

Electronic Supplementary Information (ESI)

Pd(II)-catalyzed coupling of C-H bonds of carboxamides with iodoazobenzenes toward modified azobenzenes

Sonam Suwasia, Sugumar Venkataramani* and Srinivasarao Arulananda Babu*

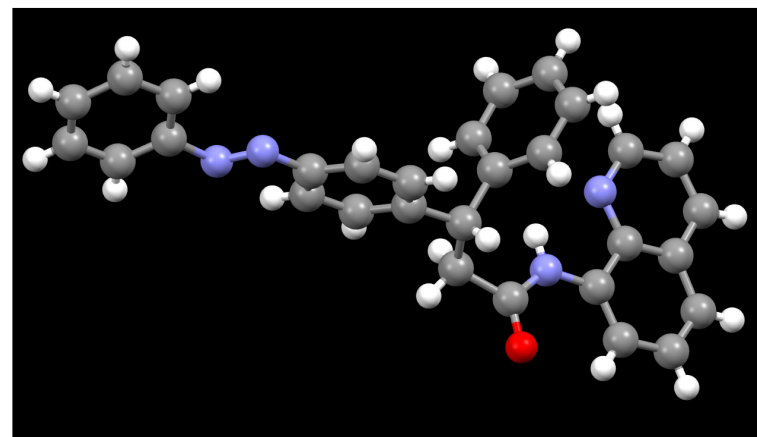
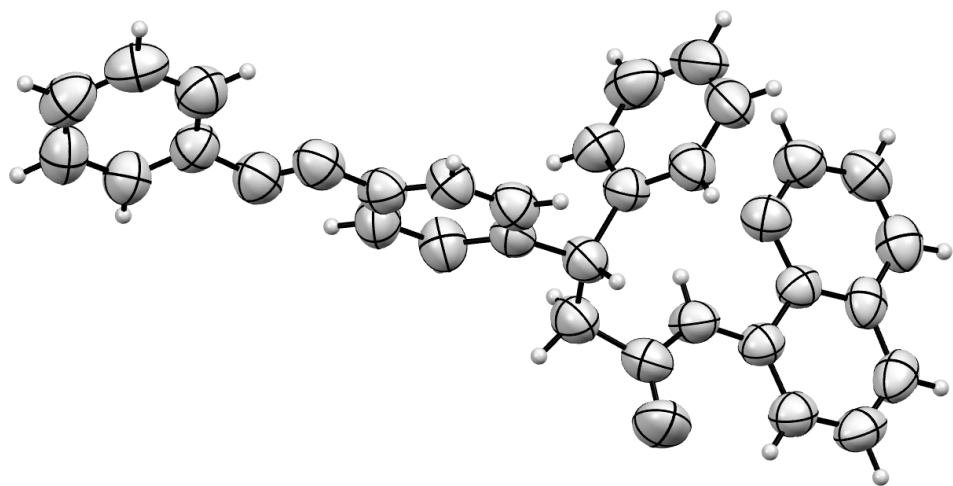
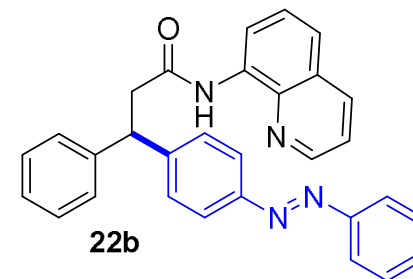
Department of Chemical Sciences, Indian Institute of Science Education and Research (IISER) Mohali, Knowledge City, Sector 81, SAS Nagar, Mohali, Manauli P.O., Punjab, India, 140306. E-mail: sugumarv@iisermohali.ac.in, sababu@iisermohali.ac.in.

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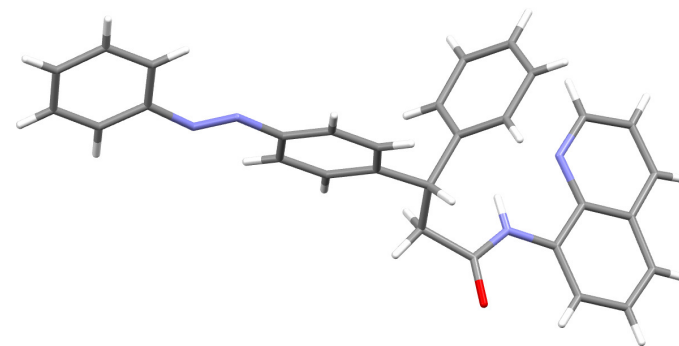
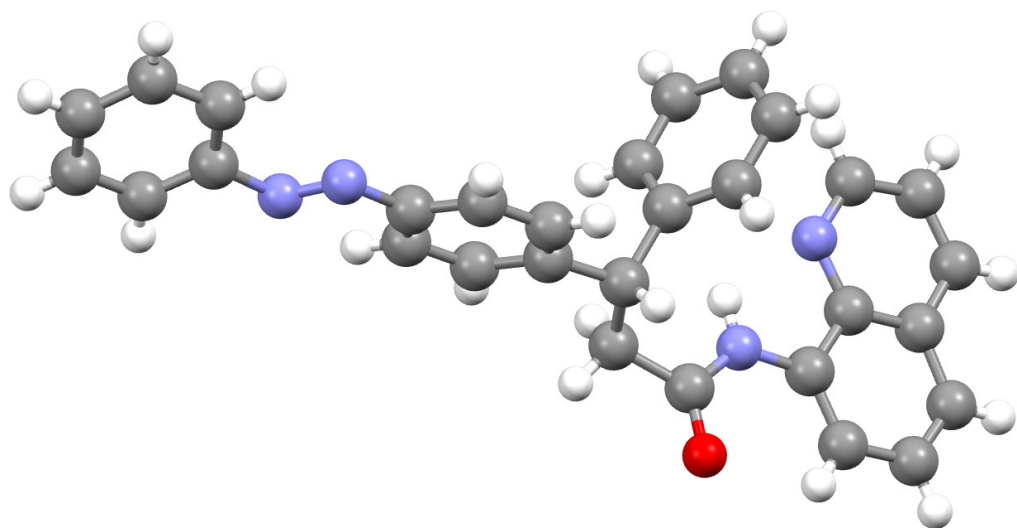
| | |
|---|----------------|
| X-ray structure and brief crystal data of compound 22b | = page2-3 |
| Copies of ¹ H and ¹³ C NMR of compounds | = page 4-364 |
| UV-Vis absorption chart of compounds | = page 365-374 |
| Figures related to photoswitching and kinetics studies | = Page 375-384 |

X-ray structure of compound **22b**

CCDC 2233013



Ellipsoid probability 50%

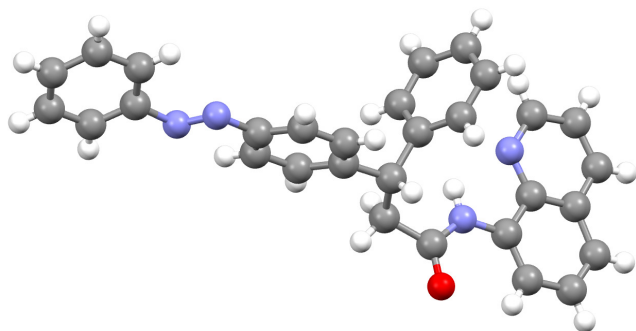
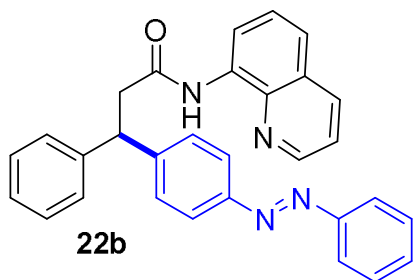


checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ss_305

Brief crystal data of compound **22b**

CCDC 2233013



THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: ss_305

Bond precision: C-C = 0.0067 Å Wavelength=0.71073
Cell: a=15.231(2) b=8.7746(10) c=18.051(3)
alpha=90 beta=101.917(14) gamma=90
Temperature: 298 K

| | Calculated | Reported |
|------------------------|--------------|--------------|
| Volume | 2360.5(6) | 2360.5(6) |
| Space group | P 21/c | P 1 21/c 1 |
| Hall group | -P 2ybc | -P 2ybc |
| Moiety formula | C30 H24 N4 O | C30 H24 N4 O |
| Sum formula | C30 H24 N4 O | C30 H24 N4 O |
| Mr | 456.53 | 456.53 |
| Dx, g cm ⁻³ | 1.285 | 1.285 |
| Z | 4 | 4 |
| Mu (mm ⁻¹) | 0.080 | 0.080 |
| F000 | 960.0 | 960.0 |
| F000' | 960.35 | |
| h, k, lmax | 23, 13, 27 | 21, 12, 26 |
| Nref | 8825 | 8213 |
| Tmin, Tmax | 0.976, 0.976 | 0.291, 1.000 |
| Tmin' | 0.976 | |

Correction method= # Reported T Limits: Tmin=0.291 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.931 Theta(max)= 32.867

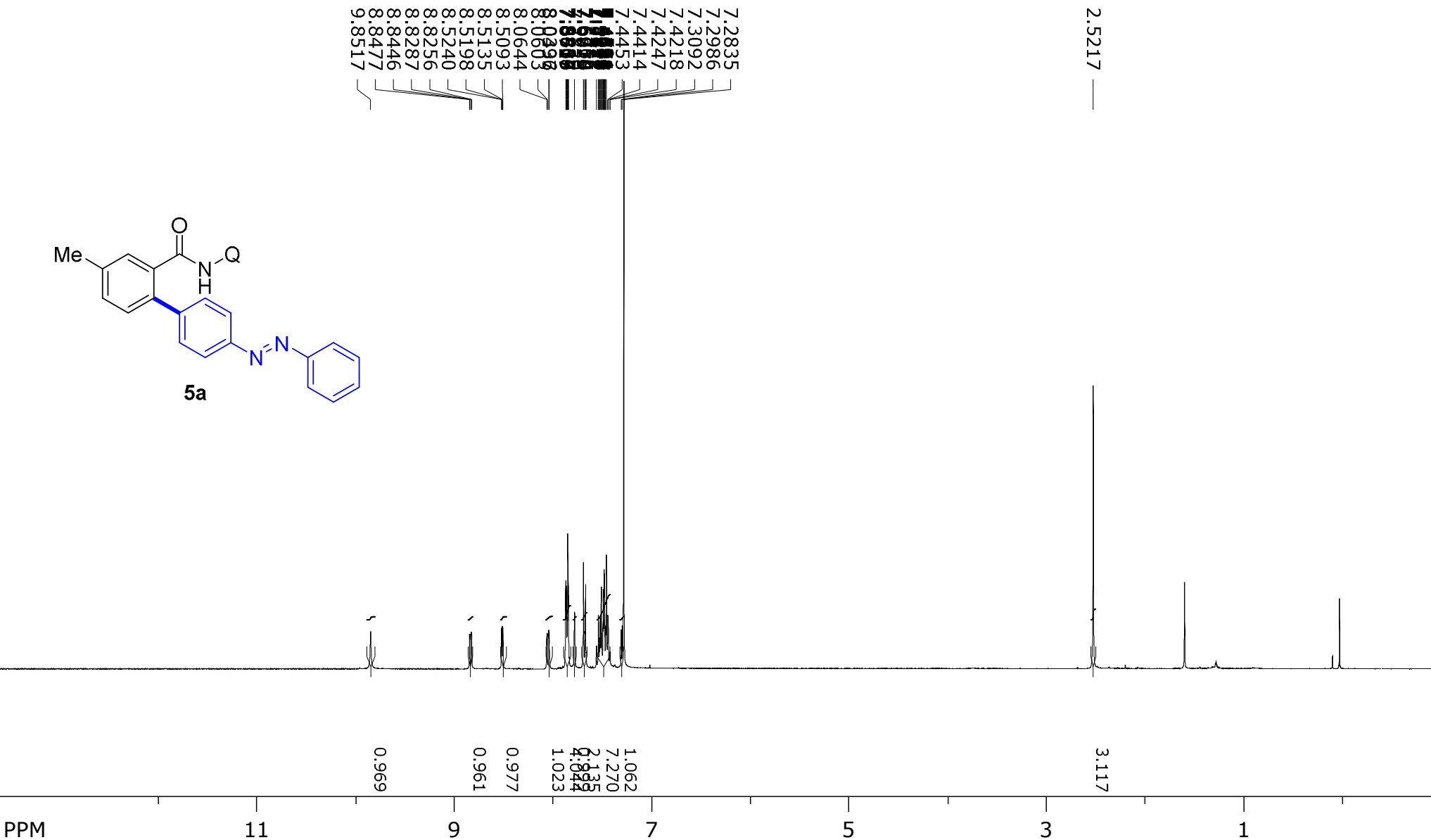
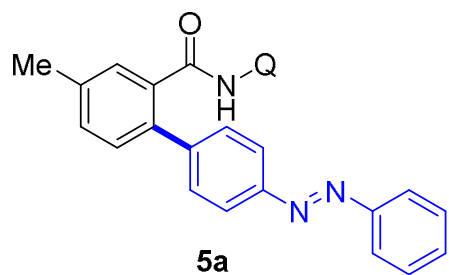
R(reflections)= 0.1101(1931)

wR2(reflections)=
0.4230(8213) 3

S = 0.928

Npar= 316

SpinWorks 4: S S 38 P
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 16

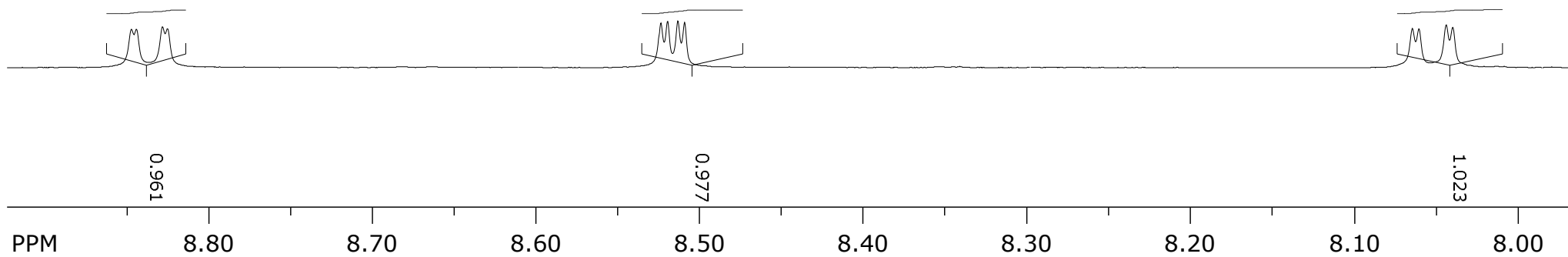
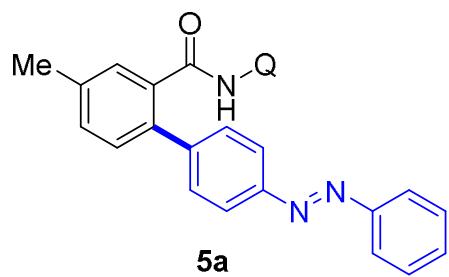


SpinWorks 4: S S 38 P
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 16

8.8256
8.8287
8.8446
8.8477

8.5093
8.5135
8.5198
8.5240

8.0396
8.0437
8.0603
8.0644



SpinWorks 4: S S 38 P
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 16

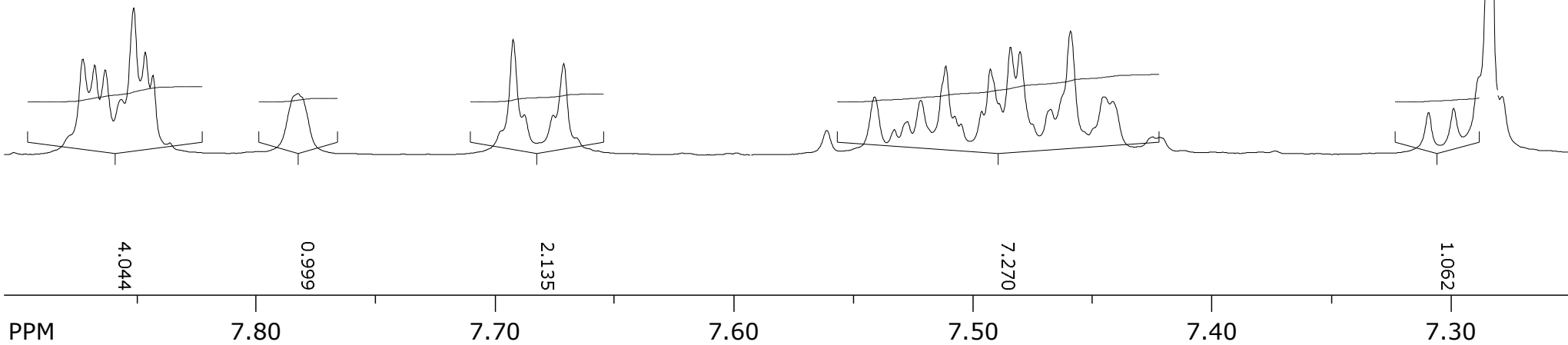
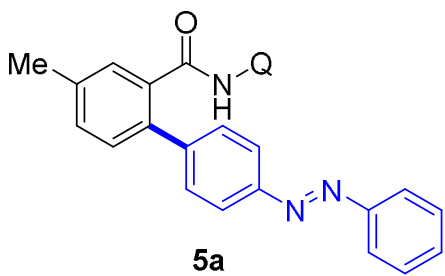
7.8434
7.8467
7.8515
7.8567
7.8635
7.8678
7.8729

7.7829

7.6660
7.6714
7.6758
7.6879
7.6926

7.4218
7.4247
7.4414
7.4453
7.4591
7.4674
7.4752
7.4803
7.4842
7.4891
7.4927
7.4963
7.5049
7.5077
7.5113
7.5218
7.5275
7.5329
7.5412
7.5612

7.2835
7.2986
7.3092

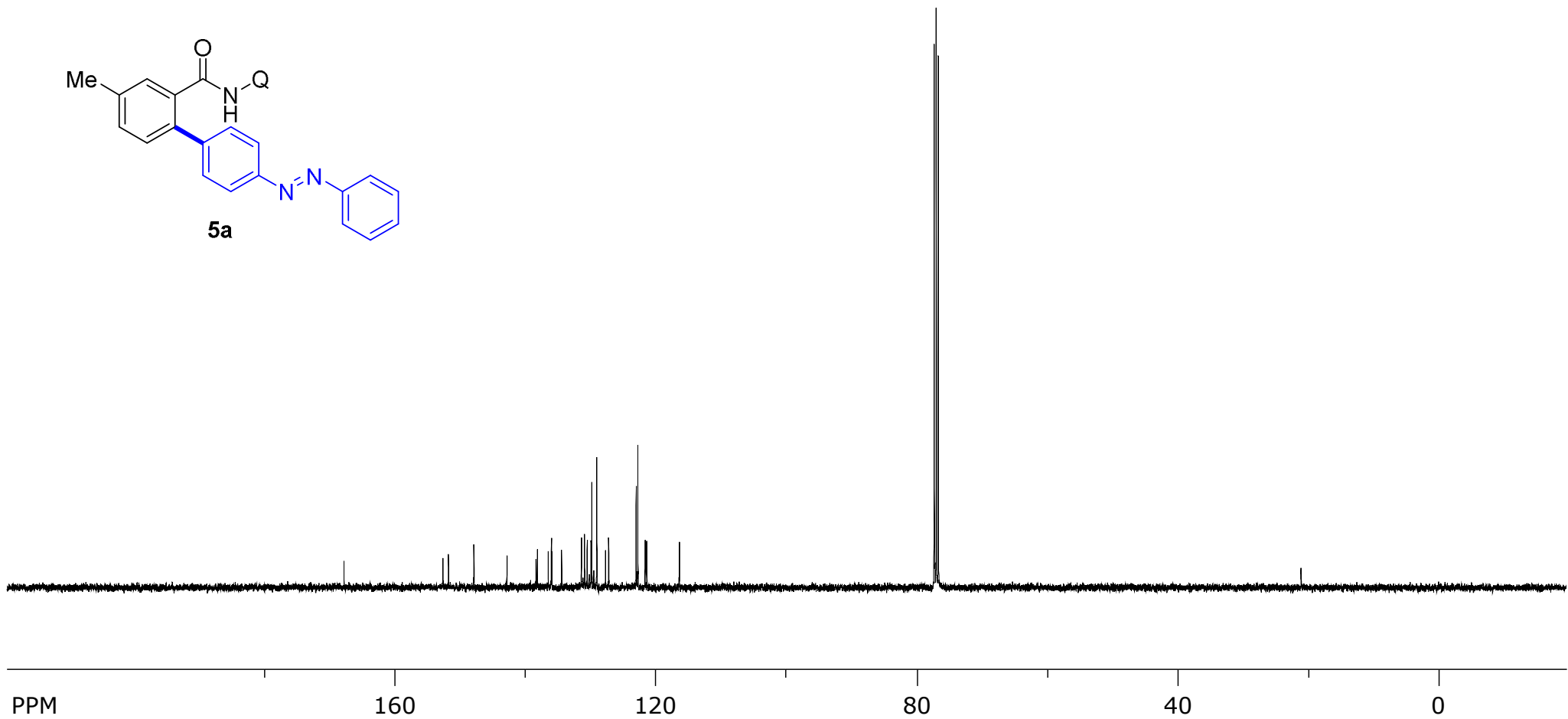
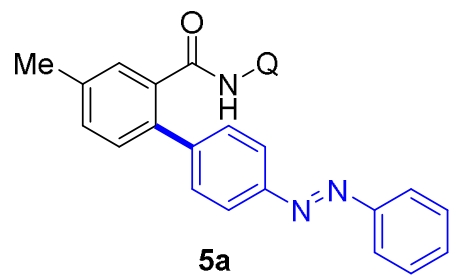


SpinWorks 4: SS 38 P
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 8

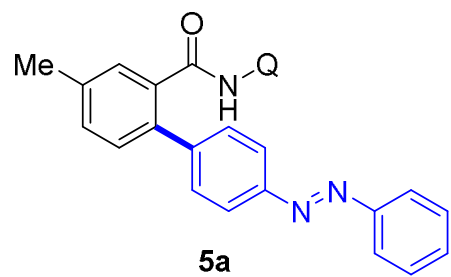
116.399
121.420
121.680
122.769
123.045
127.257
127.754
129.074
130.930
131.430
131.430
134.461
135.970
136.029
136.511
138.203
138.406
142.847
147.903
151.800
152.650
167.800

76.732
77.050
77.368

21.146



SpinWorks 4: SS 38 P
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 8



167.800 —

151.800 —
152.650 —

147.903 —

142.847 —

138.406 —
138.203 —
136.511 —
136.029 —
135.970 —

134.461 —

131.436 —

130.948 —

130.554 —

129.953 —

129.830 —

129.074 —

127.754 —

127.257 —

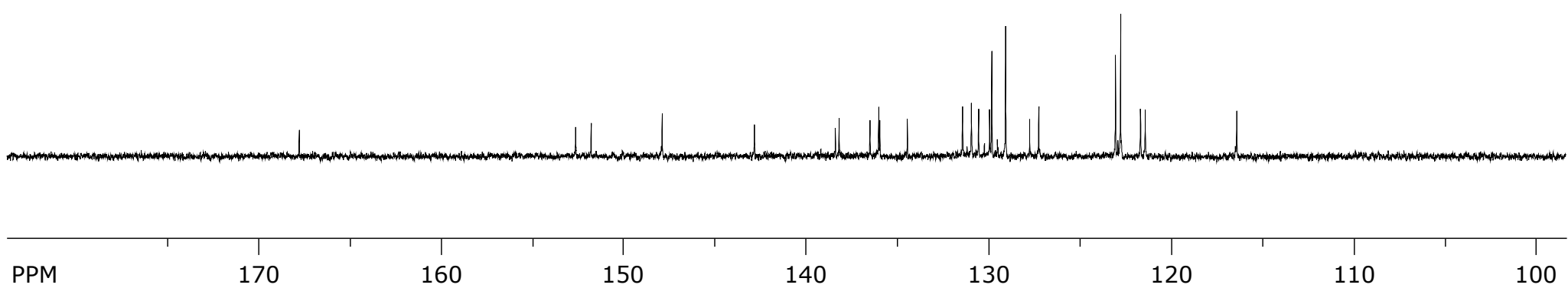
123.045 —

122.769 —

121.680 —

121.420 —

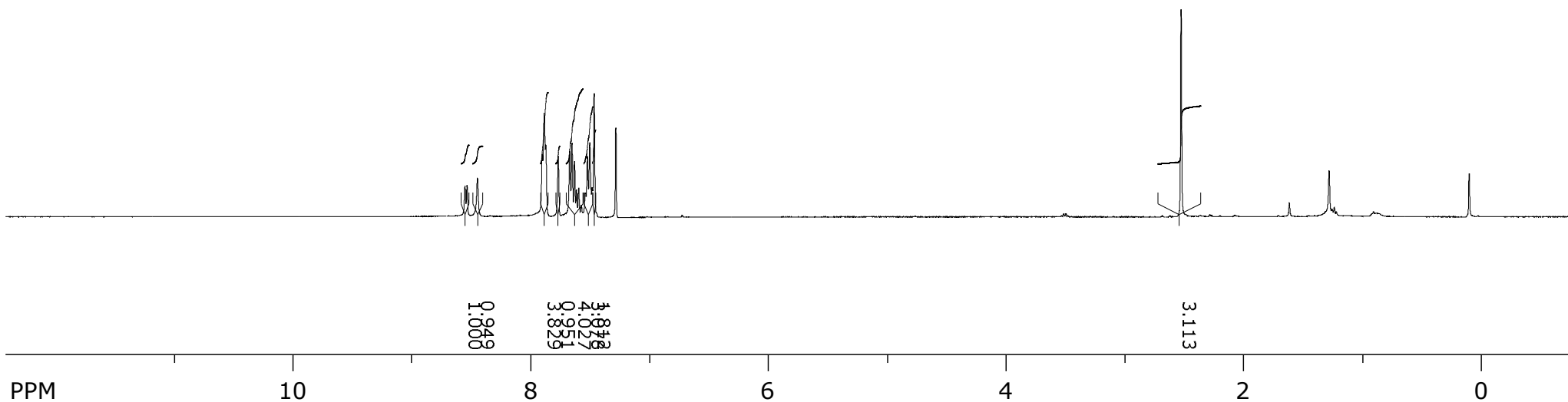
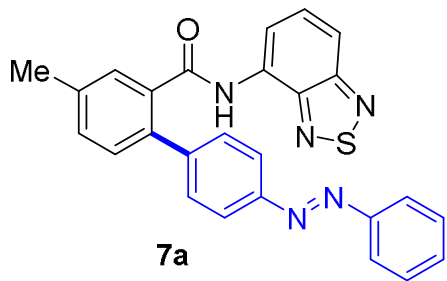
116.399 —



SpinWorks 4: SS 176 P REP
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 4

7.2861
7.4680
7.4843
7.4851
7.5043
7.5244
7.5409
7.5558
7.6546
7.6735
7.7705
7.8748
7.8885
7.9050
8.4507
8.5384
8.5558

2.5256



PPM

10

8

6

4

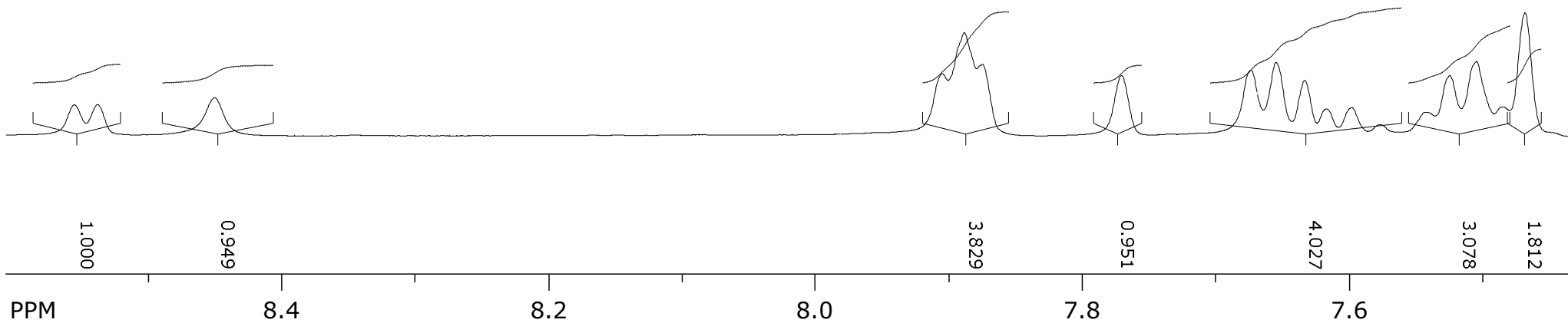
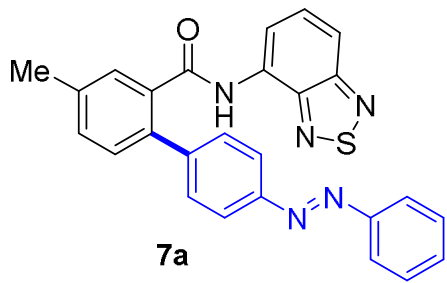
2

0

9

SpinWorks 4: SS 176 P REP
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 4

| | | | | | |
|--------|--------|--------|--------|--------|--------|
| 8.5384 | 8.4507 | 7.8748 | 7.7705 | 7.5244 | 7.4680 |
| 8.5558 | | 7.8885 | | 7.5409 | 7.4843 |
| | | 7.9050 | | 7.5432 | 7.4851 |
| | | | | 7.5789 | 7.5043 |
| | | | | 7.5979 | |
| | | | | 7.6169 | |
| | | | | 7.6331 | |
| | | | | 7.6546 | |
| | | | | 7.6735 | |

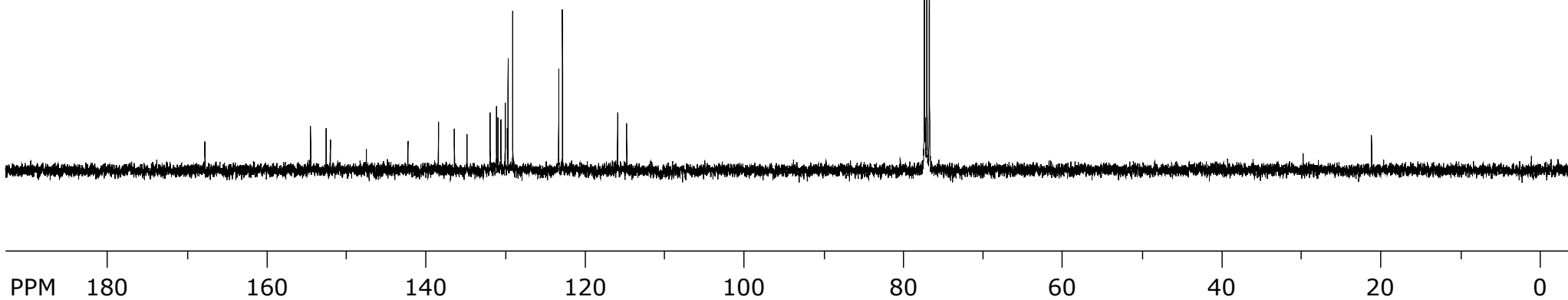
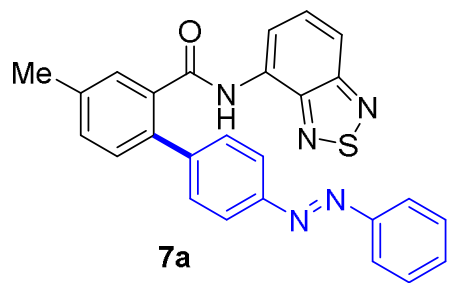


SpinWorks 4: SS 176 P REP
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 4

167.817
154.526
152.049
147.508
142.298
138.465
136.452
134.864
131.957
131.152
130.982
130.596
130.062
129.782
129.707
129.118
129.336
122.861
115.933
114.783

76.725
77.042
77.360

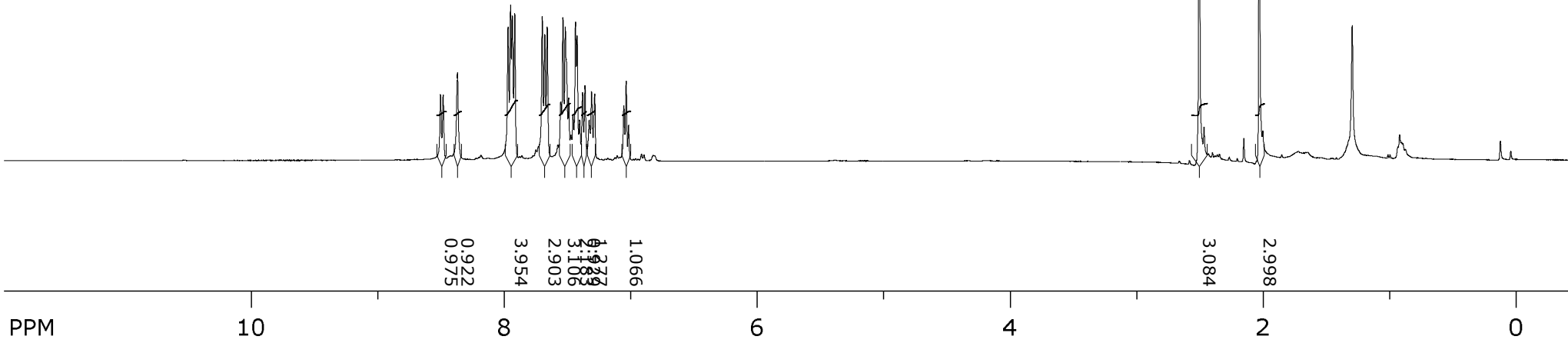
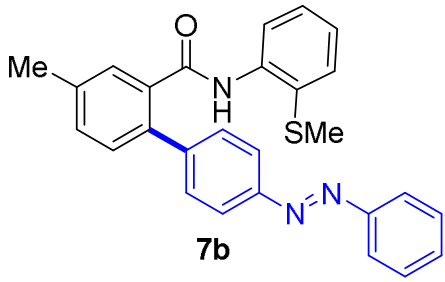
21.134



SpinWorks 4: S S 138 P
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 27

7.0185
7.0374
7.0559
7.2866
7.3109
7.3299
7.3633
7.3827
7.3910
7.3910
7.3910
7.3910
7.6623
7.6814
7.7014
7.9189
7.9382
7.9519
8.3728
8.4857
8.5062

1.2917
2.0272
2.5024



SpinWorks 4: S S 138 P
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 27

8.4857
8.5062

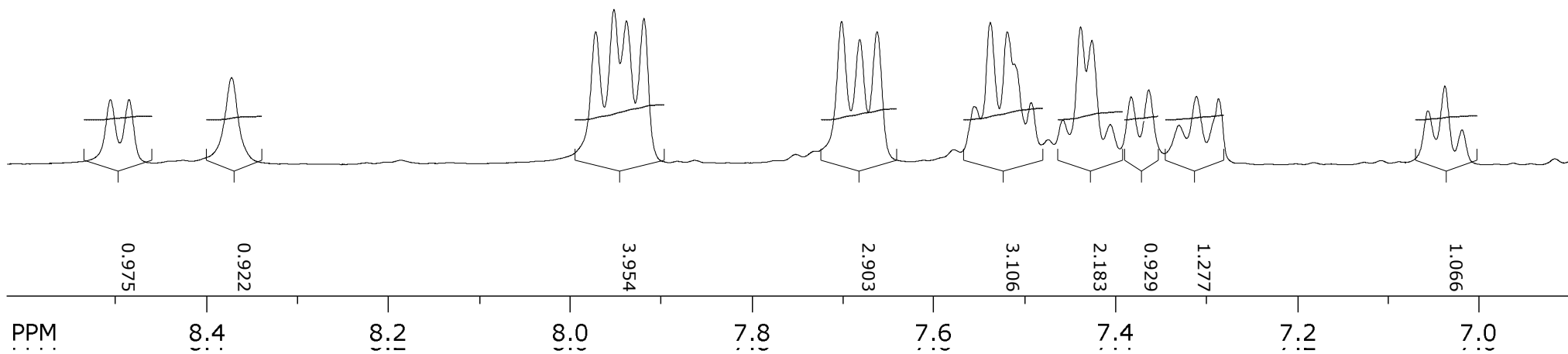
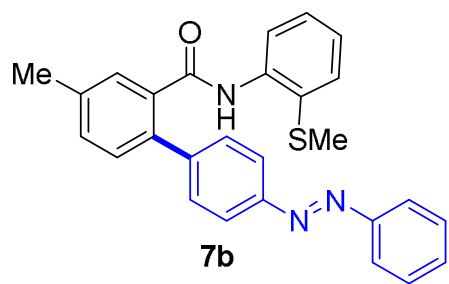
8.3728

7.9189
7.9382
7.9519
7.9720

7.6623
7.6814
7.7014

7.2866
7.3109
7.3299
7.3633
7.3827
7.4057
7.4258
7.4383
7.4578
7.4926
7.5113
7.5191
7.5376
7.5553

7.0185
7.0374
7.0559

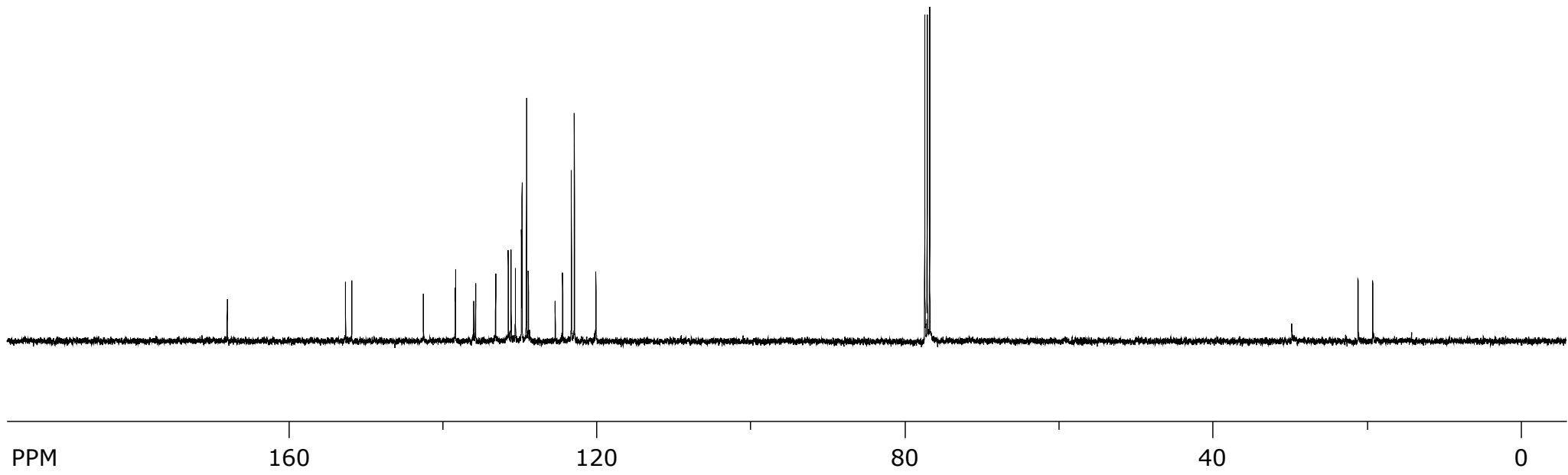
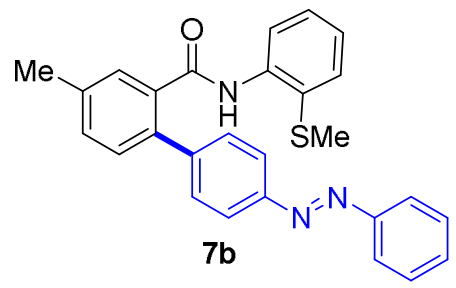


SpinWorks 4: S S 138 P
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 27

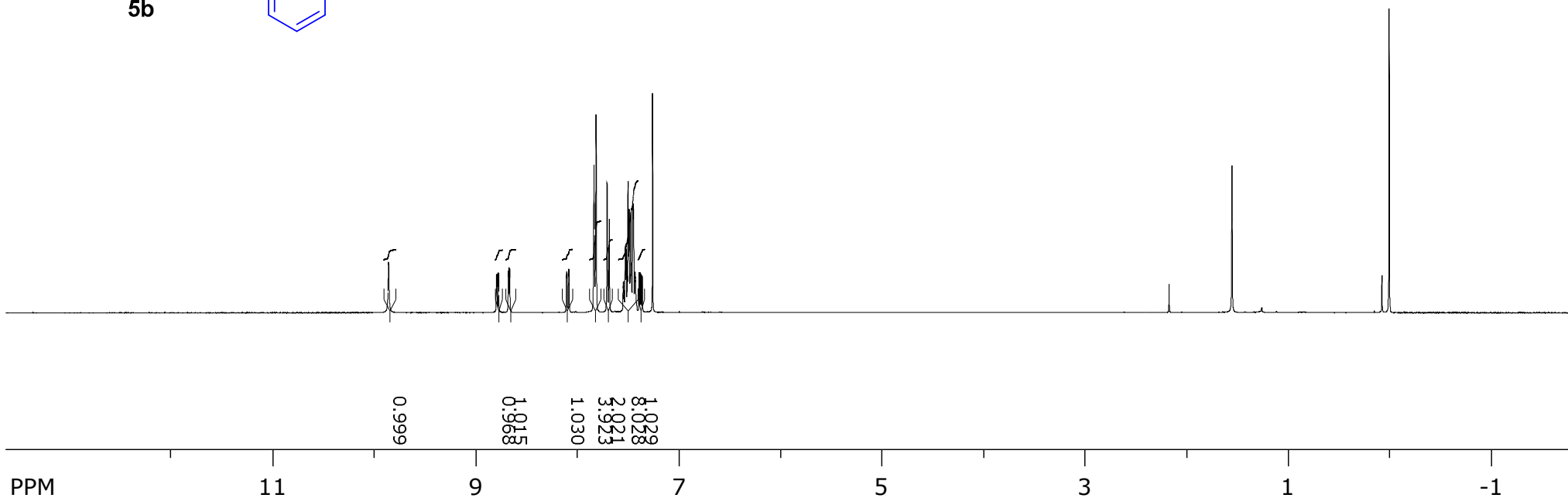
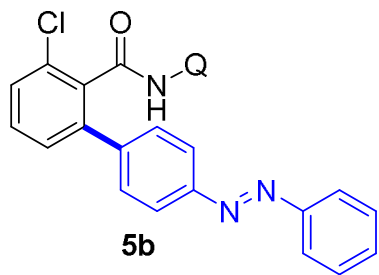
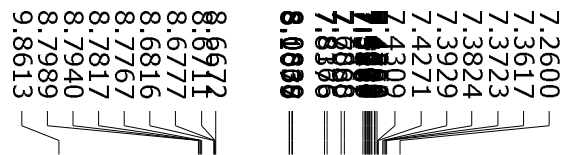
167.992
152.624
151.826
142.521
138.376
138.351
135.987
135.751
133.136
131.499
131.136
130.578
129.716
129.131
128.893
125.407
124.444
123.304
122.912
120.113

76.772
77.090
77.407

19.234
21.136



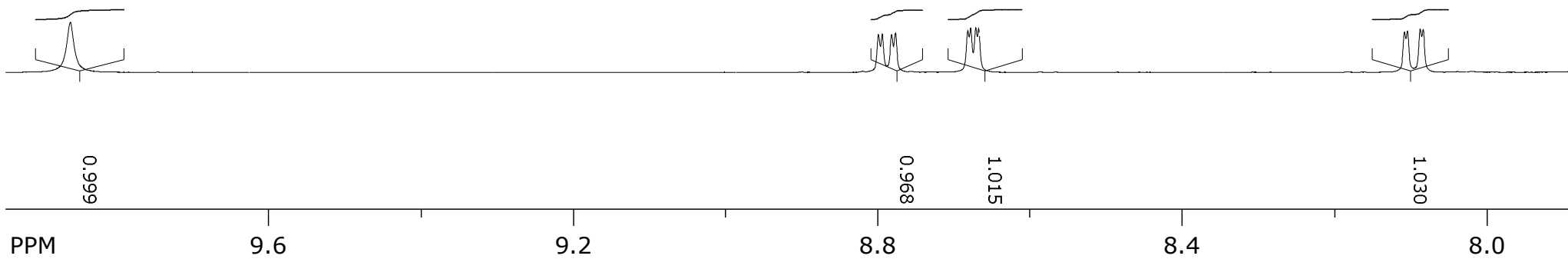
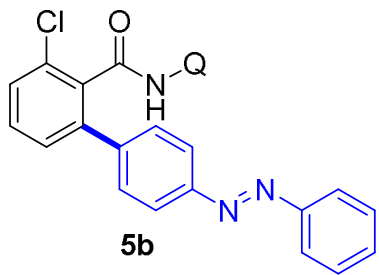
SS-41-p rep



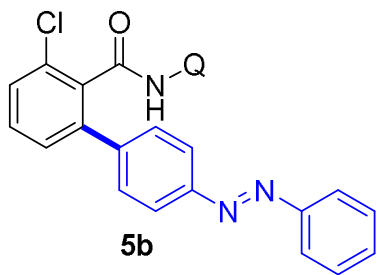
9.8613

8.6672
8.6711
8.6777
8.6816
8.7767
8.7817
8.7940
8.7989

8.0830
8.0868
8.1037
8.1075



SpinWorks 4: DC-175



7.8376

7.8166

7.7080

7.6868

7.5467

7.5305

7.5197

7.5097

7.5022

7.4968

7.4908

7.4812

7.4736

7.4551

7.4500

7.4350

7.4309

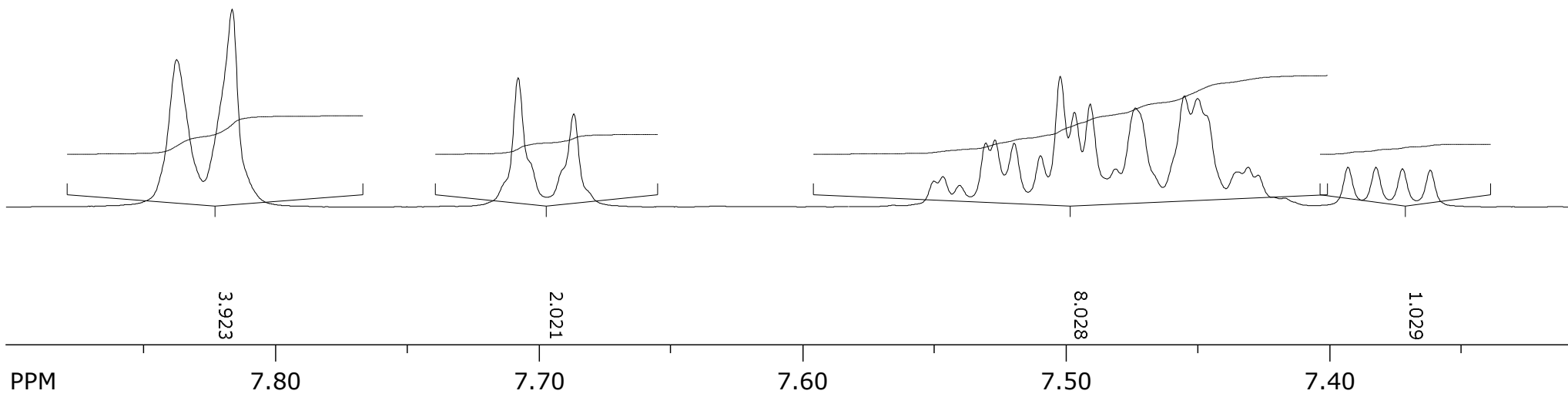
7.4271

7.3929

7.3824

7.3723

7.3617

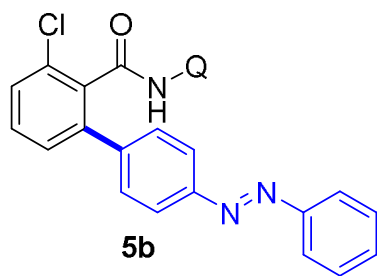


SpinWorks 4: SS 41 P REP

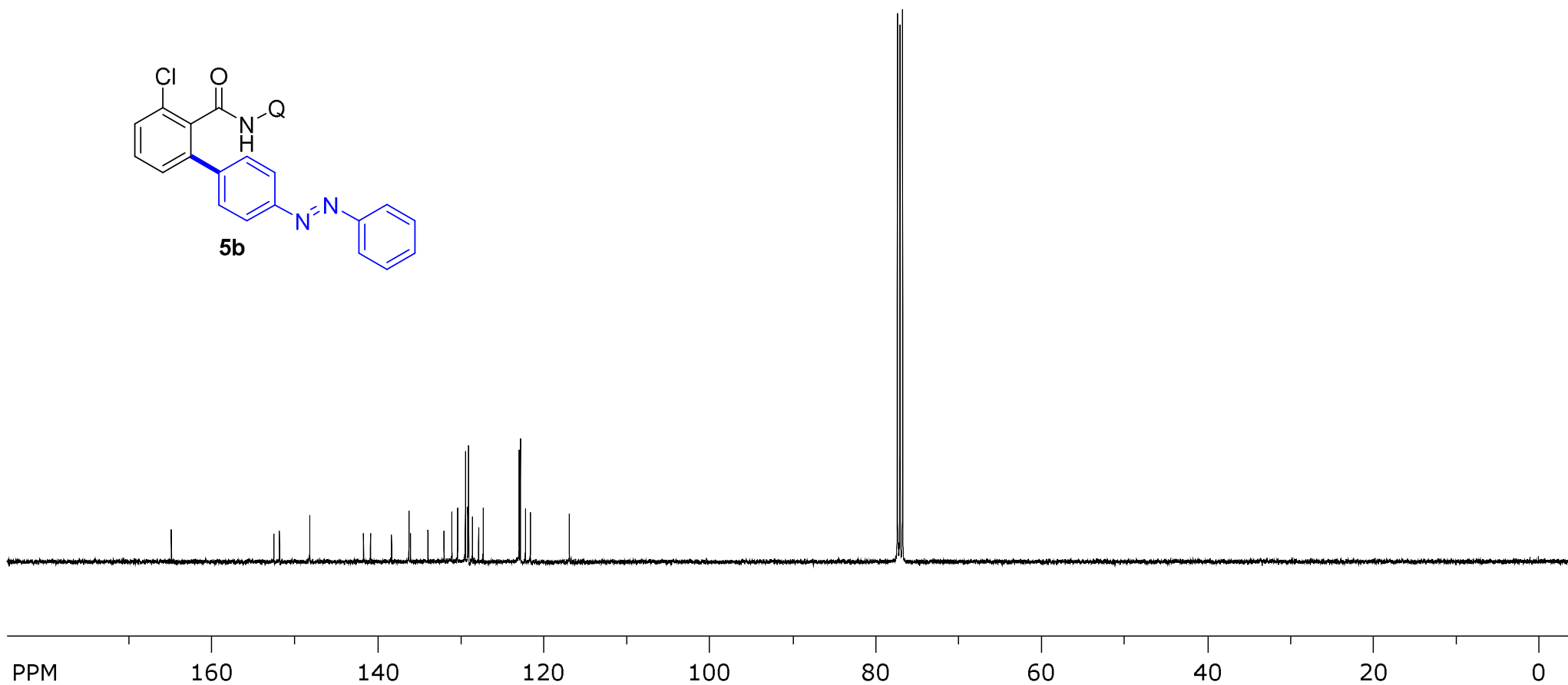
C13CPD CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 59

164.942
152.566
151.894
148.235
141.760
140.915
138.381
136.275
133.989
133.076
132.047
131.105
130.405
129.489
128.622
127.882
127.313
122.988
122.835
122.223
121.626
116.934

76.734
77.051
77.369



5b



SpinWorks 4: SS 41 P REP
C13CPD CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 59

164.942

151.894
152.566

148.235

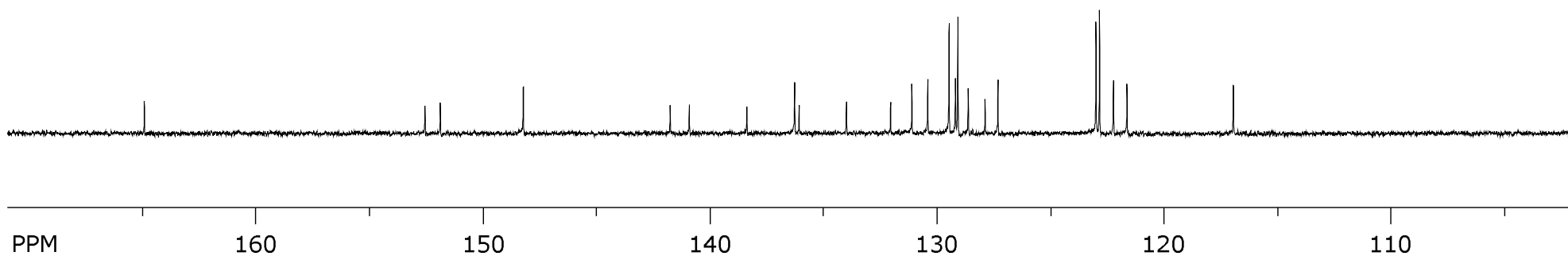
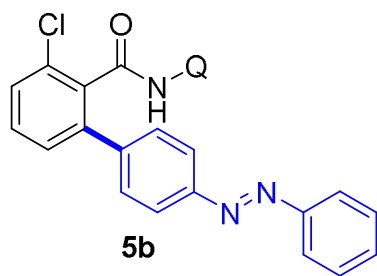
140.915
141.760

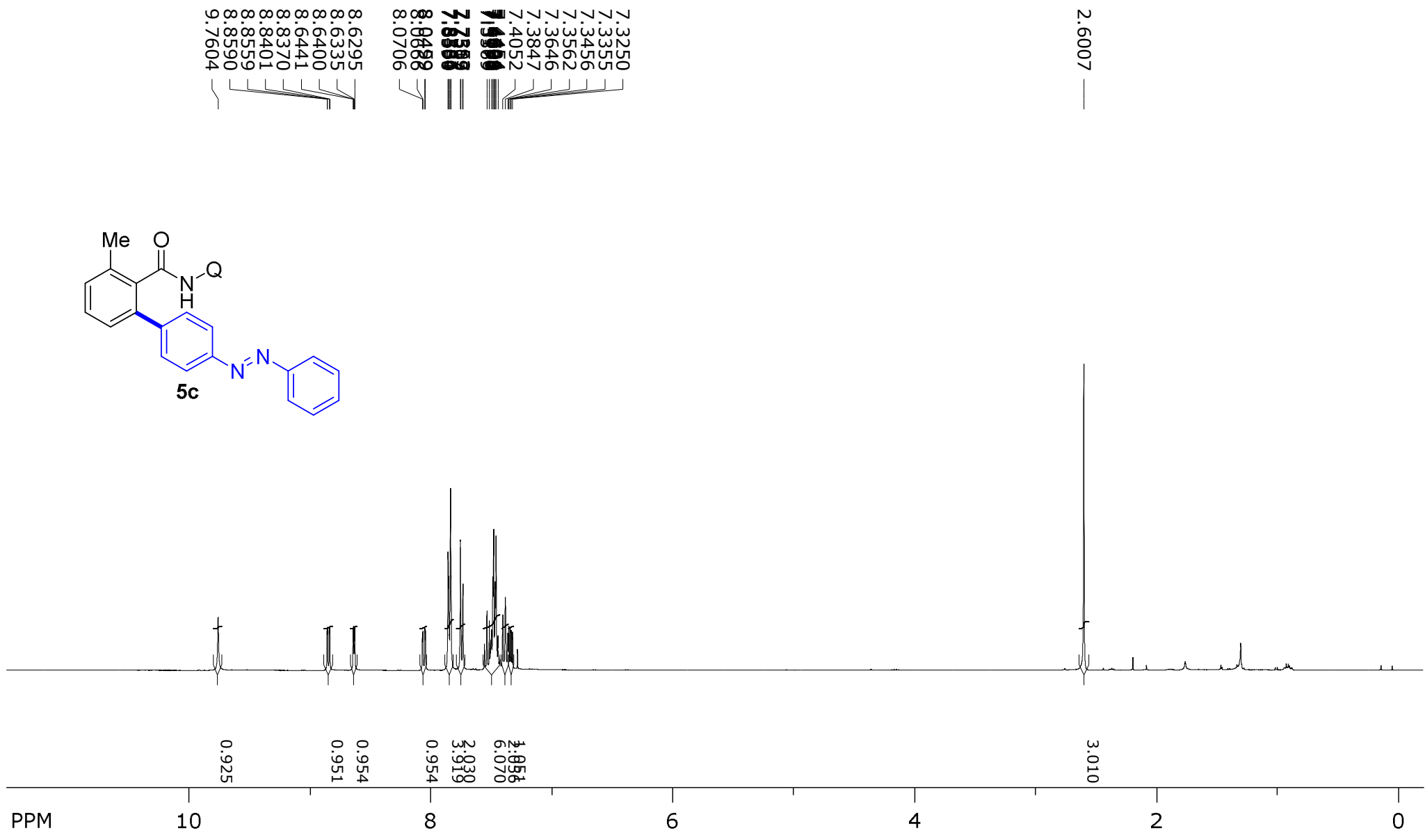
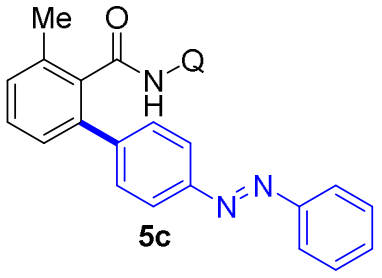
138.381
136.076
136.275

133.989
132.047
131.105
130.405
129.467
129.186
129.080
128.622
127.882
127.313

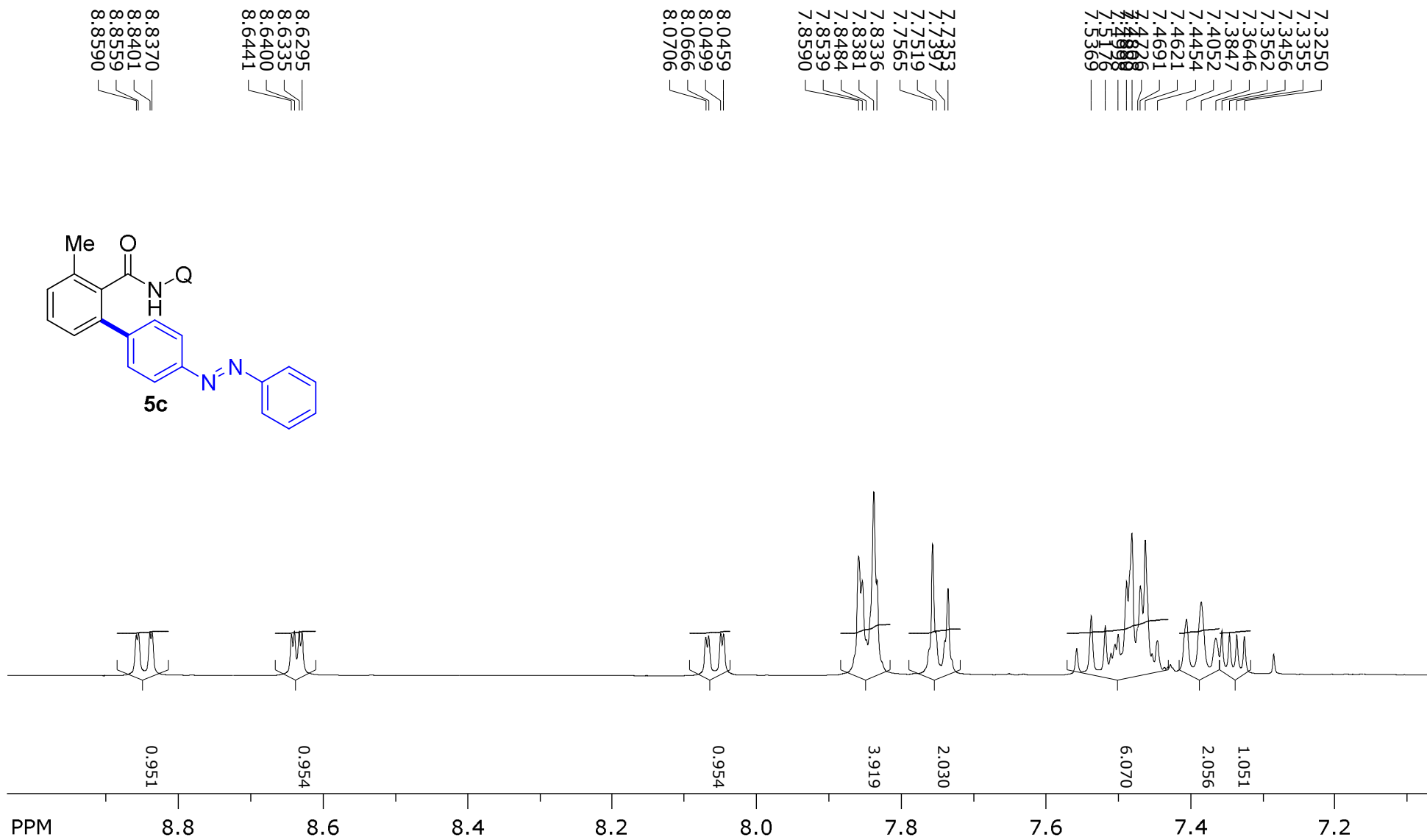
122.988
122.835
122.223
121.626

116.934



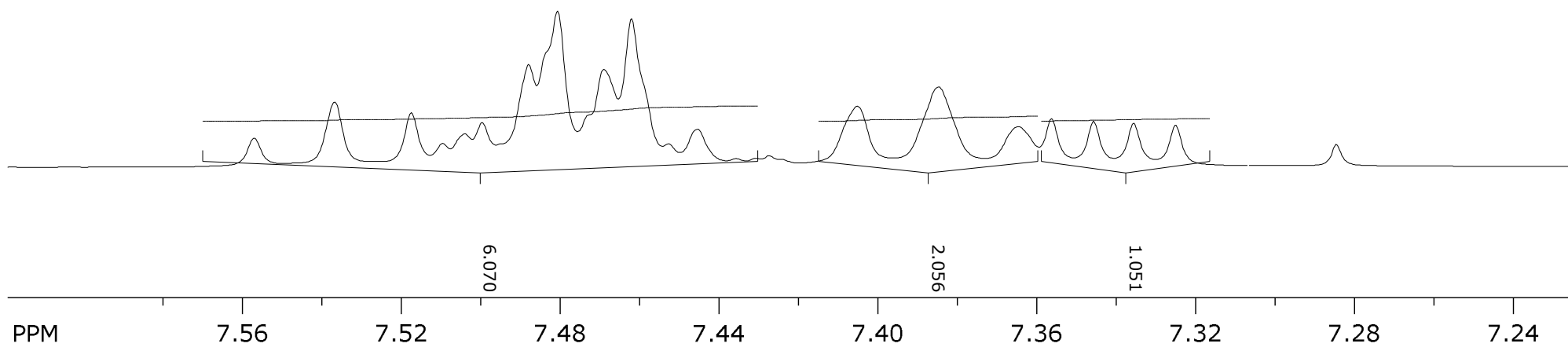
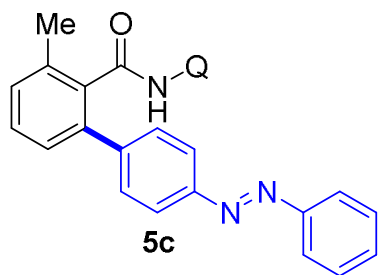


SpinWorks 4: ss-68-p (trans2)



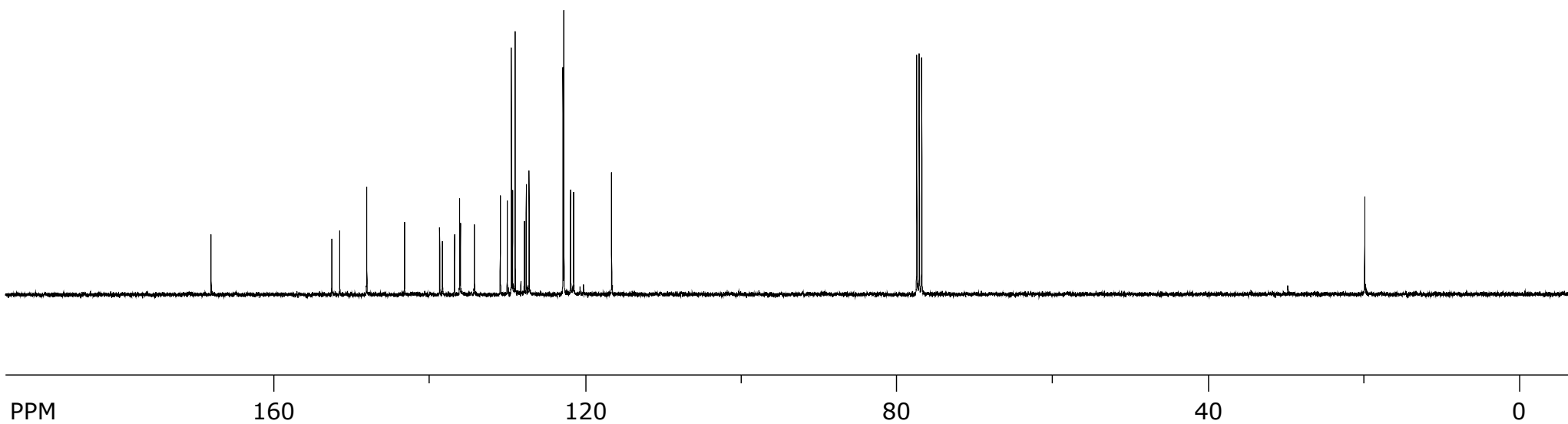
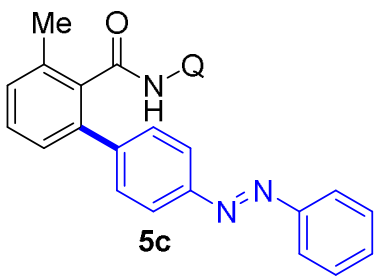
SpinWorks 4: ss-68-p (trans2)

7.5369 —
7.5176 —
7.4998 —
7.4880 —
7.4808 —
7.4726 —
7.4691 —
7.4621 —
7.4454 —
7.4052 —
7.3847 —
7.3646 —
7.3562 —
7.3456 —
7.3355 —
7.3250 —

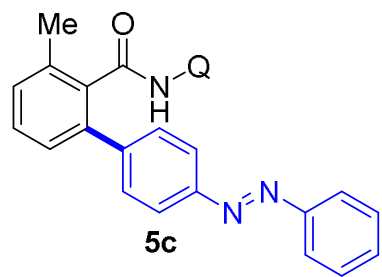


SpinWorks 4: SS 68 P
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 58

168.127 —
152.610
148.116
143.261
138.747
138.403
136.845
136.170
136.082
134.287
130.953
130.061
129.950
127.847
127.622
127.249
122.896
122.787
121.943
121.532
116.655
76.799
77.116
77.435
19.873 —



SpinWorks 4: SS 68 P
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 58



168.127 —

151.595 —
152.610 —

148.116 —

143.261 —

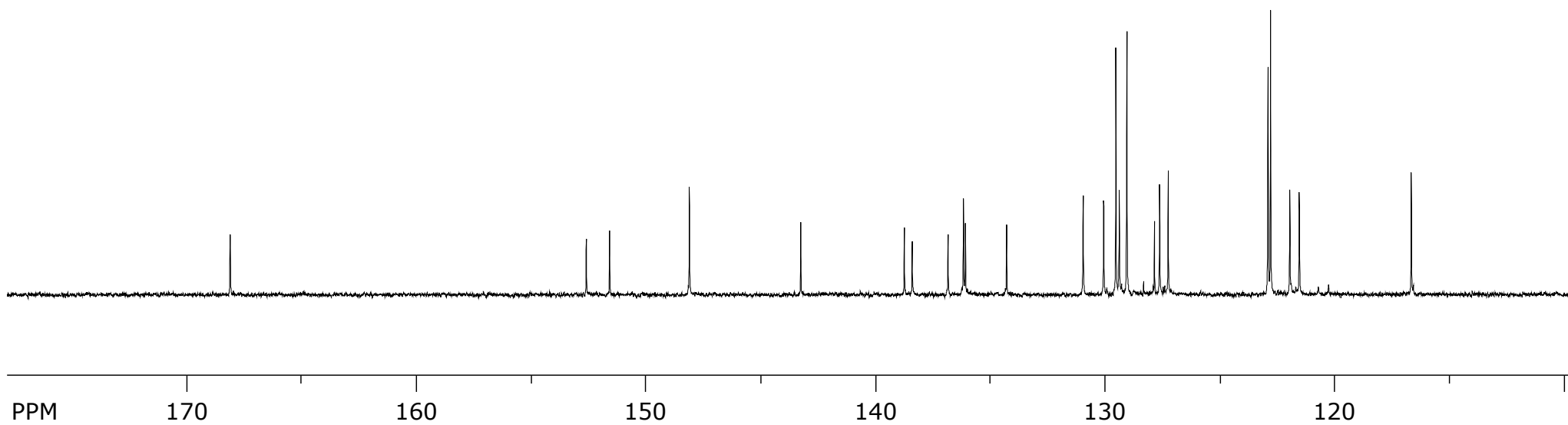
138.747 —
138.403 —
136.845 —
136.170 —
136.082 —

134.287 —

130.953 —
130.061 —
129.526 —
129.380 —
129.050 —
127.847 —
127.622 —
127.249 —

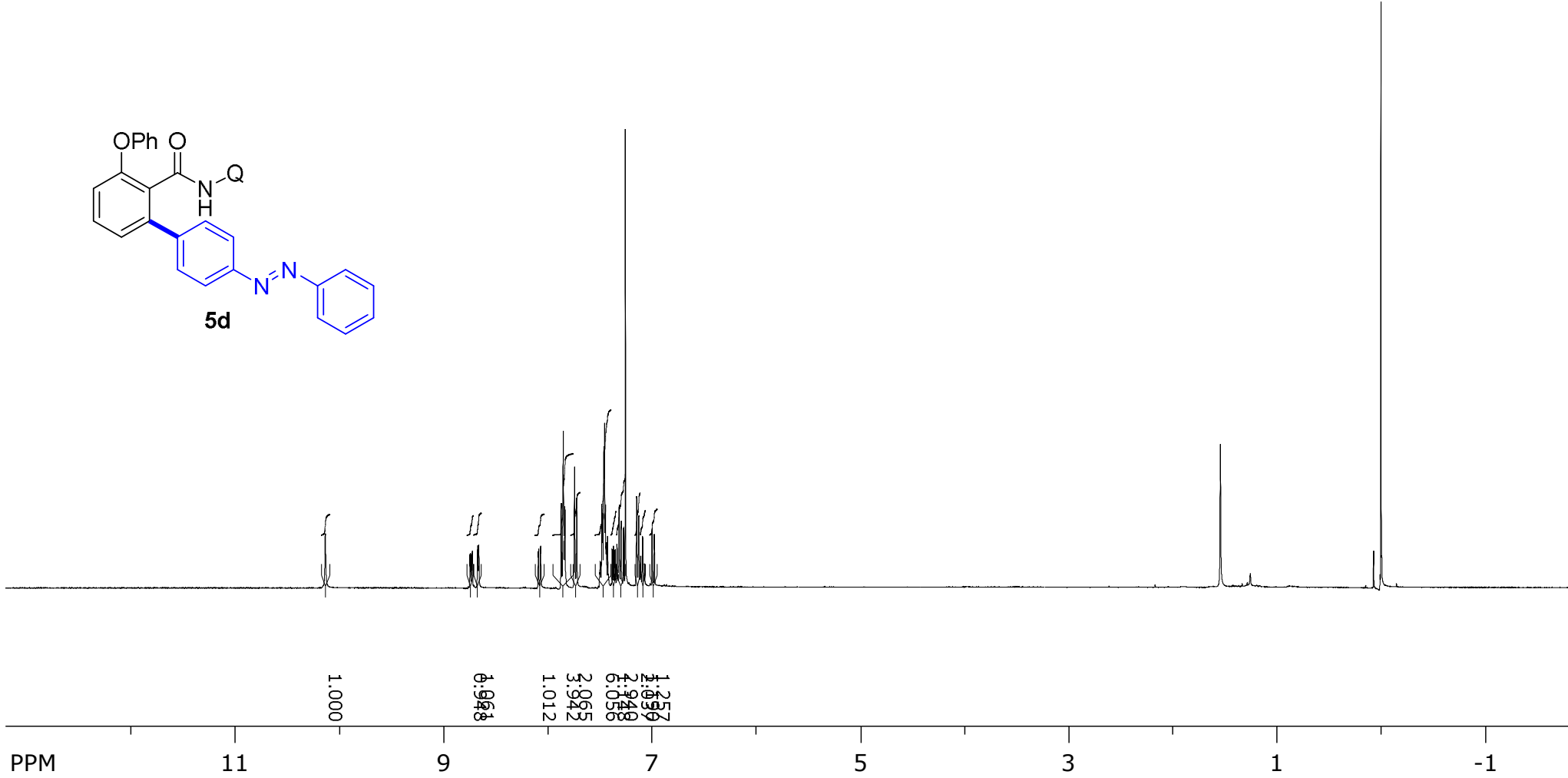
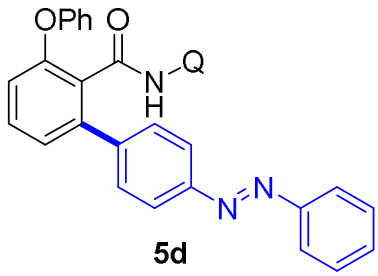
122.896 —
122.787 —
121.943 —
121.532 —

116.655 —

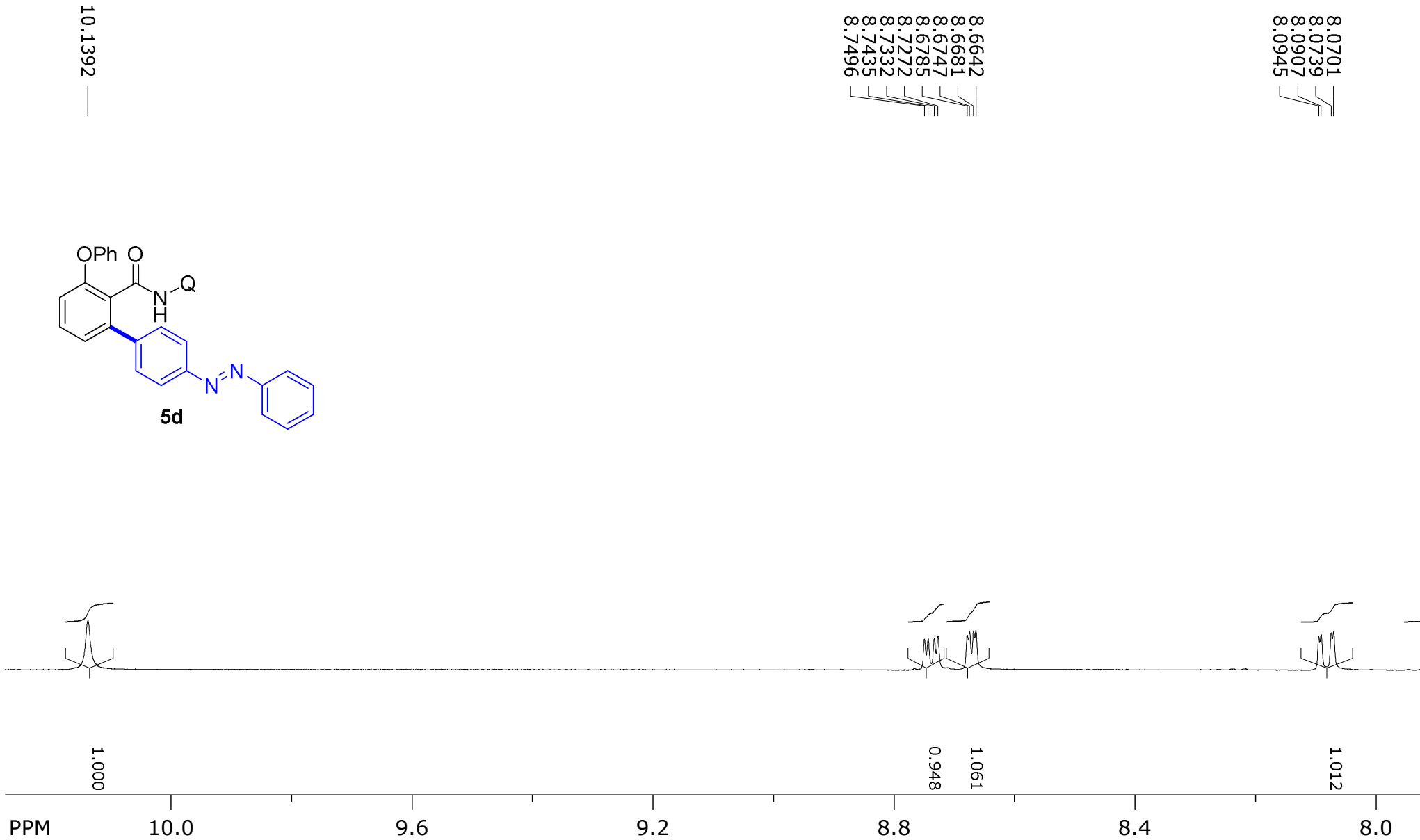
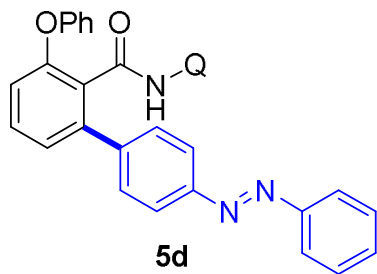


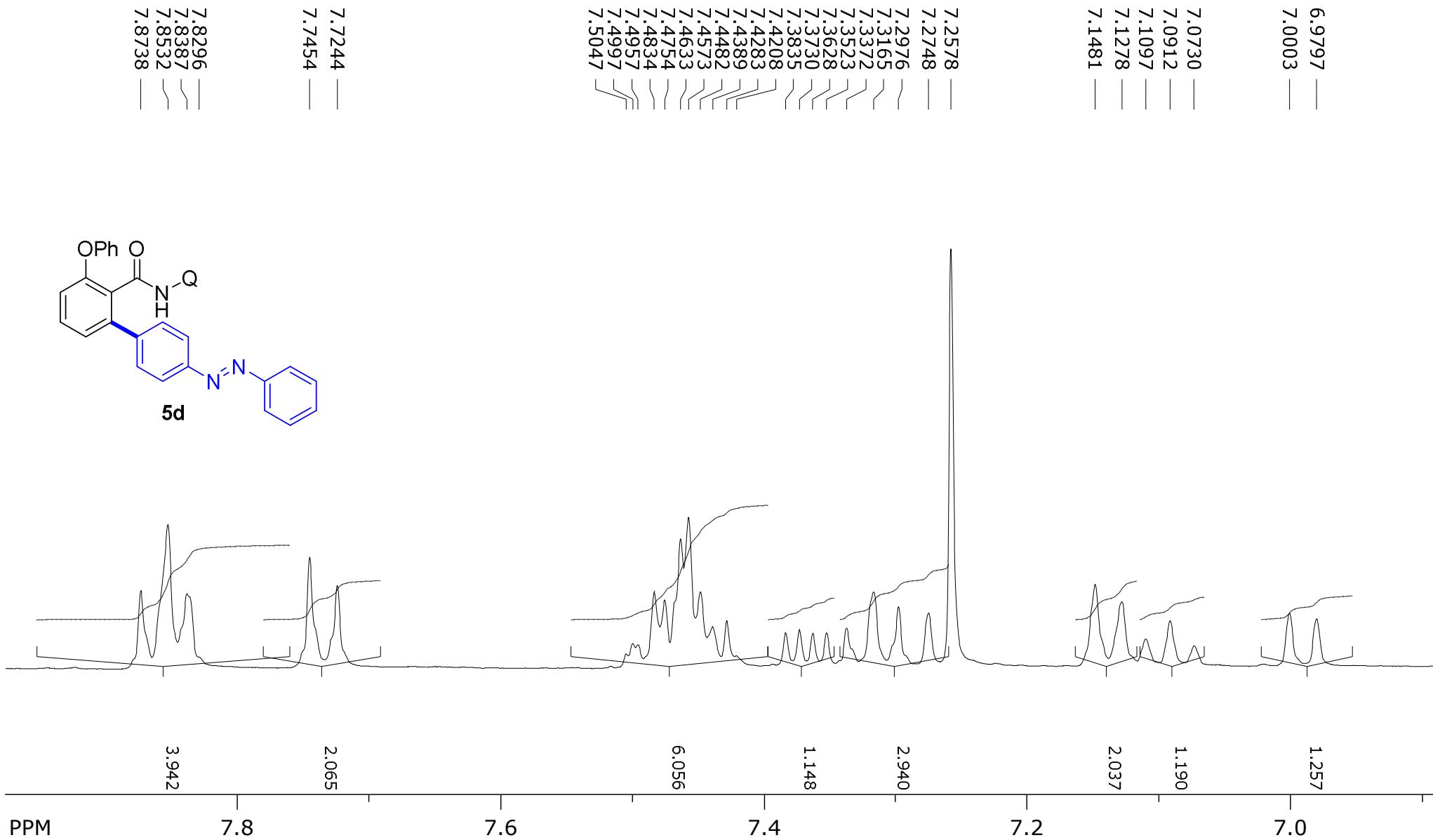
SpinWorks 4: DC-176
SS-78-p rep

8.66842
8.66811
8.67477
8.6785
8.7272
8.7332
8.7435
8.7496
10.1392
6.9797
7.0003
7.0730
7.0912
7.1097
7.1278
7.1481
7.2578
7.3014
7.3014
7.3014
8.0909



SpinWorks 4: DC-176

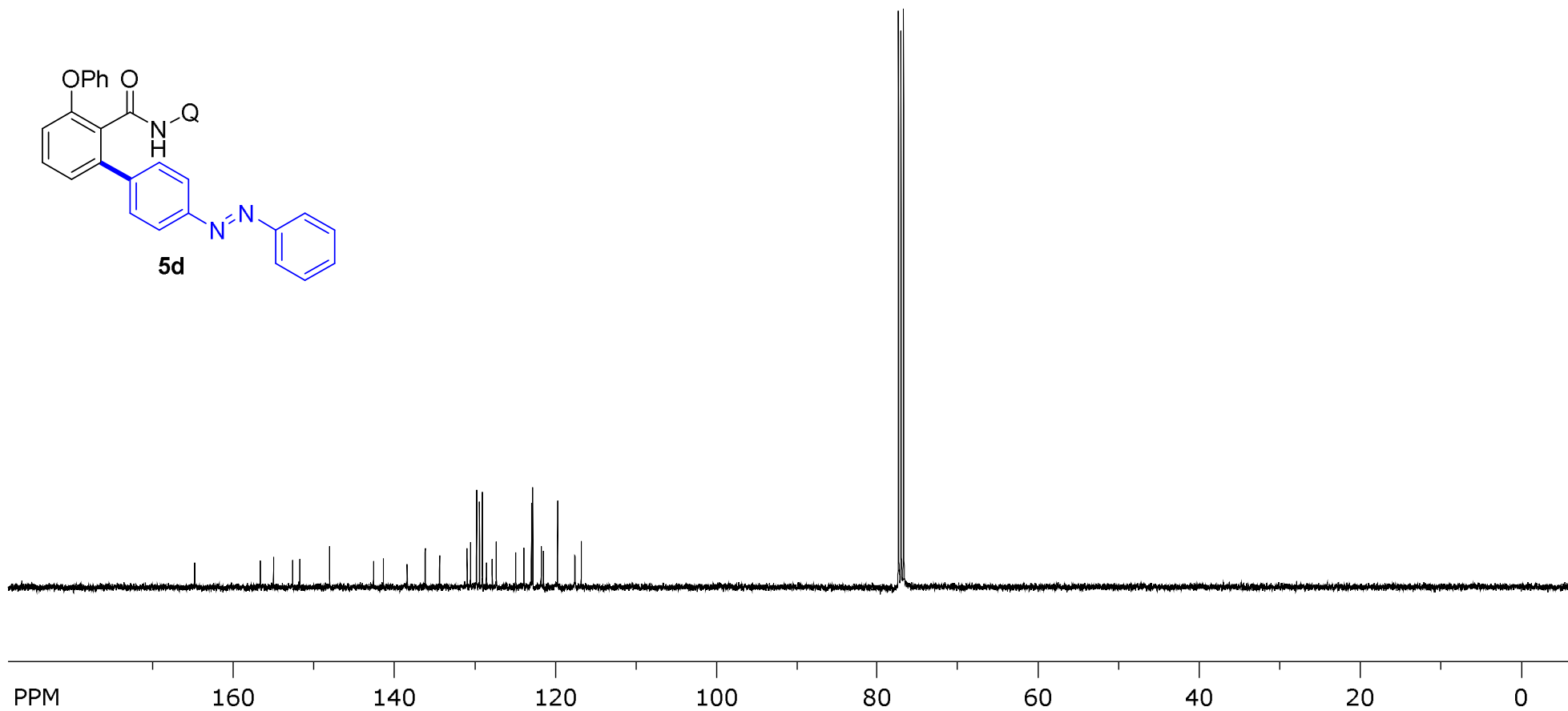
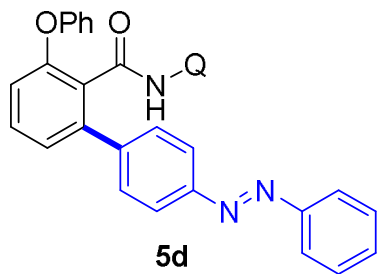




SpinWorks 4: SS 78 P REP
C13CPD CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 49

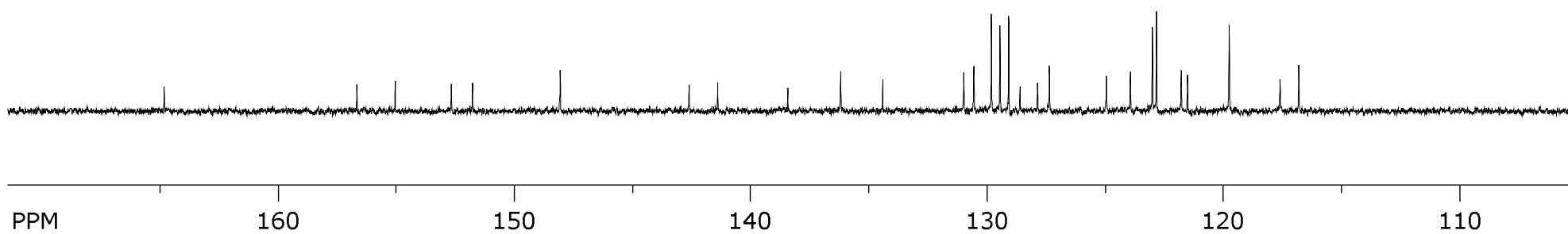
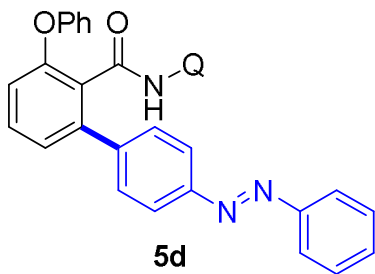
116.790
117.583
119.738
121.505
121.767
122.819
122.986
123.922
124.940
126.819
126.819
129.806
130.550
130.980
134.407
136.188
138.426
141.393
142.608
148.065
151.774
152.672
155.050
156.671
164.831

76.732
77.049
77.367



SpinWorks 4: SS 78 P REP
C13CPD CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 49

164.831 —
156.671 —
155.050 —
152.672 —
151.774 —
148.065 —
142.608 —
141.393 —
138.426 —
136.188 —
134.407 —
130.980 —
130.550 —
129.806 —
129.445 —
129.074 —
128.595 —
127.854 —
127.356 —
124.940 —
123.922 —
122.986 —
122.819 —
121.767 —
121.505 —
119.738 —
117.583 —
116.790 —

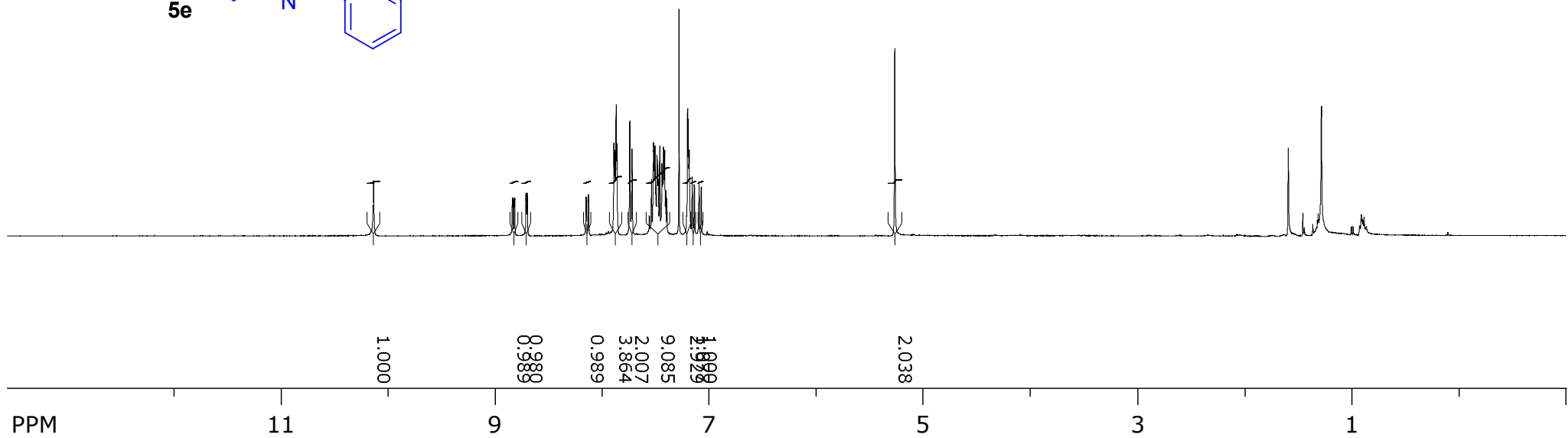
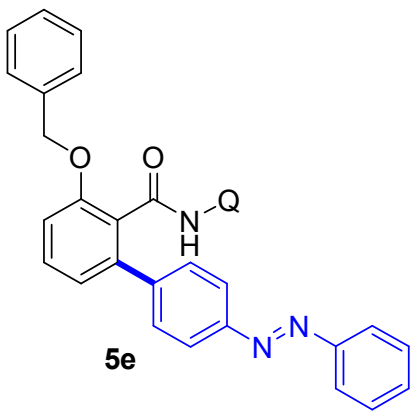


SpinWorks 4: SS-779
PROTON_32 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 2

8.7001
8.7040
8.7105
8.7144
8.8190
8.8235
8.8368
8.8413
10.1387

8.1889
7.7234
7.6918
7.1920
7.1874
7.1596
7.1406
7.0960
7.0754

5.2672

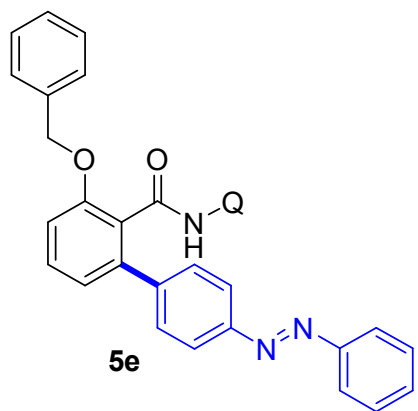


SpinWorks 4: SS-779
PROTON_32 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 2

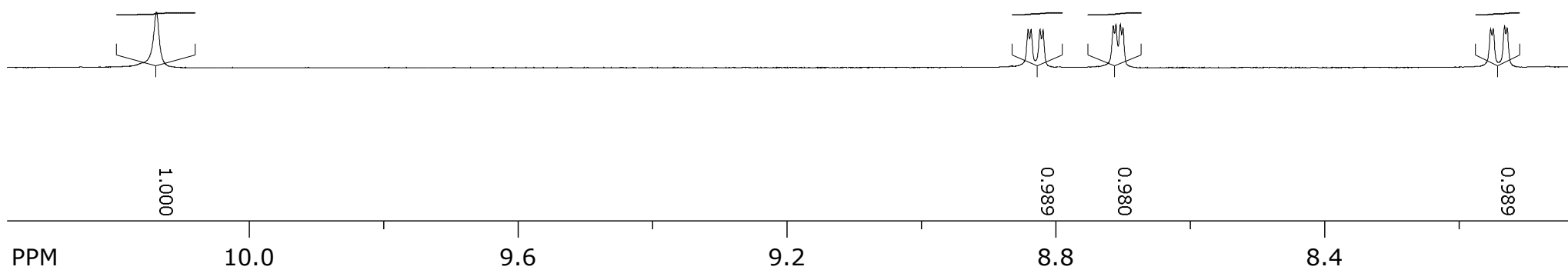
10.1387

8.7001
8.7040
8.7105
8.7144
8.8190
8.8235
8.8368
8.8413

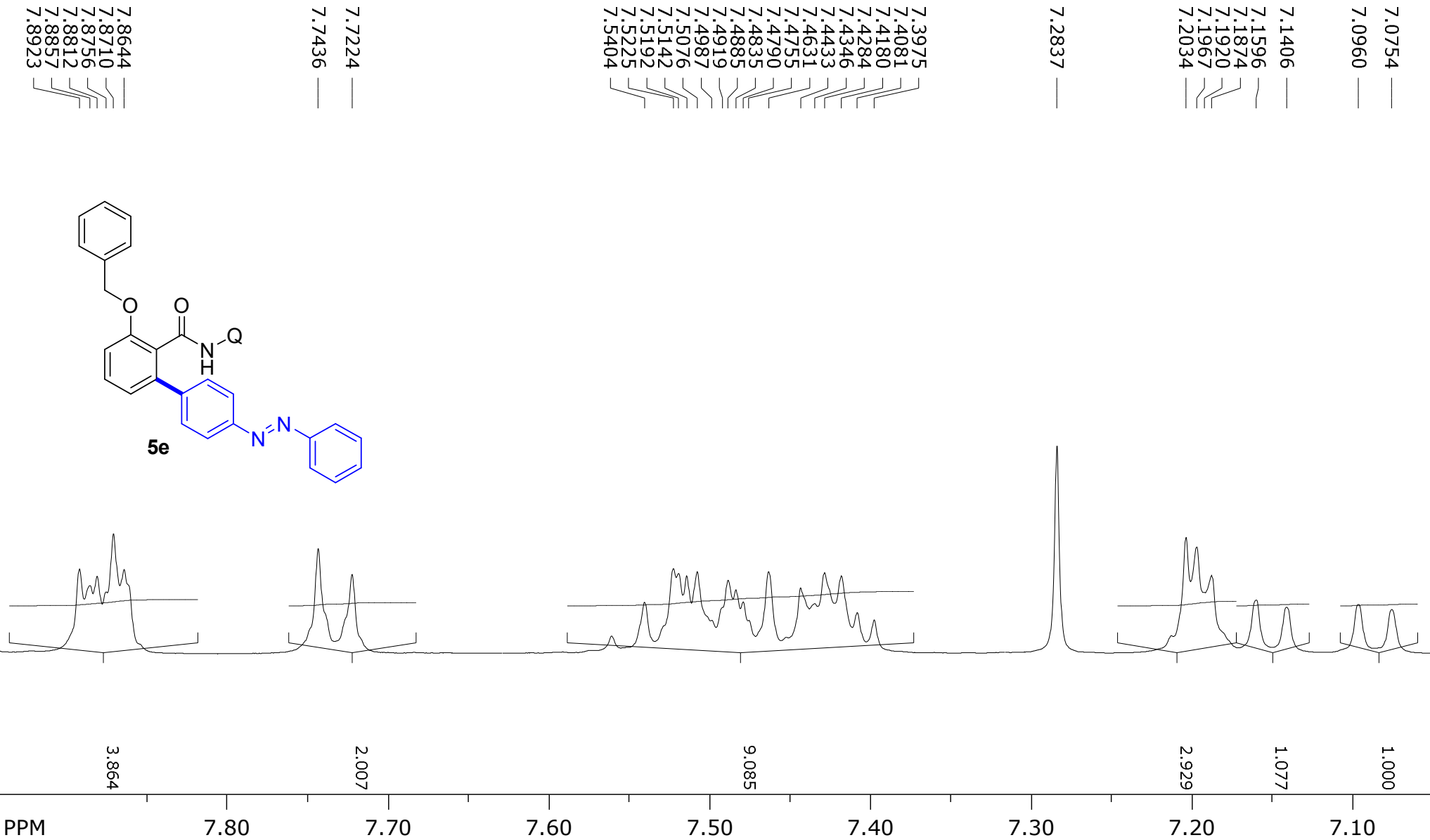
8.1282
8.1320
8.1489
8.1527



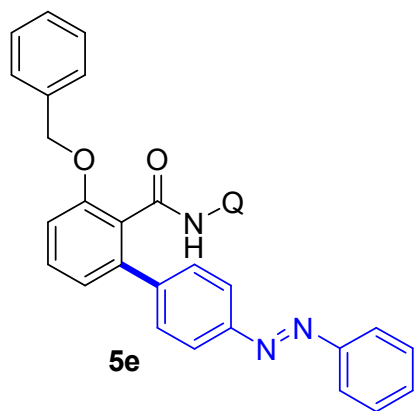
5e



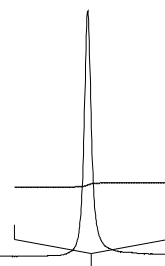
SpinWorks 4: SS-779
PROTON_32 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 2



SpinWorks 4: SS-779
PROTON_32 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 2



5.2672



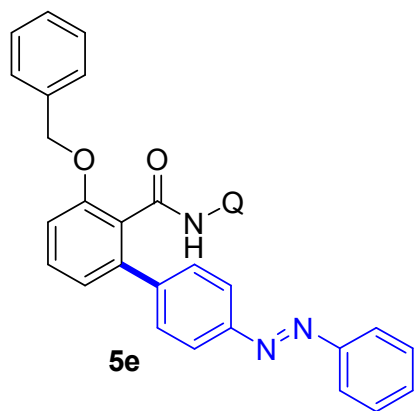
2.038

PPM 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6

SpinWorks 4: SS 779
C13CPD CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 1

112.288
116.781
121.480
121.665
122.805
122.857
126.890
126.892
130.921
134.589
136.219
136.680
138.433
141.072
142.966
148.013
151.693
152.692
155.756
165.600

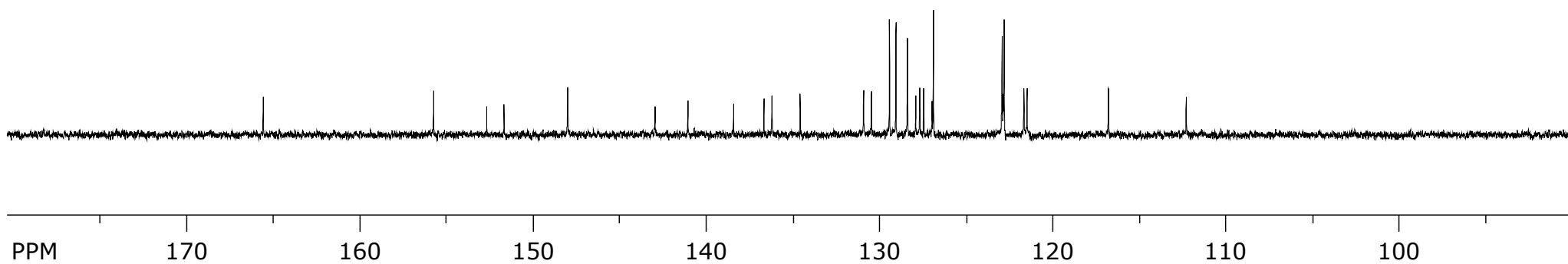
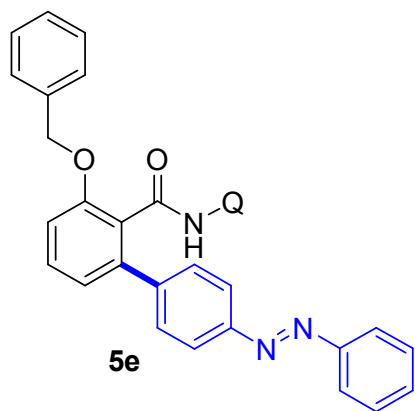
70.542
76.732
77.049
77.367



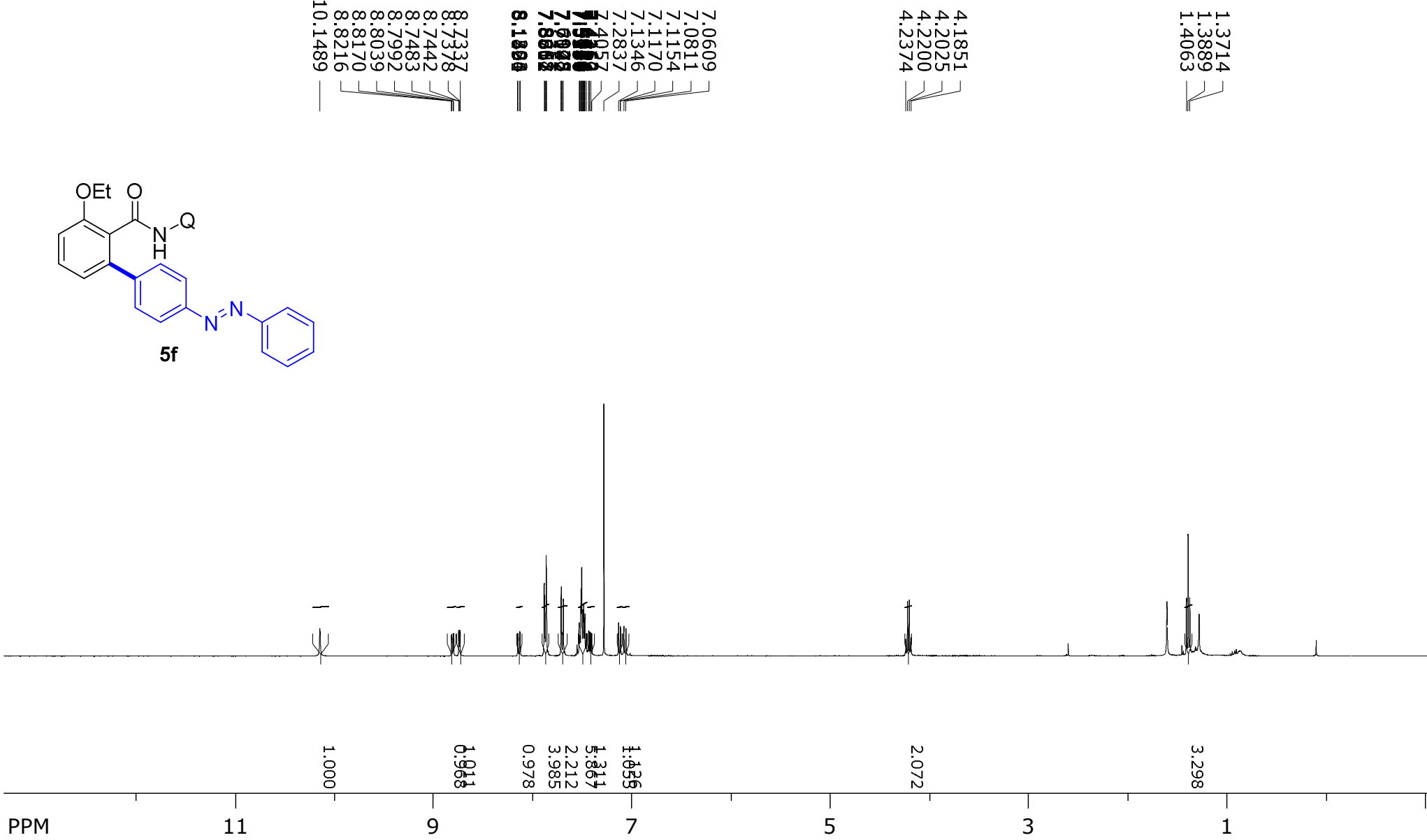
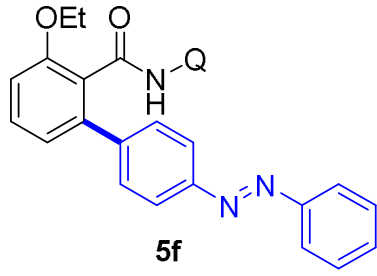
PPM 160 120 80 40 0

SpinWorks 4: SS 779
C13CPD CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 1

165.600 —
155.756 —
151.693 —
152.692 —
148.013 —
142.966 —
141.072 —
138.433 —
136.680 —
134.589 —
130.921 —
130.472 —
129.428 —
129.058 —
128.388 —
127.911 —
127.680 —
127.455 —
126.971 —
126.890 —
122.928 —
122.857 —
122.805 —
121.665 —
121.480 —
116.781 —
112.288 —



SpinWorks 4: SS-801
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 2

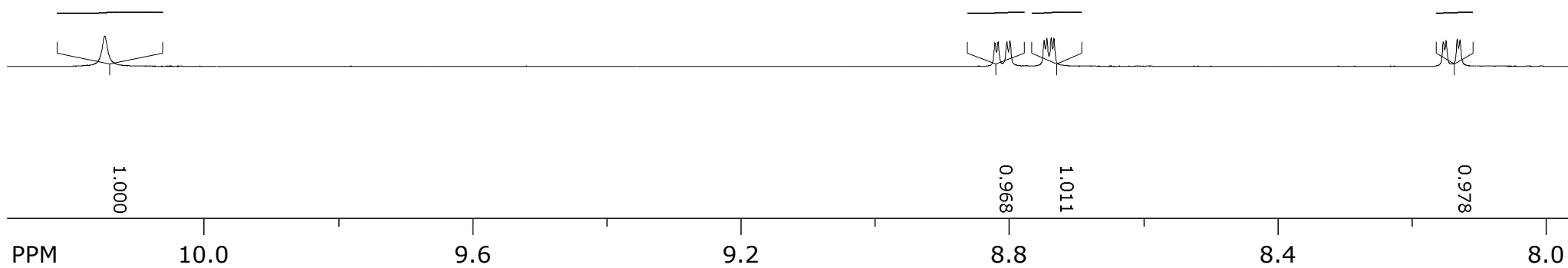
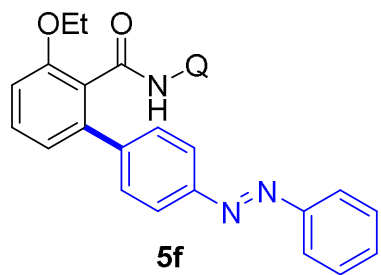


SpinWorks 4: SS-801
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 2

10.1489

8.7337
8.7378
8.7442
8.7483
8.7992
8.8039
8.8170
8.8216

8.1283
8.1324
8.1490
8.1531



SpinWorks 4: SS-801
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 2

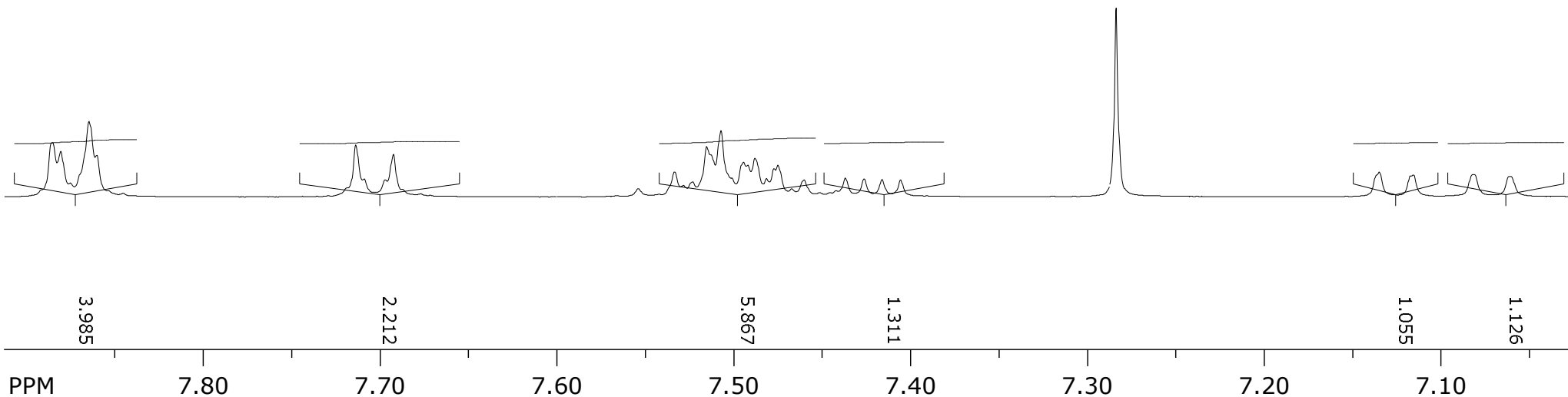
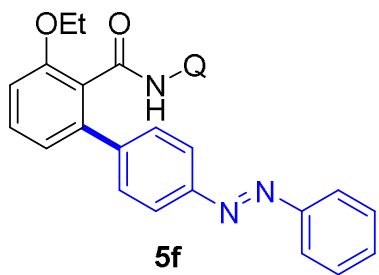
7.86608
7.86552
7.87572
7.88112
7.88661

7.69228
7.69775
7.7095
7.7142
7.7192

7.4057
7.4162
7.4263
7.4369
7.4604
7.4751
7.4774
7.4816
7.4882
7.4923
7.4946
7.5013
7.5074
7.5132
7.5154
7.5235
7.5286
7.5336

7.2837

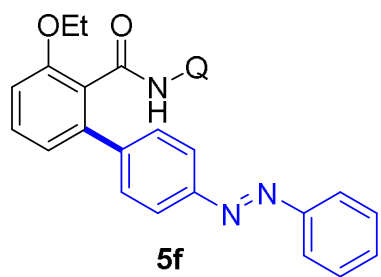
7.0609
7.0811
7.1154
7.1346



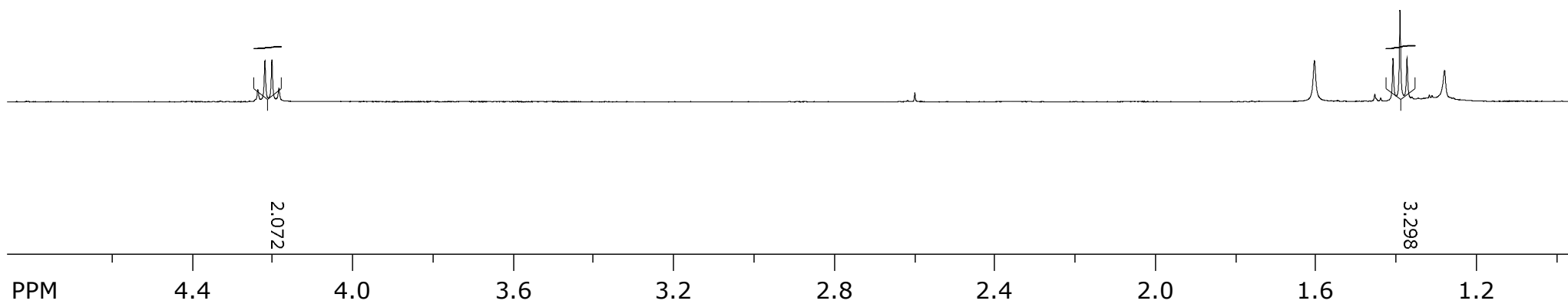
SpinWorks 4: SS-801
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 2

4.1851
4.2025
4.2200
4.2374

1.3714
1.3889
1.4063



5f

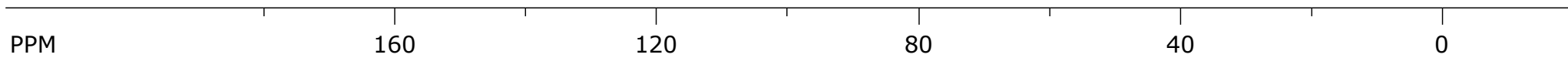
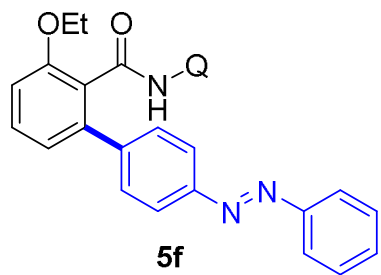


SpinWorks 4: SS-801
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 33

111.673
116.741
121.485
121.546
122.517
122.789
122.889
126.520
127.420
129.048
129.368
130.513
130.875
134.717
136.215
138.522
141.264
143.342
148.014
151.628
152.712
156.196
165.619

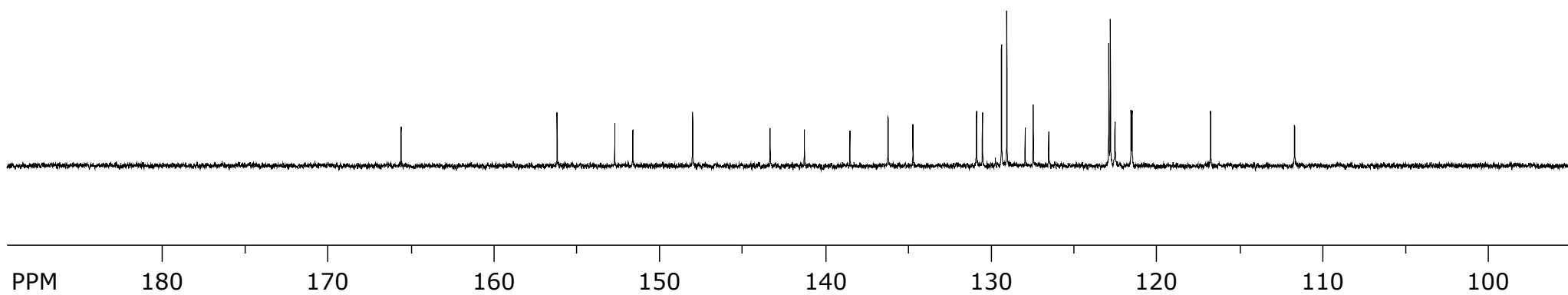
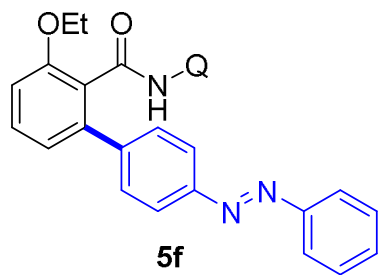
64.628
76.733
77.051
77.369

14.696



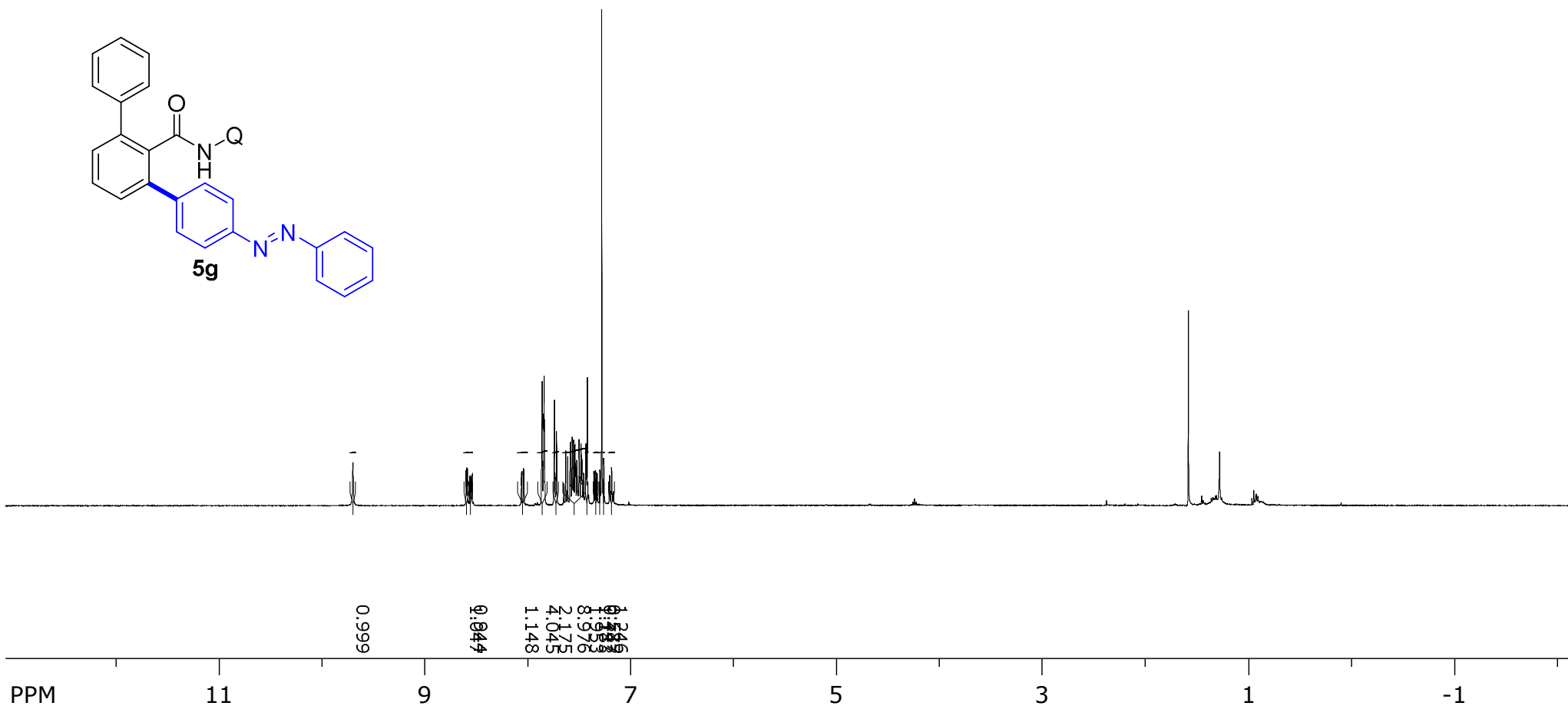
SpinWorks 4: SS-801
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 33

165.619 —
156.196 —
151.628 —
152.712 —
148.014 —
143.342 —
141.264 —
138.522 —
136.215 —
134.717 —
130.875 —
130.513 —
129.368 —
129.043 —
127.940 —
126.520 —
122.889 —
122.789 —
121.517 —
121.485 —
121.546 —
116.741 —
111.673 —



SpinWorks 4: SS 796
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 1

8.5436
8.5576
8.5576
8.5661
8.5888
8.5930
8.5994
8.6035
9.7031
8.0648
7.9988
7.9988
7.9988
7.9988
7.9988
7.9988
7.9988
7.9988
7.9988
7.9988
7.2062
7.2090
7.2032
7.1877
7.1722
7.1697
7.1667

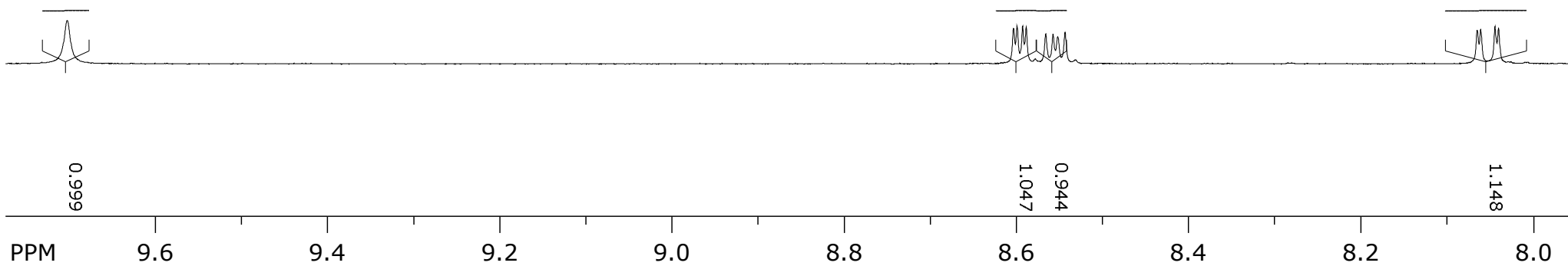
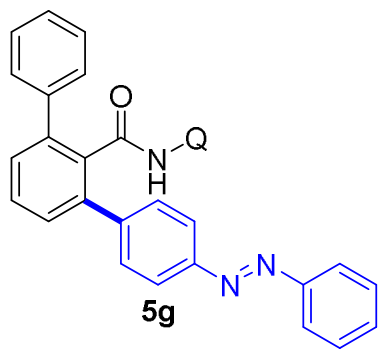


SpinWorks 4: SS 796
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 1

9.7031

8.5436
8.5521
8.5576
8.5661
8.5888
8.5930
8.5994
8.6035

8.0400
8.0441
8.0607
8.0648



SpinWorks 4: SS 796
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 1

7.8375
7.8430
7.8476
7.8516
7.8593
7.8641
7.8686

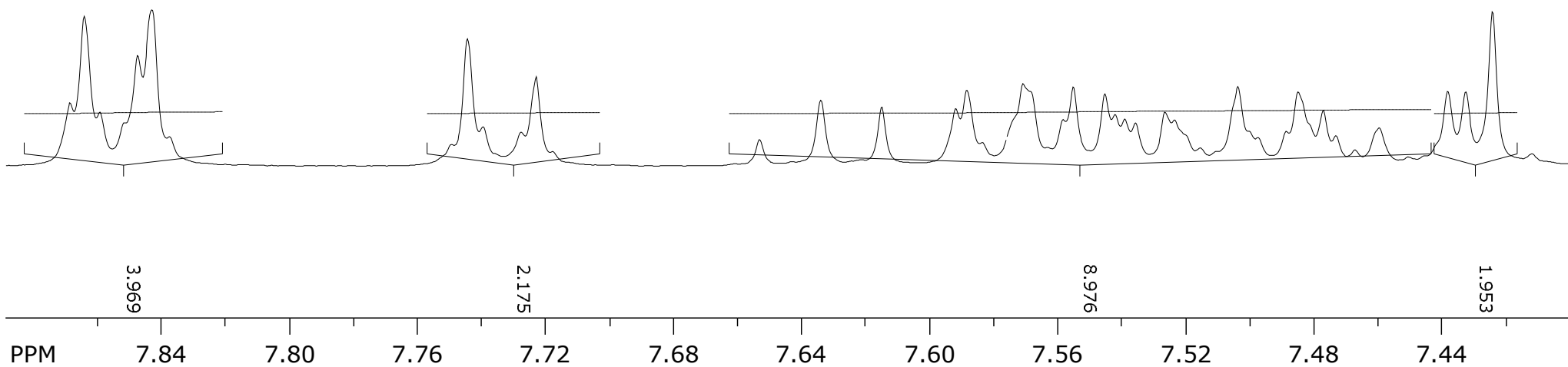
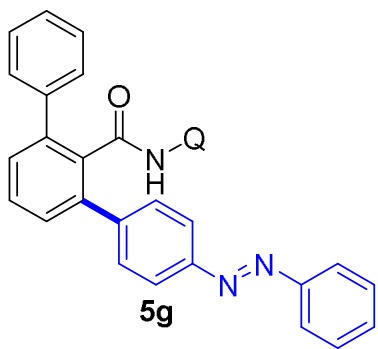
7.7230
7.7277
7.7395
7.7444

7.6532
7.6340
7.6150

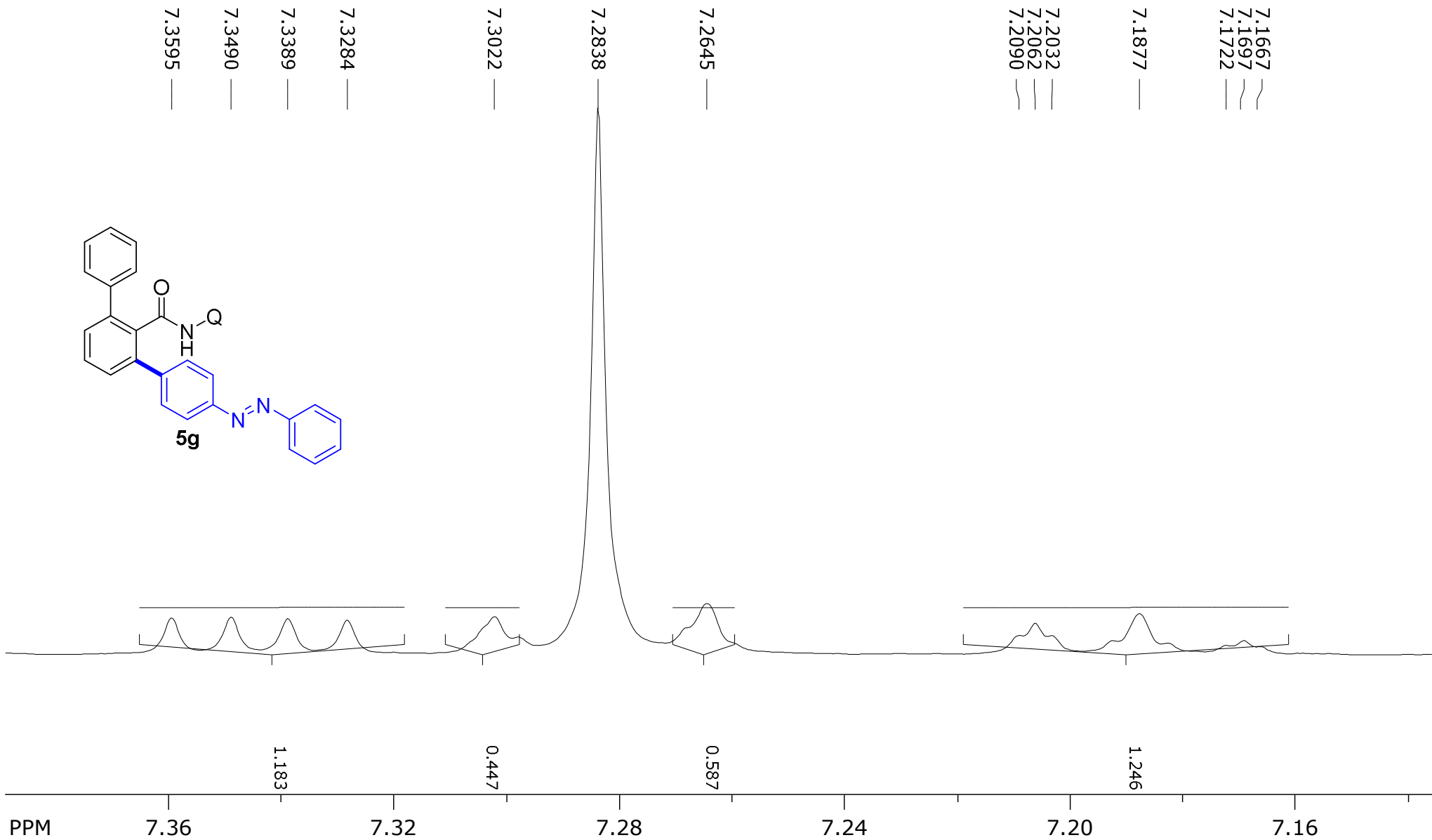
7.5836
7.5884
7.5918
7.5708
7.5583
7.5551
7.5452
7.5420
7.5390
7.5357
7.5264
7.5234

7.5036
7.4973
7.4885
7.4769
7.4730
7.4595

7.4240
7.4325
7.4381



SpinWorks 4: SS 796
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 1

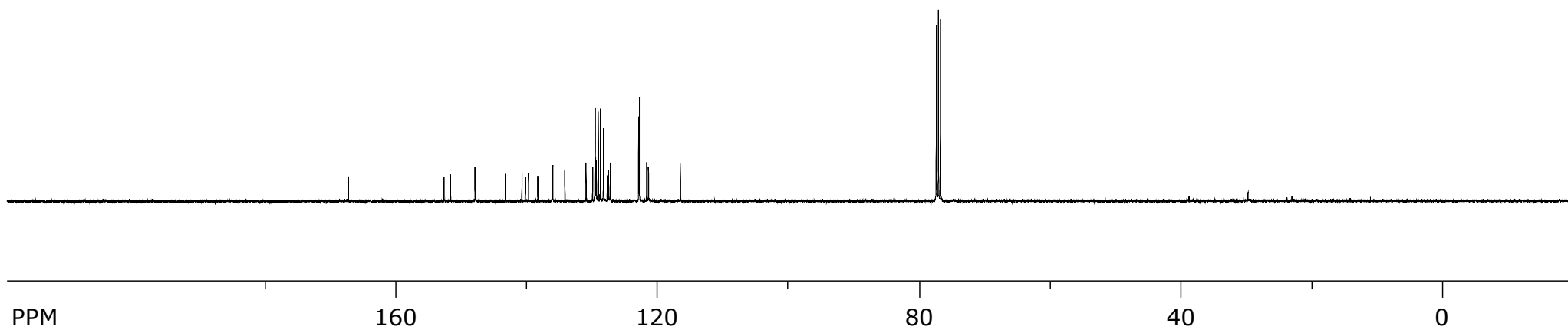
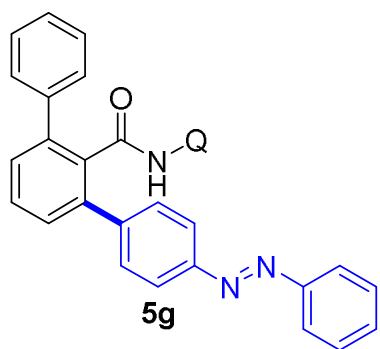


SpinWorks 4: SS-796

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 19

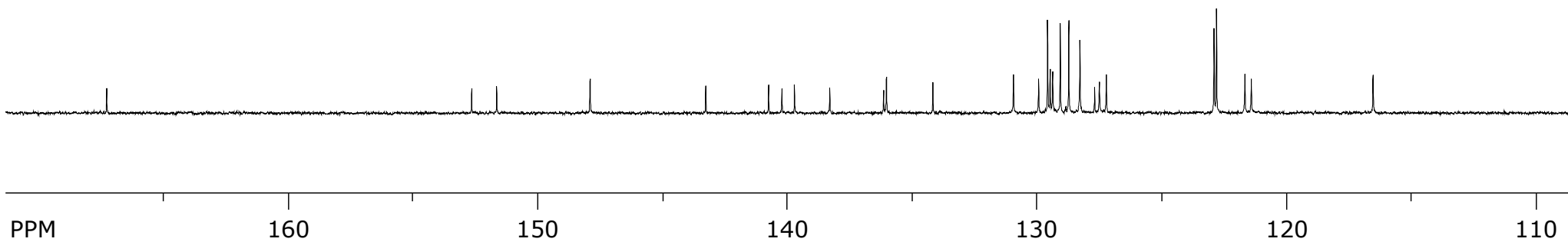
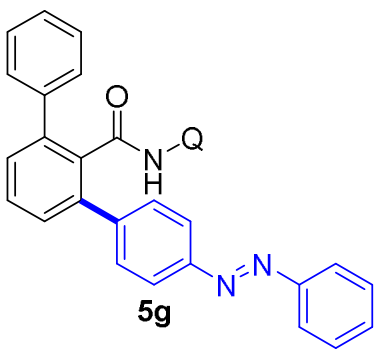
116.519
121.402
121.658
122.795
122.896
127.214
127.493
127.684
127.684
127.684
127.684
134.170
136.031
136.141
138.304
139.718
140.224
140.754
143.276
147.916
151.660
152.662
167.296

76.753
77.071
77.389



SpinWorks 4: SS-796
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 19

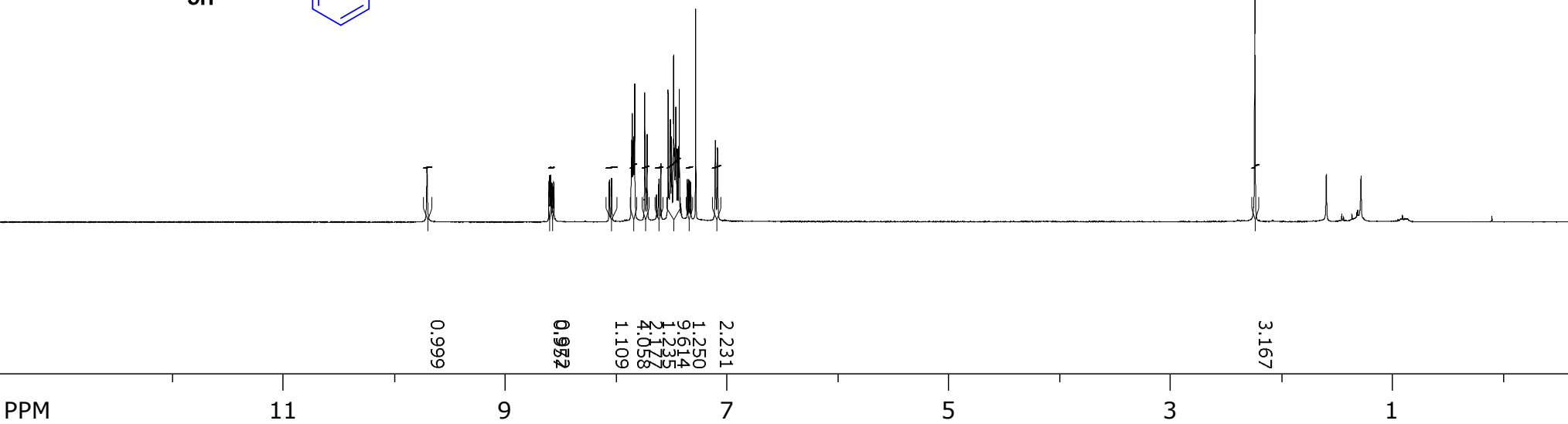
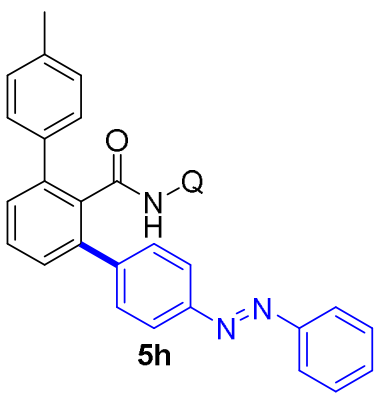
167.296 —
151.660 —
152.662 —
147.916 —
143.276 —
139.718 —
140.224 —
140.754 —
138.304 —
136.031 —
136.141 —
134.170 —
130.939 —
129.929 —
129.566 —
129.364 —
129.061 —
128.717 —
128.273 —
128.684 —
127.493 —
127.214 —
121.402 —
121.658 —
122.795 —
122.896 —
116.519 —



SpinWorks 4: SS 797
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 2

8.5696
8.5790
8.5855
8.5917
8.5959
8.6023
8.6064
9.7070
8.0608
7.9808
7.9608
7.9408
7.9208
7.3585
7.3480
7.3379
7.3273
7.2837
7.1053
7.0856

