

Supporting Information

Sulfonate derived phosphoramidates as active intermediates in the enzymatic primer-extension of DNA

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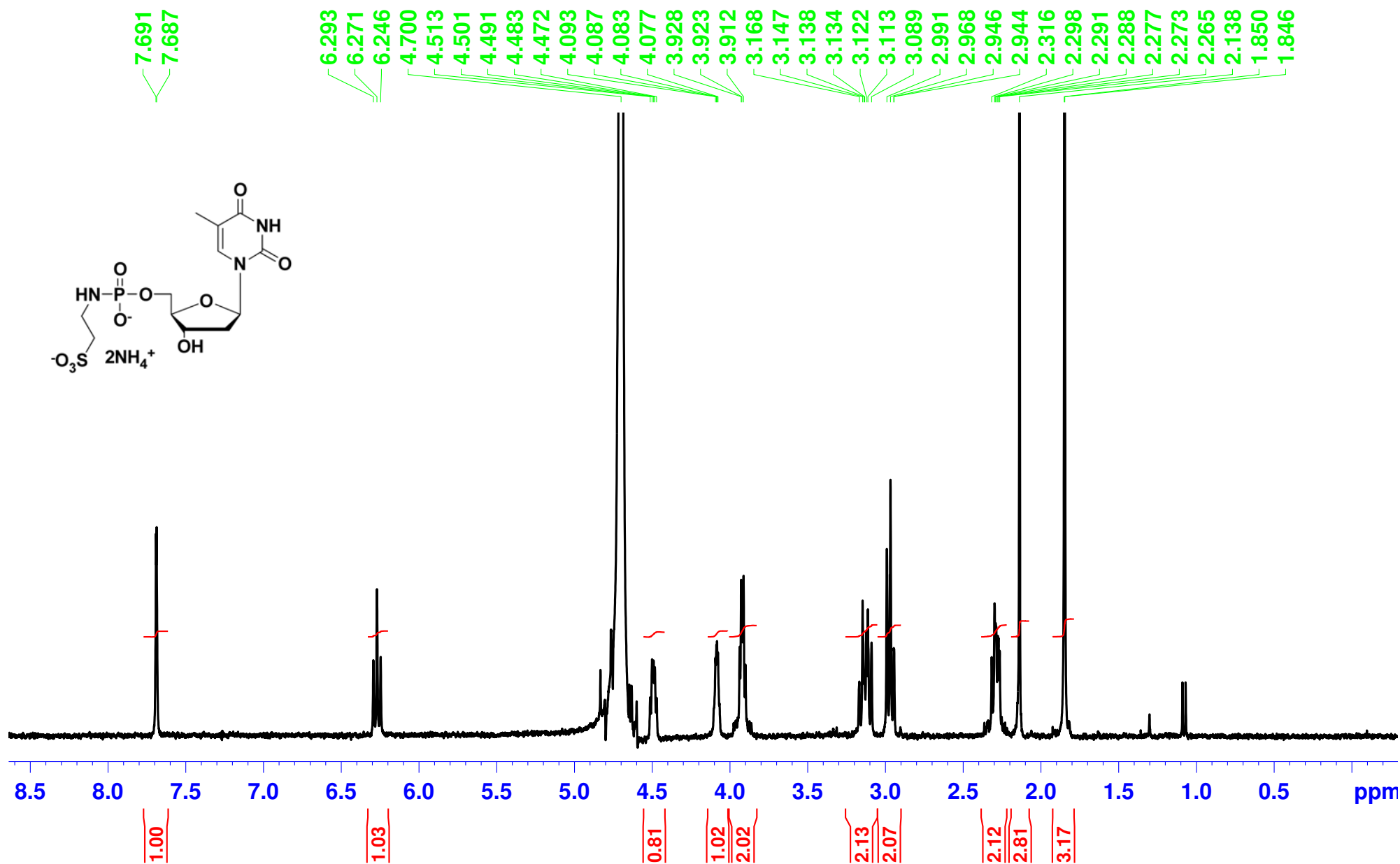
NMR spectra of the compounds.....S3-S85

Kinetic experiment data of enzymatic incorporation of compound **28** and dGTP.....S86

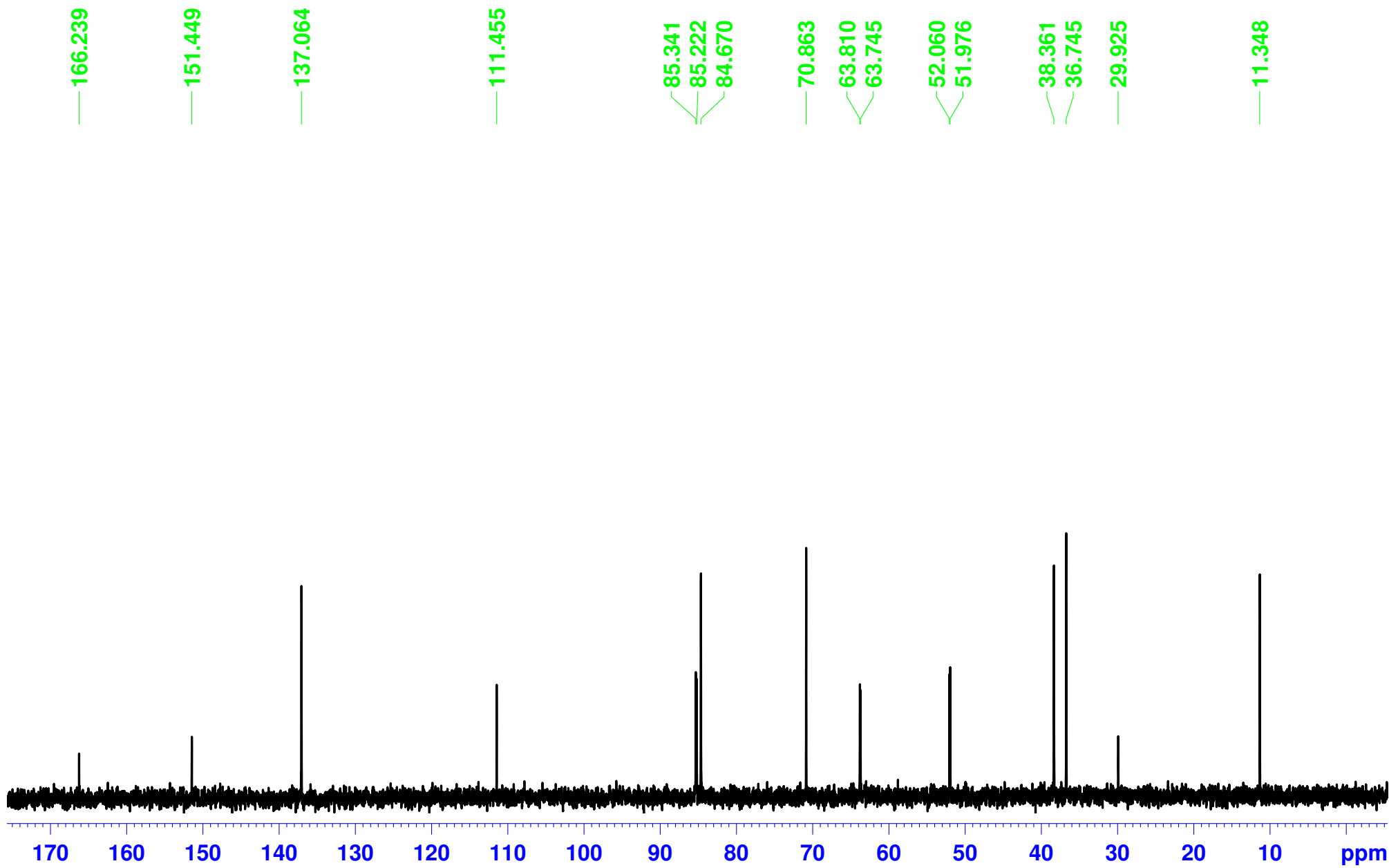
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18	¹ H and ¹³ C	S44-S45
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33	^1H , ^{13}C and ^{31}P	S80-S82
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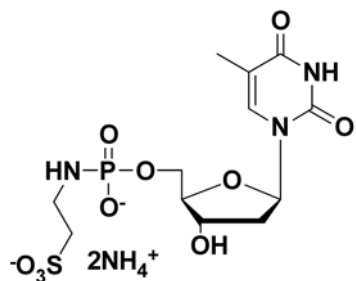
Compound 1 in D2O
1H spectrum - 300 MHz



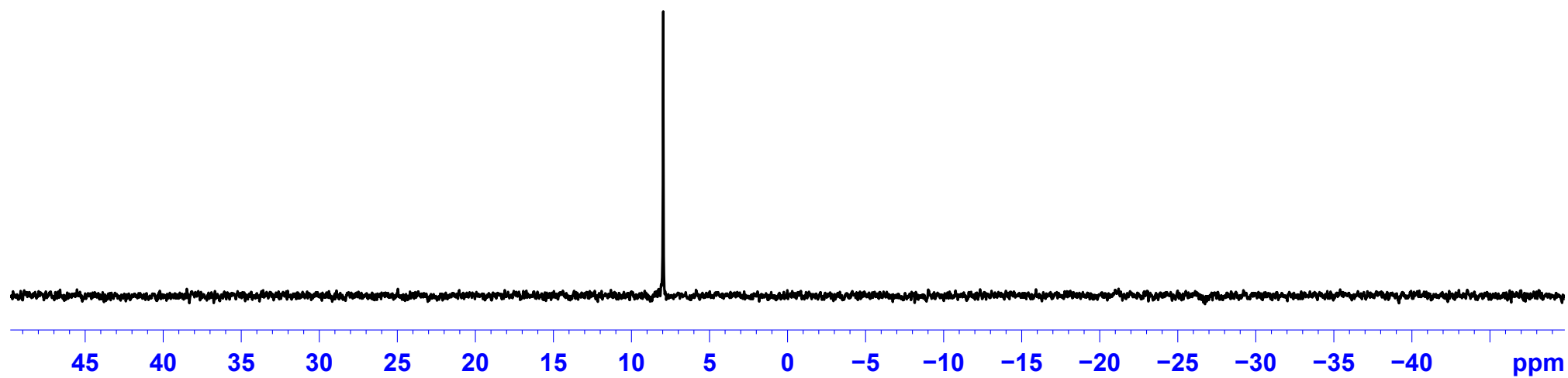
Compound 1 in D2O
13C spectrum - 75 MHz



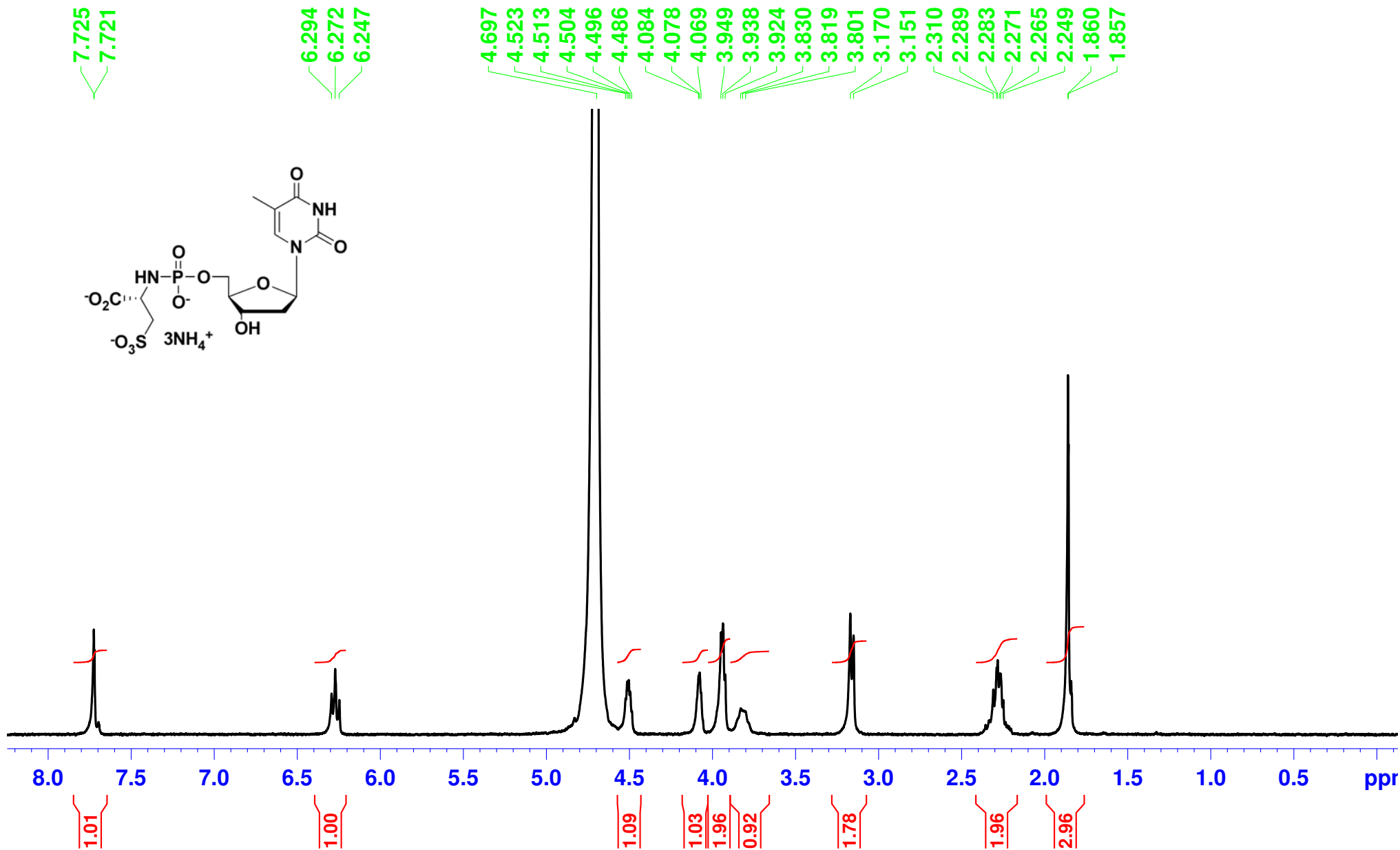
Compound 1 in D2O
31P spectrum - 121 MH



7.964



Compound 2 in D2O
1H spectrum - 300 MHz



Compound 2 in D2O
13C spectrum - 75 MHz

178.627

166.282

151.476

137.154

111.470

85.527

85.403

84.596

70.892

63.694

54.599

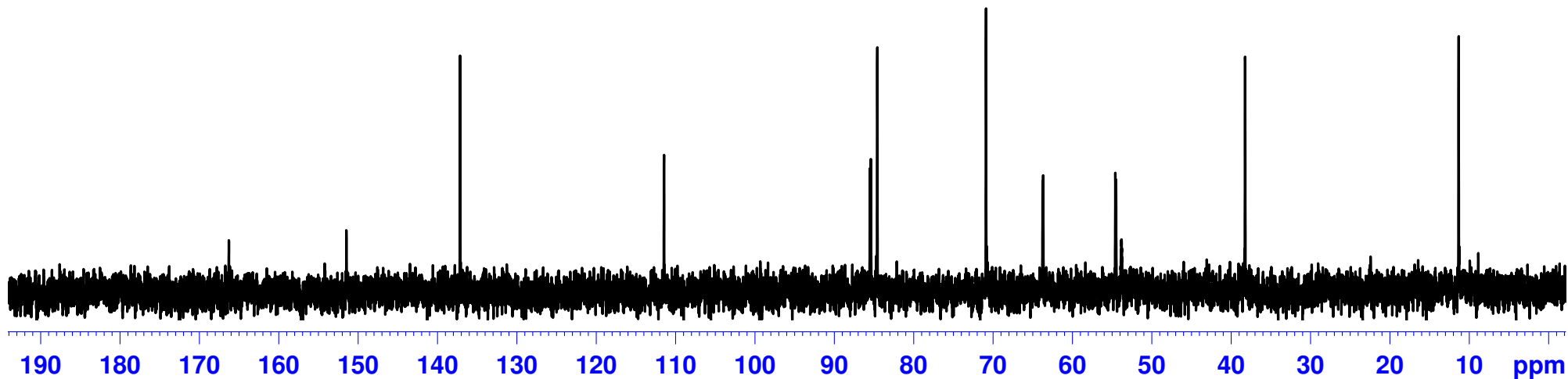
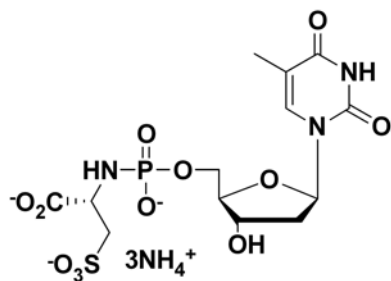
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53.857

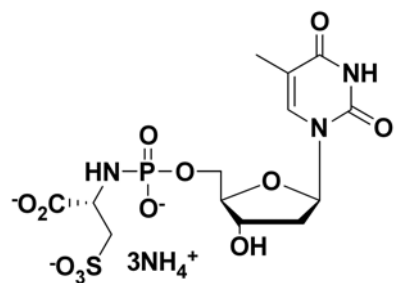
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38.248

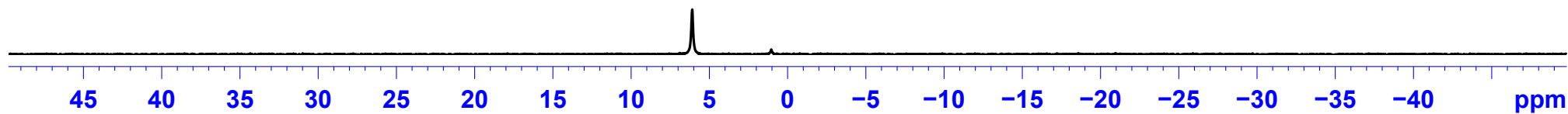
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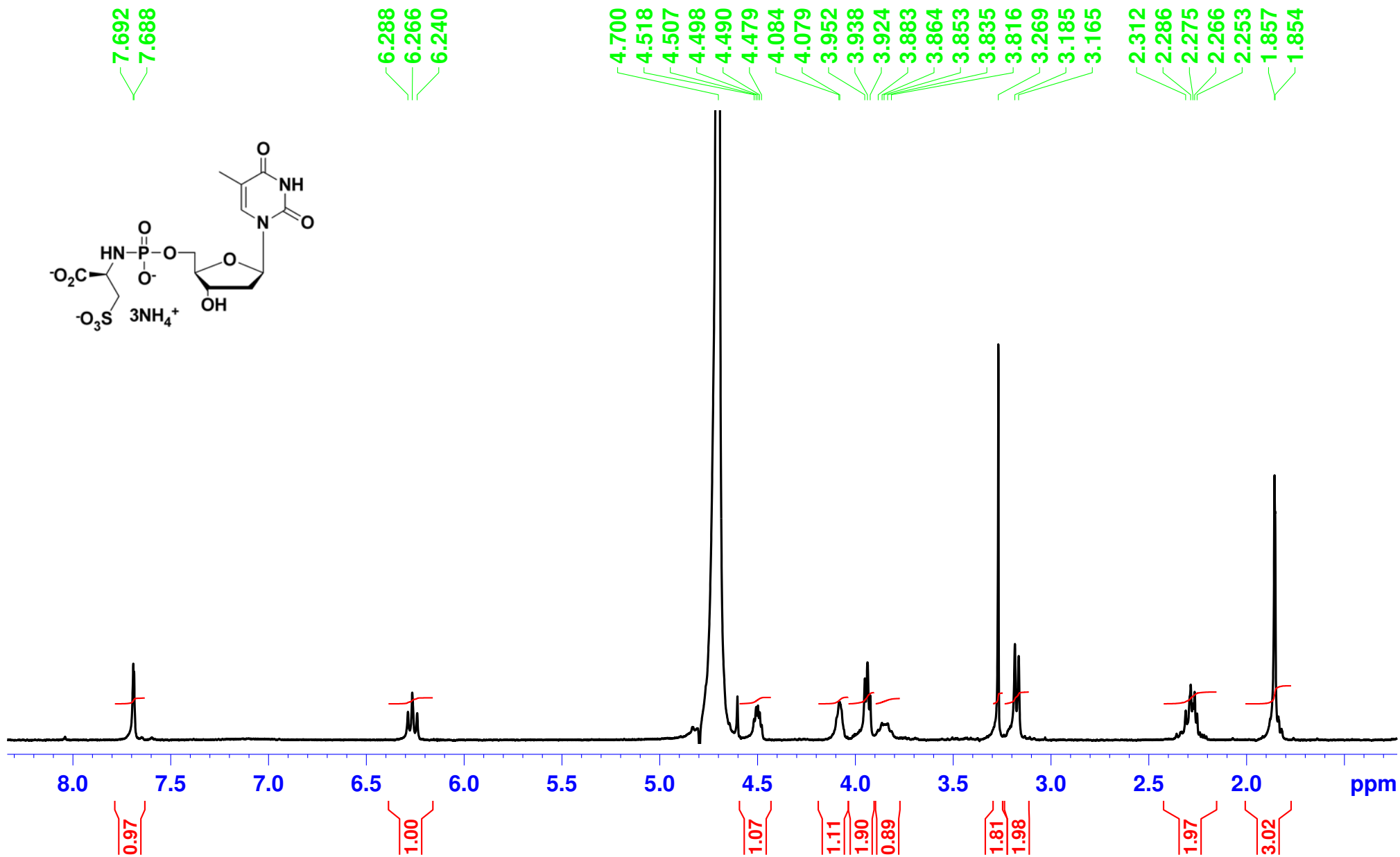
Compound 2 in D2O
31P spectrum - 121 MHz



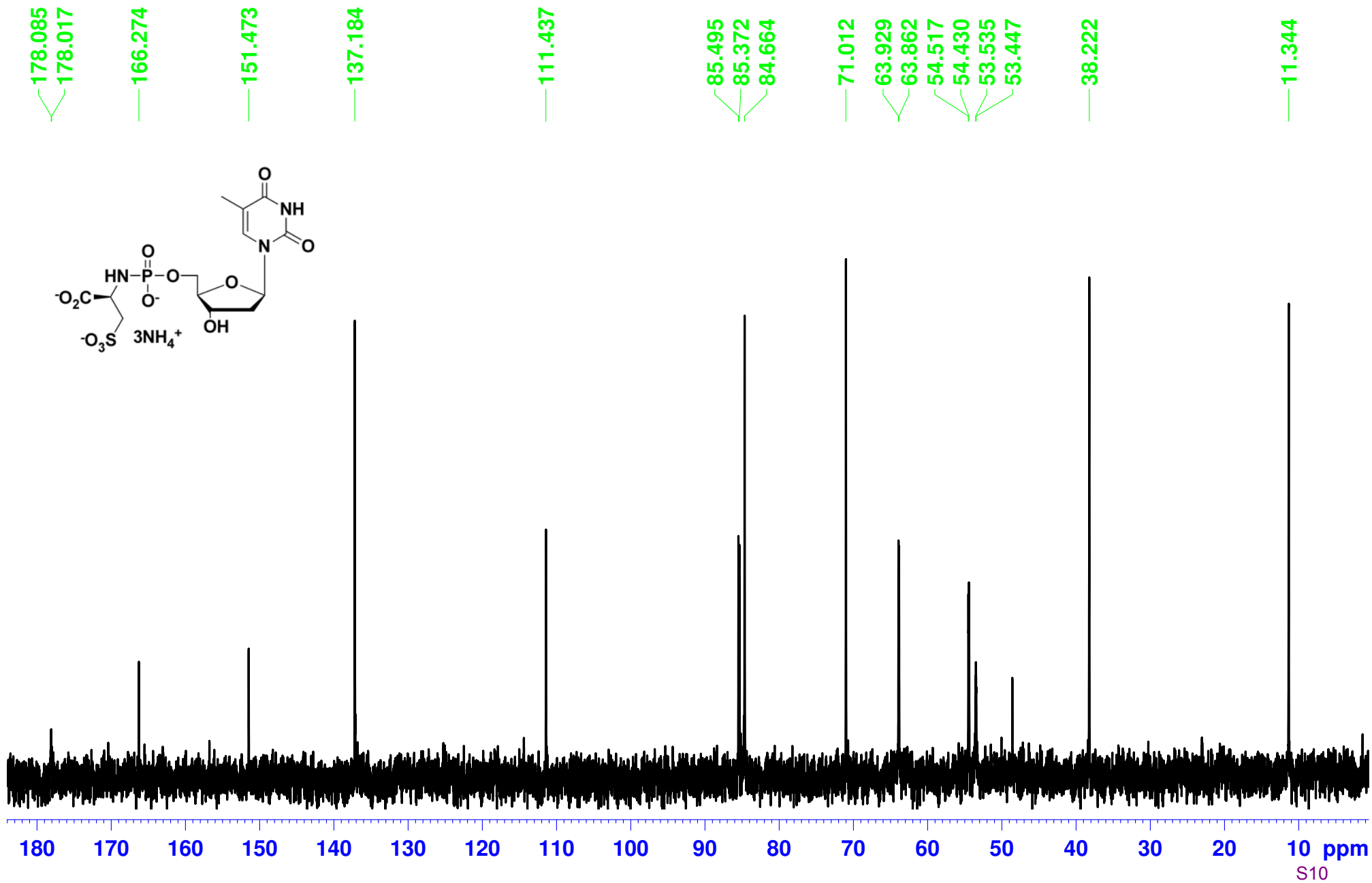
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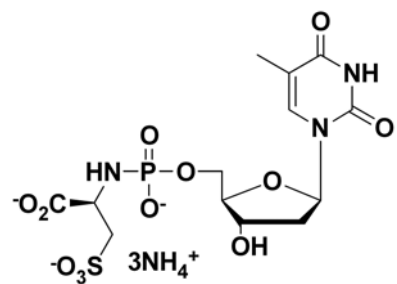
Compound 3 in D2O
1H spectrum - 300 MHz



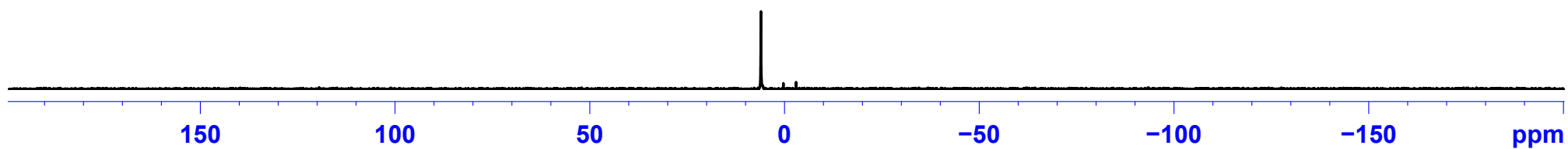
Compound 3 in D2O
13C spectrum - 75 MHz



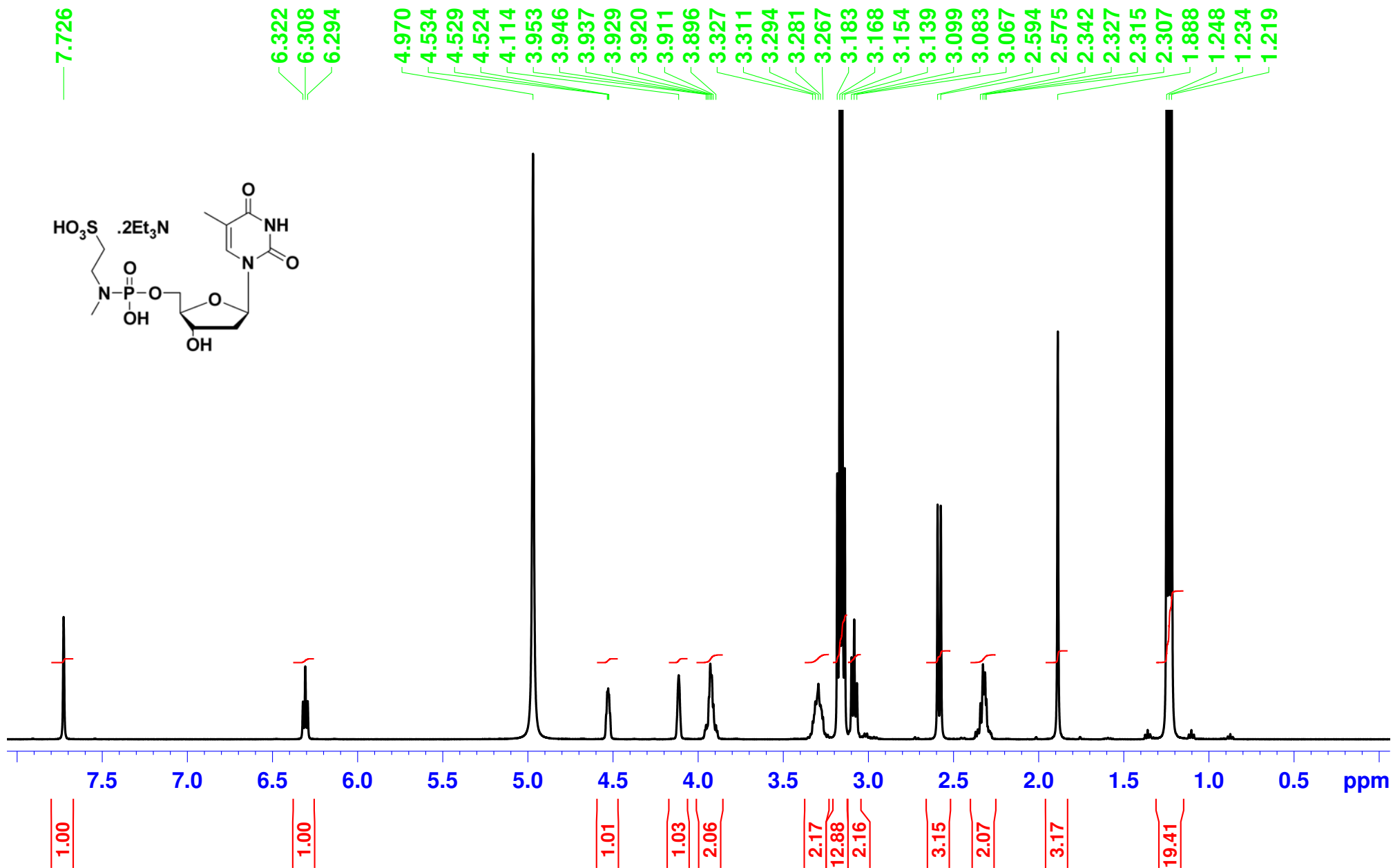
Compound 3 in D2O
31P spectrum - 121 MHz



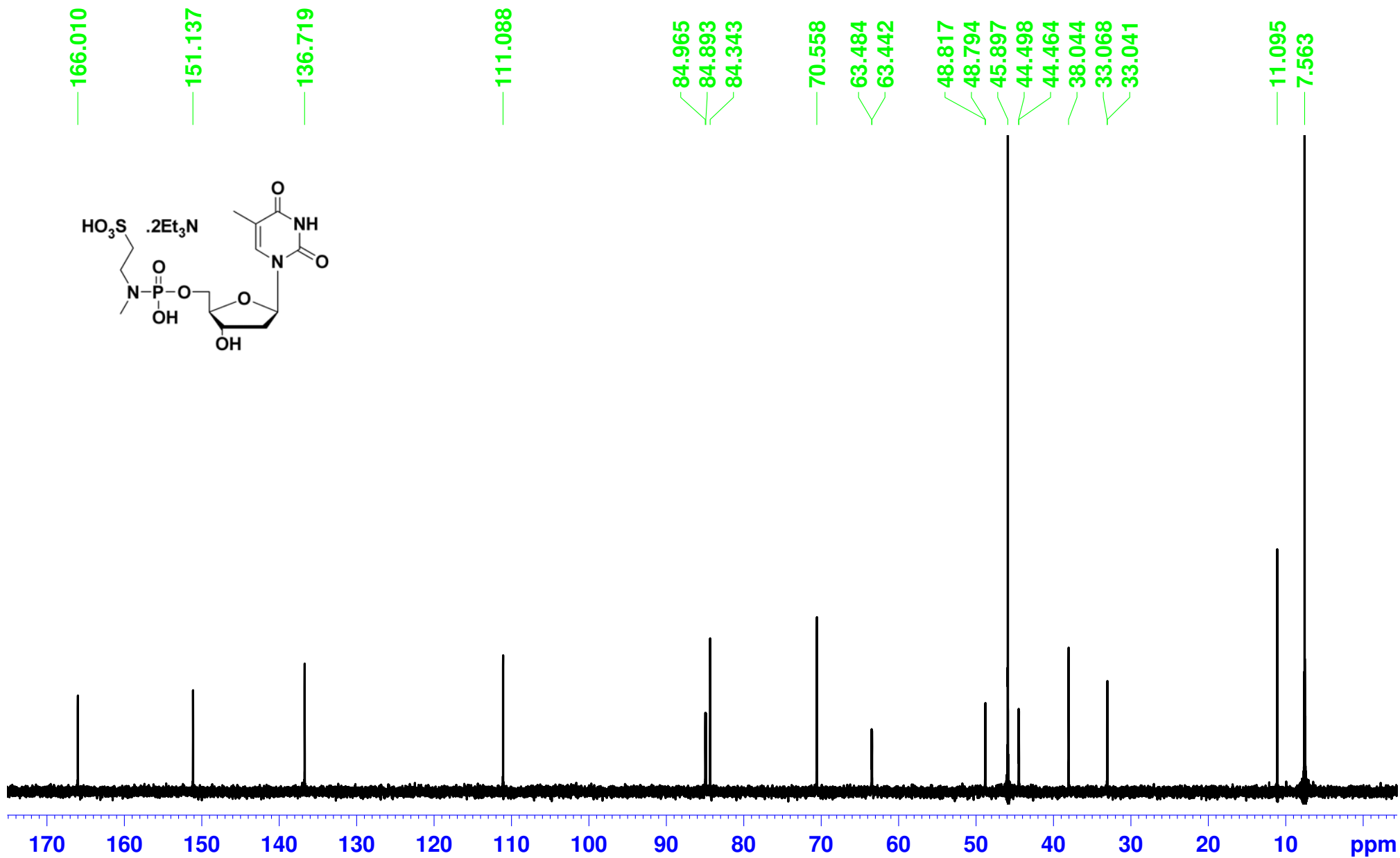
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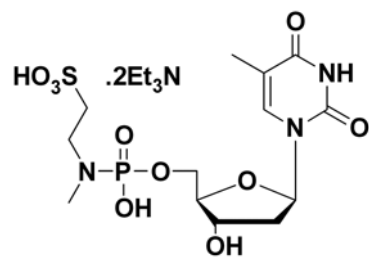
Compound 4 in D2O
1H spectrum - 500 MHz @ 6 C



