Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

The Supporting Information for

Design, synthesis and properties of near-infrared molecular switches containing fluorene ring

Peng Chen, Hai-Ming Wang and Sean Xiao-An Zhang*

TABLE OF CONTENT:

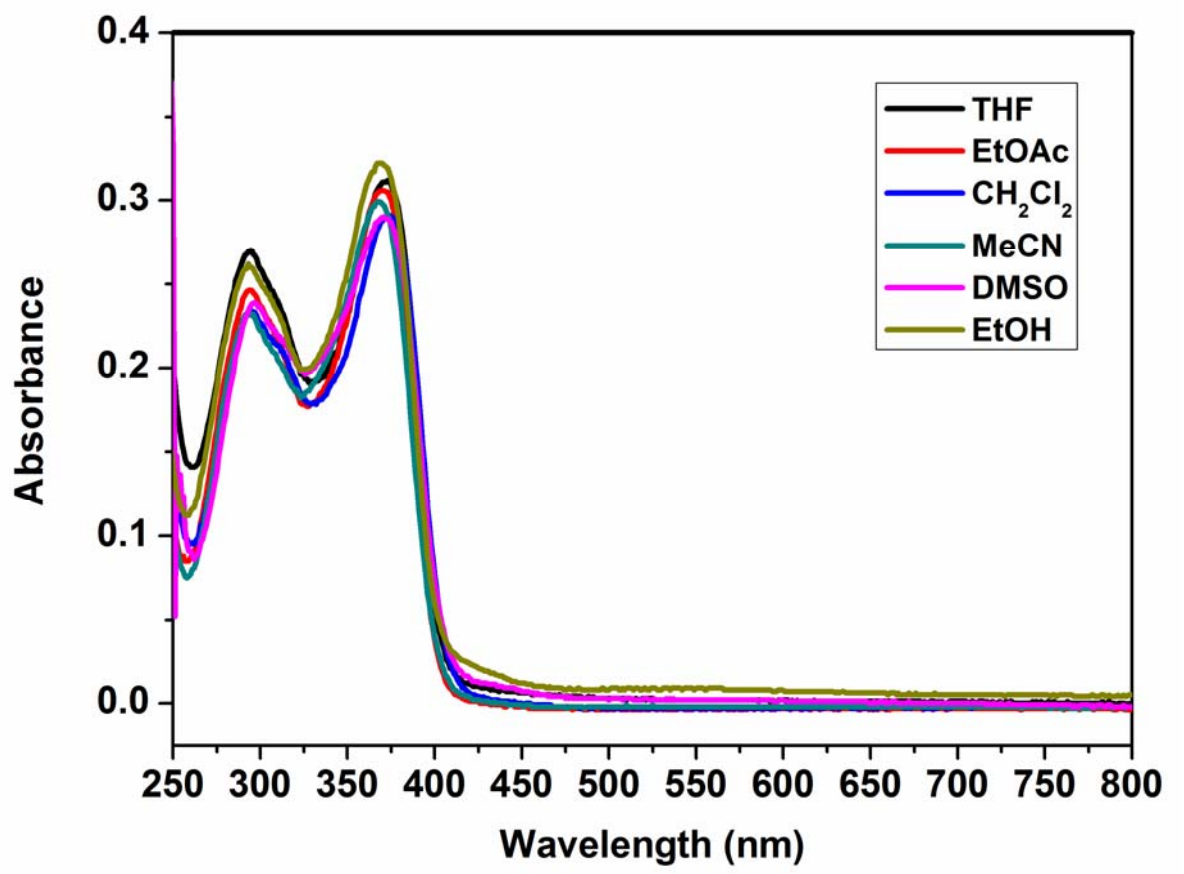


Fig. S1 UV-visible absorption spectra of **IB** in different solvents at the concentration of 0.01 mM.

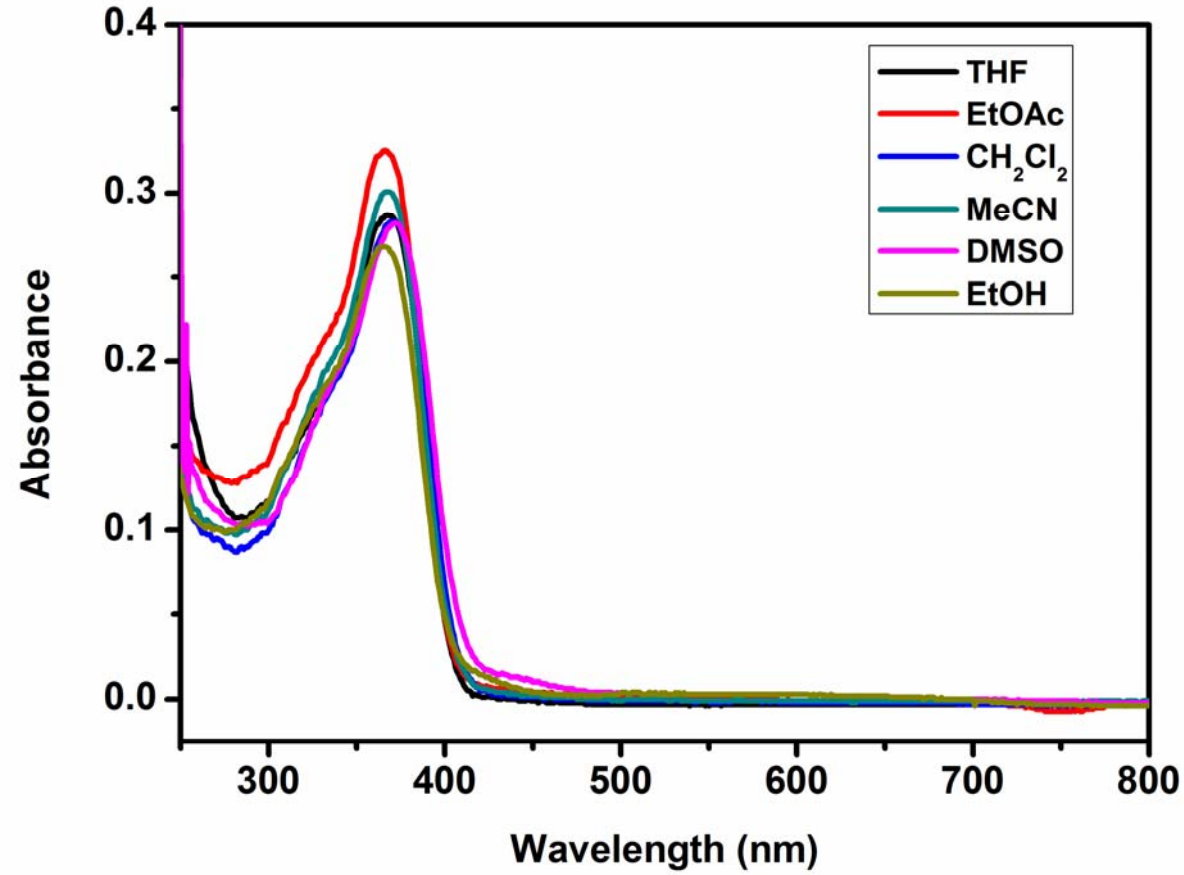


Fig. S2 UV-visible absorption spectra of **IIB** in different solvents at the concentration of 0.01 mM.

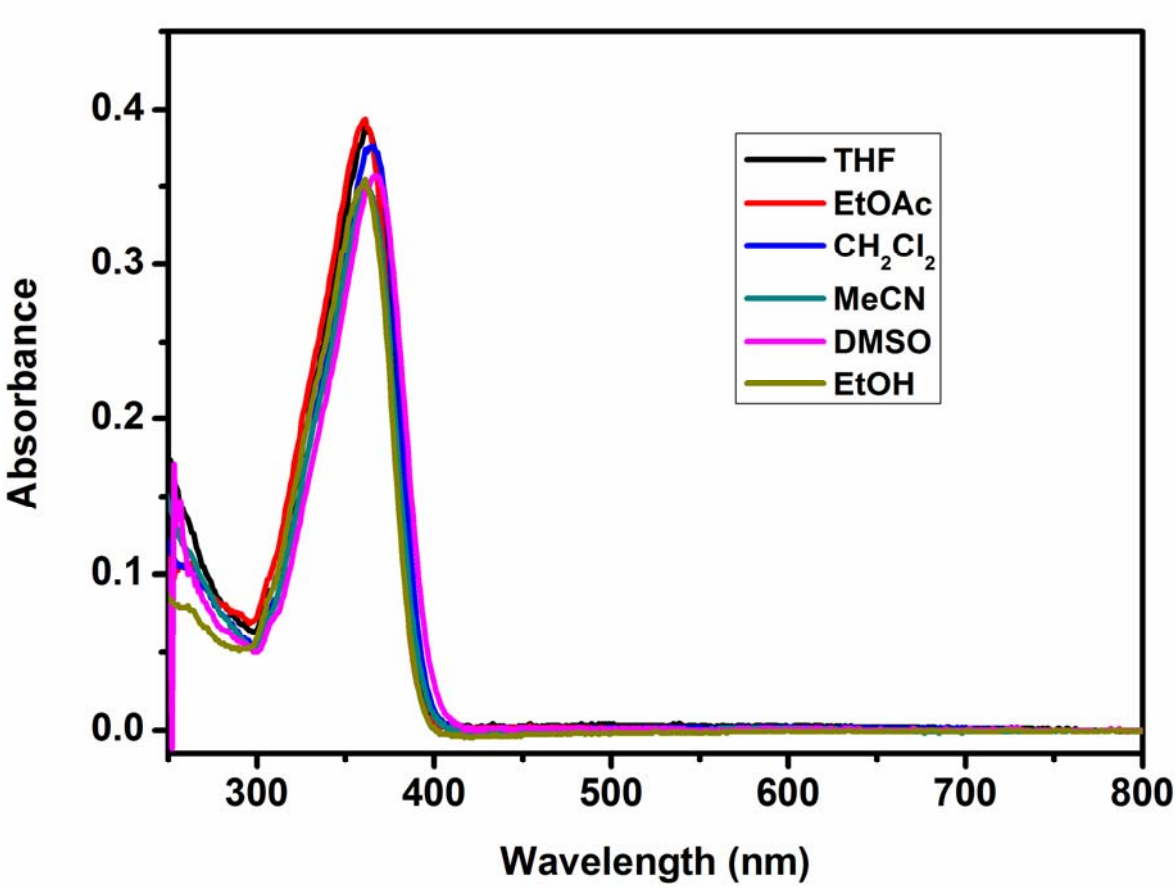
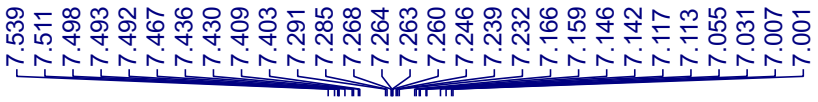


