Supplementary material

Synthesis of mixed dinucleotides by mechanochemistry

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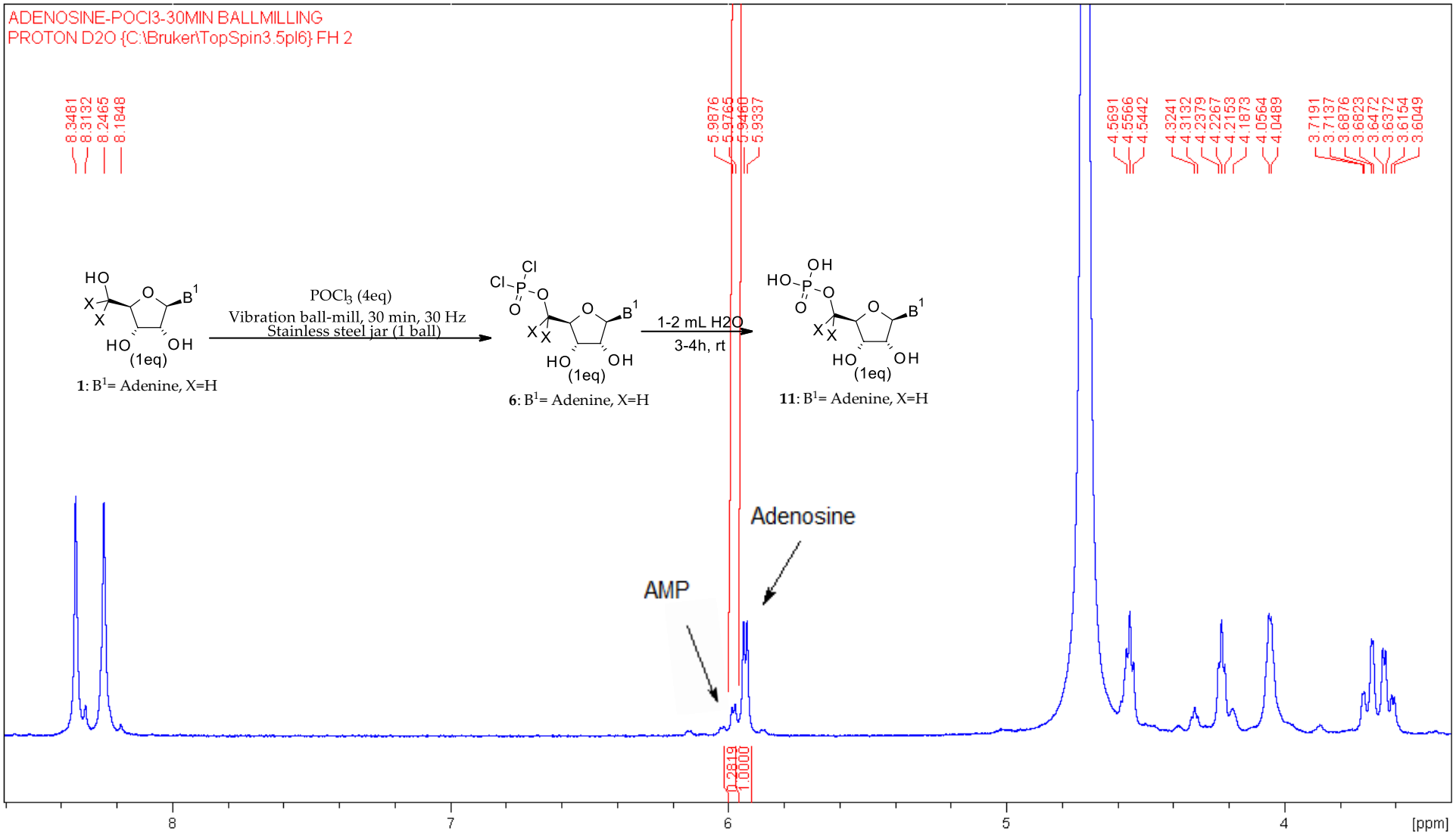
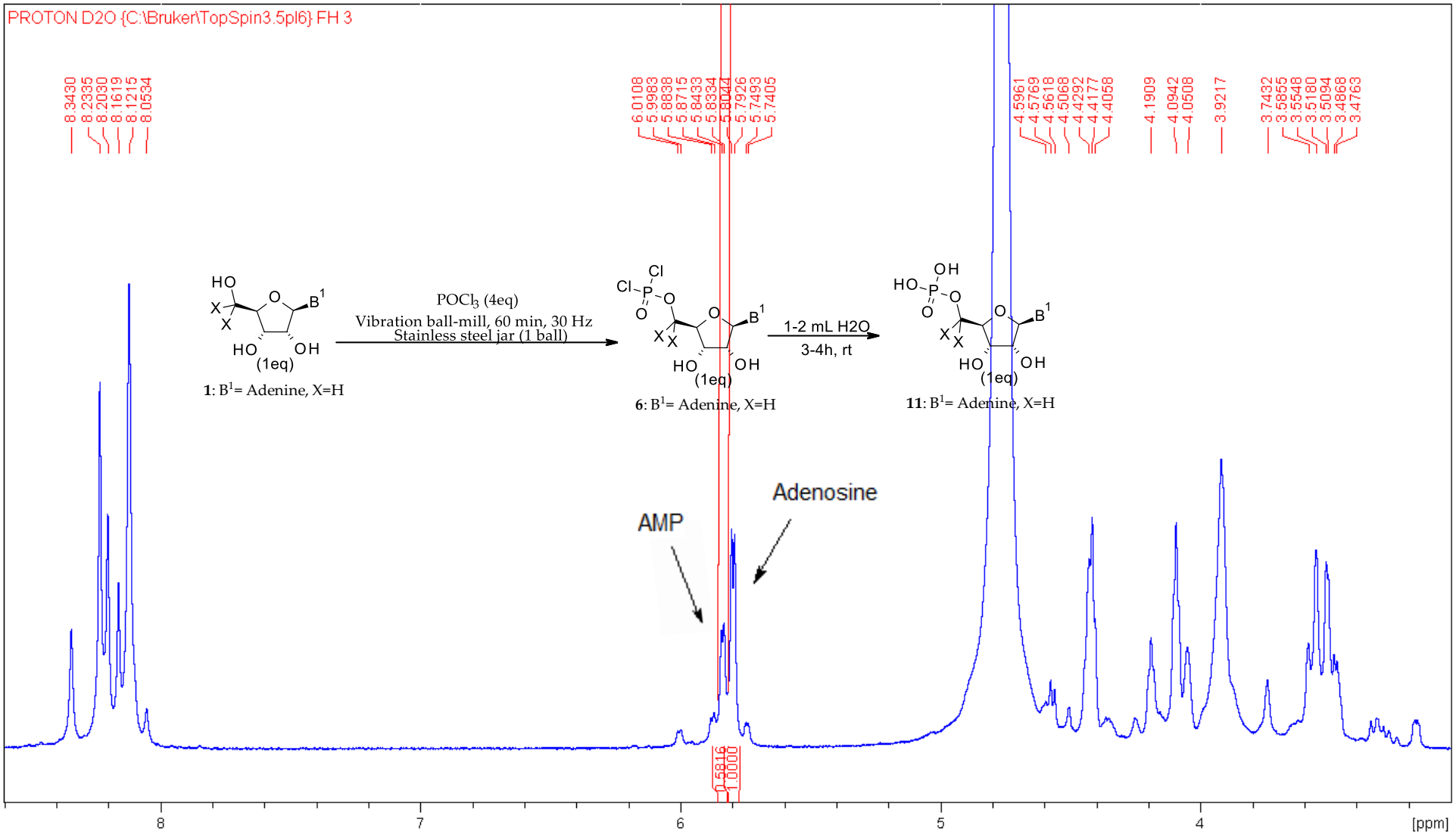
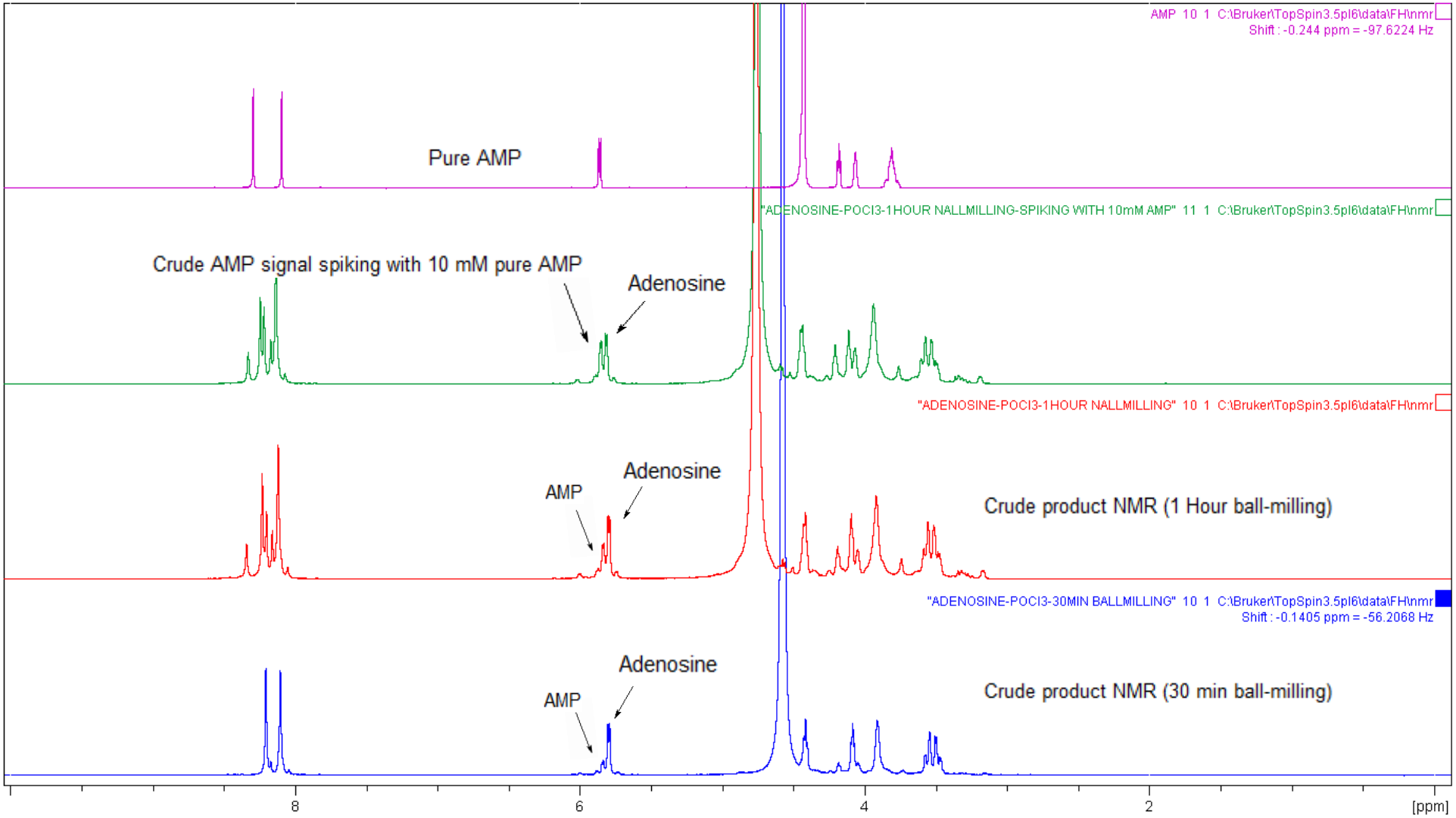
* Correspondence: mmigaud@southalabama.edu;



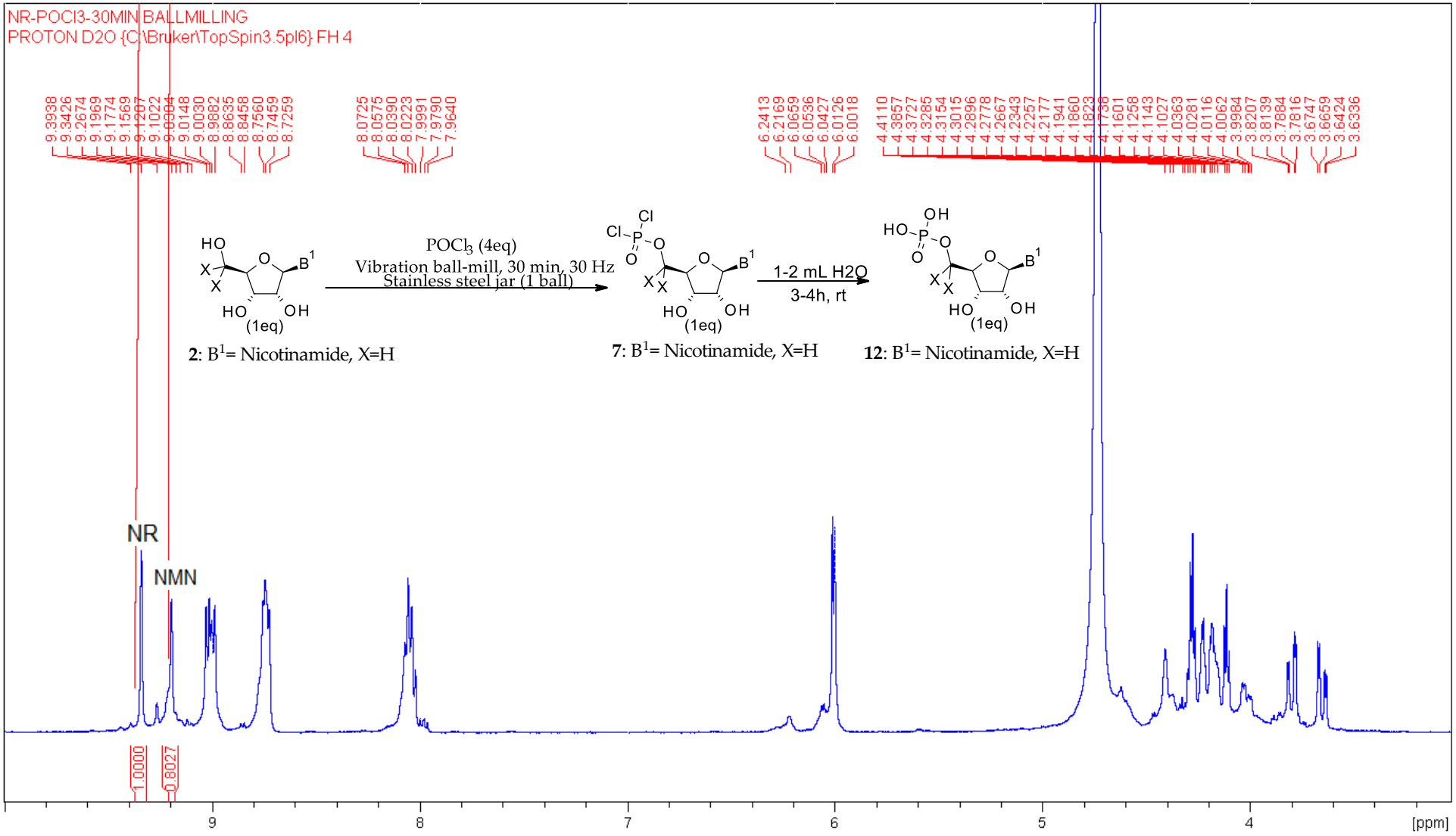
Compound 11: ^{1}H-NMR of crude product after 30 minutes of ball-milling (D_2O)



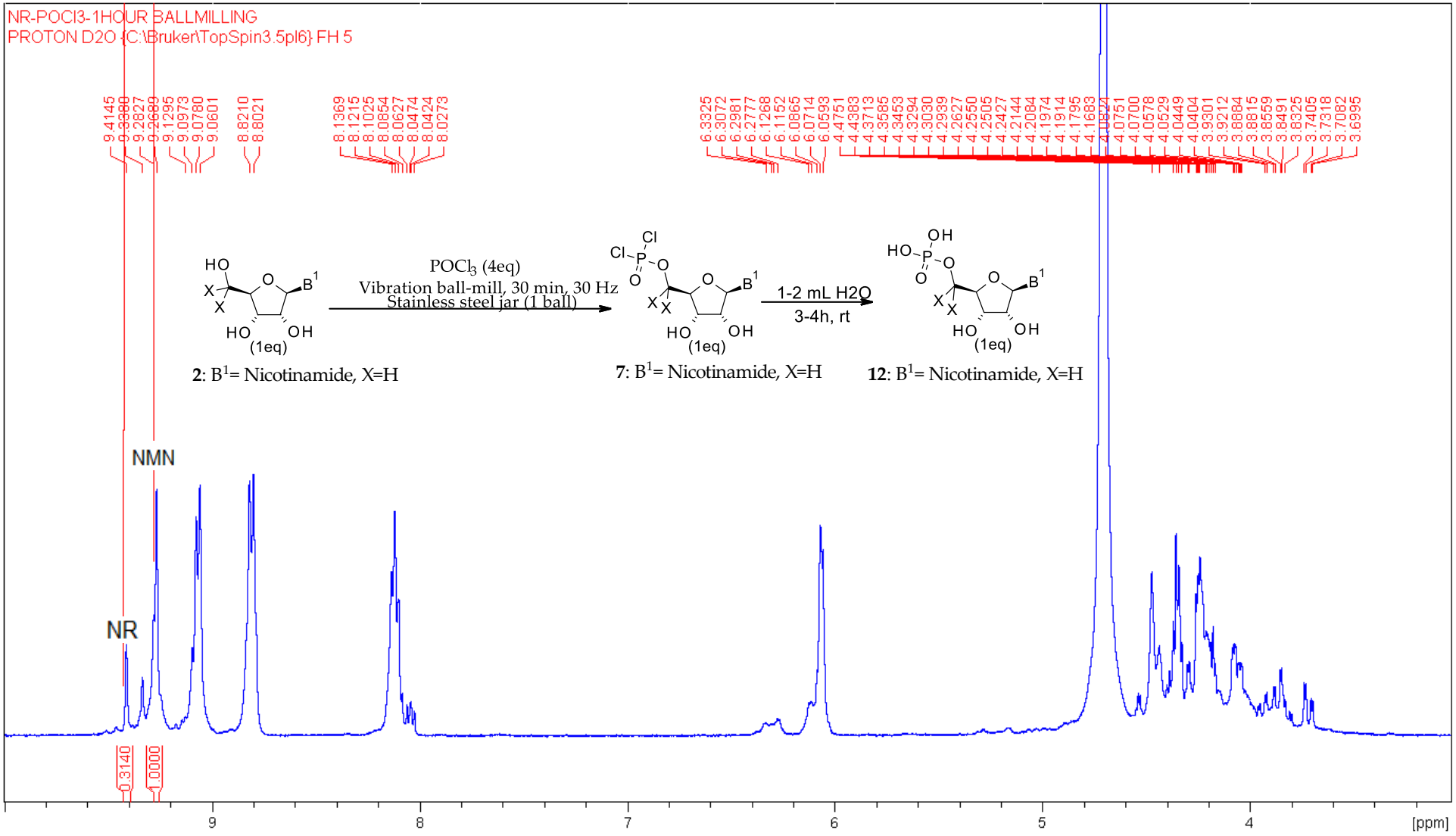
Compound 11: ^{1}H-NMR of crude product after 1 hour of ball-milling (D_2O)



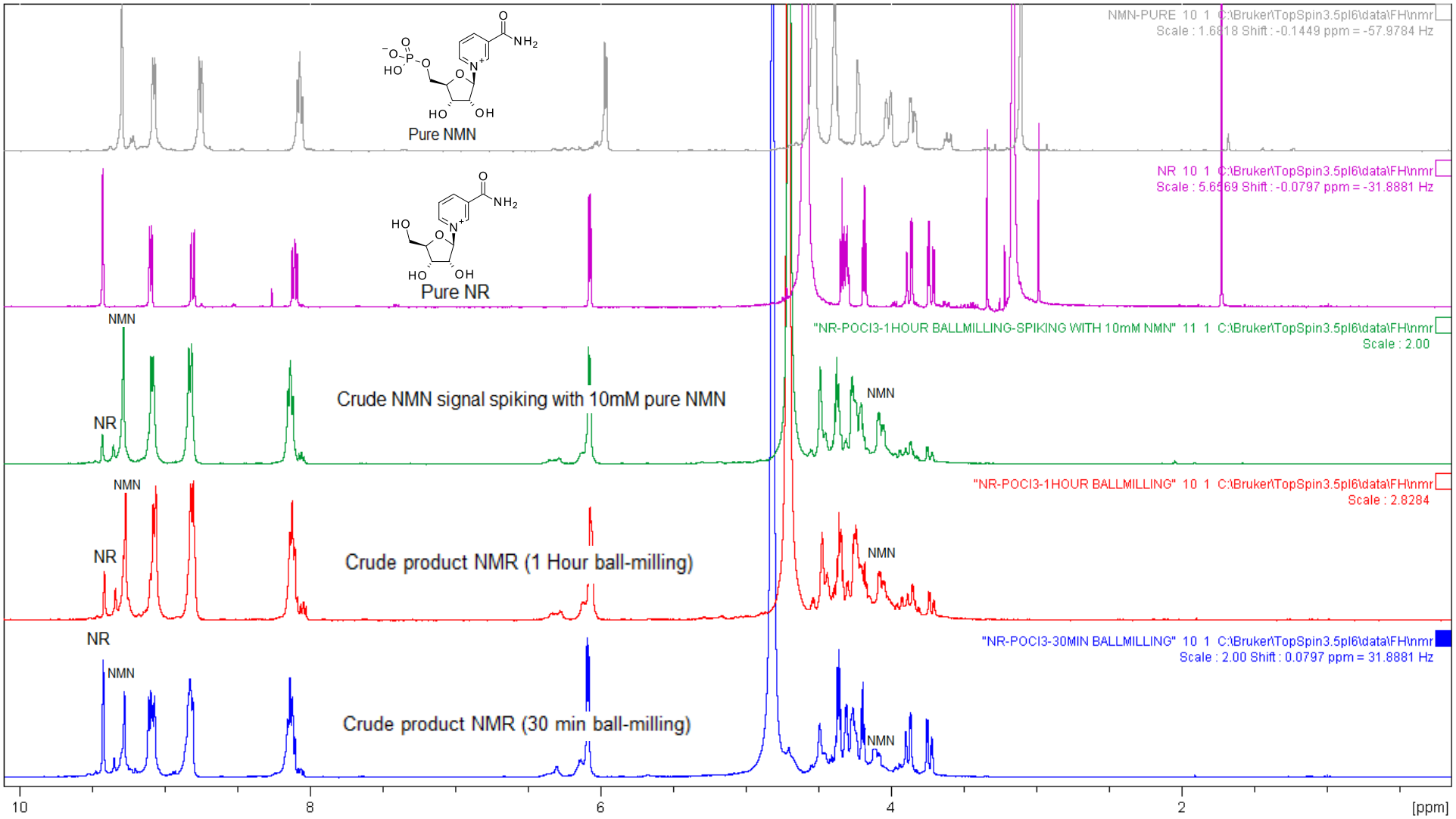
Compound 11: AMP Signals from a one-hour ball-milling crude product spiked with 10 mM pure AMP (D_2O)



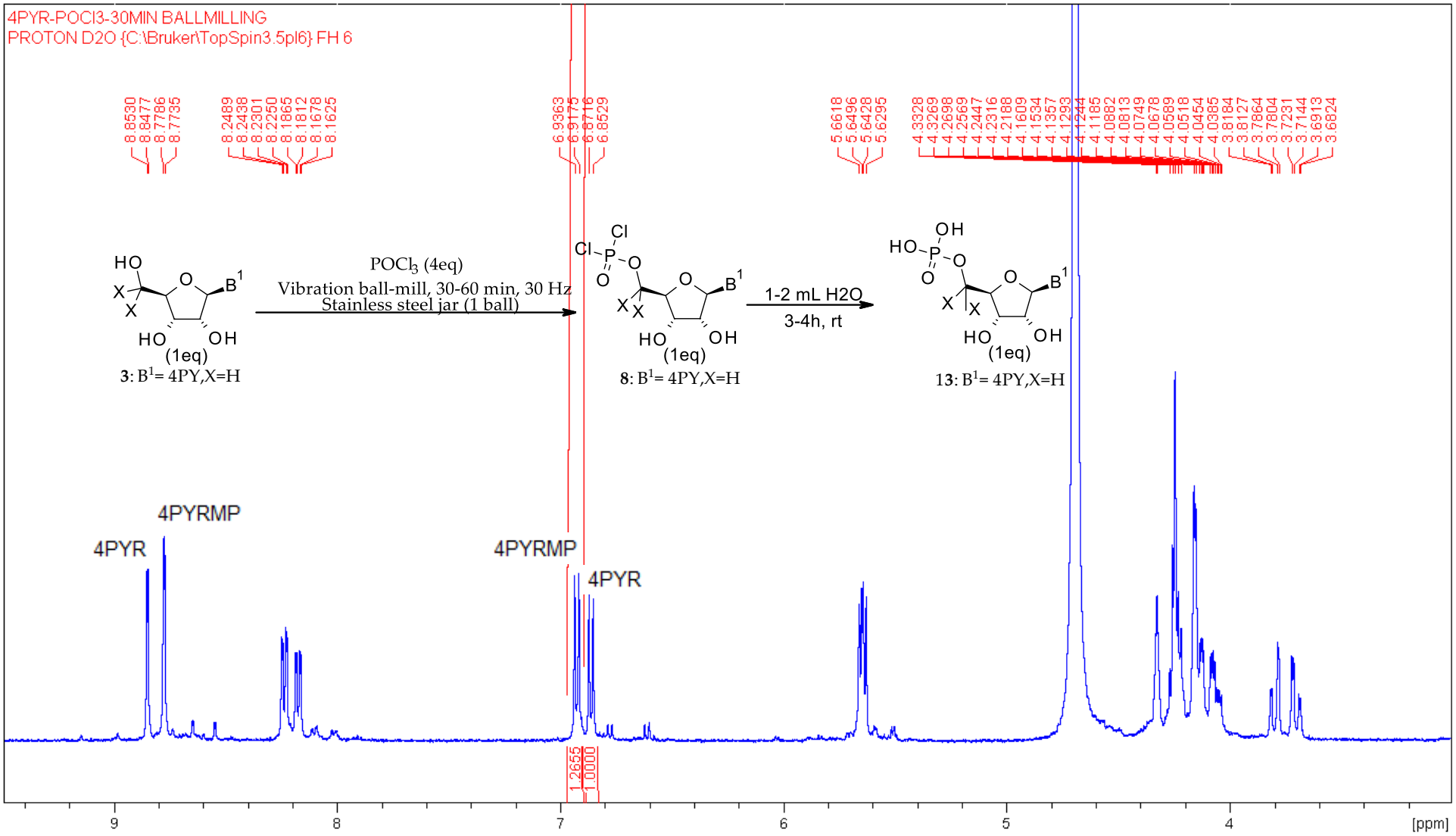
Compound 12: ^{1}H-NMR of crude product after 30 minutes of ball-milling (D_2O)



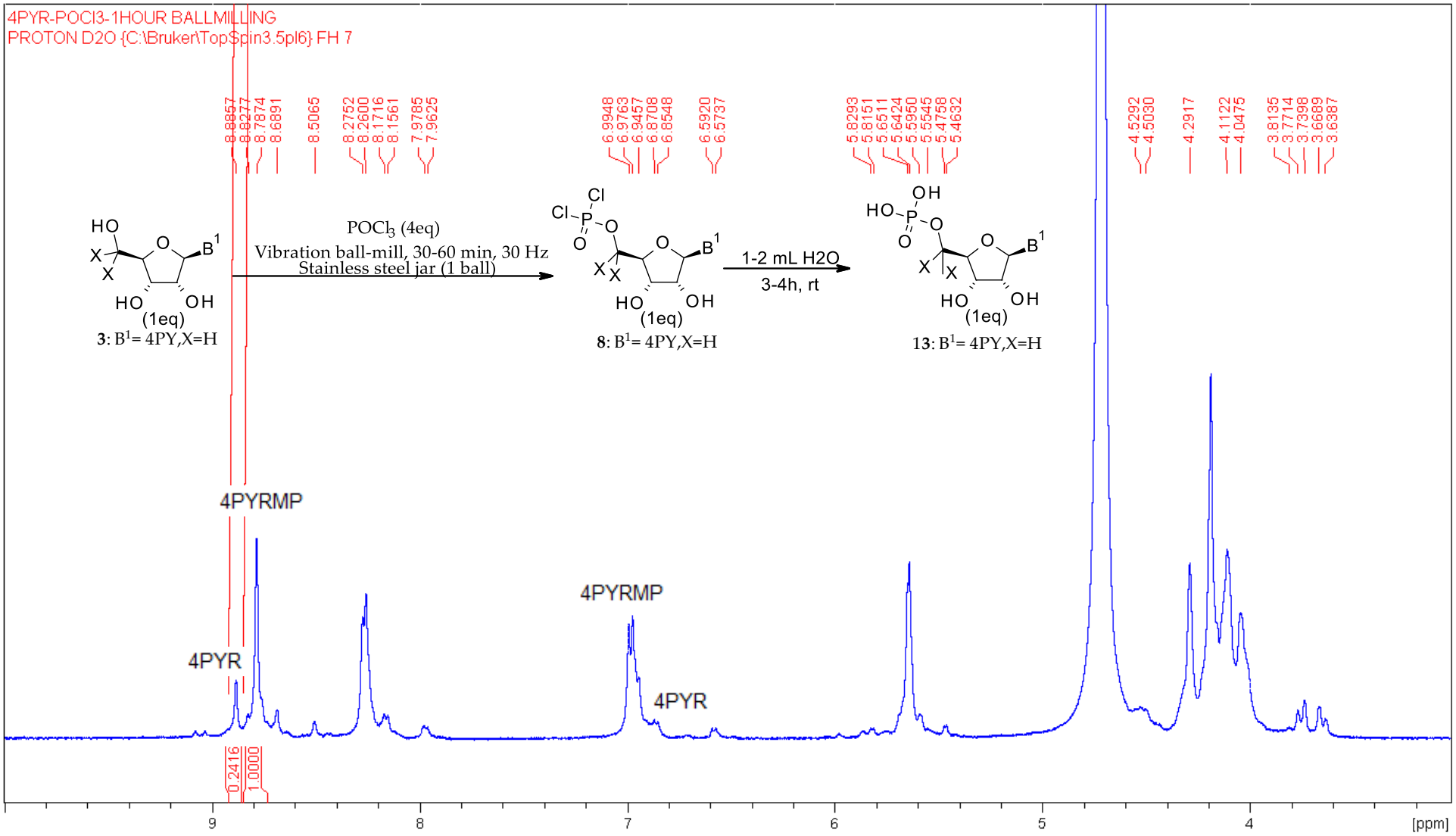
Compound 12: ^{1}H-NMR of crude product after 1 hour of ball-milling (D_2O)



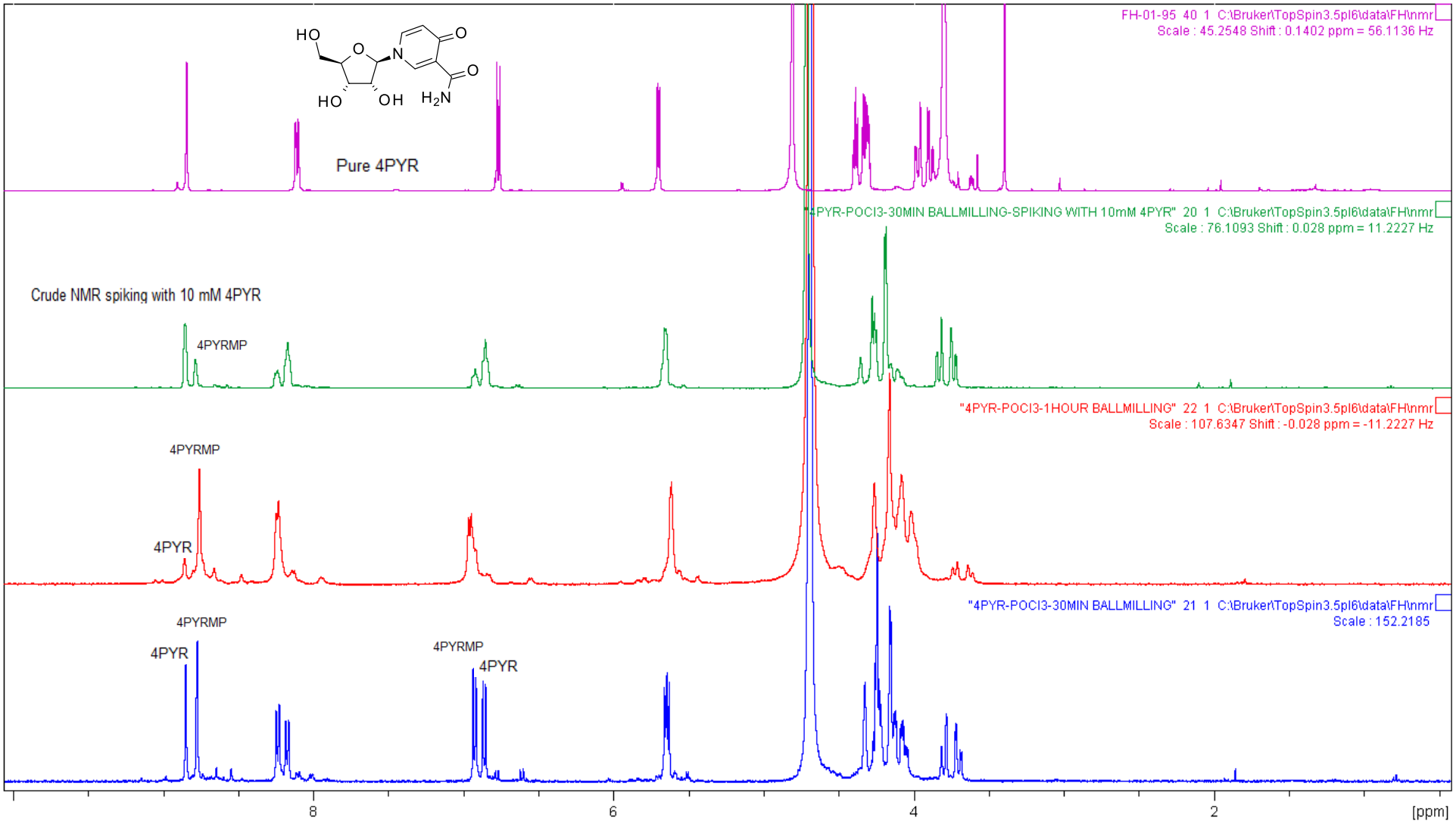
Compound 12: NMN Signals from a one-hour ball-milling crude product spiked with 10 mM pure NMN (D_2O)



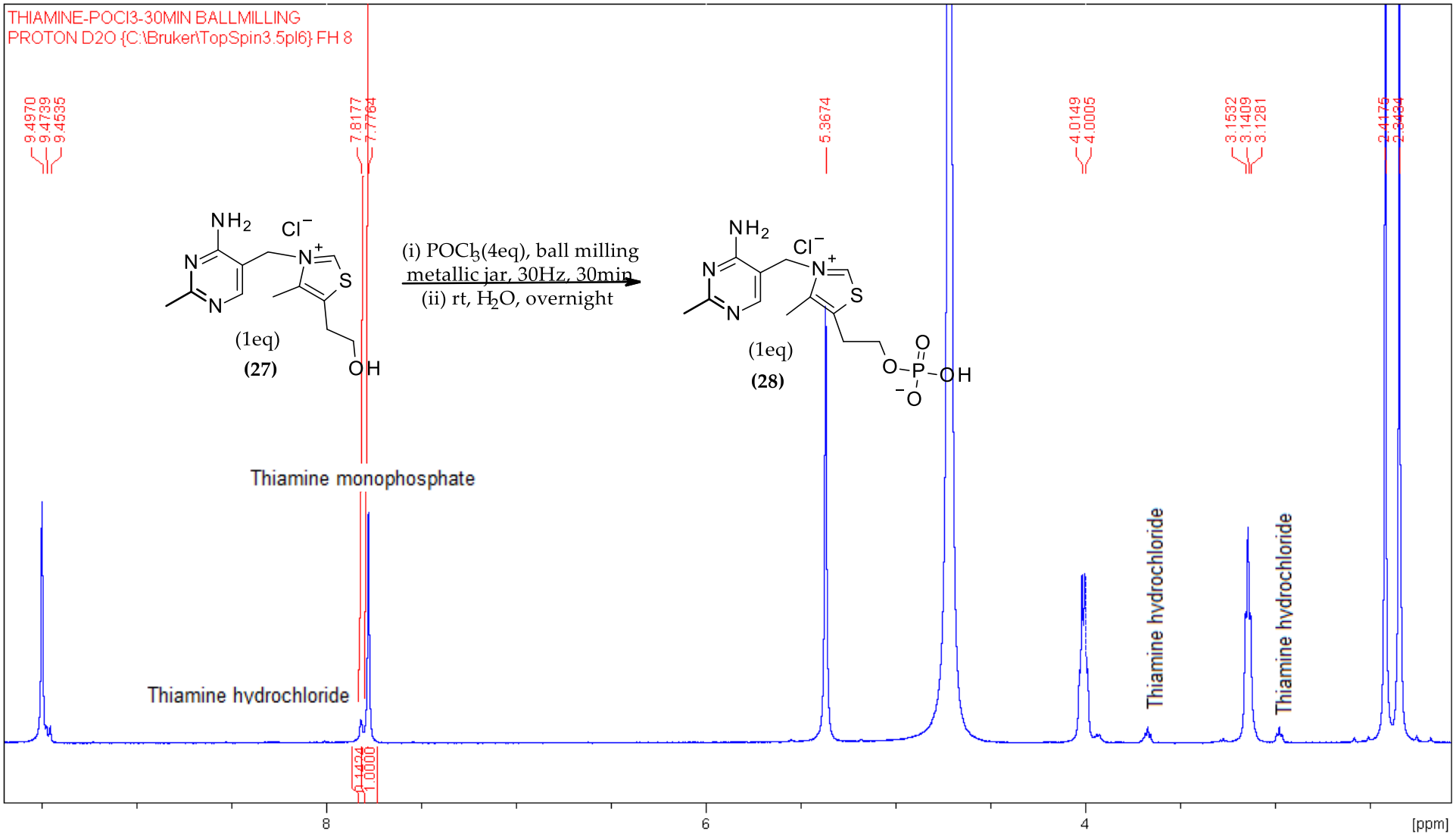
Compound 13: ^{1}H-NMR of crude product after 30 minutes of ball-milling (D_2O)



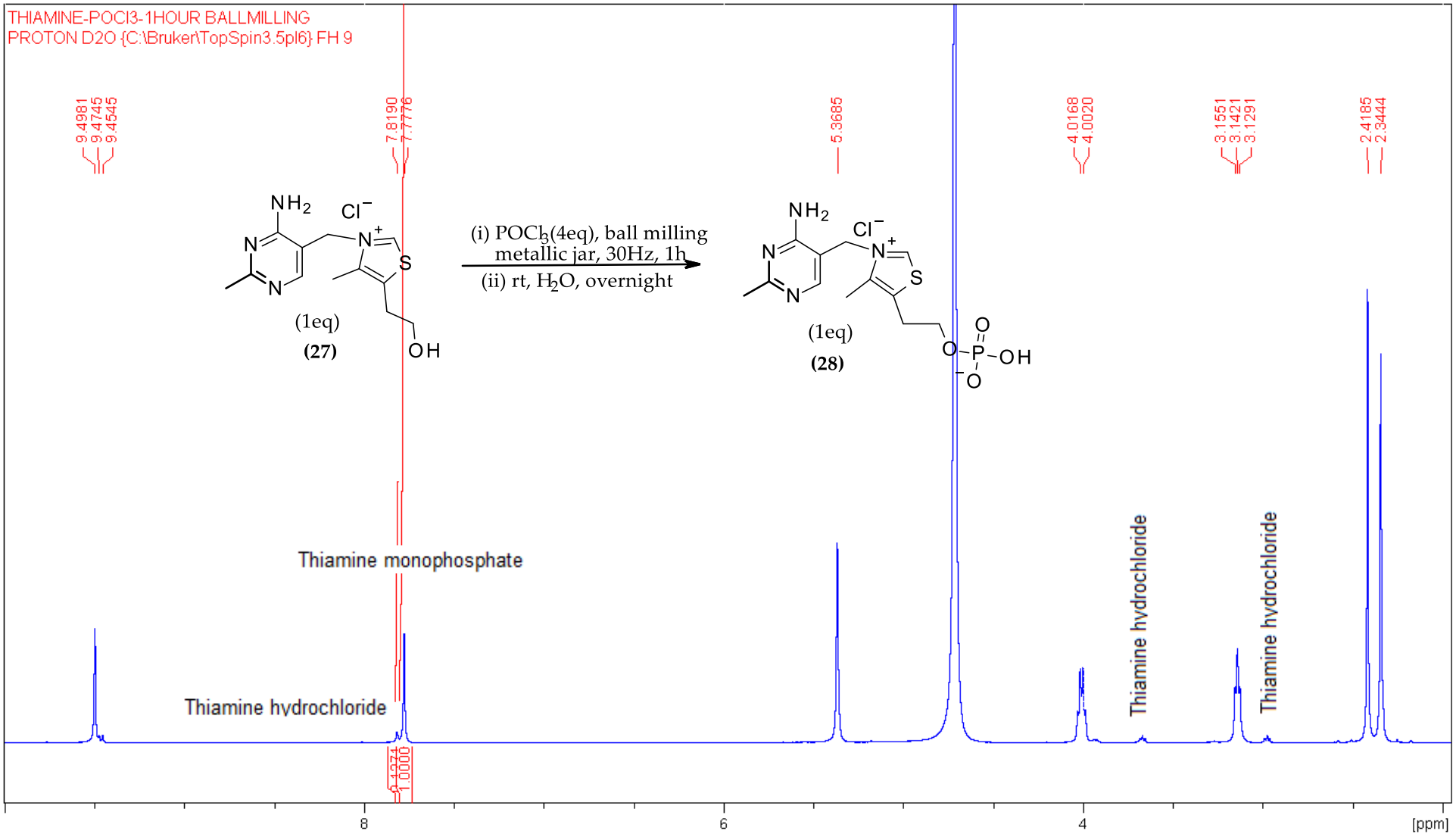
Compound 13: ^{1}H-NMR of crude product after 1 hour of ball-milling (D_2O)



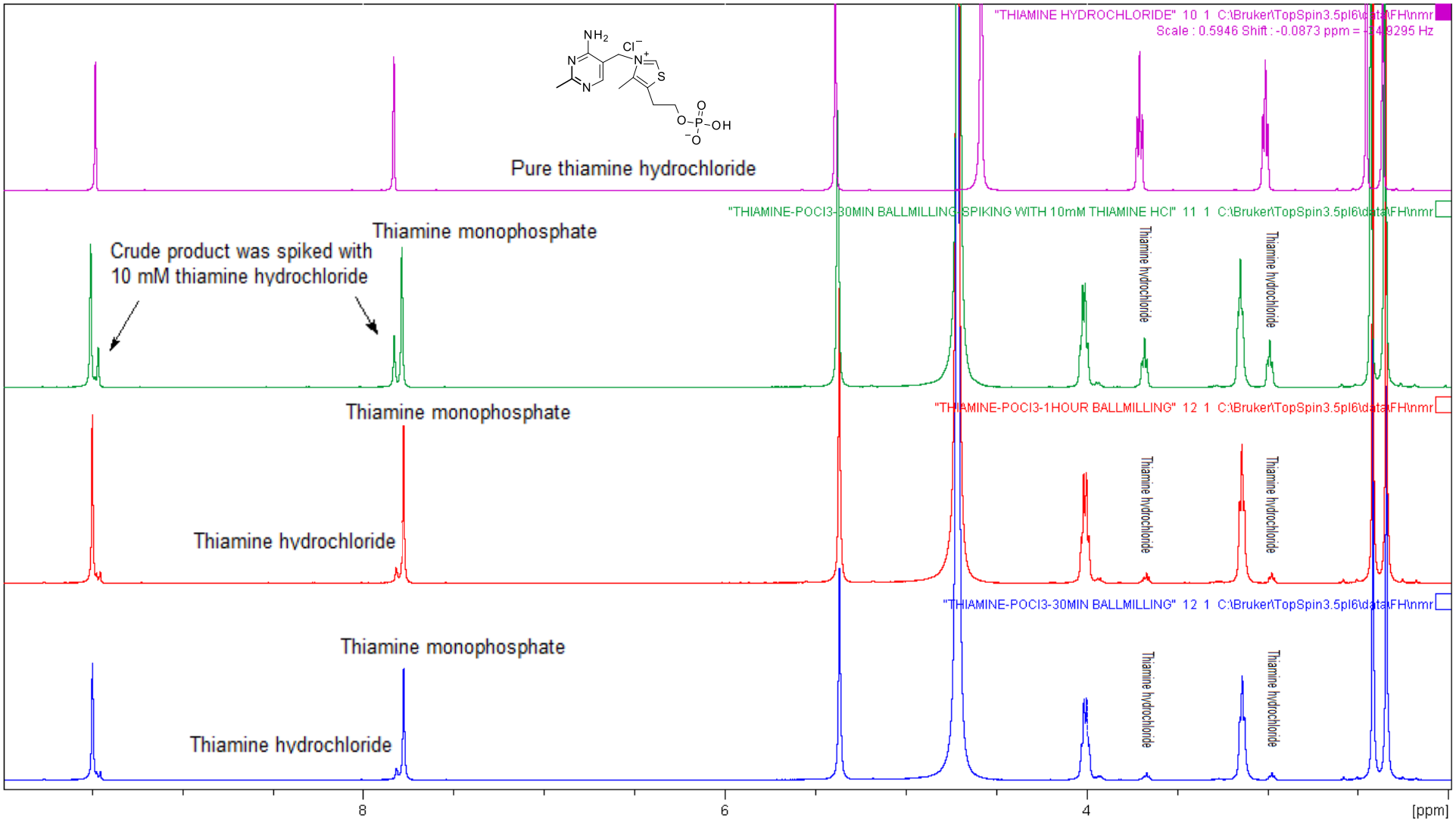
Compound 13: 4PYR Signals from a one-hour ball-milling crude product spiked with 10 mM pure 4PYR (D_2O)



