

ELECTRONIC SUPPORTING INFORMATION (ESI) to:

***In vivo* photoacoustic tumor tomography using a quinoline-annulated porphyrin as NIR molecular contrast agent**

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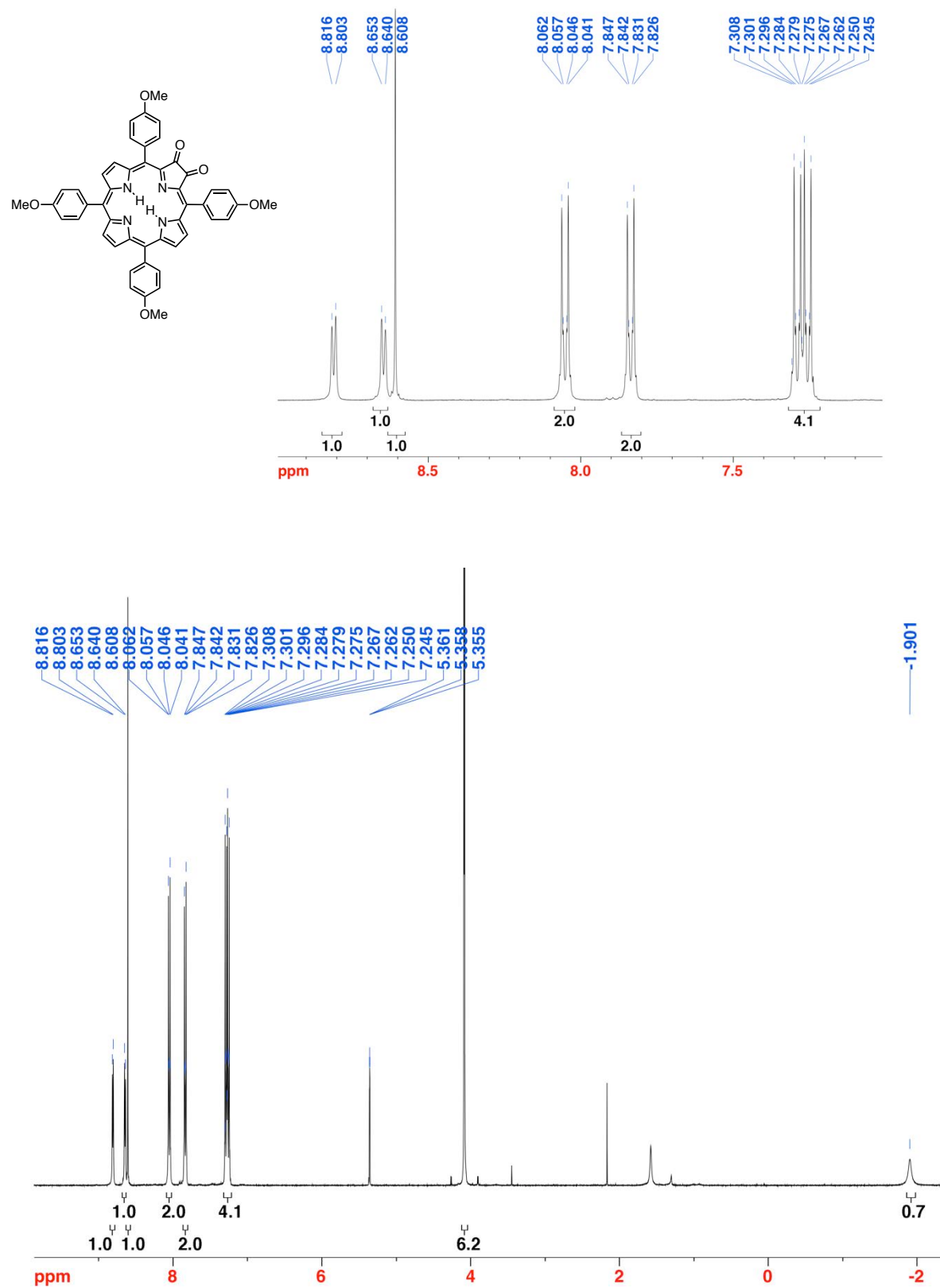


Figure S1. ^1H NMR spectrum (400 MHz, CD_2Cl_2) of **8**.

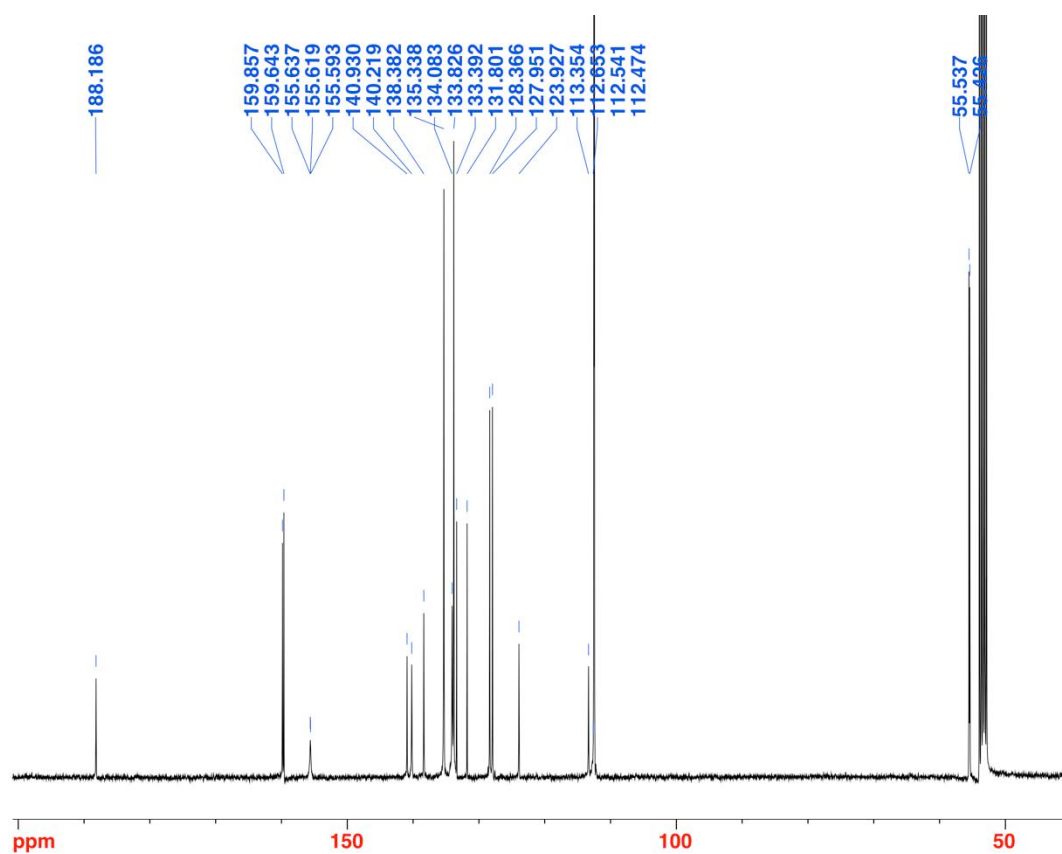
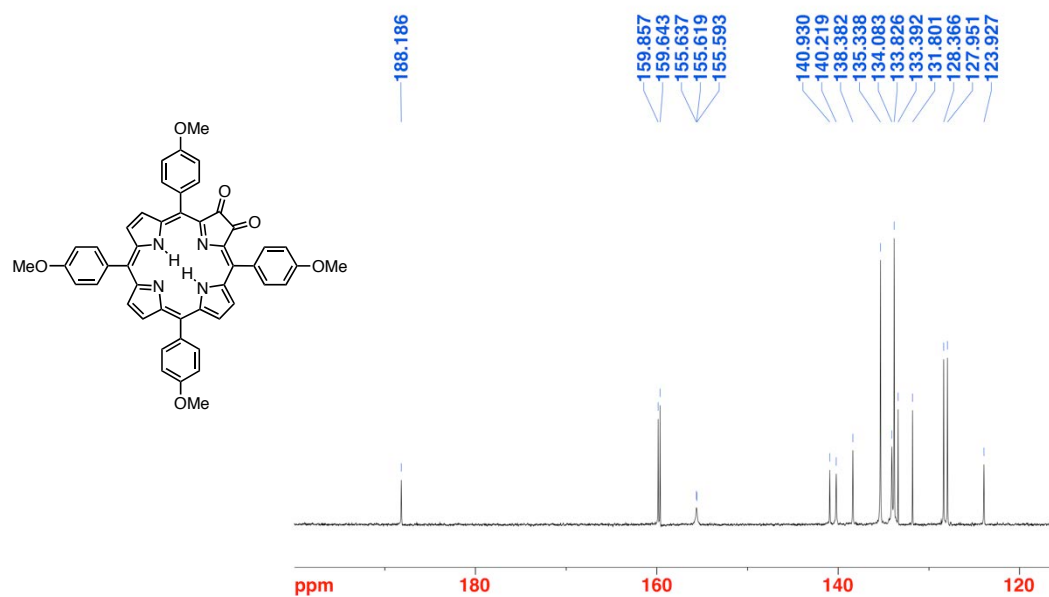


Figure S2. ^{13}C NMR spectrum (100 MHz, CD_2Cl_2) of **8**.

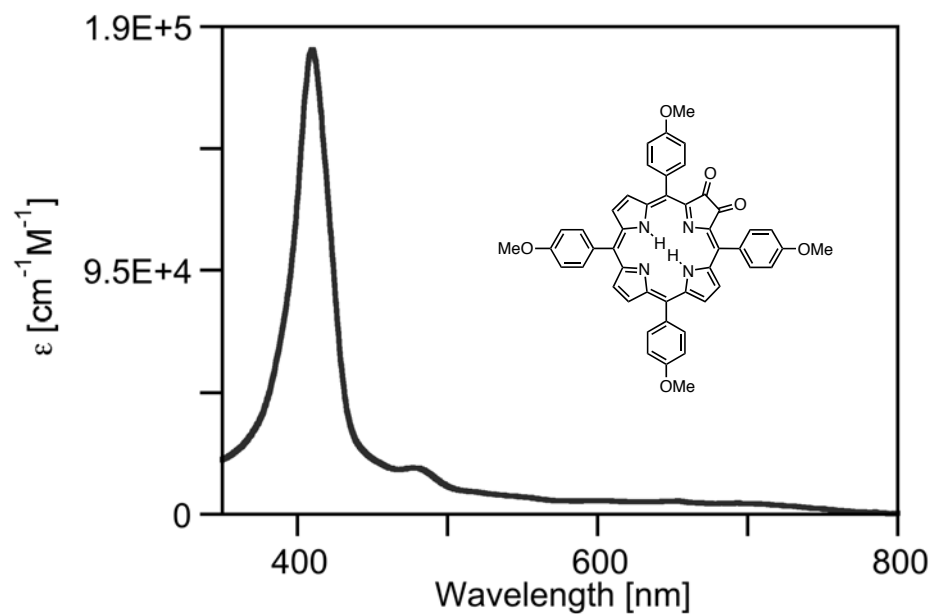


Figure S3. UV-vis spectrum (CH_2Cl_2) of **8**.

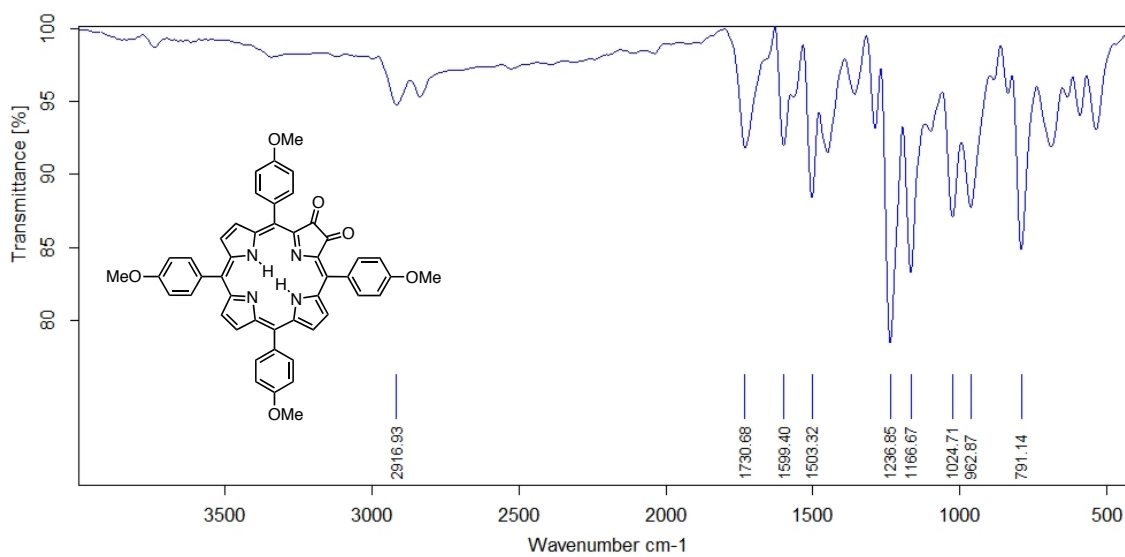


Figure S4. FT-IR spectrum (neat, diamond ATR) of **8**.

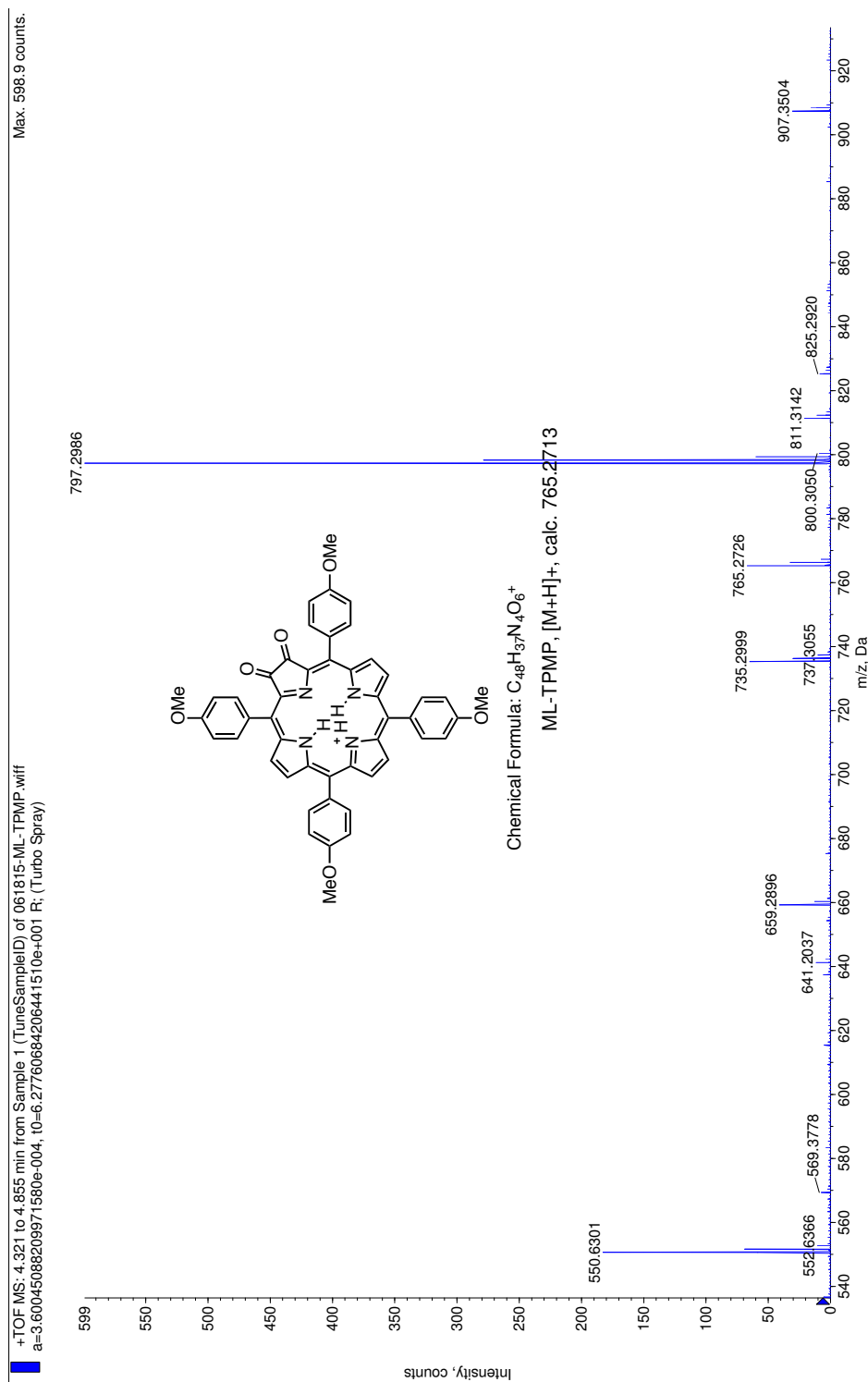


Figure S5. HR-MS (ESI^+ , 100% CH_3CN , TOF) of **8**.

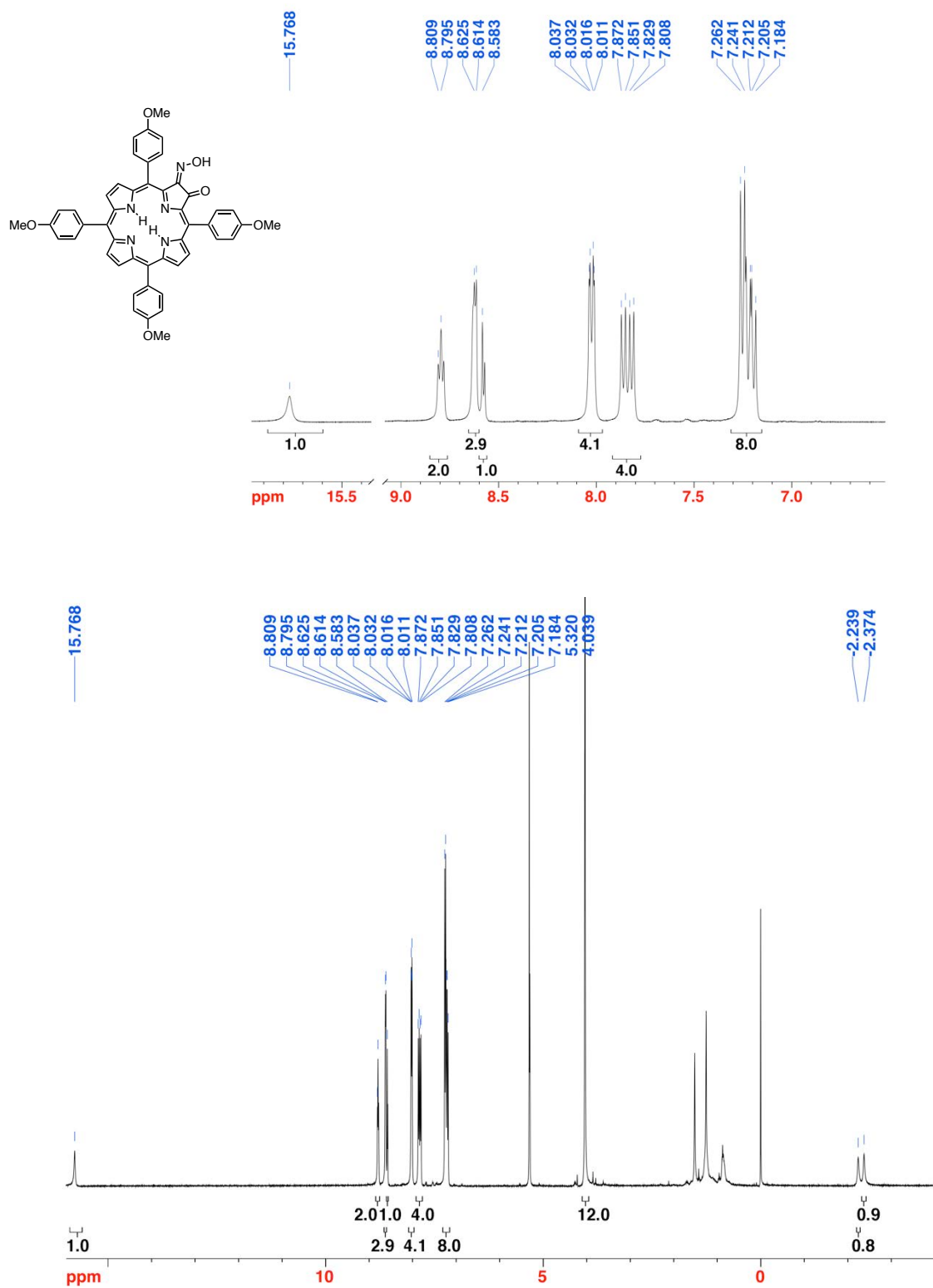


Figure S6. ^1H NMR spectrum (400 MHz, CD_2Cl_2) of **9**.

