Dalton Transactions

ARTICLE

Electronic Supporting Information for:

Carbyne Decorated Porphyrins

Benjamin J. Frogley,[a] Anthony F. Hill [a†]

Selected NMR, IR and Electronic spectra

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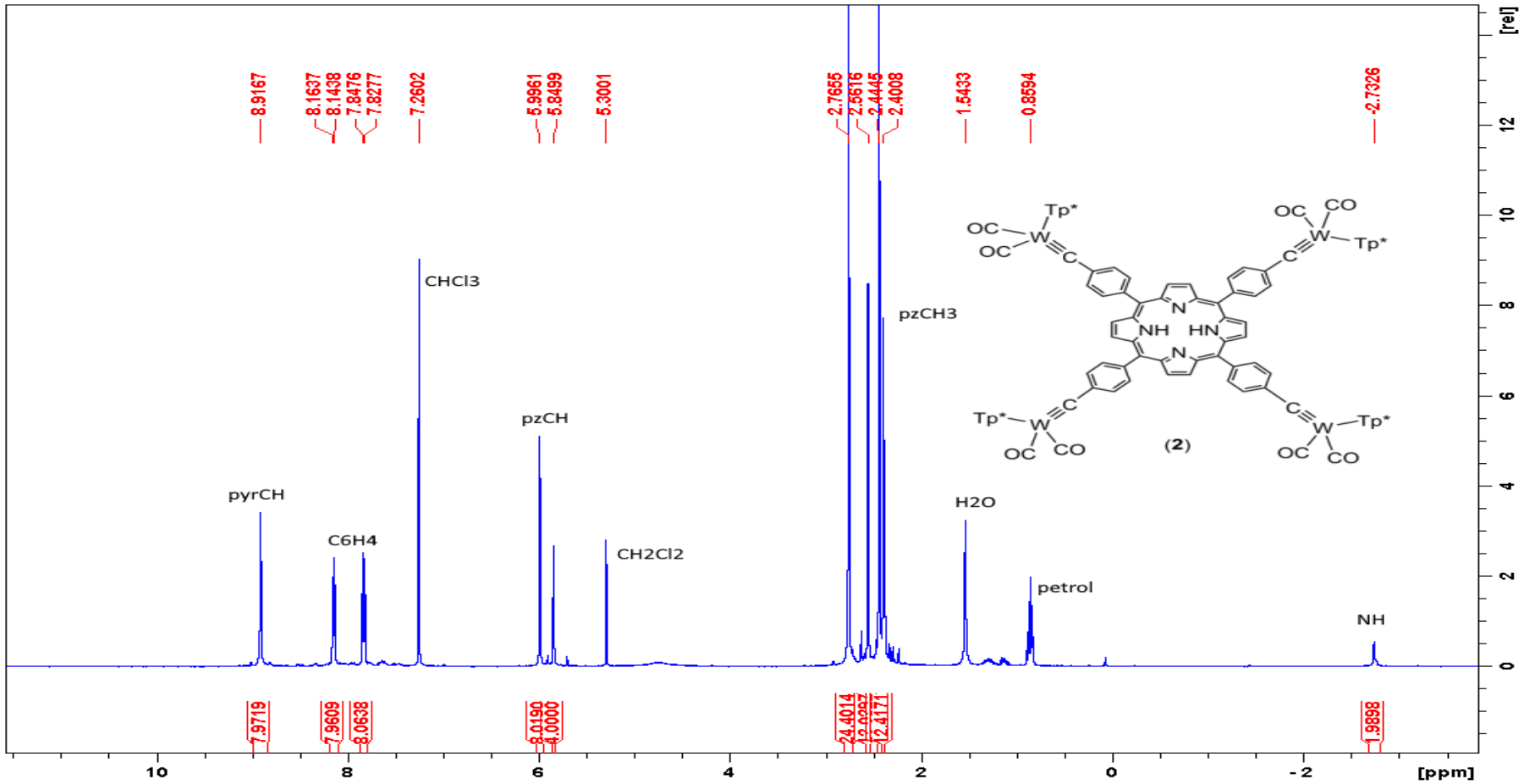

Figure S1. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 25 °C, δ) of **2**.

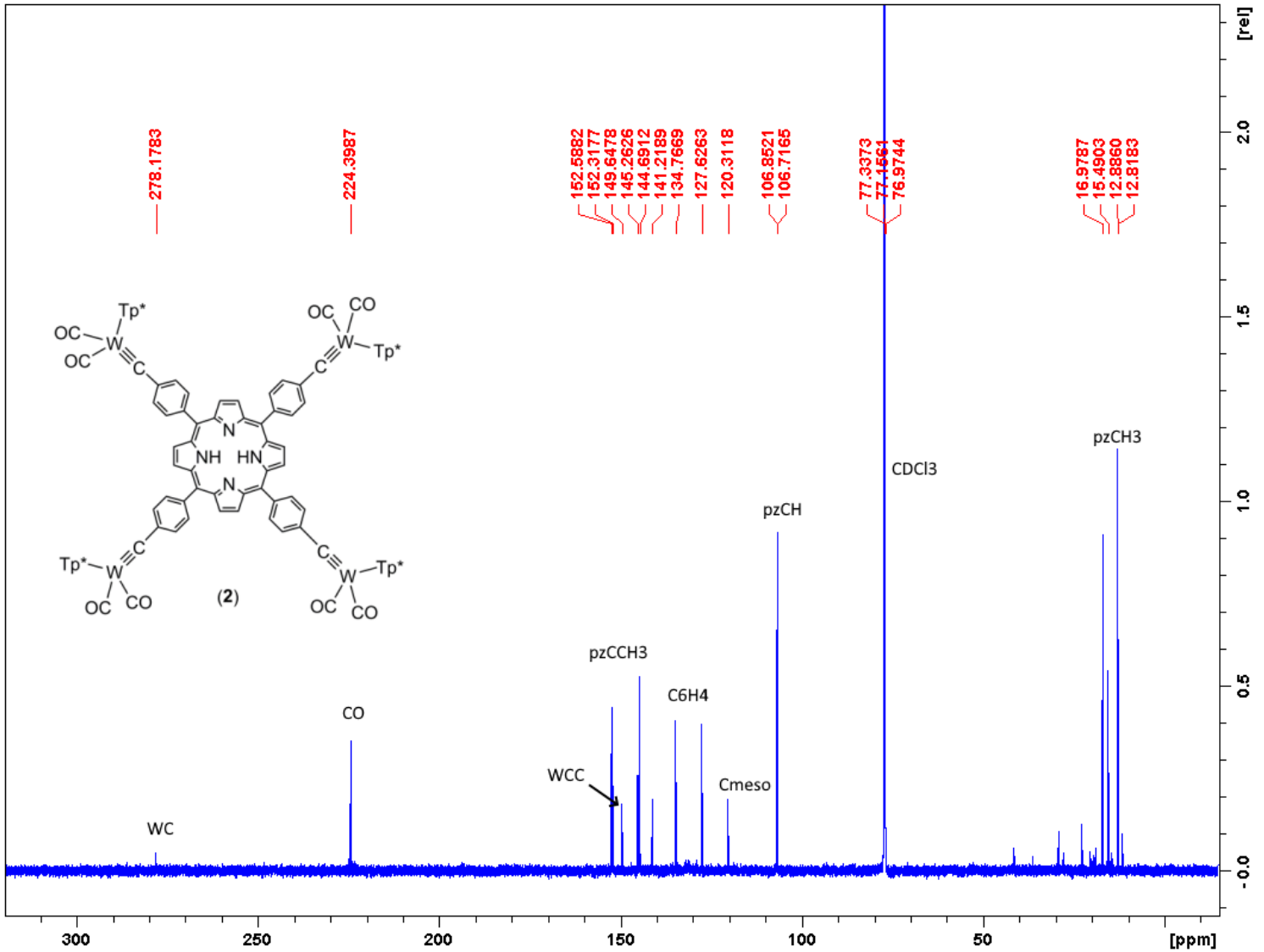

Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, $CDCl_3$, 25 °C, δ) of **2**.

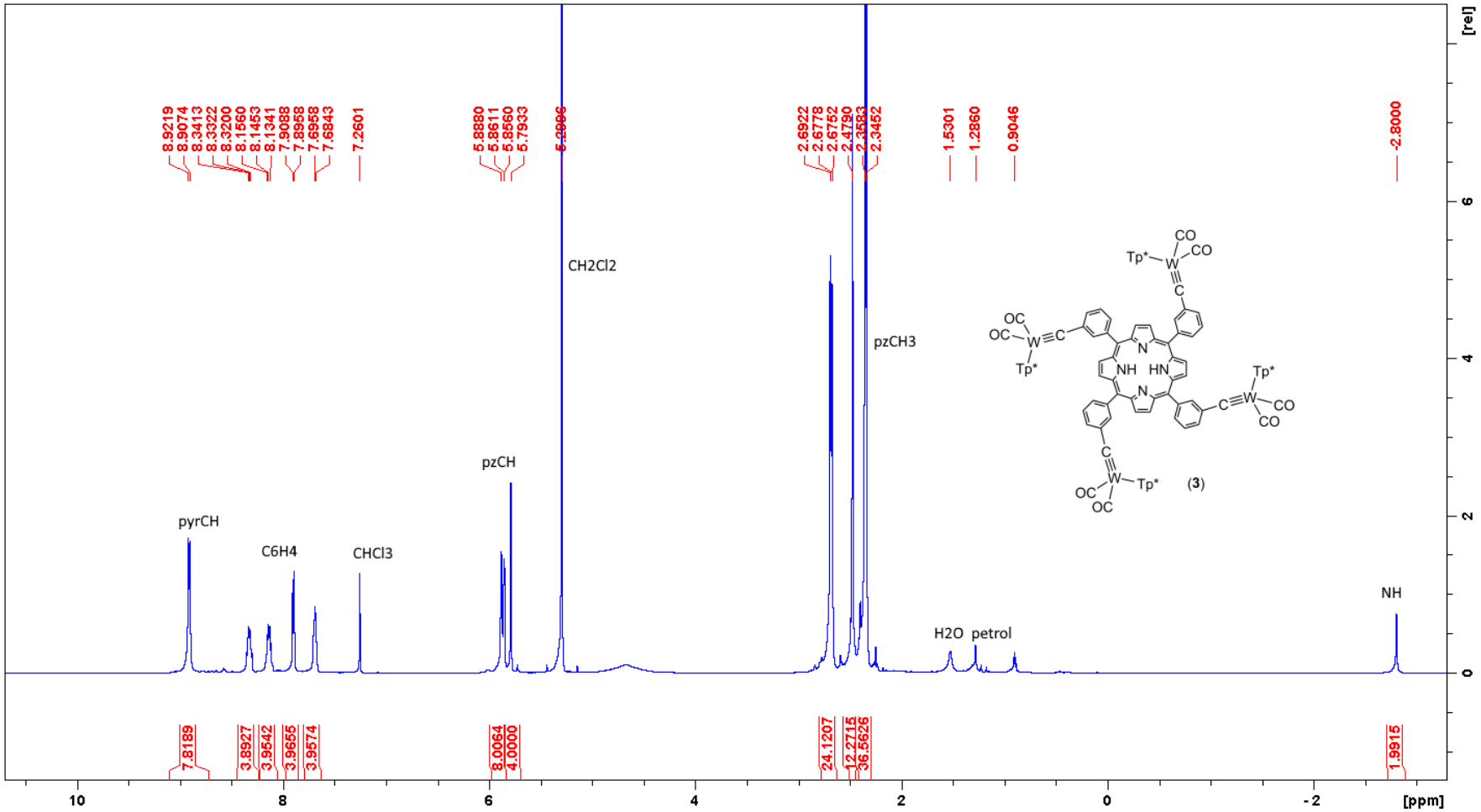

Figure S3. ^{1}H NMR spectrum (600 MHz, $CDCl_3$, 25 °C, δ) of **3**.

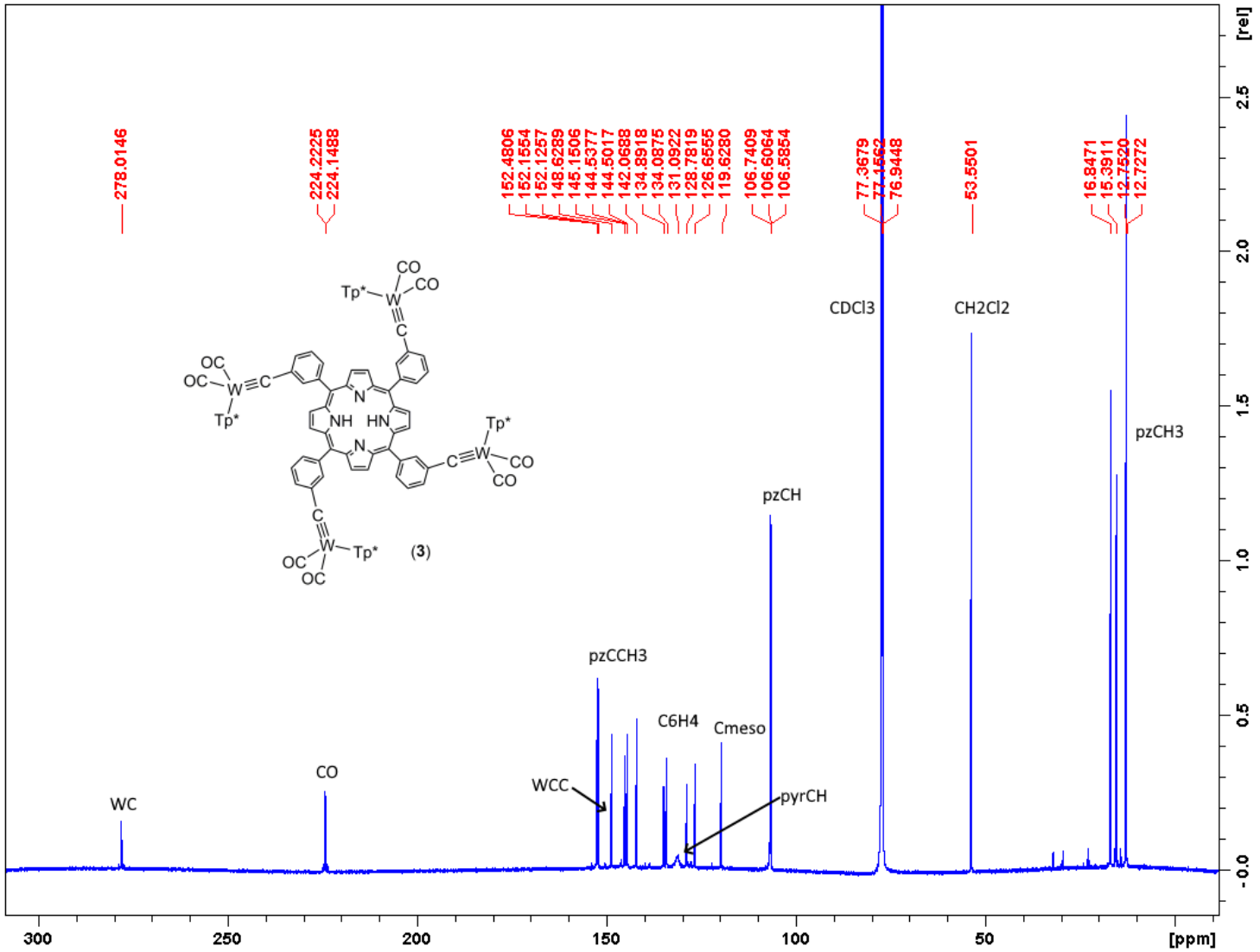

Figure S4. $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, $CDCl_3$, 25 °C, δ) of **3**.

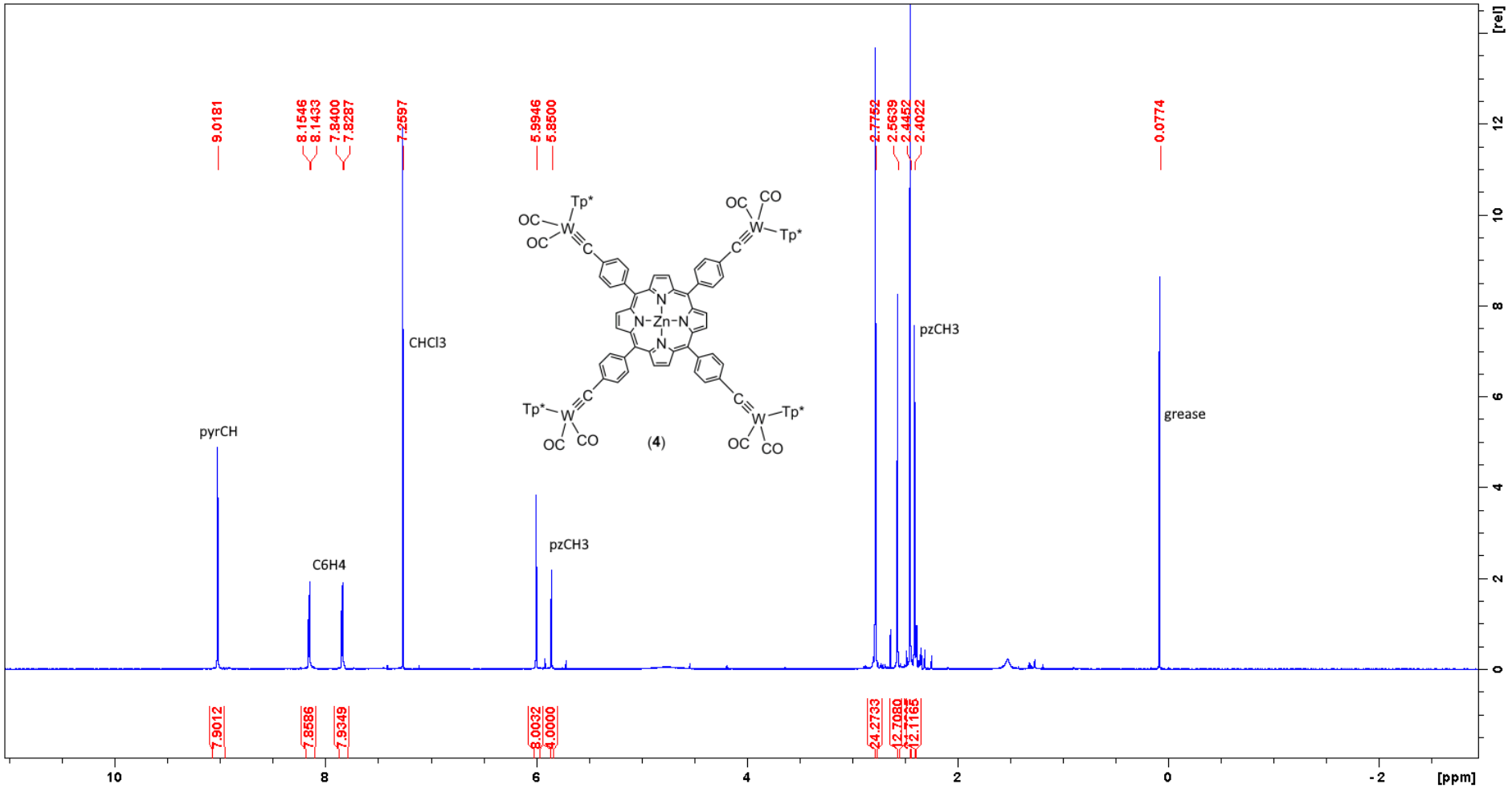

Figure S5 ^{1}H NMR spectrum (700 MHz, $CDCl_3$, 25 °C, δ) of **4**.

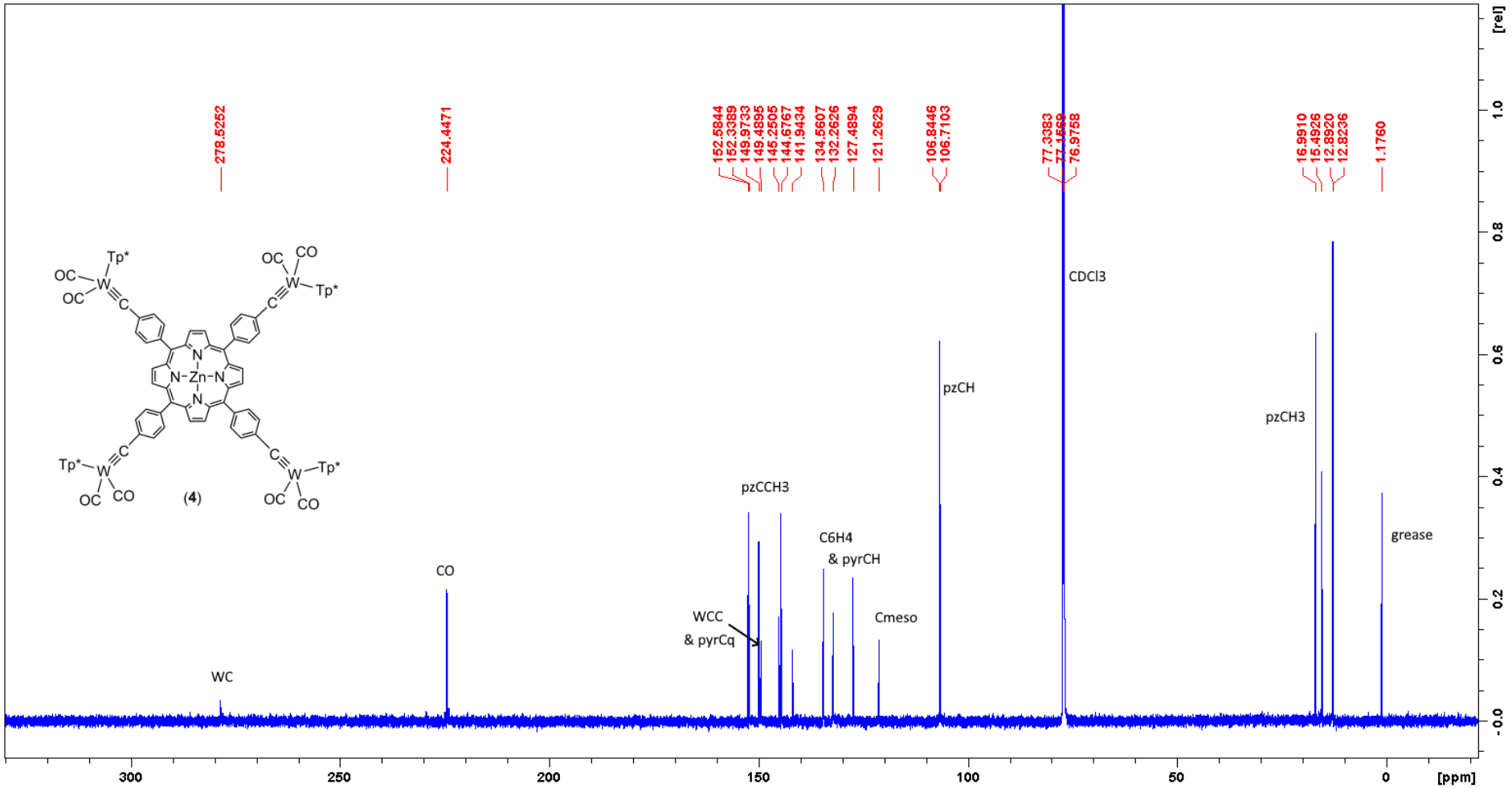

Figure S6. $^{13}C\{^{1}H\}$ NMR spectrum (176 MHz, $CDCl_3$, 25 °C, δ) of **4**.

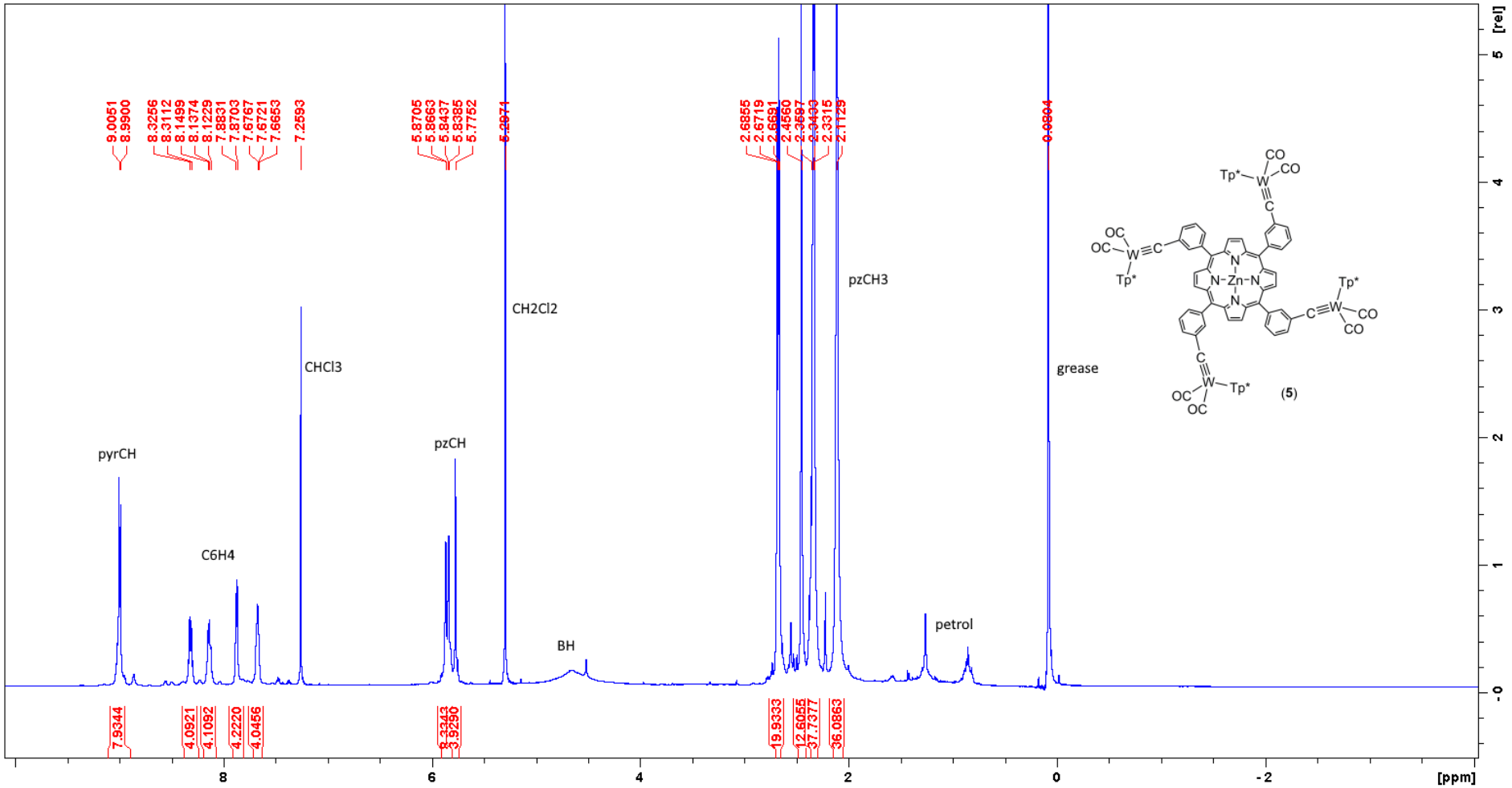

Figure S7. ^{1}H NMR spectrum (700 MHz, $CDCl_3$, 25 °C, δ) of **5**.

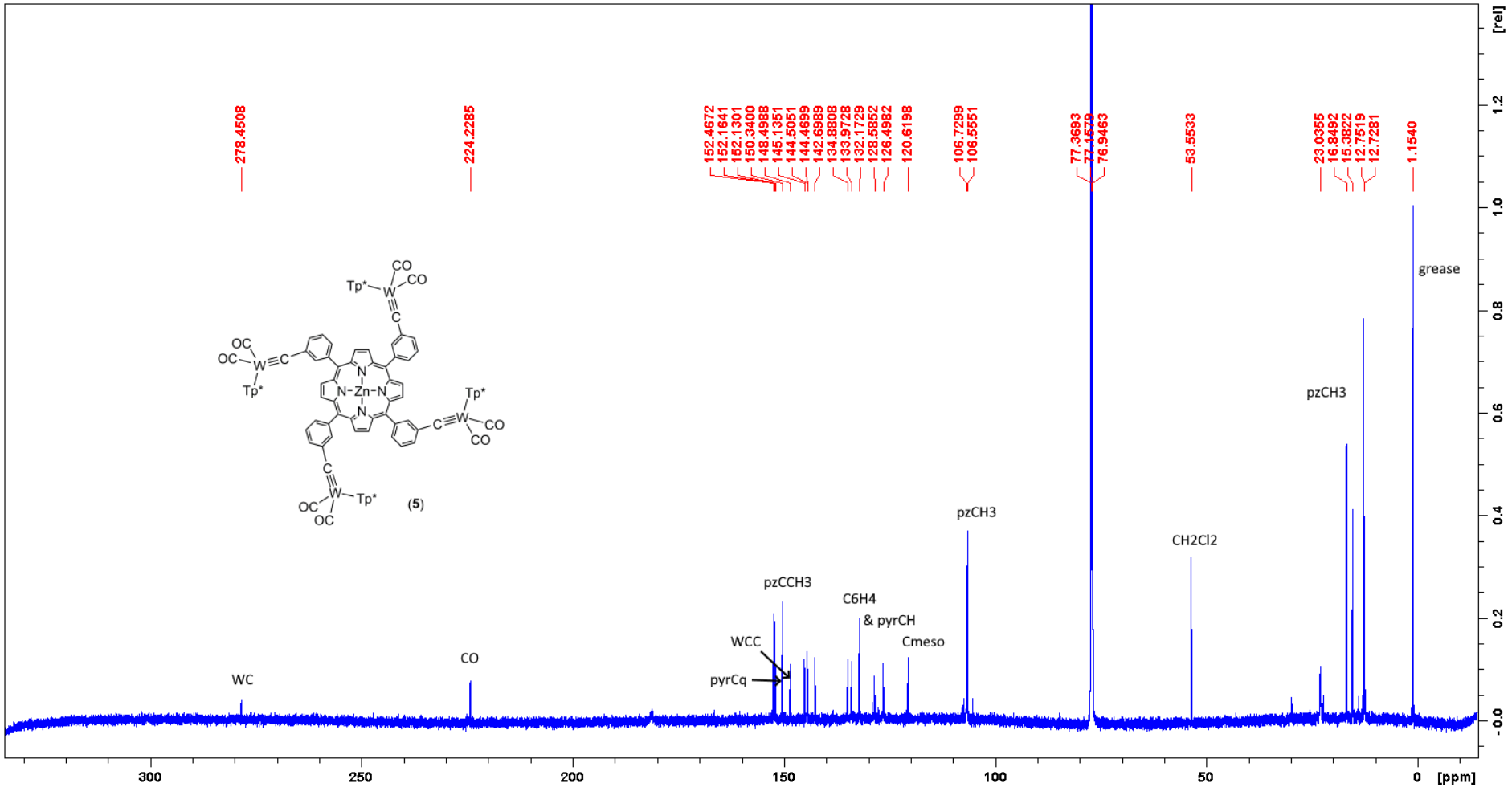

Figure S8. $^{13}C\{^{1}H\}$ NMR spectrum (176 MHz, $CDCl_3$, 25 °C, δ) of **5**.