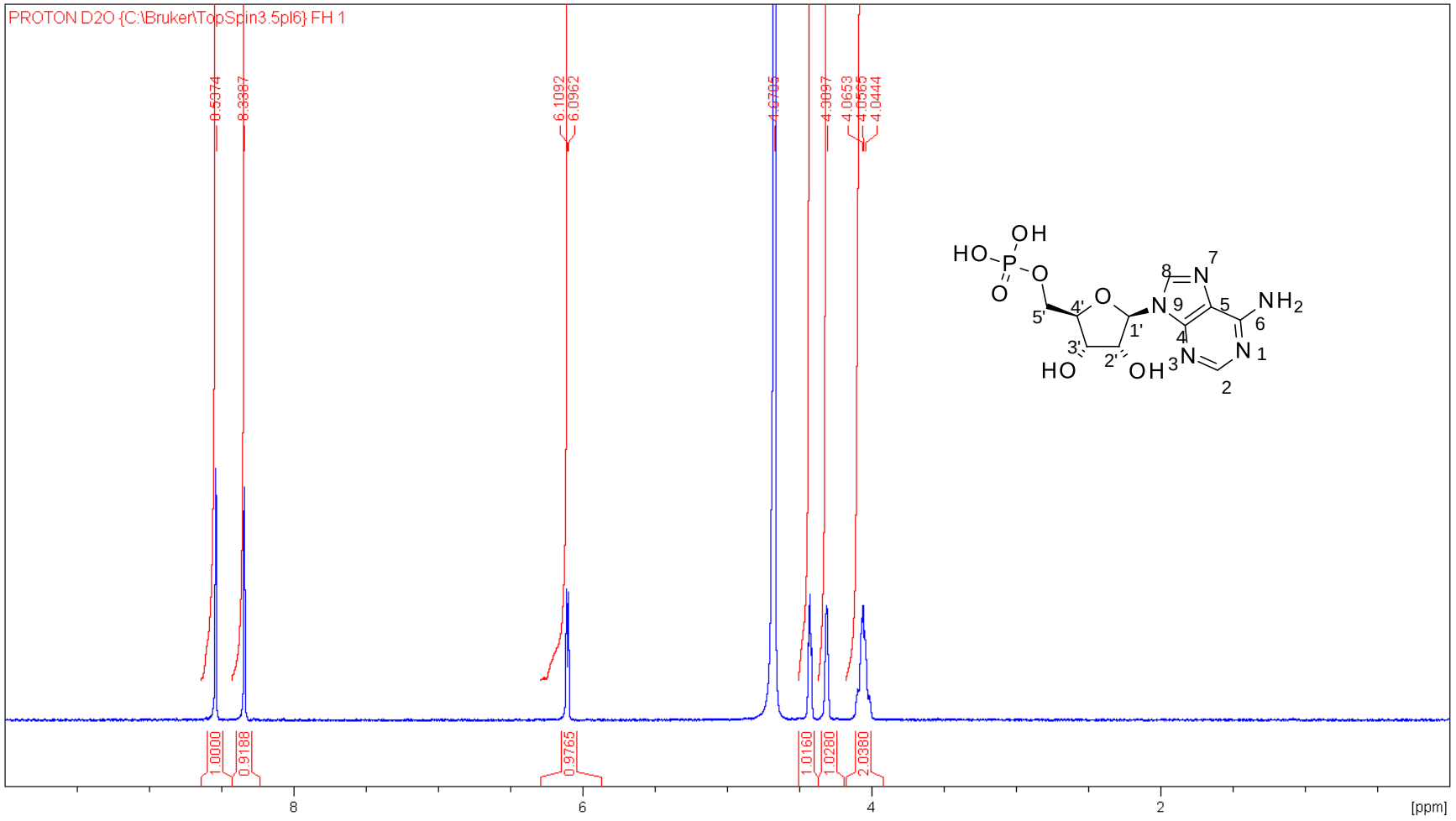
Compound 28: ^{1}H-NMR of crude product after 30 minutes of ball-milling (D_2O)



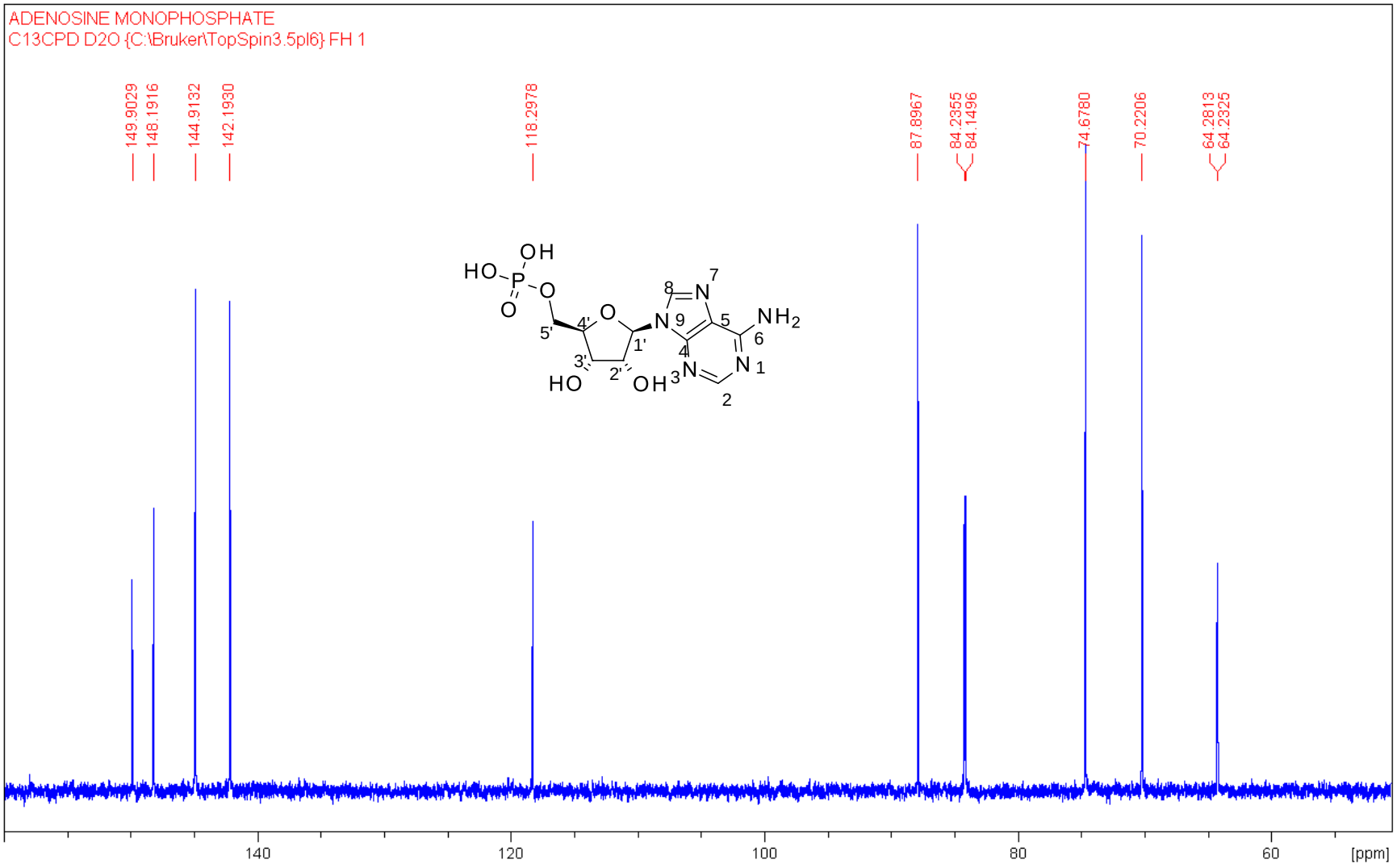
Compound 28: ^{1}H-NMR of crude product after 1 hour of ball-milling (D_2O)



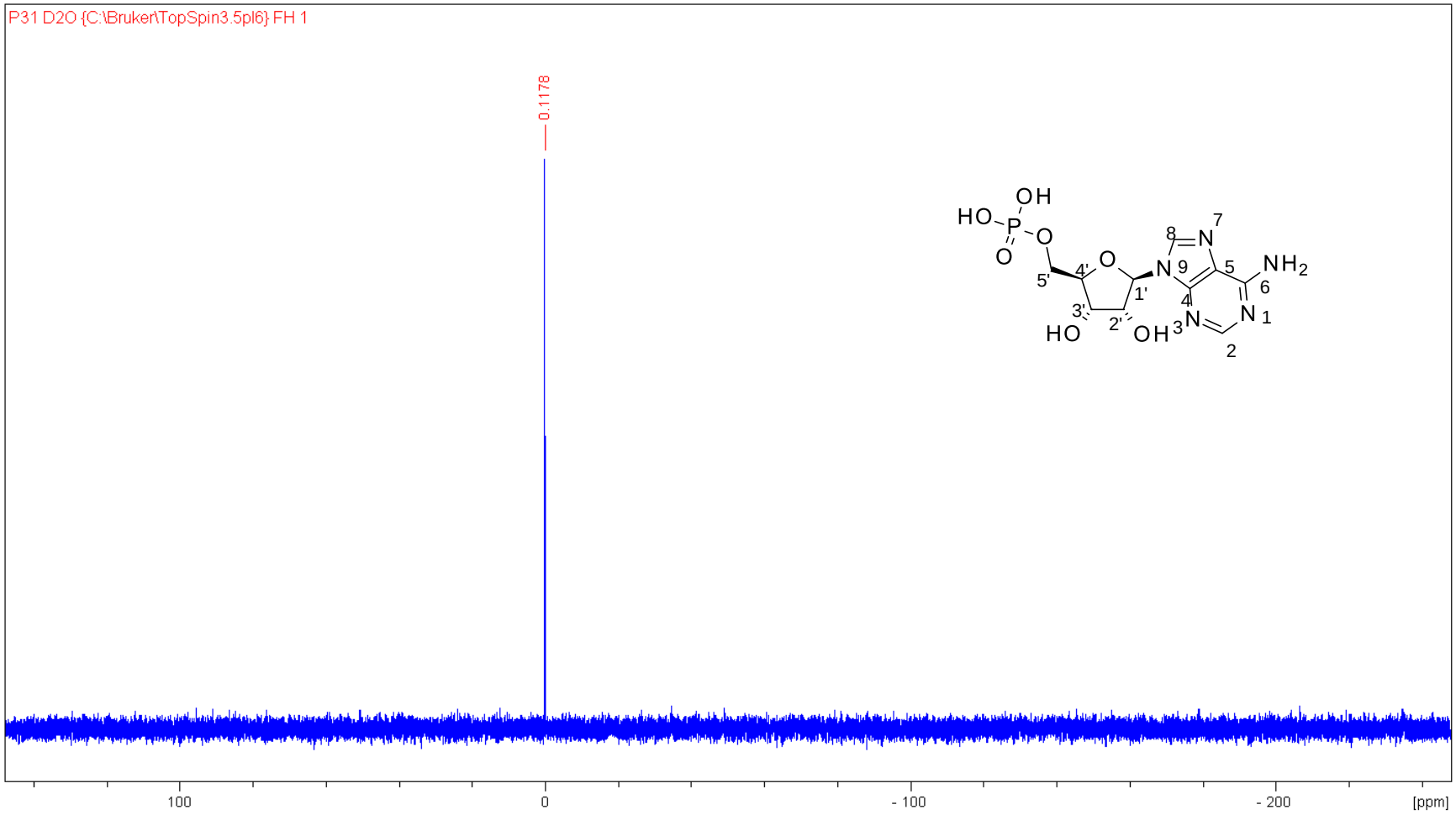
Compound 28: Thiamine Signals from a one-hour ball-milling crude product spiked with 10 mM pure thiamine hydrochloride (D_2O)



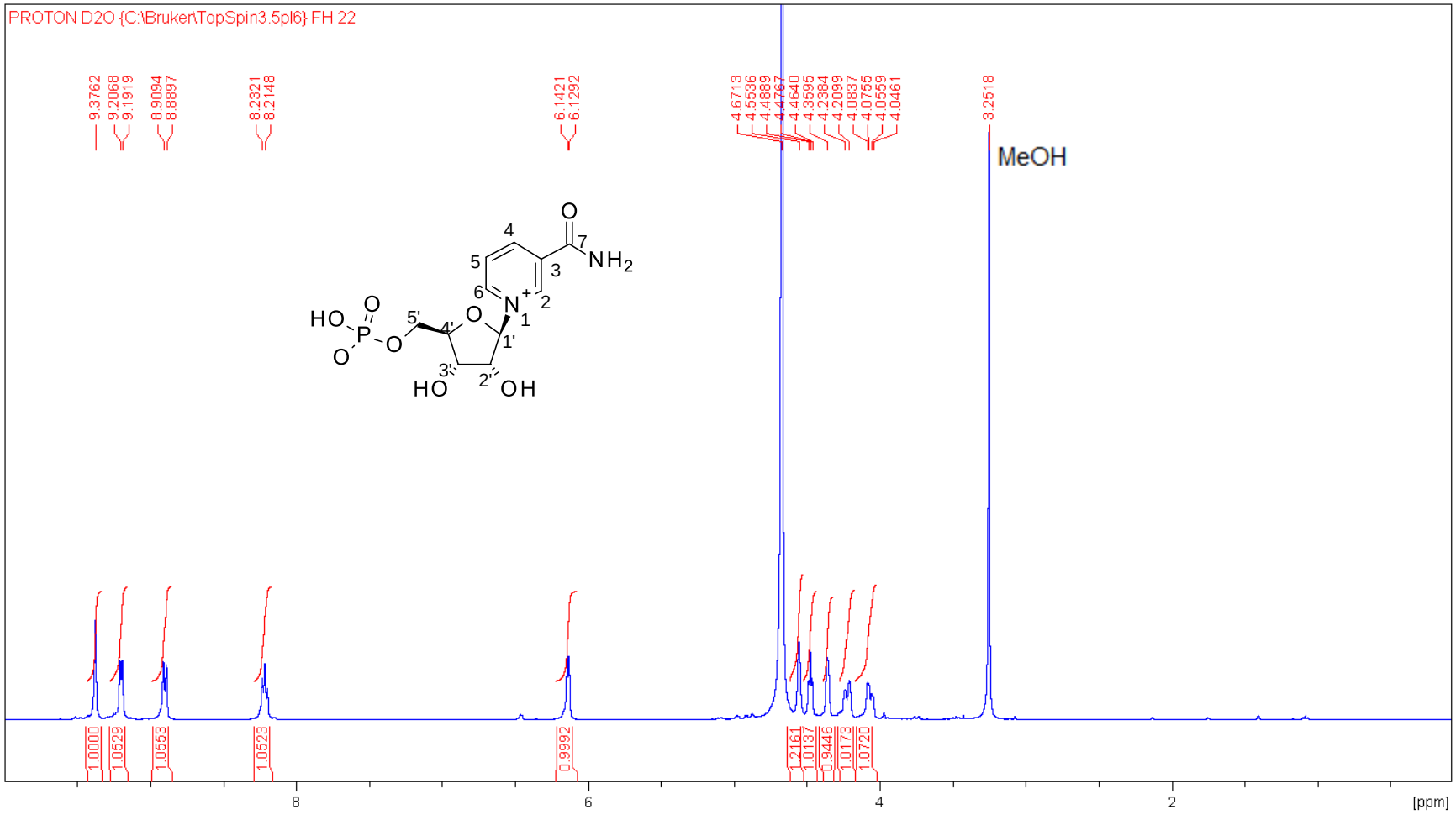
Compound 11. 400 MHz ^{1}H NMR spectrum in D_2O



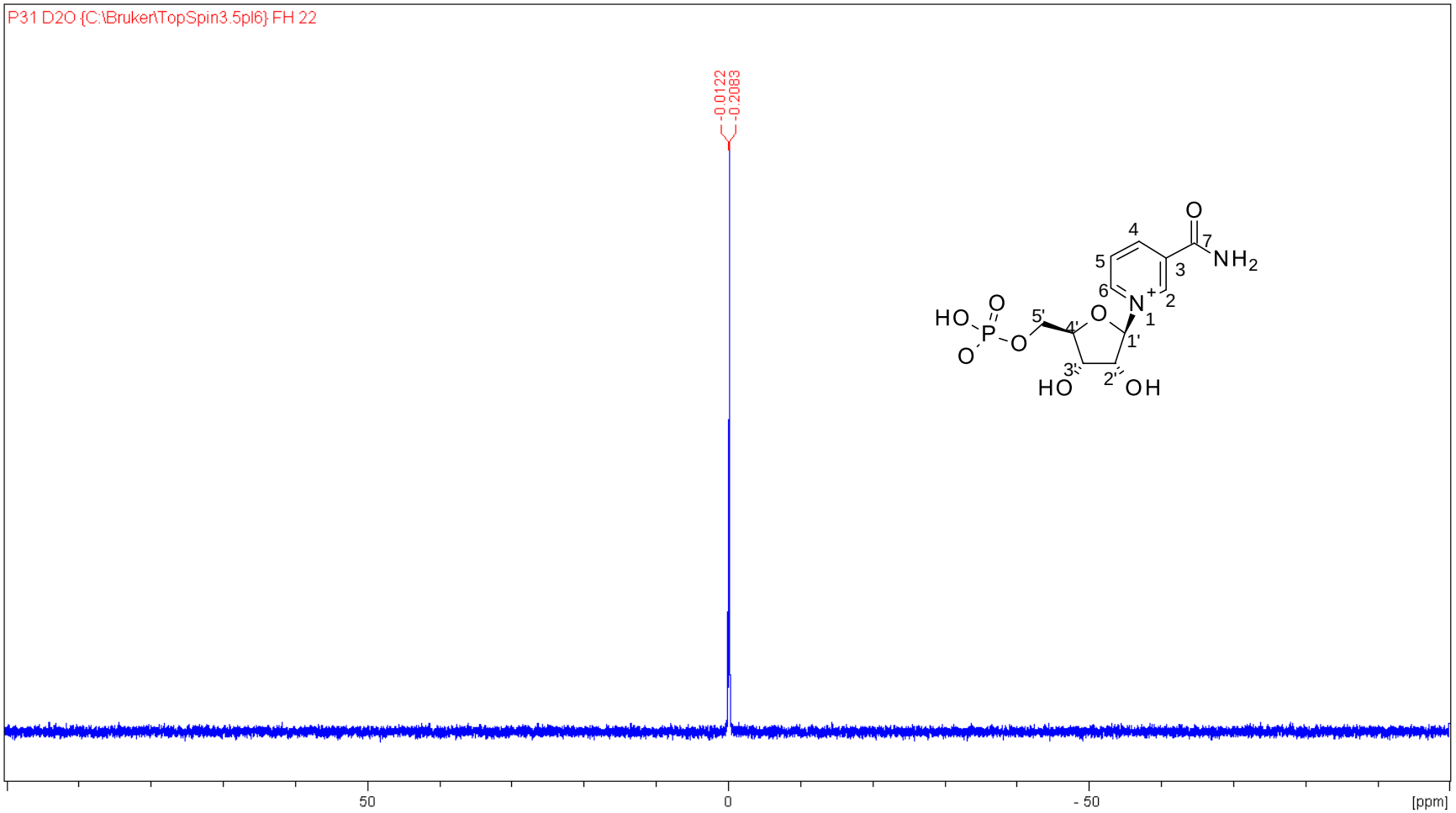
Compound 11. 100 MHz ^{13}C NMR spectrum in D_2O



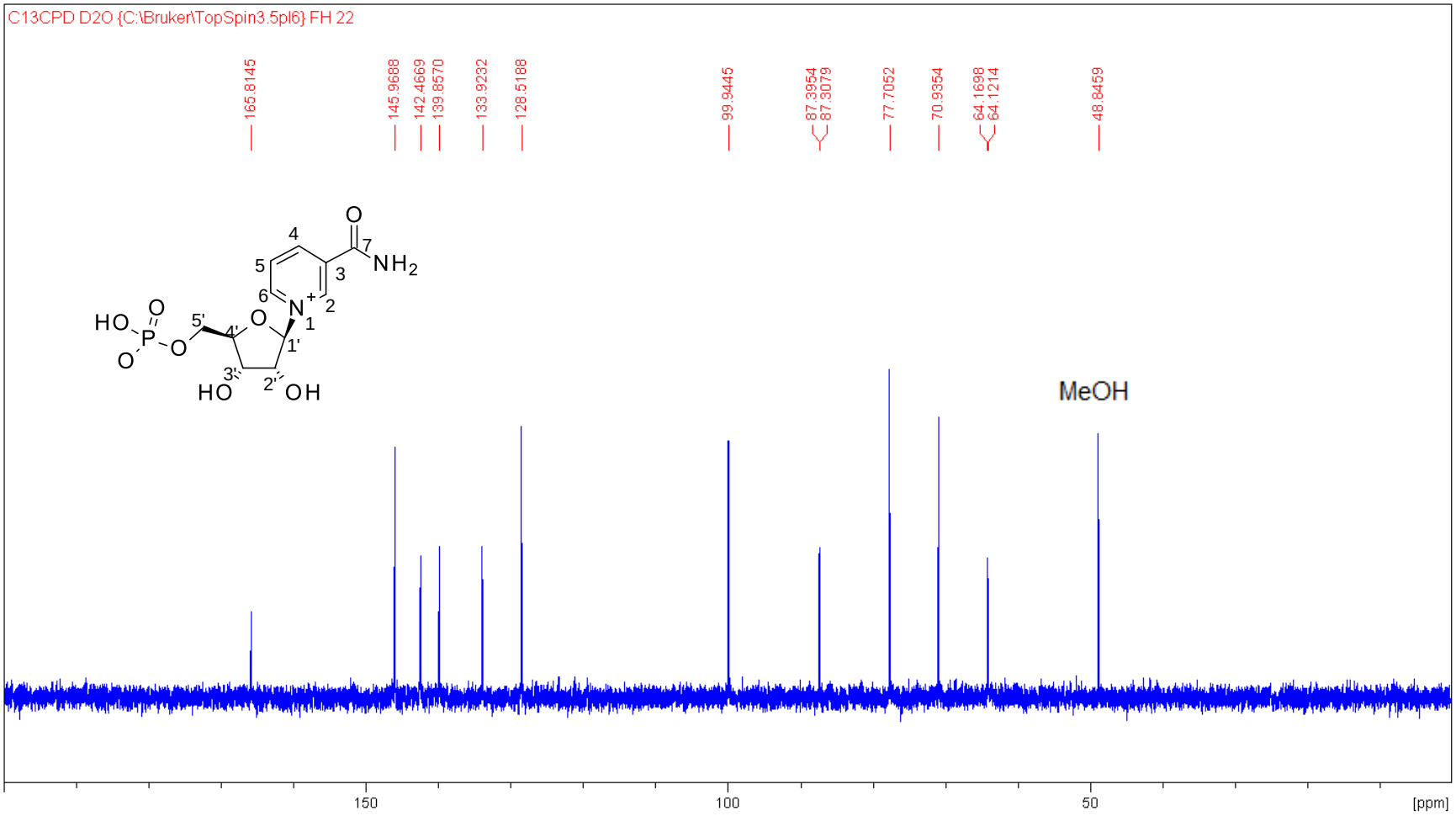
Compound 11. 162 MHz ^{31}PNMR spectrum in D_2O



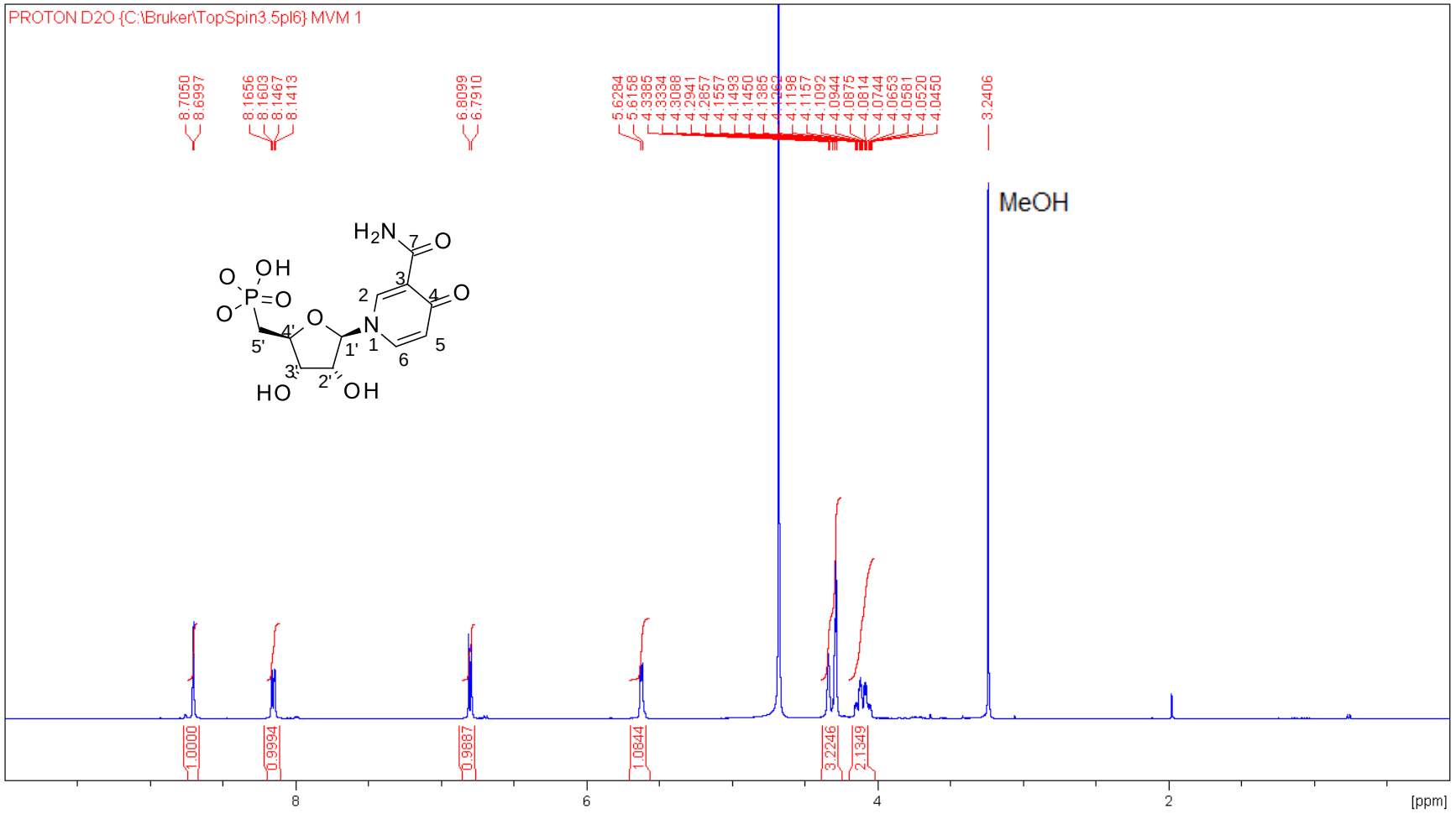
Compound 12. 400 MHz 1H NMR spectrum in D_2O



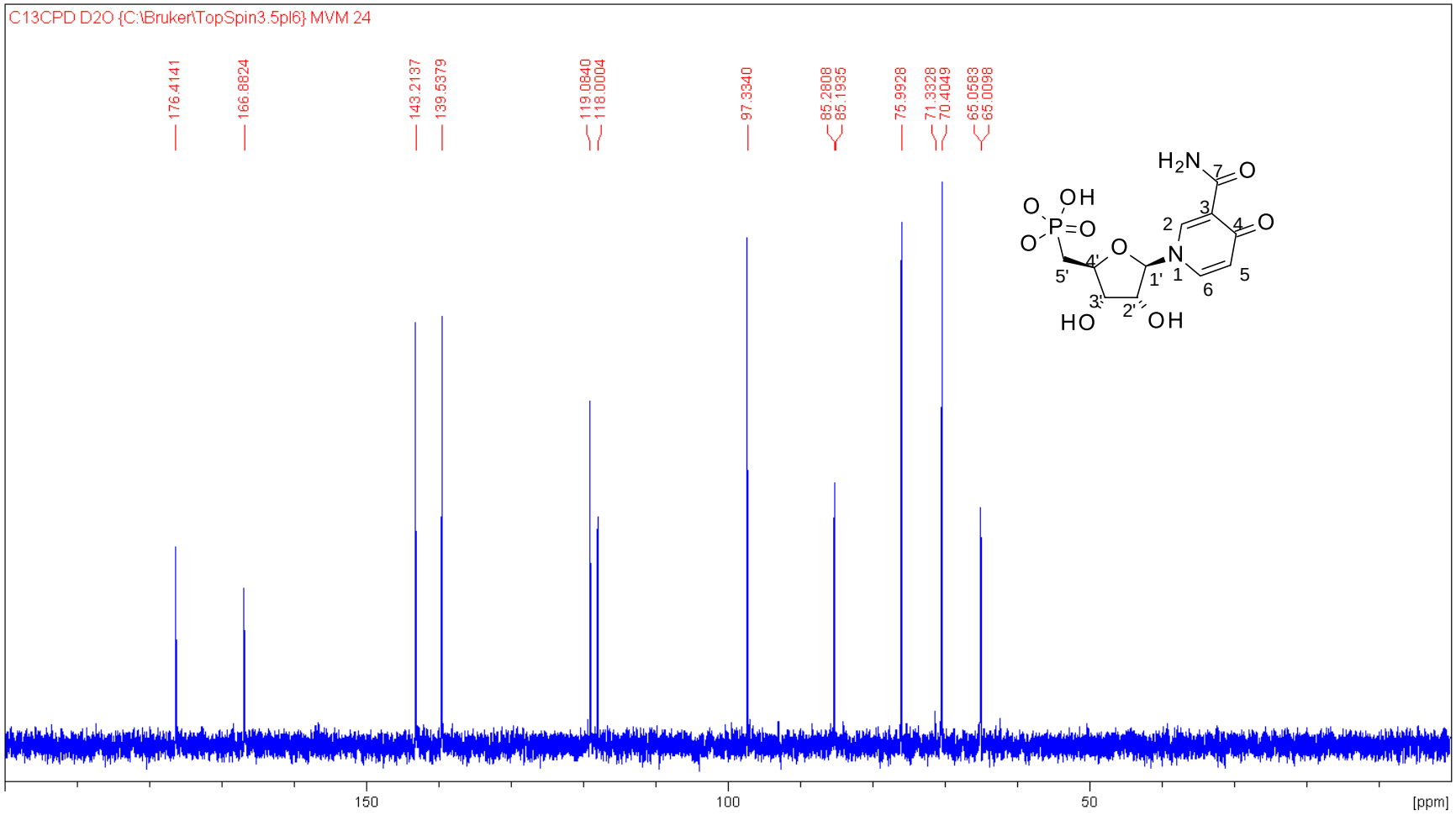
Compound12. 162 MHz ^{31}PNMR spectrum in D_2O



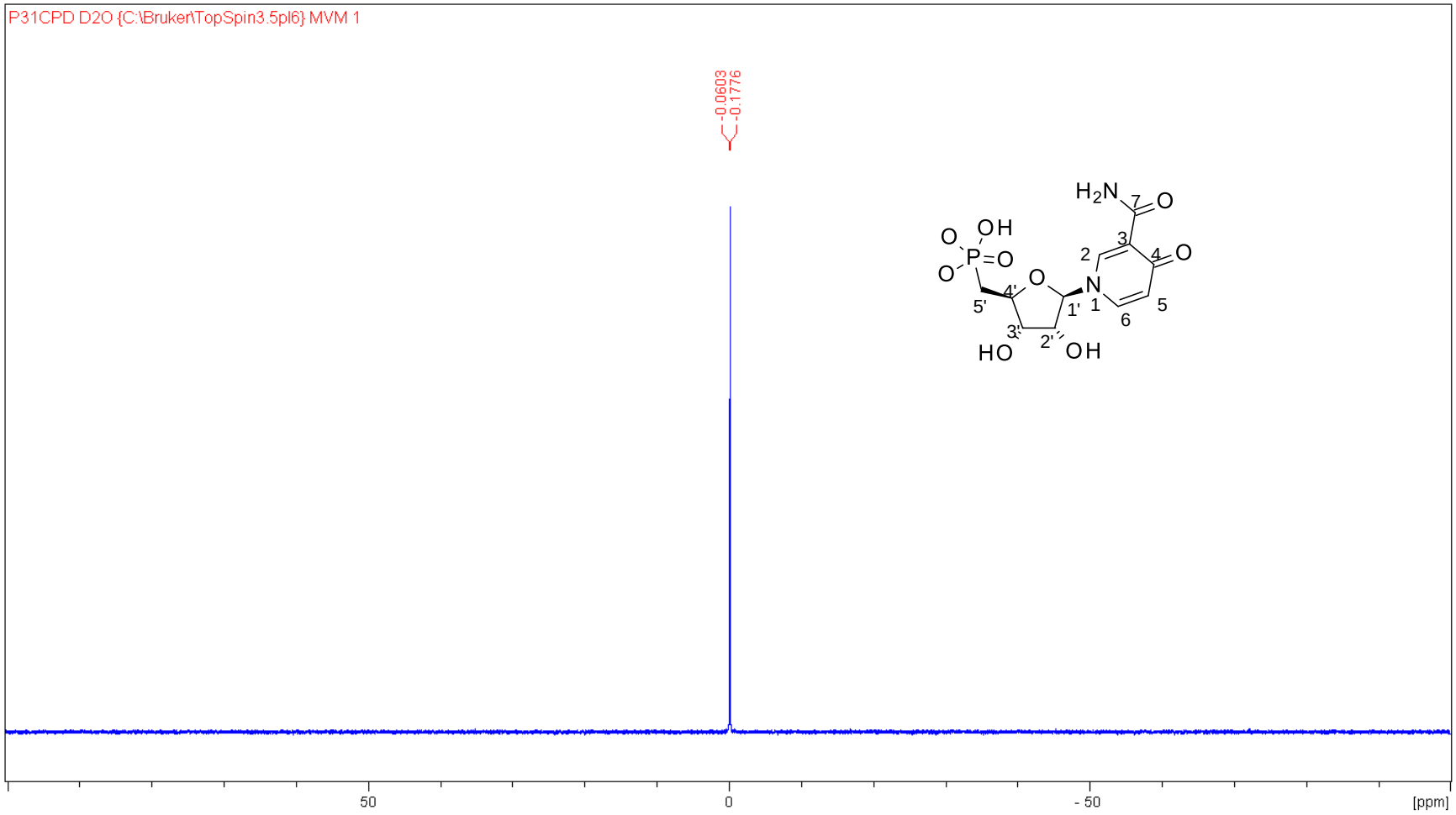
Compound 12. 100 MHz ^{13}C NMR spectrum in D_2O



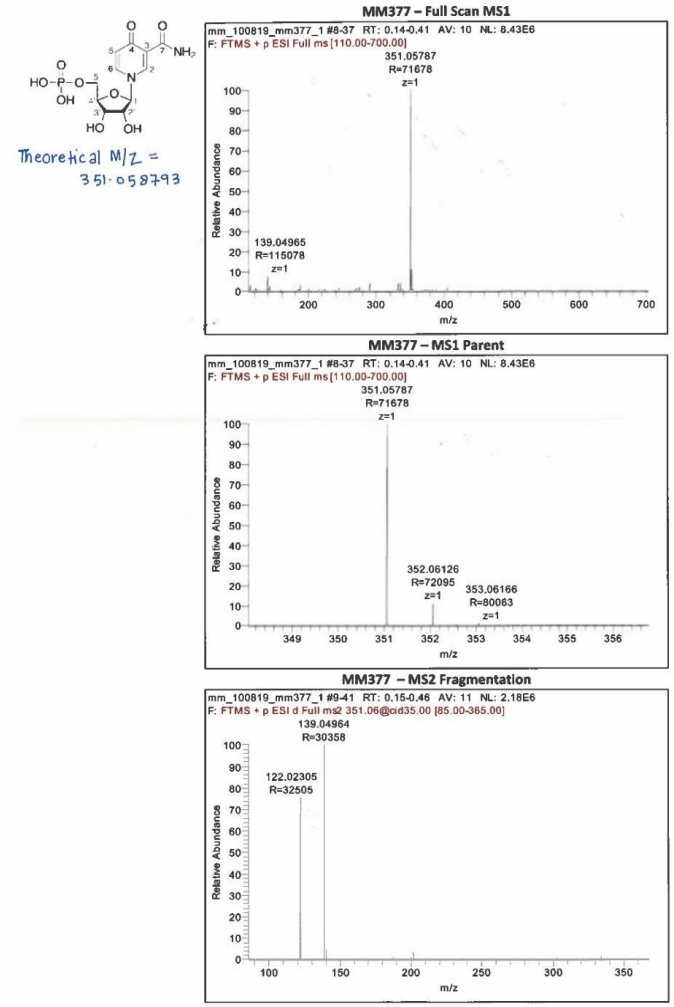
Compound 13. 400 MHz ^{1}H NMR spectrum in D_2O



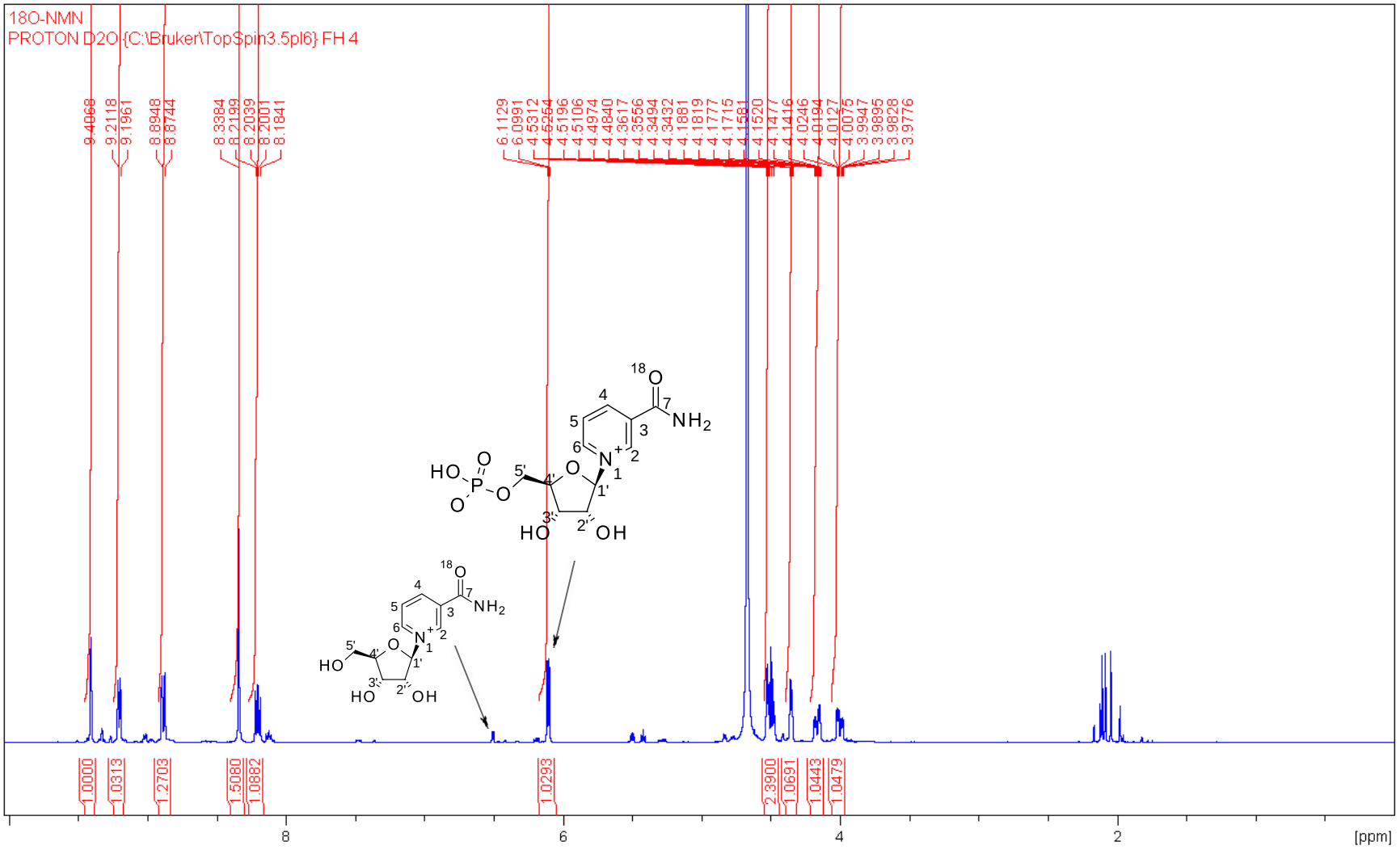
Compound 13. 100 MHz ^{13}C NMR spectrum in D_2O



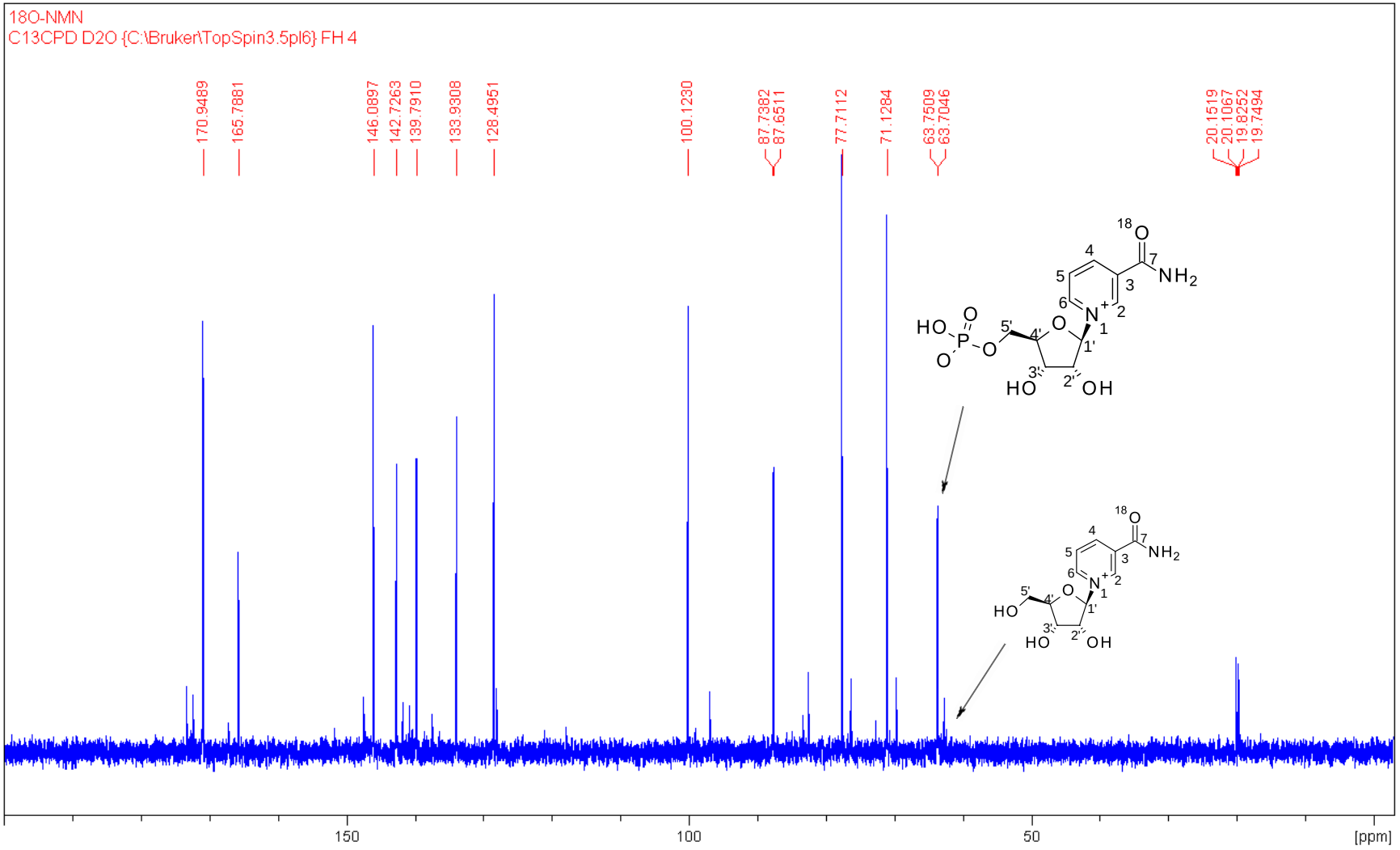
Compound 13. 162 MHz ^{31}P NMR spectrum in D_2O