Fig. S3 UV-visible absorption spectra of **IIIB** in different solvents at the concentration of 0.01 mM.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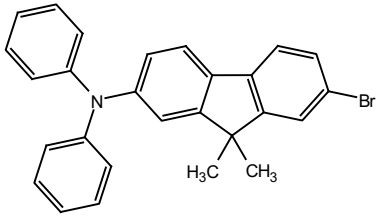
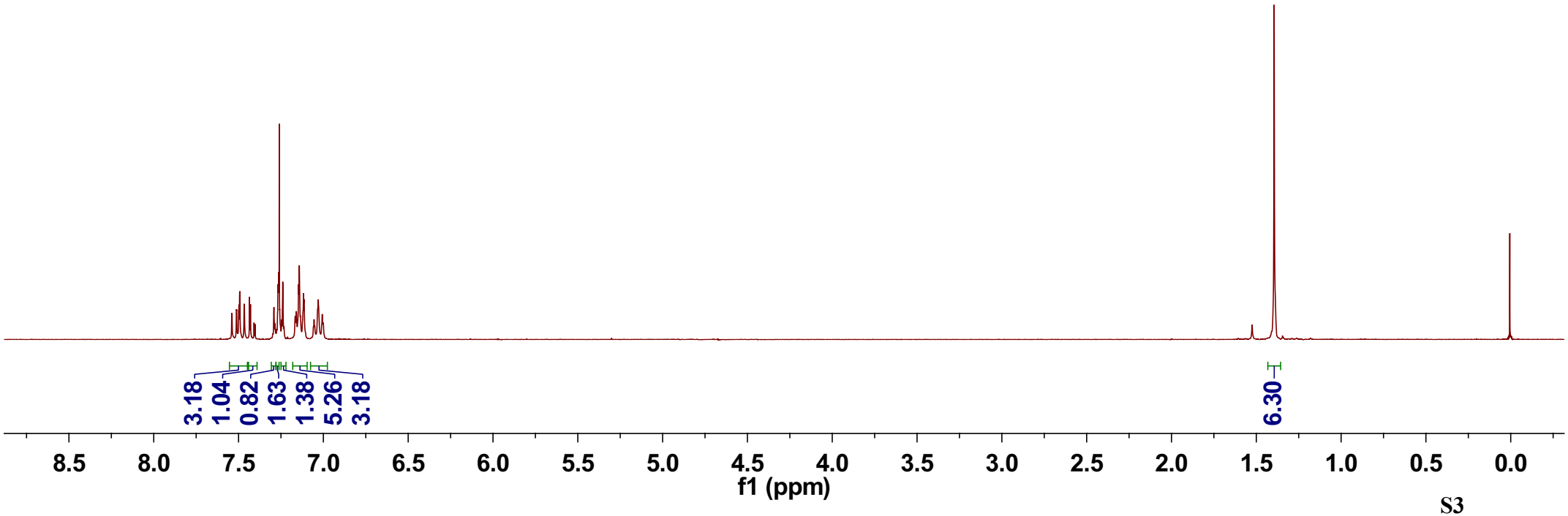
7.498
7.493
7.492
7.467
7.436
7.430
7.409
7.403
7.291
7.285
7.268
7.264
7.263
7.260
7.246
7.239
7.232
7.166
7.159
7.146
7.142
7.117
7.113
7.055
7.031
7.007
7.001
1.395
0.006


N
Br
H3C
CH3

2: in $CDCl_3$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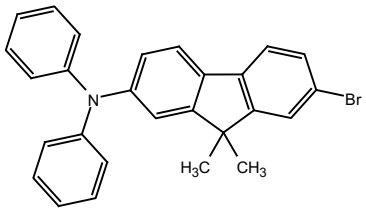
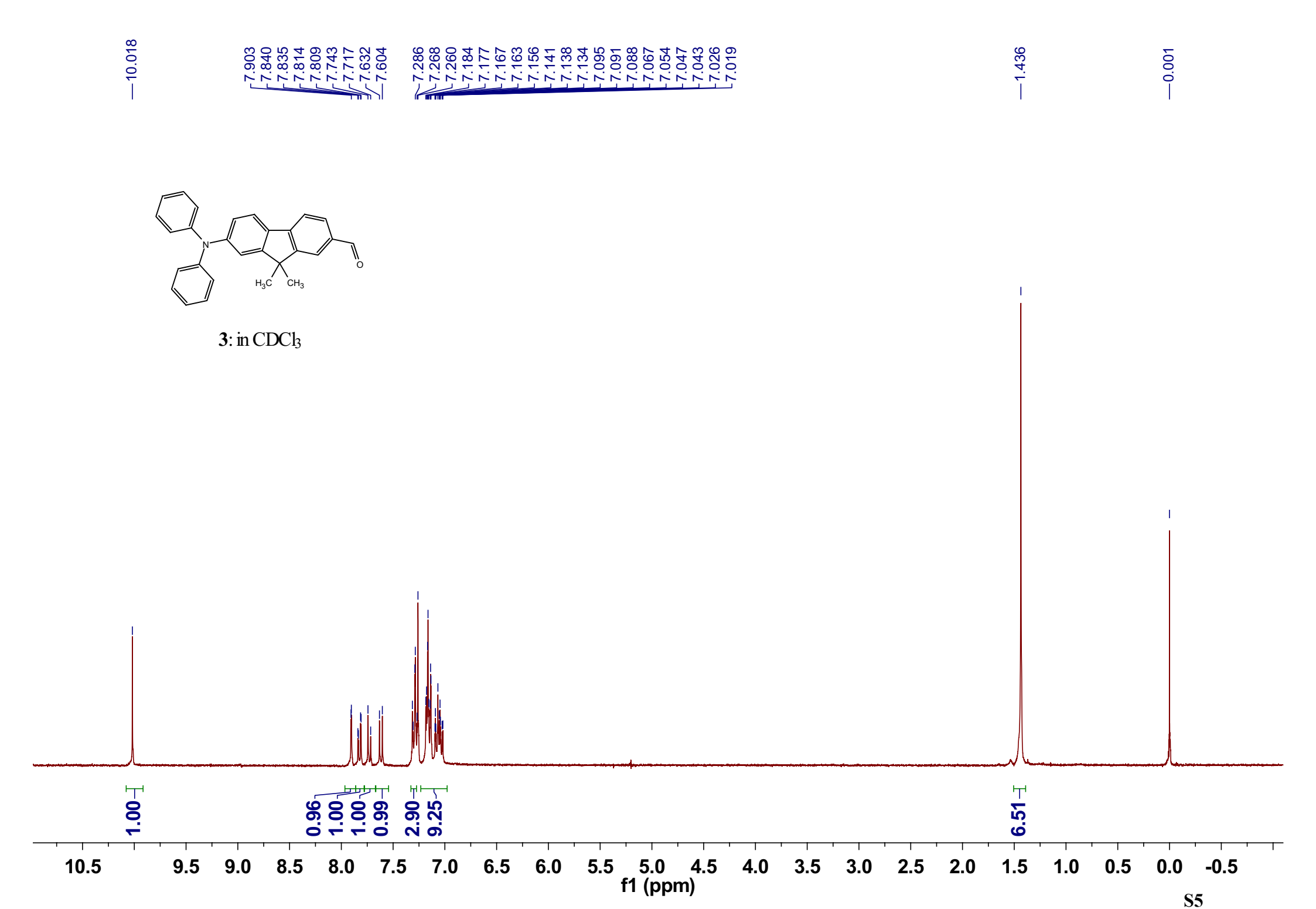
1.04
0.82
1.63
1.38
5.26
3.18
6.30
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


N
Br
H3C
CH3

2: in $CDCl_3$

155.55
154.66
147.83
138.02
132.76
129.23
124.21
122.80
120.69
120.05
118.16
77.25
77.00
76.75
47.01
26.90
155
145
135
125
115
105
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
f1 (ppm)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7.840
7.835
7.814
7.809
7.743
7.717
7.632
7.604
7.286
7.268
7.260
7.184
7.177
7.167
7.163
7.156
7.141
7.138
7.134
7.095
7.091
7.088
7.067
7.054
7.047
7.043
7.026
7.019
1.436
0.001
N
O
H3C
CH3
1.00
0.96
1.00
1.00
0.99
2.90
9.25
6.51
10.5
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
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0.5
0.0
-0.5
f1 (ppm)