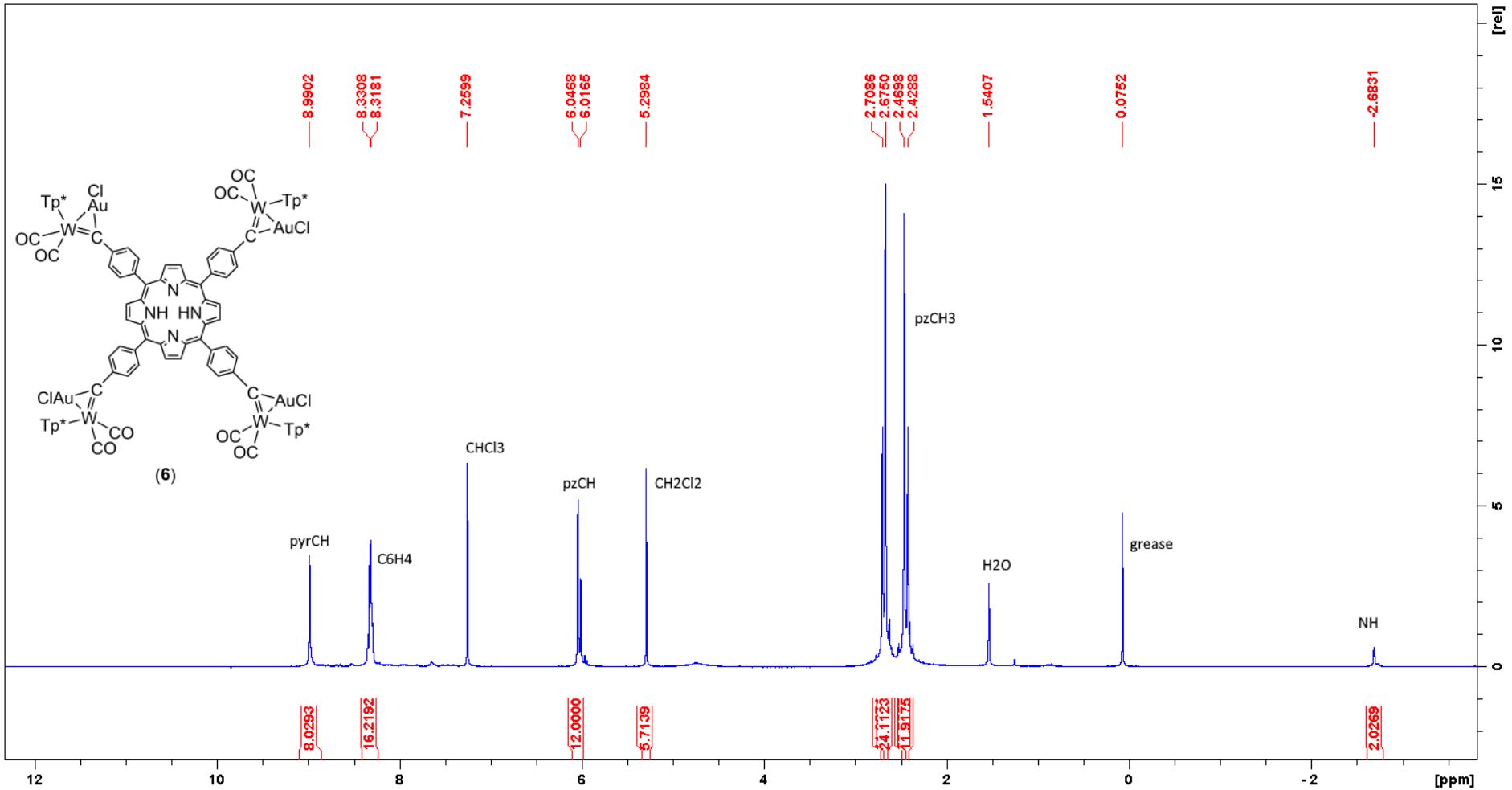

Figure S9. ^{1}H NMR spectrum (600 MHz, $CDCl_3$, 25 °C, δ) of **6**.

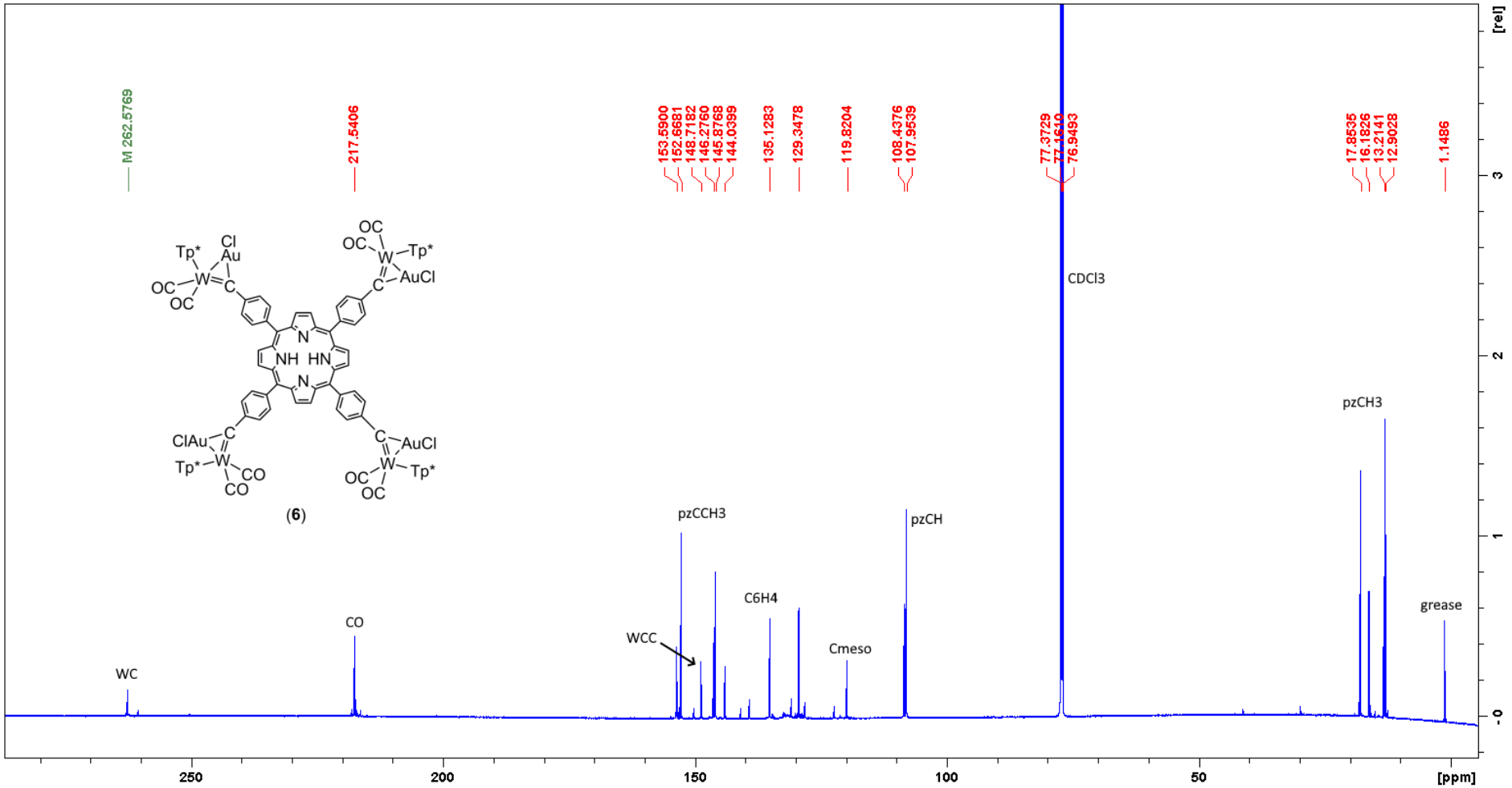

Figure S10. $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, $CDCl_3$, 25 °C, δ) of **6**.

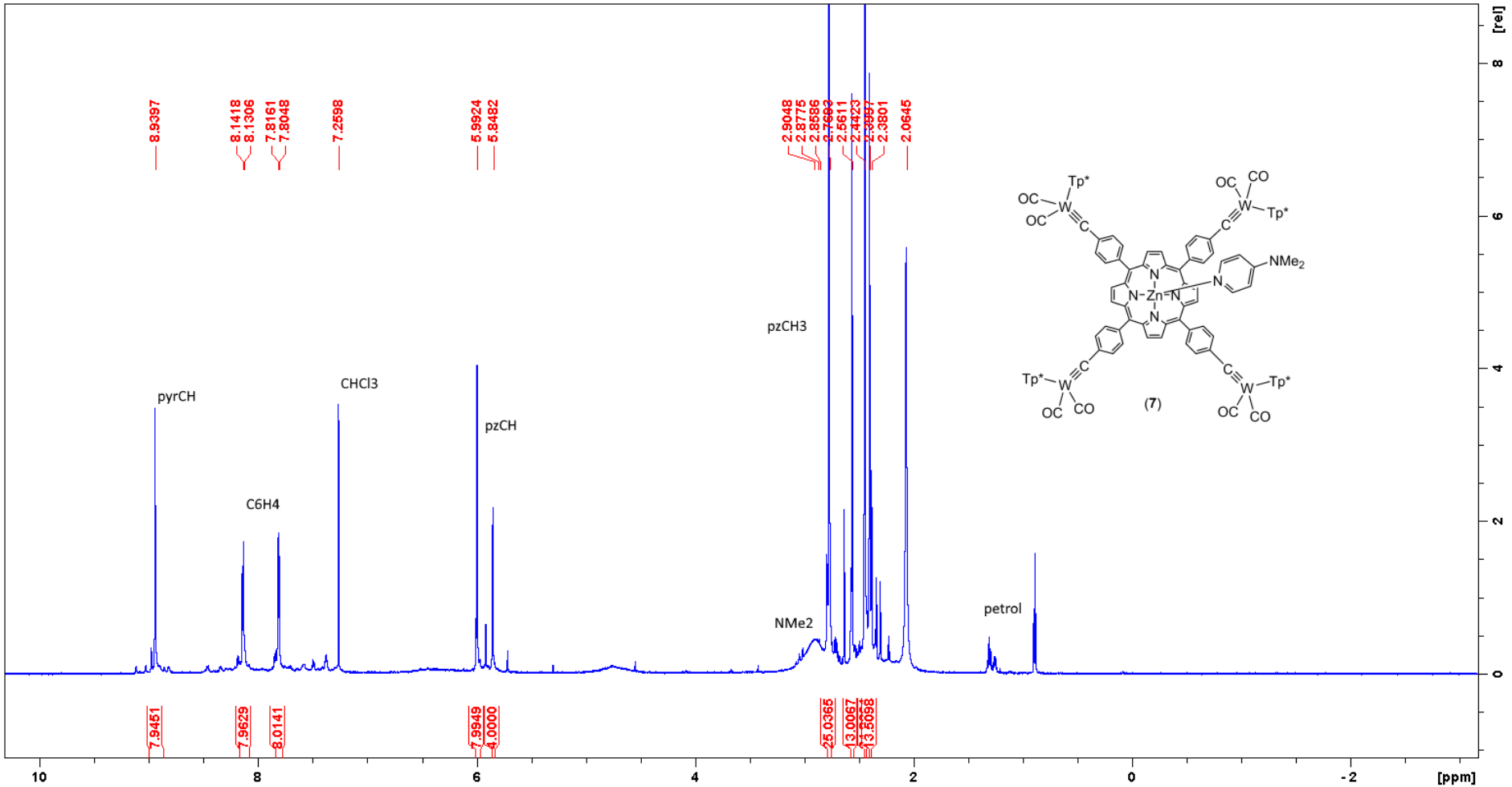

Figure S11. ^{1}H NMR spectrum (700 MHz, $CDCl_3$, 20 °C, δ) of **7** (**4** in the presence of excess 4-DMAP).

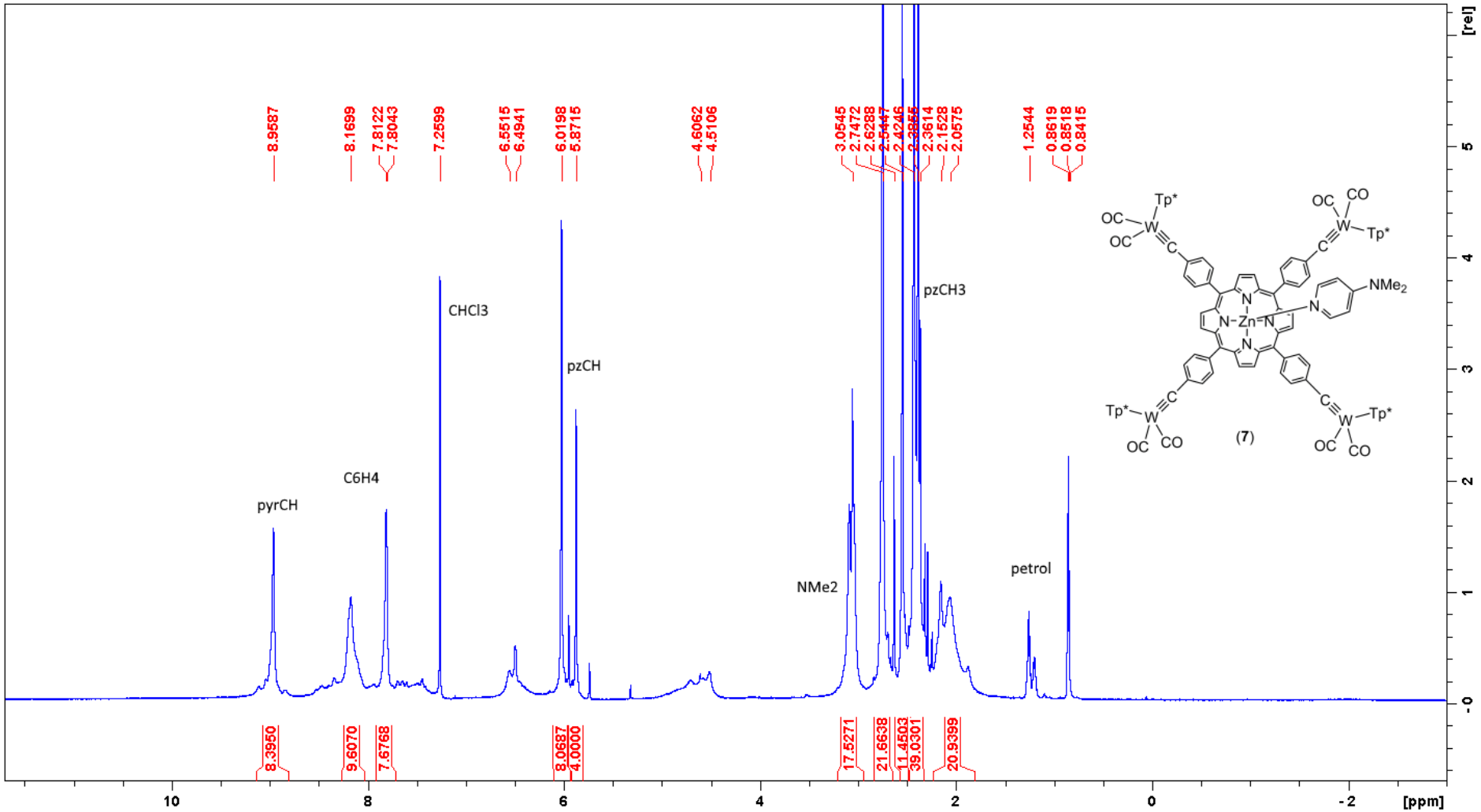

Figure S12. ^{1}H NMR spectrum (700 MHz, $CDCl_3$, –60 °C, δ) of **7** (**4** in the presence of excess 4-DMAP).

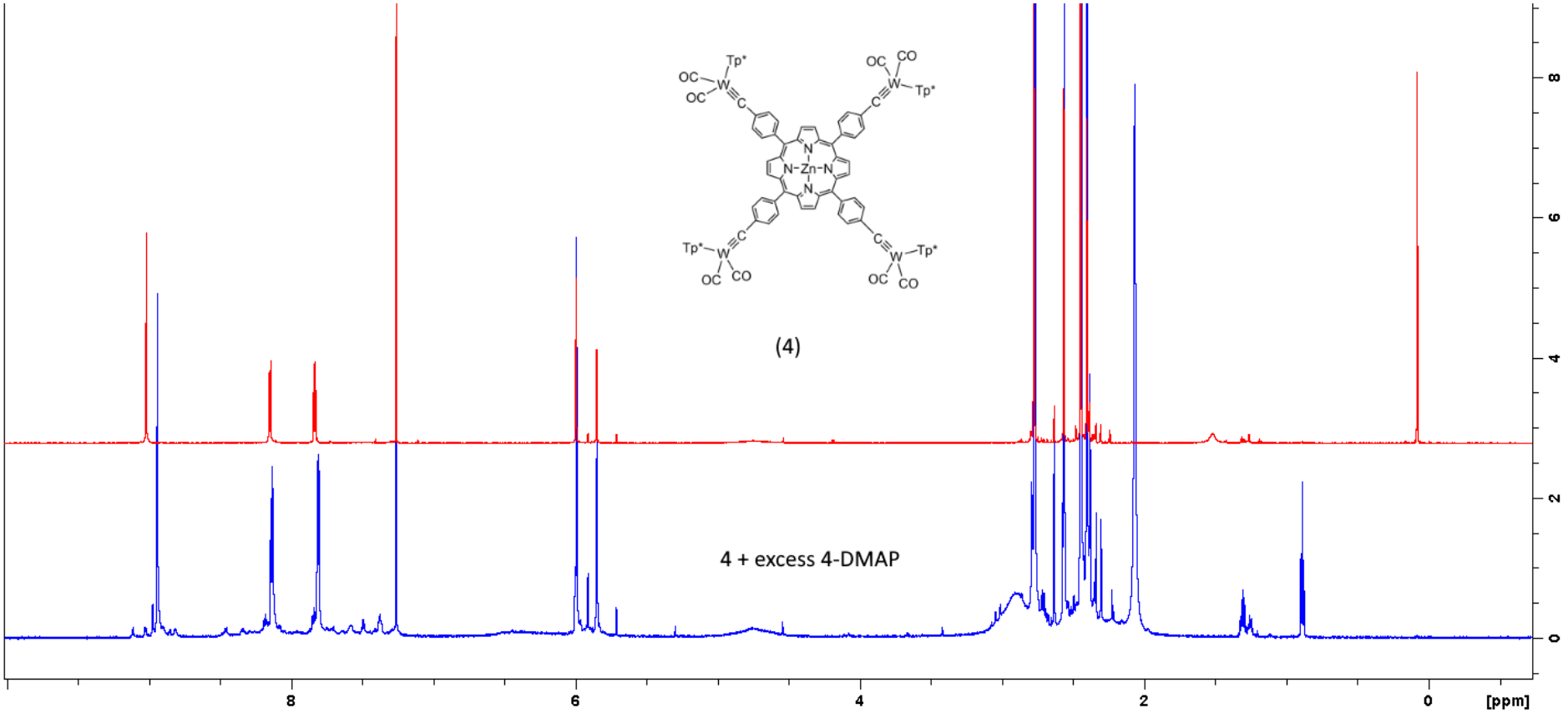

Figure S13. Comparison of ^{1}H NMR spectra of **4** and **7** (a mixture of **4** and excess 4-DMAP) at 25 °C.

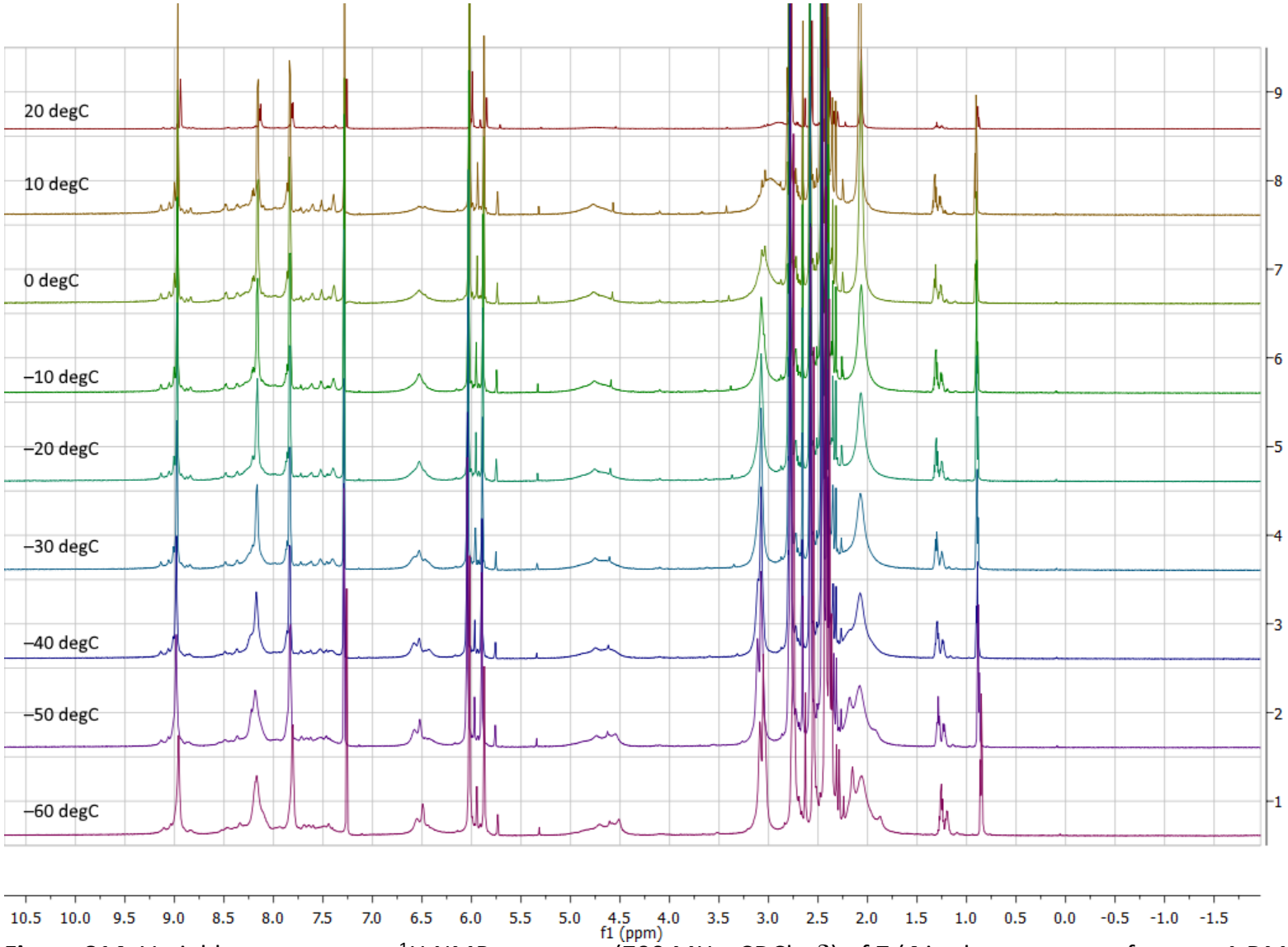

Figure S14. Variable-temperature ^{1}H NMR spectrum (700 MHz, $CDCl_3$, δ) of **7** (**4** in the presence of excess 4-DMAP).

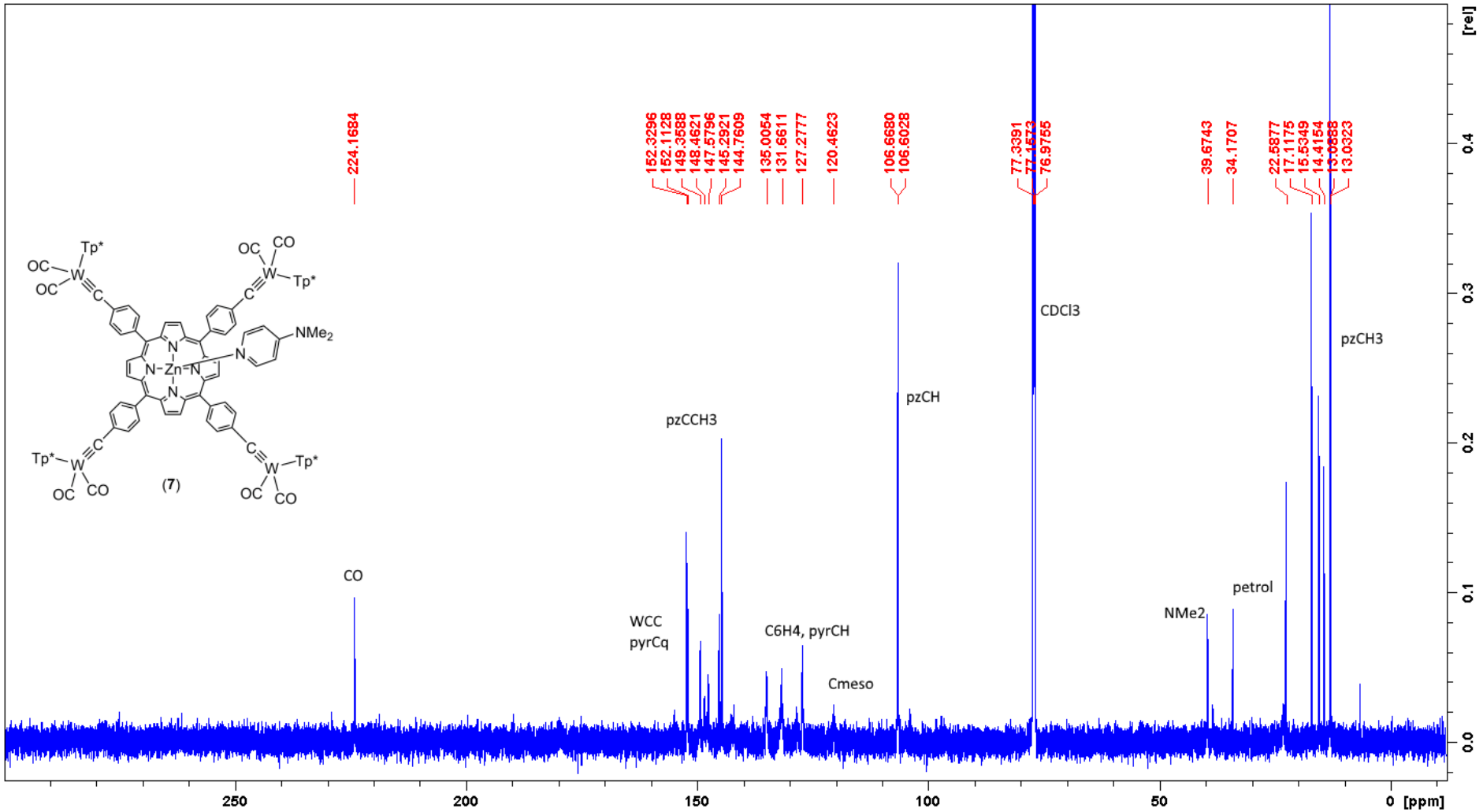

Figure S15. $^{13}C\{^{1}H\}$ NMR spectrum (176 MHz, $CDCl_3$, –60 °C, δ) of **7** (**4** in the presence of excess 4-DMAP).

