Tumor-Targeting Photosensitisers for One- and Two-photon Activated Photodynamic Therapy

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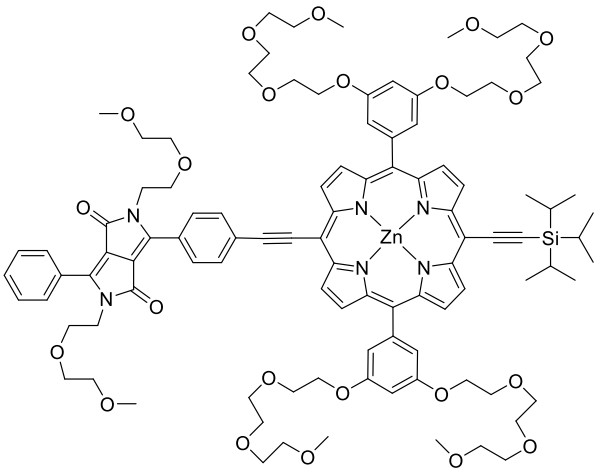
Supporting information



DPP-ZnP

Scheme S 1. Chemical structure of the PS **DPP-ZnP**

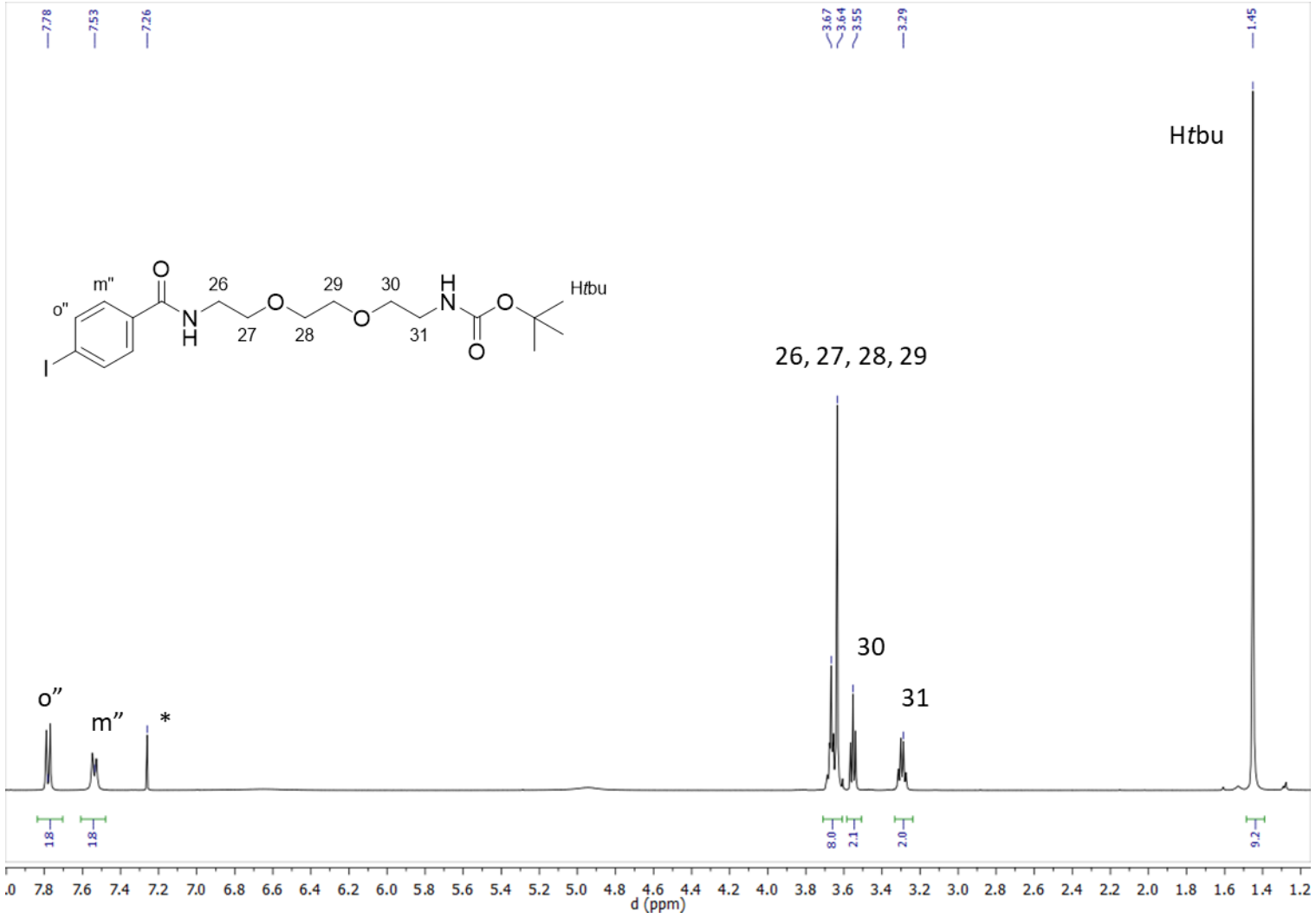


Figure S 1. ^{1}H NMR ($CDCl_3$, 400 MHz, 333 K) spectrum of **4**

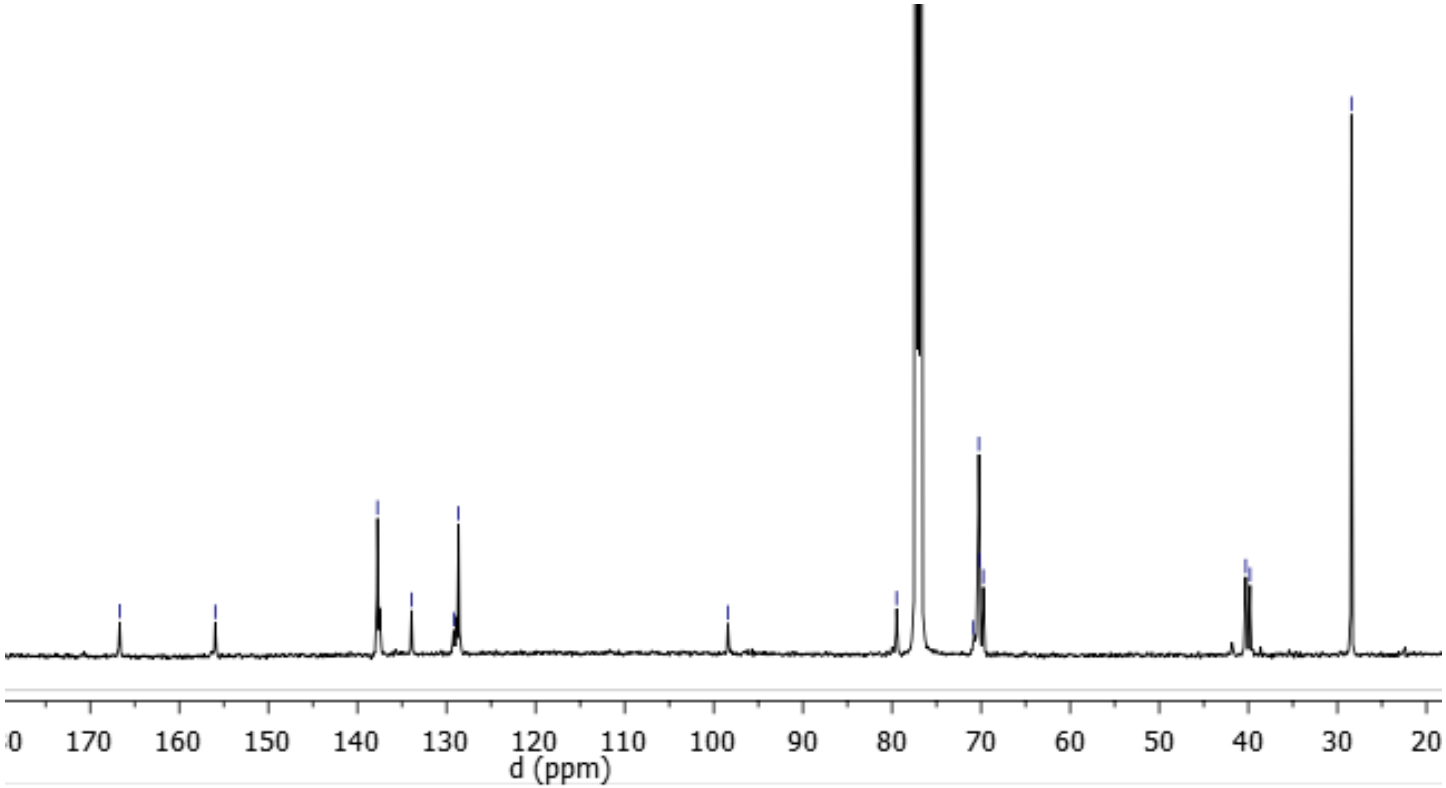


Figure S 2. ^{13}C NMR ($CDCl_3$, 125 MHz, 298 K) spectrum of **4**

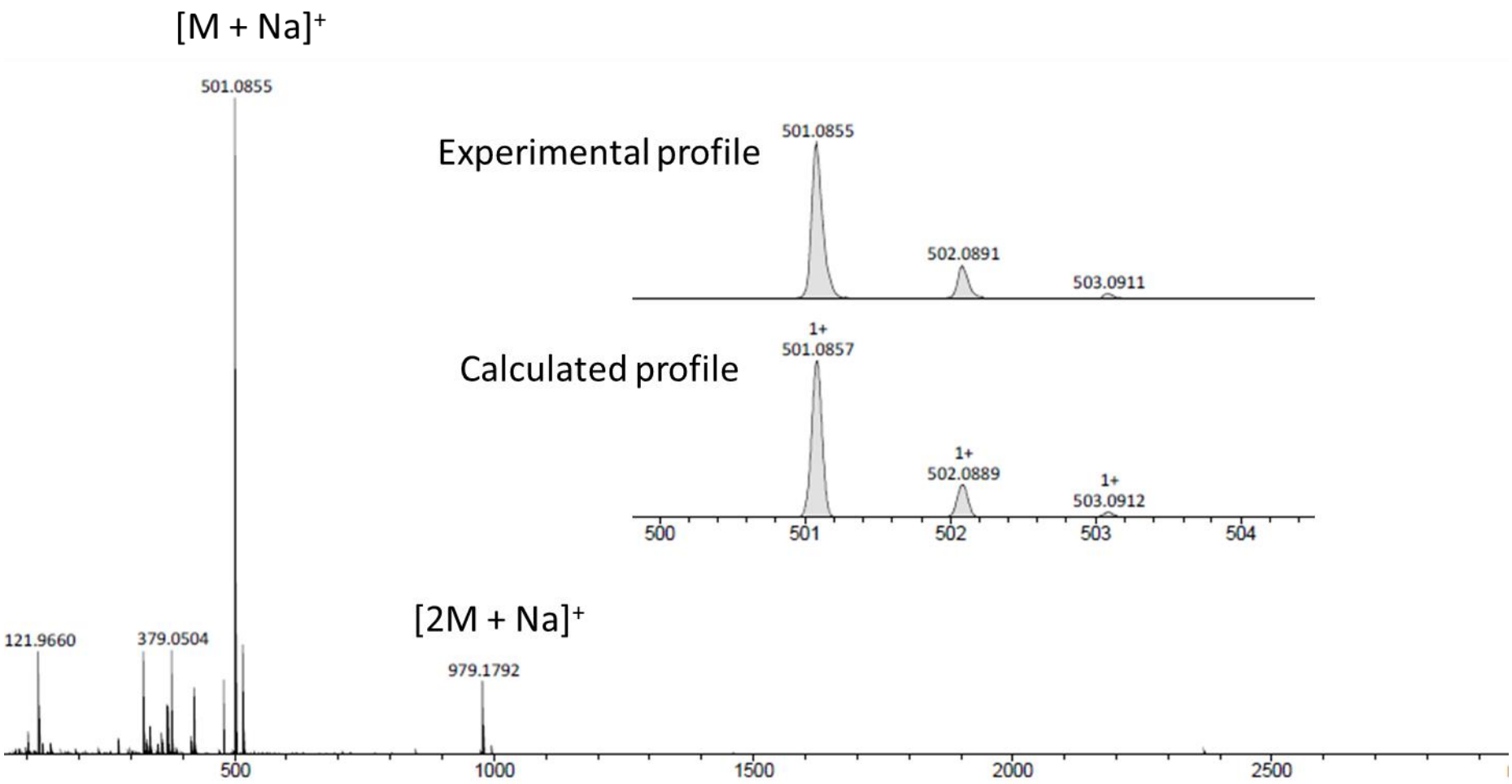


Figure S 3. HR ES-MS of **4** and the corresponding calculated profile for $[M + Na]^+$

