

Palladium-catalyzed intramolecular C-H arylation of
2-halo-N-Boc-N-arylbenzamides for the synthesis of N-H
phenanthridinones

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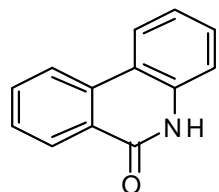
Sichuan University and Collaborative Innovation Center, Chengdu 610041, China

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Contents

Copies of NMR Spectra of 30 N-H Phenanthridinones

S2



5aa

DMSO-D6

11.691
8.526
8.506
8.407
8.387
8.341
8.322
7.881
7.862
7.845
7.671
7.652
7.634
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7.479
7.386
7.366
7.290
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7.253
3.341
2.509
-0.000

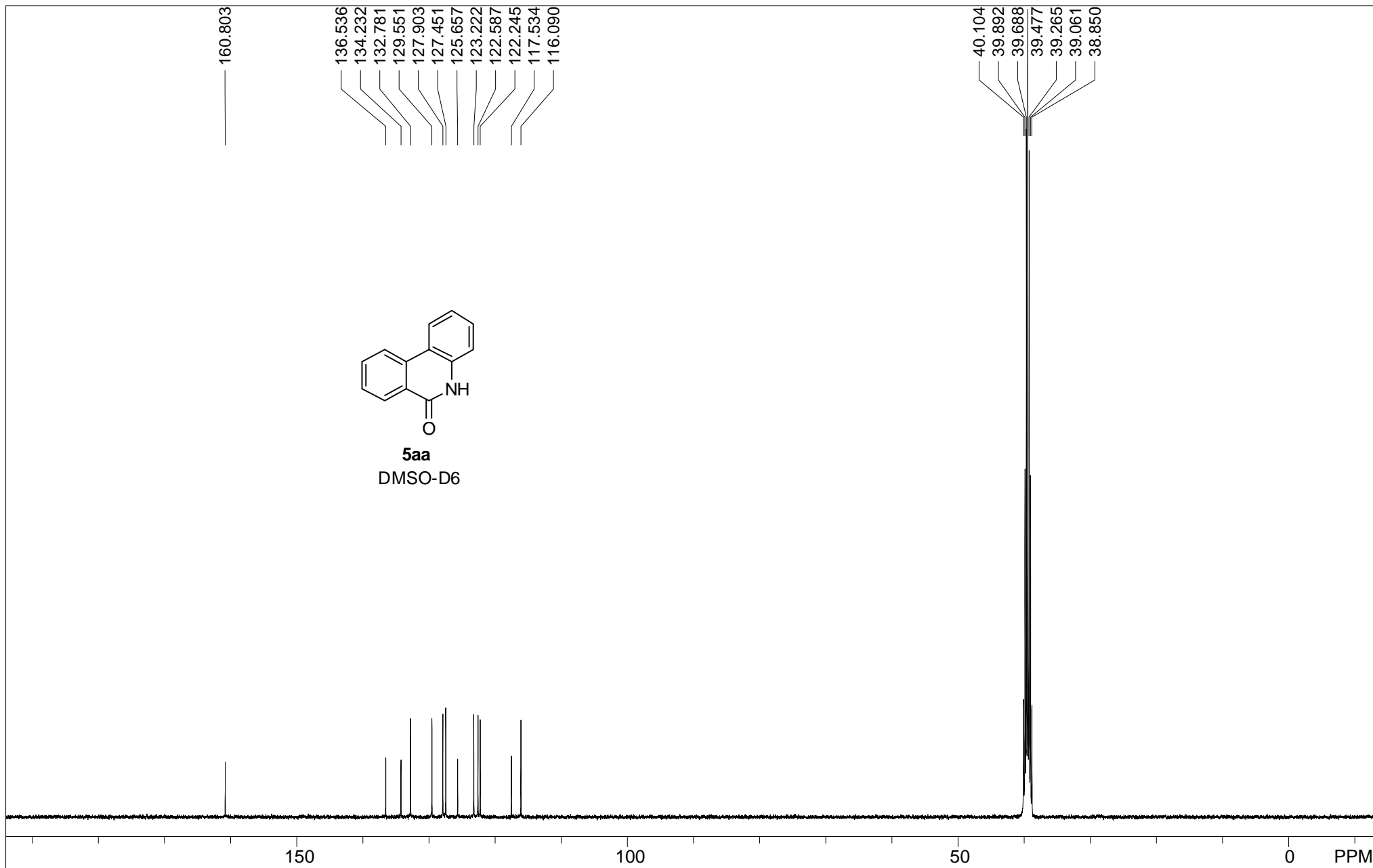
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1.02
0.40
0.200

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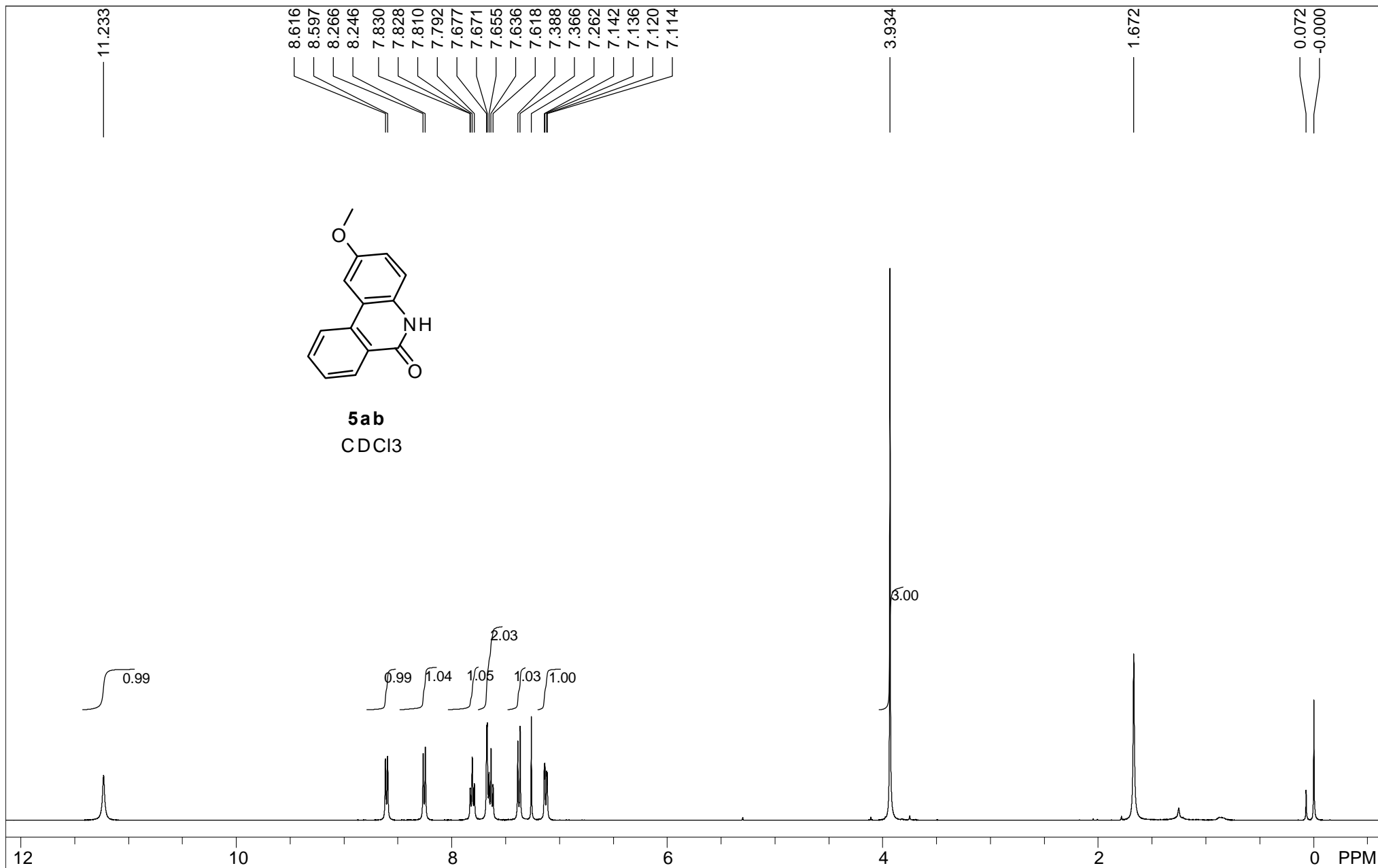
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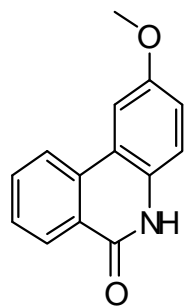
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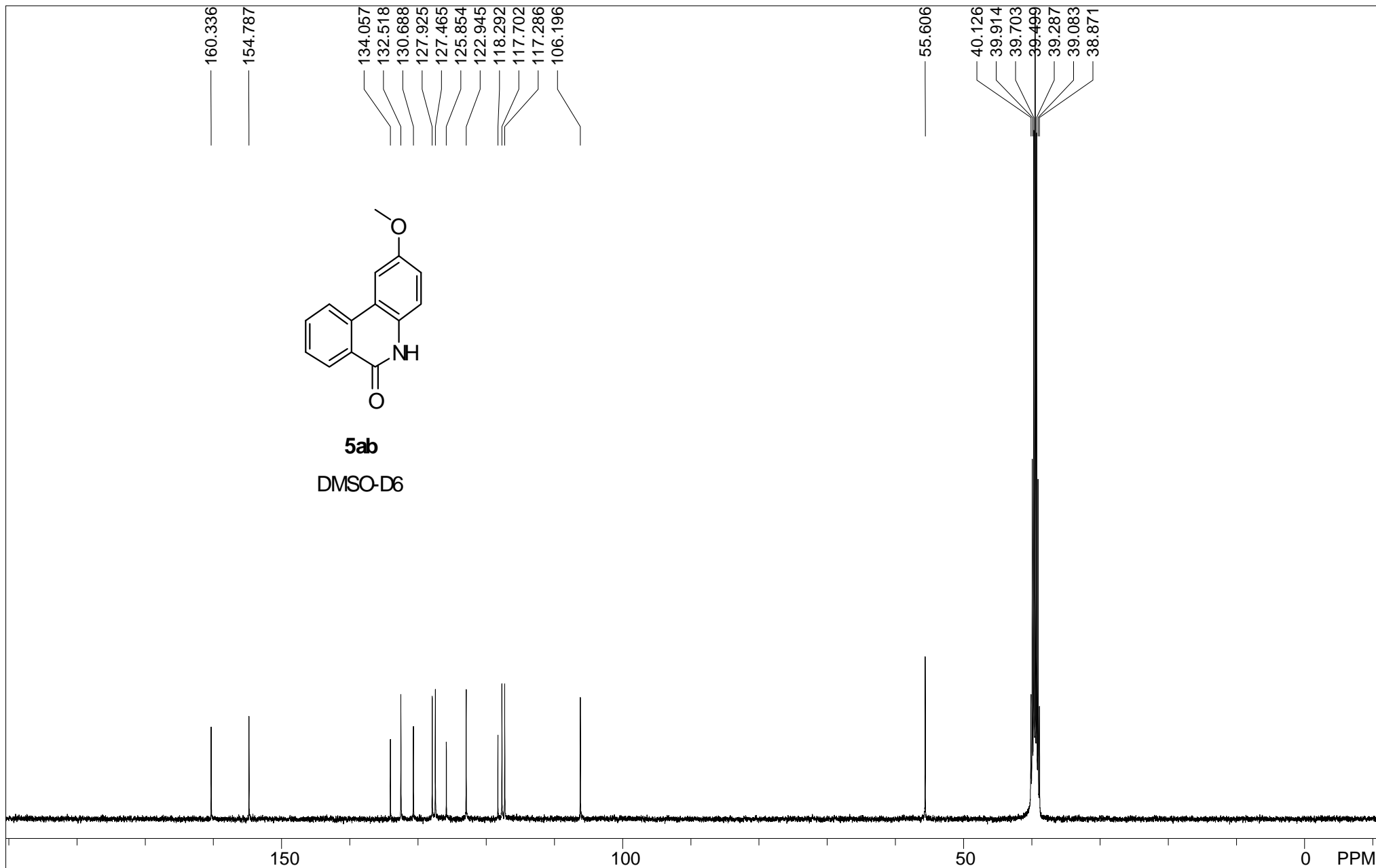
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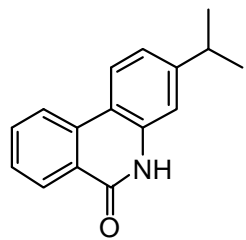
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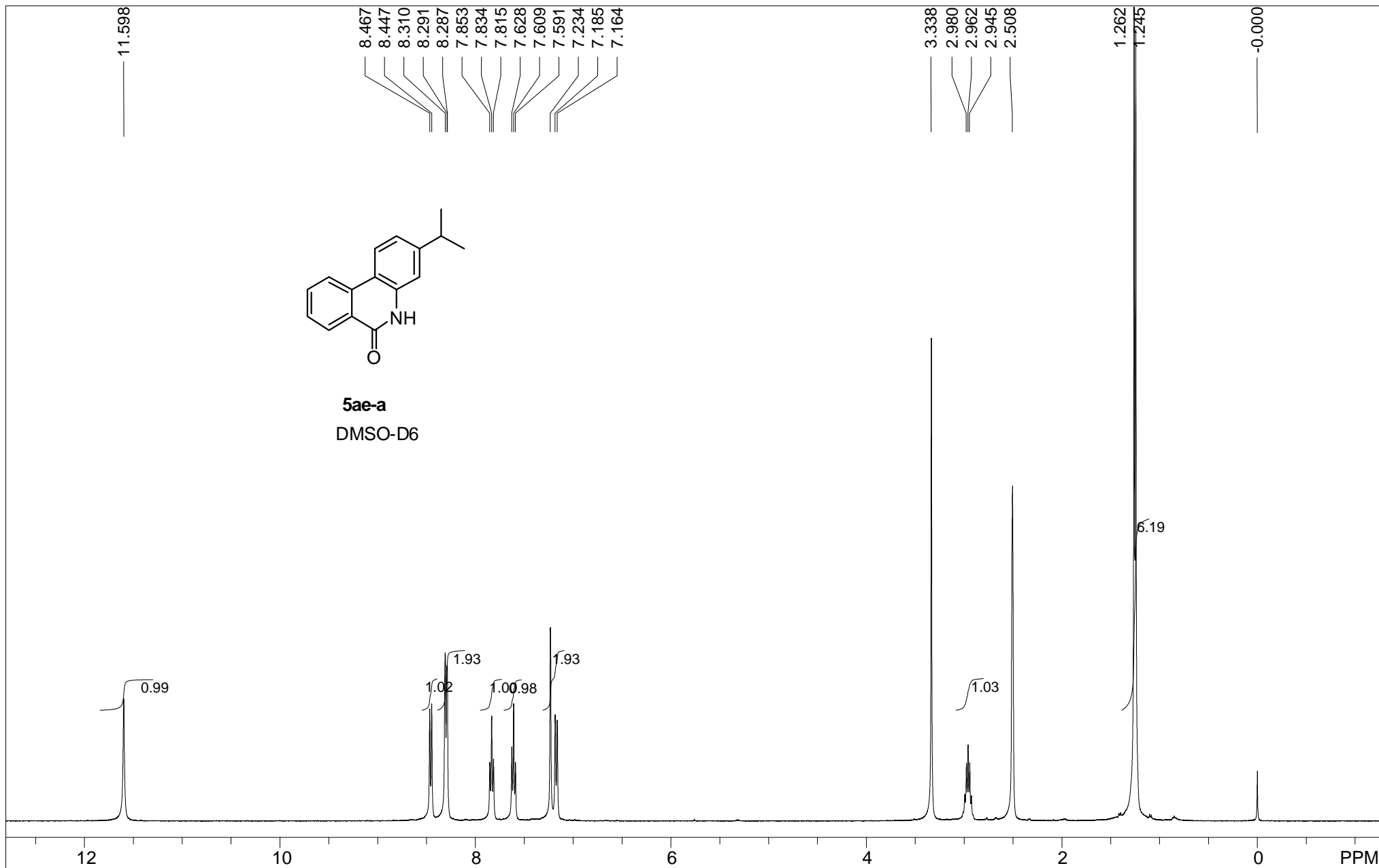


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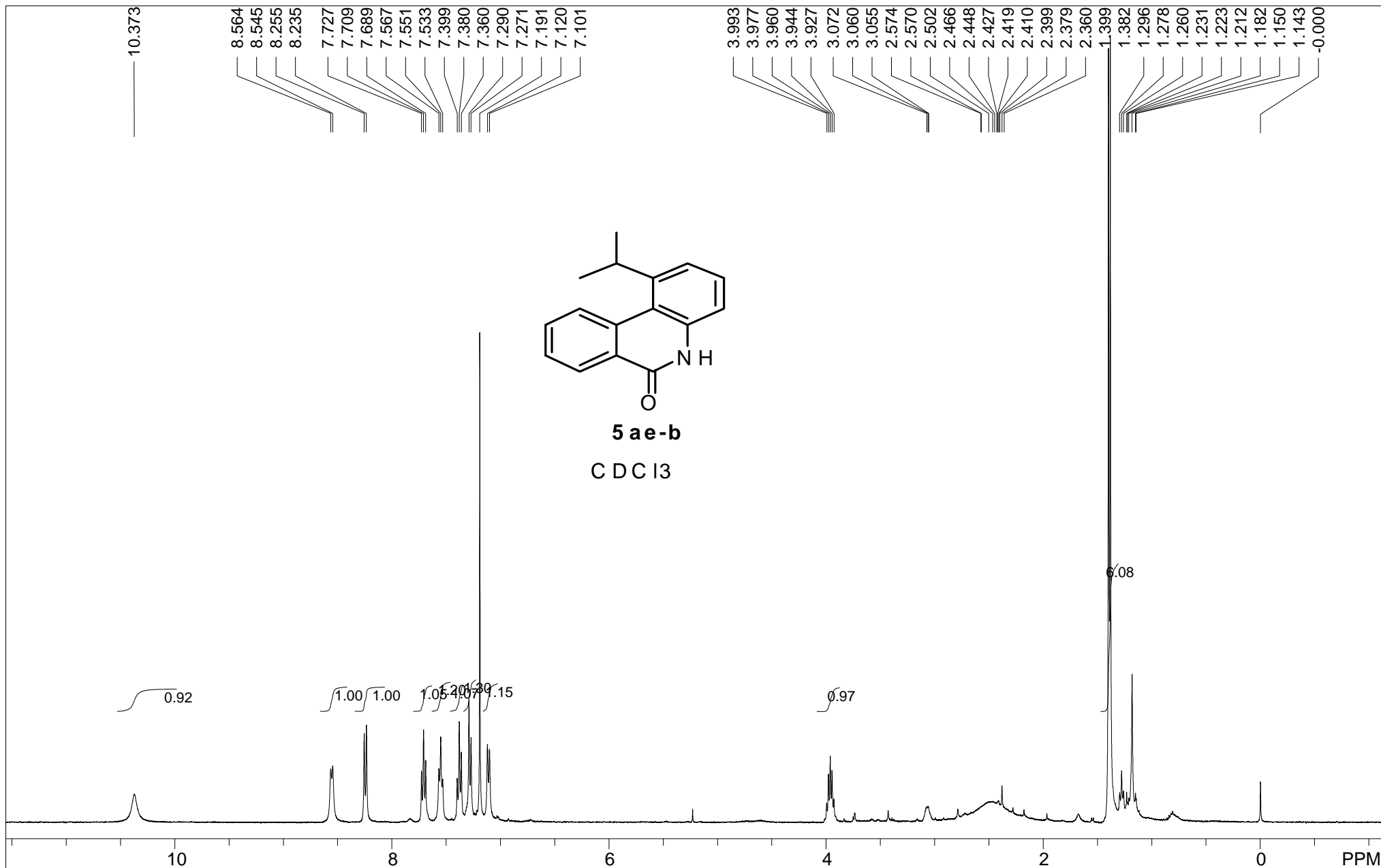


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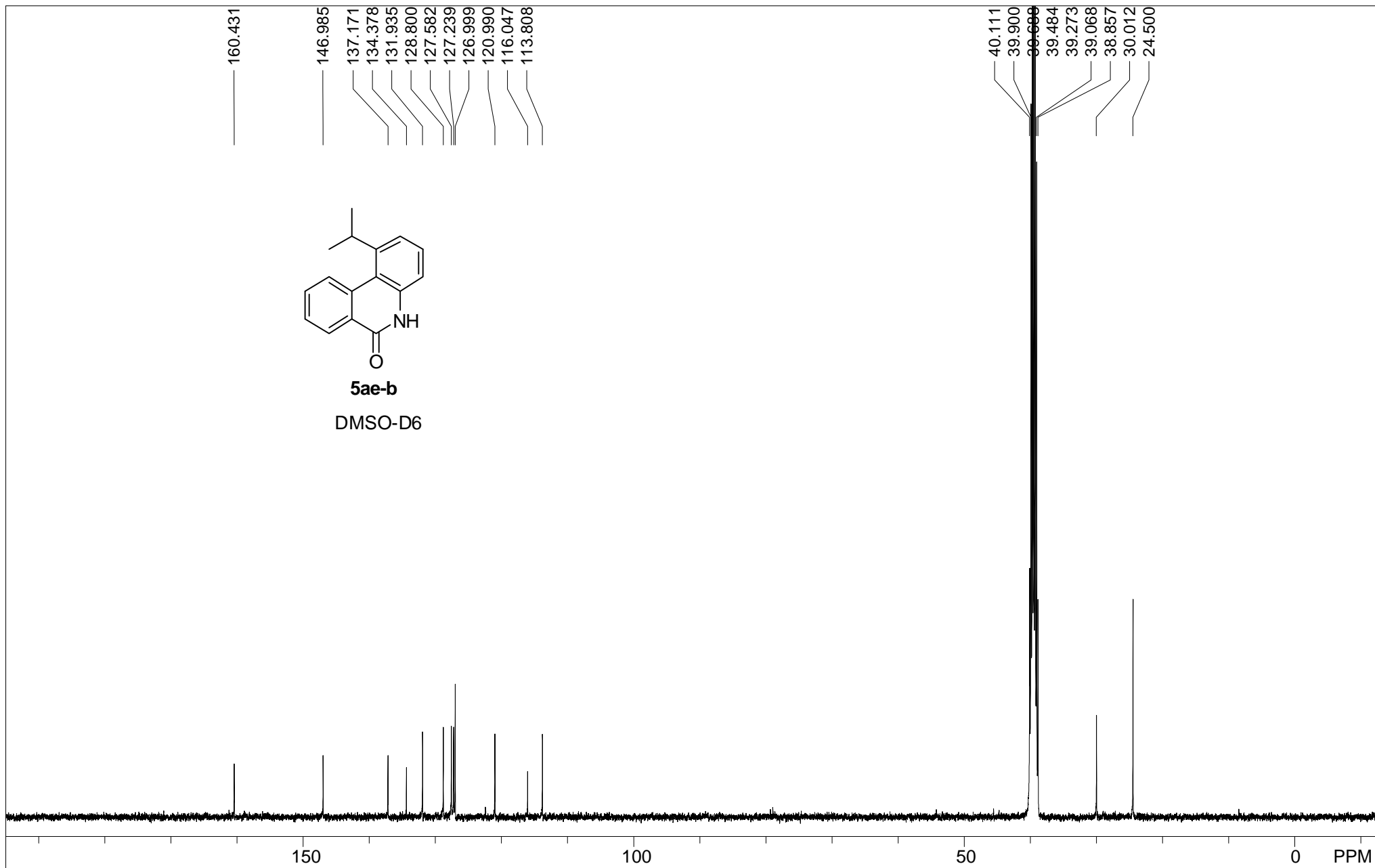


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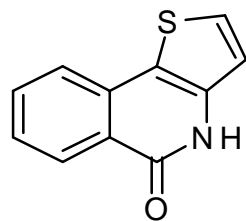


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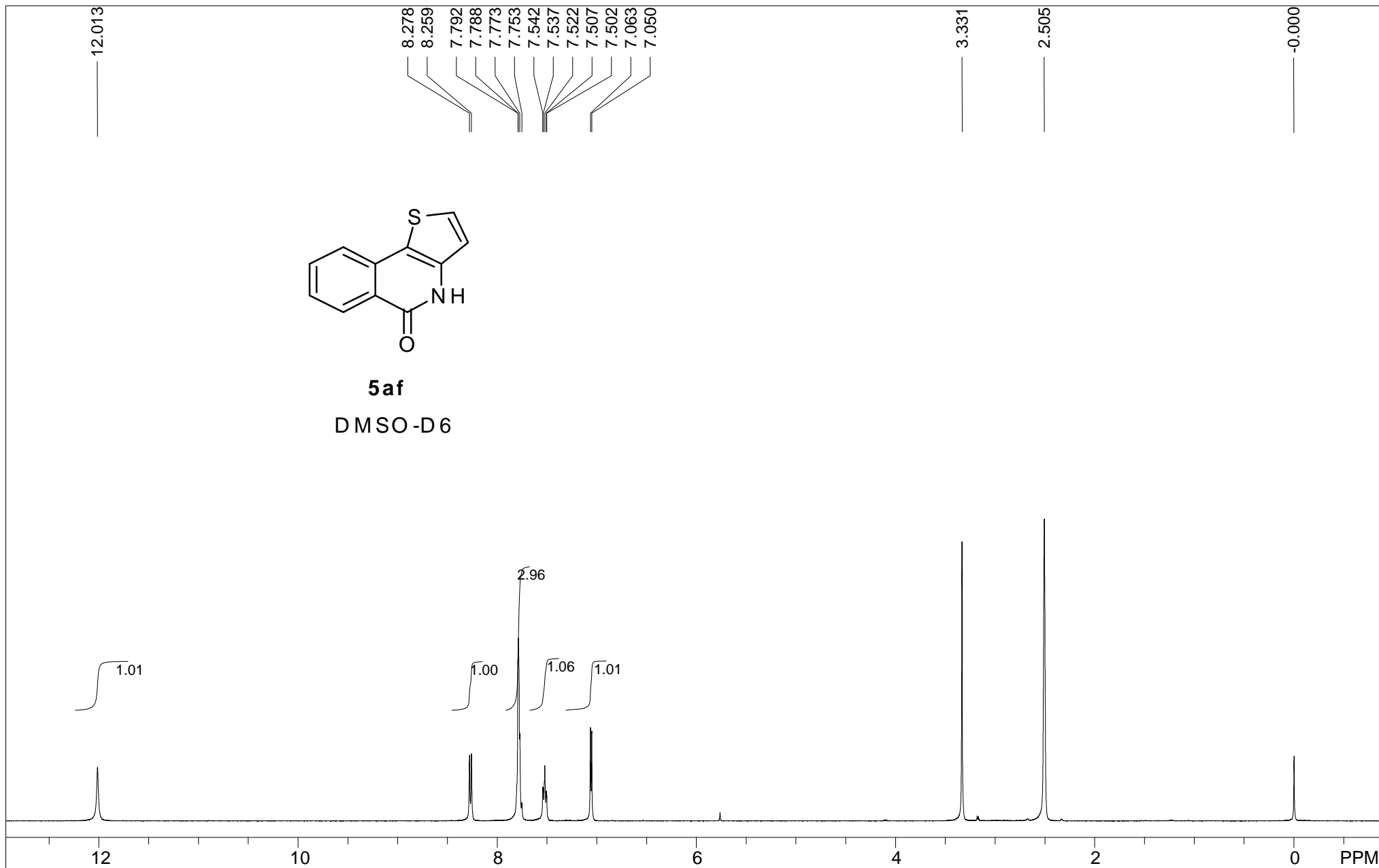


