Supporting Information

for

Effects of anion complexation on the photoreactivity of bisureido- and bisthioureido-substituted dibenzobarrelene derivatives

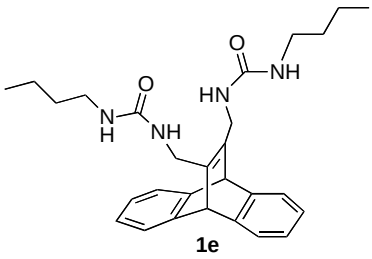
Heiko Ihmels* and Jia Luo

Address: Organic Chemistry II, University of Siegen, Adolf-Reichwein-Str. 2, D-57068 Siegen, Germany

Email: Heiko Ihmels* - ihmels@chemie.uni-siegen.de

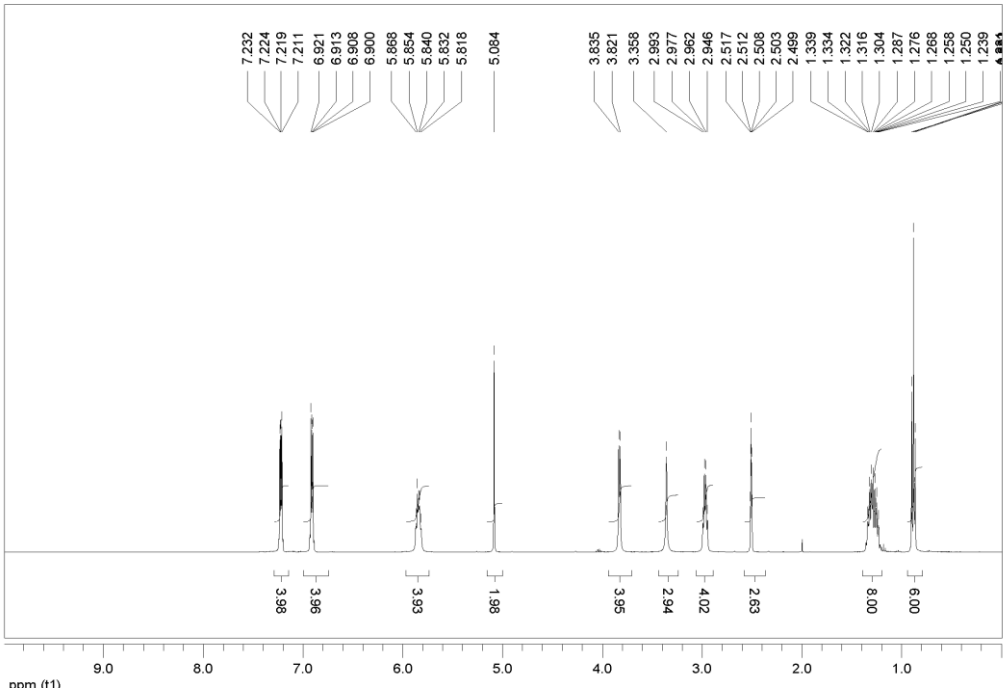
* Corresponding author

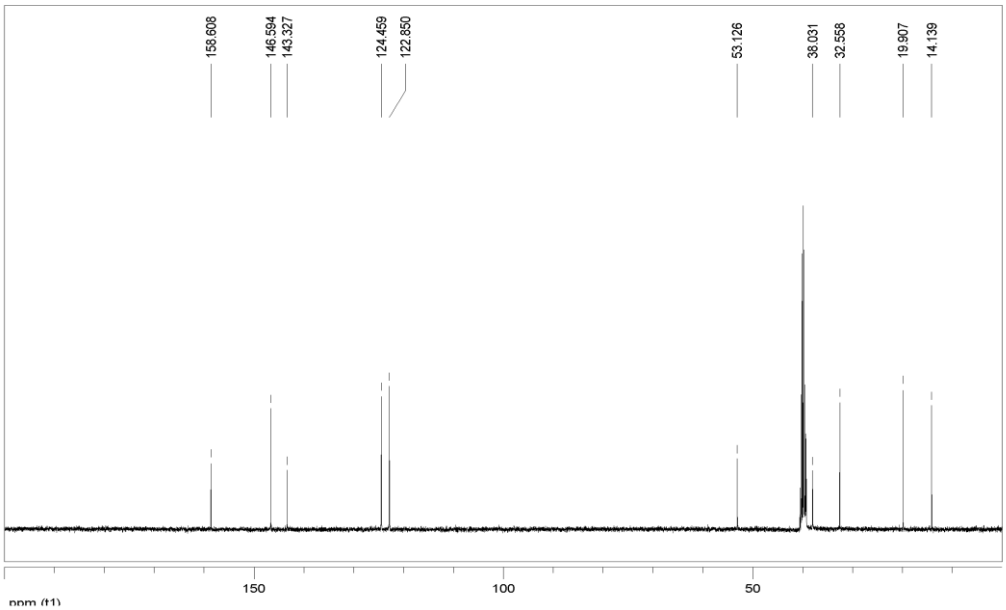
^{1}H NMR and ^{13}C NMR Spectra of Dibenzobarrelene and Semibullvalene Derivatives

