

Supplementary Materials

for

Ruthenafuran Complexes Supported by the Bipyridine-Bis(diphenylphosphino)methane Ligand Set: Synthesis and Cytotoxicity Studies

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Table of Contents	
	Page
NMR spectra of complex 1	S3–S11
NMR spectra of complex 2	S12–S20
NMR spectra of complex [3] (OTf) ₂	S21–S26
NMR spectra of complex [4] (OTf)	S27–S35
NMR spectra of complex [5] (OTf)	S36–S44
NMR spectra of complex [6] (OTf)	S45–S53
NMR spectra of complex [7] (OTf)	S54–S62
NMR spectra of complex [8] (OTf)	S63–S71
Experimental and simulated mass spectra of [1–Cl] ⁺	S72–S73
Experimental and simulated mass spectra of [2–Cl] ⁺	S74–S75
Experimental and simulated mass spectra of [3] ²⁺	S76–S77
Experimental and simulated mass spectra of [4] ⁺	S78–S79
Experimental and simulated mass spectra of [5] ⁺	S80–S81
Experimental and simulated mass spectra of [6] ⁺	S82–S83
Experimental and simulated mass spectra of [7] ⁺	S84–S85
Experimental and simulated mass spectra of [8] ⁺	S86–S87

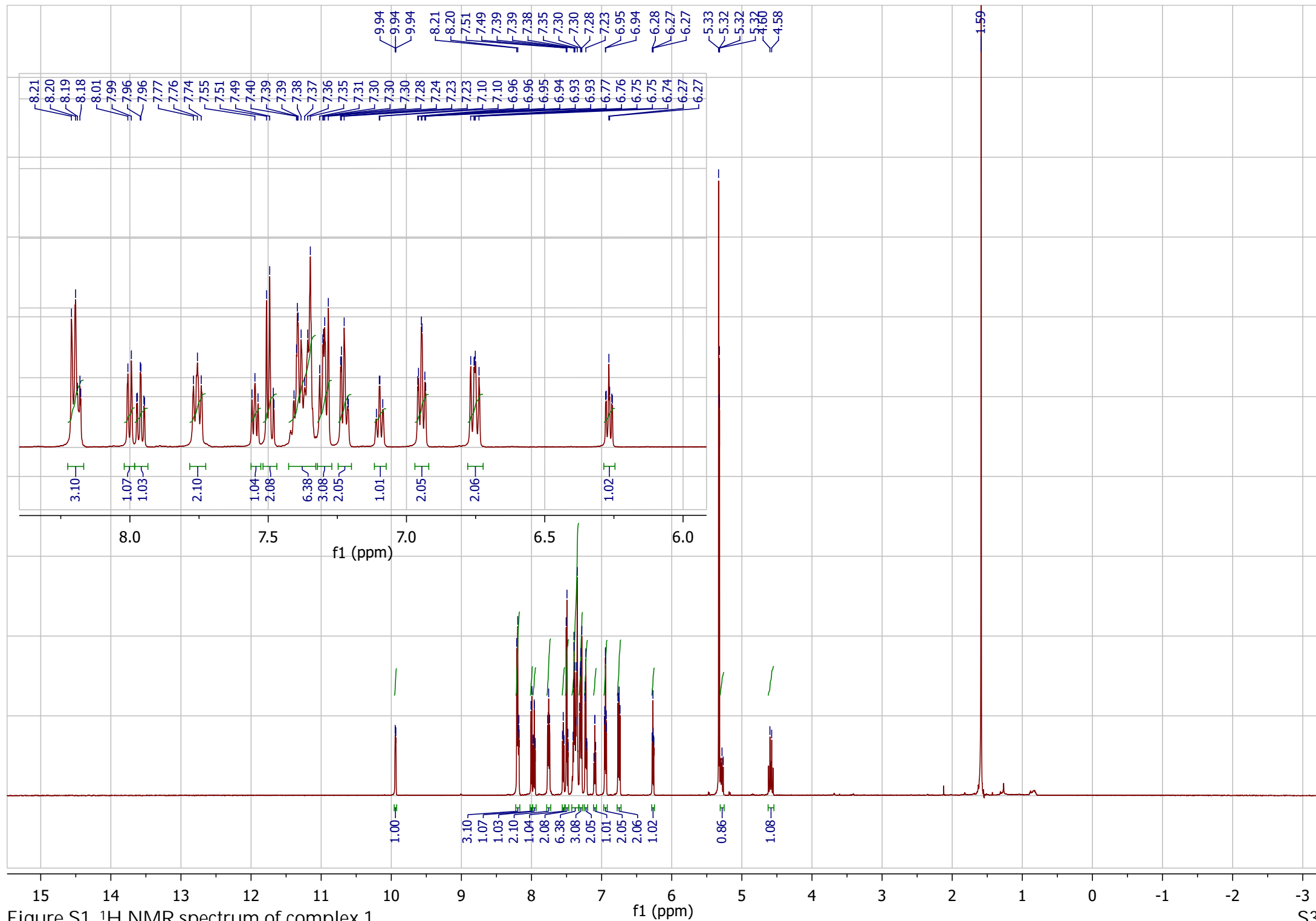


Figure S1. ^1H NMR spectrum of complex 1.

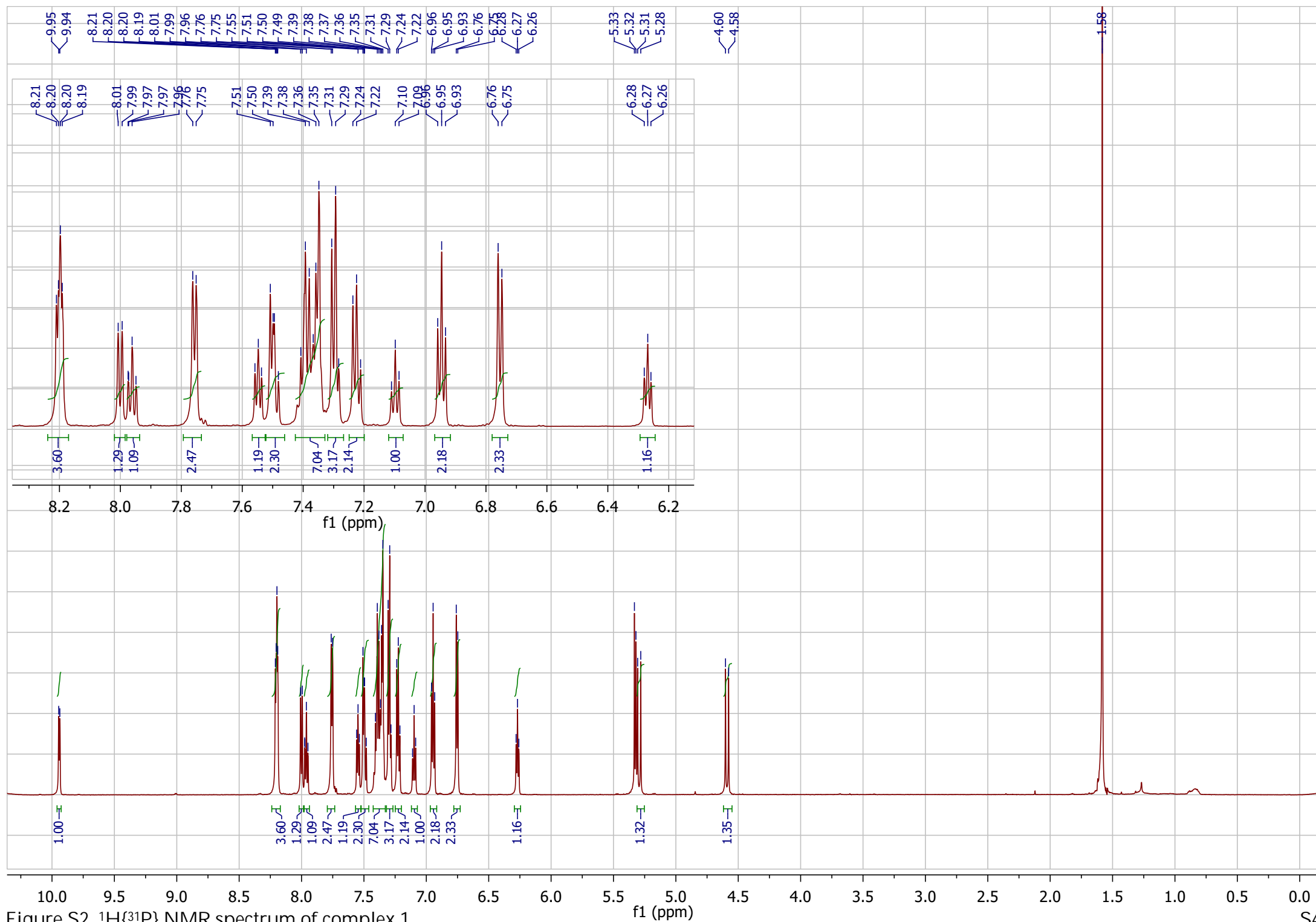
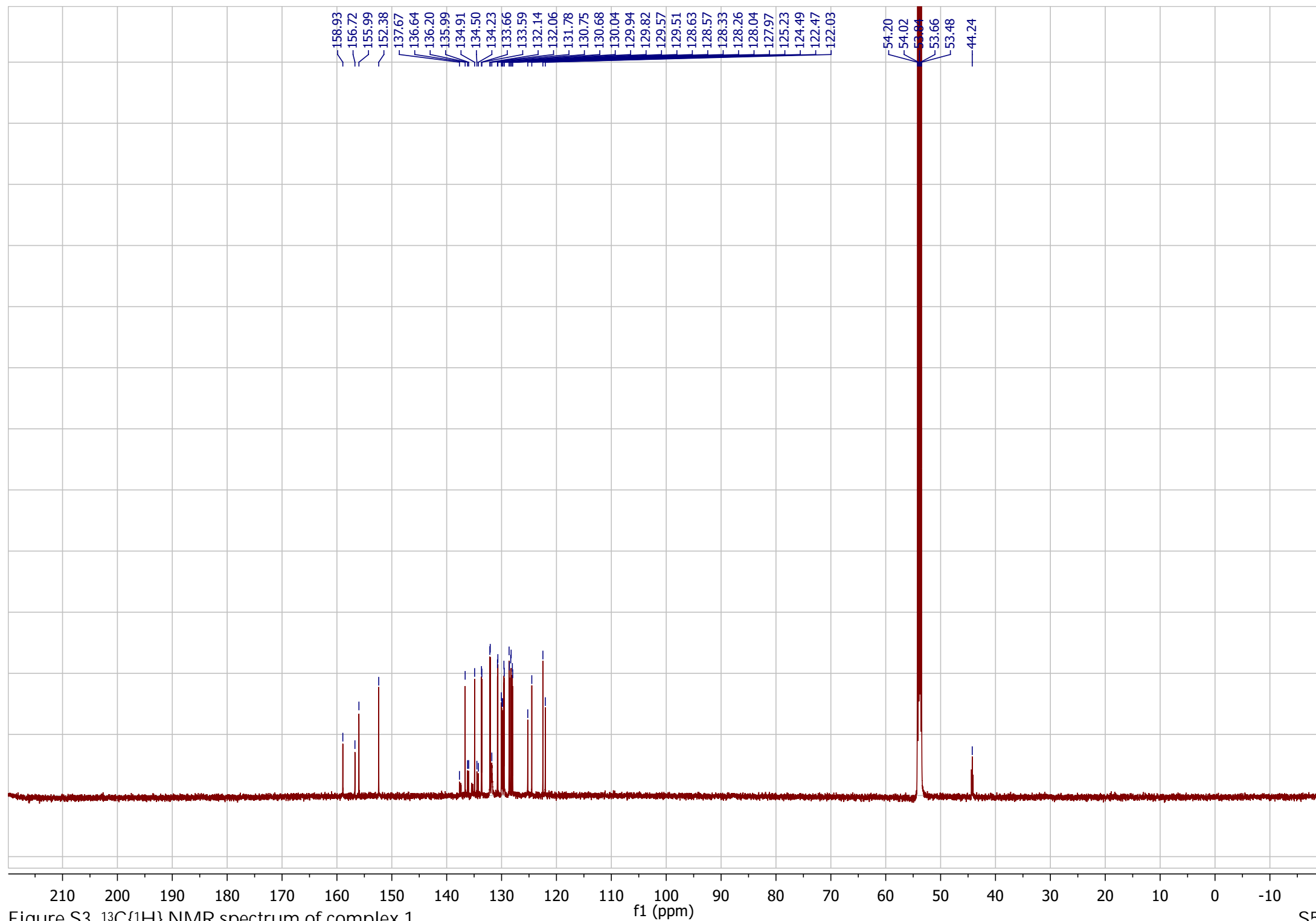


Figure S2. $^1\text{H}\{^{31}\text{P}\}$ NMR spectrum of complex 1.



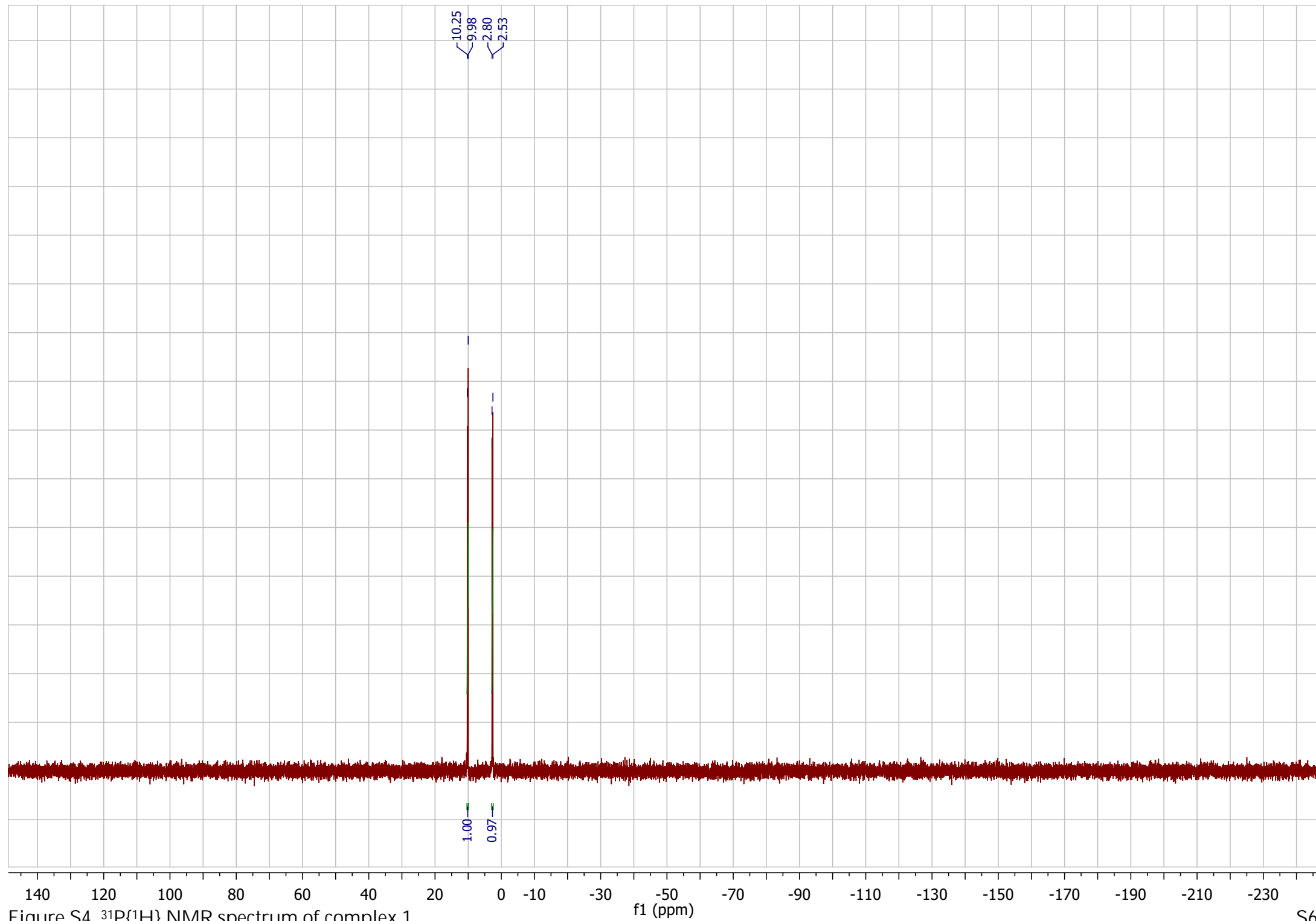


Figure S4. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of complex 1.

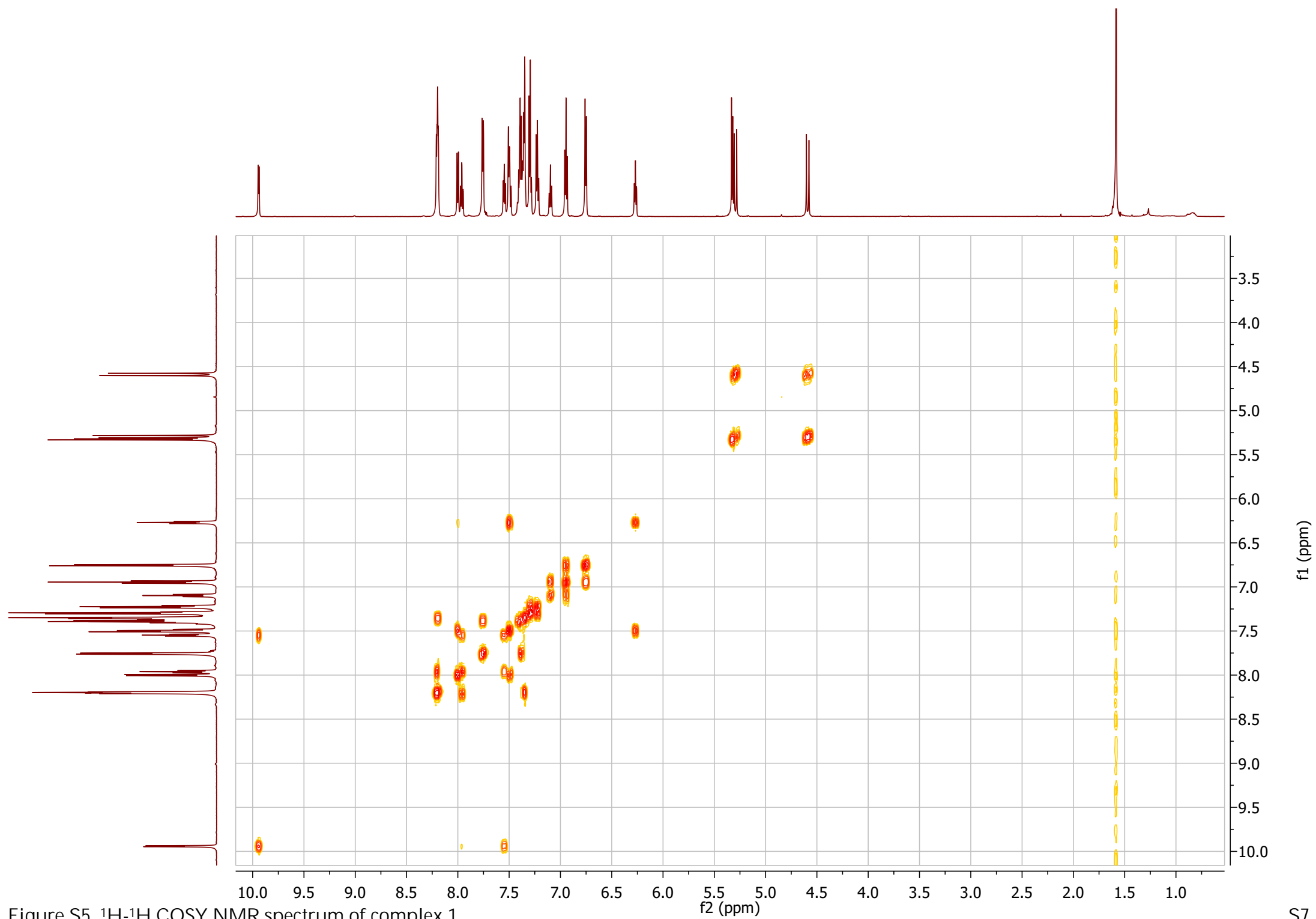


Figure S5. ${}^1\text{H}$ - ${}^1\text{H}$ COSY NMR spectrum of complex 1.

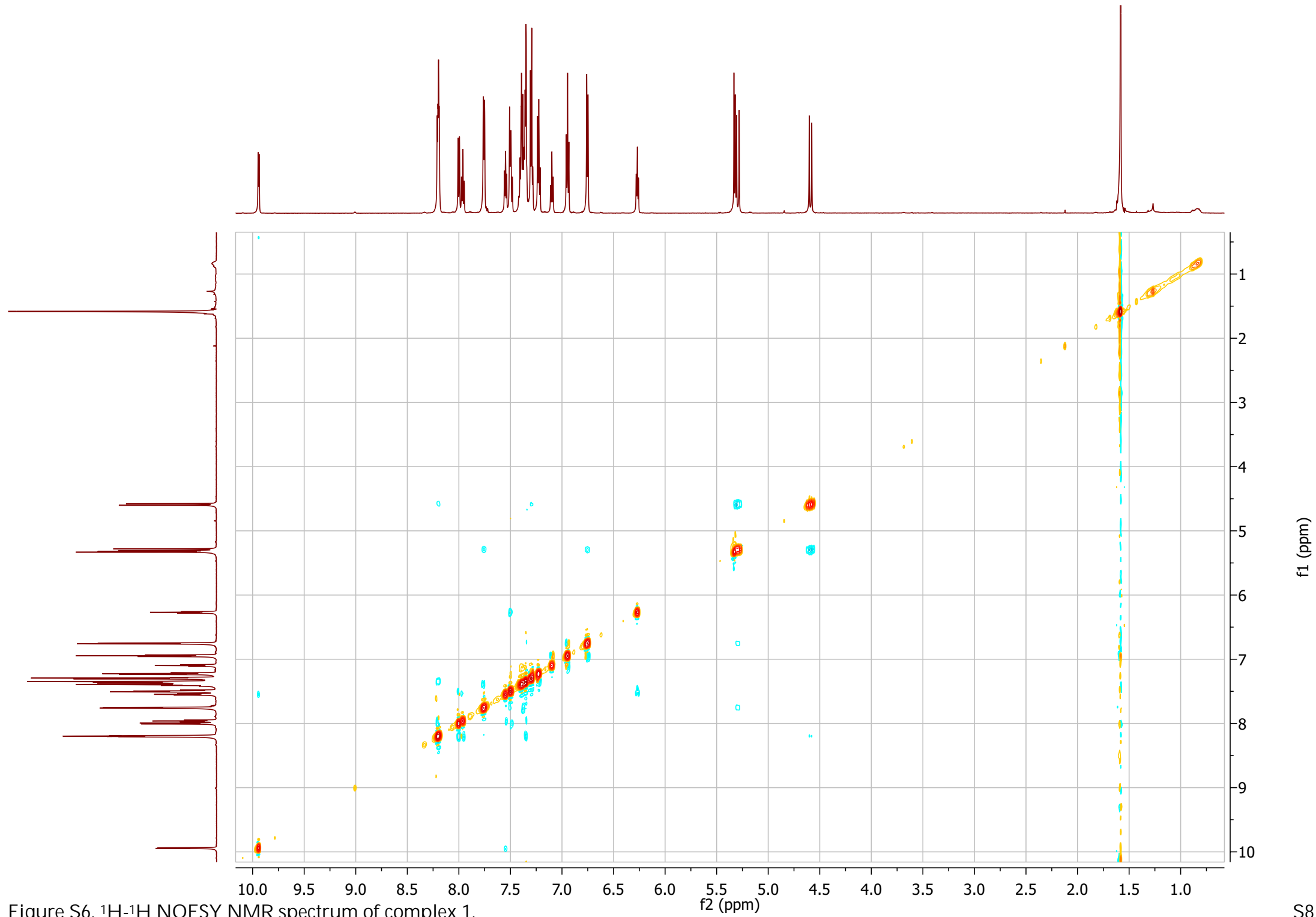


Figure S6. ^1H - ^1H NOESY NMR spectrum of complex 1.

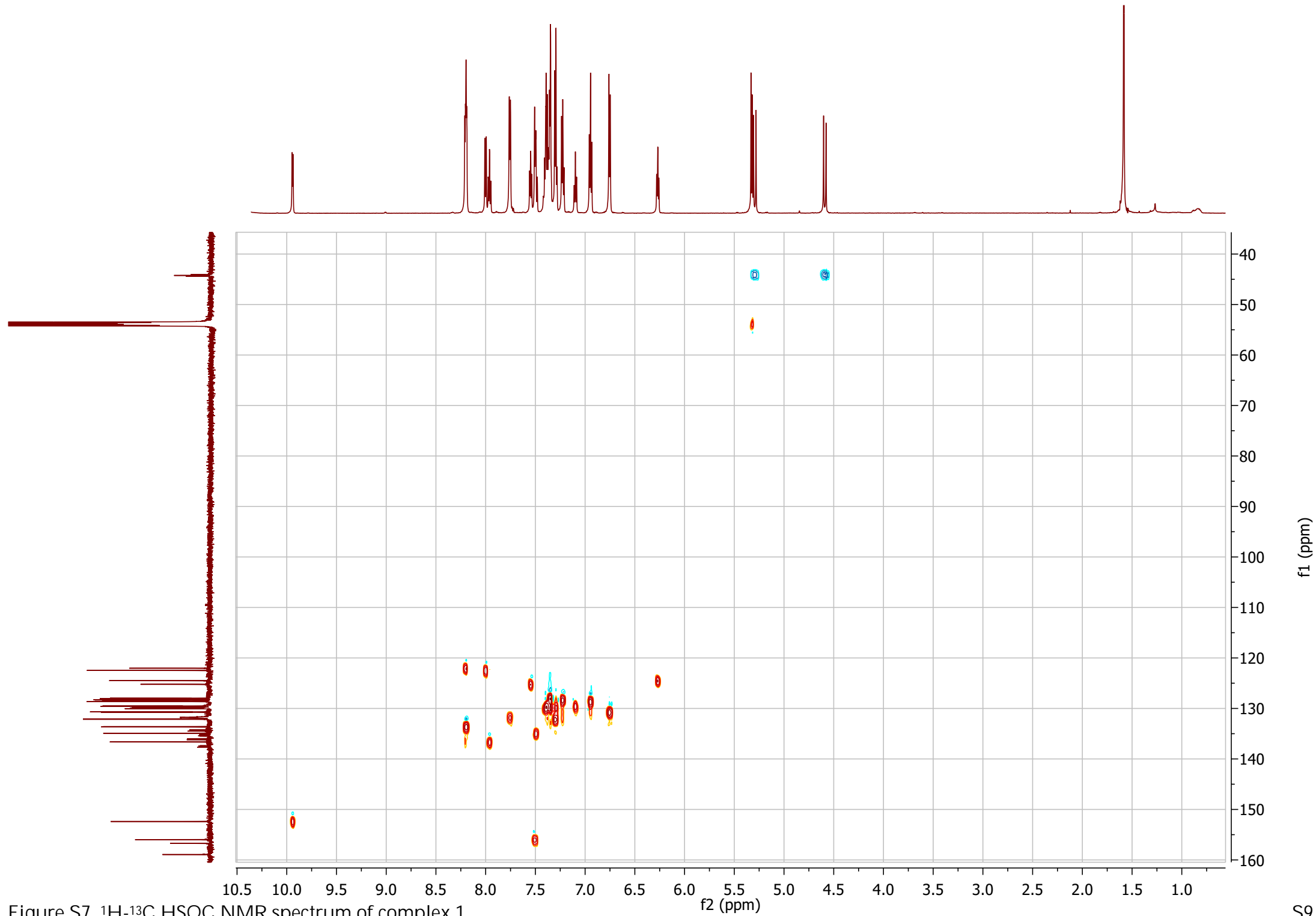
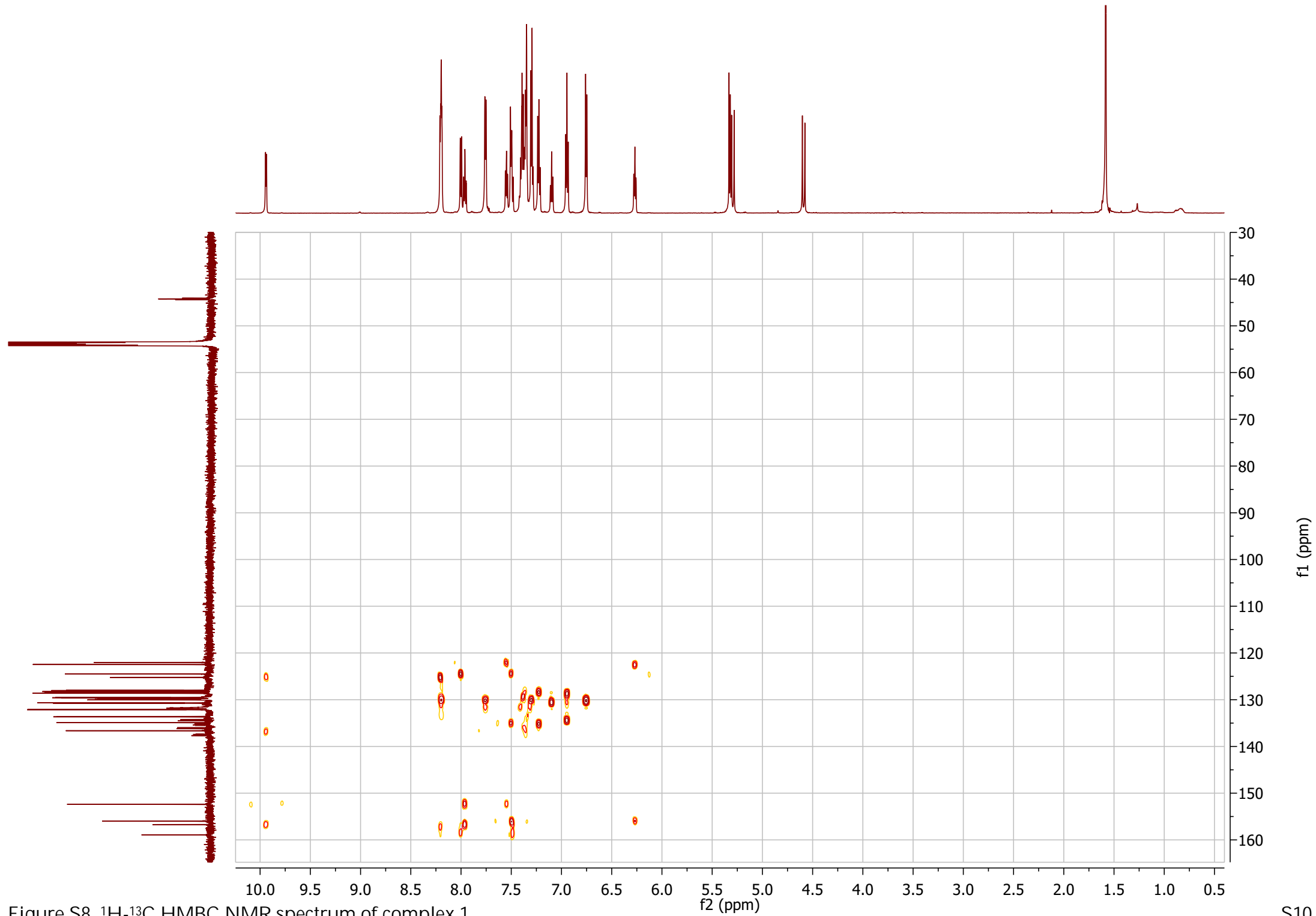


Figure S7. ^1H - ^{13}C HSQC NMR spectrum of complex 1.



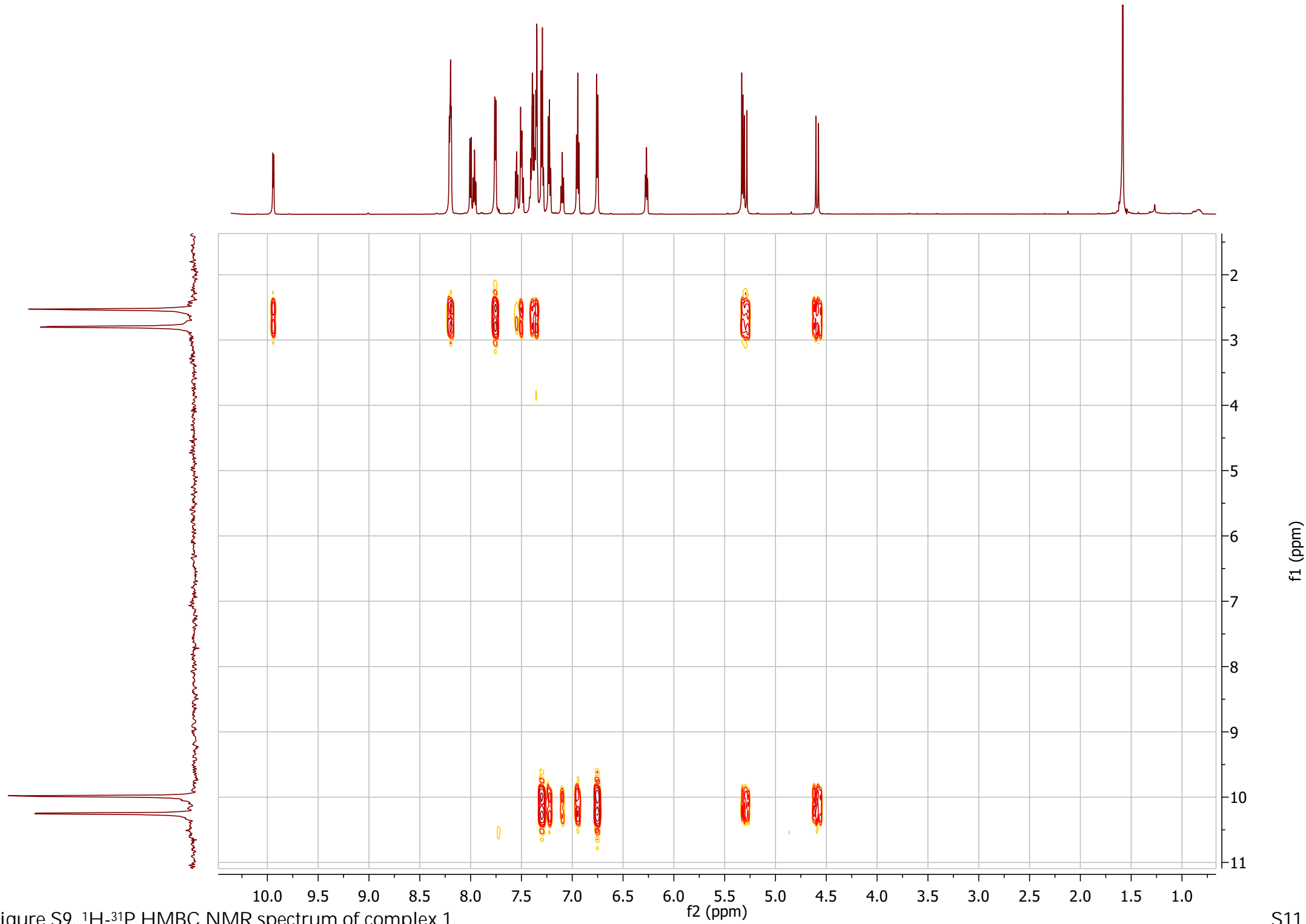
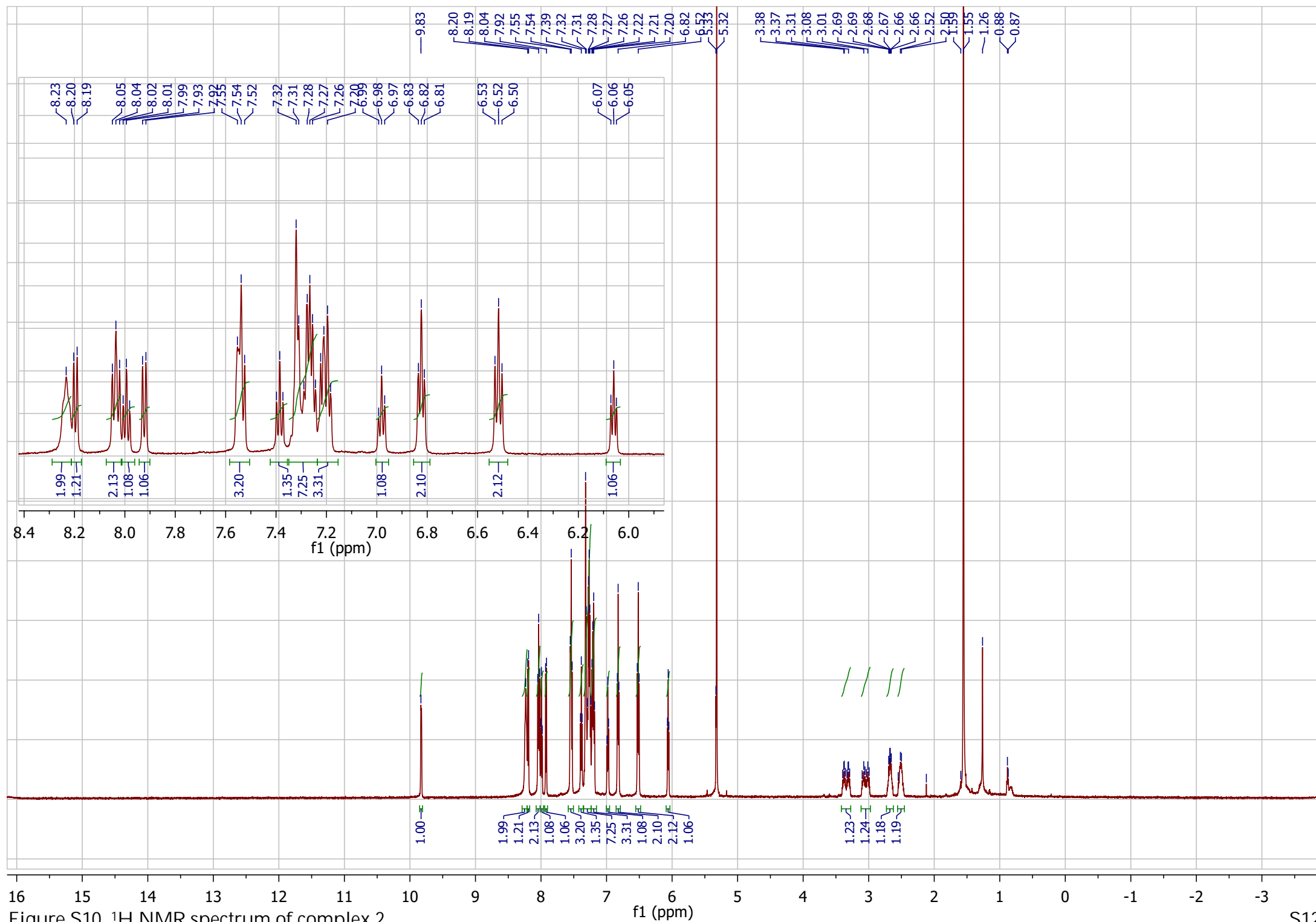


Figure S9. ^1H - ^{31}P HMBC NMR spectrum of complex 1.