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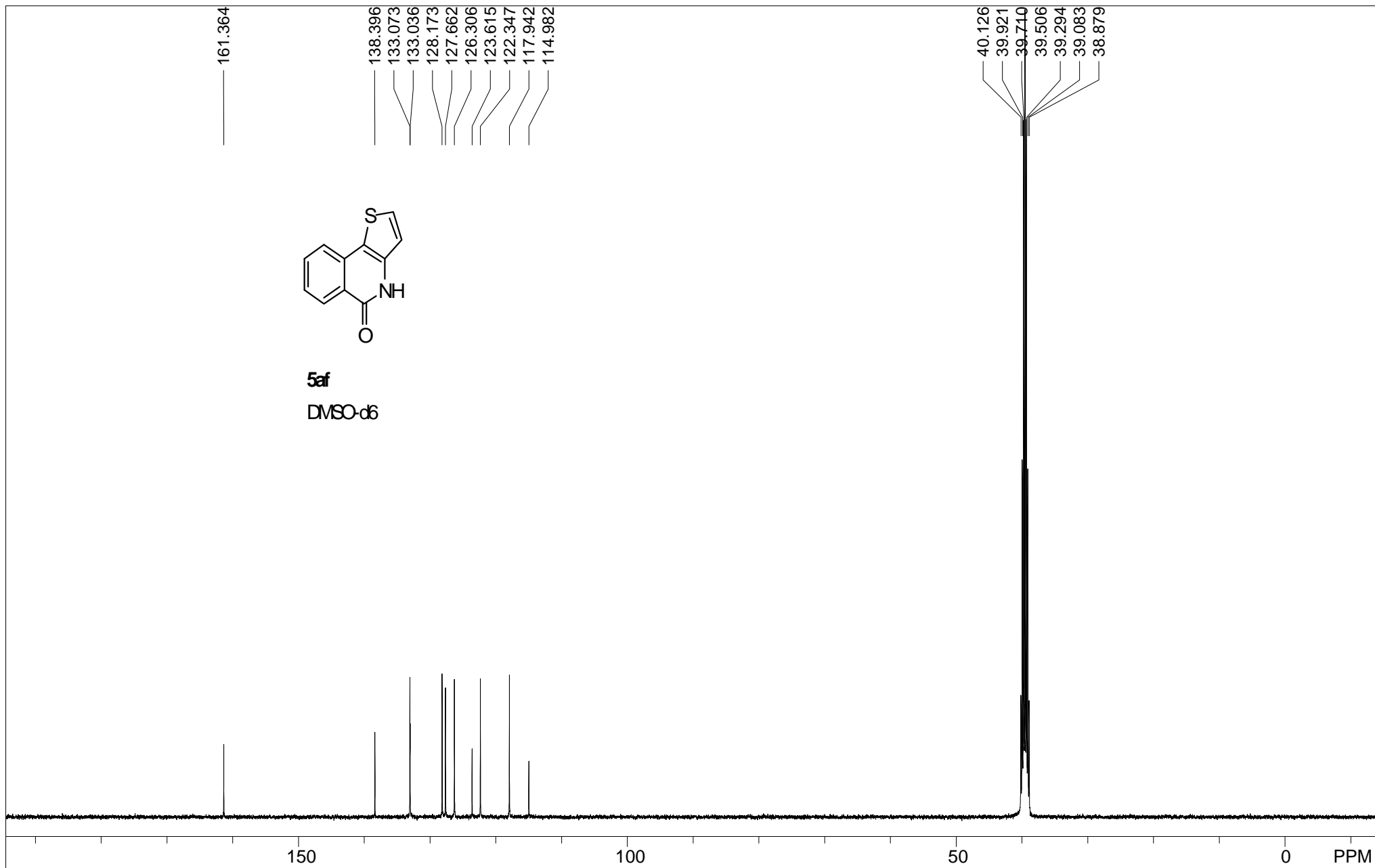


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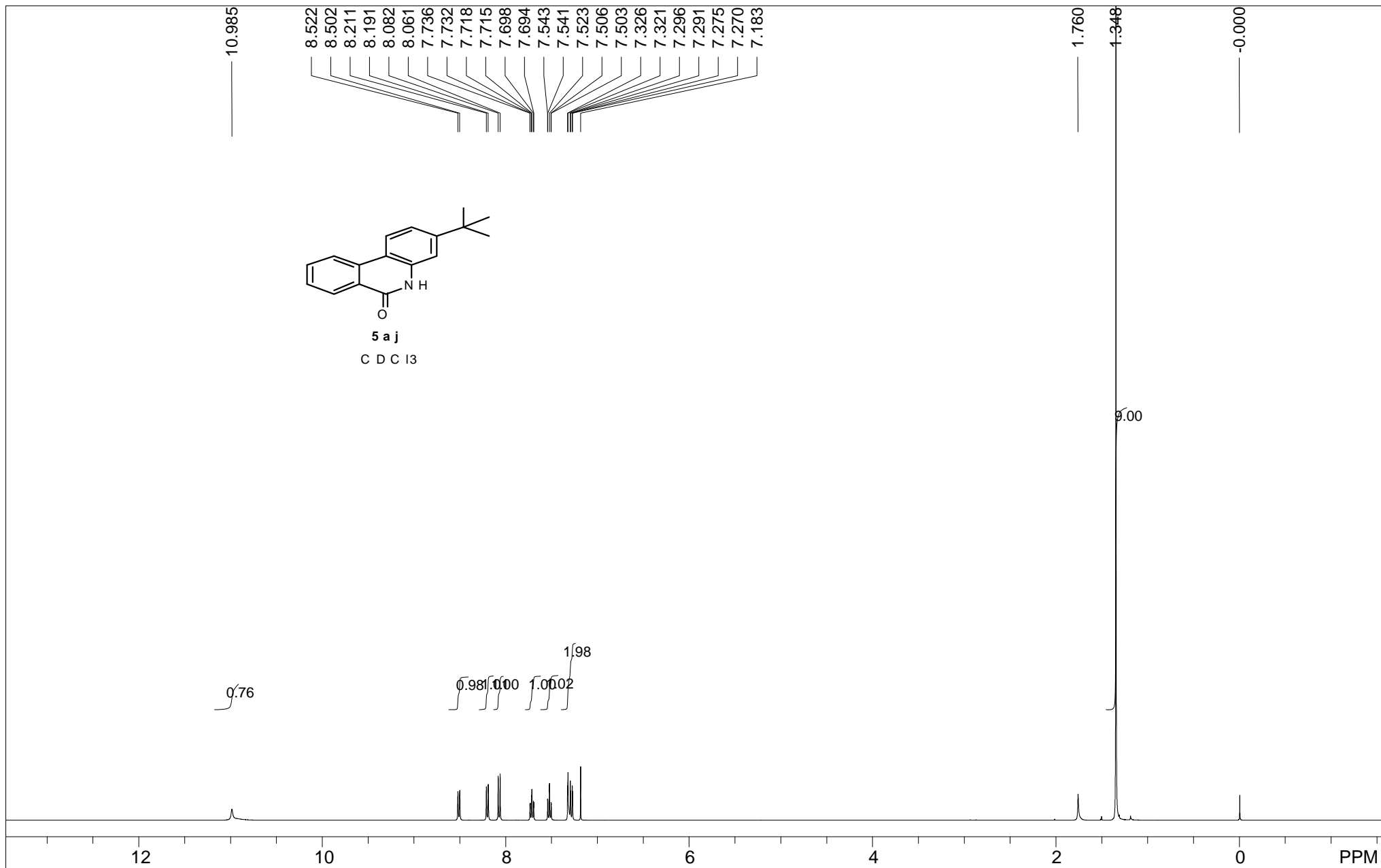


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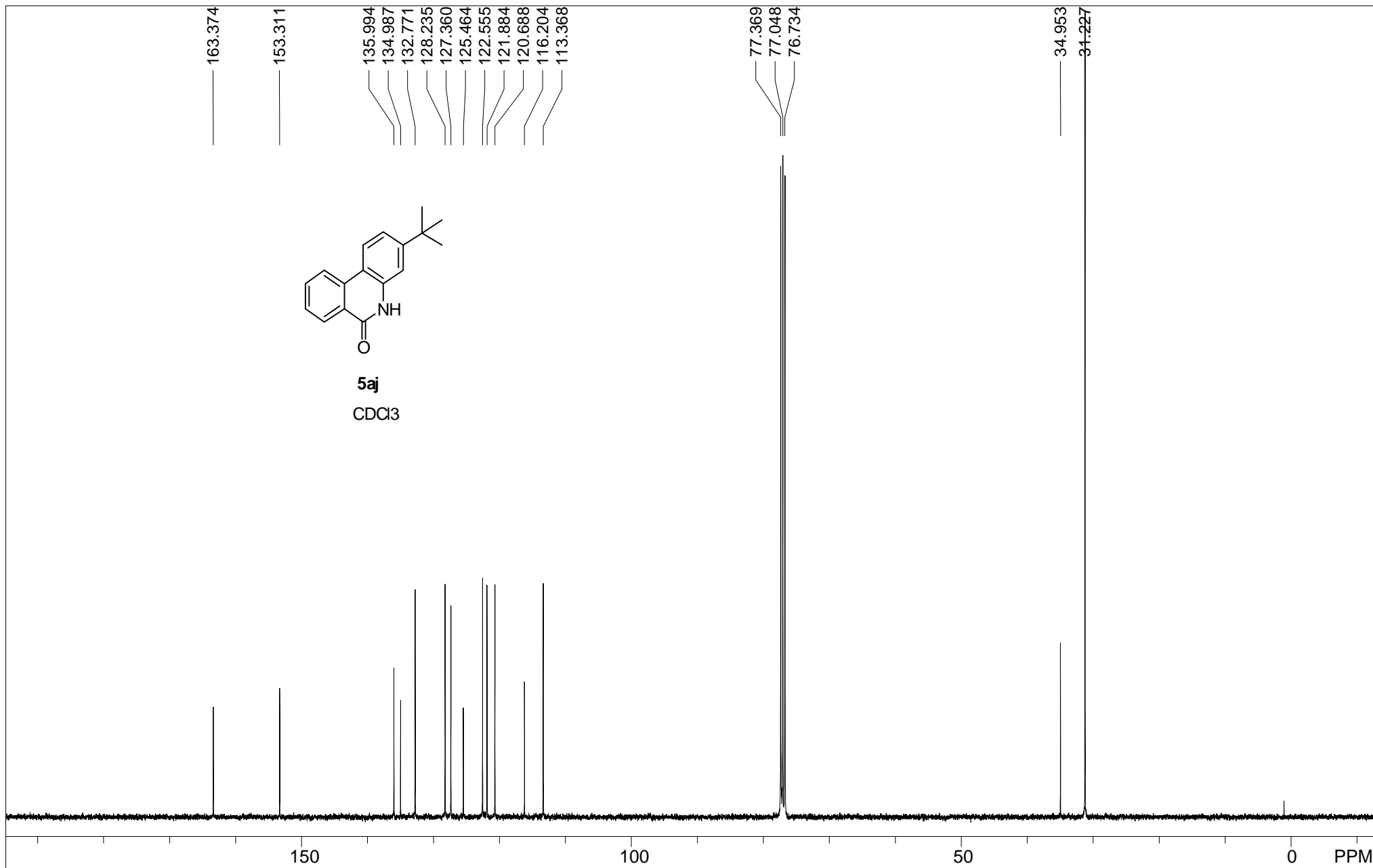
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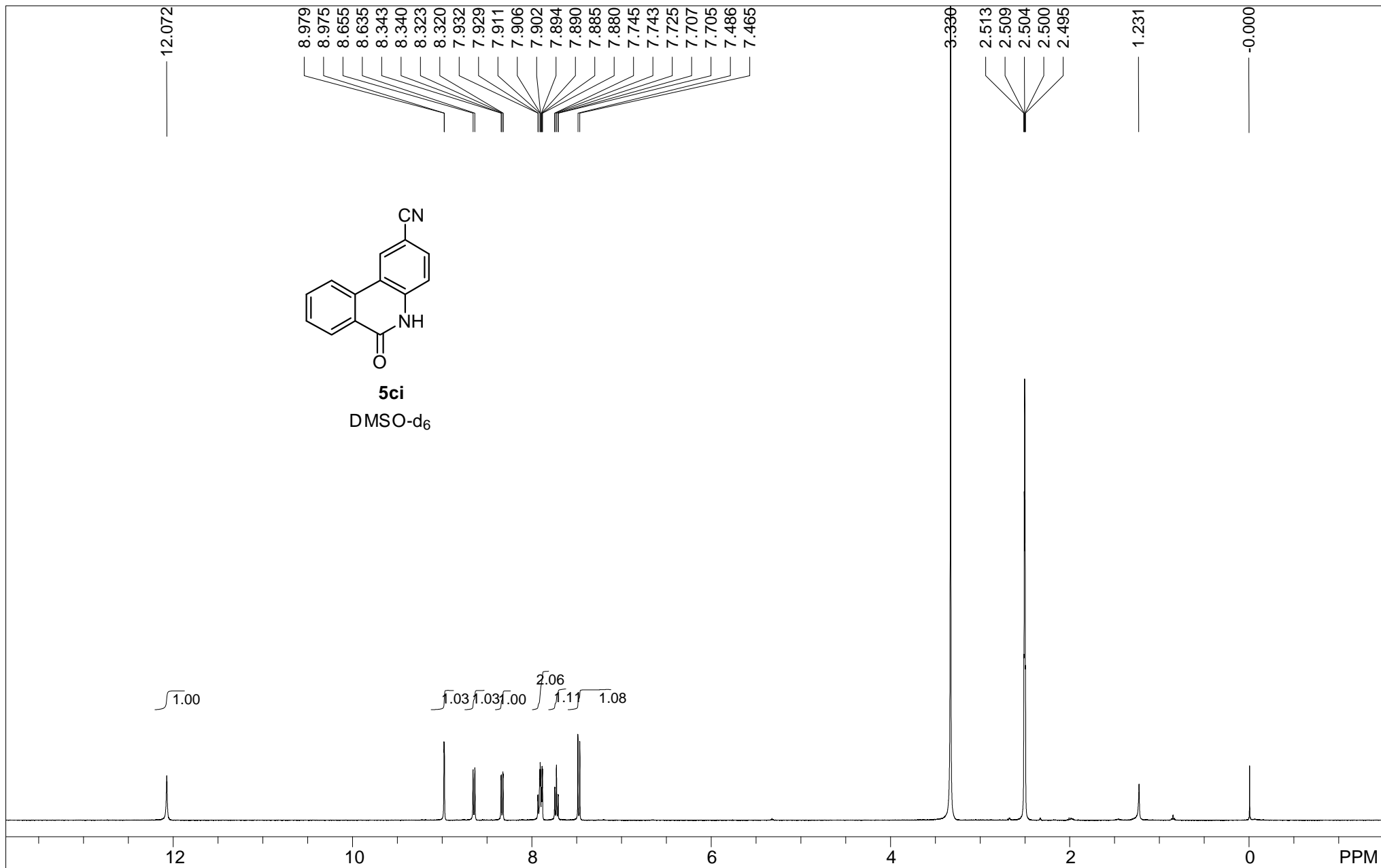
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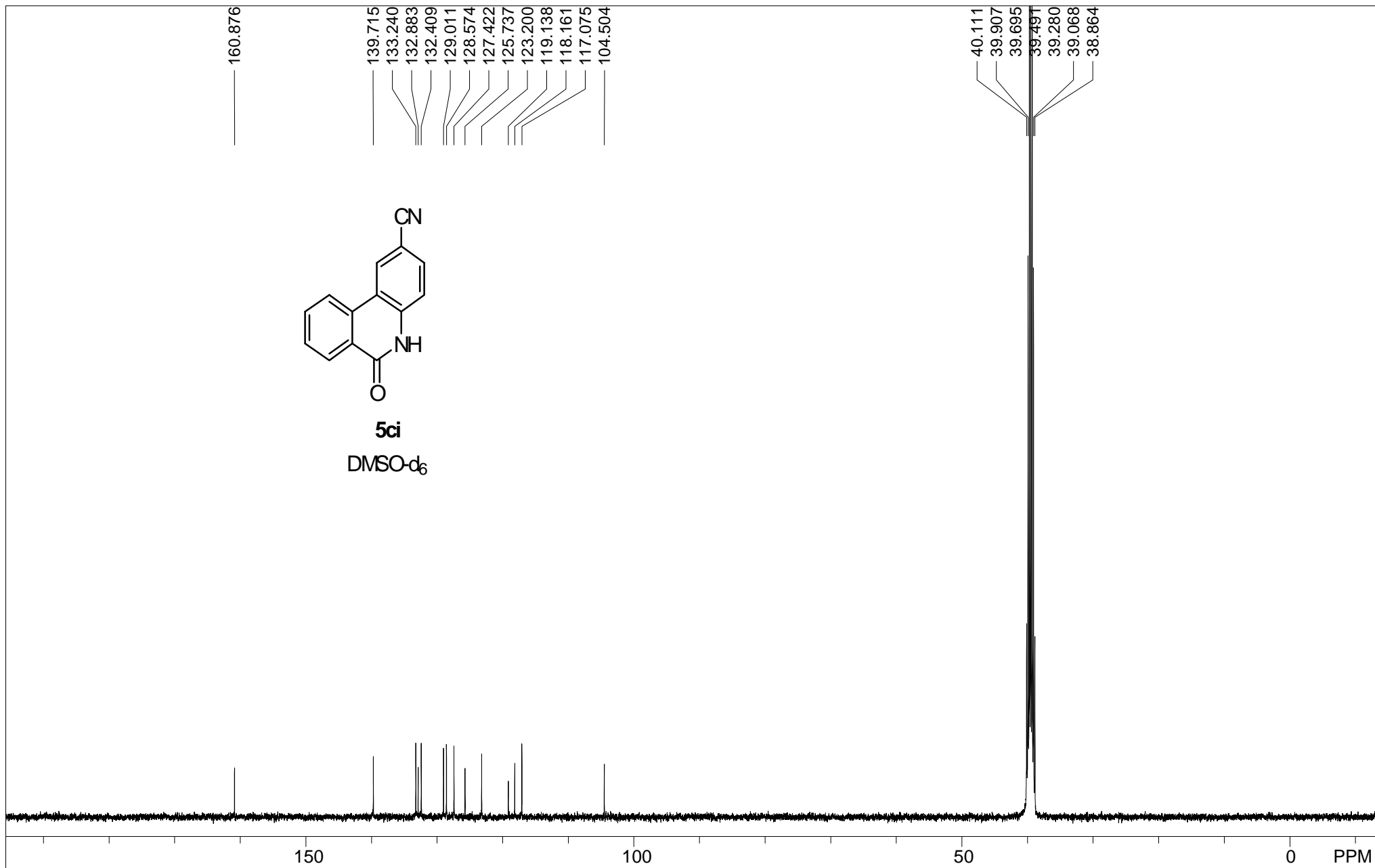
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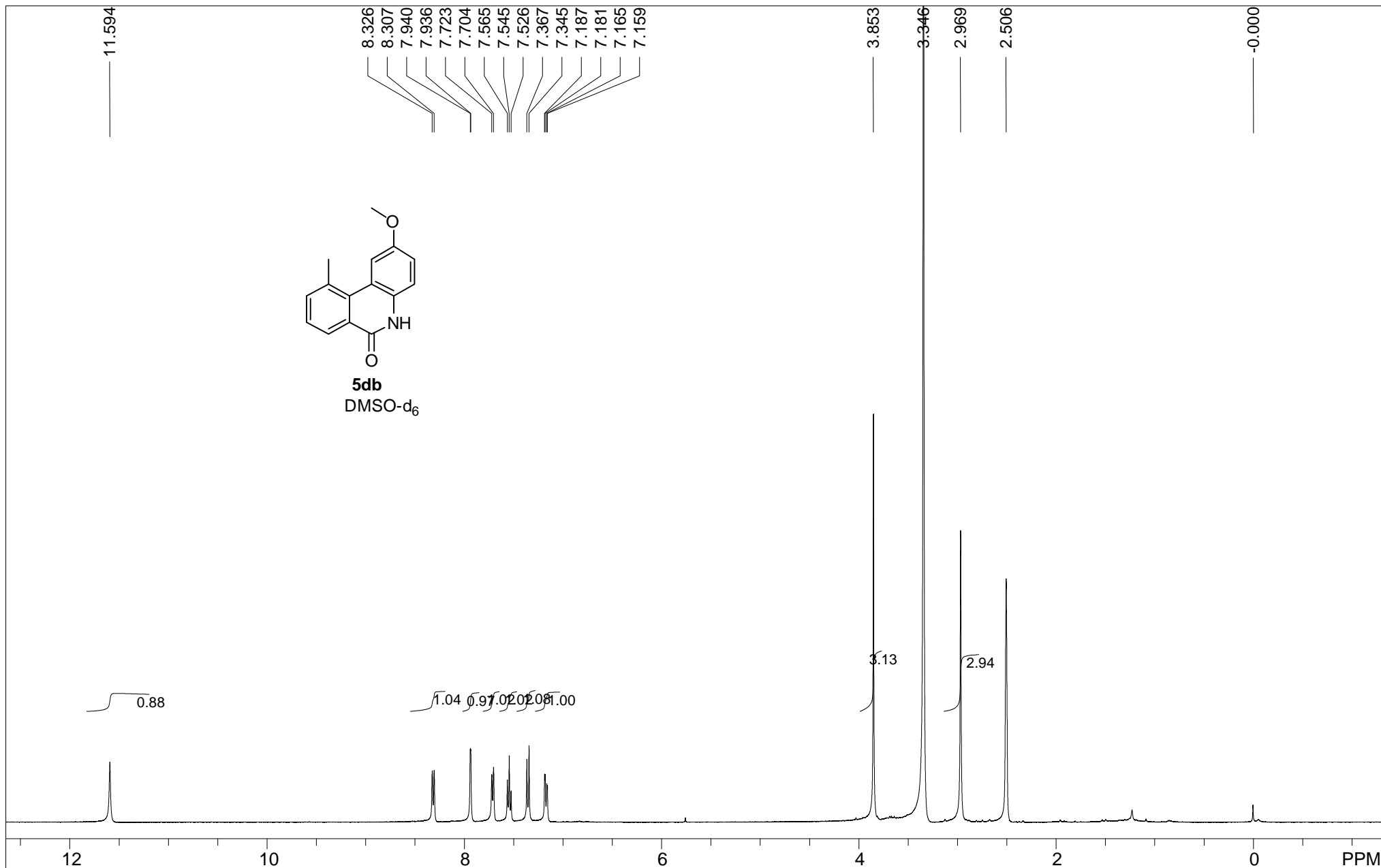
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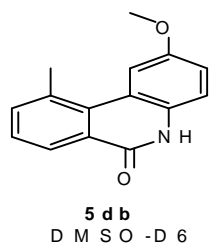
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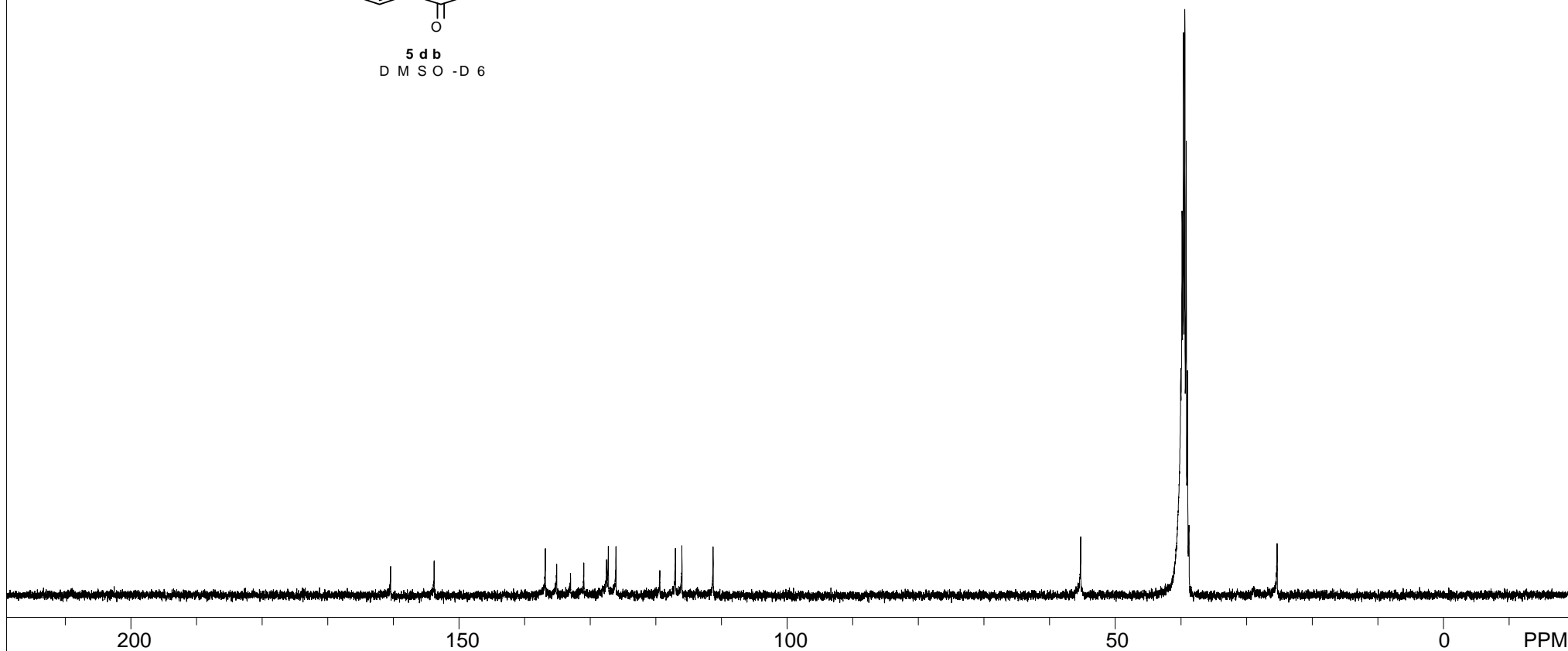
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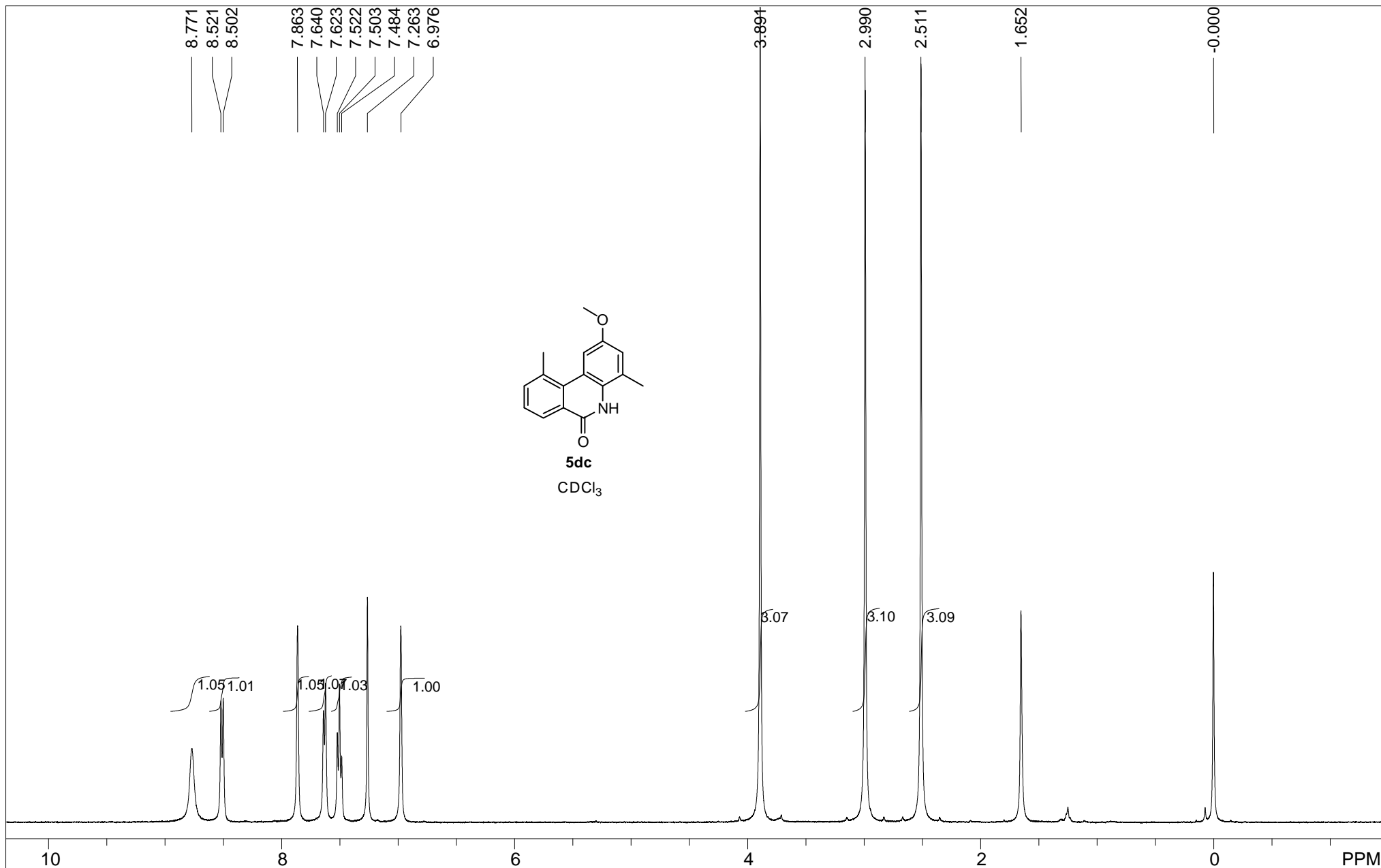
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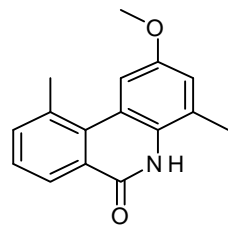
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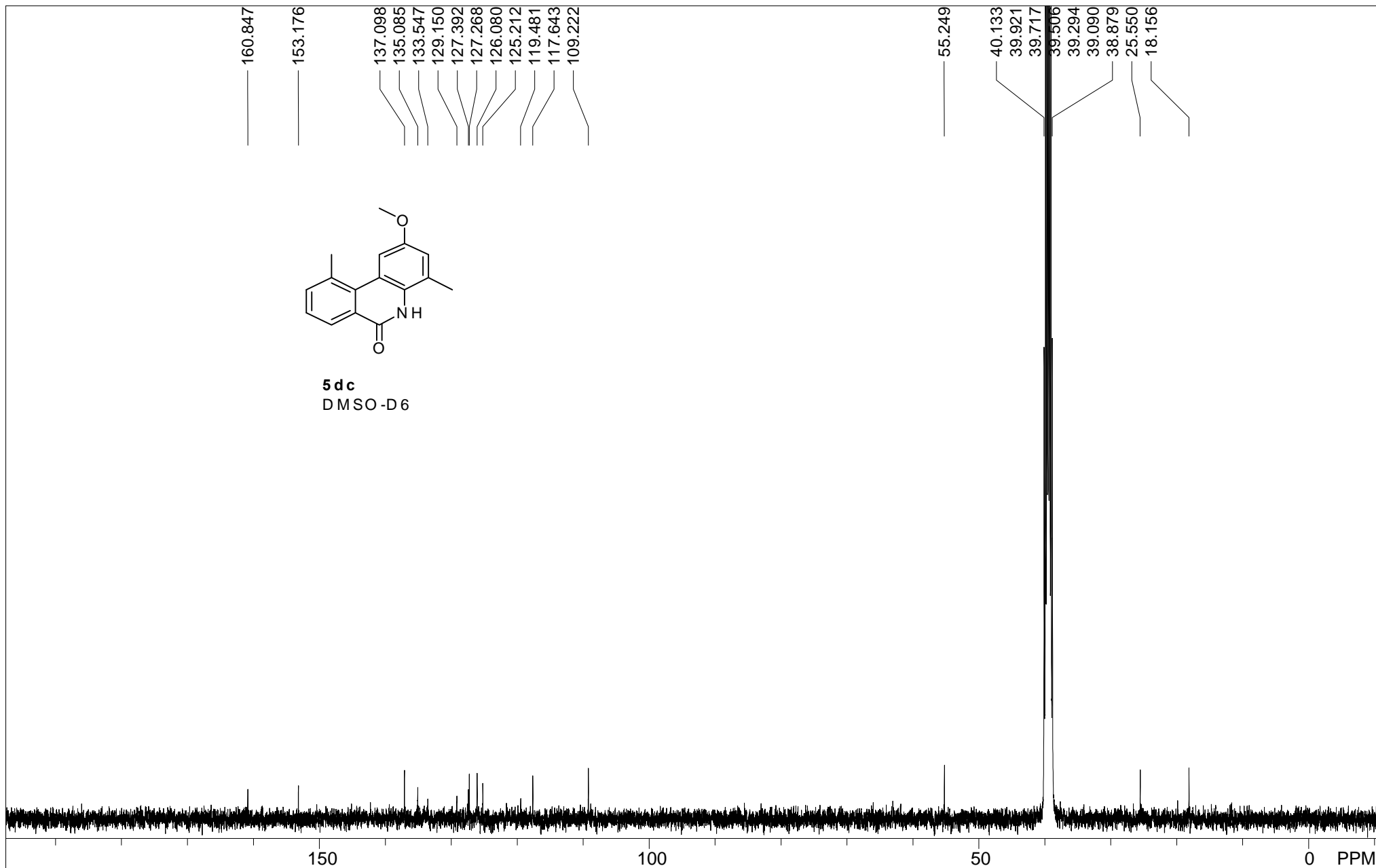