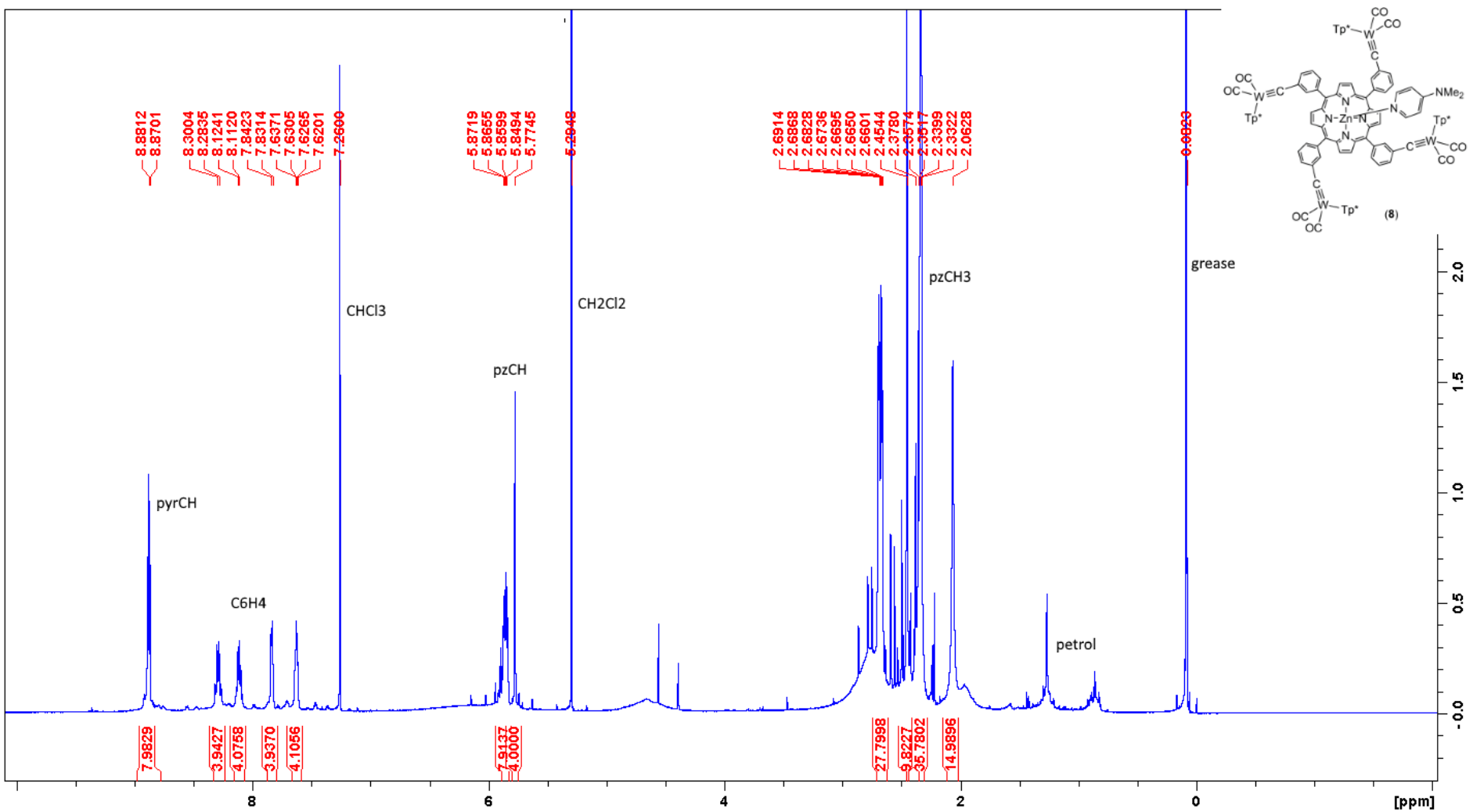

Figure S16. ^{1}H NMR spectrum (700 MHz, $CDCl_3$, 25 °C, δ) of **8** (**5** in the presence of excess 4-DMAP).

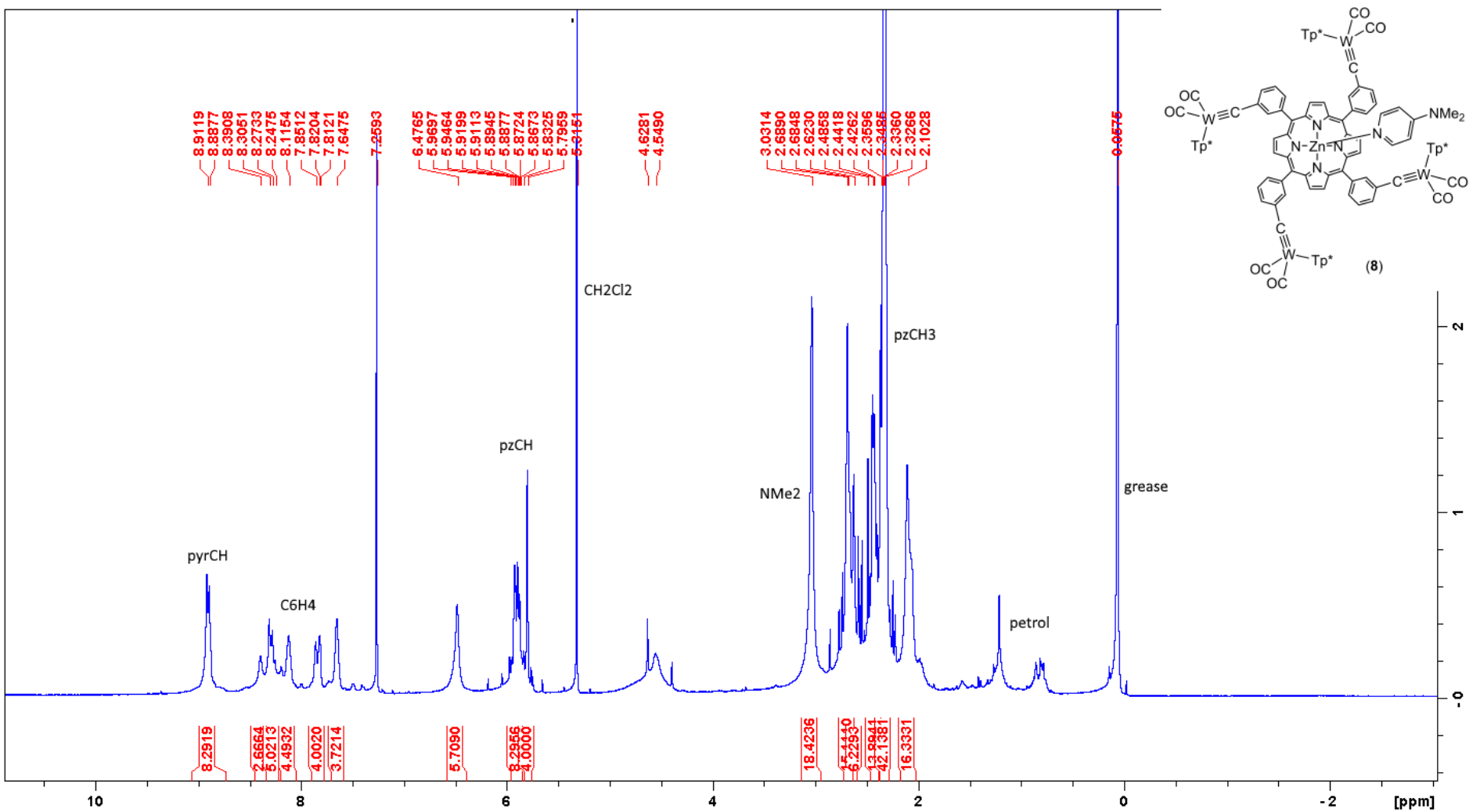

Figure S17. ^{1}H NMR spectrum (700 MHz, $CDCl_3$, –60 °C, δ) of **8** (**5** in the presence of excess 4-DMAP).

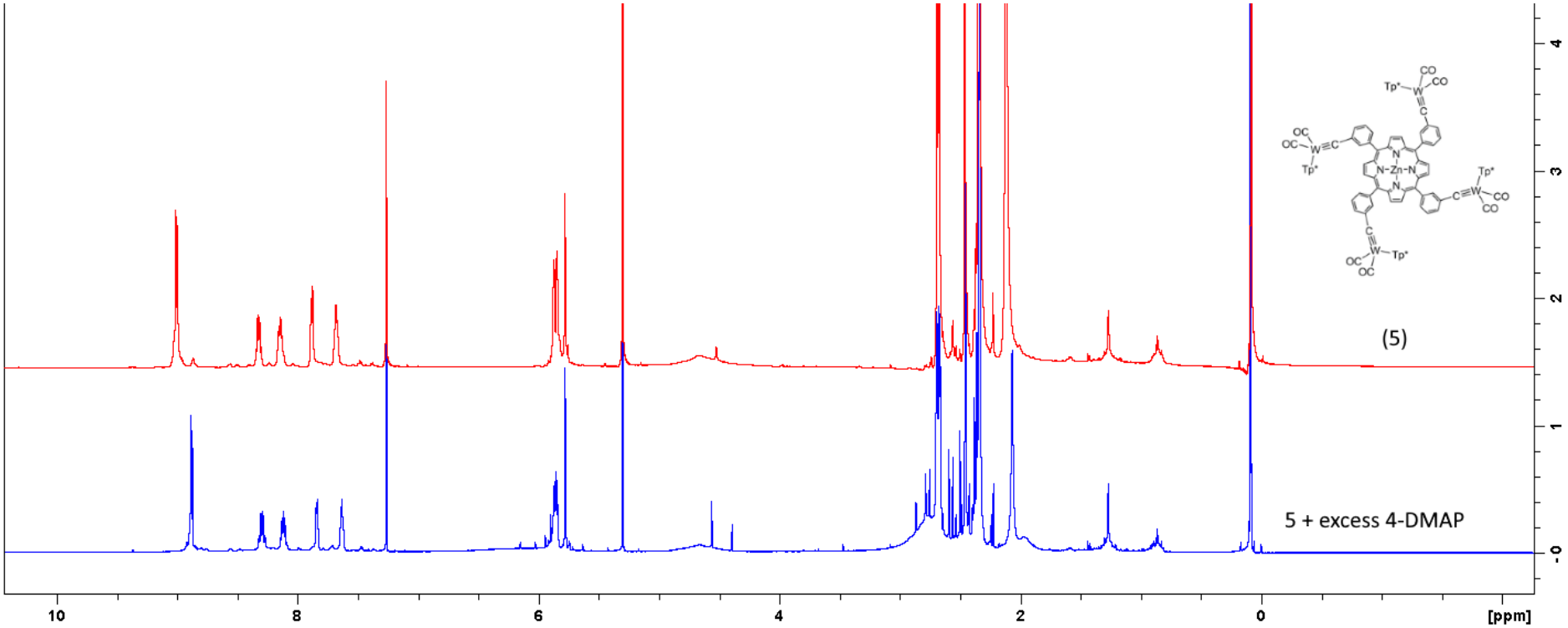

Figure S18. Comparison of ^{1}H NMR spectra of **5** and **8** (a mixture of **5** and excess 4-DMAP) at 25 °C.

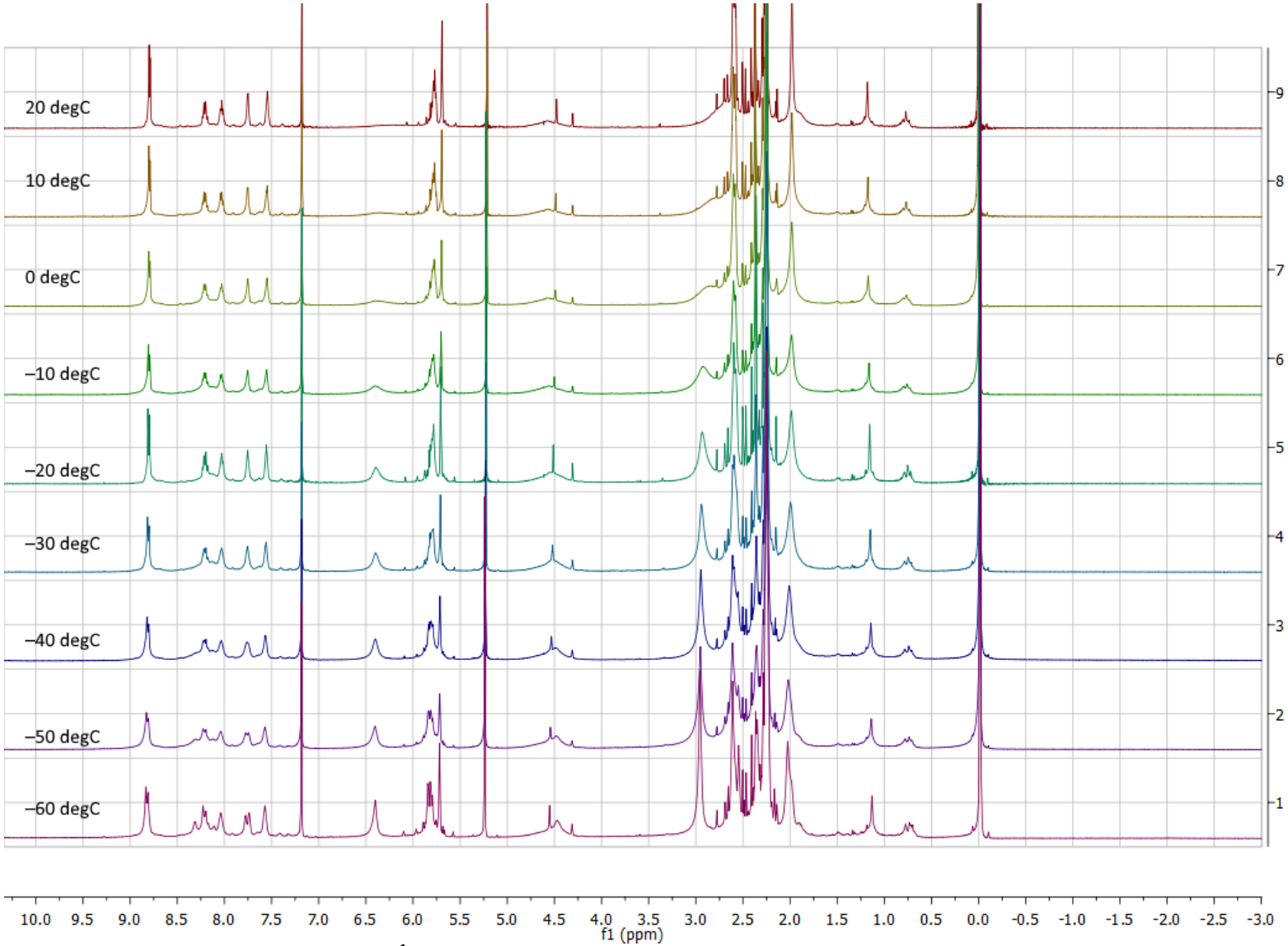

Figure S19. Variable-temperature ^{1}H NMR spectrum (700 MHz, $CDCl_3$, δ) of **8** (**5** in the presence of excess 4-DMAP).

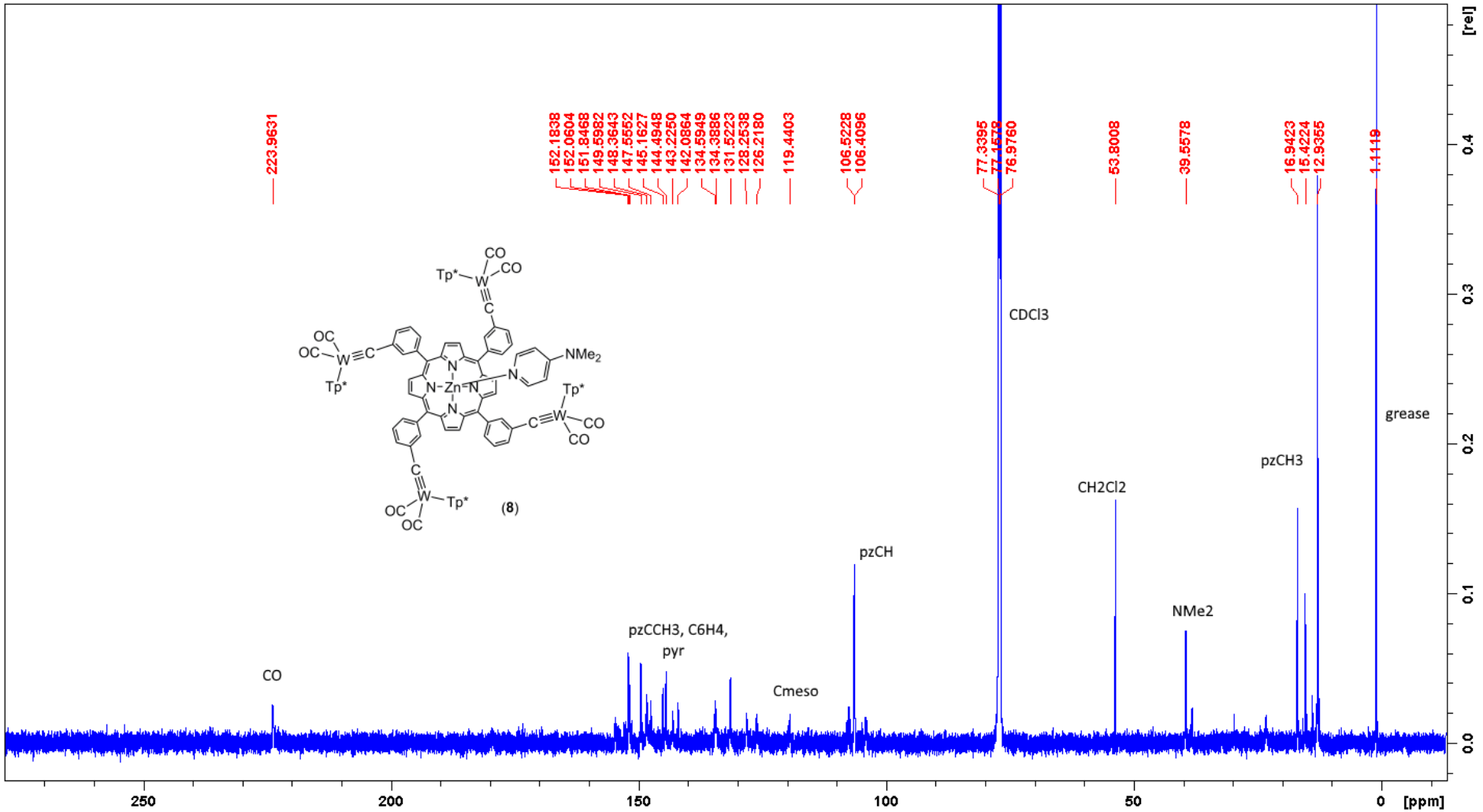

Figure S20. $^{13}C\{^{1}H\}$ NMR spectrum (176 MHz, $CDCl_3$, –60 °C, δ) of **8** (**5** in the presence of excess 4-DMAP).

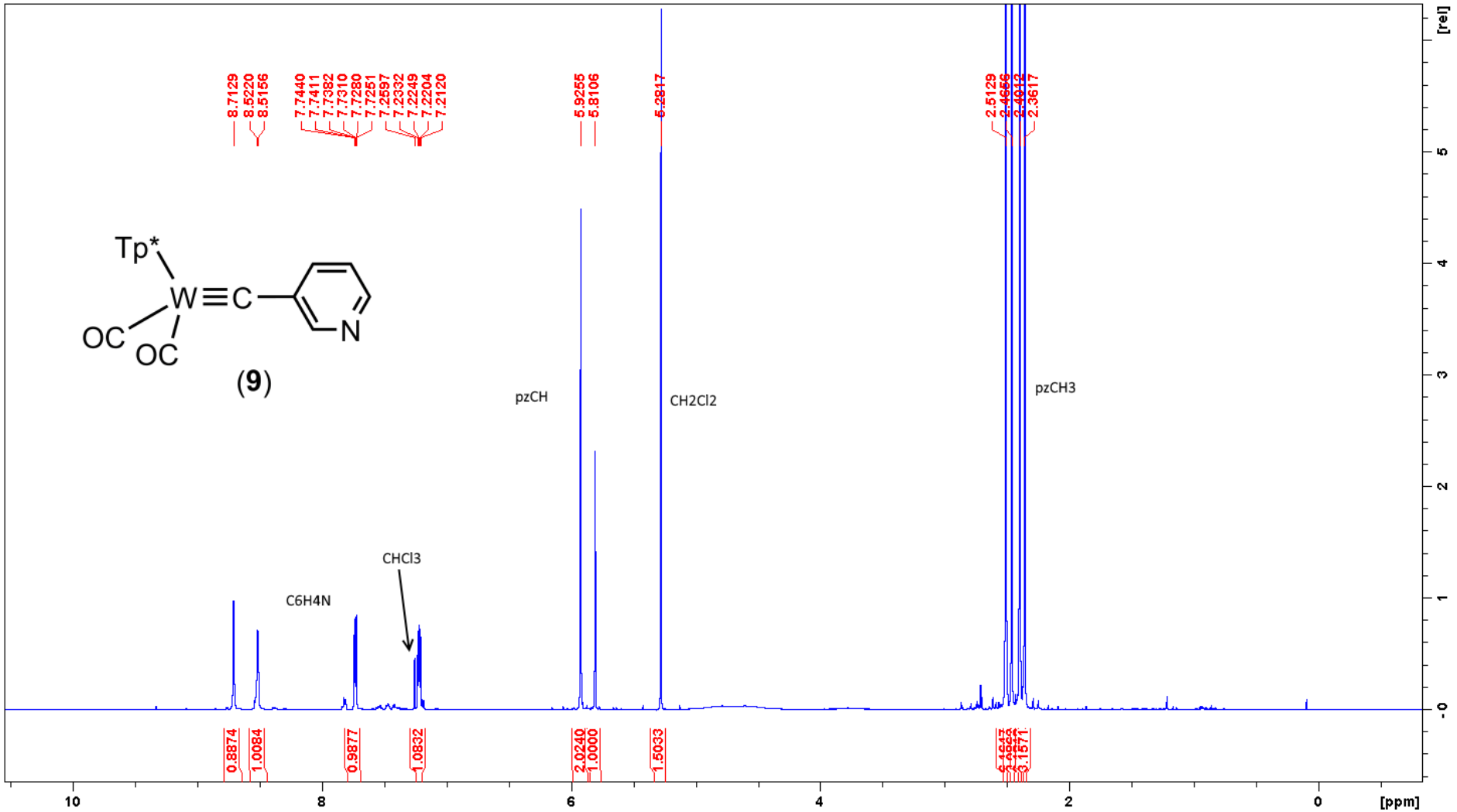

Figure S21. ^{1}H NMR spectrum (600 MHz, $CDCl_3$, 25 °C, δ) of $[NC_5H_4\{C{\equiv}W(CO)_2(Tp^*)\}\text{-}3]$ (**9**).

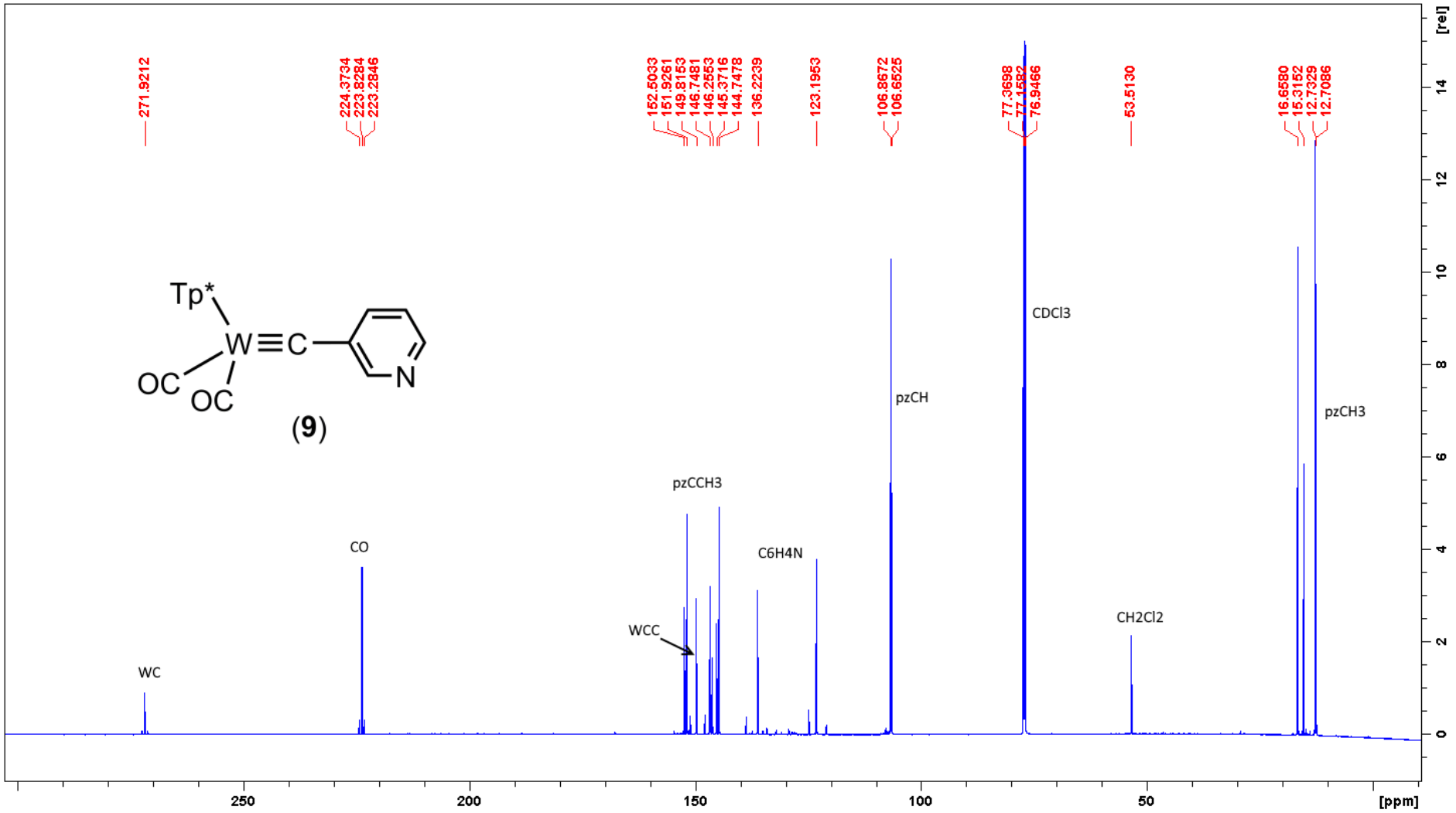

Figure S22. $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, $CDCl_3$, 25 °C, δ) of $[NC_5H_4\{C{\equiv}W(CO)_2(Tp^*)\}\text{-}3]$ (**9**).

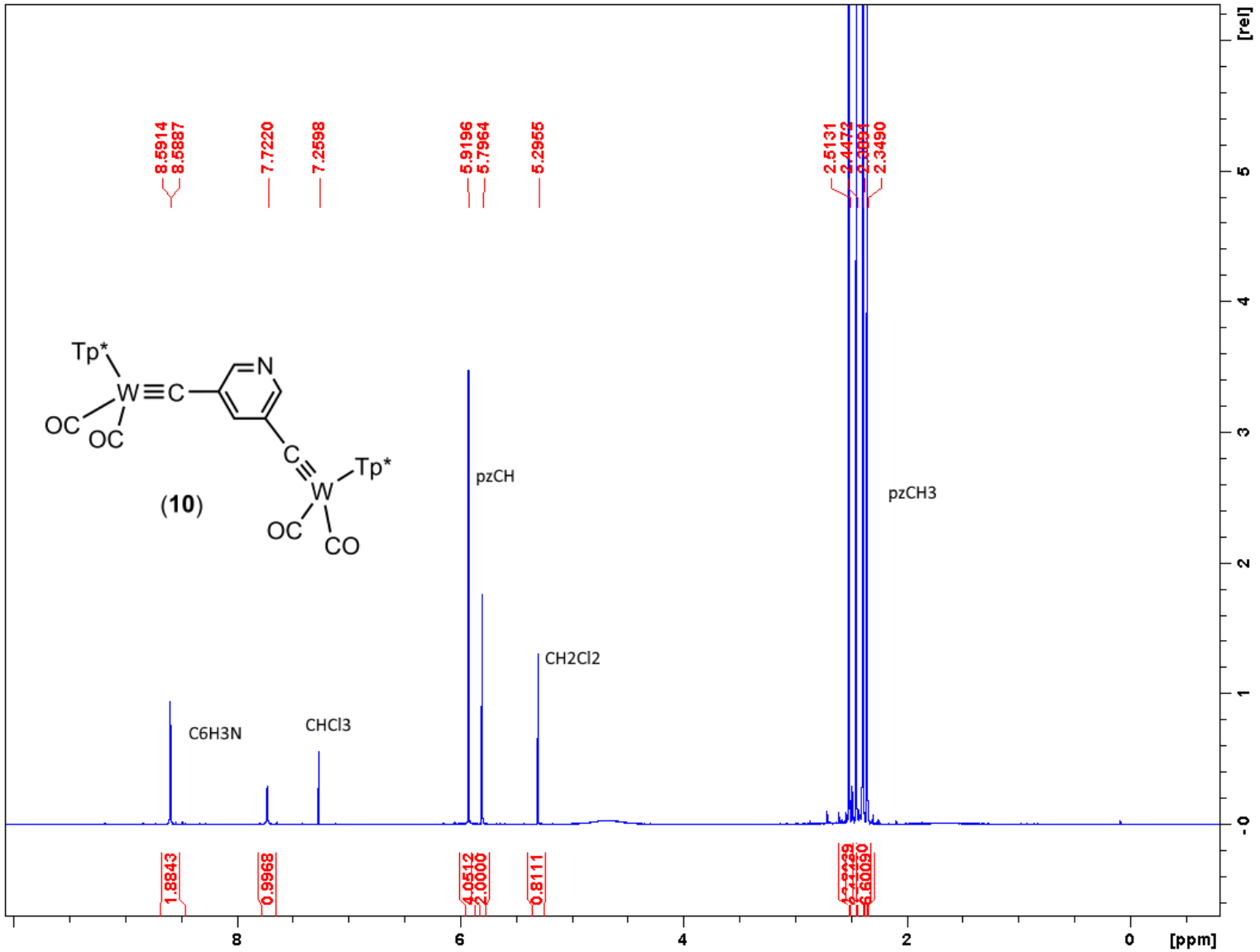

Figure S23. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 25 °C, δ) of $[NC_5H_3\{C{\equiv}W(CO)_2(Tp^*)\}_2\text{-}3,5]$ (**10**).