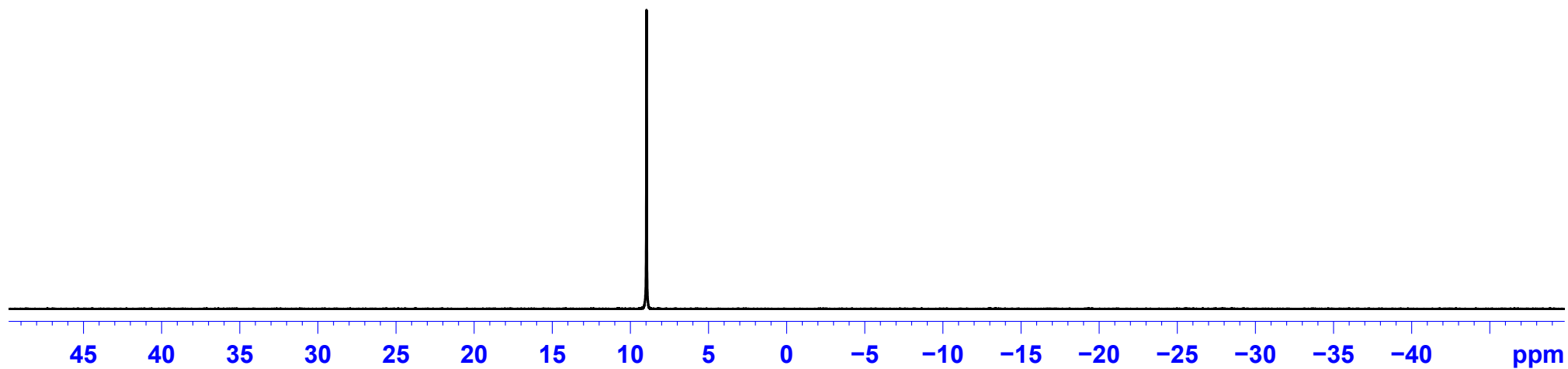
Compound 4 in D2O
13C spectrum - 125 MHz @ 6 C



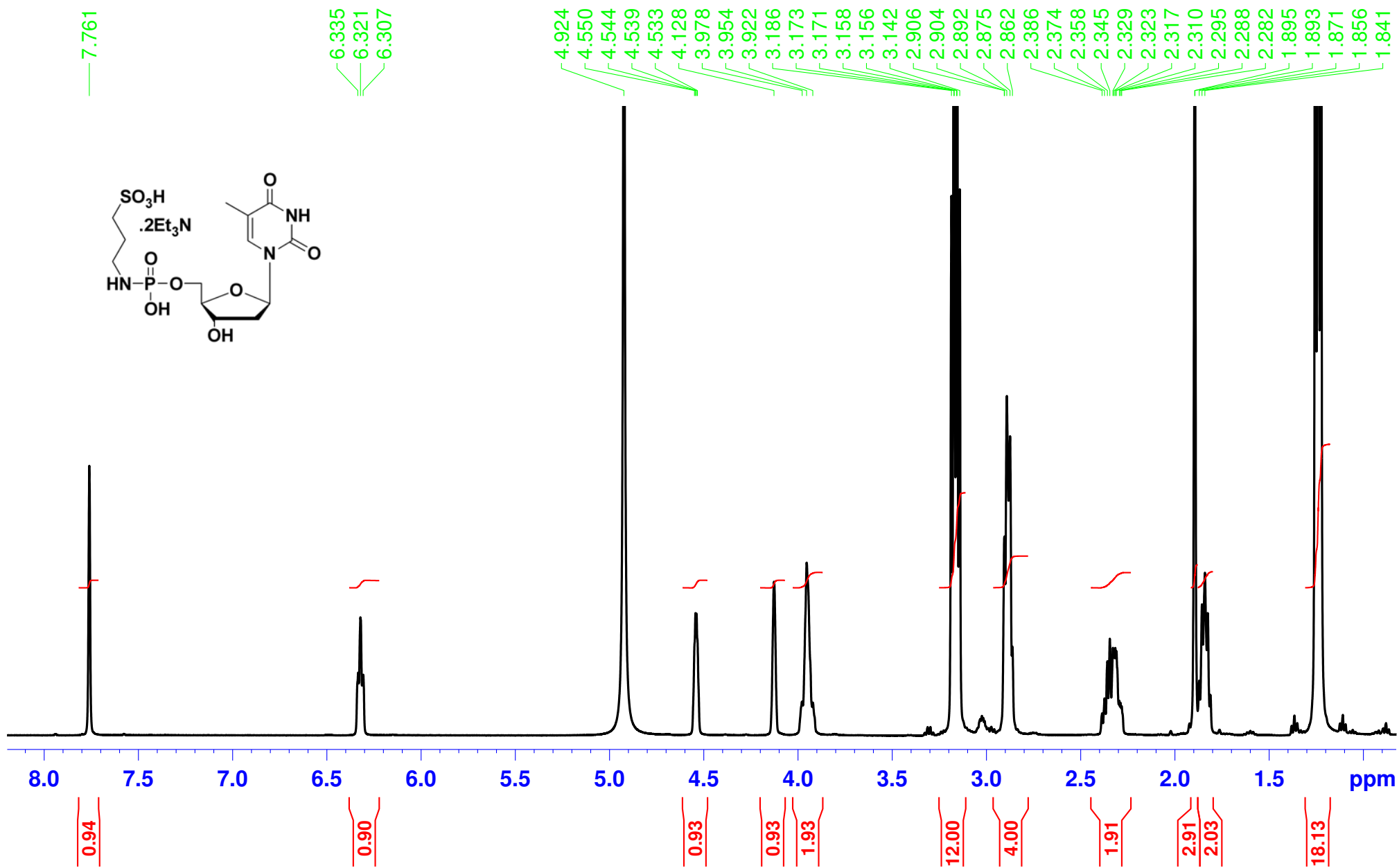
Compound 4 in D2O
31P spectrum - 202 MHz @ 6 C



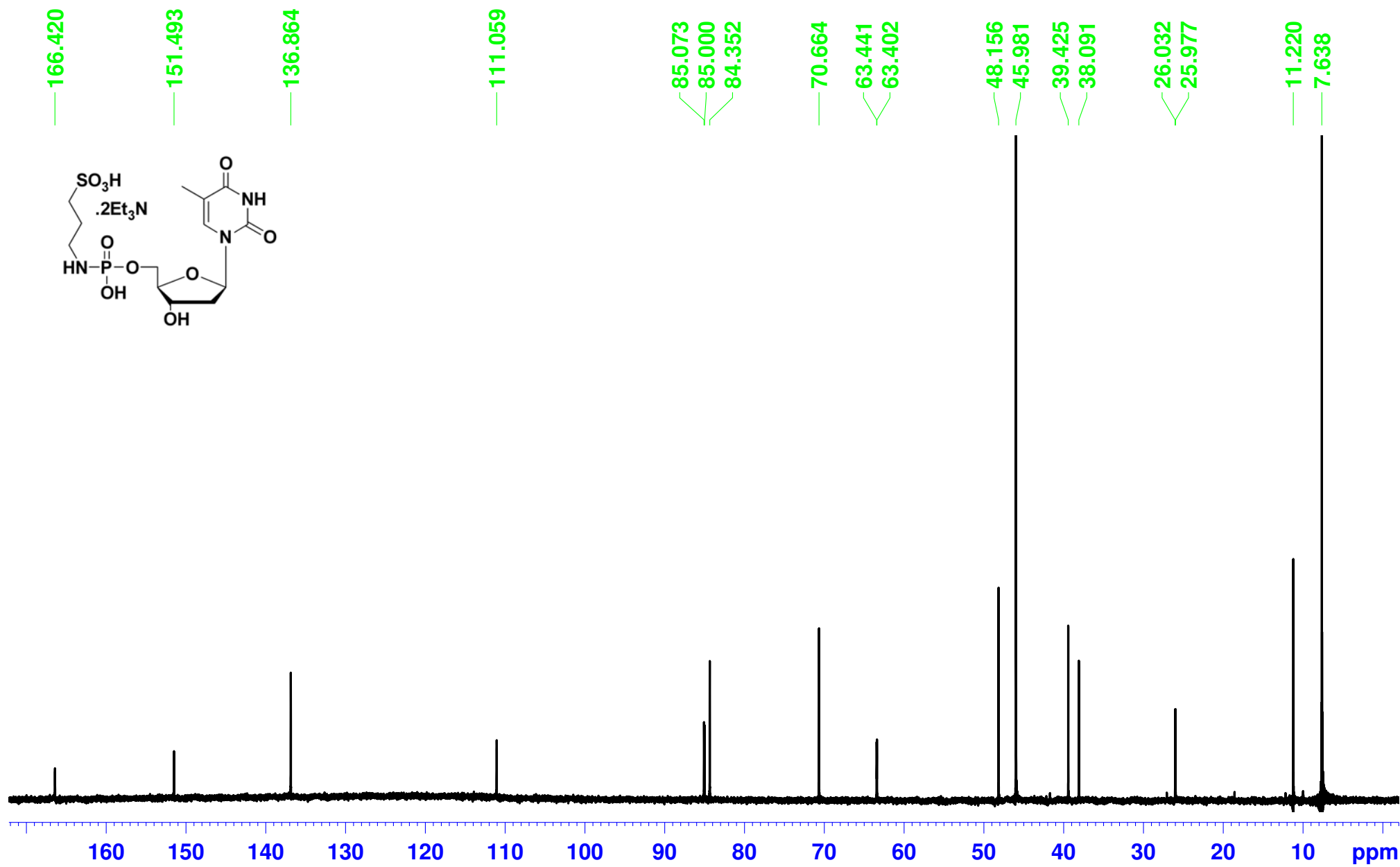
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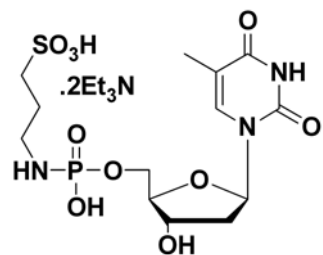
Compound 5 in D2O
1H spectrum - 500 MHz @ 10C



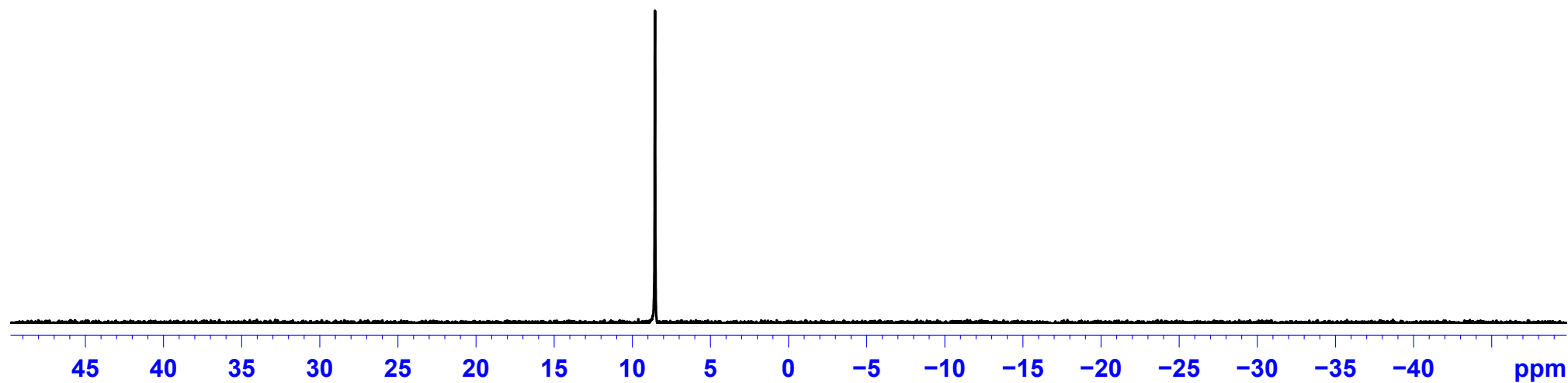
Compound 5 in D2O
13C spectrum - 125 MHz @ 10C



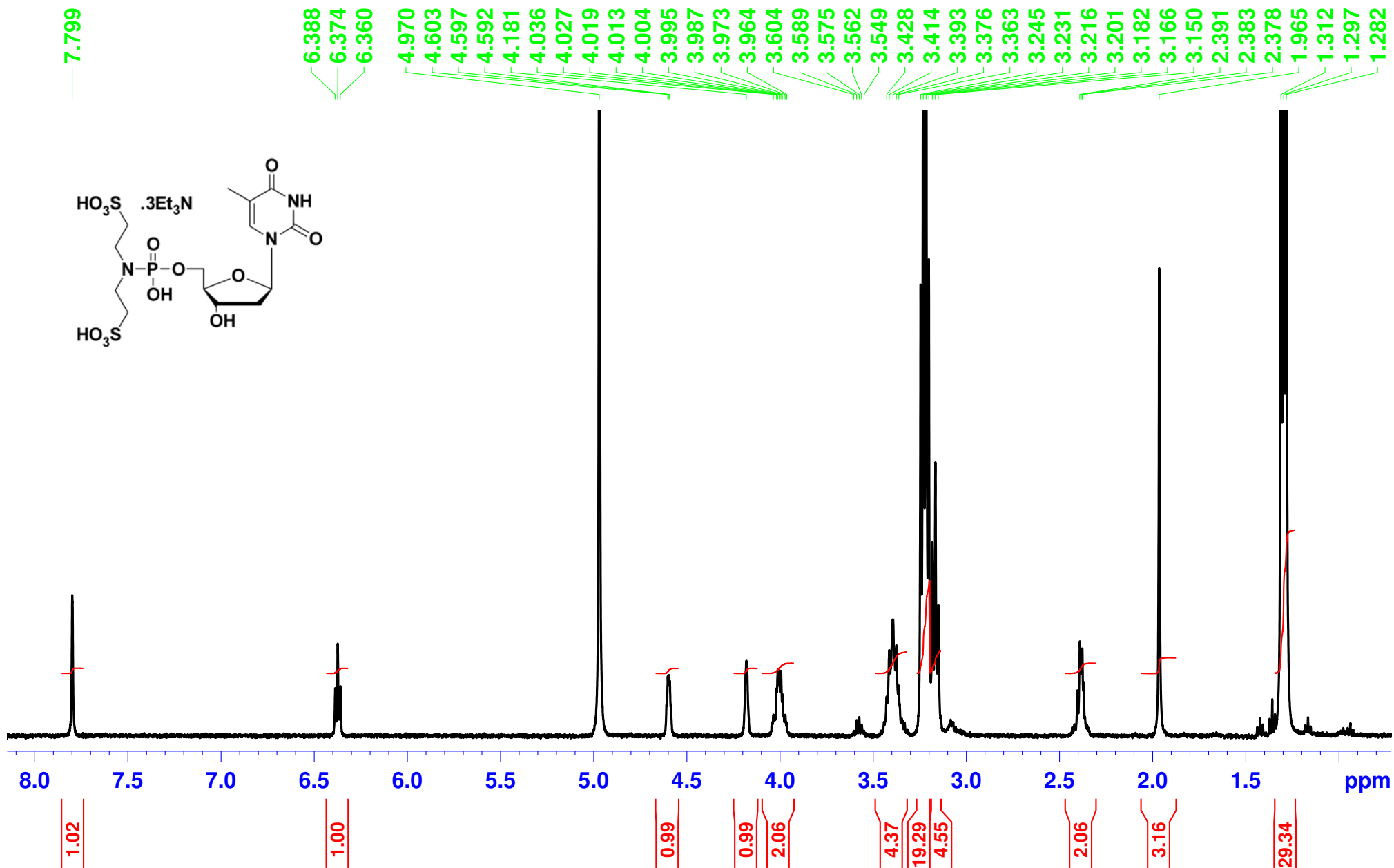
Compound 5 in D2O
31P spectrum - 202 MHz @ 10C



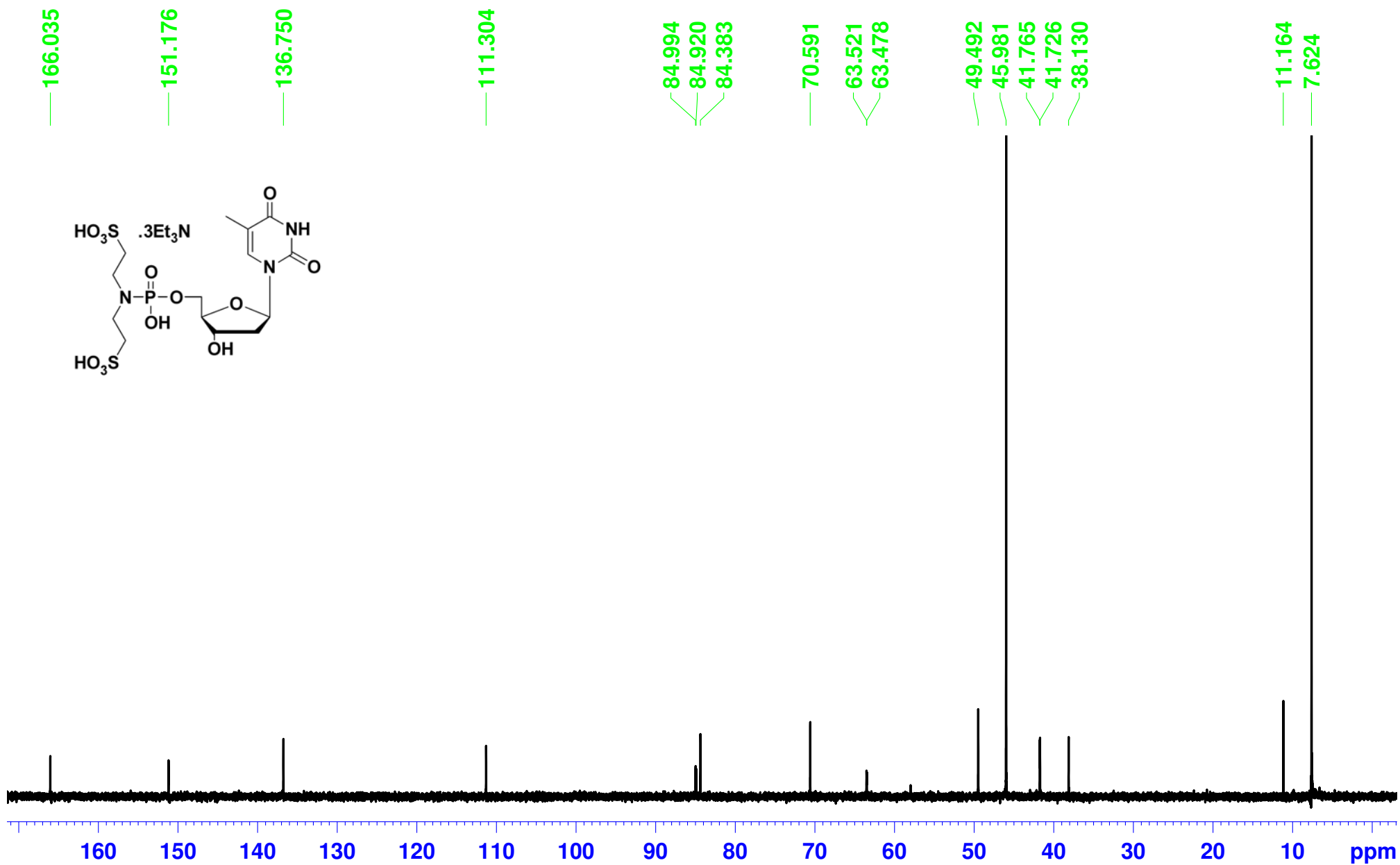
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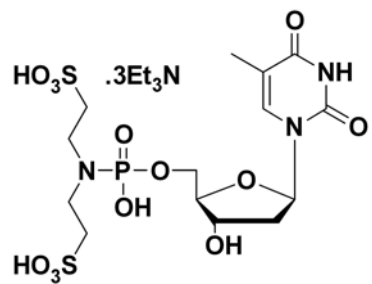
Compound 6 in D2O
1H spectrum - 500 MHz @ 6C



Compound 6 in D2O
13C spectrum - 125 MHz @ 6C



Compound 6 in D2O
31P spectrum - 202 MHz @ 6C

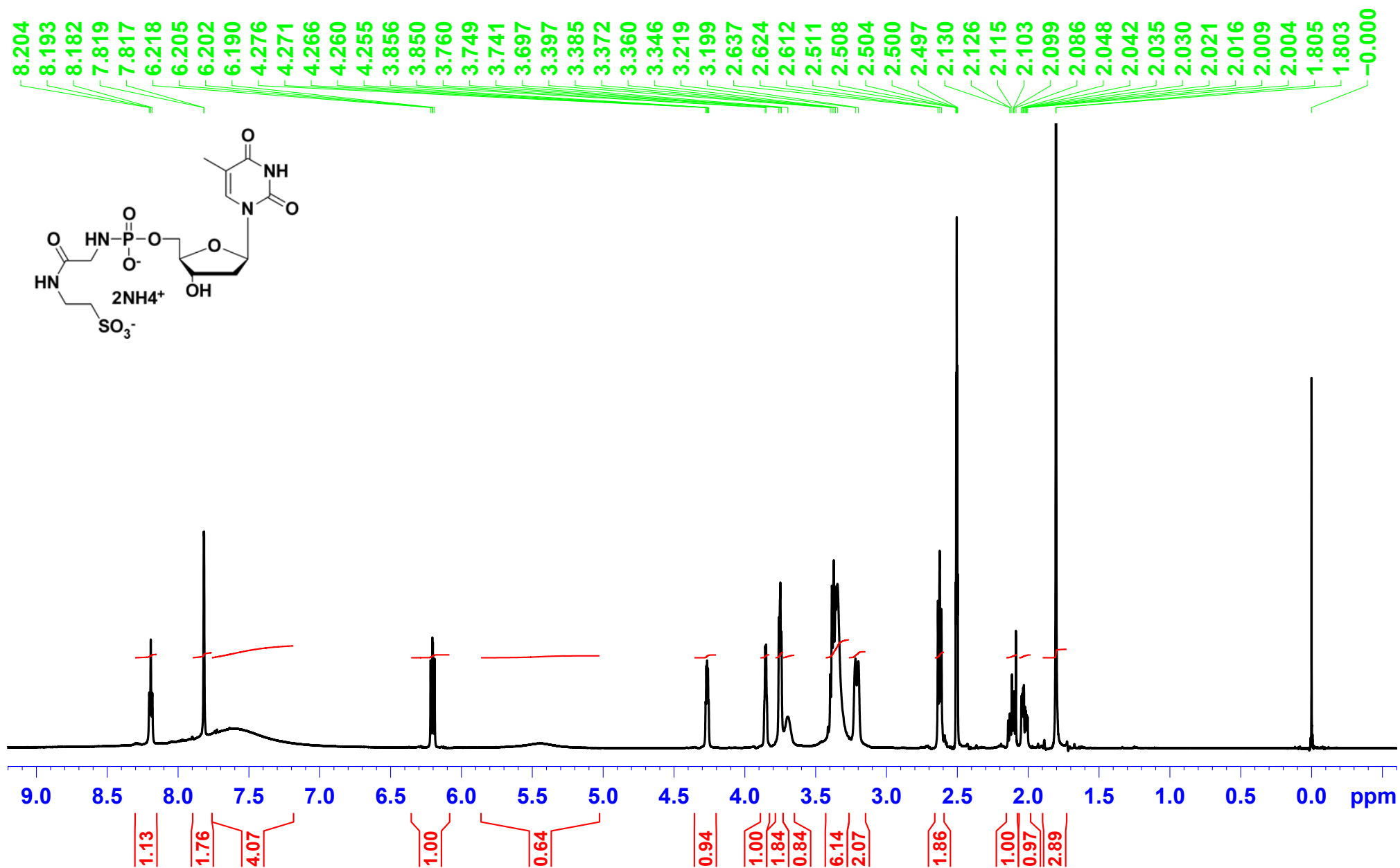


7.382



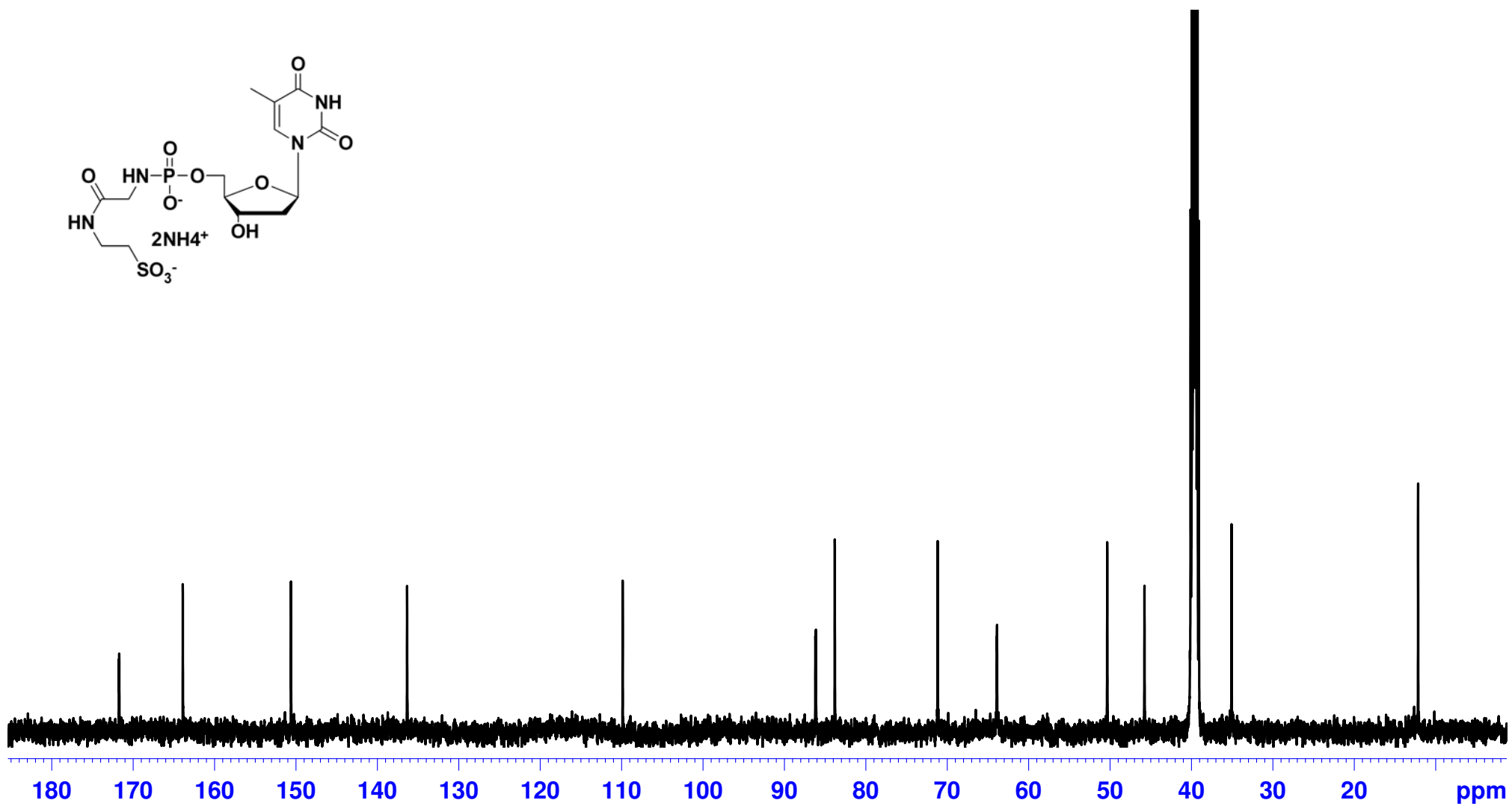
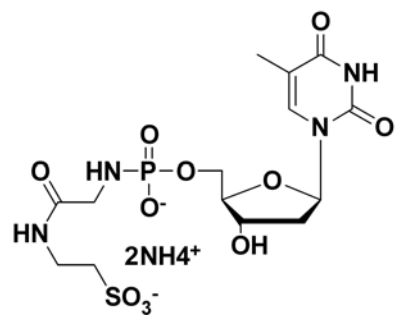
45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 ppm

Compound 16a in DMSO-d6
1H spectrum - 500 MHz @ 20C

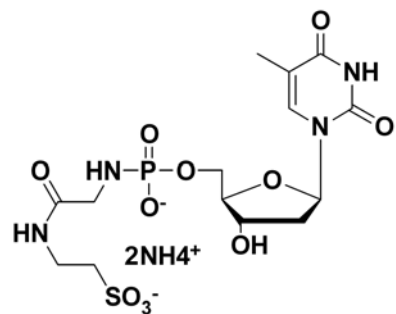


Compound 16a in DMSO-d6
13C spectrum - 125 MHz @ 20 C

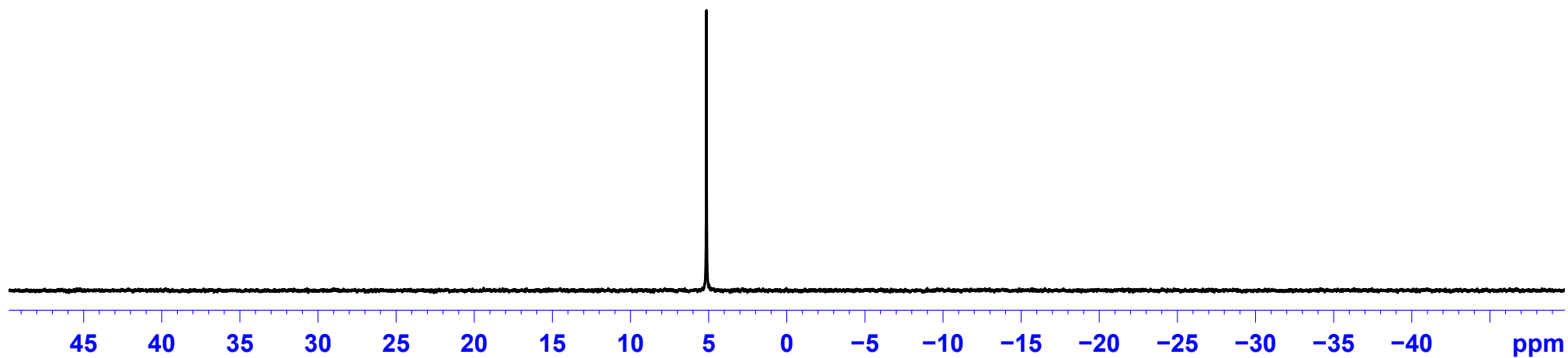
171.768
171.719
163.908
150.621
136.356
109.875
86.200
86.138
83.816
71.182
63.924
63.885
50.350
45.775
40.100
39.933
39.766
39.599
39.432
39.265
39.099
35.077
12.158



