

Electronic supplementary information

Synthesis and investigation of singlet oxygen production efficiency of photosensitizers based on meso-phenyl-2,5-thienylene linked porphyrin oligomer and polymers

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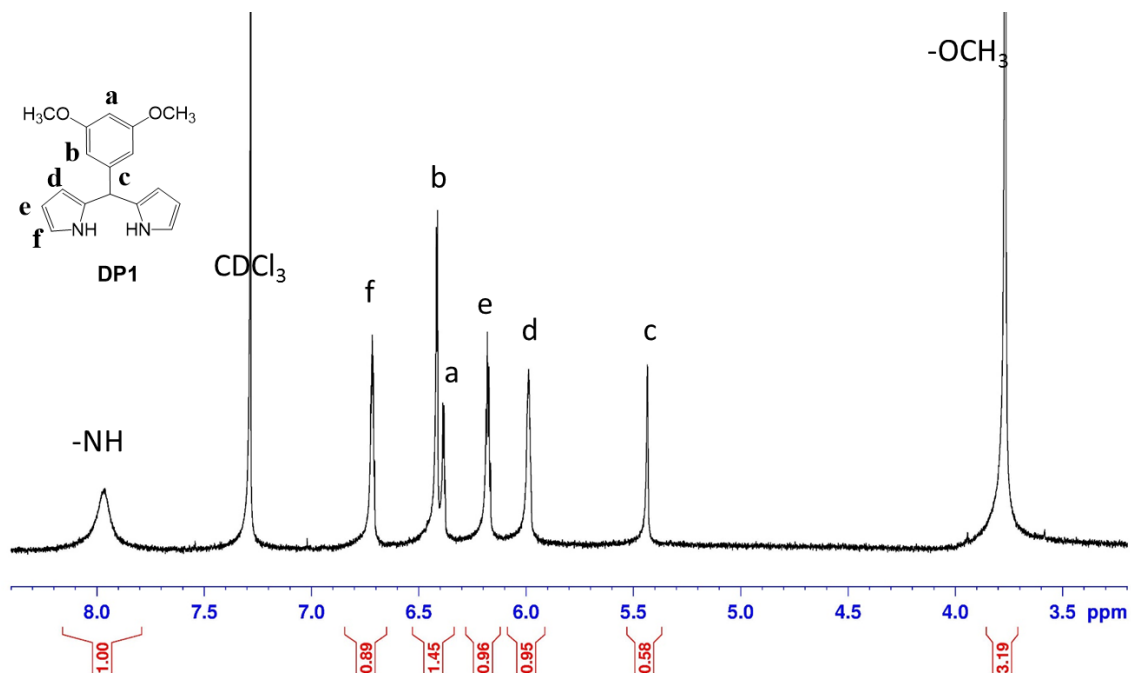