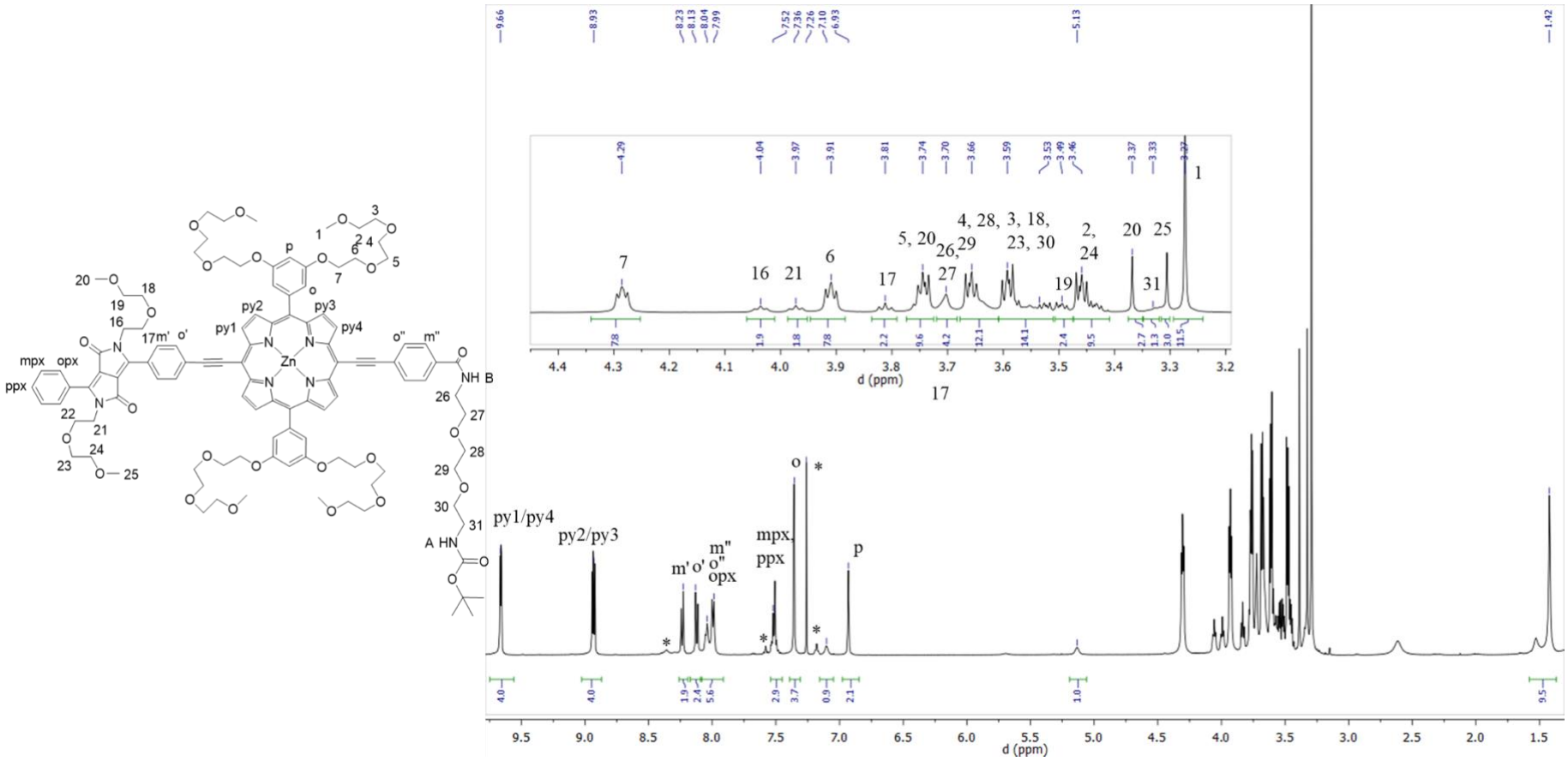


Figure S 4. ^{1}H NMR ($CDCl_3$/pyridine-d_5, 500 MHz, 298 K) spectrum of **6**

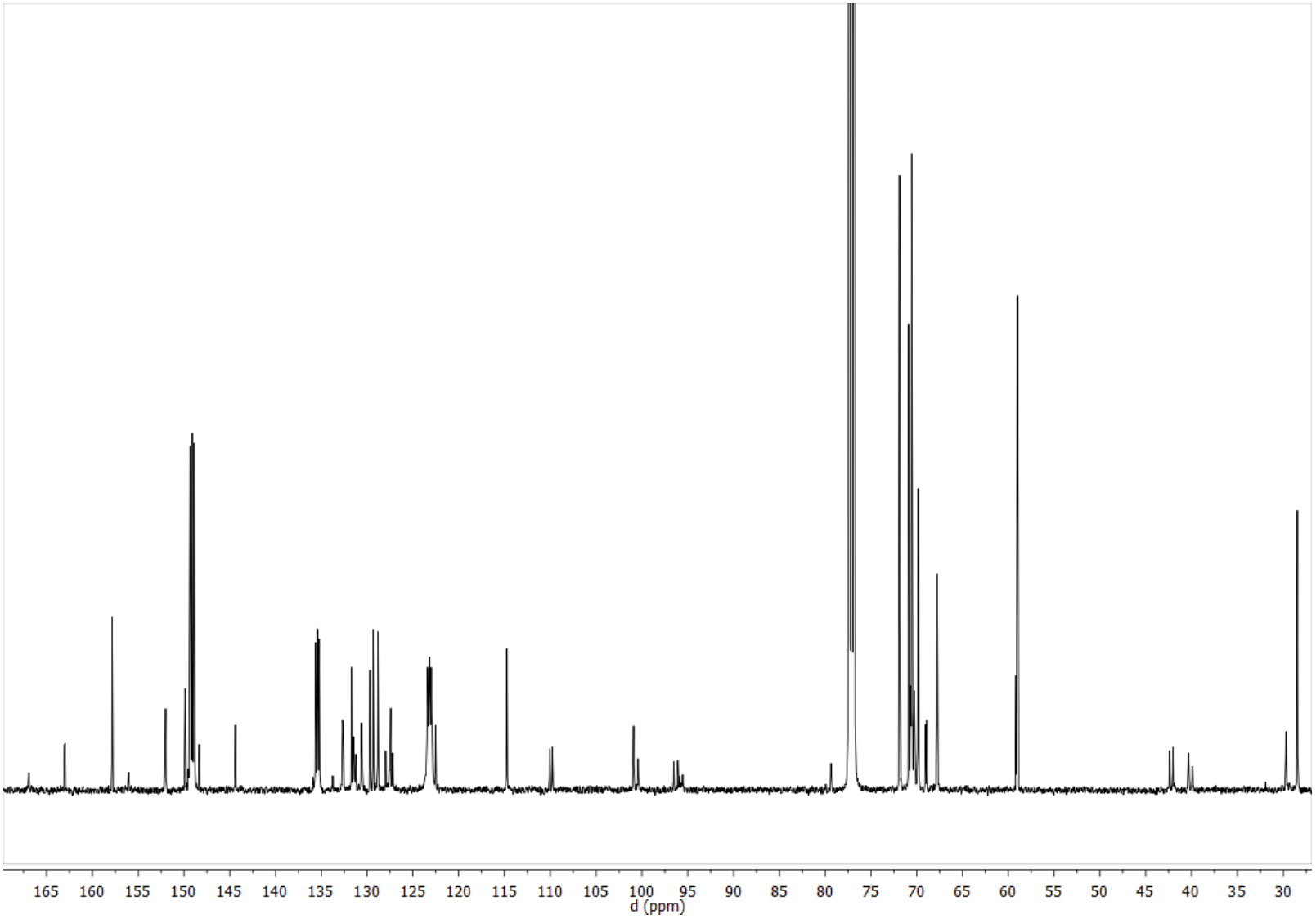


Figure S 5. ^{13}C NMR ($CDCl_3$/pyridine-d_5, 125 MHz, 298 K) spectrum of **6**