2.2392

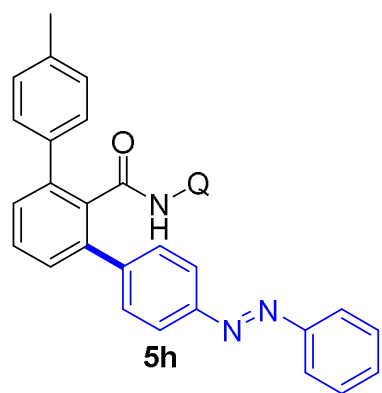


SpinWorks 4: SS 797
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 2

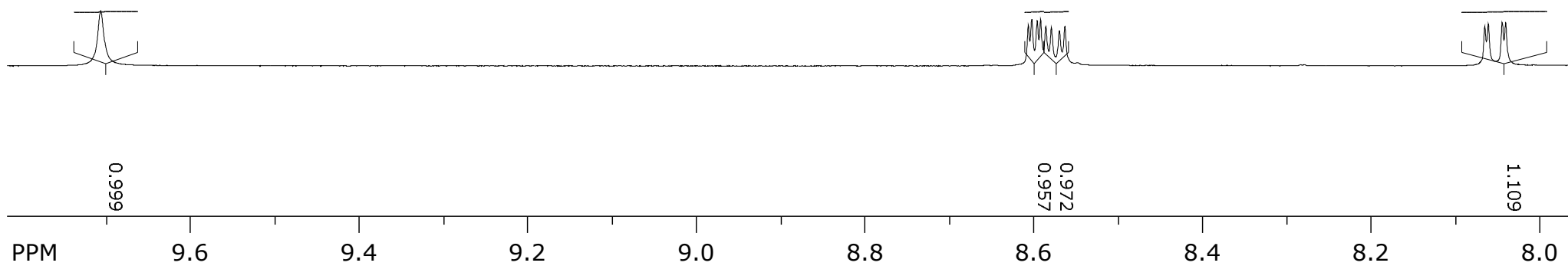
9.7070

8.5631
8.5696
8.5790
8.5855
8.5917
8.5959
8.6023
8.6064

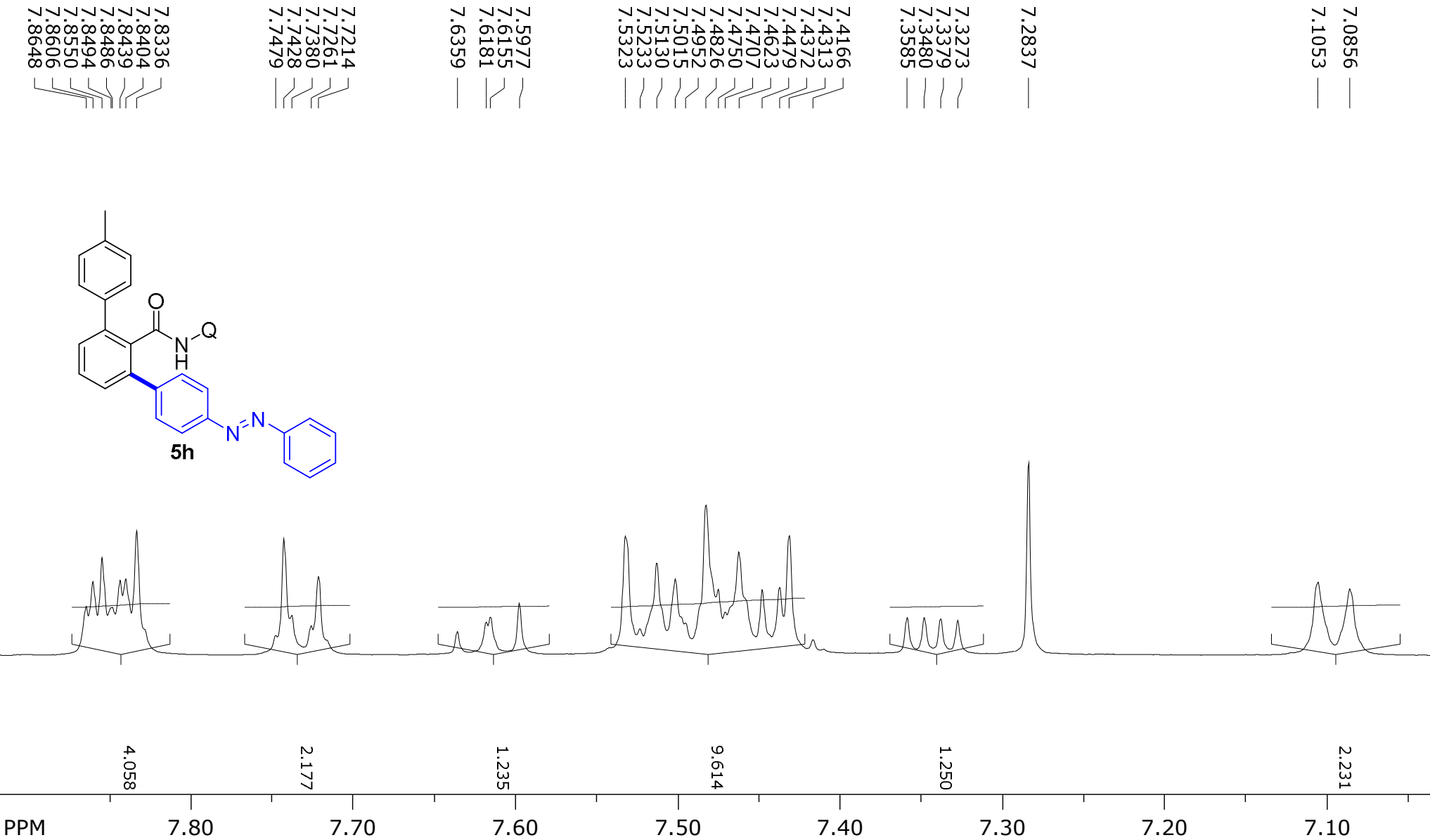
8.0400
8.0442
8.0607
8.0648



5h



SpinWorks 4: SS 797
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 2



7.83336
7.84404
7.84339
7.84886
7.84994
7.85550
7.86006
7.86648

7.72114
7.7261
7.7380
7.7428
7.7479

7.6359
7.5977
7.6155
7.6181

7.5323
7.5233
7.5130
7.5015
7.4952
7.4826
7.4750
7.4707
7.4623
7.4479
7.4372
7.4313
7.4166

7.3585
7.3480
7.3379
7.3273

7.2837

7.1053
7.0856

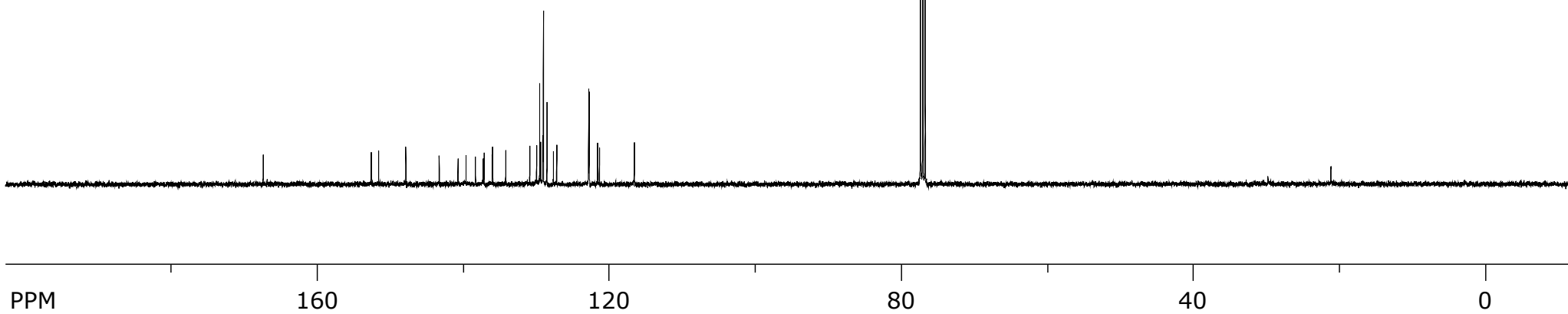
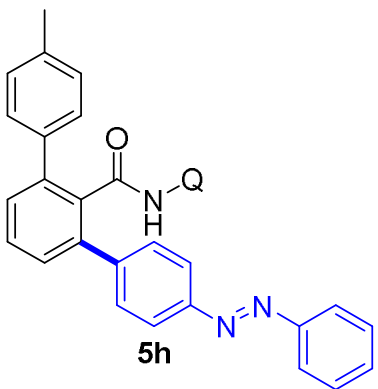
SpinWorks 4: SS-797

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 2

167.461
152.654
151.618
147.908
143.327
140.758
139.639
138.355
137.301
137.172
136.000
134.221
130.918
128.559
127.688
127.227
122.854
122.777
121.622
121.369
116.590

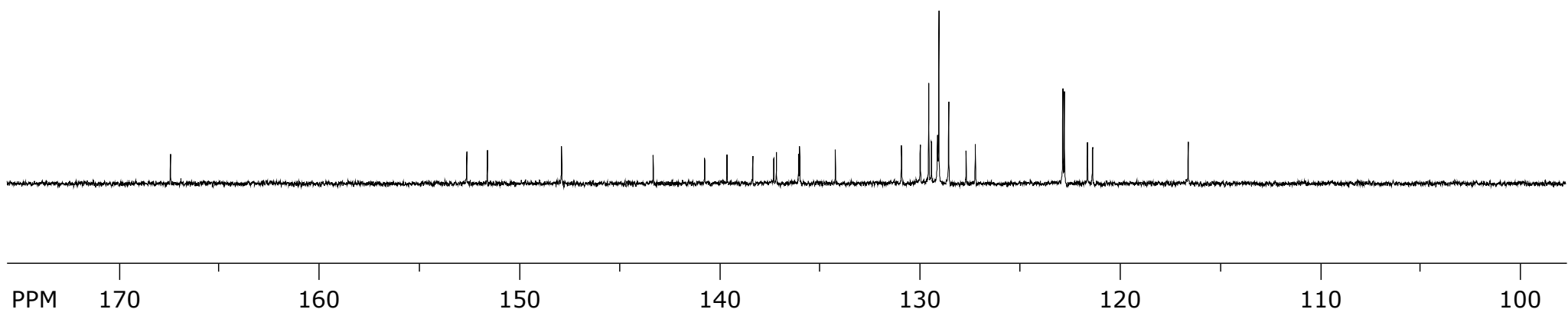
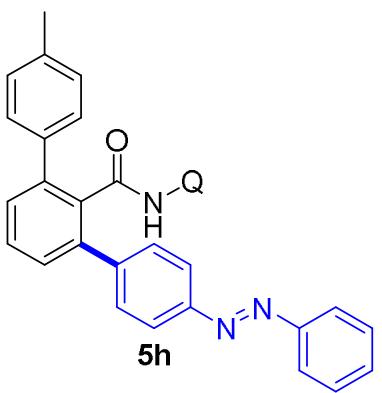
76.732
77.049
77.367

21.110



SpinWorks 4: SS-797
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 2

167.461 —
151.618 —
152.654 —
147.908 —
143.327 —
140.758 —
139.639 —
138.355 —
137.301 —
137.172 —
136.060 —
136.007 —
134.221 —
130.918 —
129.978 —
129.554 —
129.420 —
129.119 —
129.051 —
128.559 —
127.688 —
127.227 —
122.854 —
121.622 —
121.369 —
116.590 —



SpinWorks 4: ss-743 rep
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 2

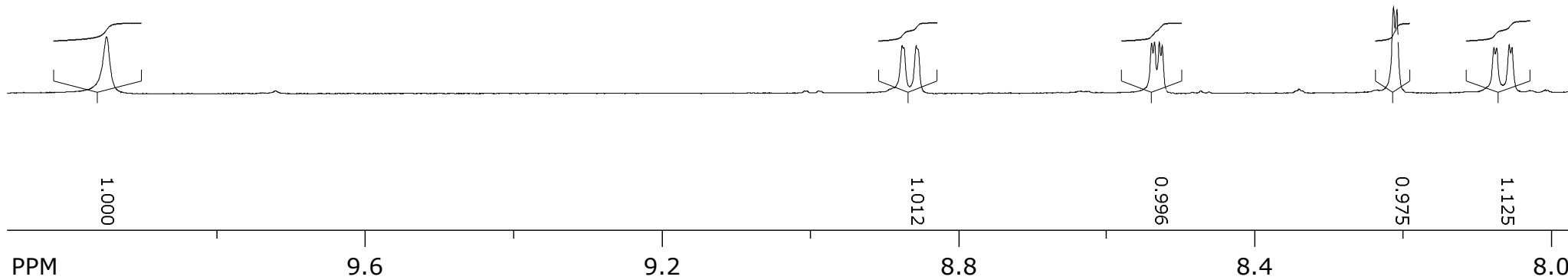
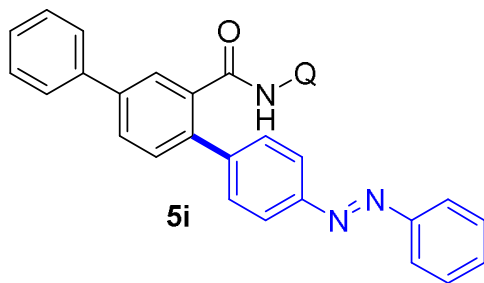
9.9496

8.8546
8.8570
8.8736
8.8759

8.5249
8.5288
8.5354
8.5393

8.2083
8.2128

8.0529
8.0566
8.0736
8.0773



SpinWorks 4: ss-743 rep
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 2

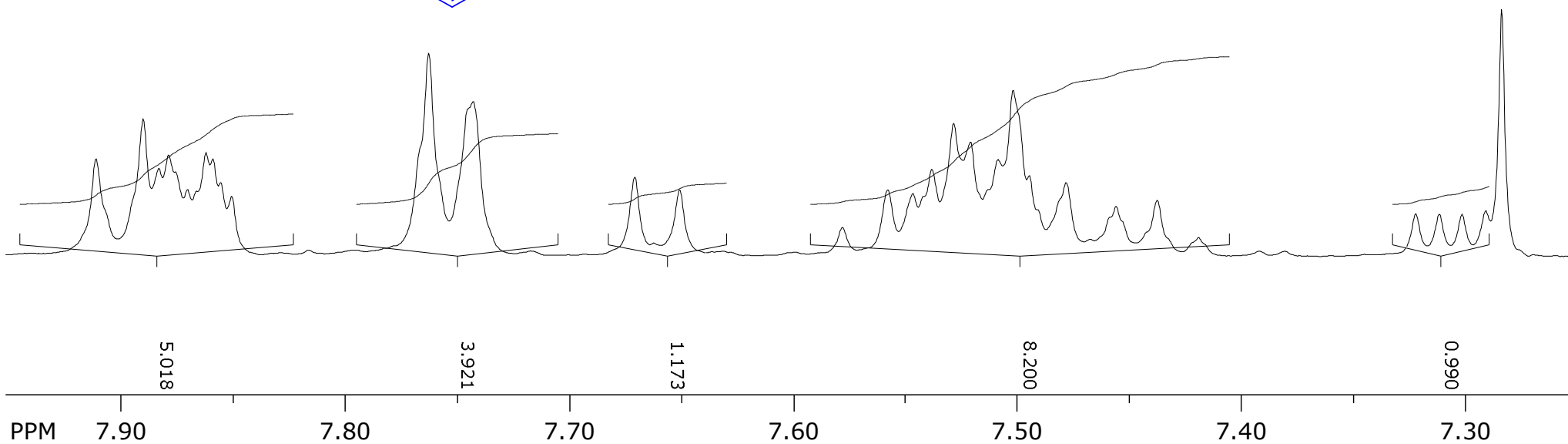
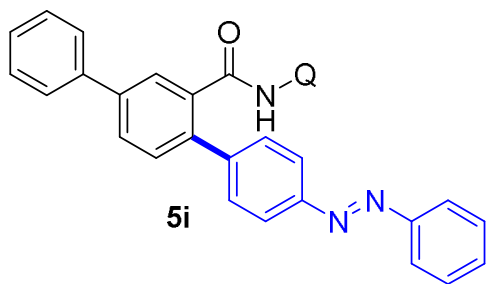
7.8509
7.8559
7.8593
7.8624
7.8665
7.8707
7.8761
7.8791
7.8835
7.8905
7.9115

7.7431
7.7629

7.6508
7.6709

7.5781
7.5579
7.5466
7.5417
7.5382
7.5284
7.5209
7.5128
7.5086
7.5019
7.4946
7.4909
7.4782
7.4673
7.4559
7.4375
7.4190

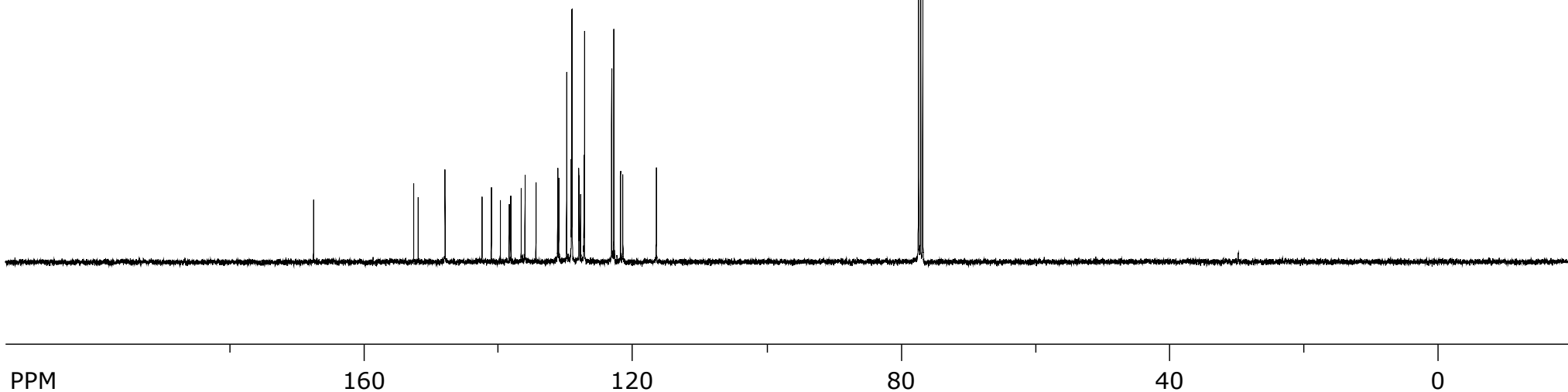
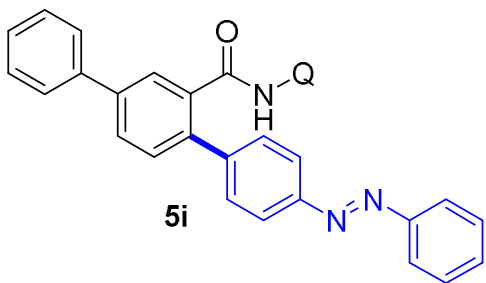
7.2836
7.2907
7.3013
7.3114
7.3220



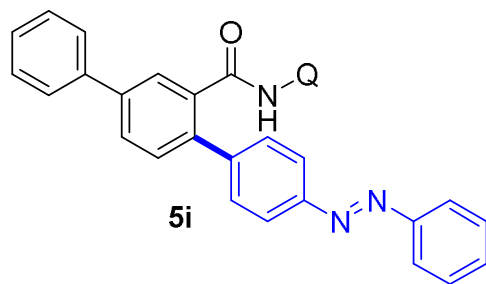
SpinWorks 4: 88-743REP
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 10

116.487
121.482
121.828
122.827
123.153
127.203
127.273
127.787
127.898
131.098
131.098
134.433
136.063
136.641
138.166
138.427
139.730
141.083
142.466
147.979
151.988
152.660
167.573

76.774
77.092
77.409



SpinWorks 4: 88-743REP
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 10



167.573

151.988
152.660

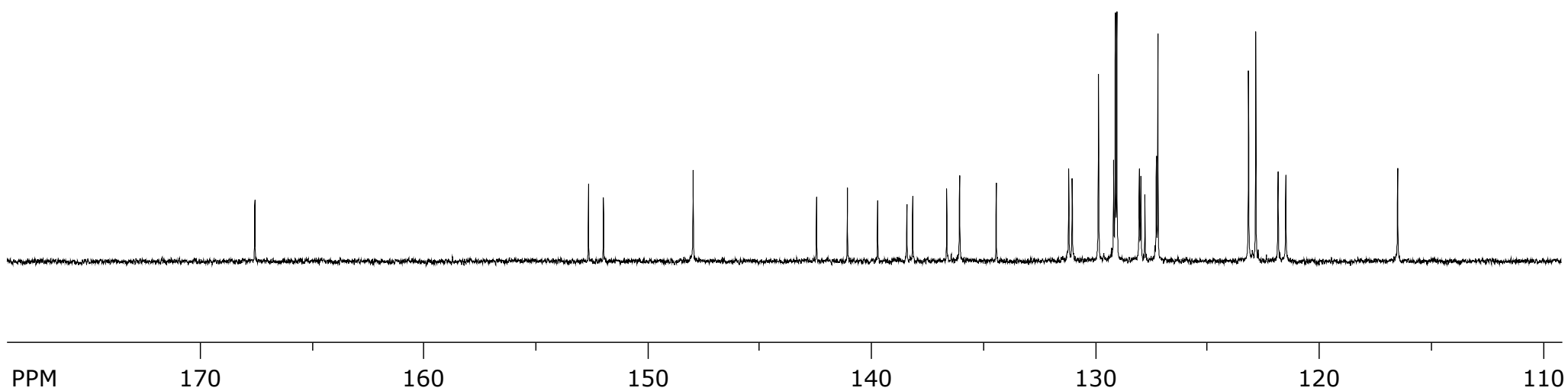
147.979

142.466
136.065
136.641
138.166
138.427
139.730
141.083

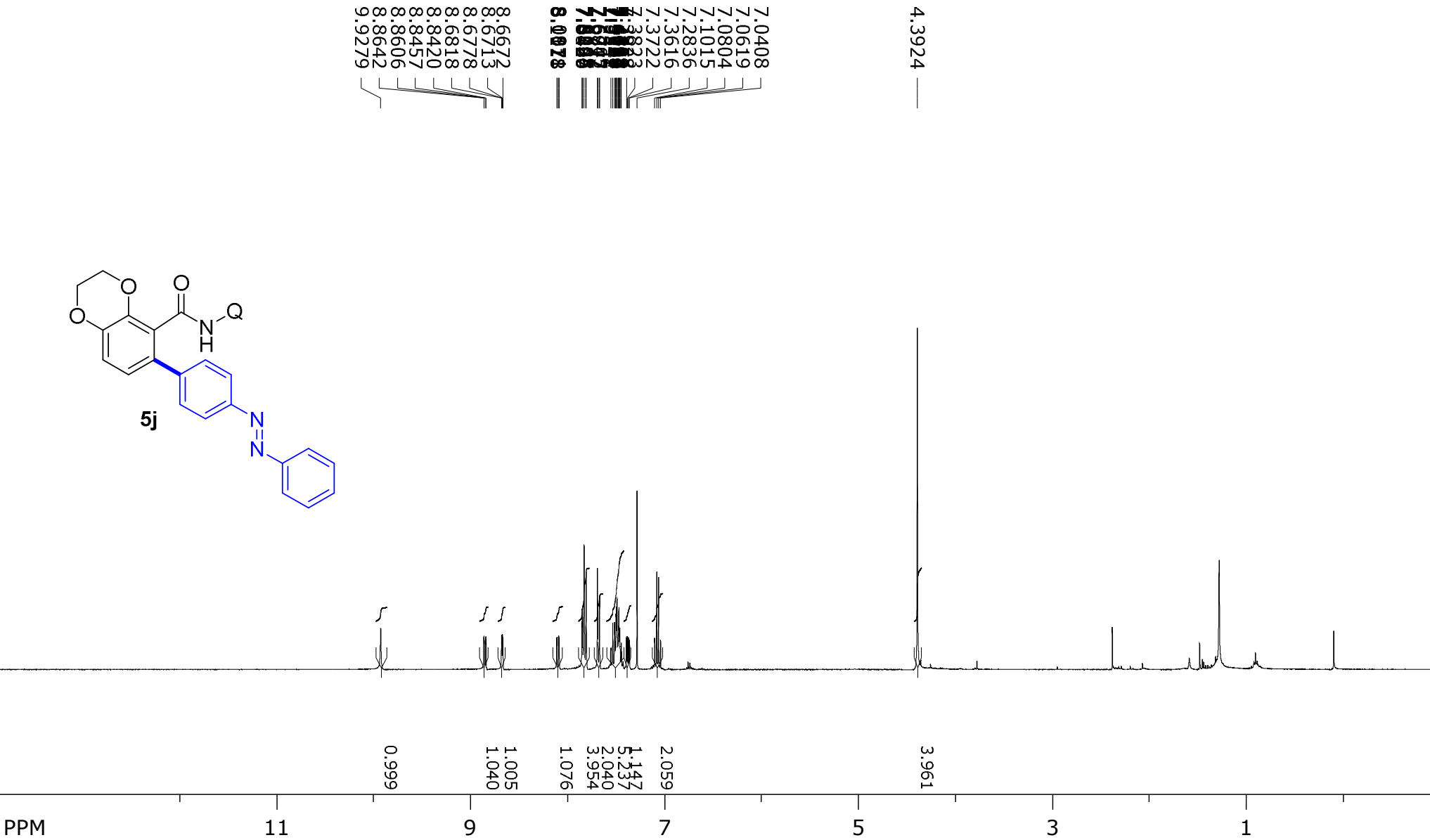
134.433
131.190
129.857
131.036
129.181
129.104
129.038
128.037
127.967
127.787
127.273
127.203

123.153
121.828
121.482
122.827

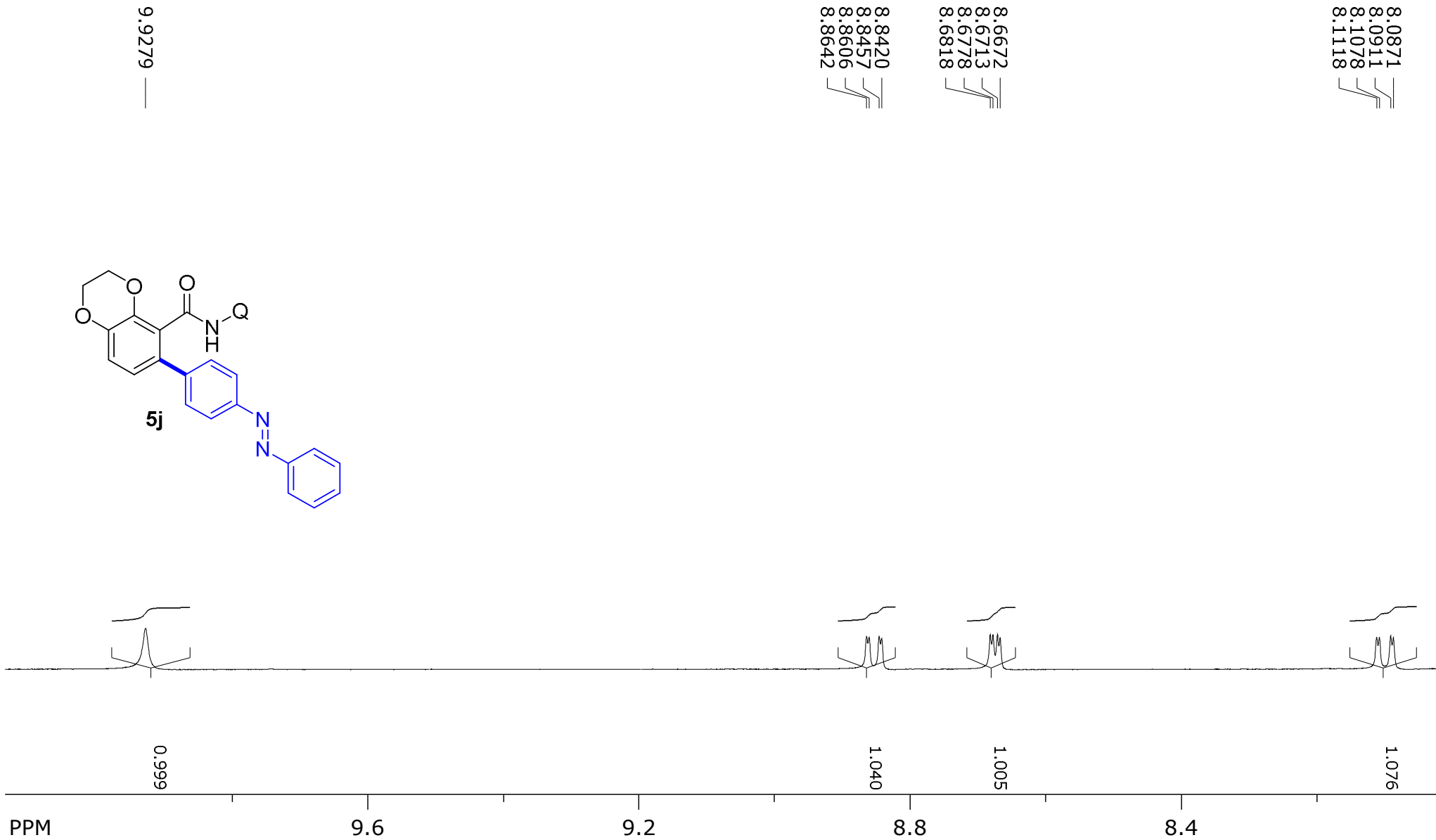
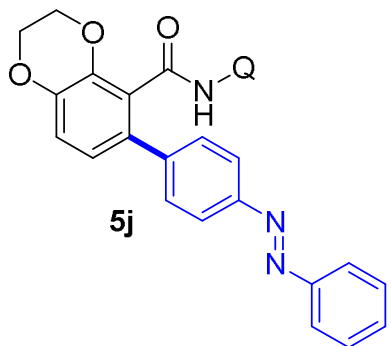
116.487



SpinWorks 4: SS 744
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 1



SpinWorks 4: SS 744
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 1



SpinWorks 4: SS 744
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 1

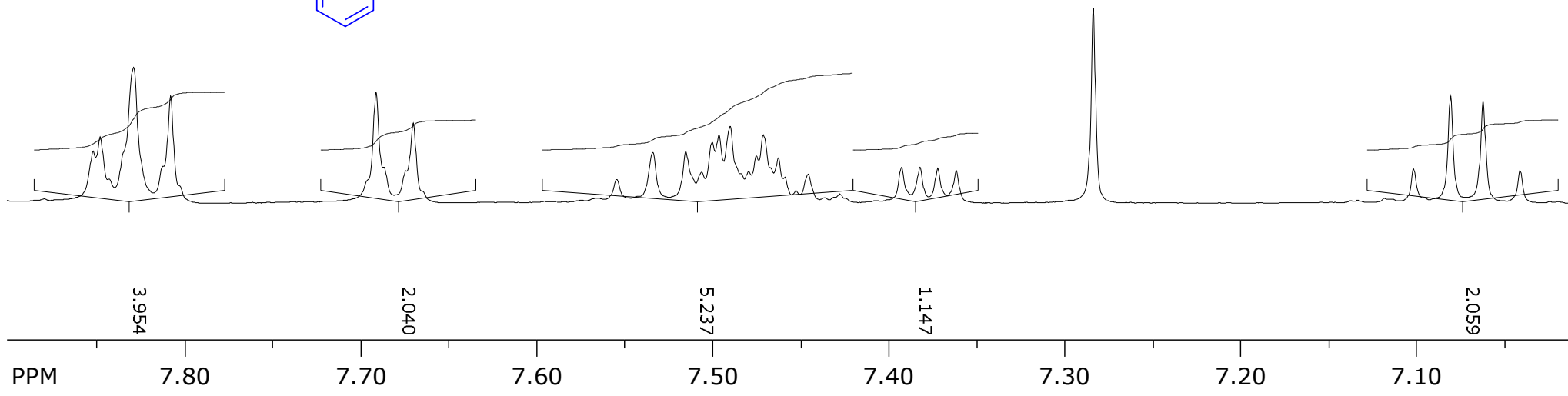
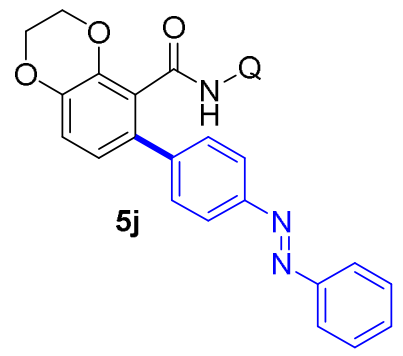
7.8085
7.8128
7.8297
7.8435
7.8485
7.8526

7.6705
7.6747
7.6872
7.6917

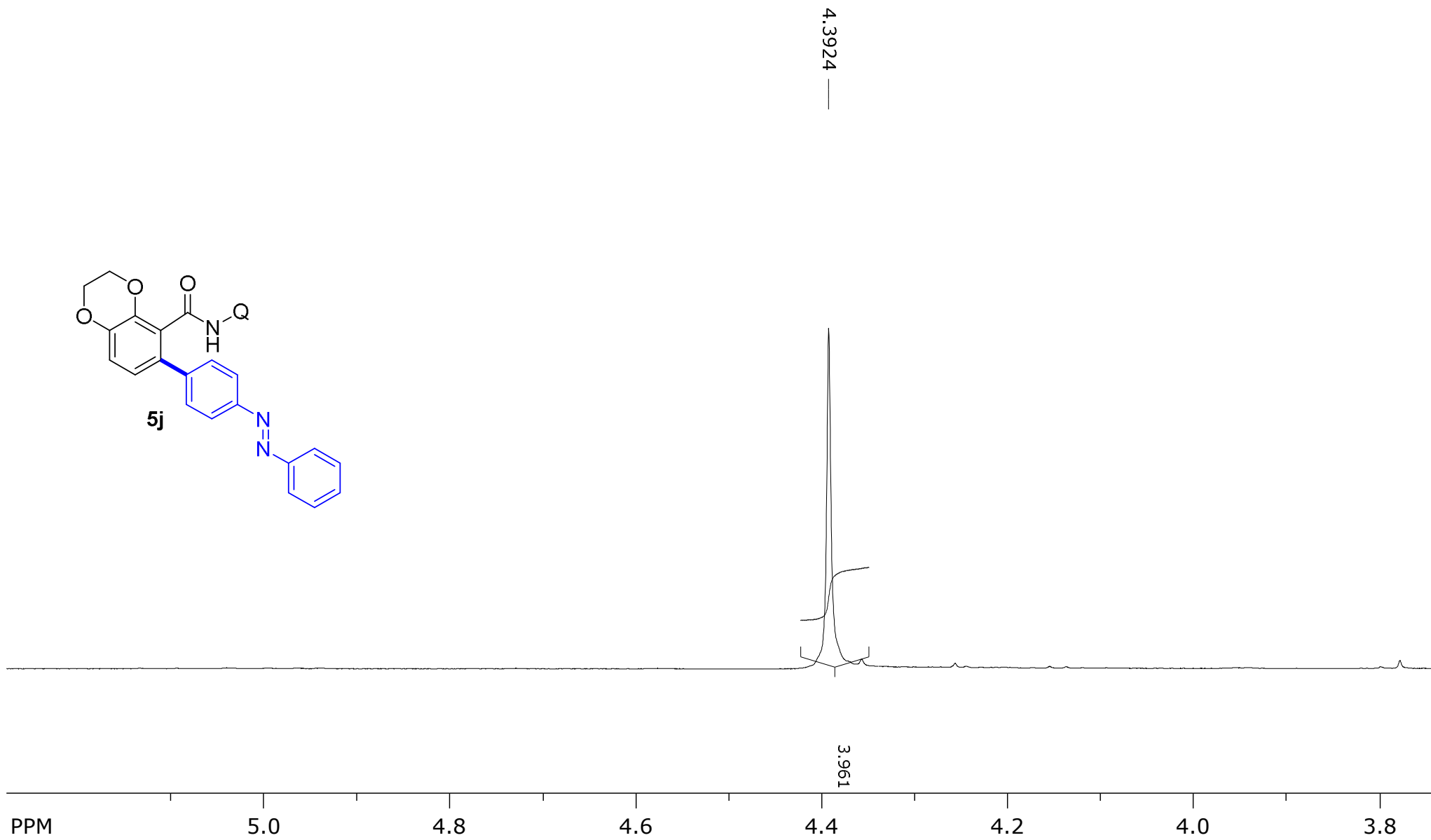
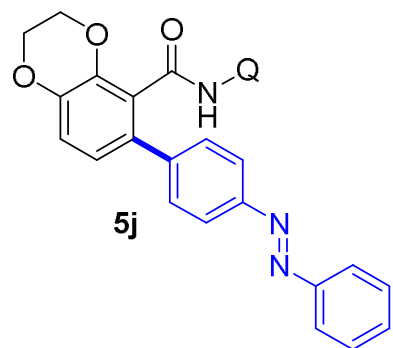
7.5547
7.5342
7.5154
7.5065
7.5005
7.4966
7.4902
7.4797
7.4753
7.4714
7.4628
7.4591
7.4528
7.4459
7.3928
7.3823
7.3722
7.3616

7.2836

7.1015
7.0804
7.0619
7.0408



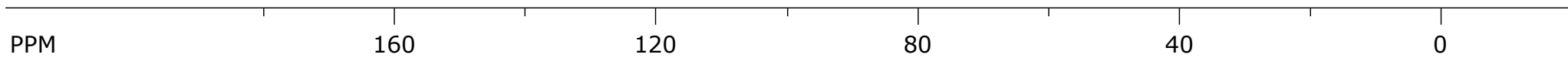
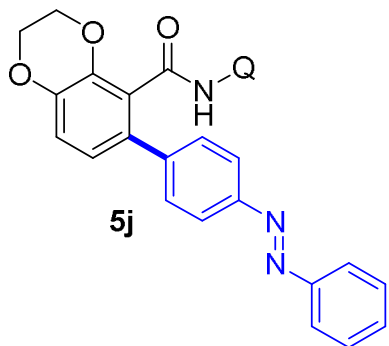
SpinWorks 4: SS 744
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 1



SpinWorks 4: SS 744
C13CPD CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 29

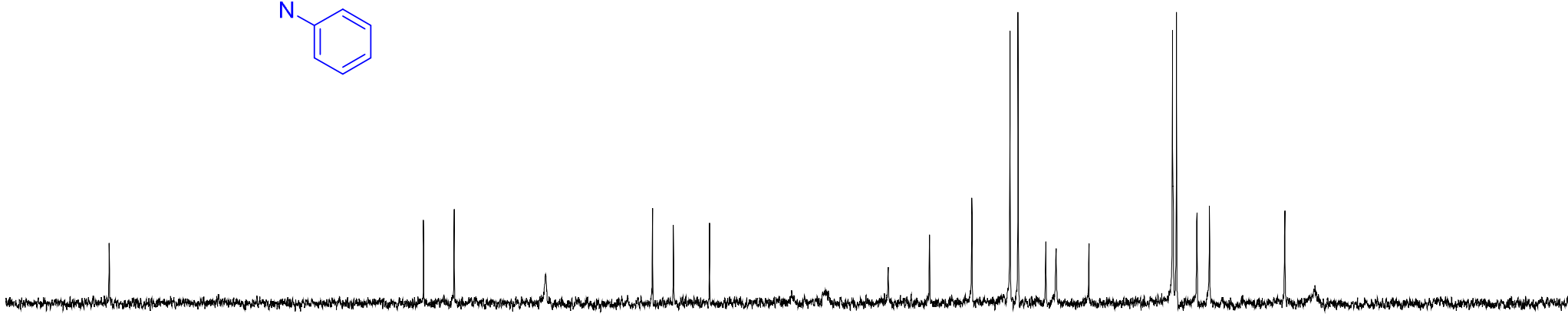
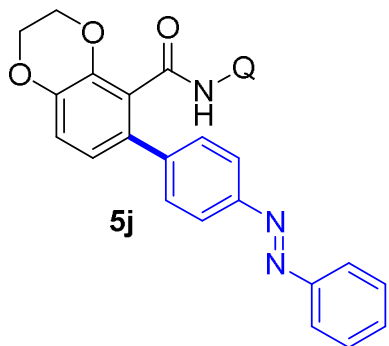
117.245
118.454
121.445
121.942
122.755
122.891
122.911
126.235
127.028
127.038
129.008
130.877
132.559
134.201
136.660
137.993
141.291
142.727
143.558
147.798
151.433
152.649
165.127

64.271
64.670
76.744
77.062
77.380



SpinWorks 4: SS 744
C13CPD CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 29

165.127 —
152.649 —
151.433 —
147.798 —
143.558 —
142.727 —
141.291 —
137.993 —
136.660 —
134.201 —
132.559 —
130.877 —
129.363 —
129.041 —
127.942 —
127.536 —
126.235 —
122.911 —
122.891 —
122.755 —
121.942 —
121.445 —
118.454 —
117.245 —



PPM

160

150

140

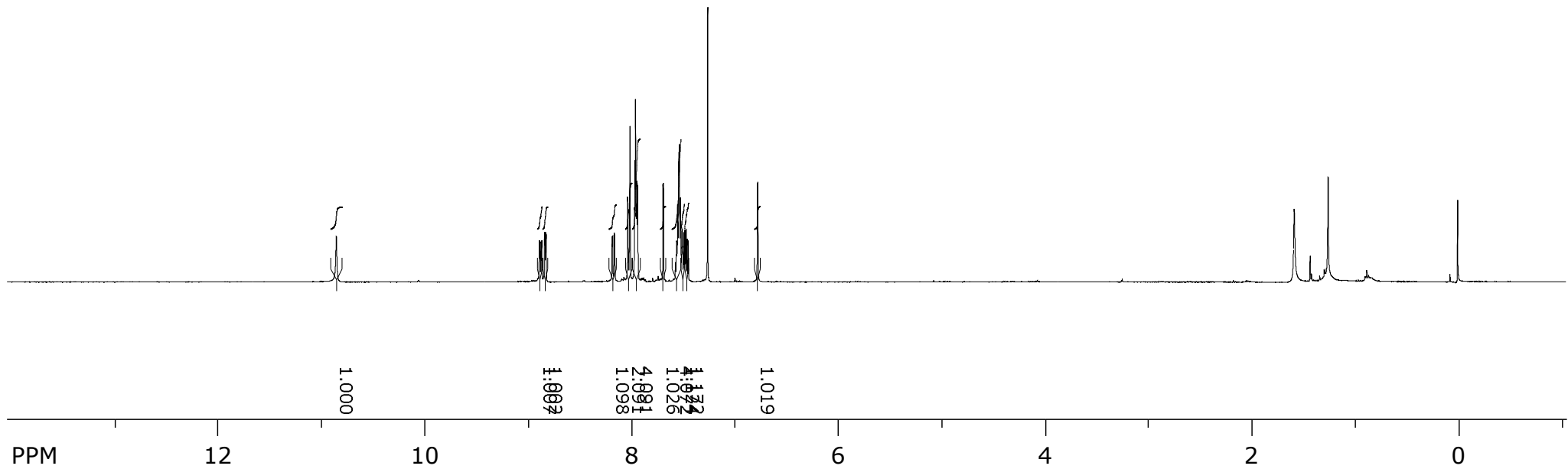
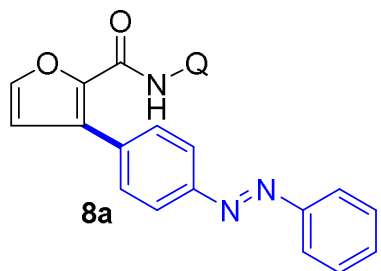
130

120

110

SpinWorks 4: SS 70
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 19

10.8598
8.8297
8.8337
8.8402
8.8443
8.8721
8.8782
8.8885
8.8946
8.1888
8.1888
8.1888
7.6928
7.4947
7.4852
7.4745
7.4644
7.4538
7.2661
6.7796
6.7840
7.7796
7.2661
7.4538
7.4644
7.4745
7.4852
7.4947
7.6928
8.1888
8.1888
8.1888

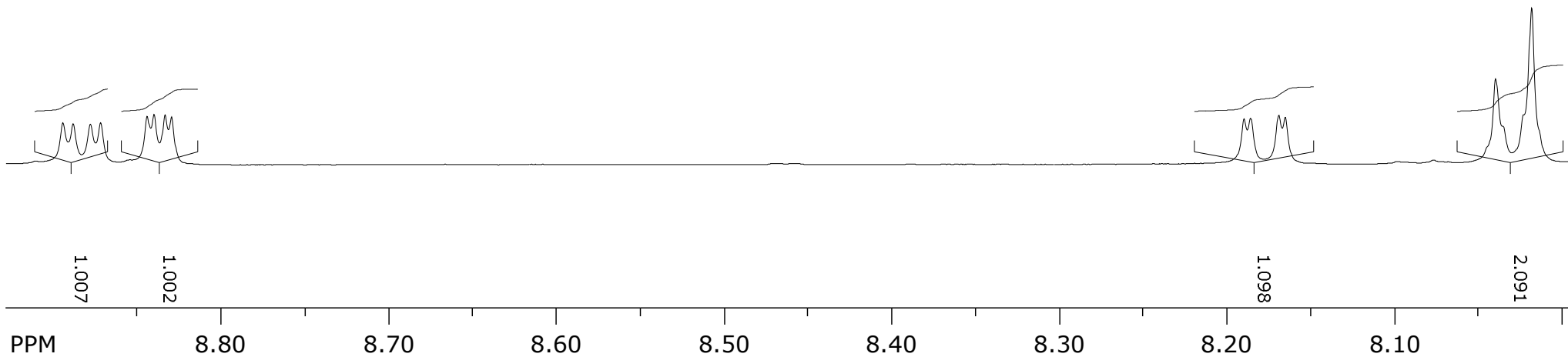
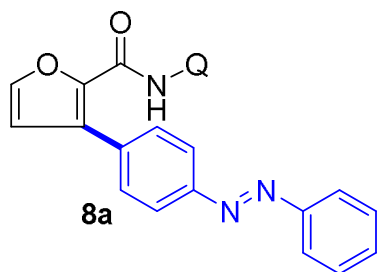


SpinWorks 4: SS 70
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 19

8.8297
8.8337
8.8402
8.8443
8.8721
8.8782
8.8885
8.8946

8.1649
8.1689
8.1856
8.1896

8.0180
8.0225
8.0352
8.0394

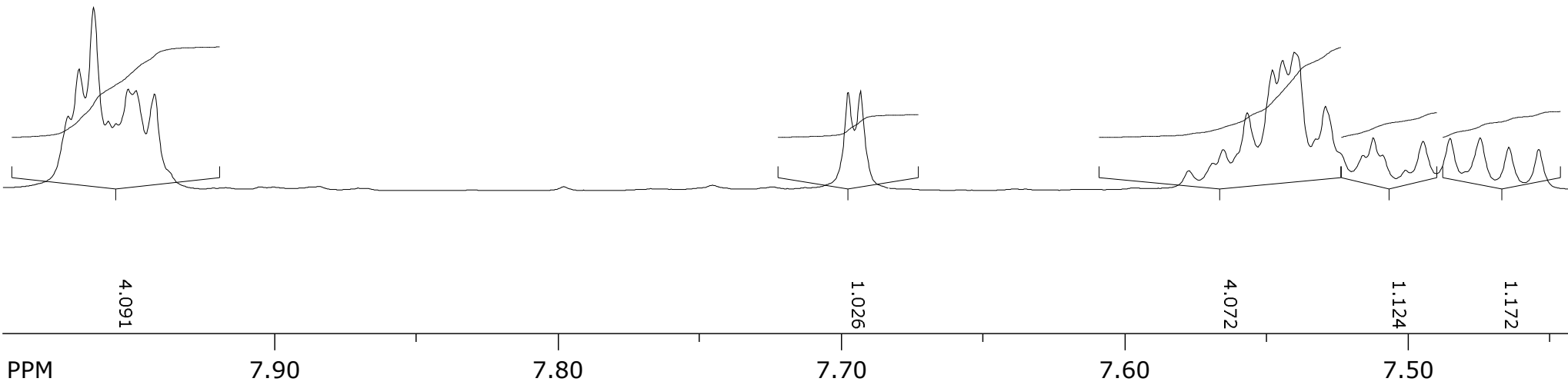
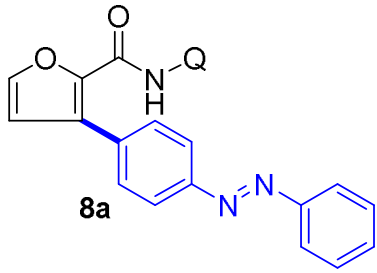


SpinWorks 4: SS 70
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 19

7.9425
7.9491
7.9518
7.9561
7.9589
7.9640
7.9692
7.9730

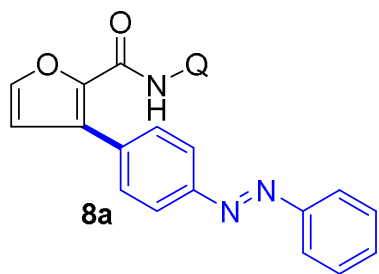
7.6933
7.6976

7.4538
7.4644
7.4745
7.4852
7.4947
7.5090
7.5123
7.5159
7.5291
7.5324
7.5400
7.5443
7.5478
7.5567
7.5652
7.5689



SpinWorks 4: SS-70-REP
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 1

114.789
116.773
121.689
121.773
122.813
122.941
127.415
128.036
129.116
130.380
131.038
131.466
134.374
134.607
136.343
138.744
142.277
143.558
148.348
152.231
152.779
156.772



76.718
77.035
77.353

PPM

160

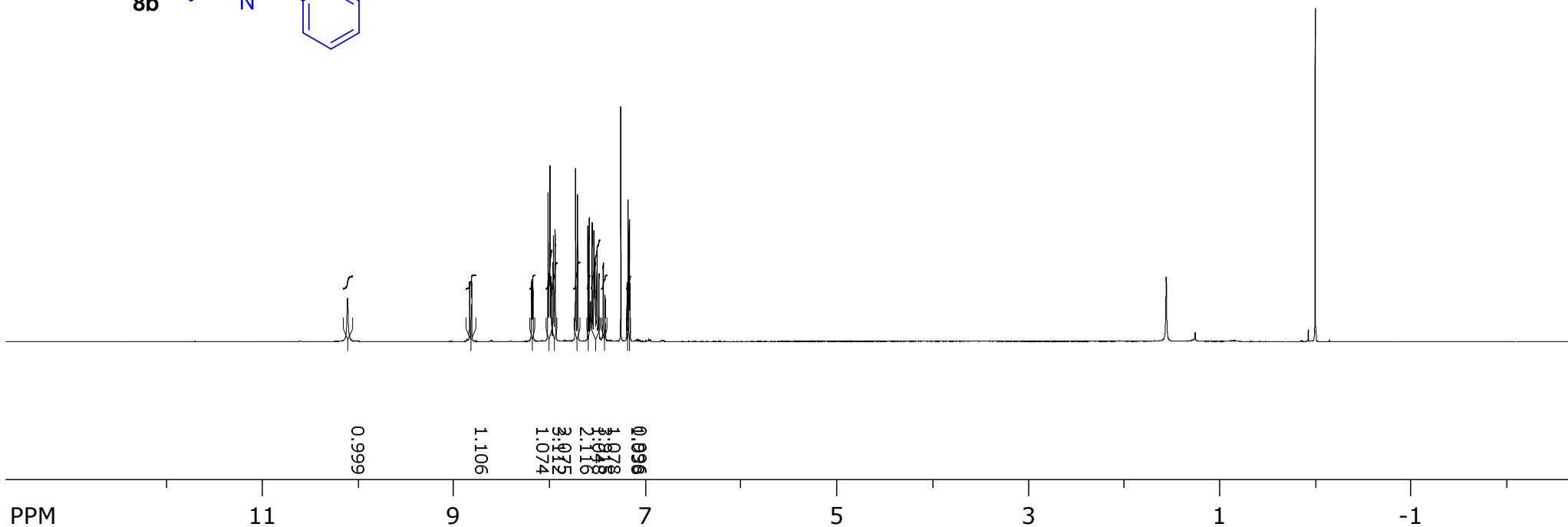
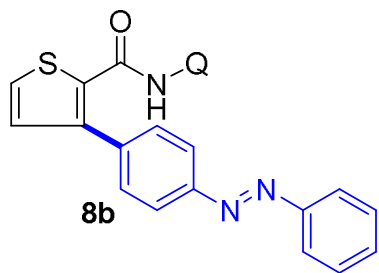
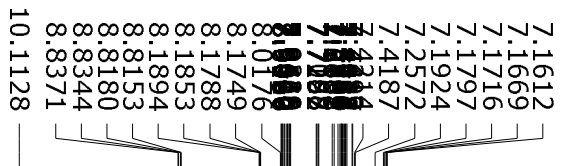
120

80

40

0

SS-42 p rep

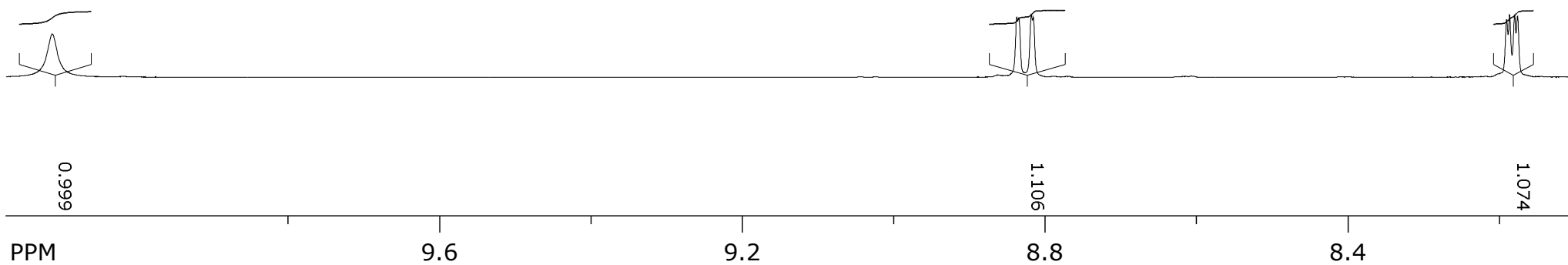
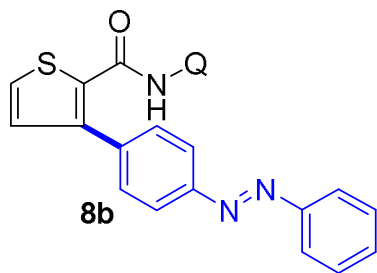


SpinWorks 4: DC-178

10.1128

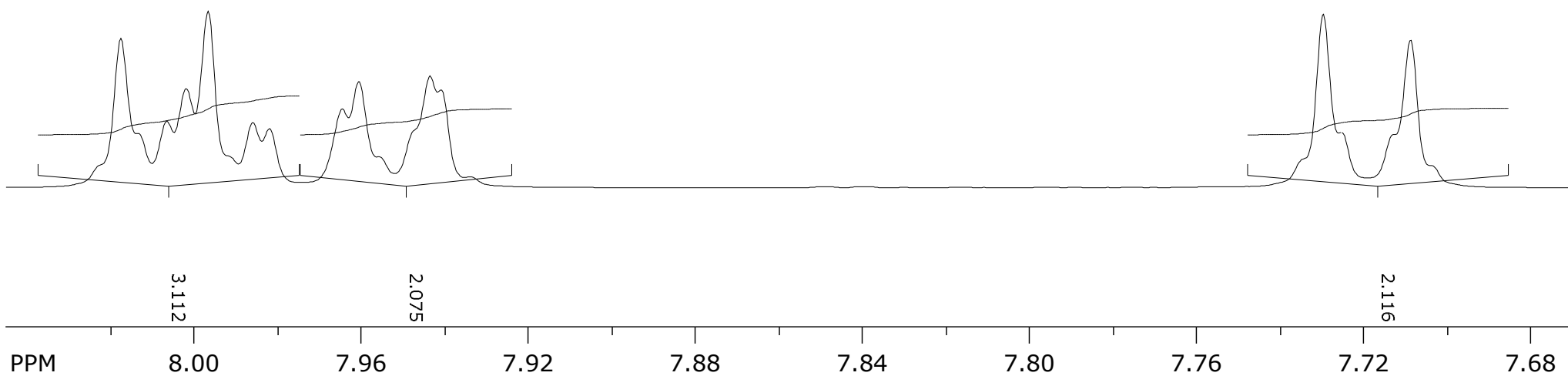
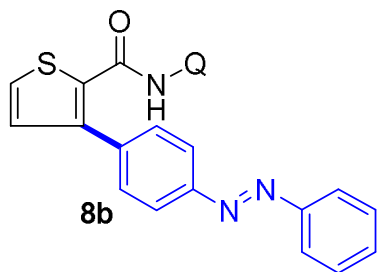
8.8153
8.8180
8.8344
8.8371

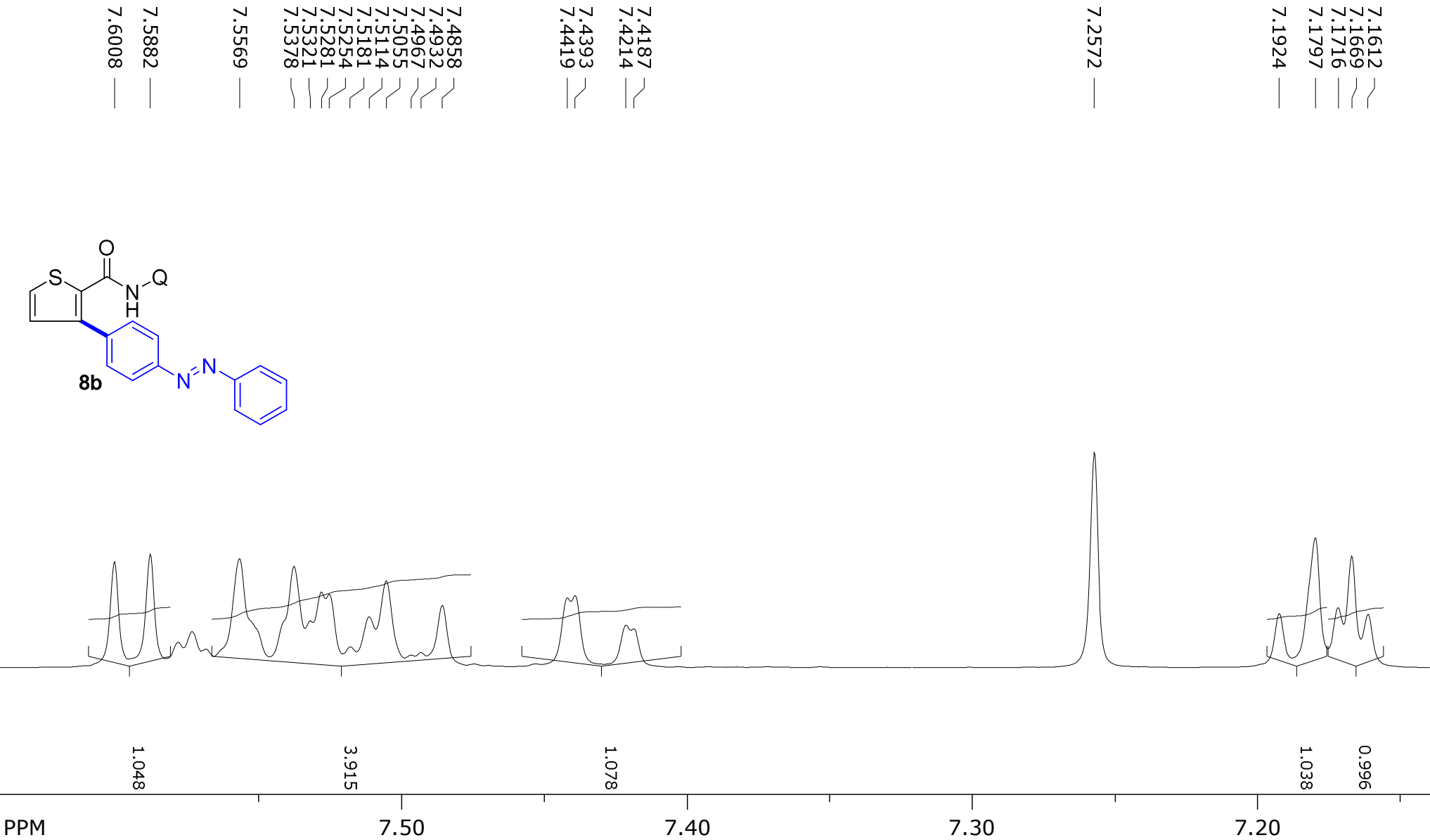
8.1749
8.1788
8.1853
8.1894



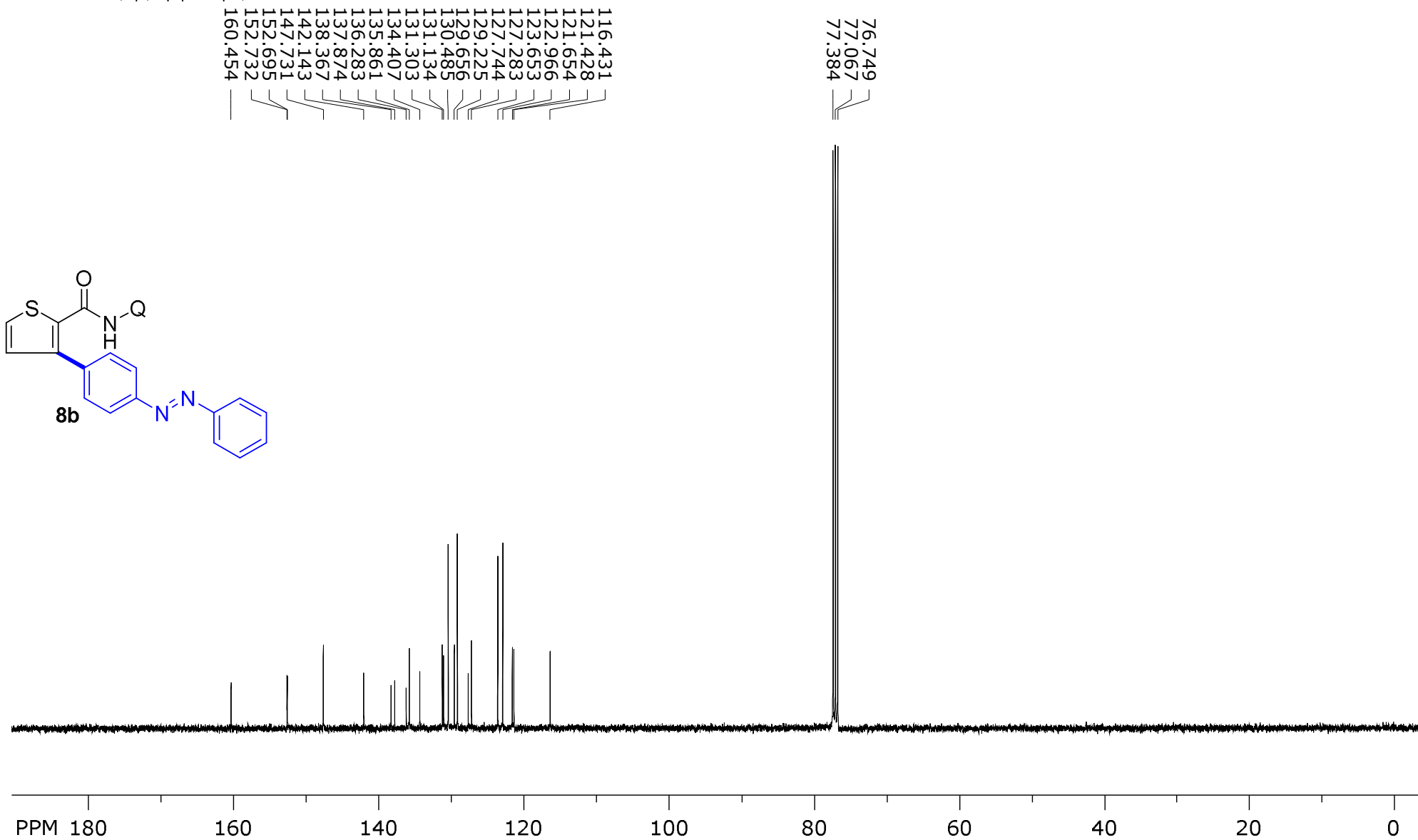
7.93339 —
7.9410 —
7.9436 —
7.9558 —
7.9606 —
7.9646 —
7.9820 —
7.9860 —
7.9967 —
8.0020 —
8.0066 —
8.0136 —
8.0176 —

7.7087 —
7.7128 —
7.7252 —
7.7296 —



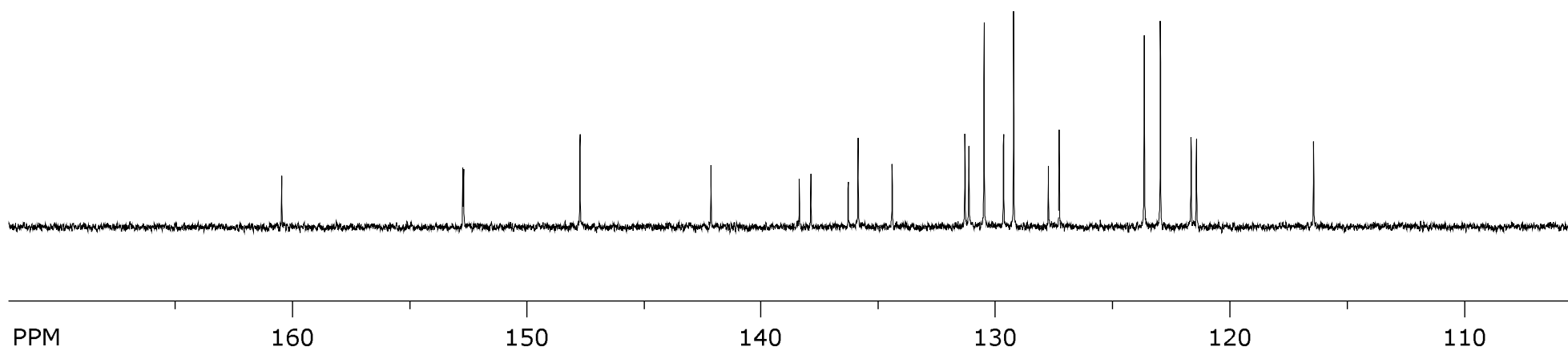
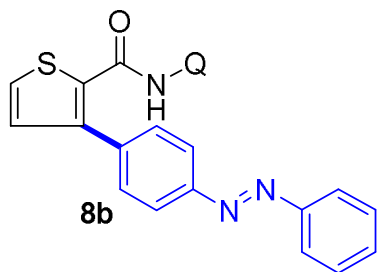


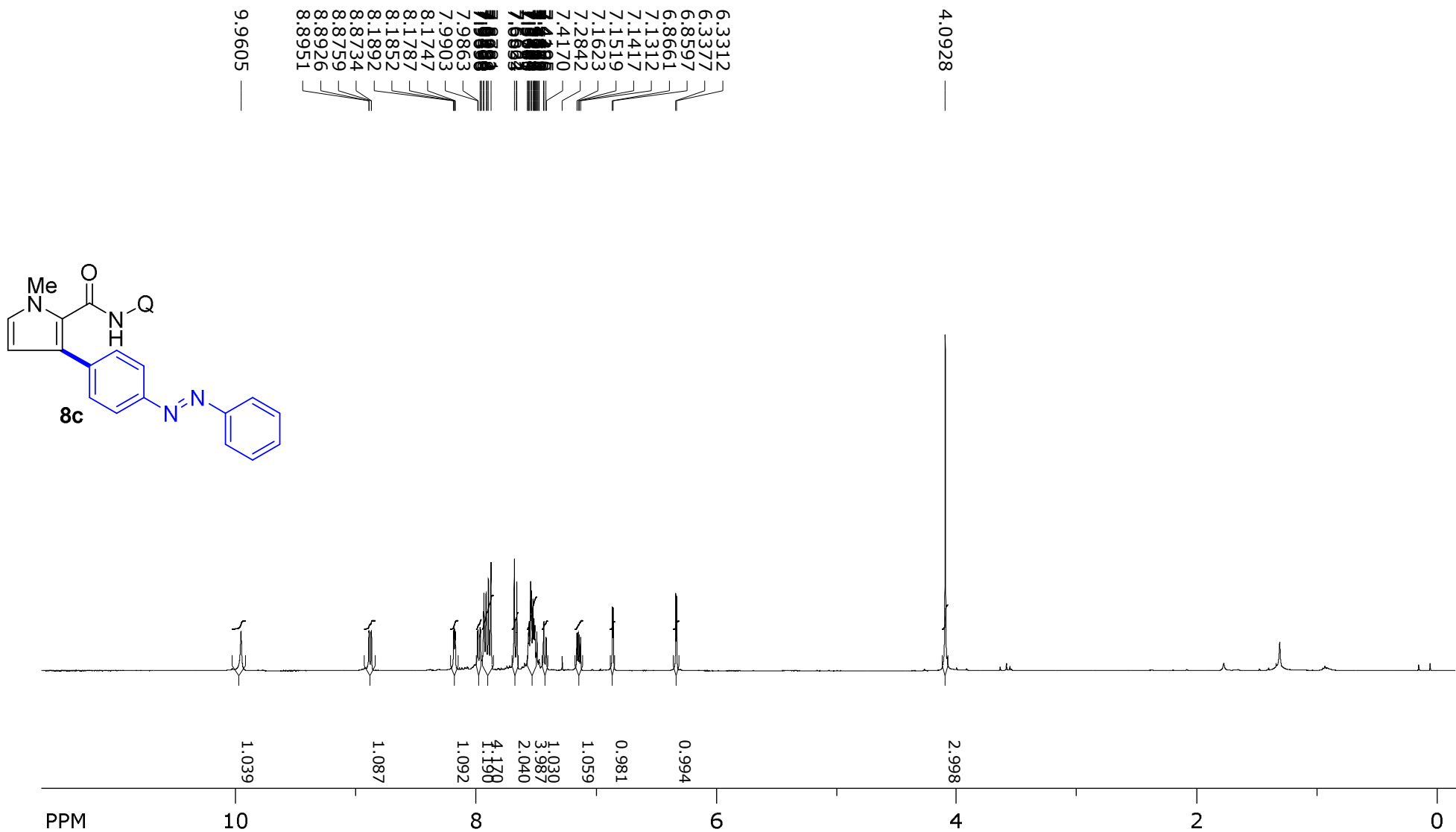
SpinWorks 4: SS 42 P REP
C13CPD CDCI3 /opt/topspin3.5pl2/nmrdata nmrsu 58



SpinWorks 4: SS 42 P REP
C13CPD CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 58

160.454 —
152.695 —
152.732 —
147.731 —
142.143 —
138.367 —
137.874 —
136.283 —
135.861 —
134.407 —
131.303 —
131.134 —
130.485 —
129.656 —
129.225 —
127.744 —
127.283 —
123.653 —
122.966 —
121.654 —
121.428 —
116.431 —

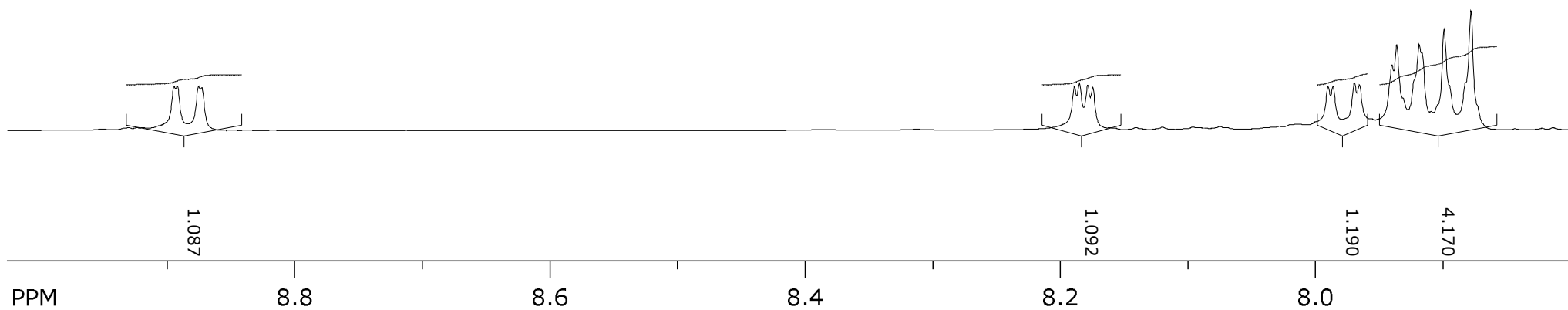
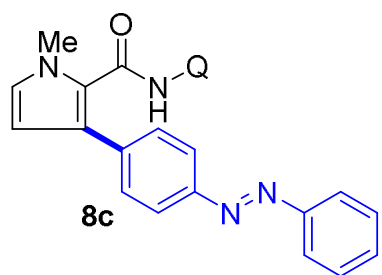


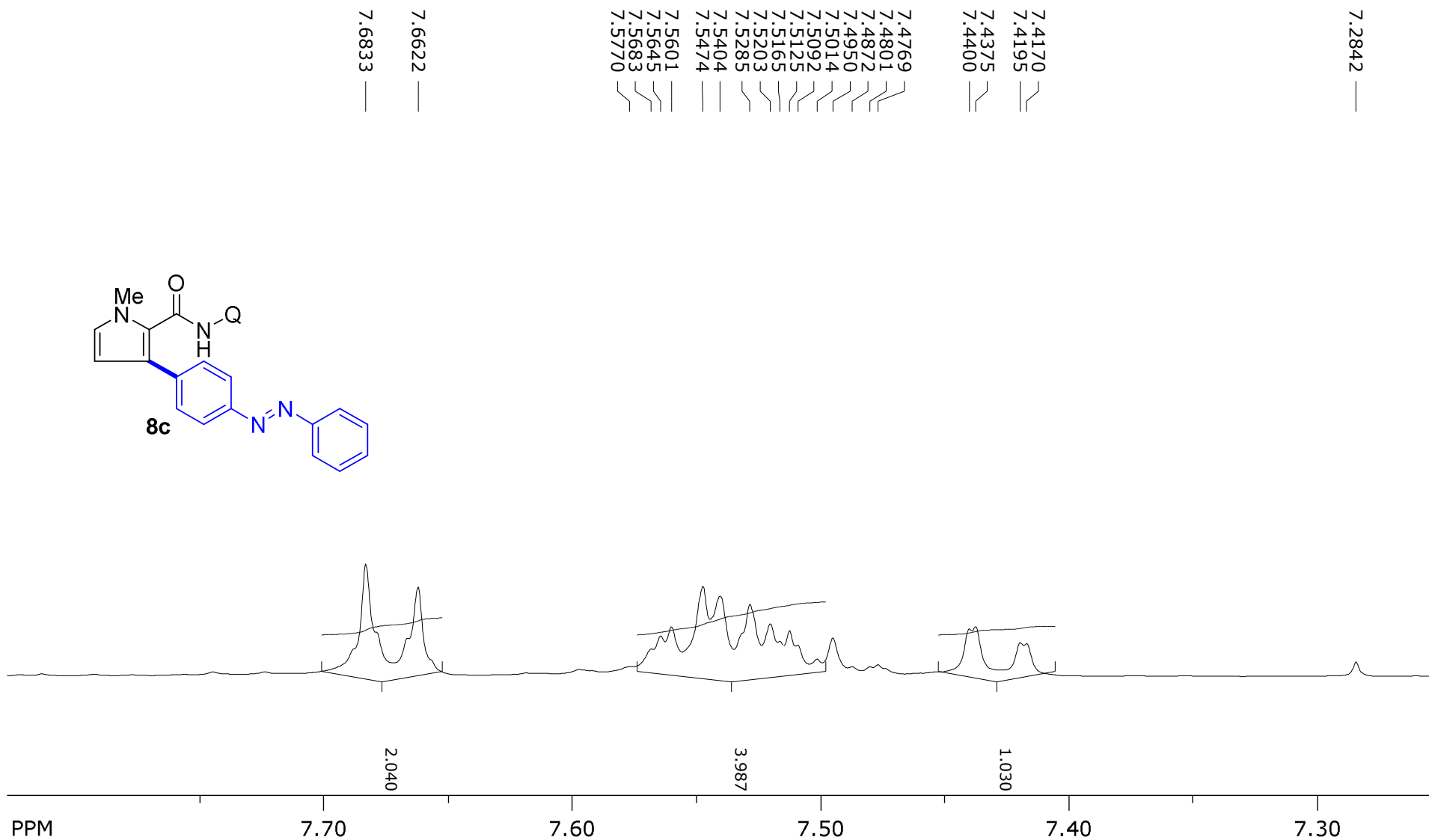


8.8734
8.8759
8.8926
8.8951

8.1747
8.1787
8.1852
8.1892

7.8781
7.8992
7.9094
7.9188
7.9364
7.9400
7.9563
7.9656
7.9696
7.9863
7.9903





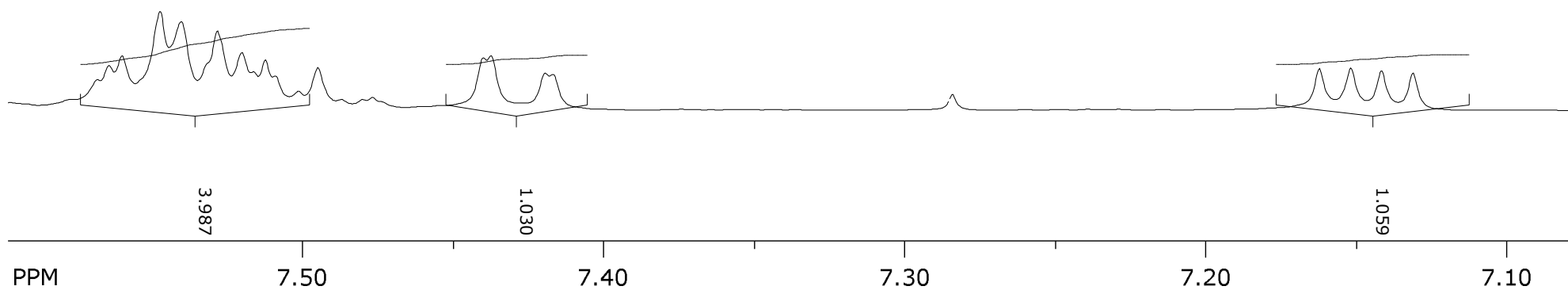
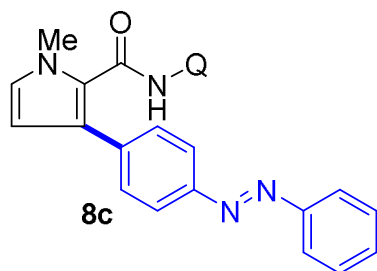
SpinWorks 4: SS-71-P

7.4769
7.4801
7.4872
7.4950
7.5014
7.5092
7.5125
7.5165
7.5203
7.5285
7.5404
7.5474
7.5601
7.5645
7.5683
7.5770

7.4375
7.4170
7.4195
7.4400

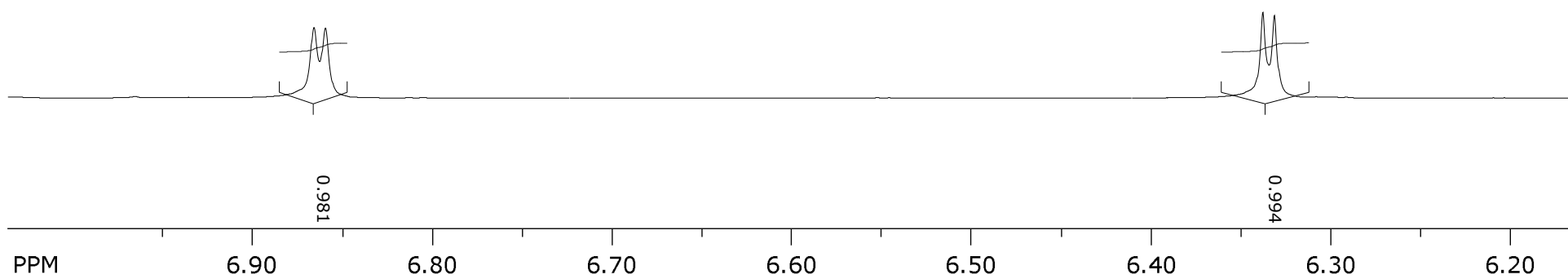
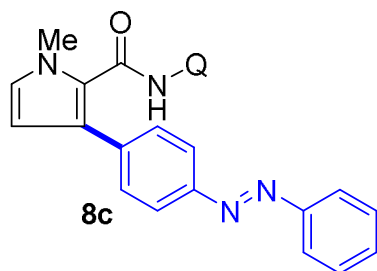
7.2842

7.1312
7.1417
7.1519
7.1623



6.8597
6.8661

6.3312
6.3377

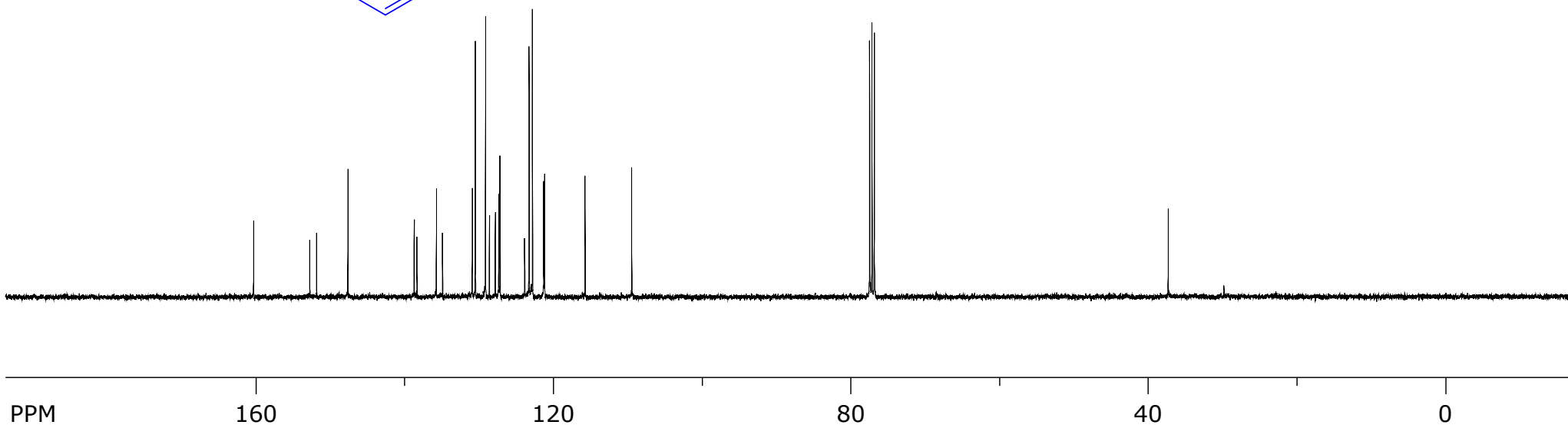
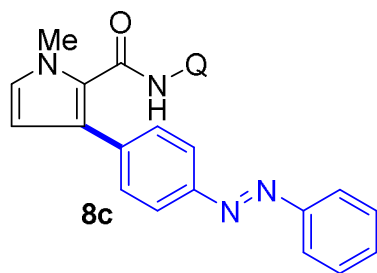


SpinWorks 4: SS 71 P
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 17

109.451
115.722
121.177
121.294
122.804
123.253
123.859
127.171
127.330
127.812
128.606
129.132
130.493
130.905
134.909
135.740
138.346
138.728
147.638
151.855
152.779
160.332

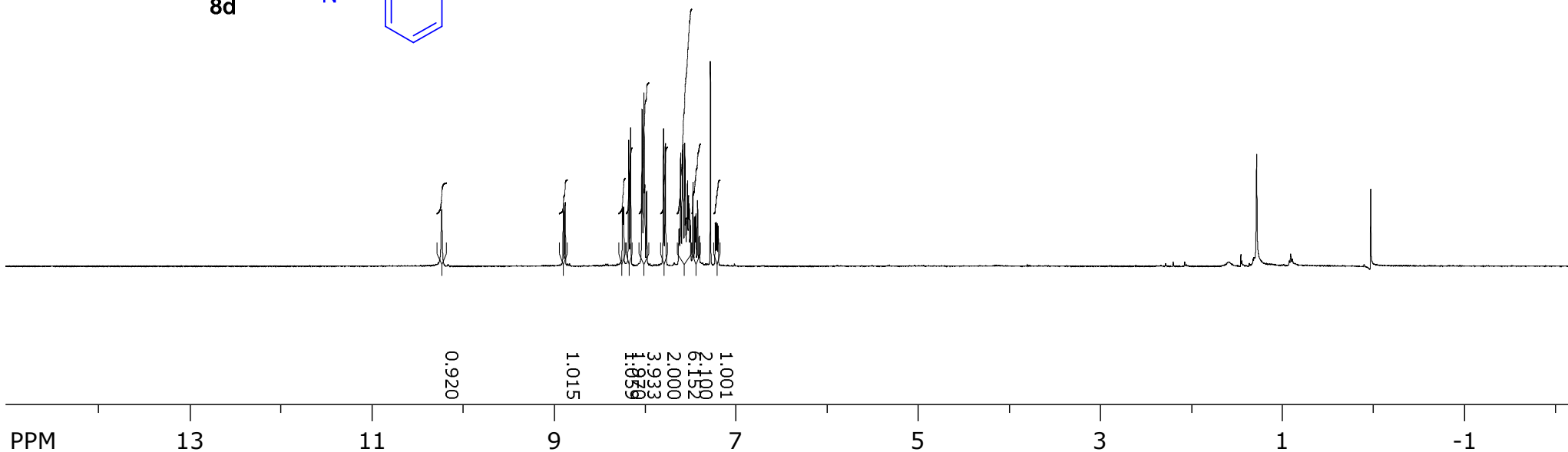
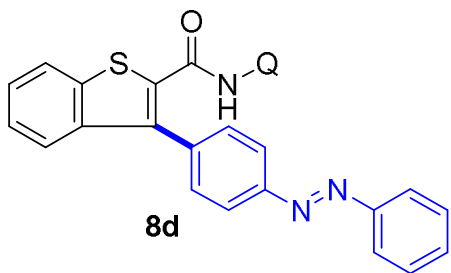
76.797
77.115
77.432

37.256



SpinWorks 4: SS 754
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 3

10.2371
8.8994
8.8805
8.2485
8.2388
8.1816
8.1612
8.0339
8.0149
8.0052
7.9955
7.9858
7.4249
7.4062
7.2833
7.2296
7.2191
7.2089
7.1984



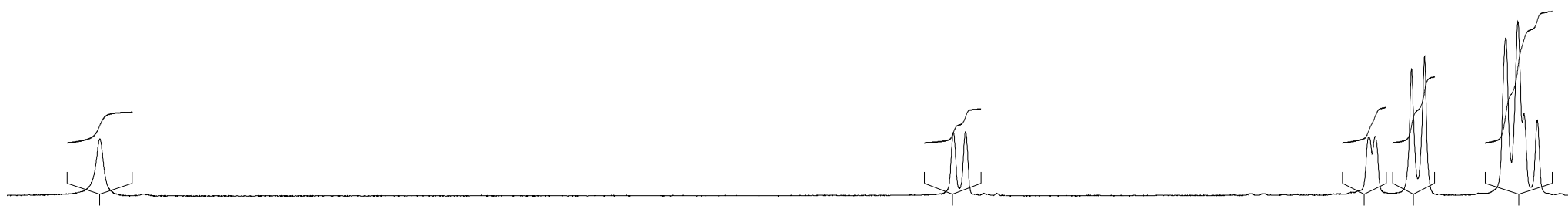
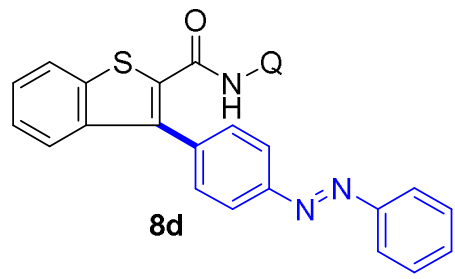
SpinWorks 4: SS 754
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 3

10.2371

8.8805
8.8994

8.1612
8.1816
8.2388
8.2485

7.9845
8.0052
8.0149
8.0339



0.920

1.015

1.059

1.970

3.933

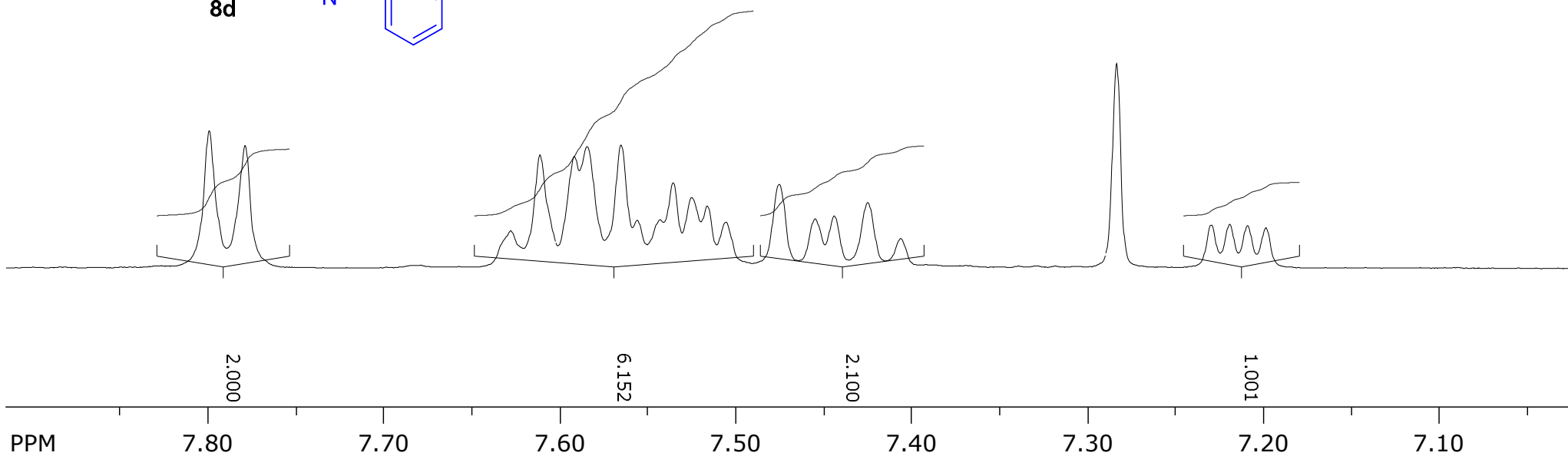
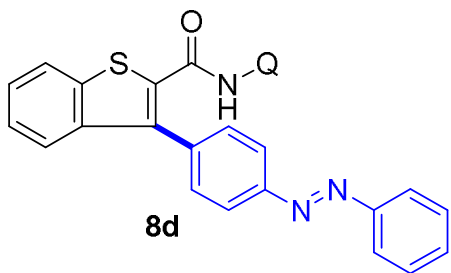
PPM 10.0 9.6 9.2 8.8 8.4 8.0

SpinWorks 4: SS 754
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 3

7.7791
7.7995

7.6280
7.6113
7.5918
7.5845
7.5653
7.5560
7.5430
7.5356
7.5251
7.5162
7.5056
7.4753
7.4549
7.4440
7.4249
7.4062

7.2833
7.1984
7.2089
7.2191
7.2296

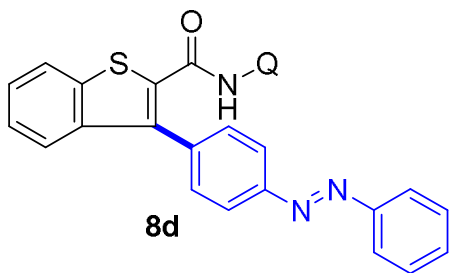


SpinWorks 4: SS-754

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 3

116.633
121.440
121.841
122.634
123.028
124.025
124.699
124.968
125.194
125.224
131.454
131.854
134.864
135.864
136.312
136.964
137.181
138.392
140.190
140.711
147.736
152.720
153.149
160.718

76.747
77.065
77.383



PPM

160

120

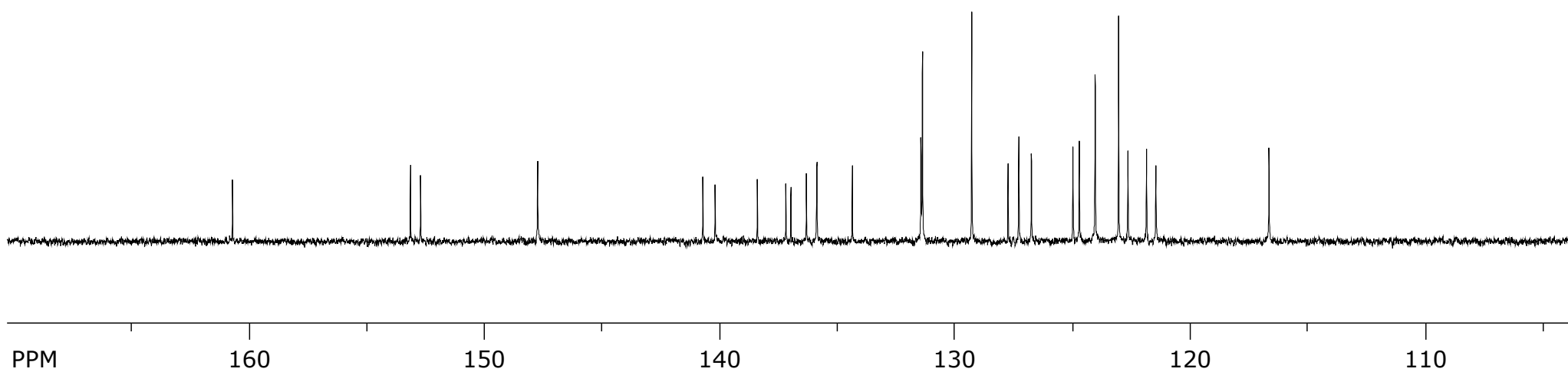
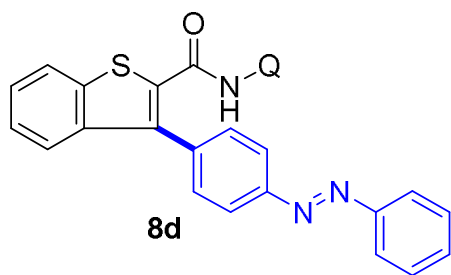
80

40

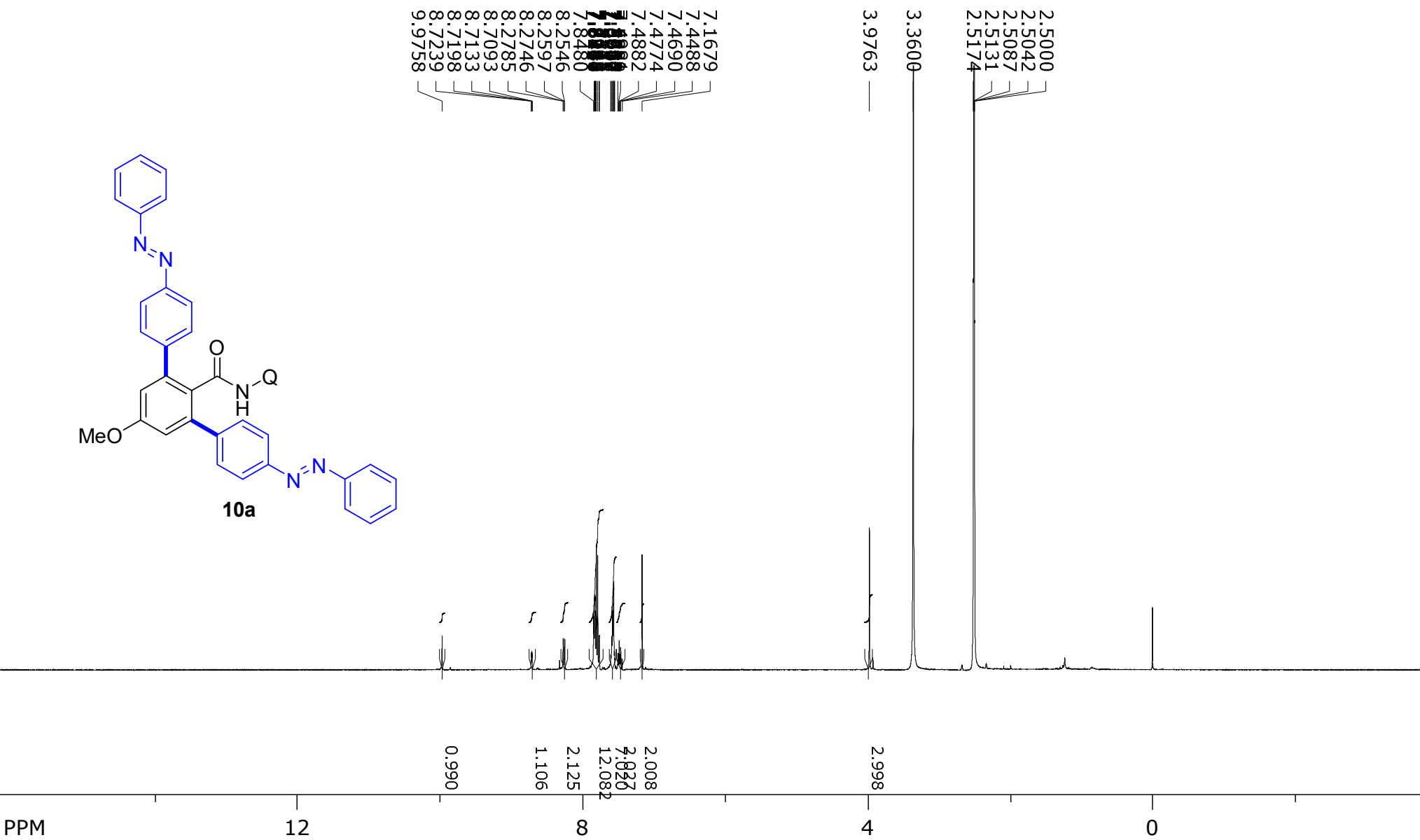
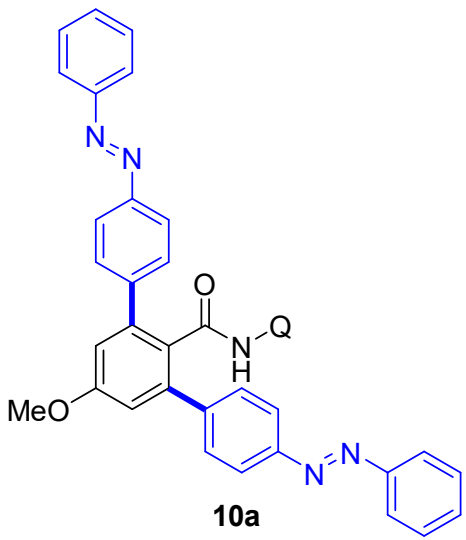
0

SpinWorks 4: SS-754
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 3

160.718 —
152.720 —
153.149 —
147.736 —
140.711 —
140.190 —
138.392 —
137.181 —
136.964 —
136.312 —
135.864 —
134.352 —
131.434 —
131.372 —
129.272 —
127.731 —
127.272 —
126.737 —
124.968 —
124.699 —
124.025 —
123.028 —
122.634 —
121.841 —
121.440 —
116.633 —



SpinWorks 4: SS 62 (III) P
PROTON DMSO /opt/topspin3.5pl2/nmrdata nmrsu 13

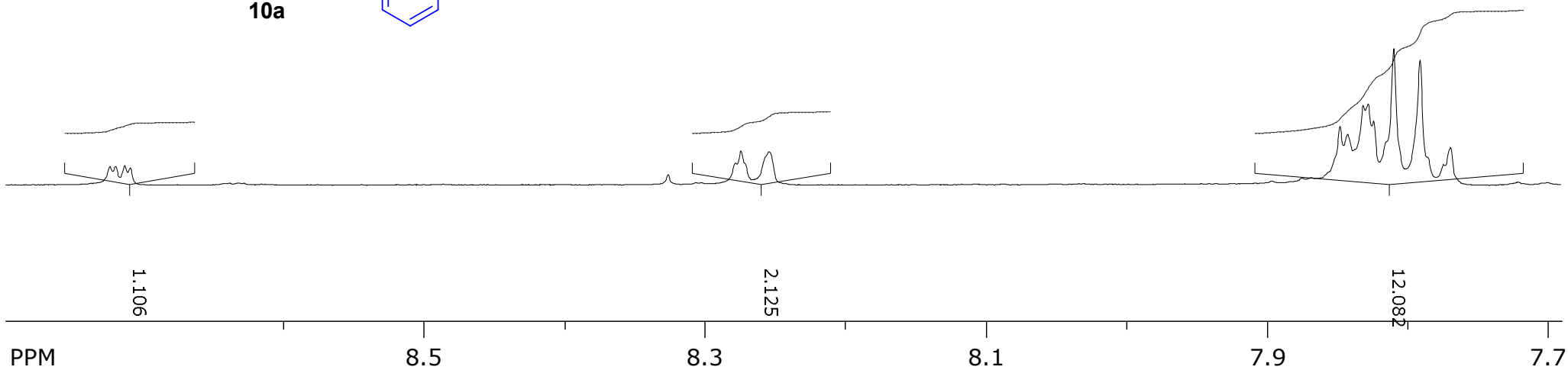
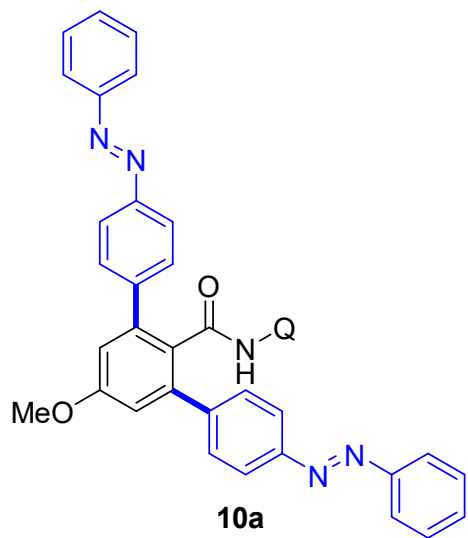


SpinWorks 4: SS 62 (III) P
PROTON DMSO /opt/topspin3.5pl2/nmrdata nmrsu 13

8.7093
8.7133
8.7198
8.7239

8.2546
8.2597
8.2746
8.2785

7.7693
7.7743
7.7910
7.8097
7.8148
7.8241
7.8280
7.8315
7.8426
7.8480

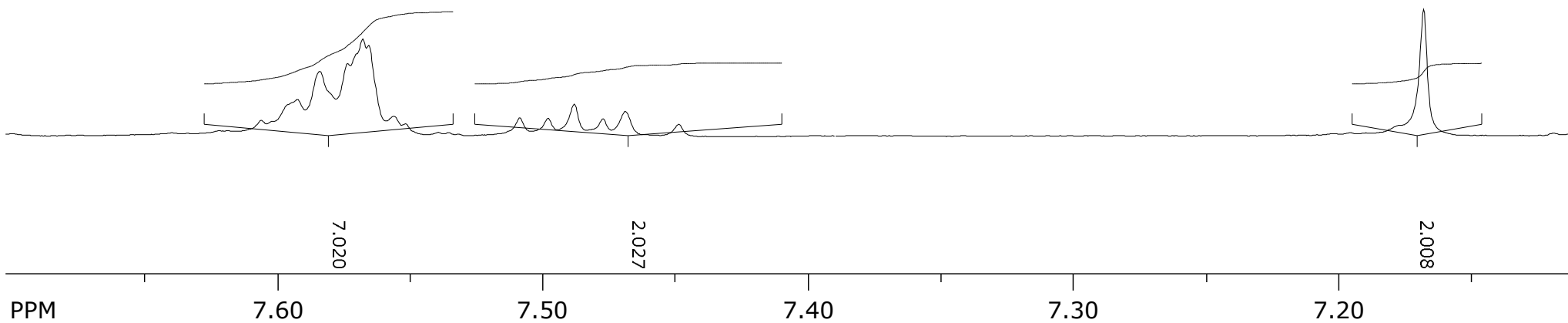
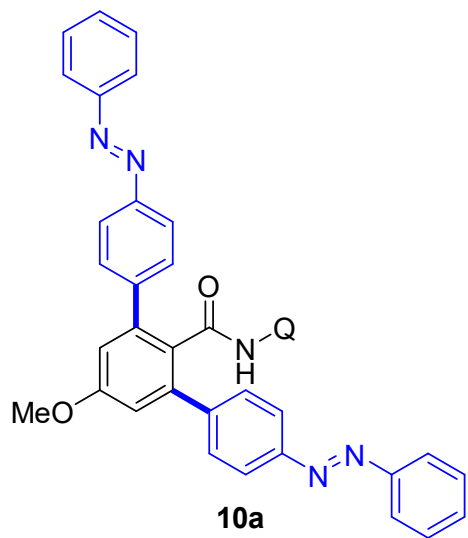


SpinWorks 4: SS 62 (III) P
PROTON DMSO /opt/topspin3.5pl2/nmrdata nmrsu 13

7.5518
7.5562
7.5657
7.5680
7.5737
7.5842
7.5927
7.6017
7.6063

7.4488
7.4690
7.4774
7.4882
7.4981
7.5088

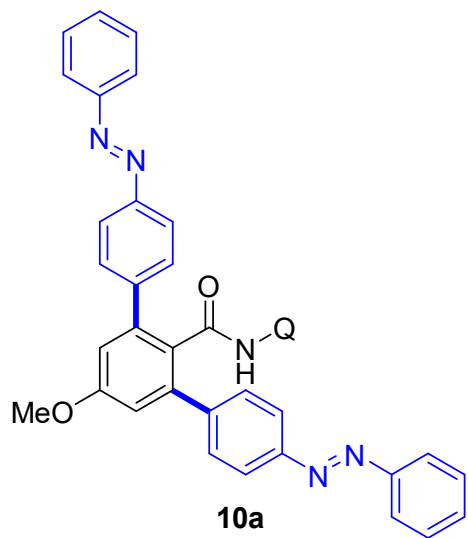
7.1679



SpinWorks 4: SS 62 III P
C13CPD DMSO /opt/topspin3.5pl2/nmrdata nmrsu 24

114.984
116.782
121.977
122.355
122.914
126.749
128.772
129.450
129.665
131.589
133.849
136.322
138.086
140.783
143.111
148.804
151.043
151.897
159.462
166.573

38.894
39.102
39.311
39.520
39.728
39.937
40.146
55.681



PPM

160

120

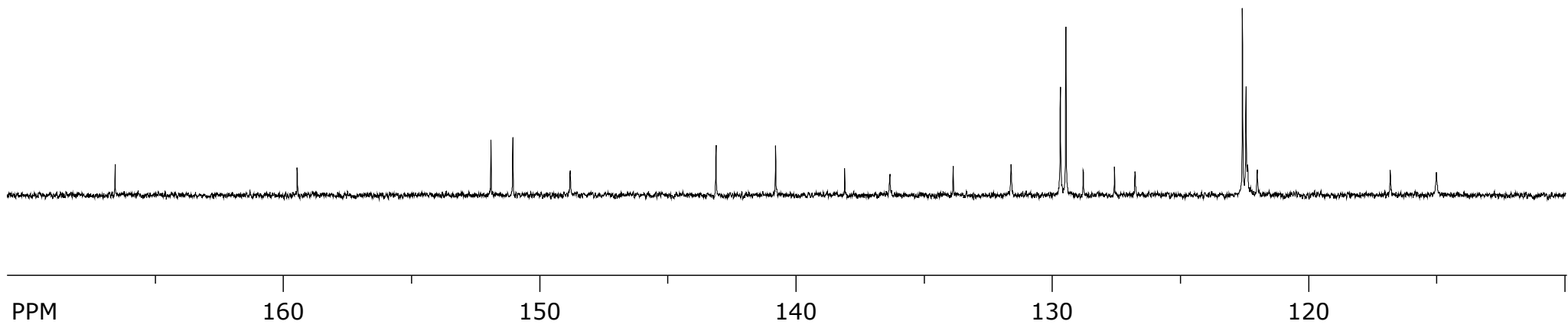
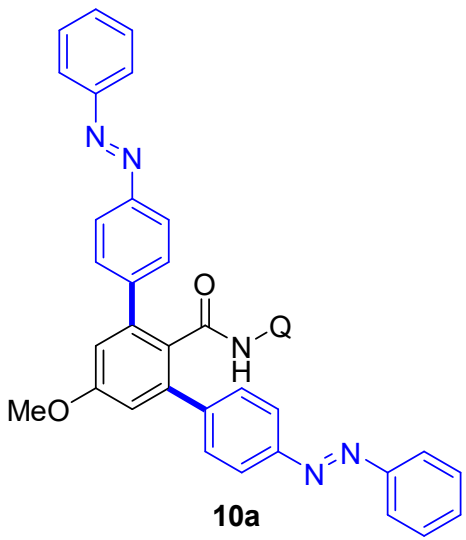
80

40

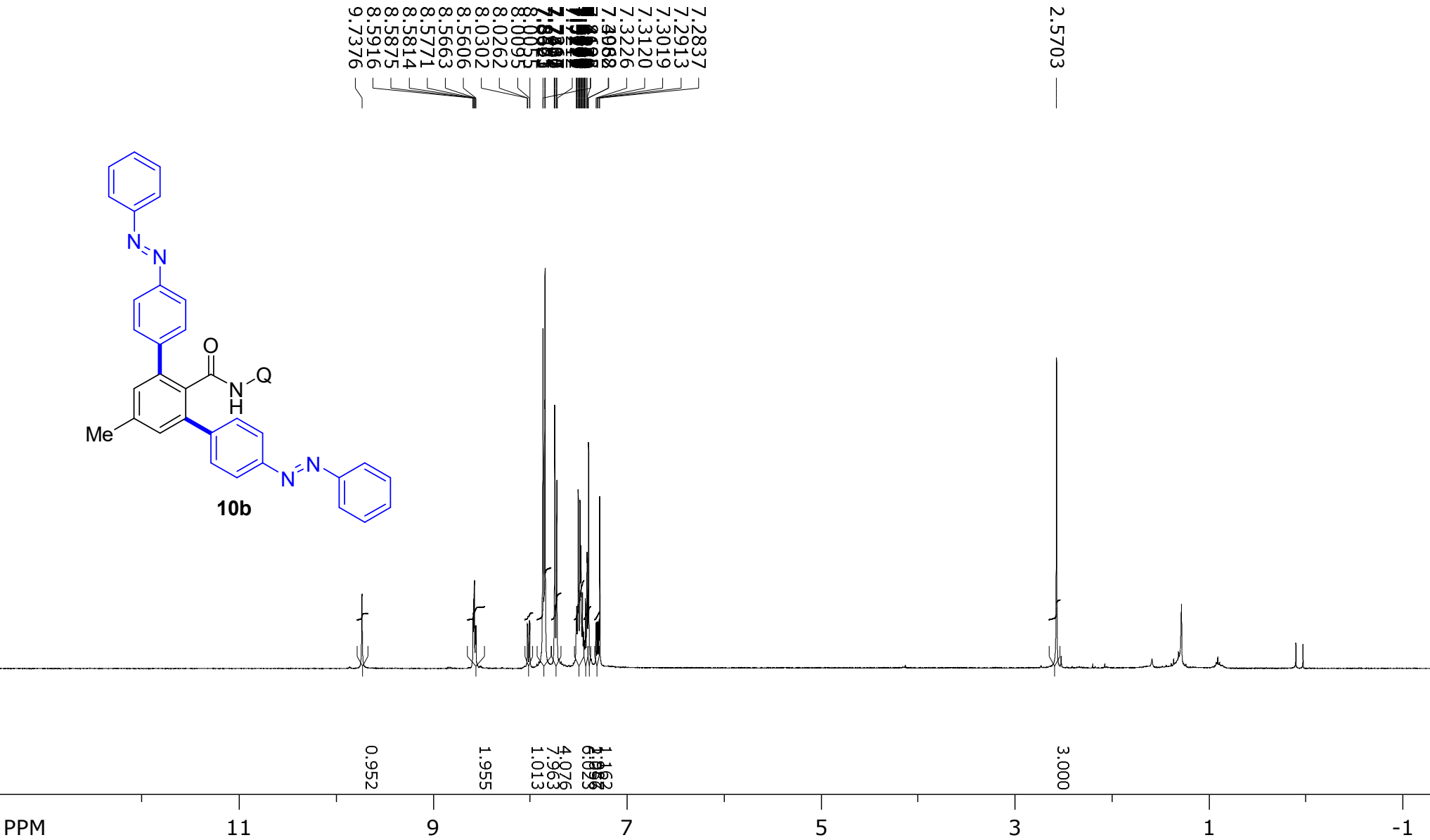
0

SpinWorks 4: SS 62 III P
C13CPD DMSO /opt/topspin3.5pl2/nmrdata nmrsu 24

166.573 —
159.462 —
151.043 —
151.897 —
148.804 —
143.111 —
140.783 —
138.086 —
136.322 —
133.849 —
131.589 —
129.665 —
129.450 —
128.772 —
127.552 —
126.749 —
122.554 —
122.416 —
122.355 —
121.977 —
116.782 —
114.984 —



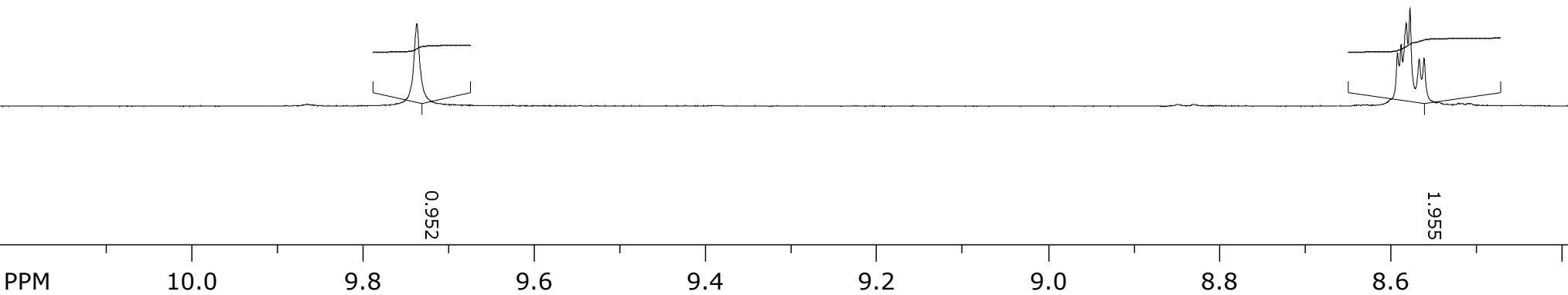
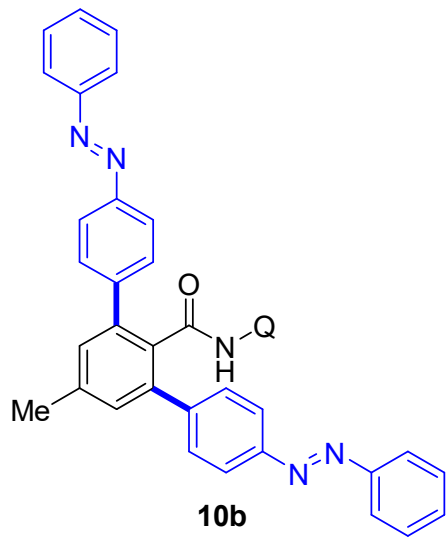
SpinWorks 4: SS-69-III
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 53



SpinWorks 4: SS-69-III
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 53

9.7376 —

8.5606
8.5663
8.5771
8.5814
8.5875
8.5916



0.952

1.955

PPM

10.0

9.8

9.6

9.4

9.2

9.0

8.8

8.6

SpinWorks 4: SS-69-III
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 53

8.0262
8.0302

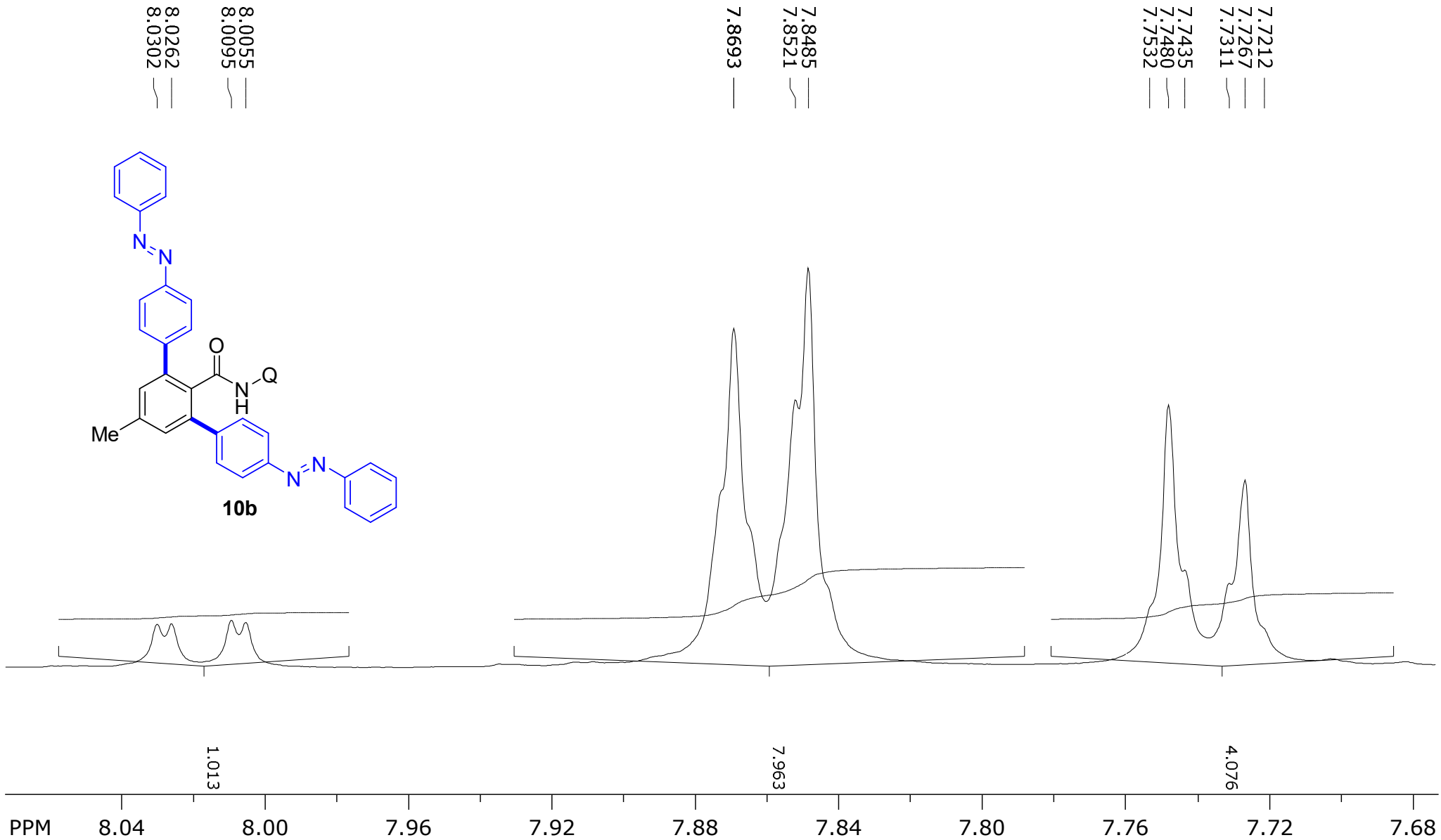
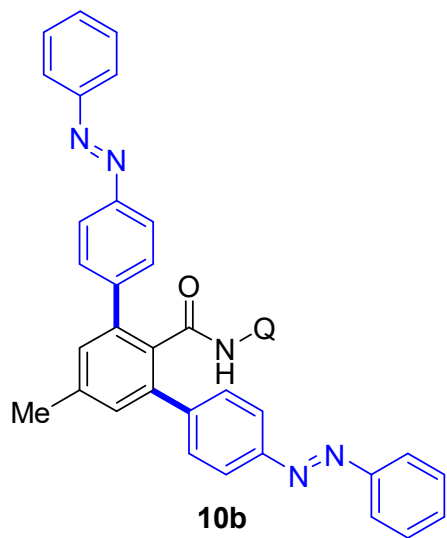
8.0055
8.0095

7.8693

7.8485
7.8521

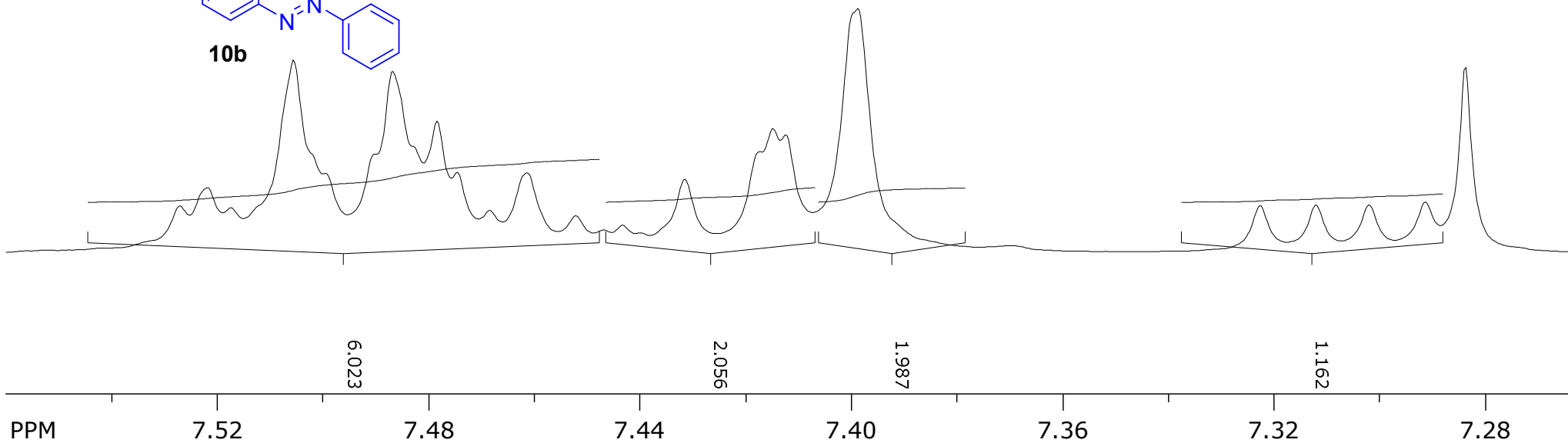
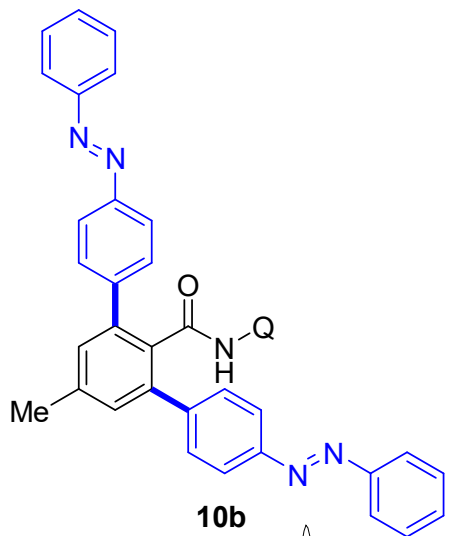
7.7435
7.7480
7.7532

7.7212
7.7267
7.7311



SpinWorks 4: SS-69-III
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 53

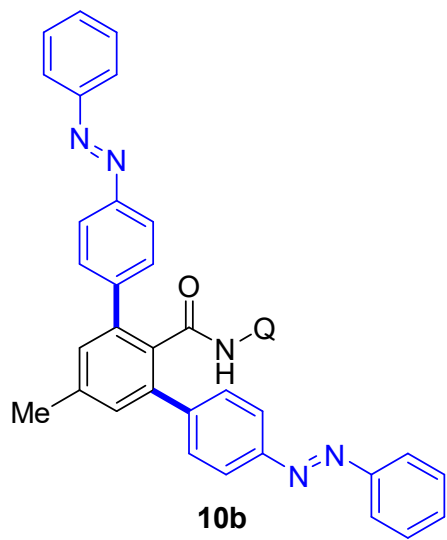
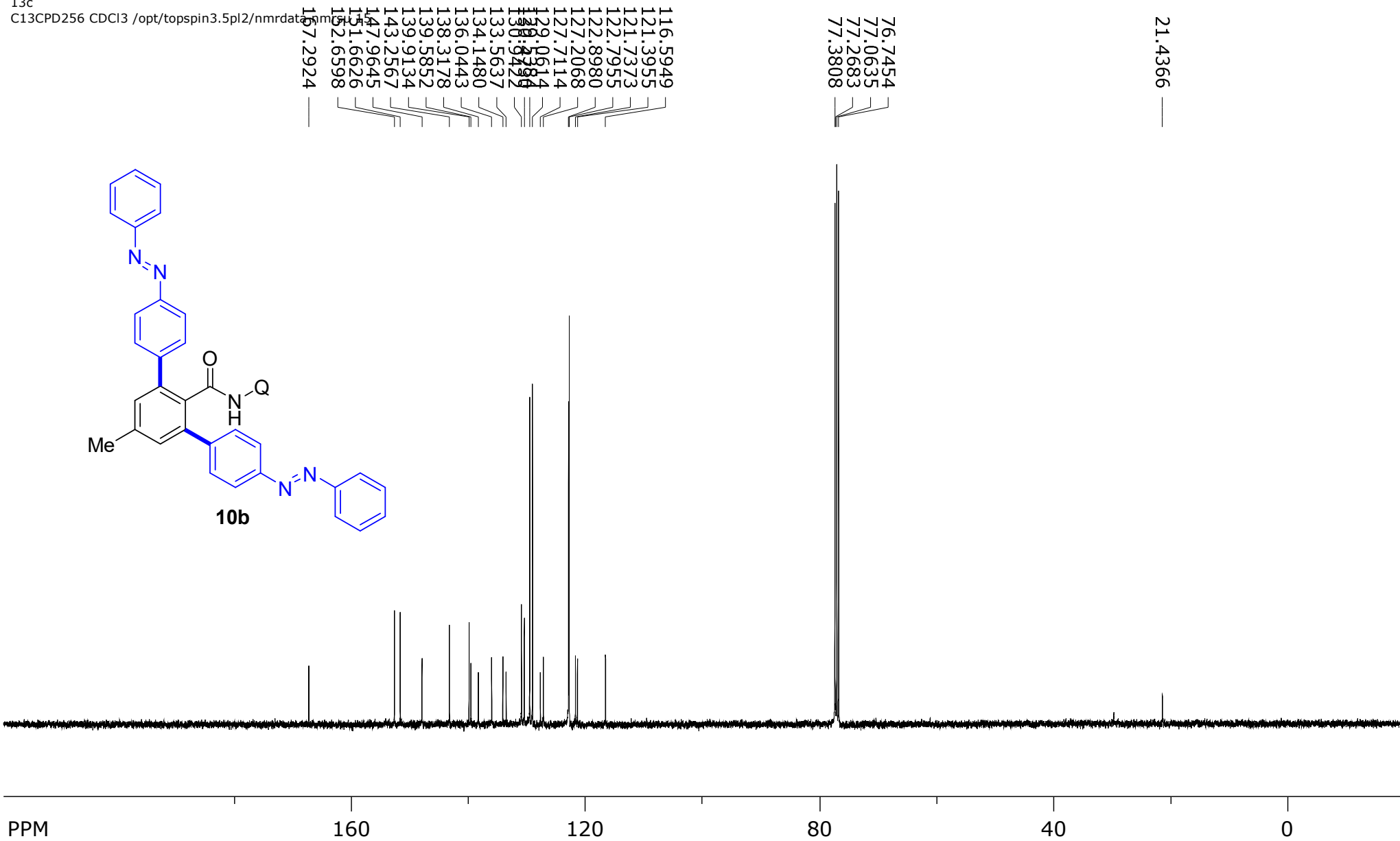
7.5272
7.5220
7.5175
7.5057
7.4996
7.4903
7.4869
7.4785
7.4747
7.4685
7.4614
7.4522
7.4469
7.4434
7.4400
7.4316
7.4174
7.4149
7.4125
7.4062
7.3988
7.3226
7.3120
7.3019
7.2913
7.2837



SpinWorks 4: ss 69-ii-p

13c

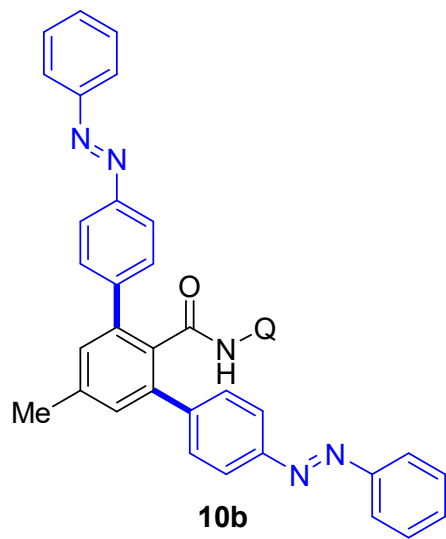
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata/nmrdata



SpinWorks 4: ss 69-ii-p

13c

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 15



187.2924

151.6626
152.6598

147.9645

143.2567

139.5852
139.9134

138.3178

136.0443

133.5637
134.1480

130.9422

130.4730

129.5384

127.7114

127.2068

122.8980

122.7955

121.7373

121.3955

116.5949

PPM

160

150

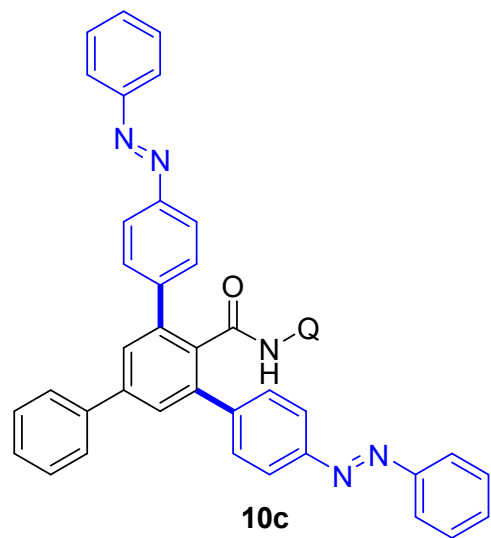
140

130

120

110

SpinWorks 4: SS-772
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 57



10c



PPM

12

8

4

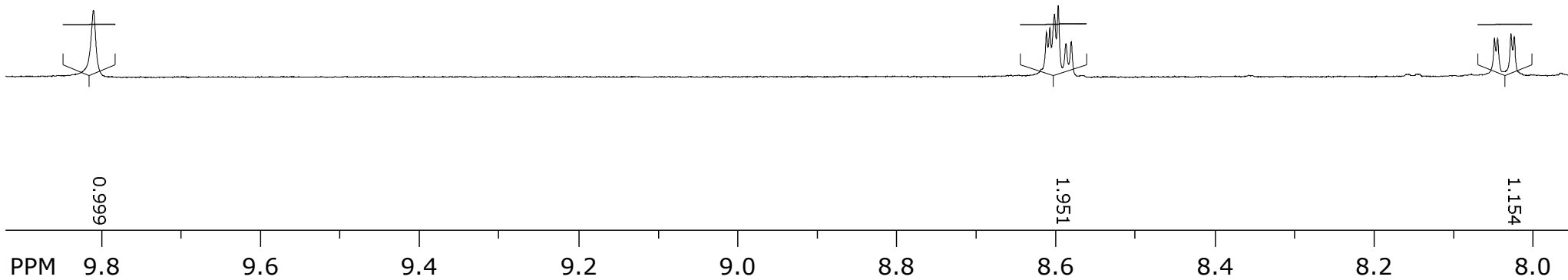
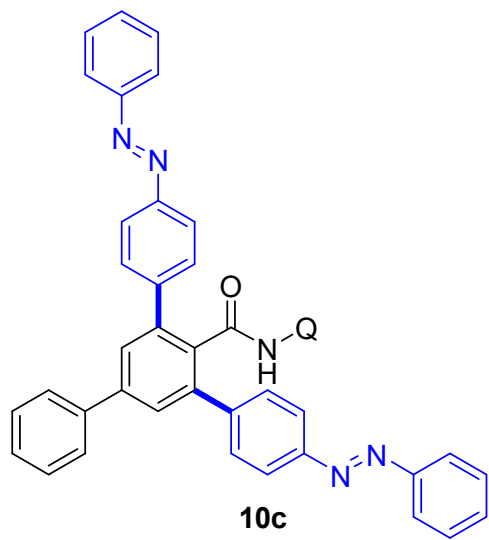
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SpinWorks 4: SS-772
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 57

8.5805
8.5871
8.5967
8.6013
8.6075
8.6116

8.0232
8.0273
8.0439
8.0480

9.8105



SpinWorks 4: SS-772
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 57

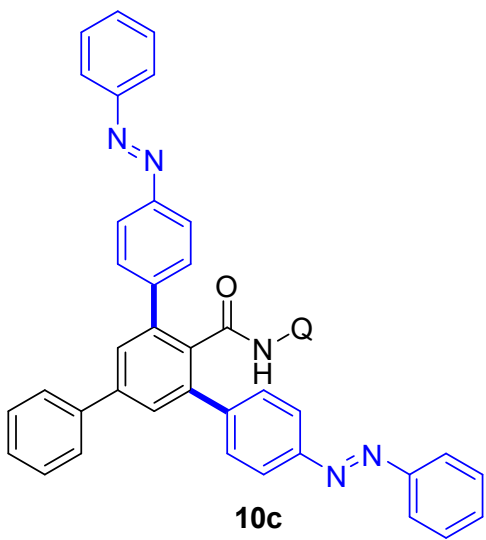
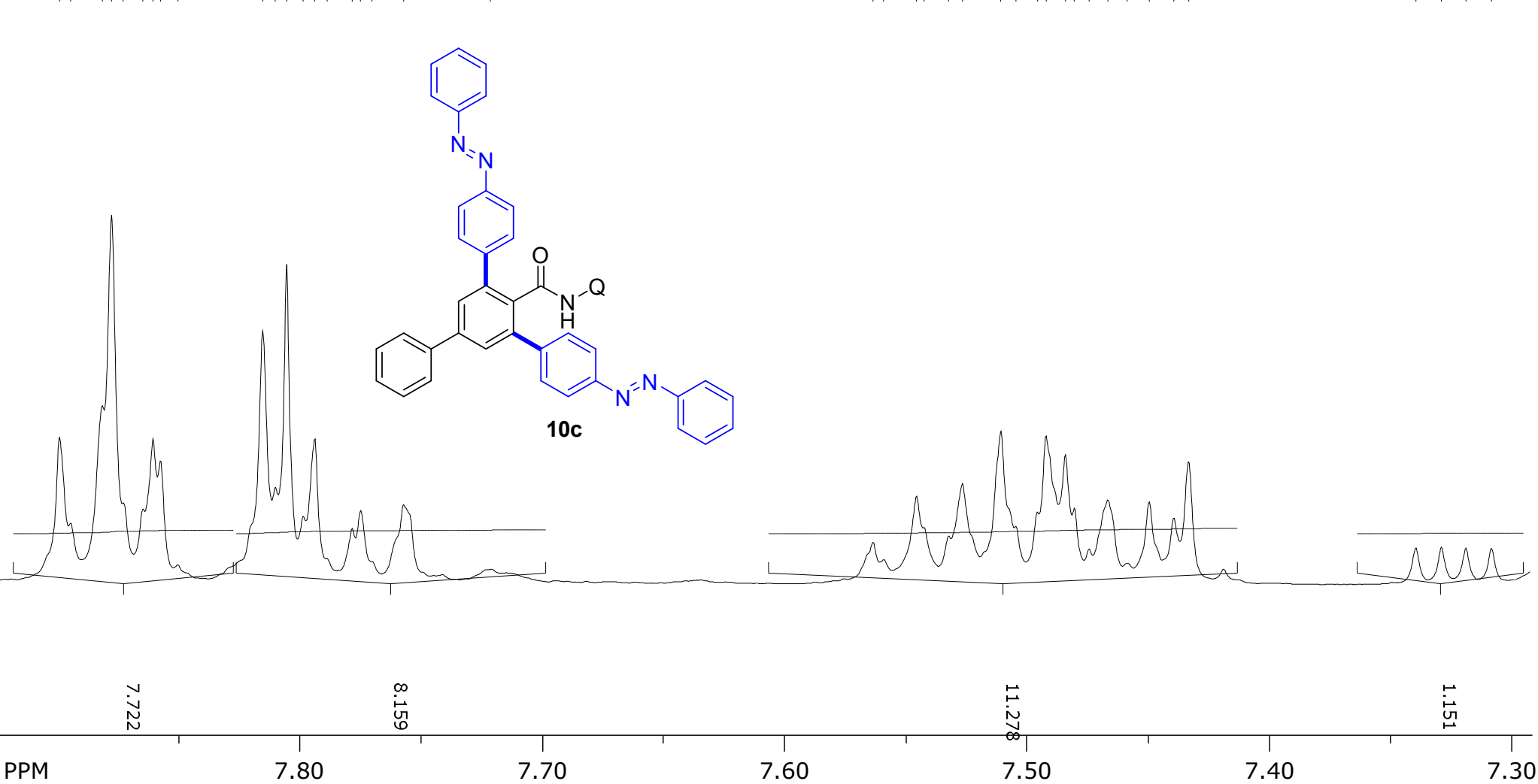
7.8505
7.8576
7.8608
7.8649
7.8731
7.8779
7.8817
7.8948
7.8994

7.8155
7.8103
7.8056
7.7988
7.7940
7.7889
7.7786
7.7751
7.7704
7.7574

7.7215

7.5266
7.5322
7.5425
7.5455
7.5591
7.5635
7.5107
7.5045
7.4956
7.4920
7.4841
7.4803
7.4743
7.4666
7.4586
7.4495
7.4393
7.4332

7.3082
7.3187
7.3288
7.3394

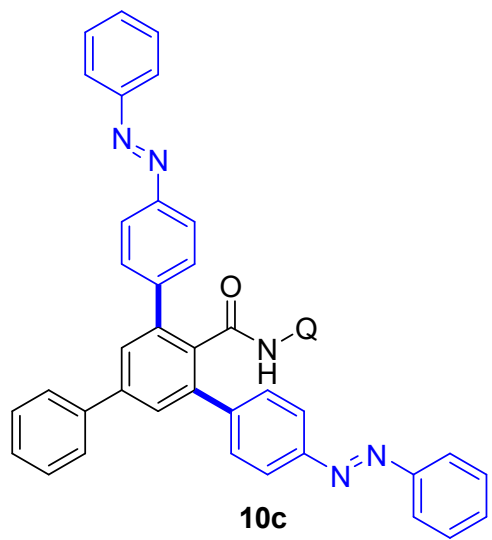


SpinWorks 4: SS-772

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 9

116.695
121.467
121.897
122.836
123.013
127.223
127.410
127.744
129.009
129.009
131.057
134.920
136.096
138.328
139.823
140.520
142.570
143.066
148.046
151.794
152.646
167.061