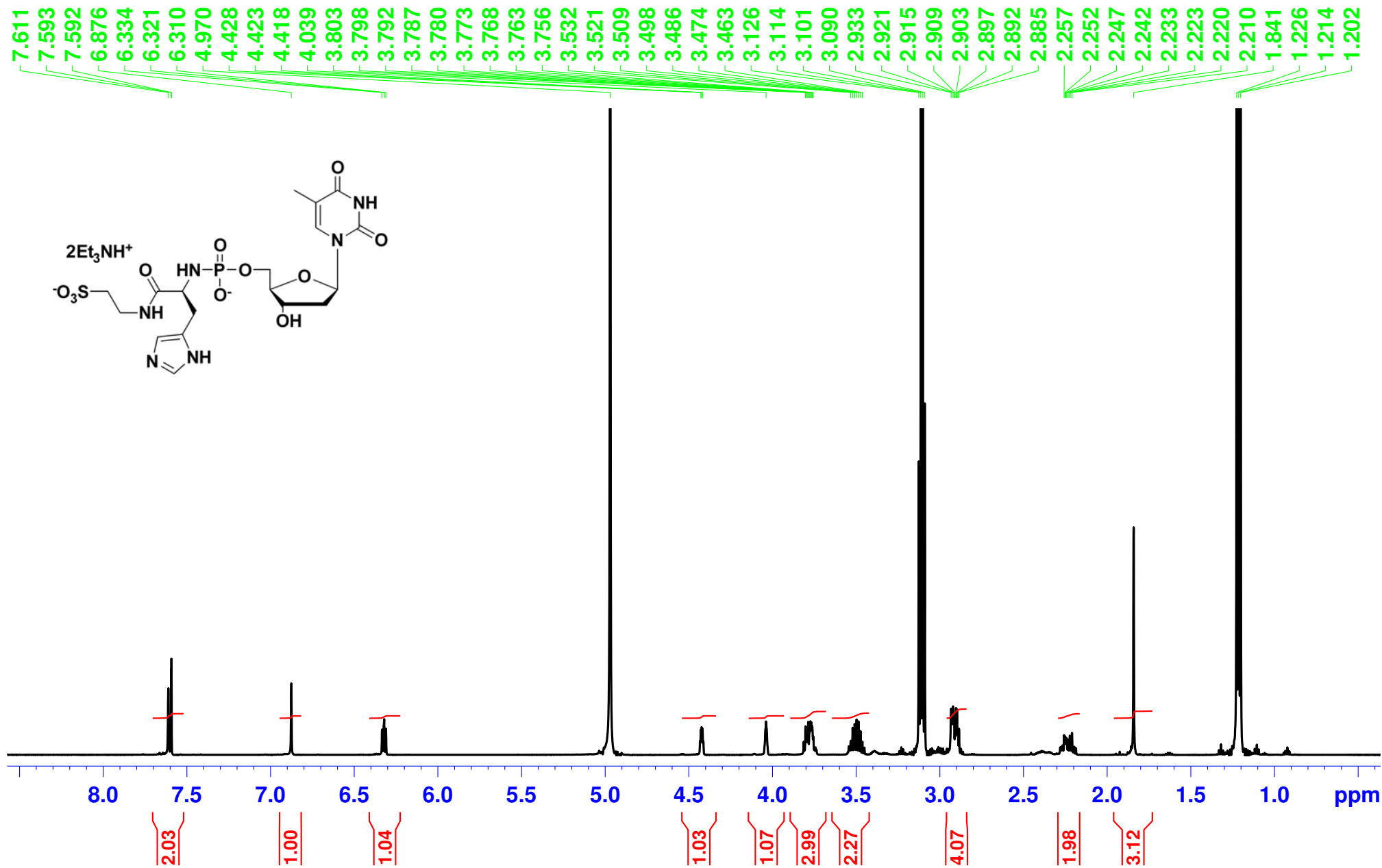
Compound 16a in DMSO-d6
31P spectrum - 202 MHz @ 20C



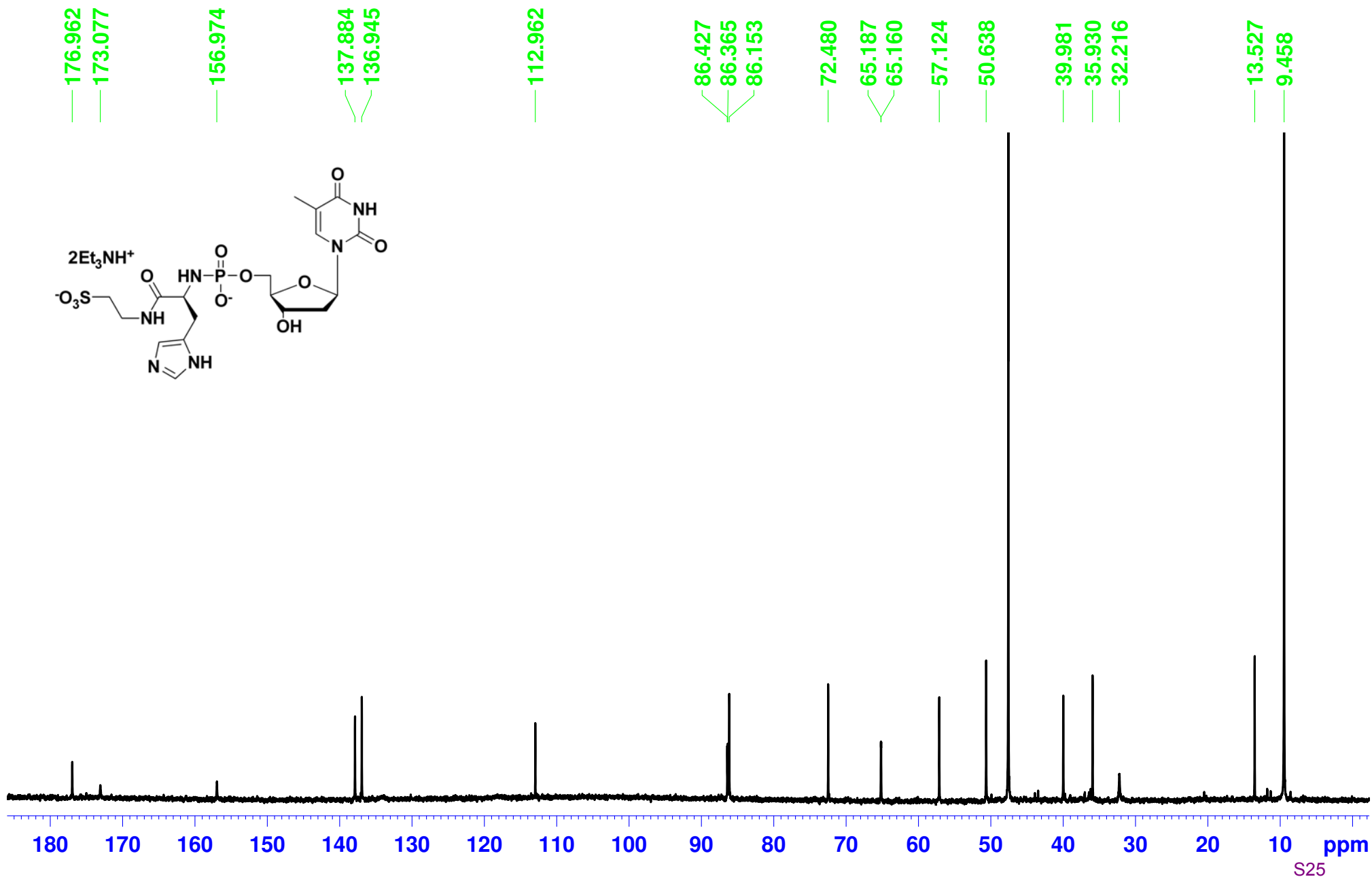
5.138



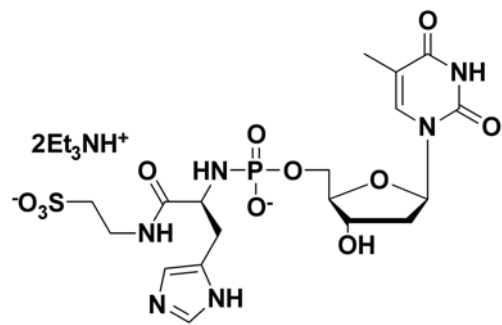
Compound 8 in D2O
1H spectrum - 600 MHz @ 25 C



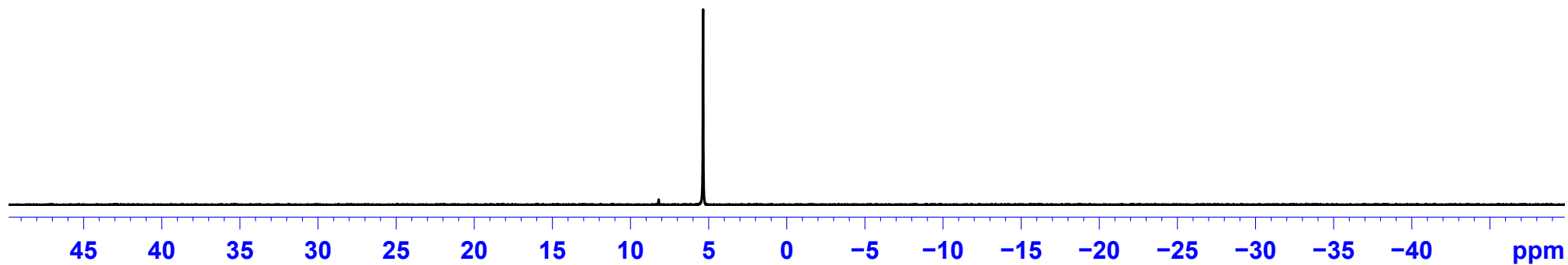
Compound 8 in D2O
13C spectrum - 150 MHz @ 25 C



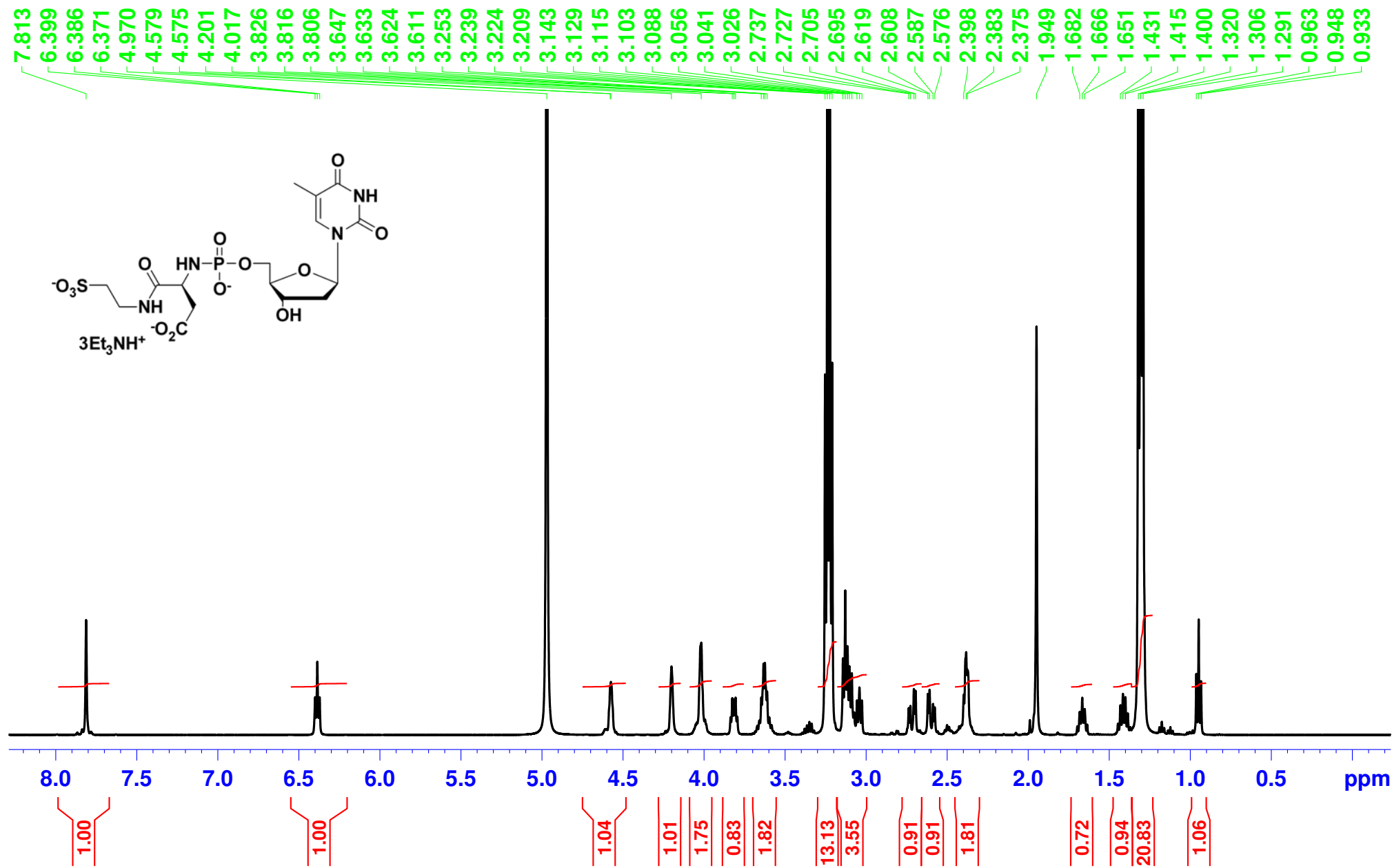
Compound 8 in D2O
31P spectrum - 202 MHz @ 6 C



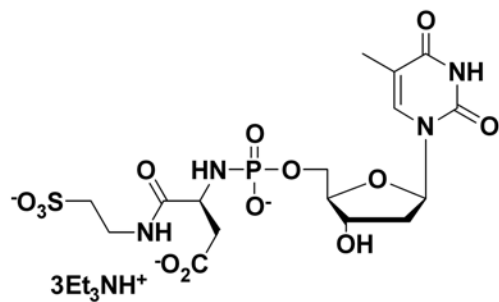
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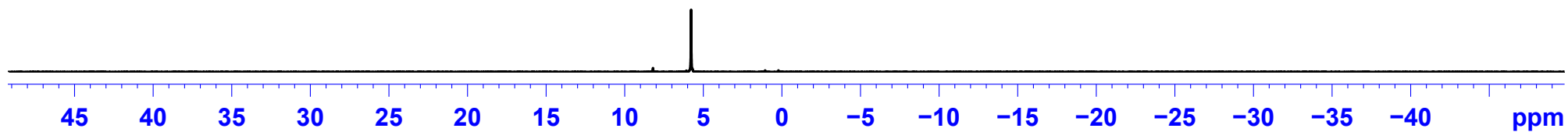
Compound 9 in D2O
H1 spectrum - 500 MHz @ 6 C



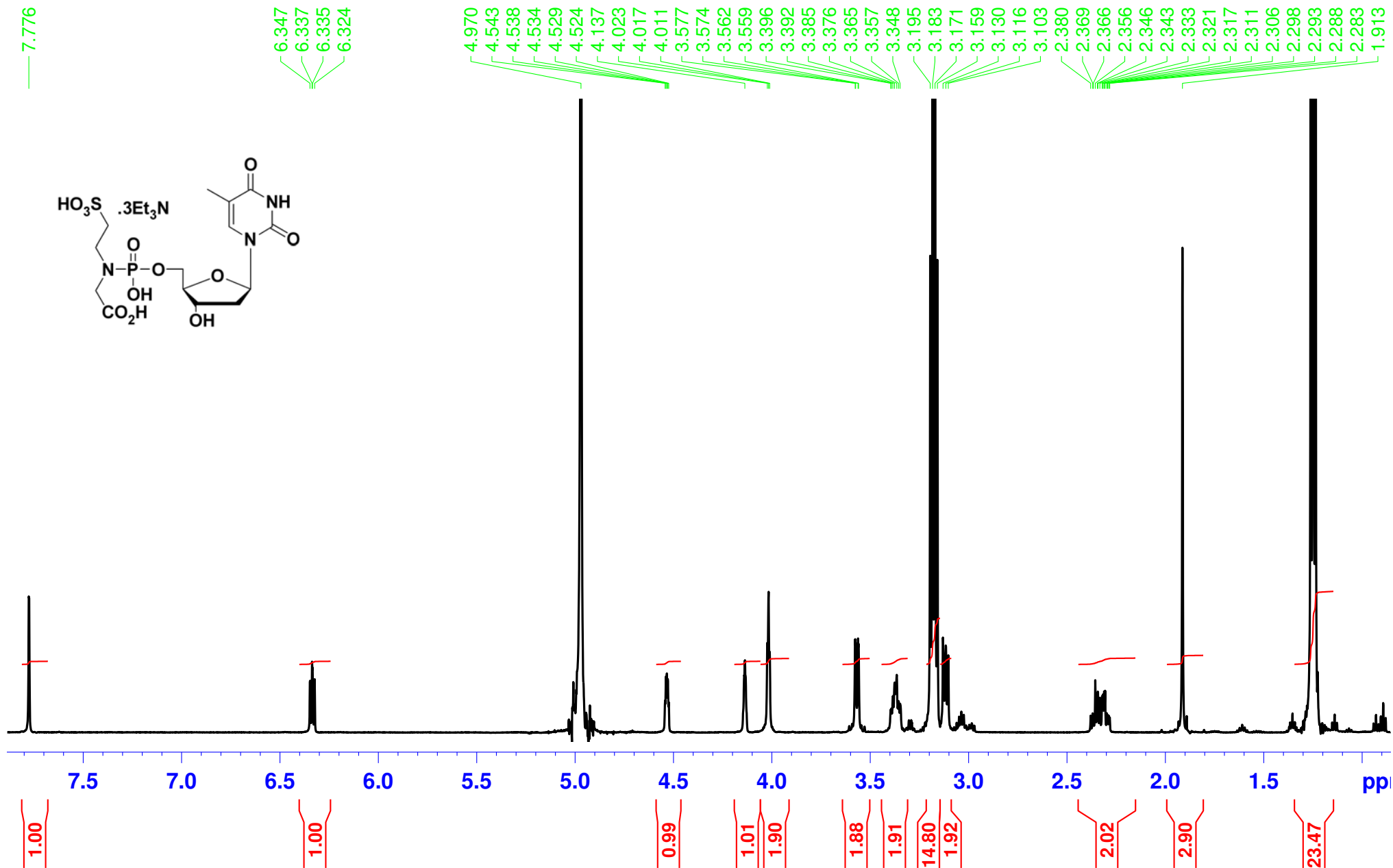
Compound 9 in D2O
31P spectrum - 202 MHz @ 6 C



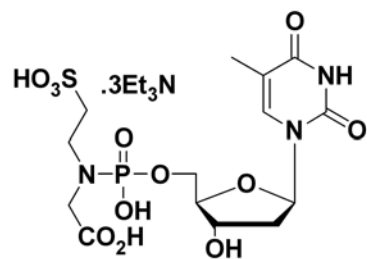
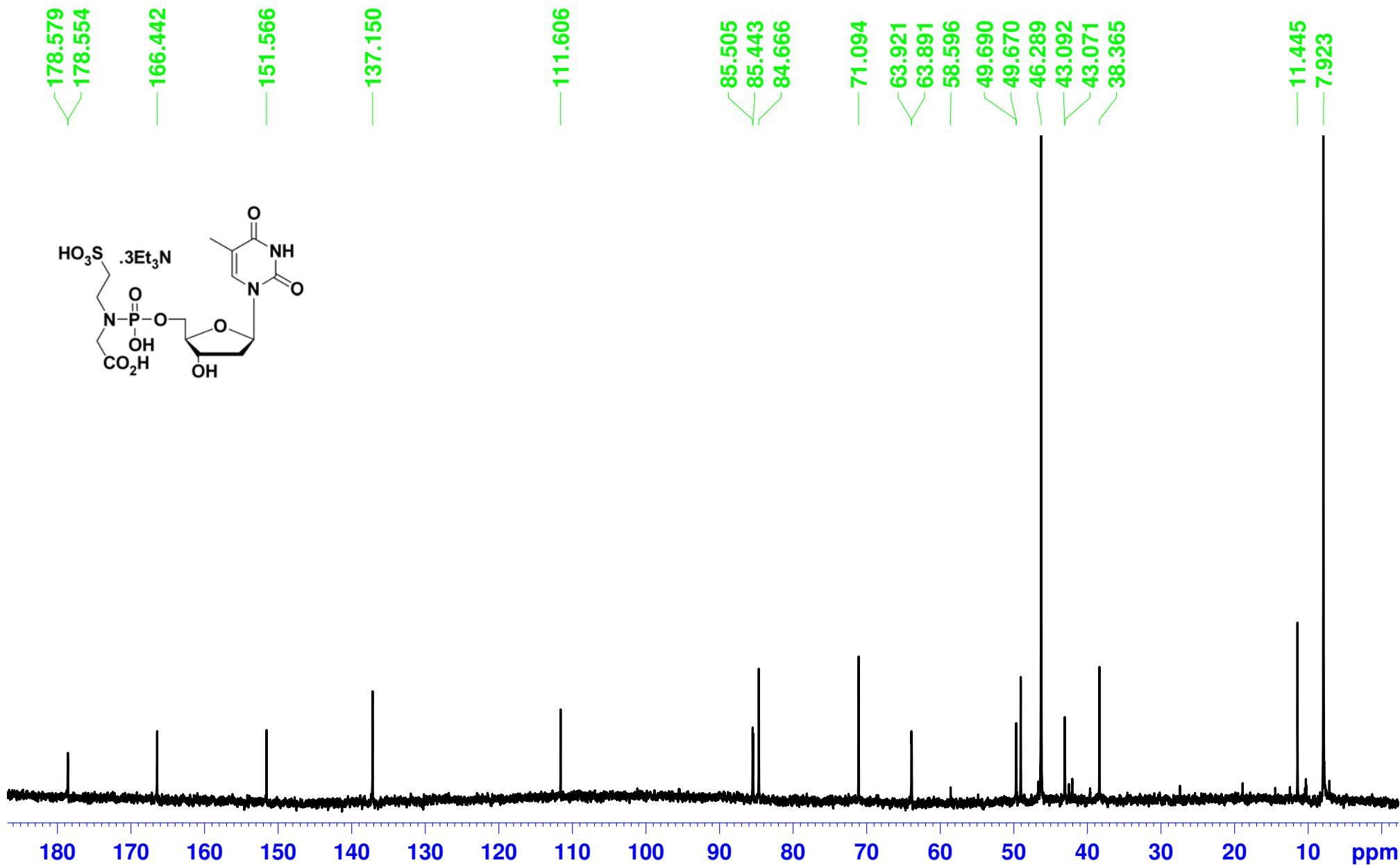
— 5.781



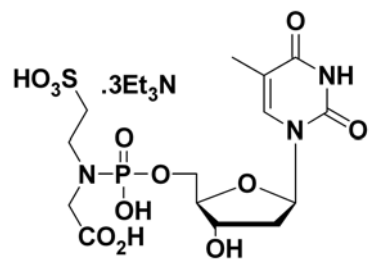
Compound 10 in D2O
1H spectrum - 600 MHz @ 6C



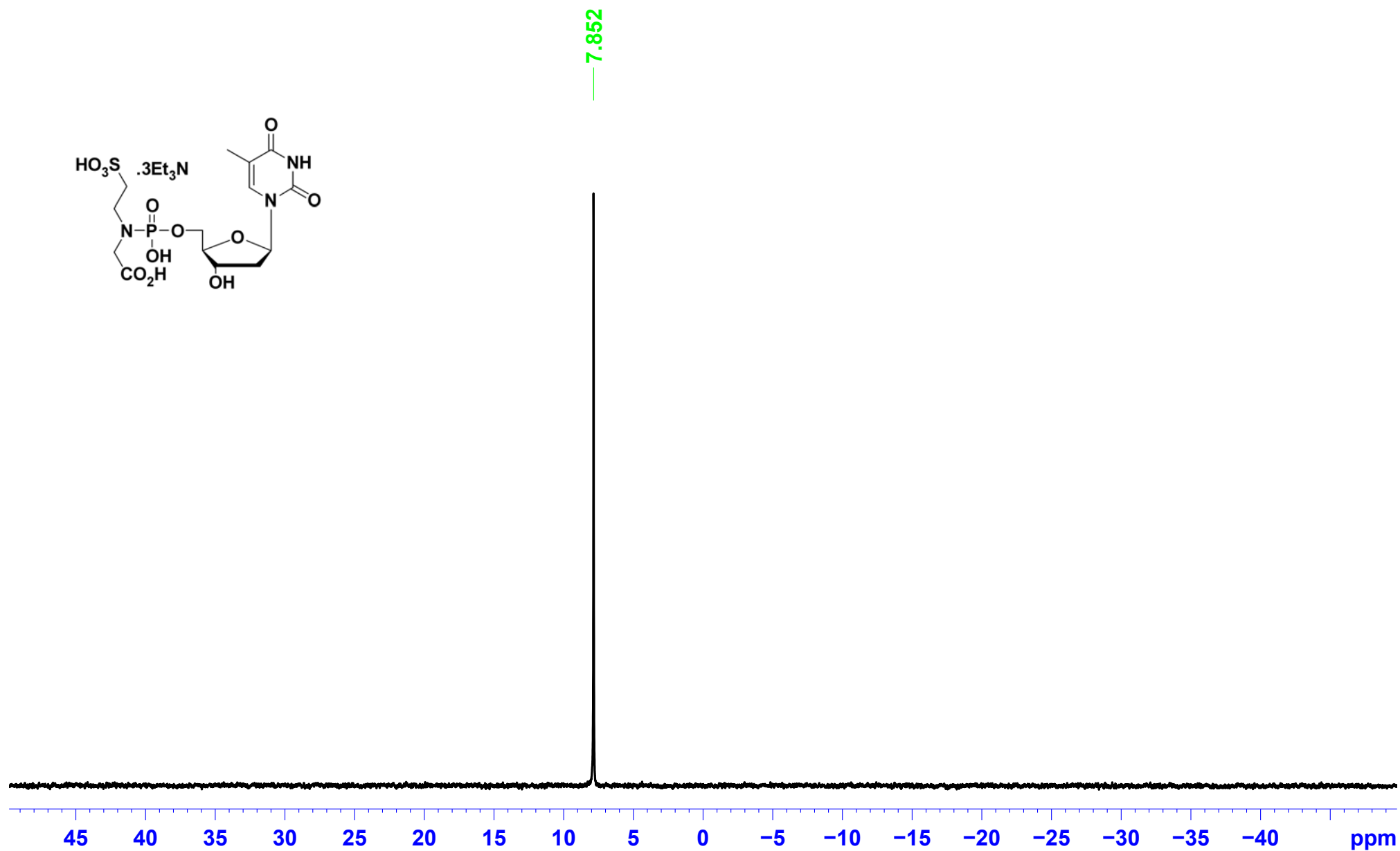
Compound 10 in D2O
13C spectrum - 150 MHz @ 6C



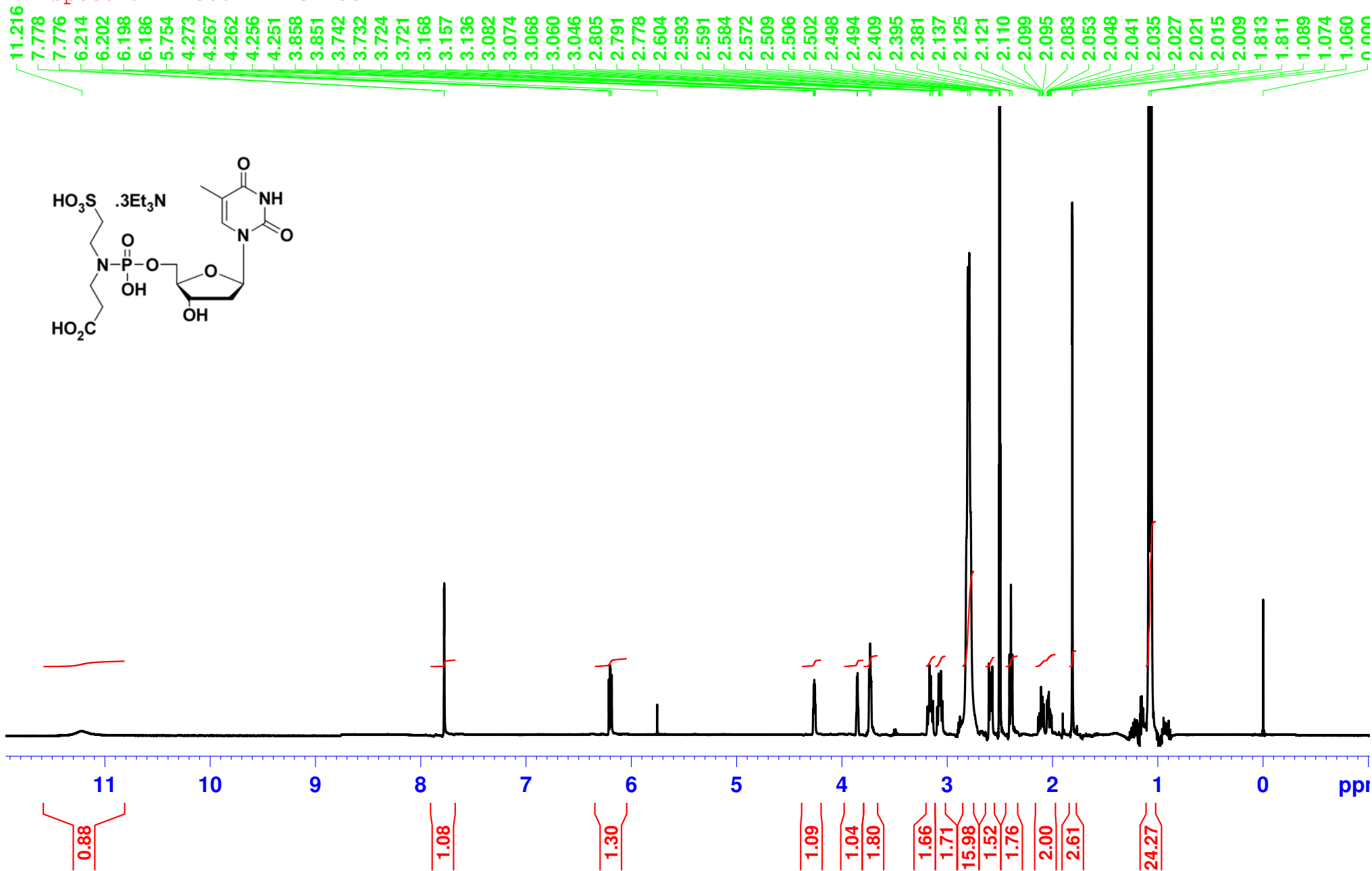
Compound 10 in D2O
31P spectrum - 202 MHz @ 6C



7.852



Compound 11 in DMSO-d6
1H spectrum - 500 MHz @ 25C



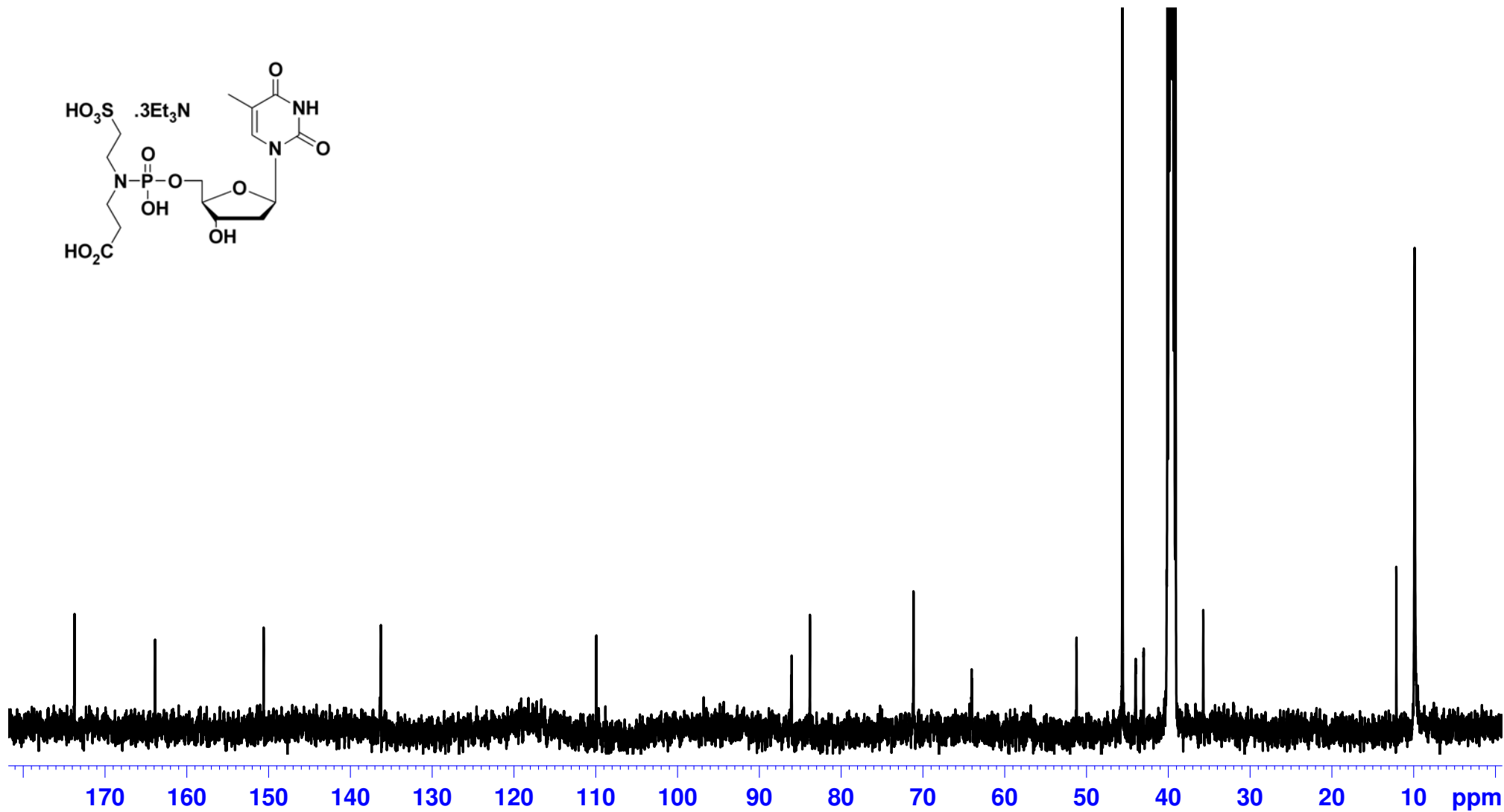
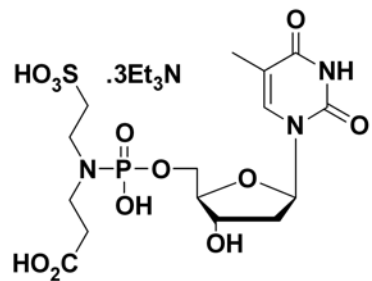
Compound 11 in DMSO-d6
13C spectrum - 125 MHz @ 25C