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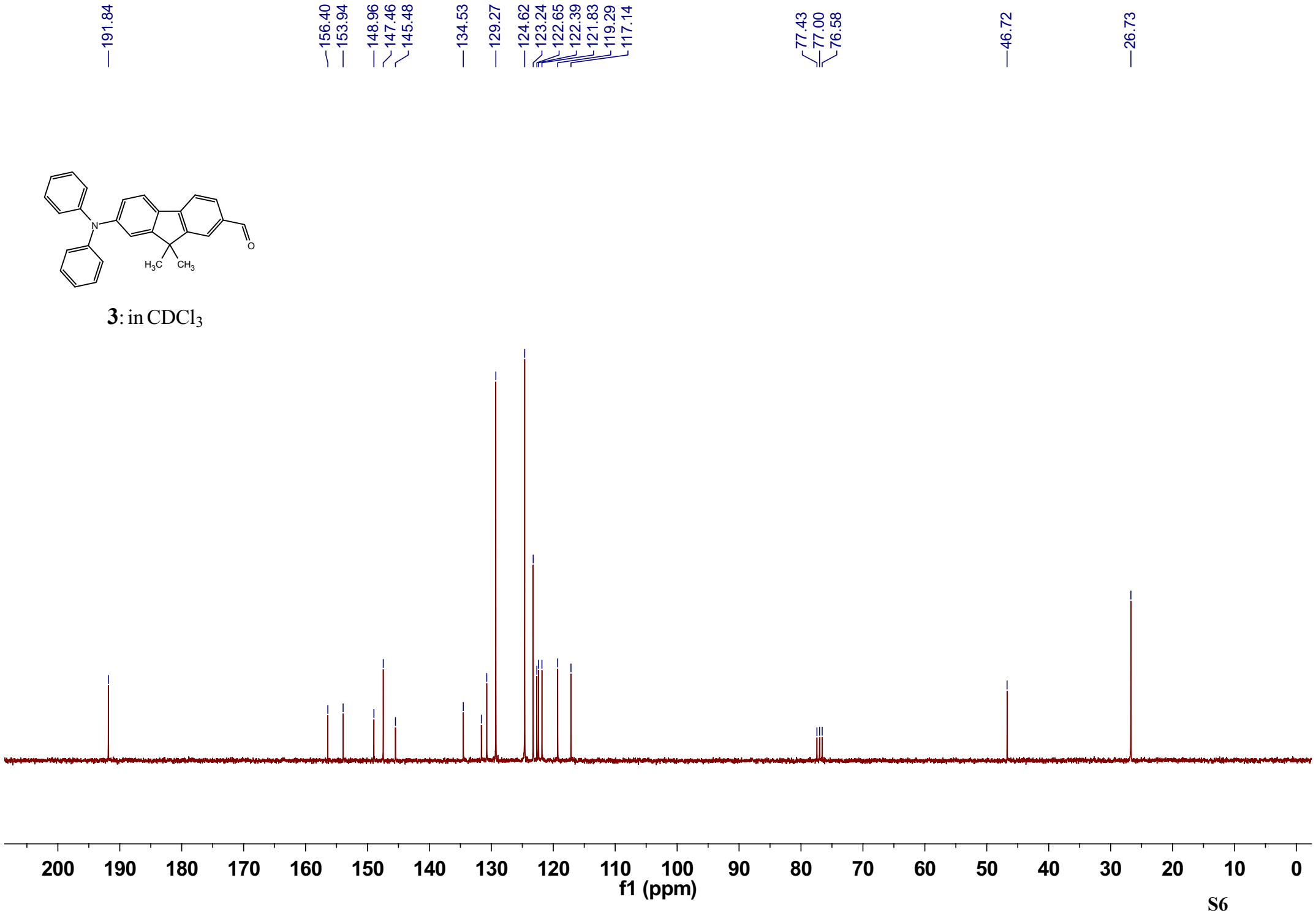
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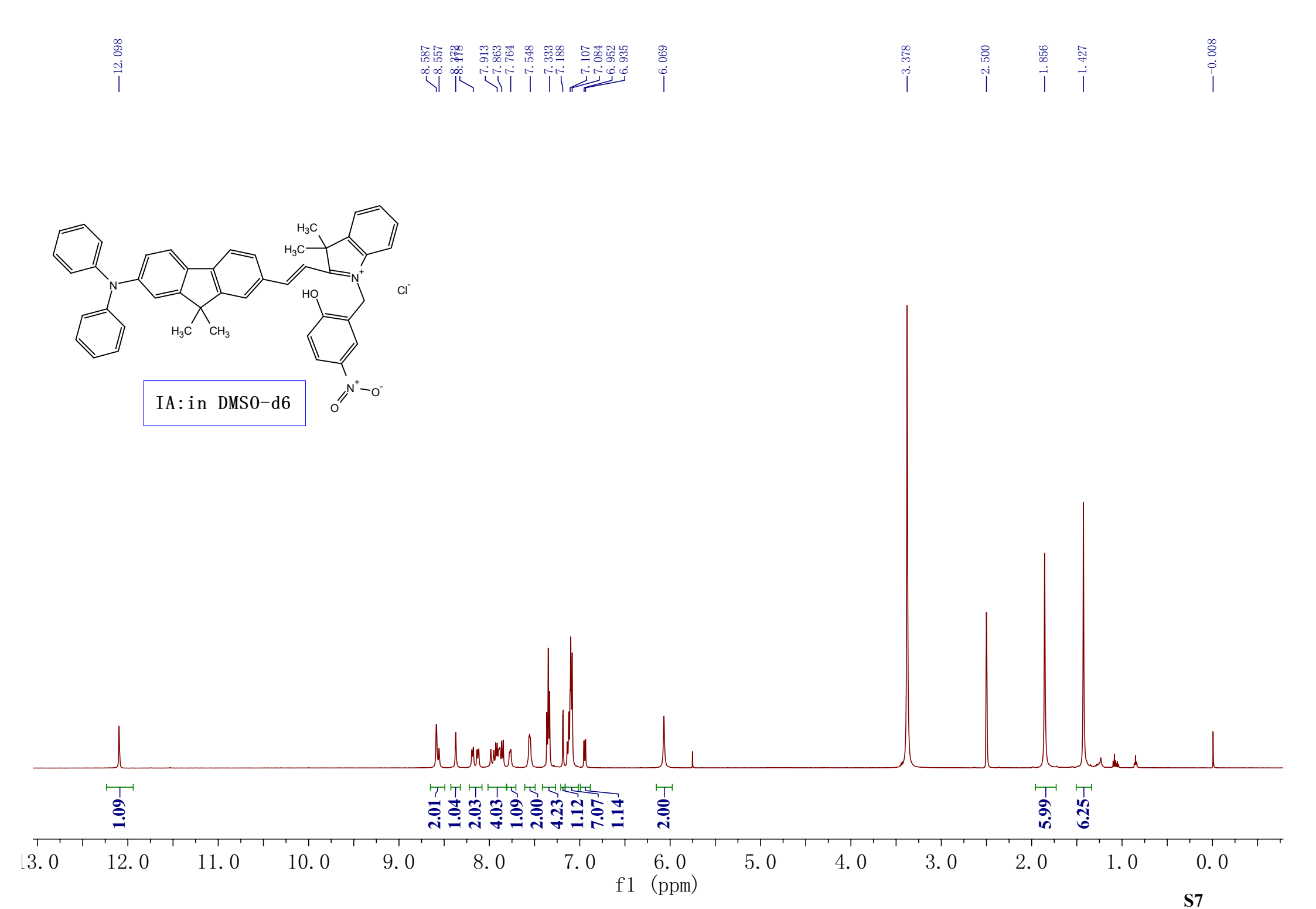
156.40
153.94
148.96
147.46
145.48
134.53
129.27
124.62
123.24
122.65
122.39
121.83
119.29
117.14
77.43
77.00
76.58
46.72
26.73
N
O
H3C
CH3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