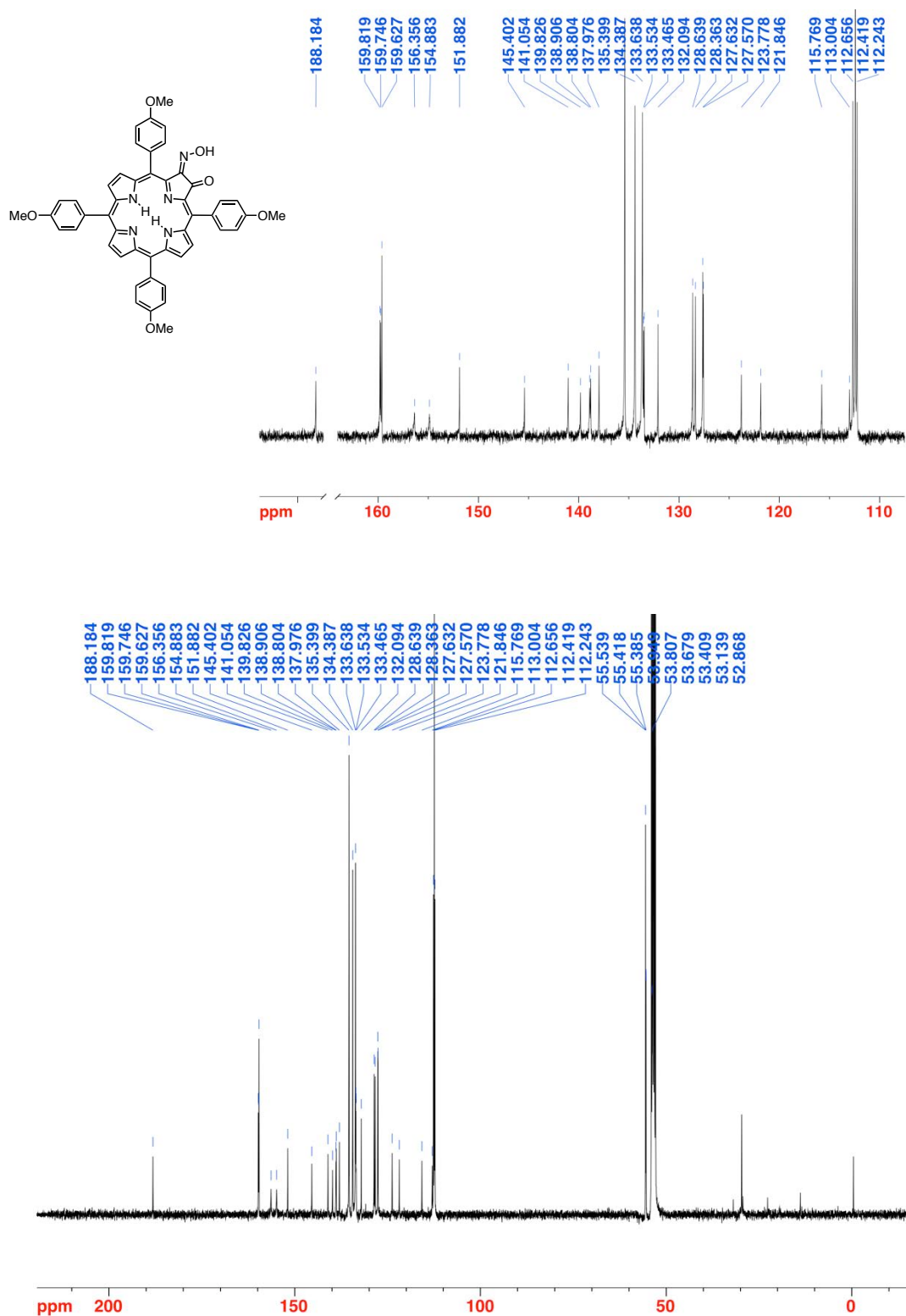


Figure S7. ^{13}C NMR spectrum (100 MHz, CD_2Cl_2) of 9.

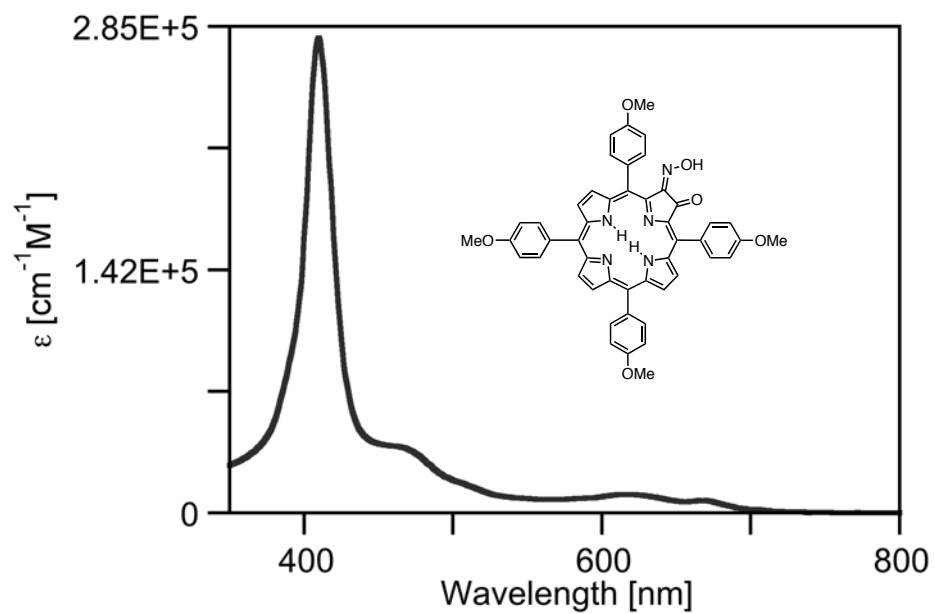


Figure S8. UV-vis spectrum (CH_2Cl_2) of **9**.

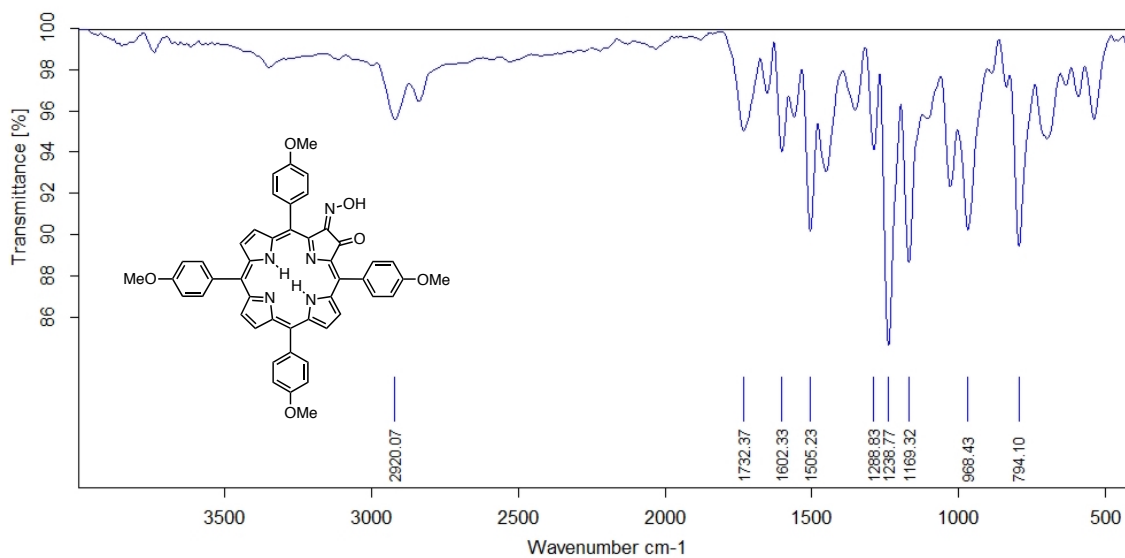


Figure S9. FT-IR spectrum (neat, diamond ATR) of **9**.

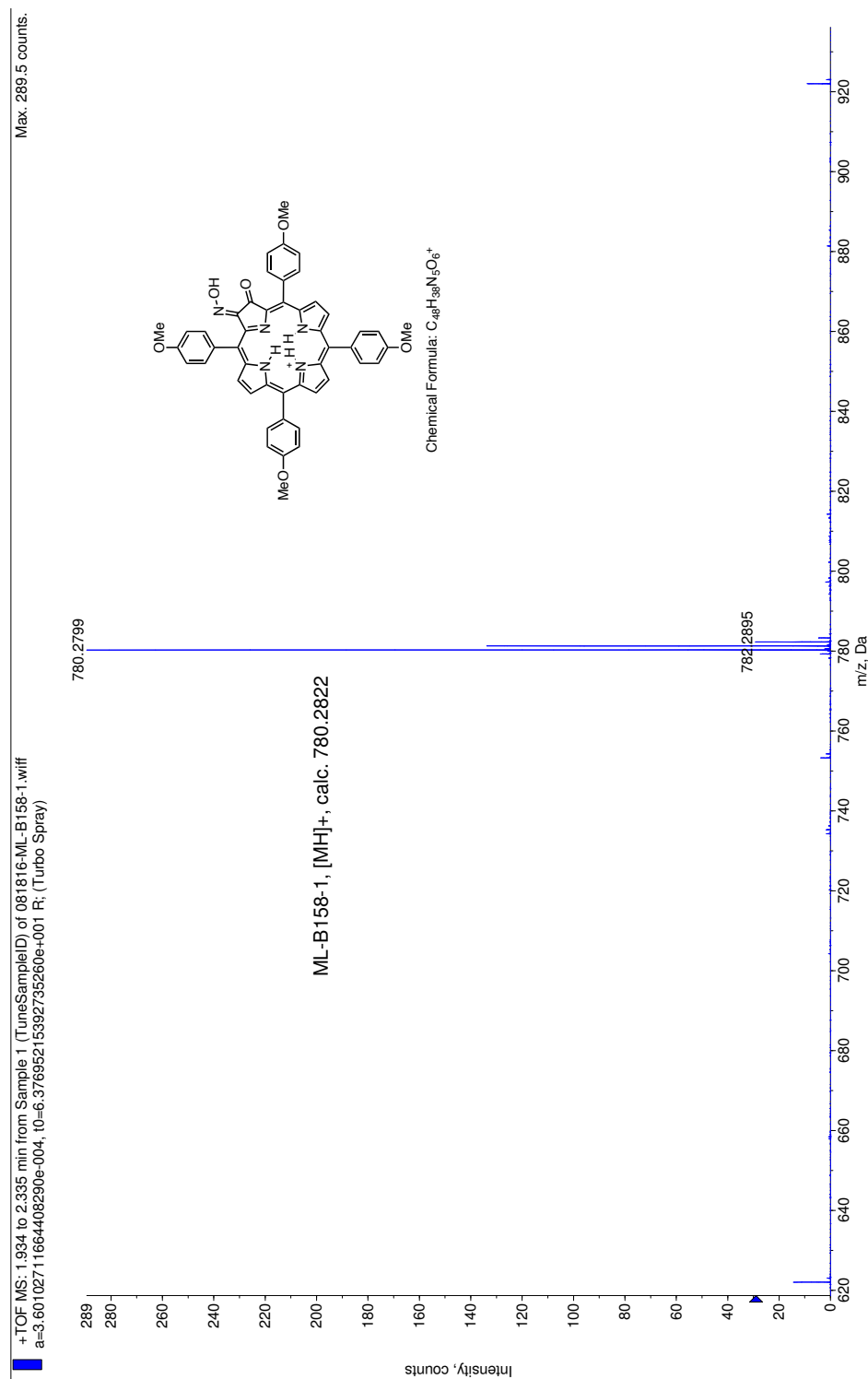


Figure S10. HR-MS (ESI⁺, 100% CH₃CN, TOF) of **9**.

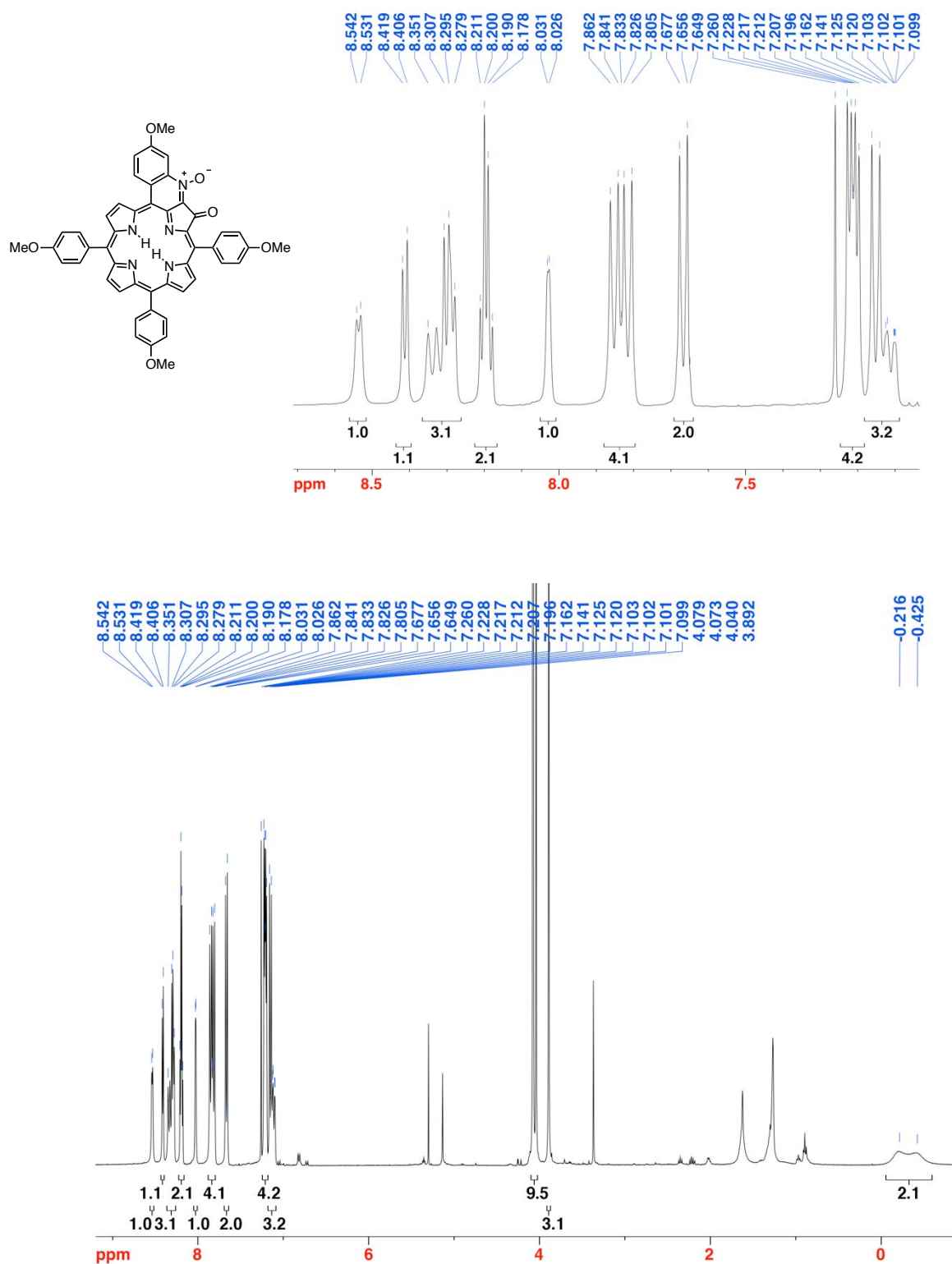


Figure S11. ¹H NMR spectrum (400 MHz, CDCl₃) of **5b**.

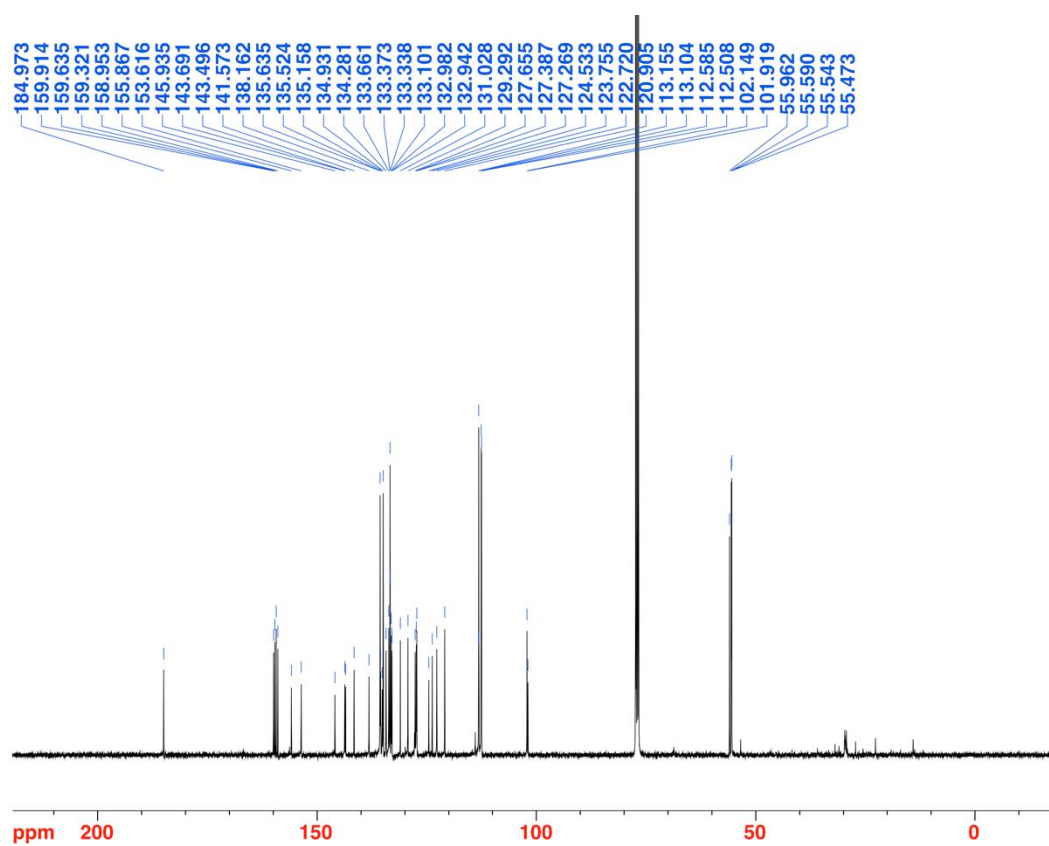
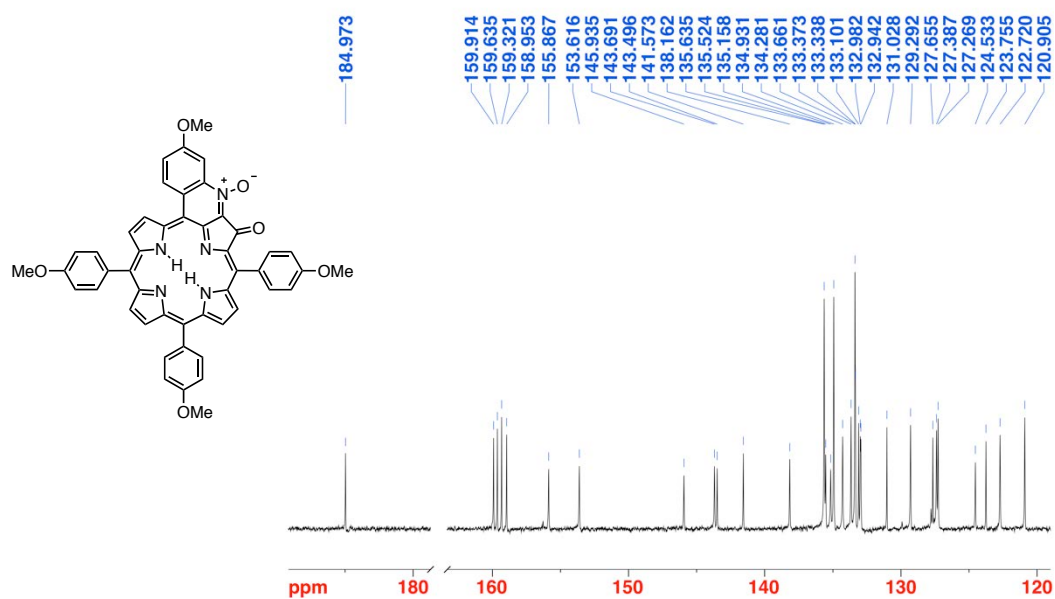


Figure S12. ^{13}C NMR spectrum (100 MHz, CDCl_3) of **5b**.