173.717
163.865
150.591
136.250

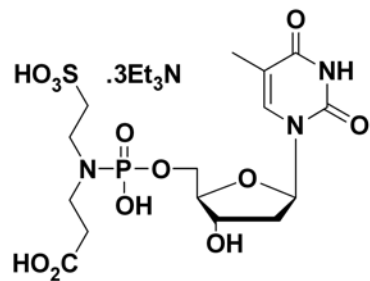
109.932

86.100
86.040
83.811

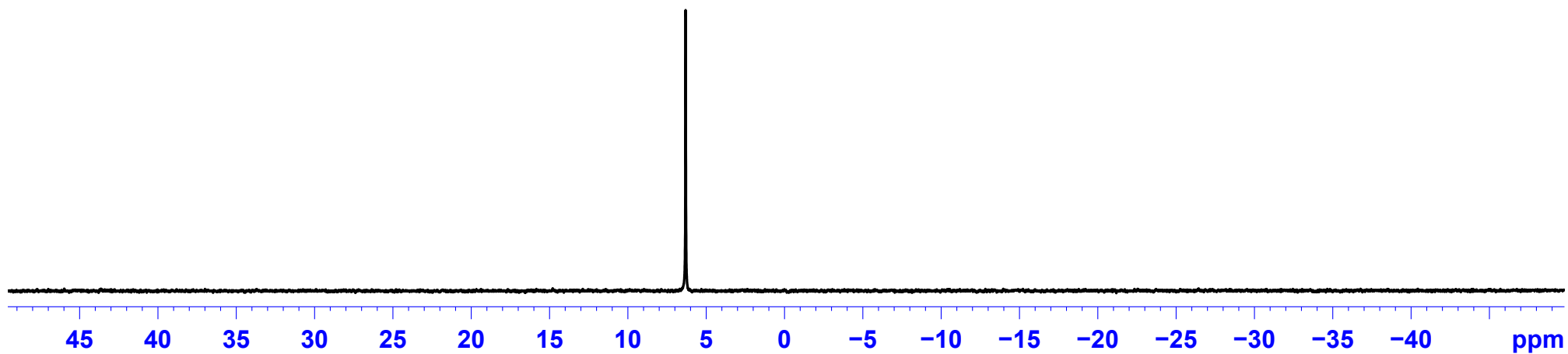
71.146
64.040
63.999
51.215
45.595
44.005
43.981
43.025
42.999
40.101
39.934
39.767
39.600
39.434
39.267
39.100
35.719
12.115
9.873



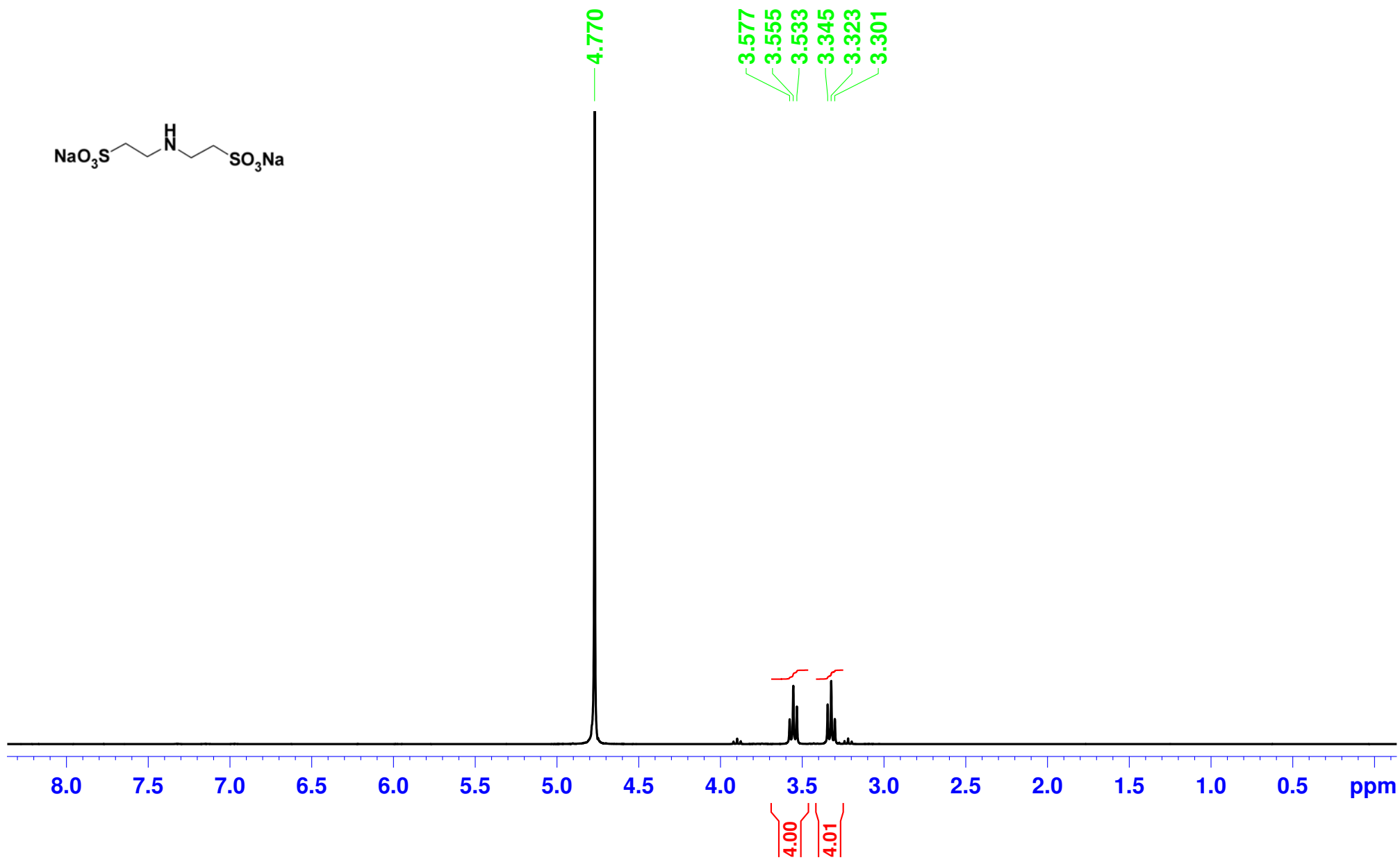
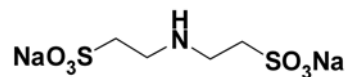
Compound 11 in DMSO-d6
31P spectrum - 125 MHz @ 25C



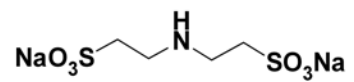
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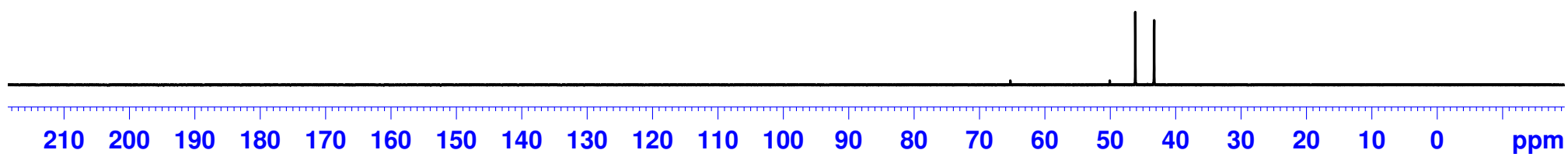
Compound 14 in D2O
1H spectrum - 300 MHz



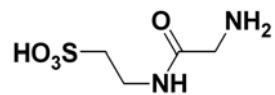
Compound 14 in D2O
13C spectrum - 75 MHz



46.179
43.300



Compound 16a in D2O
1H spectrum - 300 MHz



4.790

3.824

3.688

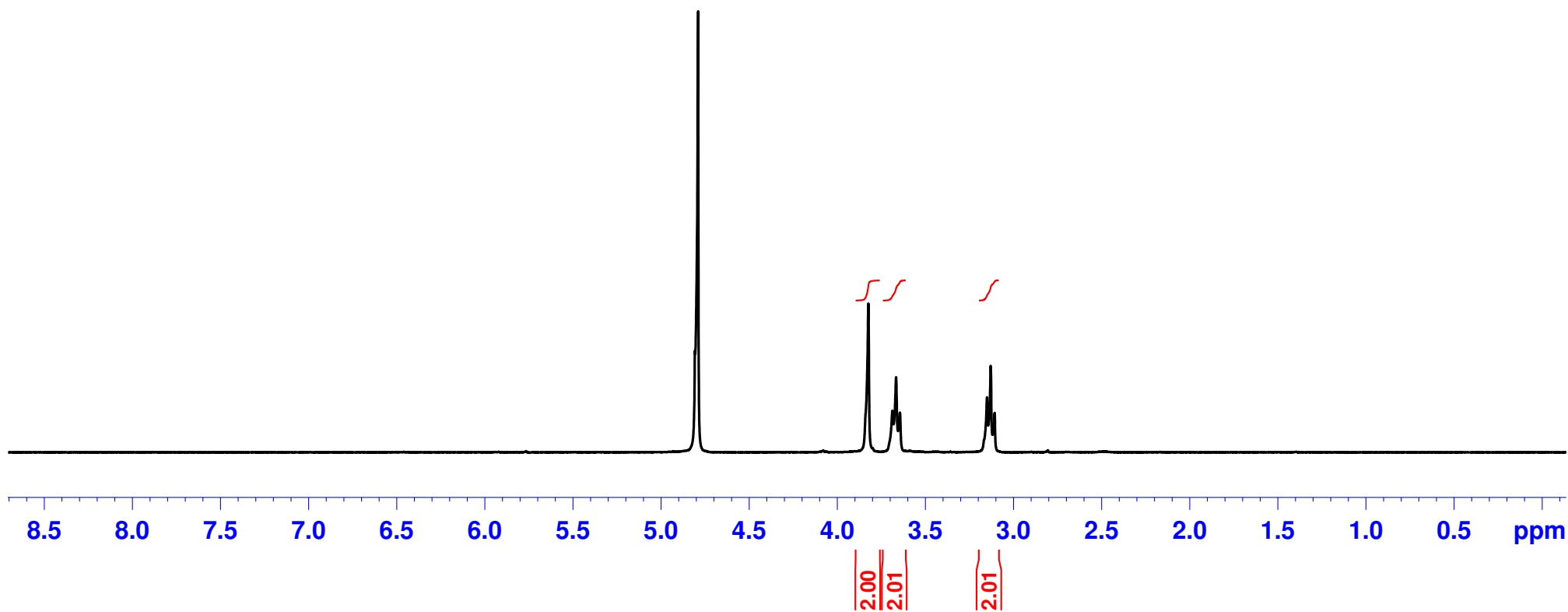
3.667

3.645

3.151

3.130

3.107



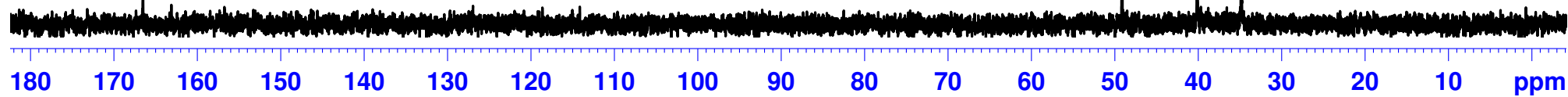
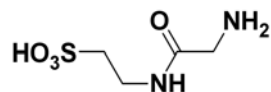
Compound 16a in D2O
13C spectrum - 75 MHz

166.506

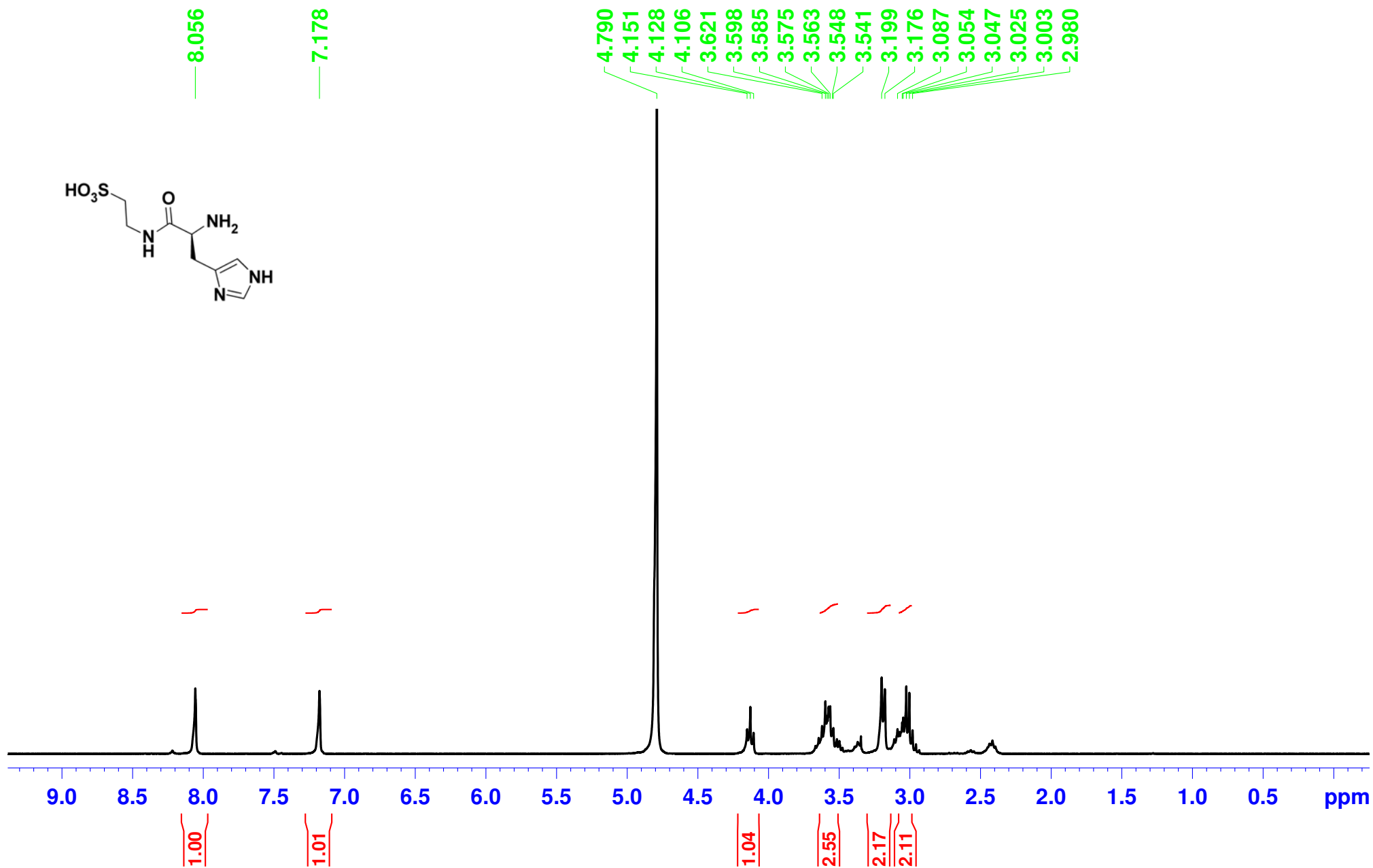
49.134

40.123

34.847



Compound 16b in D2O
1H spectrum - 300 MHz



Compound 16b in D2O
13C spectrum - 75 MHz

169.563

135.360

129.642

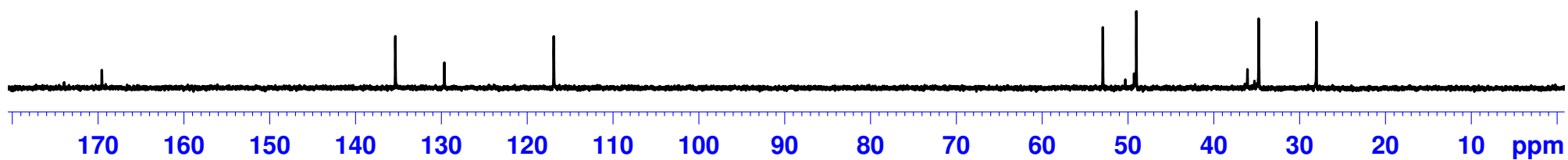
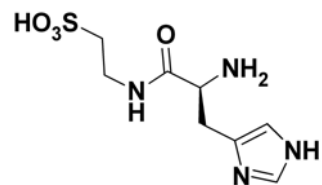
116.916

52.931

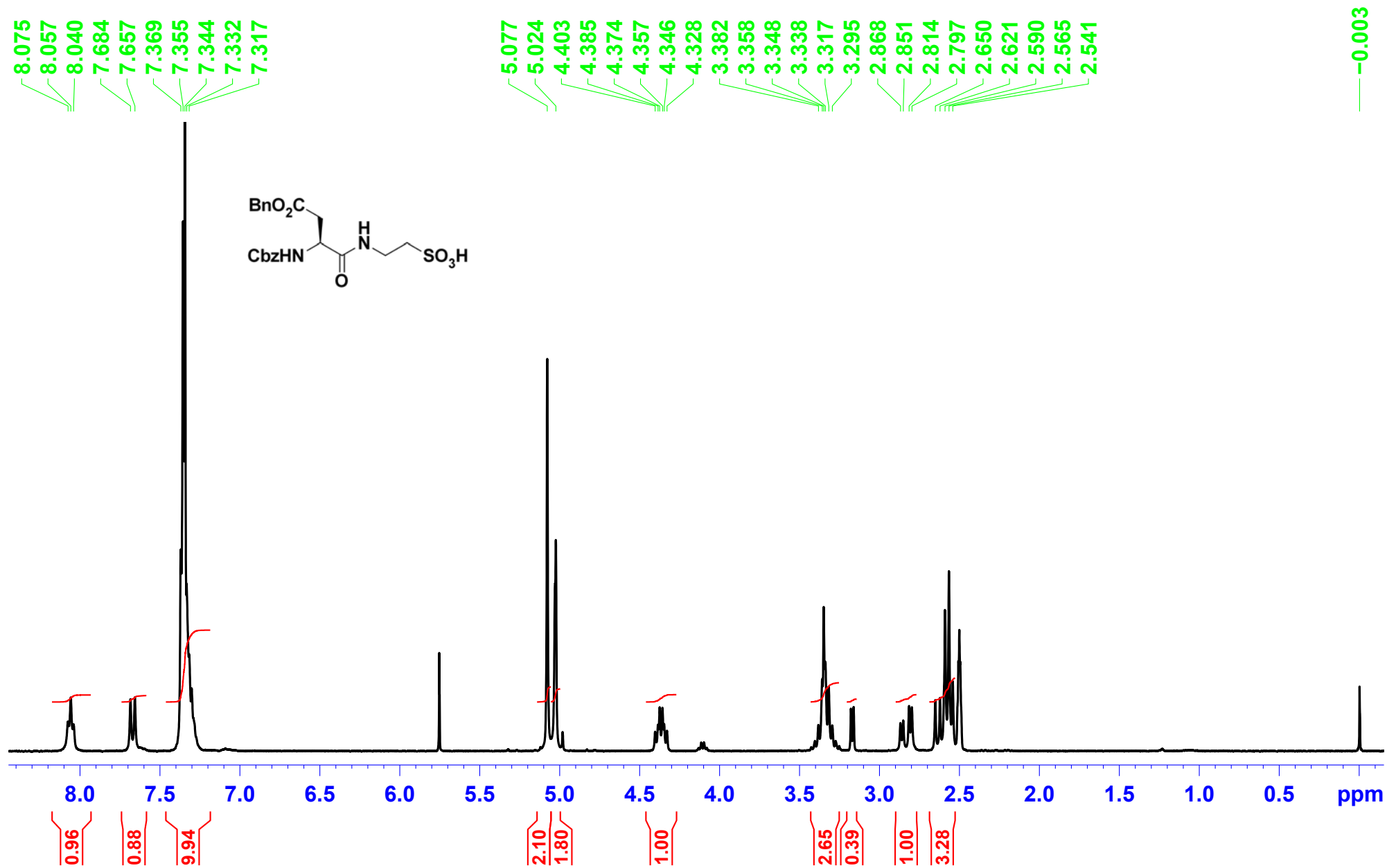
49.028

34.777

28.050



Compound 17 in DMSO-d6
1H spectrum - 300 MHz



Compound 17 in DMSO-d6
13C spectrum - 75 MHz

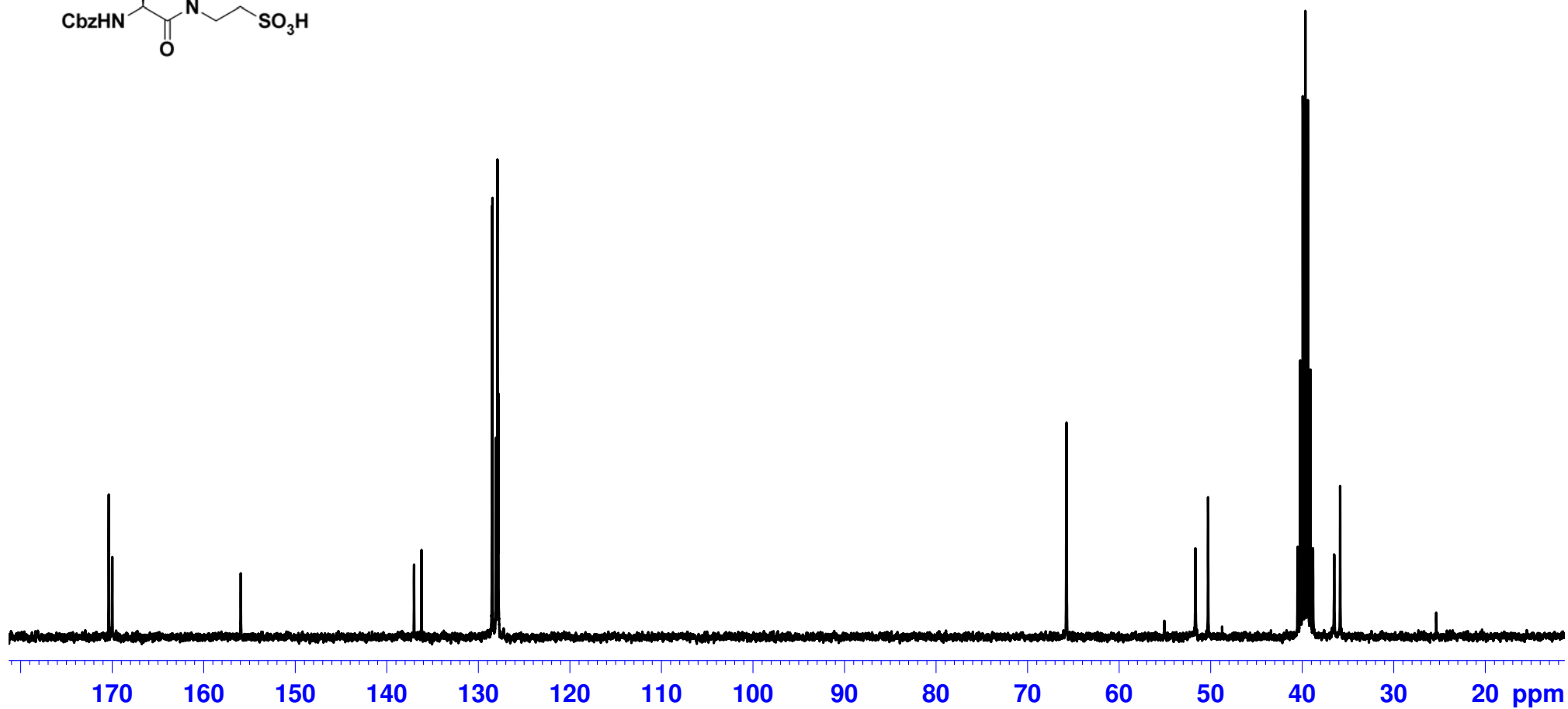
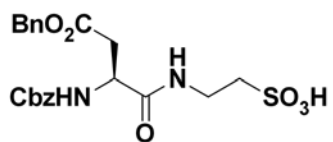
170.372
169.987

155.952

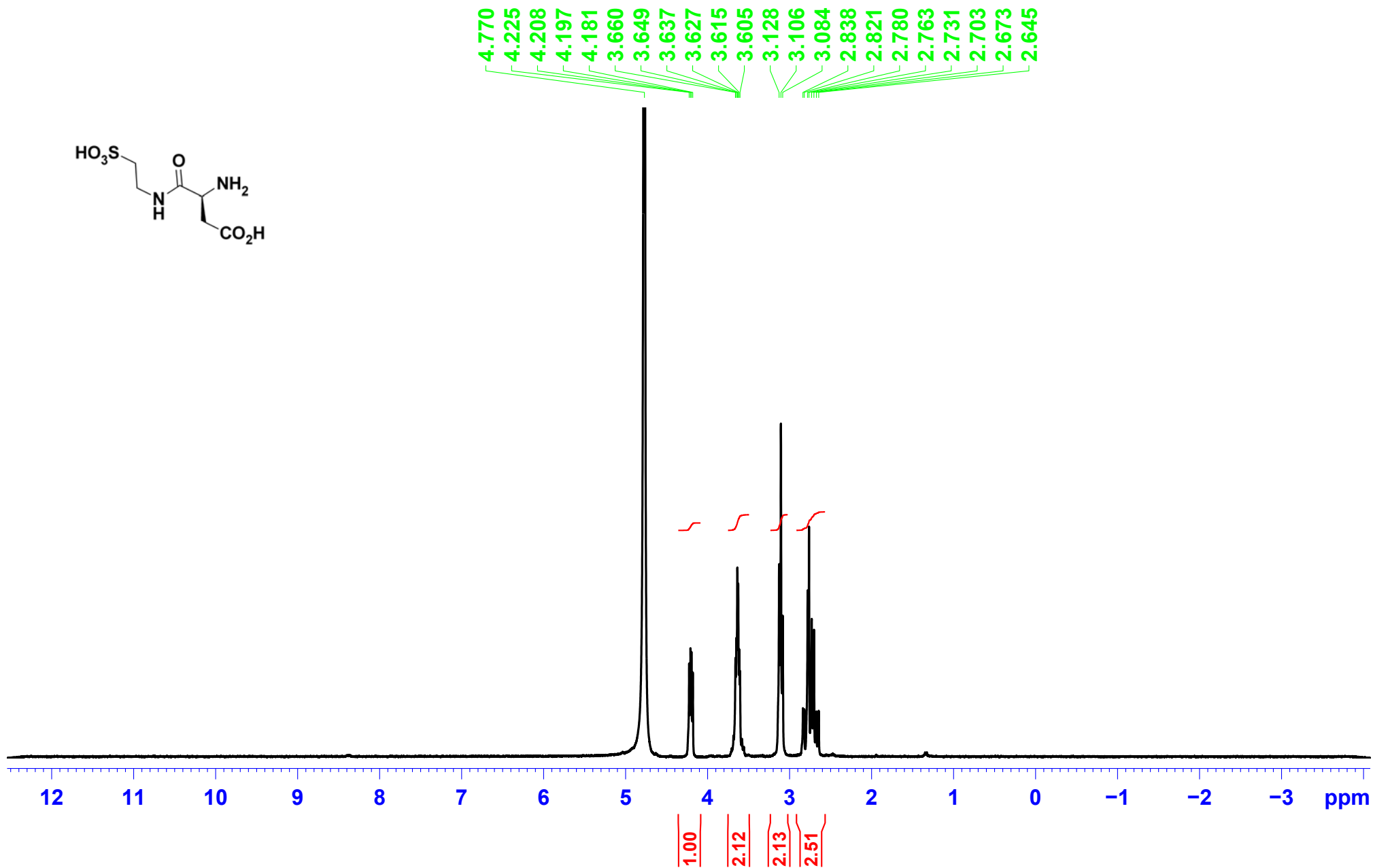
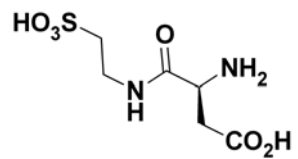
137.018
136.203
128.506
128.459
128.061
127.912
127.814

65.740

51.661
50.281
40.492
40.215
39.936
39.658
39.380
39.101
38.823
36.503
35.853



Compound 18 in D2O
1H spectrum - 300 MHz

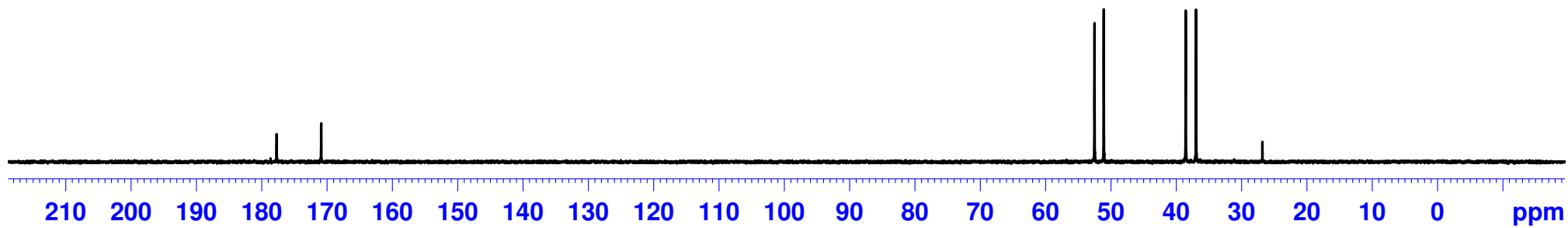
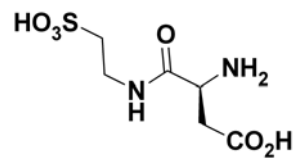


Compound 18 in D2O
13C spectrum - 75 MHz

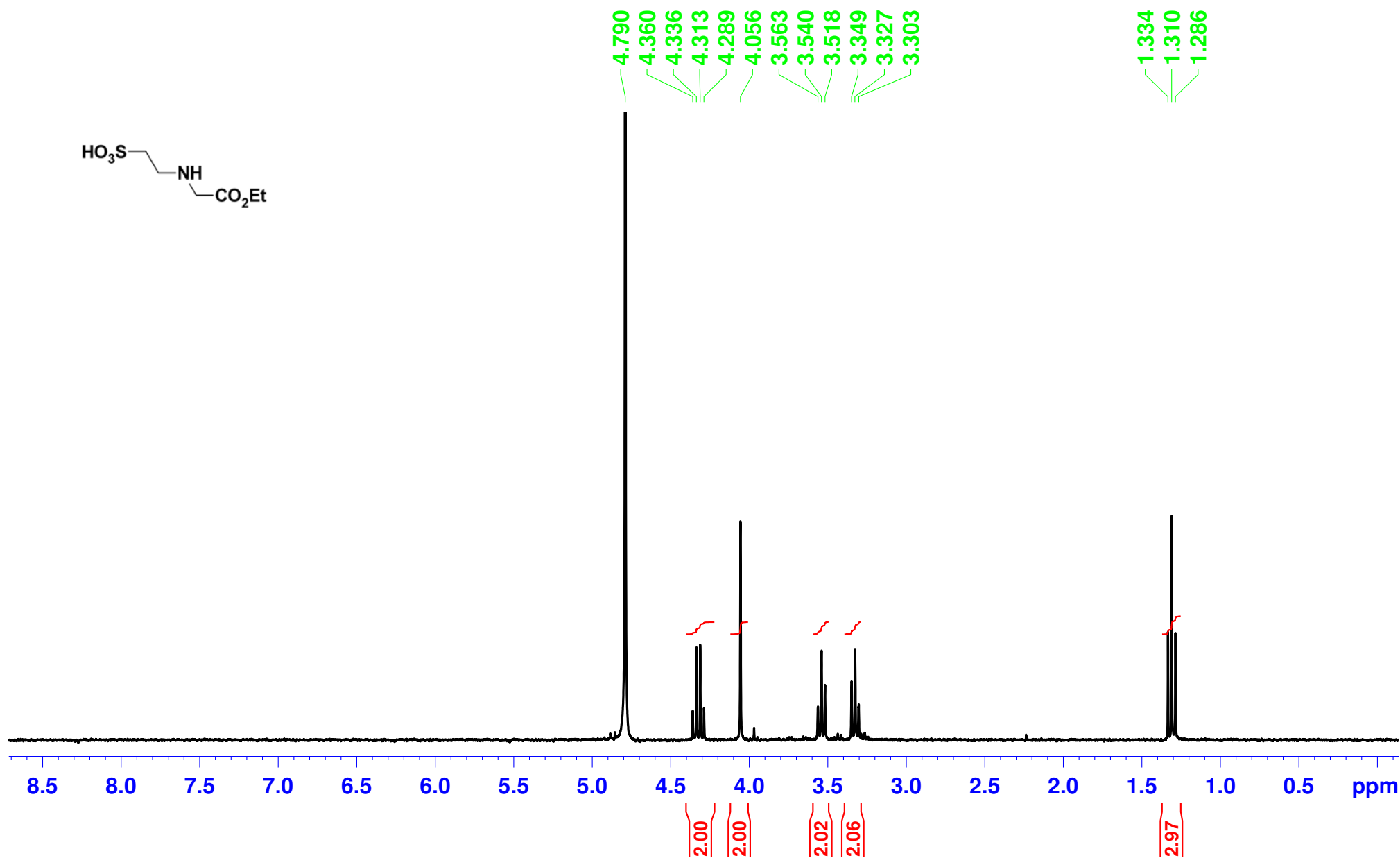
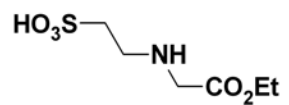
177.726
170.905