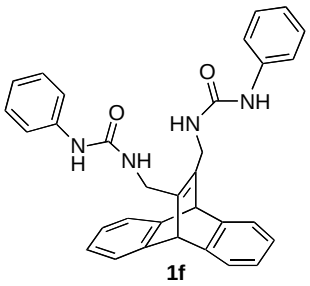


1e

in $(CD_3)_2SO$

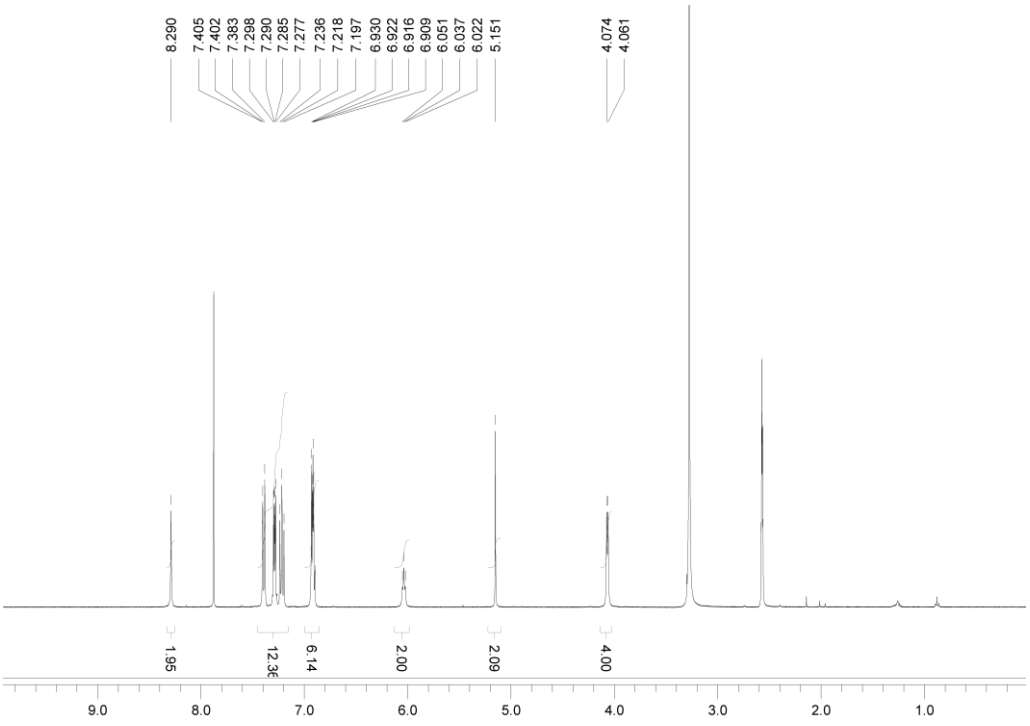






1f

(in $(CD_3)_2SO$)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7.402
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7.290
7.285
7.277
7.236
7.218
7.197
6.930
6.922
6.916
6.909
6.051
6.037
6.022
5.151
4.074
4.061
1.95
12.36
6.14
2.00
2.09
4.00
9.0
8.0
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6.0
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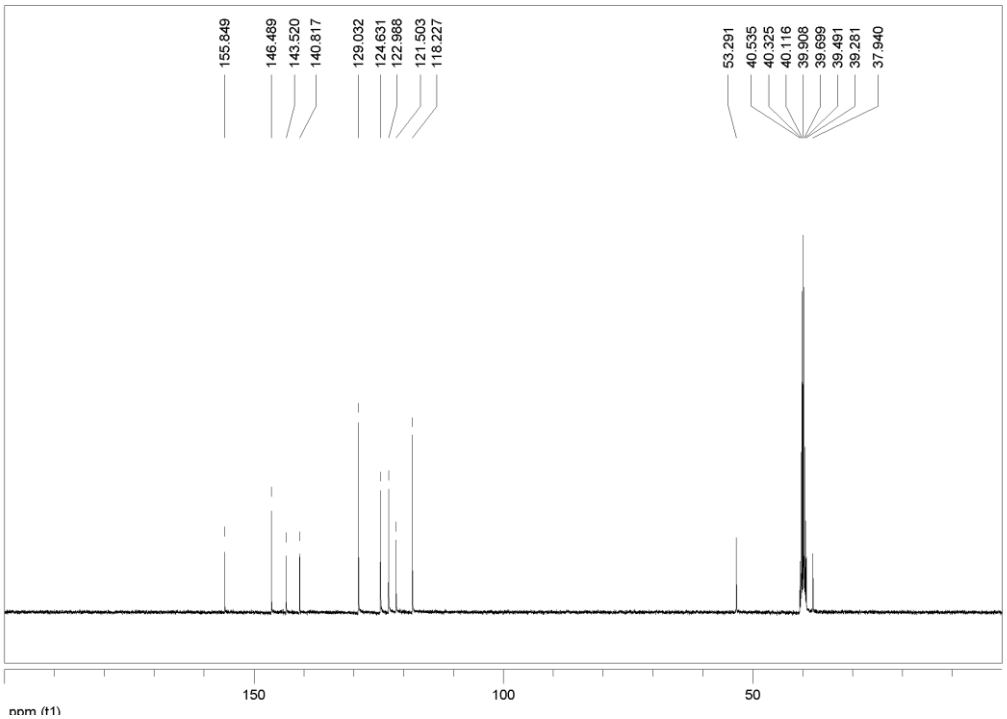
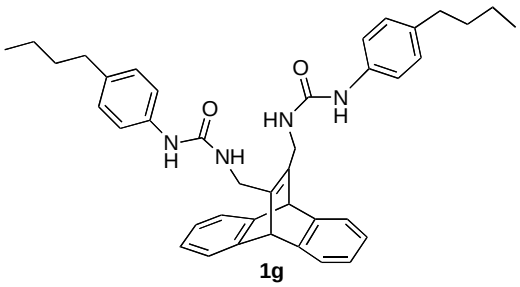
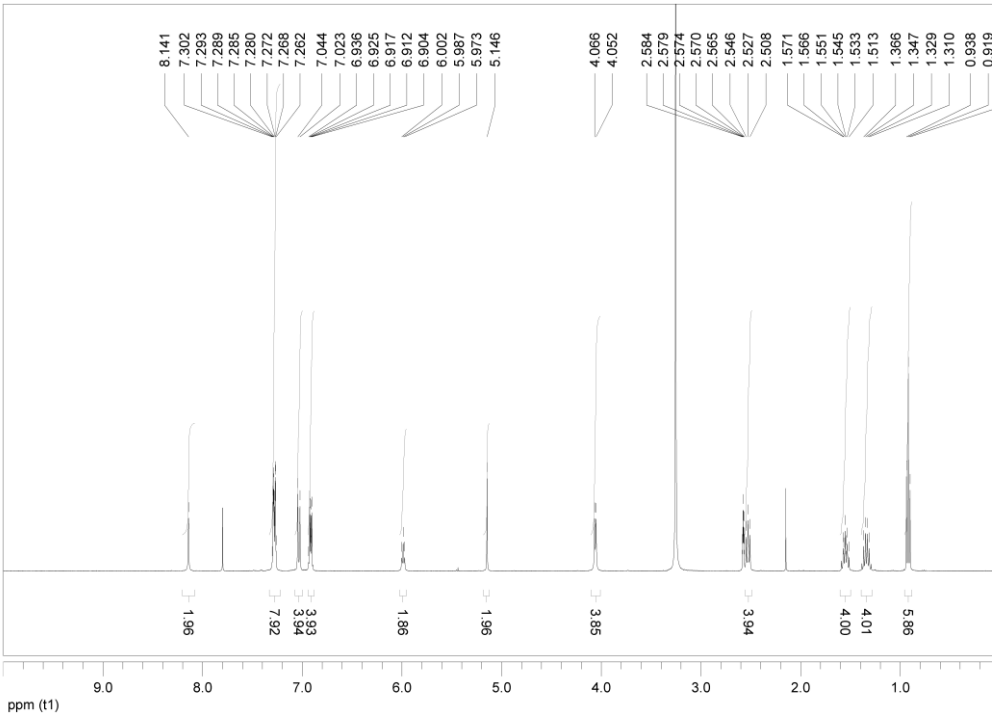
4.0
3.0
2.0
1.0


155.849
146.489
143.520
140.817
129.032
124.631
122.988
121.503
118.227
53.291
40.535
40.325
40.116
39.908
39.699
39.491
39.281
37.940
150
100
50
ppm (t1)


O
N
H
HN
O
N
H
N
H
NH

1g

in $(CD_3)_2SO$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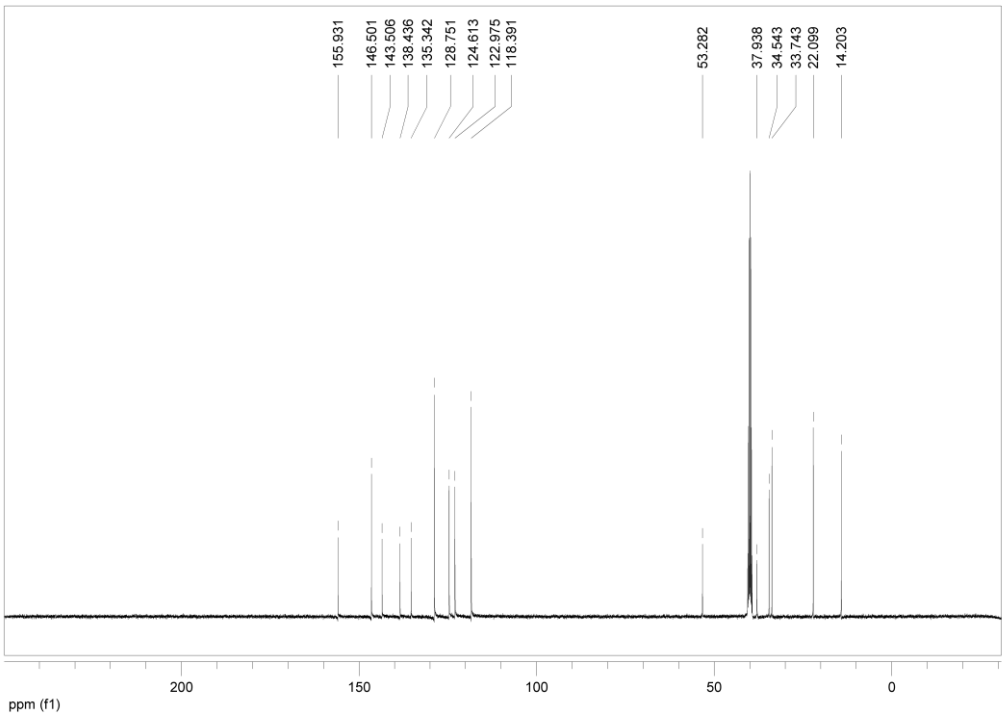
7.293
7.289
7.285
7.280
7.272
7.268
7.262
7.044
7.023
6.936
6.925
6.917
6.912
6.904
6.002
5.987
5.973
5.146
4.066
4.052
2.584
2.579
2.574
2.570
2.565
2.546
2.527
2.508
1.571
1.566
1.551
1.545
1.533
1.513
1.366
1.347
1.329
1.310
0.938
0.919
1.96
7.22
3.63
3.64
1.88
1.96
3.85
3.64
4.00
4.01
5.98
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (t1)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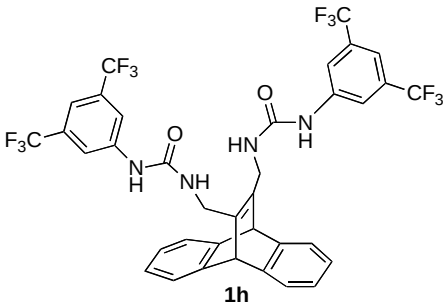
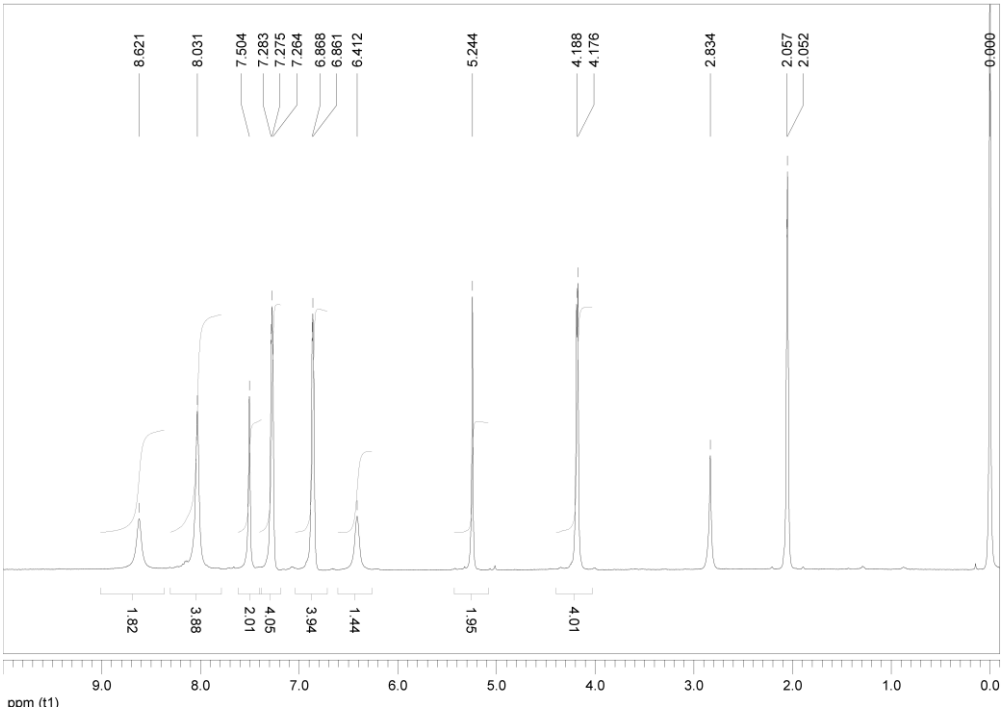
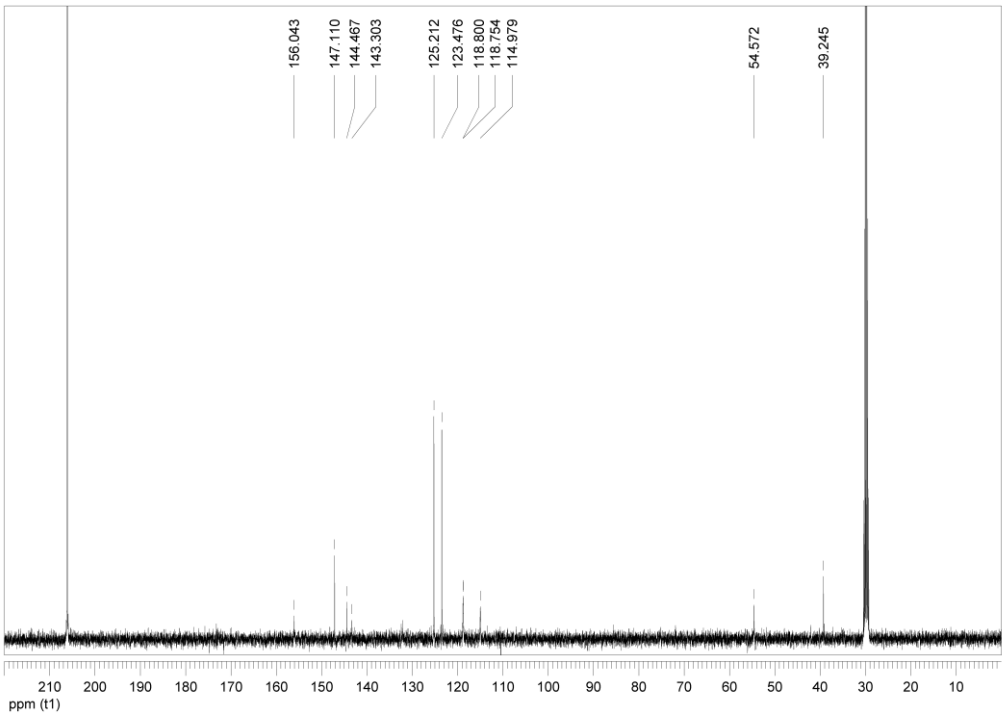
146.501
143.506
138.436
135.342
128.751
124.613
122.975
118.391
53.282
37.938
34.543
33.743
22.099
14.203
200
150
100
50
0
ppm (f1)