Figure S1: ¹H-NMR (400 MHz, CDCl₃, 25 °C) spectrum of DP1

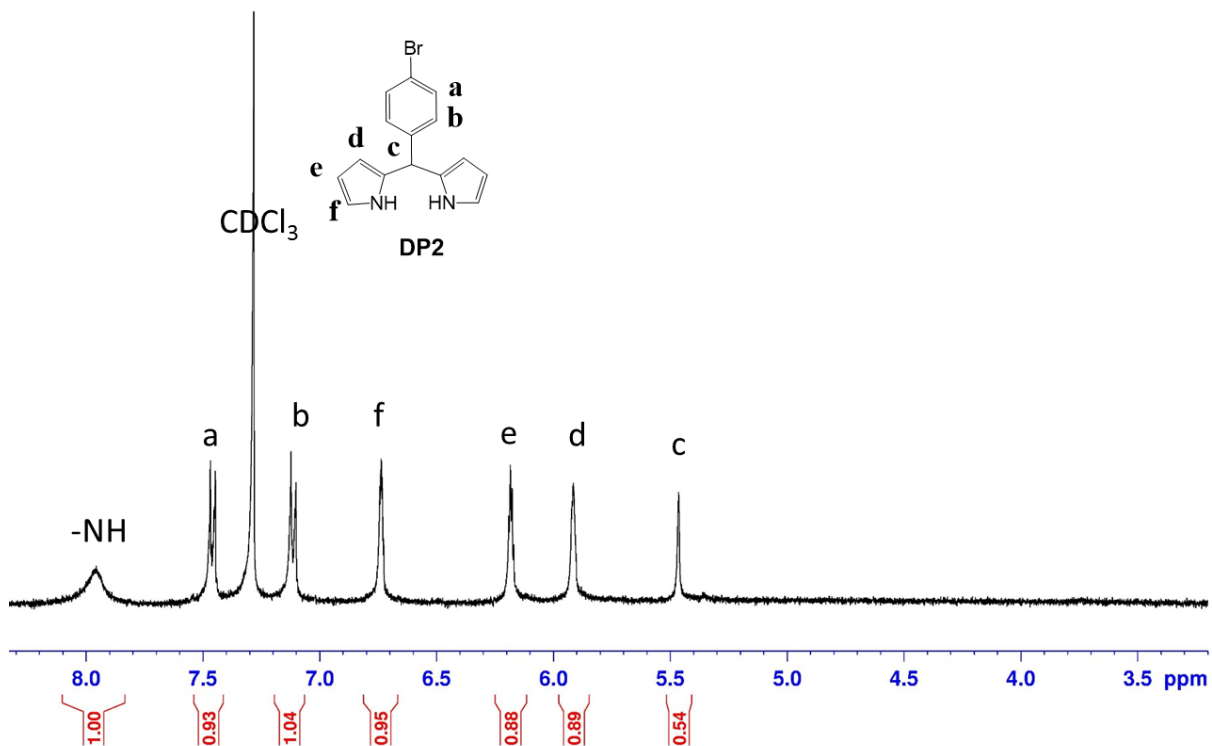


Figure S2: ¹H-NMR (400 MHz, CDCl₃, 25 °C) spectrum of DP2

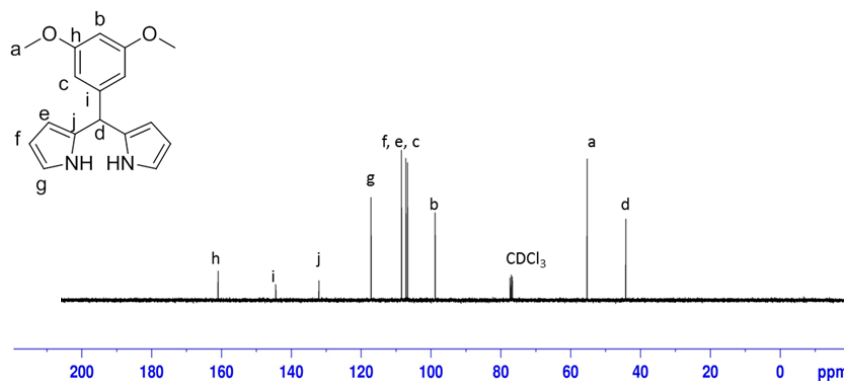


Figure S3: ^{13}C -NMR (100 MHz, CDCl₃, 25 °C) spectrum of DP1

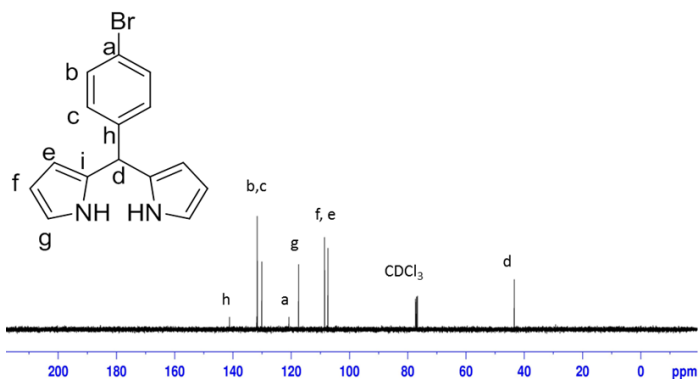


Figure S4: ^{13}C -NMR (100 MHz, CDCl₃, 25 °C) spectrum of DP2.

