

ELECTRONIC SUPPORTING INFORMATION (ESI) to:

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

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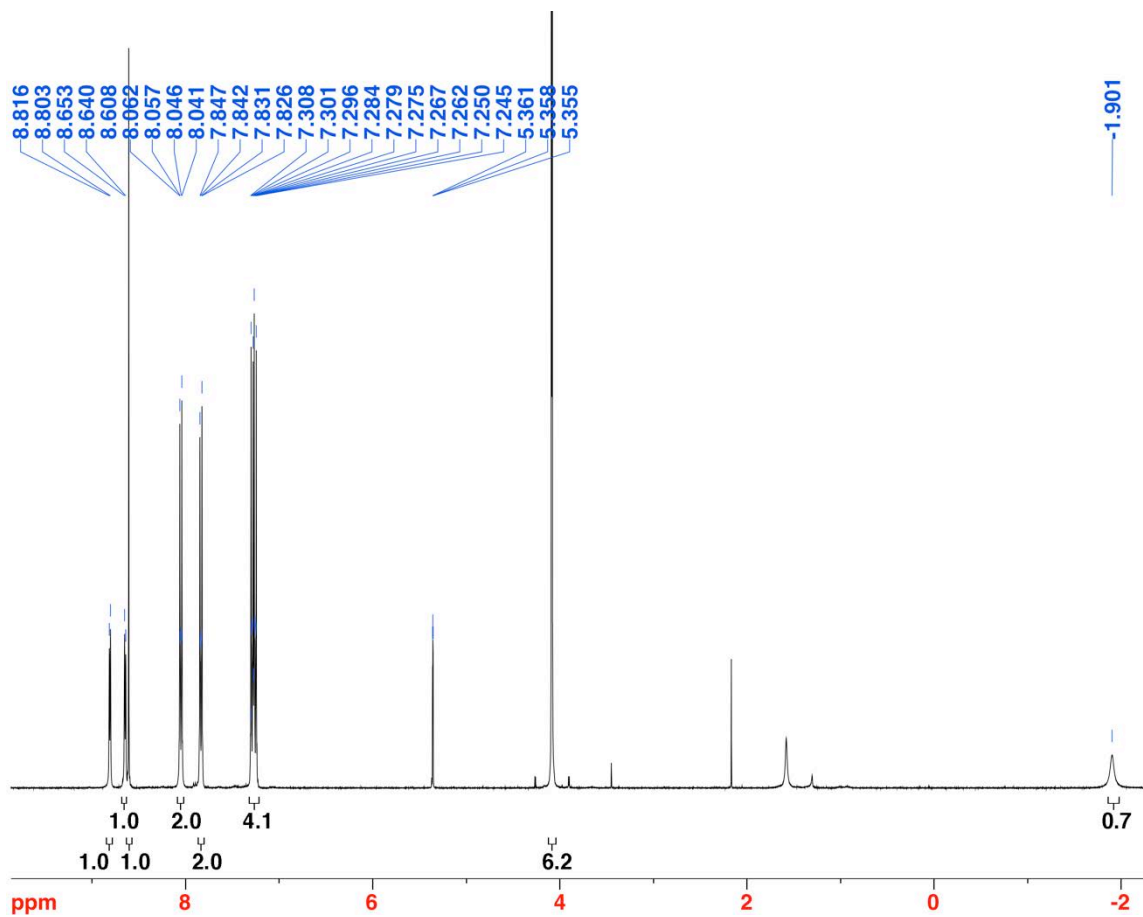
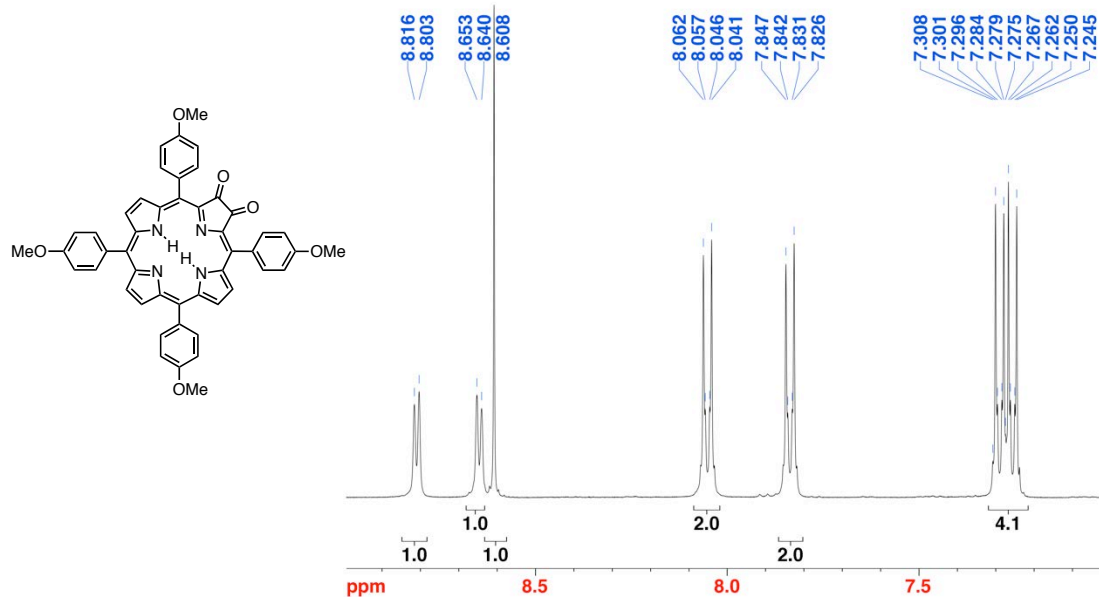


Figure S1. ¹H NMR spectrum (400 MHz, CD₂Cl₂) of **8**.

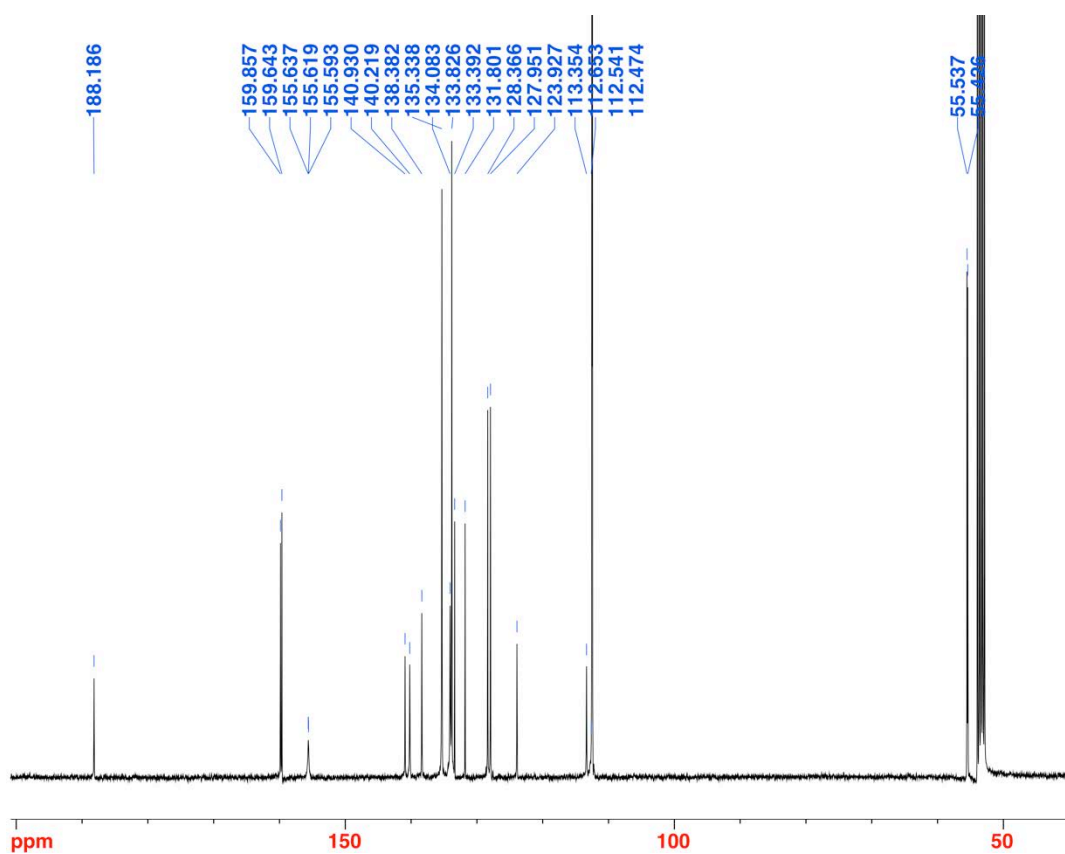
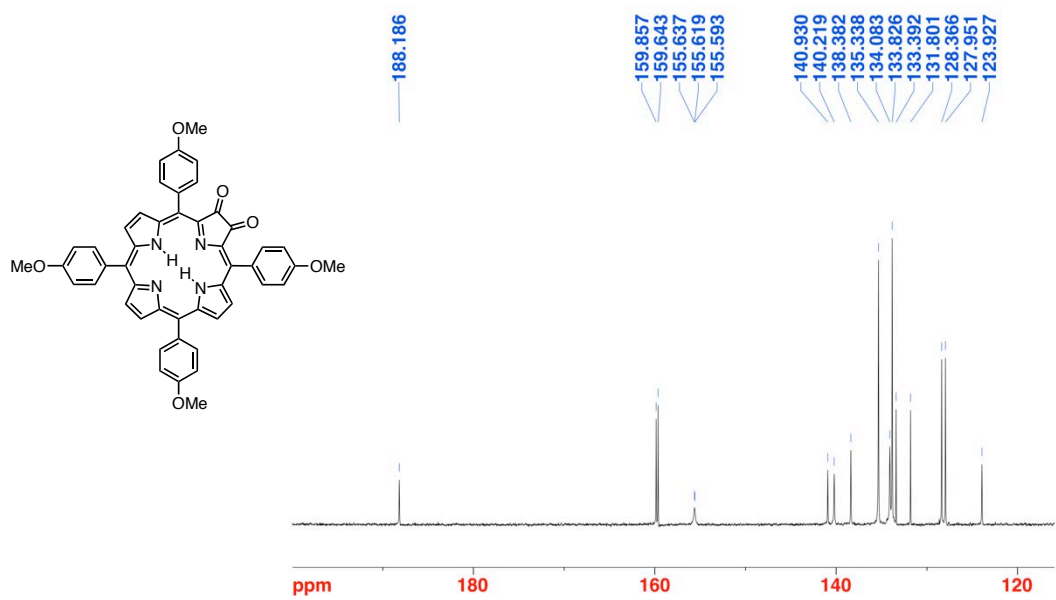


Figure S2. ¹³C NMR spectrum (100 MHz, CD₂Cl₂) of 8.

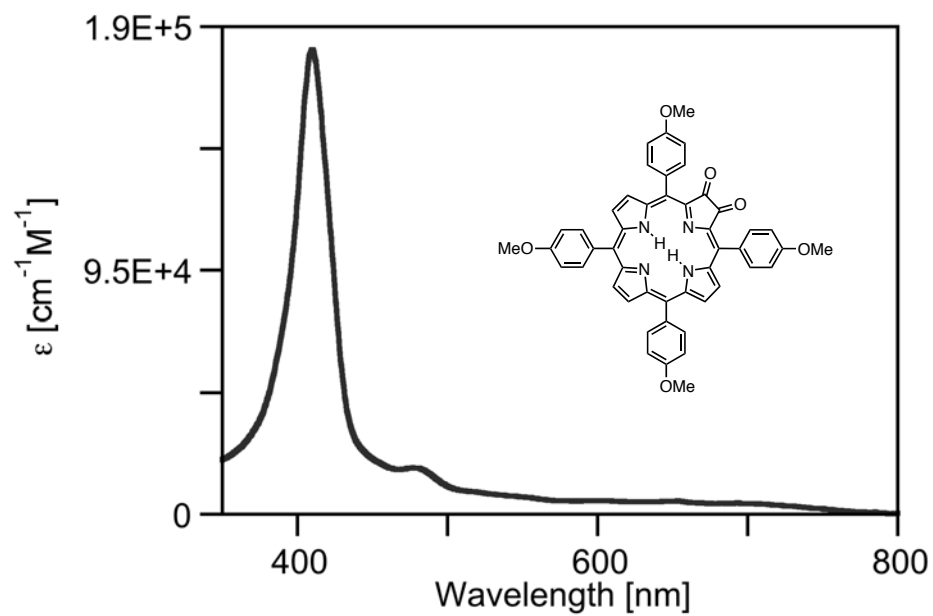


Figure S3. UV-vis spectrum (CH_2Cl_2) of **8**.

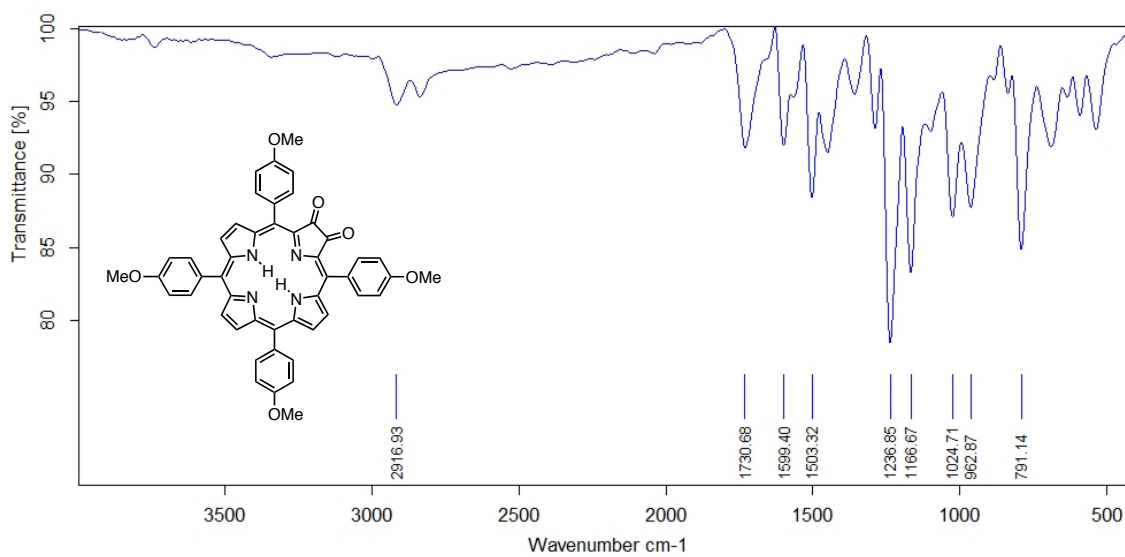


Figure S4. FT-IR spectrum (neat, diamond ATR) of **8**.

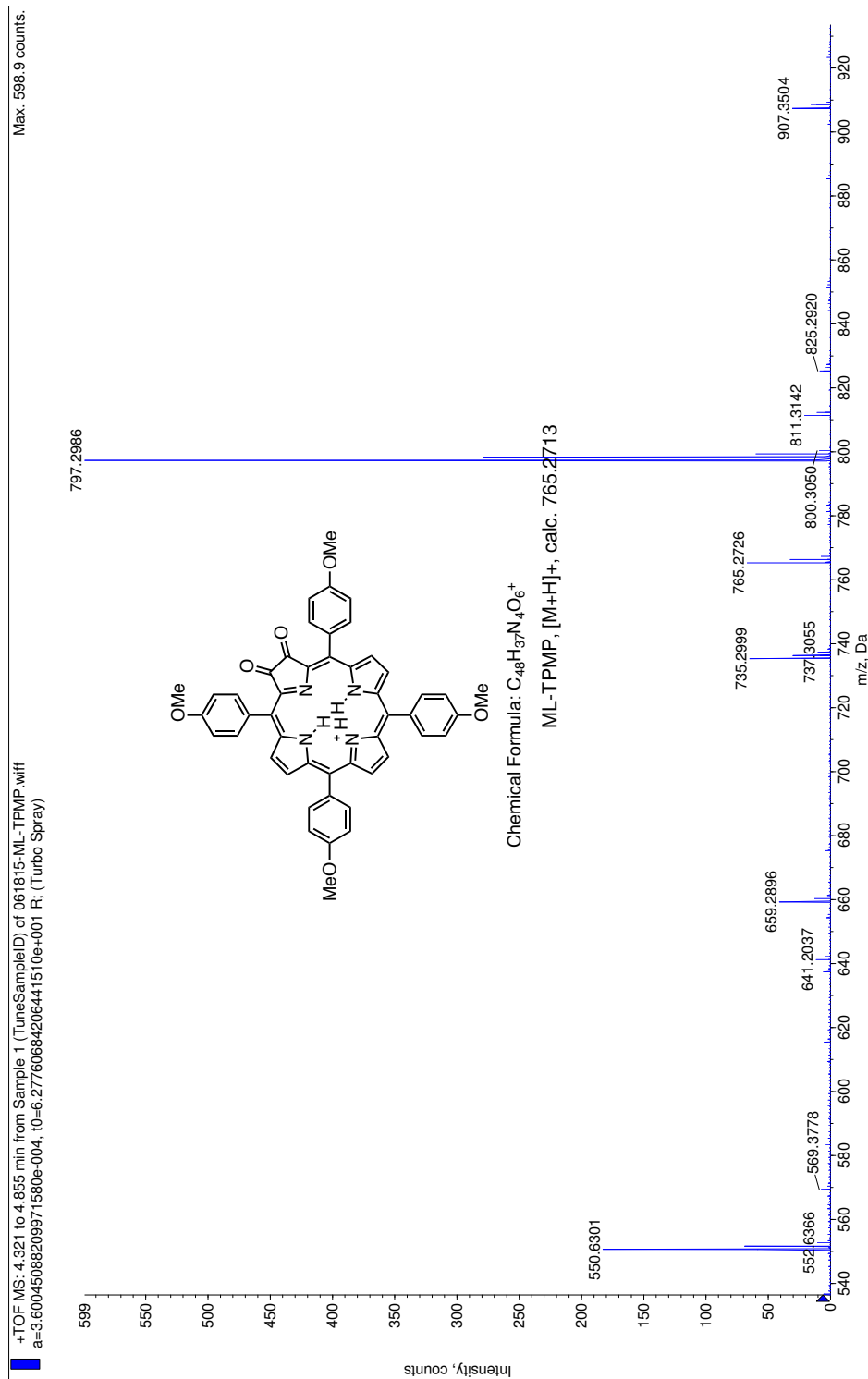


Figure S5. HR-MS (ESI⁺, 100% CH₃CN, TOF) of **8**.

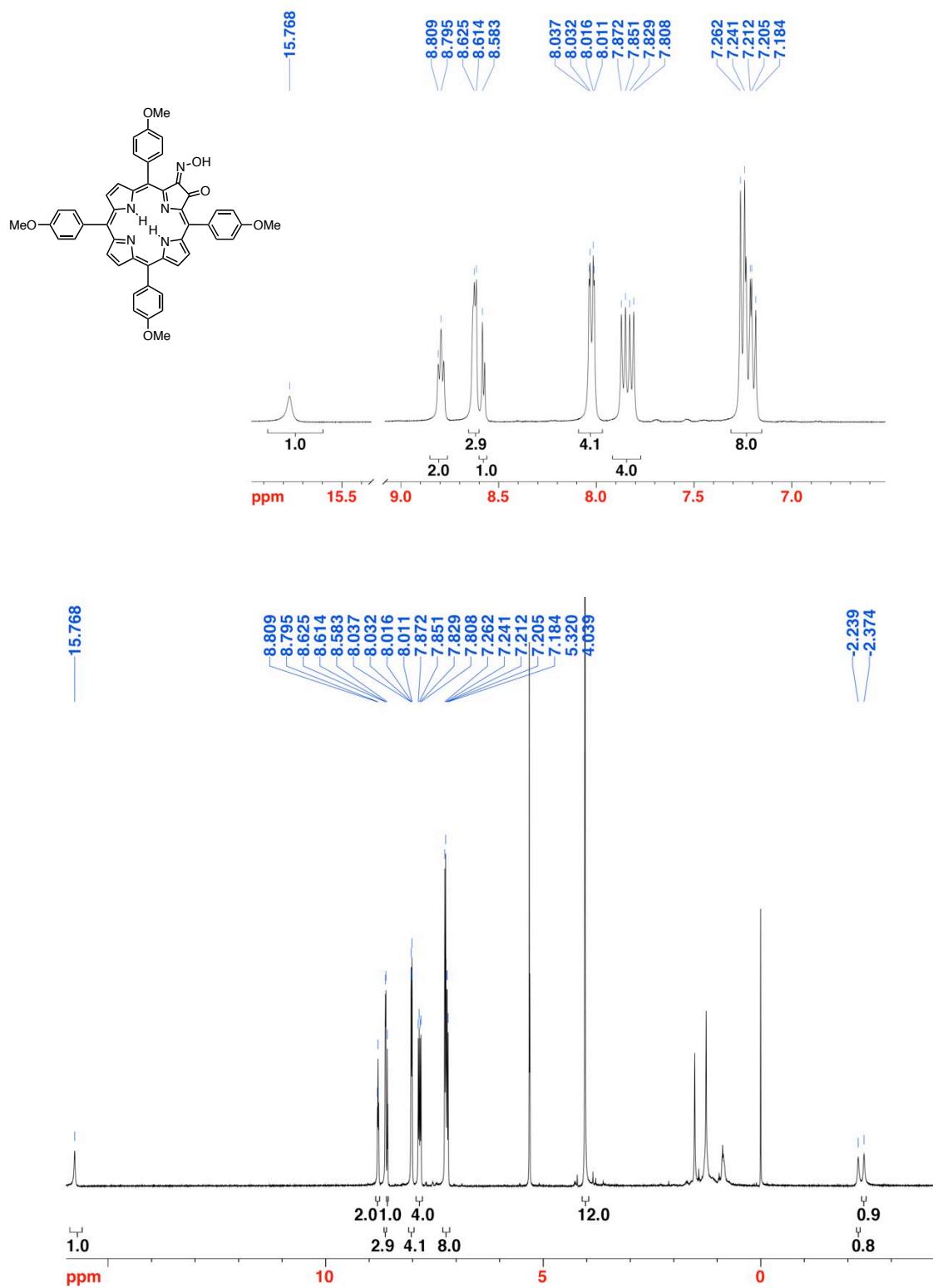


Figure S6. ^1H NMR spectrum (400 MHz, CD_2Cl_2) of **9**.

