Supporting Information for

Biosurfactant-functionalized porphyrin chromophore that forms *J*-aggregates

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Affiliations

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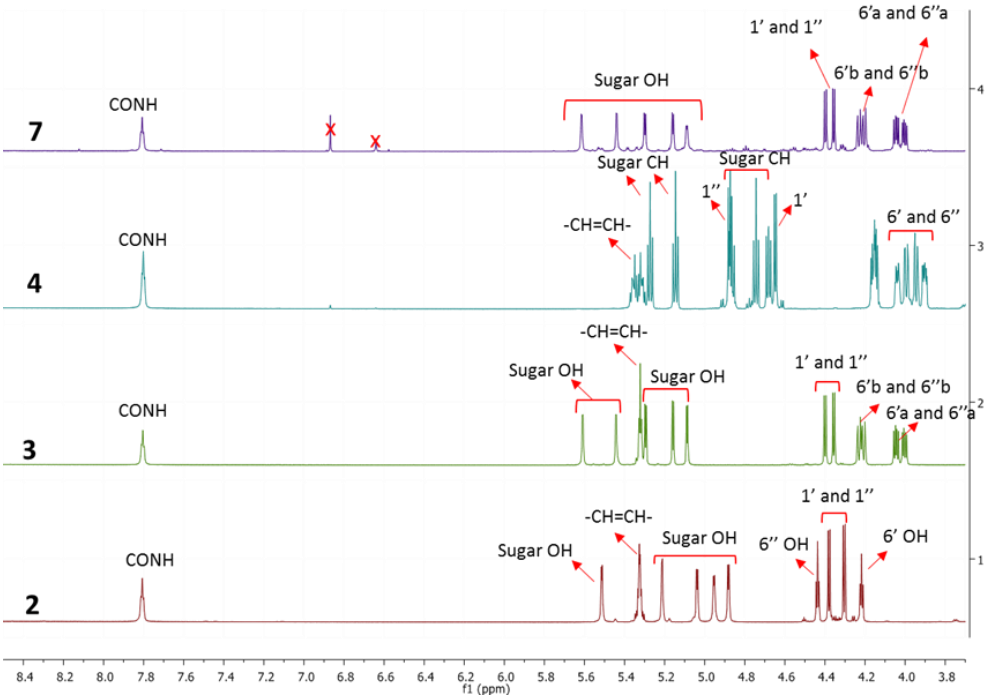


Figure SI-1. Stacked ^{1}H NMR (800 MHz, DMSO-d_6) spectra (partial) of sophorolipids derivatives **2**, **3**, **4** and **7** (bottom to top).

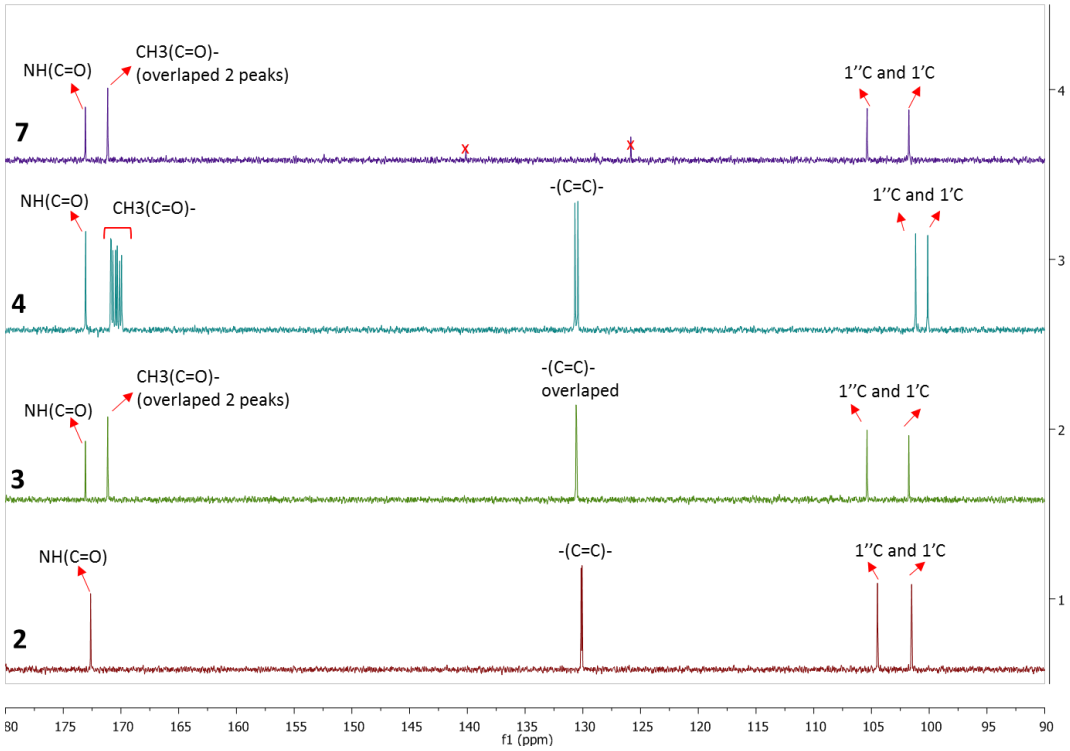


Figure SI-2. Stacked ^{13}C NMR (800 MHz, DMSO-d_6) spectra (partial) of sophorolipids derivatives **2**, **3**, **4** and **7** (bottom to top).

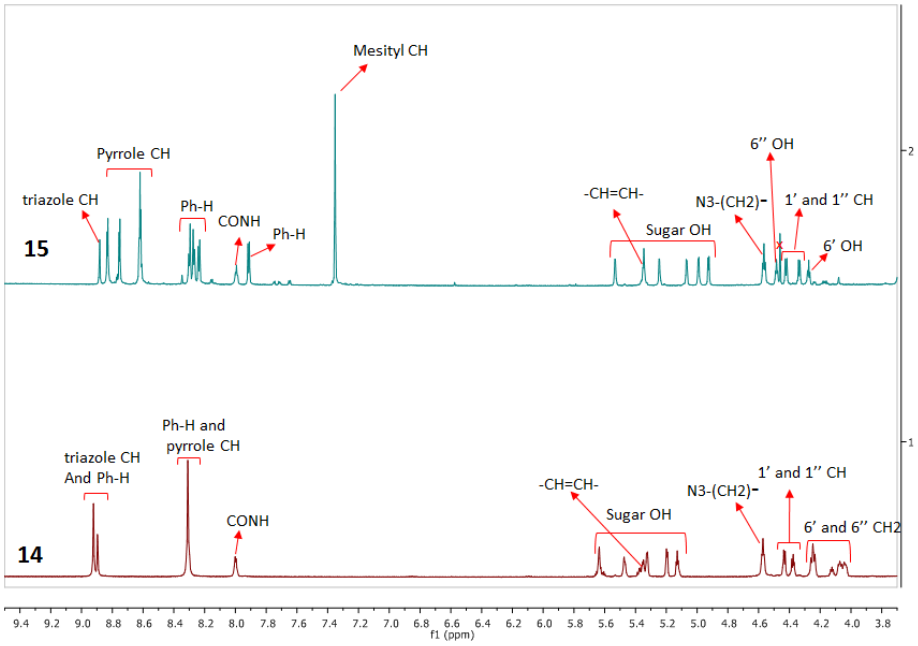


Figure SI-3. Stacked ^{1}H NMR spectra *(*800 MHz, DMSO-*d*6 *solvent)* (partial) of **14** (tetra-conjugated compound) and **15** (mono-conjugated compound) (bottom to top).

Figure SI-4. Displays the optical density spectra of 2 x10^{-6} M Compound **11** in varying organic solvents and their mixture (1:1 v/v) with water. **11** in neat 1,4-dioxane and DMSO exhibit a slight red-shift of the Soret band amounting to 4 nm and 6 nm, respectively. Comparatively, **11** in 1,4-dioxane/water (1:1 v/v) presents minimal spectral change compared to neat 1,4-dioxane solution while **11** in the DMSO-water relative to neat DMSO exhibits an optical density decrease, which may be attributed to solvatochromism effects and slight monomer aggregation [1].

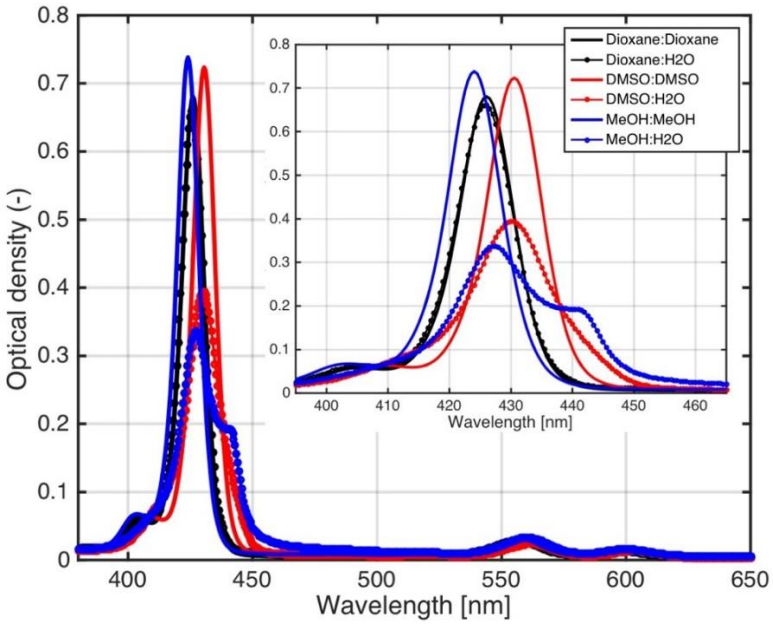
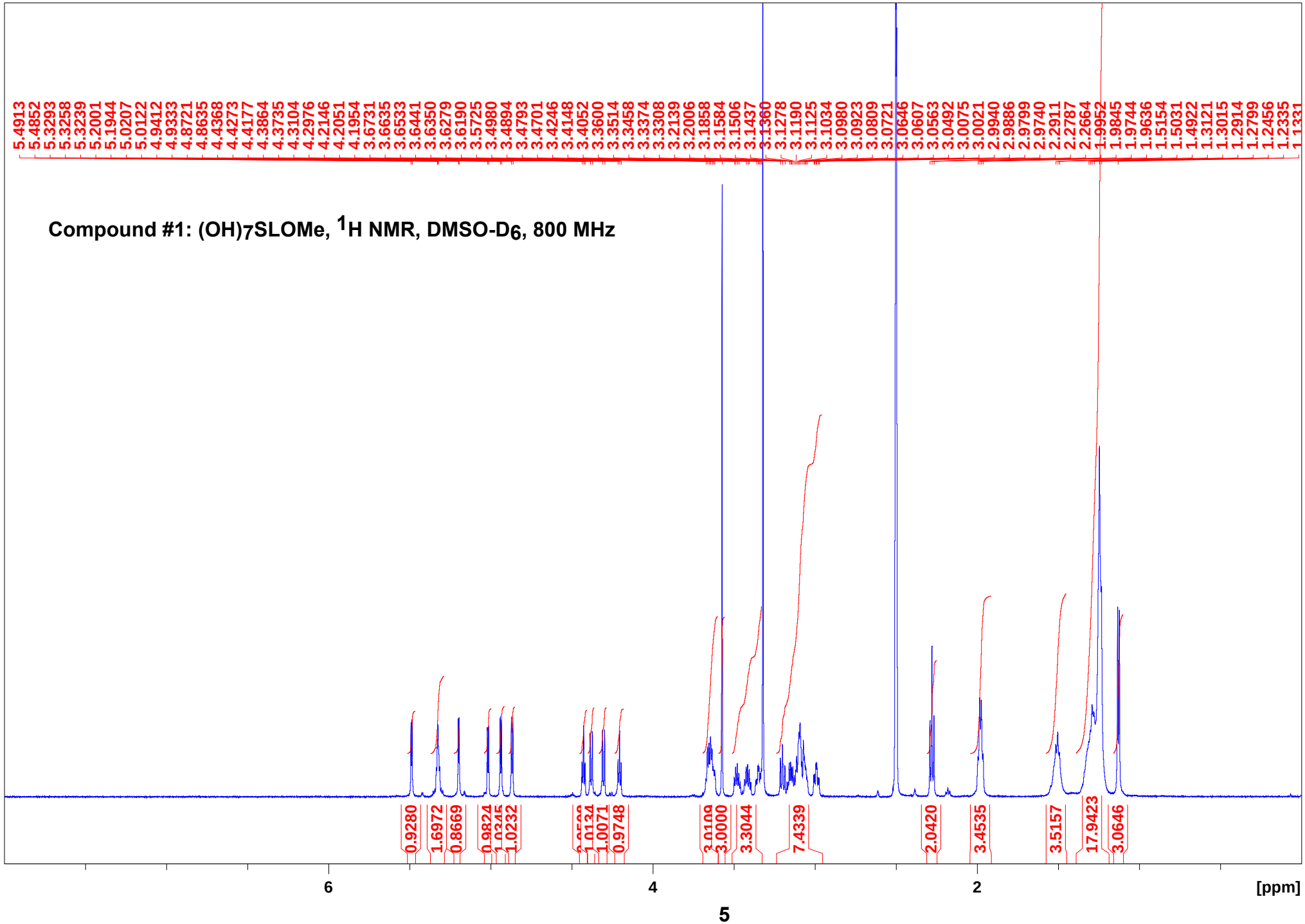