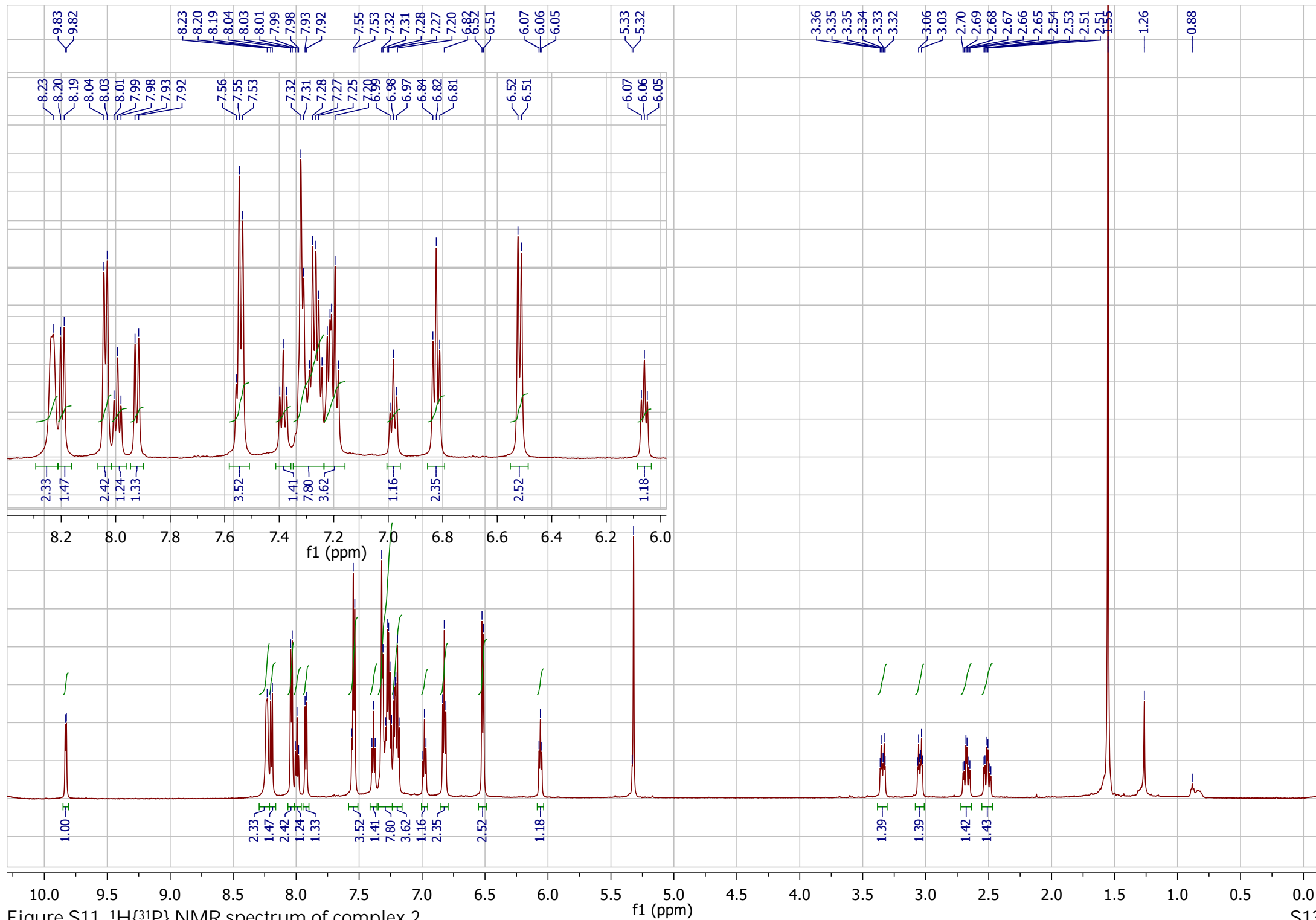


Figure S11. $^1\text{H}\{^{31}\text{P}\}$ NMR spectrum of complex 2.

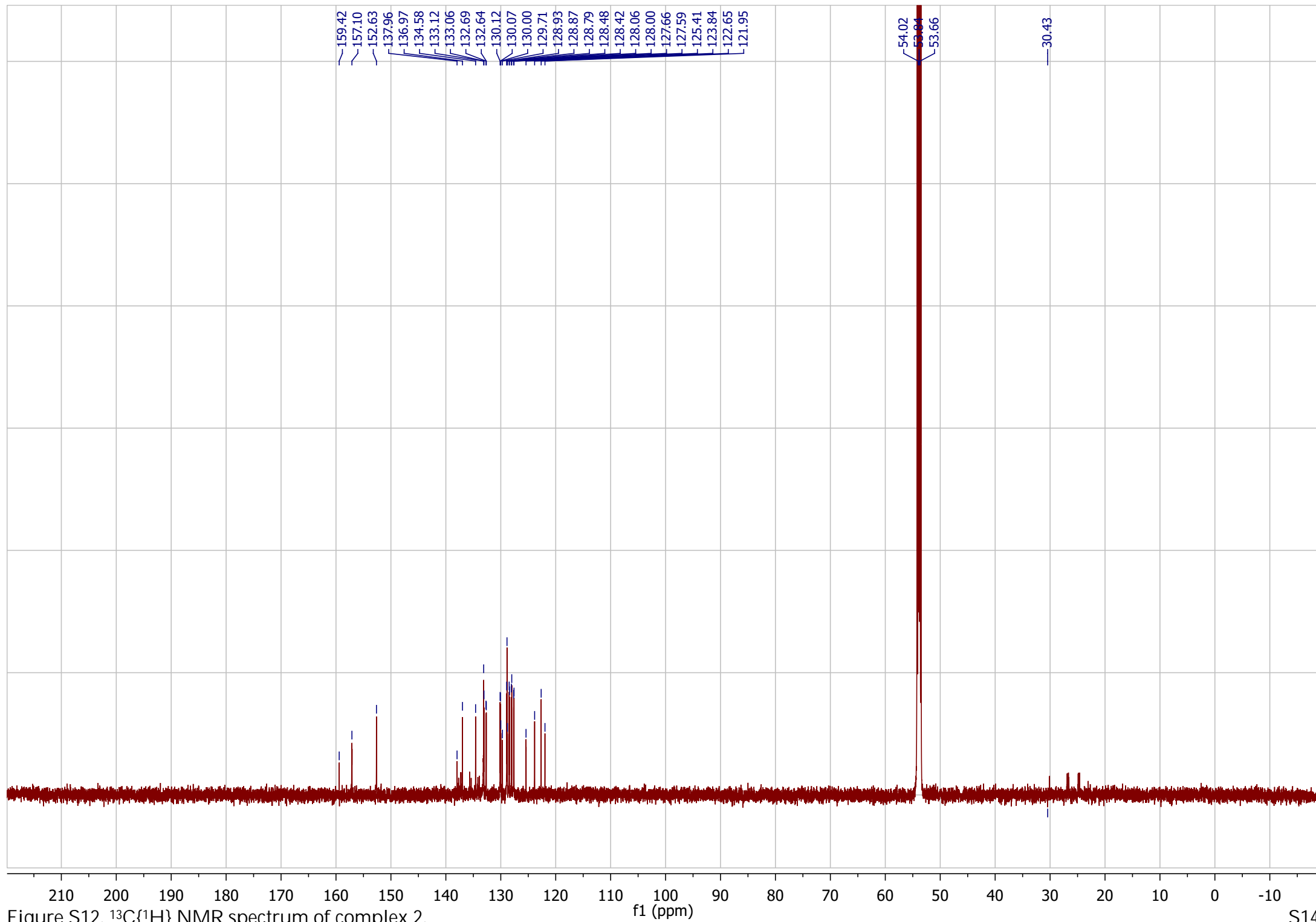


Figure S12. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of complex 2.

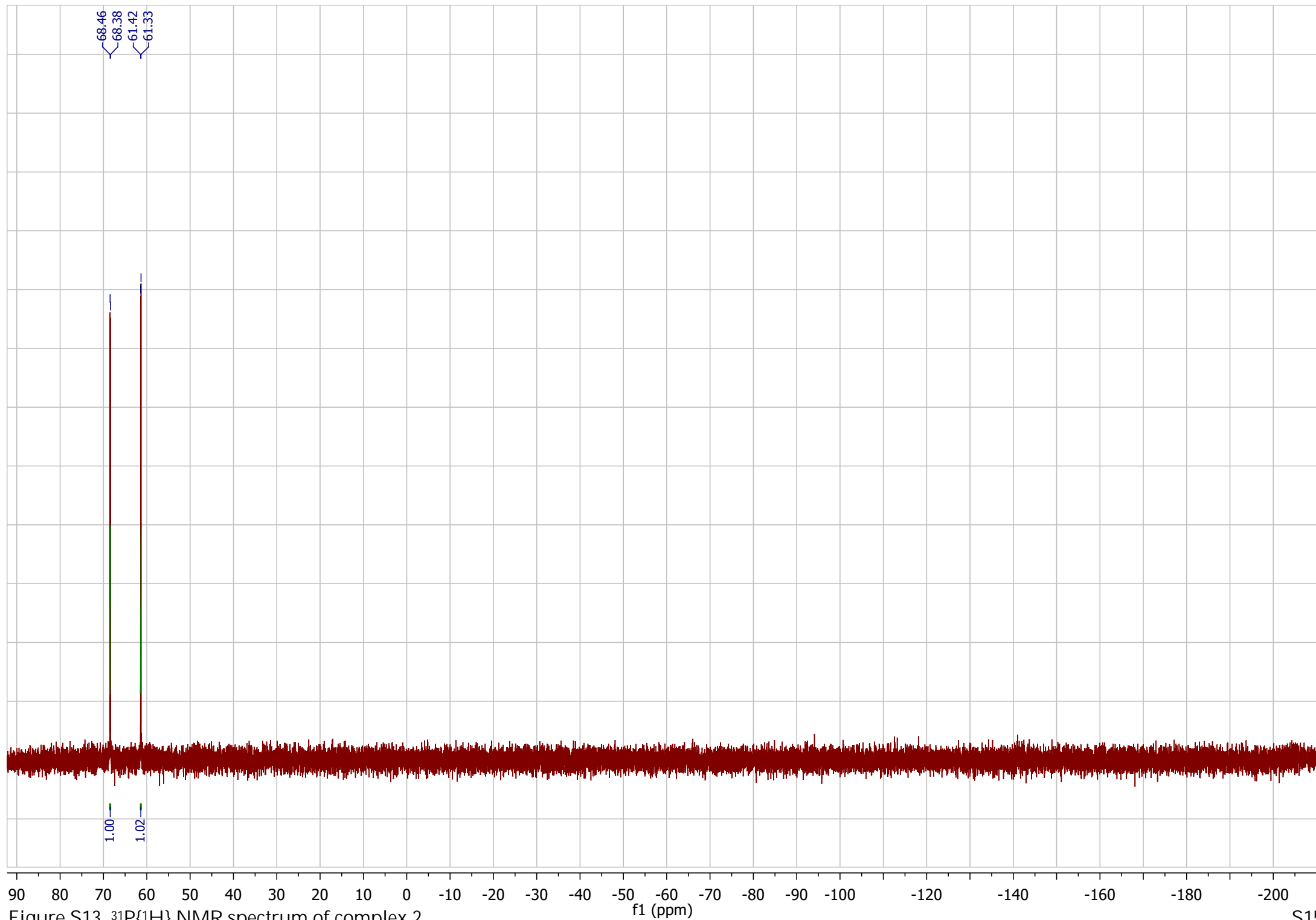
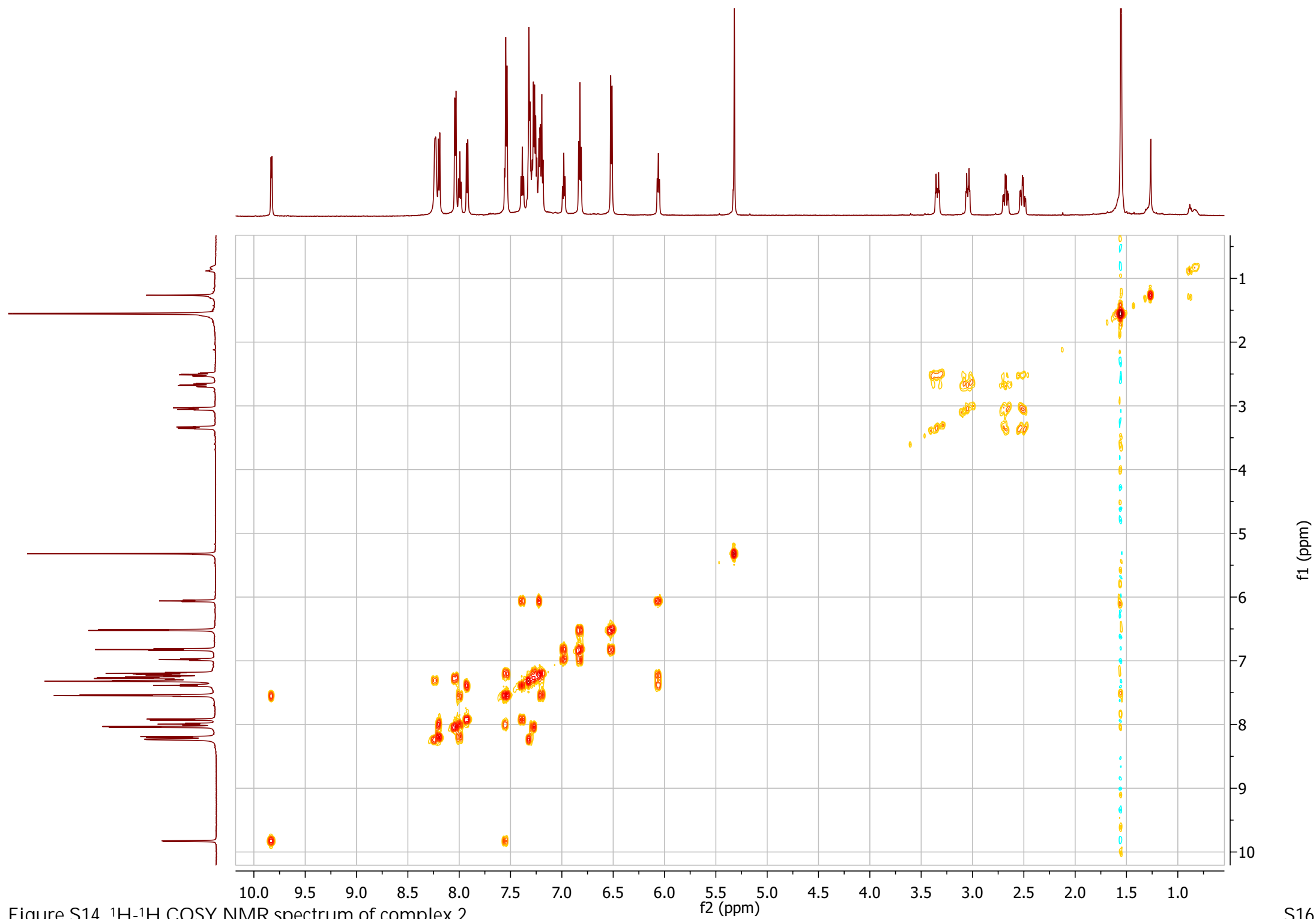
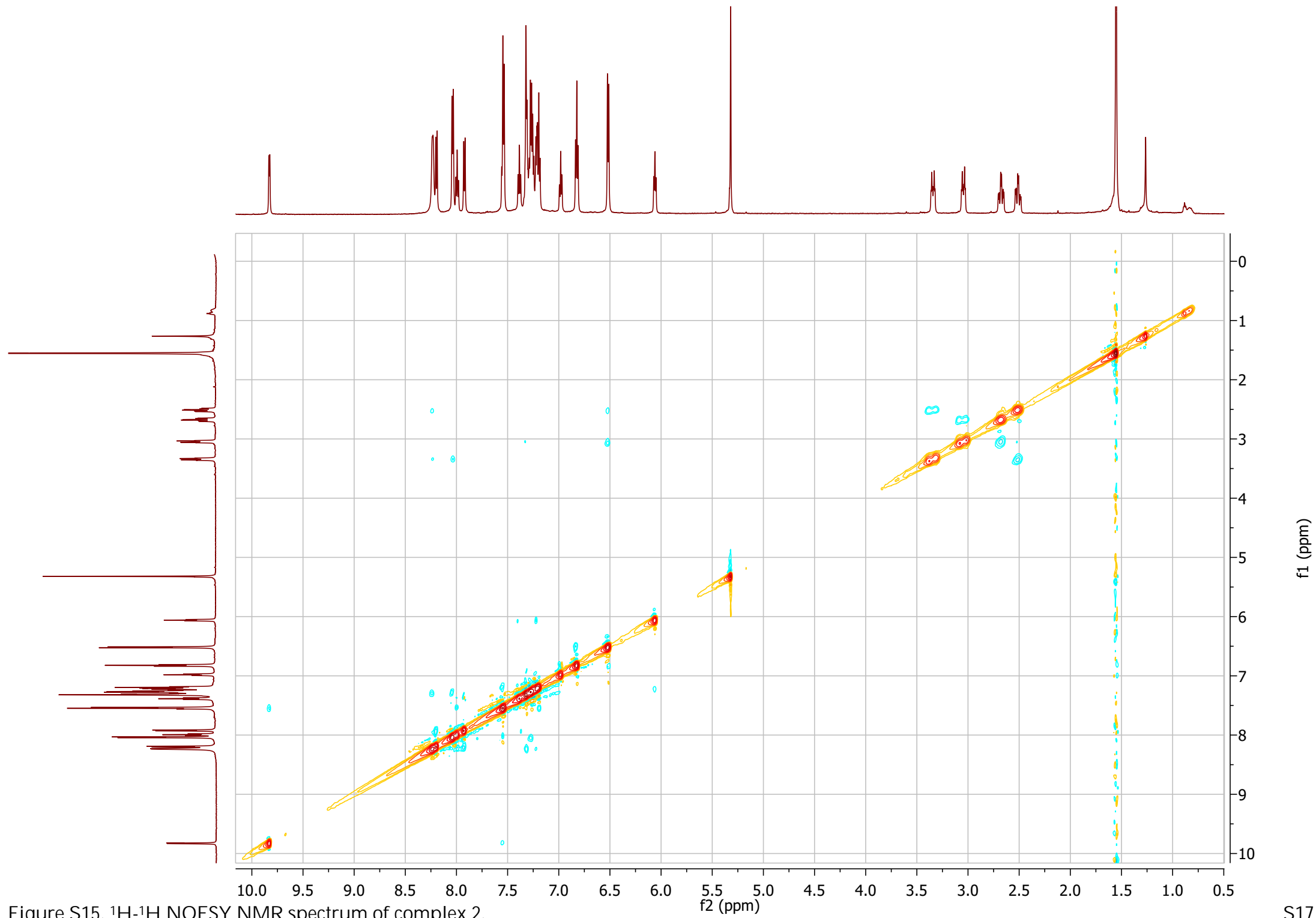


Figure S13. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of complex 2.





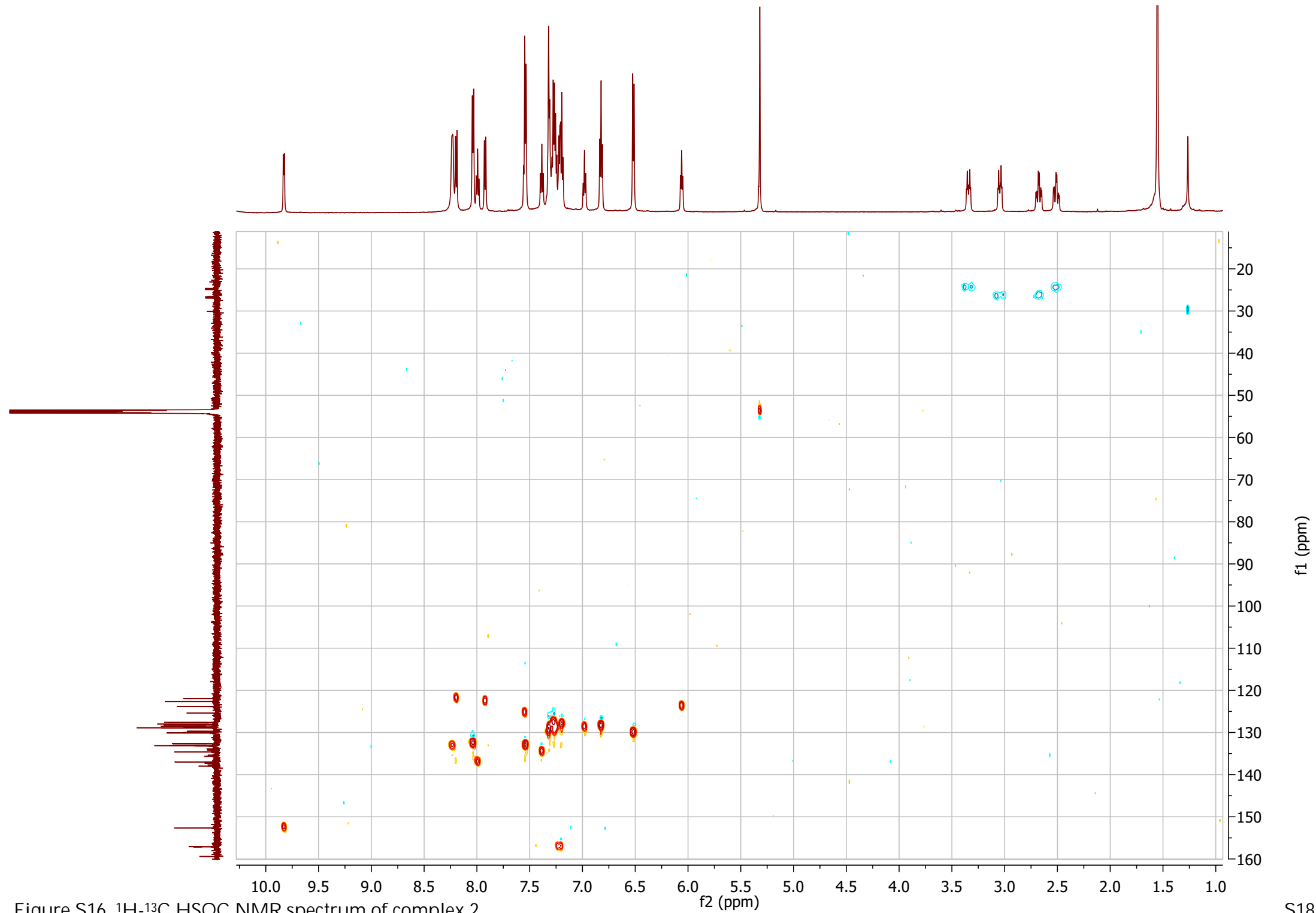
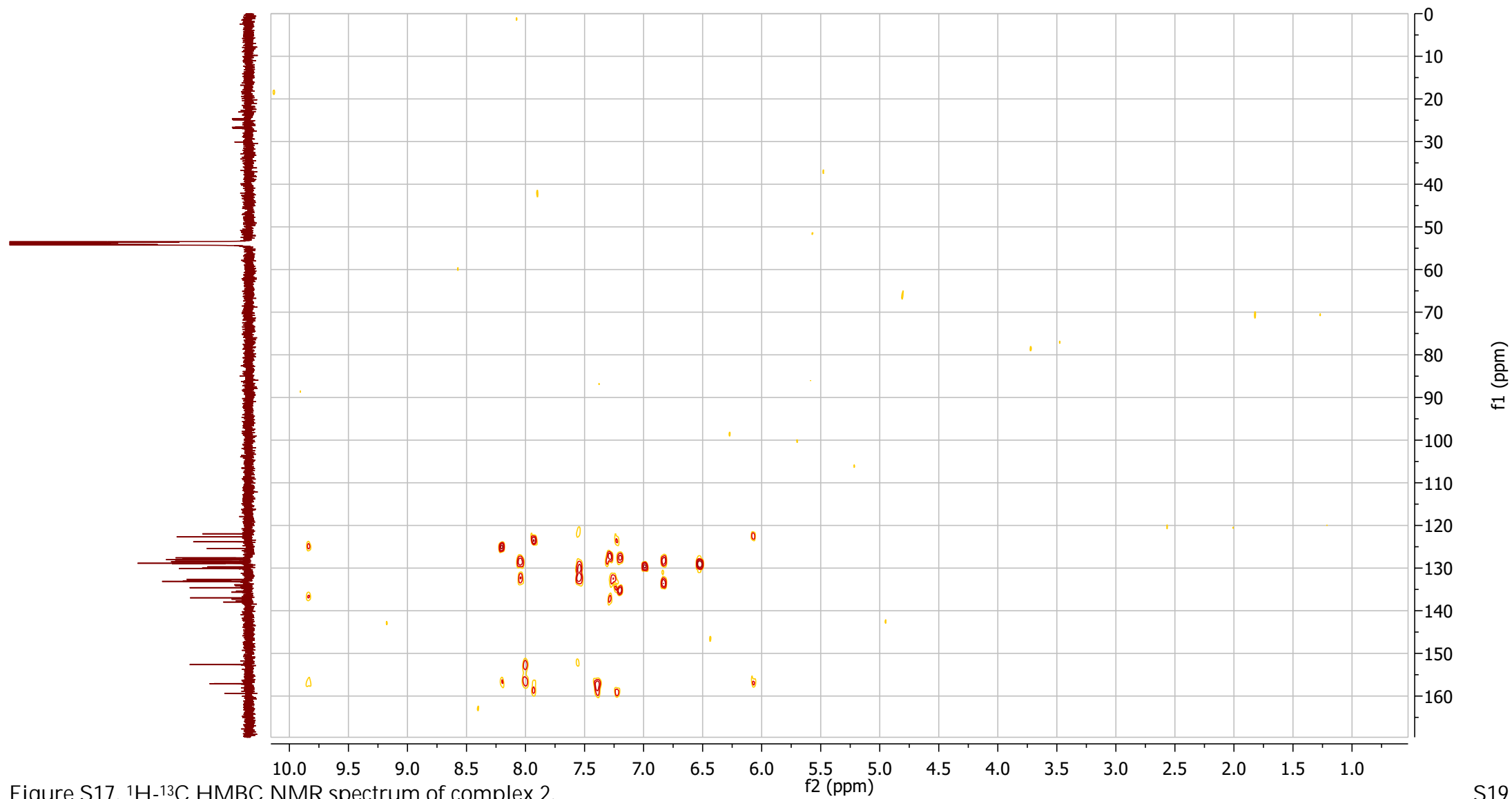


Figure S16. ^1H - ^{13}C HSQC NMR spectrum of complex 2.



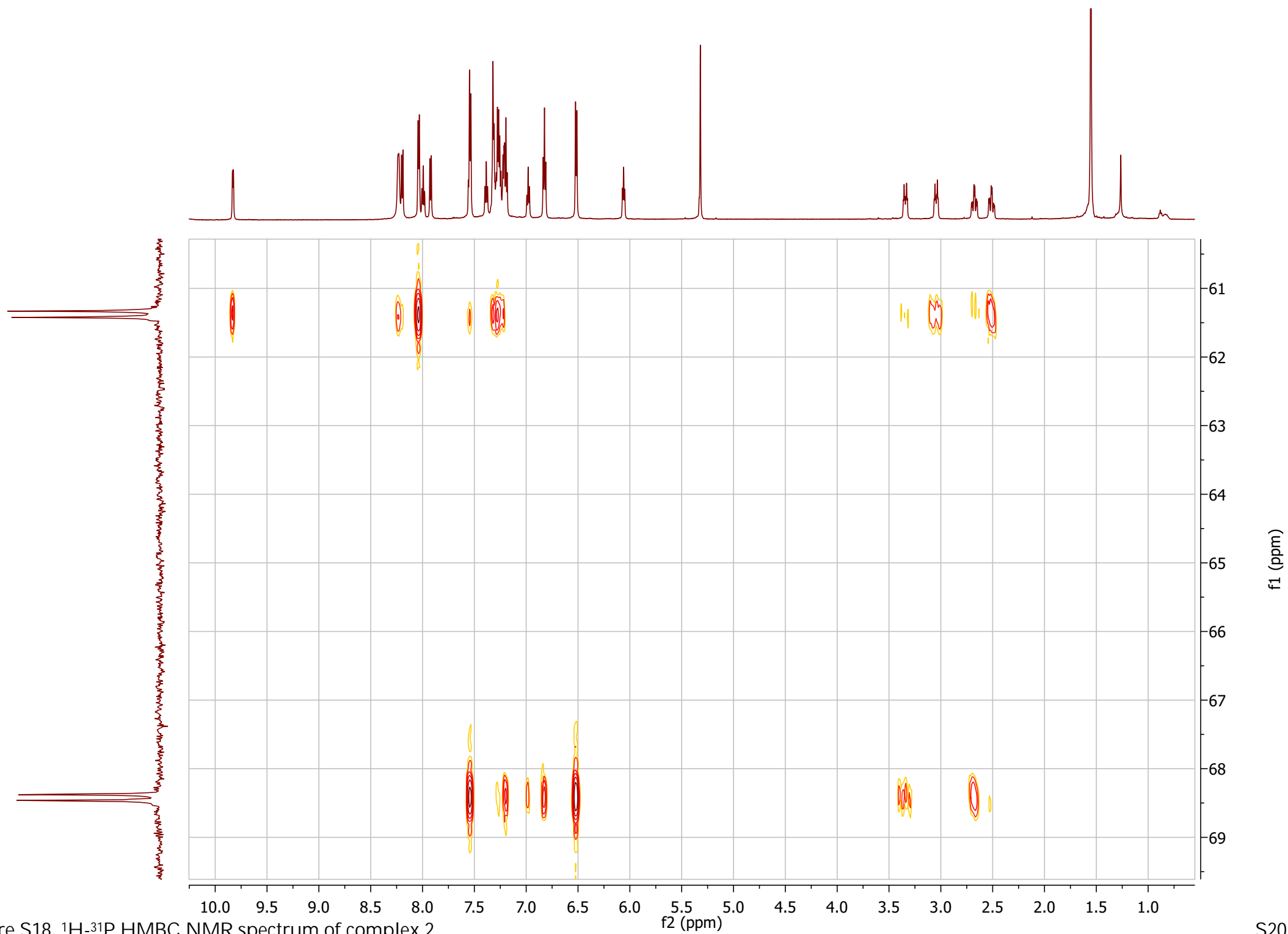
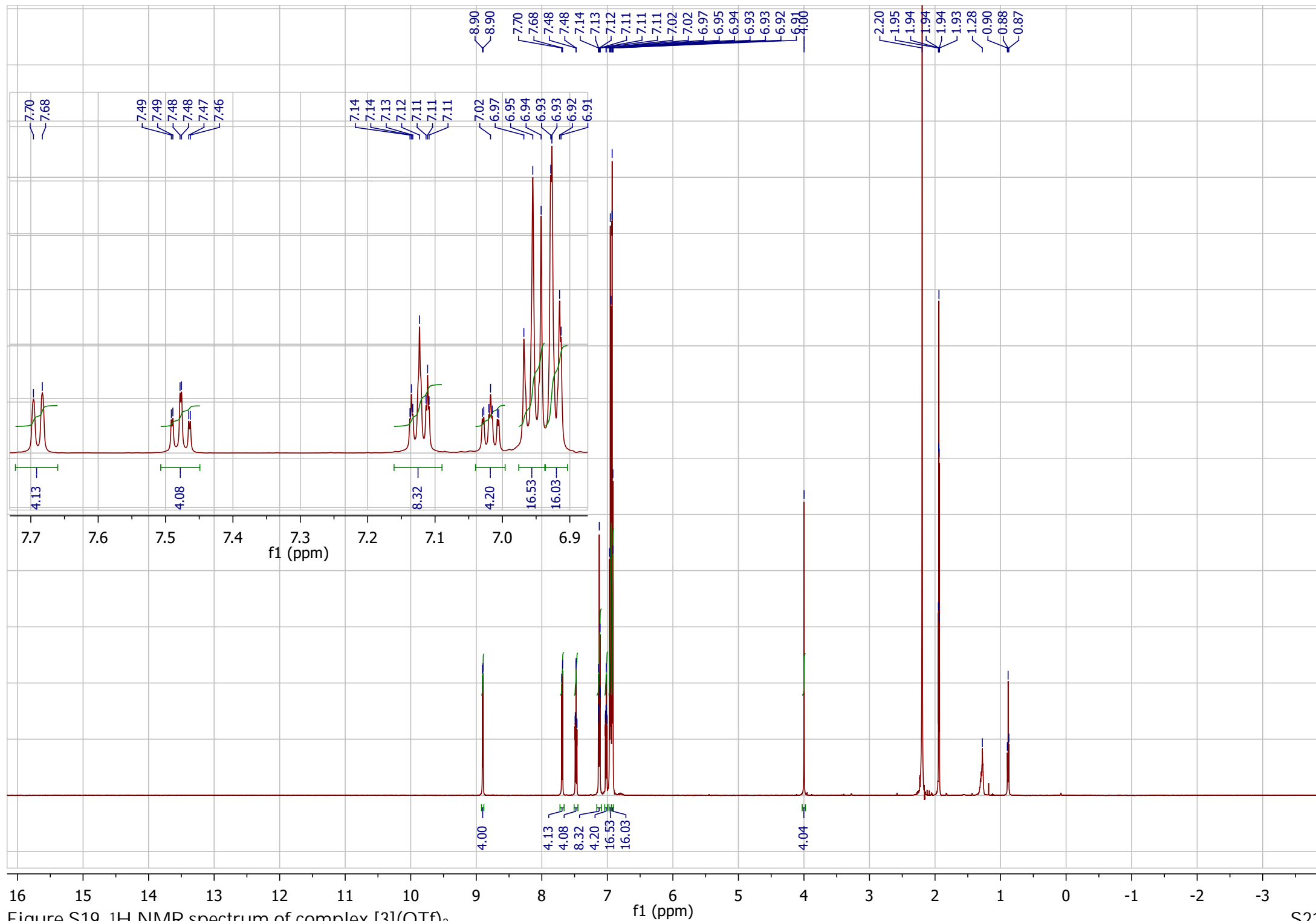


Figure S18. ^1H - ^{31}P HMBC NMR spectrum of complex 2.