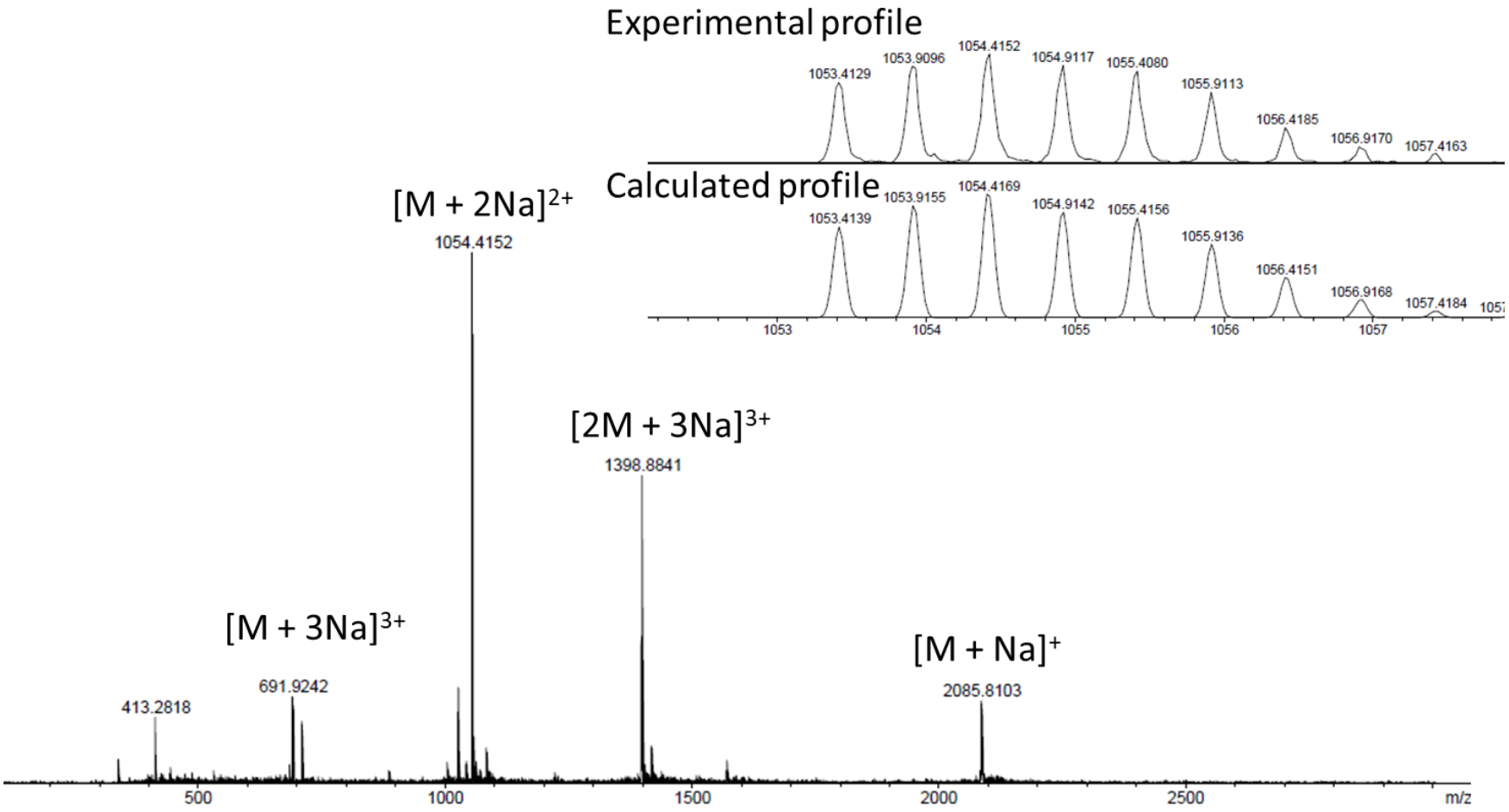


Figure S 6. HR ES-MS of **6** and the corresponding calculated profile for $[M + 2\ Na]^{2+}/2$

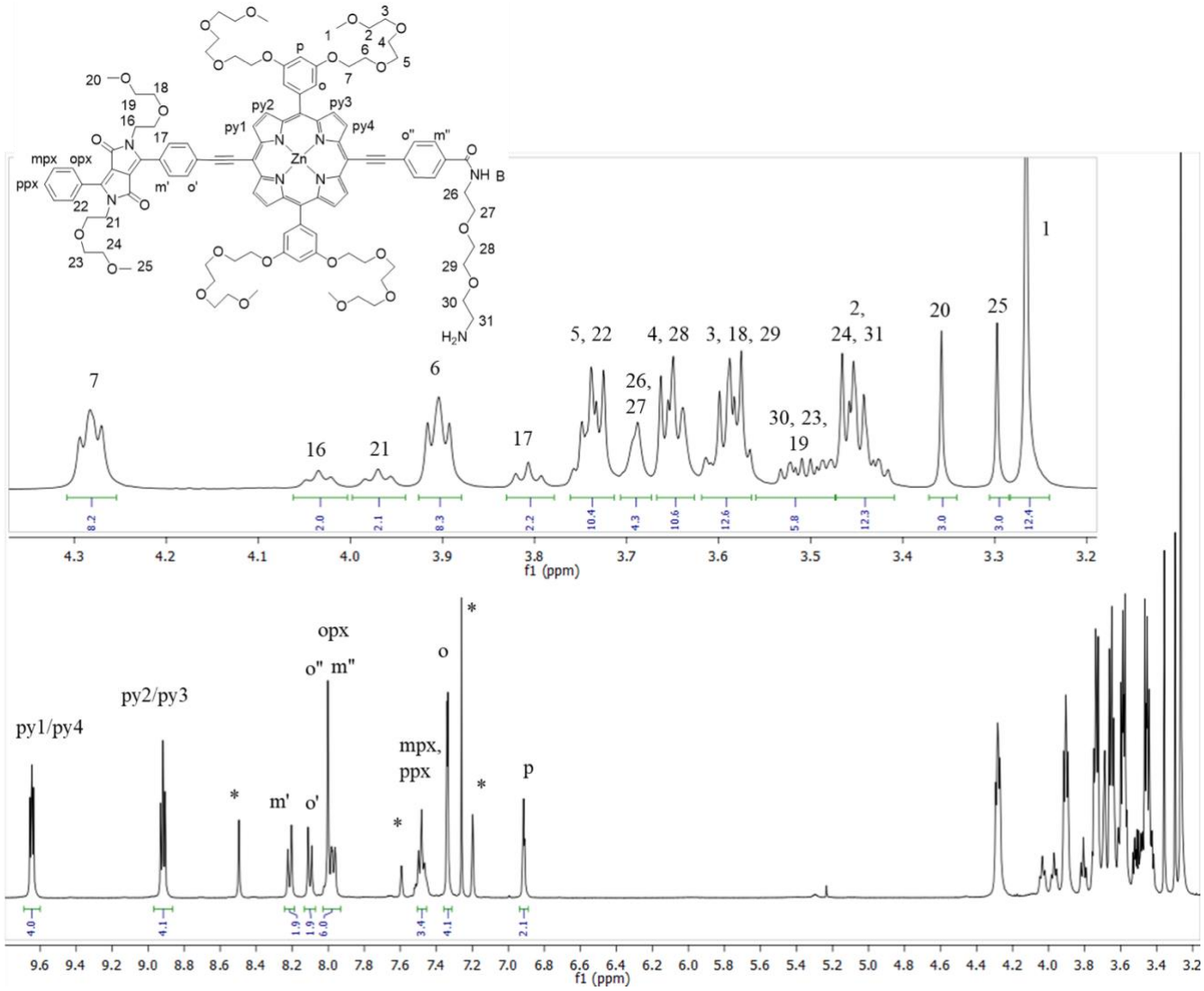


Figure S 7. ^{1}H NMR ($CDCl_3^*$/pyridine-d_5^*, 400 MHz, 298 K) spectrum of **7**

