

Poecillastrosides, Steroidal Saponins from the Mediterranean Deep-Sea Sponge *Poecillastra compressa* (Bowerbank, 1866)

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Compound Formula	Name	RT	Algorithm
C ₄₀ H ₆₈ O ₁₃	Poecillastroside A	6.251	Spectrum Extraction

6
x10
MS Spectrum

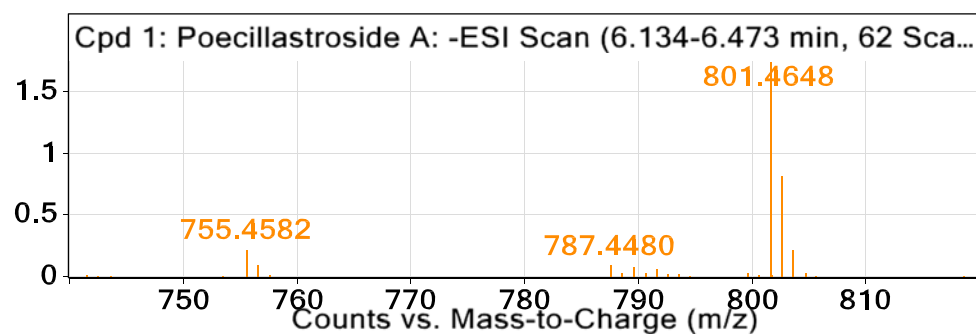


Figure S1. (-)-HRESIMS analysis of 1.