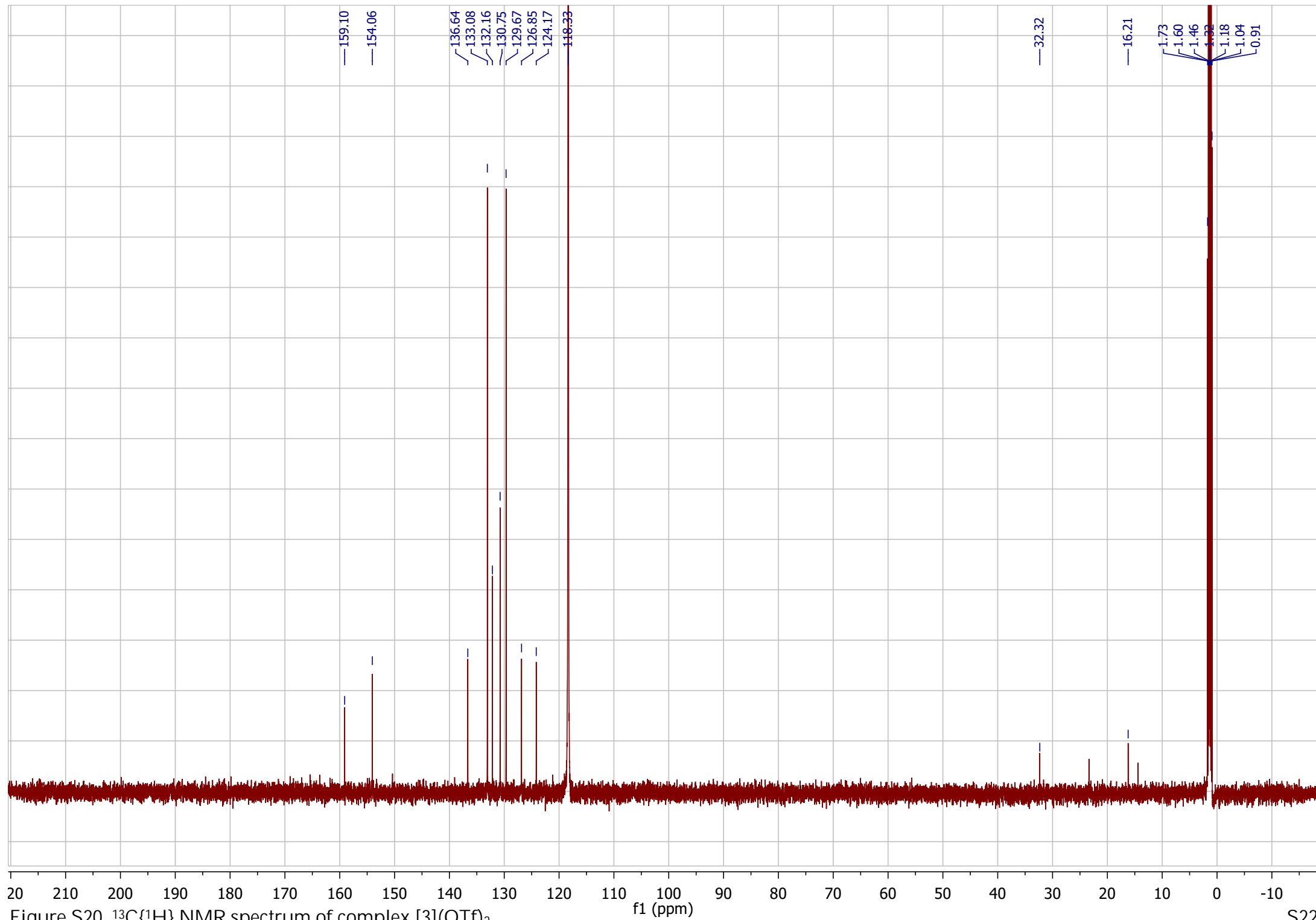


Figure S20. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of complex $[3](\text{OTf})_2$.

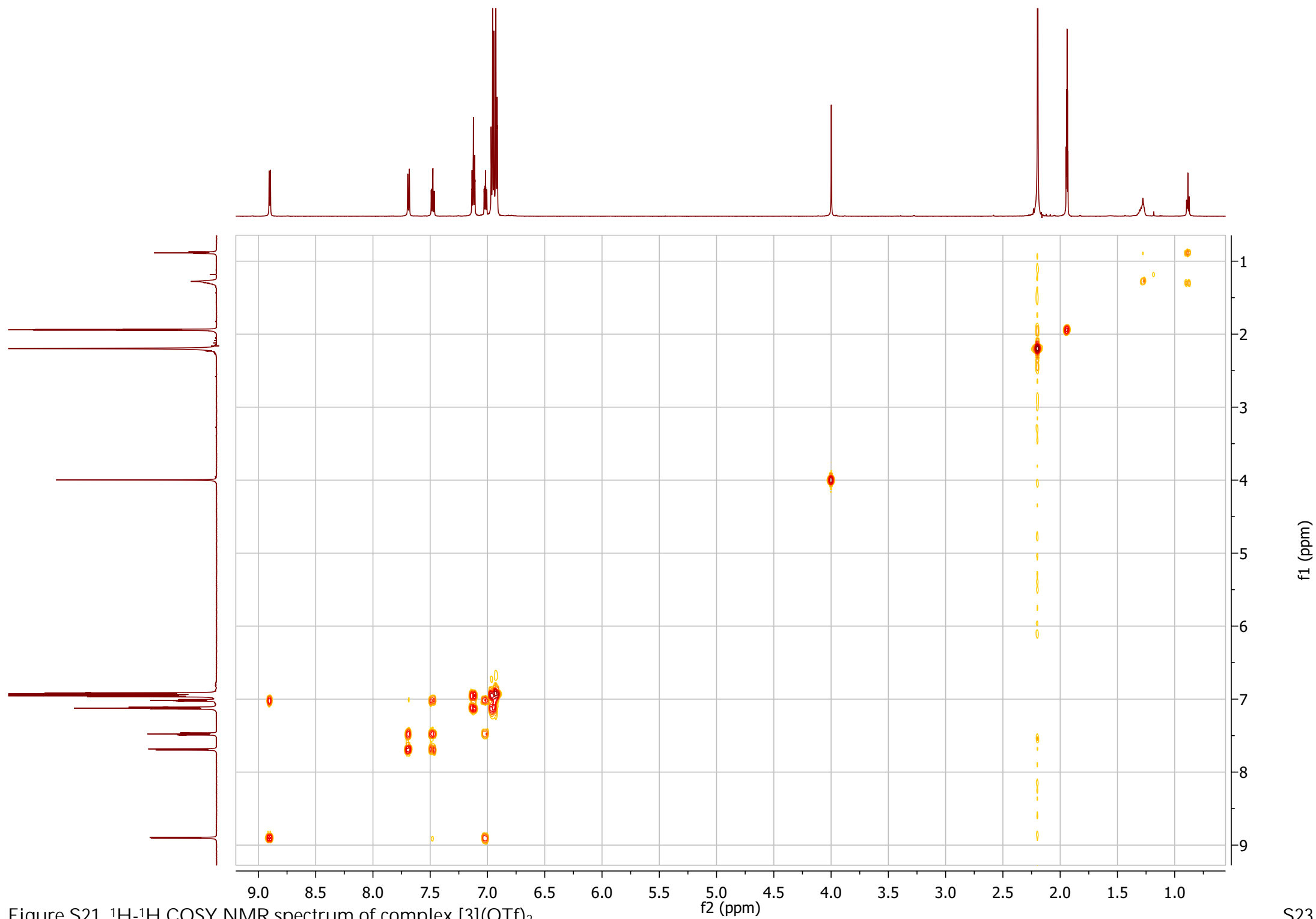


Figure S21. ^1H - ^1H COSY NMR spectrum of complex $[3](\text{OTf})_2$.

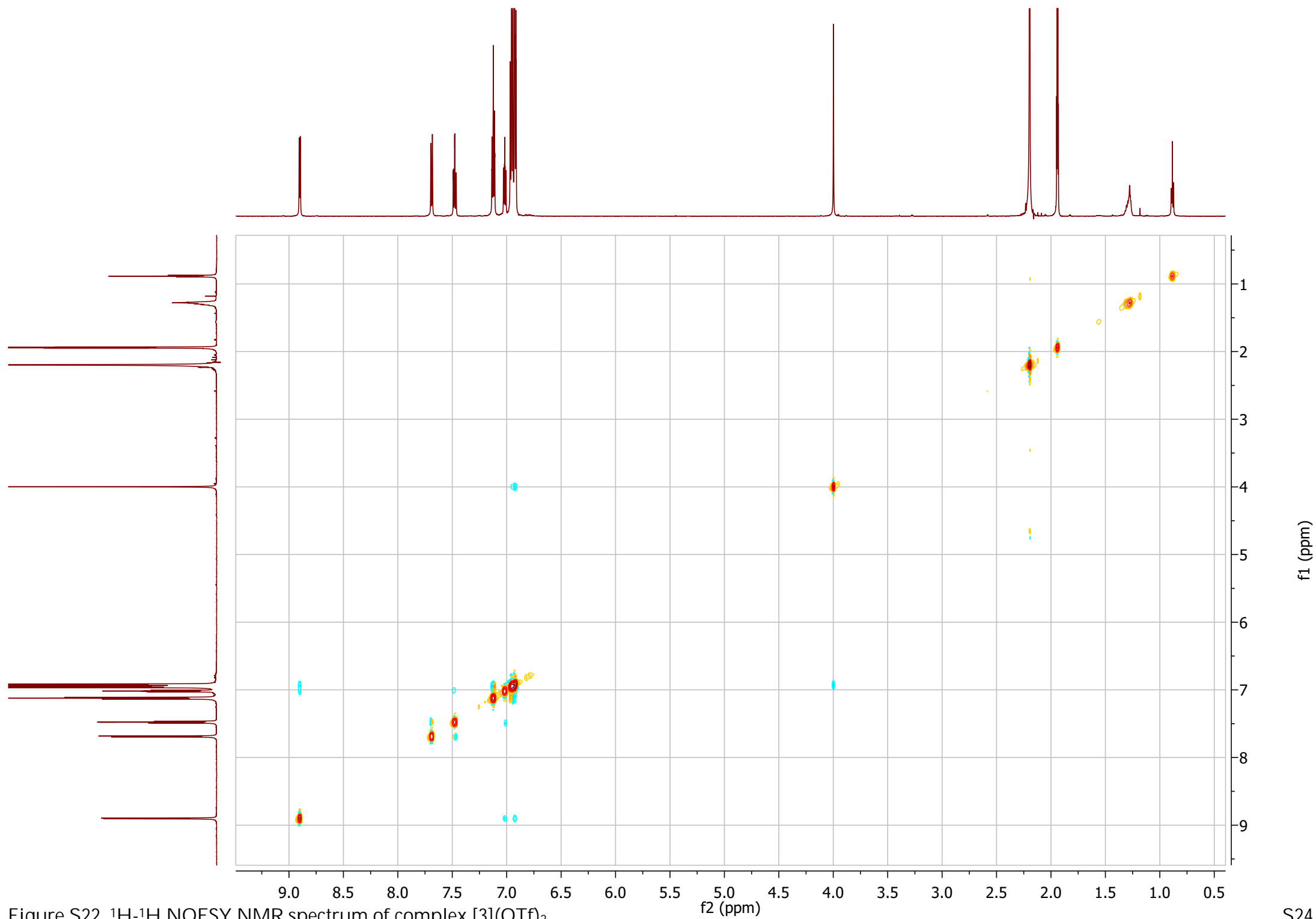


Figure S22. ^1H - ^1H NOESY NMR spectrum of complex $[3](\text{OTf})_2$.

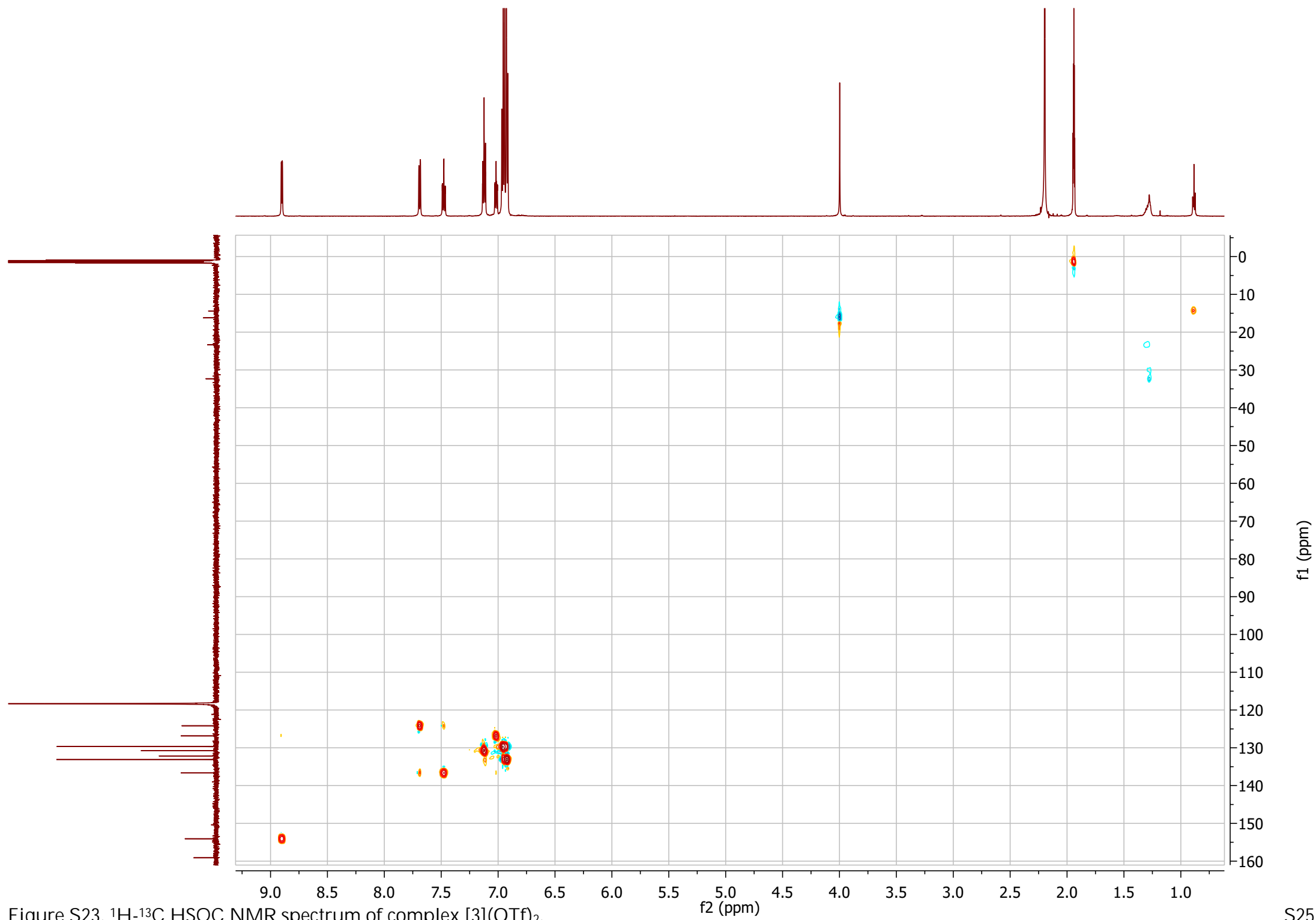
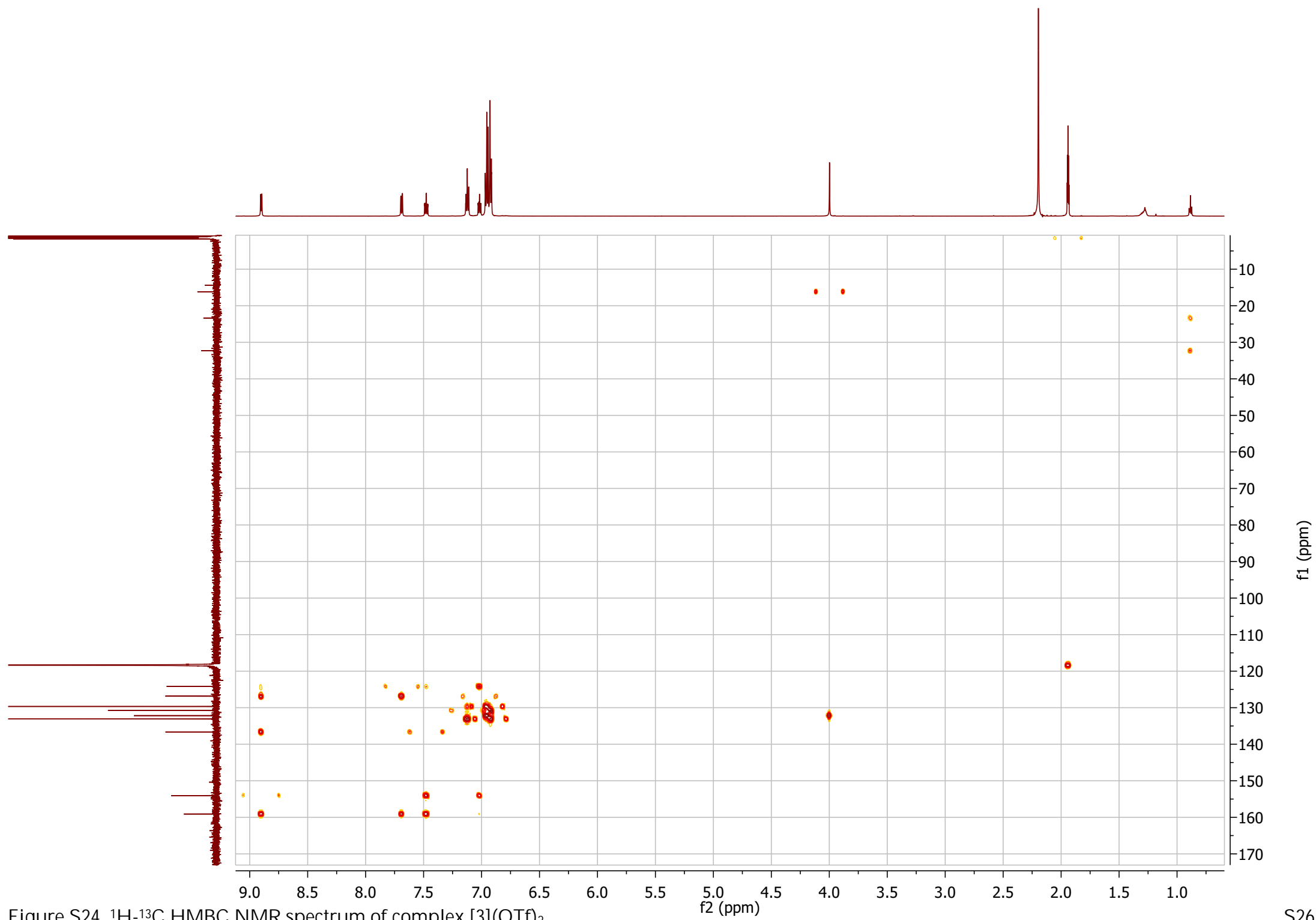


Figure S23. ^1H - ^{13}C HSQC NMR spectrum of complex $[3](\text{OTf})_2$.



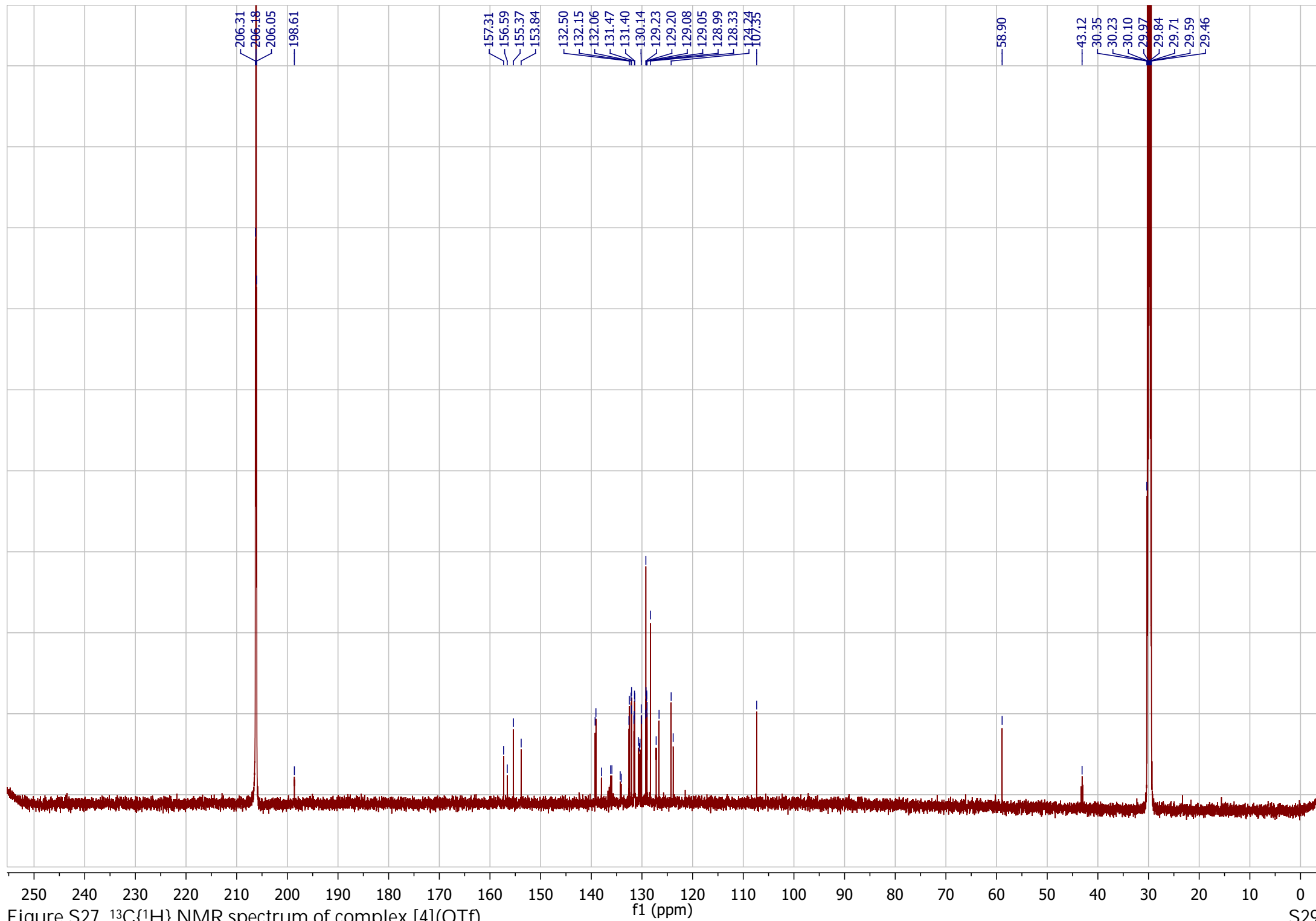


Figure S27. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of complex [4](OTf).

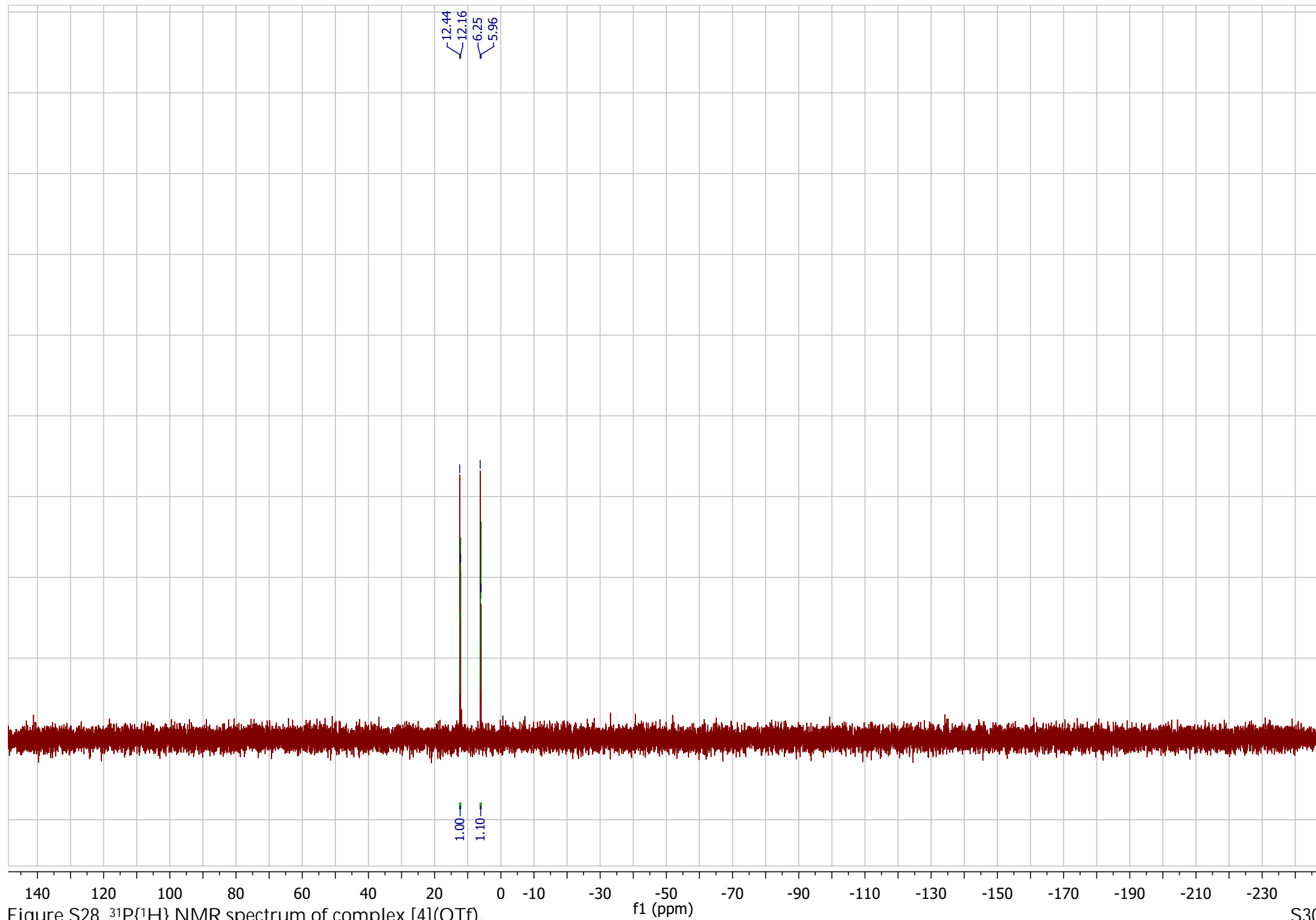


Figure S28. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of complex [4](OTf).

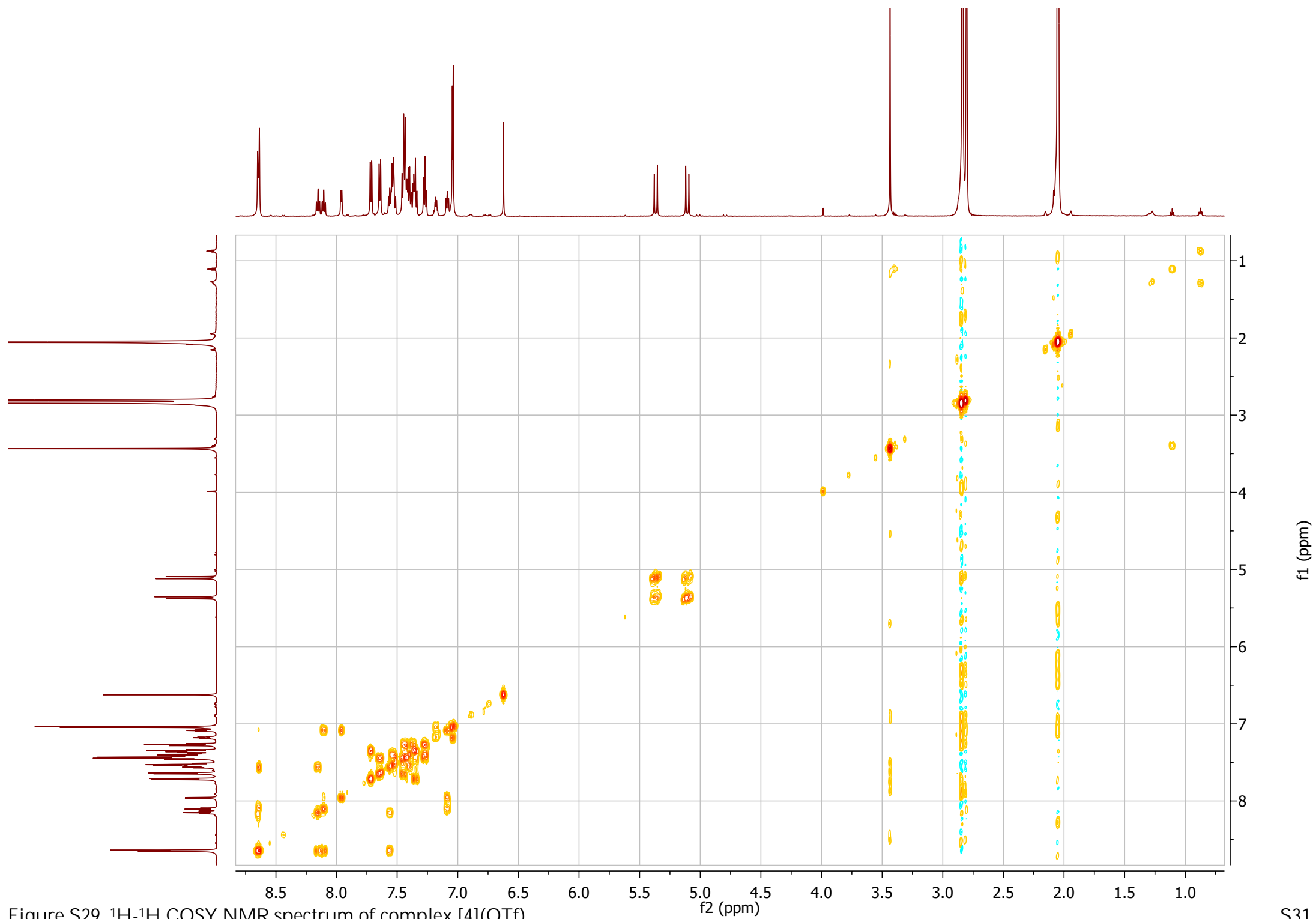
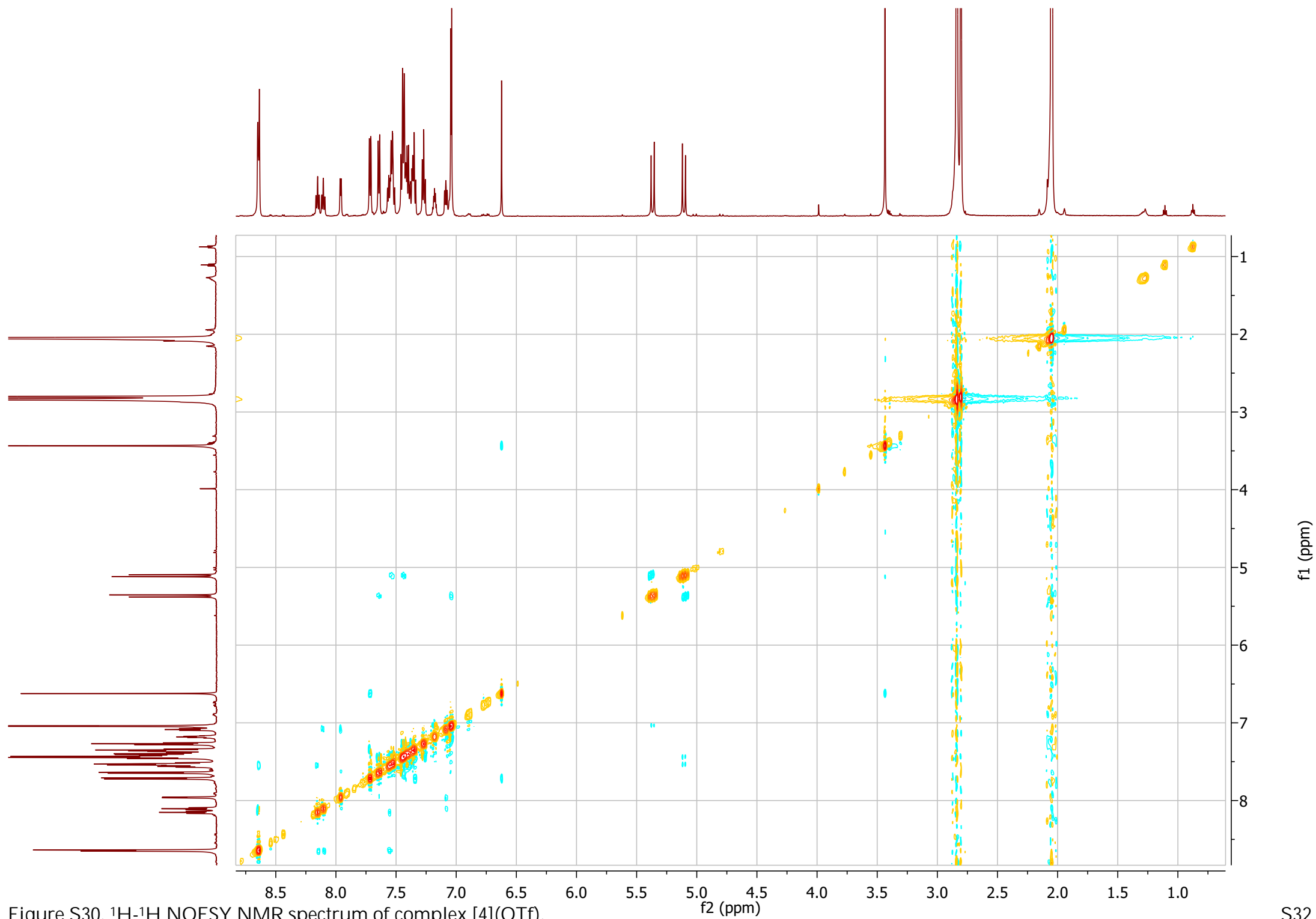


Figure S29. ^1H - ^1H COSY NMR spectrum of complex $[4](\text{OTf})$.



