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Electronic Supplementary Information

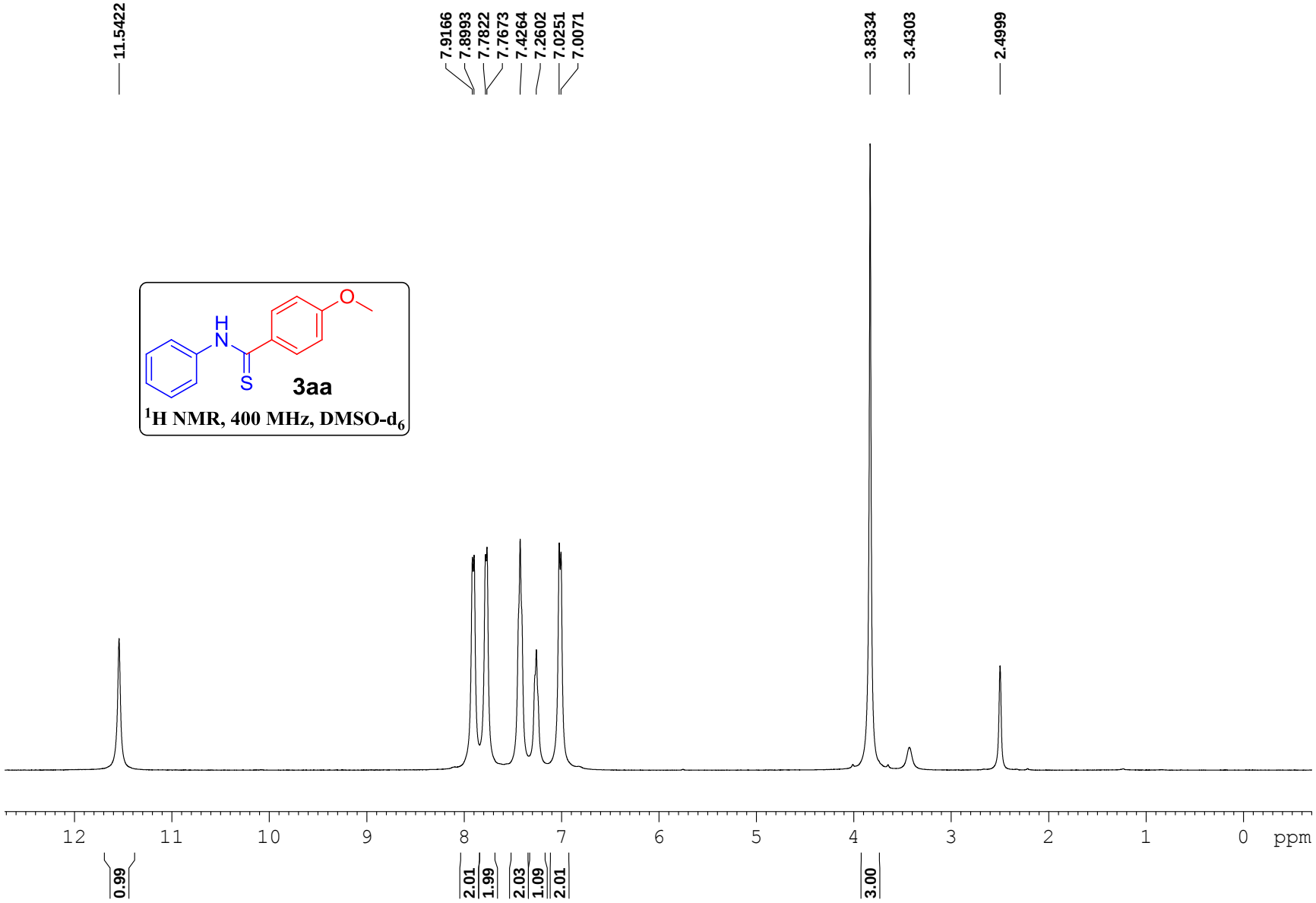
A metal-free and a solvent-free synthesis of thio-amides and amides: An efficient Friedel-Crafts arylation of isothiocyanates and isocyanates

Begur Vasanthkumar Varun, Ankush Sood and Kandikere Ramaiah Prabhu*

Department of Organic Chemistry
Indian Institute of Science
Bangalore 560 012, Karnataka
India.