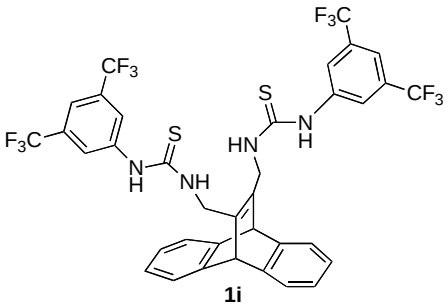


1h

in $(CD_3)_2CO$

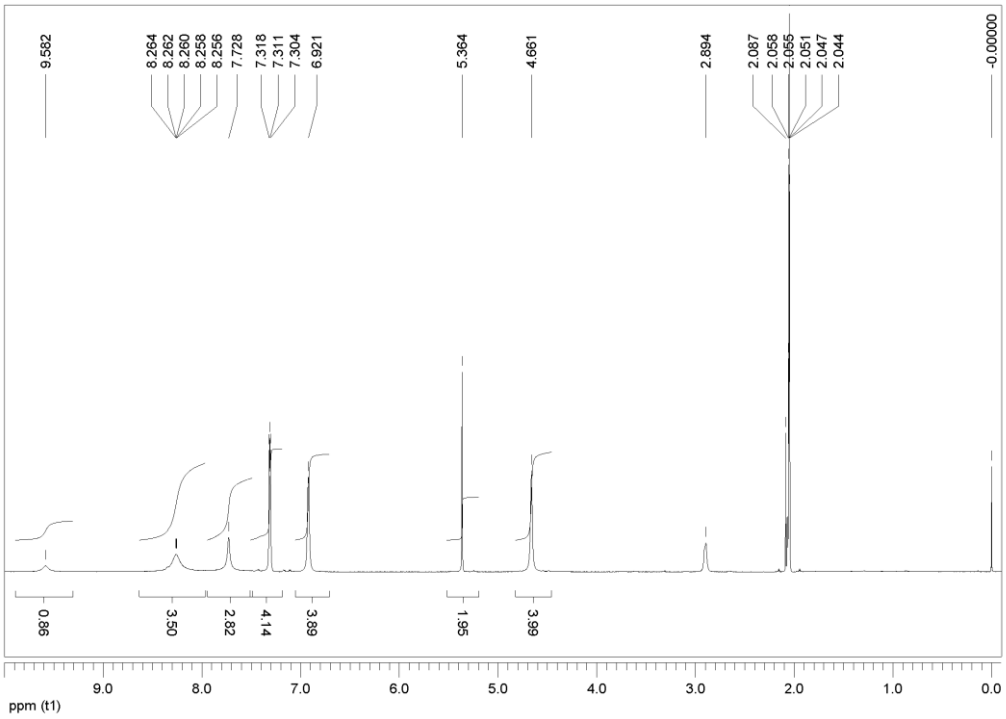

8.621
8.031
7.504
7.283
7.275
7.264
6.868
6.861
6.412
5.244
4.188
4.176
2.834
2.057
2.052
0.000
1.82
3.88
2.01
4.05
3.94
1.44
1.95
4.01
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


156.043
147.110
144.467
143.303
125.212
123.476
118.800
118.754
114.979
54.572
39.245
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm (t1)