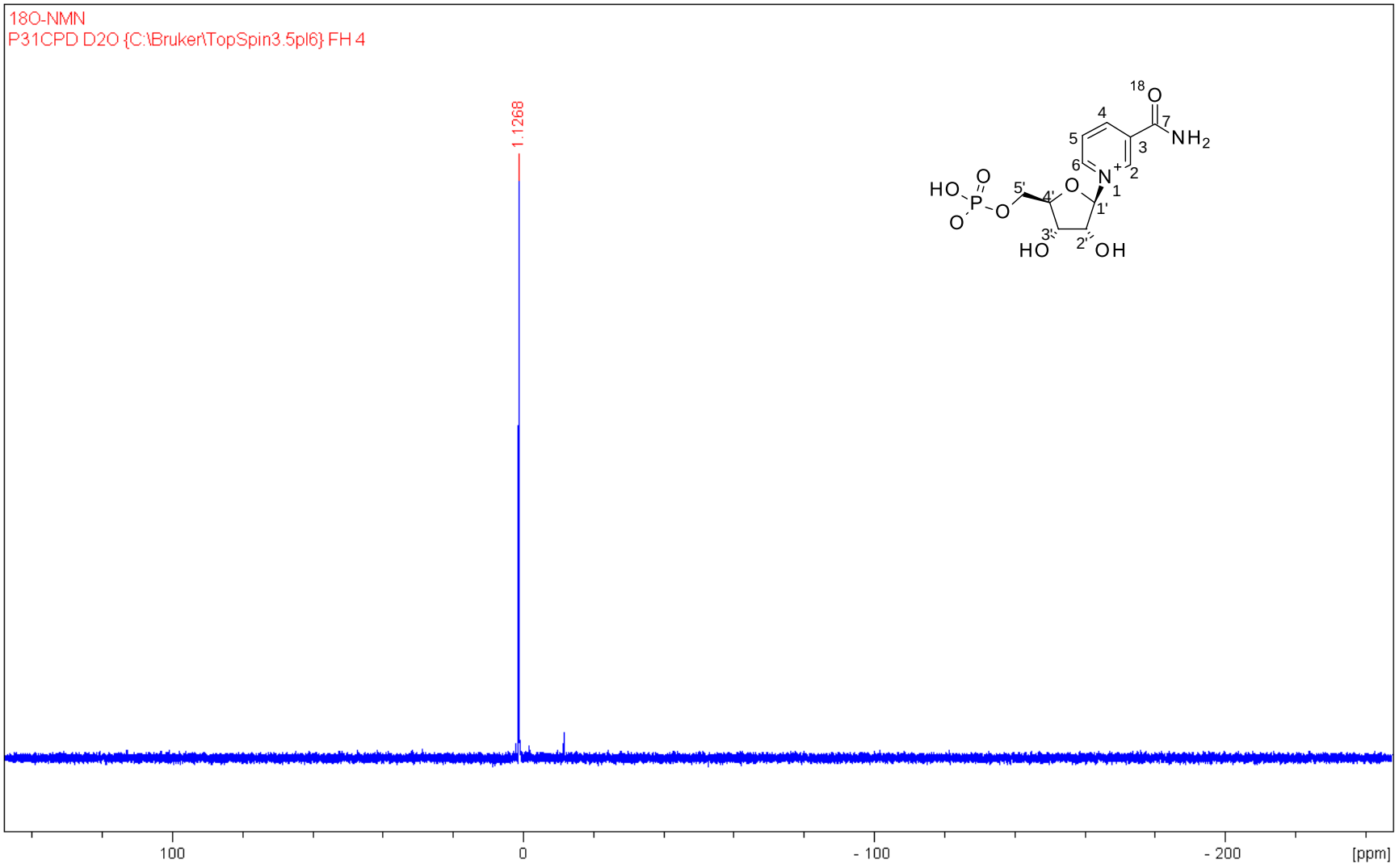
Compound 13. HRMS spectra



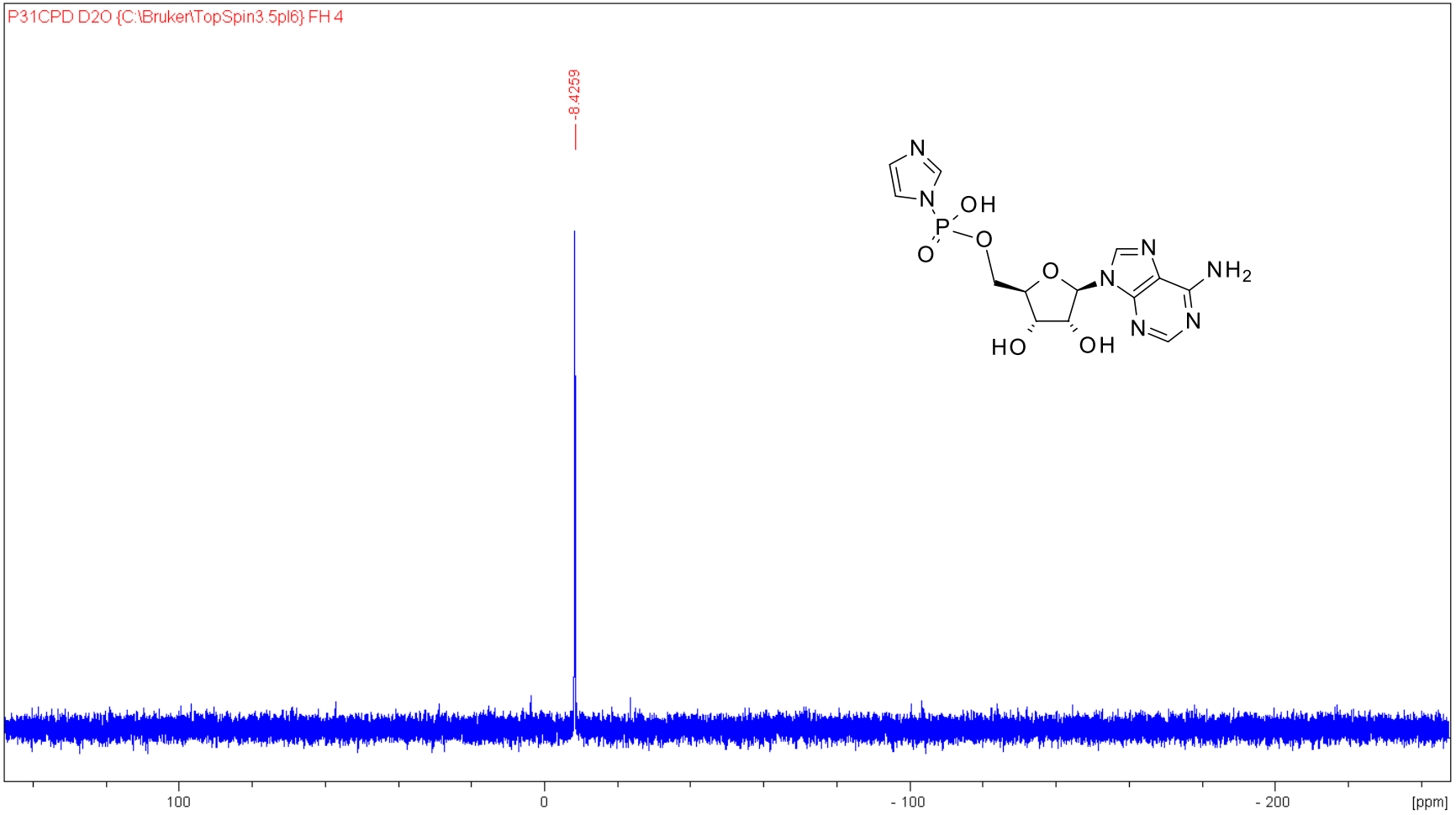
Compound 15. 400 MHz ^{1}H NMR spectrum in D_2O



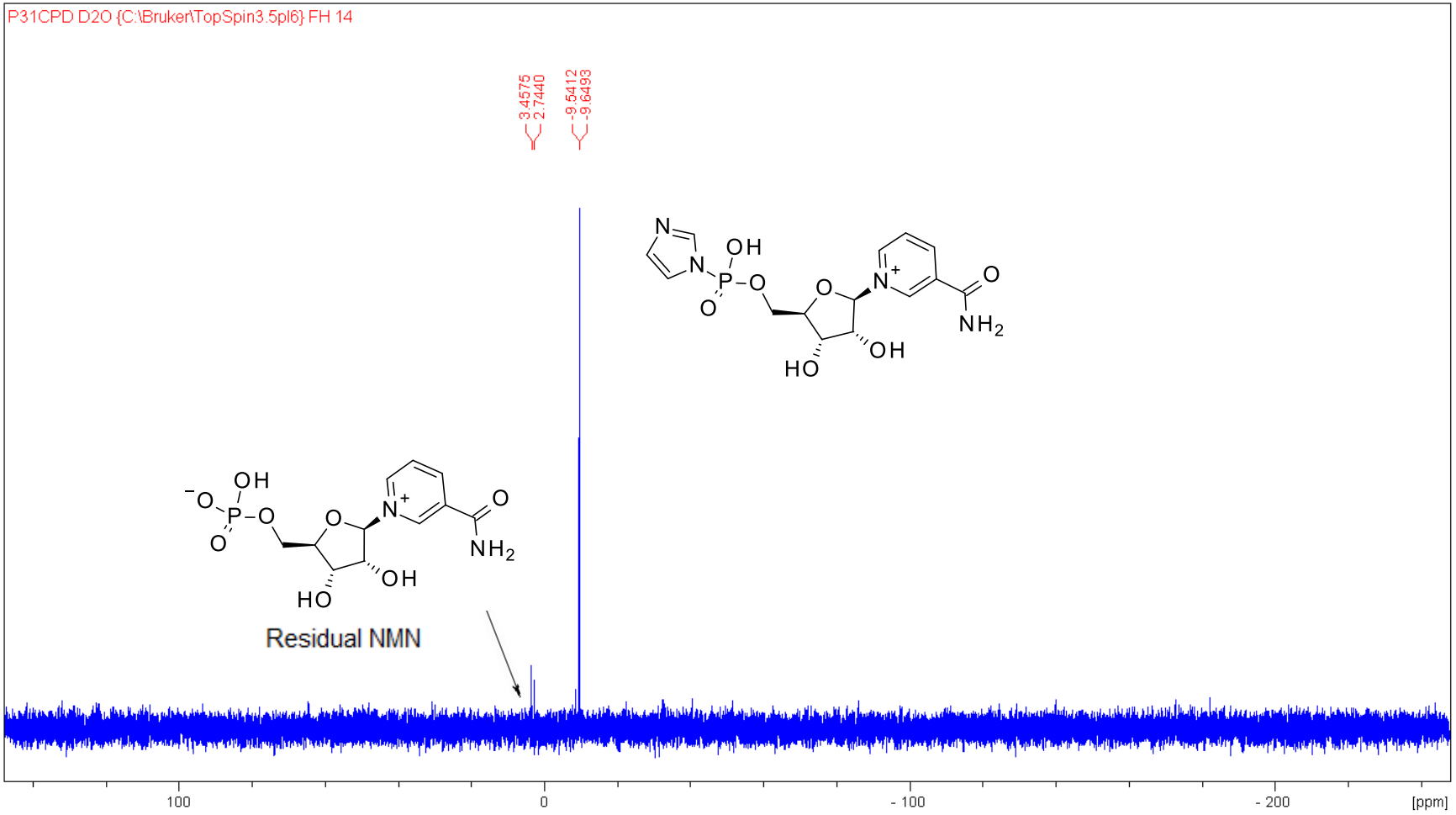
Compound 15. 100 MHz ^{1}H NMR spectrum in D_2O



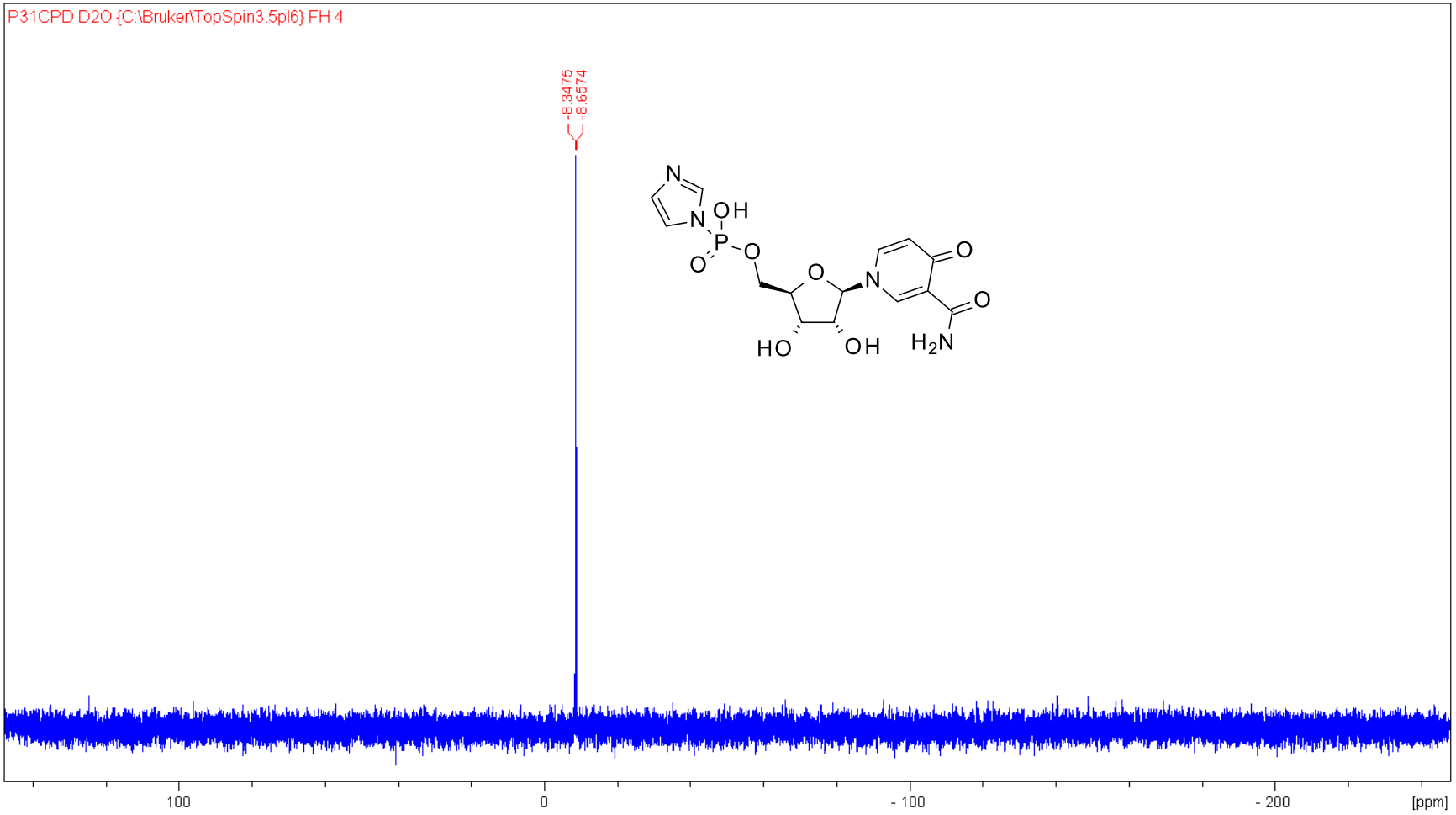
Compound 15. 162 MHz ^{31}P NMR spectrum in D_2O



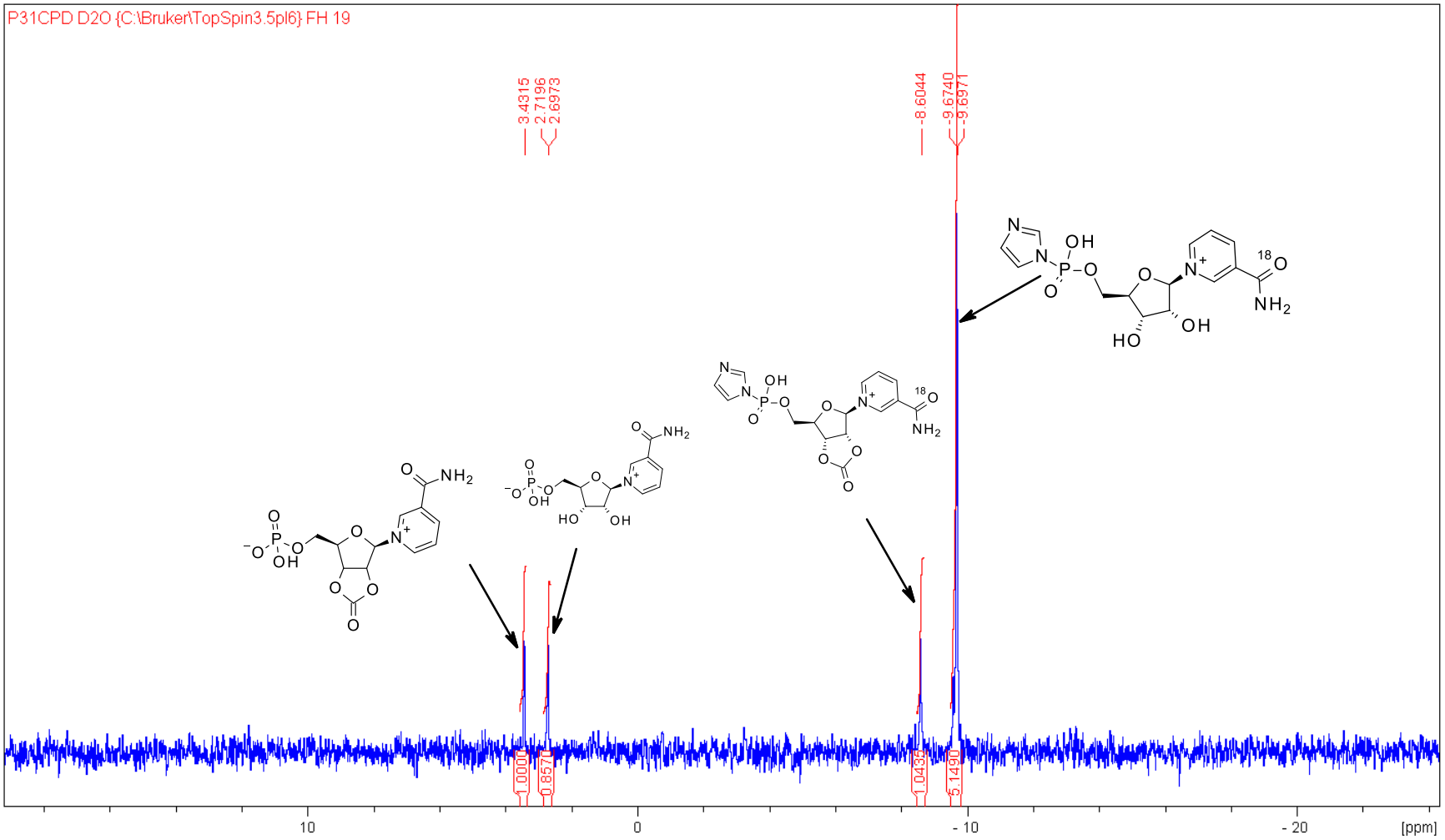
Compound 16. 162 MHz ^{31}P NMR spectrum in D_2O



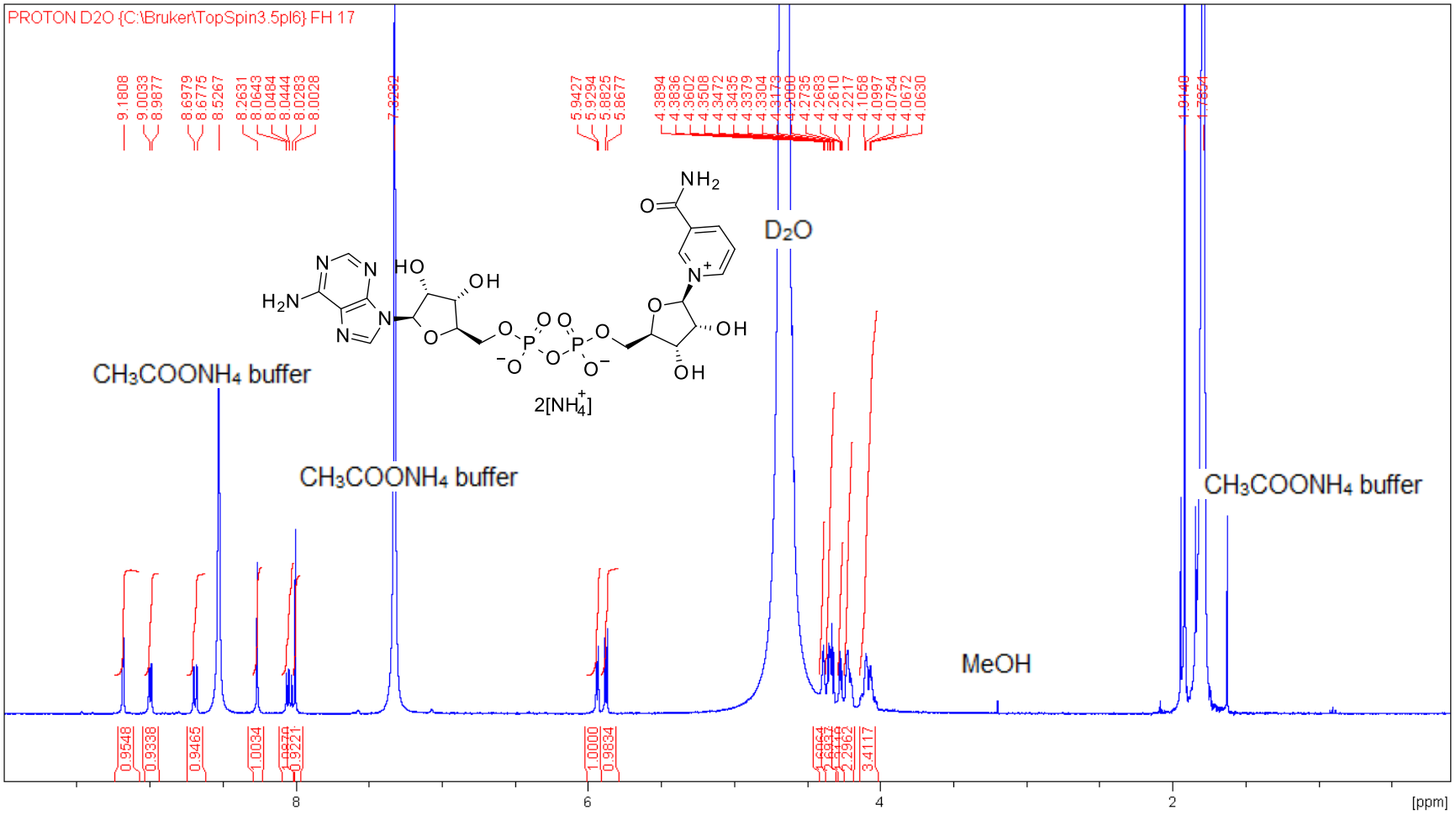
Compound 17. 162 MHz ^{31}P NMR spectrum in D_2O



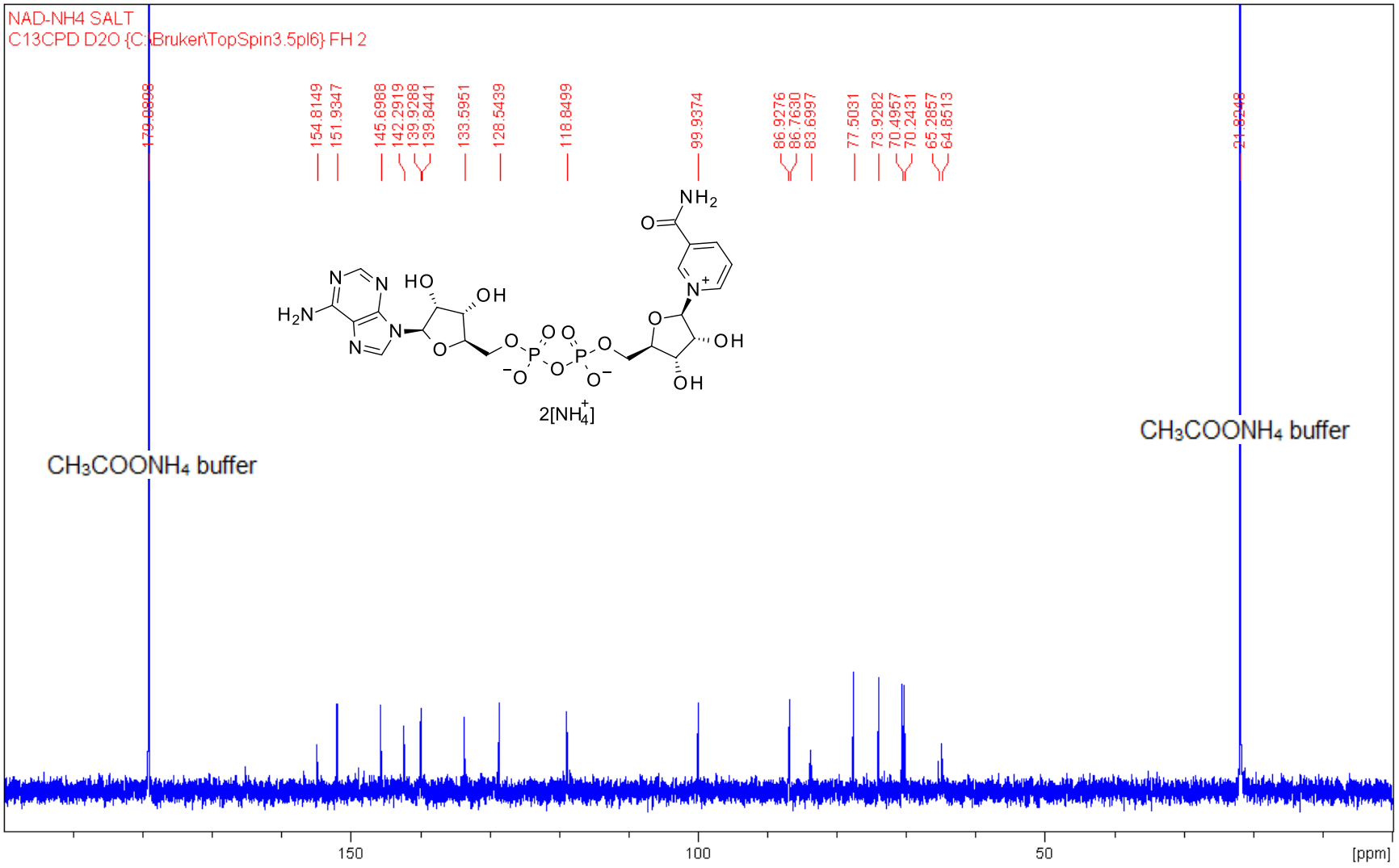
Compound 18. 162 MHz ^{31}P NMR spectrum in D_2O



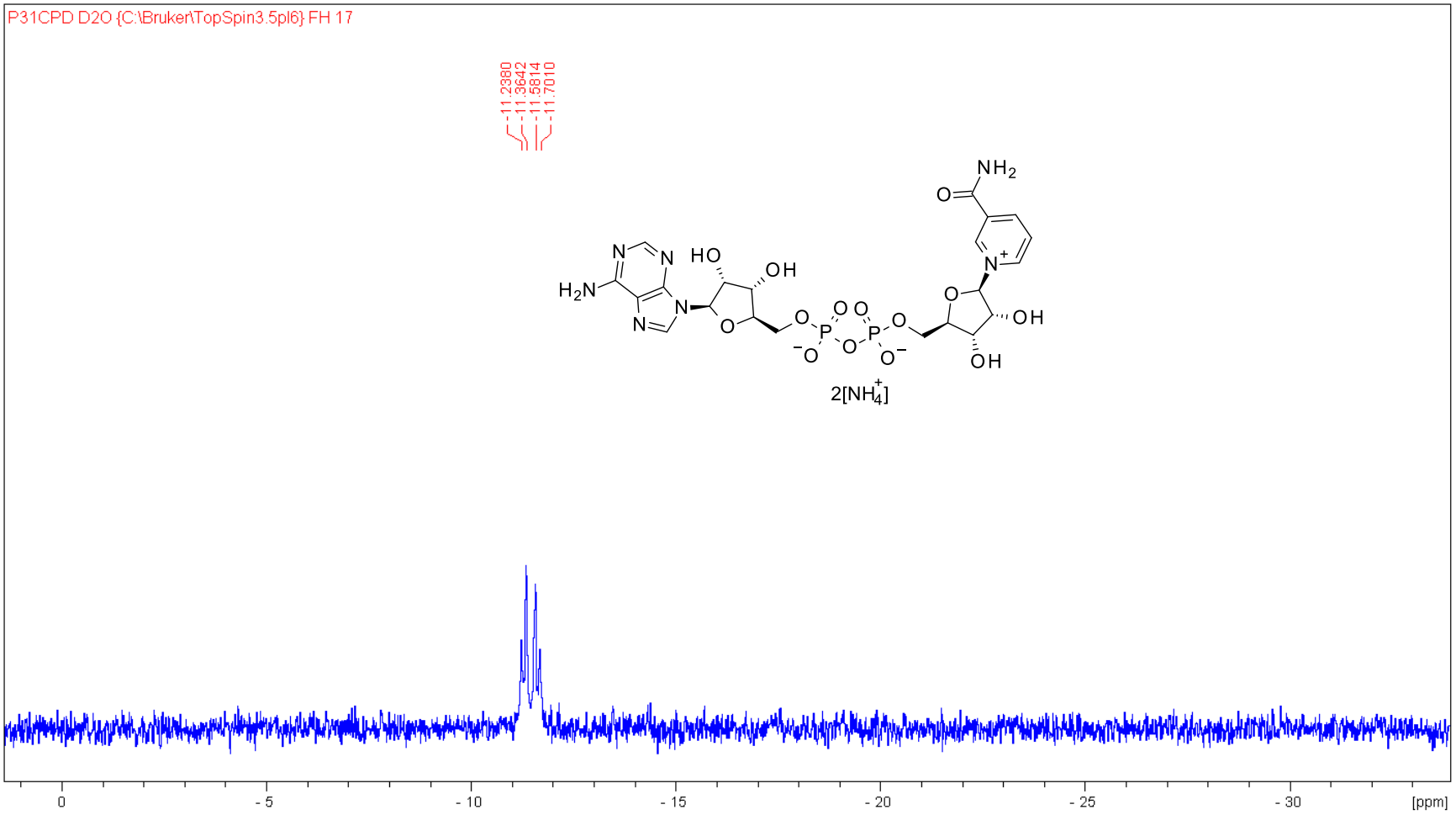
Compound 19. 162 MHz ^{31}P NMR spectrum in D_2O



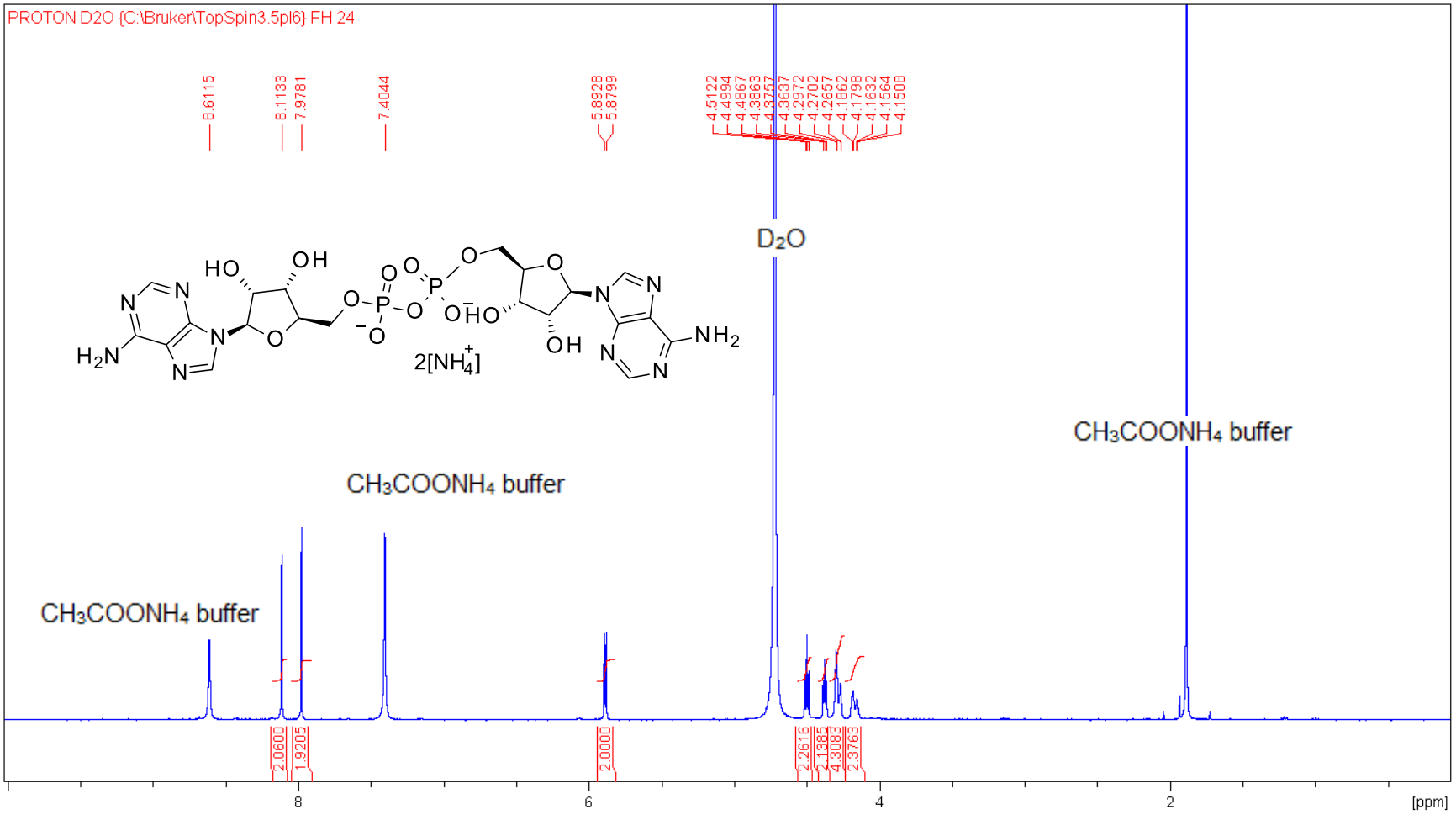
Compound 20. 400 MHz ^{1}H NMR spectrum in D_2O



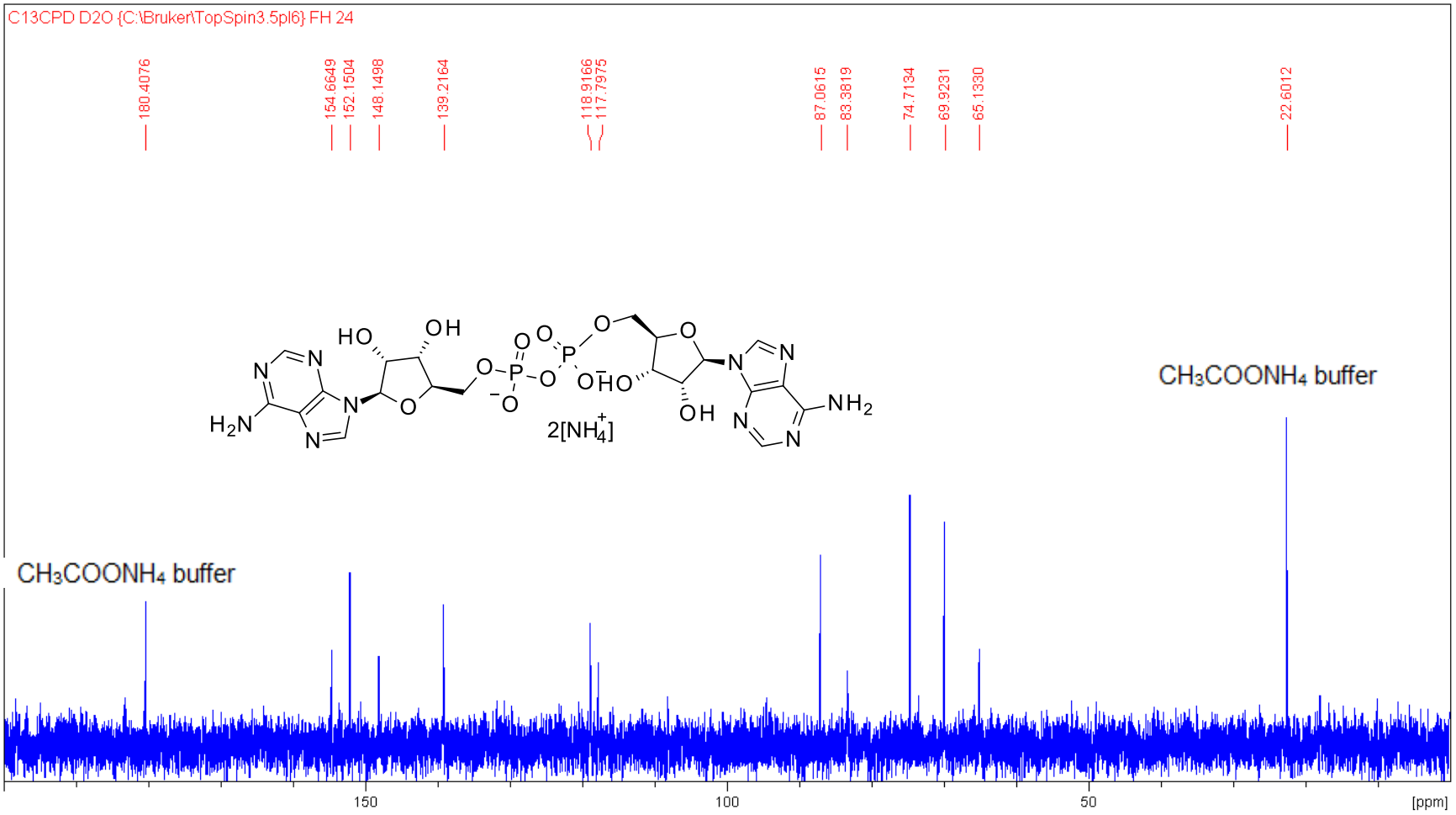
Compound 20. 100 MHz ^{13}C NMR spectrum in D_2O



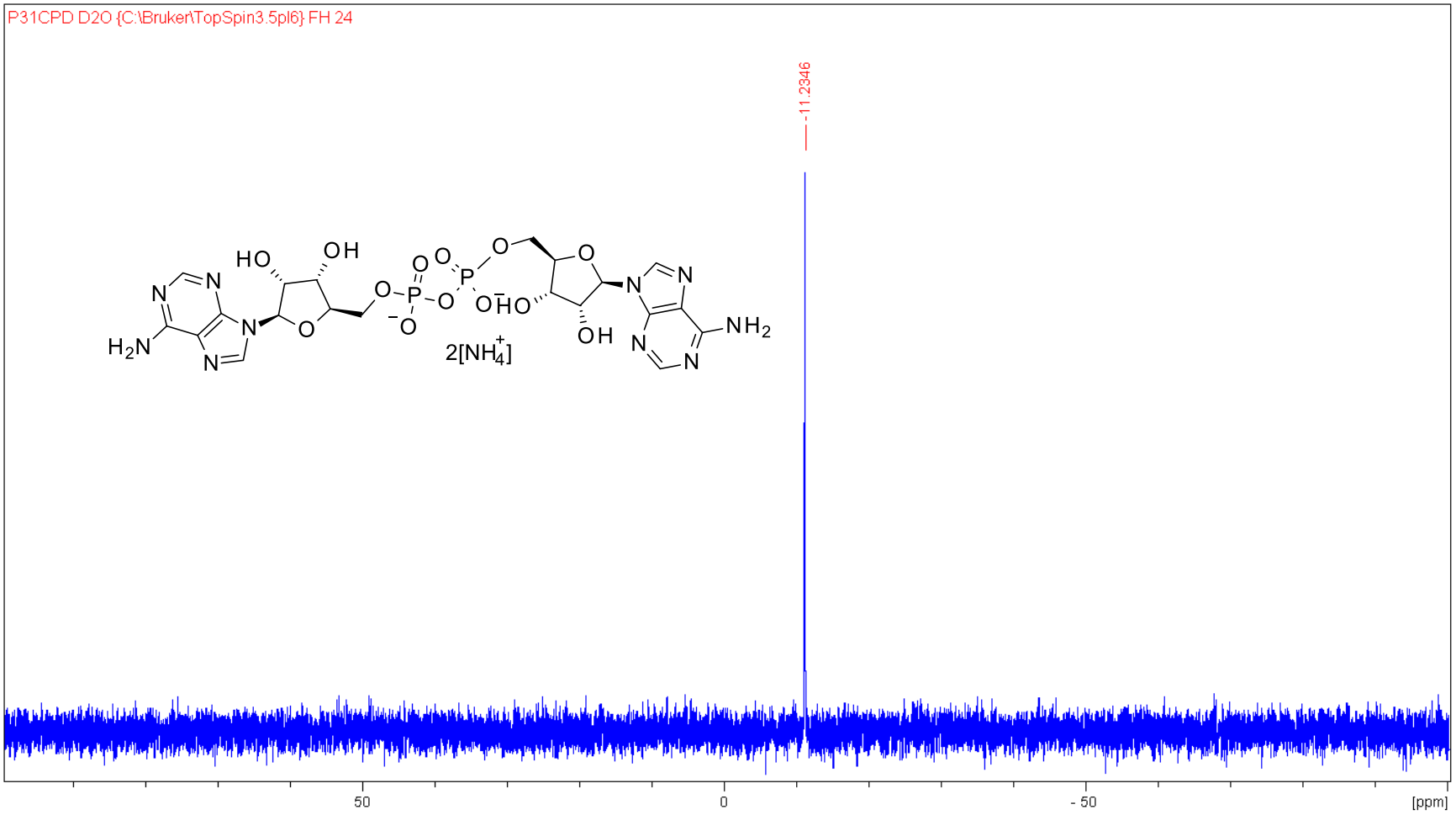
Compound 20. 162MHz ^{31}P NMR spectrum in D_2O



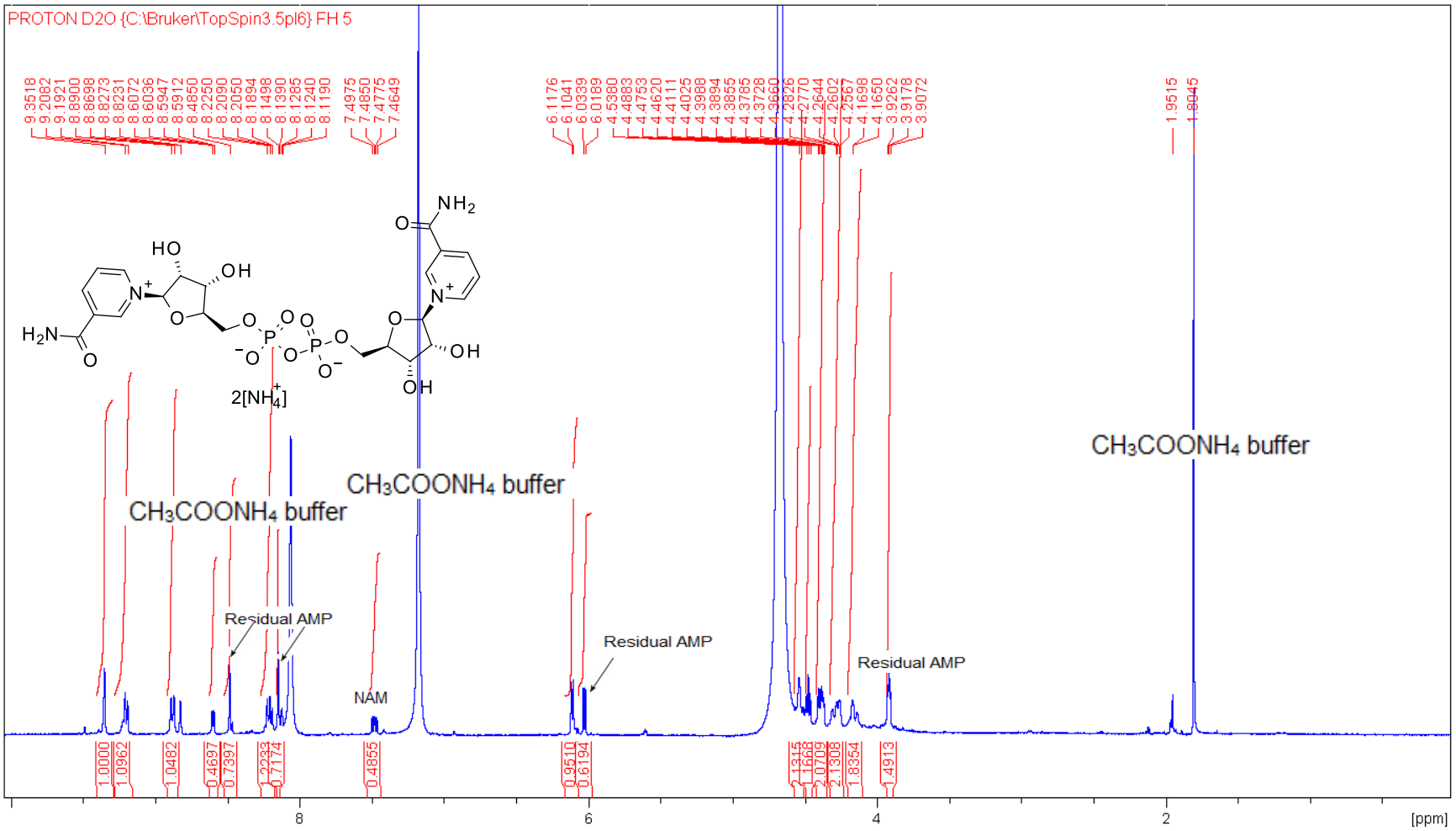
Compound 21. 400 MHz ^{1}H NMR spectrum in D_2O



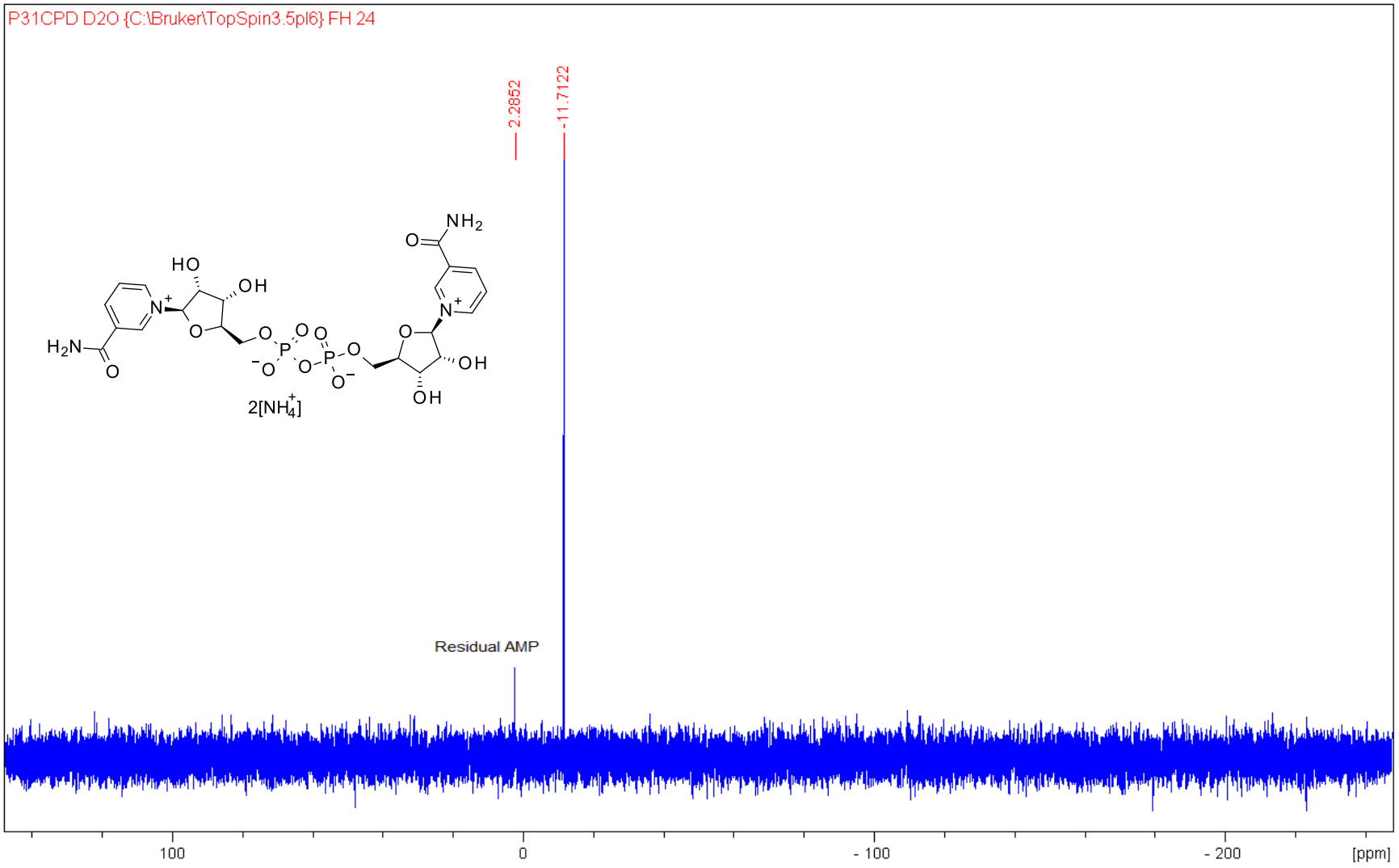
Compound 21. 100 MHz ^{13}C NMR spectrum in D_2O