Figure SI-4. Solvent-dependent absorption spectra (2x10^{-6} M) of compound **11**, expansion of the Soret region shown in inset.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5.3258
5.3239
5.2001
5.1944
5.0207
5.0122
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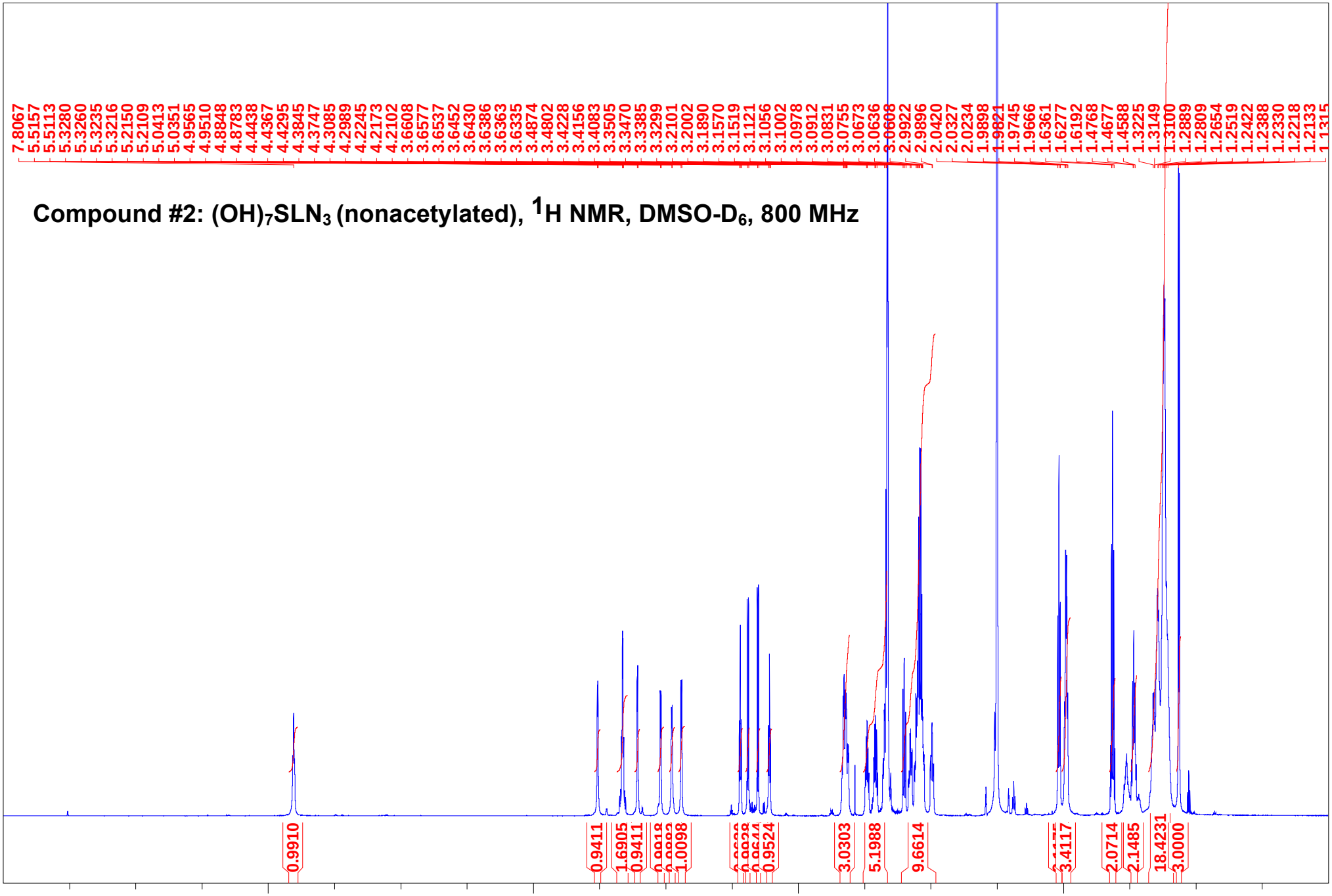
4.9333
4.8721
4.8635
4.4368
4.4273
4.4177
4.3864
4.3735
4.3104
4.2976
4.2146
4.2051
4.1954
4.1148
3.6731
3.6635
3.6533
3.6441
3.6350
3.6279
3.6190
3.5725
3.4980
3.4894
3.4793
3.4701
3.4246
3.4148
3.4052
3.3600
3.3514
3.3458
3.3374
3.3308
3.2139
3.2006
3.1858
3.1584
3.1506
3.1437
3.1360
3.1278
3.1190
3.1125
3.1034
3.0980
3.0923
3.0809
3.0721
3.0646
3.0607
3.0563
3.0492
3.0075
3.0021
2.9940
2.9886
2.9799
2.9740
2.2911
2.2787
2.2664
1.9952
1.9845
1.9744
1.9636
1.5154
1.5031
1.4922
1.3121
1.3015
1.2914
1.2799
1.2456
1.2335
1.1331
Compound #1: (OH)7SLOMe, 1H NMR, DMSO-D6, 800 MHz
0.9280
1.6972
0.8669
0.9824
1.0345
1.0232
1.0134
1.0071
0.9748
3.0109
3.0000
3.3044
7.4339
2.0420
3.4535
3.5157
17.9423
3.0646
6
4
2
[ppm]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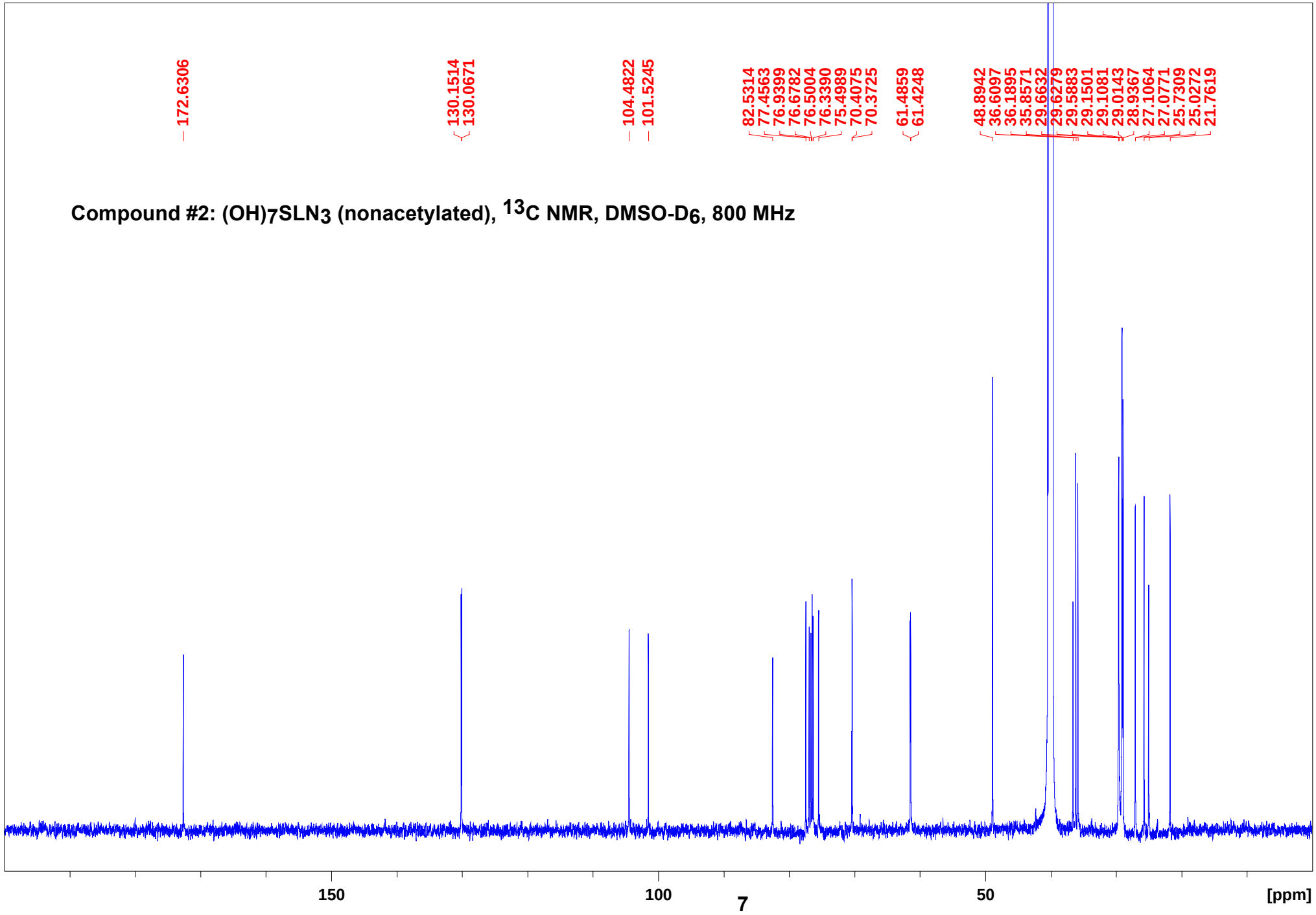
5.5113
5.3280
5.3260
5.3235
5.3216
5.2150
5.2109
5.0413
5.0351
4.9565
4.9510
4.8848
4.8783
4.4438
4.4367
4.4295
4.3845
4.3747
4.3085
4.2989
4.2245
4.2173
4.2102
3.6608
3.6577
3.6537
3.6452
3.6430
3.6386
3.6363
3.6335
3.4874
3.4802
3.4228
3.4156
3.4083
3.3505
3.3470
3.3385
3.3299
3.2101
3.2002
3.1890
3.1570
3.1519
3.1121
3.1056
3.1002
3.0978
3.0912
3.0831
3.0755
3.0673
3.0636
3.0608
2.9922
2.9896
2.0420
2.0327
2.0234
1.9898
1.9821
1.9745
1.9666
1.6361
1.6277
1.6192
1.4768
1.4677
1.4588
1.3225
1.3149
1.3100
1.2889
1.2809
1.2654
1.2519
1.2422
1.2388
1.2330
1.2218
1.2133
1.1315
Compound #2: (OH)7SLN3 (nonacetylated), 1H NMR, DMSO-D6, 800 MHz
0.9910
0.9411
1.6905
0.9411
1.0098
0.9524
3.0303
5.1988
9.6614
3.4117
2.0714
2.1485
18.4231
3.0000
8
6
4
2
[ppm]


172.6306
130.1514
130.0671
104.4822
101.5245
82.5314
77.4563
76.9399
76.6782
76.5004
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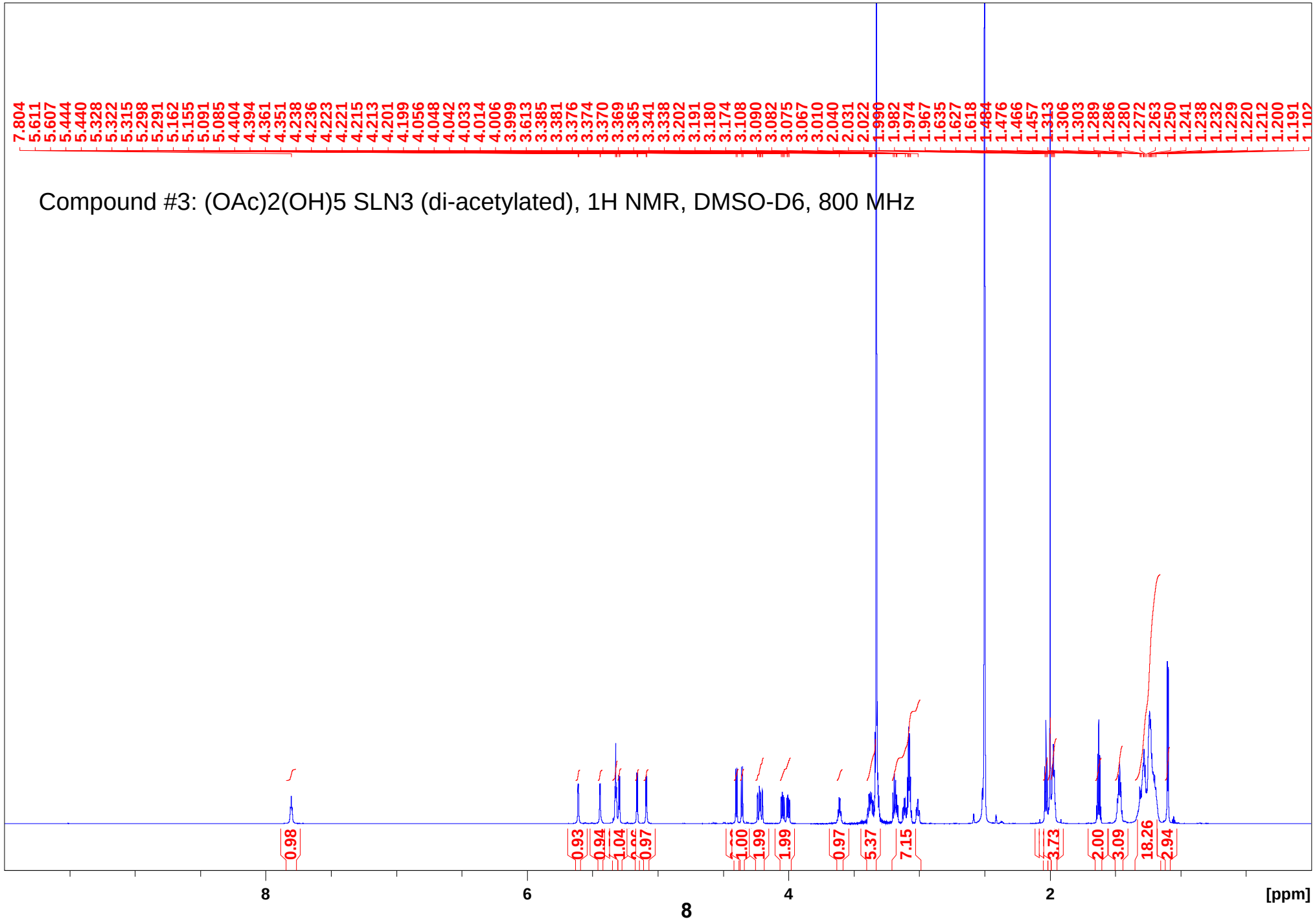
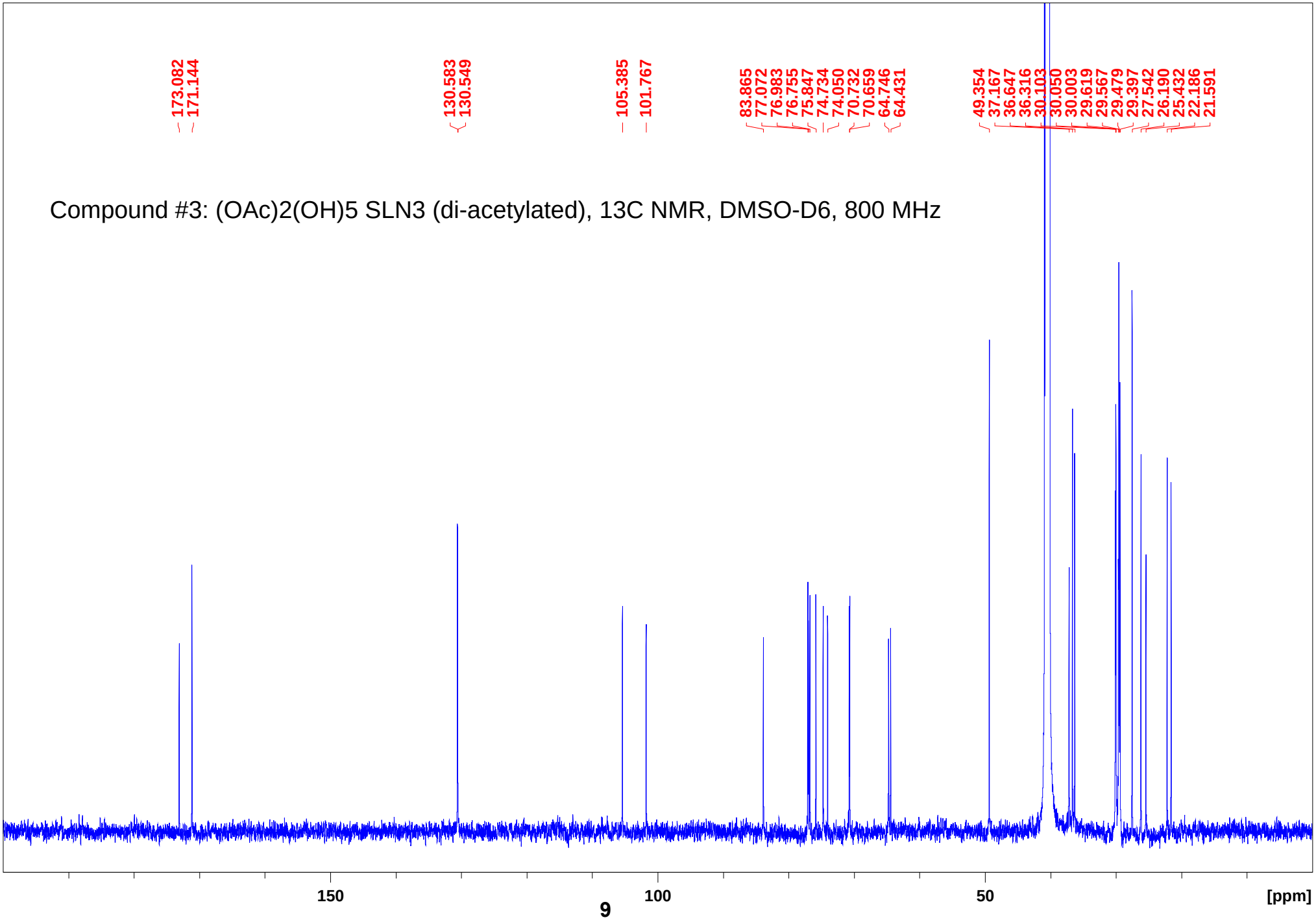
75.4989
70.4075
70.3725
61.4859
61.4248
48.8942
36.6097
36.1895
35.8571
29.6632
29.6279
29.5883
29.1501
29.1081
29.0143
28.9367
27.1064
27.0771
25.7309
25.0272
21.7619
Compound #2: (OH)7SLN3 (nonacetylated), 13C NMR, DMSO-D6, 800 MHz
150
100
50
[ppm]