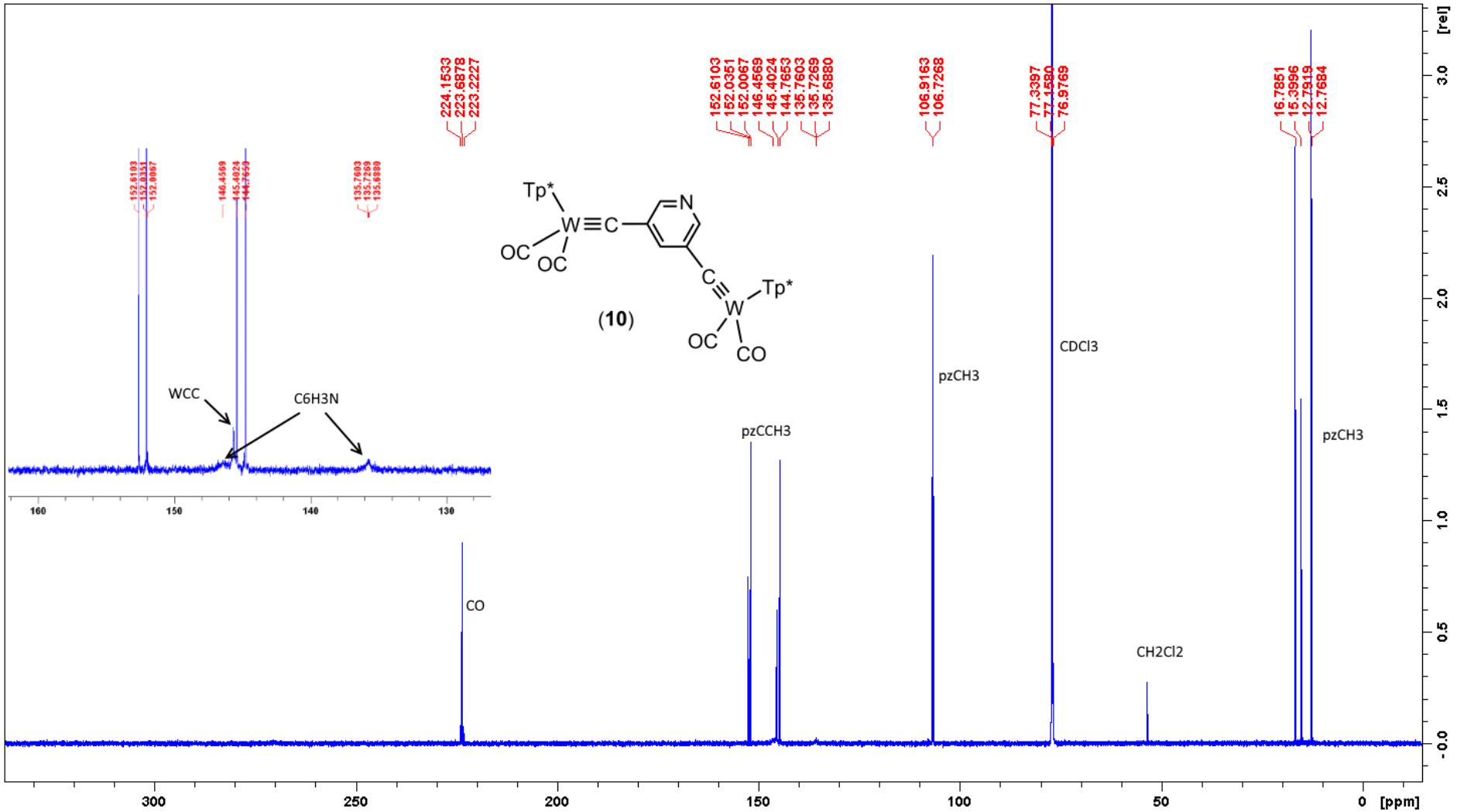

Figure S24. $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, $CDCl_3$, 25 °C, δ) of $[NC_5H_3\{C{\equiv}W(CO)_2(Tp^*)\}_2\text{-}3,5]$ (**10**).

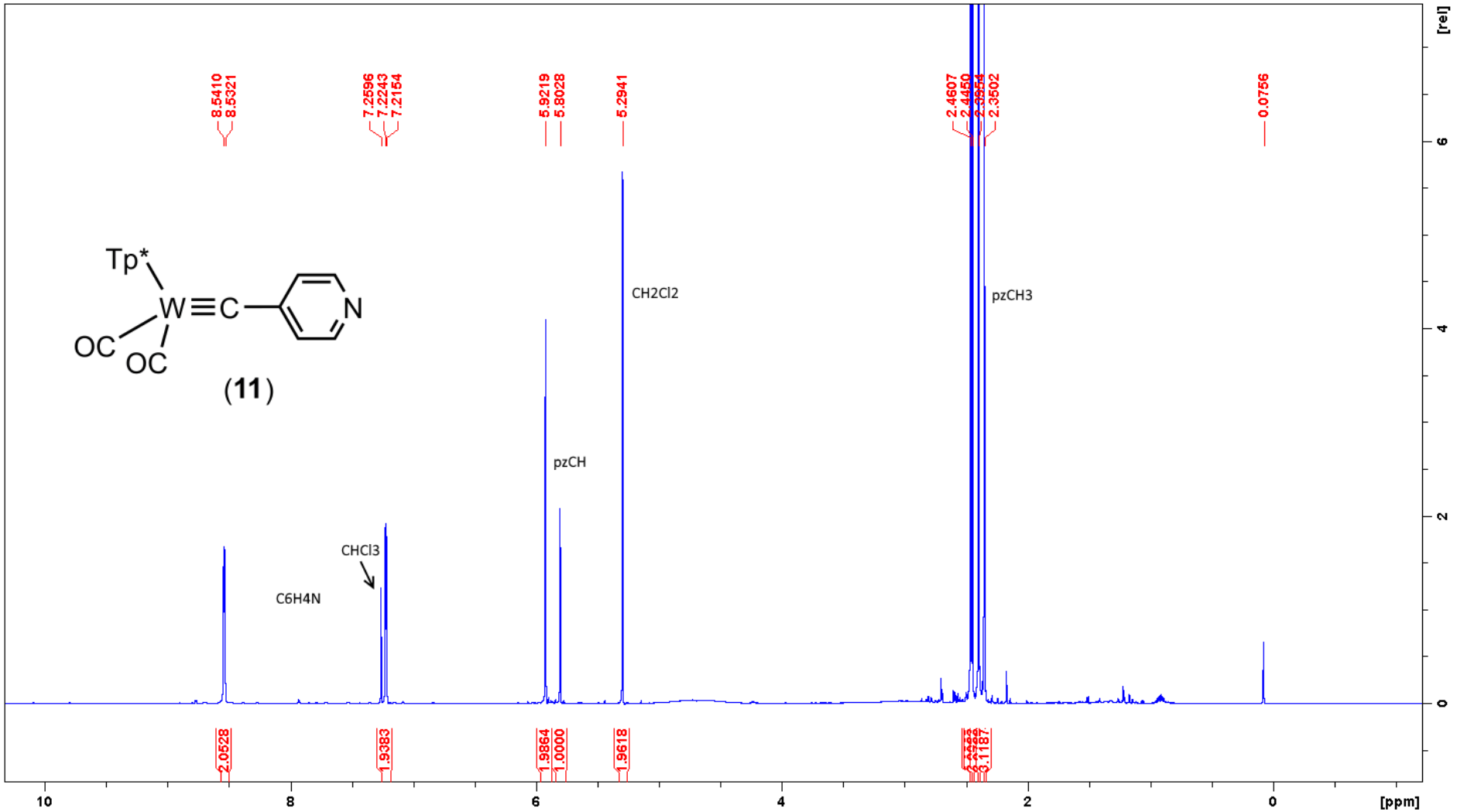

Figure S25. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 25 °C, δ) of $[NC_5H_4\{C{\equiv}W(CO)_2(Tp^*)\}\text{-}4]$ (**11**).

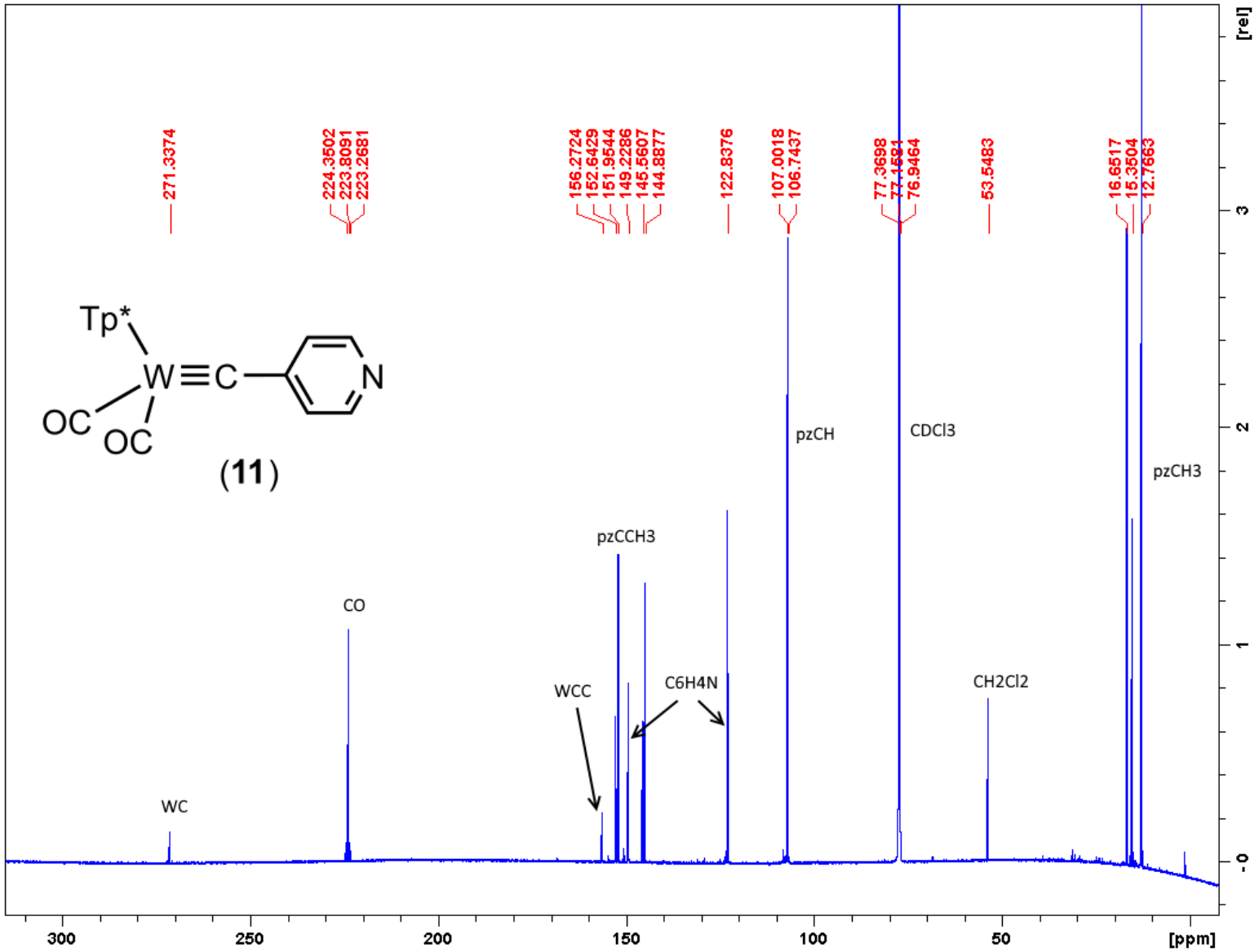

Figure S26. $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, $CDCl_3$, 25 °C, δ) of $[NC_5H_4\{C{\equiv}W(CO)_2(Tp^*)\}\text{-}4]$ (**11**).

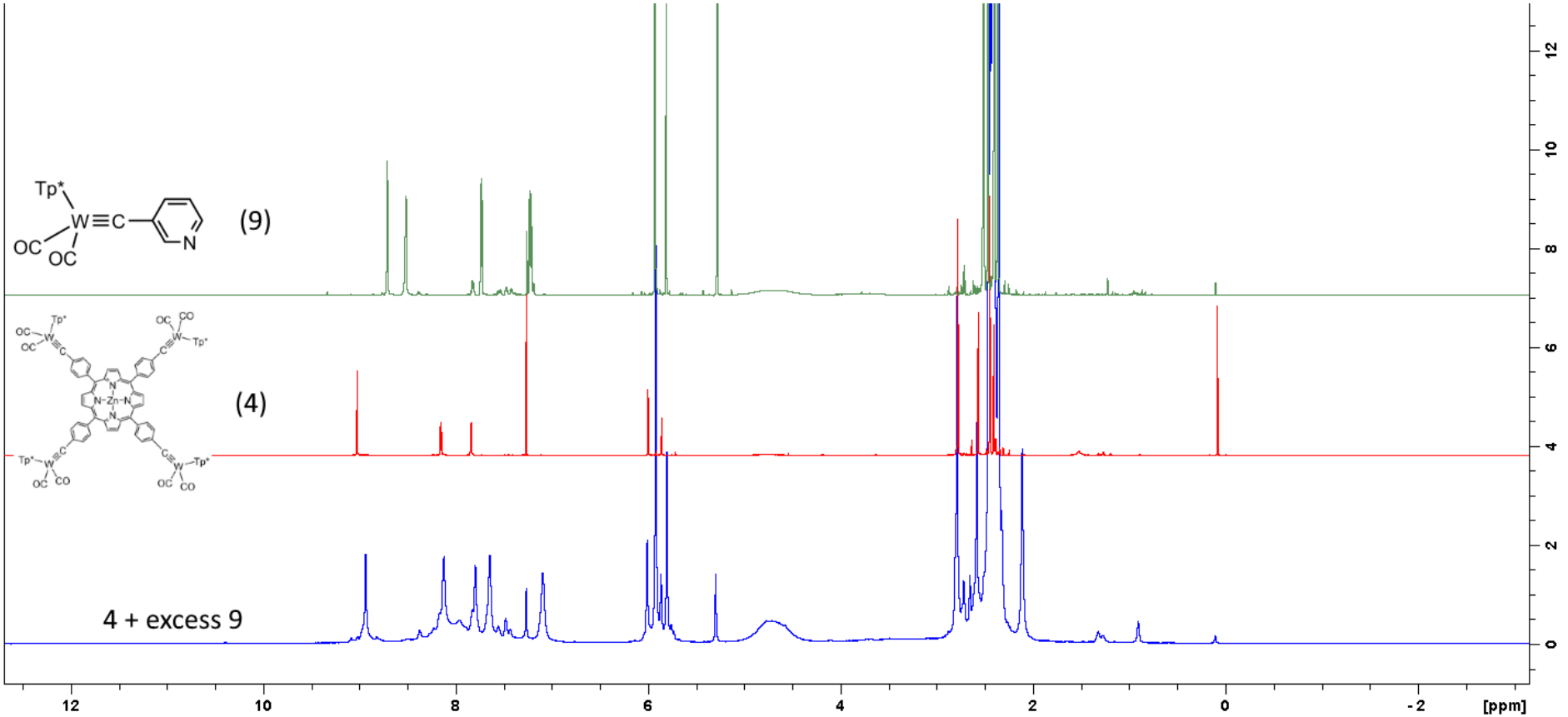

Figure S27. Comparison of ^{1}H NMR spectra at 25 °C of **4**, **9** and a mixture of **4** and excess **9**.

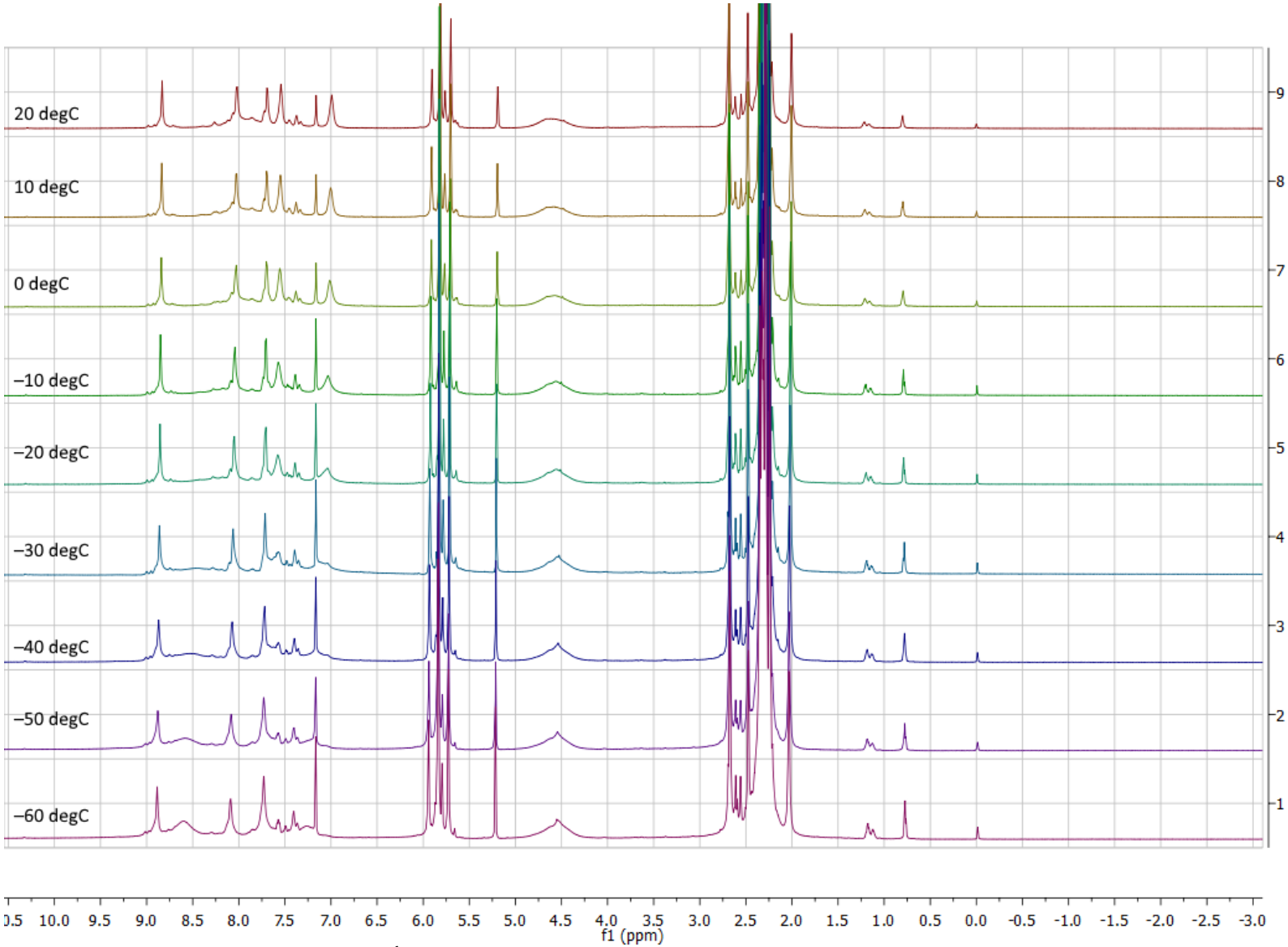

Figure S28. Variable-temperature ^{1}H NMR spectrum (700 MHz, $CDCl_3$, δ) of a mixture of **4** and excess **9**.

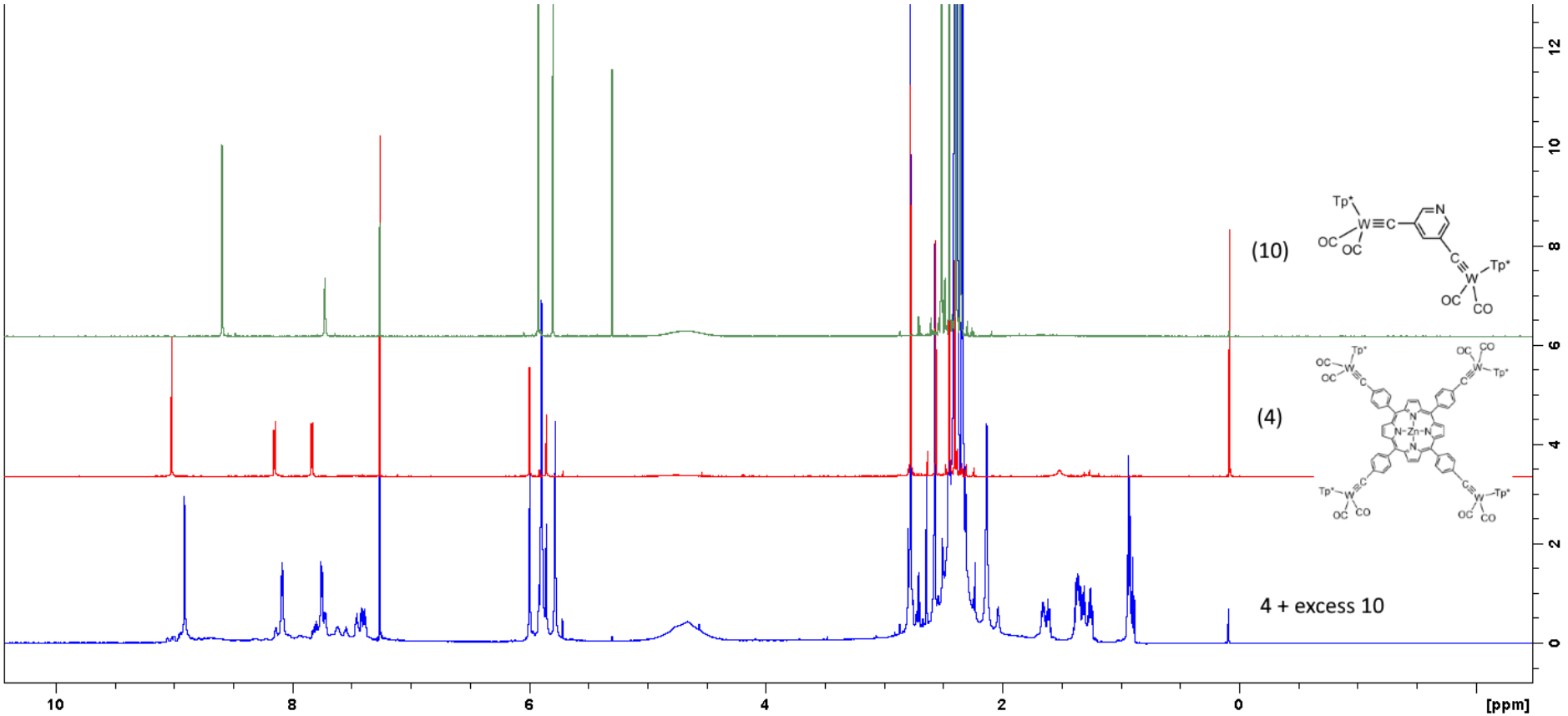

Figure S29. Comparison of ^{1}H NMR spectra at 25 °C of **4**, **10** and a mixture of **4** containing excess **10**.

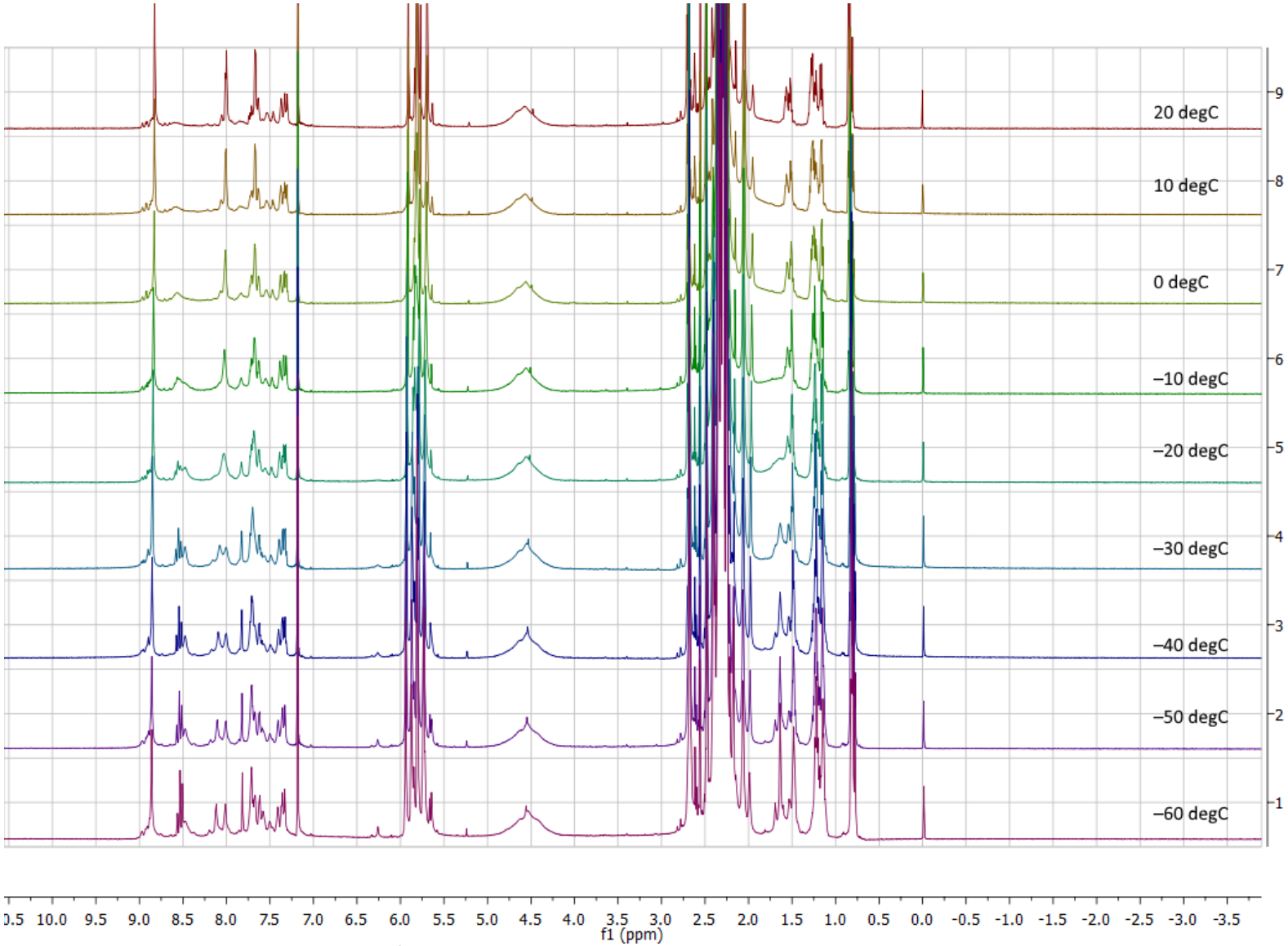

Figure S30. Variable-temperature ^{1}H NMR spectrum (700 MHz, $CDCl_3$, δ) of a solution of **4** containing excess **10**.

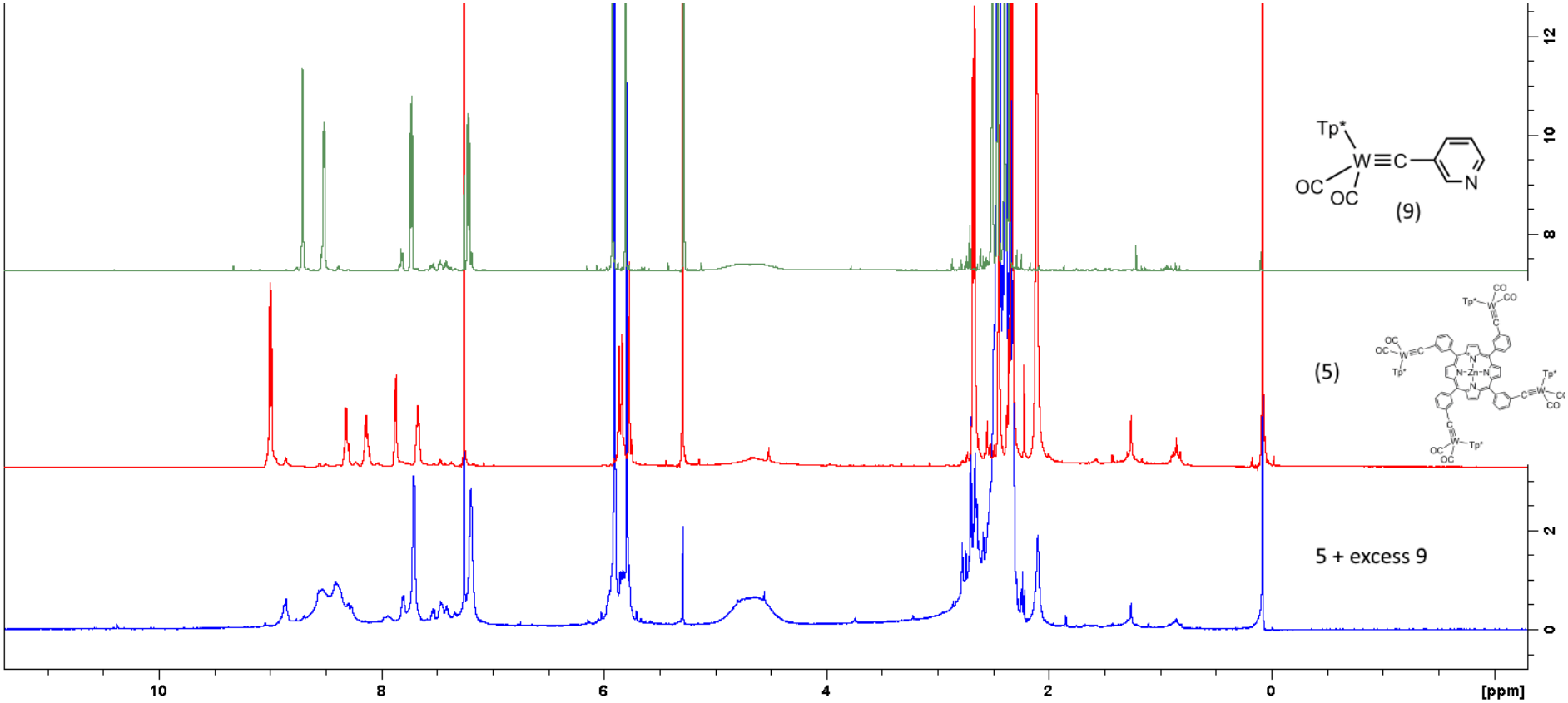

Figure S31. Comparison of ^{1}H NMR spectra at 25 °C of **5**, **9** and a mixture of **5** and excess **9**.