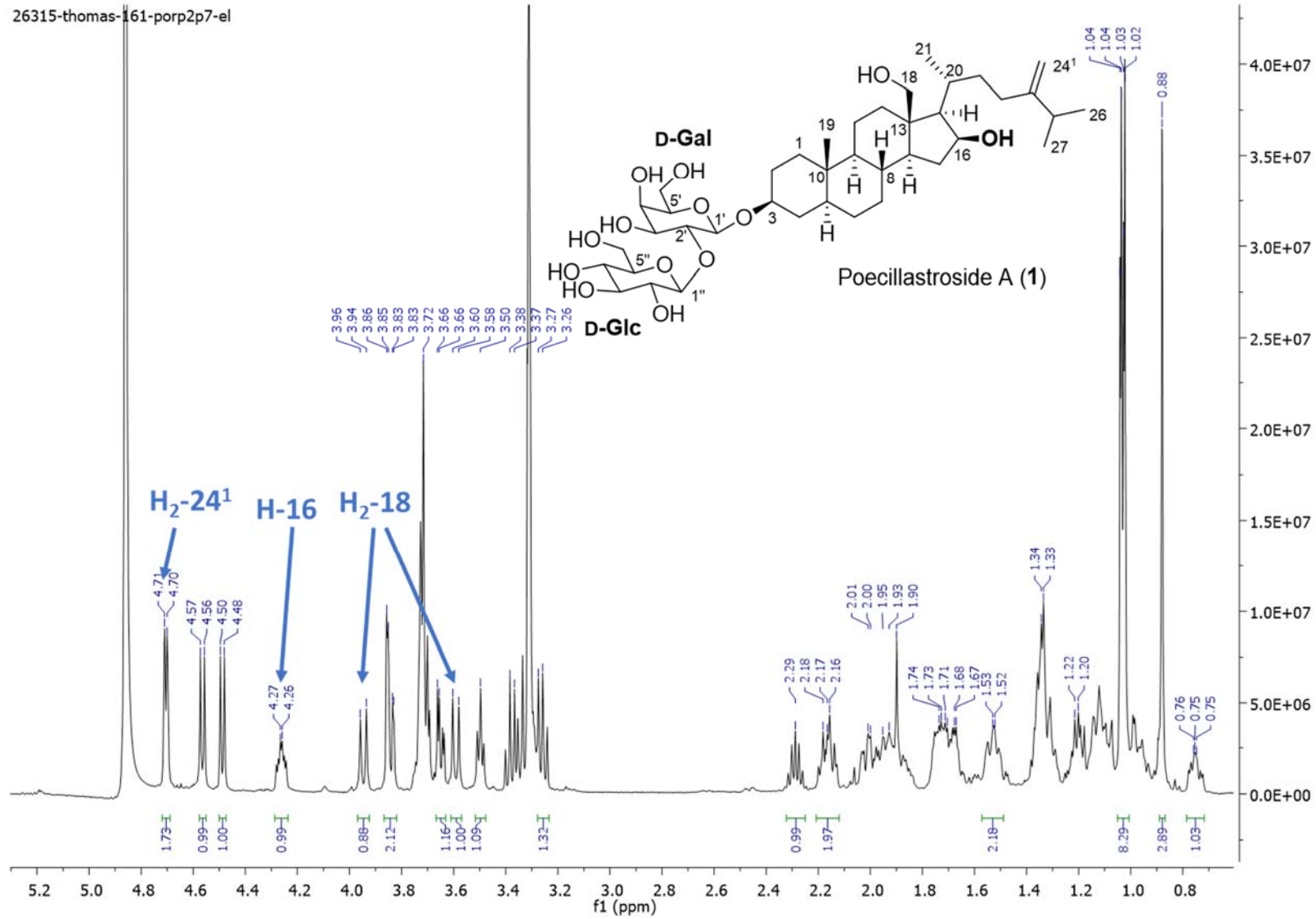


Figure S2. ¹H NMR spectrum of **1** at 500 MHz in CD₃OD

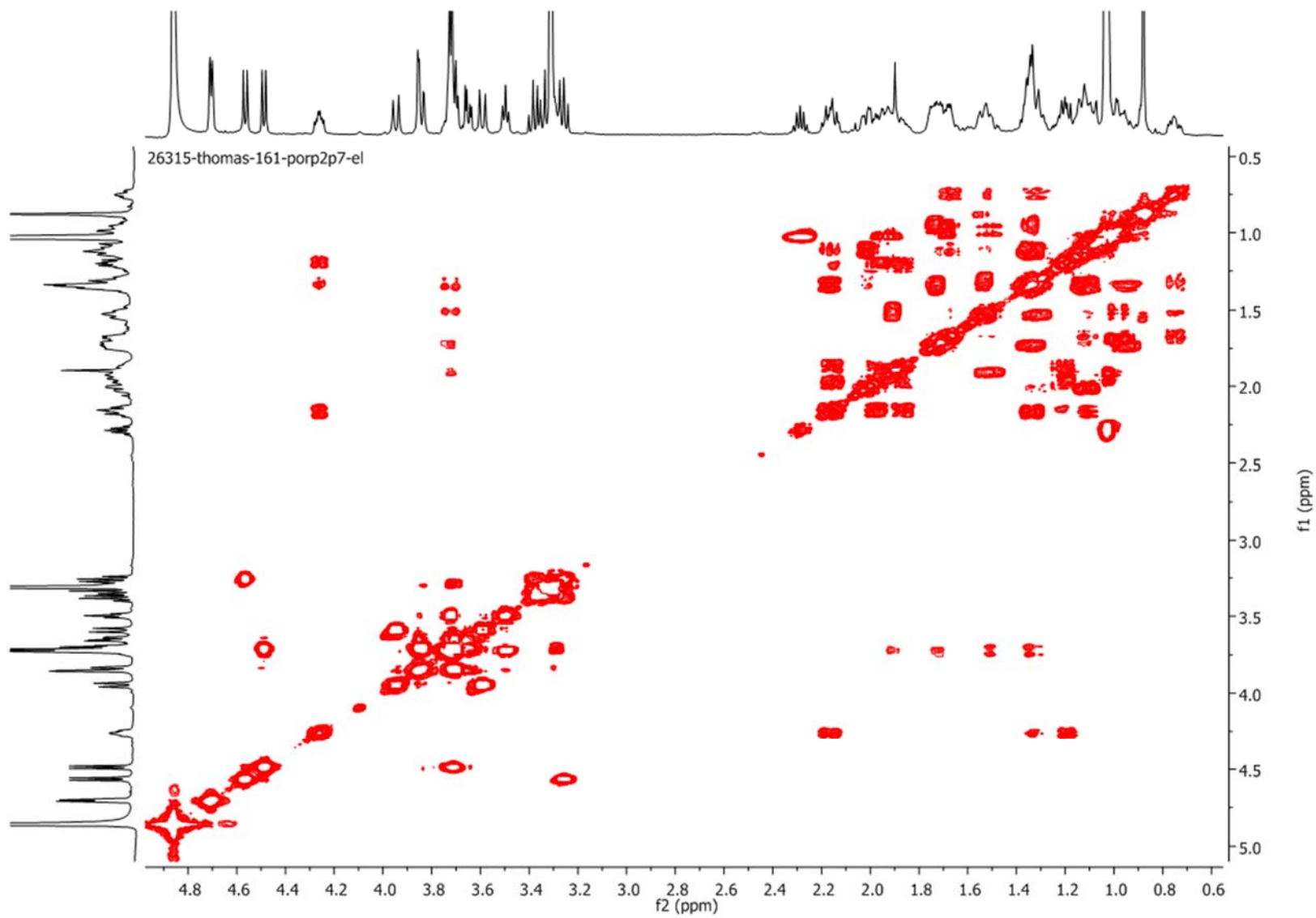


Figure S3. COSY NMR spectrum of **1** at 500 MHz in CD₃OD

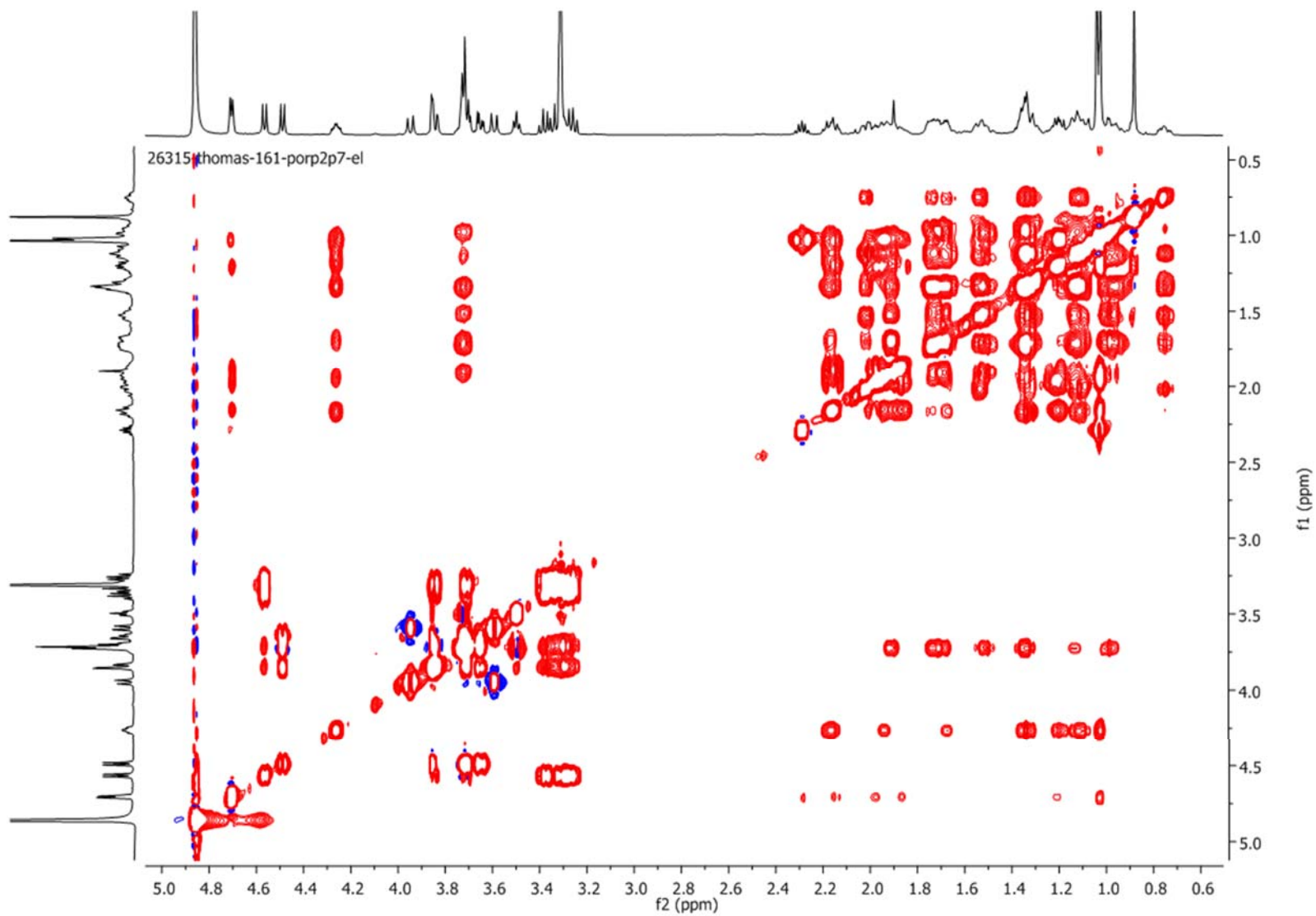


Figure S4. TOCSY NMR spectrum of **1** at 500 MHz in CD₃OD

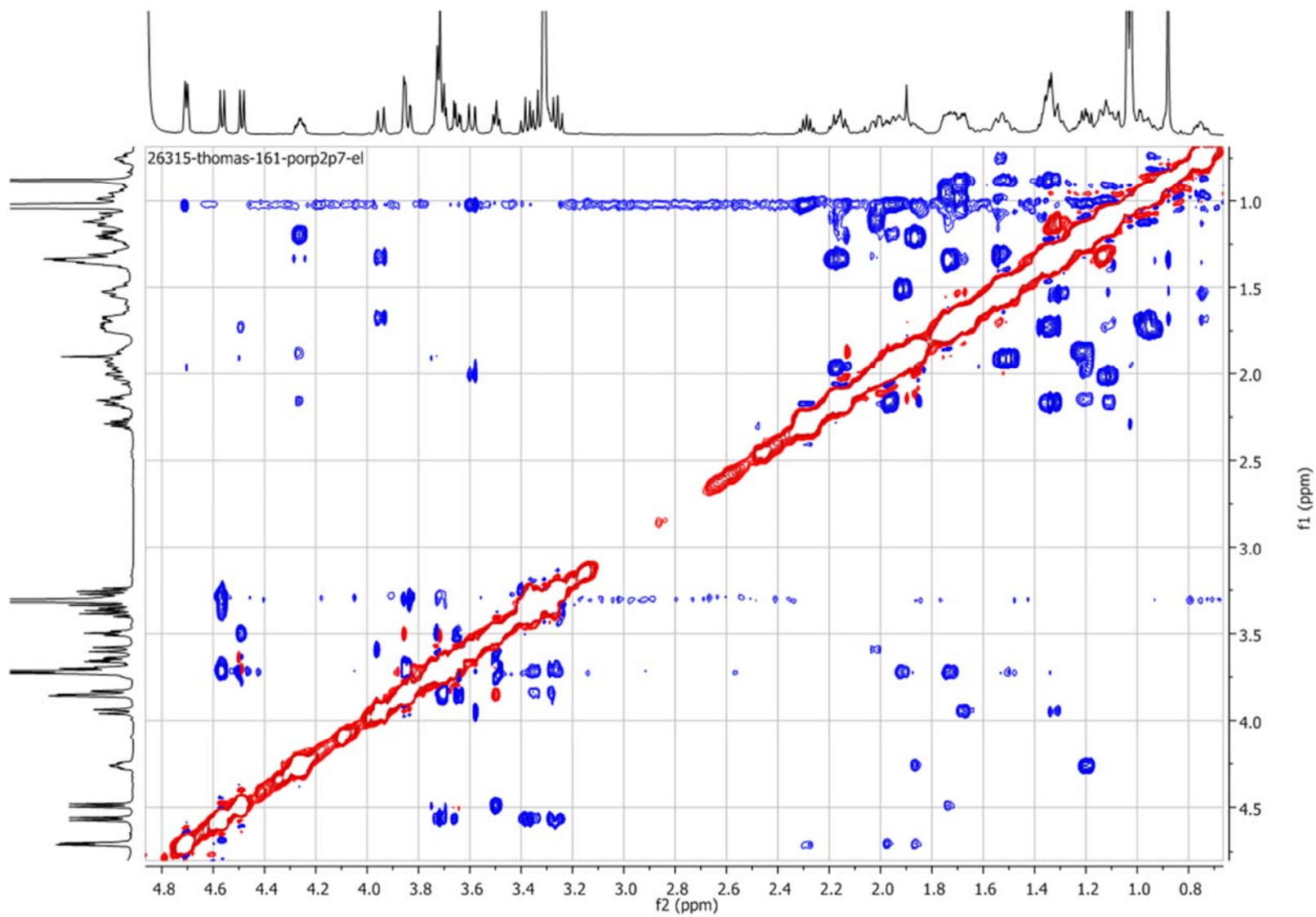


Figure S5. NOESY NMR spectrum of 1 at 500 MHz in CD₃OD

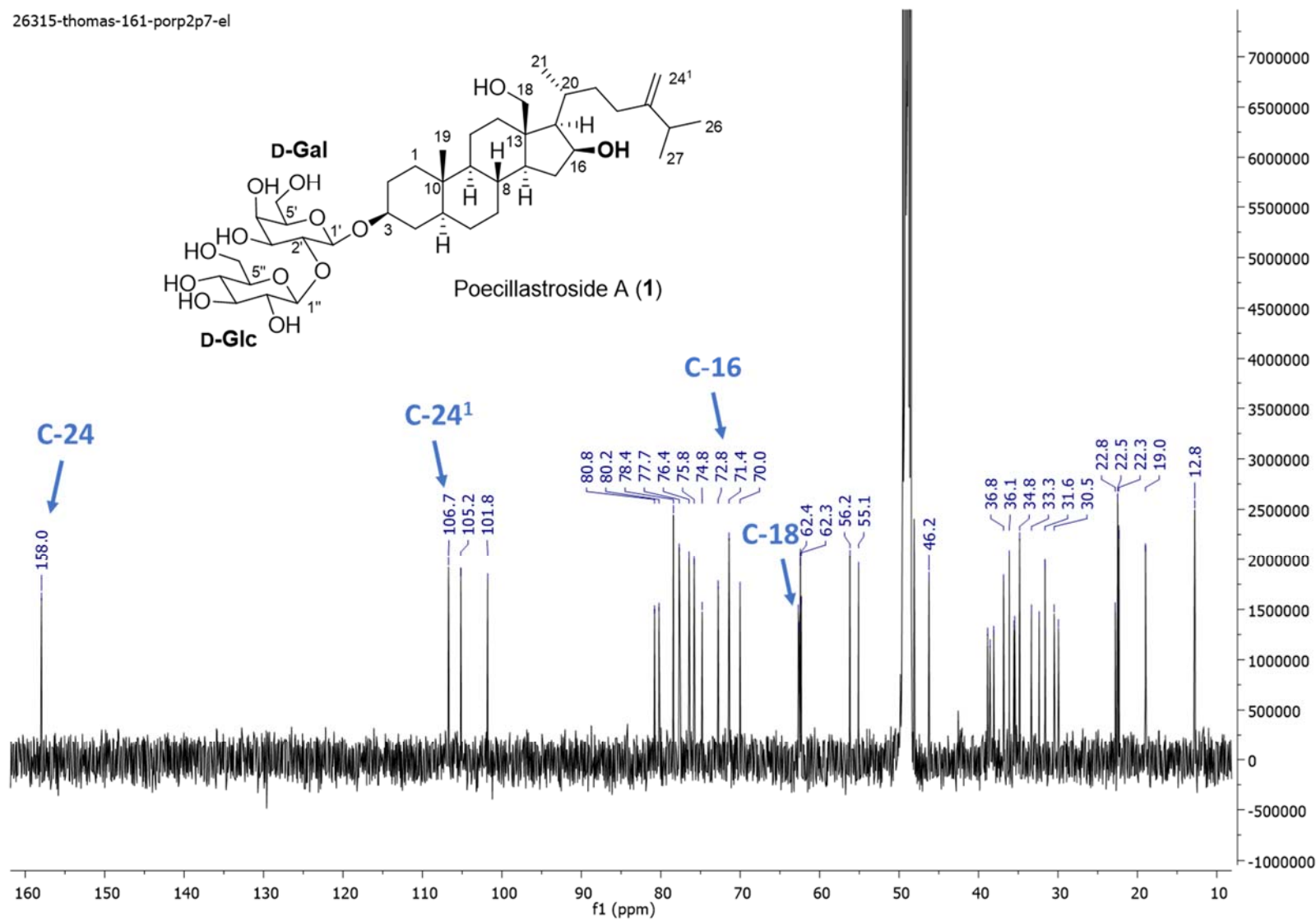


Figure S6. ^{13}C NMR spectrum of **1** at 125 MHz in CD_3OD

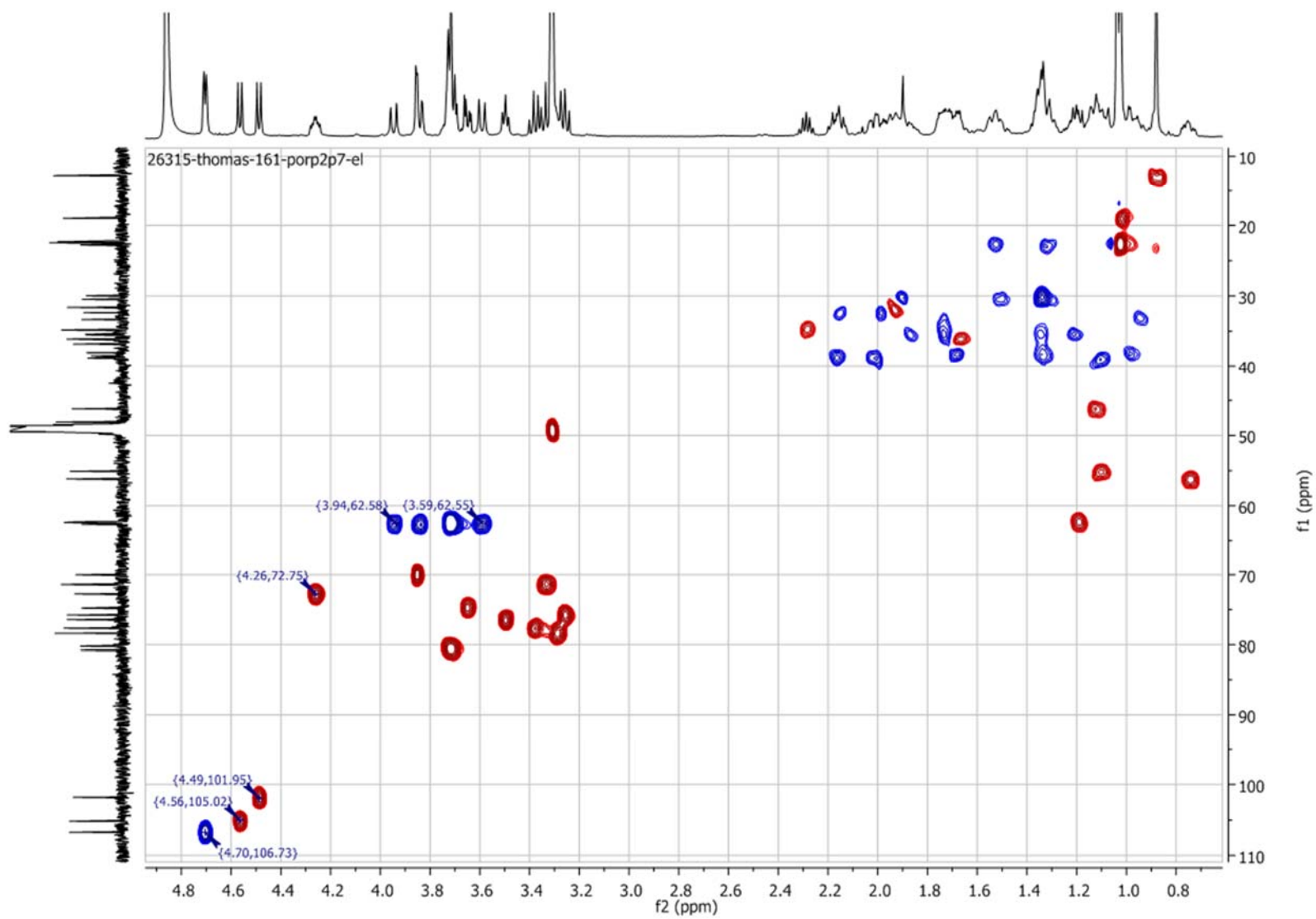


Figure S7. HSQC NMR spectrum of **1** at 500 MHz in CD₃OD

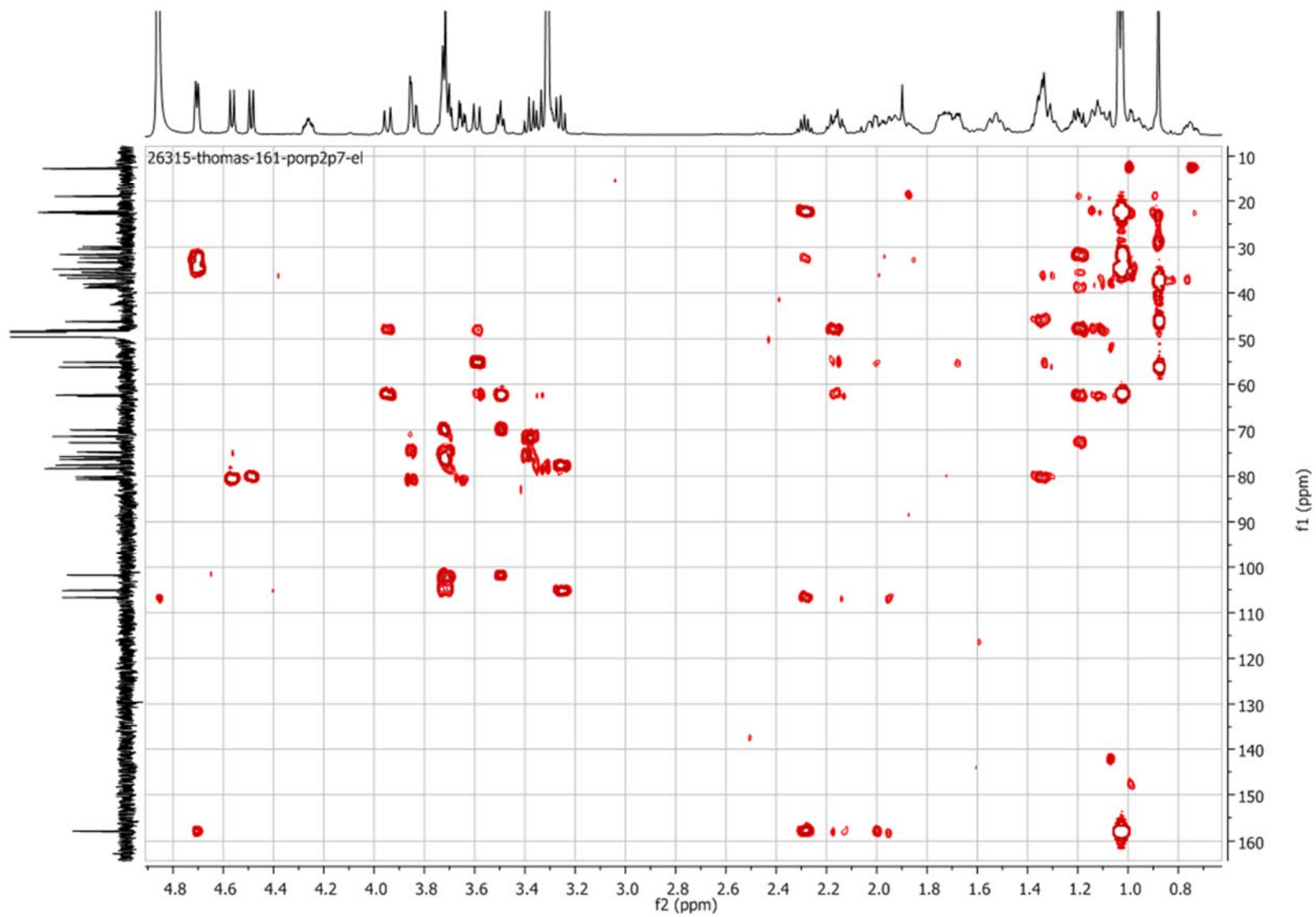


Figure S8. HMBC spectrum of 1 at 500 MHz in CD₃OD

Compound Formula	Name	RT	Algorithm
C ₄₁ H ₇₀ O ₁₃	Poecillastroside B	6.581	Spectrum Extraction

6
x10
MS Spectrum

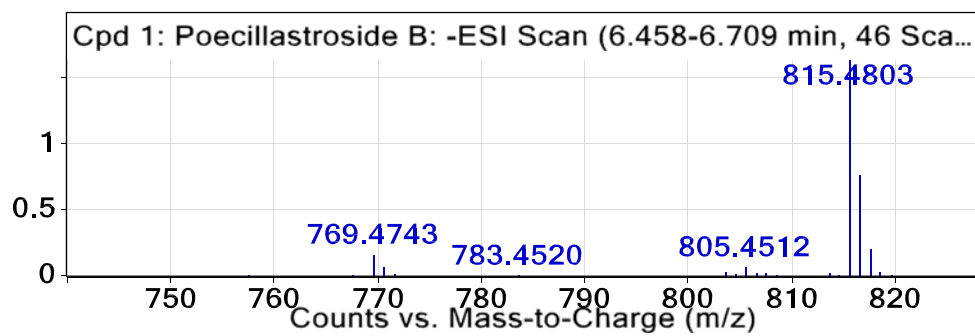


Figure S9. (-)-HRESIMS analysis of 2.