3: in $CDCl_3$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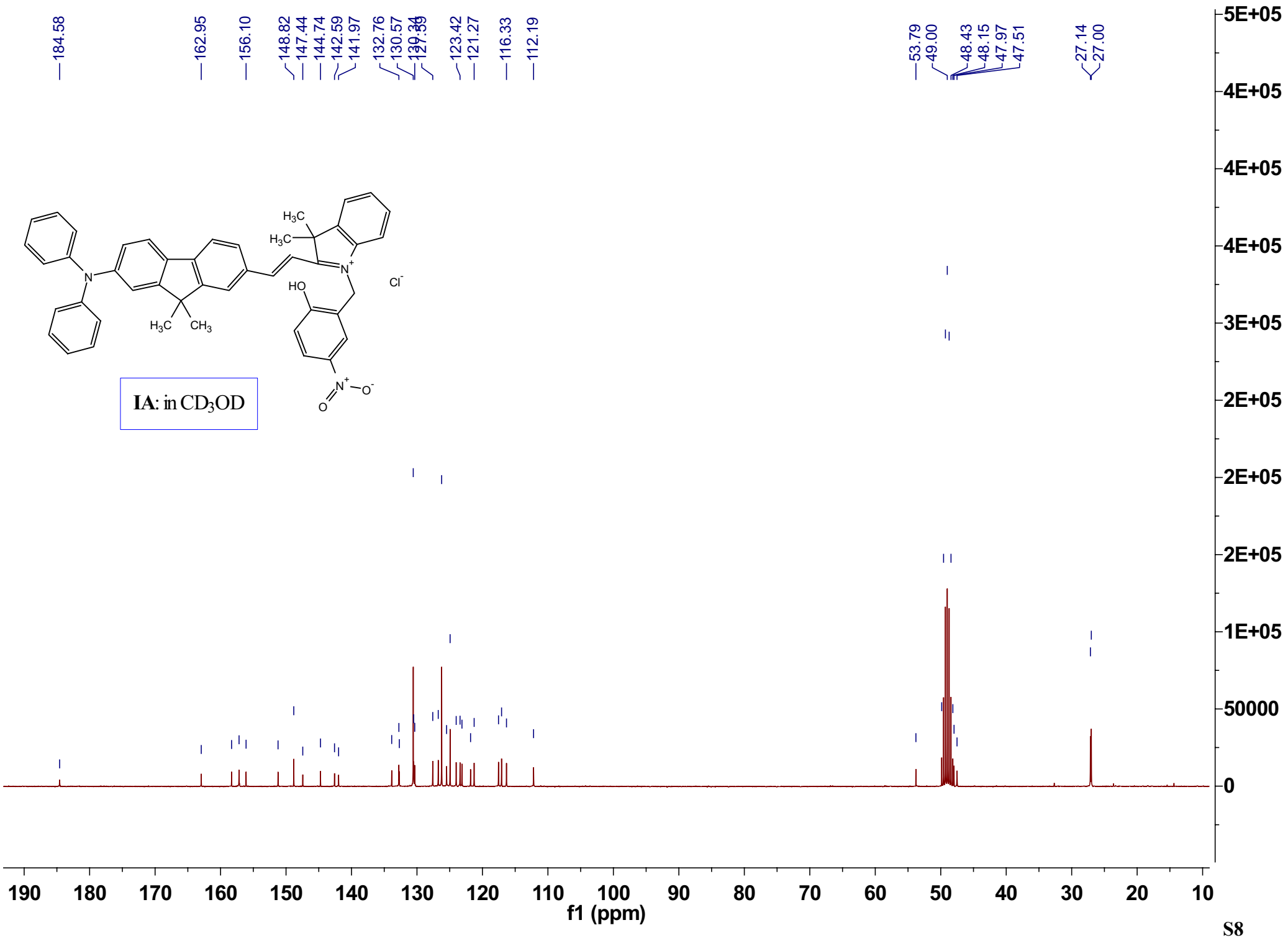
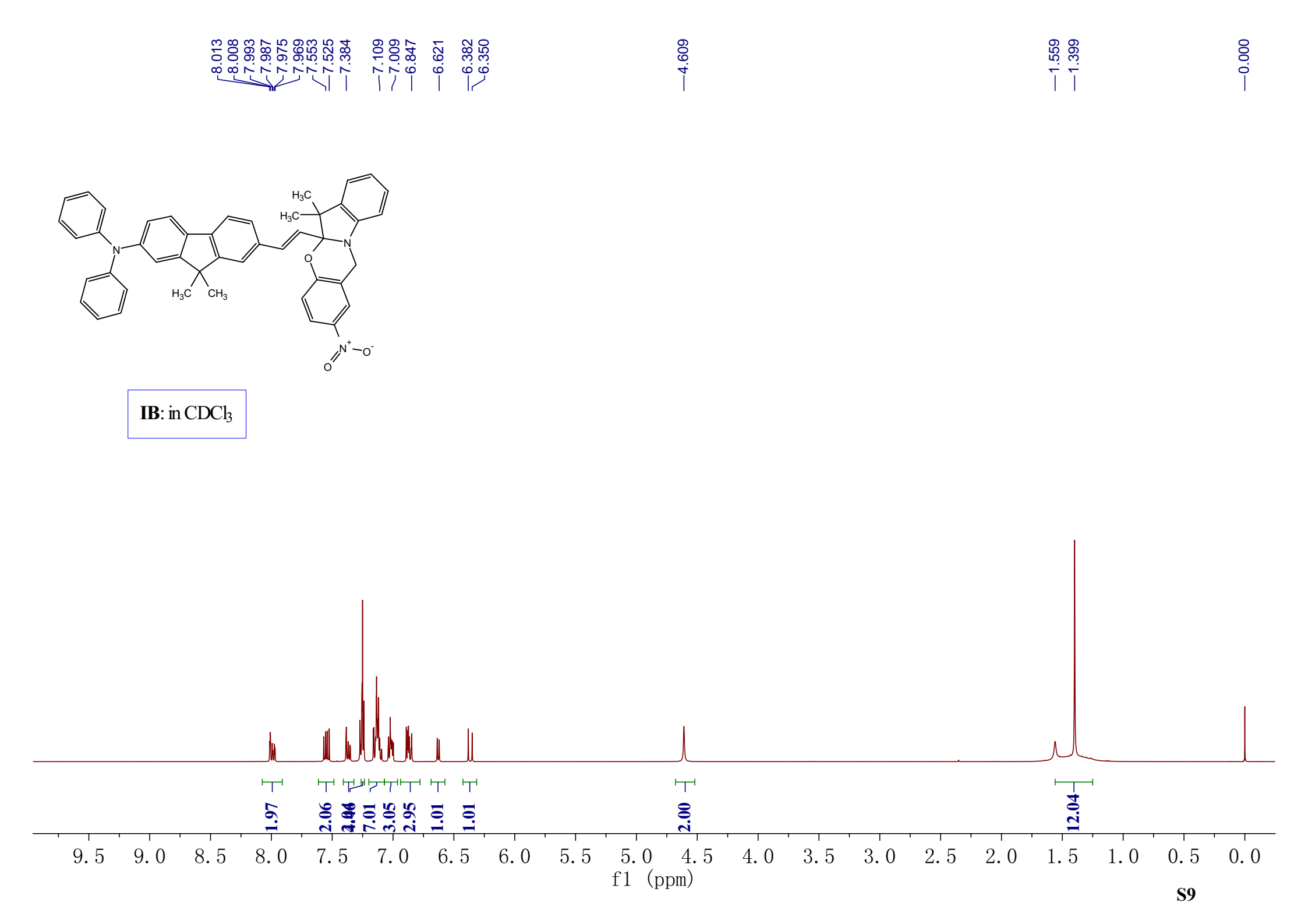
8.557
7.913
7.863
7.764
7.548
7.333
7.188
7.107
7.084
6.952
6.935
6.069
3.378
2.500
1.856
1.427
0.008
IA:in DMSO-d6
1.09
2.01
1.04
2.03
4.03
1.09
2.00
4.23
1.12
7.07
1.14
2.00
5.99
6.25
f1 (ppm)