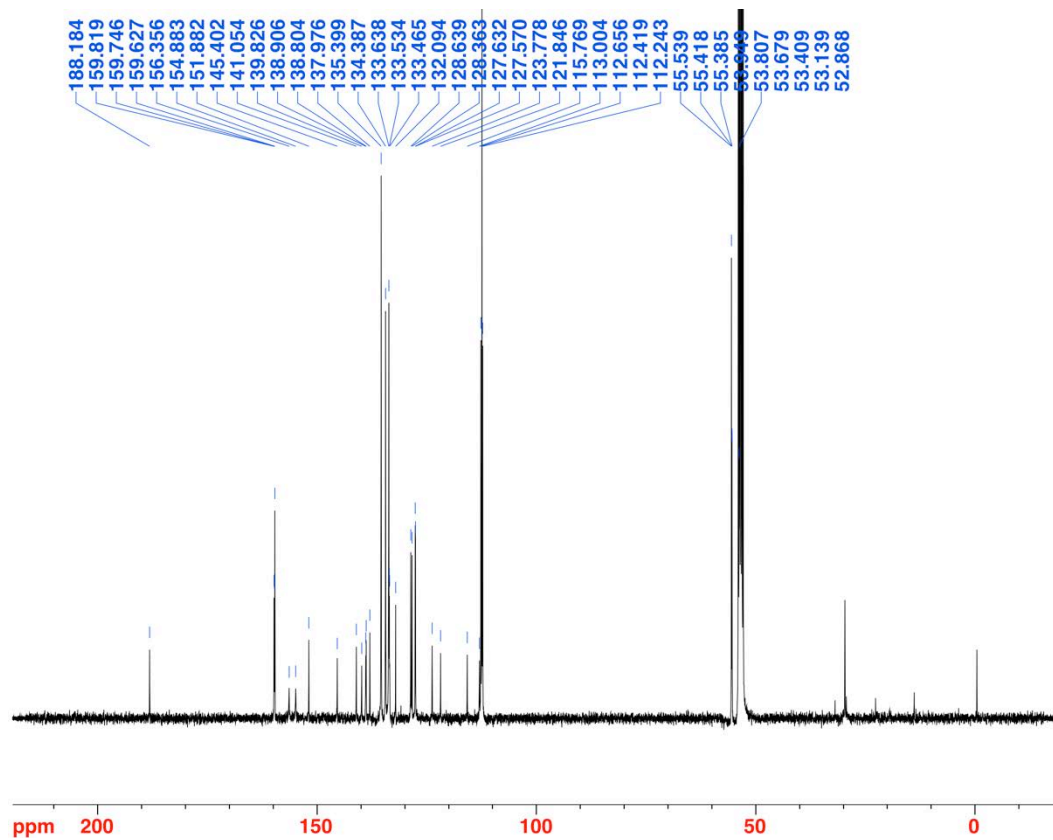
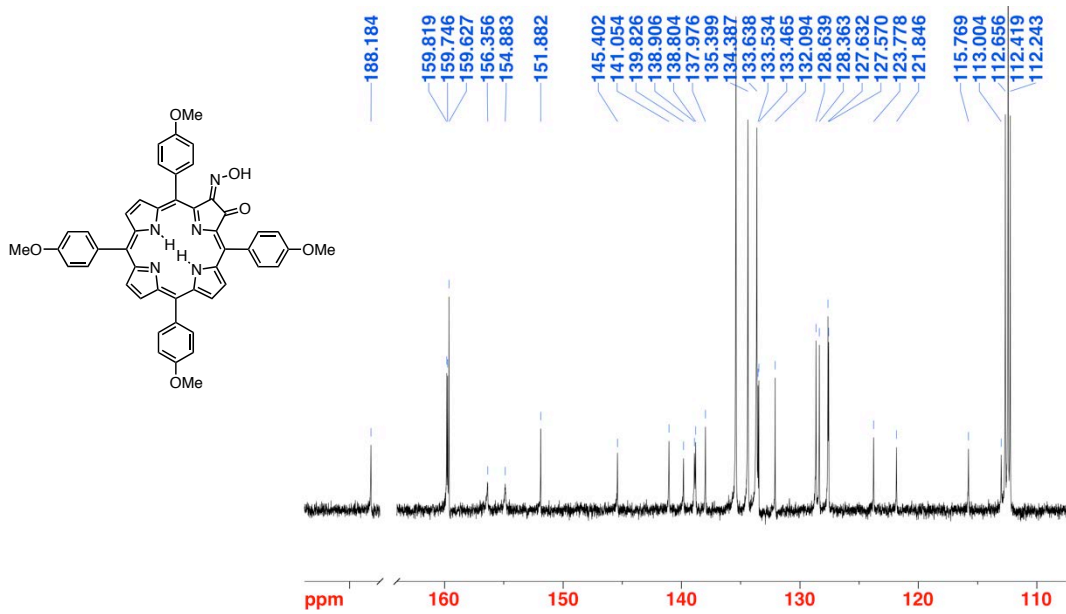


Figure S7. ^{13}C NMR spectrum (100 MHz, CD_2Cl_2) of 9.

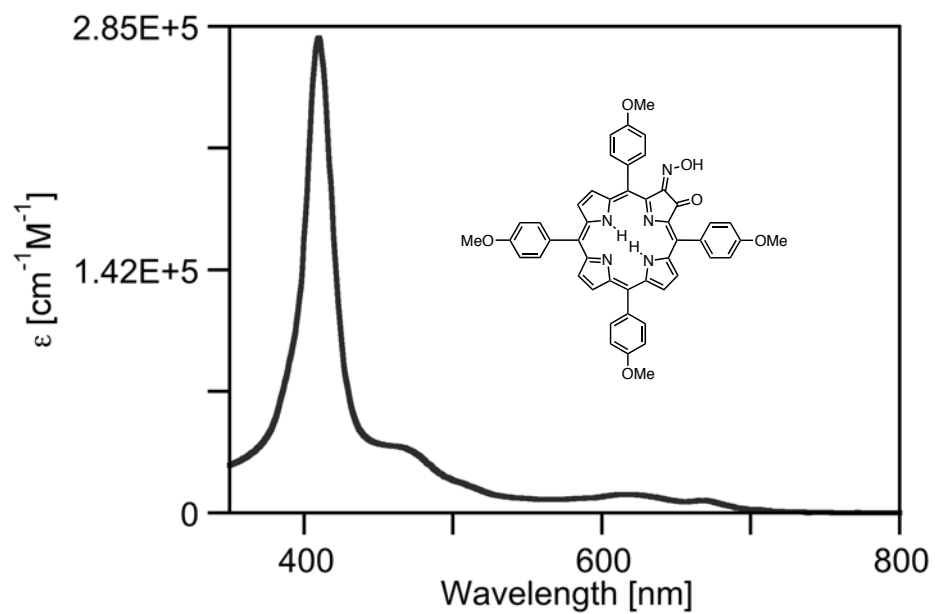


Figure S8. UV-vis spectrum (CH_2Cl_2) of **9**.

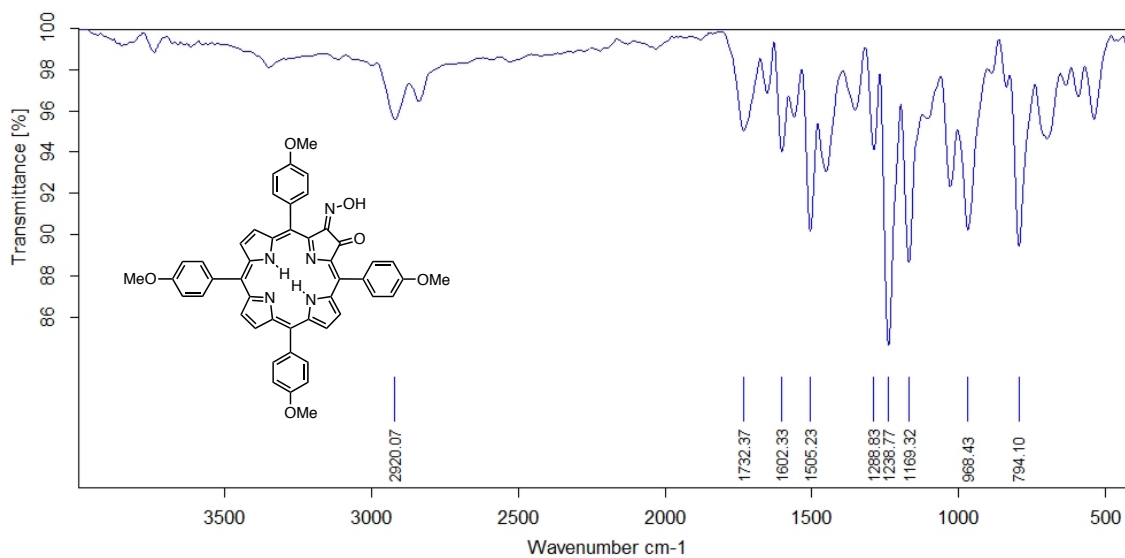


Figure S9. FT-IR spectrum (neat, diamond ATR) of **9**.

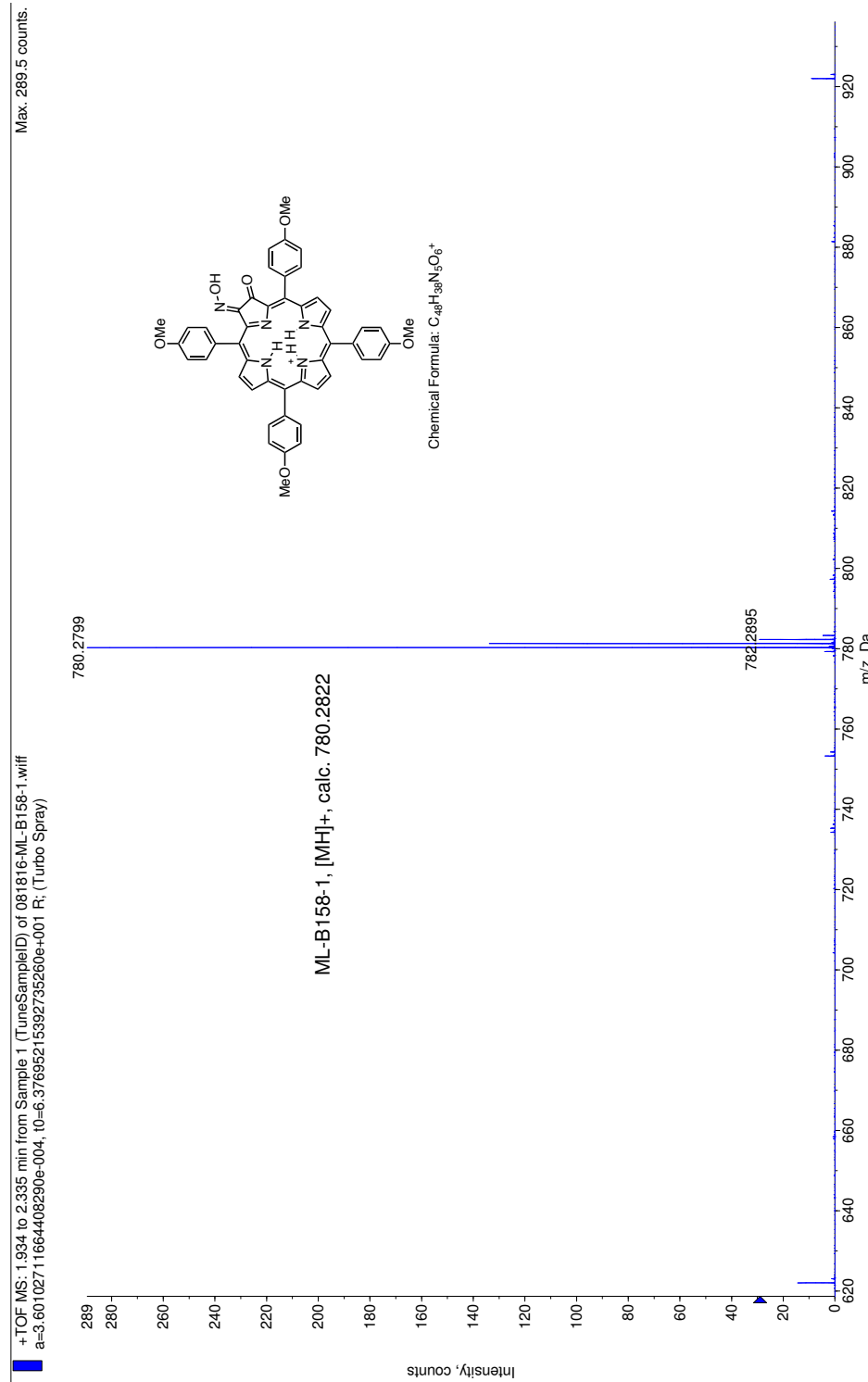


Figure S10. HR-MS (ESI⁺, 100% CH₃CN, TOF) of **9**.

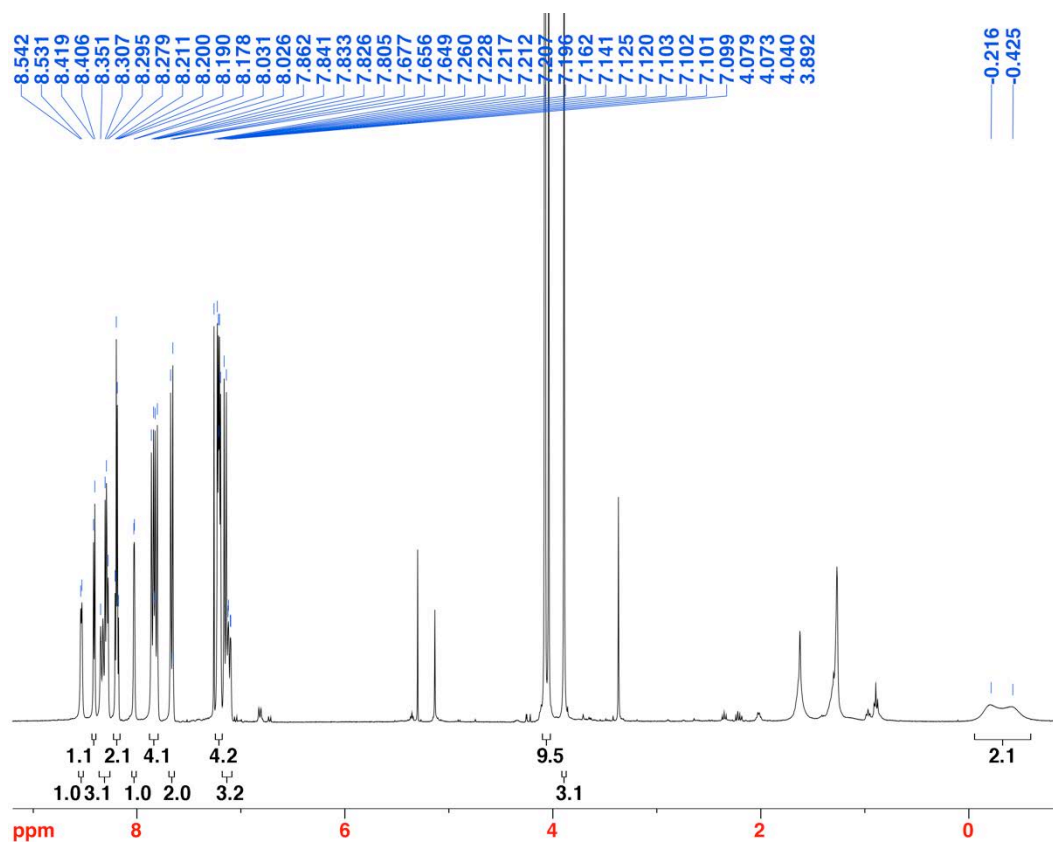
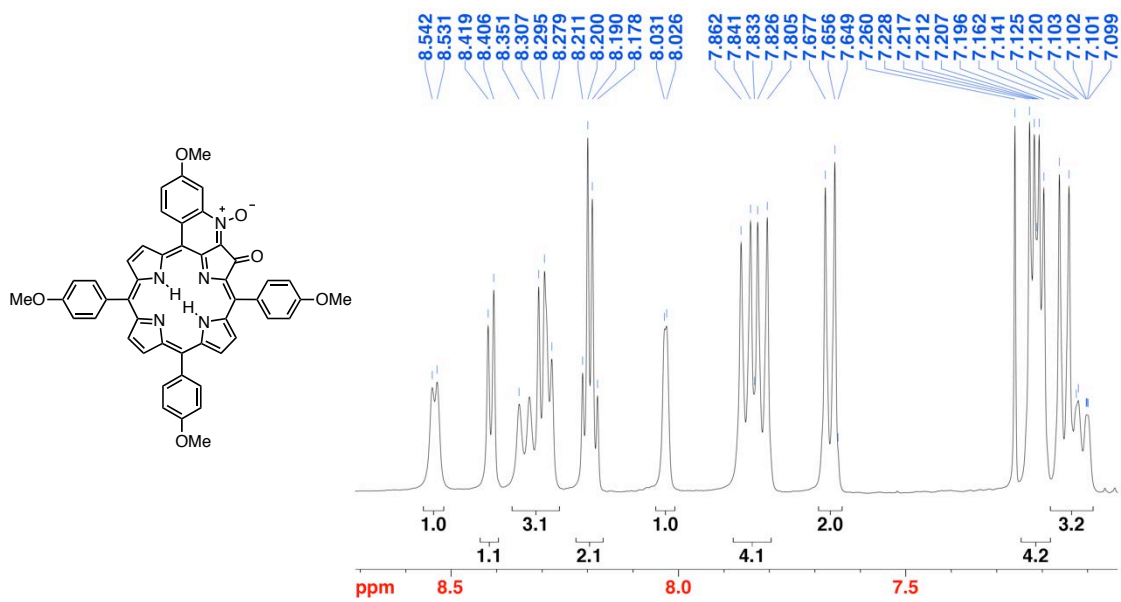


Figure S11. ¹H NMR spectrum (400 MHz, CDCl₃) of 5b.