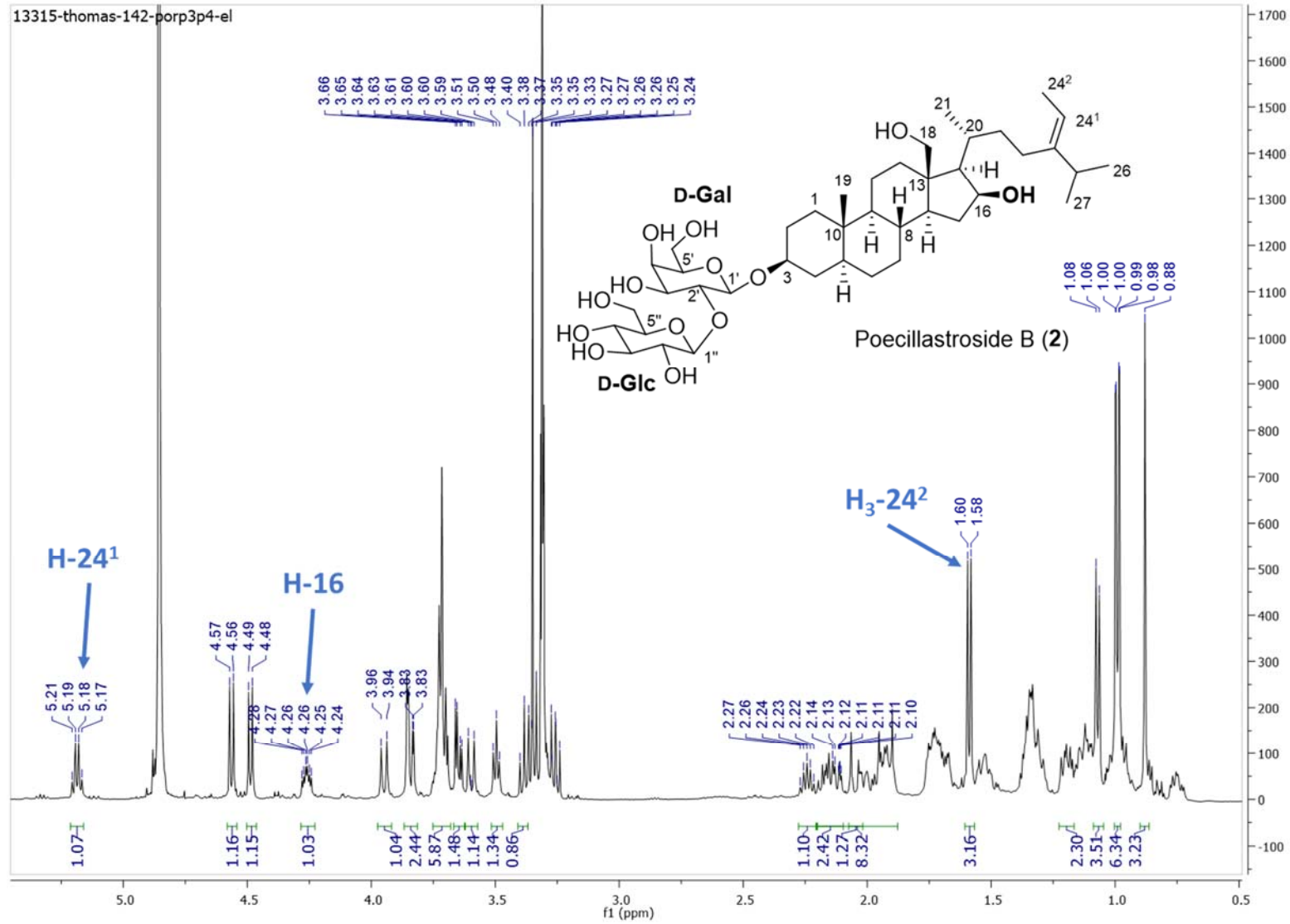


Figure S10. ¹H NMR spectrum of 2 at 500 MHz in CD₃OD

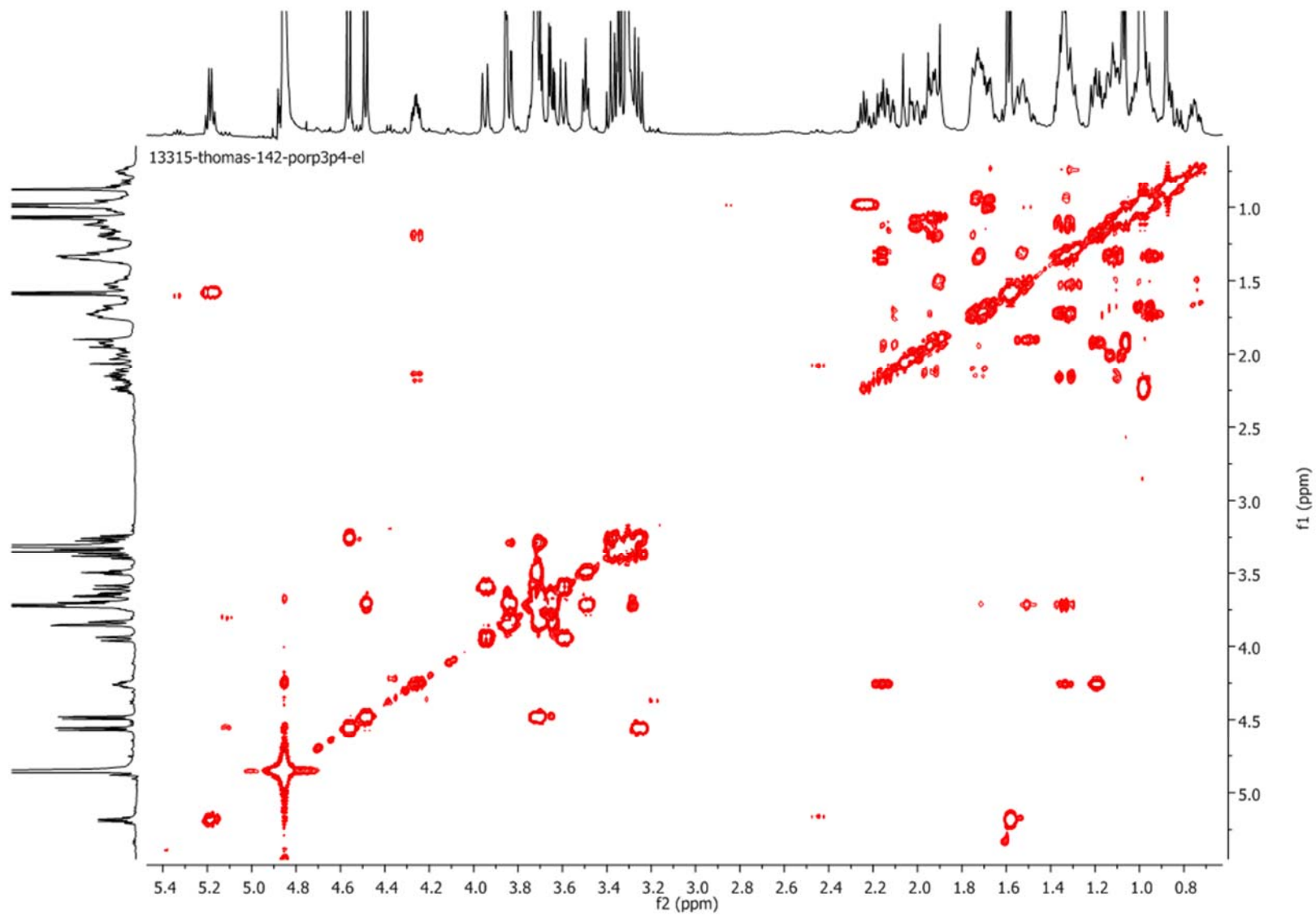


Figure S11. COSY NMR spectrum of **2** at 500 MHz in CD₃OD

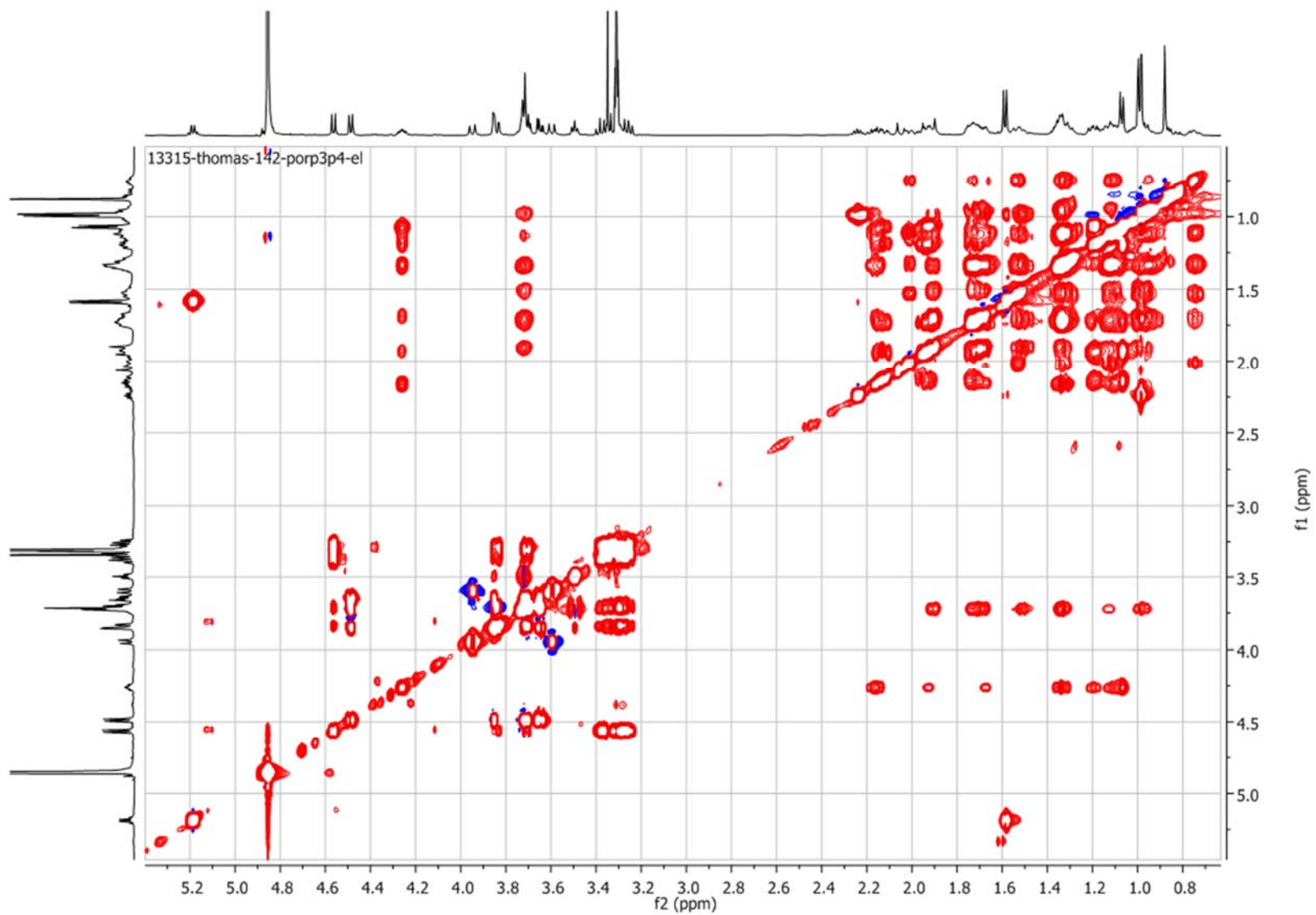


Figure S12. TOCSY NMR spectrum of **2** at 500 MHz in CD₃OD

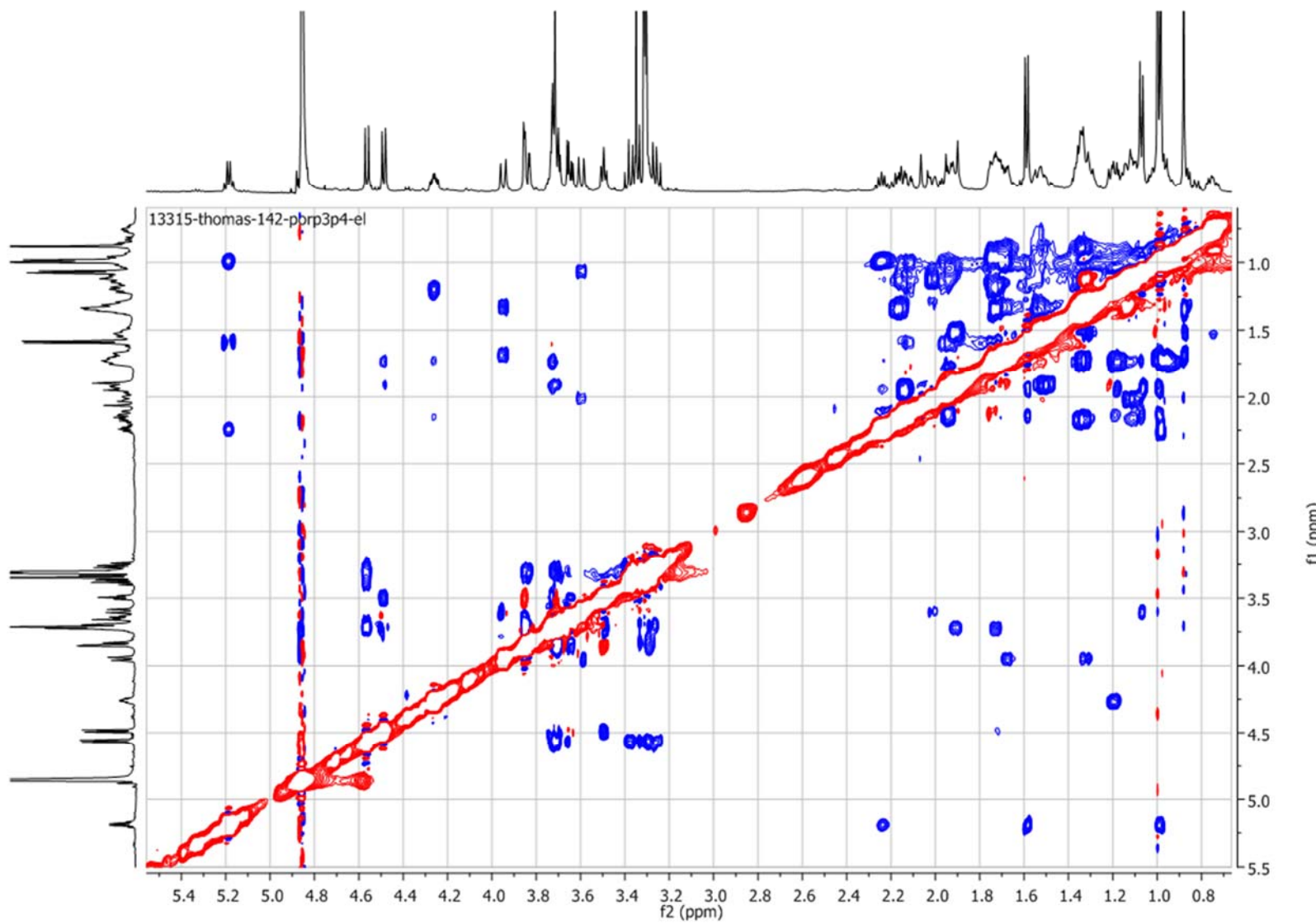


Figure S13. NOESY NMR spectrum of **2** at 500 MHz in CD₃OD

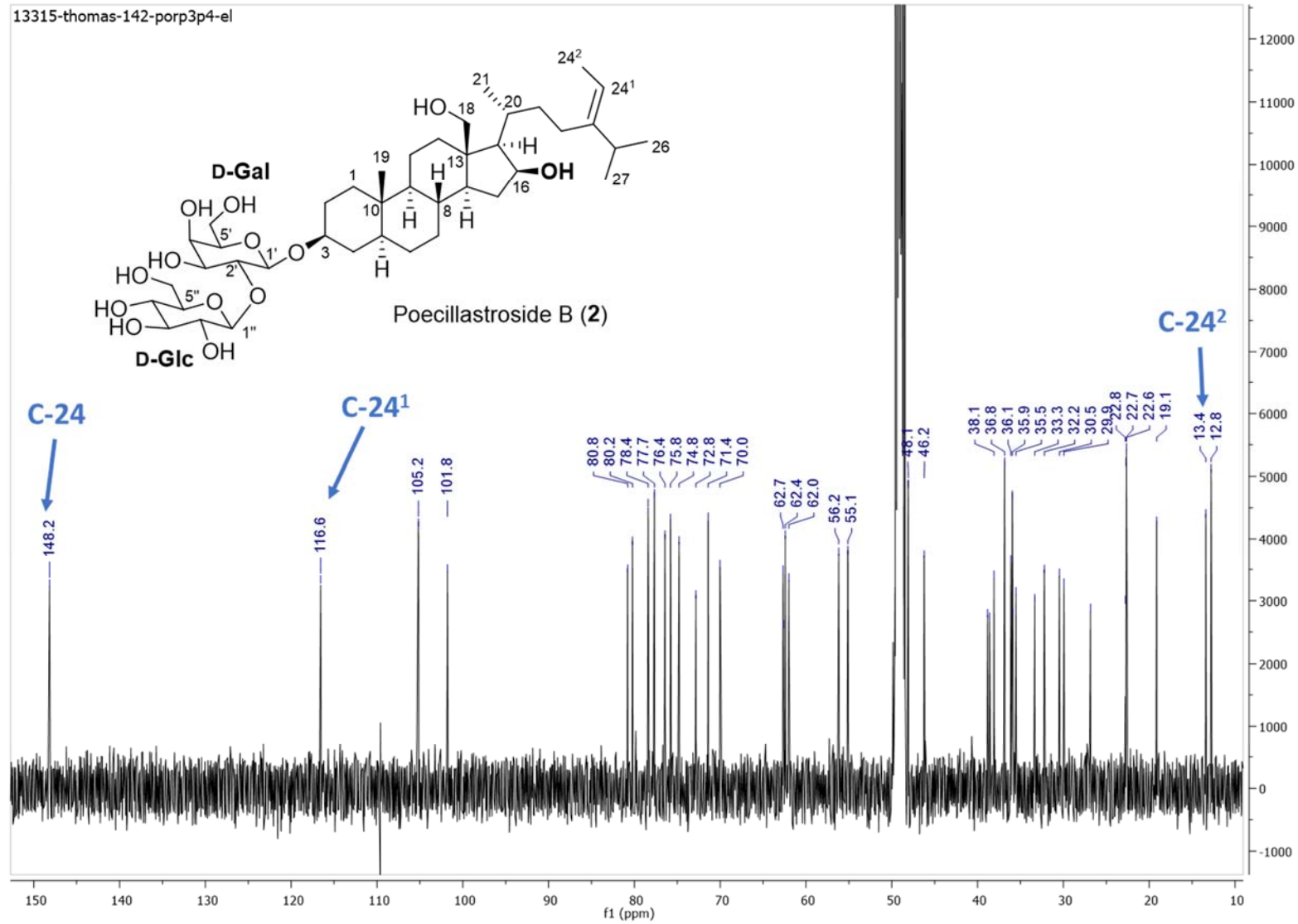


Figure S14. ^{13}C NMR spectrum of **2** at 125 MHz in CD_3OD

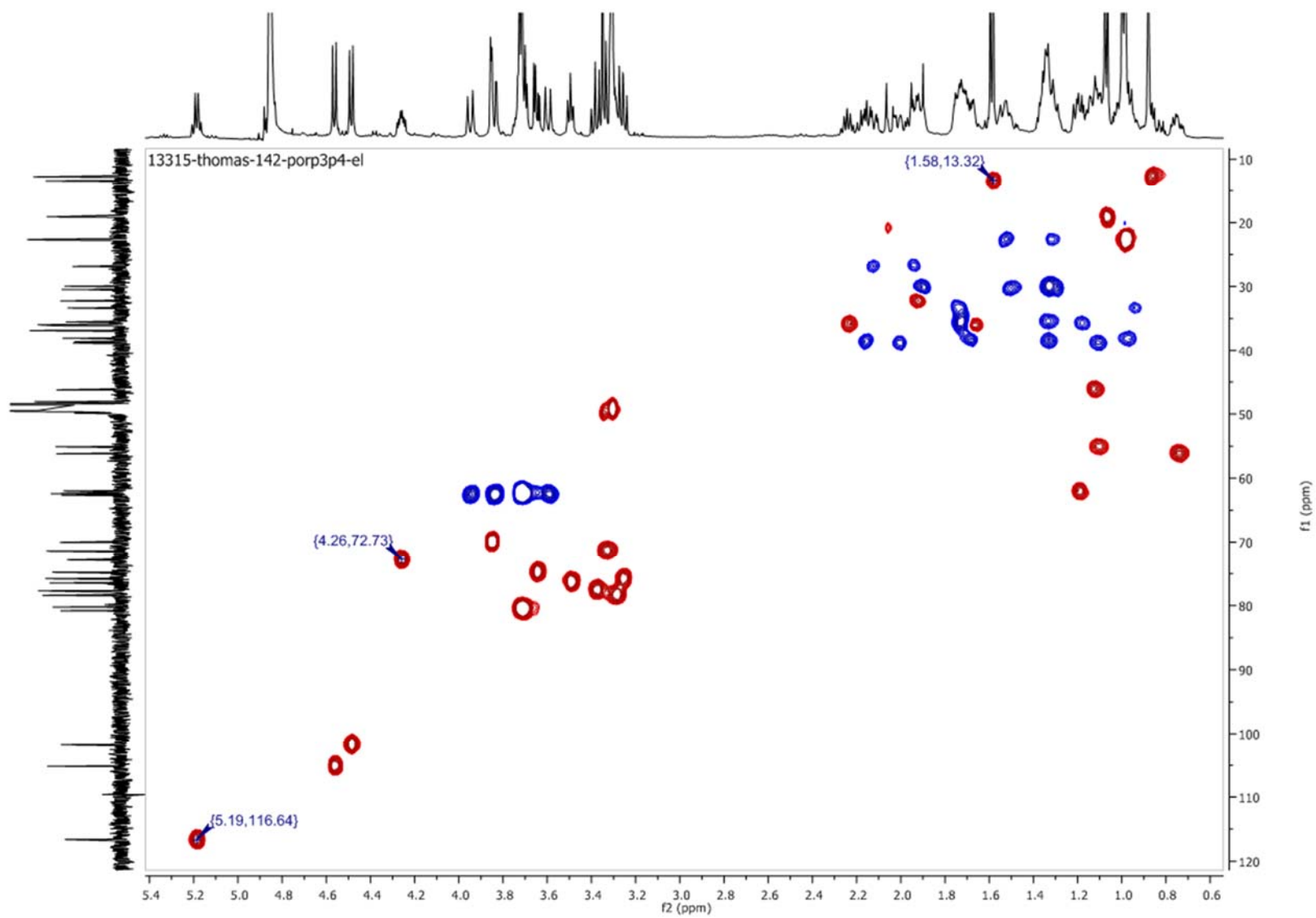


Figure S15. HSQC NMR spectrum of **2** at 500 MHz in CD₃OD

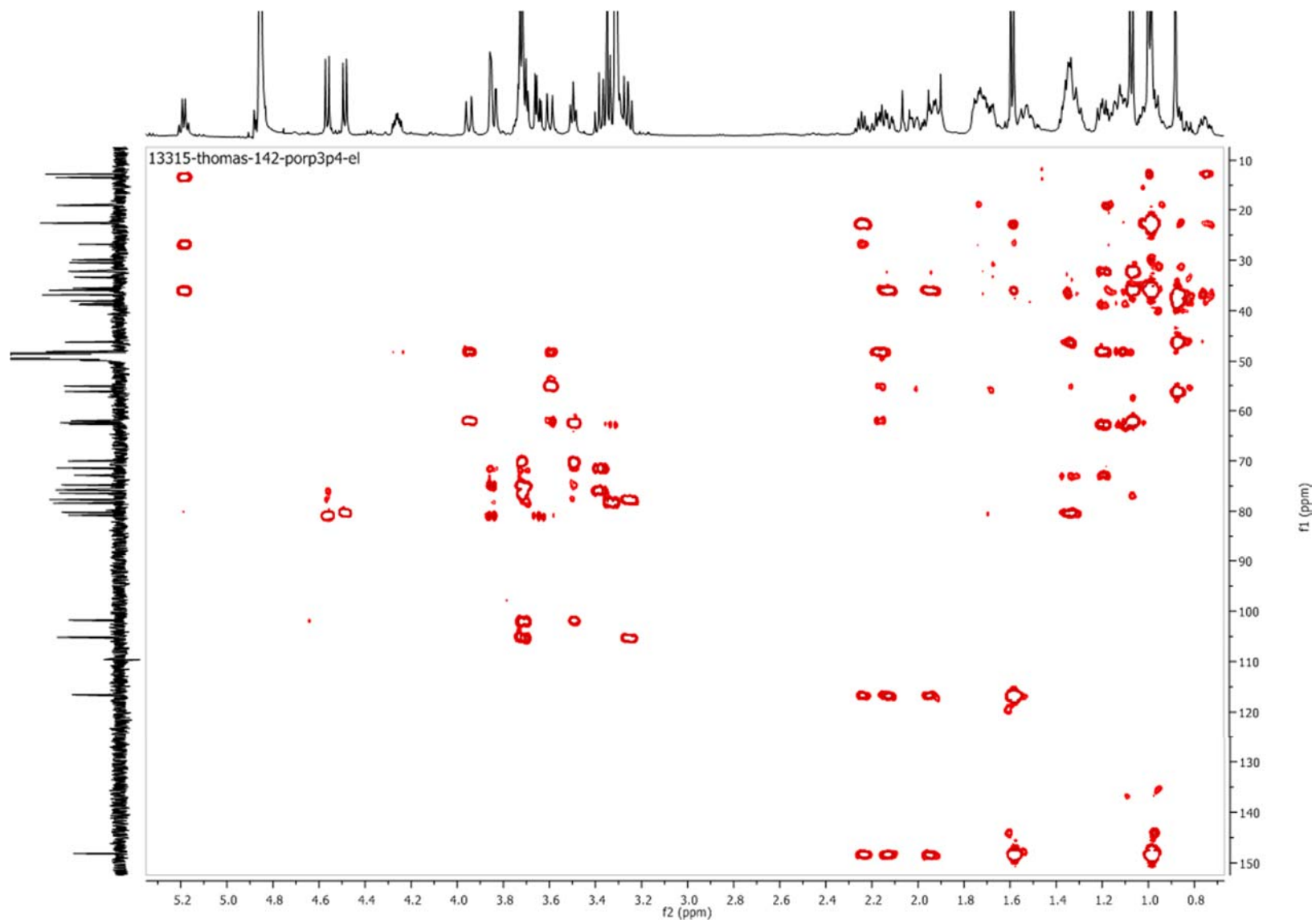


Figure S16. HMBC spectrum of 2 at 500 MHz in CD₃OD

Compound Formula	Name	RT	Algorithm
C ₄₁ H ₇₀ O ₁₃	Poecillastroside C	6.559	Spectrum Extraction

6
x10
MS Spectrum

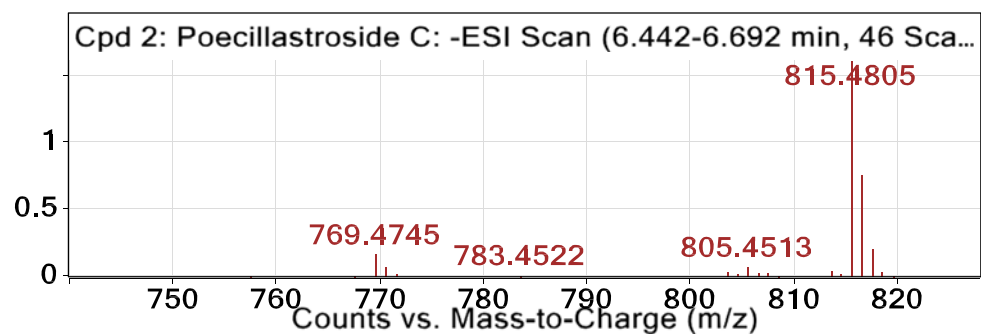


Figure S17. (-)-HRESIMS analysis of 3.