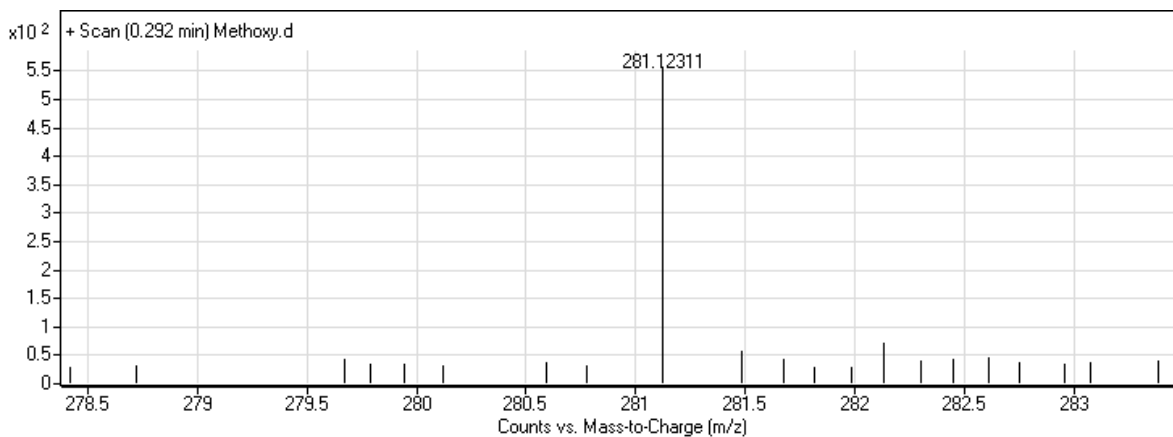


Figure S5: ESI spectrum of DP1

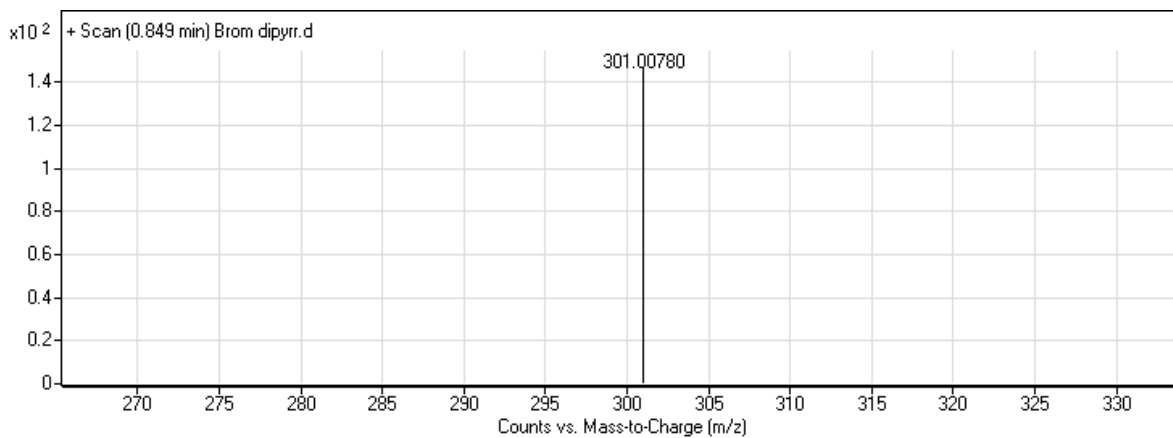


Figure S6: ESI-mass spectrum of DP2.

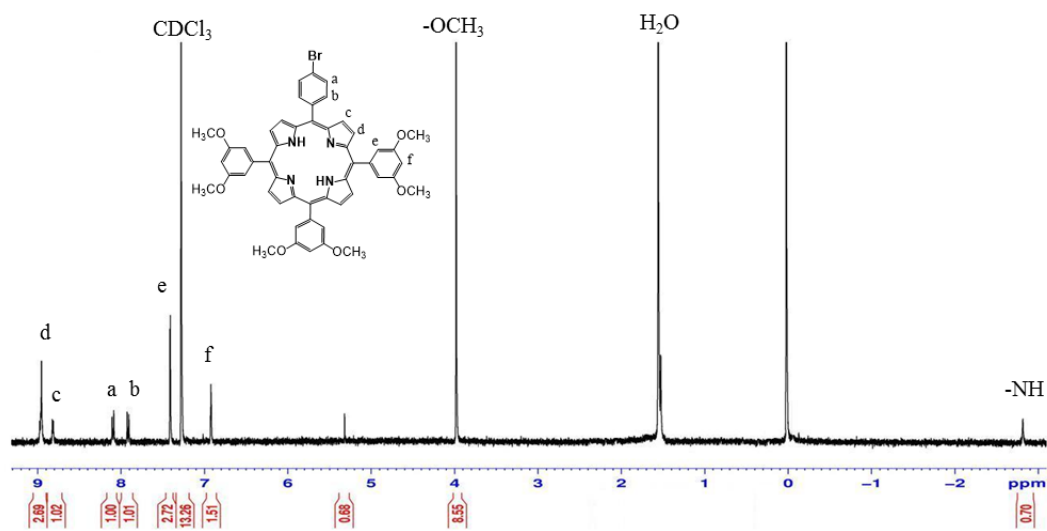


Figure S7: ¹H NMR spectrum (400 MHz, CDCl₃, 25 °C) of P1.

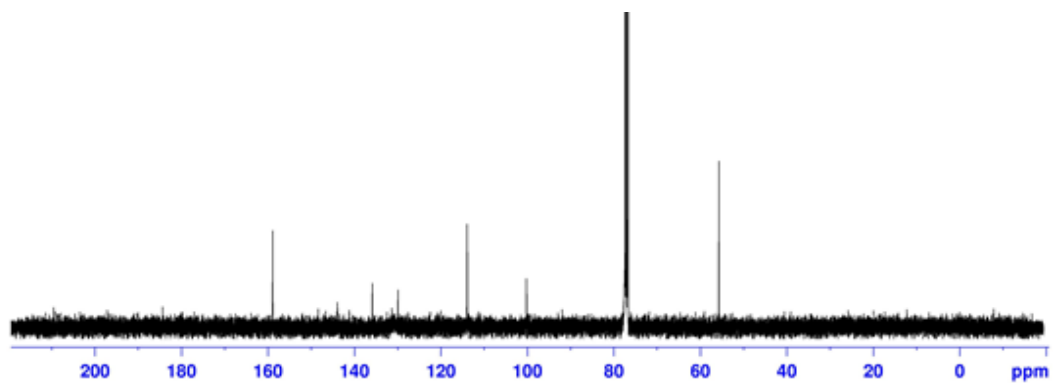


Figure S8: ¹³C NMR spectrum (100 MHz, CDCl₃, 25 °C) of P1.