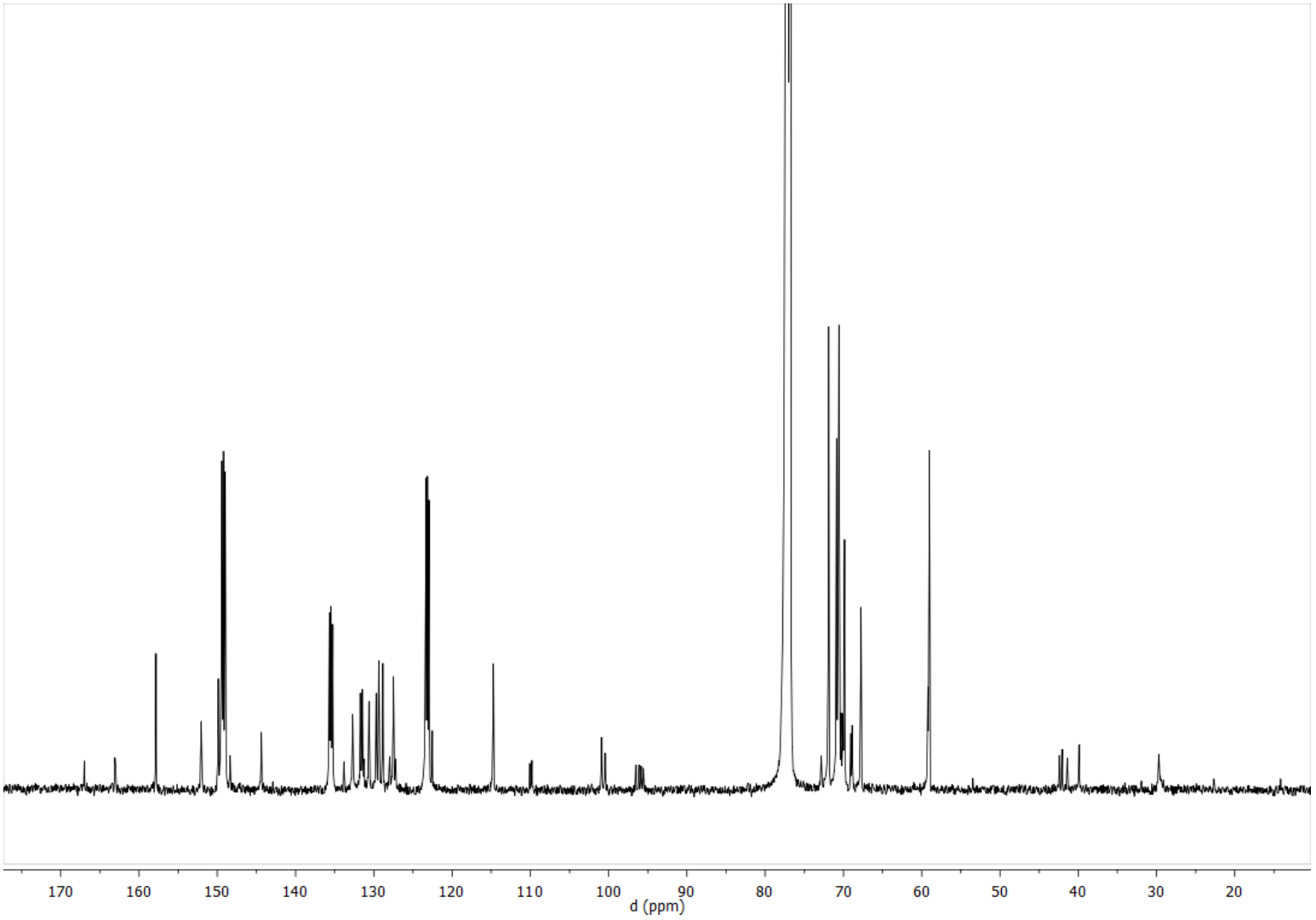


Figure S 8. ^{13}C NMR ($CDCl_3^*$/pyridine-d_5^*, 125 MHz, 298 K) spectrum of **7**

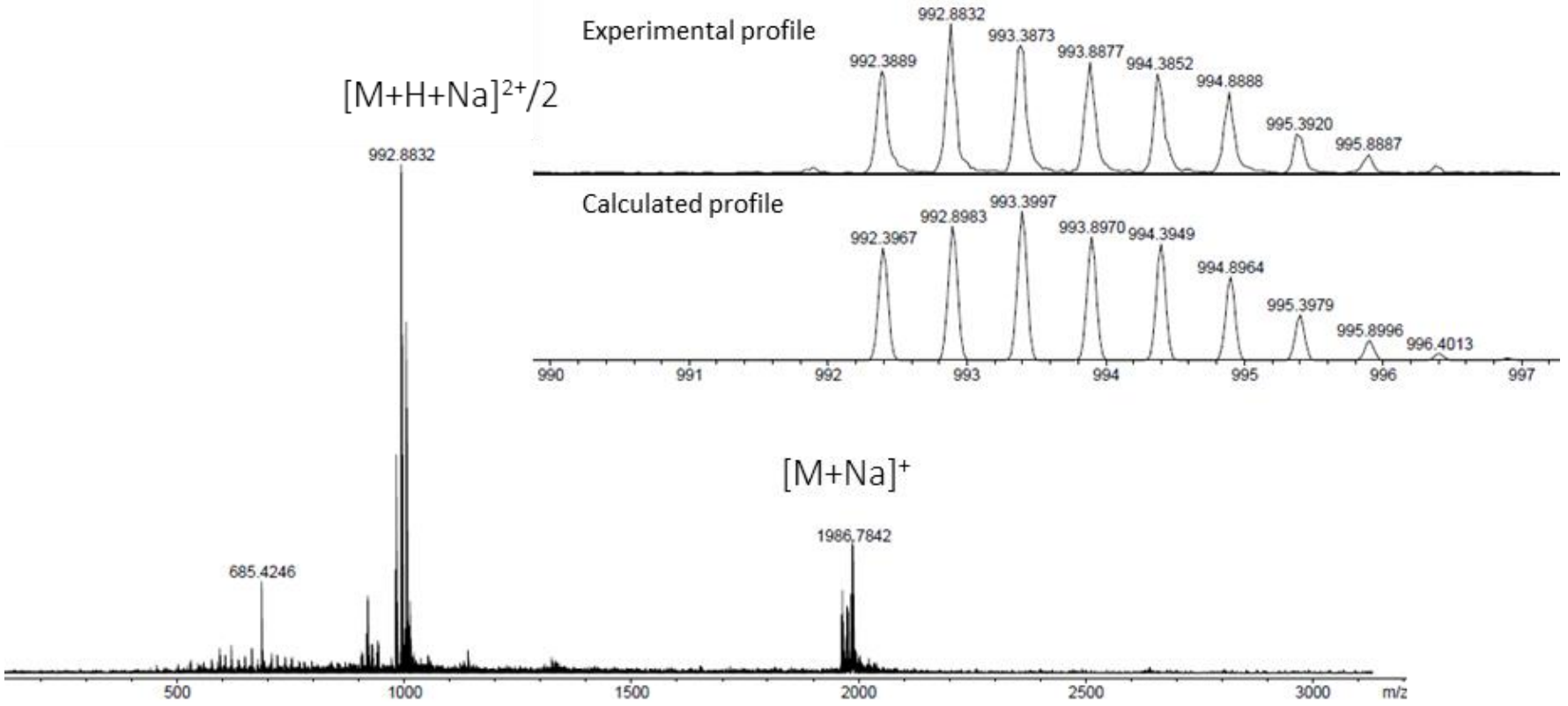


Figure S 9. HR ES-MS of **7** and the corresponding calculated profile for $[M+H+Na]^{2+}/2$.