7.804
5.611
5.607
5.444
5.440
5.328
5.322
5.315
5.298
5.291
5.162
5.155
5.091
5.085
4.404
4.394
4.361
4.351
4.238
4.236
4.223
4.221
4.215
4.213
4.201
4.199
4.056
4.048
4.042
4.033
4.014
4.006
3.999
3.613
3.385
3.381
3.376
3.374
3.370
3.369
3.365
3.341
3.338
3.202
3.191
3.180
3.174
3.108
3.090
3.082
3.075
3.067
3.010
2.040
2.031
2.022
1.990
1.982
1.974
1.967
1.635
1.627
1.618
1.484
1.476
1.466
1.457
1.313
1.306
1.303
1.289
1.286
1.280
1.272
1.263
1.250
1.241
1.238
1.232
1.229
1.220
1.212
1.200
1.191
1.102
Compound #3: (OAc)2(OH)5 SLN3 (di-acetylated), 1H NMR, DMSO-D6, 800 MHz
0.98
0.93
0.94
1.04
0.97
1.00
1.99
1.99
0.97
5.37
7.15
3.73
2.00
3.09
18.26
2.94
8
6
4
2
[ppm]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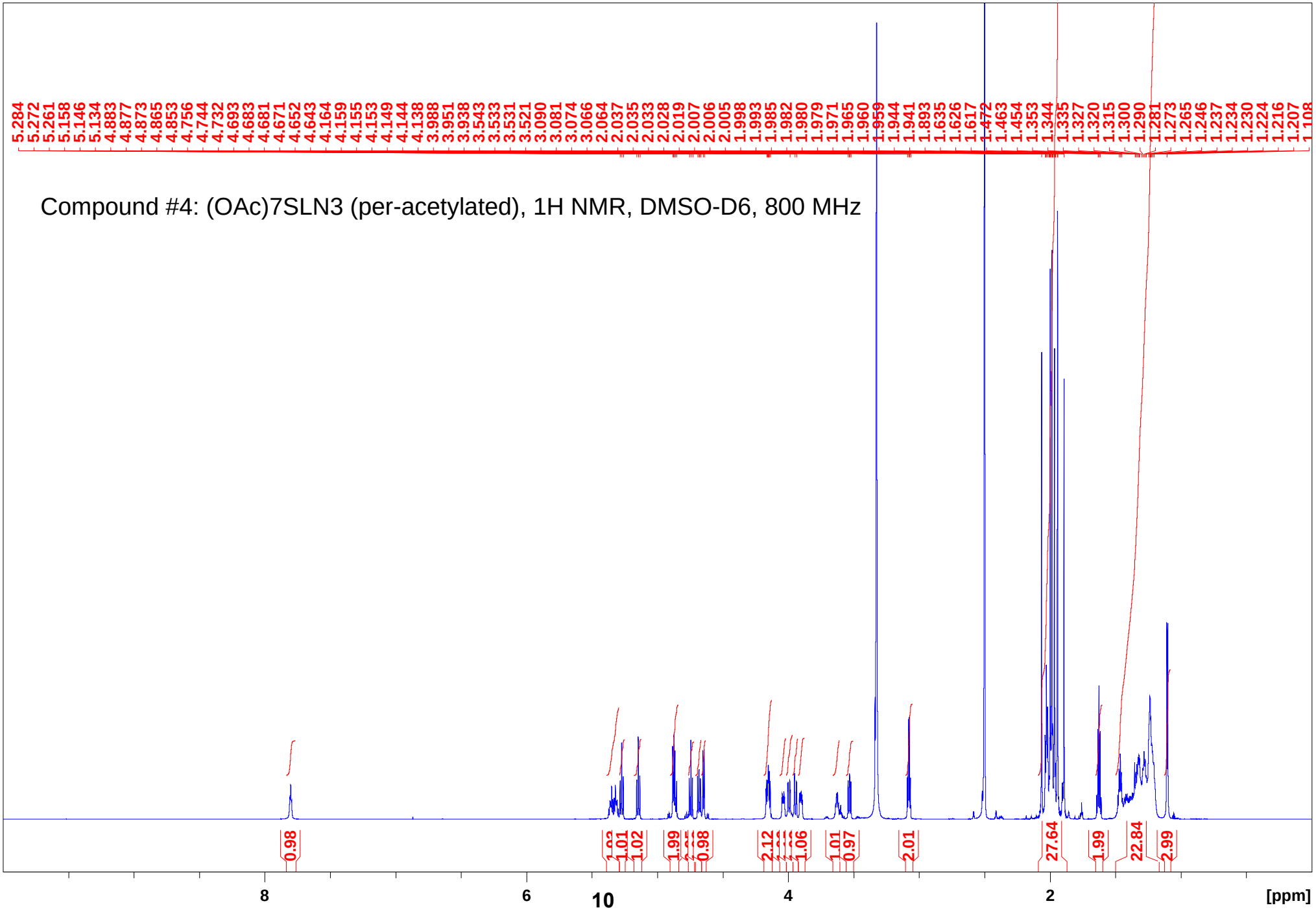
130.583
130.549
105.385
101.767
83.865
77.072
76.983
76.755
75.847
74.734
74.050
70.732
70.659
64.746
64.431
49.354
37.167
36.647
36.316
30.103
30.050
30.003
29.619
29.567
29.479
29.397
27.542
26.190
25.432
22.186
21.591
Compound #3: (OAc)2(OH)5 SLN3 (di-acetylated), 13C NMR, DMSO-D6, 800 MHz
150
100
50
[ppm]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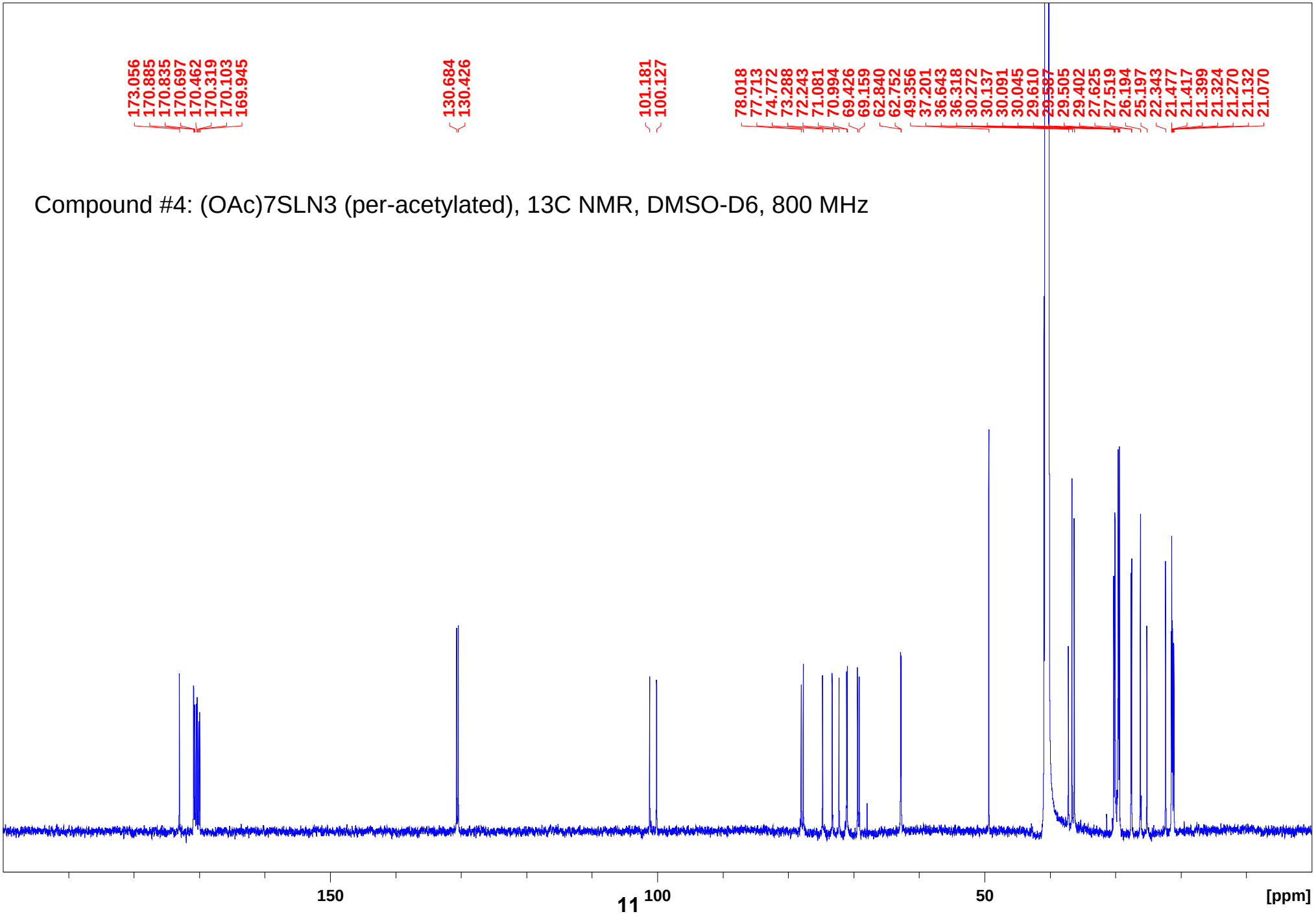
Compound #4: (OAc)7SLN3 (per-acetylated), 1H NMR, DMSO-D6, 800 MHz
0.98
1.03
1.01
1.02
1.99
0.98
2.12
1.06
1.01
0.97
2.01
27.64
1.99
22.84
2.99
8
6
10
4
2
[ppm]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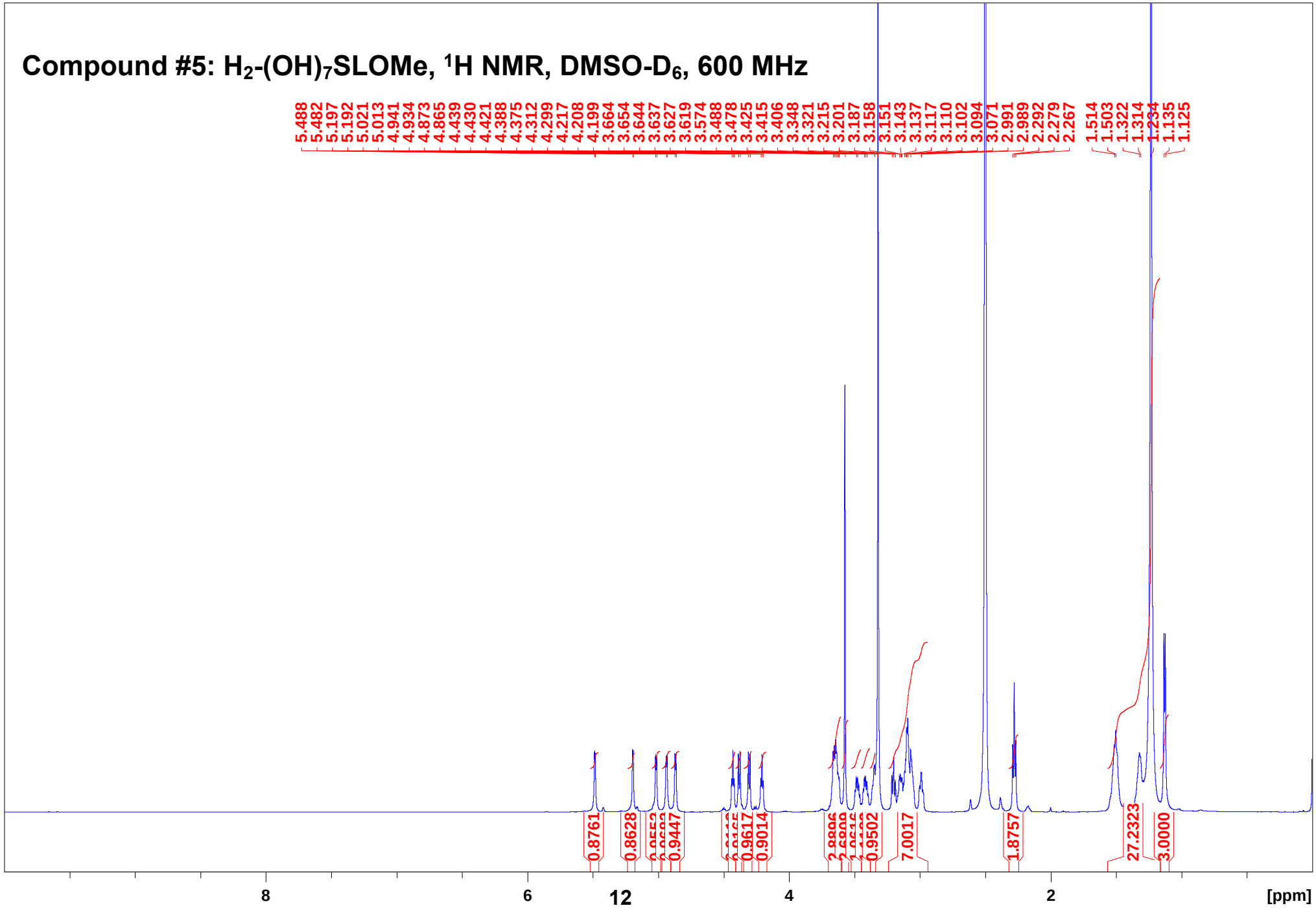
170.835
170.697
170.462
170.319
170.103
169.945
130.684
130.426
101.181
100.127
78.018
77.713
74.772
73.288
72.243
71.081
70.994
69.426
69.159
62.840
62.752
49.356
37.201
36.643
36.318
30.272
30.137
30.091
30.045
29.610
29.587
29.505
29.402
27.625
27.519
26.194
25.197
22.343
21.477
21.417
21.399
21.324
21.270
21.132
21.070
Compound #4: (OAc)7SLN3 (per-acetylated), 13C NMR, DMSO-D6, 800 MHz
150
100
50
[ppm]