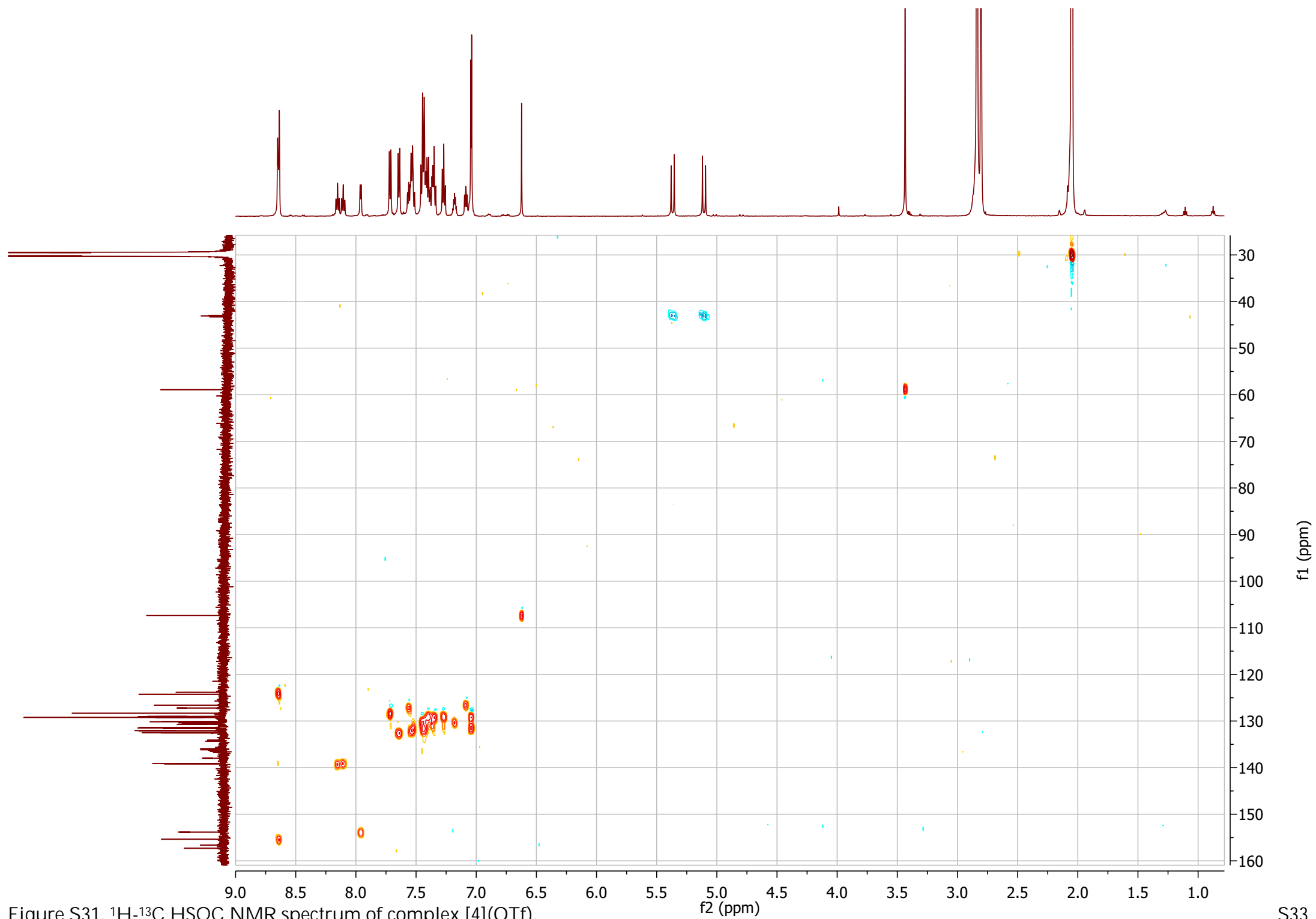
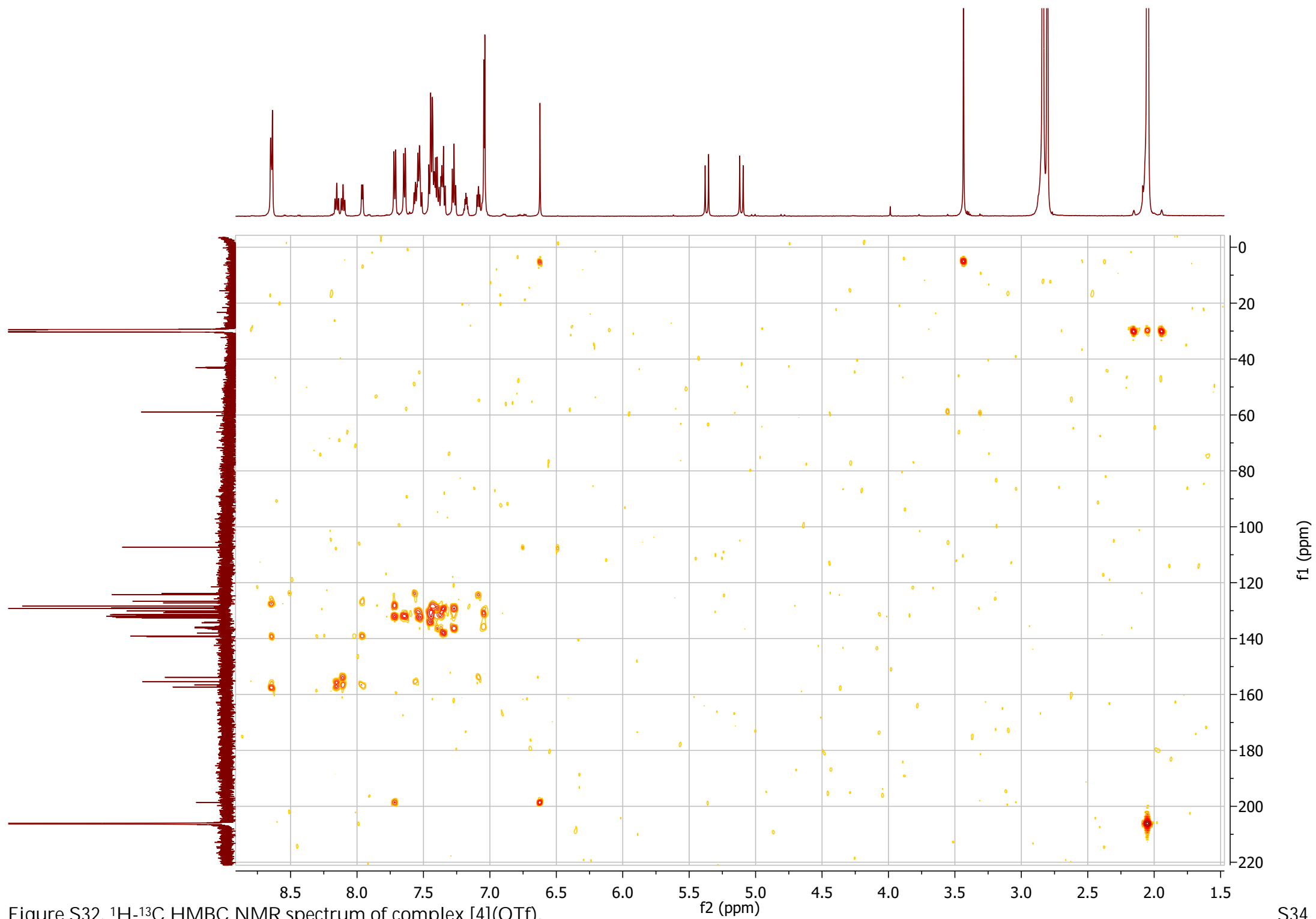


Figure S31. ^1H - ^{13}C HSQC NMR spectrum of complex [4](OTf).



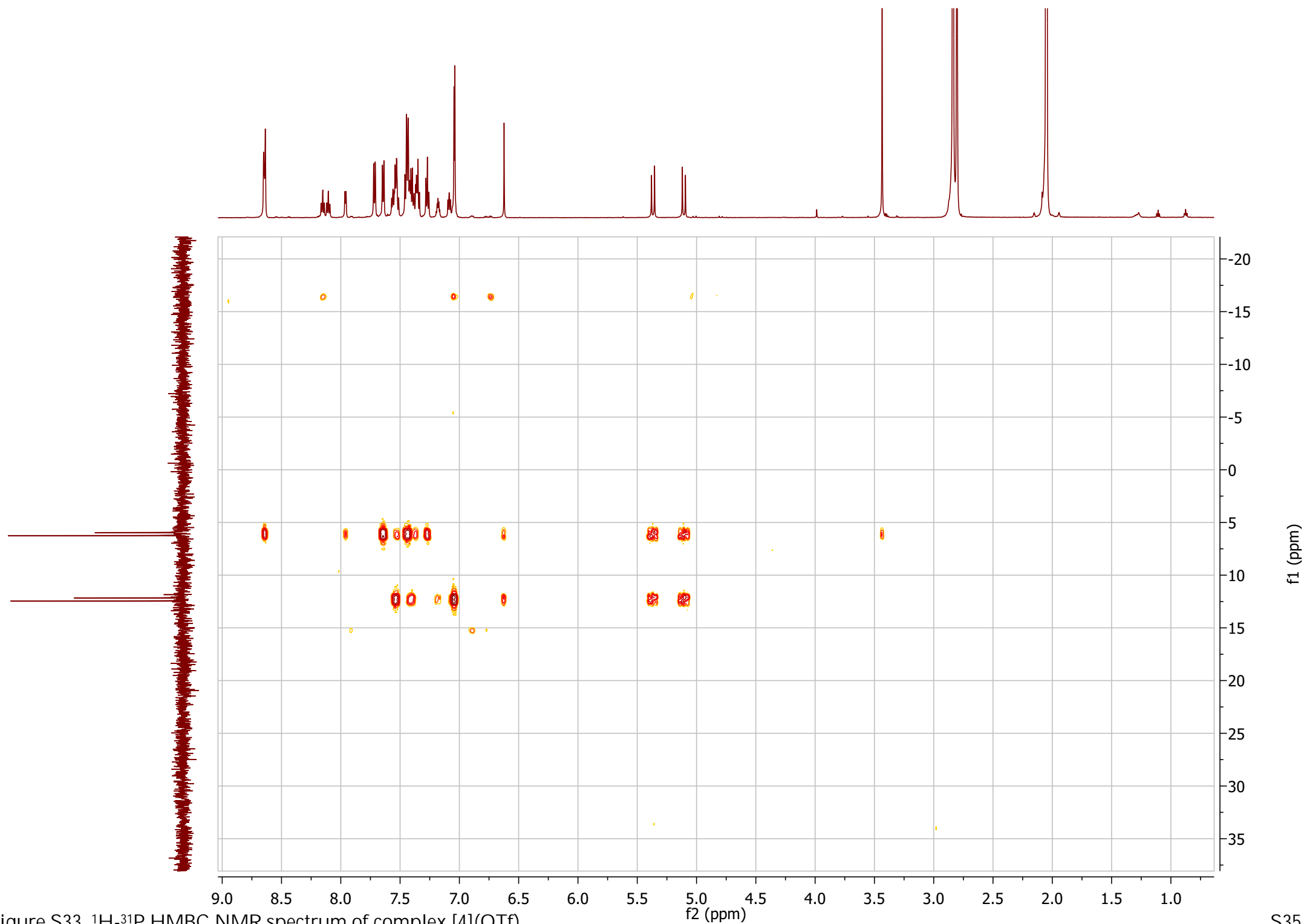


Figure S33. ^1H - ^{31}P HMBC NMR spectrum of complex $[4](\text{OTf})$.

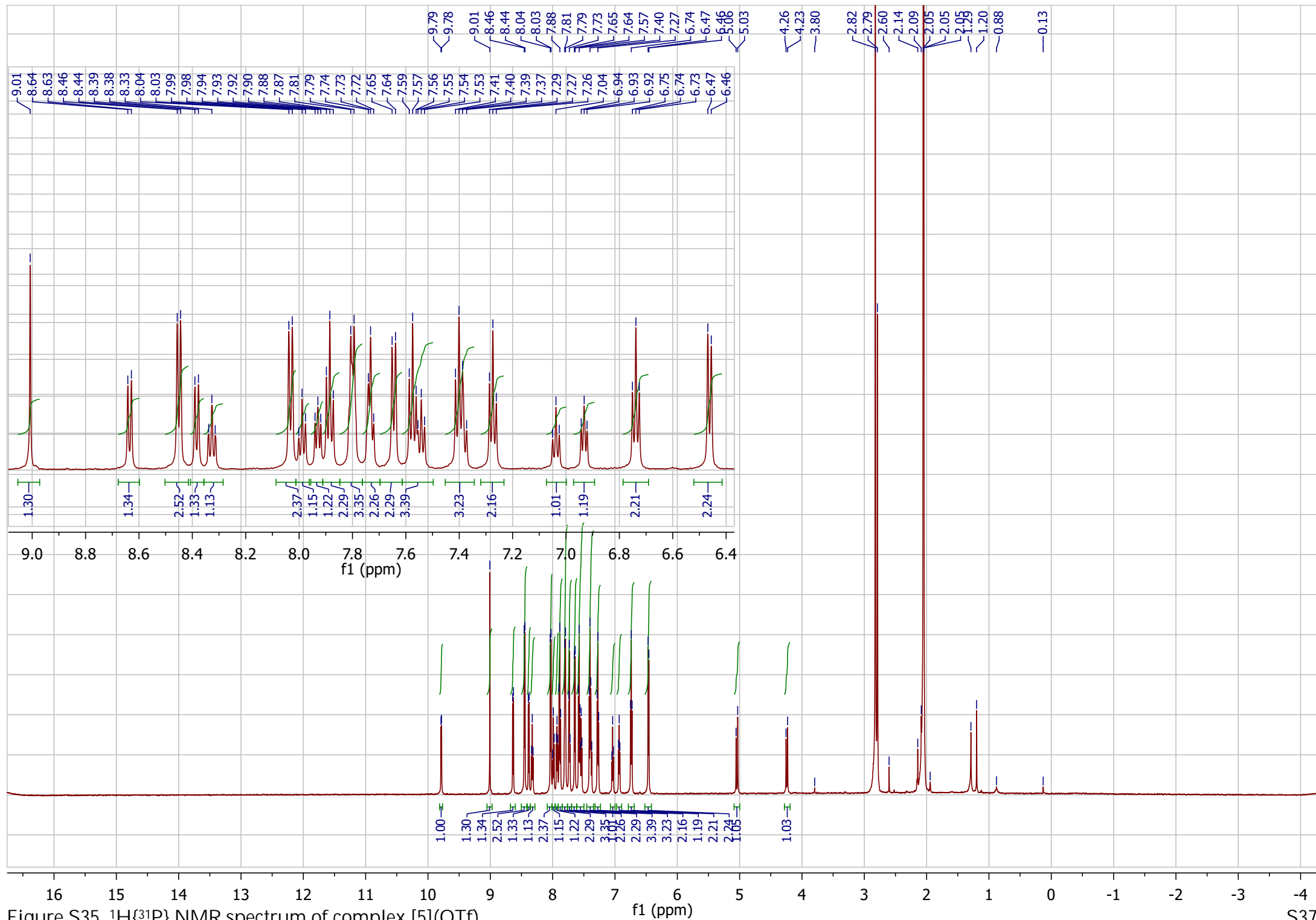


Figure S35. $^1\text{H}\{^{31}\text{P}\}$ NMR spectrum of complex [5](OTf).

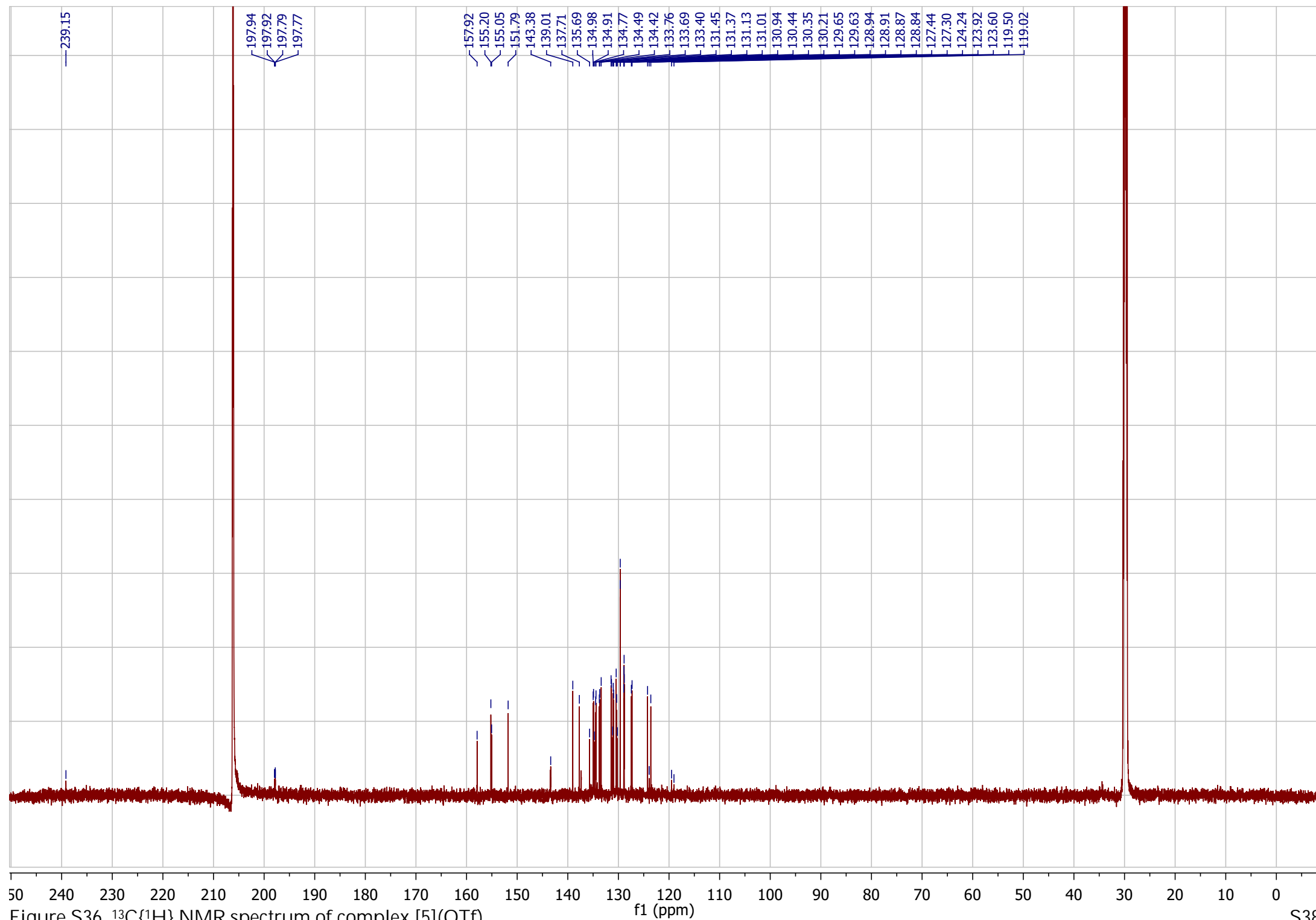


Figure S36. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of complex [5](OTf).

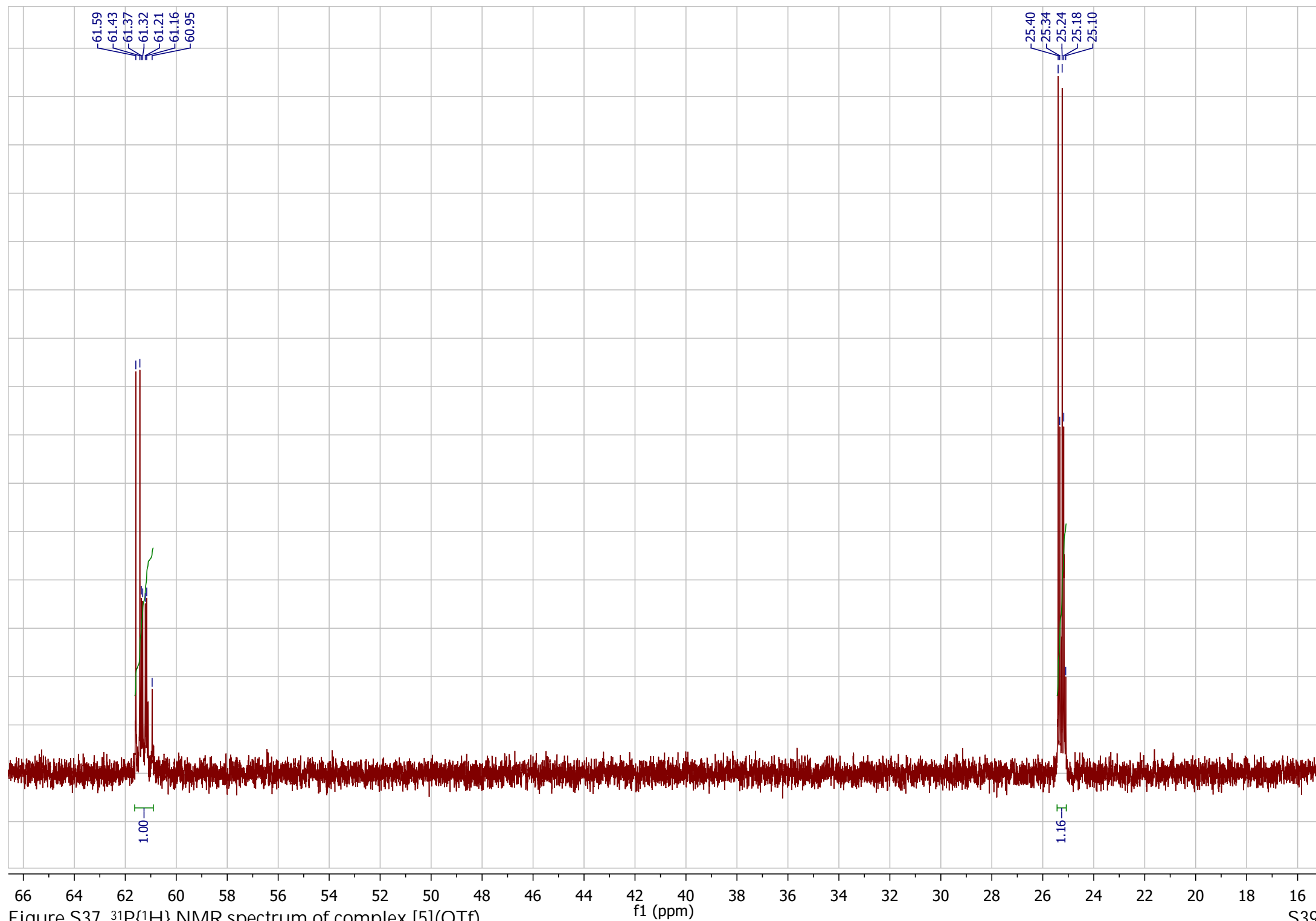


Figure S37. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of complex [5](OTf).

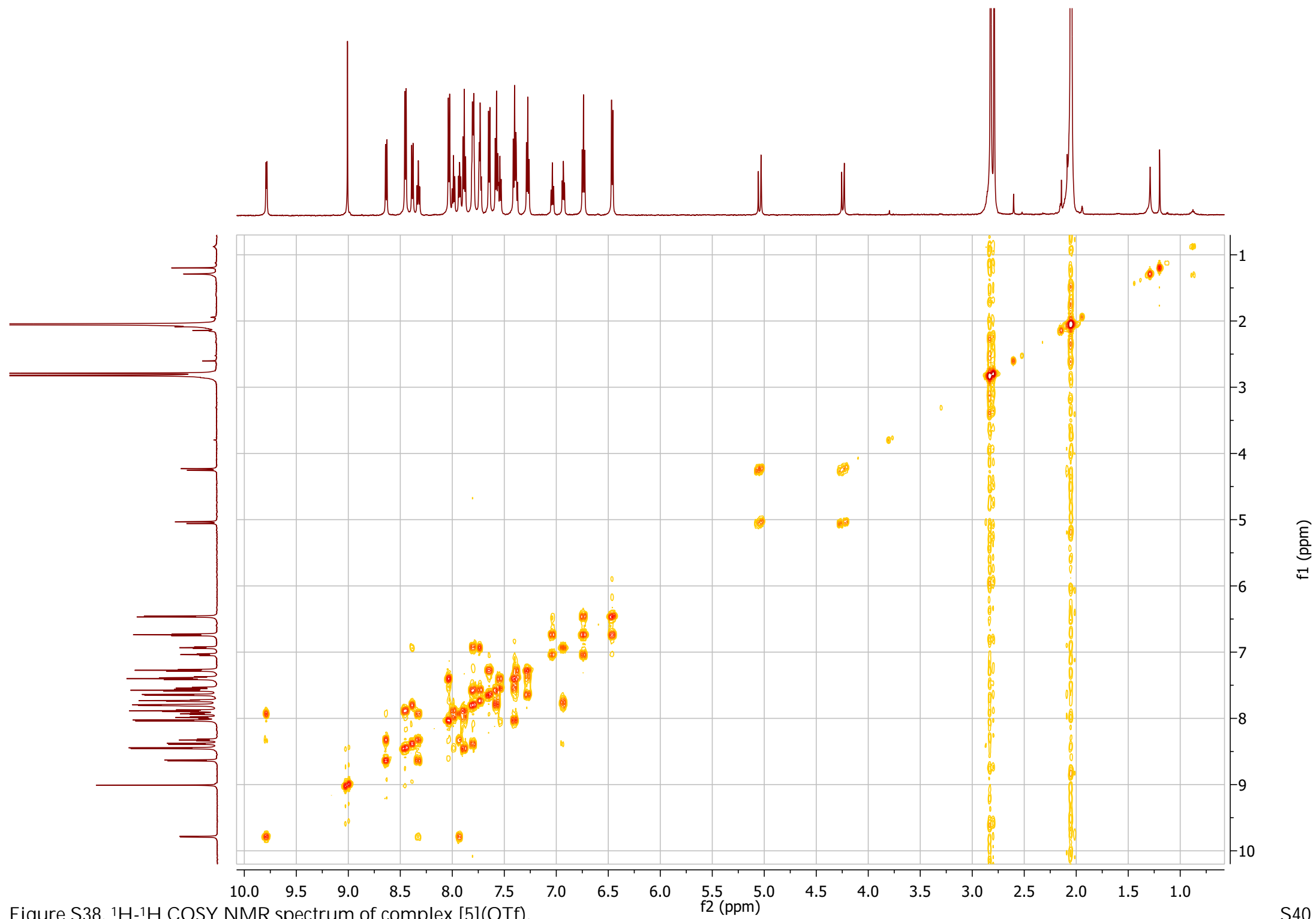
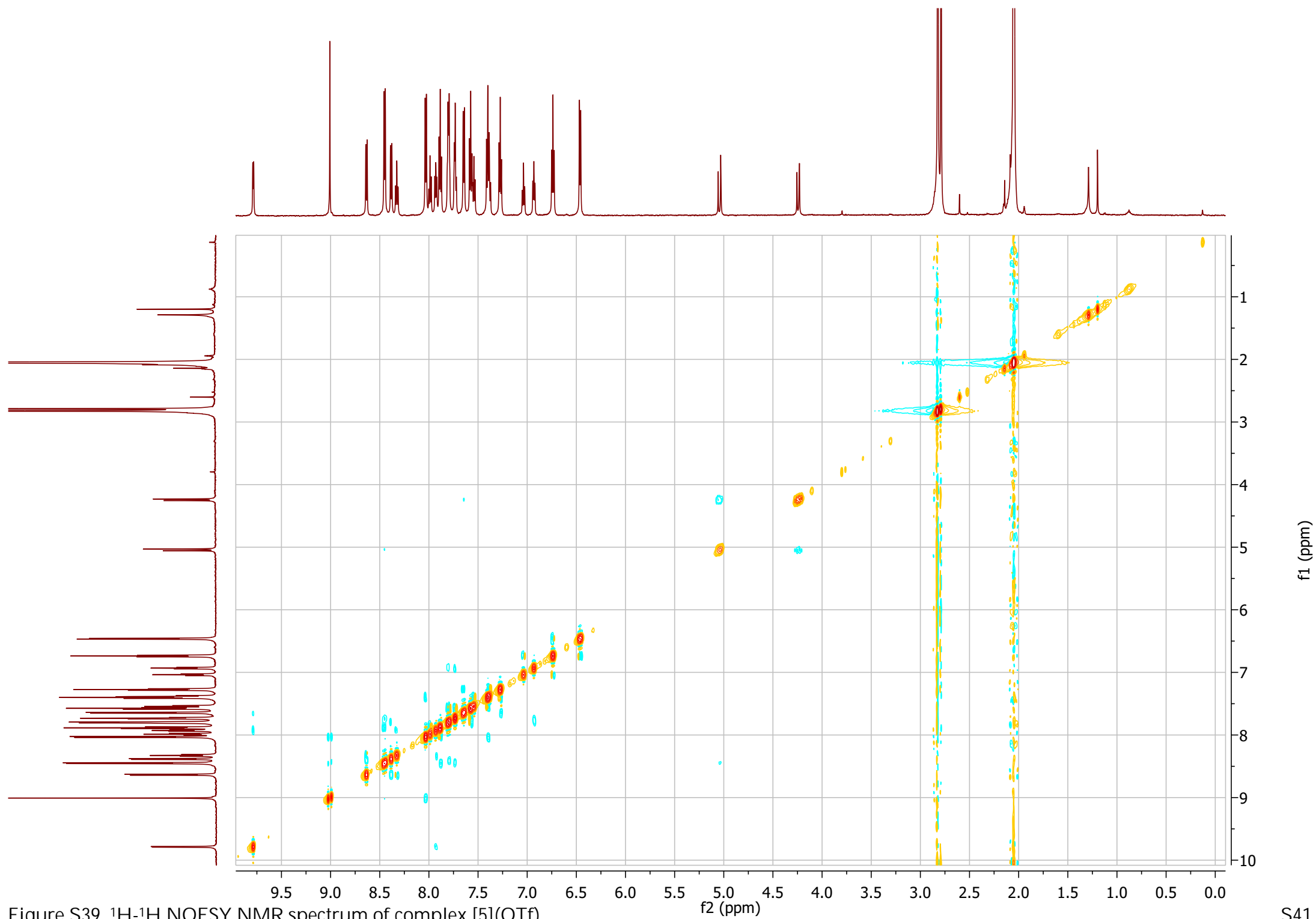


Figure S38. ^1H - ^1H COSY NMR spectrum of complex [5](OTf).



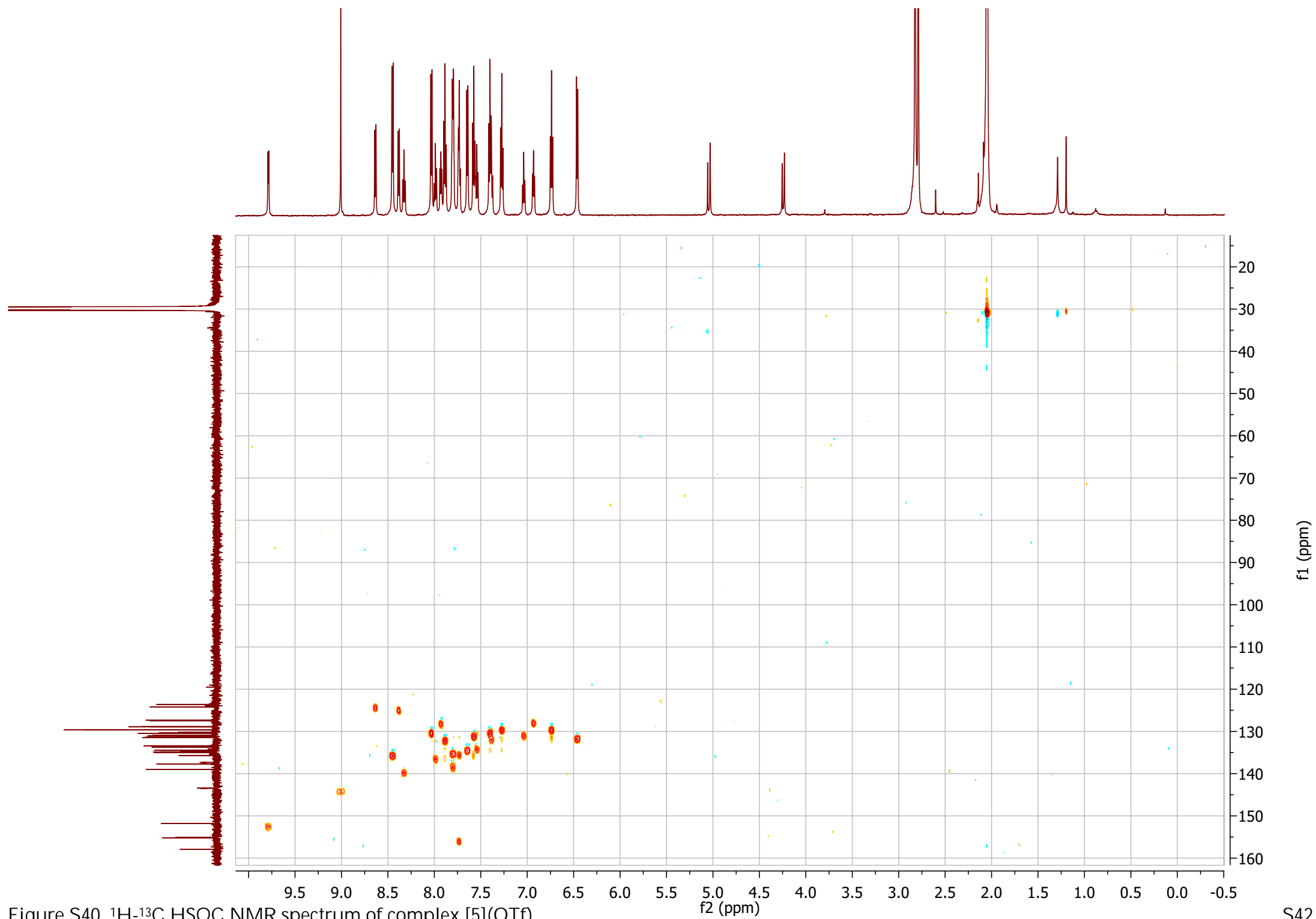


Figure S40. ^1H - ^{13}C HSQC NMR spectrum of complex [5](OTf).

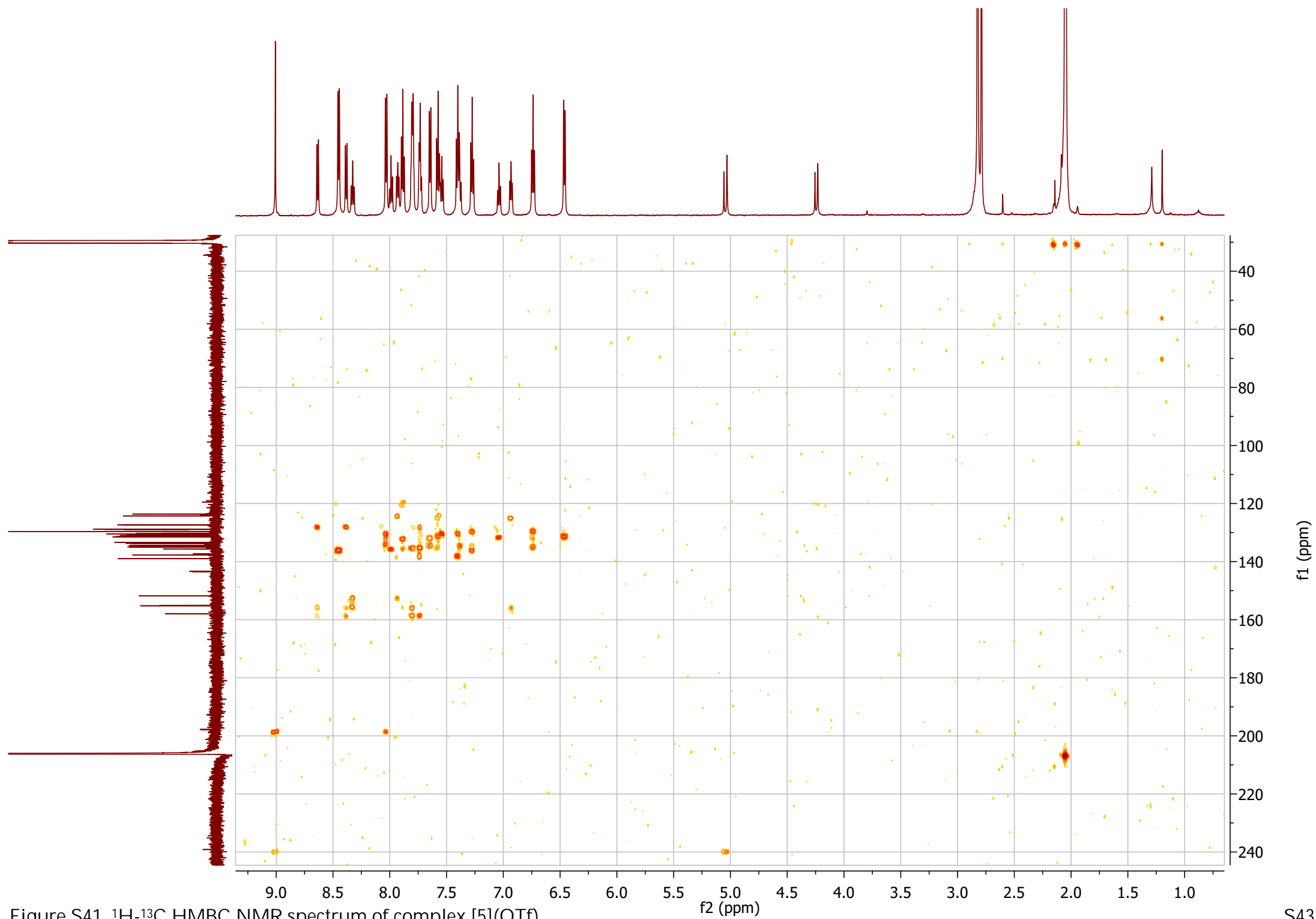


Figure S41. ^1H - ^{13}C HMBC NMR spectrum of complex [5](OTf).

