-Energy Formula into a Functional of the Electron-Density. *Phys. Rev. B* **1988**, *37*, 785-789.

4. Petersson, G. A.; Allaham, M. A. A Complete Basis Set Model Chemistry .2. Open-Shell Systems and the Total Energies of the 1st-Row Atoms. *J. Chem. Phys.* **1991**, *94*, 6081-6090.

5. Petersson, G. A.; Bennett, A.; Tensfeldt, T. G.; Allaham, M. A.; Shirley, W. A.; Mantzaris, J. A Complete Basis Set Model Chemistry .1. The Total Energies of Closed-Shell Atoms and Hydrides of the 1st-Row Elements. *J. Chem. Phys.* **1988**, *89*, 2193-2218.

6. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard, H. Puschmann, *J. Appl. Crystallogr.* **2009**, *42*, 339-341.
7. G. Sheldrick, *Acta Cryst.* **2008**, *64*, 112-122.