Compound #5: H2-(OH)7SLOMe, 1H NMR, DMSO-D6, 600 MHz
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5.482
5.197
5.192
5.021
5.013
4.941
4.934
4.873
4.865
4.439
4.430
4.421
4.388
4.375
4.312
4.299
4.217
4.208
4.199
3.664
3.654
3.644
3.637
3.627
3.619
3.574
3.488
3.478
3.425
3.415
3.406
3.348
3.321
3.215
3.201
3.187
3.158
3.151
3.143
3.137
3.117
3.110
3.102
3.094
3.071
2.991
2.989
2.292
2.279
2.267
1.514
1.503
1.322
1.314
1.234
1.135
1.125
0.8761
0.8628
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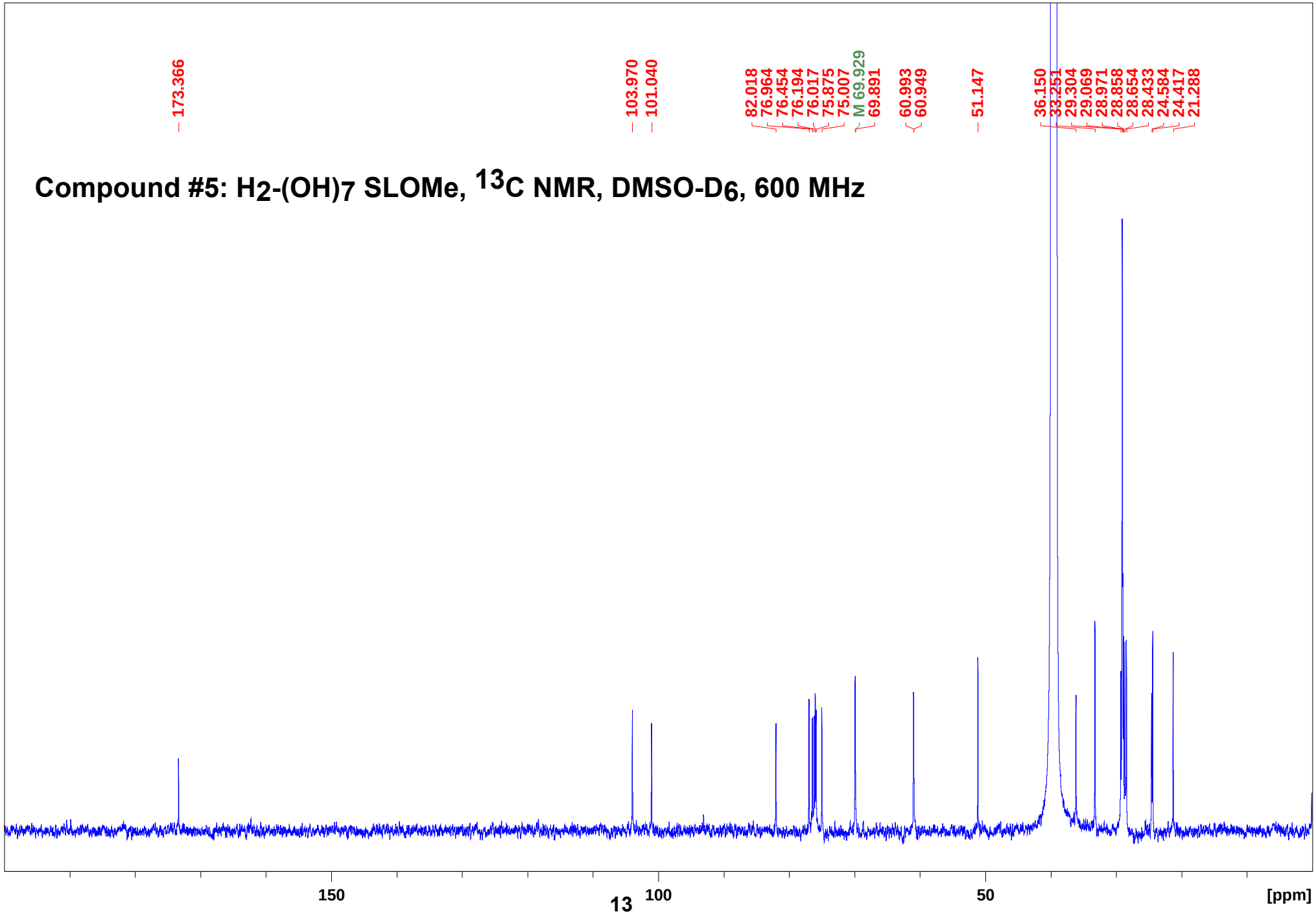
3.0000
8
6
12
4
2
[ppm]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76.454
76.194
76.017
75.875
75.007
M 69.929
69.891
60.993
60.949
51.147
36.150
33.251
29.304
29.069
28.971
28.858
28.654
28.433
24.584
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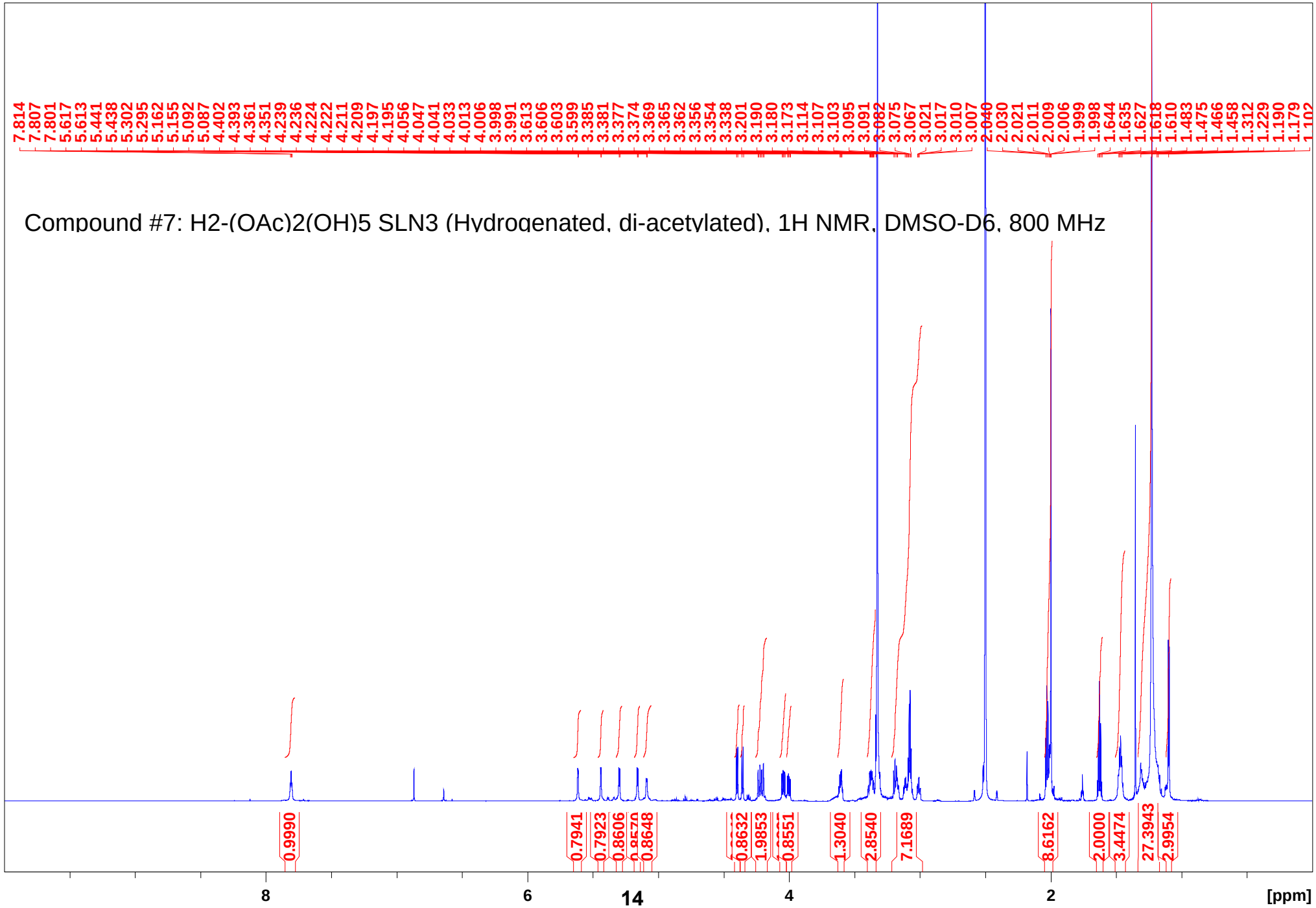
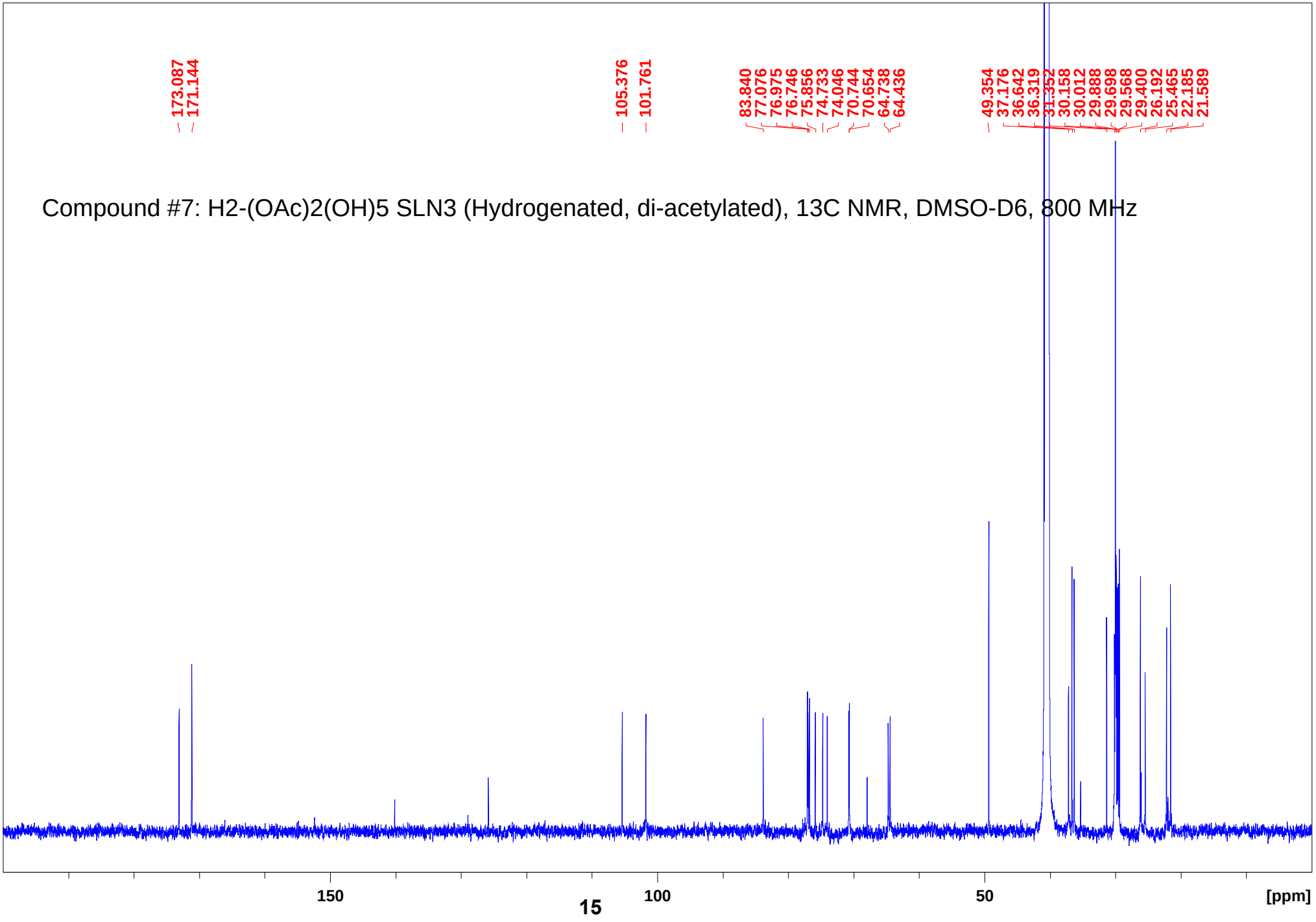
21.288
Compound #5: H2-(OH)7 SLOMe, 13C NMR, DMSO-D6, 600 MHz
150
100
50
[ppm]
13


7.814 7.807 7.801 5.617 5.613 5.441 5.438 5.302 5.295 5.162 5.155 5.092 5.087 4.402 4.393 4.361 4.351 4.239 4.236 4.224 4.222 4.211 4.209 4.197 4.195 4.056 4.047 4.041 4.033 4.013 4.006 3.998 3.991 3.613 3.606 3.603 3.599 3.385 3.381 3.377 3.374 3.369 3.365 3.362 3.356 3.354 3.338 3.201 3.190 3.180 3.173 3.114 3.107 3.103 3.095 3.091 3.082 3.075 3.067 3.021 3.017 3.010 3.007 2.040 2.030 2.021 2.011 2.009 2.006 1.999 1.998 1.644 1.635 1.627 1.618 1.610 1.483 1.475 1.466 1.458 1.312 1.229 1.190 1.179 1.102
Compound #7: H2-(OAc)2(OH)5 SLN3 (Hydrogenated, di-acetylated), 1H NMR, DMSO-D6, 800 MHz
0.9990 0.7941 0.7923 0.8606 0.8648 0.8632 1.9853 0.8551 1.3040 2.8540 7.1689 8.6162 2.0000 3.4474 27.3943 2.9954
8 6 4 2 [ppm]
14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105.376
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83.840
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76.746
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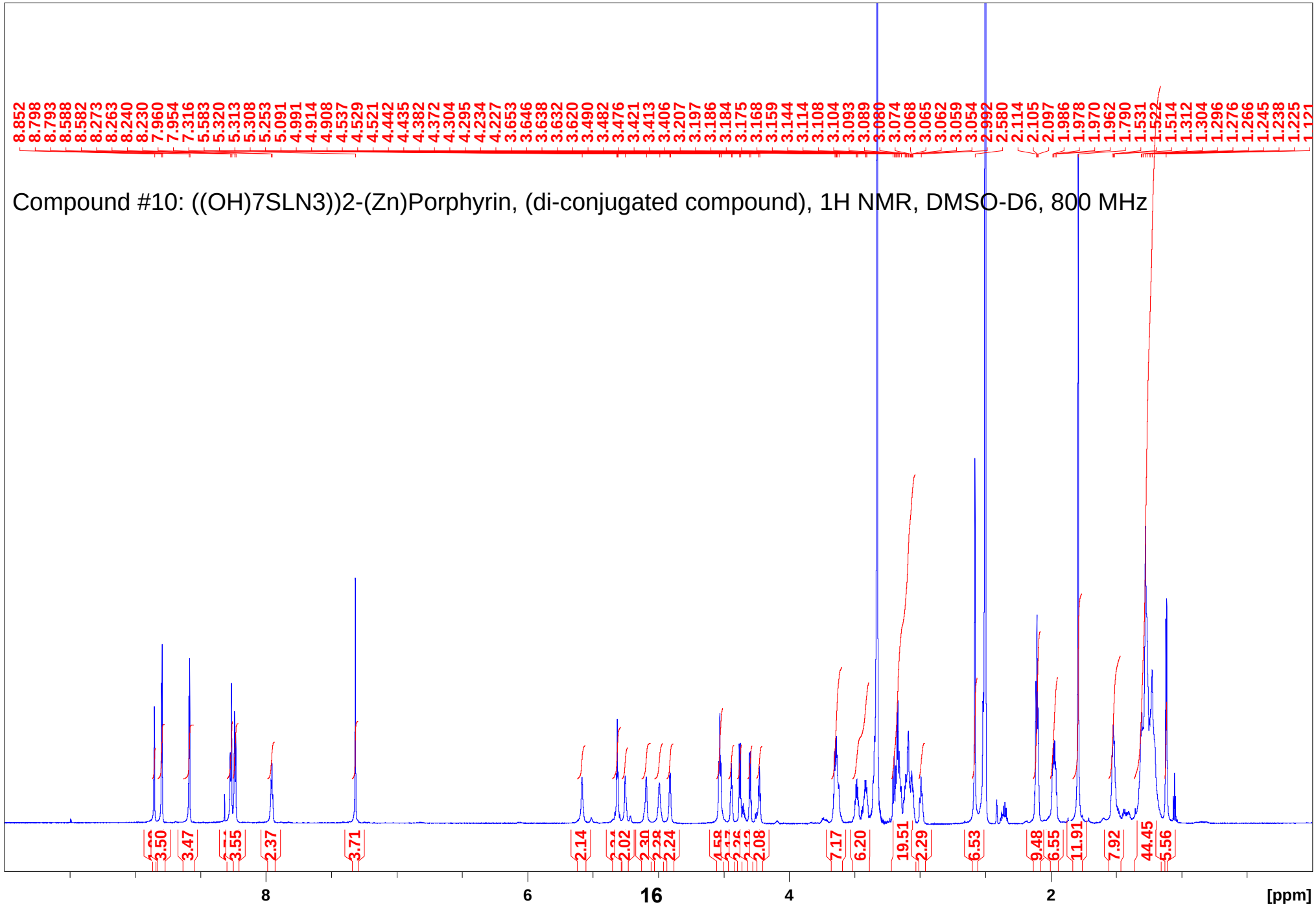
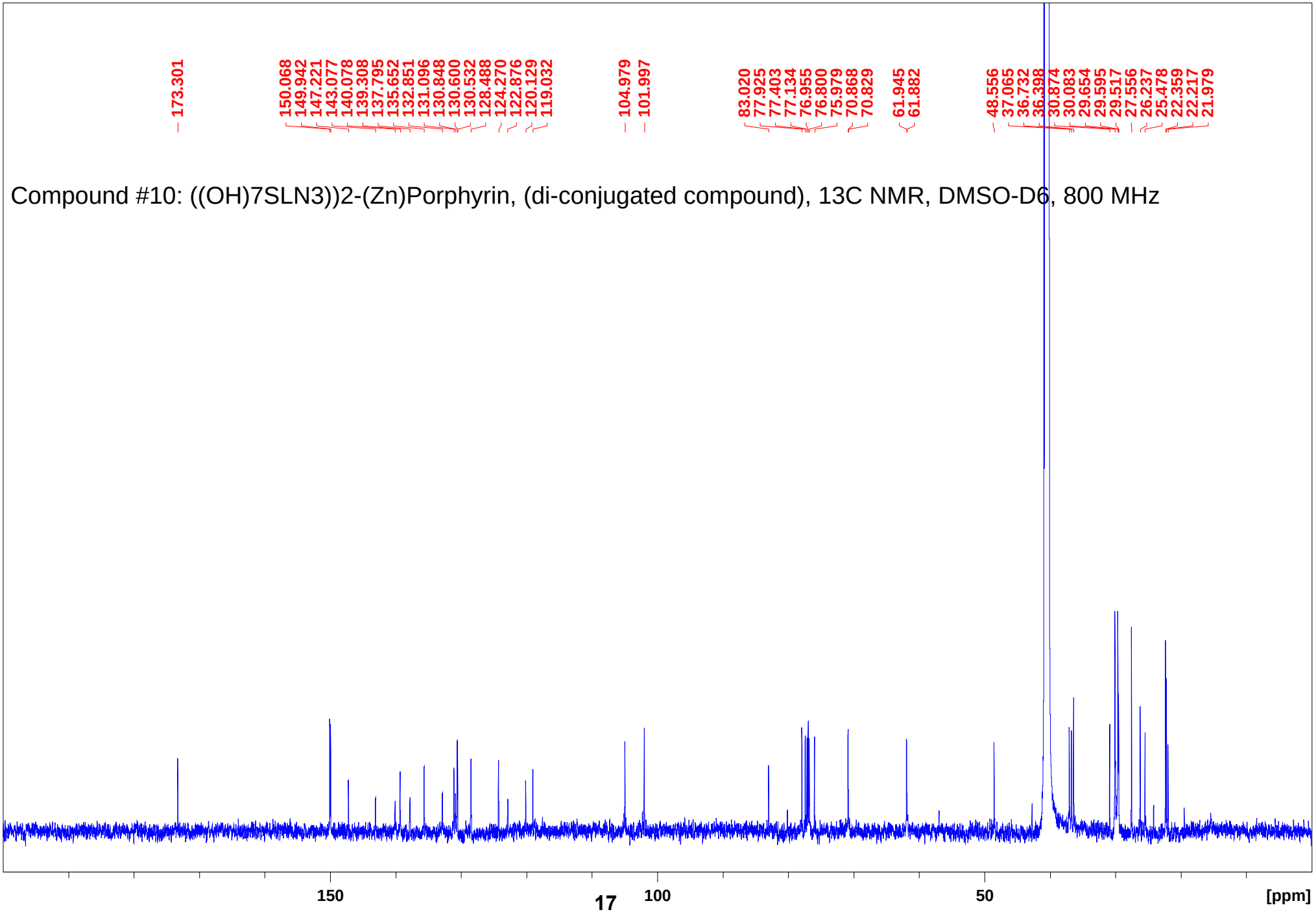
74.733
74.046
70.744
70.654
64.738
64.436
49.354
37.176
36.642
36.319
31.352
30.158
30.012
29.888
29.698
29.568
29.400
26.192
25.465
22.185
21.589
Compound #7: H2-(OAc)2(OH)5 SLN3 (Hydrogenated, di-acetylated), 13C NMR, DMSO-D6, 800 MHz
150
100
50
[ppm]