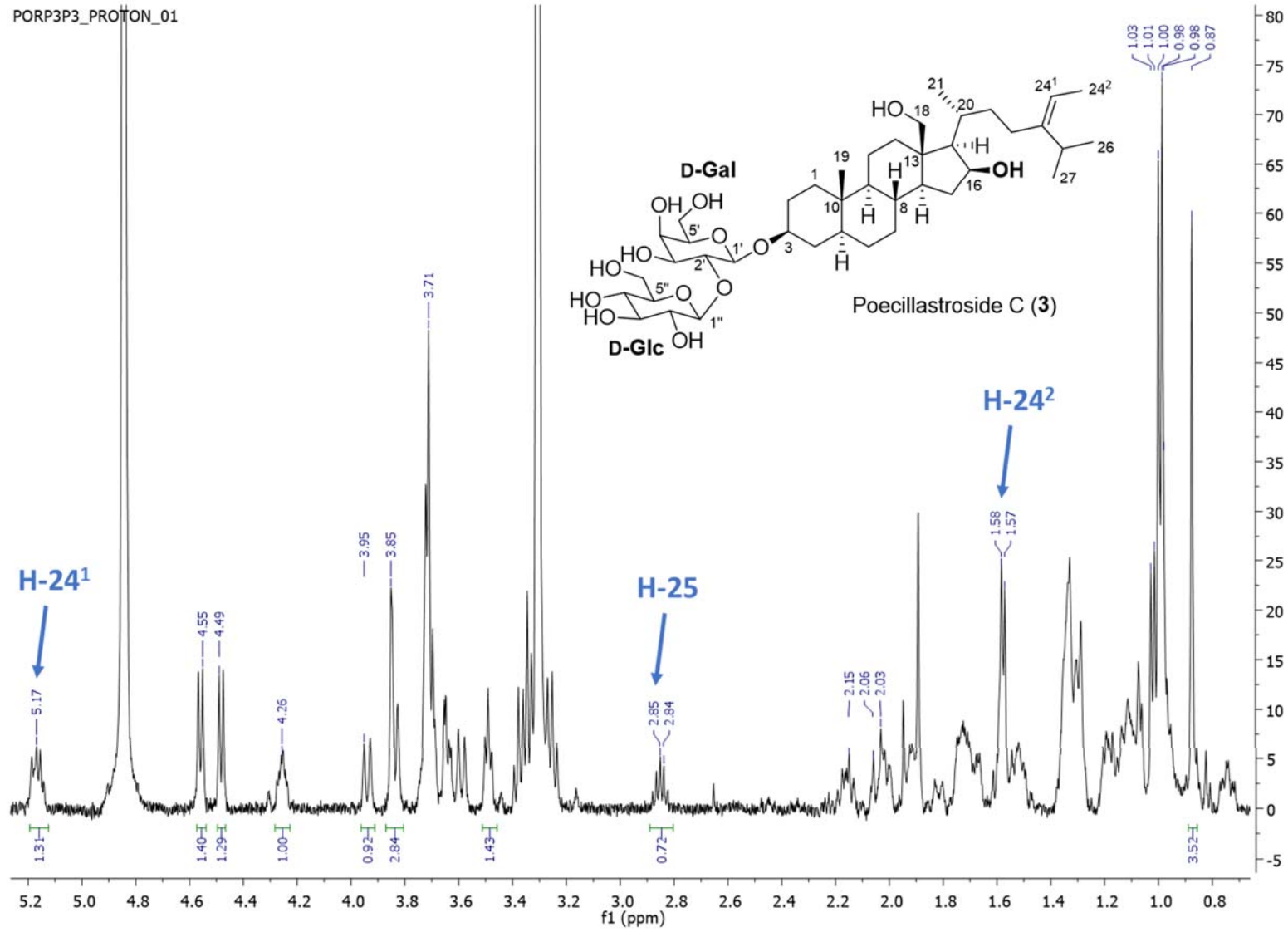


Figure S18. ¹H NMR spectrum of **3** at 500 MHz in CD₃OD

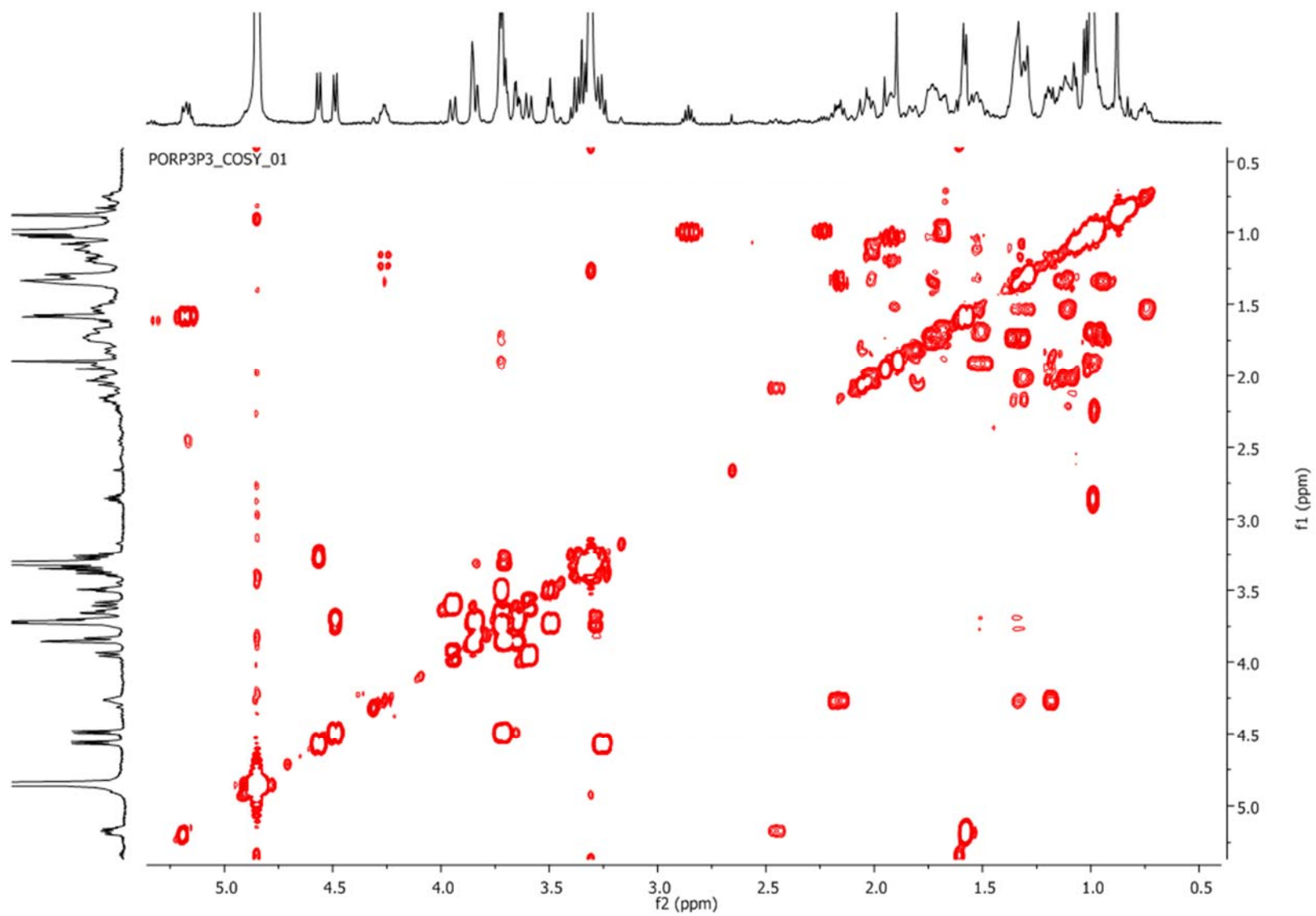


Figure S19. COSY NMR spectrum of **3** at 500 MHz in CD₃OD

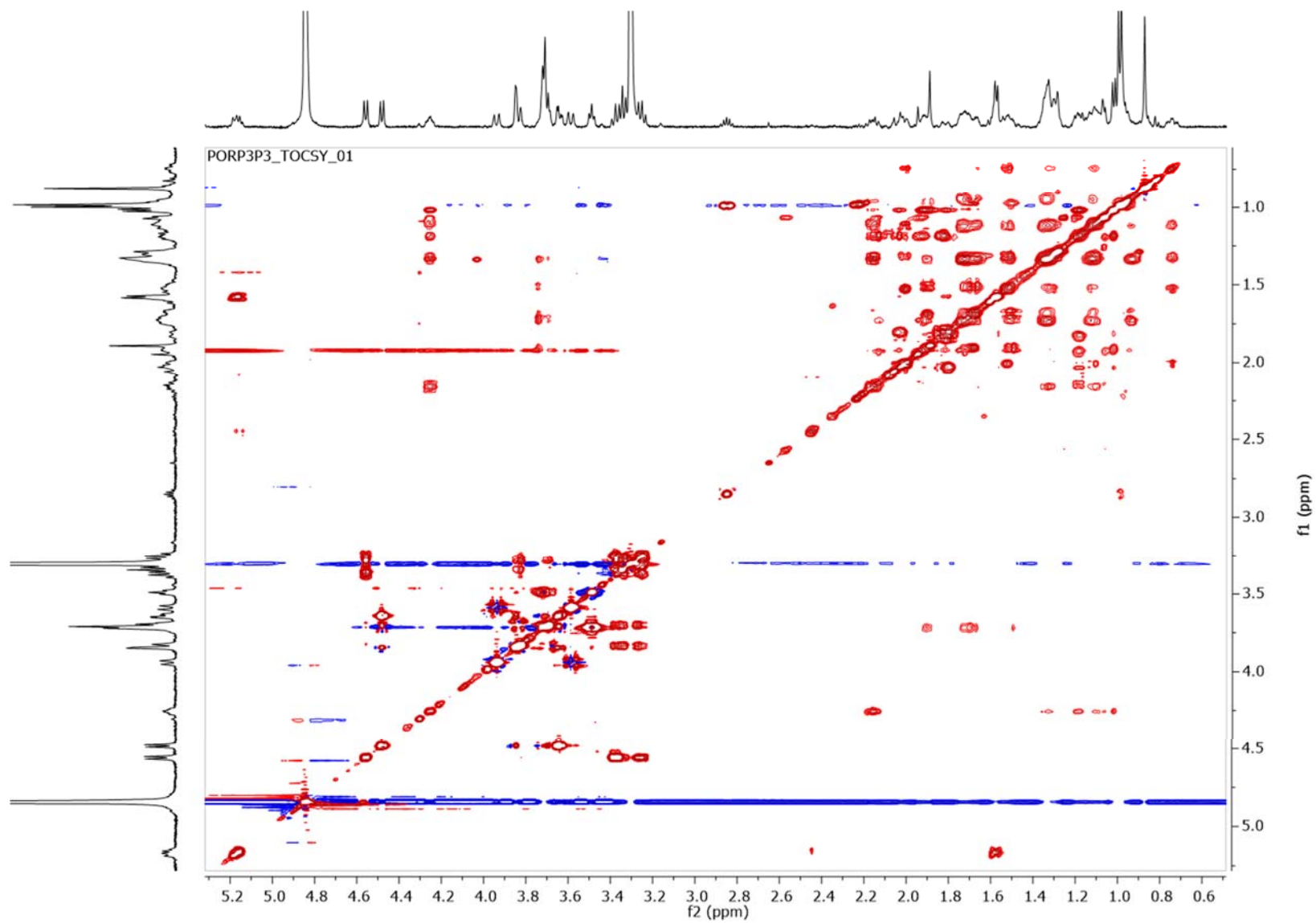


Figure S20. TOCSY NMR spectrum of 3 at 500 MHz in CD₃OD

KC_PORP3P3_CARBON_01

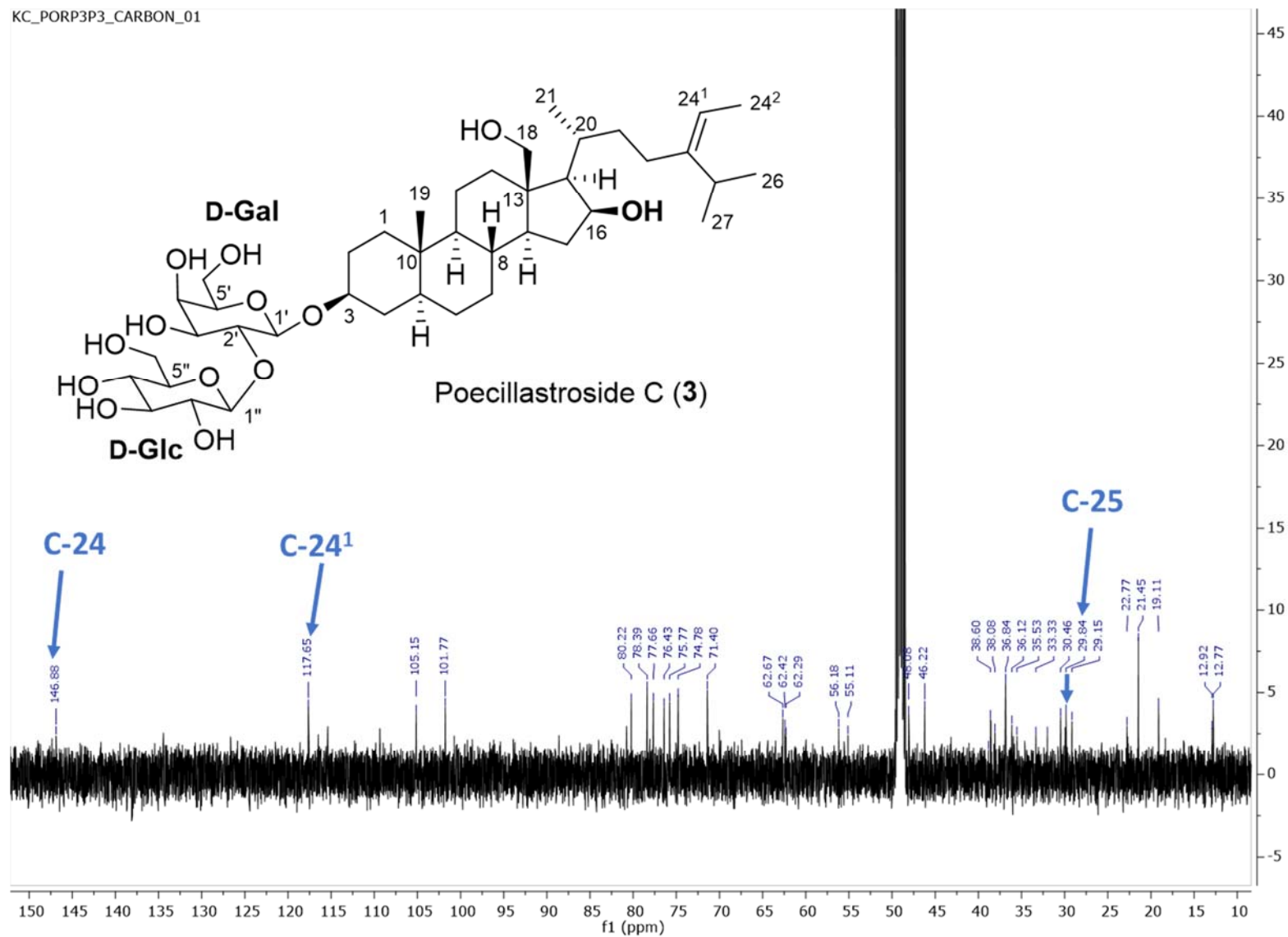


Figure S21. ¹³C NMR spectrum of 3 at 500 MHz in CD₃OD

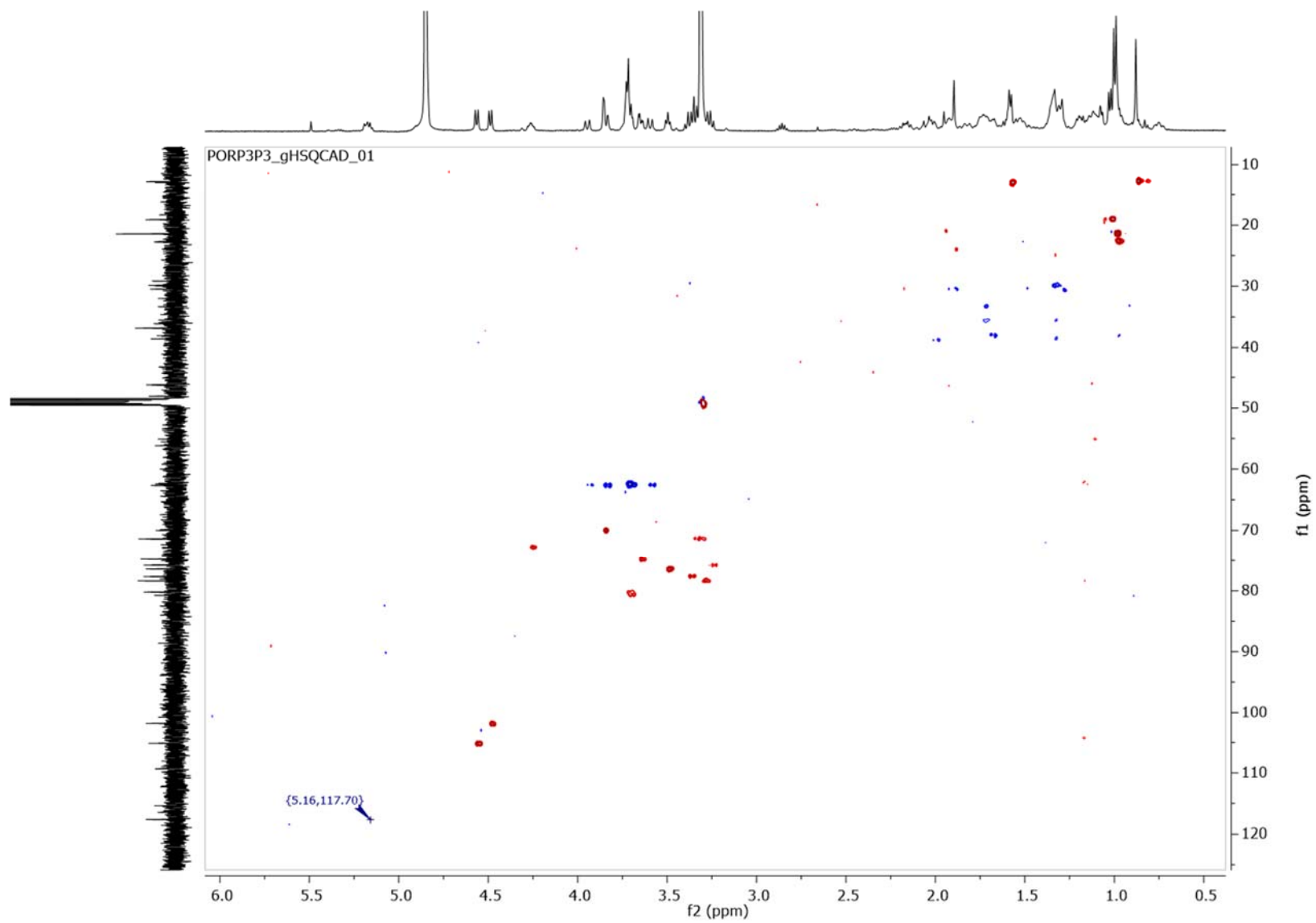


Figure S22. HSQC NMR spectrum of **3** at 500 MHz in CD_3OD

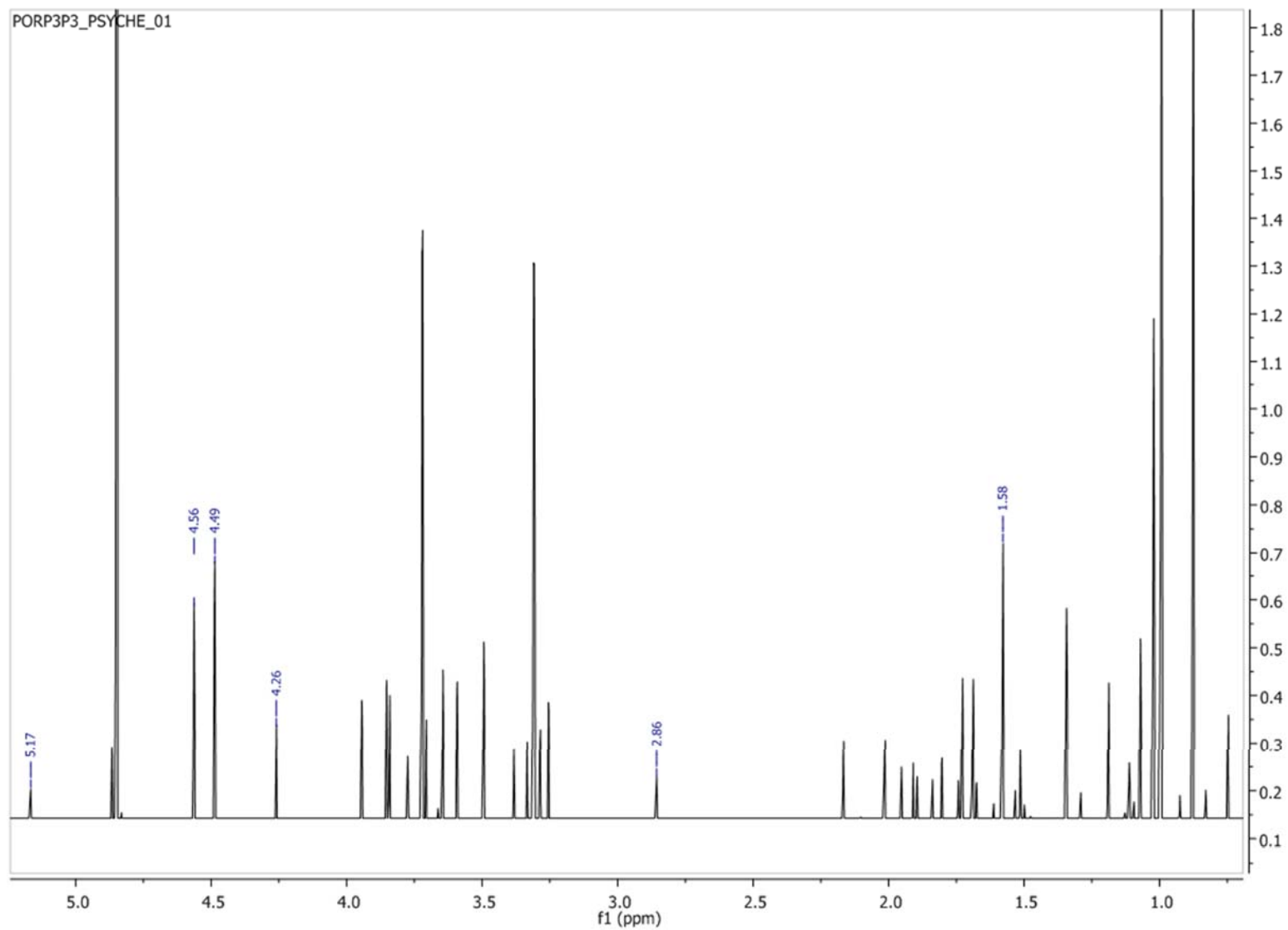


Figure S23. PSYCHE_1D NMR spectrum of **3** at 500 MHz in CD₃OD

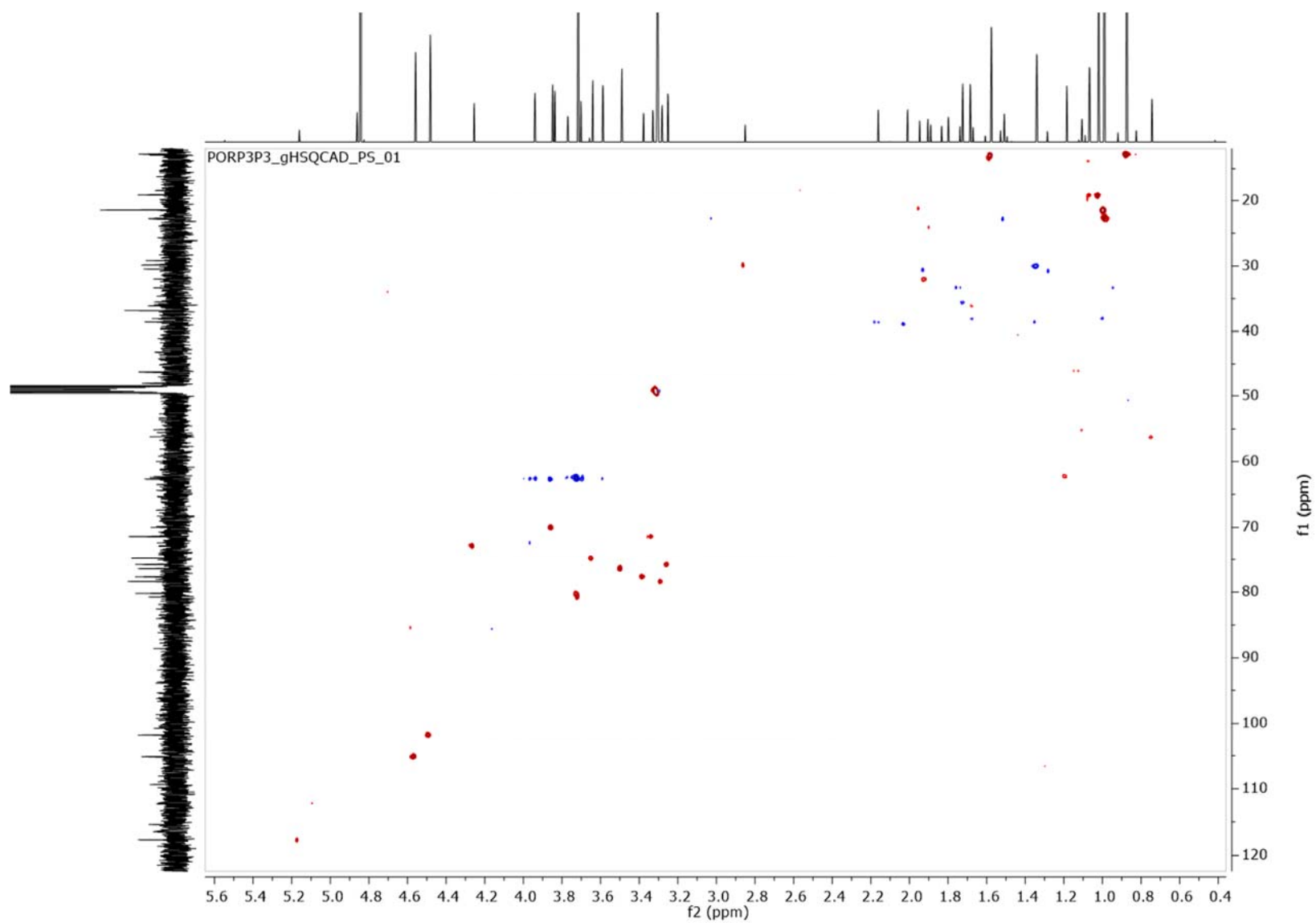


Figure S24. PS-HSQC NMR spectrum of **3** at 500 MHz in CD₃OD

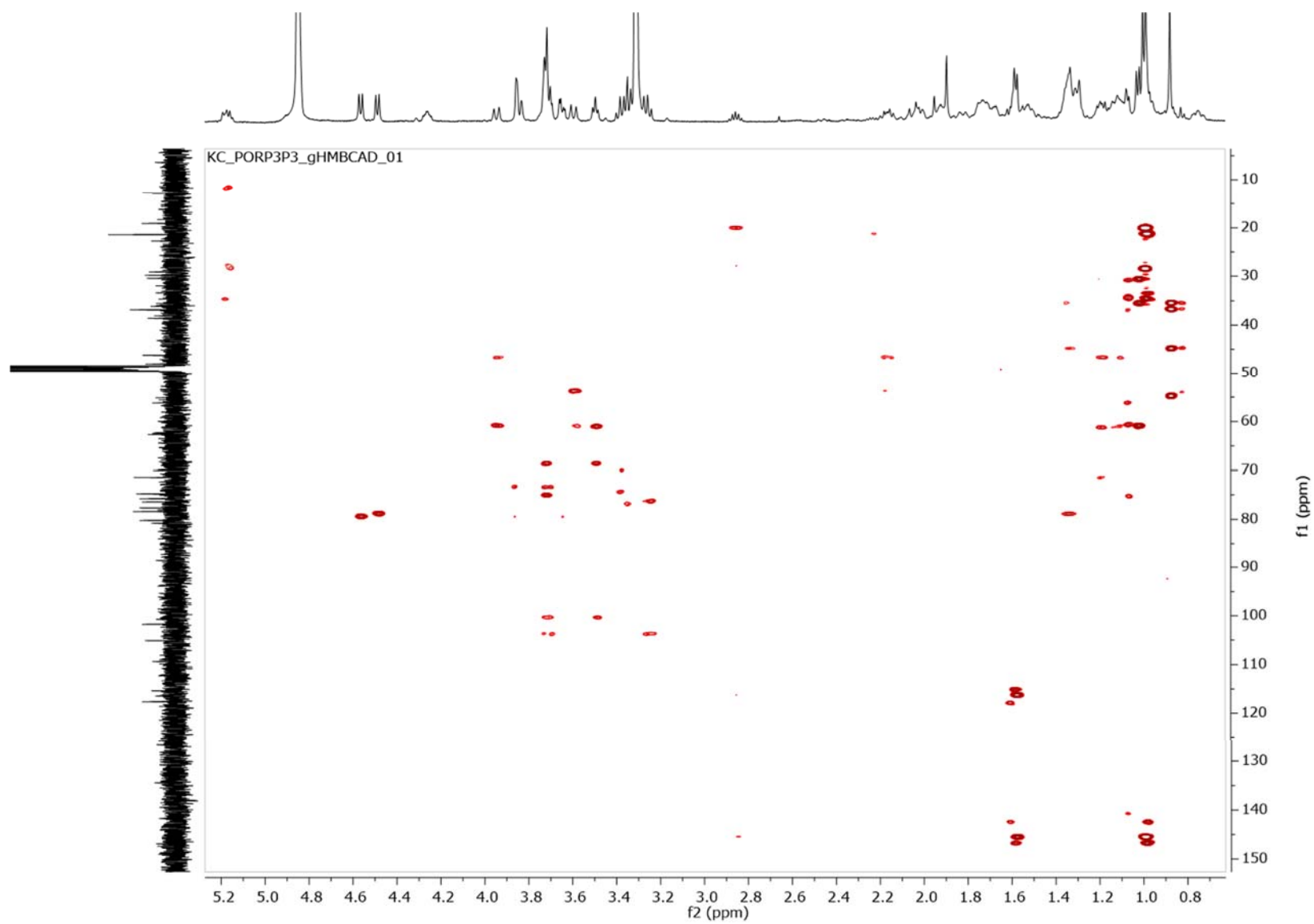


Figure S25. HMBC spectrum of **3** at 500 MHz in CD₃OD

Compound Formula	Name	RT	Algorithm
C ₄₁ H ₆₈ O ₁₃	Poecillastroside D	7.049	Spectrum Extraction

5
x10
MS Spectrum

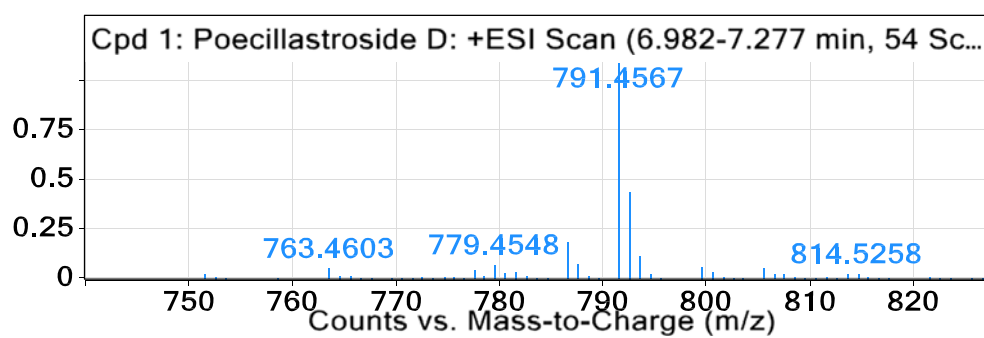


Figure S26. (+)-HRESIMS analysis of 4.