76.763
77.080
77.398



PPM

160

120

80

40

0

SpinWorks 4: SS-772
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 9

167.061

151.794
152.646

148.046

142.570
143.066

139.823
140.520

138.328

134.067
134.920

136.096

131.017

129.618

129.099

128.525

128.221

127.744

127.410

127.223

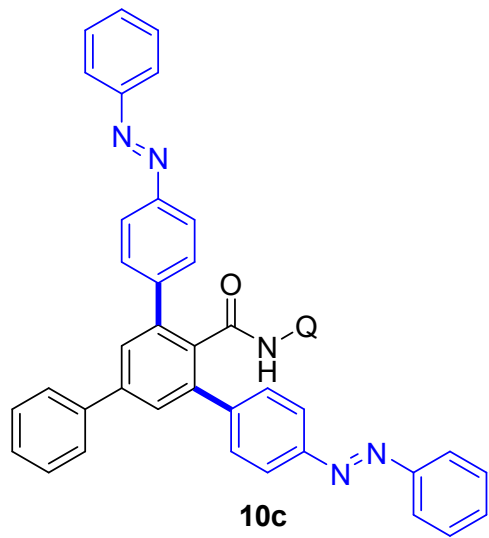
123.013

122.836

121.897

121.467

116.695



PPM

160

150

140

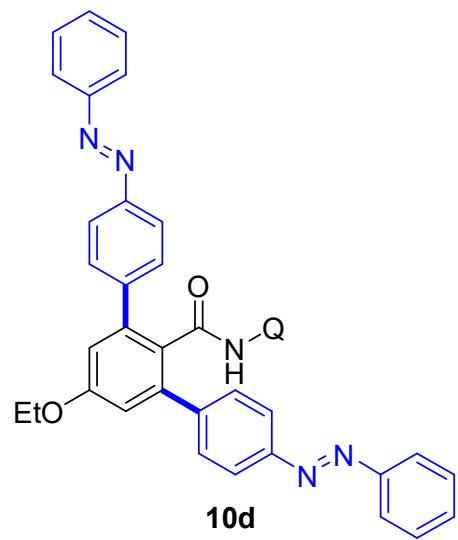
130

120

110

100

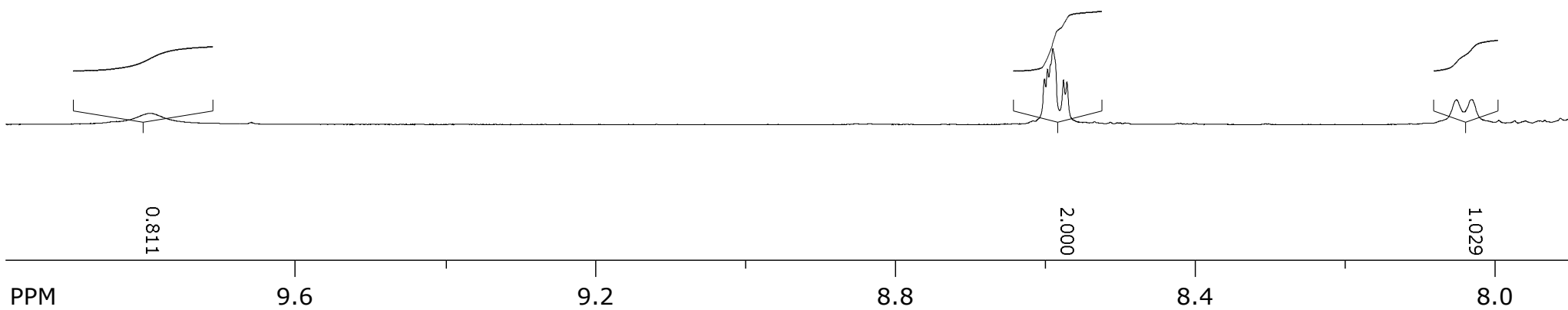
SpinWorks 4: SS-741
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 21



9.7990

8.5710
8.5756
8.5900
8.5968
8.6010

8.0306
8.0513



0.811

2.000

1.029

PPM

9.6

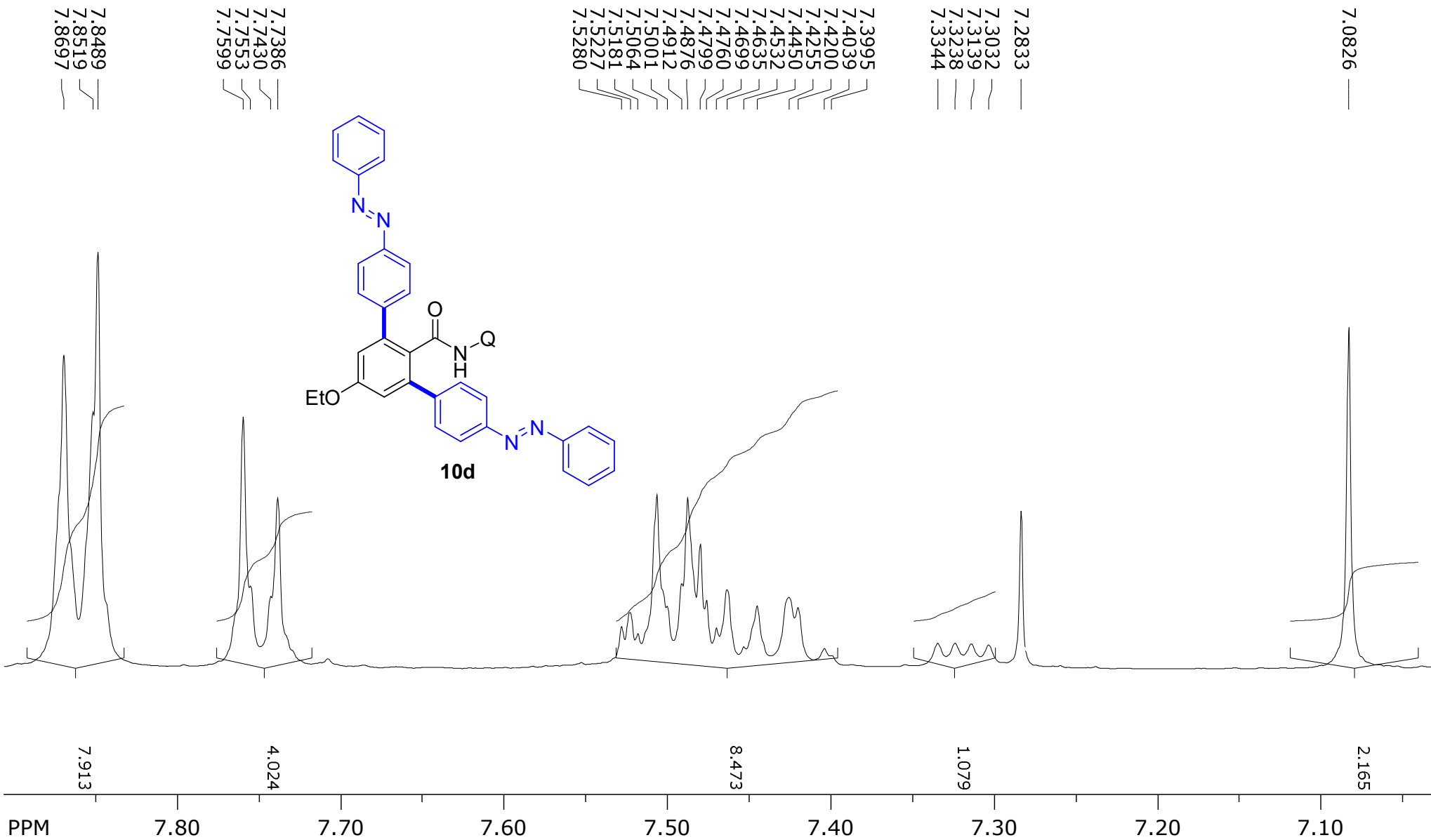
9.2

8.8

8.4

8.0

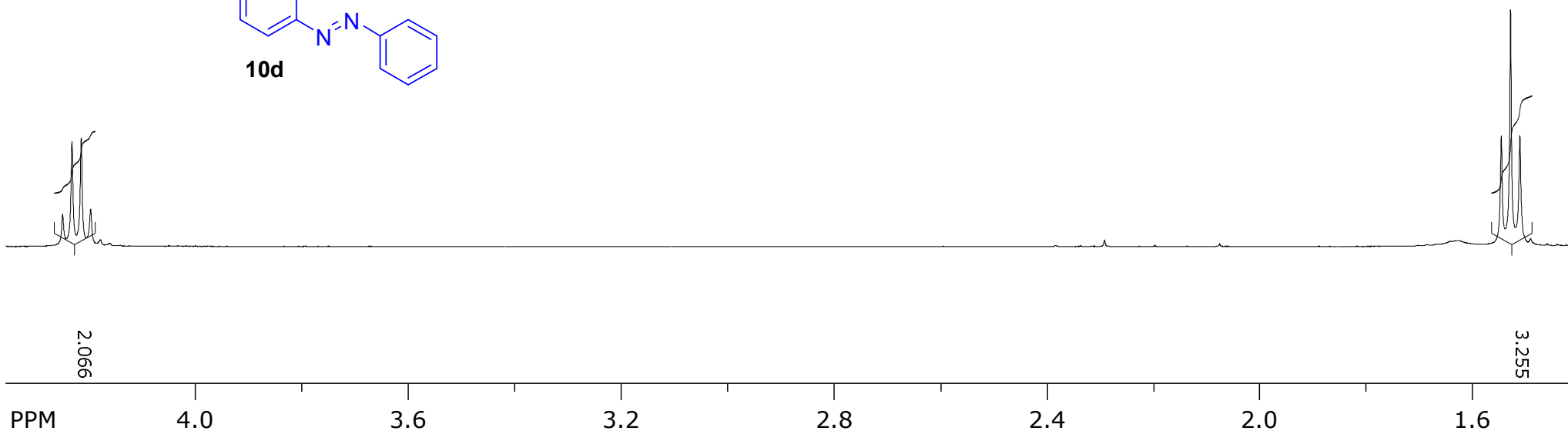
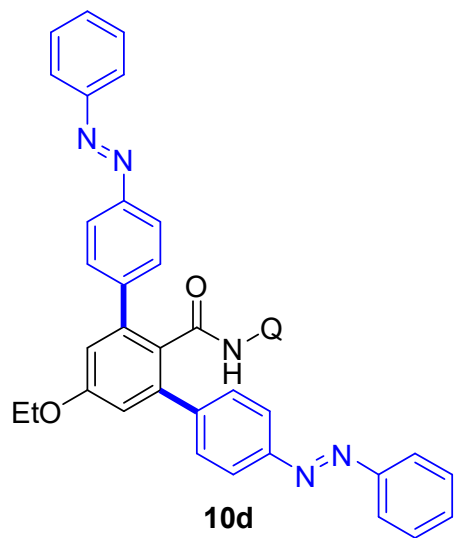
SpinWorks 4: SS-741
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 21



SpinWorks 4: SS-741
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 21

4.1968
4.2143
4.2318
4.2492

1.5107
1.5282
1.5456



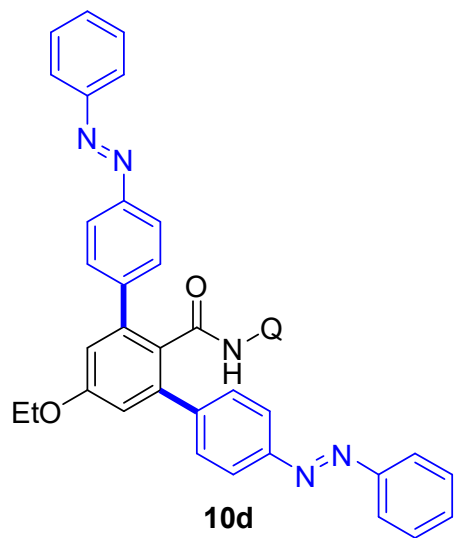
SpinWorks 4: SS 741
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 39

115.563
116.483
121.286
121.621
122.723
122.835
127.121
127.615
128.976
129.394
130.897
134.185
135.993
136.006
141.624
143.146
147.814
151.666
152.543
159.107
167.112

76.709
77.028
77.345

63.854

14.766



PPM

160

120

80

40

0

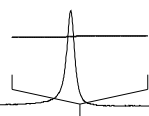
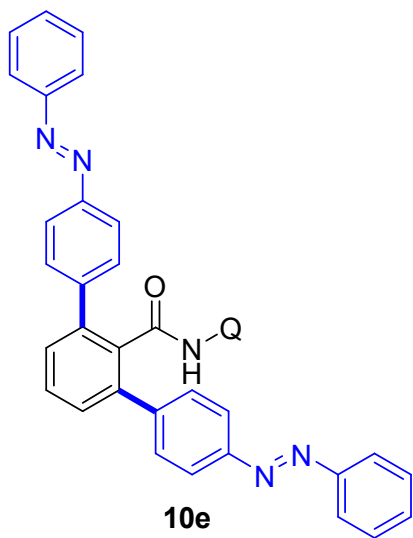
105

SpinWorks 4: SS-771
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 59

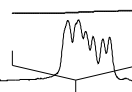
9.7618

8.5623
8.5687
8.5780
8.5848
8.5917
8.6019

8.0169
8.0374



0.999



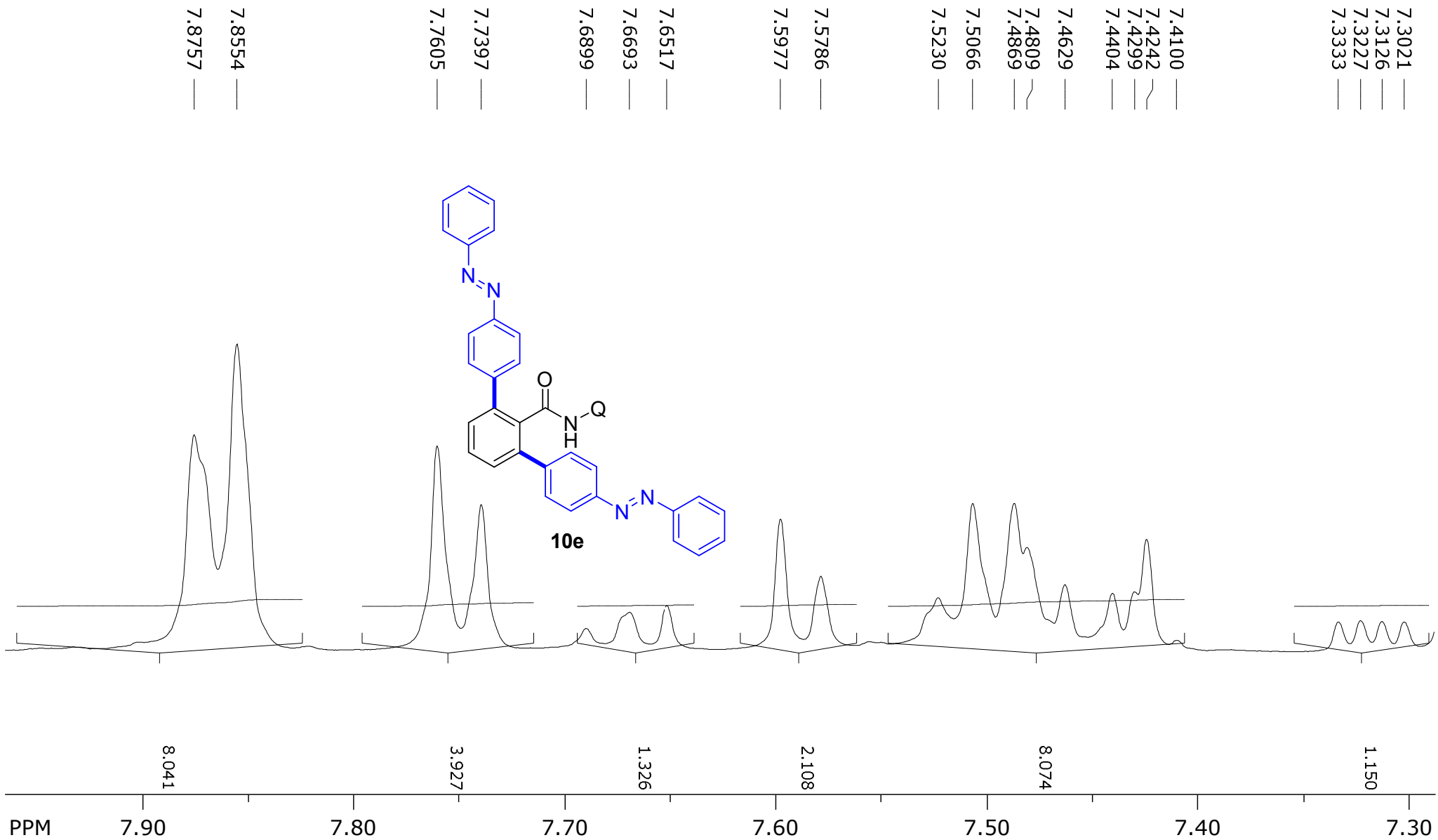
1.949



1.162

PPM 9.8 9.6 9.4 9.2 9.0 8.8 8.6 8.4 8.2 8.0

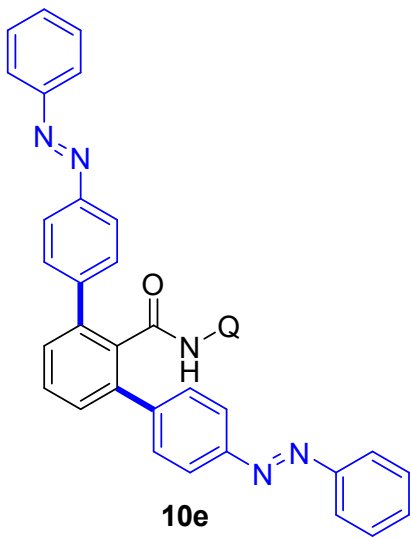
SpinWorks 4: SS-771
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 59



SpinWorks 4: SS 771
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 12

116.701
121.446
121.884
122.812
122.939
122.998
127.204
127.733
129.073
129.579
129.836
130.987
134.026
136.094
138.321
139.873
143.055
148.024
151.719
152.645
167.109

76.758
77.076
77.393



PPM

160

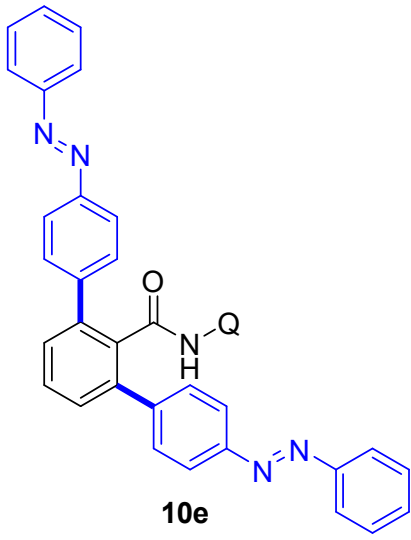
120

80

40

0

SpinWorks 4: SS 771
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 12



167.109 —

151.719 —
152.645 —

148.024 —

143.055 —

139.873 —
138.321 —

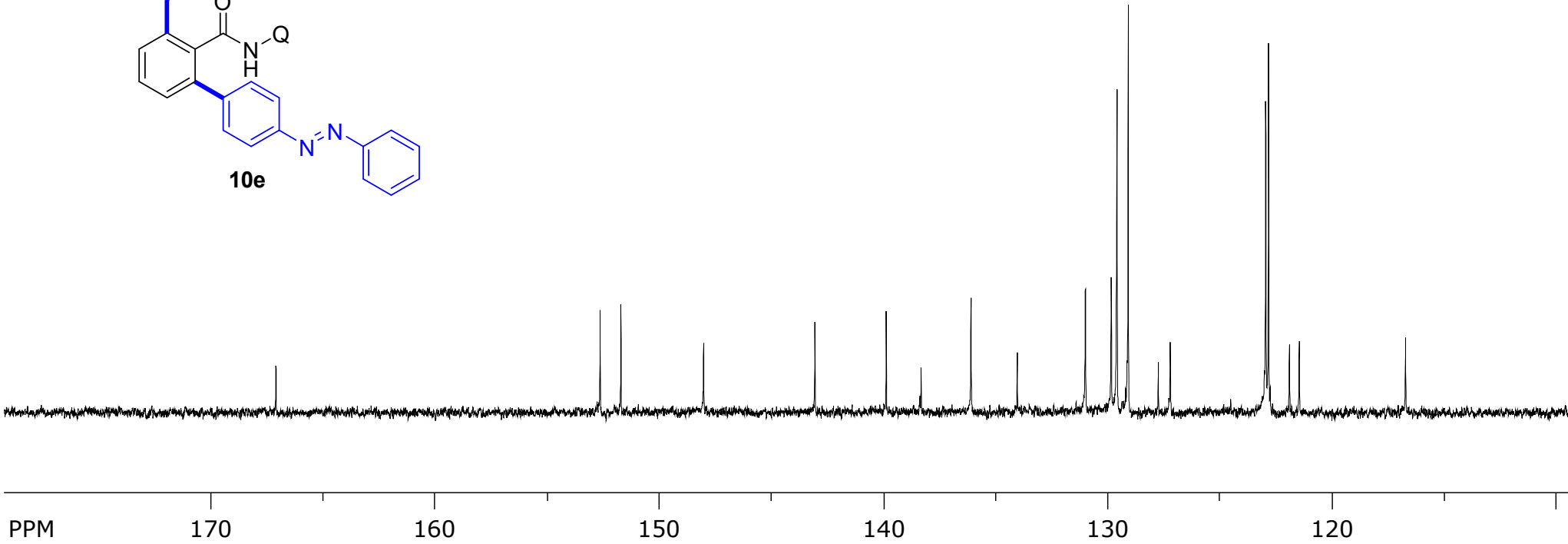
136.094 —

134.026 —

130.987 —
129.836 —
129.579 —
129.122 —
129.073 —
127.733 —
127.204 —

122.939 —
122.812 —
121.884 —
121.446 —
122.998 —

116.701 —



SpinWorks 4: SS-742-REP
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 1

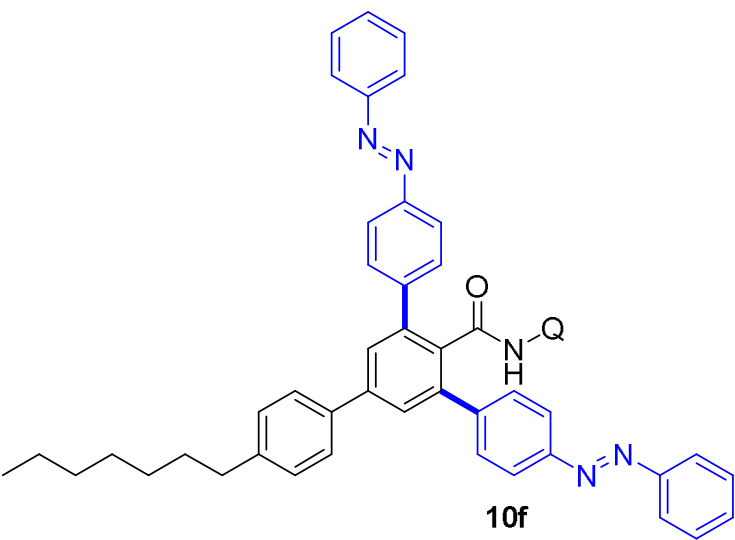
8.5968
8.6026
8.6089
8.6129
8.6192

8.0729
8.0824
8.0928

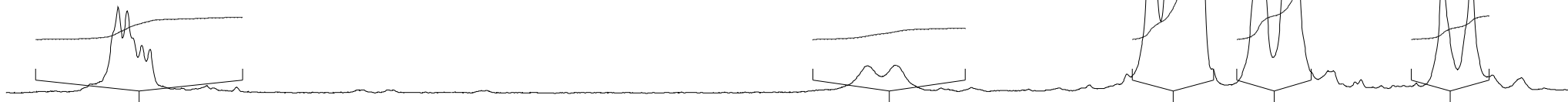
7.8574
7.8604
7.8739
7.8905
7.8950

7.7924
7.7962
7.8182

7.6688
7.6891



10f



1.967

1.000

6.963

5.107

2.089

PPM

8.4

8.2

8.0

7.8

SpinWorks 4: SS-742-REP
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 1

7.5229
7.5277
7.5327

7.5052
7.5113

7.4924

7.4805
7.4844

7.4739
7.4676

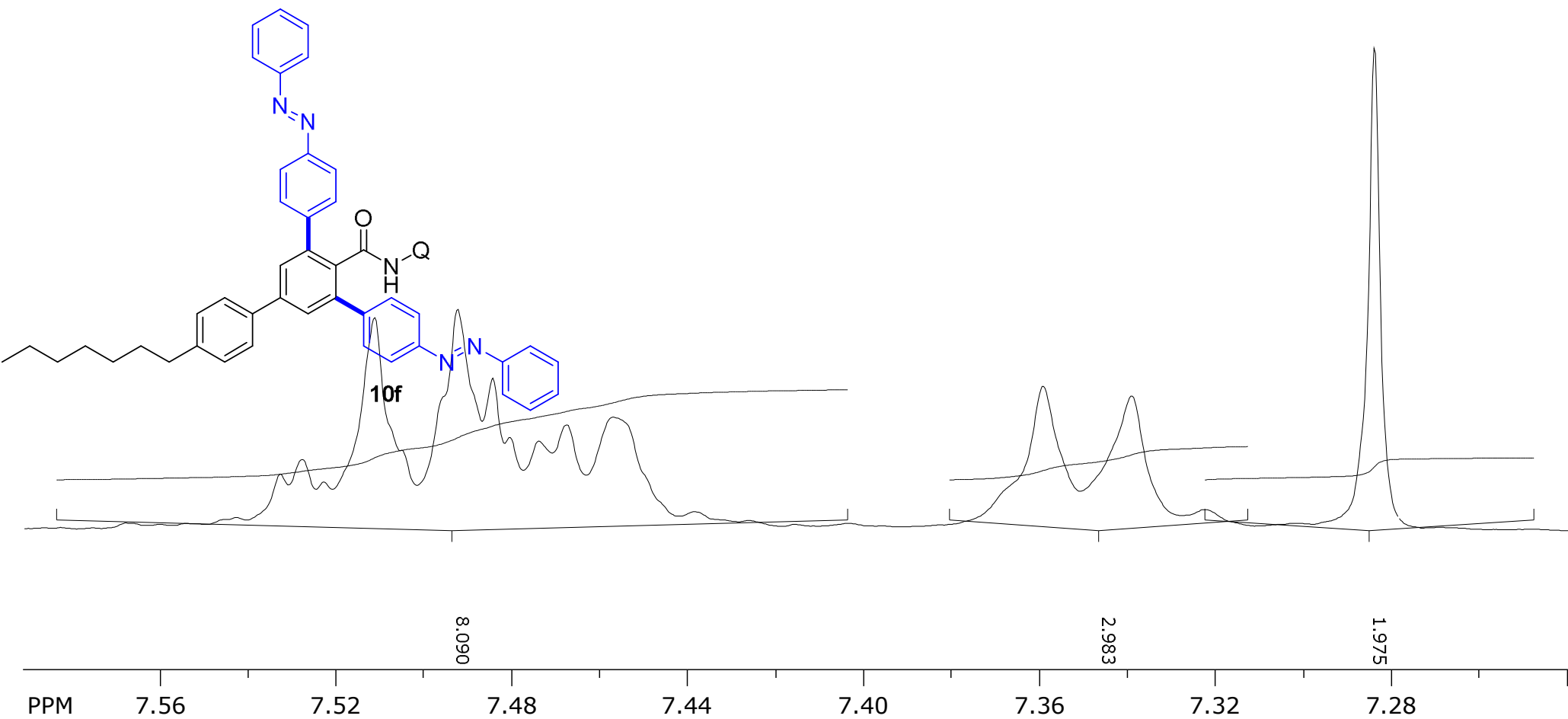
7.4570

7.3592

7.3390

7.3224

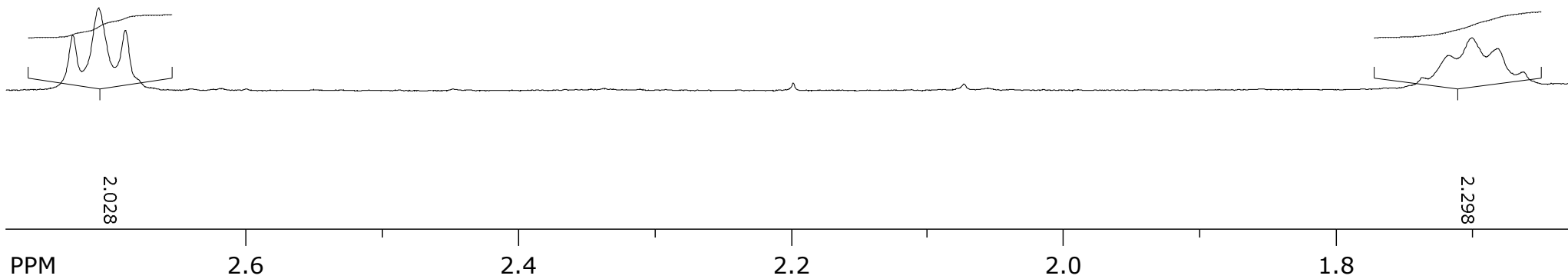
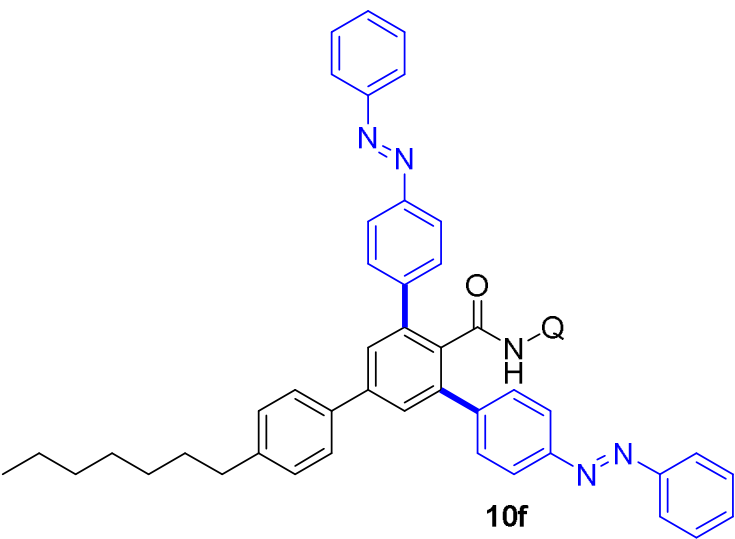
7.2838



SpinWorks 4: SS-742-REP
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 1

2.68888
2.7084
2.72273

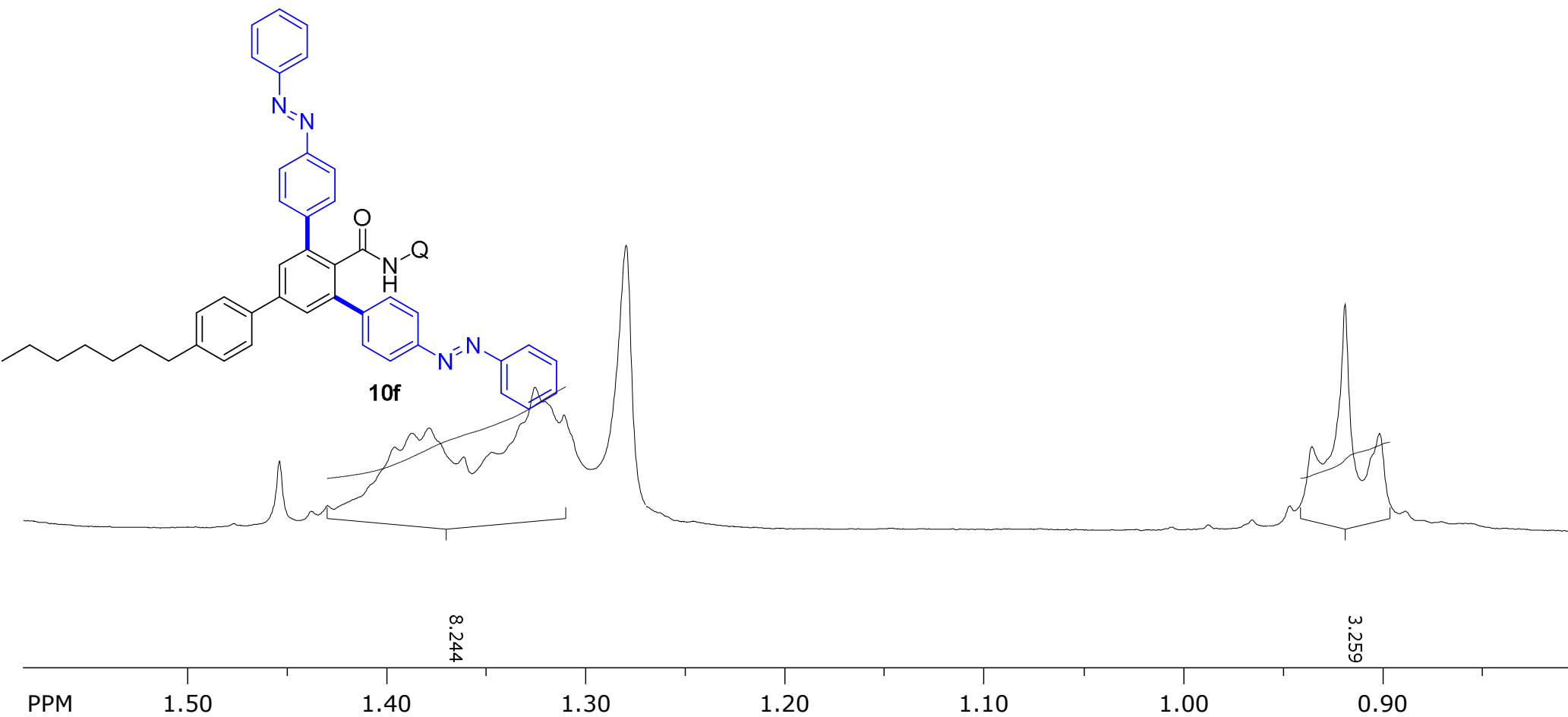
1.6627
1.6710
1.6815
1.7002
1.7124
1.7168
1.7325



SpinWorks 4: SS-742-REP
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 1

1.31110
1.3206
1.3256
1.3436
1.3470
1.3614
1.3789
1.3875
1.3962
1.4299
1.4380

0.9014
0.9187
0.9354

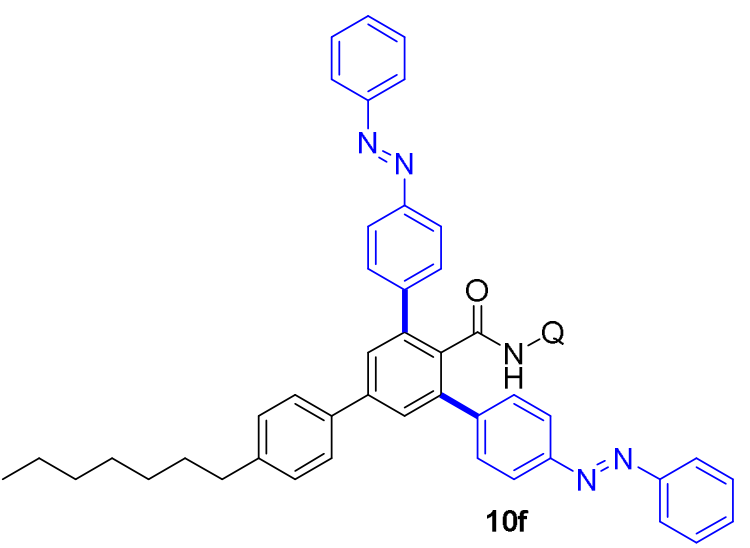


SpinWorks 4: SS-742 REP
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu_14

167.2601
152.6450
151.7417
143.2174
143.2029
142.5203
140.4322
137.0995
134.5340
131.0275
130.9750
129.0858
129.0858
127.2282
127.1845
122.9412
122.8063
121.9488
121.3598

76.7236
77.0416
77.3588

35.7010
31.8585
31.5390
29.7280
29.3581
22.7145
22.2332
14.1578

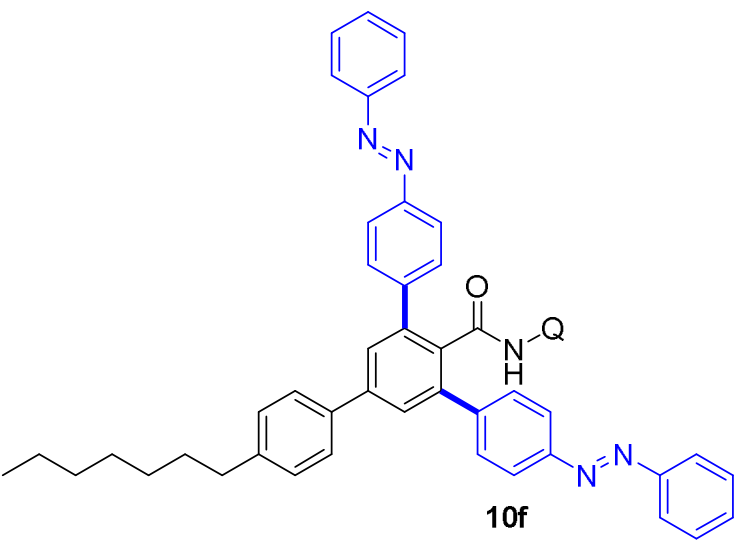


PPM

160 120 80 40 0

SpinWorks 4: SS-742 REP
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 14

167.2601 —
151.7417 —
152.6450 —
143.2174 —
142.5203 —
143.2029 —
140.4322 —
137.0995 —
134.5340 —
131.0275 —
130.9750 —
129.6858 —
129.6340 —
129.5941 —
129.5497 —
129.1363 —
129.0675 —
128.3029 —
127.8677 —
127.4760 —
127.2282 —
127.1845 —
122.9412 —
122.8063 —
121.9488 —
121.3598 —



PPM 170 160 150 140 130 120 110 100

SpinWorks 4: SS-742 REP
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 14

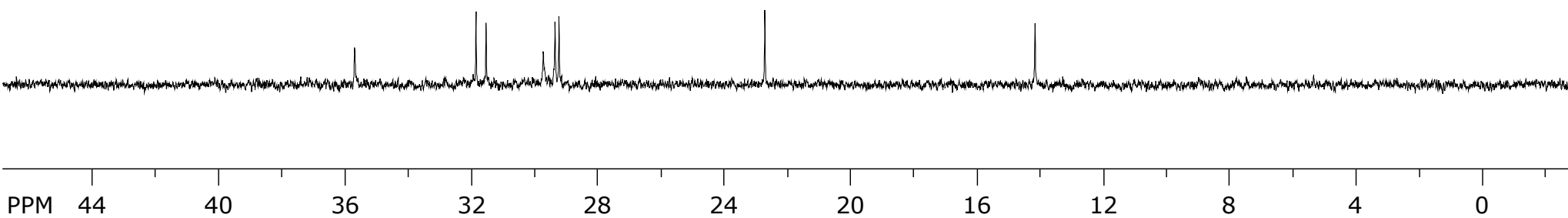
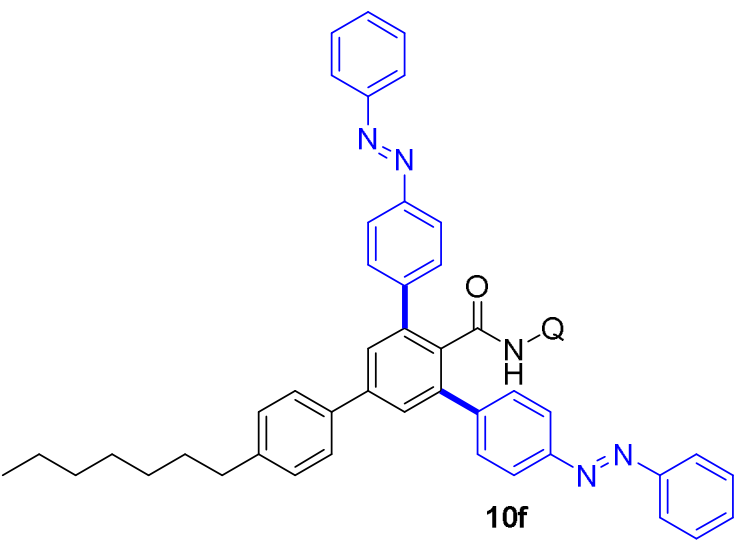
35.7010 —

31.5390 —
31.8585 —

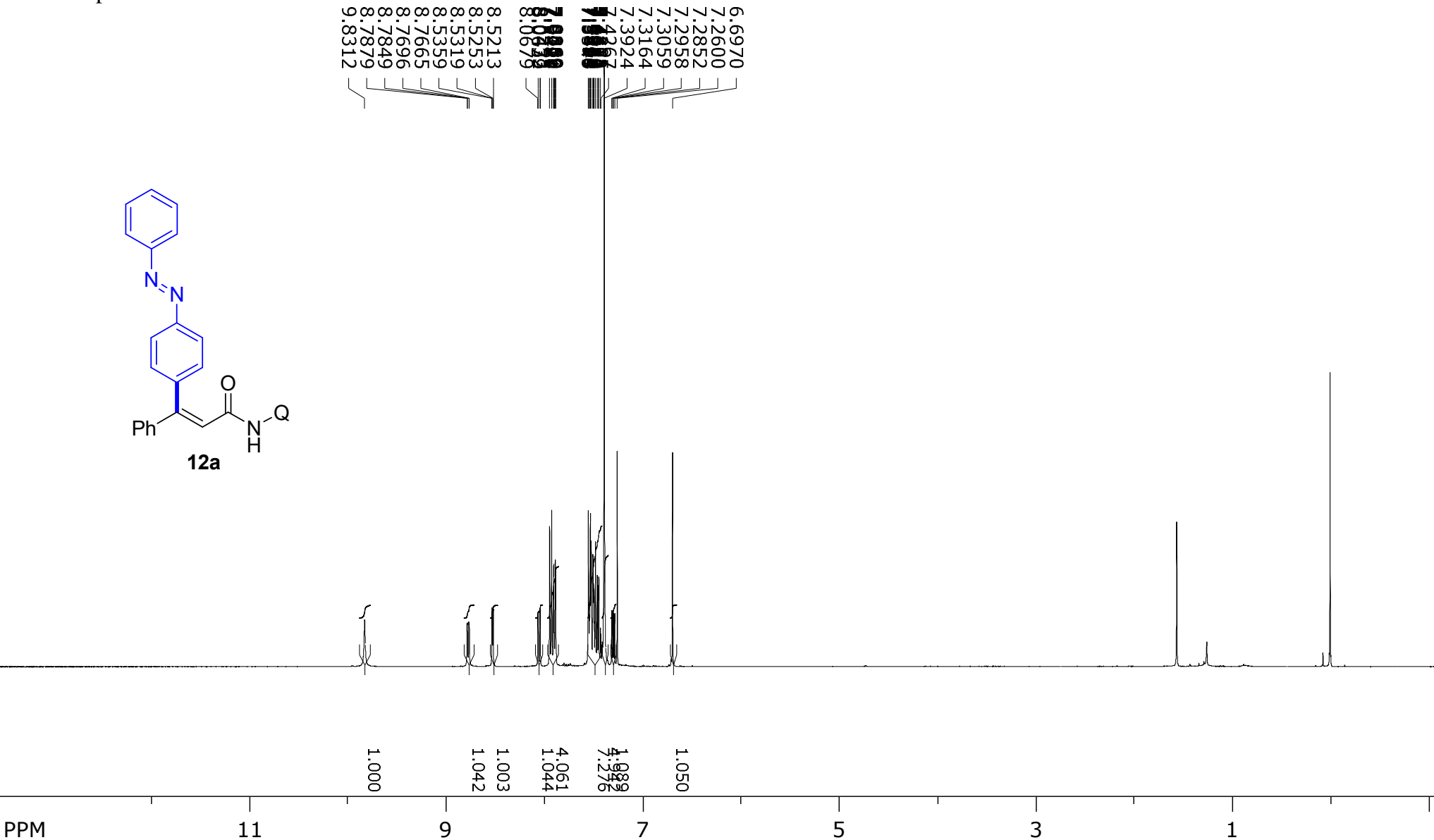
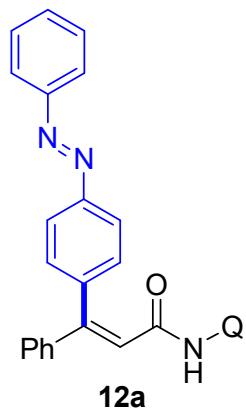
29.2332 —
29.3581 —
29.7280 —

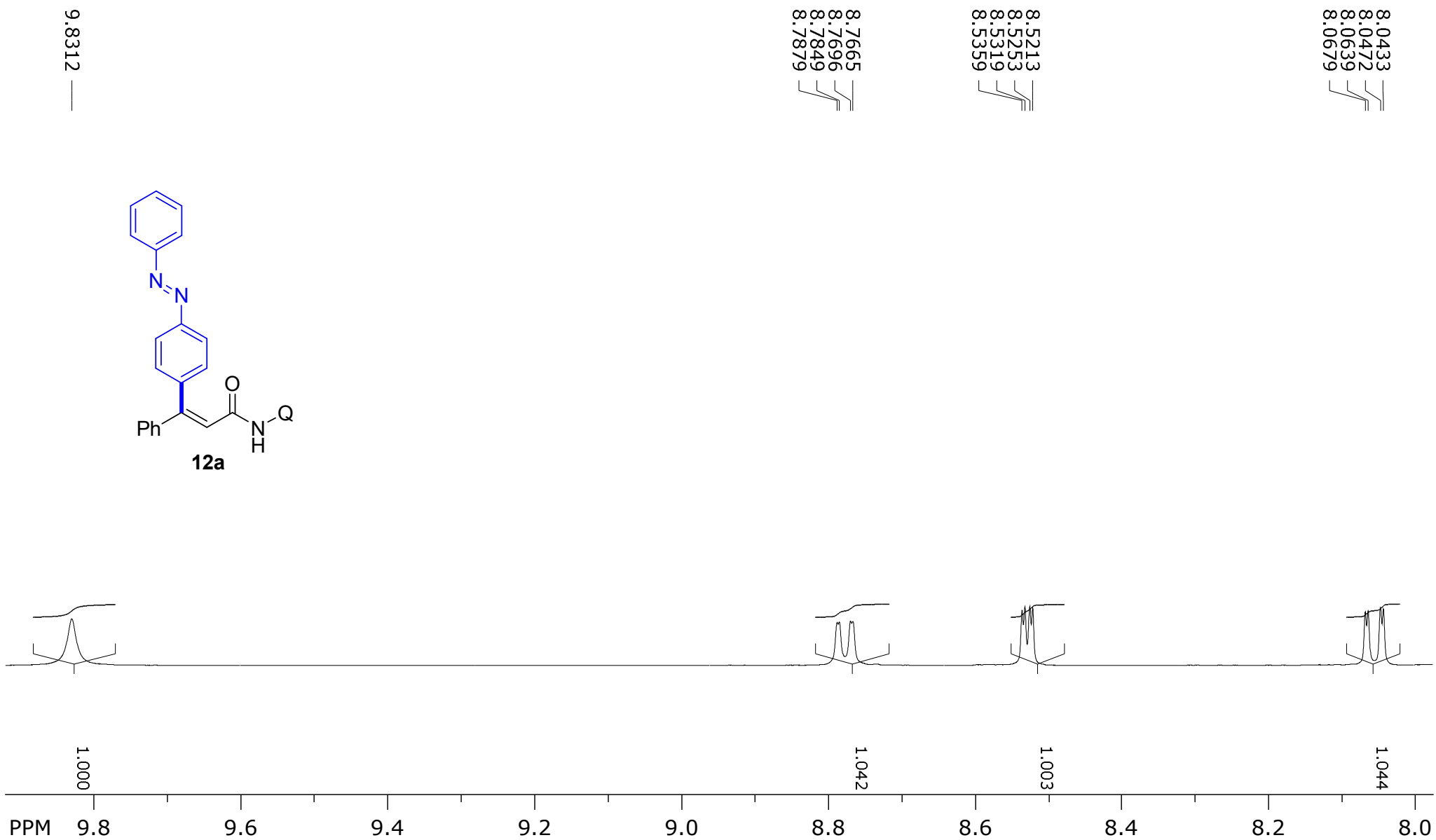
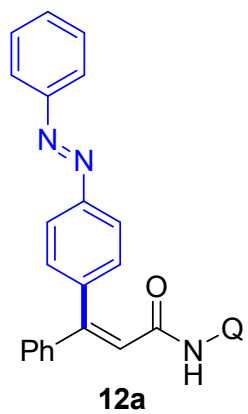
22.7145 —

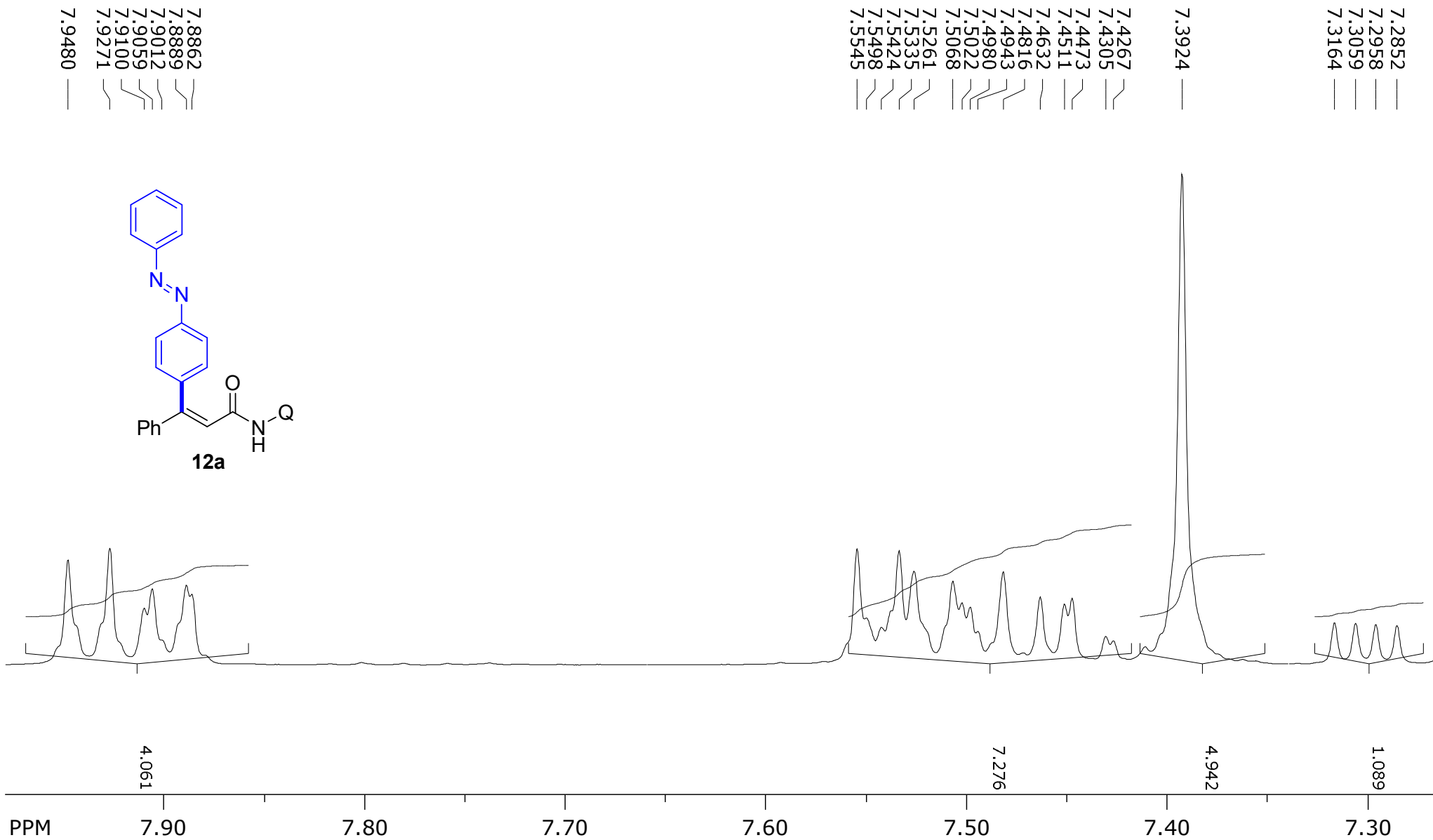
14.1578 —



SS-184-p

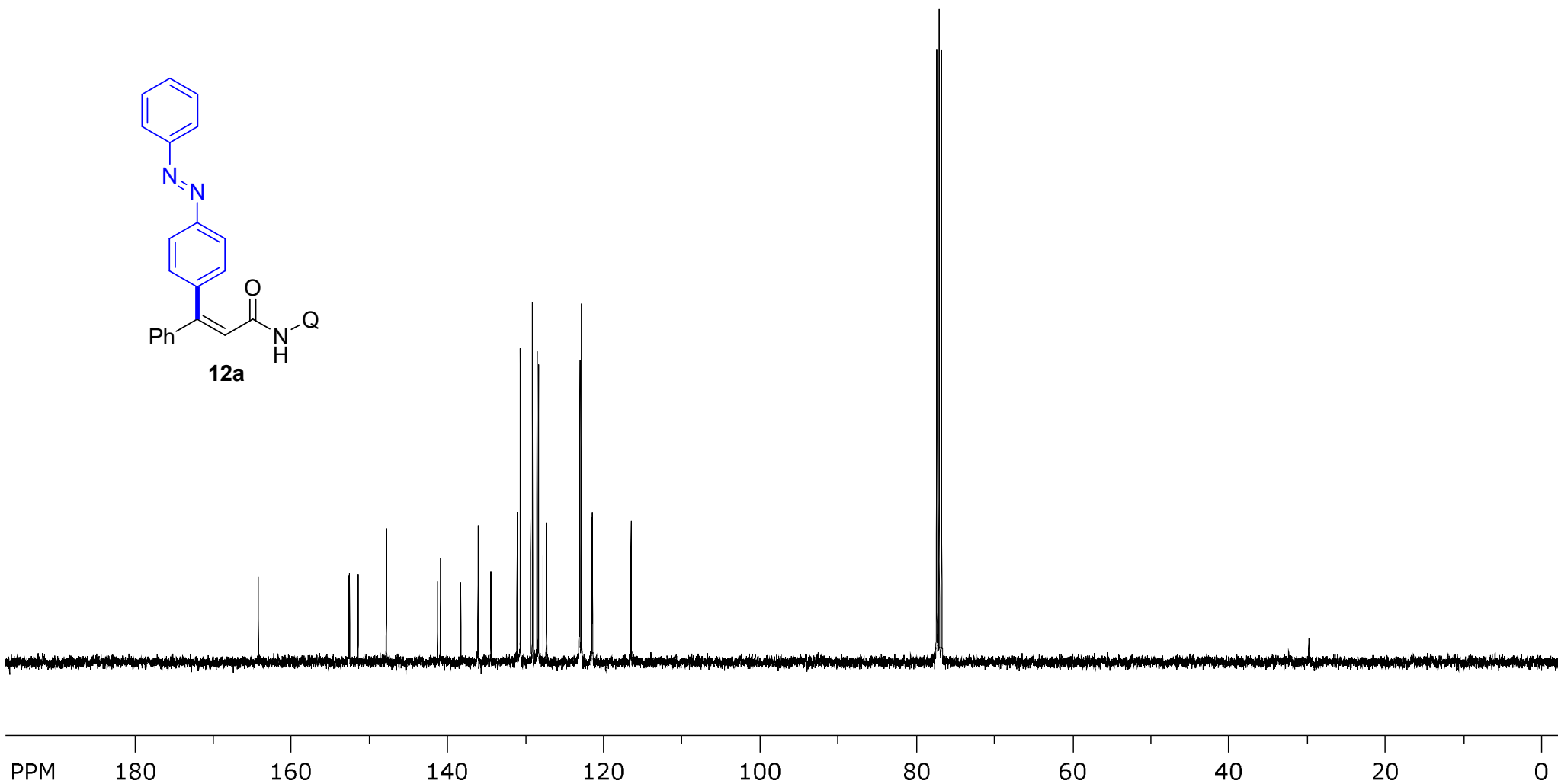
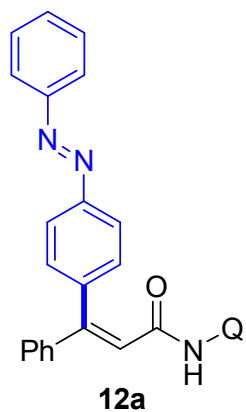




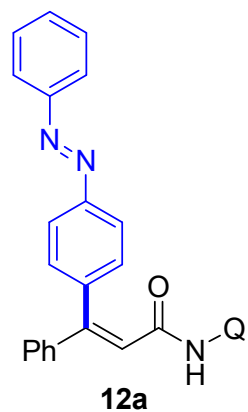


SpinWorks 4: SS 184 P
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 59

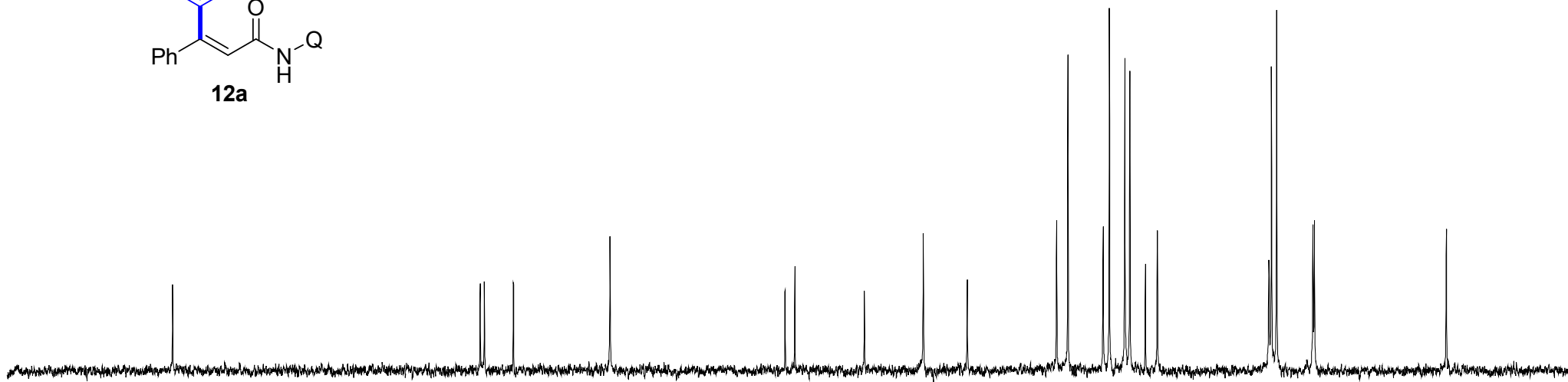
164.263
152.735
151.490
147.867
141.311
140.943
138.335
136.127
134.479
131.130
130.706
129.387
129.185
128.985
127.805
127.356
123.175
123.080
122.883
121.526
121.469
116.526
77.397
77.079
76.761



SpinWorks 4: SS 184 P
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 59



164.263 —
151.490 —
152.575 —
152.735 —
147.867 —
140.943 —
141.311 —
138.335 —
136.127 —
134.479 —
131.130 —
129.706 —
129.152 —
128.575 —
128.385 —
127.805 —
127.356 —
123.175 —
123.080 —
122.883 —
121.526 —
121.469 —
116.526 —



PPM

160

150

140

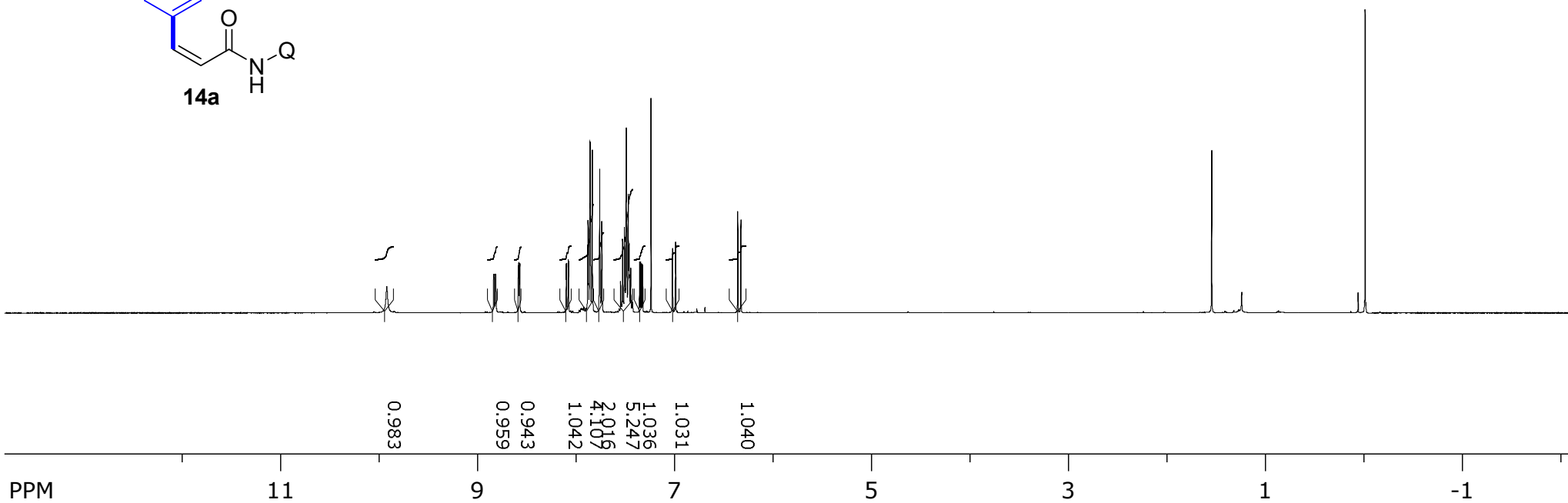
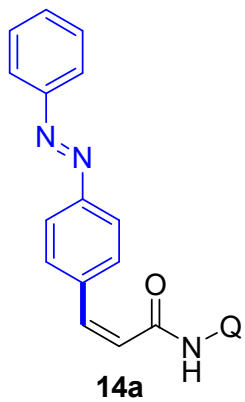
130

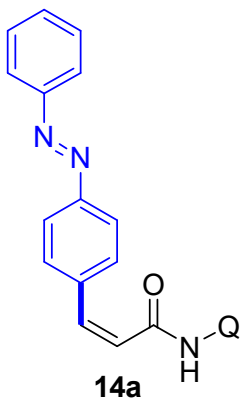
120

SpinWorks 4: DC-180

SS-185-p

6.3266
6.3579
6.9898
7.0212
7.2399
7.3243
7.3349
7.3450
7.3555
7.9100
7.9200
8.0000
8.5731
8.5771
8.5836
8.5876
8.8163
8.8191
8.8349
8.8374
9.9244





9.9244

8.8163
8.8191
8.8349
8.8374

8.5731
8.5771
8.5836
8.5876

8.0769
8.0809
8.0976
8.1016



0.983

0.959

0.943

1.042

PPM

10.0

9.6

9.2

8.8

8.4

8.0

SpinWorks 4: DC-180

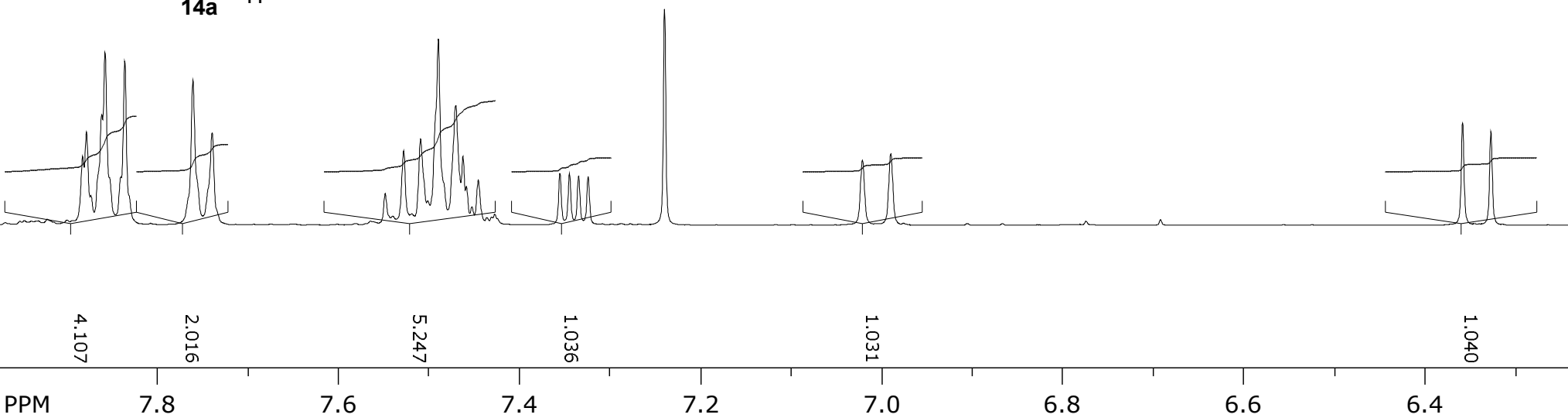
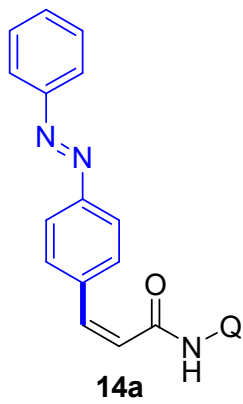
7.8363
7.8407
7.8581
7.8618
7.8739
7.8787

7.7398
7.7610

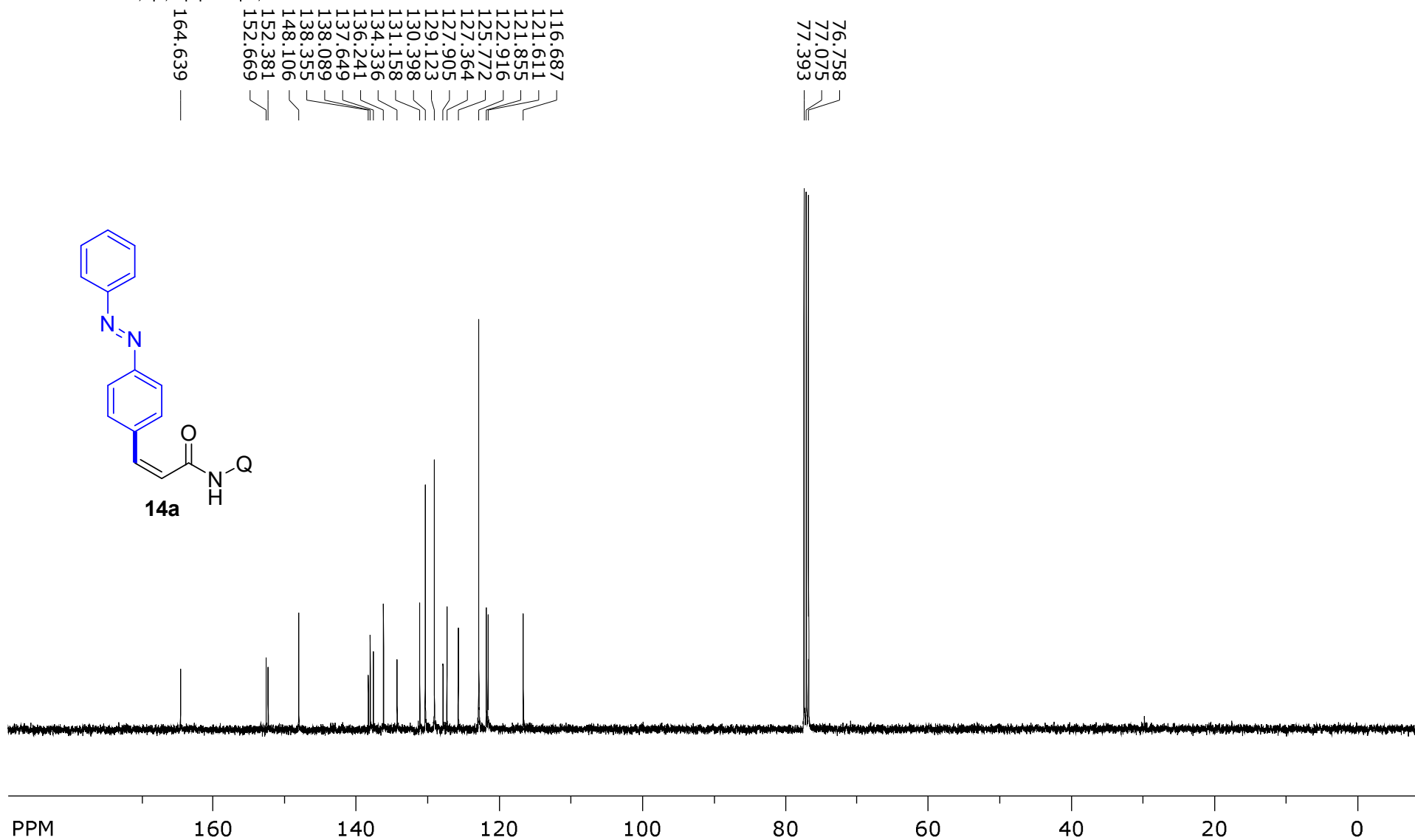
7.2399
7.3243
7.3349
7.3450
7.3555
7.4456
7.4527
7.4588
7.4626
7.4705
7.4898
7.5015
7.5094
7.5281
7.5485

6.9898
7.0212

6.3266
6.3579

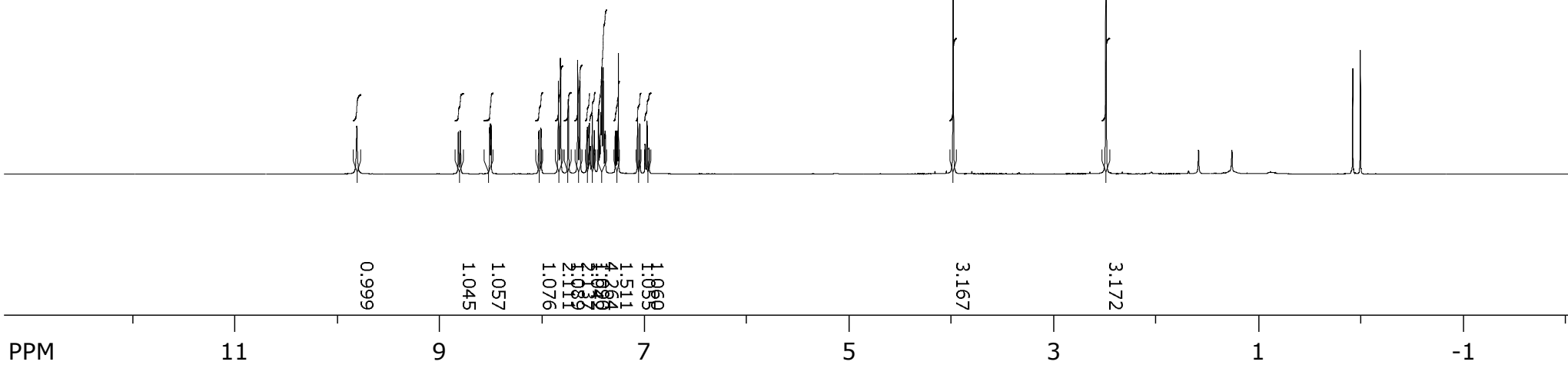
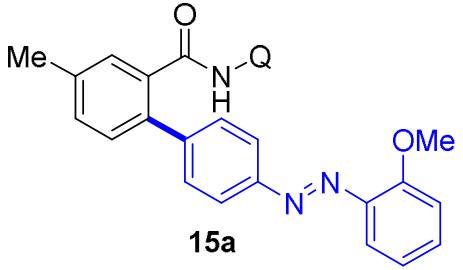


SpinWorks 4: SS 185 P
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 60



SS-116-p

6.9555
6.9735
6.9936
7.0446
7.0650
7.2537
7.2634
7.2835
7.2836
7.2837
7.2838
7.2839
7.2840
7.2841
7.2842
7.2843
7.2844
7.2845
7.2846
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7.2862
7.2863
7.2864
7.2865
7.2866
7.2867
7.2868
7.2869
7.2870
7.2871
7.2872
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7.2900
7.2901
7.2902
7.2903
7.2904
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7.2975
7.2976
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7.2979
7.2980
7.2981
7.2982
7.2983
7.2984
7.2985
7.2986
7.2987
7.2988
7.2989
7.2990
7.2991
7.2992
7.2993
7.2994
7.2995
7.2996
7.2997
7.2998
7.2999
8.0325
8.0325
8.4975
8.4975
8.5015
8.5015
8.5080
8.5080
8.5120
8.5120
8.7978
8.7978
8.7998
8.7998
8.8167
8.8167
8.8186
8.8186
9.8107
9.8107

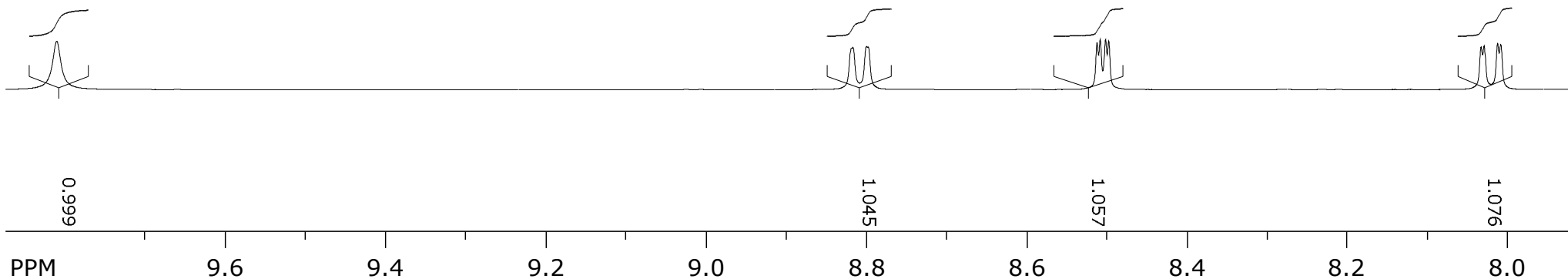
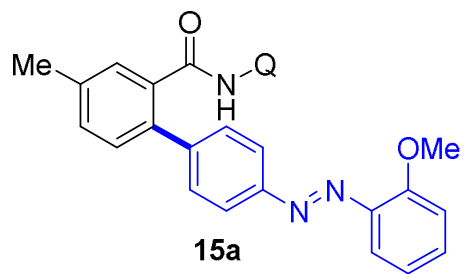


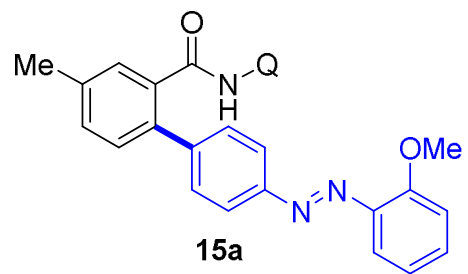
9.8107

8.7978
8.7998
8.8167
8.8186

8.4975
8.5015
8.5080
8.5120

8.0080
8.0118
8.0286
8.0325





7.8193
7.8402

7.7438

7.6301
7.6510

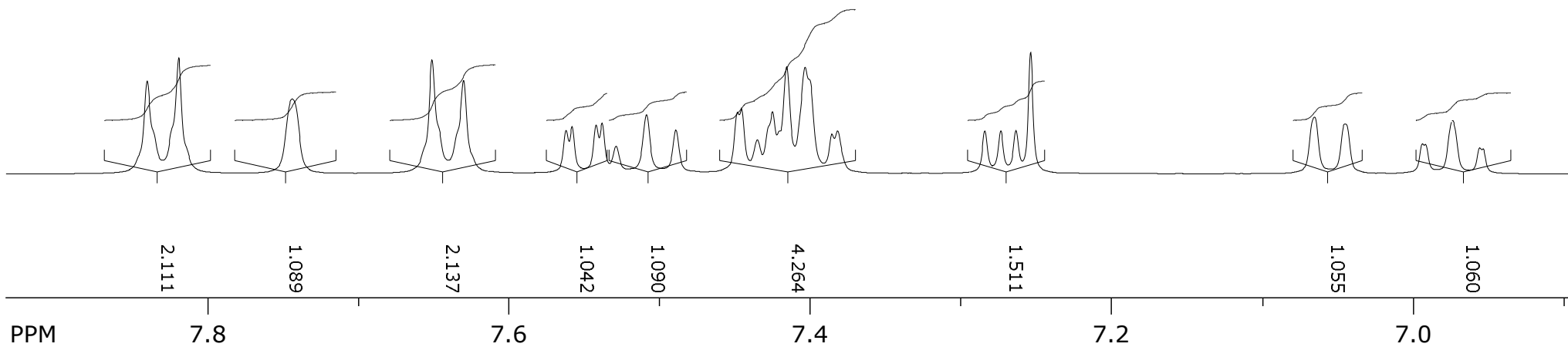
7.5621
7.5580
7.5421
7.5381
7.5289
7.5087
7.4892

7.4483
7.4455
7.4351
7.4249
7.4156
7.4033
7.3818
7.3856

7.2840
7.2735
7.2634
7.2537

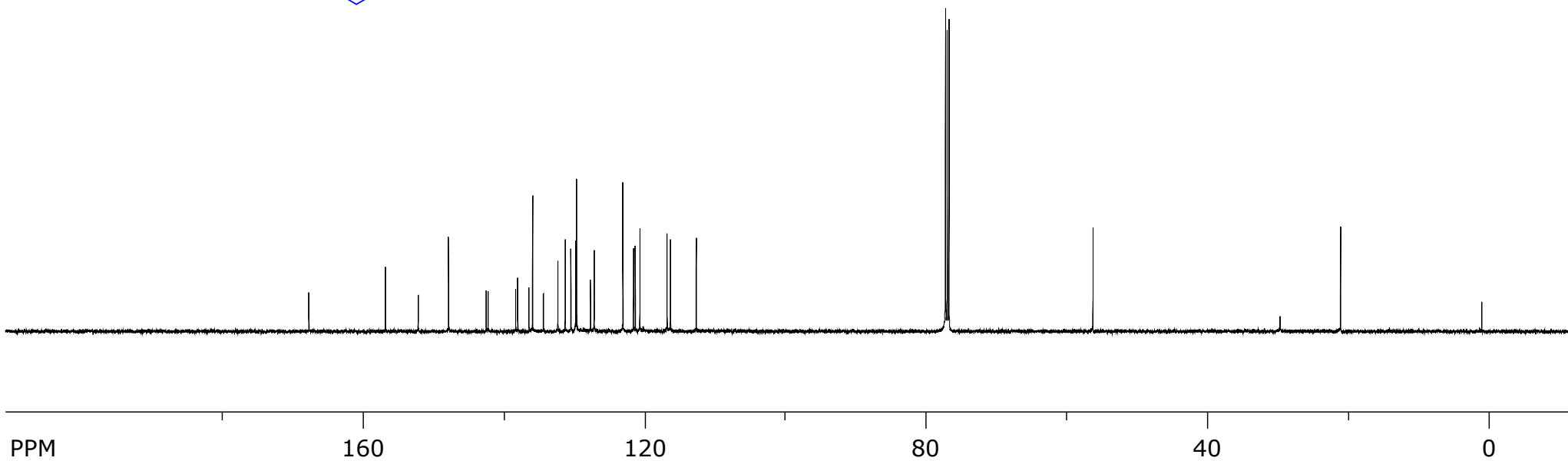
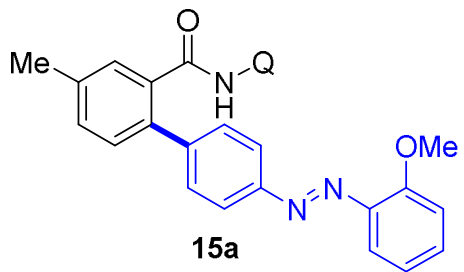
7.0650
7.0446

6.9936
6.9735
6.9555



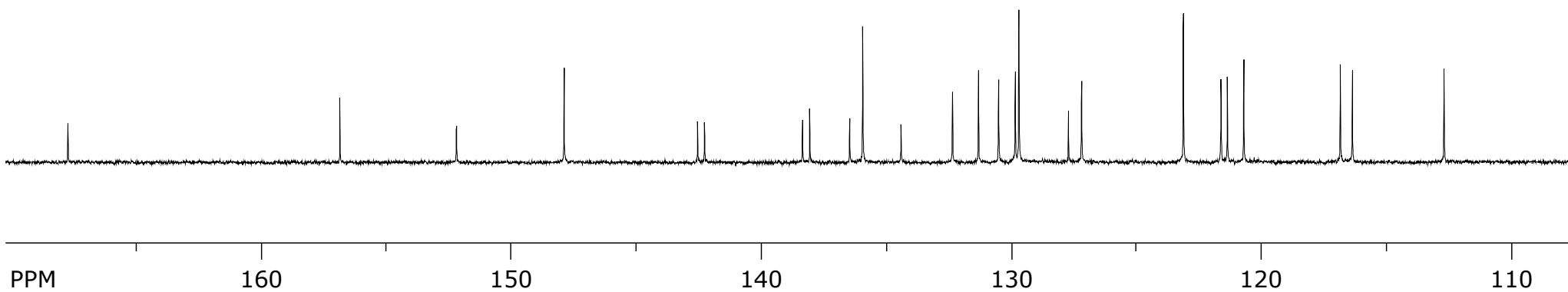
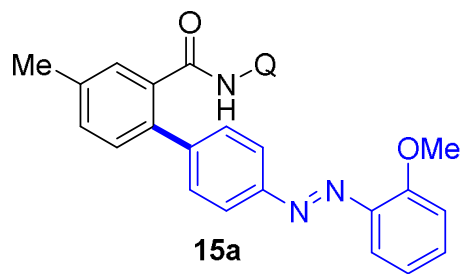
SpinWorks 4: SV100702
C13CPD CDCl3 {D:\Spectra} nmr 2

167.752 —
156.862 —
152.202 —
147.893 —
142.547 —
138.350 —
138.061 —
136.463 —
135.940 —
134.408 —
132.351 —
129.992 —
129.592 —
127.708 —
127.180 —
123.110 —
121.605 —
121.348 —
120.691 —
116.827 —
116.349 —
112.675 —
76.745 —
77.000 —
77.254 —
56.278 —
21.077 —

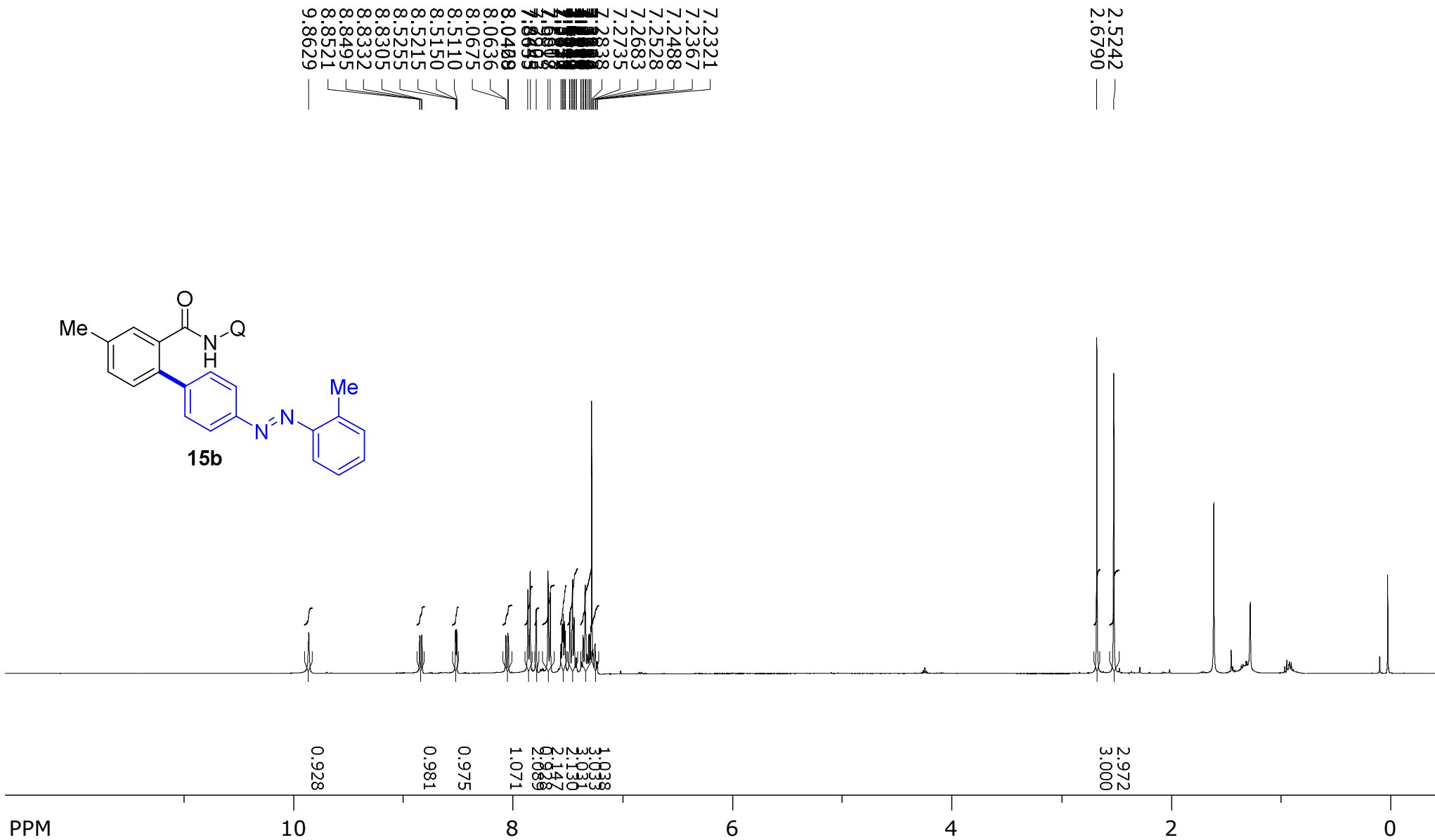


SpinWorks 4: SV100702
C13CPD CDCl3 {D:\Spectra} nmr 2

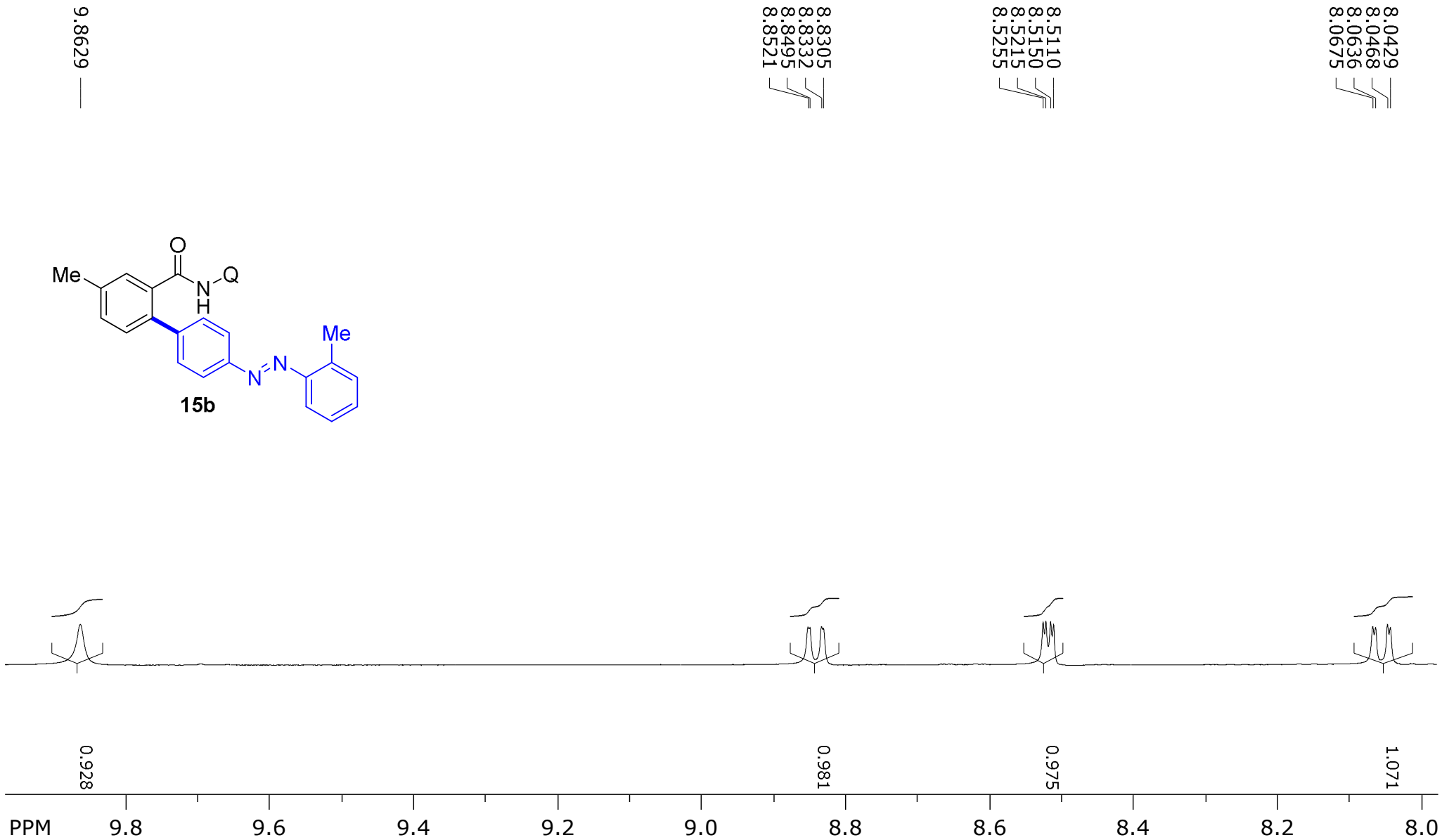
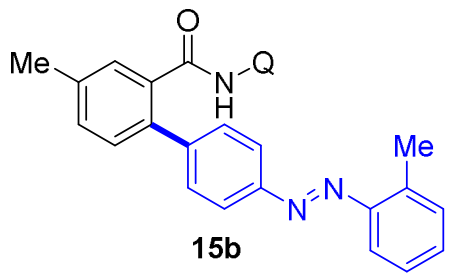
167.752 —
156.862 —
152.202 —
147.893 —
142.275 —
142.547 —
138.061 —
138.350 —
136.463 —
135.940 —
134.408 —
132.351 —
131.311 —
130.504 —
129.840 —
129.692 —
127.708 —
127.180 —
123.110 —
121.605 —
121.348 —
120.691 —
116.827 —
116.349 —
112.675 —



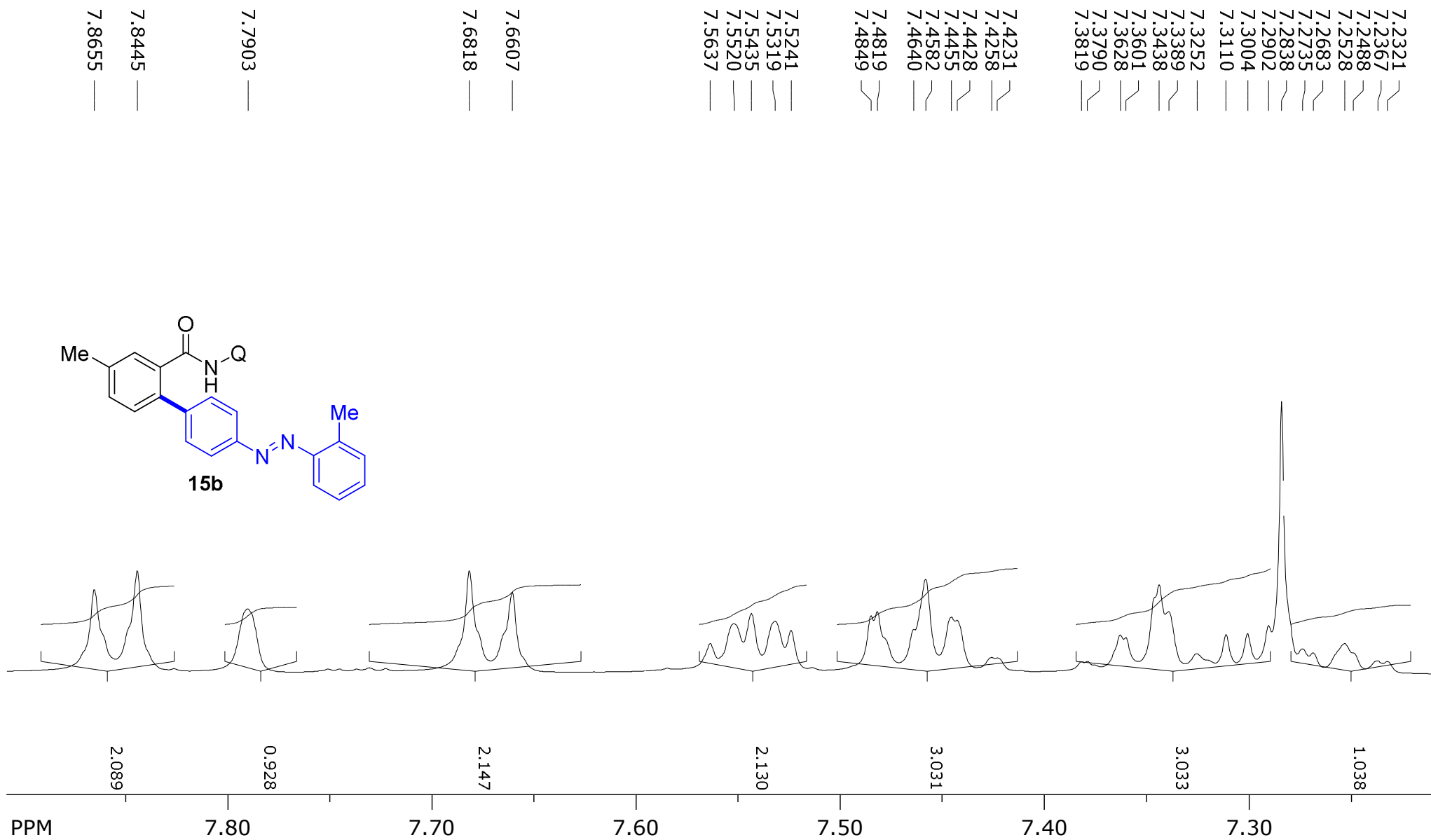
SpinWorks 4: SS-198(ii)
{PROTON 64} CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 1



SpinWorks 4: SS-198(ii)
{PROTON 64} CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 1



SpinWorks 4: SS-198(ii)
{PROTON 64} CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 1

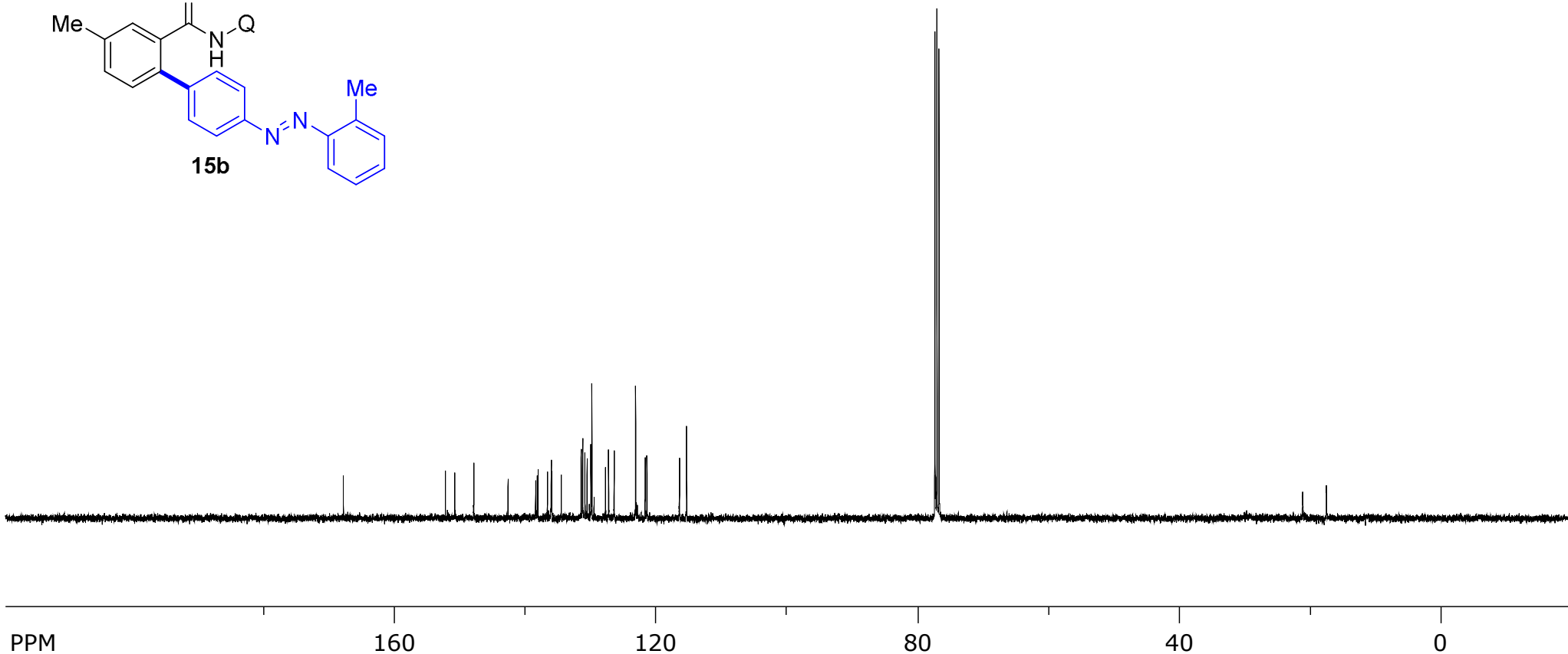
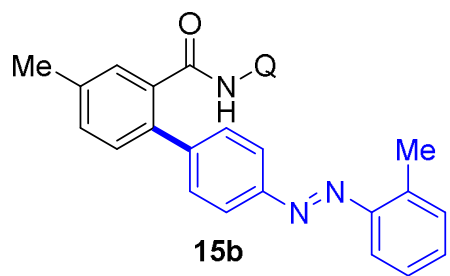


SpinWorks 4: SS-198-REP
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 23

115.334
116.422
121.403
121.675
123.123
126.410
127.264
127.754
129.812
130.812
131.812
134.489
134.989
136.024
136.613
138.053
138.168
138.428
142.636
147.868
150.766
152.201
167.803

76.740
77.057
77.375

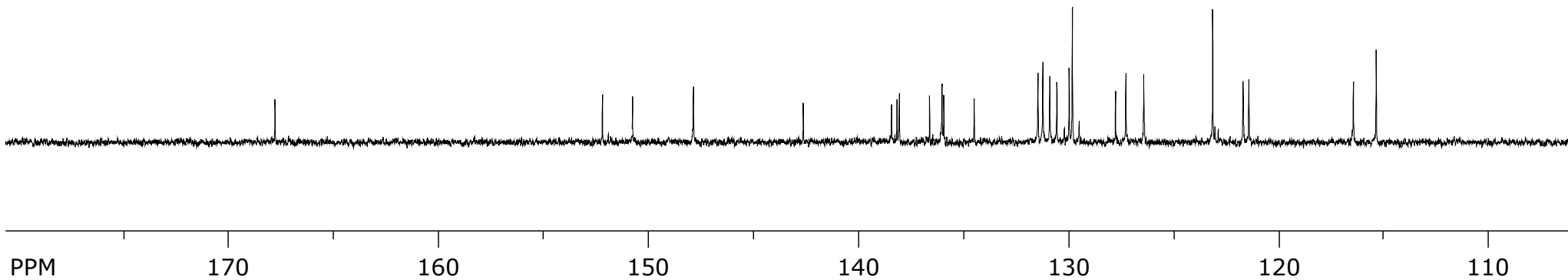
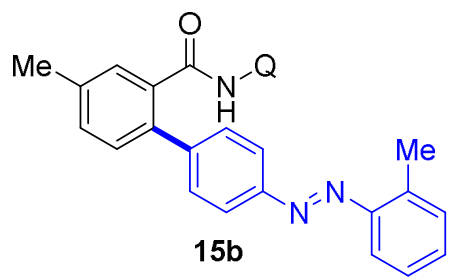
17.524
21.167



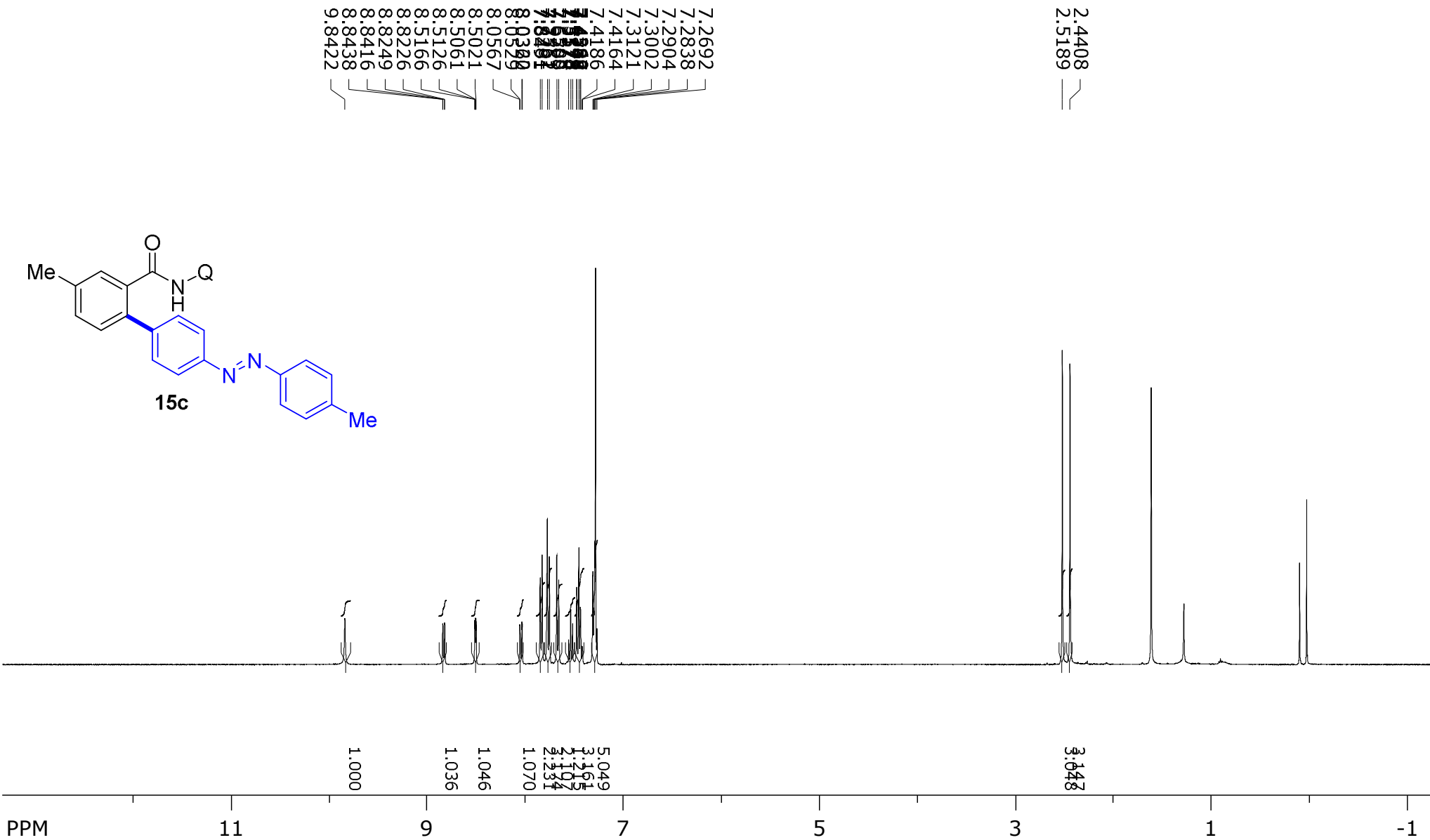
PPM

SpinWorks 4: SS-198-REP
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 23

167.803 —
152.201 —
150.766 —
147.868 —
142.636 —
138.428 —
138.168 —
138.053 —
136.613 —
136.024 —
135.934 —
134.489 —
131.452 —
131.221 —
130.889 —
130.552 —
129.963 —
129.812 —
127.754 —
127.264 —
126.410 —
123.123 —
121.675 —
121.403 —
116.422 —
115.334 —



SpinWorks 4: SS-117-P REP
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 5

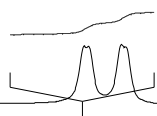
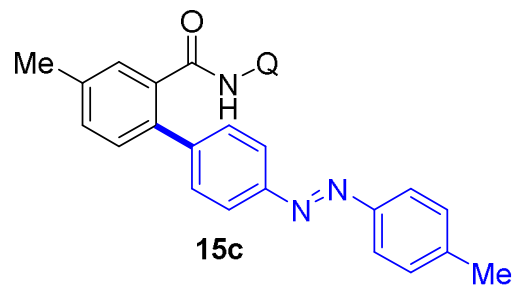


SpinWorks 4: SS-117-P REP
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 5

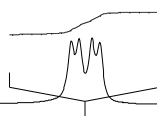
8.8226
8.8249
8.8416
8.8438

8.5021
8.5061
8.5126
8.5166

8.0322
8.0360
8.0529
8.0567



1.036



1.046



1.070

PPM

8.8

8.6

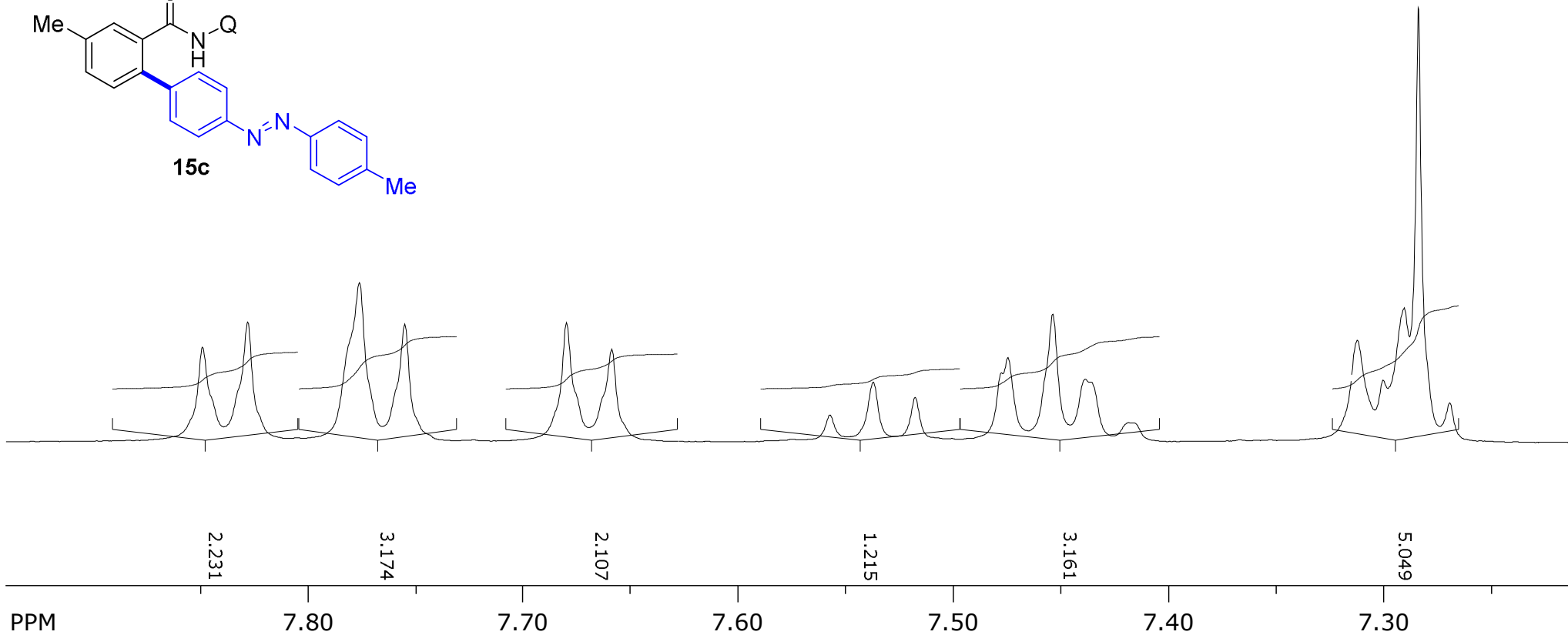
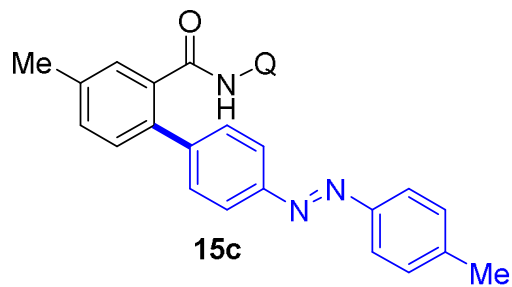
8.4

8.2

8.0

SpinWorks 4: SS-117-P REP
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 5

7.8491 —
7.8281 —
7.7762 —
7.7551 —
7.6799 —
7.6588 —
7.5574 —
7.5373 —
7.5178 —
7.4776 —
7.4747 —
7.4538 —
7.4387 —
7.4360 —
7.4186 —
7.4164 —
7.3121 —
7.3002 —
7.2904 —
7.2838 —
7.2692 —



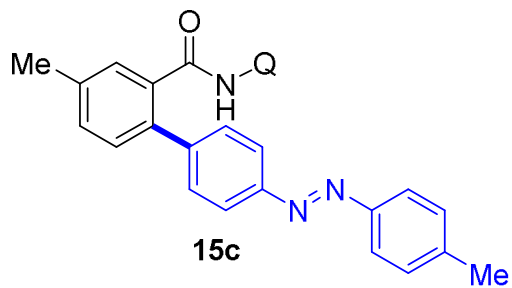
SpinWorks 4: SS-117

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 24

116.389
121.407
121.658
122.787
122.921
127.242
127.752
129.730
130.910
131.910
134.479
135.959
136.001
136.561
138.133
138.410
141.534
142.524
147.901
150.770
151.886
167.817

76.739
77.057
77.260
77.375

21.135
21.536



PPM

160

120

80

40

0

SpinWorks 4: SS-117

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 24

167.817

150.770
151.886

147.901

141.534
142.524

138.410

136.001
135.957
138.133

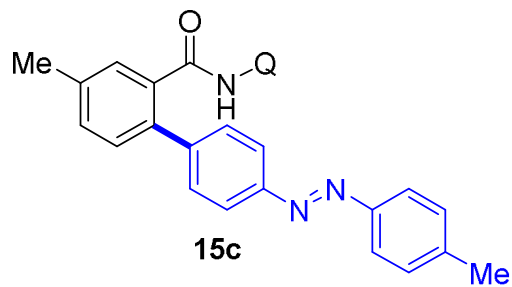
134.479

131.416
129.962
129.730
129.801

127.752
127.242

122.921
121.658
122.787

116.389



15c

PPM

160

150

140

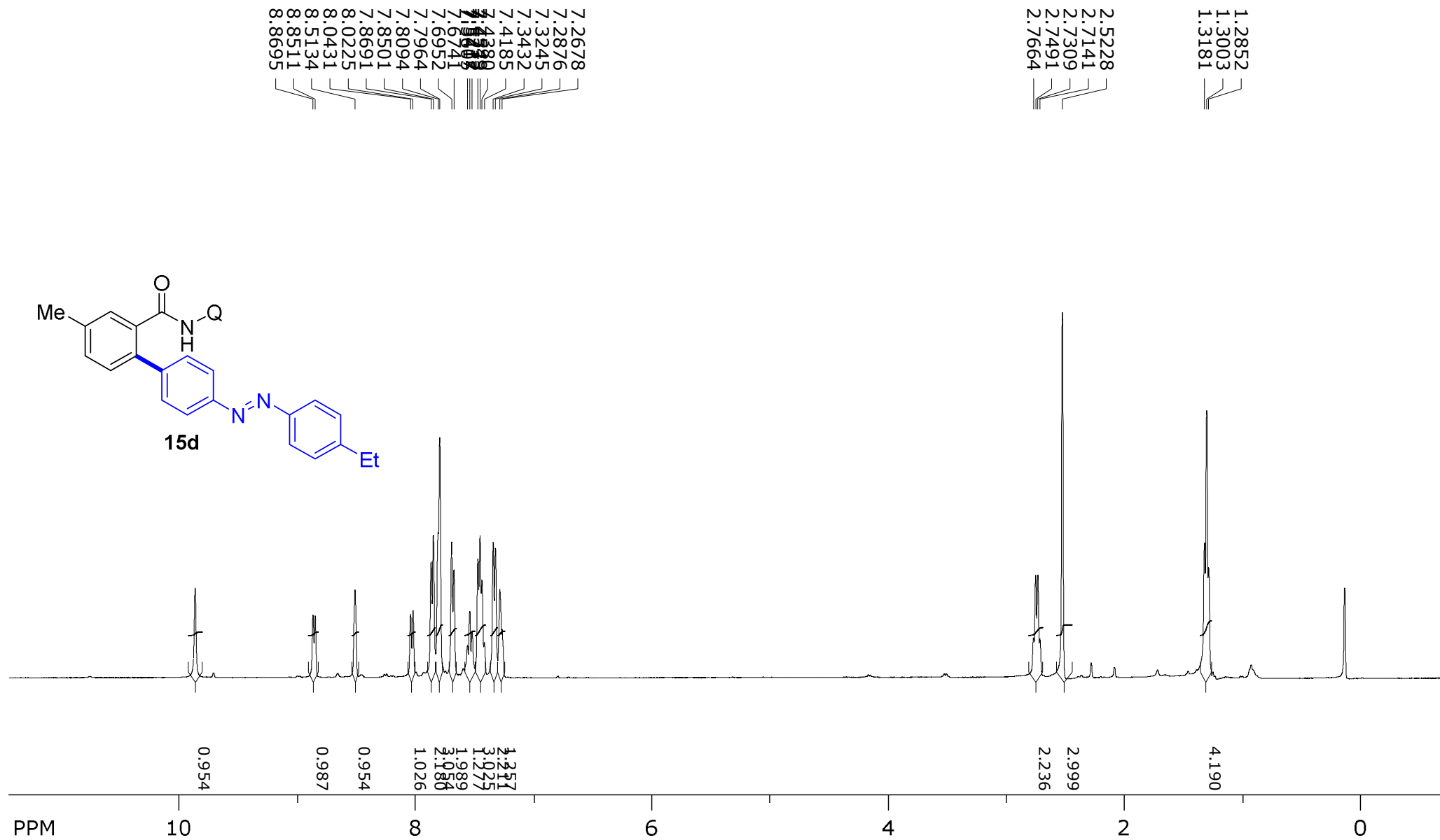
130

120

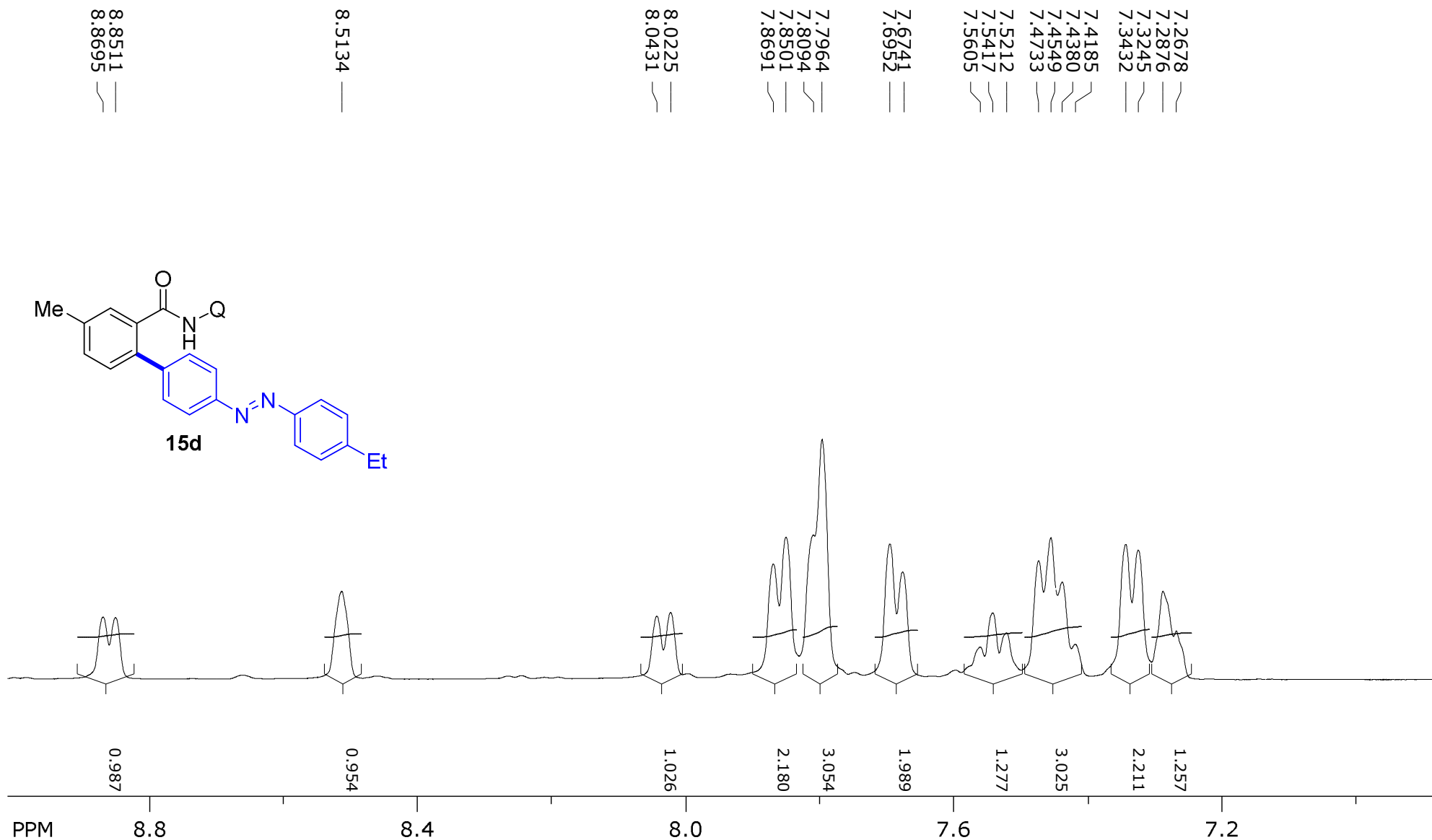
110

100

SpinWorks 4: SS 197 P
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 51



SpinWorks 4: SS 197 P
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 51



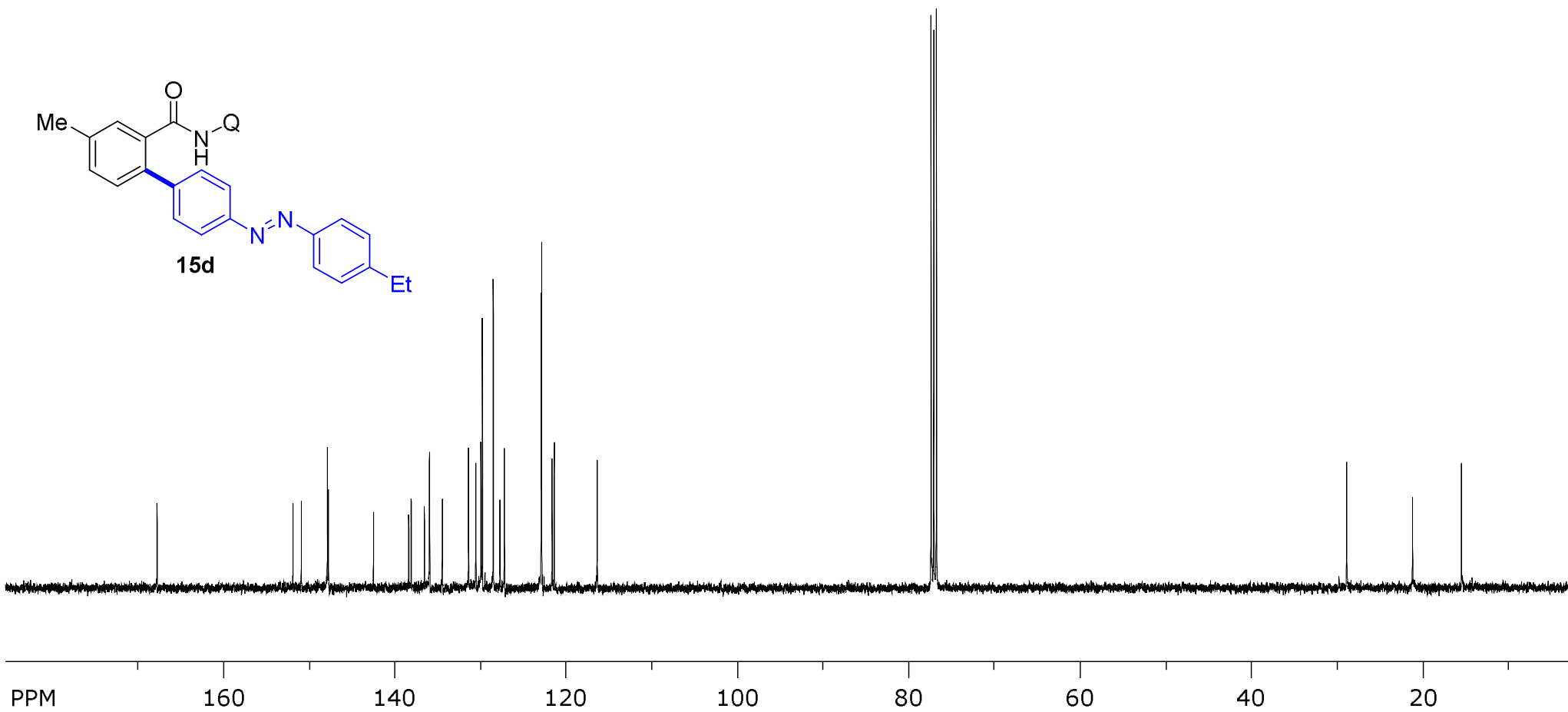
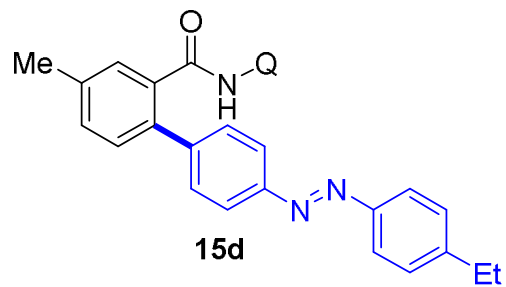
SpinWorks 4: SS 197 P

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 51

167.8097
151.9312
150.9631
147.9044
147.7901
142.5281
138.4185
138.1314
136.5809
136.0009
135.9565
134.4947
131.4293
130.9749
129.8133
128.5448
127.7548
127.2428
122.9340
122.8846
121.6672
121.4163
116.3959

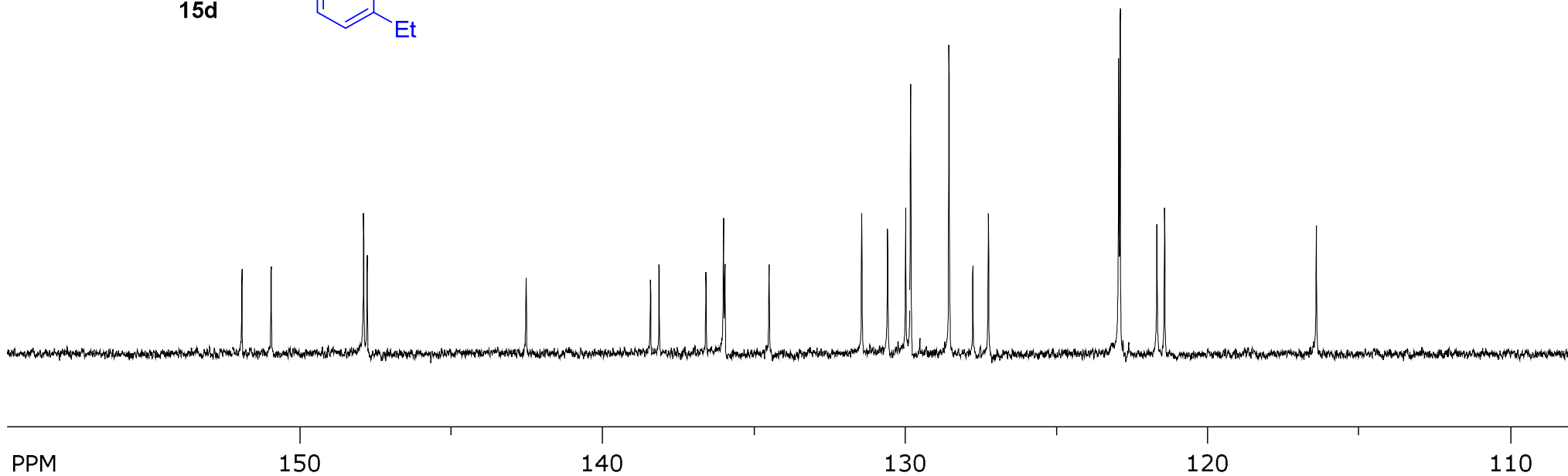
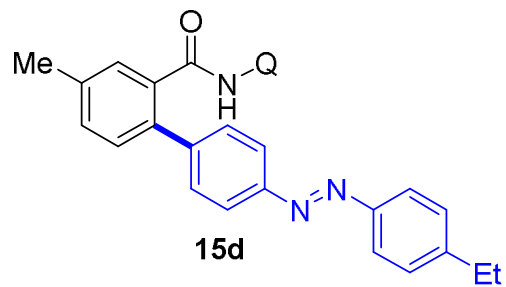
76.7637
77.0811
77.3989

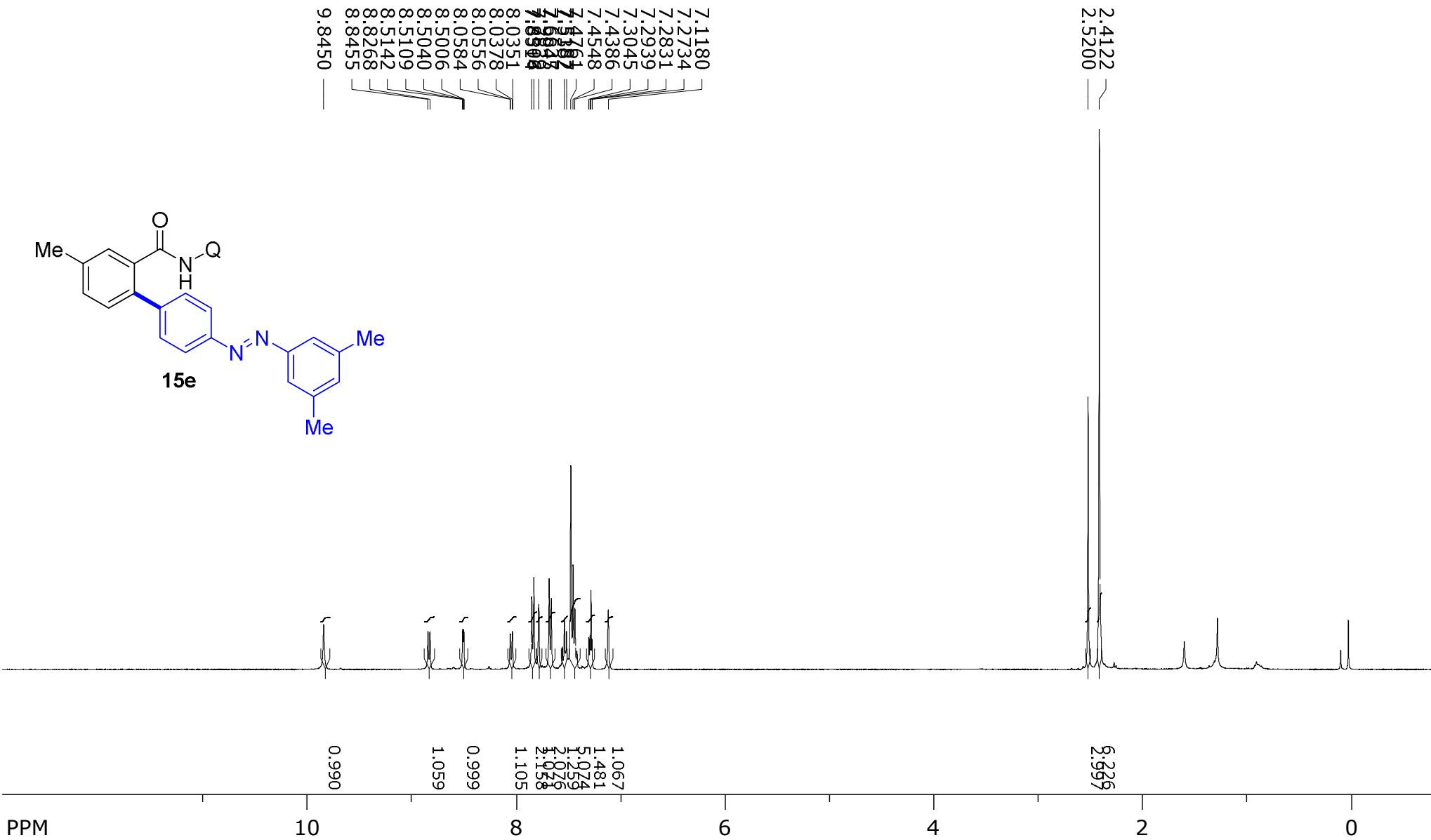
28.8538
21.1530
15.4403



SpinWorks 4: SS 197 P
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata/nmr su 51

147.7901
147.9044
150.9631
151.9312
142.5281
138.4185
138.1314
136.5809
136.0009
135.9565
134.4947
131.4293
130.5745
129.9776
129.8133
128.5448
127.7548
127.2428
122.9340
122.8846
121.6672
121.4163
116.3959



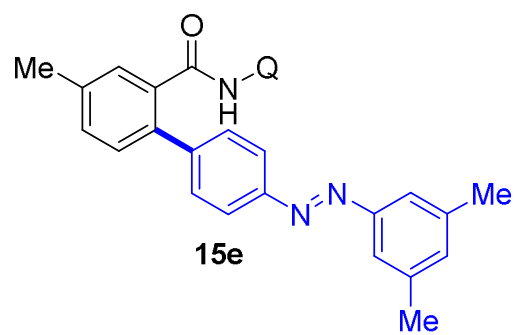


9.8450

8.8268
8.8455

8.5006
8.5040
8.5109
8.5142

8.0351
8.0378
8.0556
8.0584



0.990

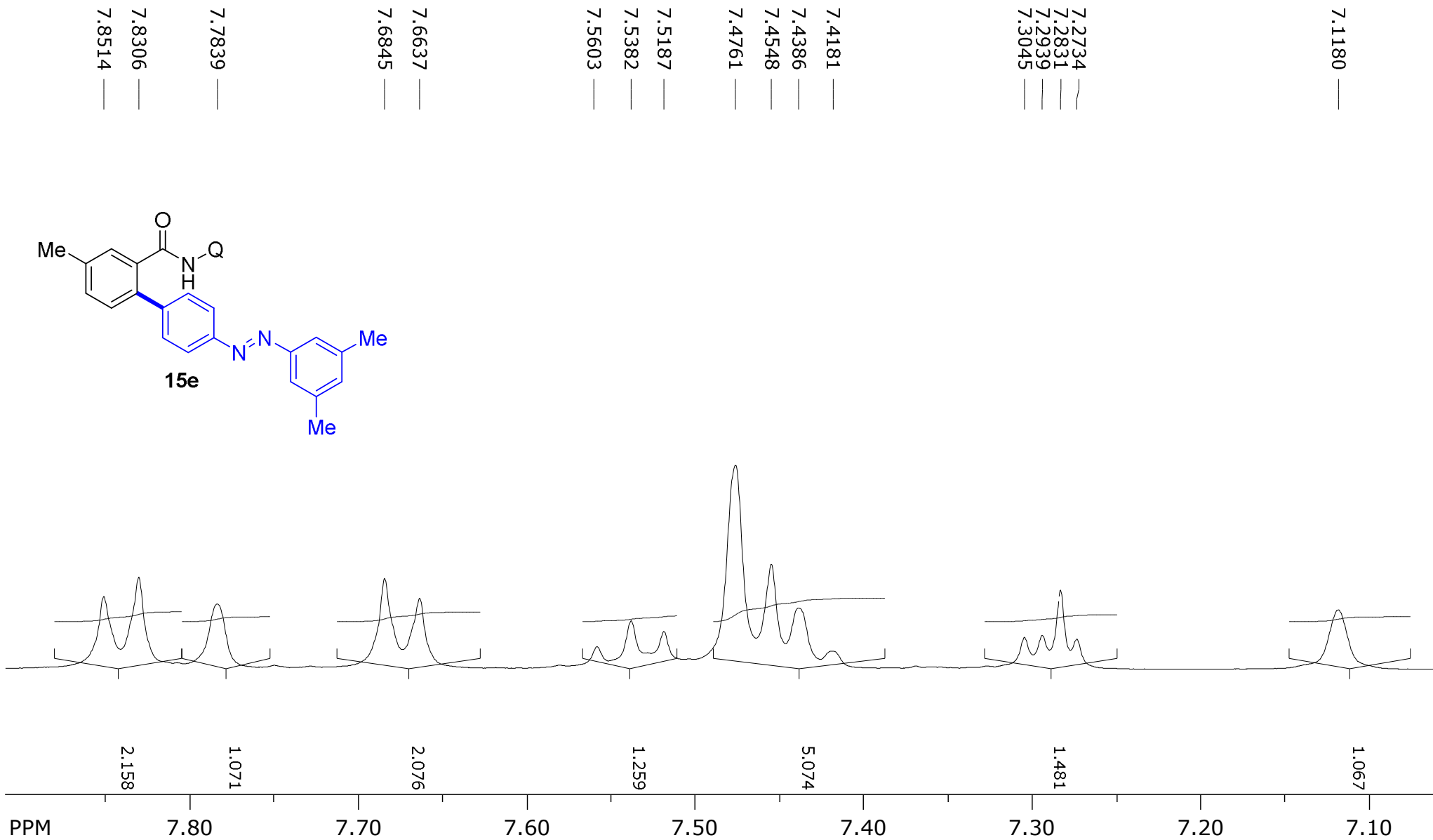
1.059

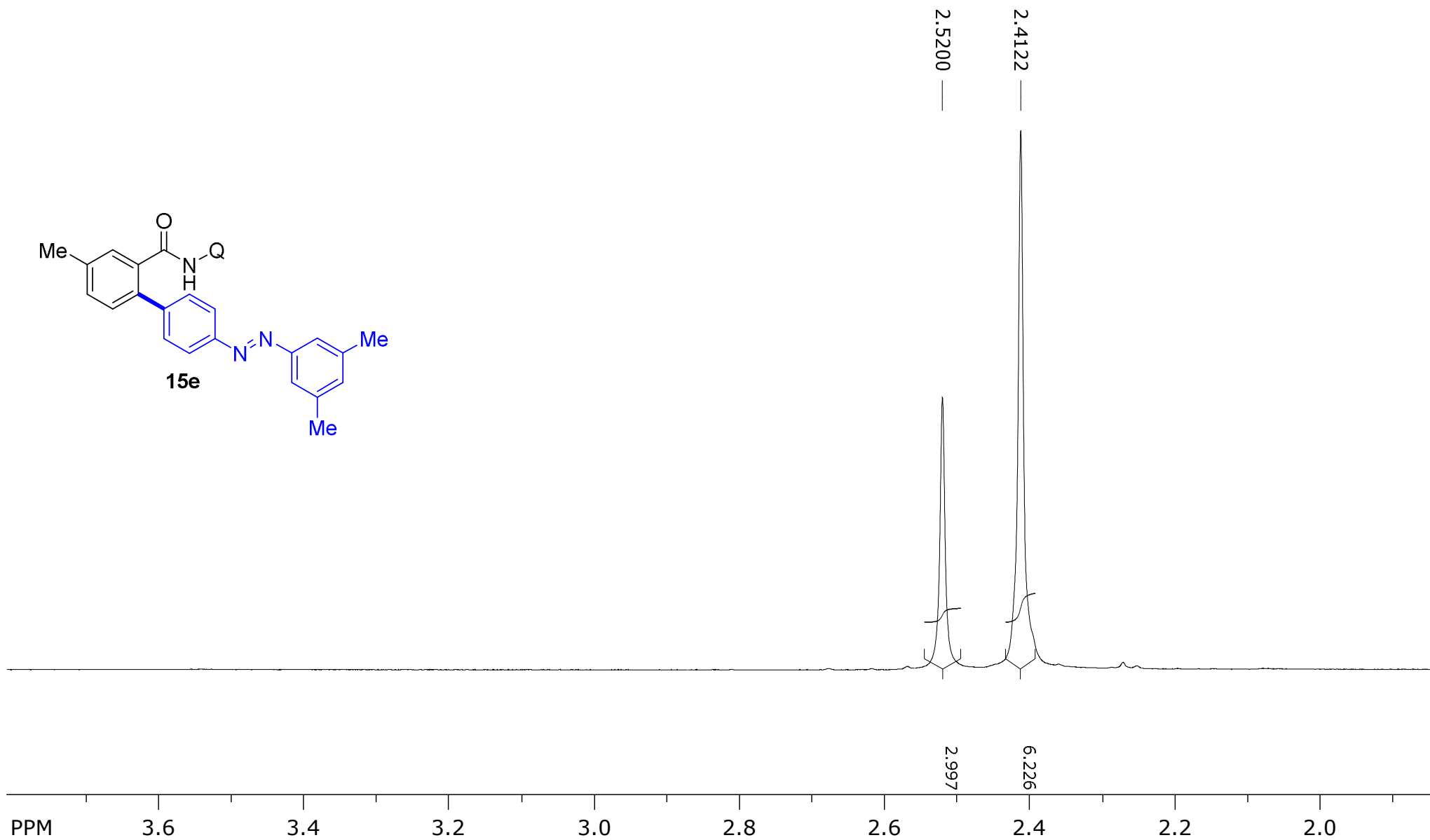
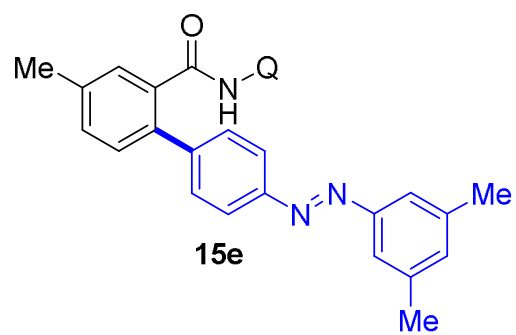
0.999