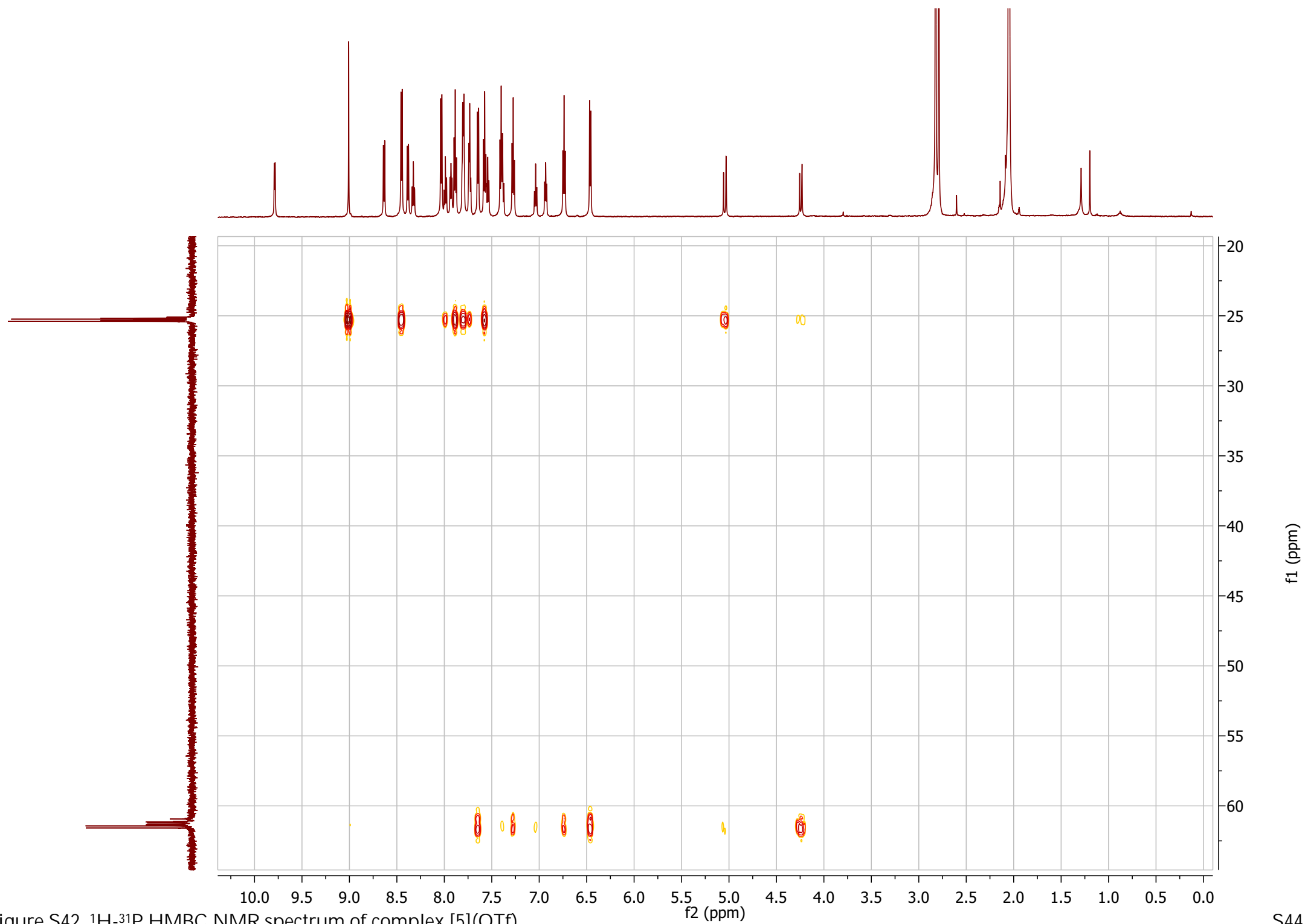


Figure S42. ^1H - ^{31}P HMBC NMR spectrum of complex $[5](\text{OTf})$.

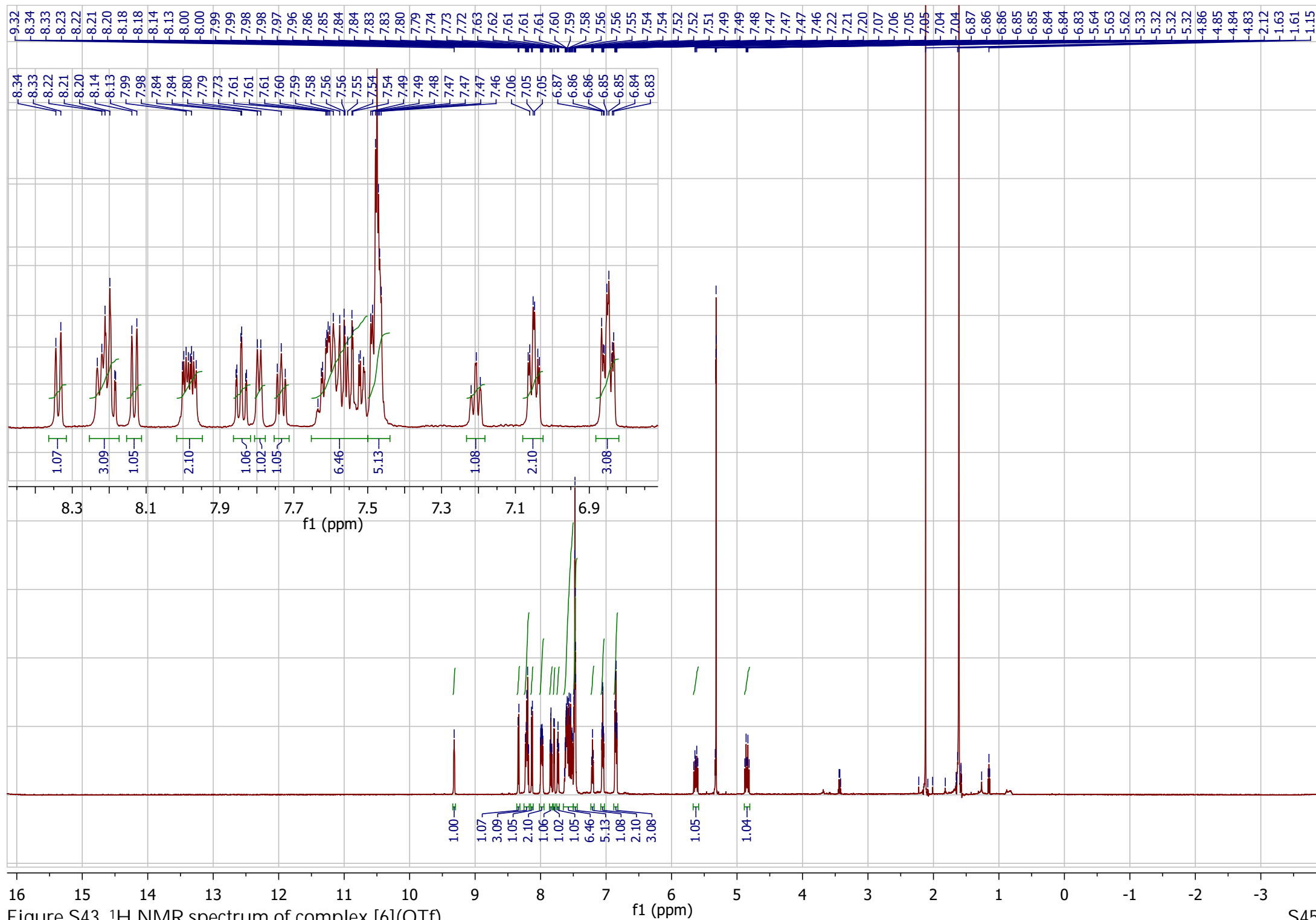


Figure S43. ^1H NMR spectrum of complex $[6](\text{OTf})$.

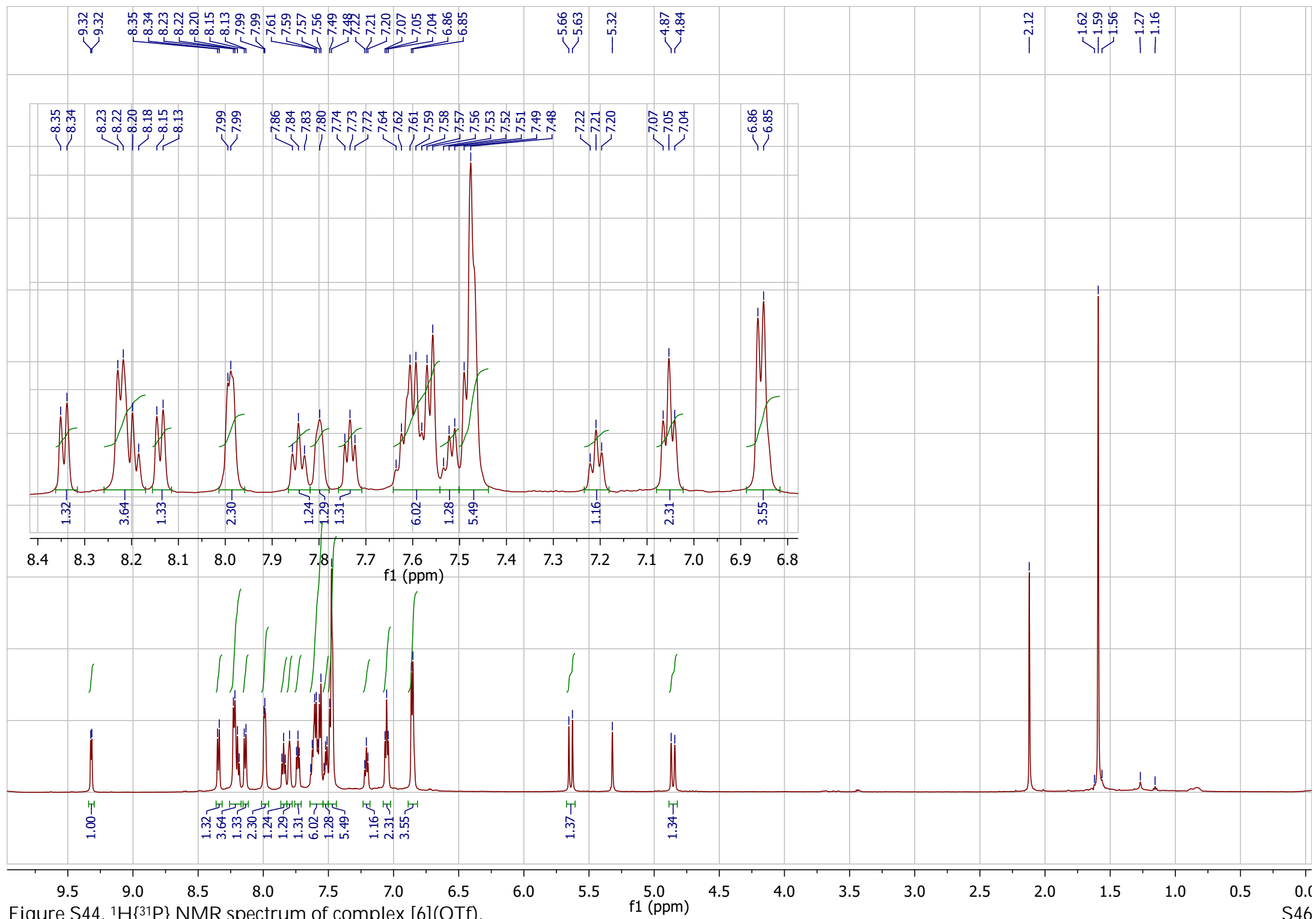


Figure S44. $^1\text{H}\{^{31}\text{P}\}$ NMR spectrum of complex $[6](\text{OTf})$.

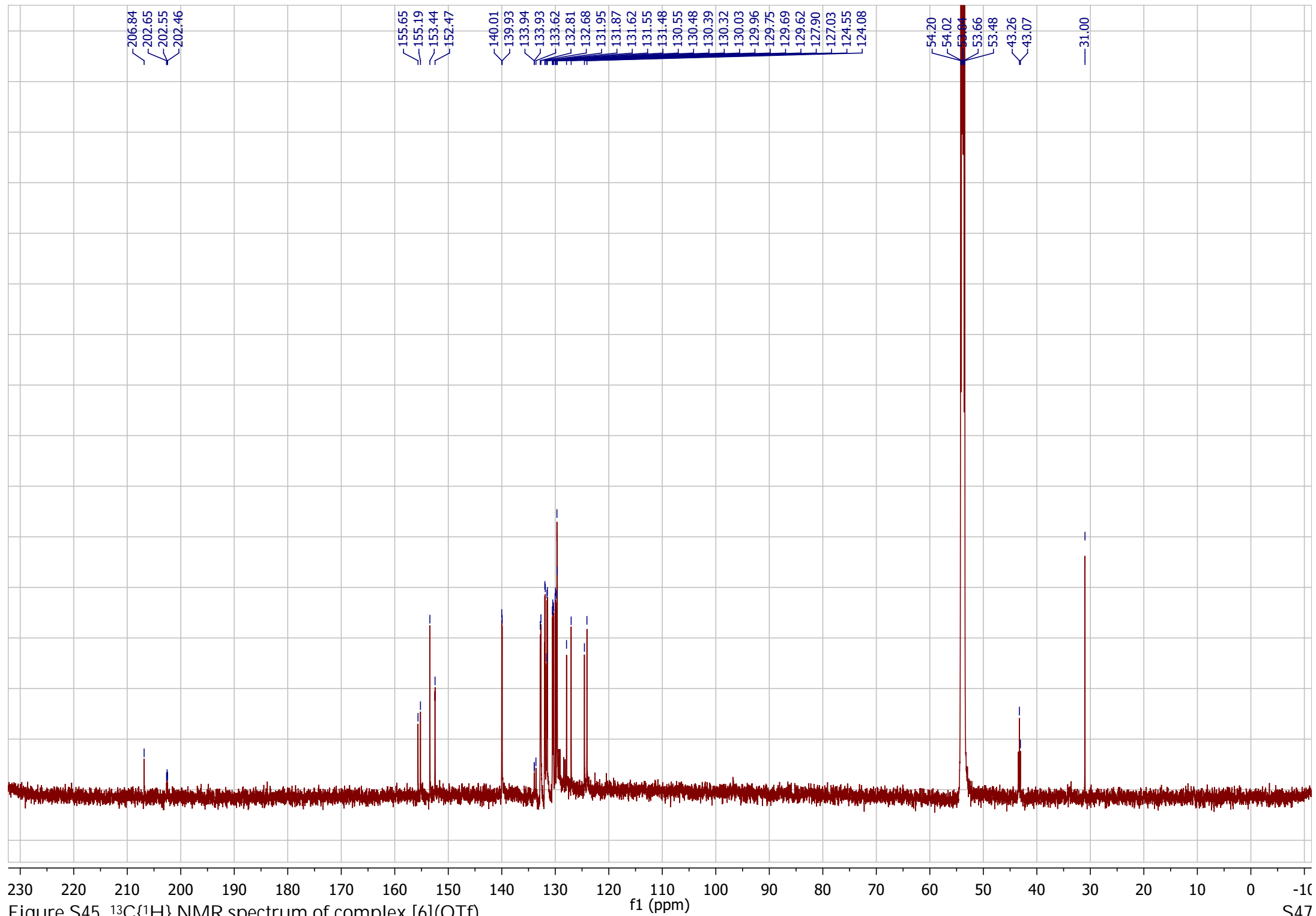


Figure S45. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of complex [6](OTf).

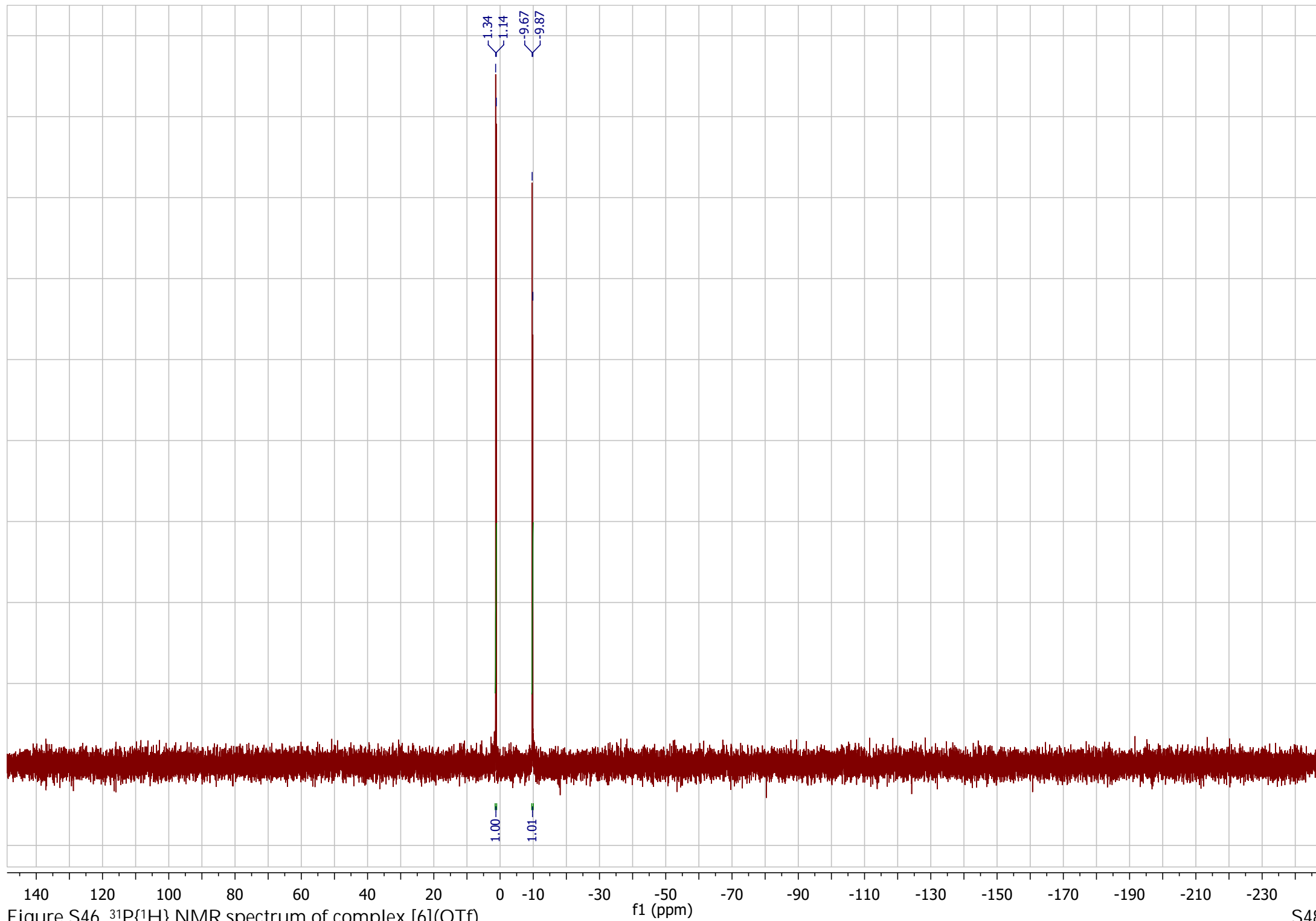
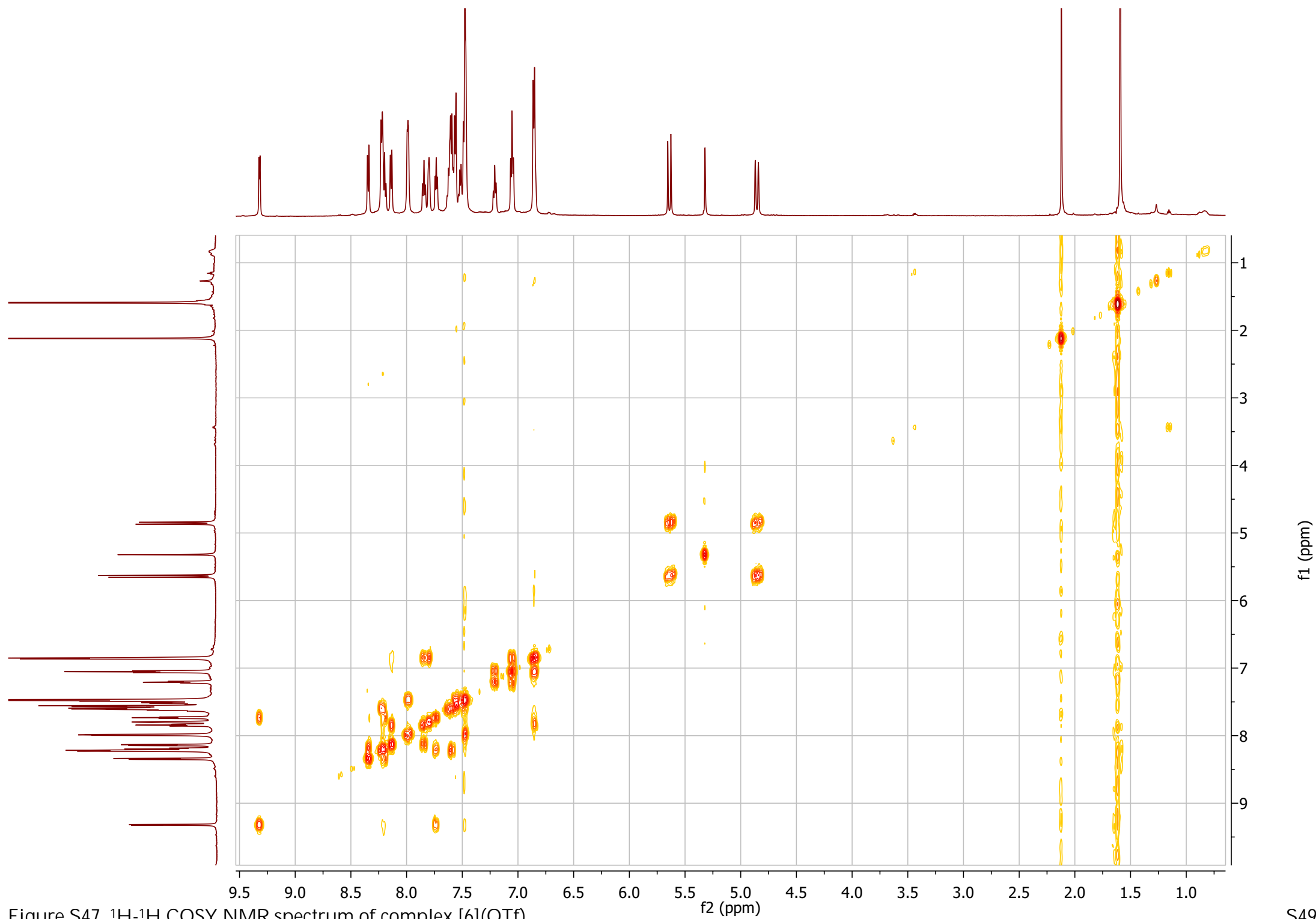


Figure S46. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of complex [6](OTf).



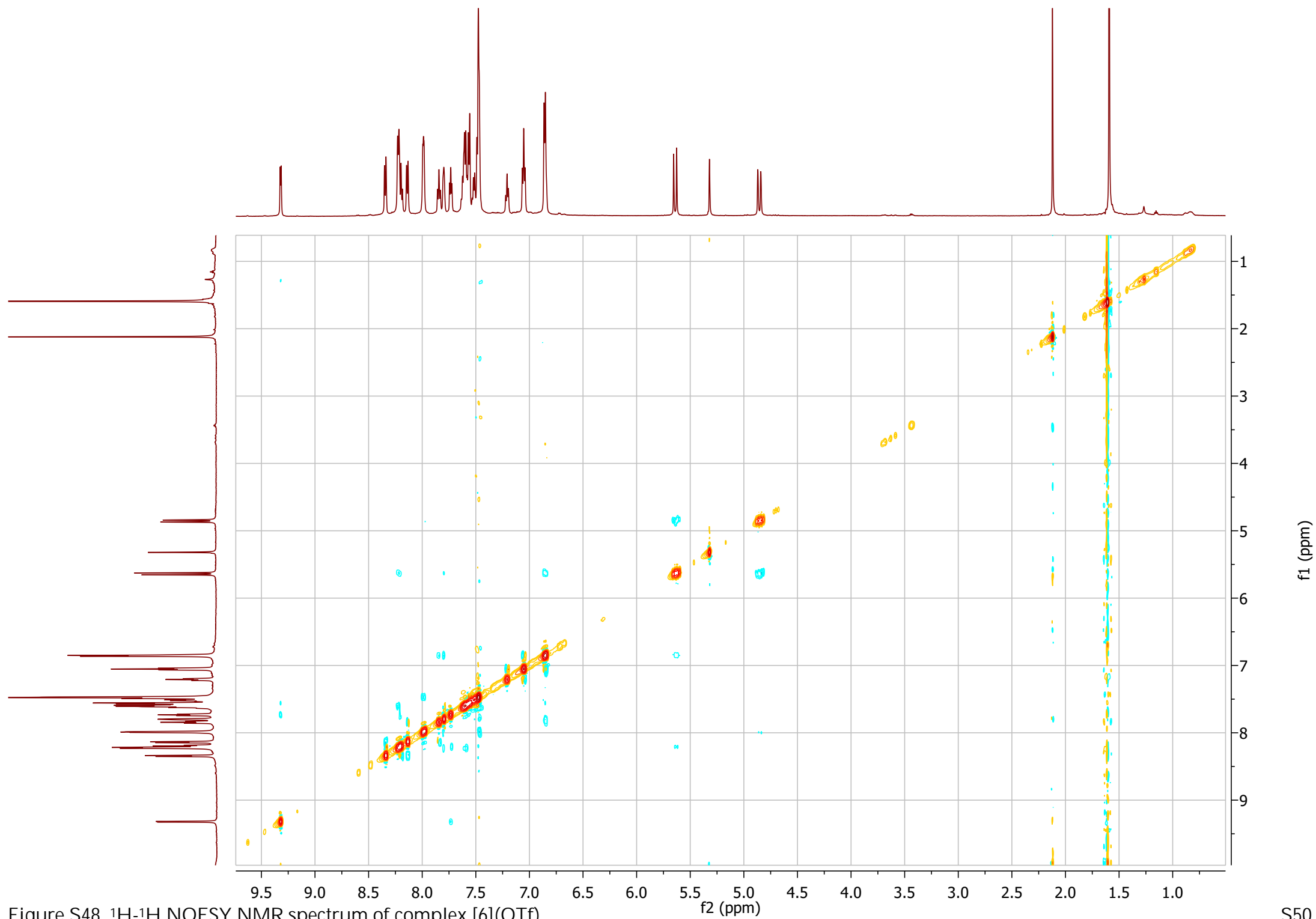
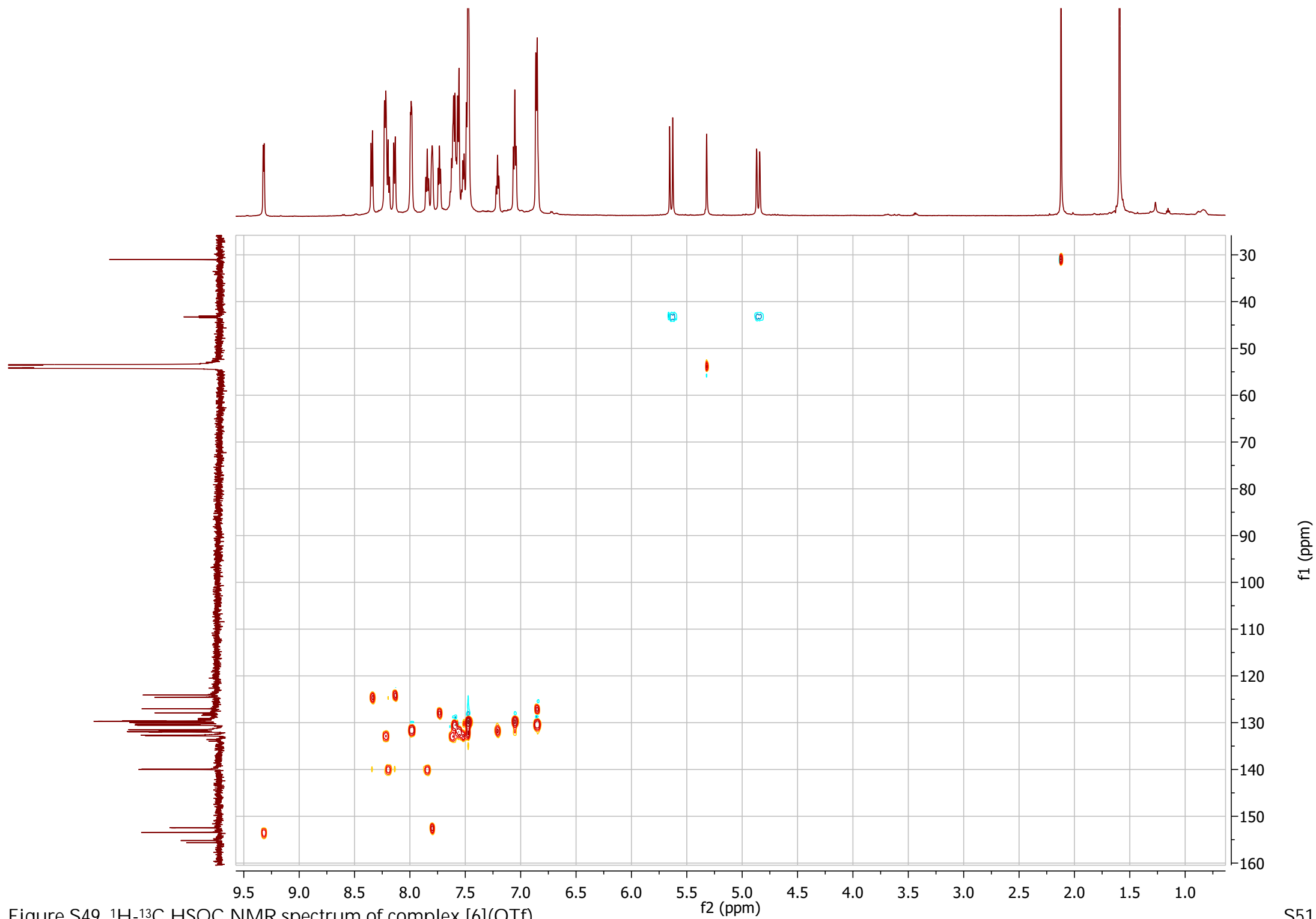


Figure S48. ^1H - ^1H NOESY NMR spectrum of complex $[6](\text{OTf})$.



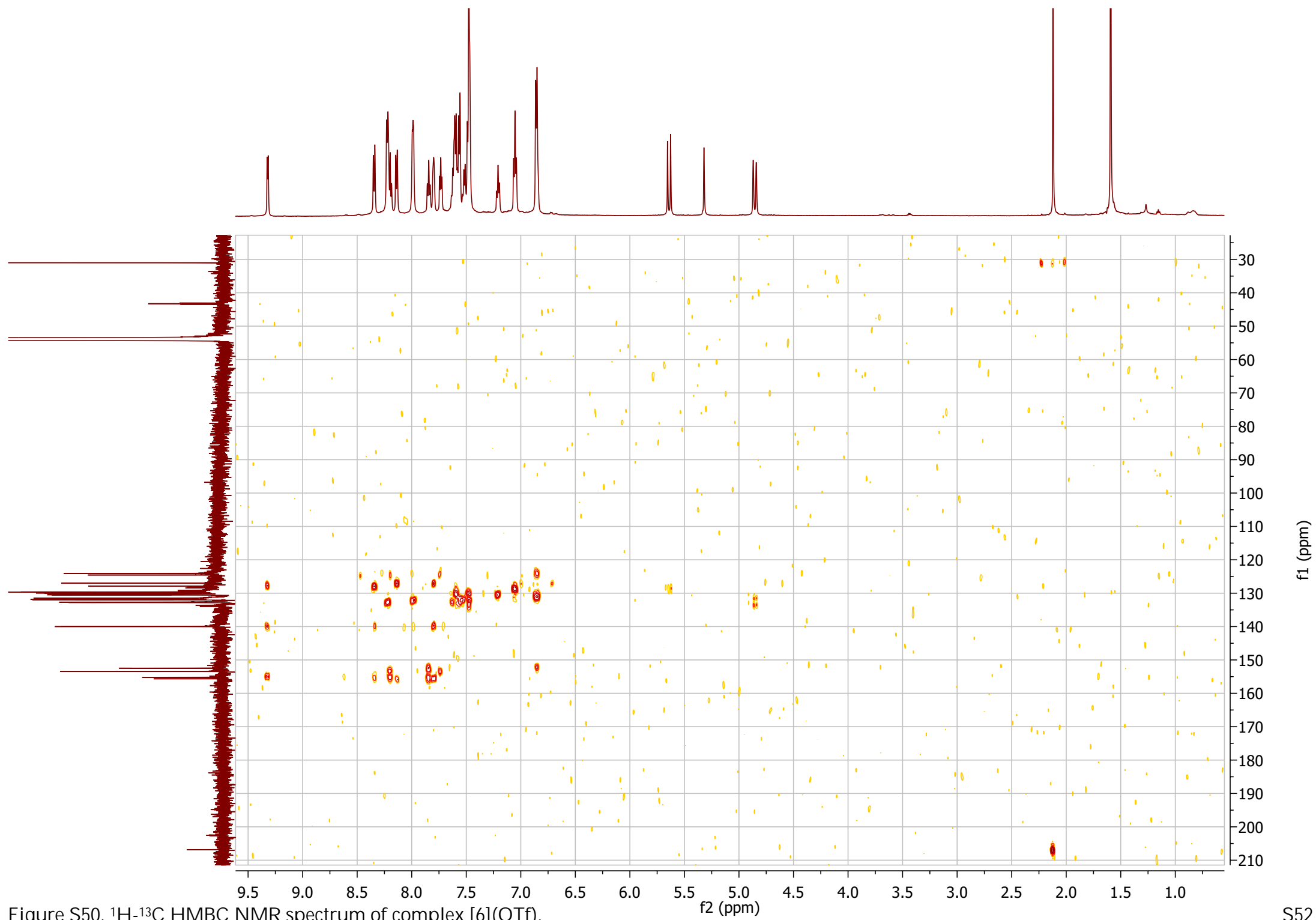
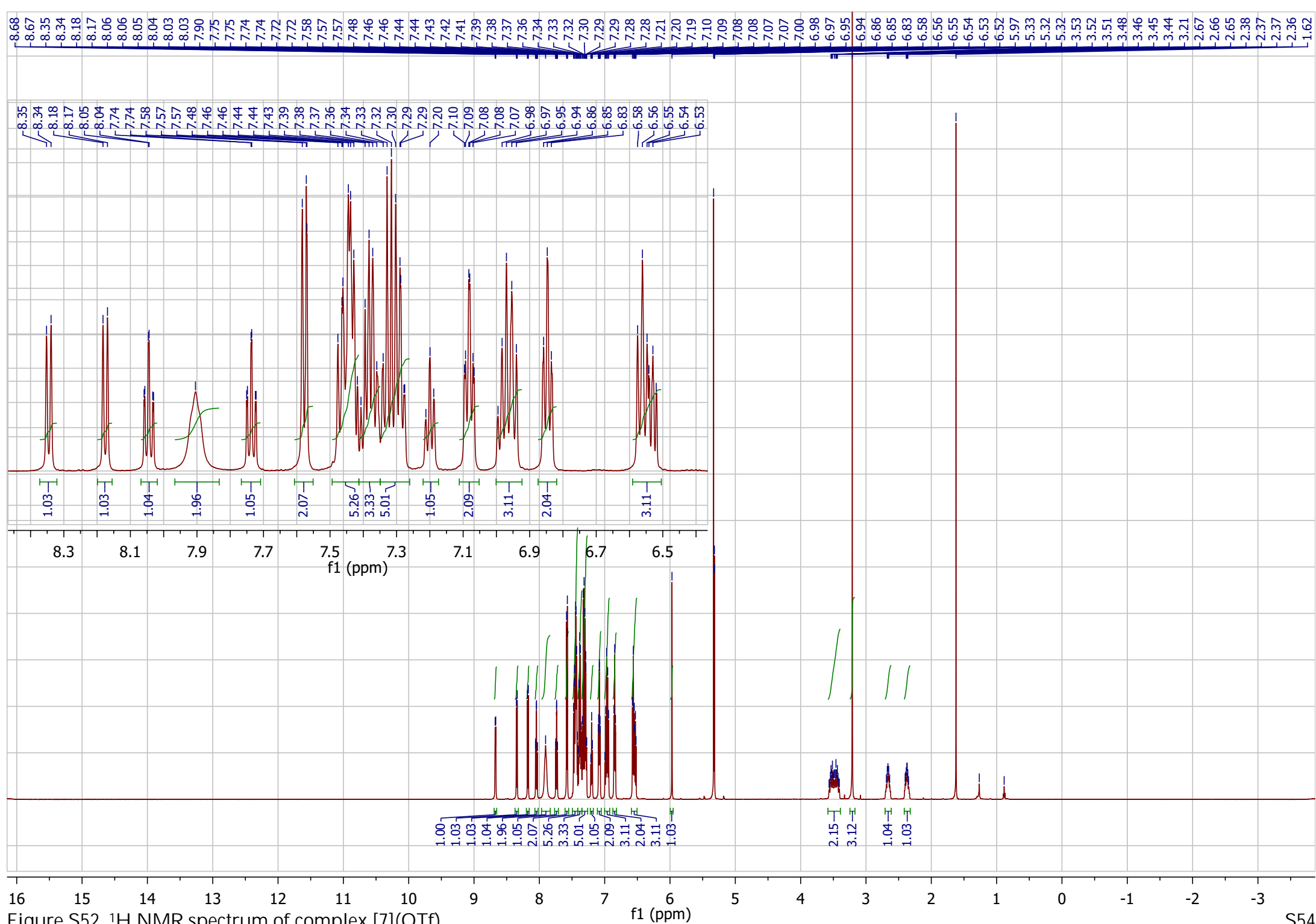




Figure S51. ^1H - ^{31}P HMBC NMR spectrum of complex $[6](\text{OTf})$.