e-mail: prabhu@orgchem.iisc.ernet.in

Contents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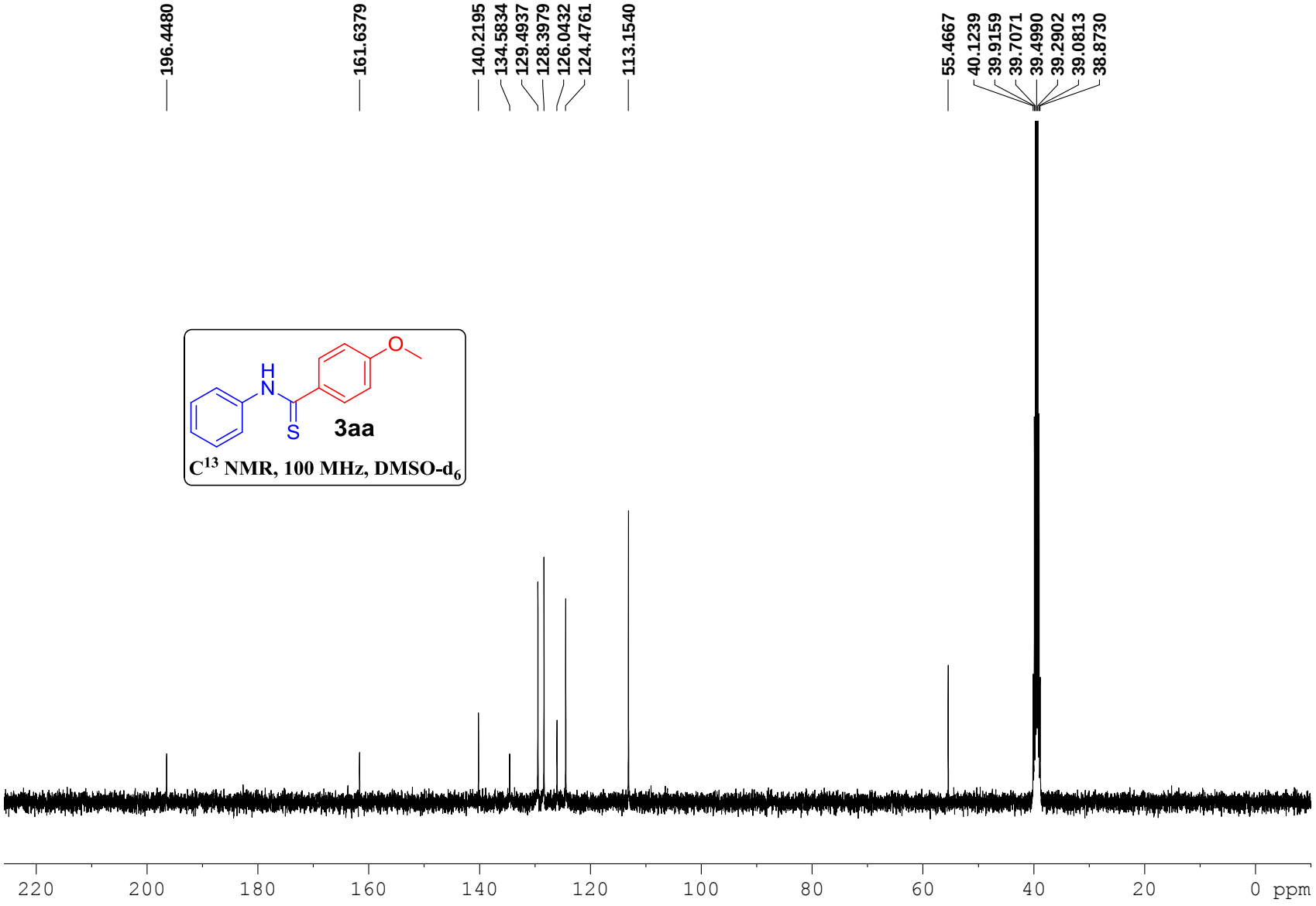
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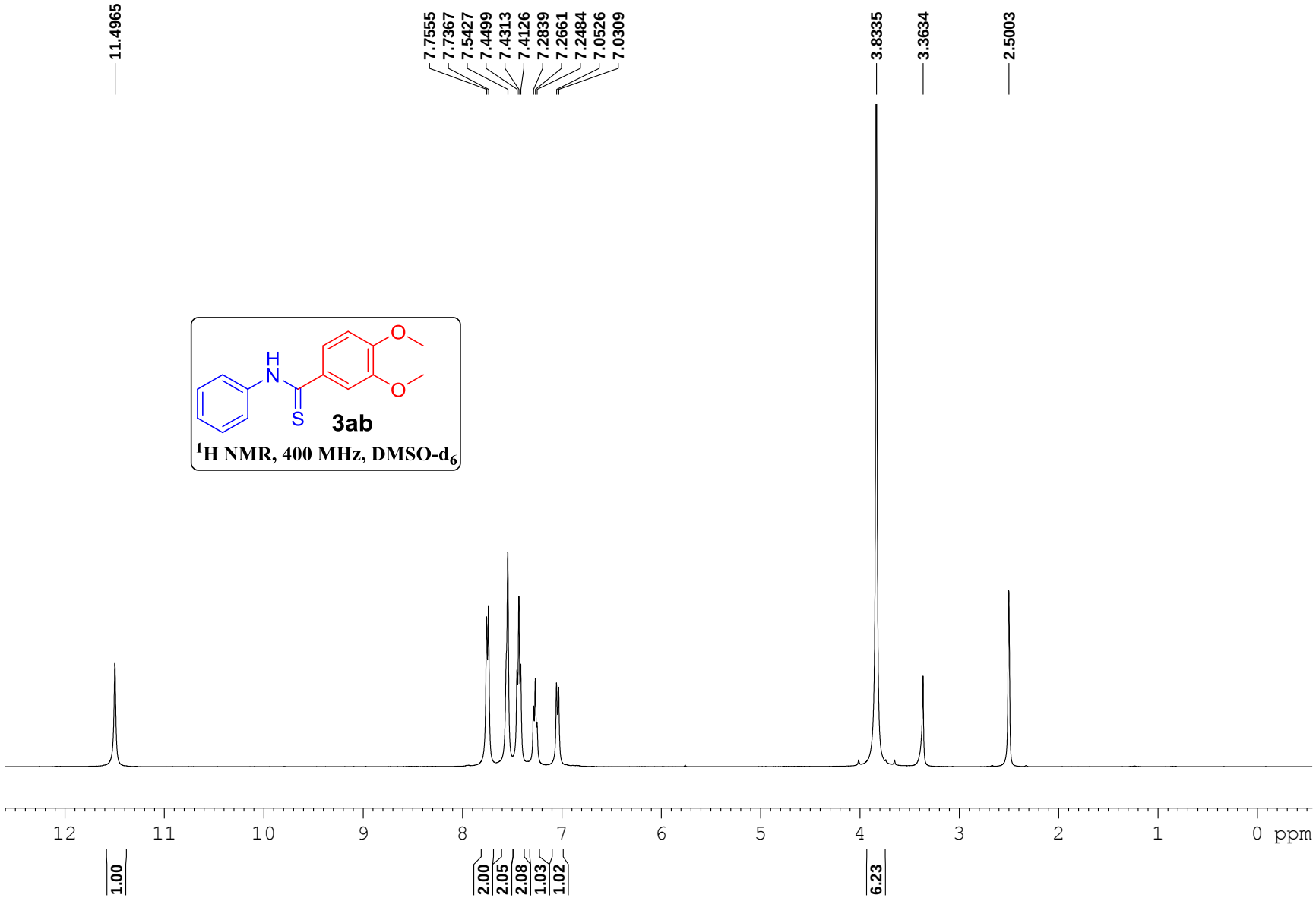
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2.5003
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S
O
O
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11
10
9
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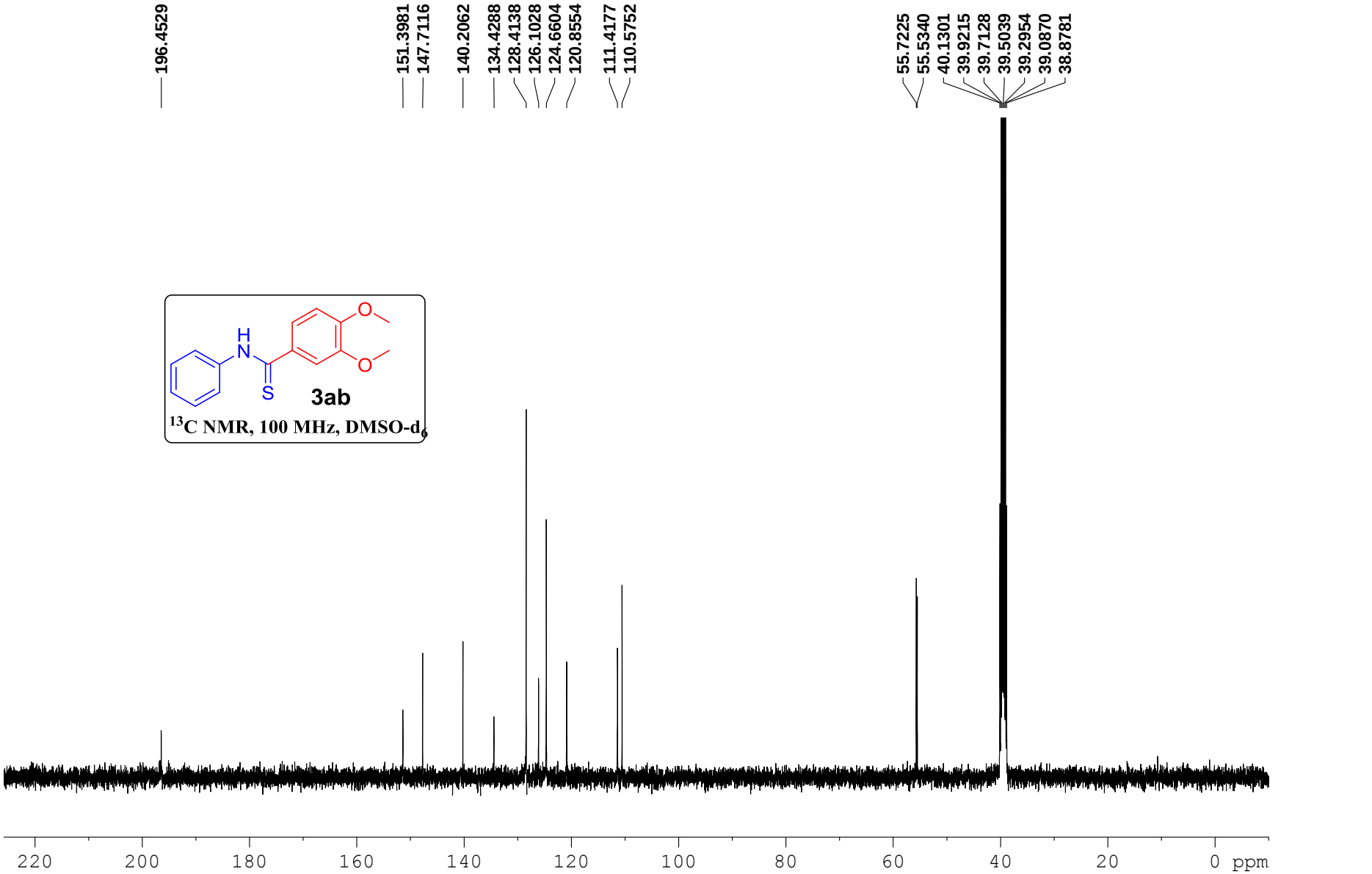
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H
N
S
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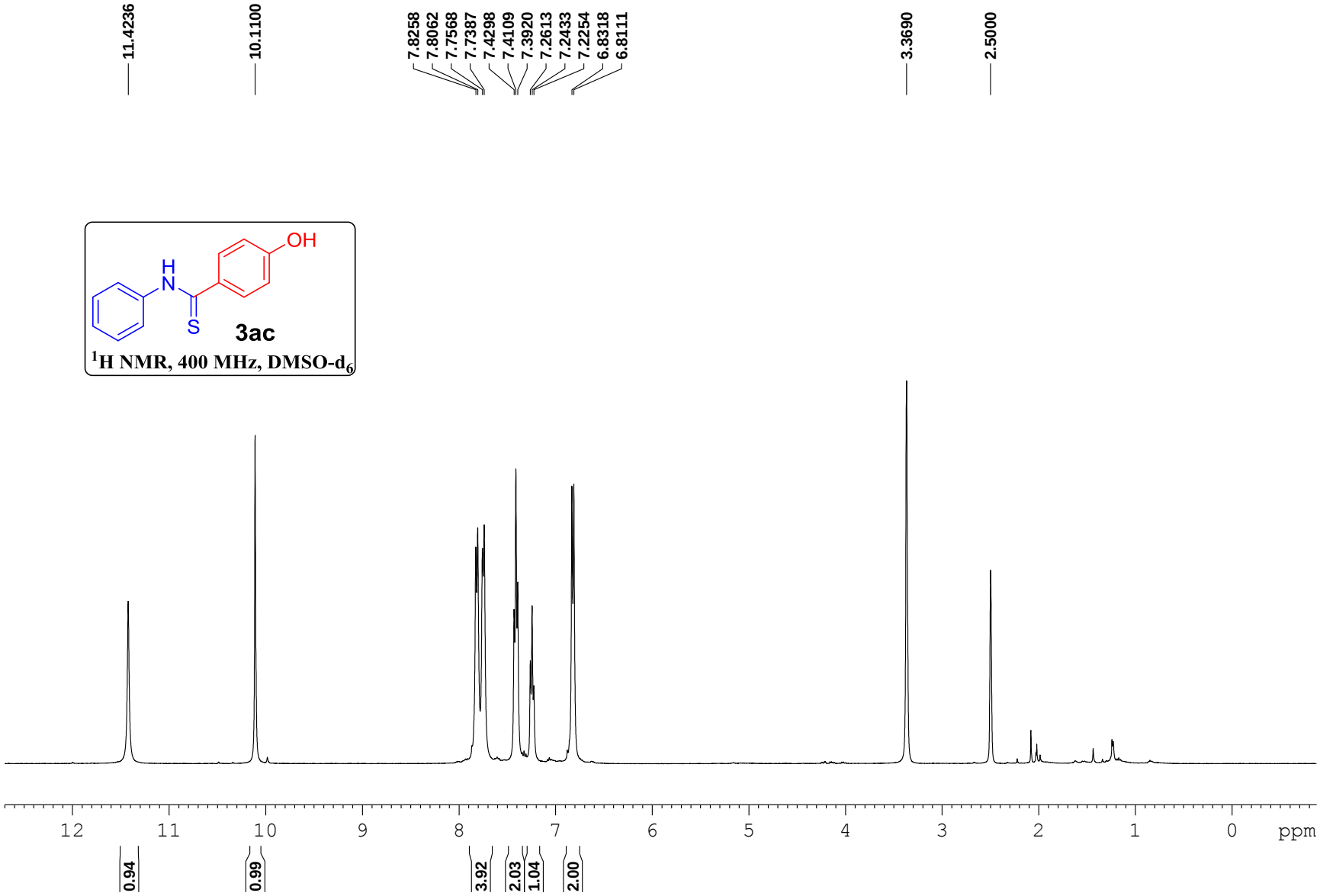
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N
S
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11
10
9
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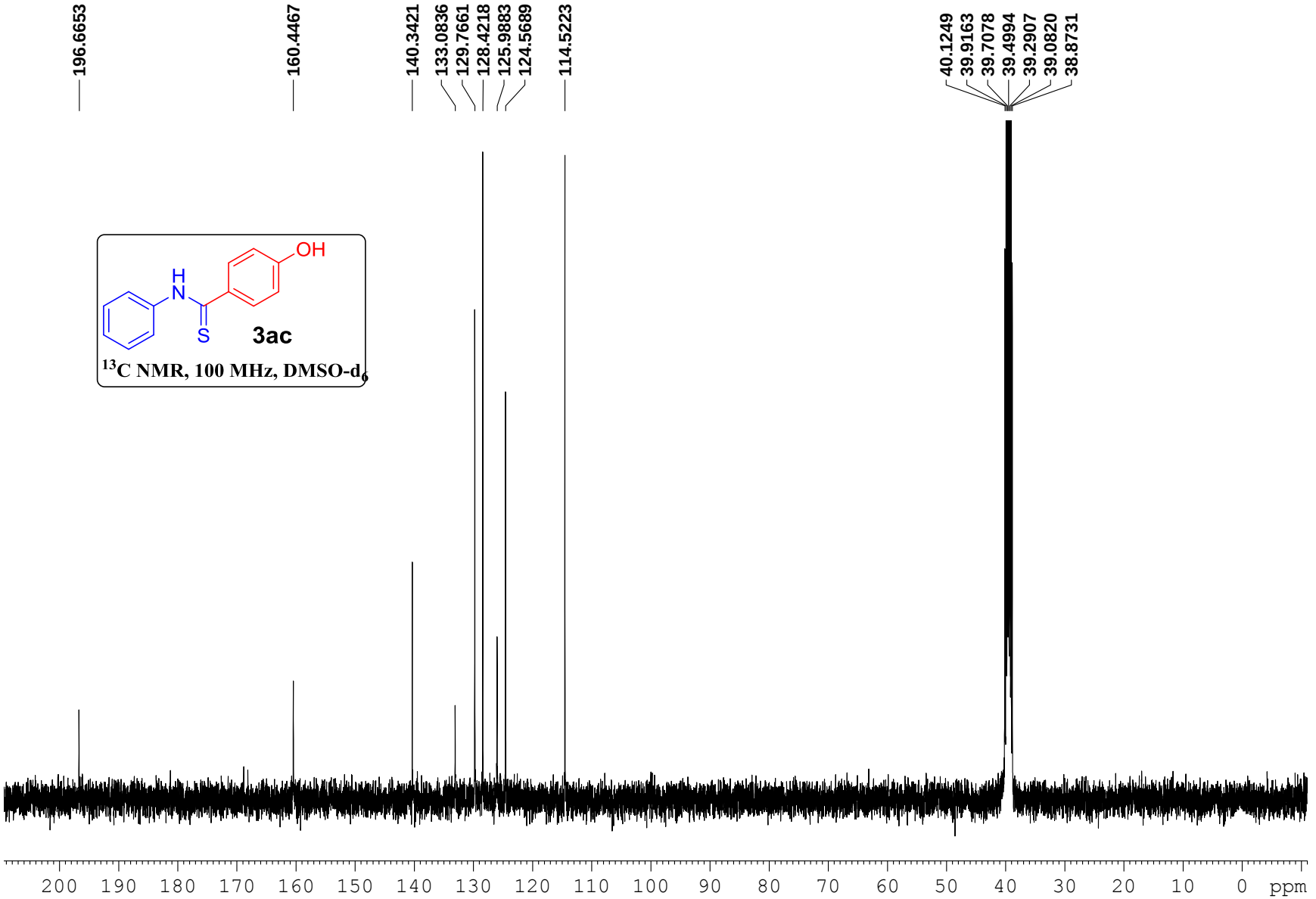
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N
S
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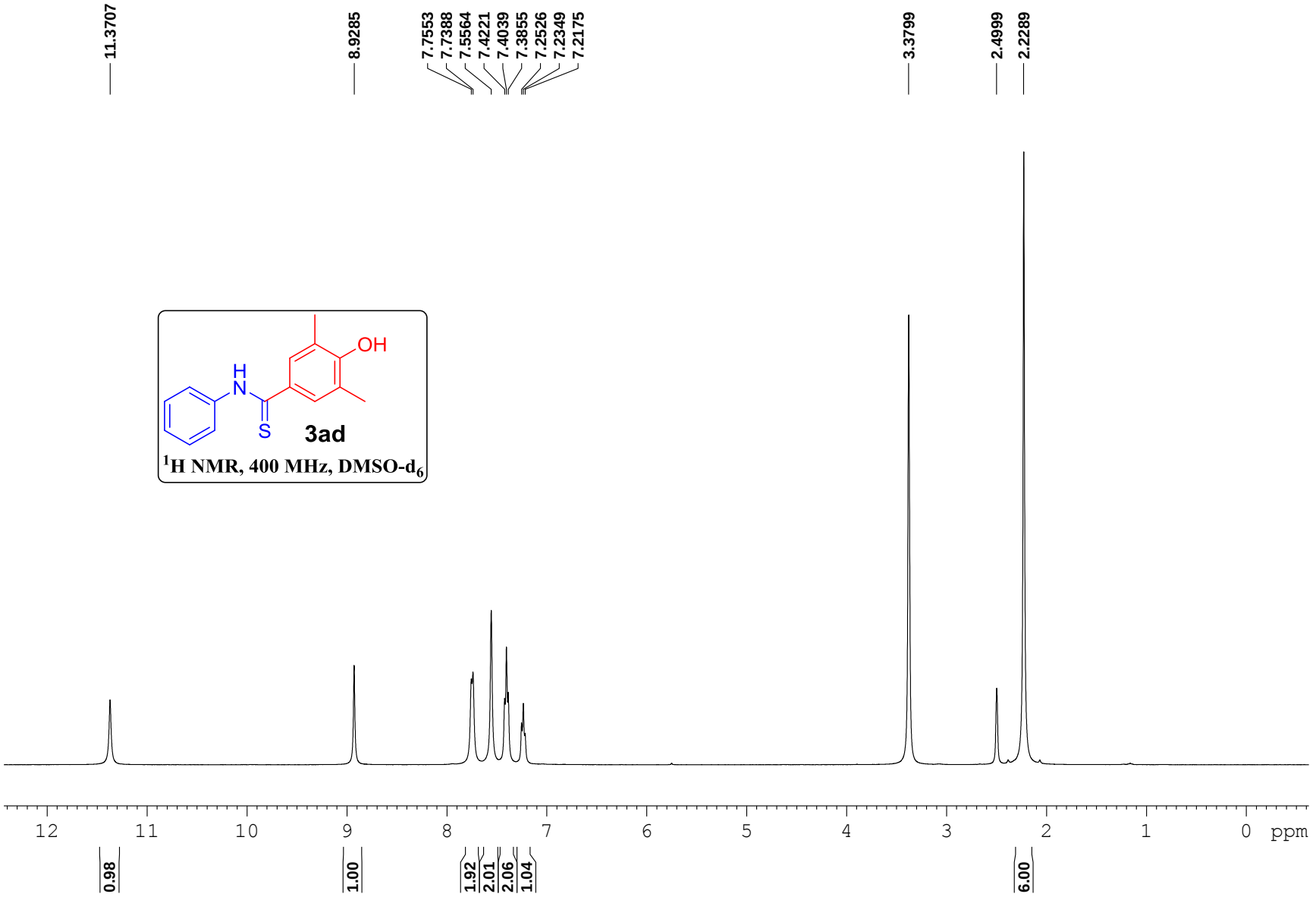
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S
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10
9
8
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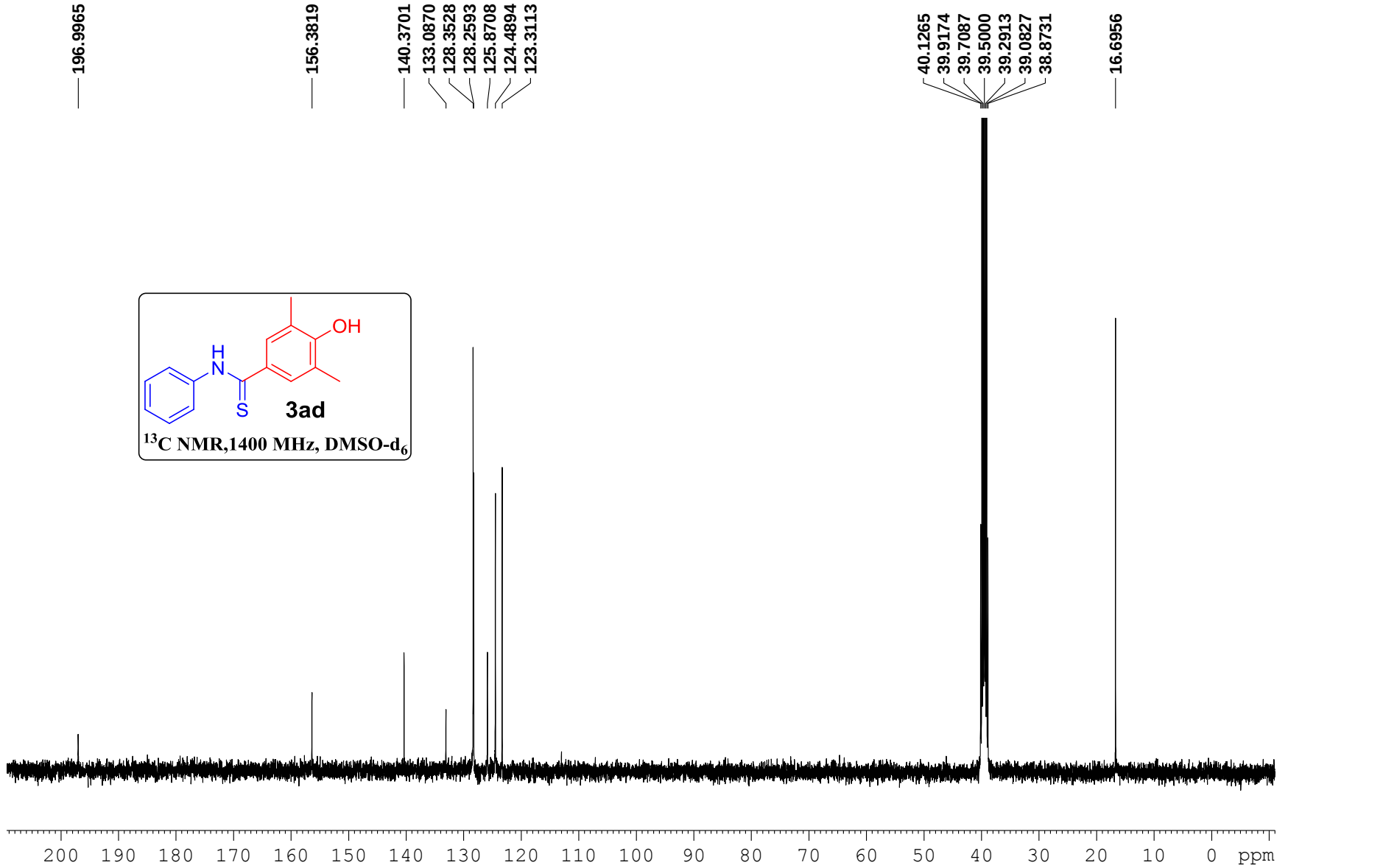
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S
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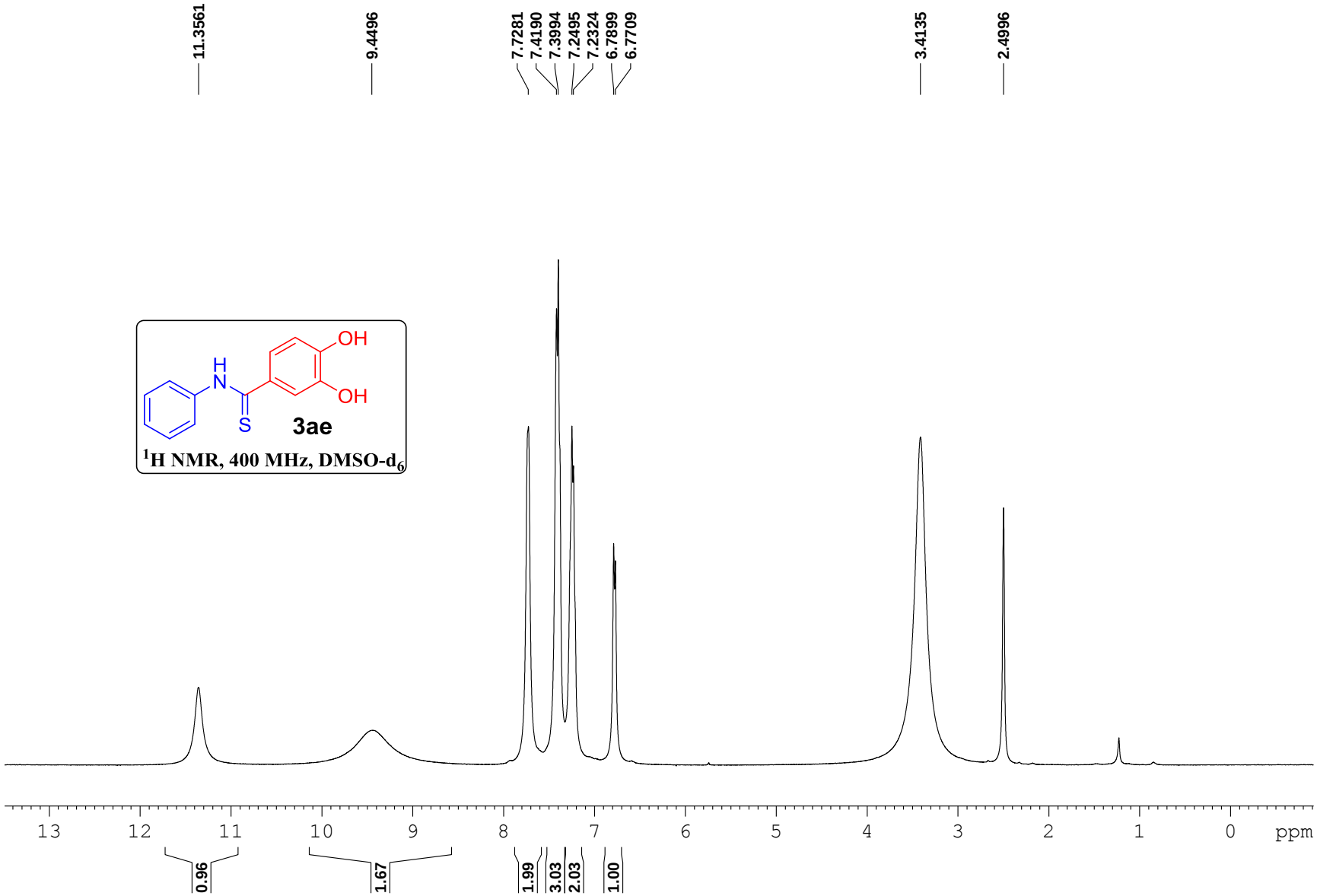
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H
N
S
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13
12
11
10
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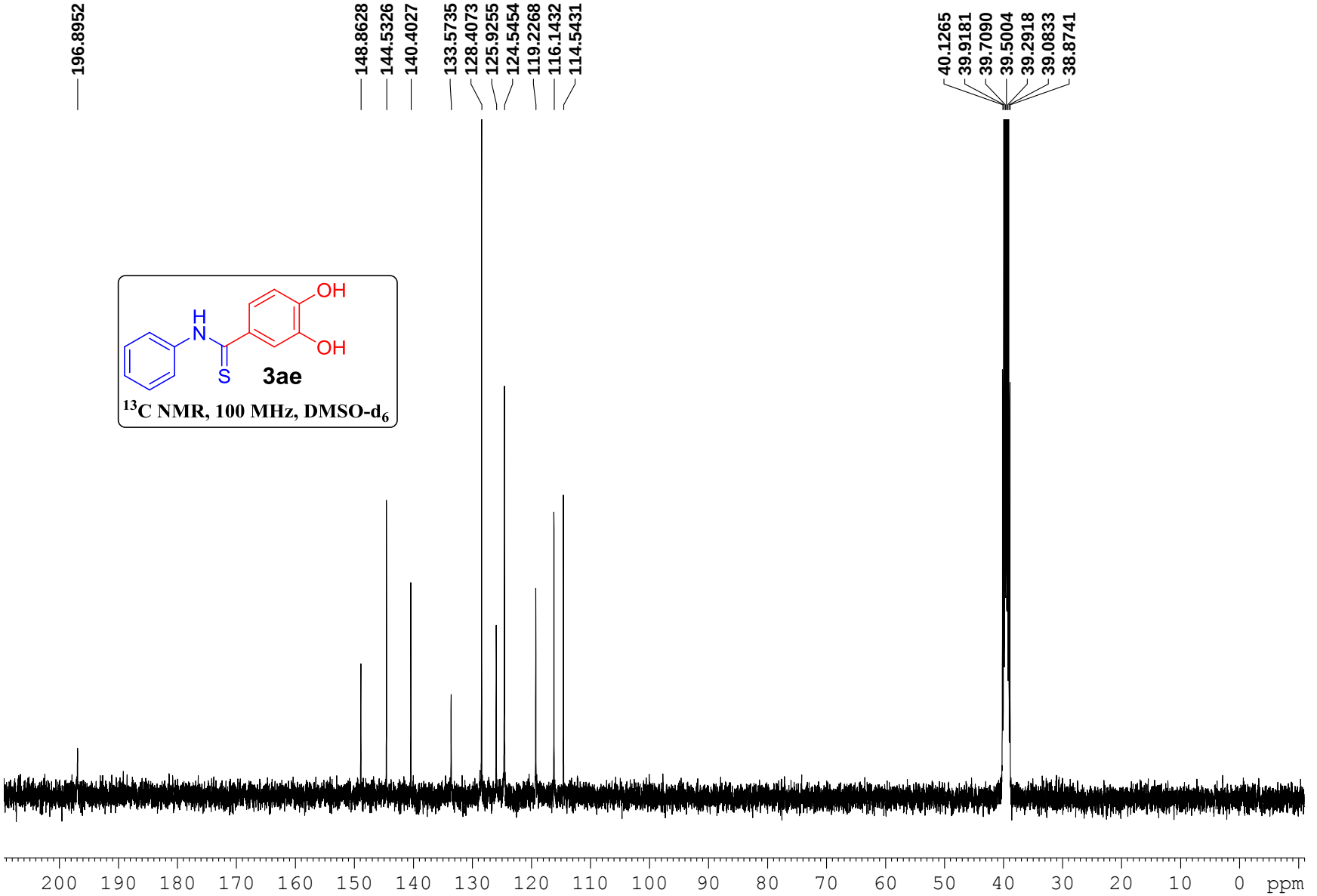
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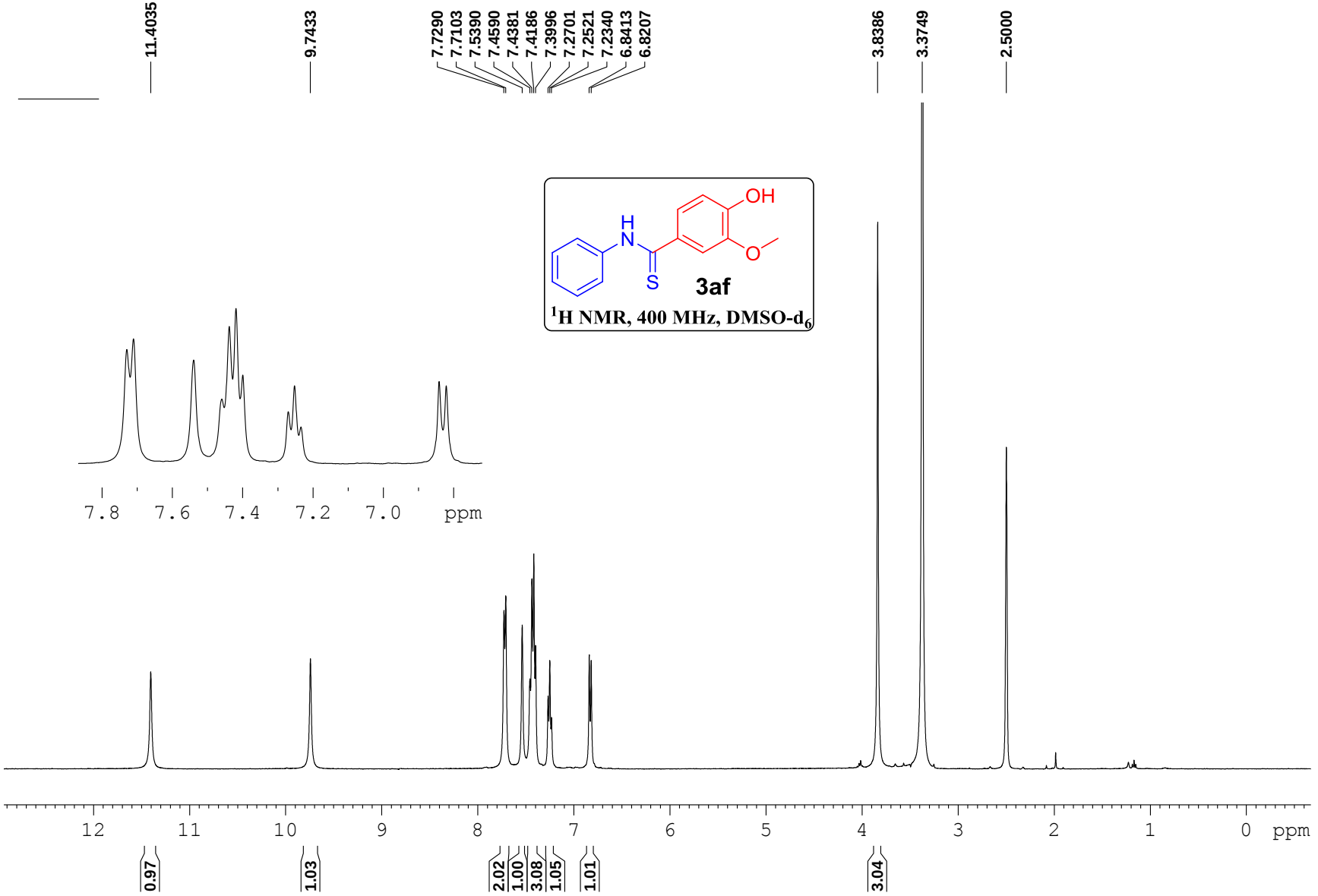
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OH
H
N
O
S
3af
1H NMR, 400 MHz, DMSO-d6
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7.6
7.4
7.2
7.0
ppm
12
11
10
9
8
7
6
5
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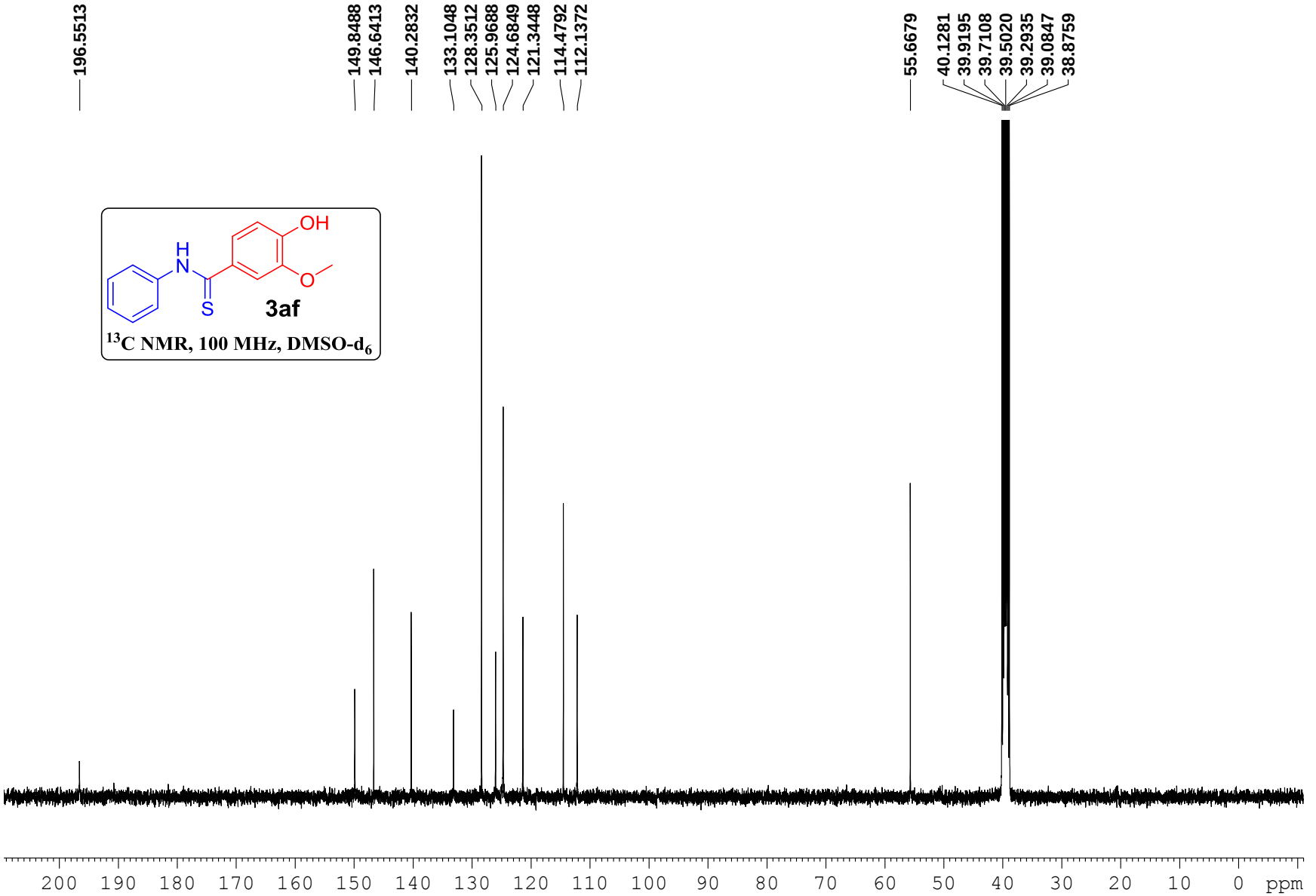
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O
S
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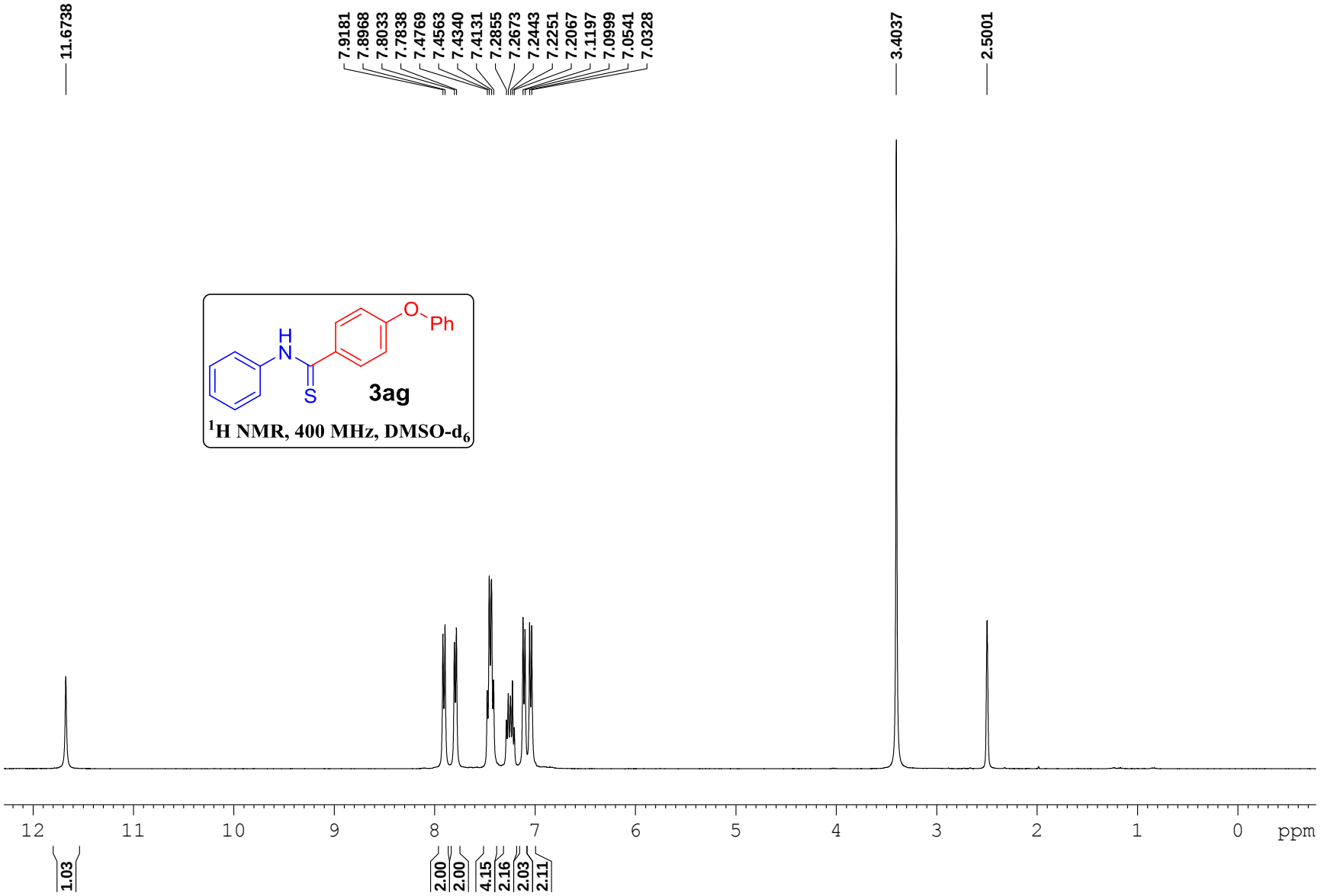
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3.4037
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O
Ph
H
N
S
3ag
1H NMR, 400 MHz, DMSO-d6
12
11
10
9
8
7
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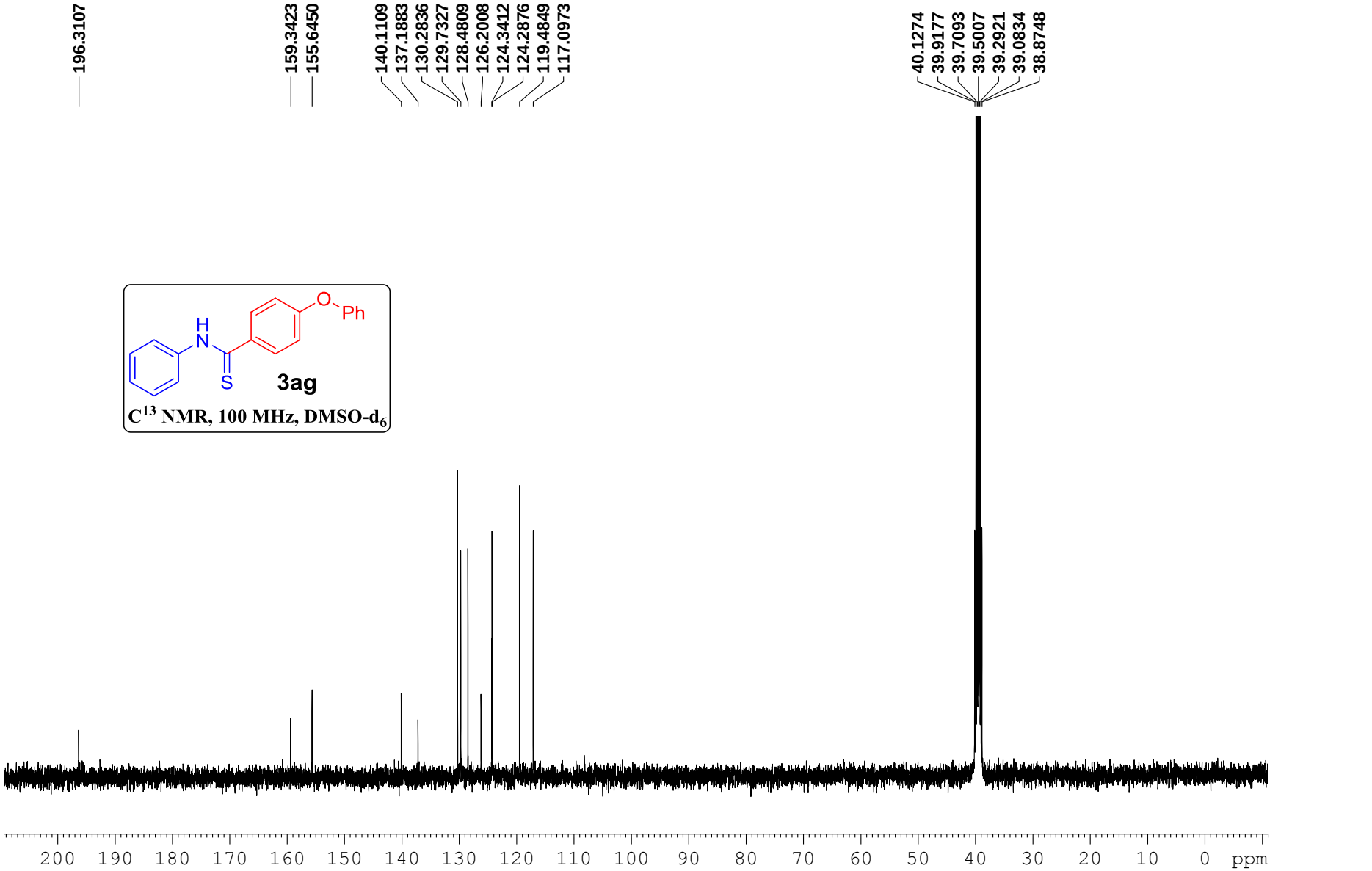
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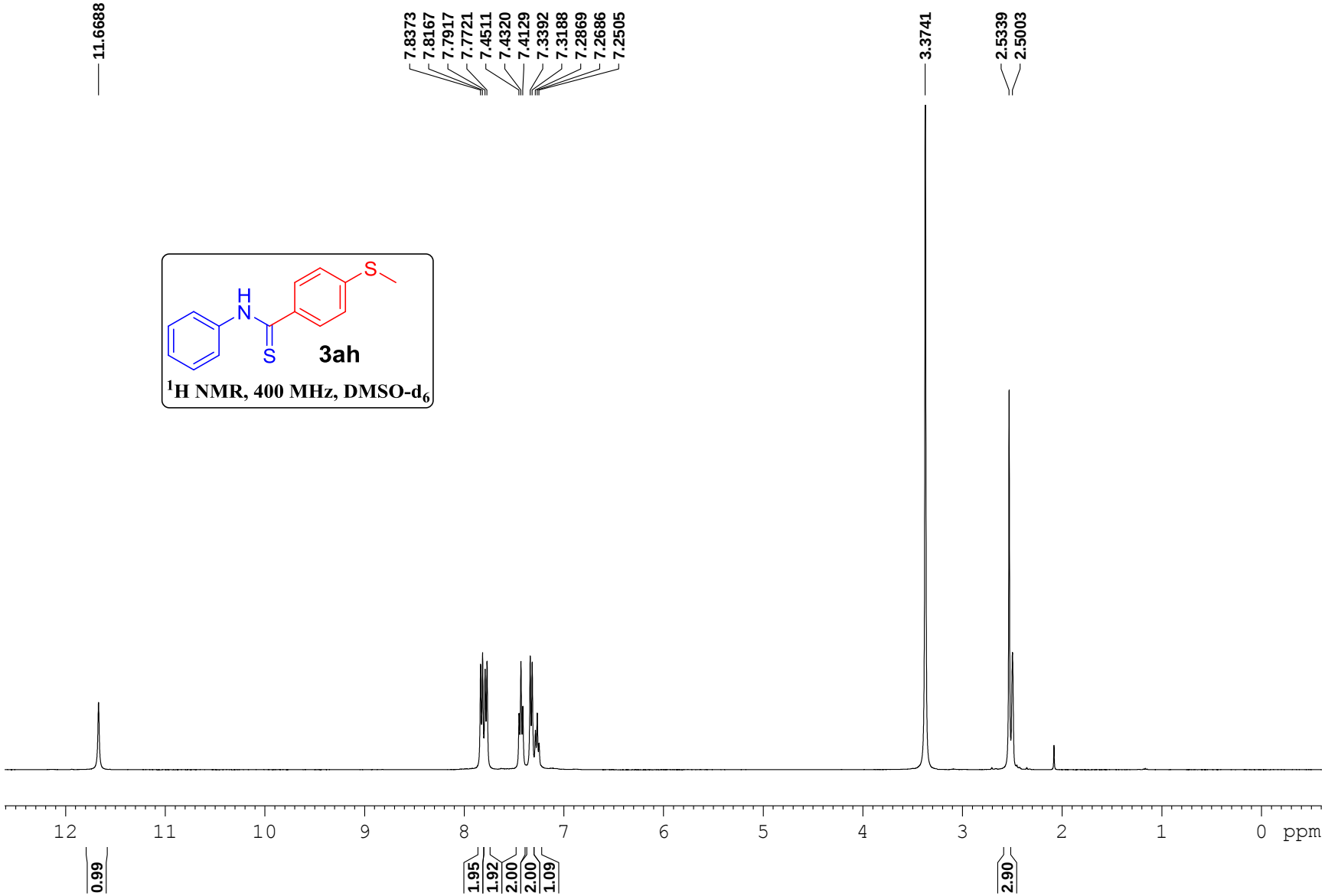
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7.2686
7.2505
3.3741
2.5339
2.5003
H
N
S
S
3ah
1H NMR, 400 MHz, DMSO-d6
12
11
10
9
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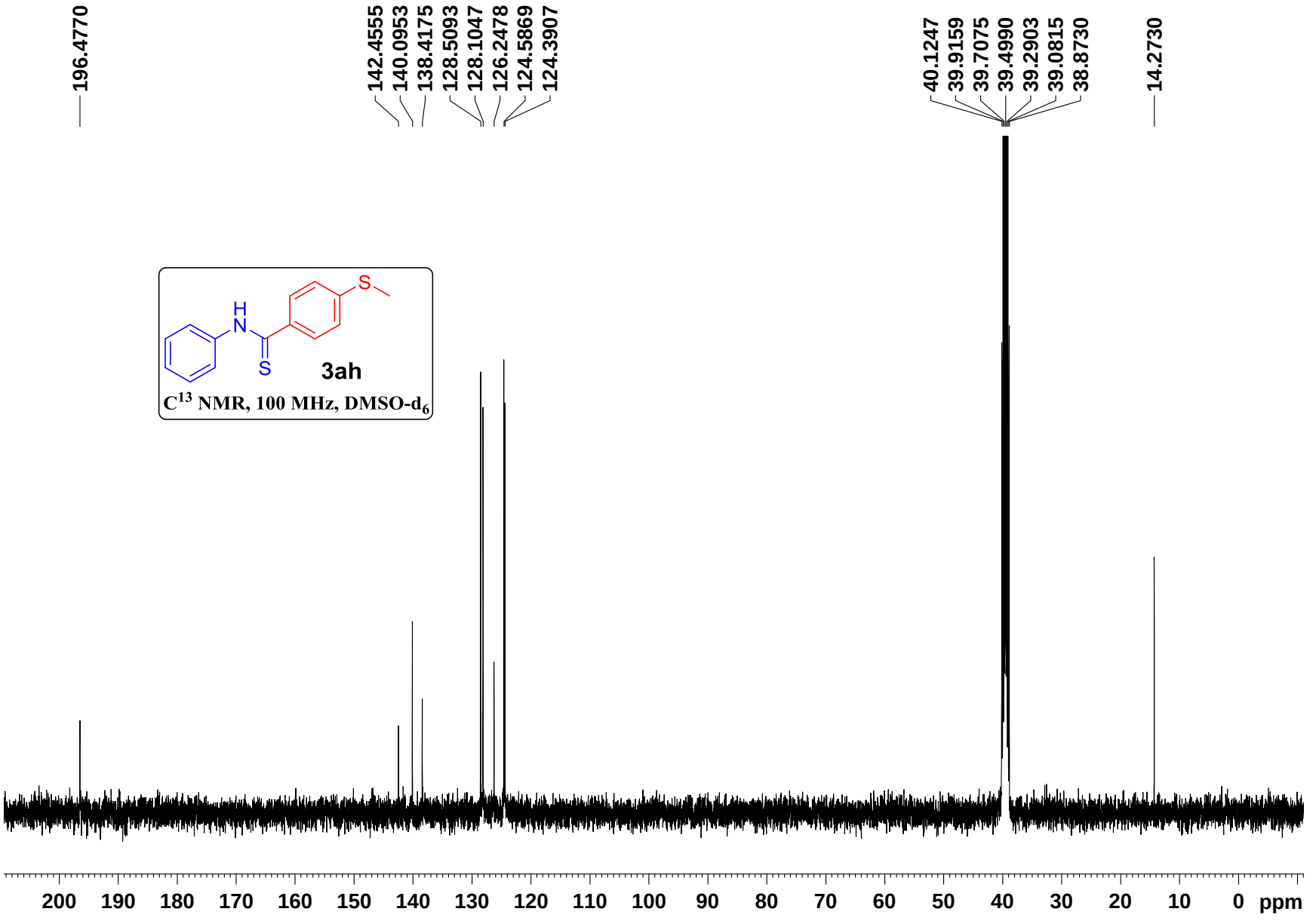
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39.4990
39.2903
39.0815
38.8730
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S
S
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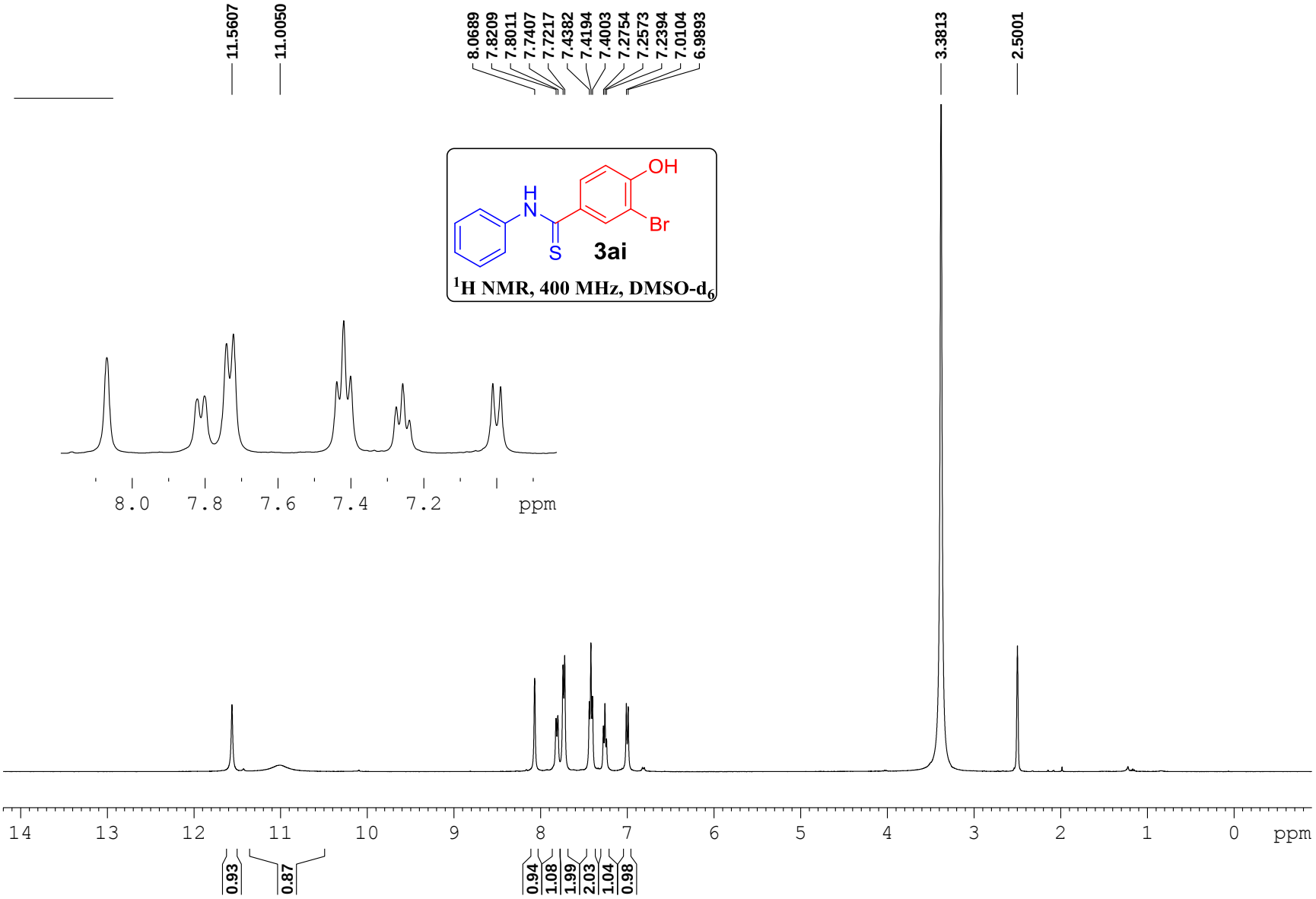
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H