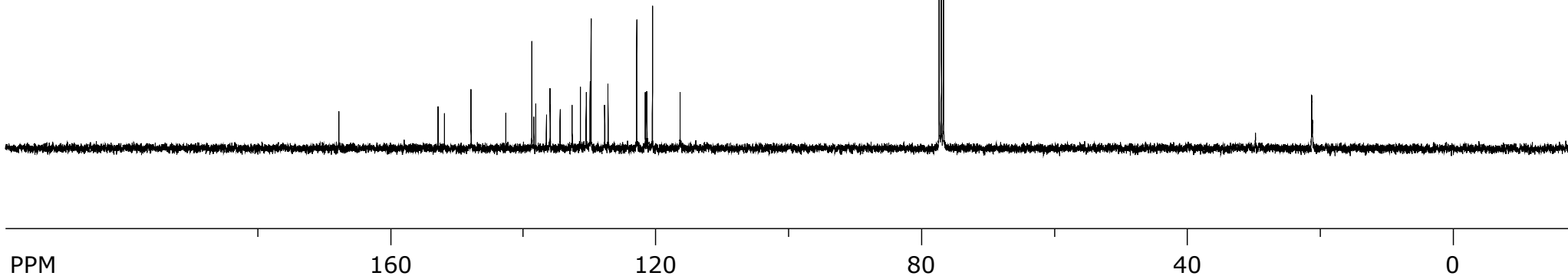
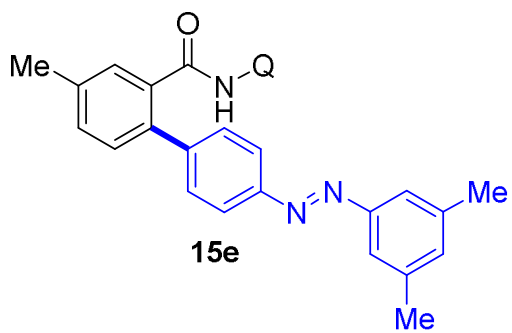
1.105

PPM 9.6 9.2 8.8 8.4 8.0

SpinWorks 4: ss 134 II -P







PPM

160

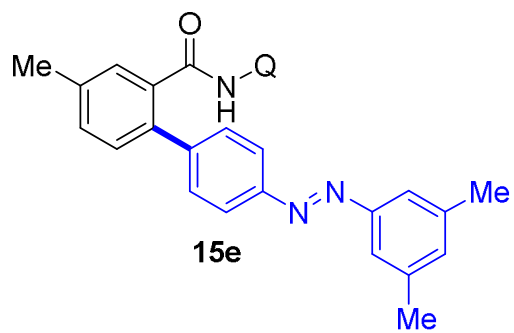
120

80

40

0

SpinWorks 4: ss-134-ii-p



167.794

151.897
152.875

147.890

142.647

138.745
138.420
138.153
136.547
136.000
135.972

134.481

132.671

131.419

130.558

129.974

129.821

127.758

127.247

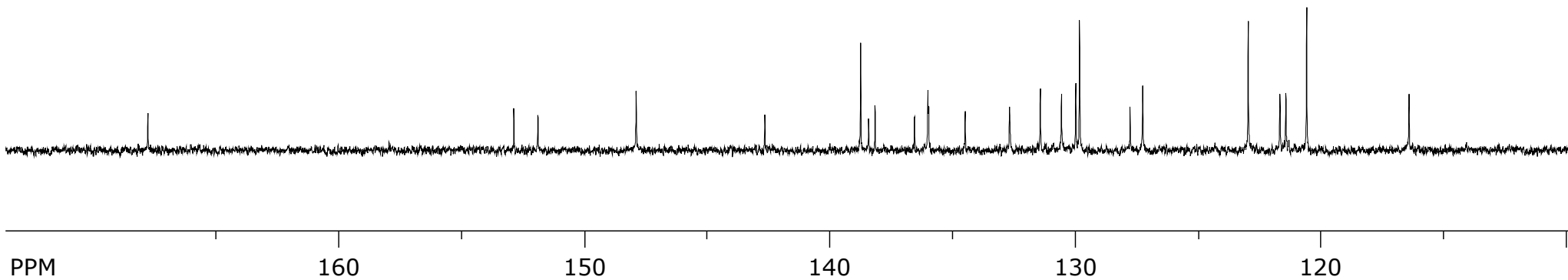
122.946

121.655

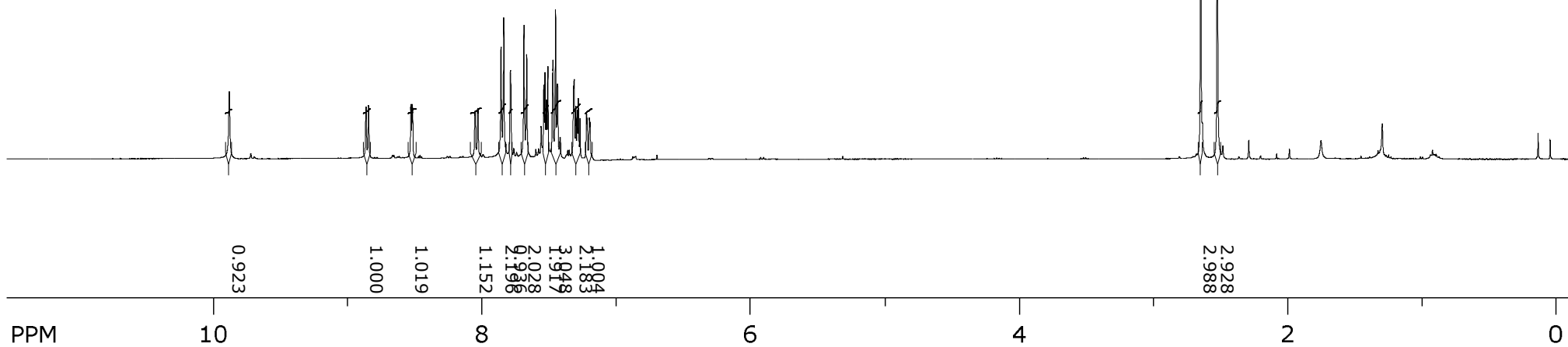
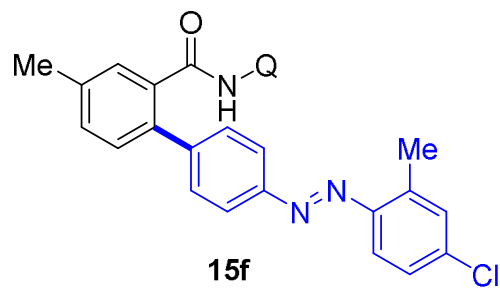
121.413

120.562

116.392



9.8846
8.8663
8.8476
8.5324
8.5287
8.5183
8.0549
8.0343
8.0308
7.8603
7.8094
7.6994
7.6484
7.5974
7.3024
7.2919
7.2848
7.2712
7.2231
7.2178
7.2016
2.6472
2.5228

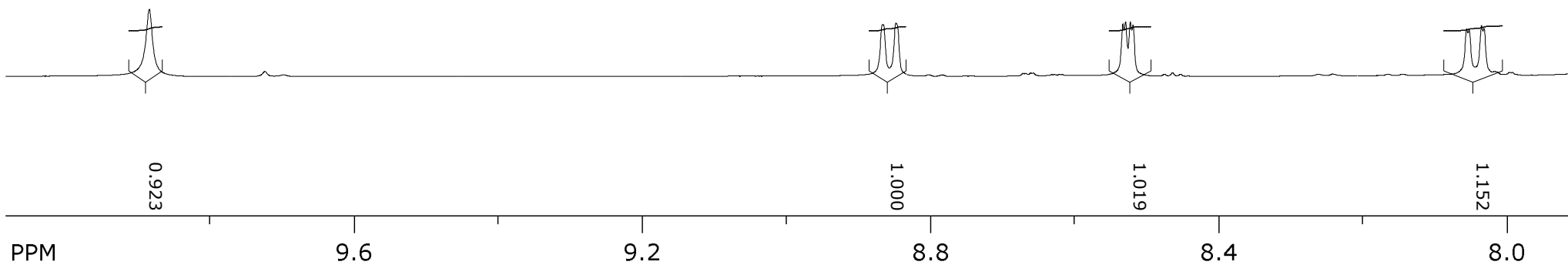
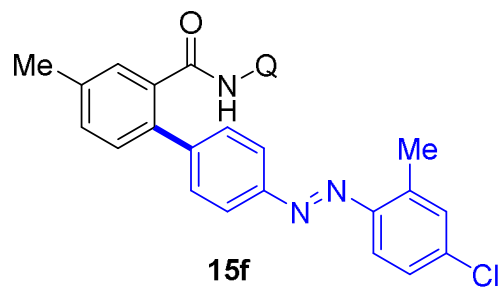


9.8846

8.8476
8.8663

8.5183
8.5220
8.5287
8.5324

8.0308
8.0343
8.0515
8.0549



7.8394
7.8603

7.7892

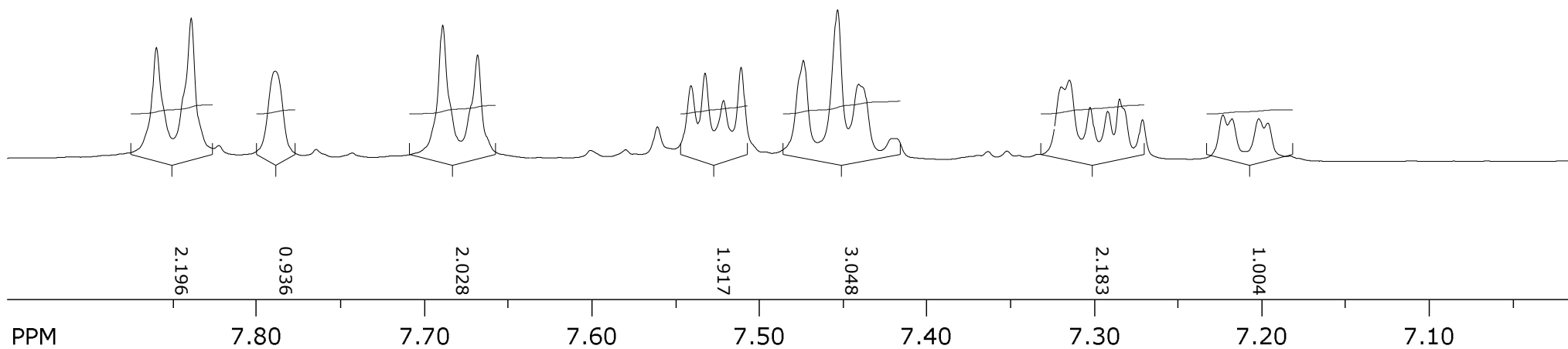
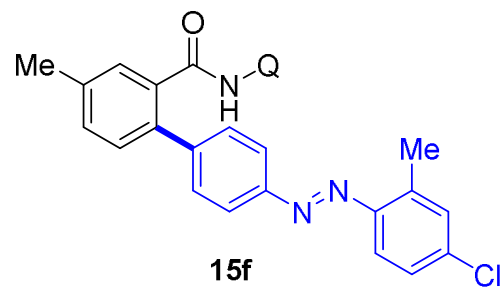
7.6684
7.6893

7.5109
7.5214
7.5325
7.5408

7.4736
7.4407
7.4534

7.3195
7.3148
7.3024
7.2919
7.2848
7.2712

7.2016
7.2178
7.2231

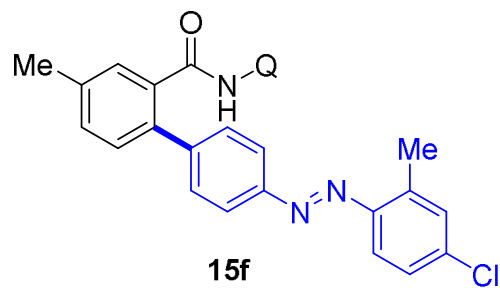


SpinWorks 4: SS 206 P
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 58

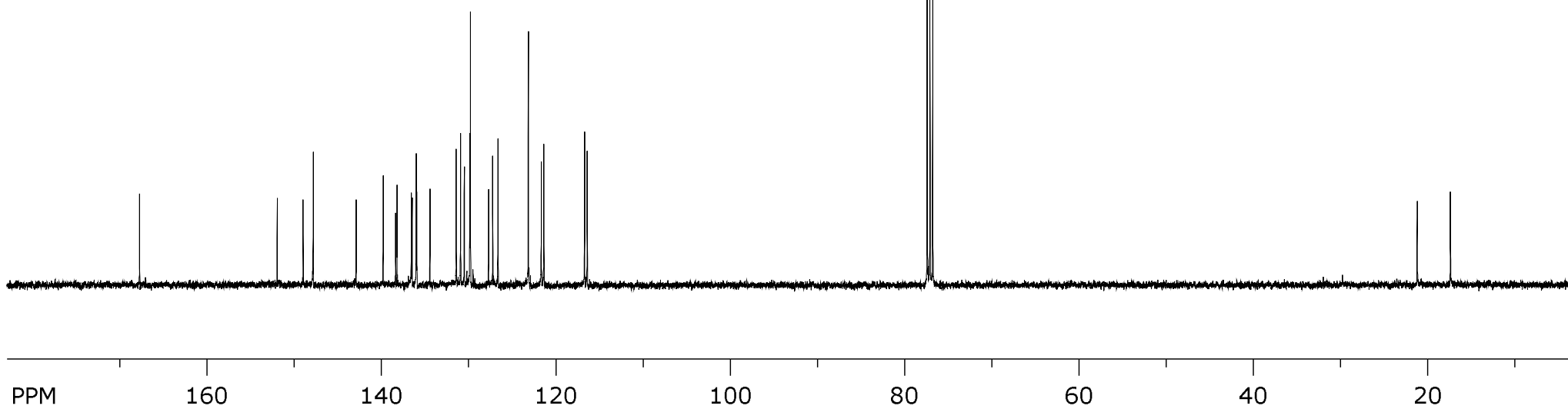
167.805
152.018
149.036
147.877
142.955
139.851
138.419
138.244
136.628
136.532
135.092
134.484
134.484
129.904
129.904
129.838
127.760
127.282
126.675
123.194
121.706
121.410
116.733
116.436

76.780
77.098
77.415

17.370
21.176

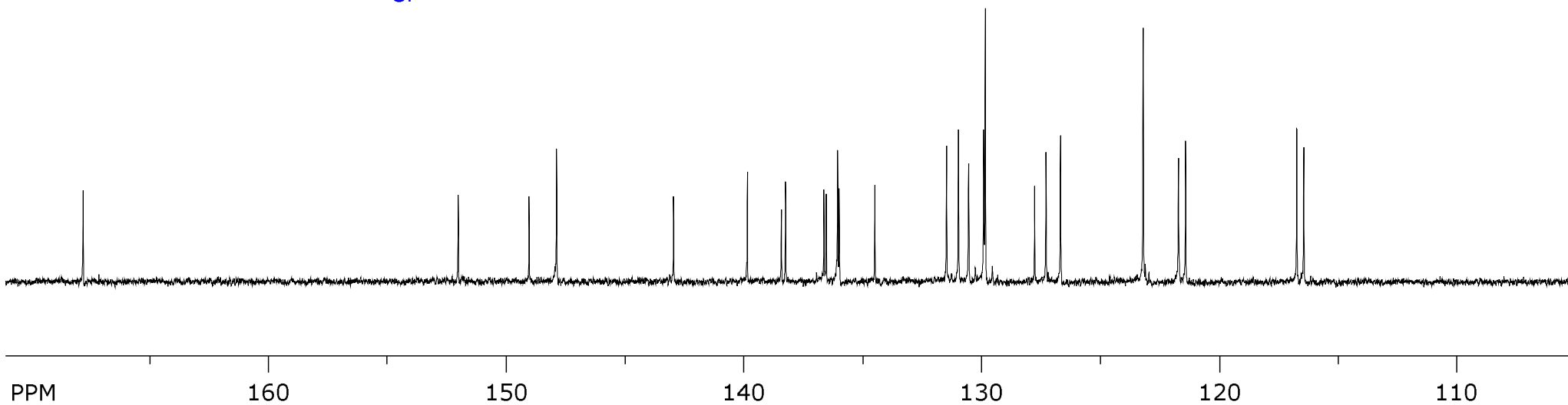
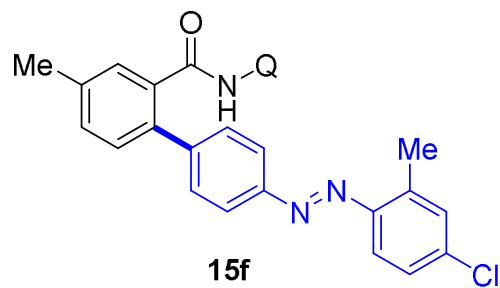


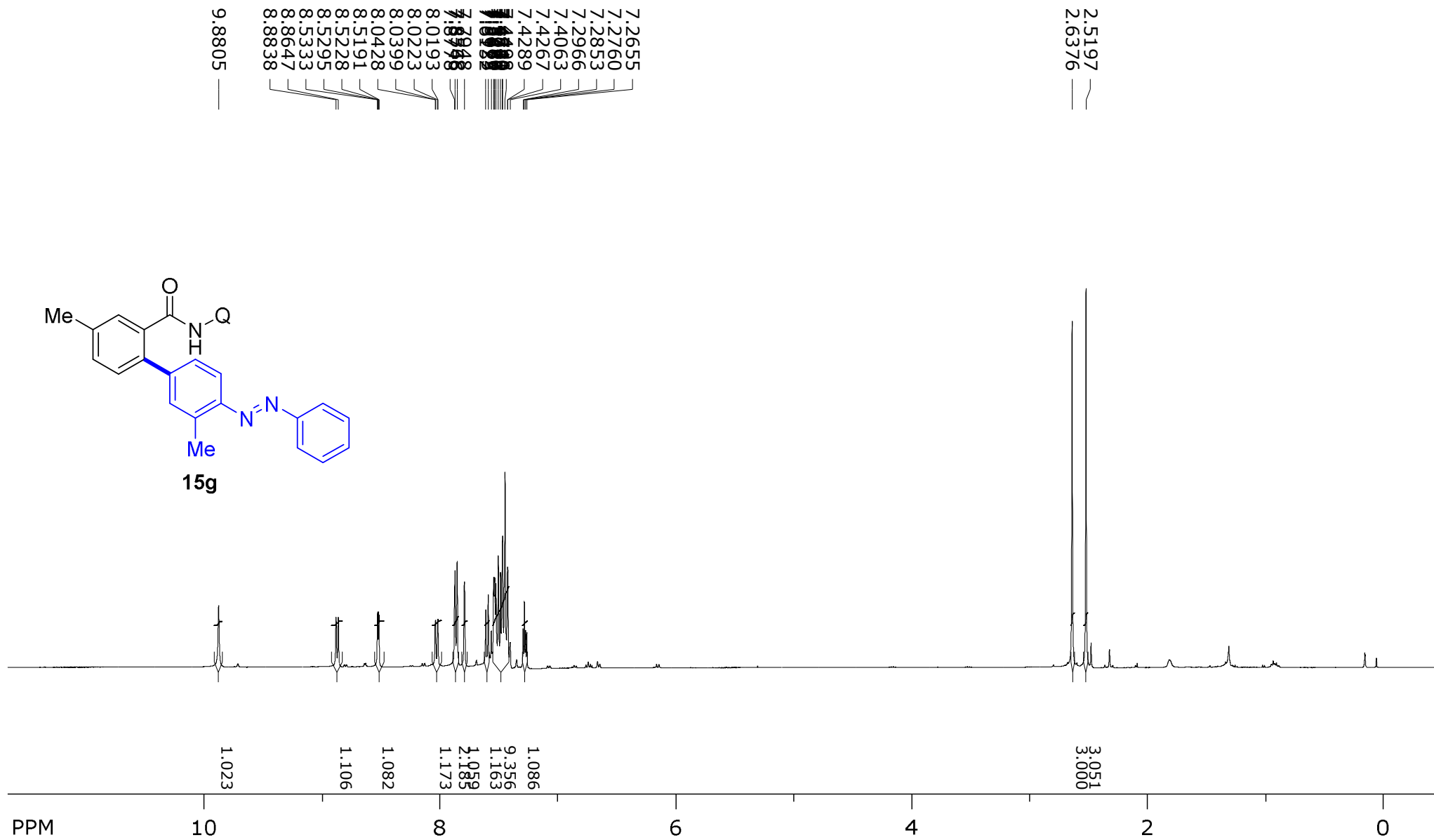
15f

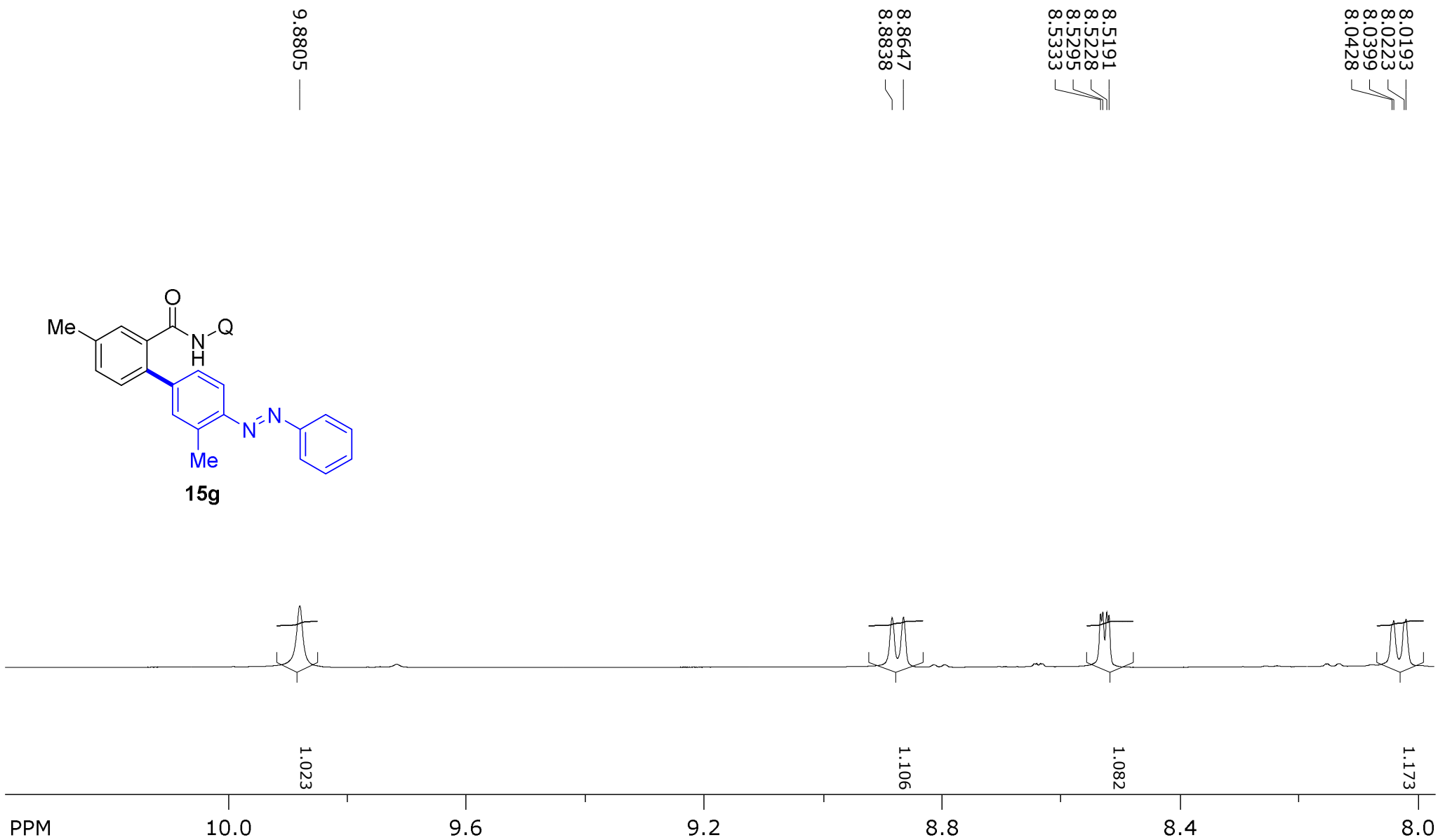
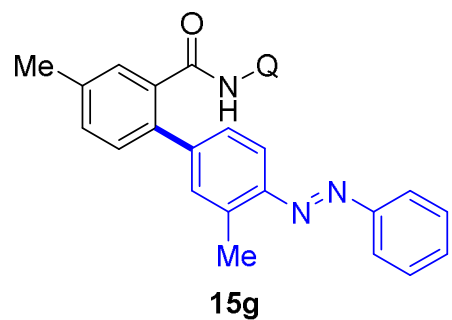


SpinWorks 4: SS 206 P
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 58

167.805 —
152.018 —
149.036 —
147.877 —
142.955 —
139.851 —
138.419 —
136.628 —
136.532 —
135.985 —
134.484 —
131.466 —
130.969 —
130.539 —
129.904 —
129.838 —
127.760 —
126.675 —
123.194 —
121.410 —
121.706 —
116.733 —
116.436 —







7.8568
7.8746
7.8778

7.7948

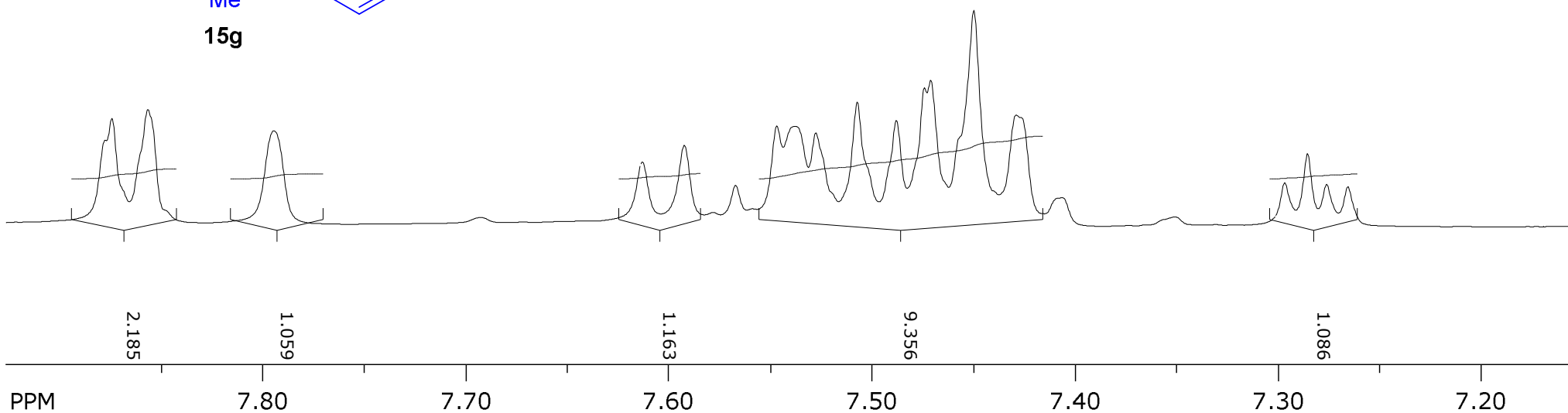
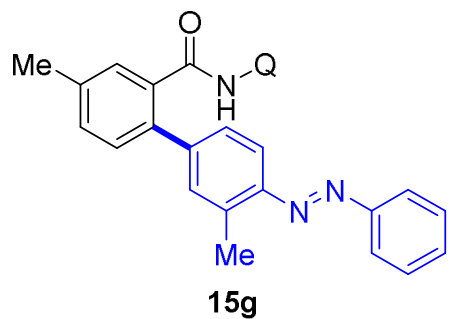
7.6132
7.5925

7.5672
7.5277
7.5380
7.5469

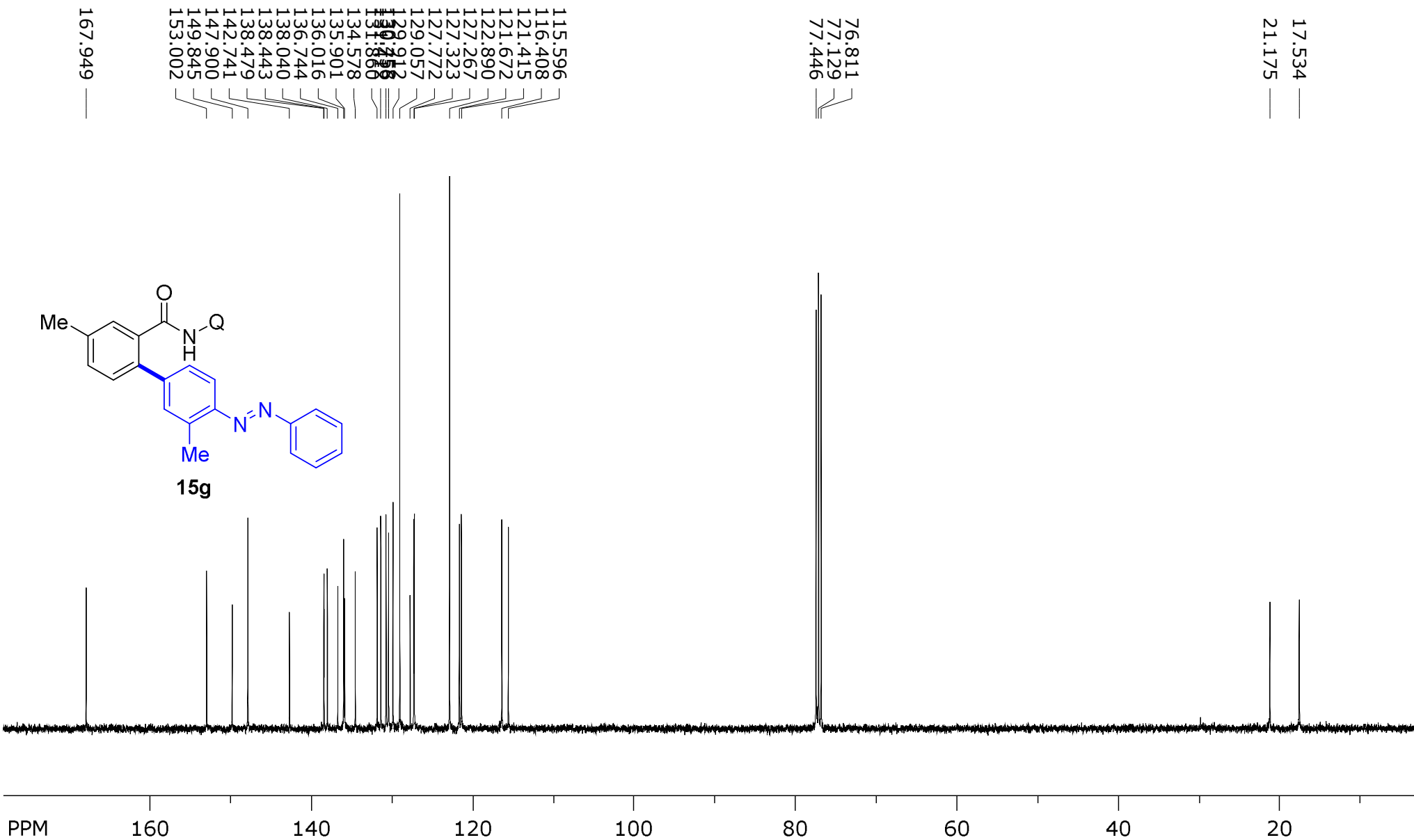
7.5072
7.4880
7.4710
7.4741

7.4498
7.4267
7.4289

7.2655
7.2760
7.2853
7.2966



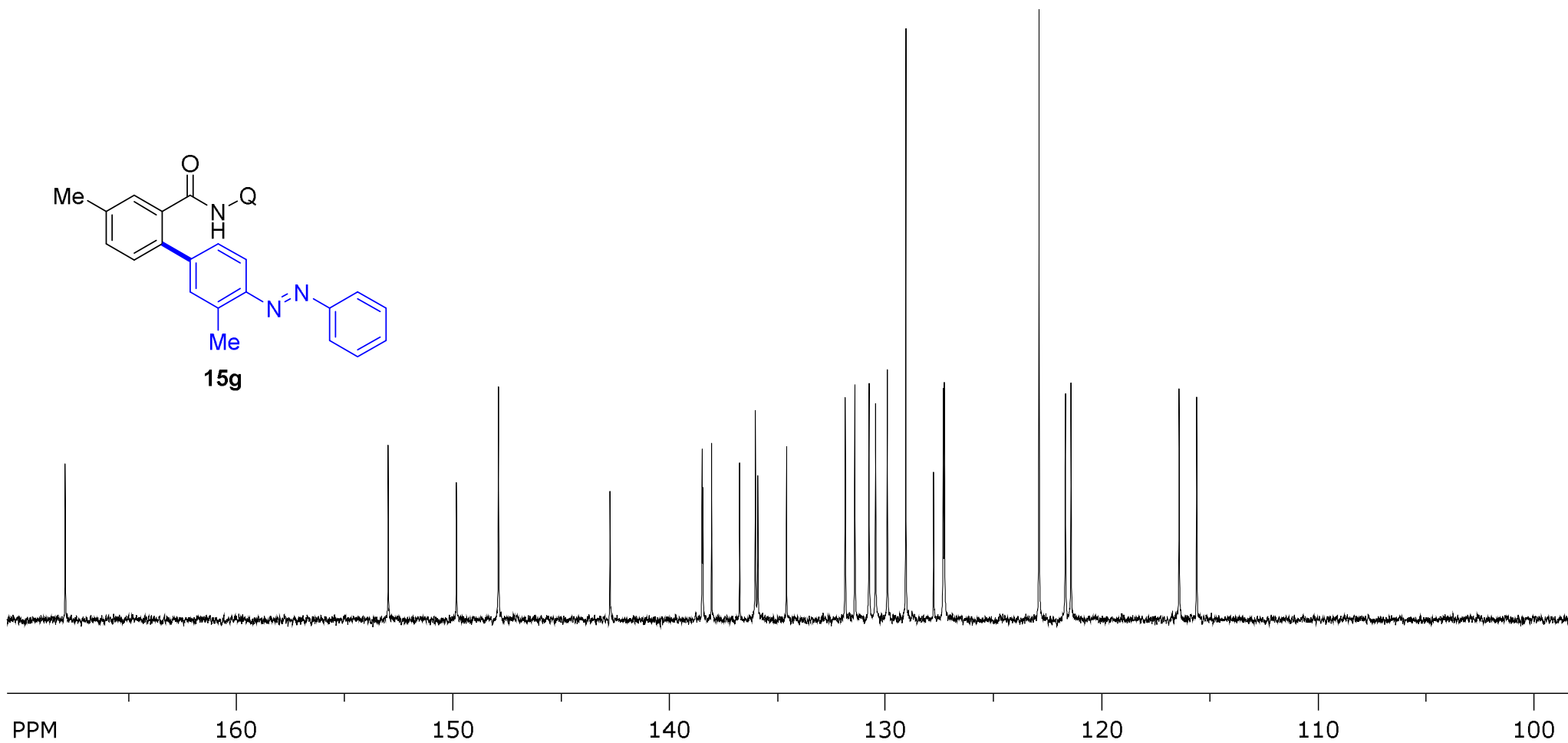
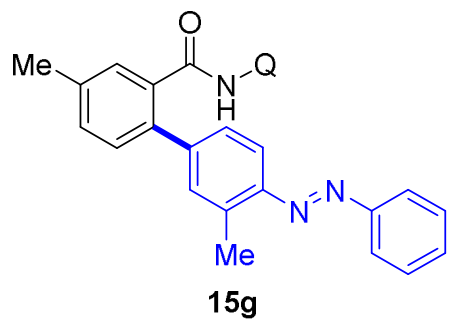
SpinWorks 4: SS 207 P
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 59



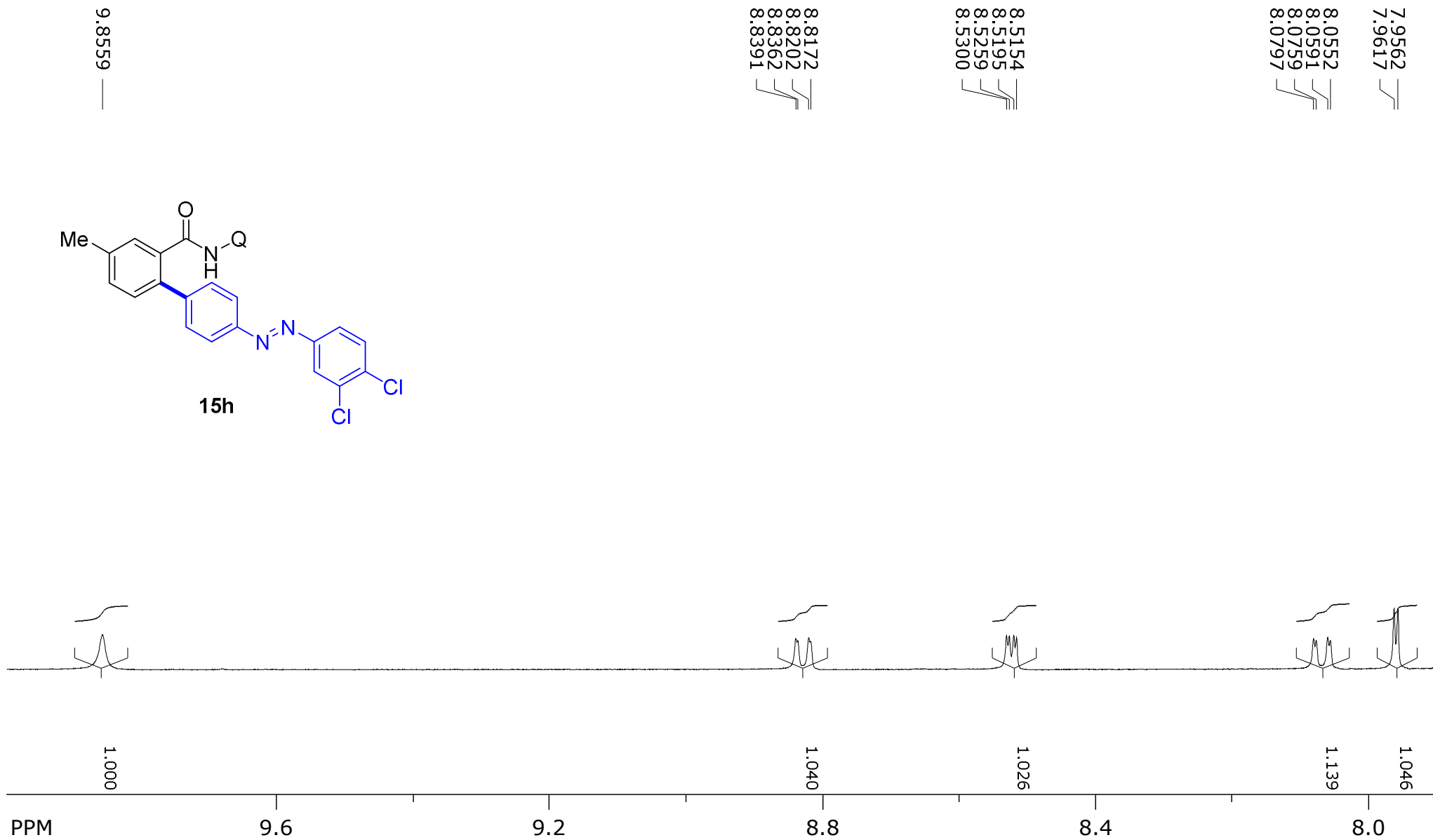
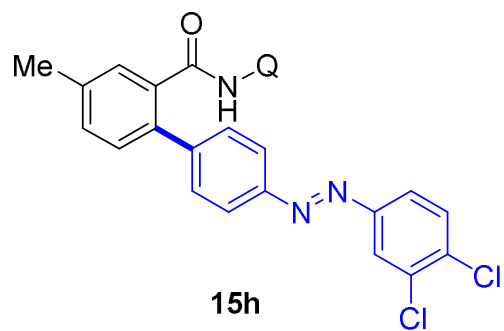
SpinWorks 4: SS 207 P

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 59

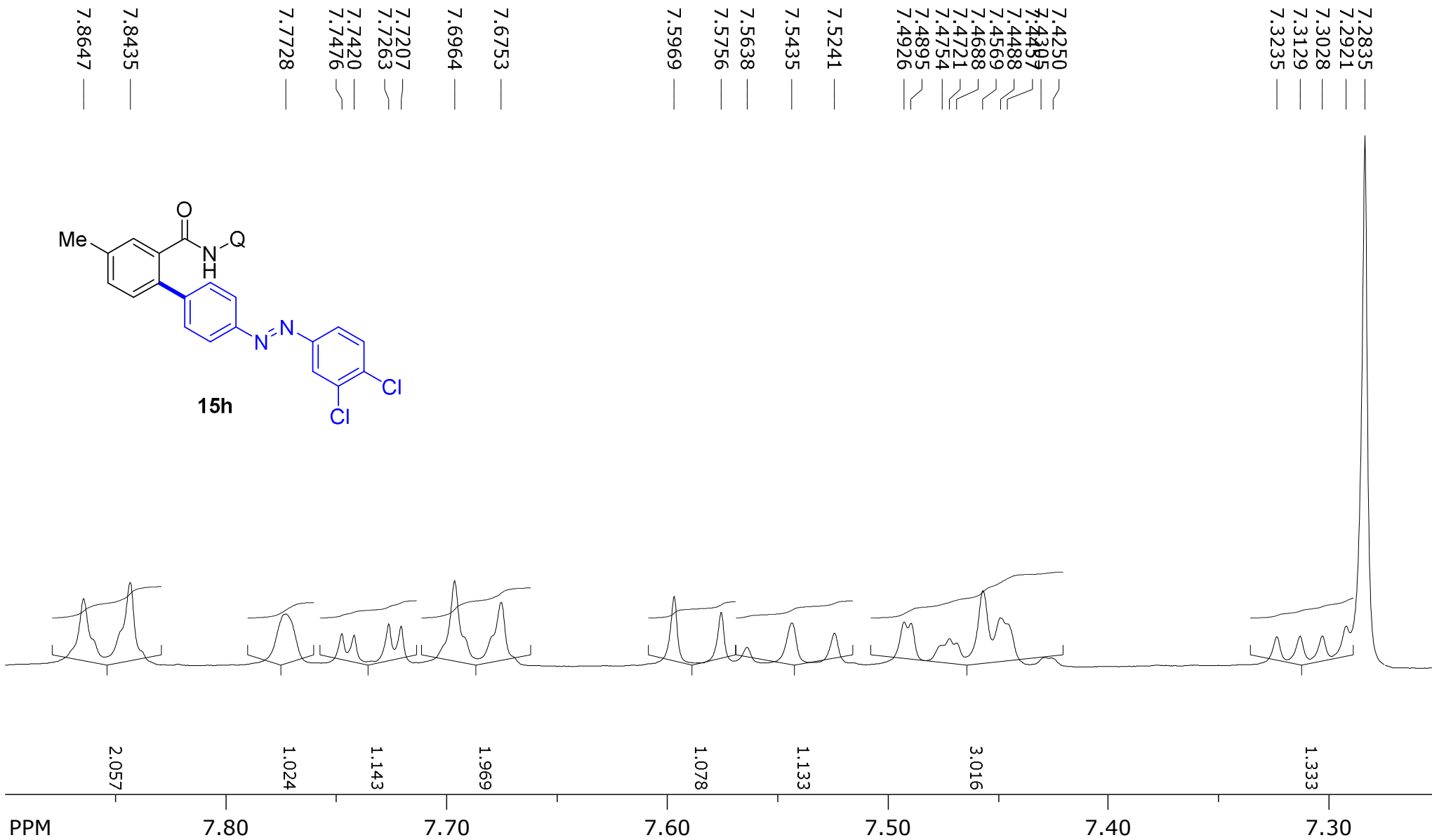
167.949 —
153.002 —
149.845 —
147.900 —
142.741 —
138.479 —
138.443 —
138.040 —
136.744 —
136.016 —
135.901 —
134.578 —
131.860 —
131.412 —
130.756 —
129.912 —
129.057 —
127.772 —
127.323 —
127.267 —
122.890 —
121.672 —
121.415 —
116.408 —
115.596 —



SpinWorks 4: SS-752 II
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 1



SpinWorks 4: SS-752 II
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 1

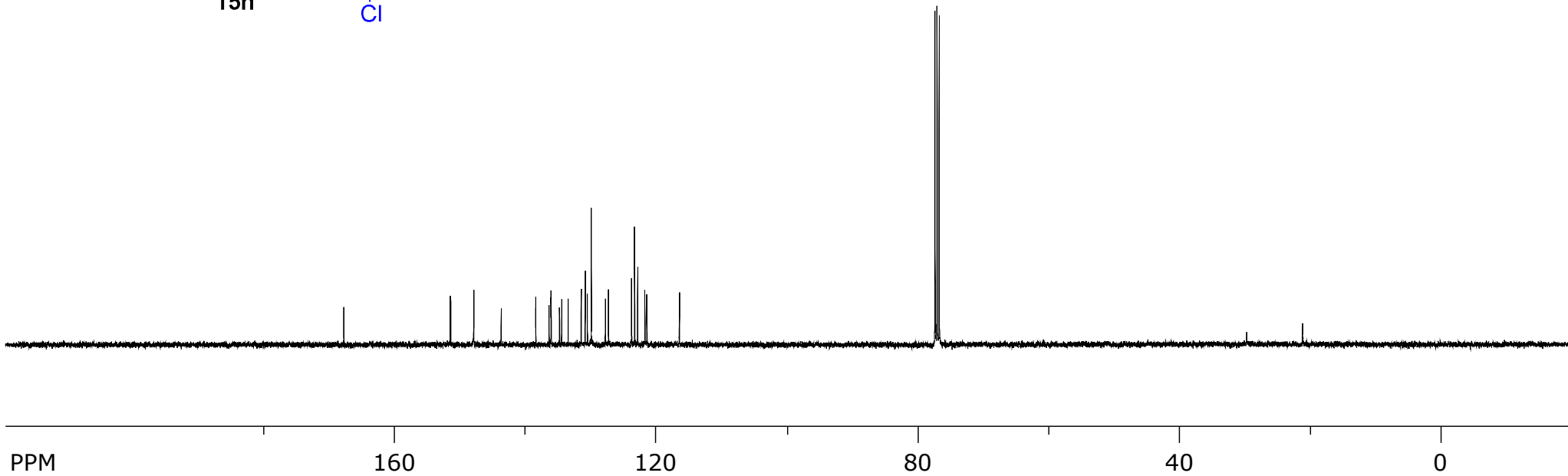
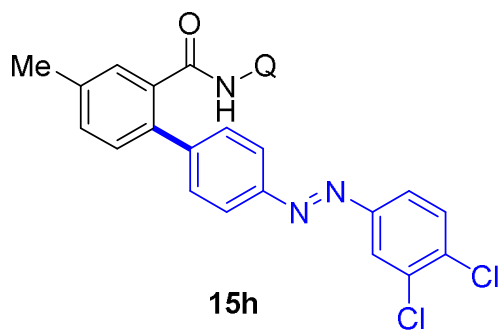


SpinWorks 4: SS 752 II
C13CPD CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 8

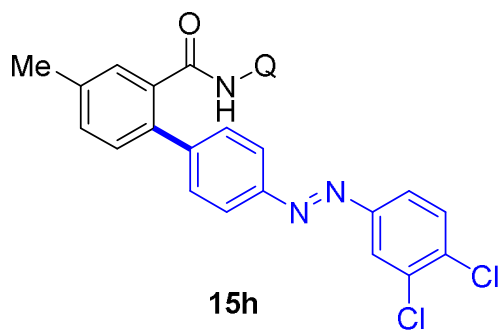
116.432
121.420
121.713
122.822
123.288
123.755
127.288
127.766
129.907
130.805
131.714
134.764
136.042
136.073
136.353
138.380
138.409
143.688
147.881
151.375
151.476
167.730

76.732
77.048
77.367

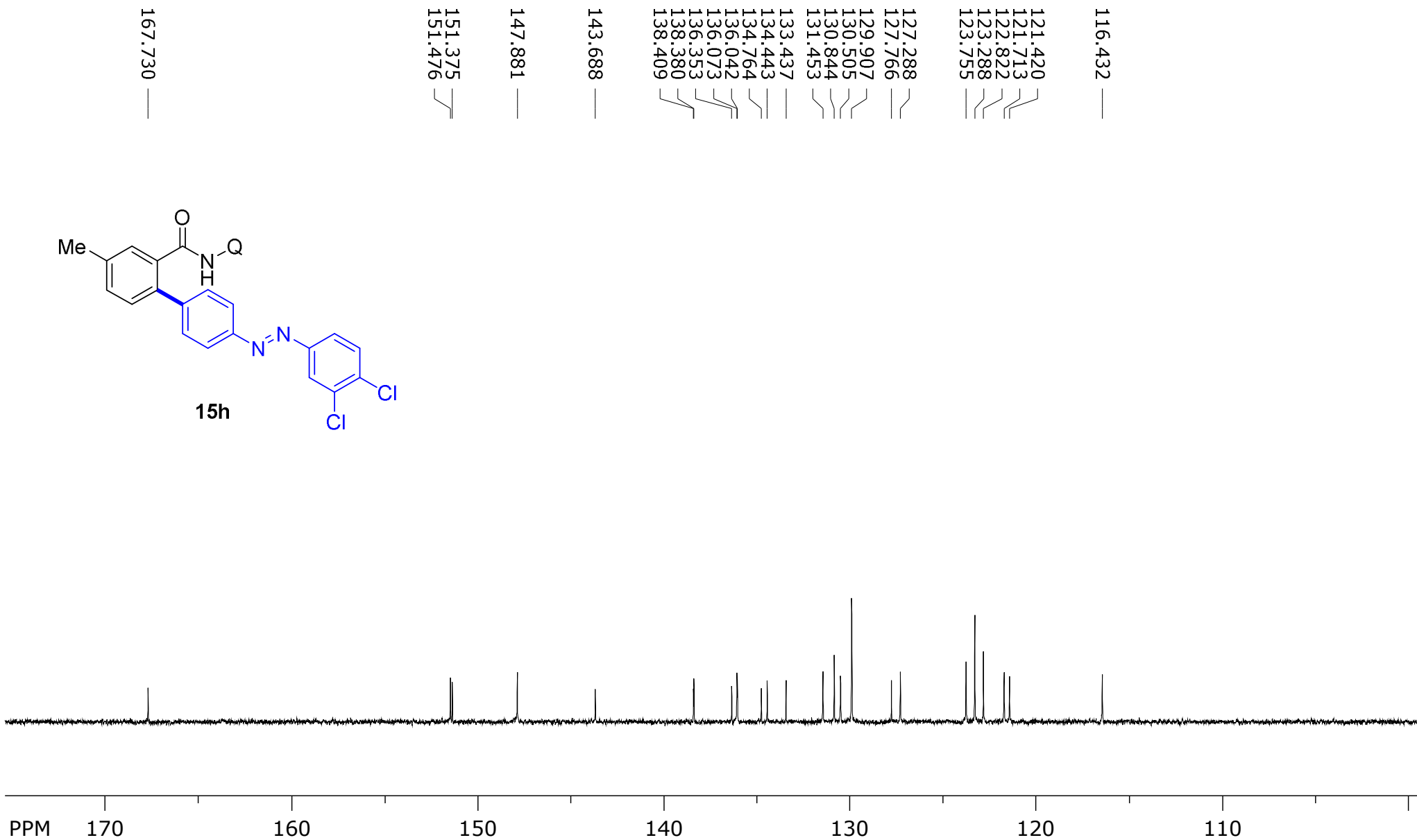
21.152



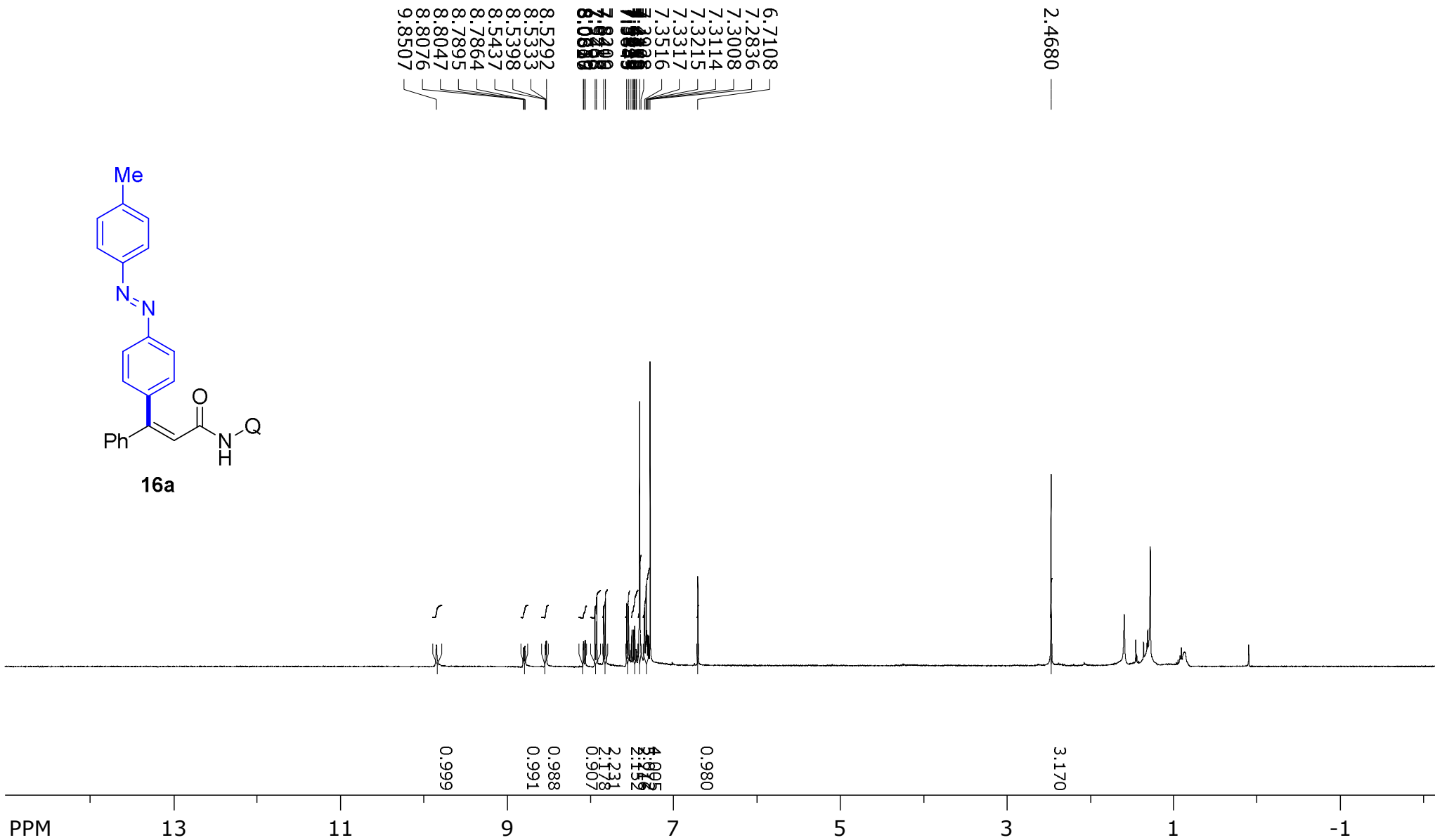
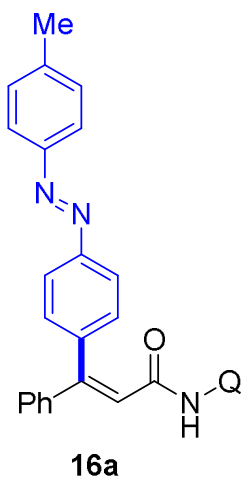
SpinWorks 4: SS 752 II
C13CPD CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 8



15h



SpinWorks 4: SS 763
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 18



SpinWorks 4: SS 763
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 18

9.8507

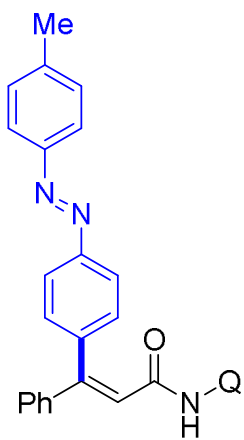
8.7864
8.7895
8.8047
8.8076

8.5292
8.5333
8.5398
8.5437

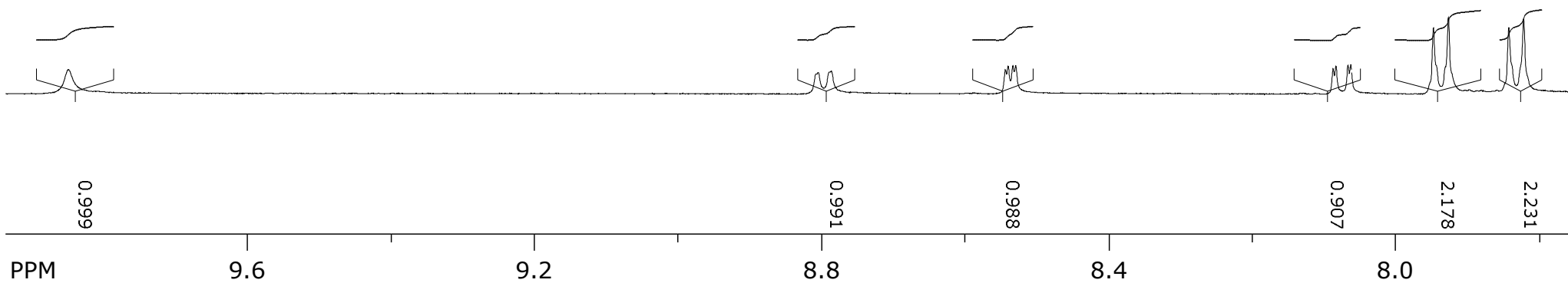
8.0619
8.0659
8.0827
8.0866

7.9258
7.9468

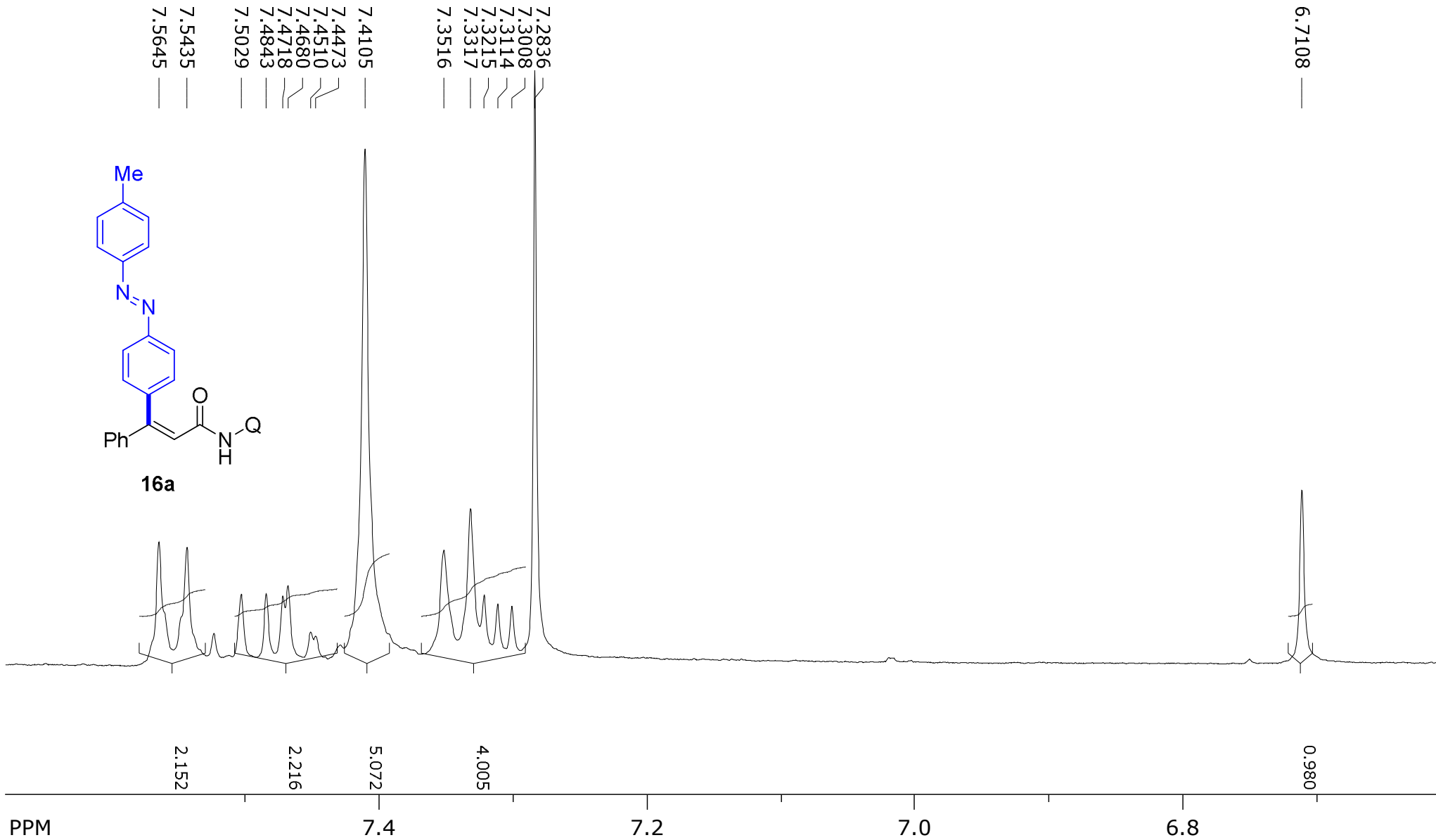
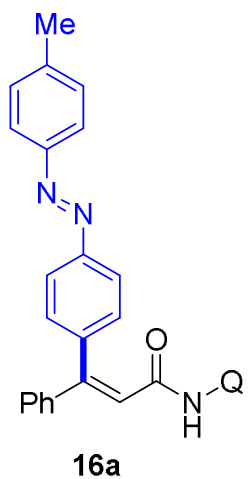
7.8209
7.8416

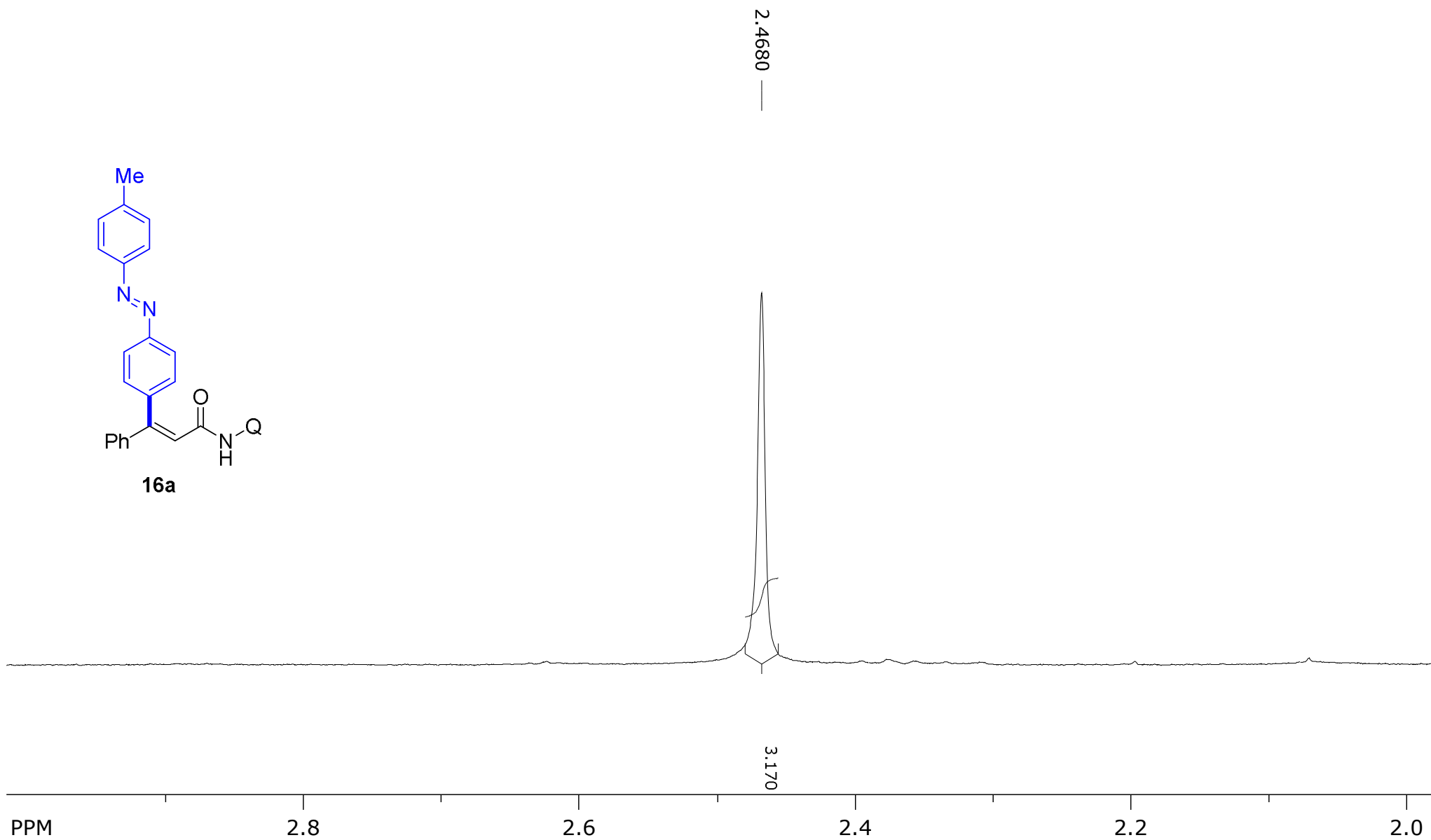
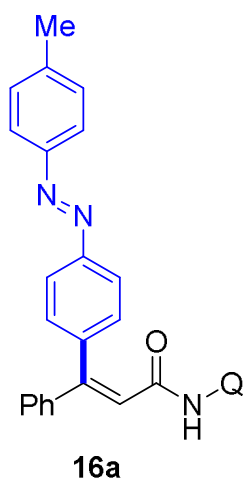


16a



SpinWorks 4: SS 763
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 18





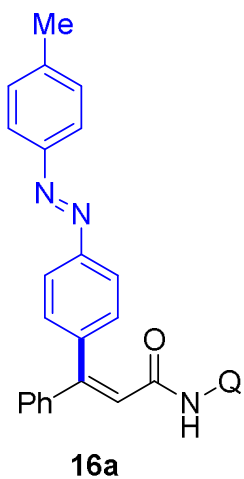
SpinWorks 4: SS-763

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 39

116.489
121.437
121.469
122.890
122.953
123.190
127.340
127.790
129.349
129.379
130.676
134.483
136.082
138.333
140.927
140.986
141.740
147.849
150.850
151.421
152.680
164.312

21.564

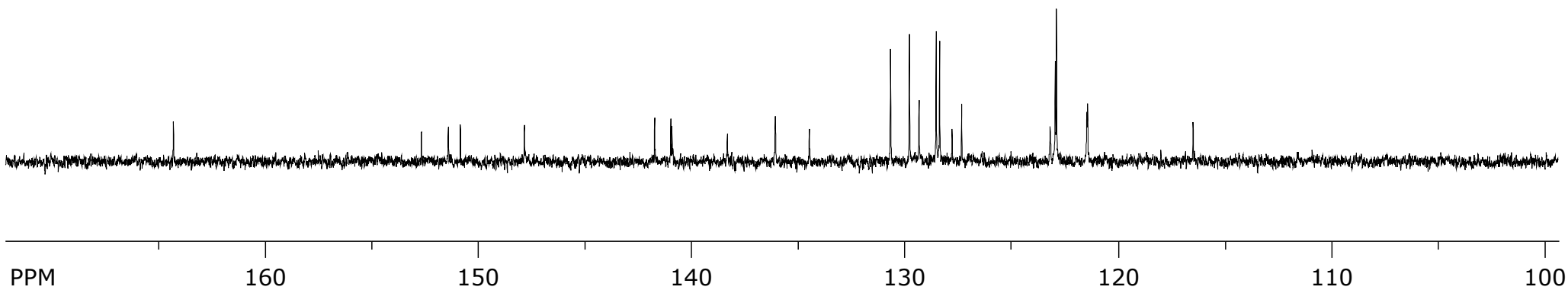
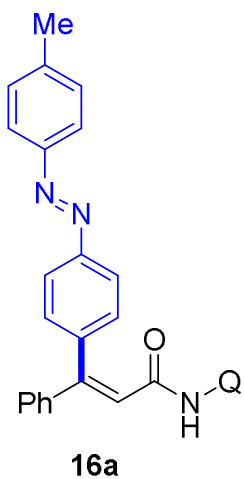
76.722
77.039
77.357



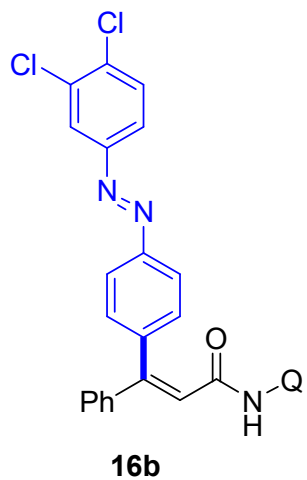
PPM 160 120 80 40 0

SpinWorks 4: SS-763
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 39

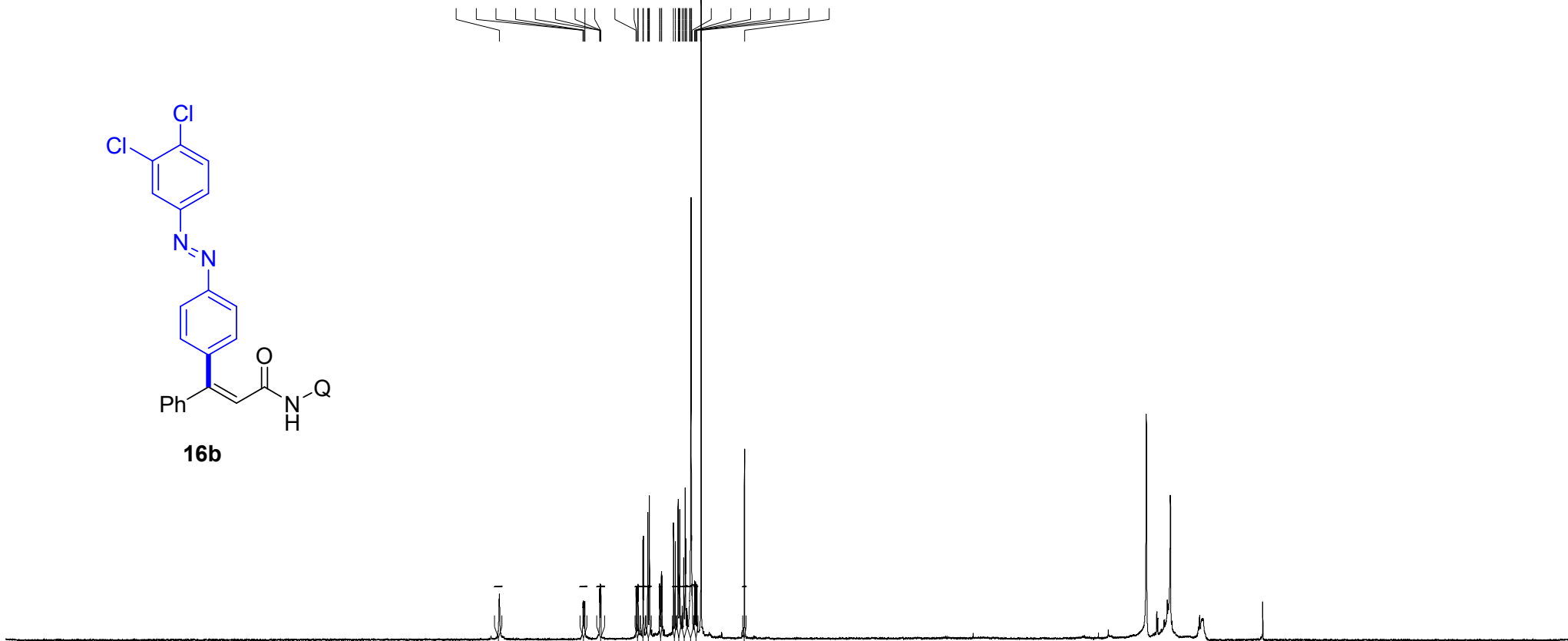
164,312 —
150,850 —
151,421 —
152,680 —
147,849 —
140,927 —
140,986 —
141,740 —
138,333 —
136,082 —
134,483 —
130,676 —
129,791 —
128,540 —
128,378 —
127,790 —
127,340 —
123,190 —
122,953 —
122,890 —
121,469 —
121,437 —
116,489 —



SpinWorks 4: SS 770
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 2



9.8665
8.7957
8.7911
8.7783
8.5819
8.5779
8.5714
8.5674
8.1145
8.0009
7.9969
7.9929
7.3981
7.3676
7.3569
7.3469
7.3363
7.2841
6.7288



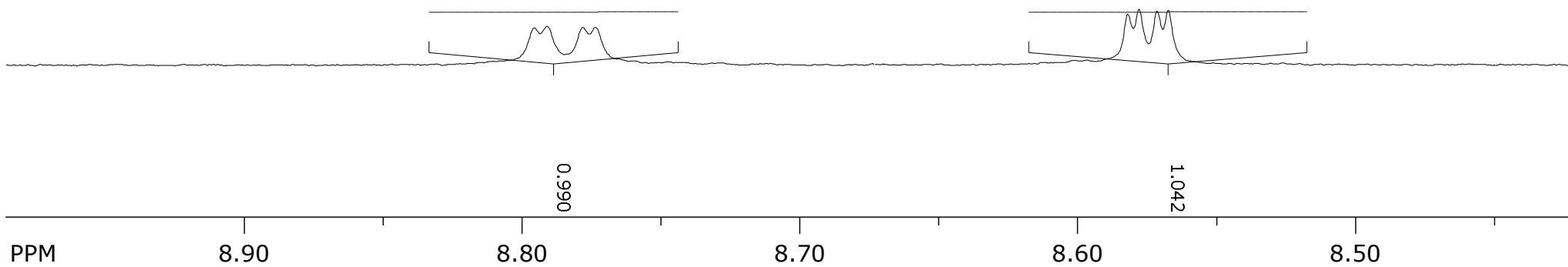
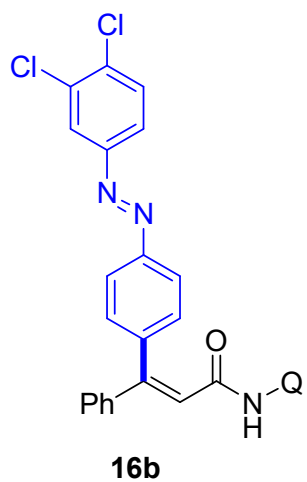
0.877
1.042
0.990
1.019
1.027
1.035
1.043
0.911

PPM 12 8 4 0

SpinWorks 4: SS 770
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 2

8.7726
8.7783
8.7911
8.7957

8.5674
8.5714
8.5779
8.5819



SpinWorks 4: SS 770
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 2

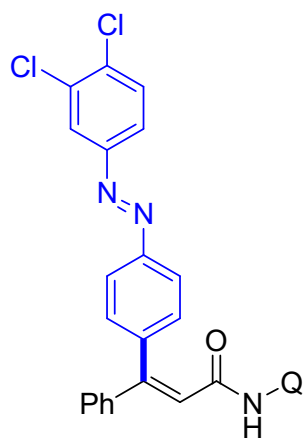
8.1105
8.1145

8.0899
8.0939

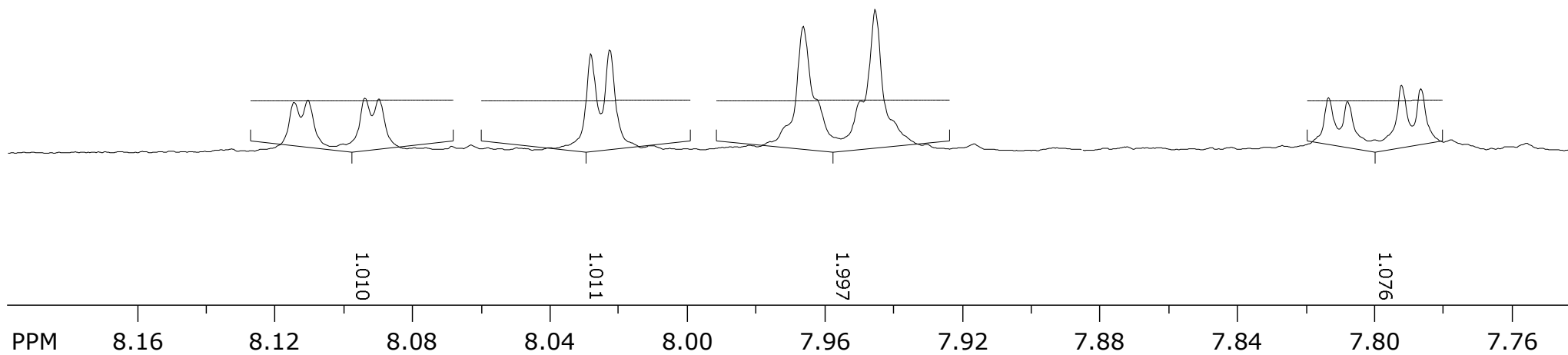
8.0226
8.0282

7.9454
7.9496
7.9600
7.9663

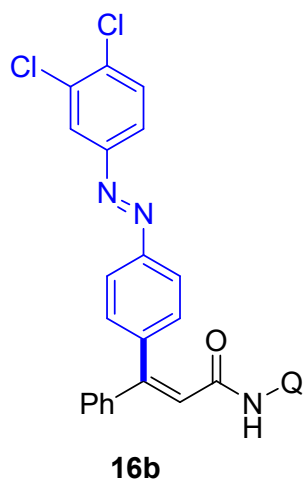
7.7865
7.7921
7.8079
7.8134



16b



SpinWorks 4: SS 770
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 2



7.6361

7.6148

7.5781

7.5724

7.5611

7.5572

7.5262

7.5056

7.4876

7.4821

7.4663

7.4307

7.4272

7.4125

7.4053

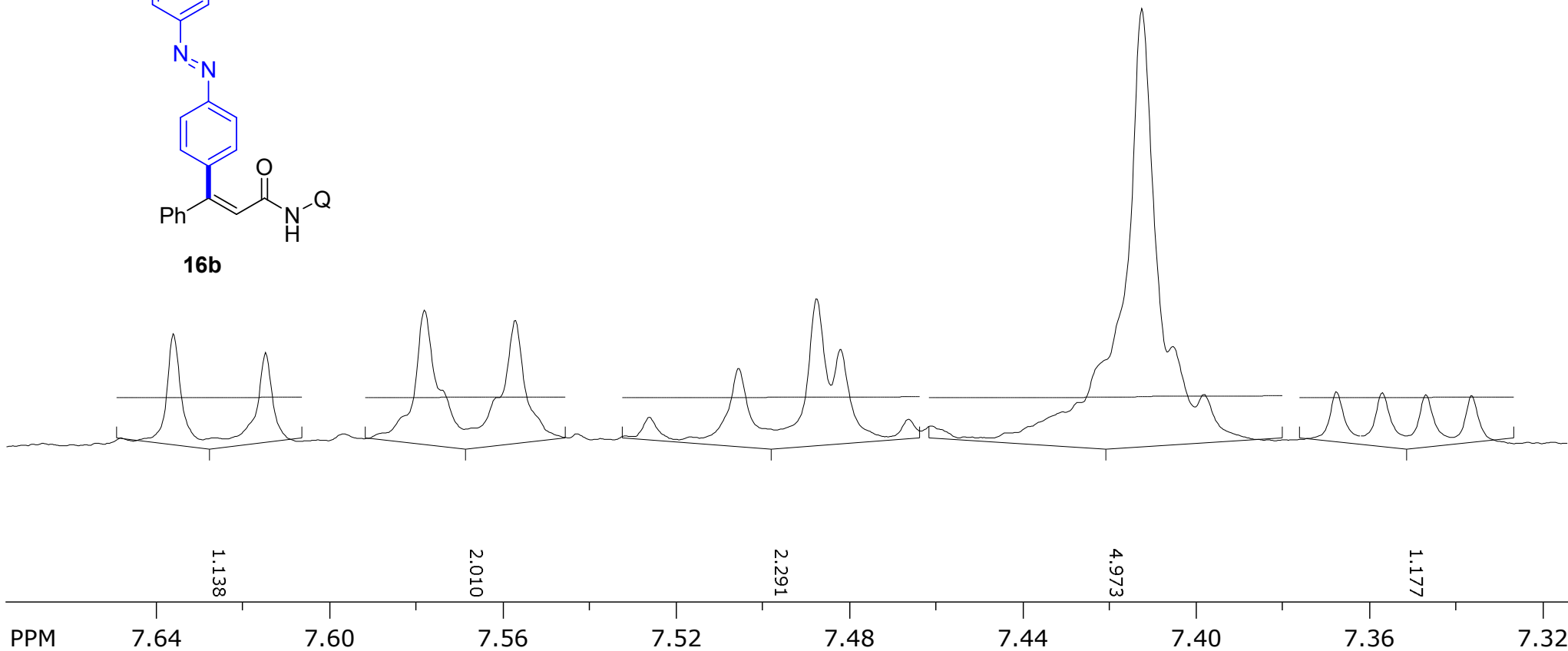
7.3981

7.3676

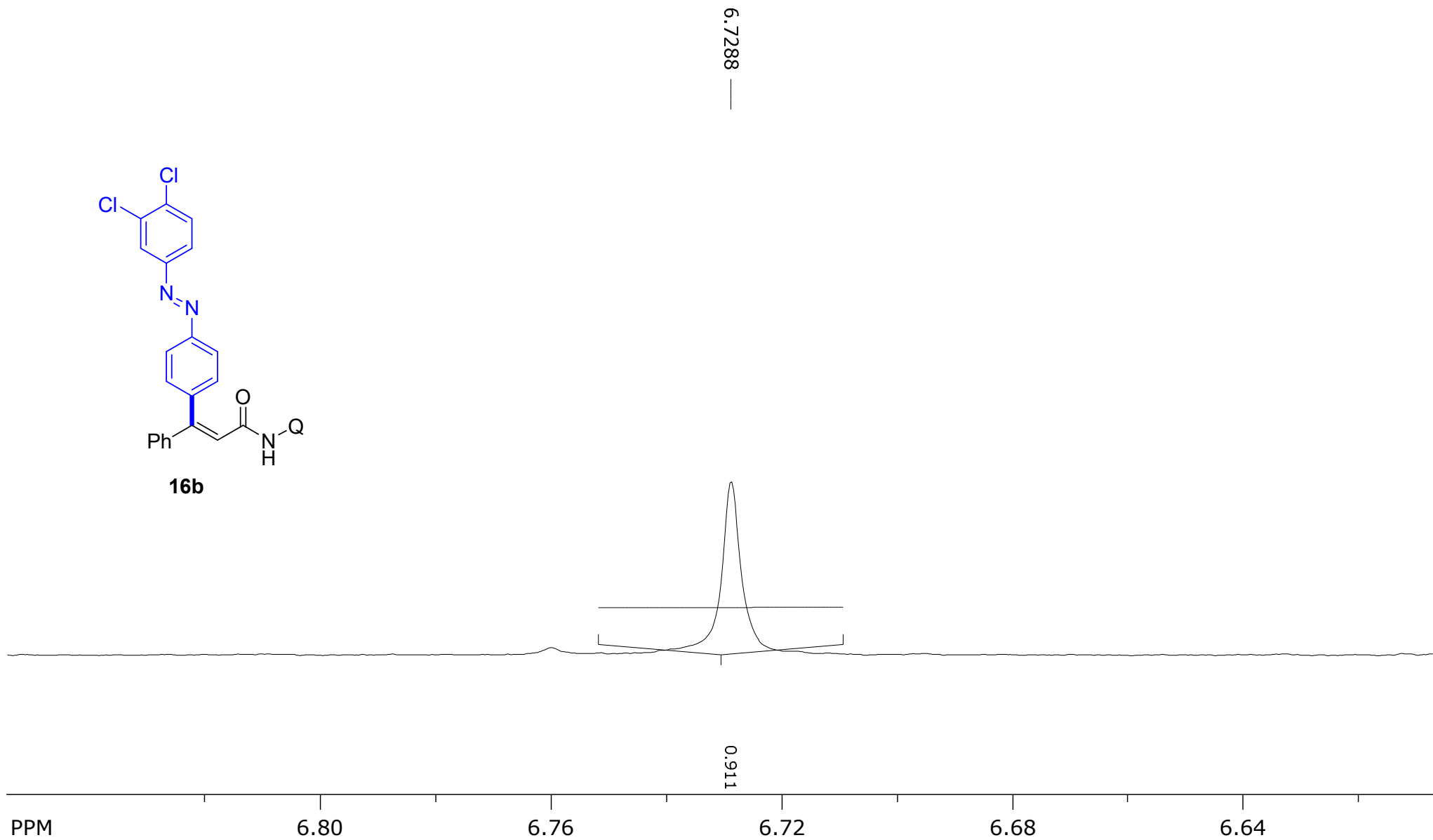
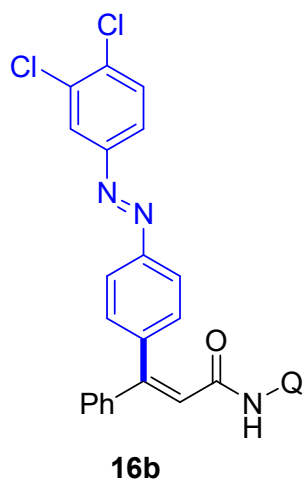
7.3569

7.3469

7.3363



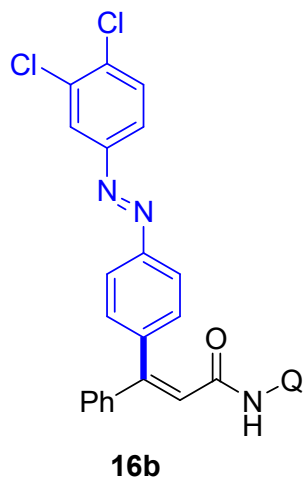
SpinWorks 4: SS 770
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 2



SpinWorks 4: SS-770
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 40

116.572
121.479
121.577
122.874
123.098
123.258
123.887
127.372
127.849
128.250
130.550
133.515
134.419
134.966
136.197
138.326
140.795
142.251
147.848
151.536
151.589
152.060
164.082

76.731
77.049
77.367



PPM

160

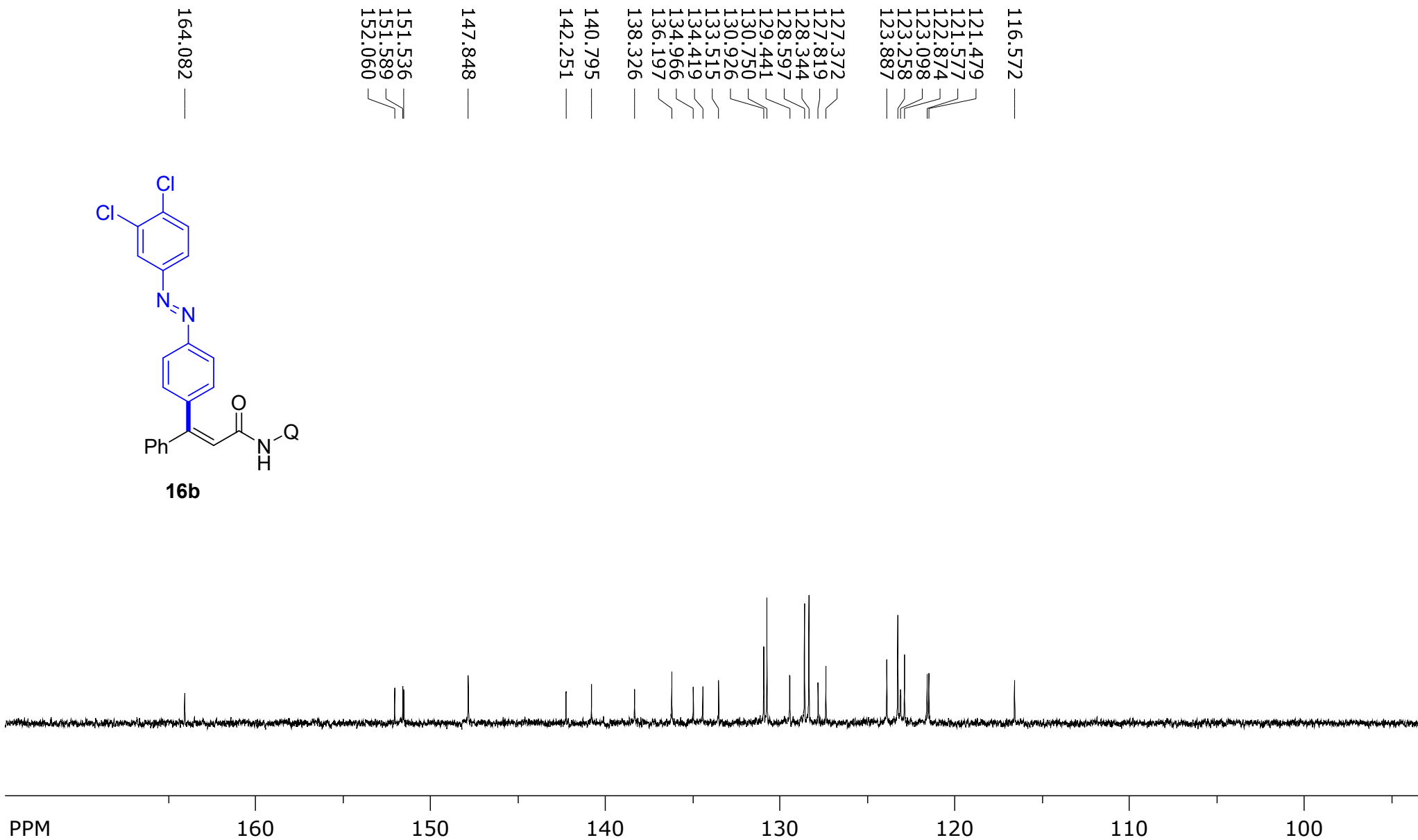
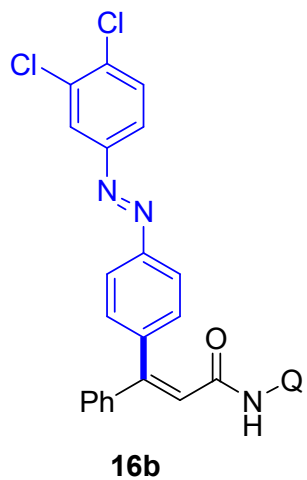
120

80

40

0

SpinWorks 4: SS-770
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 40



PPM

160

150

140

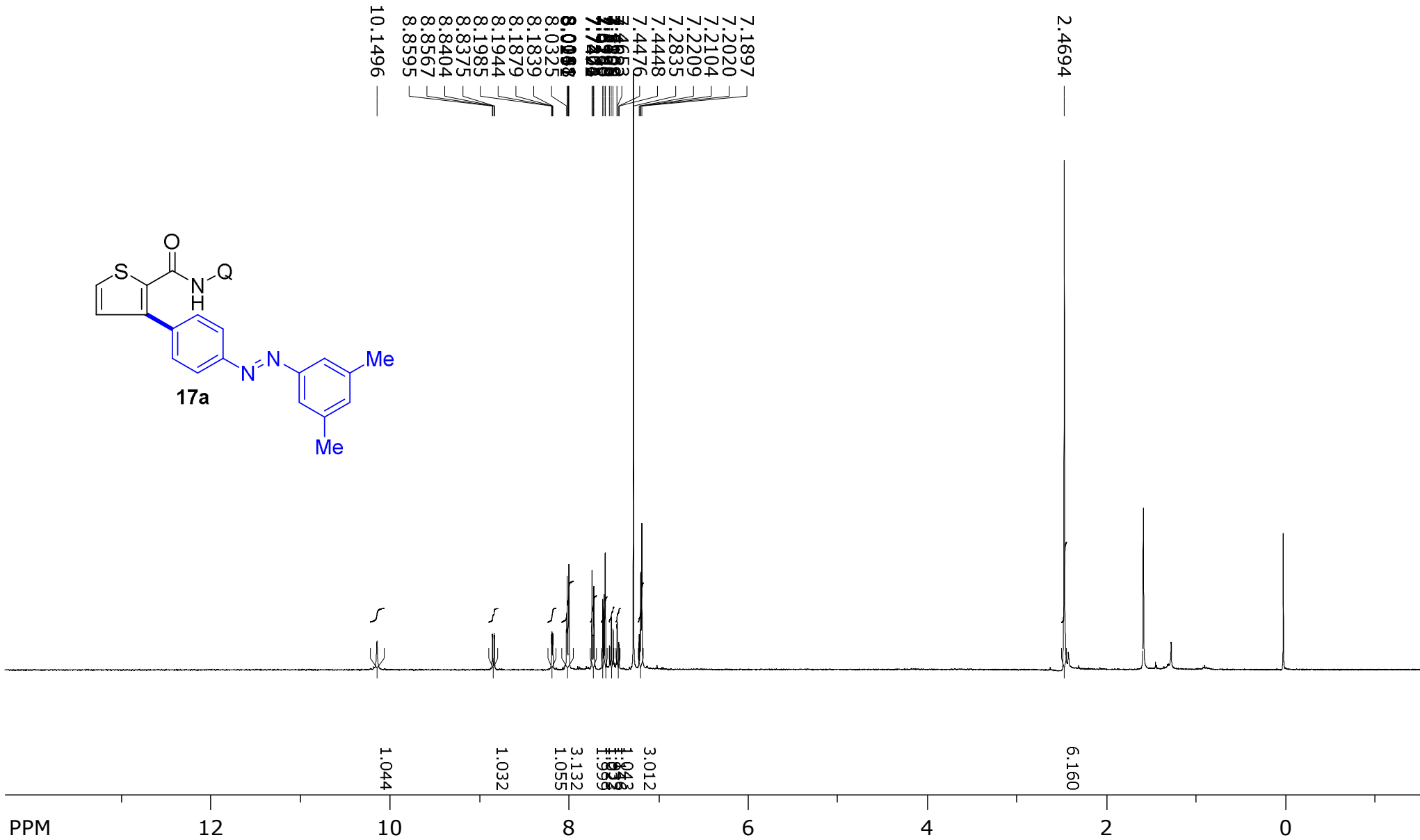
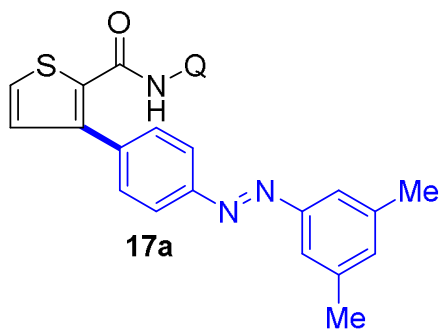
130

120

110

100

SpinWorks 4: SS-762 REP
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 33

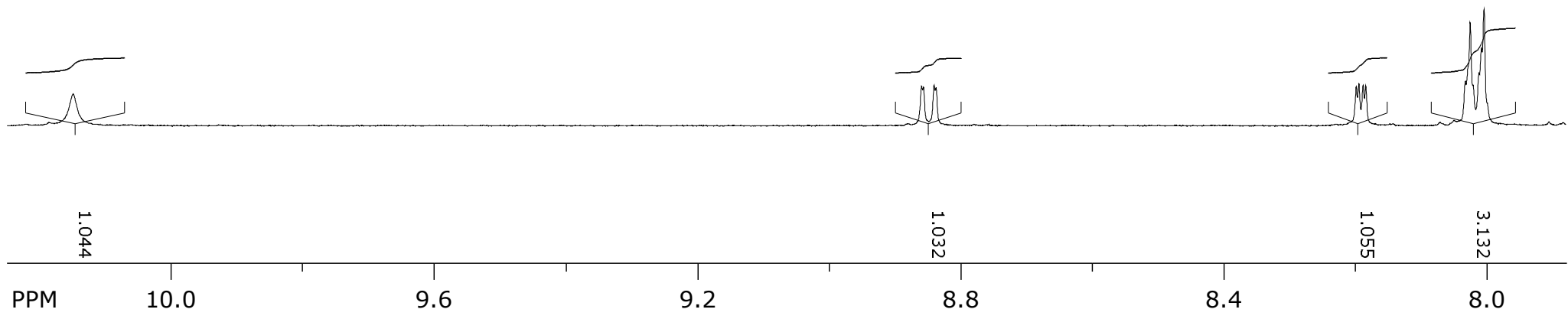
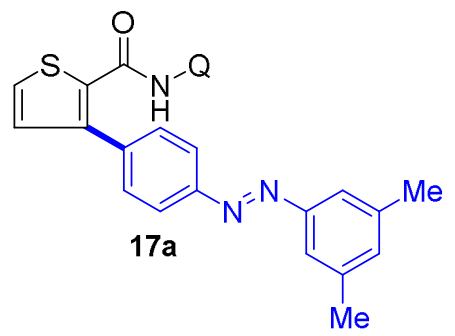


SpinWorks 4: SS-762 REP
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 33

10.1496

8.8375
8.8404
8.8567
8.8595

8.0041
8.0081
8.0118
8.0207
8.0251
8.0325
8.1839
8.1879
8.1944
8.1985



SpinWorks 4: SS-762 REP
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 33

7.7261
7.7304
7.7426
7.7472

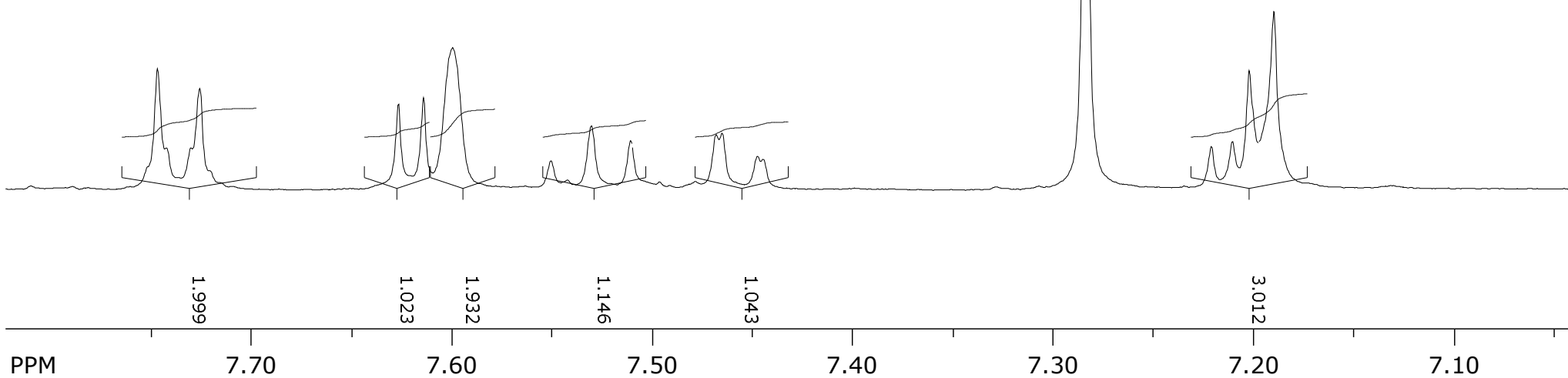
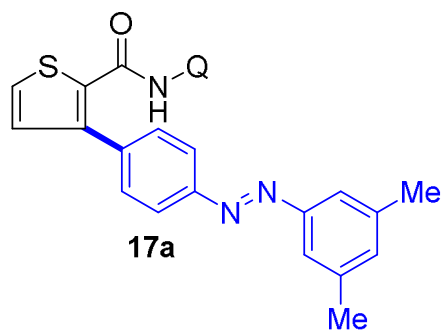
7.5998
7.6143
7.6269

7.5506
7.5305
7.5109

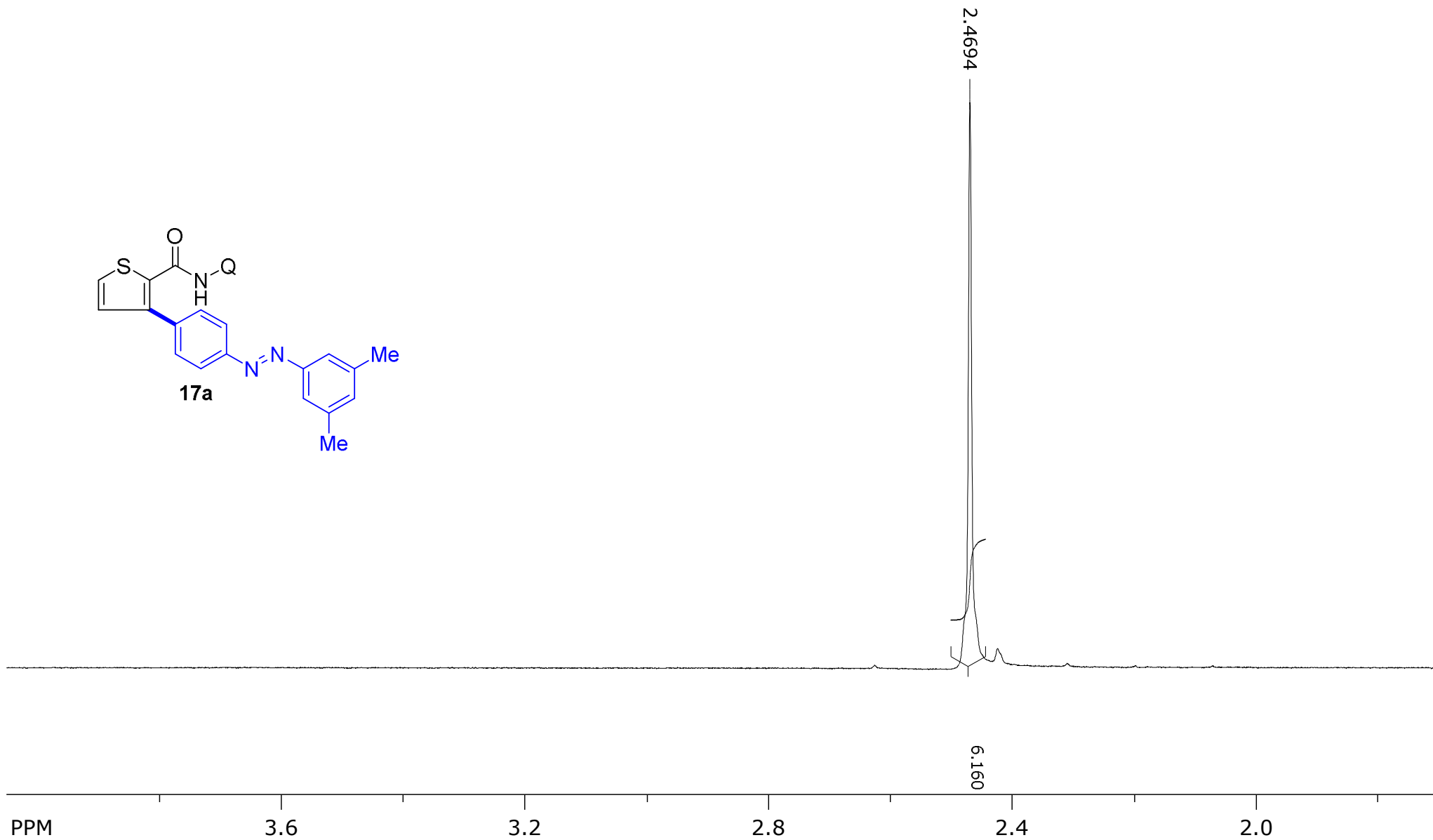
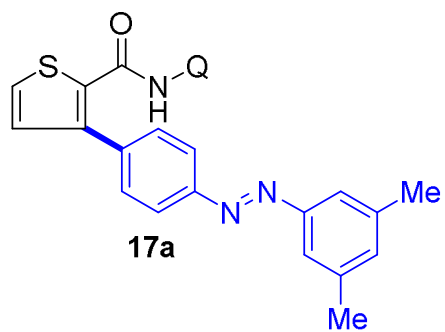
7.4448
7.4476
7.4653
7.4682

7.2835

7.1897
7.2020
7.2104
7.2209



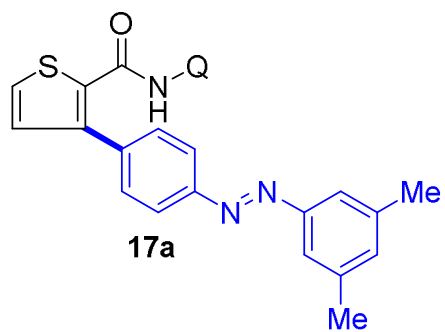
SpinWorks 4: SS-762 REP
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 33



SpinWorks 4: SS-762

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 41

116.410
120.741
121.428
121.614
123.552
127.264
127.732
129.614
130.458
131.998
134.428
135.818
136.274
137.676
138.368
138.917
142.167
147.744
152.815
160.448



76.722
77.041
77.357

21.331

PPM

160

120

80

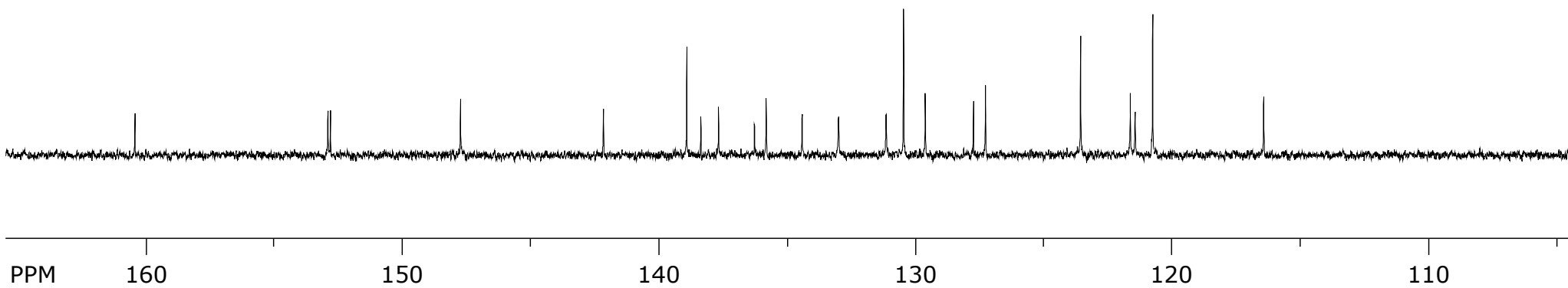
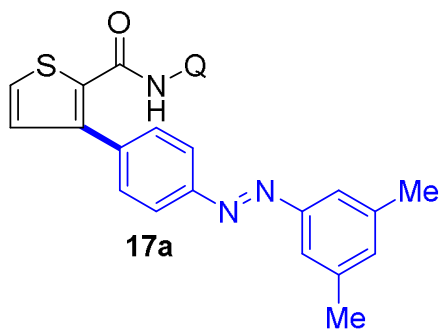
40

0

185

SpinWorks 4: SS-762
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 41

160.448 —
152.815 —
152.917 —
147.744 —
142.167 —
138.917 —
138.368 —
137.676 —
136.274 —
135.818 —
134.420 —
132.998 —
131.139 —
130.458 —
129.614 —
127.732 —
127.264 —
123.552 —
121.614 —
121.428 —
120.741 —
116.410 —



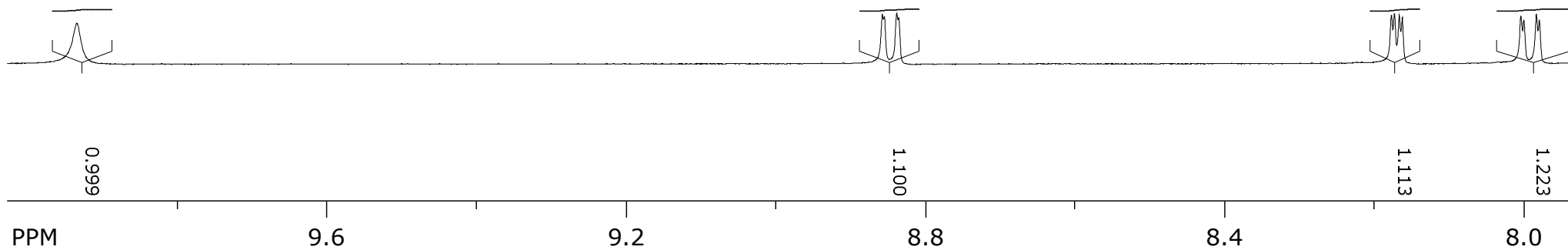
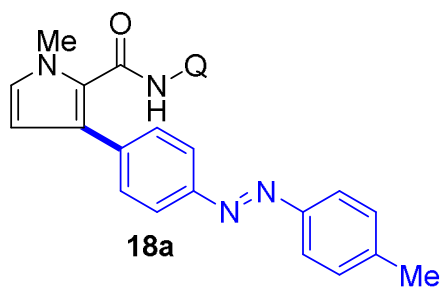
SpinWorks 4: SS-758
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 4

9.9353

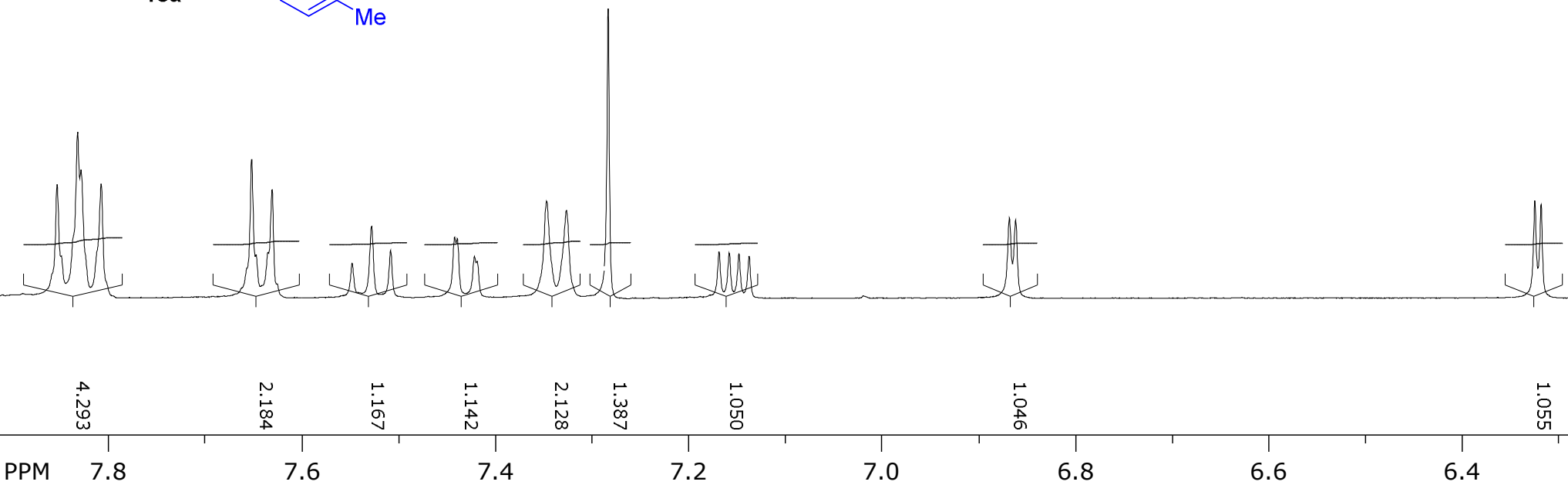
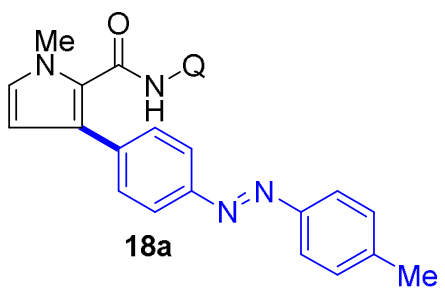
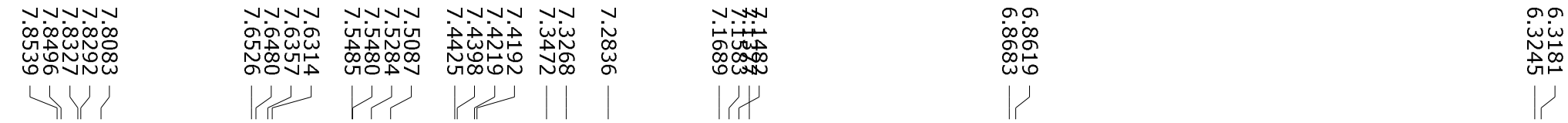
8.8356
8.8383
8.8549
8.8575

8.1621
8.1662
8.1726
8.1766

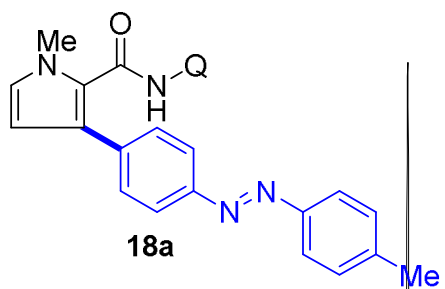
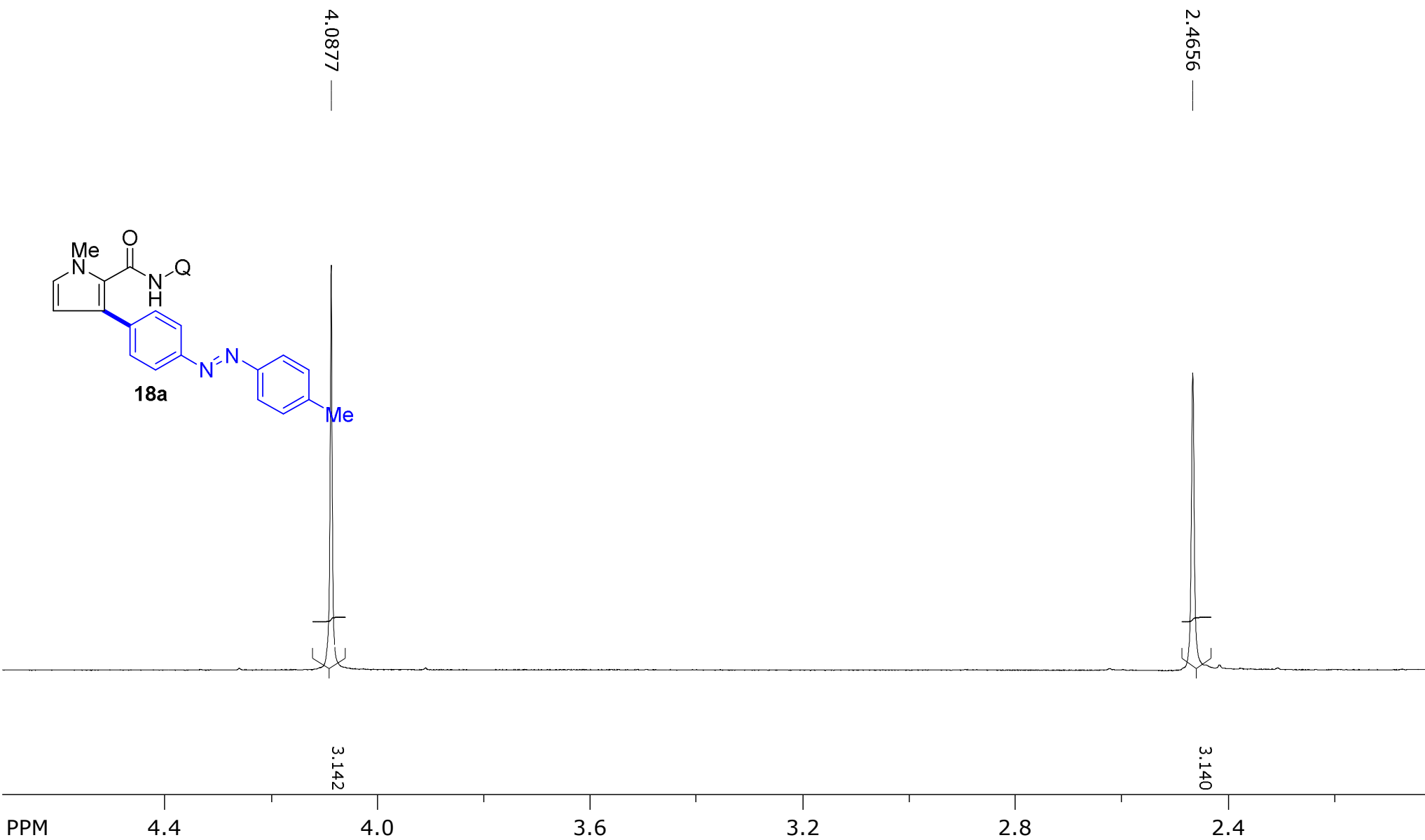
7.9788
7.9828
7.9995
8.0035



SpinWorks 4: SS-758
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 4



SpinWorks 4: SS-758
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 4



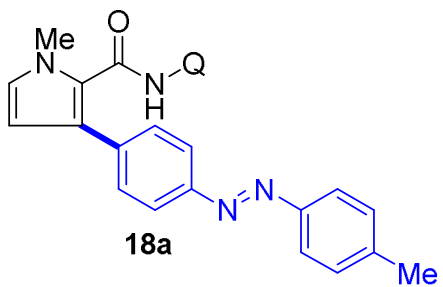
SpinWorks 4: SS758
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 40

109.430
115.688
121.128
121.282
122.789
123.101
123.801
127.143
137.281
137.281
128.682
129.766
130.450
134.900
135.705
138.339
138.375
141.452
147.650
150.877
151.910
160.345

76.735
77.052
77.370

37.259

21.491



PPM

160

120

80

40

0

SpinWorks 4: SS758
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 40

160.345

150.877
151.910

147.650

141.452

138.339
138.375

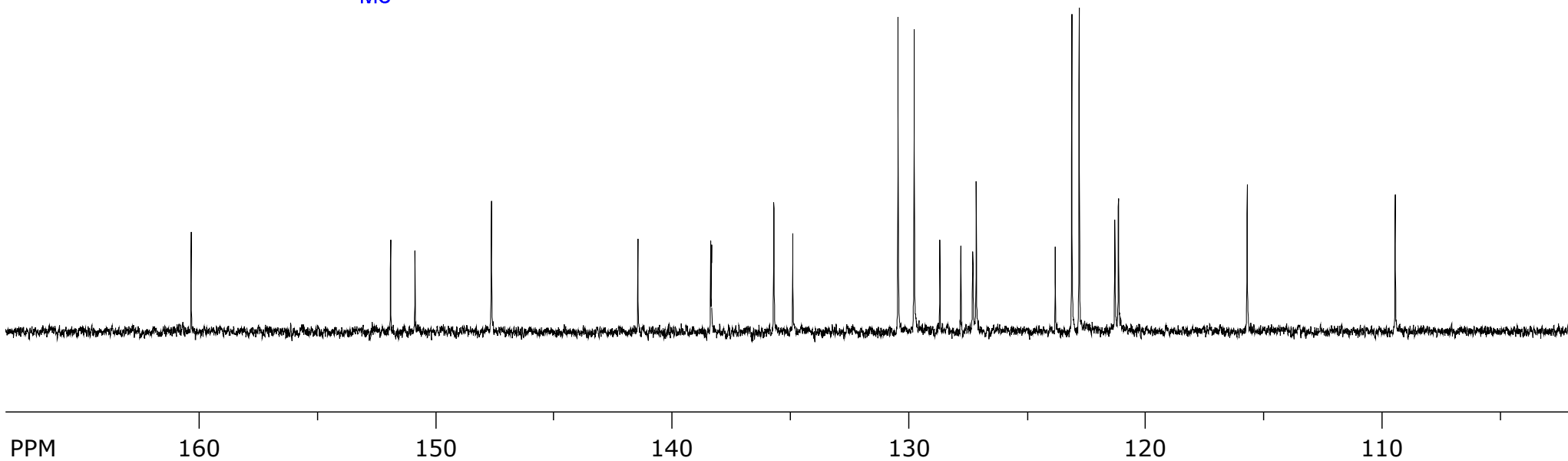
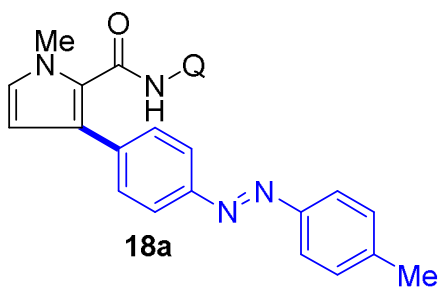
134.900
135.705

127.143
127.291
127.795
128.682
129.766
130.450

123.801
121.128
121.282
122.789
123.101

115.688

109.430



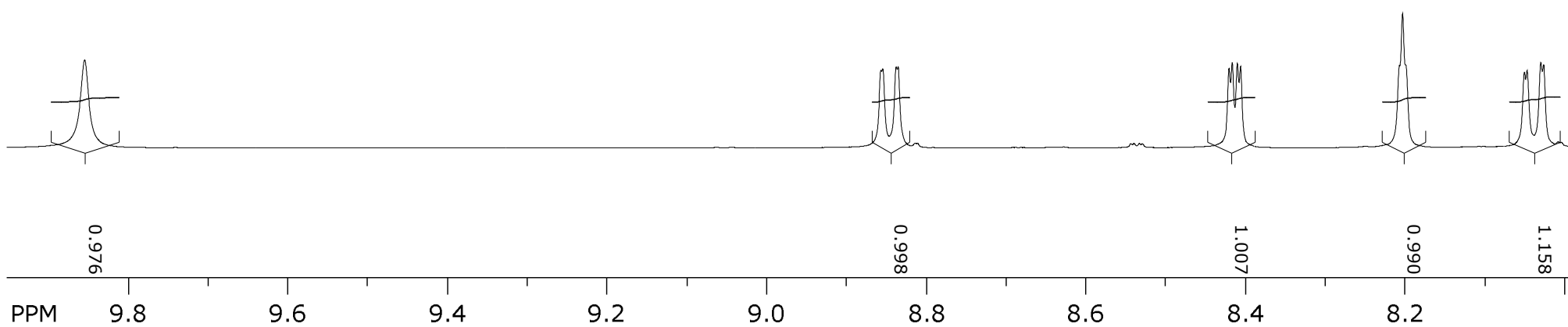
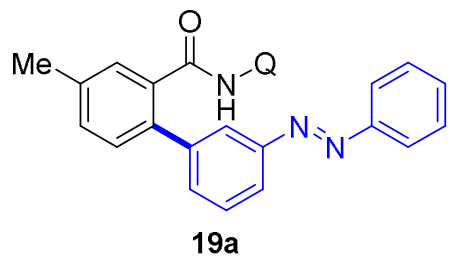
9.8551

8.8351
8.8376
8.8542
8.8566

8.4057
8.4096
8.4161
8.4200

8.1986
8.2024
8.2064

8.0256
8.0292
8.0463
8.0499



7.8984
7.9015
7.9182
7.9223

7.8160

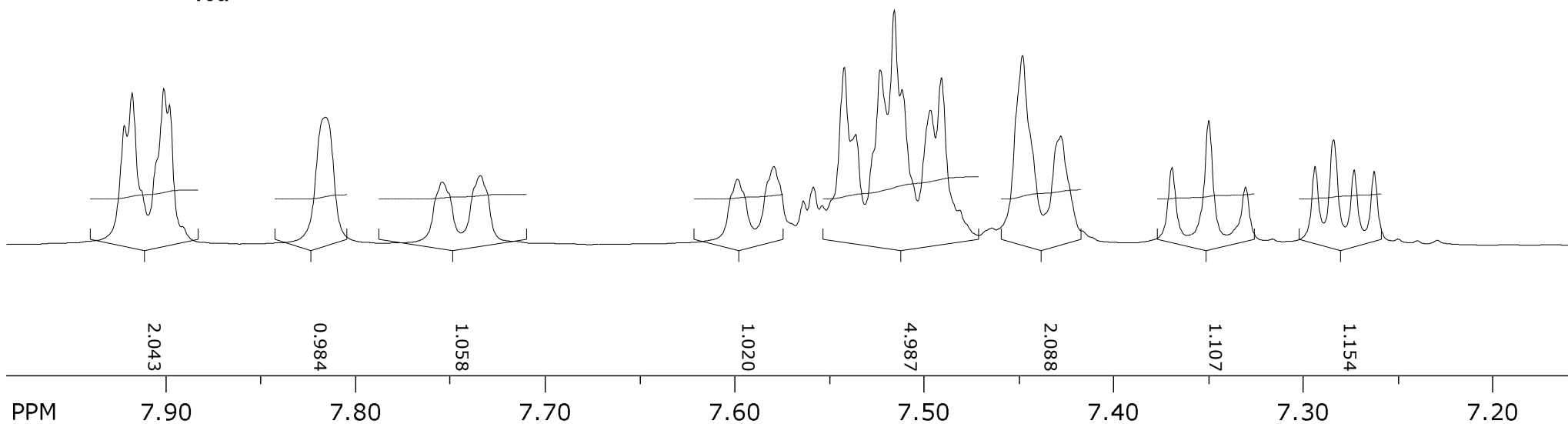
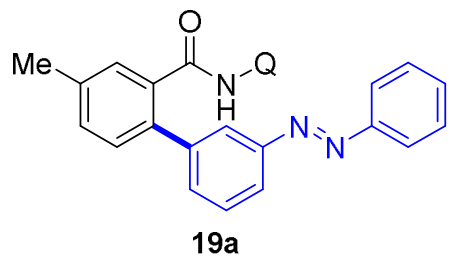
7.7343
7.7545

7.5985
7.5793
7.5638
7.5584
7.5539
7.5422
7.5361
7.5232
7.5158
7.5117
7.4967
7.4909

7.4481
7.4278

7.3692
7.3497
7.3303

7.2624
7.2730
7.2838
7.2936



SpinWorks 4: SS 243 P
C13CPD CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 51

167.751

152.616
152.905

147.864

141.116

138.069
138.398

136.659

135.966
134.490

131.767
131.487

131.088
130.662

129.961
129.131

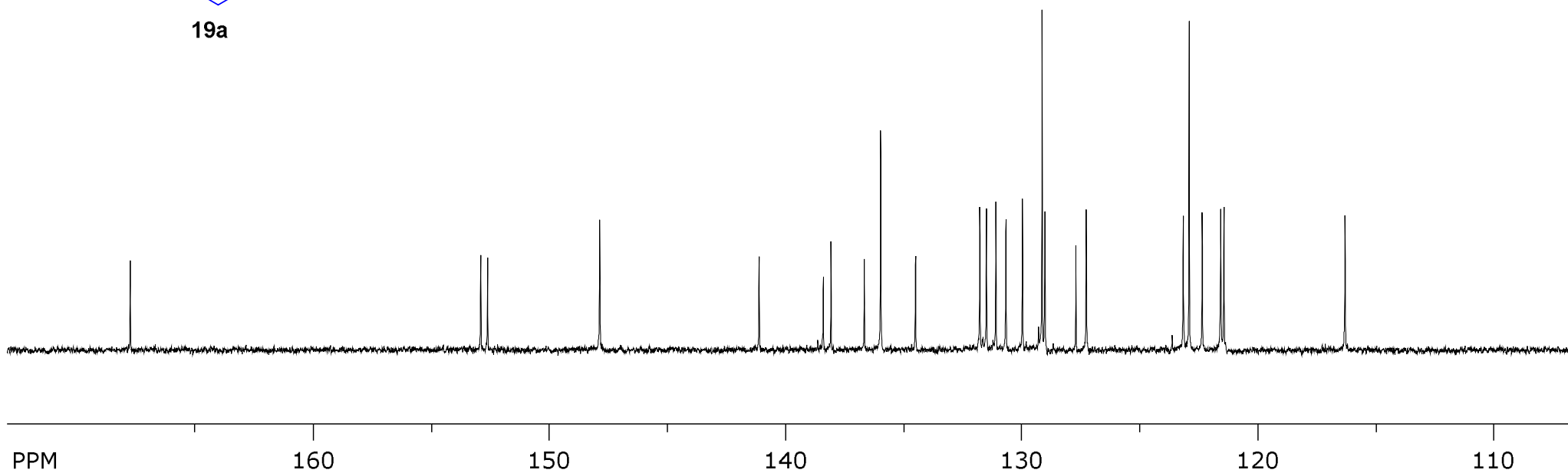
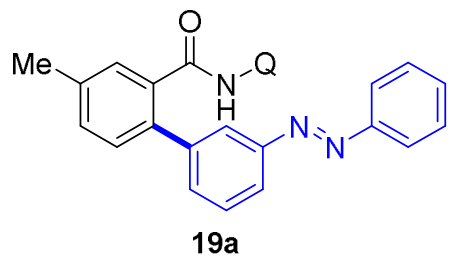
129.012
127.698

127.260

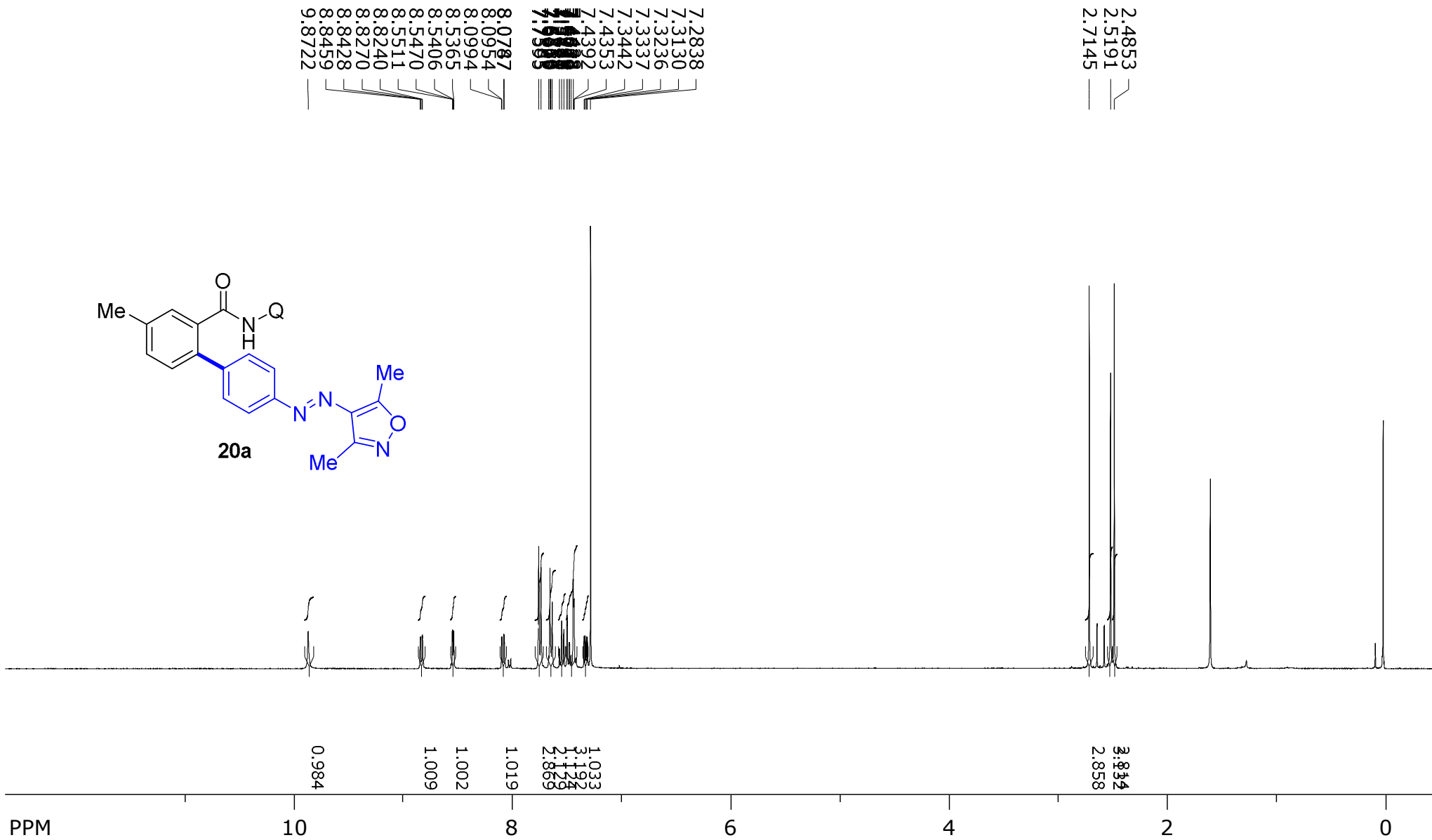
123.149
122.899

121.567
121.429

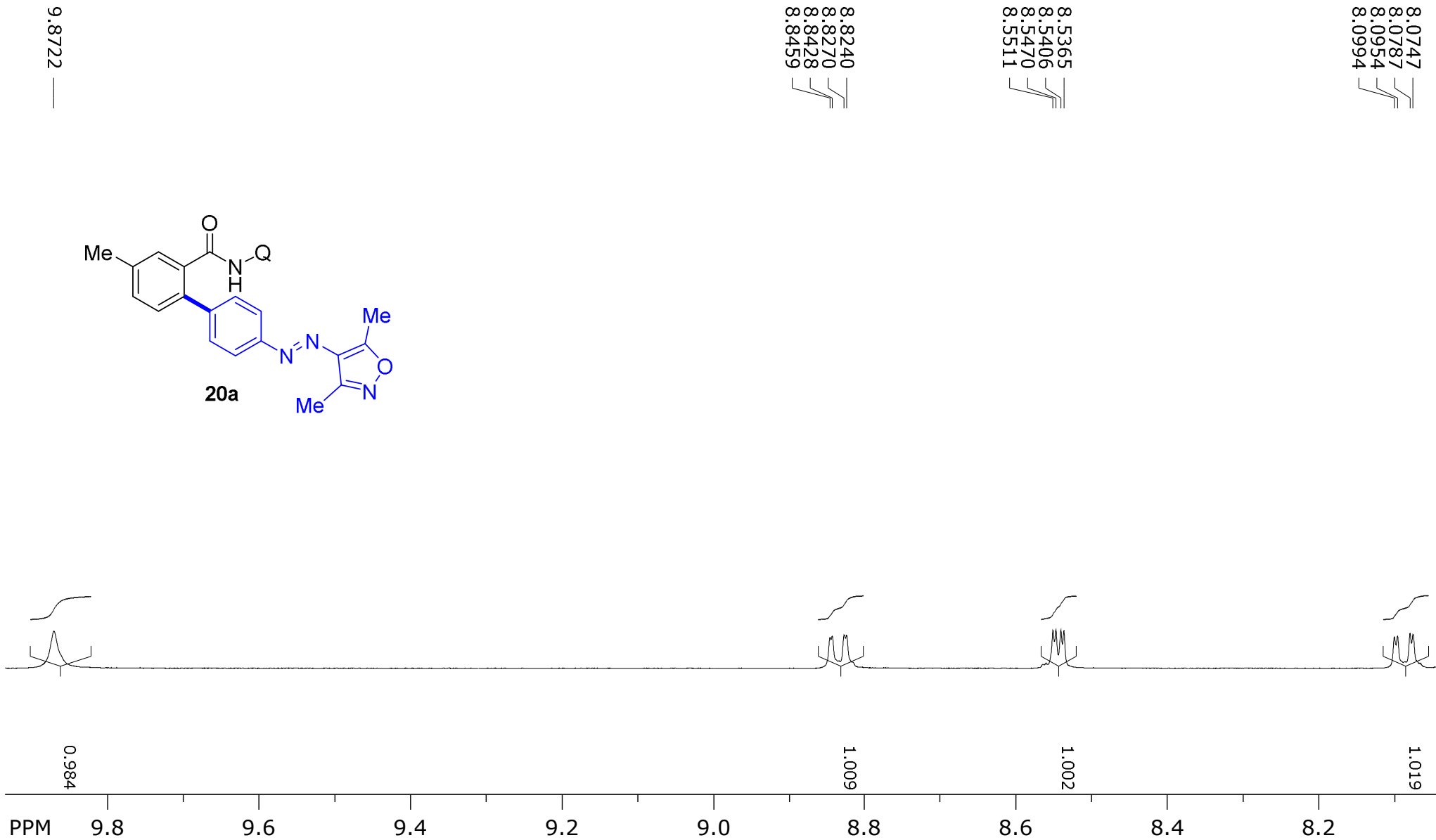
116.297



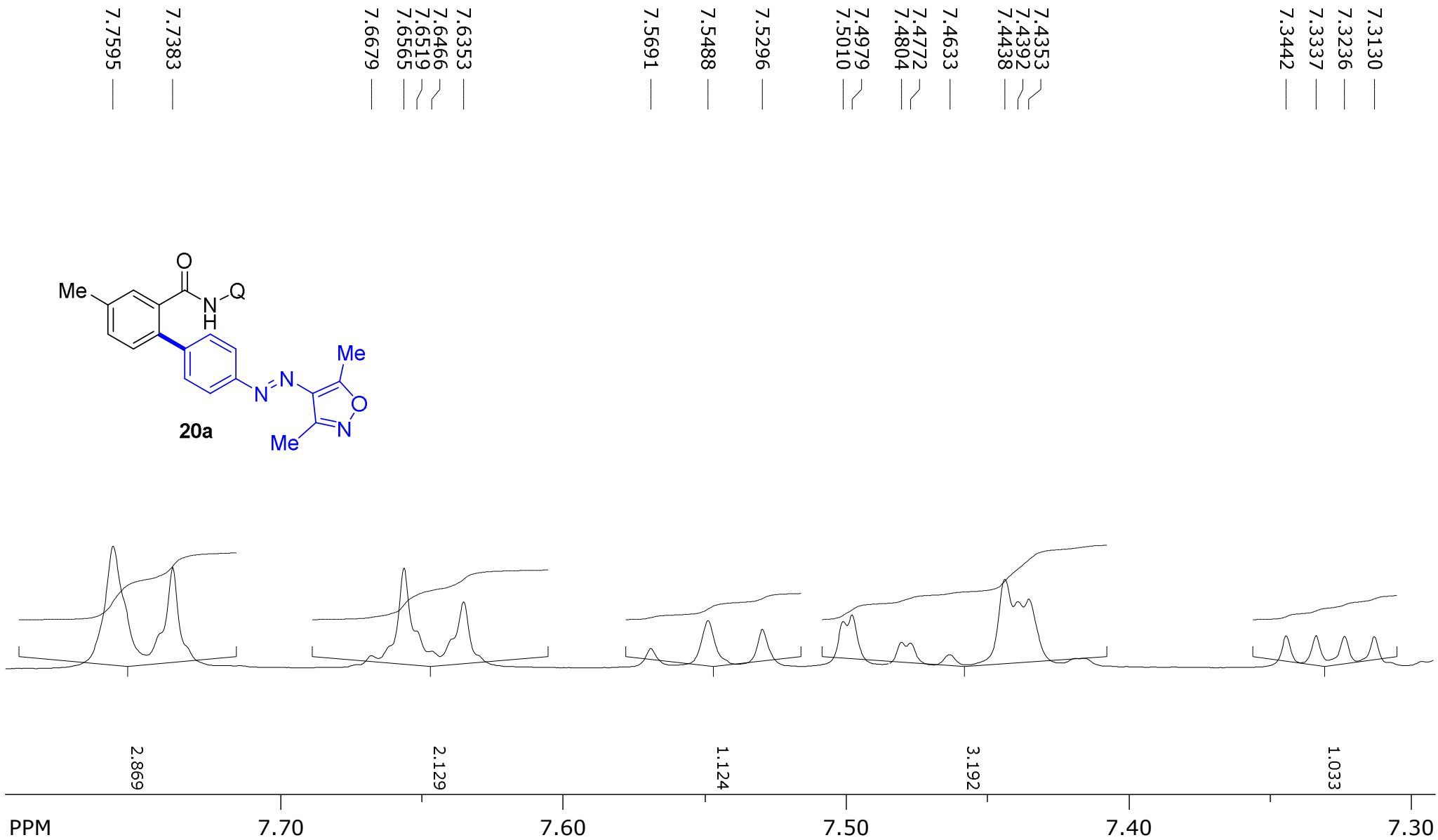
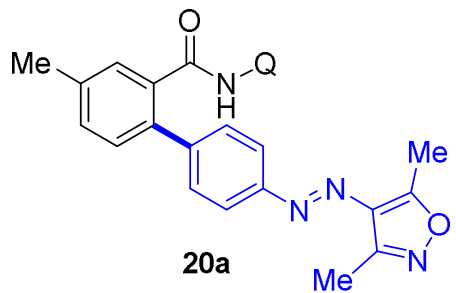
SpinWorks 4: SS 64 PSPLIT
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 1