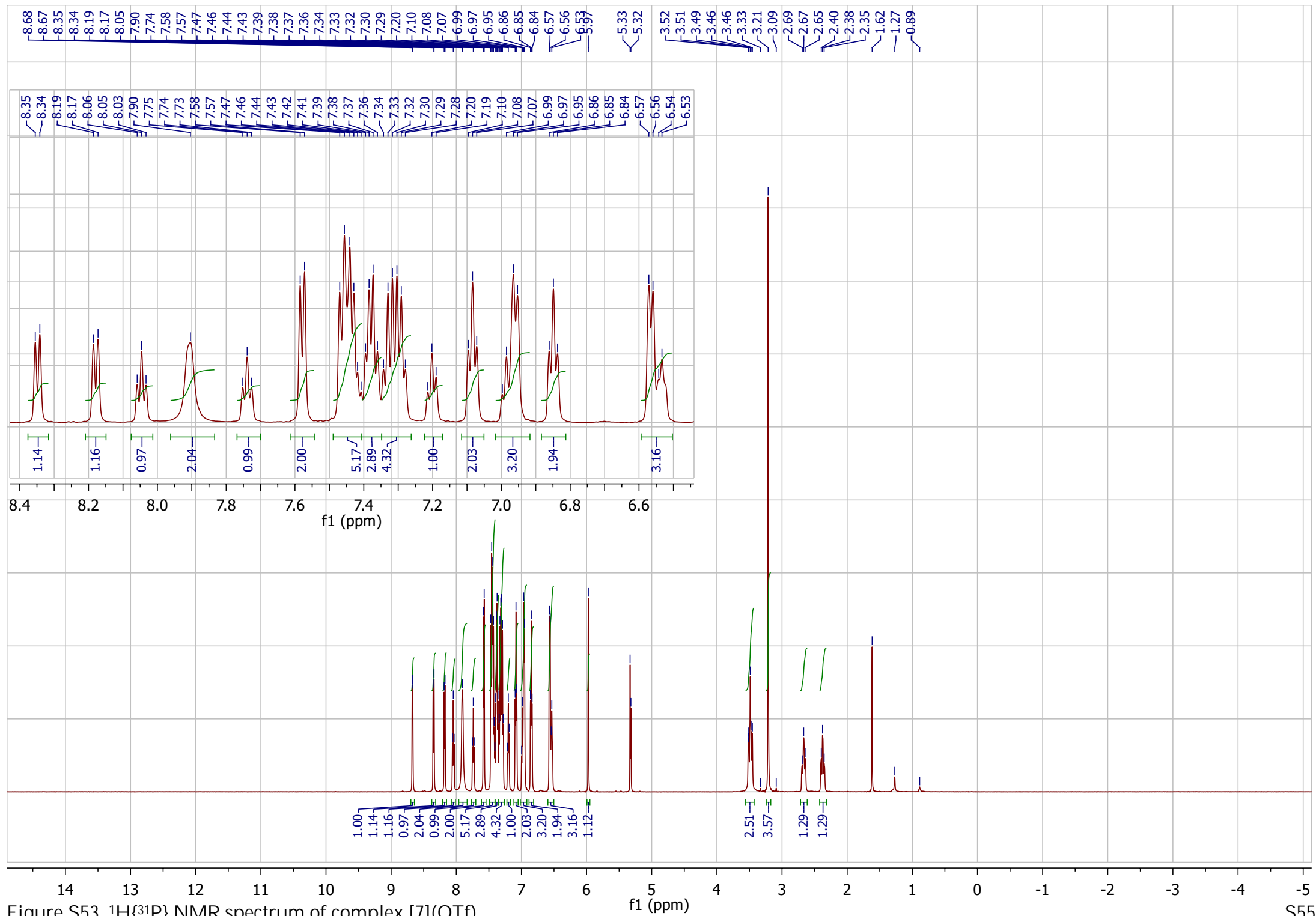


Figure S53. $^1\text{H}\{^{31}\text{P}\}$ NMR spectrum of complex [7](OTf).

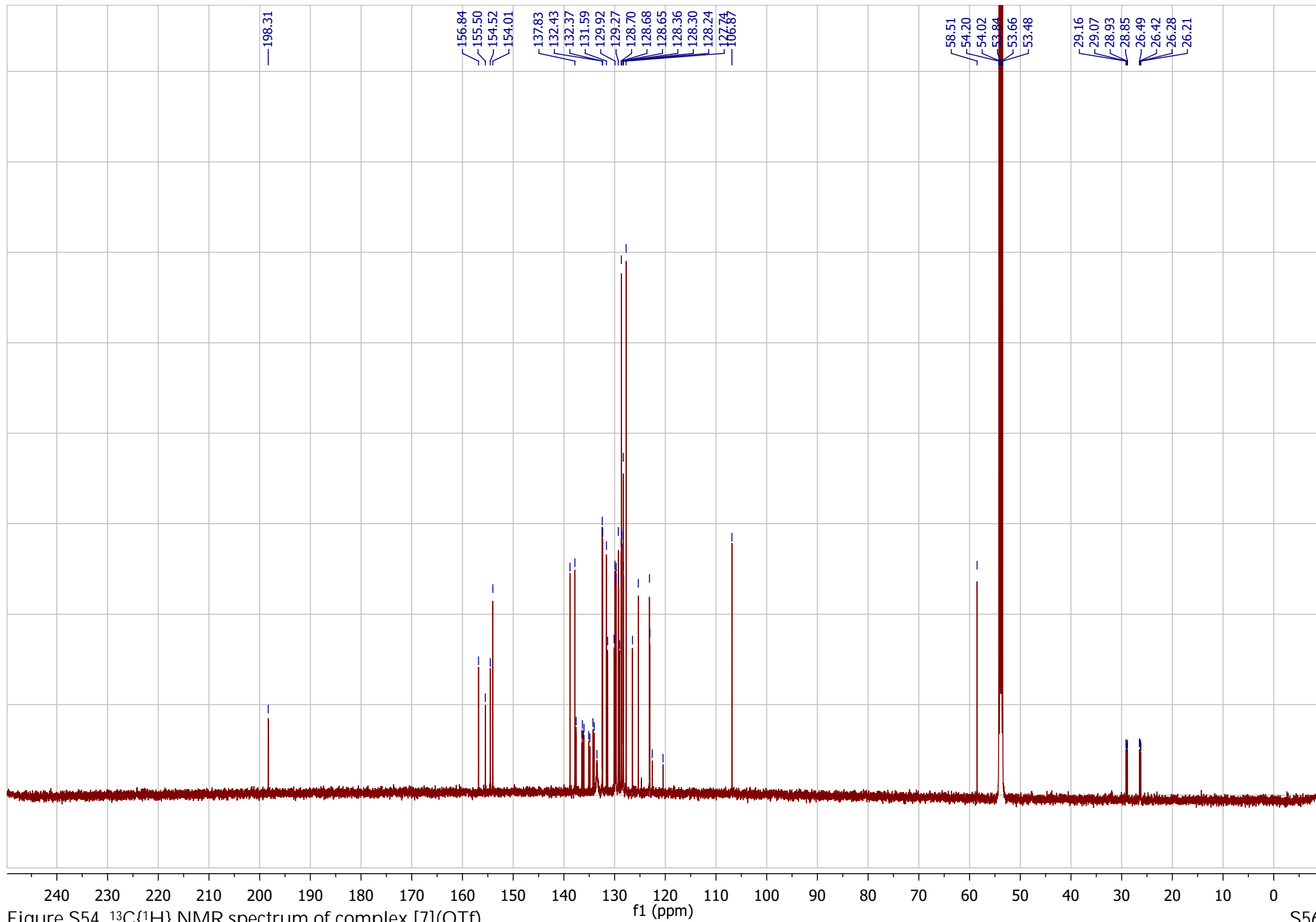


Figure S54. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of complex [7](OTf).

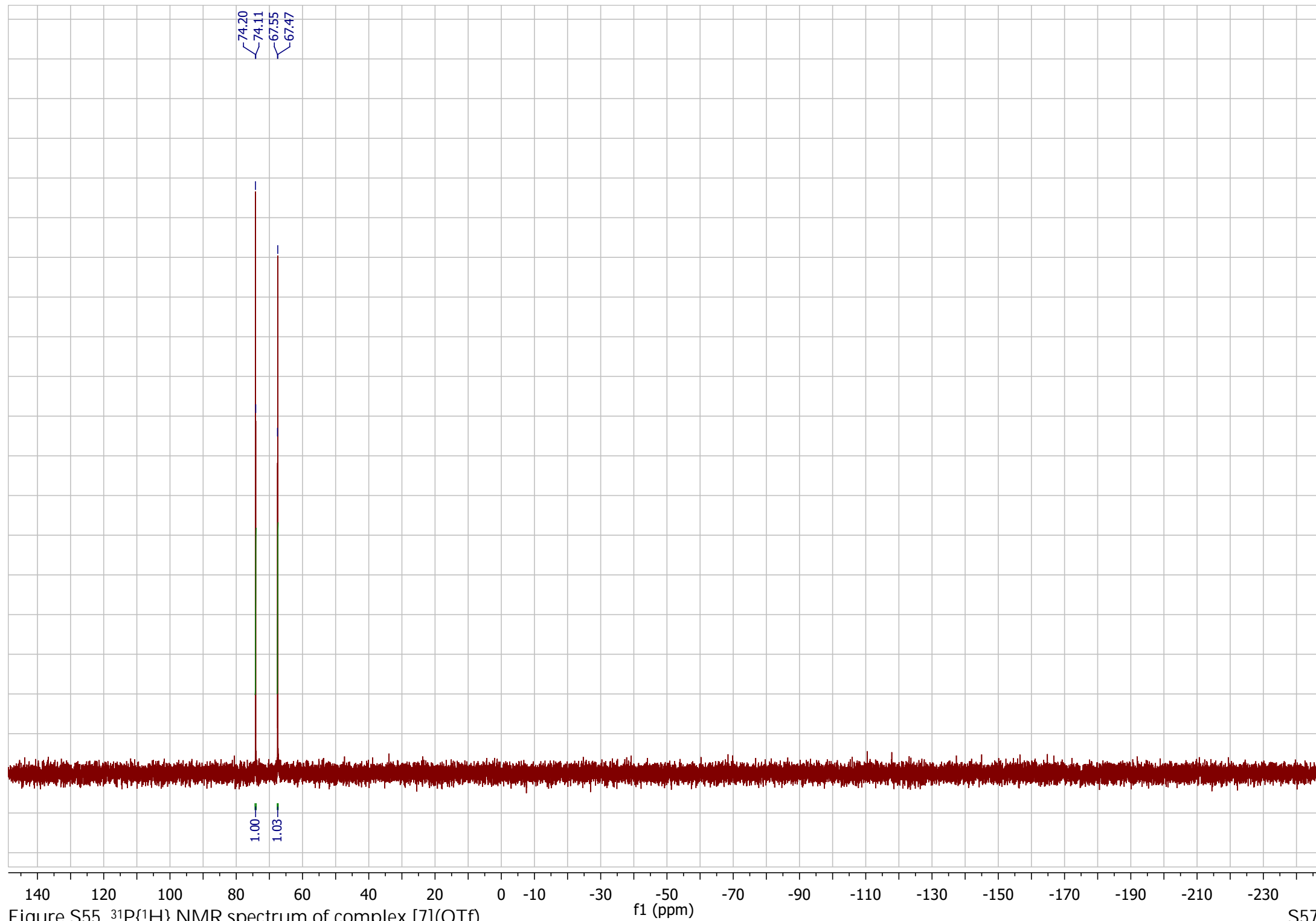
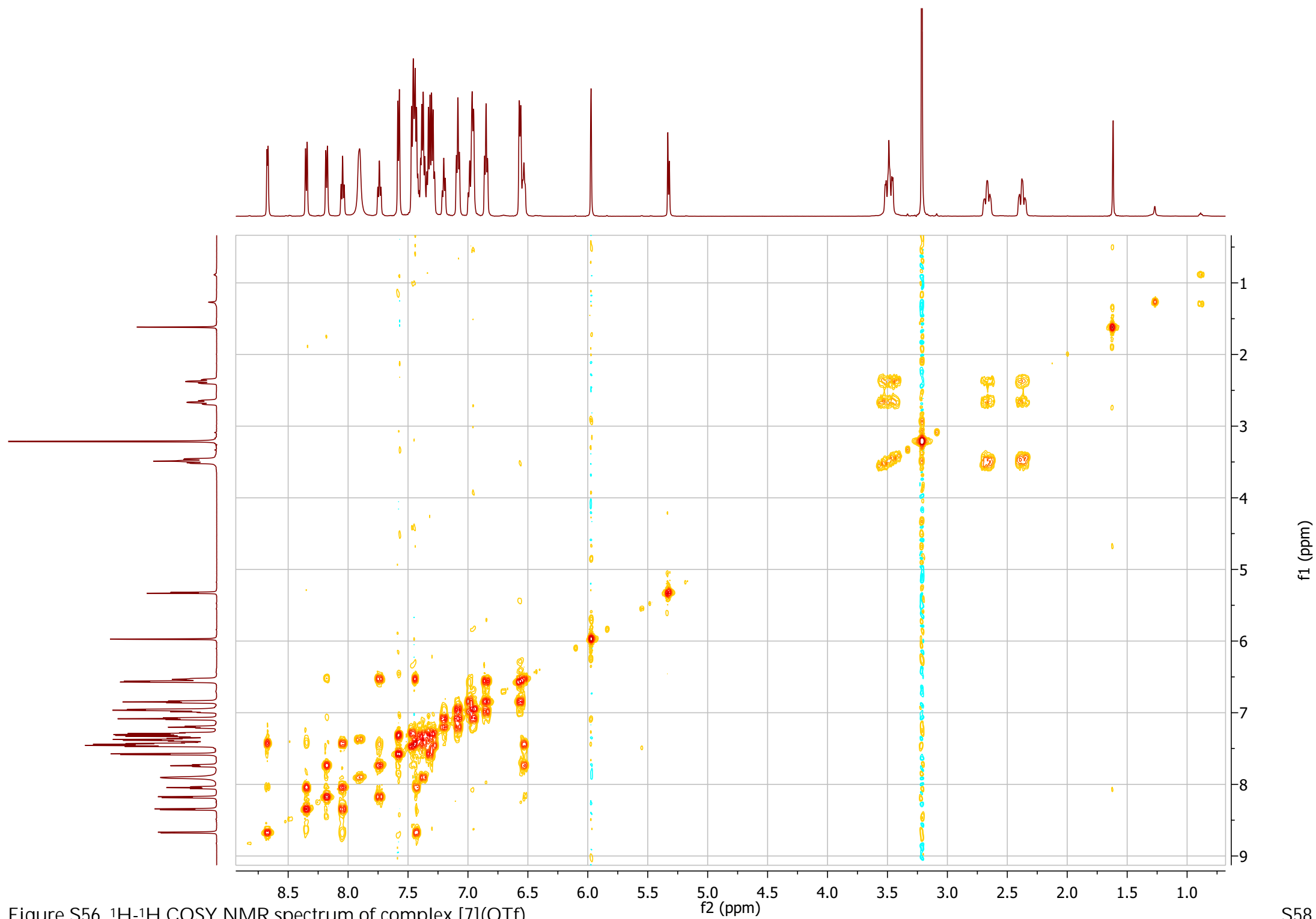


Figure S55. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of complex [7](OTf).



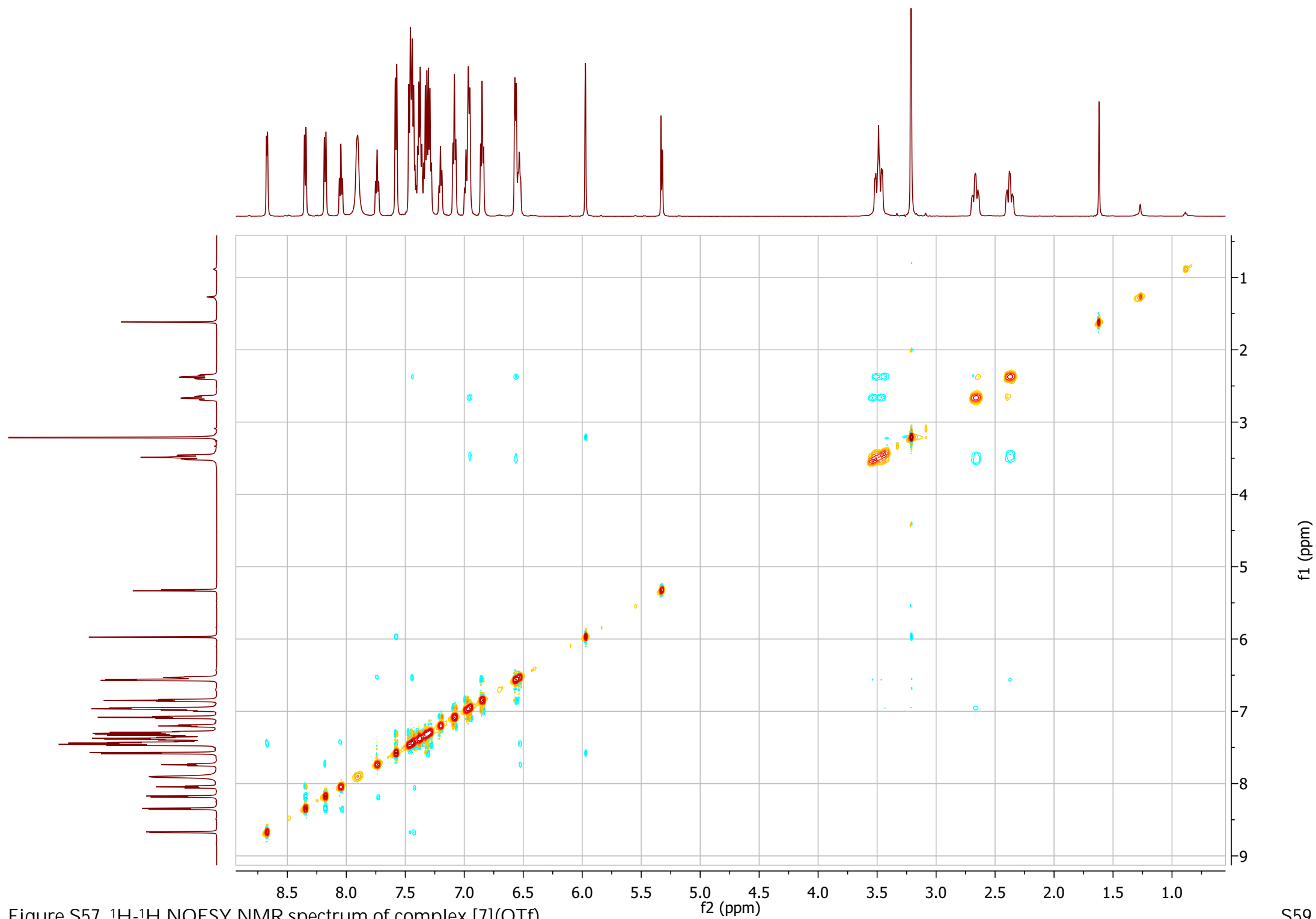
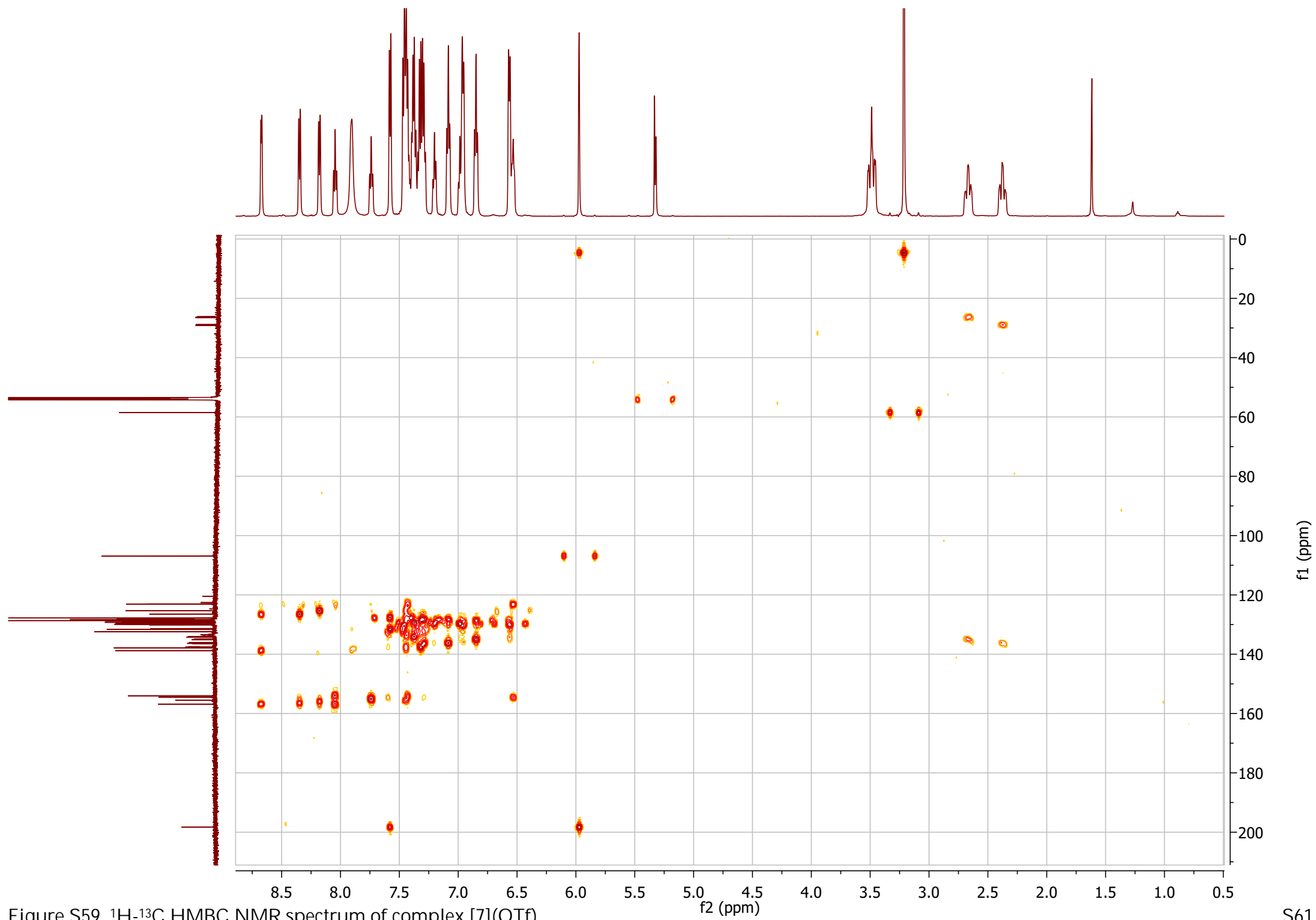


Figure S57. ^1H - ^1H NOESY NMR spectrum of complex $[7](\text{OTf})$.



Figure S58. ^1H - ^{13}C HSQC NMR spectrum of complex $[7](\text{OTf})$.



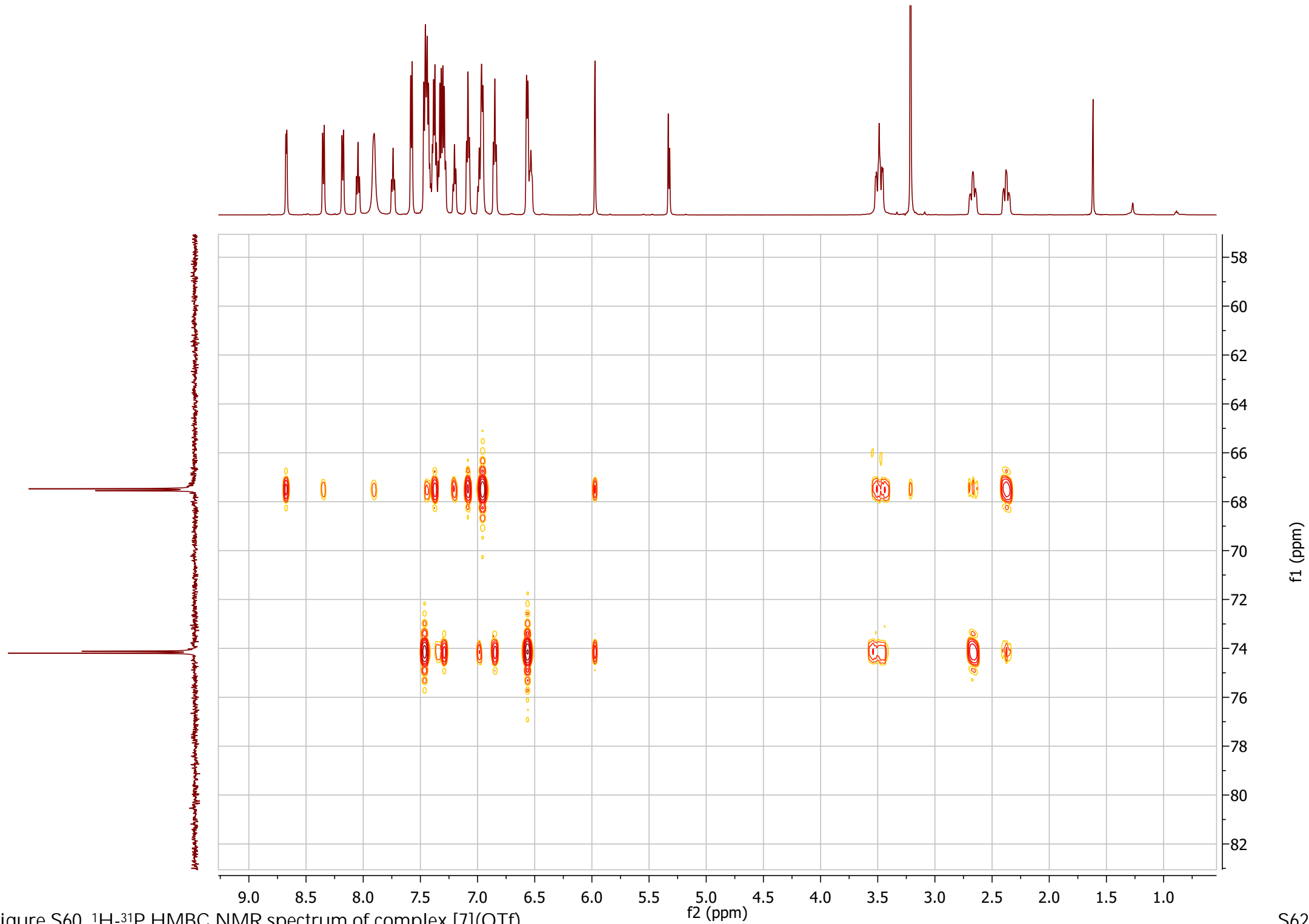
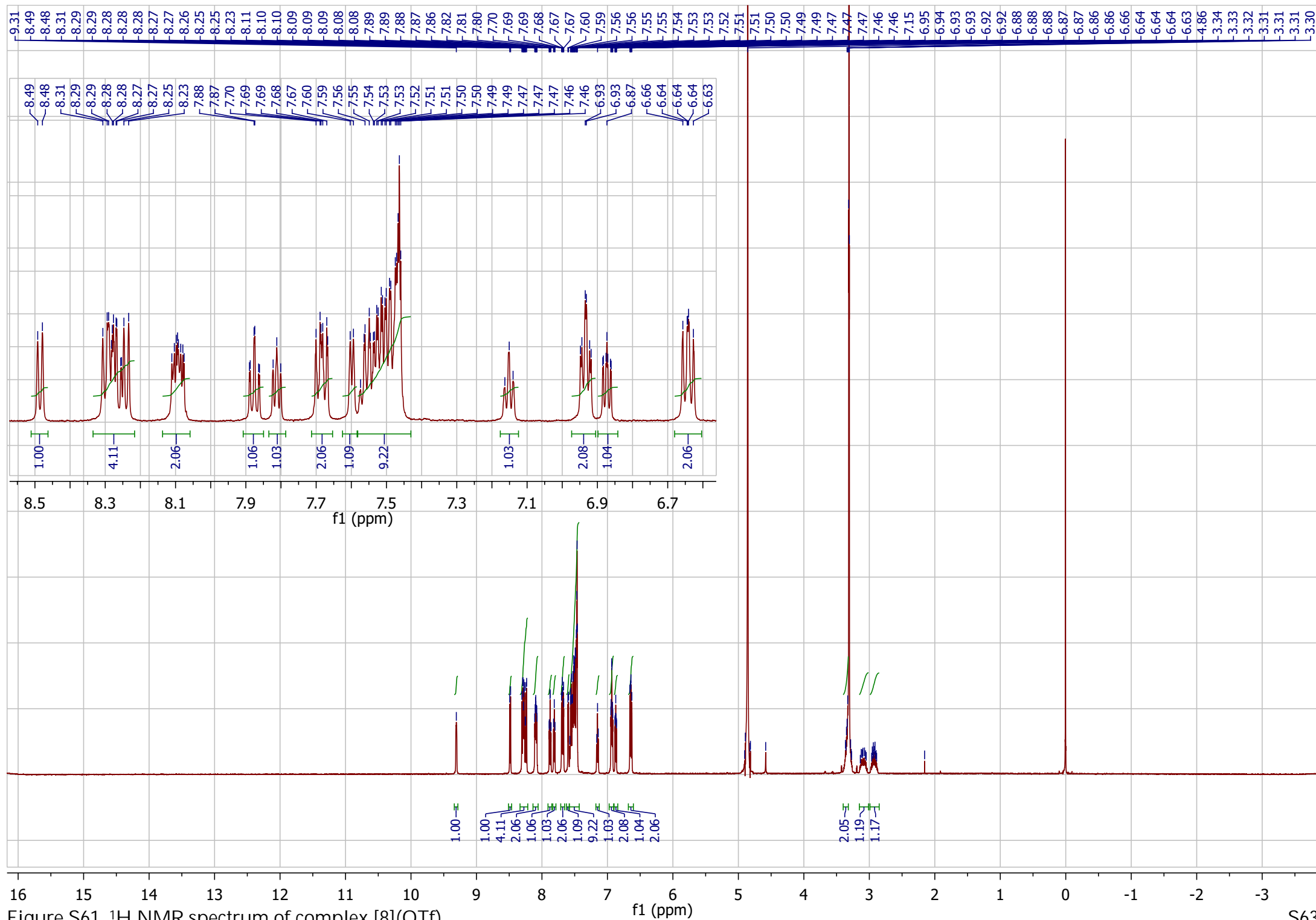


Figure S60. ^1H - ^{31}P HMBC NMR spectrum of complex $[7](\text{OTf})$.





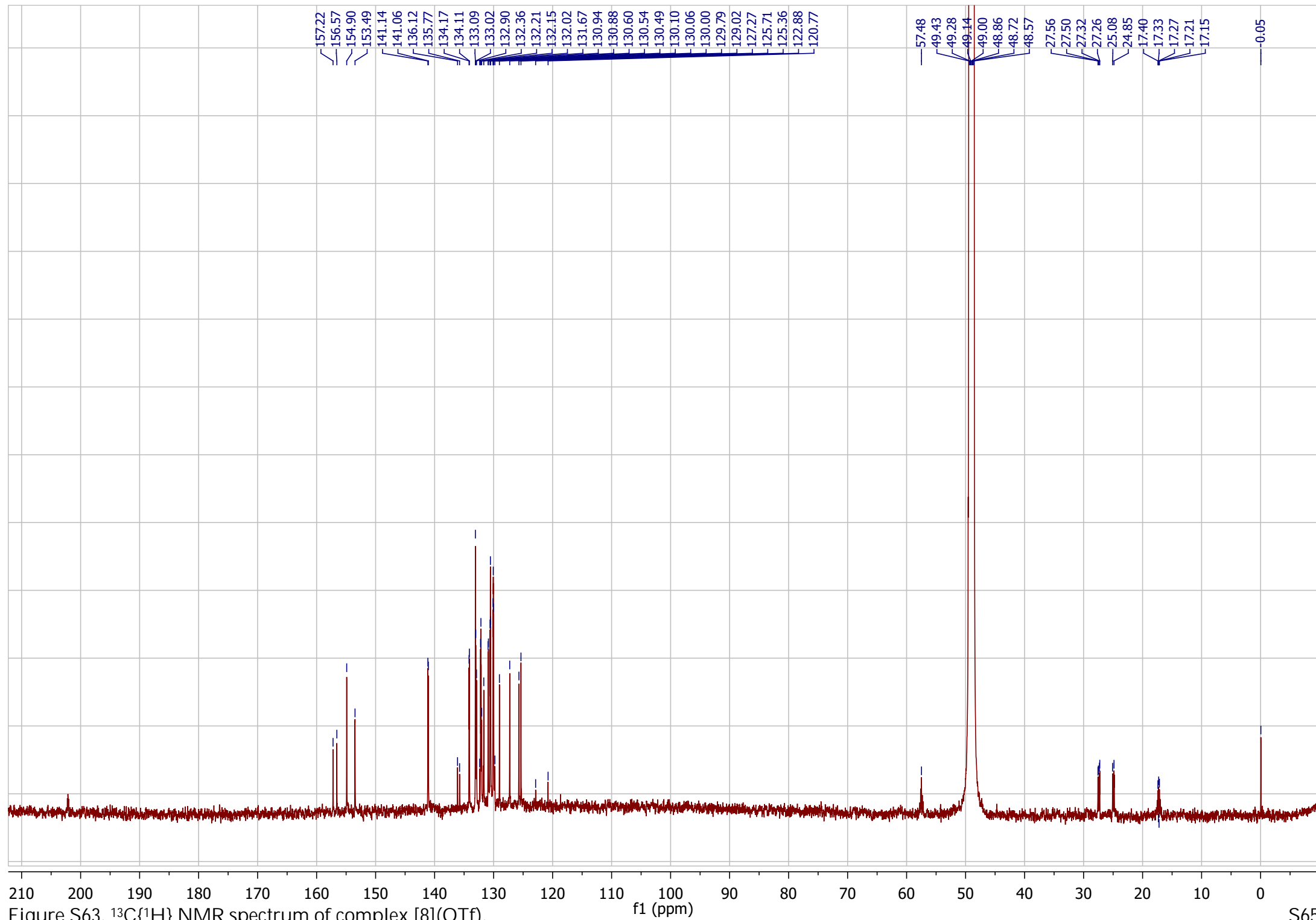


Figure S63. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of complex [8](OTf).