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Br
S
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14
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10
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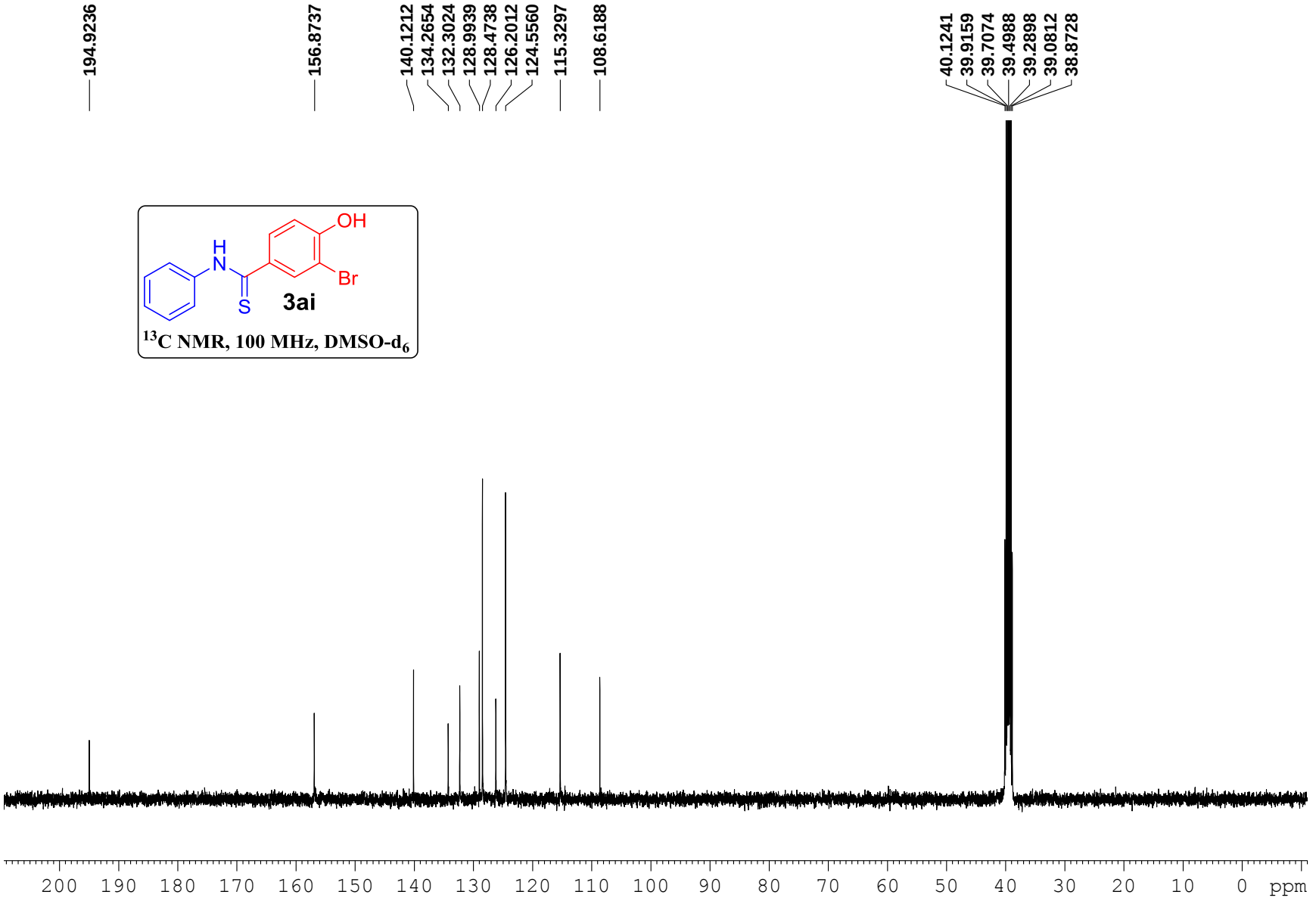
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39.2898
39.0812
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Br
S
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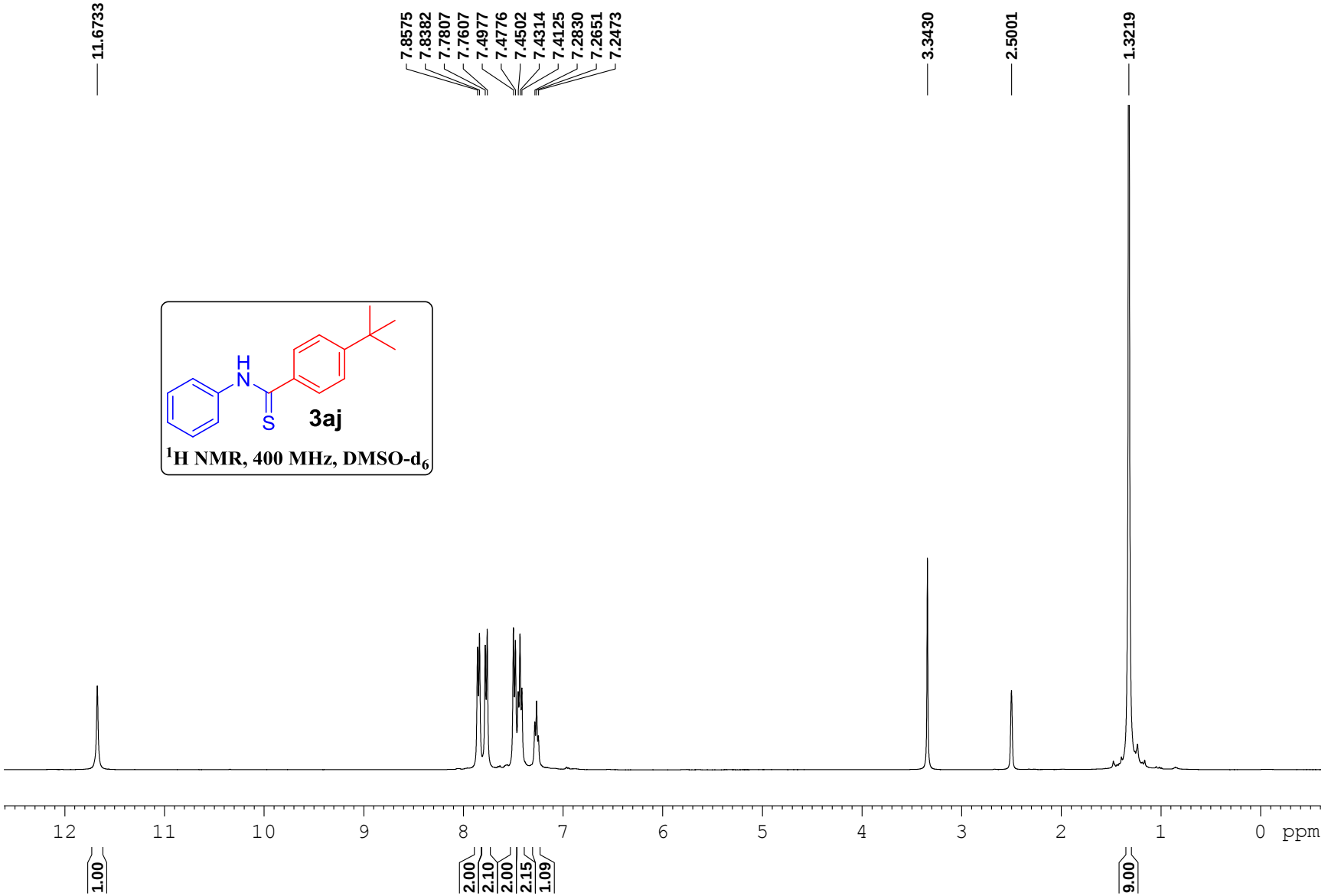
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3.3430
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1.3219
3aj
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12
11
10
9
8
7
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5
4
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ppm
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2.10
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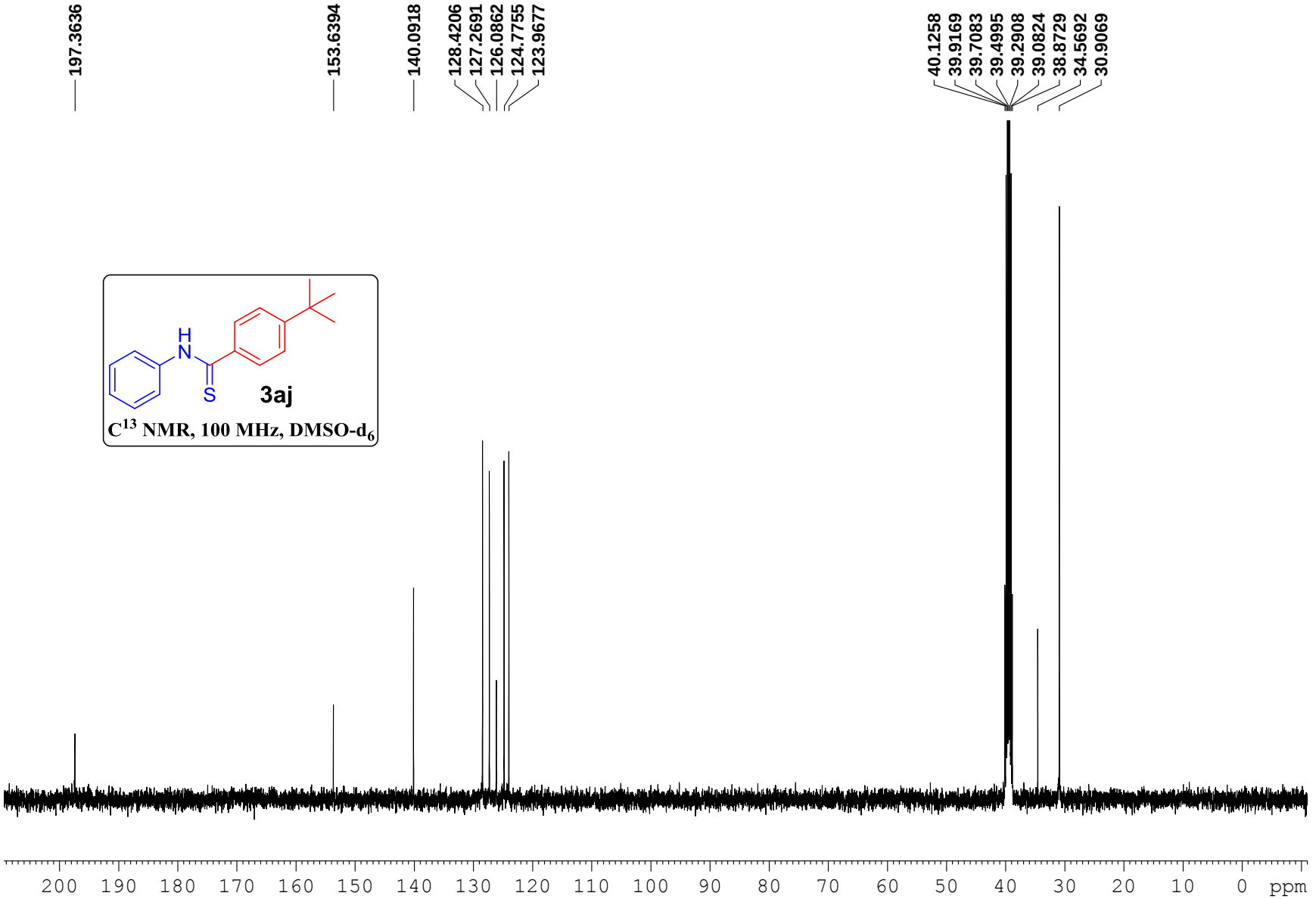
1.09
9.00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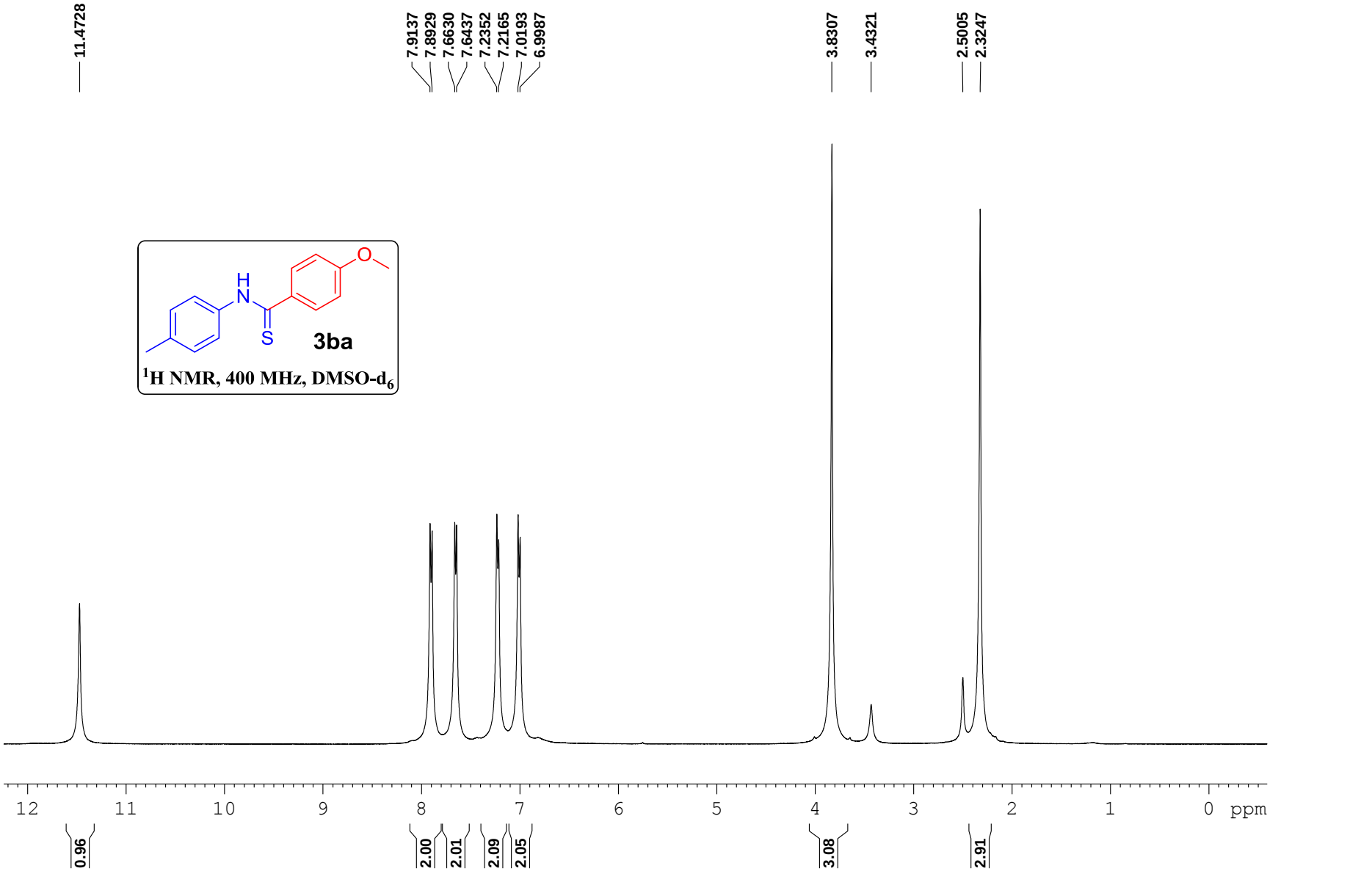
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2.3247
3ba
^{1}H NMR, 400 MHz, DMSO-d$_6$
12
11
10
9
8
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3
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2.01
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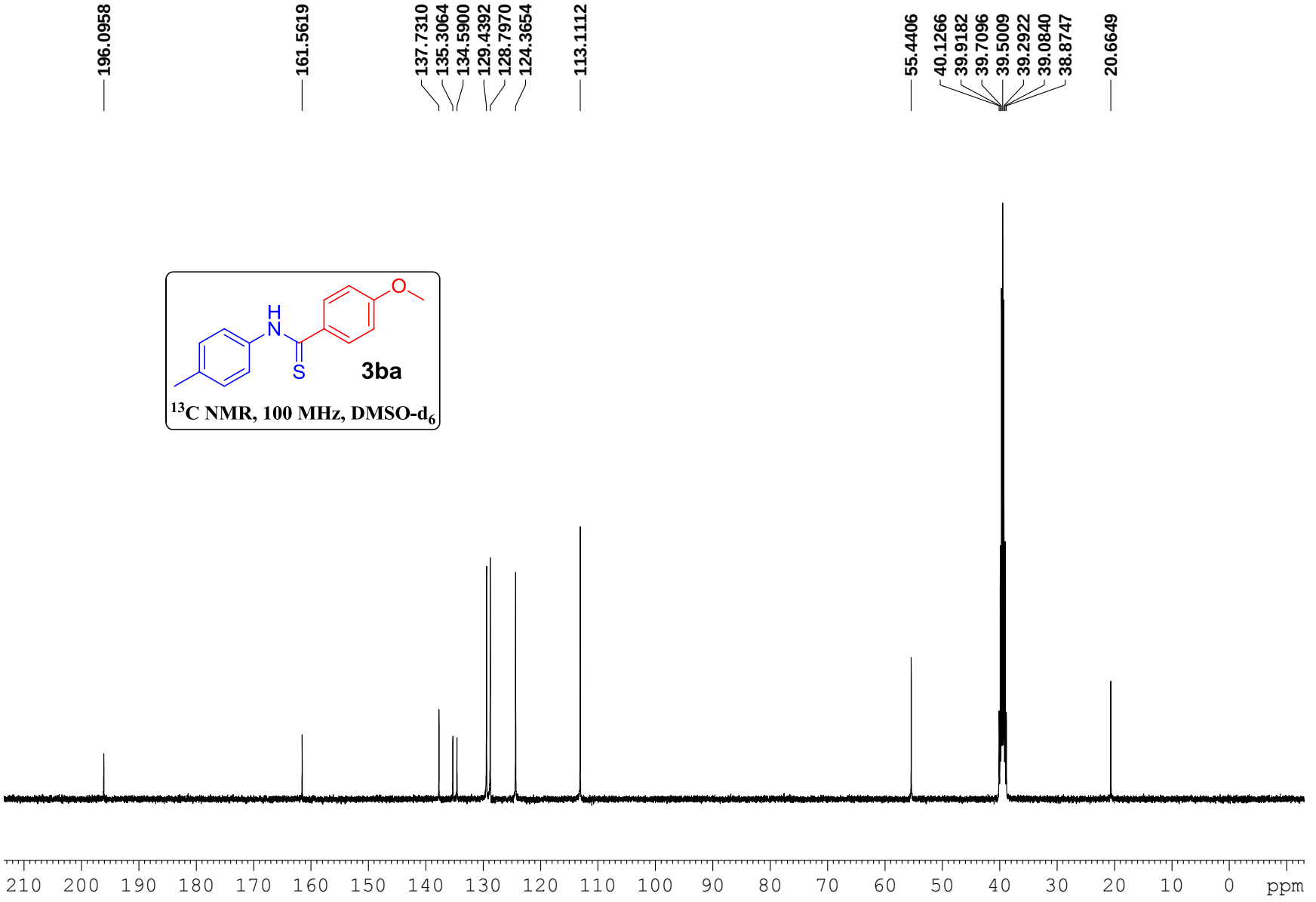
2.05
3.08
2.91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39.5009
39.2922
39.0840
38.8747
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S
O
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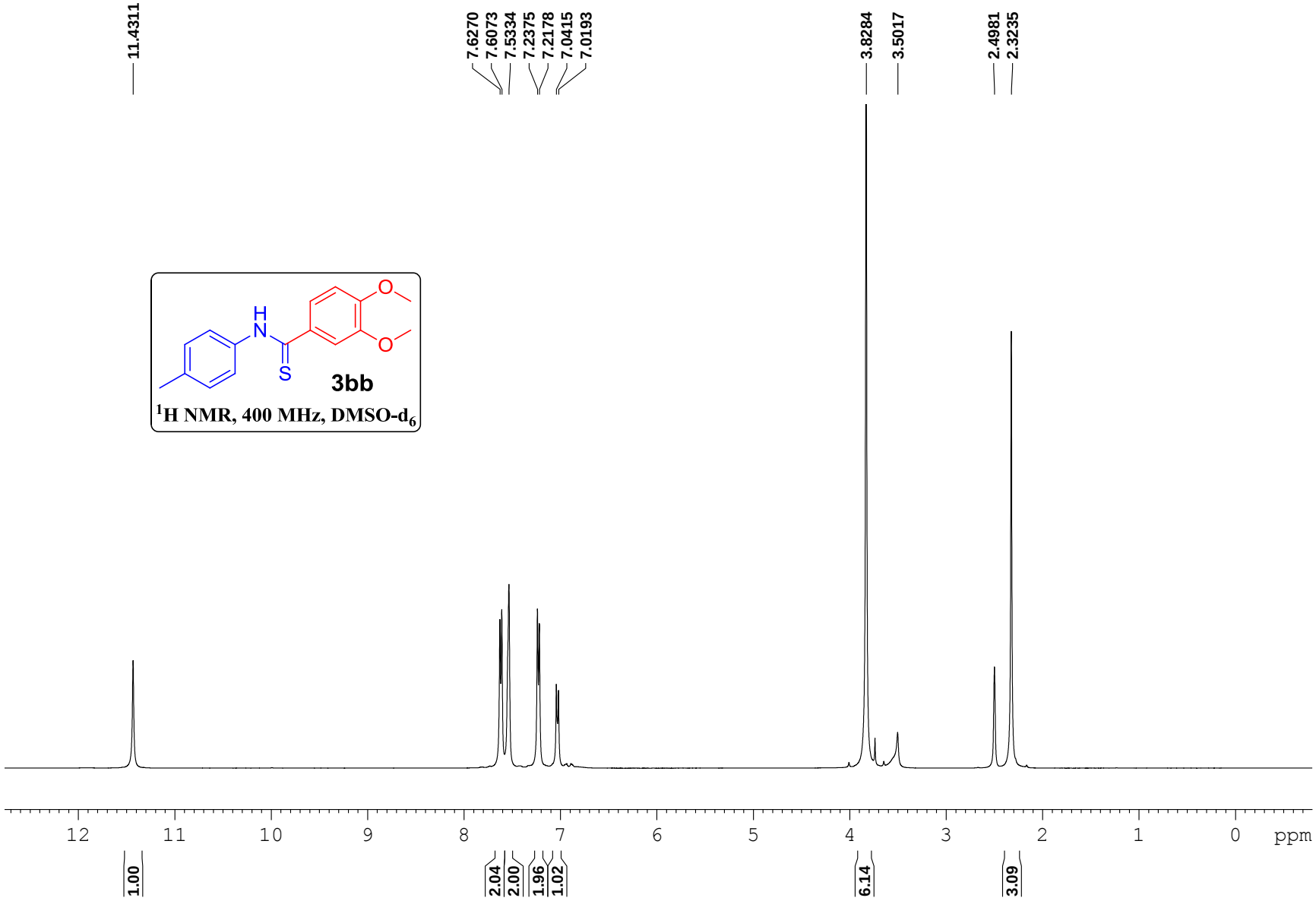
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2.4981
2.3235
3bb
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12
11
10
9
8
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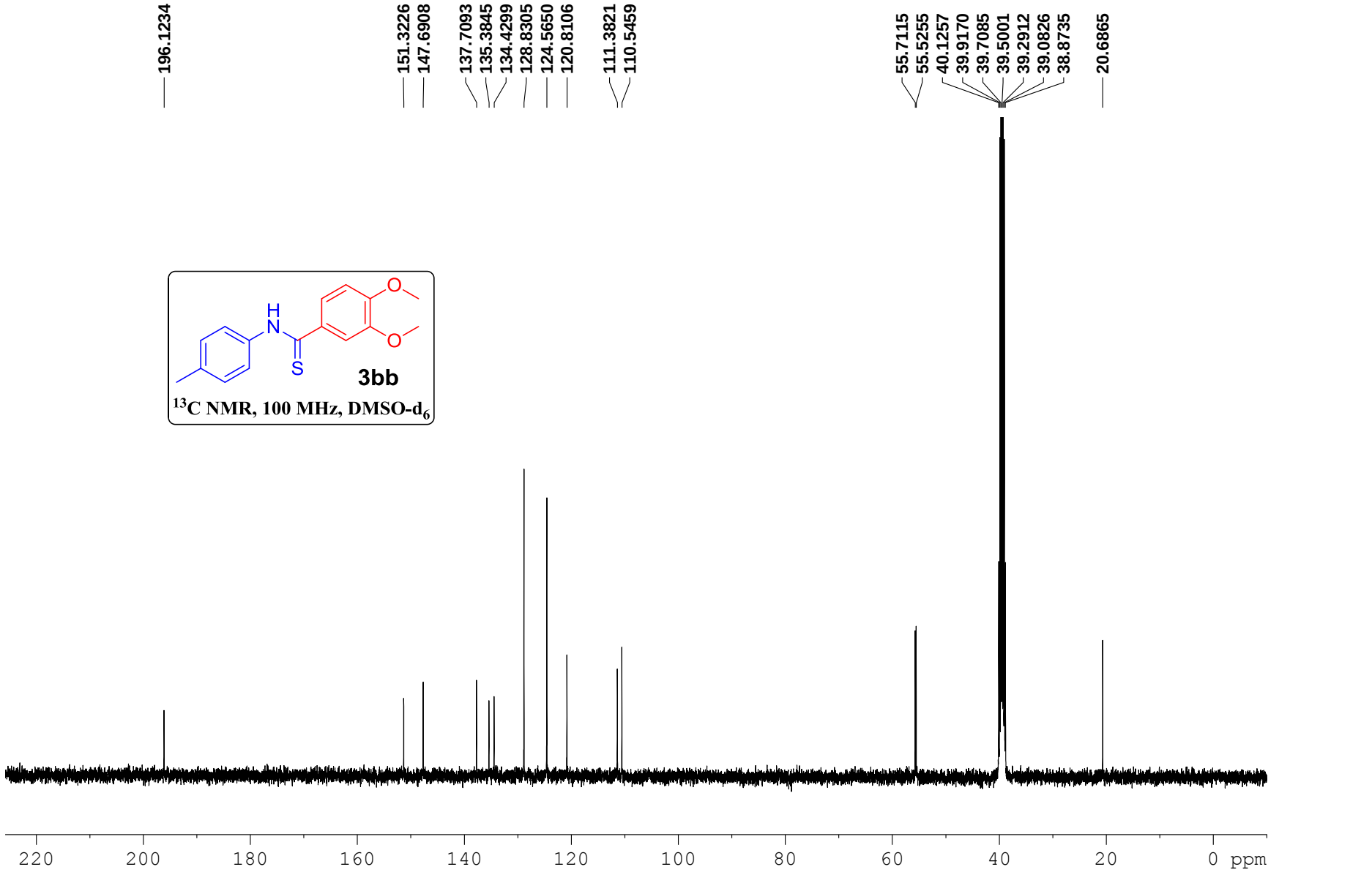
2.04
2.00
1.96
1.02
6.14
3.09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55.5255
40.1257
39.9170
39.7085
39.5001
39.2912
39.0826
38.8735
20.6865
H
N
S
O
O
3bb
13C NMR, 100 MHz, DMSO-d6
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180
160
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120
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80
60
40
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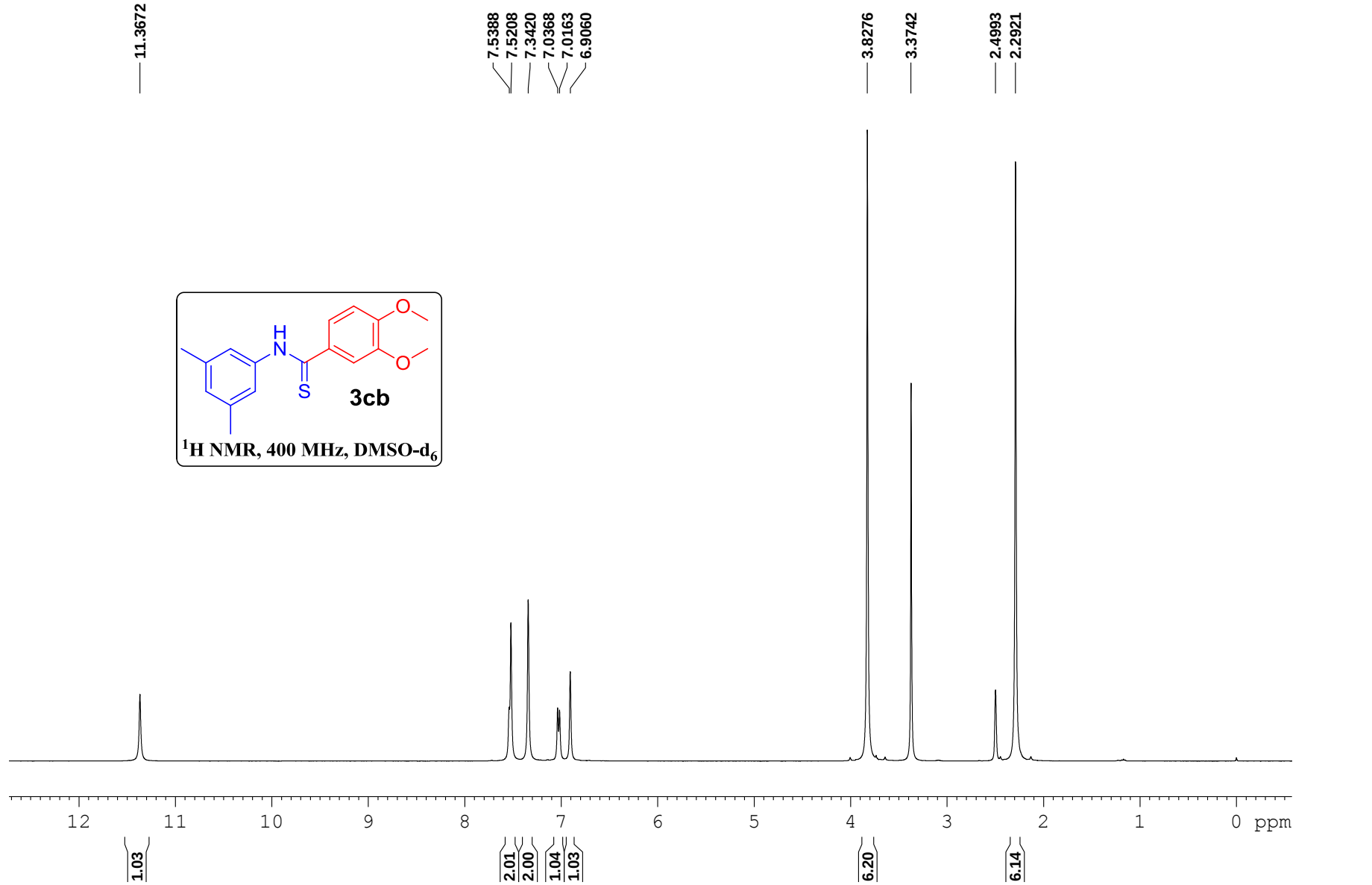
0 ppm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3cb
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11
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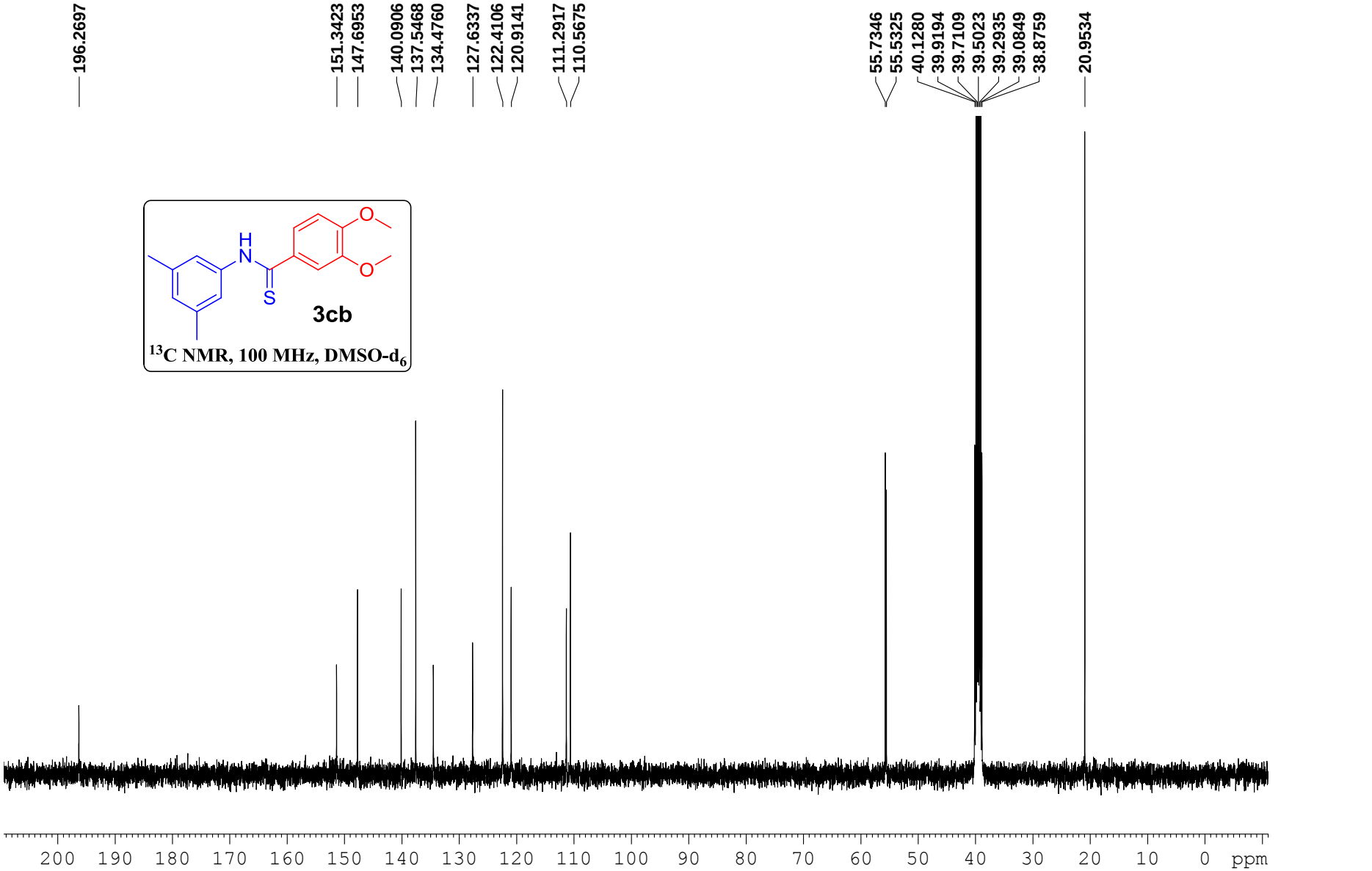
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39.5023
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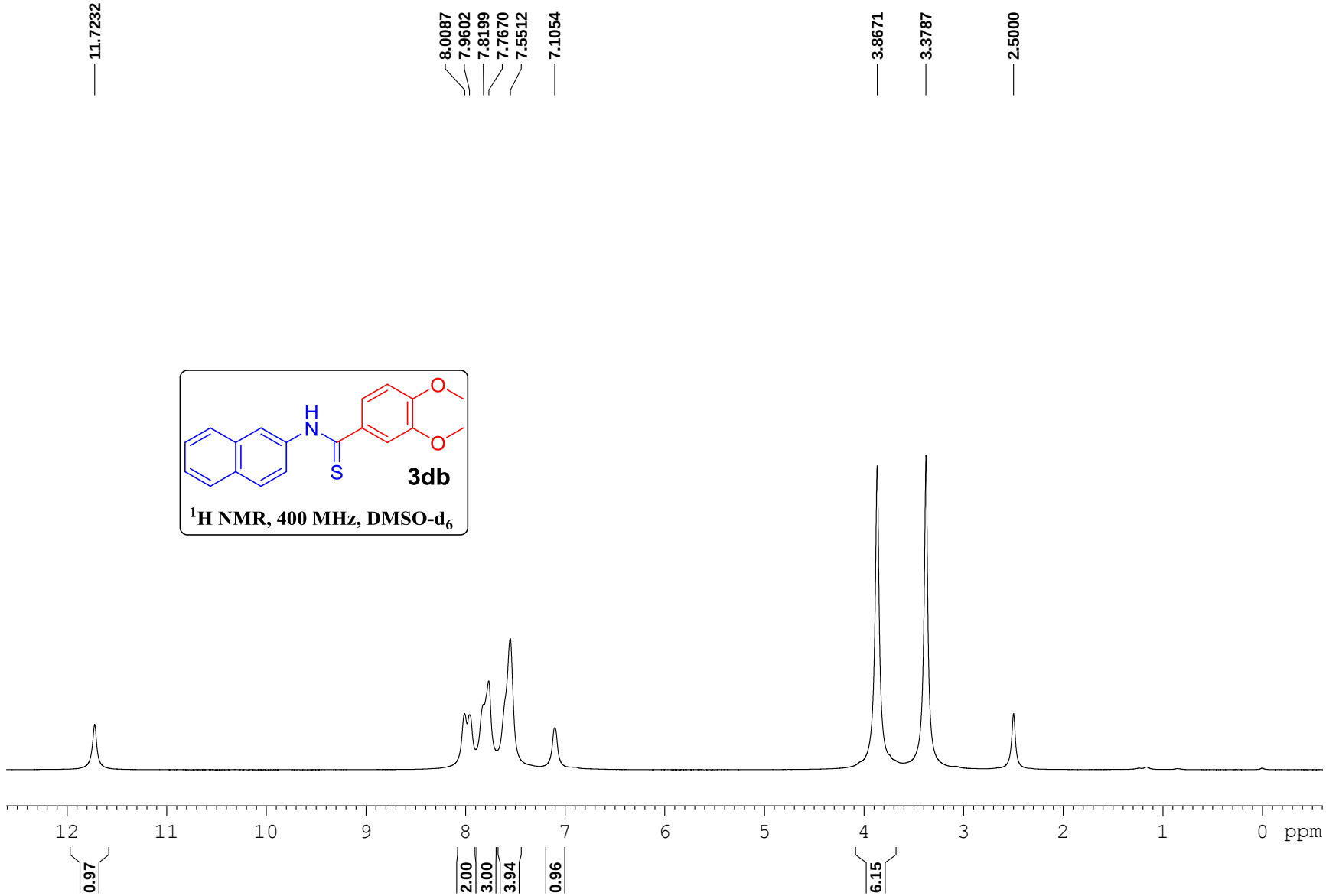
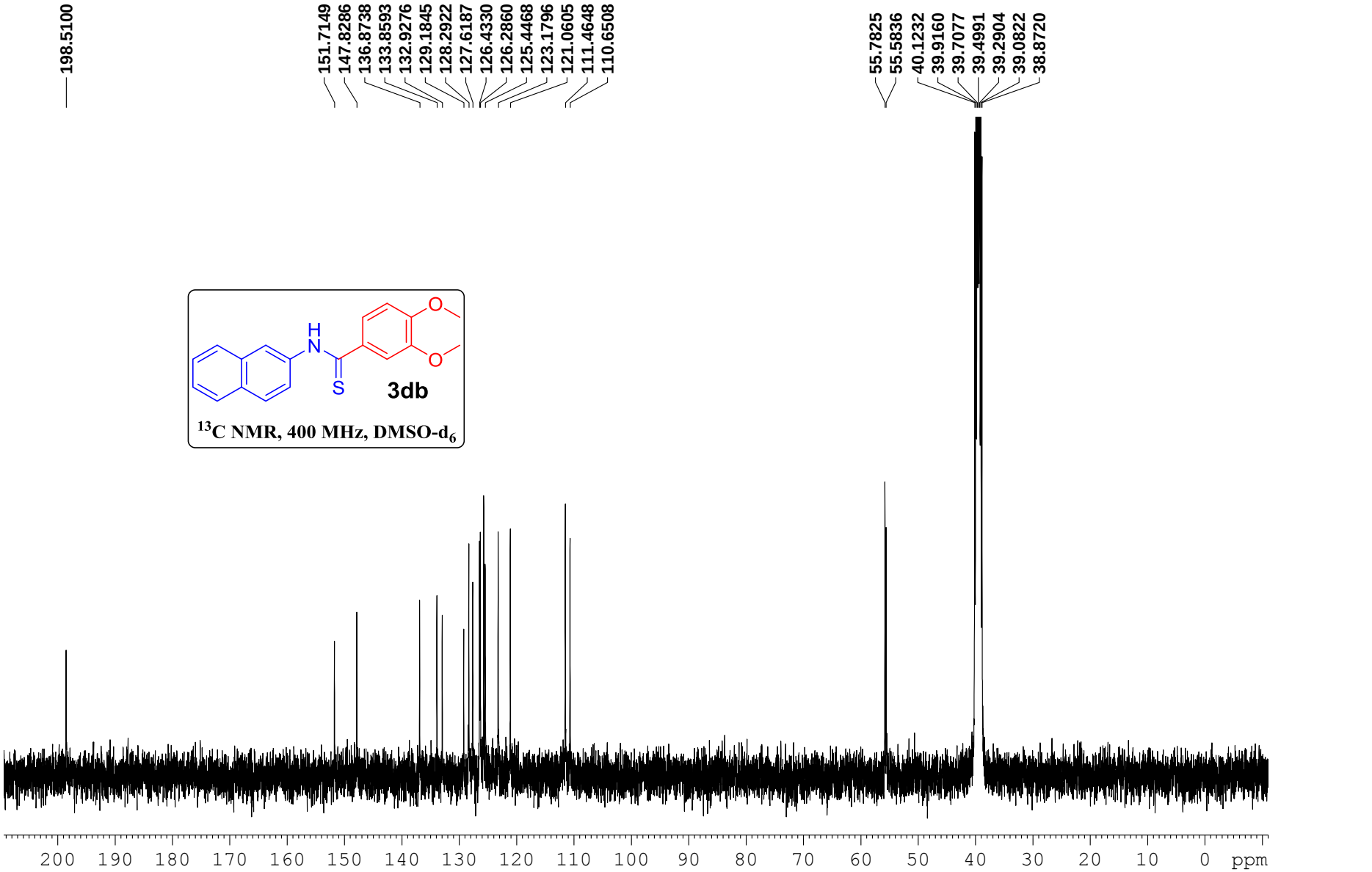
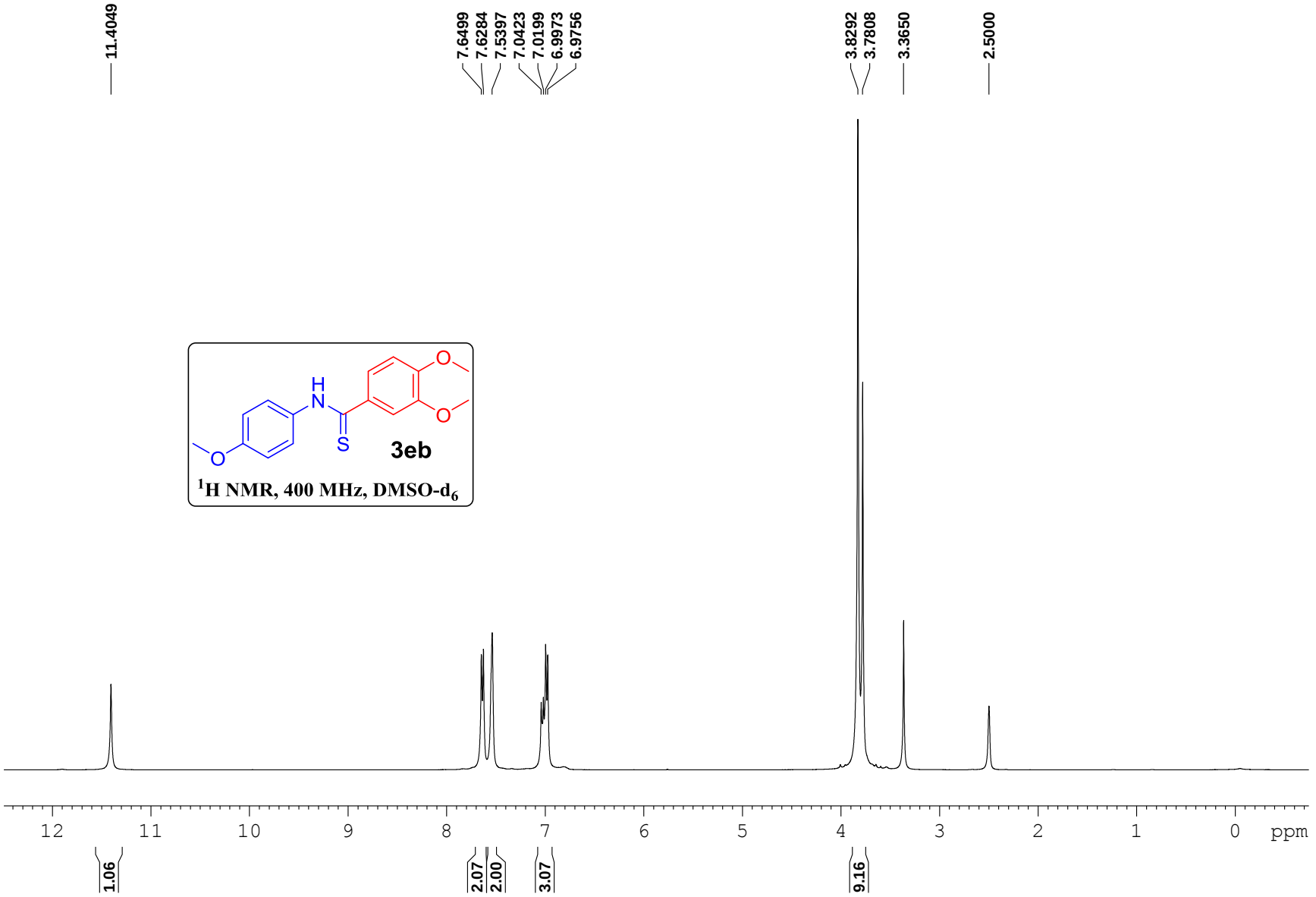
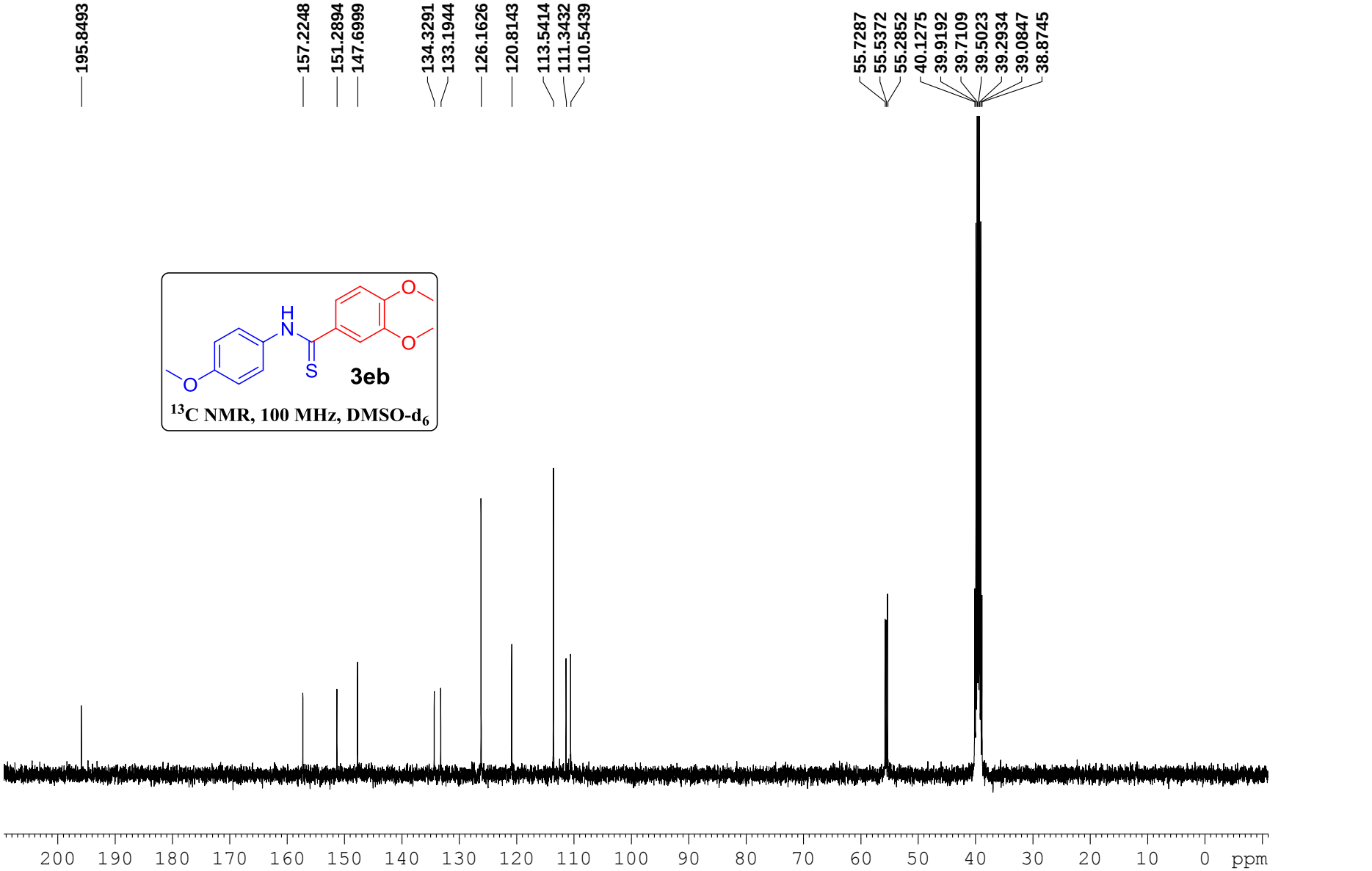
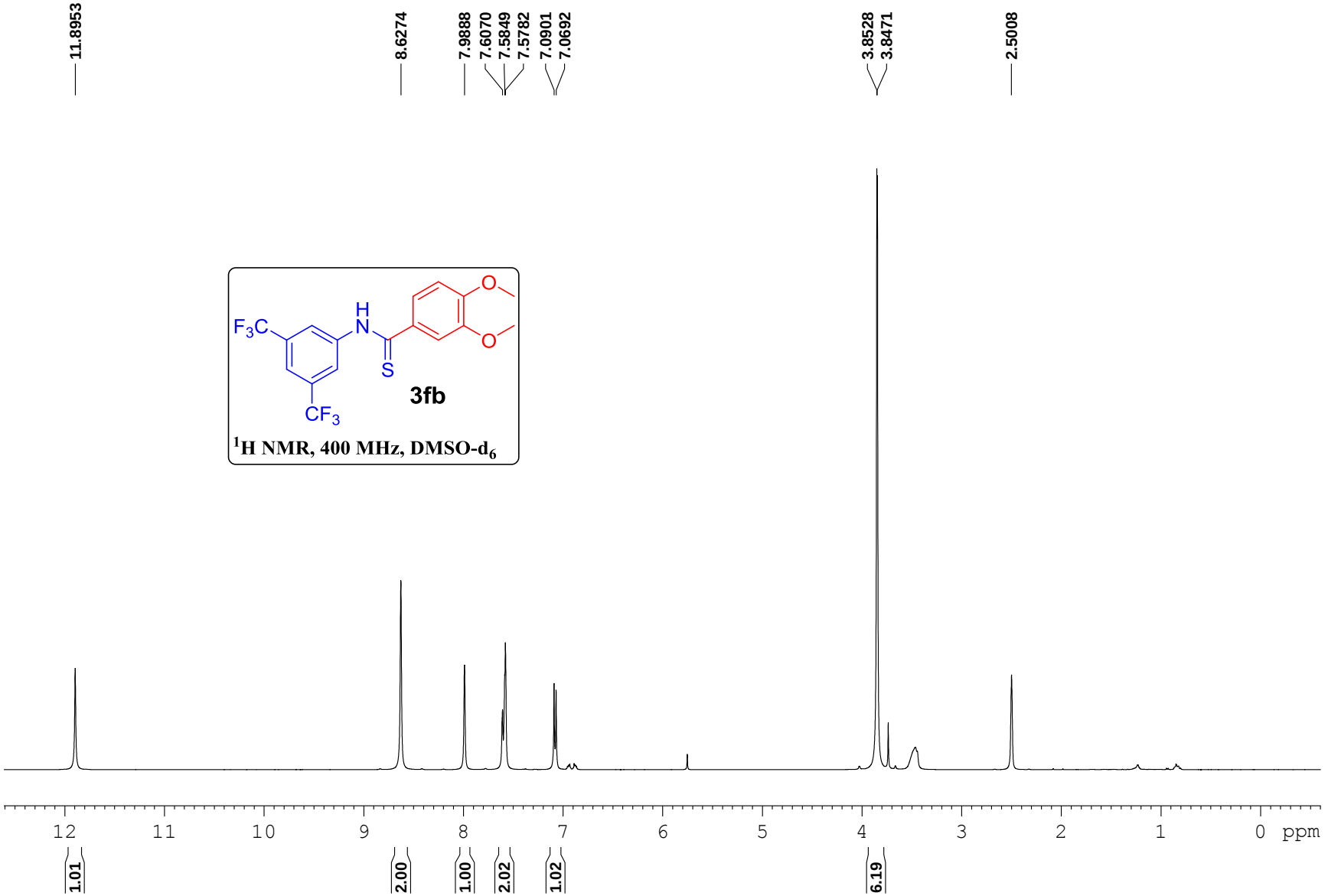
39.0849
38.8759
20.9534
H
N
S
O
O
3cb
13C NMR, 100 MHz, DMSO-d6
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