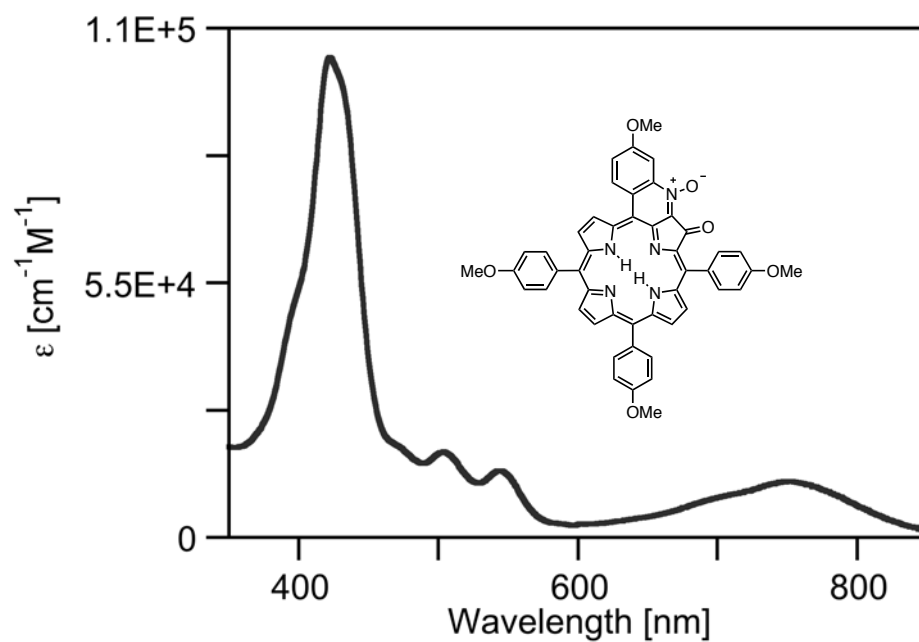


Figure S13. UV-vis spectrum (CH_2Cl_2) of **5b**.

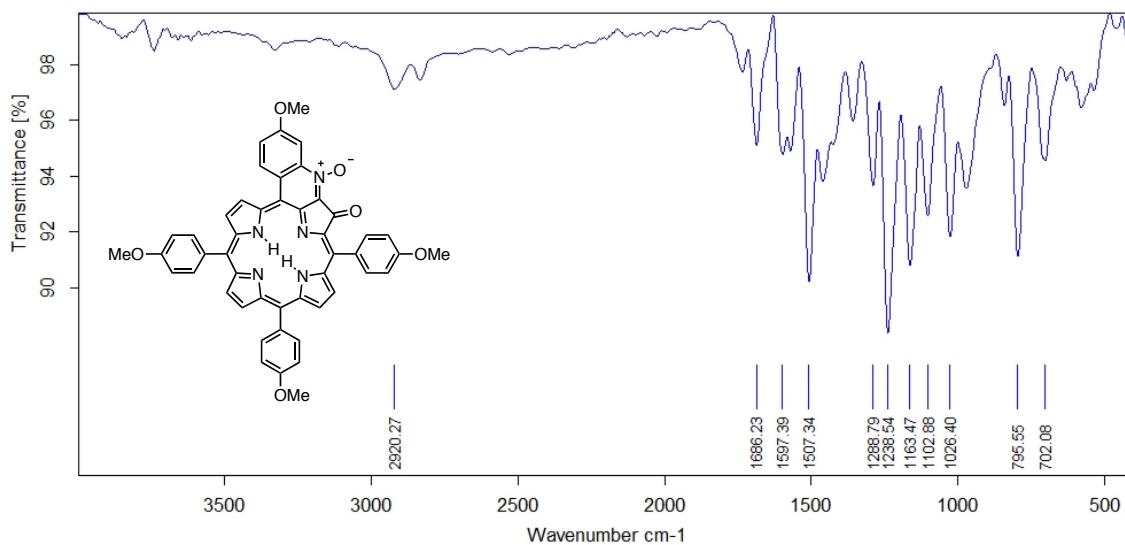


Figure S14. FT-IR spectrum (neat, diamond ATR) of **5b**.

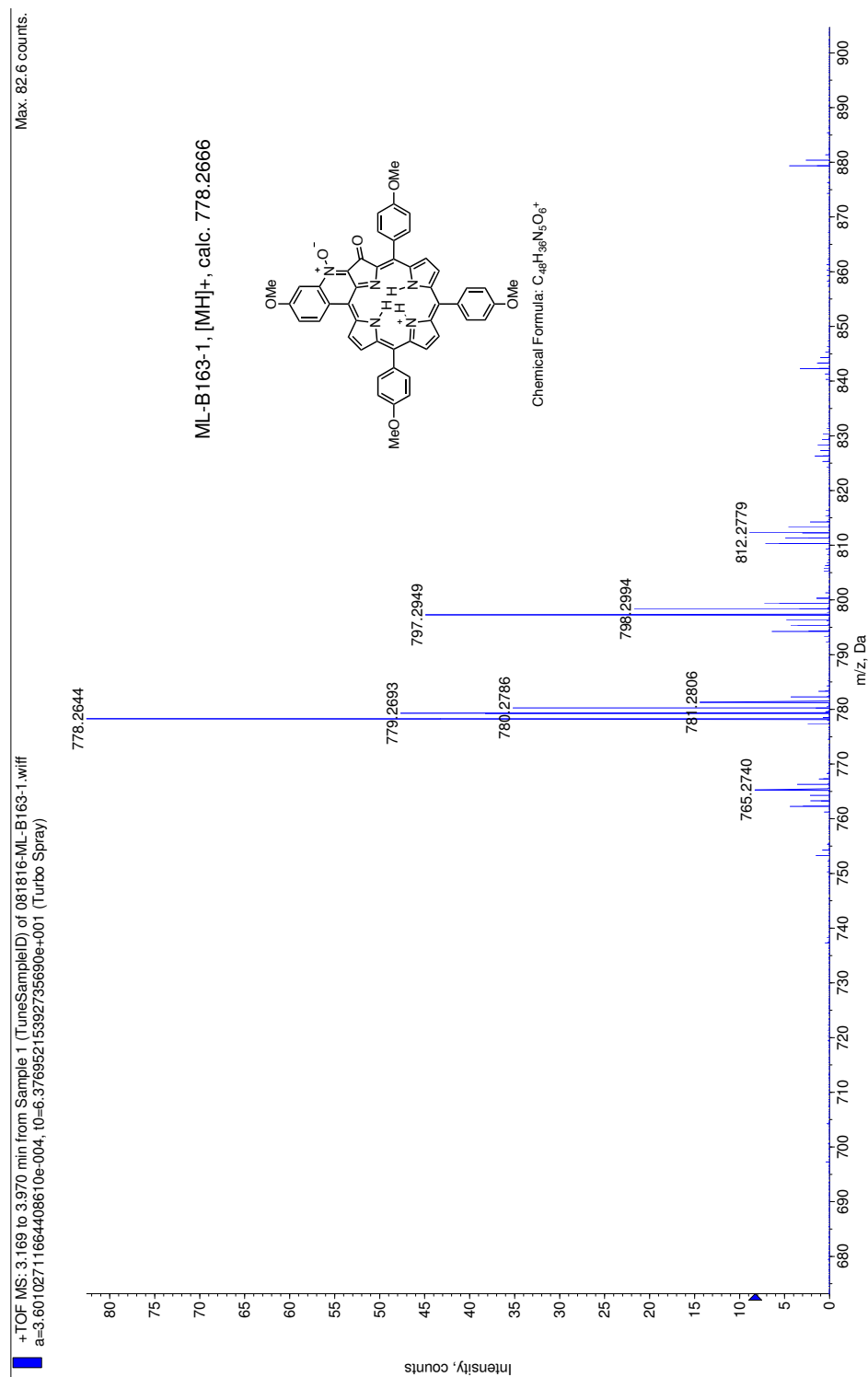


Figure S15. HR-MS (ESI⁺, 100% CH₃CN, TOF) of **5b**.

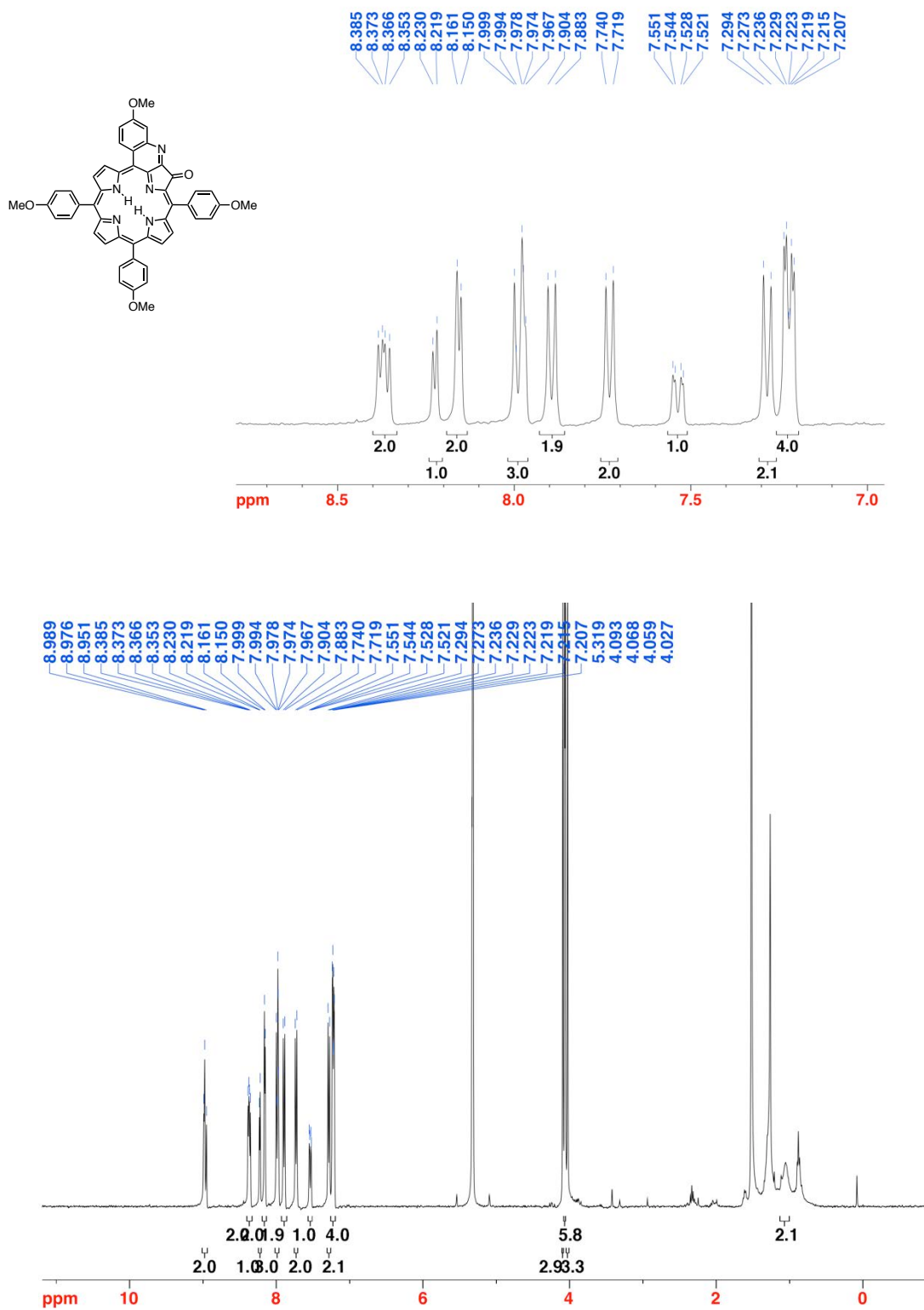


Figure S16. ^1H NMR spectrum (400 MHz, CD_2Cl_2) of **4b**.

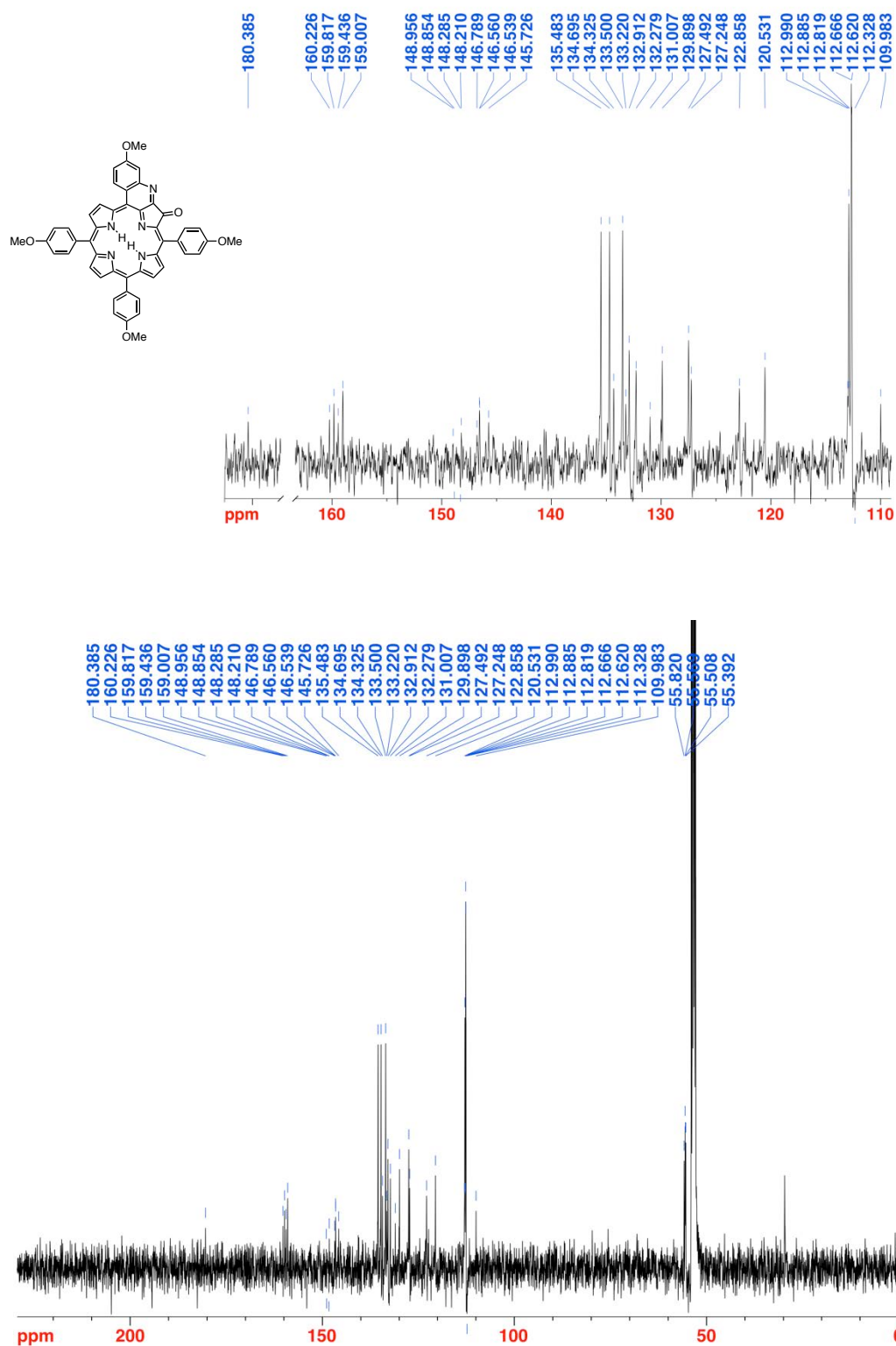


Figure S17. ^{13}C NMR spectrum (100 MHz, CD_2Cl_2) of **4b** (the compound has limited solubility).

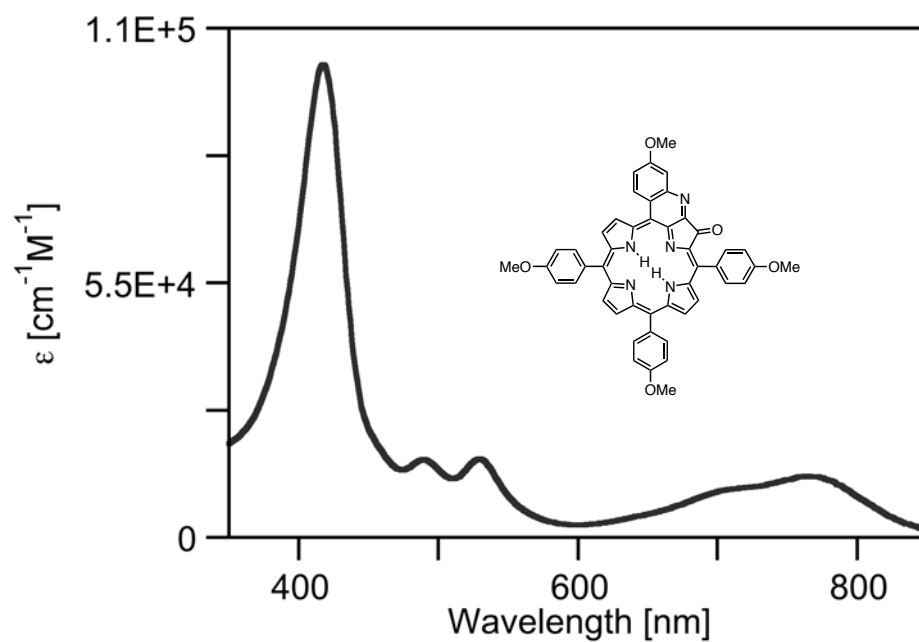


Figure S18. UV-vis spectrum (CH_2Cl_2) of **4b**.