8.852 8.798 8.793 8.588 8.582 8.273 8.263 8.240 8.230 7.960 7.954 7.316 5.583 5.320 5.313 5.308 5.253 5.091 4.991 4.914 4.908 4.537 4.529 4.521 4.442 4.435 4.382 4.372 4.304 4.295 4.234 4.227 3.653 3.646 3.638 3.632 3.620 3.490 3.482 3.476 3.421 3.413 3.406 3.207 3.197 3.186 3.184 3.175 3.168 3.159 3.144 3.114 3.108 3.104 3.093 3.089 3.080 3.074 3.068 3.065 3.062 3.059 3.054 2.992 2.580 2.114 2.105 2.097 1.986 1.978 1.970 1.962 1.790 1.531 1.522 1.514 1.312 1.304 1.296 1.276 1.266 1.245 1.238 1.225 1.121
Compound #10: ((OH)7SLN3))2-(Zn)Porphyrin, (di-conjugated compound), 1H NMR, DMSO-D6, 800 MHz
3.50 3.47 3.55 2.37 3.71 2.14 2.02 2.08 7.17 6.20 19.51 2.29 6.53 9.48 6.55 11.91 7.92 44.45 5.56
8 6 16 4 2 [ppm]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140.078
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137.795
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132.851
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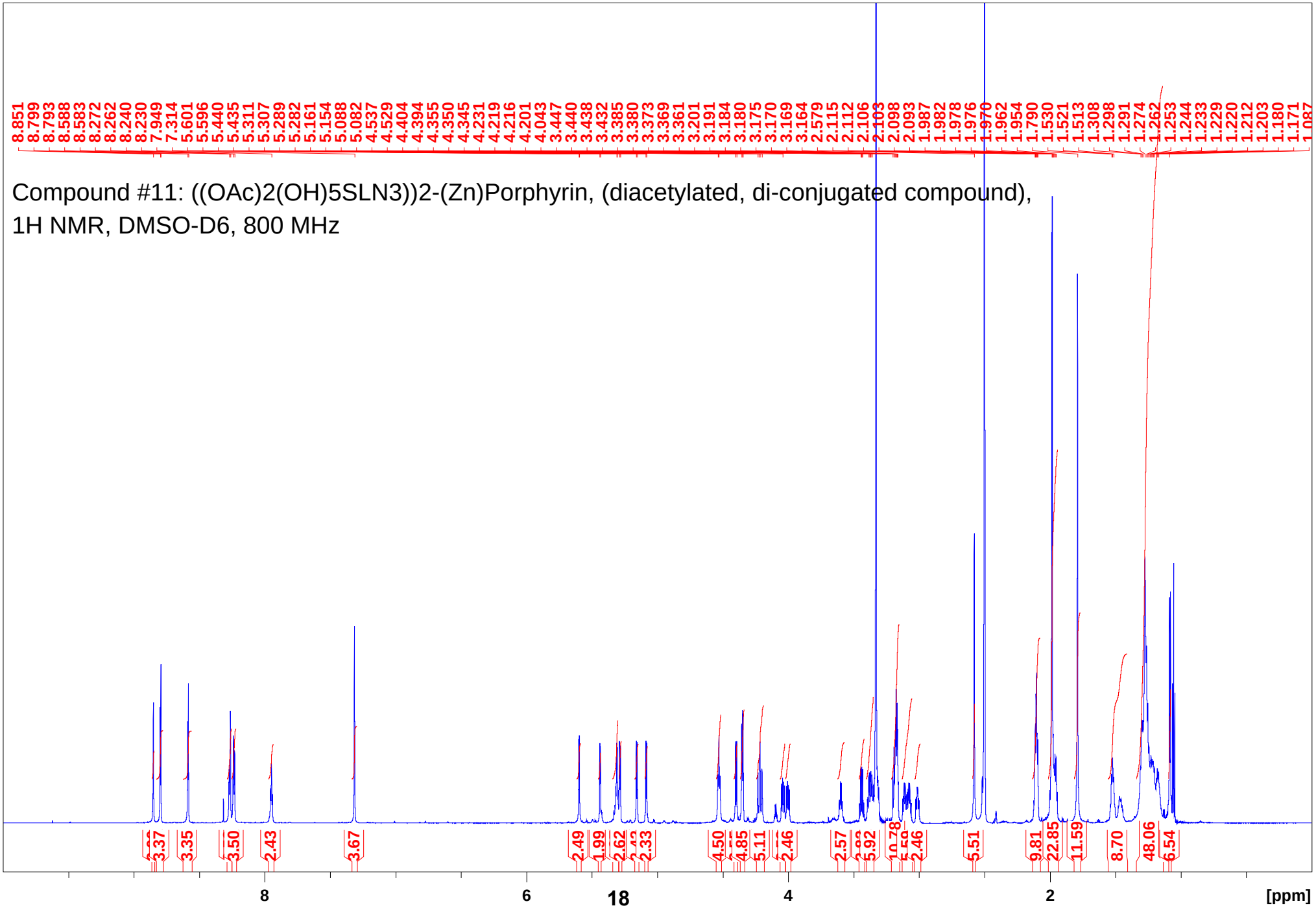
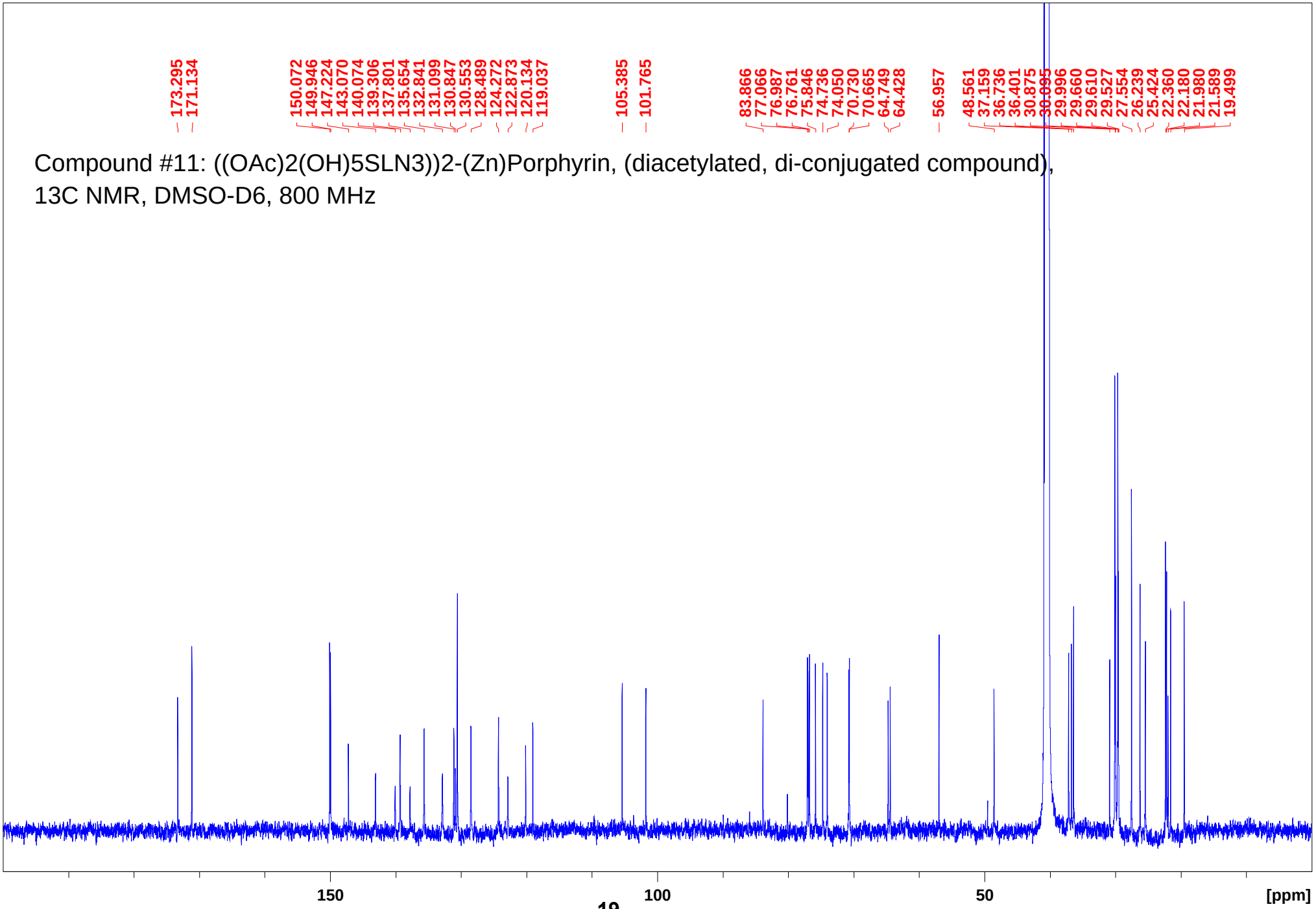
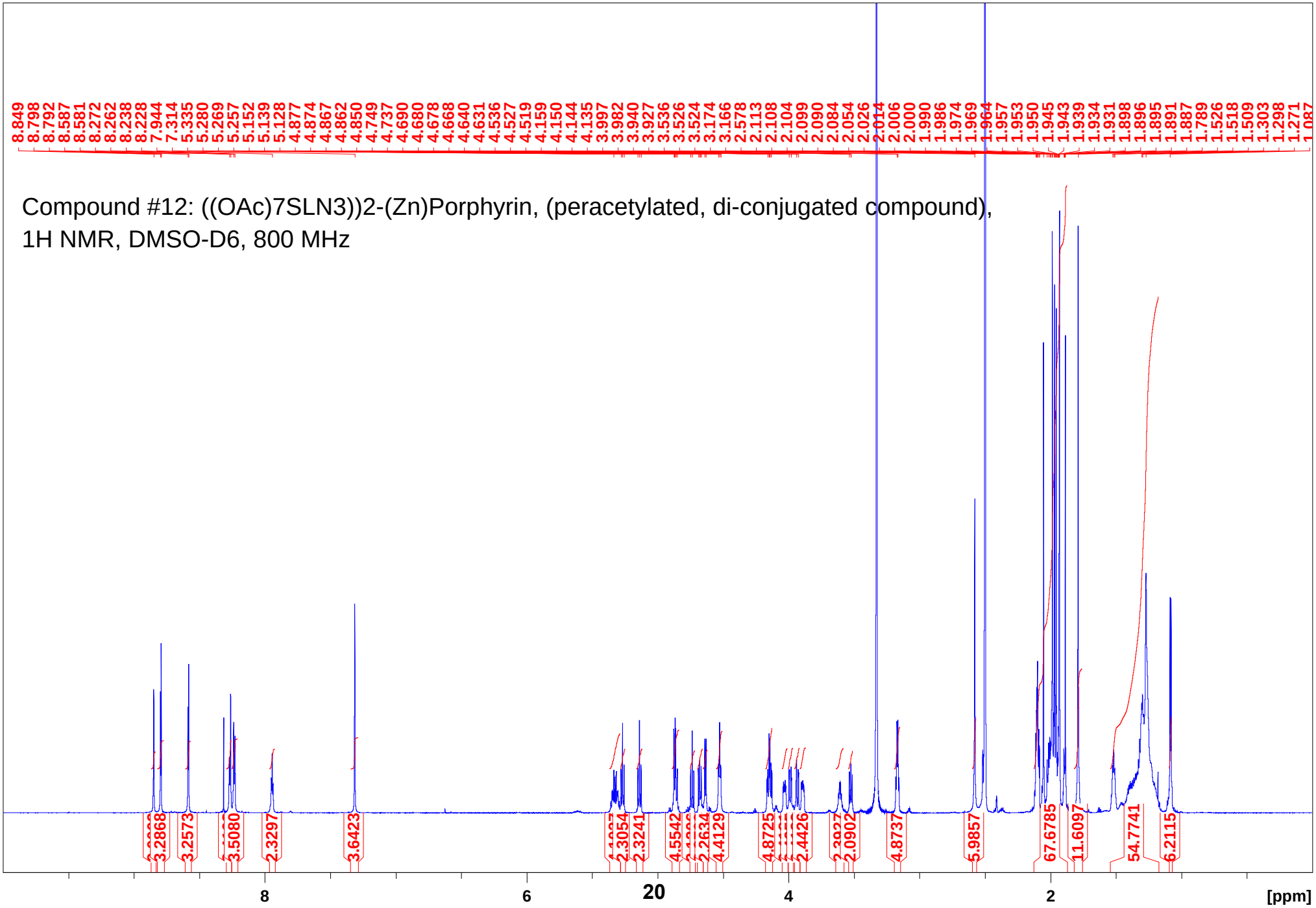
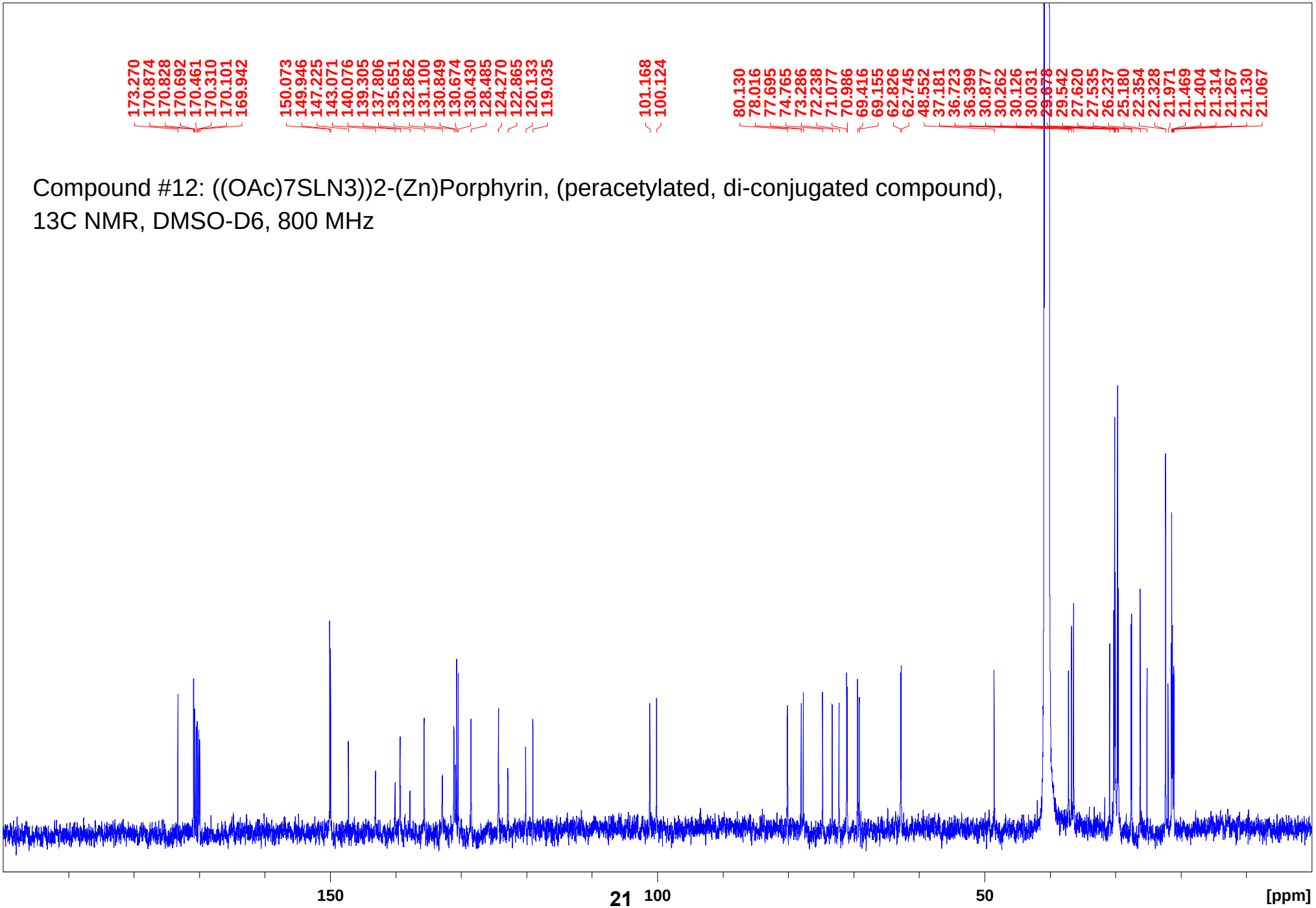
130.848
130.600
130.532
128.488
124.270
122.876
120.129
119.032
104.979
101.997
83.020
77.925
77.403
77.134
76.955
76.800
75.979
70.868
70.829
61.945
61.882
48.556
37.065
36.732
36.398
30.874
30.083
29.654
29.595
29.517
27.556
26.237
25.478
22.359
22.217
21.979
Compound #10: ((OH)7SLN3))2-(Zn)Porphyrin, (di-conjugated compound), 13C NMR, DMSO-D6, 800 MHz
150
100
50
[ppm]