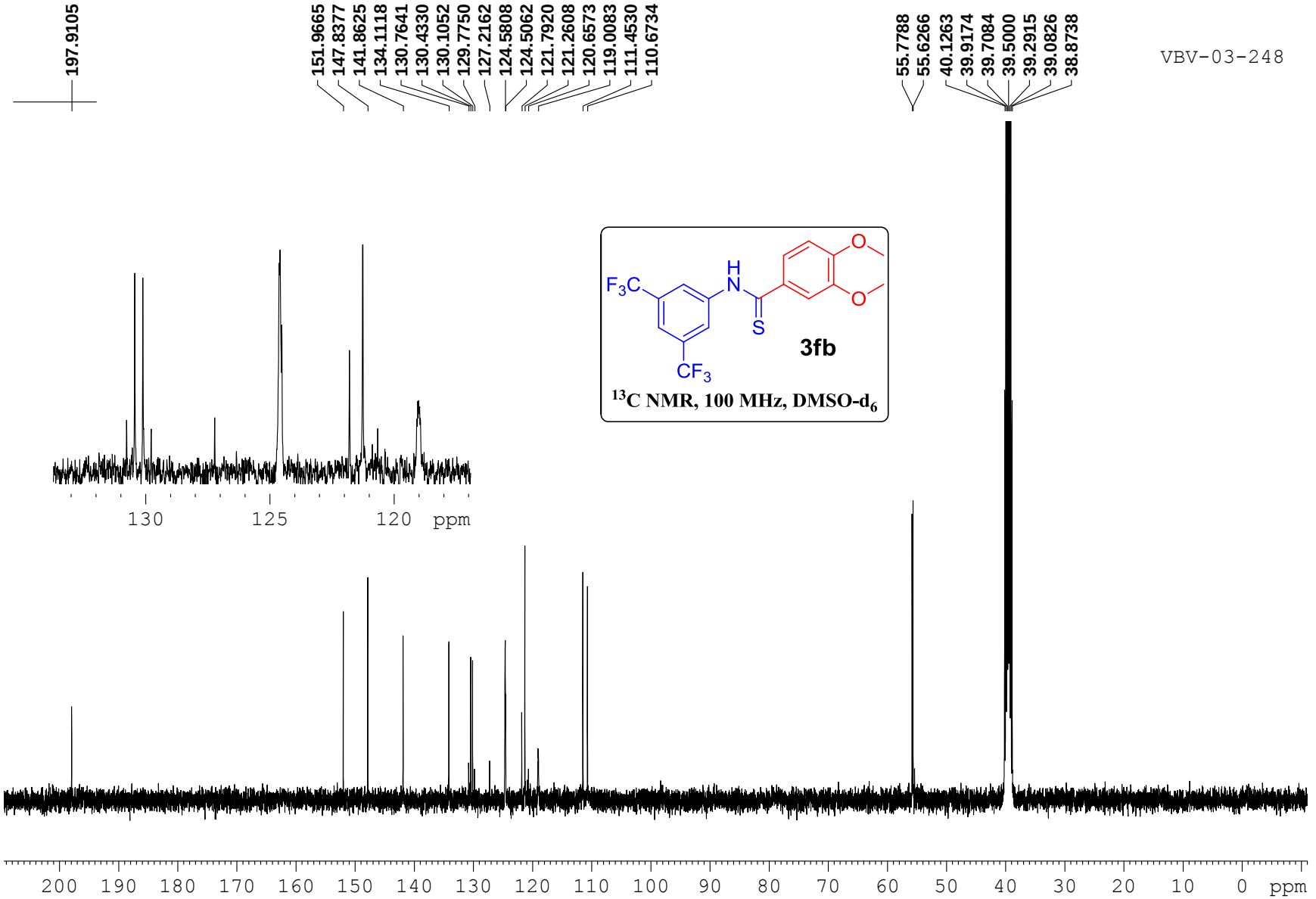

11.7232
8.0087
7.9602
7.8199
7.7670
7.5512
7.1054
3.8671
3.3787
2.5000
3db
^{1}H NMR, 400 MHz, DMSO-d$_6$
12
11
10
9
8
7
6
5
4
3
2
1
0 ppm
0.97
2.00
3.00
3.94
0.96
6.15

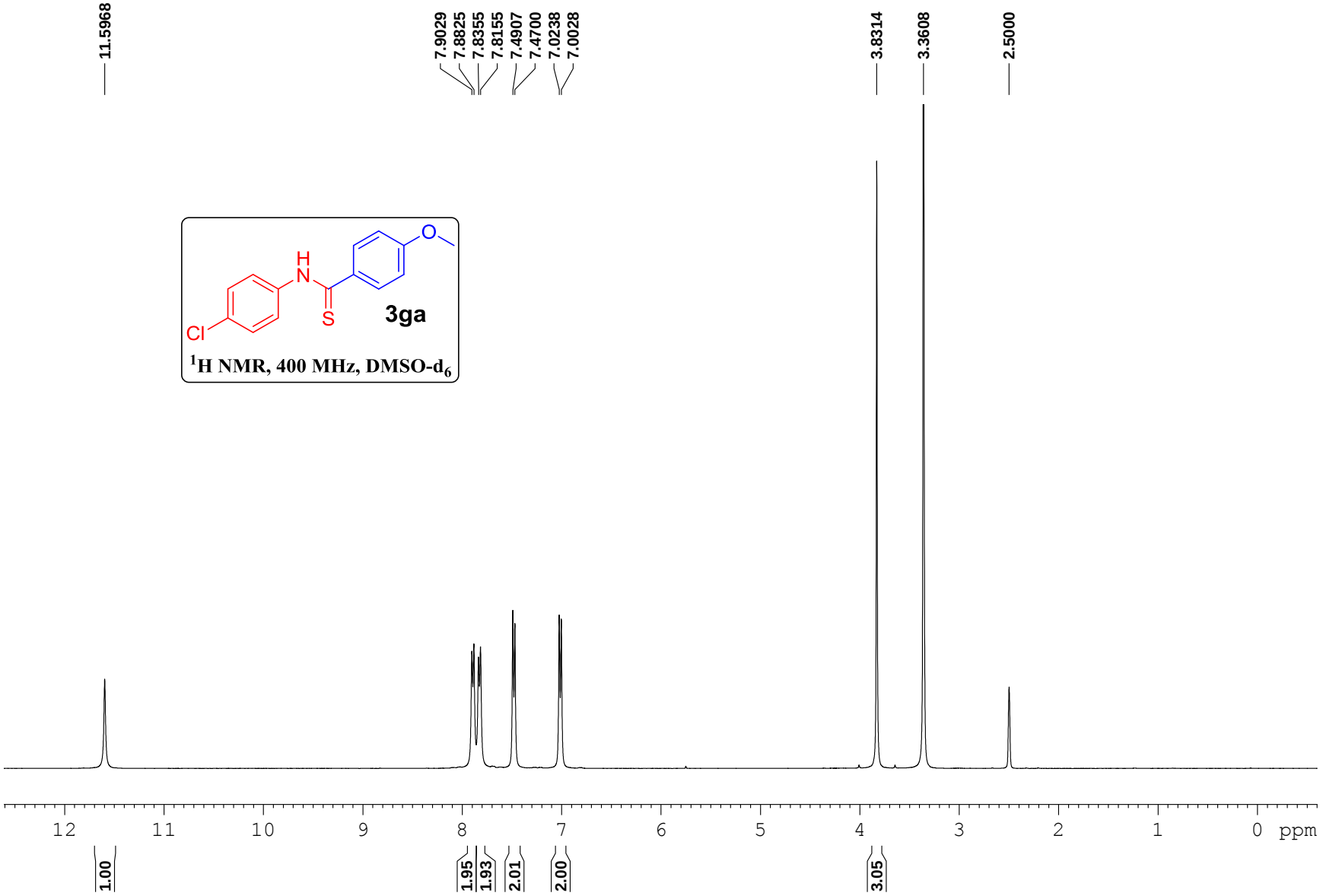

198.5100
151.7149
147.8286
136.8738
133.8593
132.9276
129.1845
128.2922
127.6187
126.4330
126.2860
125.4468
123.1796
121.0605
111.4648
110.6508
55.7825
55.5836
40.1232
39.9160
39.7077
39.4991
39.2904
39.0822
38.8720
H
N
S
O
O
3db
^{13}C NMR, 400 MHz, DMSO-d$_6$
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

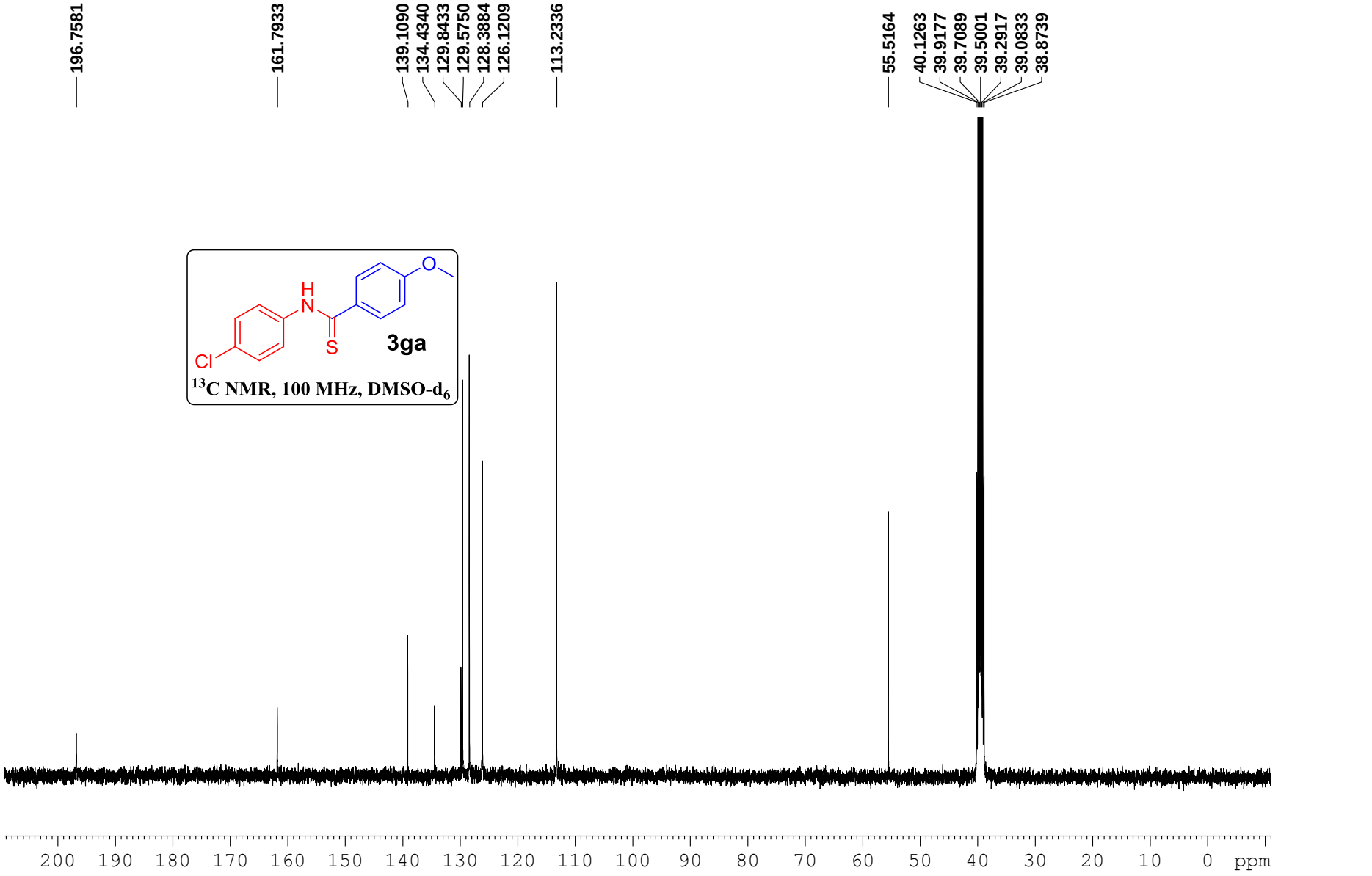

11.4049
7.6499
7.6284
7.5397
7.0423
7.0199
6.9973
6.9756
3.8292
3.7808
3.3650
2.5000
3eb
1H NMR, 400 MHz, DMSO-d6
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.06
2.07
2.00
3.07
9.16

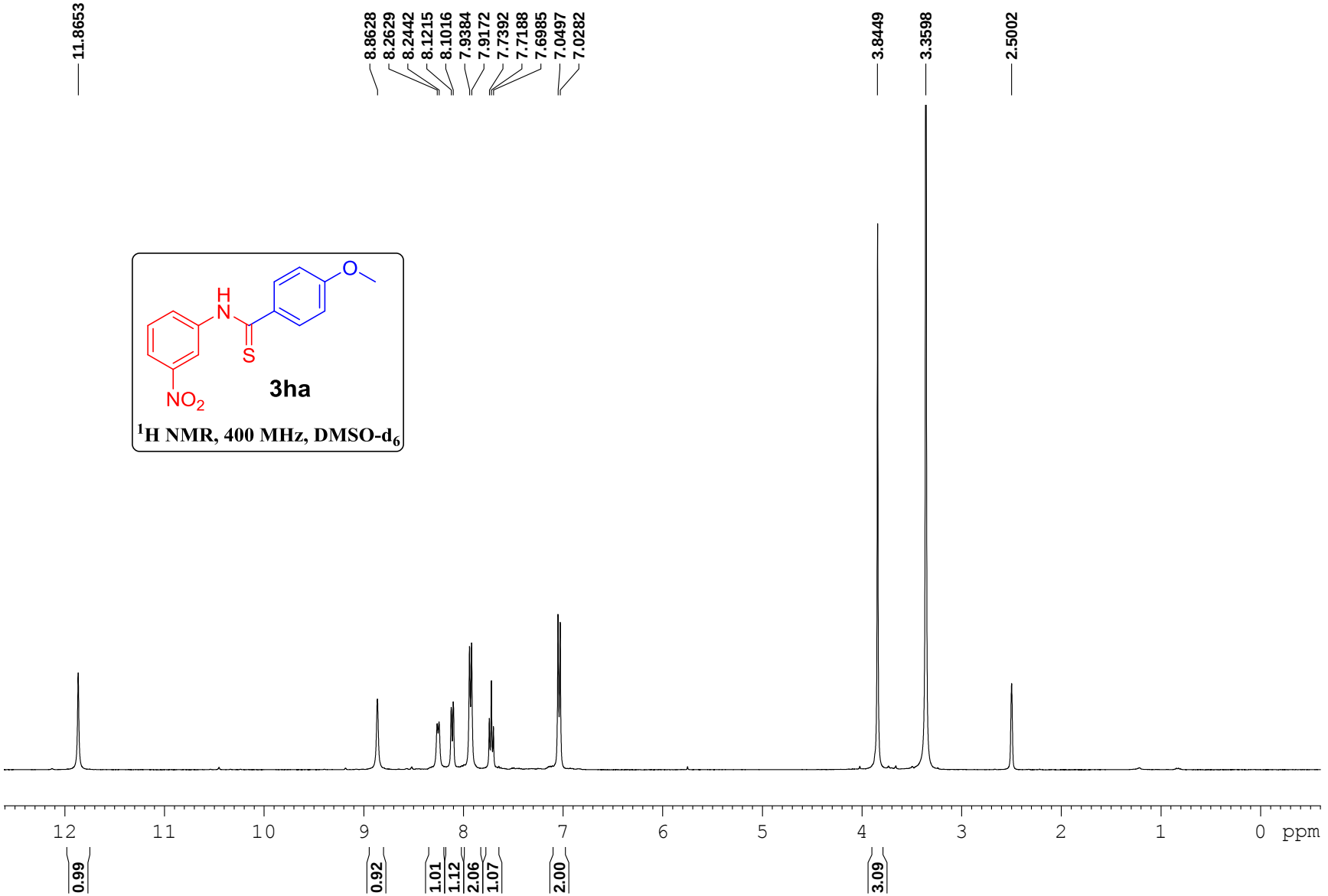

195.8493
157.2248
151.2894
147.6999
134.3291
133.1944
126.1626
120.8143
113.5414
111.3432
110.5439
55.7287
55.5372
55.2852
40.1275
39.9192
39.7109
39.5023
39.2934
39.0847
38.8745
H
N
S
O
O
O
3eb
13C NMR, 100 MHz, DMSO-d6
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

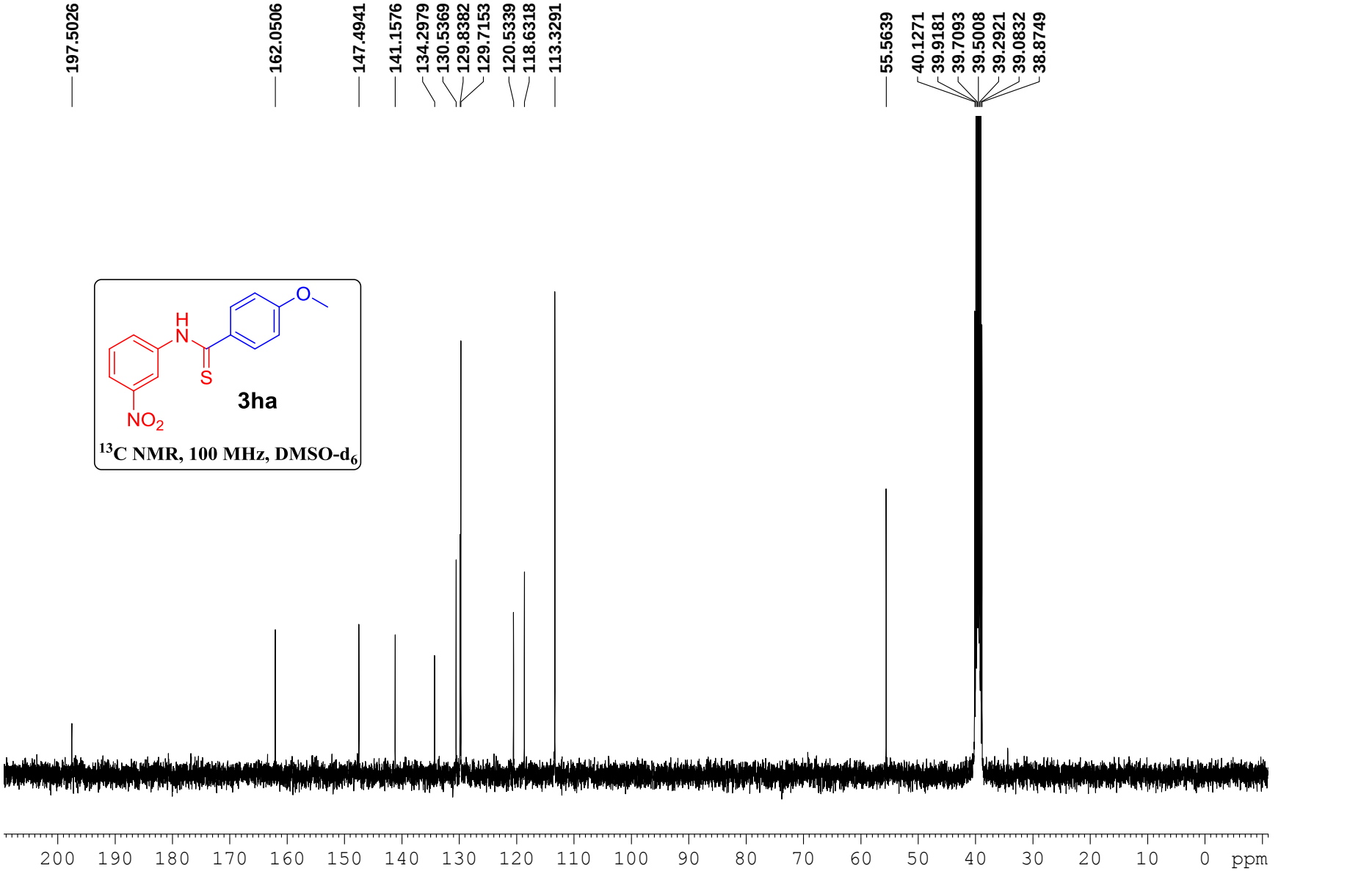

11.8953
8.6274
7.9888
7.6070
7.5849
7.5782
7.0901
7.0692
3.8528
3.8471
2.5008
F3C
H
N
S
O
O
CF3
3fb
1H NMR, 400 MHz, DMSO-d6
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.01
2.00
1.00
2.02
1.02
6.19