184.58
162.95
156.10
148.82
147.44
144.74
142.59
141.97
132.76
130.57
123.42
121.27
116.33
112.19
53.79
49.00
48.43
48.15
47.97
47.51
27.14
27.00
5E+05
4E+05
4E+05
4E+05
3E+05
2E+05
2E+05
2E+05
1E+05
50000
0
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)
IA: in CD3OD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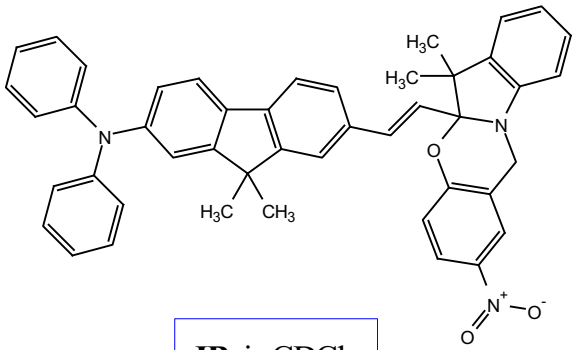
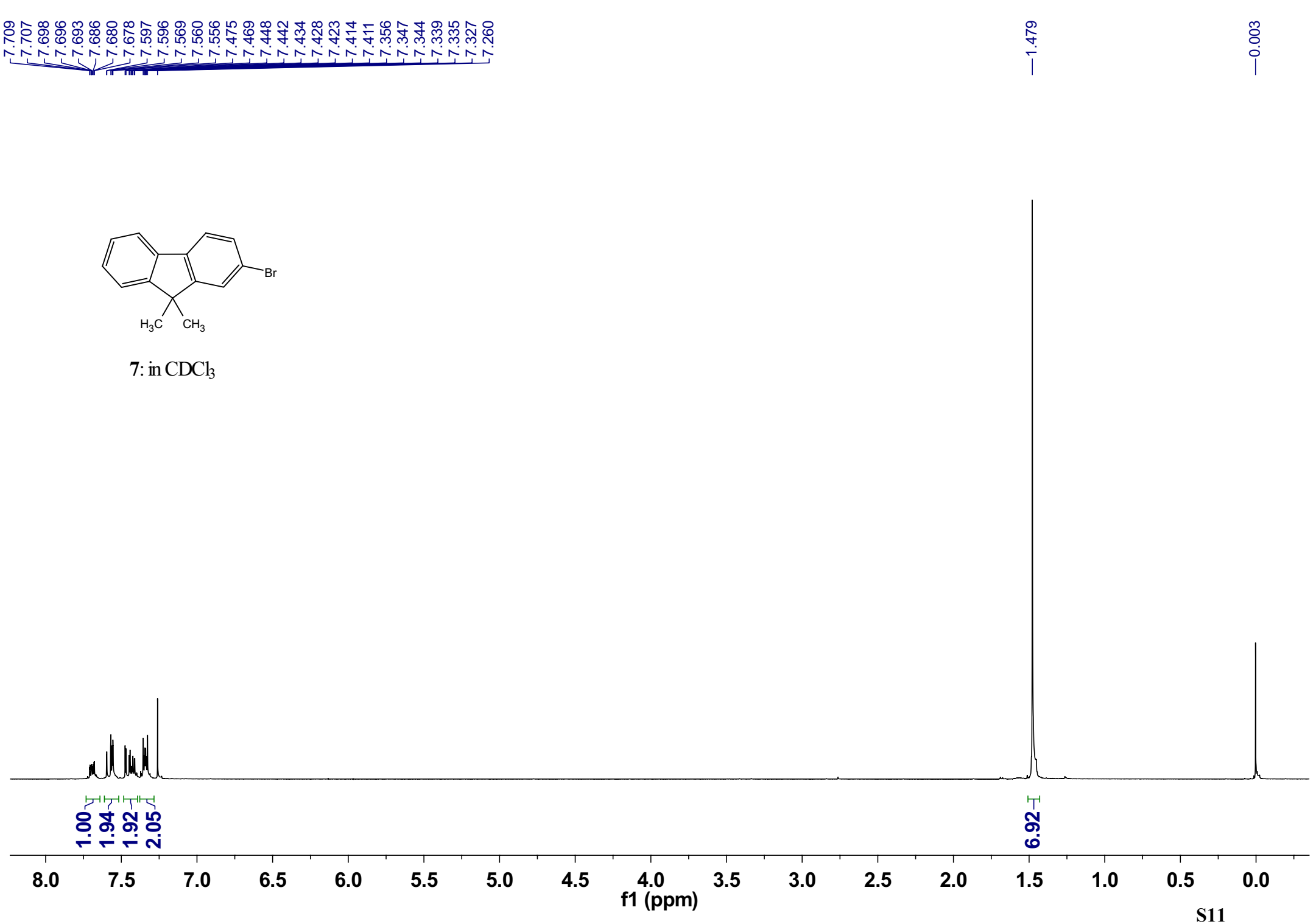
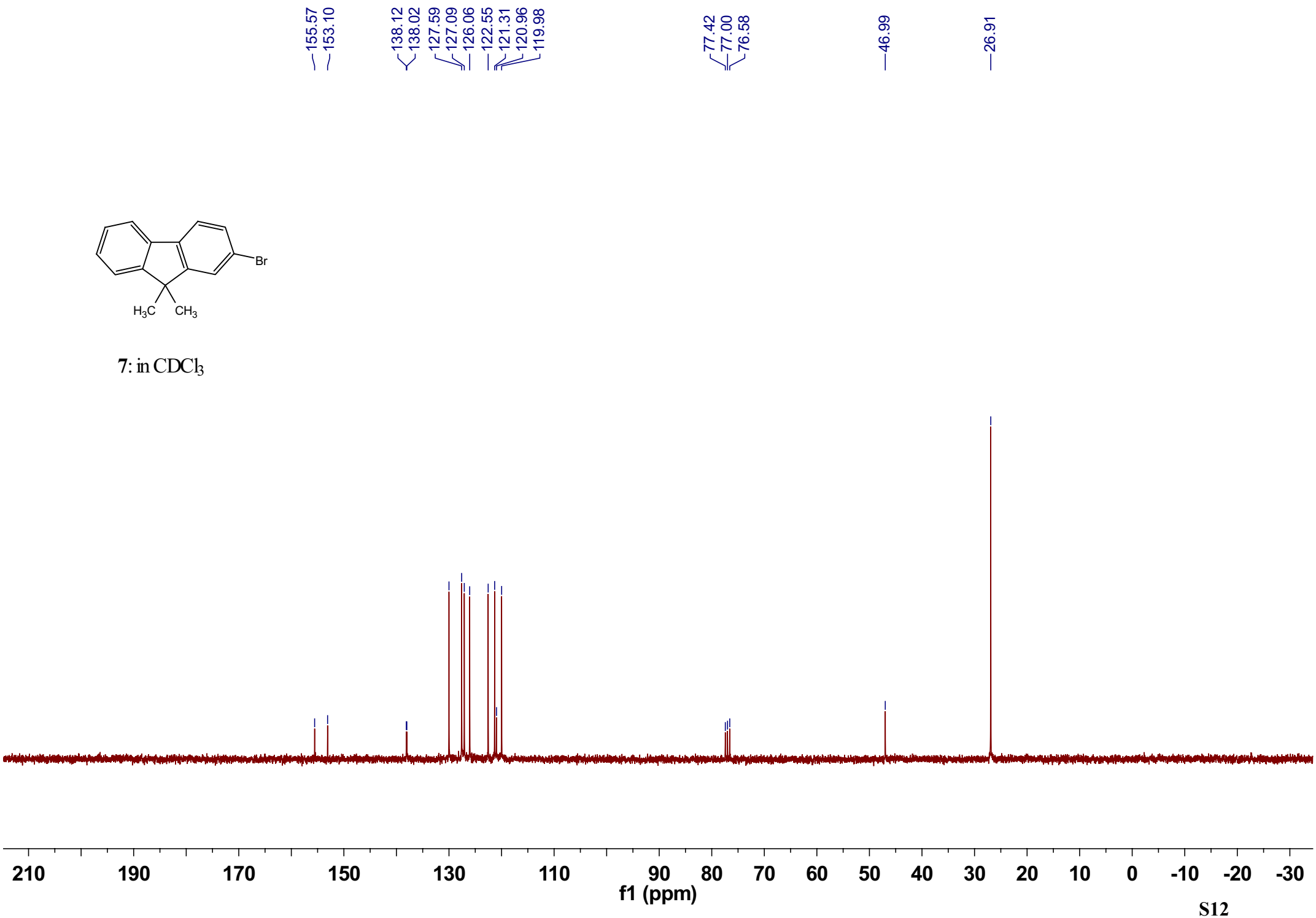
8.008
7.993
7.987
7.975
7.969
7.553
7.525
7.384
7.109
7.009
6.847
6.621
6.382
6.350
4.609
1.559
1.399
0.000
H3C
H3C
N
O
H3C
CH3
N+
O-
O
IB: in CDCl3
1.97
2.06
7.01
3.05
2.95
1.01
1.01
2.00
12.04
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)



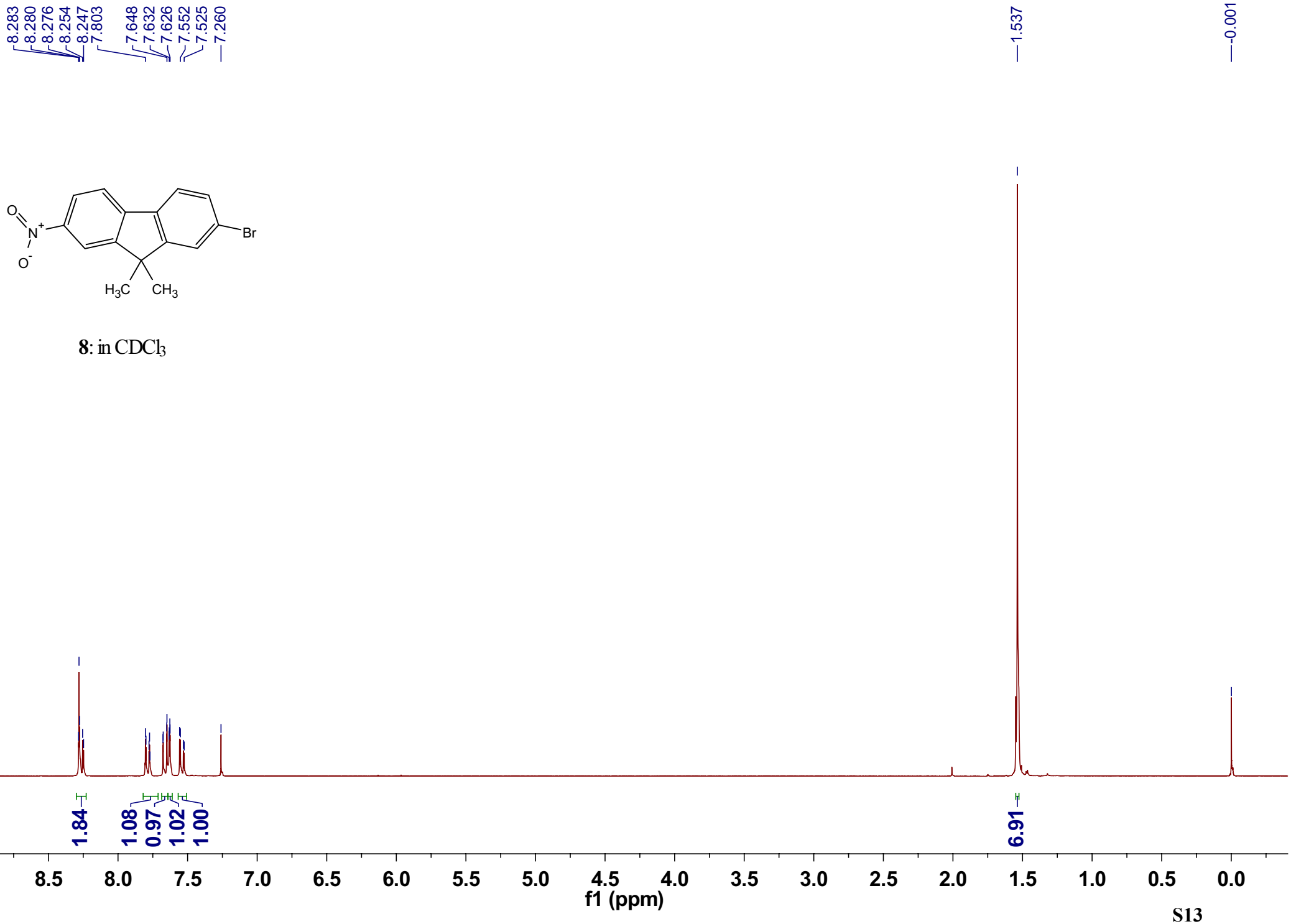
IB: in $CDCl_3$

159.23
154.02
147.81
147.70
146.42
140.55
139.76
138.22
136.54
133.07
129.21
123.95
122.99
122.54
120.87
120.65
119.51
117.61
108.74
103.92
77.25
77.00
76.75
50.11
46.75
40.67
27.01
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