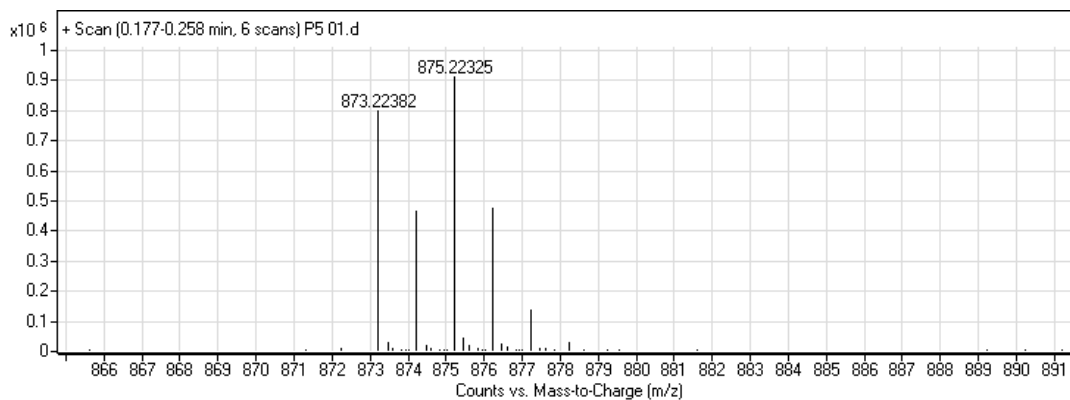


Figure S9: ESI-mass spectrum of P1.

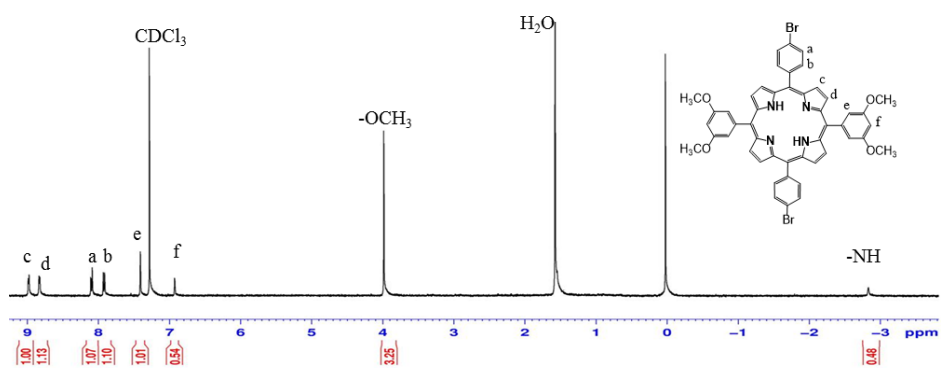


Figure S10: ¹H NMR spectrum (400 MHz, CDCl₃, 25 °C) of P2.

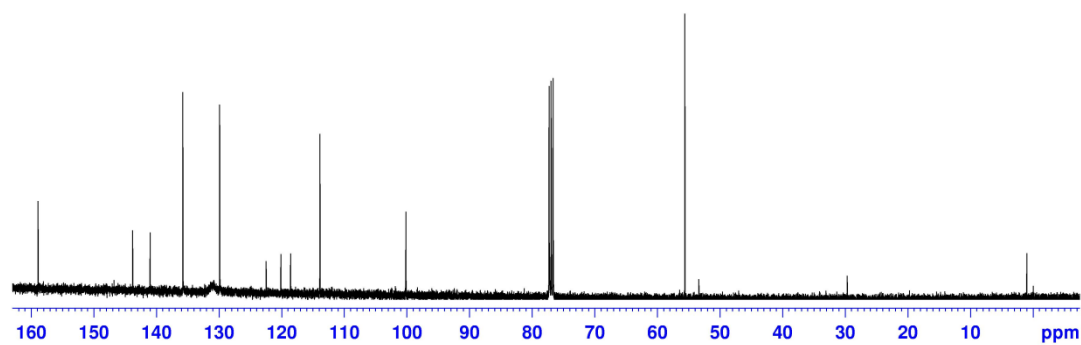


Figure S11: ¹³C NMR spectrum (100 MHz, CDCl₃, 25 °C) of P2.

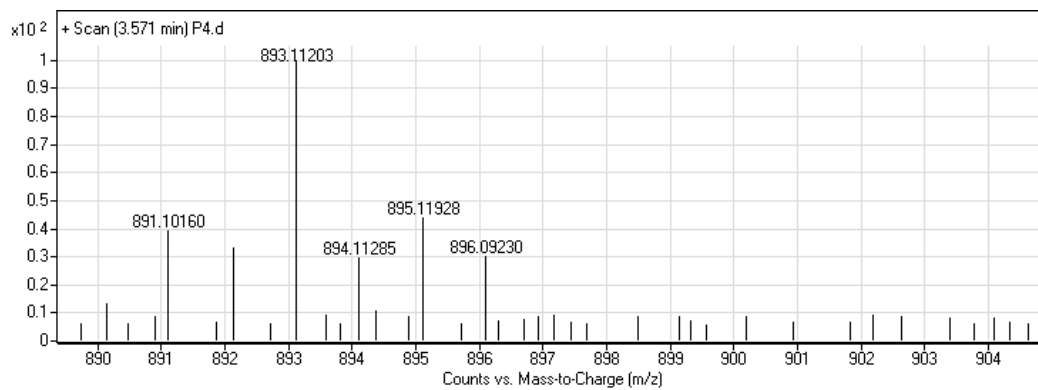


Figure S12: ESI-mass spectrum of **P2**.