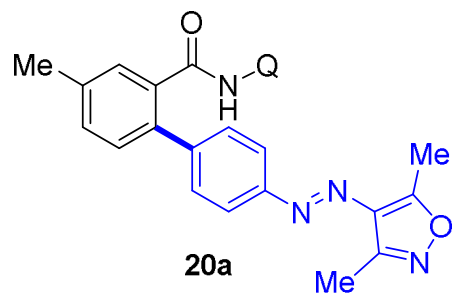
SpinWorks 4: SS 64 PSPLIT
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 1



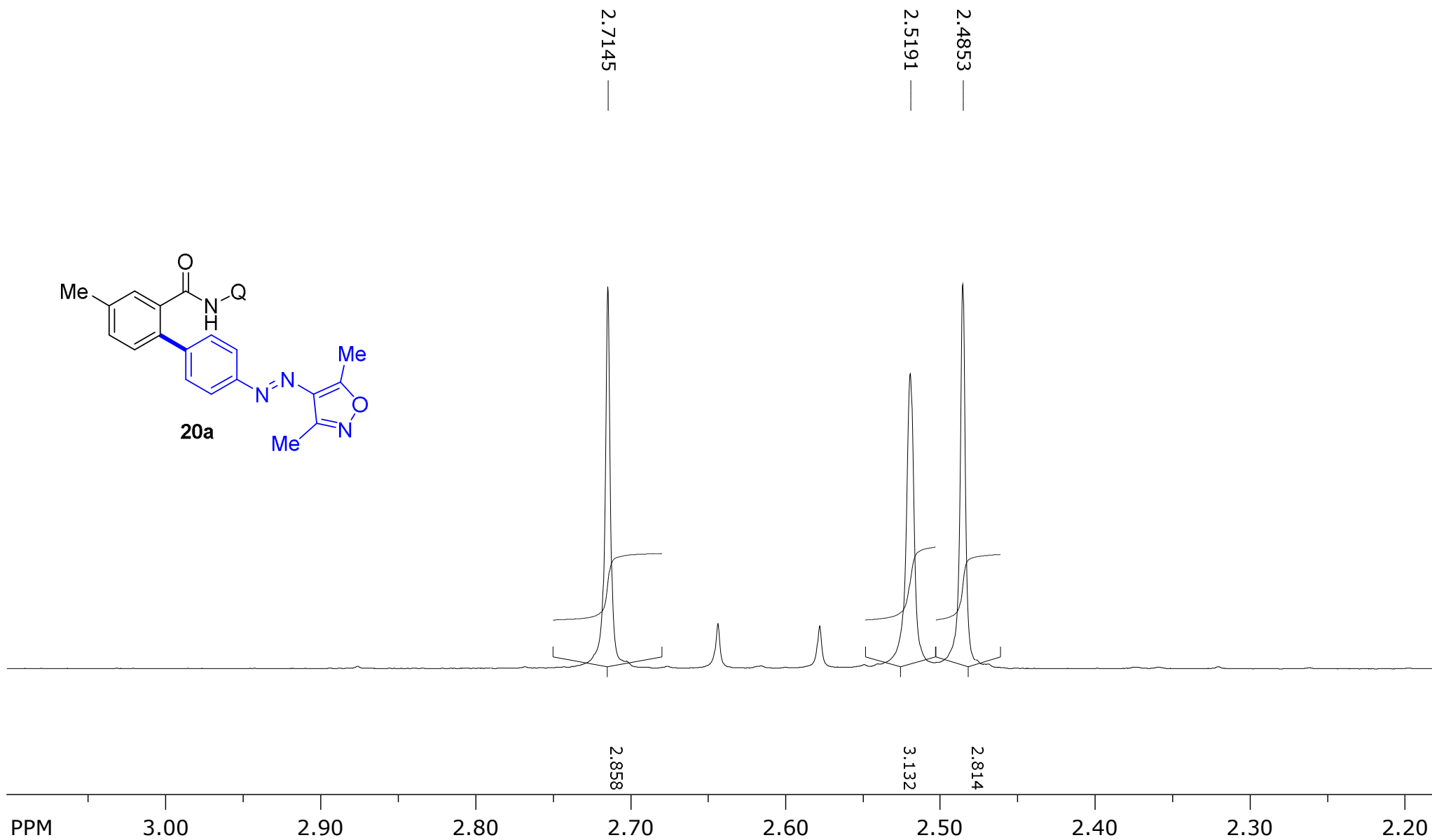
SpinWorks 4: SS 64 PSPLIT
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 1



SpinWorks 4: SS 64 PSPLIT
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 1



20a

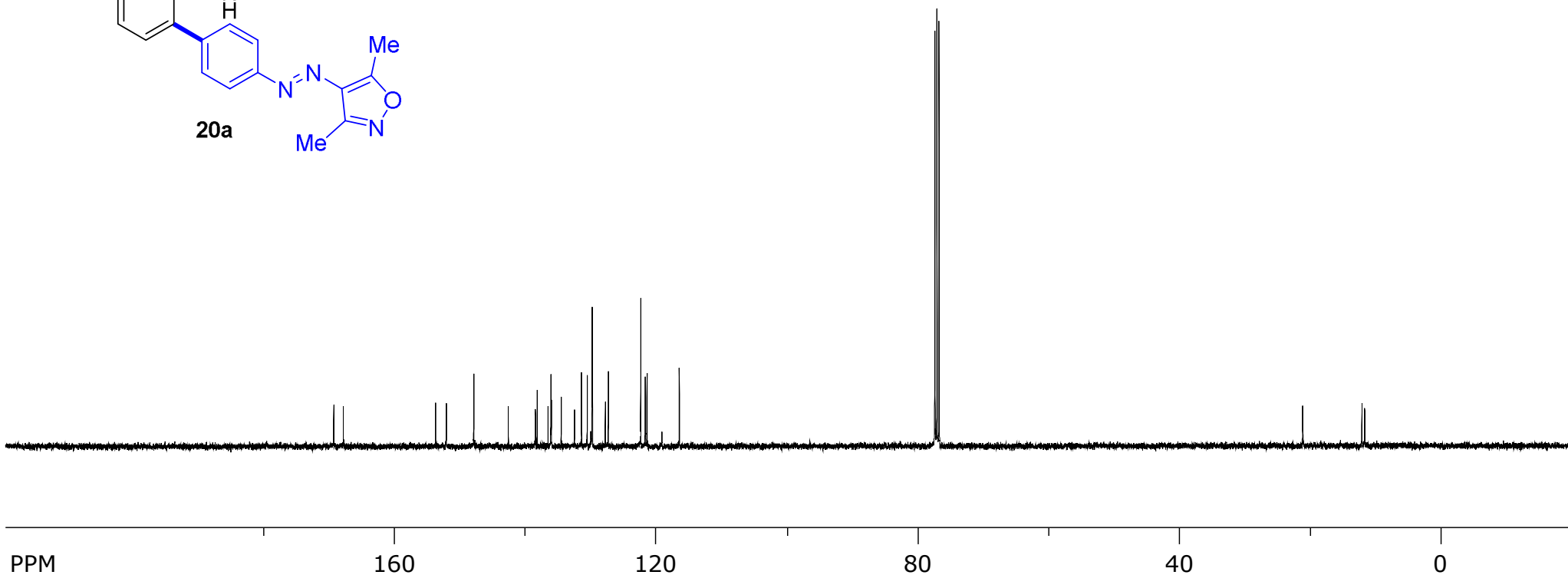
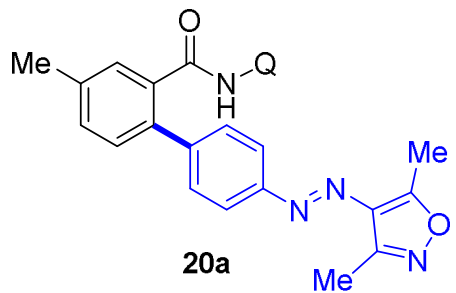


SpinWorks 4: SS 64 P TRANS 3
C13CPD CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 1

116.450
121.400
121.663
122.355
127.311
127.775
129.744
129.797
131.230
131.230
134.517
136.017
136.076
136.533
138.192
138.445
142.589
147.869
152.074
153.700
167.829
169.289

76.742
77.061
77.378

21.151
11.666
12.102



PPM

160

120

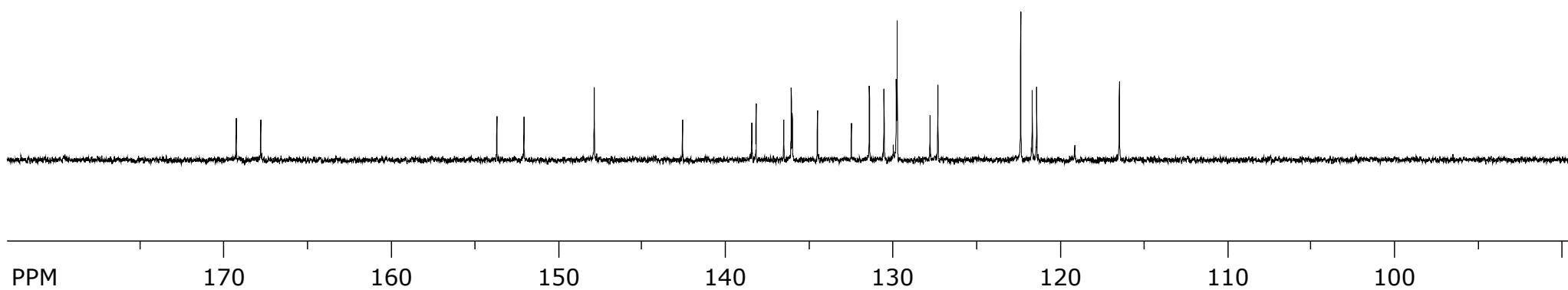
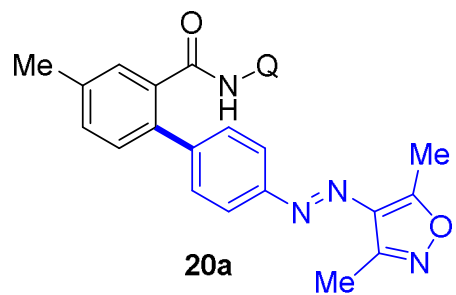
80

40

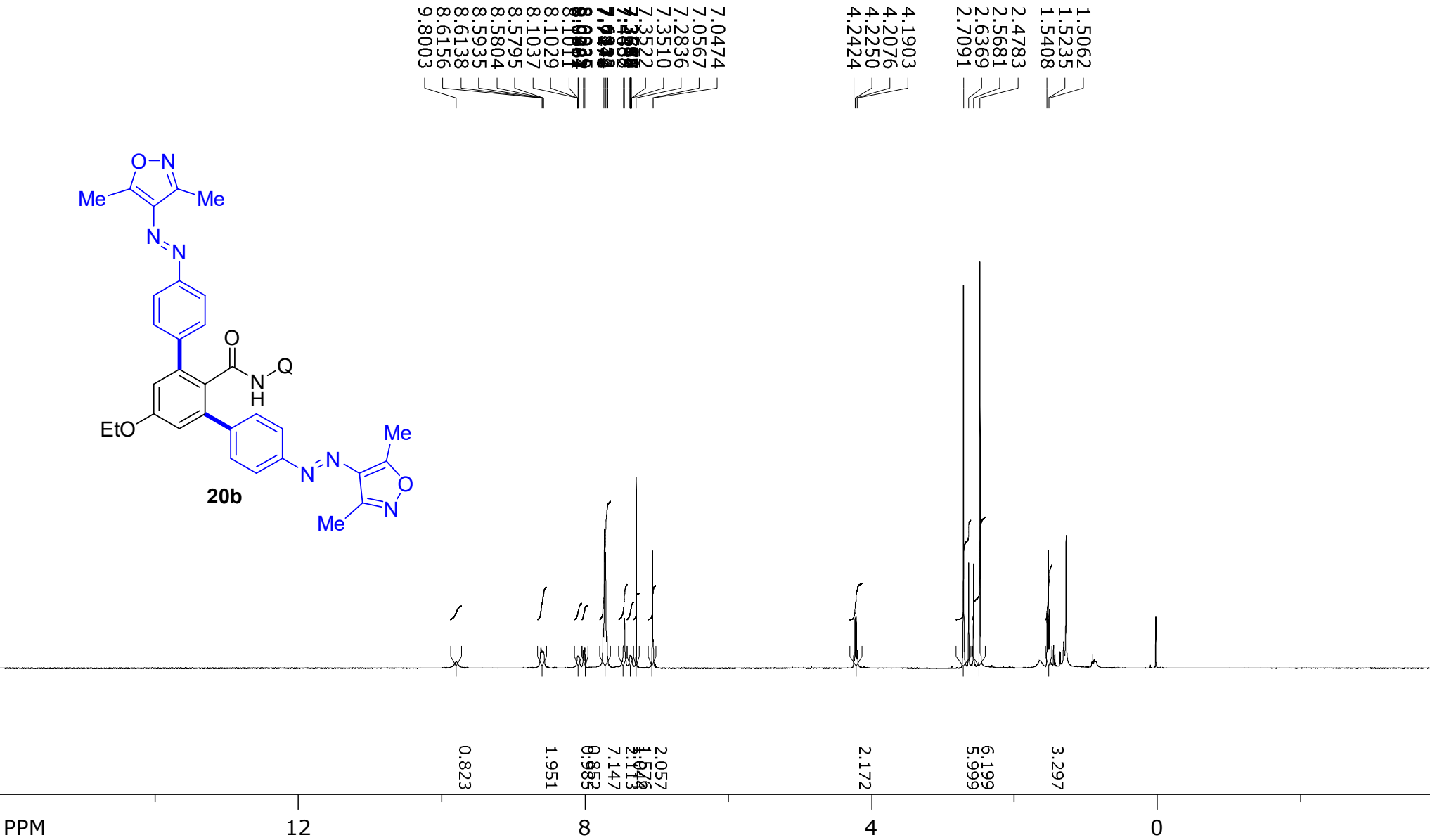
0

SpinWorks 4: SS 64 P TRANS 3
C13CPD CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 1

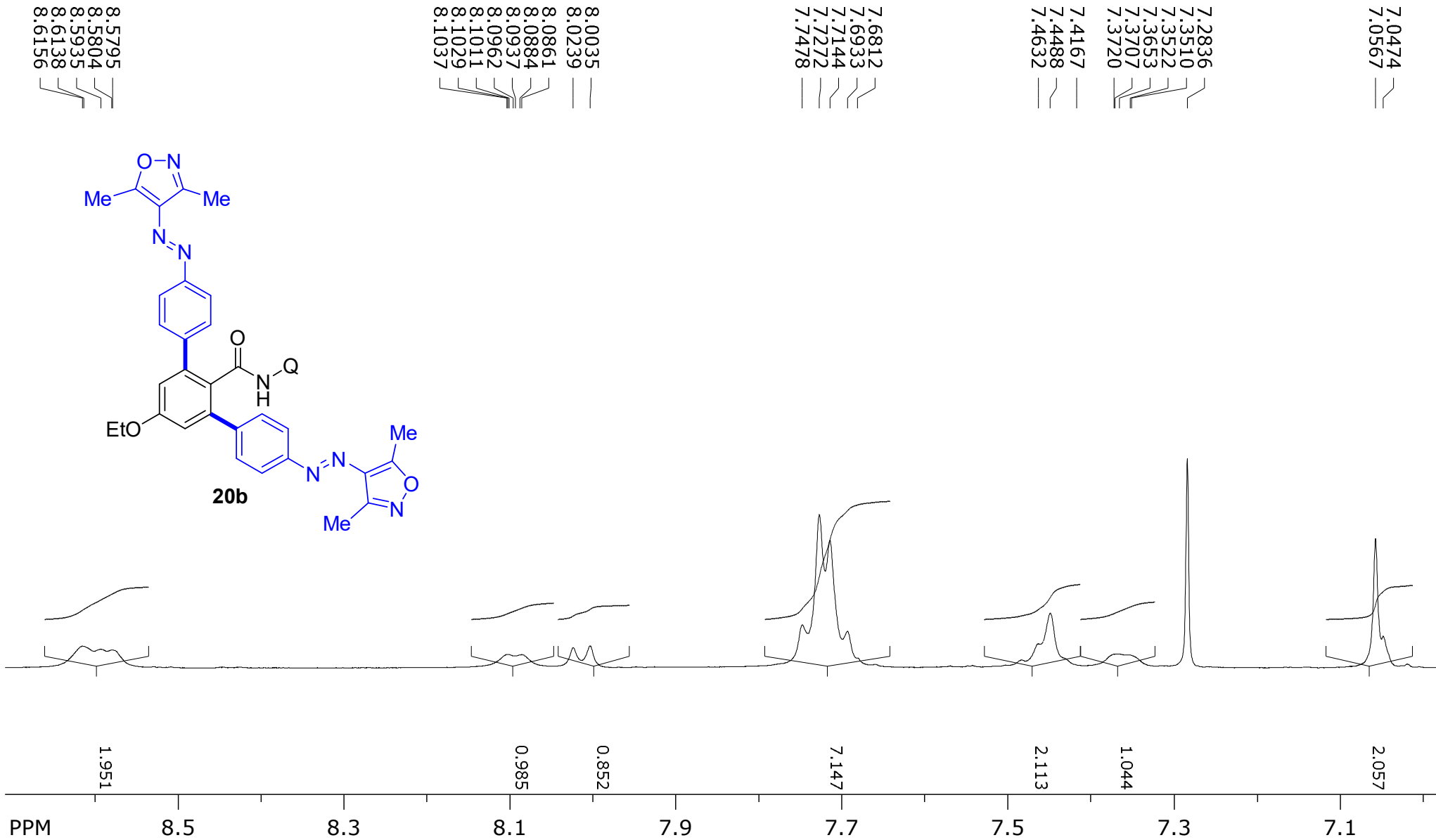
167,829 —
169,289 —
152,074 —
153,700 —
147,869 —
142,589 —
138,445 —
136,533 —
136,076 —
136,017 —
134,517 —
132,490 —
131,410 —
130,534 —
129,797 —
129,744 —
127,775 —
127,311 —
122,355 —
121,663 —
121,400 —
116,450 —



SpinWorks 4: SS-749-REP
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 31



SpinWorks 4: SS-749-REP
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 31

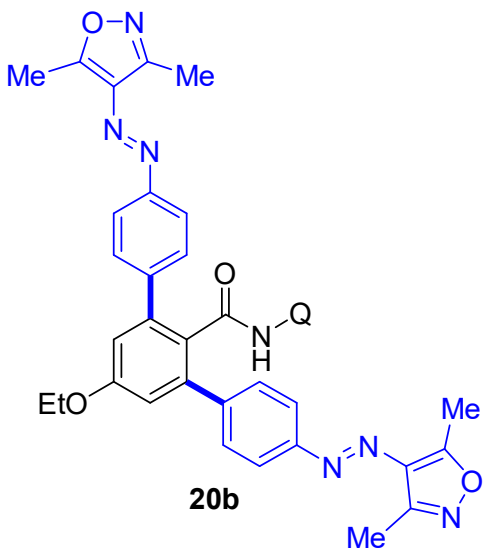


SpinWorks 4: SS-749-REP
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 31

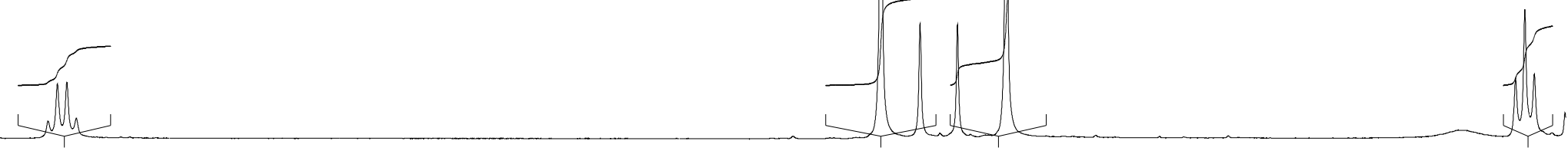
4.1903
4.2076
4.2250
4.2424

2.4783
2.5681
2.6369
2.7091

1.5062
1.5235
1.5408



20b



2.172

5.999

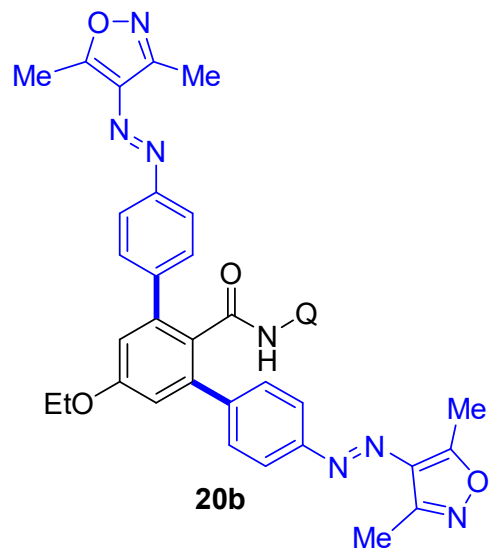
6.199

3.297

PPM 4.0 3.6 3.2 2.8 2.4 2.0 1.6

SpinWorks 4: SS-749
C13CPD CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 22

115.575
118.930
121.300
121.741
121.803
122.202
127.525
127.895
128.889
129.430
129.682
132.479
141.669
142.904
144.141
147.862
152.003
153.686
159.184
167.365
169.361



76.733
77.051
77.368
63.943
11.672
12.086
14.837

PPM

160

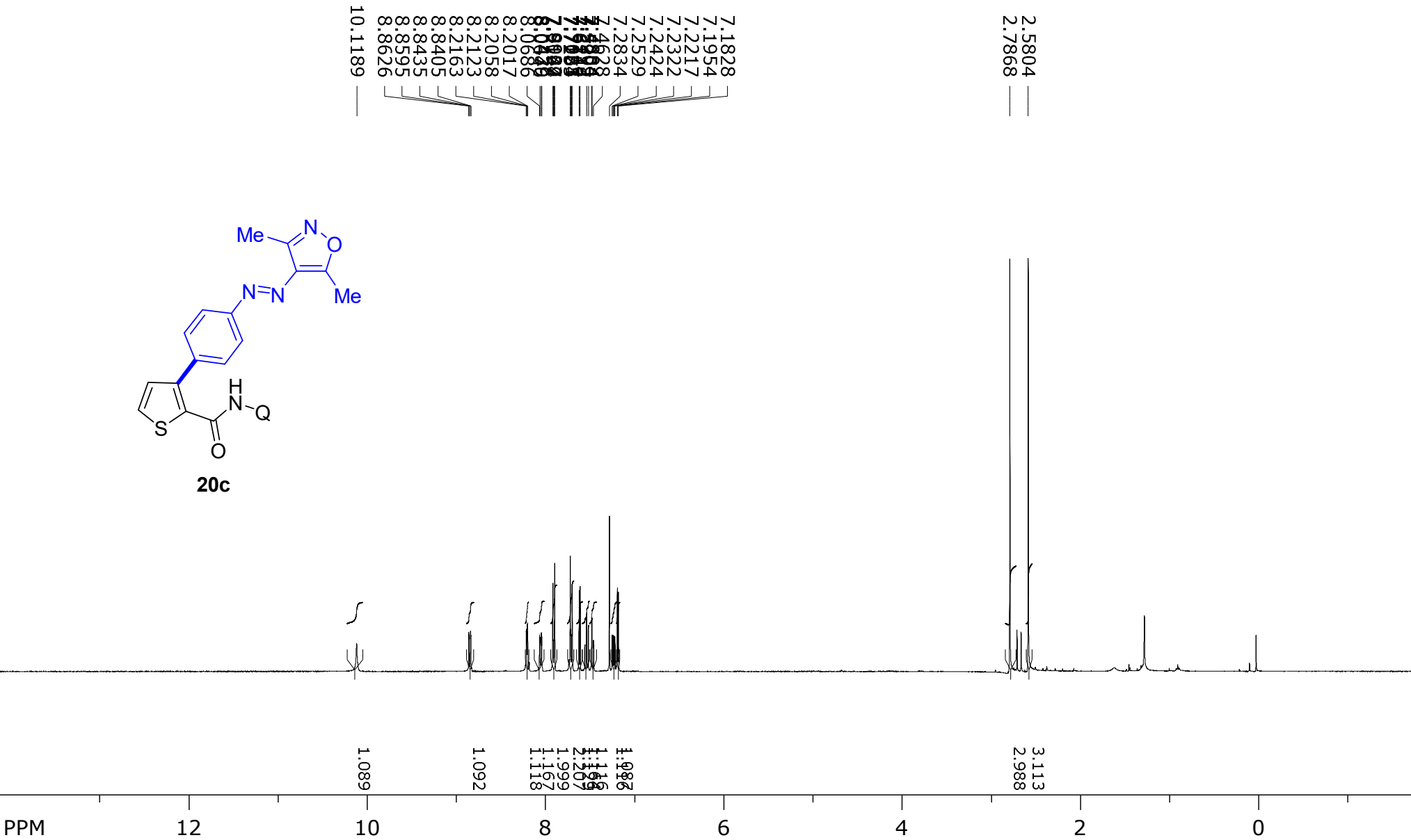
120

80

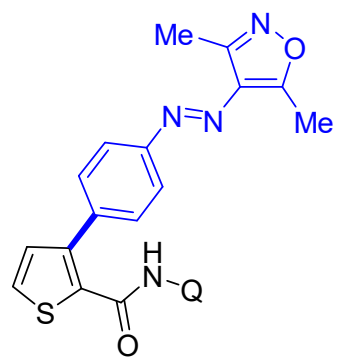
40

0

SpinWorks 4: SS 747
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 60



SpinWorks 4: SS 747
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 60



20c

10.1189

8.8405
8.8435
8.8595
8.8626

8.0439
8.0479
8.0646
8.0686
8.2017
8.2058
8.2123
8.2163

1.089

1.092

1.118

1.167

PPM

10.0

9.6

9.2

8.8

8.4

8.0

SpinWorks 4: SS 747
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 60

7.8982
7.9027
7.9149
7.9194

7.7021
7.7065
7.7184
7.7233

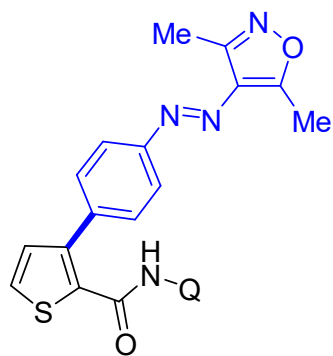
7.6114
7.6240

7.5605
7.5399

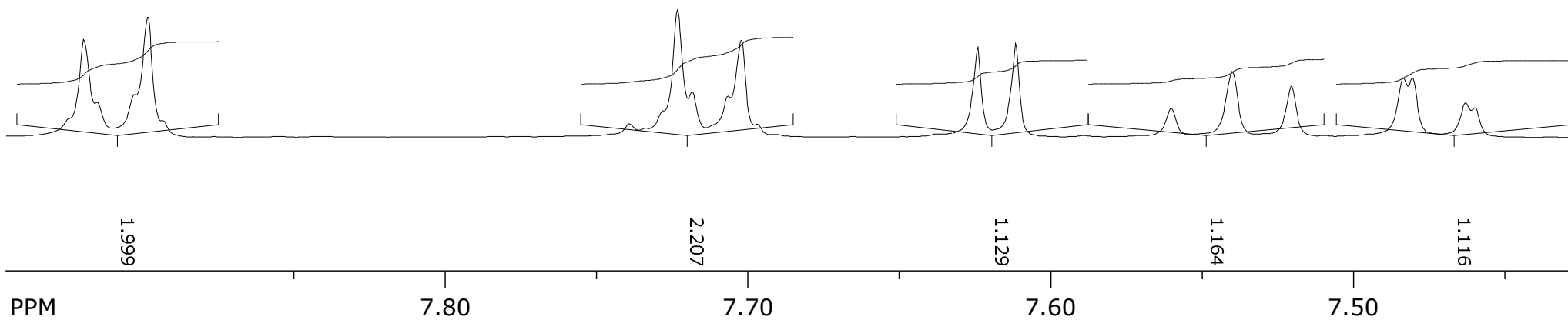
7.5203

7.4804
7.4834

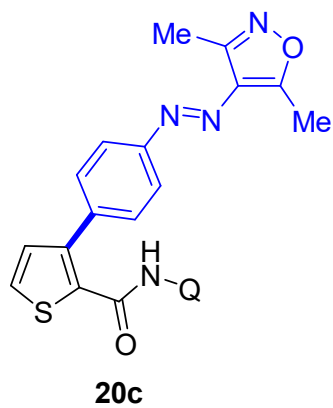
7.4594
7.4628



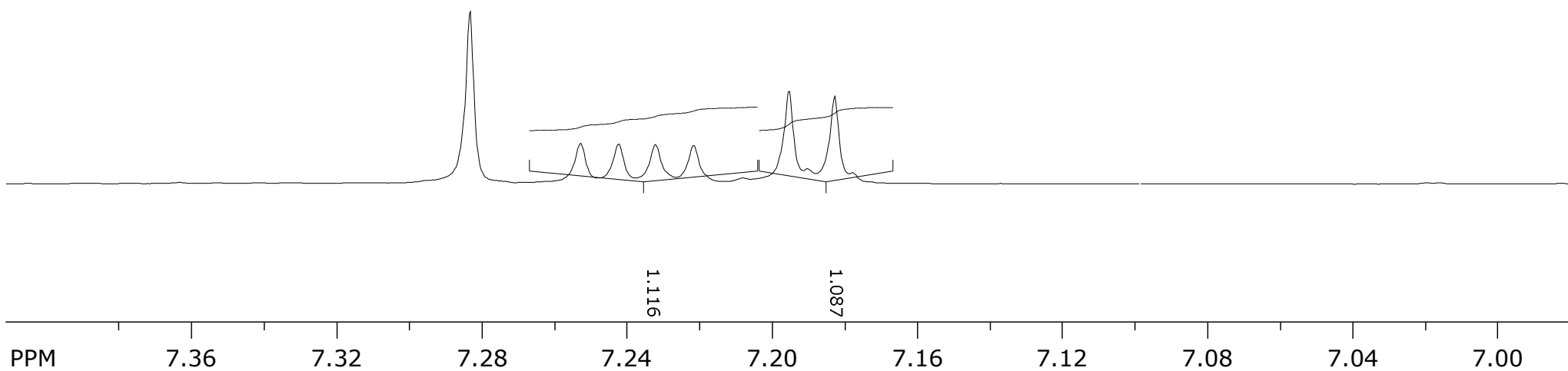
20c



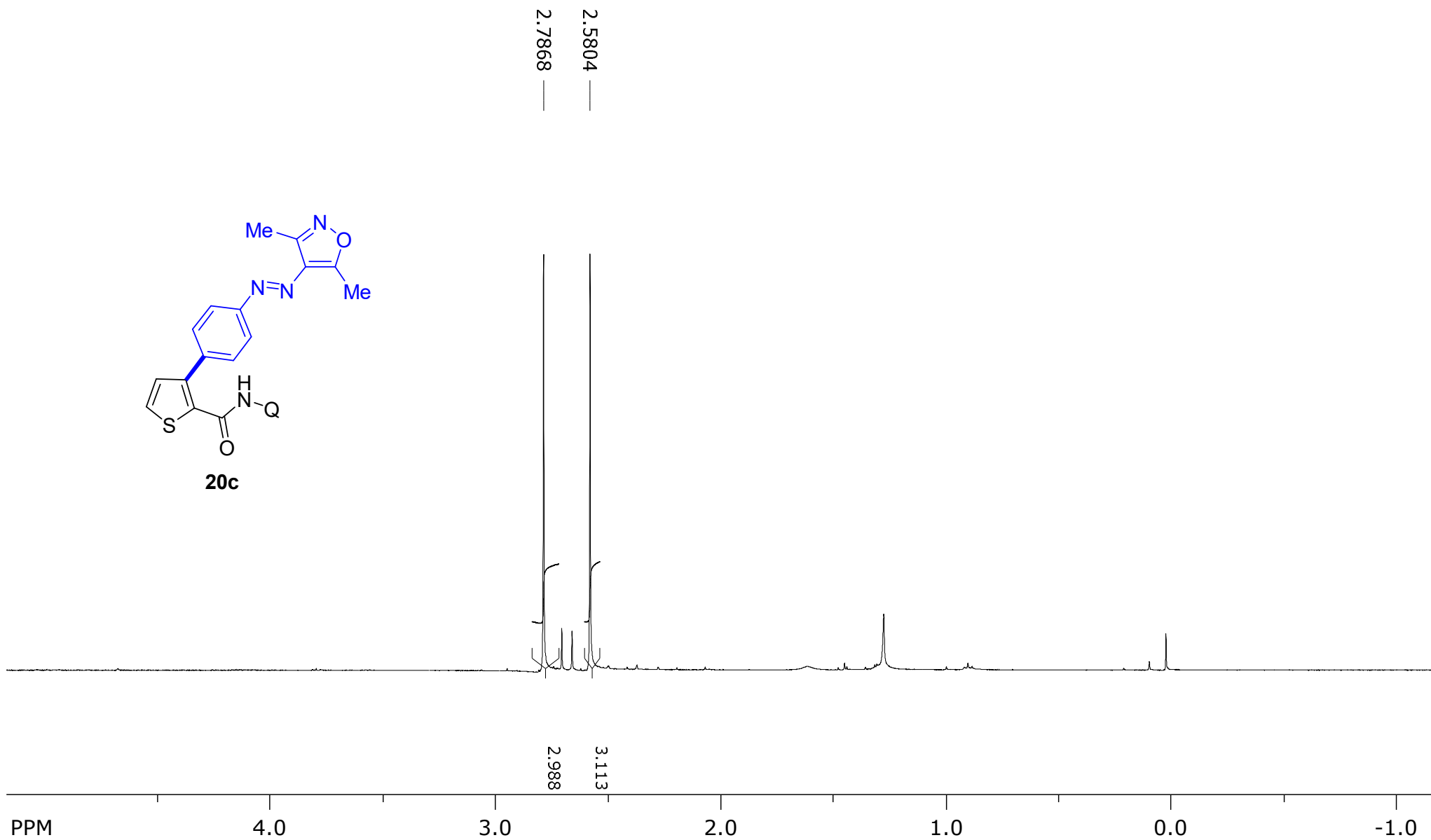
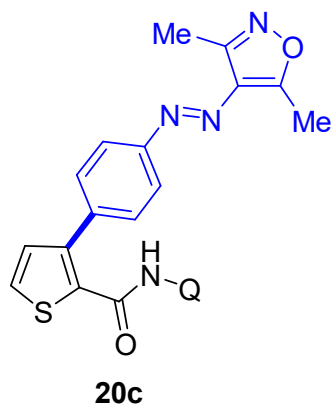
SpinWorks 4: SS 747
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 60



7.2834 —
7.2529 —
7.2424 —
7.2322 —
7.2217 —
7.1954 —
7.1828 —



SpinWorks 4: SS 747
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 60



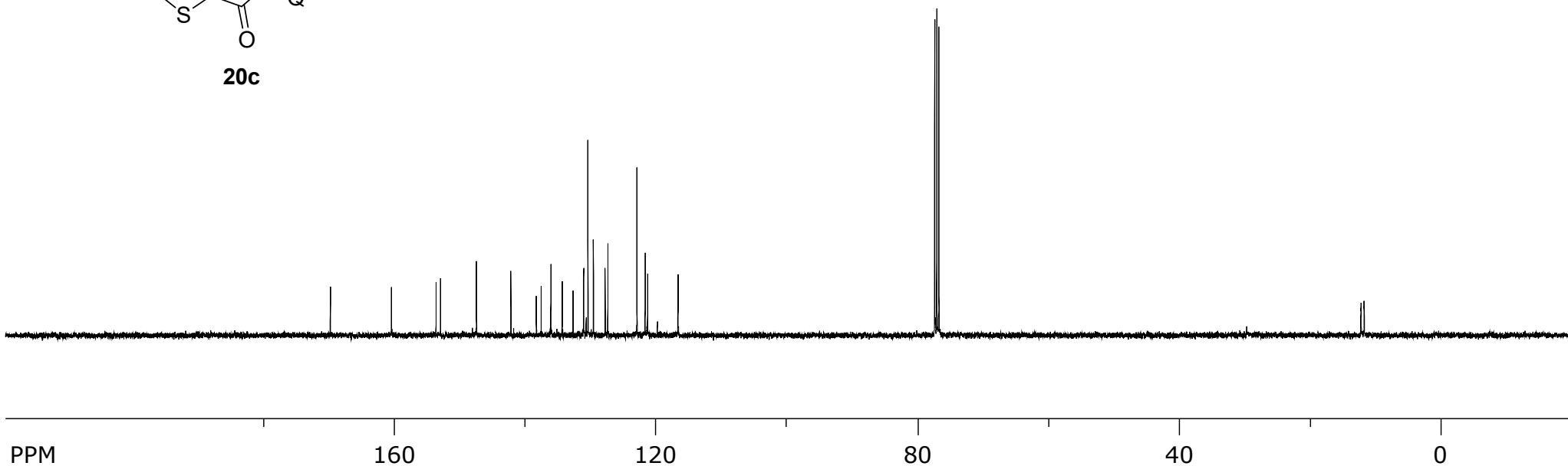
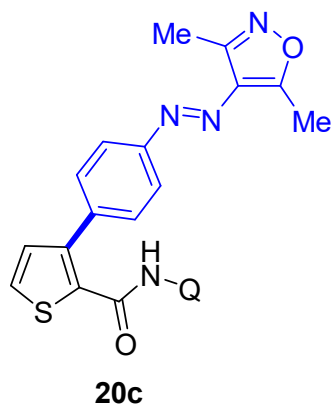
SpinWorks 4: SS 747

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 30

116.642
121.297
121.679
122.928
127.381
127.783
129.584
130.415
131.079
132.697
134.361
136.086
137.564
138.302
142.190
147.468
152.969
153.651
160.460
169.803

76.770
77.087
77.405

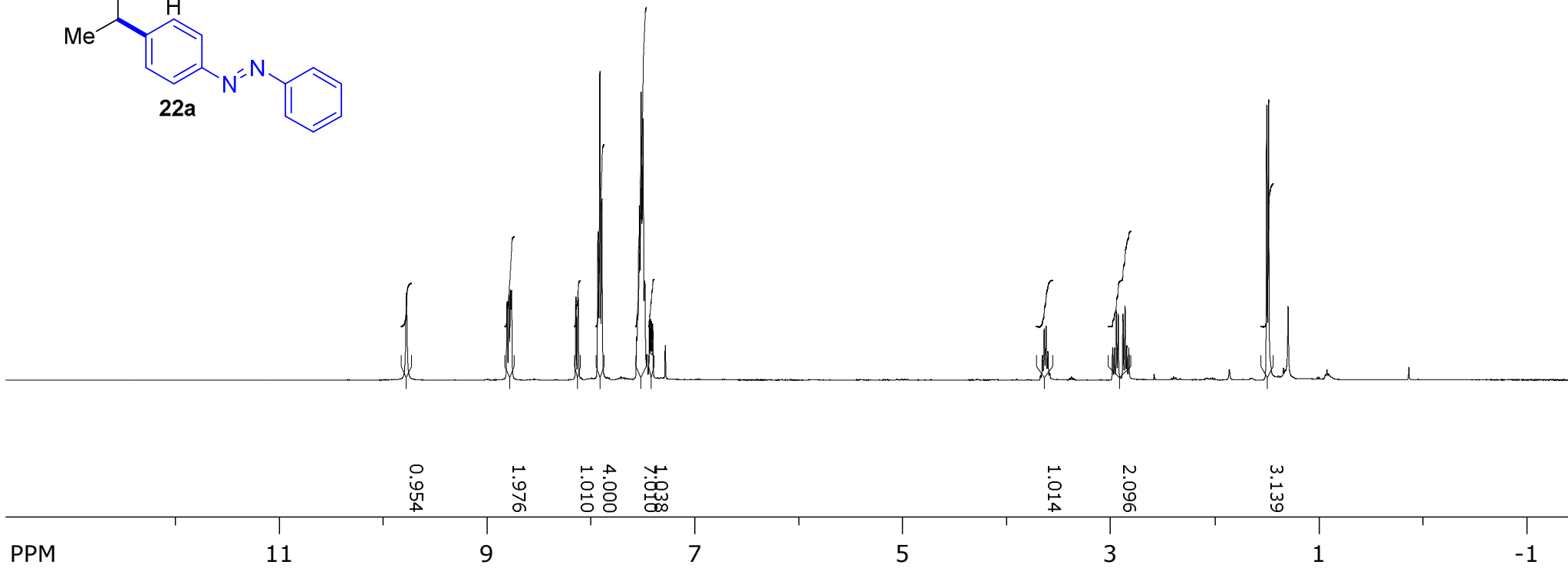
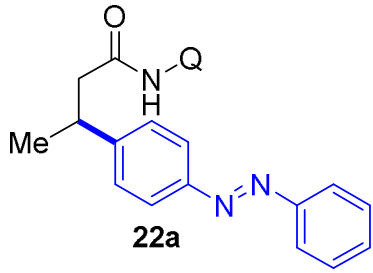
11.741
12.223



SpinWorks 4: SS 296 P
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 51

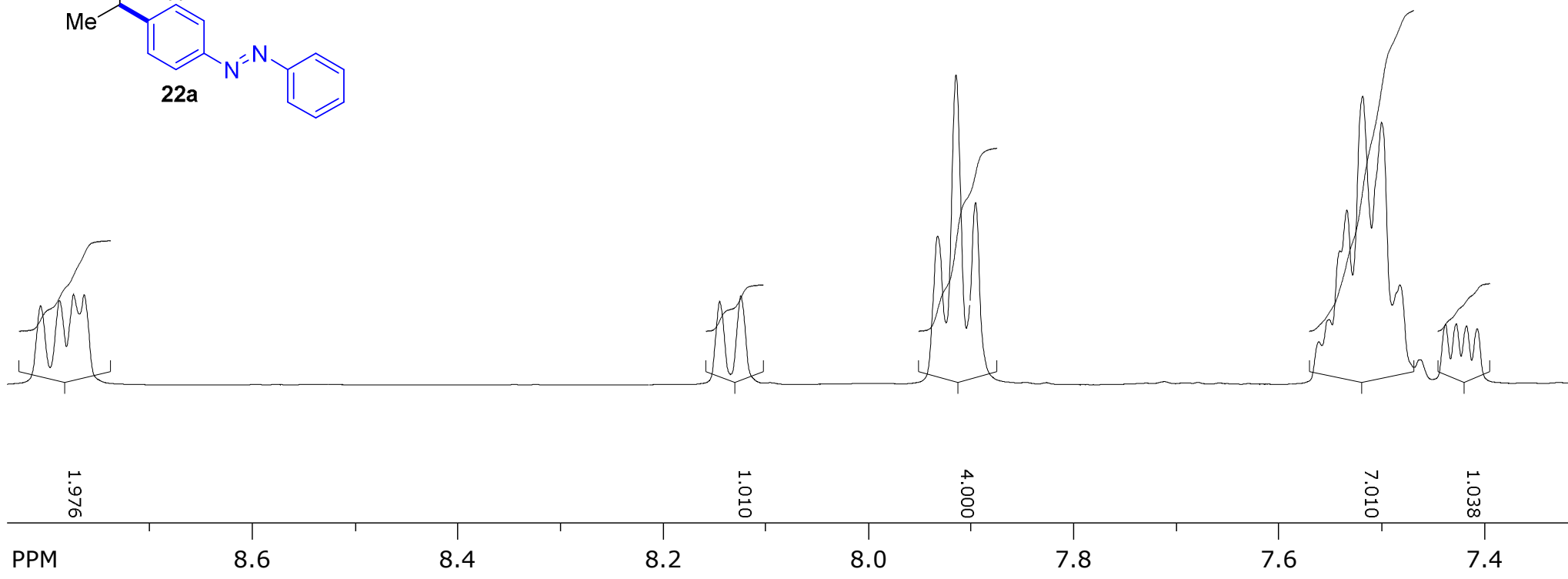
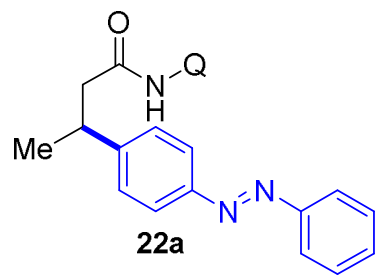
7.4063
7.4168
7.4208
7.4208
7.4208
7.5508
7.5616
7.8954
7.9145
7.9325
8.1244
8.1450
8.7646
8.7749
8.7886
8.8071
9.7758

1.4804
1.4977
2.0335
2.0618
2.0719
2.0748
2.0748
2.0748
3.6569
3.6945
3.6945
3.6945



SpinWorks 4: SS 296 P
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 51

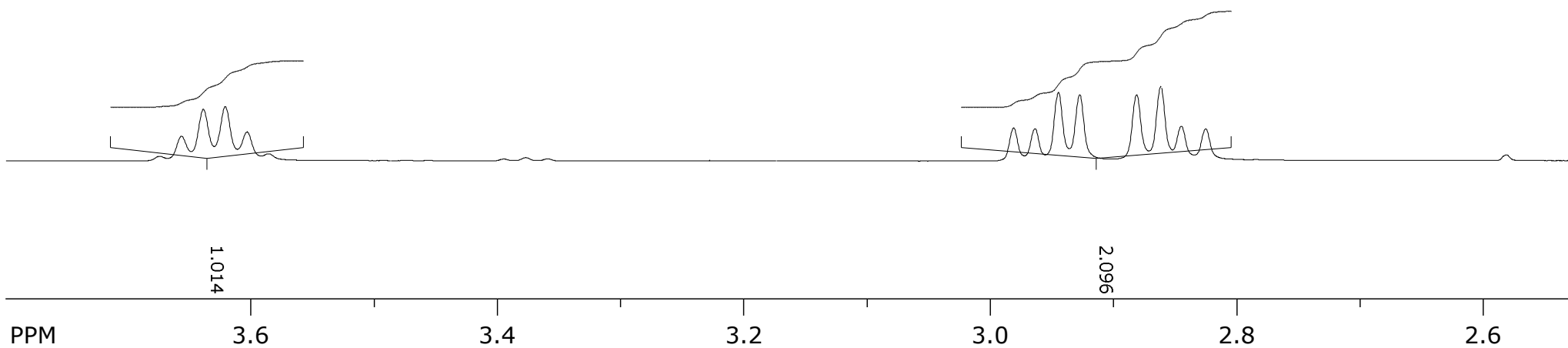
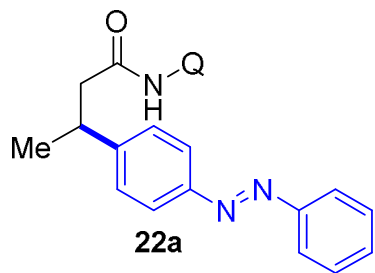
8.7646
8.7749
8.7886
8.8071
8.1244
8.1450
7.8954
7.9145
7.9325
7.4063
7.4168
7.4269
7.4373
7.4818
7.4996
7.5181
7.5334
7.5404
7.5508
7.5616



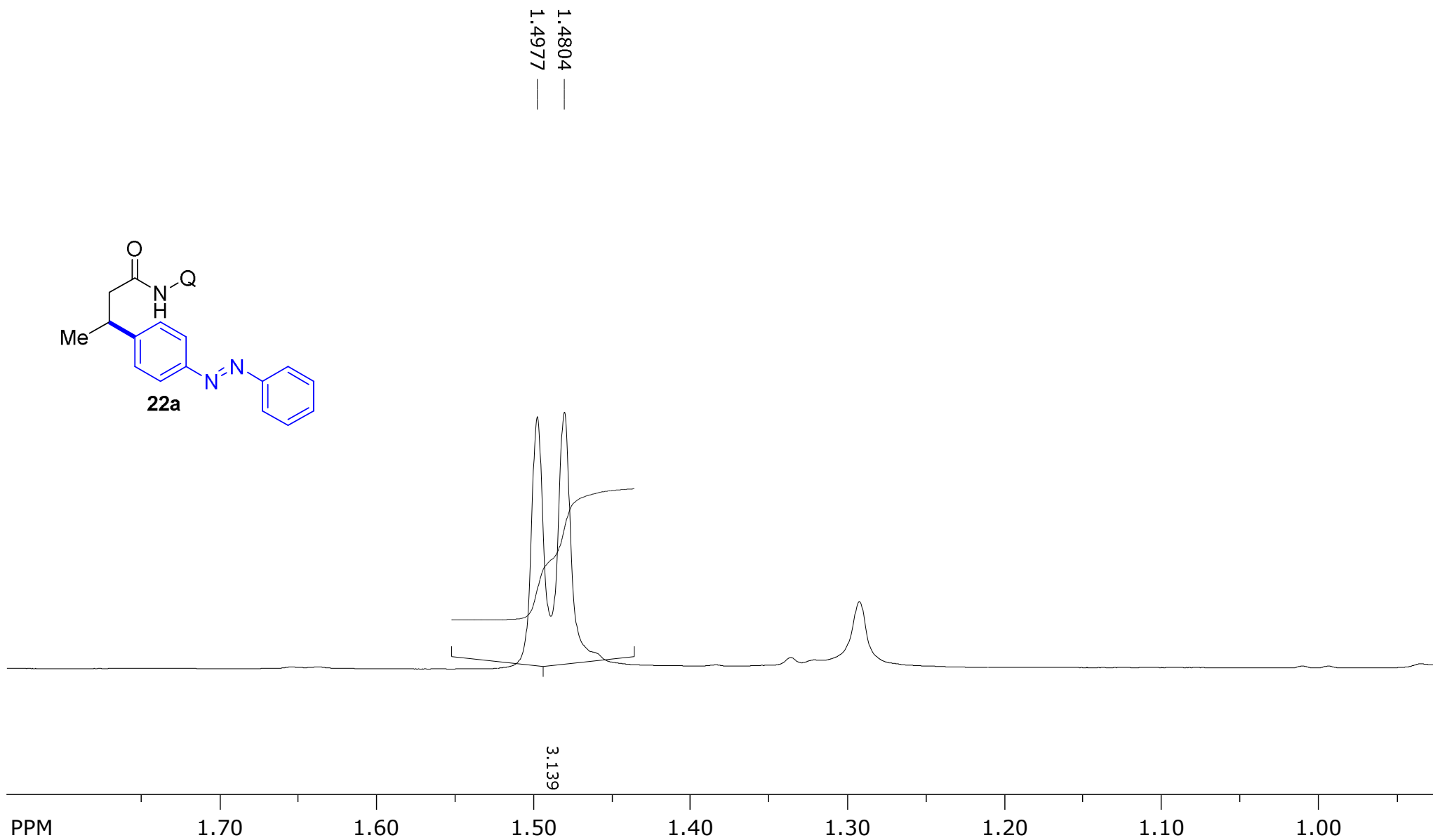
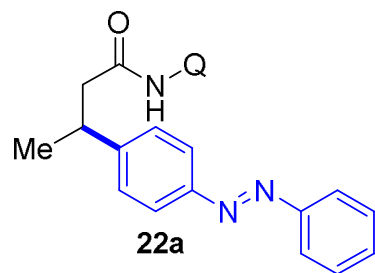
SpinWorks 4: SS 296 P
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 51

3.5845
3.6011
3.6211
3.6389
3.6569
3.6746

2.9270
2.9443
2.9633
2.9835
2.8242
2.8429
2.8612
2.8808

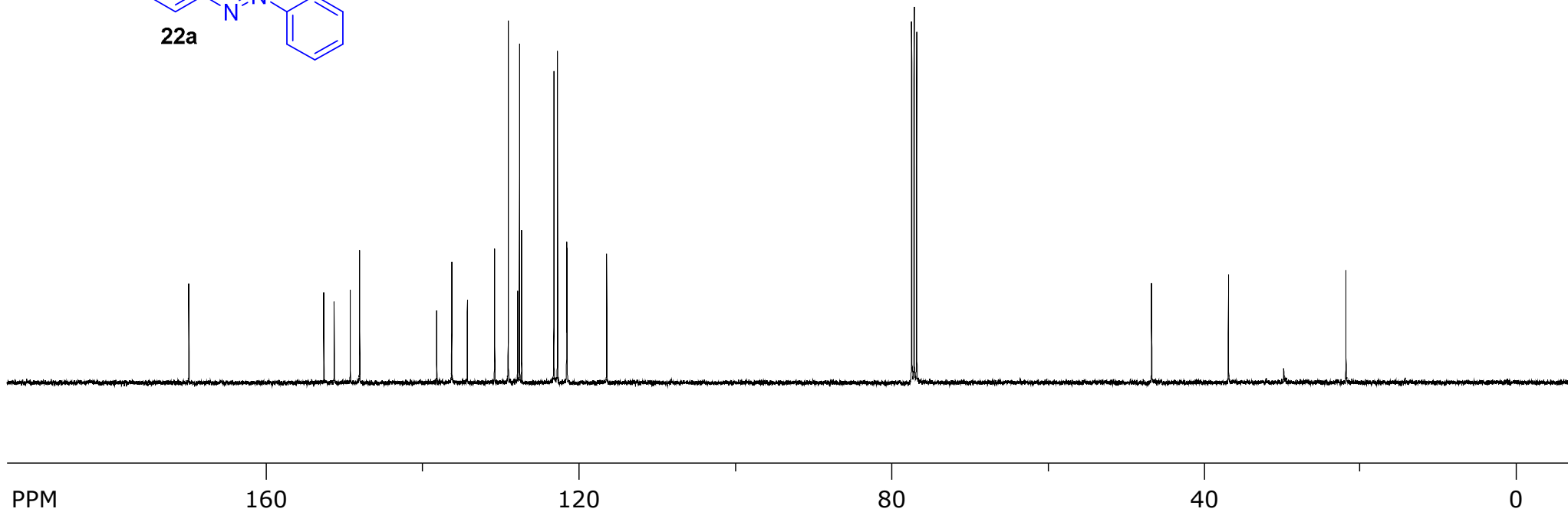
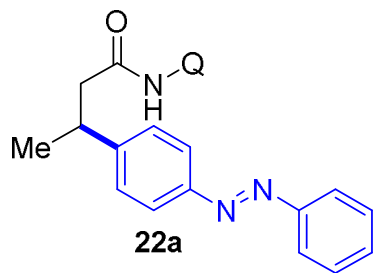


SpinWorks 4: SS 296 P
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 51



SpinWorks 4: SS 296 P
C13CPD CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 51

170.017 —
148.135 —
149.338 —
151.398 —
152.723 —
138.264 —
136.341 —
134.344 —
130.844 —
129.099 —
127.897 —
127.663 —
127.387 —
123.253 —
122.784 —
121.605 —
121.561 —
116.487 —
76.789 —
77.106 —
77.424 —
46.685 —
36.843 —
21.792 —

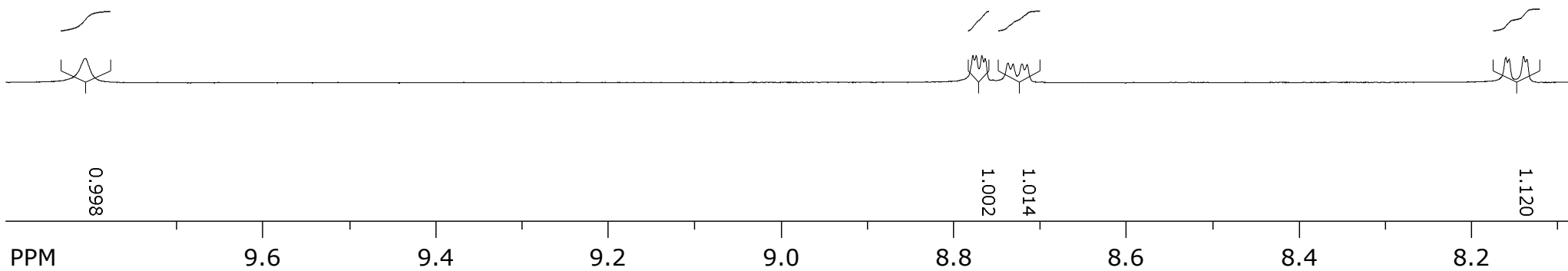
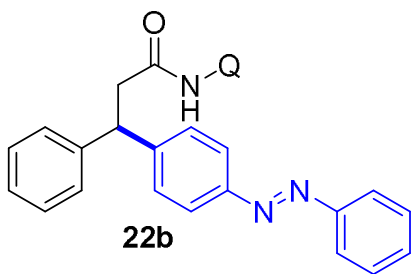


SpinWorks 4: SS 305 P REP
1H

9.8070

8.7148
8.7207
8.7311
8.7371
8.7633
8.7671
8.7738
8.7777

8.1353
8.1392
8.1560
8.1599

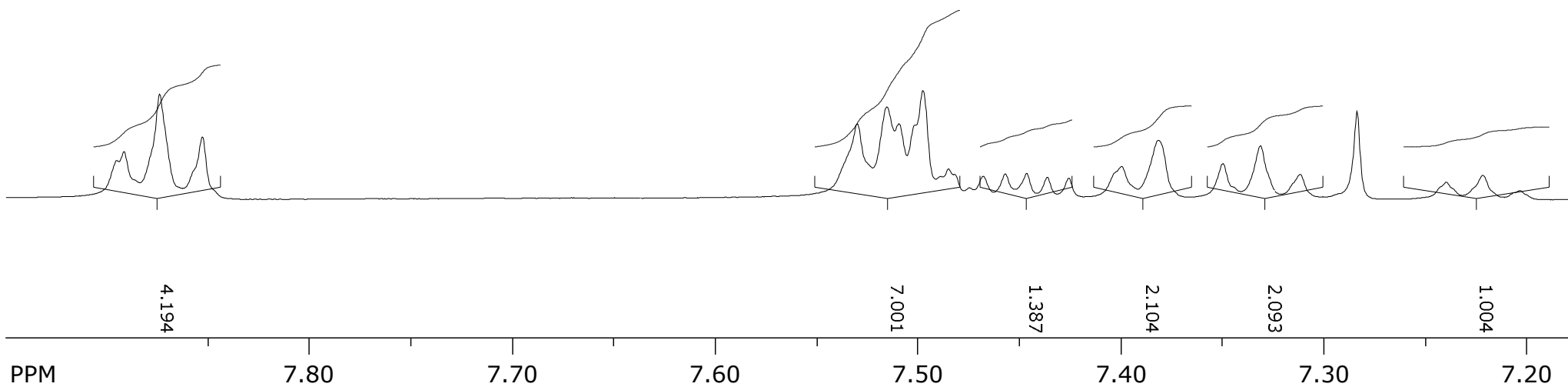
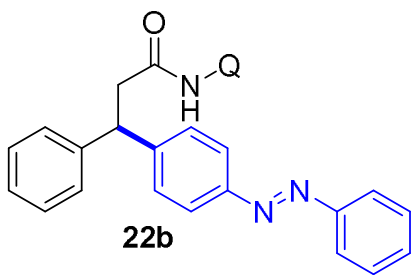


220

SpinWorks 4: SS 305 P REP
1H

7.8529 —
7.8740 —
7.8916 —
7.8952 —

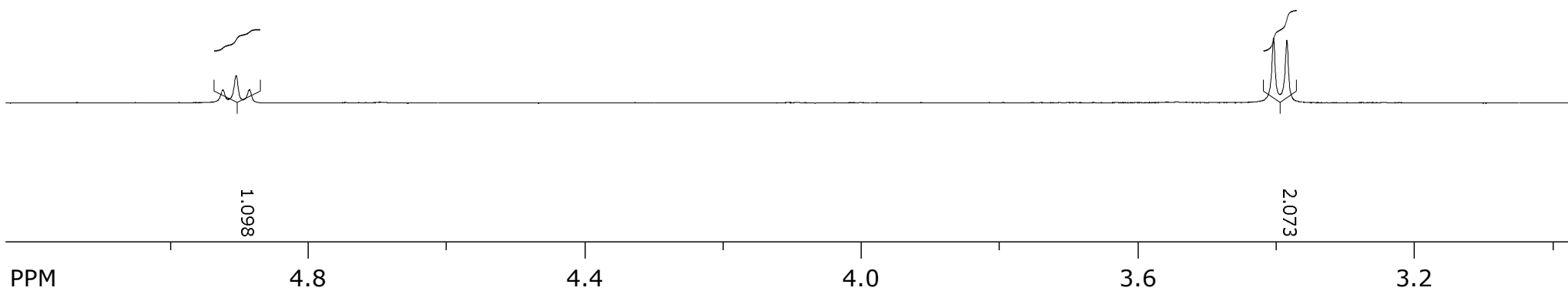
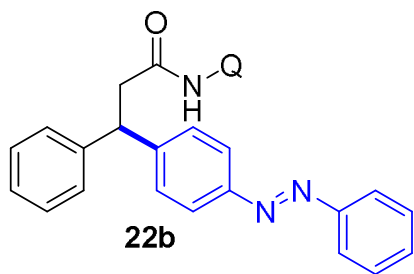
7.2034 —
7.2215 —
7.2395 —
7.2835 —
7.3116 —
7.3311 —
7.3497 —
7.3814 —
7.3996 —
7.4257 —
7.4362 —
7.4464 —
7.4569 —
7.4678 —
7.4820 —
7.4849 —
7.4888 —
7.4976 —
7.5013 —
7.5094 —
7.5154 —
7.5299 —



SpinWorks 4: SS 305 P REP
1H

4.8857
4.9049
4.9241

3.3841
3.4034



SpinWorks 4: SV100706
C13CPD CDCl3 {D:\Spectra} nmr 6

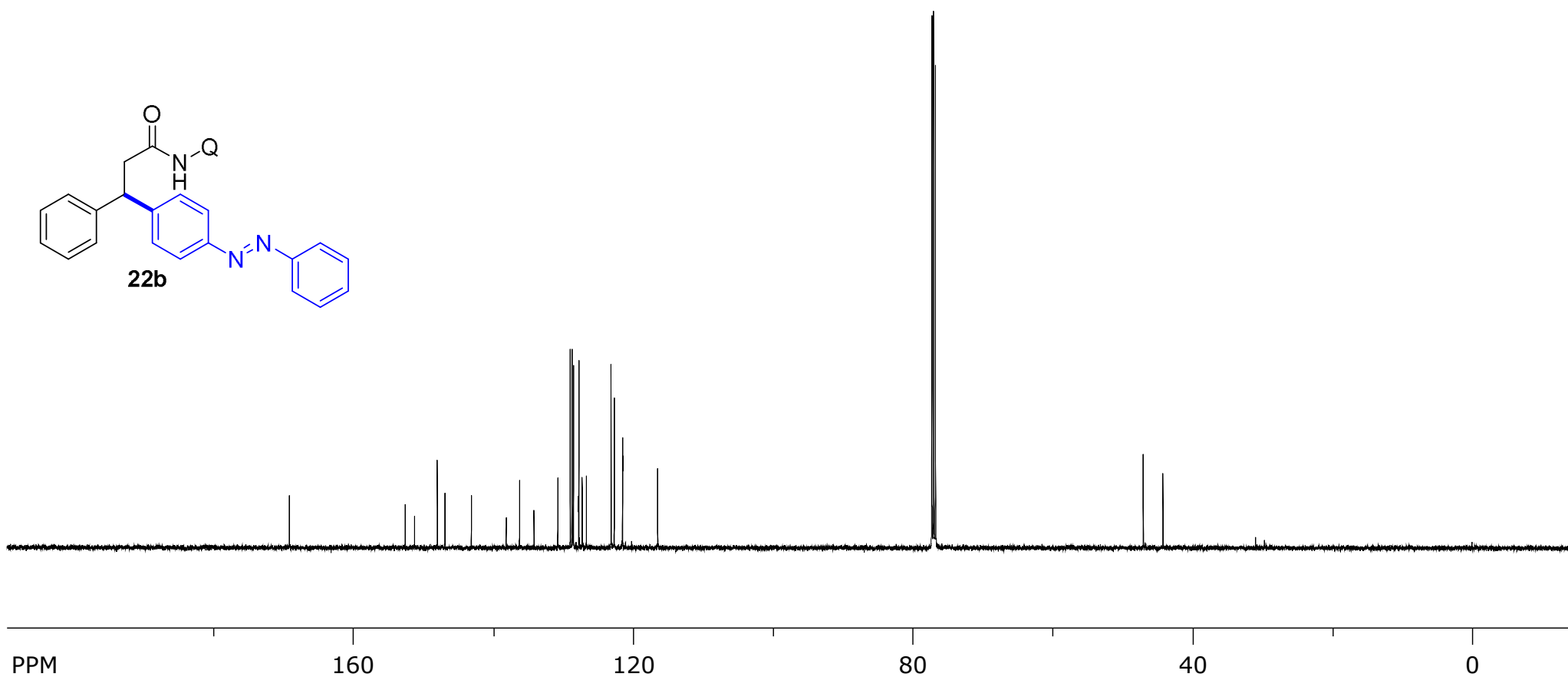
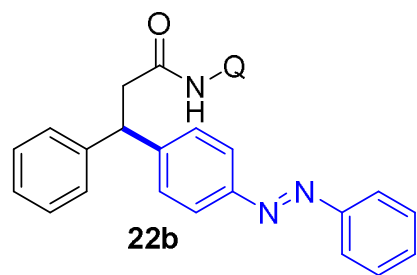
SS-305

169.271

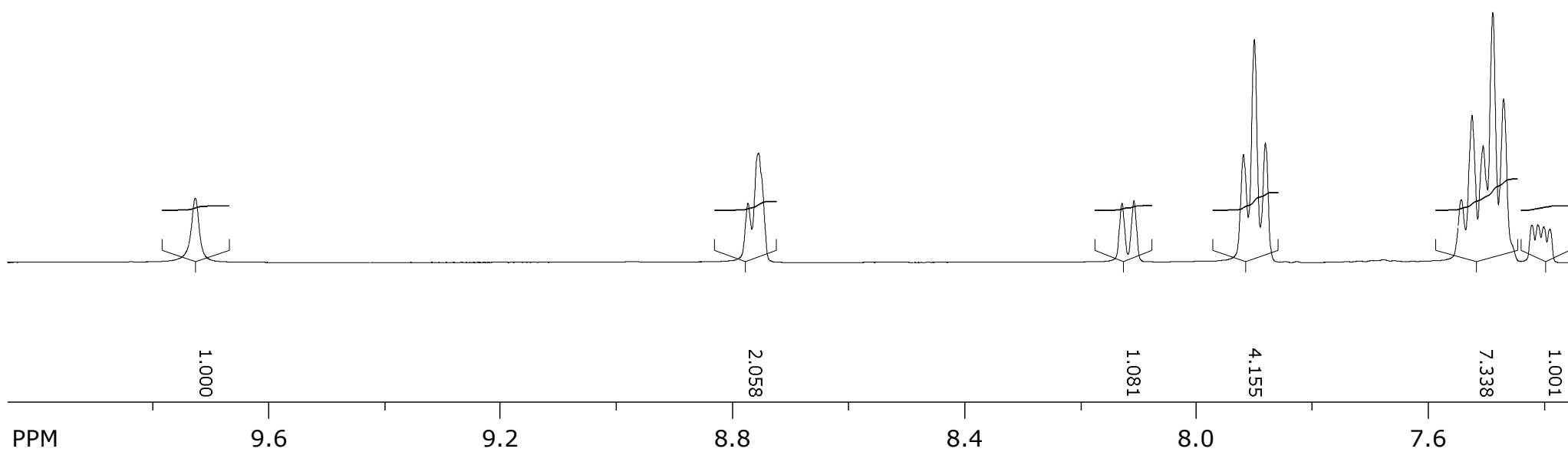
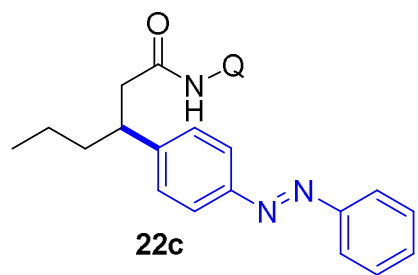
152.709
151.350
148.098
147.002
143.228
138.242
136.328
134.252
130.854
129.065
128.786
128.814
127.842
127.363
126.765
123.223
122.771
121.585
121.571
116.563

77.308
77.055
76.801

47.057
44.245



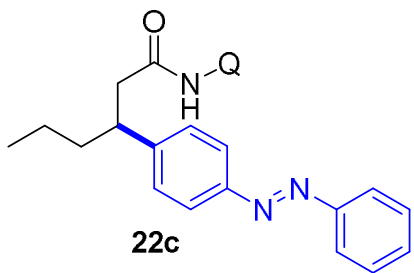
SpinWorks 4: SS 297 P
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 38



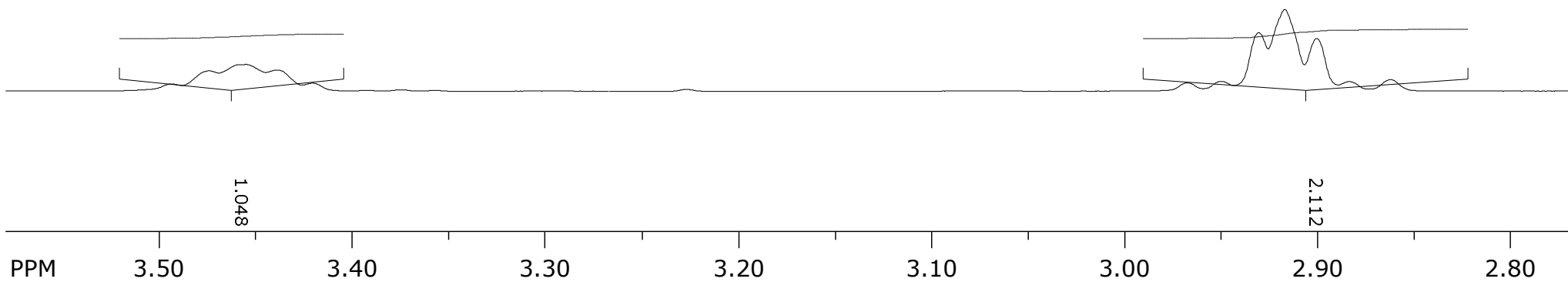
SpinWorks 4: SS 297 P
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 38

3.4211
3.4396
3.4552
3.4588
3.4744

2.8628
2.8836
2.9005
2.9170
2.9305
2.9499
2.9675



22c

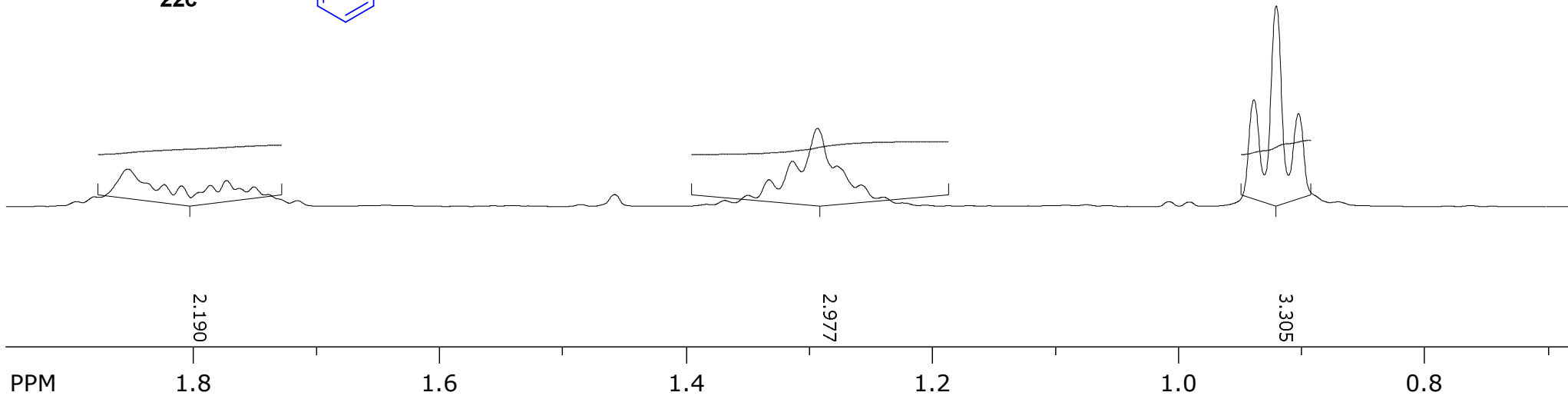
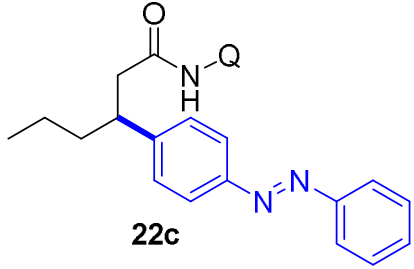


SpinWorks 4: SS 297 P
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 38

1.7400
1.7511
1.7631
1.7734
1.7865
1.7950
1.8099
1.8241
1.8534
1.8812

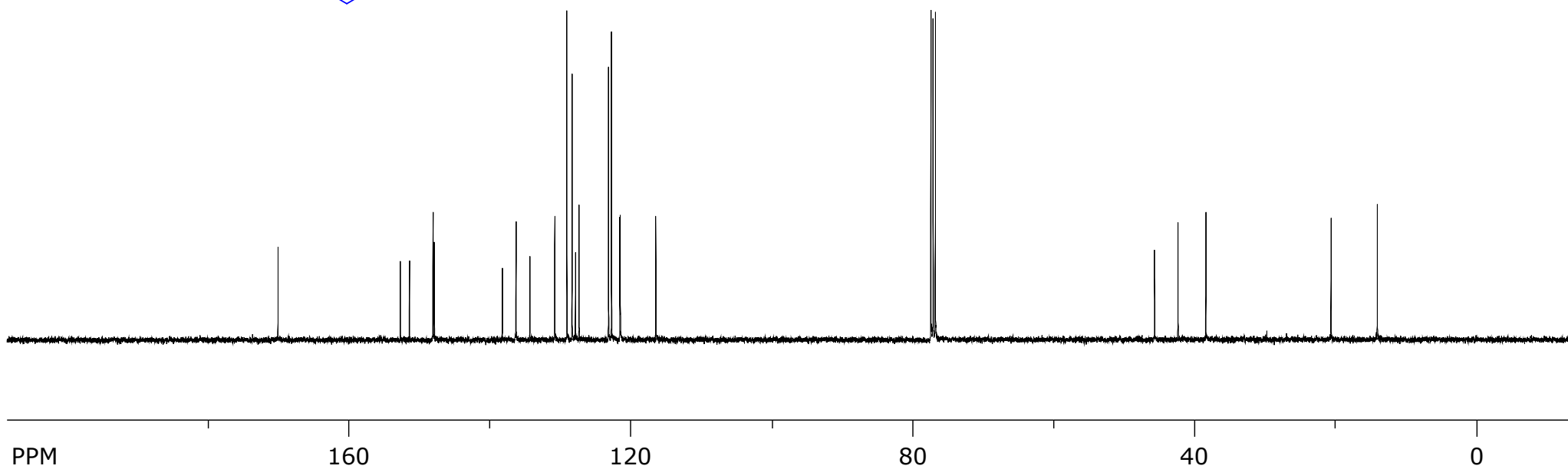
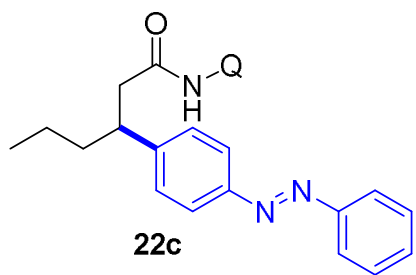
1.2396
1.2579
1.2776
1.2933
1.3136
1.3326
1.3498

0.9024
0.9205
0.9387



SpinWorks 4: SS 297 P
C13CPD CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 38

170.096 —
152.737 —
151.438 —
148.093 —
147.905 —
138.243 —
136.304 —
134.342 —
130.808 —
129.085 —
128.352 —
127.875 —
127.363 —
123.181 —
122.756 —
121.566 —
121.502 —
116.458 —
76.785 —
77.103 —
77.420 —
45.663 —
42.342 —
38.382 —
20.618 —
14.052 —

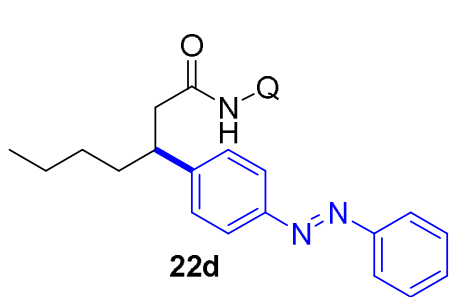


SpinWorks 4: SV030702
1H_8scan CDCl3 {D:\Spectra} nmr 26

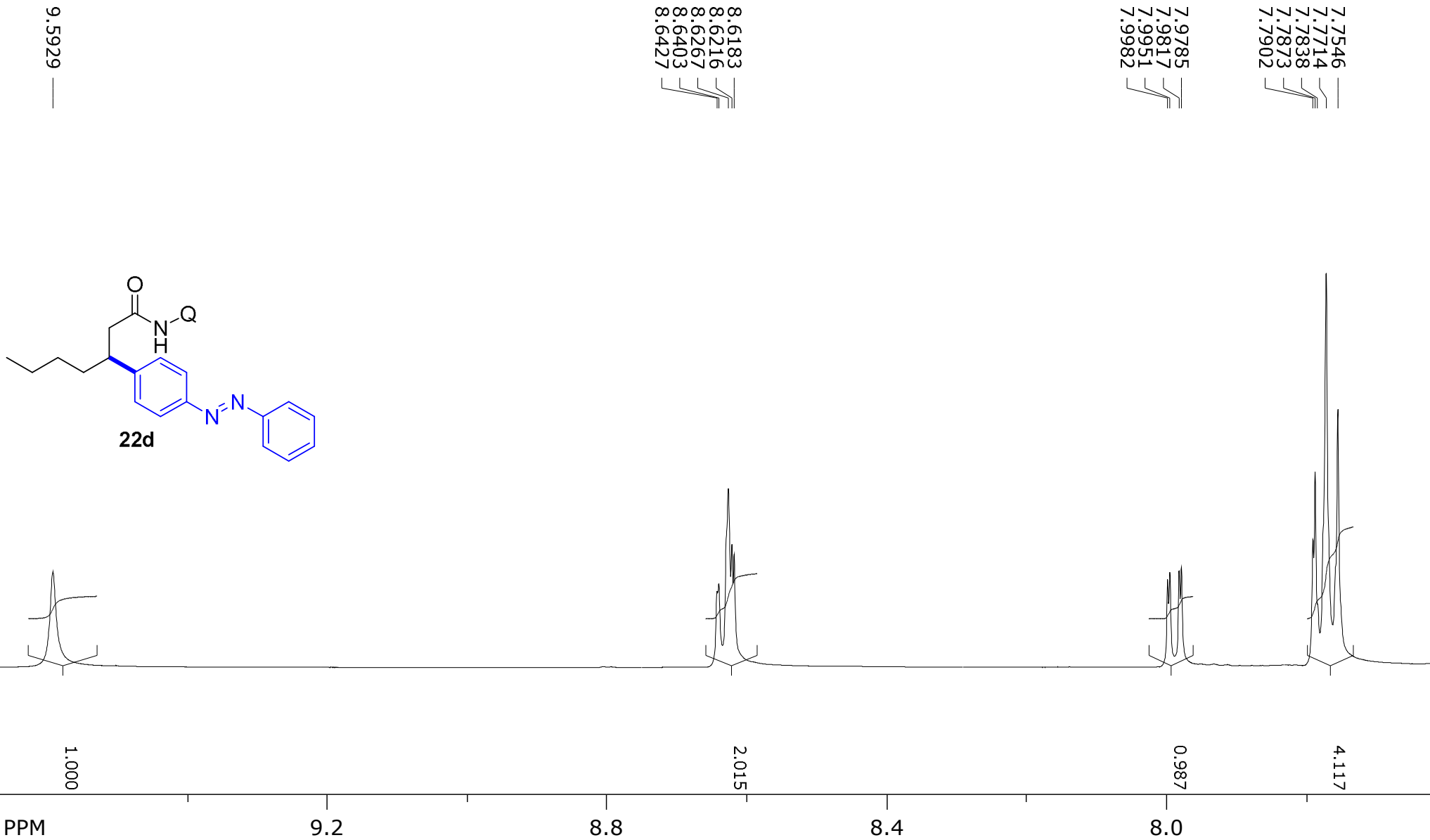
SS-302

7.1554
7.1509
7.1464
7.1419
7.1374
7.7902
7.9785
7.9817
7.9951
7.9982
8.6183
8.6216
8.6267
8.6403
8.6427
9.5929

0.7272
0.7417
0.7555
1.0581
1.0612
1.0715
1.0759
1.0805
1.0851
1.0897
1.0943
1.0989
1.1035
1.1081
1.1127
1.1173
1.1219
1.1265
1.1311
1.1357
1.1403
1.1449
1.1495
1.1541
1.1587
1.1633
1.1679
1.1725
1.1771
1.1817
1.1863
1.1909
1.1955
1.2001
1.2047
1.2093
1.2139
1.2185
1.2231
1.2277
1.2323
1.2369
1.2415
1.2461
1.2507
1.2553
1.2599
1.2645
1.2691
1.2737
1.2783
1.2829
1.2875
1.2921
1.2967
1.3013
1.3059
1.3105
1.3151
1.3197
1.3243
1.3289
1.3335
1.3381
1.3427
1.3473
1.3519
1.3565
1.3611
1.3657
1.3703
1.3749
1.3795
1.3841
1.3887
1.3933
1.3979
1.4025
1.4071
1.4117
1.4163
1.4209
1.4255
1.4301
1.4347
1.4393
1.4439
1.4485
1.4531
1.4577
1.4623
1.4669
1.4715
1.4761
1.4807
1.4853
1.4899
1.4945
1.4991
1.5037
1.5083
1.5129
1.5175
1.5221
1.5267
1.5313
1.5359
1.5405
1.5451
1.5497
1.5543
1.5589
1.5635
1.5681
1.5727
1.5773
1.5819
1.5865
1.5911
1.5957
1.6003
1.6049
1.6095
1.6141
1.6187
1.6233
1.6279
1.6325
1.6371
1.6417
1.6463
1.6509
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1.6601
1.6647
1.6693
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1.6785
1.6831
1.6877
1.6923
1.6969
1.7015
1.7061
1.7107
1.7153
1.7199
1.7245
1.7291
1.7337
1.7383
1.7429
1.7475
1.7521
1.7567
1.7613
1.7659
1.7705
1.7751
1.7797
1.7843
1.7889
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1.9959
2.0005
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2.0879
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2.1937
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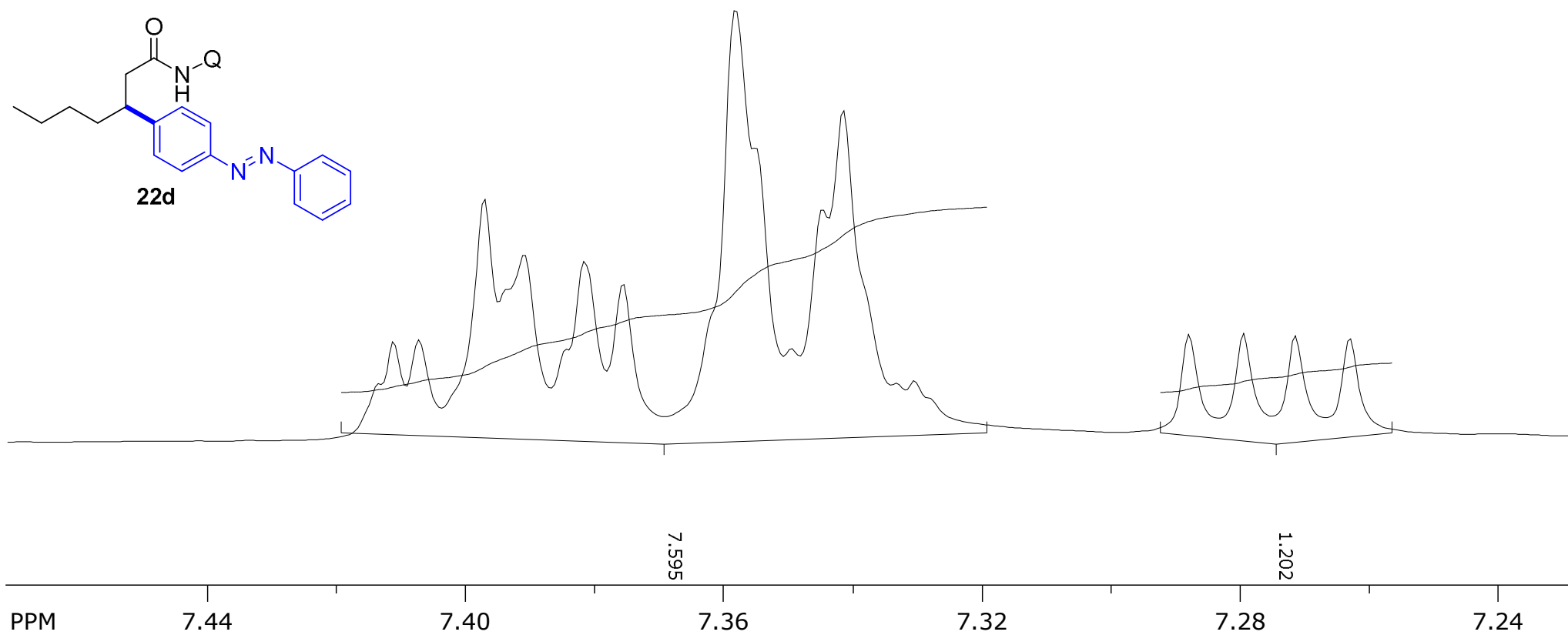
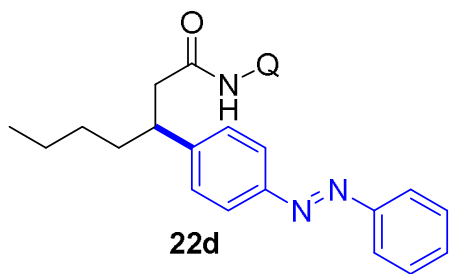


SpinWorks 4: SV030702
1H_8scan CDCl3 {D:\Spectra} nmr 26

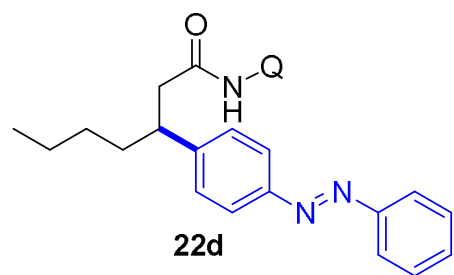


SpinWorks 4: SV030702
1H_8scan CDCl3 {D:\Spectra} nmr 26

7.4073 —
7.4112 —
7.4134 —
7.3909 —
7.3936 —
7.3971 —
7.3816 —
7.3843 —
7.3756 —
7.3552 —
7.3582 —
7.3495 —
7.3447 —
7.3415 —
7.3333 —
7.3305 —
7.2879 —
7.2795 —
7.2714 —
7.2630 —

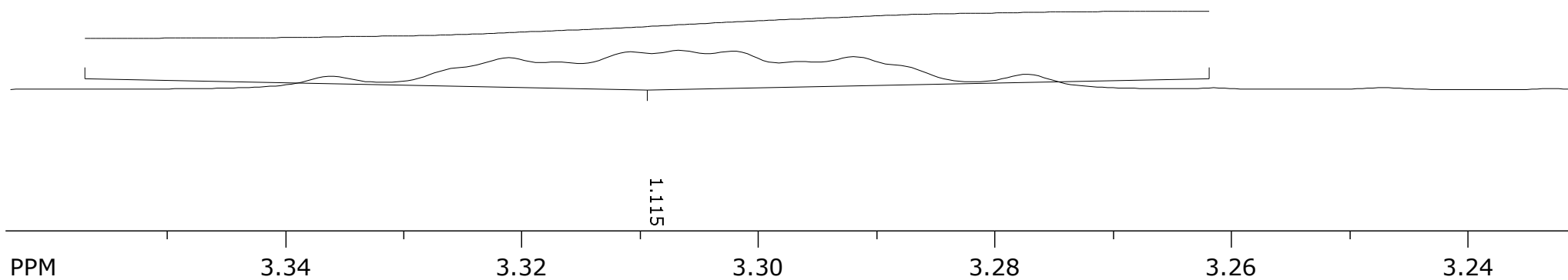


SpinWorks 4: SV030702
1H_8scan CDCl3 {D:\Spectra} nmr 26



22d

3.2773 —
3.2918 —
3.2965 —
3.3022 —
3.3068 —
3.3107 —
3.3171 —
3.3211 —



PPM

3.34

3.32

3.30

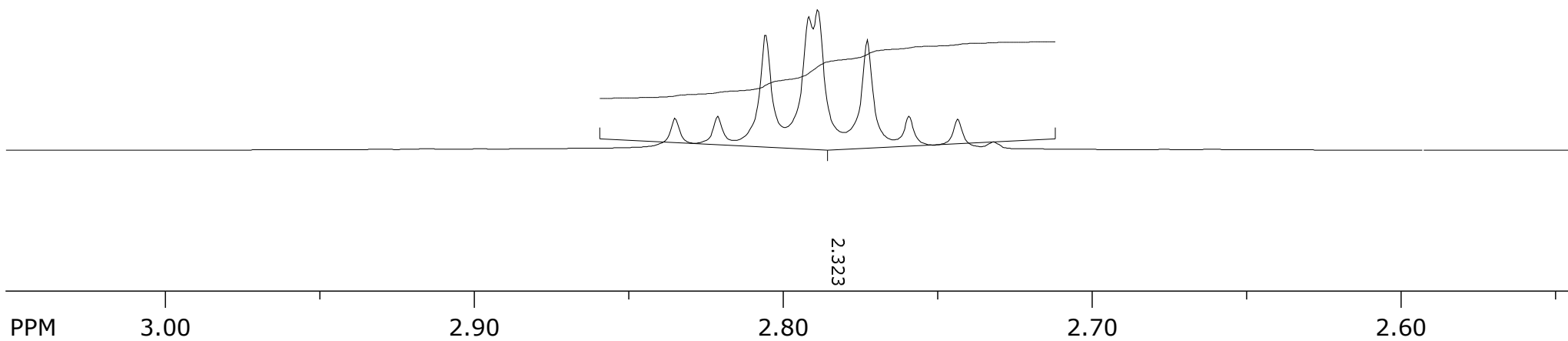
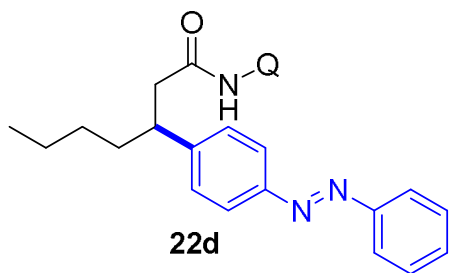
3.28

3.26

3.24

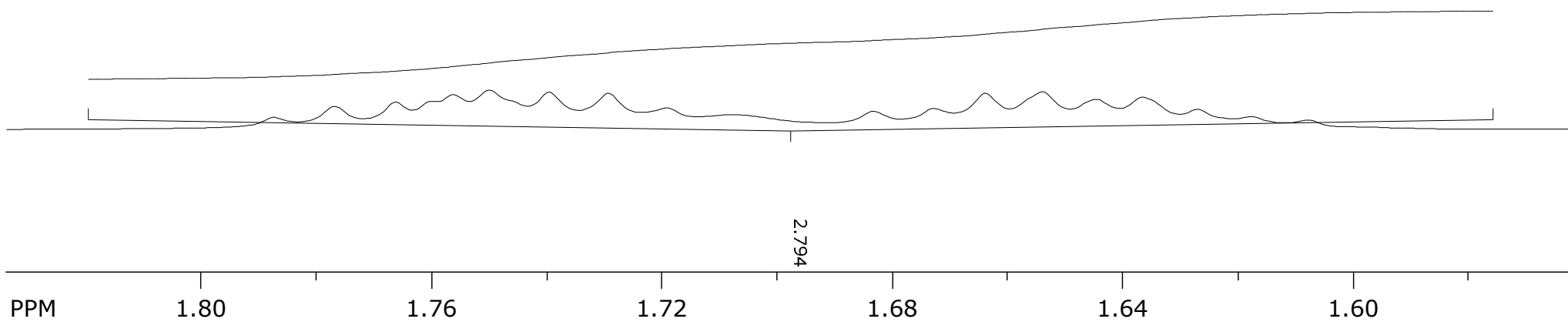
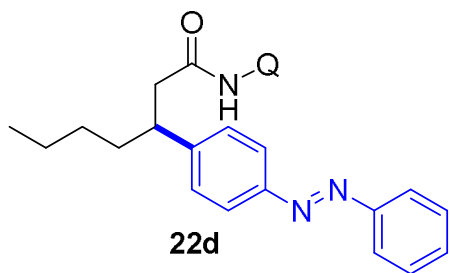
SpinWorks 4: SV030702
1H_8scan CDCl3 {D:\Spectra} nmr 26

2.7436 —
2.7594 —
2.7729 —
2.7889 —
2.7918 —
2.8059 —
2.8214 —
2.8352 —



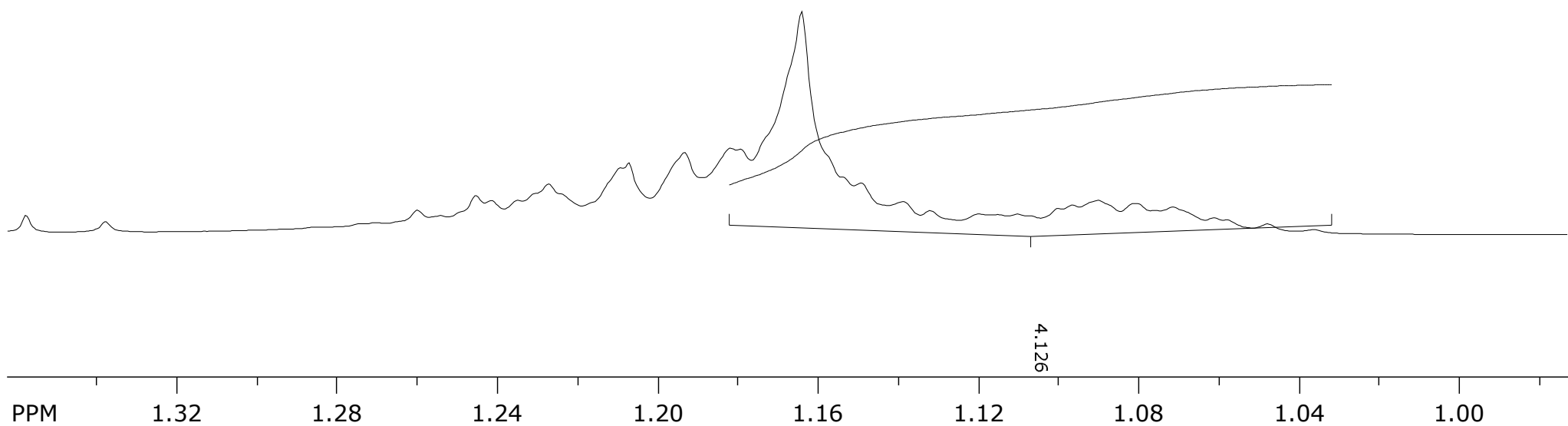
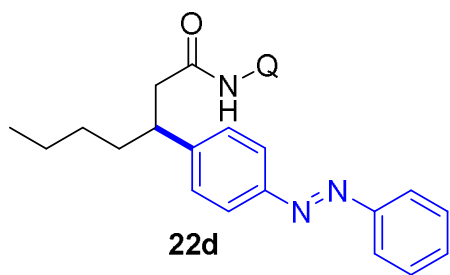
SpinWorks 4: SV030702
1H_8scan CDCl3 {D:\Spectra} nmr 26

1.7769 —
1.7663 —
1.7600 —
1.7563 —
1.7500 —
1.7396 —
1.7293 —
1.7192 —
1.7076 —
1.6833 —
1.6728 —
1.6638 —
1.6539 —
1.6446 —
1.6365 —
1.6270 —



SpinWorks 4: SV030702
1H_8scan CDCl3 {D:\Spectra} nmr 26

1.0581
1.0612
1.0715
1.0759
1.0805
1.0901
1.0965
1.1000
1.1073
1.1103
1.1152
1.1199
1.1321
1.1389
1.1493
1.1540
1.1642
1.1795
1.1819
1.1934
1.2073
1.2093
1.2273
1.2349
1.2416
1.2454
1.2543
1.2600

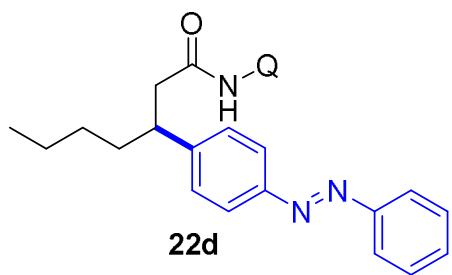


SpinWorks 4: SV030702
1H_8scan CDCl3 {D:\Spectra} nmr 26

0.7555

0.7417

0.7272



22d



3.161

PPM

0.76

0.74

0.72

0.70

0.68

SpinWorks 4: SV030702
C13CPD CDCl3 {D:\Spectra} nmr 26

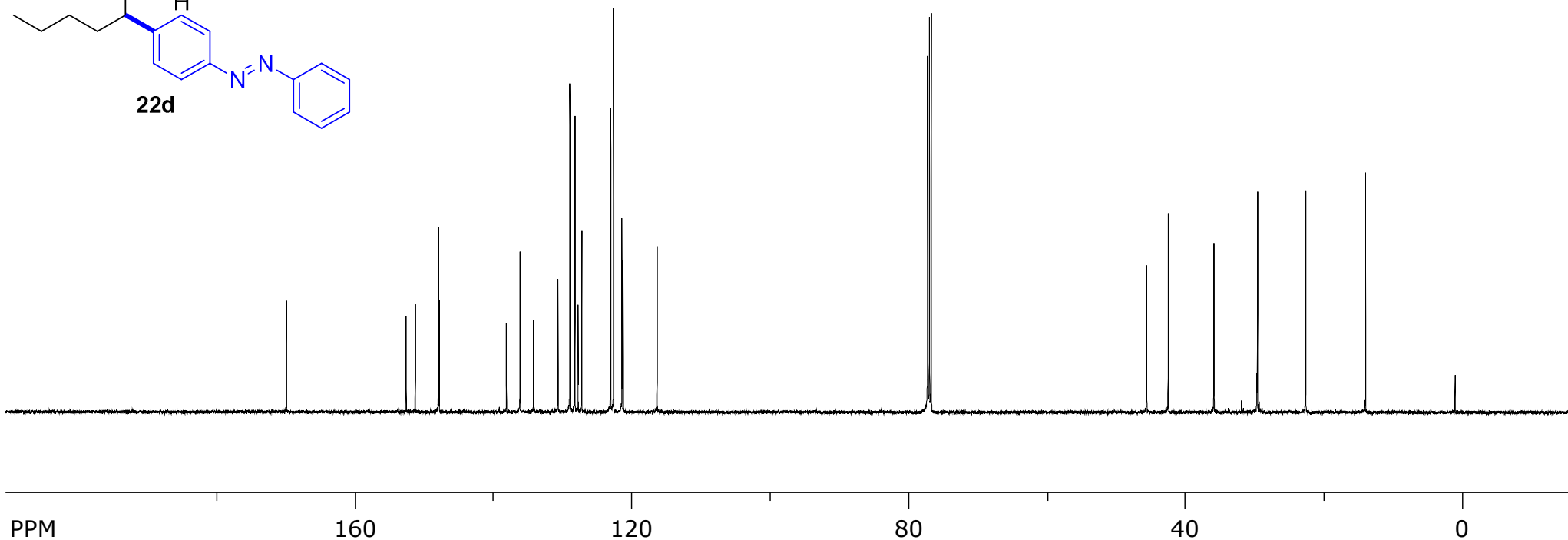
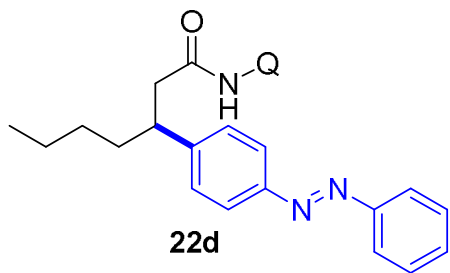
SS-302

169.991 —

116.381
121.390
121.460
122.663
123.093
127.274
127.787
128.258
128.988
130.703
134.265
136.200
138.167
147.863
147.990
151.360
152.664

76.749
77.003
77.258

42.482
45.593
35.857
29.559
22.575
13.939



PPM

160

120

80

40

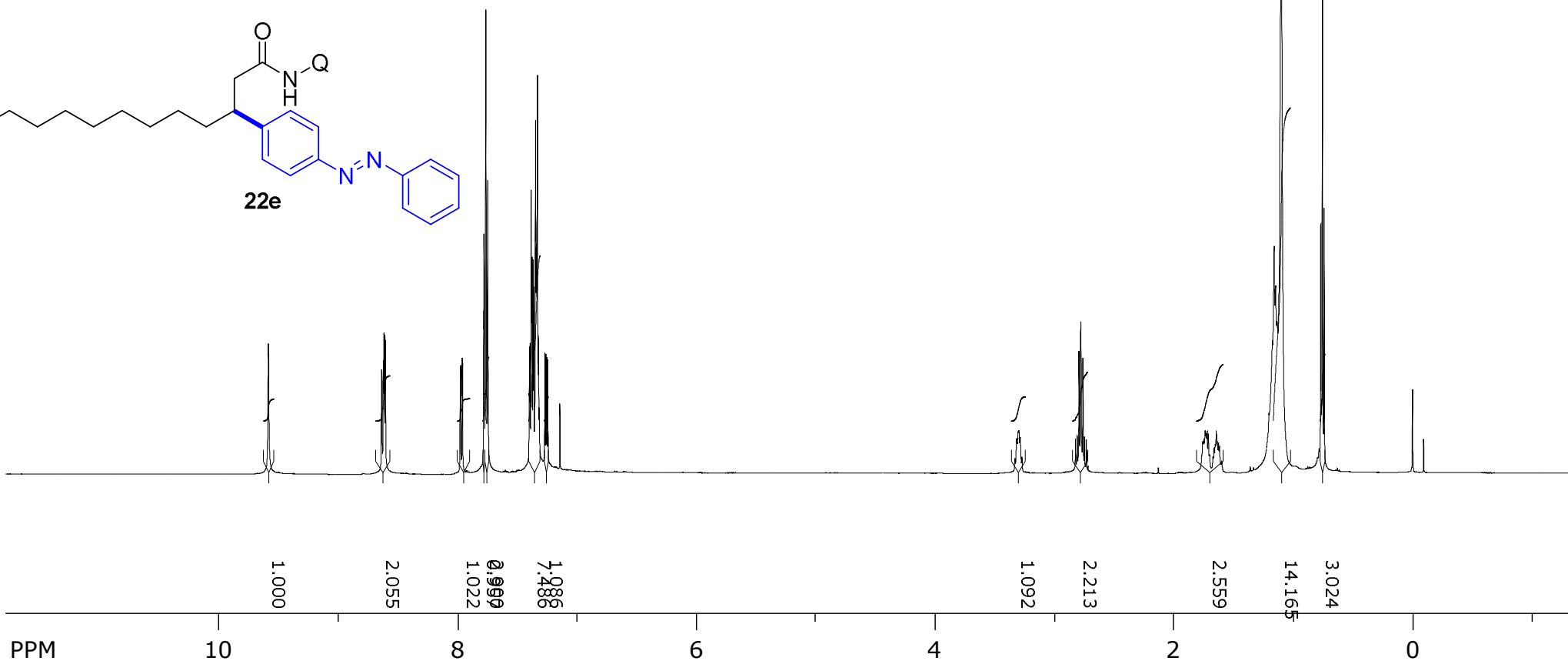
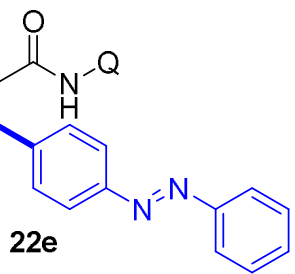
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SpinWorks 4: SV030704
1H_8scan CDCl3 {D:\Spectra} nmr 28

SS-299

9.5882
8.6381
8.6230
8.6184
8.6151
8.6099
8.6067
7.9806
7.9774
7.9699
7.7809
7.1451
7.1400

1.9984
1.9984
1.9984
1.9984
1.6255
1.6169
1.5979
1.1587
1.1465
1.1358
1.10997
0.7679
0.7542
0.7398

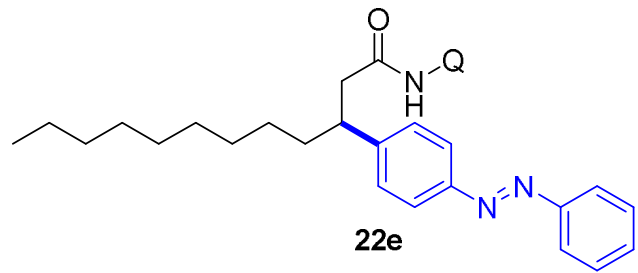


SpinWorks 4: SV030704
1H_8scan CDCl3 {D:\Spectra} nmr 28

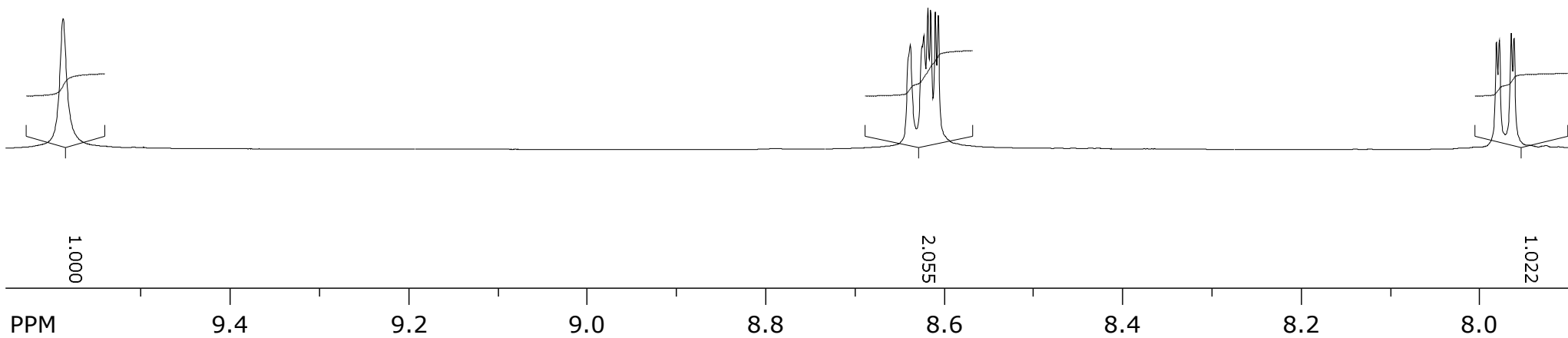
9.5882

8.6067
8.6099
8.6151
8.6184
8.6230
8.6250
8.6381

7.9609
7.9641
7.9774
7.9806

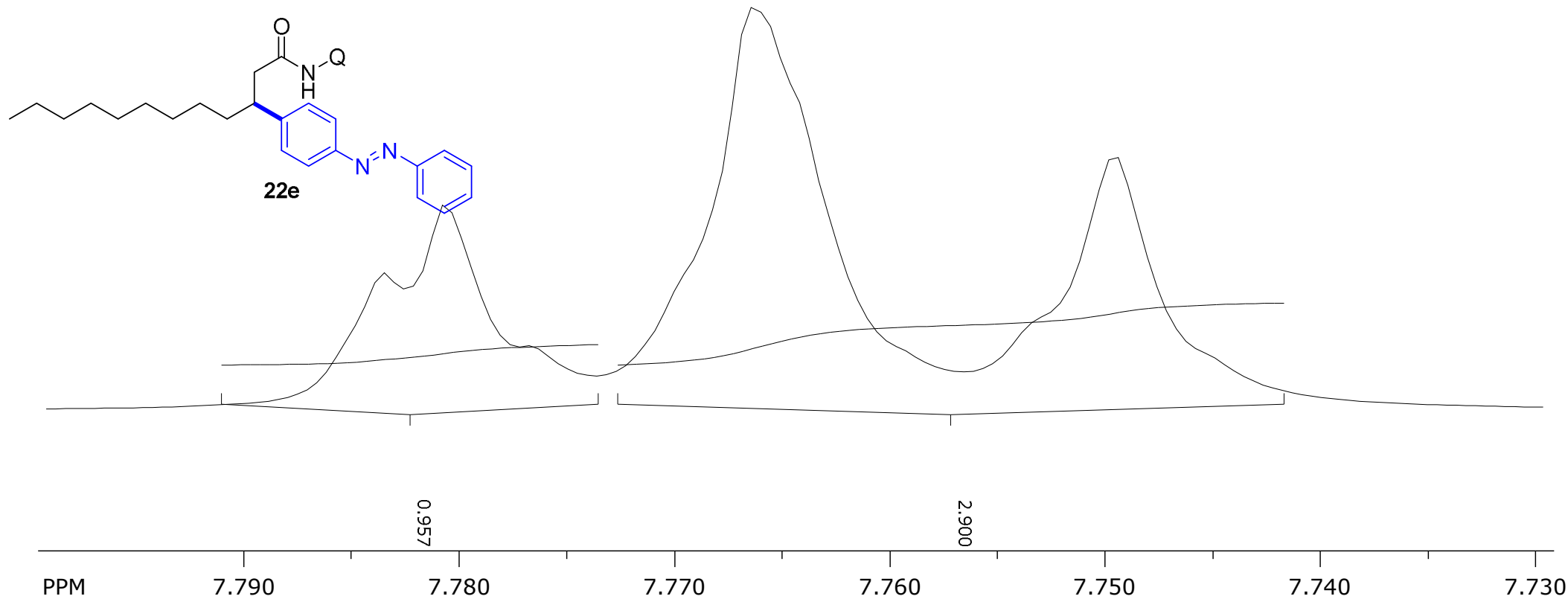


22e



SpinWorks 4: SV030704
1H_8scan CDCl3 {D:\Spectra} nmr 28

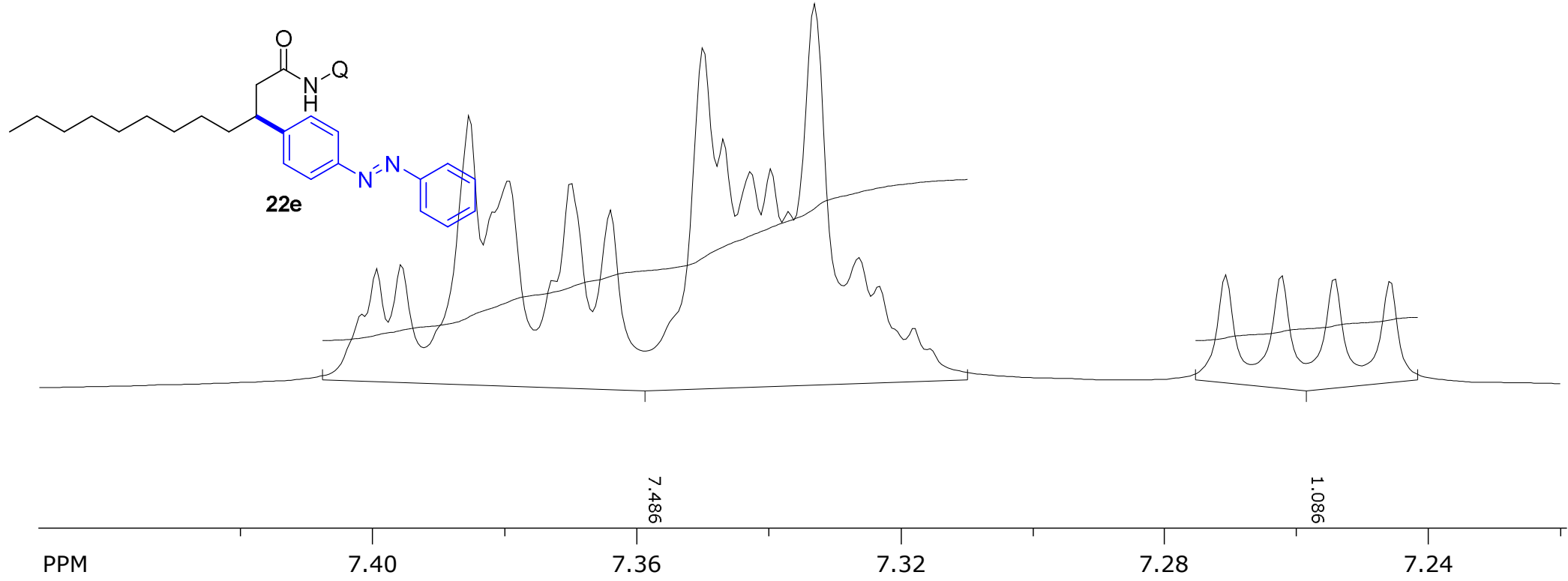
7.7835 —
7.7807 —
7.7768 —
7.7701 —
7.7663 —
7.7534 —
7.7496 —
7.7444 —



SpinWorks 4: SV030704

1H_8scan CDCl3 {D:\Spectra} nmr 28

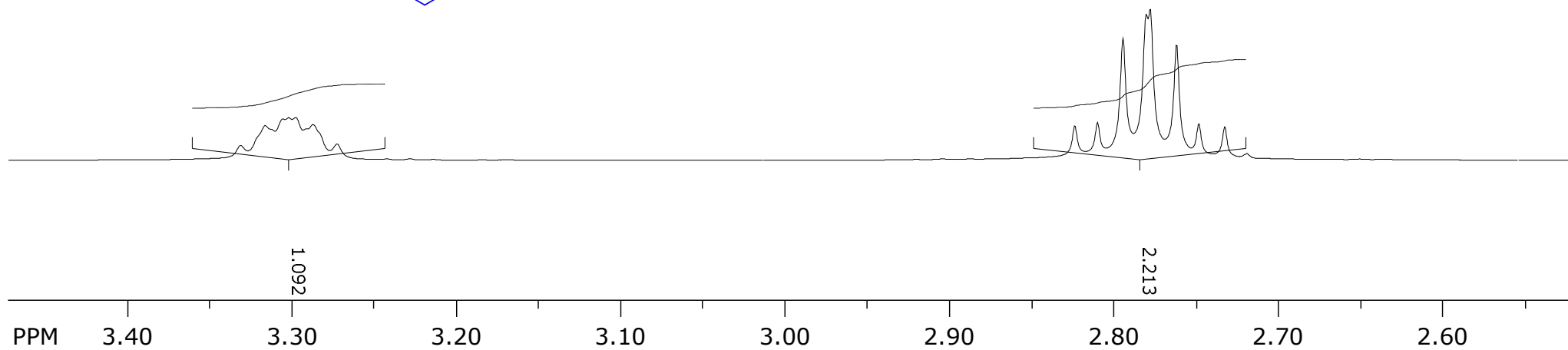
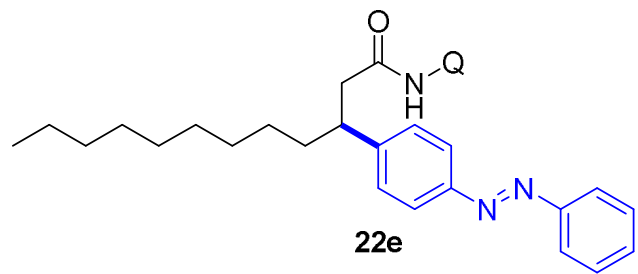
7.3957 —
7.3995 —
7.4017 —
7.3795 —
7.3818 —
7.3854 —
7.3700 —
7.3728 —
7.3641 —
7.3500 —
7.3469 —
7.3428 —
7.3371 —
7.3331 —
7.3233 —
7.3264 —
7.3180 —
7.3157 —
7.2708 —
7.2623 —
7.2543 —
7.2458 —



SpinWorks 4: SV030704
1H_8scan CDCl3 {D:\Spectra} nmr 28

3.2726
3.2872
3.2912
3.2977
3.3020
3.3056
3.3163
3.3314

2.7324
2.7482
2.7617
2.7778
2.7801
2.7943
2.8098
2.8237

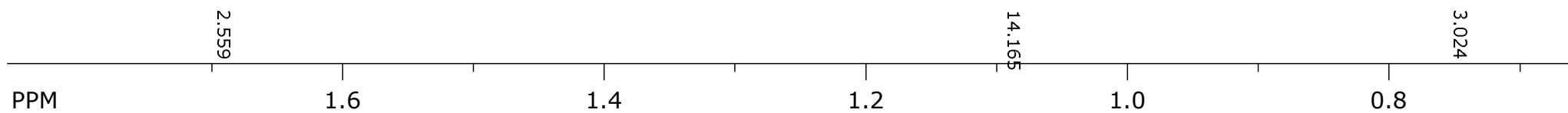
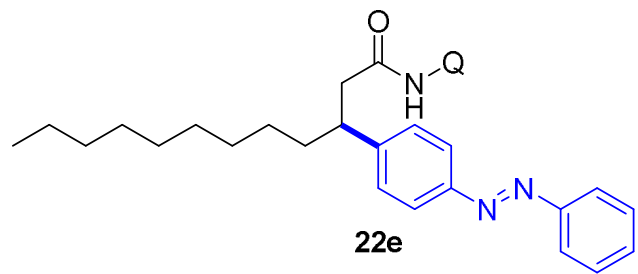


SpinWorks 4: SV030704
1H_8scan CDCl3 {D:\Spectra} nmr 28

1.5979
1.6169
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1.6362
1.6436
1.6523
1.6624
1.6714
1.7001
1.7102
1.7206
1.7305
1.7368
1.7473
1.7563

1.0997
1.1358
1.1465
1.1587

0.7398
0.7542
0.7679



SpinWorks 4: SV030704
C13CPD CDCl3 {D:\Spectra} nmr 28
SS-299

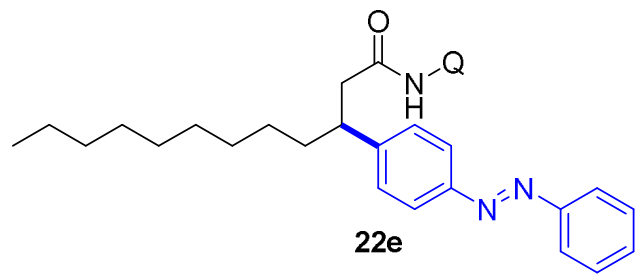
170.003

152.672
151.358
147.986
147.886
138.176
136.196
134.278
130.703
128.986
128.259
127.791
127.276
123.103
122.669
121.455
121.392
116.390

77.274
77.020
76.765

45.602
42.513

36.151
31.808
29.497
29.474
29.445
29.221
27.378
22.616
14.077



22e

PPM

160

120

80

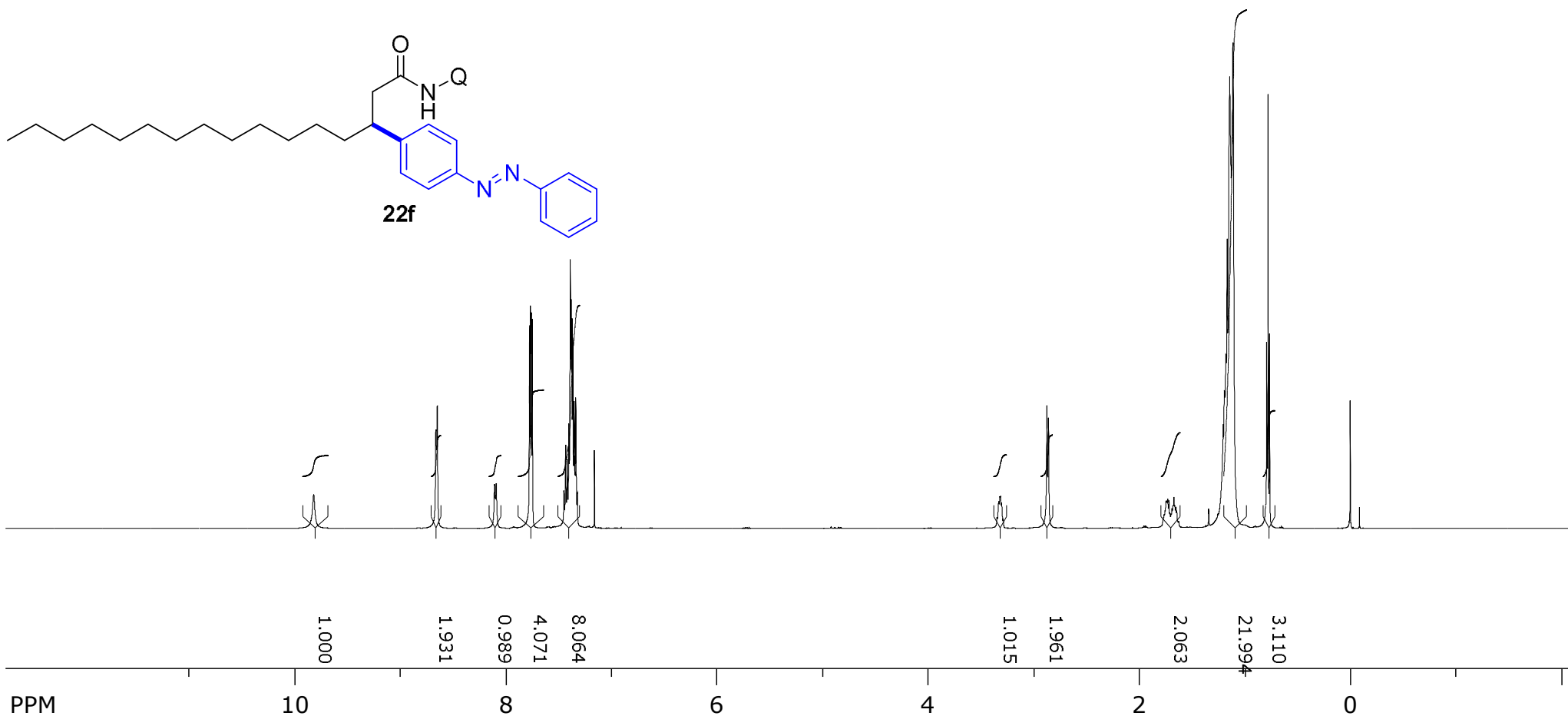
40

0

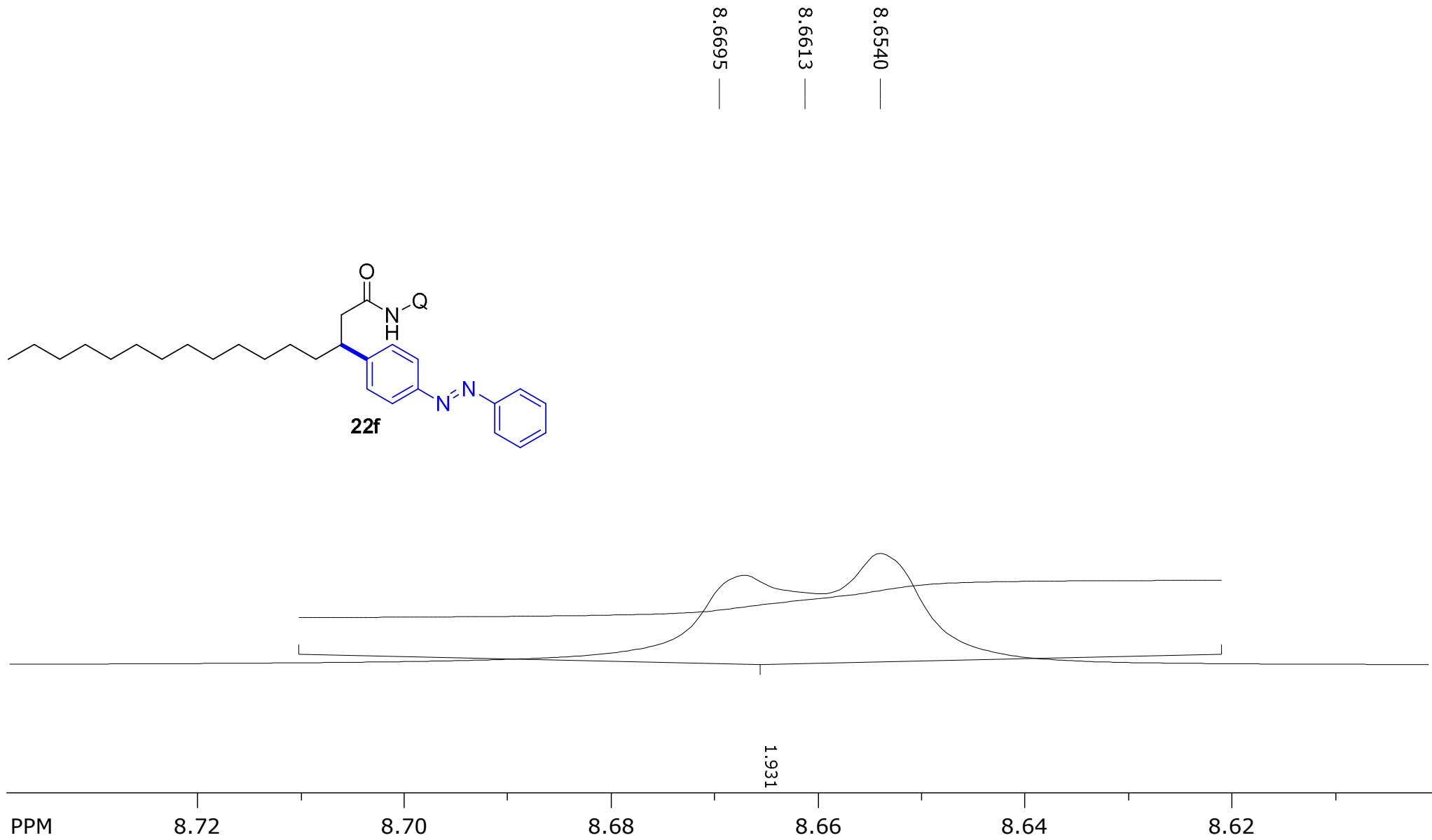
SpinWorks 4: SV070701
 1H_8scan CDCl3 {D:\Spectra} nmr 27

SS-300

| | | | | | | | | | | | | | | | | | | | | |
|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| 9.8253 | 8.6672 | 8.6613 | 8.6540 | 8.1104 | 8.0950 | 7.7810 | 7.7781 | 7.7739 | 7.7639 | 7.1638 | 2.8092 | 2.0220 | 1.9990 | 1.1781 | 1.1661 | 1.1429 | 1.1110 | 0.7923 | 0.7786 | 0.7644 |
|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|



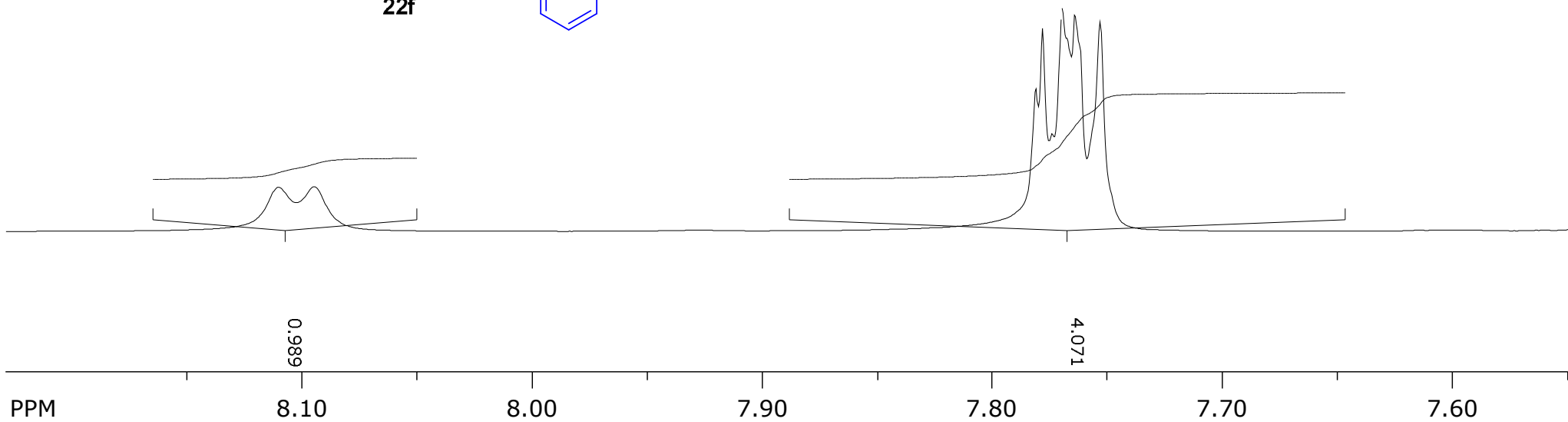
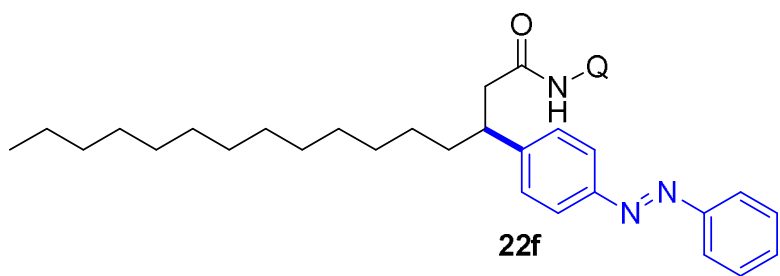
SpinWorks 4: SV070701
1H_8scan CDCl3 {D:\Spectra} nmr 27



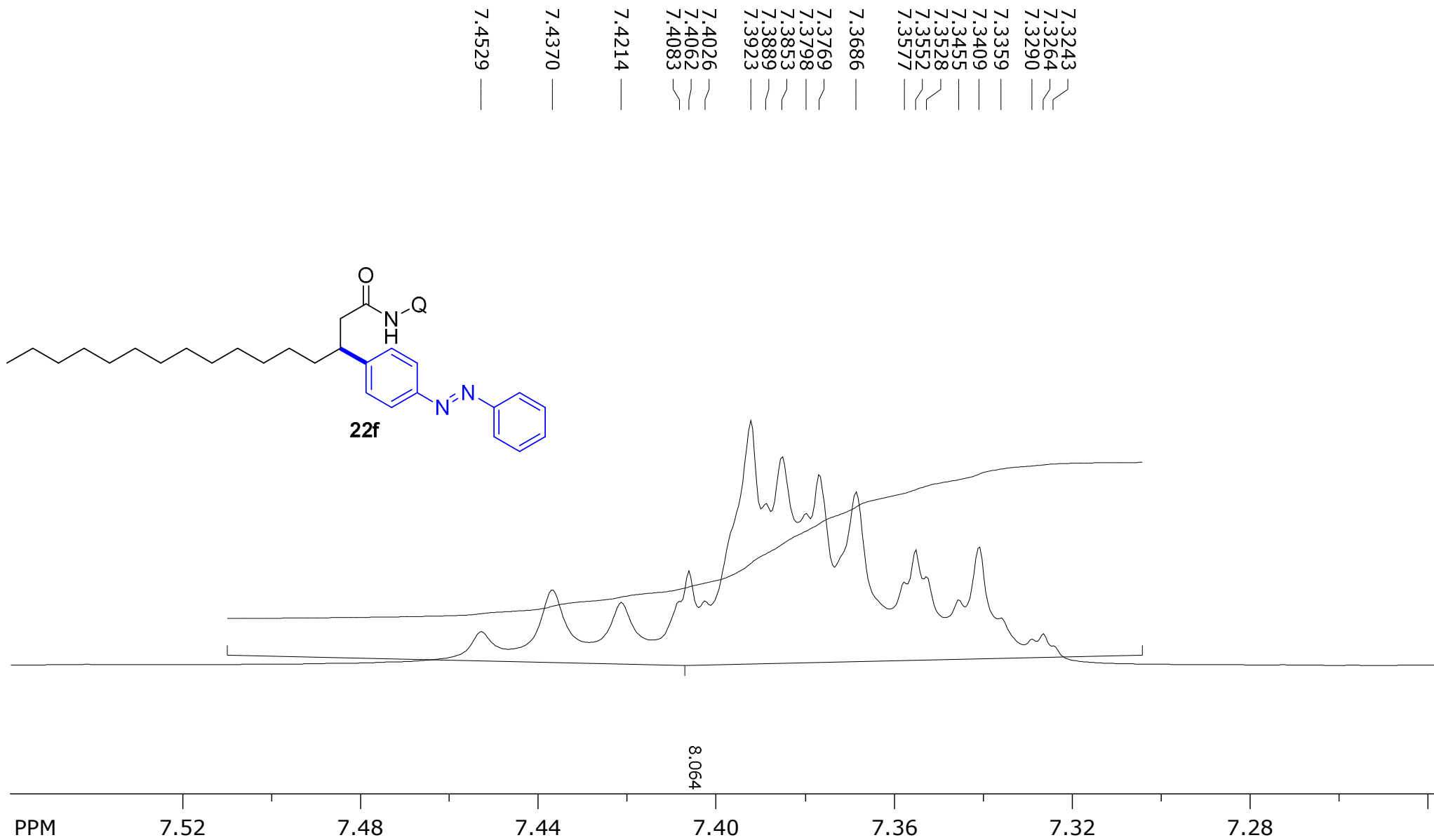
SpinWorks 4: SV070701
1H_8scan CDCl3 {D:\Spectra} nmr 27