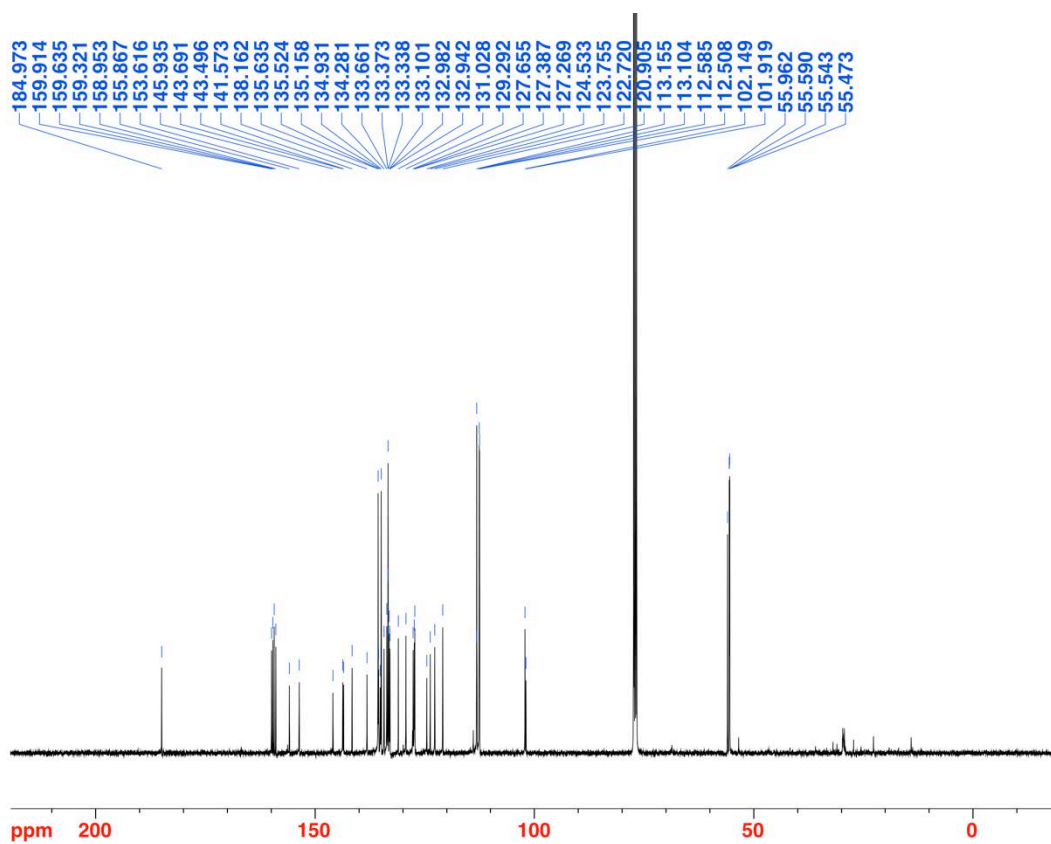
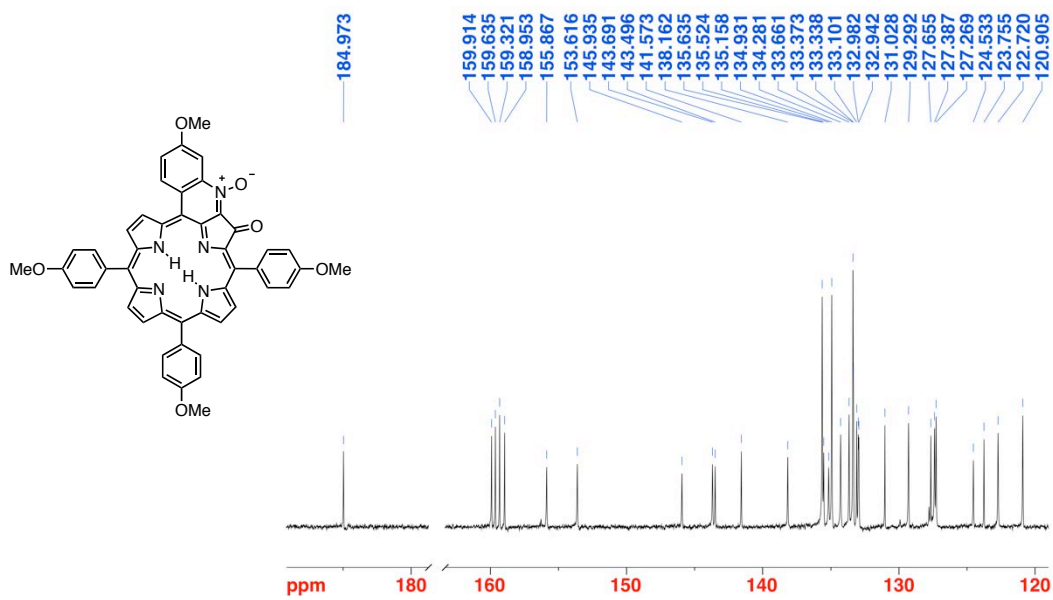


Figure S12. ¹³C NMR spectrum (100 MHz, CDCl₃) of 5b.

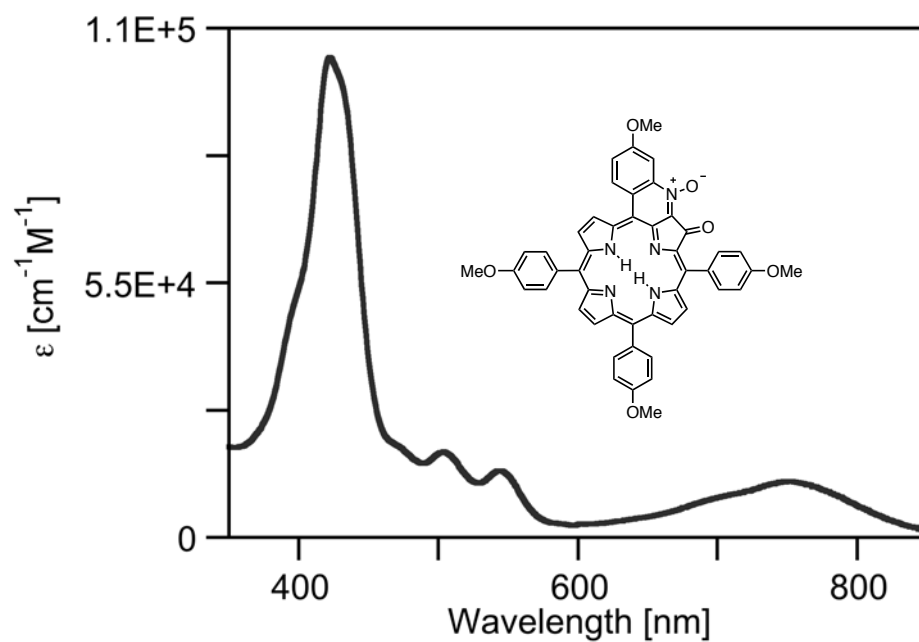


Figure S13. UV-vis spectrum (CH_2Cl_2) of **5b**.

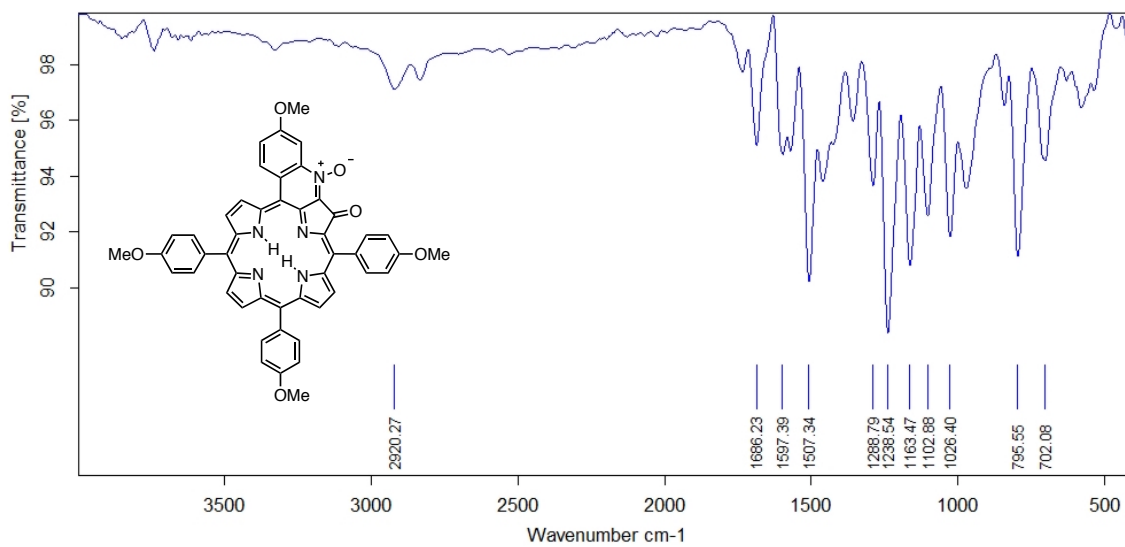


Figure S14. FT-IR spectrum (neat, diamond ATR) of **5b**.

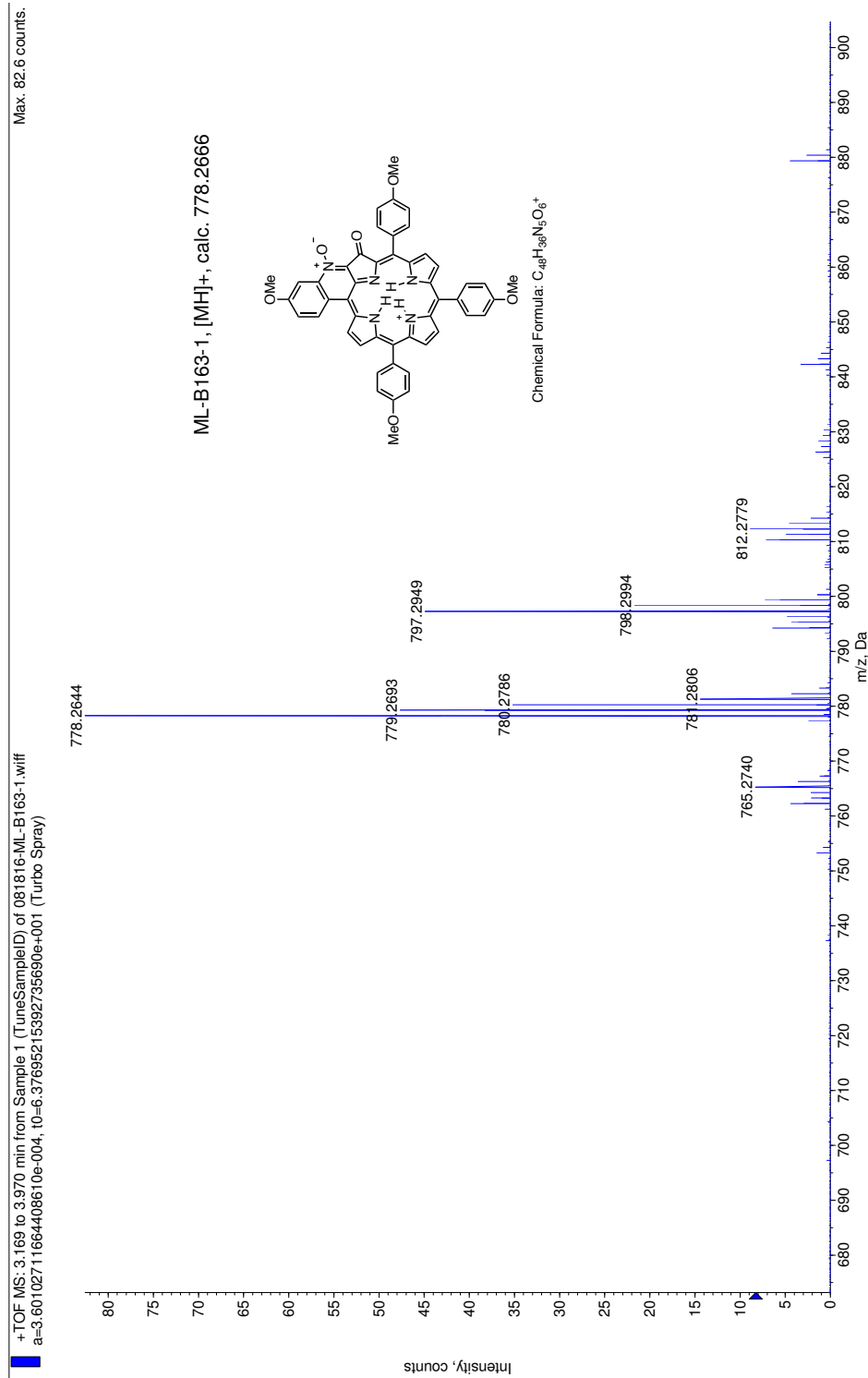


Figure S15. HR-MS (ESI⁺, 100% CH₃CN, TOF) of **5b**.

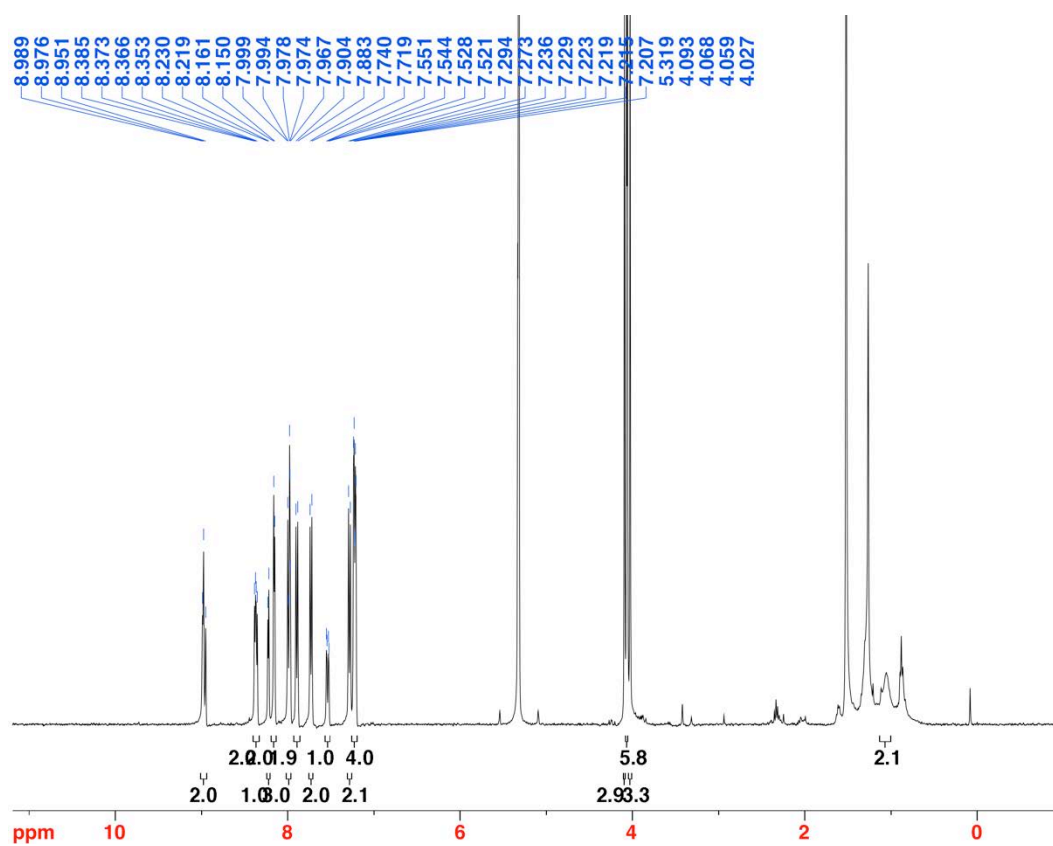
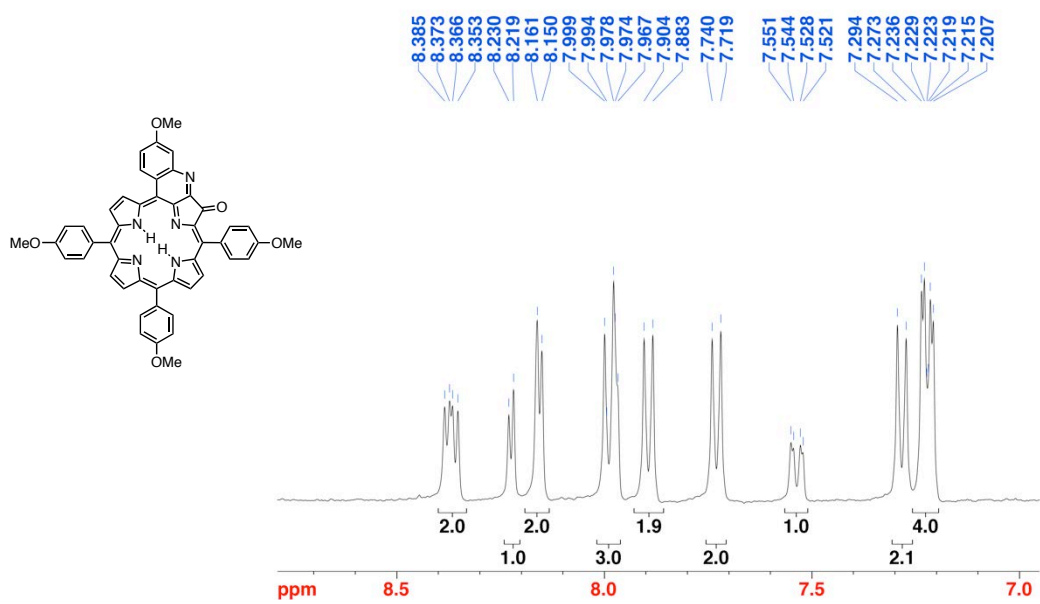


Figure S16. $^1\text{H NMR}$ spectrum (400 MHz, CD_2Cl_2) of **4b**.

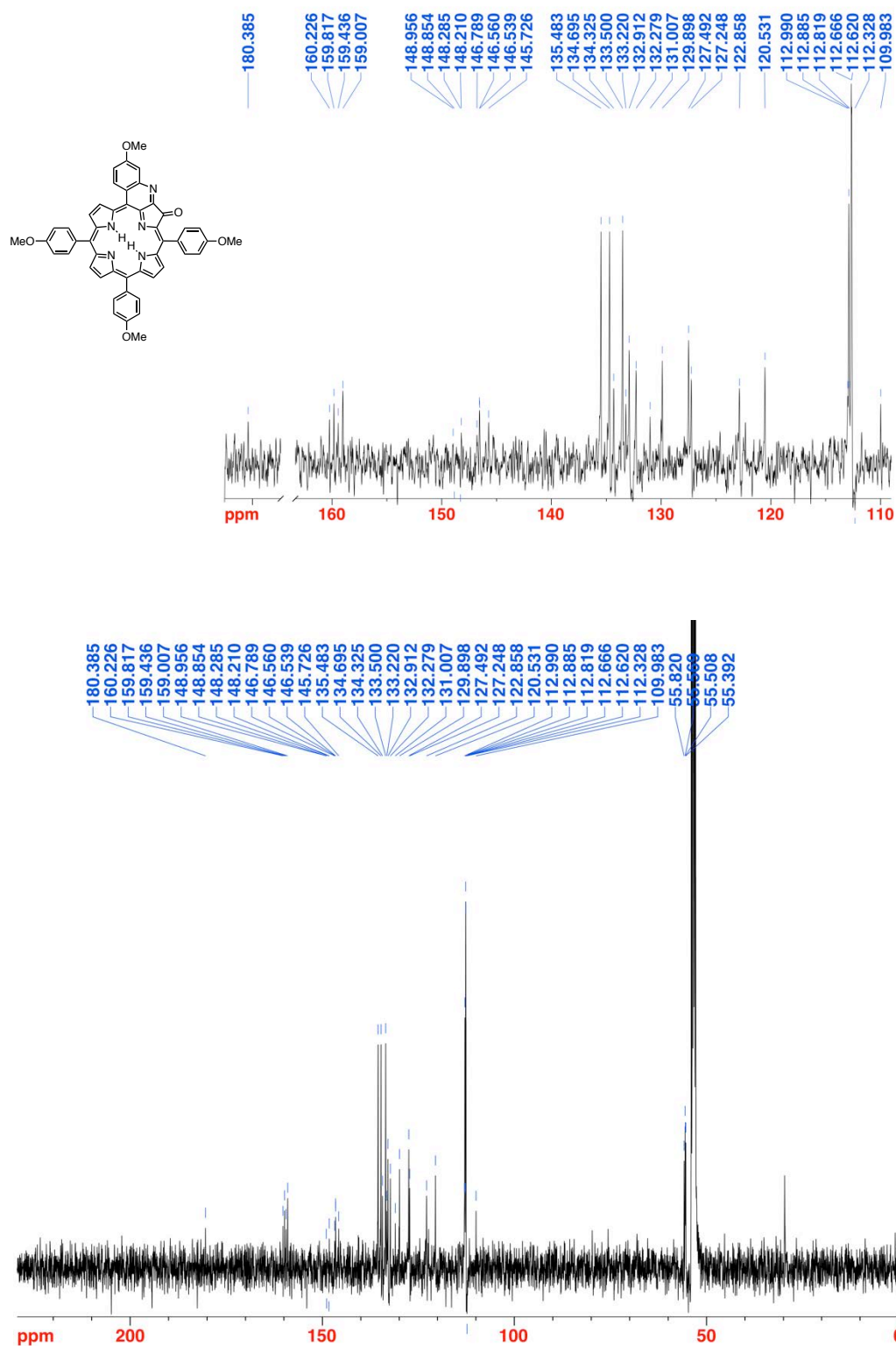


Figure S17. ¹³C NMR spectrum (100 MHz, CD₂Cl₂) of **4b** (the compound has limited solubility).

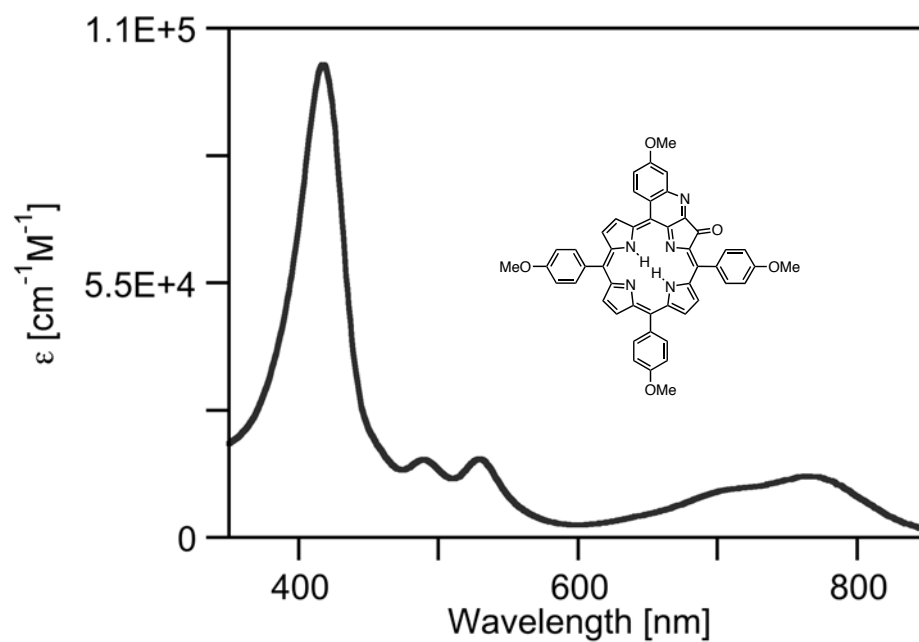


Figure S18. UV-vis spectrum (CH_2Cl_2) of **4b**.