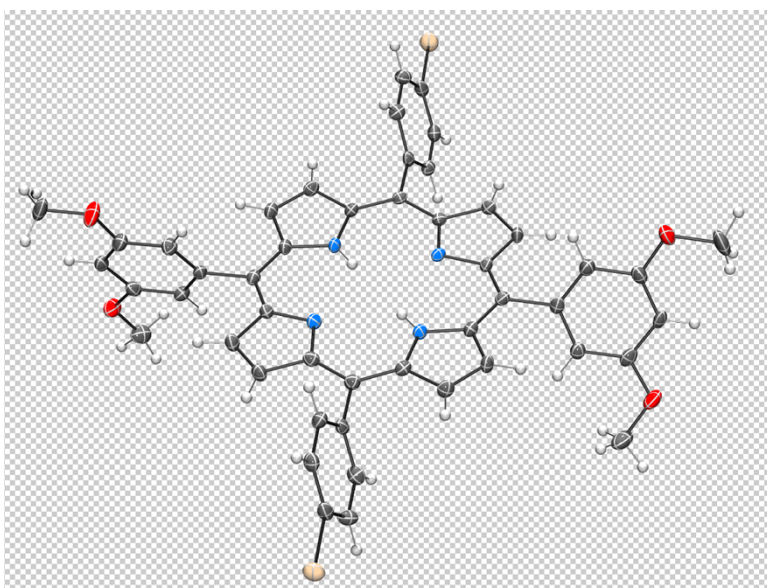


Figure S13: Structure of compound **P2** by single crystal XRD (Determined by Dr. Kitchen, University of Southampton, United Kingdom).

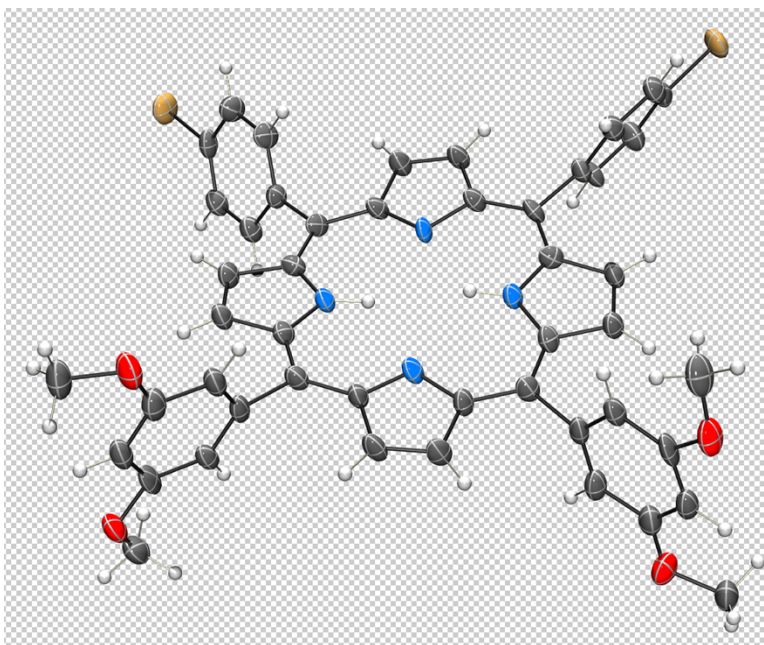


Figure S14: Structure of compound **P5** by single crystal XRD (Determined by Dr. Kitchen, University of Southampton, United Kingdom).

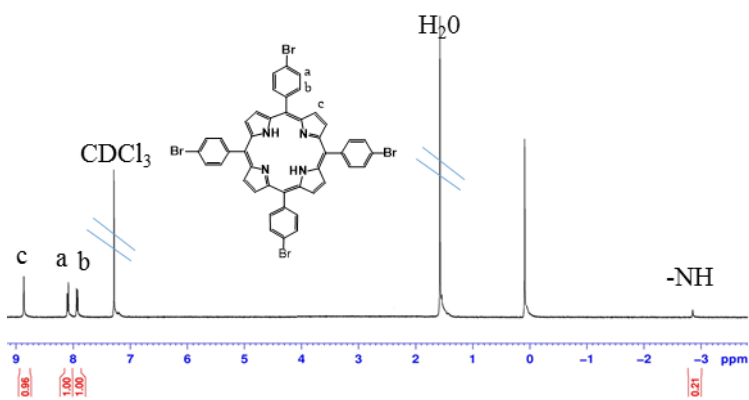


Figure S15: ^1H NMR spectrum (400 MHz, CDCl_3 , 25 °C) of **P4**.