8.0950 —
8.1104 —

7.7530 —
7.7640 —
7.7676 —
7.7695 —
7.7739 —
7.7781 —
7.7810 —



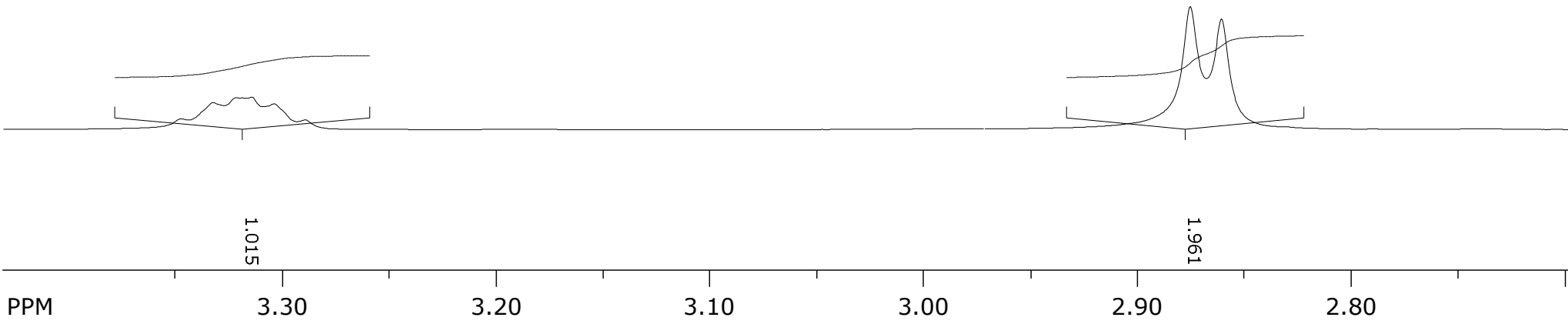
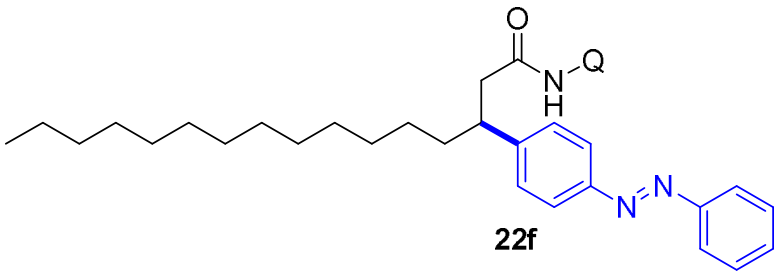
SpinWorks 4: SV070701
1H_8scan CDCl3 {D:\Spectra} nmr 27



SpinWorks 4: SV070701
1H_8scan CDCl3 {D:\Spectra} nmr 27

3.2896
3.3039
3.3146
3.3189
3.3218
3.3327
3.3476

2.8605
2.8752



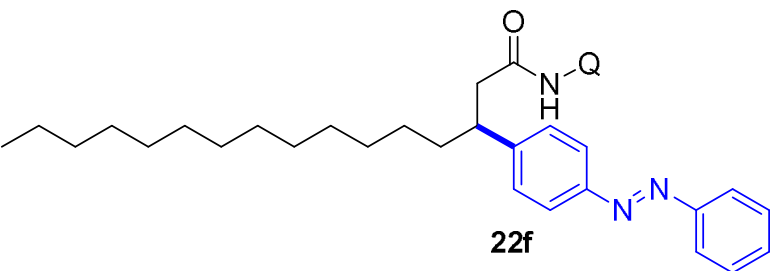
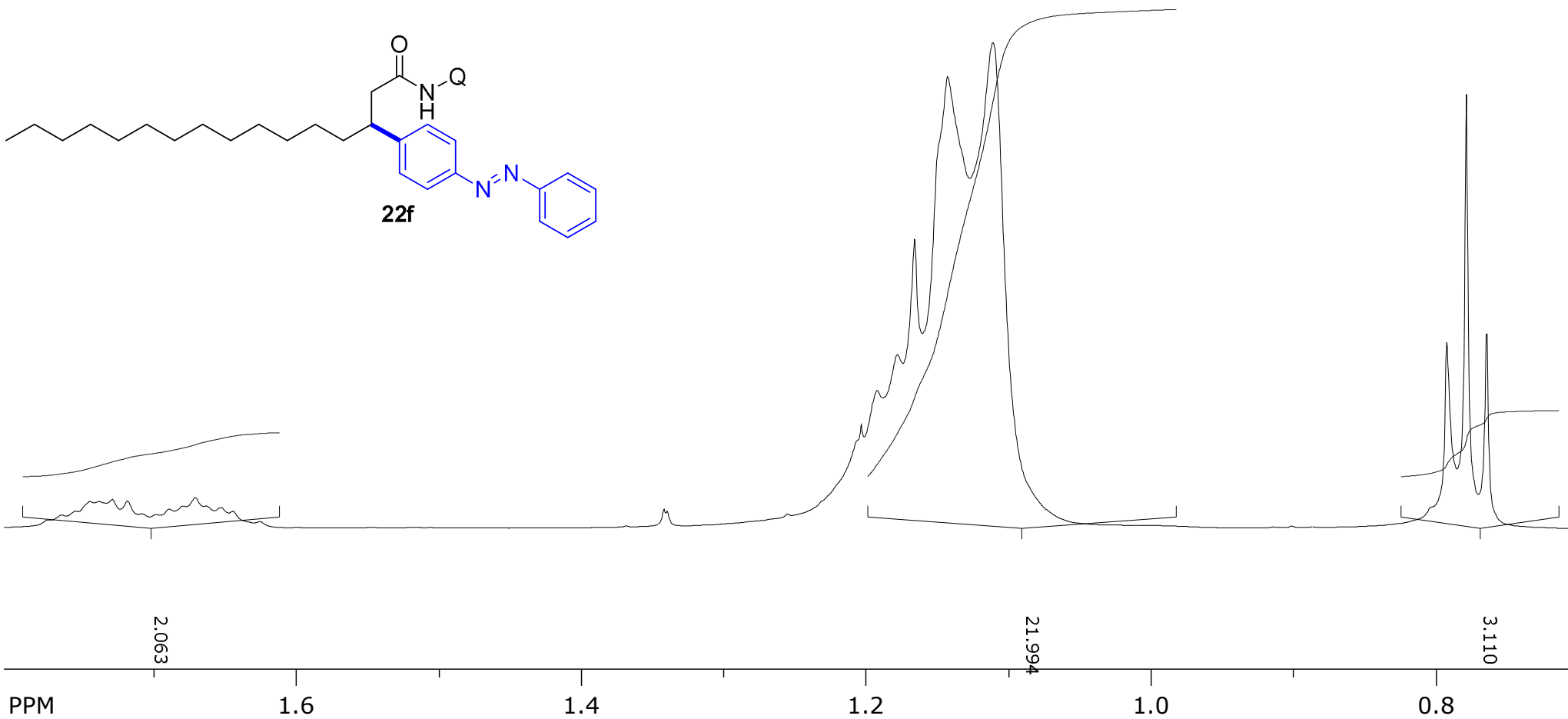
SpinWorks 4: SV070701

1H_8scan CDCl3 {D:\Spectra} nmr 27

1.64448
1.65333
1.66336
1.67113
1.67917
1.68977
1.69889
1.70877
1.71889
1.72995
1.73889
1.74522
1.75159
1.75792
1.77444

1.2554
1.2035
1.1924
1.1781
1.1661
1.1429
1.1110

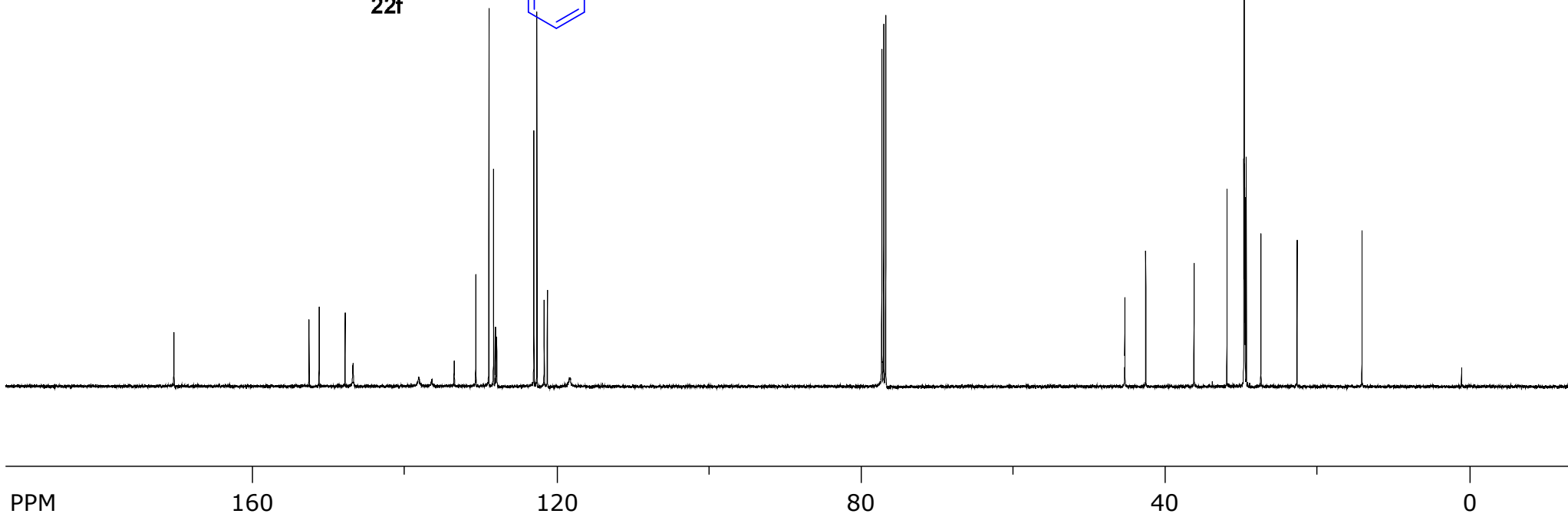
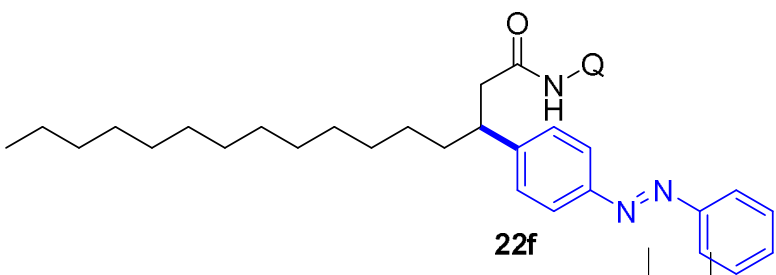
0.7644
0.7786
0.7923



SpinWorks 4: SV070701
C13CPD CDCl3 {D:\Spectra} nmr 27

SS-300

170.423
152.642
151.315
147.906
146.831
138.204
136.489
133.546
130.695
128.982
128.357
128.128
127.963
123.058
121.695
118.310
79.000
45.308
42.551
36.198
31.868
29.598
29.529
29.503
29.450
27.392
22.643
14.097



SpinWorks 4: SV070701
C13CPD CDCl3 {D:\Spectra} nmr 27

170.423

152.642
151.315

147.906
146.831

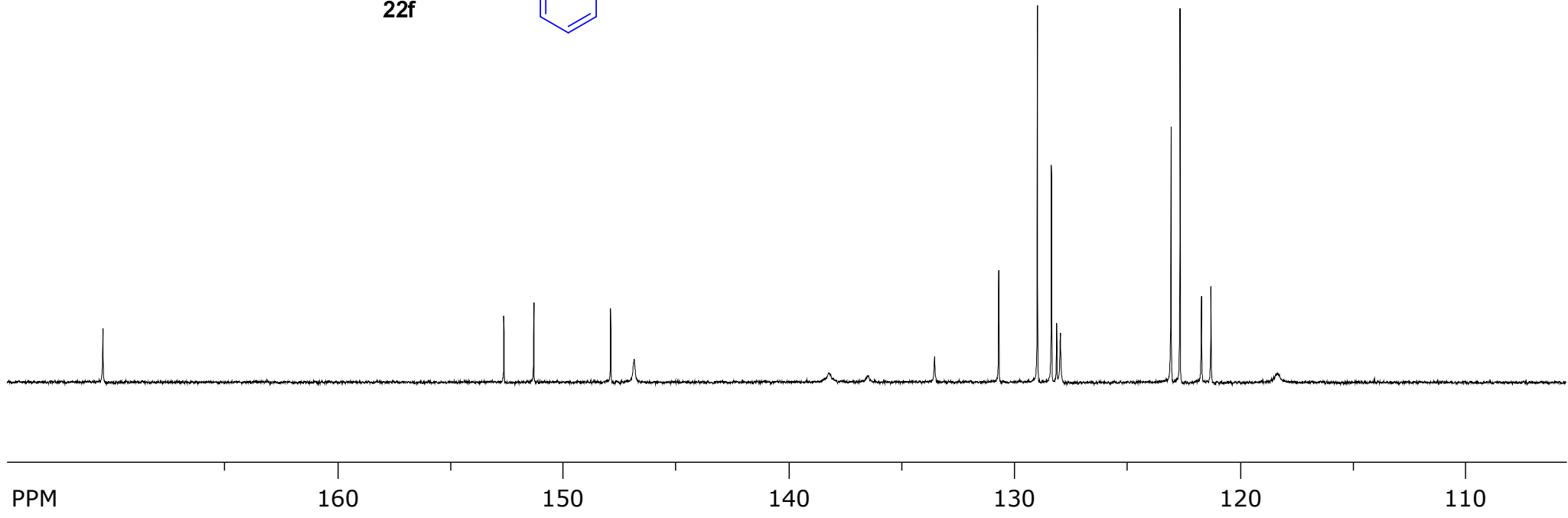
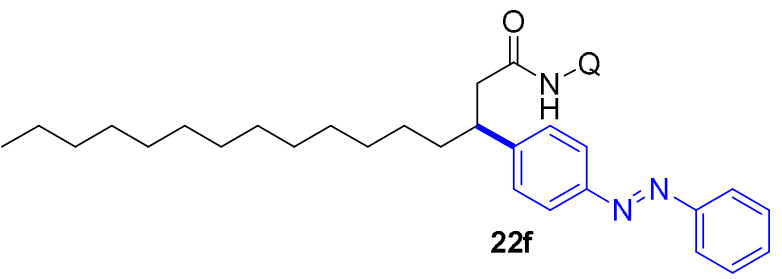
138.204
136.489

133.546

130.695
128.982
128.357
128.128
127.963

123.058
122.655
121.706
121.285

118.310



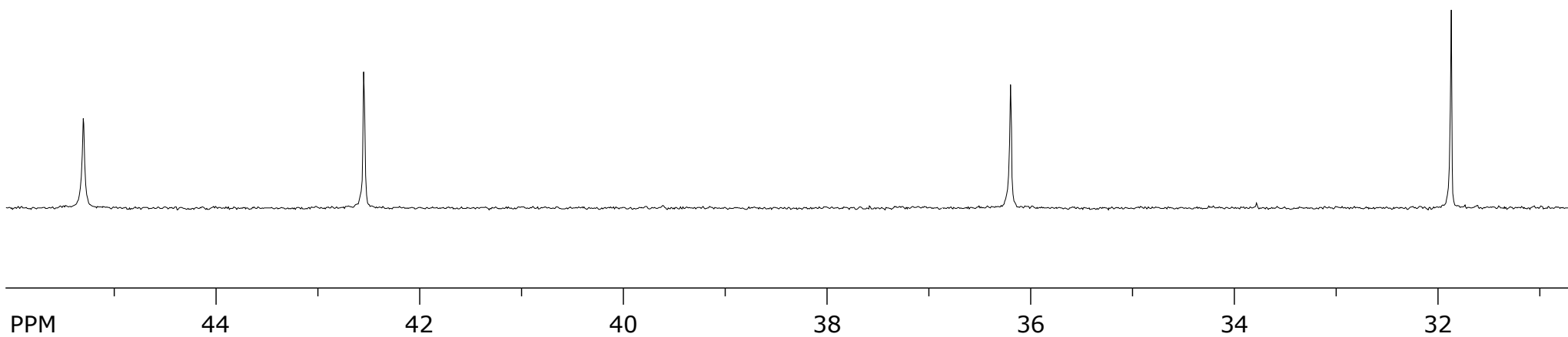
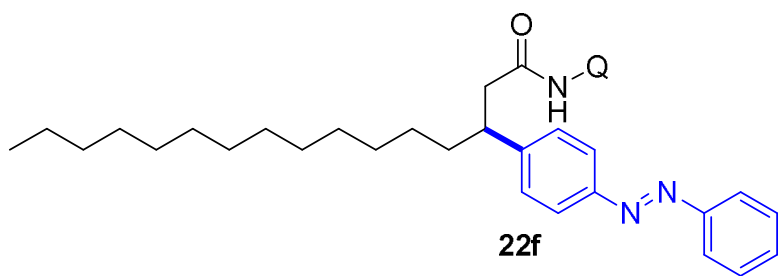
SpinWorks 4: SV070701
C13CPD CDCl3 {D:\Spectra} nmr 27

45.308

42.551

36.198

31.868



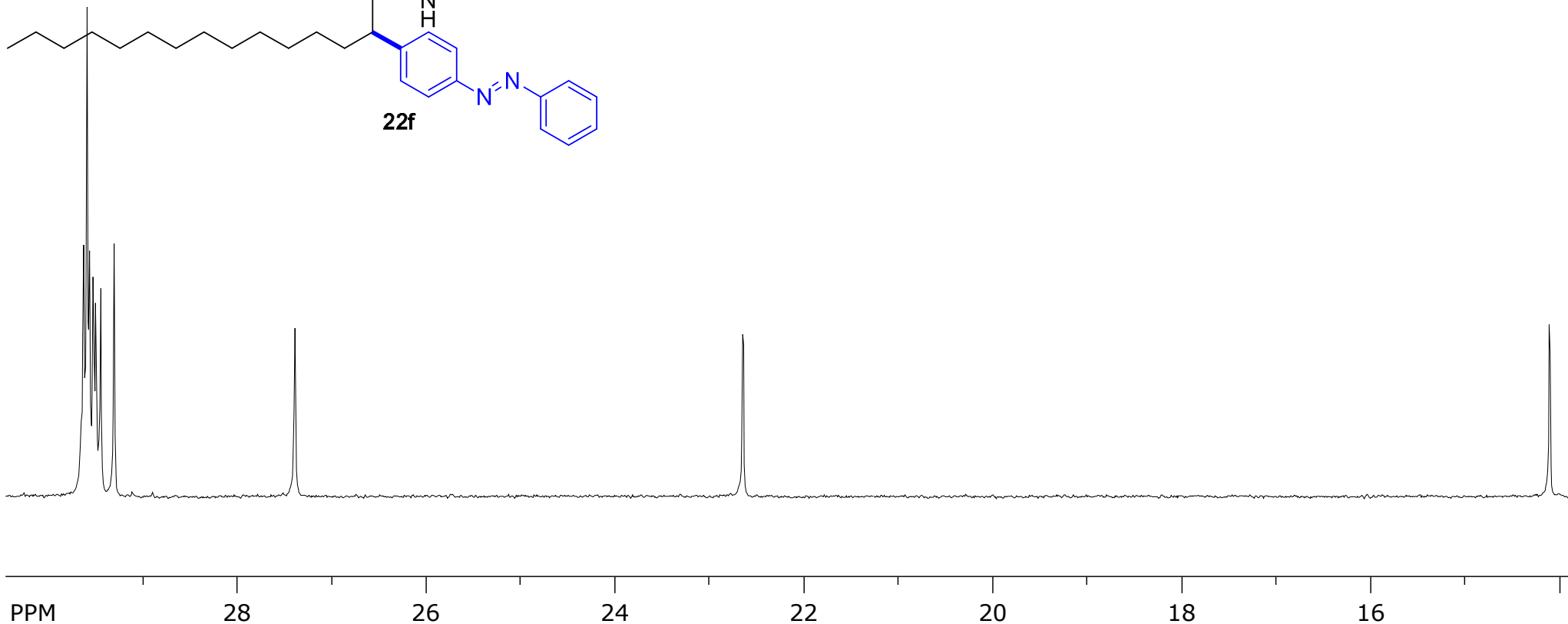
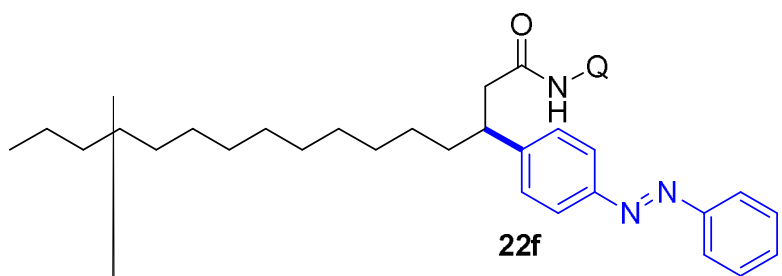
SpinWorks 4: SV070701
C13CPD CDCl3 {D:\Spectra} nmr 27

29.306
29.450
29.503
29.529
29.568
29.594
29.630
29.659

27.392

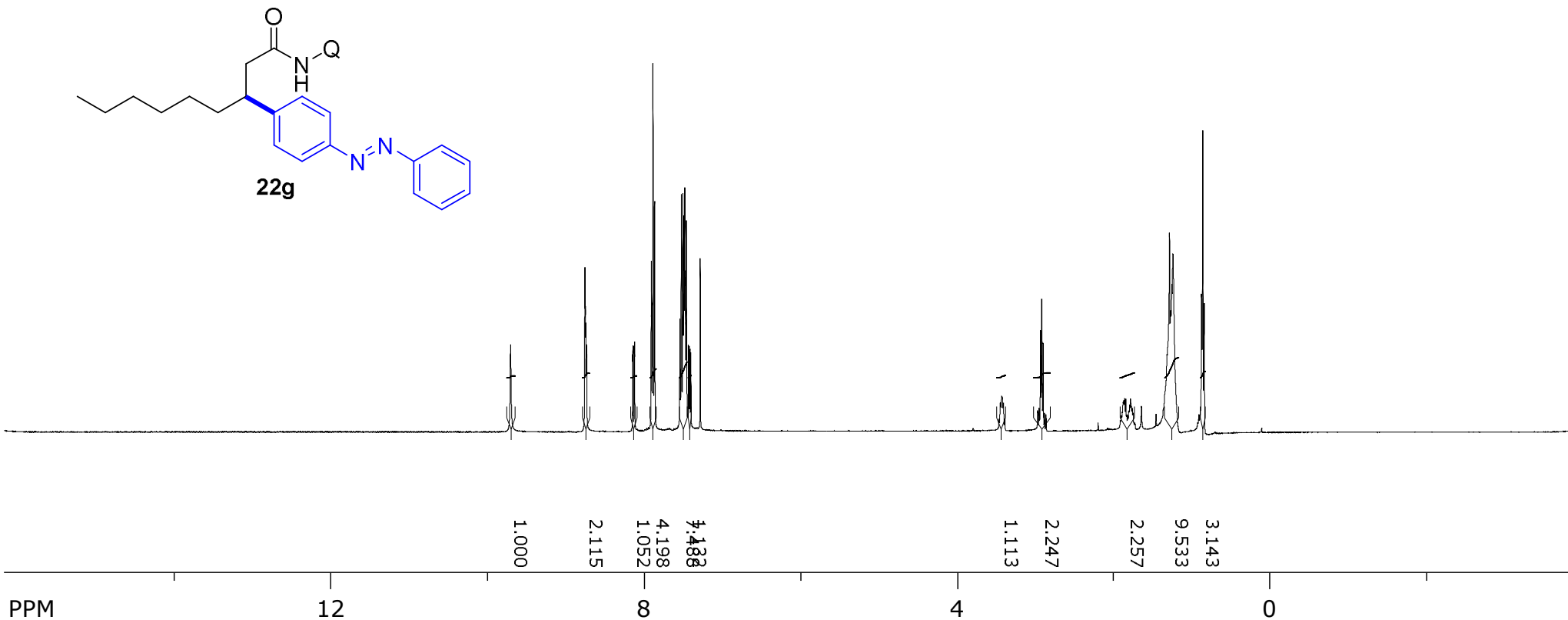
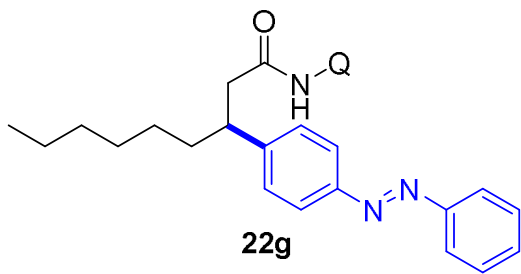
22.643

14.097



PPM 28 26 24 22 20 18 16

SpinWorks 4: SS 767
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 39

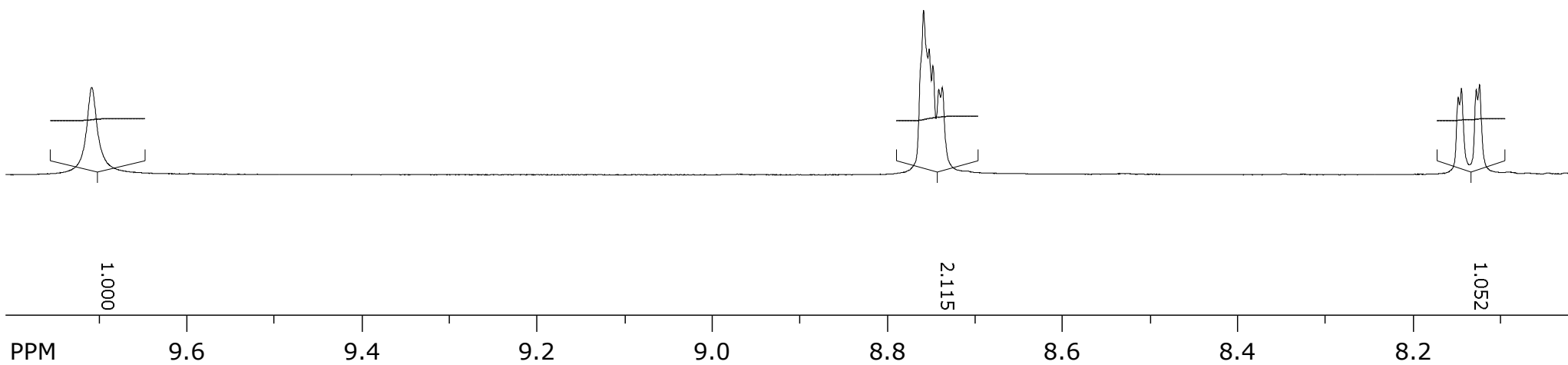
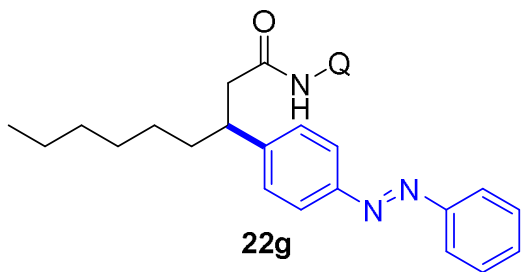


SpinWorks 4: SS 767
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 39

9.7092

8.7374
8.7413
8.7480
8.7523
8.7586

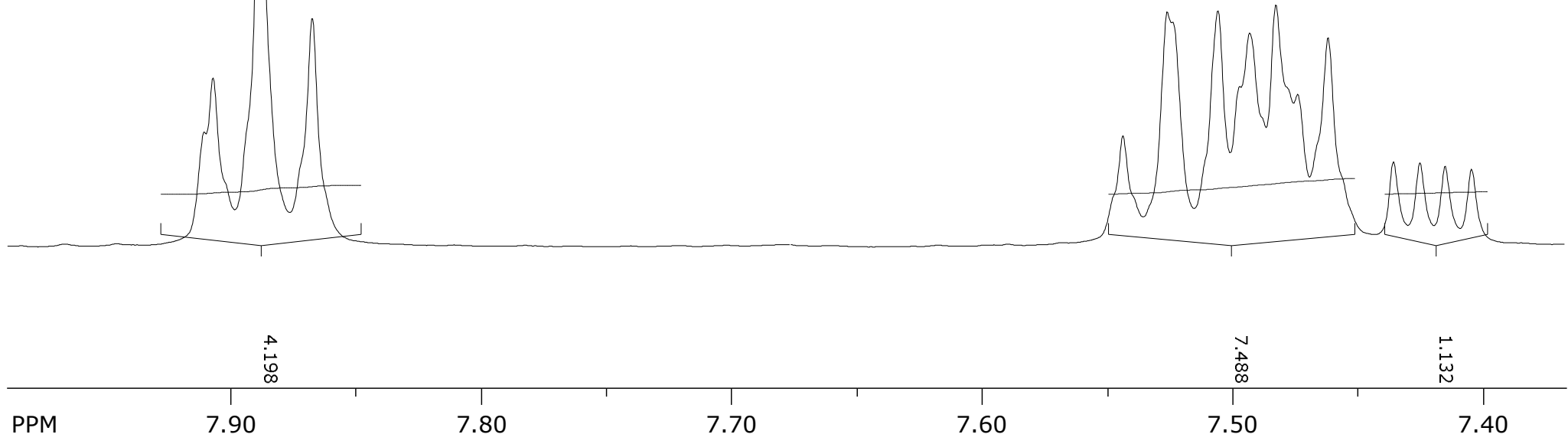
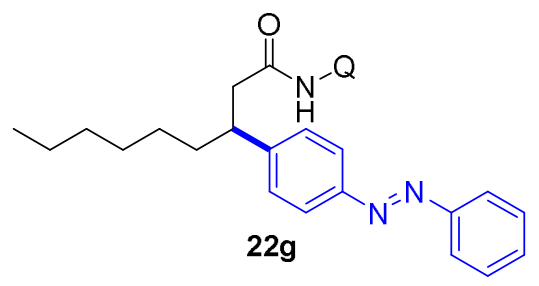
8.1235
8.1272
8.1442
8.1479



SpinWorks 4: SS 767
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 39

7.8677 —
7.8886 —
7.9073 —
7.9109 —

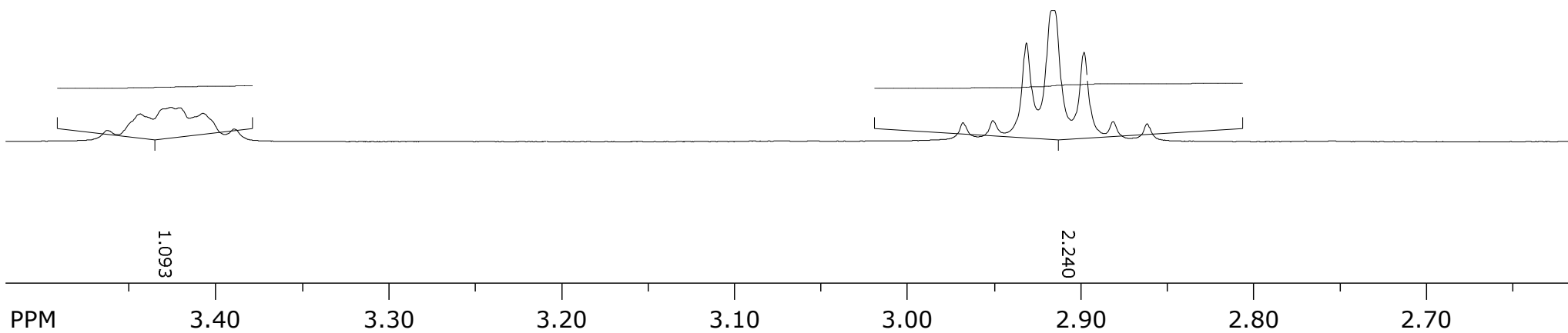
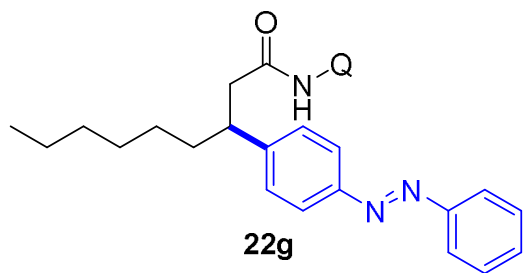
7.4045 —
7.4151 —
7.4252 —
7.4357 —
7.4618 —
7.4740 —
7.4827 —
7.4931 —
7.4971 —
7.5059 —
7.5239 —
7.5261 —
7.5438 —



SpinWorks 4: SS 767
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 39

3.4077
3.4126
3.4212
3.4263
3.4306
3.4442

2.8616
2.8812
2.8981
2.9168
2.9314
2.9506
2.9680

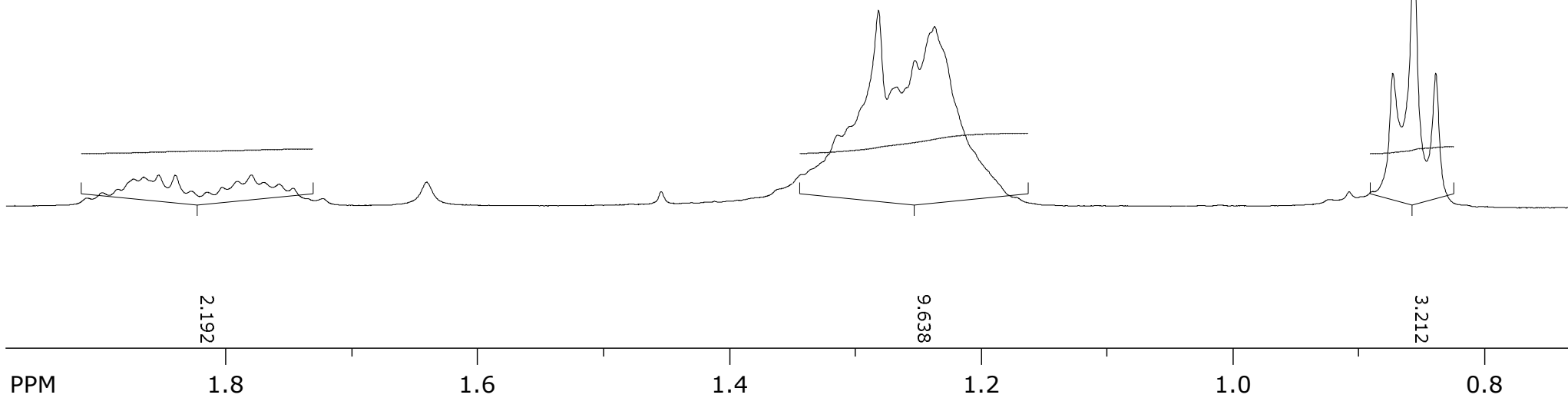
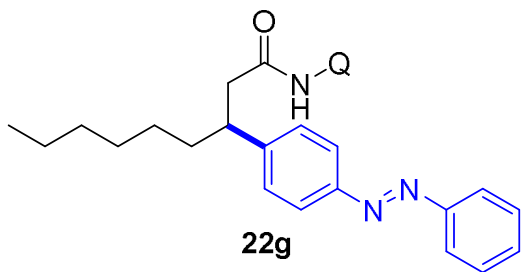


SpinWorks 4: SS 767
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 39

1.7582
1.7706
1.7805
1.7917
1.8036
1.8410
1.8541
1.8599
1.8662
1.8742
1.8869

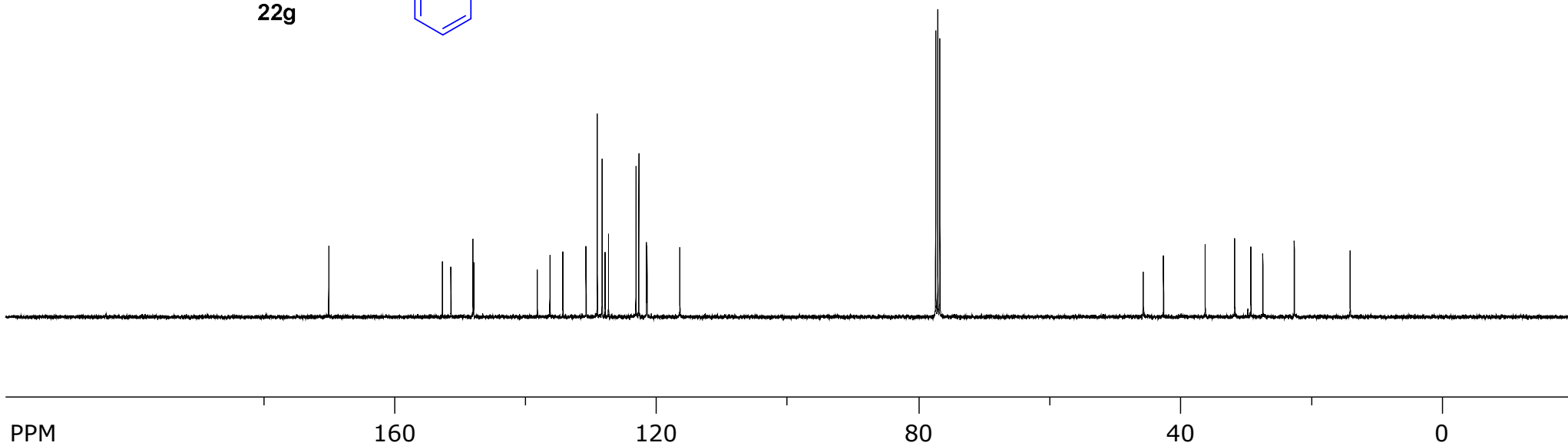
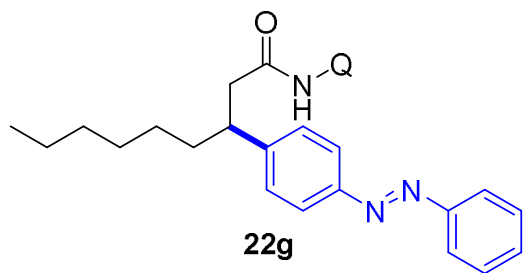
1.2372
1.2404
1.2528
1.2673
1.2818
1.3145
1.3430

0.8386
0.8561
0.8727



SpinWorks 4: SS 767

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 15

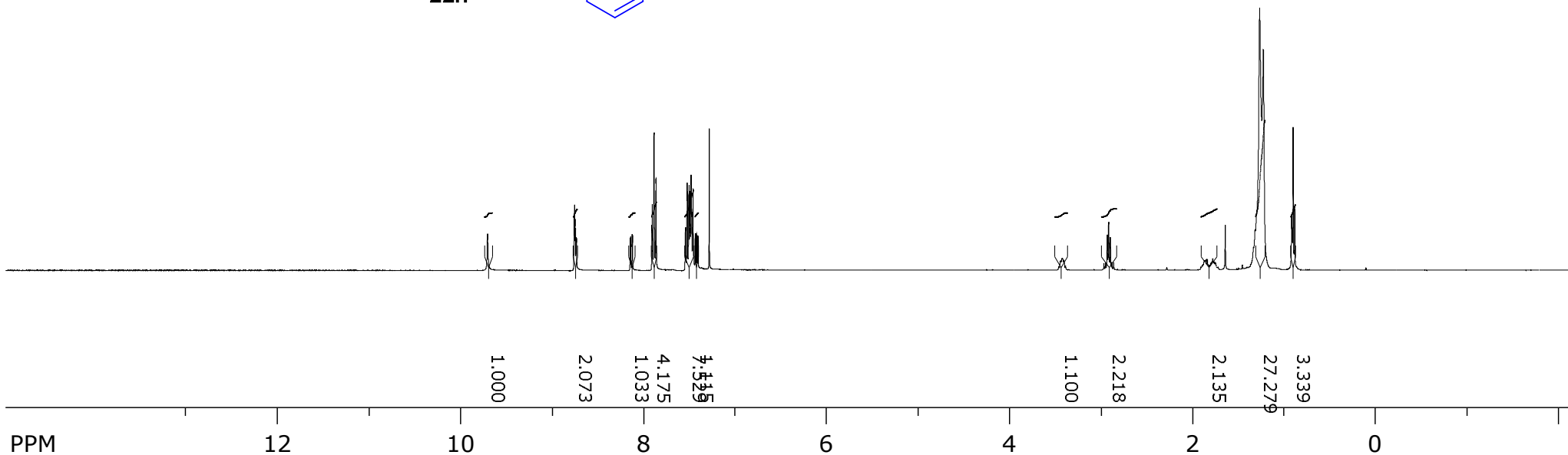
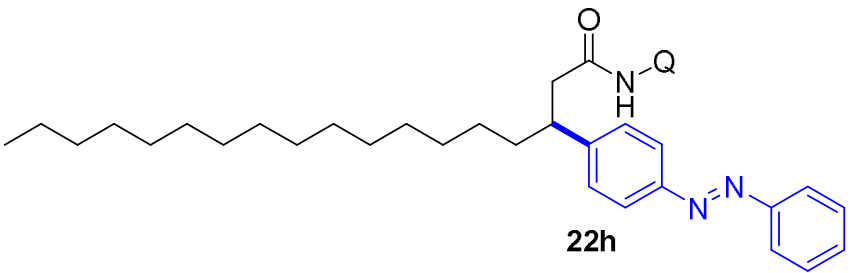


SpinWorks 4: SS-757
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 2

7.2834
7.1900
7.1004
8.1232
8.1438
8.1479
8.7358
8.7400
8.7472
8.7516
8.7579
8.7618
9.7076

1.9808
3.4000

0.8795
0.8971
0.9138
1.2232
1.2640
1.6396
1.7433
1.7541
1.7670
1.8000



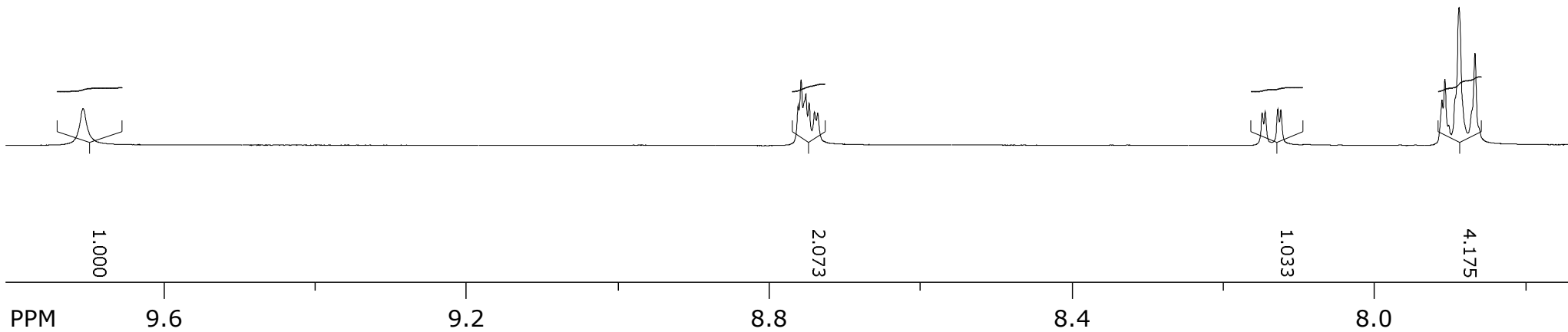
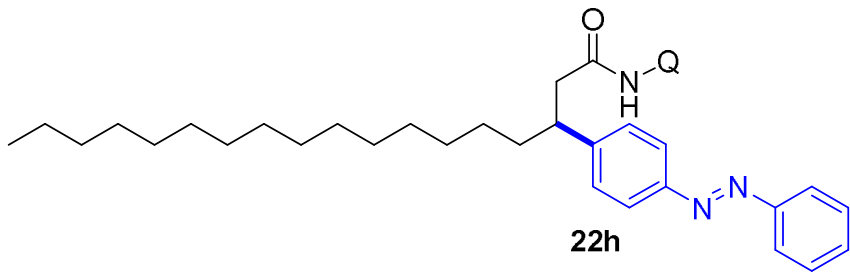
SpinWorks 4: SS-757
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 2

9.7076

8.7358
8.7400
8.7472
8.7516
8.7579
8.7618

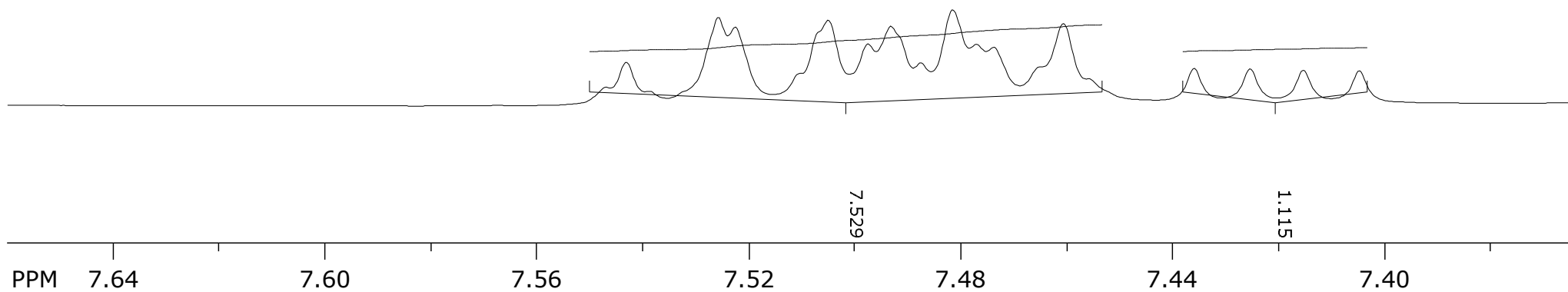
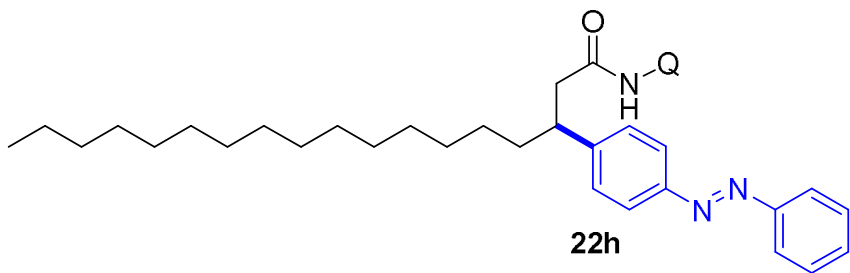
8.1231
8.1272
8.1438
8.1479

7.8664
7.8874
7.9012
7.9063
7.9100



SpinWorks 4: SS-757
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 2

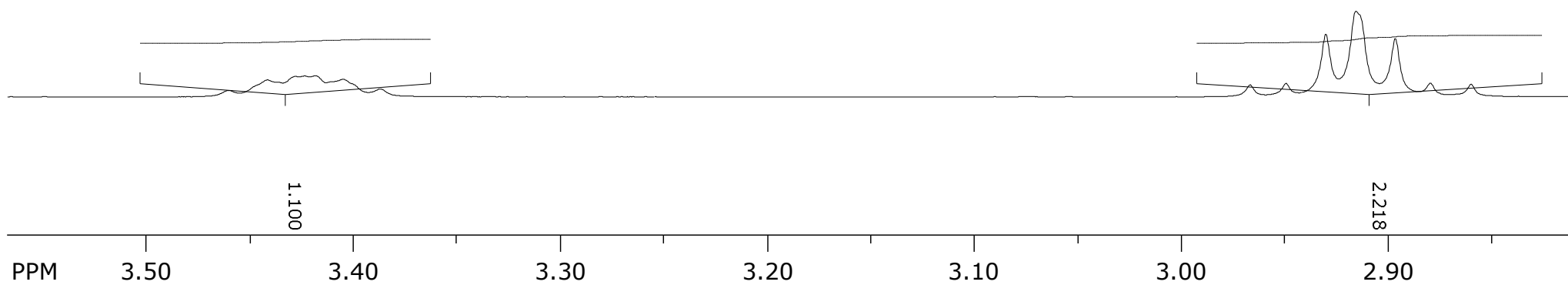
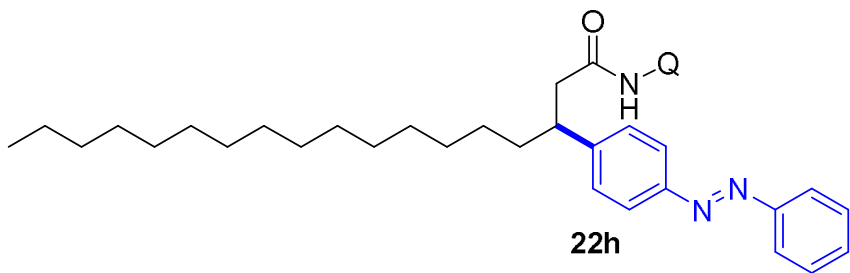
7.5389 —
7.5432 —
7.5469 —
7.5226 —
7.5258 —
7.5102 —
7.5050 —
7.4975 —
7.4932 —
7.4875 —
7.4815 —
7.4770 —
7.4737 —
7.4606 —
7.4559 —
7.4359 —
7.4253 —
7.4152 —
7.4046 —



SpinWorks 4: SS-757
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 2

3.4051
3.4185
3.4236
3.4281
3.4369
3.4416

2.8598
2.8795
2.8964
2.9154
2.9300
2.9492
2.9666

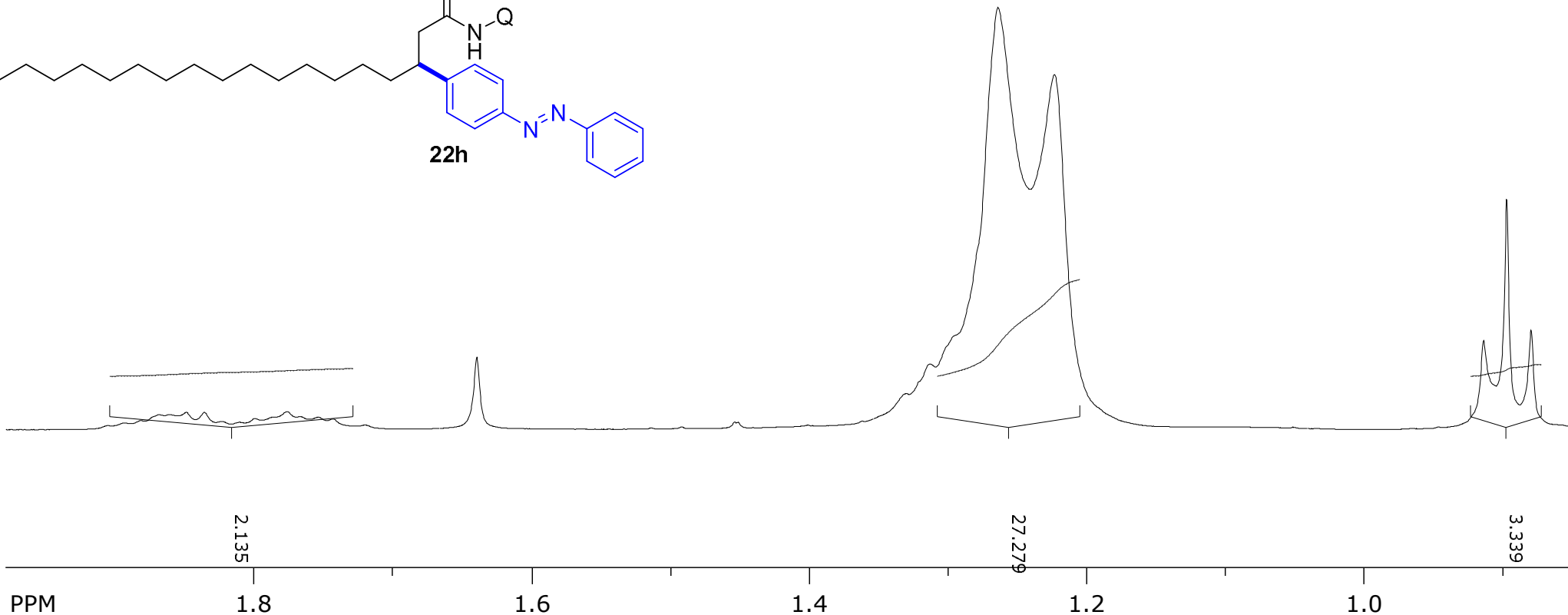
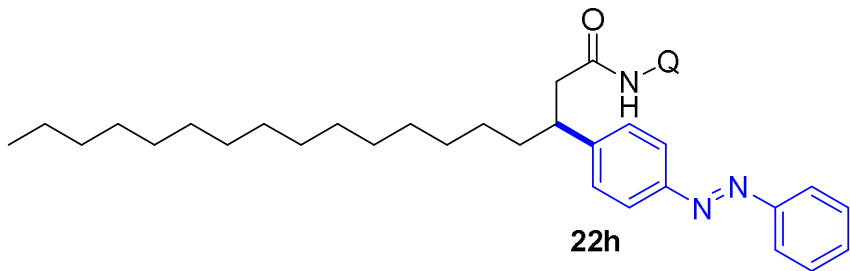


SpinWorks 4: SS-757
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 2

1.7433
1.7541
1.7670
1.7763
1.7855
1.7866
1.7997
1.8361
1.8492
1.8543
1.8552
1.8616
1.8686

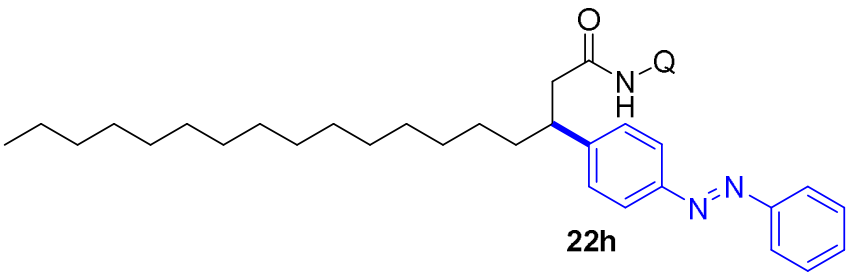
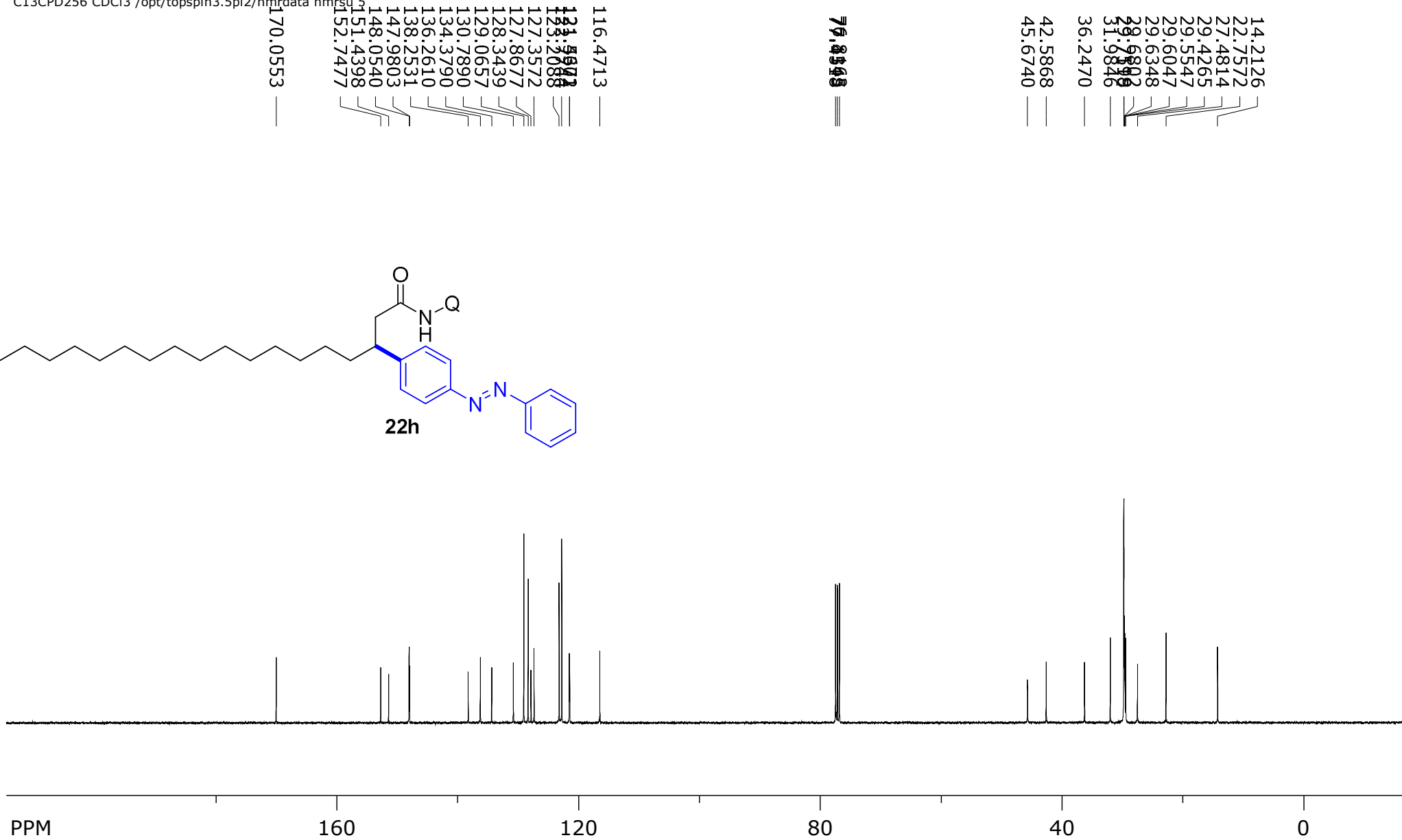
1.2232
1.2640

0.8795
0.8971
0.9138



SpinWorks 4: SS-757

C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu_5



PPM

160

120

80

40

0

SpinWorks 4: SS-757
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 5

170.0553

151.4398
152.7477

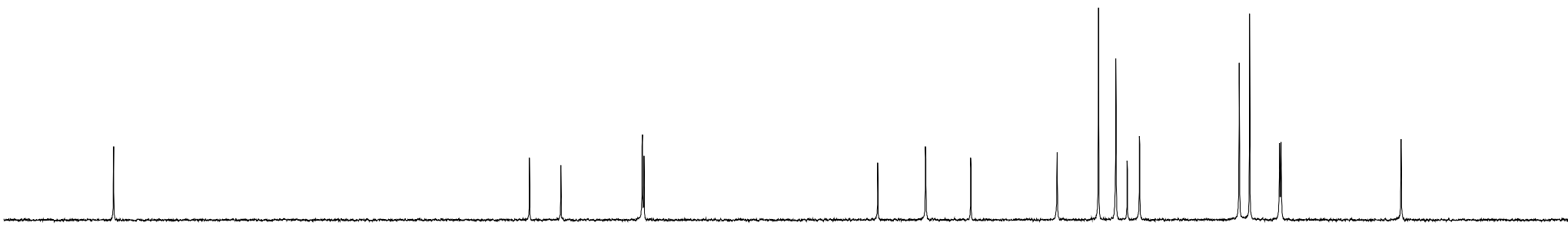
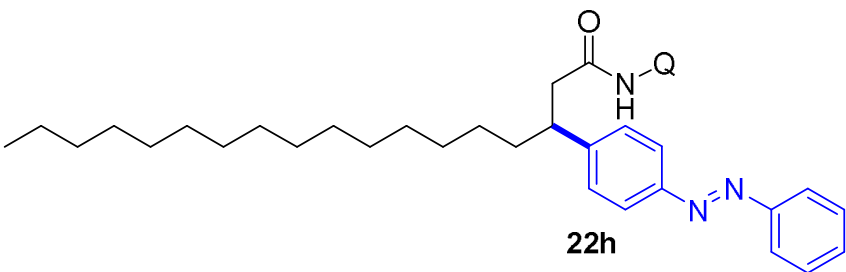
147.9803
148.0540

138.2531
136.2610
134.3790

130.7890
129.0657
128.3439
127.8677
127.3572

123.2088
122.7744
121.5302
121.4671

116.4713



PPM 160 150 140 130 120

SpinWorks 4: SS-757
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 5

45.6740

42.5868

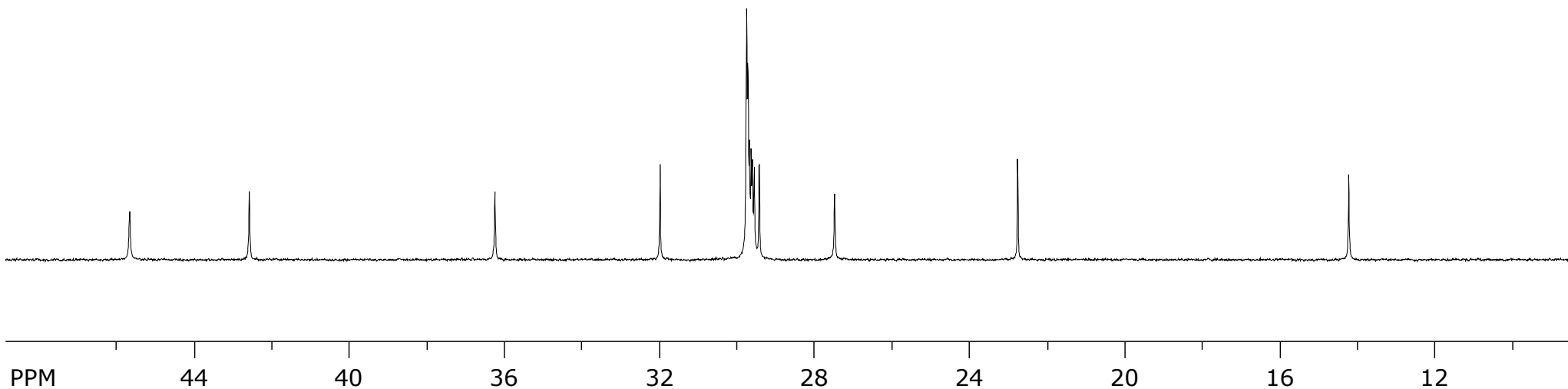
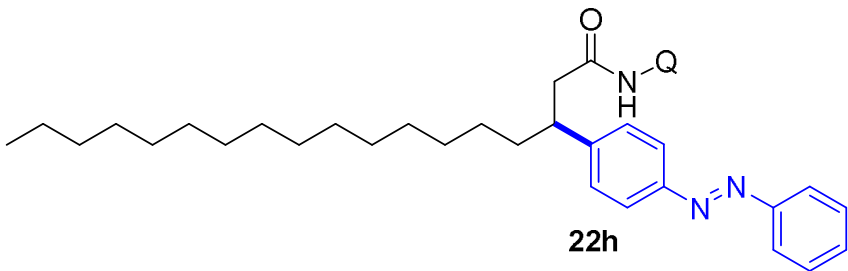
36.2470

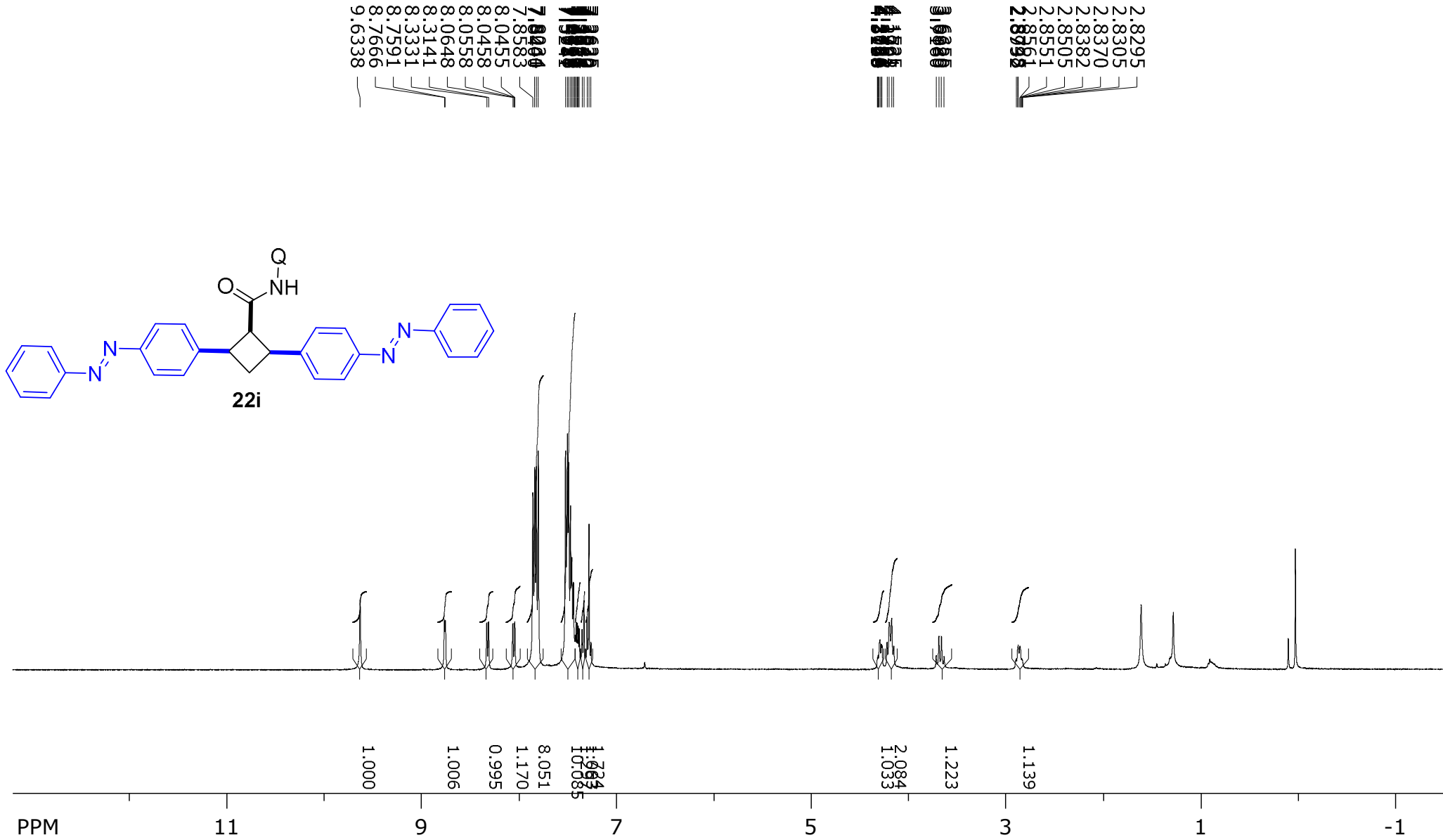
31.9846

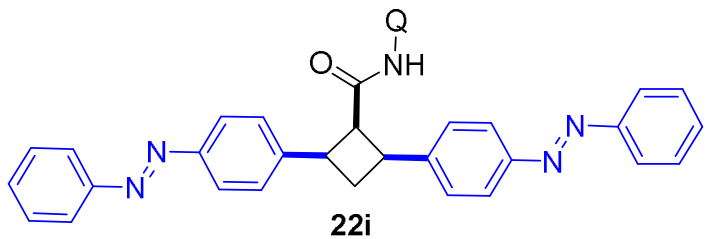
27.4814
29.4265
29.5547
29.6047
29.6348
29.6802
29.7199
29.7518

22.7572

14.2126





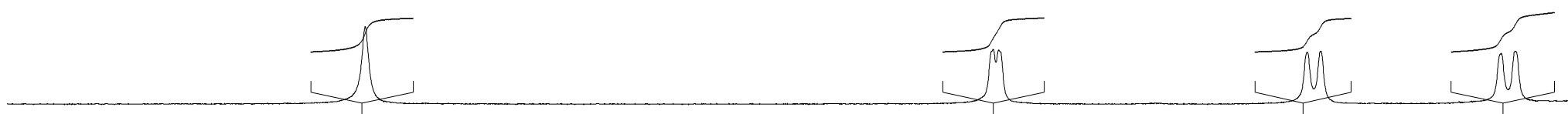


9.6338

8.7591
8.7666

8.3141
8.3331

8.0455
8.0458
8.0558
8.0648



1.000

1.006

0.995

1.170

PPM

9.6

9.2

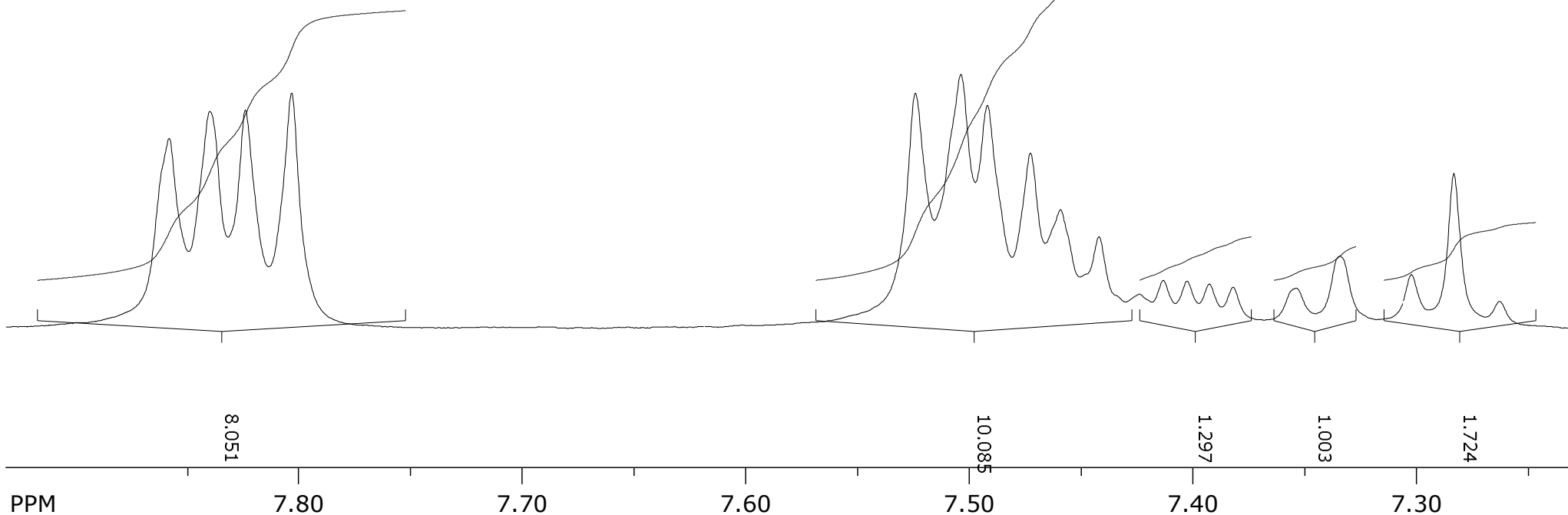
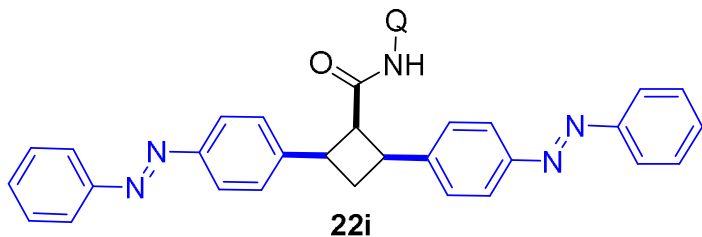
8.8

8.4

8.0

7.8034
7.8241
7.8400
7.8583

7.2625
7.2830
7.3020
7.3340
7.3534
7.3818
7.3925
7.4025
7.4131
7.4238
7.4419
7.4591
7.4726
7.4918
7.5037
7.5241



PPM

7.80

7.70

7.60

7.50

7.40

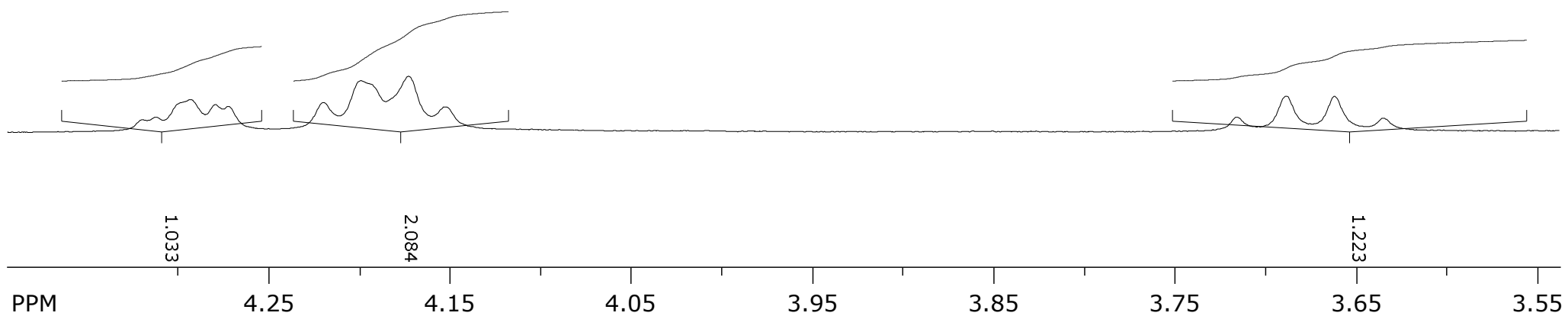
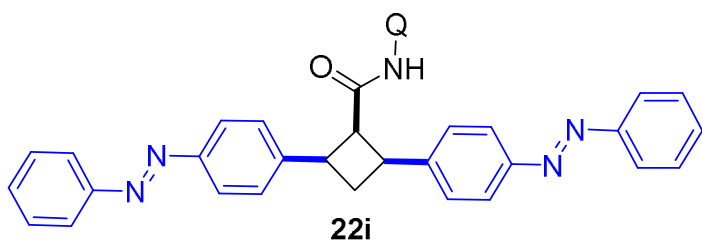
7.30

SpinWorks 4: SS-304-P2-REP

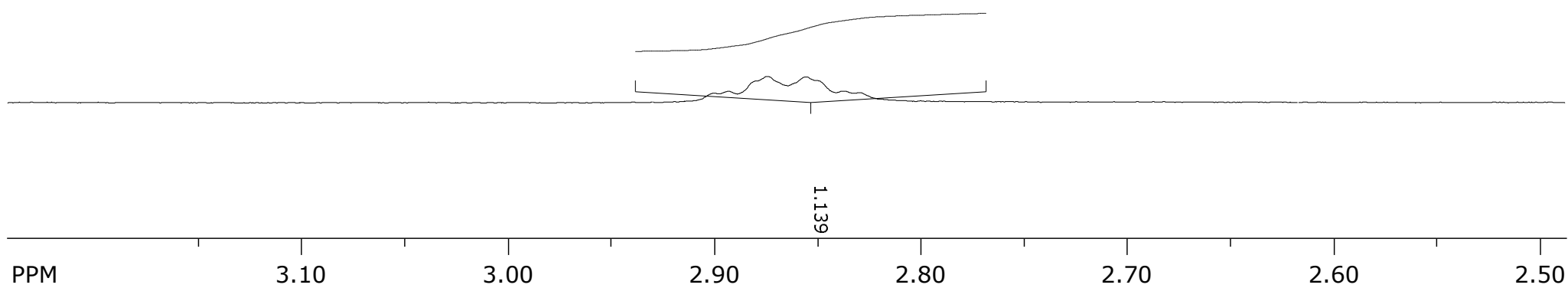
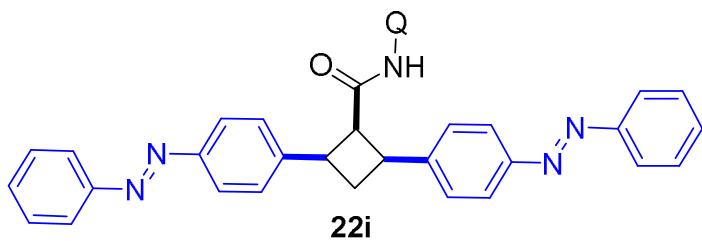
4.2727
4.2796
4.2934
4.3086
4.3125
4.3168
4.3199

4.2201
4.1995
4.1731
4.1525

3.7160
3.6885
3.6620
3.6355

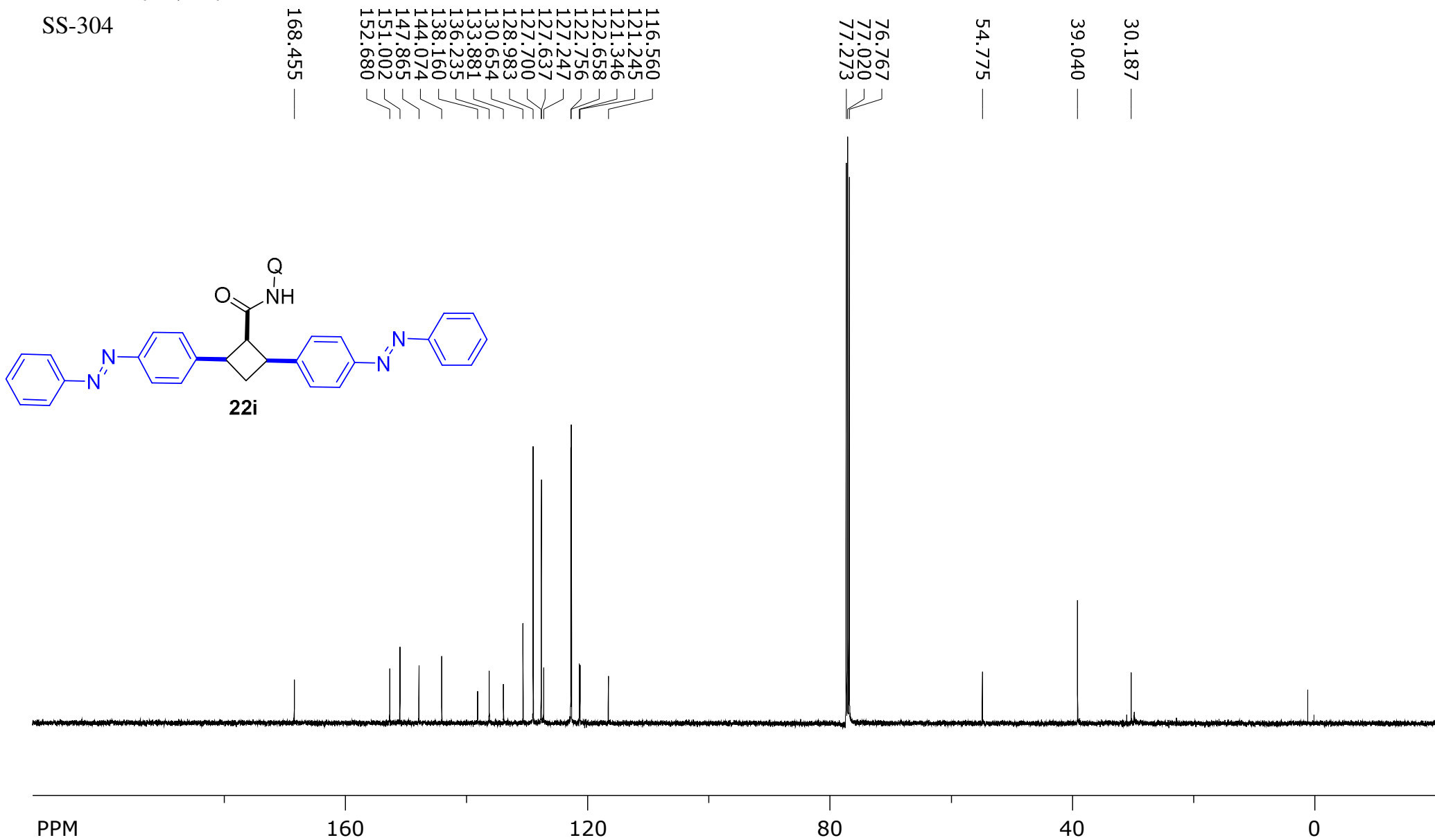


2.8295
2.8305
2.8370
2.8382
2.8505
2.8551
2.8561
2.8745
2.8798
2.8932

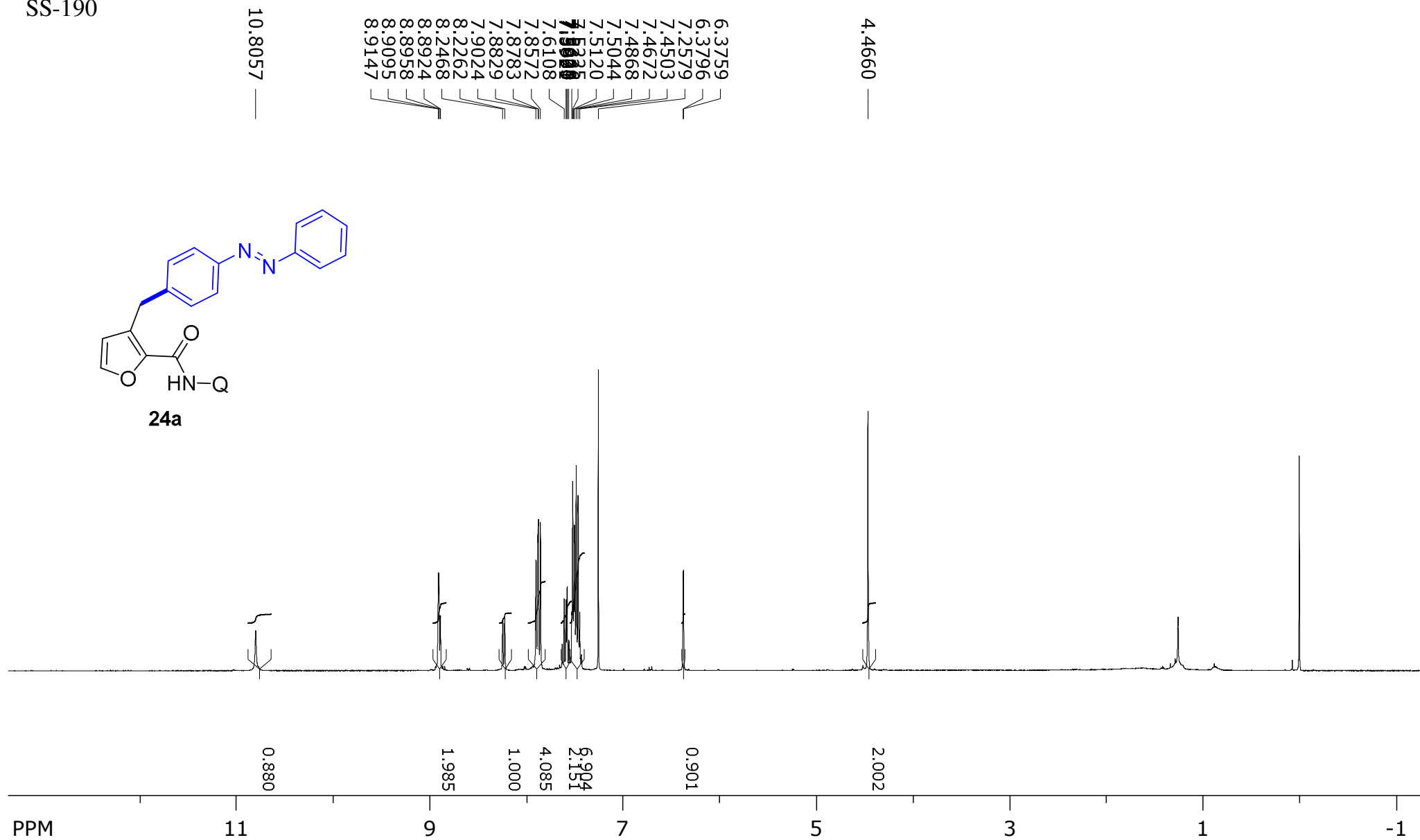
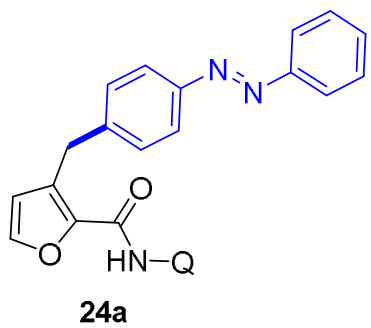


SpinWorks 4: SV100707
C13CPD CDCl3 {D:\Spectra} nmr 7

SS-304



SS-190

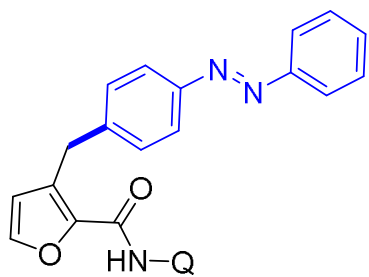


8.8924
8.8958
8.9095
8.9147

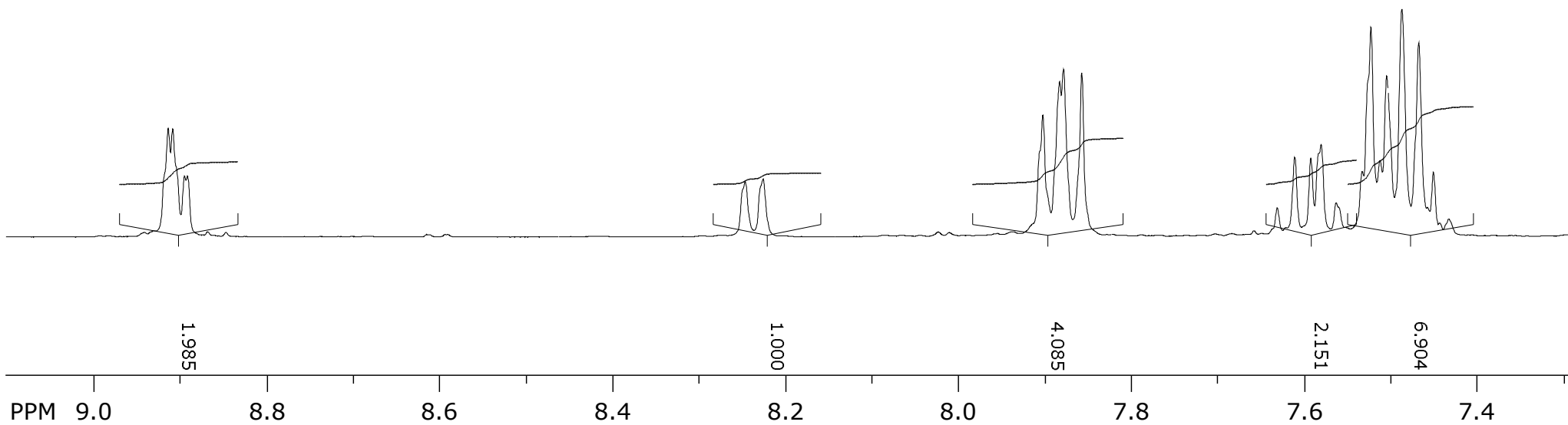
8.2262
8.2468

7.8572
7.8783
7.8829
7.9024

7.4503
7.4672
7.4868
7.5044
7.5120
7.5225
7.5326
7.5628
7.5803
7.5830
7.5921
7.6108

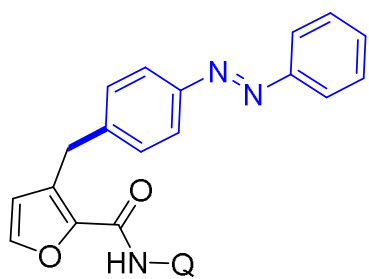


24a

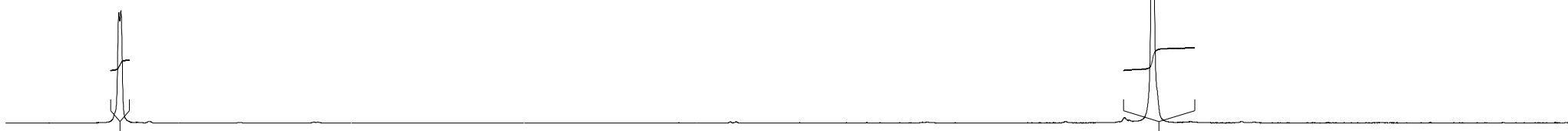


6.3759
6.3796

4.4660



24a



0.901

2.002

PPM

6.0

5.6

5.2

4.8

4.4

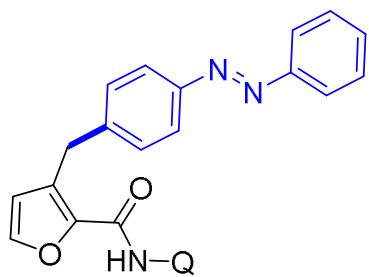
4.0

SpinWorks 4: SS190 P
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 49

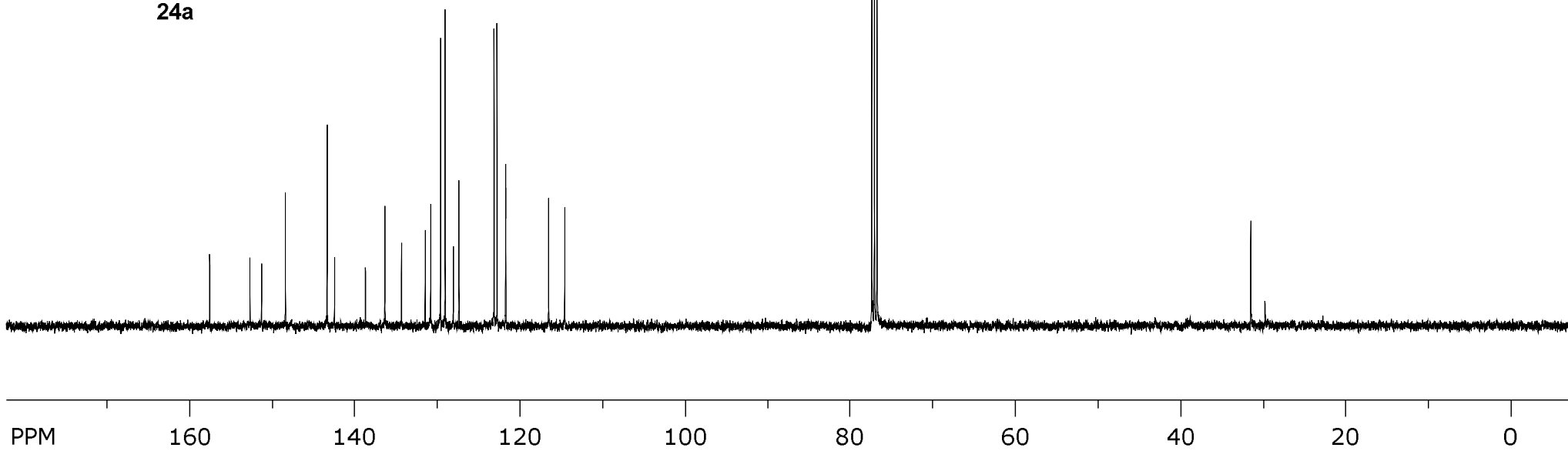
114.592
116.547
121.728
121.752
122.796
123.152
127.404
128.083
129.081
129.633
130.827
131.499
134.374
136.377
138.738
142.483
143.375
148.431
151.322
152.720
157.609

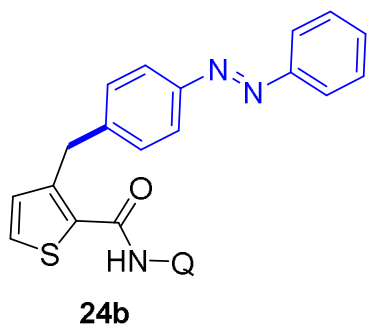
76.756
77.073
77.391

31.471

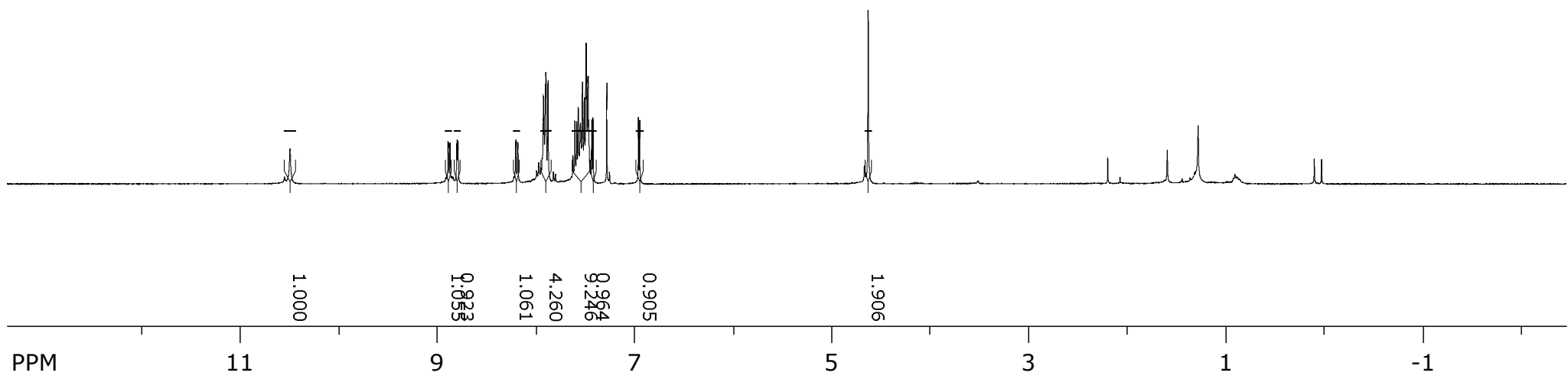


24a





| | | | | | | | | | | | | | | | | |
|---------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| 10.5008 | 8.8960 | 8.8923 | 8.8775 | 8.8739 | 8.8080 | 8.8041 | 8.7936 | 8.2009 | 7.9907 | 7.4728 | 7.4662 | 7.4367 | 7.4240 | 7.2837 | 6.9500 | 4.6296 |
|---------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|

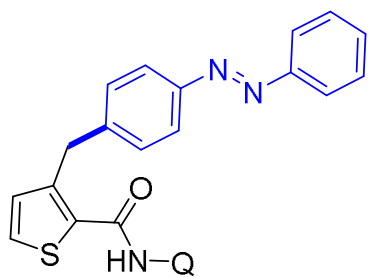


SpinWorks 4: ss-179-p

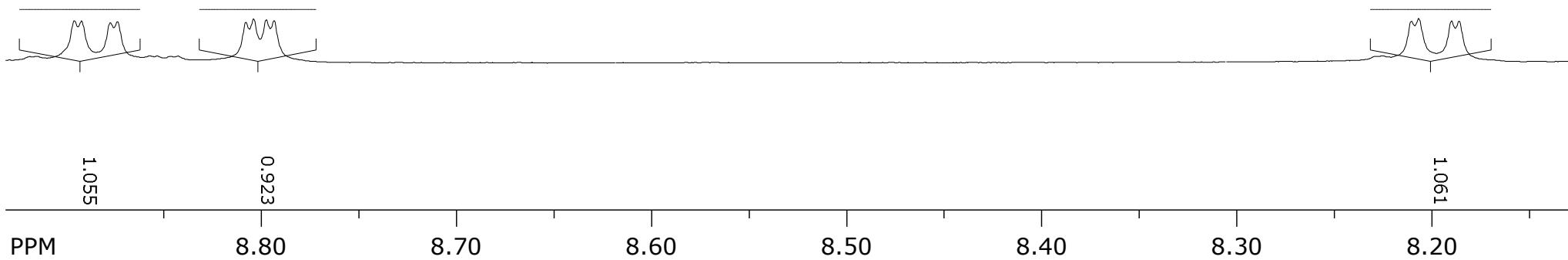
8.8739
8.8775
8.8923
8.8960

8.7936
8.7976
8.8041
8.8080

8.1861
8.1899
8.2067
8.2105

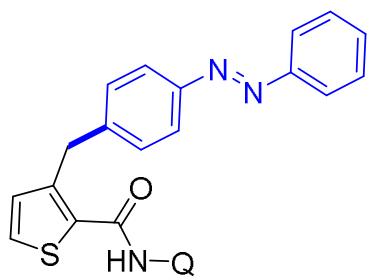


24b

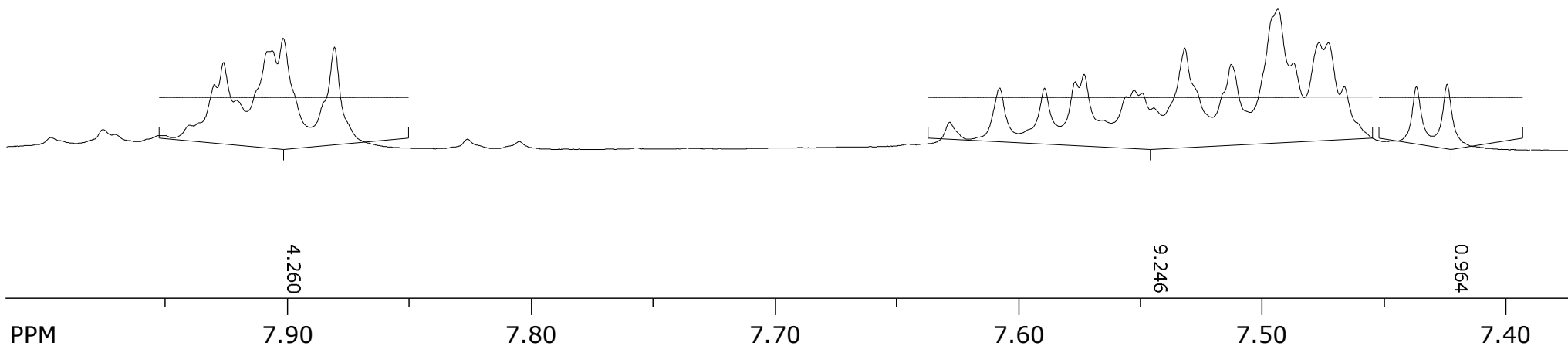


7.9017
7.9063
7.9082
7.9209
7.9263
7.9300
7.9402
7.8807

7.4240
7.4367
7.4662
7.4728
7.4767
7.4871
7.4936
7.5127
7.5317
7.5444
7.5492
7.5525
7.5558
7.5656
7.5730
7.5767
7.5892
7.6077
7.6282

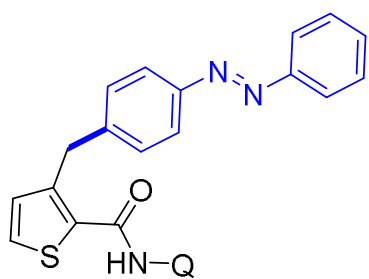


24b

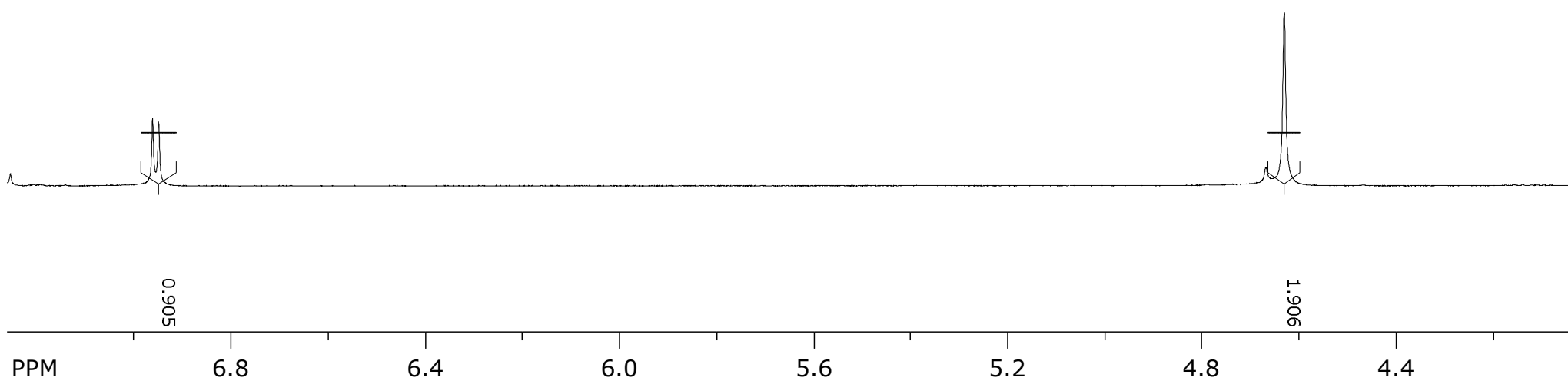


6.9500
6.9627

4.6296



24b

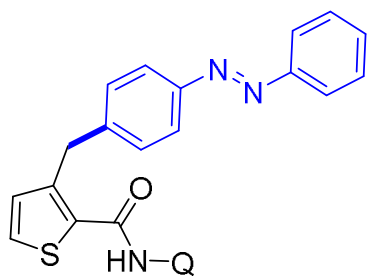


SpinWorks 4: SS 179 P
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 24

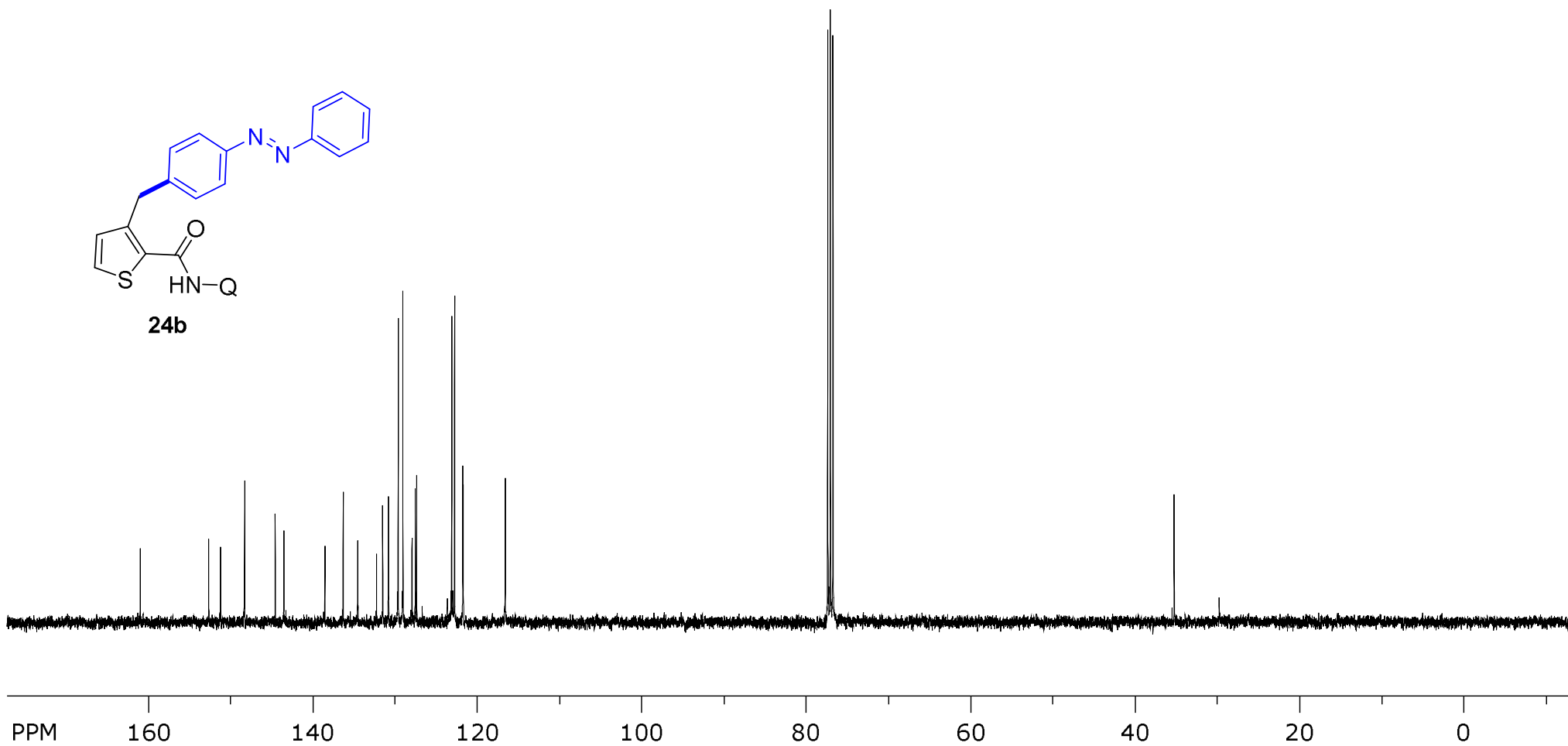
116.628
121.744
121.801
122.796
123.147
127.415
127.577
127.981
129.086
129.662
130.841
131.552
132.298
134.590
136.362
138.581
143.574
144.625
148.353
151.277
152.719
161.052

76.755
77.072
77.390

35.234

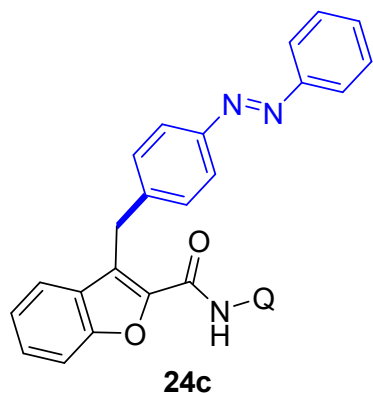


24b



SpinWorks 4: DC-195

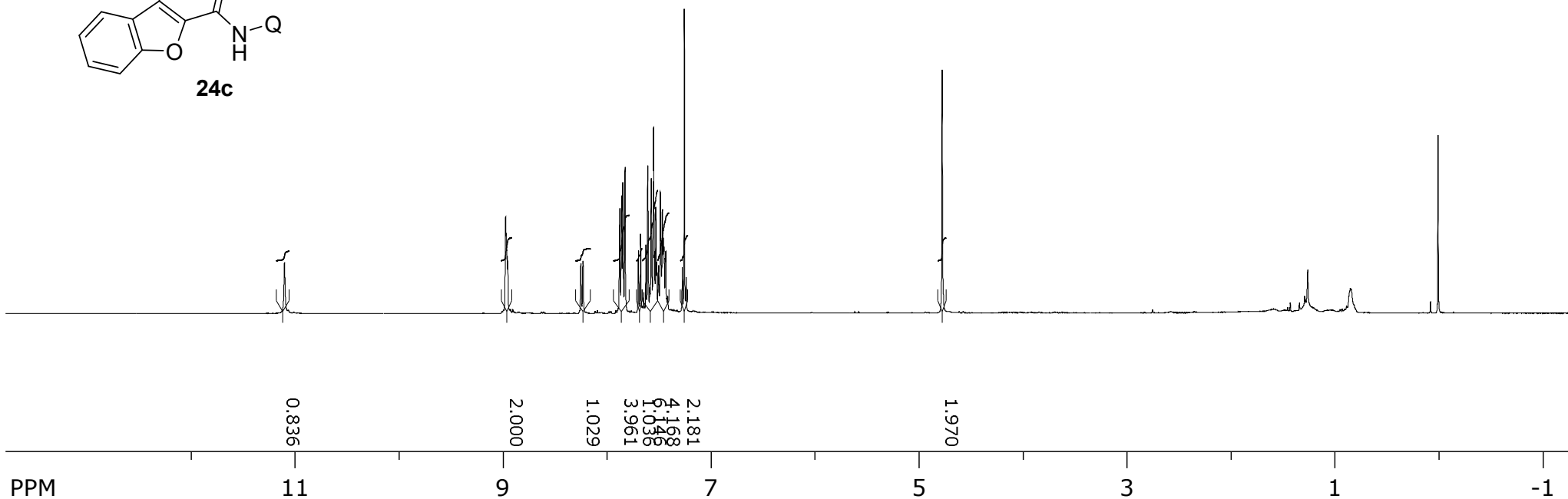
SS-180 rep



11.1062

7.2389
7.2564
7.2765
7.4350
7.4406
7.4521
7.4590
7.8276
7.8485
7.8598
7.8781
8.2315
8.2521
8.9558
8.9611
8.9661
8.9719
8.9775

4.7743

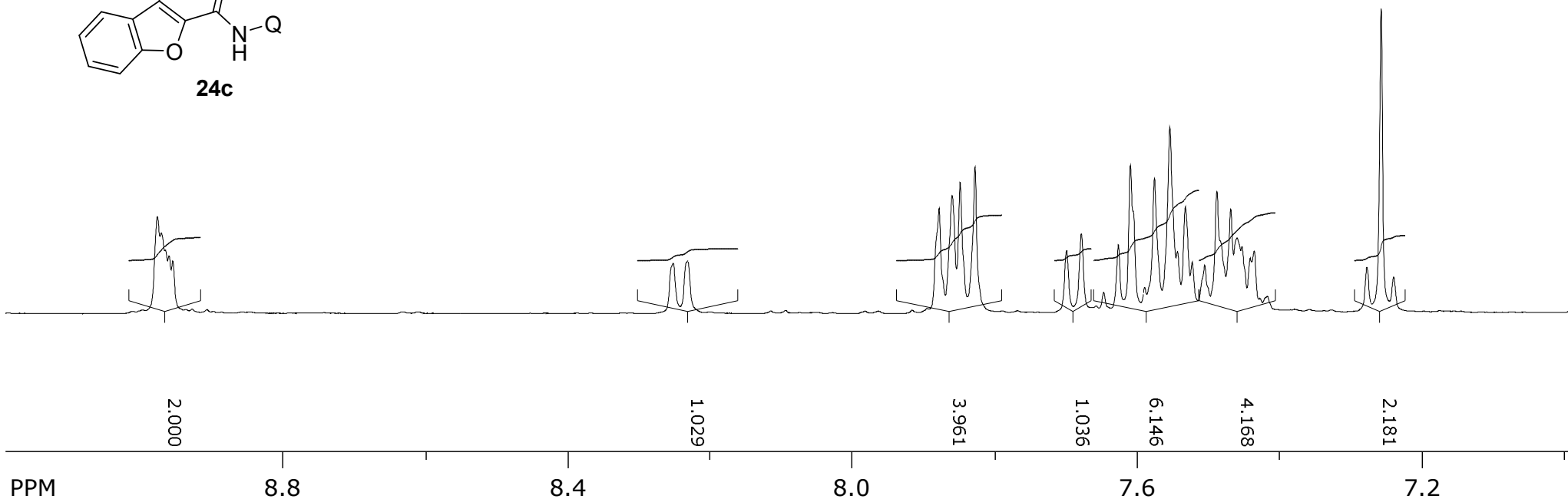
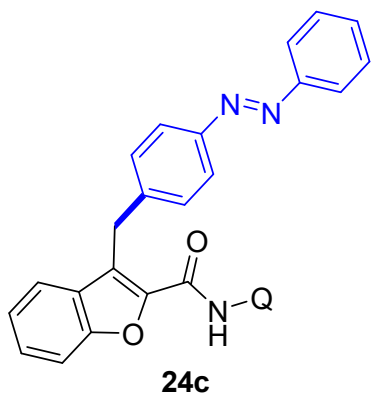


8.9558
8.9611
8.9661
8.9719
8.9775

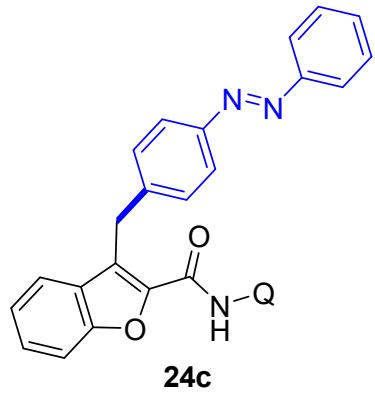
8.2315
8.2521

7.8276
7.8485
7.8598
7.8781

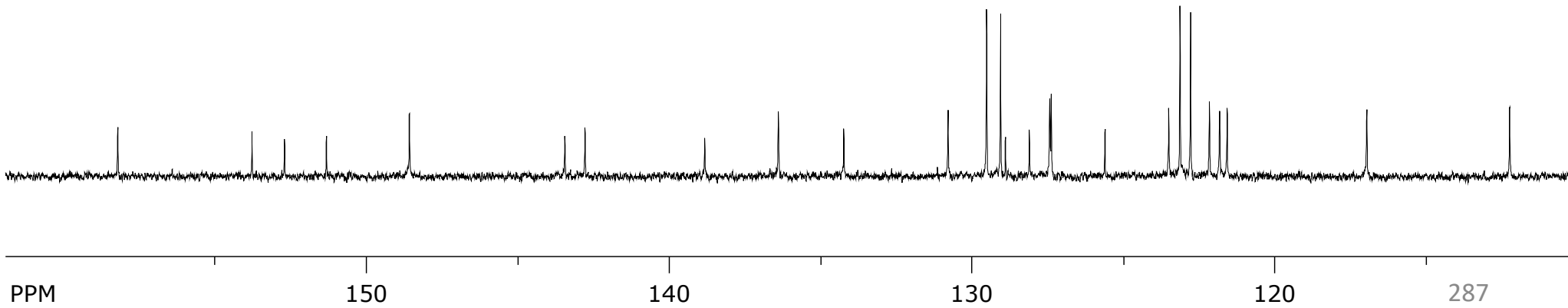
7.2389
7.2564
7.2765
7.4350
7.4406
7.4521
7.4590
7.4680
7.4874
7.5046
7.5221
7.5318
7.5430
7.5536
7.5752
7.6091
7.6260
7.6781
7.6988



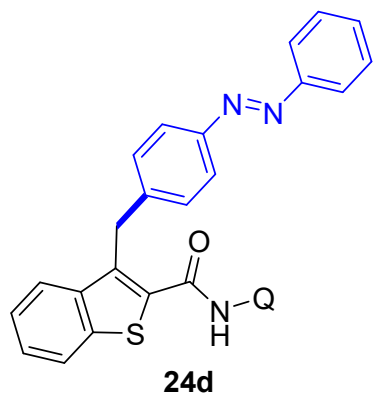
SpinWorks 4: SS 180 P
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 23



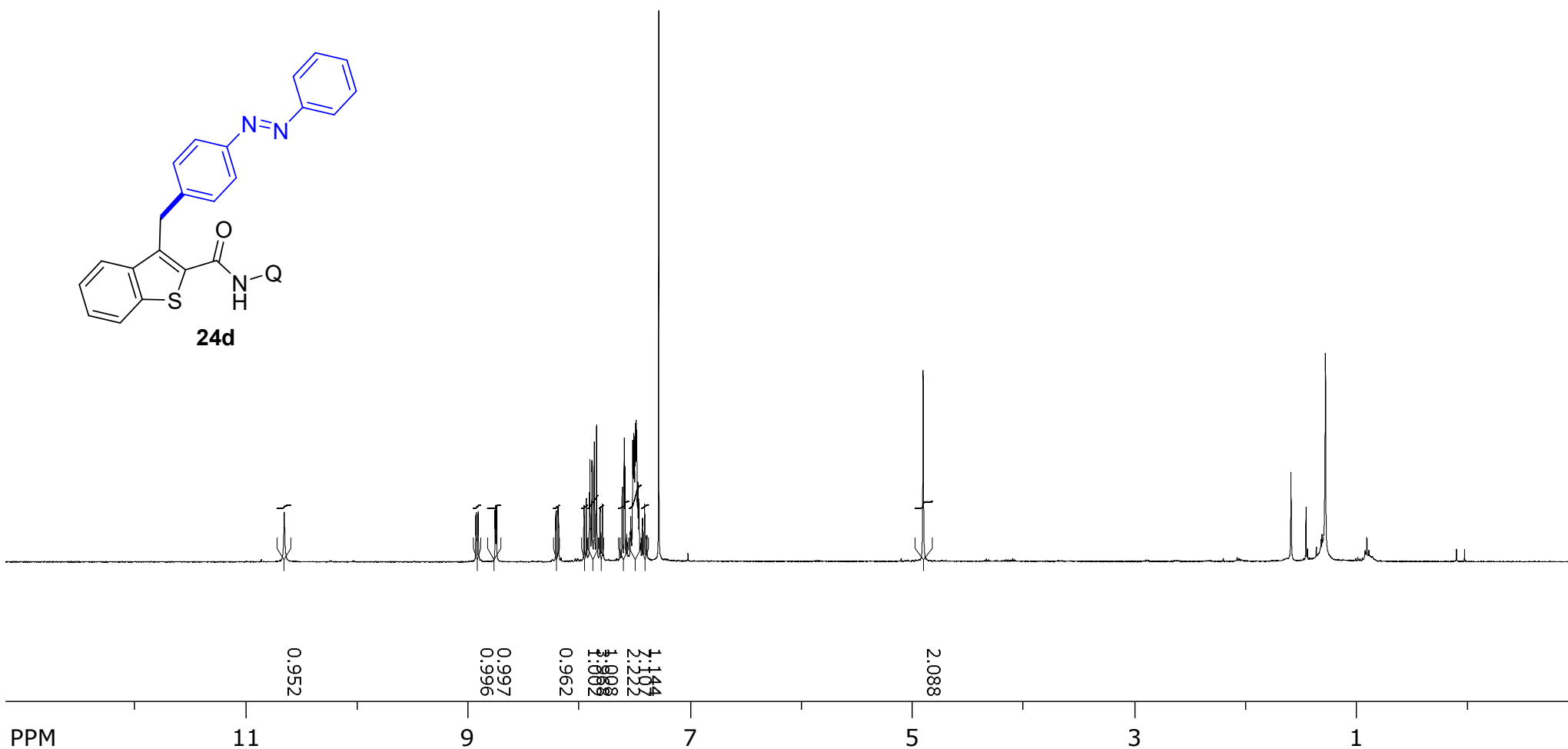
158.225 —
151.328 —
152.717 —
153.789 —
148.588 —
142.786 —
143.450 —
138.829 —
136.394 —
134.234 —
130.788 —
129.516 —
129.054 —
128.893 —
128.103 —
127.431 —
127.380 —
125.605 —
123.496 —
123.123 —
122.775 —
122.154 —
121.814 —
121.568 —
116.956 —
112.233 —



SpinWorks 4: SS-775-REP S1
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 32



10.6575
8.7433
8.7474
8.7539
8.7580
8.9090
8.9138
8.9266
8.9314
9.2894
9.2914
9.2934
9.2954
9.2974
7.4305
7.4279
7.4102
7.4080
7.3926
7.3897
7.2838
4.9013

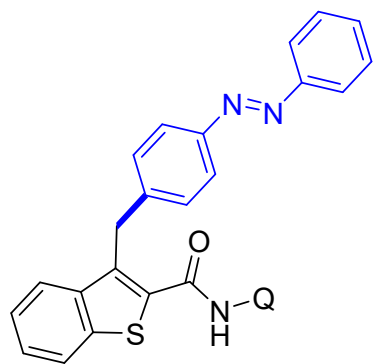


SpinWorks 4: SS-775-REP S1
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 32

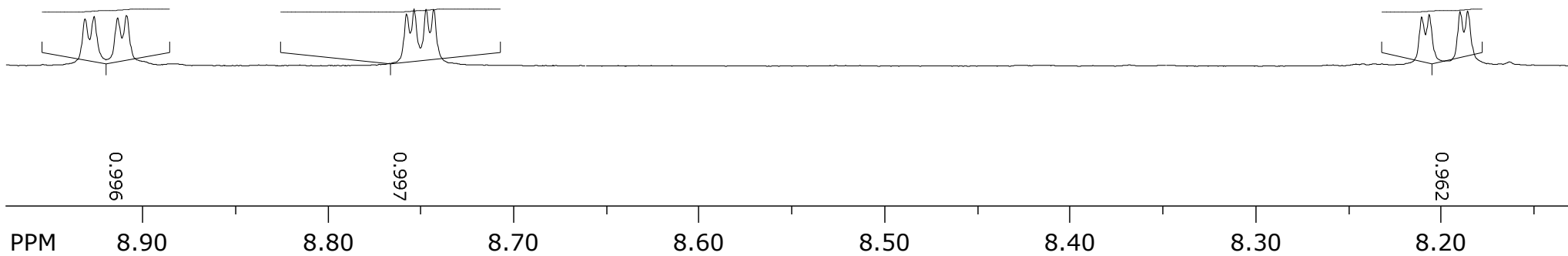
8.9090
8.9138
8.9266
8.9314

8.7433
8.7474
8.7539
8.7580

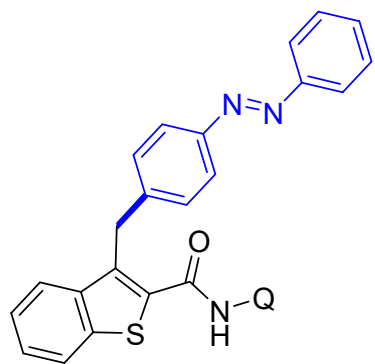
8.1856
8.1897
8.2064
8.2104



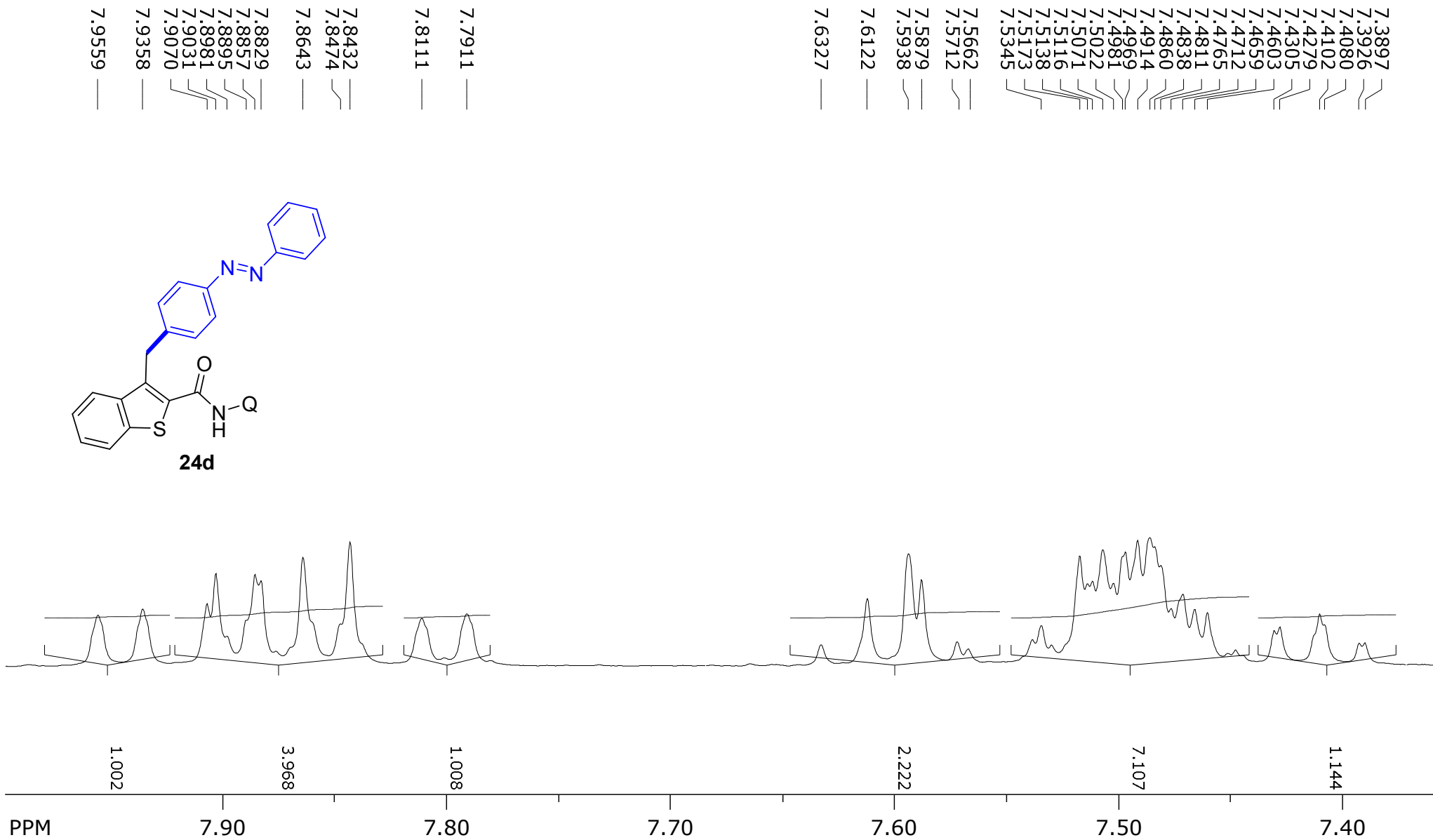
24d



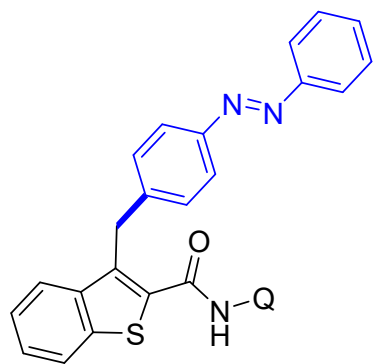
SpinWorks 4: SS-775-REP S1
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 32



24d



SpinWorks 4: SS-775 REP S1
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 13



24d

116.817
121.789
122.093
122.760
122.796
123.115
123.974
125.002
125.002
130.780
131.081
131.423
136.341
138.167
138.580
139.134
140.048
142.736
148.417
151.247
152.705
161.387

76.722
77.040
77.357

32.925

PPM

160

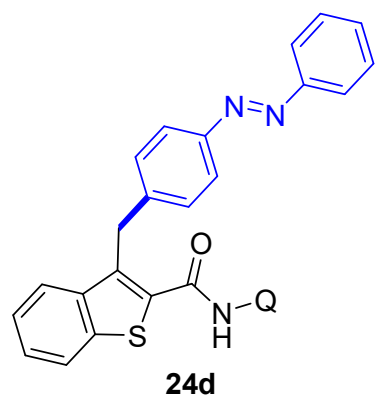
120

80

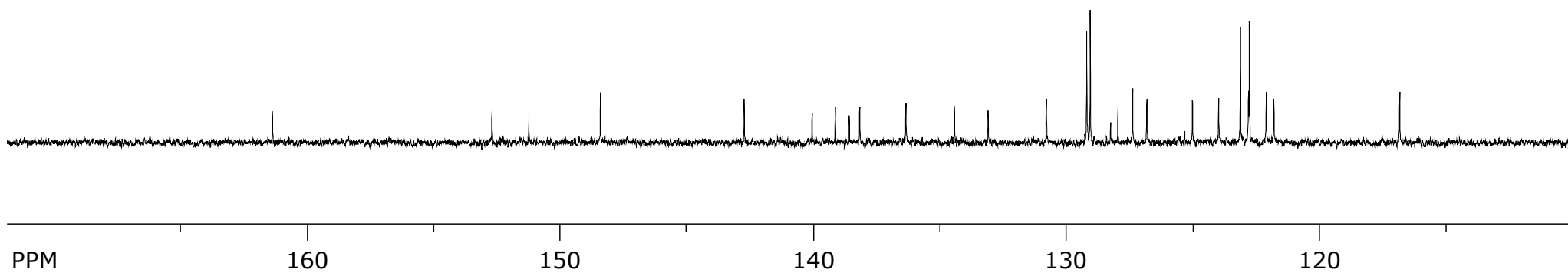
40

0

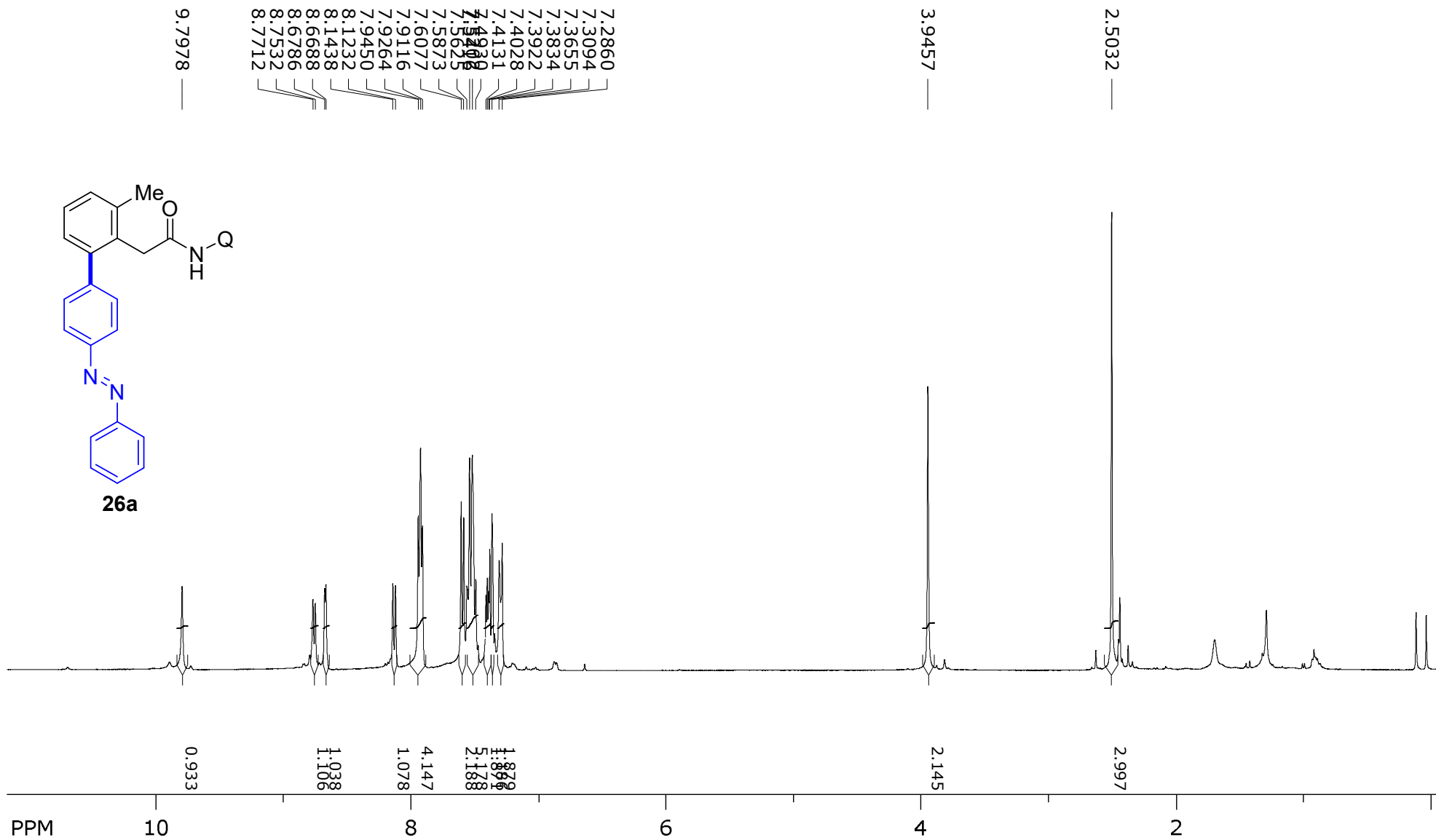
SpinWorks 4: SS-775 REP S1
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 13



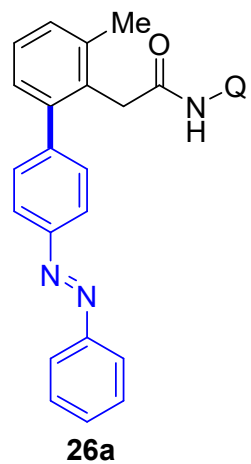
161.387 —
152.705 —
151.247 —
148.417 —
142.736 —
140.048 —
139.134 —
138.167 —
136.341 —
134.423 —
133.091 —
130.786 —
129.188 —
129.052 —
128.252 —
127.958 —
127.375 —
126.815 —
125.009 —
123.974 —
123.115 —
122.796 —
122.760 —
122.093 —
121.789 —
116.817 —



SpinWorks 4: ss-148-p
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 29



SpinWorks 4: ss-148-p
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 29



9.7978

8.6688
8.6786
8.7532
8.7712

8.1232
8.1438

7.9116
7.9264
7.9450

7.2860
7.3094
7.3655
7.3834
7.3922
7.4028
7.4131
7.4930
7.5202
7.5416
7.5625
7.5873
7.6077