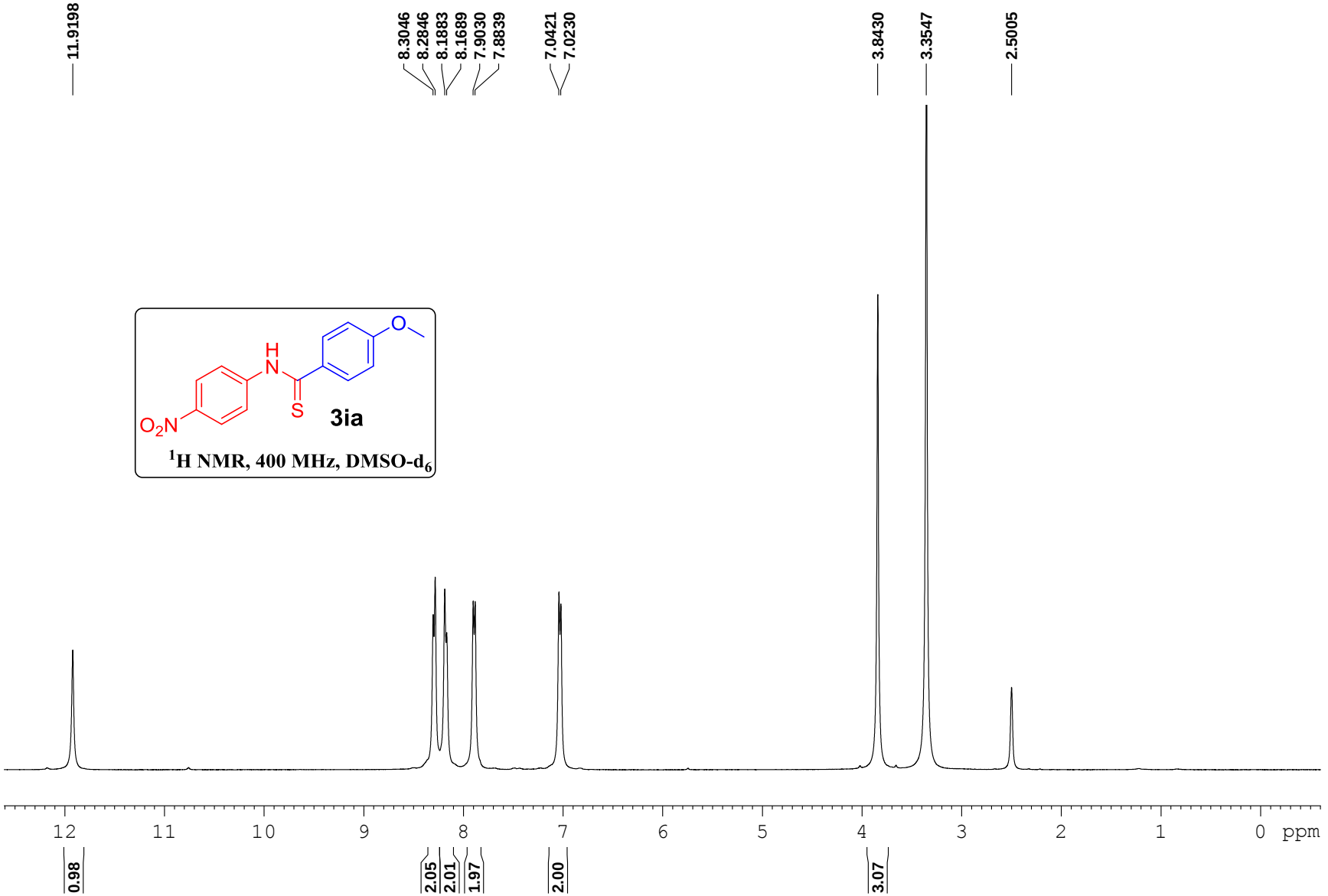

197.9105
151.9665
147.8377
141.8625
134.1118
130.7641
130.4330
130.1052
129.7750
127.2162
124.5808
124.5062
121.7920
121.2608
120.6573
119.0083
111.4530
110.6734
55.7788
55.6266
40.1263
39.9174
39.7084
39.5000
39.2915
39.0826
38.8738
VBV-03-248
3fb
^{13}C NMR, 100 MHz, DMSO-d$_6$
130
125
120
ppm
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

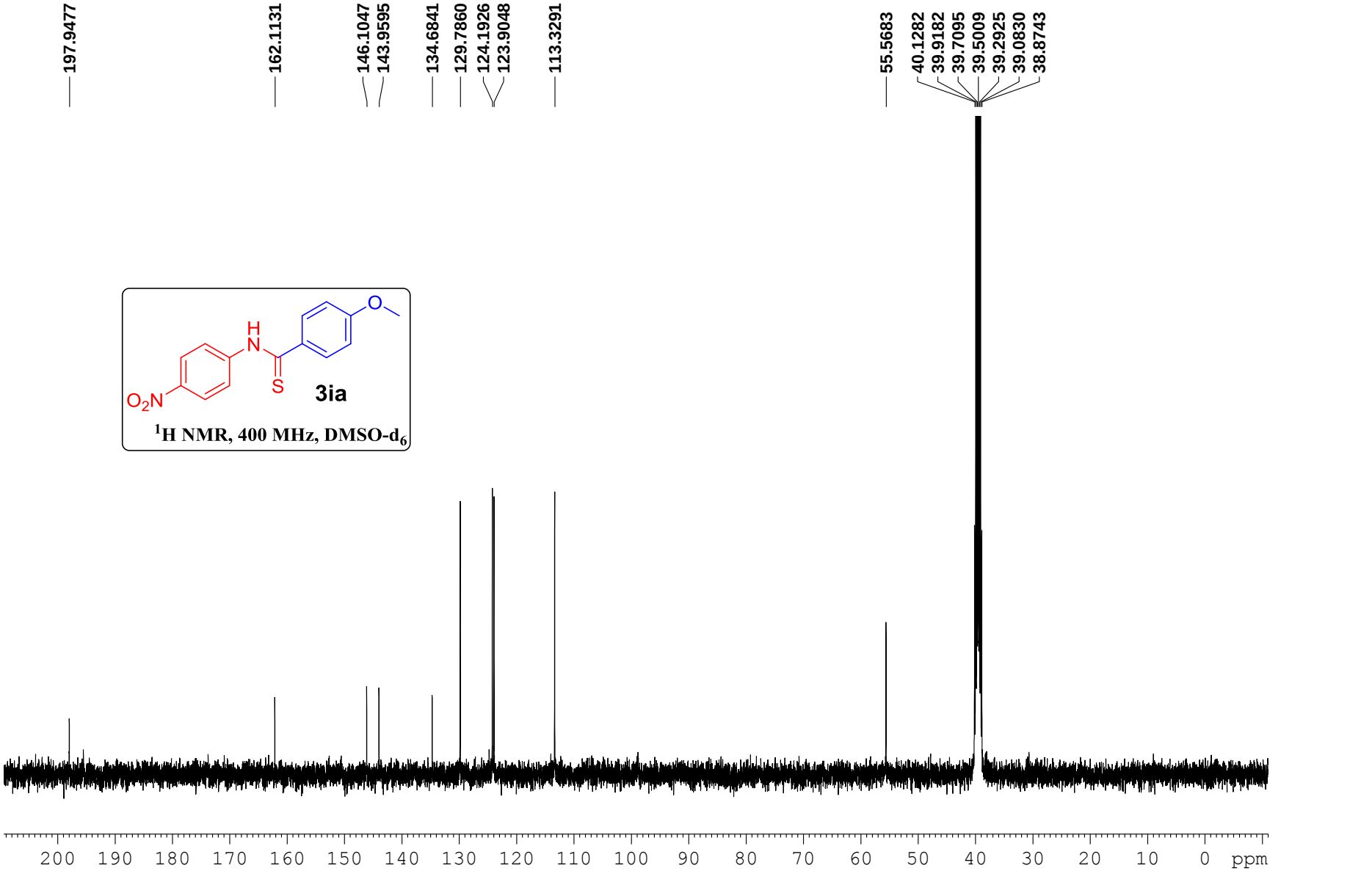

11.5968
7.9029
7.8825
7.8355
7.8155
7.4907
7.4700
7.0238
7.0028
3.8314
3.3608
2.5000
3ga
^{1}H NMR, 400 MHz, DMSO-d$_6$
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.95
1.93
2.01
2.00
3.05

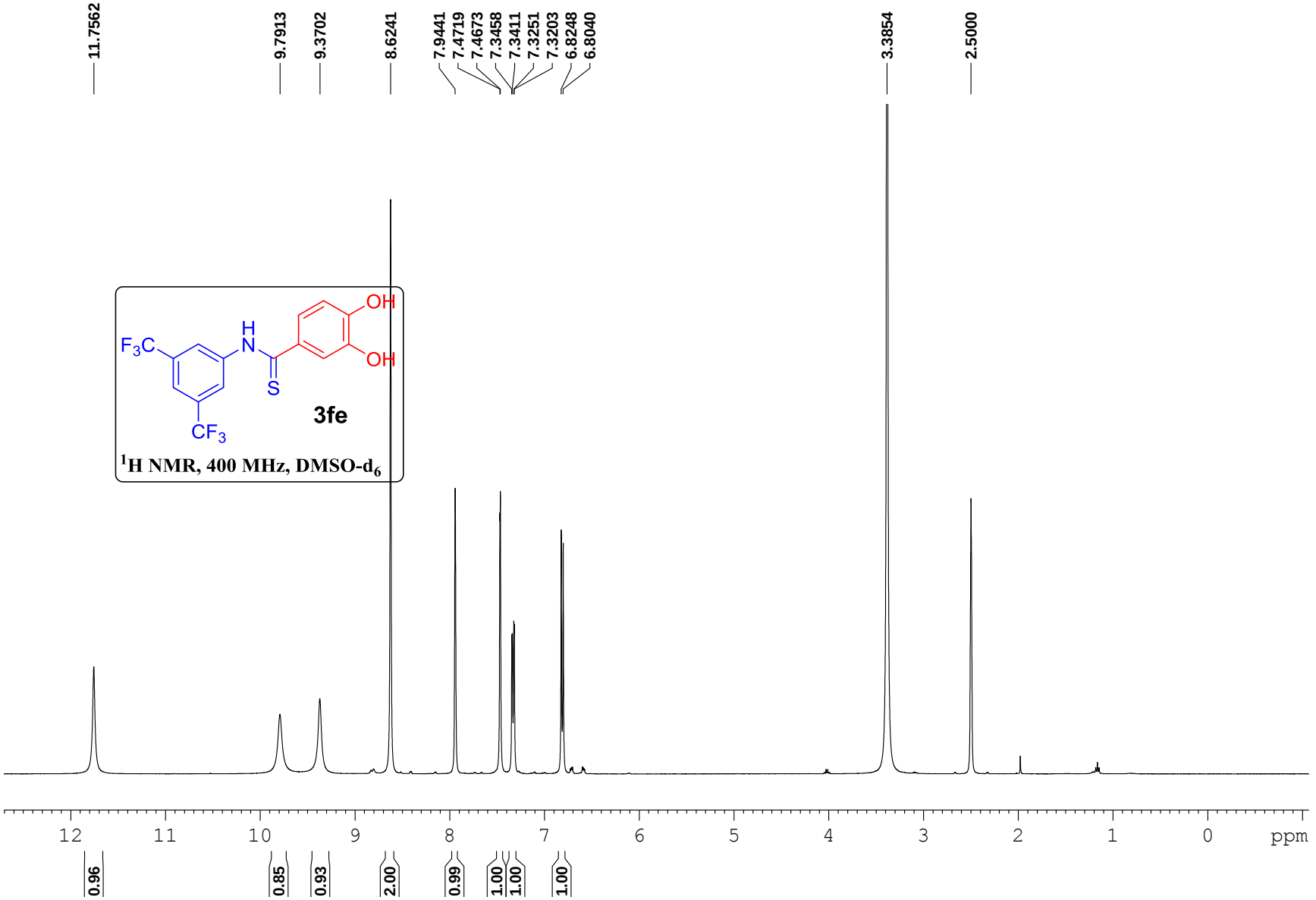

196.7581
161.7933
139.1090
134.4340
129.8433
129.5750
128.3884
126.1209
113.2336
55.5164
40.1263
39.9177
39.7089
39.5001
39.2917
39.0833
38.8739
H
N
O
S
Cl
3ga
13C NMR, 100 MHz, DMSO-d6
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

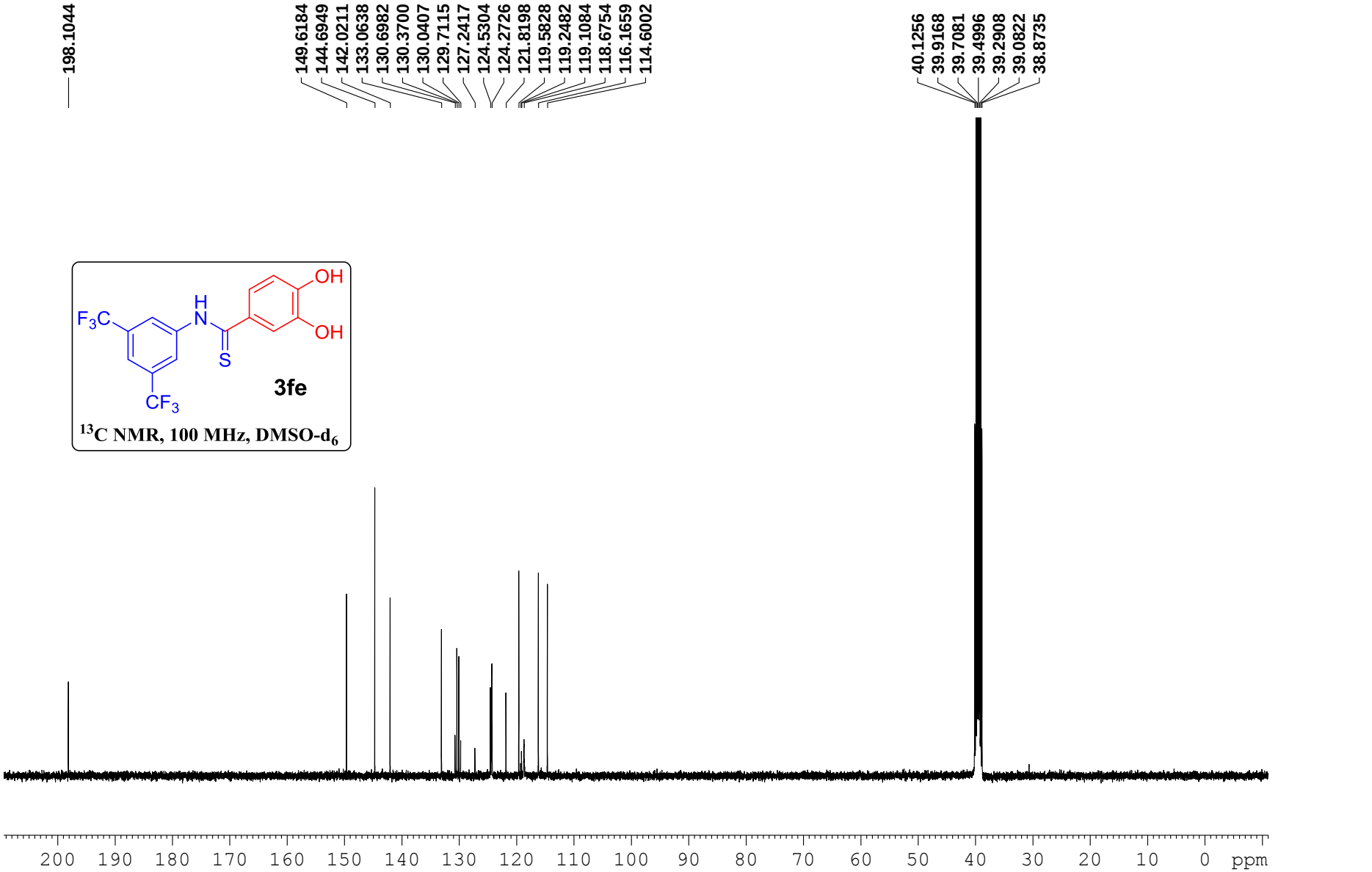

11.8653
8.8628
8.2629
8.2442
8.1215
8.1016
7.9384
7.9172
7.7392
7.7188
7.6985
7.0497
7.0282
3.8449
3.3598
2.5002
H
N
S
O
NO2
3ha
1H NMR, 400 MHz, DMSO-d6
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.99
0.92
1.01
1.12
2.06
1.07
2.00
3.09

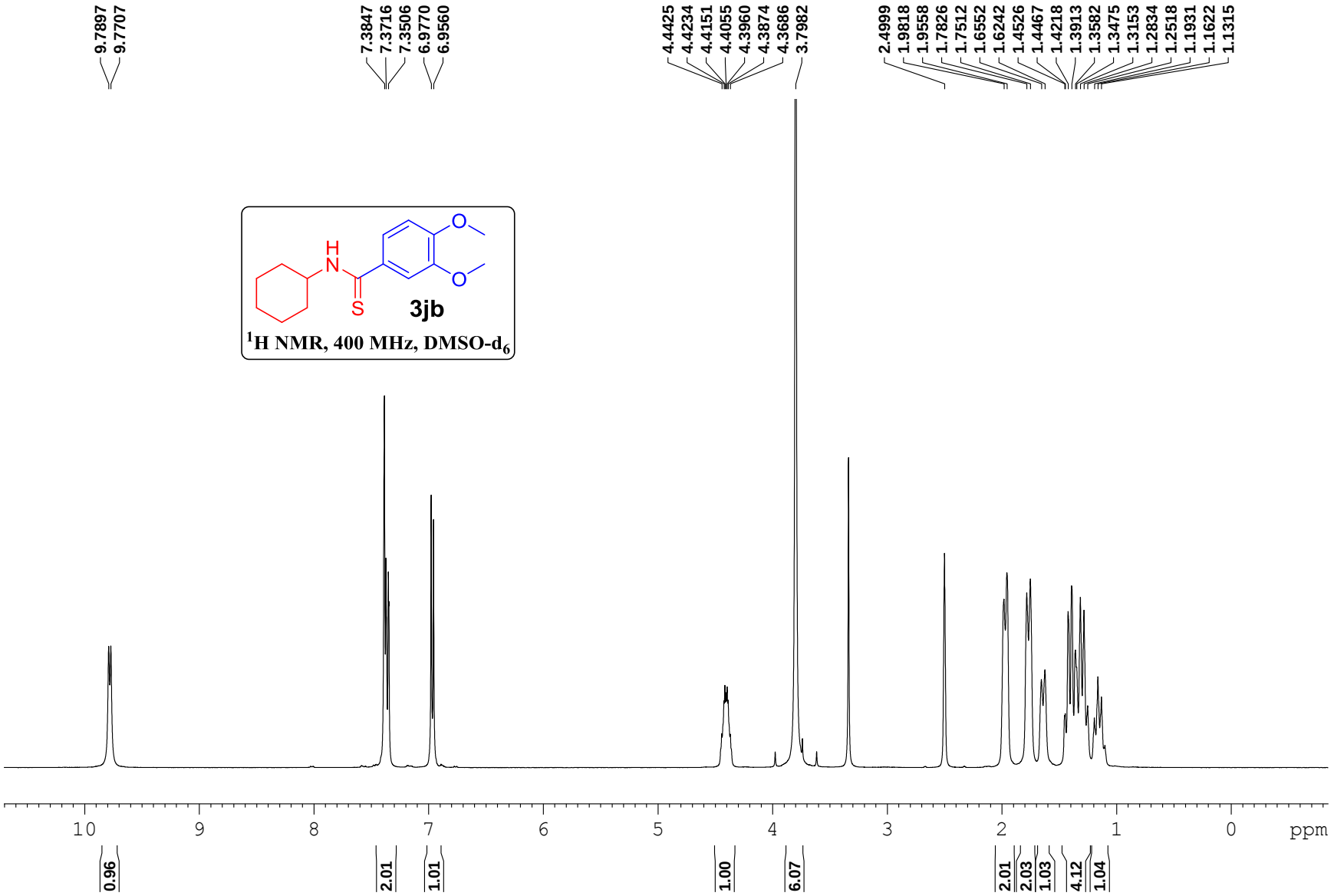

197.5026
162.0506
147.4941
141.1576
134.2979
130.5369
129.8382
129.7153
120.5339
118.6318
113.3291
55.5639
40.1271
39.9181
39.7093
39.5008
39.2921
39.0832
38.8749
H
N
S
O
NO2
3ha
13C NMR, 100 MHz, DMSO-d6
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

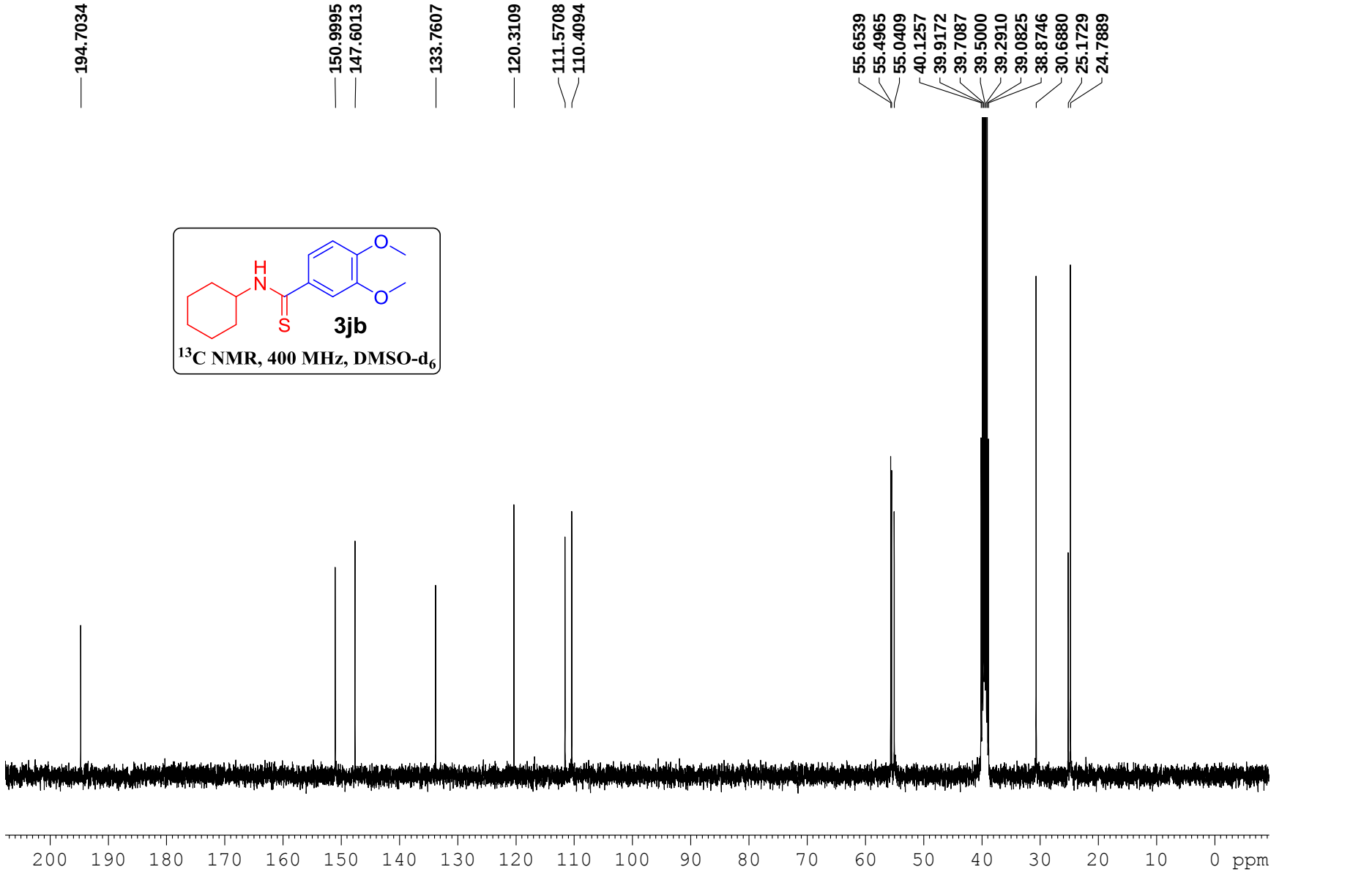

11.9198
8.3046
8.2846
8.1883
8.1689
7.9030
7.8839
7.0421
7.0230
3.8430
3.3547
2.5005
O
H
N
S
O2N
3ia
1H NMR, 400 MHz, DMSO-d6
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.98
2.05
2.01
1.97
2.00
3.07


197.9477
162.1131
146.1047
143.9595
134.6841
129.7860
124.1926
123.9048
113.3291
55.5683
40.1282
39.9182
39.7095
39.5009
39.2925
39.0830
38.8743
O
H
N
S
O2N
3ia
1H NMR, 400 MHz, DMSO-d6
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


11.7562
9.7913
9.3702
8.6241
7.9441
7.4719
7.4673
7.3458
7.3411
7.3251
7.3203
6.8248
6.8040
3.3854
2.5000
OH
OH
H
N
S
F3C
CF3
3fe
1H NMR, 400 MHz, DMSO-d6
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.96
0.85
0.93
2.00
0.99
1.00
1.00
1.00


198.1044
149.6184
144.6949
142.0211
133.0638
130.6982
130.3700
130.0407
129.7115
127.2417
124.5304
124.2726
121.8198
119.5828
119.2482
119.1084
118.6754
116.1659
114.6002
40.1256
39.9168
39.7081
39.4996
39.2908
39.0822
38.8735
OH
OH
H
N
S
F3C
CF3
3fe
13C NMR, 100 MHz, DMSO-d6
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


9.7897
9.7707
7.3847
7.3716
7.3506
6.9770
6.9560
4.4425
4.4234
4.4151
4.4055
4.3960
4.3874
4.3686
3.7982
2.4999
1.9818
1.9558
1.7826
1.7512
1.6552
1.6242
1.4526
1.4467
1.4218
1.3913
1.3582
1.3475
1.3153
1.2834
1.2518
1.1931
1.1622
1.1315
H
N
S
O
O
3jb
1H NMR, 400 MHz, DMSO-d6
10
9
8
7
6
5
4
3
2
1
0
ppm
0.96
2.01
1.01
1.00
6.07
2.01
2.03
1.03
4.12
1.04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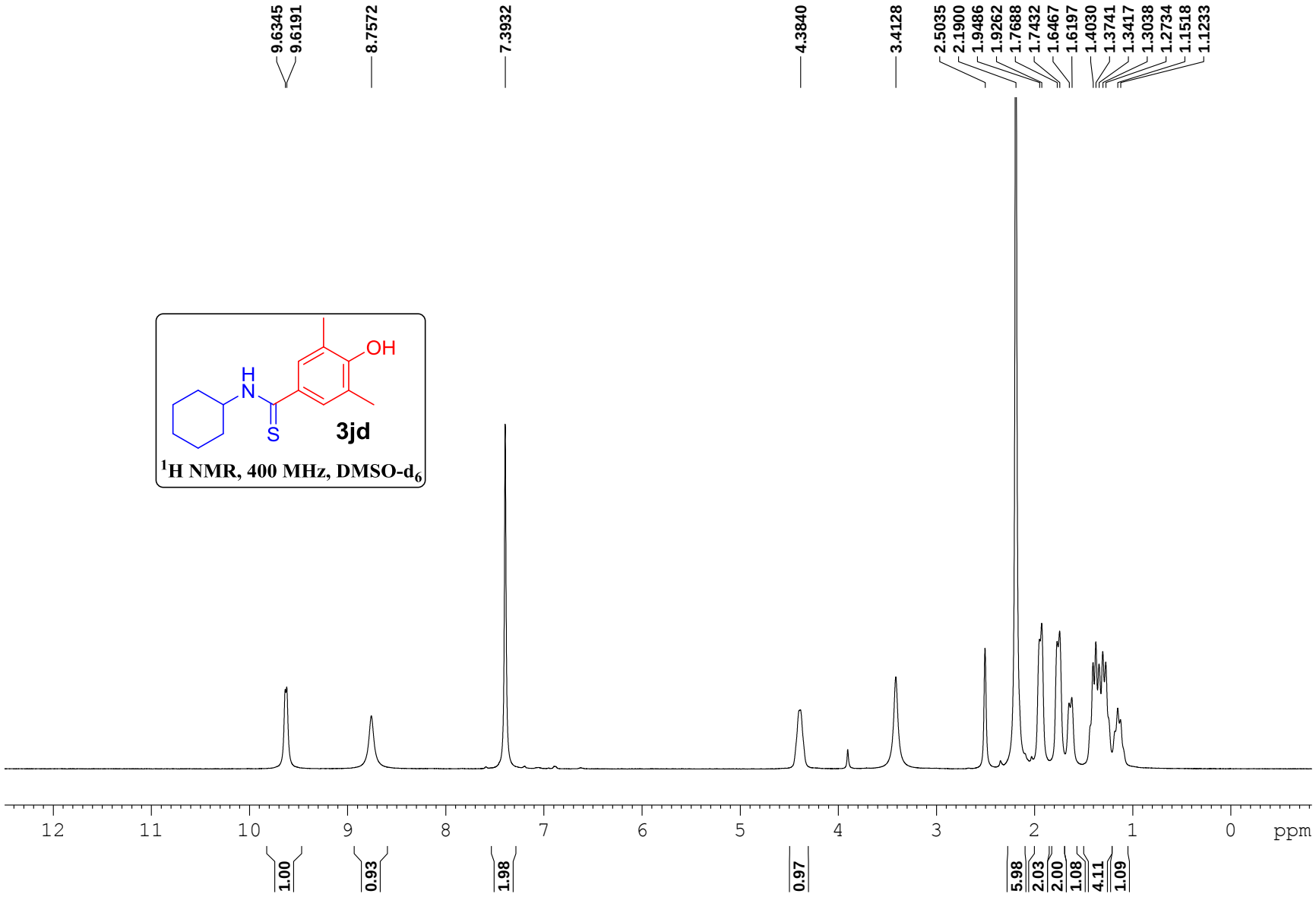
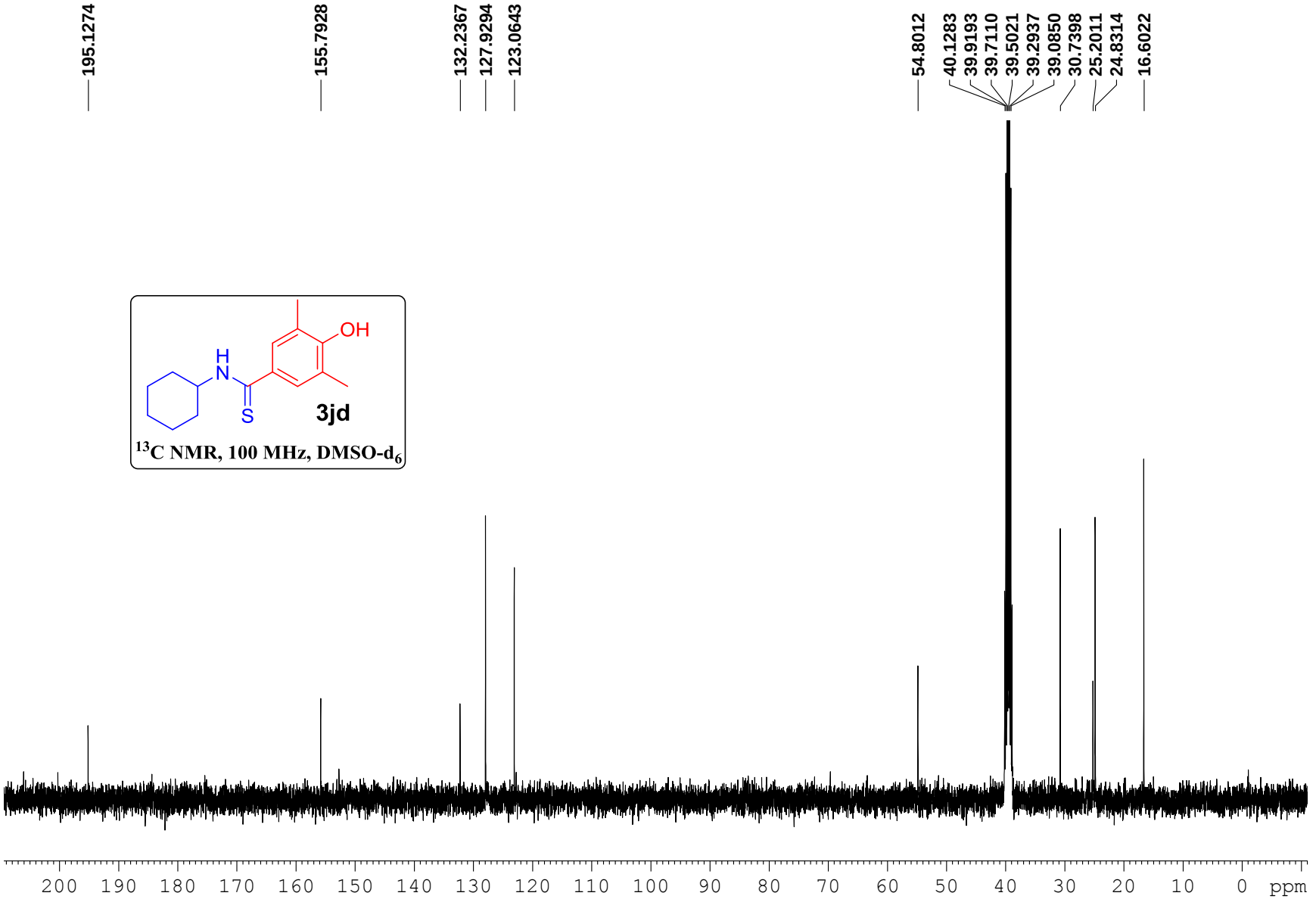
147.6013
133.7607
120.3109
111.5708
110.4094
55.6539
55.4965
55.0409
40.1257
39.9172
39.7087
39.5000
39.2910
39.0825
38.8746
30.6880
25.1729
24.7889
H
N
S
O
O
3jb
13C NMR, 400 MHz, DMSO-d6
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