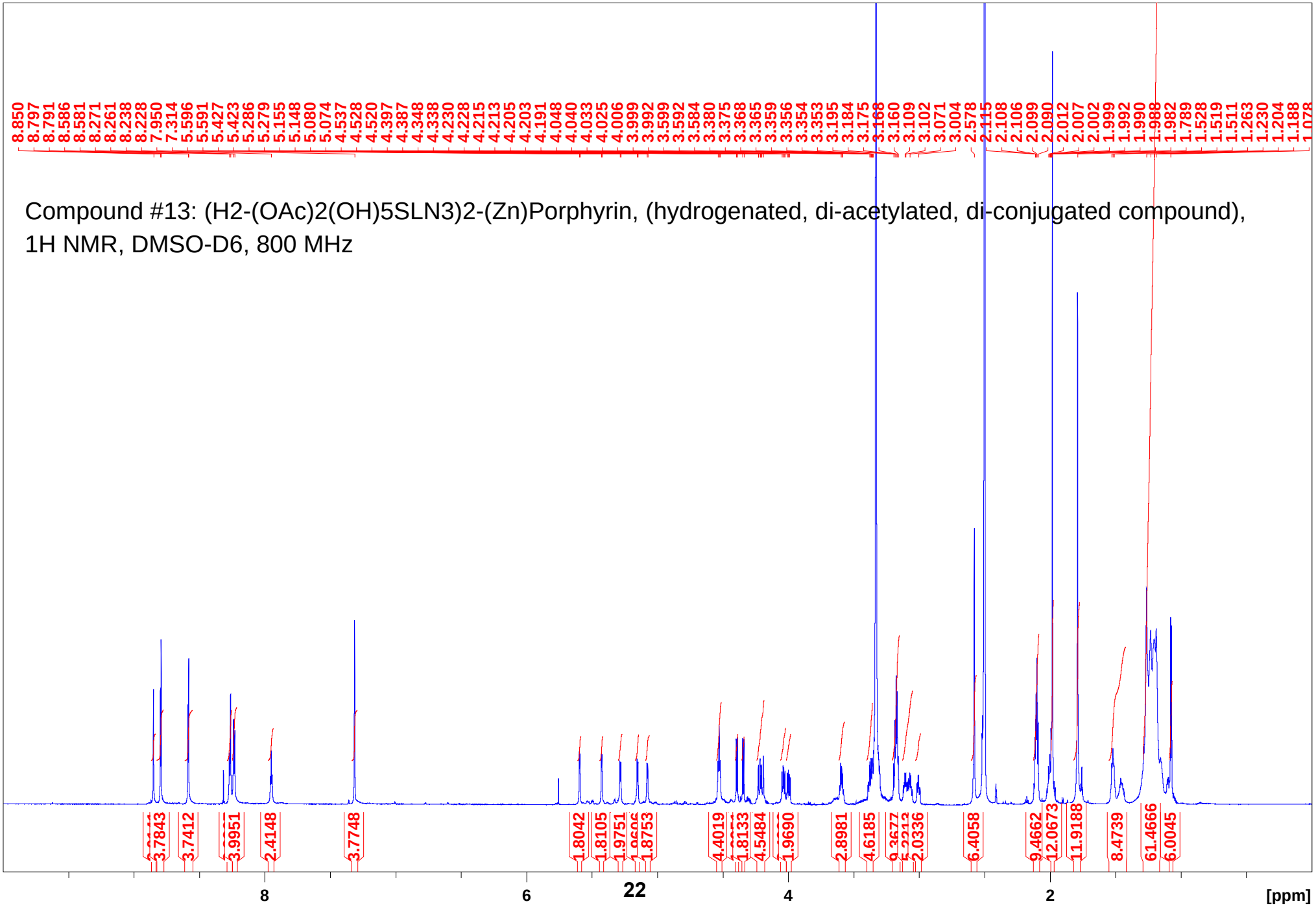

8.851 8.799 8.793 8.588 8.583 8.272 8.262 8.240 8.230 7.949 7.314 5.601 5.596 5.440 5.435 5.311 5.307 5.289 5.282 5.161 5.154 5.088 5.082 4.537 4.529 4.404 4.394 4.355 4.350 4.345 4.231 4.219 4.216 4.201 4.043 3.447 3.440 3.438 3.432 3.385 3.380 3.373 3.369 3.361 3.201 3.191 3.184 3.180 3.175 3.170 3.169 3.164 2.579 2.115 2.112 2.106 2.103 2.098 2.093 1.987 1.982 1.978 1.976 1.970 1.962 1.954 1.790 1.530 1.521 1.513 1.308 1.298 1.291 1.274 1.262 1.253 1.244 1.233 1.229 1.220 1.212 1.203 1.180 1.171 1.087
Compound #11: ((OAc)2(OH)5SLN3))2-(Zn)Porphyrin, (diacetylated, di-conjugated compound),
1H NMR, DMSO-D6, 800 MHz
3.37 3.35 3.50 2.43 3.67 2.49 1.99 2.62 2.33 4.50 4.85 5.11 2.46 2.57 5.92 10.78 2.46 5.51 9.81 22.85 11.59 8.70 48.06 6.54
8 6 4 2 [ppm]

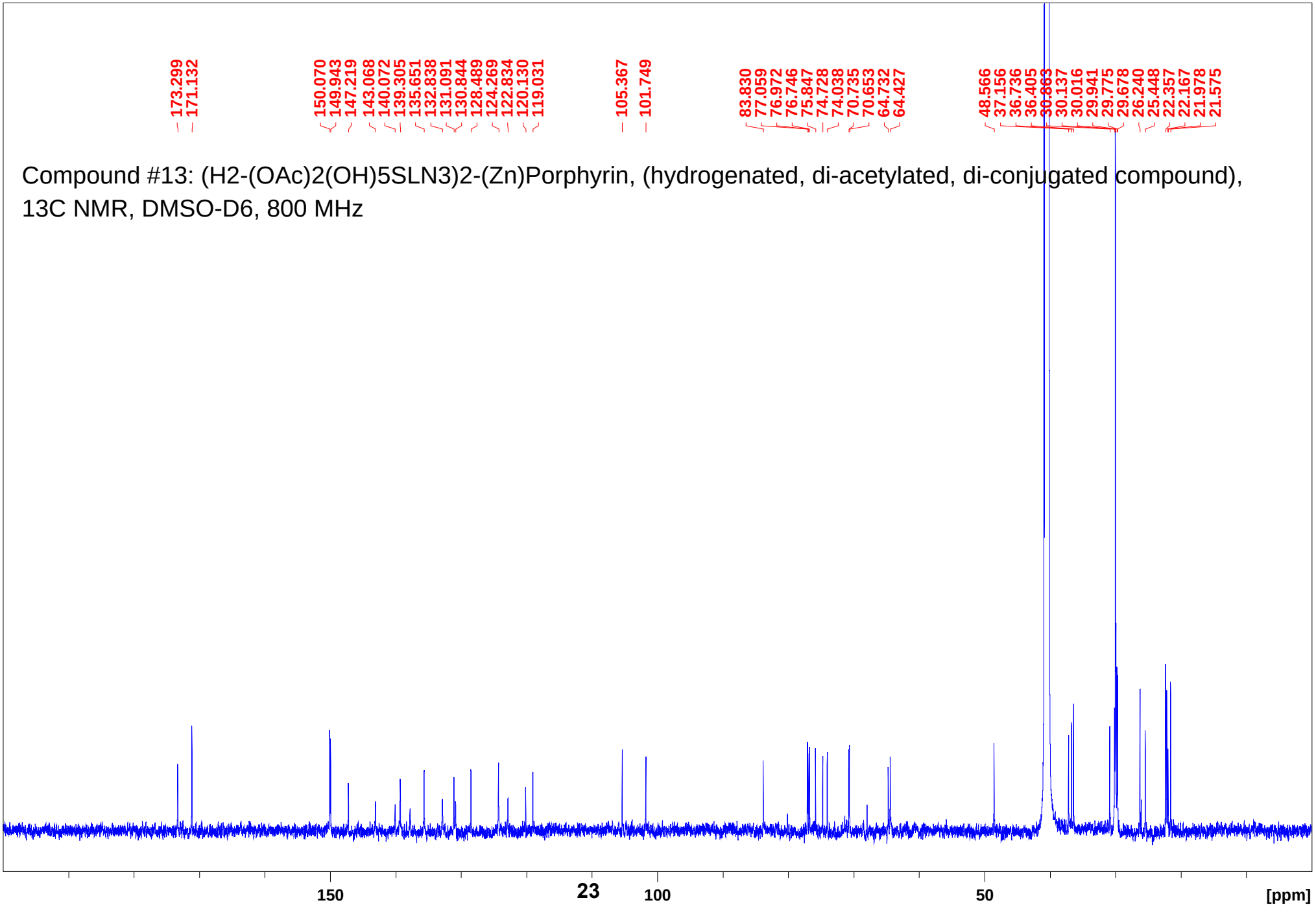


Compound #11: ((OAc)2(OH)5SLN3))2-(Zn)Porphyrin, (diacetylated, di-conjugated compound),
13C NMR, DMSO-D6, 800 MHz

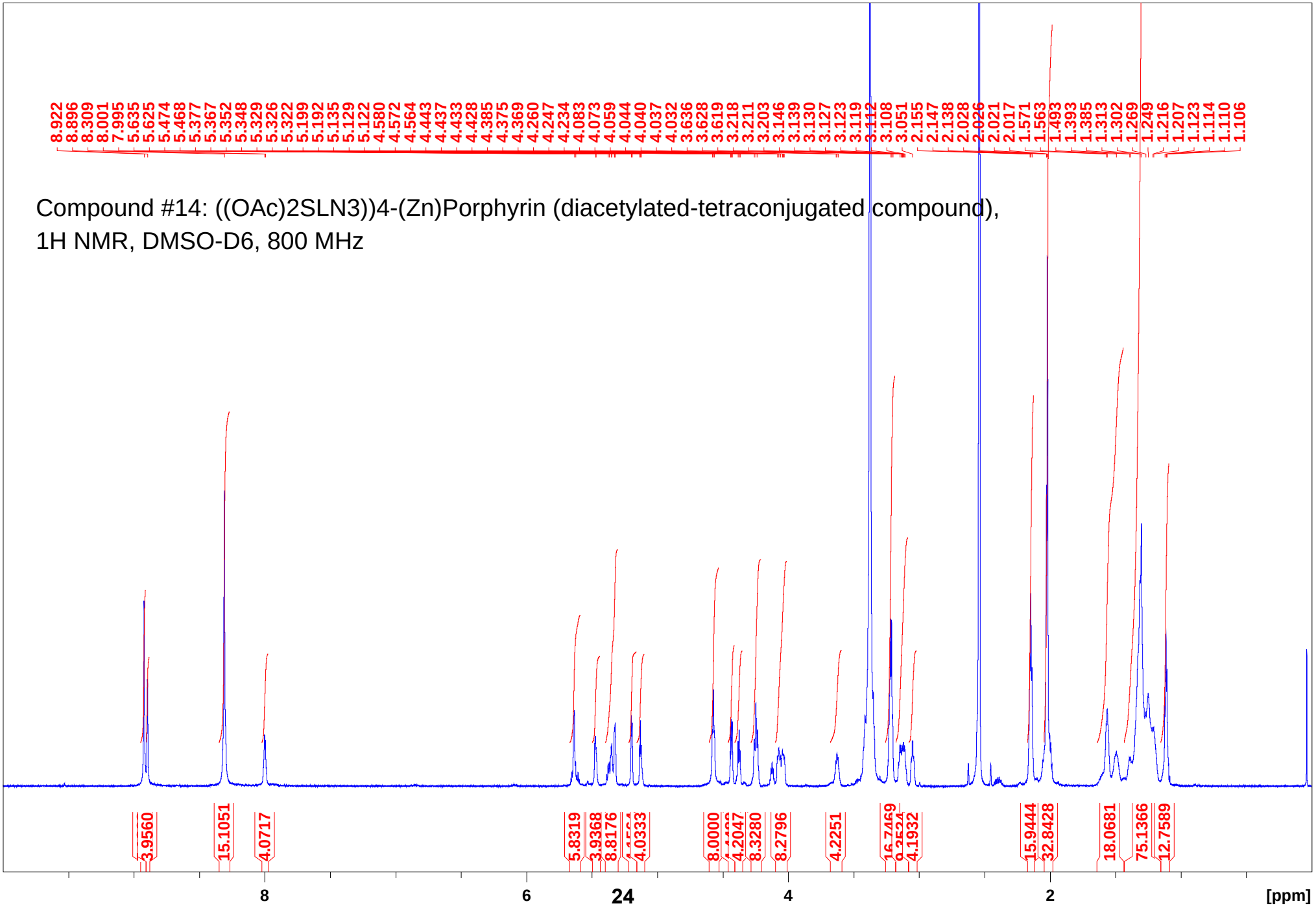

8.849 8.798 8.792 8.587 8.581 8.272 8.262 8.238 8.228 7.944 7.314 5.335 5.280 5.269 5.257 5.152 5.139 5.128 4.877 4.874 4.867 4.862 4.850 4.749 4.737 4.690 4.680 4.678 4.668 4.640 4.631 4.536 4.527 4.519 4.159 4.150 4.144 4.135 3.997 3.982 3.940 3.927 3.536 3.526 3.524 3.174 3.166 2.578 2.113 2.108 2.104 2.099 2.090 2.084 2.054 2.026 2.014 2.006 2.000 1.990 1.986 1.974 1.969 1.964 1.957 1.953 1.950 1.945 1.943 1.939 1.934 1.931 1.898 1.896 1.895 1.891 1.887 1.789 1.526 1.518 1.509 1.303 1.298 1.271 1.087
Compound #12: ((OAc)7SLN3))2-(Zn)Porphyrin, (peracetylated, di-conjugated compound),
1H NMR, DMSO-D6, 800 MHz
3.2868
3.2573
3.5080
2.3297
3.6423
2.3054
2.3241
4.5542
2.2634
4.4129
4.8725
2.4426
2.0902
4.8737
5.9857
67.6785
11.6097
54.7741
6.2115
8
6
20
4
2
[ppm]

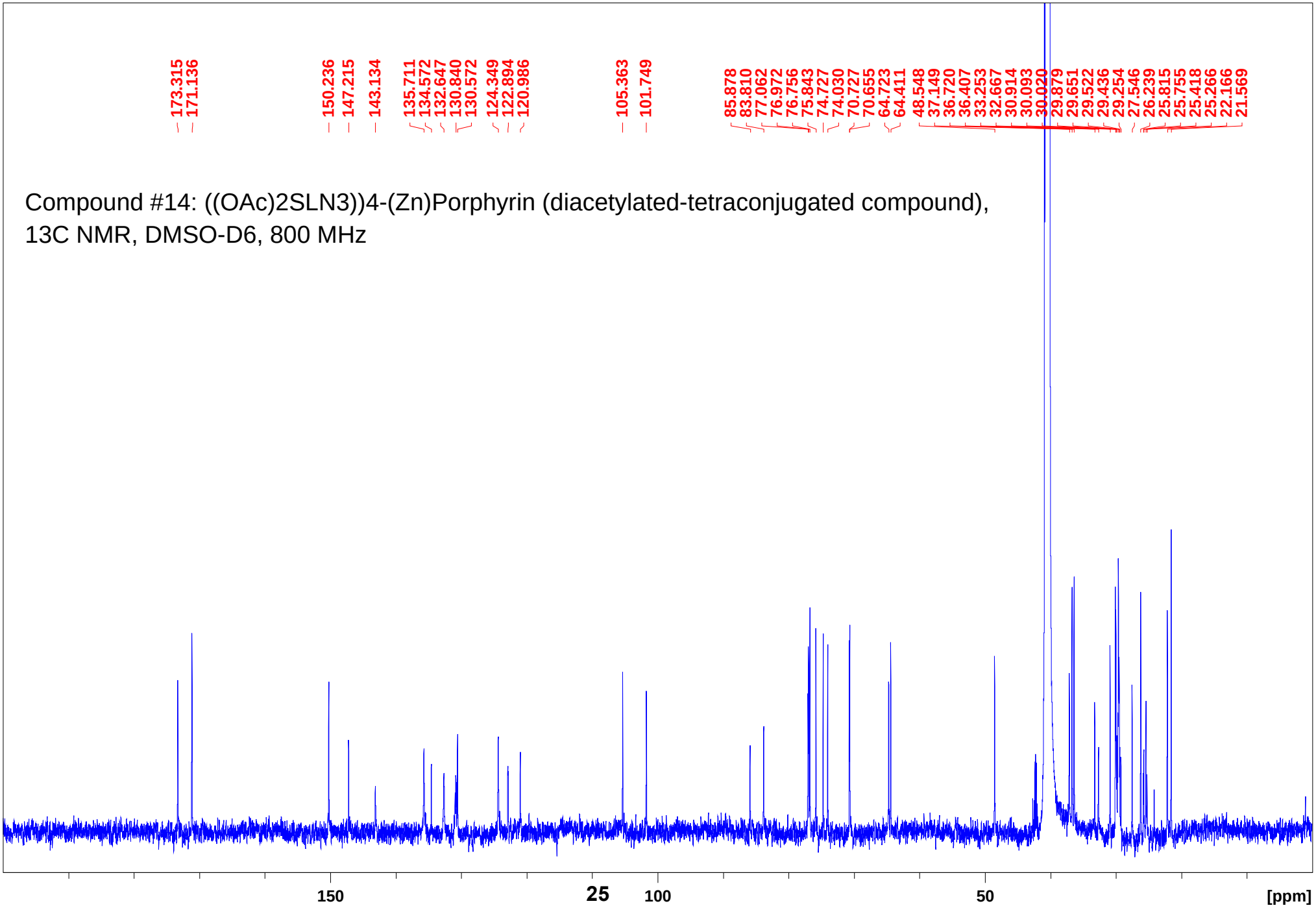

173.270
170.874
170.828
170.692
170.461
170.310
170.101
169.942
150.073
149.946
147.225
143.071
140.076
139.305
137.806
135.651
132.862
131.100
130.849
130.674
130.430
128.485
124.270
122.865
120.133
119.035
101.168
100.124
80.130
78.016
77.695
74.765
73.286
72.238
71.077
70.986
69.416
69.155
62.826
62.745
48.552
37.181
36.723
36.399
30.877
30.262
30.126
30.031
29.678
29.542
27.620
27.535
26.237
25.180
22.354
22.328
21.971
21.469
21.404
21.314
21.267
21.130
21.067
Compound #12: ((OAc)7SLN3))2-(Zn)Porphyrin, (peracetylated, di-conjugated compound),
13C NMR, DMSO-D6, 800 MHz
150
100
50
[ppm]