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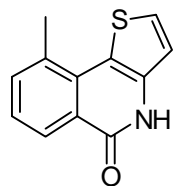


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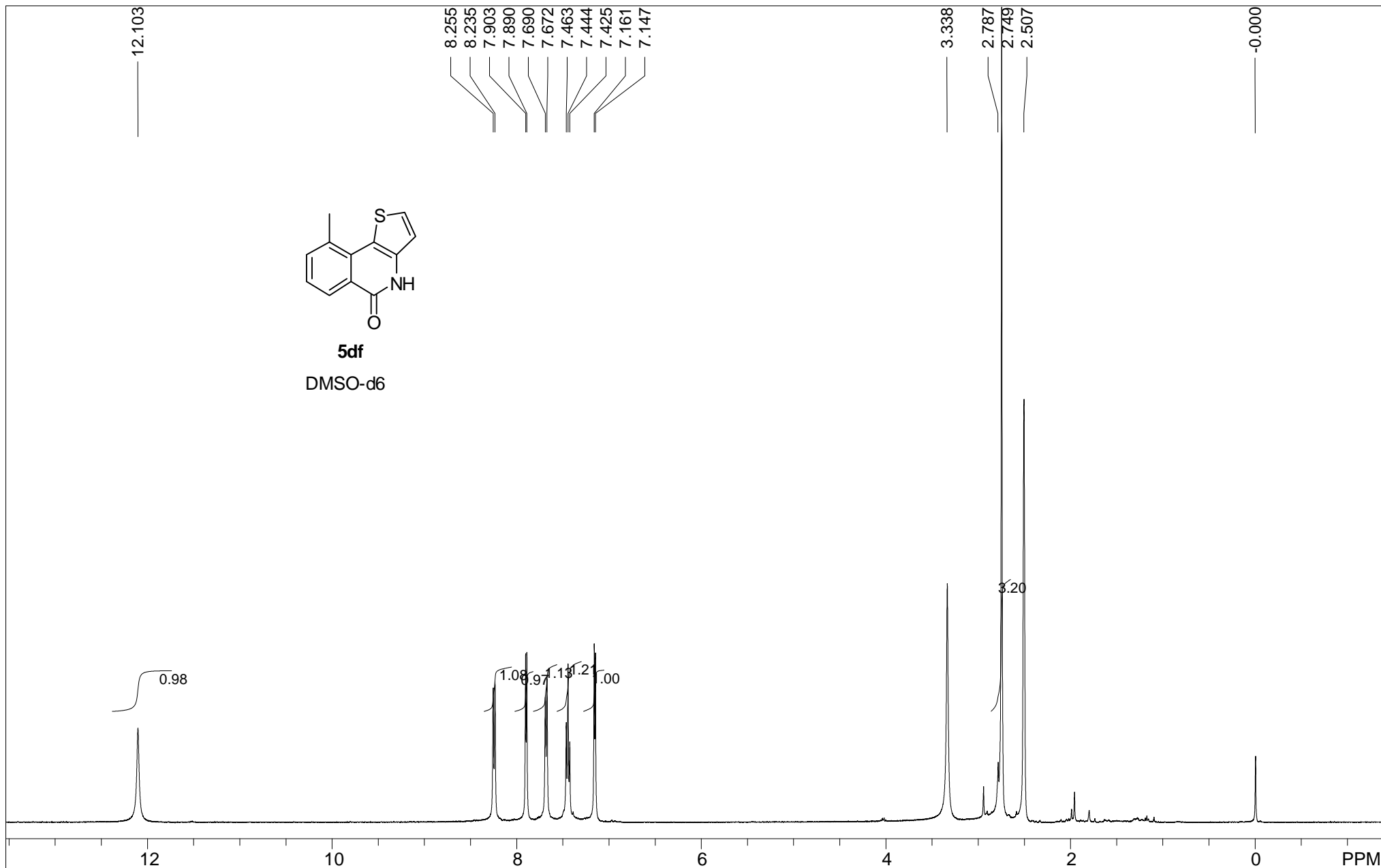


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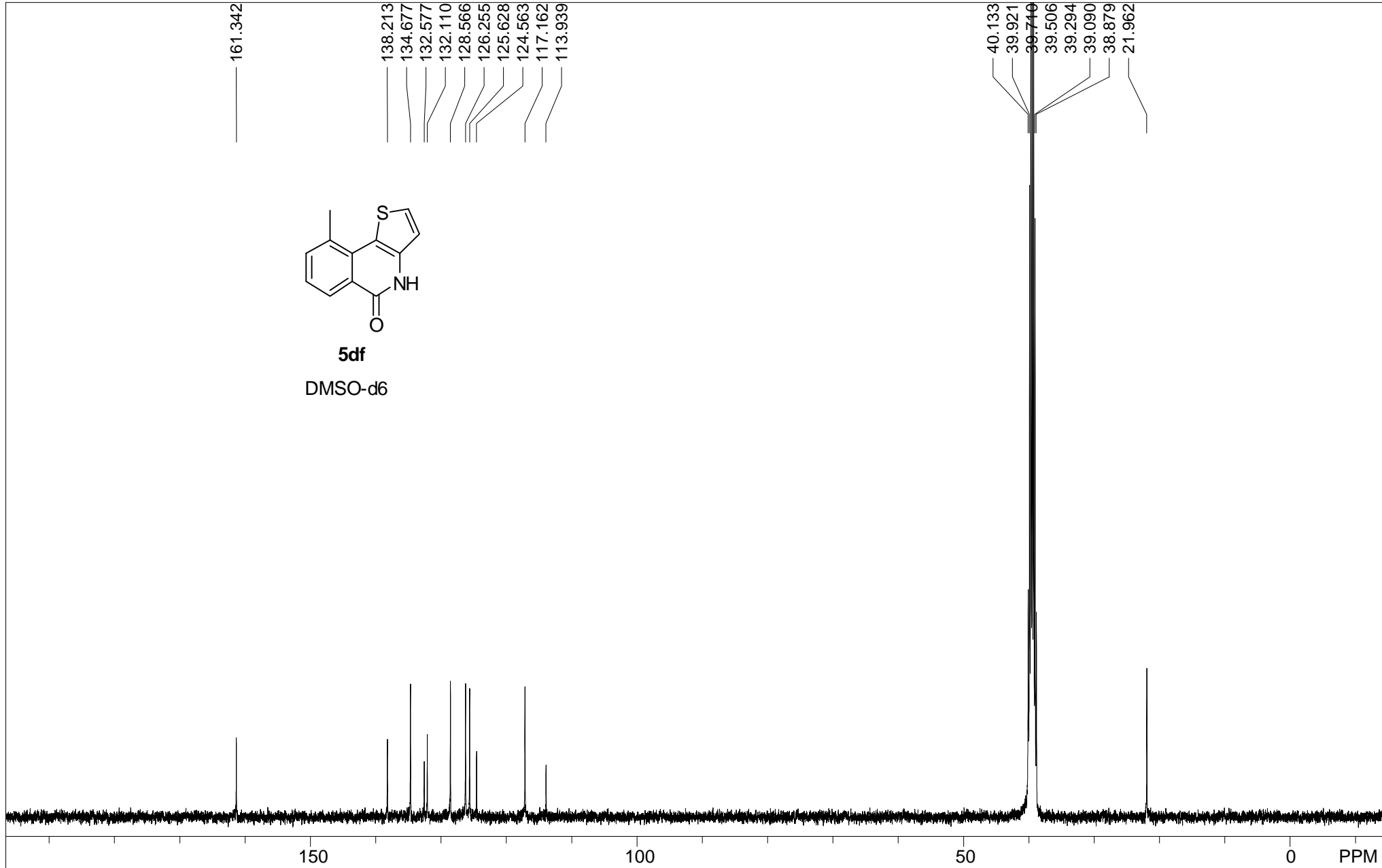


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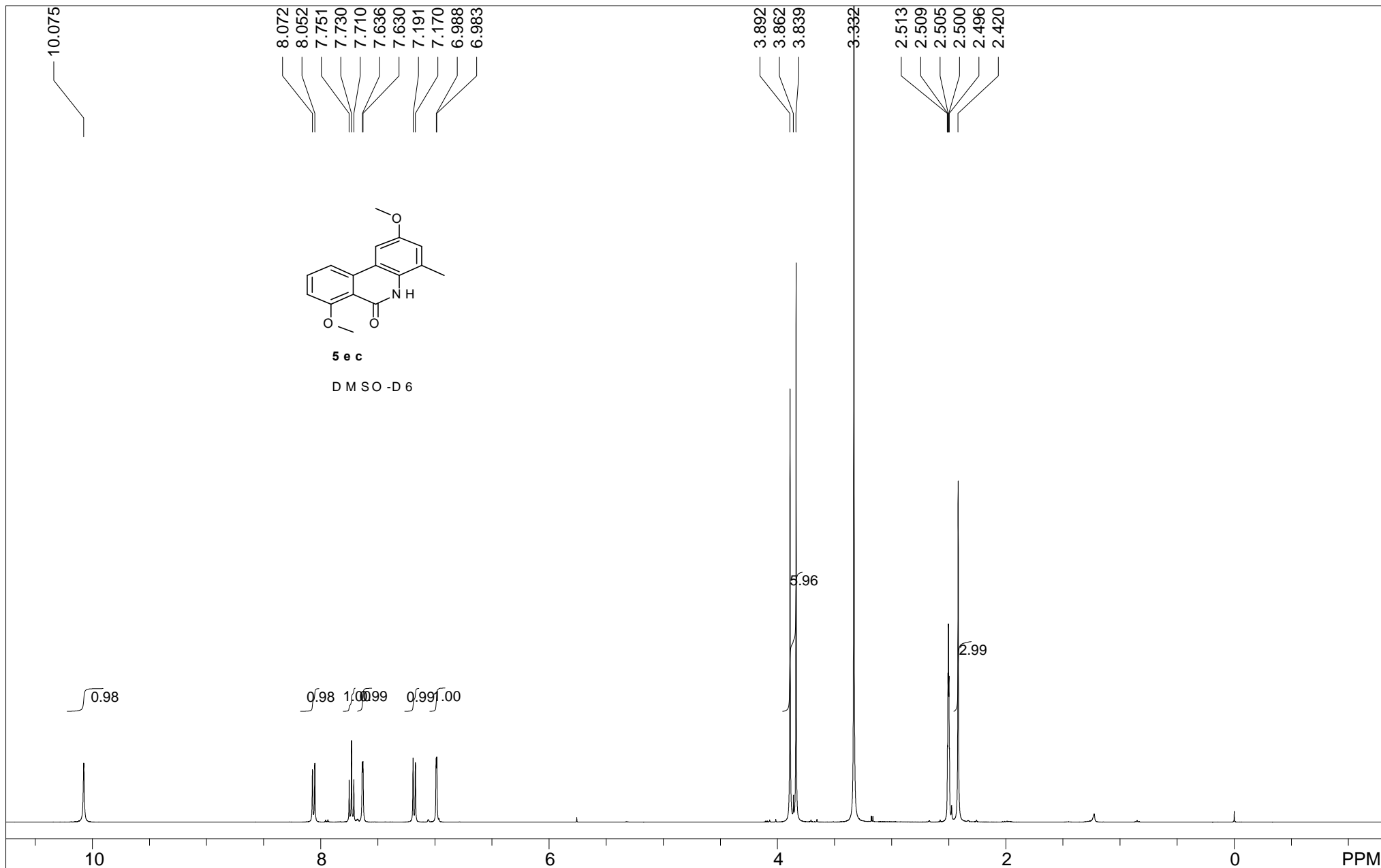
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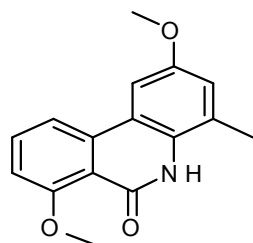
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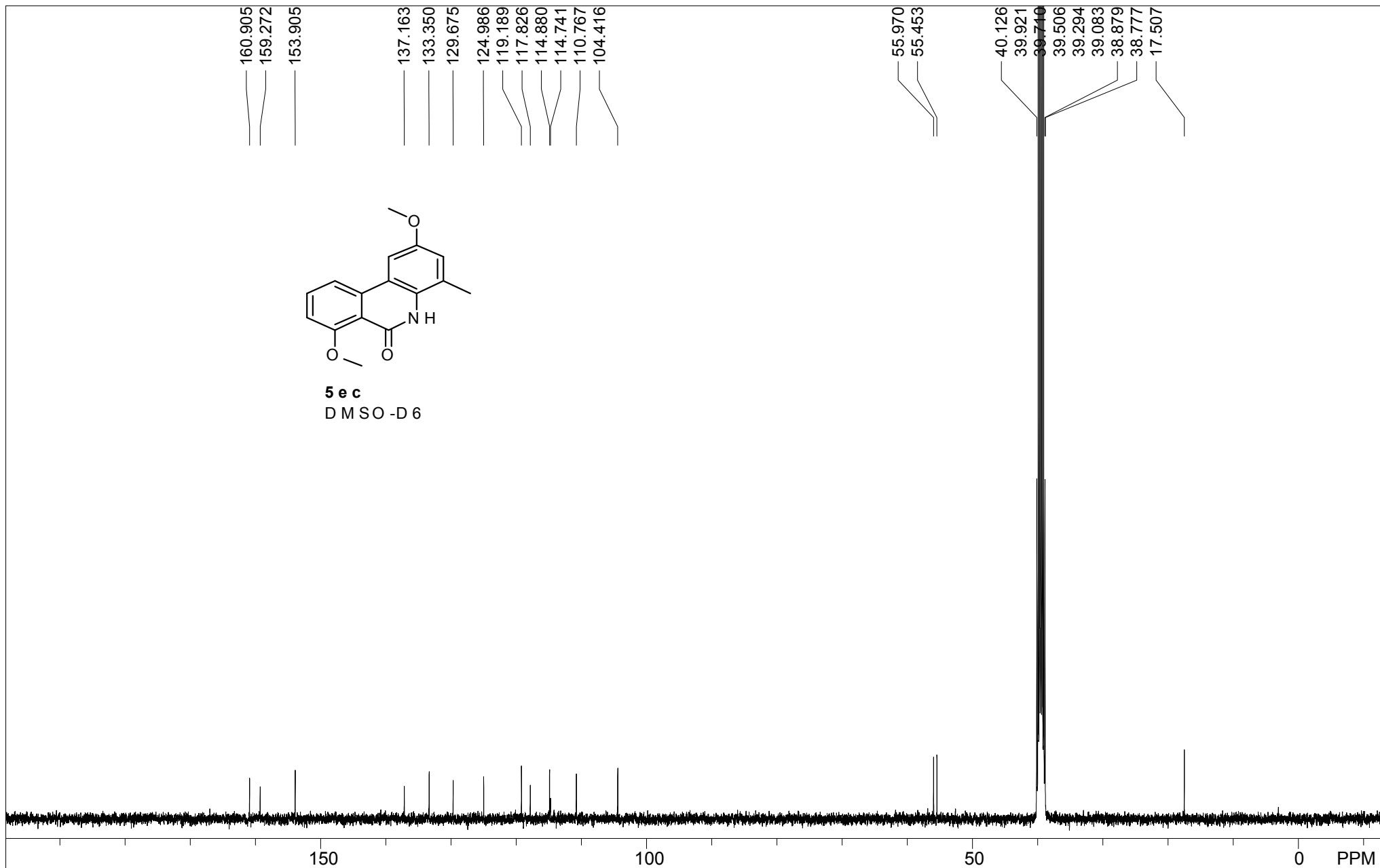


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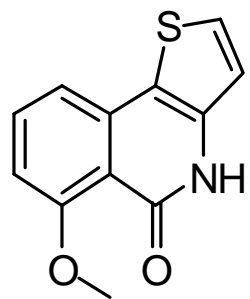


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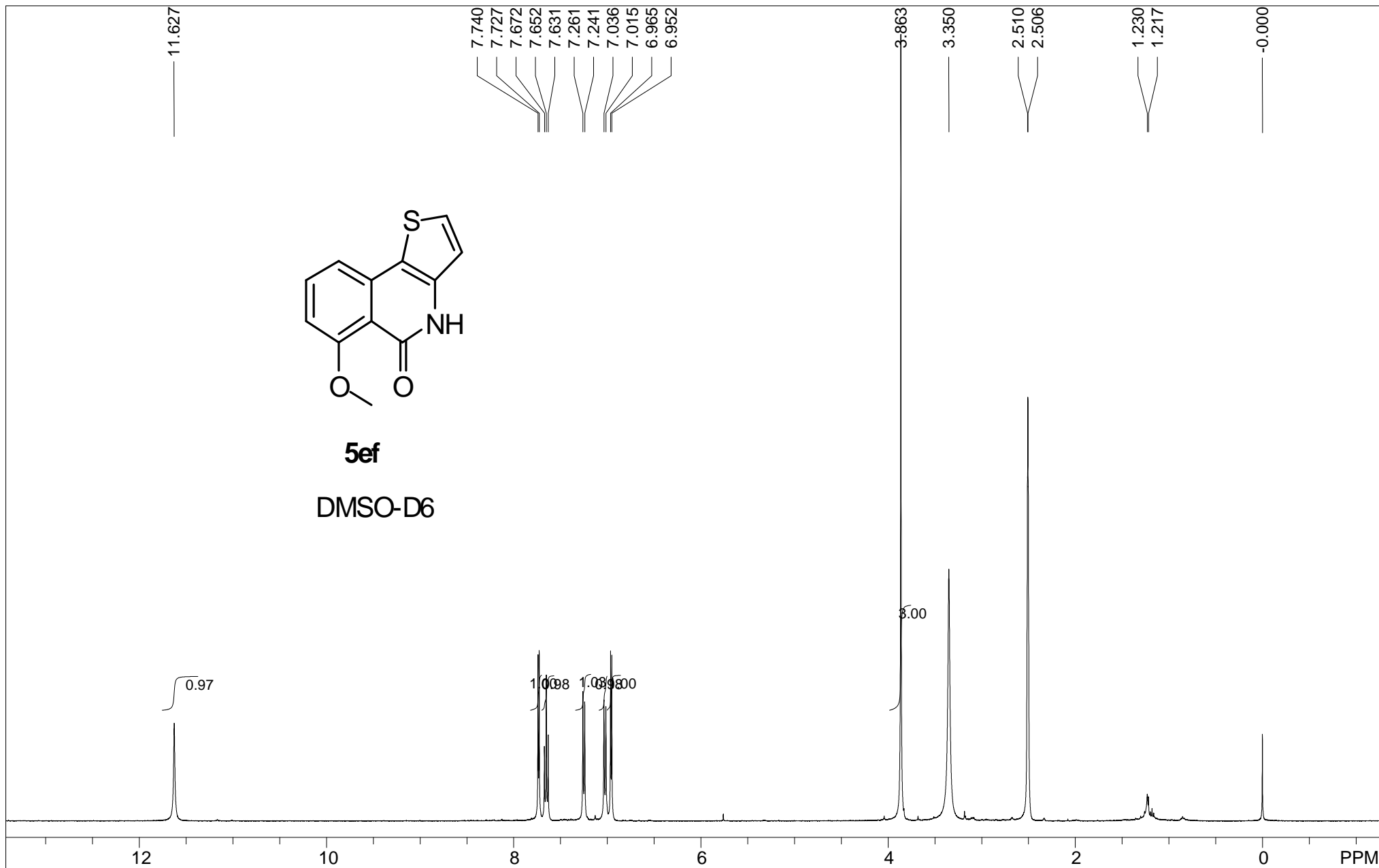
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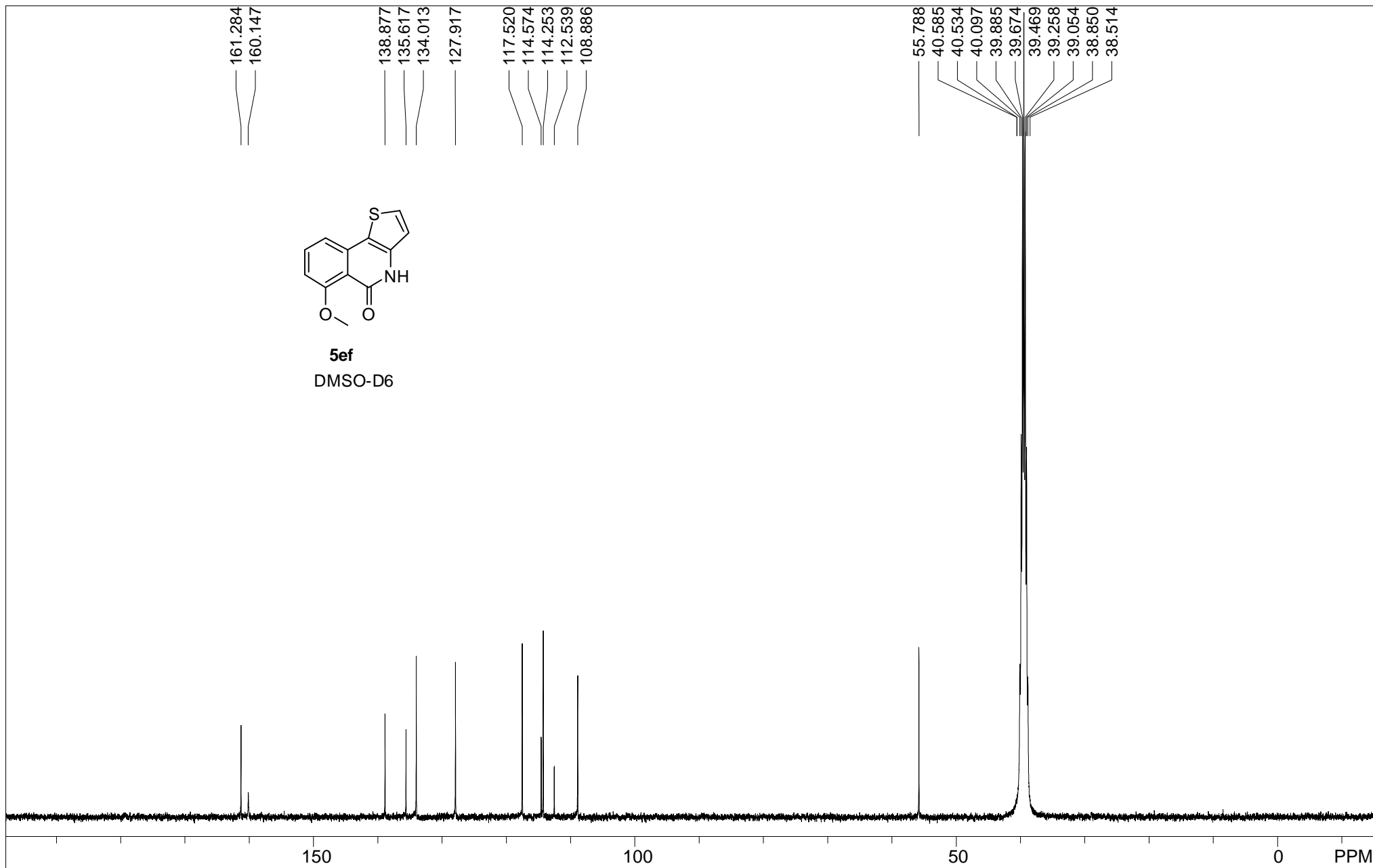
DMSO-D6