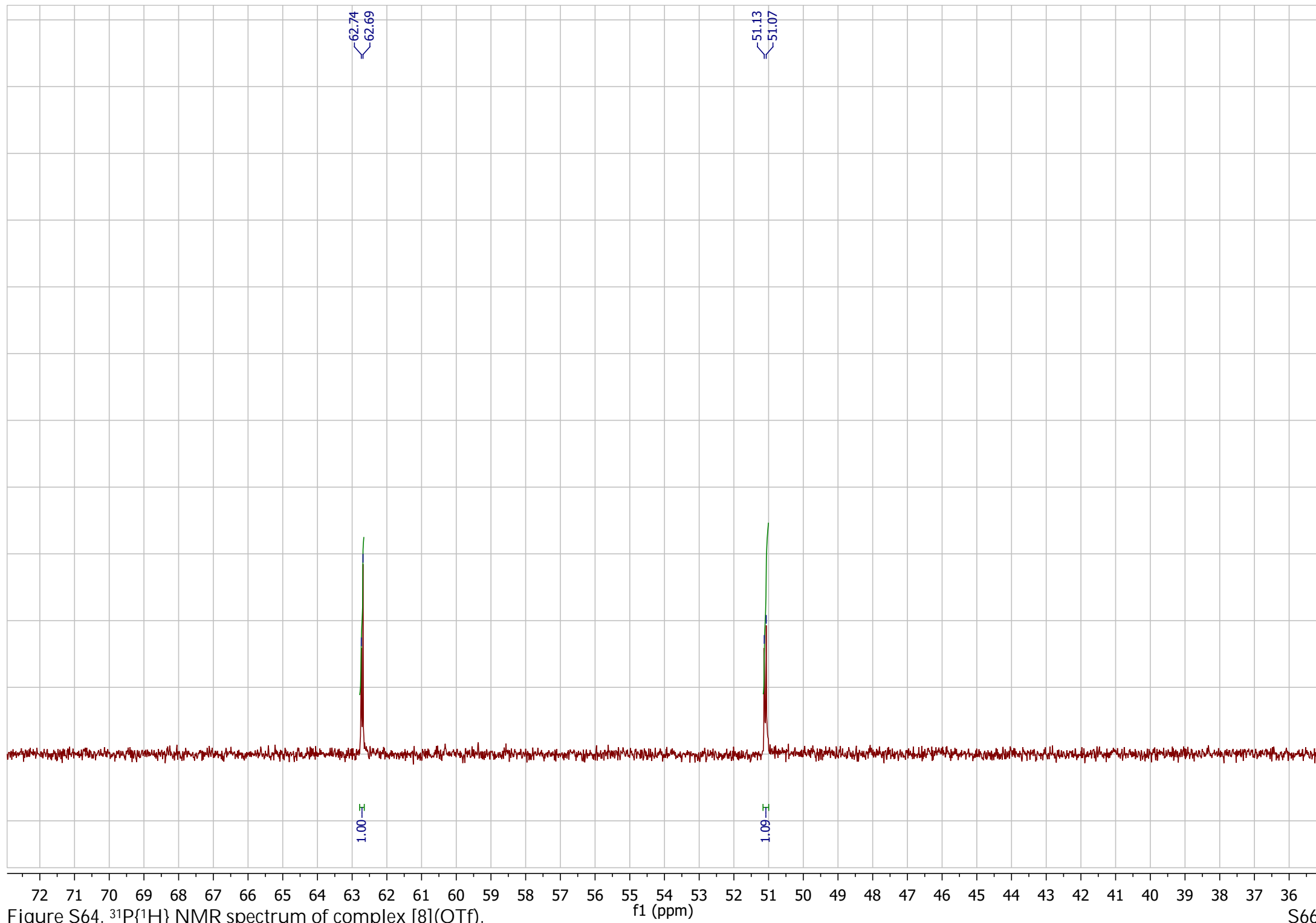
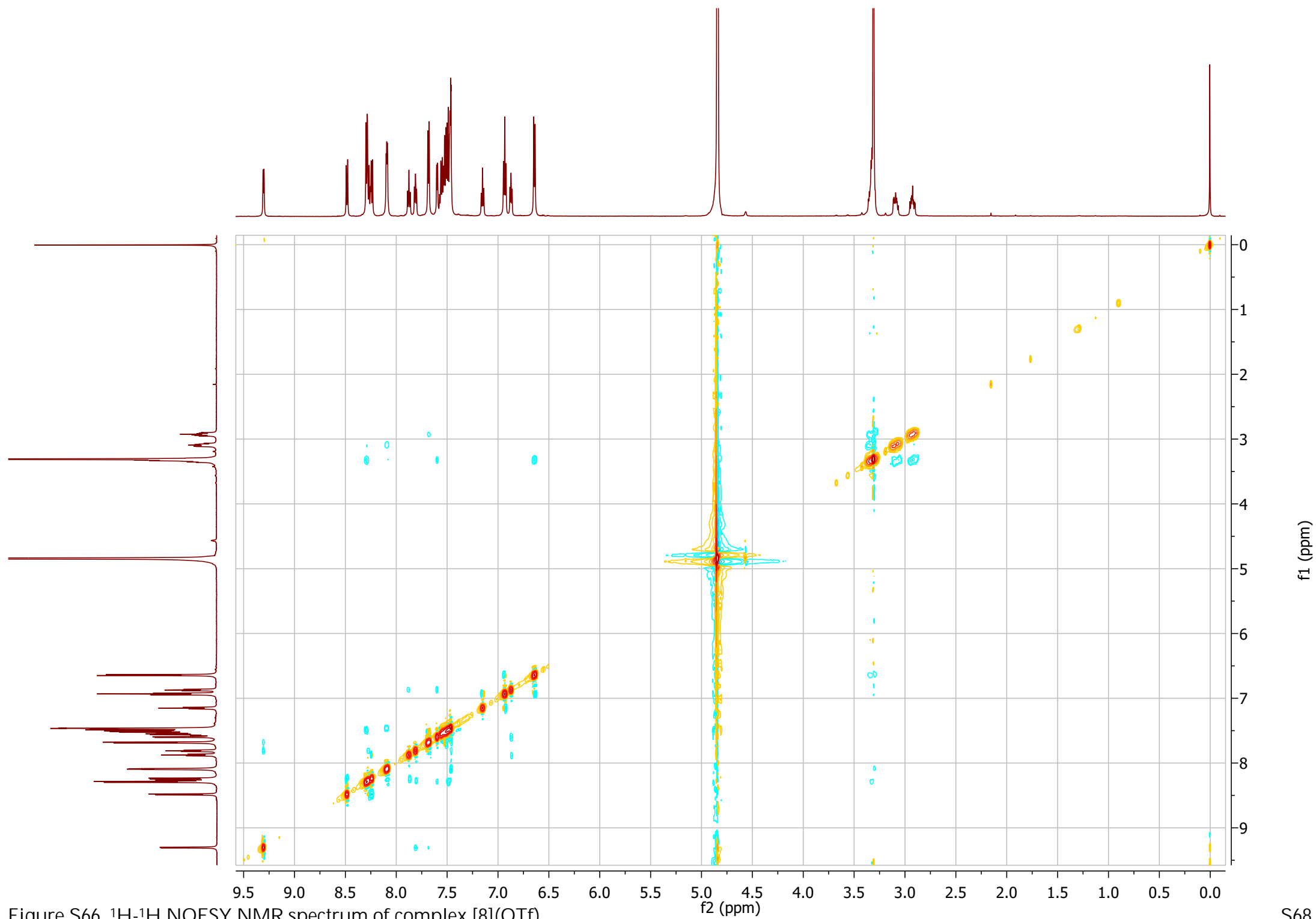


Figure S64. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of complex [8](OTf).



Figure S65. ^1H - ^1H COSY NMR spectrum of complex [8](OTf).



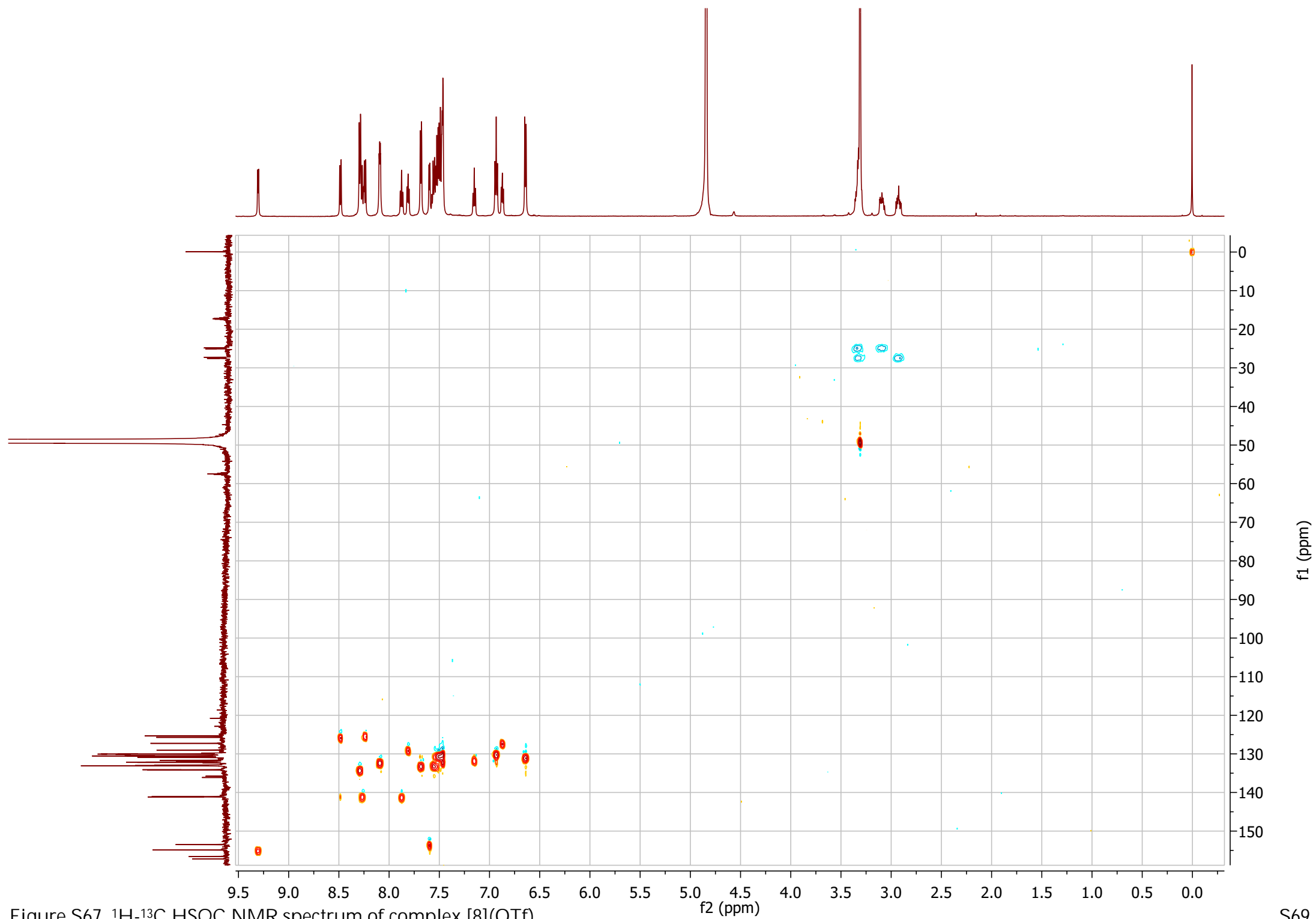


Figure S67. ^1H - ^{13}C HSQC NMR spectrum of complex $[8](\text{OTf})$.

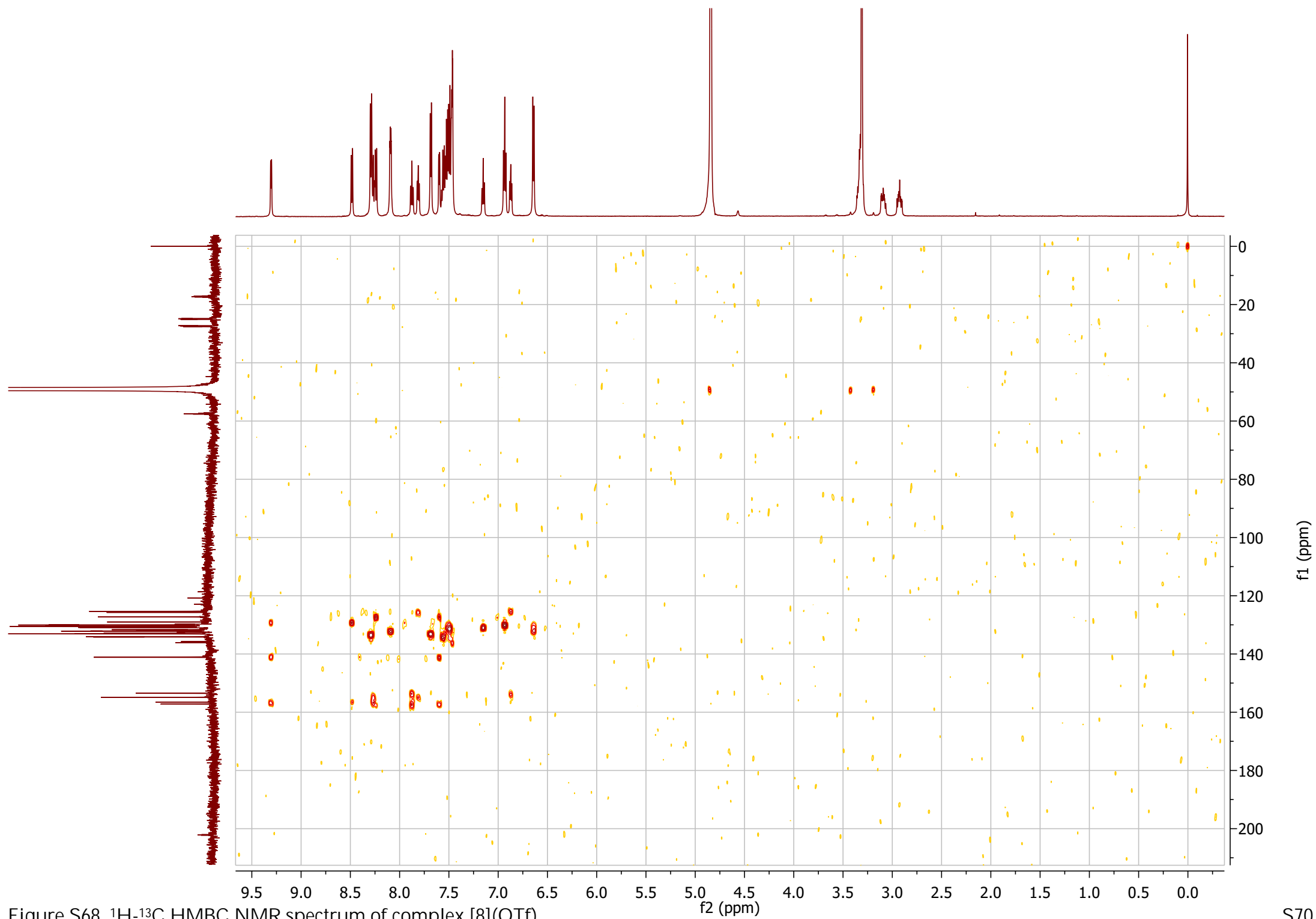


Figure S68. ^1H - ^{13}C HMBC NMR spectrum of complex $[8](\text{OTf})$.

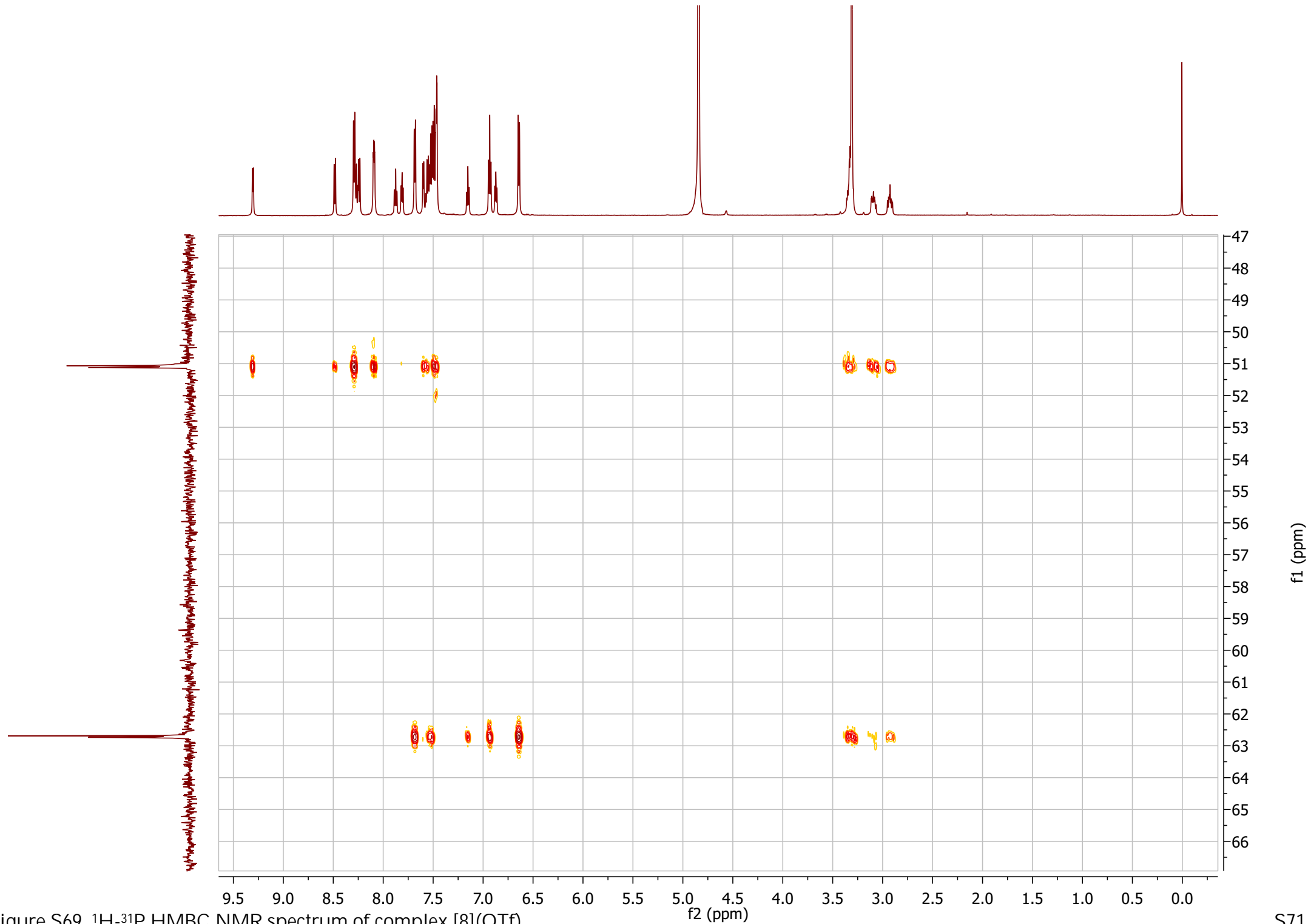


Figure S69. ^1H - ^{31}P HMBC NMR spectrum of complex $[8](\text{OTf})$.

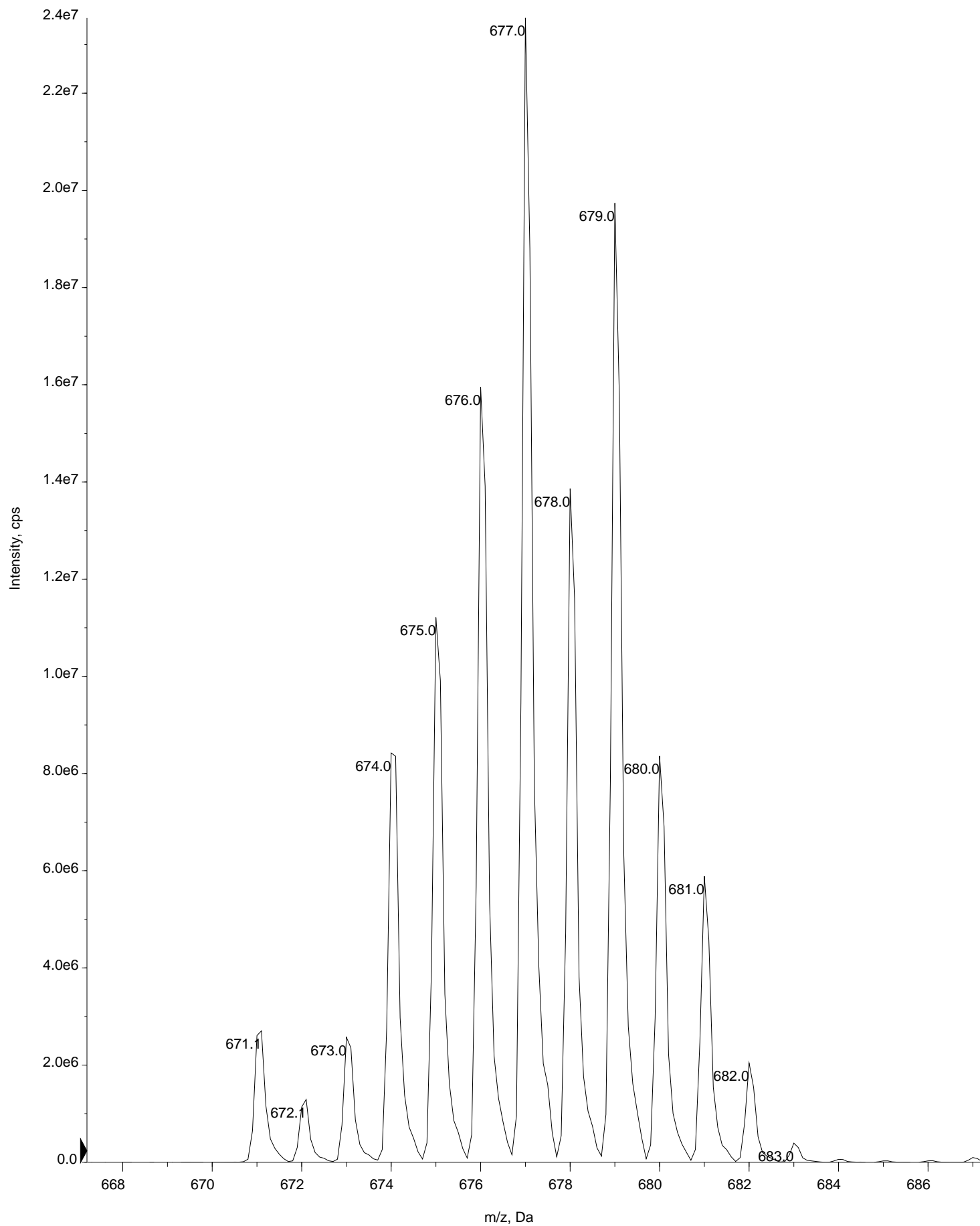


Figure S70. Experimental ESI mass spectrum of $[1\text{-Cl}]^+$ in methanol (positive mode).

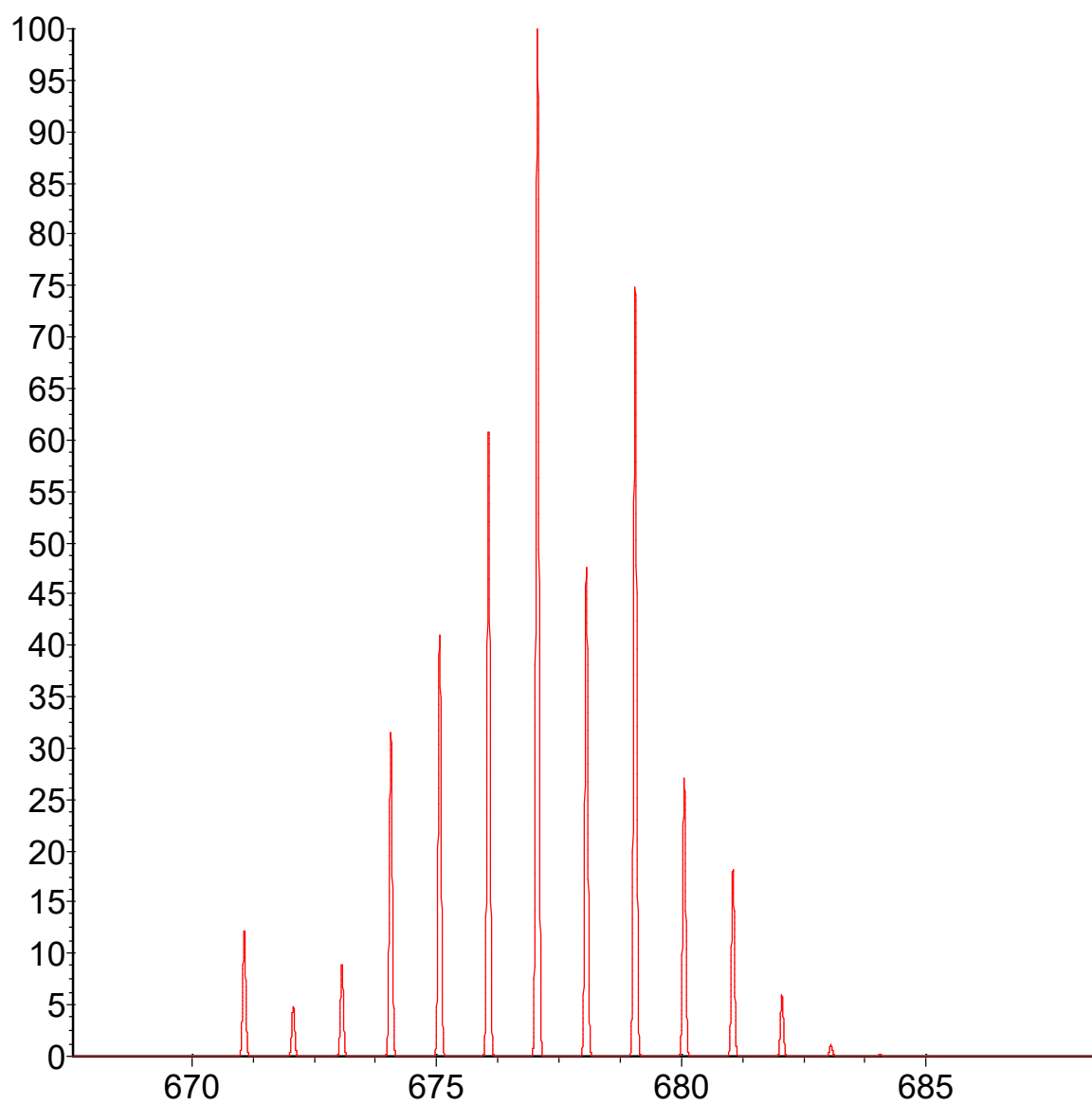


Figure S71. Simulated isotopic distribution pattern of $[1\text{-Cl}]^+$.

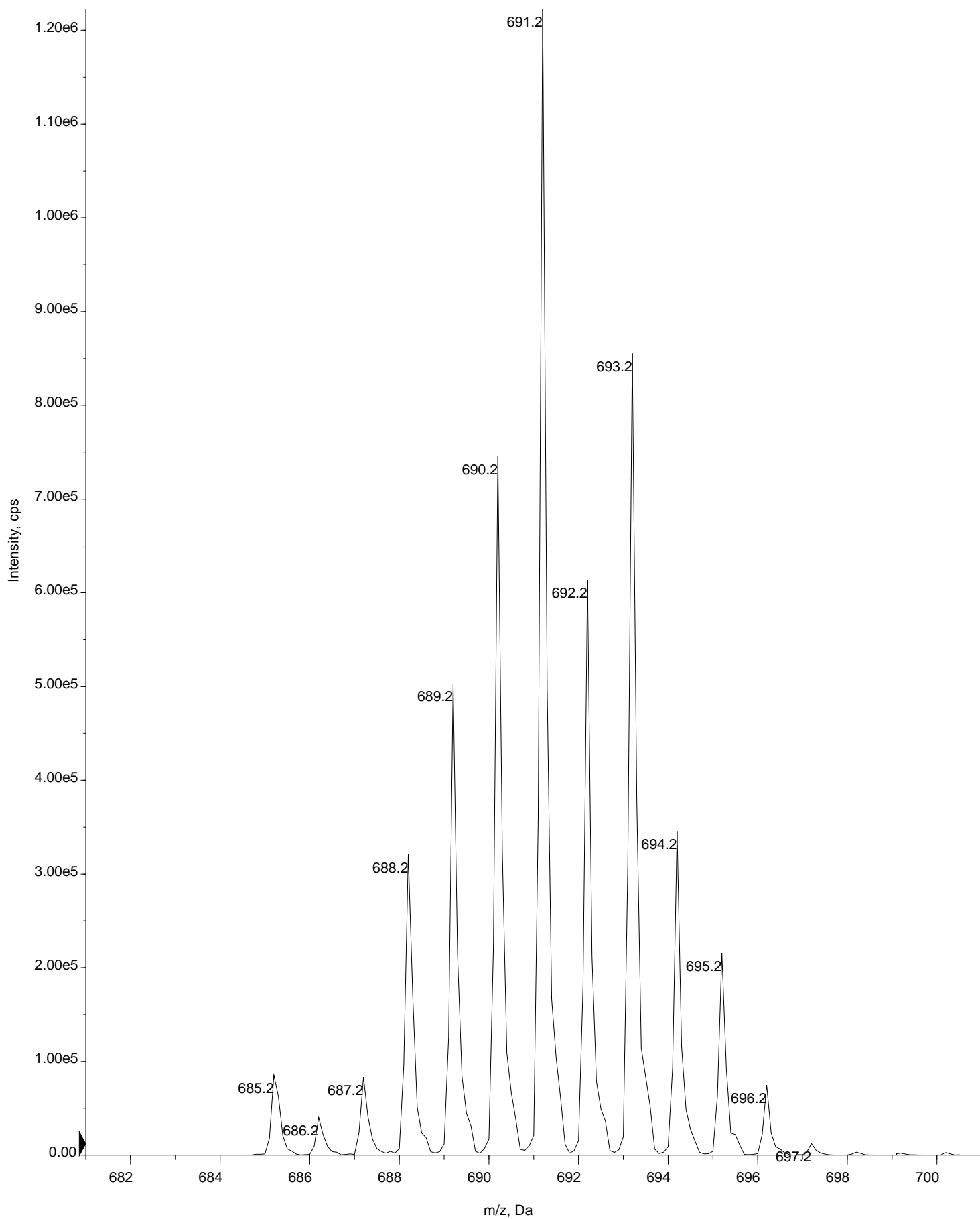


Figure S72. Experimental ESI mass spectrum of $[2\text{-Cl}]^+$ in methanol (positive mode).

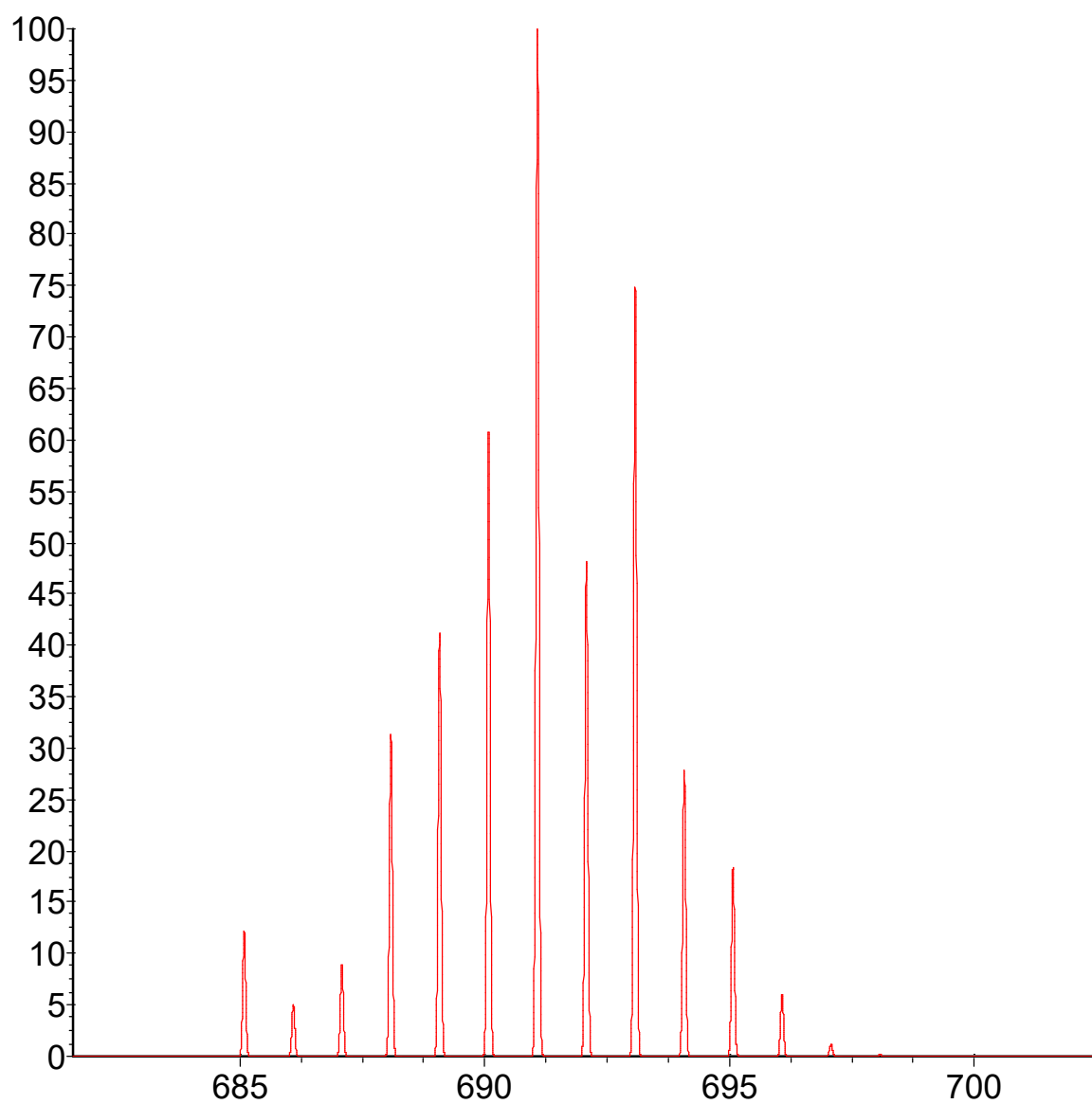


Figure S73. Simulated isotopic distribution pattern of $[2\text{-Cl}]^+$.

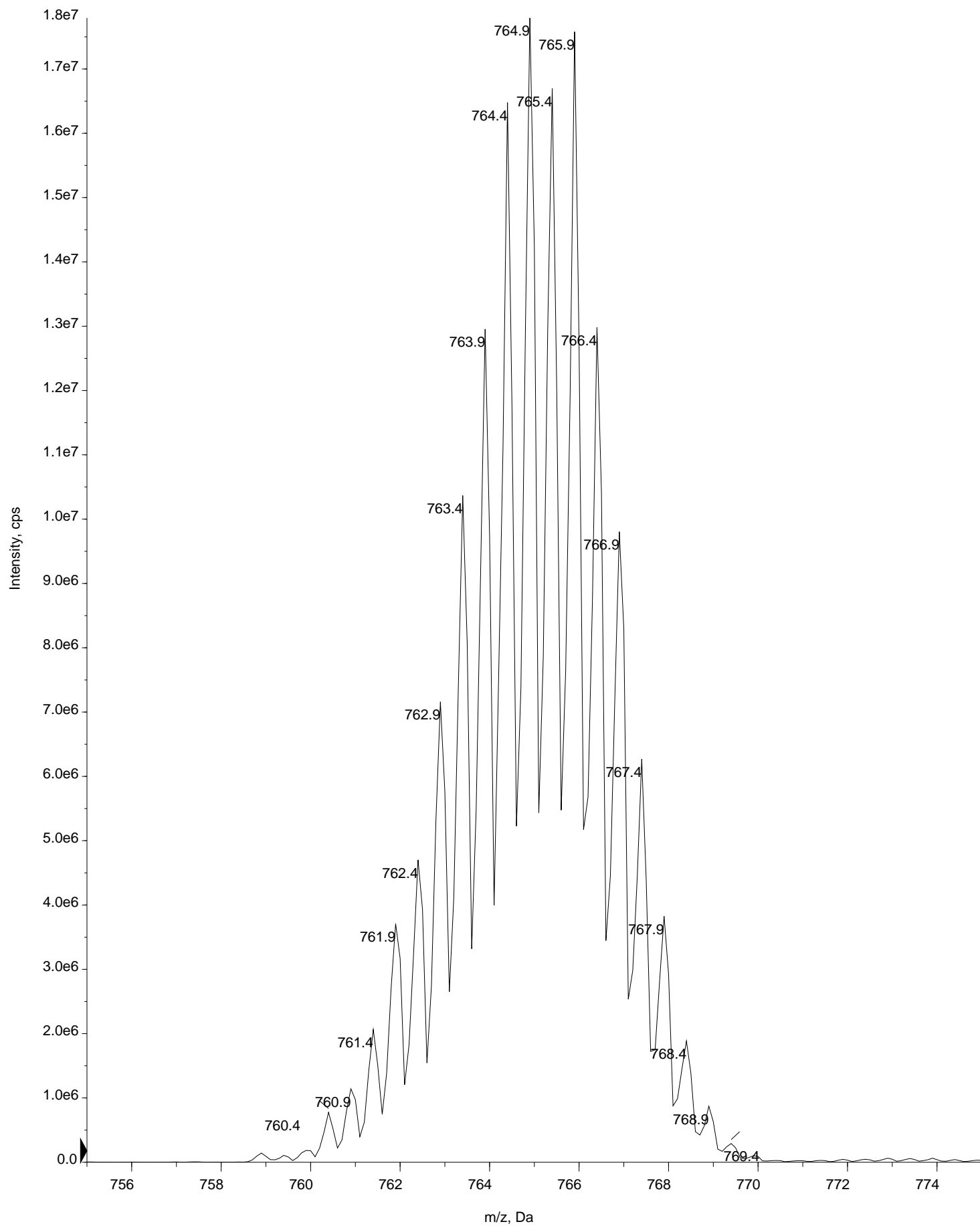


Figure S74. Experimental ESI mass spectrum of $[3]^{2+}$ in methanol (positive mode).