0.933

1.106

1.038

1.078

4.147

2.188

5.178

1.871

1.186

1.879

PPM

10.0

9.6

9.2

8.8

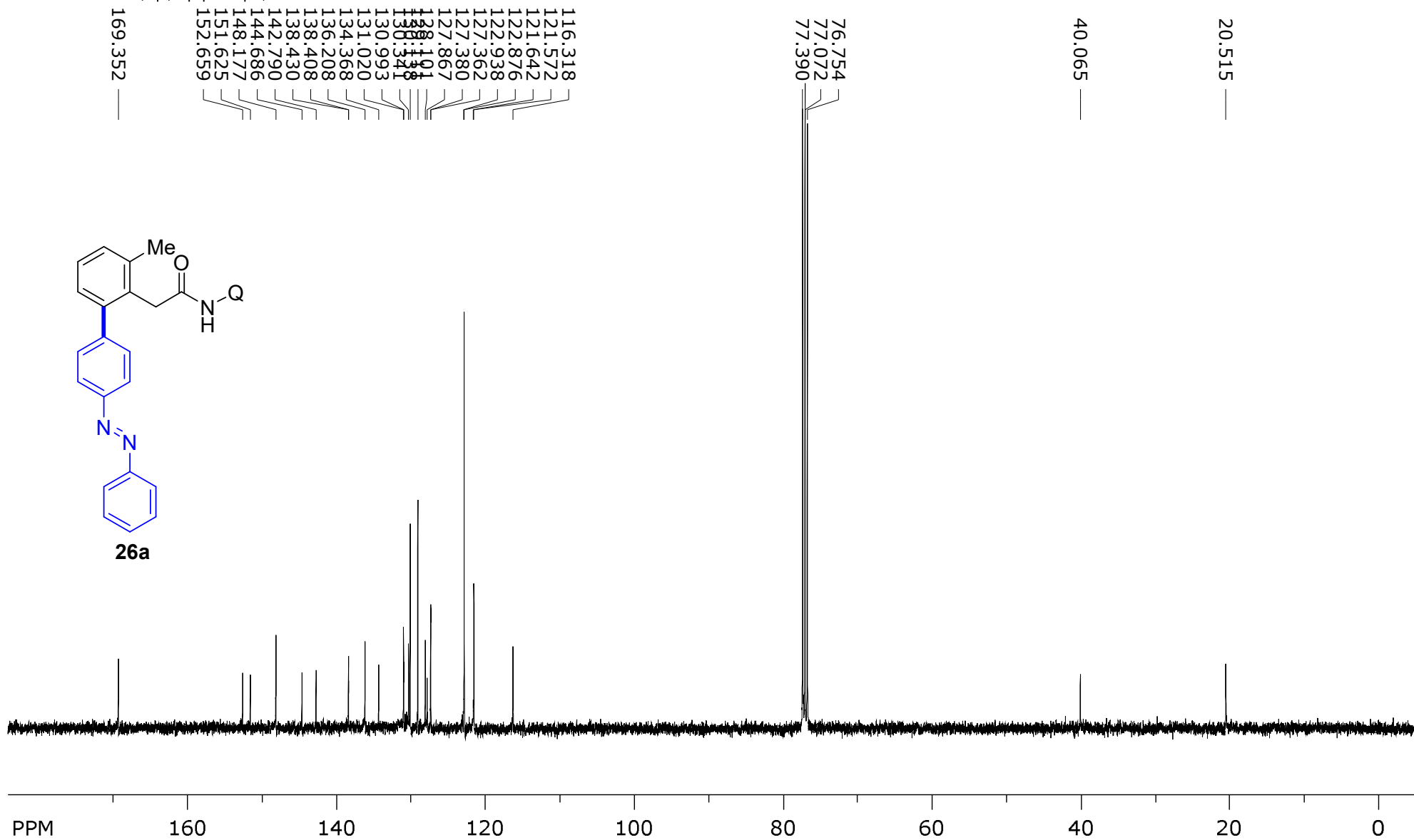
8.4

8.0

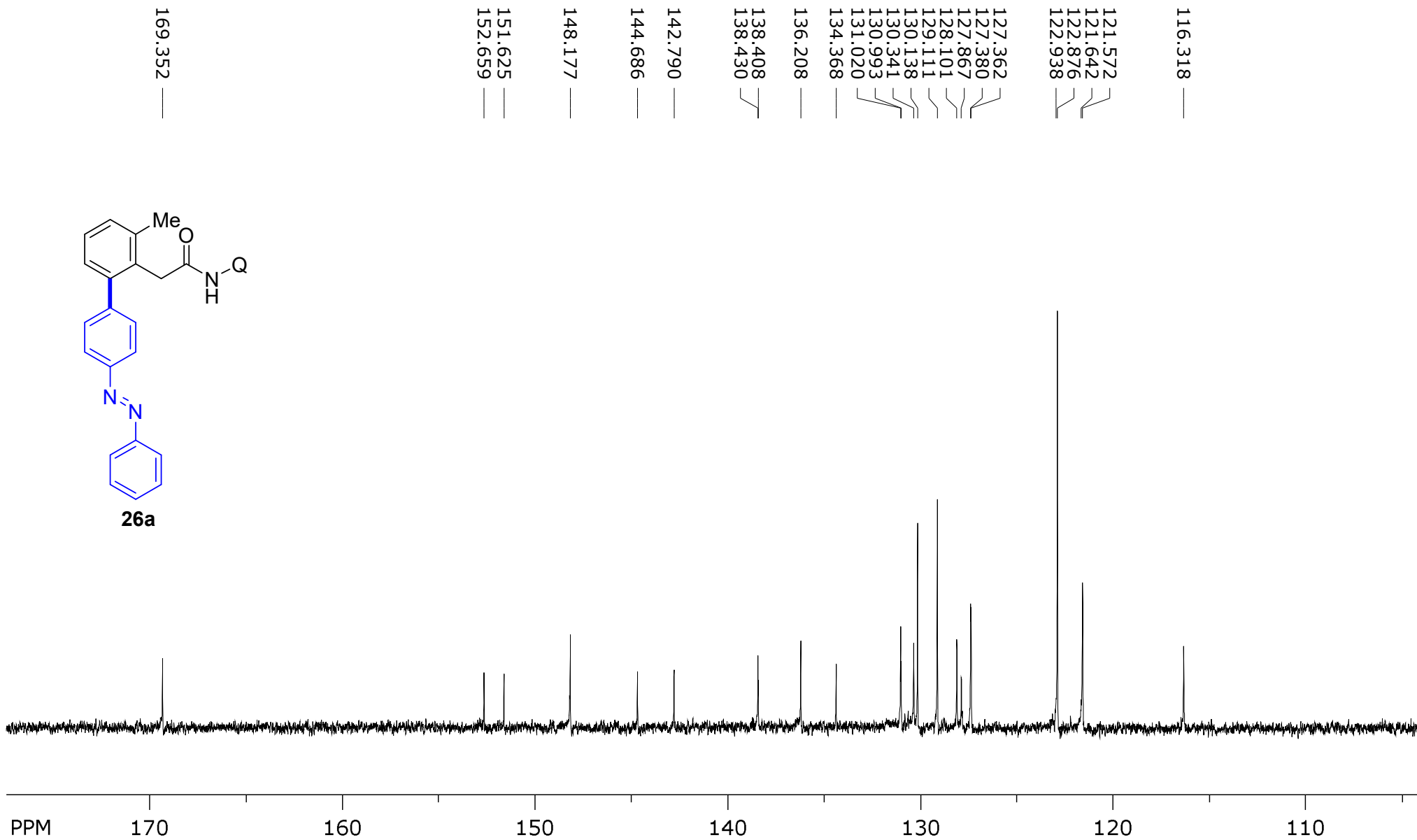
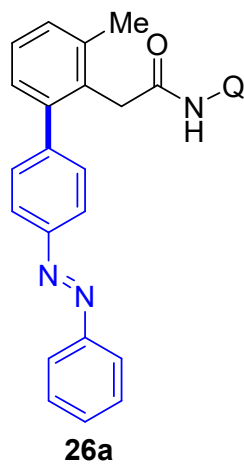
7.6

7.2

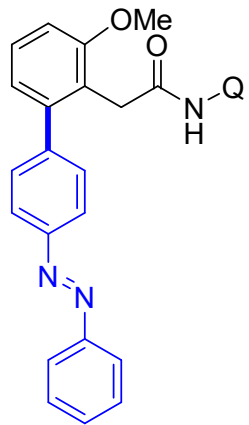
SpinWorks 4: ss-148-p
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 29



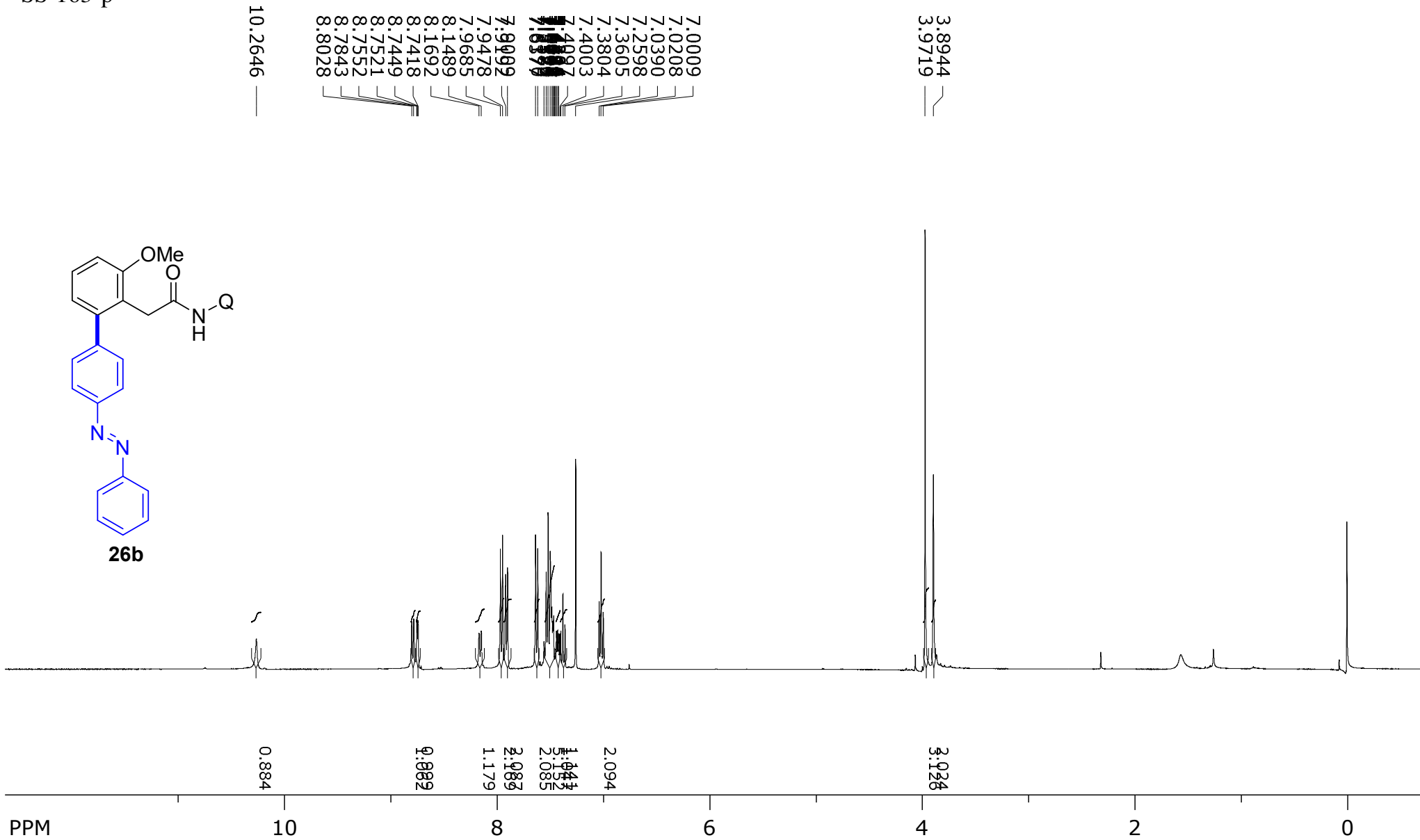
SpinWorks 4: ss-148-p
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 29



SS-163-p



26b



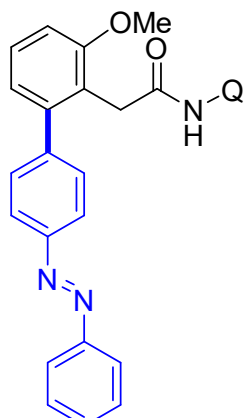
8.7418
8.7449
8.7521
8.7552
8.7843
8.8028

8.1489
8.1692

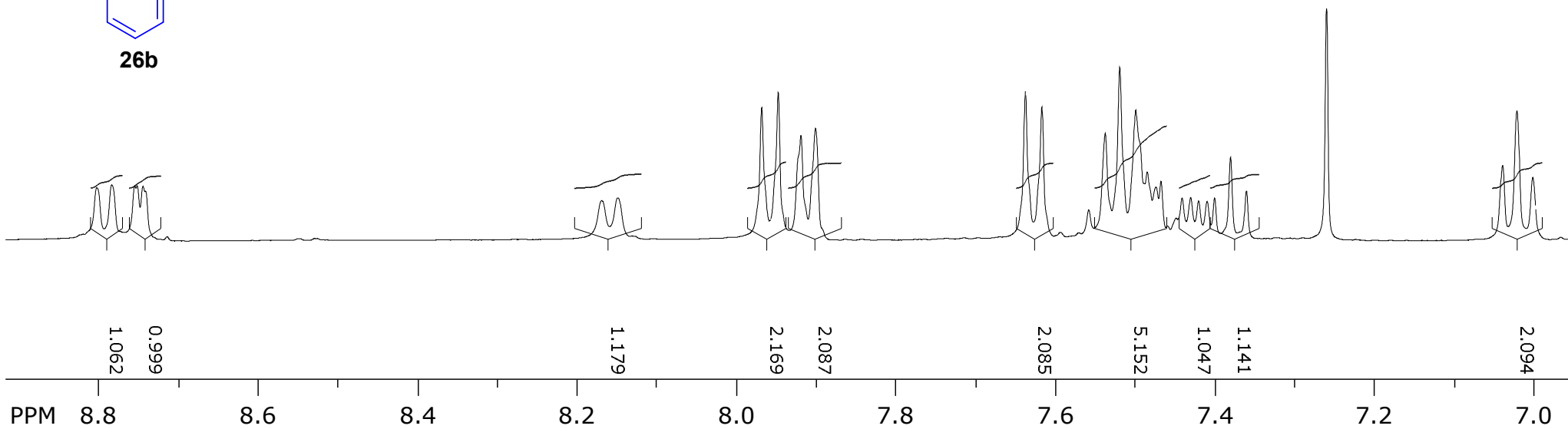
7.9009
7.9192
7.9478
7.9685

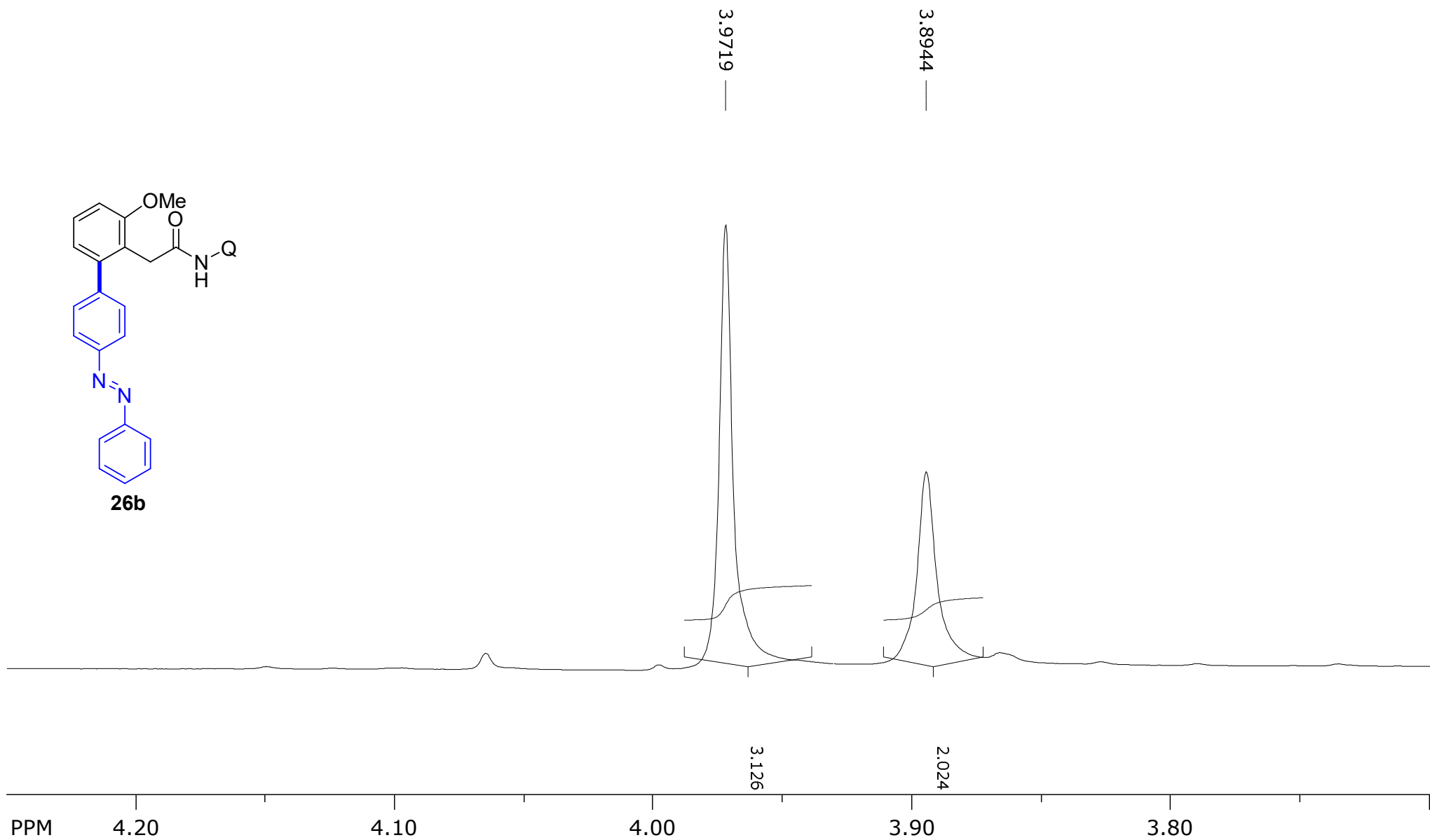
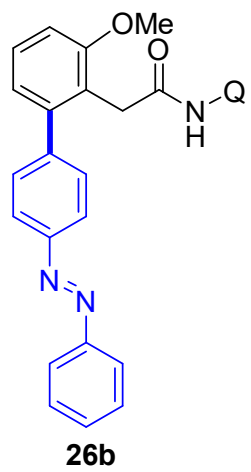
7.2598
7.3605
7.3804
7.4003
7.4097
7.4204
7.4304
7.4410
7.4485
7.4596
7.4676
7.4741
7.4848
7.4994
7.5194
7.5376
7.5582
7.6170
7.6377

7.0009
7.0208
7.0390



26b





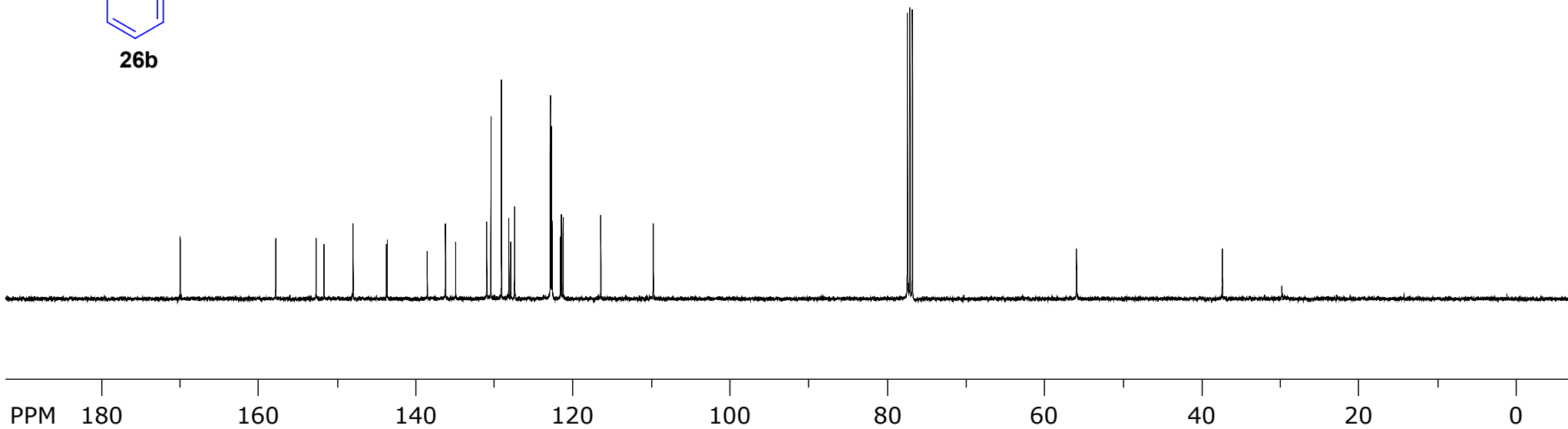
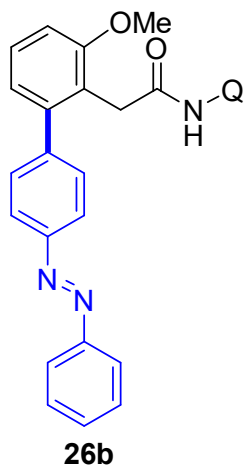
SpinWorks 4: SS 163 P
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 28

170.033
157.869
152.733
151.725
148.020
143.773
143.655
138.567
136.253
134.956
131.002
130.471
129.126
128.188
127.951
127.457
122.912
122.781
122.664
121.625
121.494
121.286
116.480
109.795

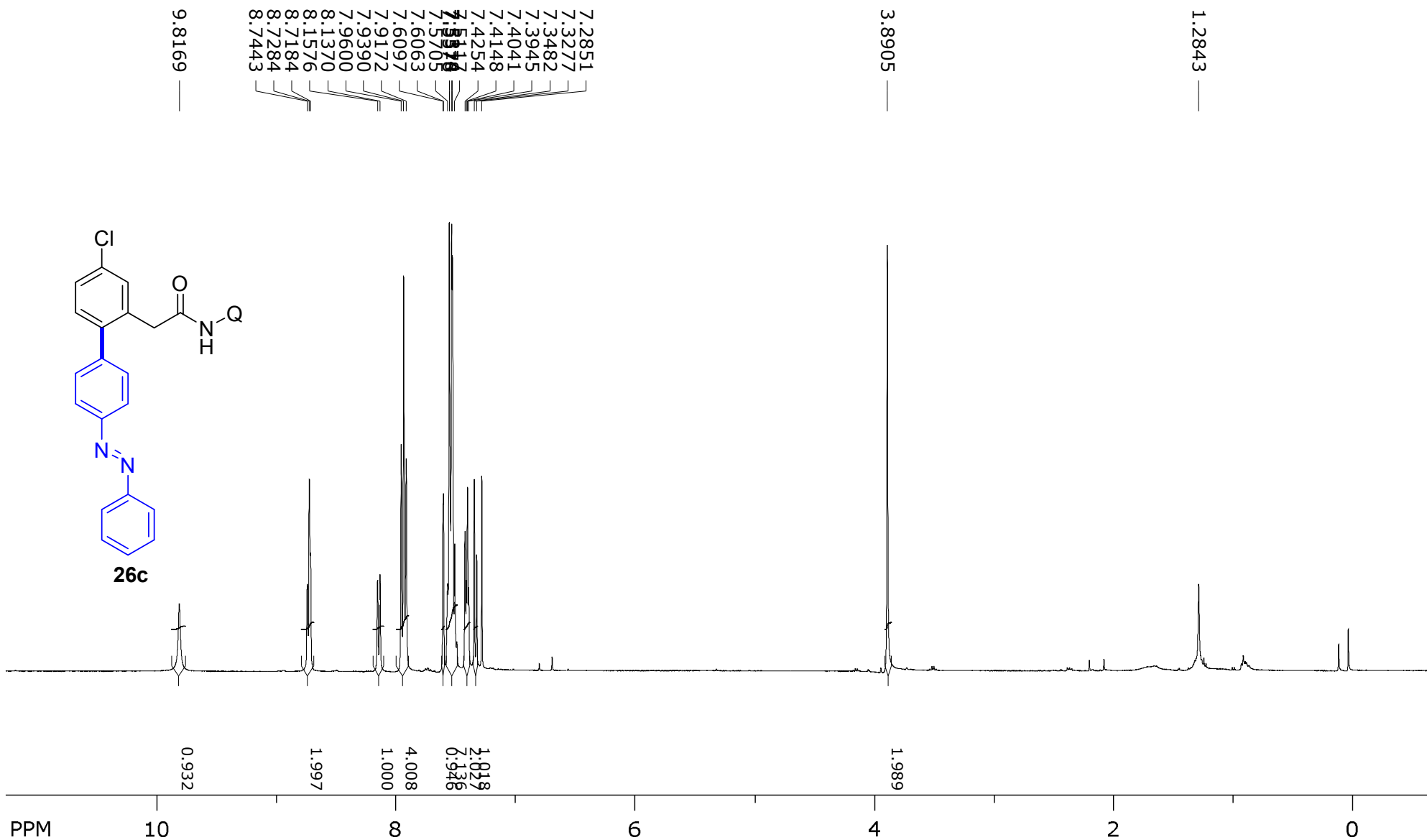
76.802
77.121
77.438

55.917

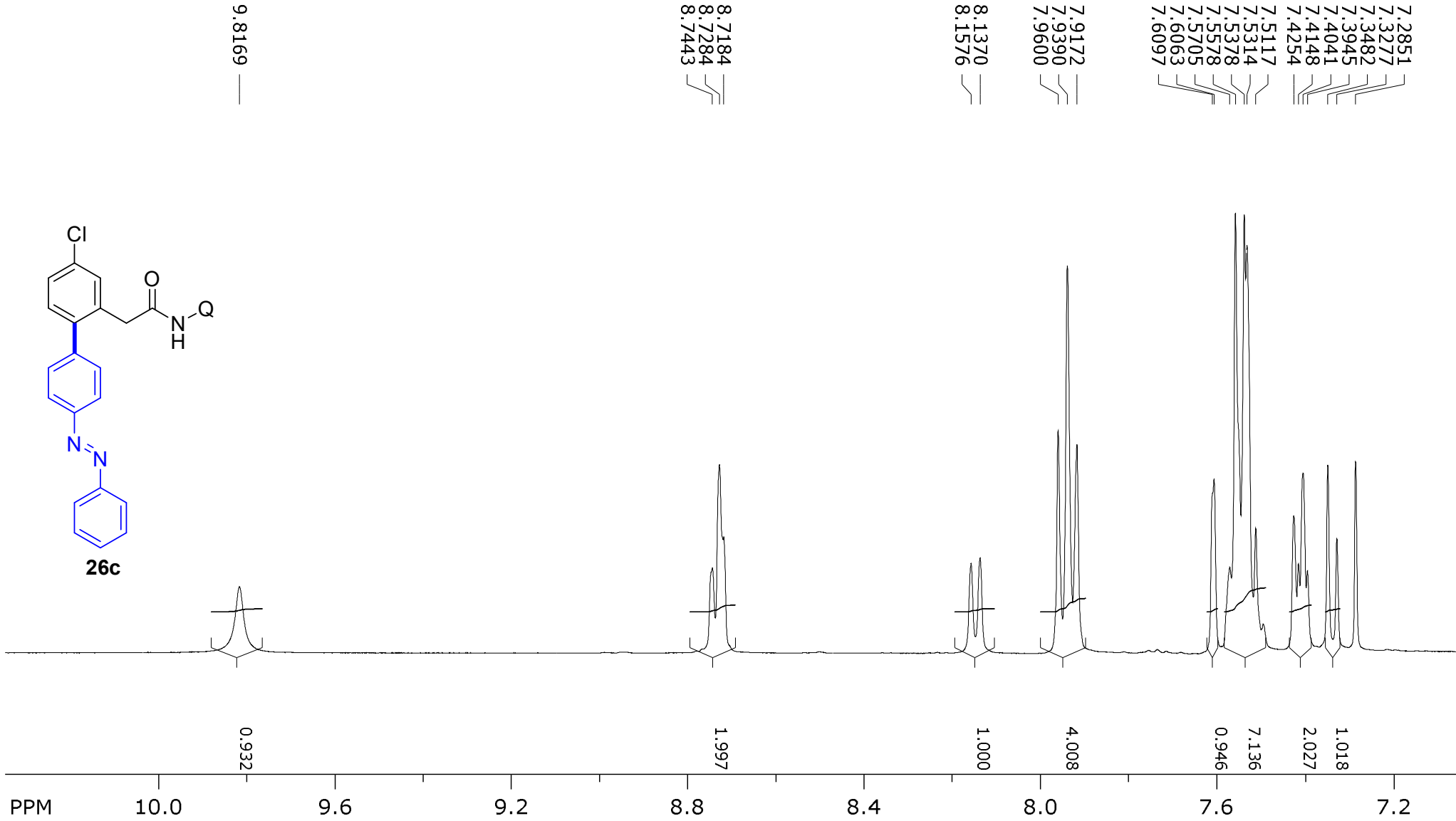
37.338



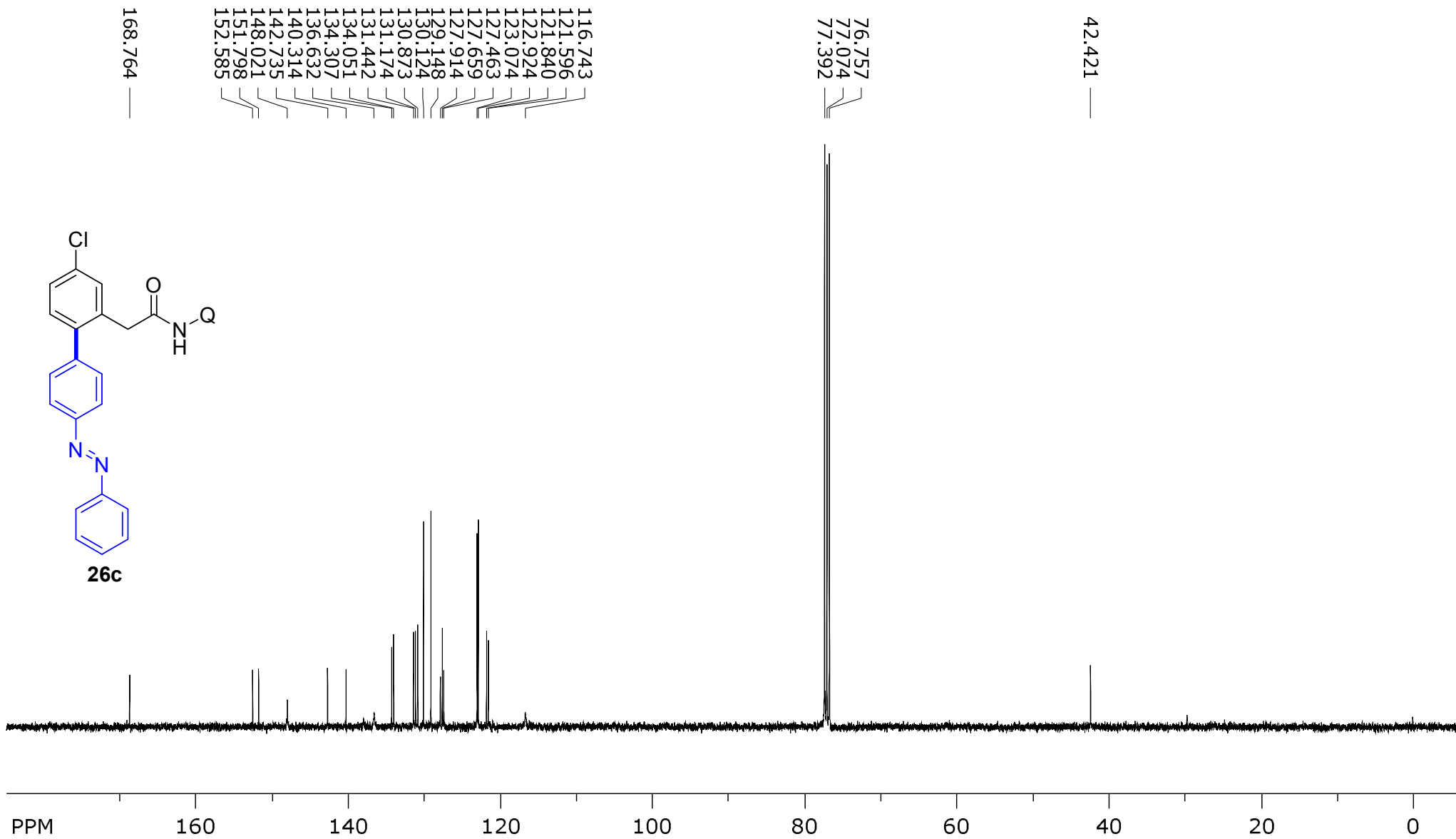
SpinWorks 4: SS-167-P
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 3



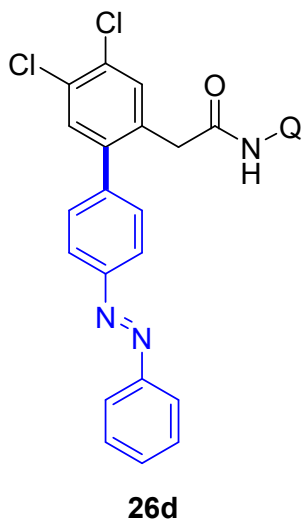
SpinWorks 4: SS-167-P
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 3



SpinWorks 4: SS-167-P
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 3

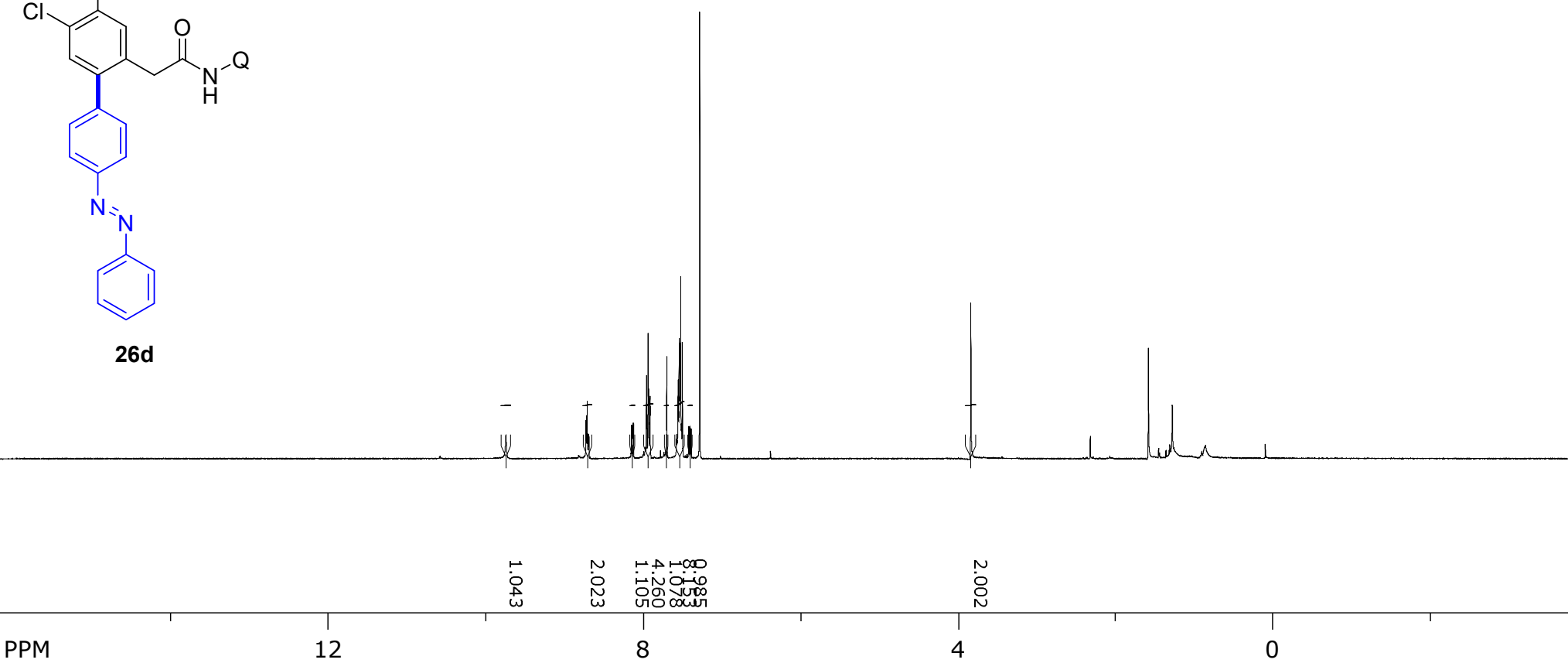


SpinWorks 4: SS 774
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 11

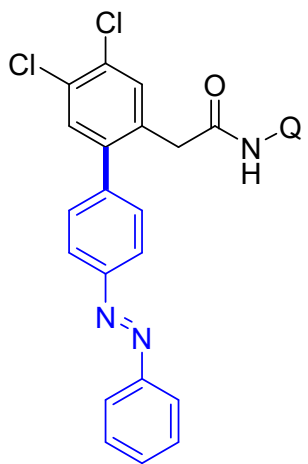


7.2837
7.3923
7.4029
7.4130
7.4236
7.4978
7.5048
7.5097
7.5100
7.5103
7.5106
7.5109
8.11508
8.6930
8.6998
8.7087
8.7152
8.7191
8.7256
8.7298
9.7478

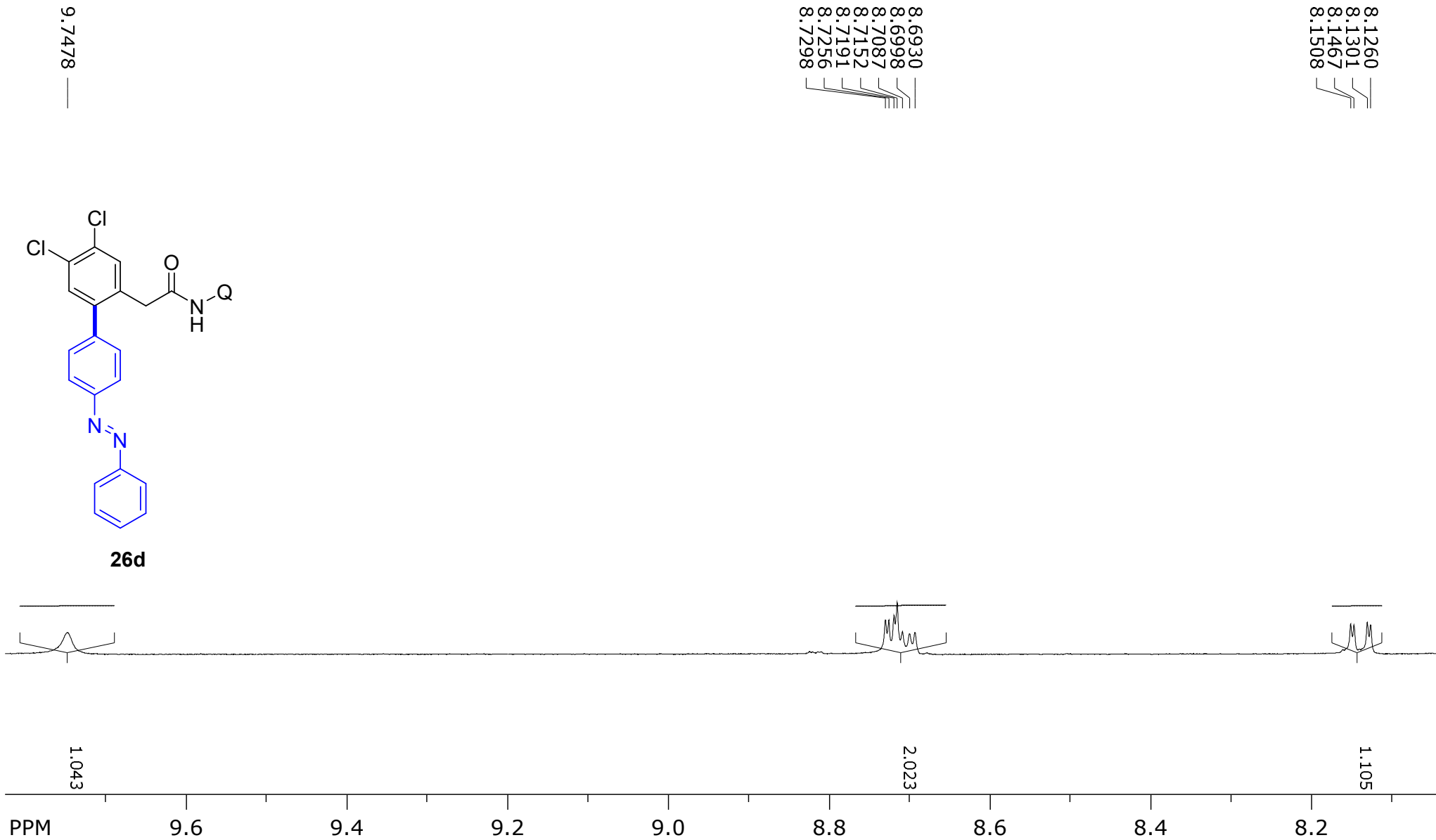
3.8369



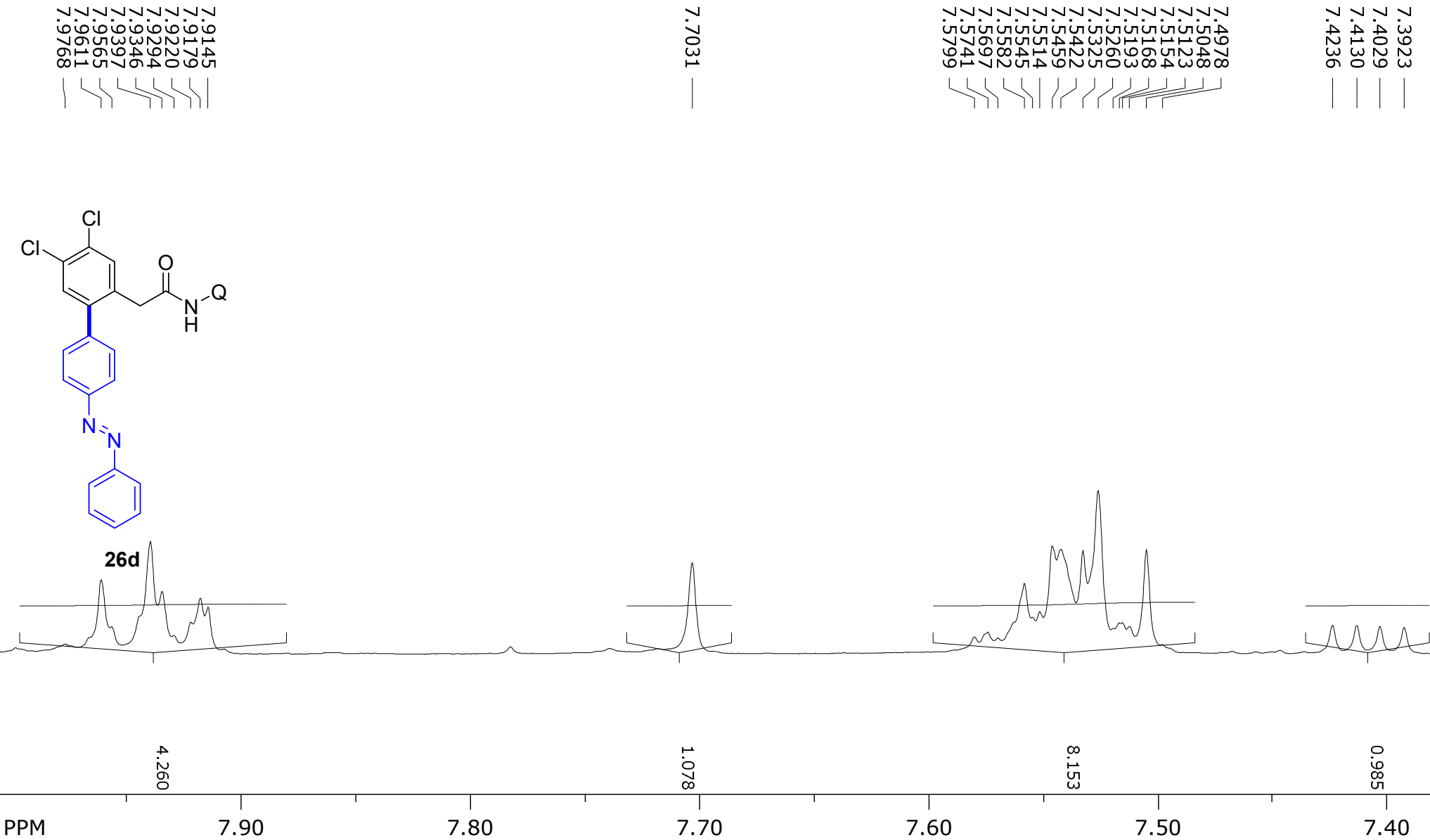
SpinWorks 4: SS 774
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 11

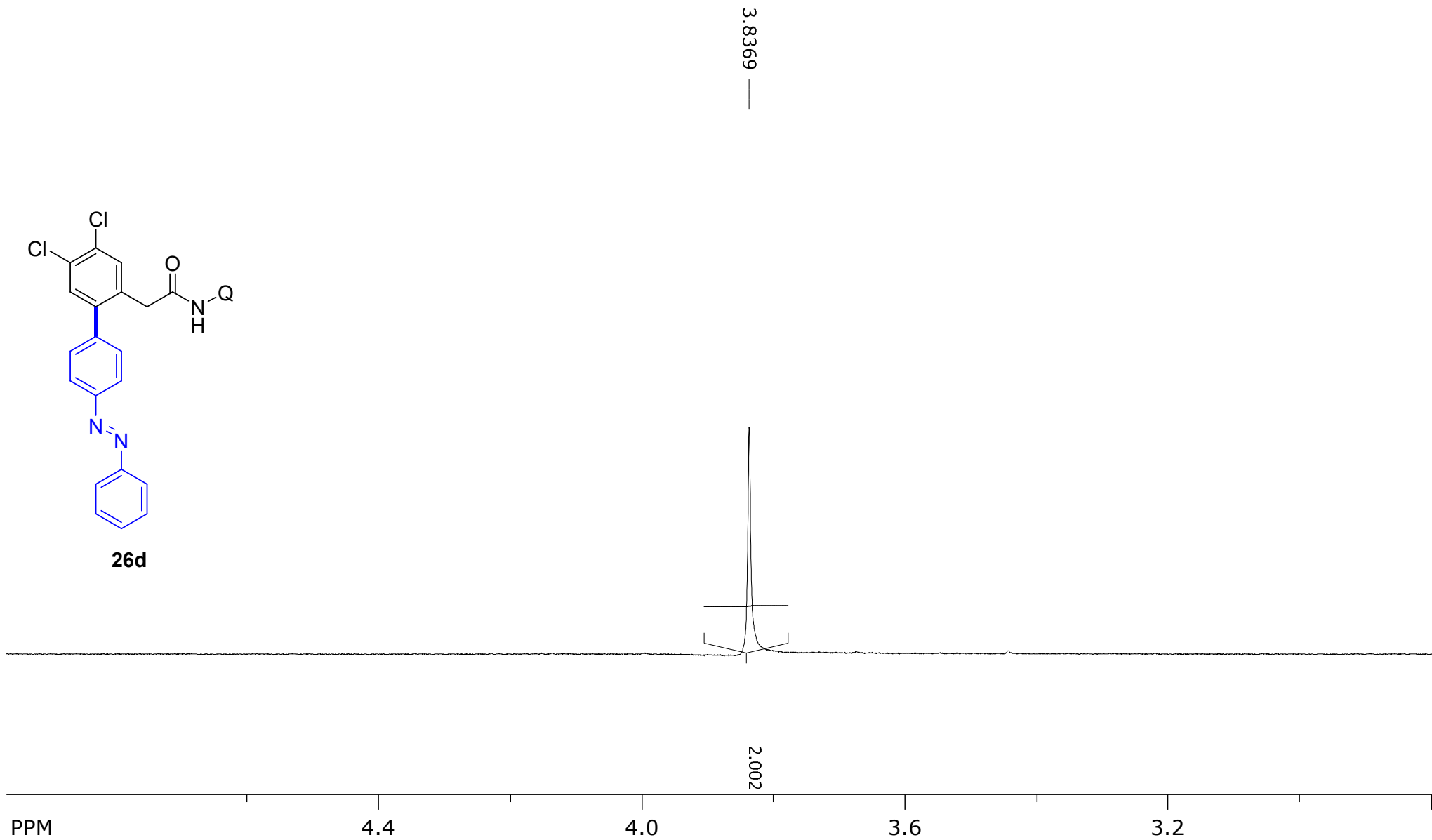
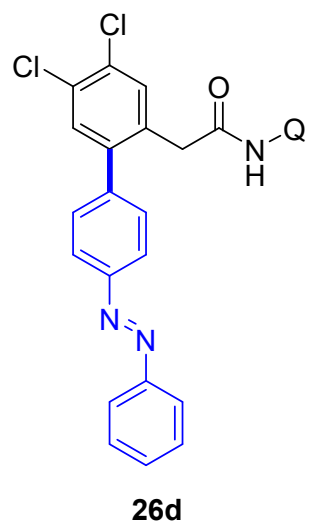


26d



SpinWorks 4: SS 774
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 11



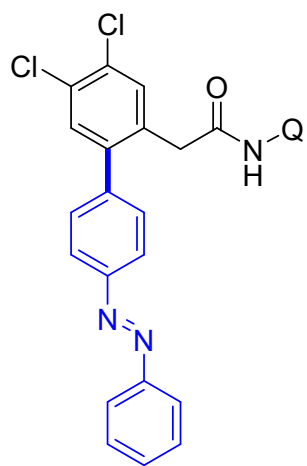


SpinWorks 4: SS 774
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 16

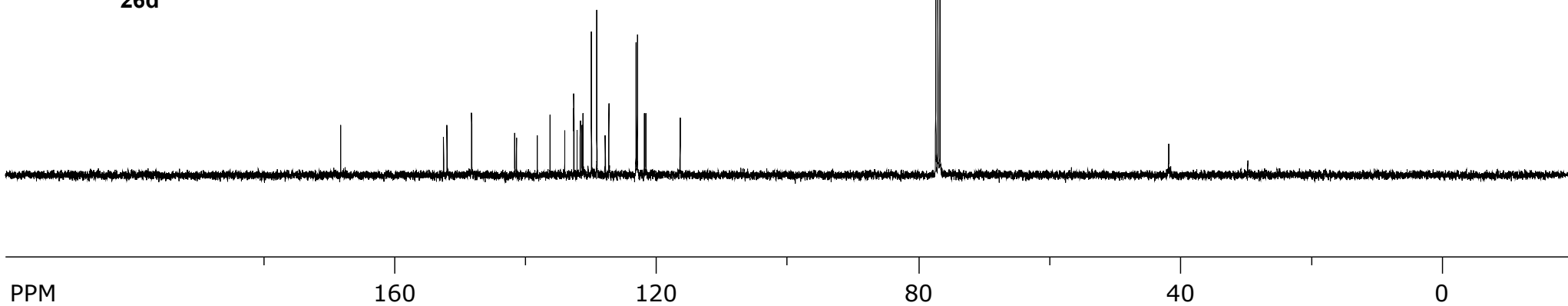
116.427
121.664
121.881
122.959
123.173
127.322
127.858
129.152
129.969
131.978
132.660
132.681
134.065
136.298
138.252
141.429
141.680
148.269
152.027
152.553
168.263

76.742
77.059
77.377

41.803

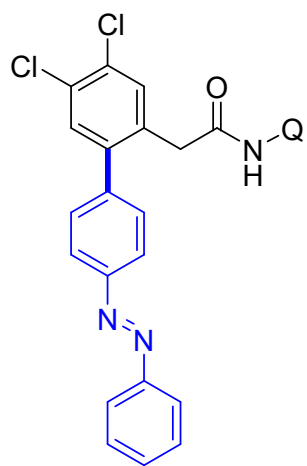


26d

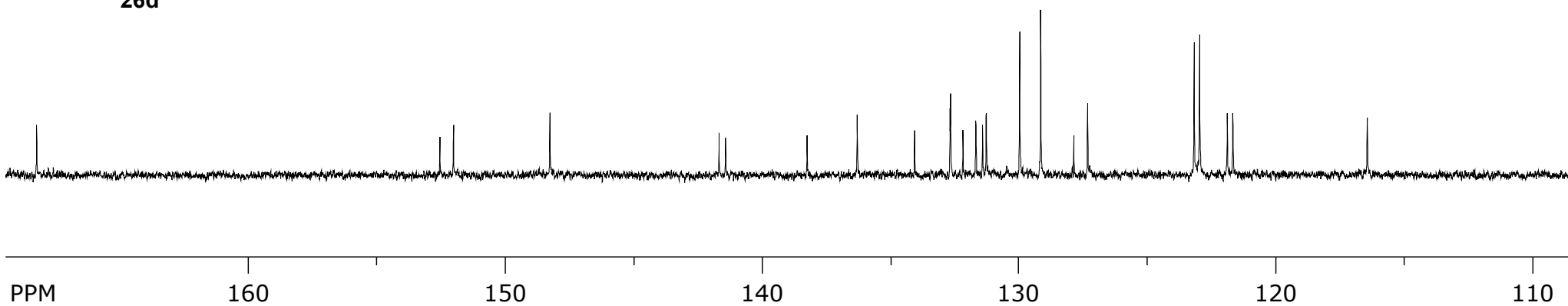


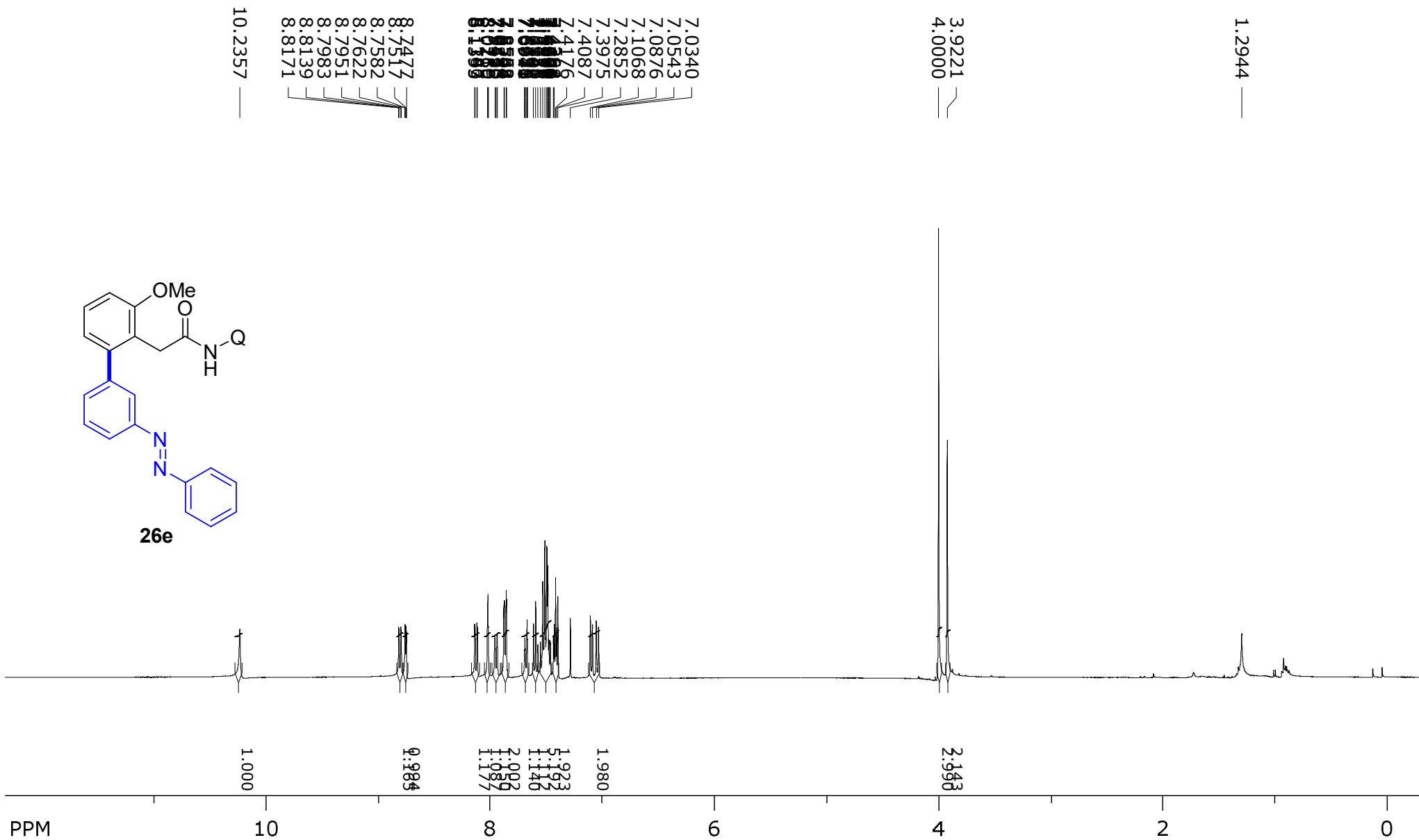
SpinWorks 4: SS 774
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 16

168.263 —
152.027 —
152.553 —
148.269 —
141.429 —
141.680 —
138.252 —
136.298 —
134.065 —
132.681 —
132.660 —
132.178 —
131.674 —
131.414 —
131.271 —
129.969 —
127.858 —
127.322 —
123.173 —
122.959 —
121.881 —
121.664 —
116.427 —



26d





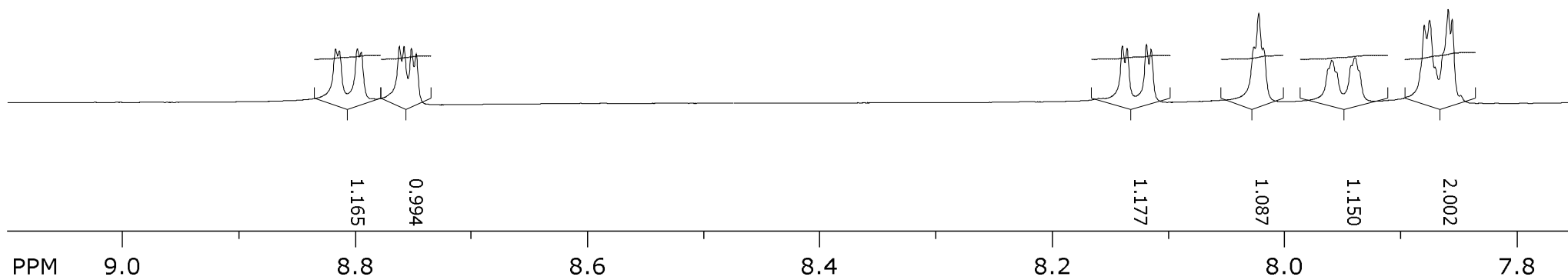
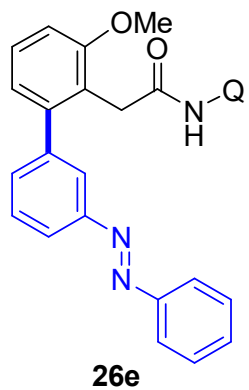
8.7477
8.7517
8.7582
8.7622
8.7951
8.7983
8.8139
8.8171

8.1146
8.1187
8.1353
8.1393

8.0180
8.0219
8.0260

7.9356
7.9423
7.9550
7.9590

7.8553
7.8588
7.8748
7.8794



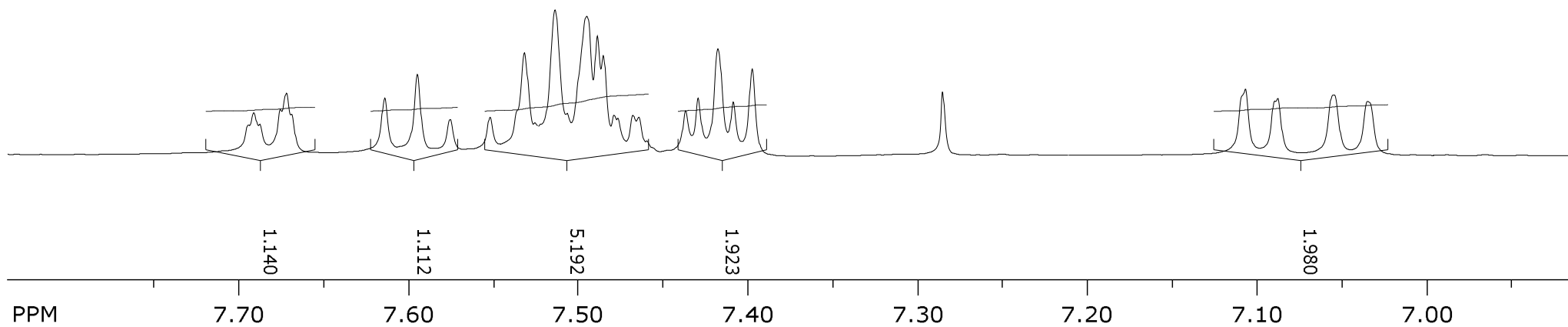
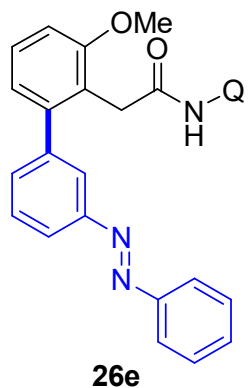
SpinWorks 4: ss-244-p

7.6691
7.6721
7.6758
7.6879
7.6912
7.6946

7.5756
7.5948
7.6142
7.5521
7.5317
7.5136
7.4951
7.4889
7.4852
7.4790
7.4768
7.4678
7.4644
7.4368
7.4294
7.4176
7.3975

7.2852

7.1068
7.0876
7.0543
7.0340



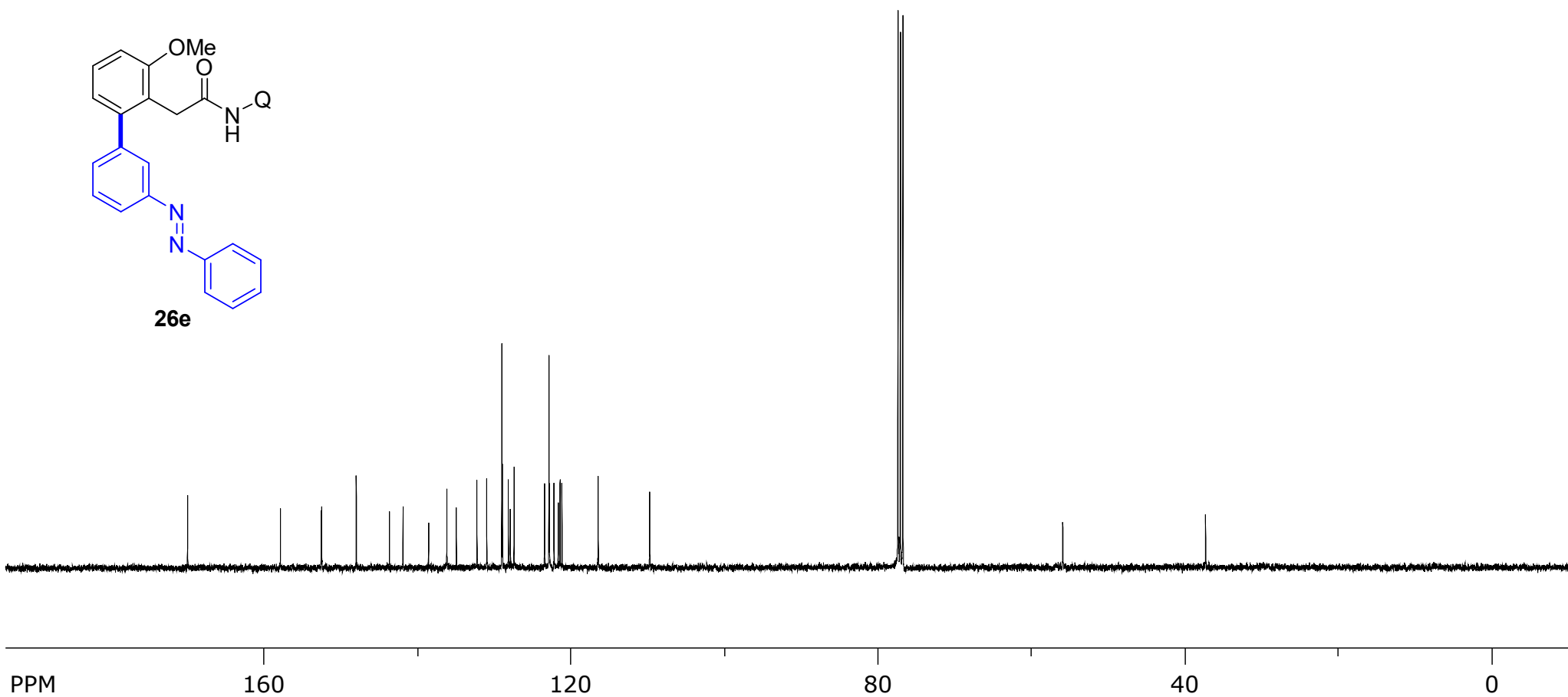
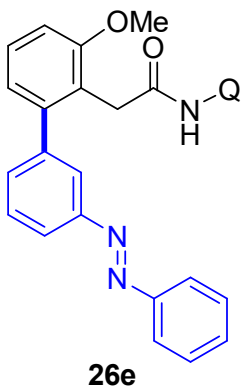
SpinWorks 4: SS 244 P
C13CPD CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 51

169.988 —
157.895 —
152.500 —
147.998 —
143.674 —
141.907 —
138.574 —
136.189 —
134.956 —
132.271 —
130.988 —
129.035 —
128.975 —
128.430 —
123.498 —
122.815 —
122.231 —
121.676 —
121.439 —
121.194 —
116.465 —
109.753 —

77.390 —
77.072 —
76.755 —

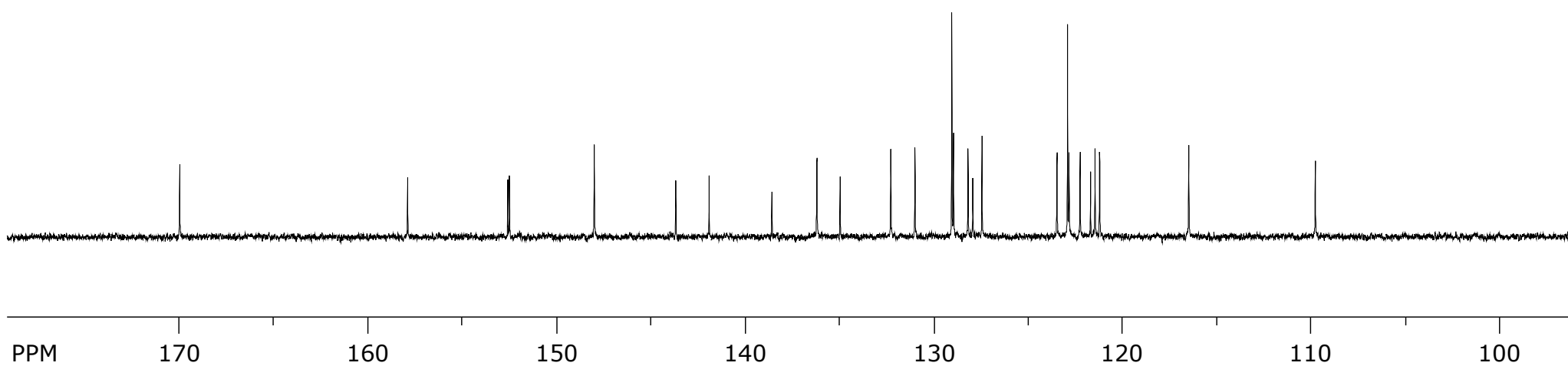
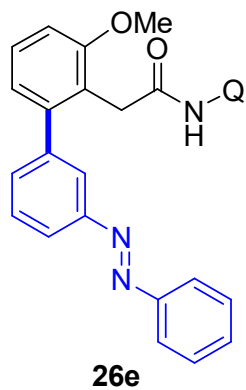
55.909 —

37.295 —

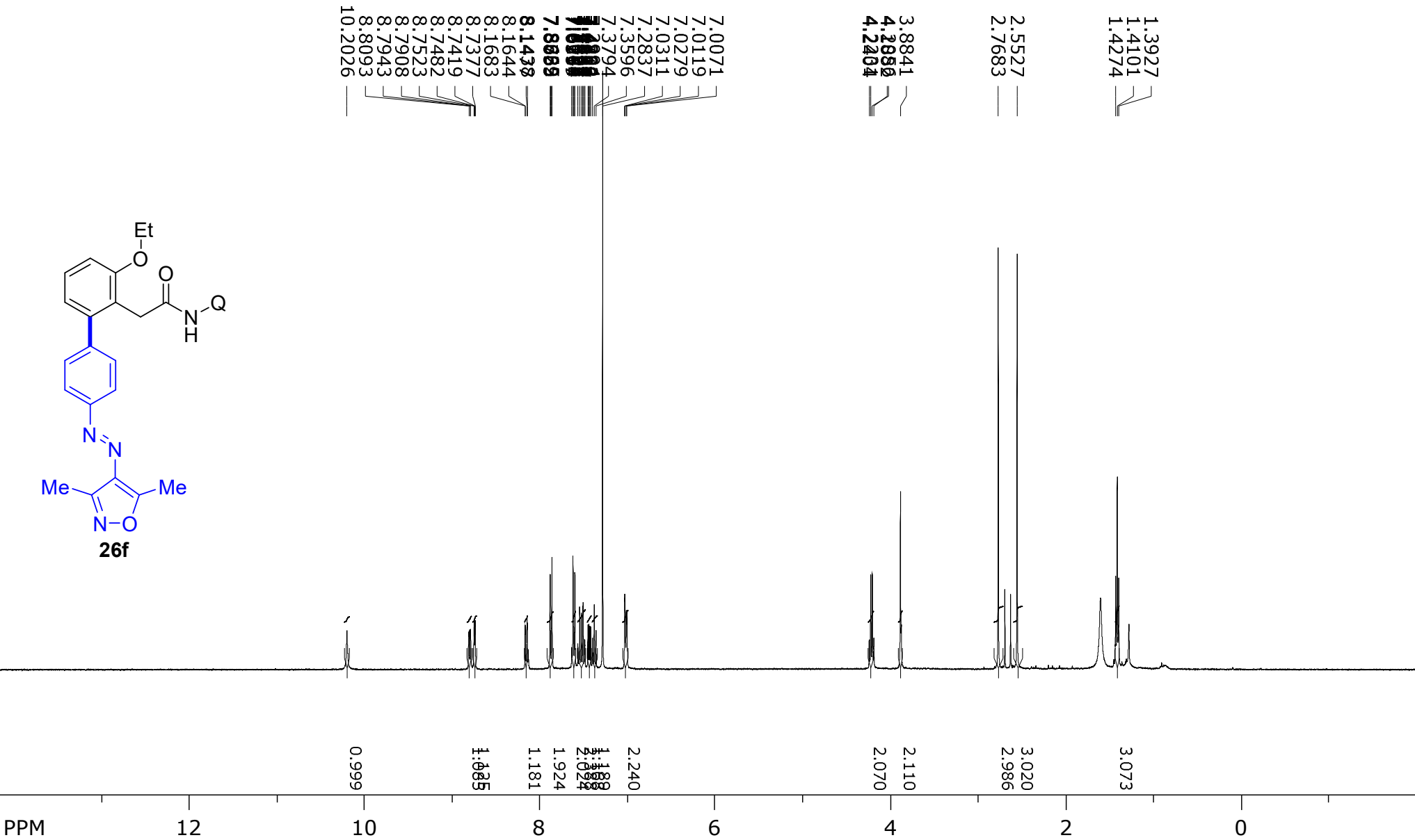


SpinWorks 4: SS 244 P
C13CPD CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 51

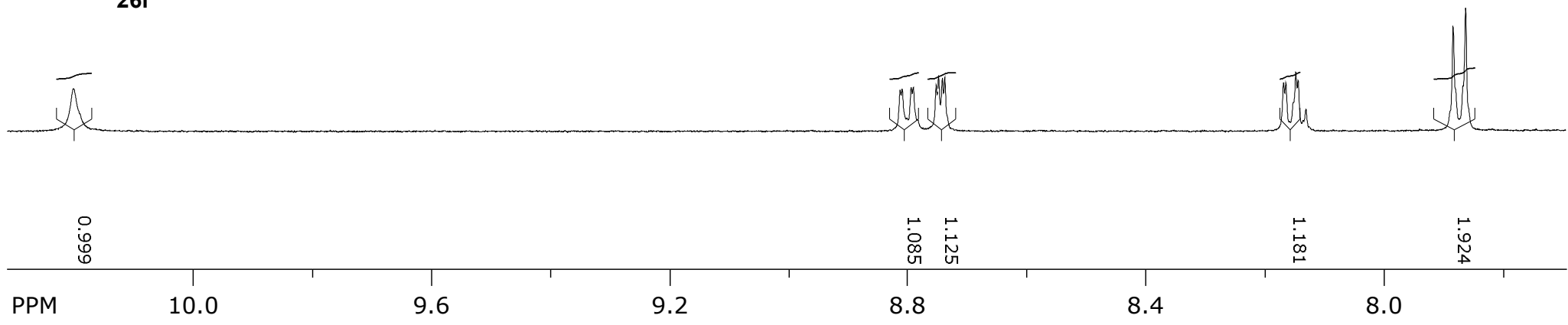
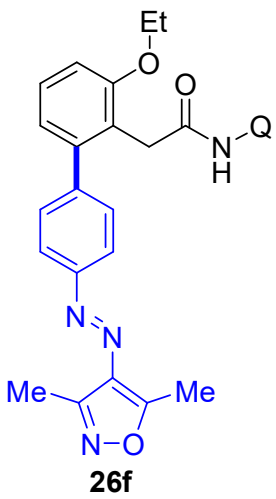
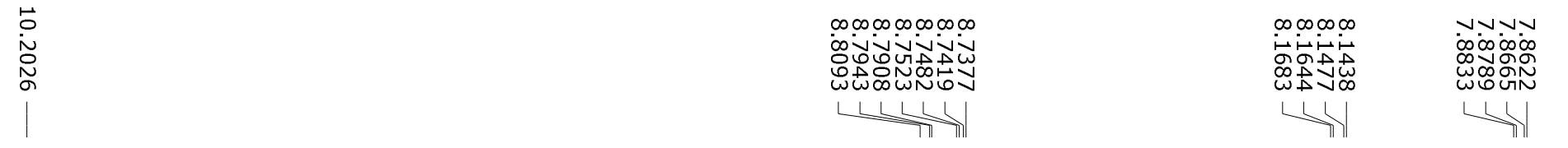
169.988 —
157.895 —
152.500 —
152.586 —
147.998 —
143.674 —
141.907 —
138.574 —
136.189 —
134.956 —
132.271 —
130.988 —
129.035 —
128.945 —
128.174 —
127.920 —
127.432 —
123.458 —
122.896 —
122.815 —
122.231 —
121.676 —
121.439 —
121.194 —
116.465 —
109.753 —



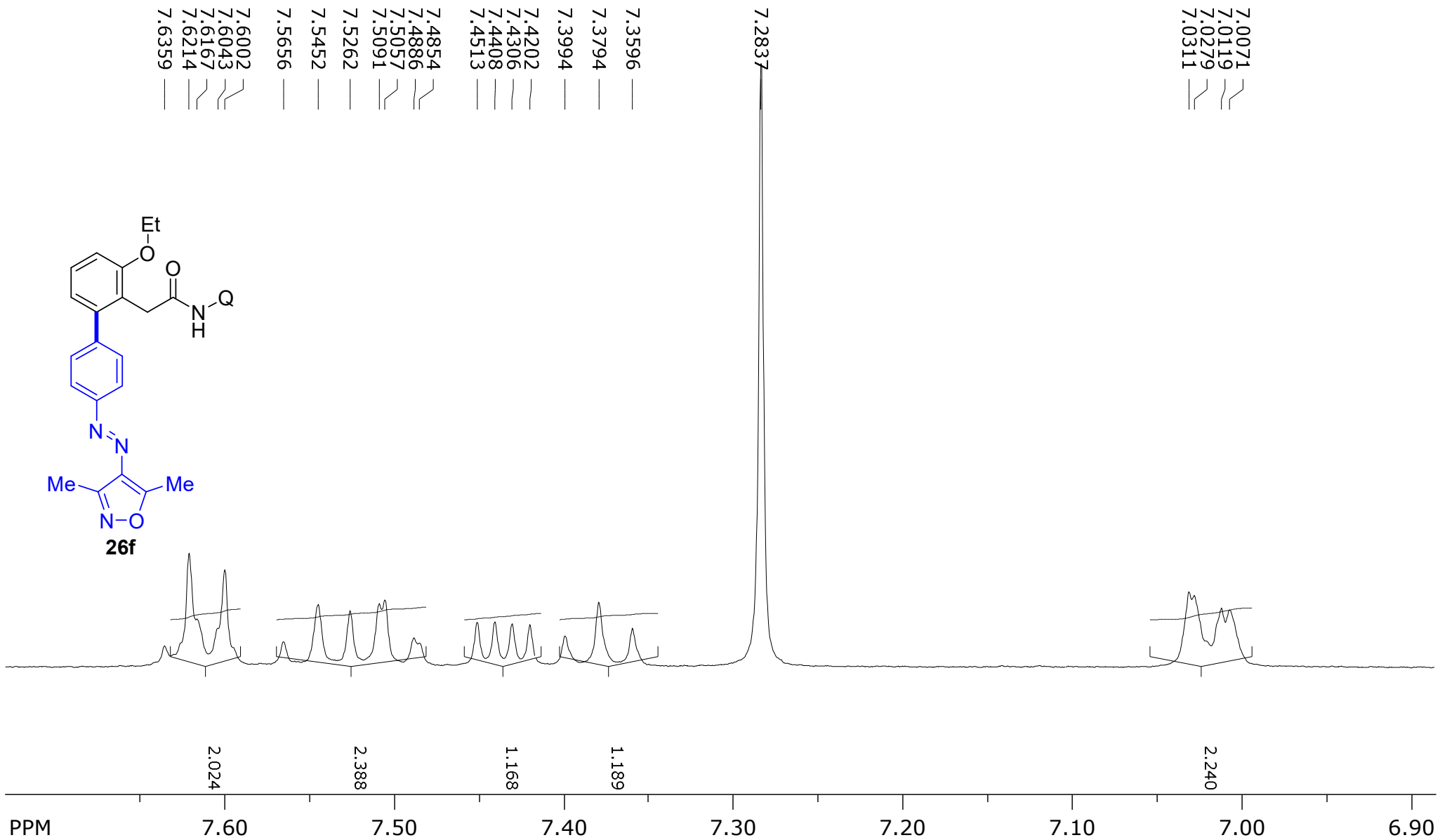
SpinWorks 4: ss-748 rep
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 3



SpinWorks 4: ss-748 rep
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 3



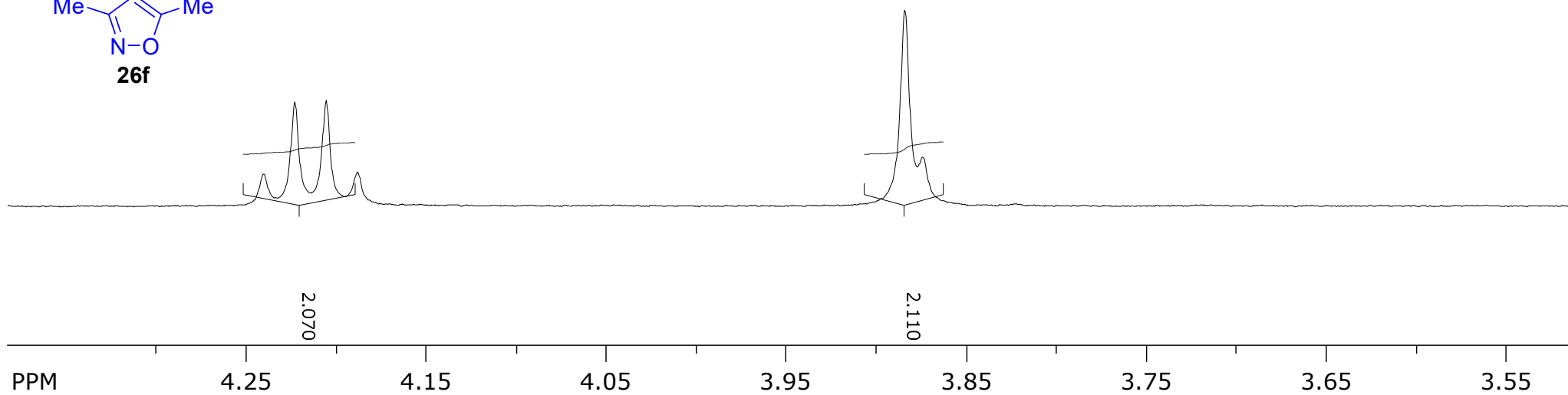
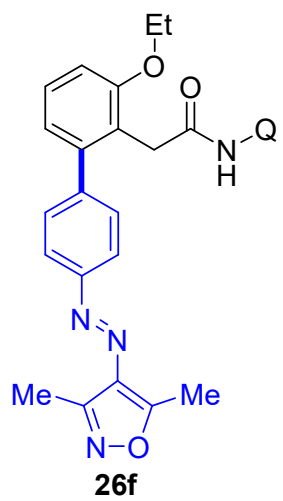
SpinWorks 4: ss-748 rep
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 3



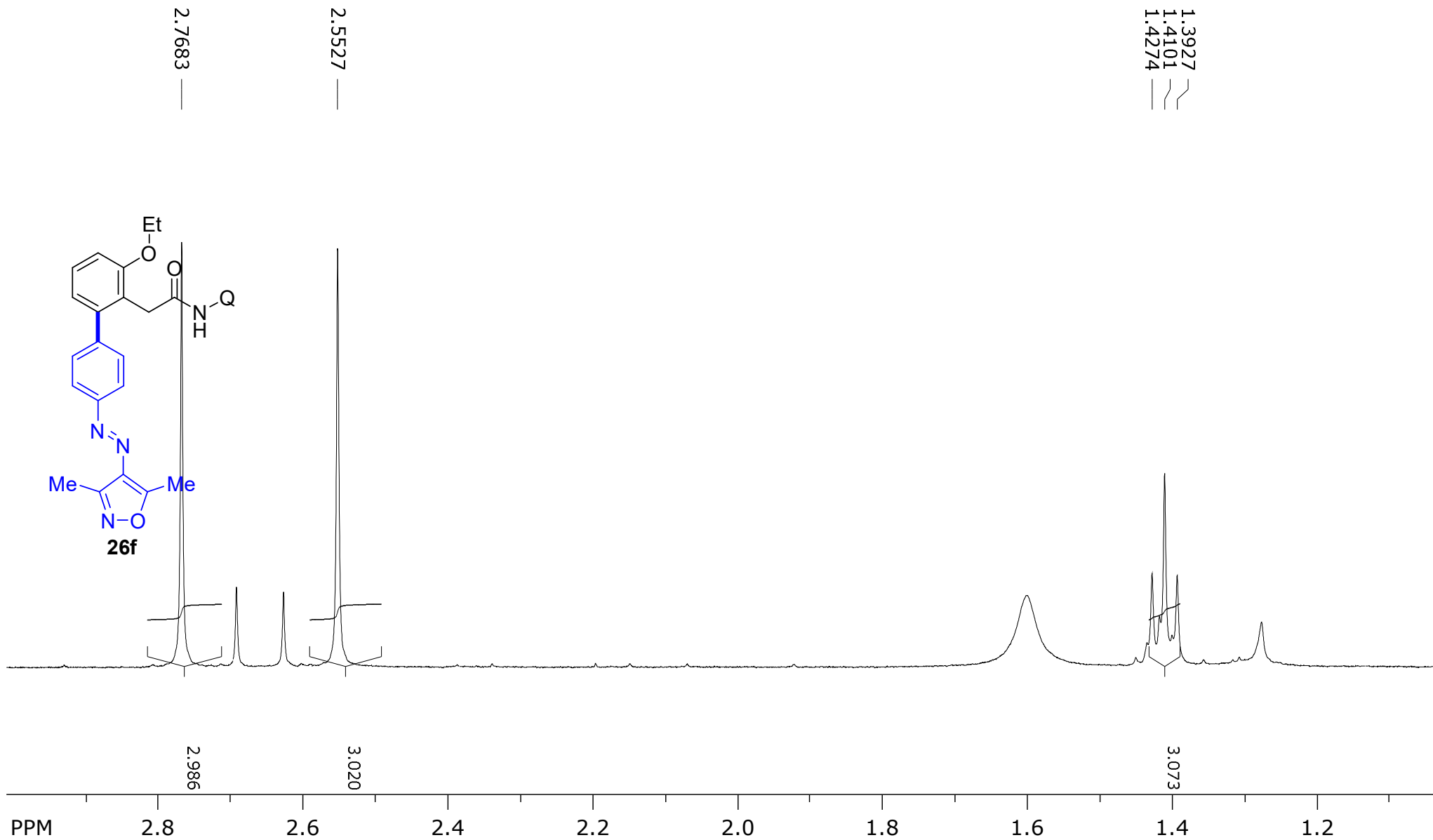
SpinWorks 4: ss-748 rep
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 3

4.1882
4.2056
4.2231
4.2404

3.8841



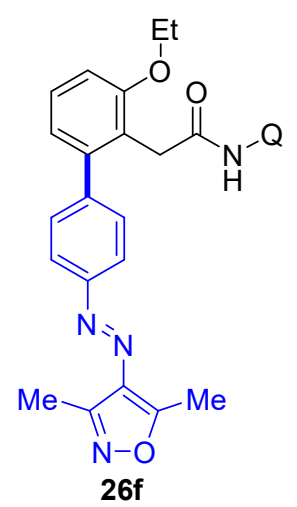
SpinWorks 4: ss-748 rep
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 3



SpinWorks 4: SS-748 REP
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 8

110.584
116.439
121.231
121.462
121.762
122.074
122.342
127.458
127.943
128.103
130.337
130.569
132.551
134.951
135.957
136.227
138.559
147.906
151.917
153.800
157.253
169.374
170.240

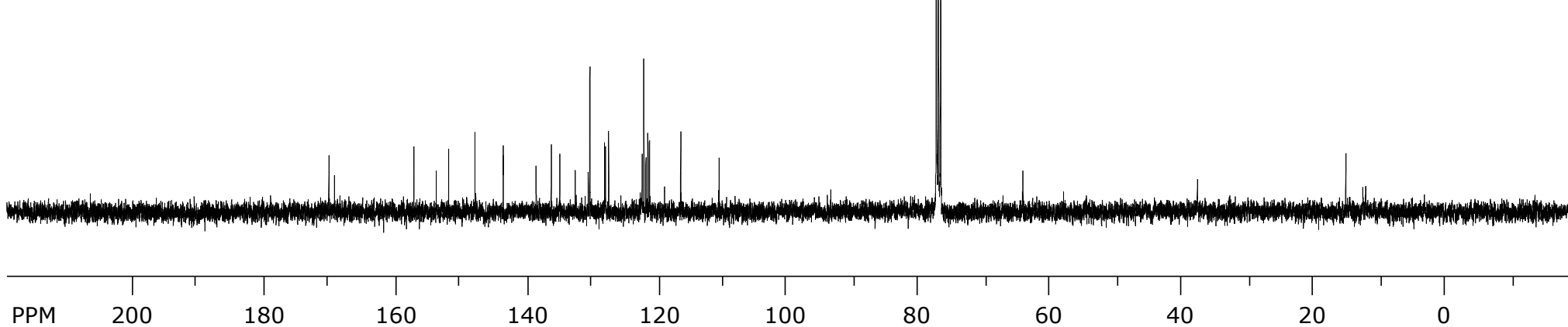
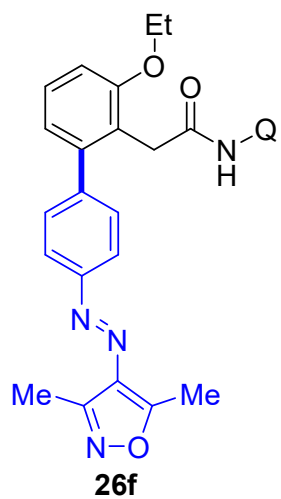
76.717
77.035
77.353
64.128
37.449
11.658
12.167
14.756



PPM 160 120 80 40 0

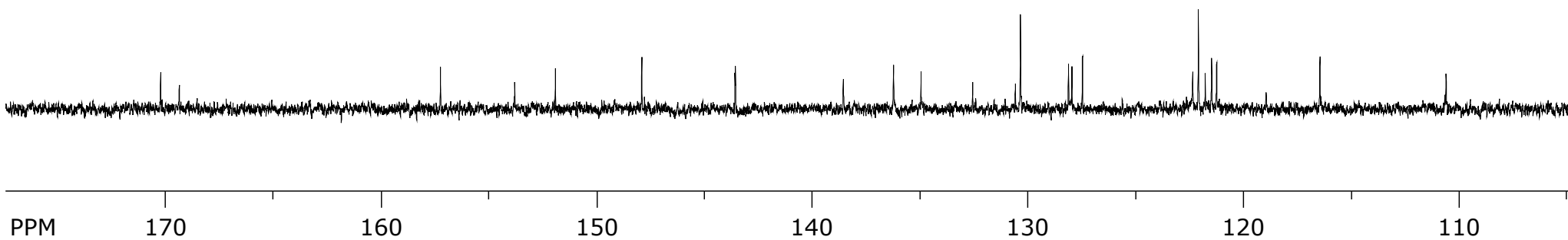
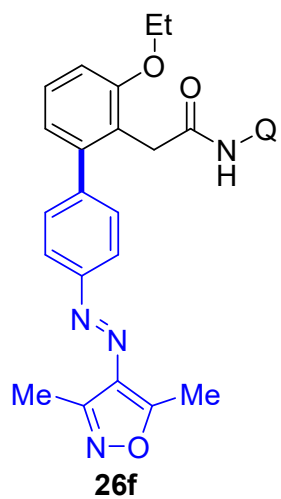
SpinWorks 3: SS-748 REP

110.5838
116.4388
121.2306
121.4618
121.7622
122.0737
122.3419
127.4576
127.9430
128.1028
130.3368
130.5687
132.5511
134.9506
136.2267
138.5591
143.5607
143.5815
147.9065
151.9168
153.8002
157.2532
169.3741
170.2400
76.7171
77.0349
77.3525
64.1282
37.4494
11.6812
11.7142
12.1309
12.1589
14.7565

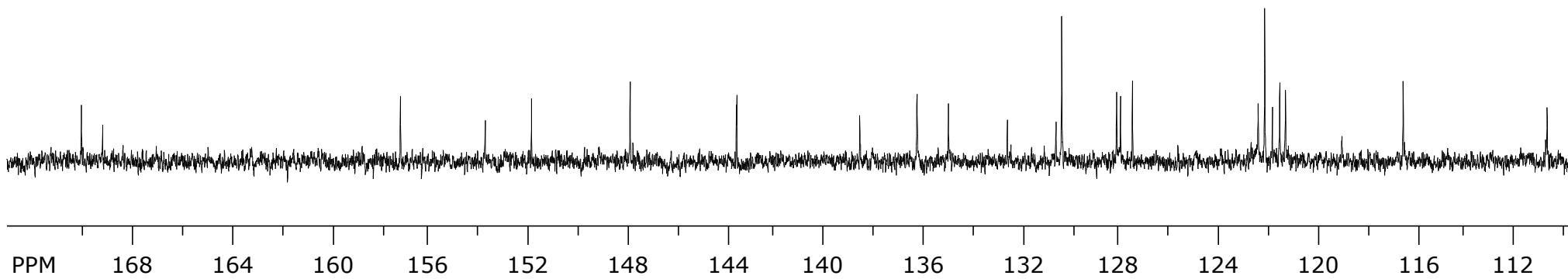
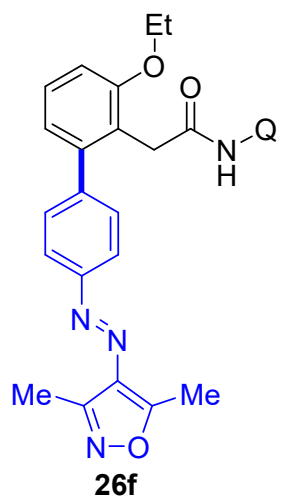
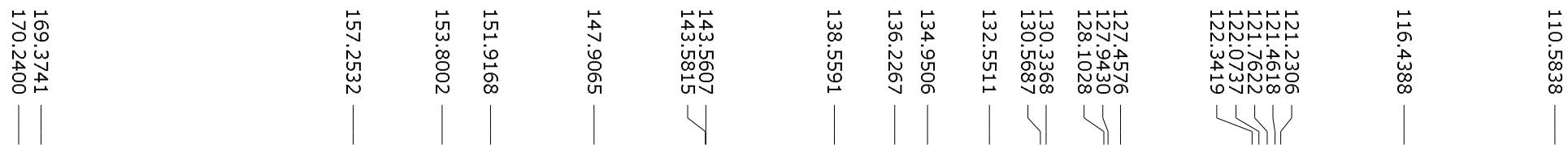


SpinWorks 4: SS-748 REP
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 8

169.374 —
170.240 —
157.253 —
153.800 —
151.917 —
147.906 —
143.567 —
138.559 —
136.227 —
134.951 —
132.551 —
130.569 —
130.337 —
128.103 —
127.943 —
127.458 —
122.342 —
122.074 —
121.762 —
121.462 —
121.231 —
116.439 —
110.584 —



SpinWorks 3: SS-748 REP



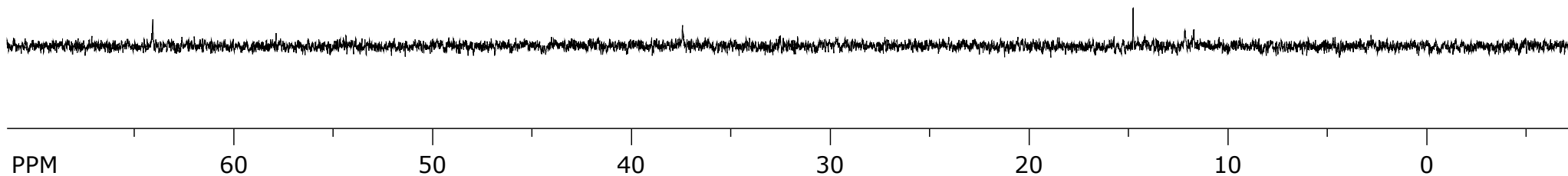
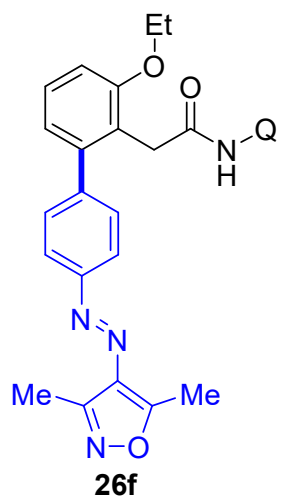
SpinWorks 4: SS-748 REP
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 8

64.128 —

37.449 —

14.756 —

11.658 —
12.167 —

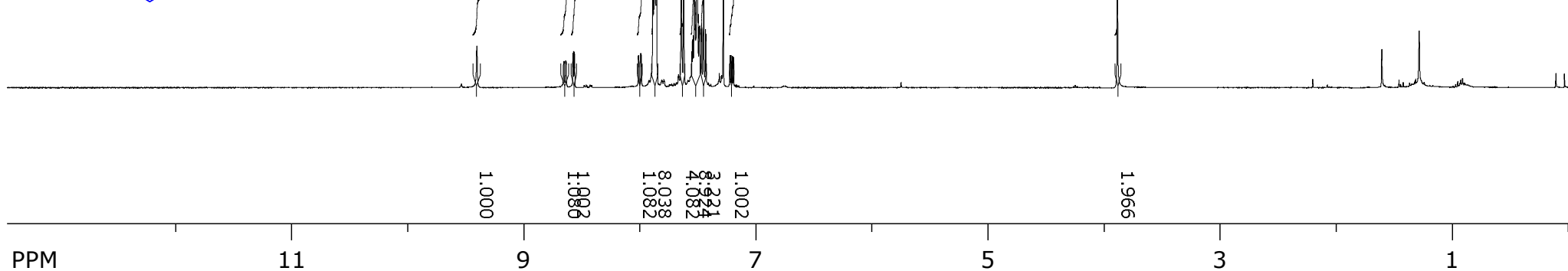
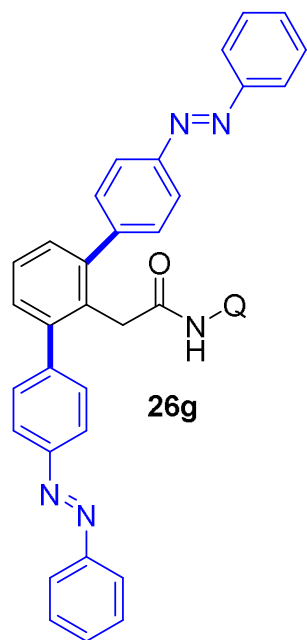


SpinWorks 4: SS-773-11
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 2

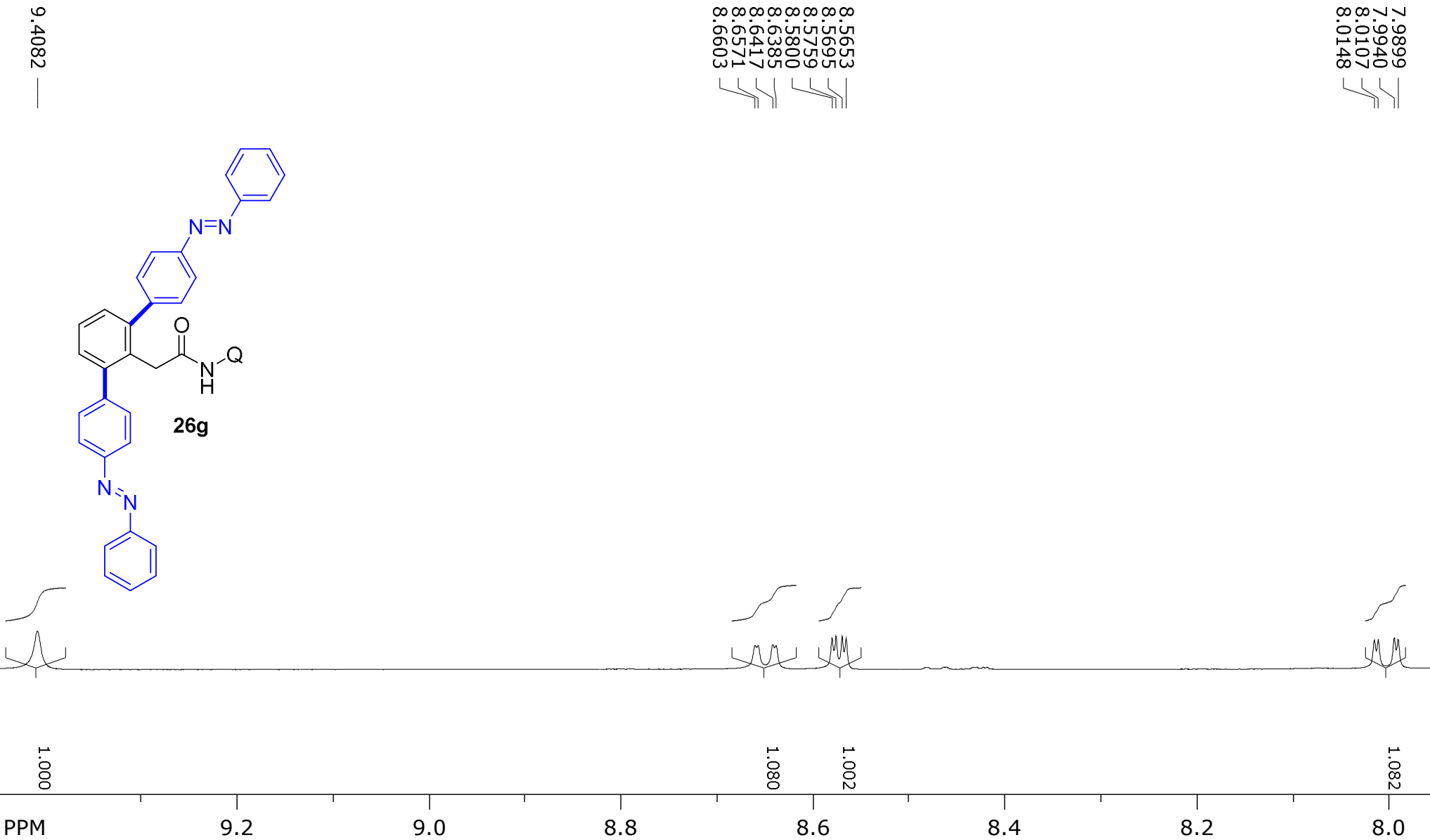
8.5693
8.5759
8.5800
8.6385
8.6417
8.6571
8.6603
9.4082

7.1945
7.2050
7.2152
7.2257
7.2836
7.4329
7.4357
7.4537
7.4620
7.4680
7.4700
7.4720
7.4740
7.4760
7.4780
7.4800
7.4820
7.4840
7.4860
7.4880
7.4900
7.4920
7.4940
7.4960
7.4980
7.5000
7.5020
7.5040
7.5060
7.5080
7.5100
7.5120
7.5140
7.5160
7.5180
7.5200
7.5220
7.5240
7.5260
7.5280
7.5300
7.5320
7.5340
7.5360
7.5380
7.5400
7.5420
7.5440
7.5460
7.5480
7.5500
7.5520
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7.5620
7.5640
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7.5700
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7.5760
7.5780
7.5800
7.5820
7.5840
7.5860
7.5880
7.5900
7.5920
7.5940
7.5960
7.5980
7.6000
7.6020
7.6040
7.6060
7.6080
7.6100
7.6120
7.6140
7.6160
7.6180
7.6200
7.6220
7.6240
7.6260
7.6280
7.6300
7.6320
7.6340
7.6360
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7.6400
7.6420
7.6440
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7.6500
7.6520
7.6540
7.6560
7.6580
7.6600
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7.6840
7.6860
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7.6900
7.6920
7.6940
7.6960
7.6980
7.7000
7.7020
7.7040
7.7060
7.7080
7.7100
7.7120
7.7140
7.7160
7.7180
7.7200
7.7220
7.7240
7.7260
7.7280
7.7300
7.7320
7.7340
7.7360
7.7380
7.7400
7.7420
7.7440
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7.8240
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7.8280
7.8300
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7.9640
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7.9960
7.9980
8.0000

3.8837



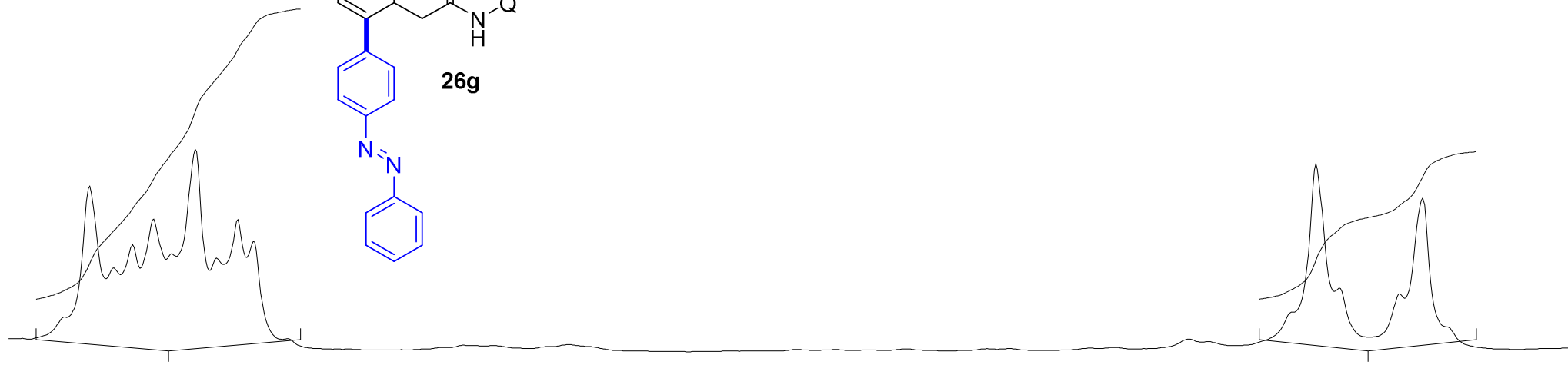
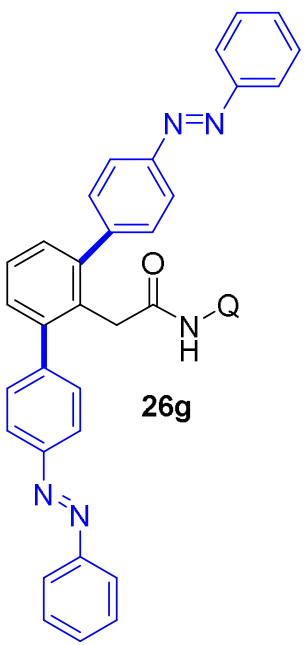
SpinWorks 4: SS-773-11
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 2



SpinWorks 4: SS-773-11
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 2

7.8499
7.8568
7.8600
7.8641
7.8684
7.8731
7.8768
7.8809
7.8847
7.8896
7.8945

7.6231
7.6278
7.6398
7.6445



8.038

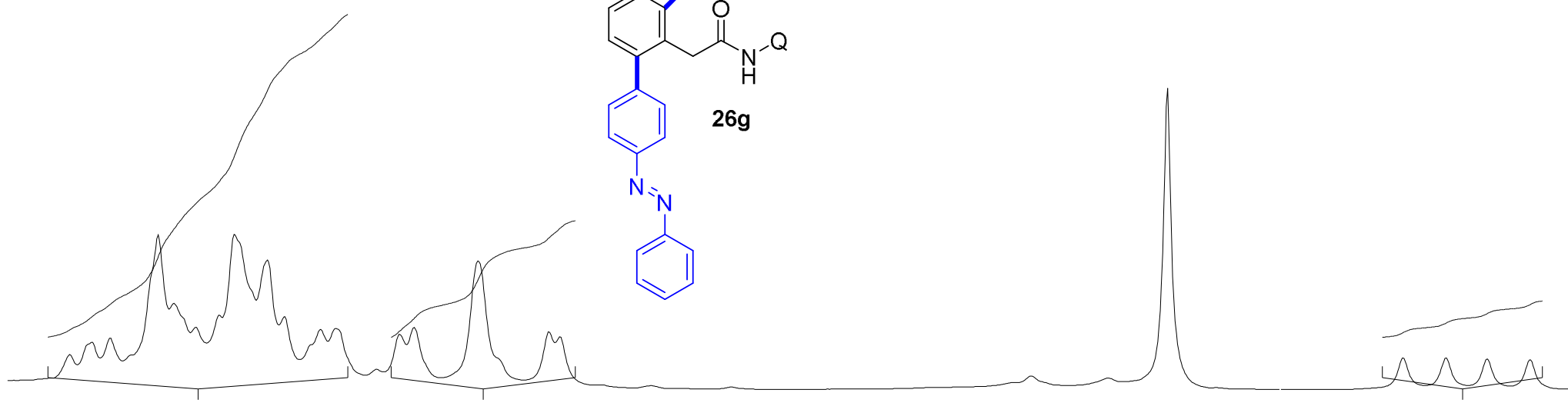
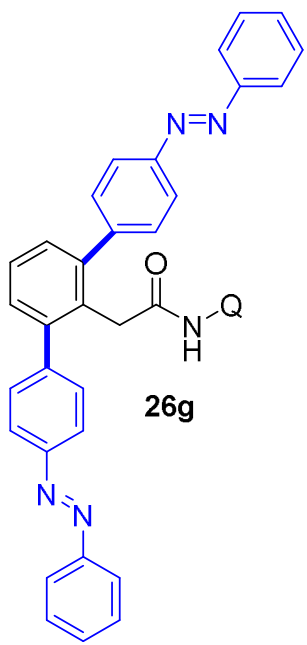
4.082

PPM 7.88 7.84 7.80 7.76 7.72 7.68 7.64 7.60

SpinWorks 4: SS-773-11
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 2

7.4329
7.4357
7.4530
7.4688
7.4723
7.4780
7.4880
7.4918
7.5007
7.5048
7.5130
7.5167
7.5224
7.5278
7.5317
7.5383
7.5435
7.5480
7.5534

7.1945
7.2050
7.2152
7.2257
7.2836



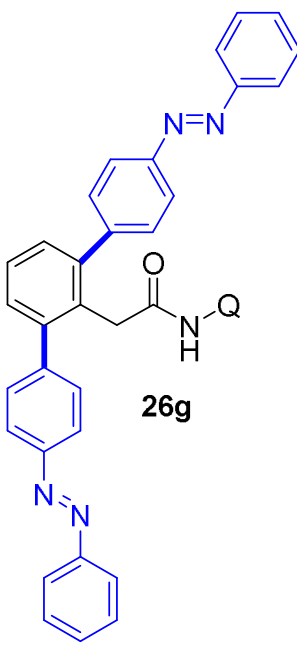
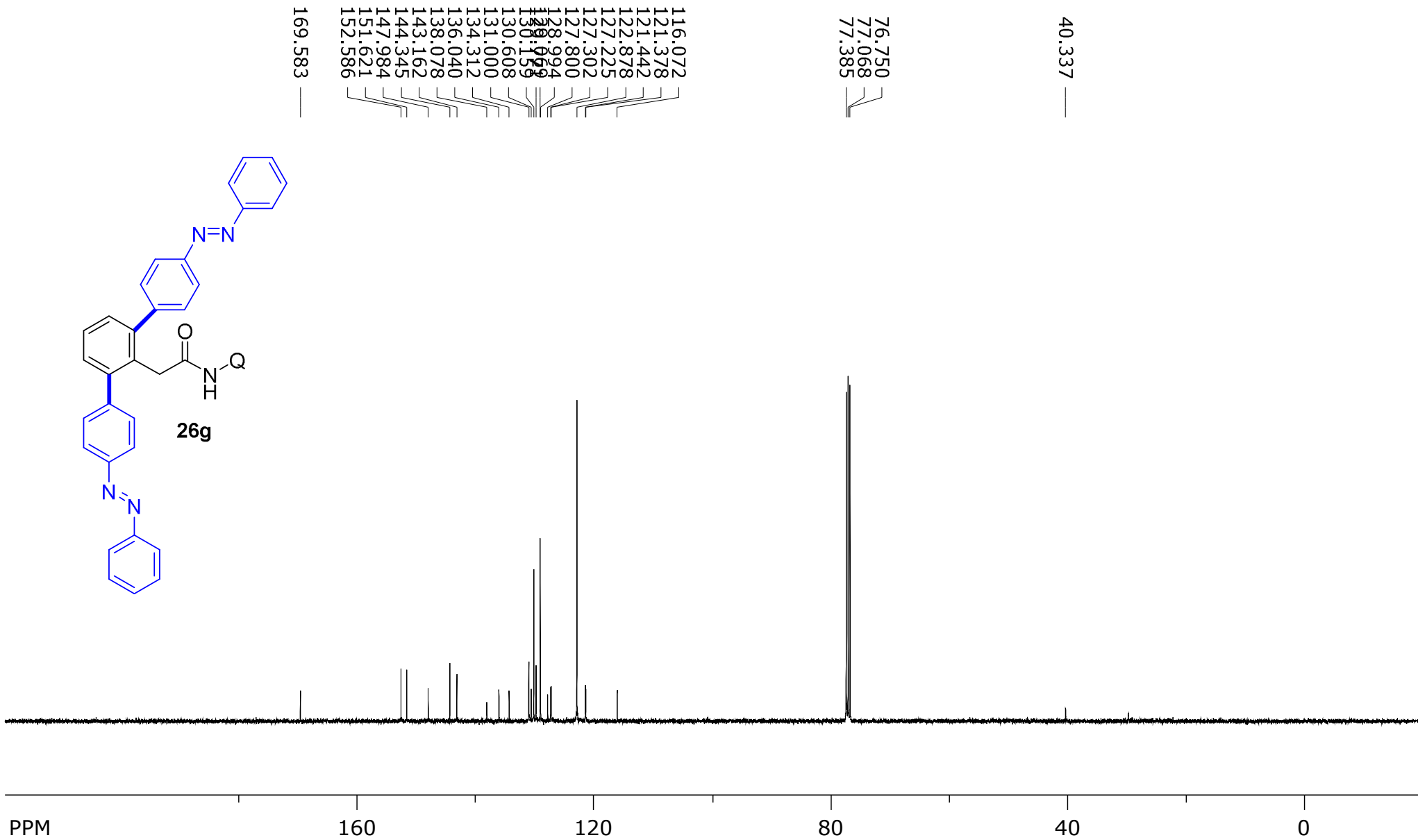
8.924

3.221

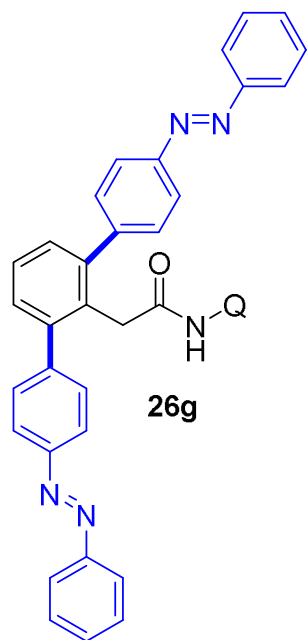
1.002

PPM 7.52 7.48 7.44 7.40 7.36 7.32 7.28 7.24 7.20

SpinWorks 4: SS 773 II A
C13CPD CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 50



SpinWorks 4: SS 773 II A
C13CPD CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 50



169.583

151.621
152.586

147.984

143.162
144.345

138.078

136.040

134.312

131.000

130.608

130.159

129.771

129.069

128.994

127.800

127.302

127.225

122.878

121.442

121.378

116.072

PPM

170

160

150

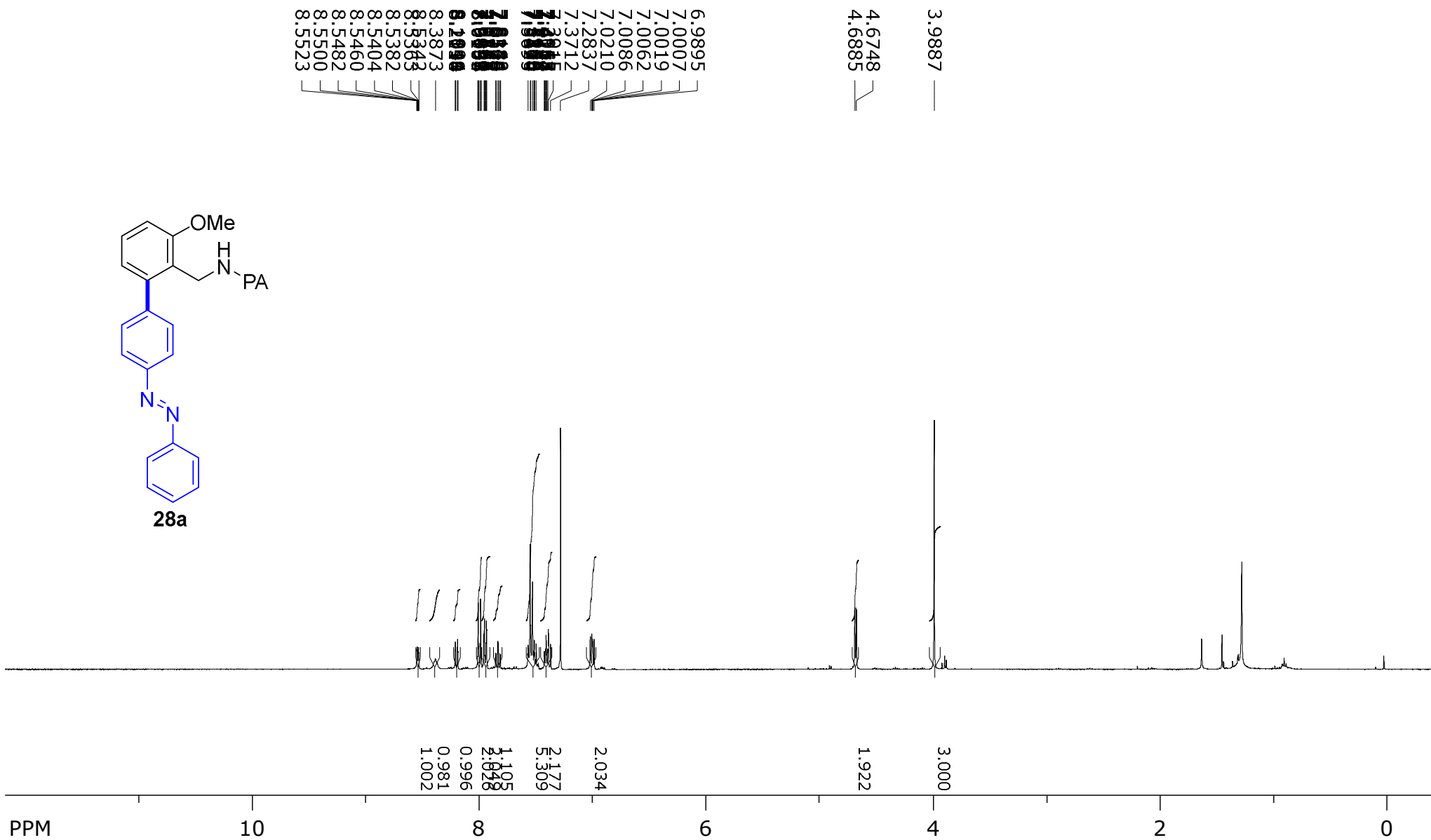
140

130

120

110

SpinWorks 4: SS 782 REP
 PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 3

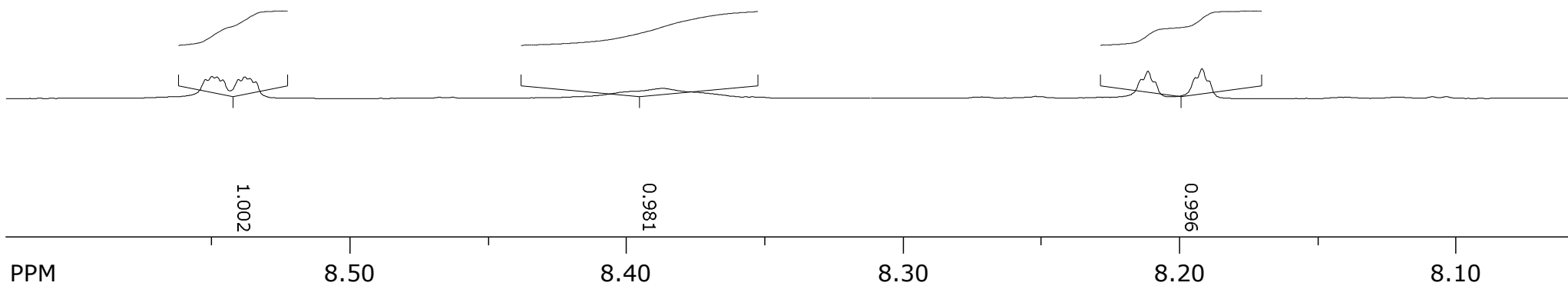
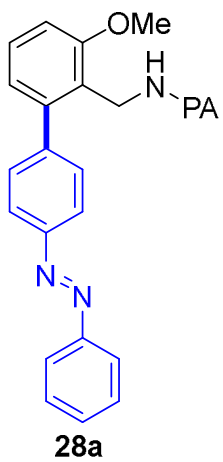


SpinWorks 4: SS 782 REP
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 3

8.5342
8.5363
8.5382
8.5404
8.5460
8.5482
8.5500
8.5523

8.3873

8.1894
8.1919
8.1941
8.2090
8.2114
8.2138



SpinWorks 4: SS 782 REP
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 3

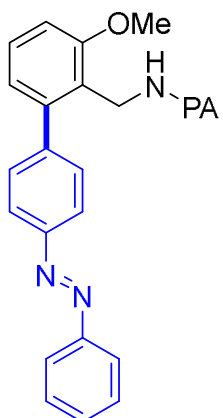
7.9840
7.9891
7.9937
8.0056
8.0103
8.0154

7.9505
7.9556
7.9594
7.9354
7.9381
7.9420

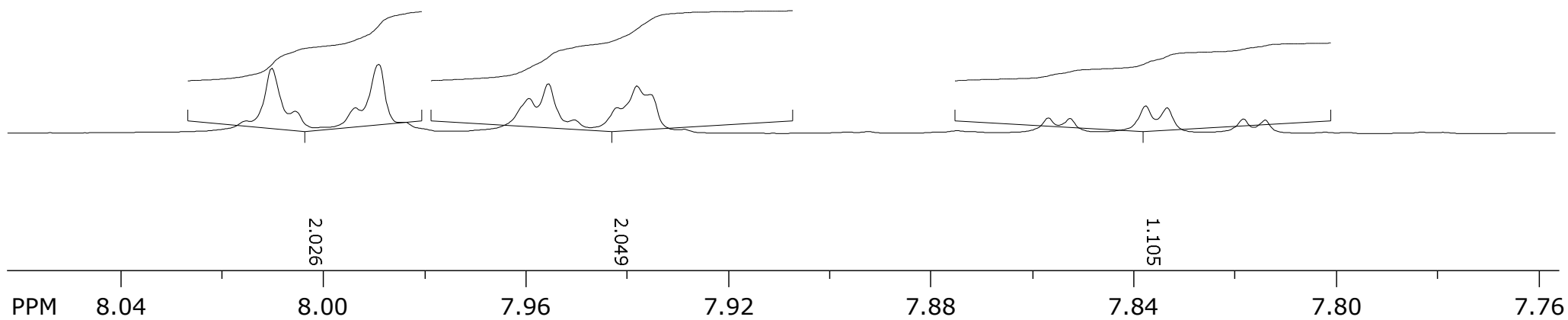
7.8525
7.8568

7.8334
7.8376

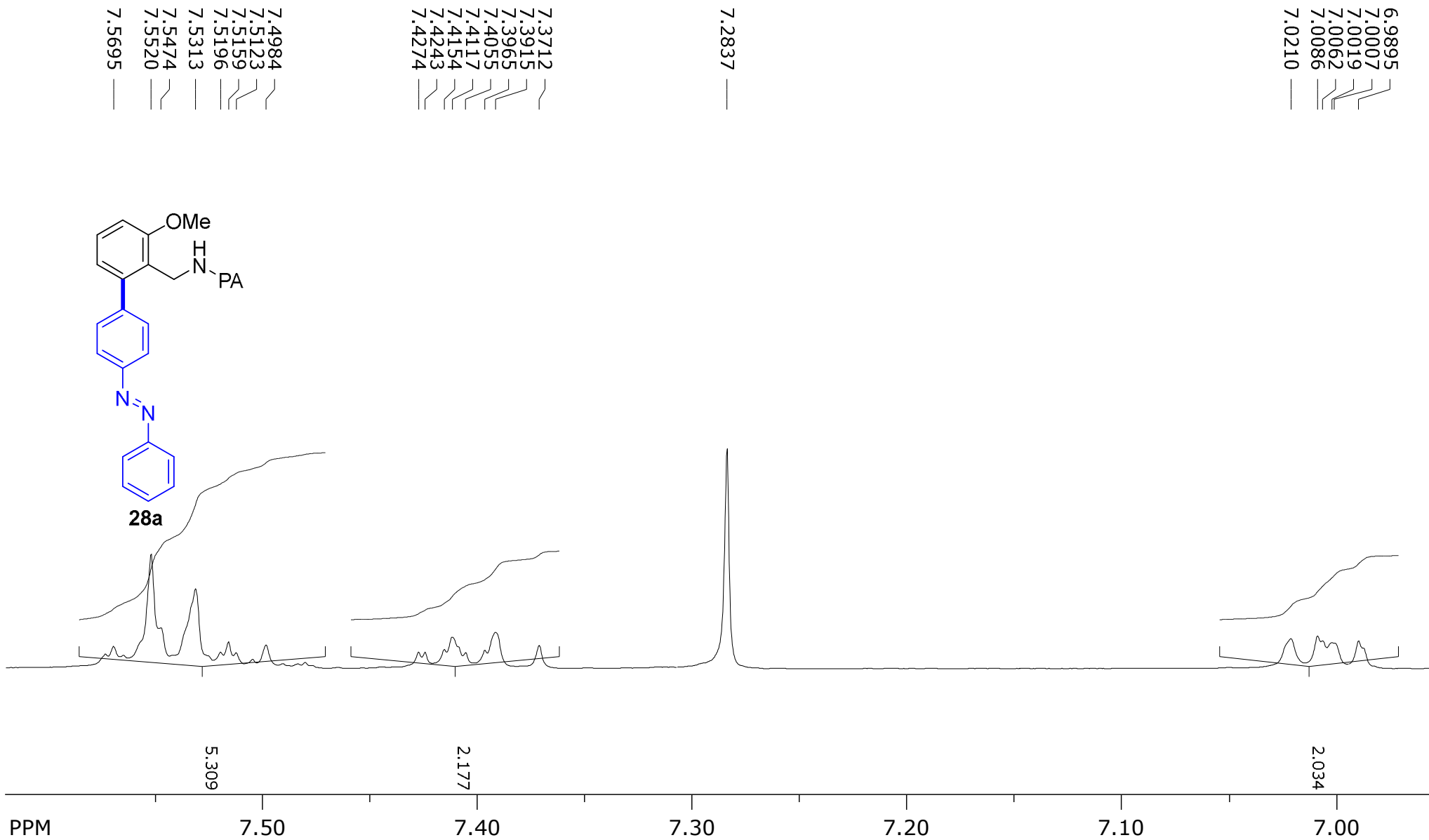
7.8140
7.8183



28a



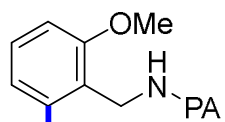
SpinWorks 4: SS 782 REP
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 3



SpinWorks 4: SS 782 REP
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 3

4.6748
4.6885

3.9887



28a



1.922

3.000

PPM

4.70

4.60

4.50

4.40

4.30

4.20

4.10

4.00

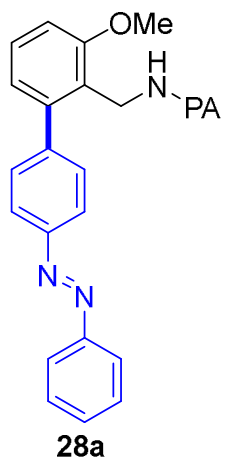
335

SpinWorks 4: ss 782 rep
C13CPD CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 1

109.965
122.281
122.561
122.867
123.660
125.905
128.612
129.100
130.115
130.924
137.215
143.194
143.375
148.035
150.280
151.704
152.767
158.791
163.433

76.722
77.040
77.358

29.727
36.837



PPM

160

120

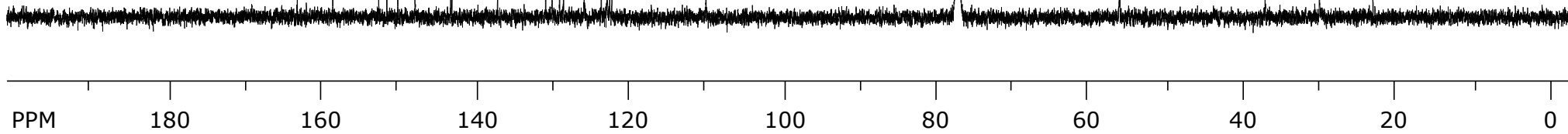
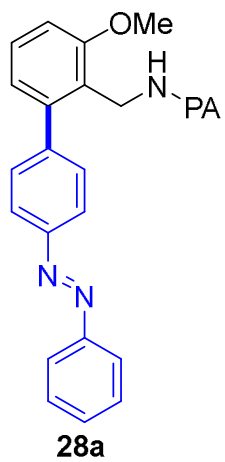
80

40

0

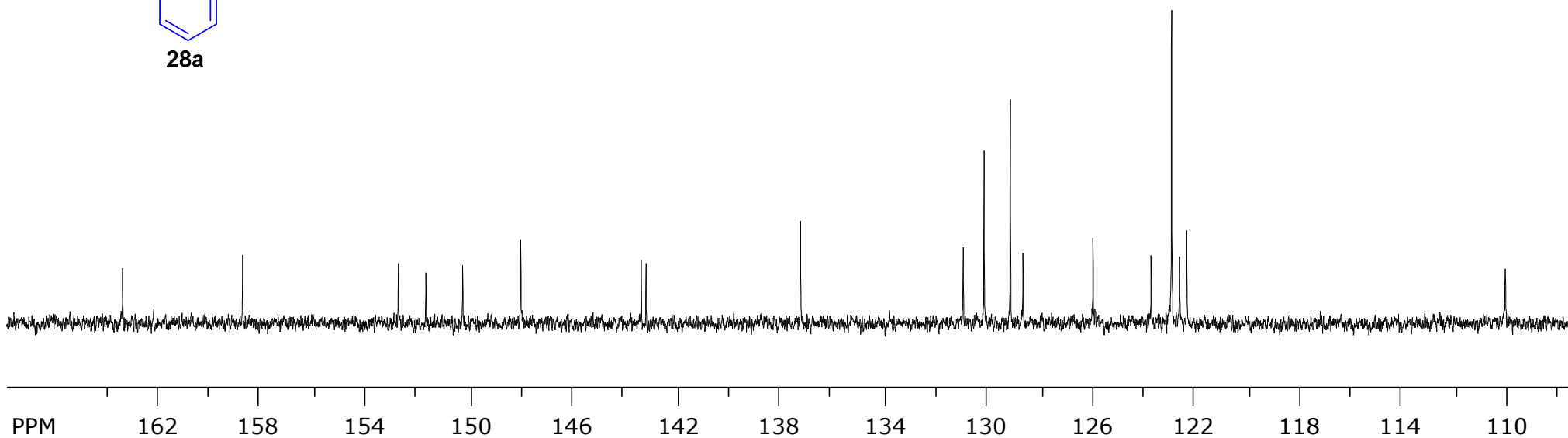
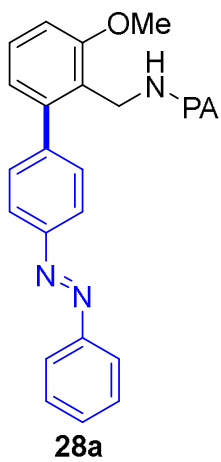
SpinWorks 3: ss 782 rep

143.1937
143.3747
148.0348
150.2803
151.7039
152.7672
158.7909
163.4334
109.9646
122.2806
122.5613
122.8674
123.6596
125.9054
128.6120
129.0998
130.1150
130.9243
137.2147
76.7223
77.0399
77.3576
55.8777
29.7265
36.8374



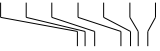
SpinWorks 3: ss 782 rep

163.4334 —
158.7909 —
152.7672 —
151.7039 —
150.2803 —
148.0348 —
143.1937 —
143.3747 —
137.2147 —
130.9243 —
129.0998 —
128.6120 —
125.9054 —
123.6596 —
122.8674 —
122.5613 —
122.2806 —
109.9646 —

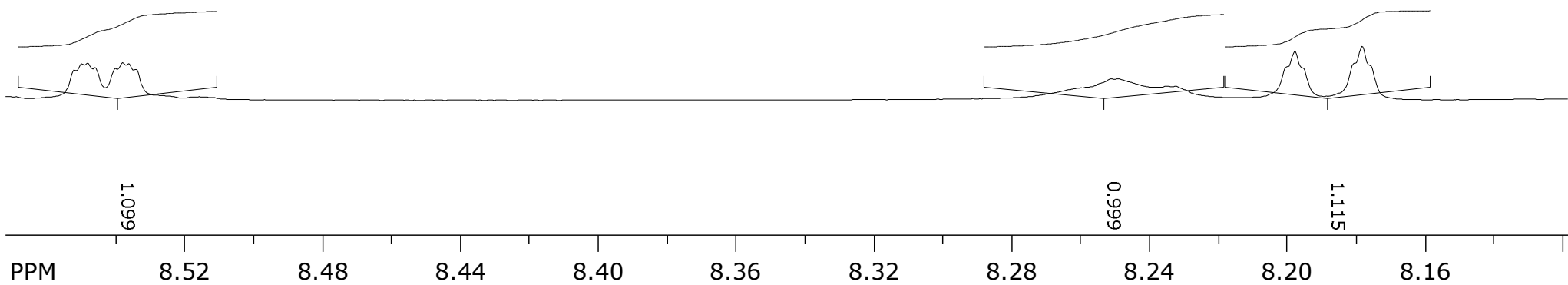
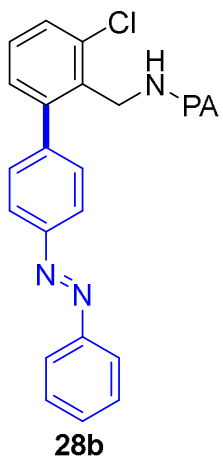


SpinWorks 4: SS-295-REP4
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 18

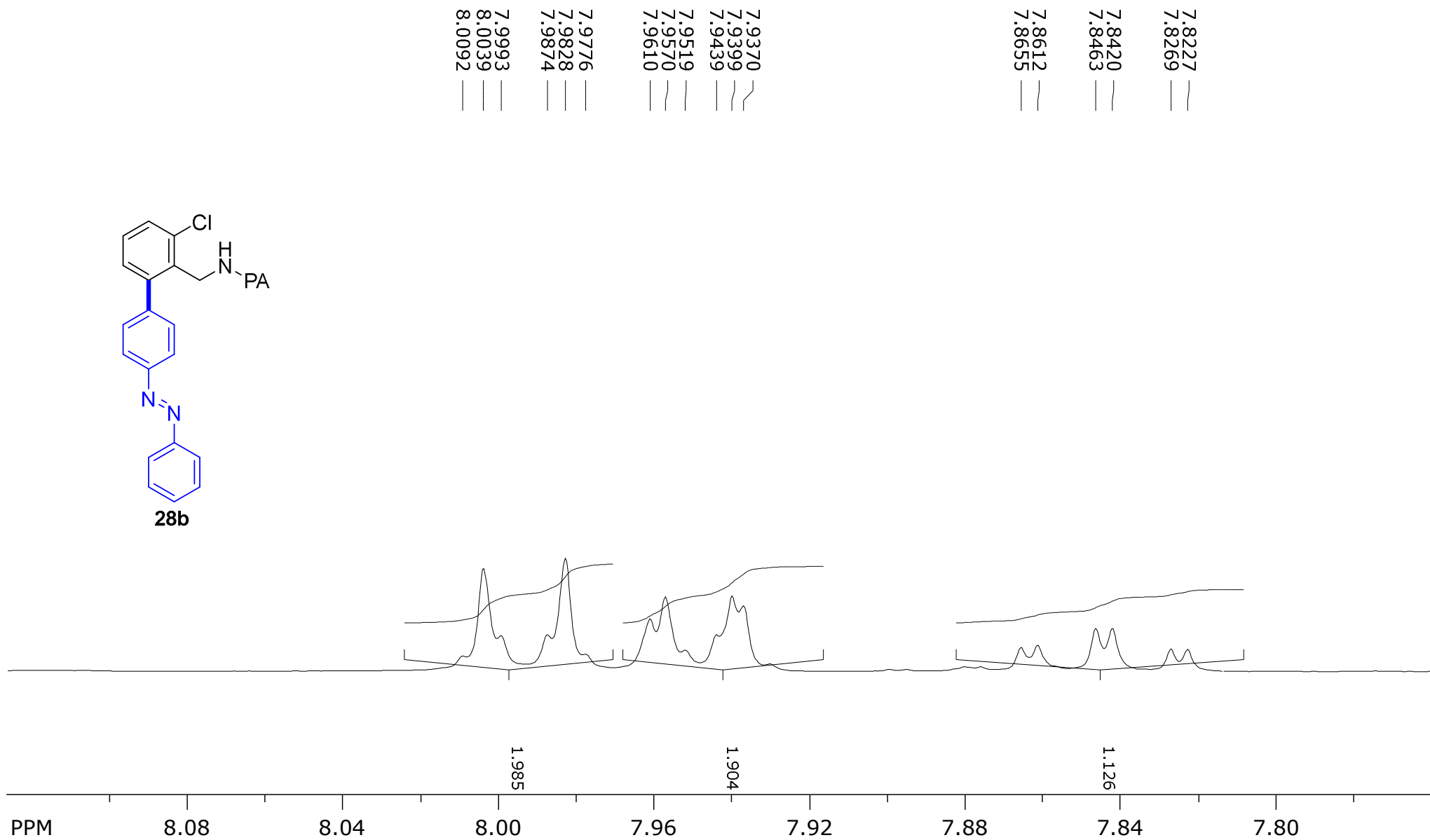
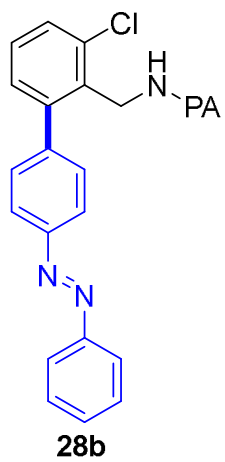
8.5343
8.5365
8.5382
8.5403
8.5462
8.5483
8.5500



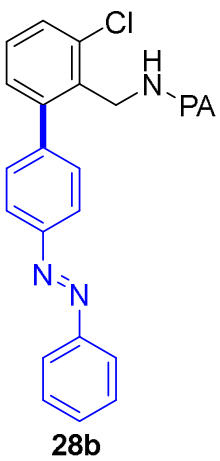
8.1782
8.1803
8.1977
8.2347
8.2510
8.2650



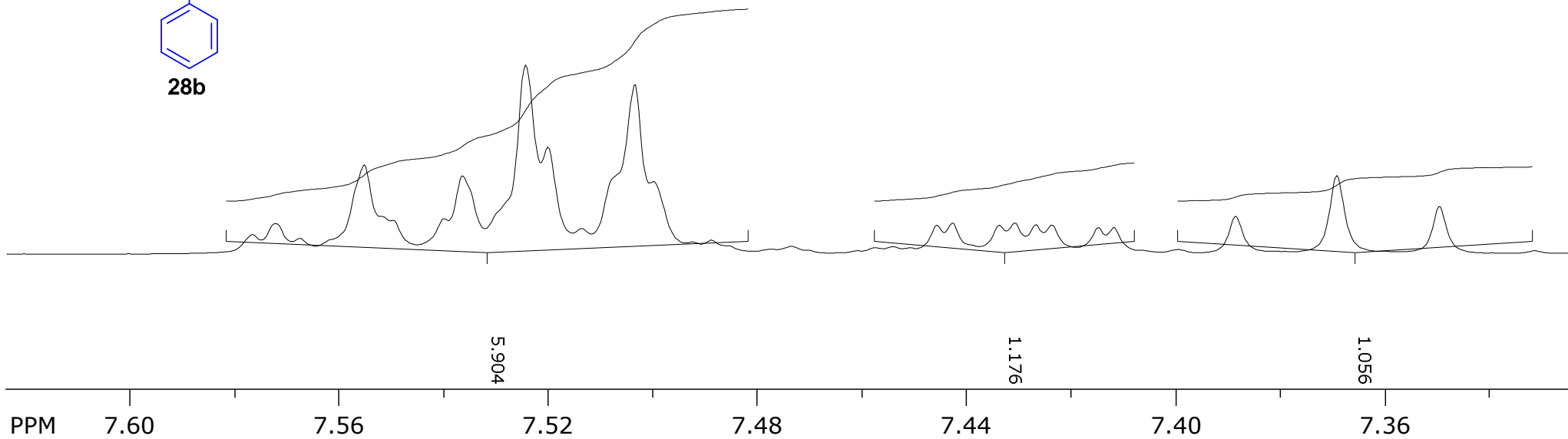
SpinWorks 4: SS-295-REP4
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 18