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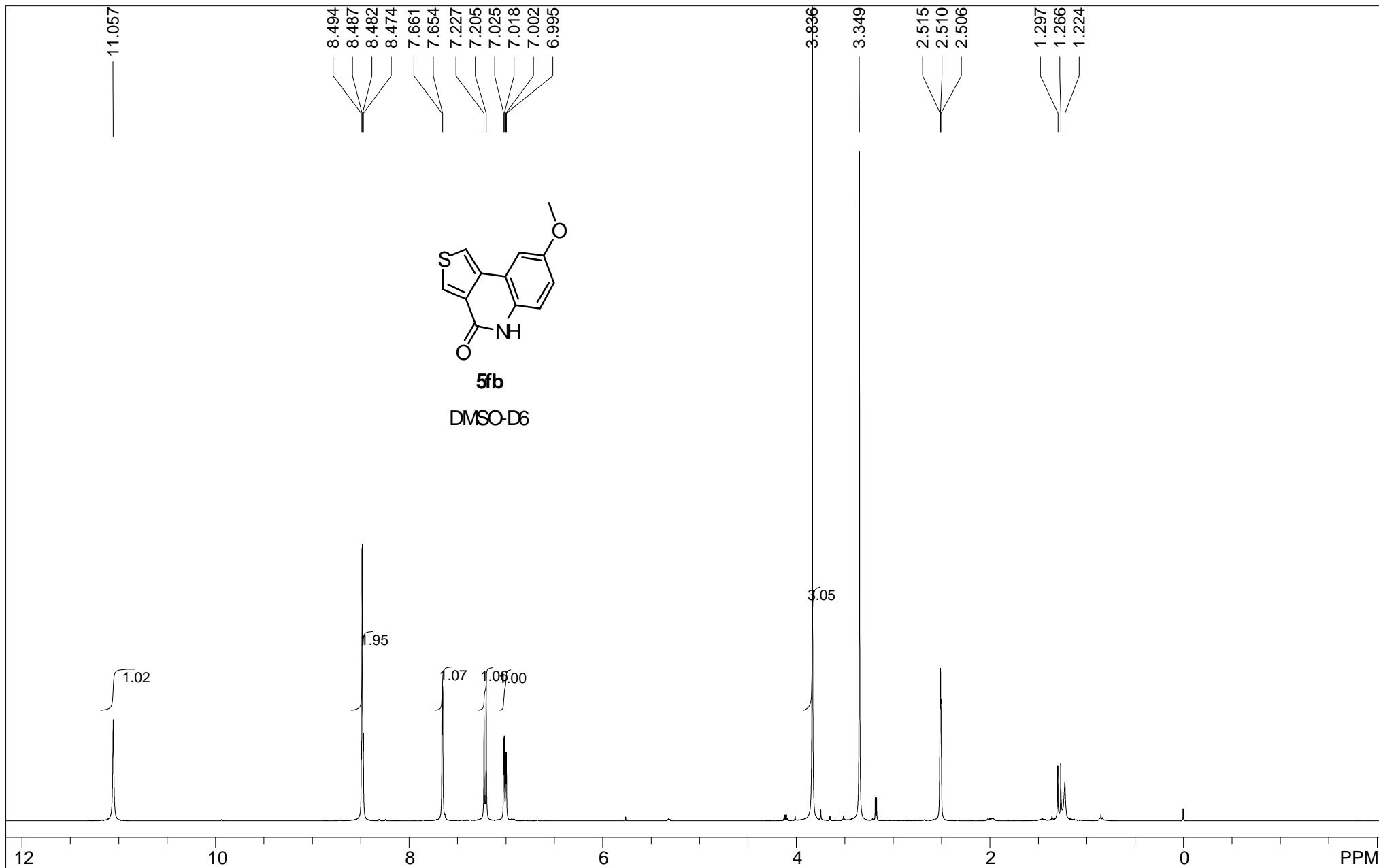
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DMSO-D6

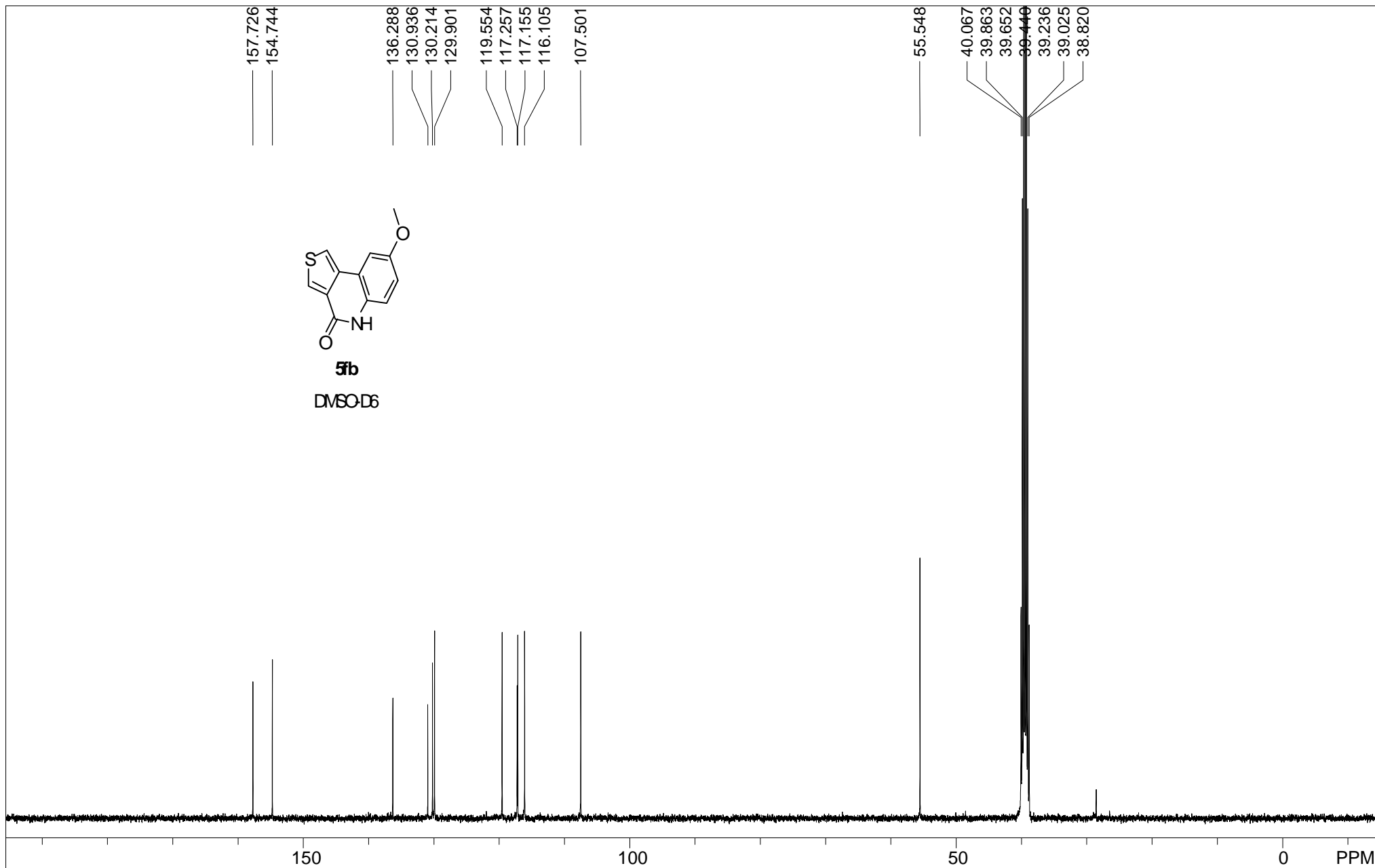
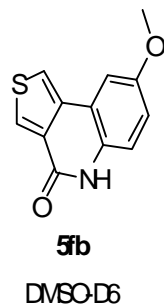
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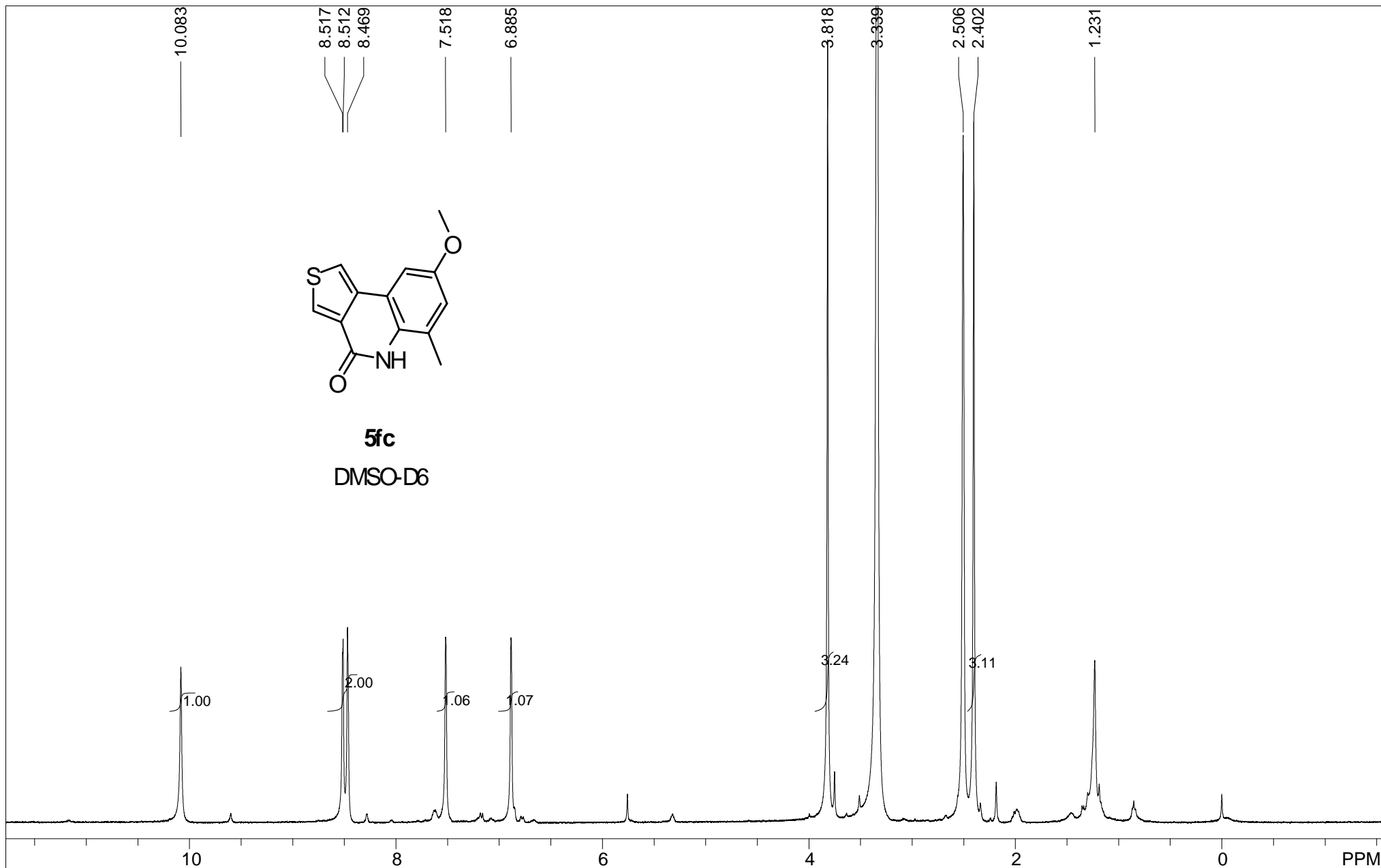
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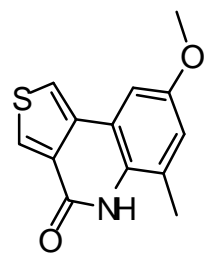
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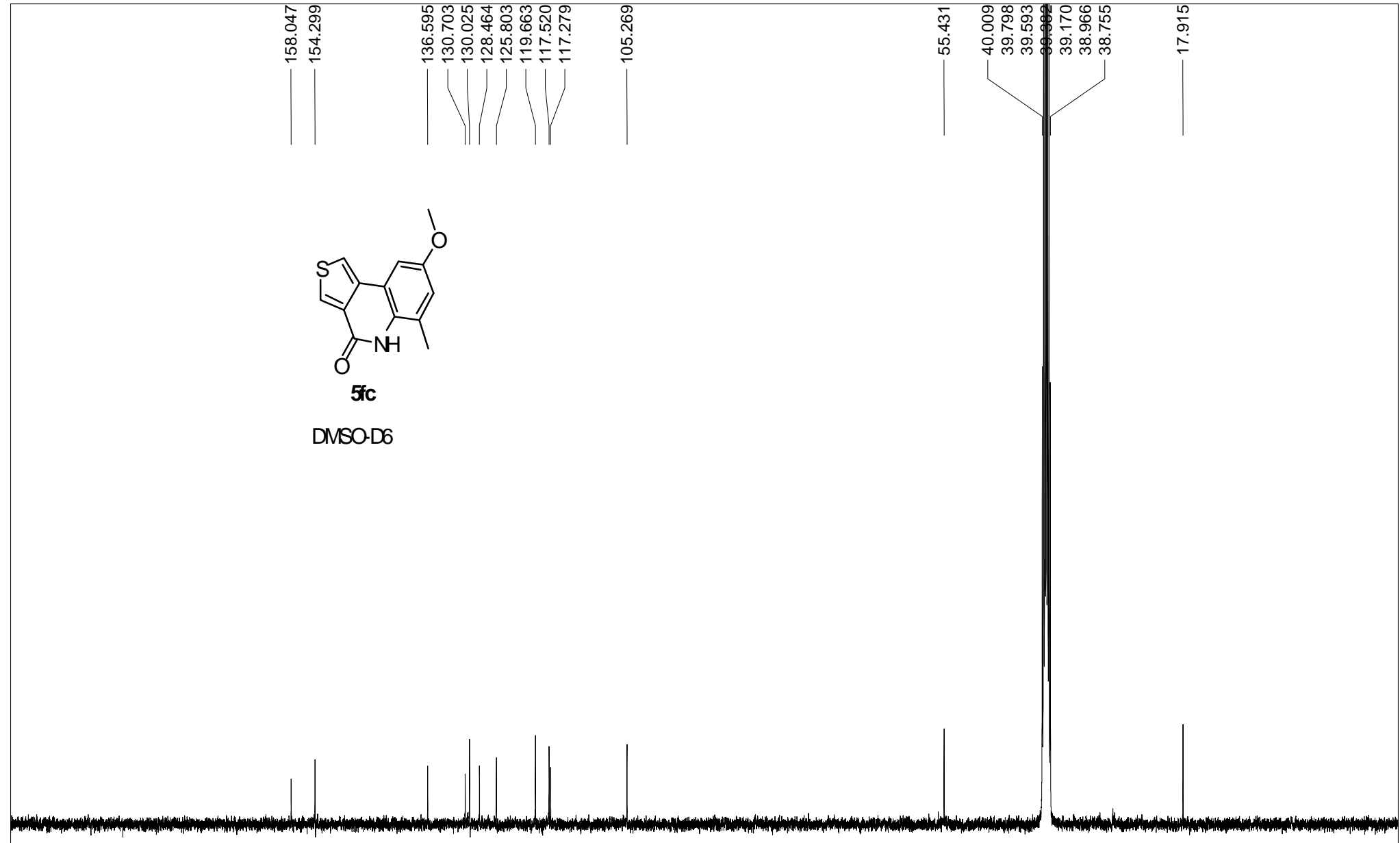


5c

DMSO-D6

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150

100

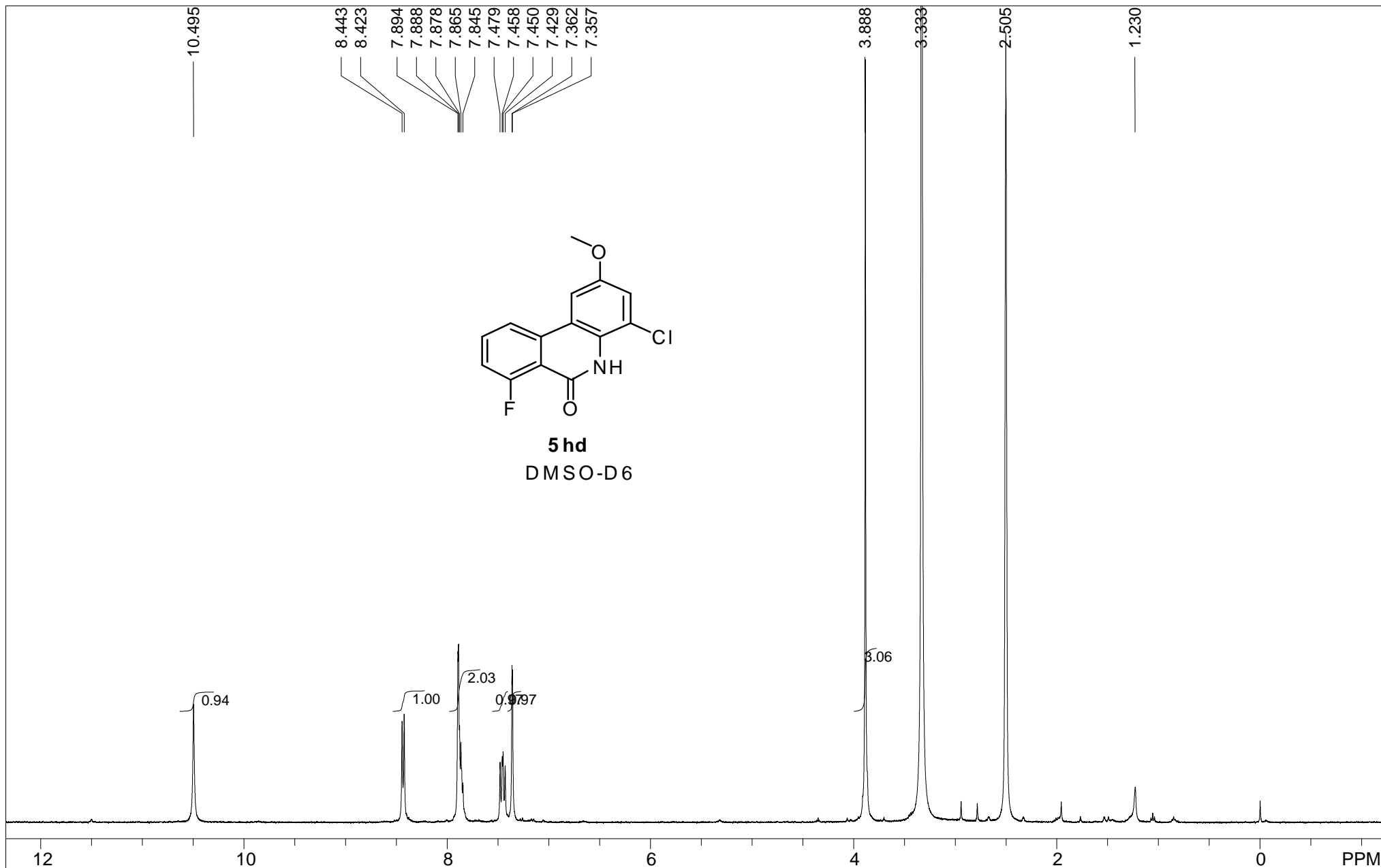
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PPM

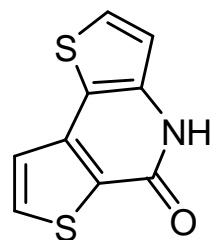
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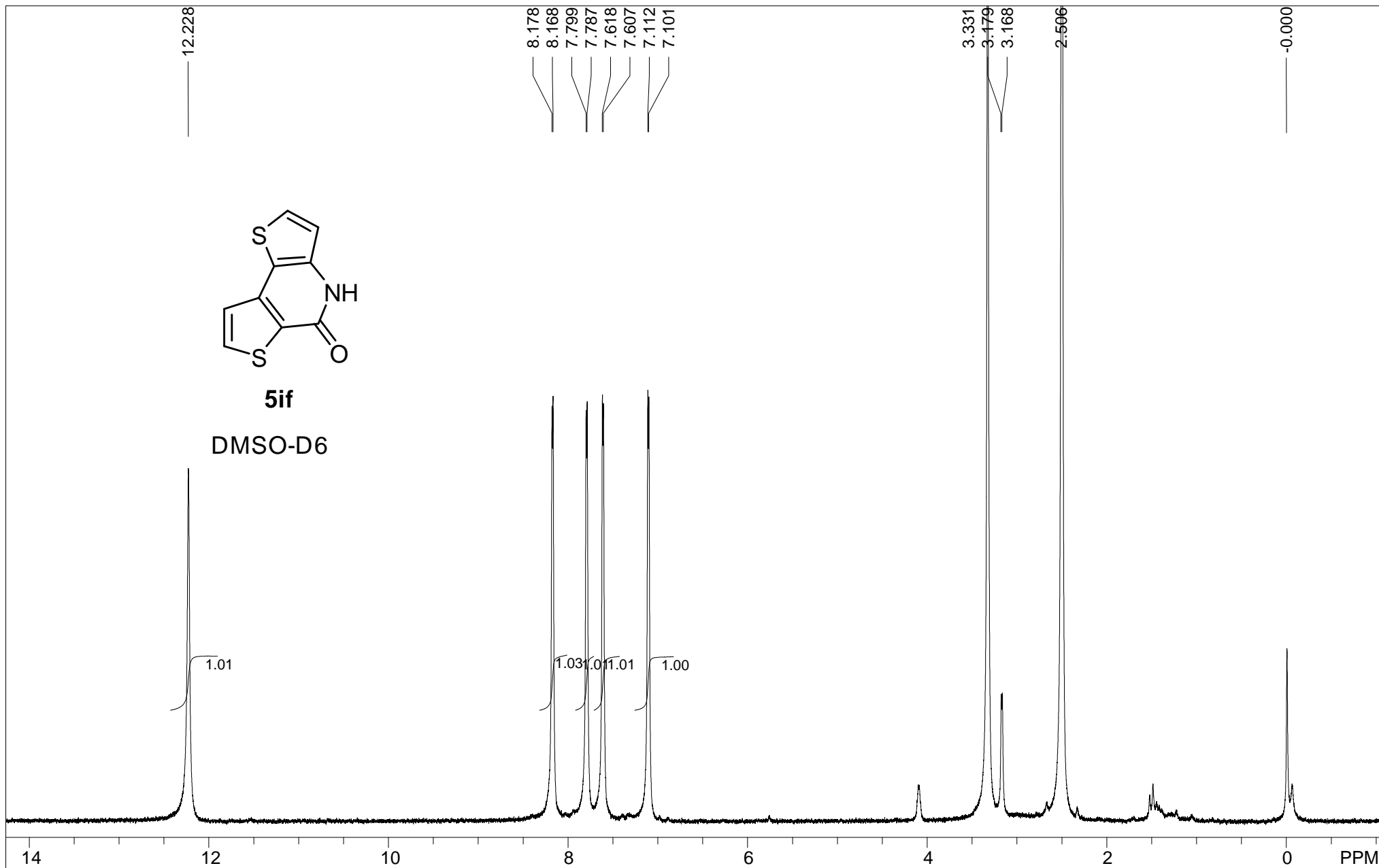
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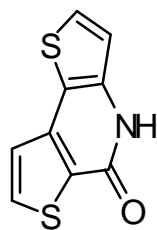