9.6345
9.6191
8.7572
7.3932
4.3840
3.4128
2.5035
2.1900
1.9486
1.9262
1.7688
1.7432
1.6467
1.6197
1.4030
1.3741
1.3417
1.3038
1.2734
1.1518
1.1233
OH
H
N
S
3jd
^{1}H NMR, 400 MHz, DMSO-d$_6$
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
0.93
1.98
0.97
5.98
2.03
2.00
1.08
4.11
1.09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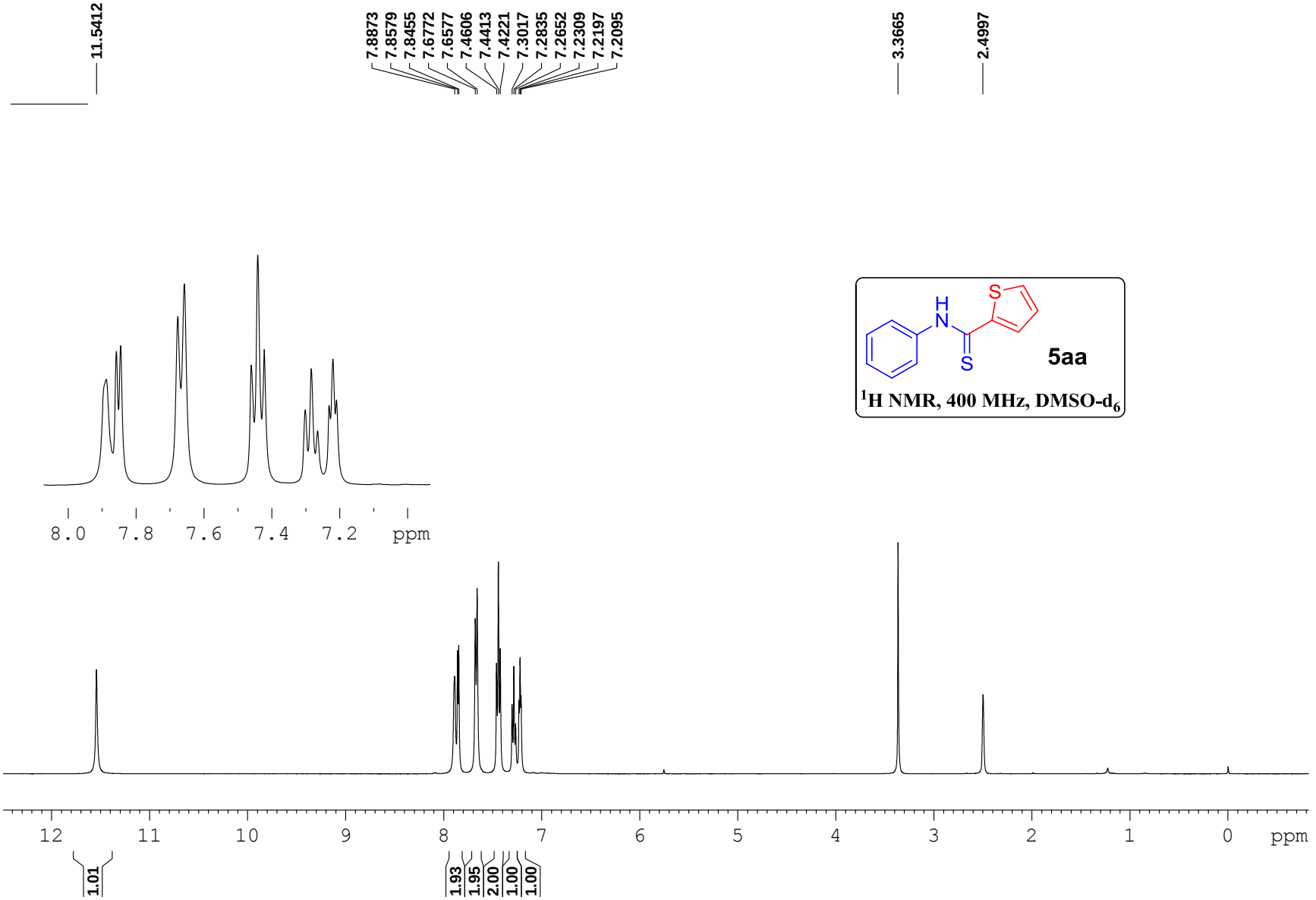
155.7928
132.2367
127.9294
123.0643
54.8012
40.1283
39.9193
39.7110
39.5021
39.2937
39.0850
30.7398
25.2011
24.8314
16.6022
OH
H
N
S
3jd
13C NMR, 100 MHz, DMSO-d6
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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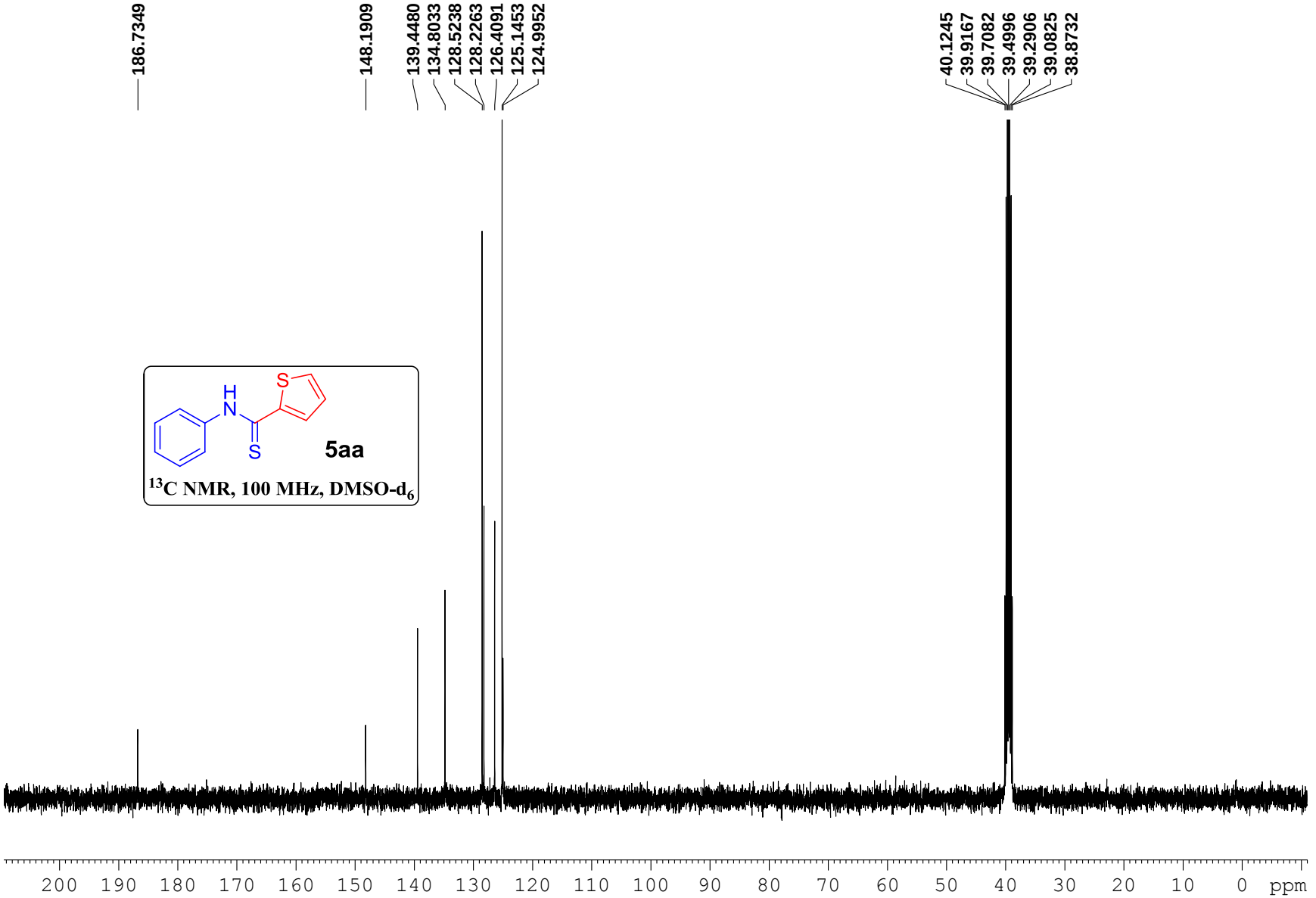
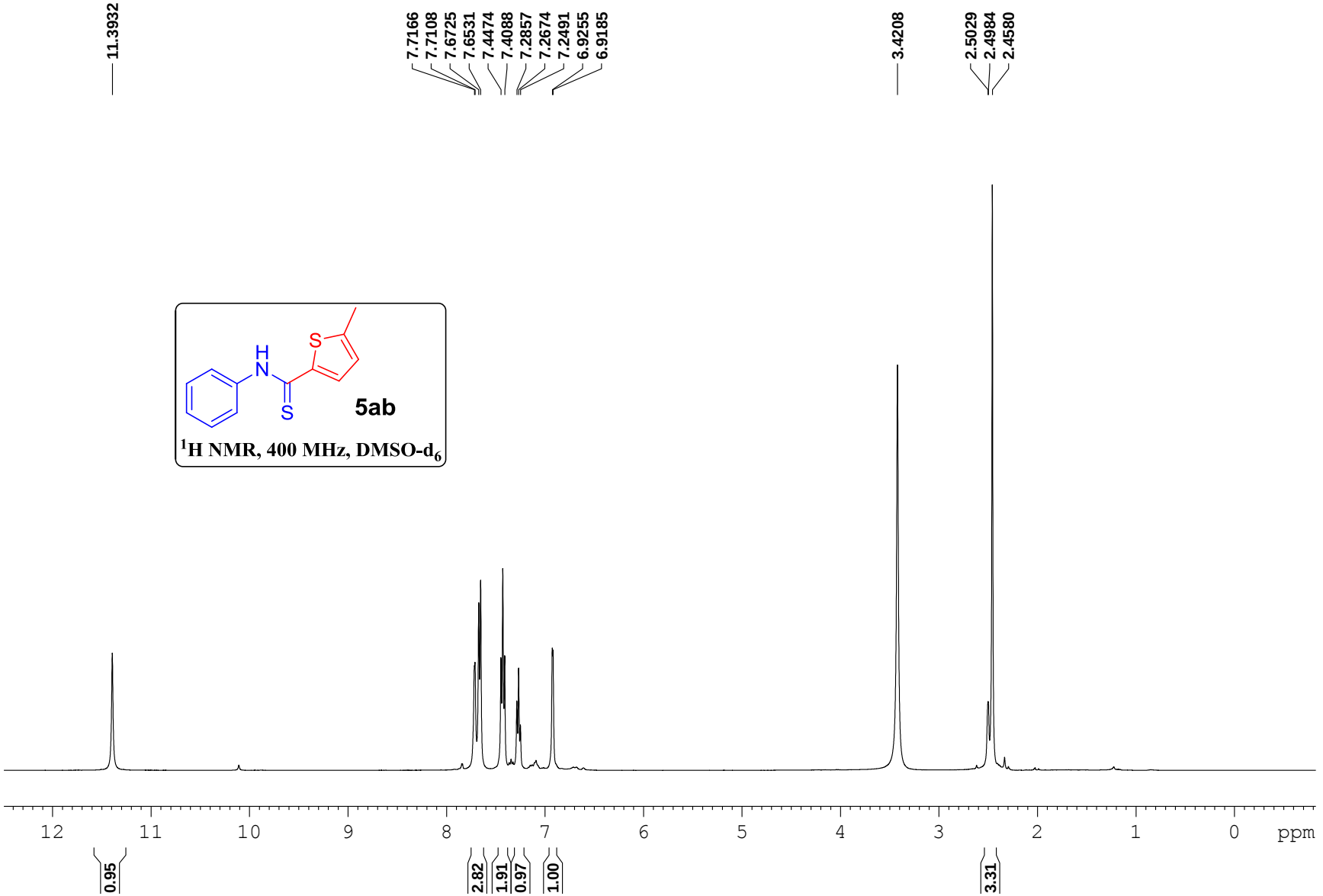
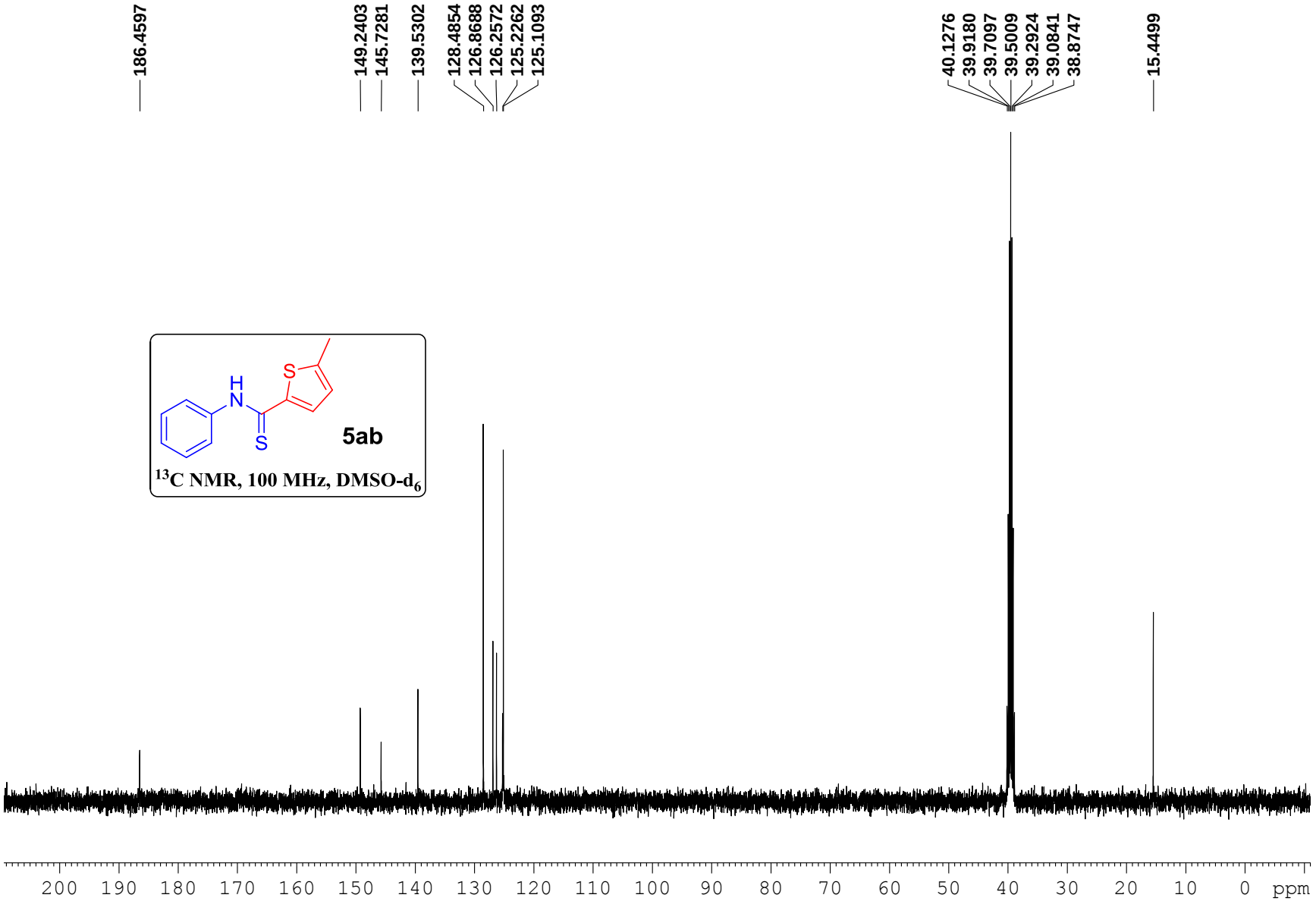
7.8873
7.8579
7.8455
7.6772
7.6577
7.4606
7.4413
7.4221
7.3017
7.2835
7.2652
7.2309
7.2197
7.2095
3.3665
2.4997
8.0
7.8
7.6
7.4
7.2
ppm
5aa
1H NMR, 400 MHz, DMSO-d6
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.01
1.93
1.95
2.00
1.00
1.00


186.7349
148.1909
139.4480
134.8033
128.5238
128.2263
126.4091
125.1453
124.9952
40.1245
39.9167
39.7082
39.4996
39.2906
39.0825
38.8732
H
N
S
S
5aa
13C NMR, 100 MHz, DMSO-d6
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


11.3932
7.7166
7.7108
7.6725
7.6531
7.4474
7.4088
7.2857
7.2674
7.2491
6.9255
6.9185
3.4208
2.5029
2.4984
2.4580
H
N
S
S
5ab
1H NMR, 400 MHz, DMSO-d6
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.95
2.82
1.91
0.97
1.00
3.31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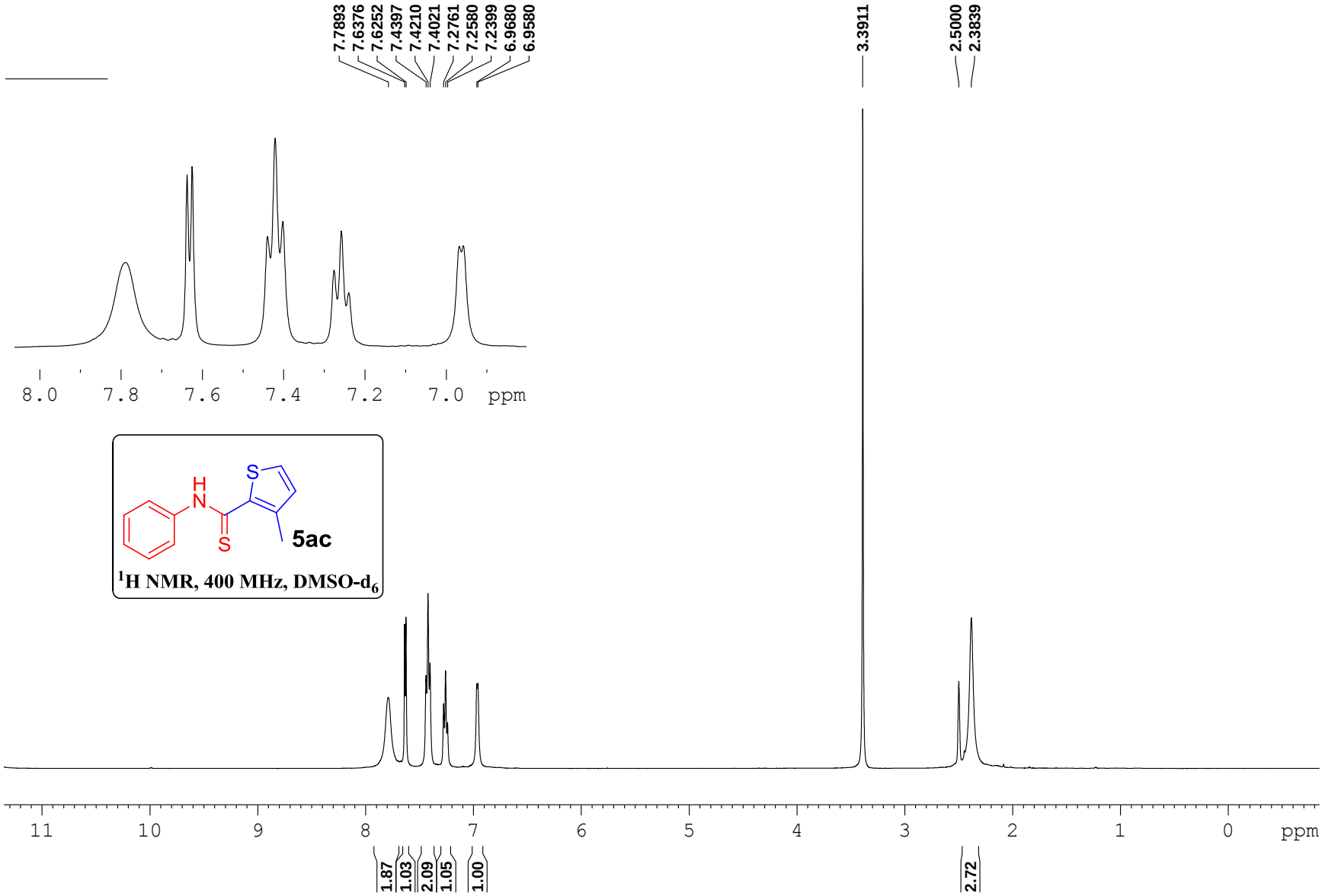
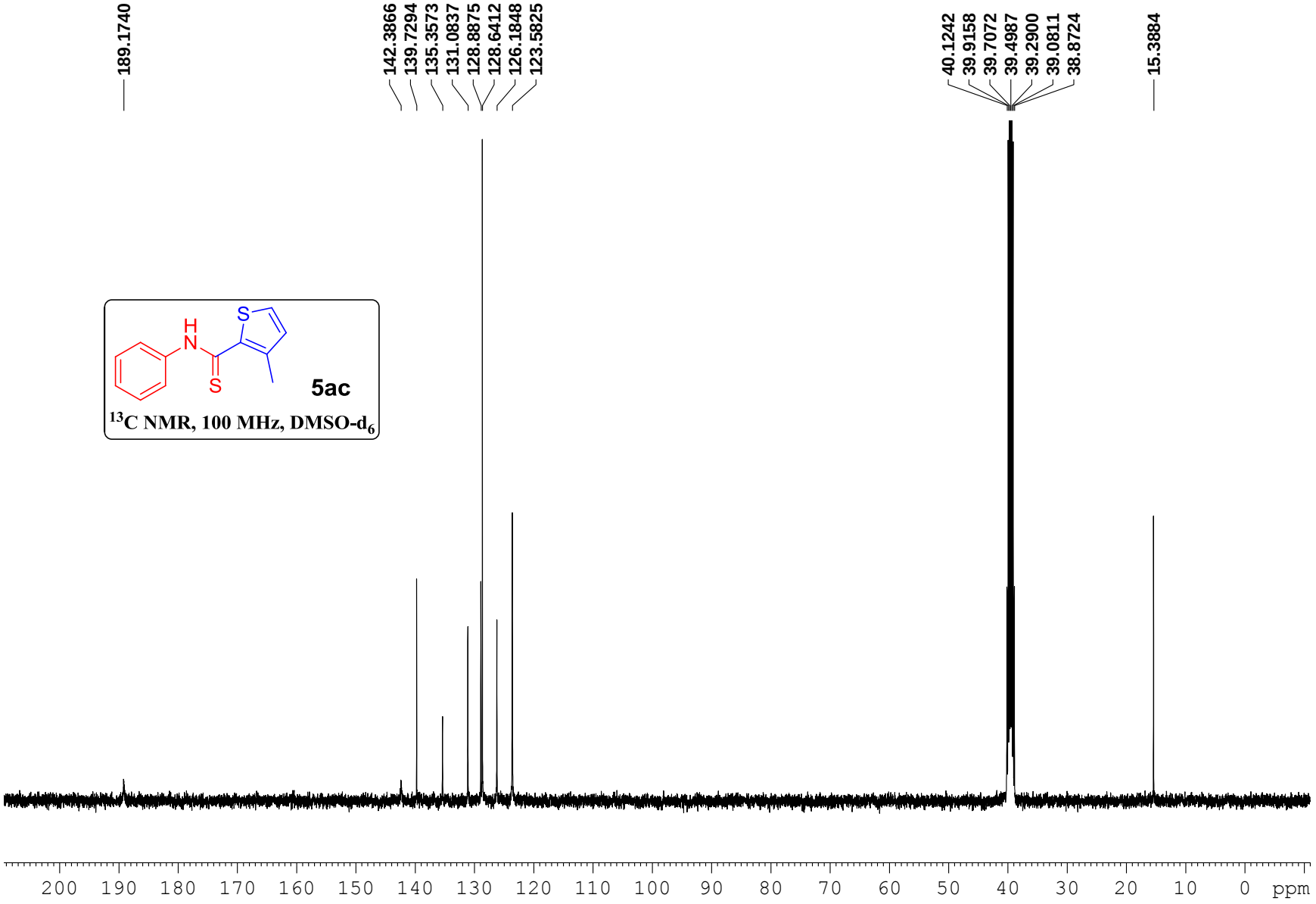
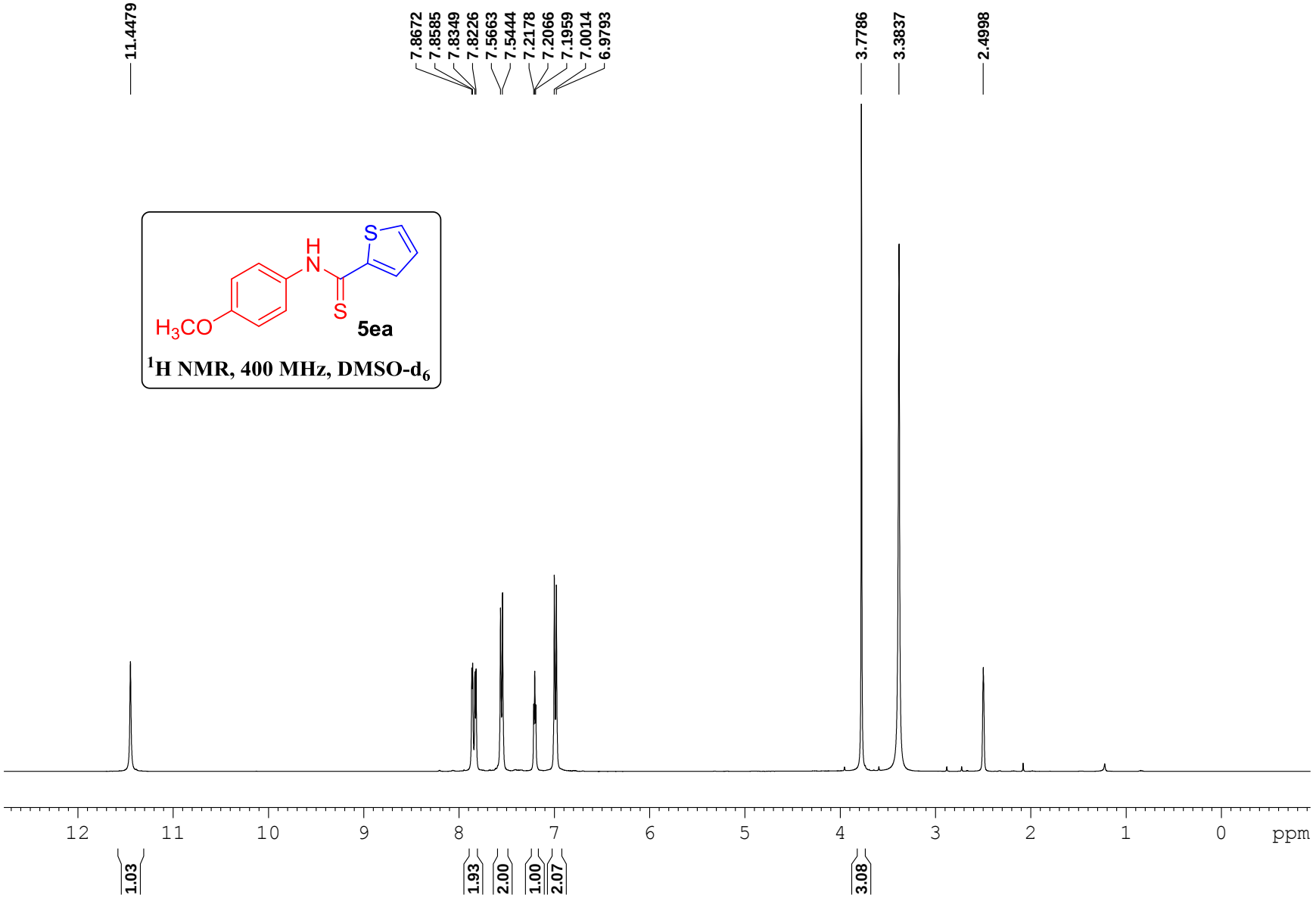
145.7281
139.5302
128.4854
126.8688
126.2572
125.2262
125.1093
40.1276
39.9180
39.7097
39.5009
39.2924
39.0841
38.8747
15.4499
5ab
13C NMR, 100 MHz, DMSO-d6
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


7.7893
7.6376
7.6252
7.4397
7.4210
7.4021
7.2761
7.2580
7.2399
6.9680
6.9580
3.3911
2.5000
2.3839
8.0
7.8
7.6
7.4
7.2
7.0
ppm
H
N
S
S
5ac
1H NMR, 400 MHz, DMSO-d6
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.87
1.03
2.09
1.05
1.00
2.72