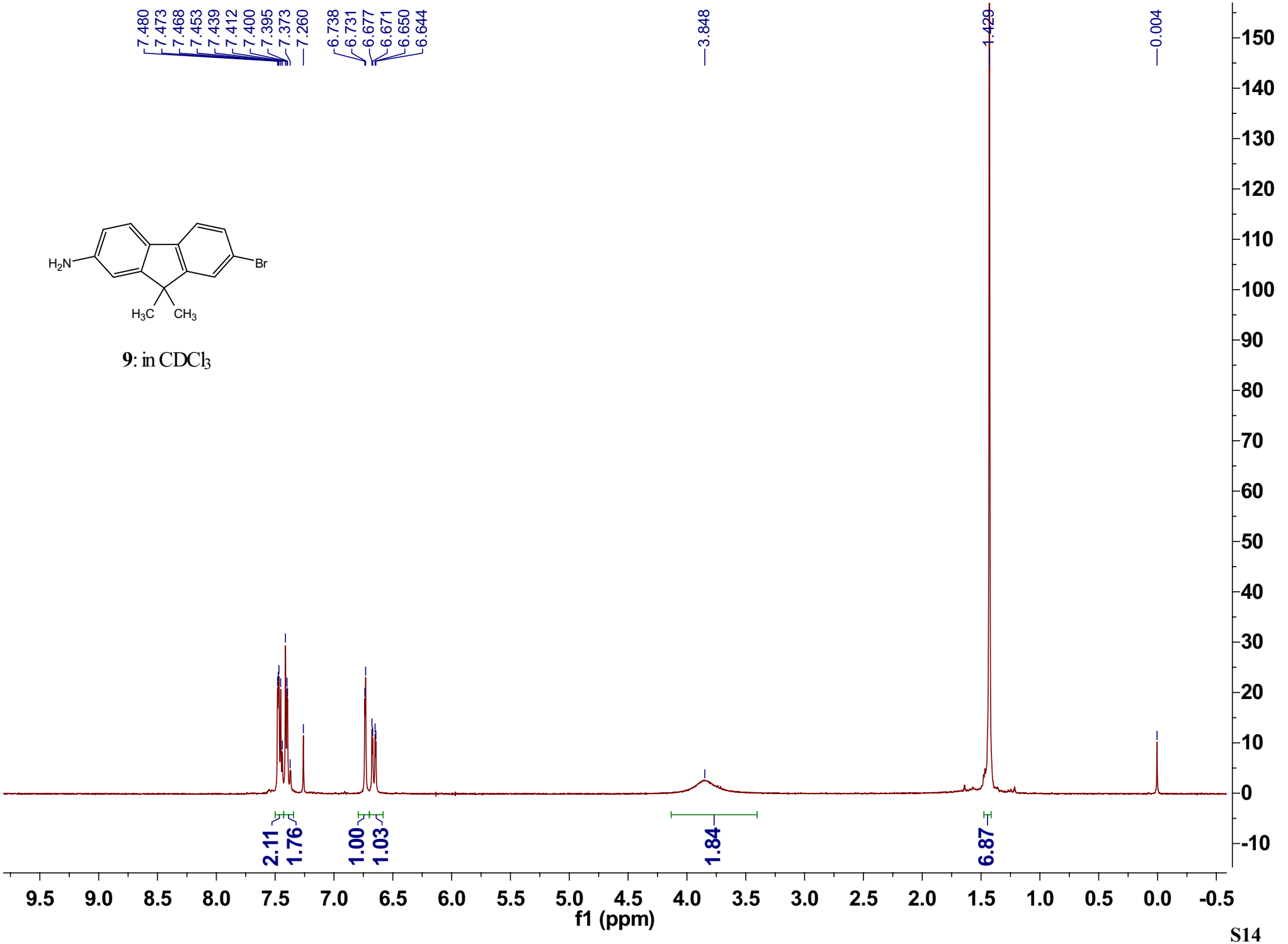

7.709
7.707
7.698
7.696
7.693
7.686
7.680
7.678
7.597
7.596
7.569
7.560
7.556
7.475
7.469
7.448
7.442
7.434
7.428
7.423
7.414
7.411
7.356
7.347
7.344
7.339
7.335
7.327
7.260
1.479
0.003
Br
H3C
CH3
7: in CDCl3
1.00
1.94
1.92
2.05
6.92
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


155.57
153.10
138.12
138.02
127.59
127.09
126.06
122.55
121.31
120.96
119.98
77.42
77.00
76.58
46.99
26.91
Br
H3C
CH3
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
f1 (ppm)

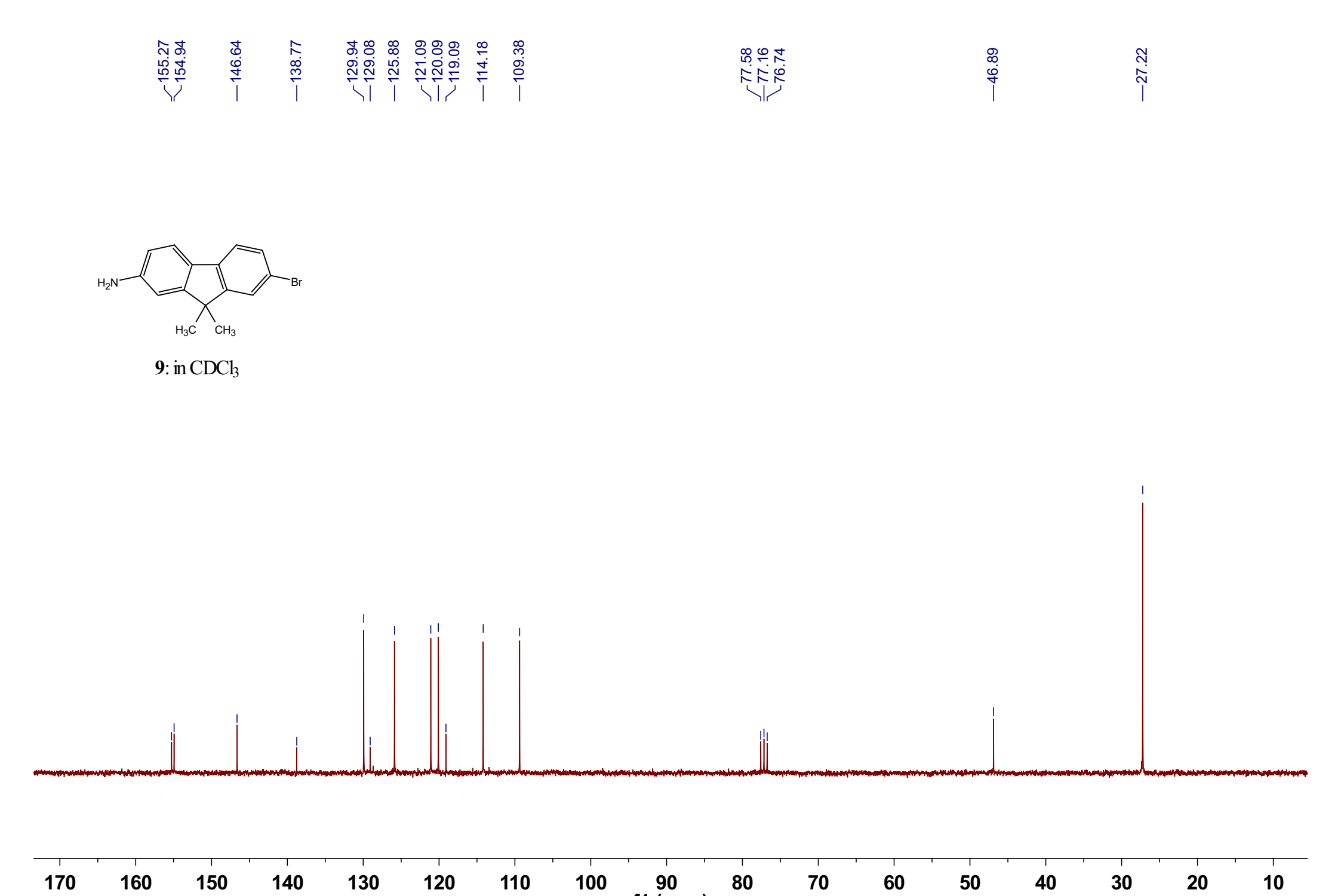
7: in $CDCl_3$


8.283
8.280
8.276
8.254
8.247
7.803
7.648
7.632
7.626
7.552
7.525
7.260
1.537
-0.001
O
N+
O-
Br
H3C
CH3
1.84
1.08
0.97
1.02
1.00
6.91
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)