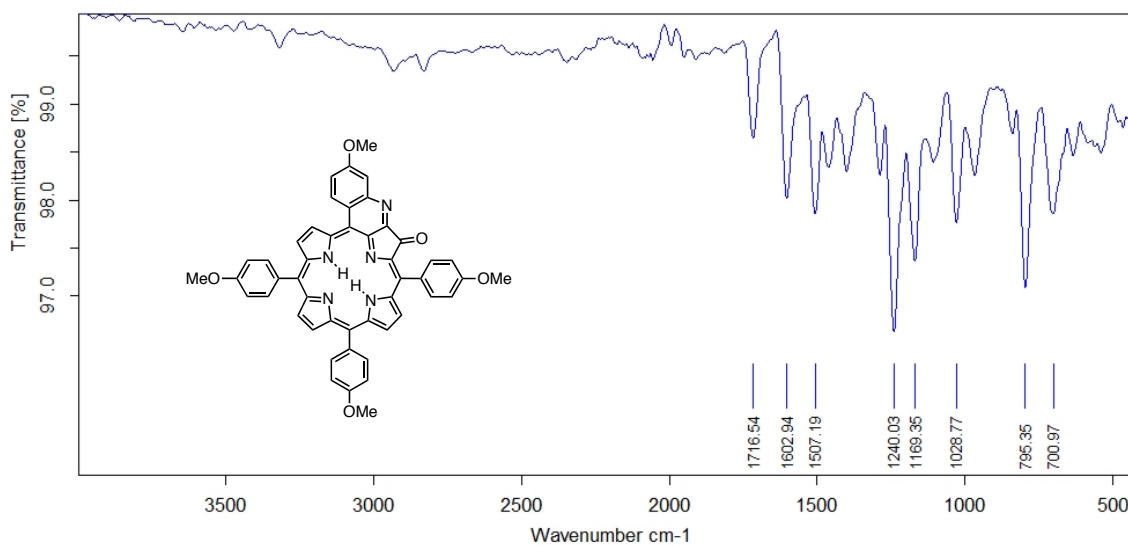


Figure S19. FT-IR spectrum (neat, diamond ATR) of **4b**.

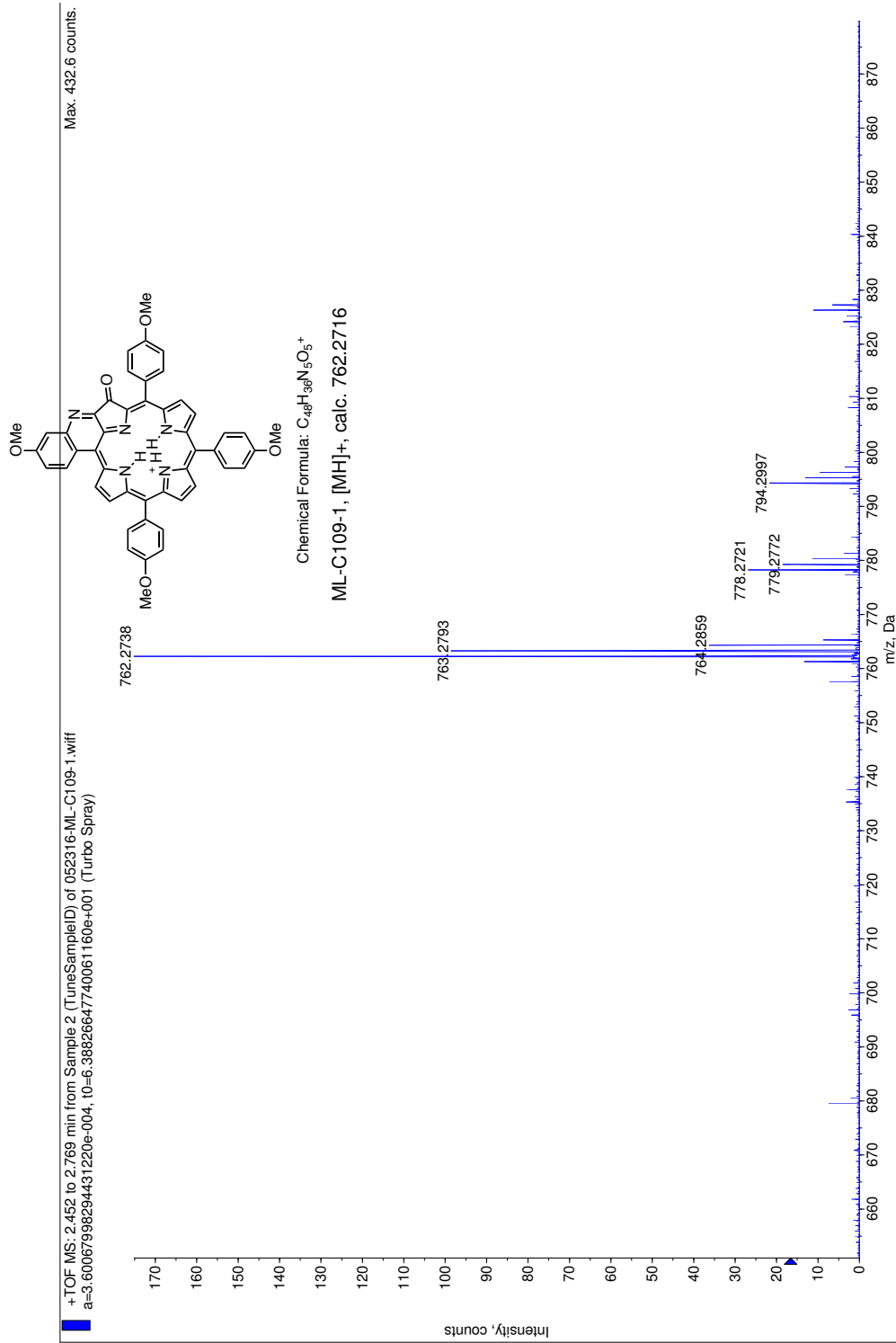


Figure S20. HR-MS (ESI^+ , 100% CH_3CN , TOF) of **4b**.

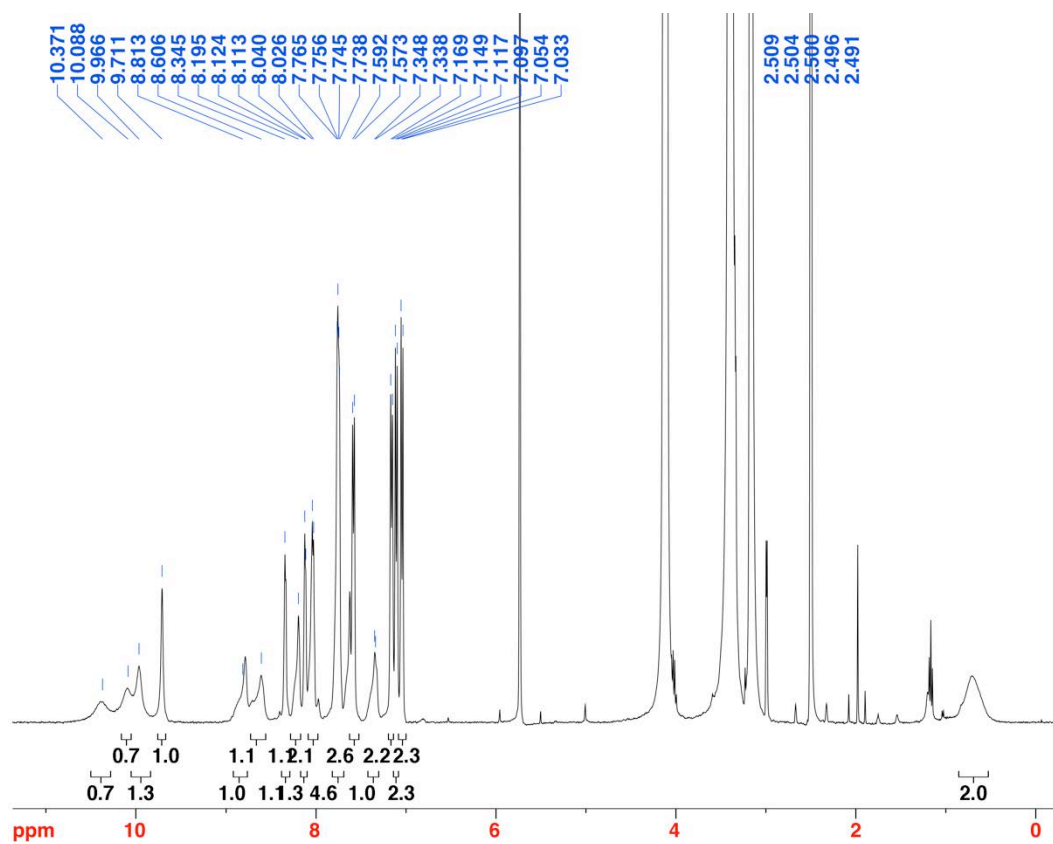
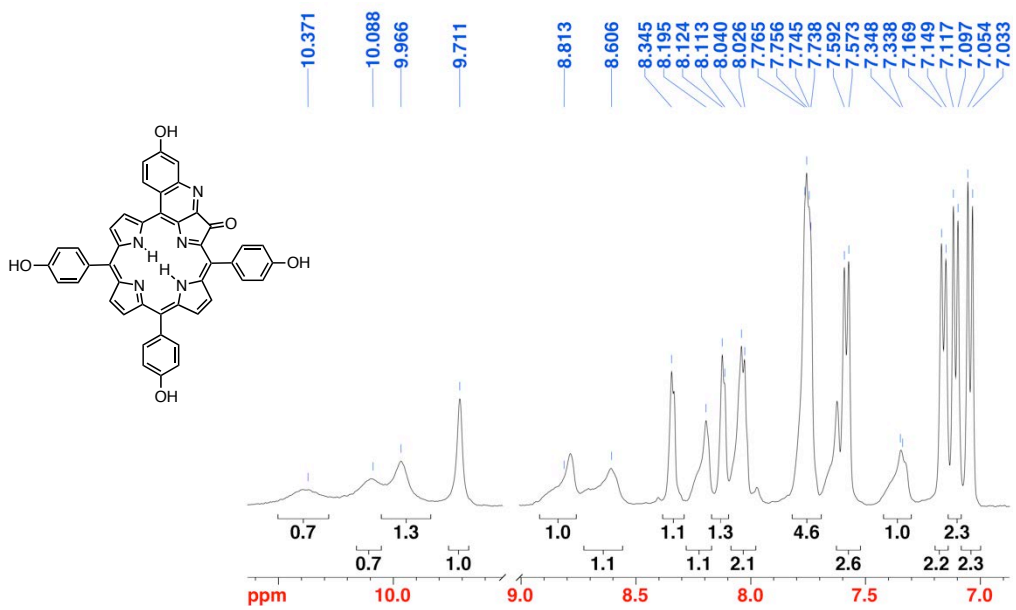


Figure S21. ¹H NMR spectrum (400 MHz, DMSO-d₆) of 4c.

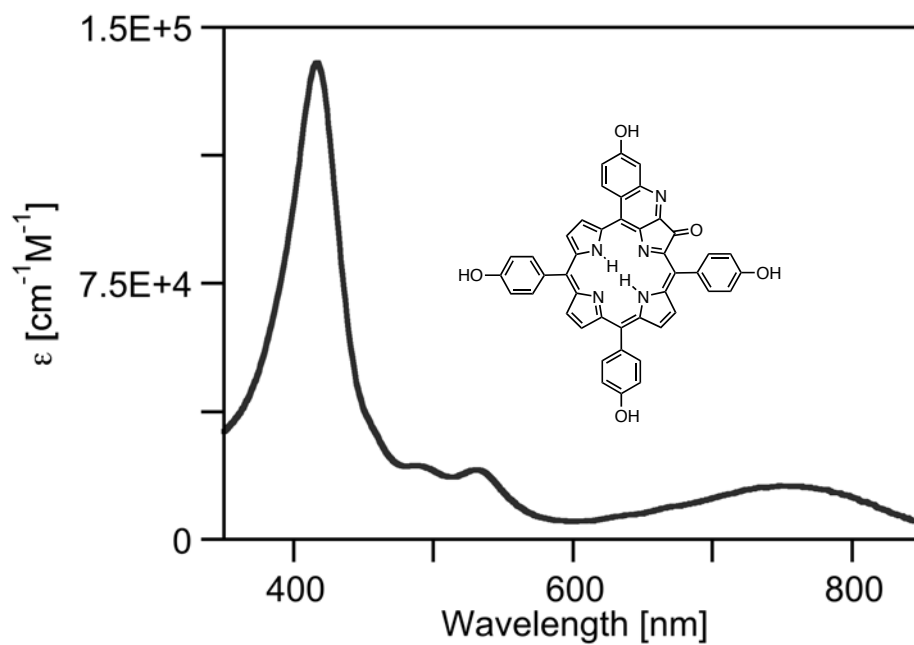


Figure S23. UV-vis spectrum (MeOH) of **4c**.

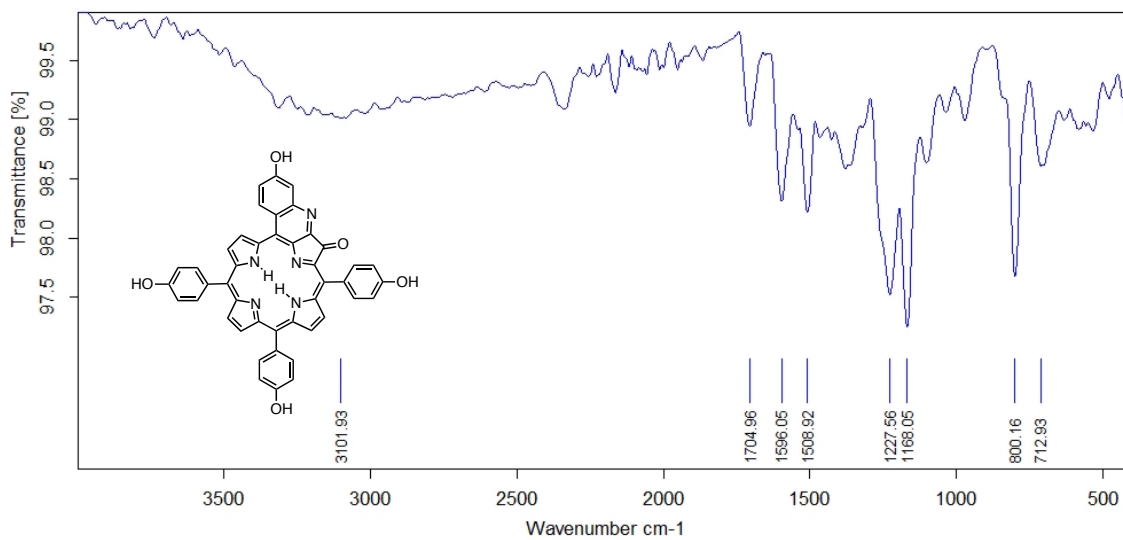


Figure S24. FT-IR spectrum (neat, diamond ATR) of **4c**.

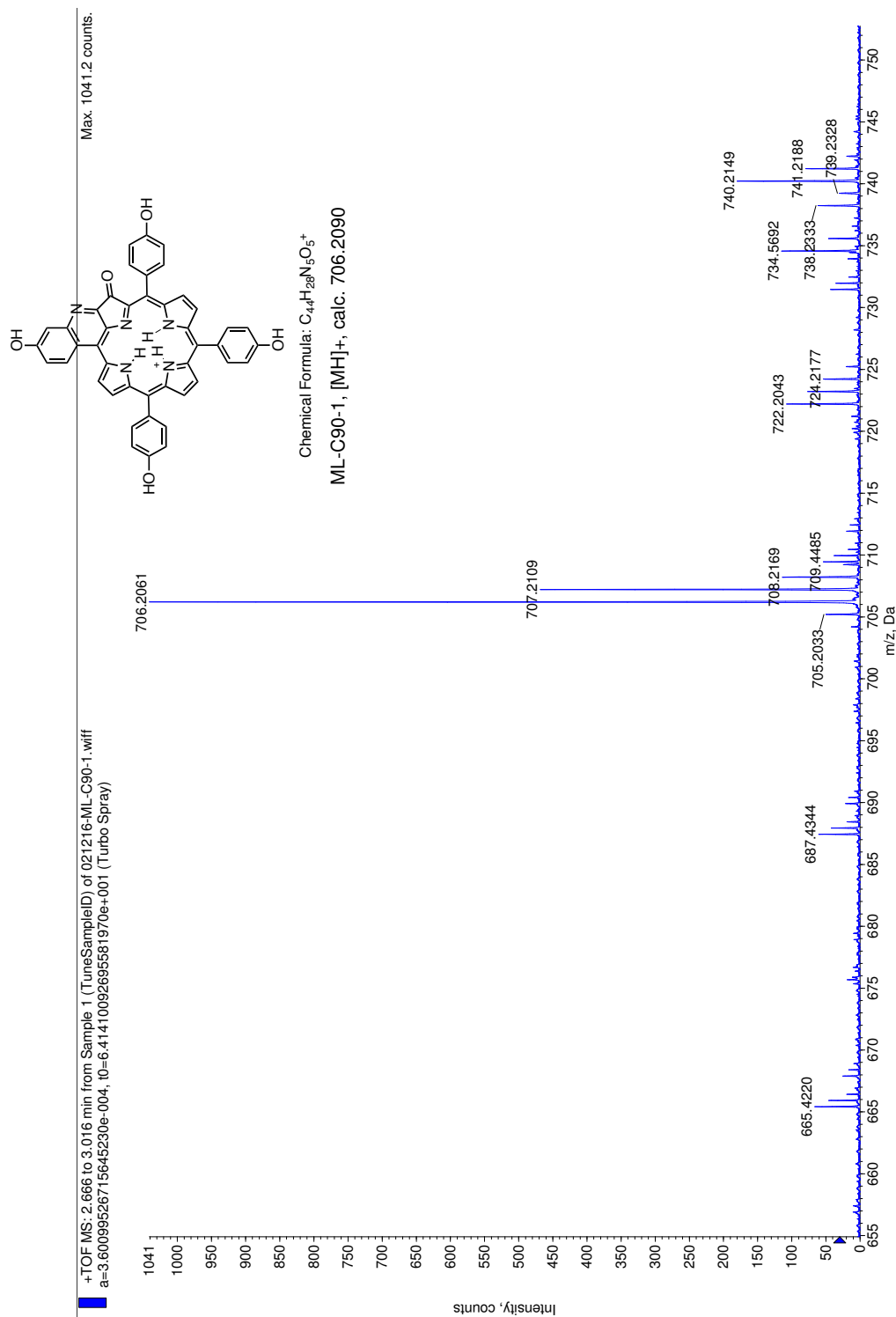


Figure S25. HR-MS (ESI^+ , 100% CH_3CN , TOF) of **4c**.