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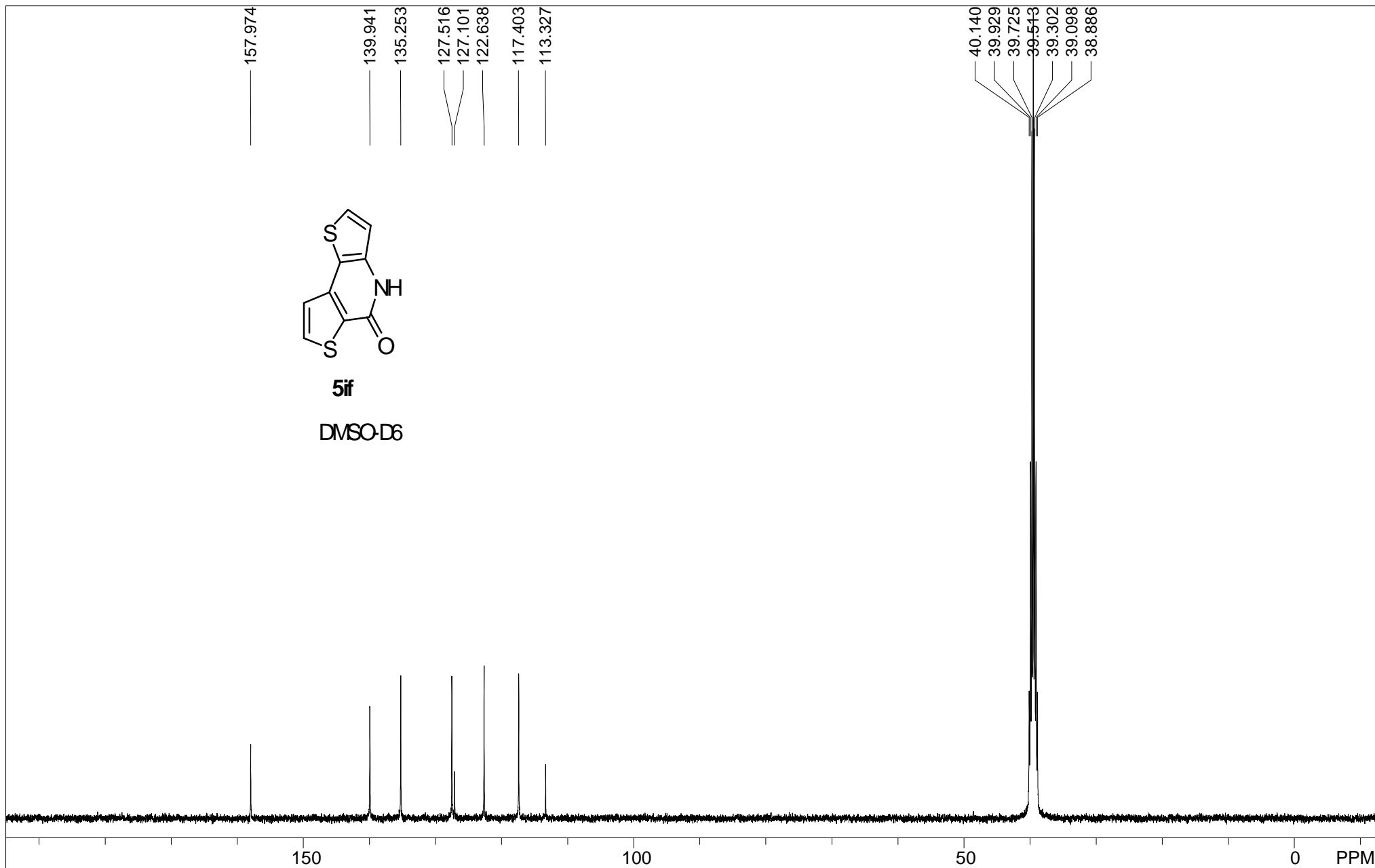


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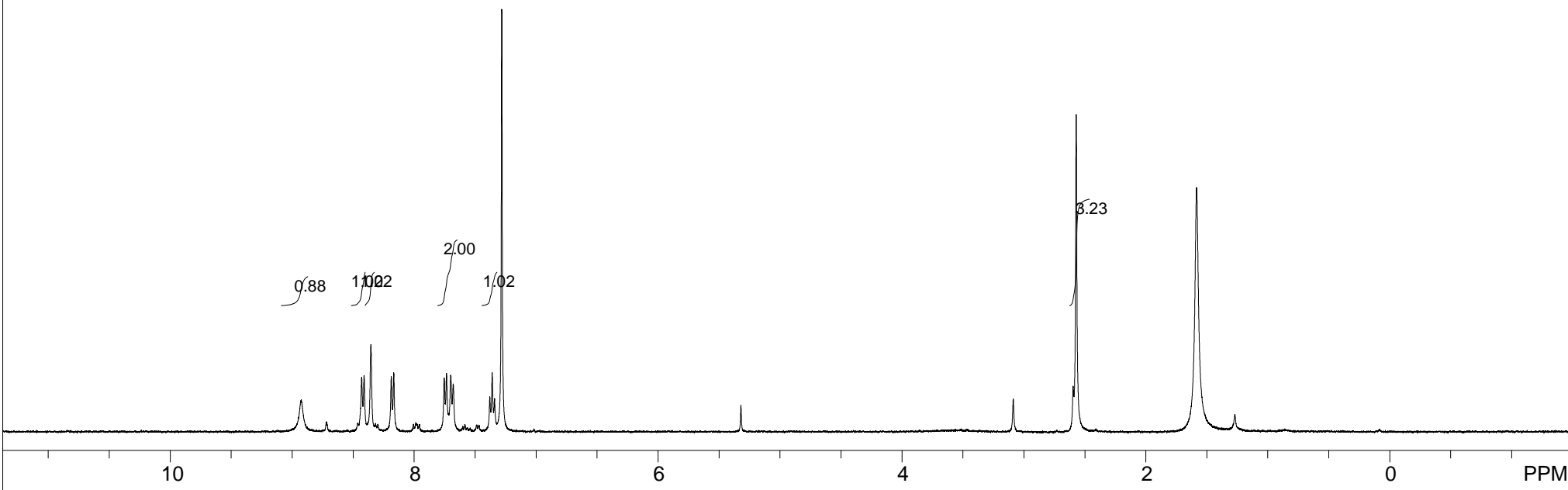
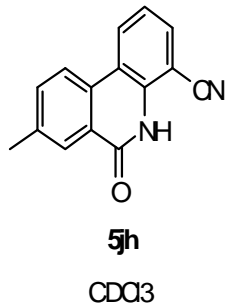
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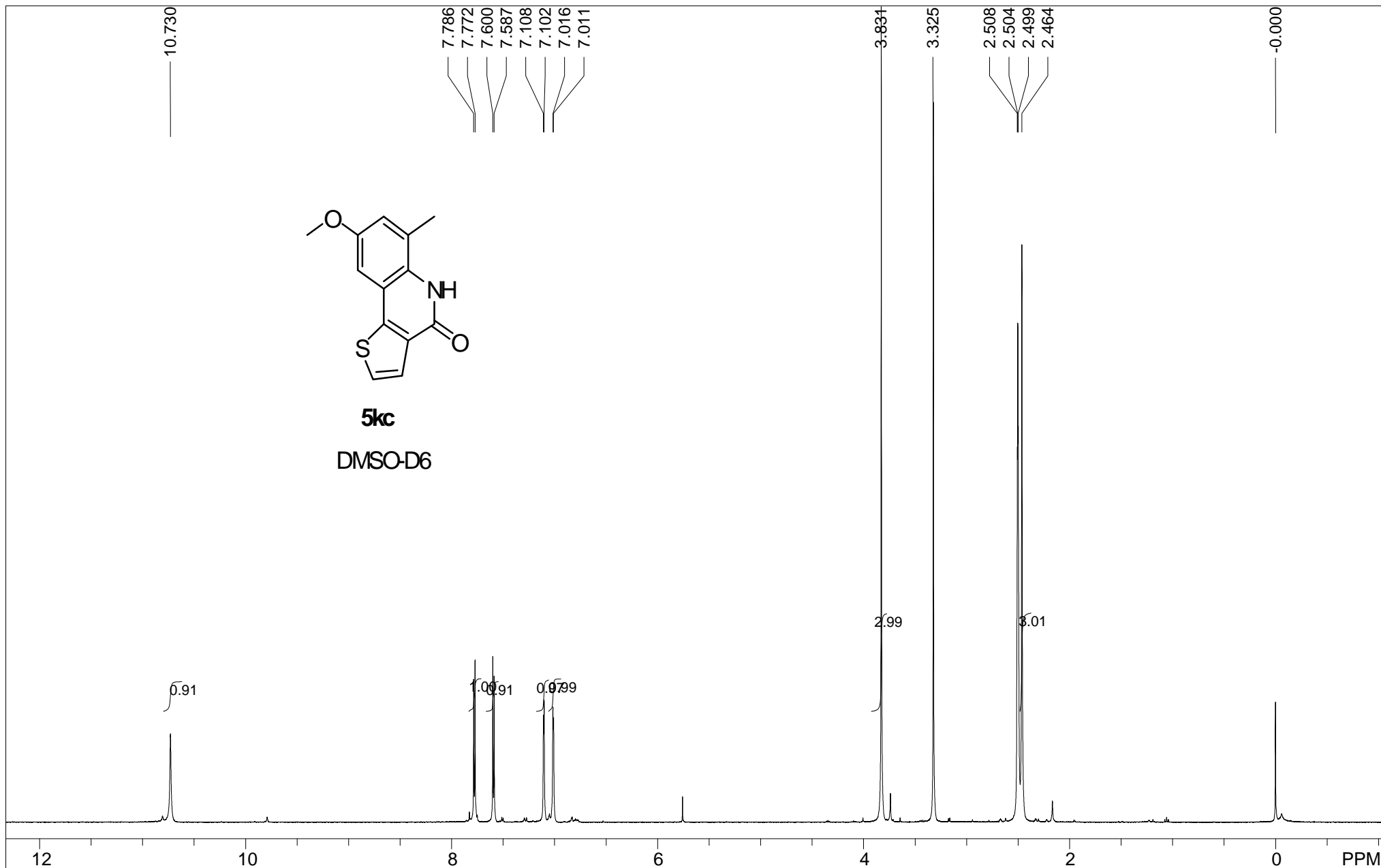
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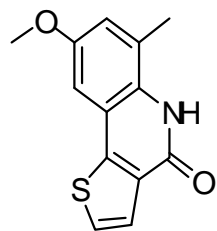


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F1: 400.160	F2: 1.000	SW1: 8224	PD: 1.0 sec	OF1: 3201.3	LB: 0.3	PTS1d: 65536
EX: zg30		PW: 12.8 us		NA: 16		Nuts - \$5jh-H1-CDCl3 10.1



USER: fx -- DATE: 2017-05-12 10:17:19.512

F1: 400.160	F2: 1.000	SW1: 8224	OF1: 3199.2	PTS1d: 65536
EX: zg30	PW: 12.8 us	PD: 1.0 sec	NA: 16	LB: 0.3
				Nuts - \$5kc-H1-DMSO 10.1

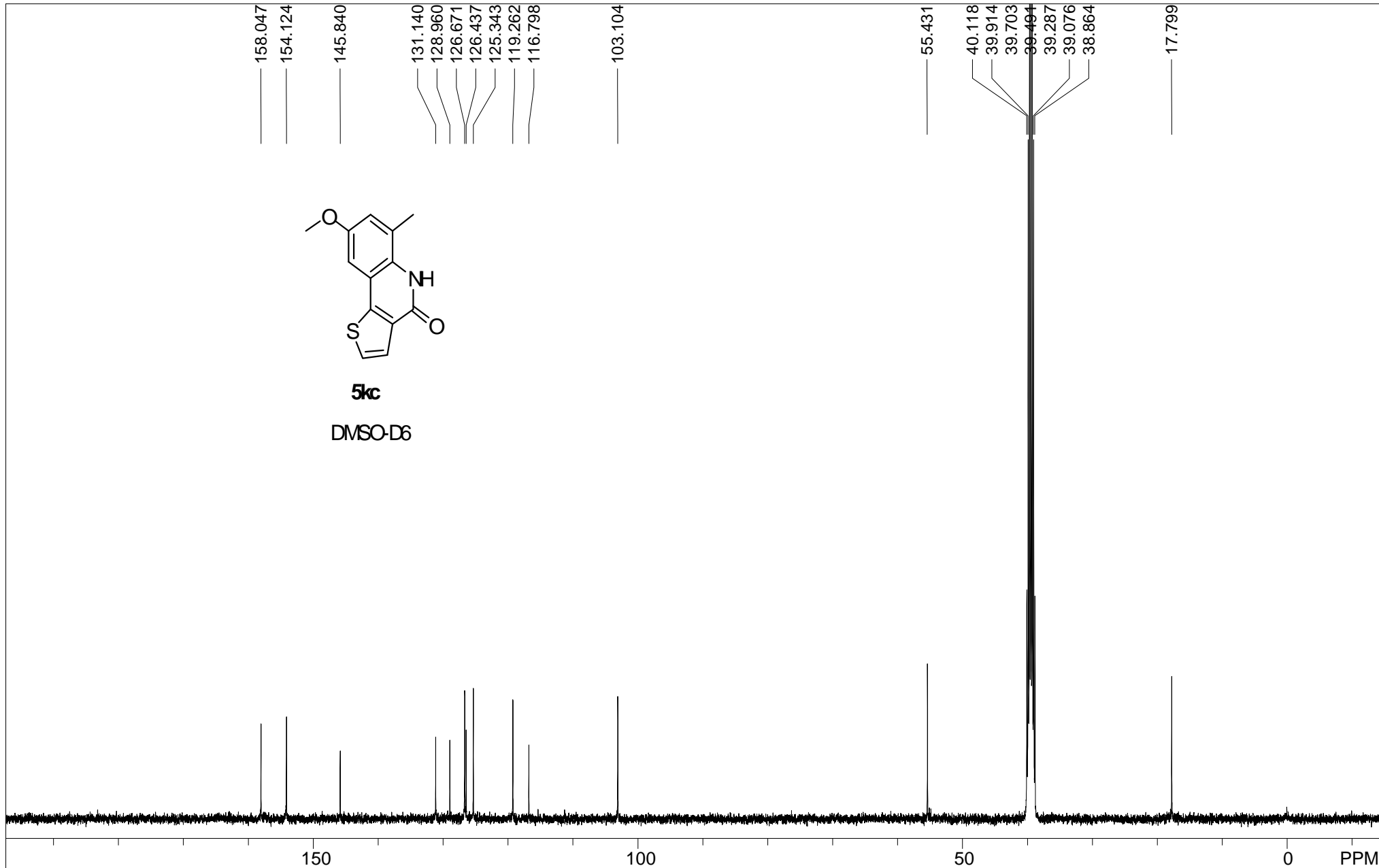


5kc

DMSO-D6

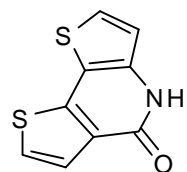
158.047
154.124
145.840
131.140
128.960
126.671
126.437
125.343
119.262
116.798
103.104

55.431
40.118
39.914
39.703
39.494
39.287
39.076
38.864
17.799



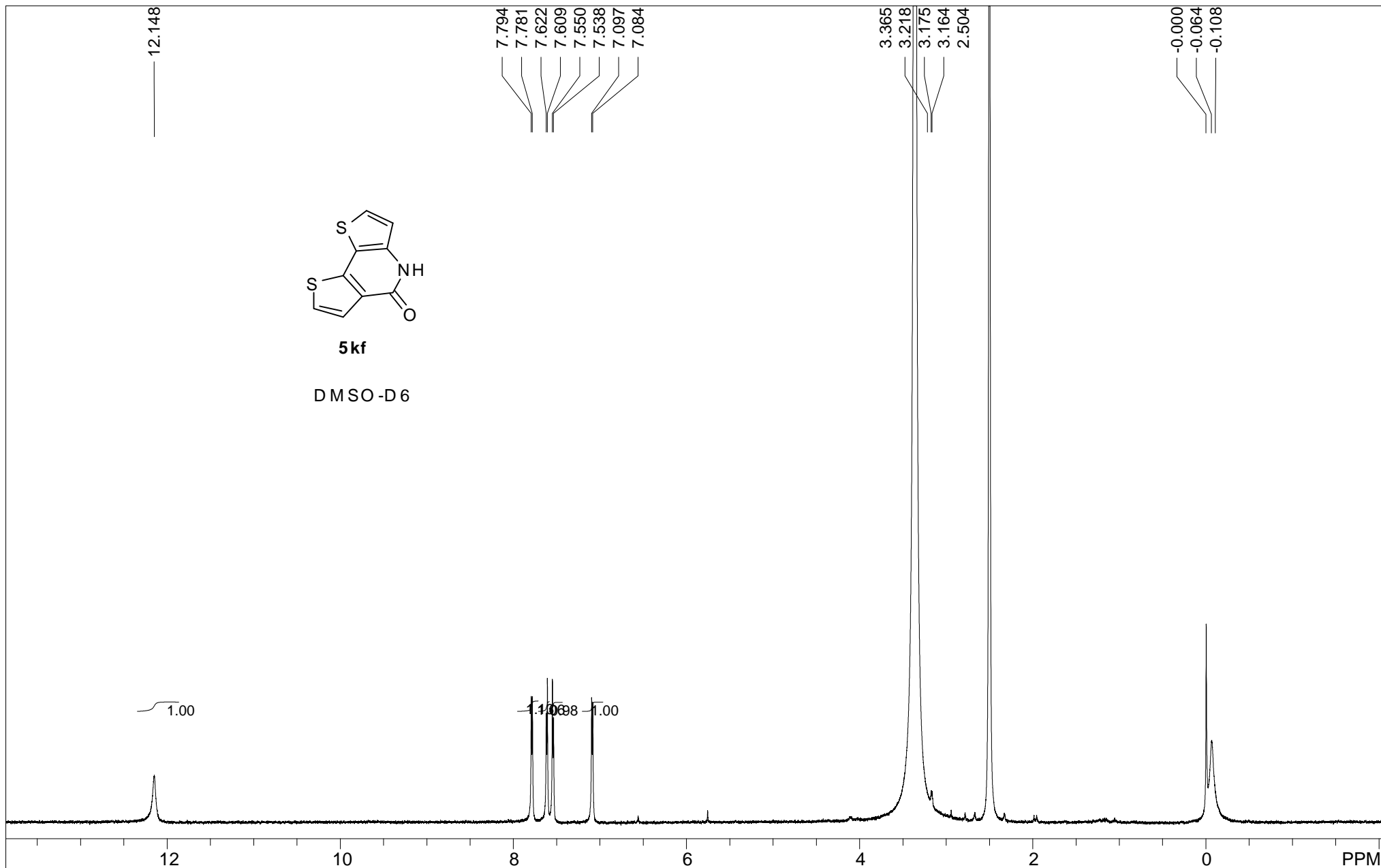
USER: fx -- DATE: 2017-05-13 00:56:44.436

F1: 100.620	F2: 1.000	SW1: 24038	OF1: 10011.3	PTS1d: 32768
EX: zgpg30	PW: 9.0 us	PD: 2.0 sec	NA: 1024	LB: 1.0 Nuts - \$SP-0011167-5kc-C13-DMSO-20170512-CT54 10.1



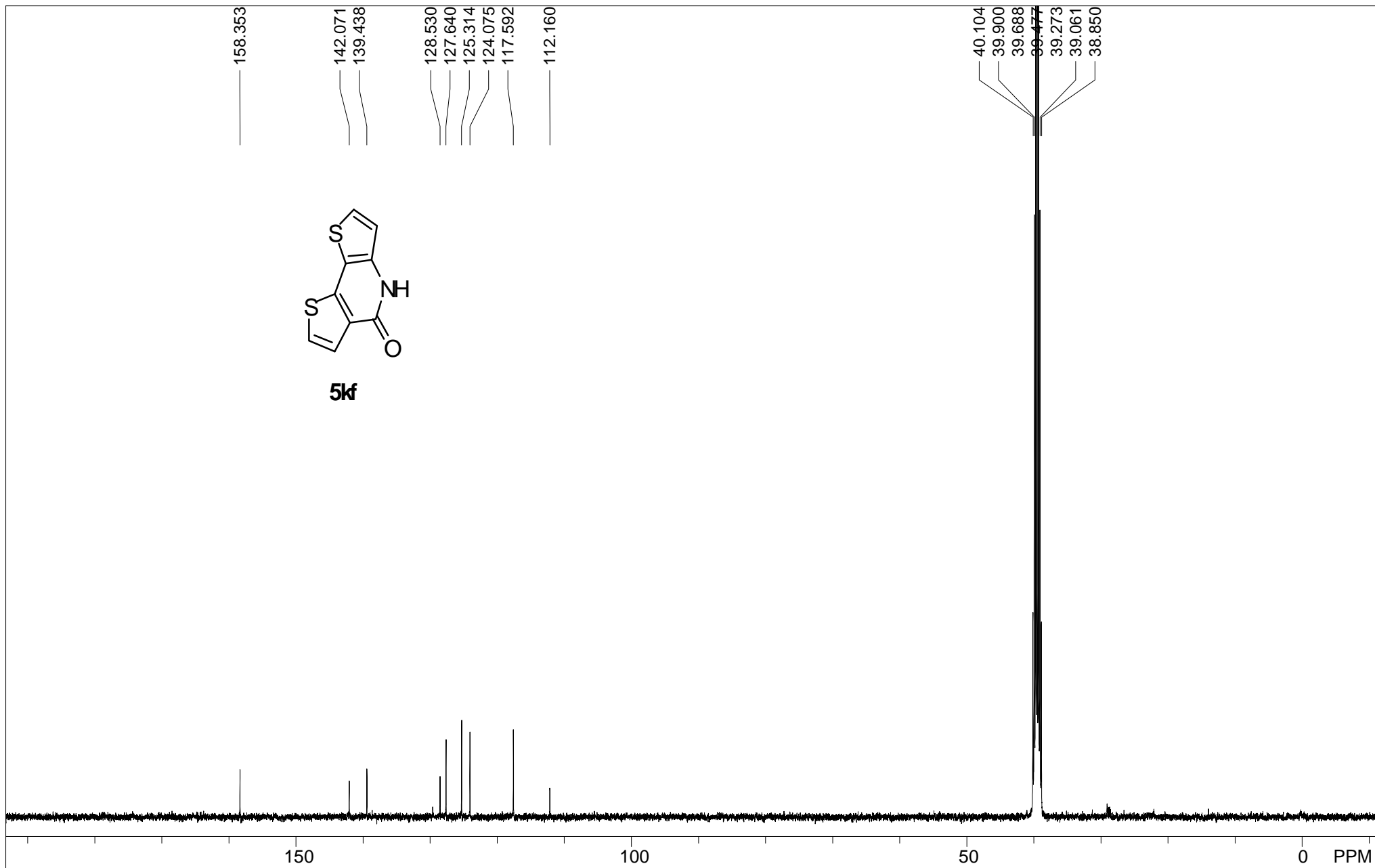
5kf

DMSO-D6



USER: fx -- DATE: 2017-05-31 12:03:36.364

F1: 400.160	F2: 1.000	SW1: 8224	OF1: 3199.9	PTS1d: 65536
EX: zg30	PW: 12.8 us	PD: 1.0 sec	NA: 16	LB: 0.3 Nuts - \$sp-0011167-5kf-H1-DMSO-20170531-CT54 10.1



USER: fx -- DATE: 2017-06-02 23:30:55.292

F1: 100.620	F2: 1.000	SW1: 24038	OF1: 10011.3	PTS1d: 32768
EX: zpgg30	PW: 9.0 us	PD: 2.0 sec	NA: 1024	LB: 1.0 Nuts - \$SP-0011167-5kf-C13-DMSO-20170602-CT54 10.1

10.912

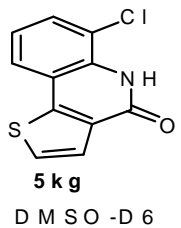
7.877
7.865
7.855
7.655
7.645
7.633
7.285
7.265
7.246