52.515
51.097

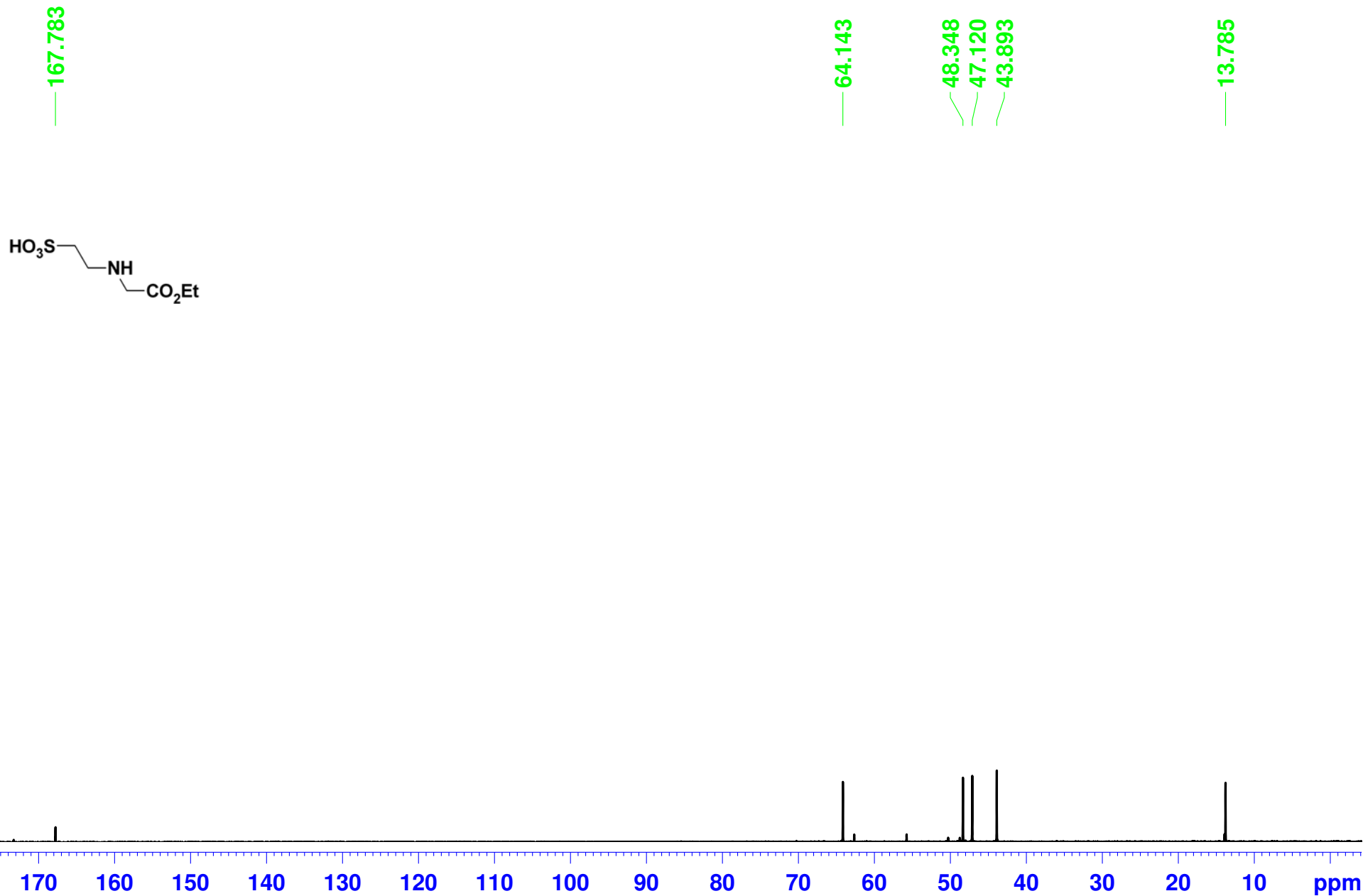
38.551
36.968



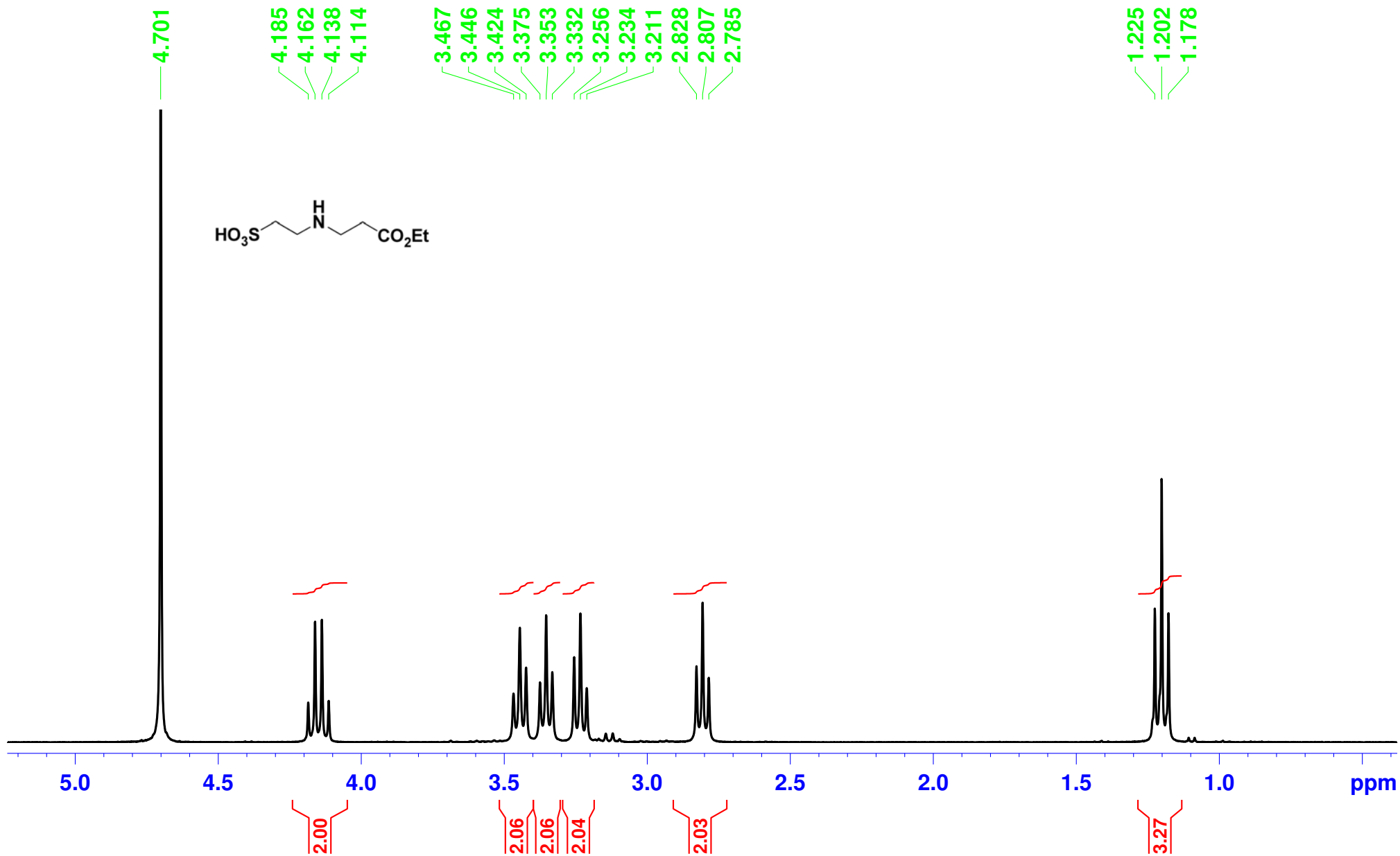
Compound 19 in D2O
1H spectrum - 300 MHz



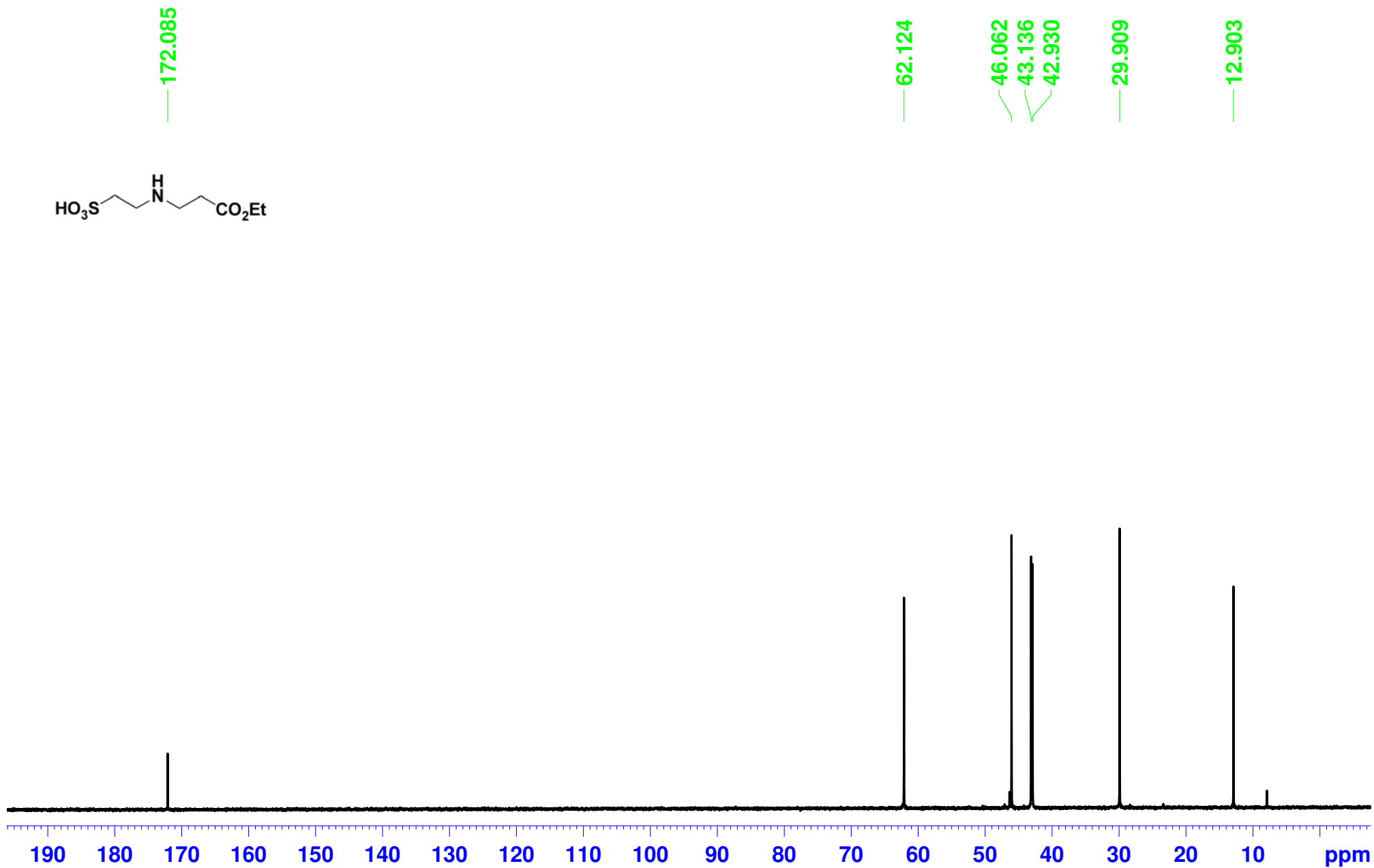
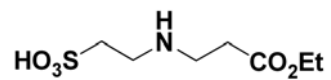
Compound 19 in D2O
13C spectrum - 75 MHz



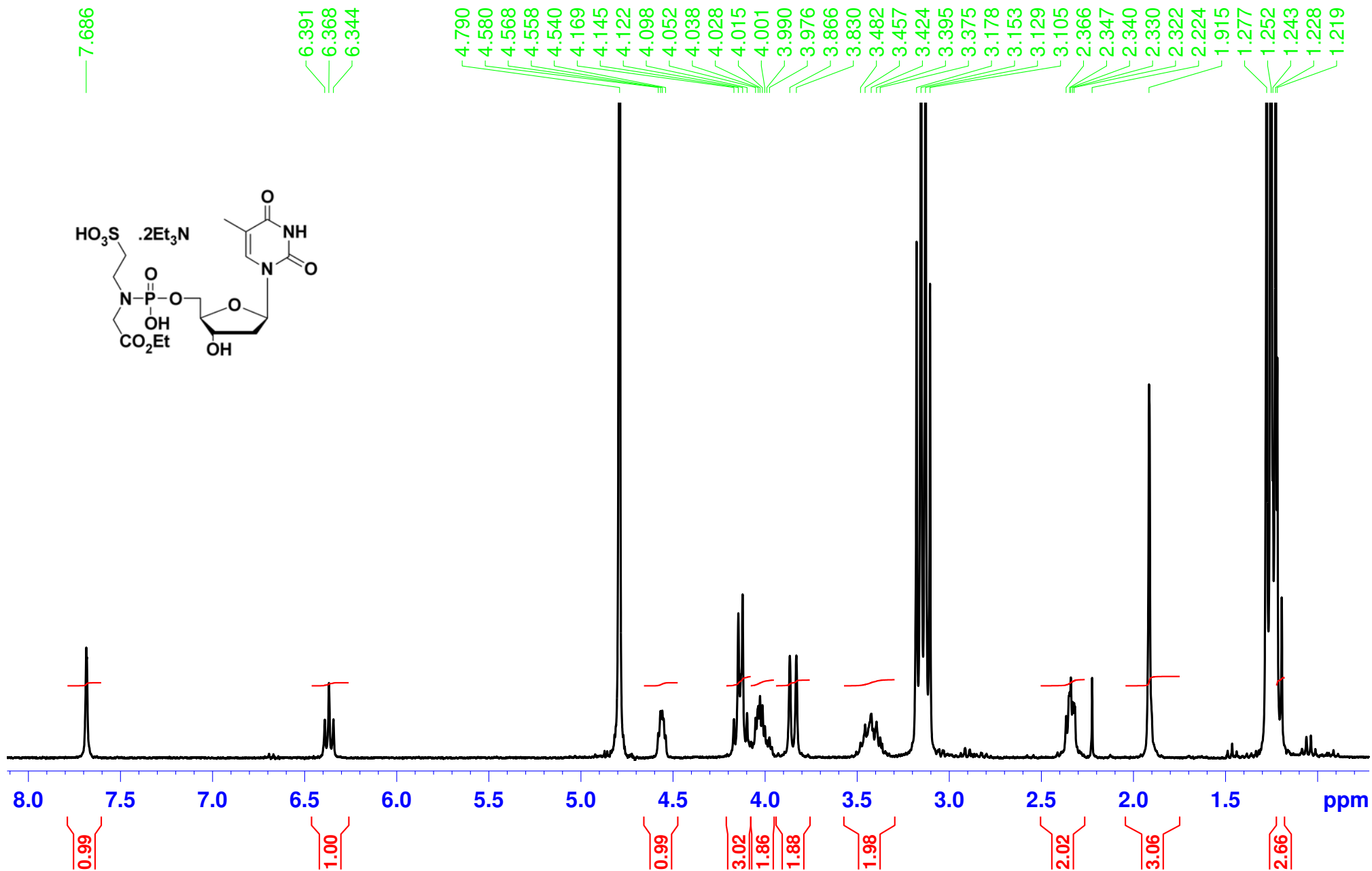
Compound 20 in D2O
1H spectrum - 300 MHz



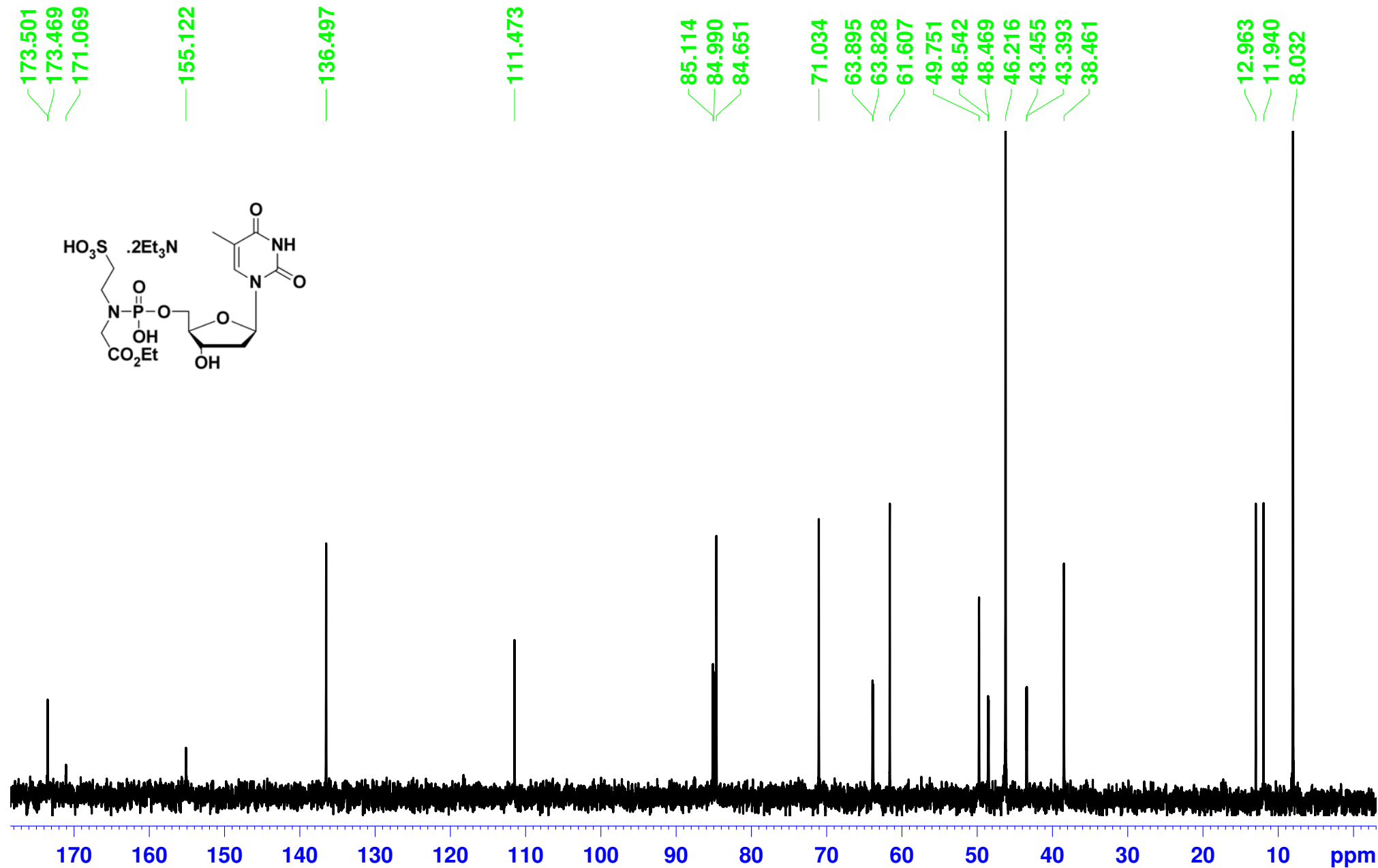
Compound 20 in D2O
13C spectrum - 75 MHz



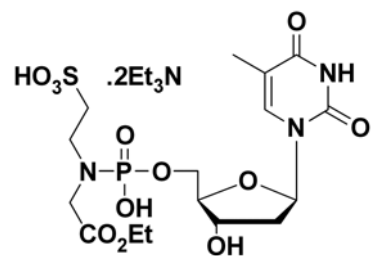
Compound 21 in D2O
1H spectrum - 300 MHz



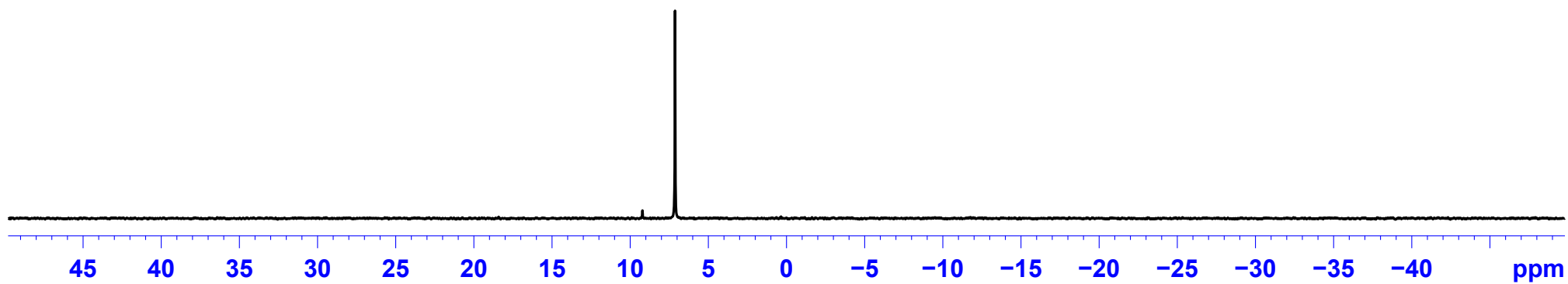
Compound 21 in D2O
13C spectrum - 75 MHz



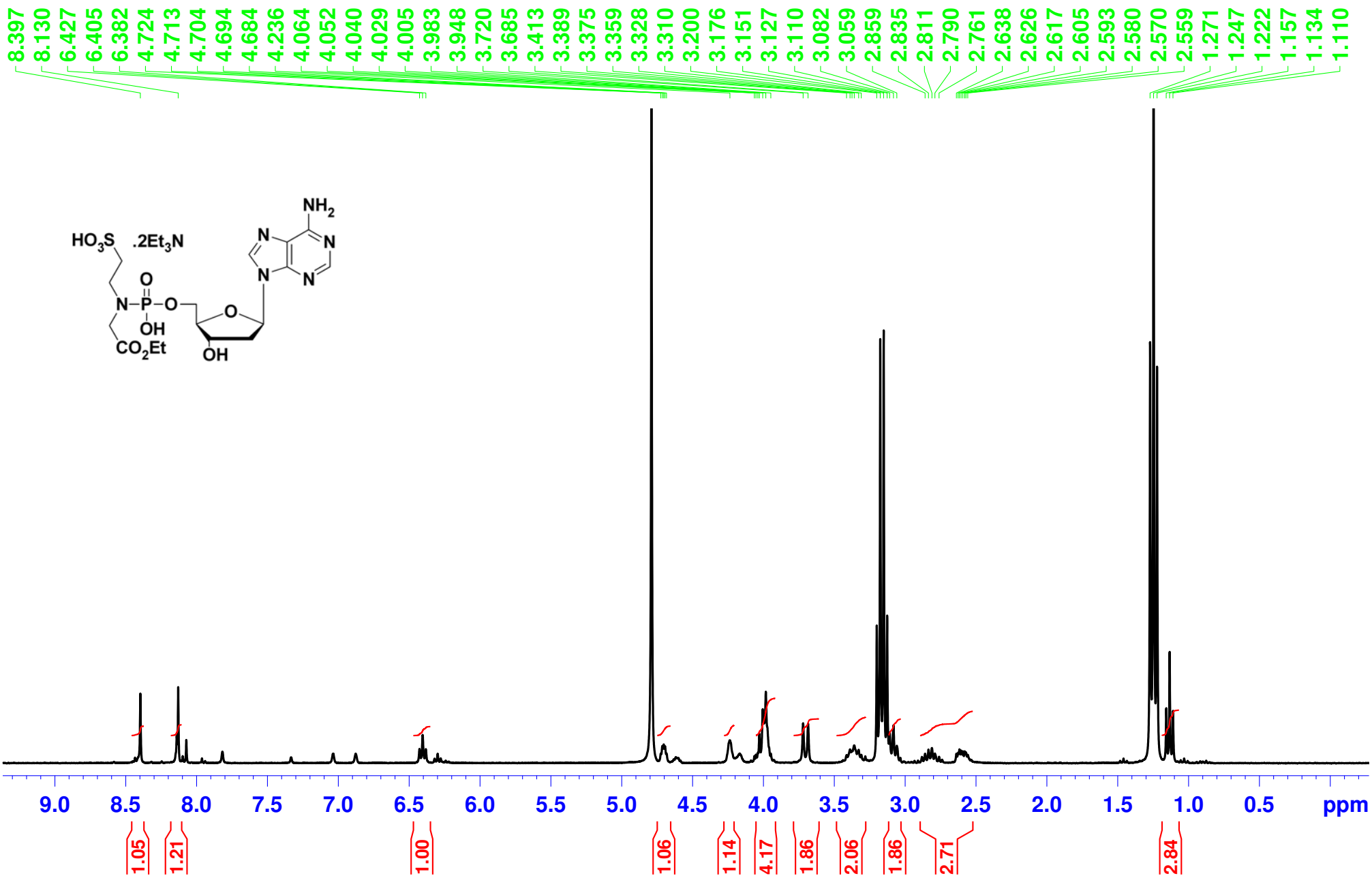
Compound 21 in D2O
31P spectrum - 121 MHz



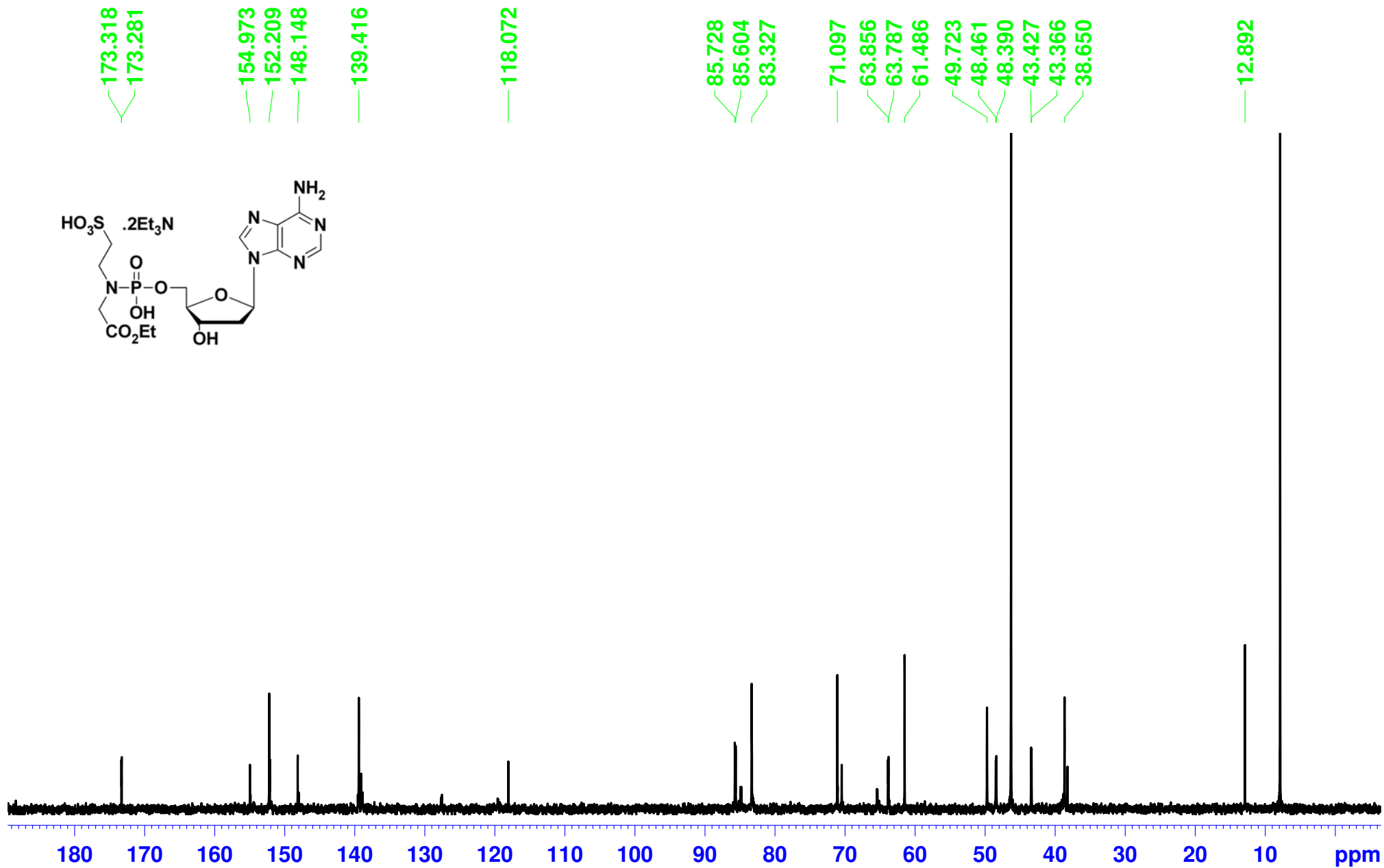
7.130



Compound 22 in D2O
1H spectrum - 300 MHz

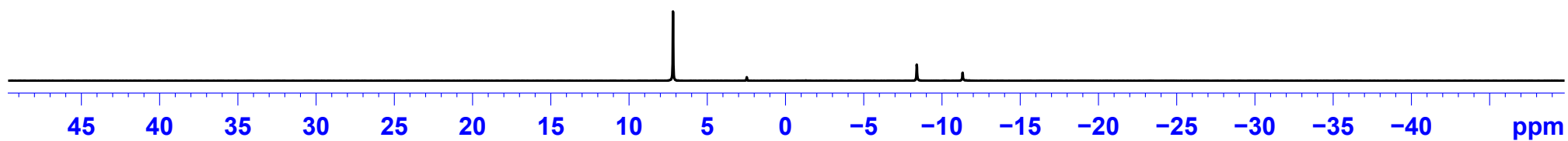
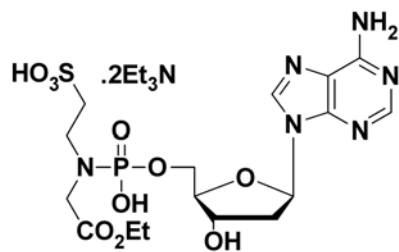