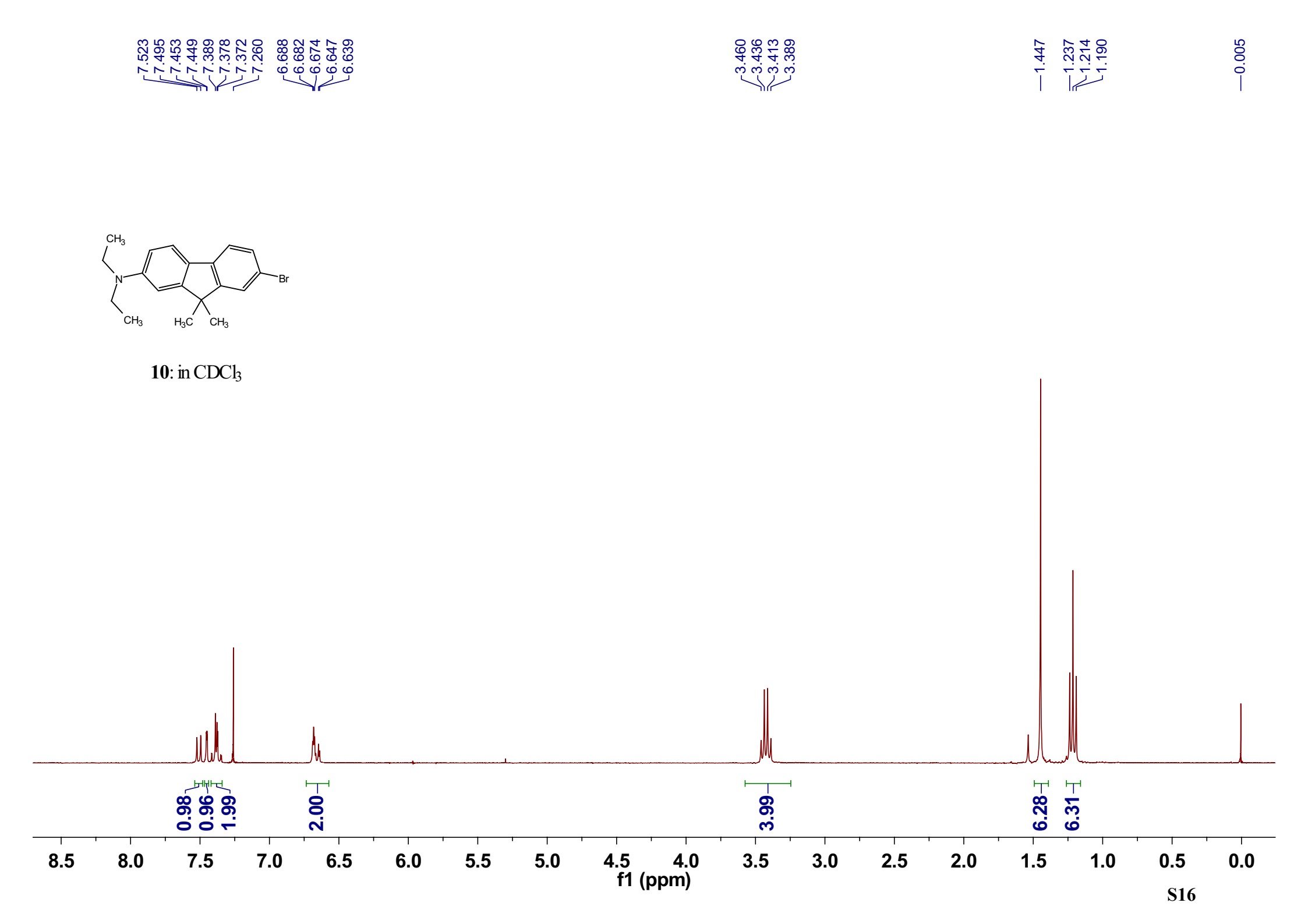
8: in $CDCl_3$


7.480
7.473
7.468
7.453
7.439
7.412
7.400
7.395
7.373
7.260
6.738
6.731
6.677
6.671
6.650
6.644
3.848
1.429
0.004
H2N
Br
H3C
CH3
2.11
1.76
1.00
1.03
1.84
6.87
f1 (ppm)

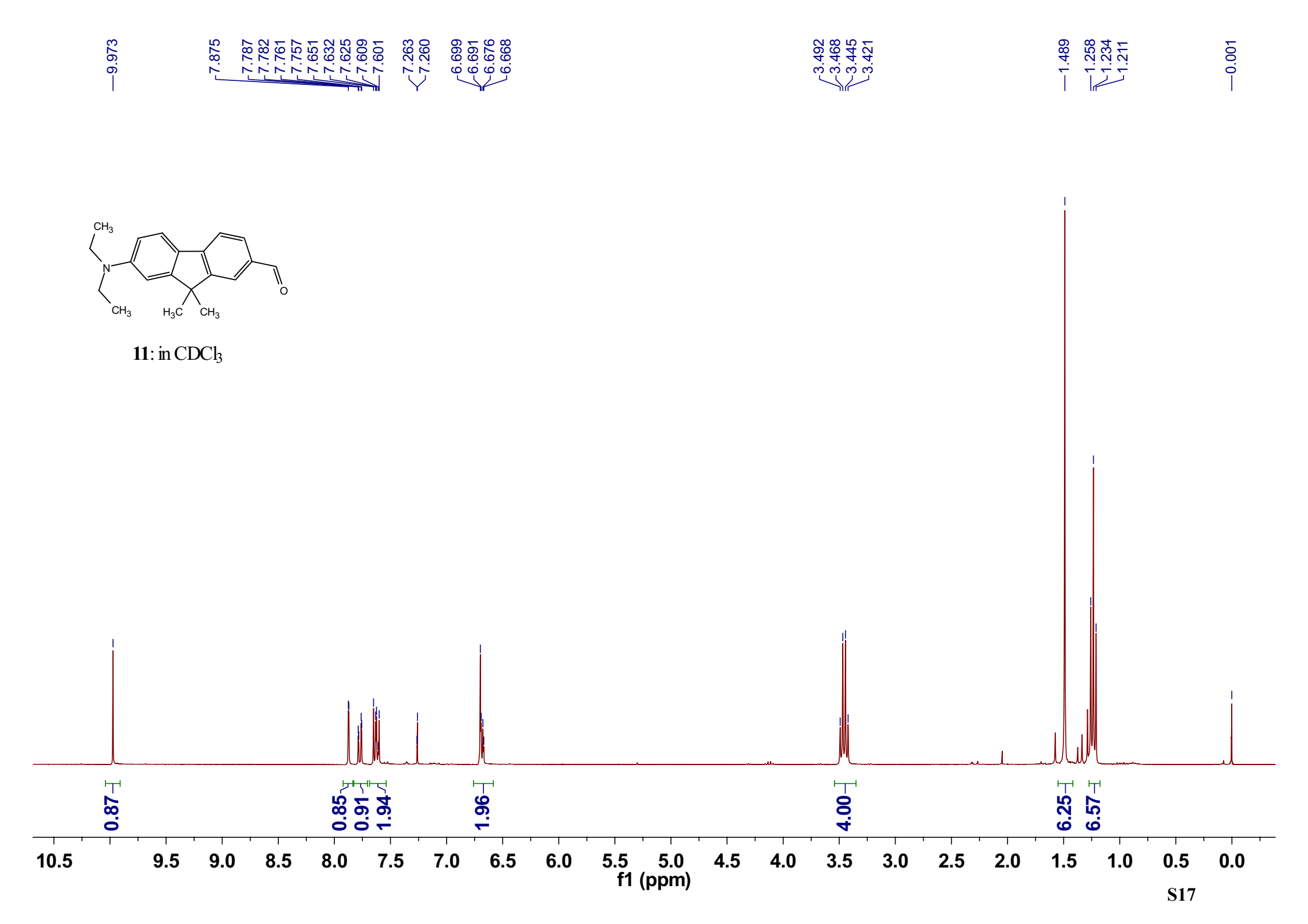
9: in $CDCl_3$


155.27
154.94
146.64
138.77
129.94
129.08
125.88
121.09
120.09
119.09
114.18
109.38
77.58
77.16
76.74
46.89
27.22
H2N
Br
H3C
CH3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