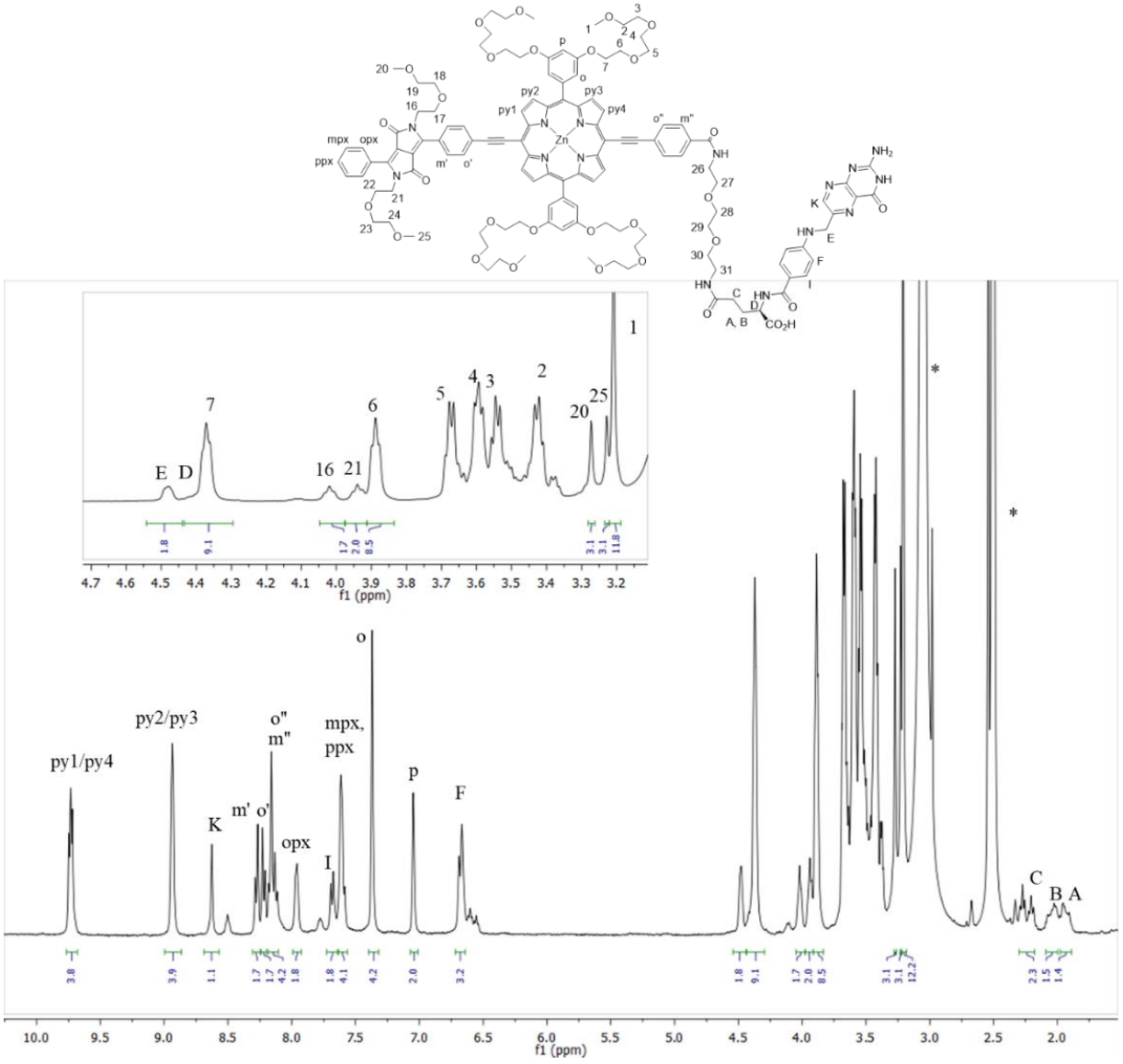


Figure S 10. ^{1}H NMR (DMSO-d_6^*, 400 MHz, 350 K) spectrum of **1**

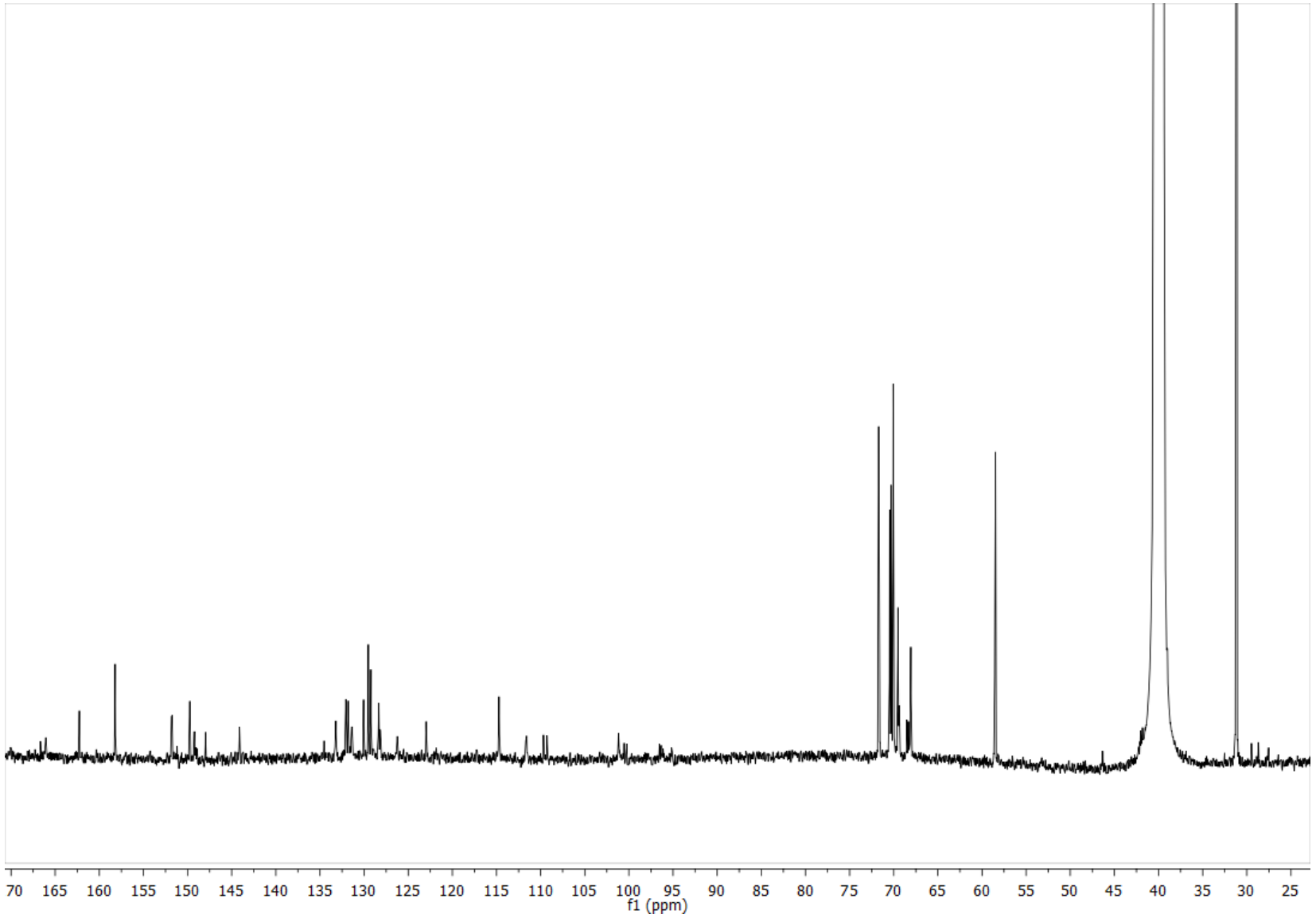


Figure S 11. ^{13}C NMR (DMSO-d_6^*, 125 MHz, 298 K) spectrum of **1**

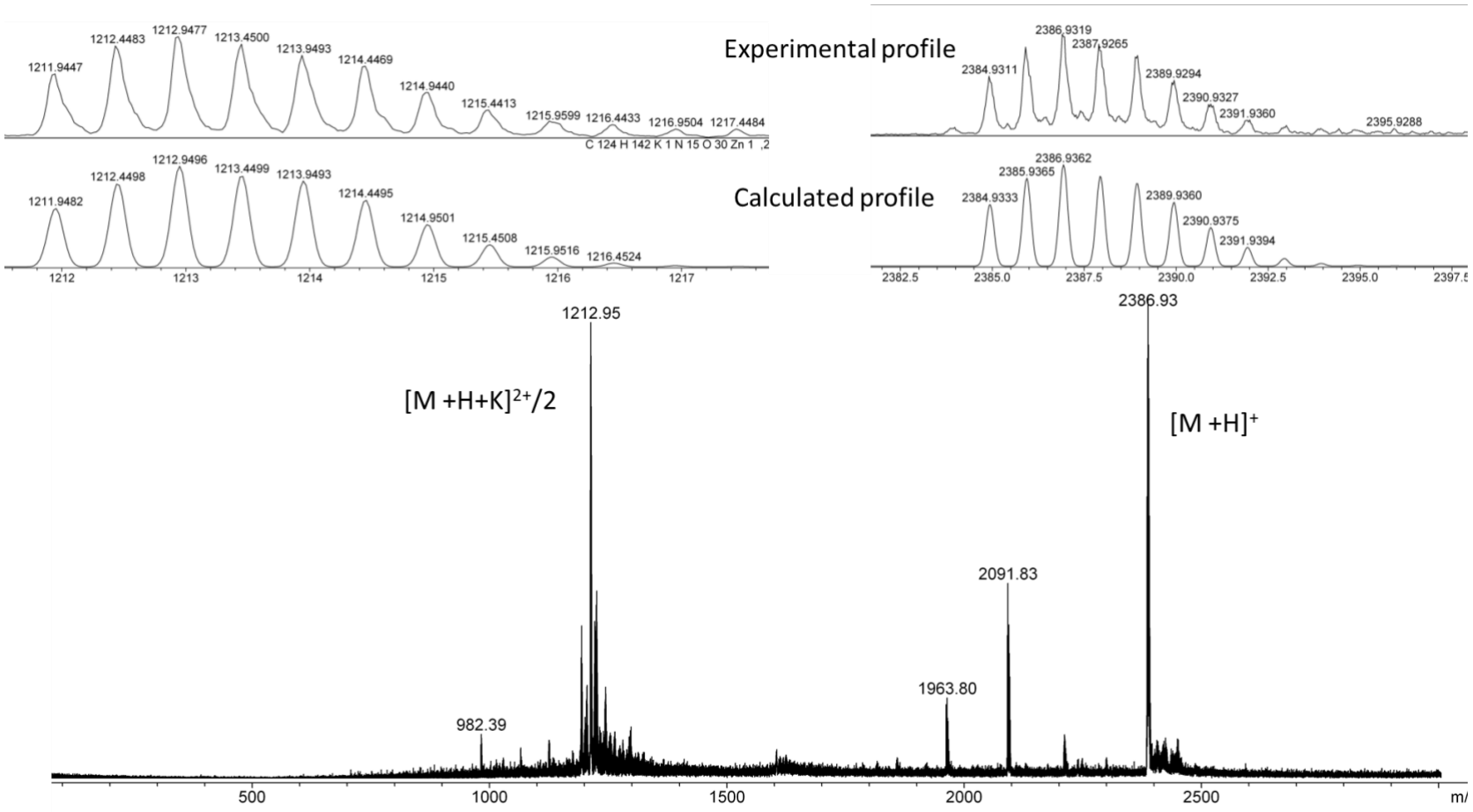


Figure S 12. HR ES-MS of **1** and the corresponding calculated profile for $[M+H+K]^{2+}/2$ and $[M+H]^{+}$