Compound 22 in D2O
13C spectrum - 75 MHz

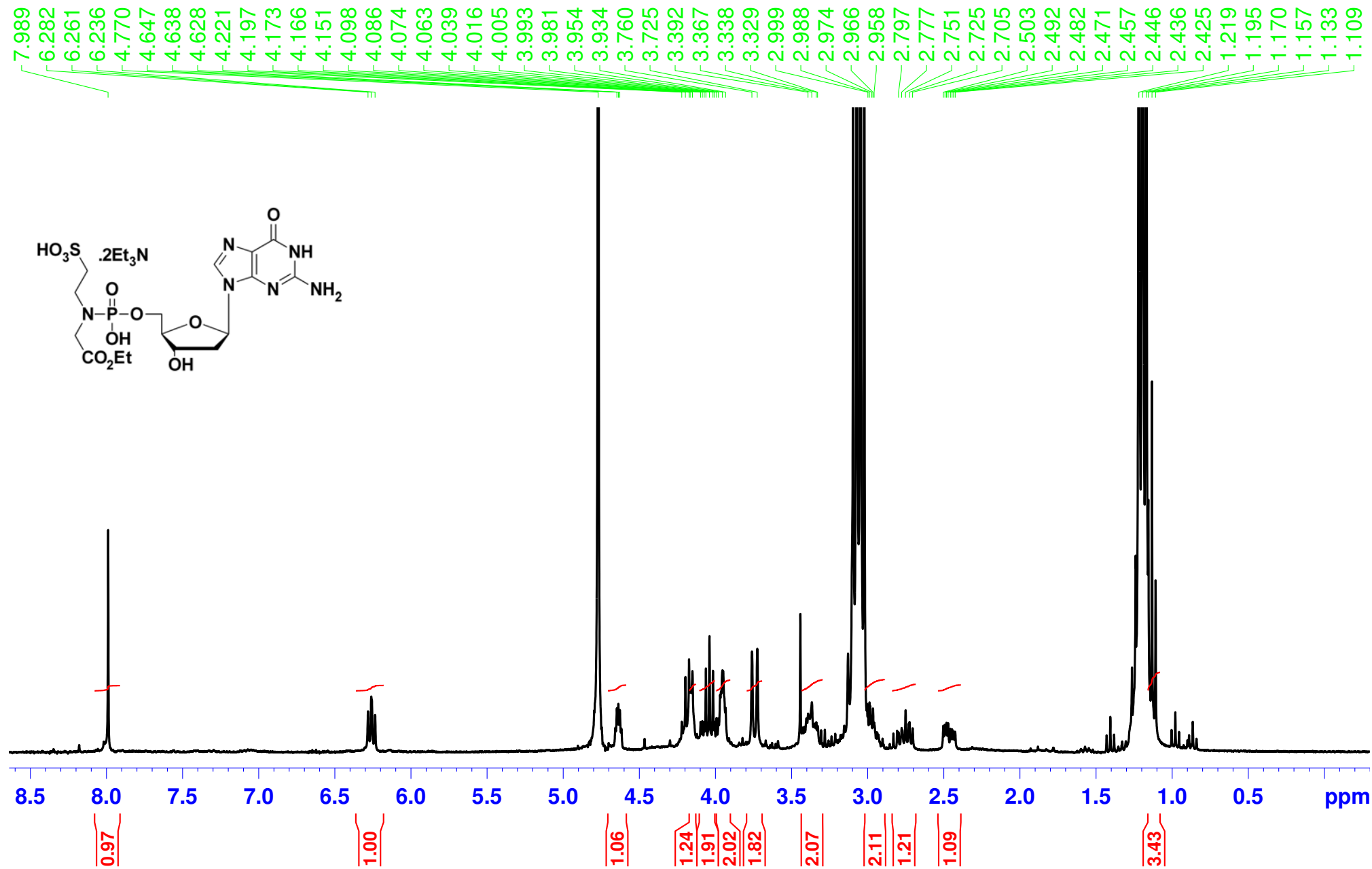


Compound 22 in D2O
31P spectrum - 121 MHz

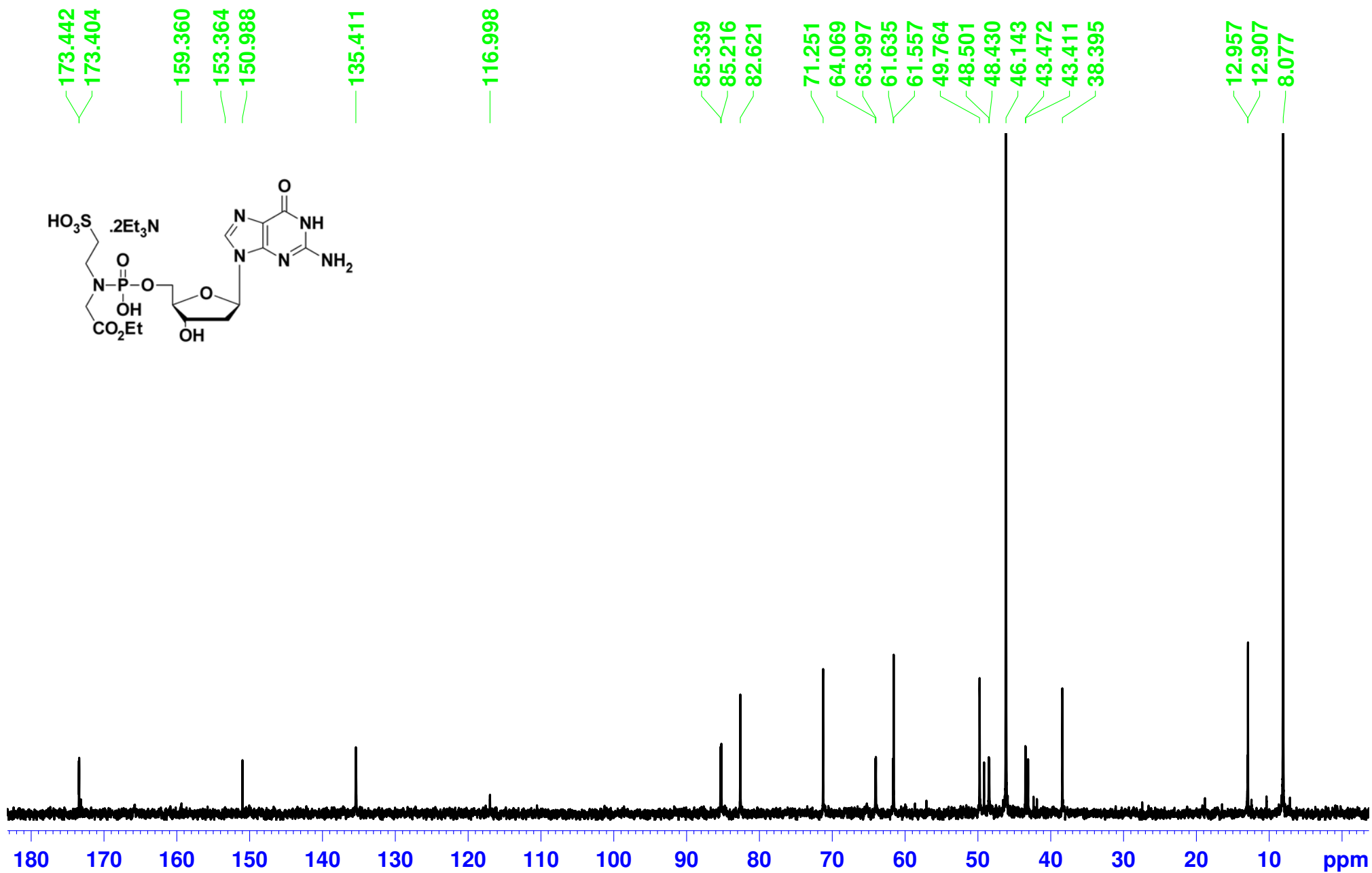
7.188



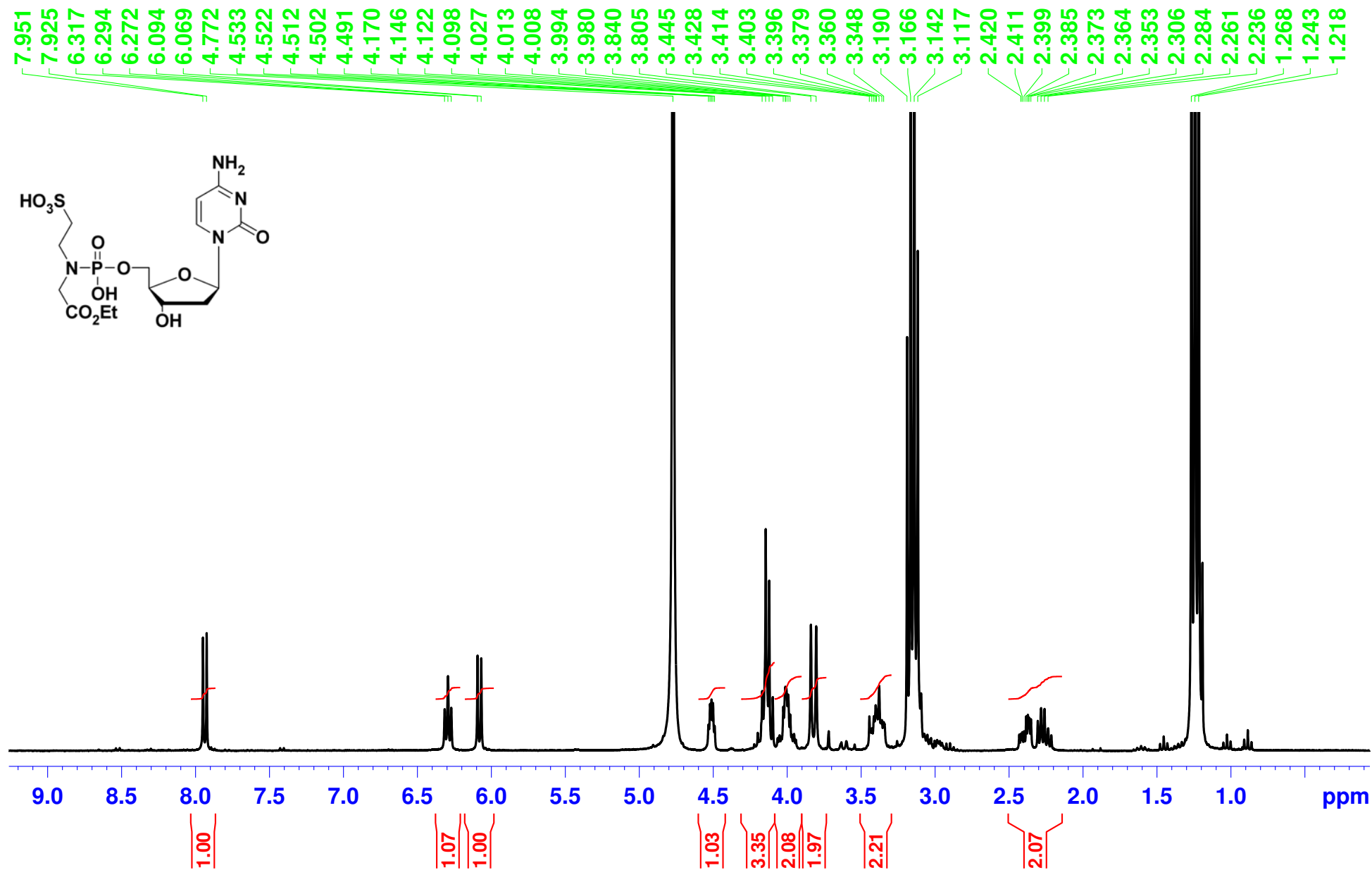
Compound 23 in D2O
1H spectrum - 300 MHz



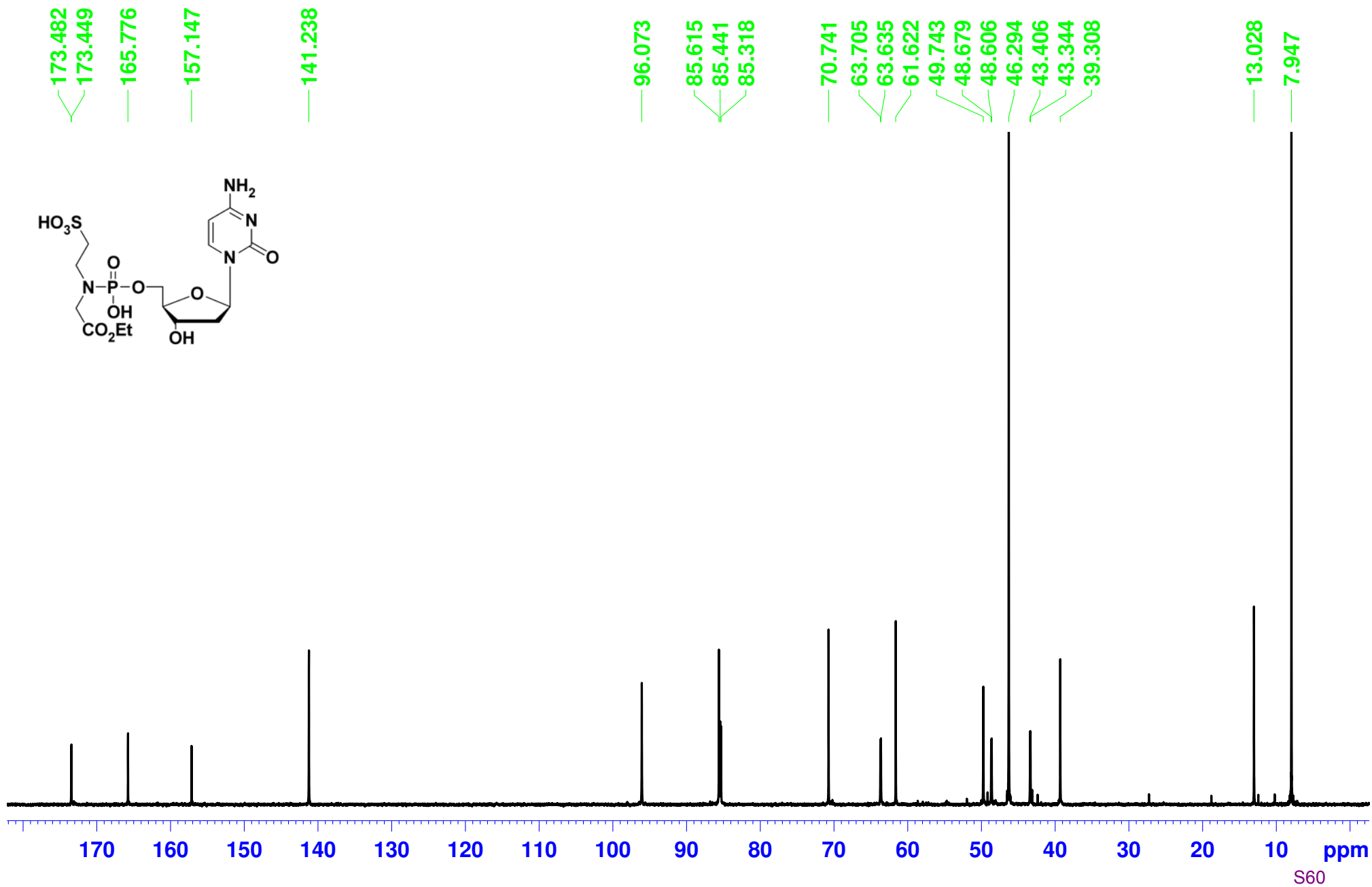
Compound 23 in D2O
13C spectrum - 75 MHz



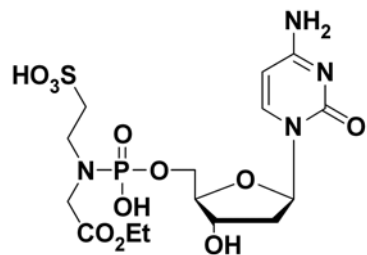
Compound 24 in D2O
1H spectrum - 300 MHz



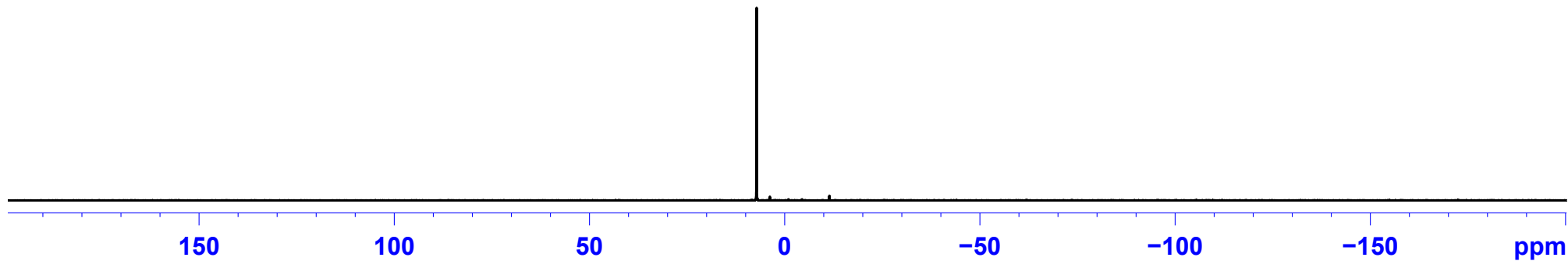
Compound 24 in D2O
13C spectrum - 75 MHz



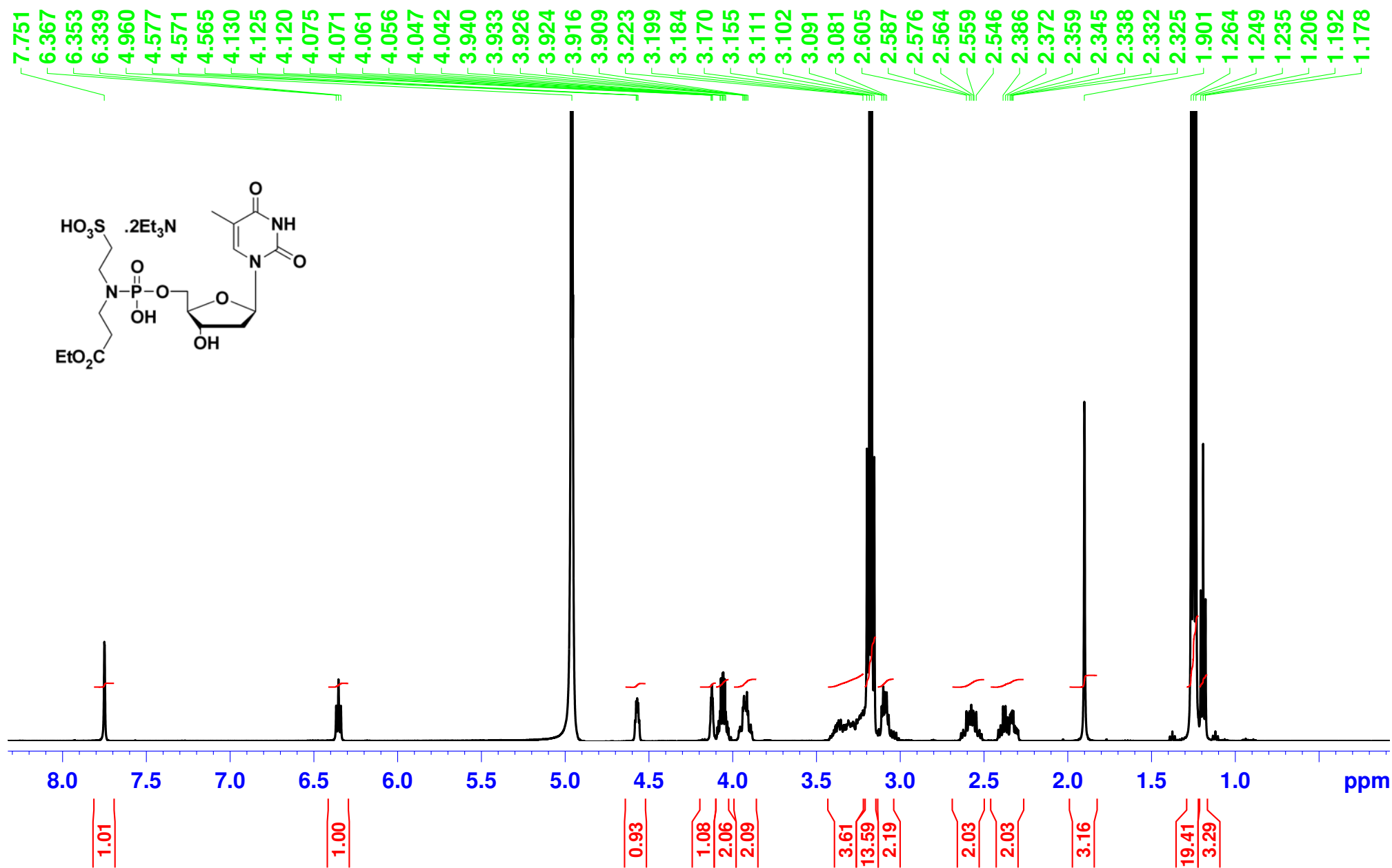
Compound 24 in D2O
31P spectrum - 121 MHz



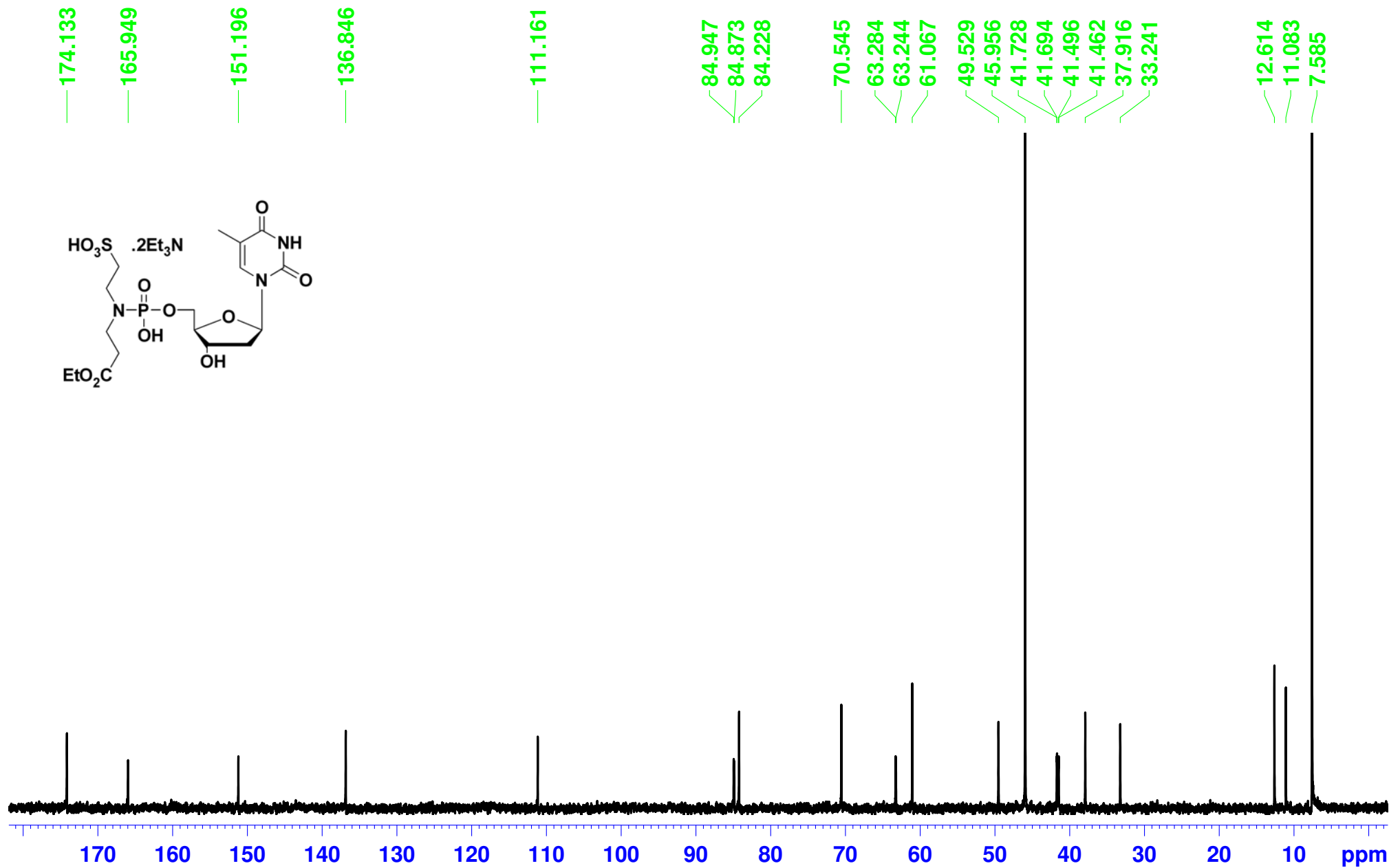
7.183



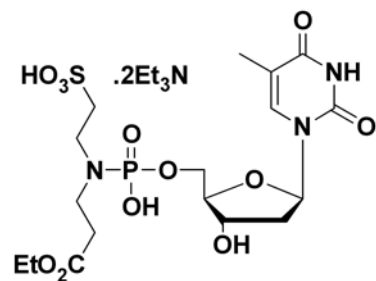
Compound 25 in D2O
1H spectrum - 500 MHz @ 6 C



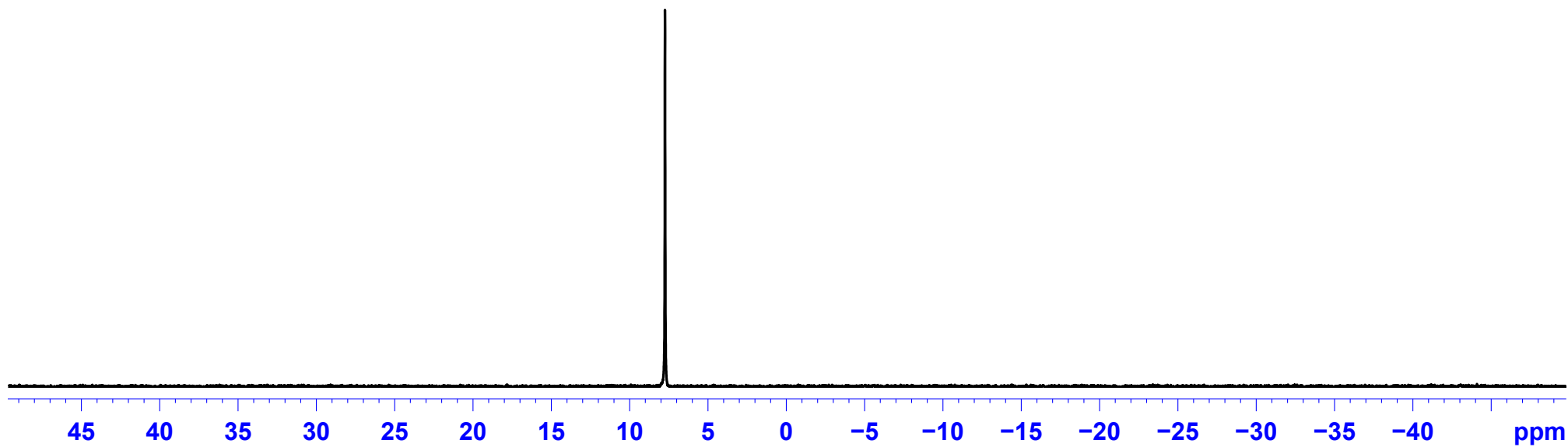
Compound 25 in D2O
1C spectrum - 125 MHz @ 6 C



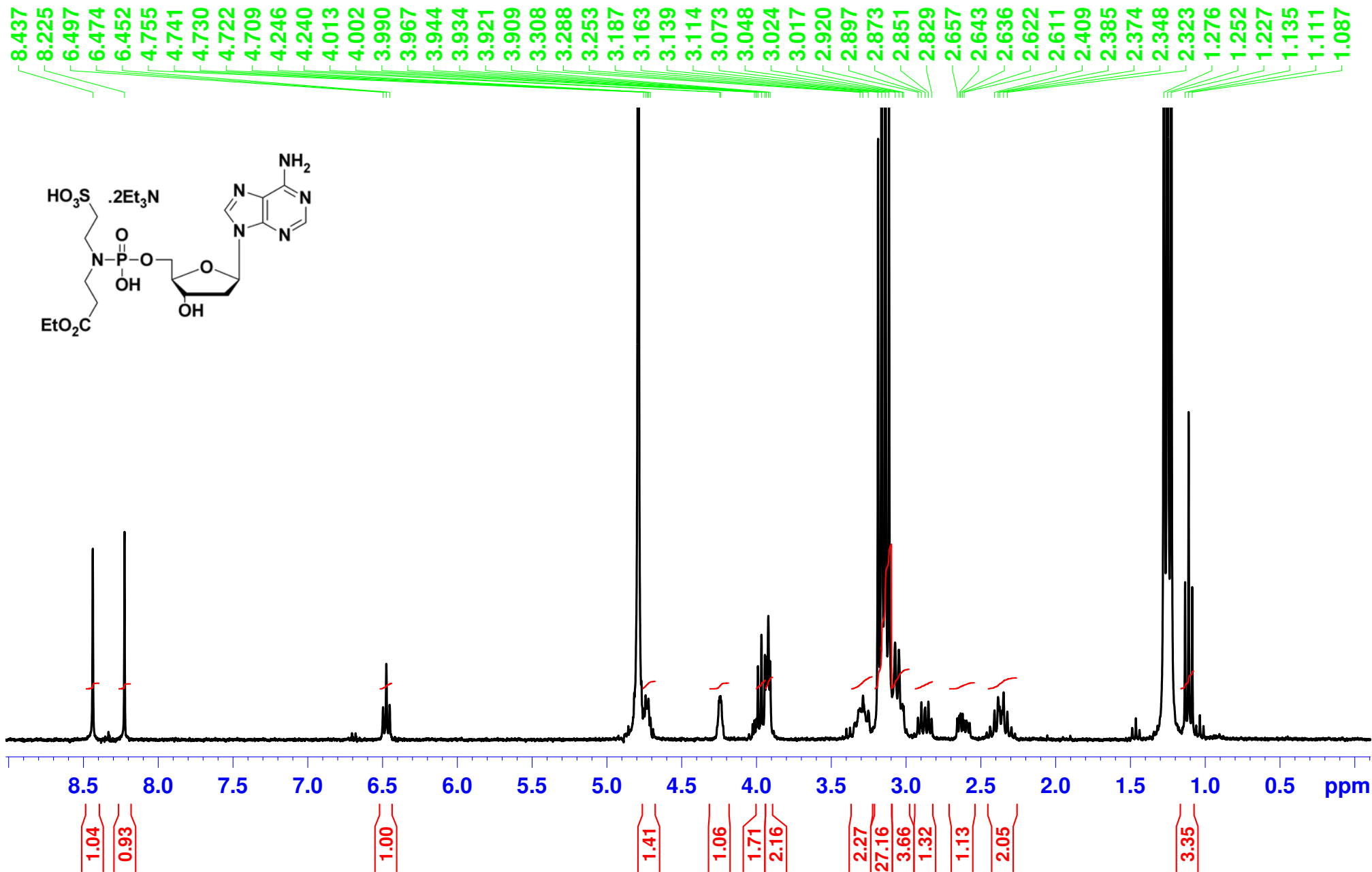
Compound 25 in D2O
31P spectrum - 202 MHz @ 6 C



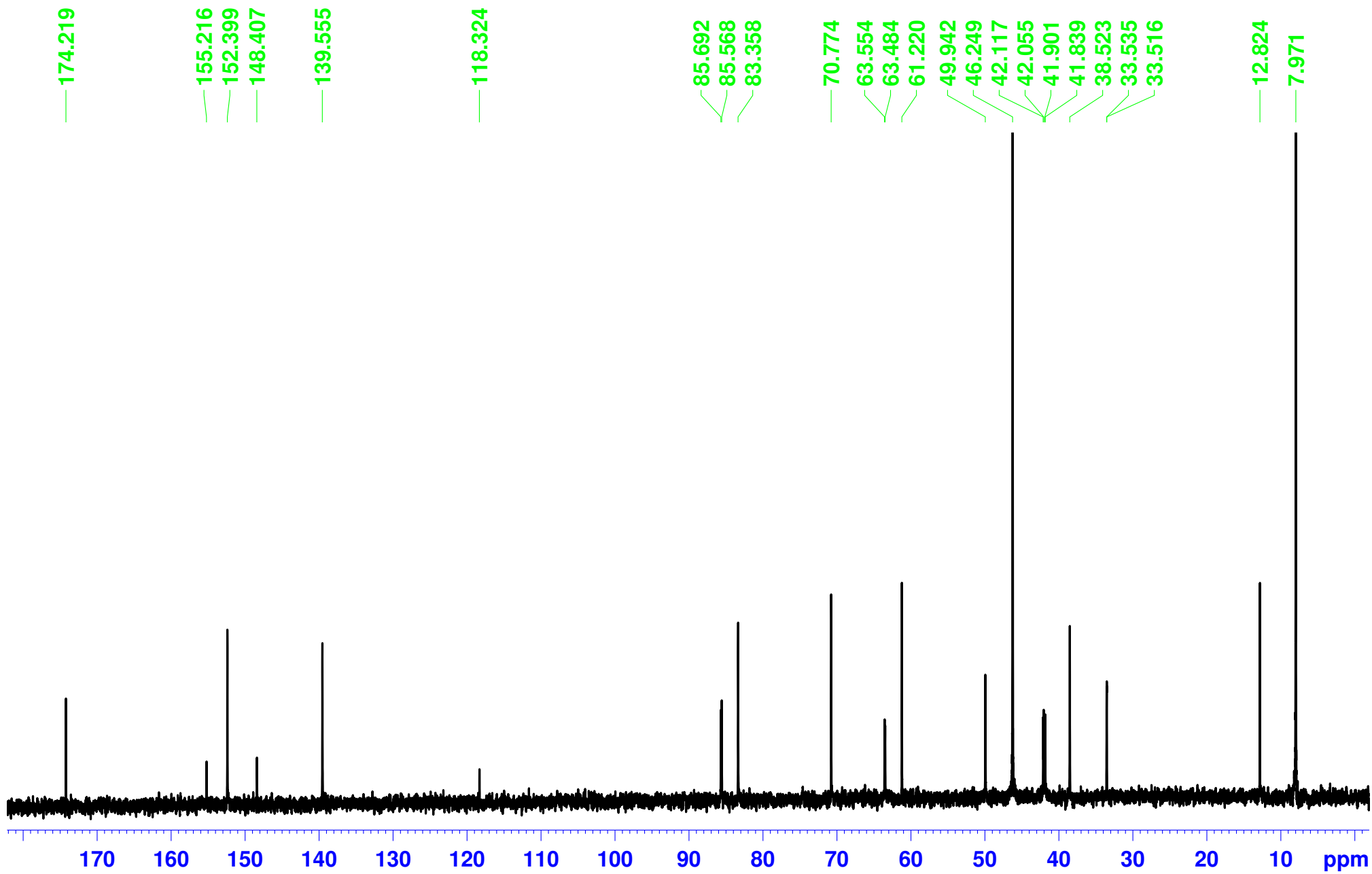
7.750



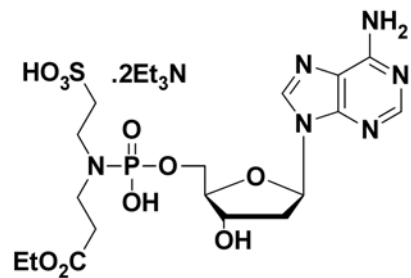
Compound 26 in D2O
1H spectrum - 300 MHz