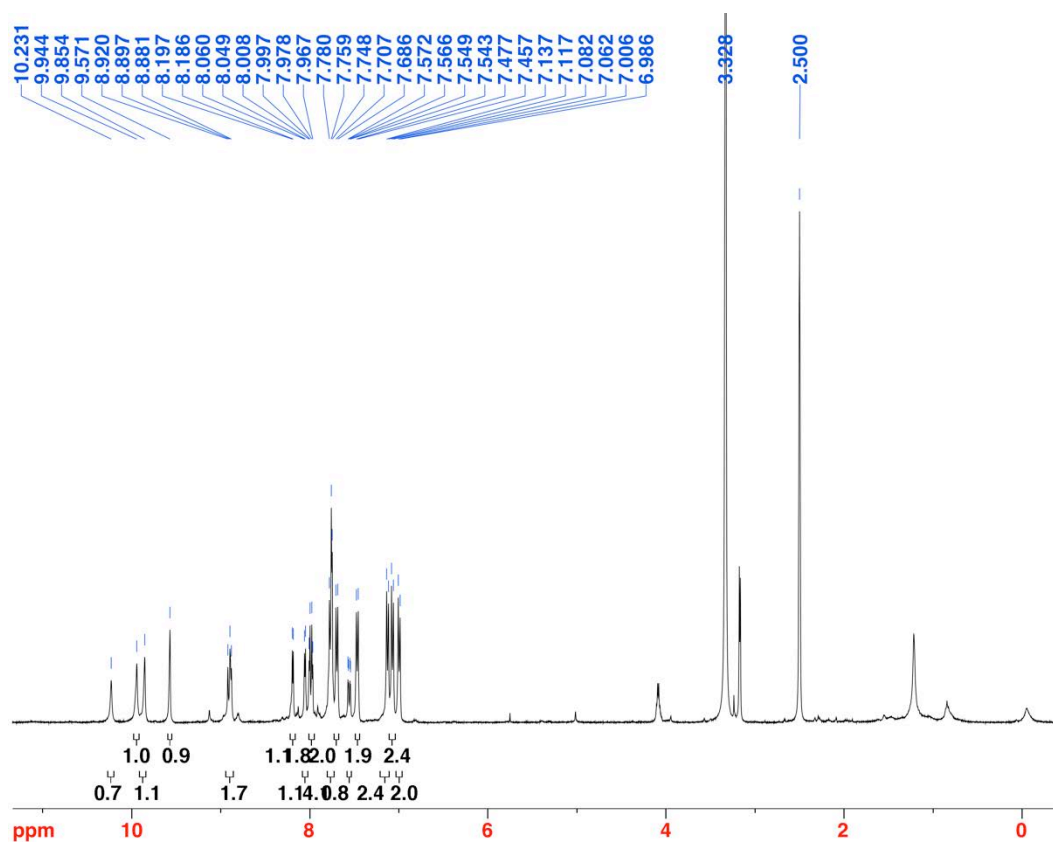
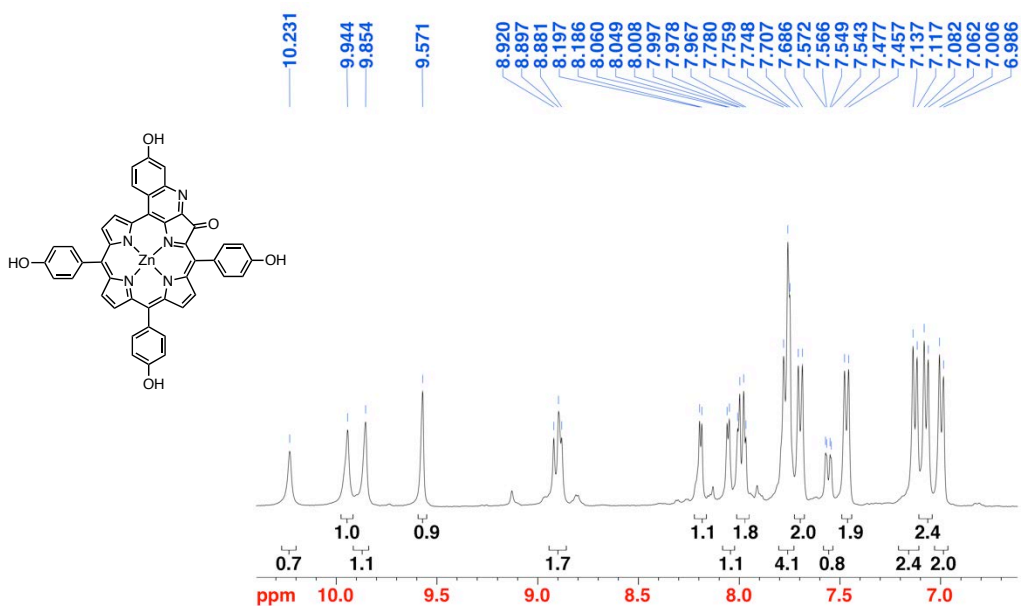


Figure S26. ¹H NMR spectrum (400 MHz, DMSO-d₆) of **4c^{Zn}**.

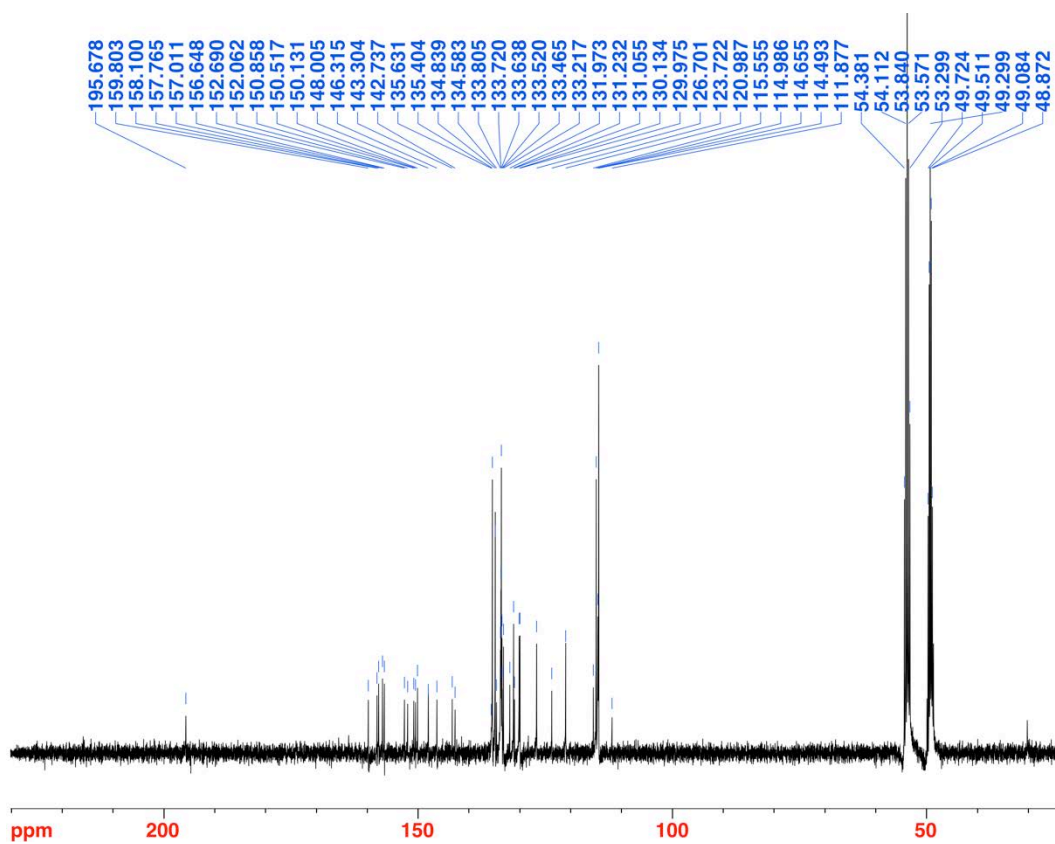
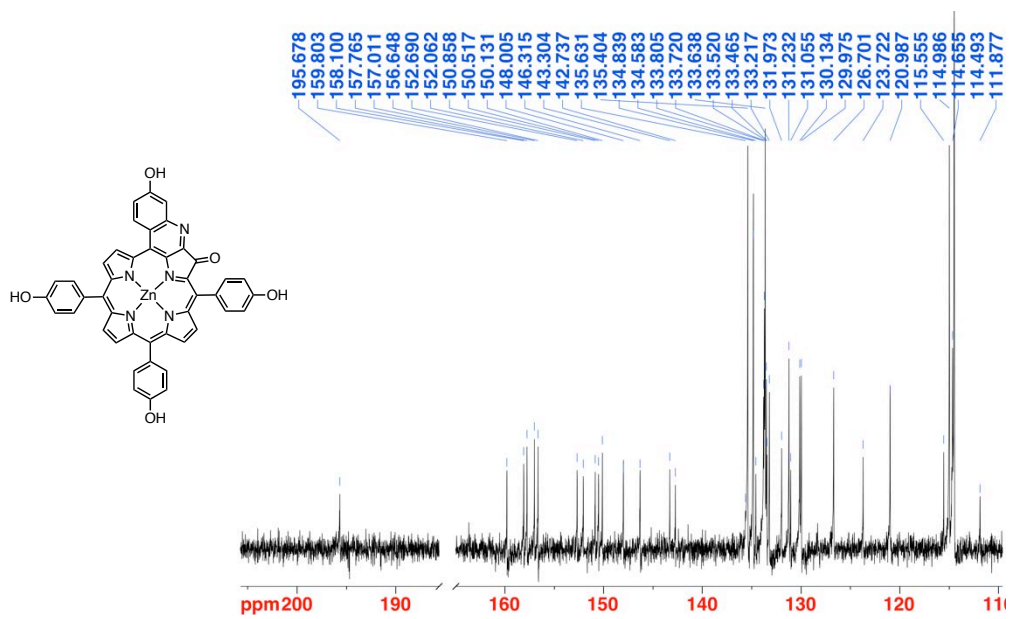


Figure S27. ^{13}C NMR spectrum (100 MHz, $CD_2Cl_2/10\%$ MeOD) of $4c^{Zn}$.

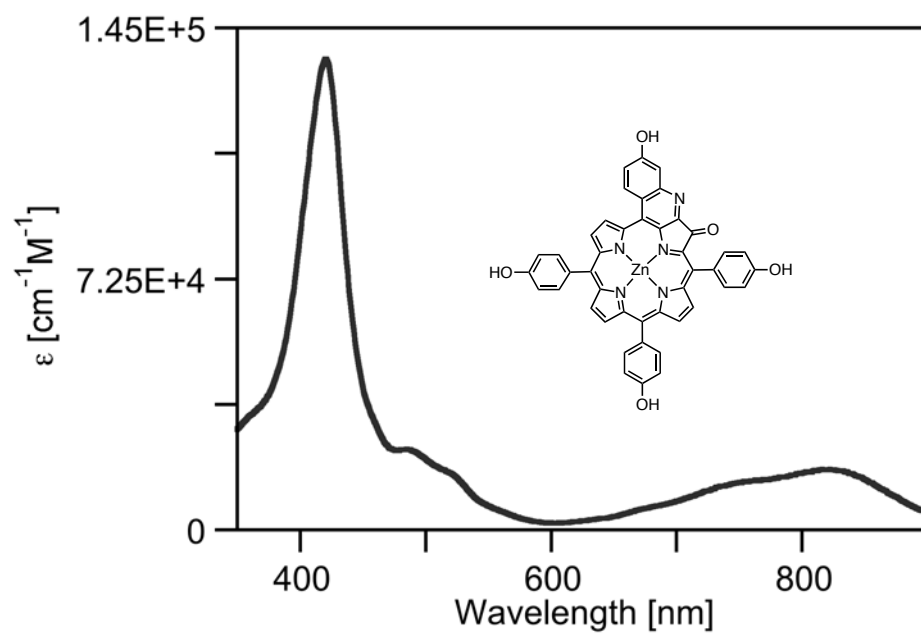


Figure S28. UV-vis spectrum (MeOH) of **4c^{Zn}**.

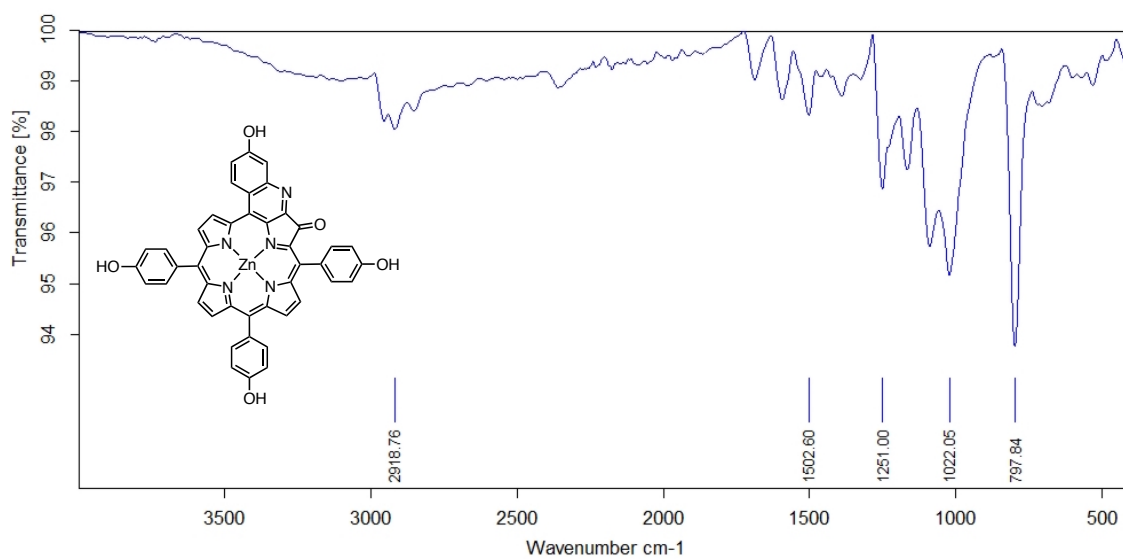


Figure S29. FT-IR spectrum (neat, diamond ATR) of **4c^{Zn}**.

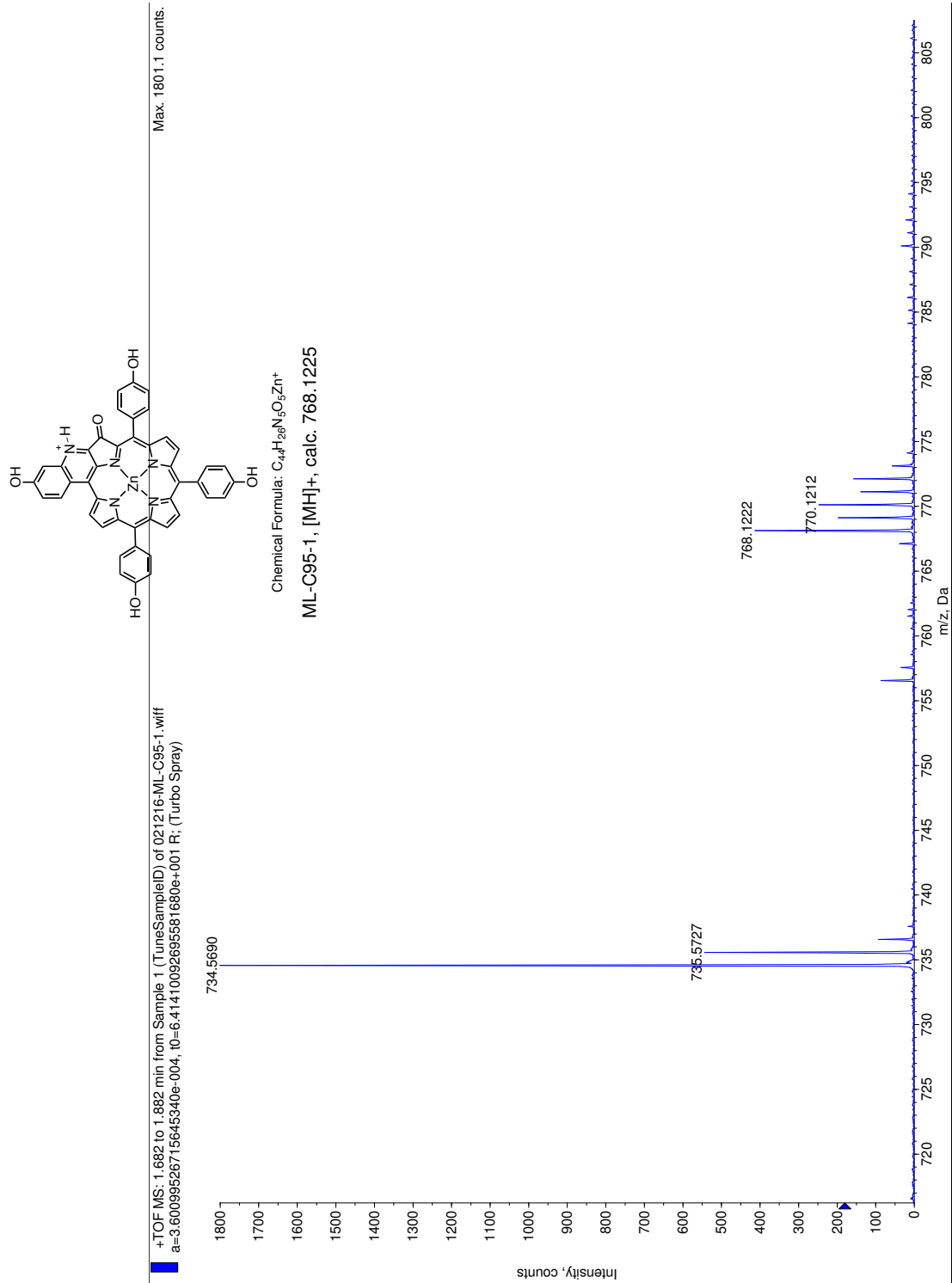


Figure S30. HR-MS (ESI⁺, 100% CH₃CN, TOF) of **4c**^{Zn}.

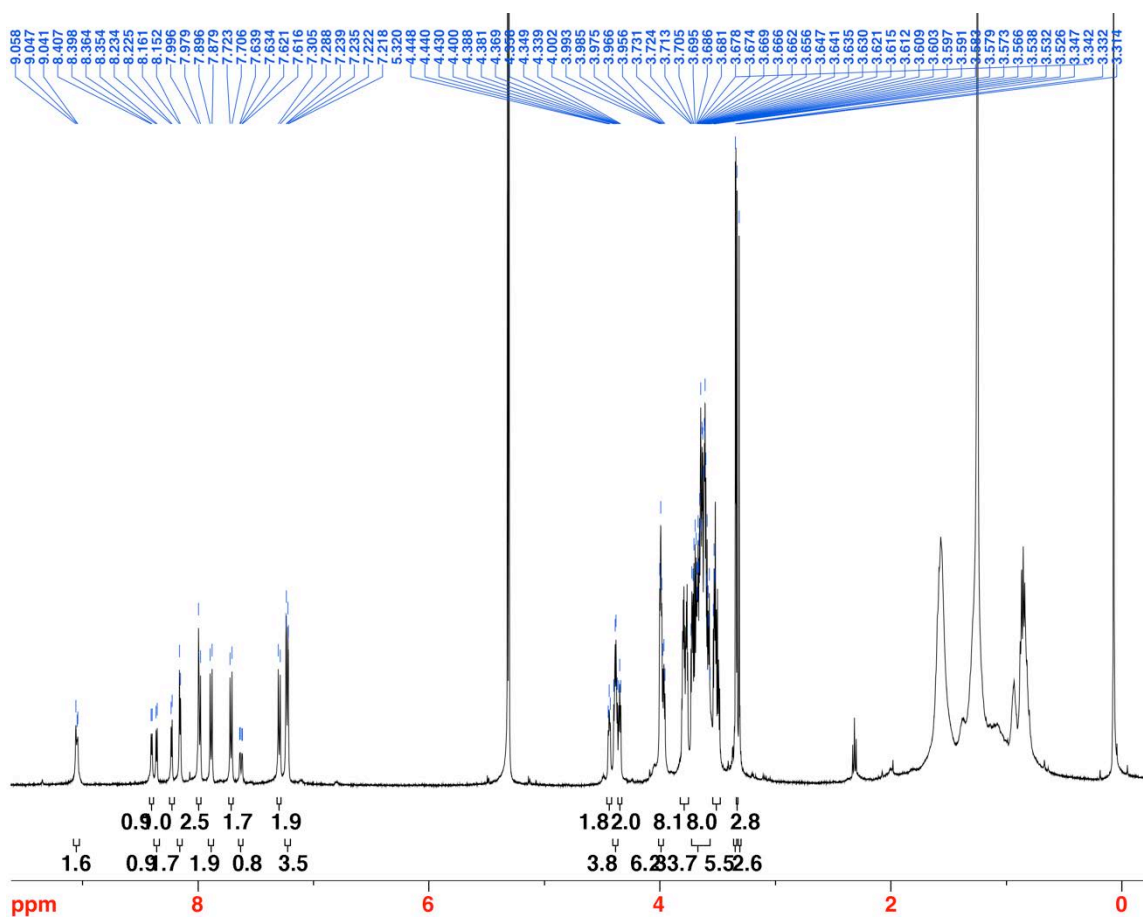
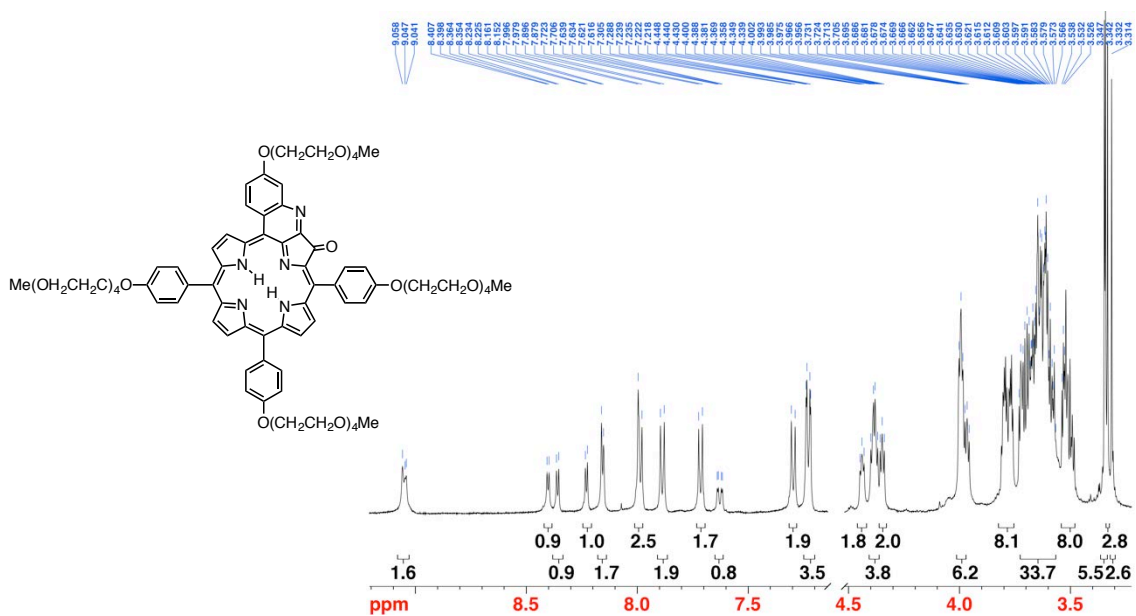


Figure S31. ¹H NMR spectrum (500 MHz, CD₂Cl₂) of 4d.