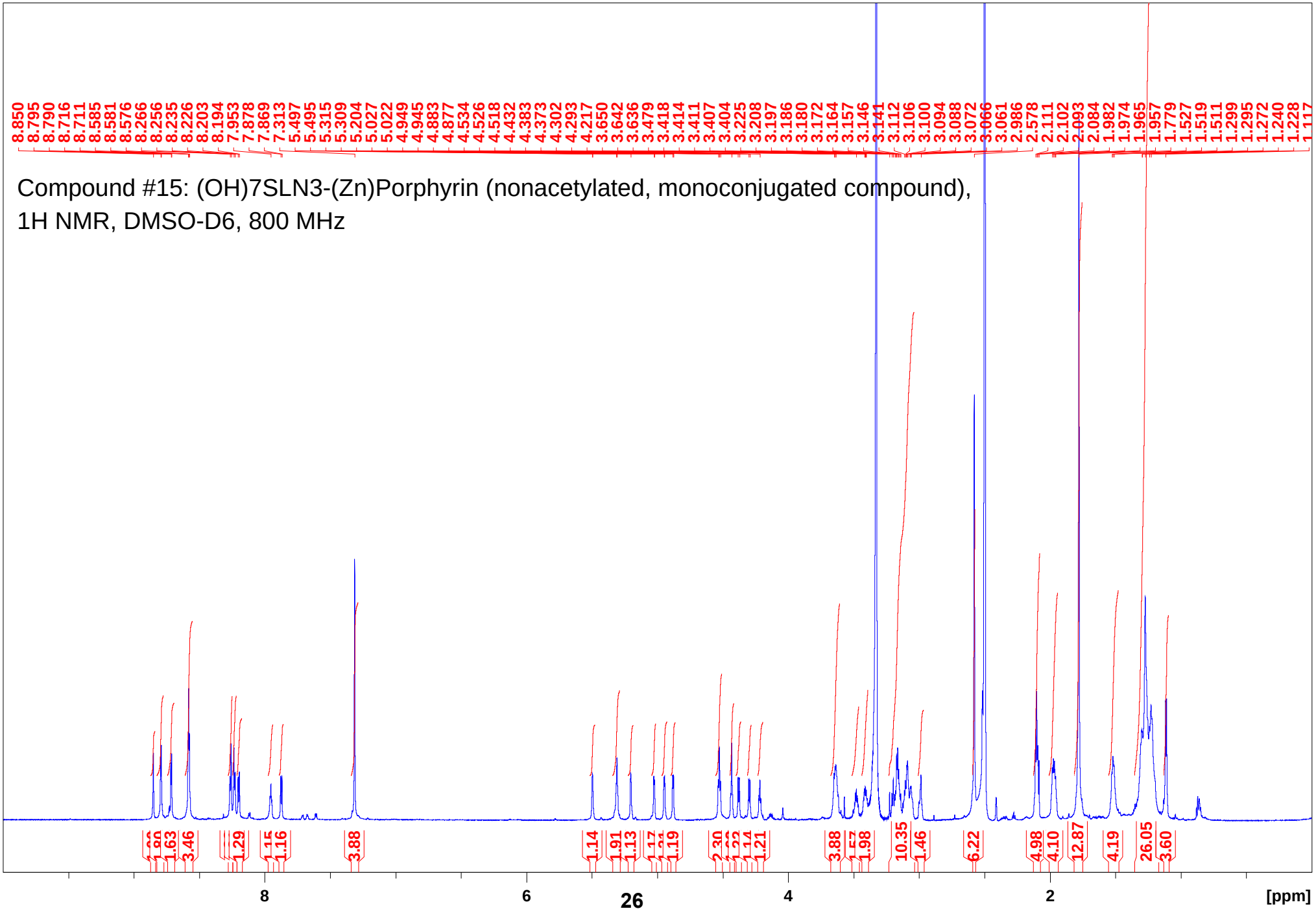

8.850 8.797 8.791 8.586 8.581 8.271 8.261 8.238 8.228 7.950 7.314 5.596 5.591 5.427 5.423 5.286 5.279 5.155 5.148 5.080 5.074 4.537 4.528 4.520 4.397 4.387 4.348 4.338 4.230 4.228 4.215 4.213 4.205 4.203 4.191 4.048 4.040 4.033 4.025 4.006 3.999 3.992 3.599 3.592 3.584 3.380 3.375 3.368 3.365 3.359 3.356 3.353 3.195 3.184 3.175 3.168 3.160 3.109 3.102 3.071 3.004 2.578 2.115 2.108 2.106 2.099 2.090 2.012 2.007 2.002 1.999 1.992 1.990 1.988 1.982 1.789 1.528 1.519 1.511 1.263 1.230 1.204 1.188 1.078
Compound #13: (H2-(OAc)2(OH)5SLN3)2-(Zn)Porphyrin, (hydrogenated, di-acetylated, di-conjugated compound),
1H NMR, DMSO-D6, 800 MHz
3.7843 3.7412 3.9951 2.4148 3.7748 1.8042 1.8105 1.9751 1.8753 4.4019 1.8133 4.5484 1.9690 2.8981 4.6185 9.3677 2.0336 6.4058 9.4662 12.0673 11.9188 8.4739 61.4666 6.0045
8 6 4 2 [ppm]

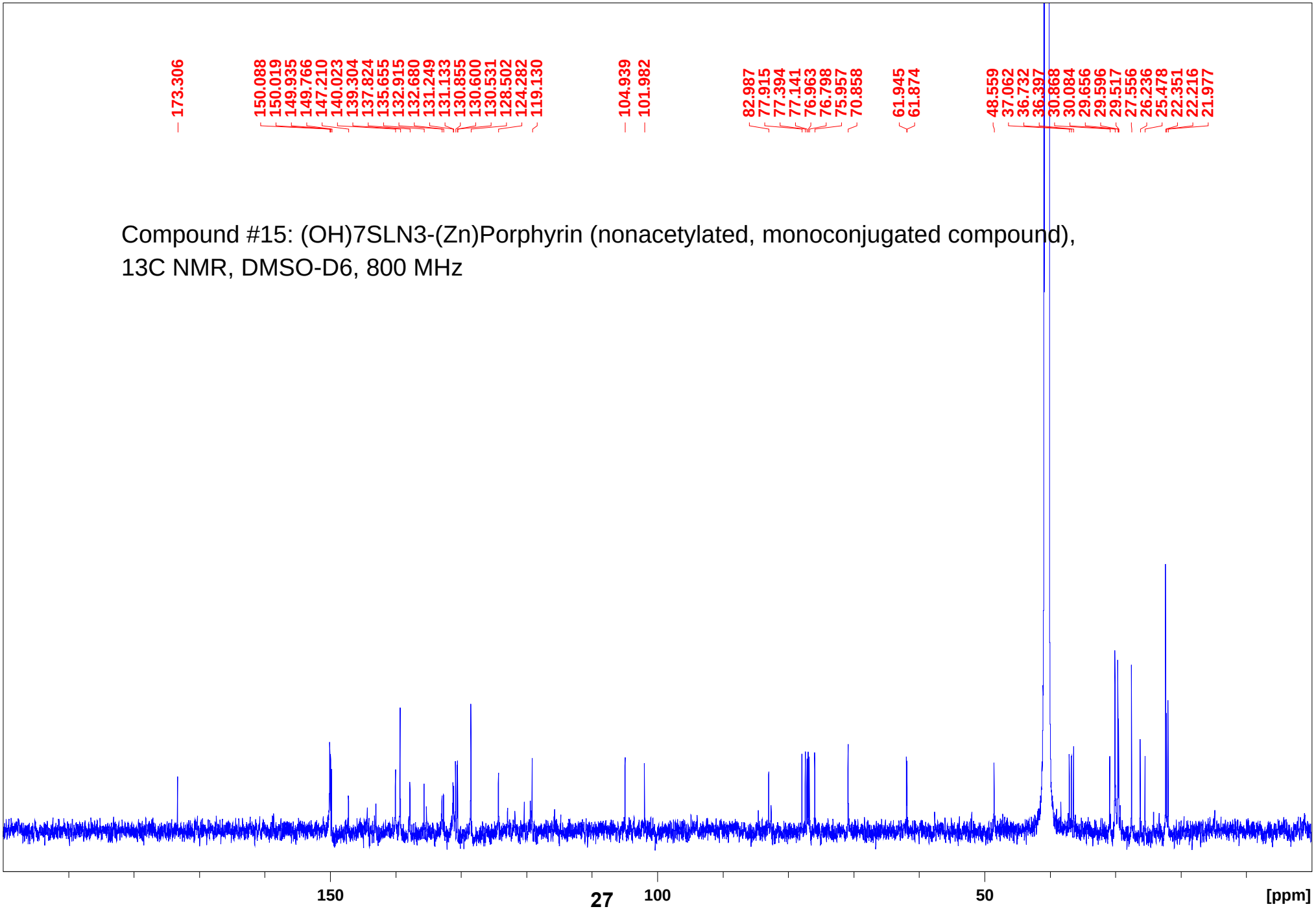


Compound #13: (H2-(OAc)2(OH)5SLN3)2-(Zn)Porphyrin, (hydrogenated, di-acetylated, di-conjugated compound), 13C NMR, DMSO-D6, 800 MHz


8.922
8.896
8.309
8.001
7.995
5.635
5.625
5.474
5.468
5.377
5.367
5.352
5.348
5.329
5.326
5.322
5.199
5.192
5.135
5.129
5.122
4.580
4.572
4.564
4.443
4.437
4.433
4.428
4.385
4.375
4.369
4.260
4.247
4.234
4.083
4.073
4.059
4.044
4.040
4.037
4.032
3.636
3.628
3.619
3.218
3.211
3.203
3.146
3.139
3.130
3.127
3.123
3.119
3.112
3.108
3.051
2.155
2.147
2.138
2.028
2.026
2.021
2.017
1.571
1.563
1.493
1.393
1.385
1.313
1.302
1.269
1.249
1.216
1.207
1.123
1.114
1.110
1.106
Compound #14: ((OAc)2SLN3))4-(Zn)Porphyrin (diacetylated-tetraconjugated compound),
1H NMR, DMSO-D6, 800 MHz
3.9560
15.1051
4.0717
5.8319
3.9368
8.8176
4.0333
8.0000
4.2047
8.3280
8.2796
4.2251
4.1932
15.9444
32.8428
18.0681
75.1366
12.7589
8
6
24
4
2
[ppm]

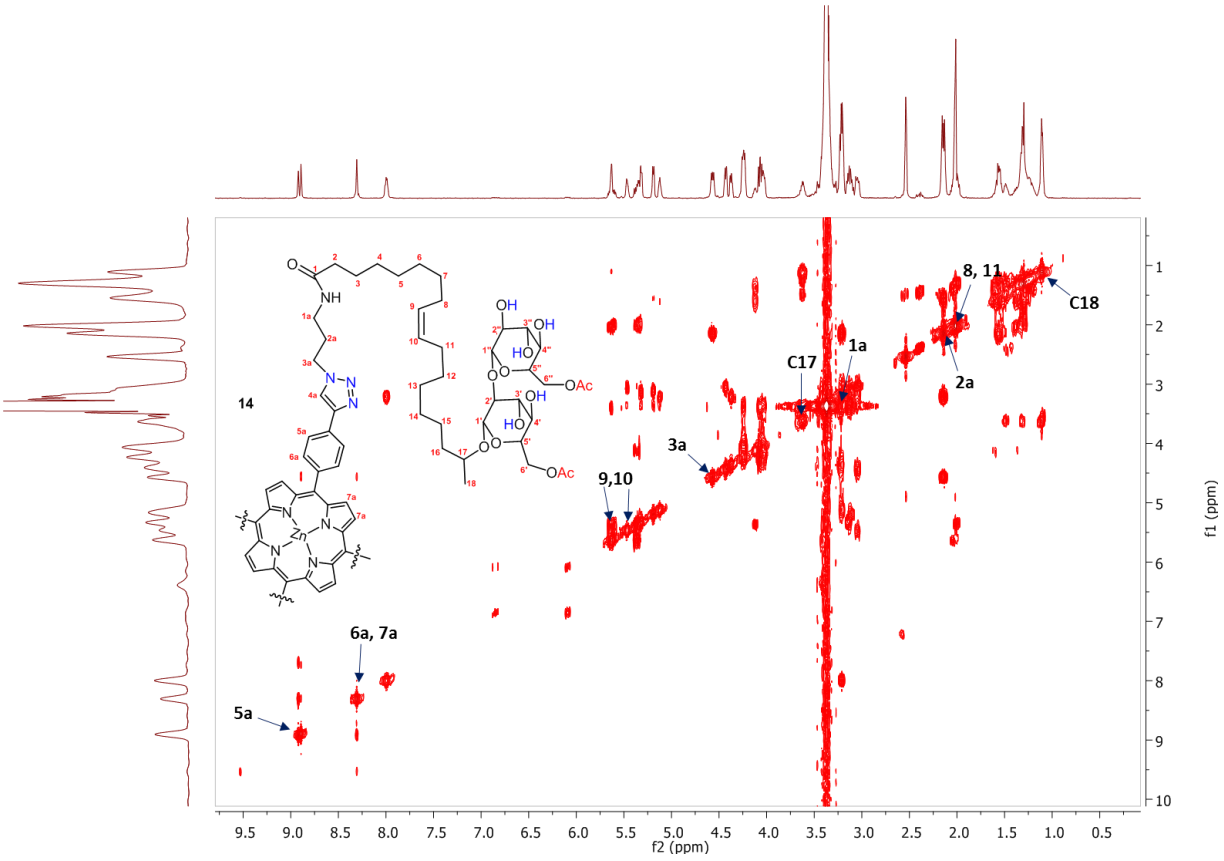

173.315
171.136
150.236
147.215
143.134
135.711
134.572
132.647
130.840
130.572
124.349
122.894
120.986
105.363
101.749
85.878
83.810
77.062
76.972
76.756
75.843
74.727
74.030
70.727
70.655
64.723
64.411
48.548
37.149
36.720
36.407
33.253
32.667
30.914
30.093
30.020
29.879
29.651
29.522
29.436
29.254
27.546
26.239
25.815
25.755
25.418
25.266
22.166
21.569
Compound #14: ((OAc)2SLN3))4-(Zn)Porphyrin (diacetylated-tetraconjugated compound),
13C NMR, DMSO-D6, 800 MHz
150
25
100
50
[ppm]


8.850 8.795 8.790 8.716 8.711 8.585 8.581 8.576 8.266 8.256 8.235 8.226 8.203 8.194 7.953 7.878 7.869 7.313 5.497 5.495 5.315 5.309 5.204 5.027 5.022 4.949 4.945 4.883 4.877 4.534 4.526 4.518 4.432 4.383 4.373 4.302 4.293 4.217 3.650 3.642 3.636 3.479 3.418 3.414 3.411 3.407 3.404 3.225 3.208 3.197 3.186 3.180 3.172 3.164 3.157 3.146 3.141 3.112 3.106 3.100 3.094 3.088 3.072 3.066 3.061 2.986 2.578 2.111 2.102 2.093 2.084 1.982 1.974 1.965 1.957 1.779 1.527 1.519 1.511 1.299 1.295 1.272 1.240 1.228 1.117
Compound #15: (OH)7SLN3-(Zn)Porphyrin (nonacetylated, monoconjugated compound),
1H NMR, DMSO-D6, 800 MHz
1.63 3.46 1.29 1.16 3.88 1.14 1.91 1.13 1.19 3.88 1.98 10.35 1.46 6.22 4.98 4.10 12.87 4.19 26.05 3.60
8 6 4 2 [ppm]

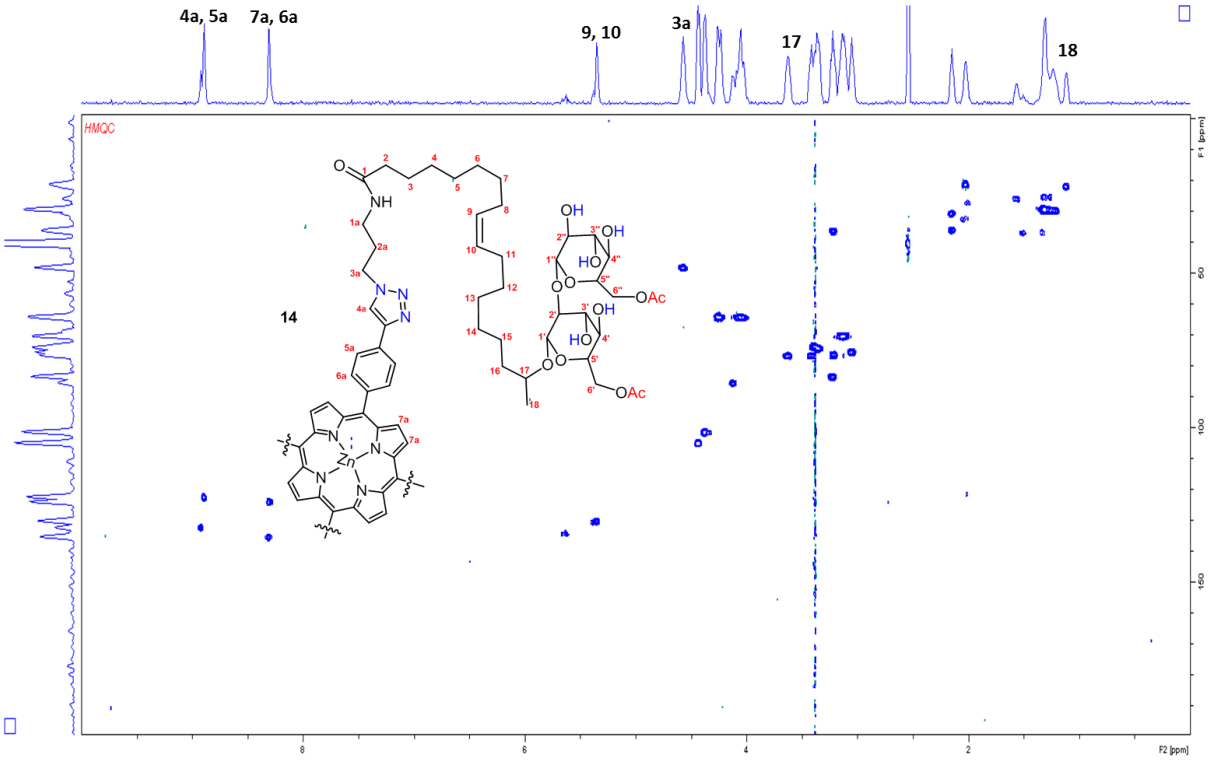


Compound #15: (OH)7SLN3-(Zn)Porphyrin (nonacetylated, monoconjugated compound),
13C NMR, DMSO-D6, 800 MHz

^{1}H-COSY, for tetra-conjugated compound (#14), 600 MHz, in DMSO-d_6.