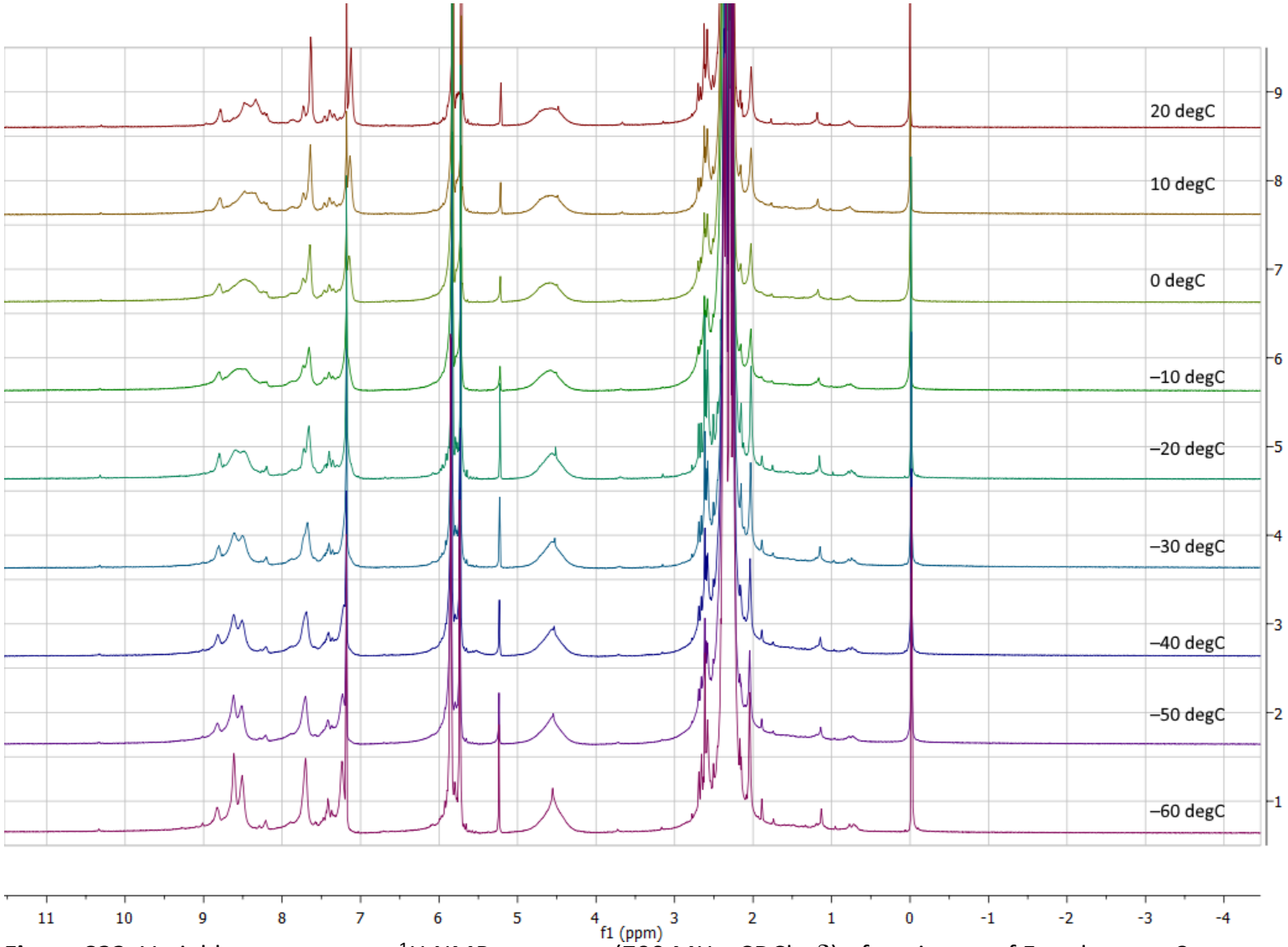

Figure S32. Variable-temperature ^{1}H NMR spectrum (700 MHz, $CDCl_3$, δ) of a mixture of **5** and excess **9**.

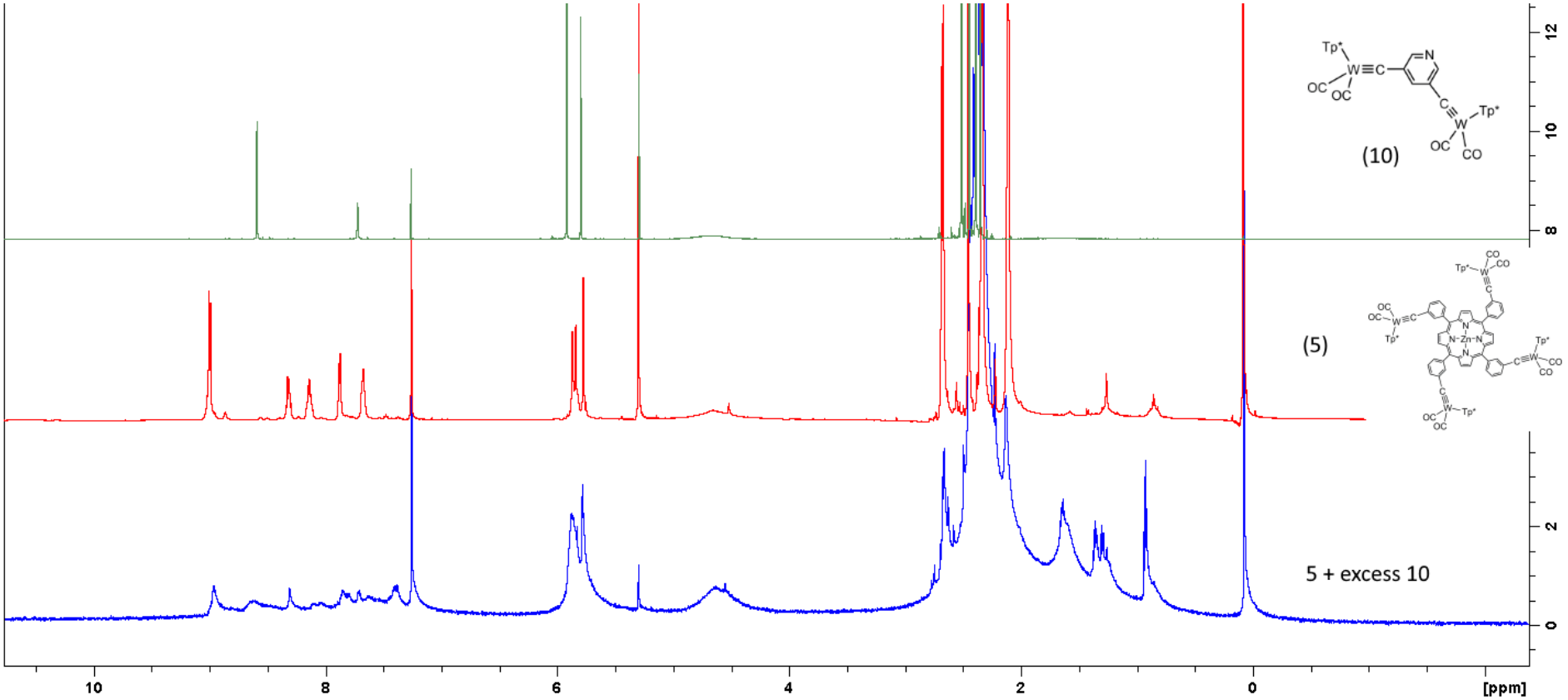

Figure S33. Comparison of ^{1}H NMR spectra at 25 °C of **5**, **10** and a mixture of **5** and excess **10**.

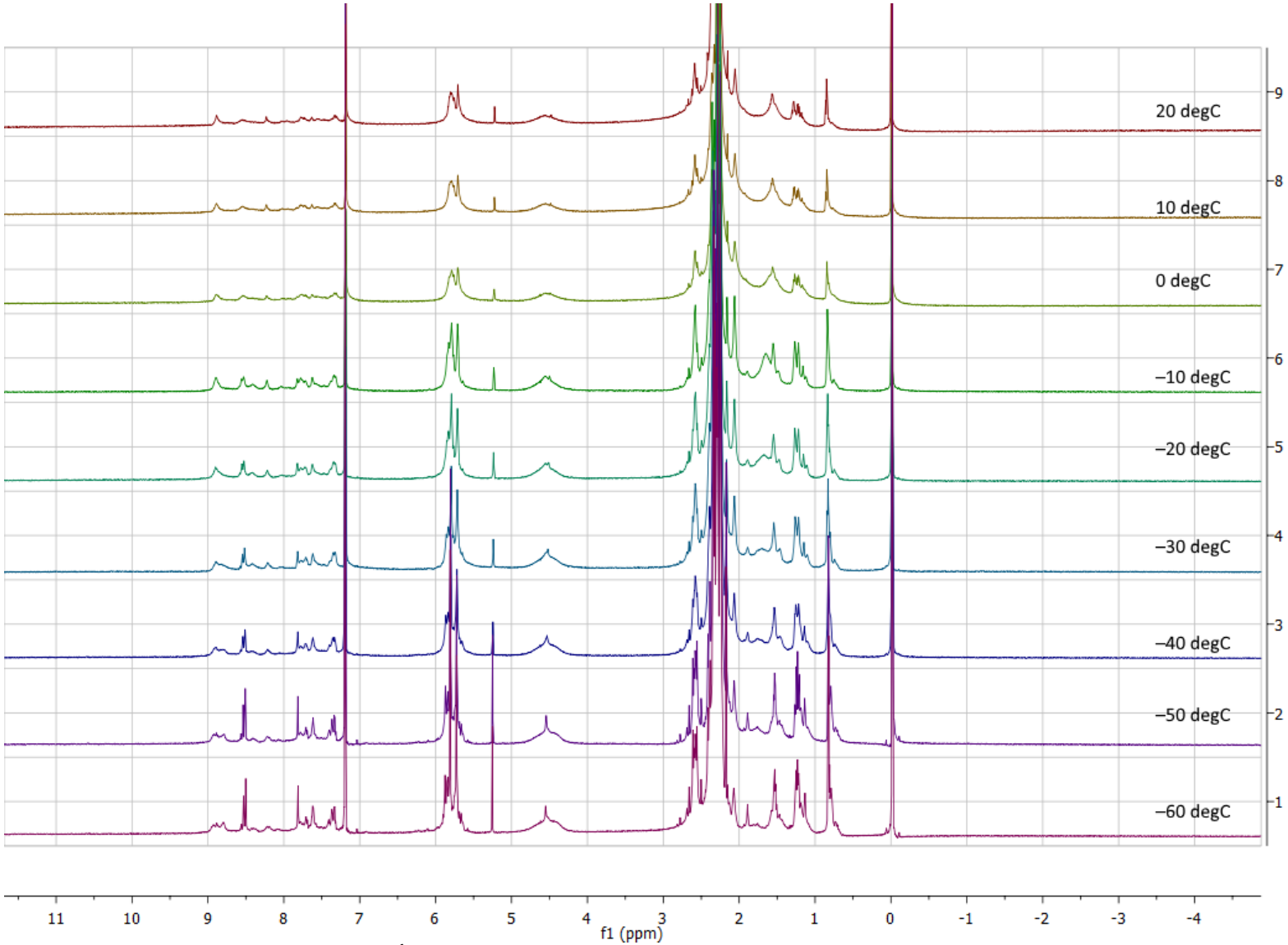

Figure S34. Variable-temperature ^{1}H NMR spectrum (700 MHz, $CDCl_3$, δ) of a mixture of **5** and excess **10**.

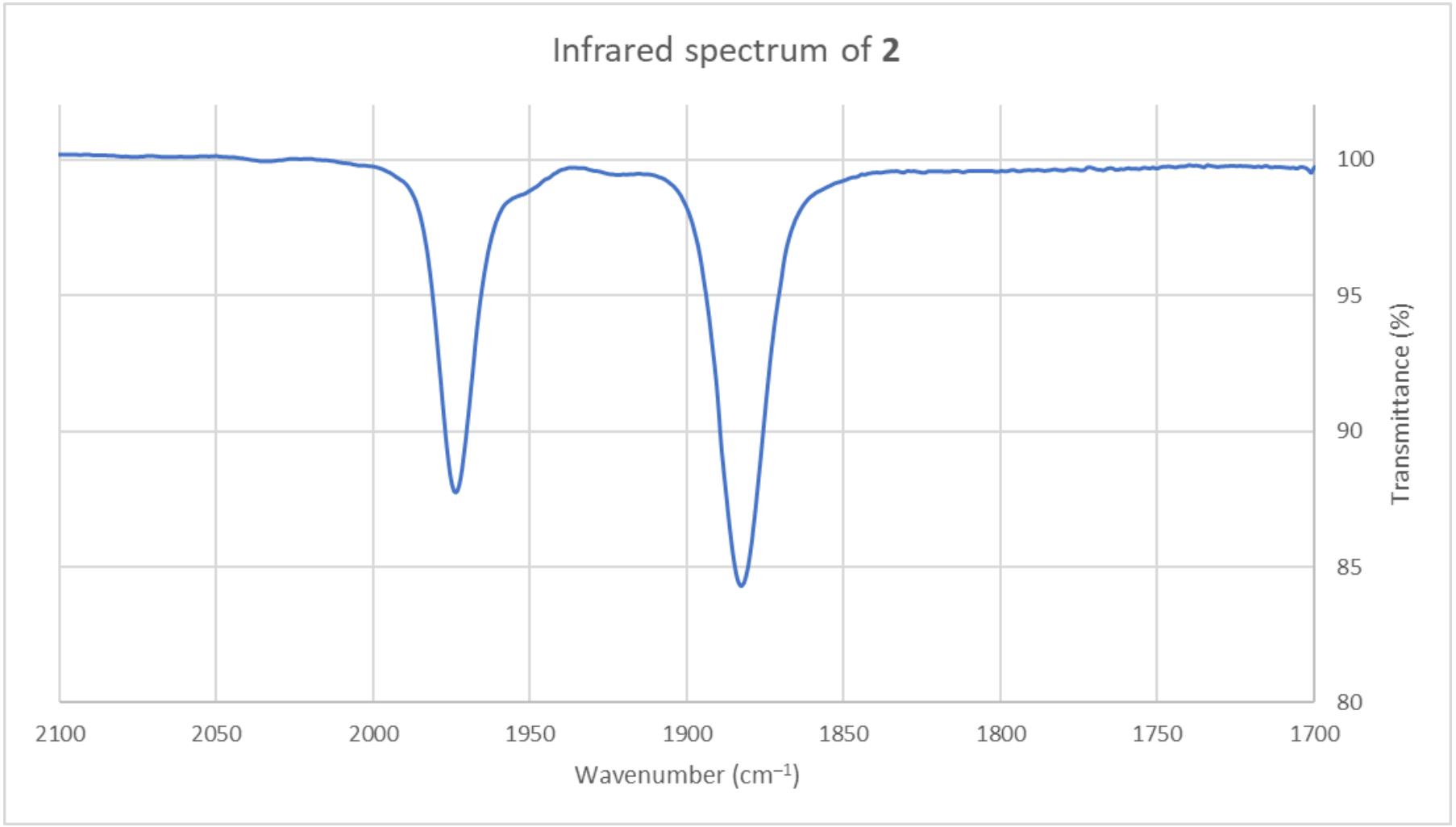

Figure S35. Infrared spectrum (CH_2Cl_2, cm^{-1}) of **2**.

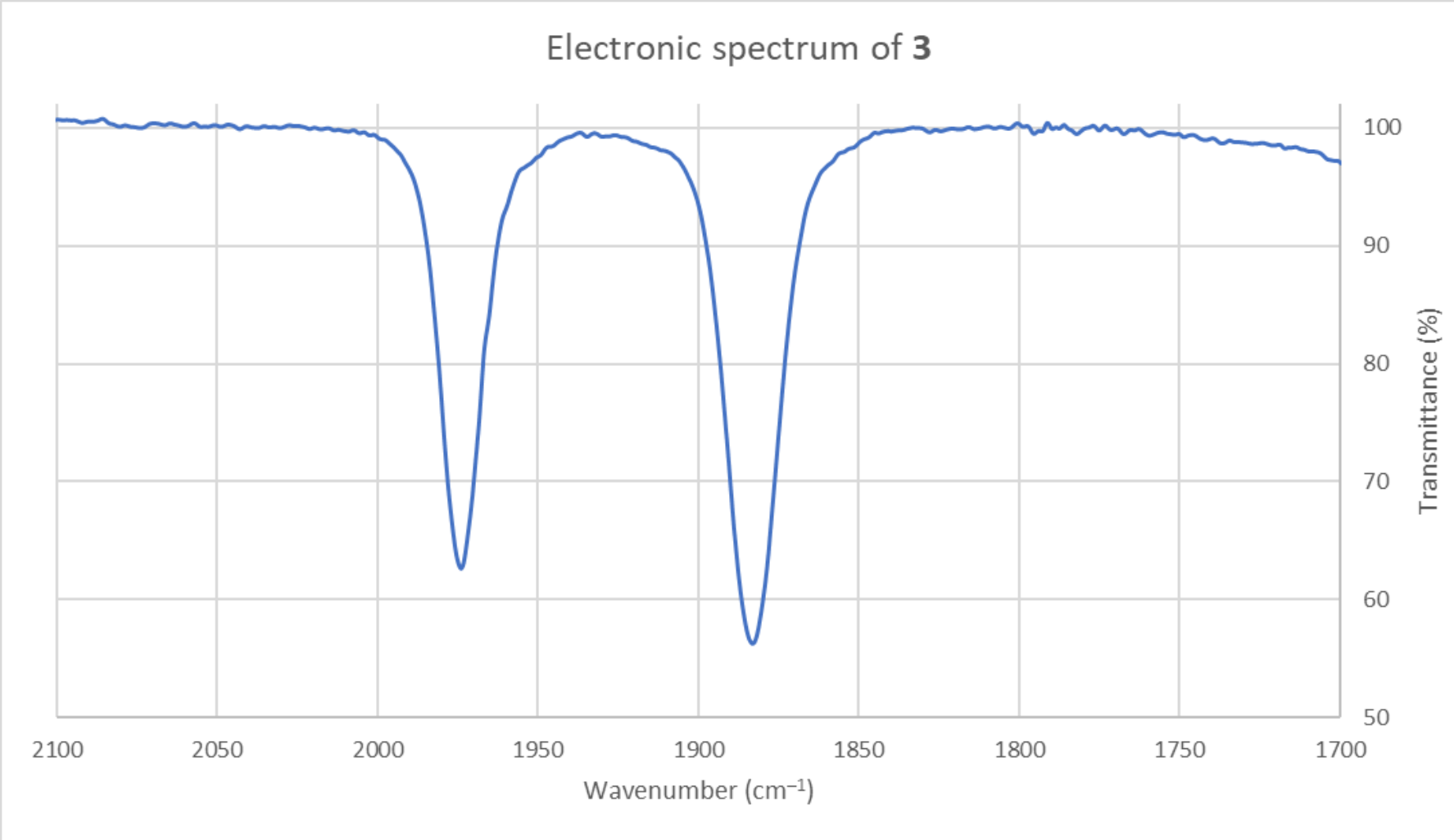

Figure S36. Infrared spectrum (CH_2Cl_2, cm^{-1}) of **3**.

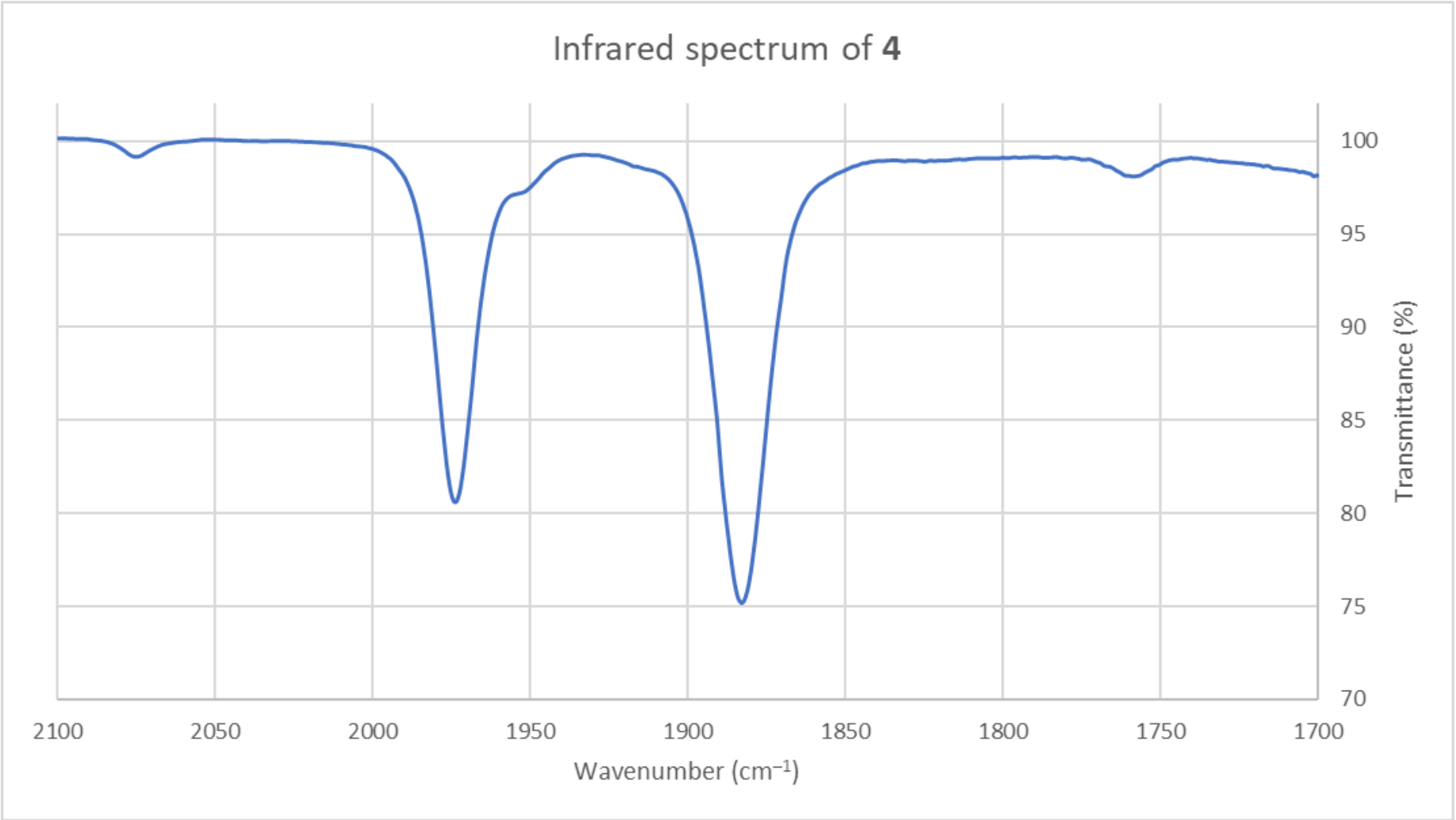

Figure S37. Infrared spectrum (CH_2Cl_2, cm^{-1}) of **4**.

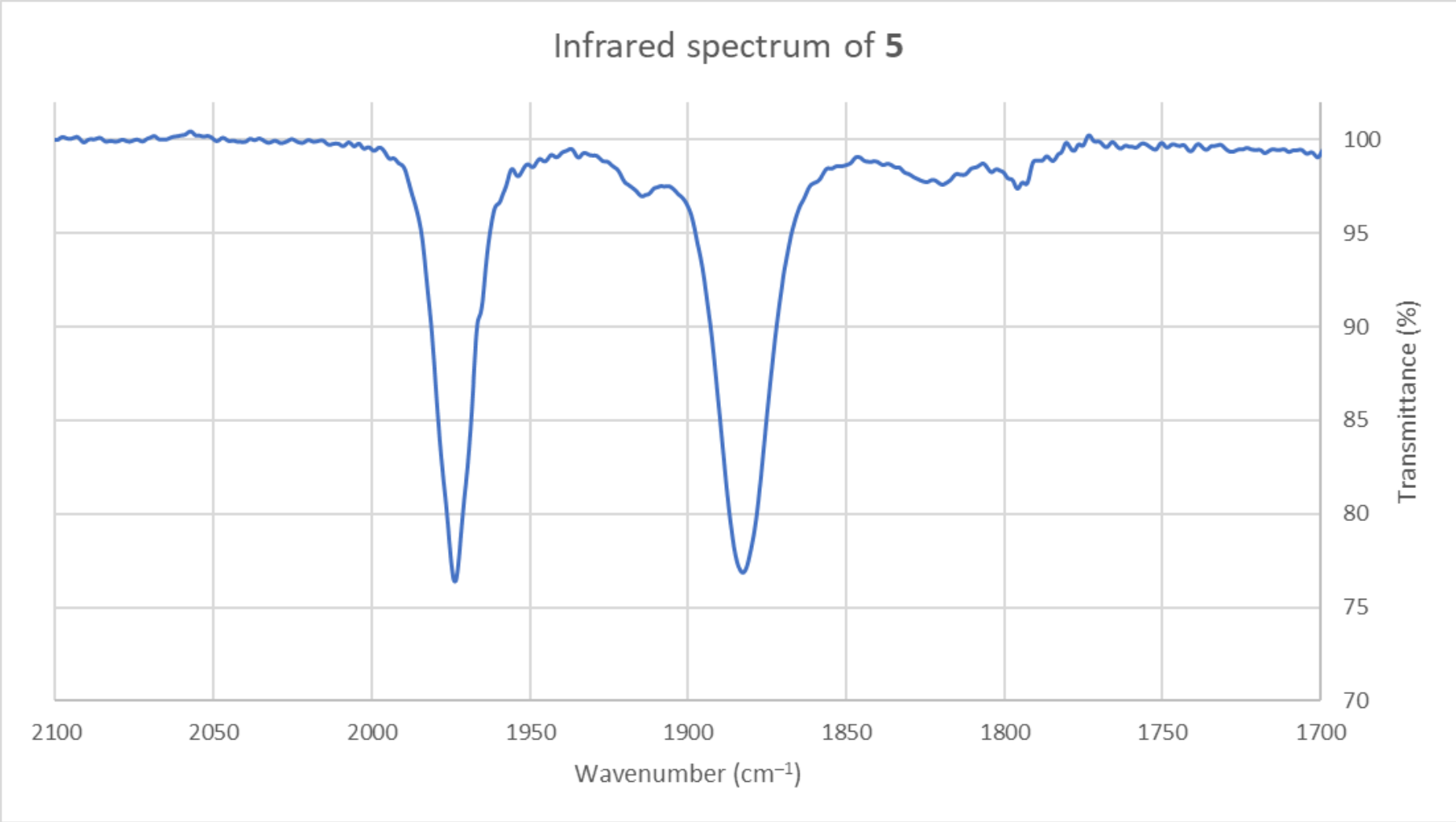

Figure S38. Infrared spectrum (CH_2Cl_2, cm^{-1}) of **5**.