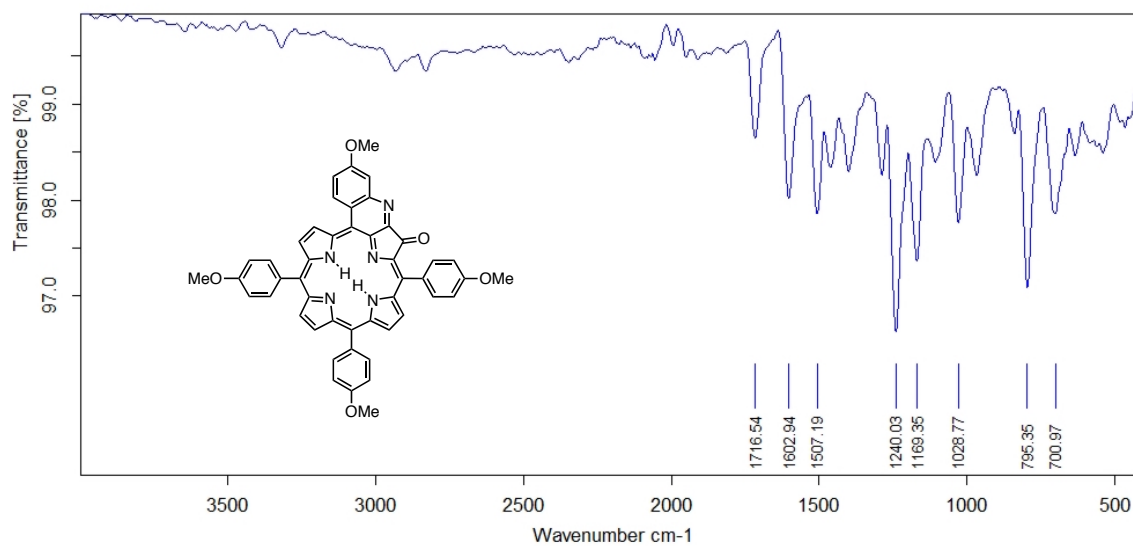


Figure S19. FT-IR spectrum (neat, diamond ATR) of **4b**.

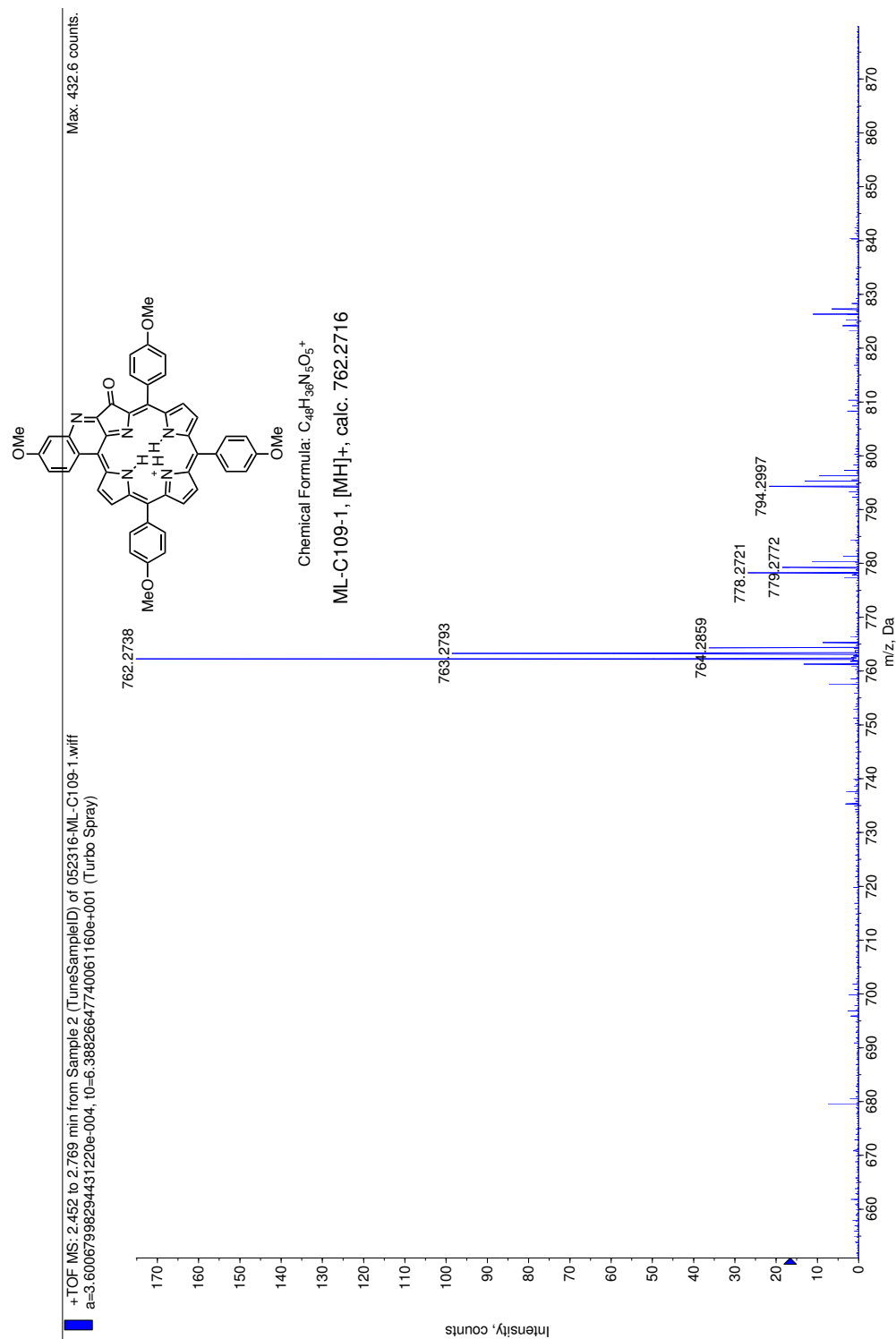


Figure S20. HR-MS (ESI^+ , 100% CH_3CN , TOF) of **4b**.

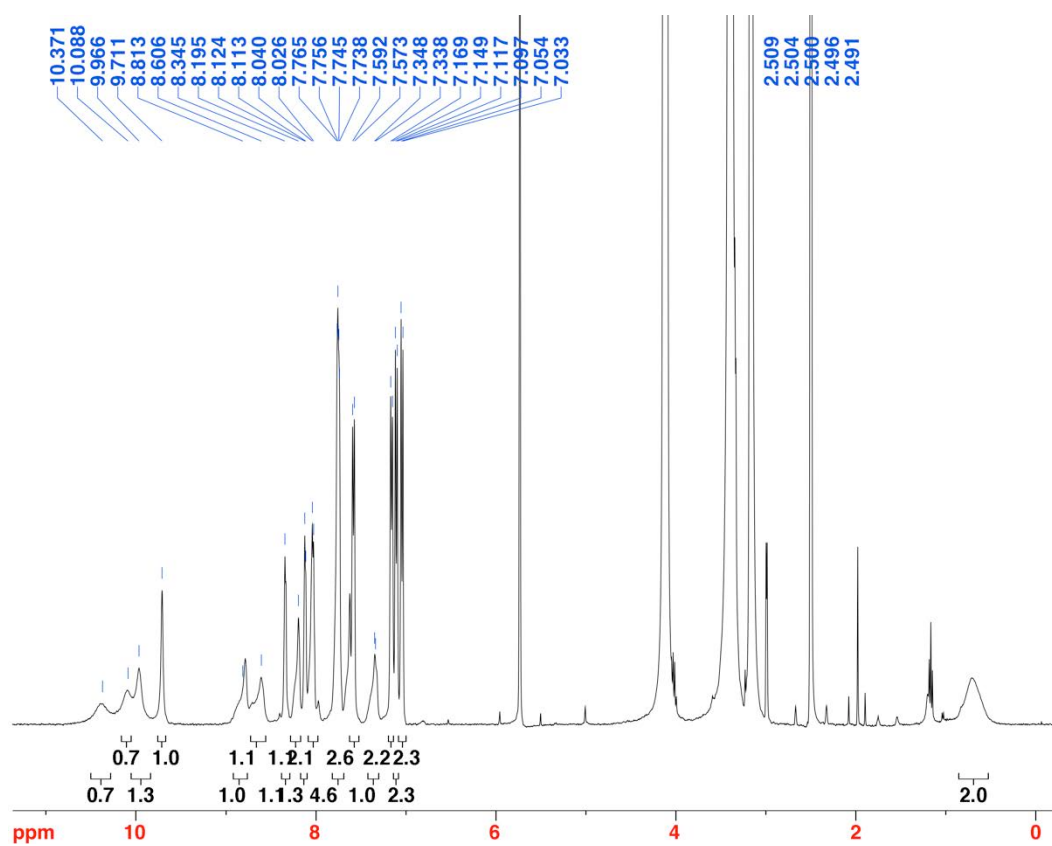
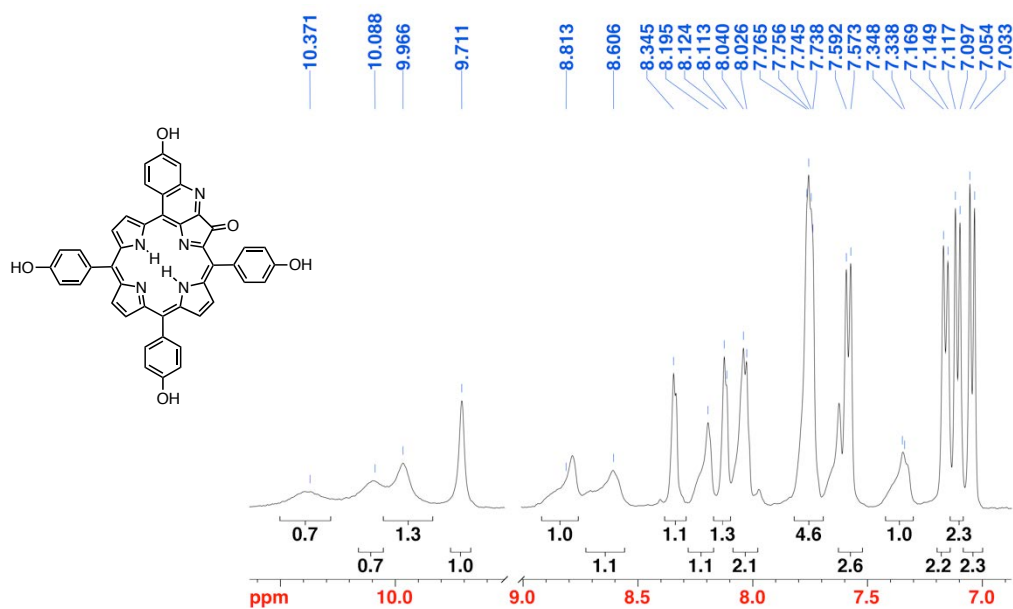


Figure S21. ^1H NMR spectrum (400 MHz, DMSO-d_6) of **4c**.

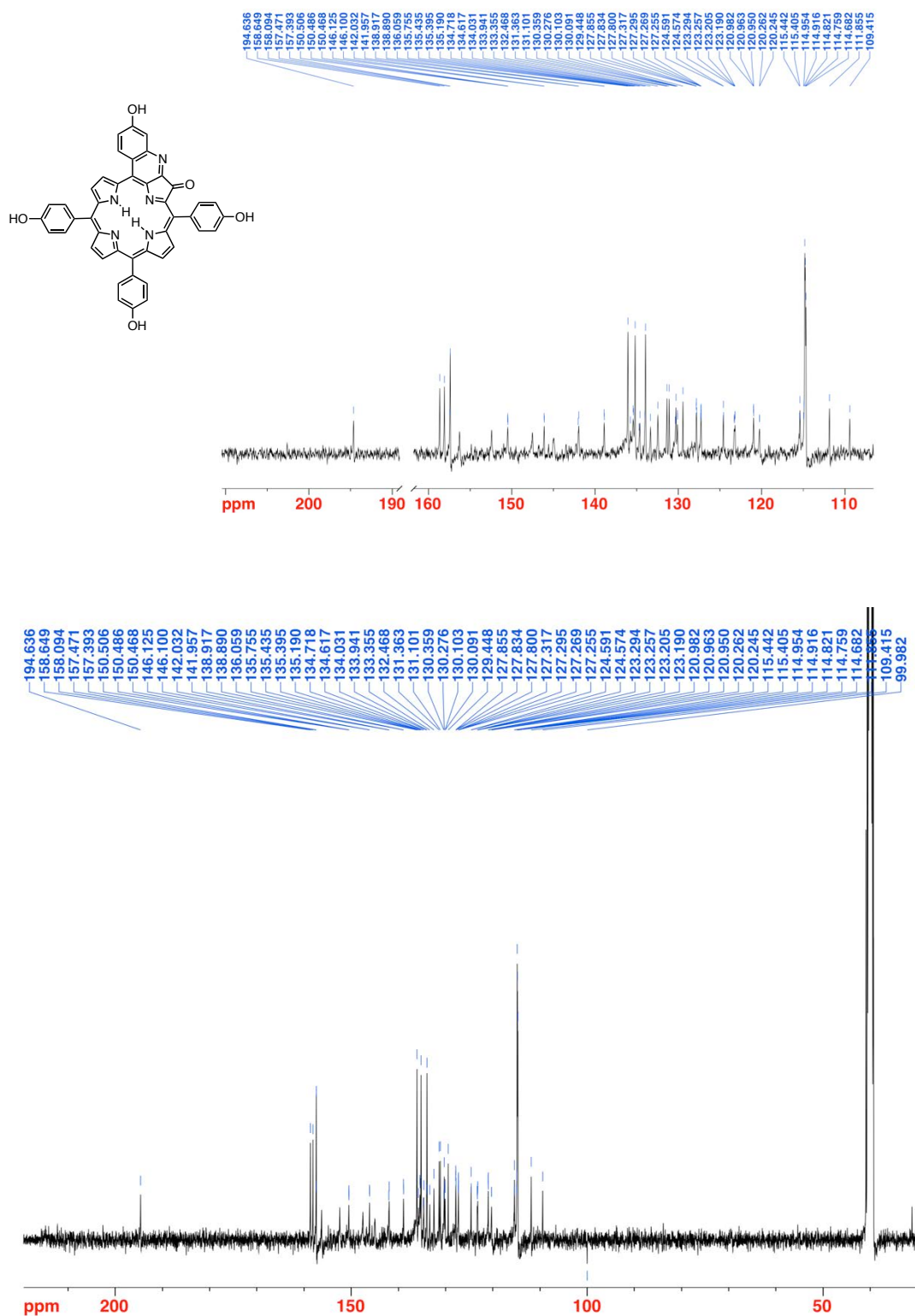


Figure S22. ¹³C NMR spectrum (100 MHz, DMSO-d₆) of 4c.

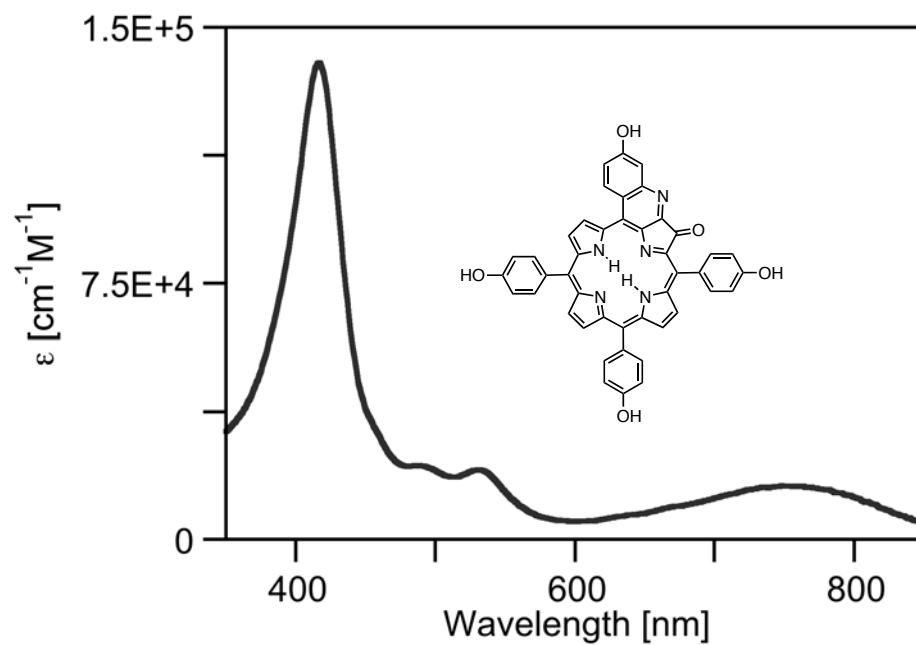


Figure S23. UV-vis spectrum (MeOH) of **4c**.

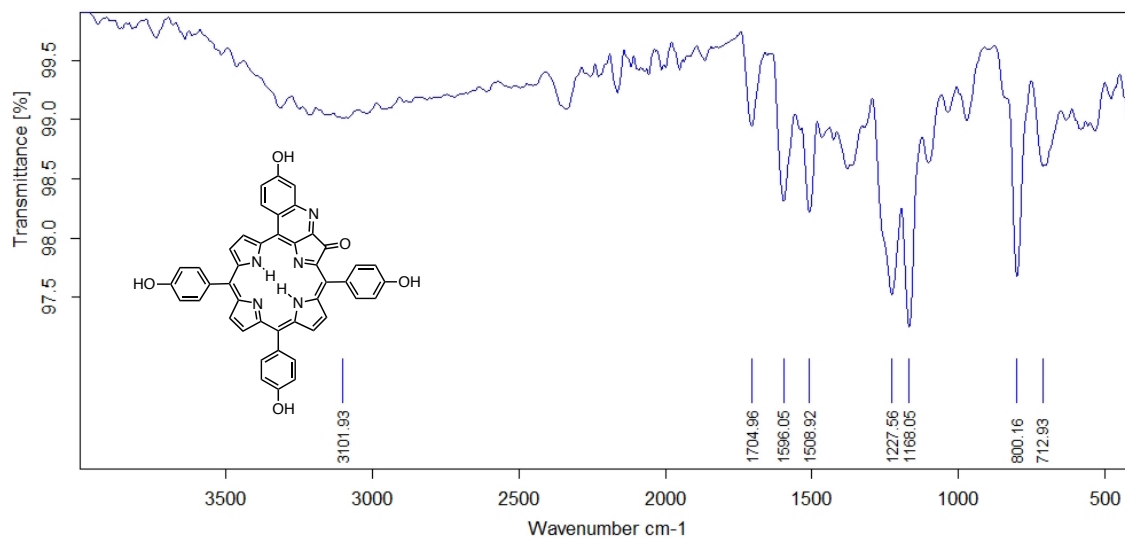


Figure S24. FT-IR spectrum (neat, diamond ATR) of **4c**.