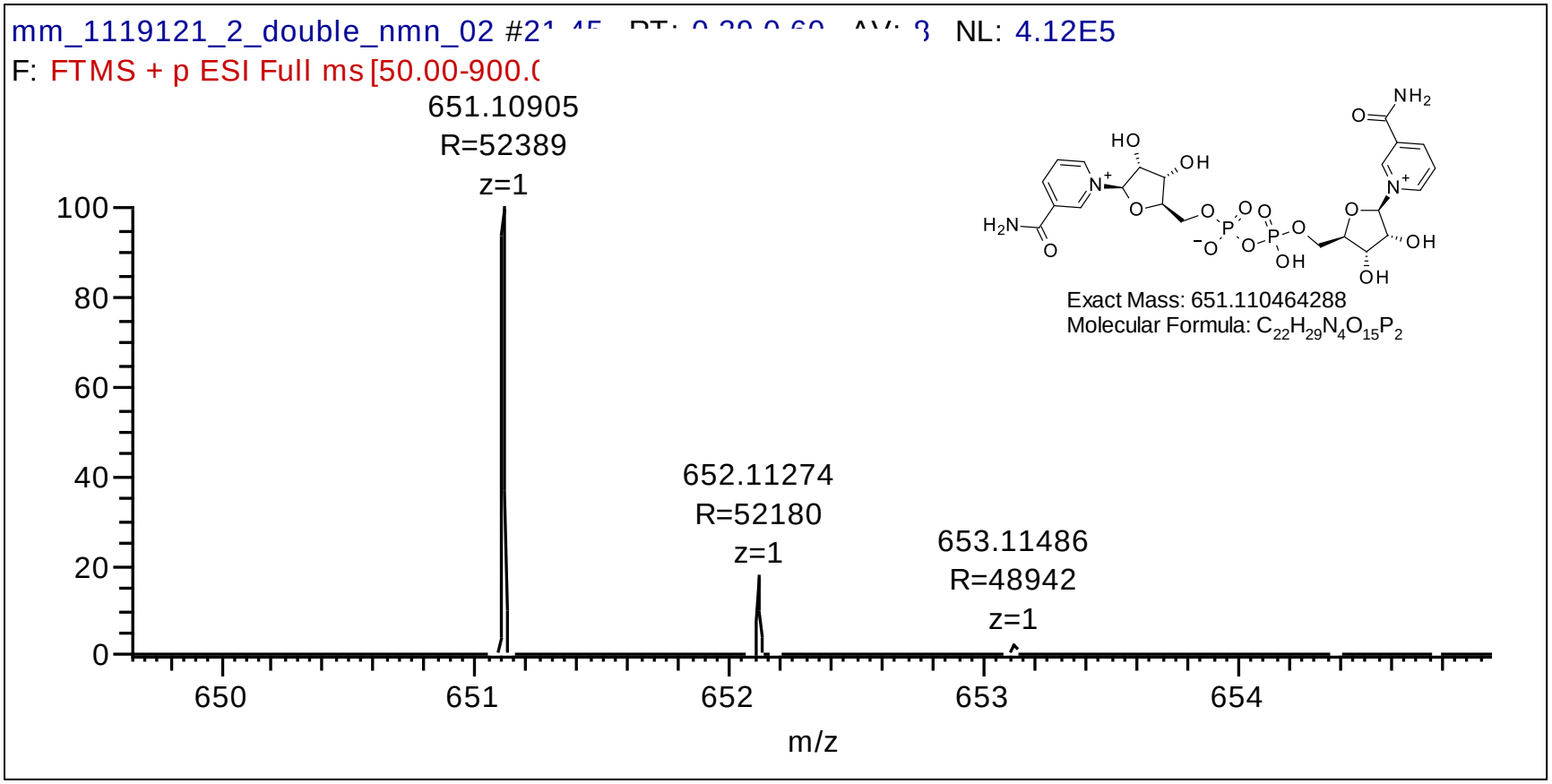
Compound 21. 162MHz ^{31}P NMR spectrum in D_2O



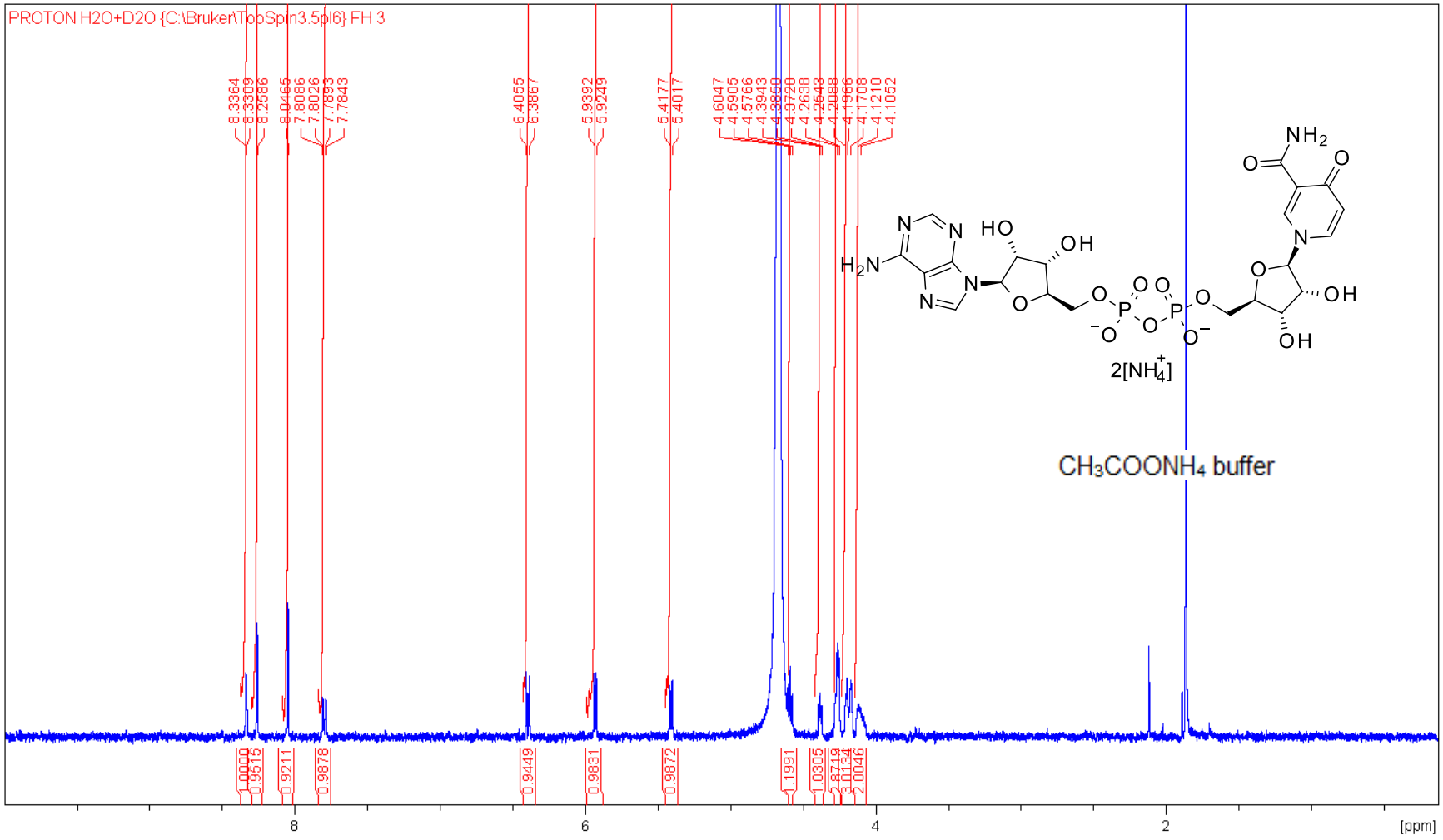
Compound 22. 400 MHz ^{1}H NMR spectrum in D_2O



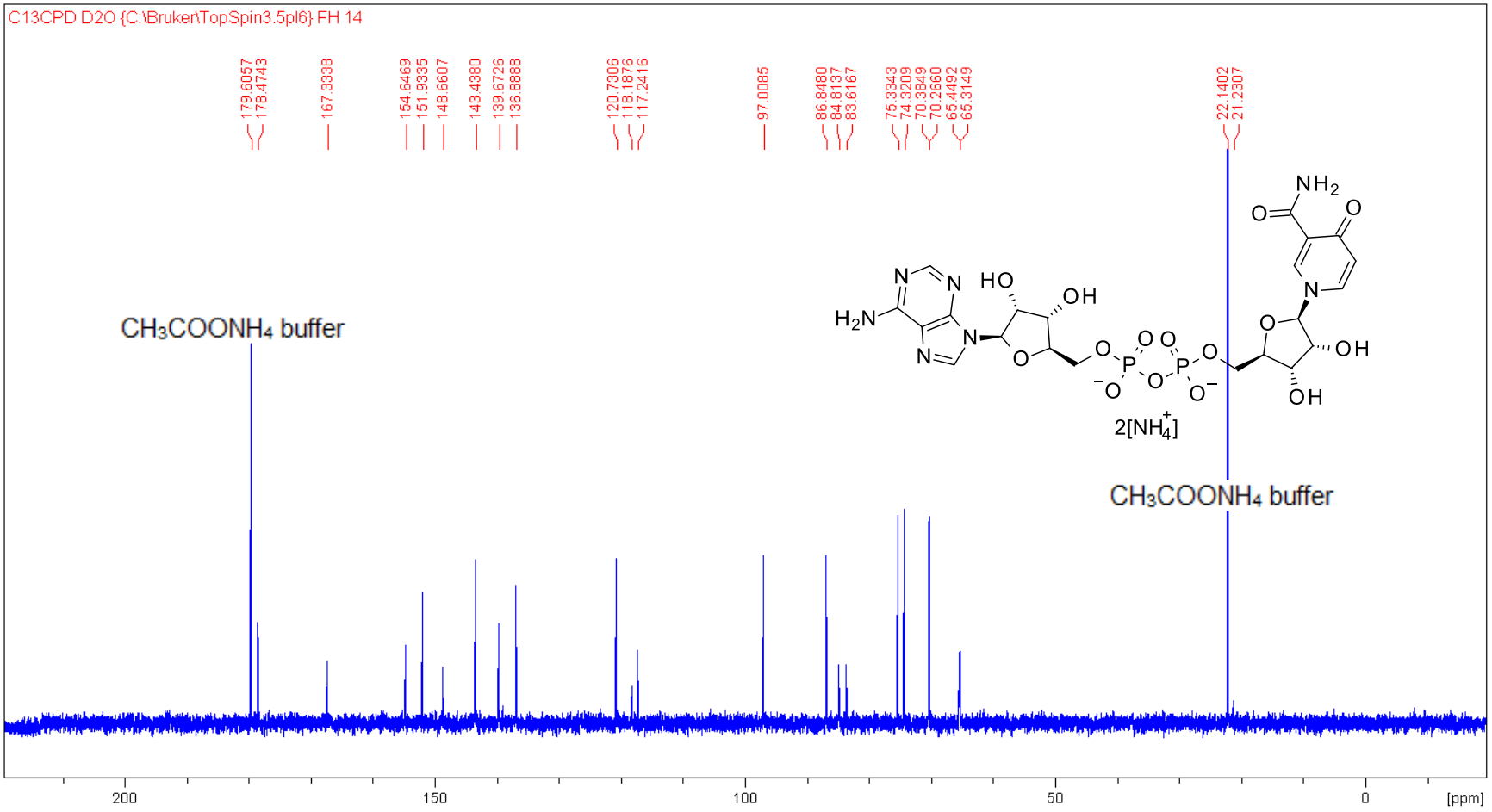
Compound 22. 162 MHz ^{31}P NMR spectrum in D_2O



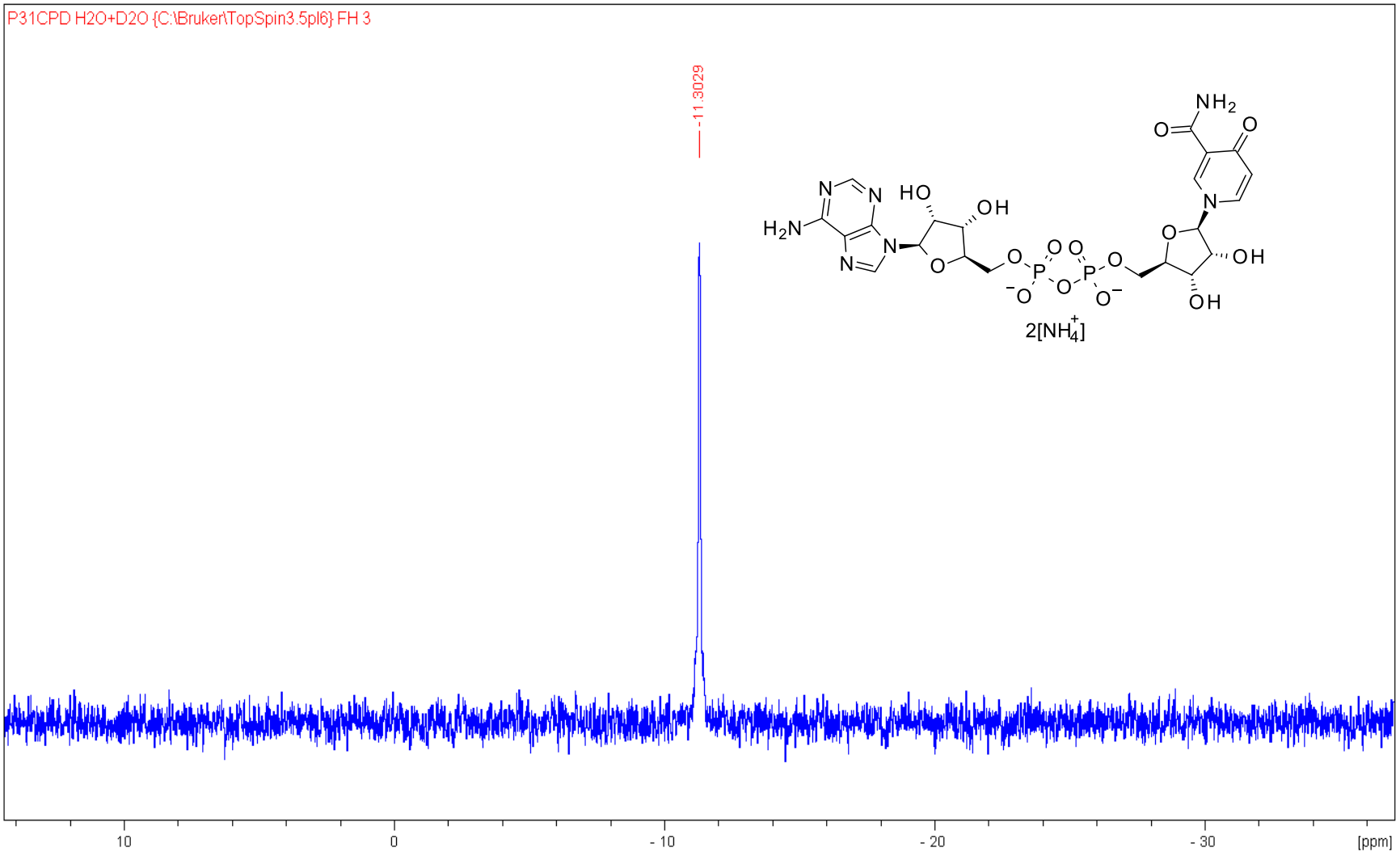
Compound 22. HRMS spectra



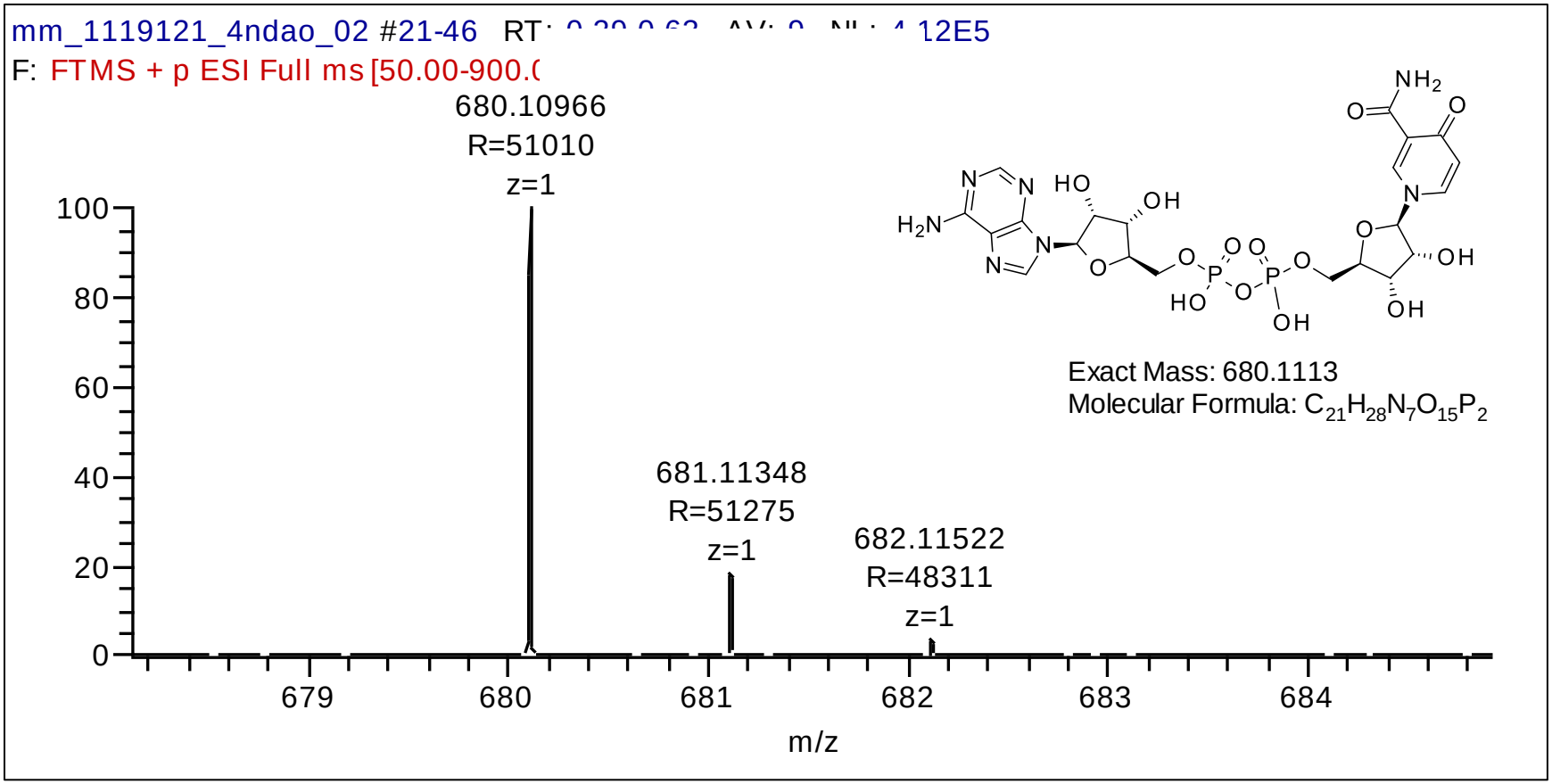
Compound 23. 400 MHz ^{1}H NMR spectrum in D_2O



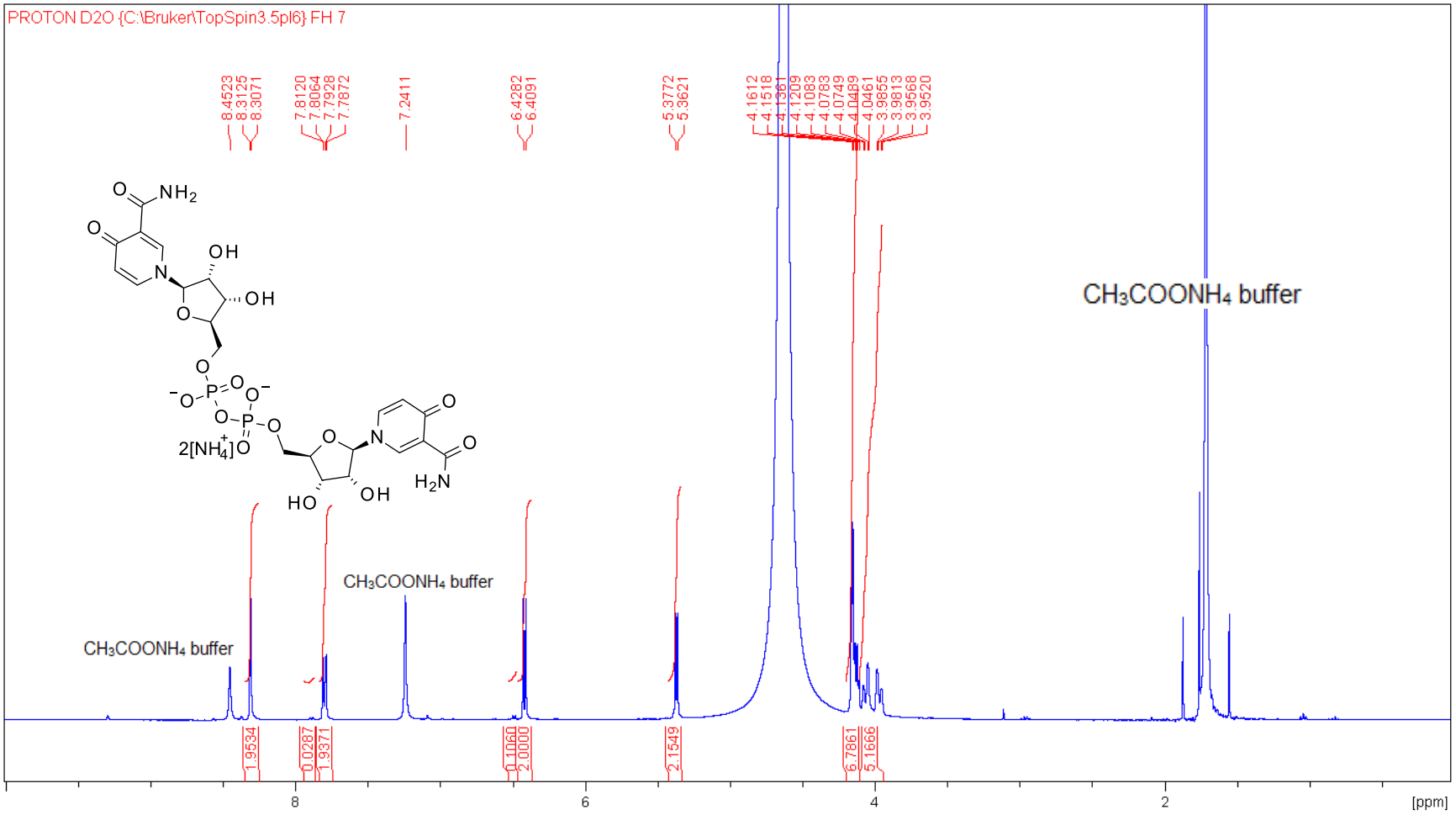
Compound 23. 100 MHz ^{13}C NMR spectrum in D_2O



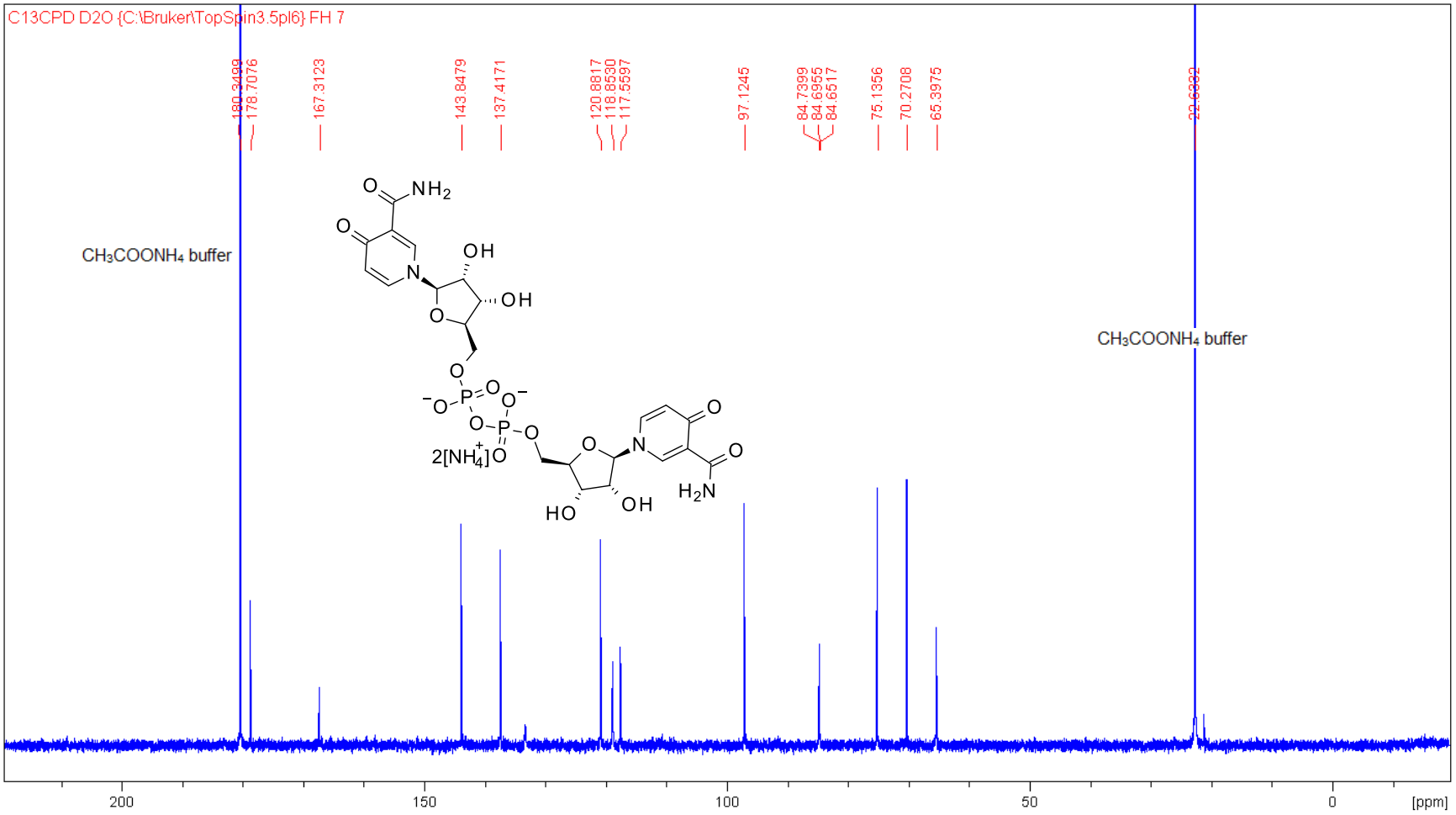
Compound 23. 162 MHz ^{31}P NMR spectrum in D_2O



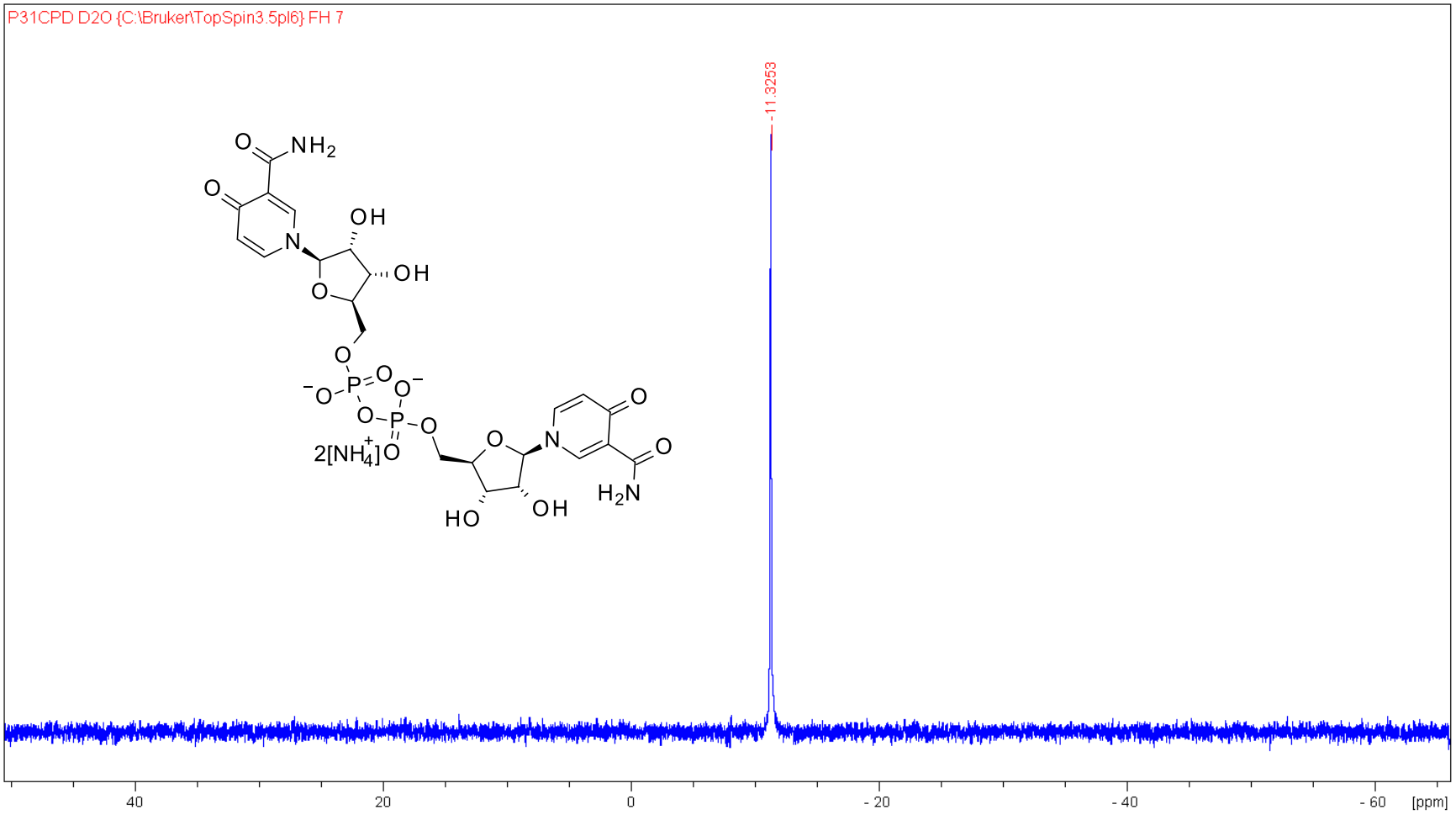
Compound 23. HRMS Spectra



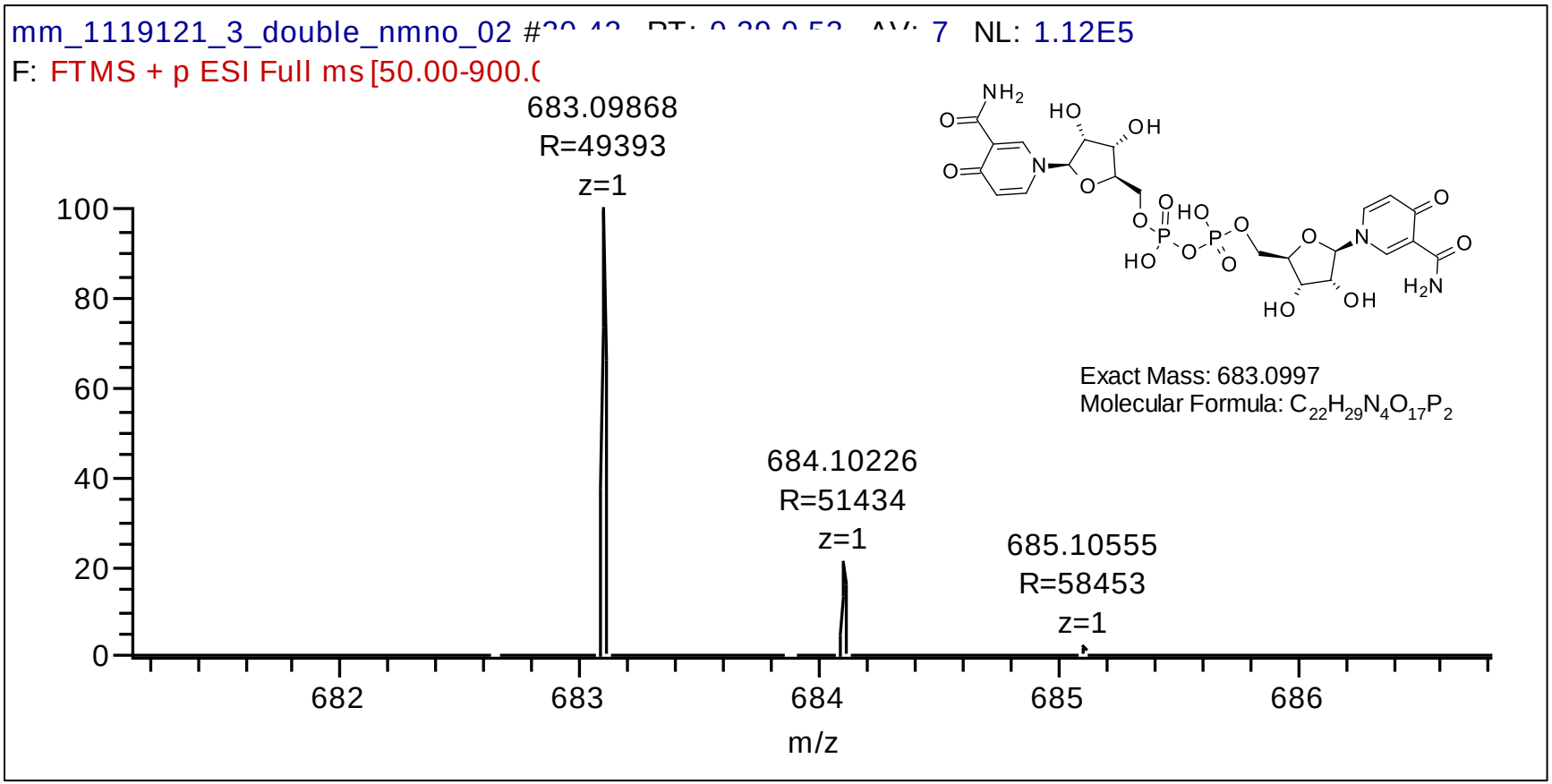
Compound 24. 400 MHz ^{1}H NMR spectrum in D_2O



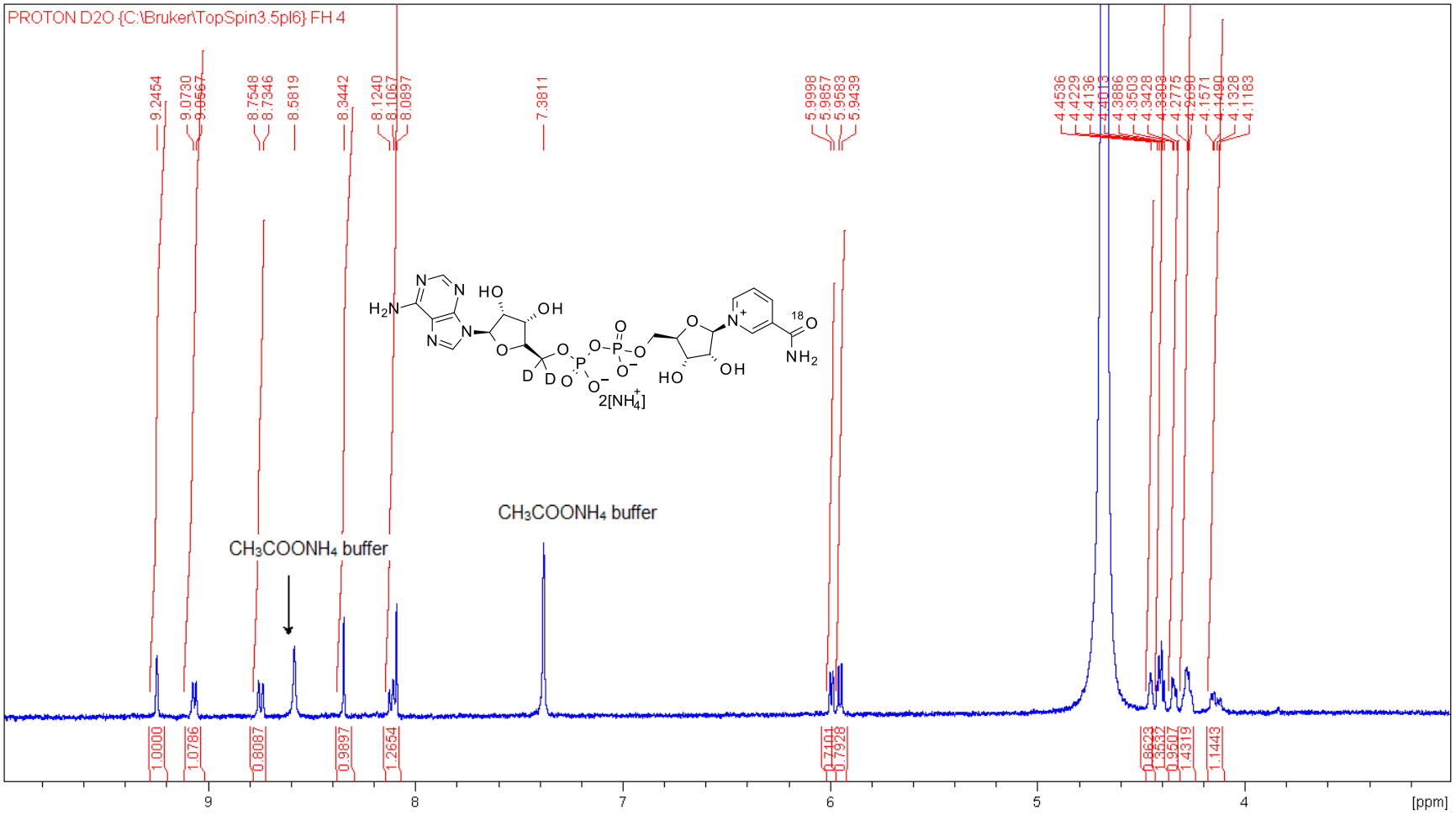
Compound 24. 100 MHz ^{13}C NMR spectrum in D_2O



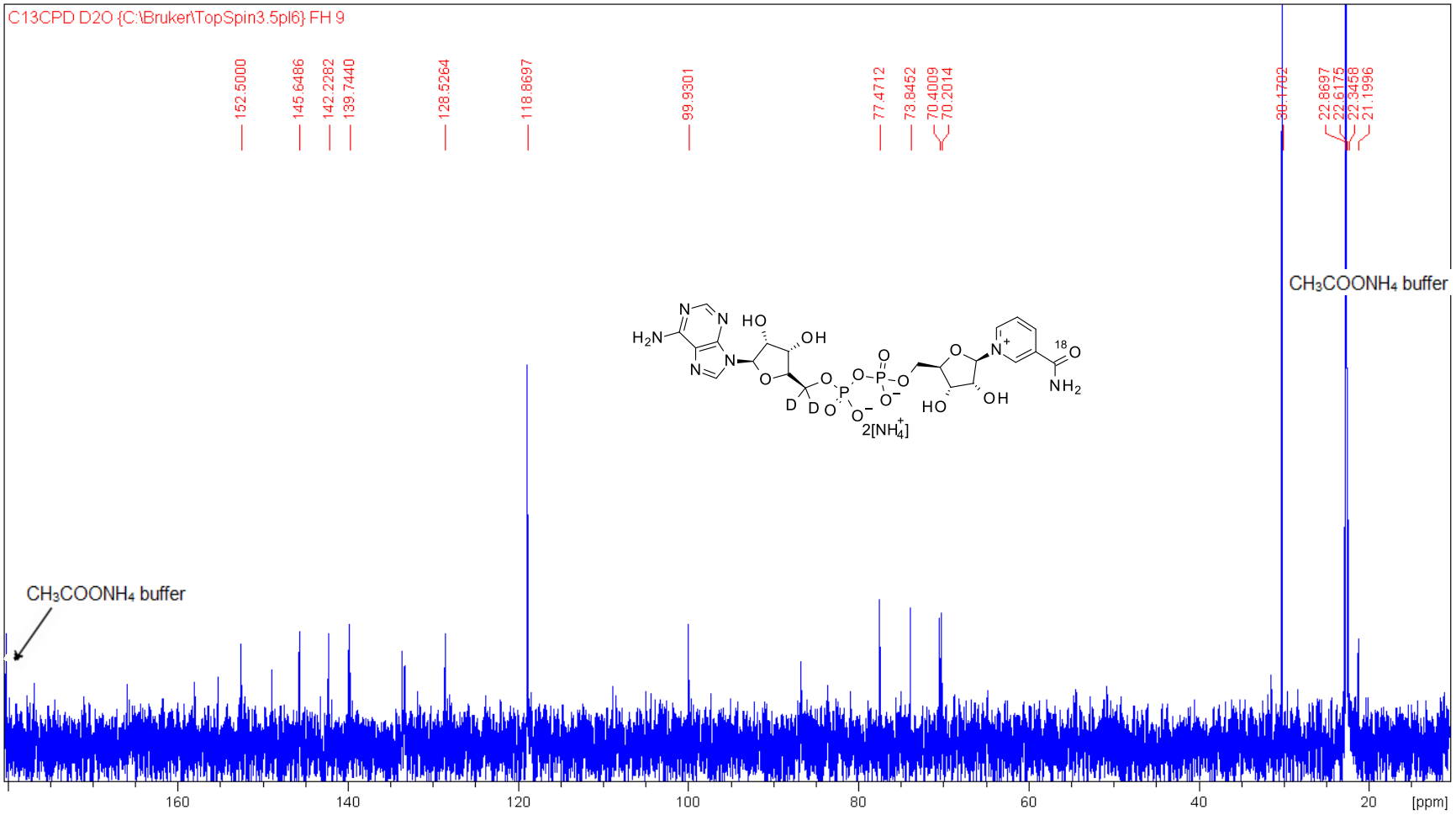
Compound 24. 162 MHz ^{31}P NMR spectrum in D_2O