189.1740
142.3866
139.7294
135.3573
131.0837
128.8875
128.6412
126.1848
123.5825
40.1242
39.9158
39.7072
39.4987
39.2900
39.0811
38.8724
15.3884
H
N
S
S
5ac
13C NMR, 100 MHz, DMSO-d6
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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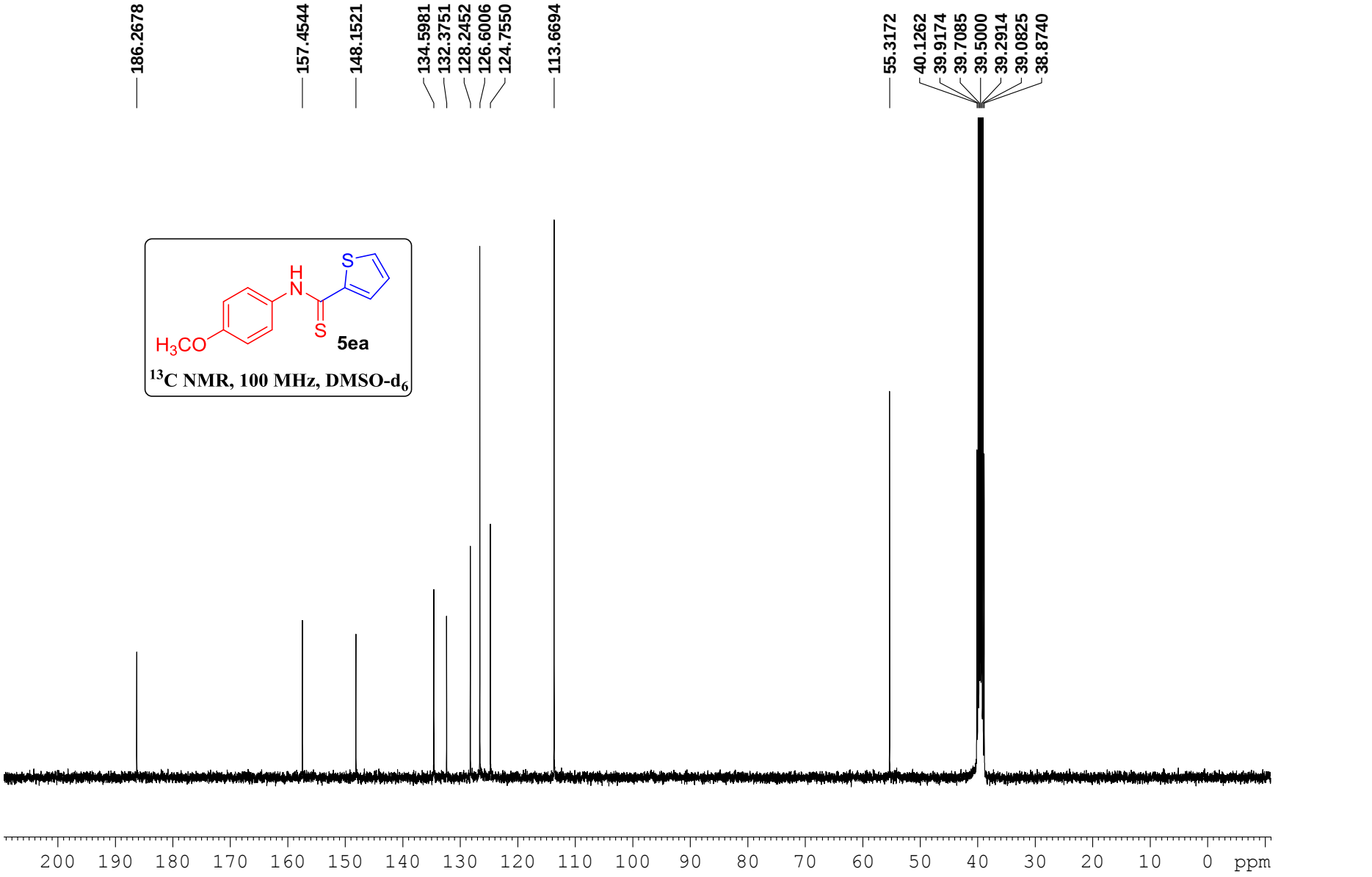
7.8672
7.8585
7.8349
7.8226
7.5663
7.5444
7.2178
7.2066
7.1959
7.0014
6.9793
3.7786
3.3837
2.4998
H
N
S
S
H3CO
5ea
1H NMR, 400 MHz, DMSO-d6
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.03
1.93
2.00
1.00
2.07
3.08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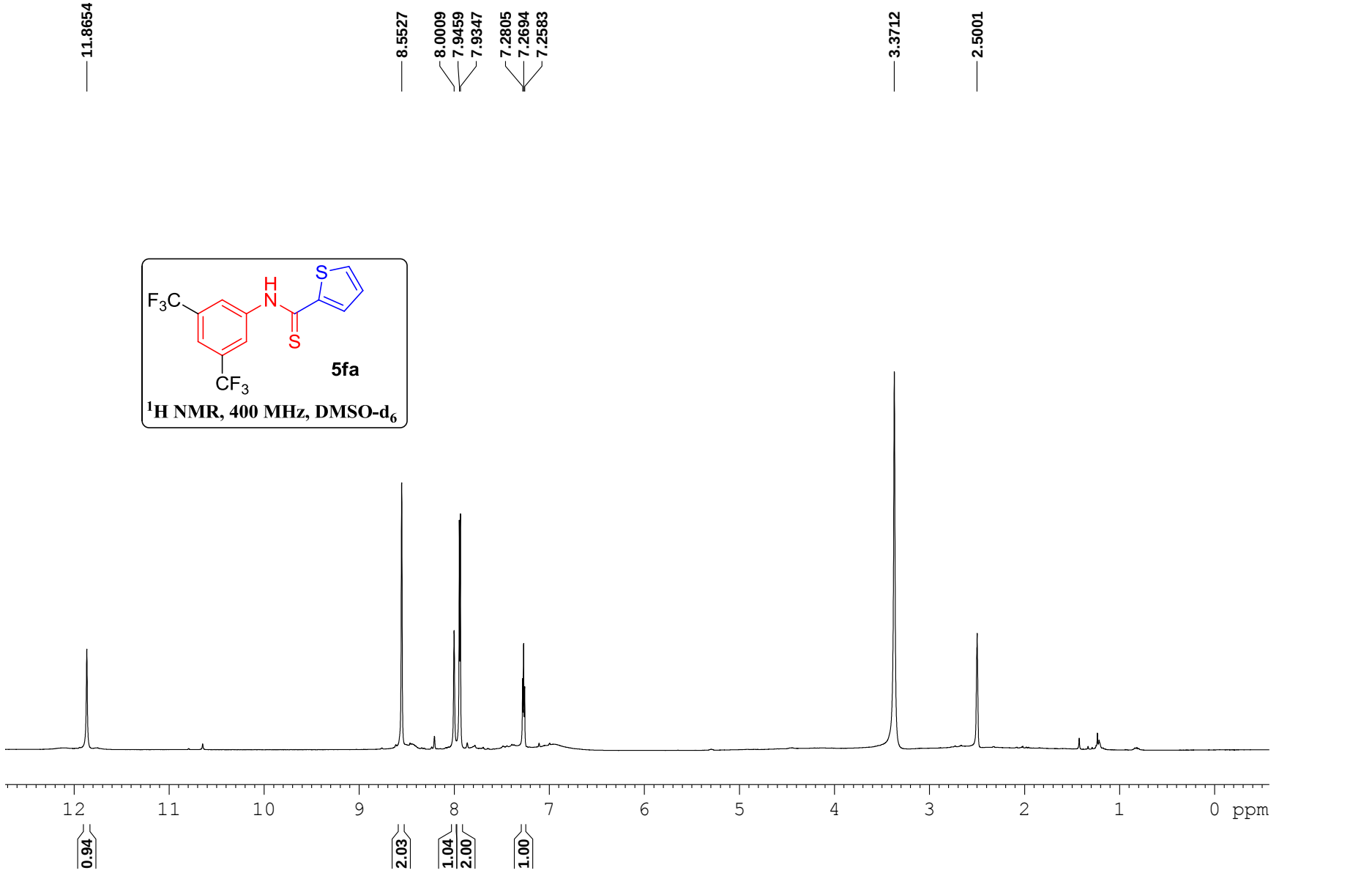
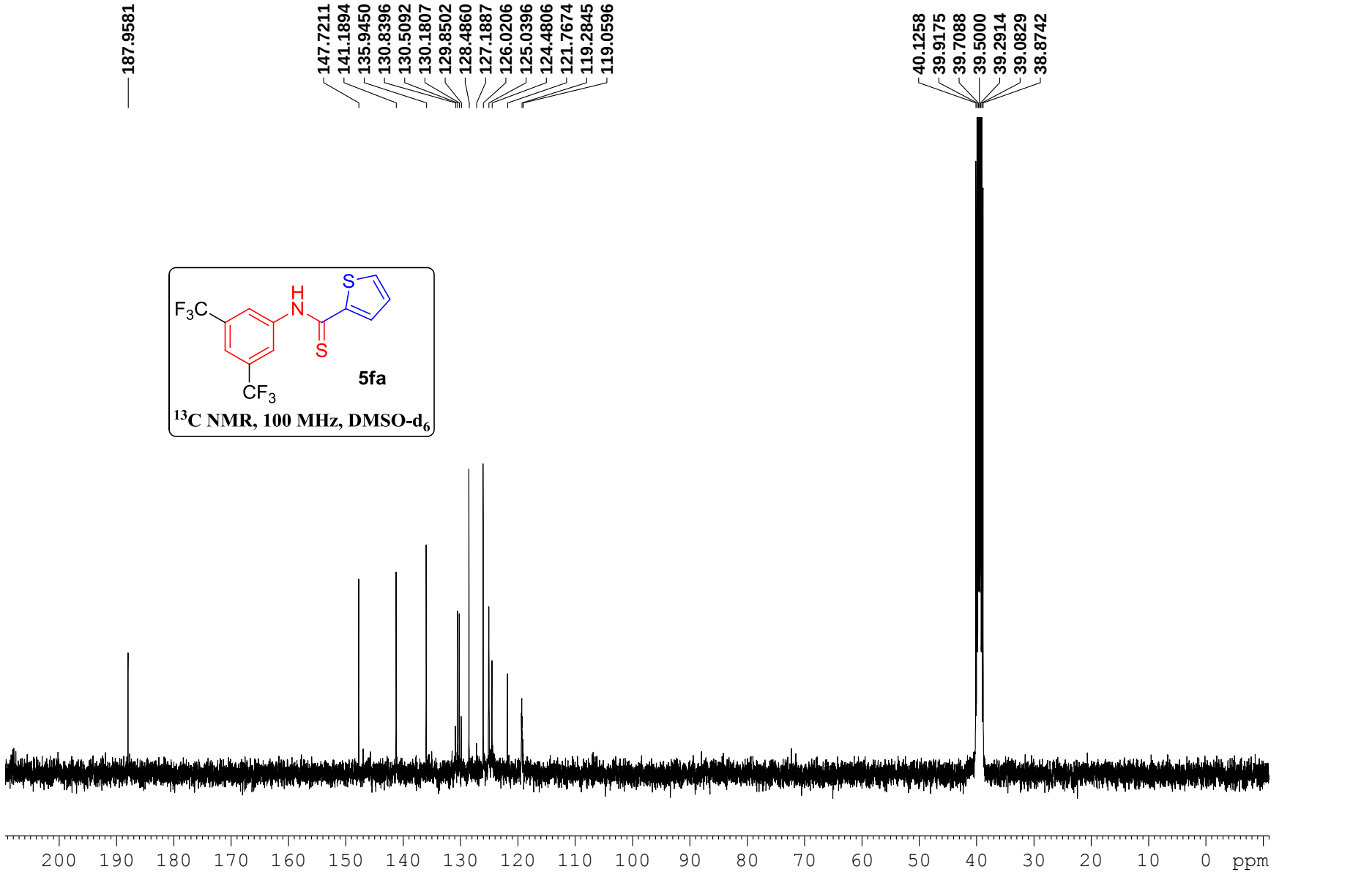
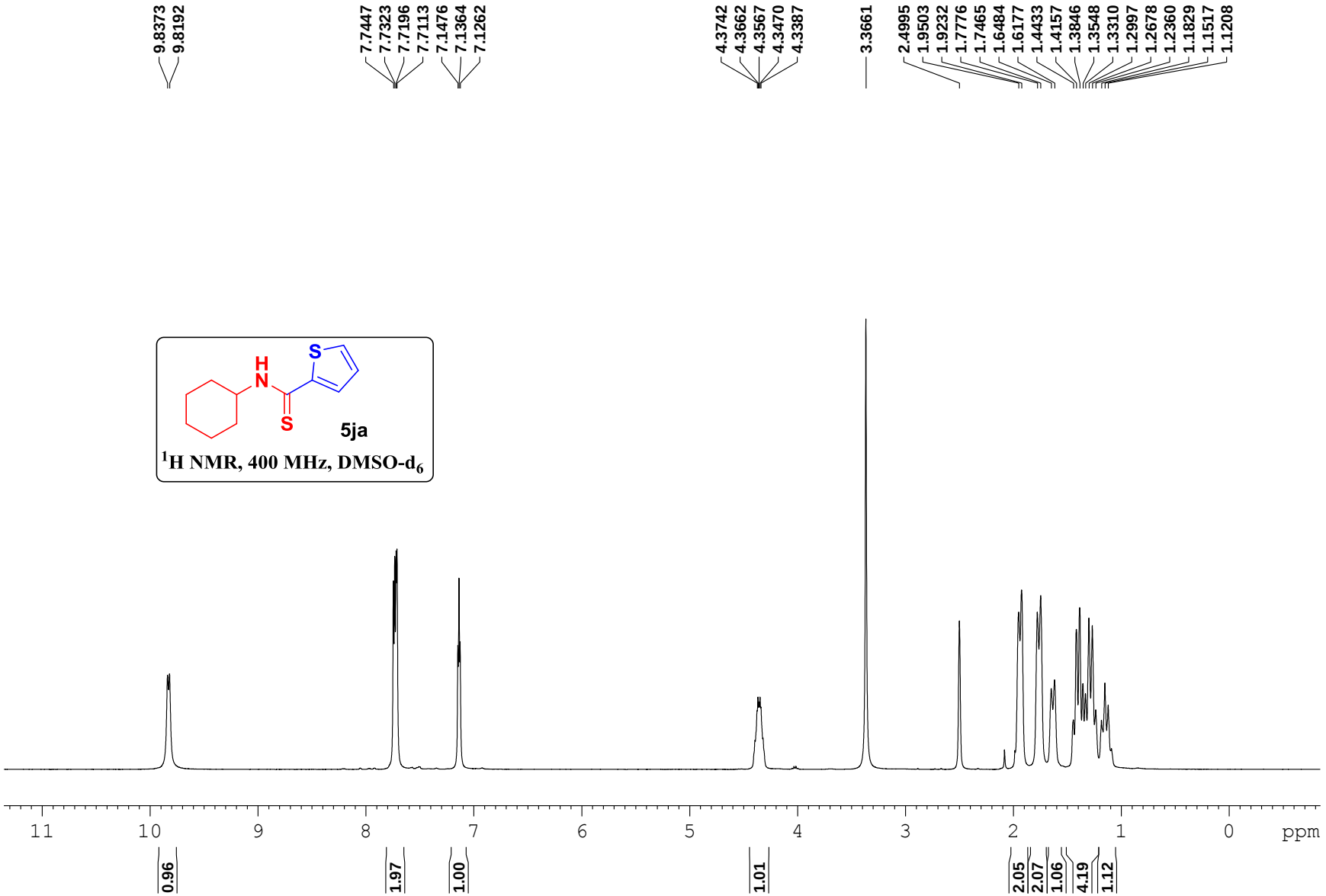
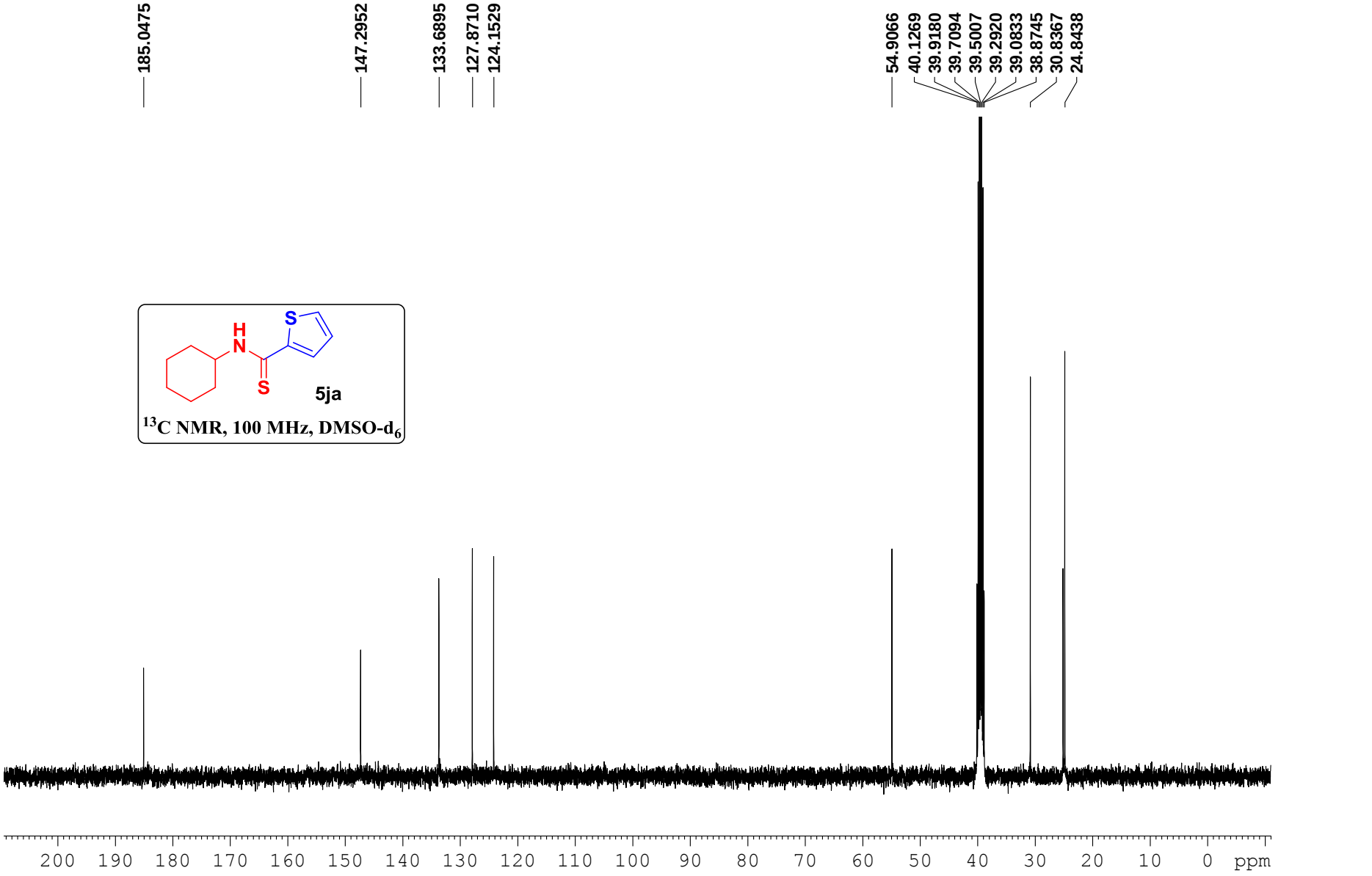
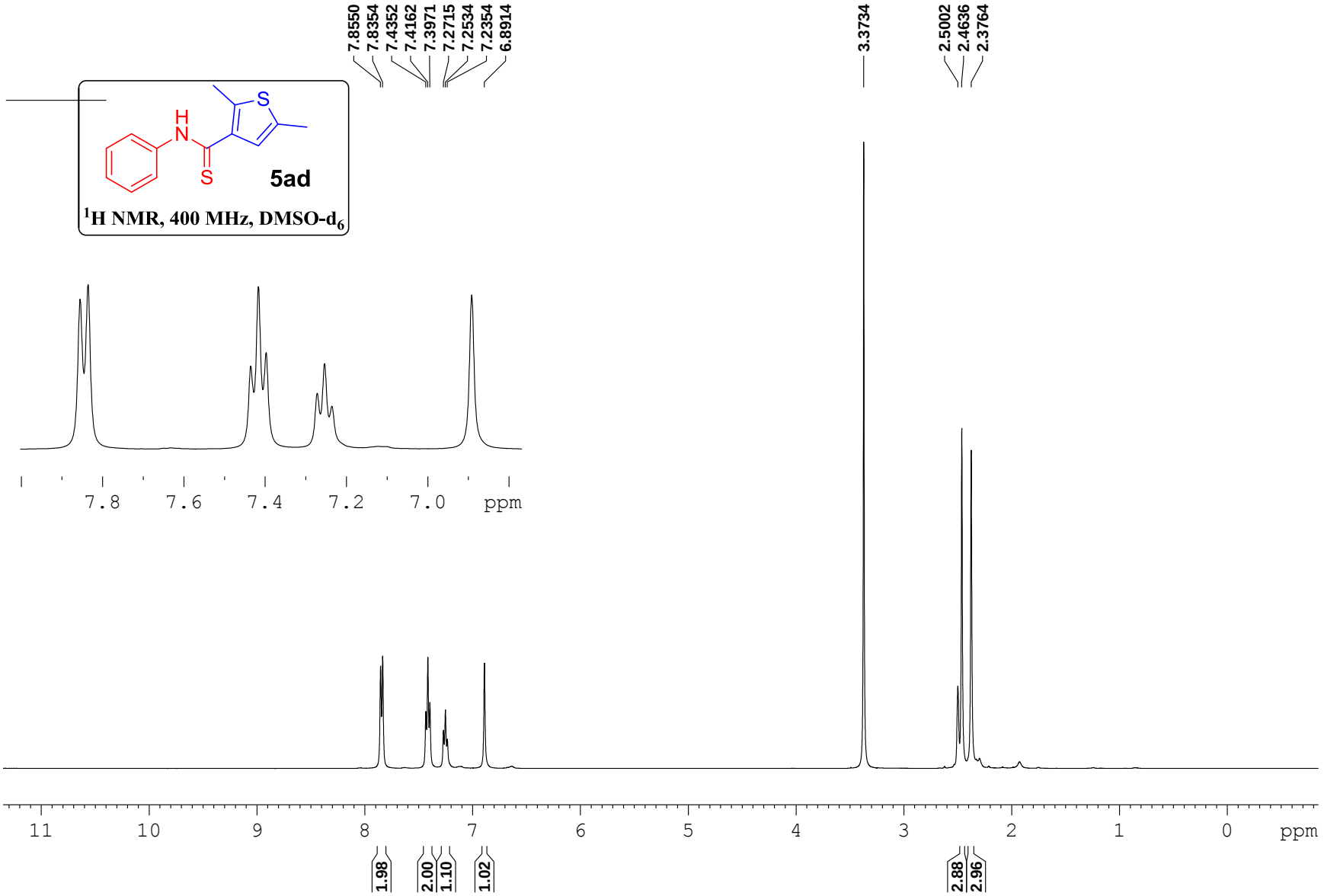
157.4544
148.1521
134.5981
132.3751
128.2452
126.6006
124.7550
113.6694
55.3172
40.1262
39.9174
39.7085
39.5000
39.2914
39.0825
38.8740
H
N
S
S
H3CO
5ea
13C NMR, 100 MHz, DMSO-d6
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

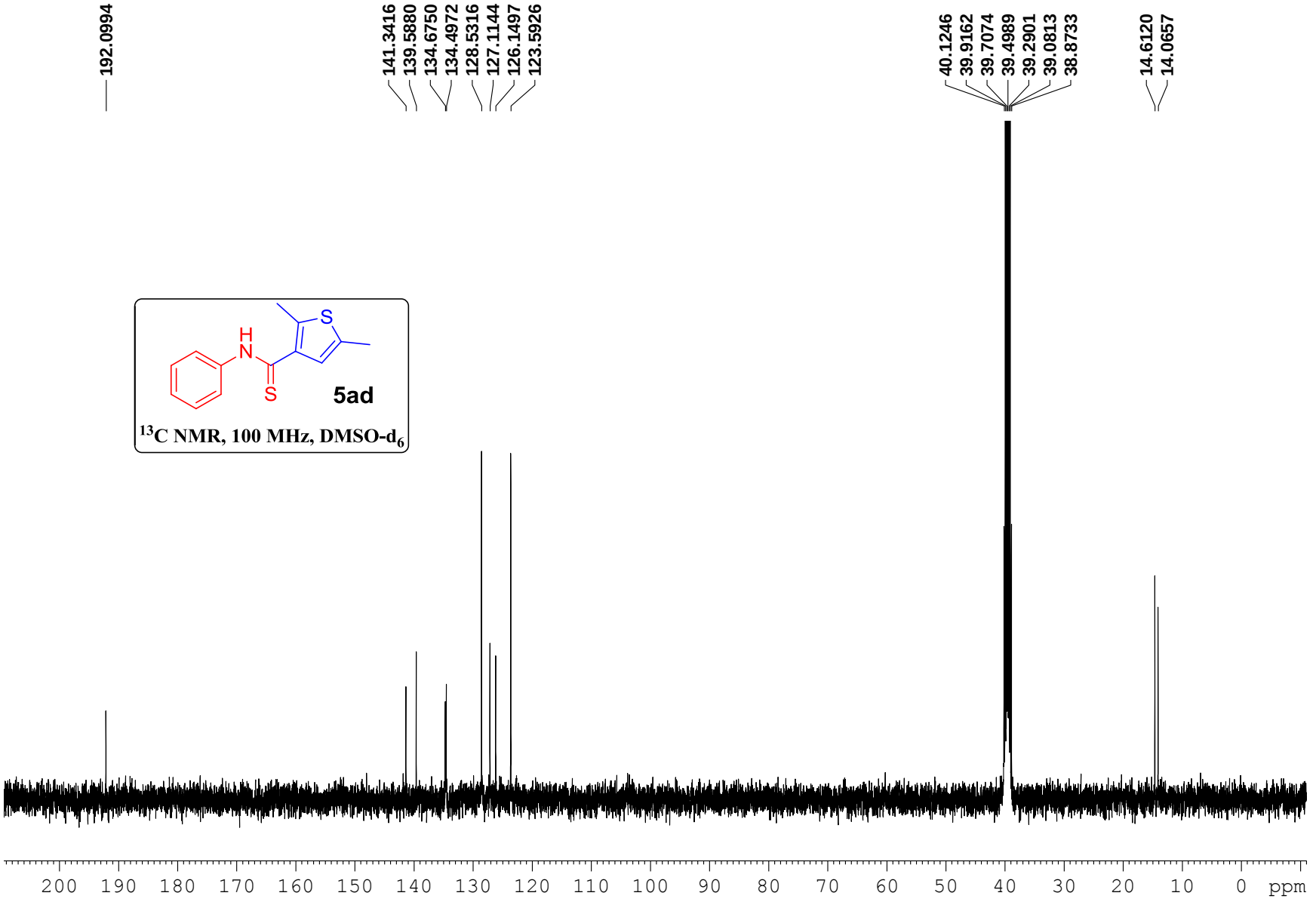

11.8654
8.5527
8.0009
7.9459
7.9347
7.2805
7.2694
7.2583
3.3712
2.5001
F3C
CF3
H
N
S
S
5fa
1H NMR, 400 MHz, DMSO-d6
12
11
10
9
8
7
6
5
4
3
2
1
0 ppm
0.94
2.03
1.04
2.00
1.00

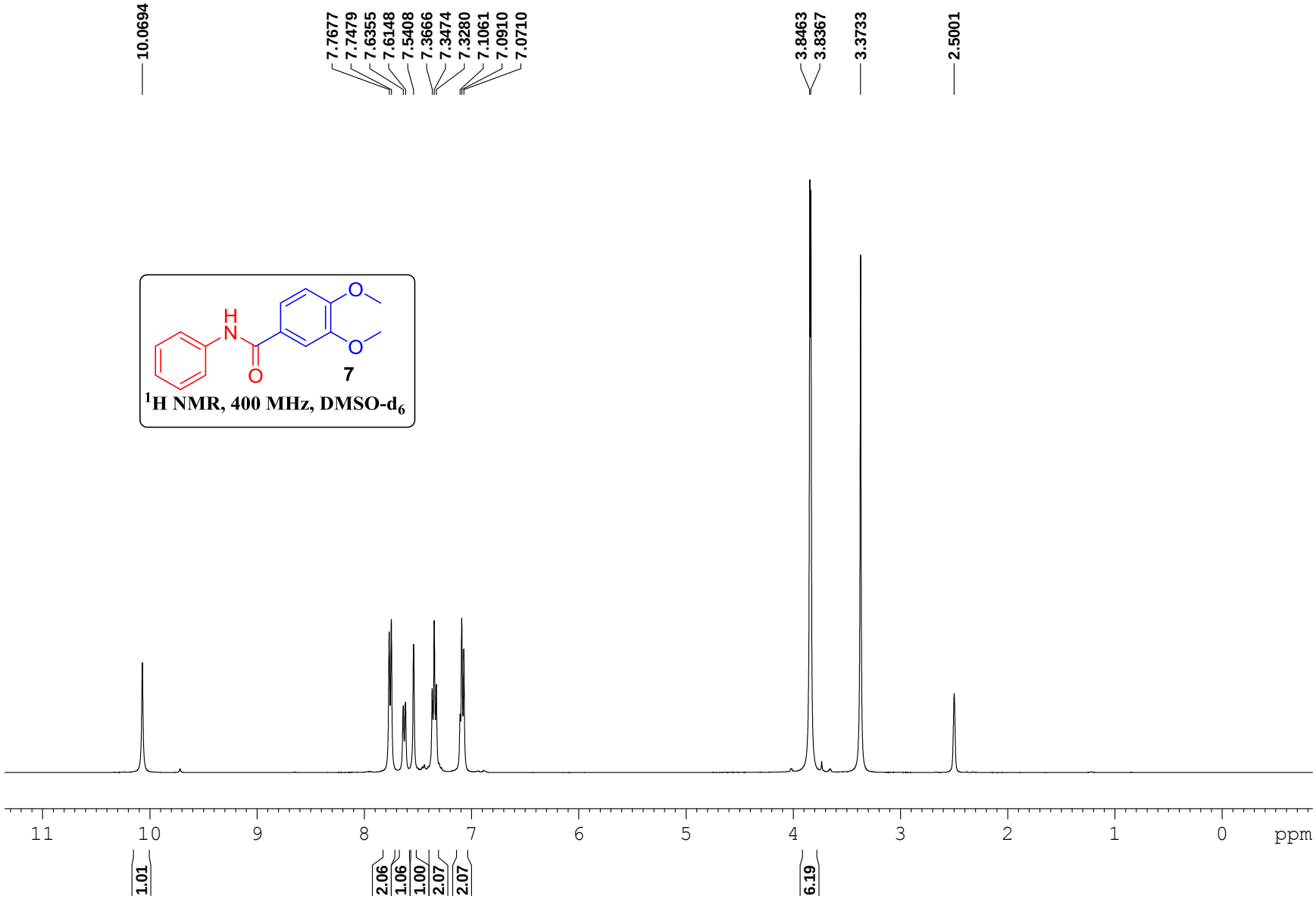

187.9581
147.7211
141.1894
135.9450
130.8396
130.5092
130.1807
129.8502
128.4860
127.1887
126.0206
125.0396
124.4806
121.7674
119.2845
119.0596
40.1258
39.9175
39.7088
39.5000
39.2914
39.0829
38.8742
F3C
H
N
S
S
CF3
5fa
13C NMR, 100 MHz, DMSO-d6
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

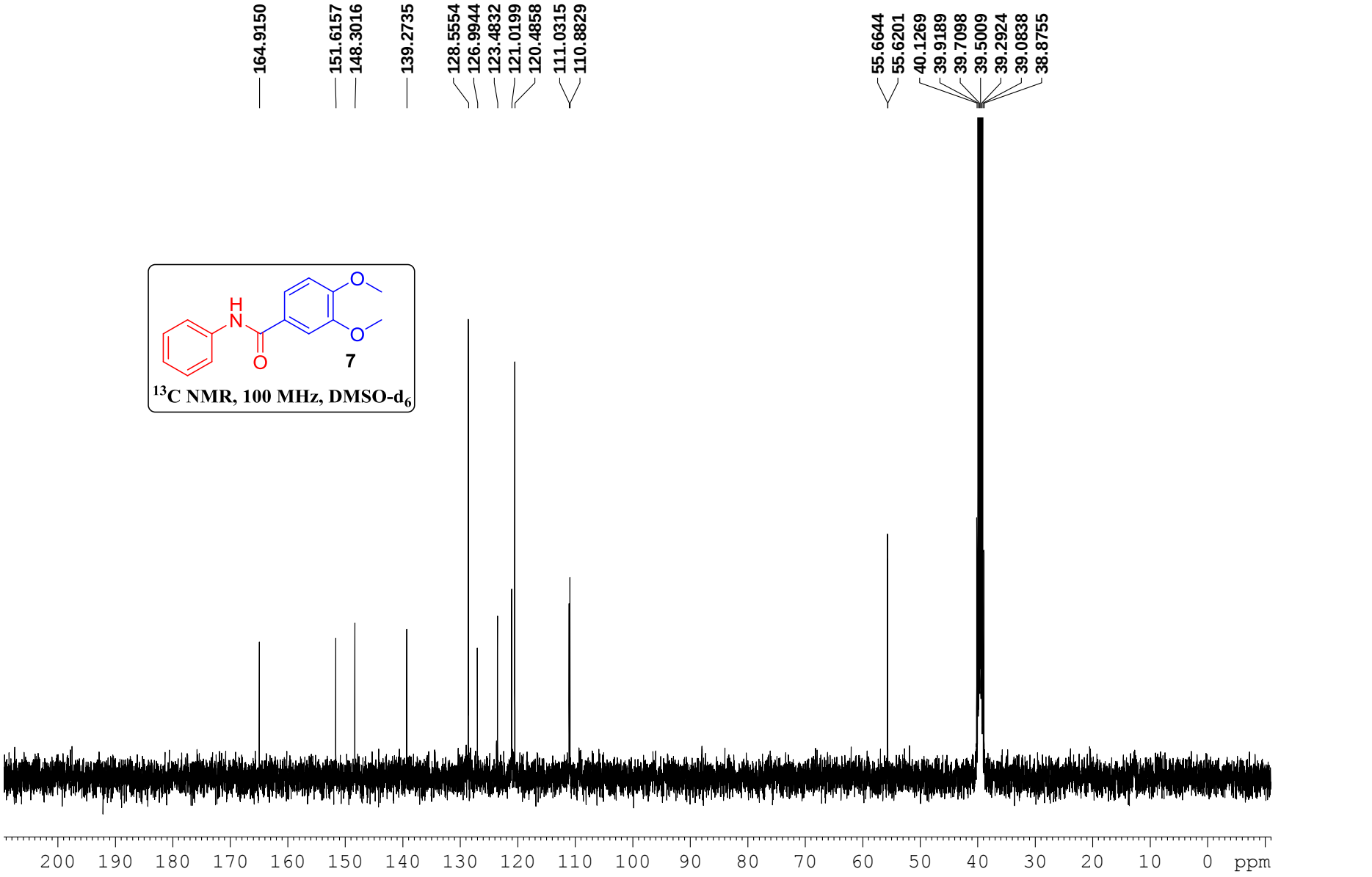

9.8373
9.8192
7.7447
7.7323
7.7196
7.7113
7.1476
7.1364
7.1262
4.3742
4.3662
4.3567
4.3470
4.3387
3.3661
2.4995
1.9503
1.9232
1.7776
1.7465
1.6484
1.6177
1.4433
1.4157
1.3846
1.3548
1.3310
1.2997
1.2678
1.2360
1.1829
1.1517
1.1208
H
N
S
S
5ja
1H NMR, 400 MHz, DMSO-d6
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.96
1.97
1.00
1.01
2.05
2.07
1.06
4.19
1.12

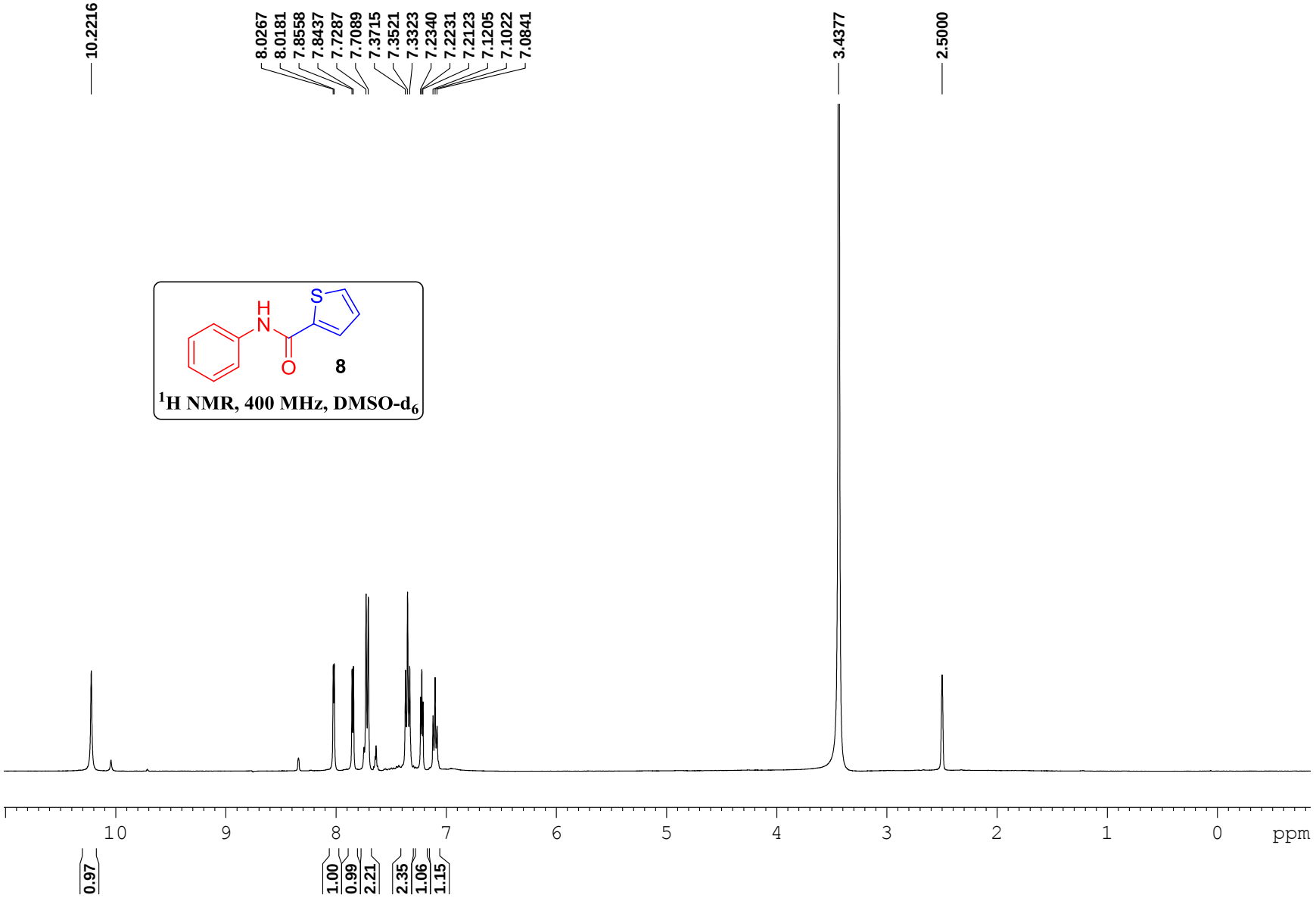

185.0475
147.2952
133.6895
127.8710
124.1529
54.9066
40.1269
39.9180
39.7094
39.5007
39.2920
39.0833
38.8745
30.8367
24.8438
H
N
S
S
5ja
13C NMR, 100 MHz, DMSO-d6
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