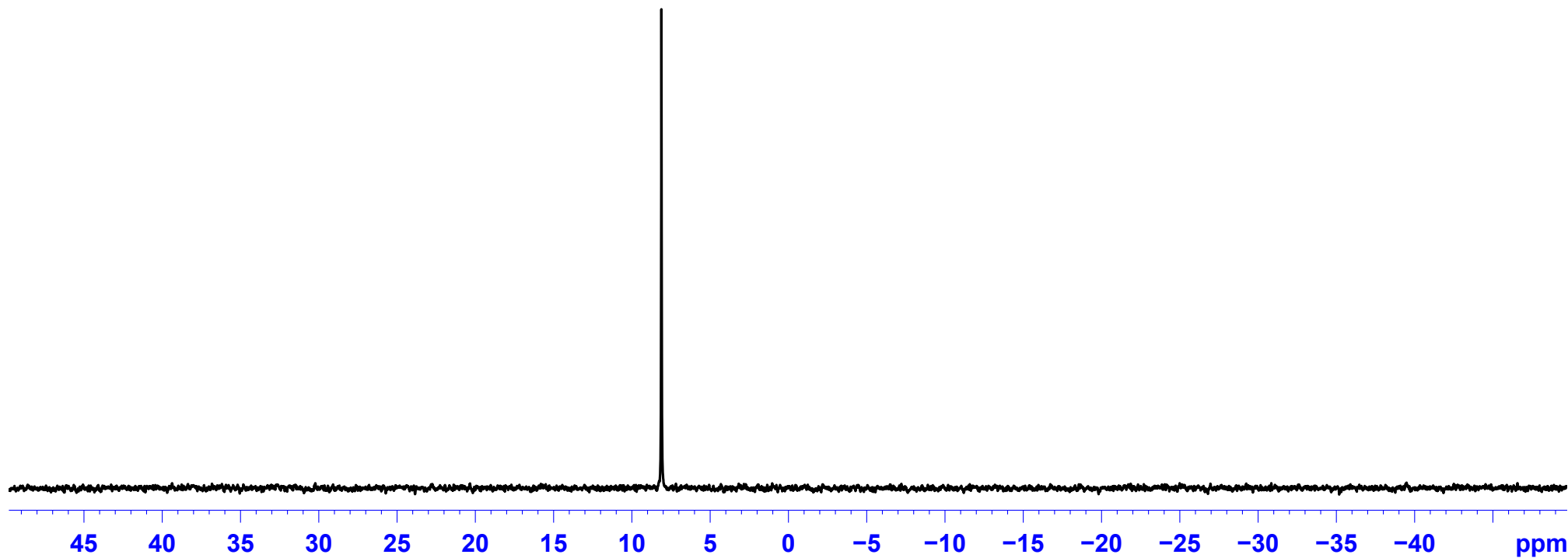
Compound 26 in D2O
13C spectrum - 75 MHz



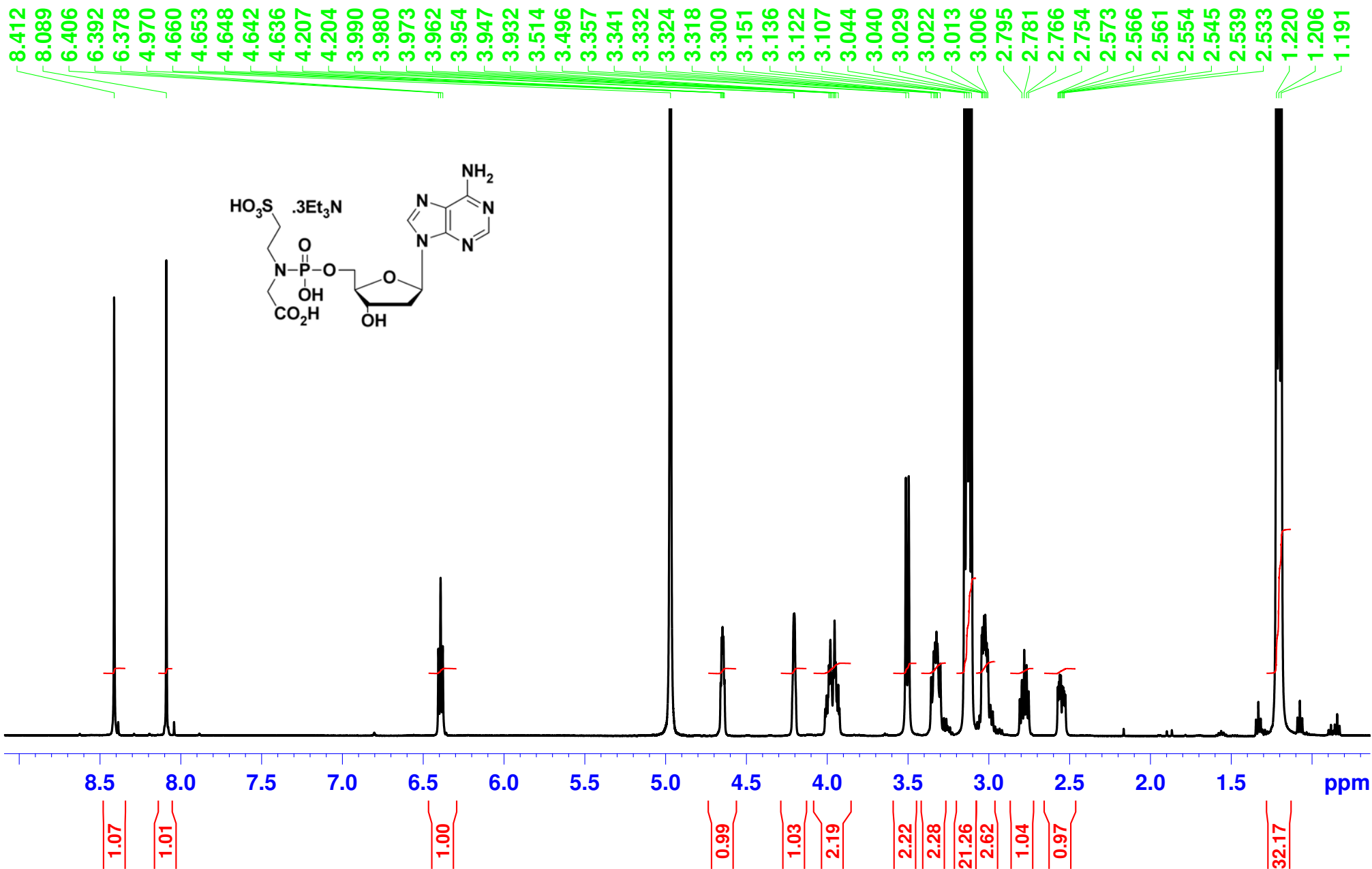
Compound 26 in D2O
31P spectrum - 121 MHz



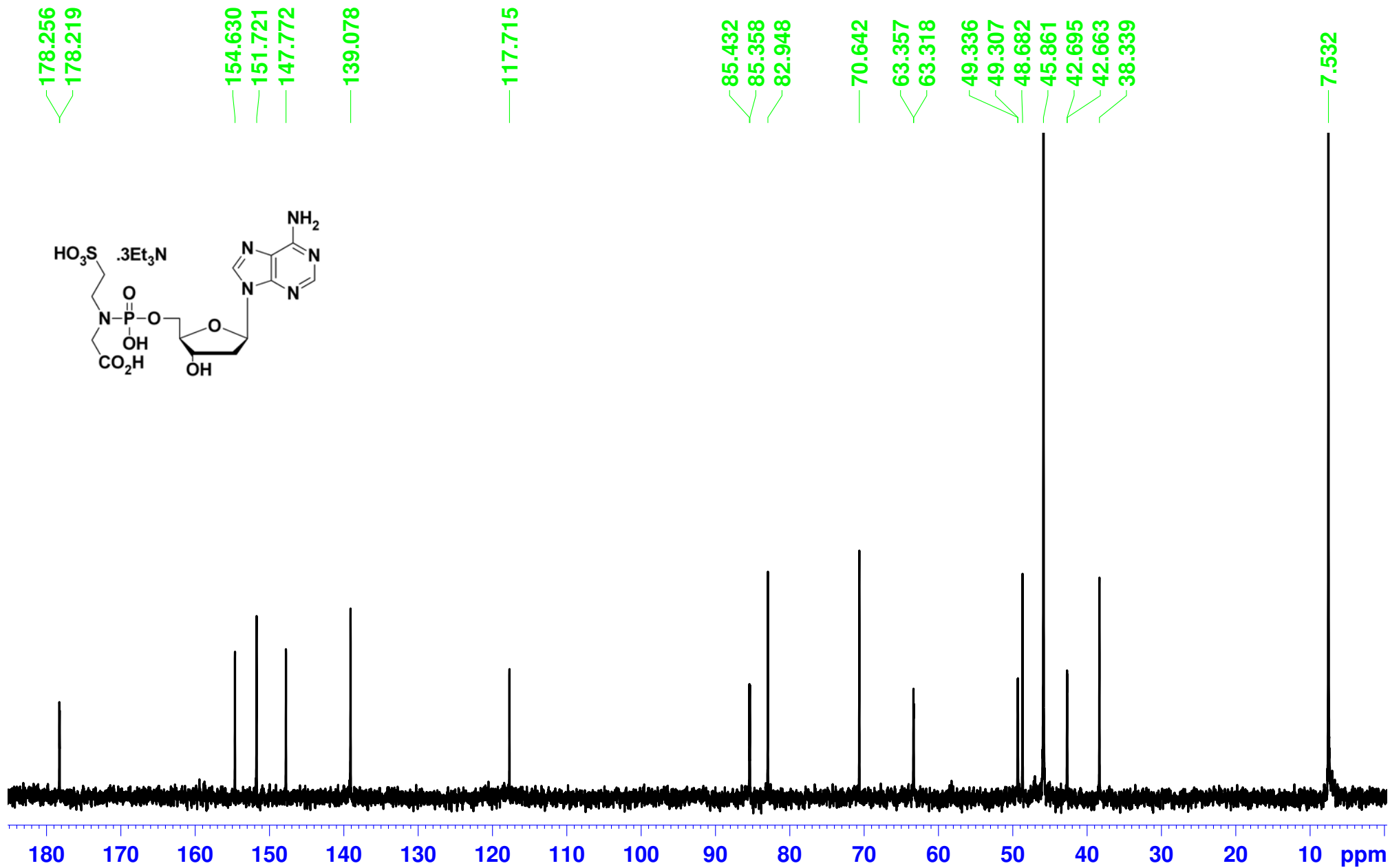
8.111



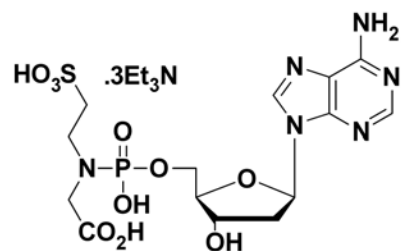
Compound 27 in D2O
1H spectrum - 500 MHz @ 6C



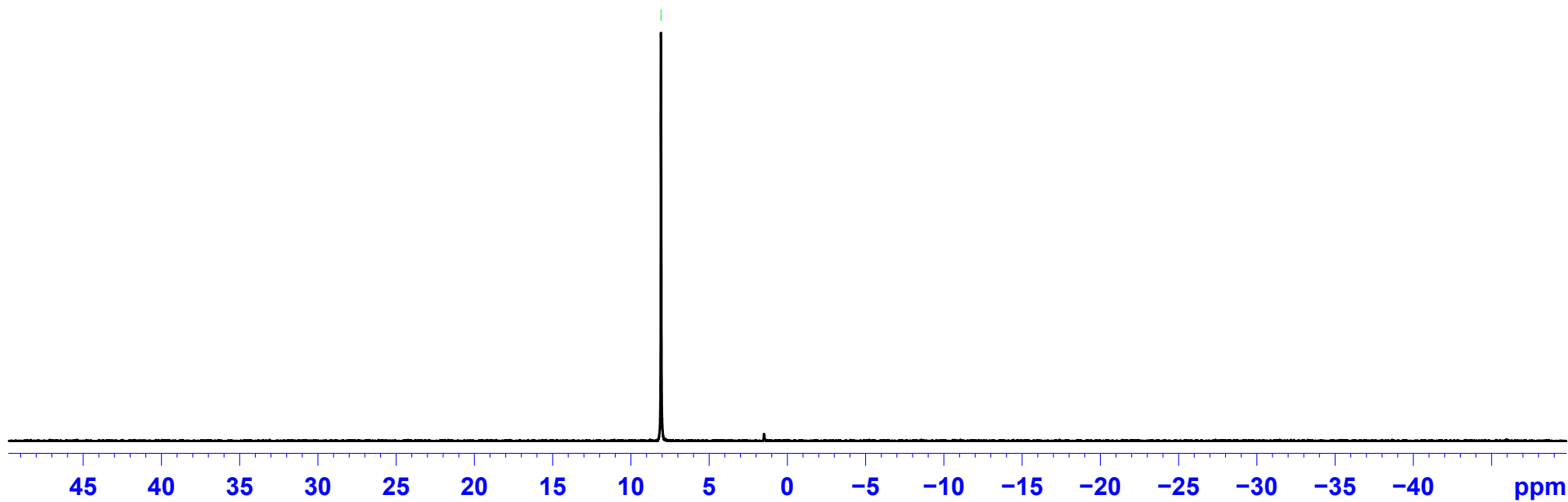
Compound 27 in D2O
13C spectrum - 125 MHz @ 6C



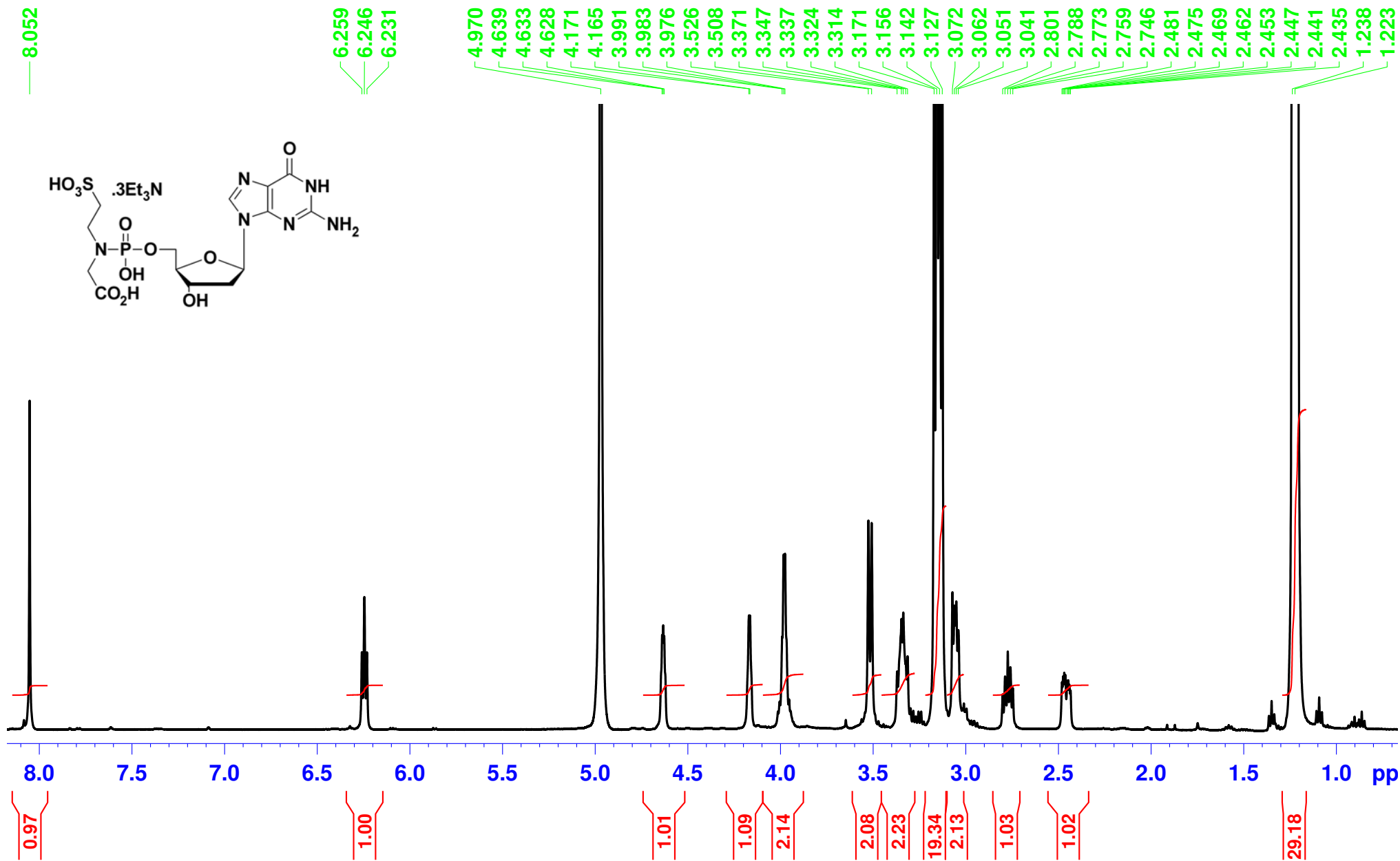
Compound 27 in D₂O
31P spectrum - 202 MHz @ 6C



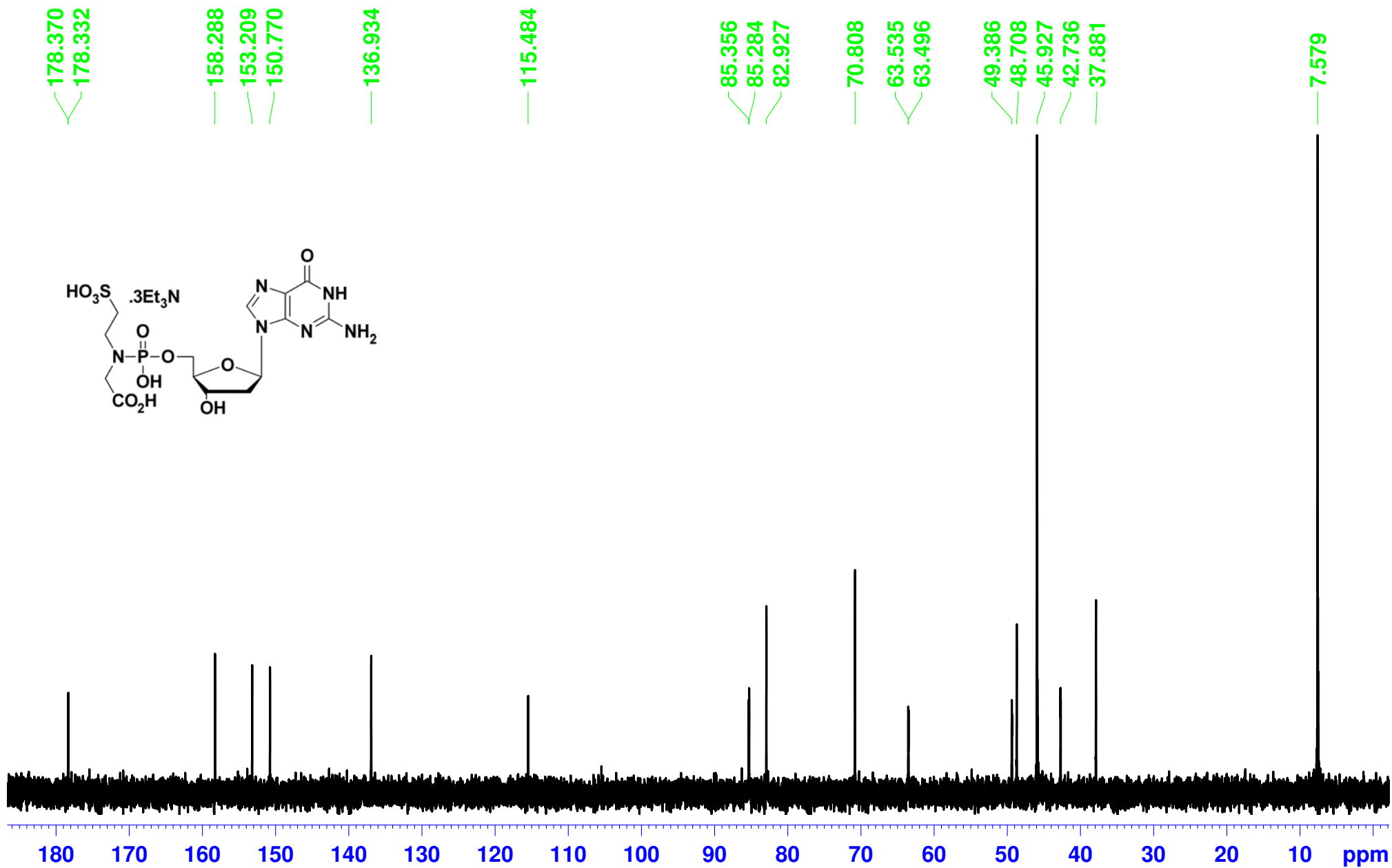
8.075



Compound 28 in D2O
1H spectrum - 500 MHz @ 5C

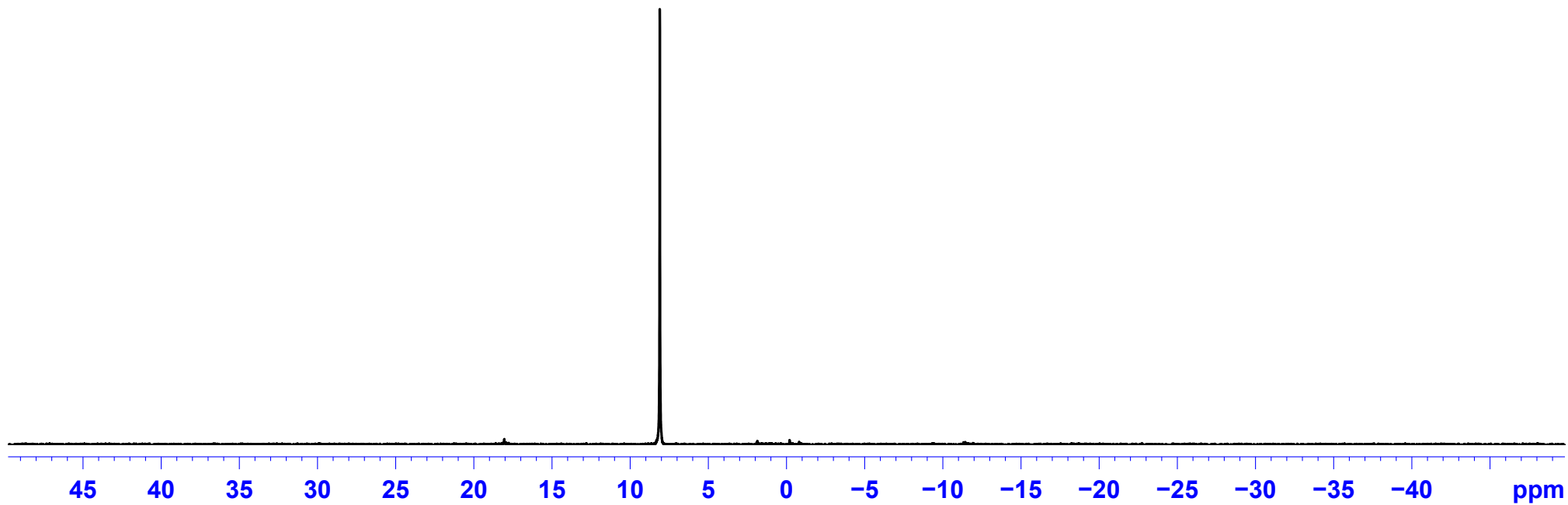
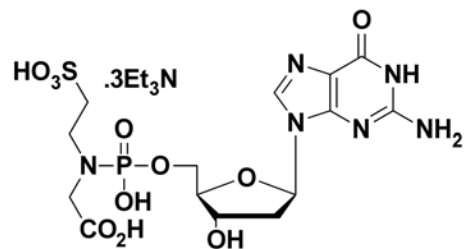


Compound 28 in D2O
13C spectrum - 125 MHz @ 5C

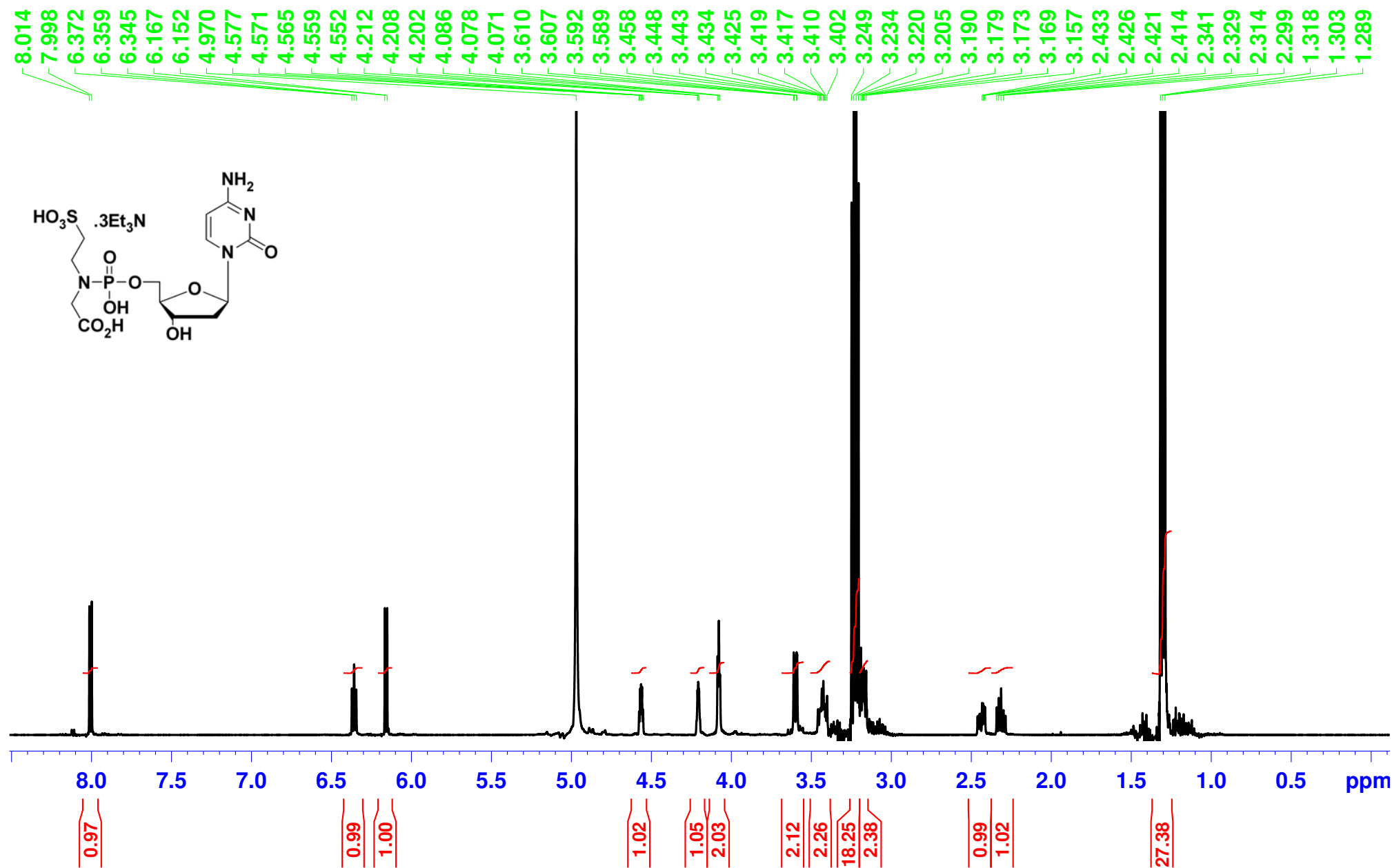


Compound 28 in D2O
31P spectrum - 202 MHz @ 5C

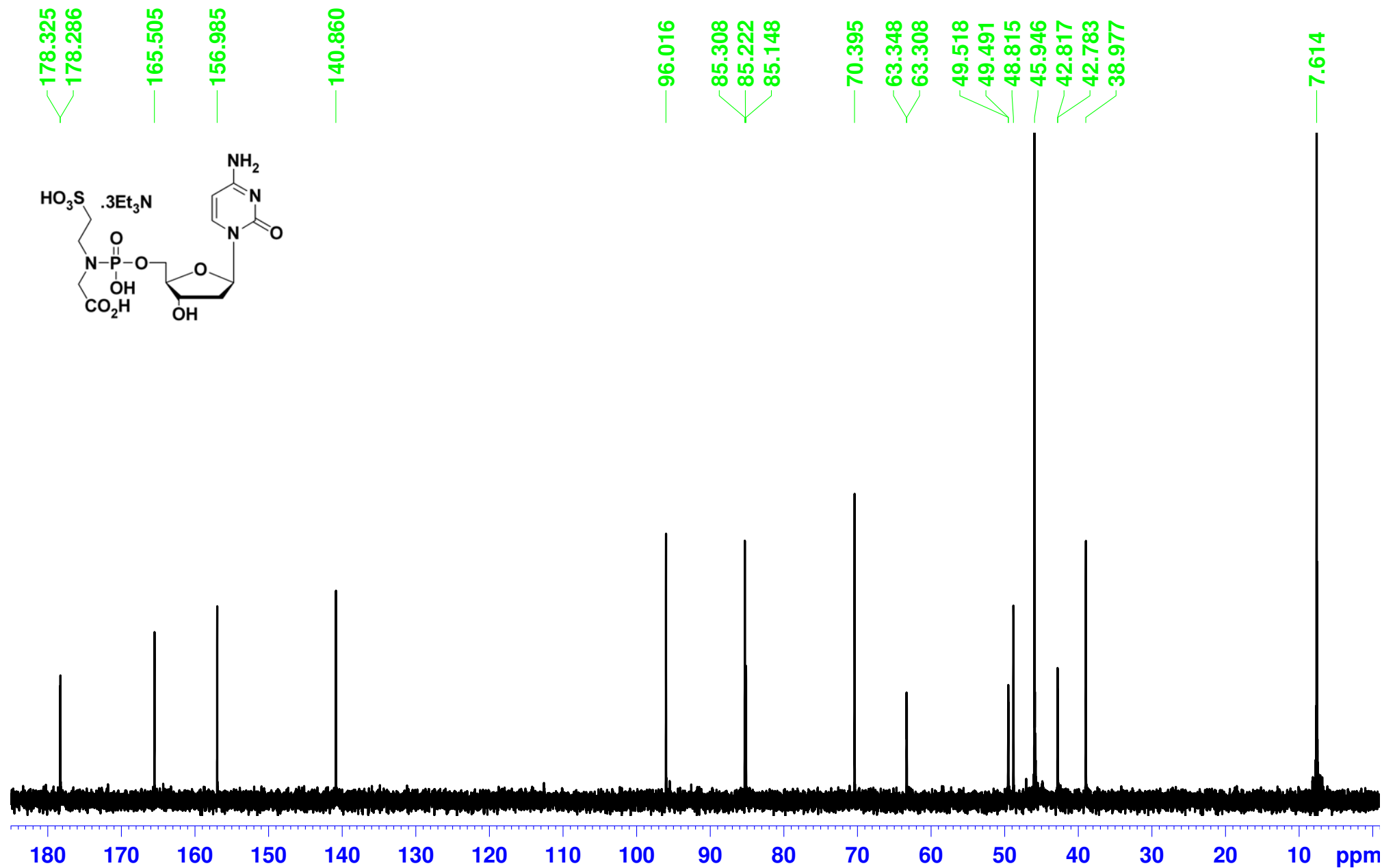
8.107



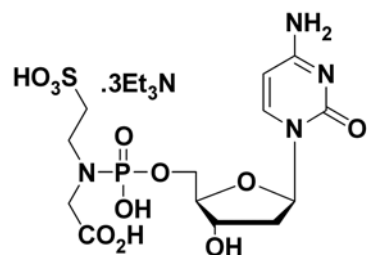
Compound 29 in D2O
1H spectrum - 500 MHz @ 6C