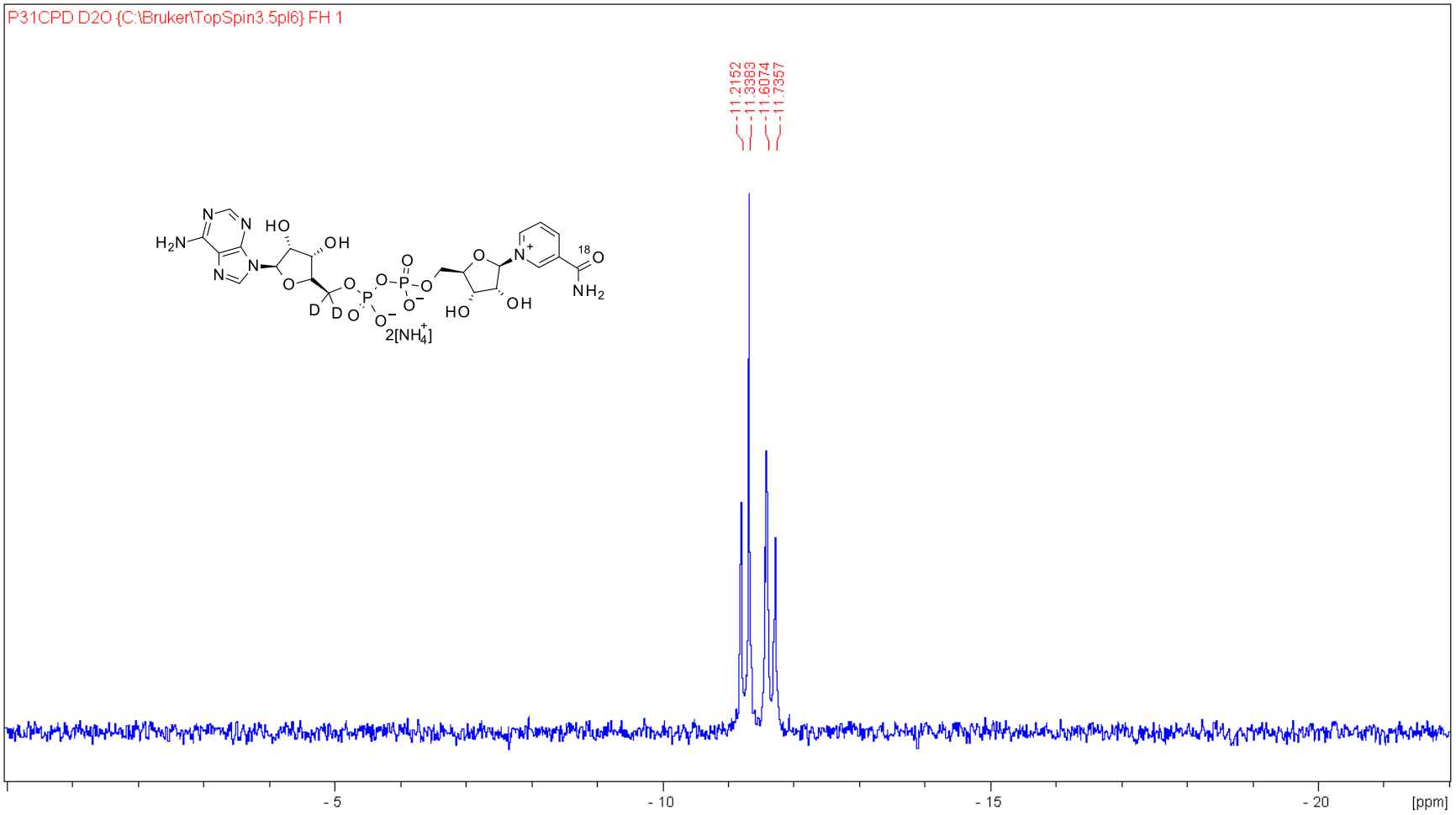
Compound 24. HRMS Sprctra



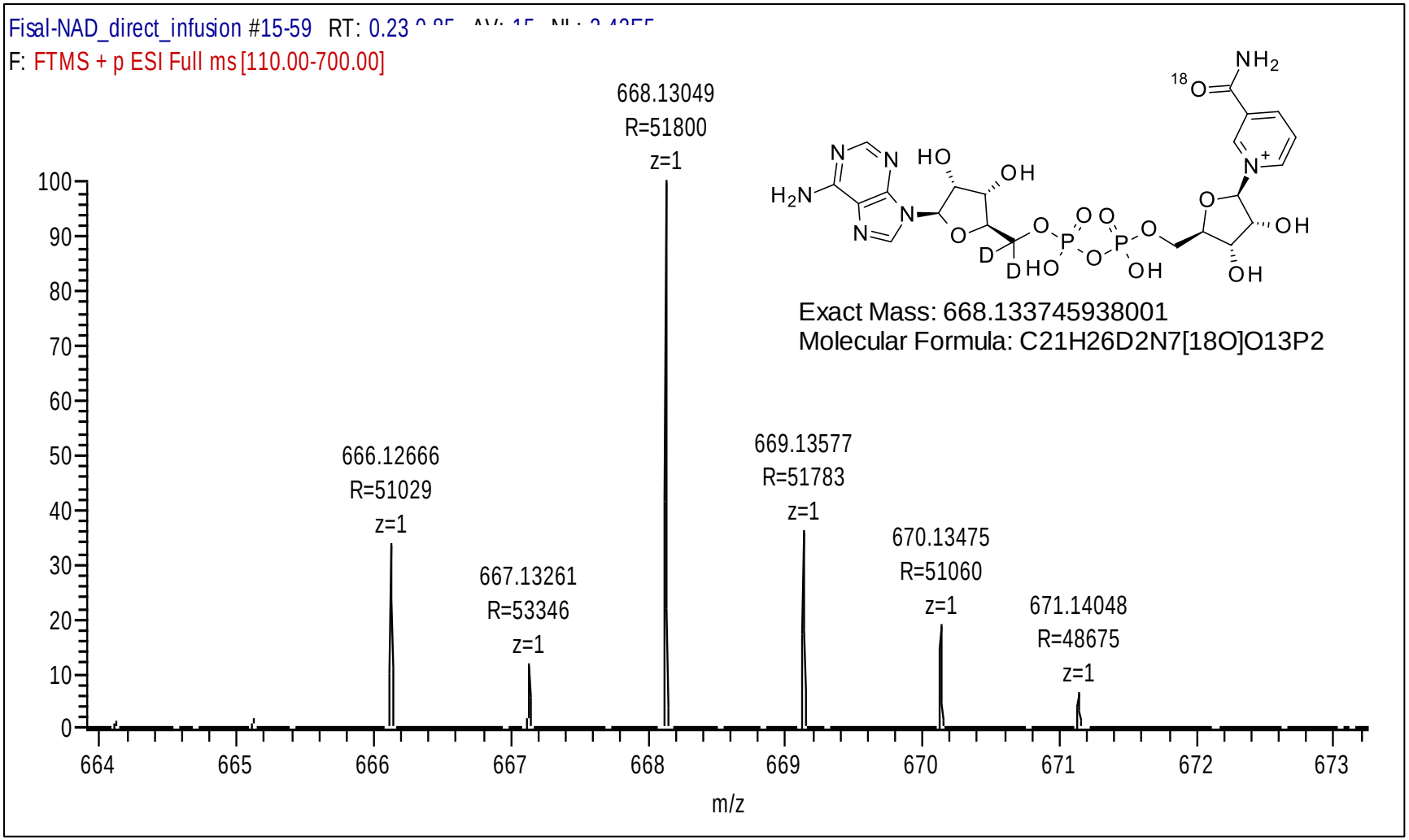
Compound 25. 400 MHz ^{1}H NMR spectrum in D_2O



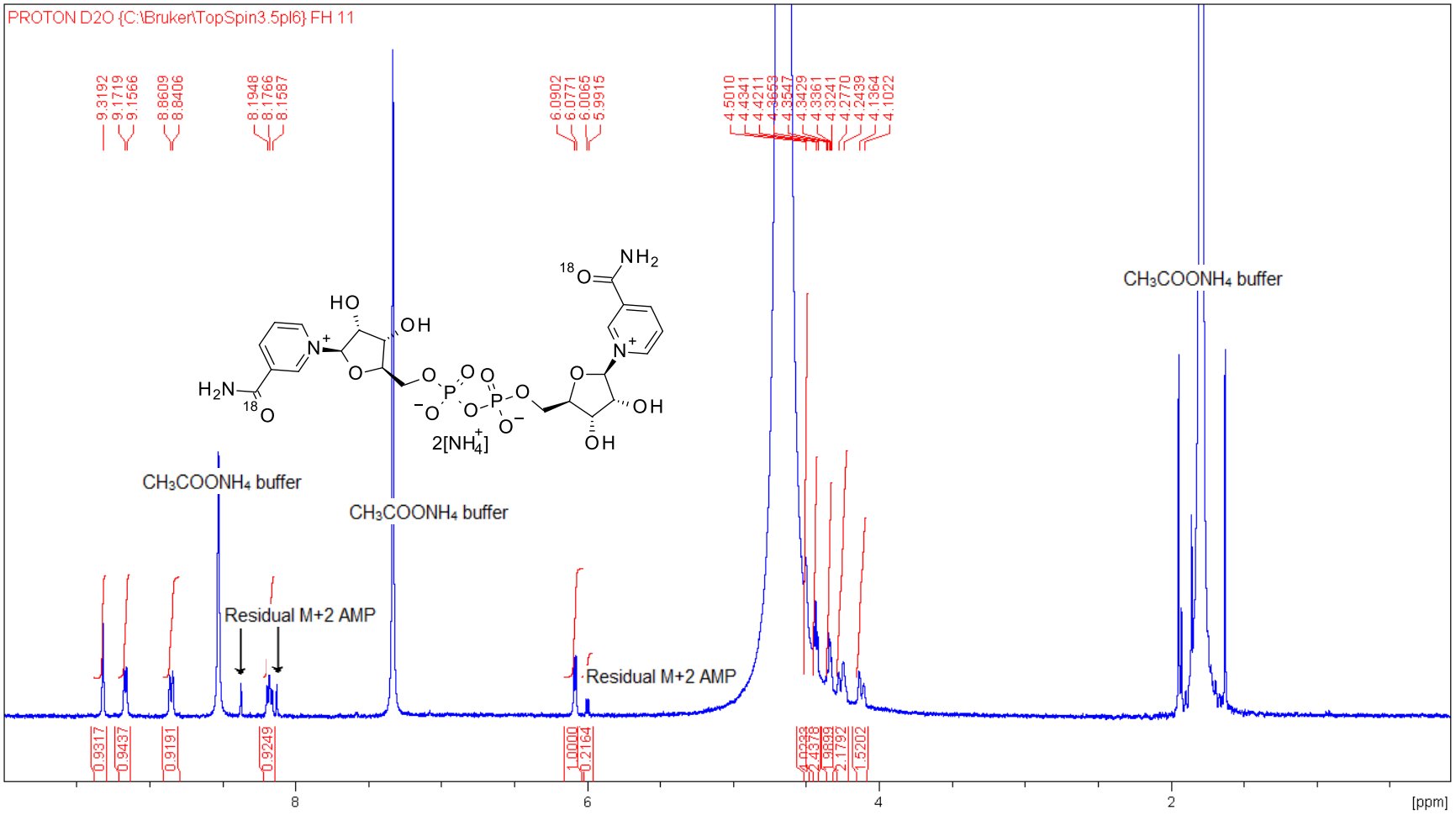
Compound 25. 100 MHz ^{13}C NMR spectrum in D_2O



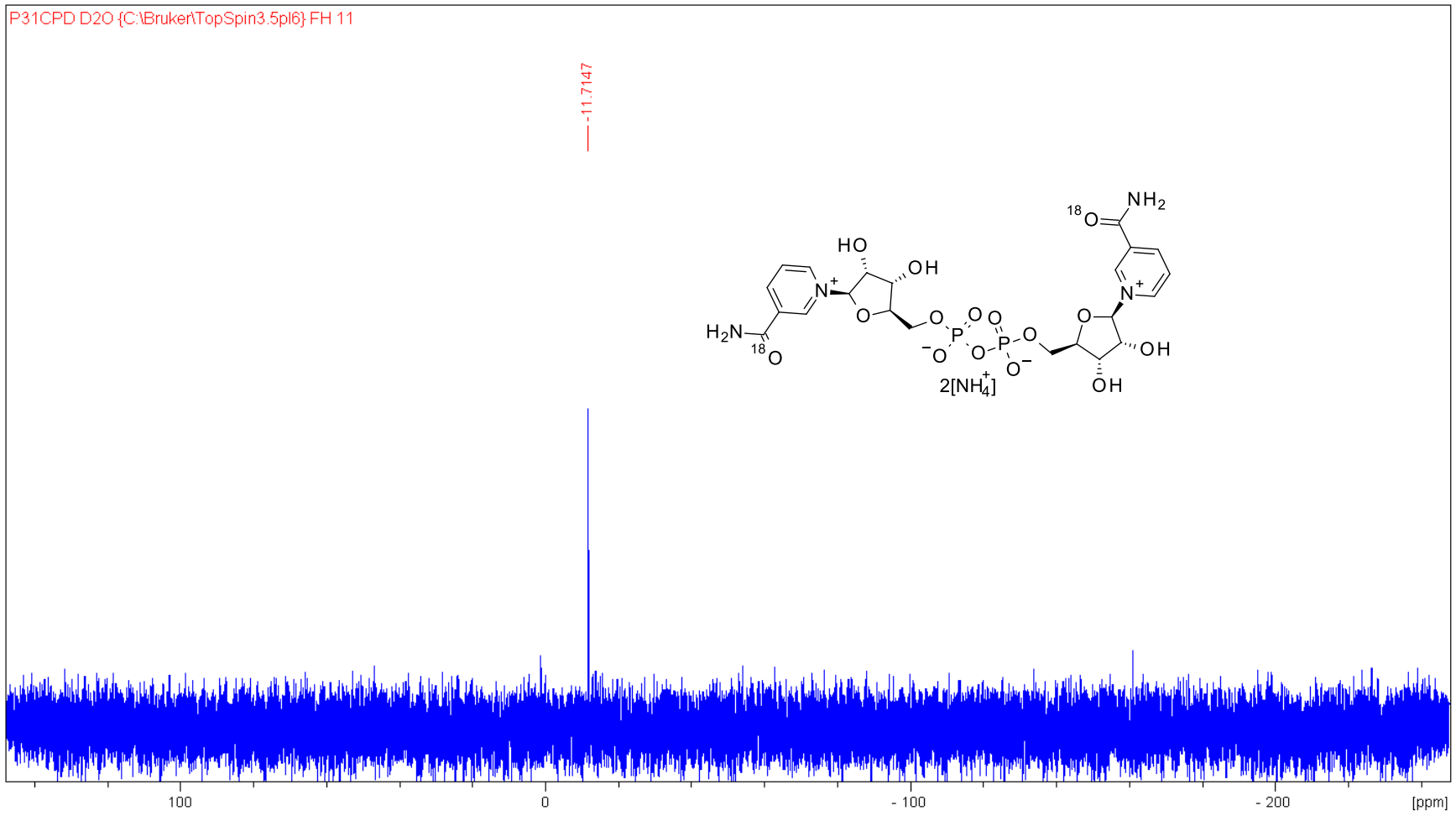
Compound 25. 162 MHz ^{31}P NMR spectrum in D_2O



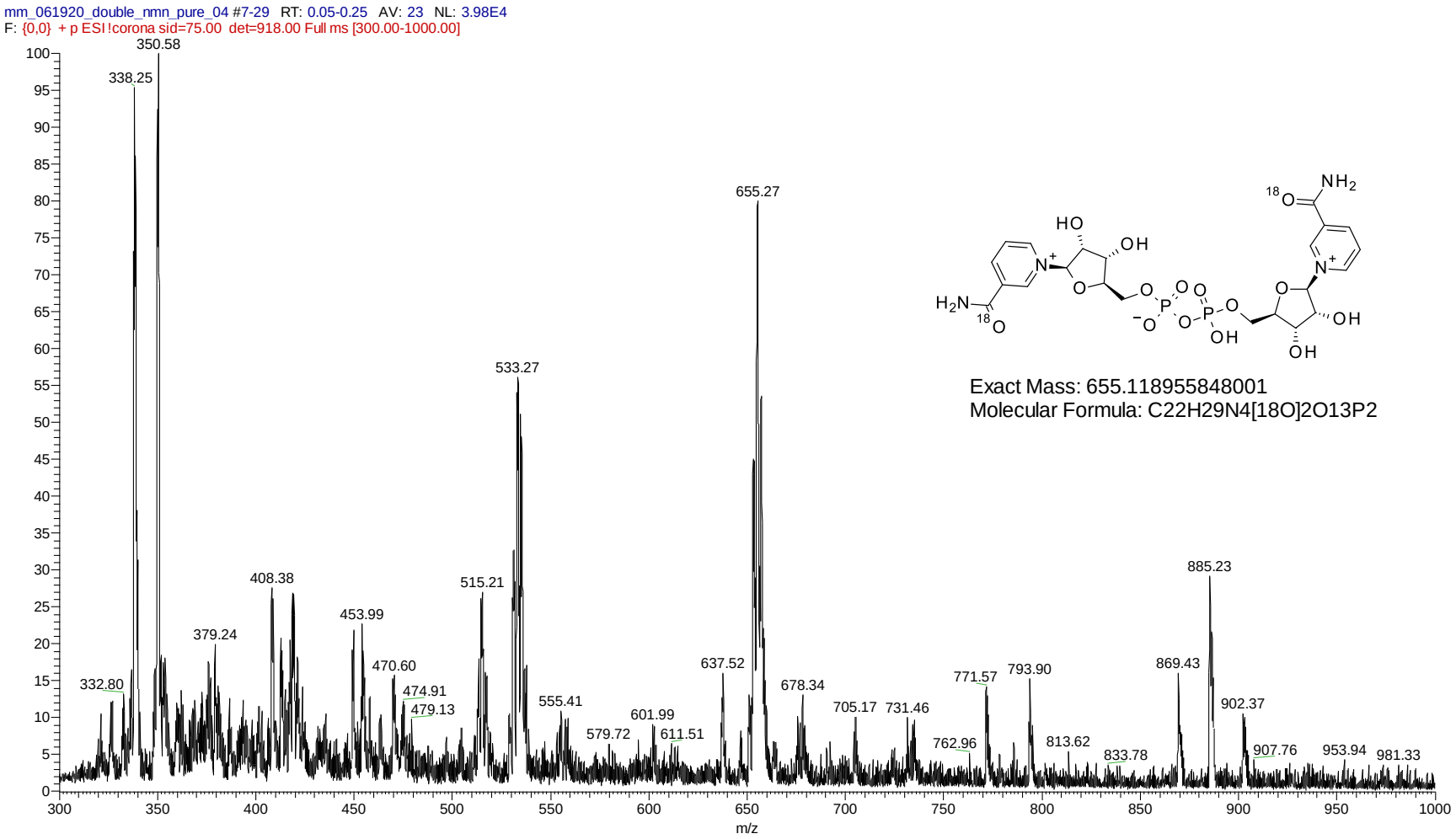
Compound 25. HRMS Spectra



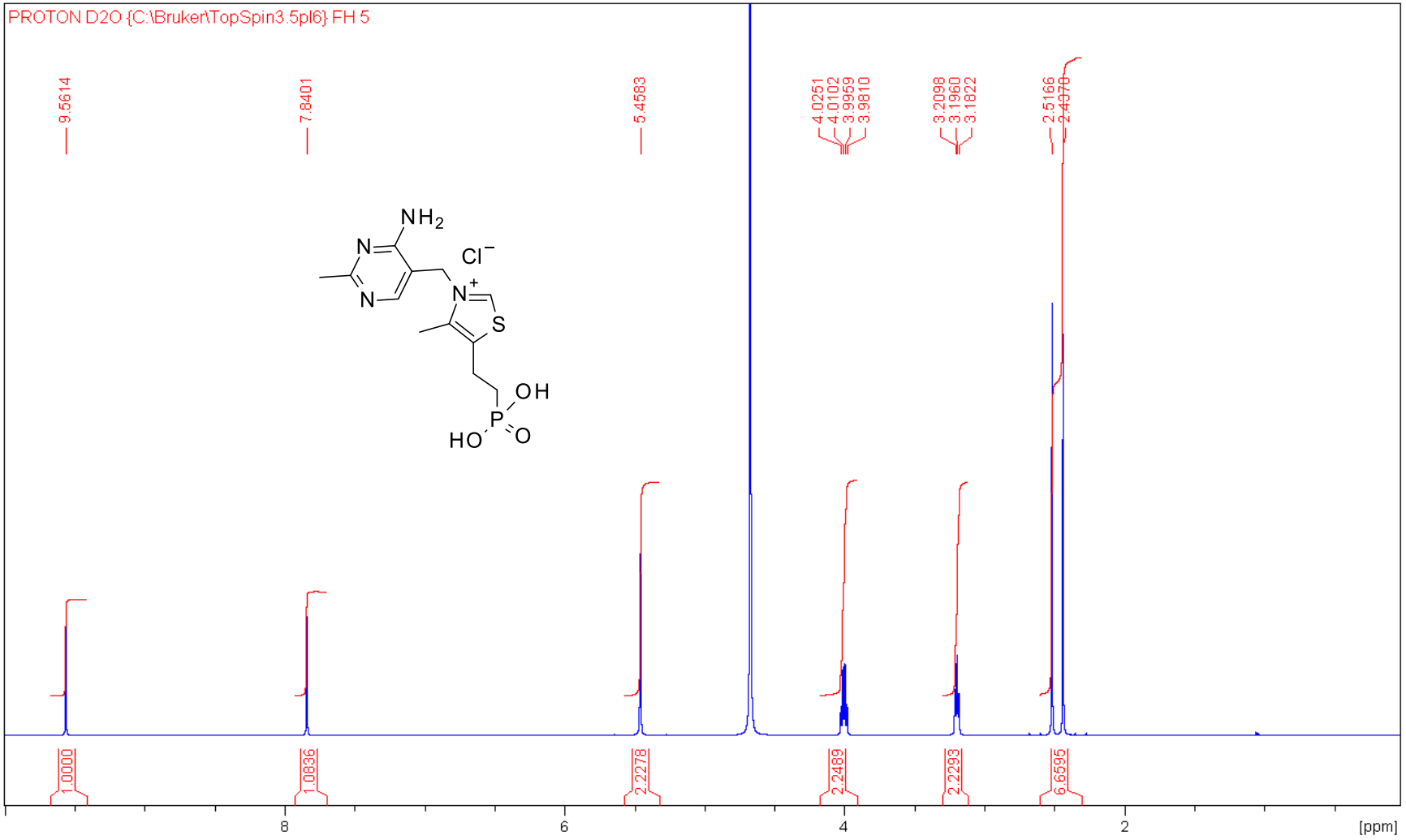
Compound 26. 400 MHz ^{1}H NMR spectrum in D_2O



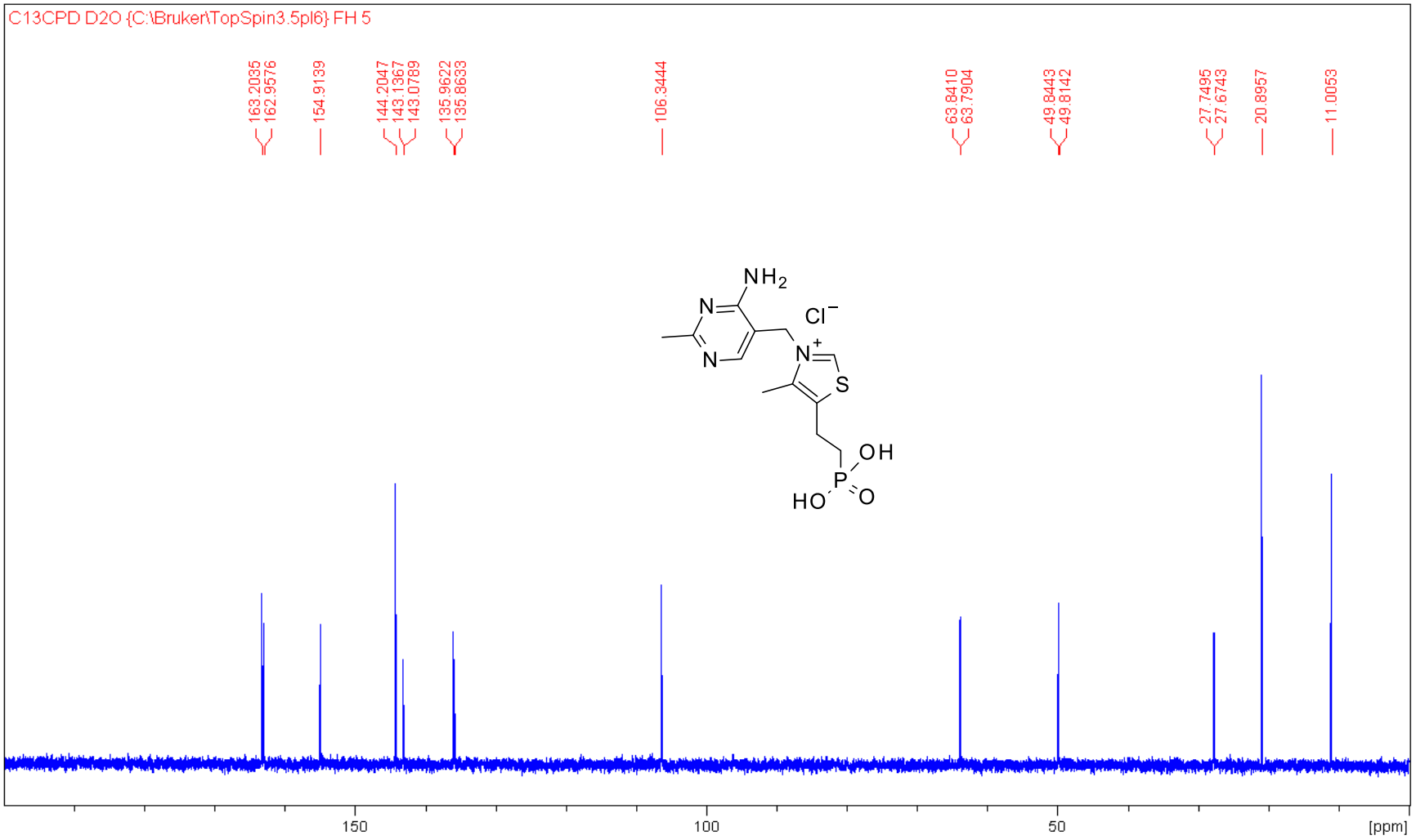
Compound 26. 162 MHz ^{31}P NMR spectrum in D_2O



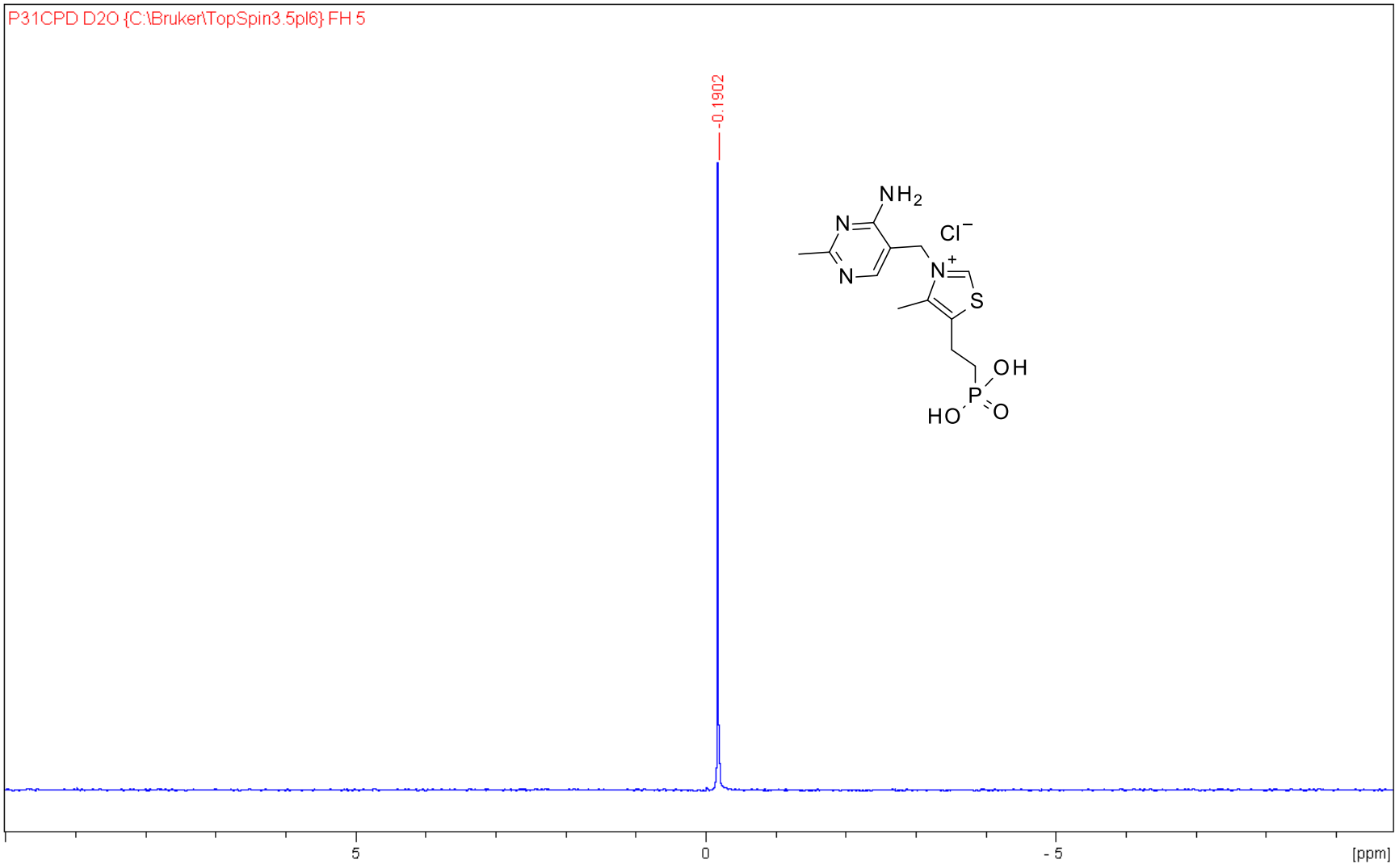
Compound 26. ESI-MS spectra



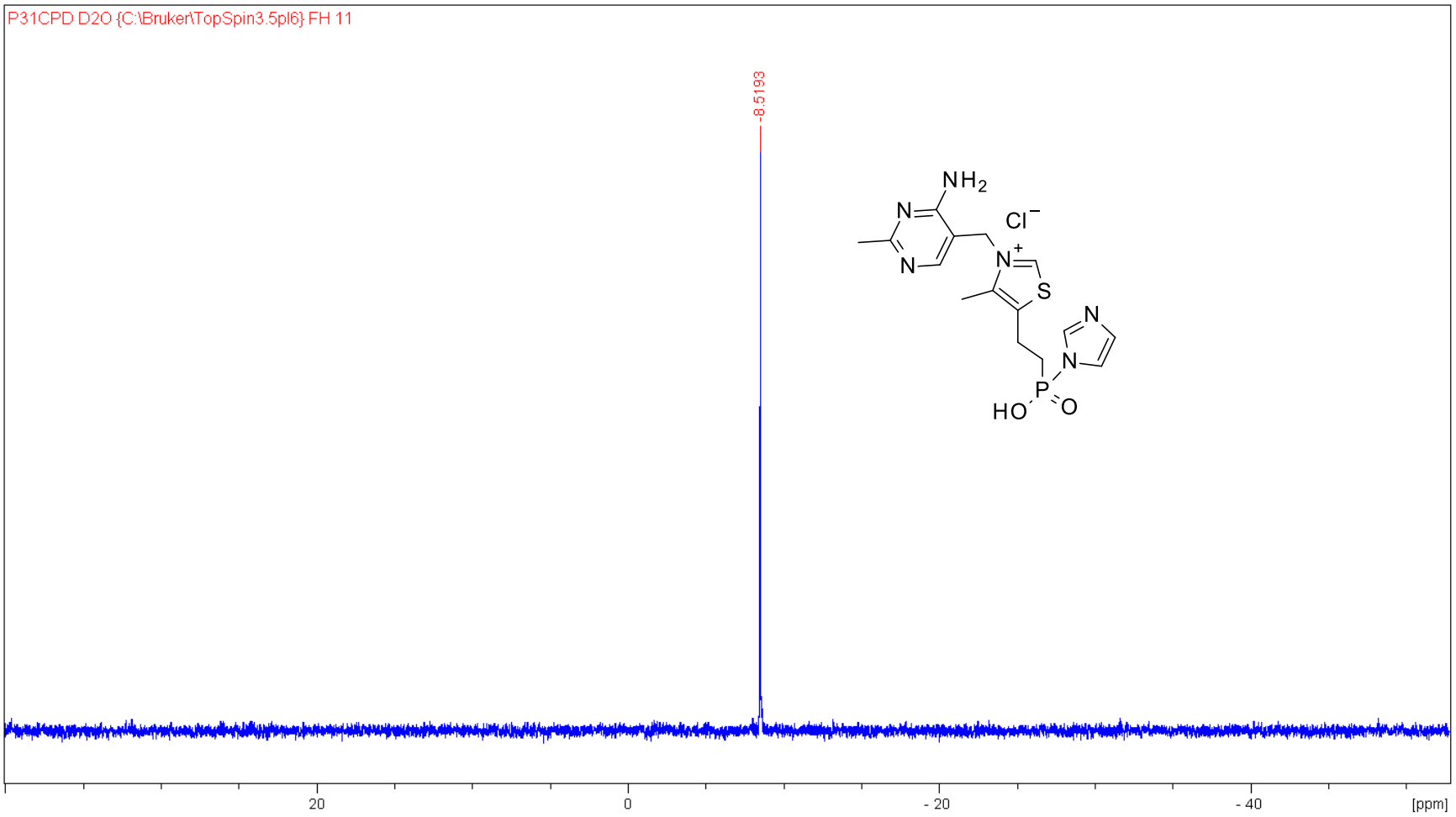
Compound 28. 400 MHz ^{1}H NMR spectrum in D_2O



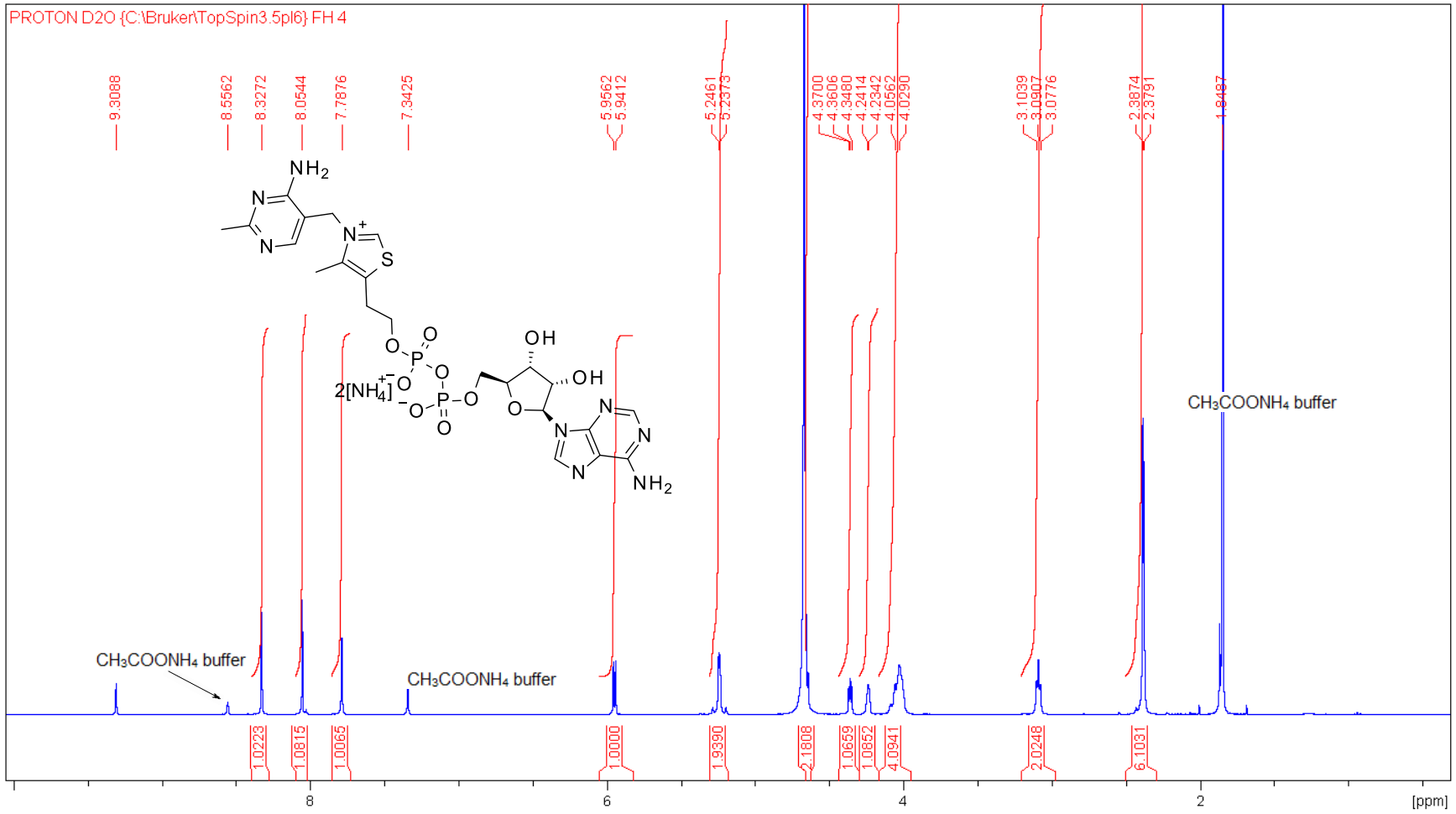
Compound 28. 100 MHz ^{13}C NMR spectrum in D_2O



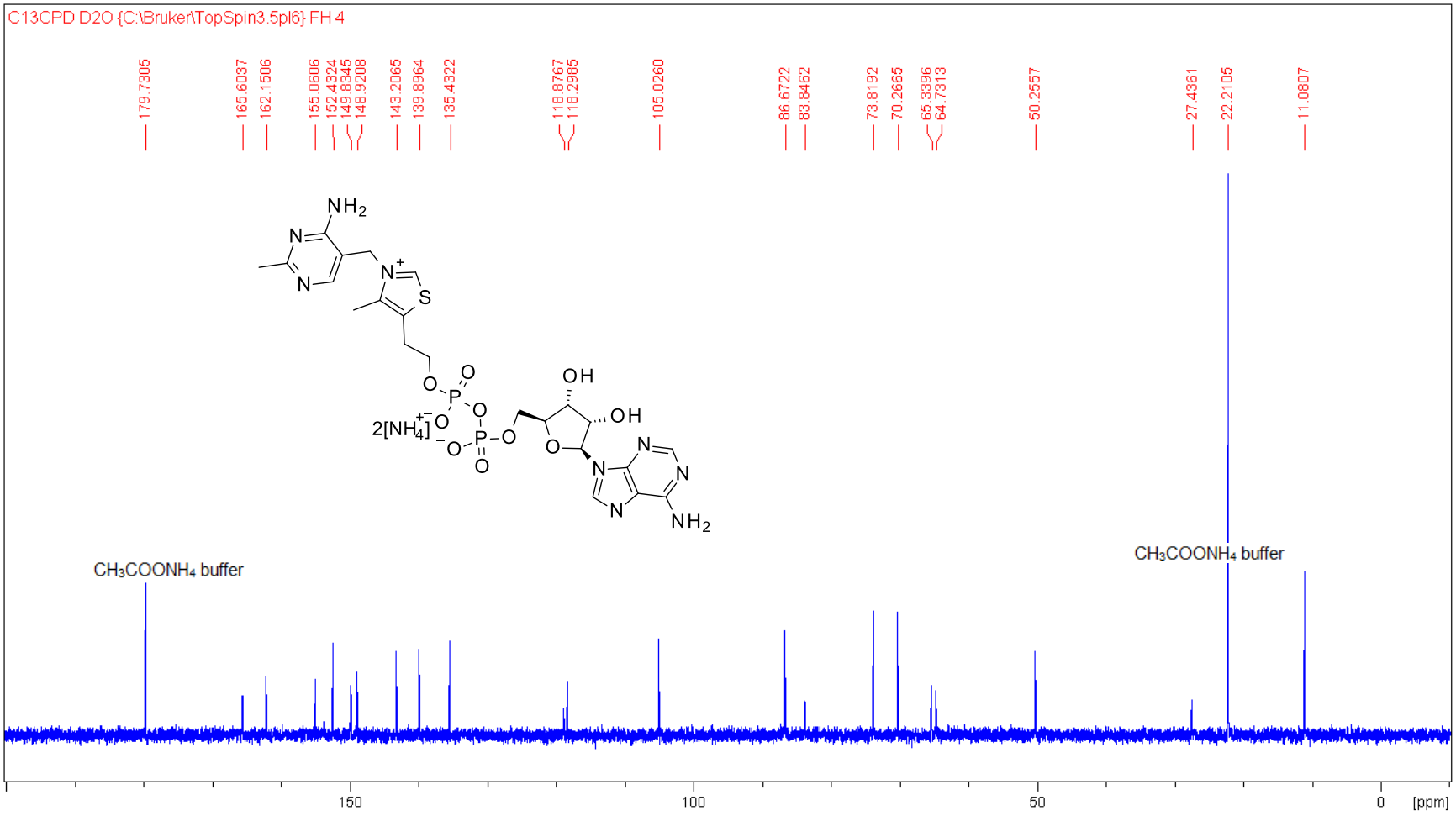
Compound 28. 162 MHz ^{31}P NMR spectrum in D_2O



Compound 29. 162 MHz ^{31}P NMR spectrum in D_2O



Compound 30a. 400 MHz ^{1}H NMR spectrum in D_2O


C13CPD D2O {C:\Bruker\TopSpin3.5pl6} FH 4
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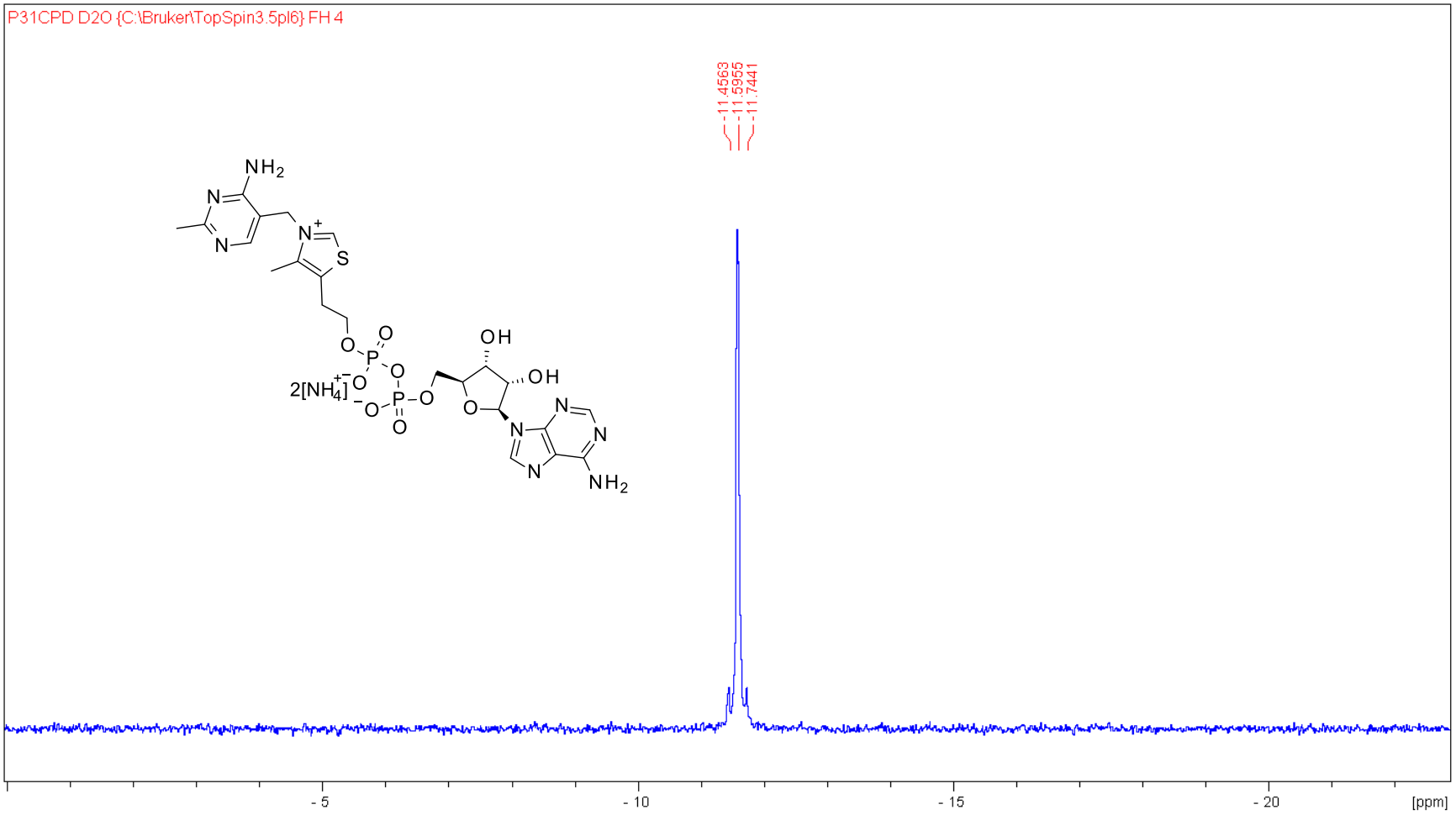
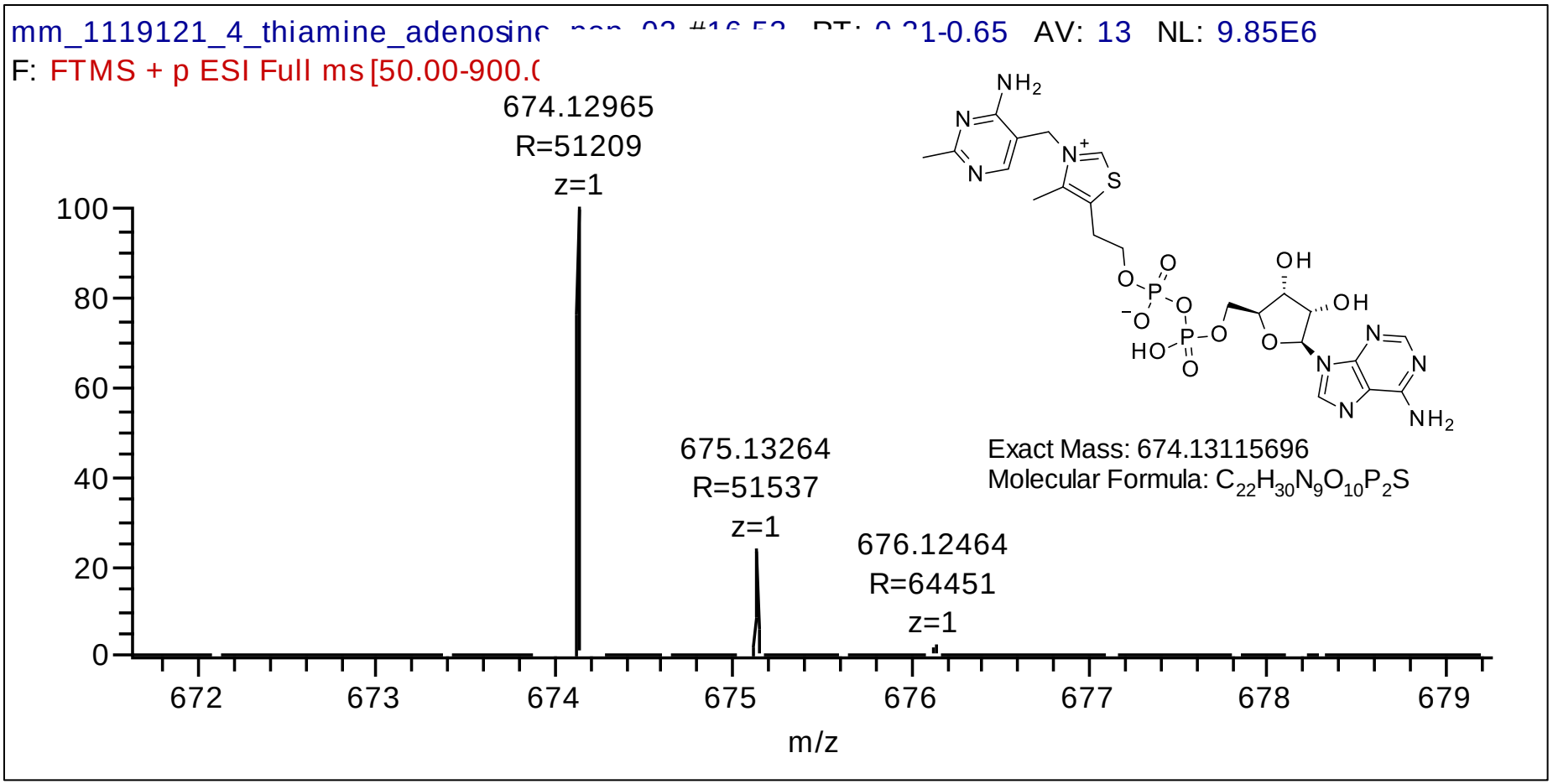
162.1506
155.0606
152.4324
149.8345
148.9208
143.2065
139.8964
135.4322
118.8767
118.2985
105.0260
86.6722
83.8462
73.8192
70.2665
65.3396
64.7313
50.2557
27.4361
22.2105
11.0807
CH3COONH4 buffer
CH3COONH4 buffer
150
100
50
0
[ppm]