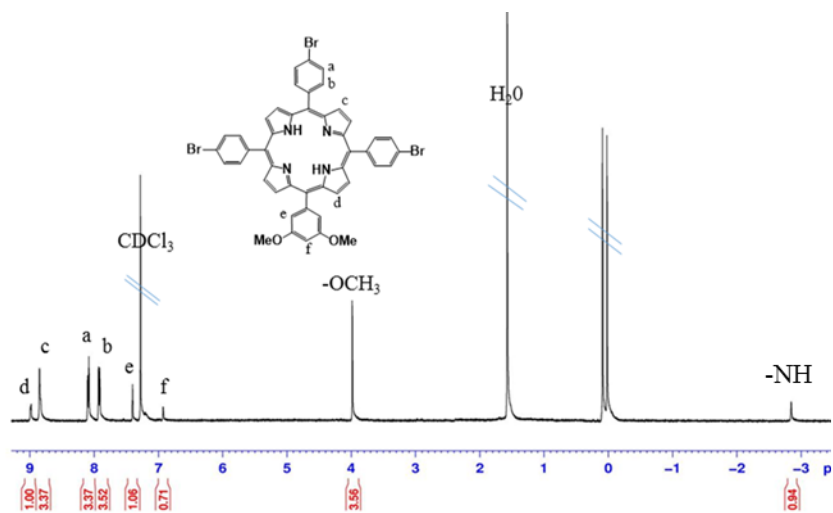


Figure S16: ^1H NMR spectrum (400 MHz, CDCl_3 , 25 $^\circ\text{C}$) of P6.

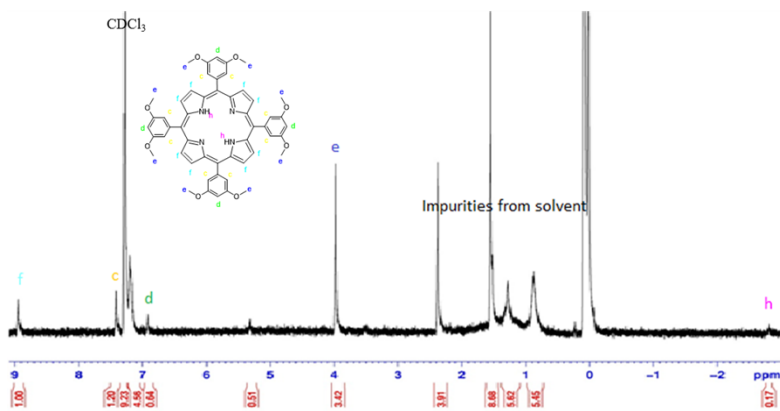


Figure S17: ^1H NMR spectrum (400 MHz, CDCl_3 , 25 $^\circ\text{C}$) of P3.

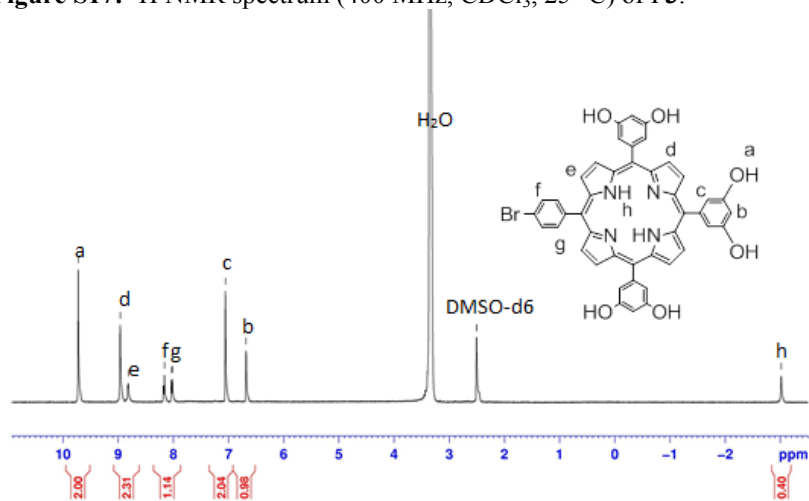


Figure S18: ^1H NMR spectrum (400 MHz, DMSO-d_6 , 25 $^\circ\text{C}$) of P1-OH.

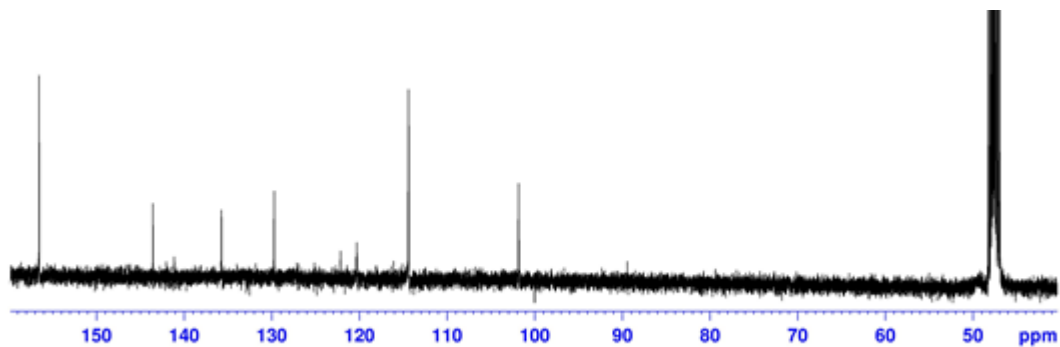


Figure S19: ^{13}C NMR spectrum (100 MHz, DMSO- d_6 , 25 $^{\circ}\text{C}$) of P1-OH.