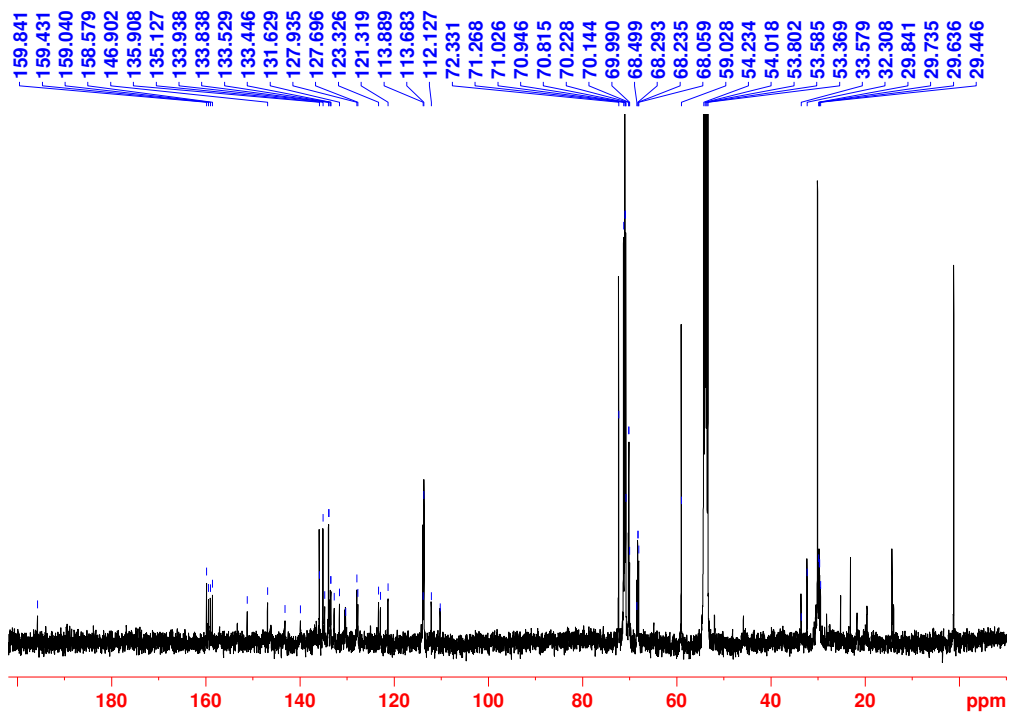
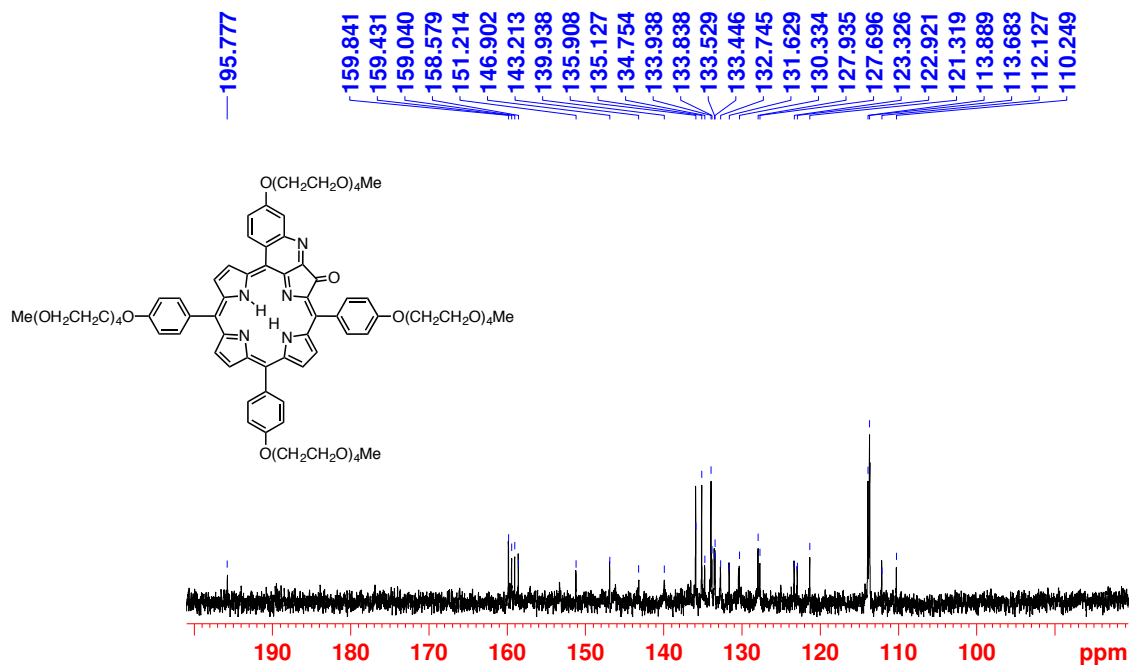


Figure S32. ¹³C NMR spectrum (125 MHz, CD₂Cl₂) of **4d**.

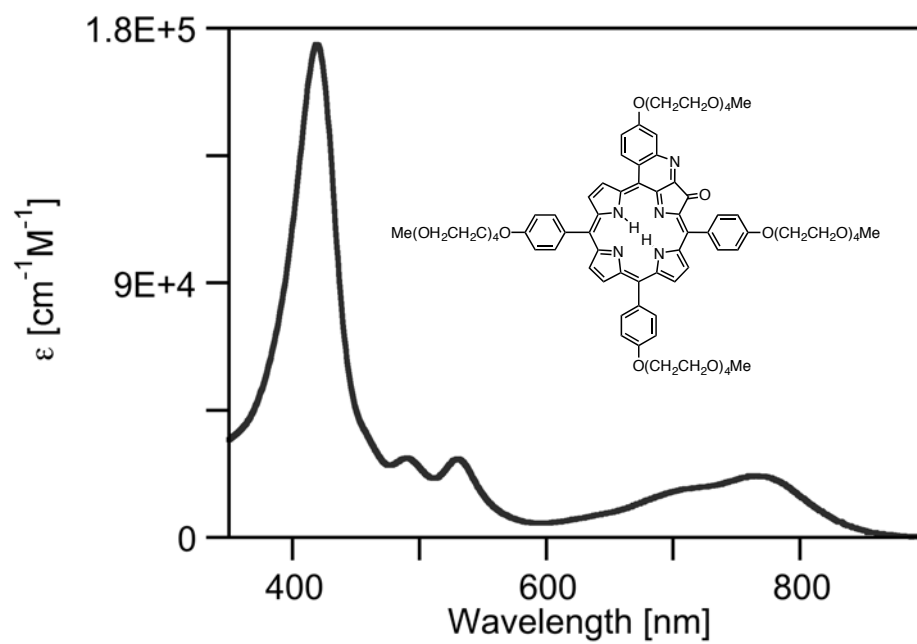


Figure S33. UV-vis spectrum (CH_2Cl_2) of **4d**.

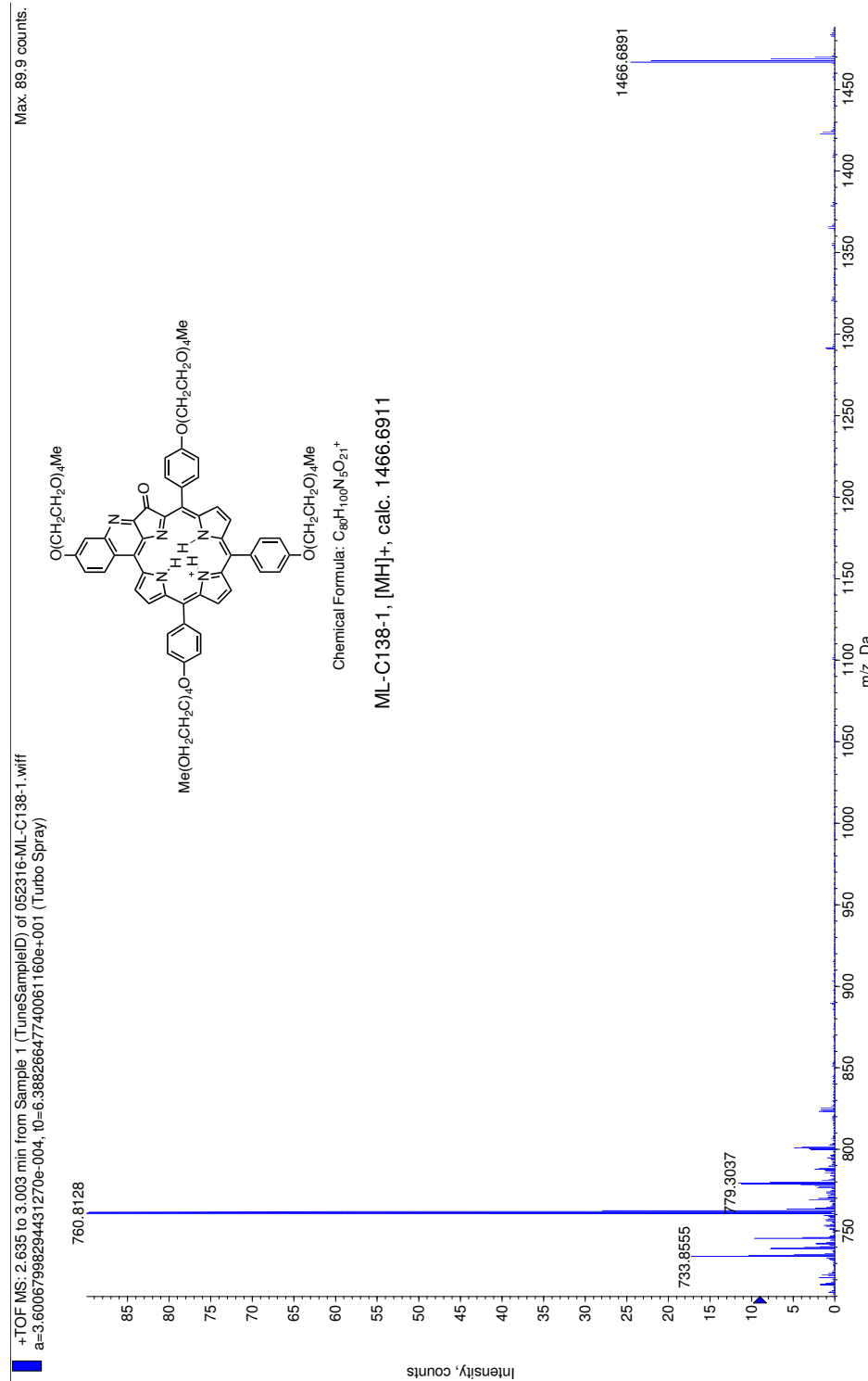


Figure S34. HR-MS (ESI⁺, 100% CH₃CN, TOF) of **4d**.

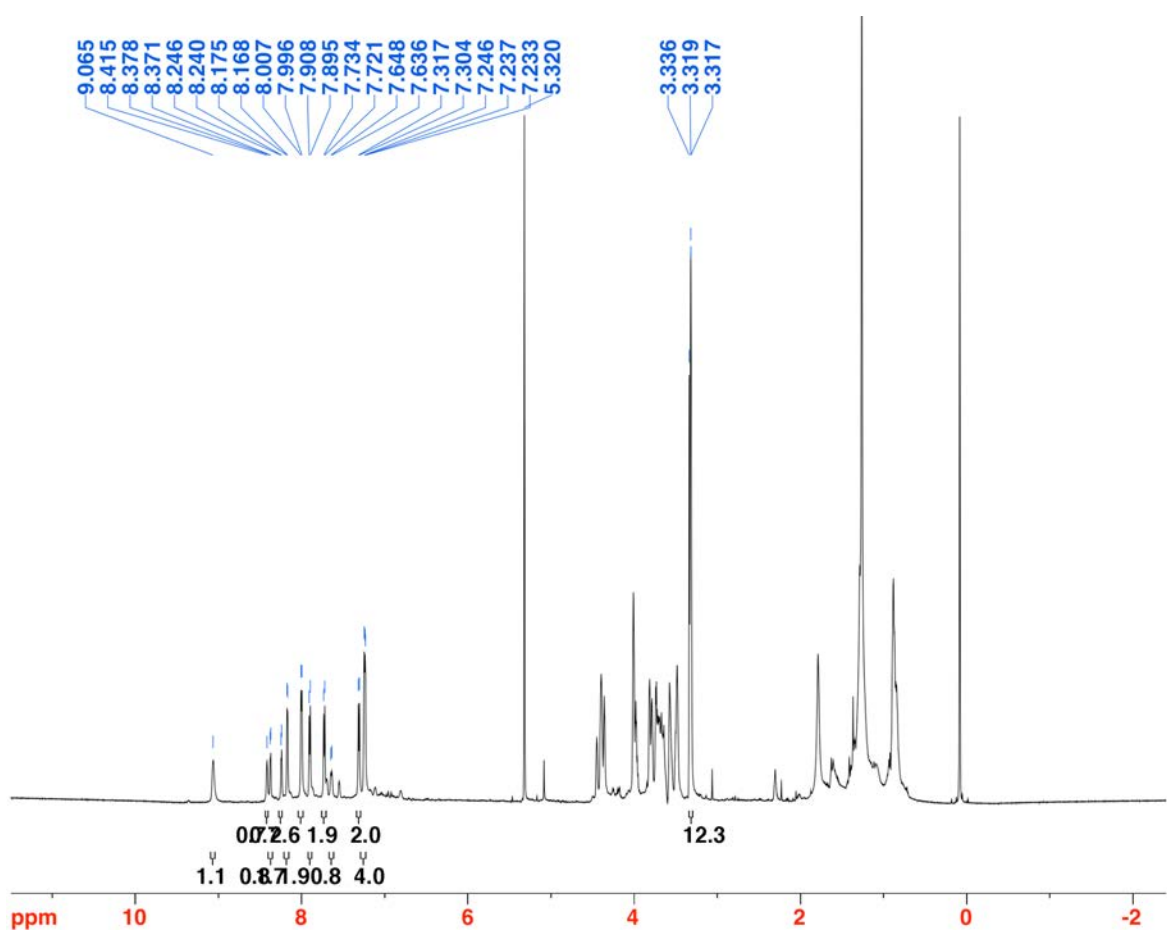
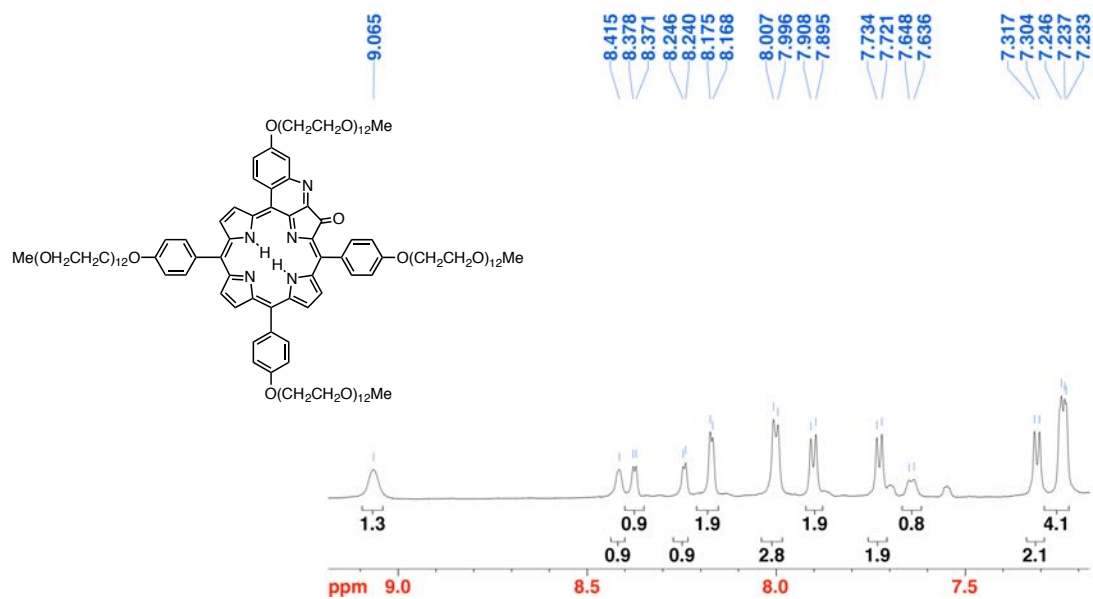


Figure S35. ^1H NMR spectrum (400 MHz, CD_2Cl_2) of **4e**.

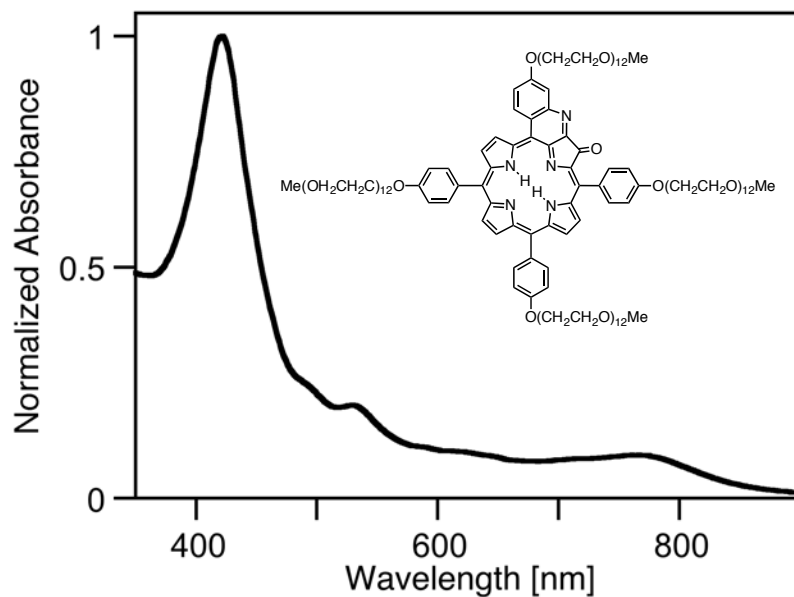


Figure S36. UV-vis spectrum (H_2O) of **4e**.

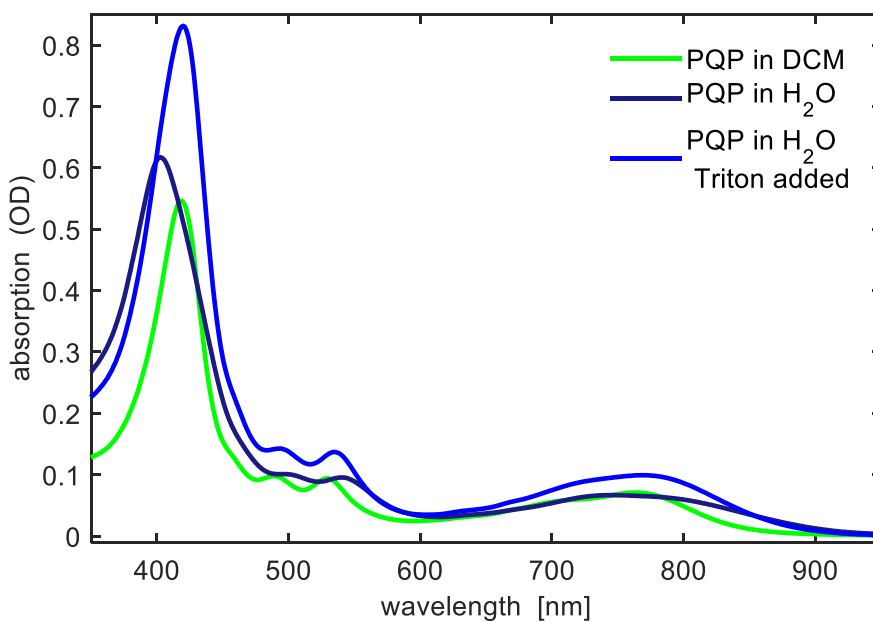


Figure S37. Absorption spectra of **4e** (PQP) in CH_2Cl_2 , H_2O and H_2O -Triton-X solutions. The change of the absorption spectrum of **4e** in H_2O after adding triton indicates that **4e** is somewhat aggregated in pure aqueous solution.