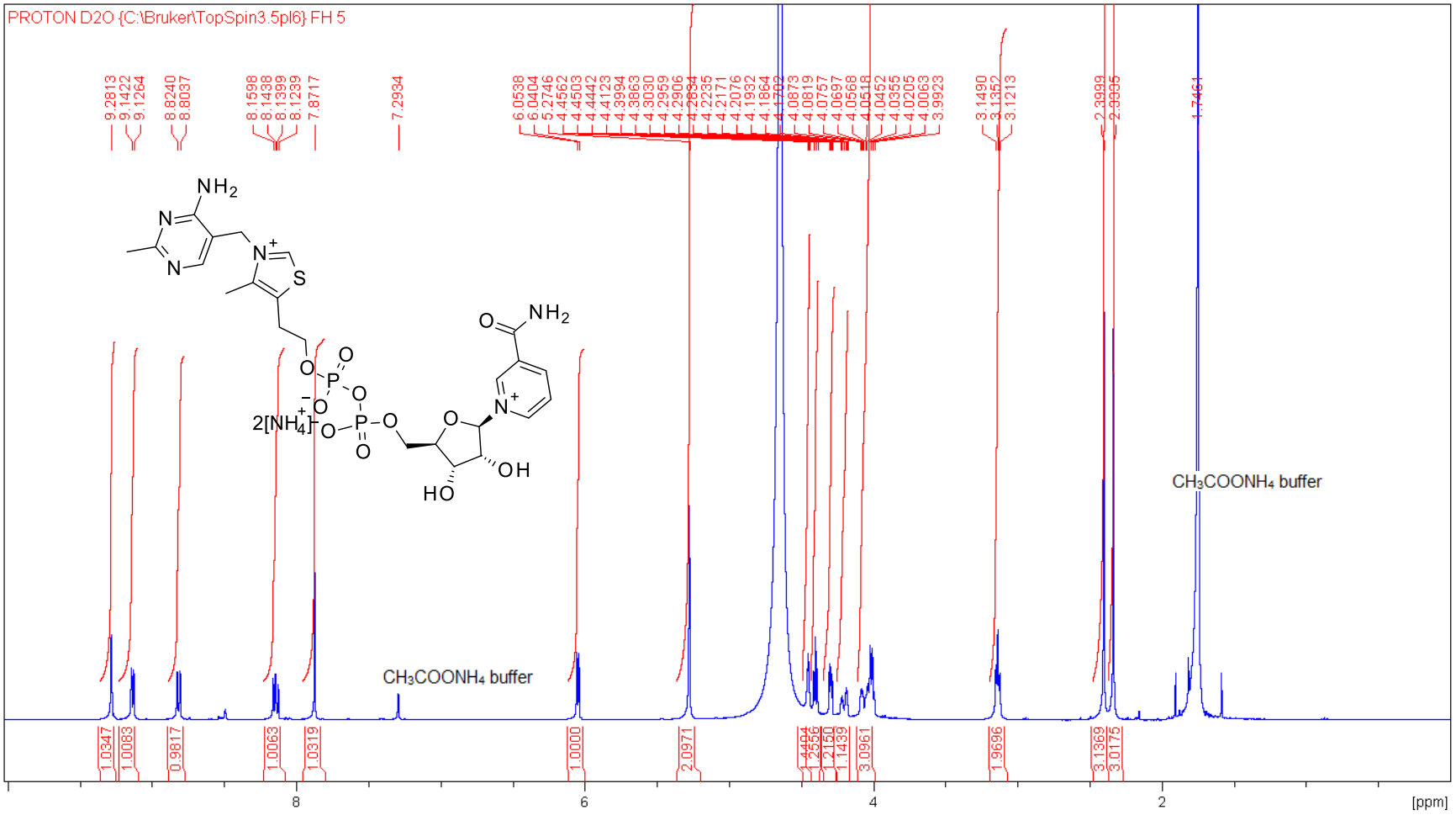
Compound 30a. 100 MHz ^{13}C NMR spectrum in D_2O



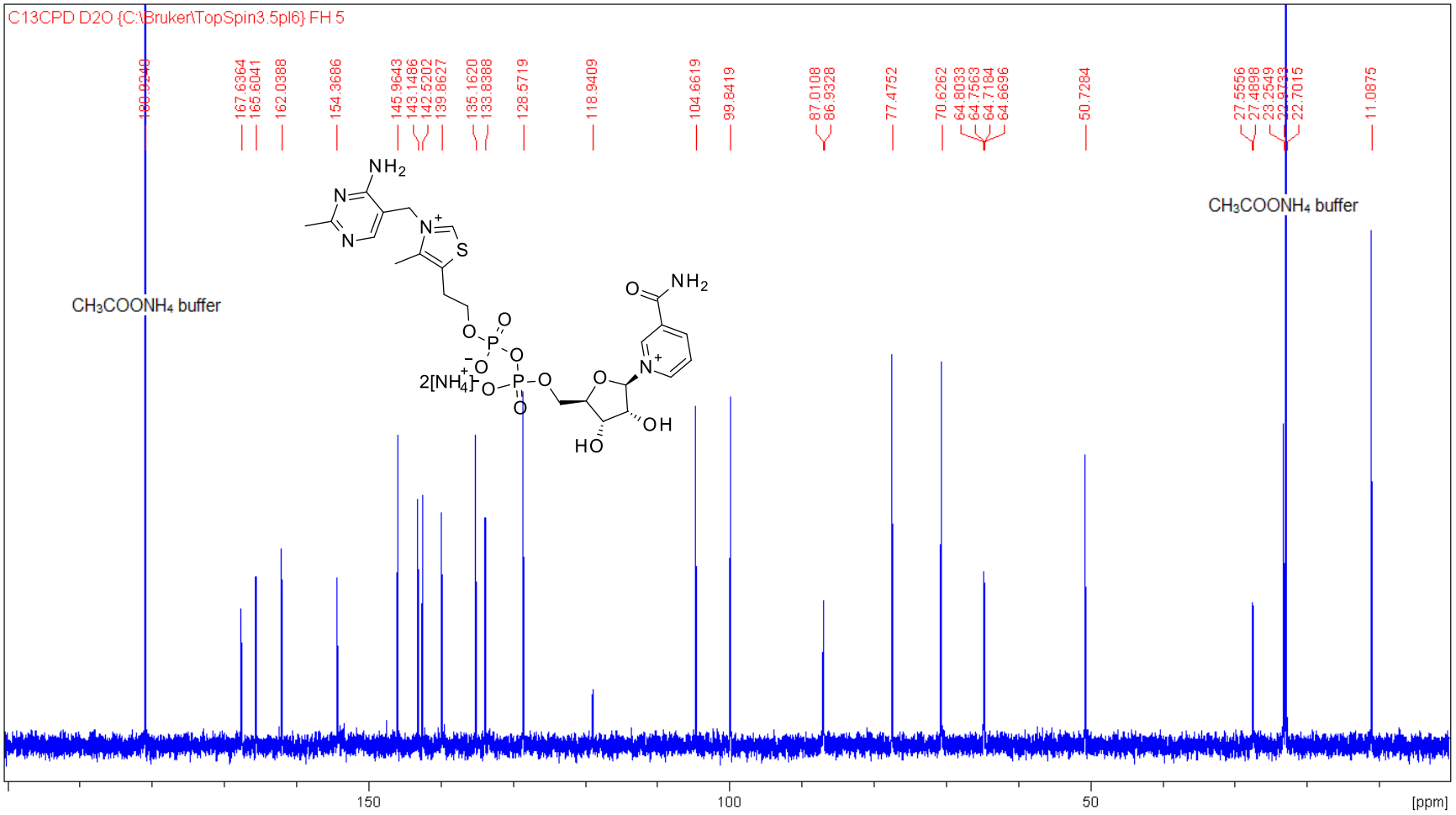
Compound 30a. 162 MHz ^{31}P NMR spectrum in D_2O



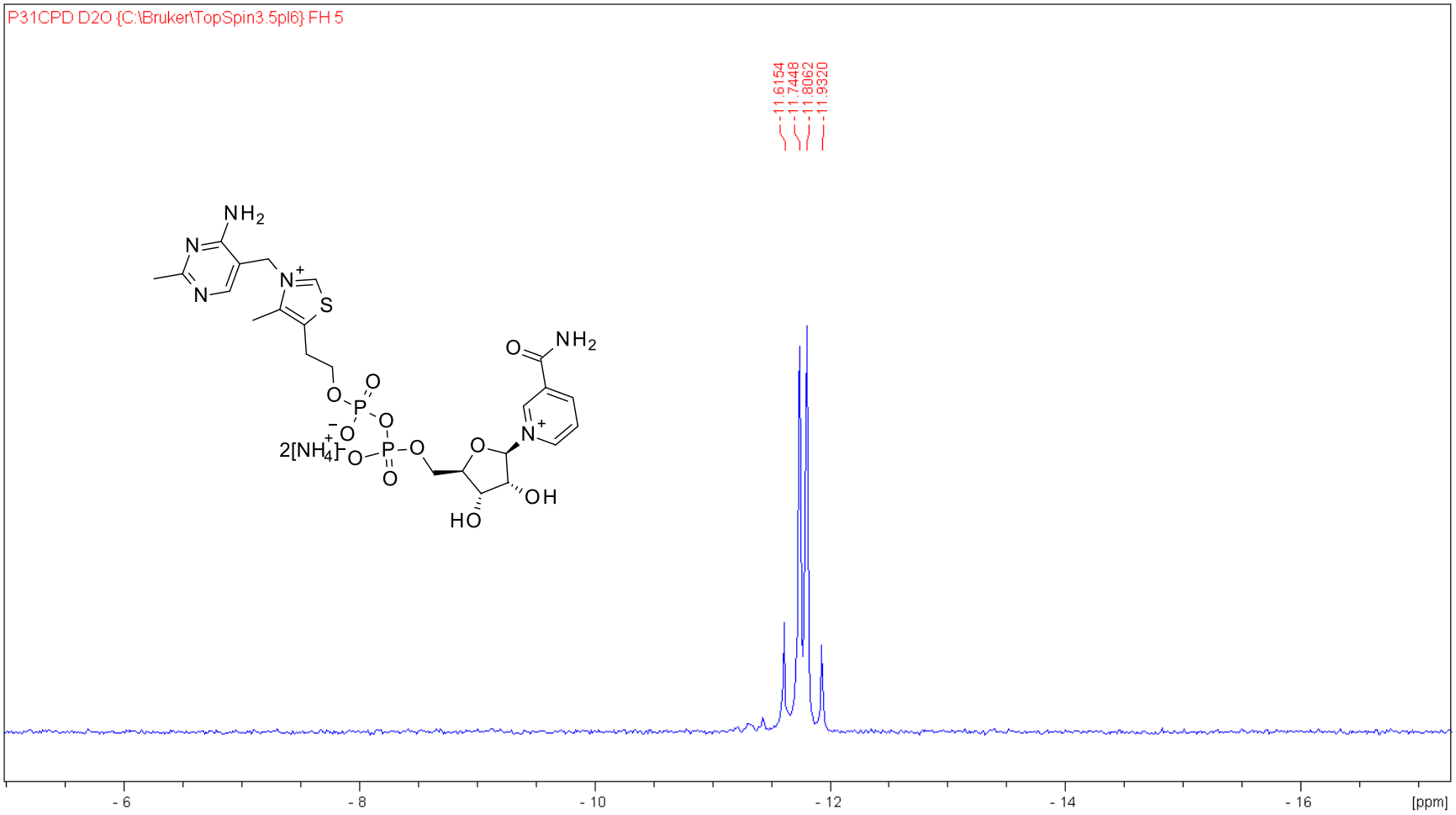
Compound 30a. HRMS spectra



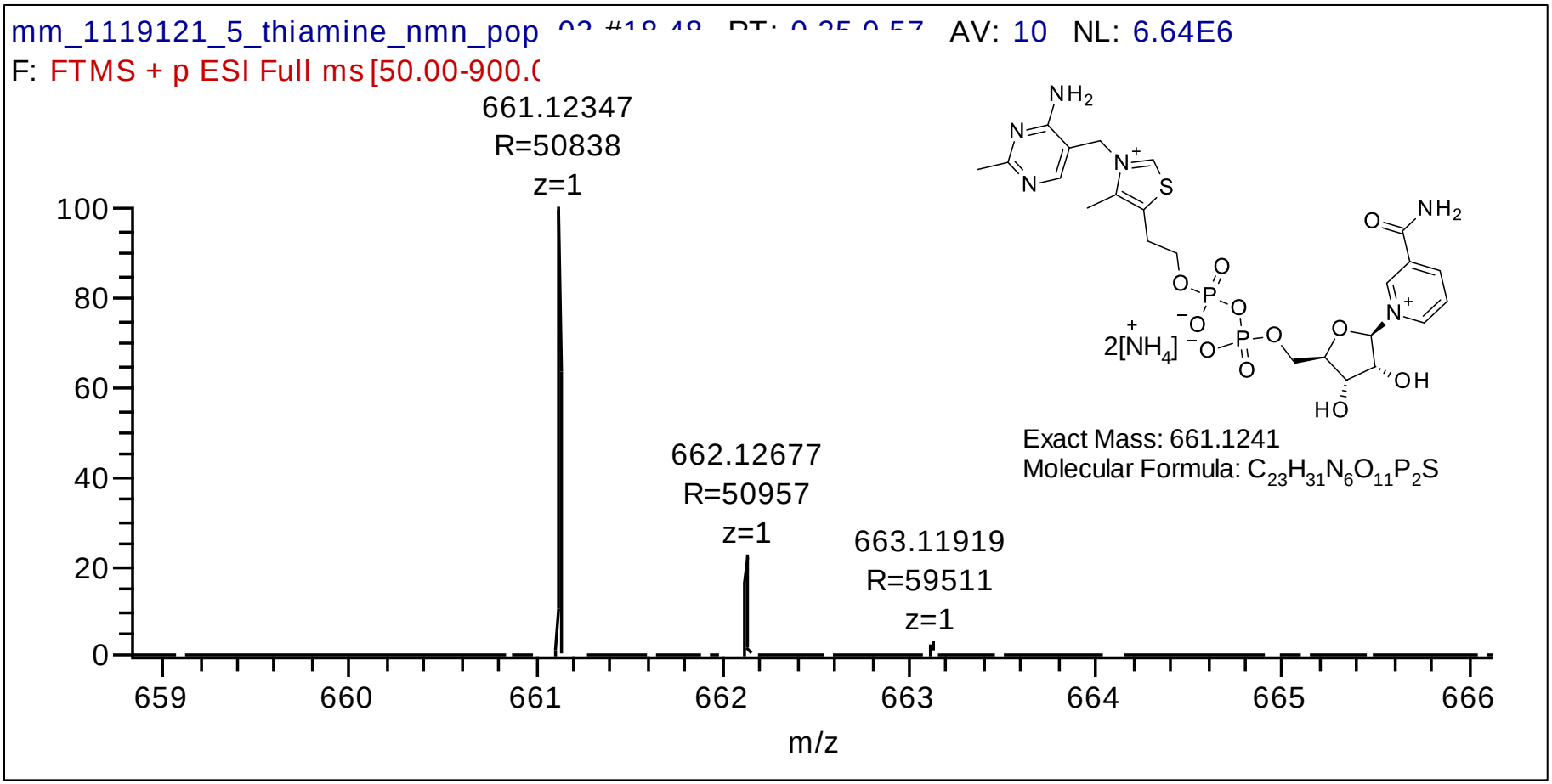
Compound 31. 400 MHz ^{1}H NMR spectrum in D_2O



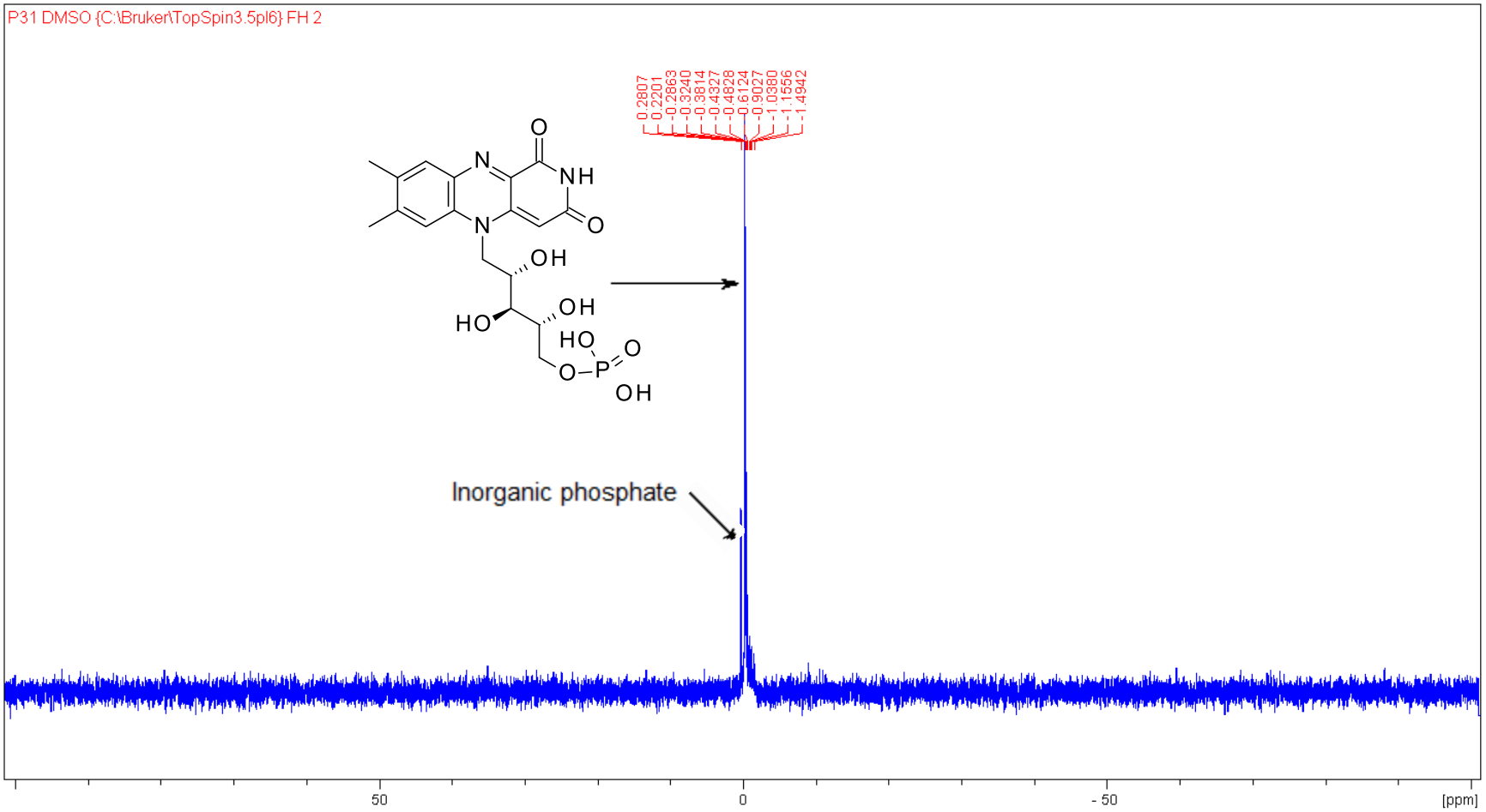
Compound 31. 100 MHz ^{13}C NMR spectrum in D_2O



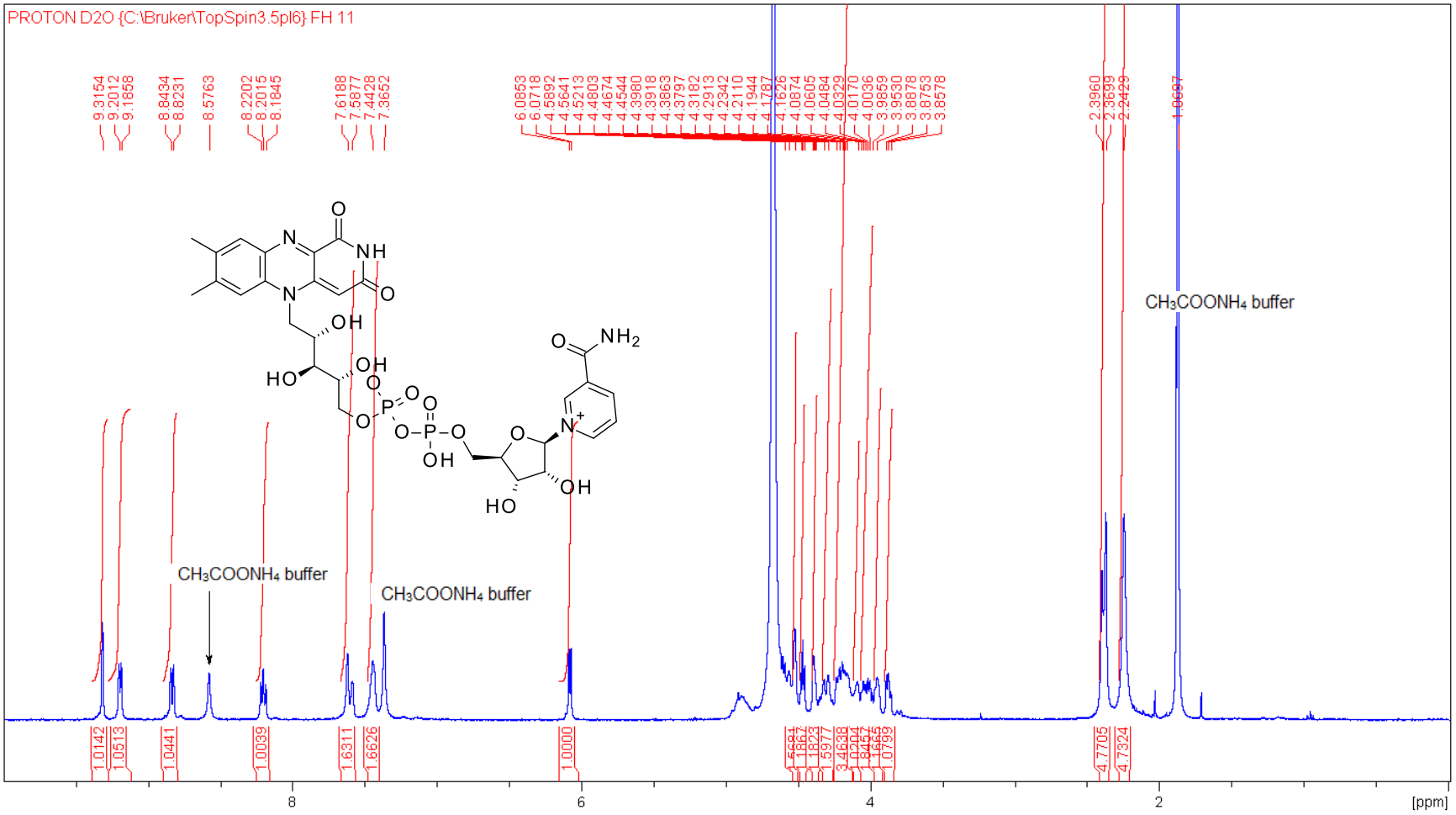
Compound 31. 162 MHz ^{31}P NMR spectrum in D_2O



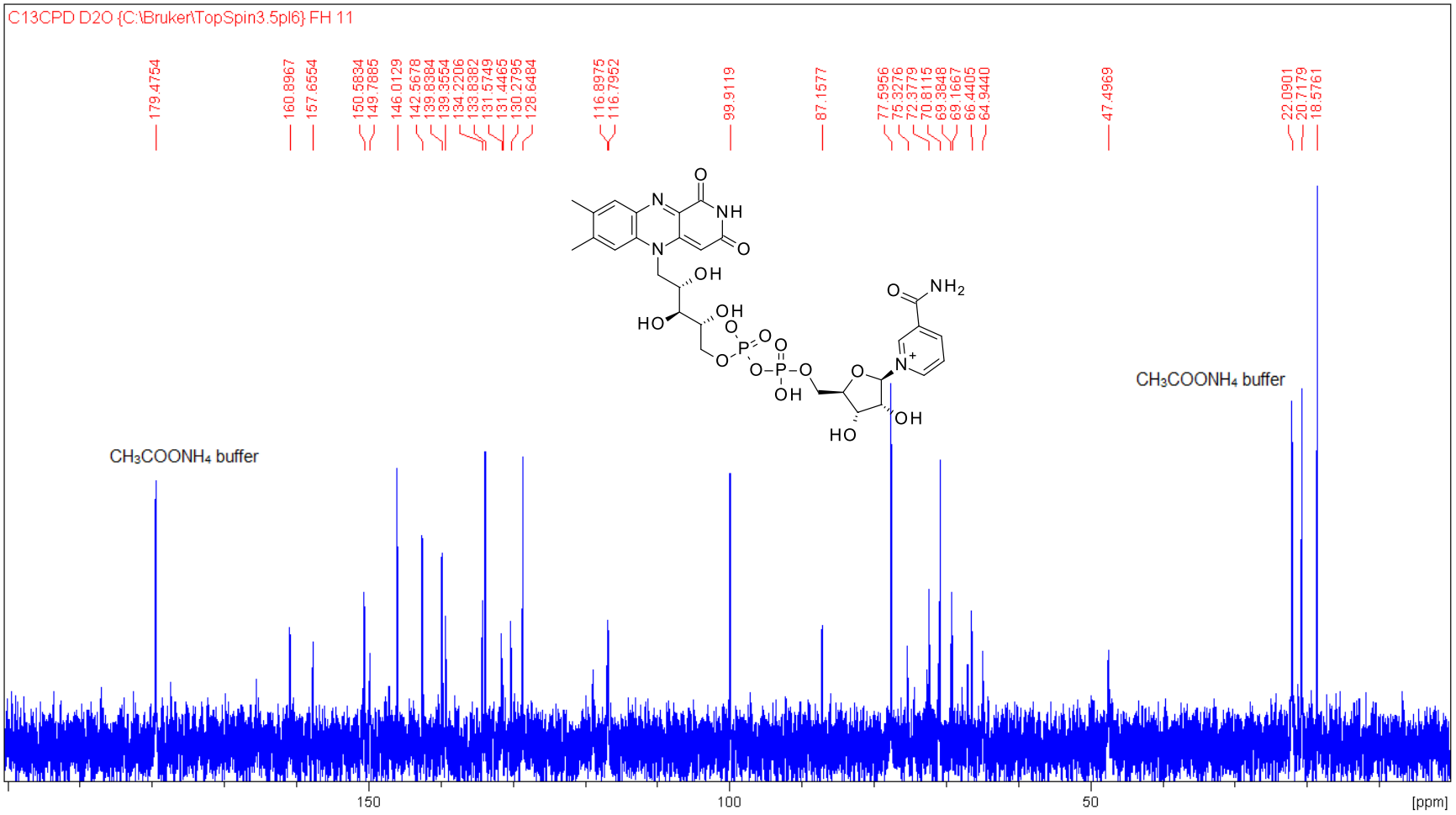
Compound 31. HRMS spectra



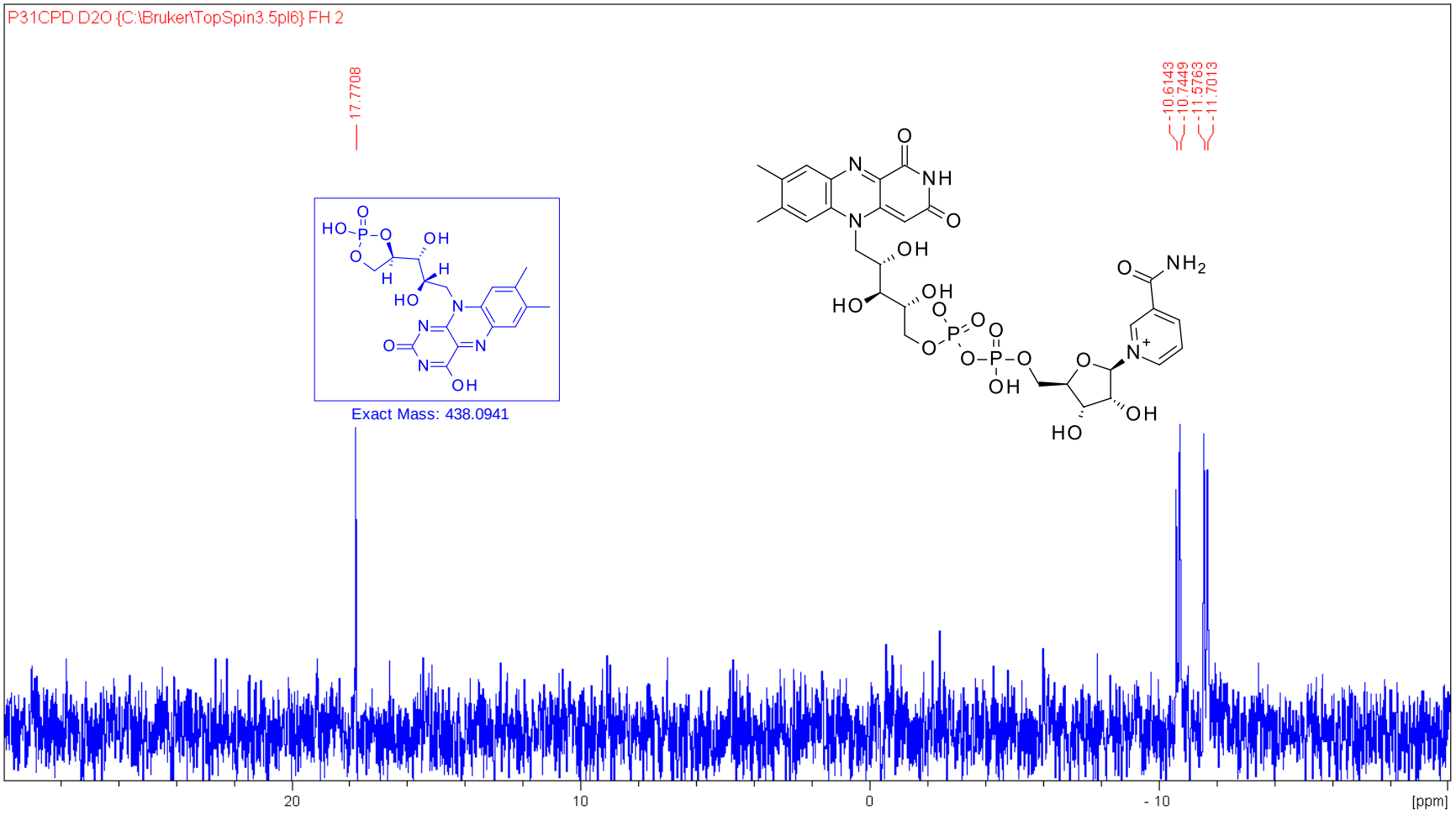
Compound 32. 162 MHz ^{31}P NMR spectrum in D_2O



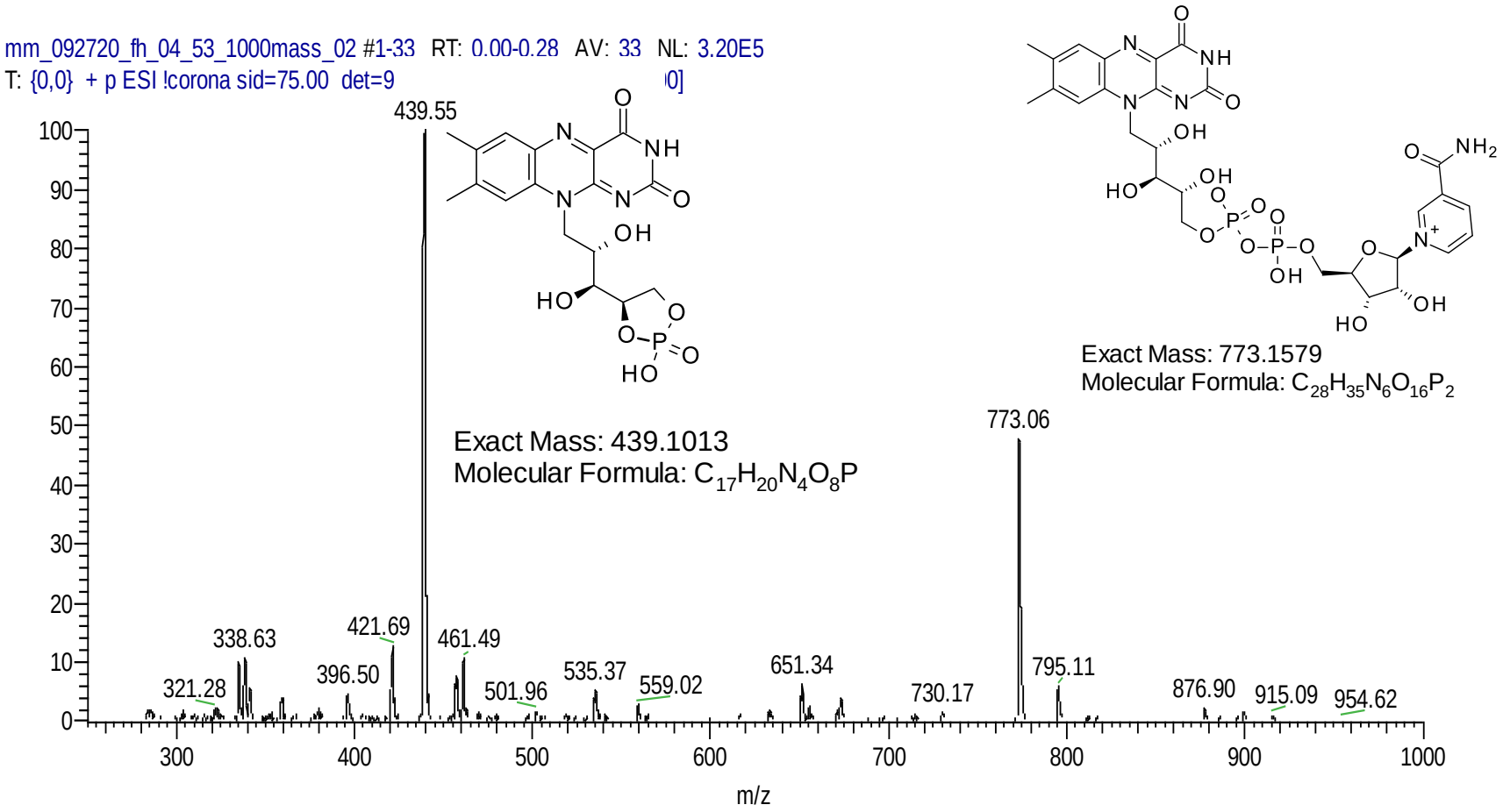
Compound33. 400 MHz ^{1}H NMR spectrum in D_2O



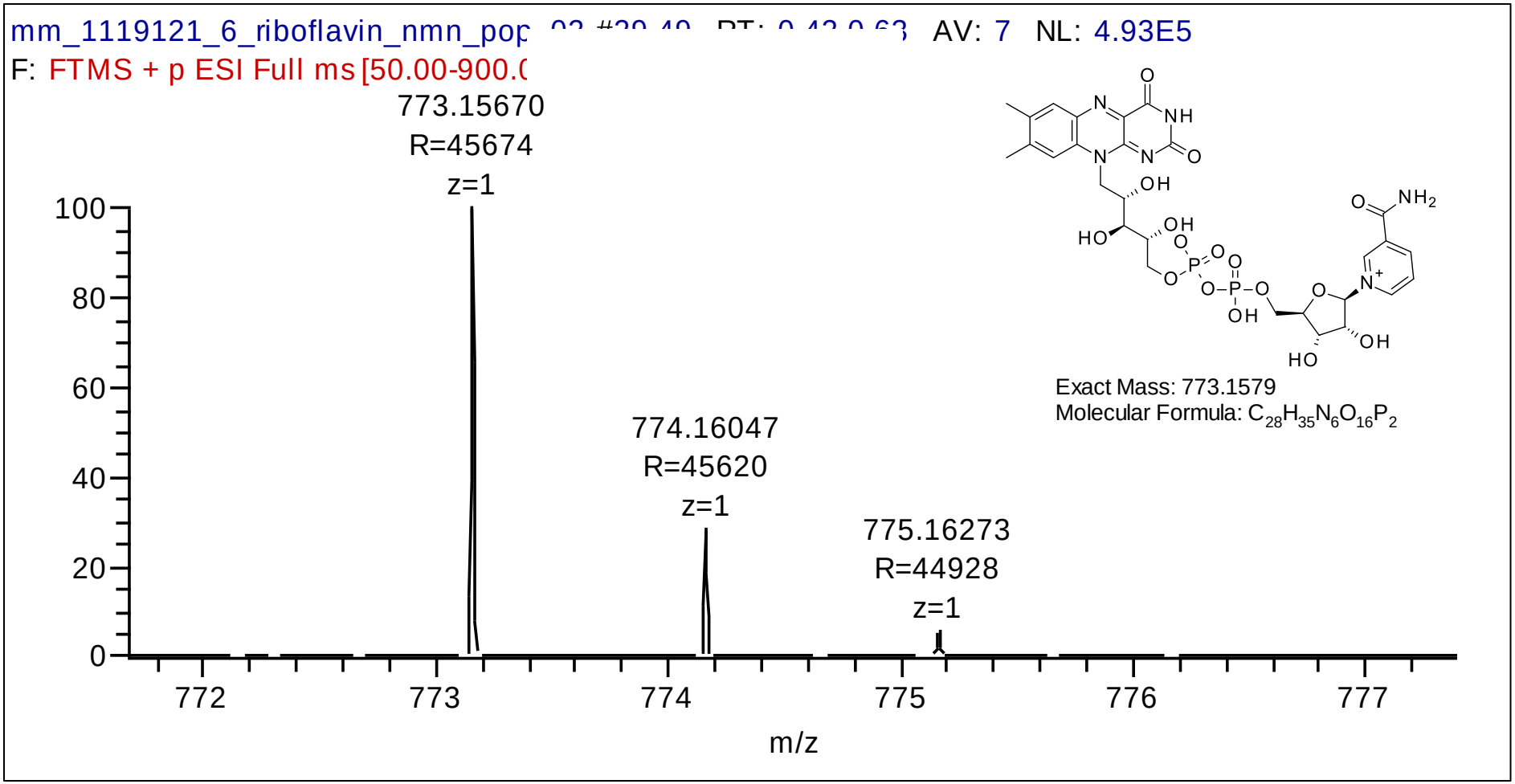
Compound 33. 100 MHz ^{13}C NMR spectrum in D_2O



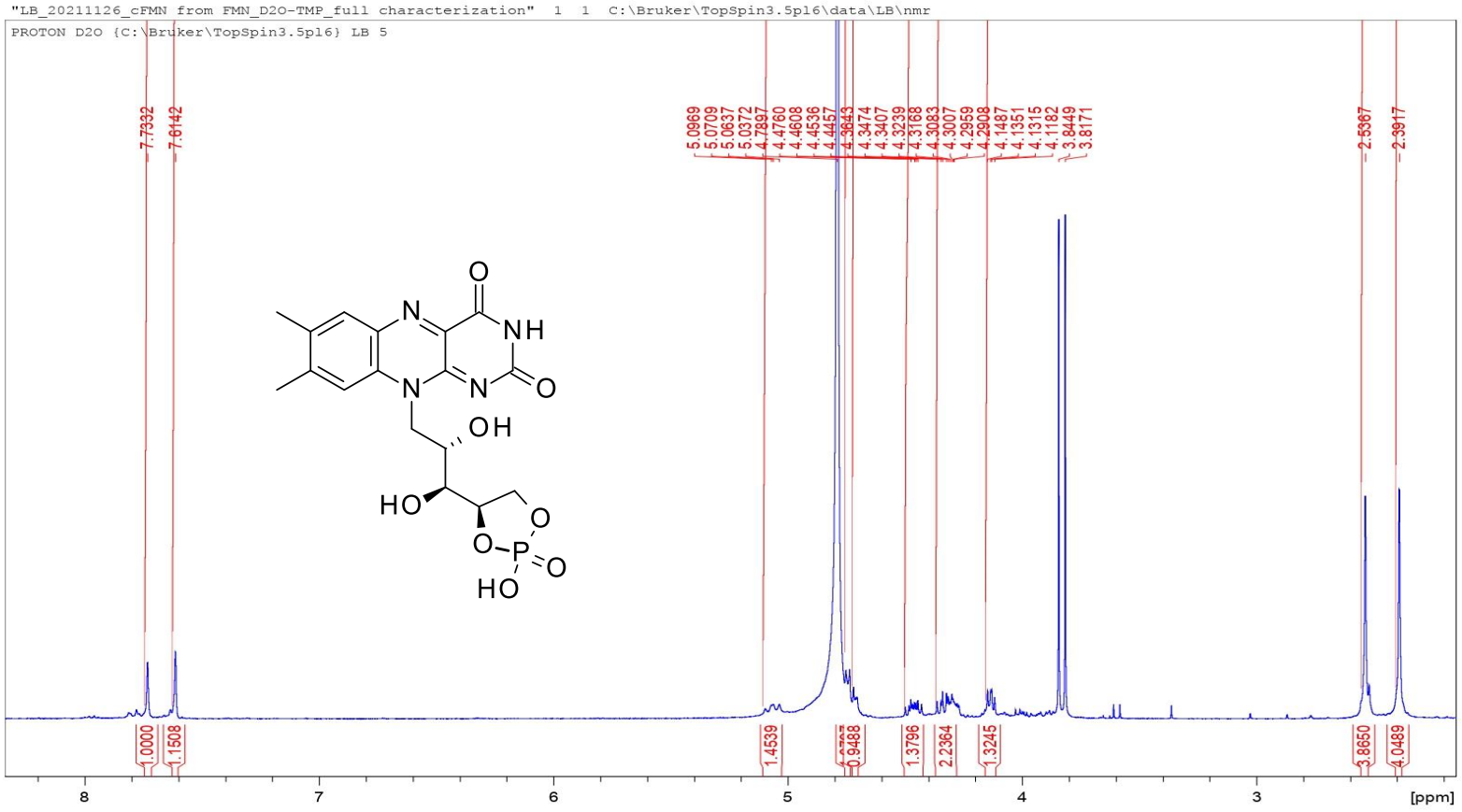
Compound 33. 162 MHz ^{31}P NMR spectrum in D_2O