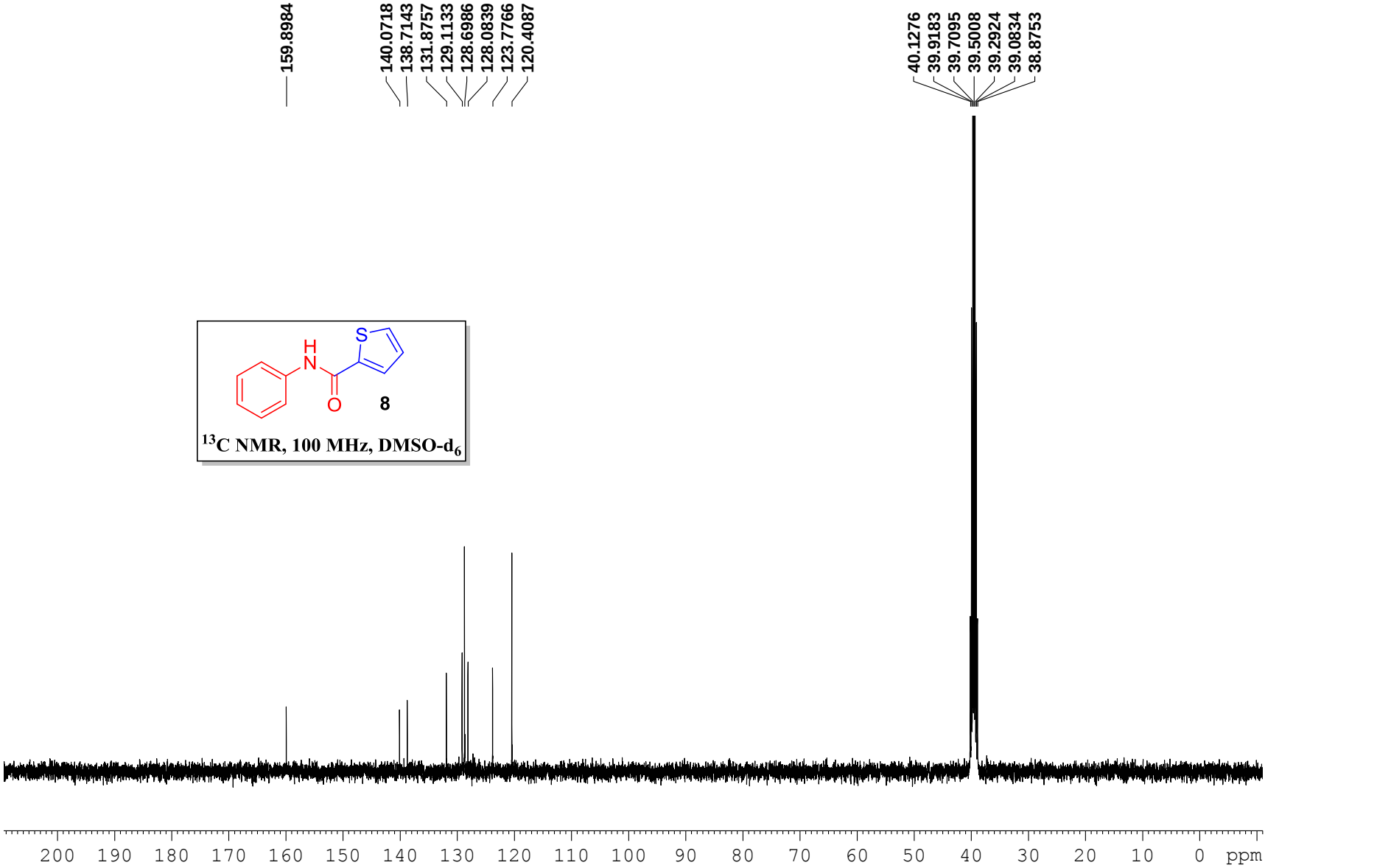

7.8550
7.8354
7.4352
7.4162
7.3971
7.2715
7.2534
7.2354
6.8914
3.3734
2.5002
2.4636
2.3764
5ad
^{1}H NMR, 400 MHz, DMSO-d$_6$
7.8
7.6
7.4
7.2
7.0
ppm
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.98
2.00
1.10
1.02
2.88
2.96

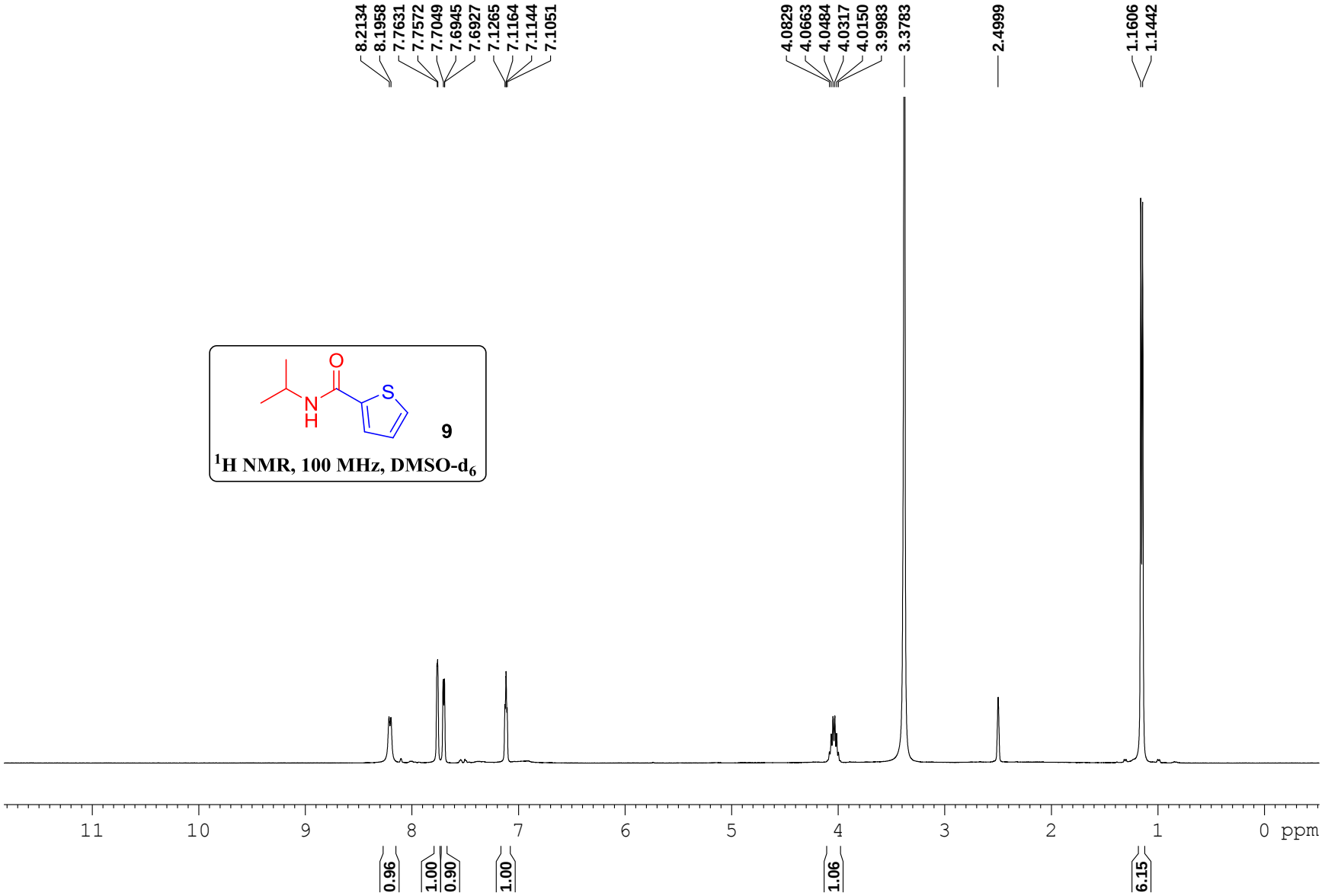

192.0994
141.3416
139.5880
134.6750
134.4972
128.5316
127.1144
126.1497
123.5926
40.1246
39.9162
39.7074
39.4989
39.2901
39.0813
38.8733
14.6120
14.0657
H
N
S
S
5ad
13C NMR, 100 MHz, DMSO-d6
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

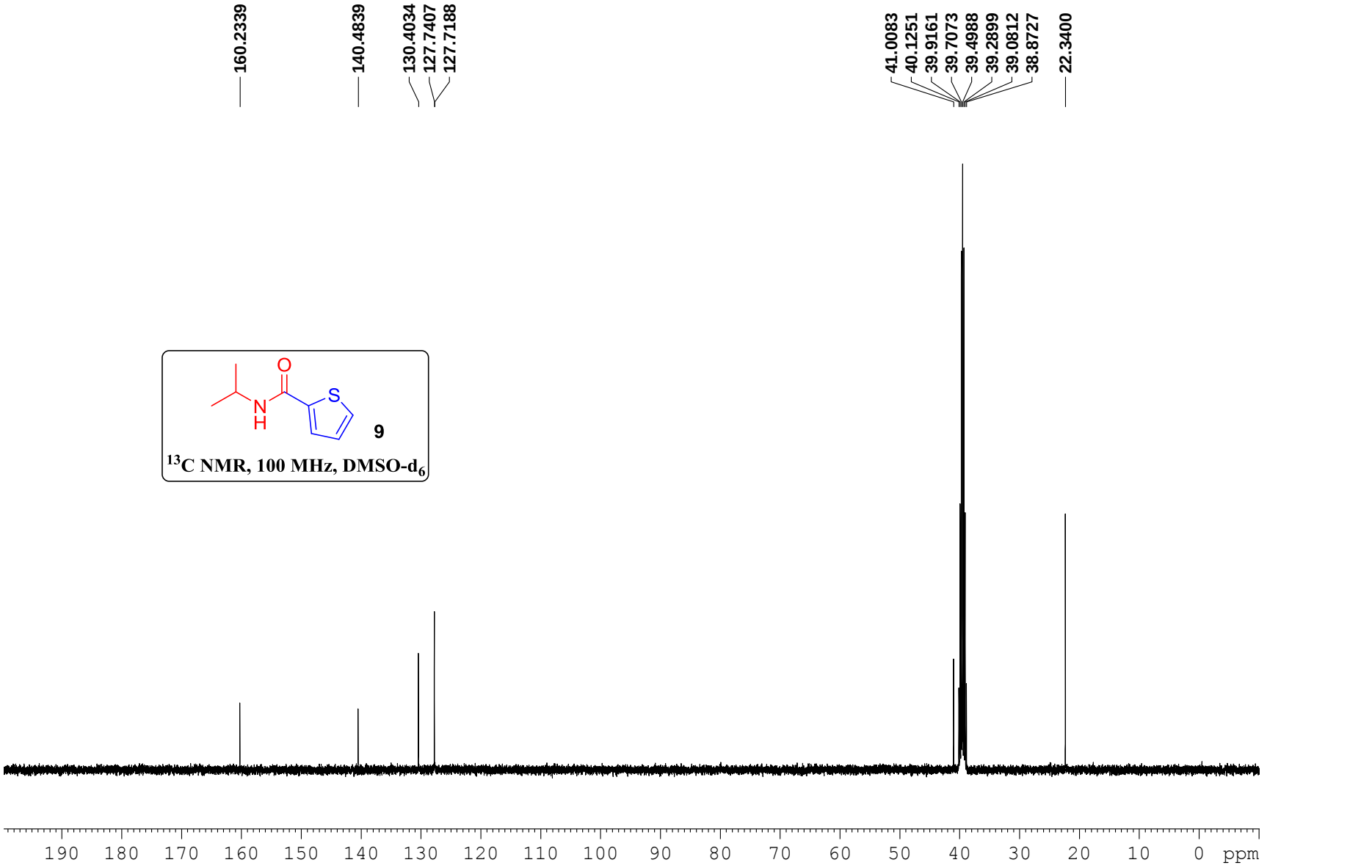

10.0694
7.7677
7.7479
7.6355
7.6148
7.5408
7.3666
7.3474
7.3280
7.1061
7.0910
7.0710
3.8463
3.8367
3.3733
2.5001
H
N
O
O
O
7
^{1}H NMR, 400 MHz, DMSO-d$_6$
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.01
2.06
1.06
1.00
2.07
2.07
6.19

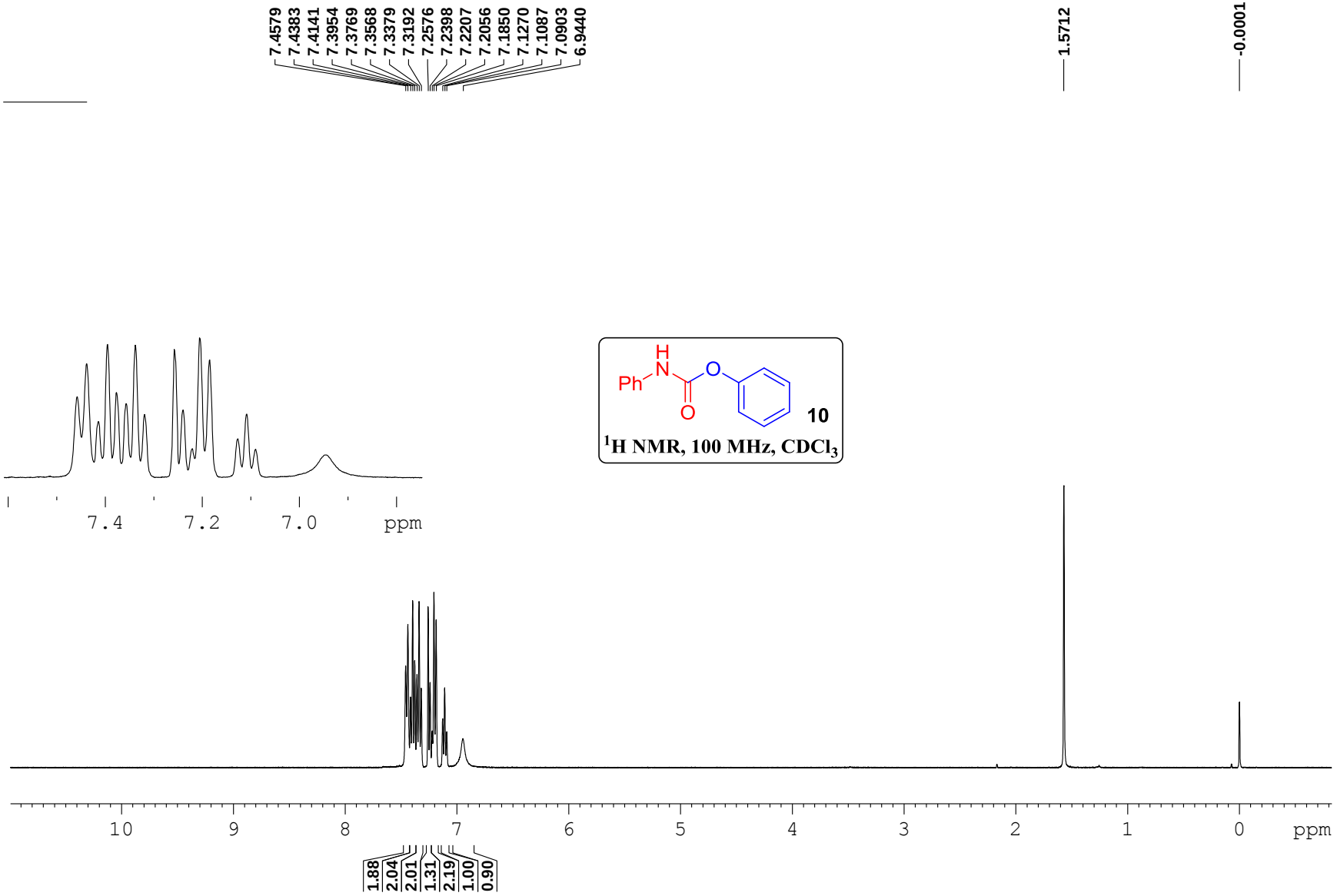

164.9150
151.6157
148.3016
139.2735
128.5554
126.9944
123.4832
121.0199
120.4858
111.0315
110.8829
55.6644
55.6201
40.1269
39.9189
39.7098
39.5009
39.2924
39.0838
38.8755
H
N
O
O
O
7
13C NMR, 100 MHz, DMSO-d6
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

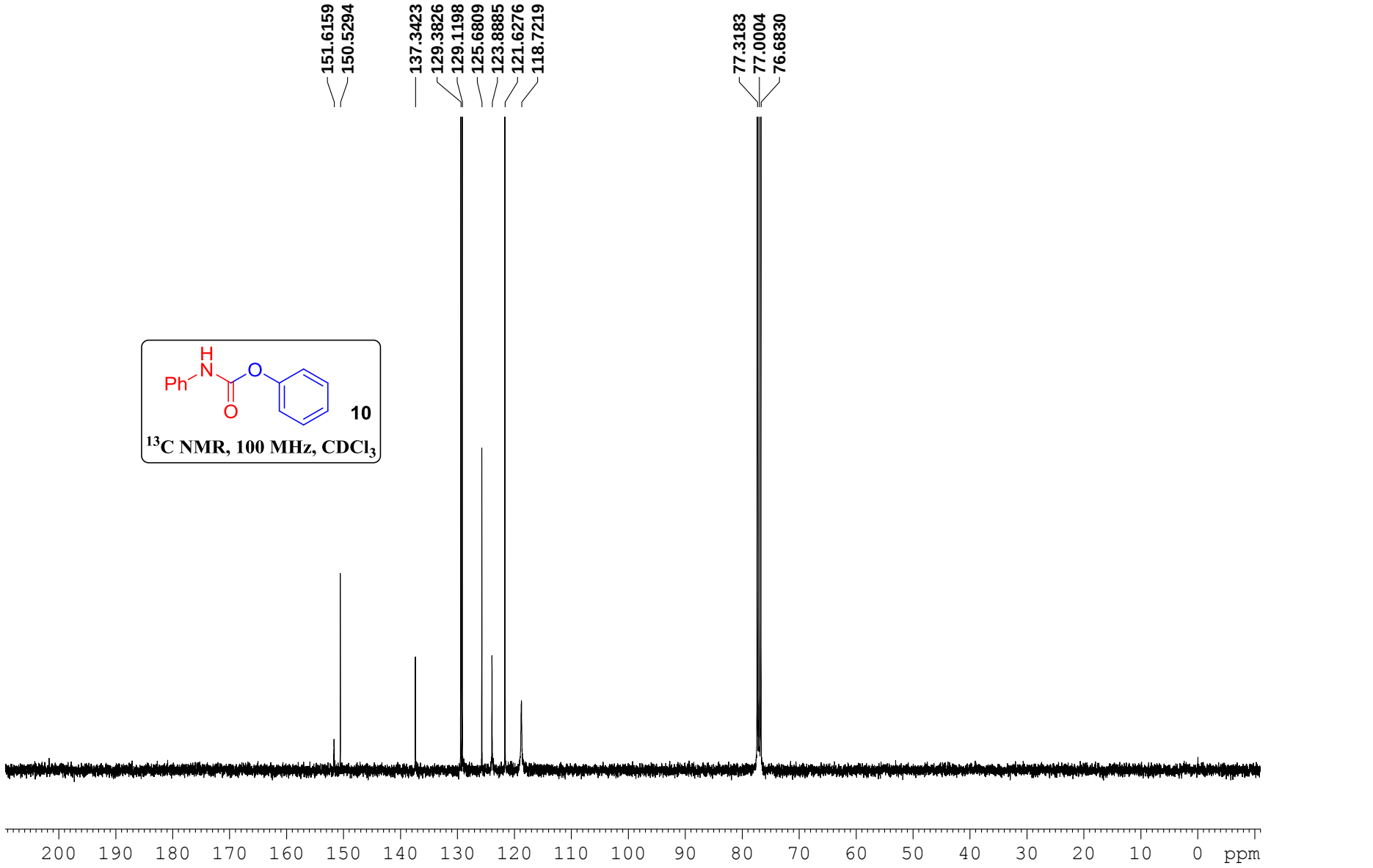

10.2216
8.0267
8.0181
7.8558
7.8437
7.7287
7.7089
7.3715
7.3521
7.3323
7.2340
7.2231
7.2123
7.1205
7.1022
7.0841
3.4377
2.5000
H
N
O
S
8
^{1}H NMR, 400 MHz, DMSO-d$_6$
10
9
8
7
6
5
4
3
2
1
0
ppm
0.97
1.00
0.99
2.21
2.35
1.06
1.15


159.8984
140.0718
138.7143
131.8757
129.1133
128.6986
128.0839
123.7766
120.4087
40.1276
39.9183
39.7095
39.5008
39.2924
39.0834
38.8753
H
N
O
S
8
^{13}C NMR, 100 MHz, DMSO-d$_6$
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

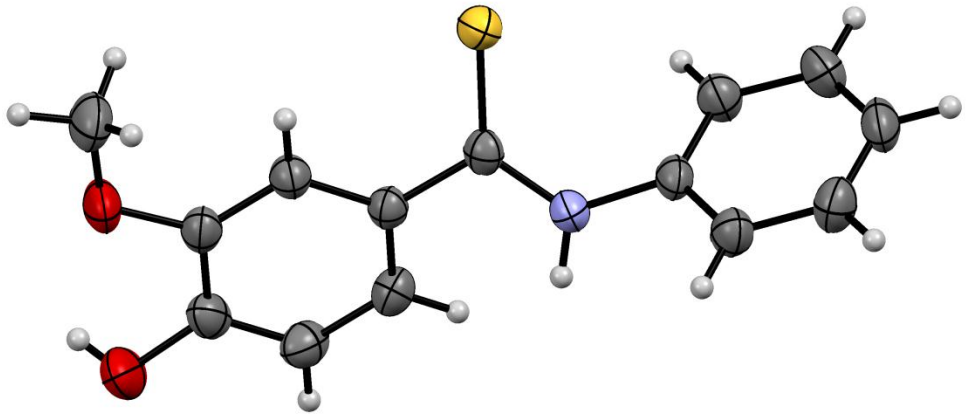

8.2134
8.1958
7.7631
7.7572
7.7049
7.6945
7.6927
7.1265
7.1164
7.1144
7.1051
4.0829
4.0663
4.0484
4.0317
4.0150
3.9983
3.3783
2.4999
1.1606
1.1442
O
N
H
S
9
1H NMR, 100 MHz, DMSO-d6
11
10
9
8
7
6
5
4
3
2
1
0 ppm
0.96
1.00
0.90
1.00
1.06
6.15


160.2339
140.4839
130.4034
127.7407
127.7188
41.0083
40.1251
39.9161
39.7073
39.4988
39.2899
39.0812
38.8727
22.3400
O
N
H
S
9
13C NMR, 100 MHz, DMSO-d6
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


7.4579
7.4383
7.4141
7.3954
7.3769
7.3568
7.3379
7.3192
7.2576
7.2398
7.2207
7.2056
7.1850
7.1270
7.1087
7.0903
6.9440
1.5712
-0.0001
Ph
N
H
O
O
10
^{1}H NMR, 100 MHz, CDCl$_3$
7.4
7.2
7.0
ppm
10
9
8
7
6
5
4
3
2
1
0
ppm
1.88
2.04
2.01
1.31
2.19
1.00
0.90


151.6159
150.5294
137.3423
129.3826
129.1198
125.6809
123.8885
121.6276
118.7219
77.3183
77.0004
76.6830
Ph
N
H
O
O
10
^{13}C NMR, 100 MHz, CDCl$_3$
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

Crystal Data and Details of the Structure Determination (3af)



Crystal Data and Details of the Structure Determination (**3af**)

Crystal Data

Formula			C14 H13 N O2 S
Formula Weight			259.31
Crystal System			monoclinic
Space group		Cc	(No. 9)
a, b, c [Angstrom]	12.7799(16)	12.8970(16)	7.5173(9)
alpha, beta, gamma [deg]	90	99.827(10)	90
V [Ang**3]			1220.8(3)
Z			4
D(calc) [g/cm**3]			1.411
Mu(MoKa) [/mm]			0.257
F(000)			544
Crystal Size [mm]		0.08 x	0.09 x 0.36

Data Collection

Temperature (K)		293
Radiation [Angstrom]	MoKa	0.71073
Theta Min-Max [Deg]		2.3, 27.7
Dataset	-16: 16 ; -15: 16 ;	-9: 8

Tot., Uniq. Data, R(int)	7068, 2641, 0.056
Observed Data [I > 0.0 sigma(I)]	2494
Refinement	
Nref, Npar	2641, 167
R, wR2, S	0.0354, 0.0866, 1.03
w = S^2^(FO^2^)+(0.0459P)^2^+0.1112P] WHERE P=(FO^2^+2FC^2^)/3 '	
Max. and Av. Shift/Error	0.00, 0.00
Flack x	0.01(5)
Min. and Max.Resd.Dens. [e/Ang^3]	-0.16, 0.30

Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms

Atom	x	y	z	U(eq) [Ang^2]
S1	0.49486(6)	0.33504(5)	0.77053(8)	0.0399(2)
O1	0.8524(2)	0.3755(2)	0.2242(3)	0.0562(8)
O2	0.88064(17)	0.34993(19)	0.5839(3)	0.0496(7)
N1	0.41690(17)	0.44857(18)	0.4838(3)	0.0342(6)
C1	0.7667(2)	0.3742(2)	0.3098(4)	0.0387(8)
C2	0.7783(2)	0.3636(2)	0.4974(4)	0.0360(8)
C3	0.6906(2)	0.3677(2)	0.5803(3)	0.0338(8)
C4	0.5895(2)	0.38163(18)	0.4782(3)	0.0302(7)
C5	0.4958(2)	0.39036(19)	0.5704(3)	0.0309(7)
C6	0.3137(2)	0.4631(2)	0.5297(3)	0.0326(7)
C7	0.2495(3)	0.3797(2)	0.5519(4)	0.0398(8)
C8	0.1477(2)	0.3968(3)	0.5850(4)	0.0449(9)
C9	0.1106(2)	0.4962(3)	0.5962(4)	0.0454(9)
C10	0.8972(3)	0.3427(3)	0.7740(5)	0.0551(11)
C11	0.5793(2)	0.3885(2)	0.2910(3)	0.0366(8)
C12	0.6671(2)	0.3846(2)	0.2087(4)	0.0405(9)
C13	0.2763(2)	0.5631(2)	0.5381(4)	0.0398(8)
C14	0.1747(3)	0.5794(3)	0.5739(4)	0.0461(9)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Hydrogen Atom Positions and Isotropic Displacement Parameters

Atom	x	y	z	U(iso) [Ang^2]
H1	0.897(4)	0.355(4)	0.294(6)	0.0690
H1A	0.42940	0.48100	0.38970	0.0410
H3	0.69860	0.36100	0.70510	0.0410
H7	0.27450	0.31240	0.54470	0.0480
H8	0.10420	0.34080	0.59970	0.0540
H9	0.04220	0.50730	0.61880	0.0540
H10A	0.87040	0.40390	0.82320	0.0820
H10B	0.97180	0.33610	0.81930	0.0820
H10C	0.86070	0.28290	0.80880	0.0820
H11	0.51220	0.39590	0.22120	0.0440
H12	0.65920	0.38890	0.08360	0.0490
H13	0.31890	0.61920	0.51990	0.0480
H14	0.14980	0.64660	0.58290	0.0550

==========

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms

(An)isotropic Displacement Parameters

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
S1	0.0346(3)	0.0470(4)	0.0382(3)	0.0077(3)	0.0065(3)	-0.0005(3)
O1	0.0456(14)	0.0697(16)	0.0597(14)	0.0148(11)	0.0272(11)	0.0164(12)
O2	0.0251(11)	0.0736(15)	0.0508(11)	0.0084(10)	0.0083(9)	0.0044(9)
N1	0.0269(11)	0.0417(12)	0.0349(10)	0.0055(9)	0.0079(9)	0.0014(9)
C1	0.0391(16)	0.0346(13)	0.0460(15)	0.0032(11)	0.0174(13)	0.0061(12)
C2	0.0290(14)	0.0340(14)	0.0447(14)	0.0024(11)	0.0059(11)	0.0018(10)
C3	0.0295(14)	0.0378(13)	0.0342(12)	0.0004(10)	0.0058(11)	0.0003(11)
C4	0.0277(13)	0.0287(13)	0.0343(12)	-0.0001(9)	0.0052(10)	0.0012(10)
C5	0.0260(13)	0.0303(12)	0.0353(12)	-0.0031(9)	0.0022(11)	-0.0035(10)
C6	0.0236(12)	0.0422(14)	0.0313(11)	0.0015(10)	0.0025(10)	0.0023(11)
C7	0.0360(15)	0.0360(14)	0.0488(15)	-0.0006(11)	0.0116(12)	-0.0004(12)
C8	0.0328(15)	0.0511(17)	0.0525(16)	0.0029(13)	0.0121(13)	-0.0065(12)
C9	0.0262(13)	0.0640(19)	0.0473(16)	0.0021(13)	0.0099(12)	0.0053(13)
C10	0.0312(17)	0.077(2)	0.0546(18)	0.0063(15)	0.0002(14)	0.0051(15)
C11	0.0335(15)	0.0364(14)	0.0386(14)	-0.0001(10)	0.0022(12)	0.0059(11)
C12	0.0477(18)	0.0402(15)	0.0351(13)	0.0018(11)	0.0111(12)	0.0112(12)
C13	0.0311(14)	0.0401(15)	0.0466(14)	0.0030(11)	0.0025(12)	-0.0007(11)
C14	0.0361(15)	0.0464(16)	0.0547(16)	0.0001(13)	0.0049(13)	0.0096(13)

==========

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for Anisotropic Atoms.Astar(i) are Reciprocal Axial Lengths and h(i) are the Reflection Indices.

Bond Distances (Angstrom)

S1	-C5	1.667(2)	C7	-C8	1.383(5)
O1	-C1	1.362(4)	C8	-C9	1.374(5)
O2	-C2	1.369(3)	C9	-C14	1.378(5)
O2	-C10	1.412(4)	C11	-C12	1.372(4)
O1	-H1	0.75(5)	C13	-C14	1.386(5)
N1	-C6	1.431(3)	C3	-H3	0.9300
N1	-C5	1.334(3)	C7	-H7	0.9300
N1	-H1A	0.8600	C8	-H8	0.9300
C1	-C12	1.373(4)	C9	-H9	0.9300
C1	-C2	1.399(4)	C10	-H10A	0.9600
C2	-C3	1.373(4)	C10	-H10B	0.9600
C3	-C4	1.397(4)	C10	-H10C	0.9600
C4	-C11	1.394(3)	C11	-H11	0.9300
C4	-C5	1.487(4)	C12	-H12	0.9300
C6	-C13	1.381(4)	C13	-H13	0.9300
C6	-C7	1.380(4)	C14	-H14	0.9300

Bond Angles (Degrees)

C2	-O2	-C10	117.1(3)	C1	-C12	-C11	120.4(3)
C1	-O1	-H1	104(4)	C6	-C13	-C14	119.6(3)
C5	-N1	-C6	127.4(2)	C9	-C14	-C13	120.1(3)
C6	-N1	-H1A	116.00	C2	-C3	-H3	120.00
C5	-N1	-H1A	116.00	C4	-C3	-H3	120.00
O1	-C1	-C2	121.5(2)	C6	-C7	-H7	120.00
O1	-C1	-C12	118.8(3)	C8	-C7	-H7	120.00
C2	-C1	-C12	119.7(3)	C7	-C8	-H8	120.00
O2	-C2	-C3	125.2(3)	C9	-C8	-H8	120.00
O2	-C2	-C1	114.8(2)	C8	-C9	-H9	120.00
C1	-C2	-C3	120.0(2)	C14	-C9	-H9	120.00
C2	-C3	-C4	120.4(2)	O2	-C10	-H10A	110.00
C3	-C4	-C5	119.8(2)	O2	-C10	-H10B	109.00
C5	-C4	-C11	121.5(2)	O2	-C10	-H10C	109.00
C3	-C4	-C11	118.8(2)	H10A	-C10	-H10B	110.00
N1	-C5	-C4	114.6(2)	H10A	-C10	-H10C	109.00
S1	-C5	-C4	121.25(18)	H10B	-C10	-H10C	109.00
S1	-C5	-N1	124.1(2)	C4	-C11	-H11	120.00

N1	-C6	-C7	121.2(2)	C12	-C11	-H11	120.00
N1	-C6	-C13	118.3(2)	C1	-C12	-H12	120.00
C7	-C6	-C13	120.3(3)	C11	-C12	-H12	120.00
C6	-C7	-C8	119.6(3)	C6	-C13	-H13	120.00
C7	-C8	-C9	120.3(3)	C14	-C13	-H13	120.00
C8	-C9	-C14	120.0(3)	C9	-C14	-H14	120.00
C4	-C11	-C12	120.7(2)	C13	-C14	-H14	120.00

Torsion Angles (Degrees)

C10	-O2	-C2	-C1	177.7(3)
C10	-O2	-C2	-C3	-2.1(4)
C6	-N1	-C5	-S1	-9.2(4)
C6	-N1	-C5	-C4	173.5(2)
C5	-N1	-C6	-C7	-54.3(4)
C5	-N1	-C6	-C13	130.5(3)
O1	-C1	-C2	-O2	-3.0(4)
O1	-C1	-C2	-C3	176.8(3)
C12	-C1	-C2	-O2	177.7(2)
C12	-C1	-C2	-C3	-2.6(4)
O1	-C1	-C12	-C11	-177.0(2)
C2	-C1	-C12	-C11	2.4(4)
O2	-C2	-C3	-C4	-179.8(2)
C1	-C2	-C3	-C4	0.5(4)
C2	-C3	-C4	-C5	-177.4(2)
C2	-C3	-C4	-C11	1.7(4)
C3	-C4	-C5	-S1	-27.2(3)

C3	-C4	-C5	-N1	150.2(2)
C11	-C4	-C5	-S1	153.7(2)
C11	-C4	-C5	-N1	-28.9(3)
C3	-C4	-C11	-C12	-1.8(4)
C5	-C4	-C11	-C12	177.3(2)
N1	-C6	-C7	-C8	-175.9(2)
C13	-C6	-C7	-C8	-0.8(4)
N1	-C6	-C13	-C14	177.0(2)
C7	-C6	-C13	-C14	1.8(4)
C6	-C7	-C8	-C9	-0.2(4)
C7	-C8	-C9	-C14	0.2(5)
C8	-C9	-C14	-C13	0.7(5)
C4	-C11	-C12	-C1	-0.2(4)
C6	-C13	-C14	-C9	-1.7(4)