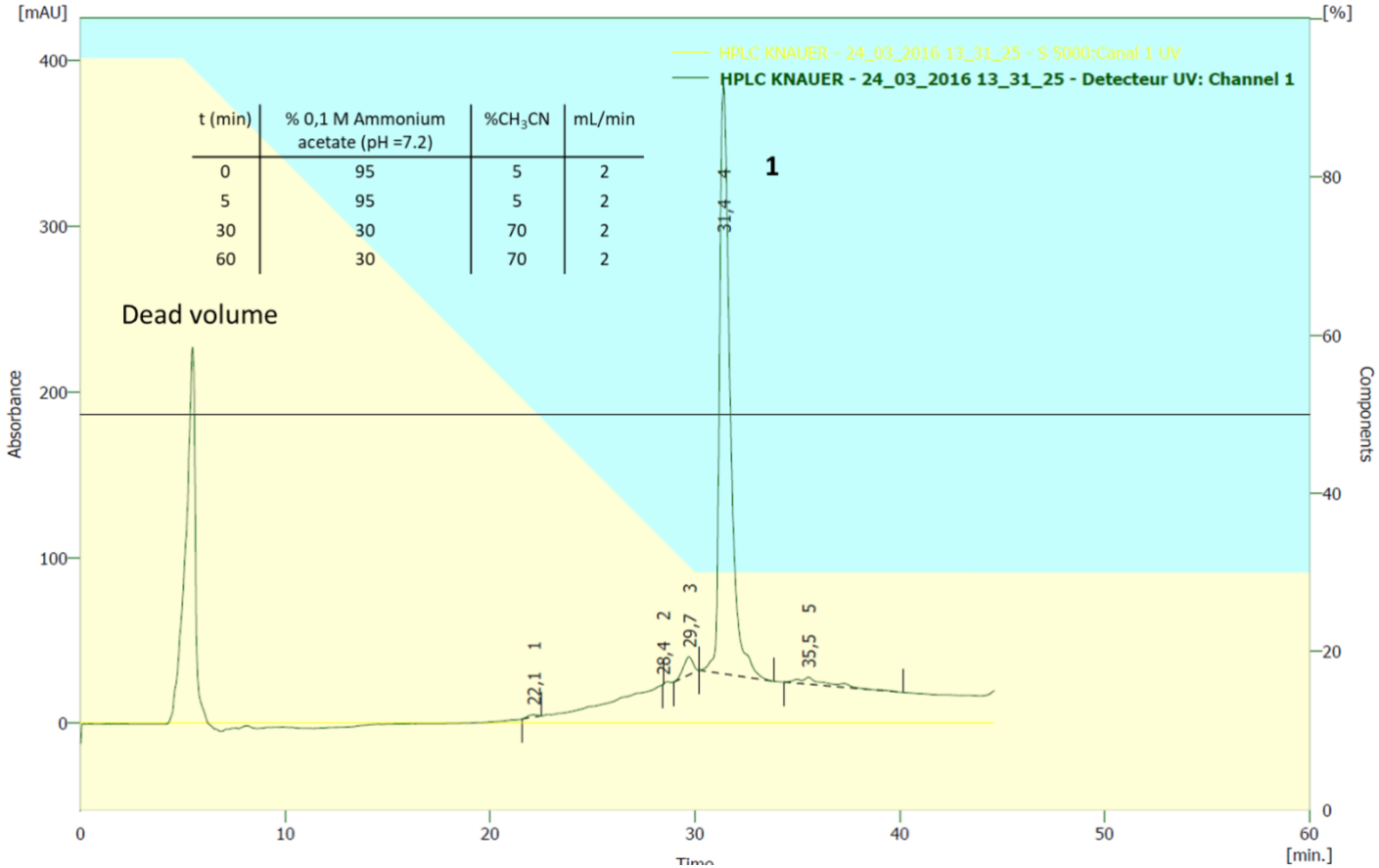


Figure S 13. HPLC chromatogram of **1** and the elution gradient

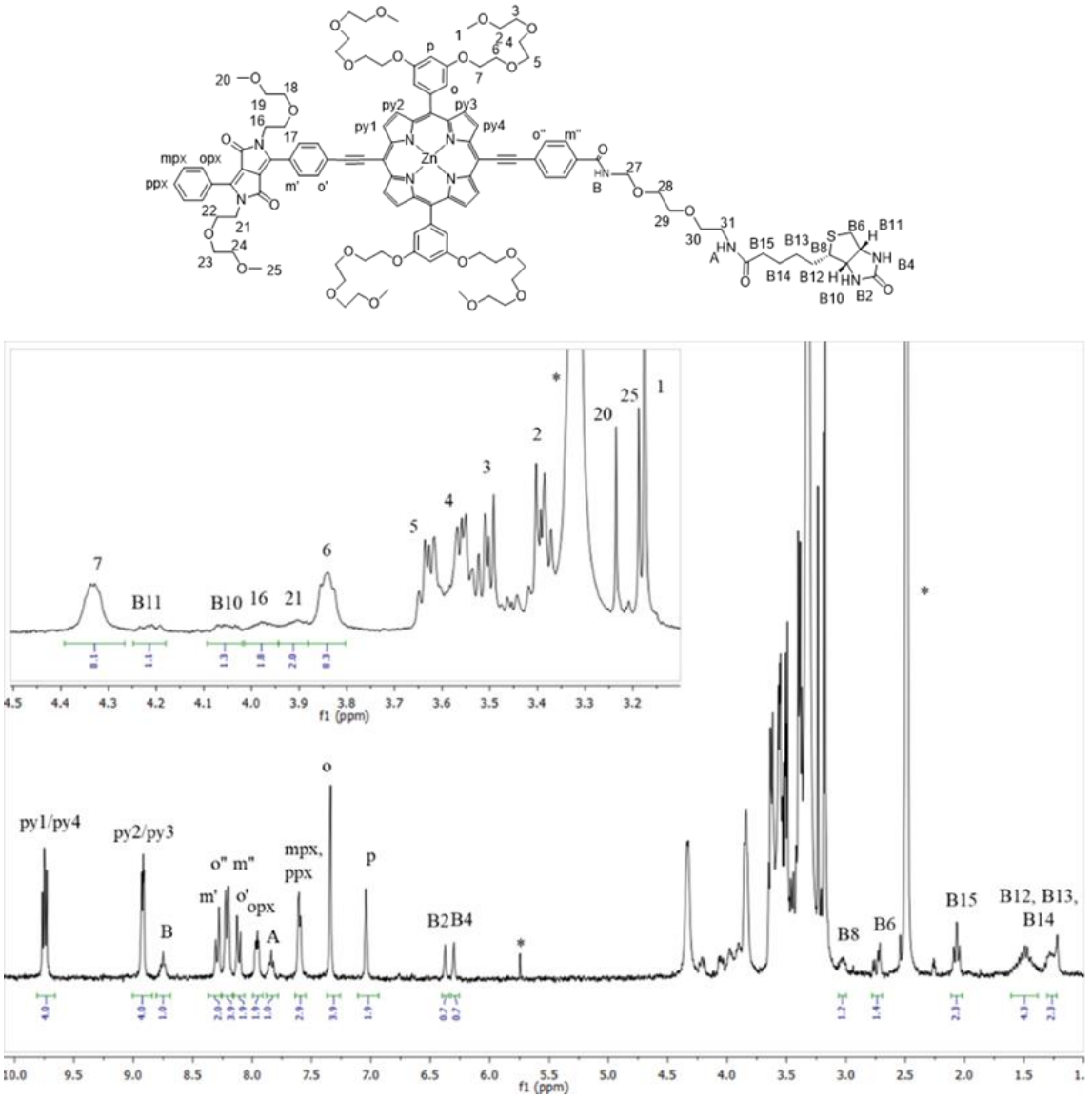


Figure S 14. ^{1}H NMR (DMSO-d_6^*, 400 MHz, 298 K) spectrum of **2**

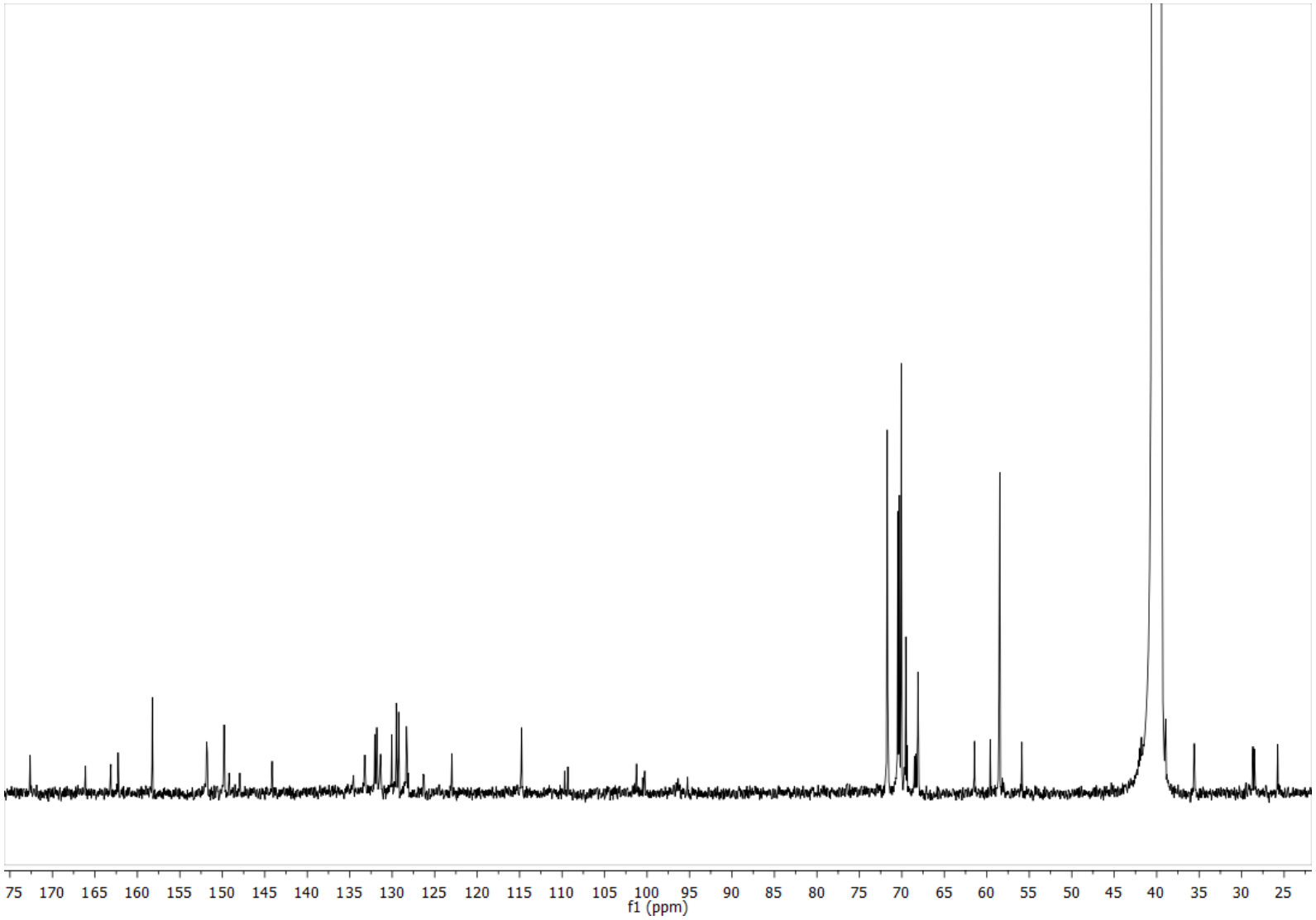


Figure S 15. ^{13}C NMR (DMSO-d_6^*, 125 MHz, 298 K) spectrum of **2**

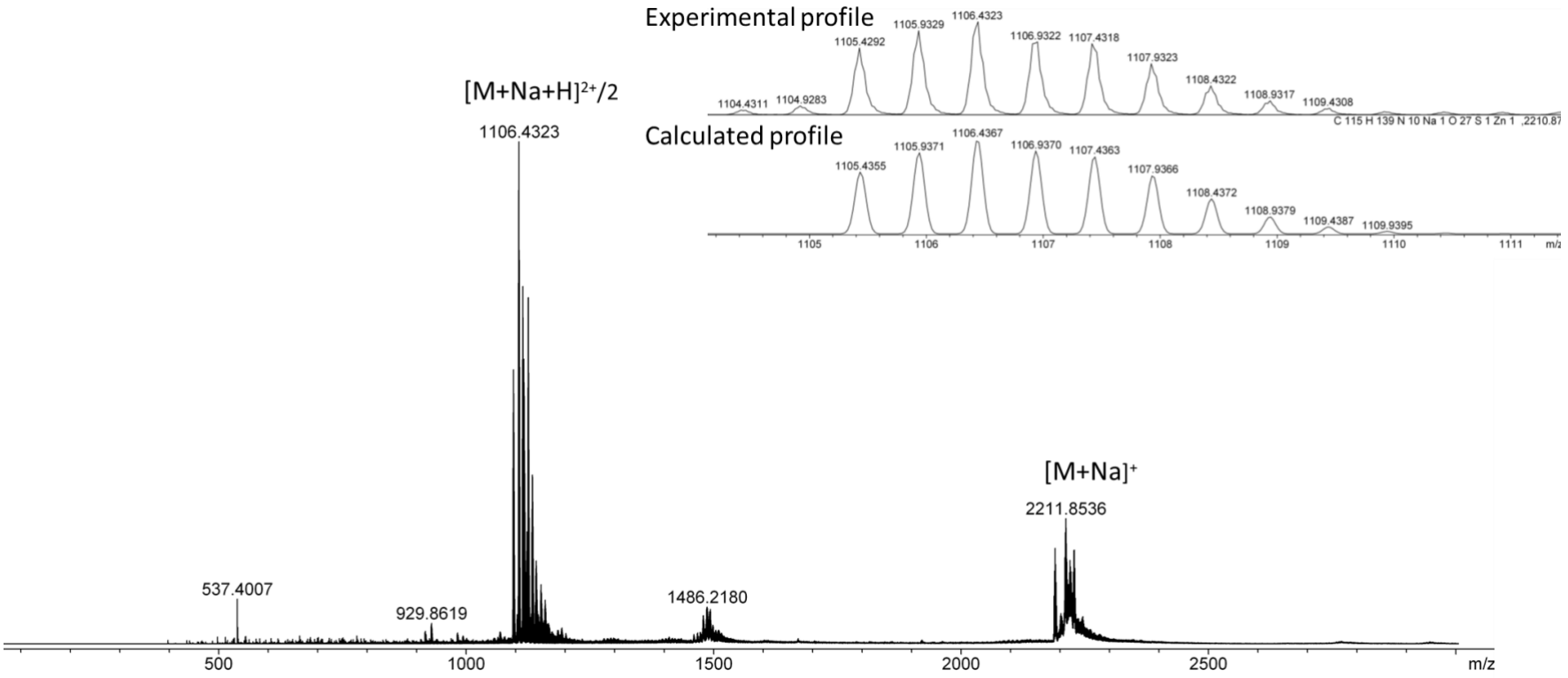


Figure S 16. HR ES-MS of **2** and the corresponding calculated profile for $[M+Na+H]^{2+}/2$