1i

in $(CD_3)_2CO$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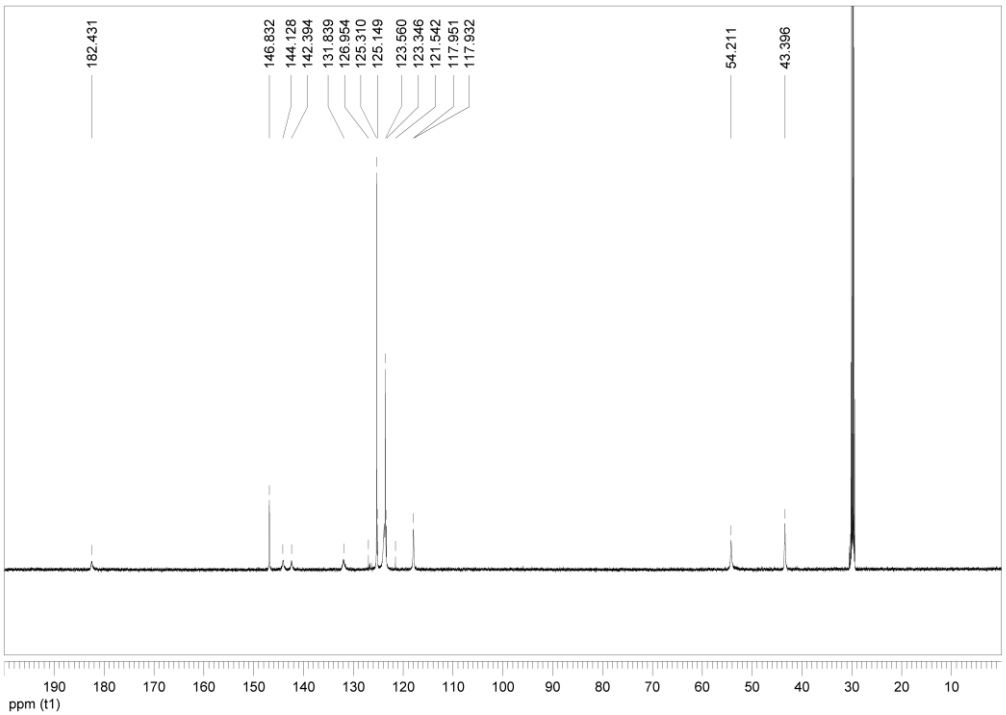
8.262
8.260
8.258
8.256
7.728
7.318
7.311
7.304
6.921
5.364
4.661
2.894
2.087
2.058
2.055
2.051
2.047
2.044
-0.00000
0.86
3.50
2.82
4.14
3.89
1.95
3.99
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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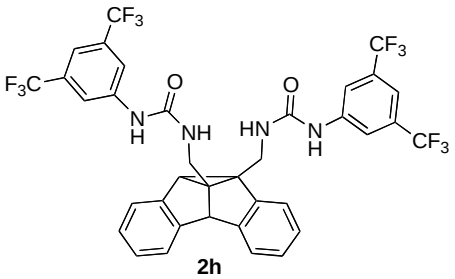
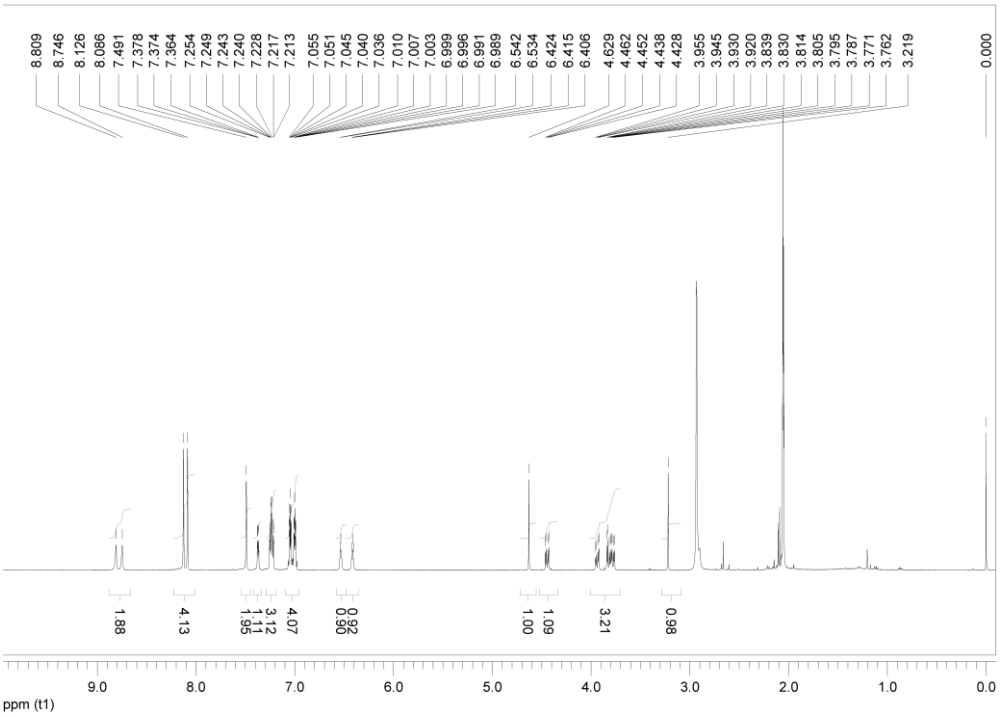
144.128
142.394
131.839
126.954
125.310
125.149
123.560
123.346
121.542
117.951
117.932
54.211
43.396
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm (t1)


CF3
F3C
O
N
H
NH
HN
O
N
H
CF3
CF3

2h

in $(CD_3)_2CO$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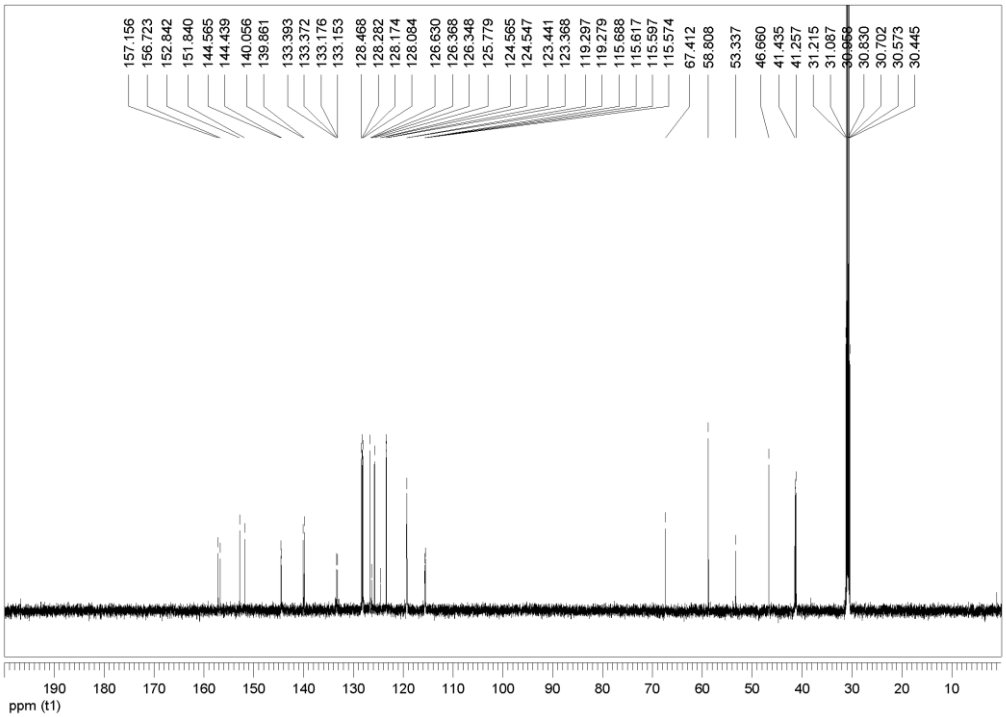
8.086
7.491
7.378
7.374
7.364
7.254
7.249
7.243
7.240
7.228
7.217
7.213
7.055
7.051
7.045
7.040
7.036
7.010
7.007
7.003
6.999
6.996
6.991
6.989
6.542
6.534
6.424
6.415
6.406
4.629
4.462
4.452
4.438
4.428
3.955
3.945
3.930
3.920
3.839
3.830
3.814
3.805
3.795
3.787
3.771
3.762
3.219
0.000
1.88
4.13
1.11
1.95
3.12
4.07
0.90
0.92
1.00
1.09
3.21
0.98
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


157.156
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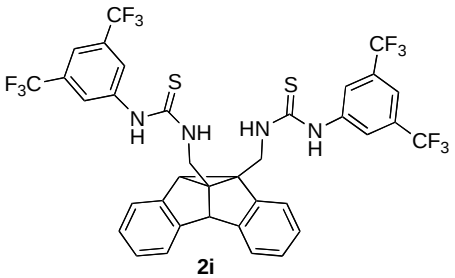
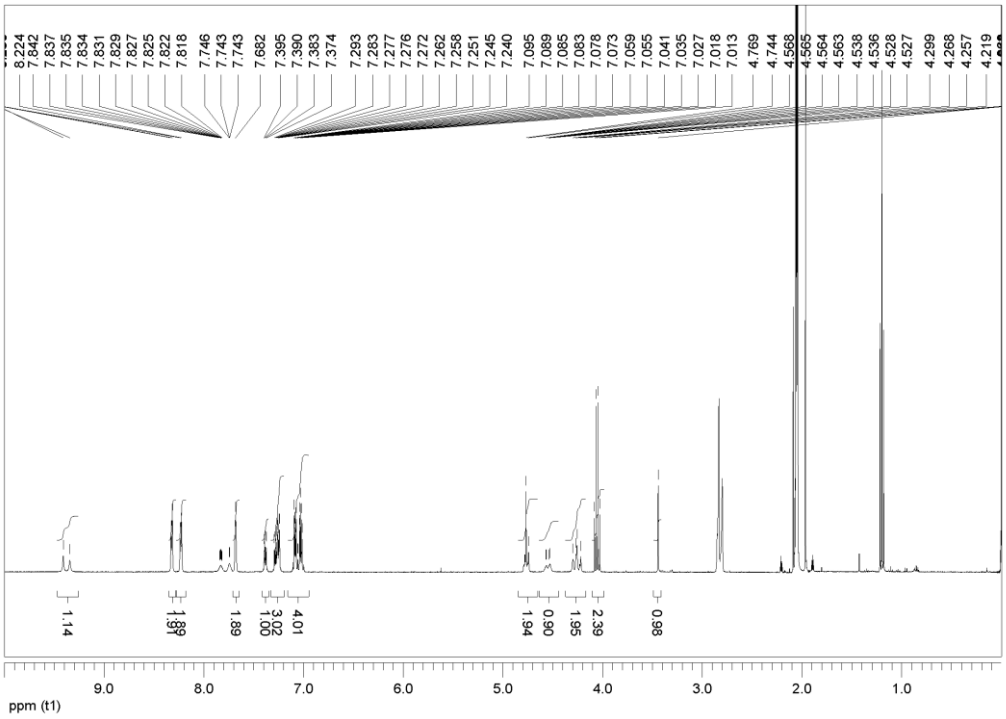
152.842
151.840
144.565
144.439
140.056
139.861
133.393
133.372
133.176
133.153
128.468
128.282
128.174
128.084
126.630
126.368
126.348
125.779
124.565
124.547
123.441
123.368
119.297
119.279
115.688
115.617
115.597
115.574
67.412
58.808
53.337
46.660
41.435
41.257
31.215
31.087
30.830
30.702
30.573
30.445
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm (t1)