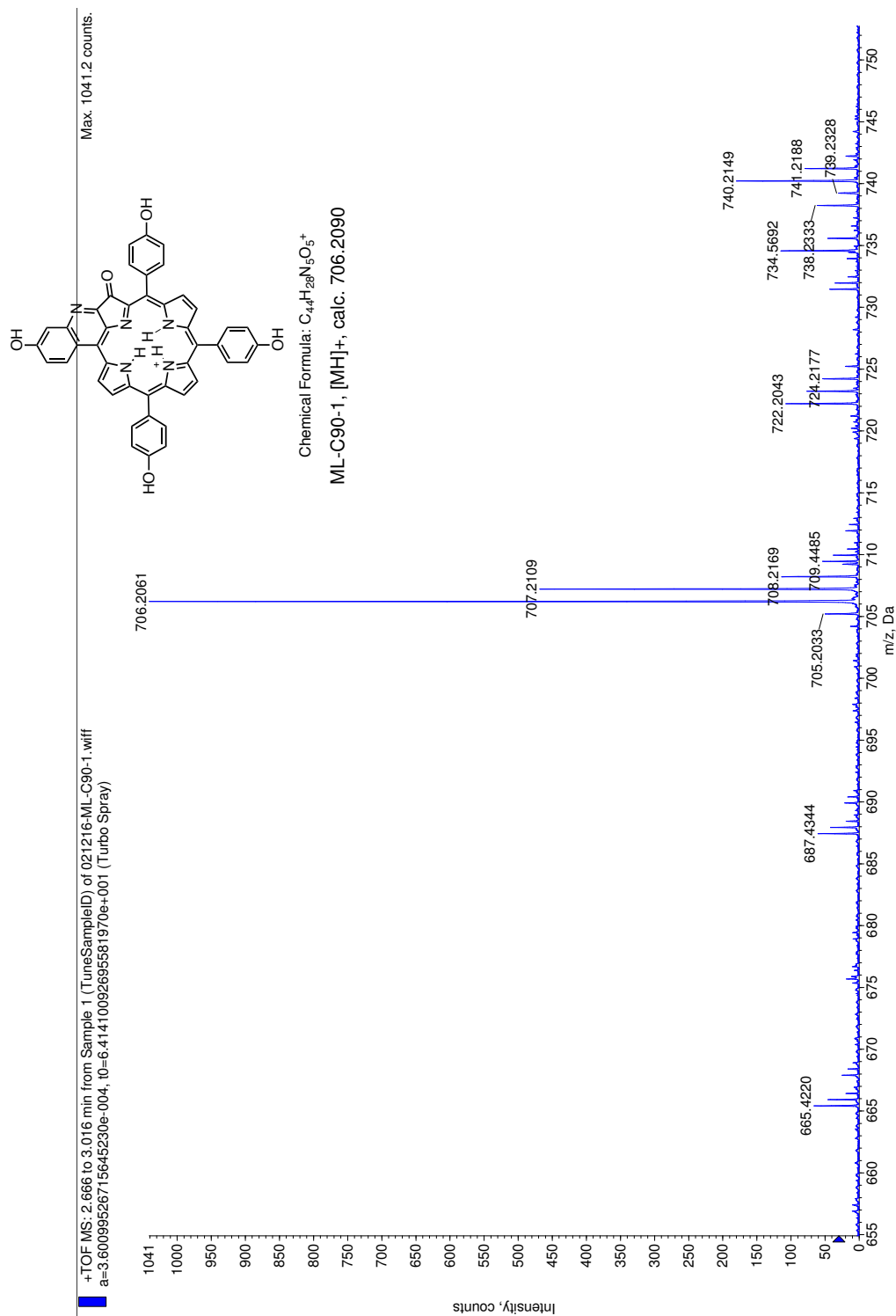


Figure S25. HR-MS (ESI^+ , 100% CH_3CN , TOF) of **4c**.

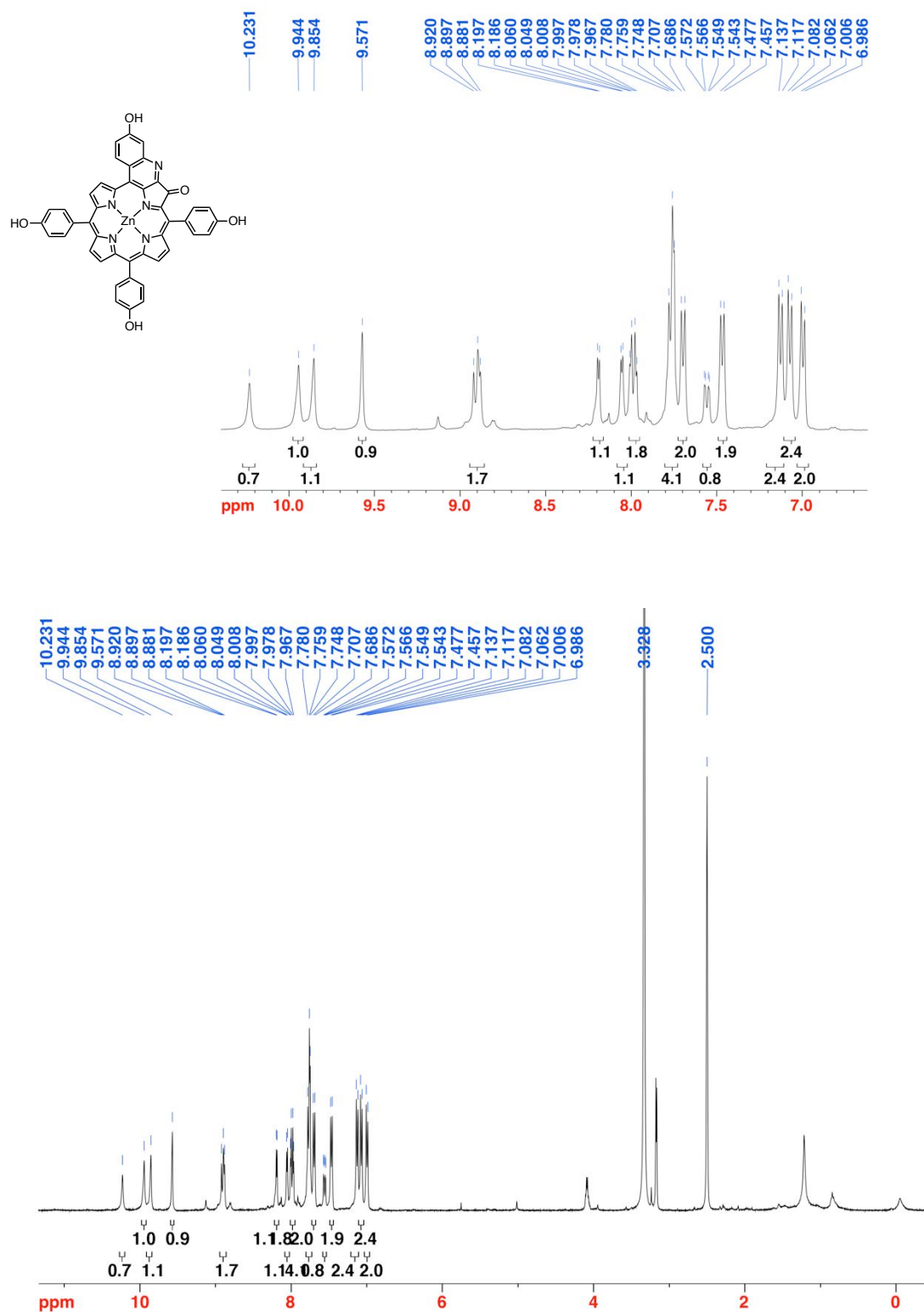


Figure S26. ¹H NMR spectrum (400 MHz, DMSO-d₆) of 4c^{Zn}.

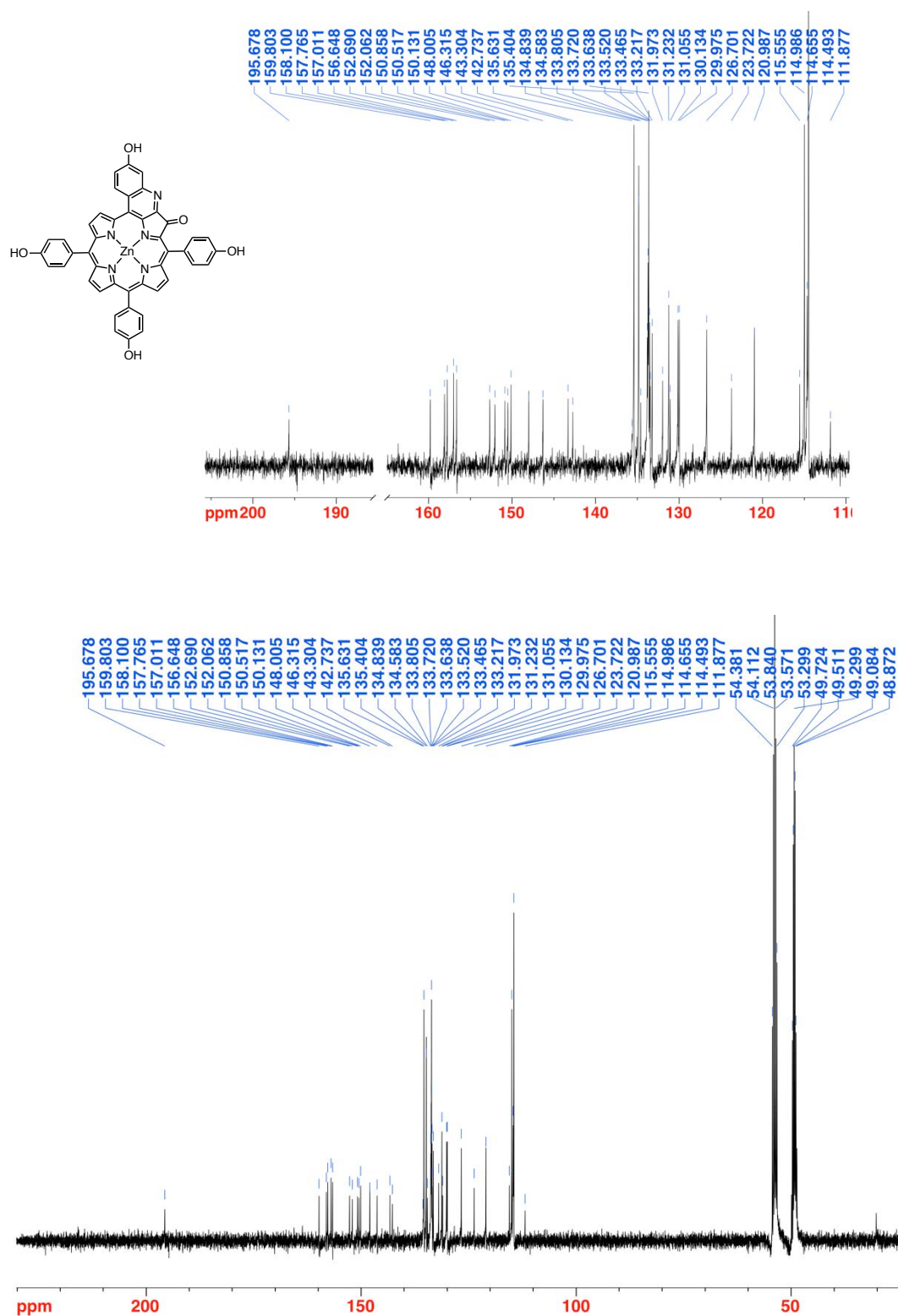


Figure S27. ¹³C NMR spectrum (100 MHz, CD₂Cl₂/10% MeOD) of **4c^{Zn}**.

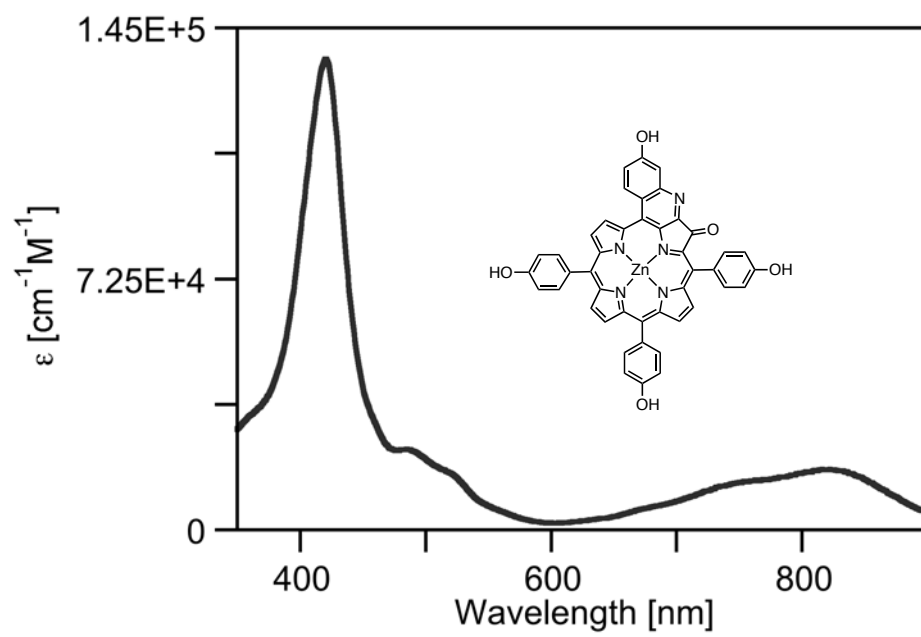


Figure S28. UV-vis spectrum (MeOH) of **4c^{Zn}**.

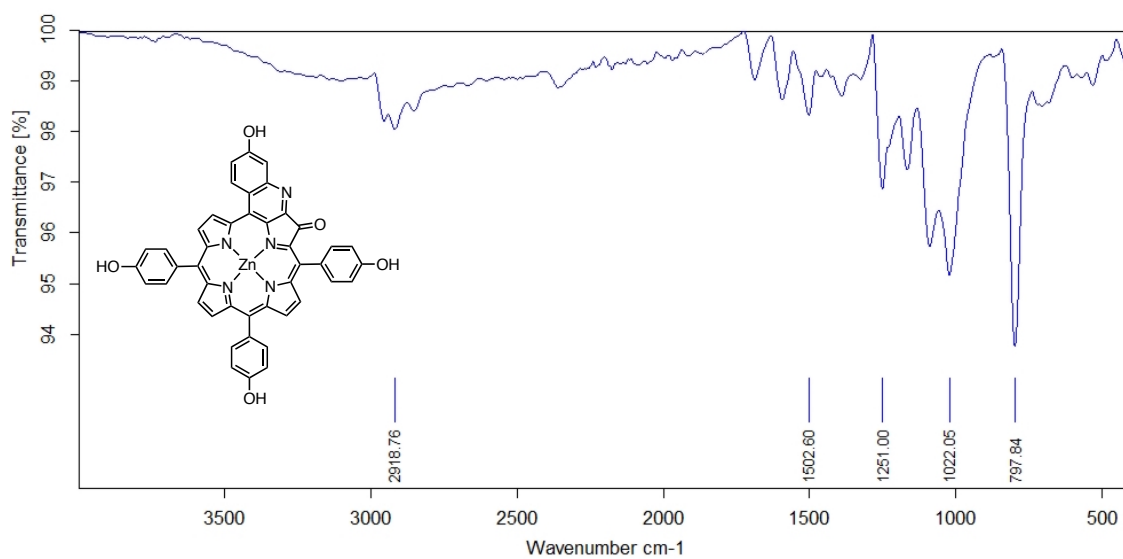


Figure S29. FT-IR spectrum (neat, diamond ATR) of **4c^{Zn}**.

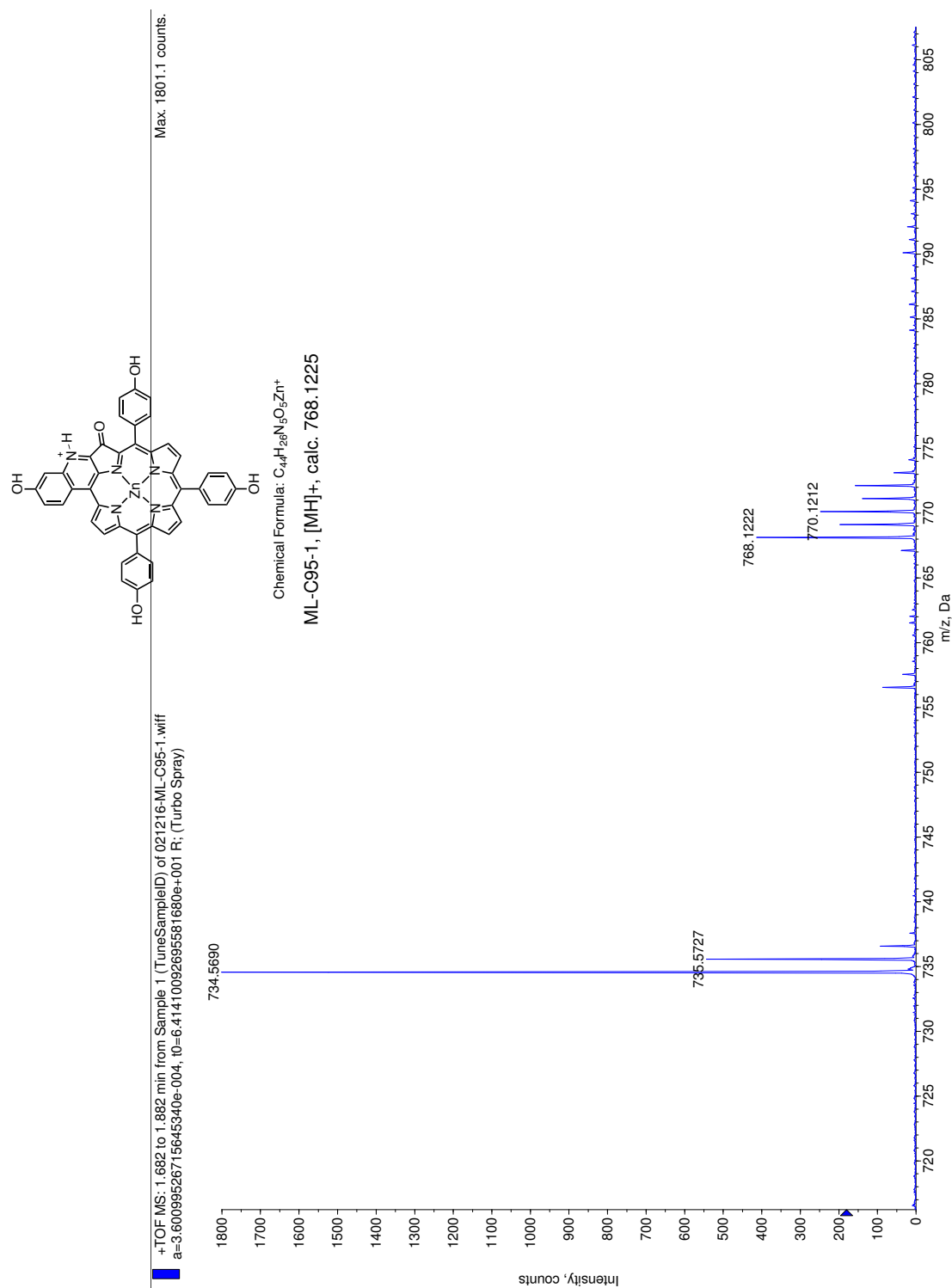


Figure S30. HR-MS (ESI^+ , 100% CH_3CN , TOF) of $4c^{Zn}$.