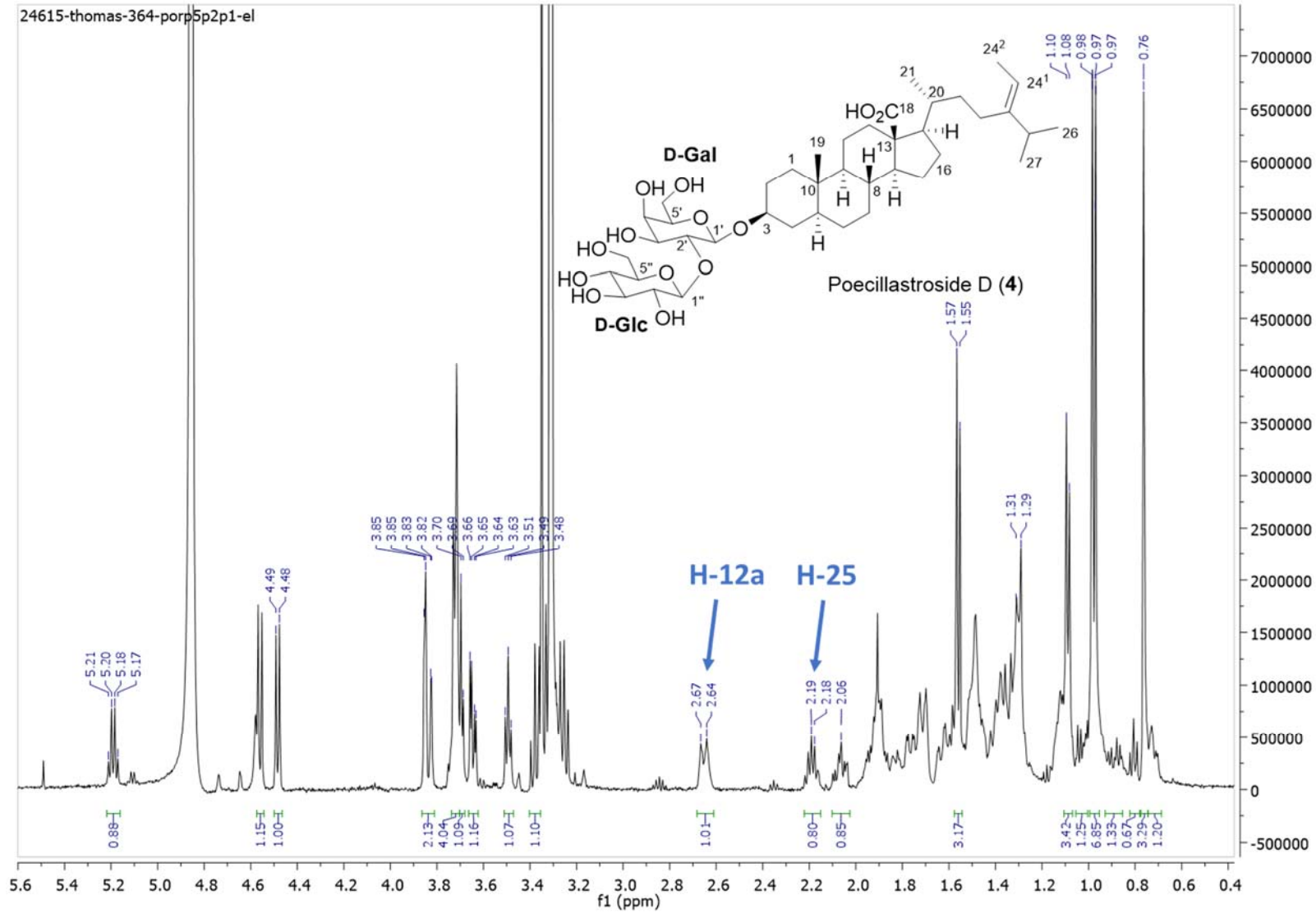


Figure S27. ¹H NMR spectrum of 4 at 500 MHz in CD₃OD

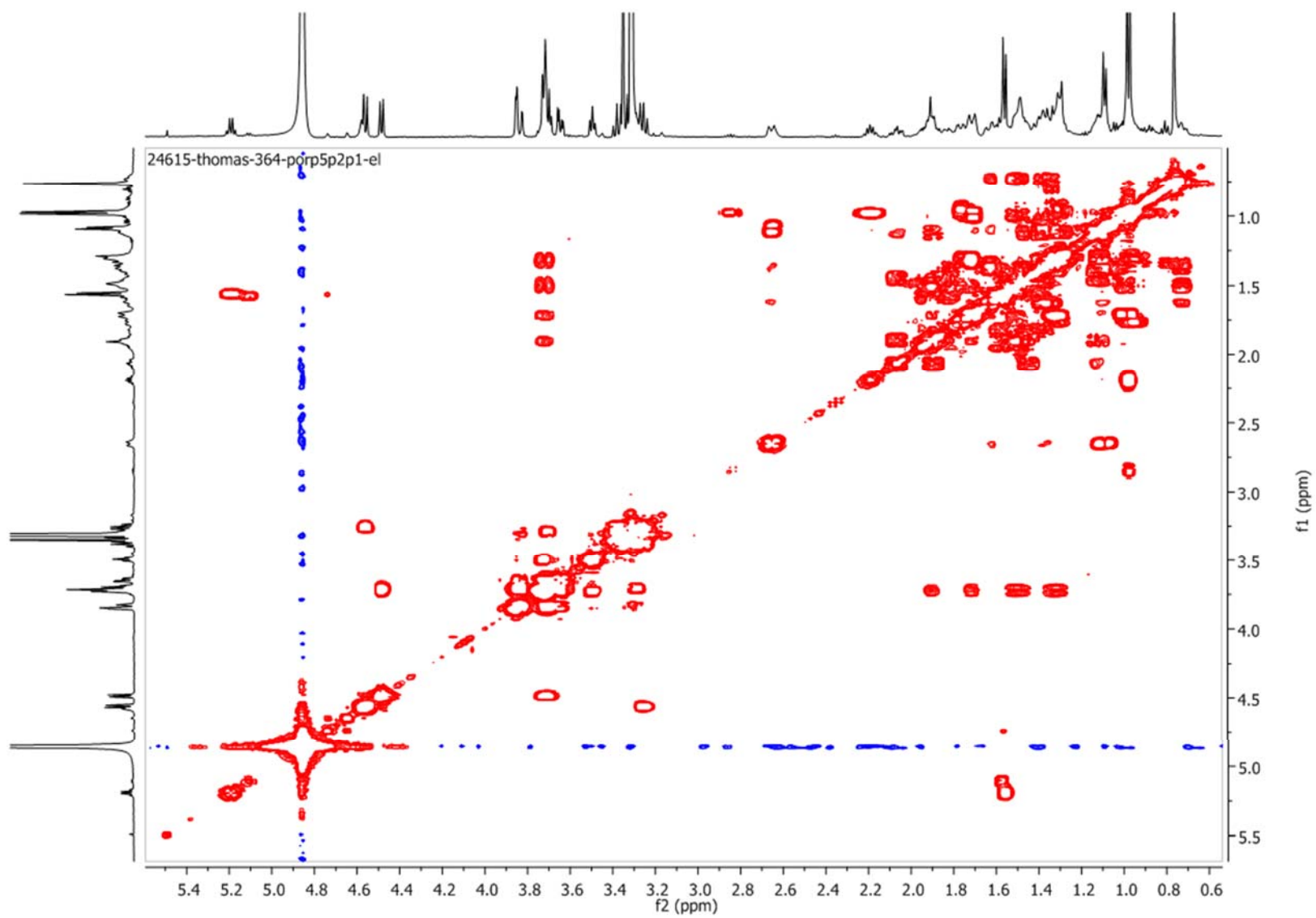


Figure S28. COSY NMR spectrum of **4** at 500 MHz in CD₃OD

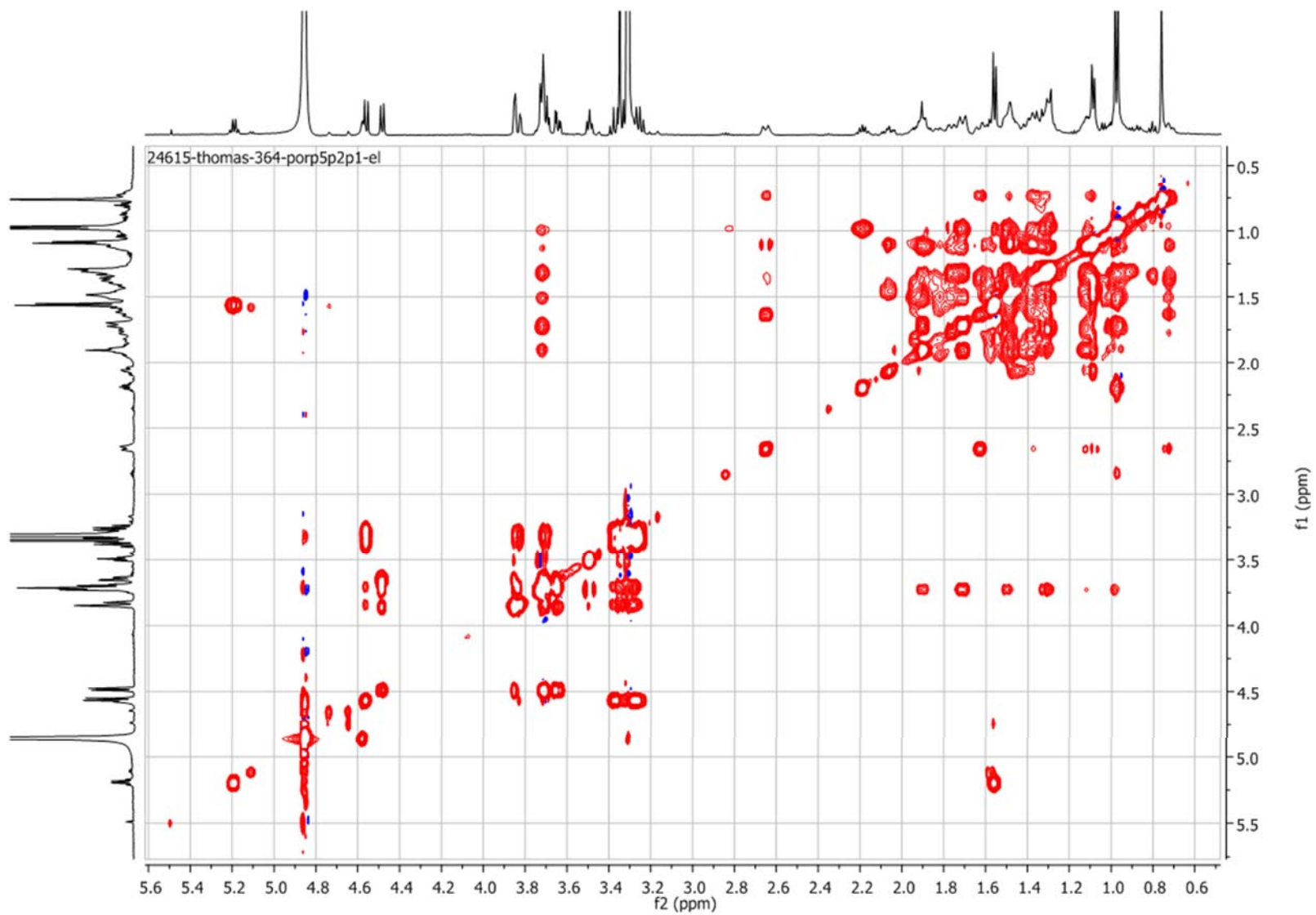


Figure S29. TOCSY NMR spectrum of **4** at 500 MHz in CD₃OD

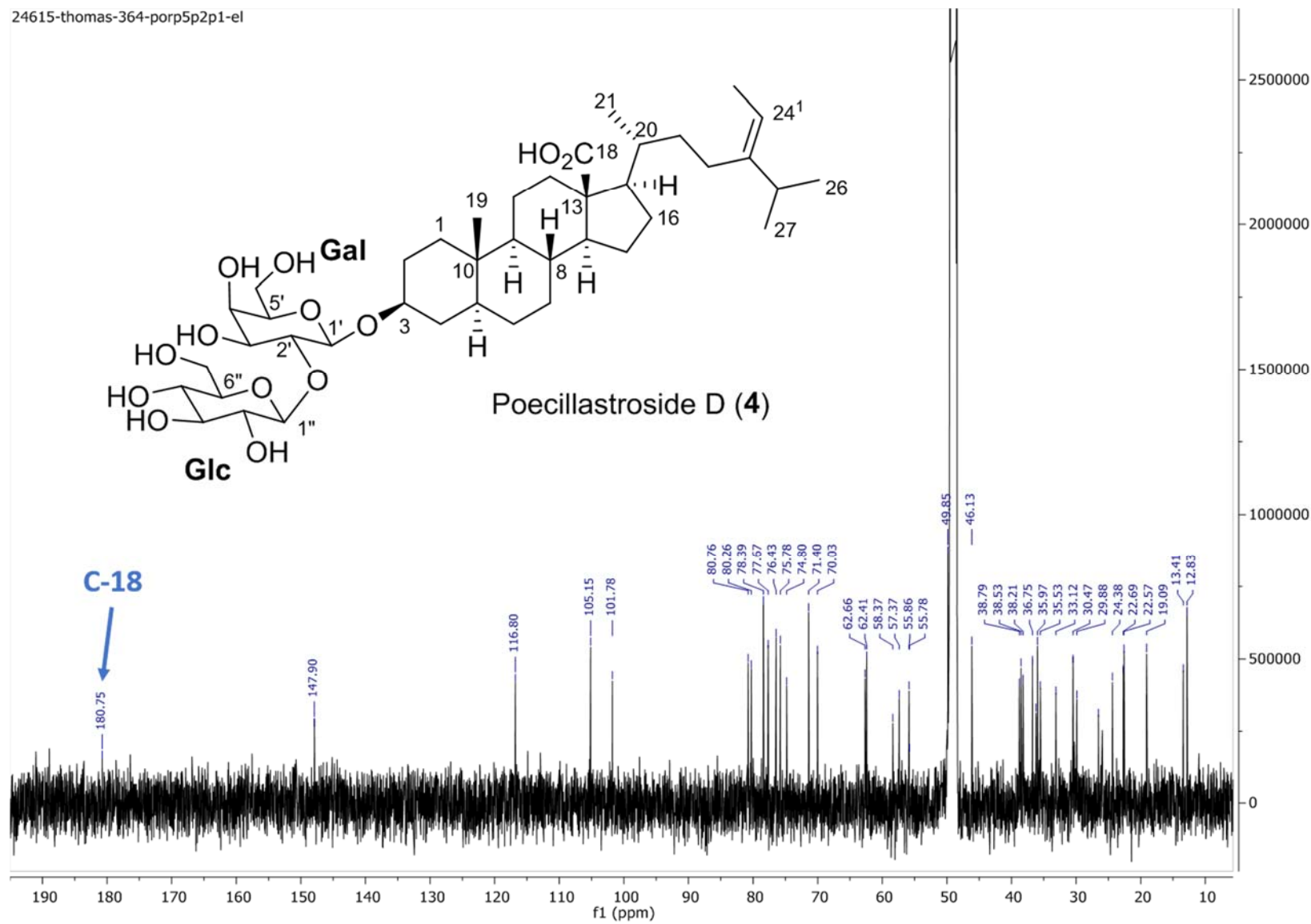


Figure S30. ¹³C NMR spectrum of 4 at 125 MHz in CD₃OD

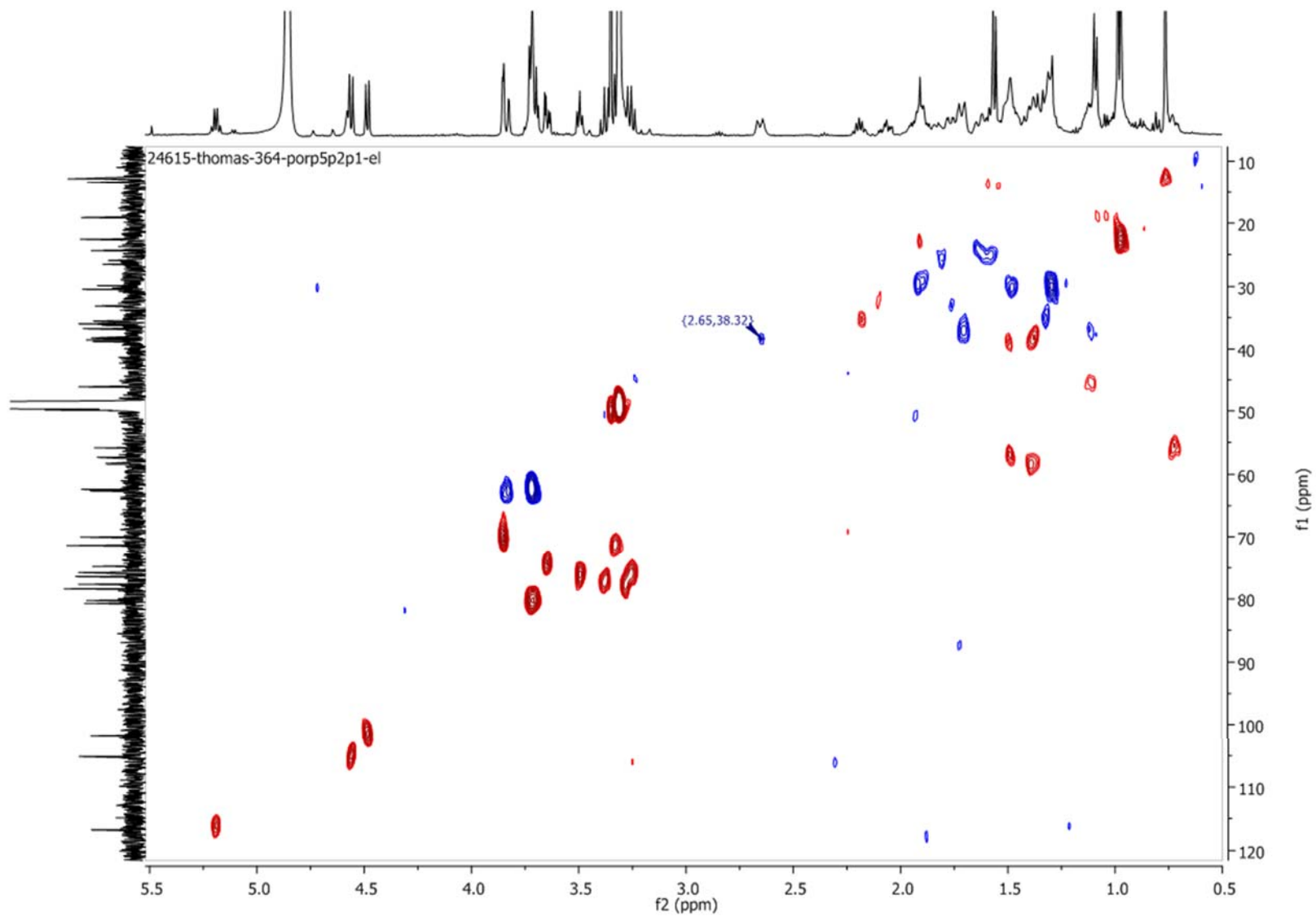


Figure S31. HSQC NMR spectrum of **4** at 500 MHz in CD₃OD

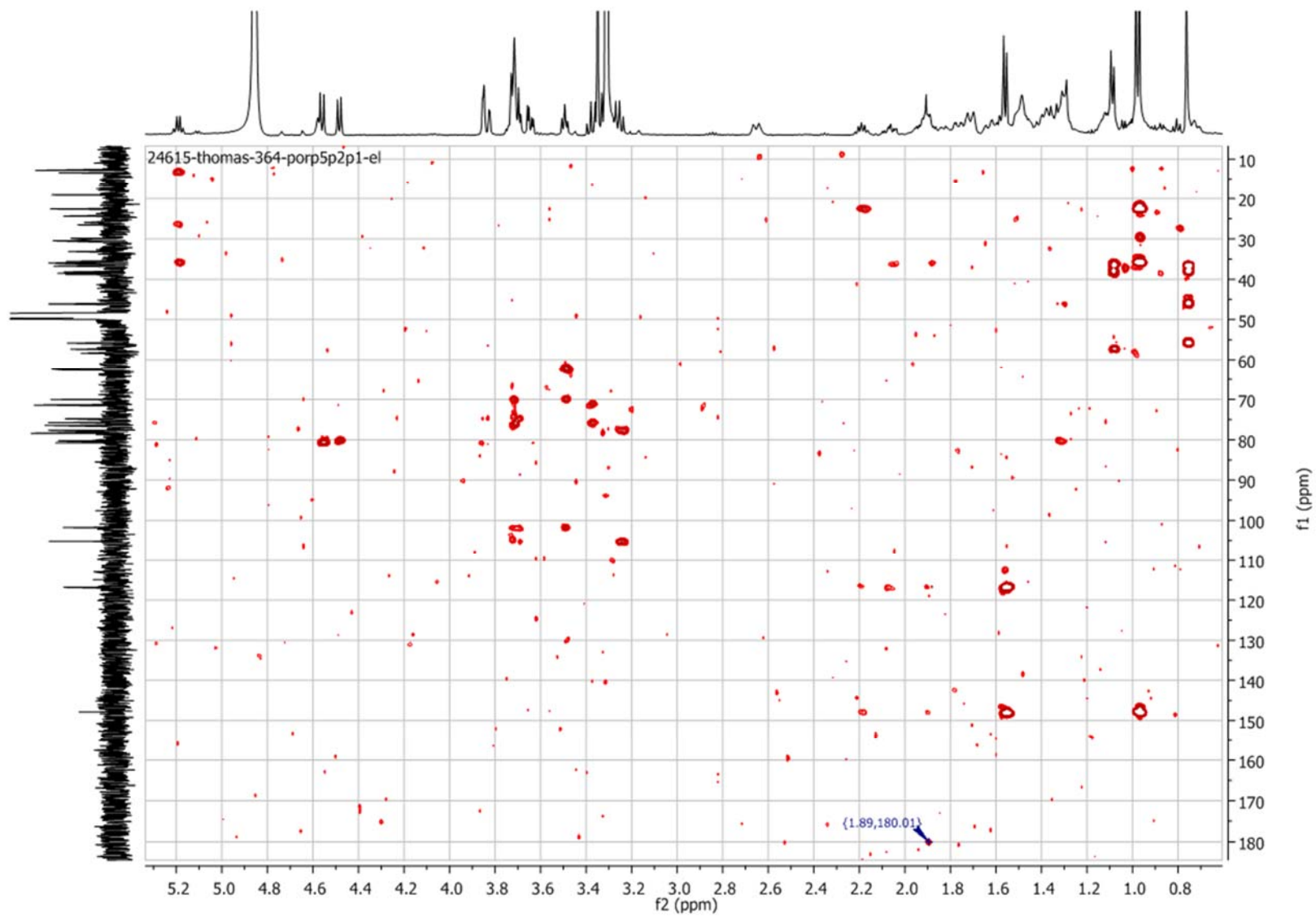


Figure S32. HMBC spectrum of **4** at 500 MHz in CD₃OD

Compound Formula	Name	RT	Algorithm
C ₄₃ H ₆₆ O ₁₅	Poecillastroside E	7.109	Spectrum Extraction

5
x10
MS Spectrum

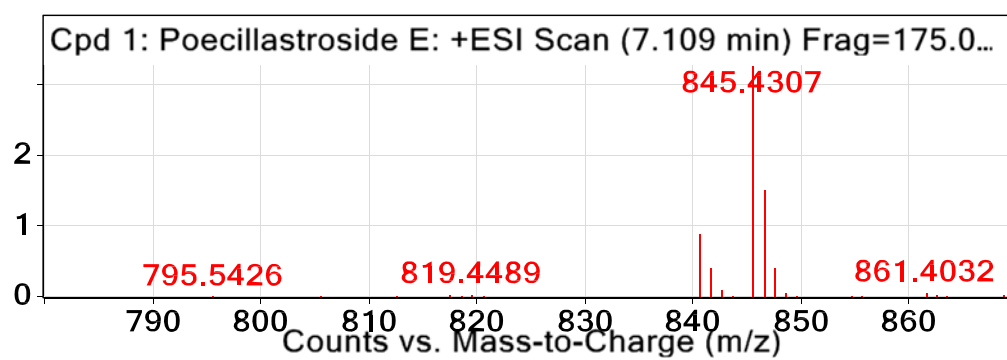


Figure S33. (+)-HRESIMS analysis of 5.