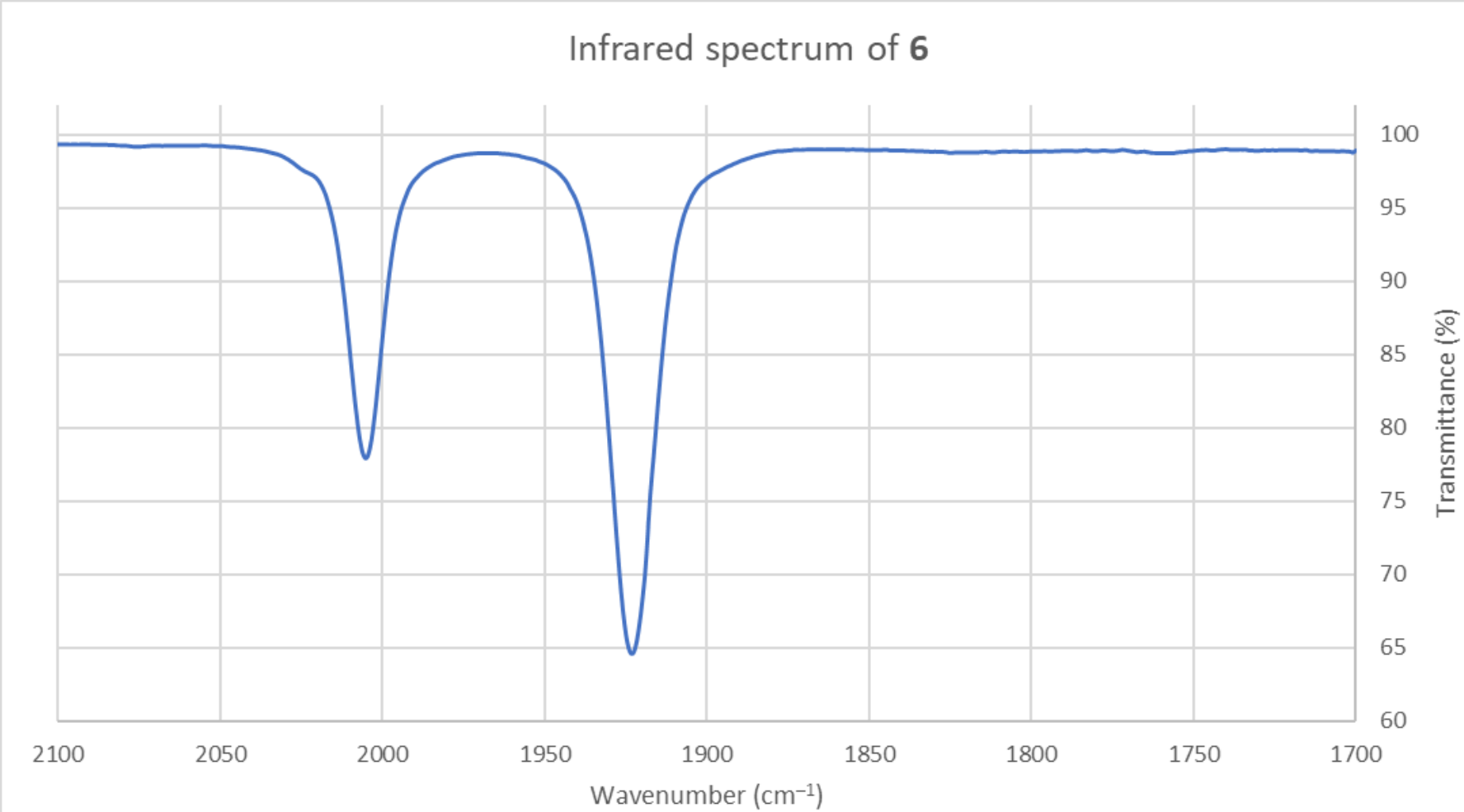

Figure S40. Infrared spectrum (CH_2Cl_2, cm^{-1}) of **6**.

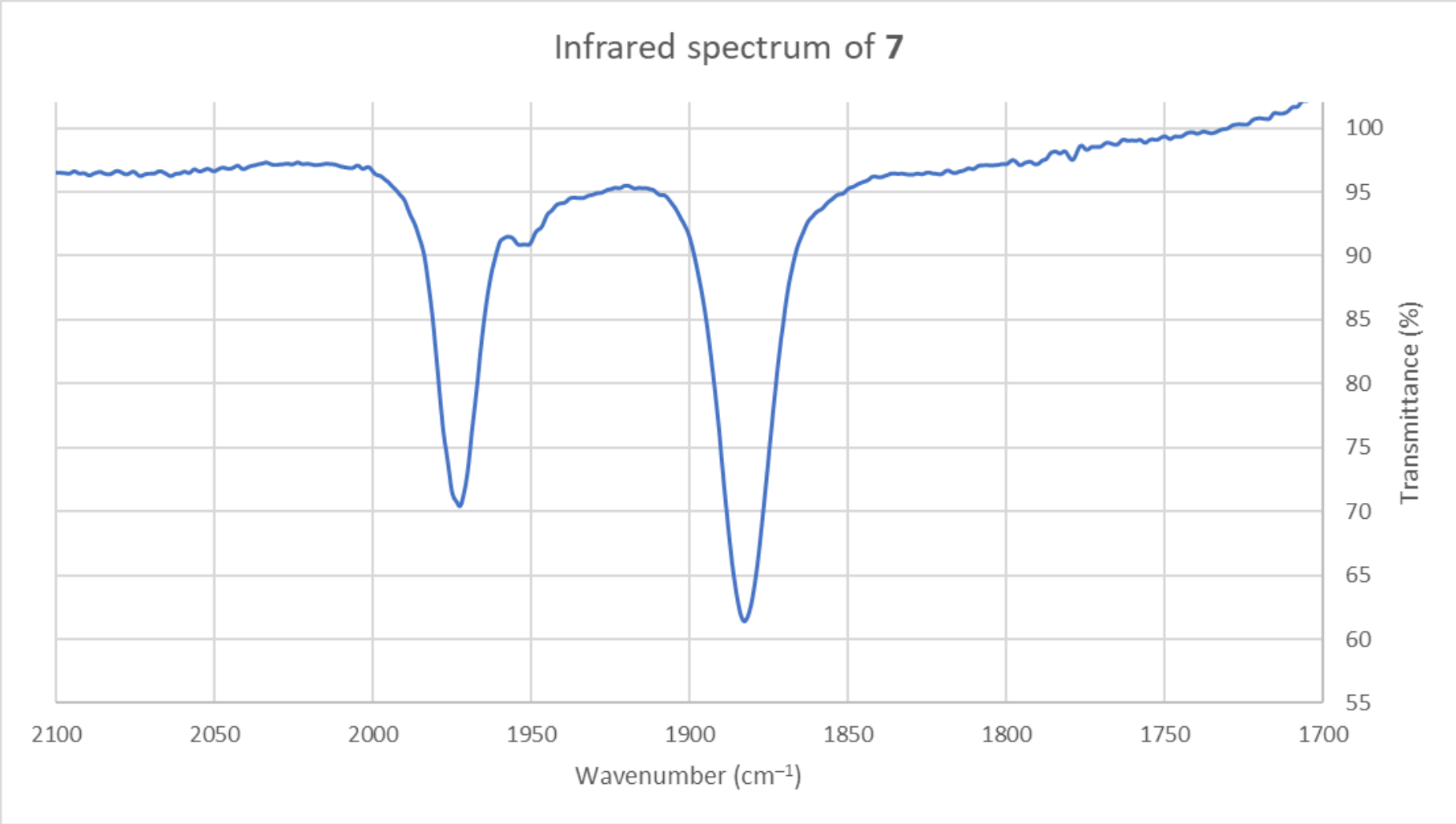

Figure S41. Infrared spectrum (CH_2Cl_2, cm^{-1}) of **7**.

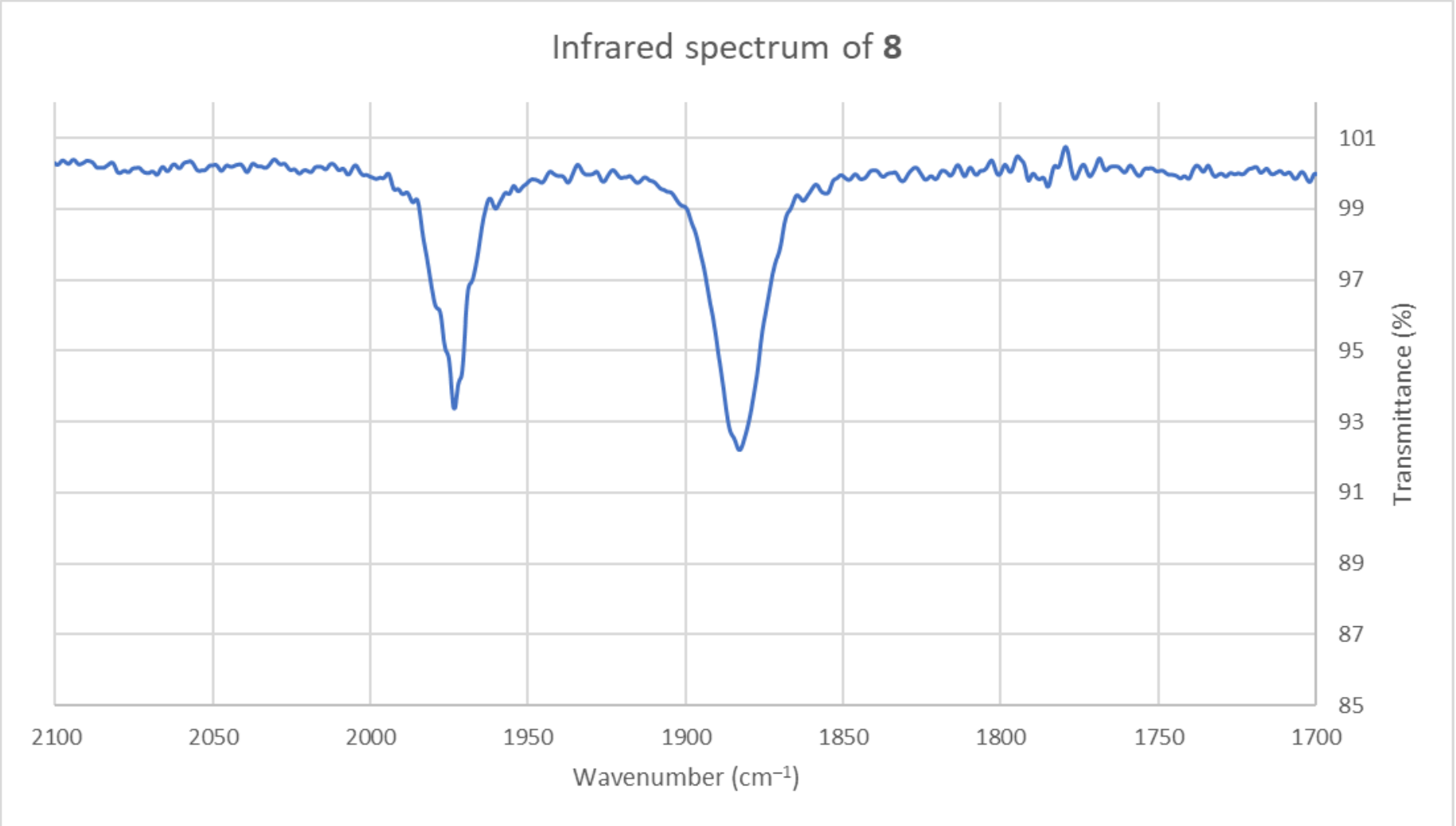

Figure S42. Infrared spectrum (CH_2Cl_2, cm^{-1}) of **8**.

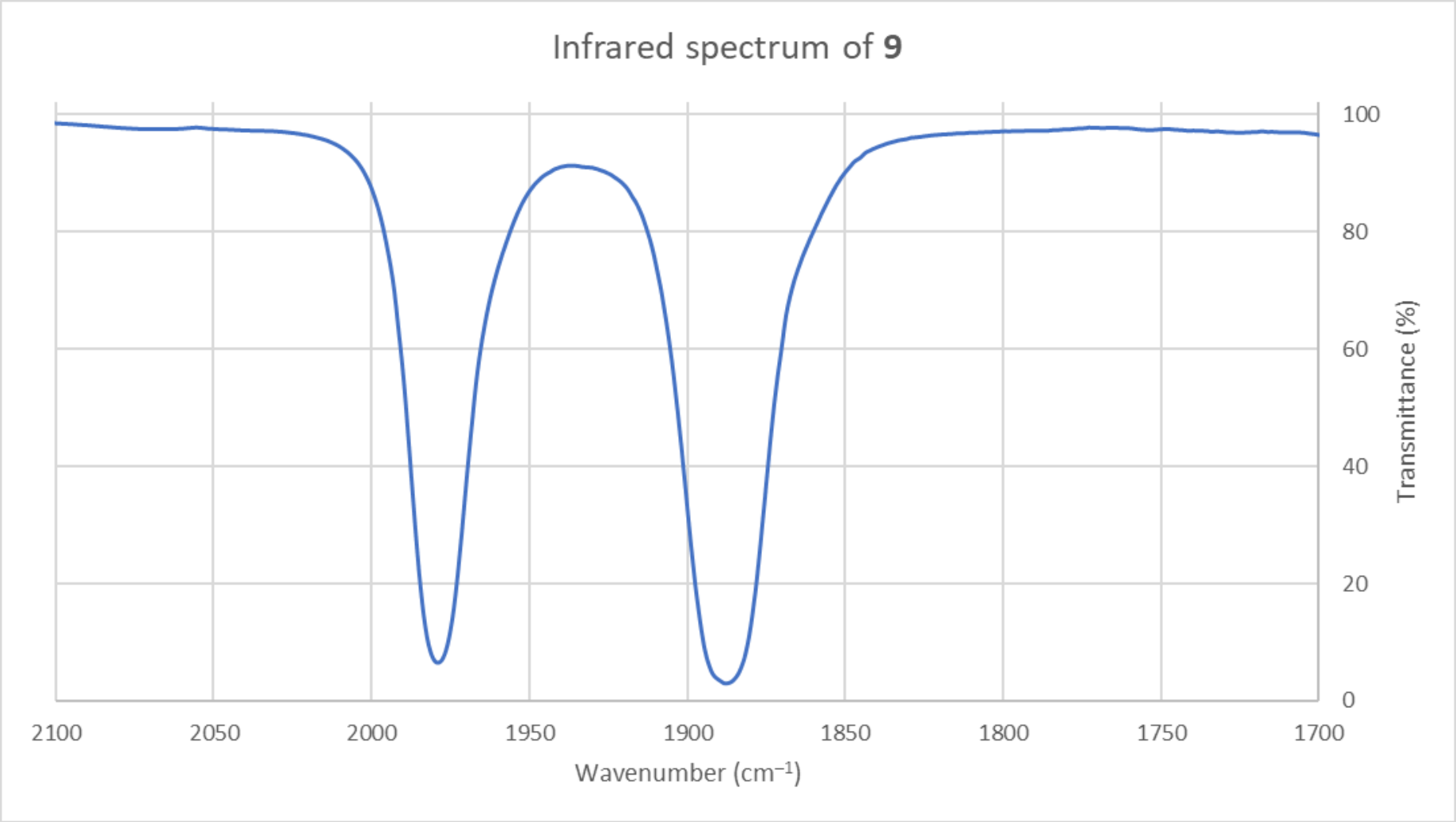

Figure S43. Infrared spectrum (CH_2Cl_2, cm^{-1}) of [NC_5H_4{C≡W(CO)$_2$(Tp*)}-3] (**9**).

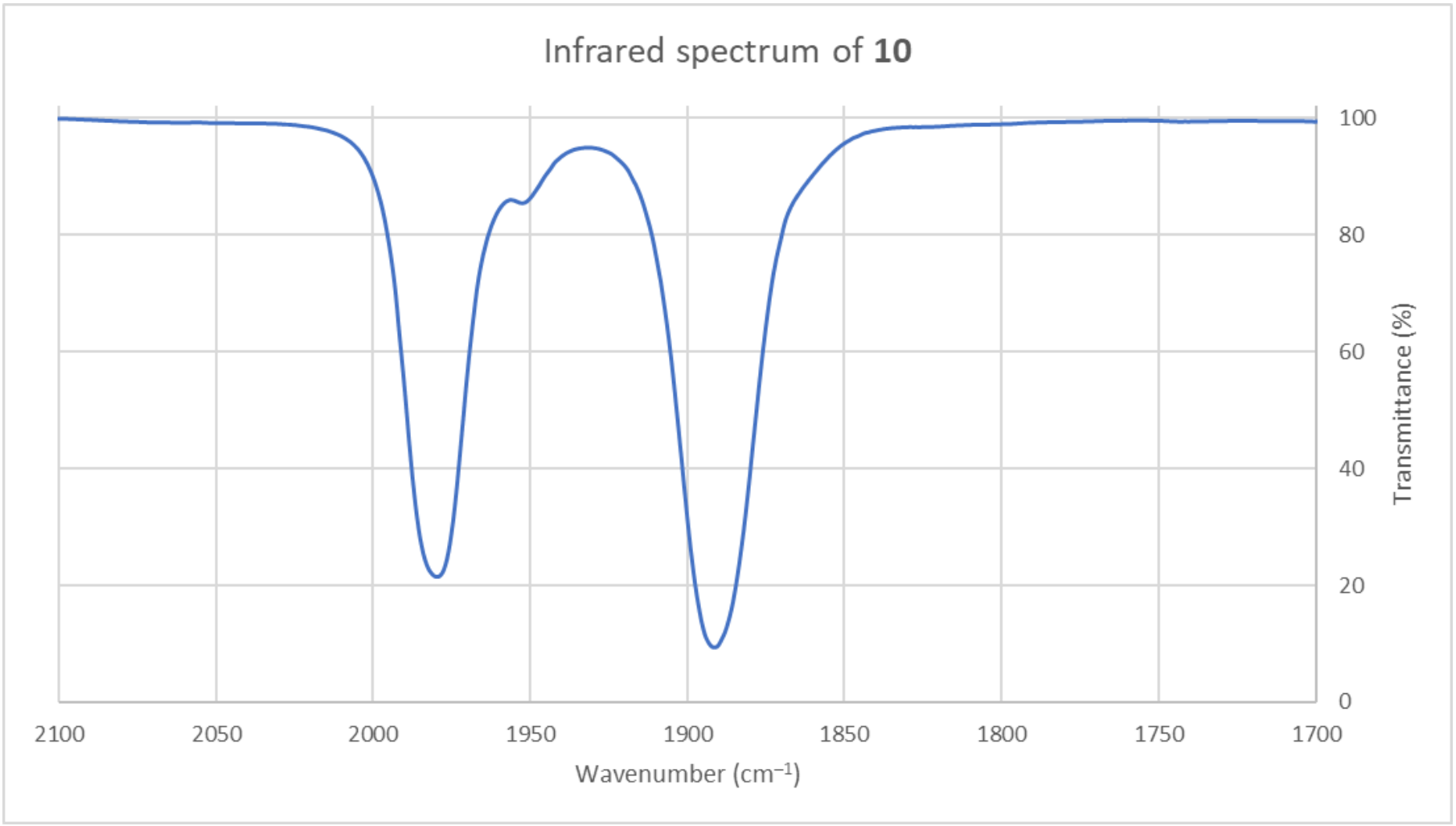

Figure S44. Infrared spectrum (CH_2Cl_2, cm^{-1}) of $[NC_5H_3\{C{\equiv}W(CO)_2(Tp^*)\}_2\text{-}3,5]$ (**10**).

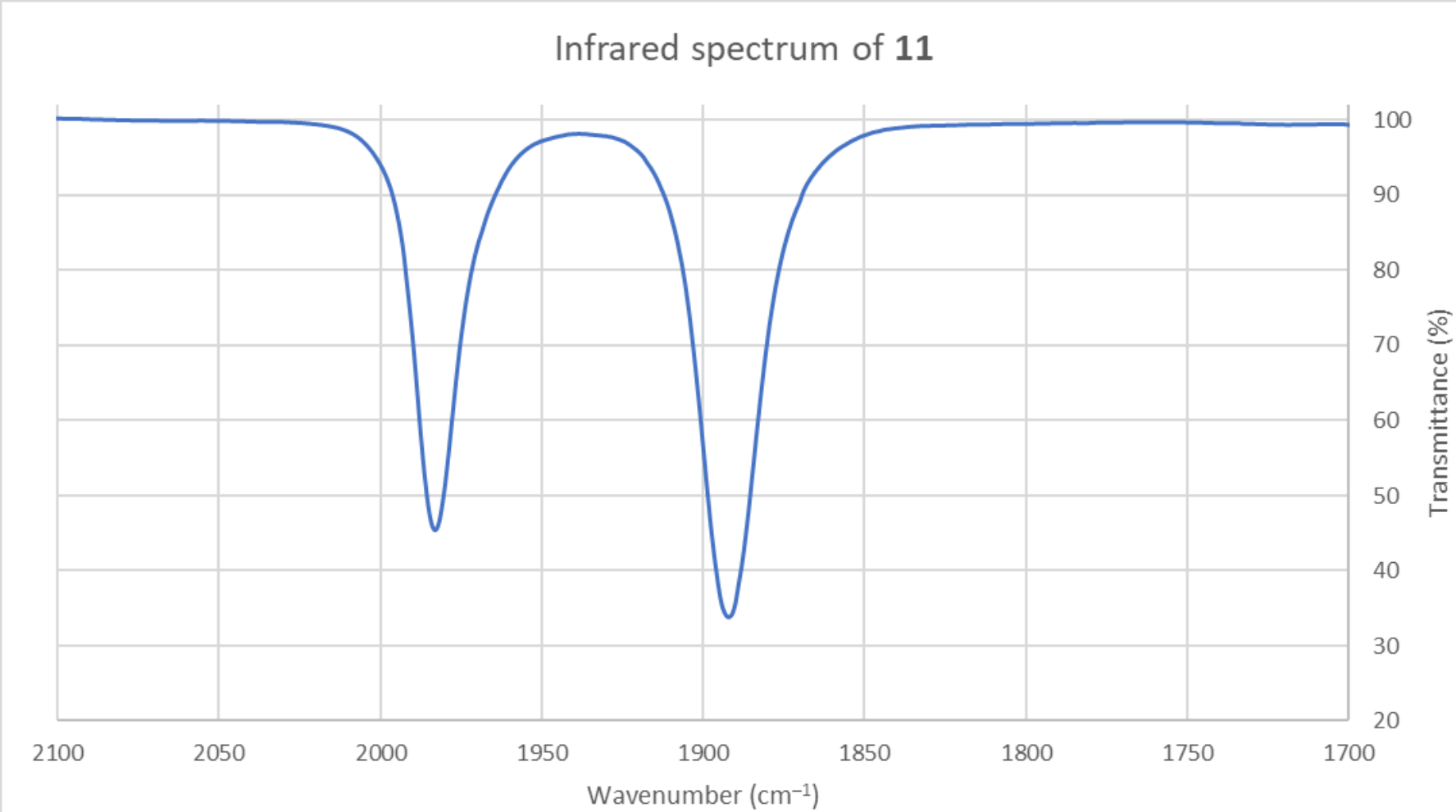

Figure S45. Infrared spectrum (CH_2Cl_2, cm^{-1}) of $[NC_5H_4\{C{\equiv}W(CO)_2(Tp^*)\}\text{-}4]$ (**11**).

Selected electronic spectra

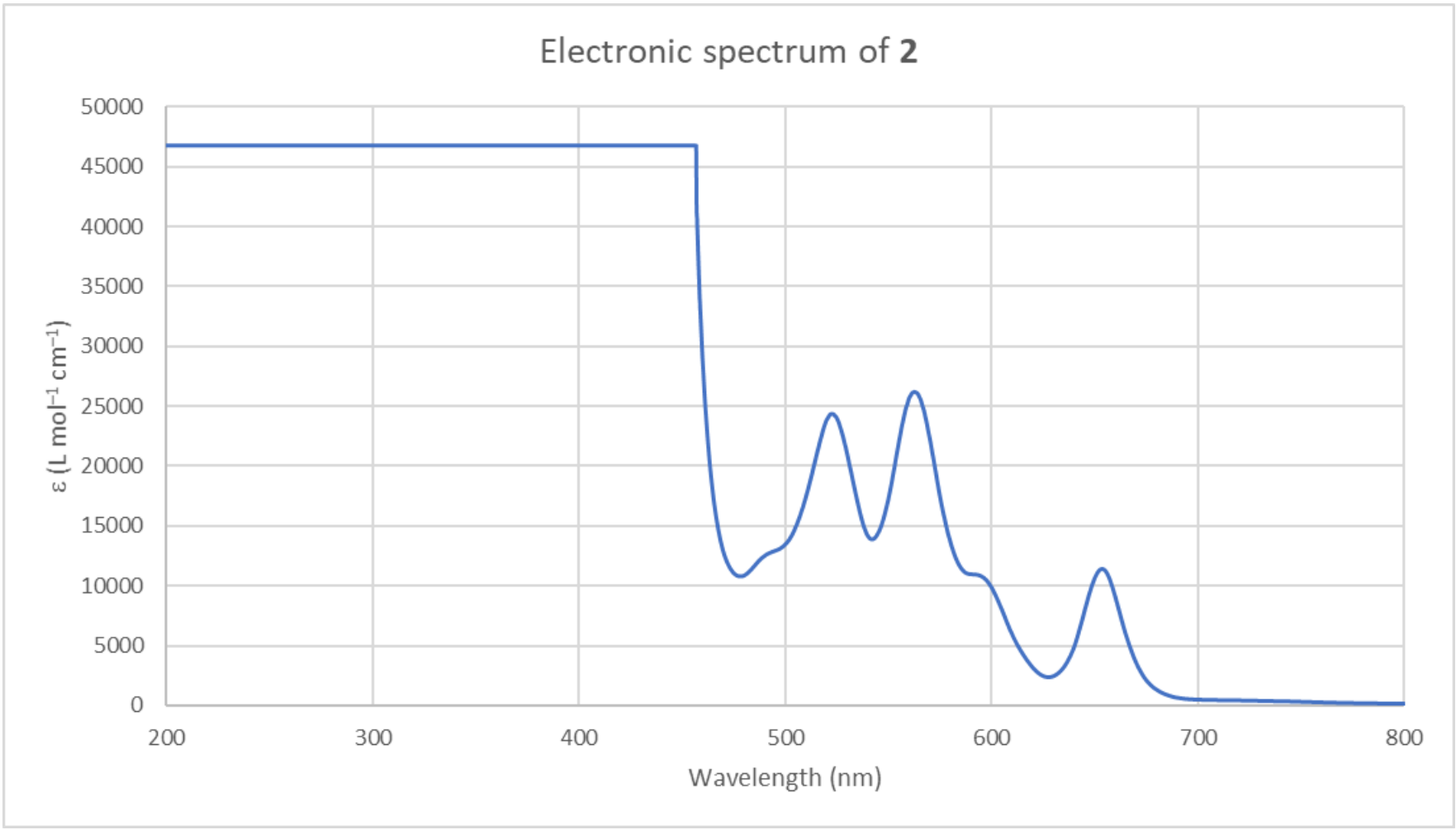

Figure S46. Electronic spectrum (CH_2Cl_2) of **2** (1.1 x 10^{-4} M).

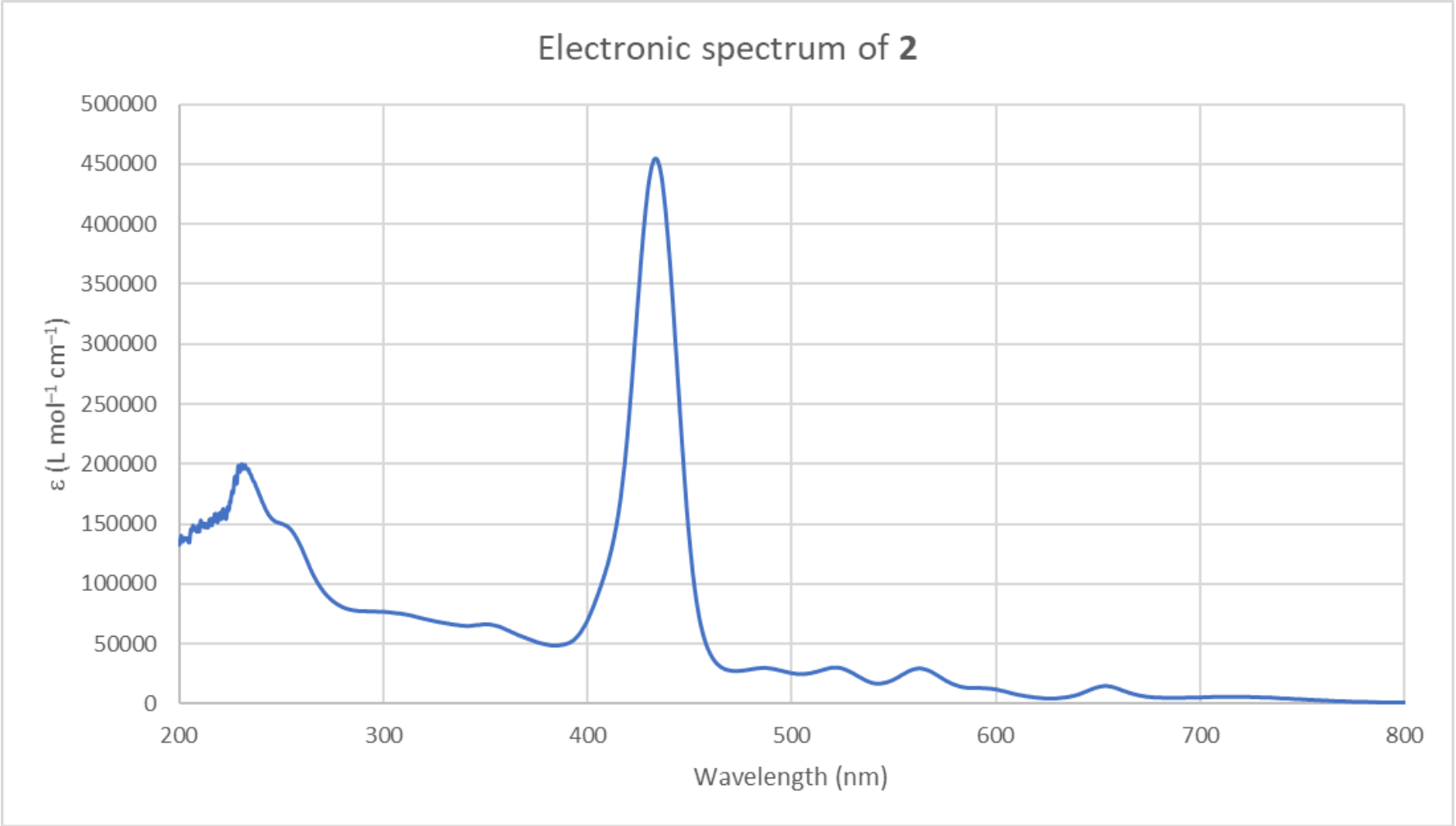

Figure S47. Electronic spectrum (CH_2Cl_2) of **2** (5.3 x 10^{-6} M).