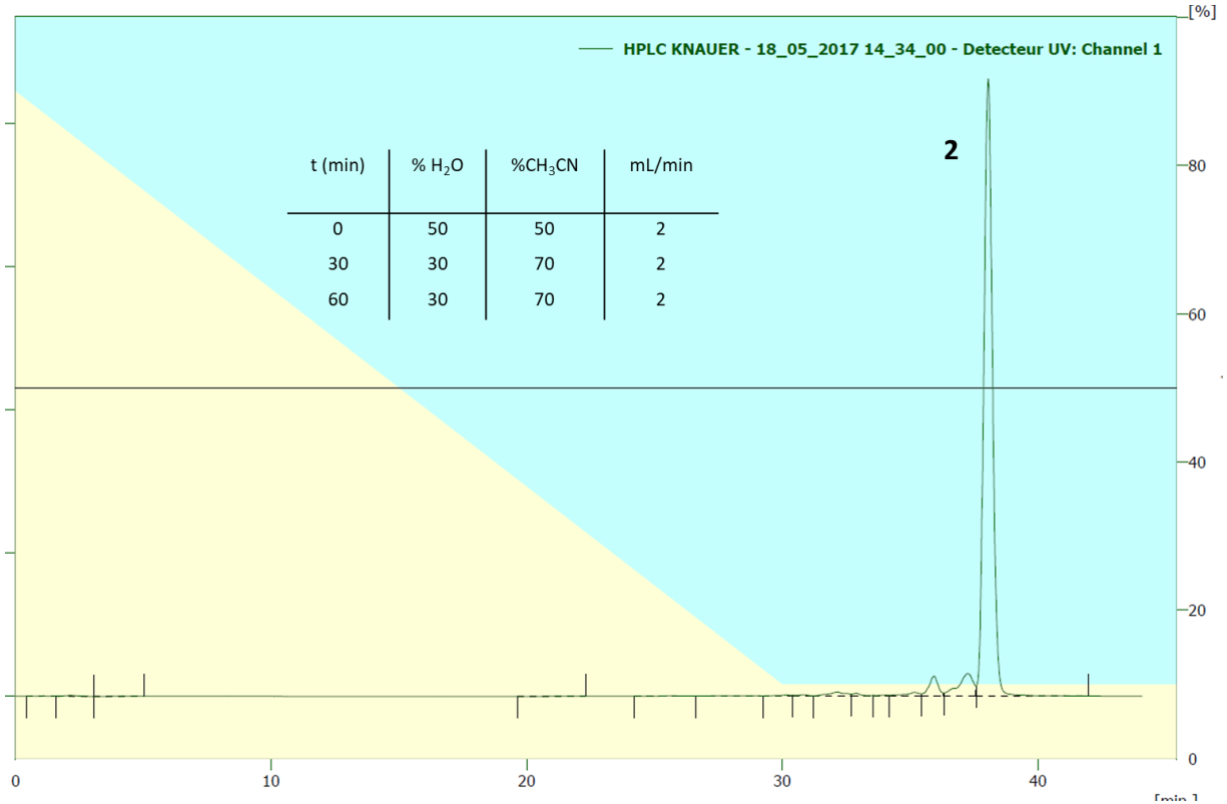


Figure S 17. HPLC chromatogram of **2** and the elution gradient

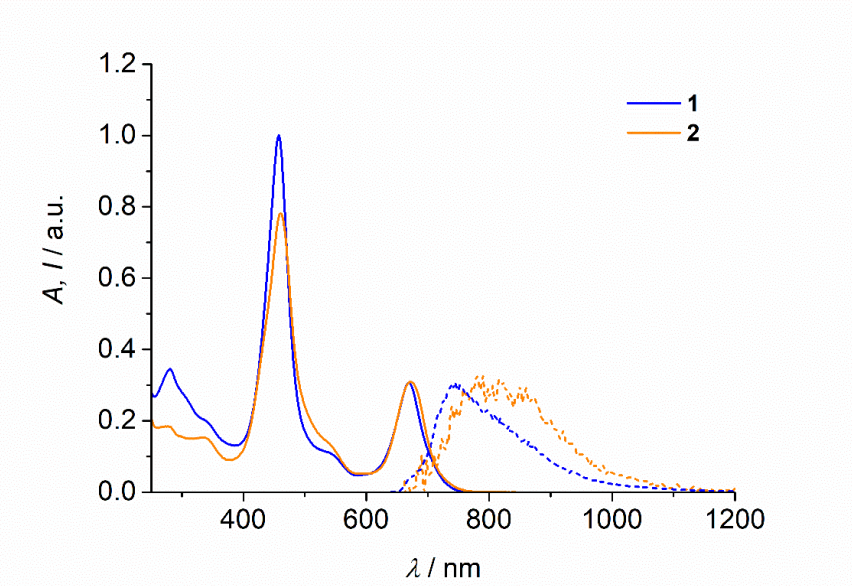


Figure S 18. Arbitrarily scaled absorption (full) and emission (dashed) spectra of **1** (blue) and **2** (orange) in H_2O added with 1% DMSO. The exact molar absorption coefficients could not be determined due to solubility reasons.