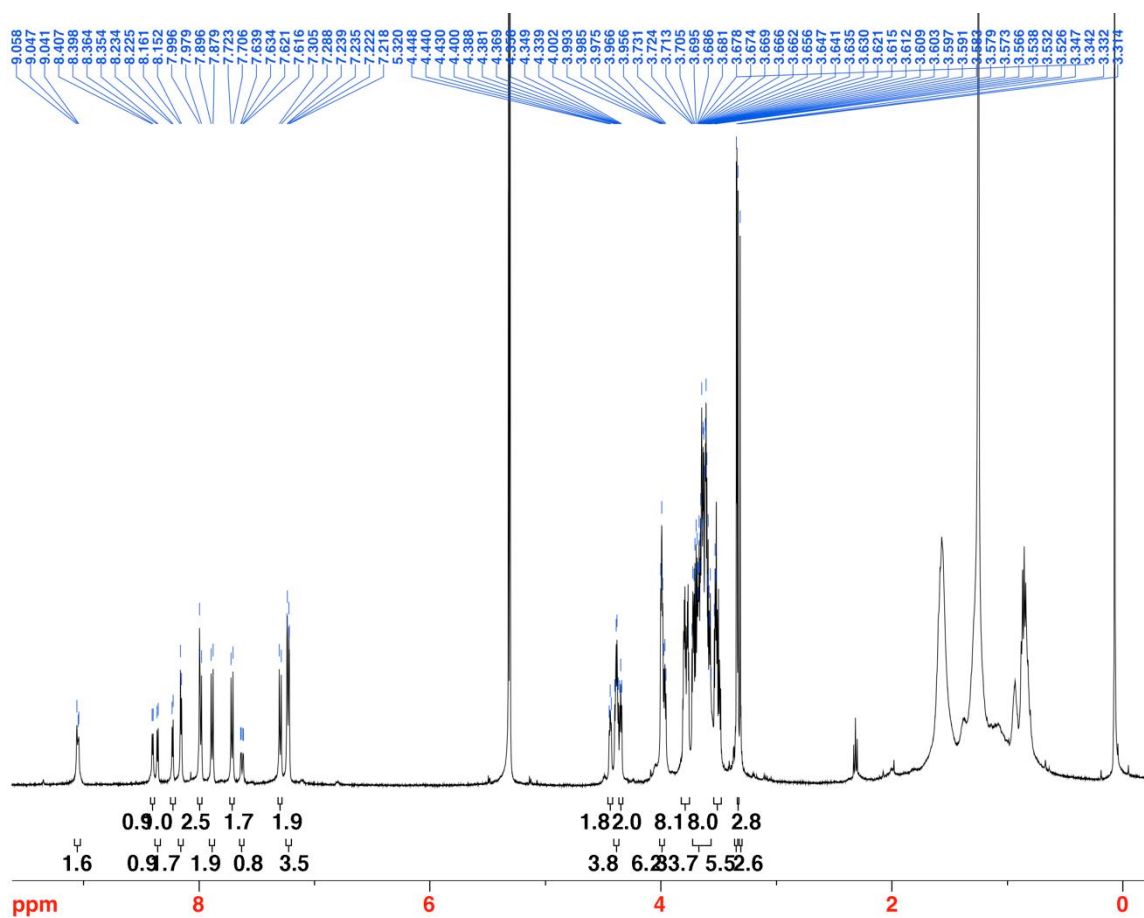
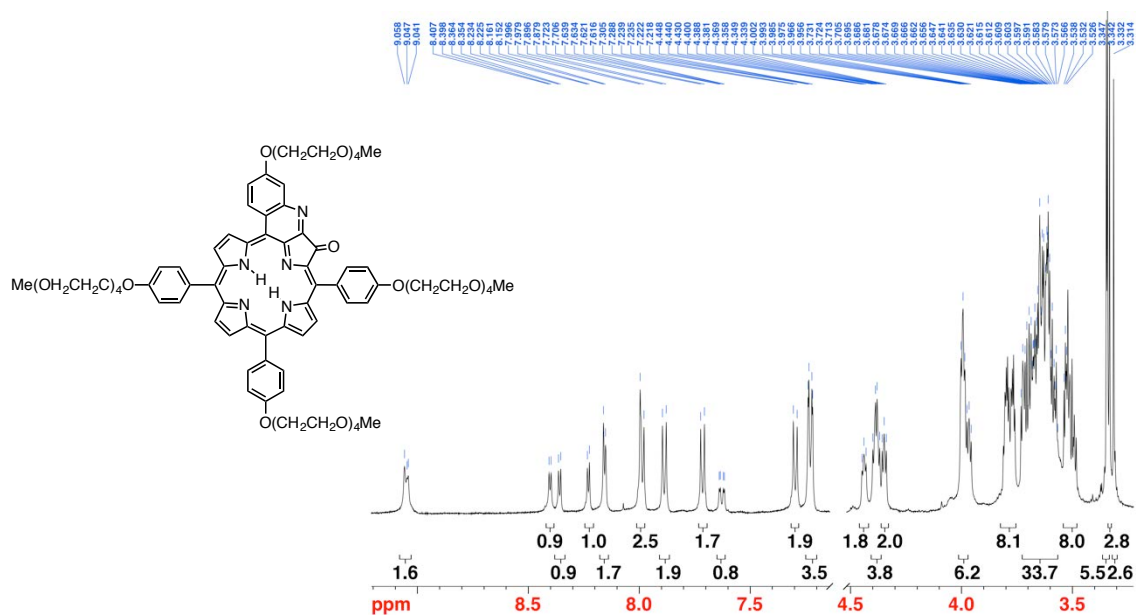


Figure S31. ¹H NMR spectrum (500 MHz, CD_2Cl_2) of **4d**.

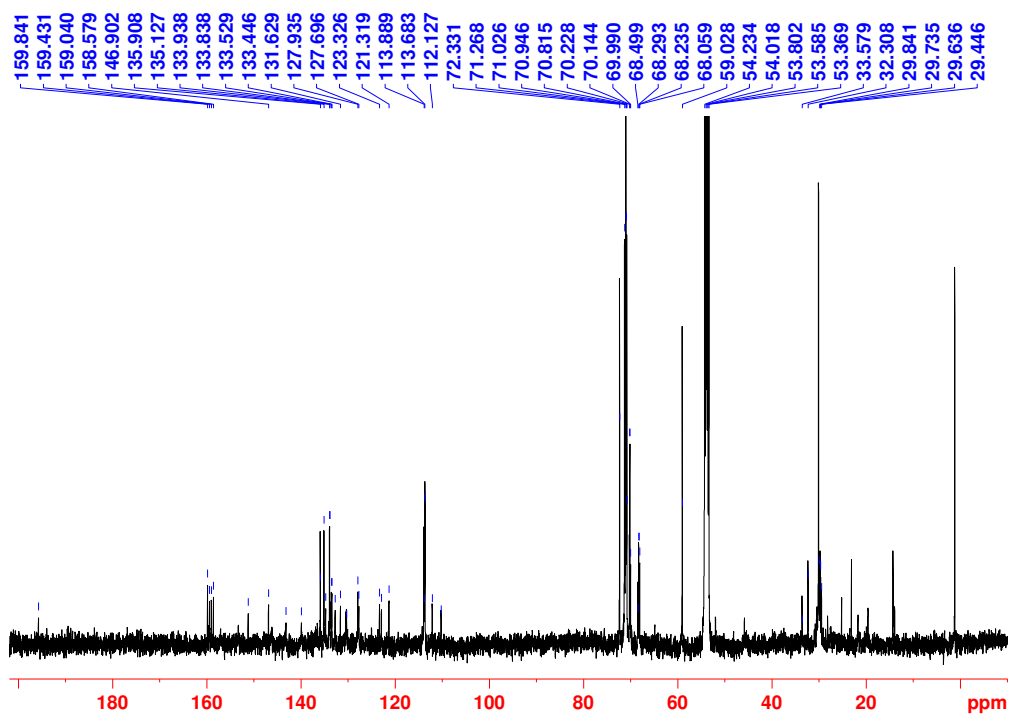
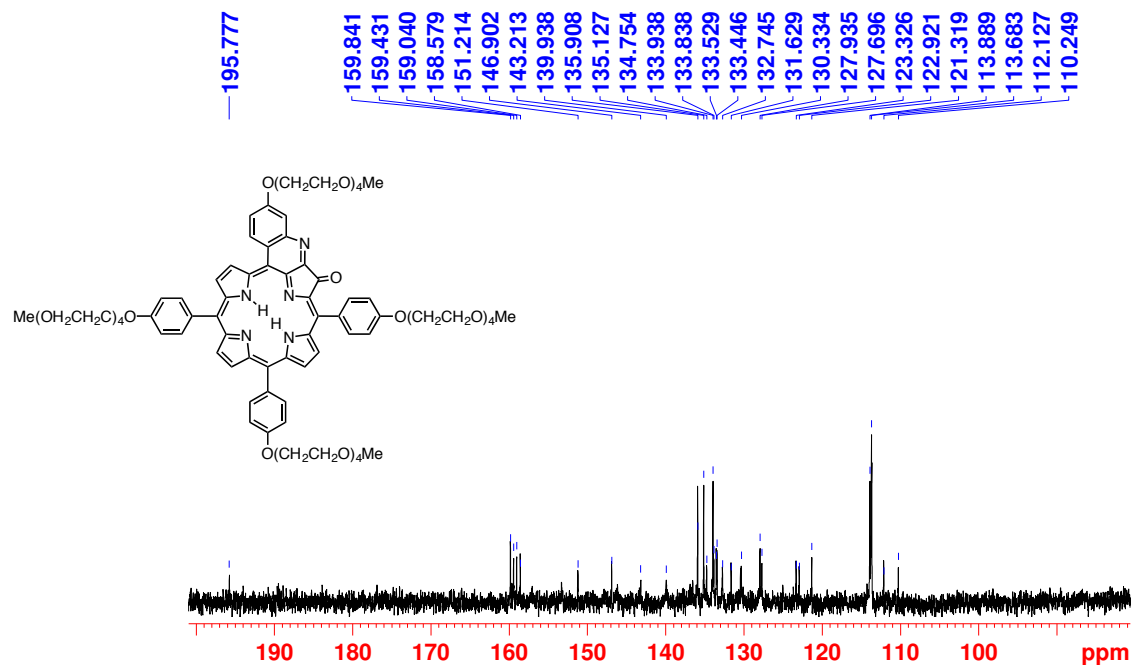


Figure S32. ^{13}C NMR spectrum (125 MHz, CD_2Cl_2) of **4d**.

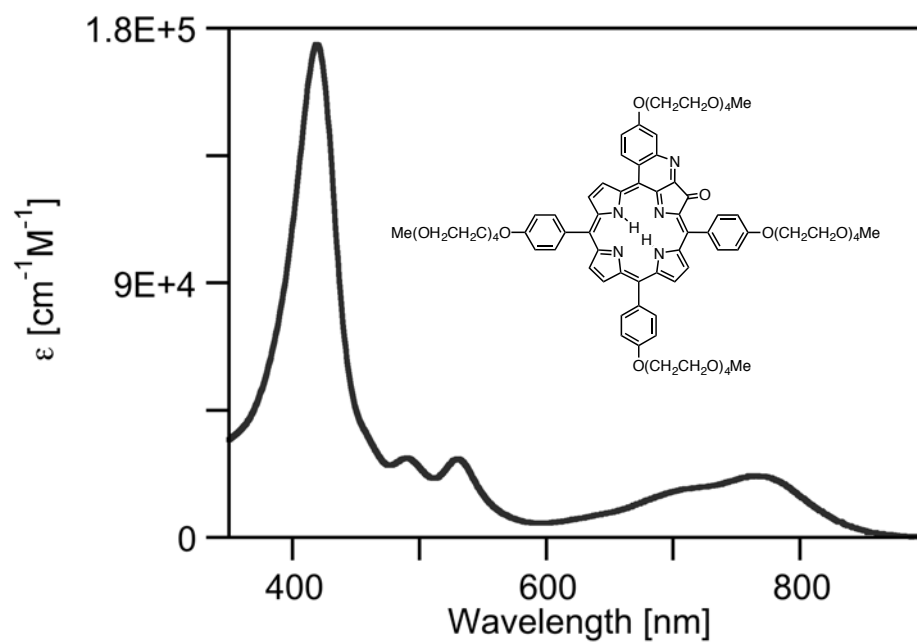


Figure S33. UV-vis spectrum (CH_2Cl_2) of **4d**.

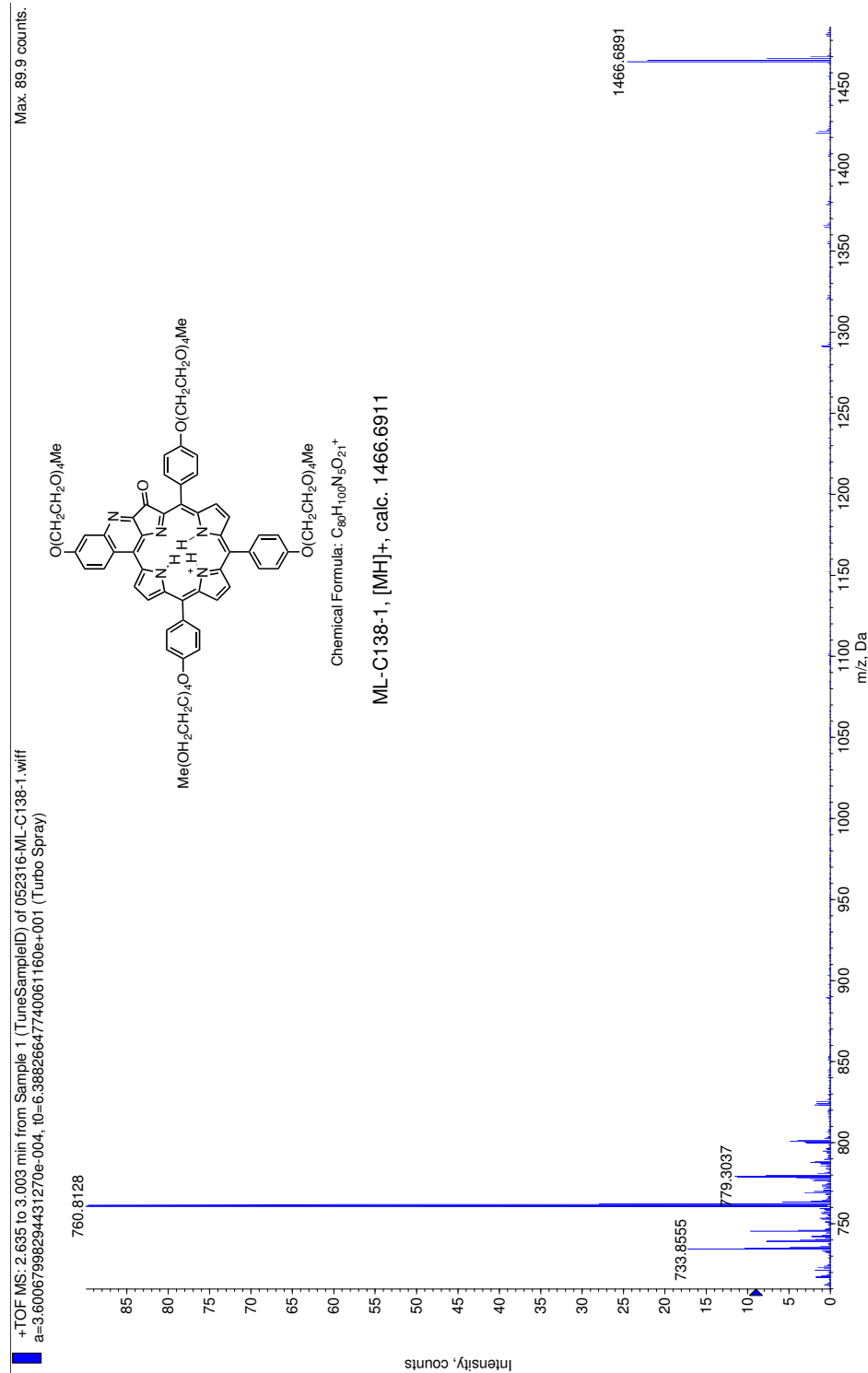


Figure S34. HR-MS (ESI⁺, 100% CH₃CN, TOF) of **4d**.

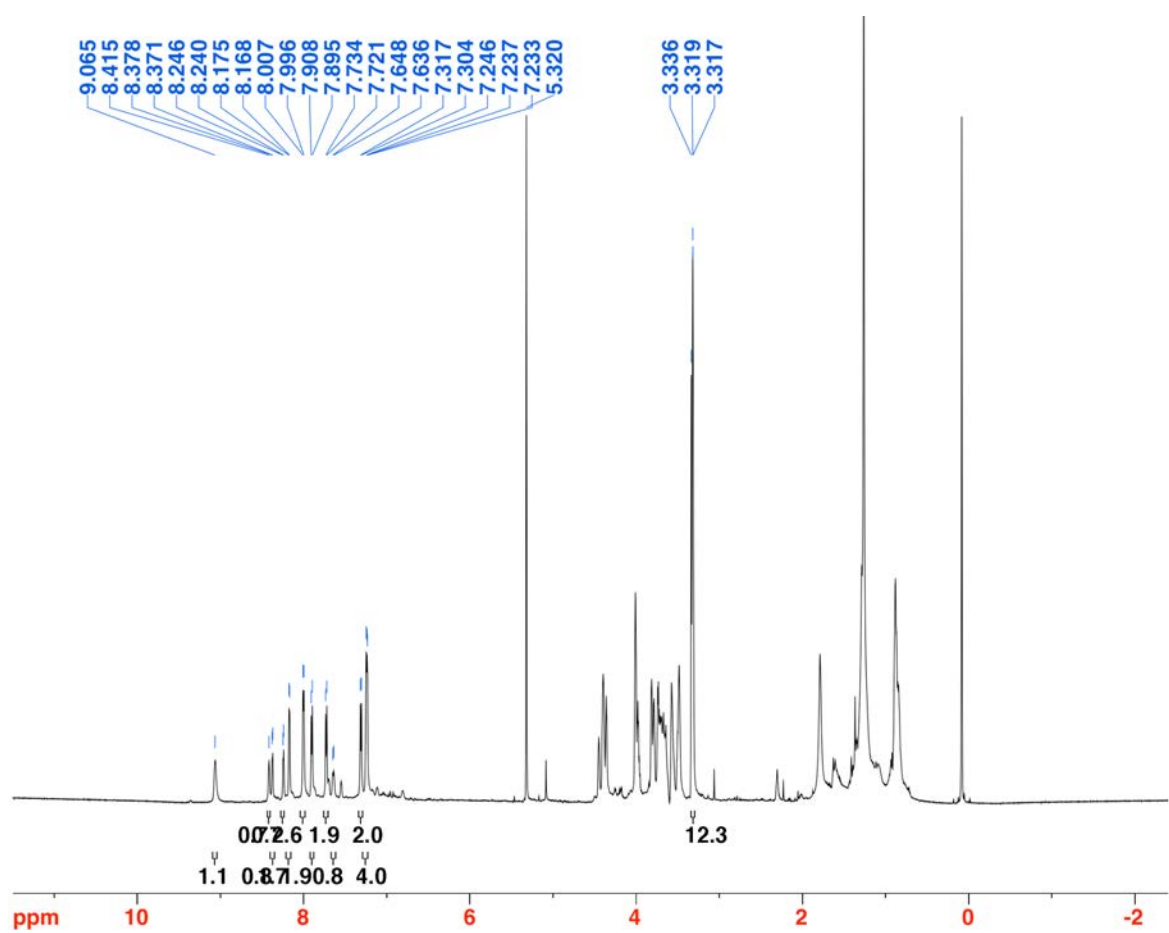
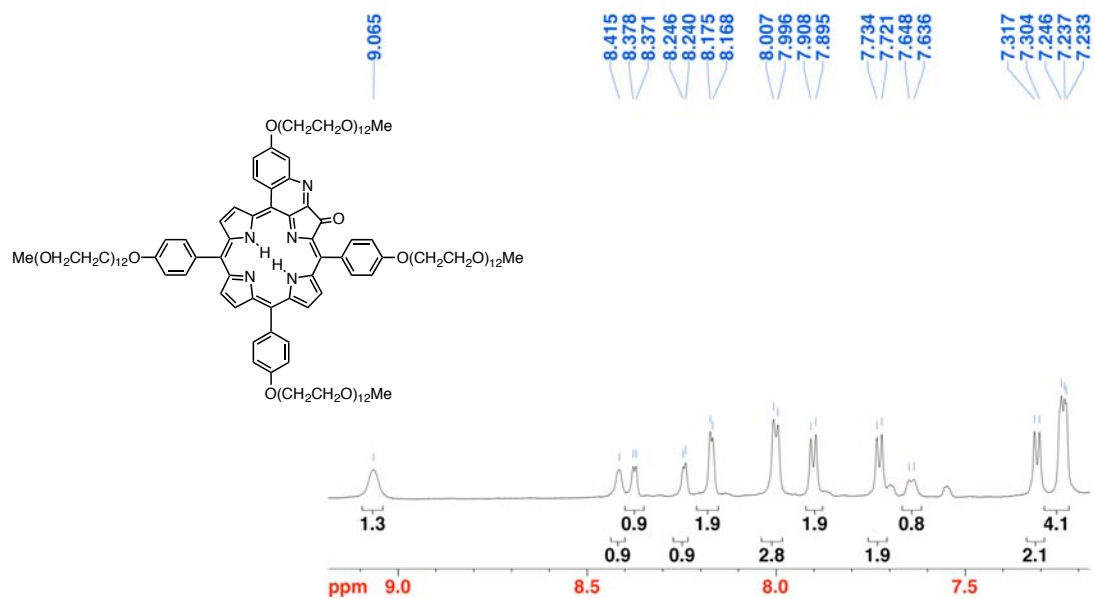


Figure S35. ^1H NMR spectrum (400 MHz, CD_2Cl_2) of **4e**.