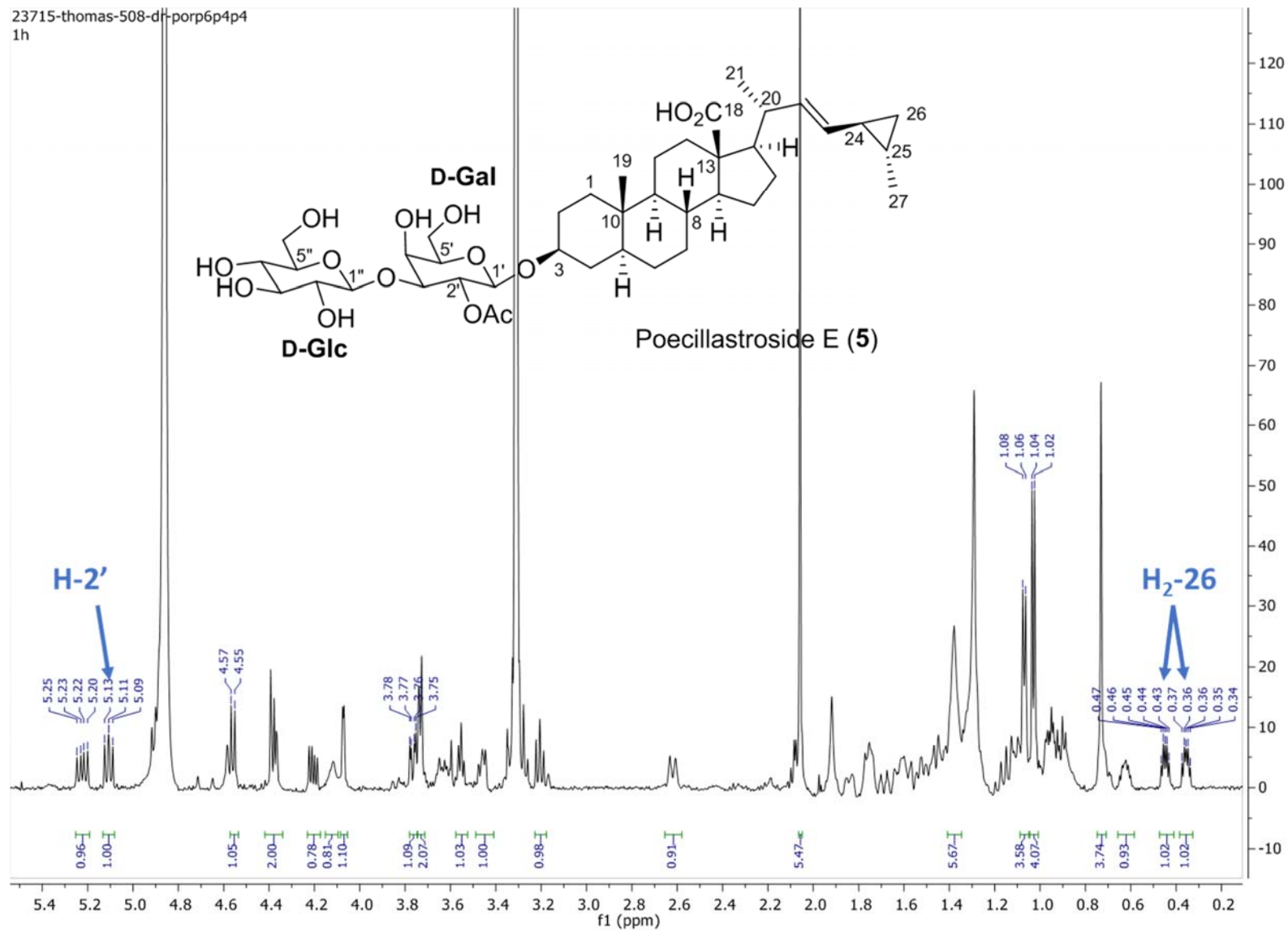


Figure S34. ¹H NMR spectrum of 5 at 500 MHz in CD₃OD

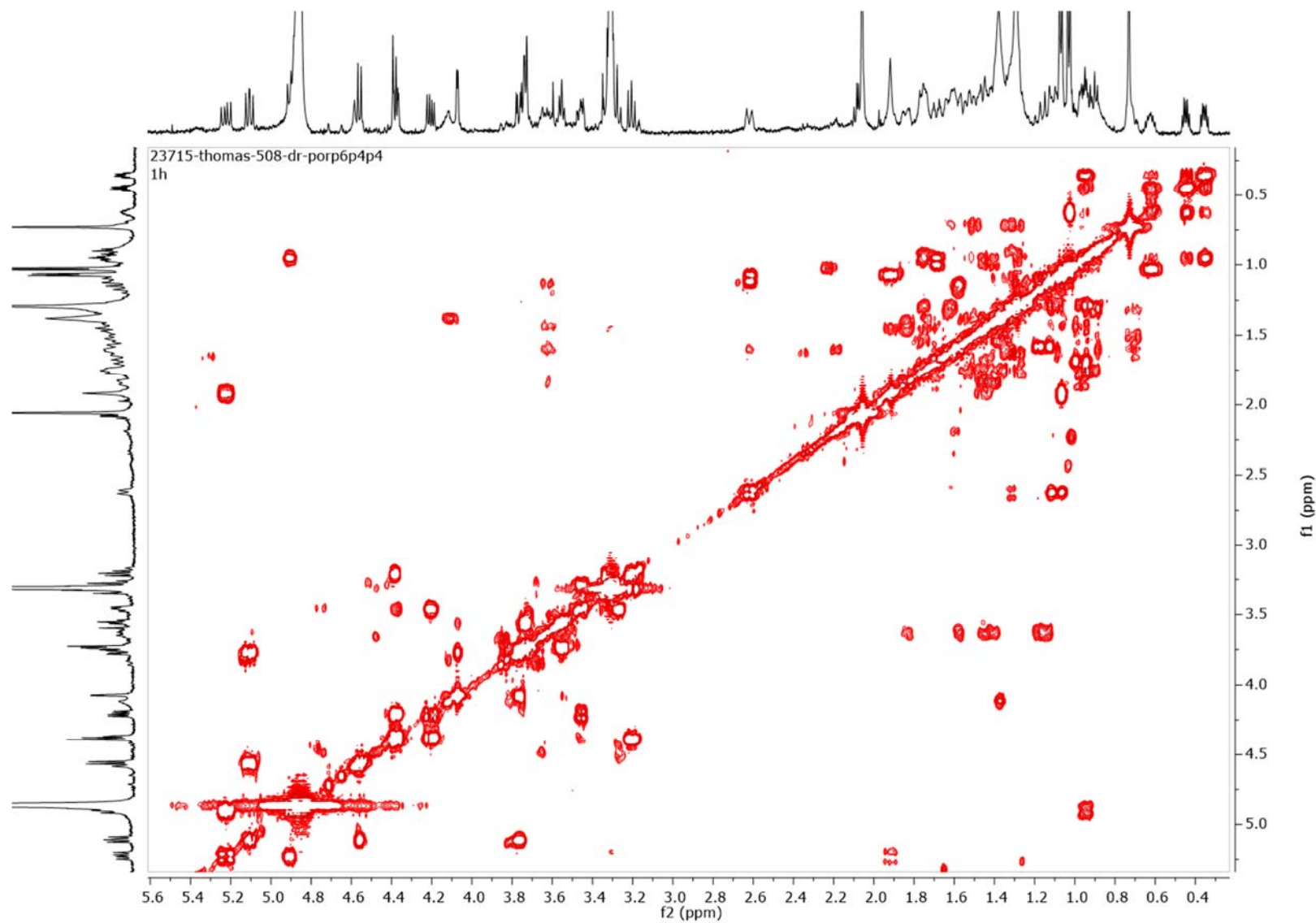


Figure S35. COSY NMR spectrum of **5** at 500 MHz in CD₃OD

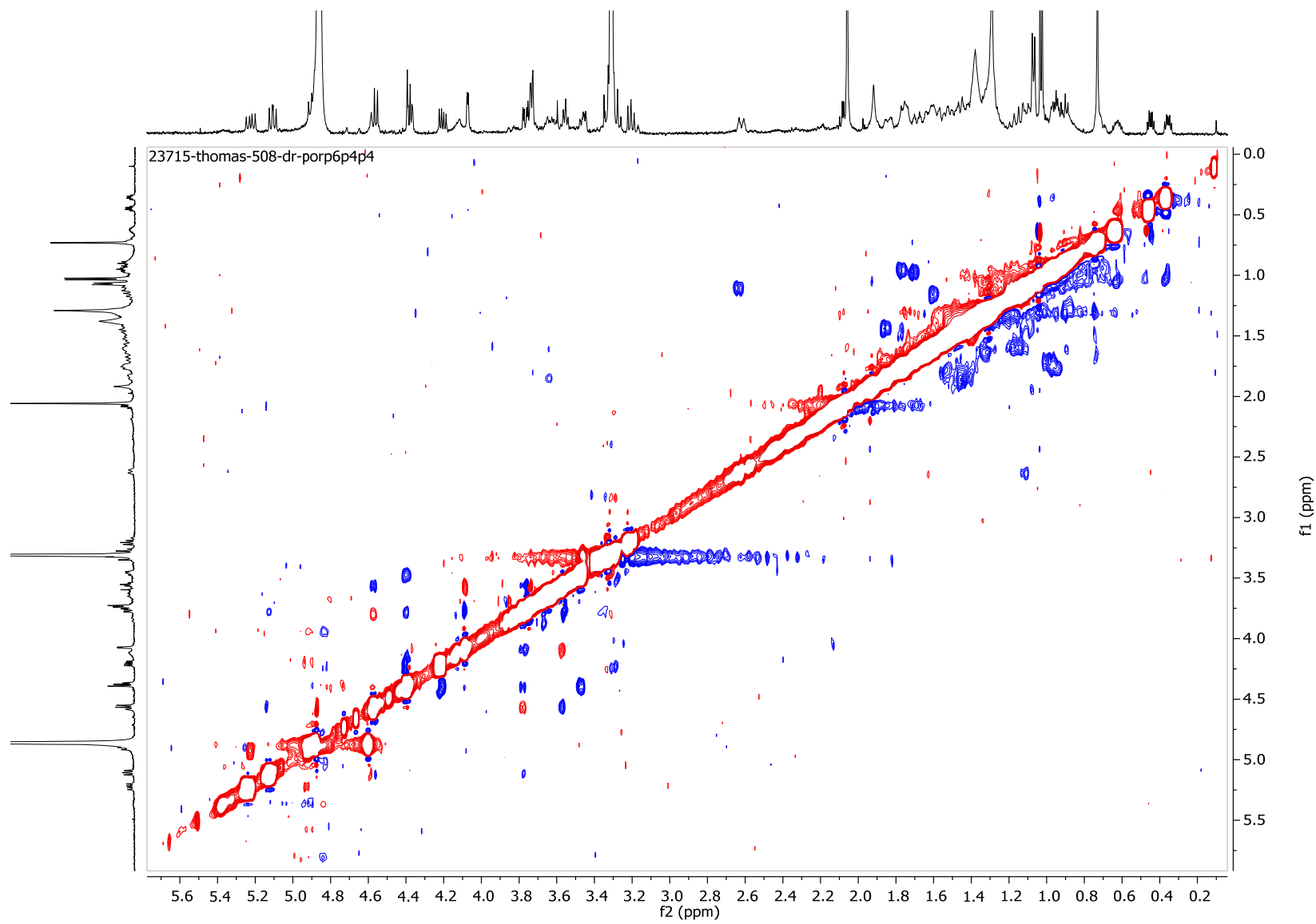


Figure S36. NOESY NMR spectrum of **5** at 500 MHz in CD₃OD

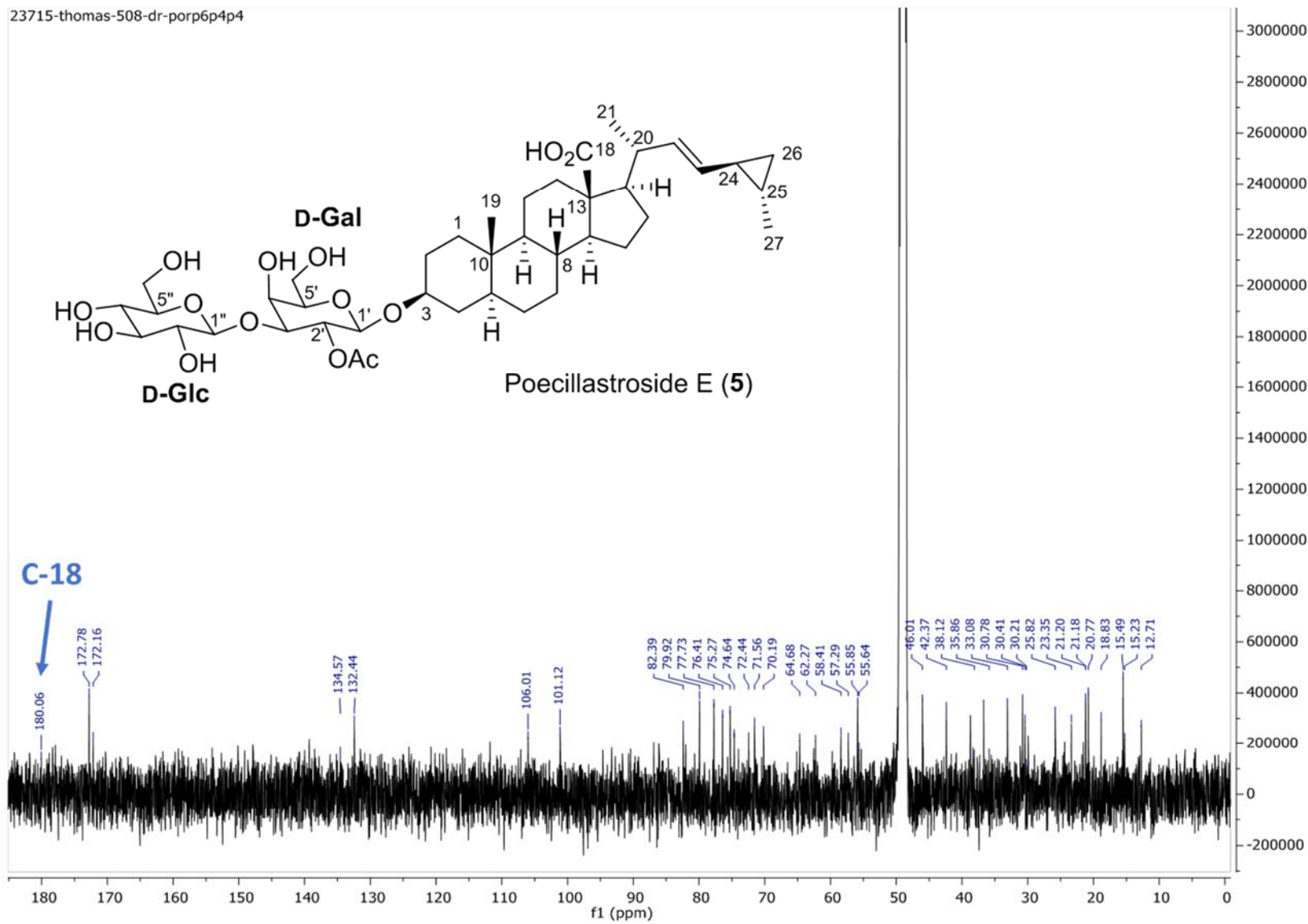


Figure S37. ^{13}C NMR spectrum of **5** at 125 MHz in CD_3OD

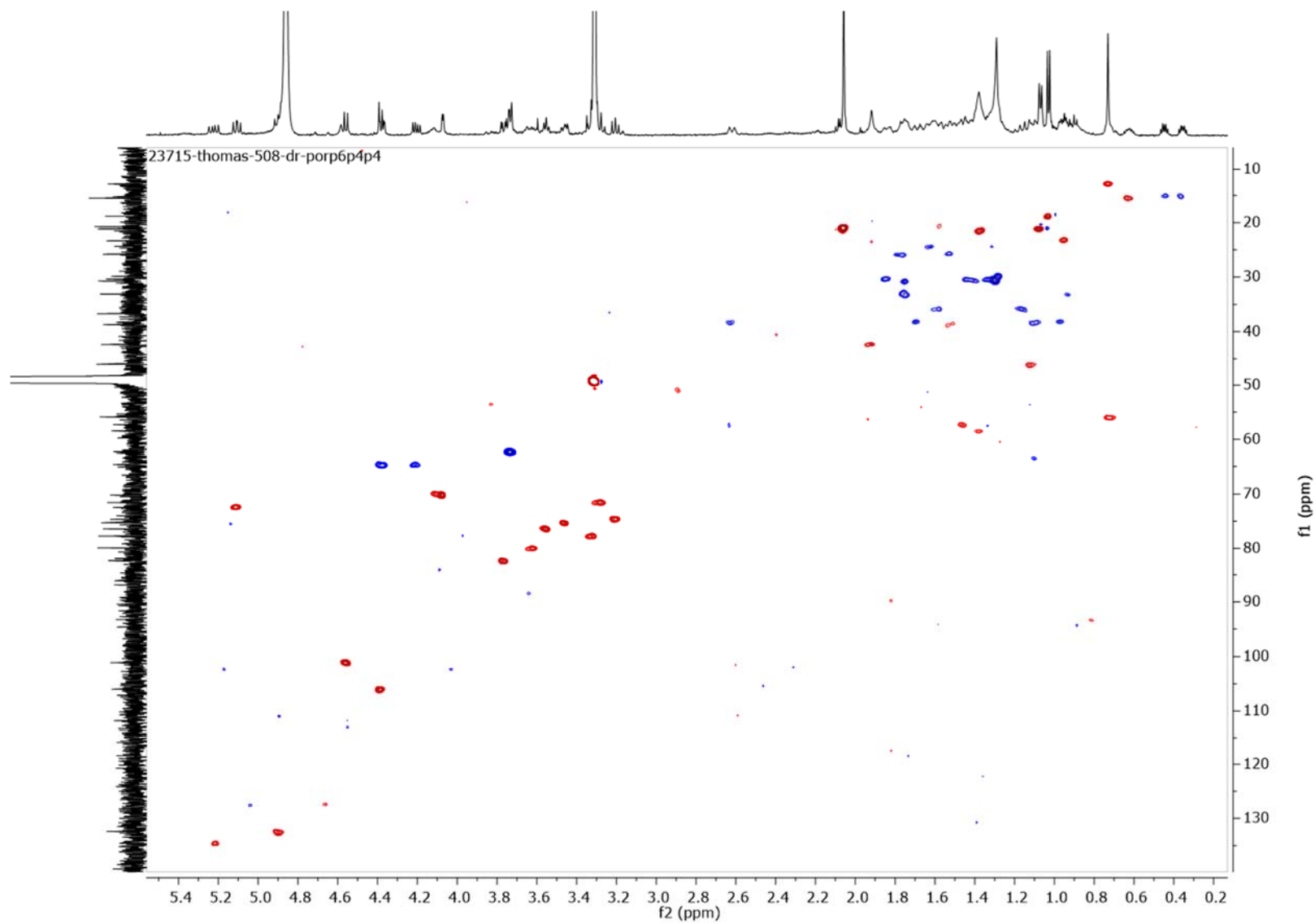


Figure S38. HSQC NMR spectrum of **5** at 500 MHz in CD₃OD

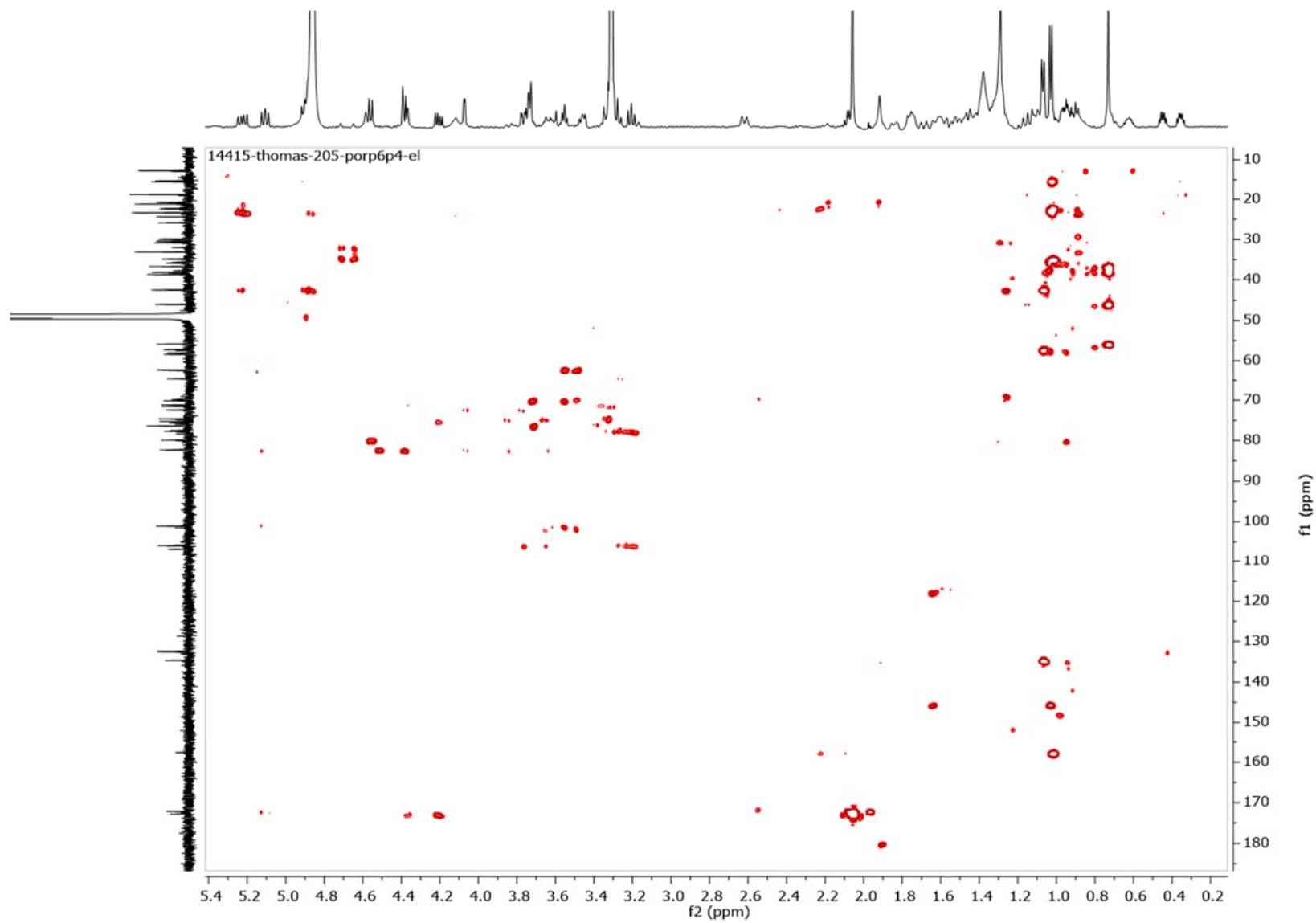


Figure S39. HMBC spectrum of 5 at 500 MHz in CD₃OD

Compound Formula	Name	RT	Algorithm
C ₄₁ H ₆₆ O ₁₃	Poecillastroside F	7.024	Spectrum Extraction

MS Spectrum

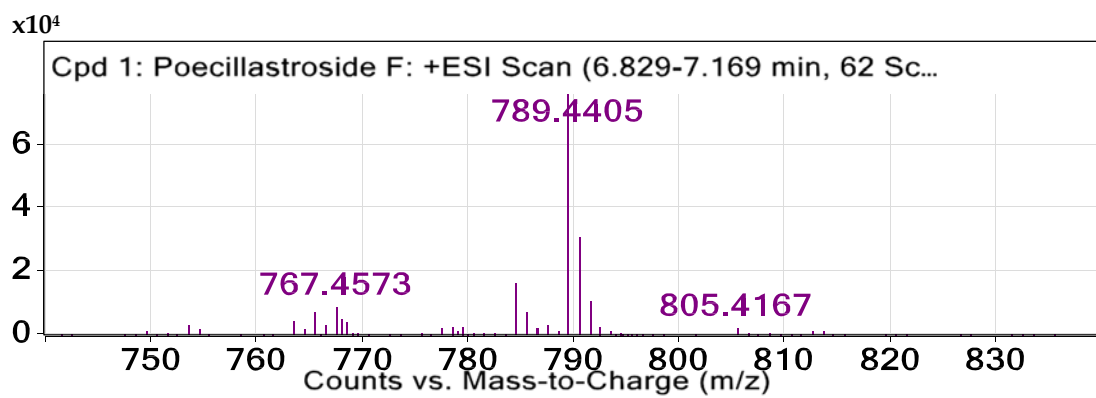


Figure S40. (+)-HRESIMS analysis of 6.