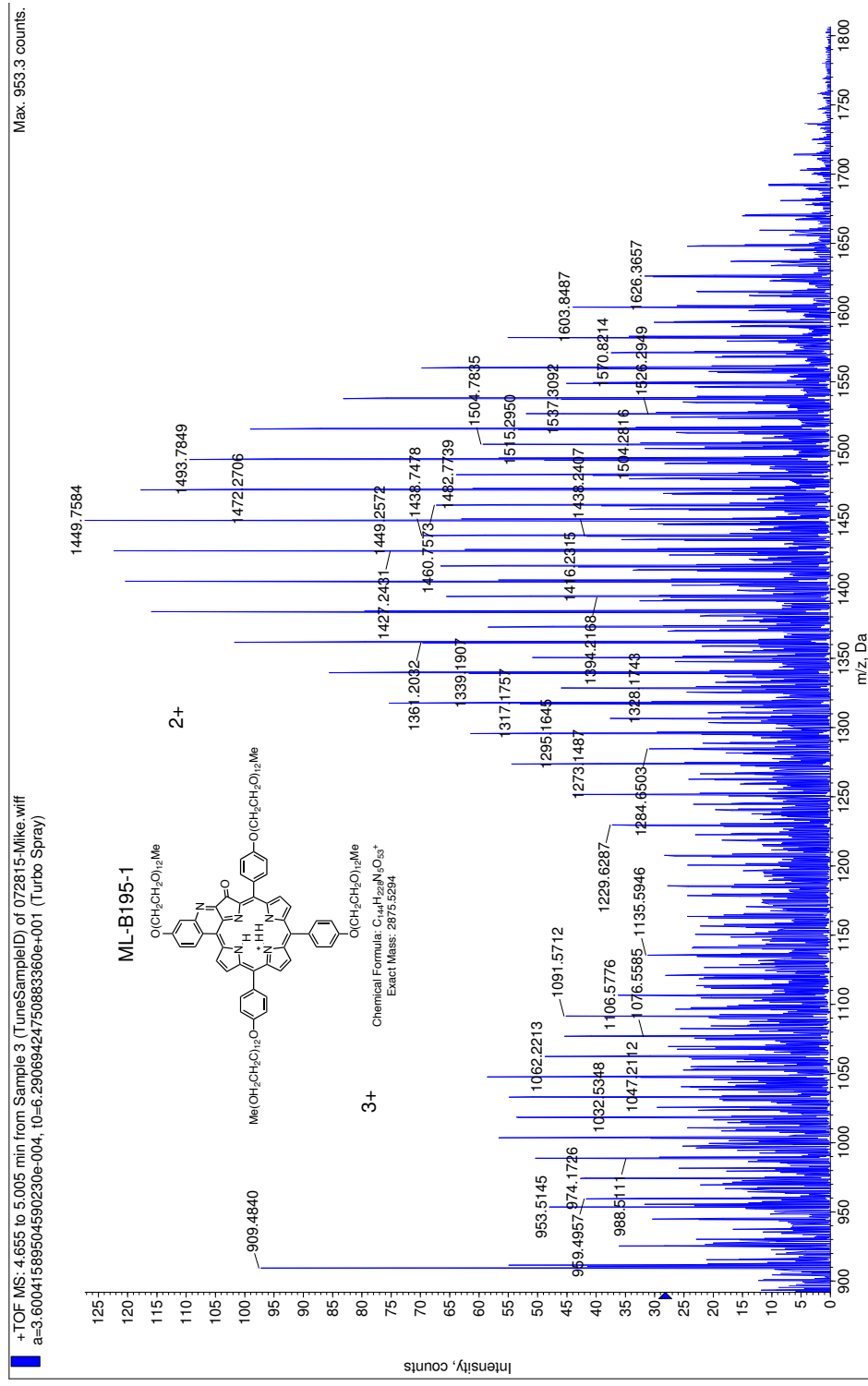


Figure S38. HR-MS (ESI⁺, 100% CH₃CN, TOF) of 4e.

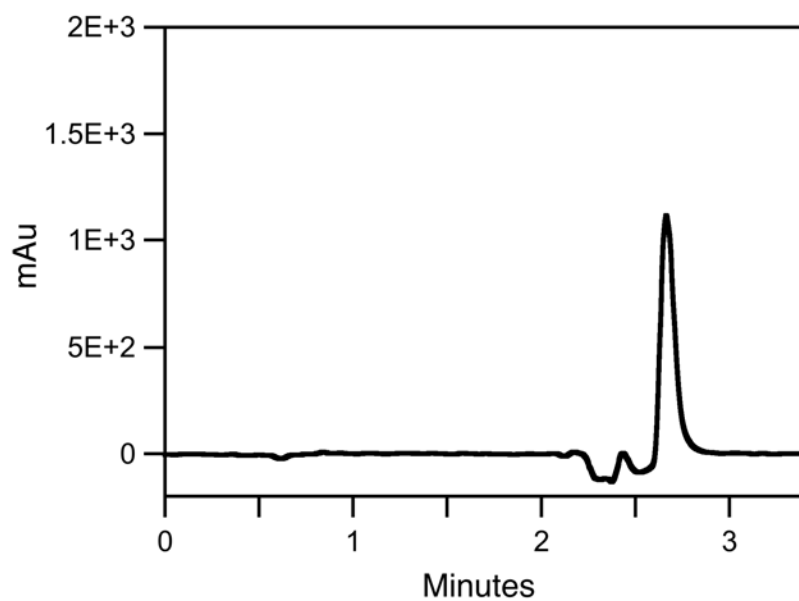


Figure S39. HPLC trace, UV-vis detector, of **4e** (silica, mobile phase: CH₂Cl₂/10% MeOH).

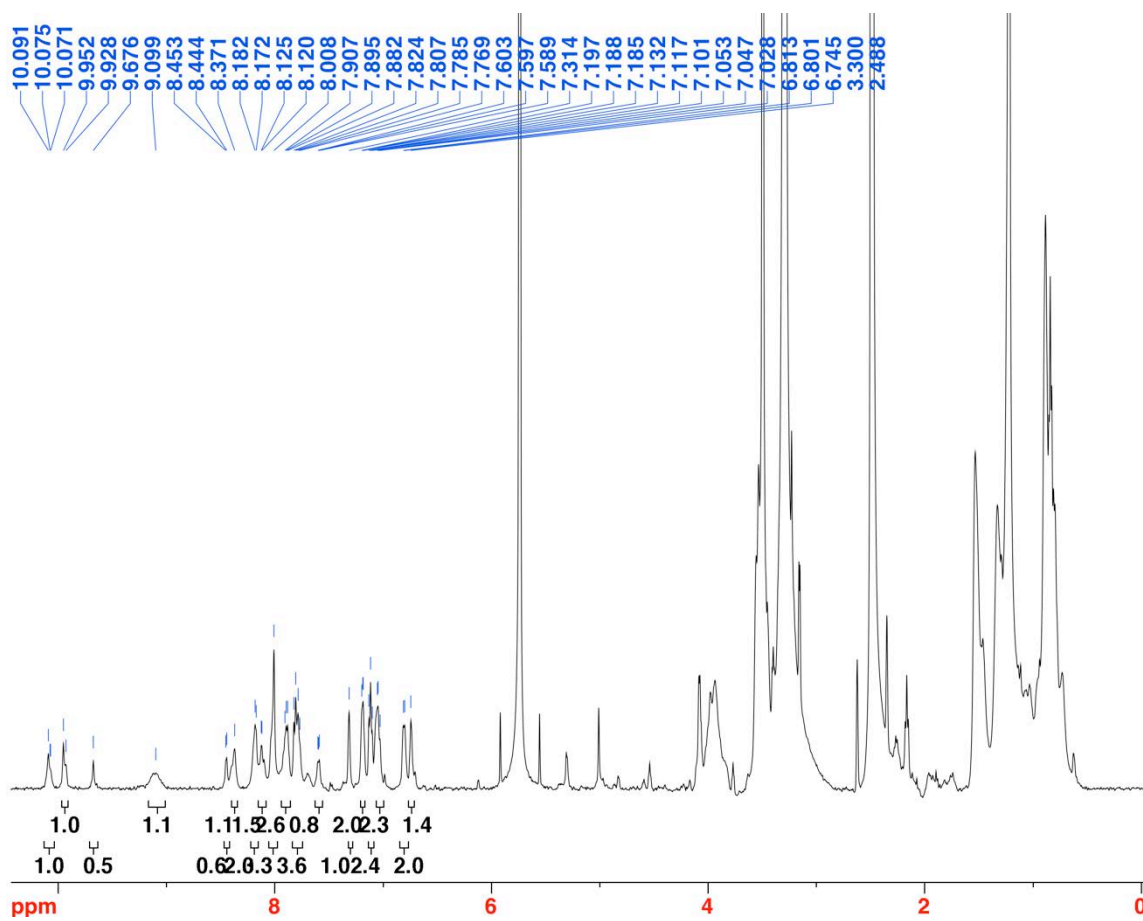
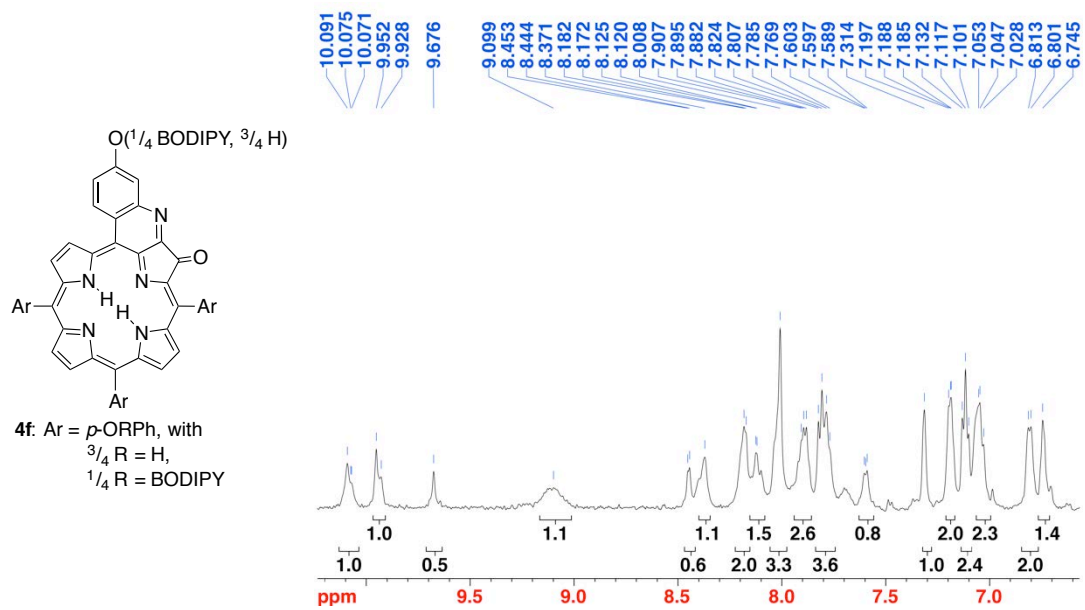


Figure S40. ¹H NMR spectrum (500 MHz, DMSO-d₆) of **4f**.

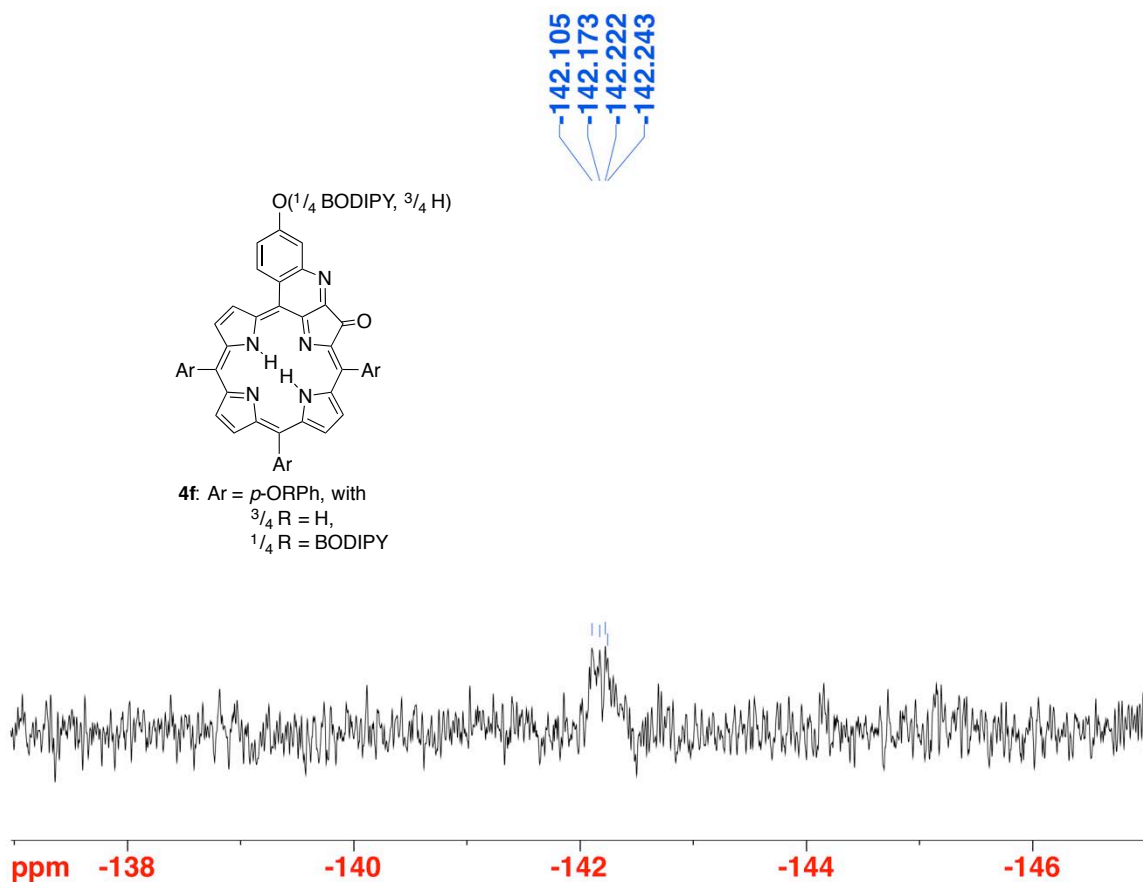


Figure S41. ^{19}F NMR spectrum (470 MHz, DMSO- d_6) of **4f**.

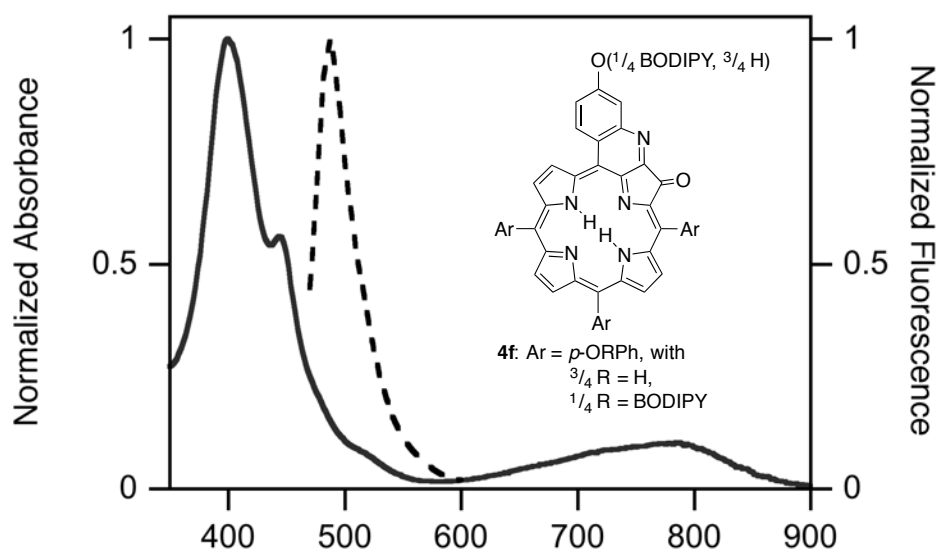


Figure S42. UV-vis and Fluorescence emission spectrum (MeOH, $\lambda_{\text{excitation}} = 441 \text{ nm}$) of **4f**.

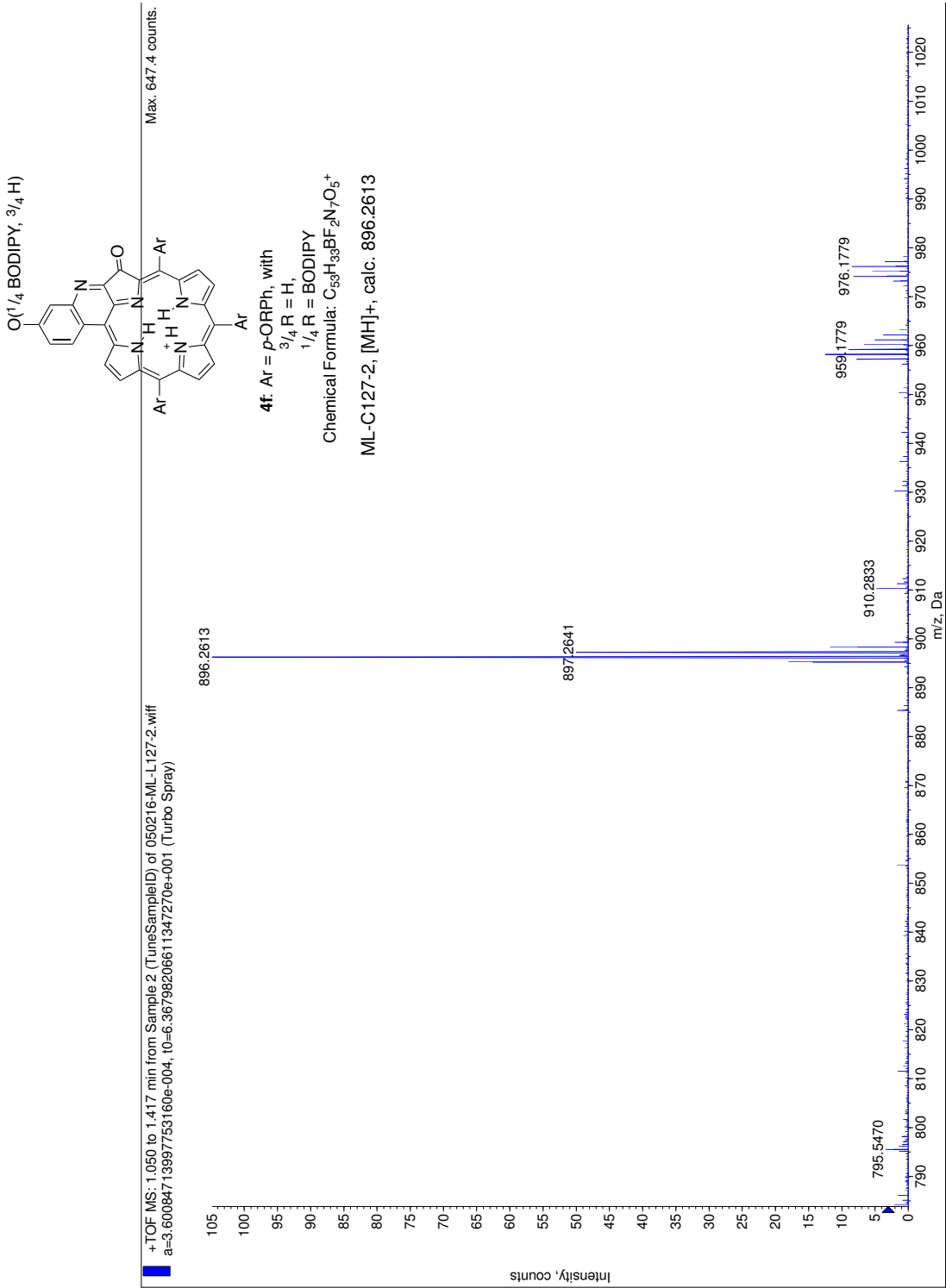


Figure S43. HR-MS (ESI+, 100% CH₃CN, TOF) of 4f.

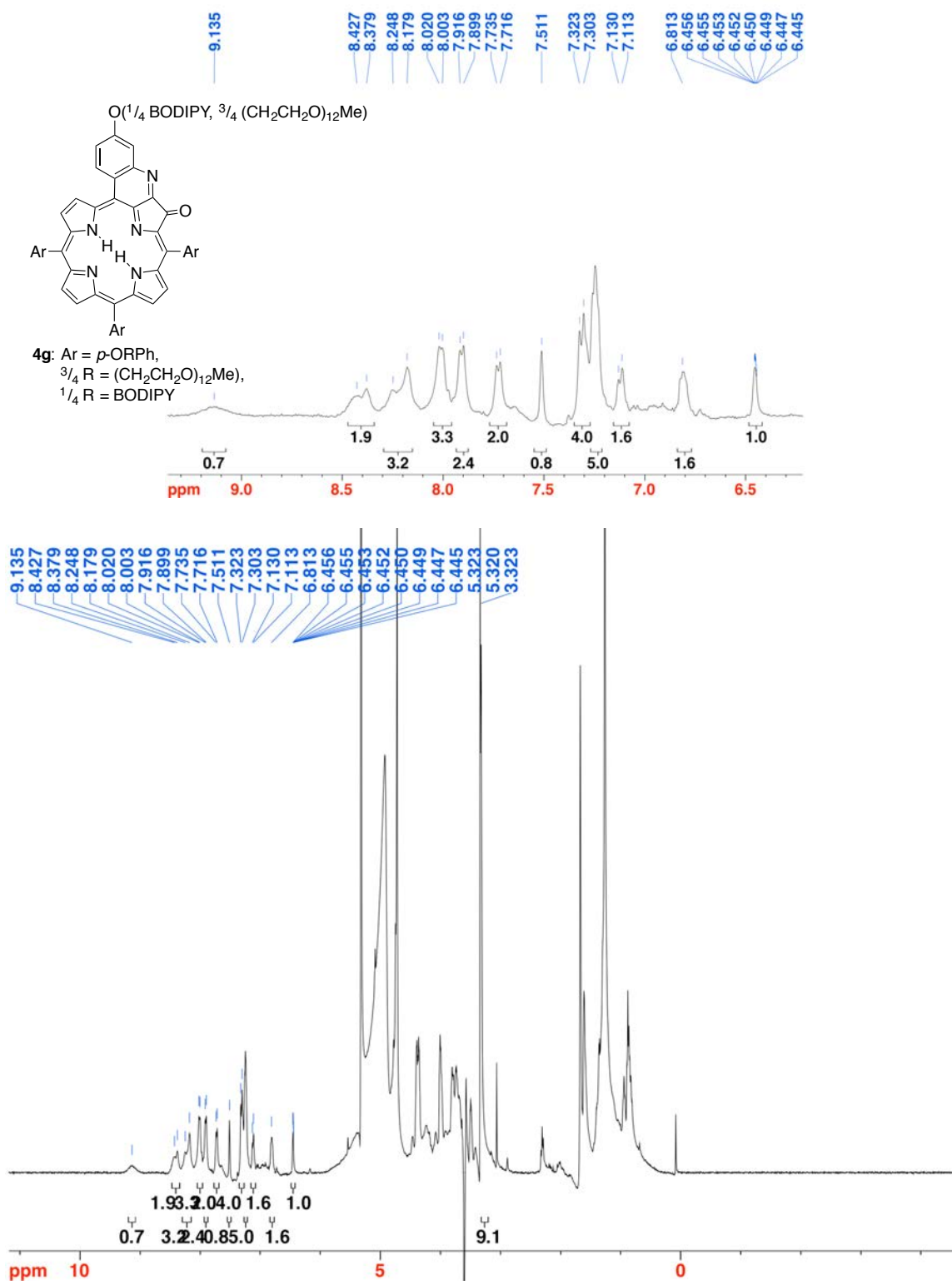


Figure S44. ¹H NMR spectrum (400 MHz, CD₂Cl₂, pre-saturated at 3.6 ppm) of **4g**.