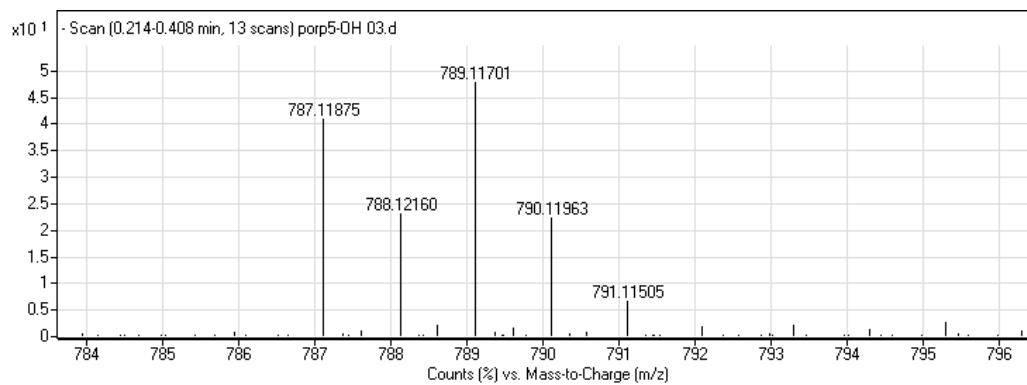


Figure S20: ESI-mass spectrum of P1-OH.

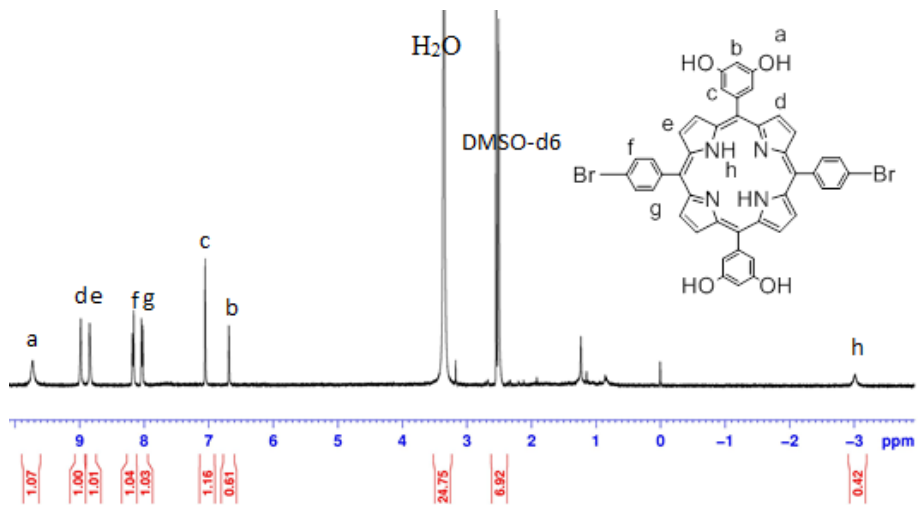


Figure S21: ^1H NMR spectrum (400 MHz, DMSO- d_6 , 25 $^{\circ}\text{C}$) of P2-OH.

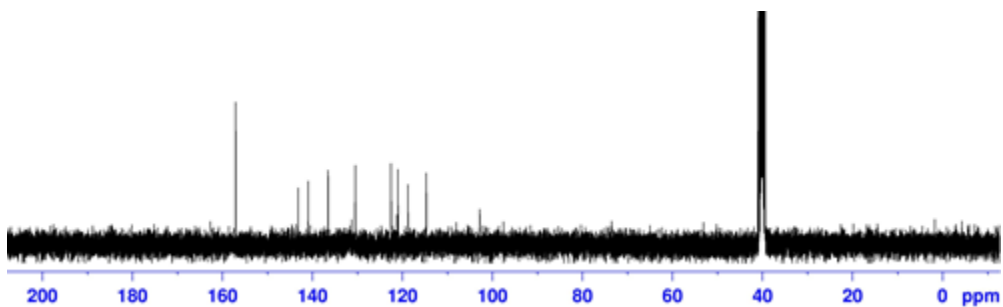


Figure S22: ^{13}C NMR spectrum (100 MHz, DMSO- d_6 , 25 $^\circ\text{C}$) of P2-OH.

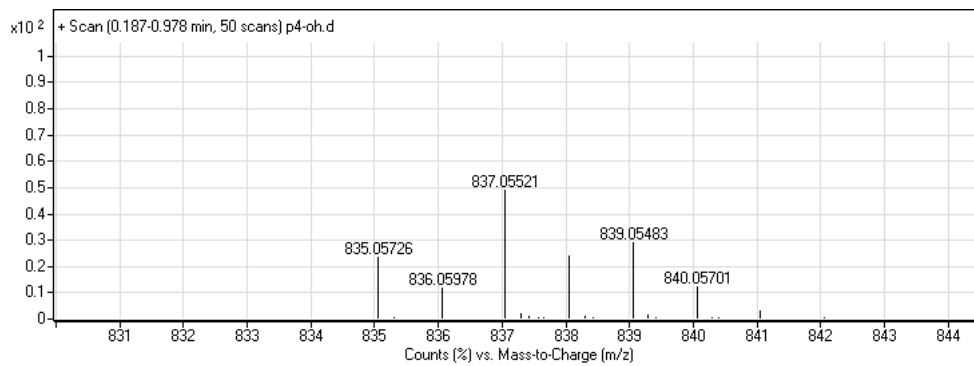


Figure S23: ESI-mass spectrum of P2-OH.