2i

in $(CD_3)_2CO$


8.224
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7.837
7.835
7.834
7.831
7.829
7.827
7.825
7.822
7.818
7.746
7.743
7.743
7.682
7.395
7.390
7.383
7.374
7.293
7.283
7.277
7.276
7.272
7.262
7.258
7.251
7.245
7.240
7.095
7.089
7.085
7.083
7.078
7.073
7.059
7.055
7.041
7.035
7.027
7.018
7.013
4.769
4.744
4.568
4.565
4.564
4.563
4.538
4.536
4.528
4.527
4.299
4.268
4.257
4.219
1.14
1.91
1.89
1.89
1.00
3.02
4.01
1.94
0.90
1.96
2.39
0.98
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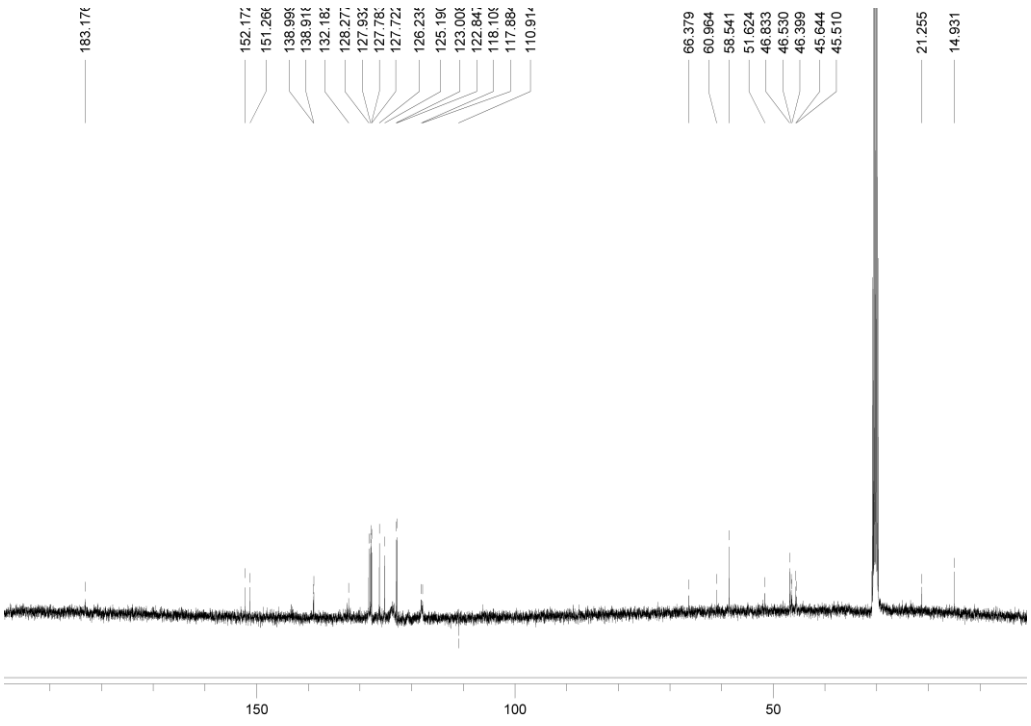
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (t1)


183.178
152.17
151.26
138.99
138.91
132.18
128.27
127.93
127.78
127.72
126.23
125.19
123.00
122.84
118.10
117.88
110.91
66.379
60.964
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46.833
46.530
46.399
45.644
45.510
21.255
14.931
150
100
50

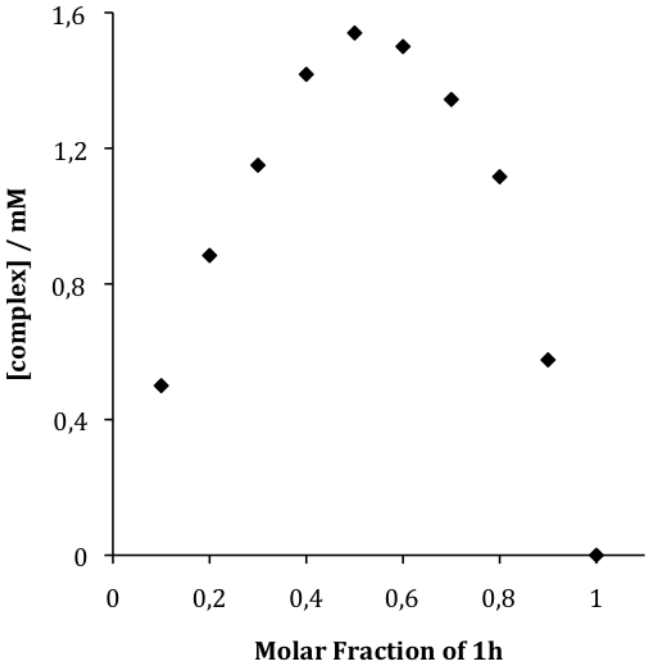
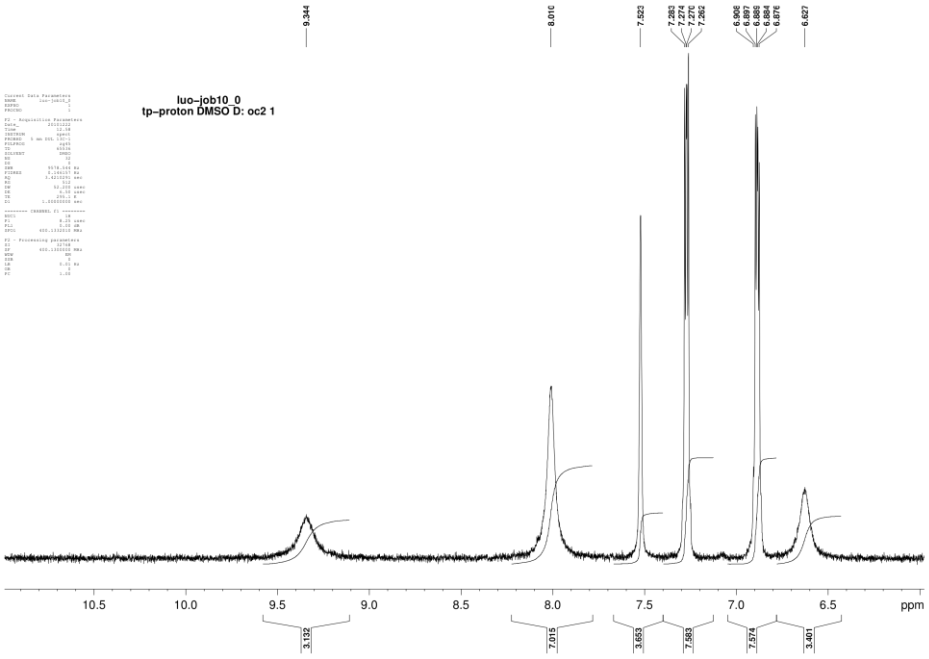
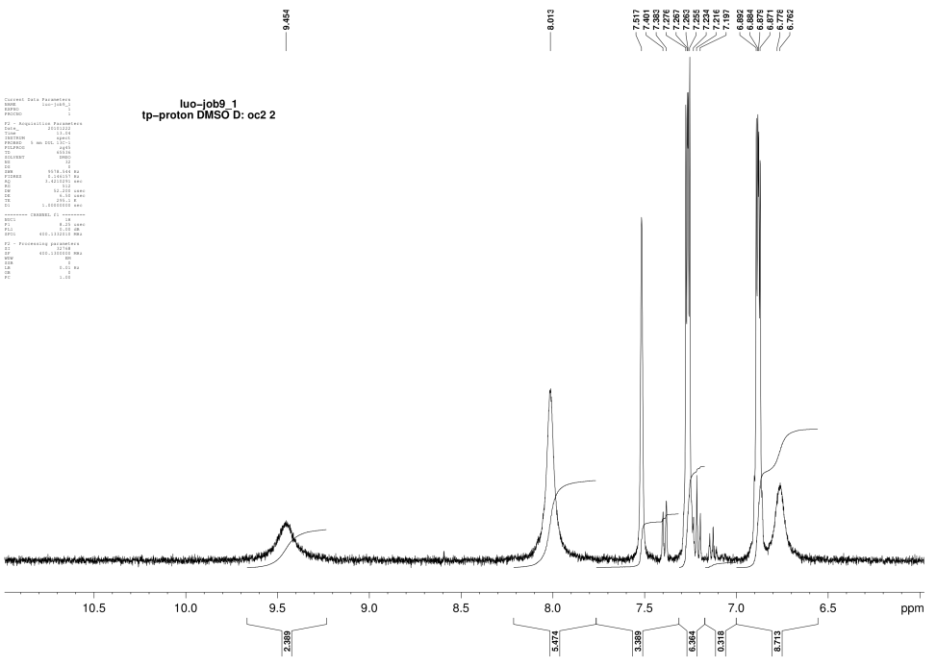
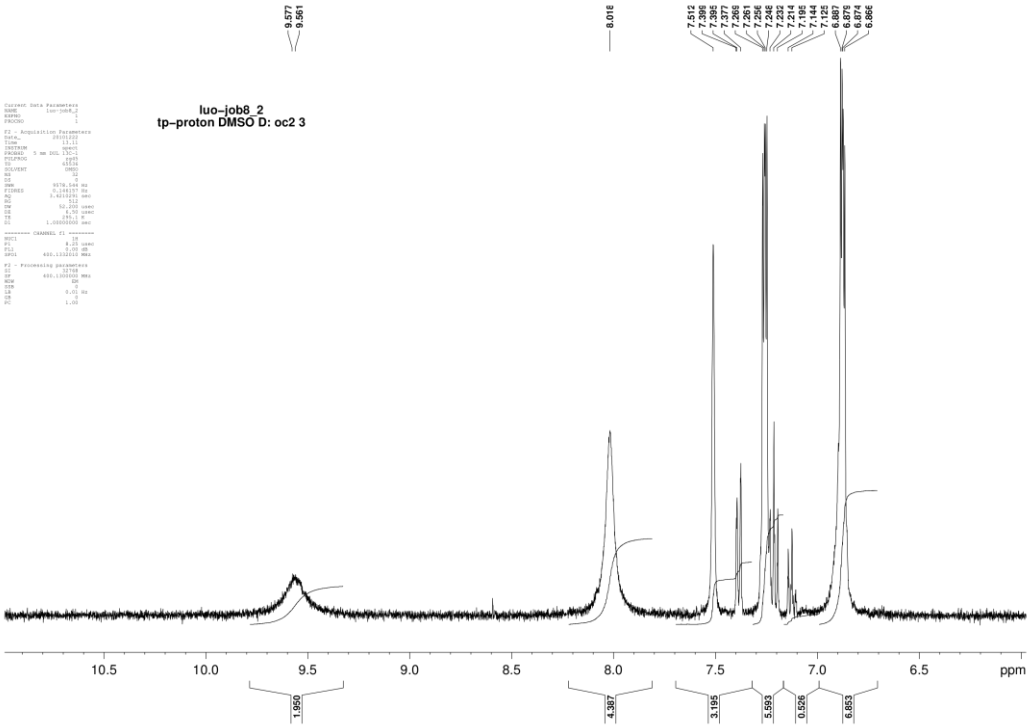