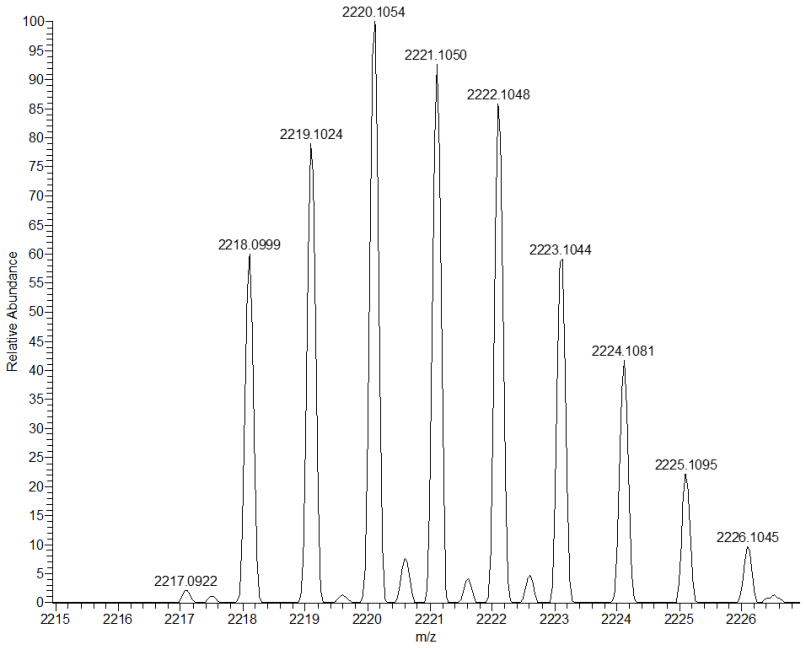
HMQC for tetraconjugated compound (#14) 600 MHz, in DMSO



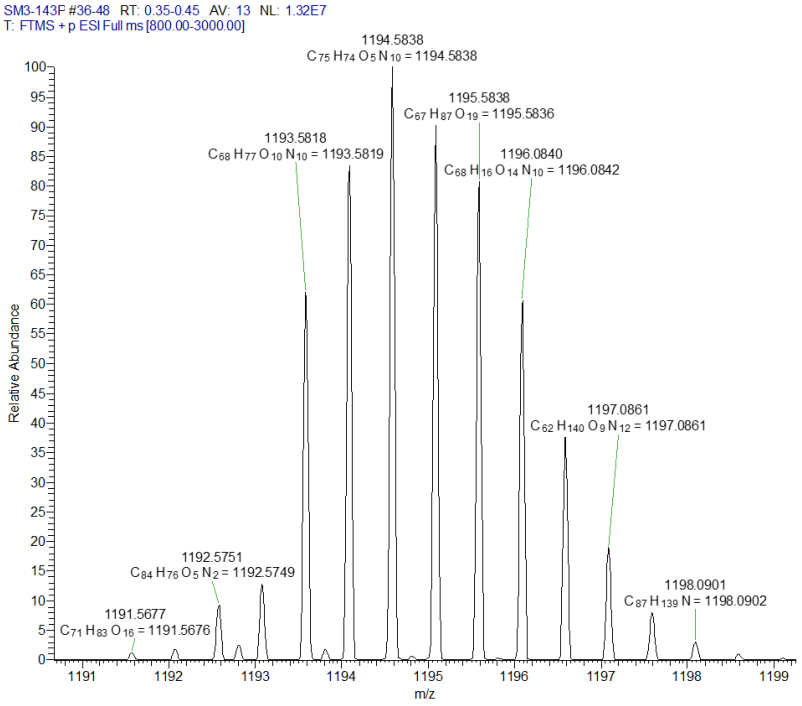
FTMS-ESI and MALDT-TOF of sophorolipids-porphyrin conjugated compounds:

Compound# 10:

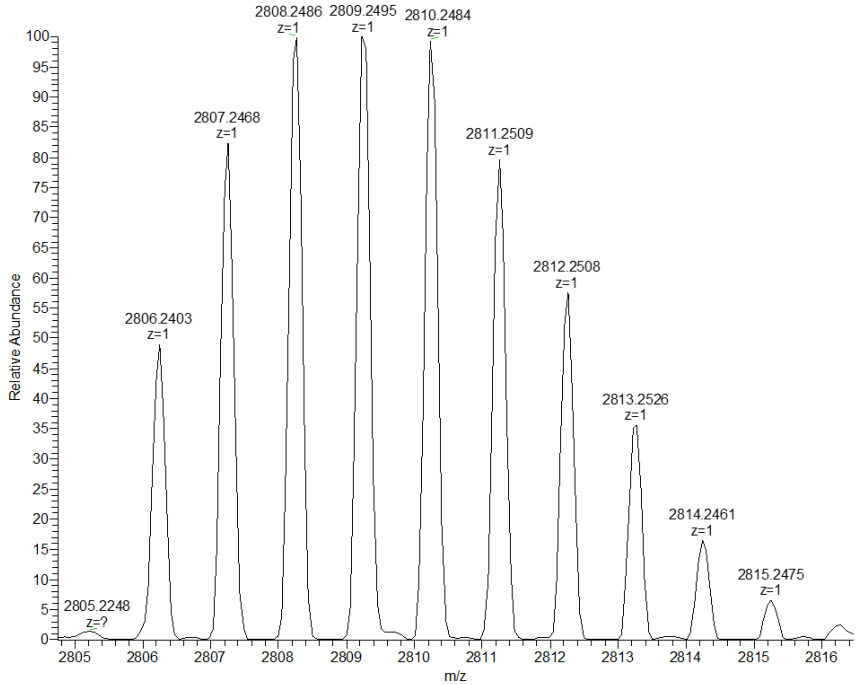
170511_4 #538-543 RT: 4.93-4.98 AV: 6 NL: 6.19E4
F: FTMS + p ESI Full ms [800.00-3000.00]



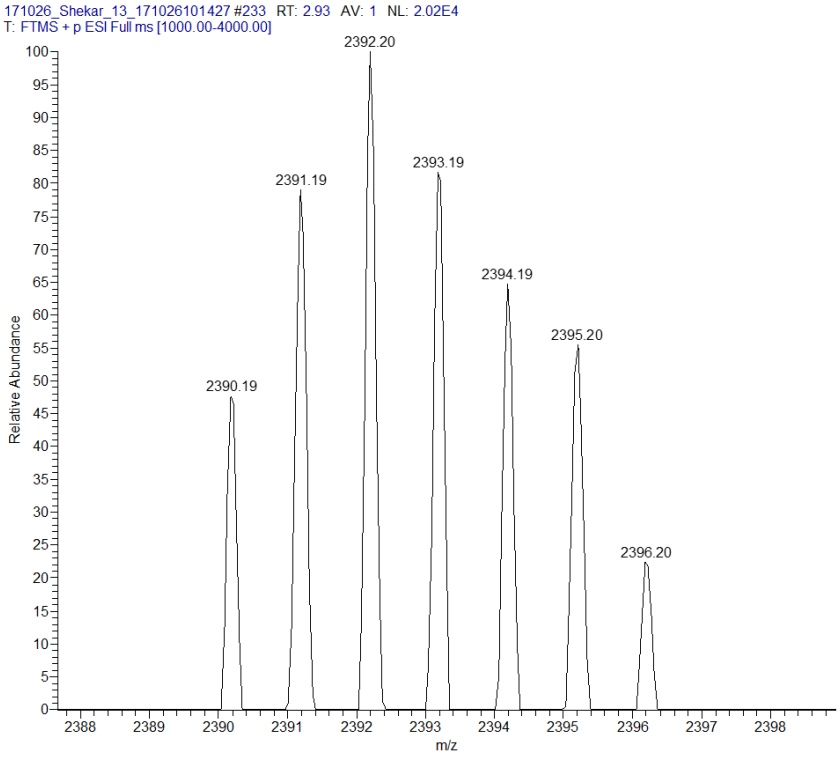
Compound# 11:



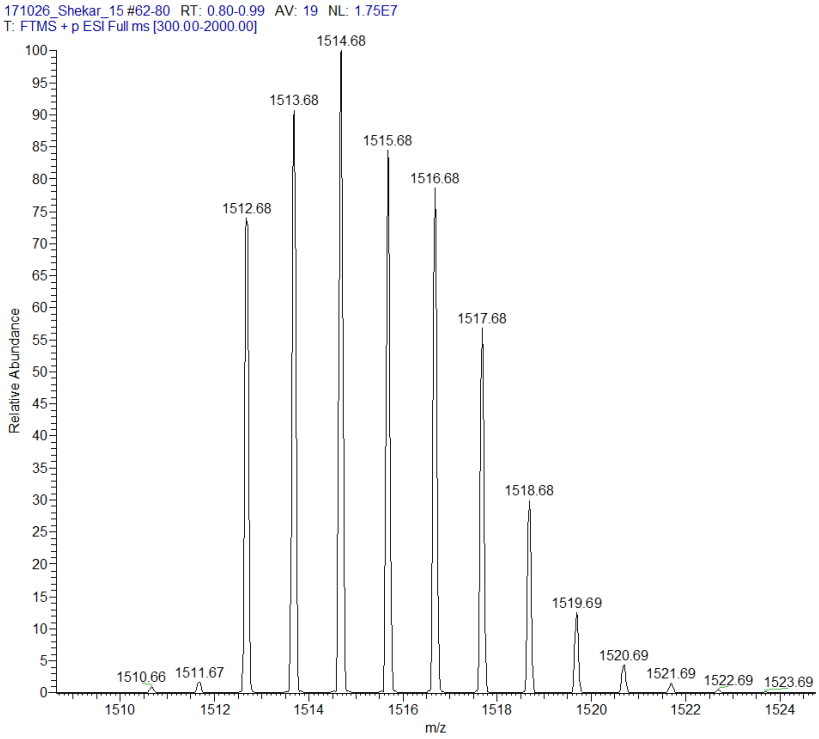
Compound# 12:



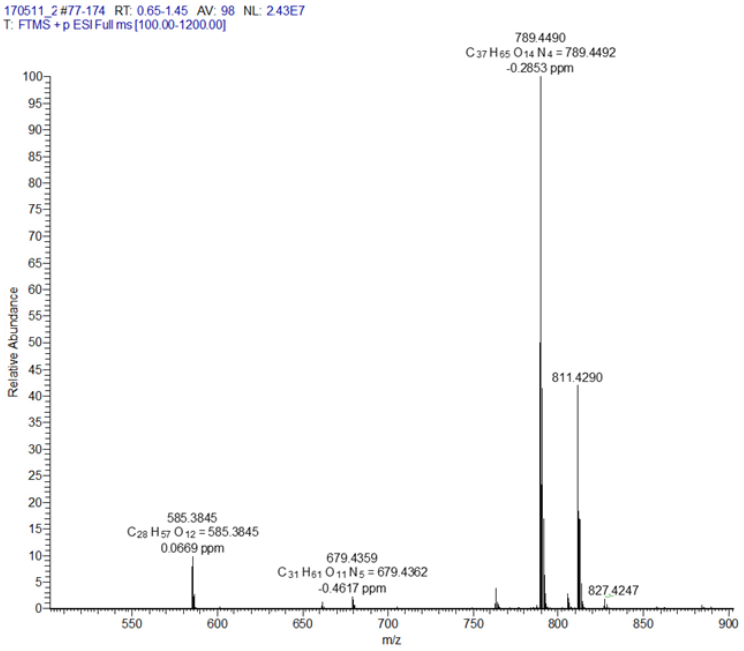
Compound# 13:



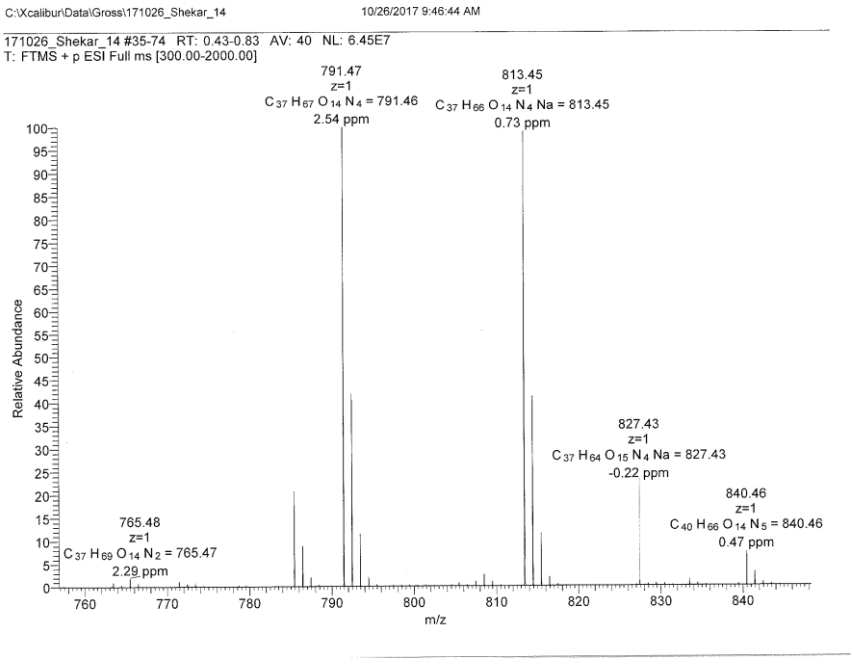
Compound# 15:



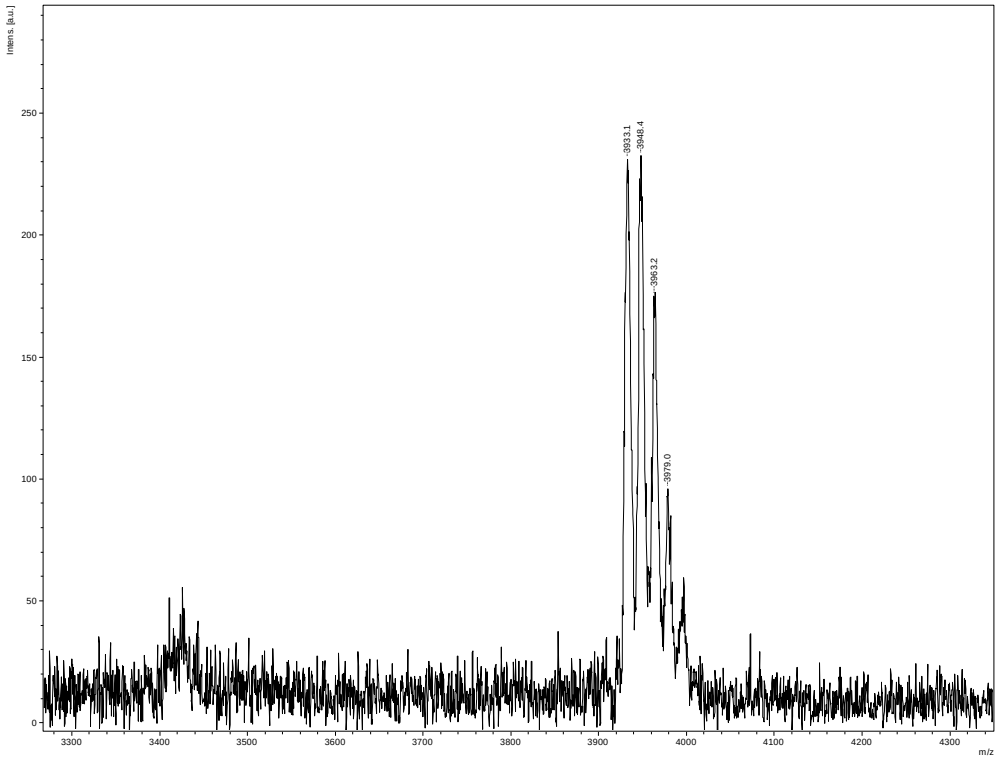
ESI-MS for compound #3:



ESI-MS for compound #7:



MALDI-TOF of compound#14



References

1. U. Siggel, U. Bindig, C. Endisch et al., *Ber. Bunsenges. Phys. Chem*., 1996,**100**, 2070.