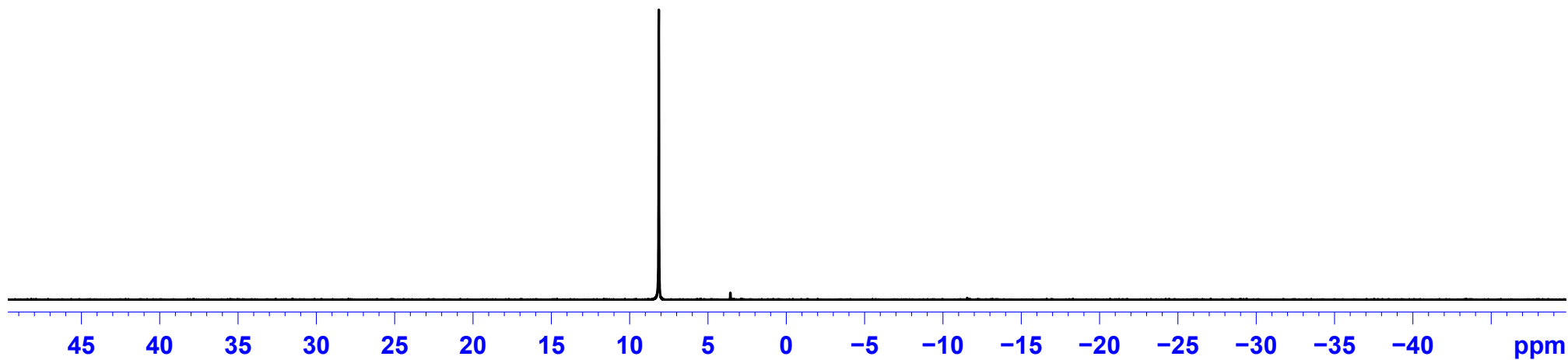
Compound 29 in D2O
13C spectrum - 125 MHz @ 6C



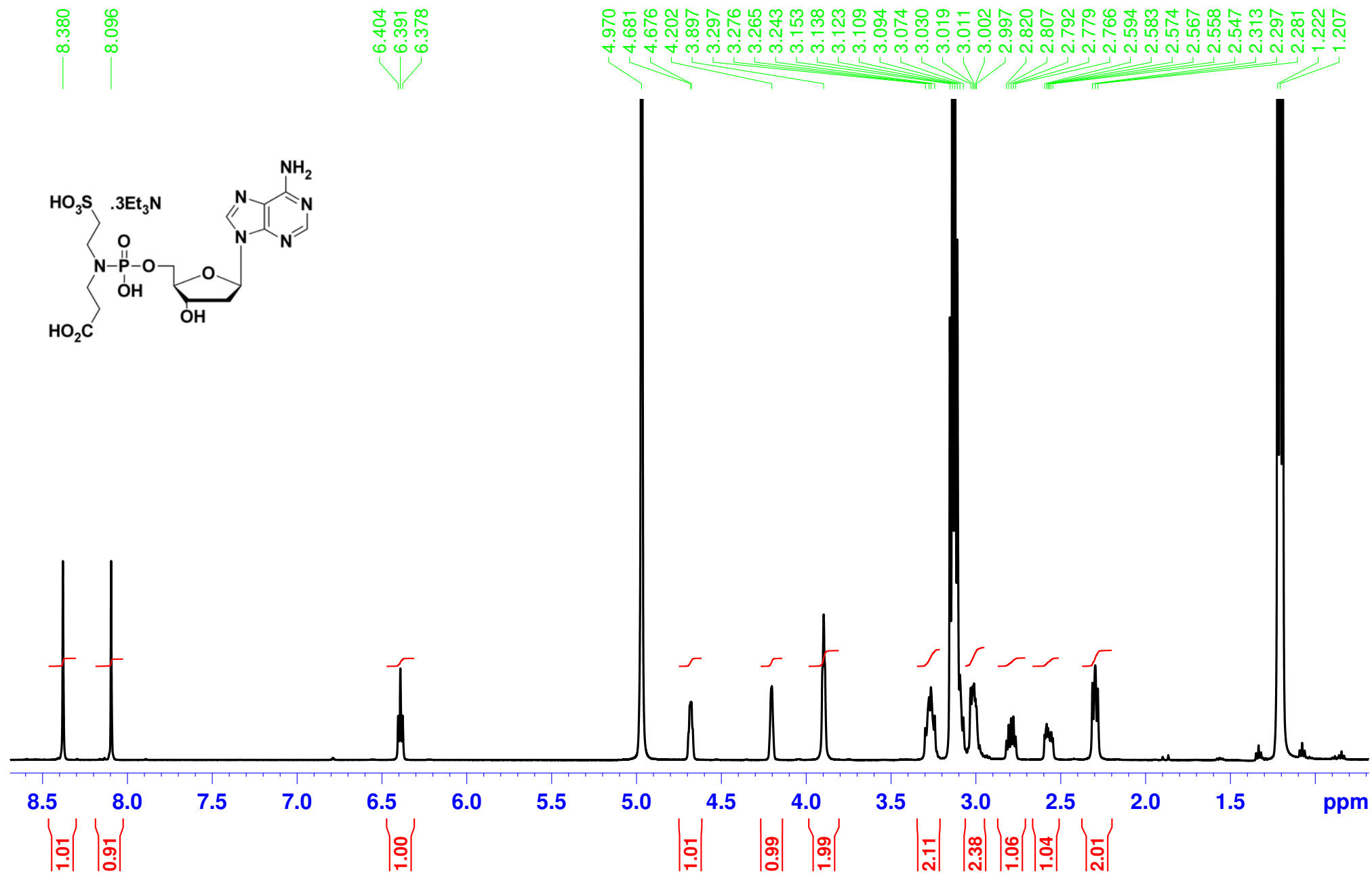
Compound 29 in D2O
31P spectrum - 202 MHz @ 6C



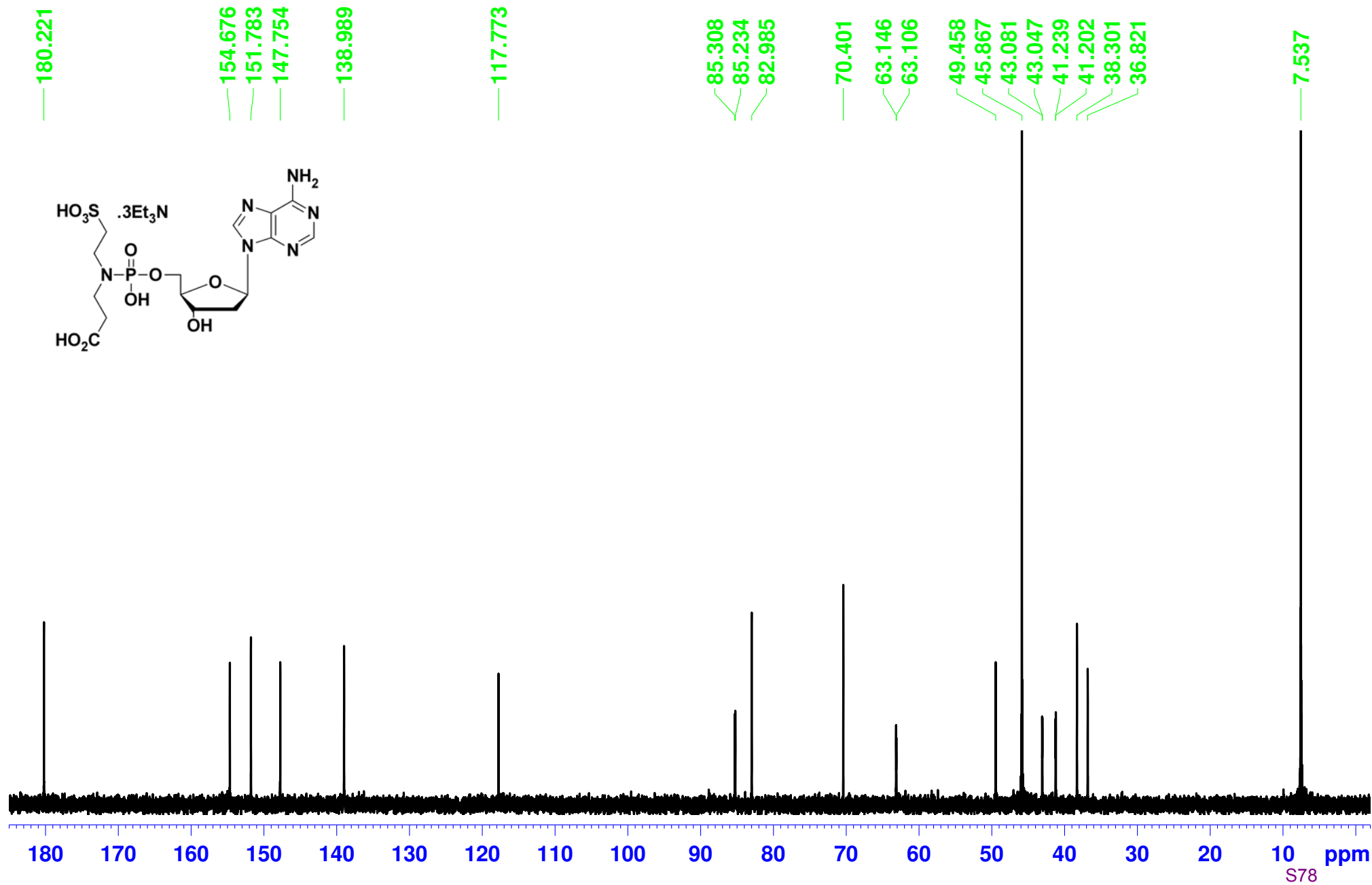
8.142



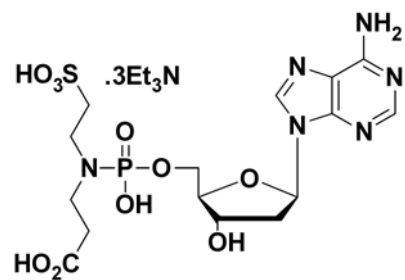
Compound 30 in D2O
1H spectrum - 500 MHz @ 5C



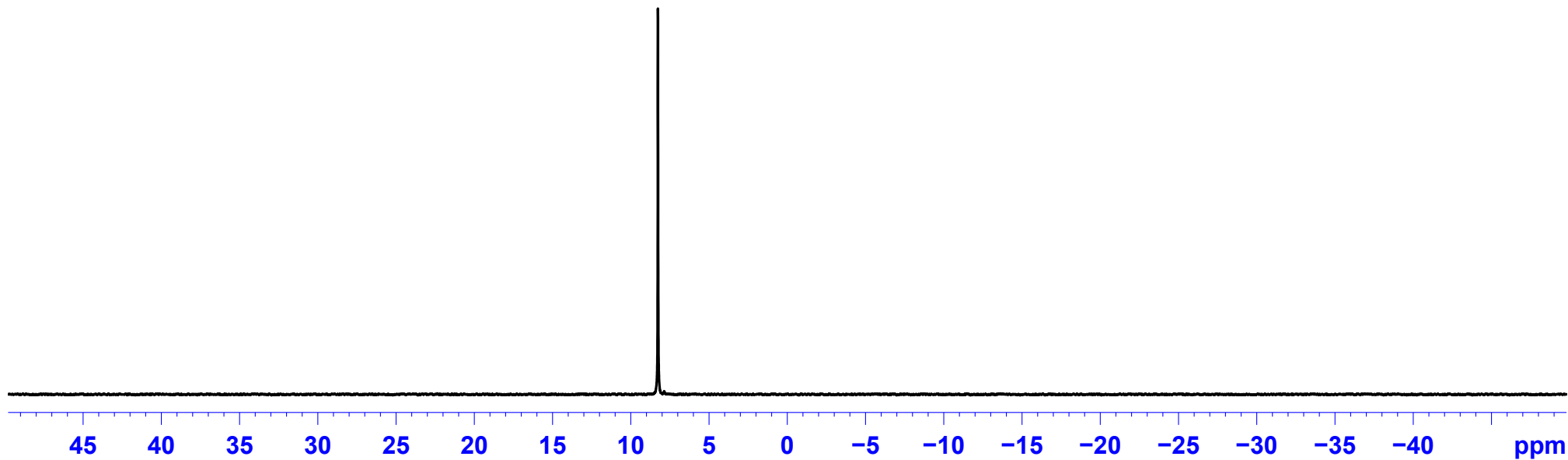
Compound 30 in D2O
13C spectrum - 125 MHz @ 5C



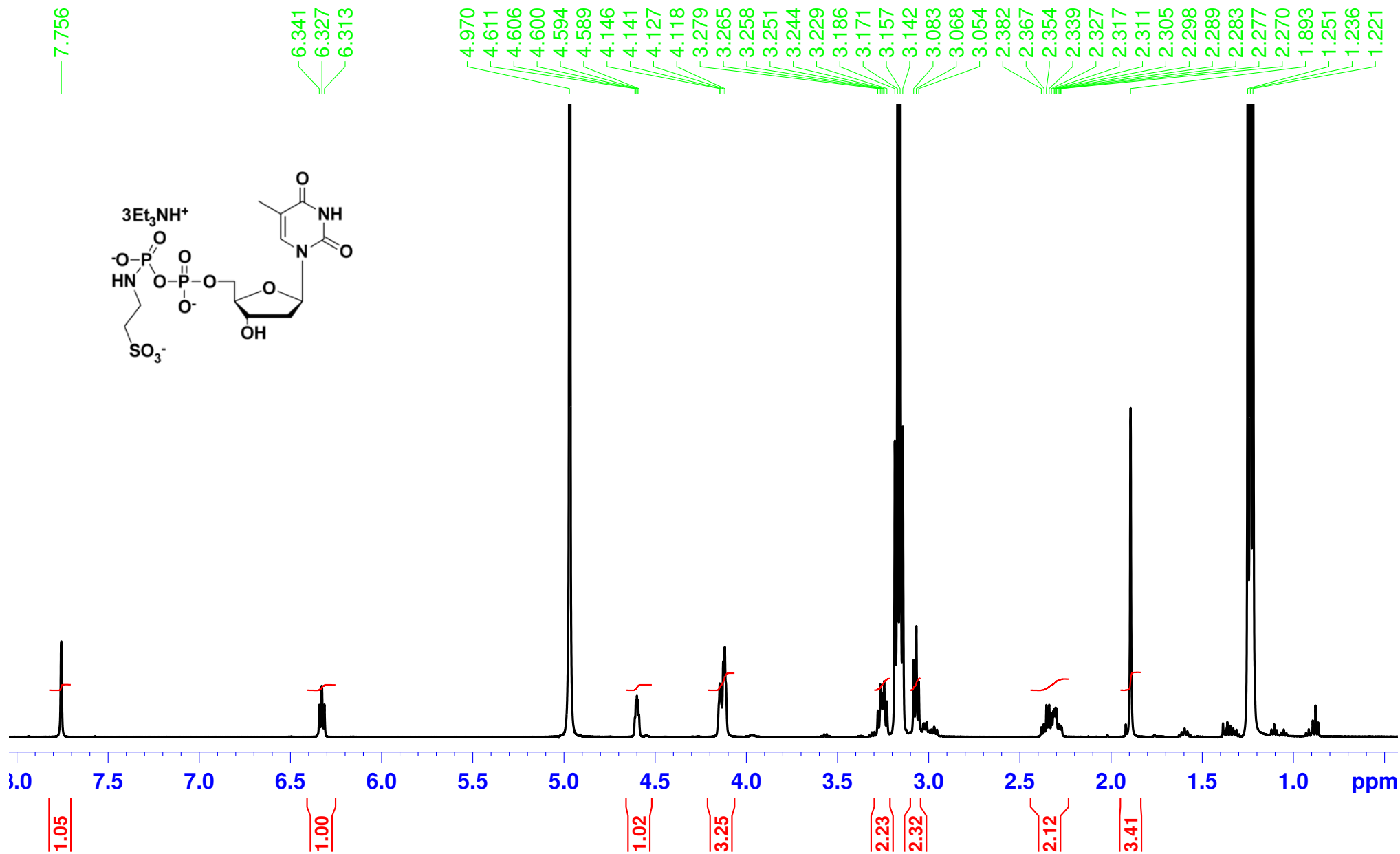
Compound 30 in D2O
31P spectrum - 202 MHz @ 5C



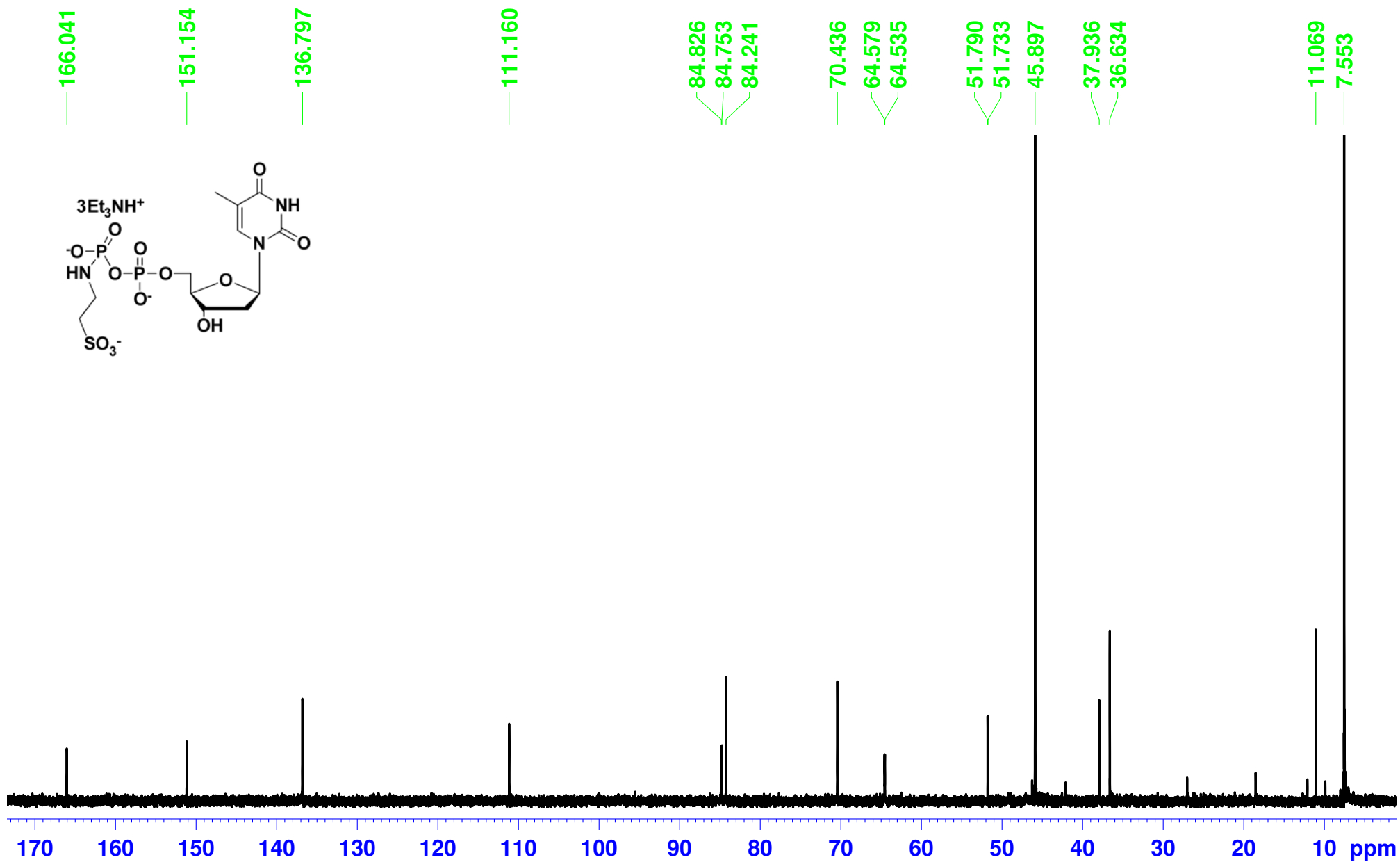
8.267



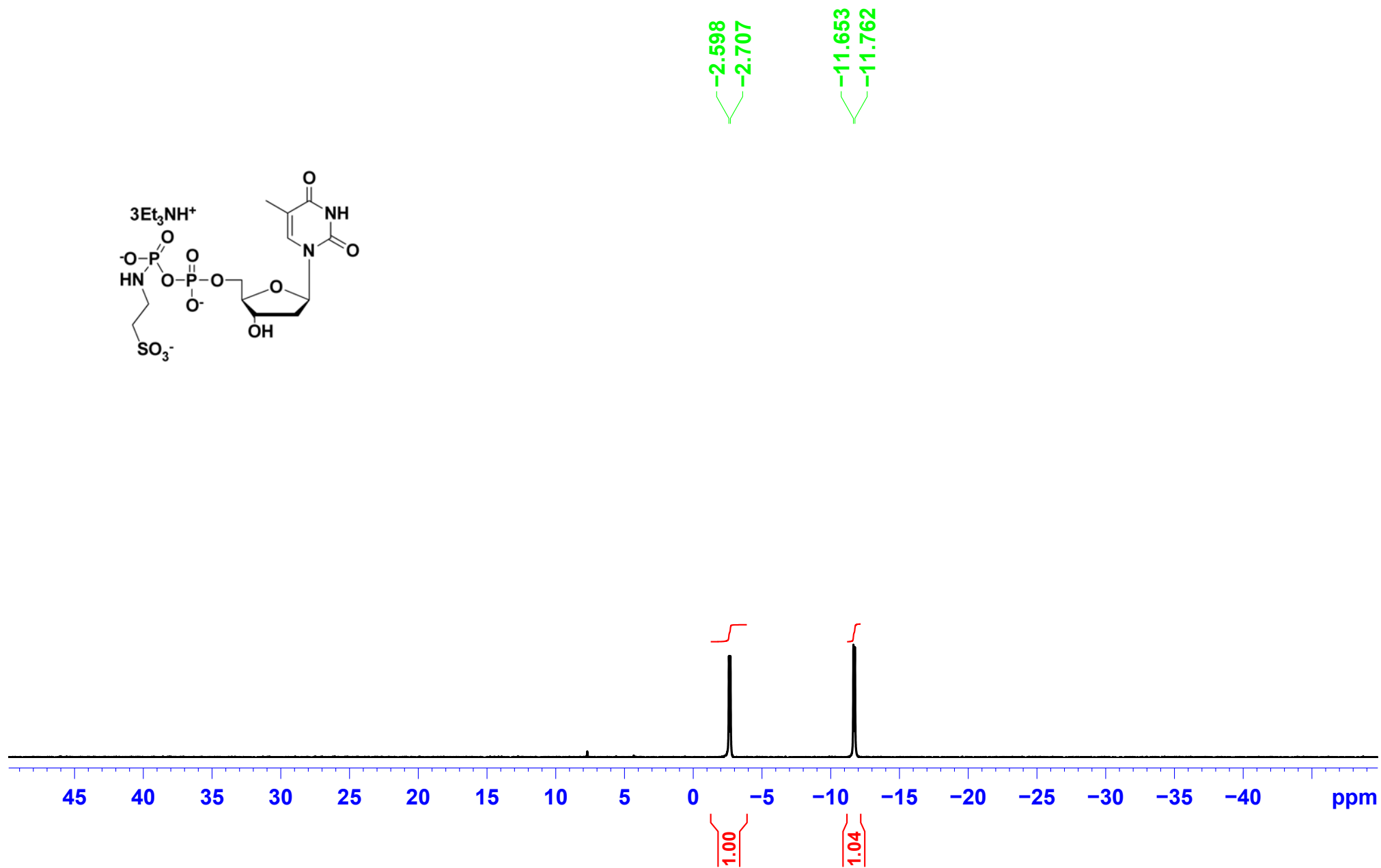
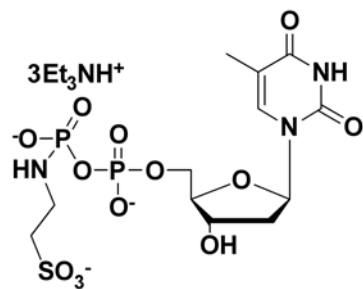
Compound 33 in D2O
1H spectrum - 500 MHz @ 6 C



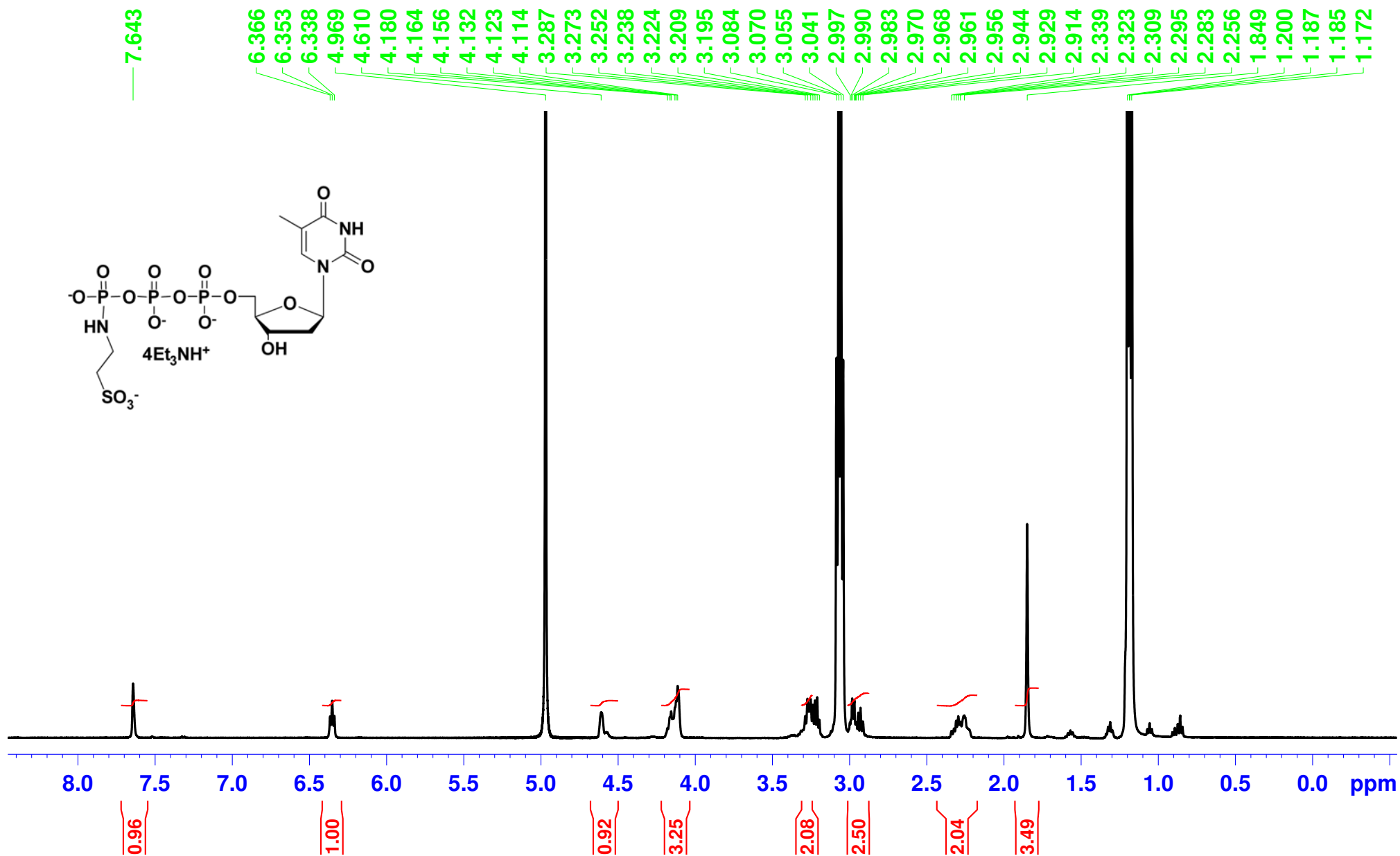
Compound 33 in D2O
13C spectrum - 125 MHz @ 6C



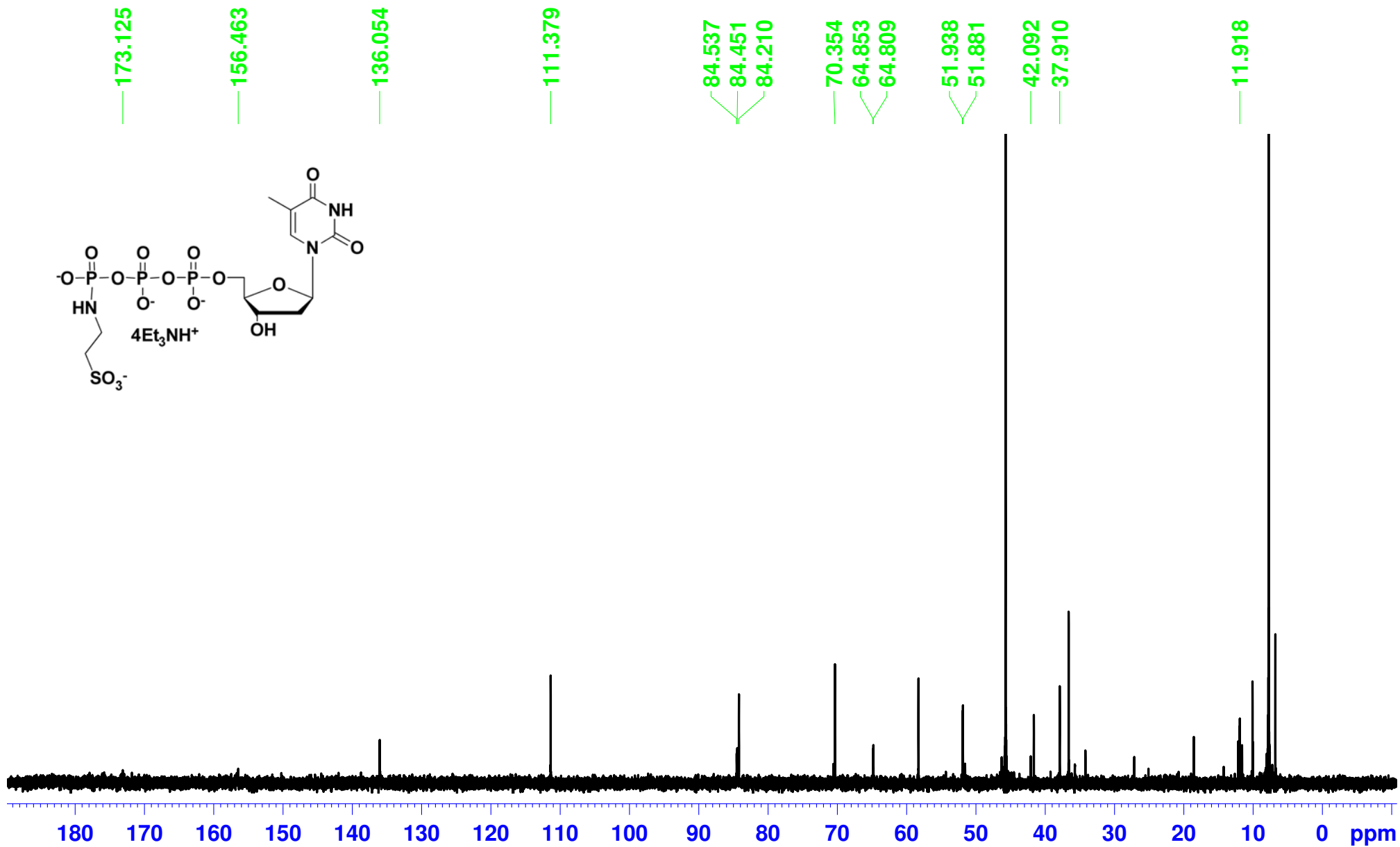
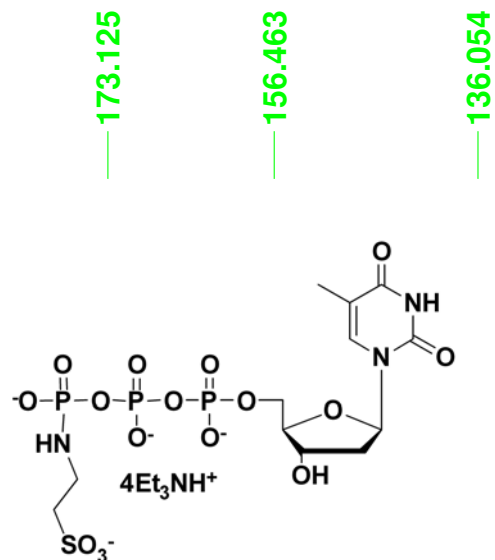
Compound 33 in D2O
31P spectrum - 202 MHz @ 6C



Compound 35 in D2O
1H spectrum - 500 MHz @ 6 C



Compound 35 in D2O
13C spectrum - 125 MHz @ 6 C



Compound 35 in D2O
31P spectrum - 202 MHz @ 6 C