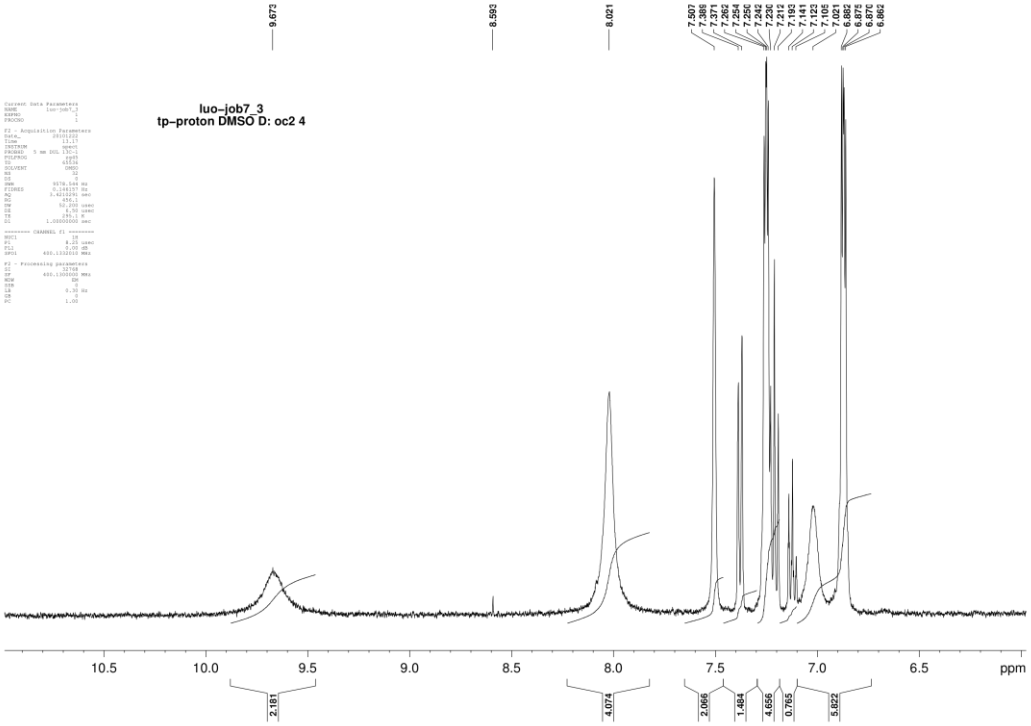
Figure S1: Job plot of **1h** with tetrabutylammonium (*S*)-mandelate (**SMD**) in $(CD_3)_2SO$, 400 MHz; determined from the ^1H NMR spectroscopic shift of the ar-NH proton at different molar fractions of **1h** (see following ^1H NMR spectra; overall concentration [**1h**] + [**SMD**] = 5.0 mM).

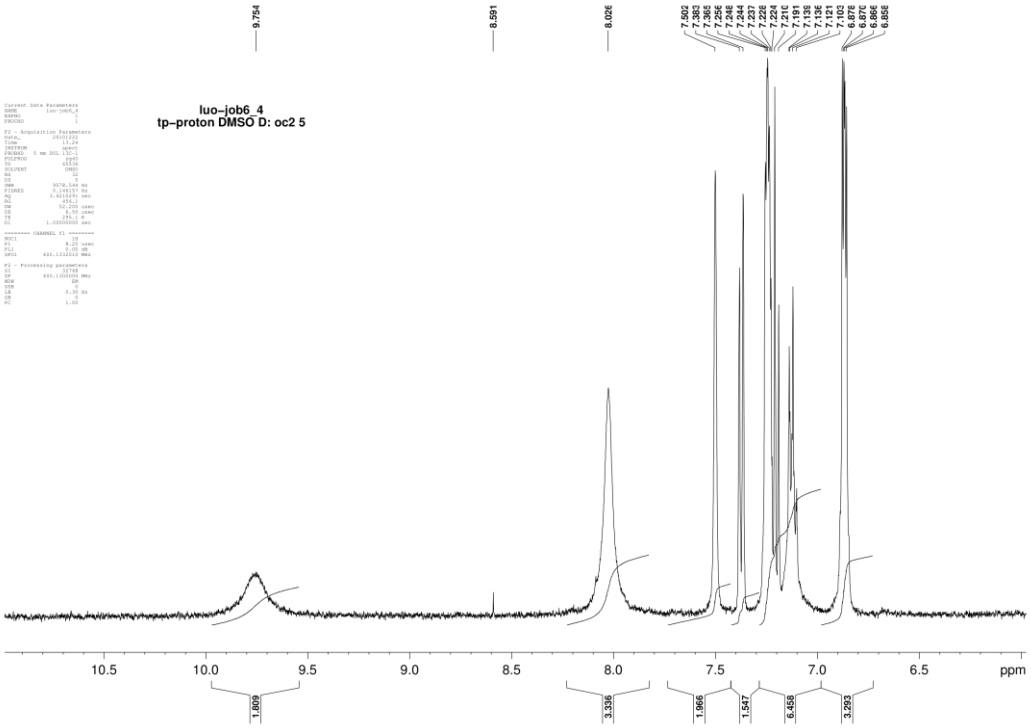
^{1}H NMR spectra of 1h with SMD at different molar ratio (1h:SMD from 10:0 to 1:9)