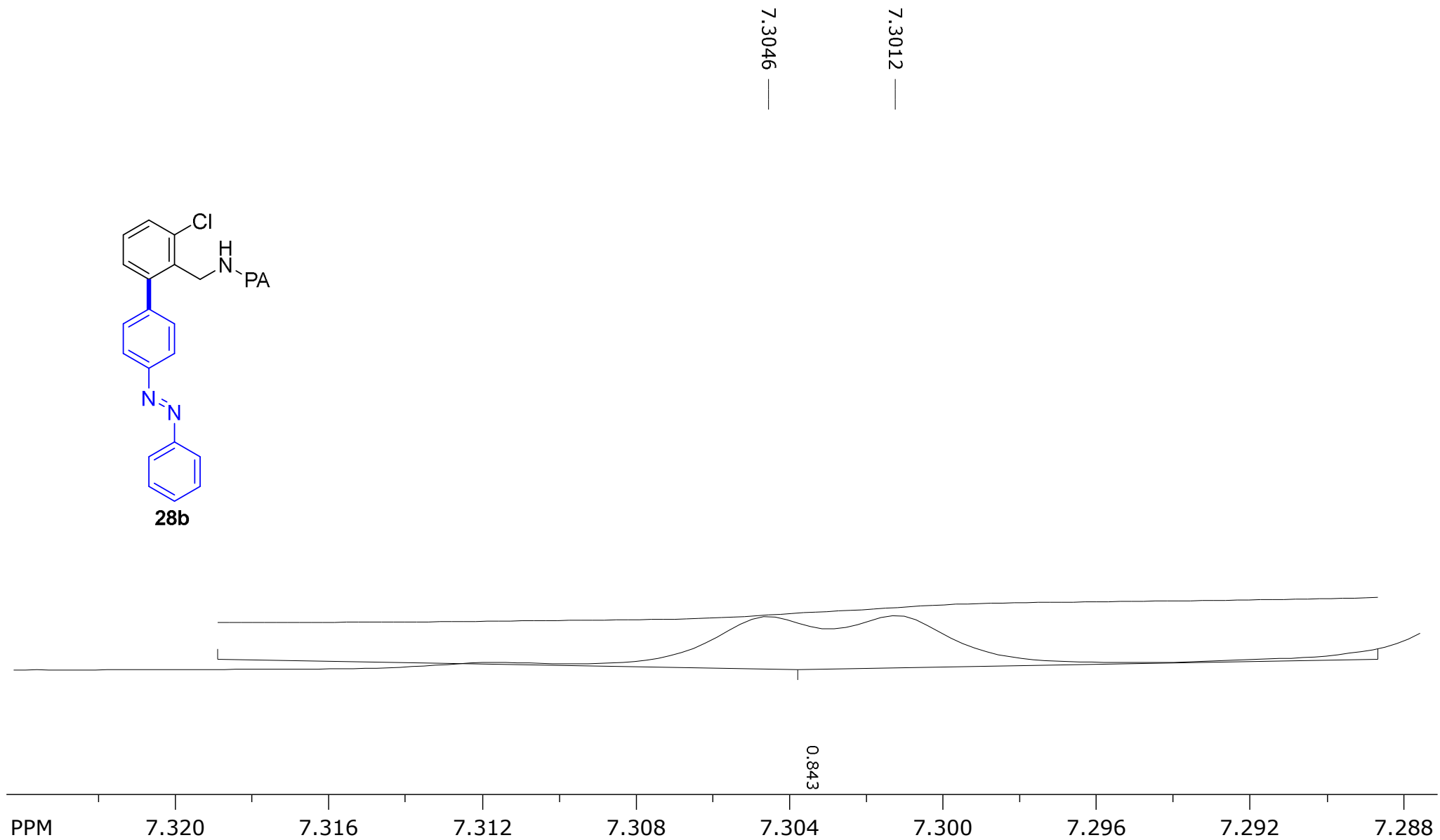
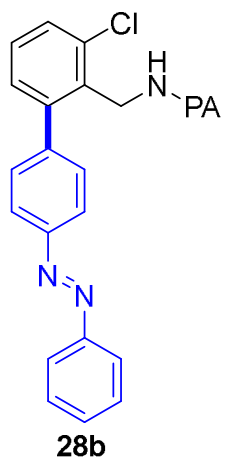
SpinWorks 4: SS-295-REP4
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 18



7.5766
7.5722
7.5676
7.5552
7.5519
7.5498
7.5400
7.5365
7.5243
7.5201
7.5136
7.4999
7.5034
7.4888
7.4457
7.4426
7.4337
7.4307
7.4267
7.4237
7.4148
7.4118
7.3885
7.3691
7.3495

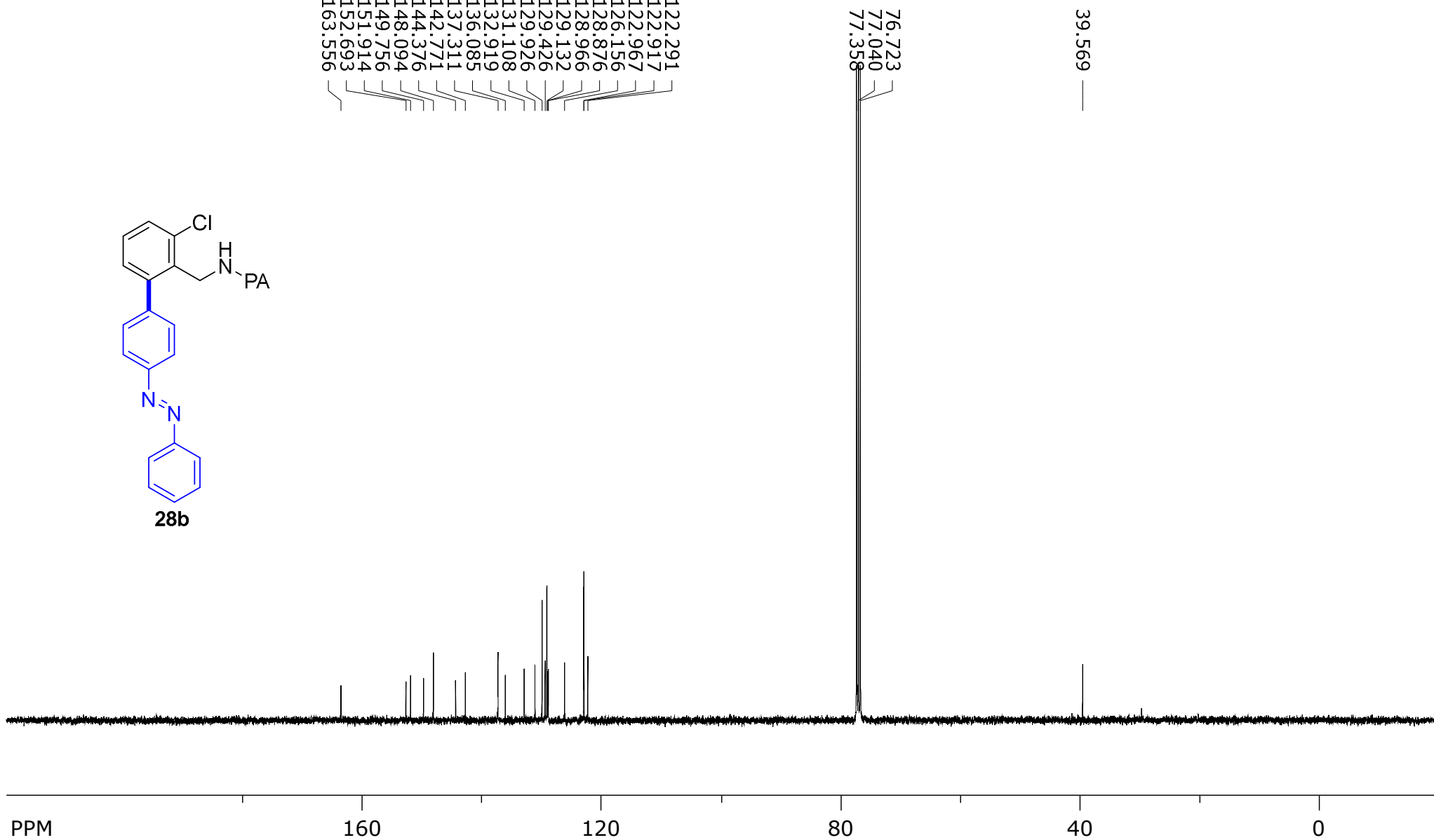
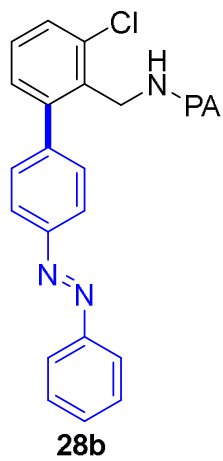


SpinWorks 4: SS-295-REP4
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 18



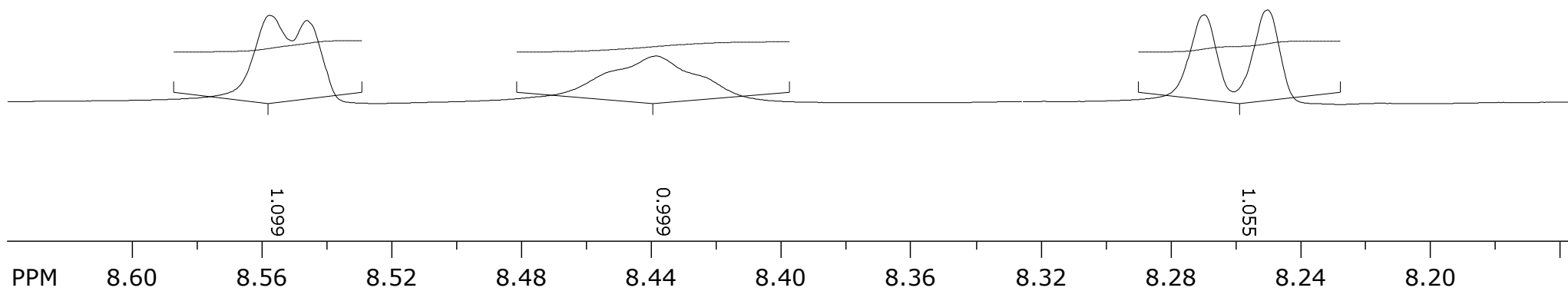
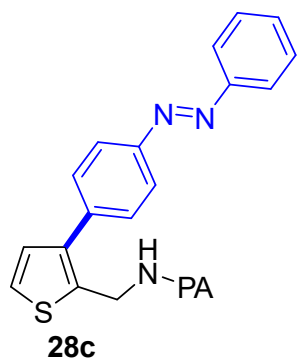
SpinWorks 4: SS-295-R4
C13CPD CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 8

122.291
122.917
122.917
122.967
126.156
128.876
128.966
129.132
129.426
129.926
131.108
132.919
136.085
137.311
142.771
144.376
148.094
149.756
151.914
152.693
163.556

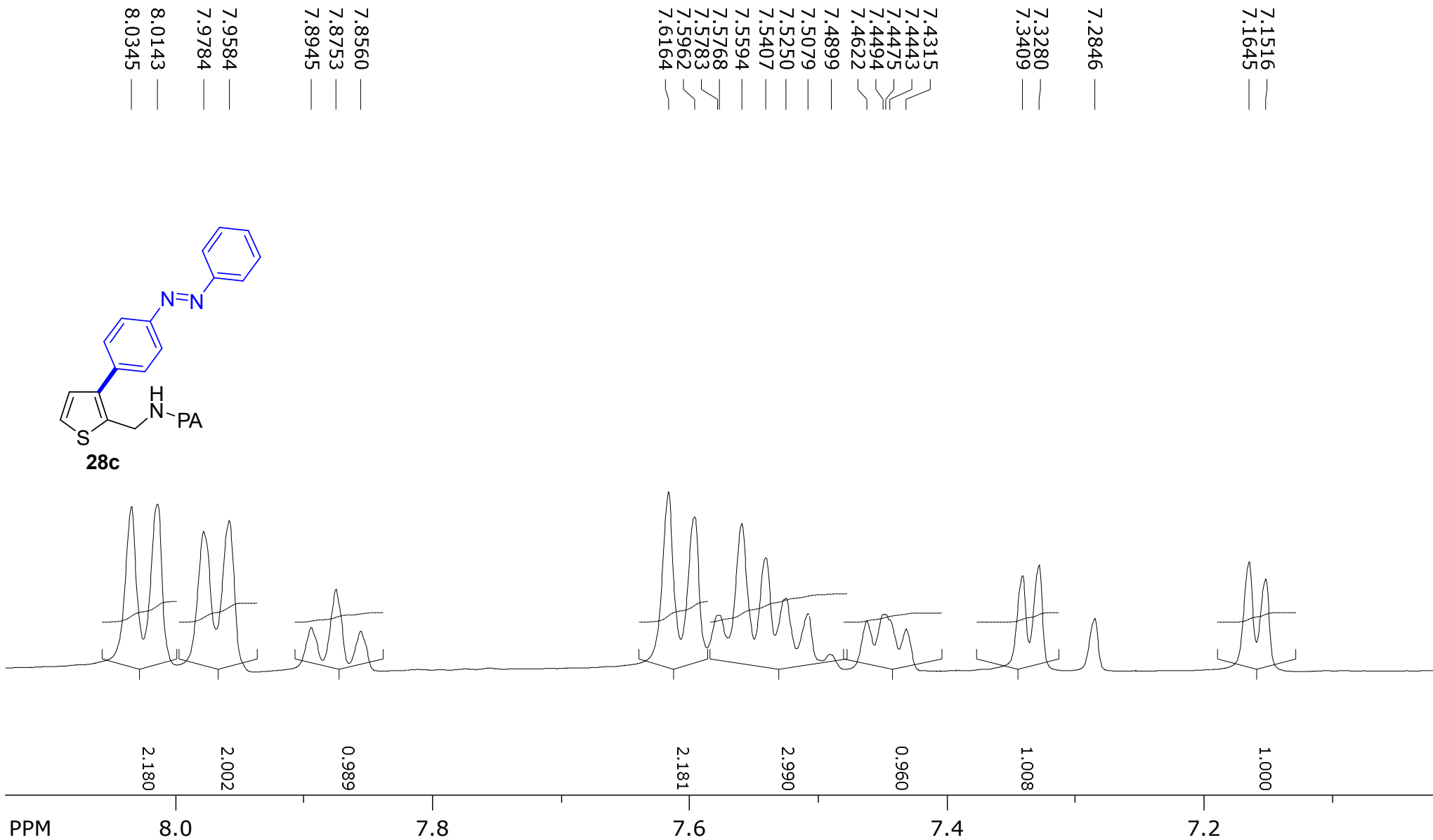
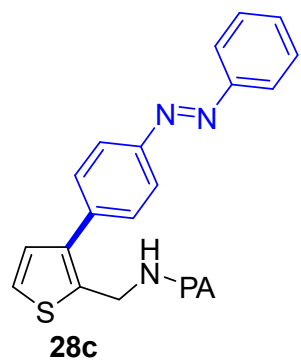


SpinWorks 4: SS 285 P
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 48

8.5577 —
8.5462 —
8.4671 —
8.4560 —
8.4386 —
8.4208 —
8.4097 —
8.2697 —
8.2502 —

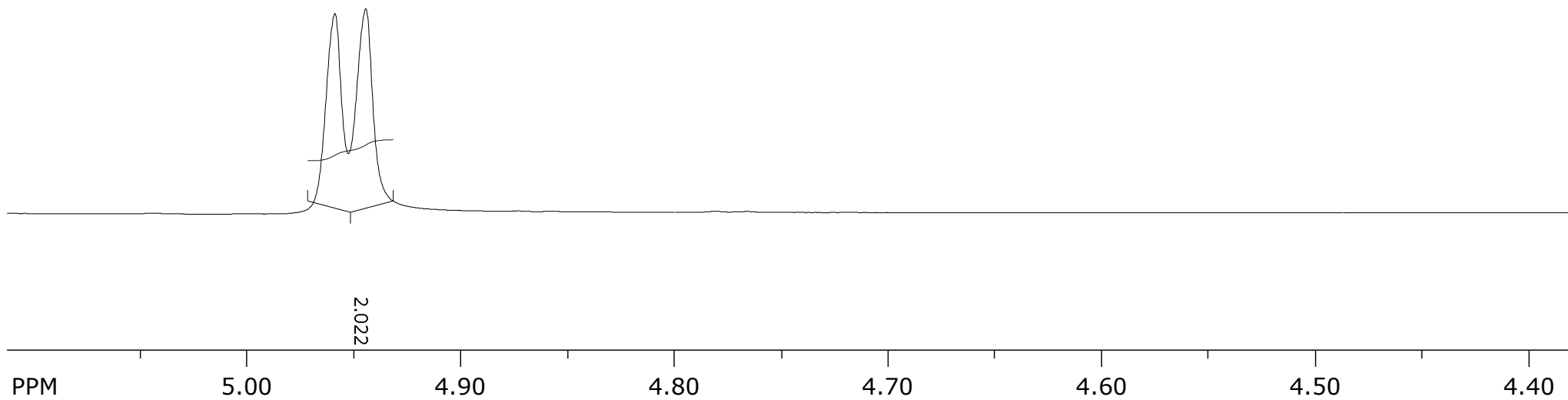
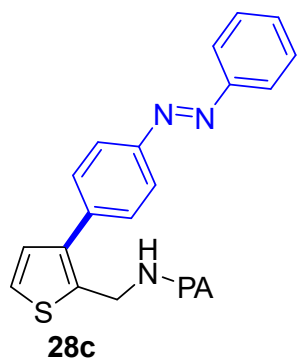


SpinWorks 4: SS 285 P
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 48



SpinWorks 4: SS 285 P
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 48

4.9446
4.9591

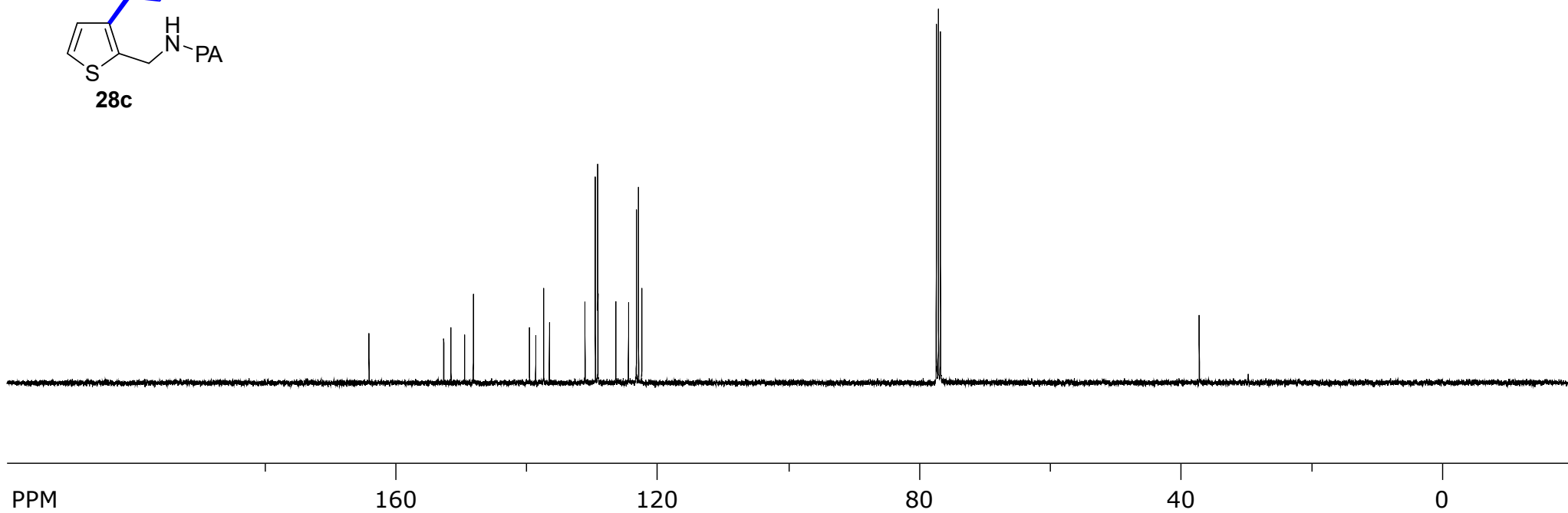
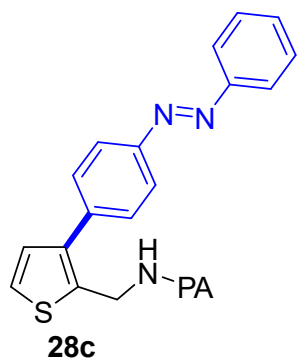


SpinWorks 4: SS 285 P
C13CPD CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 48

122.427
122.925
123.247
124.468
126.390
129.127
129.152
129.522
131.098
136.553
137.419
138.649
139.585
148.179
149.508
151.593
152.699
164.120

76.760
77.077
77.395

37.197



SpinWorks 4: SS 286 P
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 52

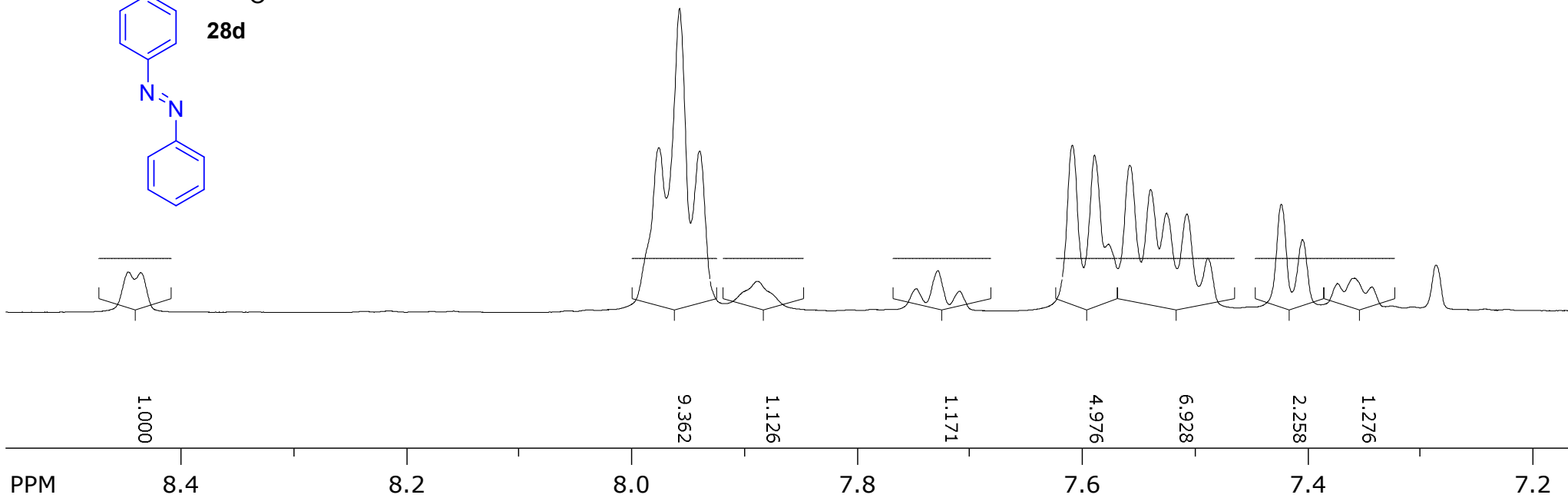
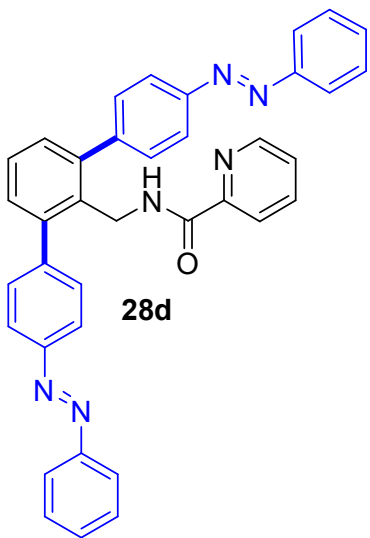
8.4364
8.4475

7.86664
7.8885
7.9071
7.9399
7.9577
7.9761

7.7088
7.7281
7.7473

7.4884
7.5069
7.5250
7.5391
7.5576
7.5766
7.5891
7.6087

7.3427
7.3581
7.3595
7.3731
7.4043
7.4231
7.2855

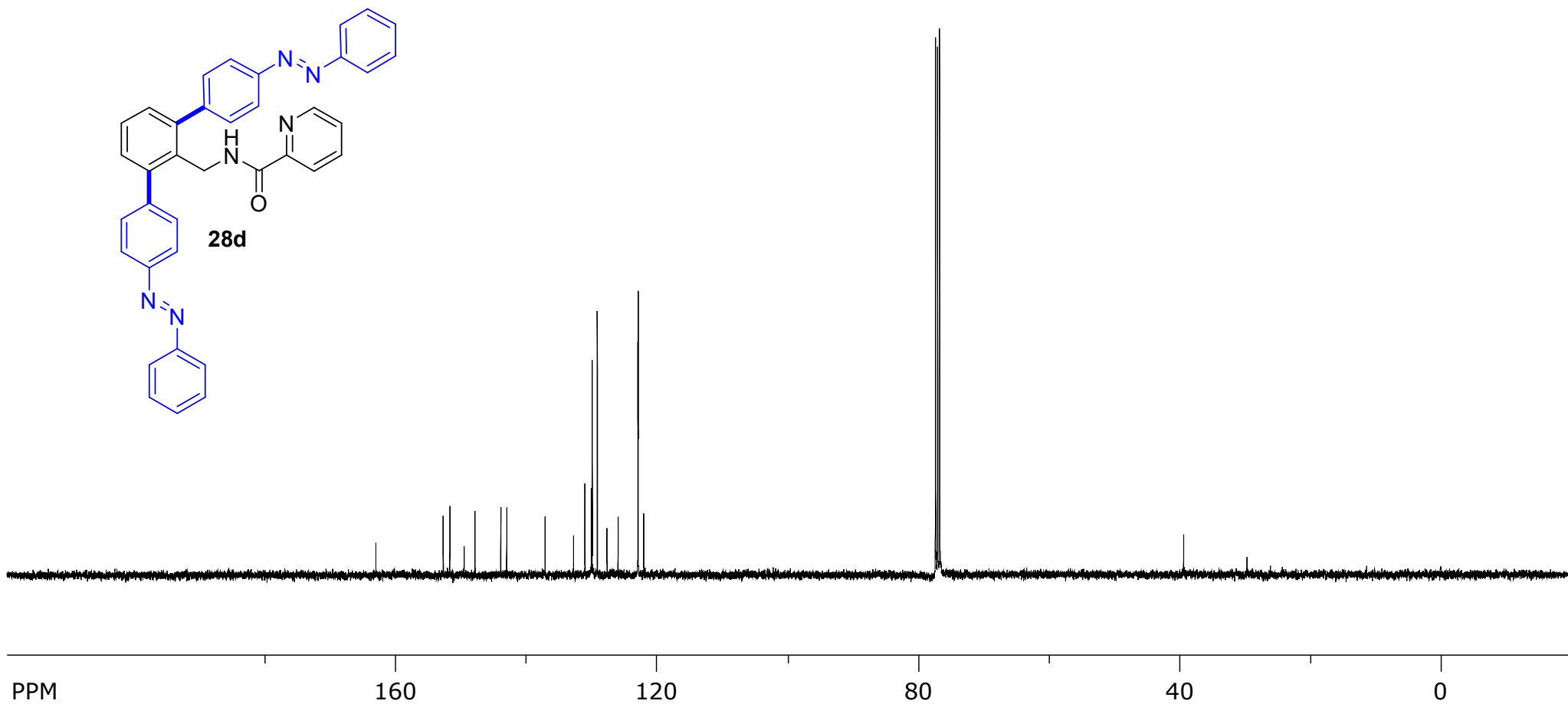
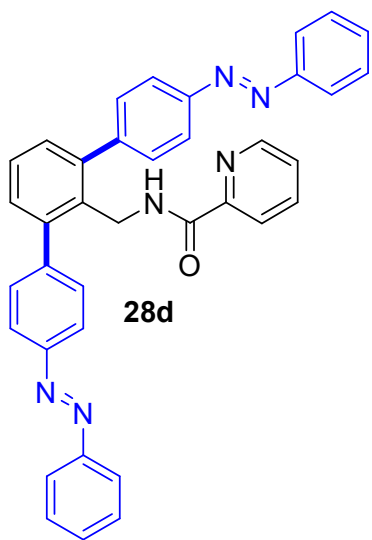


SpinWorks 4: SS 286 P
C13CPD CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 52

122.029
122.888
122.917
125.964
127.651
129.134
129.896
130.062
131.045
132.767
137.133
143.002
143.910
147.845
149.518
151.711
152.711
163.005

76.740
77.058
77.375

39.414



PPM

160

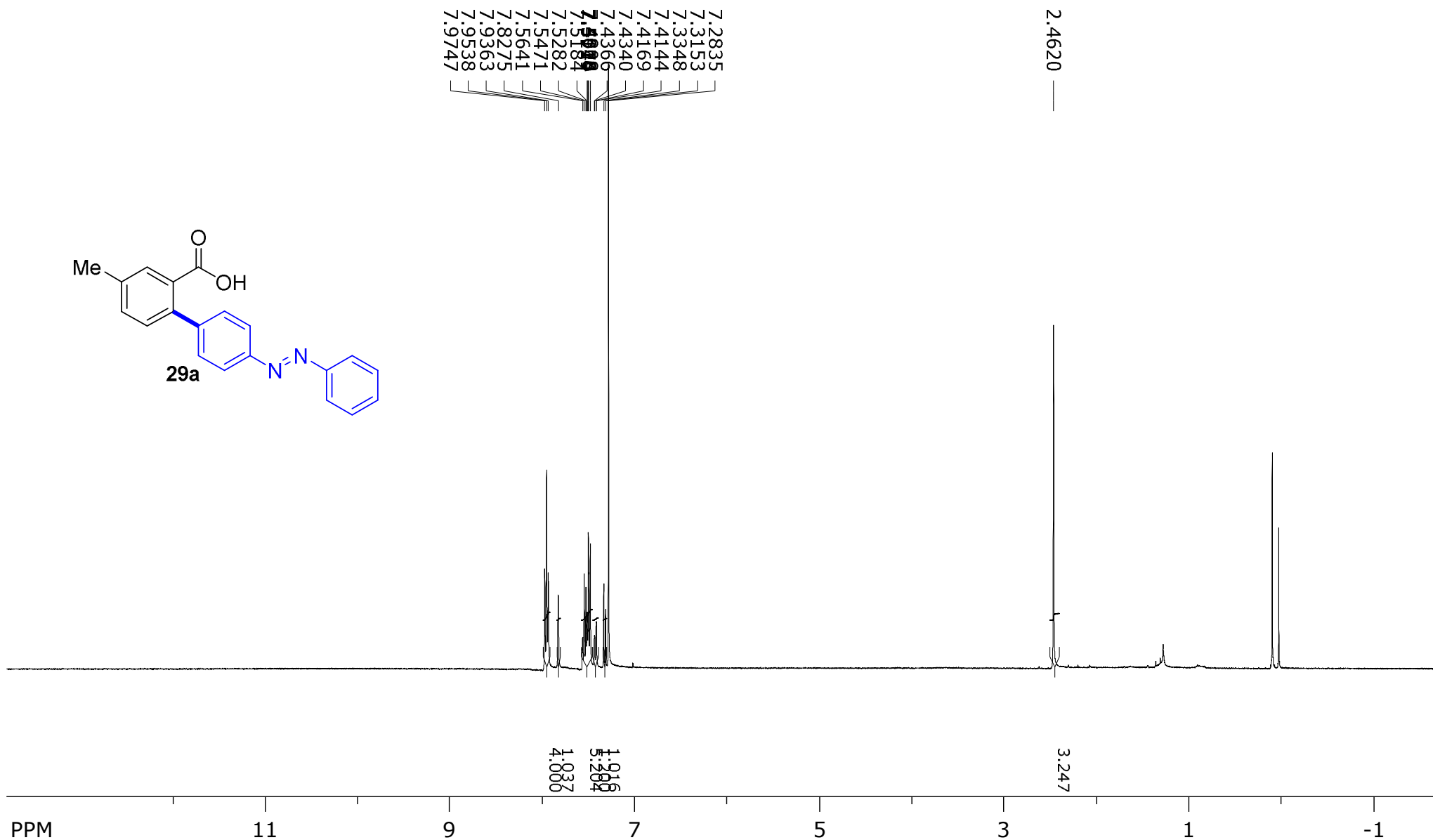
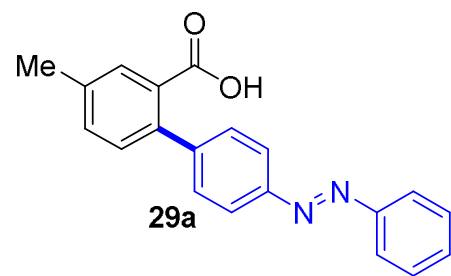
120

80

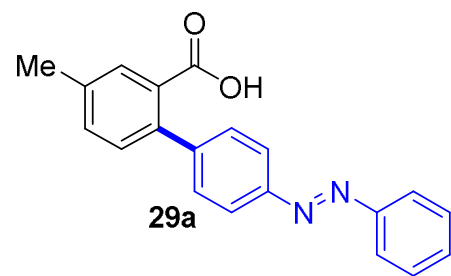
40

0

SpinWorks 4: S S 188
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 18



SpinWorks 4: S S 188
PROTON CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 18



7.9363
7.9538
7.9747

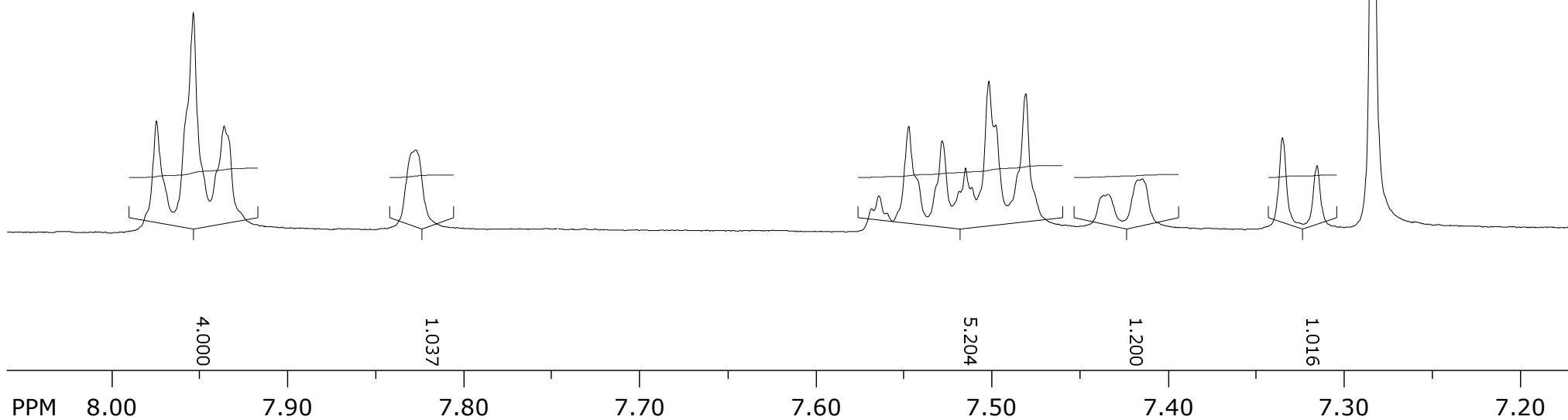
7.8275

7.4808
7.4978
7.5018
7.5114
7.5149
7.5184
7.5282
7.5471
7.5641

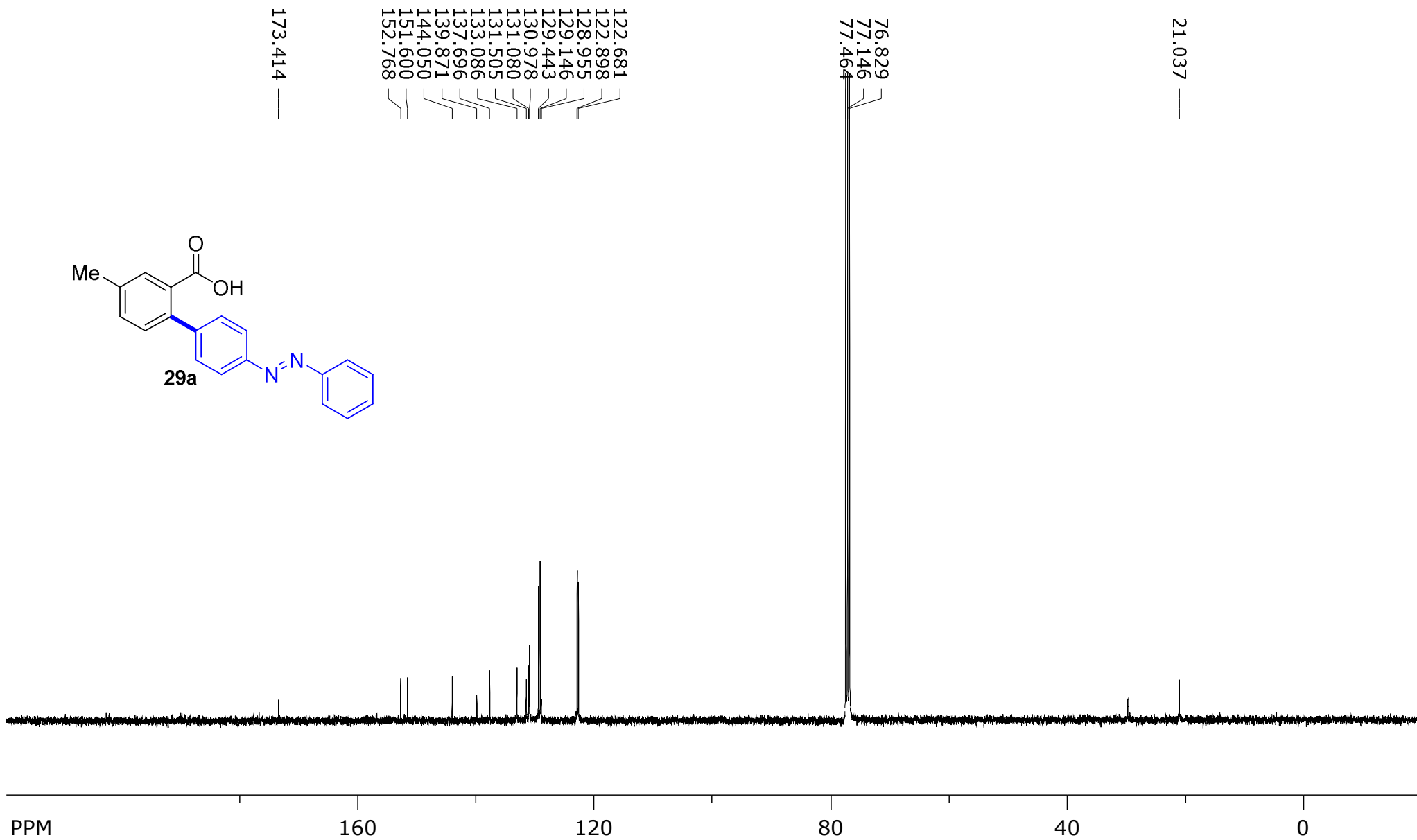
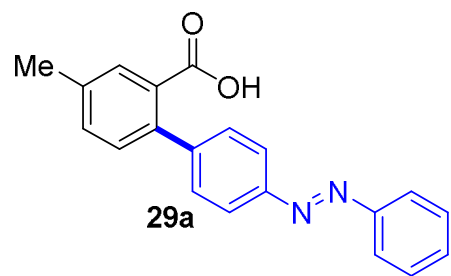
7.4144
7.4169
7.4340
7.4366

7.3153
7.3348

7.2835



SpinWorks 4: SS 188 ACID
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 48



PPM

160

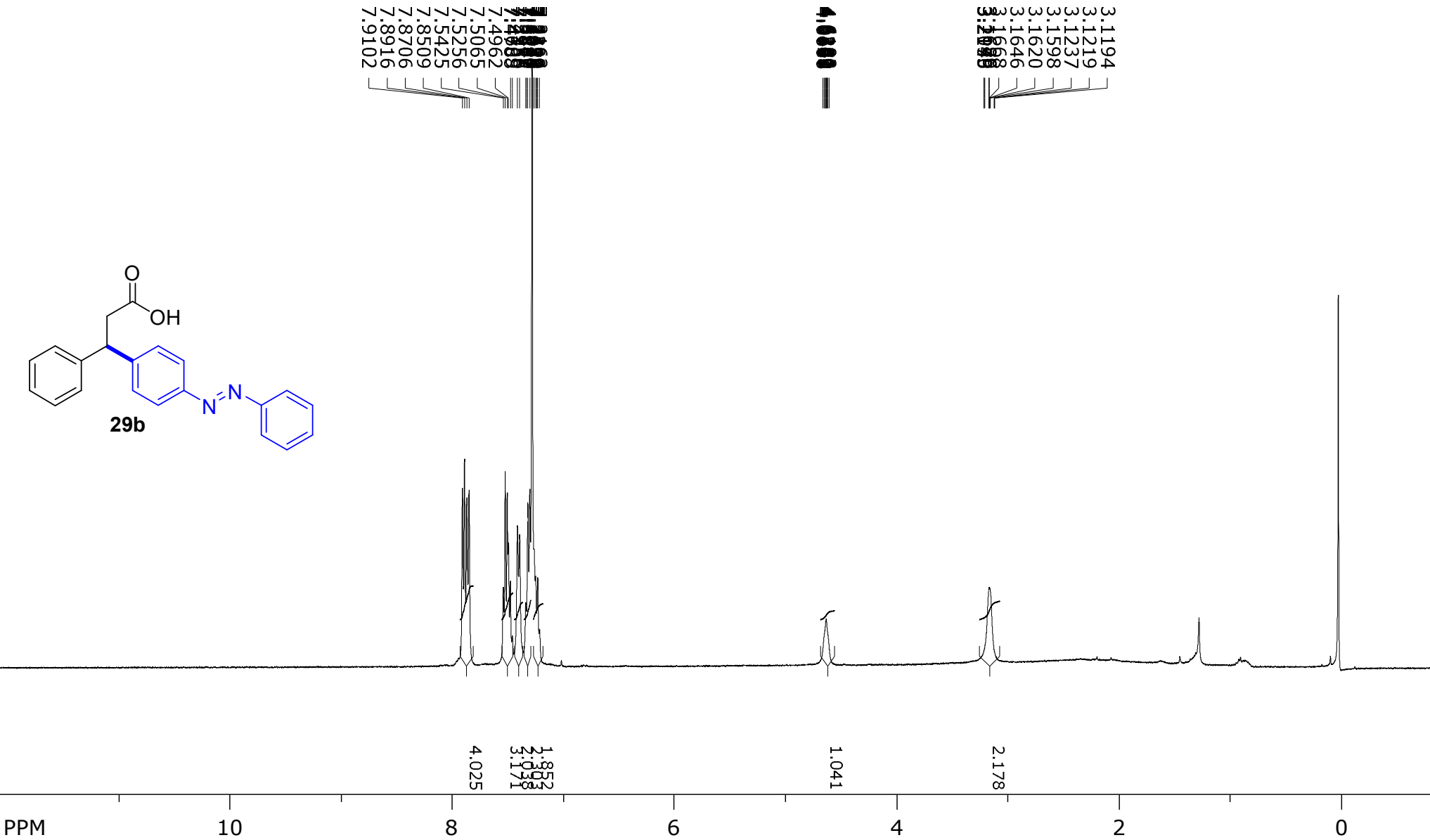
120

80

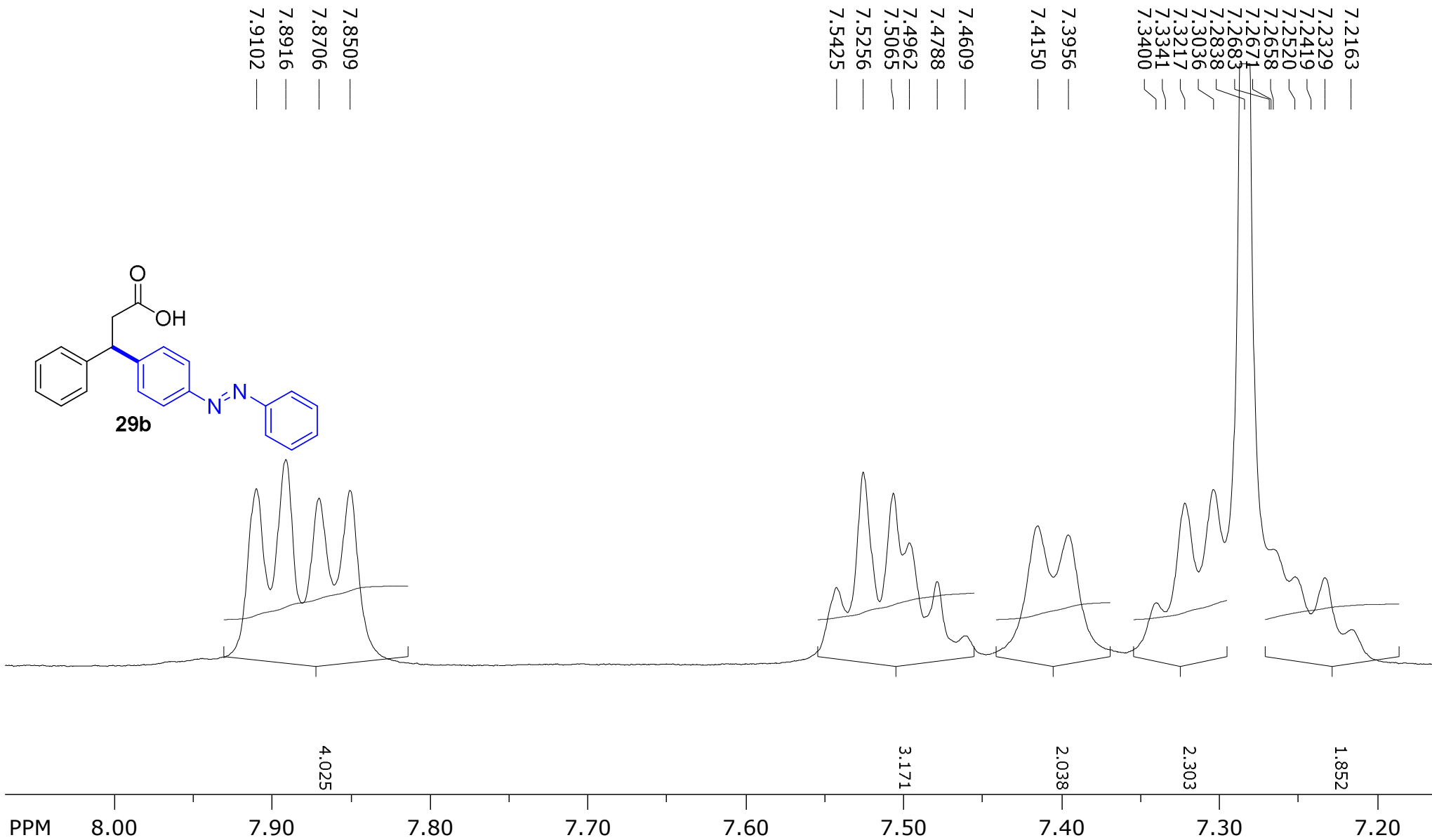
40

0

SpinWorks 4: SS-847REP2
{PROTON 64} CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 22

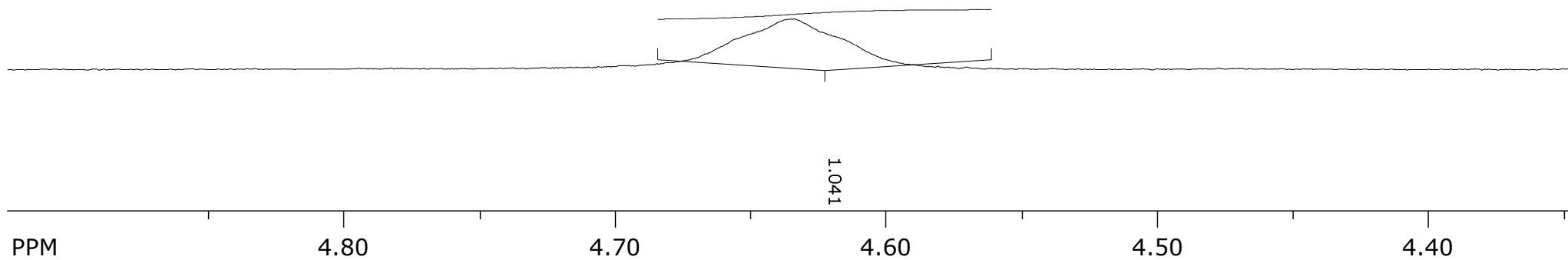
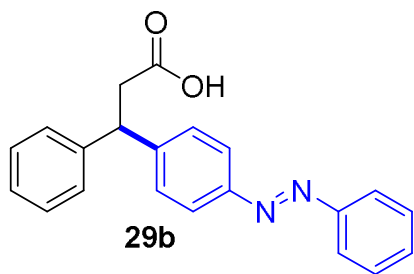


SpinWorks 4: SS-847REP2
{PROTON 64} CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 22



SpinWorks 4: SS-847REP2
{PROTON 64} CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 22

4.6102
4.6200
4.6249
4.6342
4.6352
4.6361
4.6370
4.6489
4.6523
4.6666

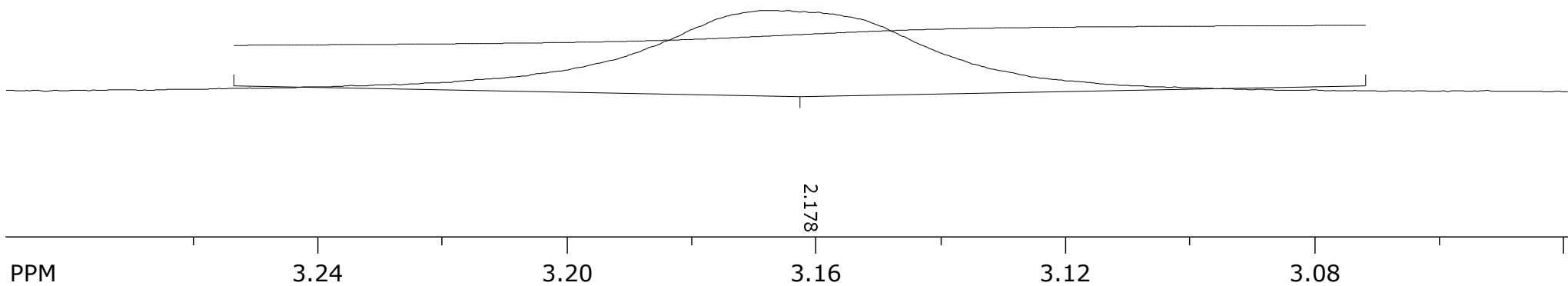
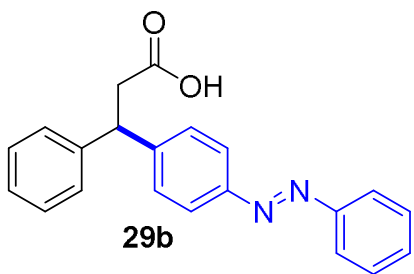


SpinWorks 4: SS-847REP2
{PROTON 64} CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 22

3.2070 —
3.2143 —
3.2155 —

3.1598 —
3.1620 —
3.1646 —
3.1668 —
3.1679 —
3.1686 —

3.1194 —
3.1219 —
3.1237 —



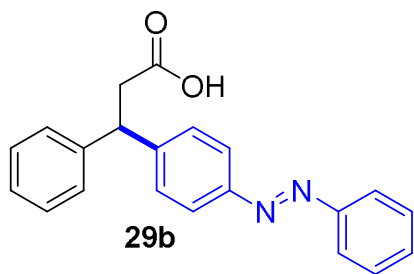
SpinWorks 4: SS-847 REP
C13CPD256 CDCl3 /opt/topspin3.5pl2/nmrdata nmrsu 31

122.806
123.174
126.887
127.650
128.421
128.782
129.089
130.938
142.721
146.381
151.398
152.680

76.722
77.040
77.357

46.550

29.725



PPM

160

120

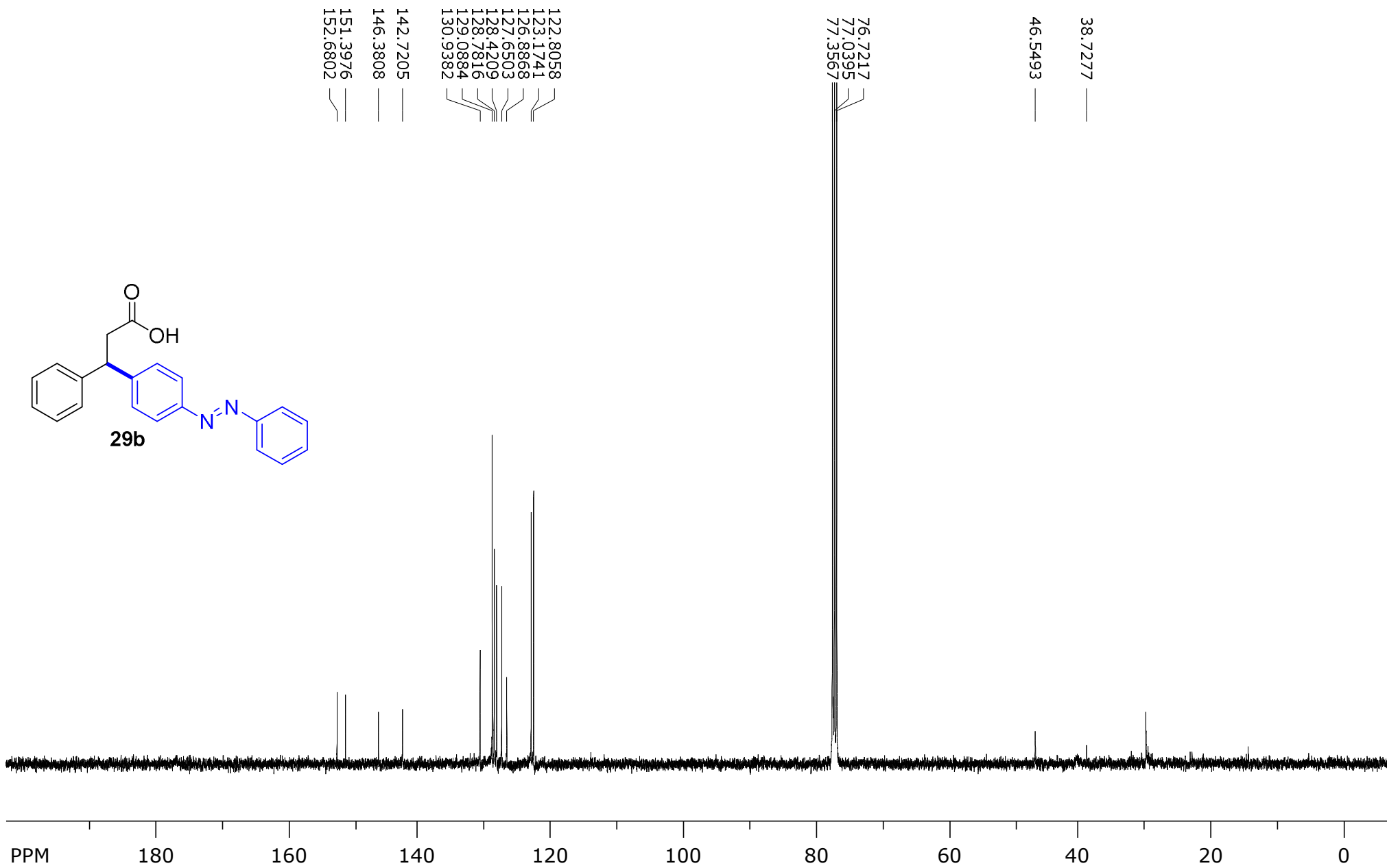
80

40

0

360

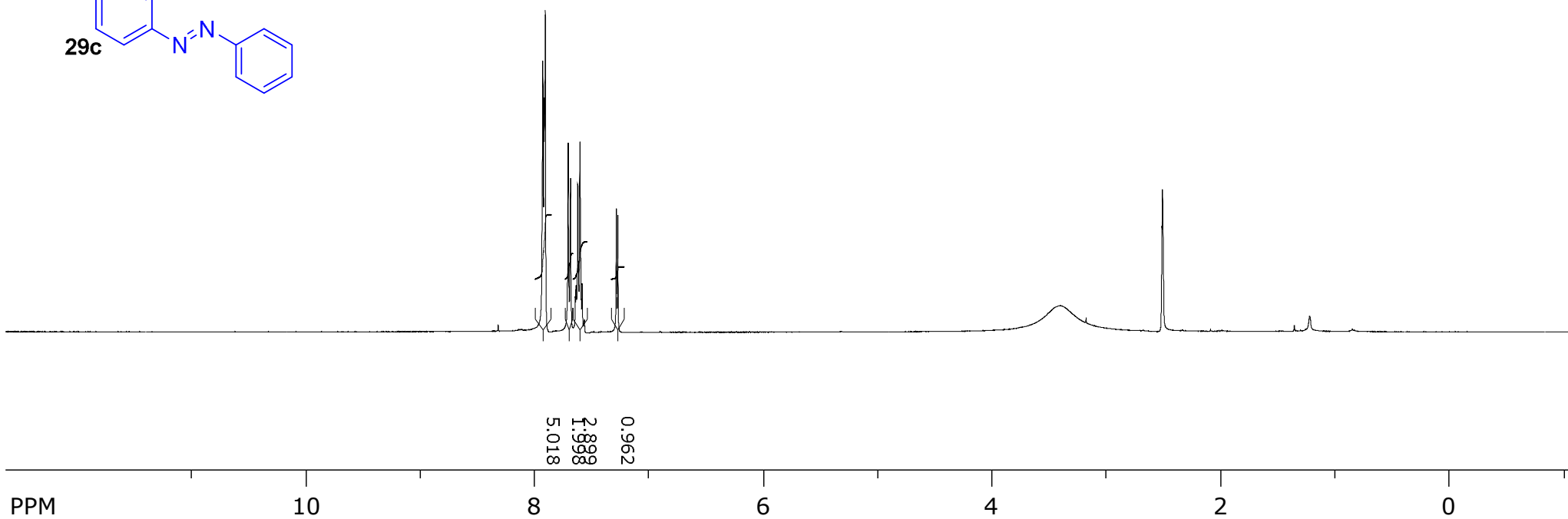
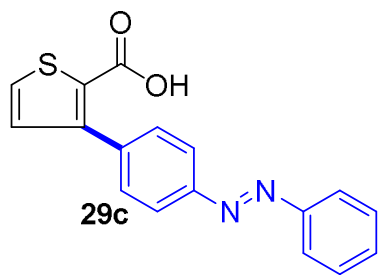
SpinWorks 3: SS-847 REP



SpinWorks 4: SS-848 REP
PROTON DMSO /opt/topspin3.5pl2/nmrdata nmrsu 2

7.2884
7.1891
7.1891
7.1891
7.1891
7.6453
7.6869
7.7080
7.9077
7.9145
7.9194
7.9298

2.5023
2.5065
2.5107
3.3308
3.3342
3.3370
3.3424
3.3449
3.3480
3.3480



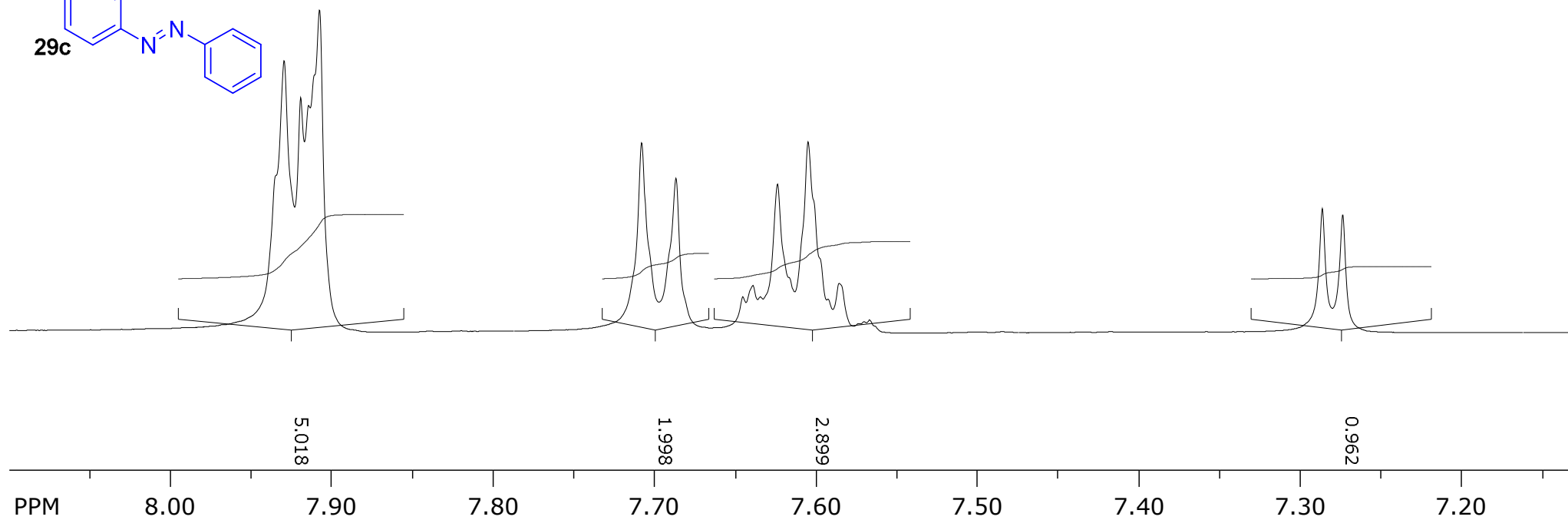
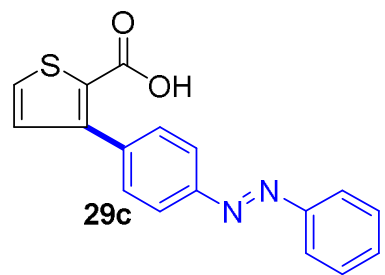
SpinWorks 4: SS-848 REP
PROTON DMSO /opt/topspin3.5pl2/nmrdata nmrsu 2

7.9077
7.9145
7.9194
7.9298

7.6869
7.7080

7.6453
7.6391
7.6345
7.6237
7.6050
7.5926
7.5857
7.5667

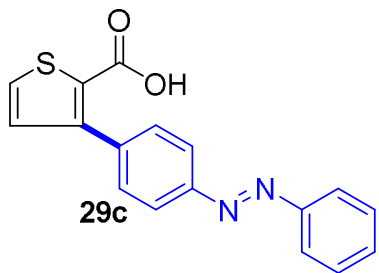
7.2734
7.2861



SpinWorks 4: SS-848 REP
C13CPD256 DMSO /opt/topspin3.5pl2/nmrdata nmrsu 2

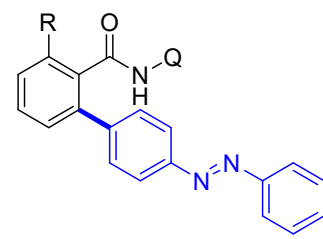
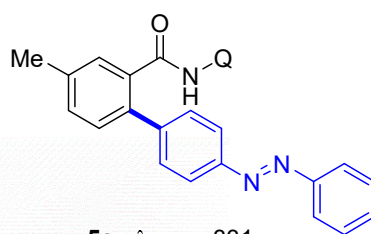
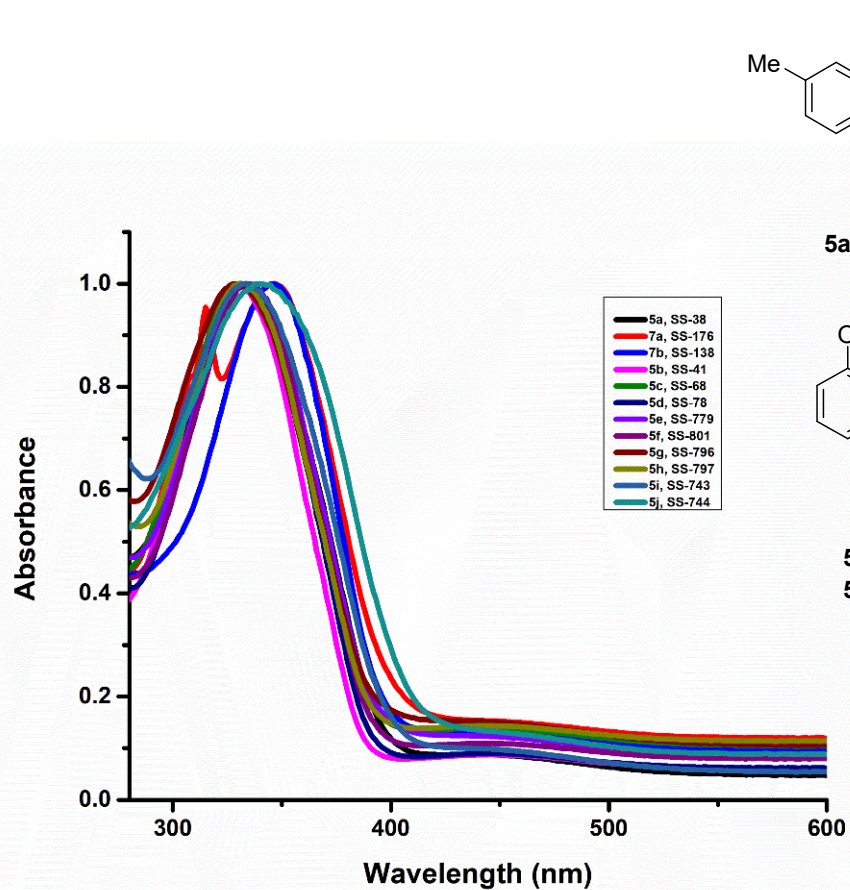
163.294 —
152.475 —
151.562 —
146.362 —
139.077 —
132.071 —
131.988 —
131.785 —
130.985 —
129.980 —
129.539 —
123.063 —
122.454 —

39.318 —
39.527 —
39.736 —
39.945 —
40.153 —
40.362 —
40.571 —

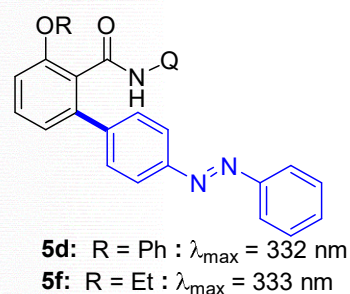
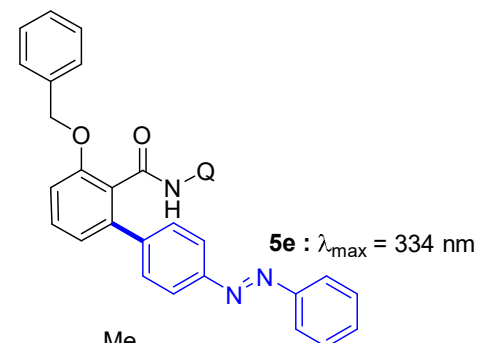


PPM 160 120 80 40 0

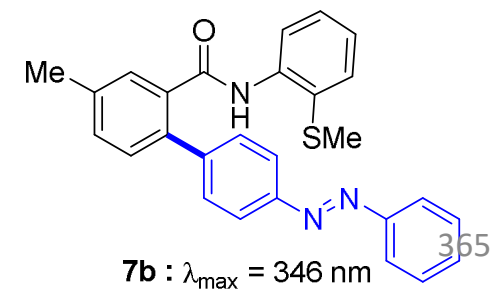
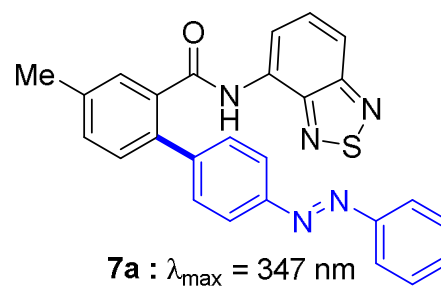
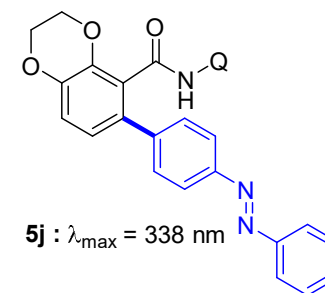
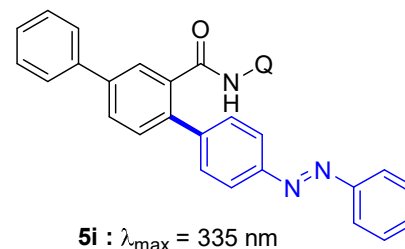
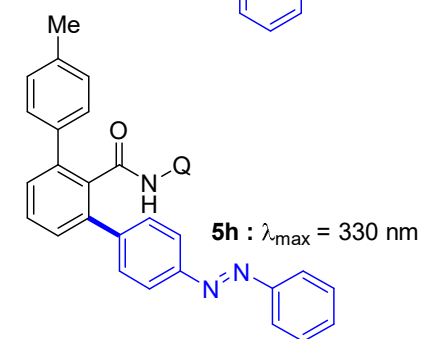
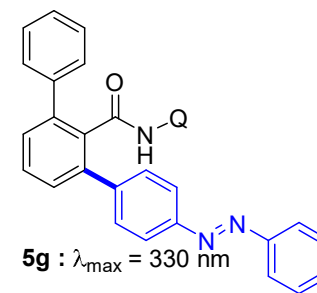
UV-Vis absorption chart (λ_{\max}) of compounds 5a-j,7a,b



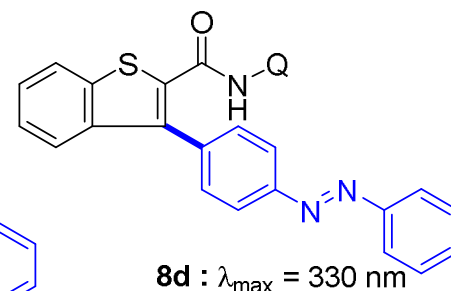
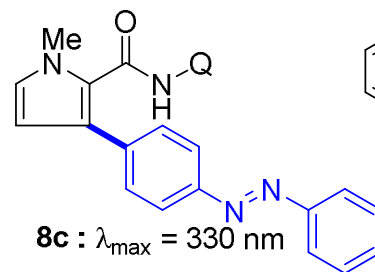
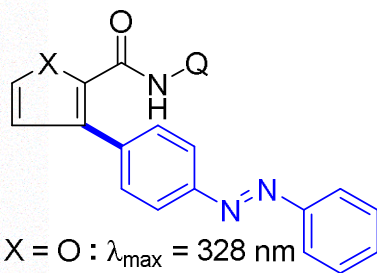
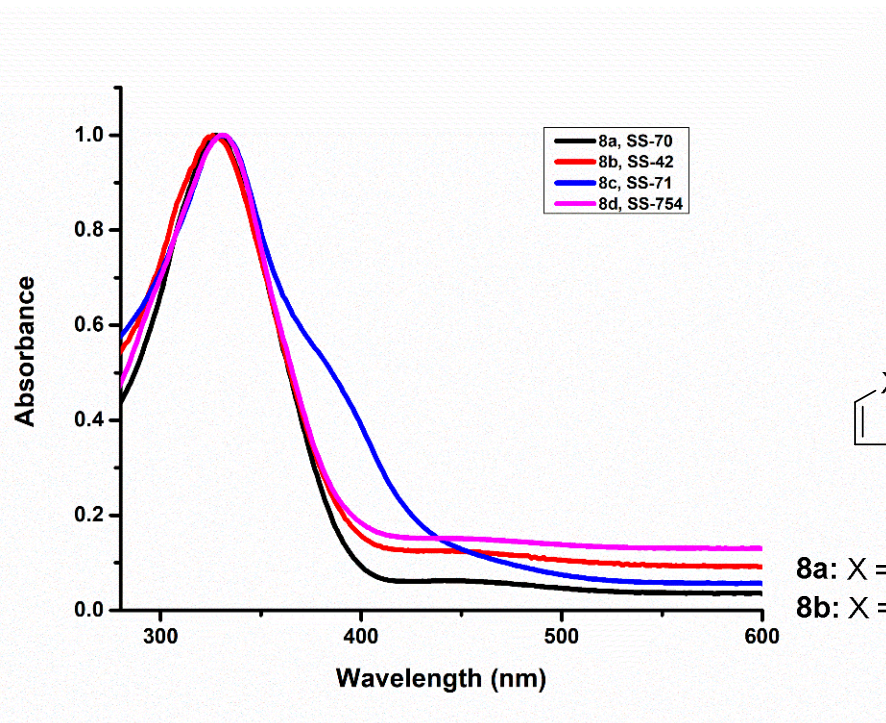
5c : R = Me : $\lambda_{\max} = 332$ nm



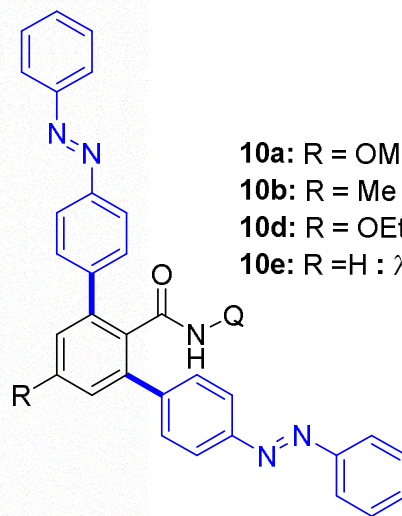
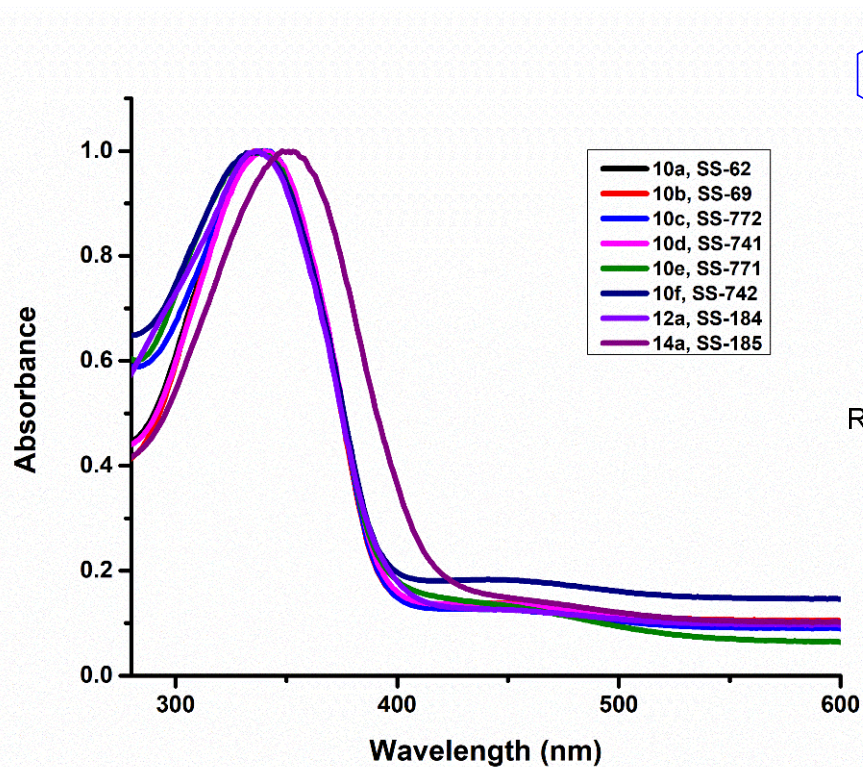
5f : R = Et : $\lambda_{\max} = 333$ nm



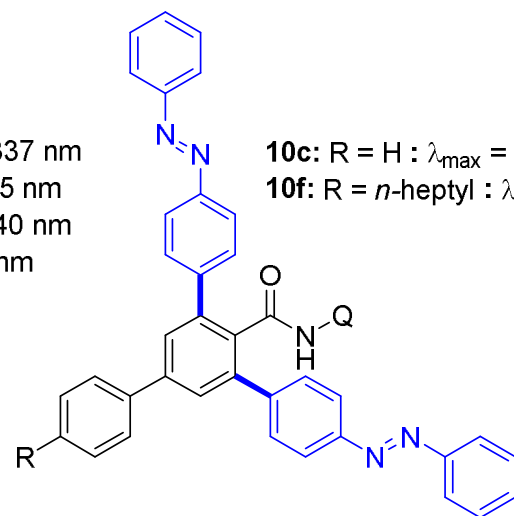
UV-Vis absorption chart (λ_{\max}) of compounds 8a-d



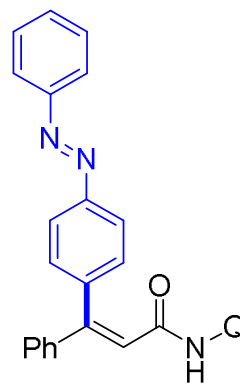
UV-Vis absorption chart (λ_{\max}) of compounds 10a-f, 12a, 14a



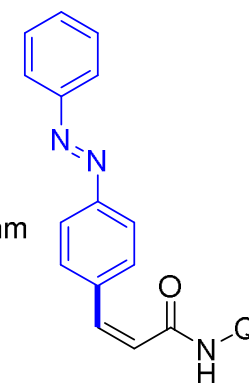
10a: R = OMe : λ_{\max} = 337 nm
10b: R = Me : λ_{\max} = 335 nm
10d: R = OEt : λ_{\max} = 340 nm
10e: R = H : λ_{\max} = 338 nm



10c: R = H : λ_{\max} = 341 nm
10f: R = *n*-heptyl : λ_{\max} = 337 nm

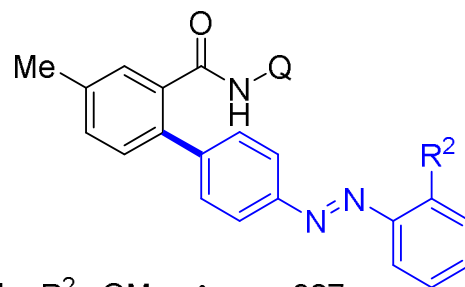
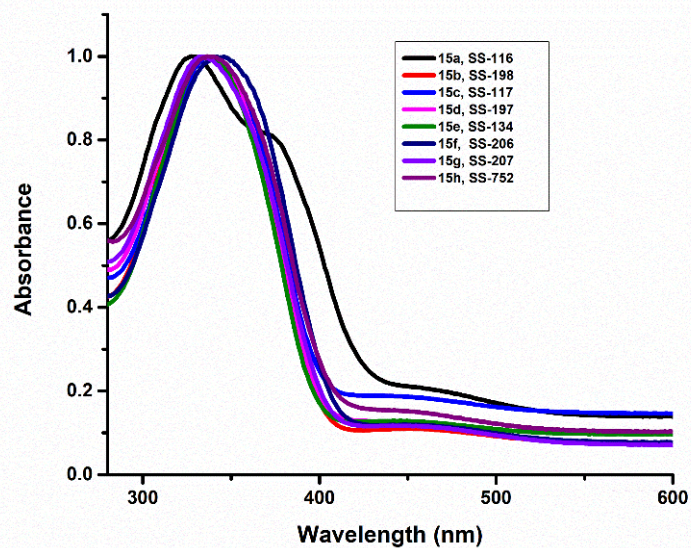


12a : λ_{\max} = 336 nm



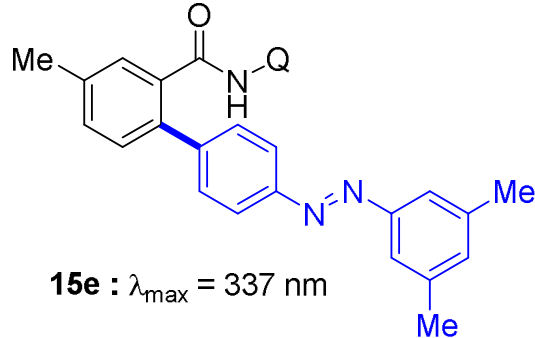
14a : λ_{\max} = 348 nm

UV-Vis absorption chart (λ_{\max}) of compounds 15a-h

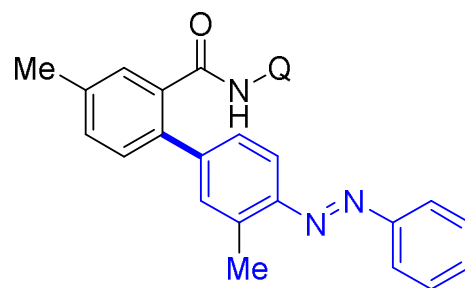


15a: R² = OMe : λ_{\max} = 327 nm

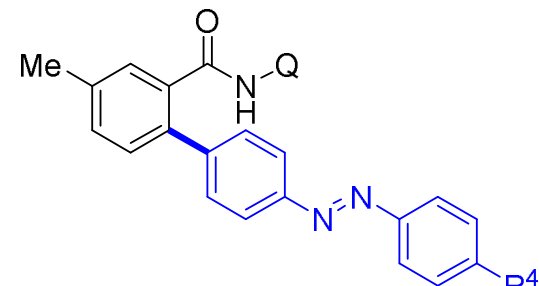
15b: R² = Me : λ_{\max} = 338 nm



15e: λ_{\max} = 337 nm

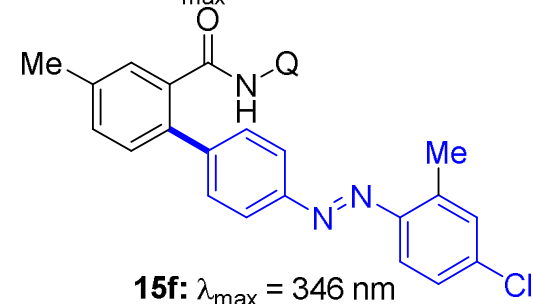


15g: λ_{\max} = 334 nm

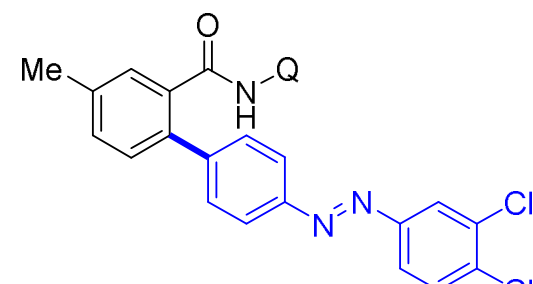


15c: R⁴ = Me : λ_{\max} = 337 nm

15d: R⁴ = Et : λ_{\max} = 335 nm

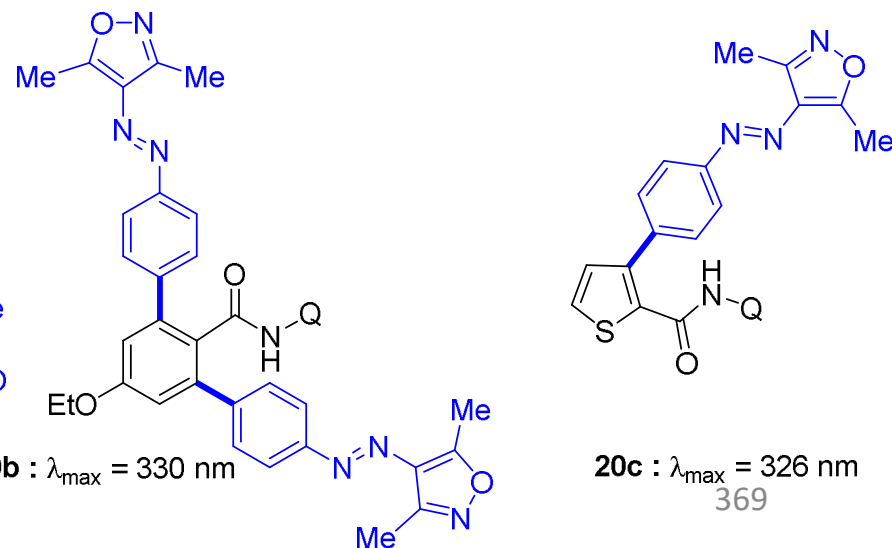
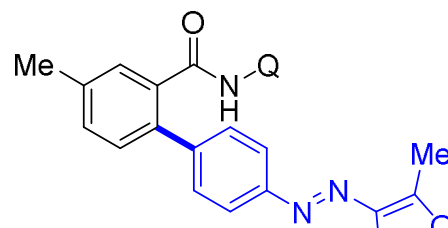
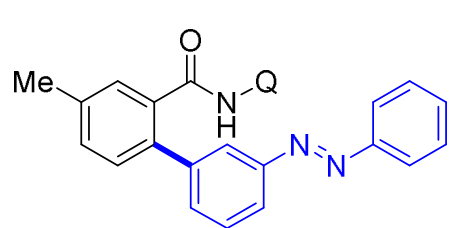
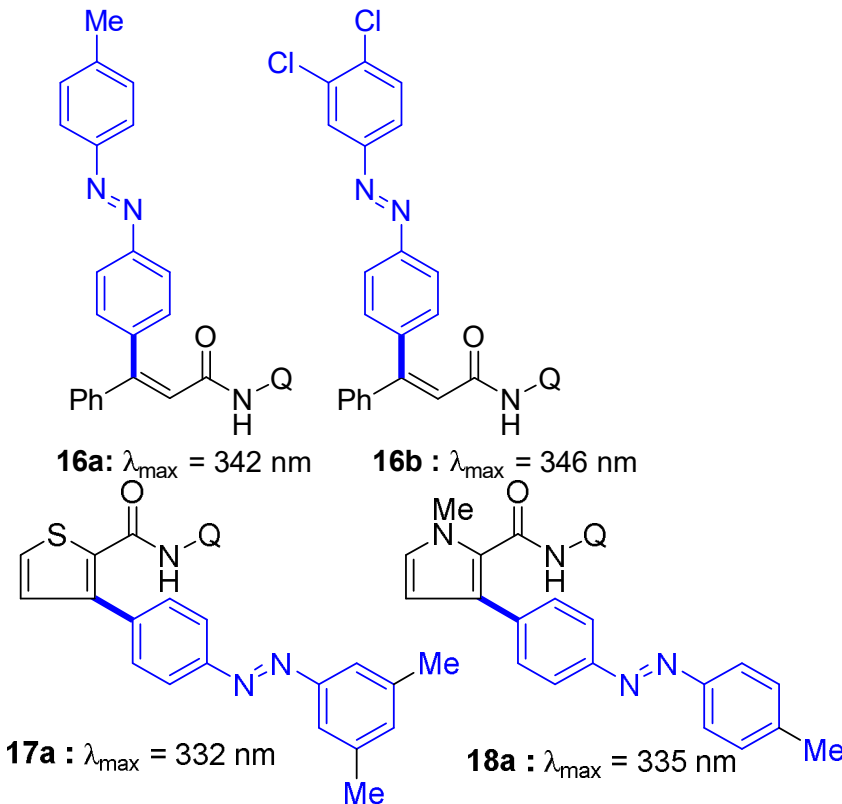
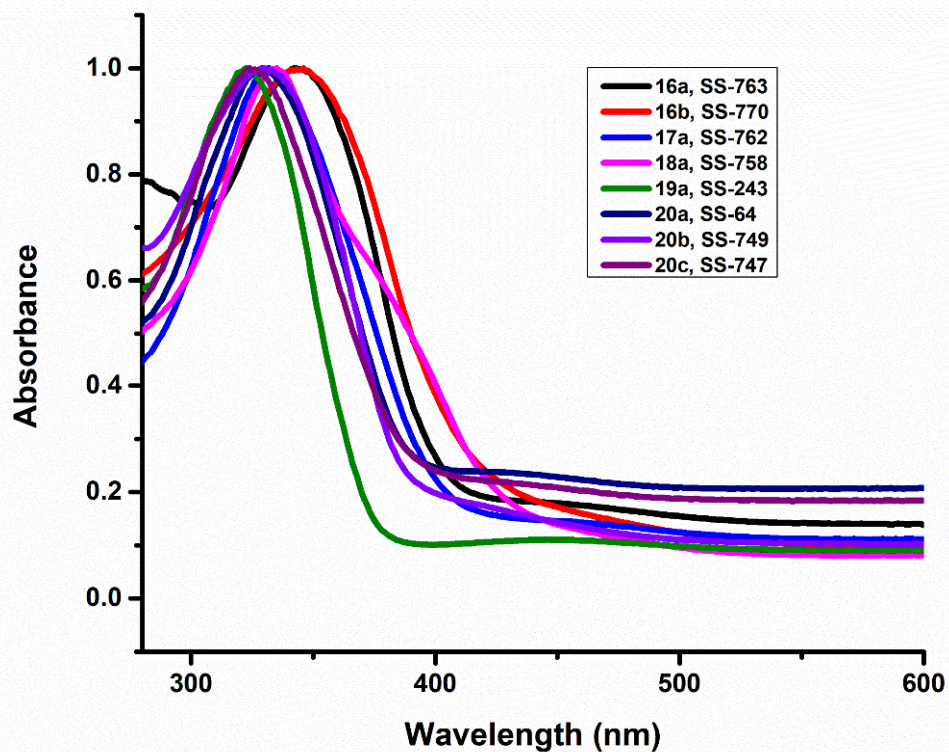


15f: λ_{\max} = 346 nm

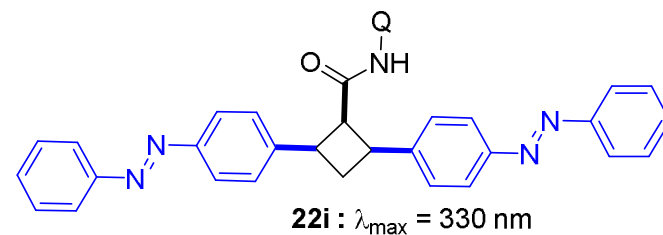
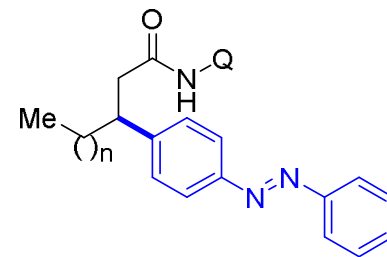
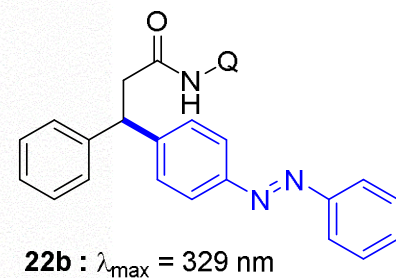
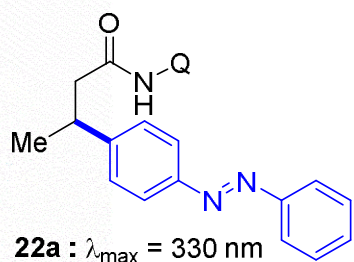
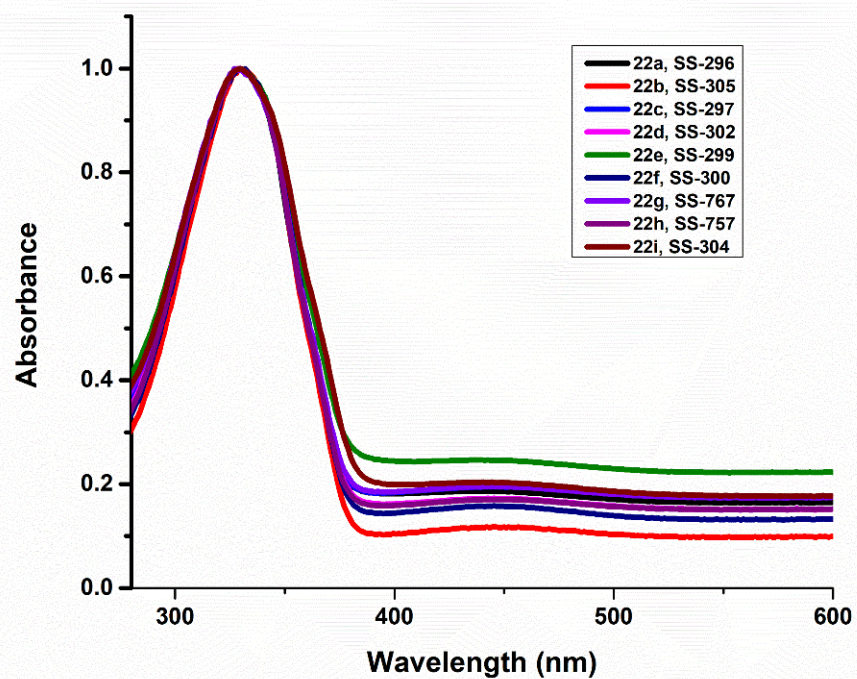


15h: λ_{\max} = 337 nm

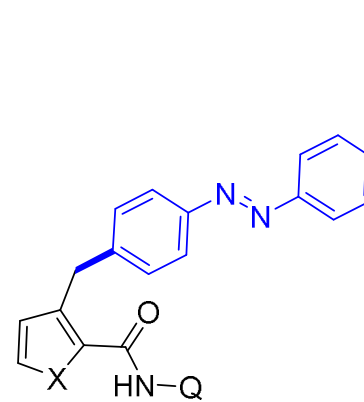
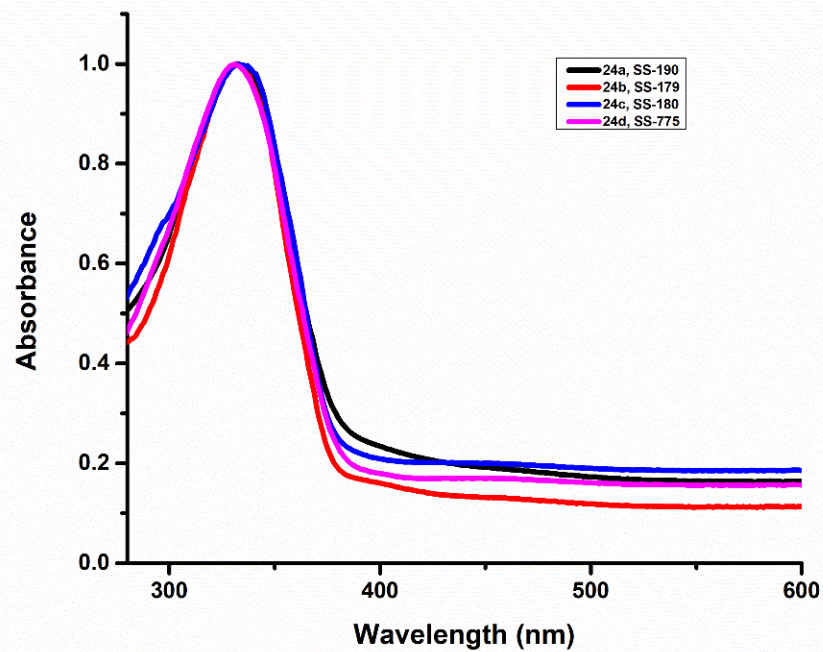
UV-Vis absorption chart (λ_{\max}) of compounds 16a-b, 17a, 18a, 19a, 20a-c



UV-Vis absorption chart (λ_{\max}) of compounds 22a-i

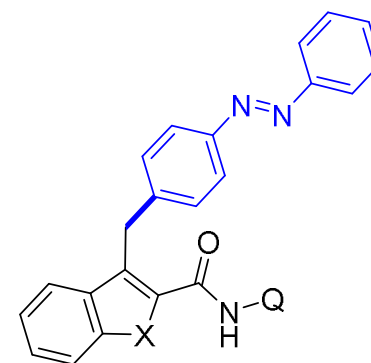


UV-Vis absorption chart (λ_{\max}) of compounds 24a-d



24a: X=O : λ_{\max} = 333 nm

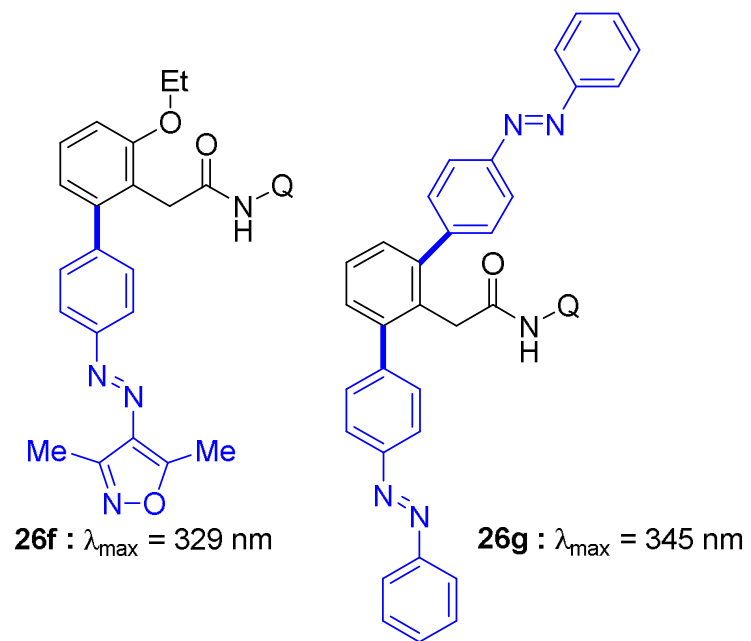
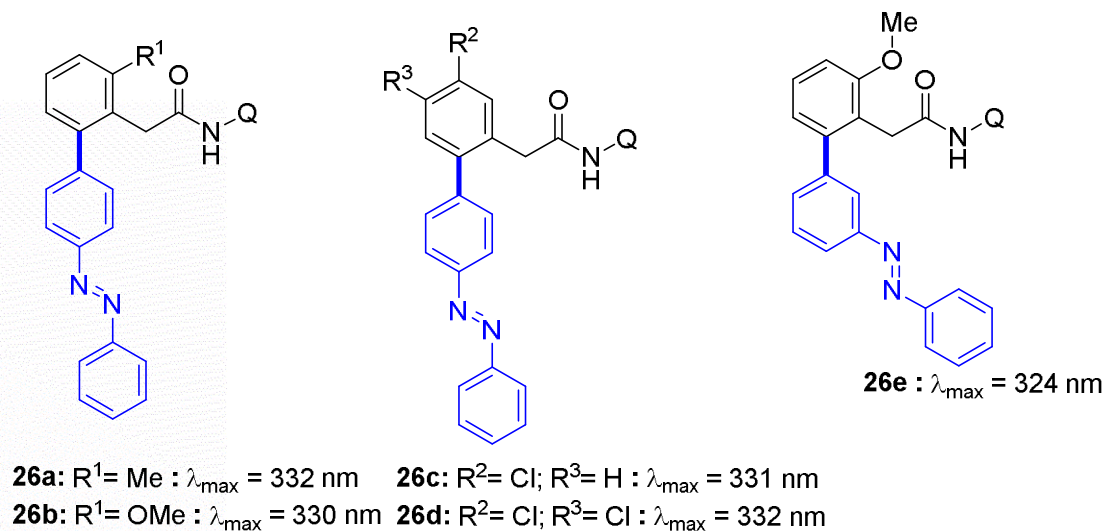
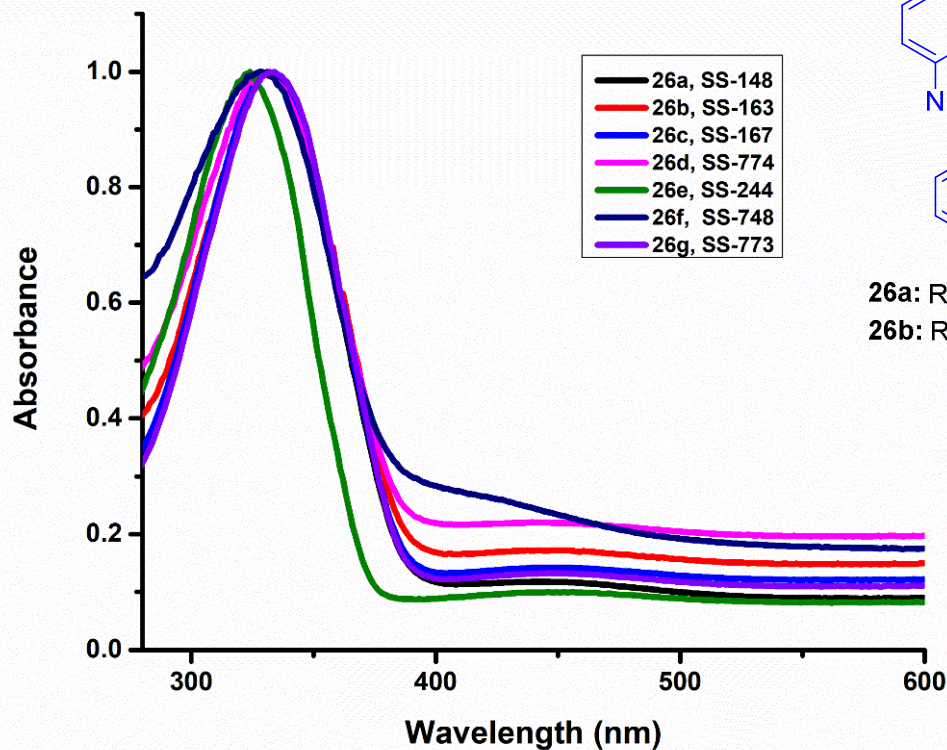
24b: X=S : λ_{\max} = 332 nm



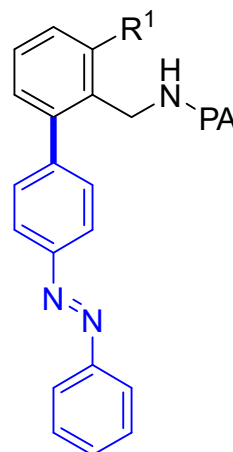
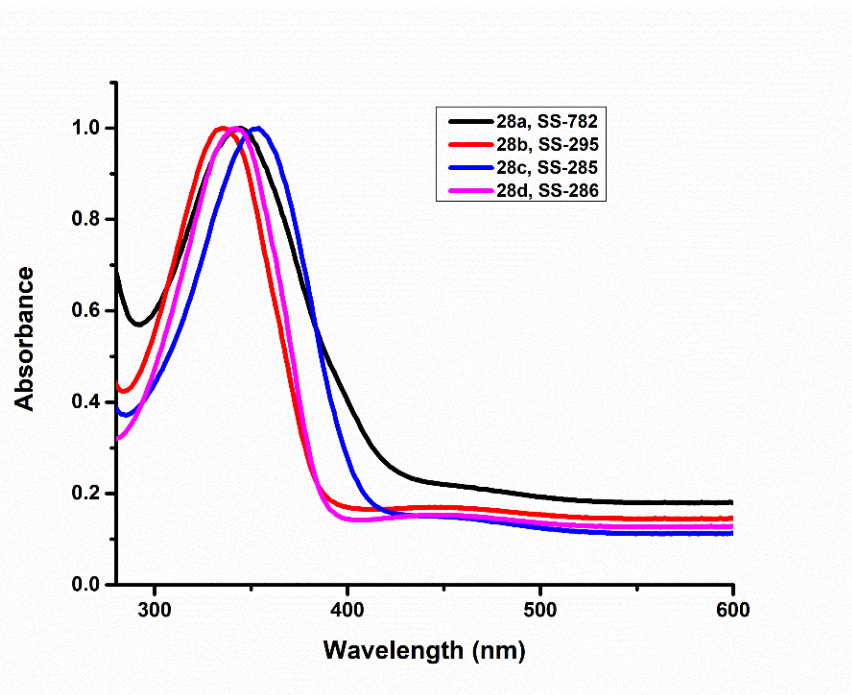
24c: X=O : λ_{\max} = 332 nm

24d: X=S : λ_{\max} = 331 nm

UV-Vis absorption chart (λ_{\max}) of compounds 26a-g

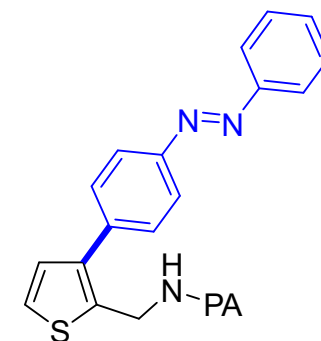


UV-Vis absorption chart (λ_{\max}) of compounds 28a-d

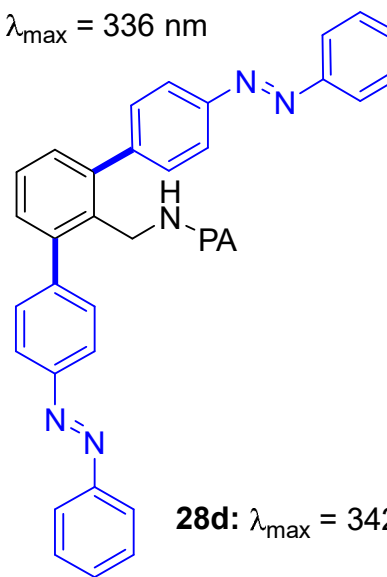


28a: R¹ = OMe : λ_{\max} = 345 nm

28b: R¹ = Cl : λ_{\max} = 336 nm

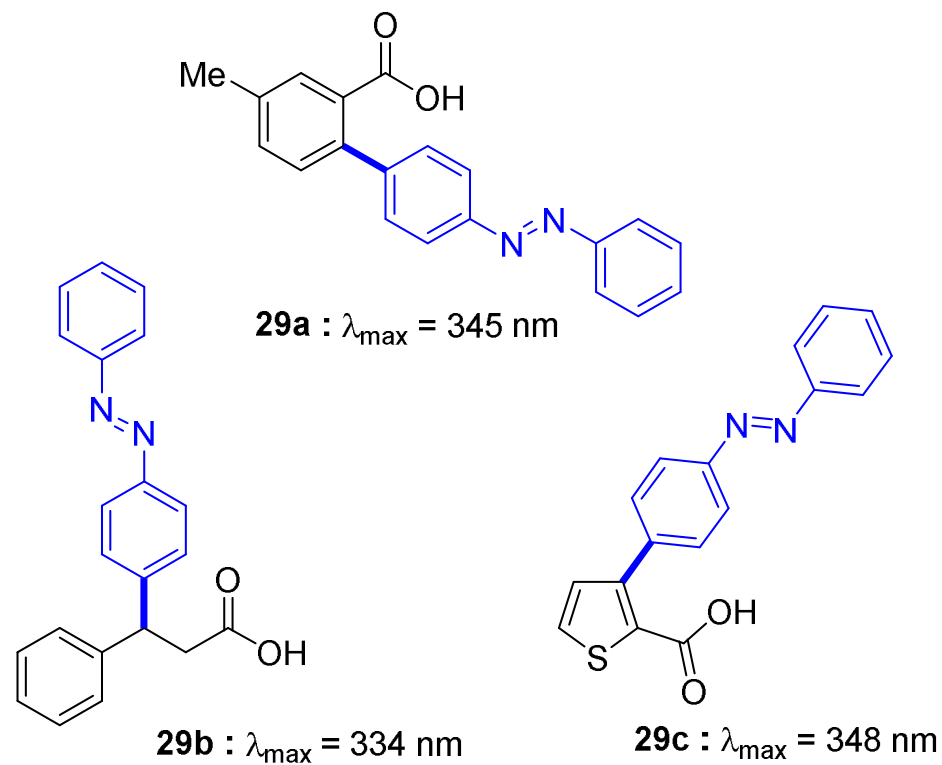
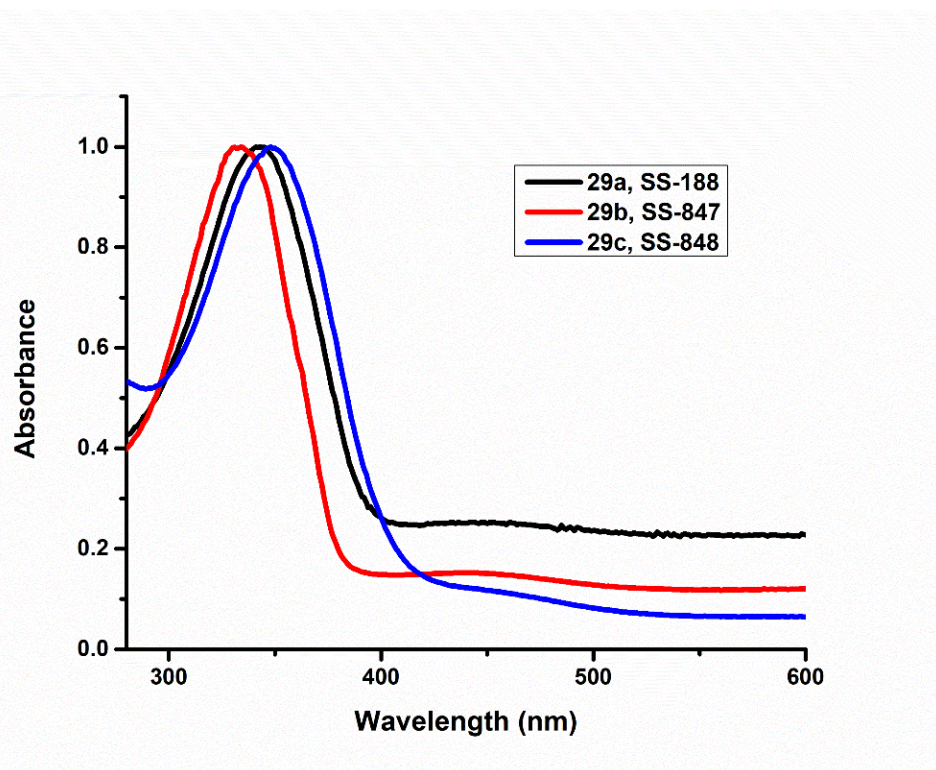


28c: λ_{\max} = 354 nm



28d: λ_{\max} = 342 nm

UV-Vis absorption chart (λ_{\max}) of compounds 29a-c



Photoswitching and kinetics experiments: UV-Vis spectroscopy

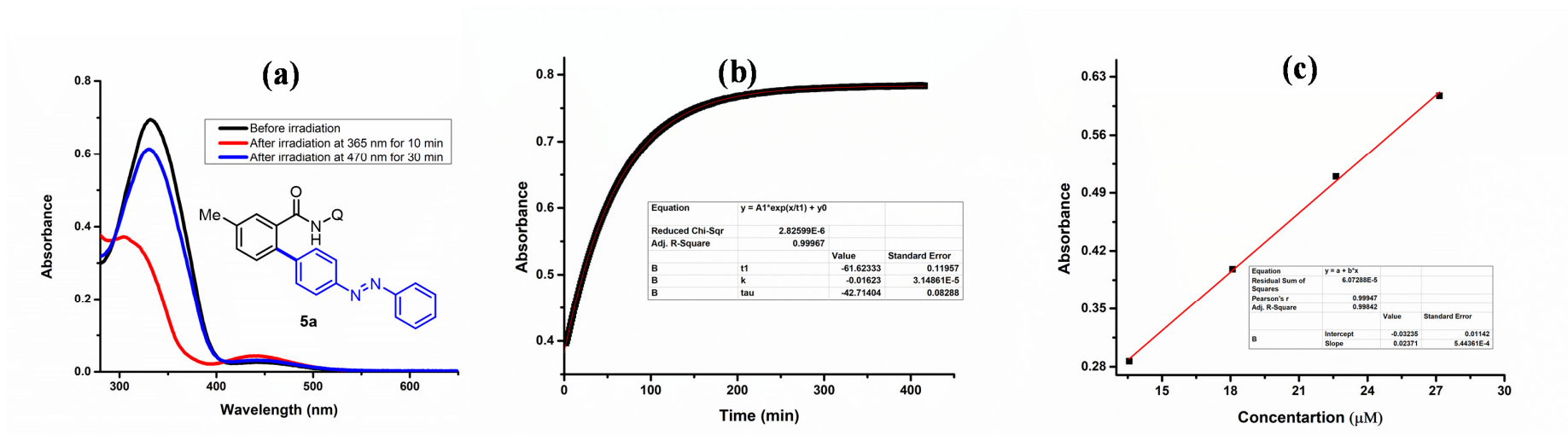


Figure S1 (a) Photoswitching behavior (forward *E-Z* and reverse *Z-E* photoisomerization) of **5a** (DMSO, 6.8 μM) at the indicated wavelengths; (b) Thermal reverse *Z-E* isomerization kinetics profile and exponential fit for the first order rate of **5a** (DMSO, 6.8 μM , 60 $^{\circ}\text{C}$, monitored at $\lambda = 331$ nm); (c) Estimation of the molar absorption coefficient of **5a** in DMSO at 331 nm.

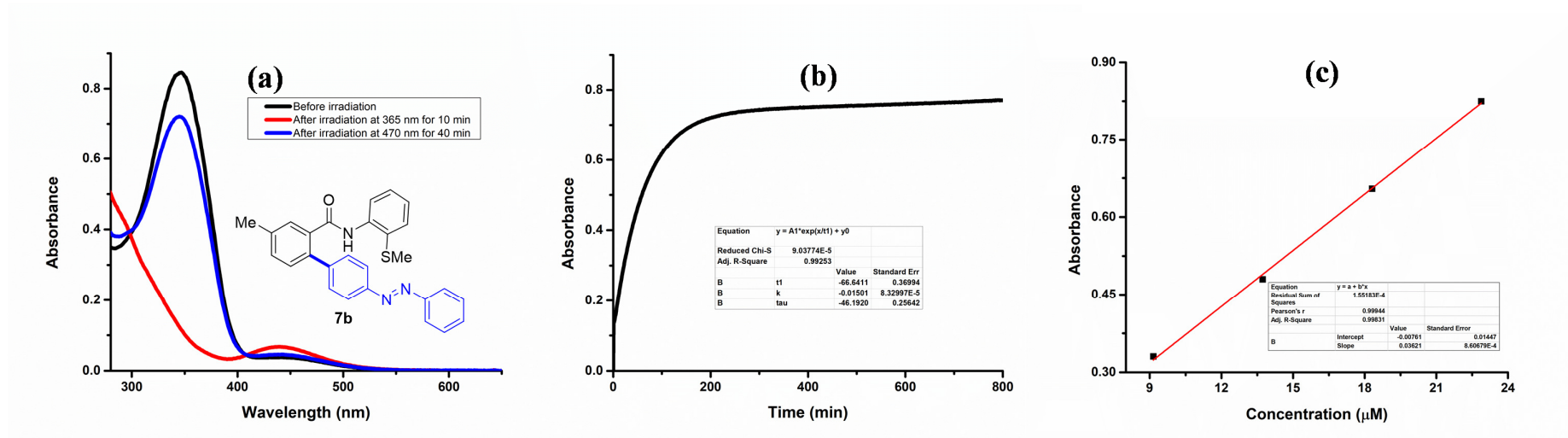


Figure S2 (a) Photoswitching behavior (forward *E-Z* and reverse *Z-E* photoisomerization) of **7b** (DMSO, 18.3 μM) at the indicated wavelengths; (b) Thermal reverse *Z-E* isomerization kinetics profile and exponential fit for the first order rate of **7b** (DMSO, 18.3 μM, 60 °C, monitored at $\lambda = 346$ nm); (c) Estimation of the molar absorption coefficient of **7b** in DMSO at 346 nm.

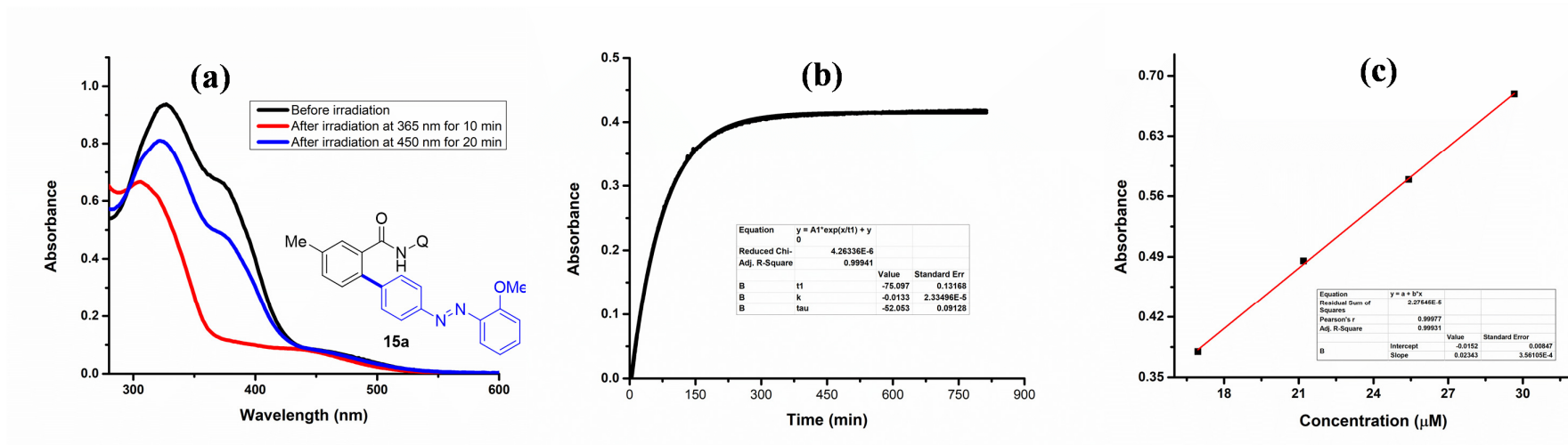


Figure S3 (a) Photoswitching behavior (forward *E-Z* and reverse *Z-E* photoisomerization) of **15a** (DMSO, 33.9 μM) at the indicated wavelengths; (b) Thermal reverse *E-Z* isomerization kinetics profile and exponential fit for the first order rate of **15a** (DMSO, 33.9 μM , 60 $^{\circ}\text{C}$, monitored at $\lambda = 327$ nm); (c) Estimation of the molar absorption coefficient of **15a** in DMSO at 327 nm.

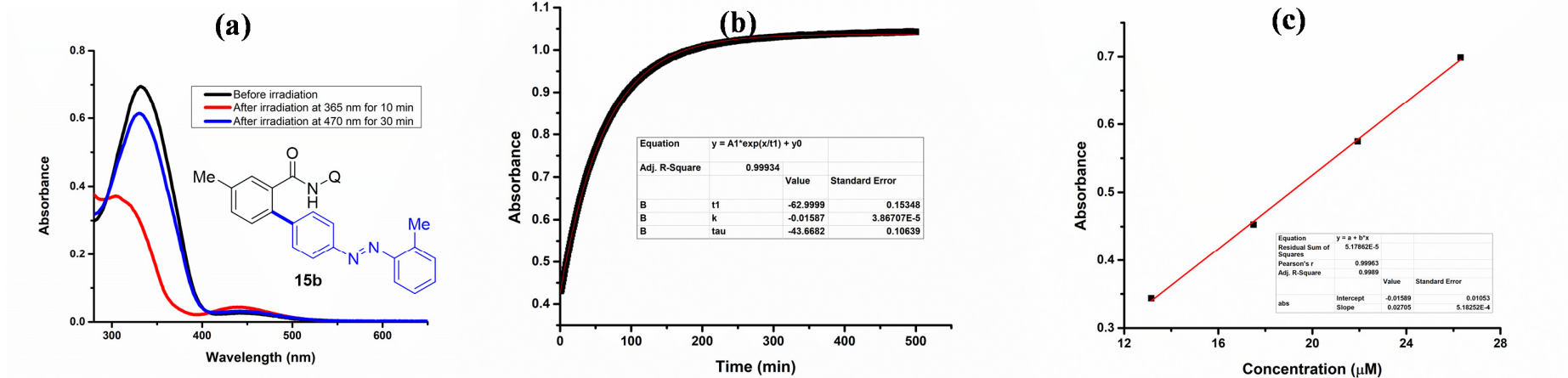


Figure S4 (a) Photoswitching behavior (forward *E-Z* and reverse *Z-E* photoisomerization) of **15b** (DMSO, 21.9 μM) at the indicated wavelengths; (b) Thermal reverse *Z-E* isomerization kinetics profile and exponential fit for the first order rate of **15b** (DMSO, 21.9 μM , 60 $^{\circ}\text{C}$, monitored at $\lambda = 338 \text{ nm}$); (c) Estimation of the molar absorption coefficient of **15b** in DMSO at 338 nm.

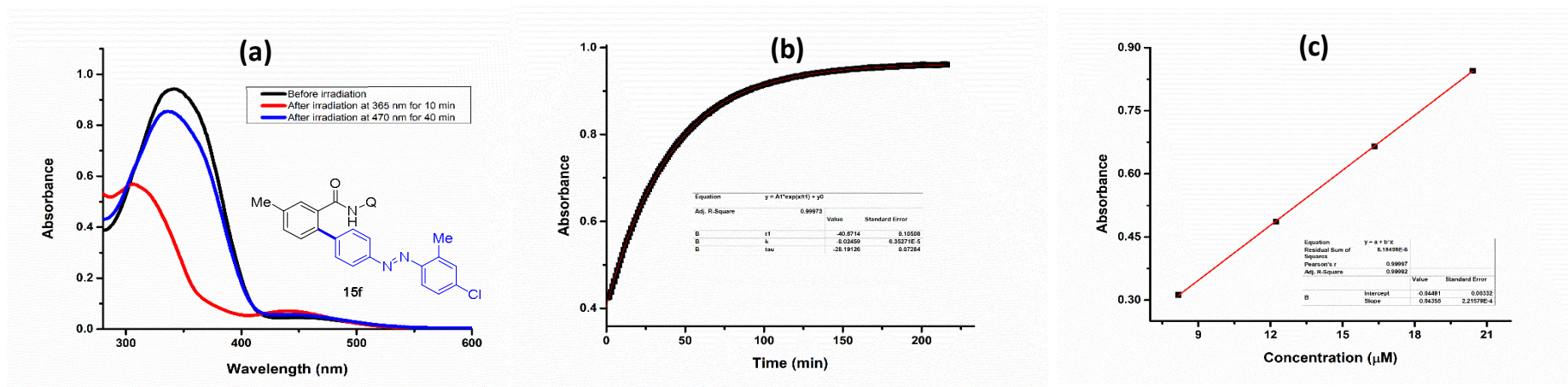


Figure S5 (a) Photoswitching behavior (forward *E-Z* and reverse *Z-E* photoisomerization) of **15f** (DMSO, 24.5 μM) at the indicated wavelengths; (b) Thermal reverse *Z-E* isomerization kinetics profile and exponential fit for the first order rate of **15f** (DMSO, 24.5 μM, 60 °C, monitored at λ = 346 nm); (c) Estimation of the molar absorption coefficient of **15f** in DMSO at 346 nm.

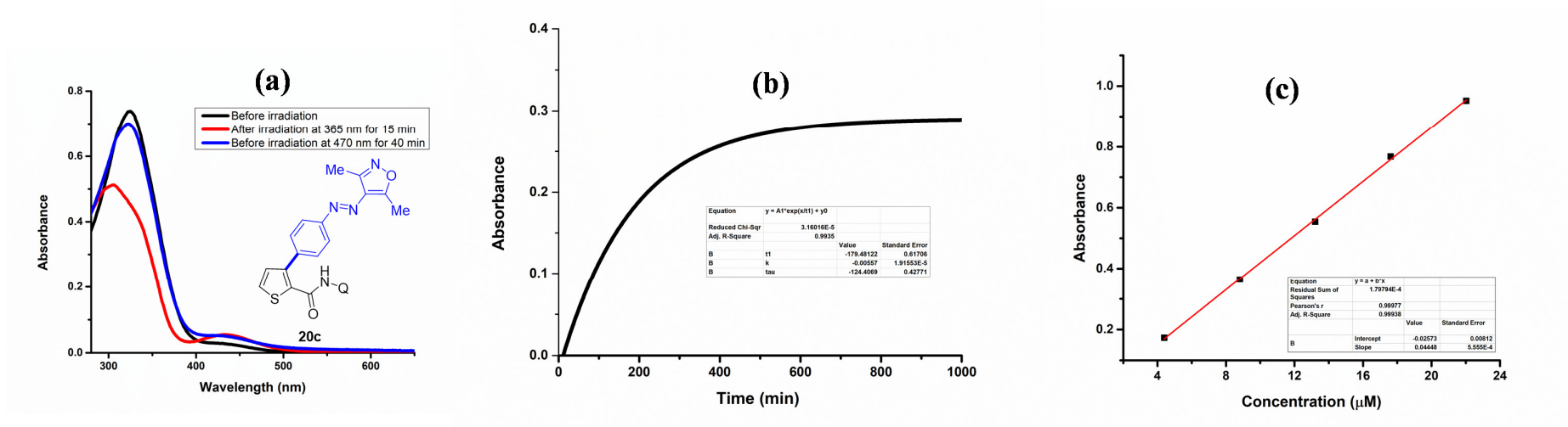


Figure S6 (a) Photoswitching behavior (forward *E-Z* and reverse *Z-E* photoisomerization) of **20c** (DMSO, 15.4 µM) at the indicated wavelengths; (b) Thermal reverse *E-Z* isomerization kinetics profile and exponential fit for the first order rate of **20c** (DMSO, 15.4 µM, 60 °C, monitored at λ = 326 nm); (c) Estimation of the molar absorption coefficient of **20c** in DMSO at 326 nm.

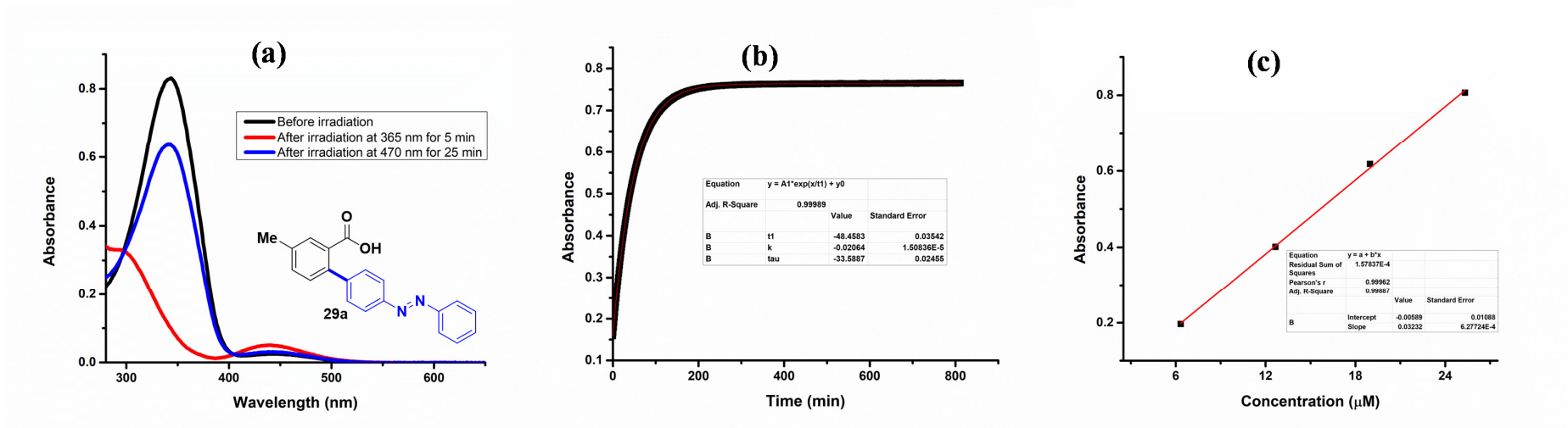


Figure S7 (a) Photoswitching behavior (forward *E-Z* and reverse *Z-E* photoisomerization) of **29a** (DMSO, 12.6 μM) at the indicated wavelengths; (b) Thermal reverse *Z-E* isomerization kinetics profile and exponential fit for the first order rate of **29a** (DMSO, 12.6 μM , 60 $^{\circ}\text{C}$, monitored at $\lambda = 345$ nm); (c) Estimation of the molar absorption coefficient of **29a** in DMSO at 345 nm.

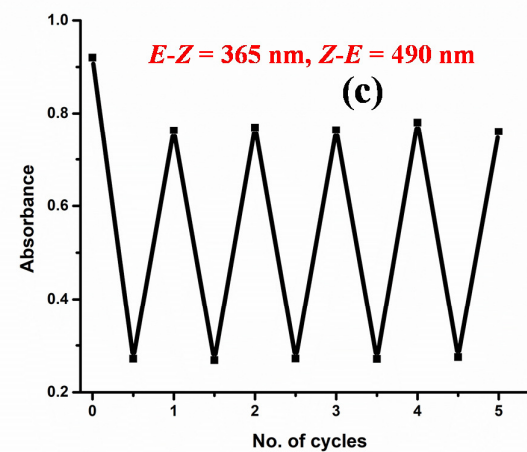
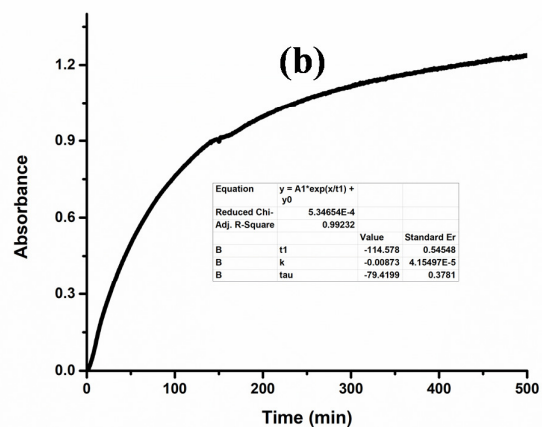
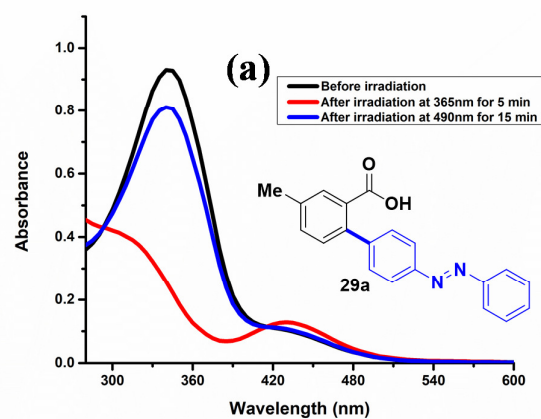


Figure S8 (a) Photoswitching behavior (forward *E-Z* and reverse *Z-E* photoisomerization) of **29a** (water at pH=7.5, concentration undetermined) at the indicated wavelengths; (b) Thermal reverse *Z-E* isomerization kinetics profile and exponential fit for the first order rate of **29a** (water at pH=7.5, concentration undetermined, 60 °C, monitored at $\lambda = 340$ nm); (c) Photoswitching stability over five cycles of **29a** by alternate irradiation for forward and reverse photoisomerization (Forward: 365 nm, reverse 490 nm) in water at pH=7.5.

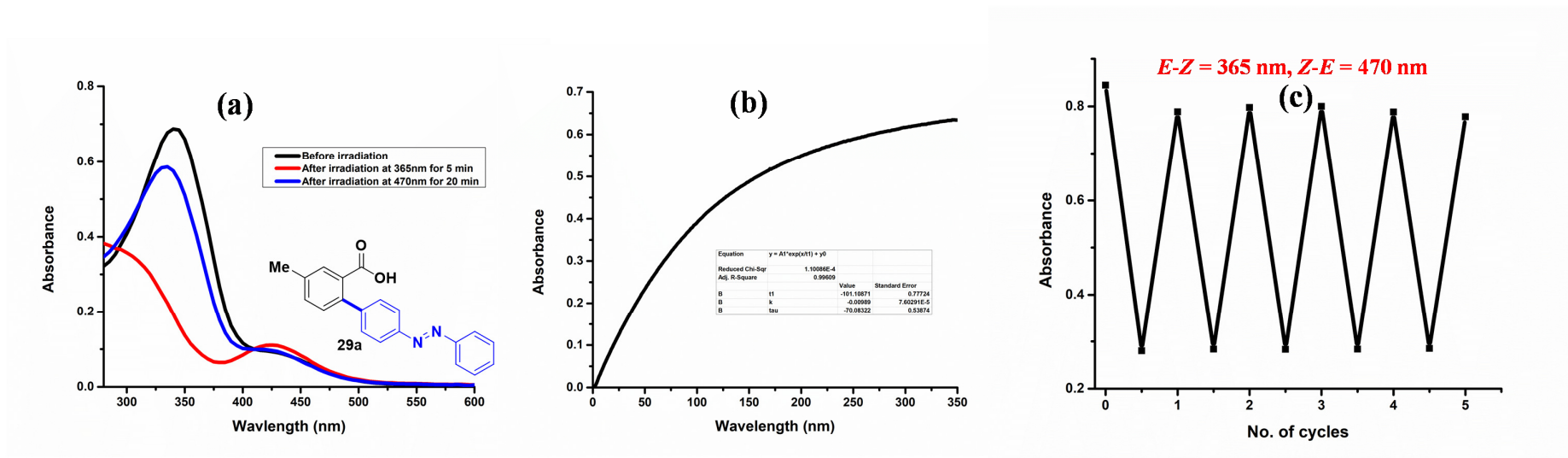


Figure S9 (a) Photoswitching behavior (forward *E-Z* and reverse *Z-E* photoisomerization) of **29a** (water at pH=9.5, concentration undetermined) at the indicated wavelengths; (b) Thermal reverse *Z-E* isomerization kinetics profile and exponential fit for the first order rate of **29a** (water at pH=9.5, concentration undetermined, 60 °C, monitored at $\lambda = 345$ nm); (c) Photoswitching stability over five cycles of **29a** by alternate irradiation for forward and reverse photoisomerization (Forward: 365 nm, reverse 470 nm) in water at pH=9.5.

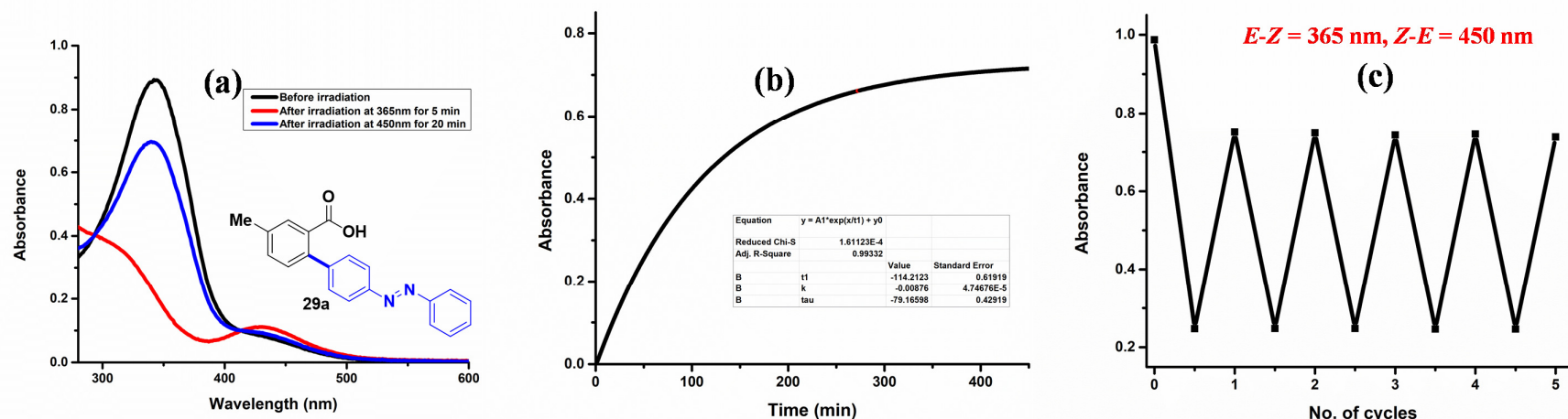


Figure S10 (a) Photoswitching behavior (forward *E-Z* and reverse *Z-E* photoisomerization) of **29a** (water at pH=12.1, concentration undetermined) at the indicated wavelengths; (b) Thermal reverse *Z-E* isomerization kinetics profile and exponential fit for the first order rate of **29a** (water at pH=12.1, concentration undetermined, 60 °C, monitored at $\lambda = 342$ nm); (c) Photoswitching stability over five cycles of **29a** by alternate irradiation for forward and reverse photoisomerization (Forward: 365 nm, reverse 450 nm) in water at pH=12.1.

The PSS composition of **29a** at different pH (7.5-12.1) has been estimated using the formula given below.

$$\% \text{ conversion of } E\text{-}Z \text{ isomers} = \left(1 - \frac{A_{\pi-\pi^*} \text{ absorption after irradiation at } 365 \text{ nm}}{A_{\pi-\pi^*} \text{ absorption before irradiation}} \right) \times 100$$

$$\% \text{ conversion of } Z\text{-}E \text{ isomers} = \left(1 - \frac{A_{\pi-\pi^*} \text{ absorption after irradiation at } 365 \text{ nm}}{A_{\pi-\pi^*} \text{ absorption after irradiation at } 450\text{--}490 \text{ nm}} \right) \times 100$$

| Sr. No. | Compound | PSS composition in solution state | |
|---------|----------------------|--------------------------------------|--------------------------------------|
| | | Forward isomerization (<i>E-Z</i>) | Reverse isomerization (<i>Z-E</i>) |
| 1. | 29a (pH=7.5) | 72 | 55 |
| 2. | 29a (pH=9.5) | 76 | 70 |
| 3. | 29a (pH=12.1) | 75 | 68 |