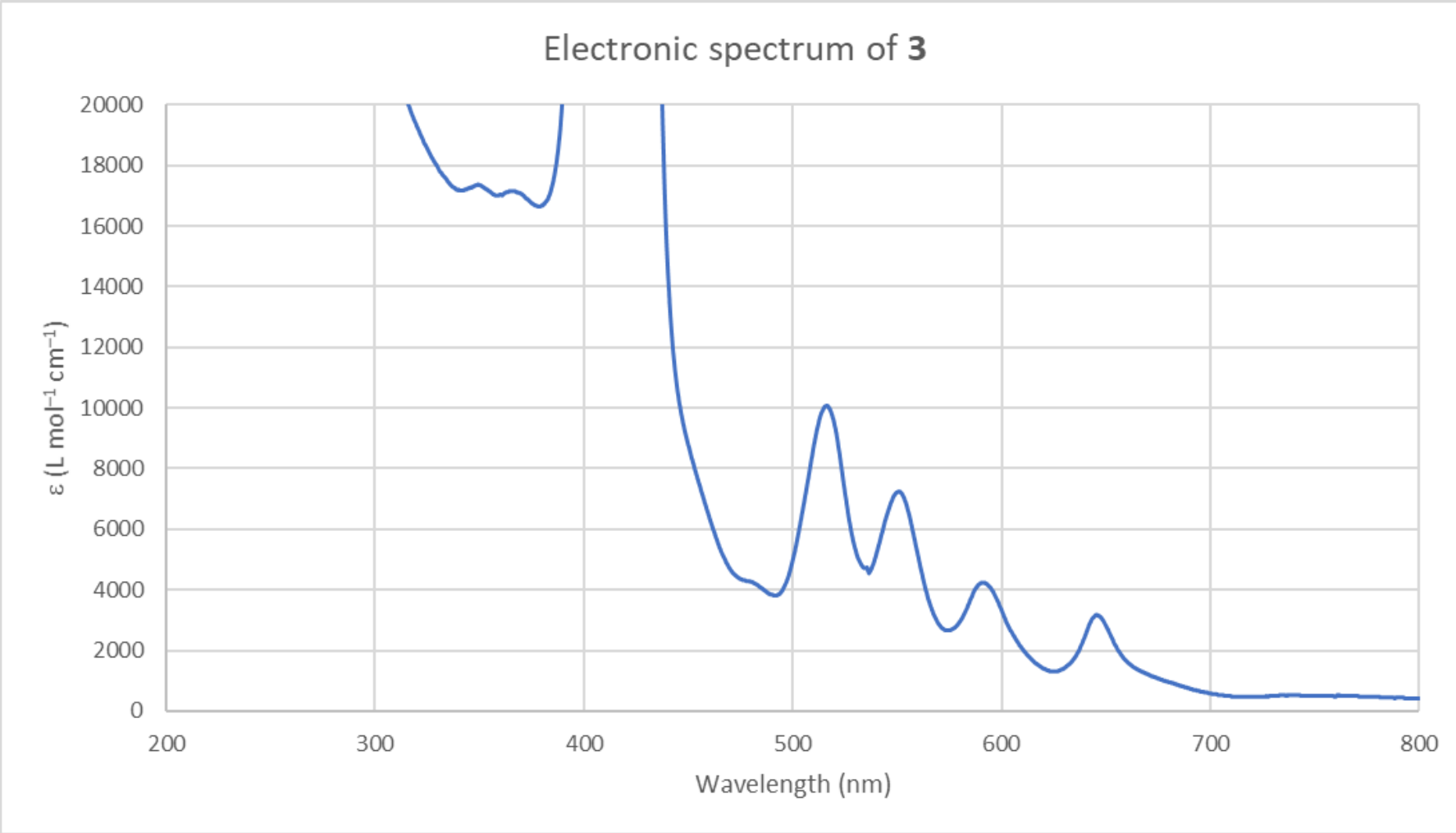

Figure S48. Electronic spectrum (CH_2Cl_2) of **3** (3.6 x 10^{-5} M).

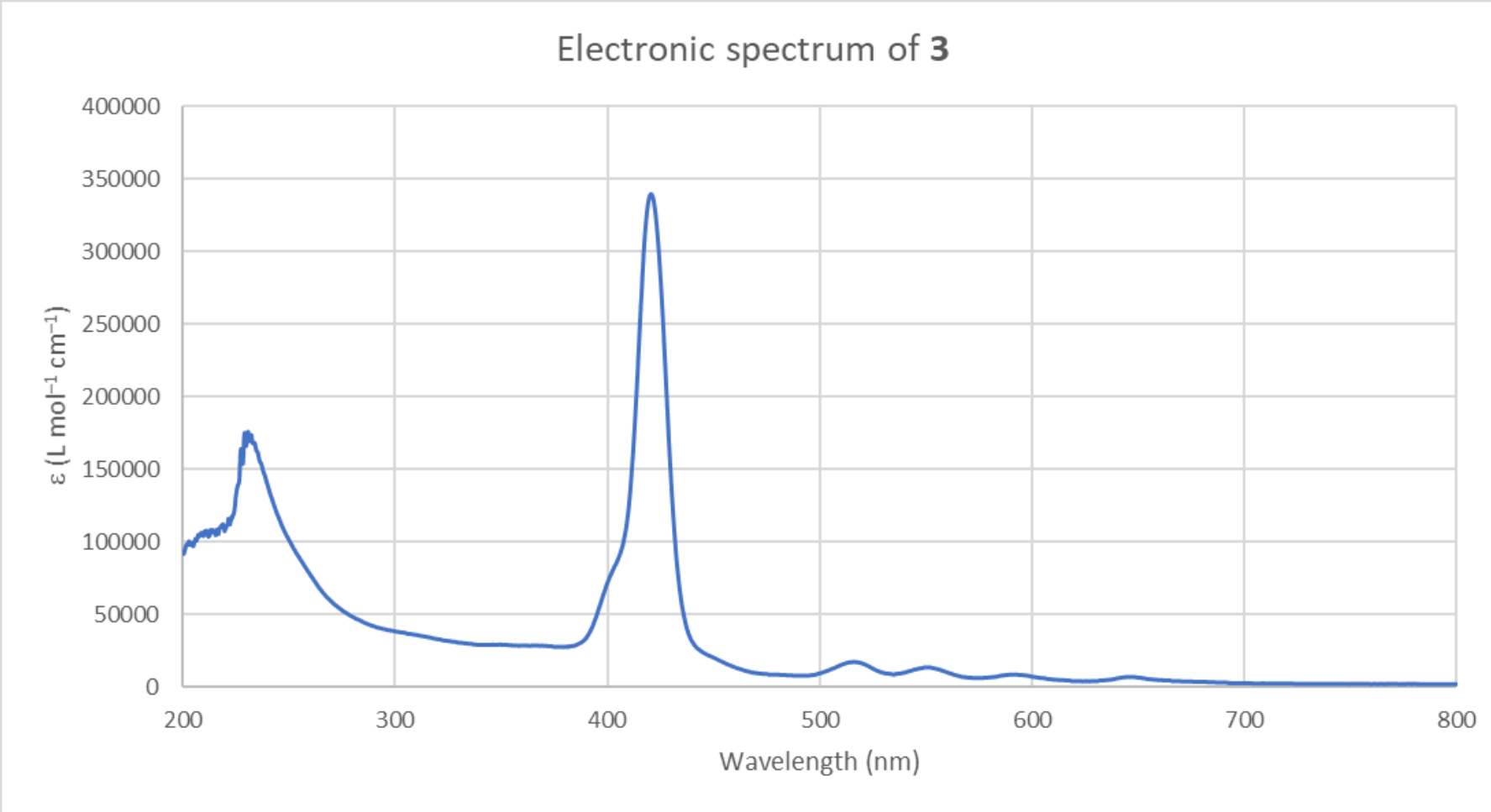

Figure S49. Electronic spectrum (CH_2Cl_2) of **3** (3.6 x 10^{-6} M).

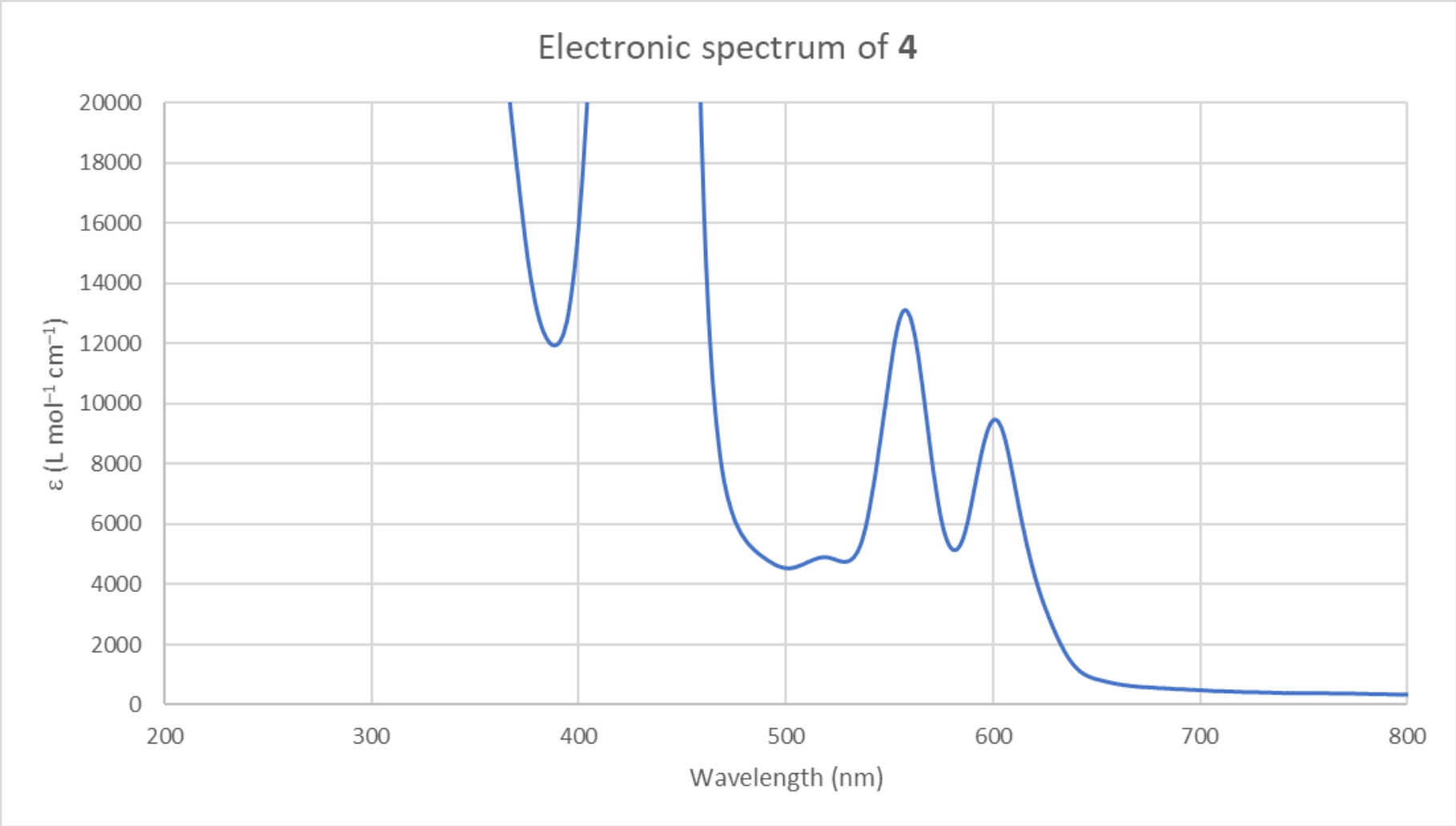

Figure S50. Electronic spectrum (CH_2Cl_2) of **4** (1.2 x 10^{-4} M).

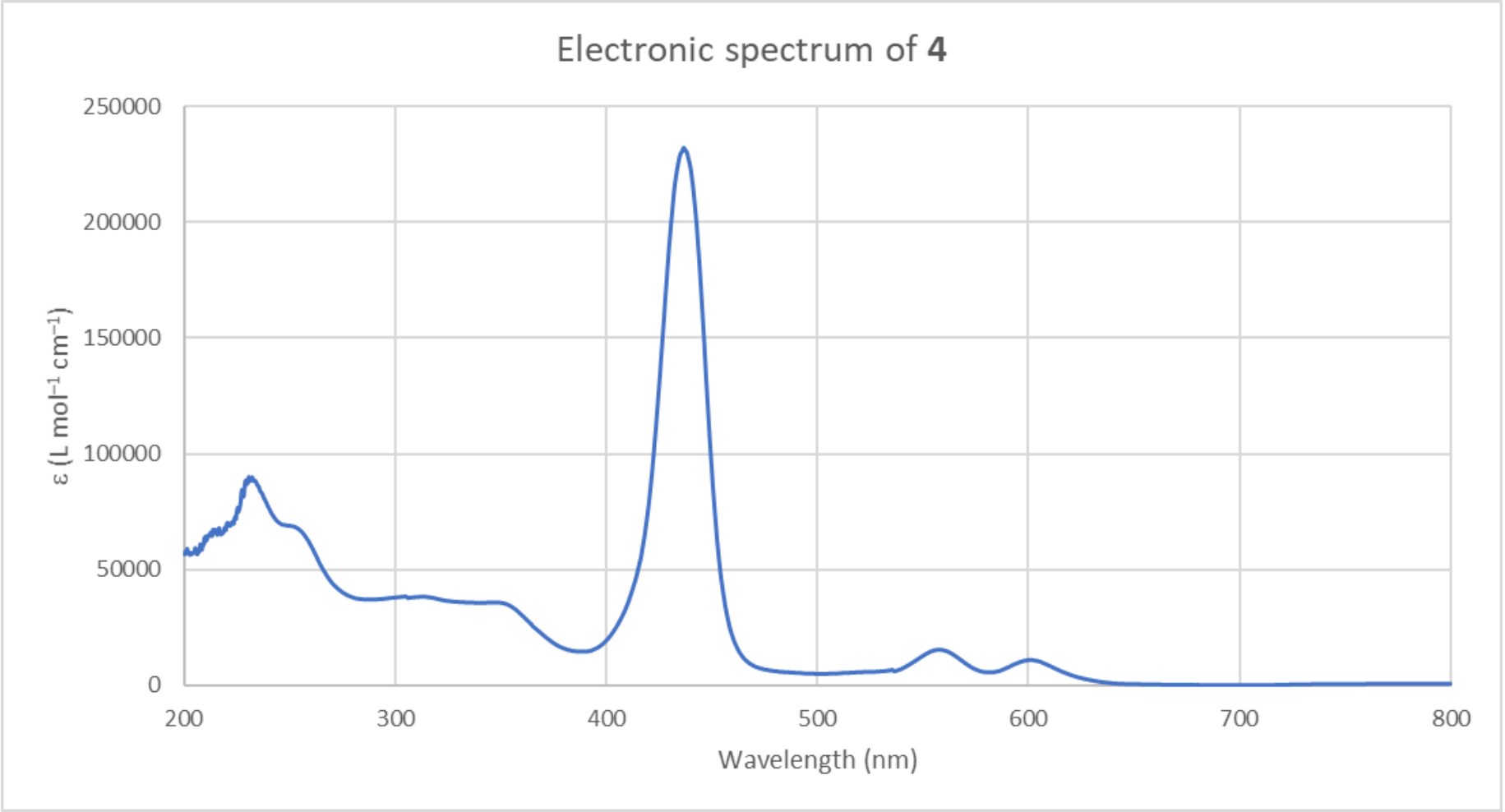

Figure S51. Electronic spectrum (CH_2Cl_2) of **4** (1.2 x 10^{-5} M).

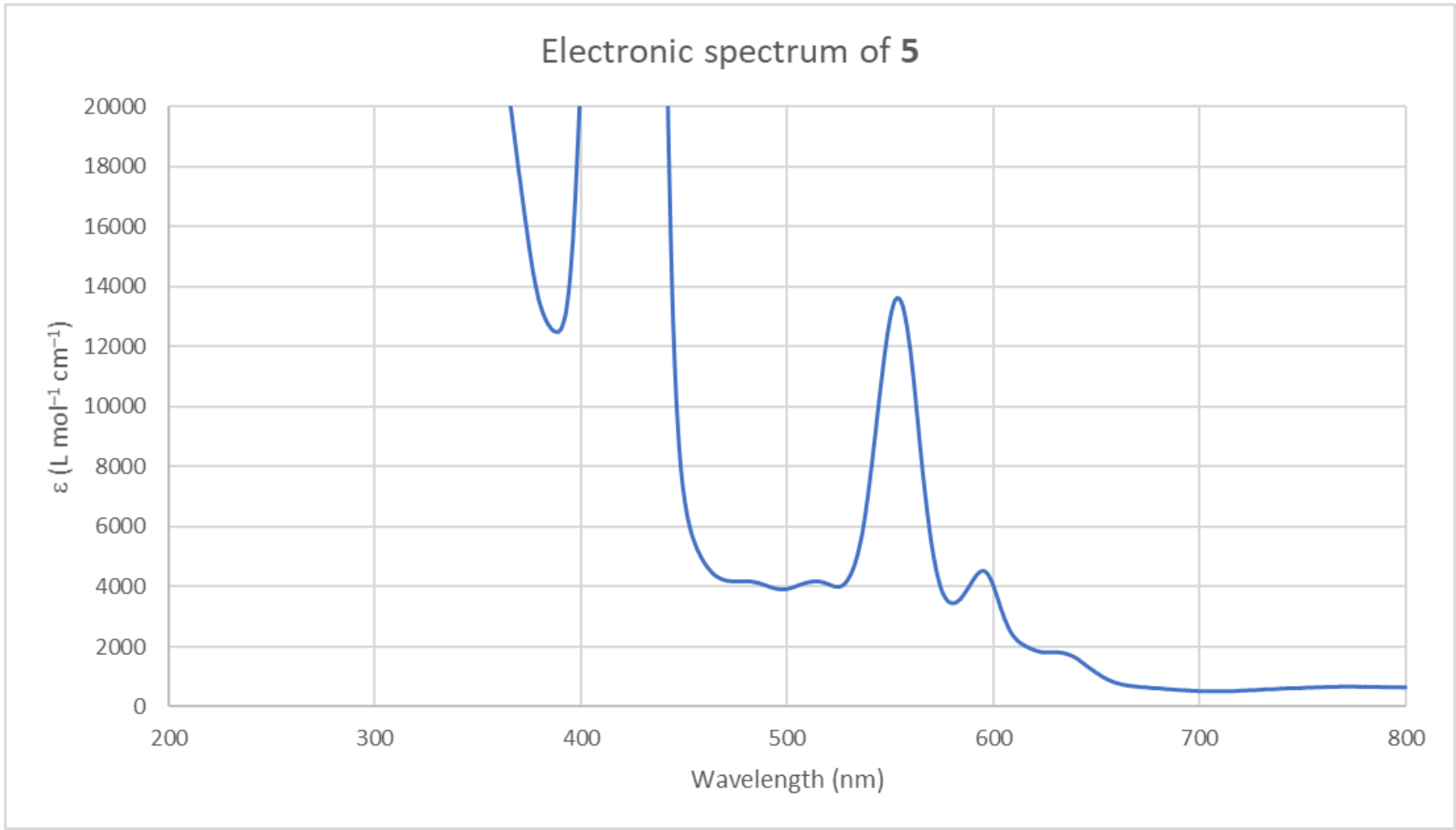

Figure S52. Electronic spectrum (CH_2Cl_2) of **5** (1.2×10^{-4} M).

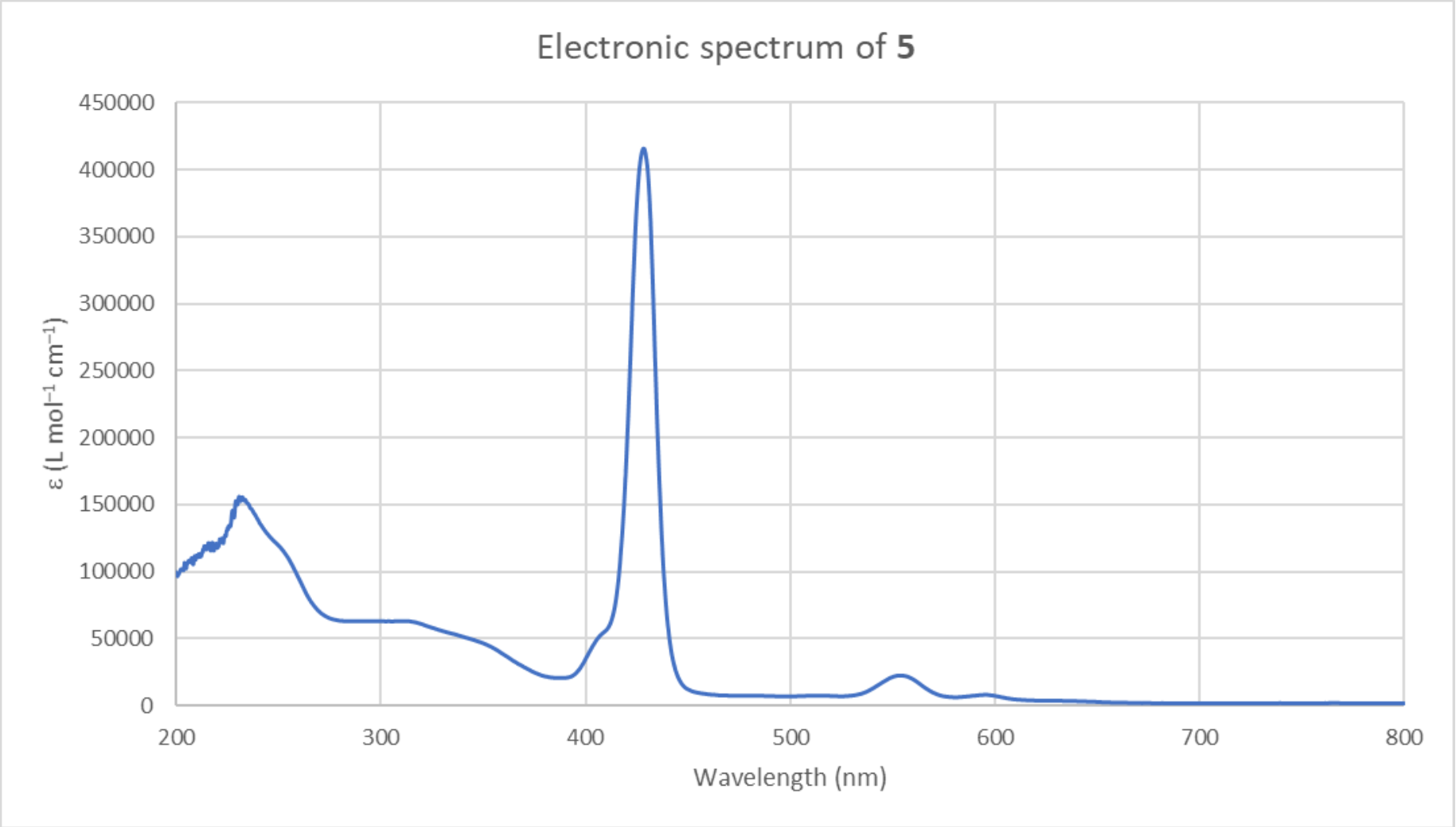

Figure S53. Electronic spectrum (CH_2Cl_2) of **5** (6.8 x 10^{-6} M).

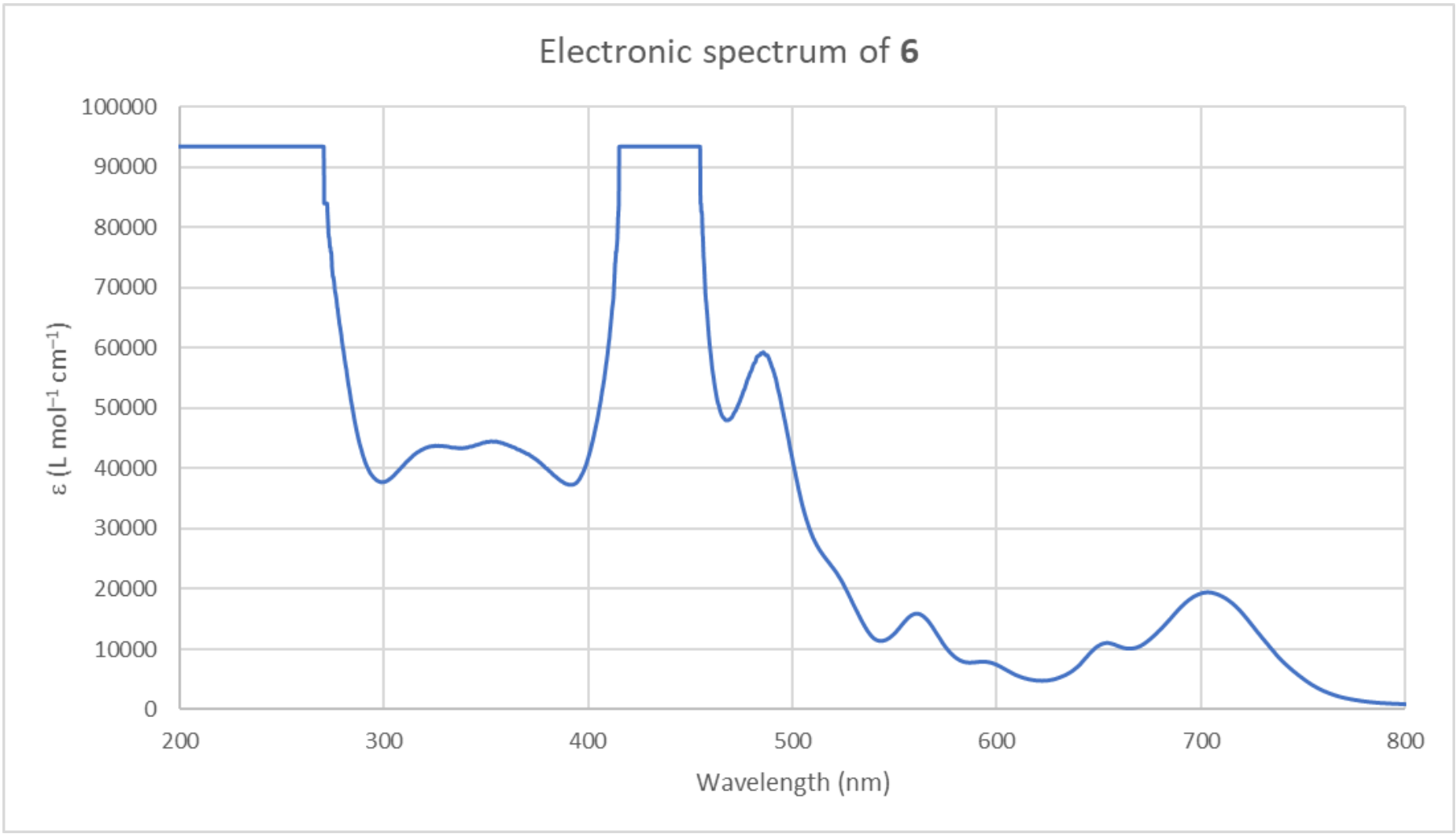

Figure S54. Electronic spectrum (CH_2Cl_2) of **6** (5.4 x 10^{-5} M).