3.331

2.505

1.240

-0.000



0.95

1.91
1.88
1.00

10

8

6

4

2

0

PPM

USER: fx -- DATE: 2017-05-24 12:11:54.260

F1: 400.160

F2: 1.000

SW1: 8224

OF1: 3199.4

PTS1d: 65536

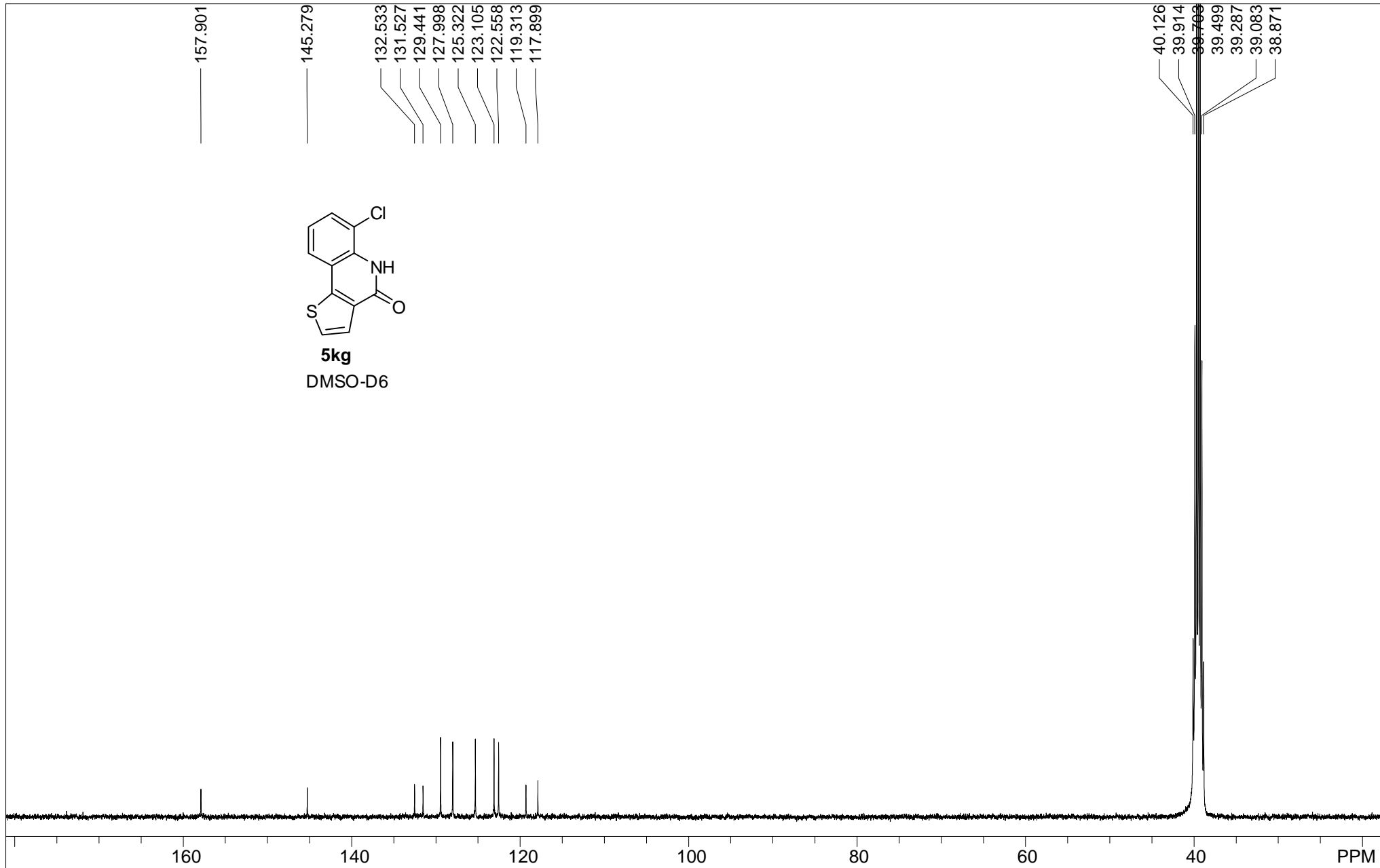
EX: zg30

PW: 12.8 us

PD: 1.0 sec

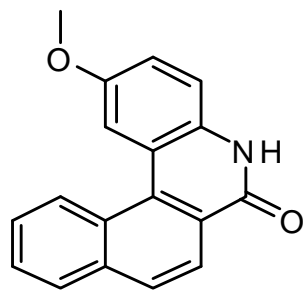
NA: 16

LB: 0.3 Nuts - \$SP-0011167-5KG-H1-DMSO-20170524-CT54 10.1

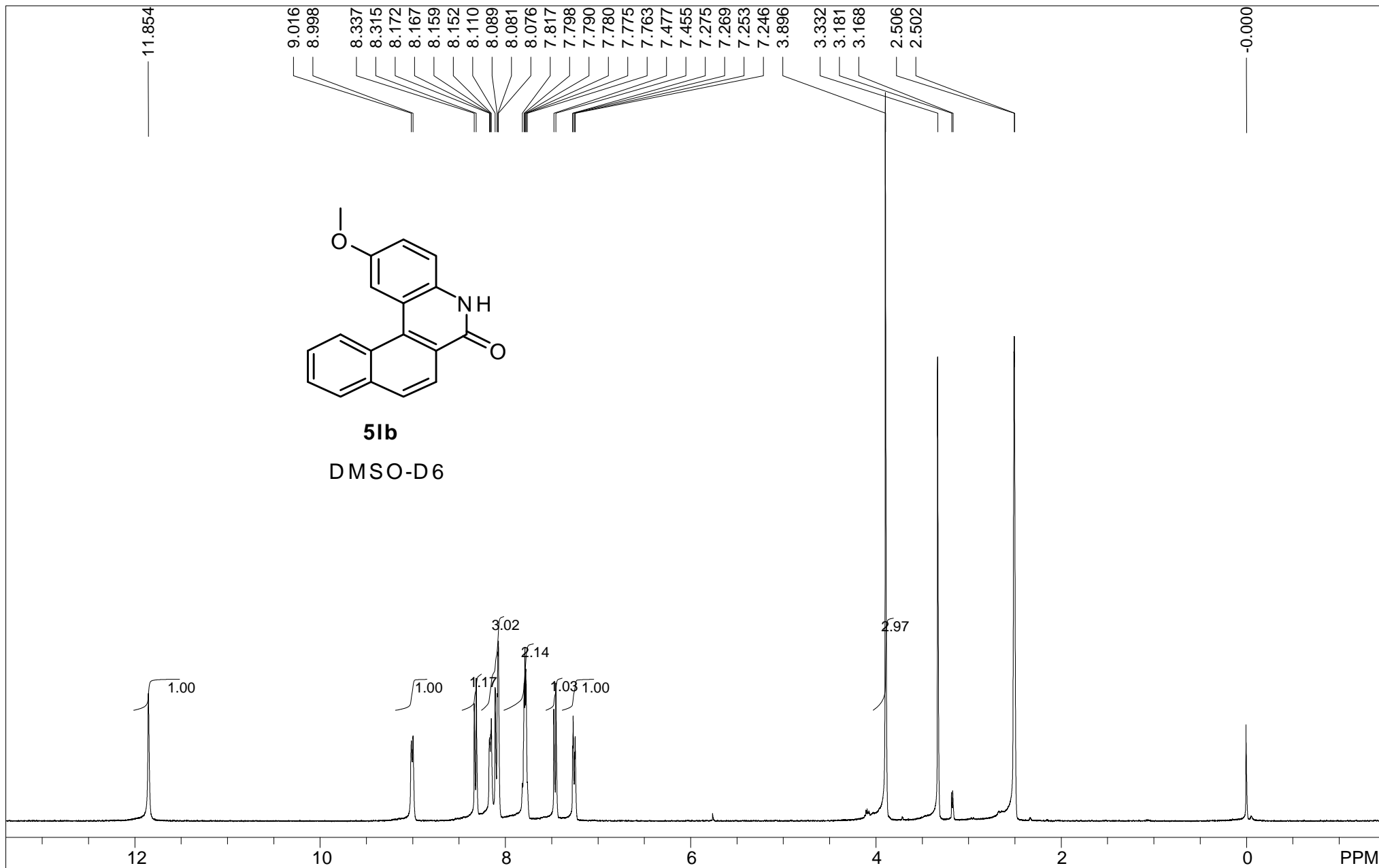


USER: fx -- DATE: 2017-05-26 02:25:40.231

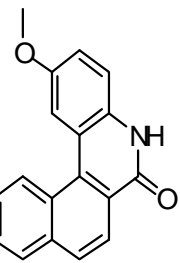
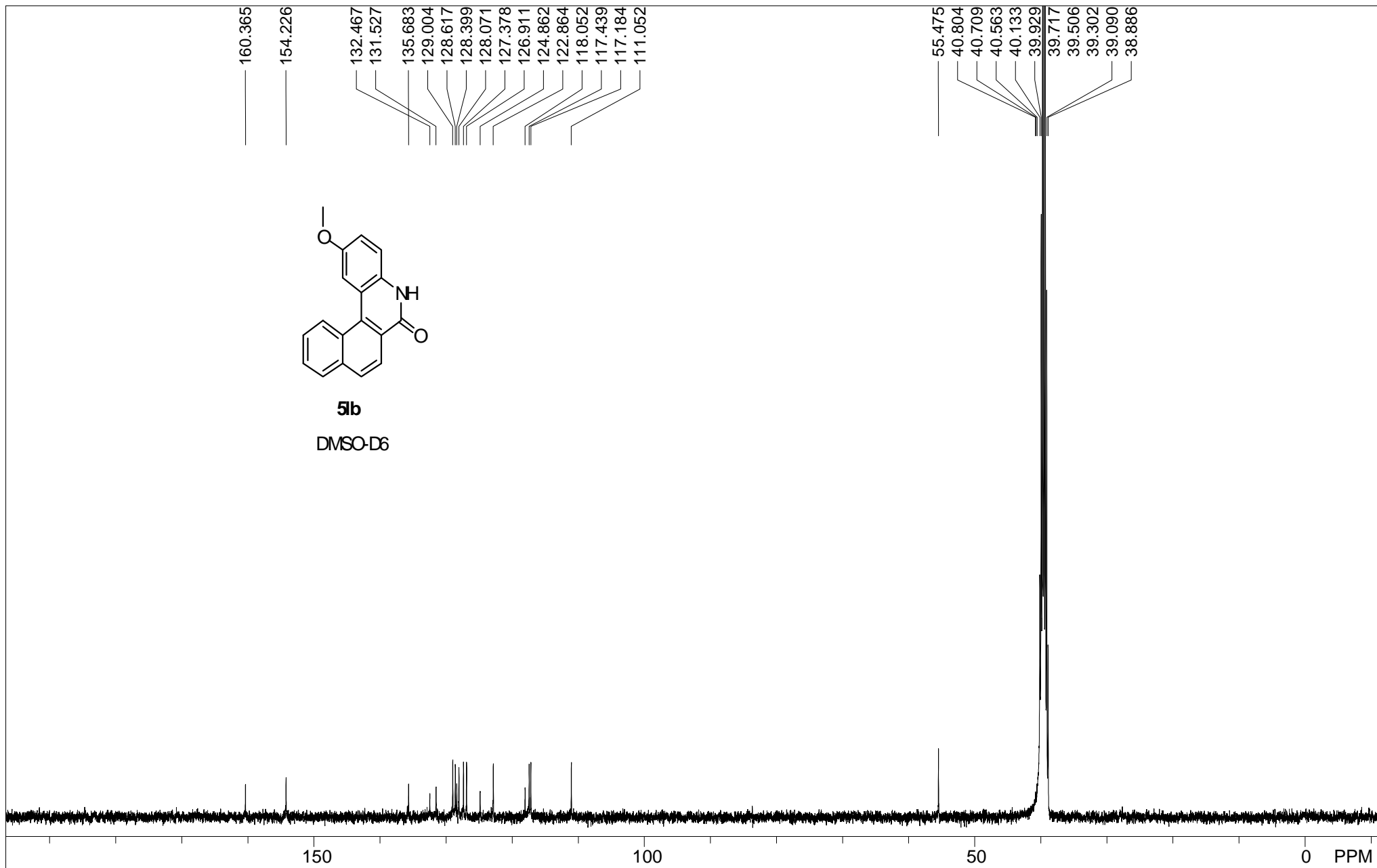
F1: 100.620	F2: 1.000	SW1: 24038	OF1: 10011.3	PTS1d: 32768
EX: zpgp30	PW: 9.0 us	PD: 2.0 sec	NA: 1024	LB: 1.0 Nuts - \$SP-0011167-5KG-C13-DMSO-20170525-CT54 10.1



5b
DMSO-D6



USER: fx -- DATE: 2017-06-06 10:27:05.525						
F1: 400.160	F2: 1.000	SW1: 8224	PD: 1.0 sec	OF1: 3198.5	LB: 0.3	PTS1d: 65536
EX: zg30		PW: 12.8 us		NA: 16		Nuts - \$5b-H1-DMSO 10.1

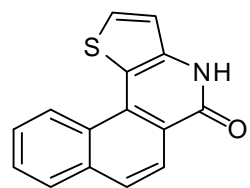


5b

DMSO-D6

USER: fx -- DATE: 2017-06-08 00:53:56.935

F1: 100.620	F2: 1.000	SW1: 24038	OF1: 10011.3	PTS1d: 32768
EX: zgpg30	PW: 9.0 us	PD: 2.0 sec	NA: 1024	LB: 1.0 Nuts - \$SP-0011167-51b-C13-DMSO-20170607-CT54 10.1



5lf

DMSO-D6

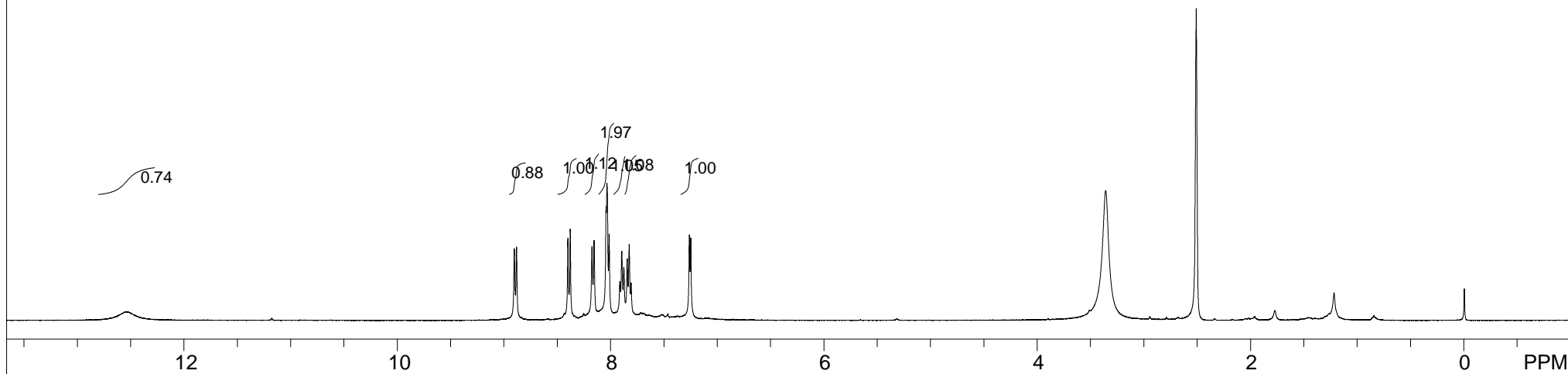
8.904
8.883
8.401
8.379
8.175
8.156
8.043
8.035
8.014
7.914
7.896
7.877
7.845
7.826
7.808
7.262
7.248

3.357

2.510

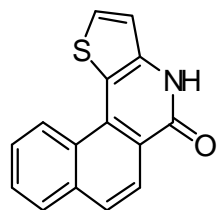
1.219

-0.000



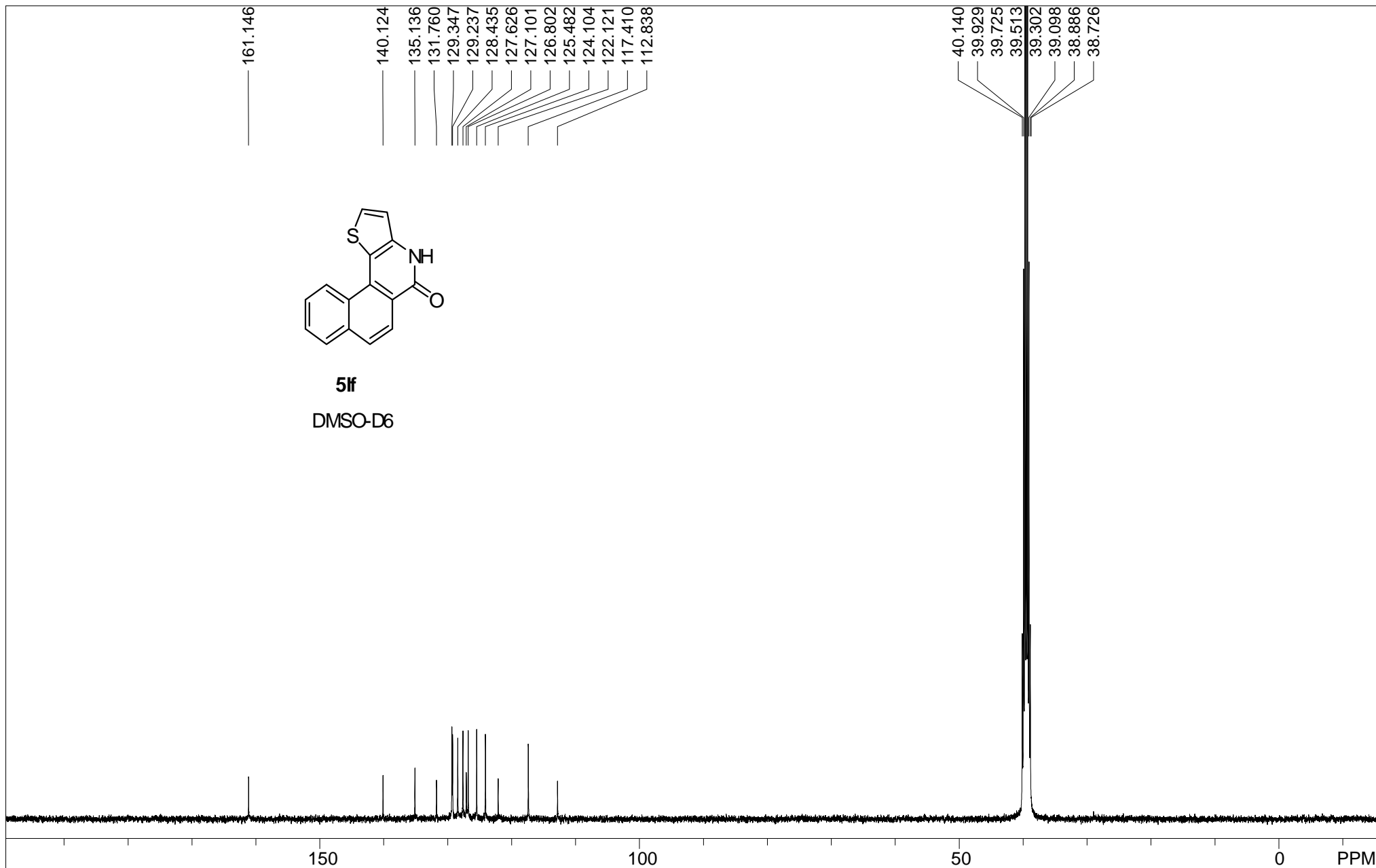
USER: fx -- DATE: 2017-06-12 11:38:57.634

F1: 400.160	F2: 1.000	SW1: 8224	OF1: 3201.5	PTS1d: 65536
EX: zg30	PW: 12.8 us	PD: 1.0 sec	NA: 16	LB: 0.3 Nuts - \$P-0011167-5LF-H1-DMSO-20170612-CT54 10.1



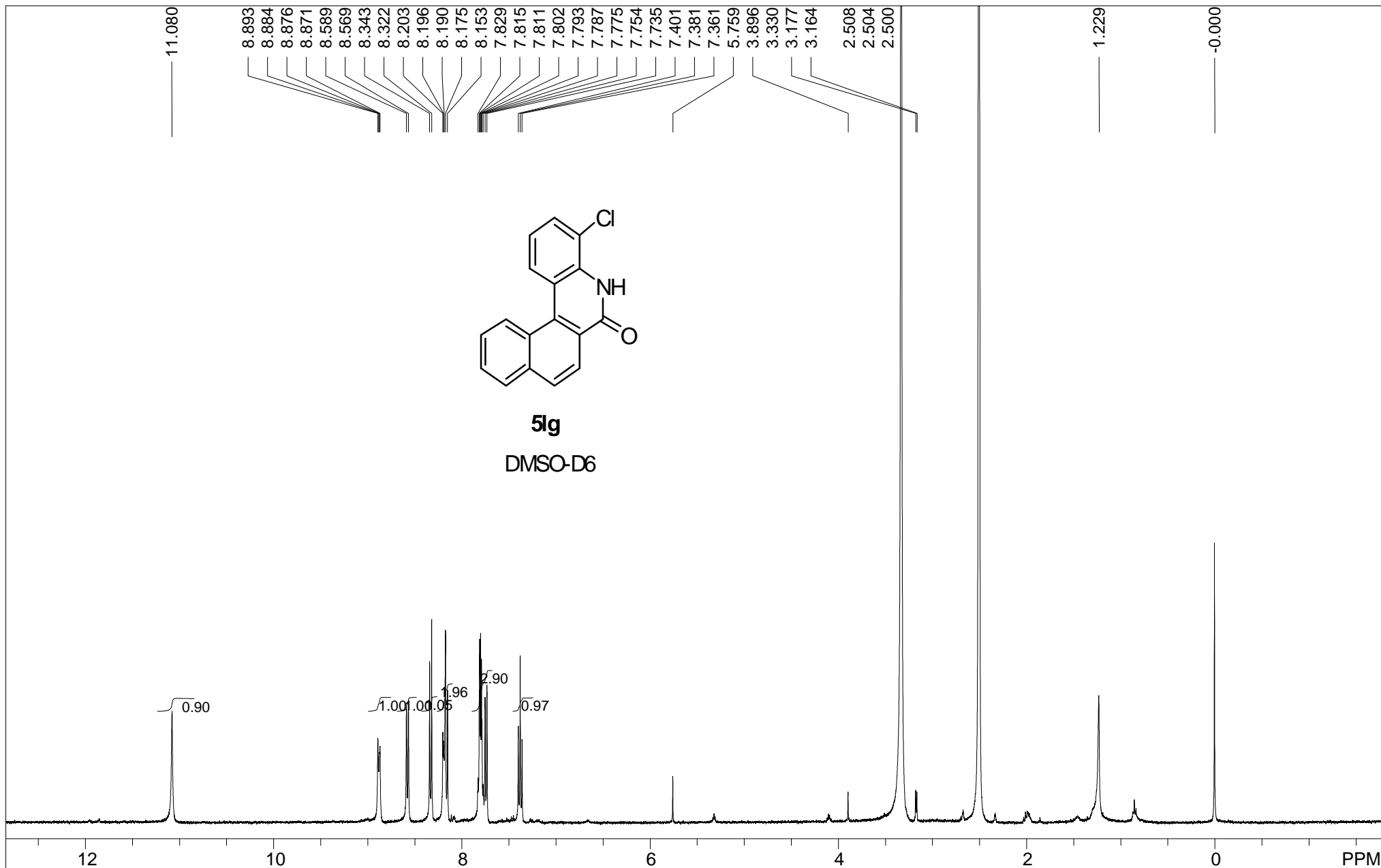
5f

DMSO-D6



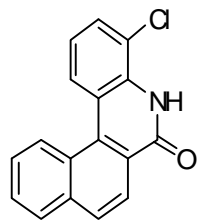
USER: fx -- DATE: 2017-06-12 22:21:16.037

F1: 100.620	F2: 1.000	SW1: 24038	OF1: 10011.3	PTS1d: 32768
EX: zgpg30	PW: 9.0 us	PD: 2.0 sec	NA: 1024	LB: 1.0 Nuts - \$SP-0011167-5f-C13-DMSO-20170612-CT54 20.1

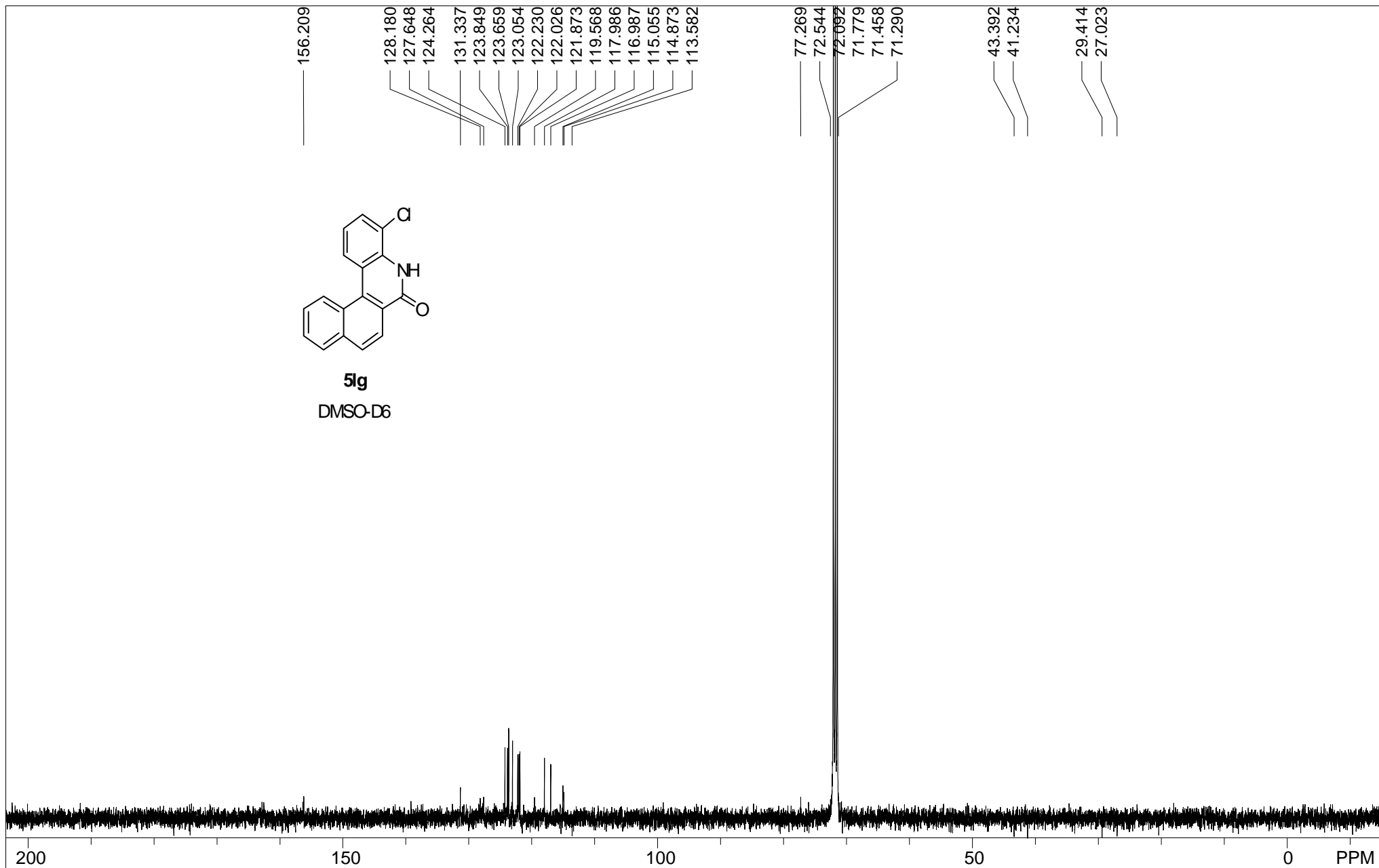


USER: fx -- DATE: 2017-06-09 14:18:41.741

F1: 400.160	F2: 1.000	SW1: 8224	OF1: 3199.1	PTS1d: 65536
EX: zg30	PW: 12.8 us	PD: 1.0 sec	NA: 16	LB: 0.3
				Nuts - \$51g-H1-DMSO 10.1

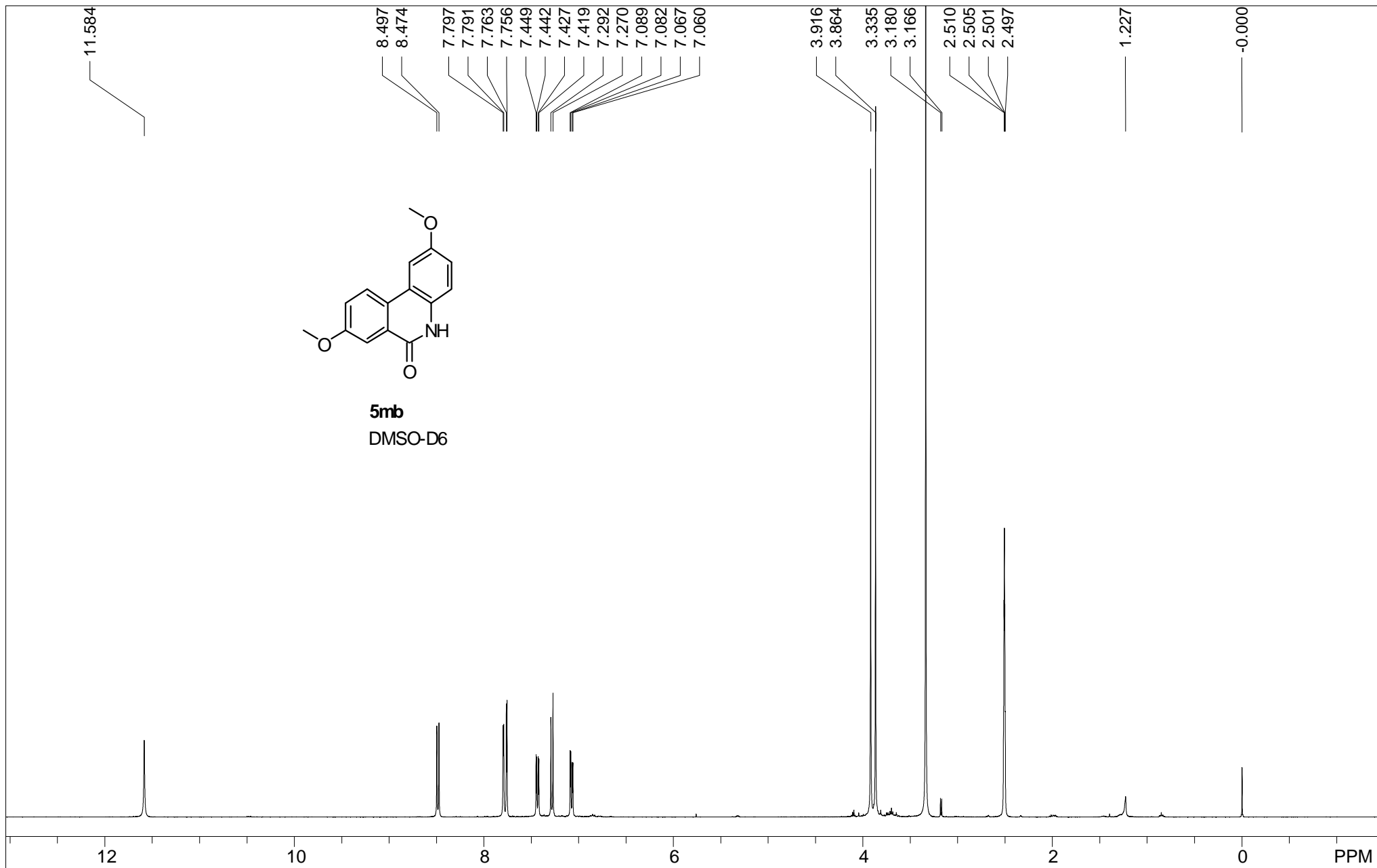


5g
DMSO-D6



USER: fx -- DATE: 2017-06-12 23:24:07.297

F1: 100.620	F2: 1.000	SW1: 24038	OF1: 10011.3	PTS1d: 32768
EX: zgpg30	PW: 9.0 us	PD: 2.0 sec	NA: 1024	LB: 1.0 Nuts - \$P-0011167-5lg-C13-CDC13-20170612-CT54 10.1