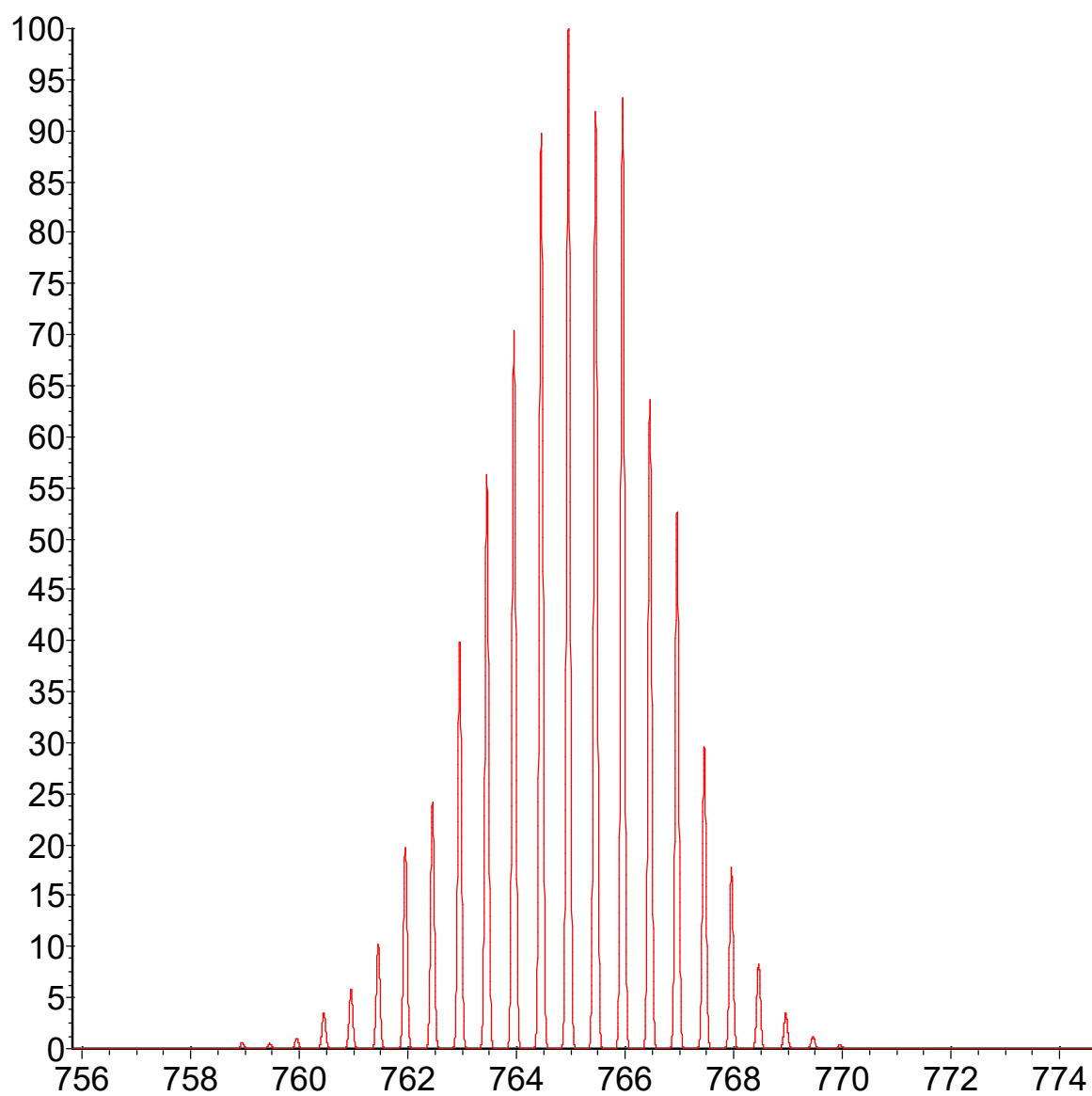


Figure S75. Simulated isotopic distribution pattern of $[3]^{2+}$.

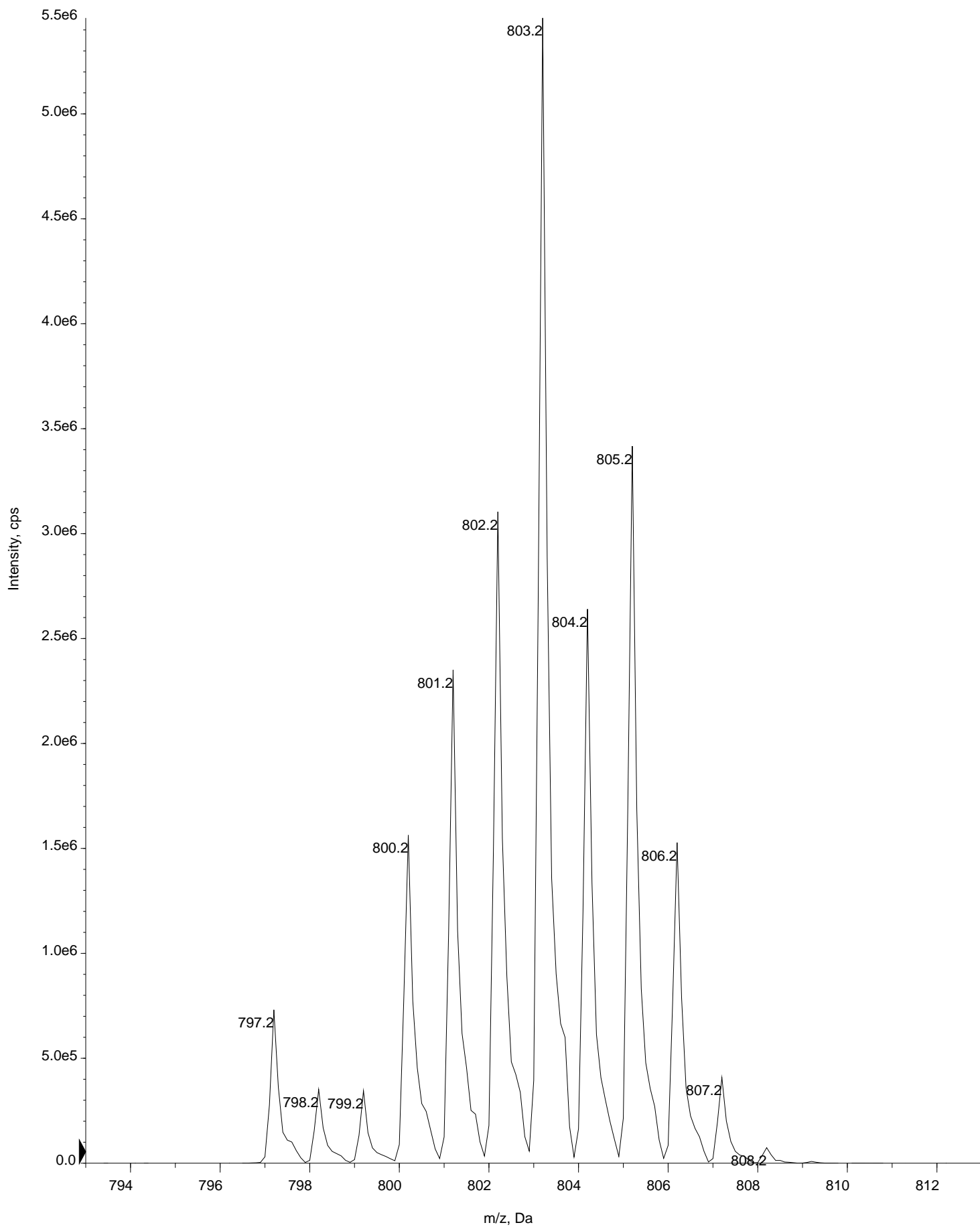


Figure S76. Experimental ESI mass spectrum of [4]⁺ in methanol (positive mode).

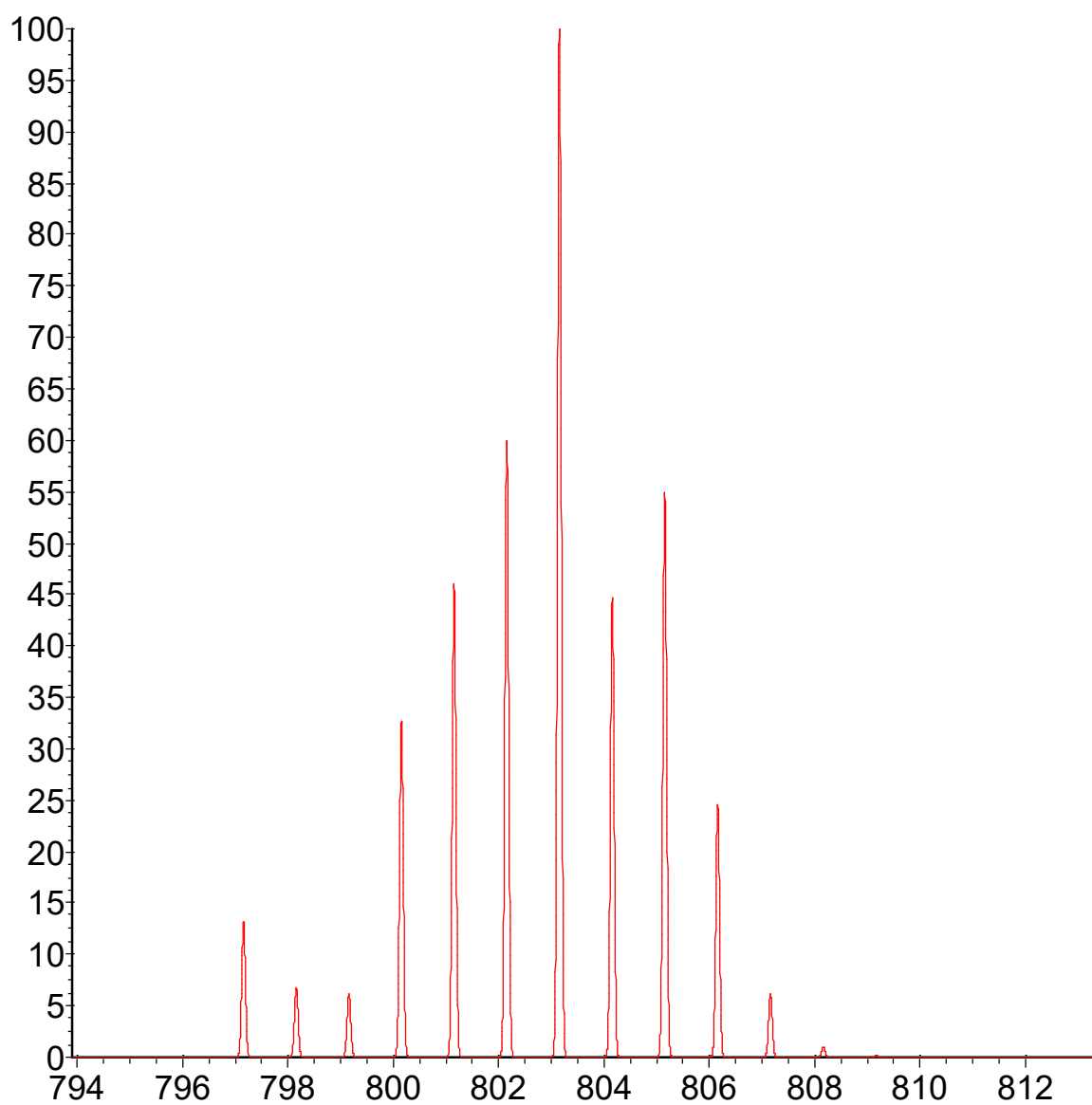


Figure S77. Simulated isotopic distribution pattern of [4]⁺.

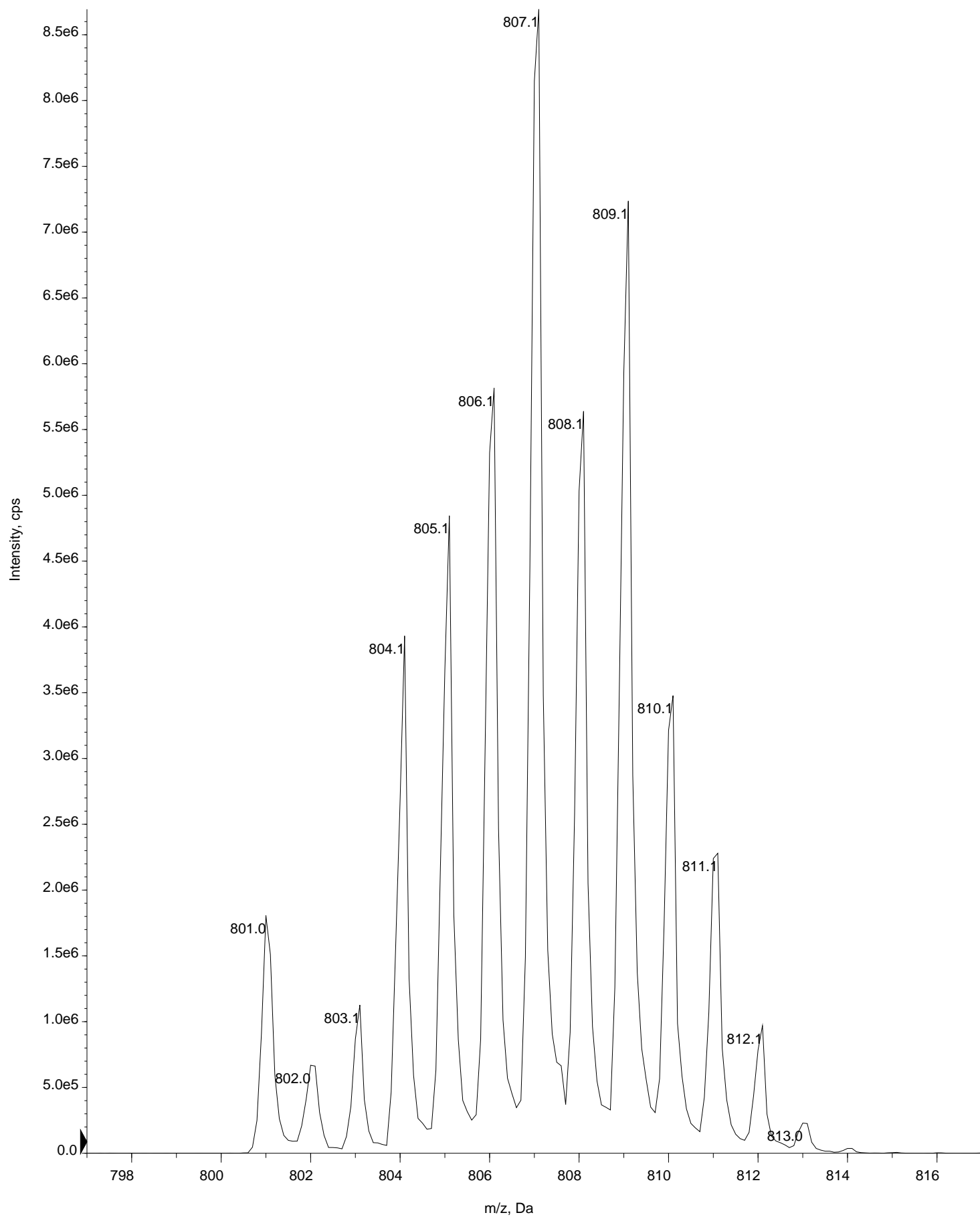


Figure S78. Experimental ESI mass spectrum of $[5]^+$ in methanol (positive mode).

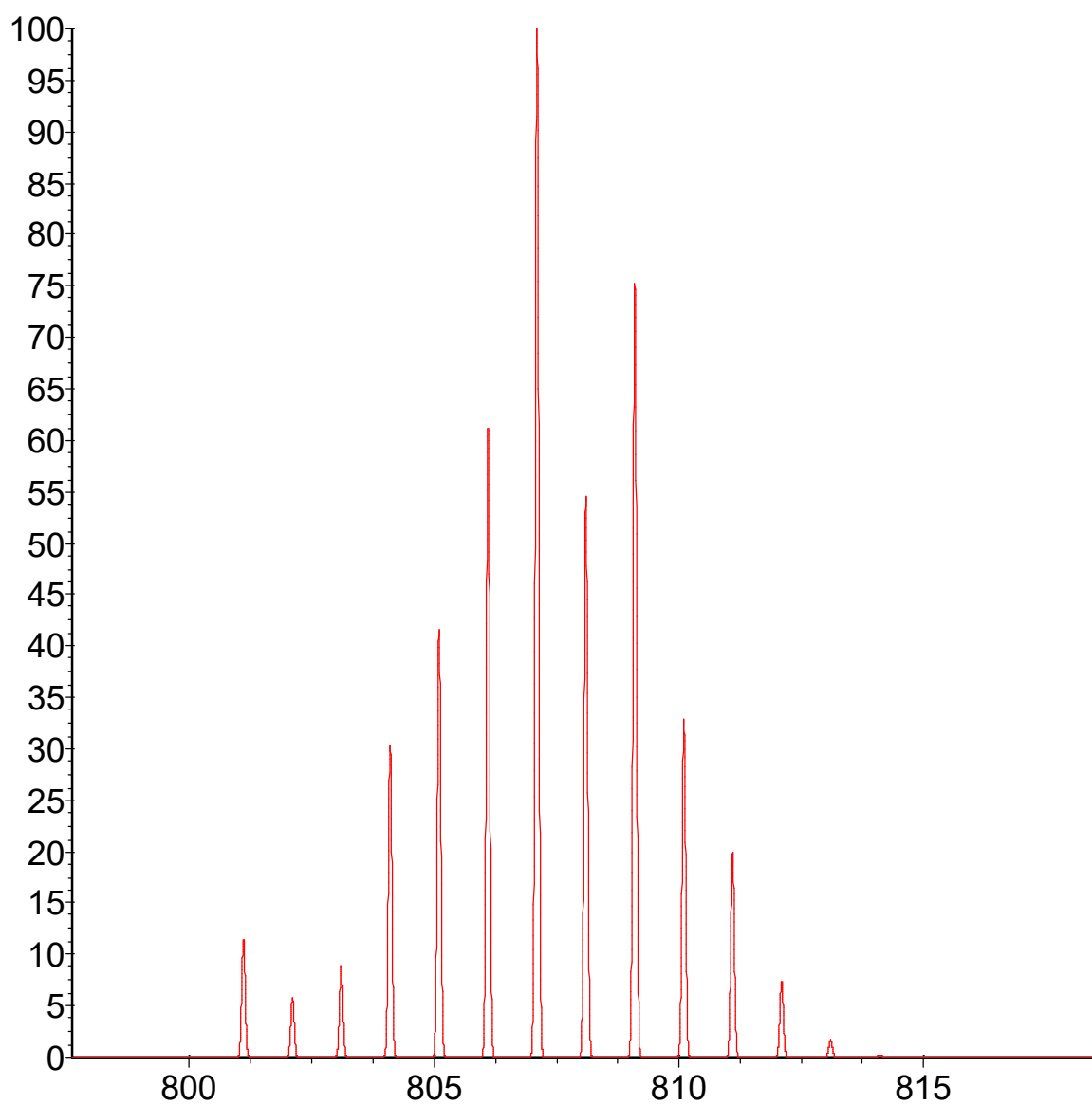


Figure S79. Simulated isotopic distribution pattern of $[5]^+$.

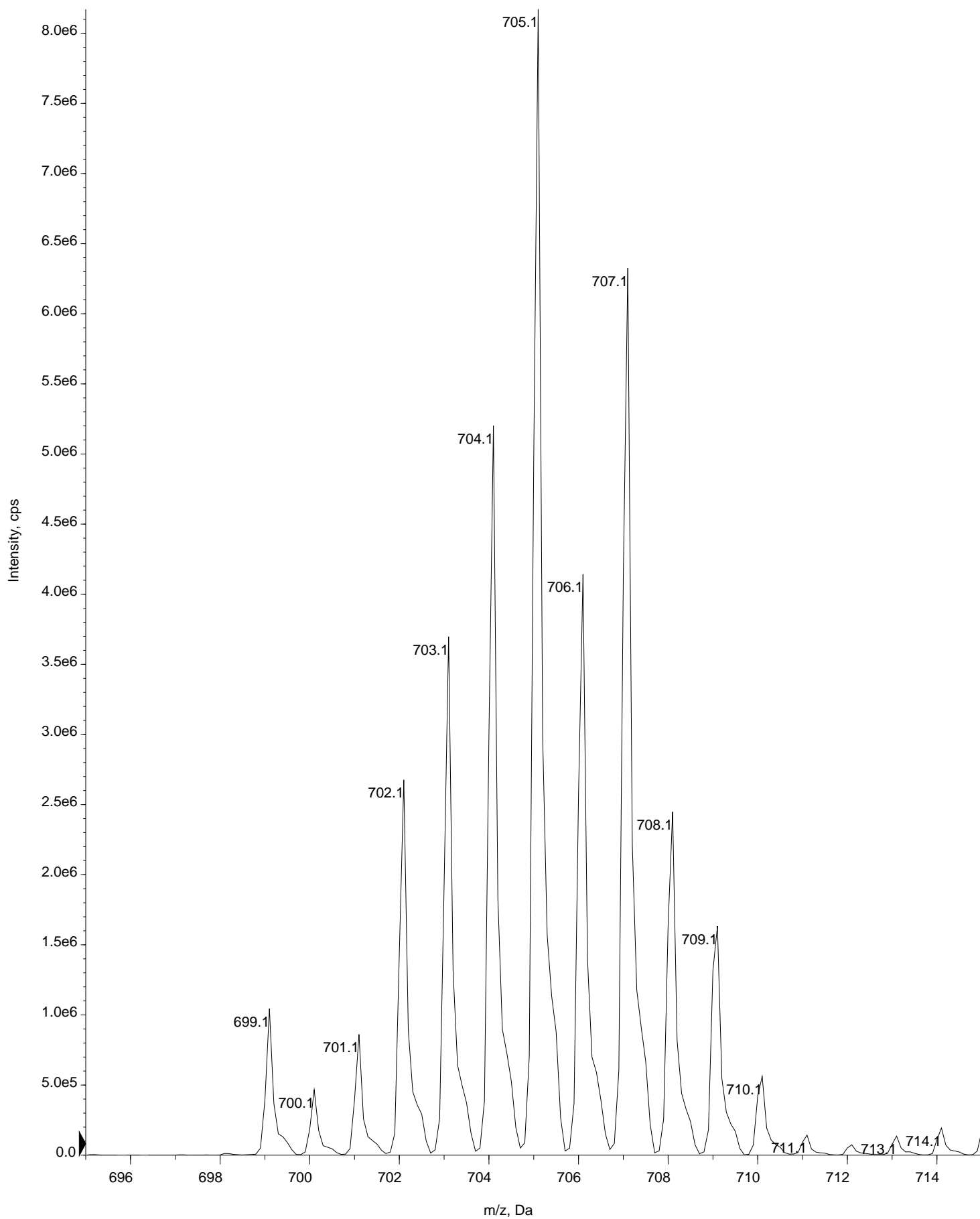


Figure S80. Experimental ESI mass spectrum of $[6]^+$ in methanol (positive mode).

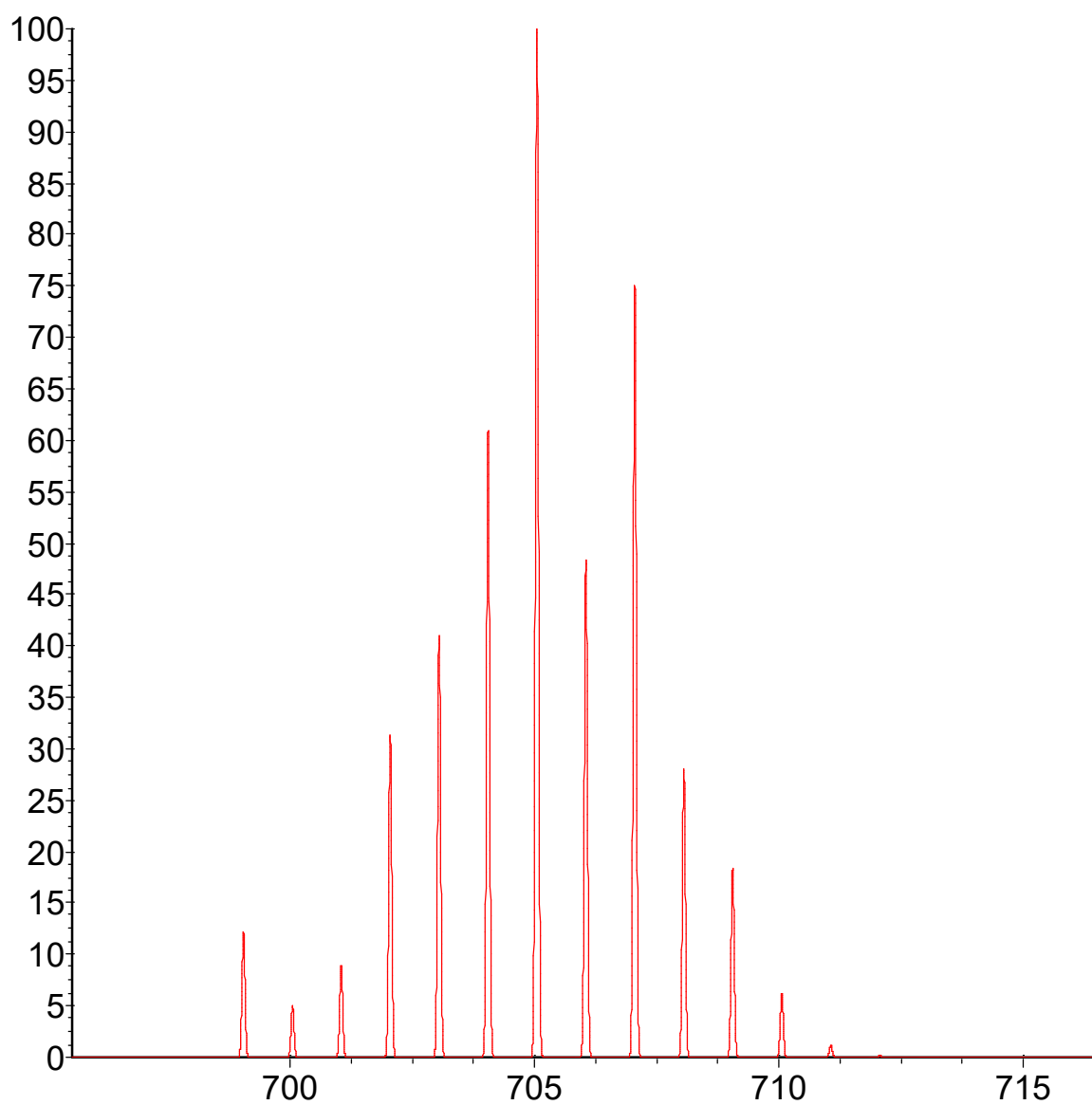


Figure S81. Simulated isotopic distribution pattern of $[6]^+$.

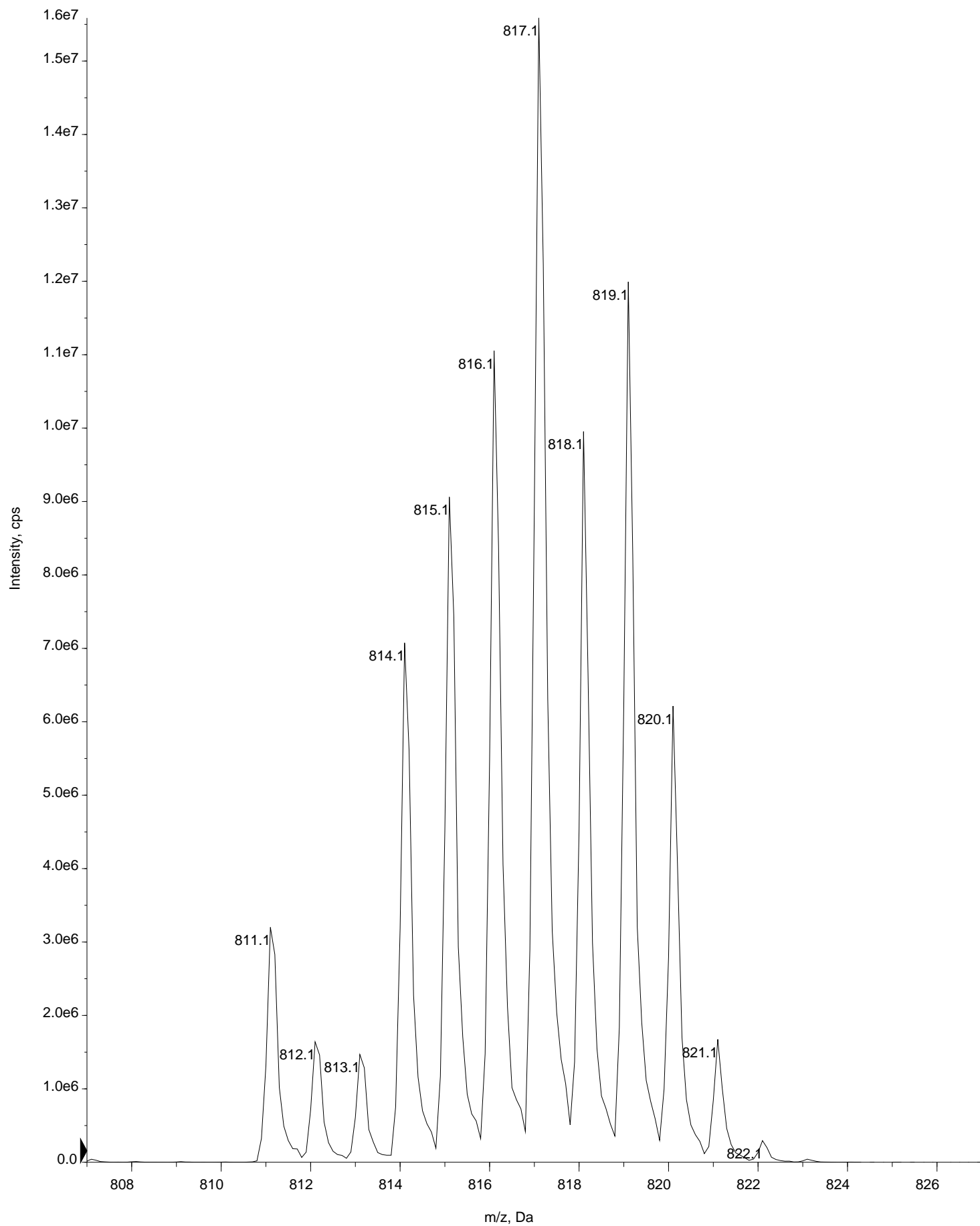


Figure S82. Experimental ESI mass spectrum of $[7]^+$ in methanol (positive mode).

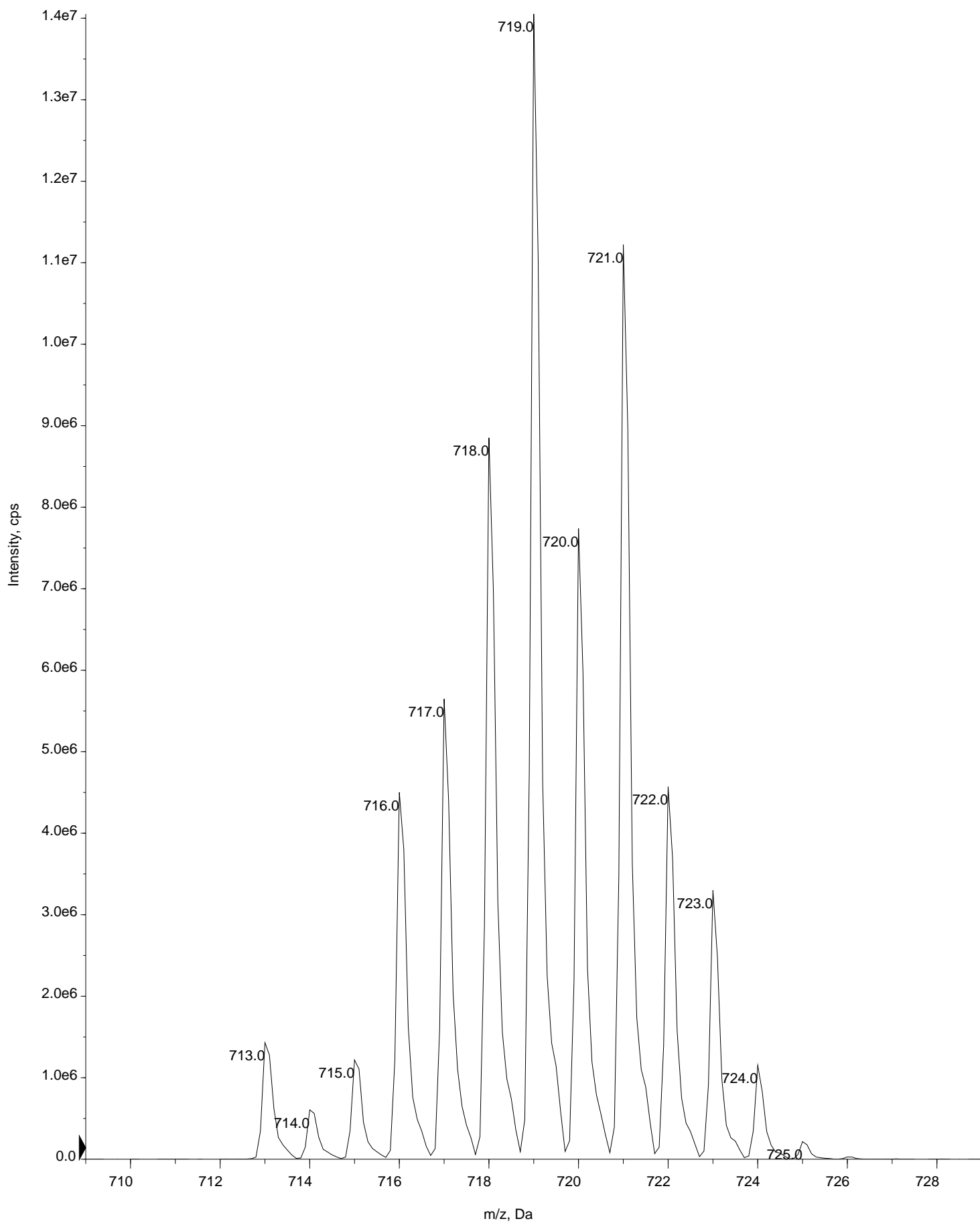


Figure S84. Experimental ESI mass spectrum of $[8]^+$ in methanol (positive mode).

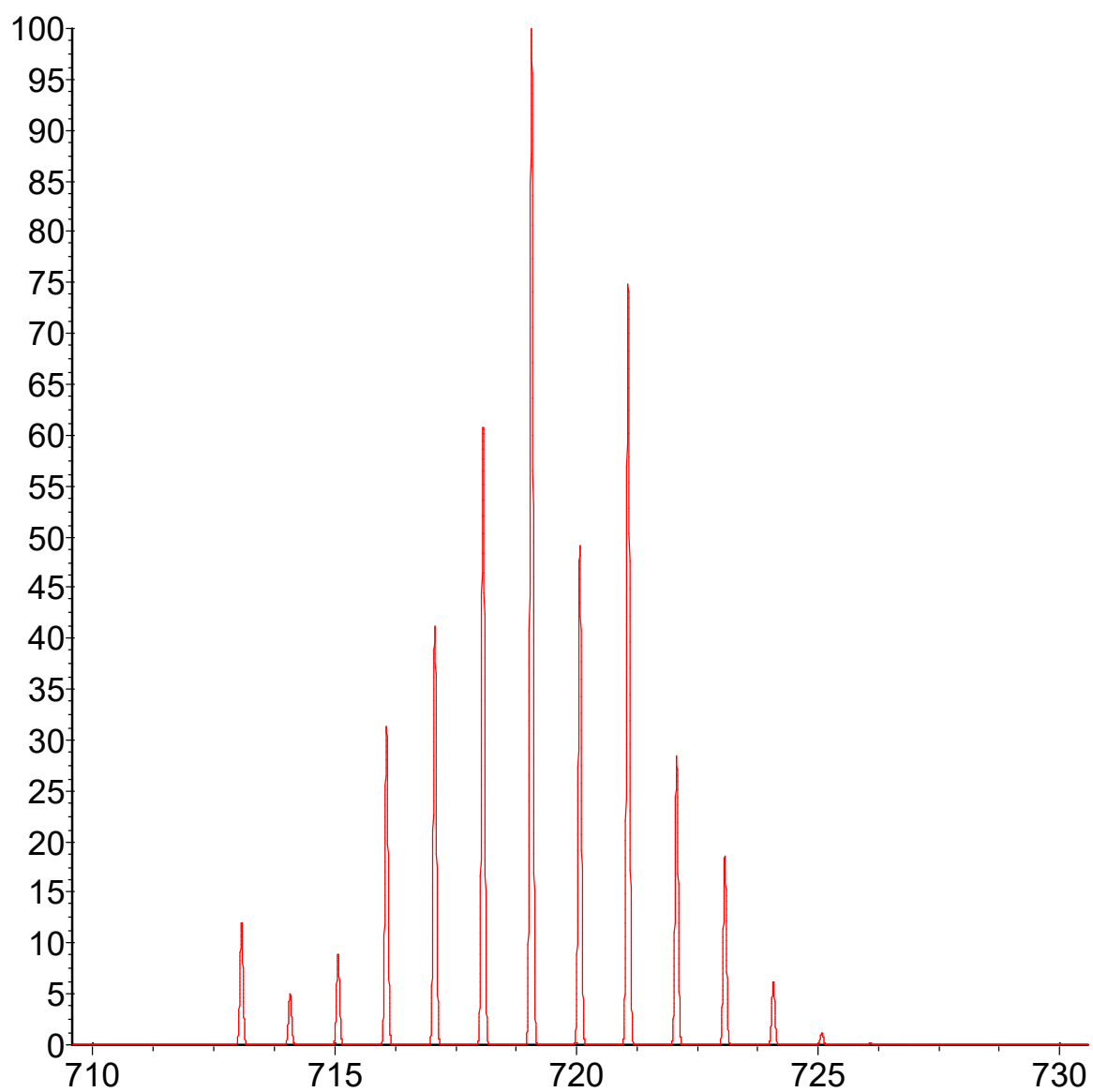


Figure S85. Simulated isotopic distribution pattern of $[8]^+$.