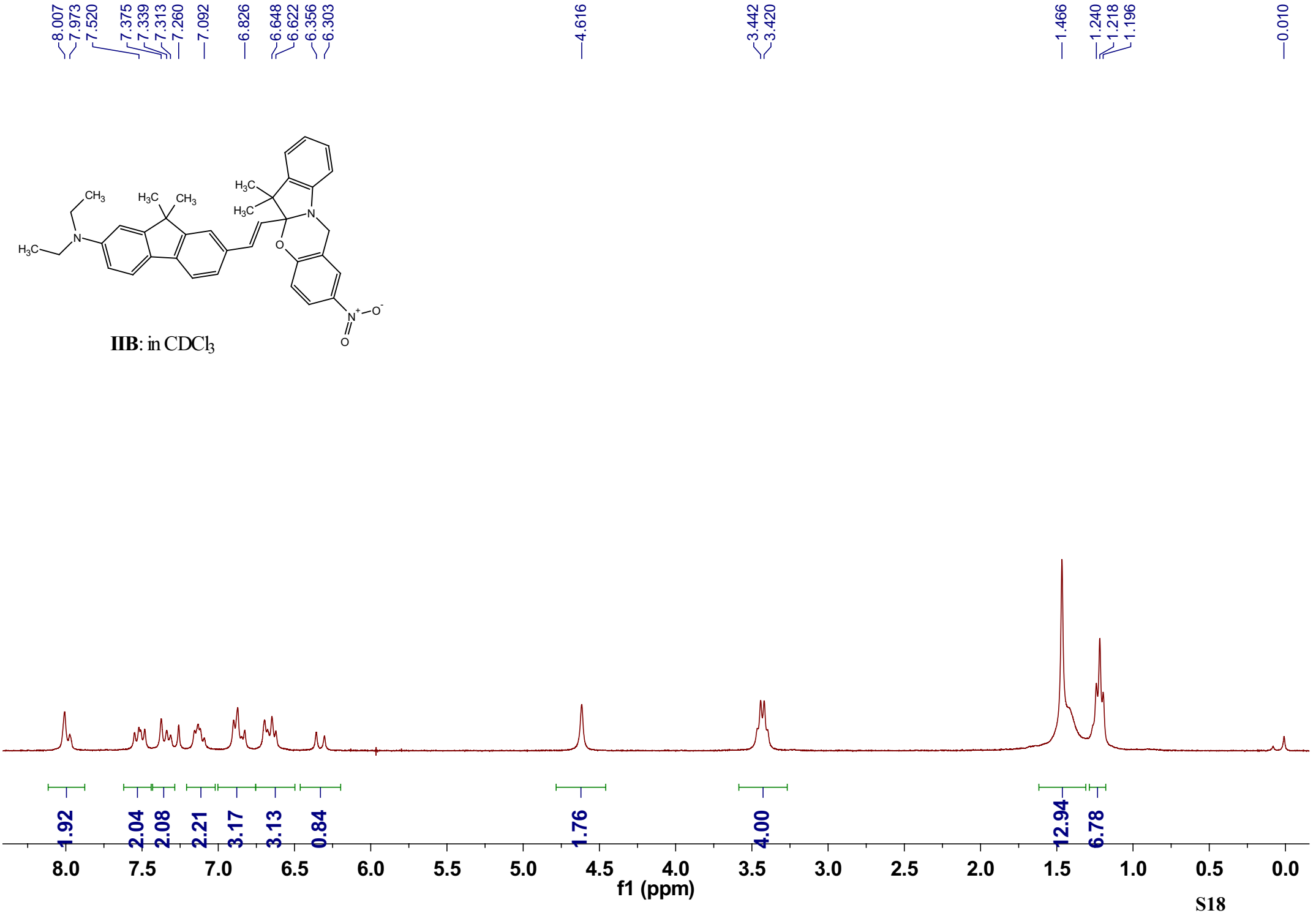
9: in $CDCl_3$


7.523
7.495
7.453
7.449
7.389
7.378
7.372
7.260
6.688
6.682
6.674
6.647
6.639
3.460
3.436
3.413
3.389
1.447
1.237
1.214
1.190
0.005
CH3
N
Br
CH3
H3C
CH3
0.98
0.96
1.99
2.00
3.99
6.28
6.31
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)

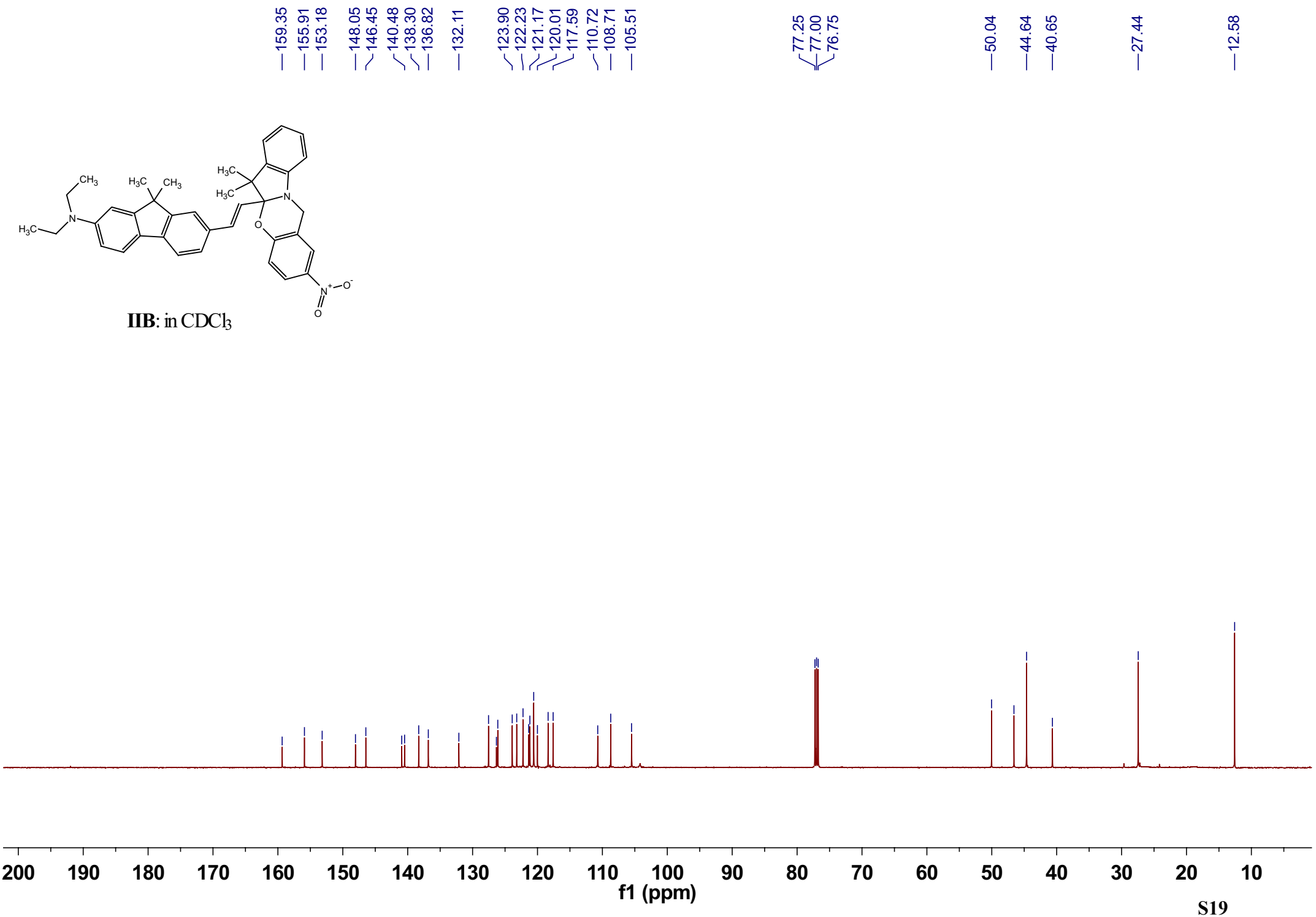
10: in $CDCl_3$


9.973
7.875
7.787
7.782
7.761
7.757
7.651
7.632
7.625
7.609
7.601
7.263
7.260
6.699
6.691
6.676
6.668
3.492
3.468
3.445
3.421
1.489
1.258
1.234
1.211
0.001
CH3
N
CH3
H3C
CH3
O
0.87
0.85
0.91
1.94
1.96
4.00
6.25
6.57
10.5
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)

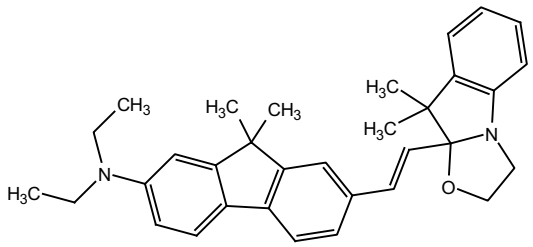
11: in $CDCl_3$


8.007
7.973
7.520
7.375
7.339
7.313
7.260
7.092
6.826
6.648
6.622
6.356
6.303
4.616
3.442
3.420
1.466
1.240
1.218
1.196
0.010
1.92
2.04
2.08
2.21
3.17
3.13
0.84
1.76
4.00
12.94
6.78
f1 (ppm)

IIB: in $CDCl_3$

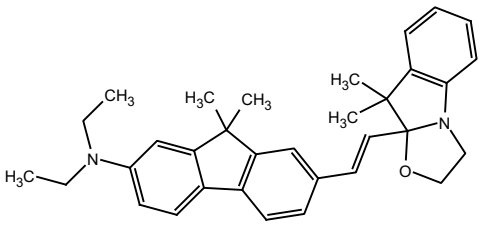

159.35
155.91
153.18
148.05
146.45
140.48
138.30
136.82
132.11
123.90
122.23
121.17
120.01
117.59
110.72
108.71
105.51
77.25
77.00
76.75
50.04
44.64
40.65
27.44
12.58
f1 (ppm)

IIB: in $CDCl_3$



IIIB: in $CDCl_3$

155.81
153.11
150.65
147.86
140.13
139.85
133.14
132.93
127.47
126.08
122.32
121.01
120.32
118.36
111.96
110.71
110.07
105.62
77.25
77.00
76.75
63.45
50.06
47.92
46.56
44.64
28.44
27.50
20.29
12.61



IIIB: in $CDCl_3$