USER: fx -- DATE: 2017-06-13 13:19:03.617

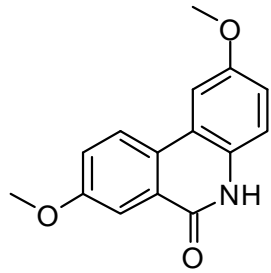
F1: 400.160	F2: 1.000	SW1: 8224	OF1: 3199.9	PTS1d: 65536
EX: zg30	PW: 12.8 us	PD: 1.0 sec	NA: 16	LB: 0.3
				Nuts - \$5mb-H1-DMSO 10.1

160.059
159.038
154.846

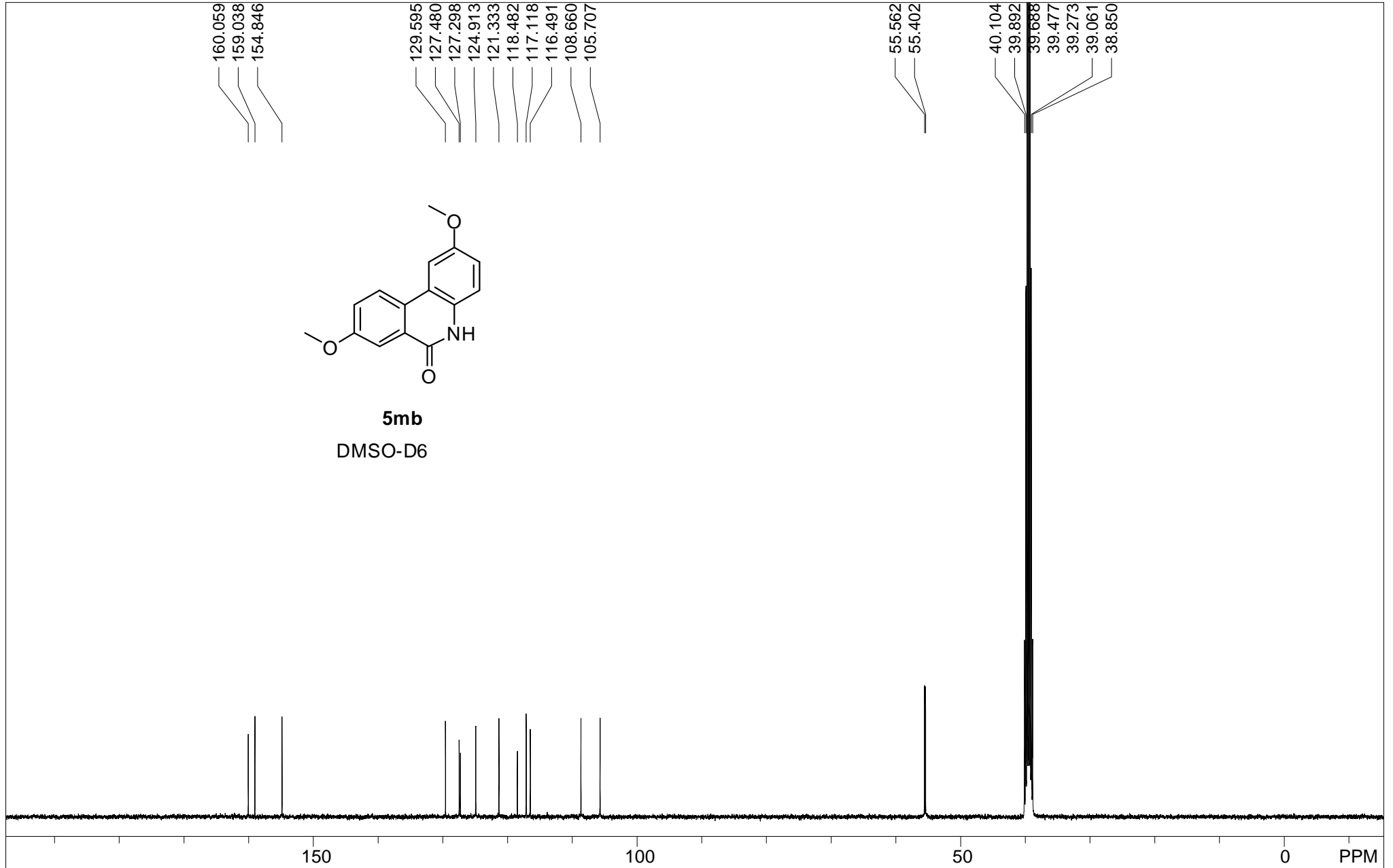
129.595
127.480
127.298
124.913
121.333
118.482
117.118
116.491
108.660
105.707

55.562
55.402

40.104
39.892
39.688
39.477
39.273
39.061
38.850

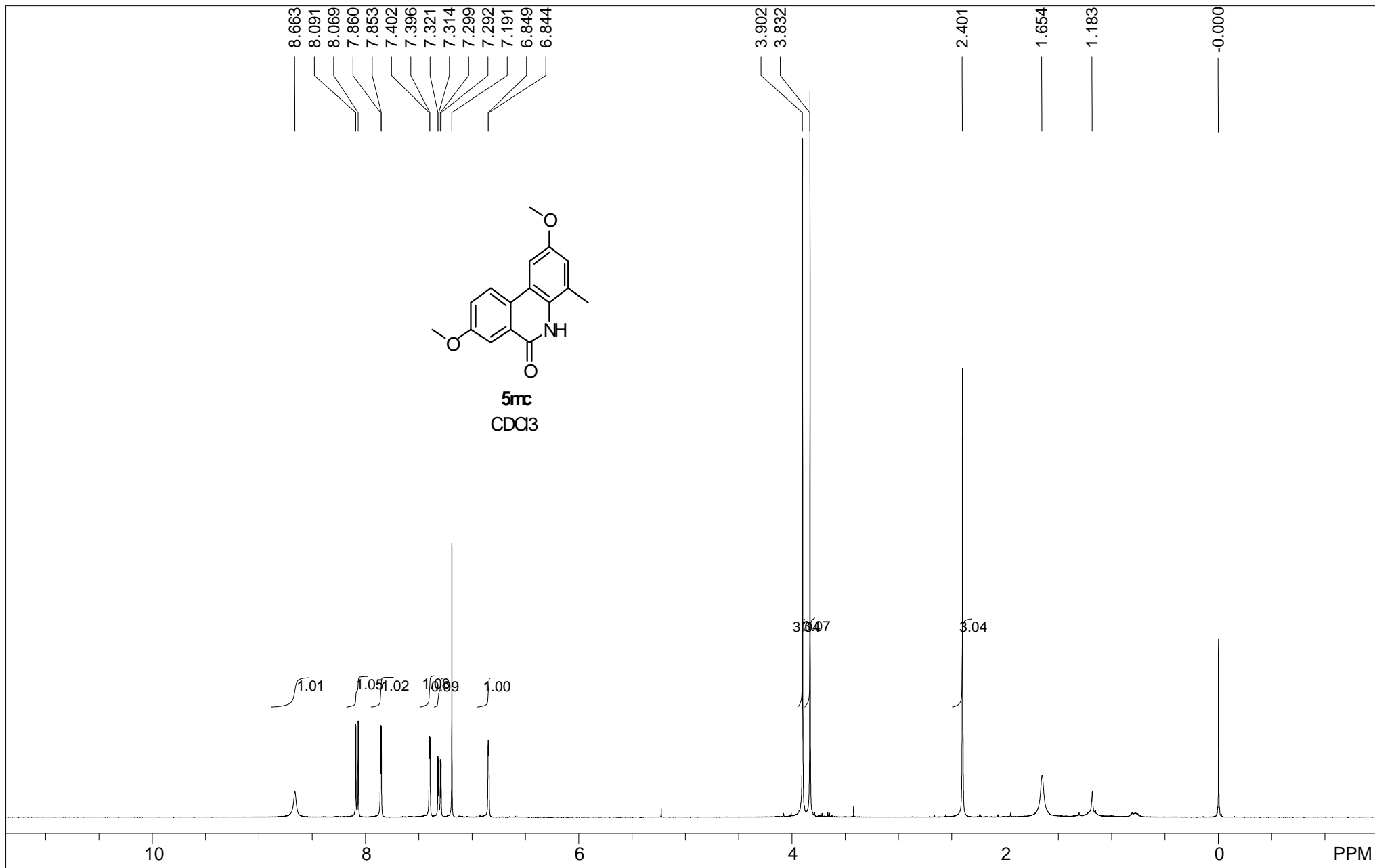


5mb
DMSO-D6



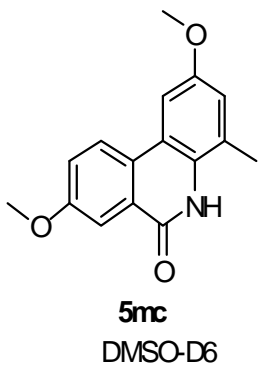
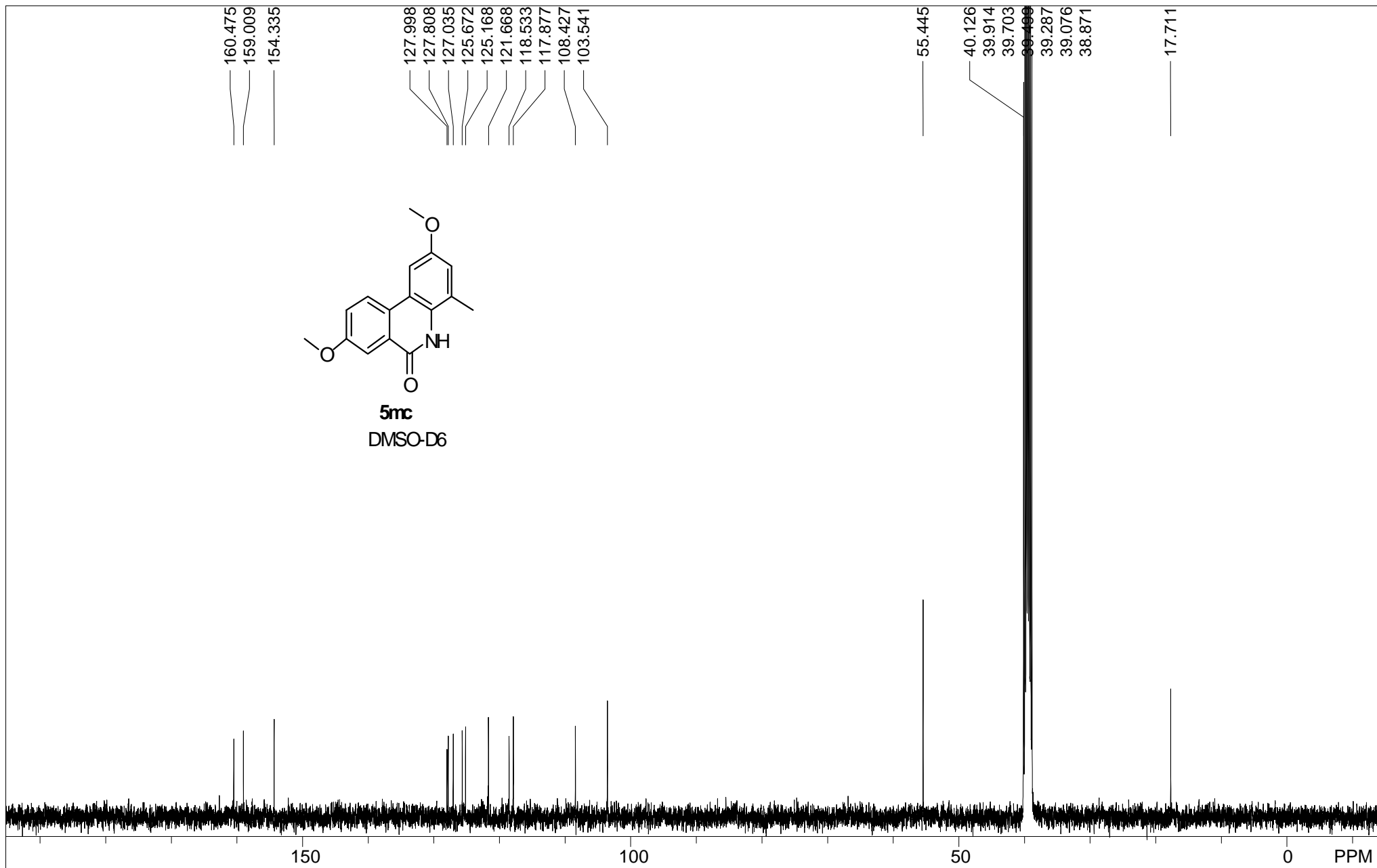
USER: fx -- DATE: 2017-06-13 23:13:35.762

F1: 100.620	F2: 1.000	SW1: 24038	OF1: 10011.3	PTS1d: 32768
EX: zgpg30	PW: 9.0 us	PD: 2.0 sec	NA: 1024	LB: 1.0Nuts - \$SP-0011167-5mb-C13-DMSO-20170613-CT54 10.1



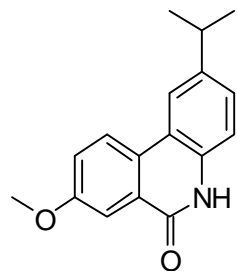
USER: fx -- DATE: 2017-06-26 13:13:21.571

F1: 400.160	F2: 1.000	SW1: 8224	OF1: 3165.3	PTS1d: 65536
EX: zg30	PW: 12.8 us	PD: 1.0 sec	NA: 16	LB: 0.3
				Nuts - \$5mc-H1-CDCl3 10.1



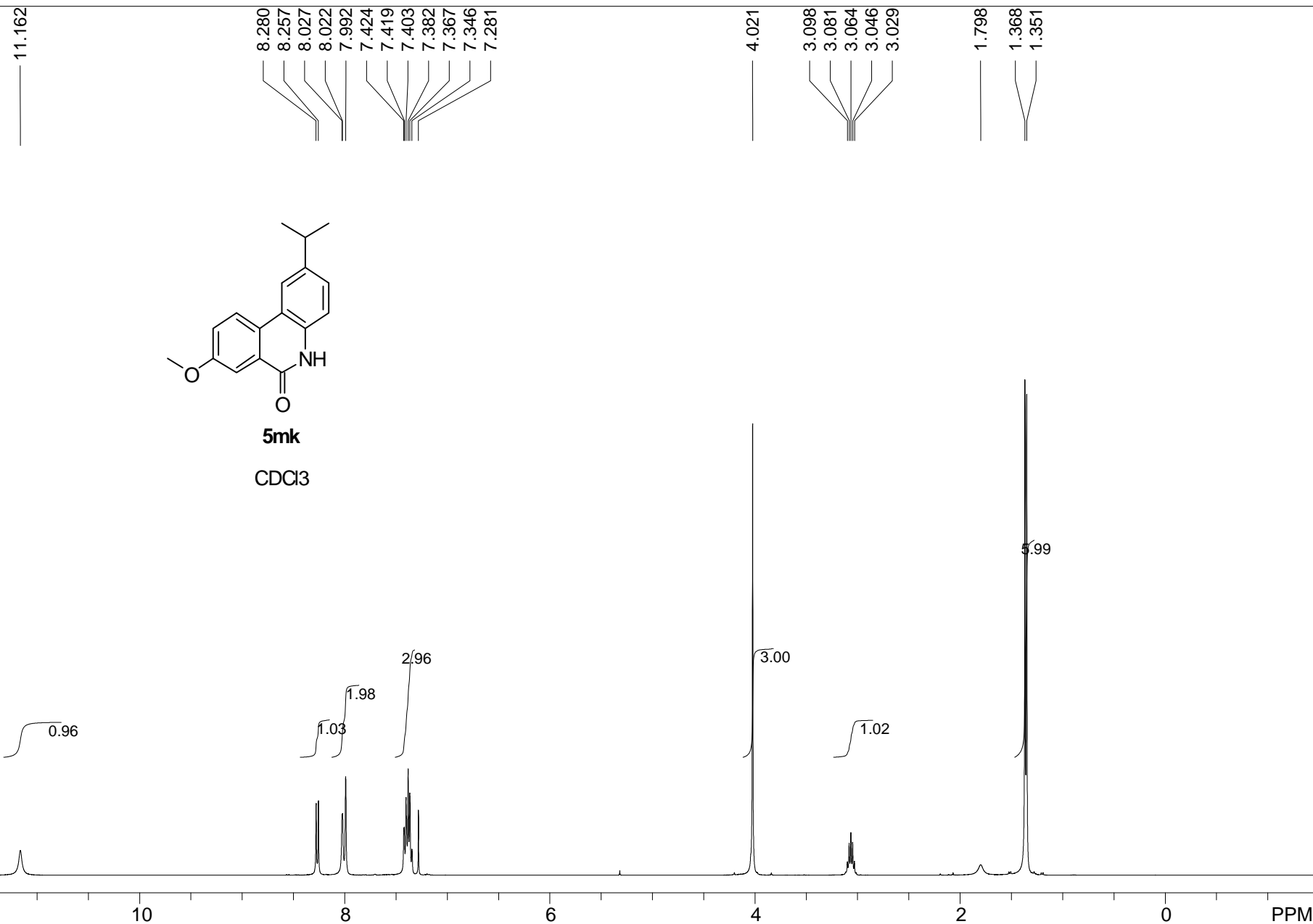
USER: fx -- DATE: 2017-06-27 00:58:21.709

F1: 100.620	F2: 1.000	SW1: 24038	OF1: 10011.3	PTS1d: 32768
EX: zgpg30	PW: 9.0 us	PD: 2.0 sec	NA: 1024	LB: 1.0Nuts - \$\$P-0011167-5mc-C13-DMSO-20170626-CT54 10.1



5mk

CDCl3



USER: fx -- DATE: 2017-06-27 09:47:08.096

F1: 400.160

F2: 1.000

SW1: 8224

OF1: 3201.3

PTS1d: 65536

EX: zg30

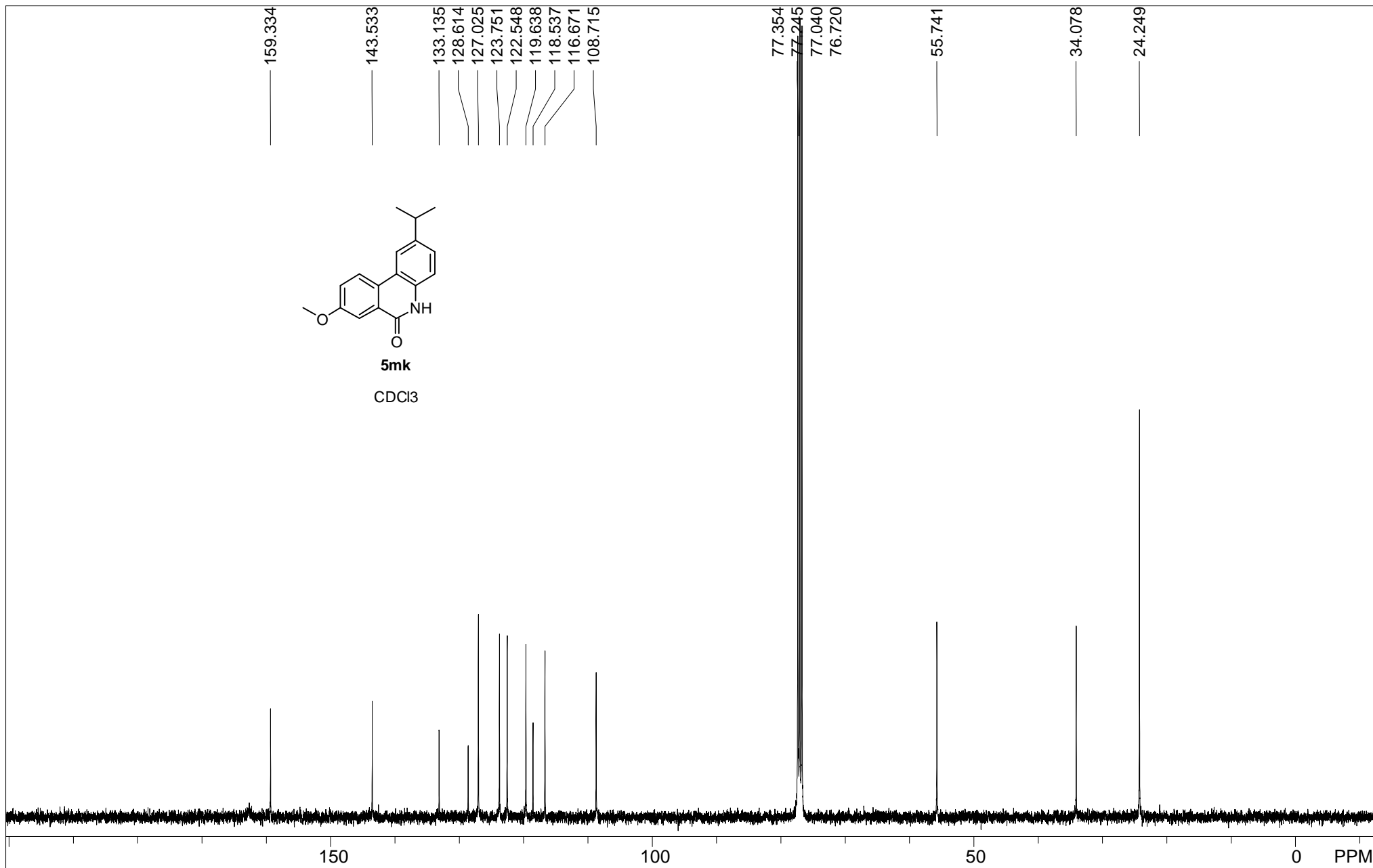
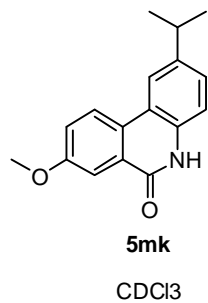
PW: 12.8 us

PD: 1.0 sec

NA: 16

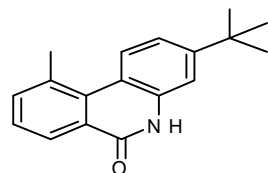
LB: 0.3

Nuts - \$5mk-H1-CDCl3 10.1



USER: fx -- DATE: 2017-06-27 21:36:55.820

F1: 100.620	F2: 1.000	SW1: 24038	OF1: 10061.6	PTS1d: 32768
EX: zgpg30	PW: 9.0 us	PD: 2.0 sec	NA: 1024	LB: 1.0Nuts - \$SP-0011167-5mk-C13-CDC13-20170627-CT54 10.1



5nj

DMSO-D6

11.577

8.397
8.375
8.303
8.285
7.702
7.684
7.526
7.507
7.488
7.454
7.450
7.336
7.331
7.314
7.309
5.758

3.336
3.088
3.072
2.920
2.505

1.337
1.229
1.203
1.185
1.167

0.96

1.02
1.02
1.01
1.98
0.97

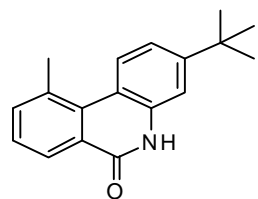
3.00

8.85

12 10 8 6 4 2 0 PPM

USER: fx -- DATE: 2017-06-30 10:46:17.194

F1: 400.160	F2: 1.000	SW1: 8224	OF1: 3199.4	PTS1d: 65536
EX: zg30	PW: 12.8 us	PD: 1.0 sec	NA: 16	LB: 0.3 Nuts - \$SP-0011167-5NJ-H1-DMSO-20170630-CT54 10.1

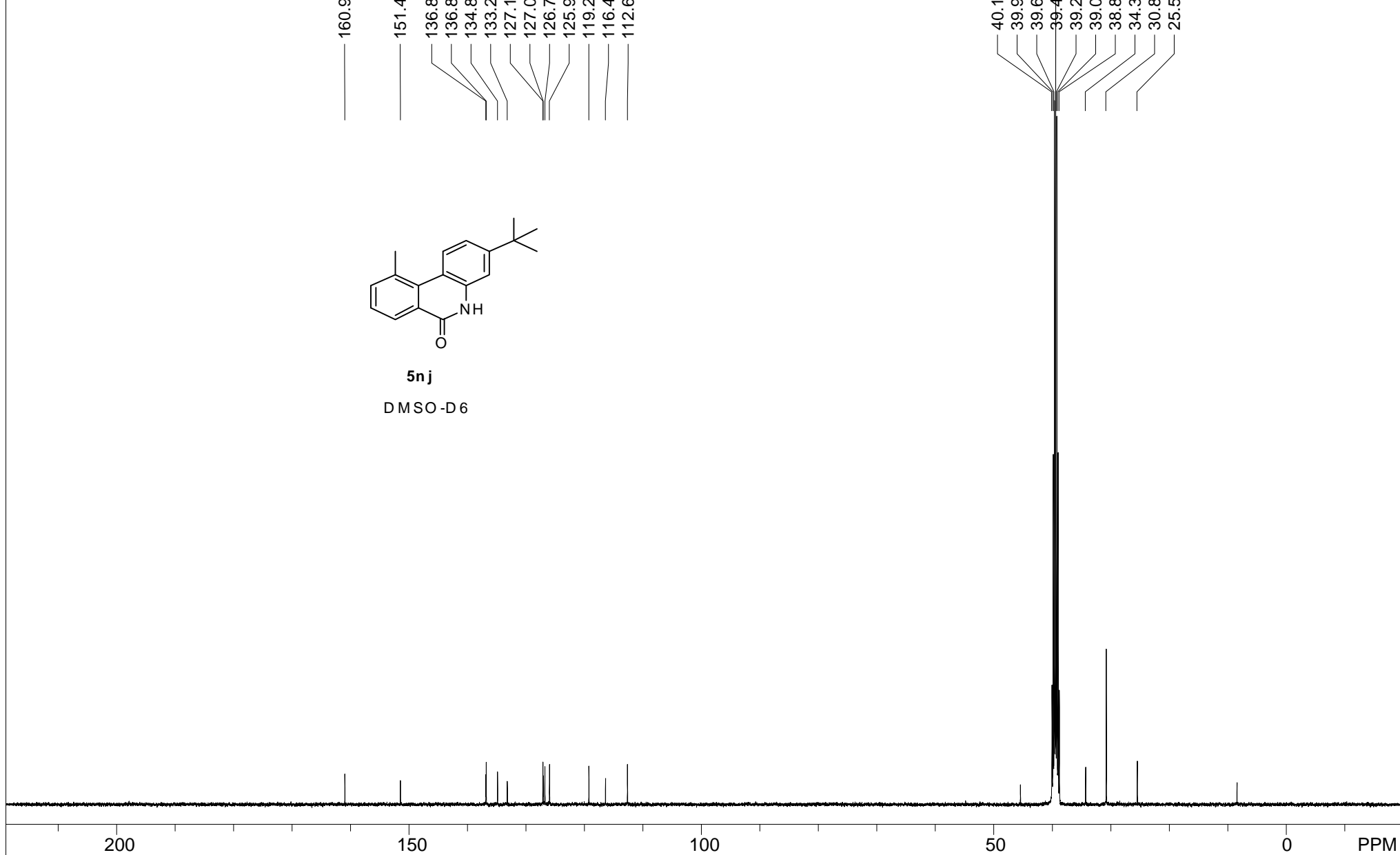


5nj

DMSO-D6

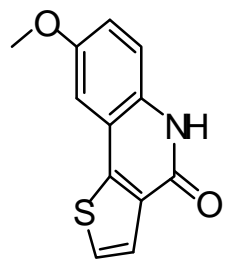
160.978
151.477
136.872
136.813
134.866
133.211
127.115
127.057
126.780
125.992
119.255
116.418
112.671