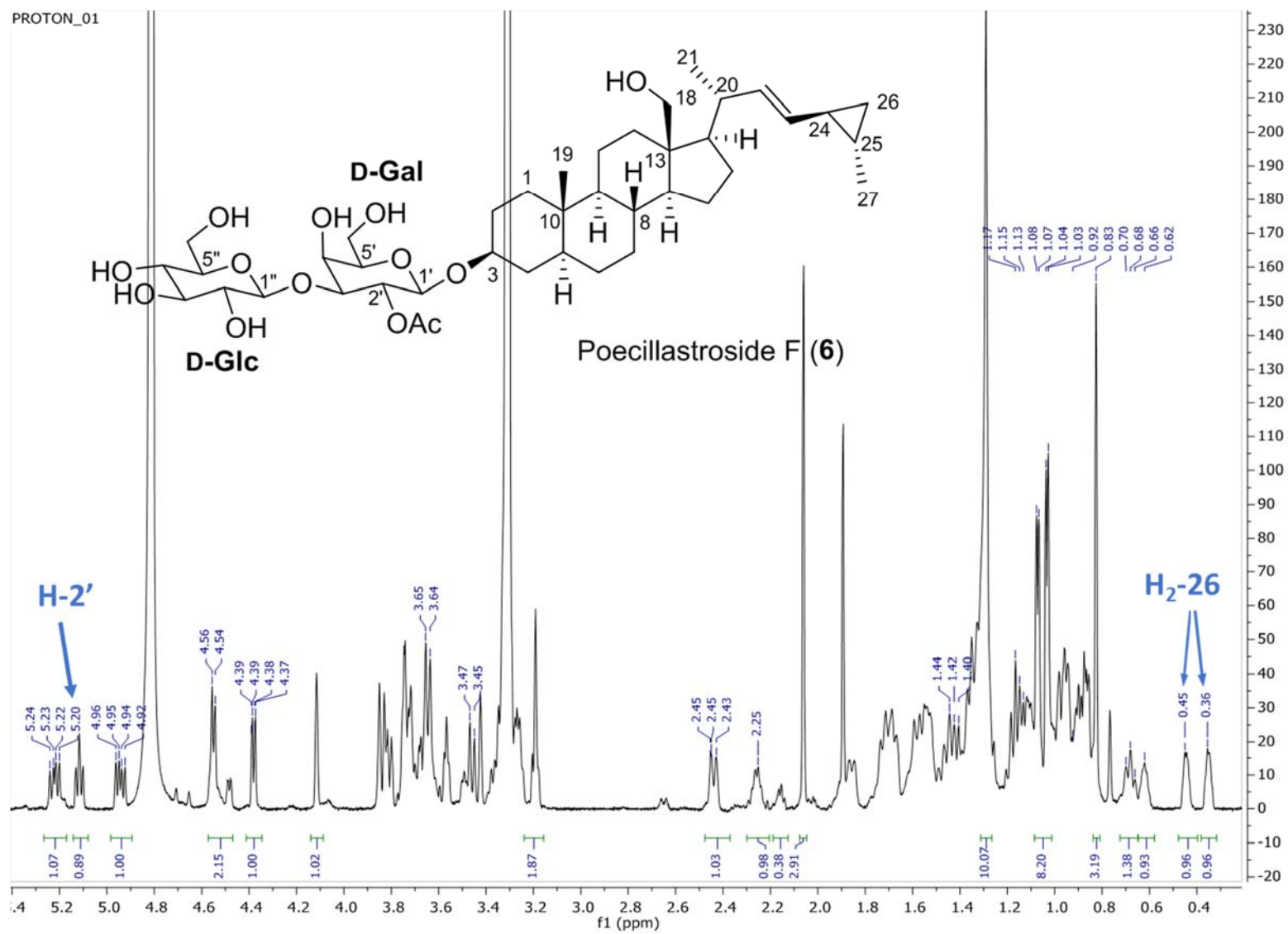


Figure S41. ¹H NMR spectrum of **6** at 600 MHz in CD₃OD

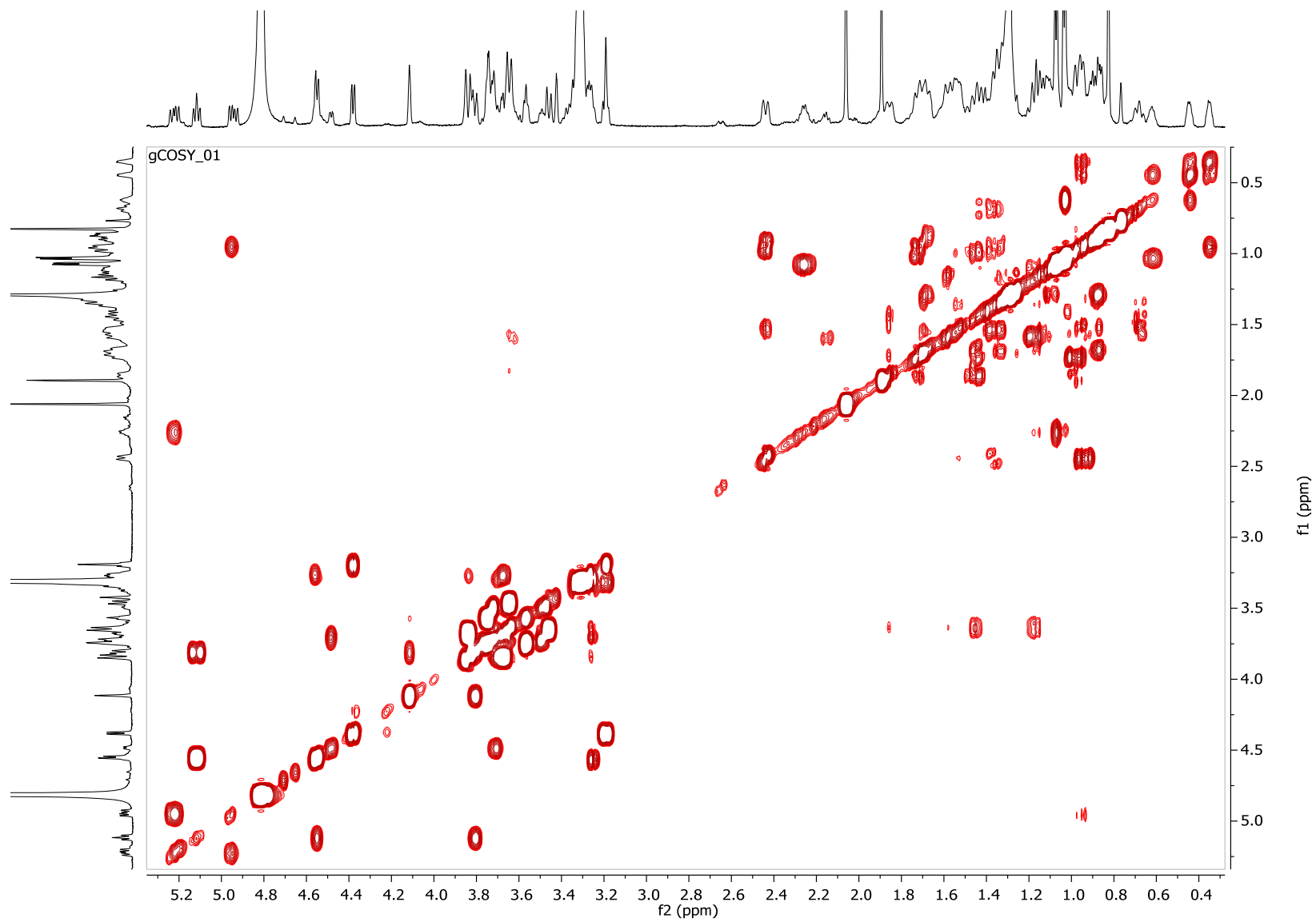


Figure S42. COSY NMR spectrum of **6** at 600 MHz in CD₃OD

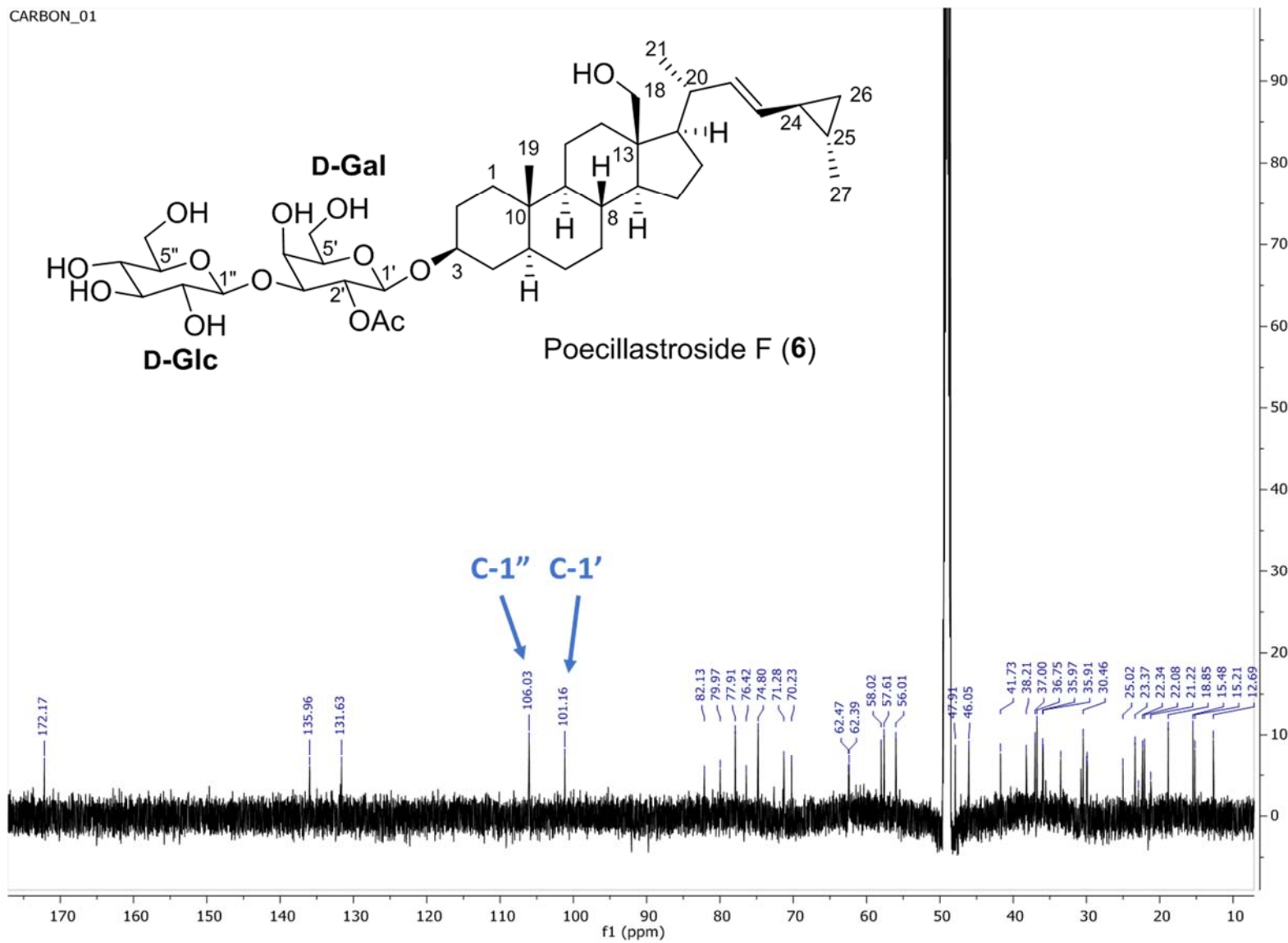


Figure S43. ^{13}C NMR spectrum of **6** at 150 MHz in CD_3OD

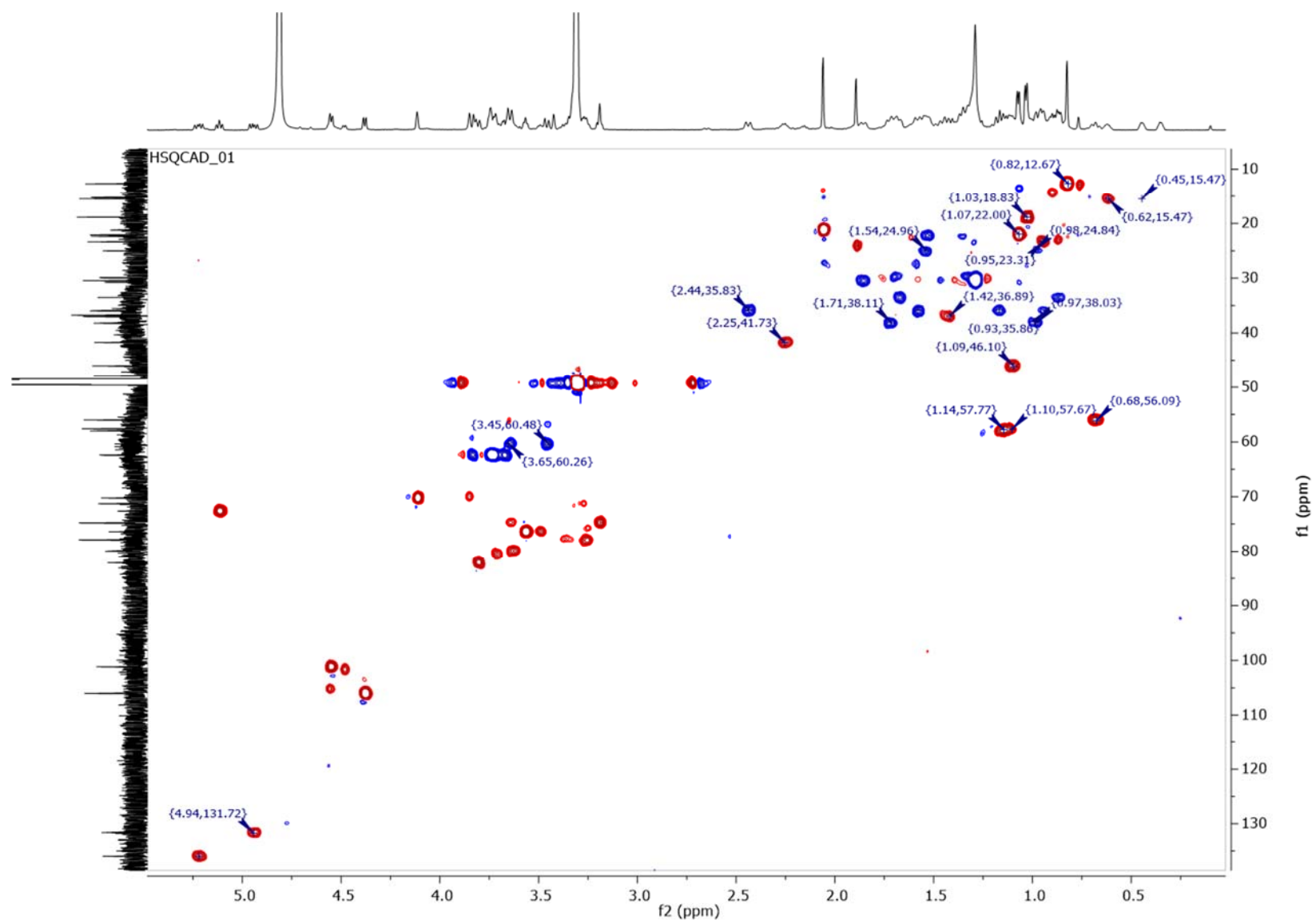


Figure S44. HSQC NMR spectrum of 6 at 600 MHz in CD₃OD

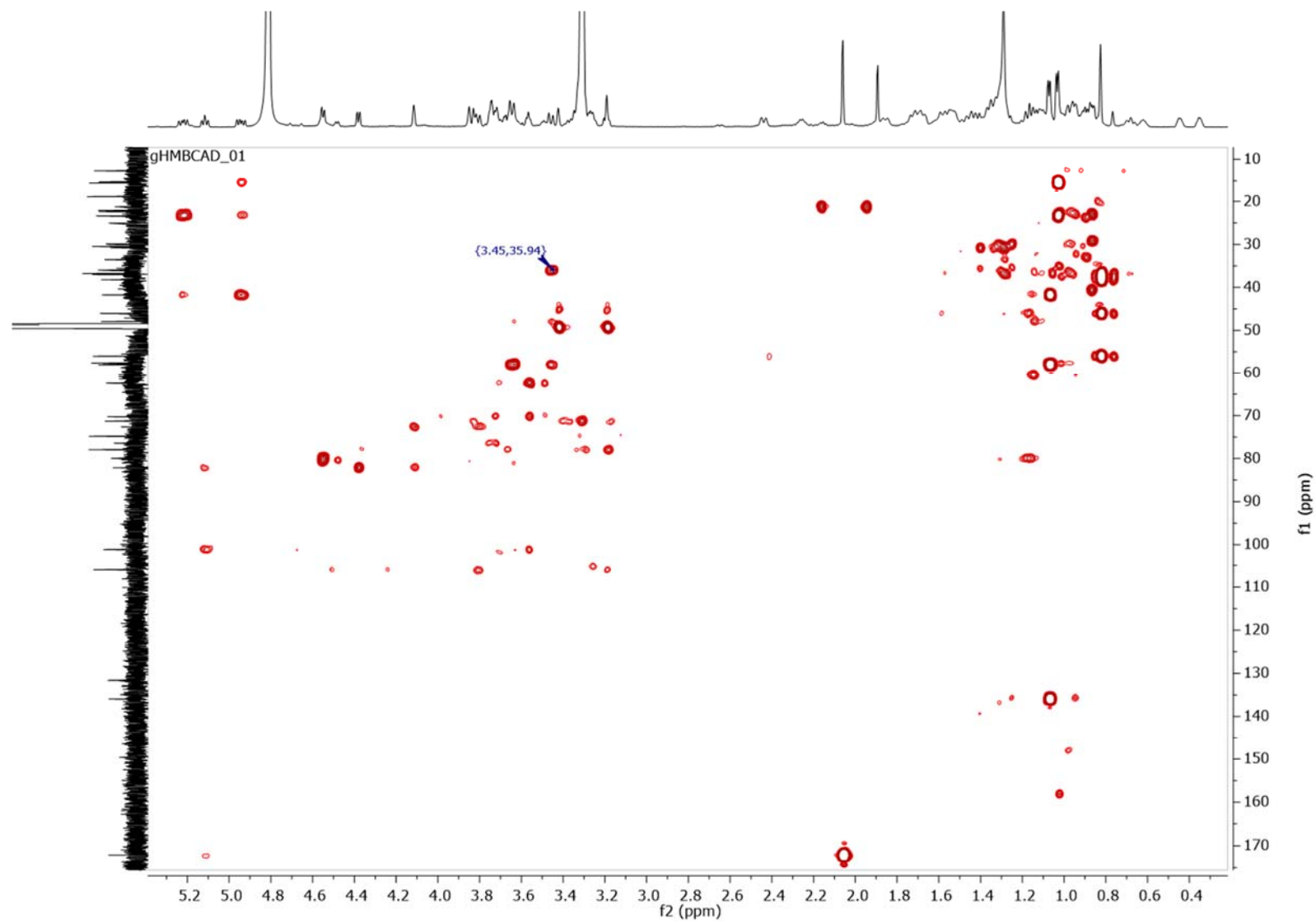


Figure S45. HMBC spectrum of 6 at 600 MHz in CD₃OD

Compound Formula	Name	RT	Algorithm
C ₄₃ H ₆₈ O ₁₄	Poecillastroside G	7.384	Spectrum Extraction

MS Spectrum

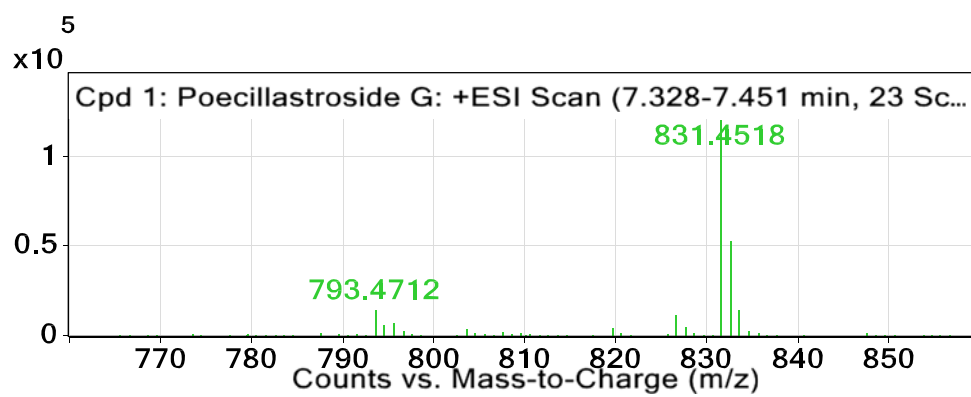


Figure S46. (+)-HRESIMS analysis of 7.