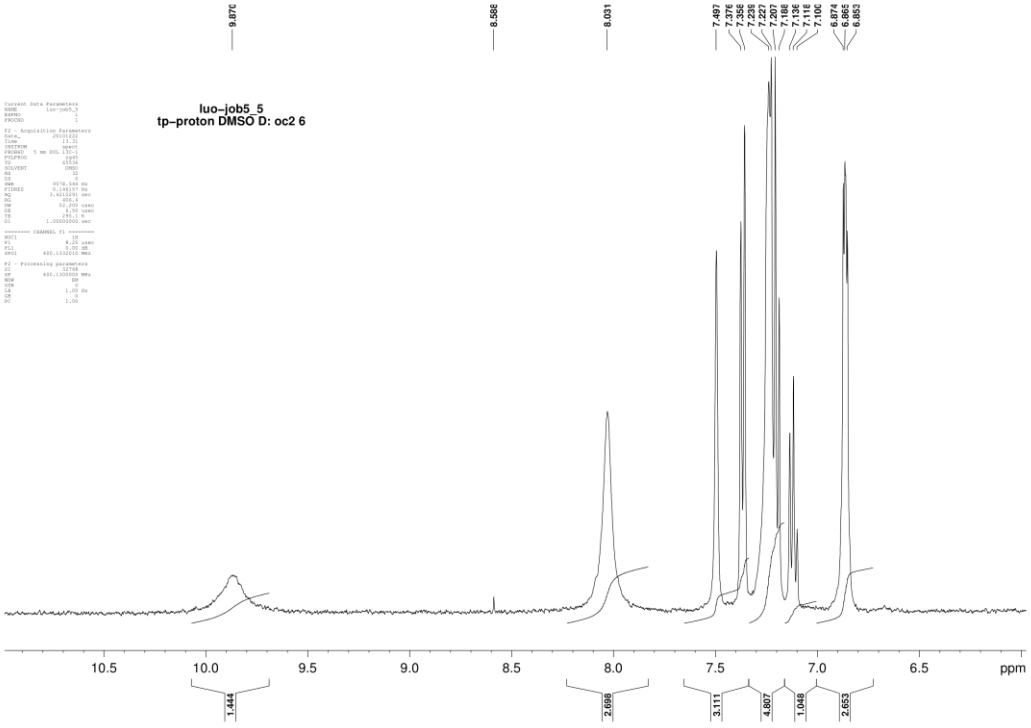


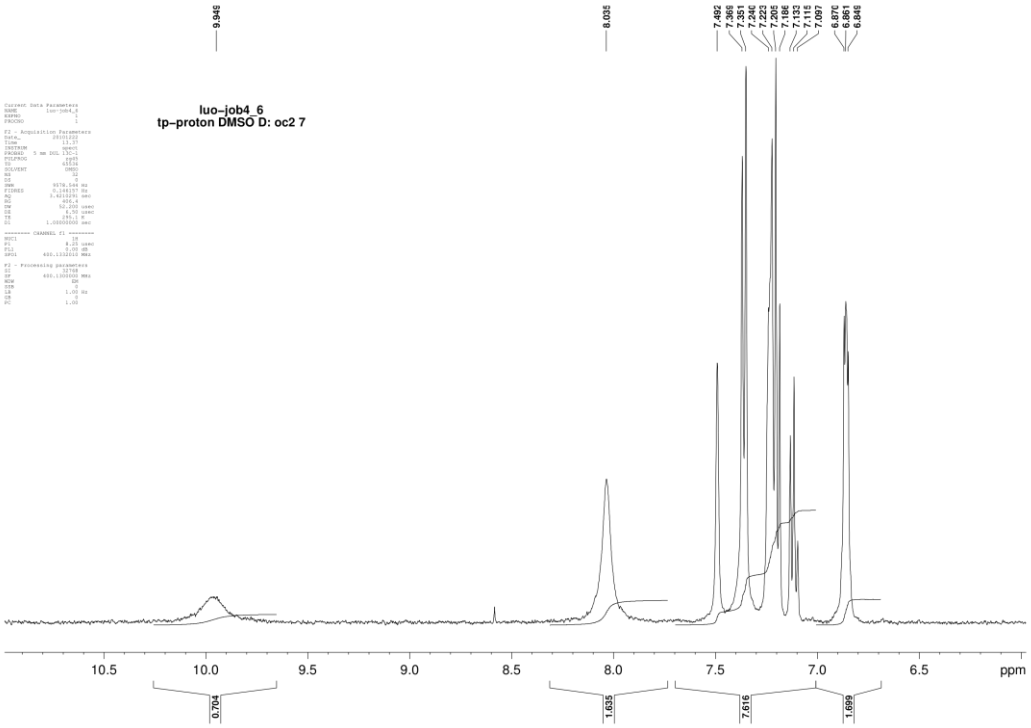


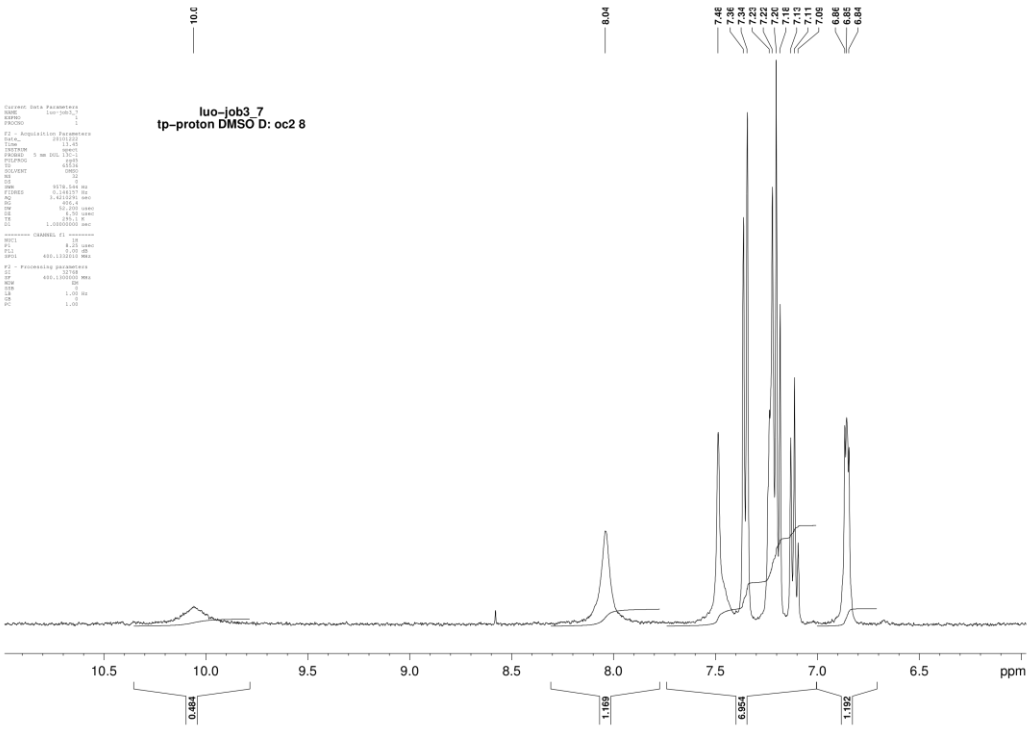

9.577
9.561
8.016
7.512
7.396
7.377
7.366
7.261
7.256
7.246
7.233
7.214
7.195
7.144
7.125
6.880
6.875
6.874
6.866
luo-job8_2
tp-proton DMSO D: oc2 3
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
ppm
1.950
4.987
3.195
5.593
0.526
6.853

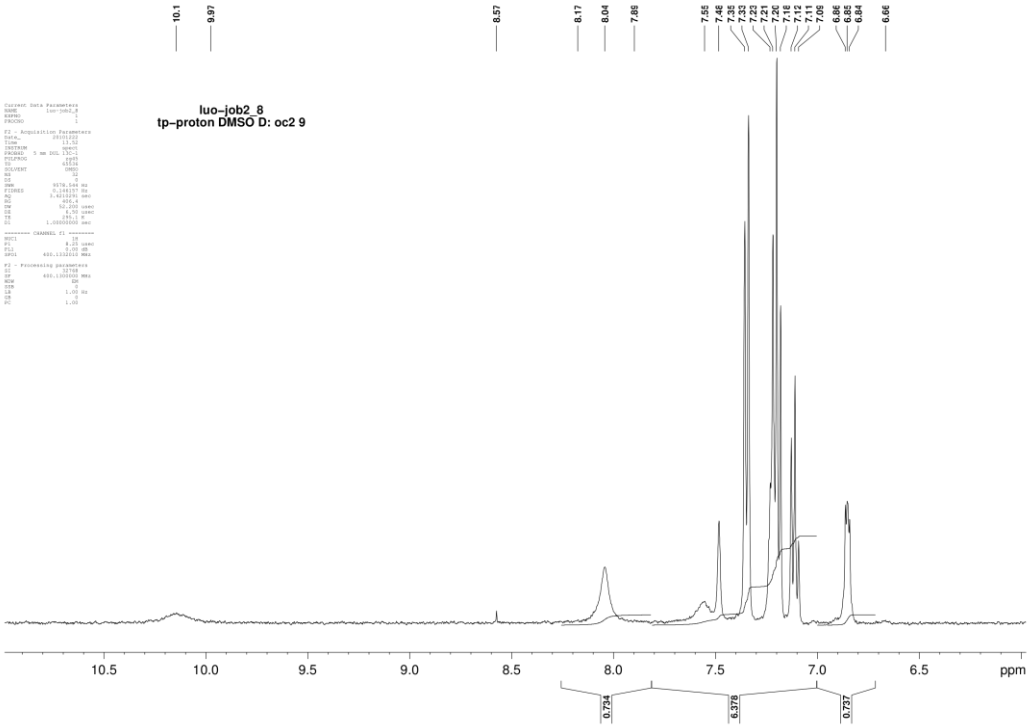

9.672
8.593
8.021
7.907
7.388
7.371
7.262
7.254
7.256
7.242
7.236
7.212
7.193
7.141
7.123
7.105
7.021
6.885
6.875
6.870
6.862
luo-job7_3
tp-proton DMSO D: oc2 4
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
ppm
2.181
4.074
2.066
1.484
4.656
0.765
5.822