40.111
39.900
39.695
39.484
39.280
39.068
38.857
34.358
30.829
25.528



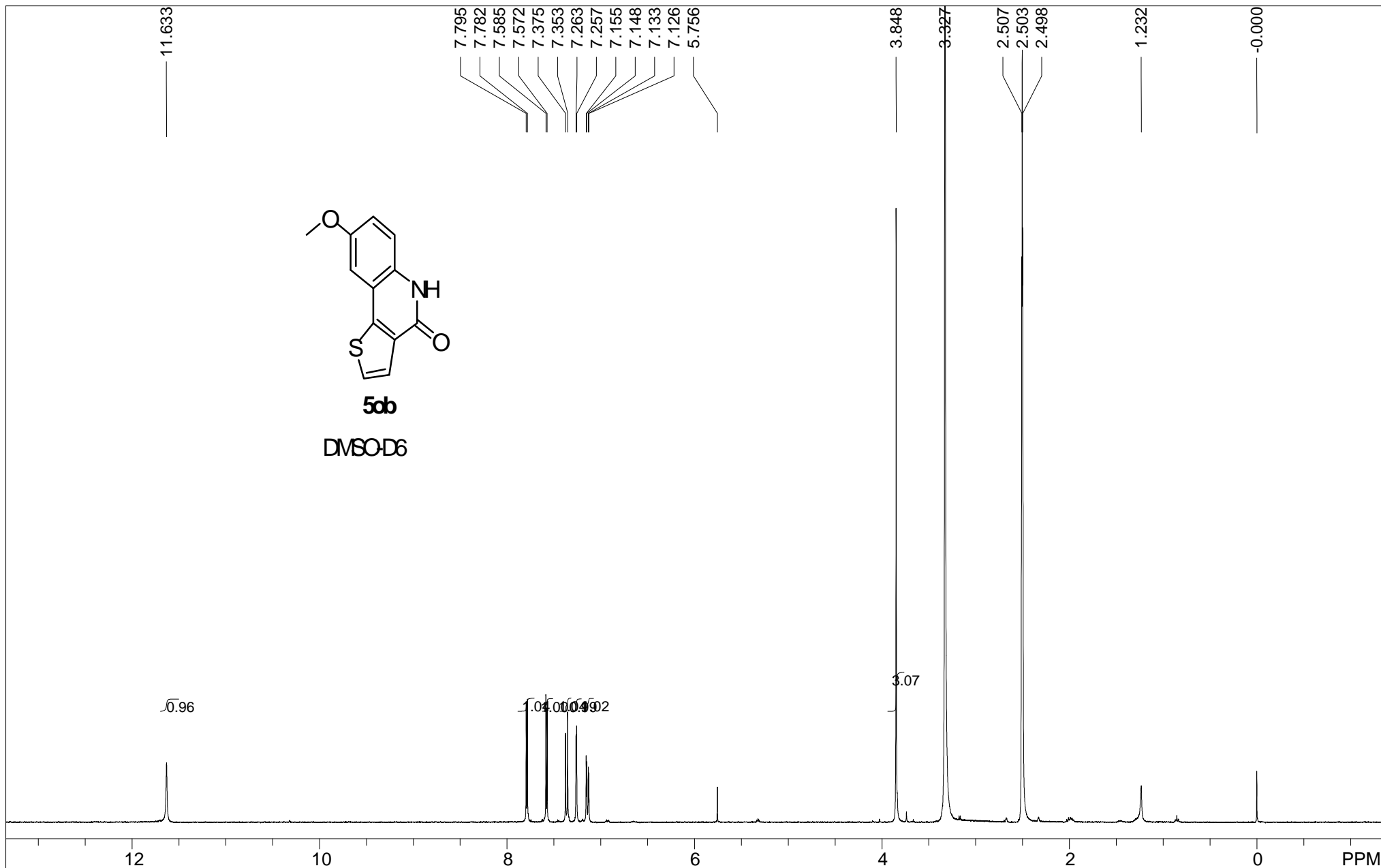
USER: fx -- DATE: 2017-07-01 03:00:19.396

F1: 100.620	F2: 1.000	SW1: 24038	OF1: 10011.3	PTS1d: 32768
EX: zgpg30	PW: 9.0 us	PD: 2.0 sec	NA: 1024	LB: 1.0Nuts - \$SP-0011167-5NJ-C13-DMSO-20170630-CT54 10.1



5b

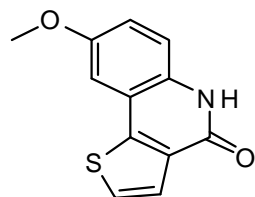
DMSO-D6



USER: fx -- DATE: 2017-07-04 11:30:08.715

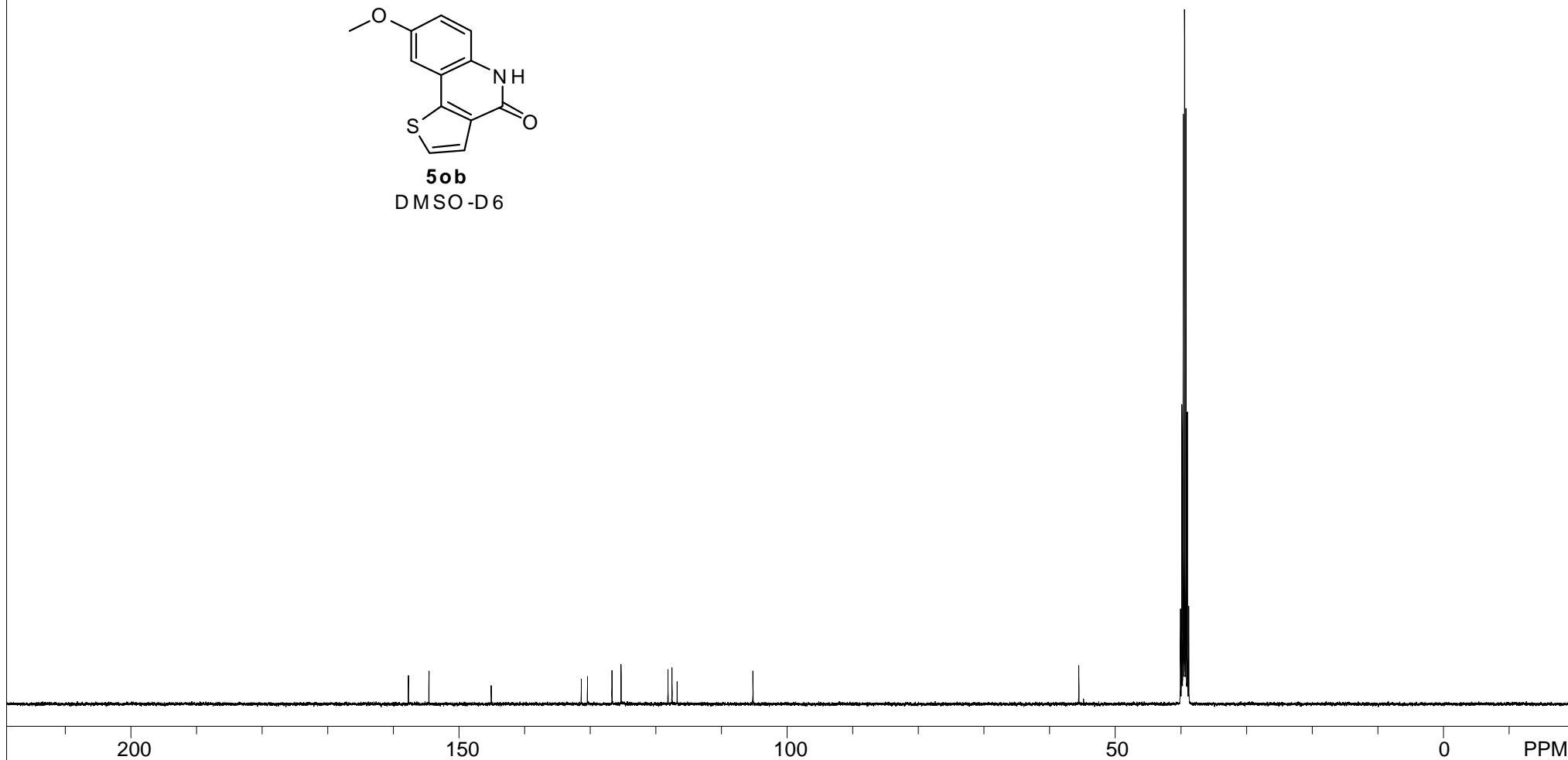
F1: 400.160	F2: 1.000	SW1: 8224	OF1: 3198.6	PTS1d: 65536
EX: zg30	PW: 12.8 us	PD: 1.0 sec	NA: 16	LB: 0.3

Nuts - \$5ob-H1-DMSO 10.1



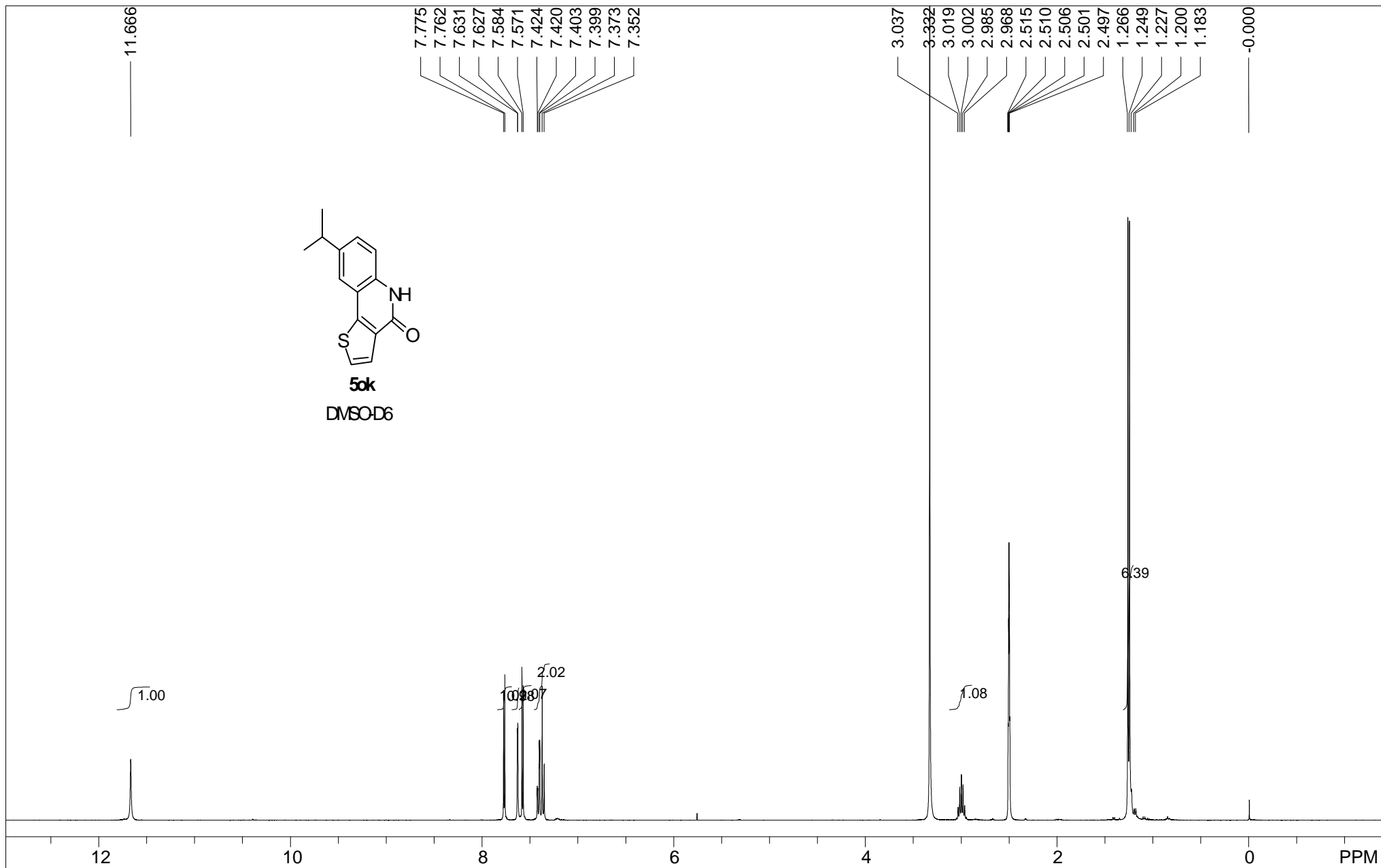
5ob
DMSO-D6

157.726
154.590
145.097
131.381
130.440
126.700
125.329
118.176
117.563
116.783
105.233
55.606
40.126
39.914
39.703
39.499
39.287
39.076
38.871



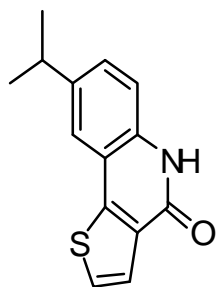
USER: fx -- DATE: 2017-07-04 21:50:03.485

F1: 100.620	F2: 1.000	SW1: 24038	OF1: 10011.3	PTS1d: 32768
EX: zgpg30	PW: 9.0 us	PD: 2.0 sec	NA: 1024	LB: 1.0Nuts - \$\$P-0011167-50B-C13-DMSO-20170704-CT54 10.1



USER: fx -- DATE: 2017-07-07 11:54:59.569

F1: 400.160	F2: 1.000	SW1: 8224	OF1: 3199.9	PTS1d: 65536
EX: zg30	PW: 12.8 us	PD: 1.0 sec	NA: 16	LB: 0.3
				Nuts - \$5ok-H1-DMSO 10.1

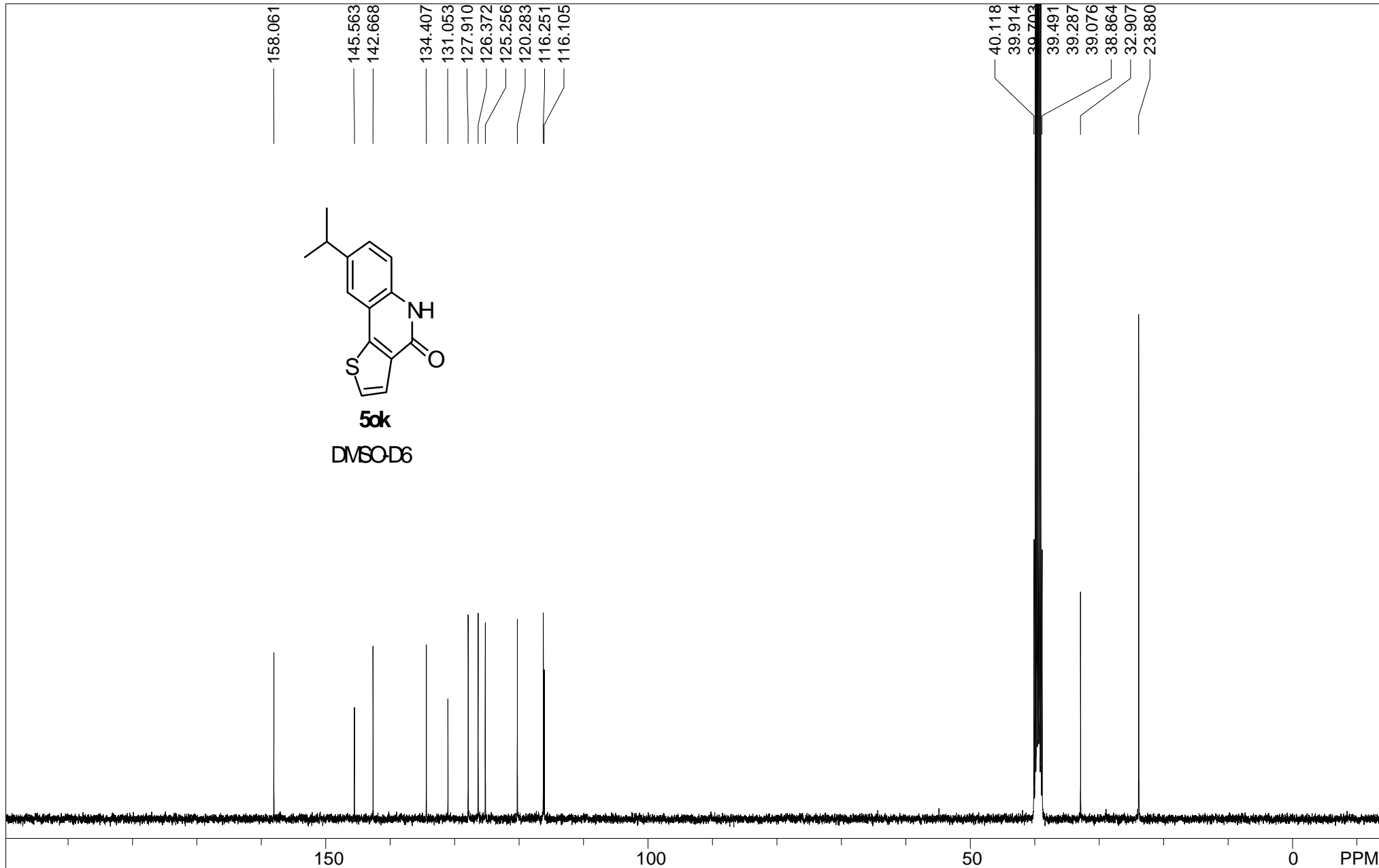


5ok

DMSO-D6

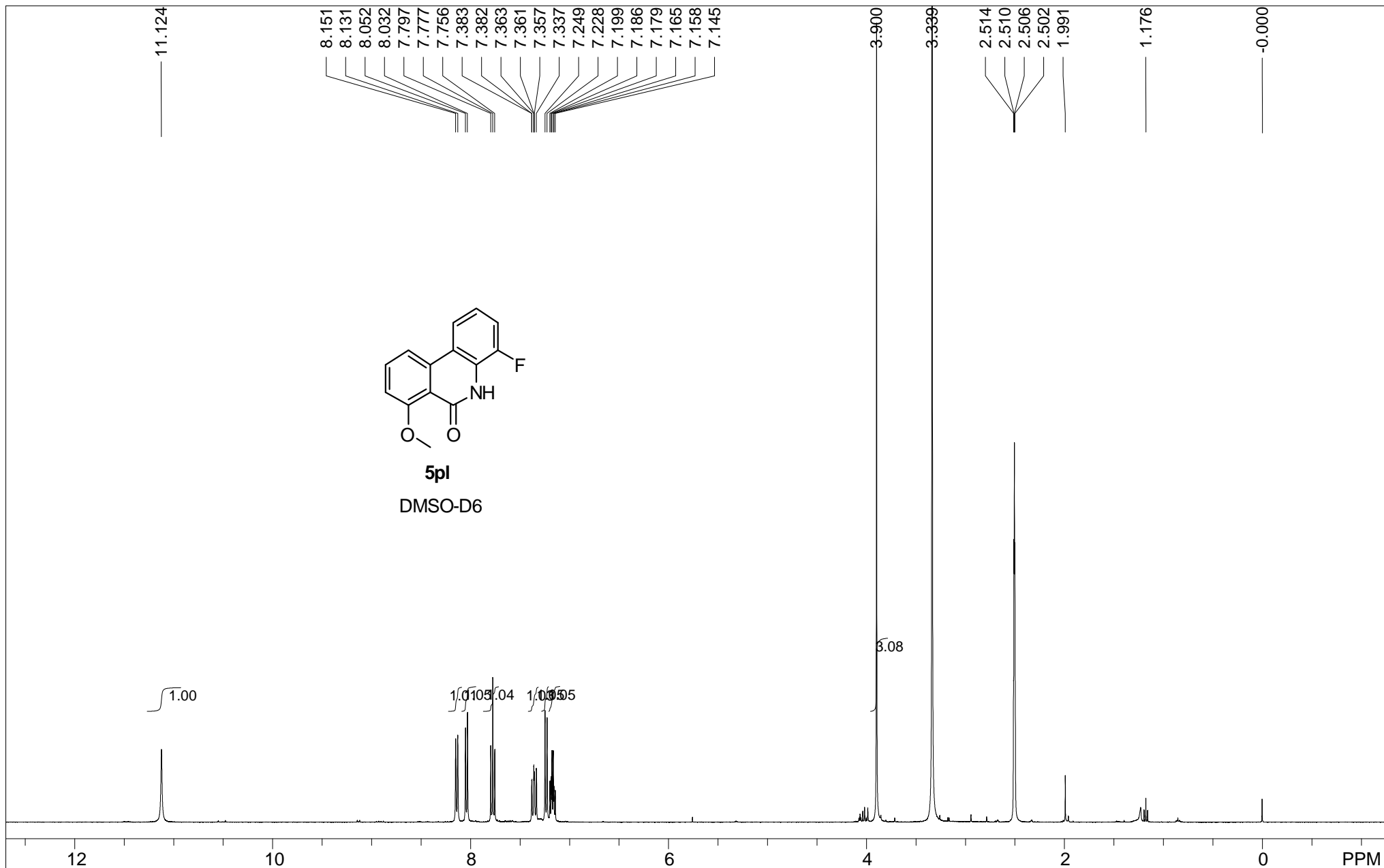
158.061
145.563
142.668
134.407
131.053
127.910
126.372
125.256
120.283
116.251
116.105

40.118
39.914
39.703
39.491
39.287
39.076
38.864
32.907
23.880



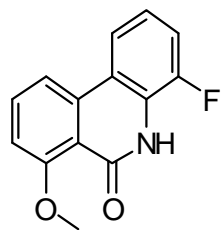
USER: fx -- DATE: 2017-07-11 03:44:16.582

F1: 100.620	F2: 1.000	SW1: 24038	OF1: 10011.3	PTS1d: 32768
EX: zpgg30	PW: 9.0 us	PD: 2.0 sec	NA: 1024	LB: 1.0 Nuts - \$SP-0011167-5ok-C13-DMSO-20170710-CT54 10.1

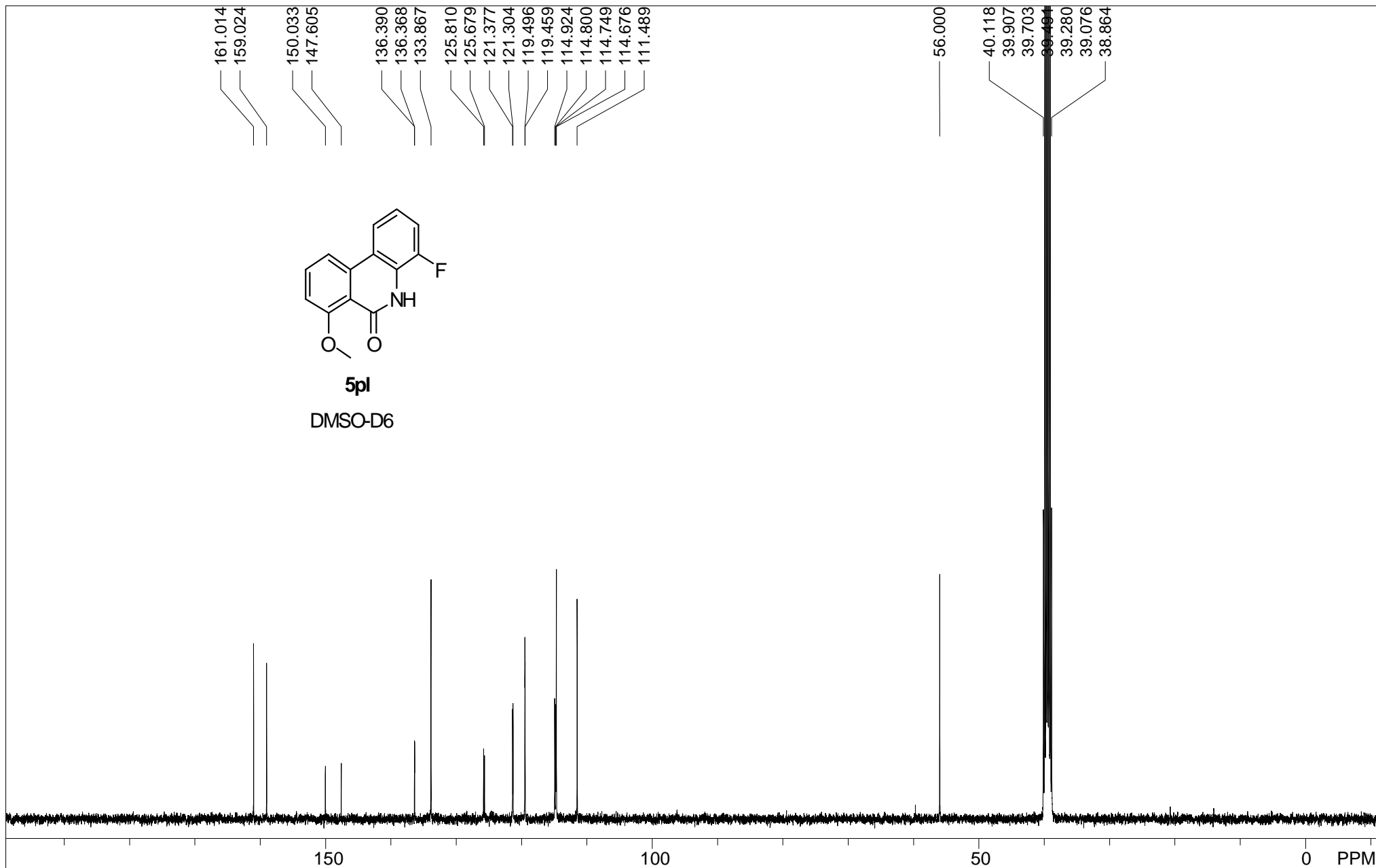


USER: fx -- DATE: 2017-07-10 10:26:18.881

F1: 400.160	F2: 1.000	SW1: 8224	OF1: 3201.1	PTS1d: 65536
EX: zg30	PW: 12.8 us	PD: 1.0 sec	NA: 16	LB: 0.3
				Nuts - \$5pl-H1-DMSO 10.1



5pl
DMSO-D6



USER: fx -- DATE: 2017-07-11 02:42:59.890

F1: 100.620	F2: 1.000	SW1: 24038	OF1: 10011.3	PTS1d: 32768
EX: zpgp30	PW: 9.0 us	PD: 2.0 sec	NA: 1024	LB: 1.0 Nuts - \$SP-0011167-5pl-C13-DMSO-20170710-CT54 20.1