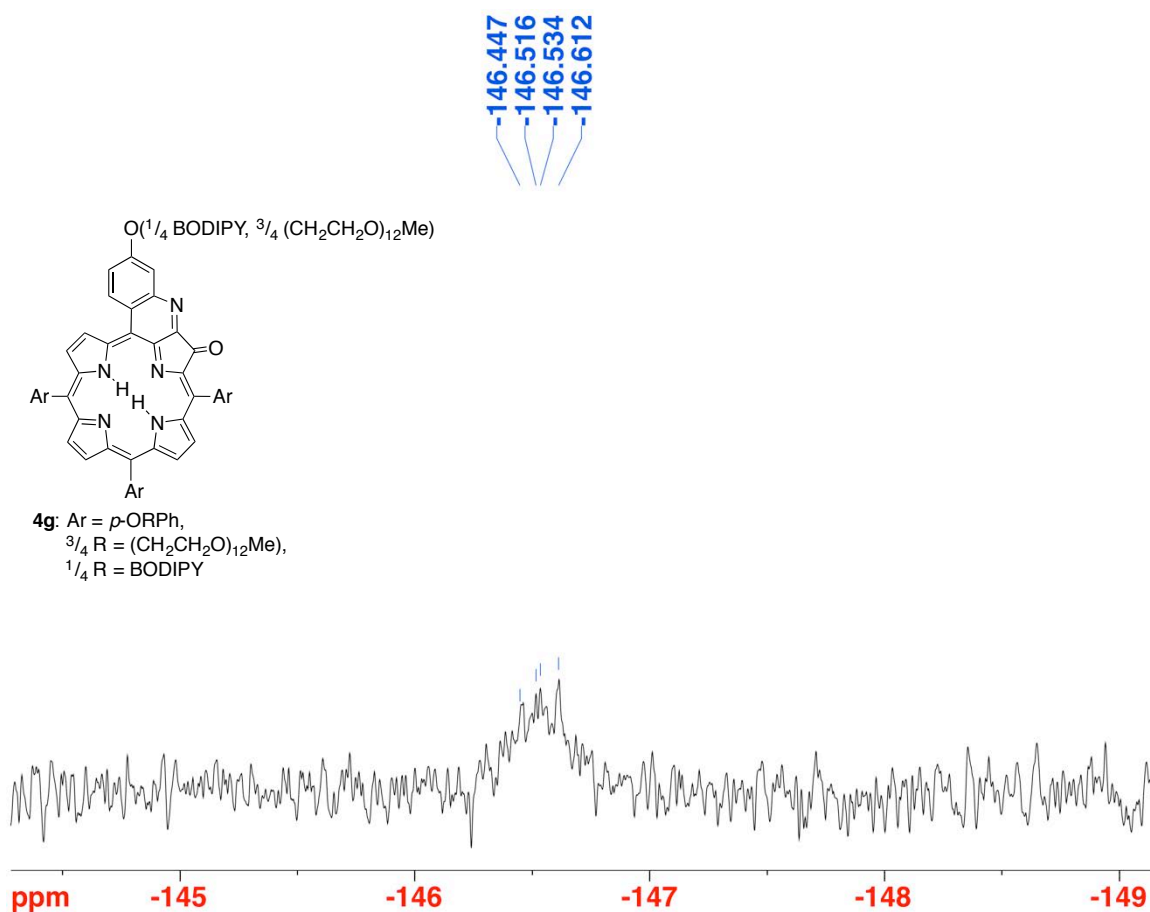


Figure S45. ¹⁹F NMR spectrum (376 MHz, CD₂Cl₂) of **4g**.

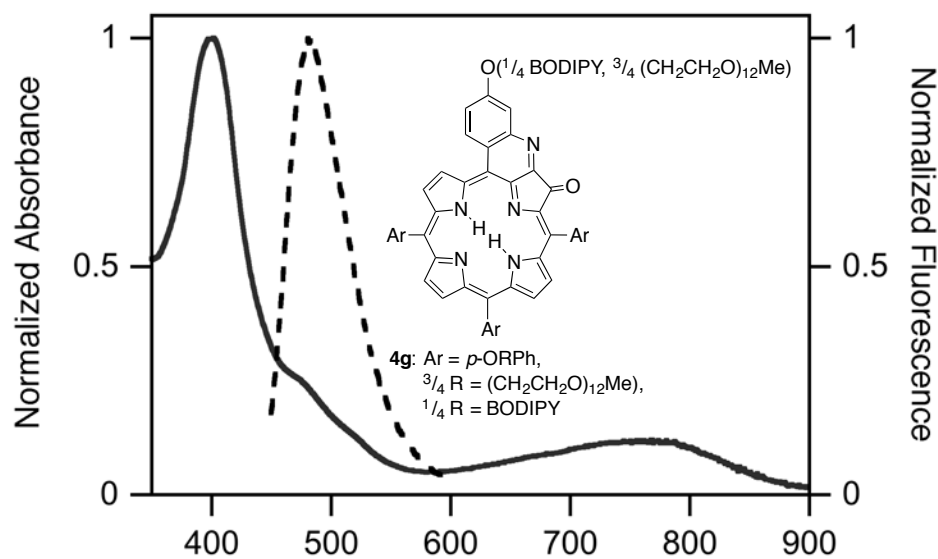
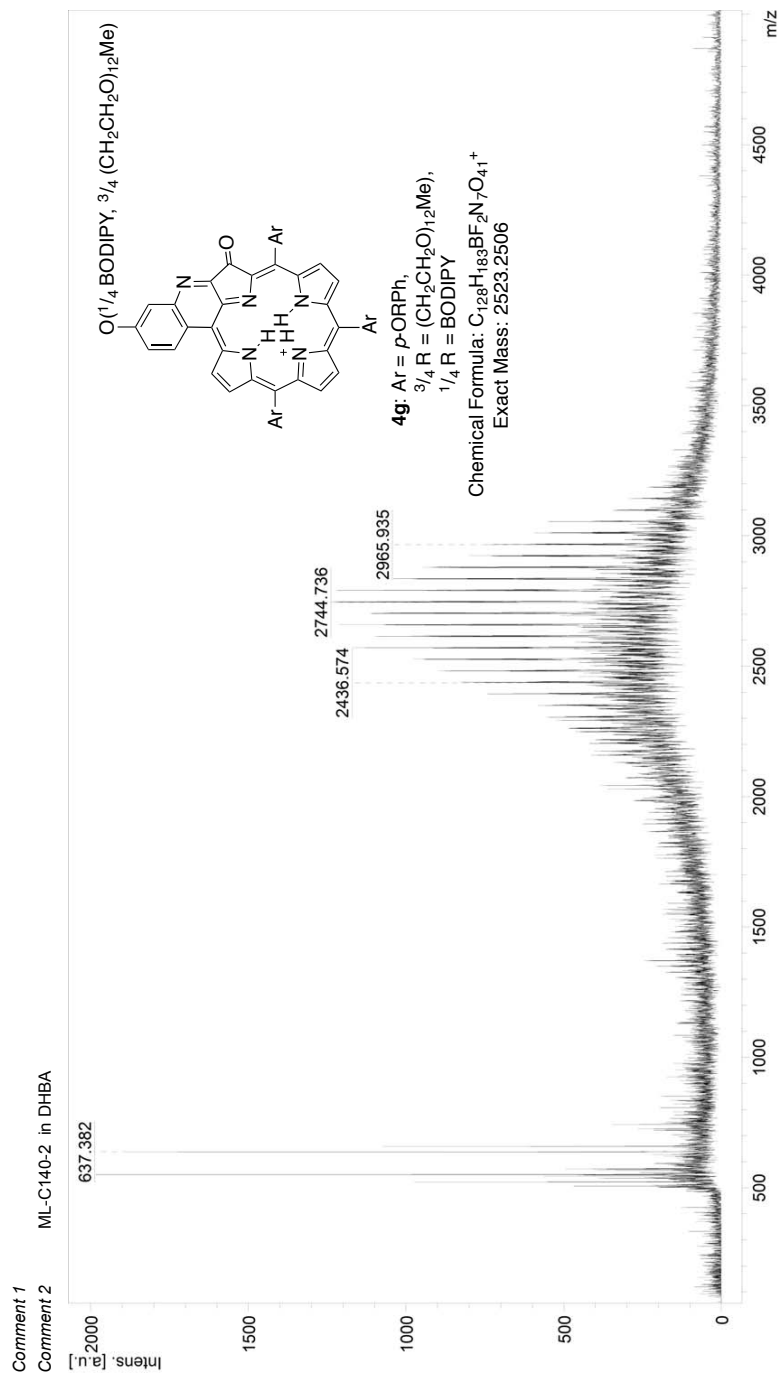


Figure S46. UV-vis and Fluorescence emission spectrum (MeOH, $\lambda_{\text{excitation}} = 441$ nm) of **4g**.

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

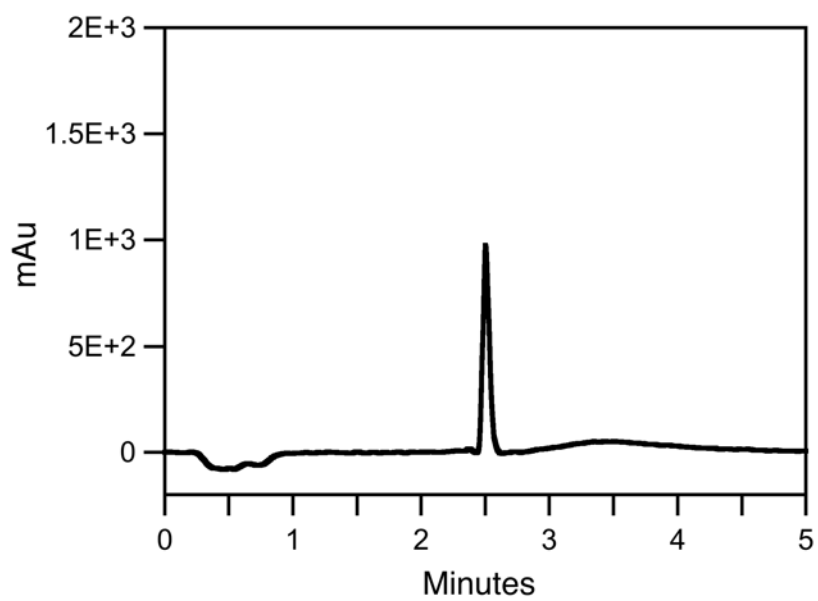


Figure S48. HPLC trace, UV-vis detector, of **4g** (silica, mobile phase: CH₂Cl₂/5% MeOH).

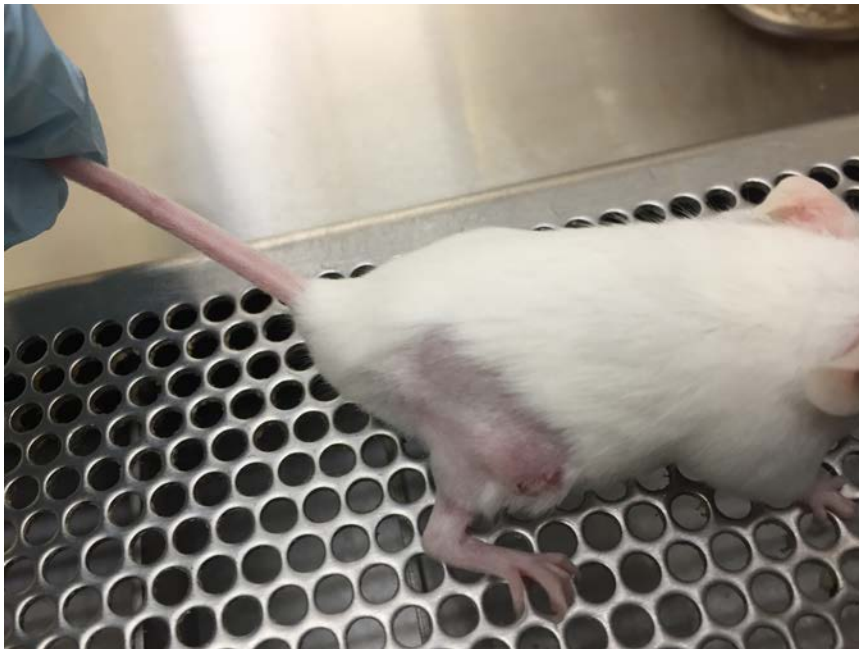


Figure S49. A mouse tumor before injection of **4e**.

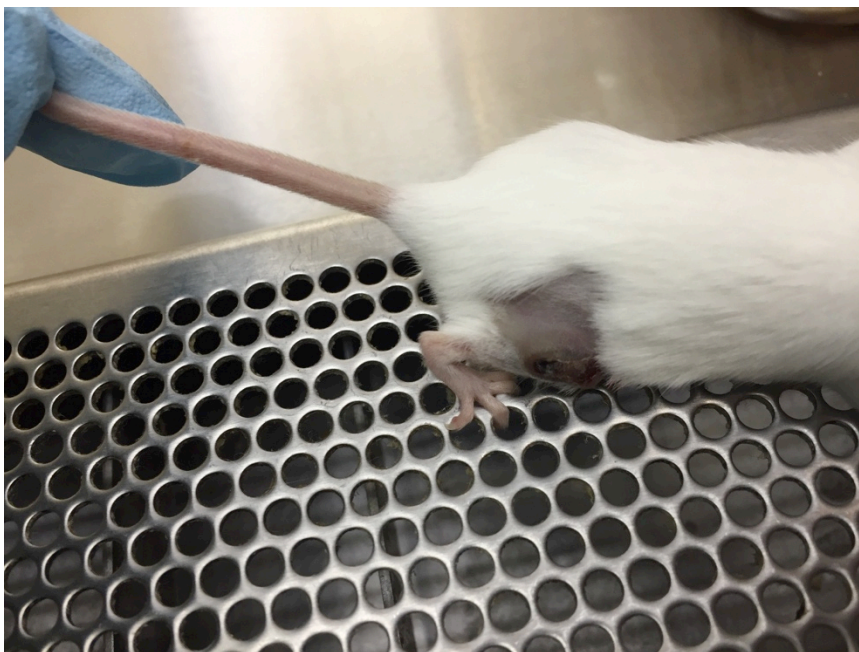


Figure S50. A mouse tumor 48 h after injection of 100 μL of a 33 mM solution of **4e** in PBS, showing the dark brown-stained tumor site.

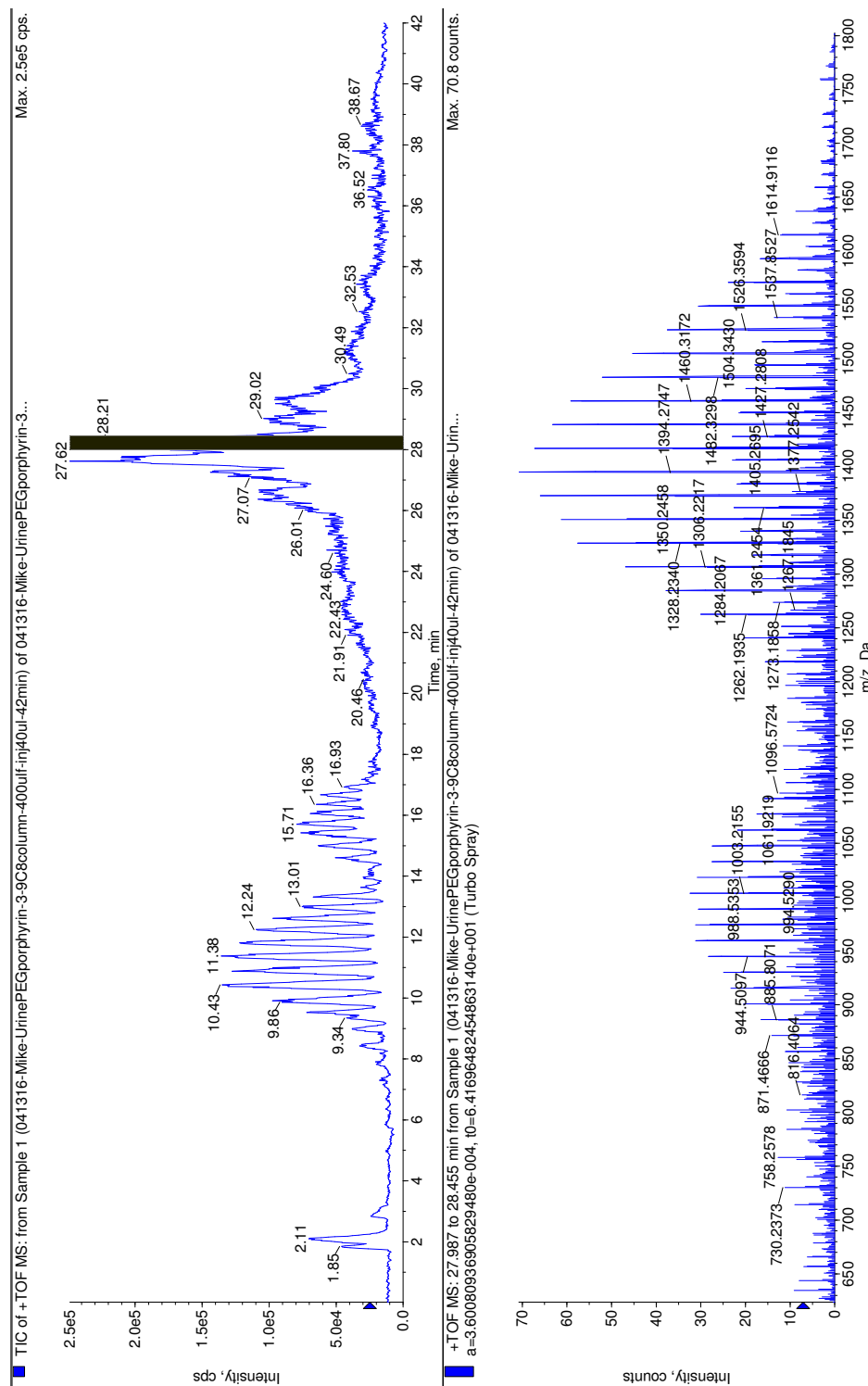


Figure S51. LC-MS of mouse urine extract (CH_2Cl_2), obtained after injection of **4e**.

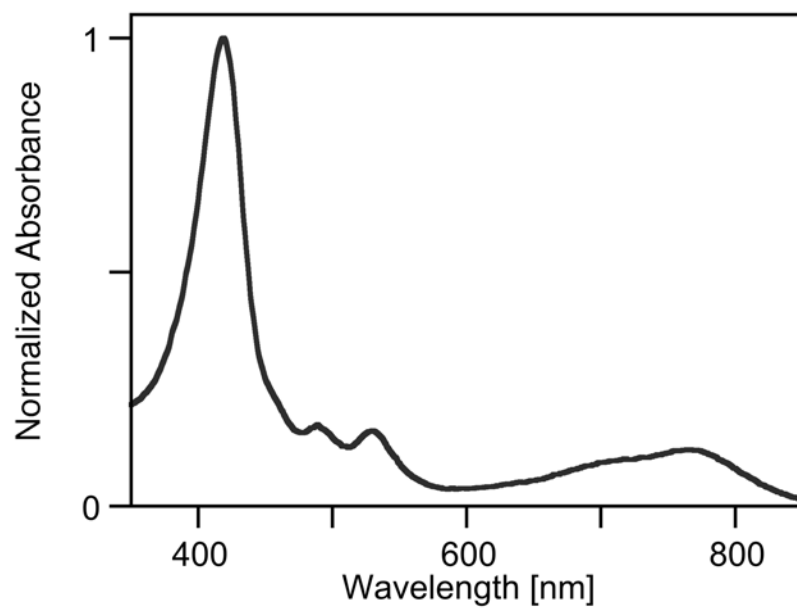


Figure S52. UV-vis spectrum (CH_2Cl_2) of mouse (diluted) urine obtained after injection of **4e**.