9.754
8.591
8.026
7.502
7.383
7.365
7.256
7.246
7.244
7.237
7.228
7.224
7.210
7.191
7.138
7.135
7.121
7.103
6.878
6.876
6.866
6.858
luo-job6_4
tp-proton DMSO D: oc2 5
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
ppm
1.809
3.336
1.956
1.547
6.458
3.293


9.676
8.588
8.031
7.497
7.376
7.358
7.228
7.227
7.207
7.188
7.136
7.114
7.106
6.874
6.865
6.853
luo-job5_5
tp-proton DMSO D: oc2 6
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
ppm
1.444
2.698
3.111
4.807
1.048
2.653


9.946
8.035
7.492
7.366
7.351
7.246
7.223
7.205
7.186
7.133
7.116
7.099
6.871
6.855
6.846
luo-job4_6
tp-proton DMSO D: oc2 7
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
ppm
0.704
1.635
7.616
1.699


10.0
8.04
7.48
7.36
7.34
7.22
7.23
7.20
7.18
7.13
7.11
7.06
6.86
6.85
6.84
luo-job3_7
tp-proton DMSO D: oc2 8
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
ppm
0.484
1.169
6.954
1.192


10.1
9.97
8.57
8.17
8.04
7.86
7.55
7.48
7.35
7.33
7.22
7.21
7.20
7.18
7.12
7.11
7.06
6.86
6.85
6.84
6.66
luo-job2_8
tp-proton DMSO D: oc2 9
10.5
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9.5
9.0
8.5
8.0
7.5
7.0
6.5
ppm
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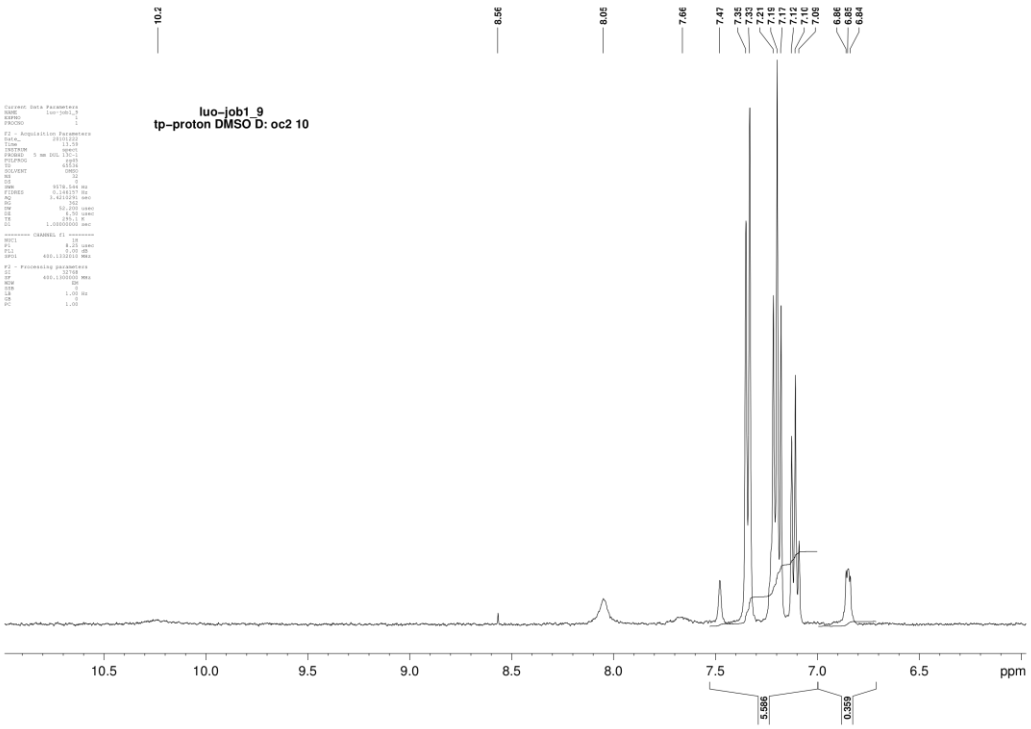
6.378
0.737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8.56
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7.66
7.47
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7.17
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7.11
7.06
6.86
6.85
6.84
luo-job1_9
tp-proton DMSO D: oc2 10
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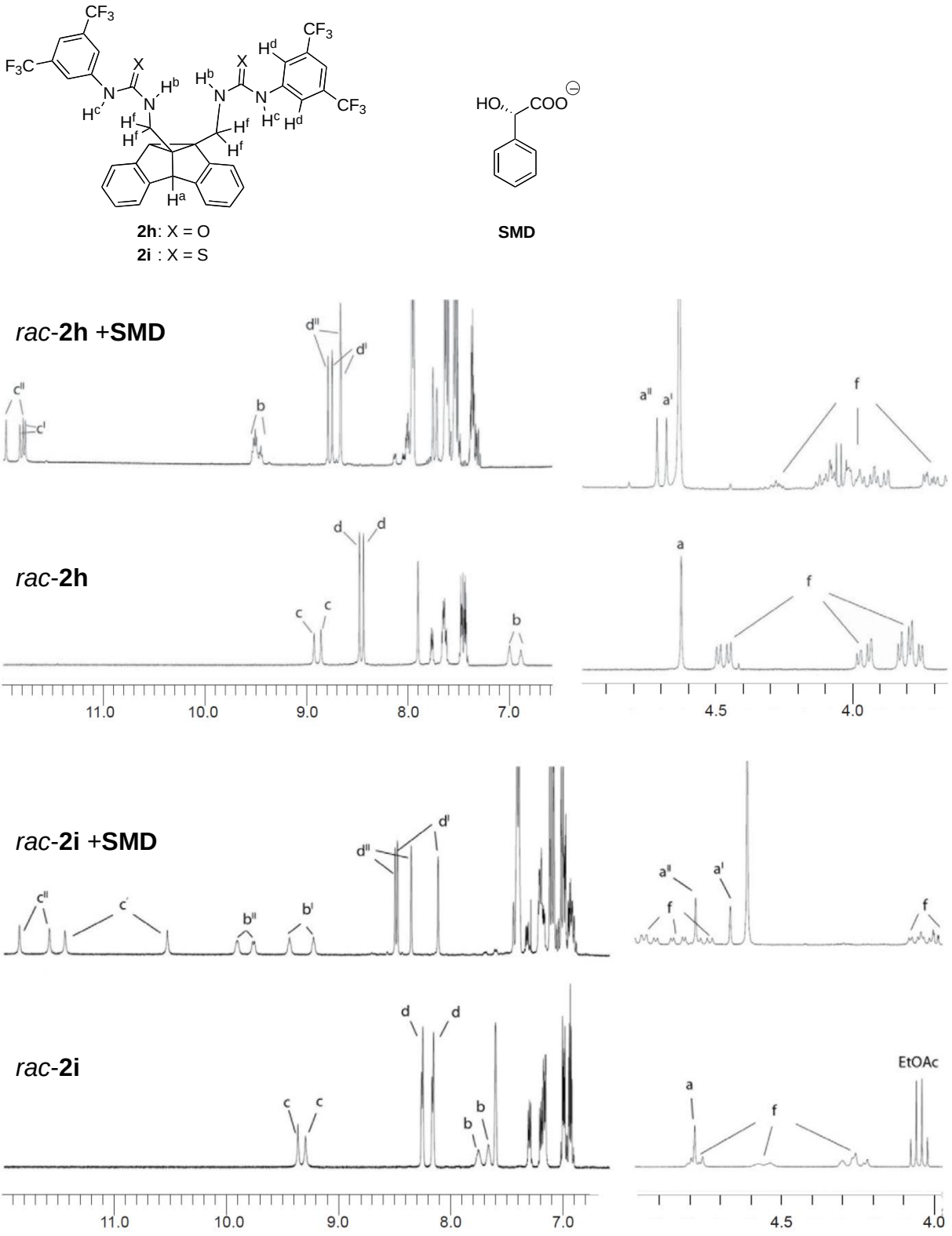

Figure S2: Tetrabutylammonium (*S*)-mandelate (**SMD**) as chiral shift reagent for the dibenzosemibullvalene derivatives **2h** and **2i**, in $(CD_3)_2CO$, 400 MHz.