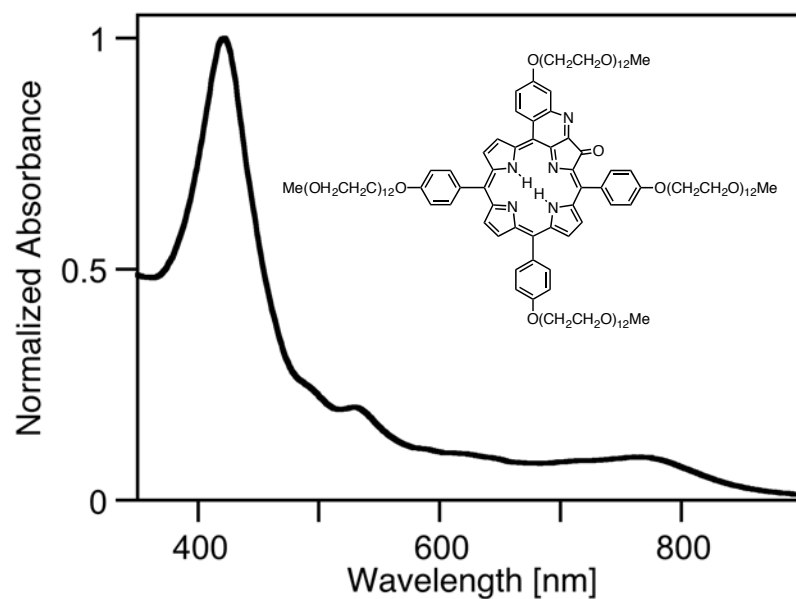


Figure S36. UV-vis spectrum (H_2O) of **4e**.

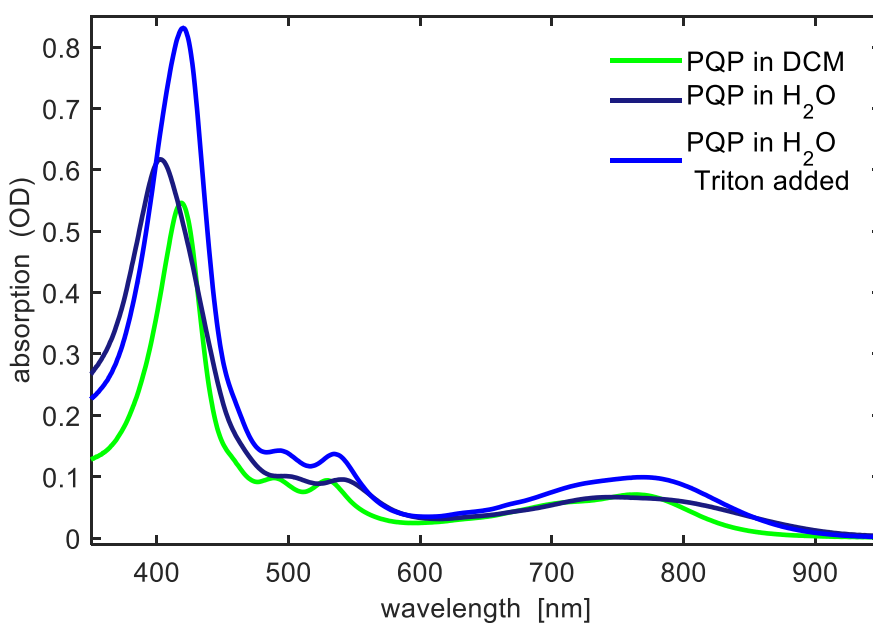


Figure S37. Absorption spectra of **4e** (PQP) in CH_2Cl_2 , H_2O and H_2O -Triton-X solutions. The change of the absorption spectrum of **4e** in H_2O after adding triton indicates that **4e** is somewhat aggregated in pure aqueous solution.

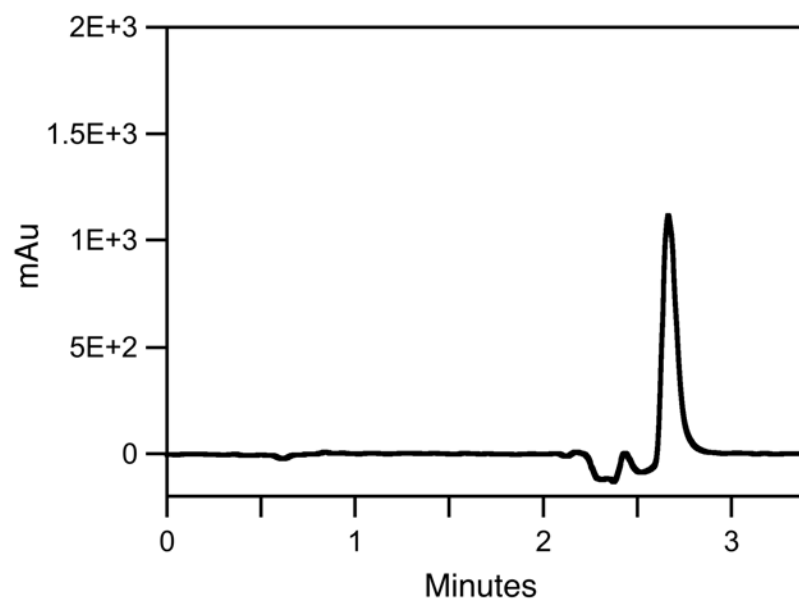


Figure S39. HPLC trace, UV-vis detector, of **4e** (silica, mobile phase: CH₂Cl₂/10% MeOH).

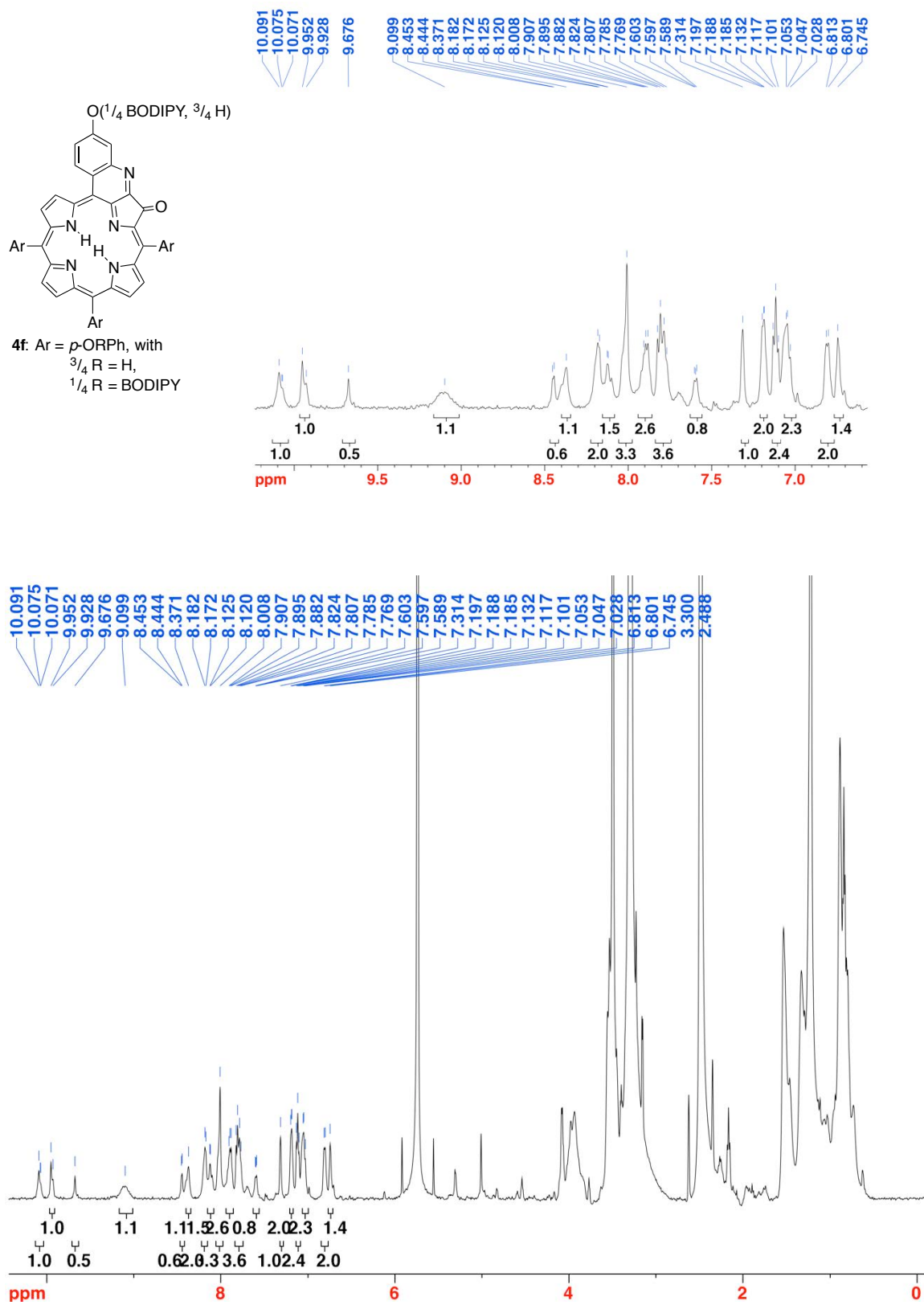


Figure S40. ^1H NMR spectrum (500 MHz, DMSO- d_6) of **4f**.

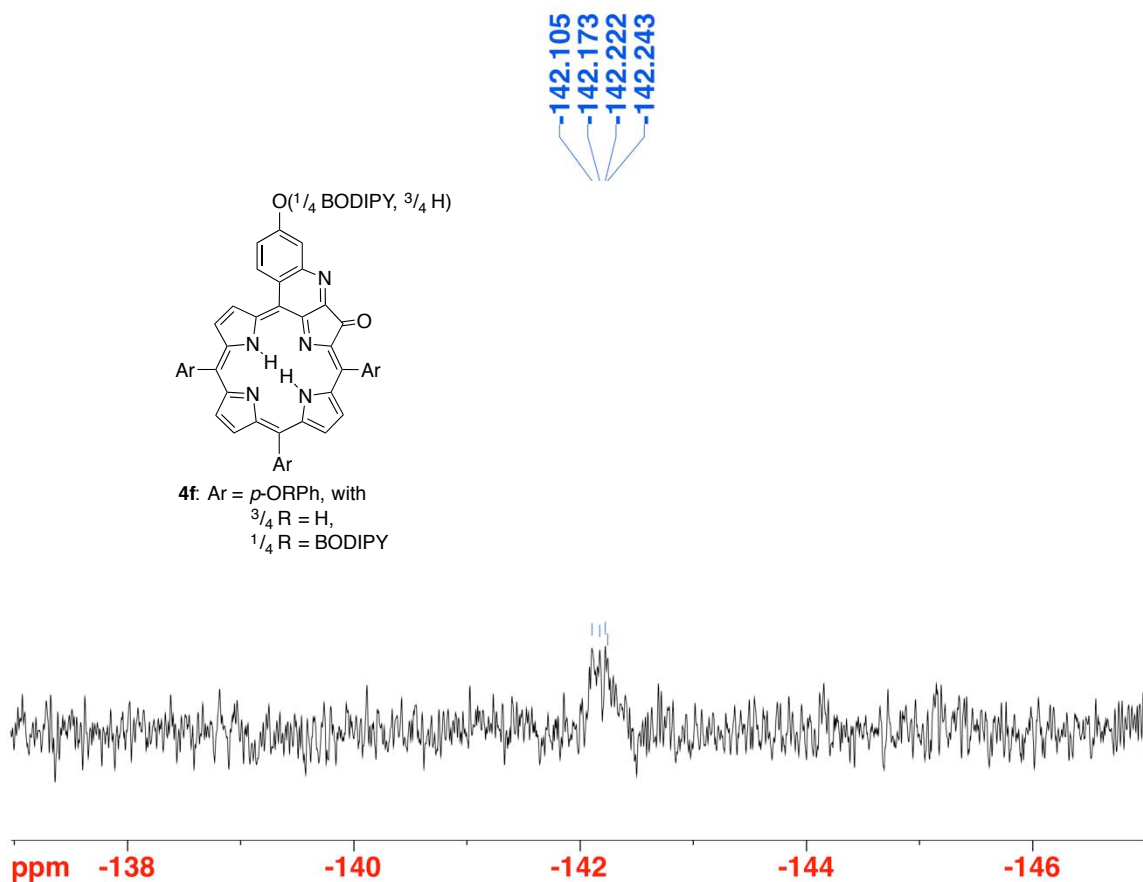


Figure S41. ^{19}F NMR spectrum (470 MHz, DMSO- d_6) of **4f**.

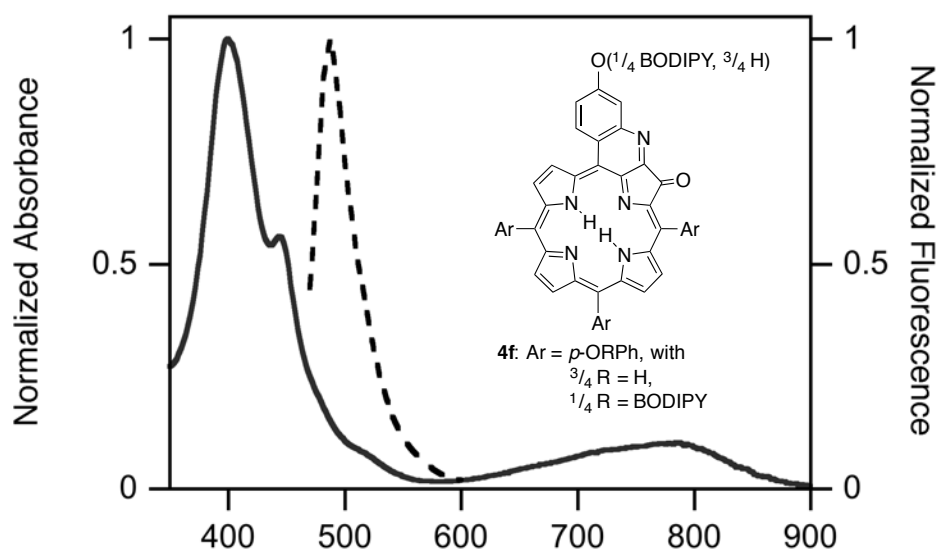


Figure S42. UV-vis and Fluorescence emission spectrum (MeOH, $\lambda_{\text{excitation}} = 441 \text{ nm}$) of **4f**.

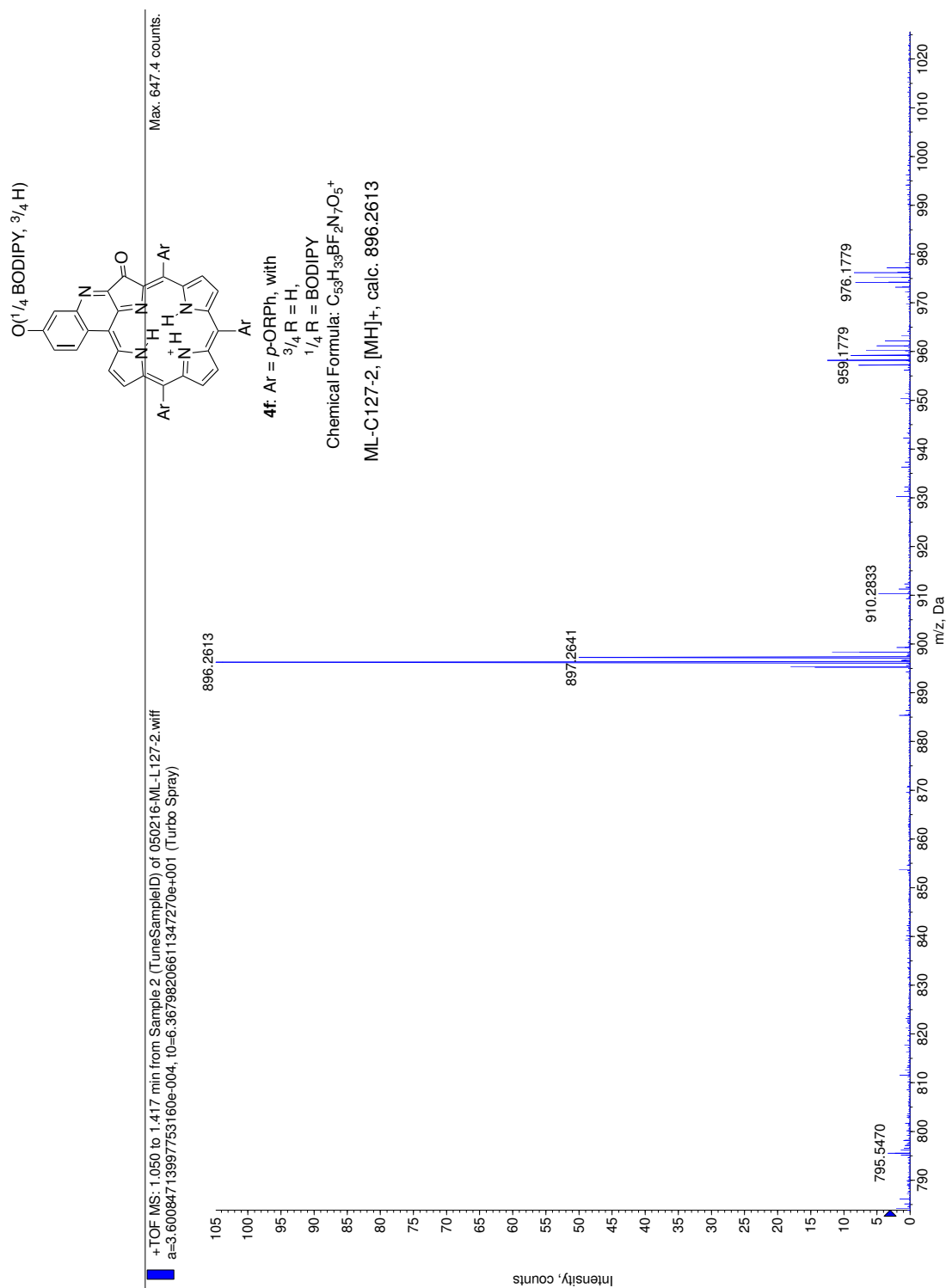


Figure S43. HR-MS (ESI+, 100% CH_3CN , TOF) of **4f**.