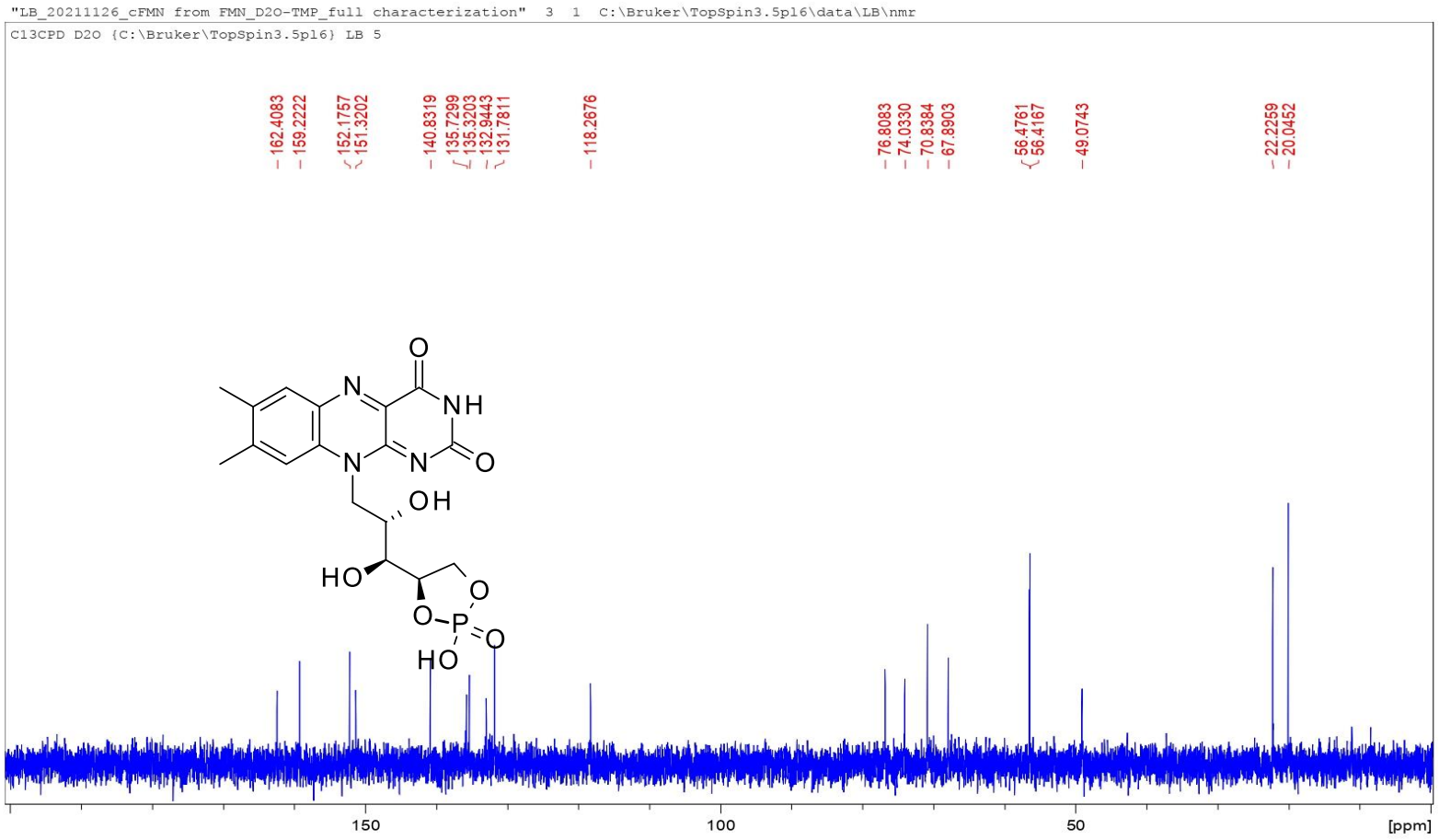
Compound 33&34. ESI-MS spectra



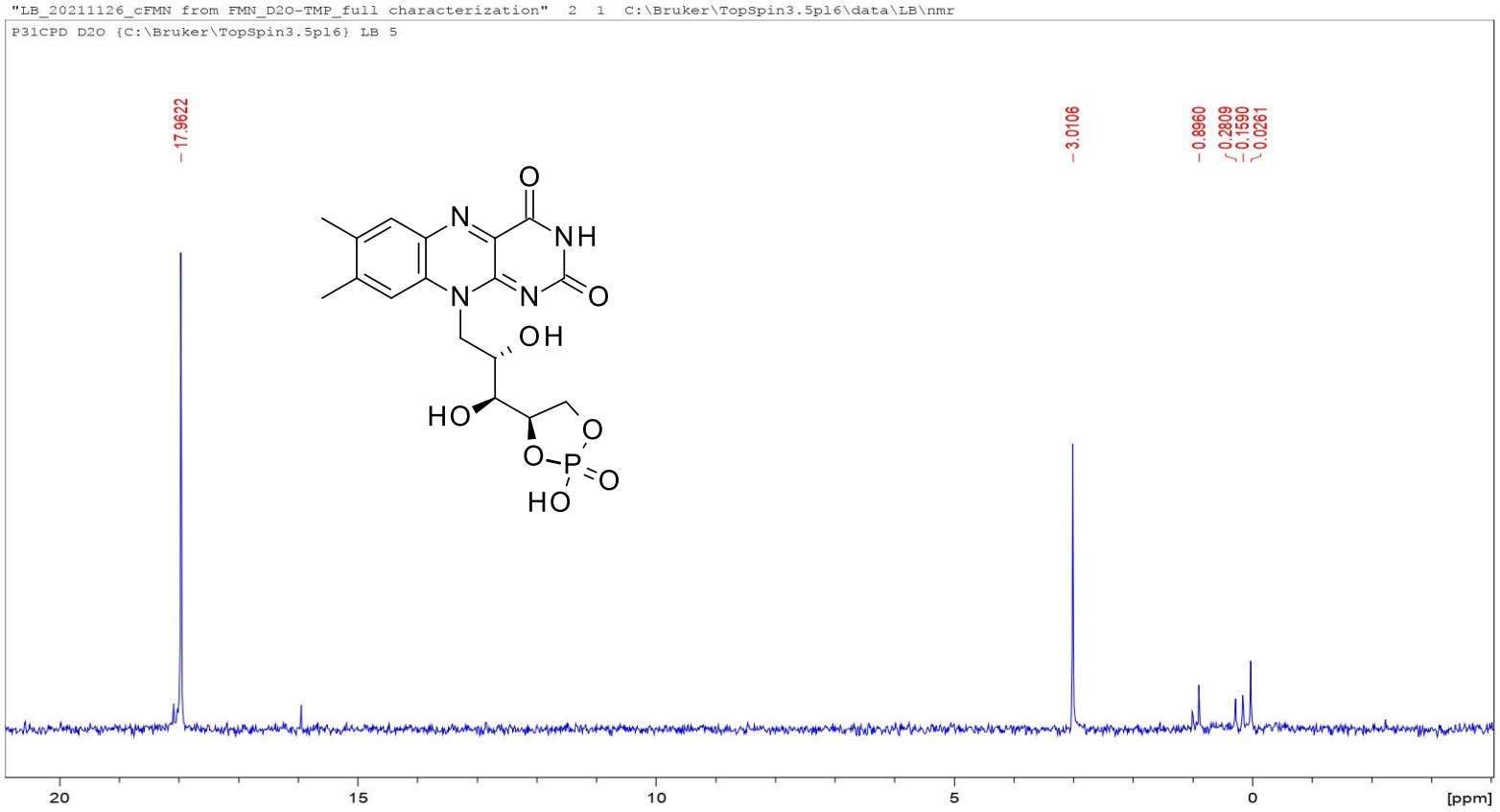
Compound 33. HRMS spectra



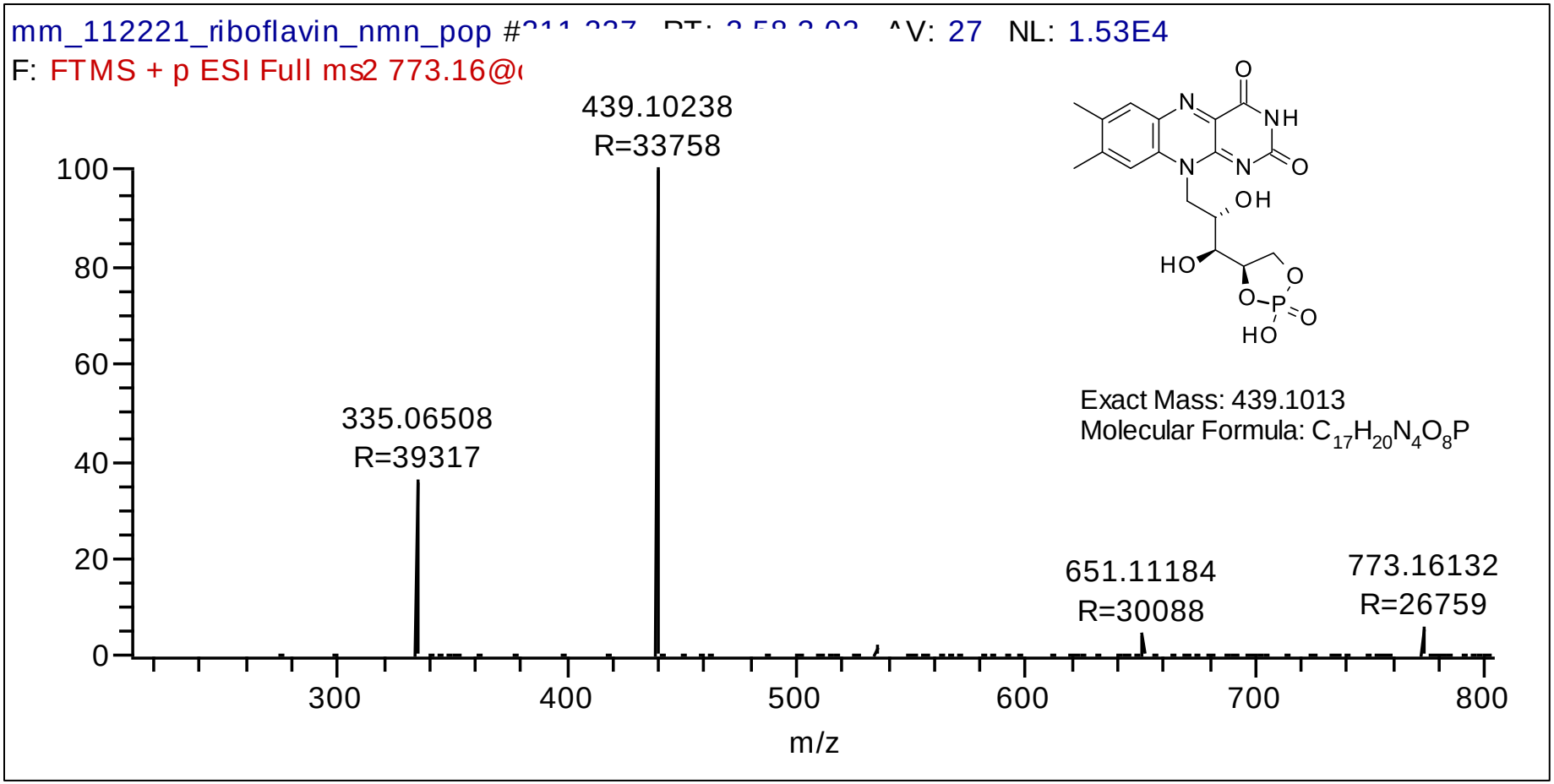
Compound 34. 400 MHz ^{1}H NMR spectrum in D_2O



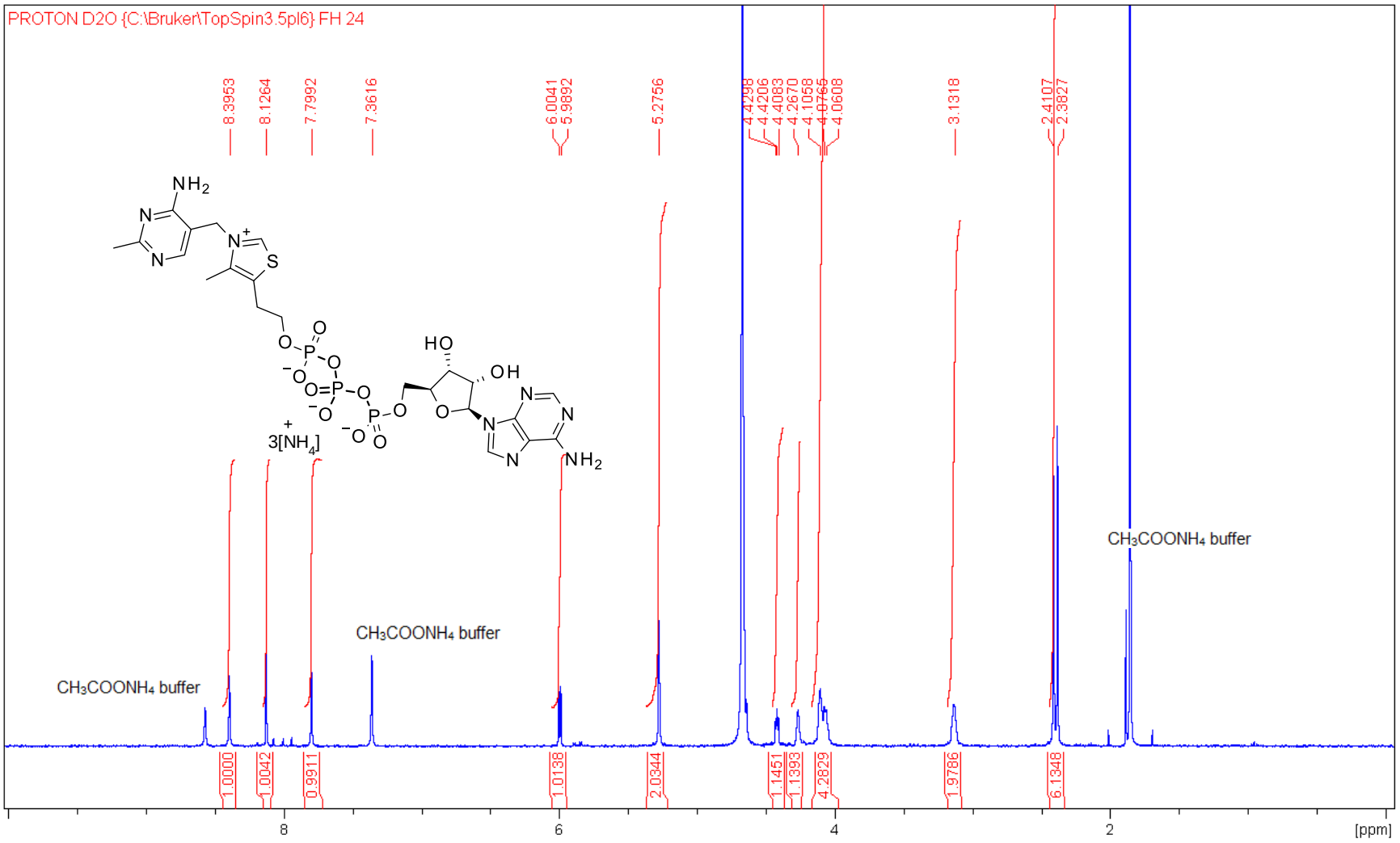
Compound 34. 100 MHz ^{13}C NMR spectrum in D_2O



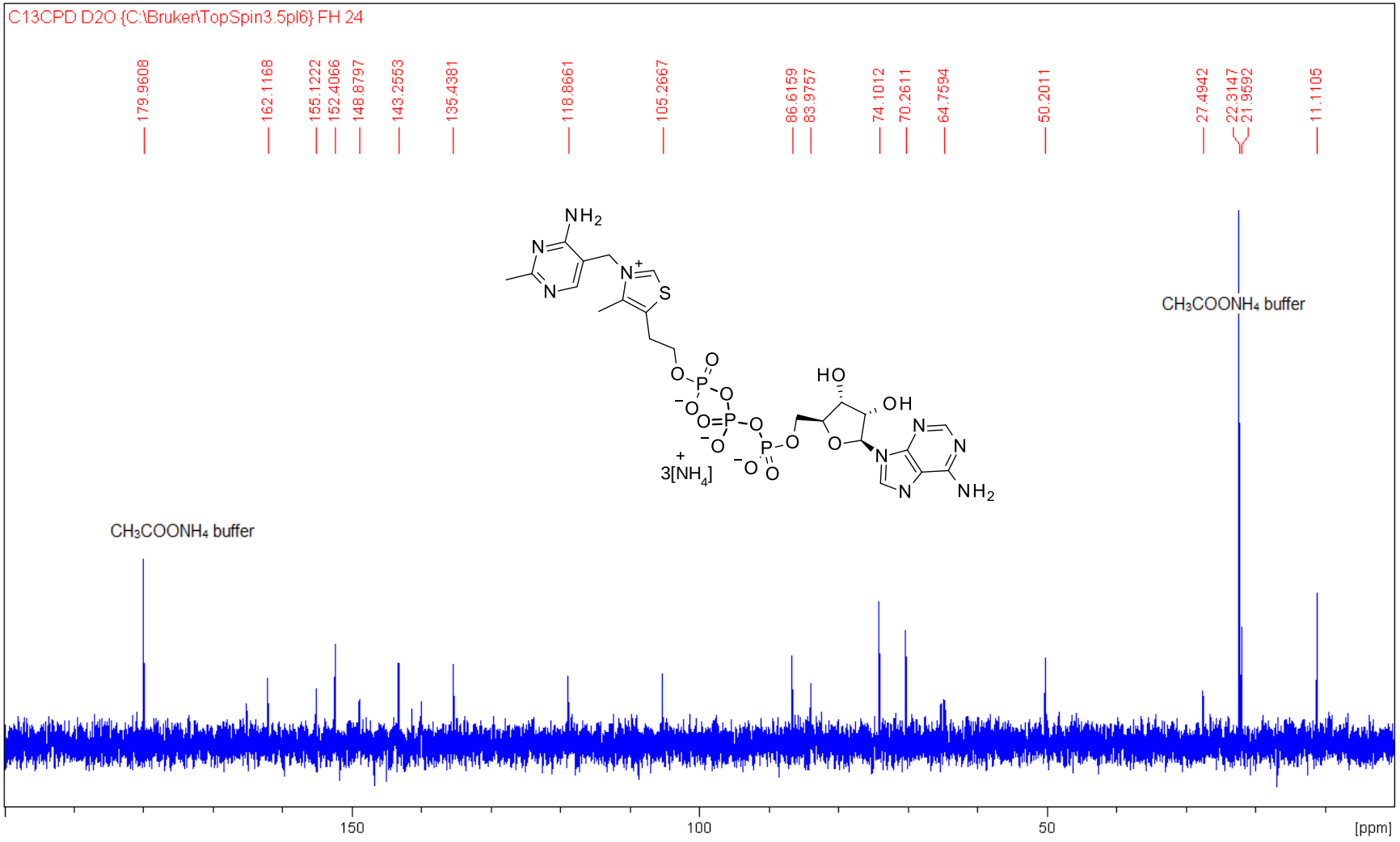
Compound 34. 162 MHz ^{31}P NMR spectrum in D_2O



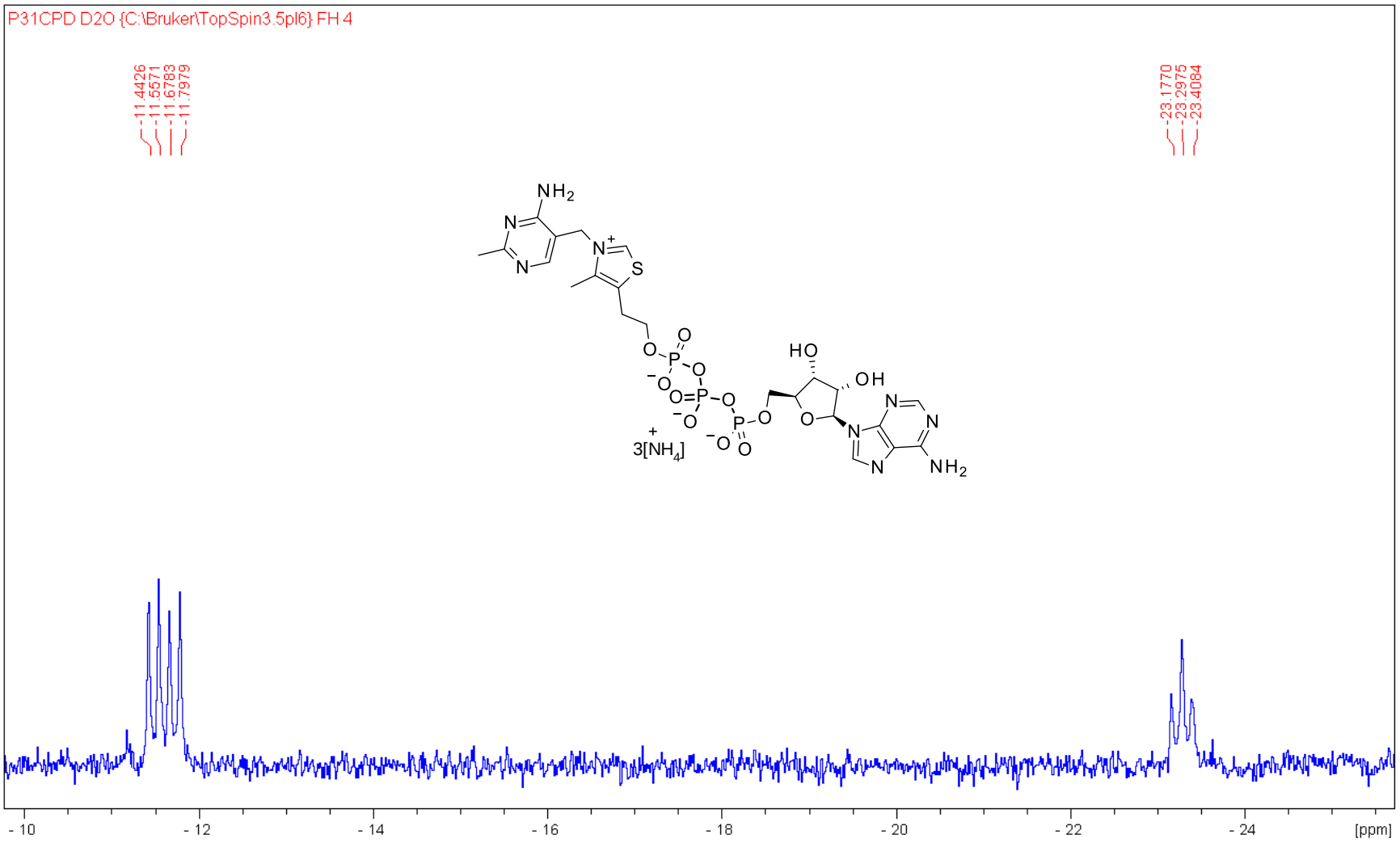
Compound 34. HRMS spectra



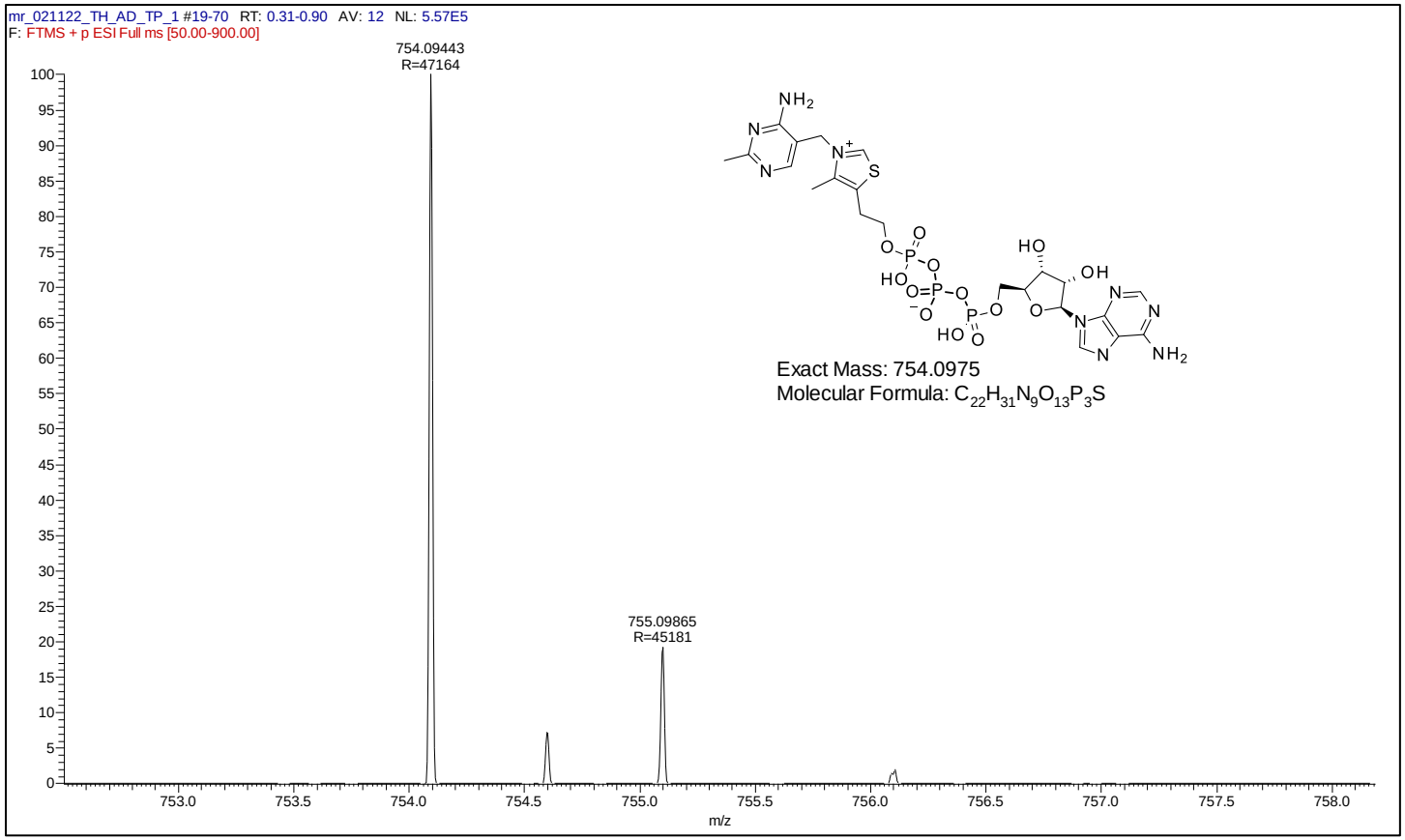
Compound 37. 400 MHz ^{1}H NMR spectrum in D_2O



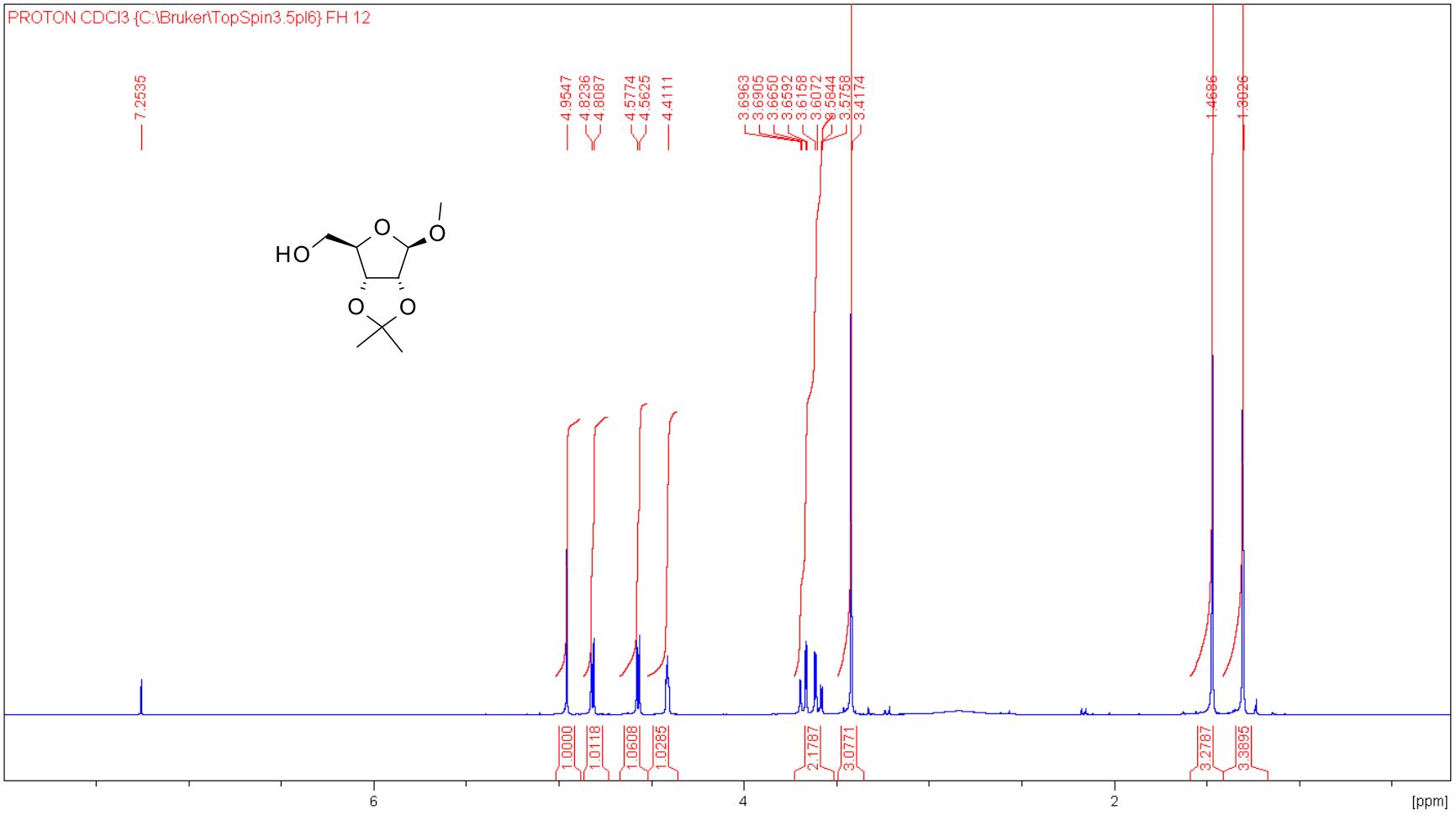
Compound 37. 100 MHz ^{13}C NMR spectrum in D_2O



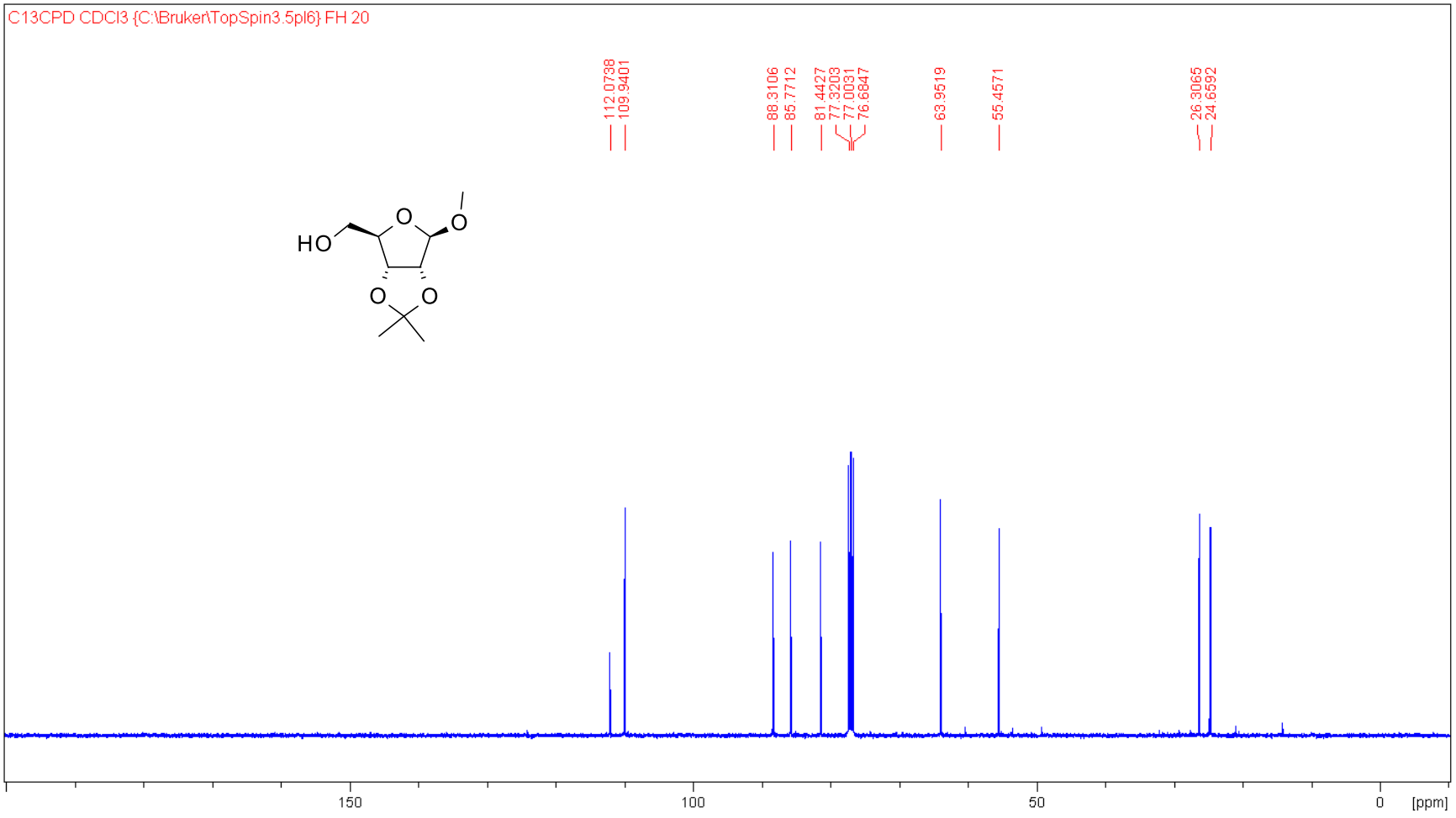
Compound 37. 162 MHz ^{31}P NMR spectrum in D_2O



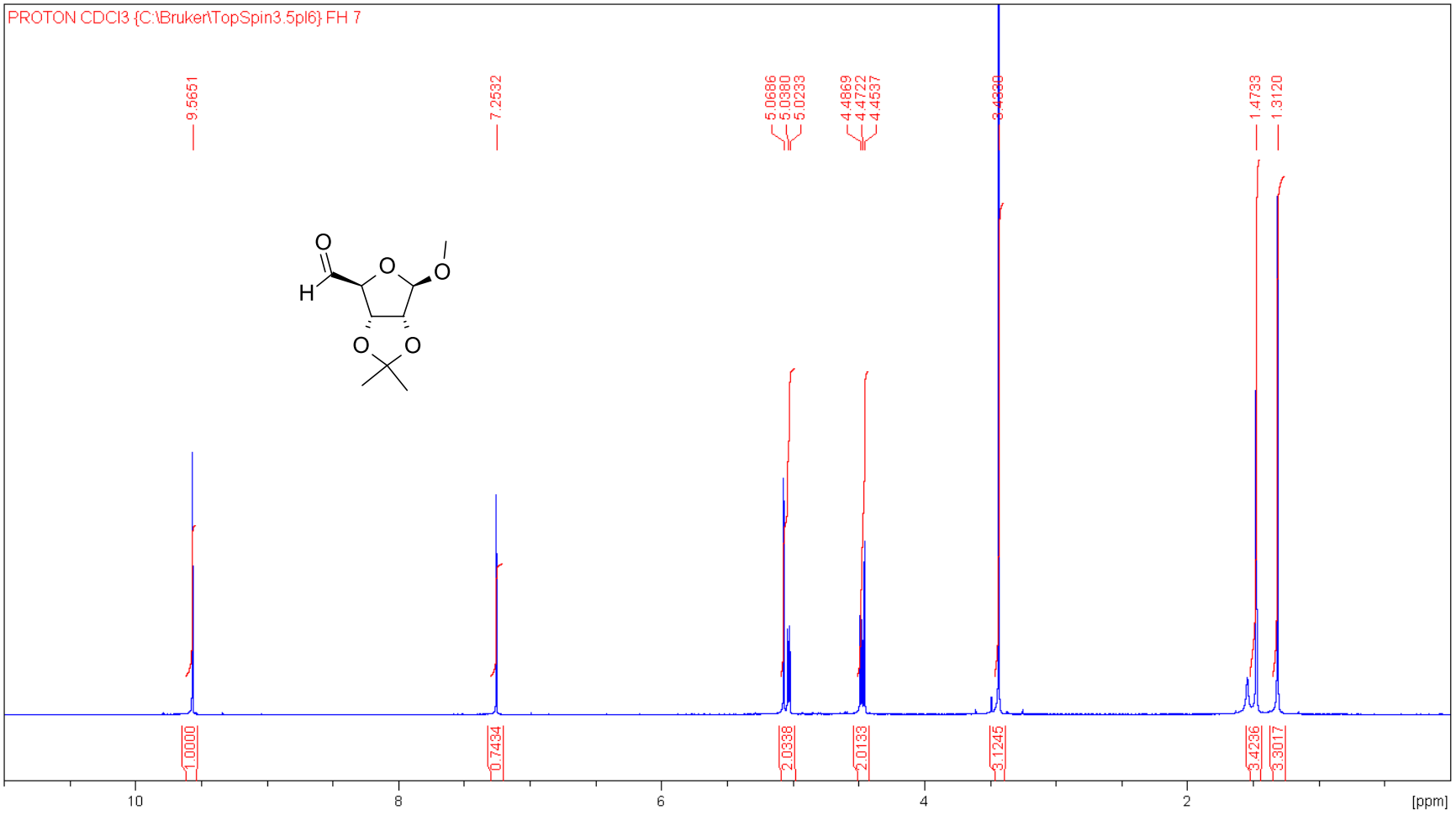
Compound 37. HRMS spectra



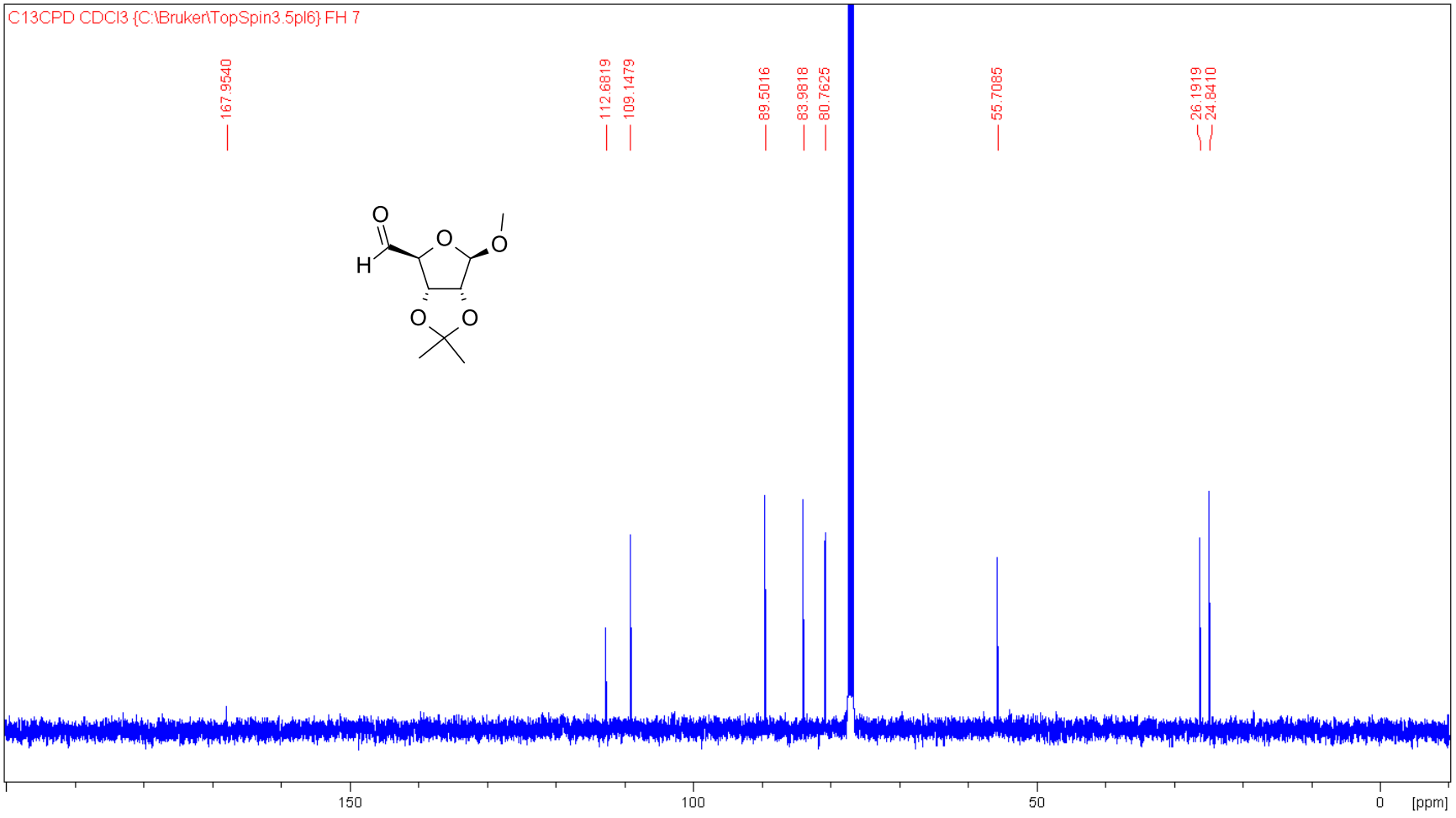
Compound 39. 400 MHz ^{1}H NMR spectrum in $CDCl_3$



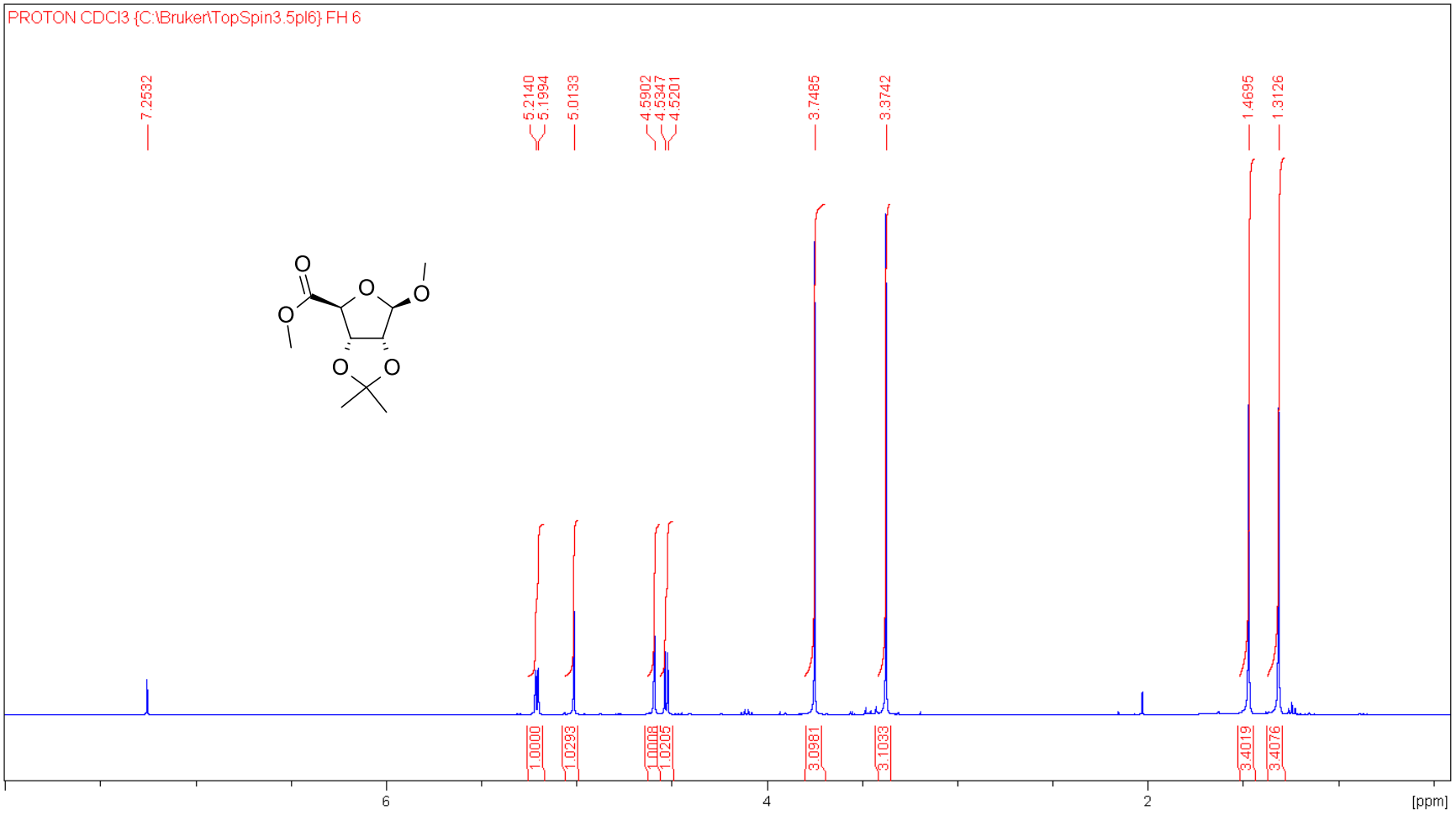
Compound 39. 100 MHz ^{31}C NMR spectrum in $CDCl_3$



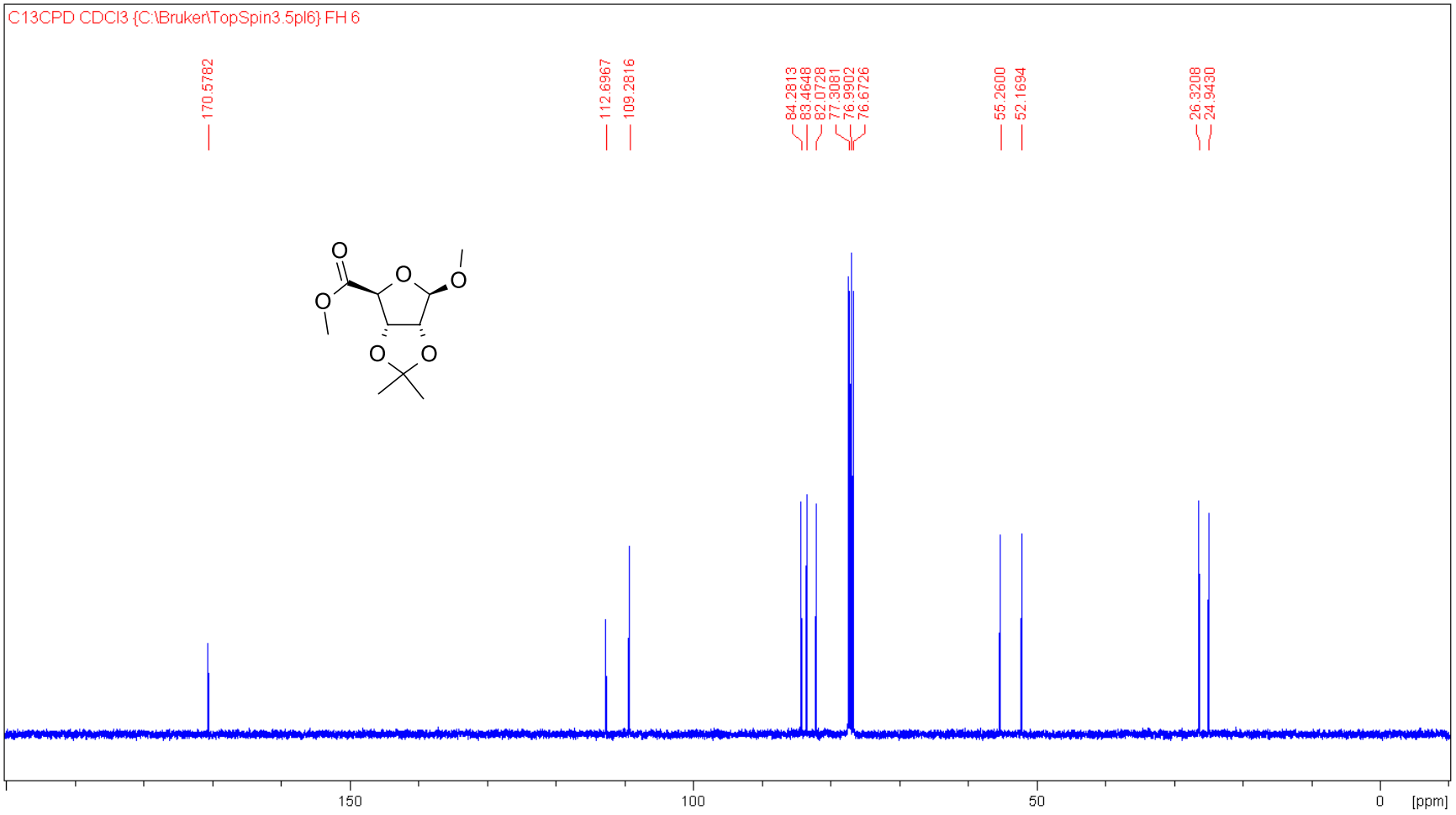
Compound 39. 400 MHz ^{1}H NMR spectrum in $CDCl_3$