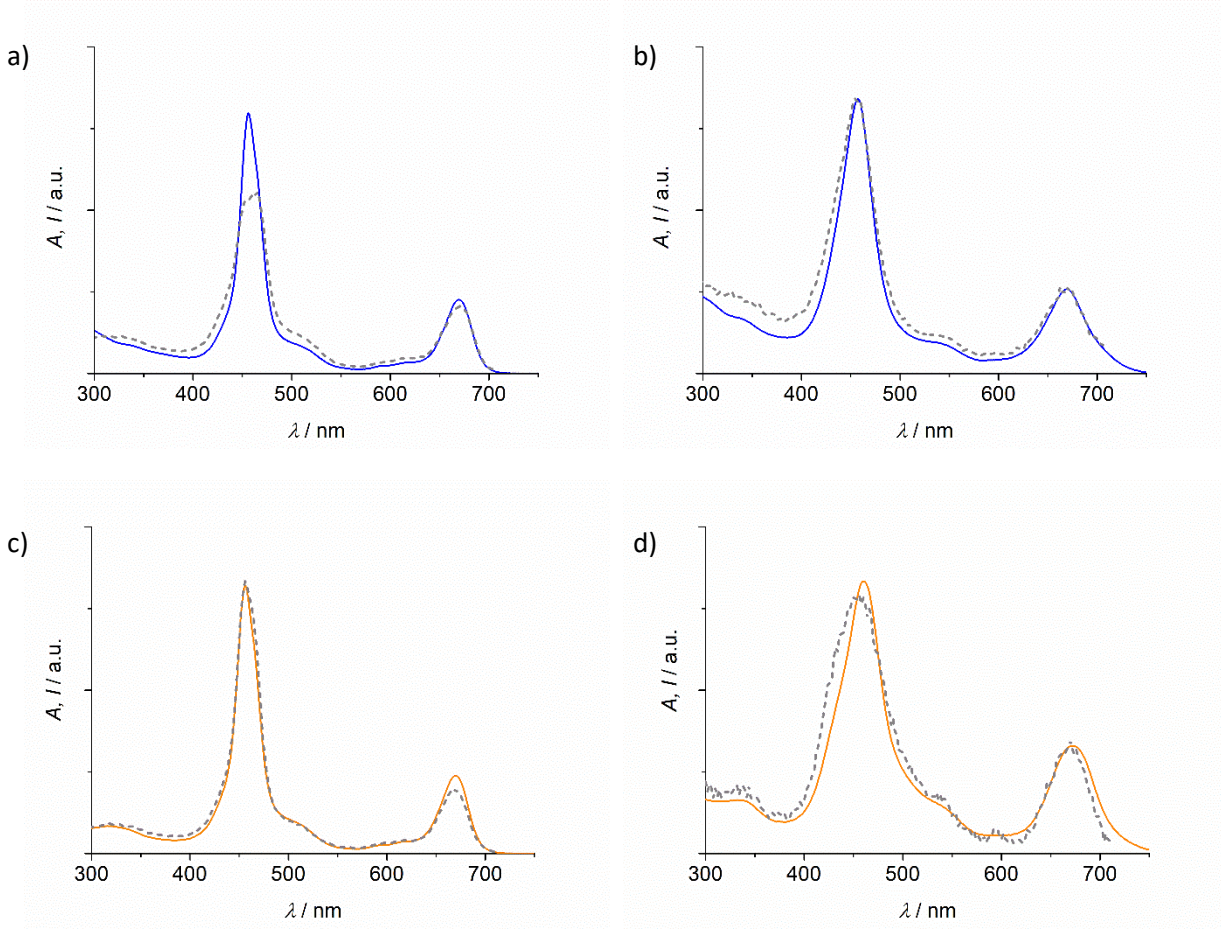


Figure S 19. Excitation (grey dashed) and arbitrarily scaled absorption (full) spectra of: a) **1** in DMSO, λ_{em}= 720 nm; b) **1** in H2O + 1% DMSO; λ_{em}= 740 nm; c) **2** in DMSO, λ_{em}= 720 nm; d) **2** in H2O + 1% DMSO, λ_{em}= 750 nm.

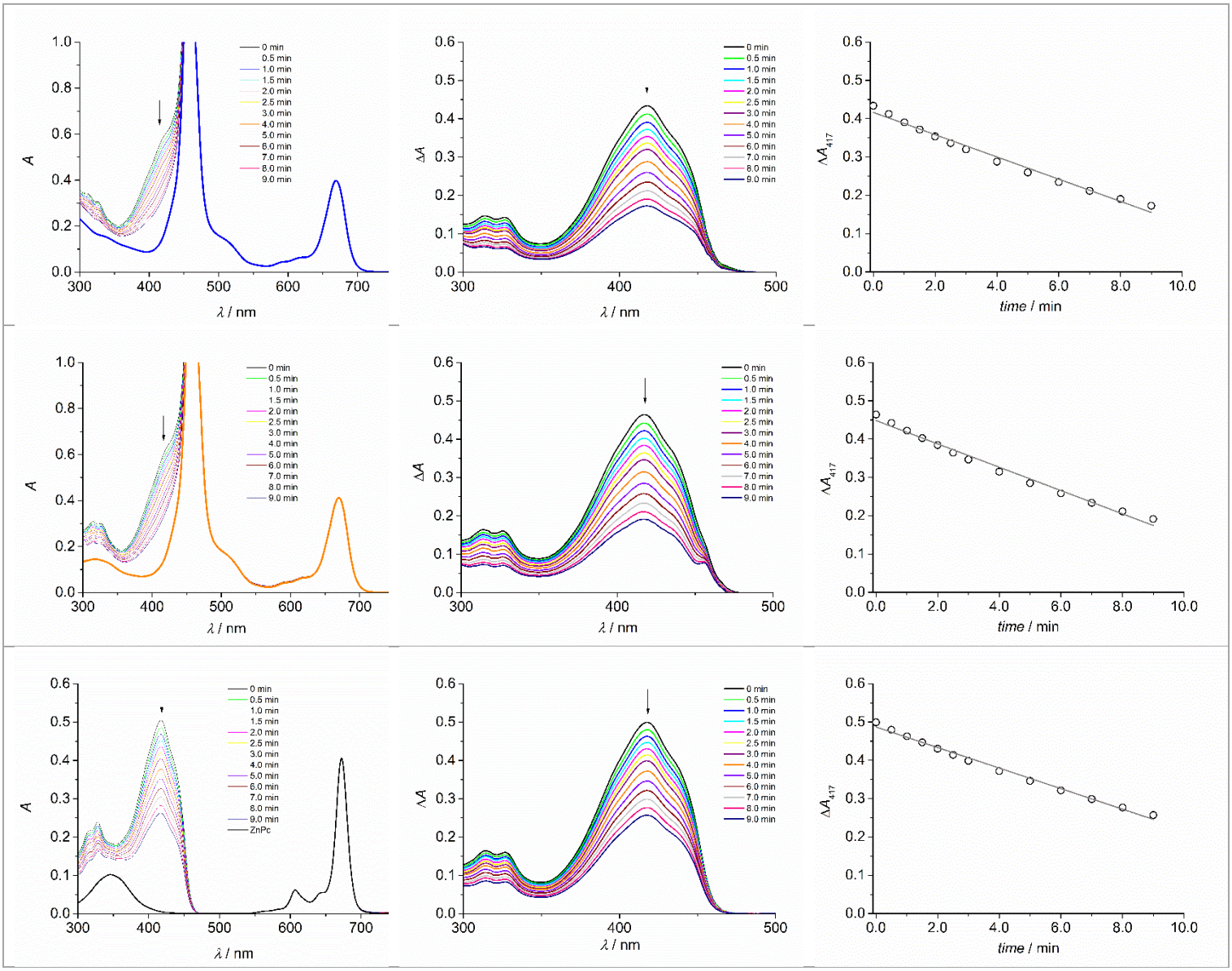


Figure S 20. Left: Absorption spectra of a DMSO solution containing the examined compound/standard and DPBF upon irradiation at 672 nm (0-9 min). Center: the same spectra subtracted by the constant contribution of the compound/standard. Right: value of DPBF absorbance at 417 nm as a function of the irradiation time. Top panel: compound **1**; middle panel: compound **2**, bottom panel: standard ZnPc.

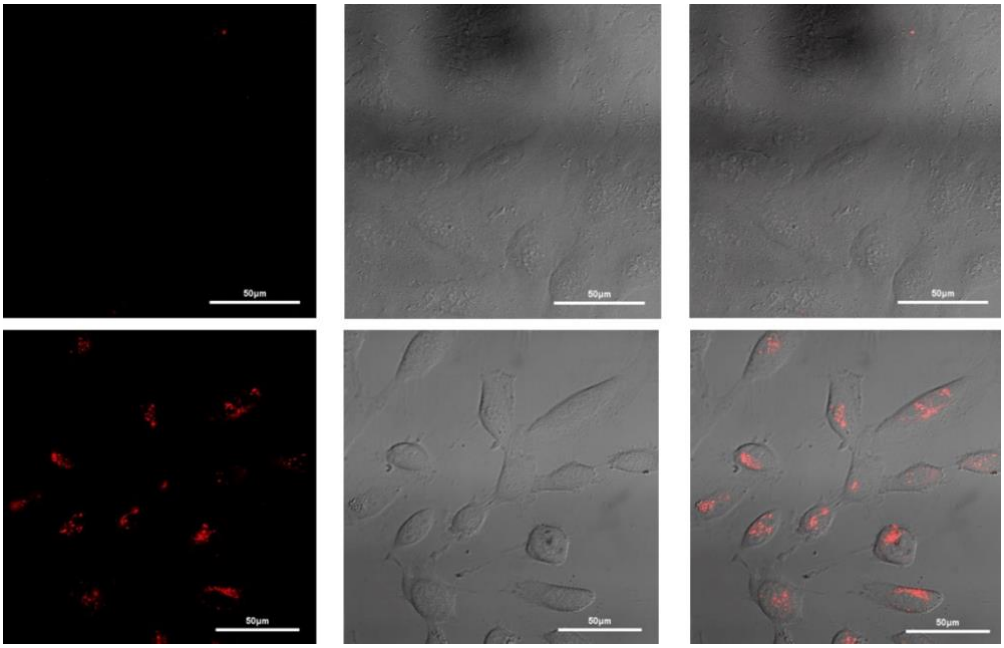


Figure S 21. Confocal and DIC images of HeLa cells incubated without (top) or with (bottom) PS **1.** (left : fluorescence image λ_{ex} = 488 nm ; λ_{em} = 700 – 1000 nm, center : DIC image, right : merge). Scale bar is 50 µm.