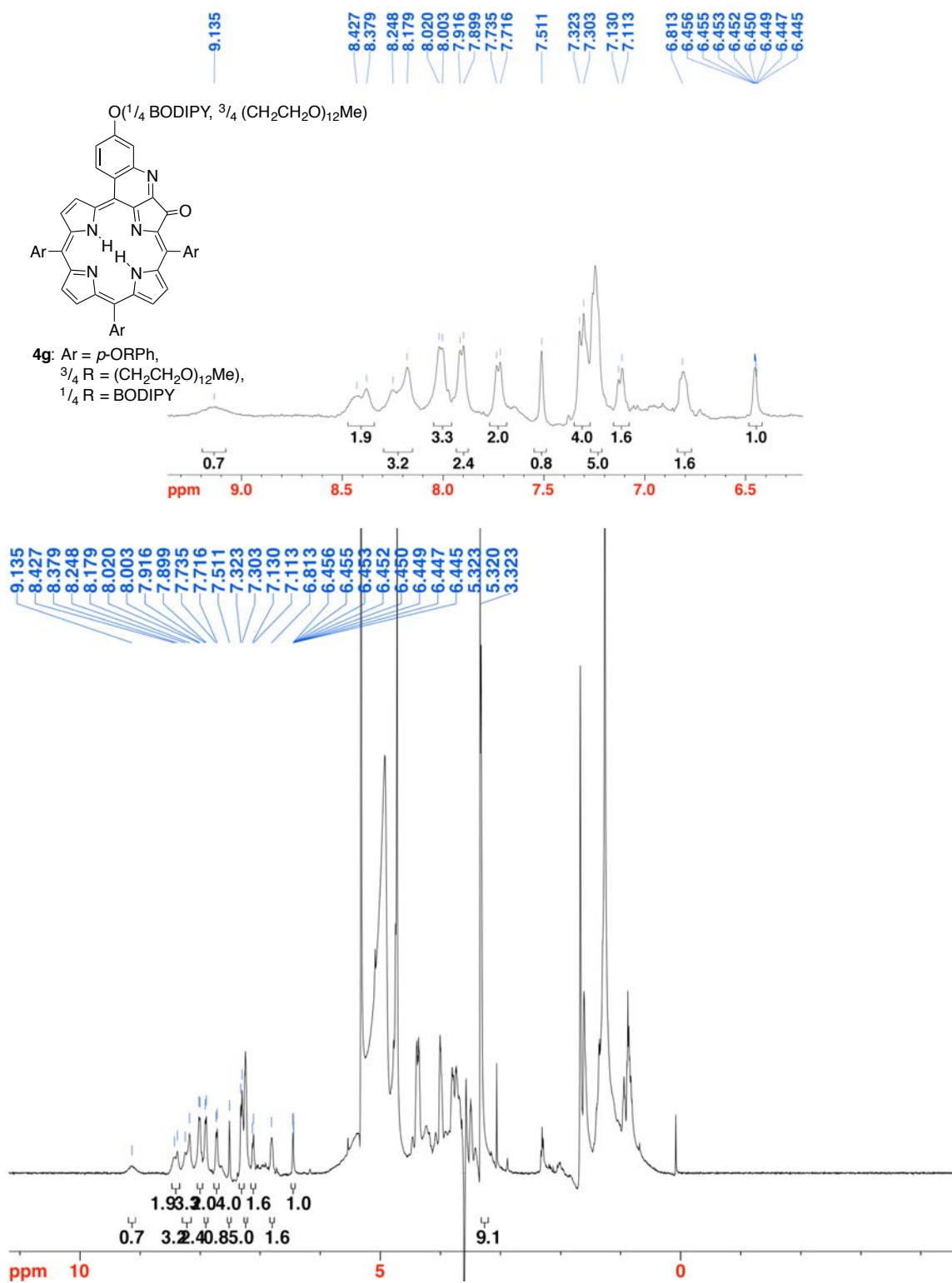


Figure S44. 1H NMR spectrum (400 MHz, CD_2Cl_2 , pre-saturated at 3.6 ppm) of **4g**.

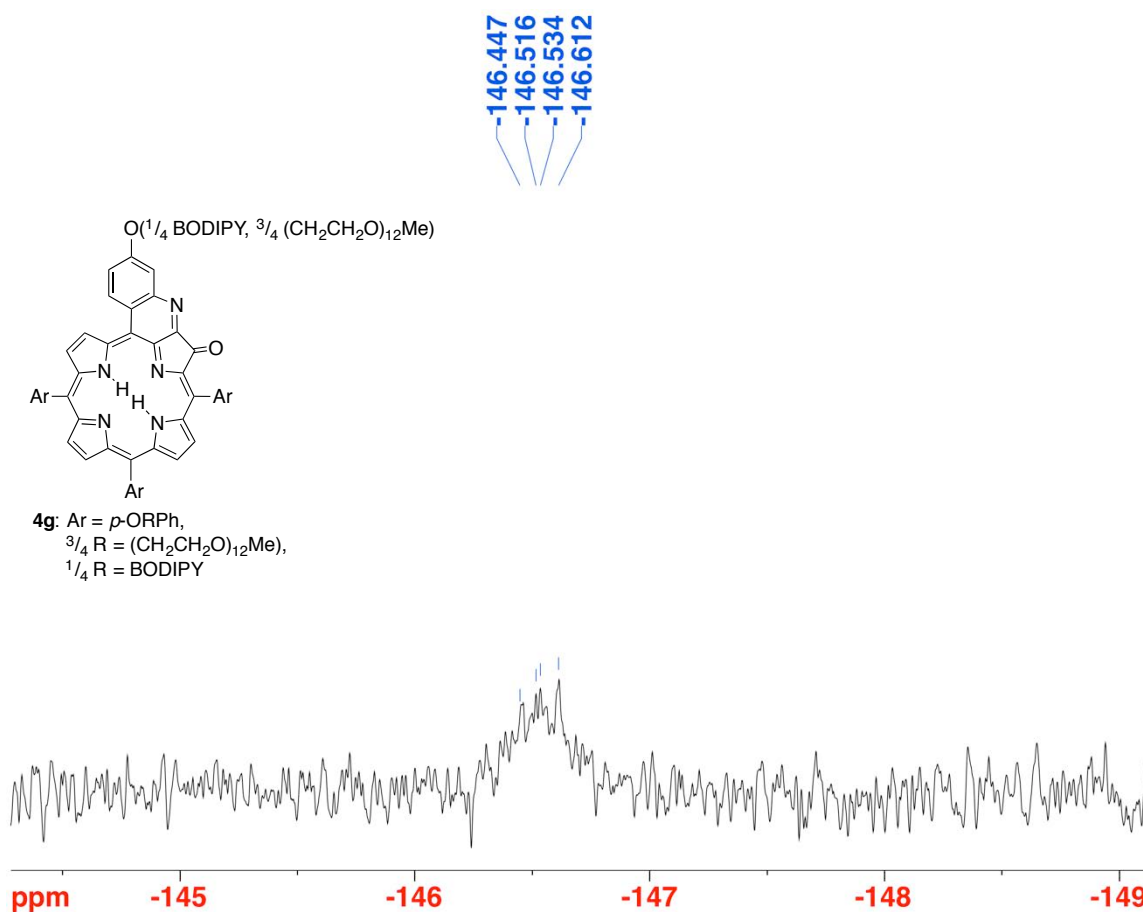


Figure S45. ^{19}F NMR spectrum (376 MHz, CD_2Cl_2) of **4g**.

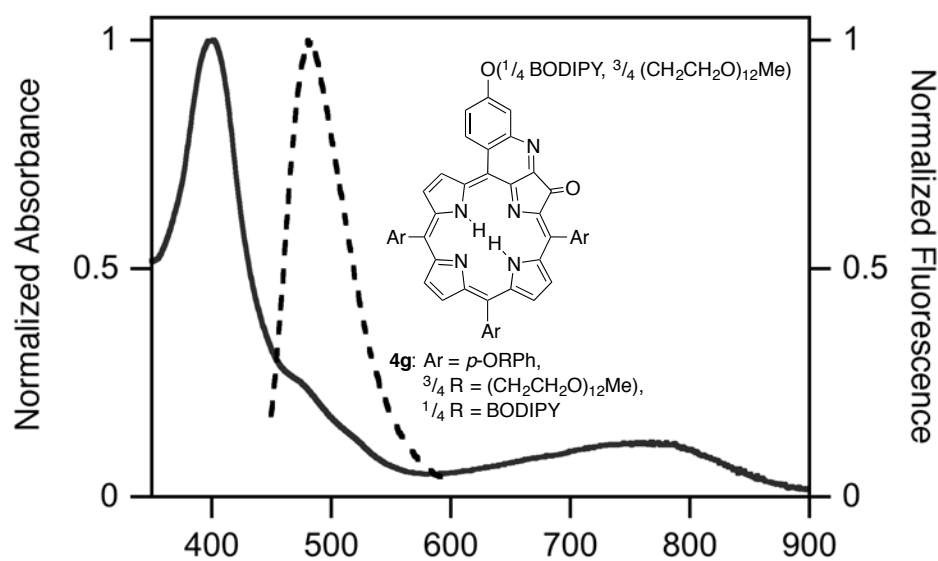


Figure S46. UV-vis and Fluorescence emission spectrum (MeOH, $\lambda_{\text{excitation}} = 441 \text{ nm}$) of **4g**.

D:\Data\Nonka\ML 090916\ML-C140-2 in DHBA\0_CS\1\1\SRref

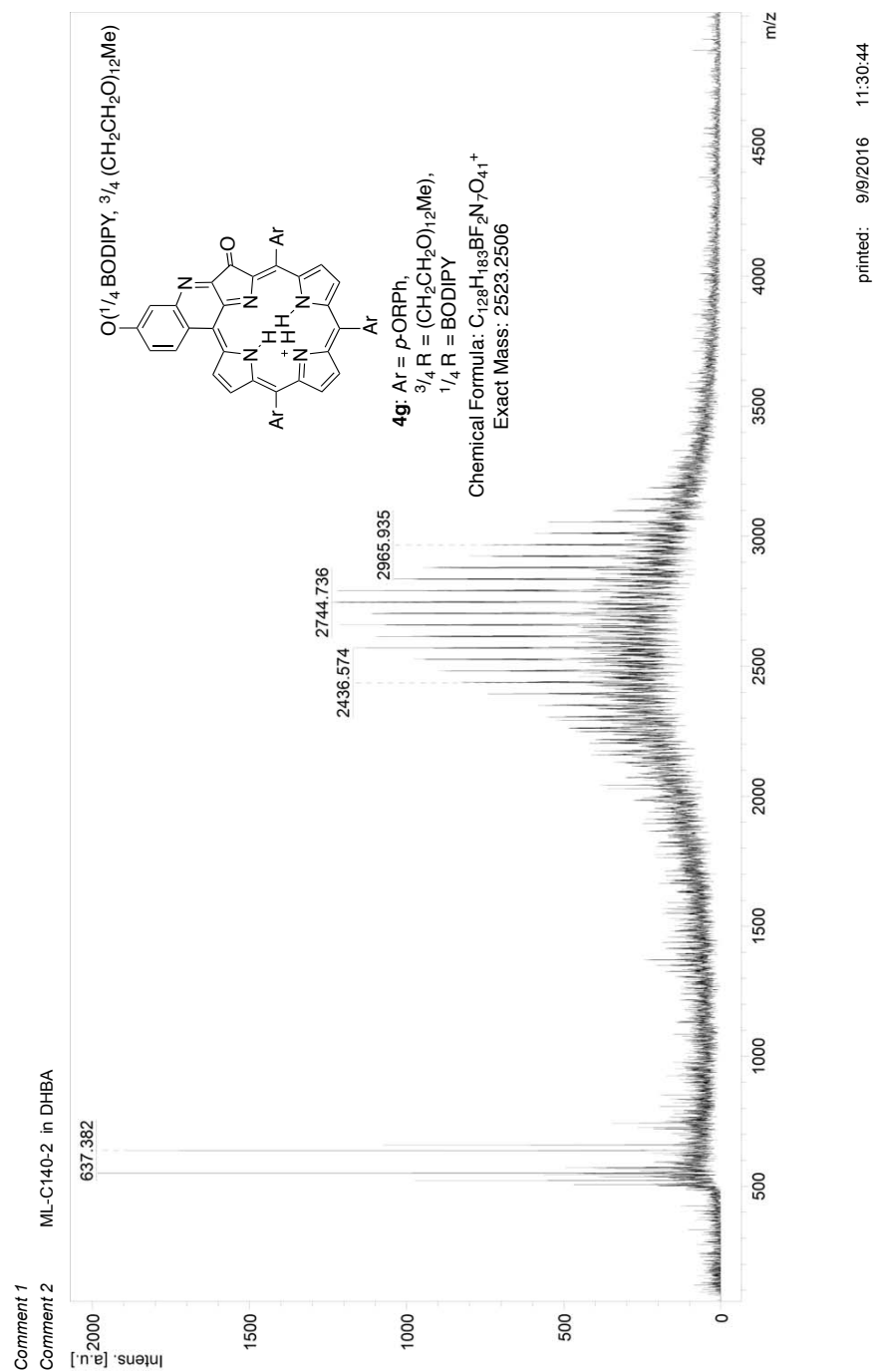


Figure S47. MALDI-TOF spectrum (100% DHBA) of **4g**.

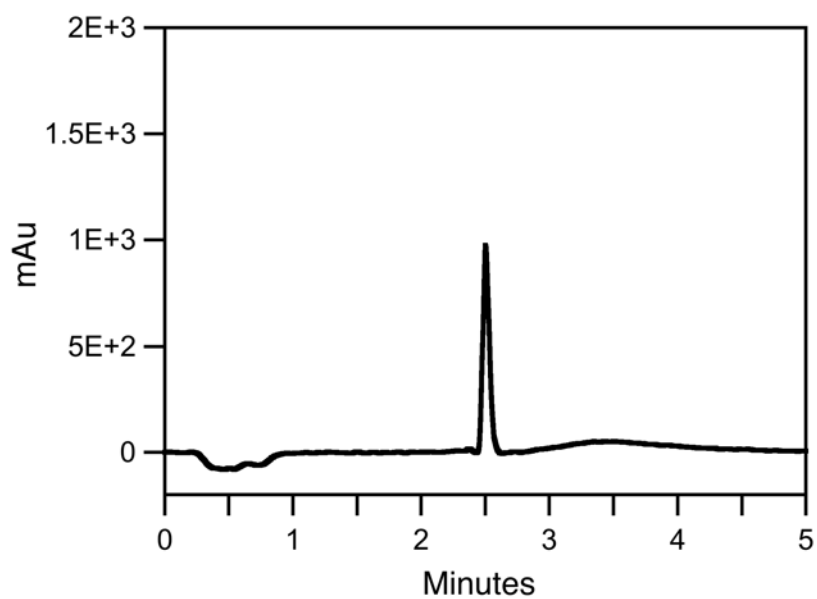


Figure S48. HPLC trace, UV-vis detector, of **4g** (silica, mobile phase: CH₂Cl₂/5% MeOH).



Figure S49. A mouse tumor before injection of **4e**.

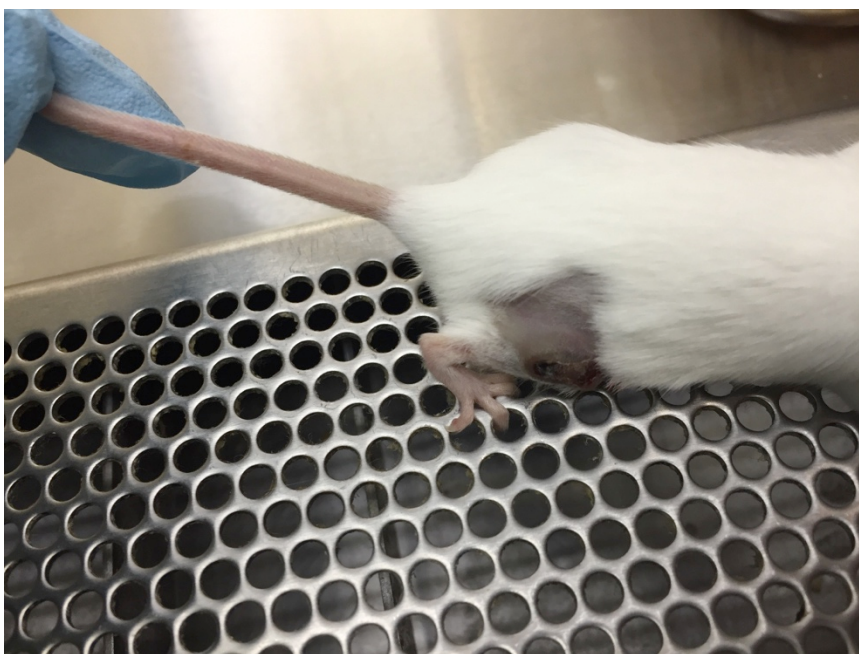


Figure S50. A mouse tumor 48 h after injection of 100 μ L of a 33 mM solution of **4e** in PBS, showing the dark brown-stained tumor site.

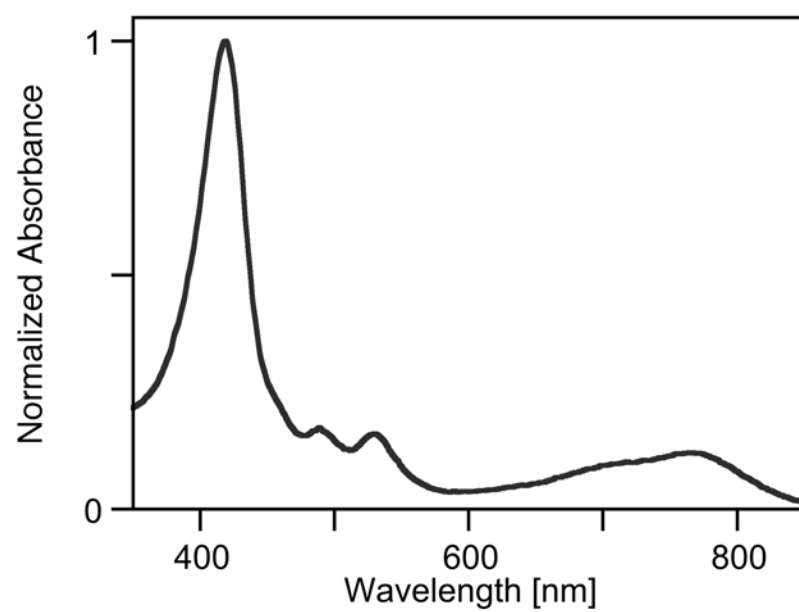


Figure S52. UV-vis spectrum (CH_2Cl_2) of mouse (diluted) urine obtained after injection of **4e**.