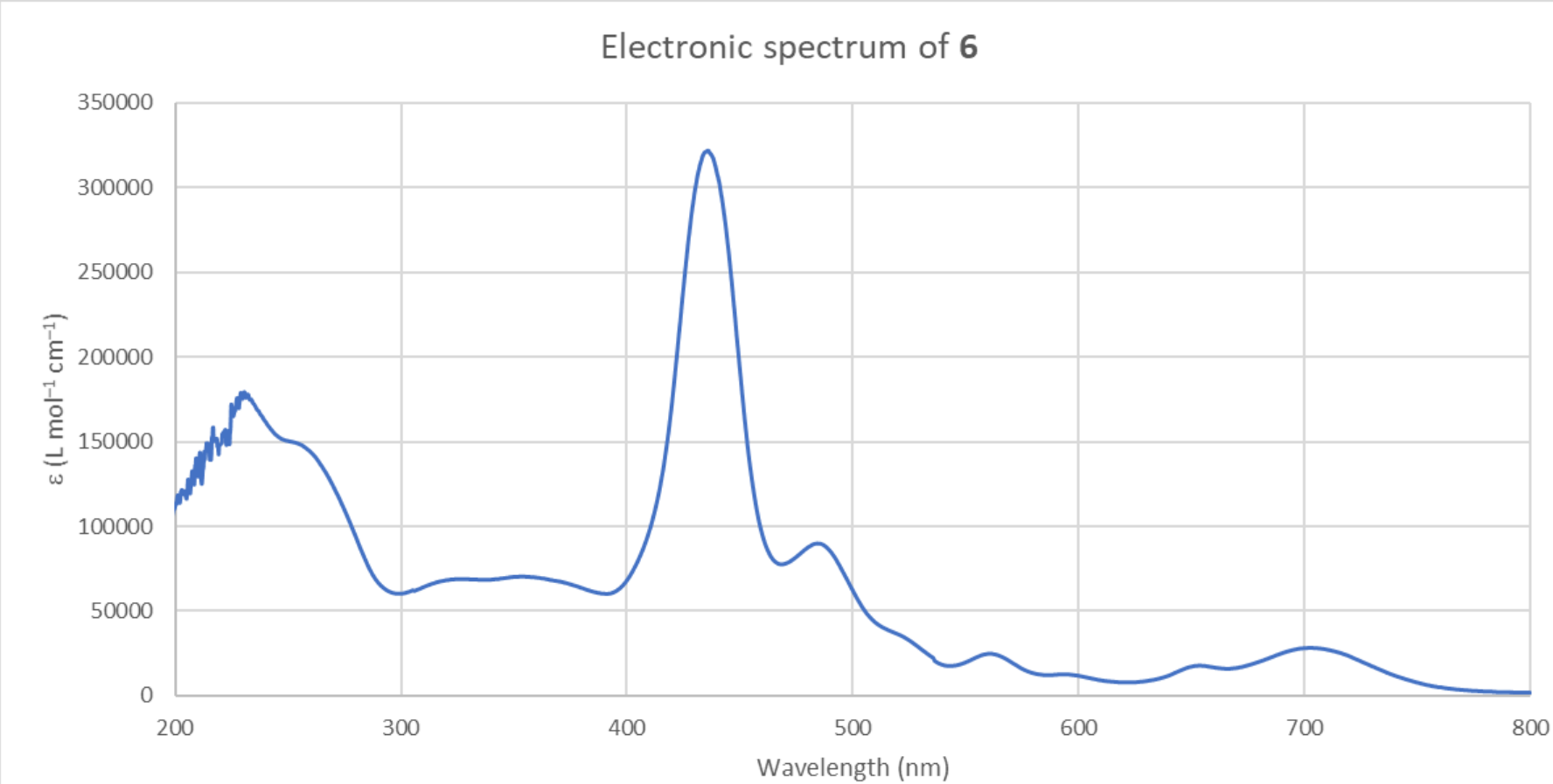

Figure S55. Electronic spectrum (CH_2Cl_2) of **6** (8.9 x 10^{-6} M).

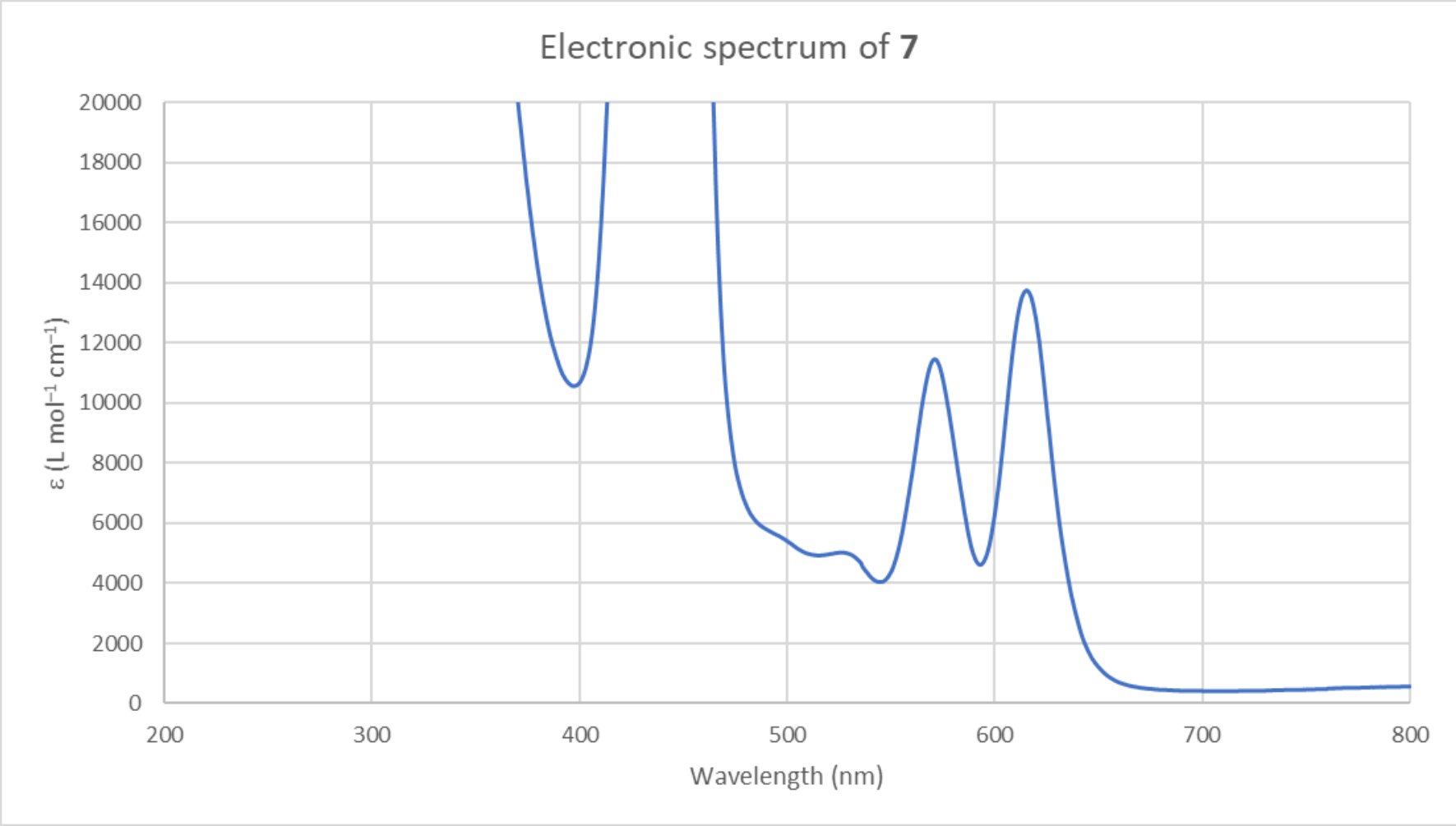

Figure S56. Electronic spectrum (CH_2Cl_2) of **3** (1.2 x 10^{-4} M) in the presence of excess 4-dimethylaminopyridine (**7**).

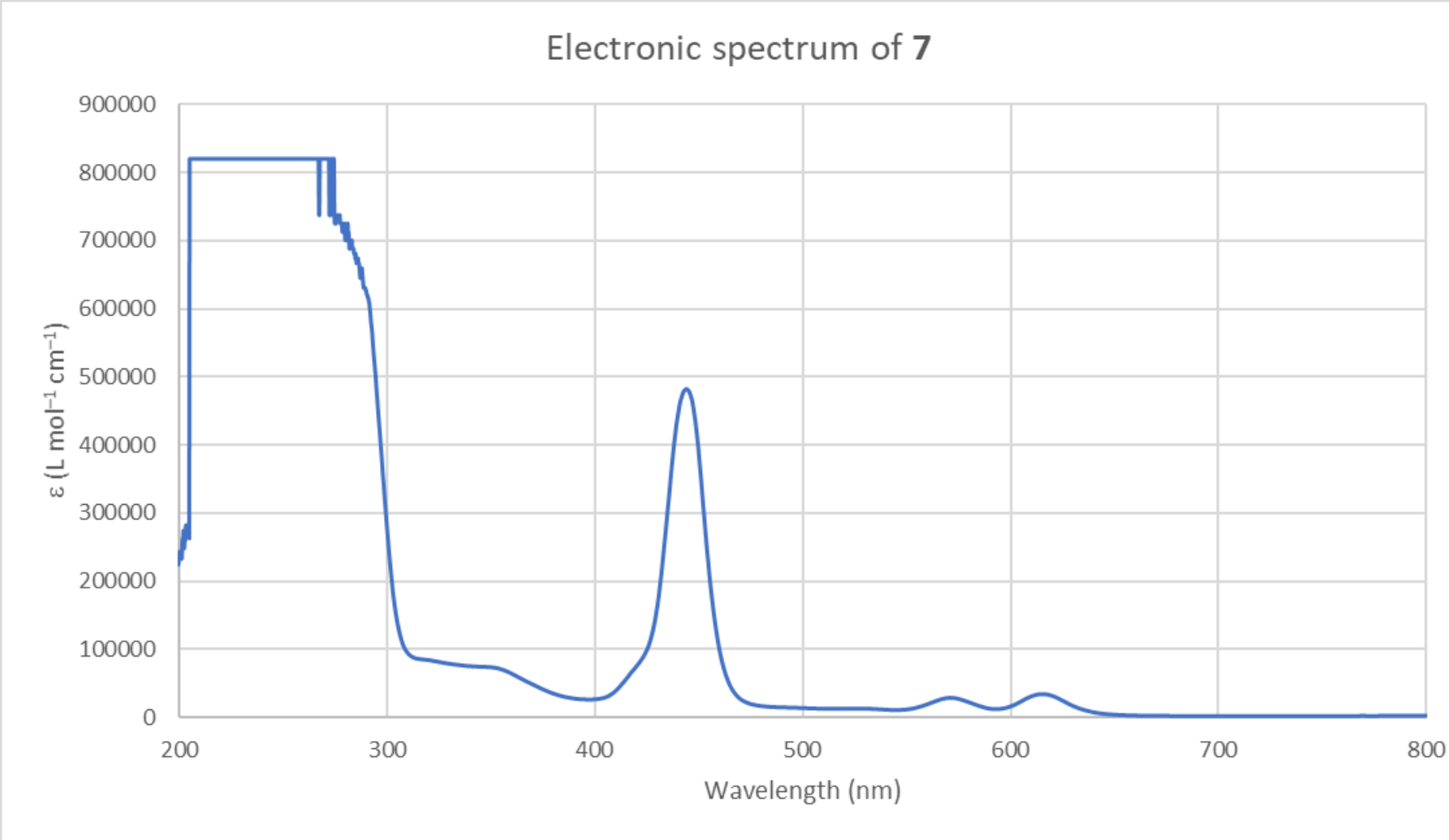

Figure S57. Electronic spectrum (CH_2Cl_2) of **3** (6.1×10^{-6} M) in the presence of excess 4-dimethylaminopyridine (**7**).

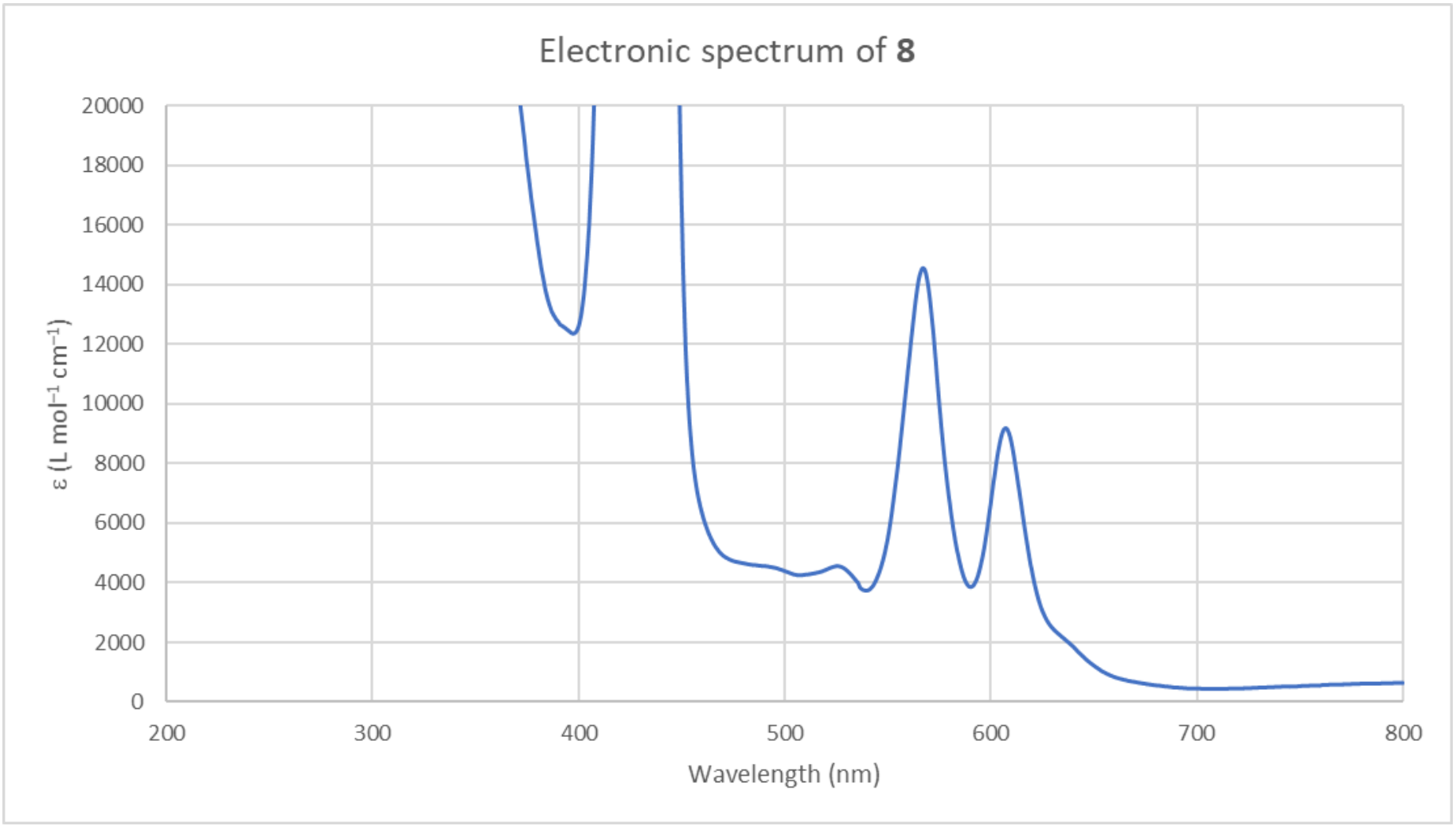

Figure S58. Electronic spectrum (CH_2Cl_2) of **4** (1.2 x 10^{-4} M) in the presence of excess 4-dimethylaminopyridine (**8**).

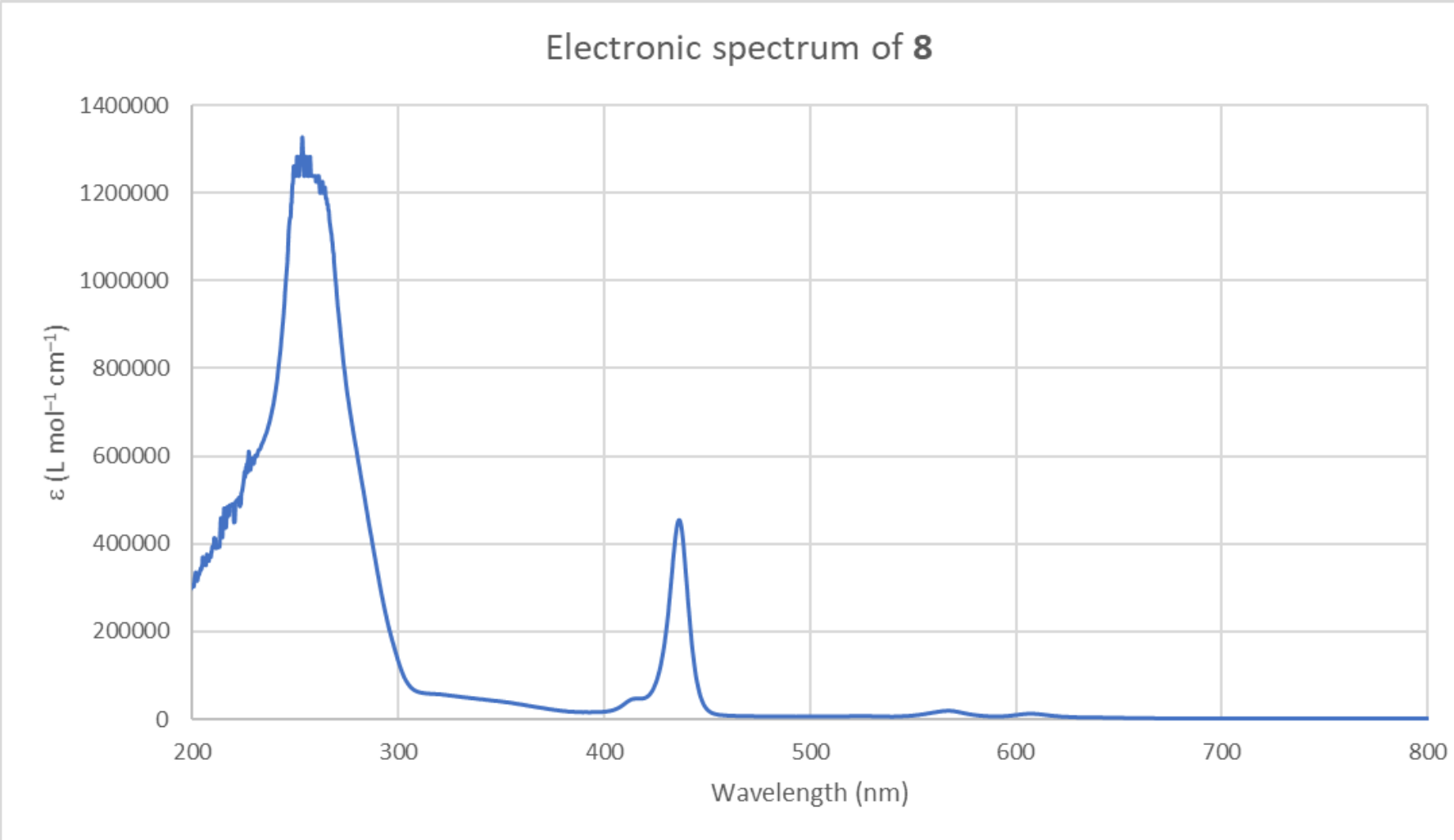

Figure S59. Electronic spectrum (CH_2Cl_2) of **4** (3.4 x 10^{-6} M) in the presence of excess 4-dimethylaminopyridine (**8**).

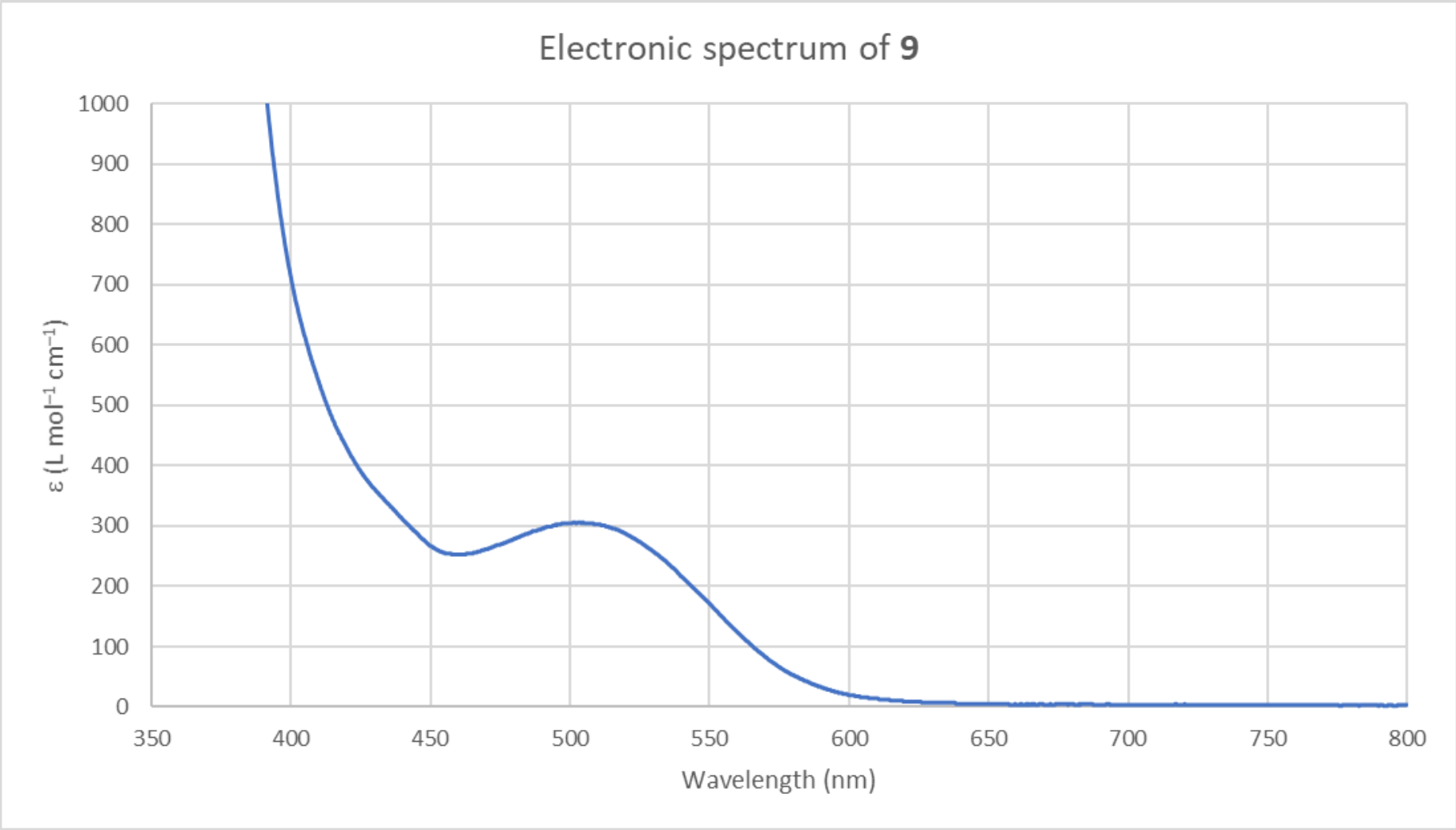

Figure S60. Electronic spectrum (CH_2Cl_2) of **9** (5.6 x 10^{-4} M).

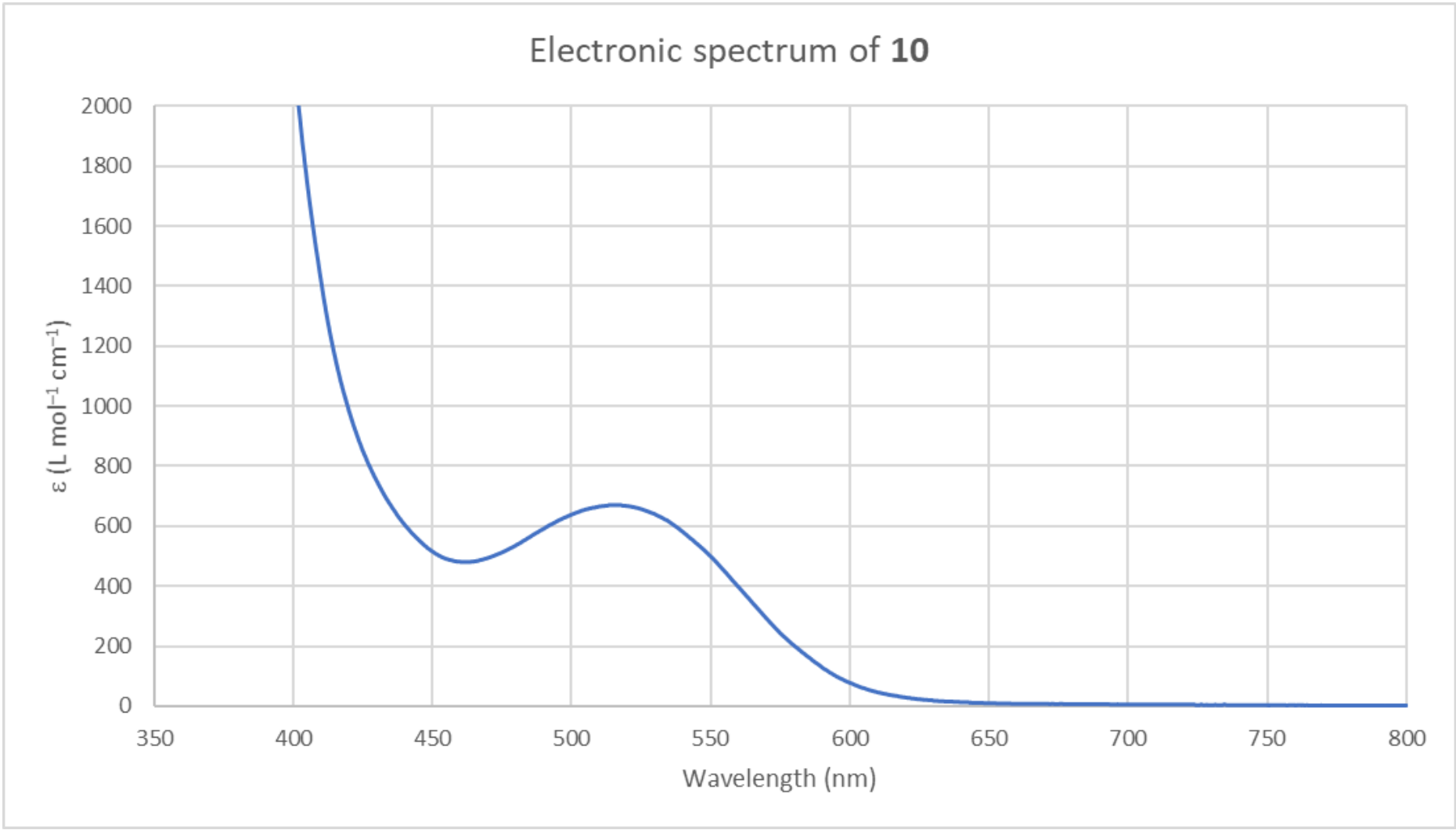

Figure S61. Electronic spectrum (CH_2Cl_2) of **10** (7.7×10^{-4} M).

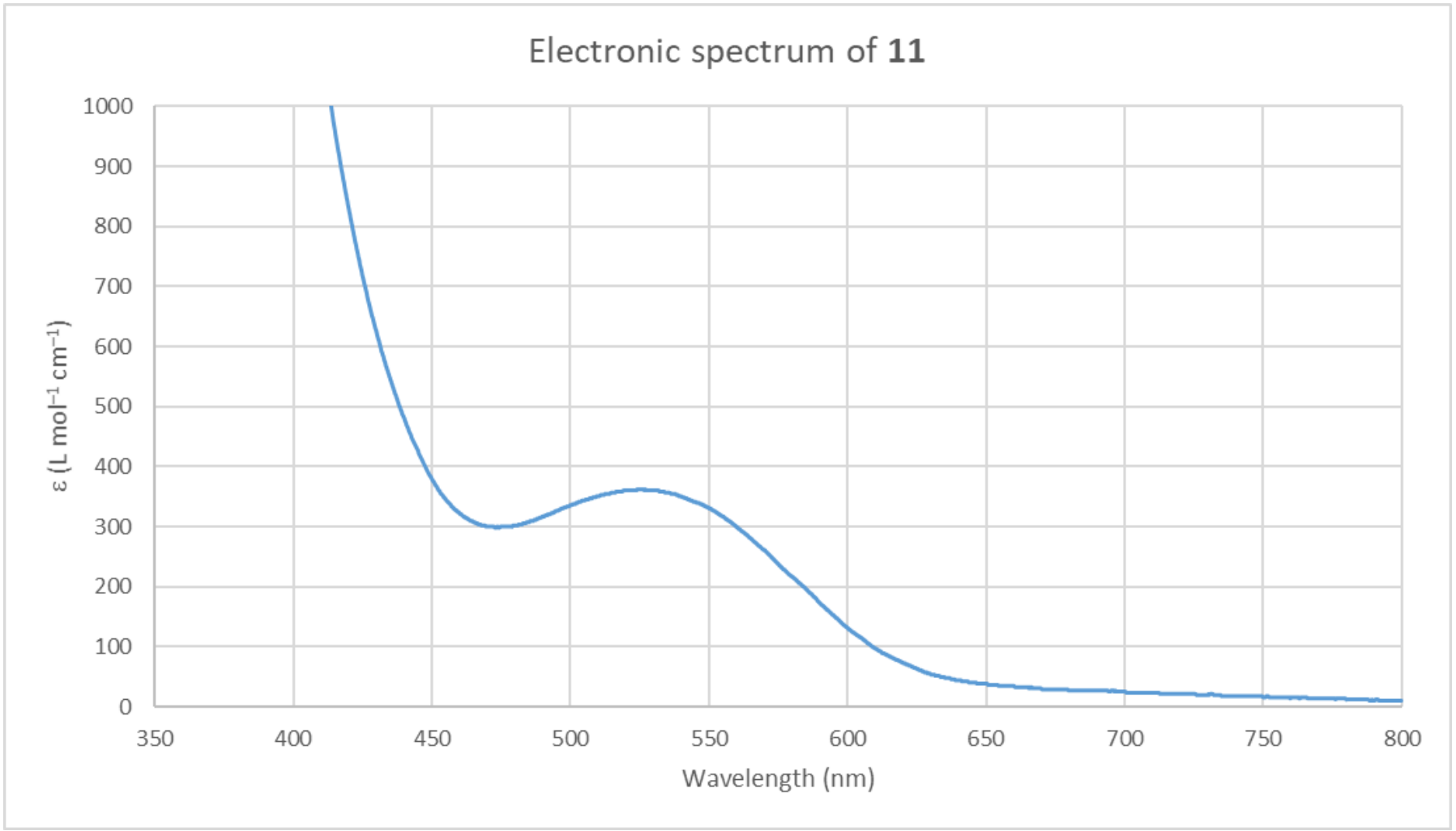

Figure S62. Electronic spectrum (CH_2Cl_2) of **11** (5.3 x 10^{-4} M).