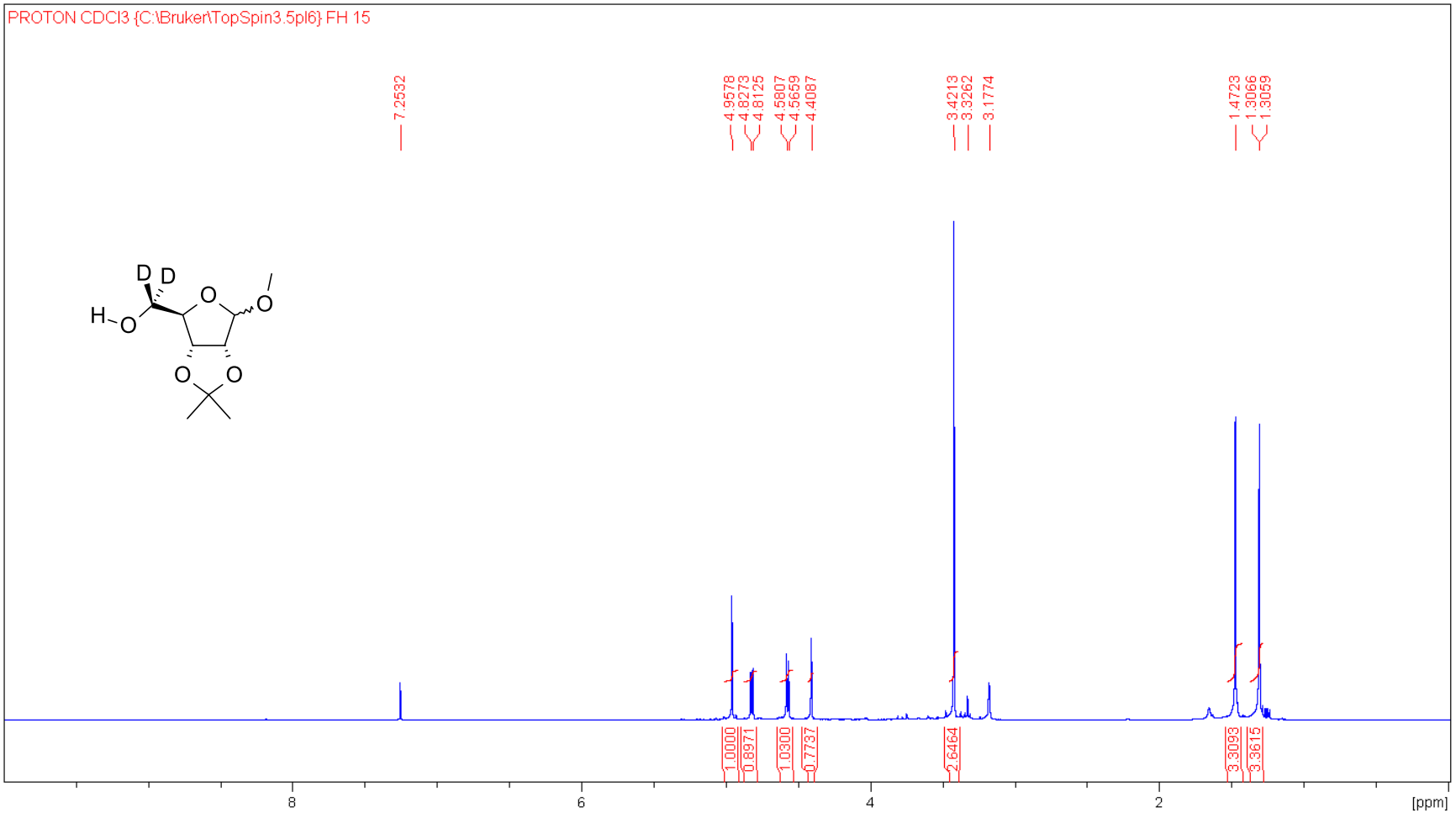
Compound 40. 100 MHz ^{31}C NMR spectrum in $CDCl_3$



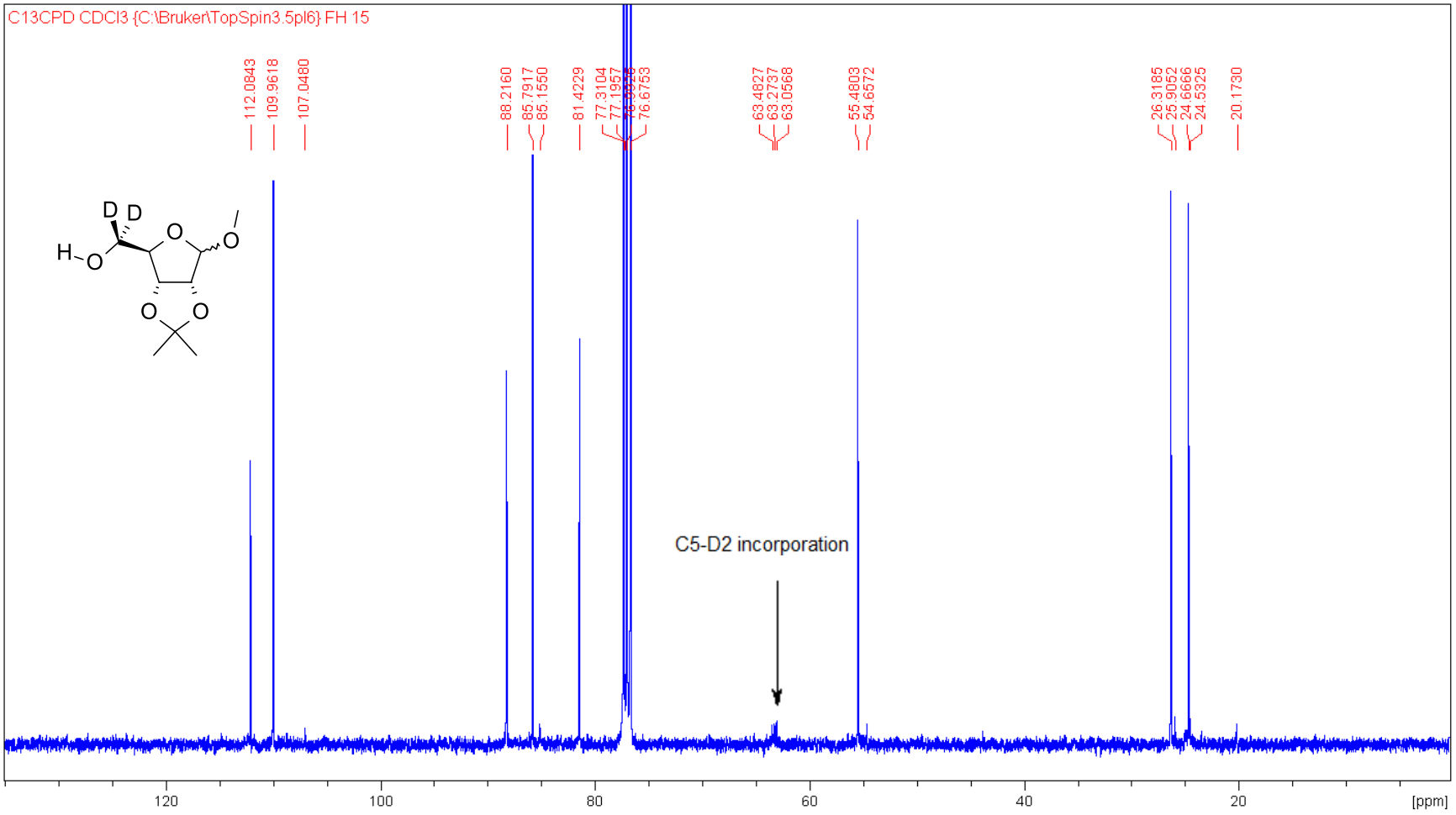
Compound 41. 400 MHz ^{1}H NMR spectrum in $CDCl_3$



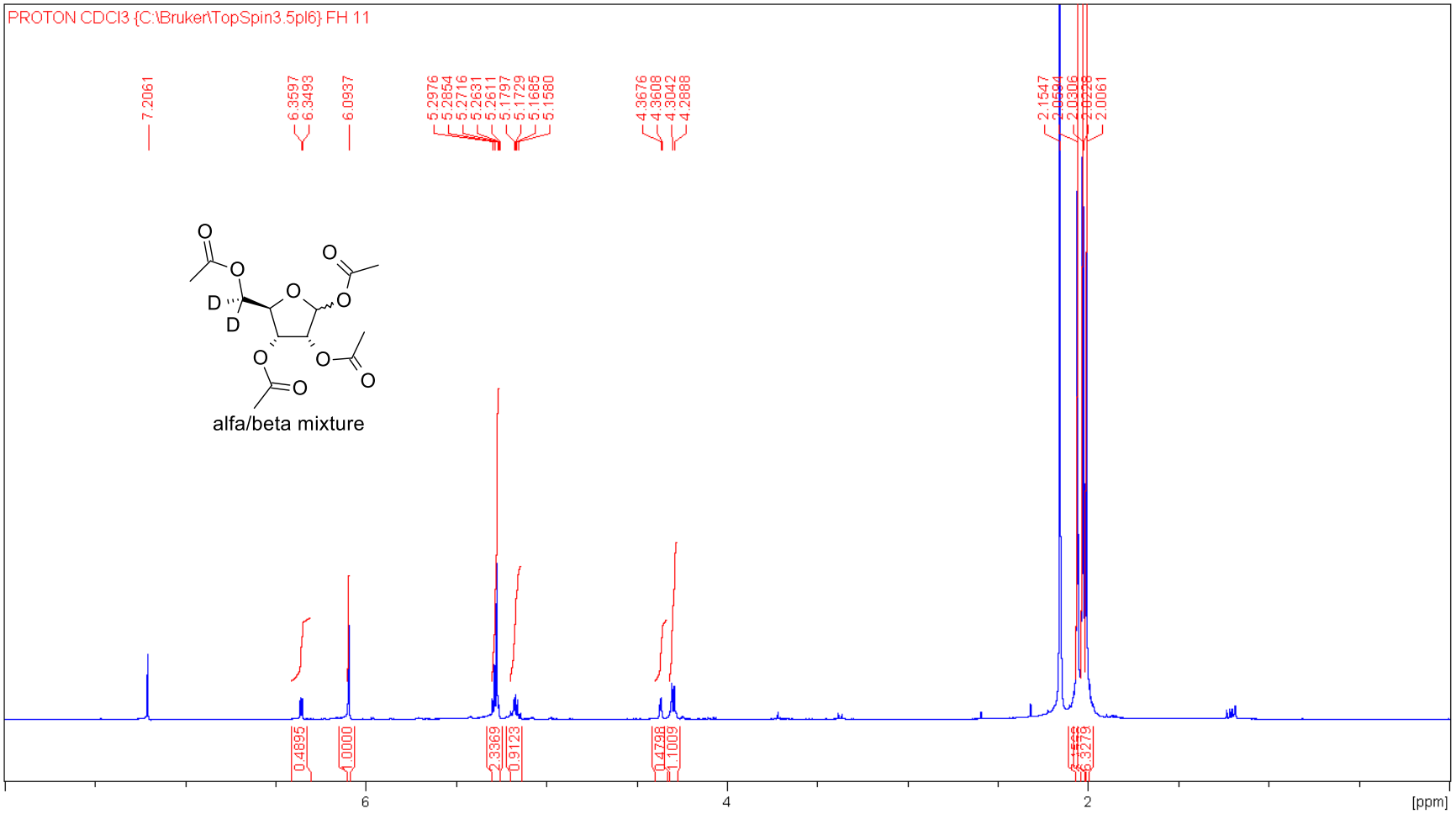
Compound 41. 100 MHz ^{31}C NMR spectrum in $CDCl_3$



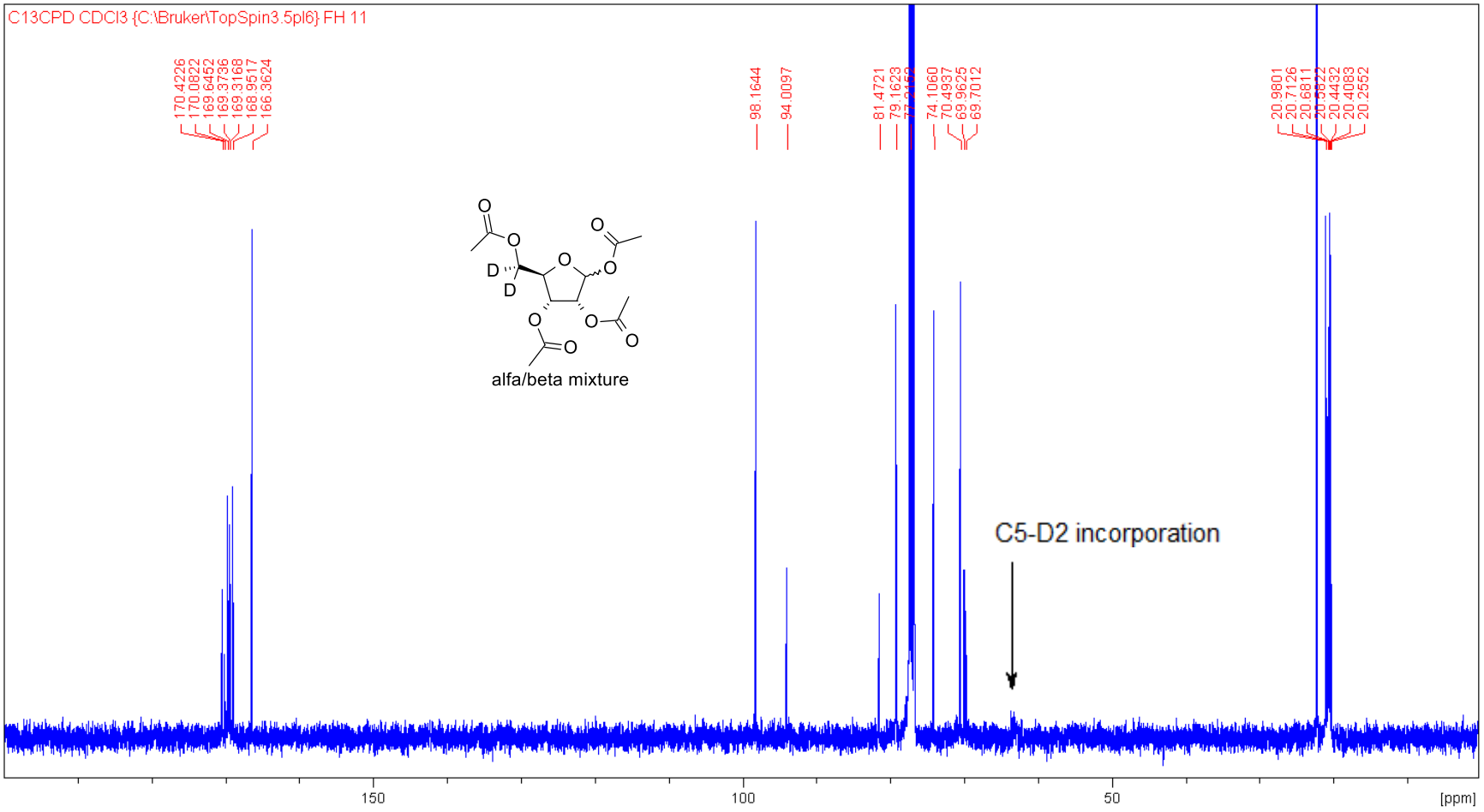
Compound 42. 400 MHz ^{1}H NMR spectrum in $CDCl_3$



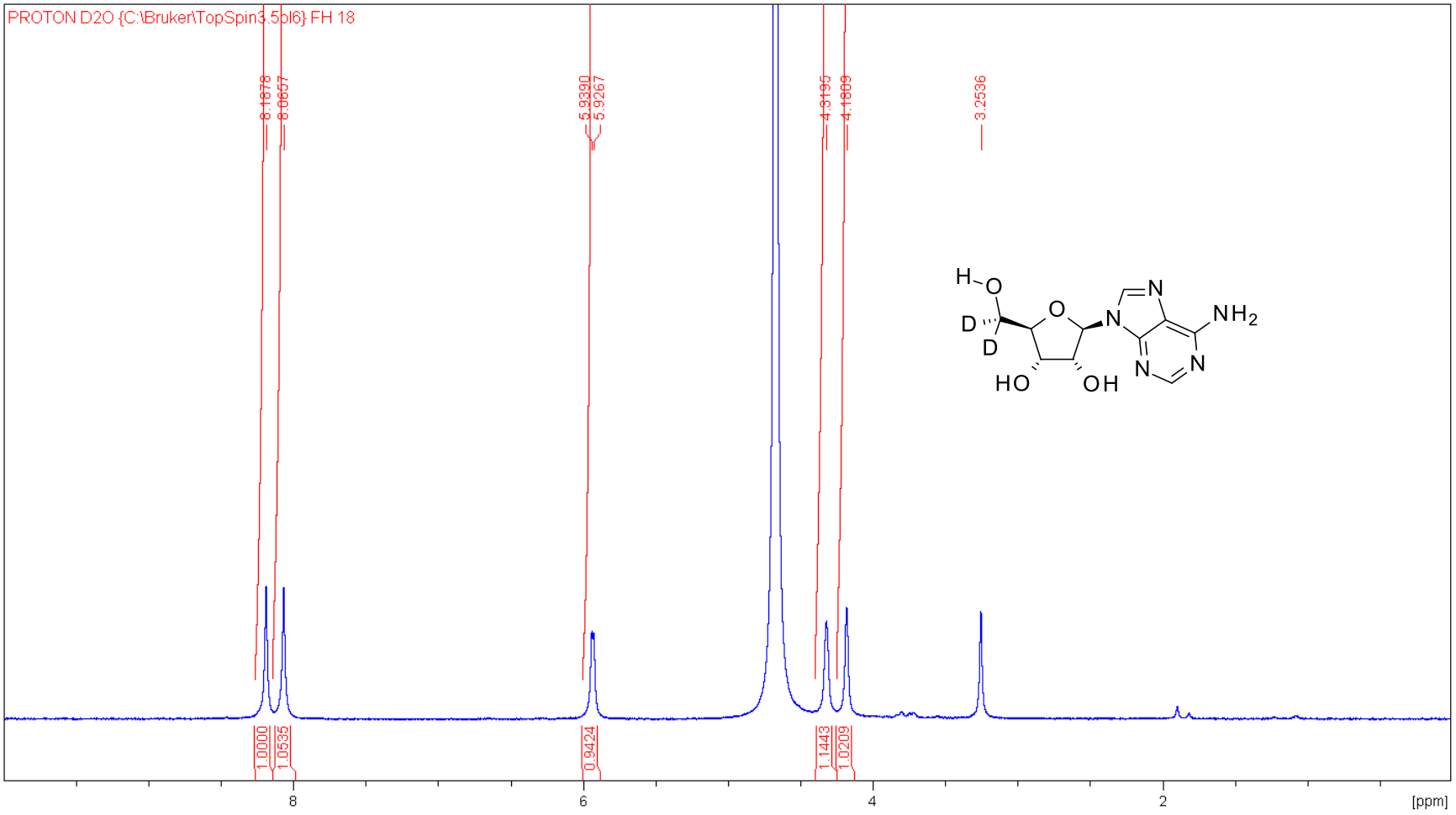
Compound 42. 100 MHz ^{31}C NMR spectrum in $CDCl_3$



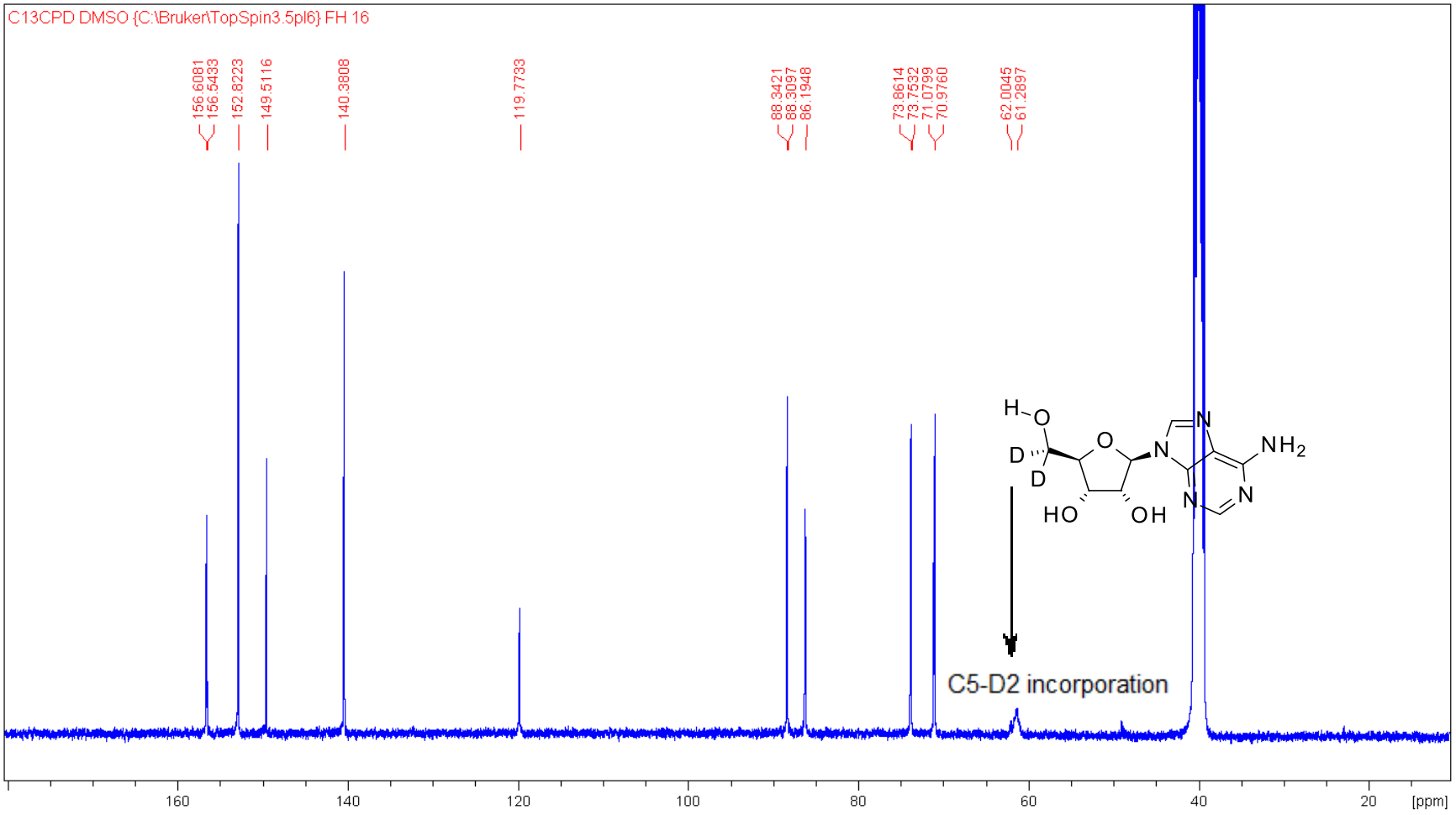
Compound 46. 400 MHz ^{1}H NMR spectrum in $CDCl_3$



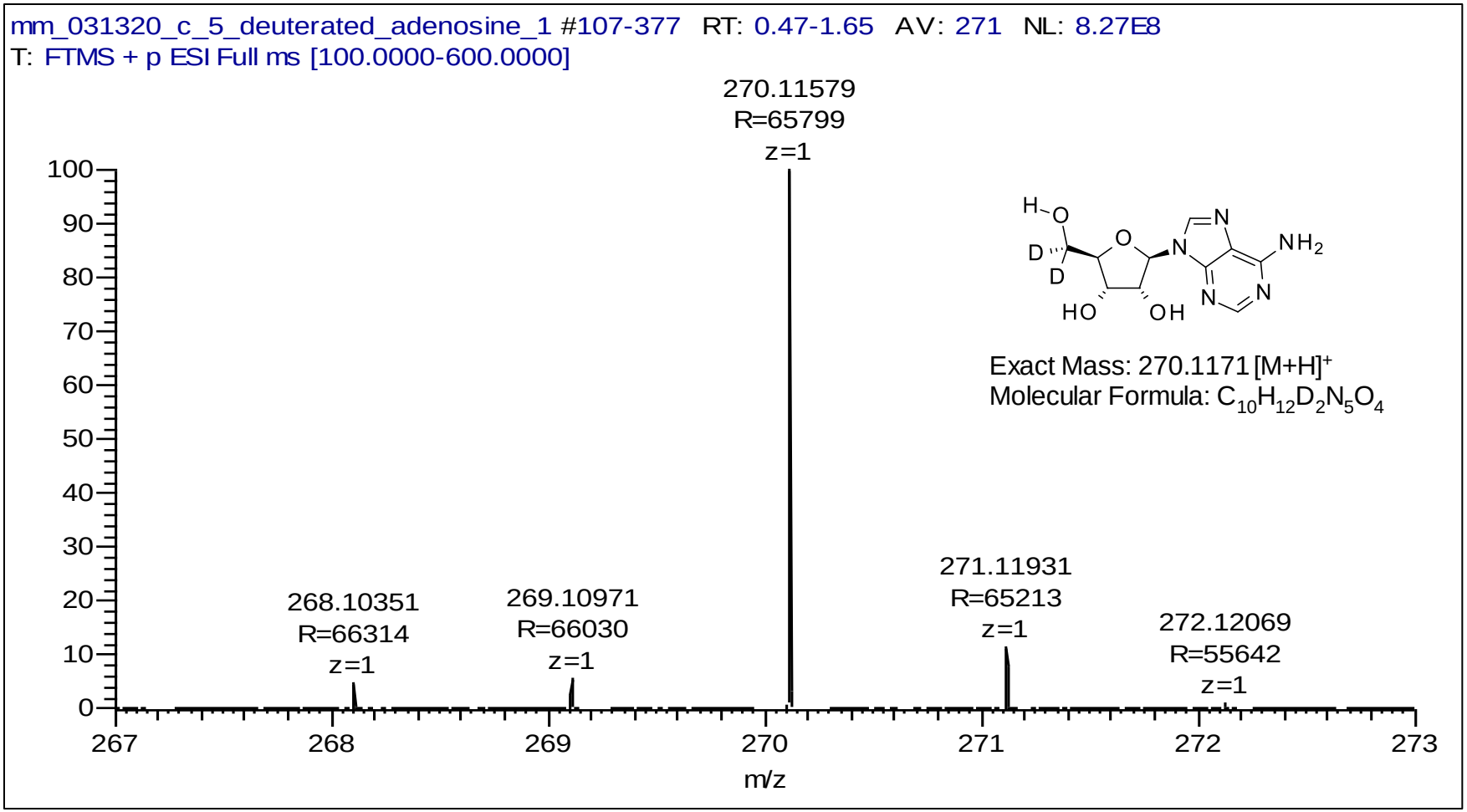
Compound 46. 100 MHz ^{31}C NMR spectrum in $CDCl_3$



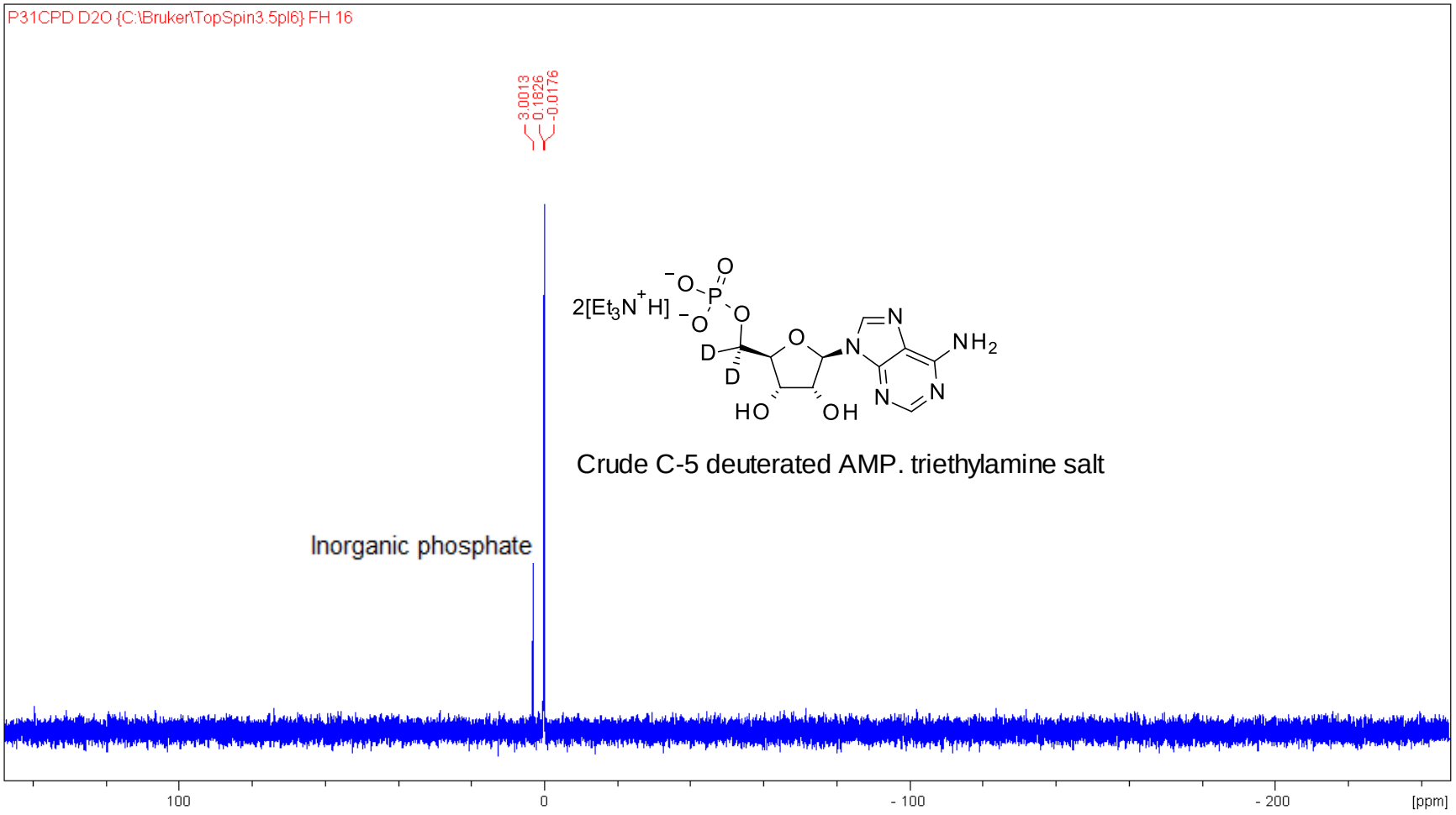
Compound 48. 400 MHz ^{1}H NMR spectrum in D_2O



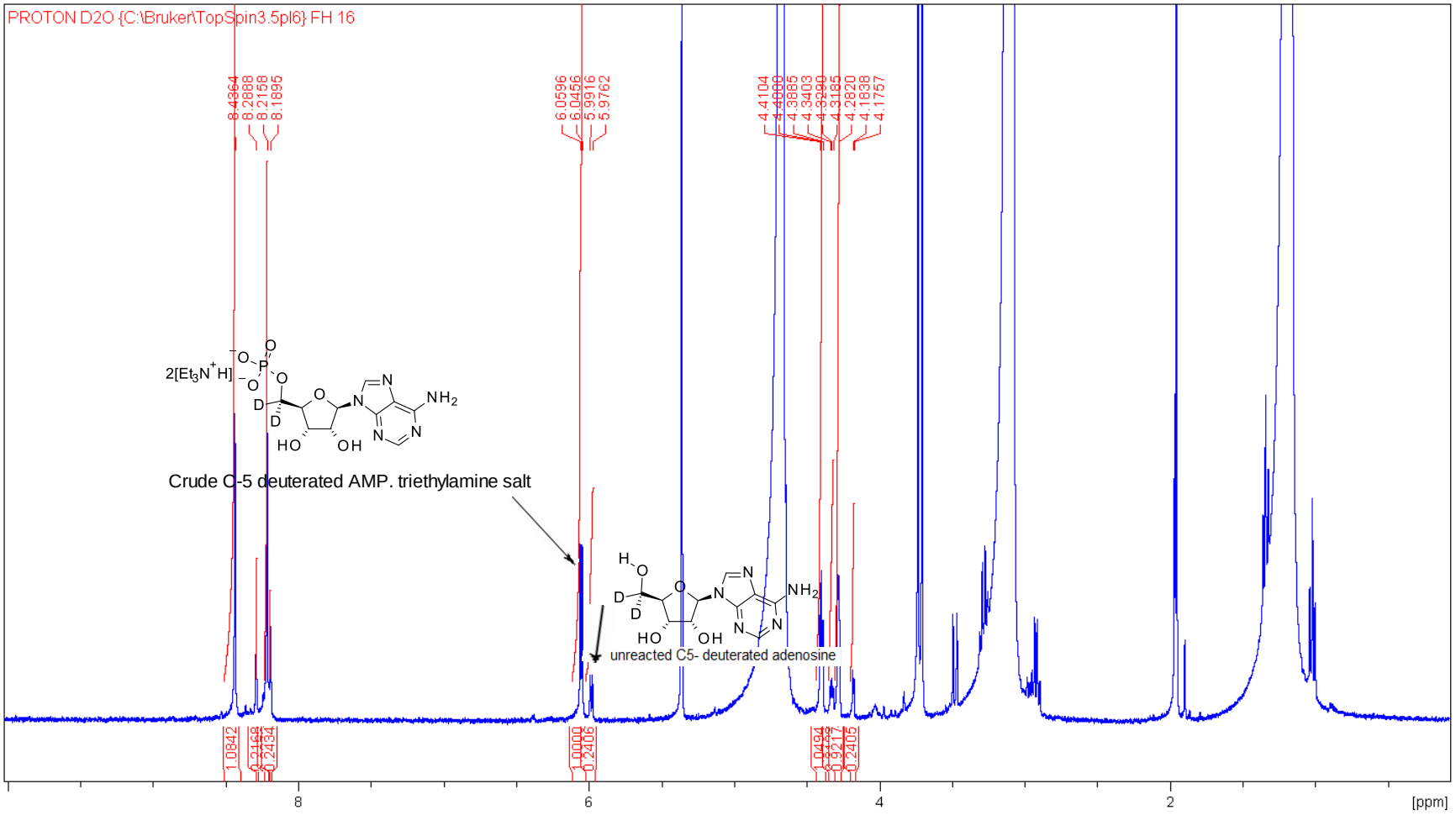
Compound 48. 100 MHz ^{31}C NMR spectrum in D_2O



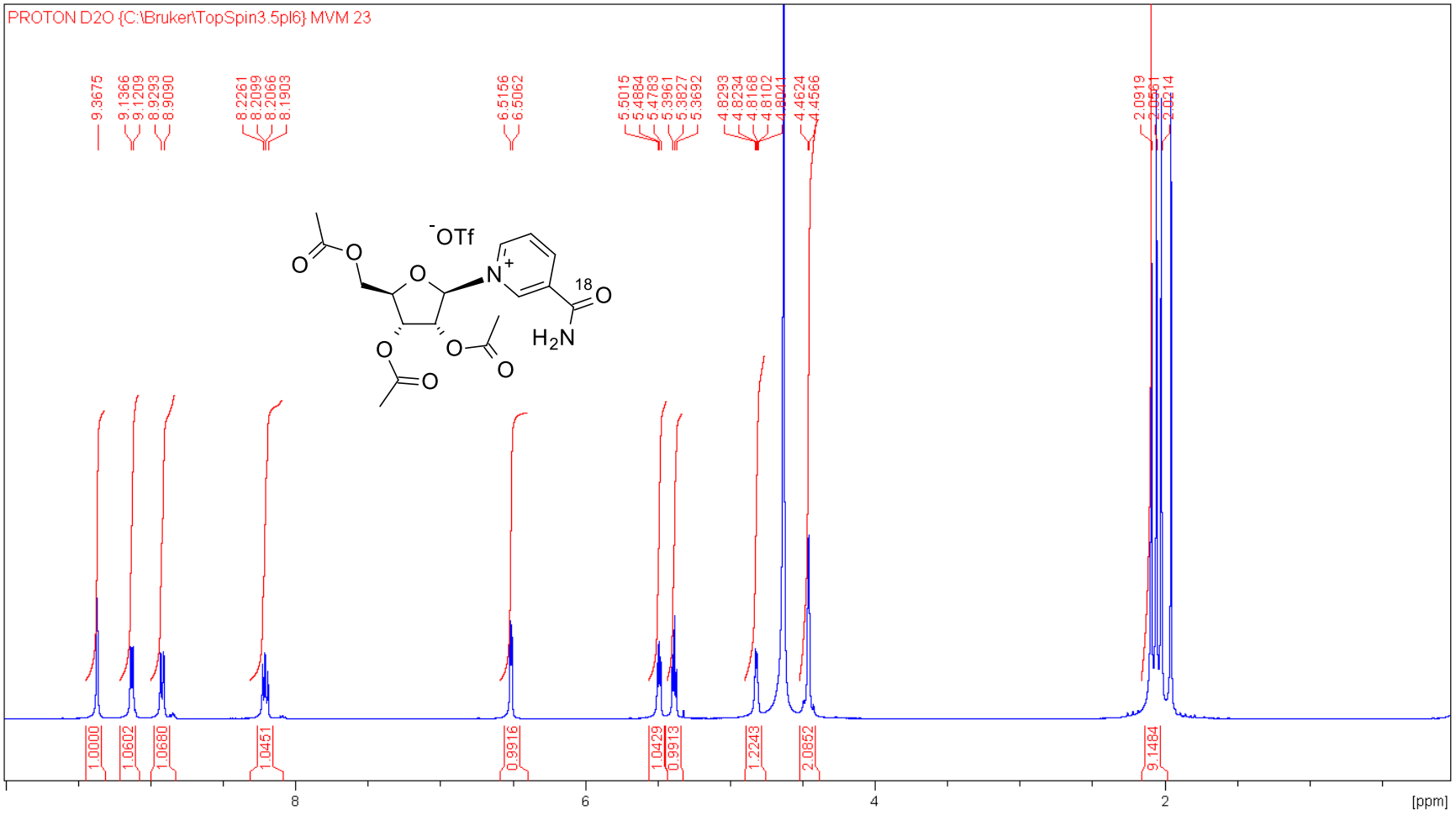
Compound 48. HRMS Spectra



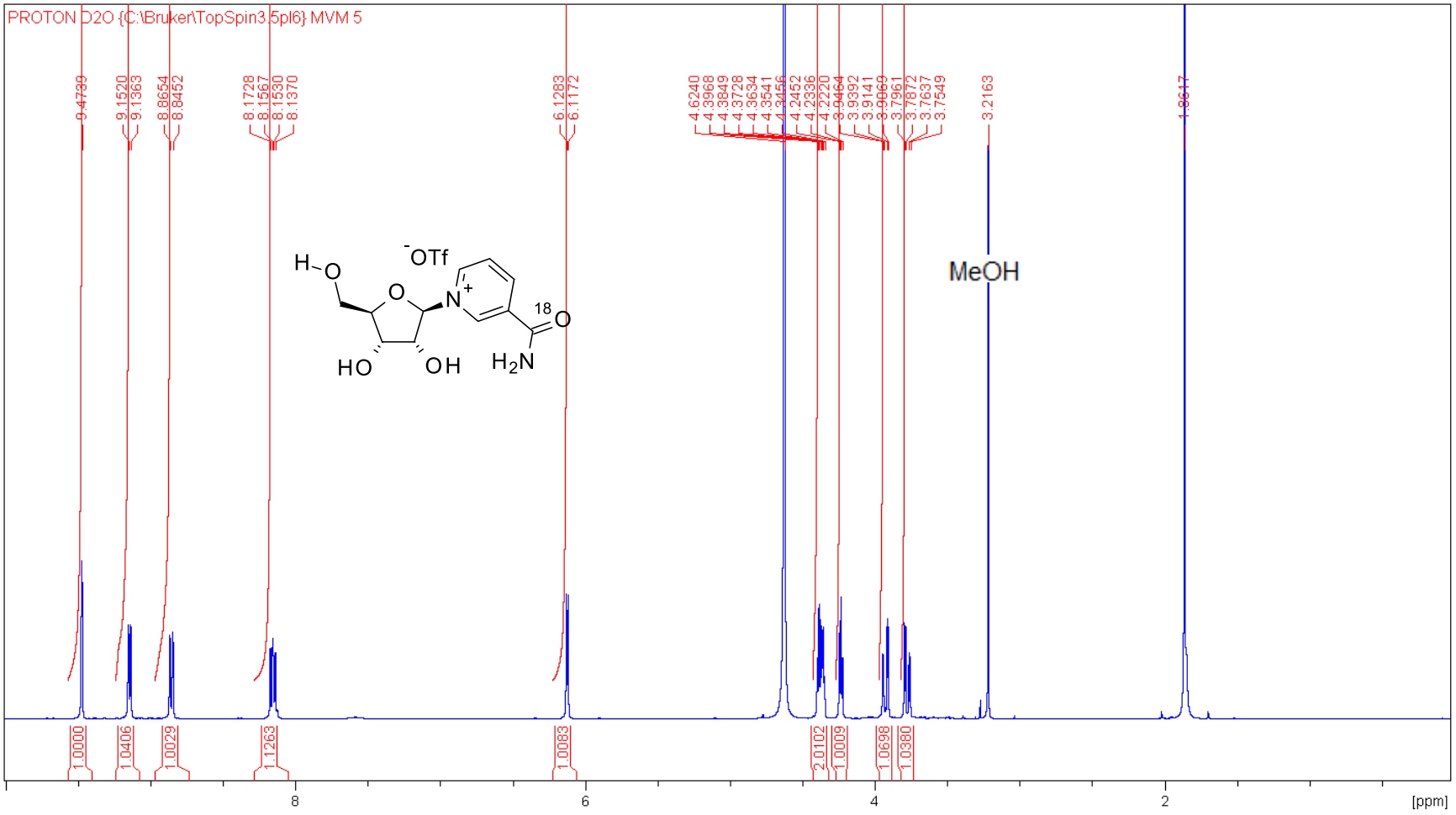
Compound 49. 162 MHz ^{31}P NMR spectrum in D_2O



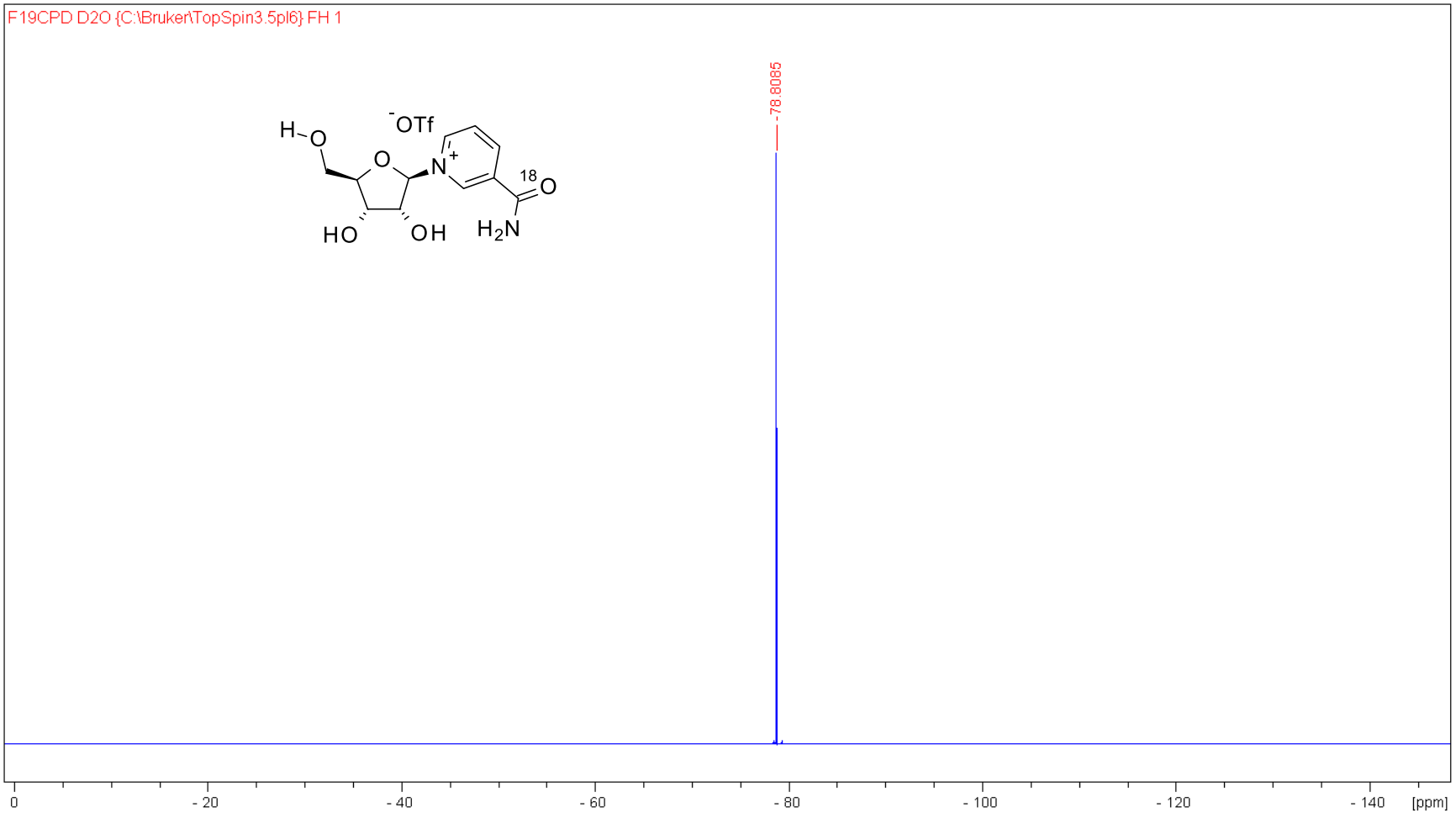
Compound 49. 400 MHz ^{1}H NMR spectrum in D_2O



Compound 53. 400 MHz ^{1}H NMR spectrum in D_2O



Compound 54. 400 MHz ^{1}H NMR spectrum in D_2O



Compound 54. 377 MHz ^{19}F NMR spectrum in D_2O