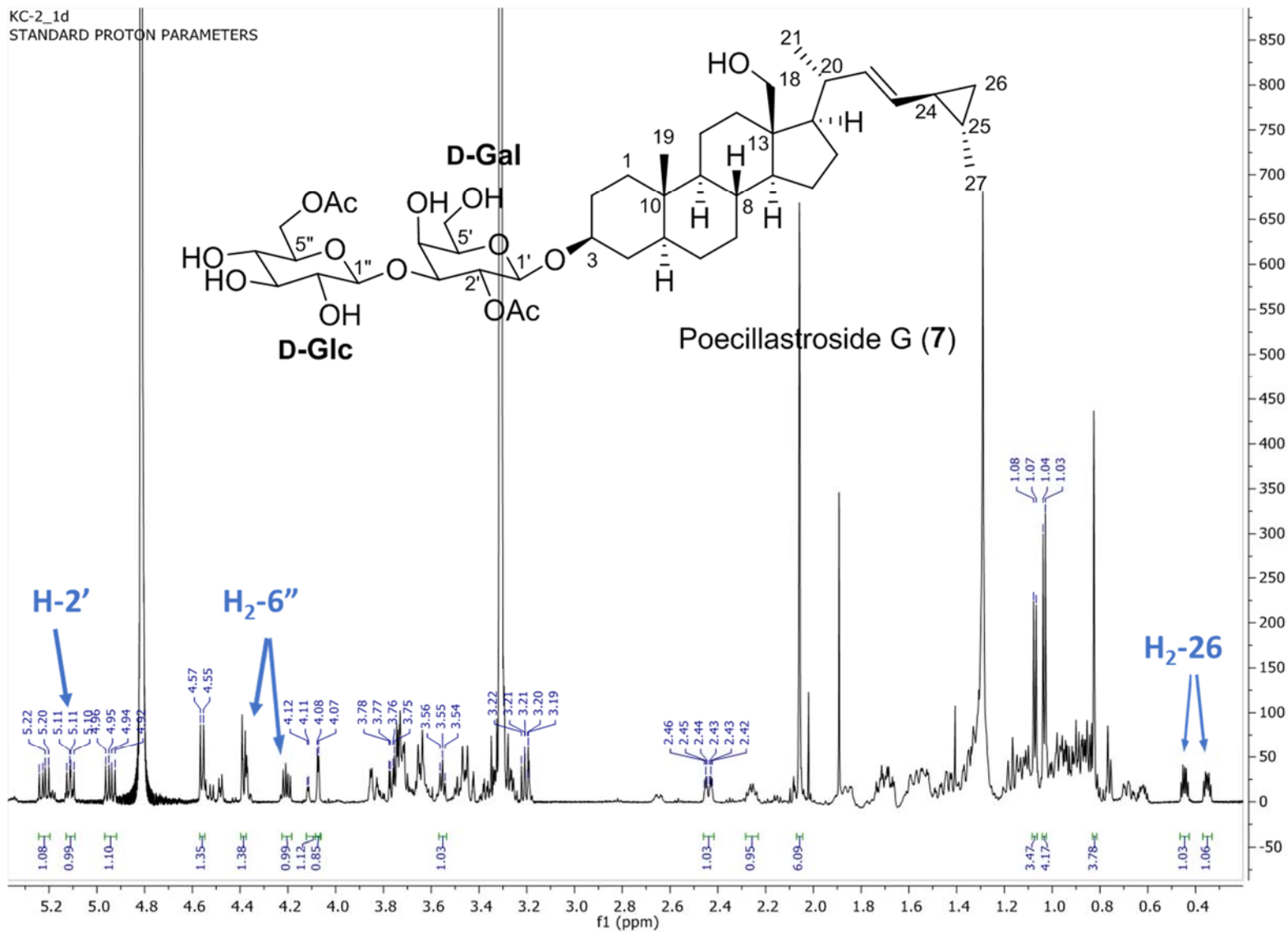


Figure S47. ¹H NMR spectrum of 7 at 600 MHz in CD₃OD

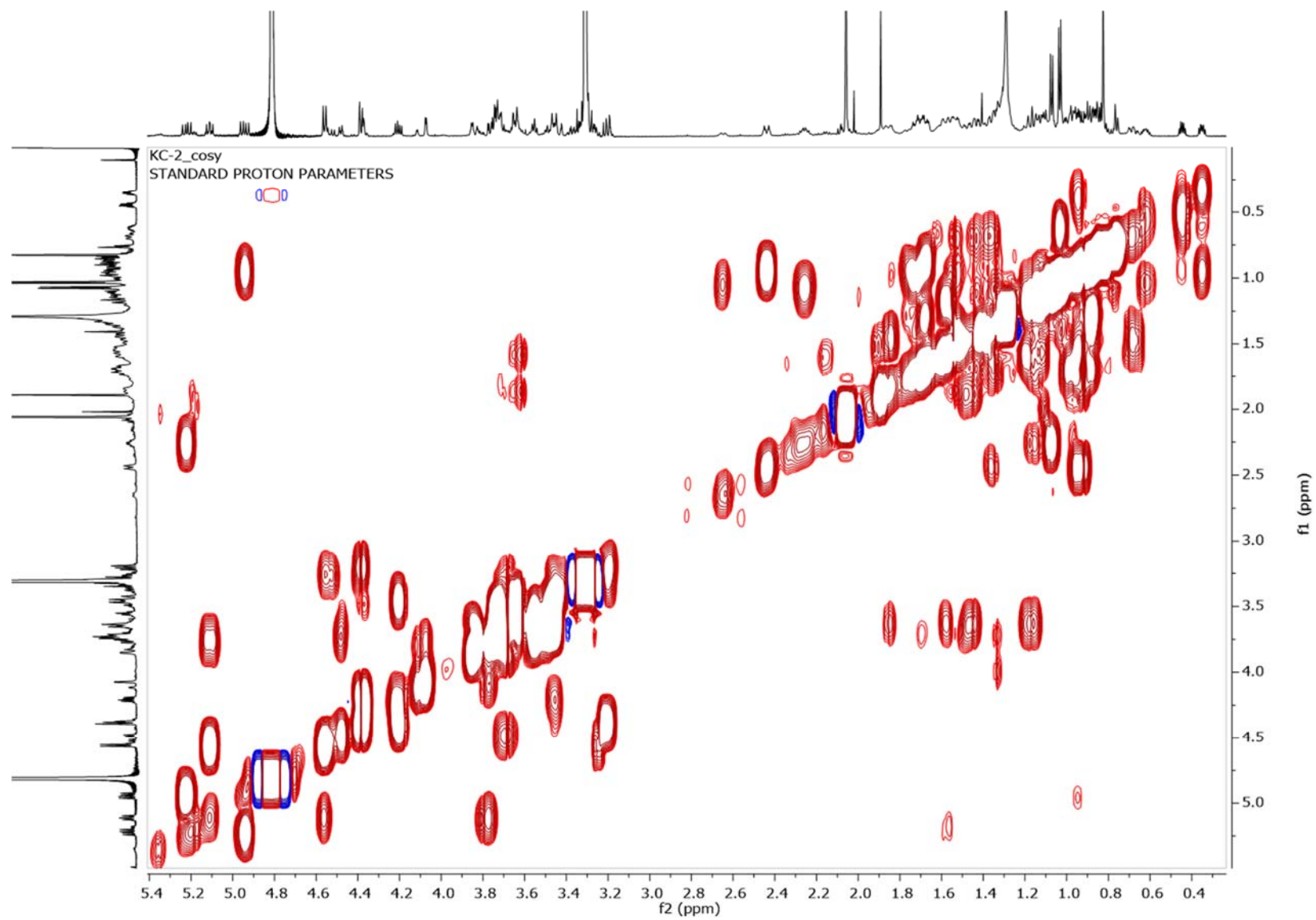


Figure S48. COSY NMR spectrum of 7 at 600 MHz in CD₃OD

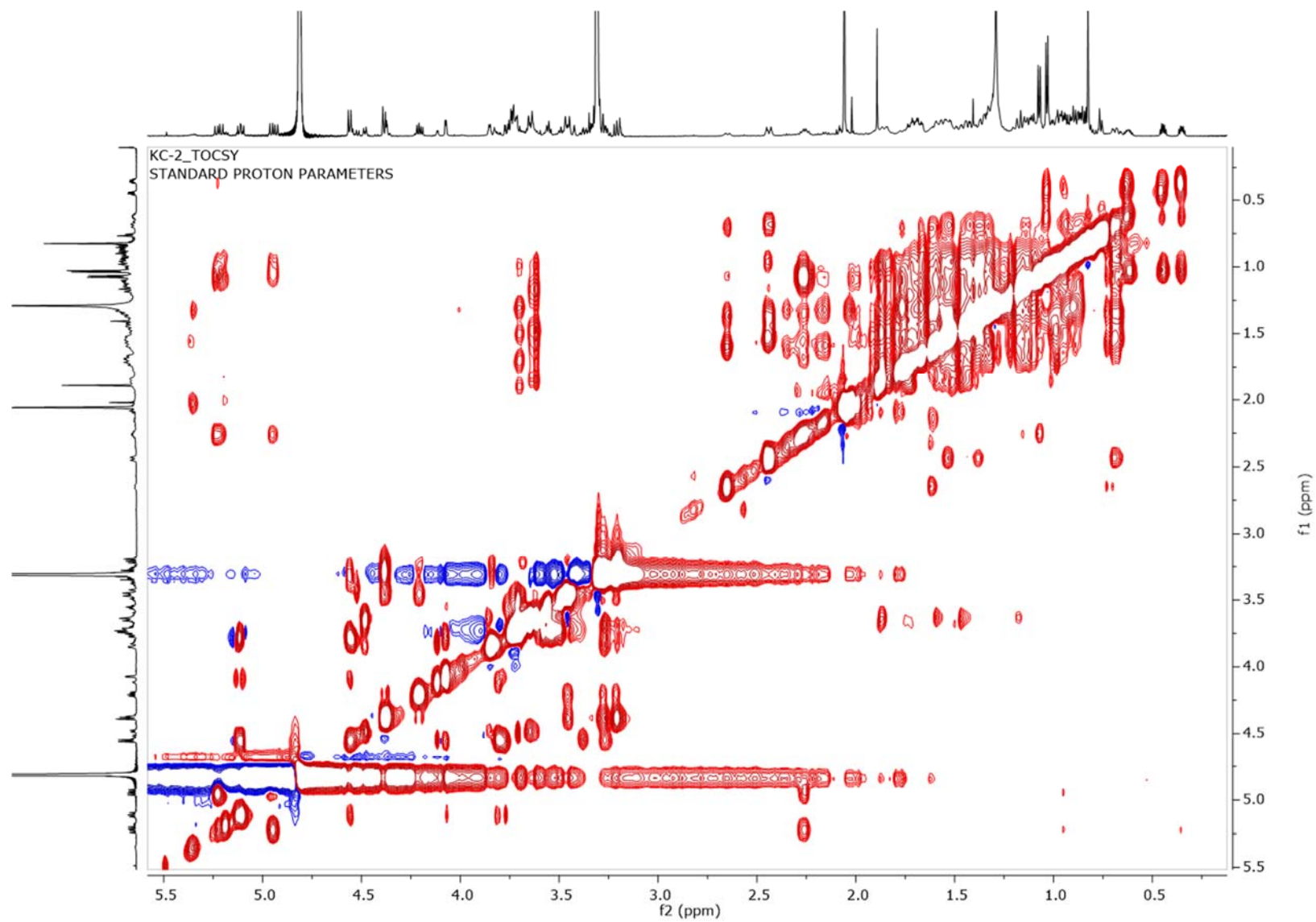


Figure S49. TOCSY NMR spectrum of 7 at 600 MHz in CD₃OD

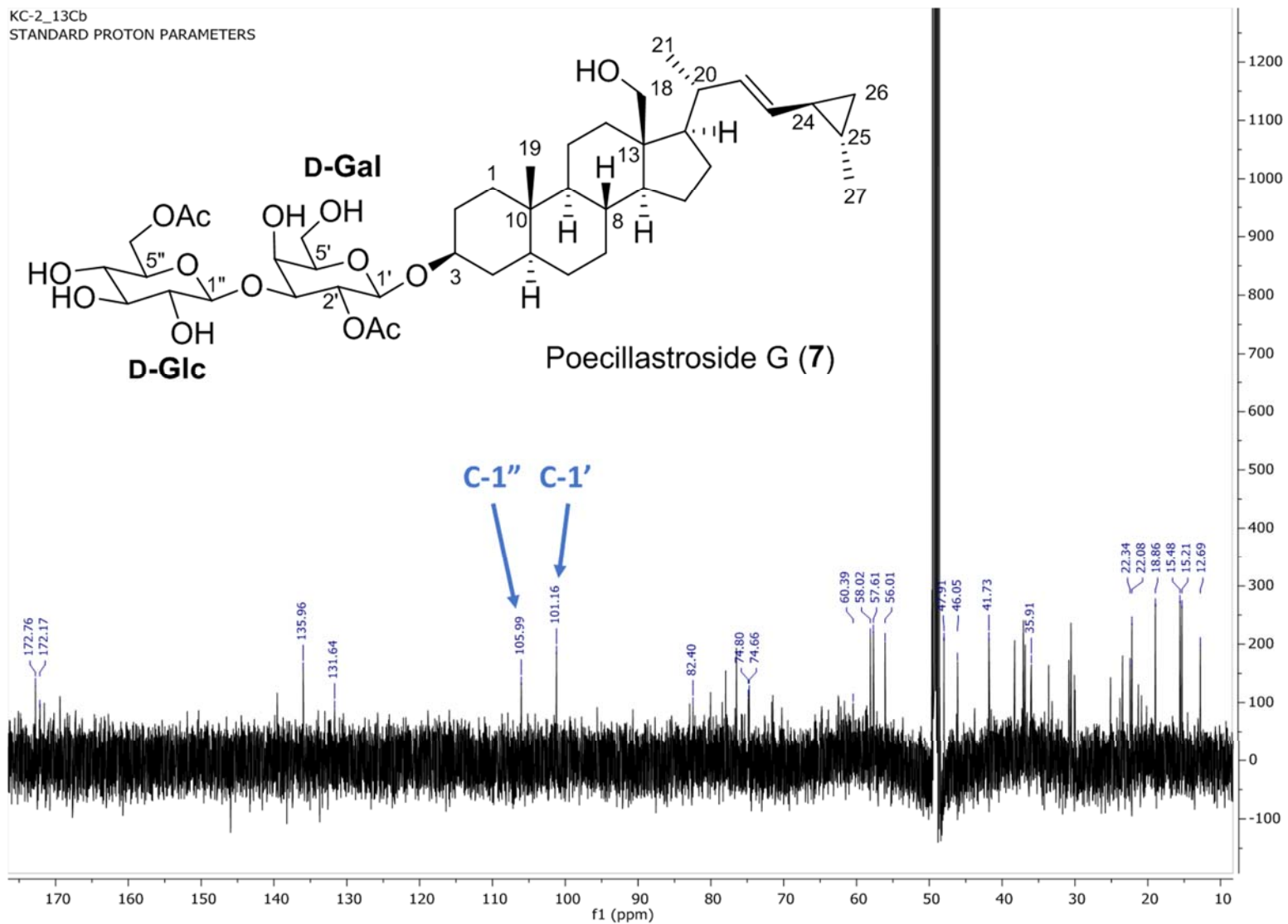


Figure S50. ¹³C NMR spectrum of 7 at 150 MHz in CD₃OD

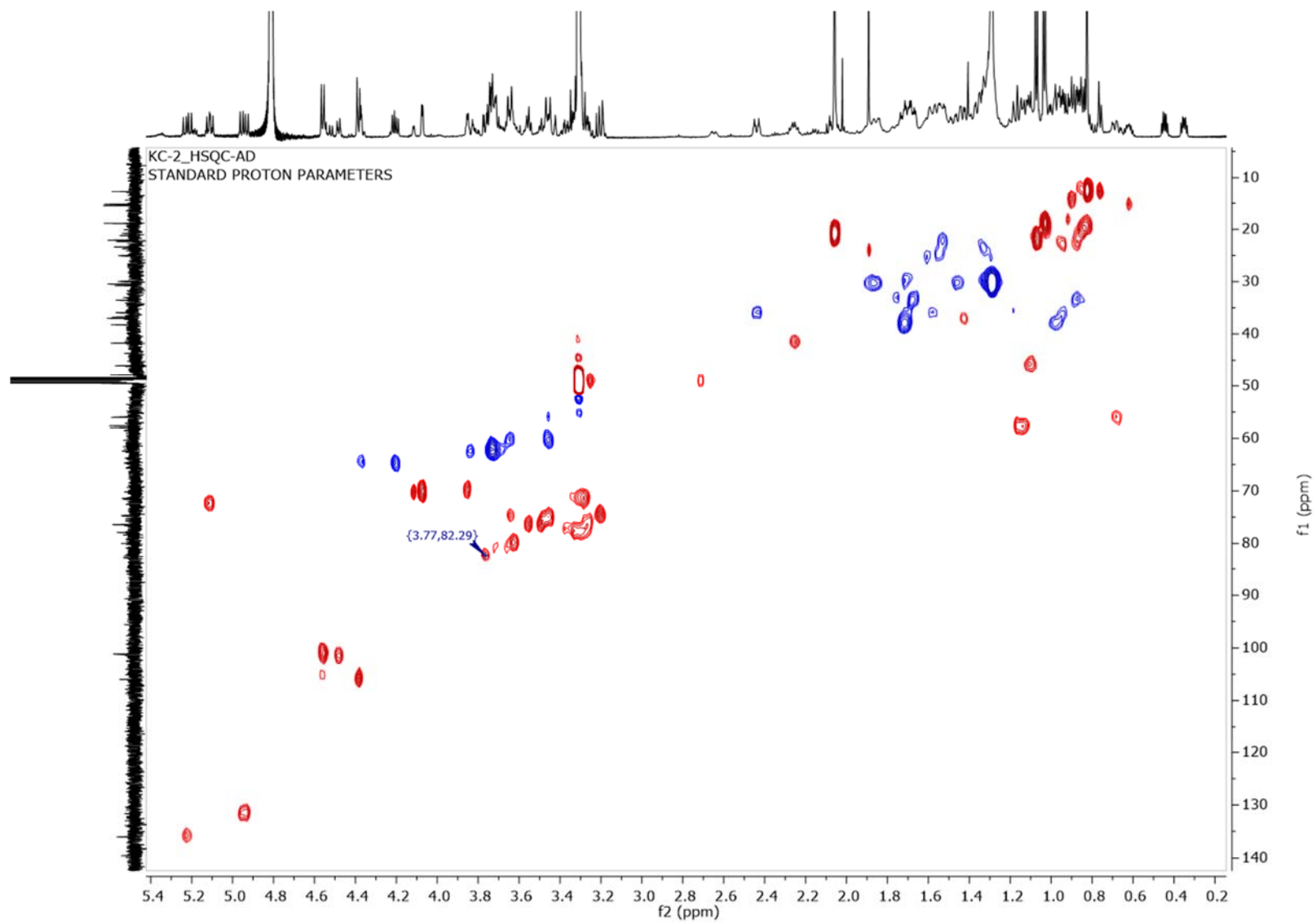


Figure S51. HSQC NMR spectrum of **7** at 600 MHz in CD₃OD

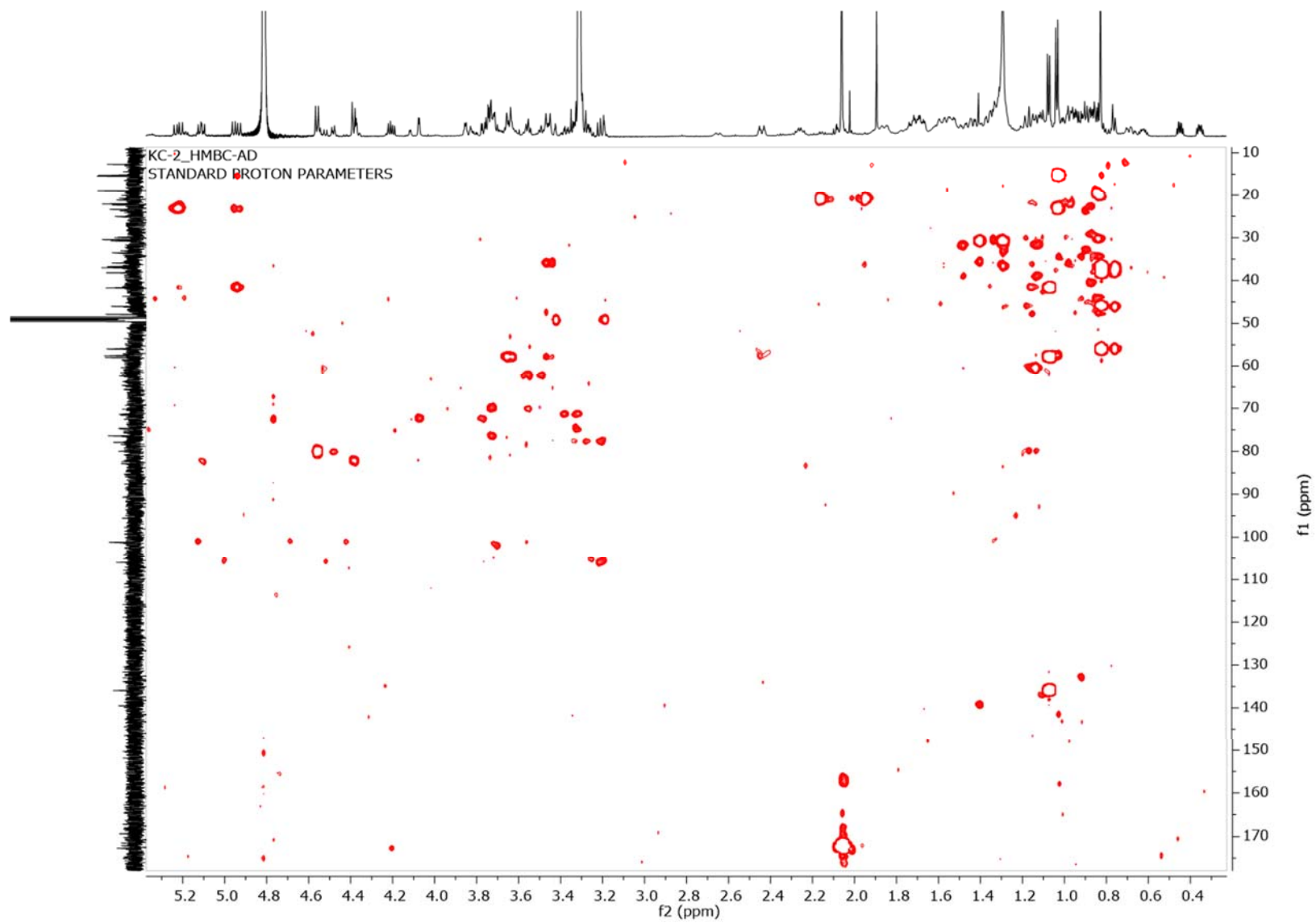


Figure S52. HMBC spectrum of 7 at 600 MHz in CD₃OD

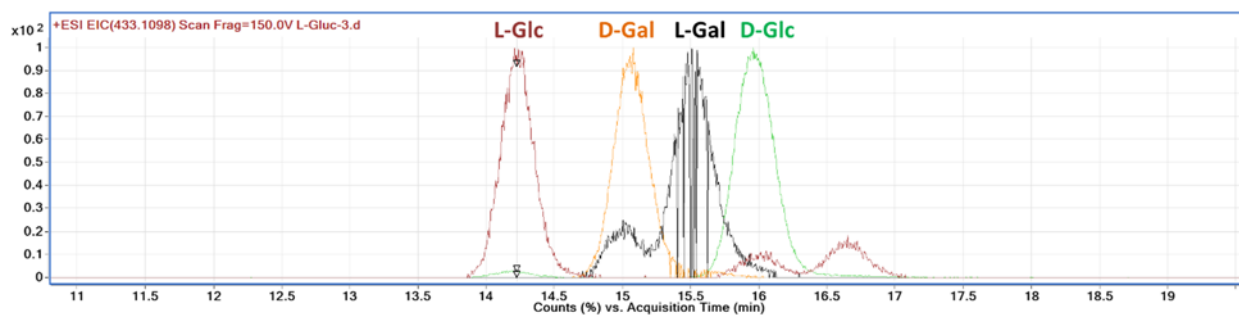


Figure S53. UPLC-qToF analysis of the four monosaccharide derivatives

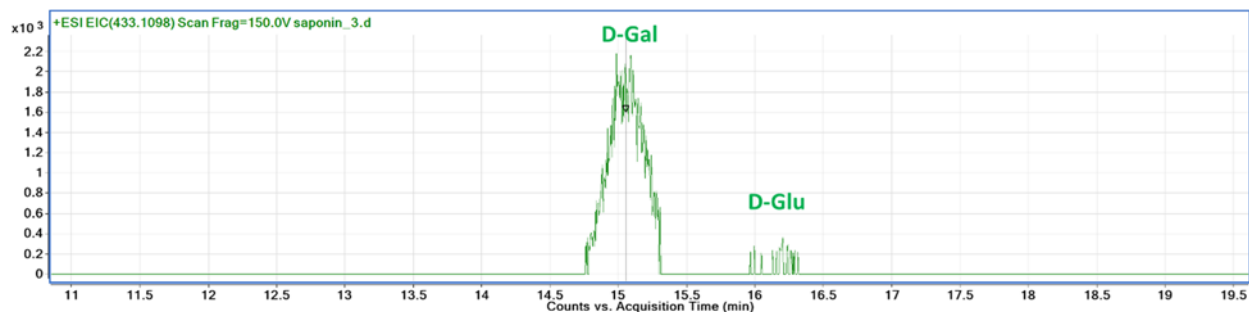


Figure S54. Absolute configuration of the pyranose moieties of 3

$\times 10^5$

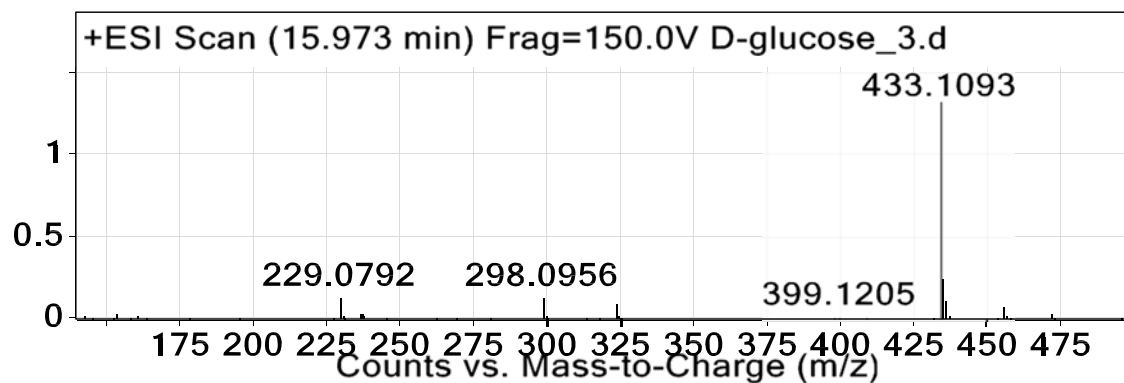


Figure S55. ESI-(+) mass spectrum of D-(+)-glucose derivative