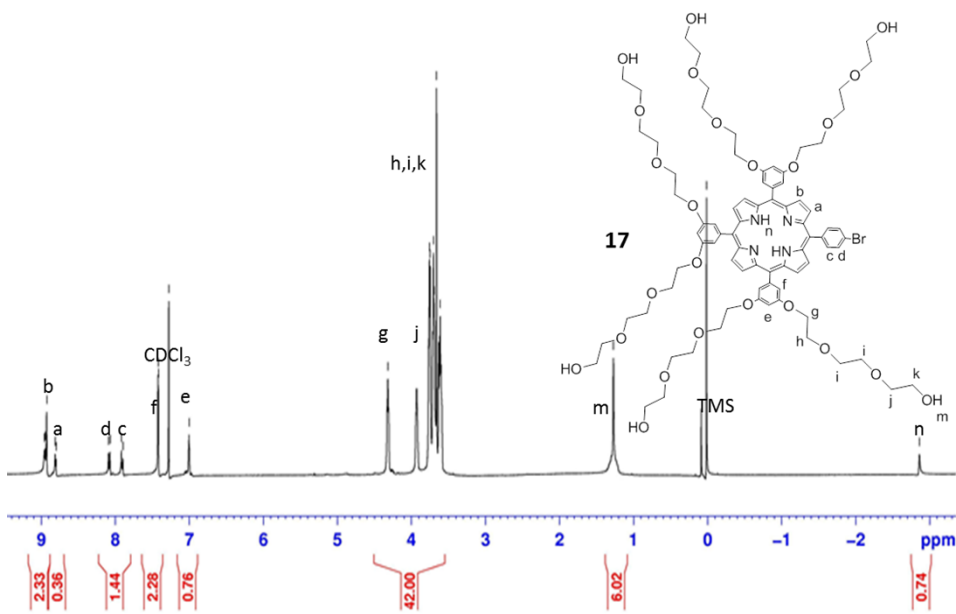


Figure S24: ^1H NMR spectrum (400 MHz, CDCl_3 , 25 $^\circ\text{C}$) of Porphyrin 1.

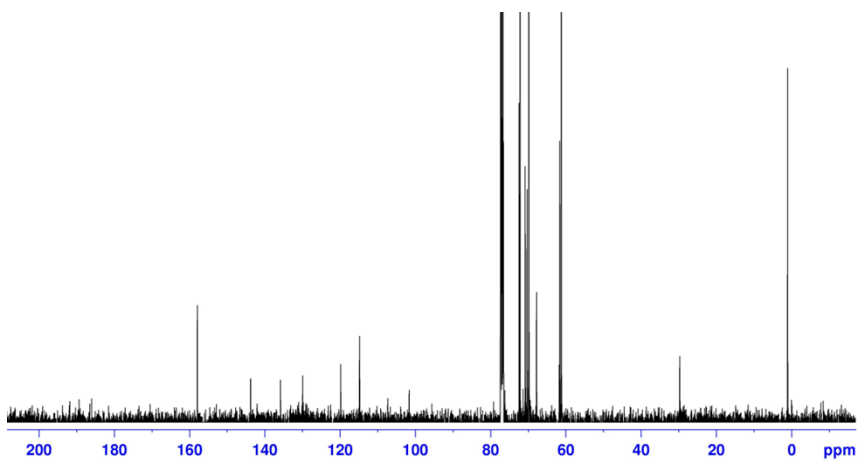


Figure S25: ¹³C NMR spectrum (100 MHz, CDCl₃, 25 °C) of **Porphyrin 1**.

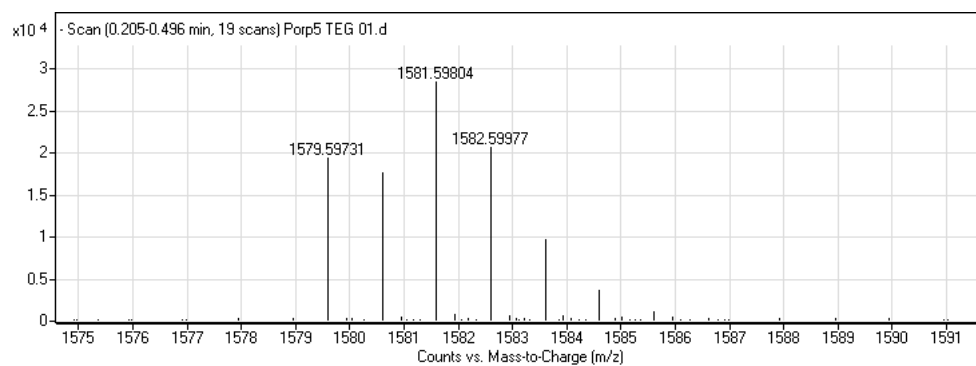


Figure S26: ESI-mass spectrum of **Porphyrin 1**.

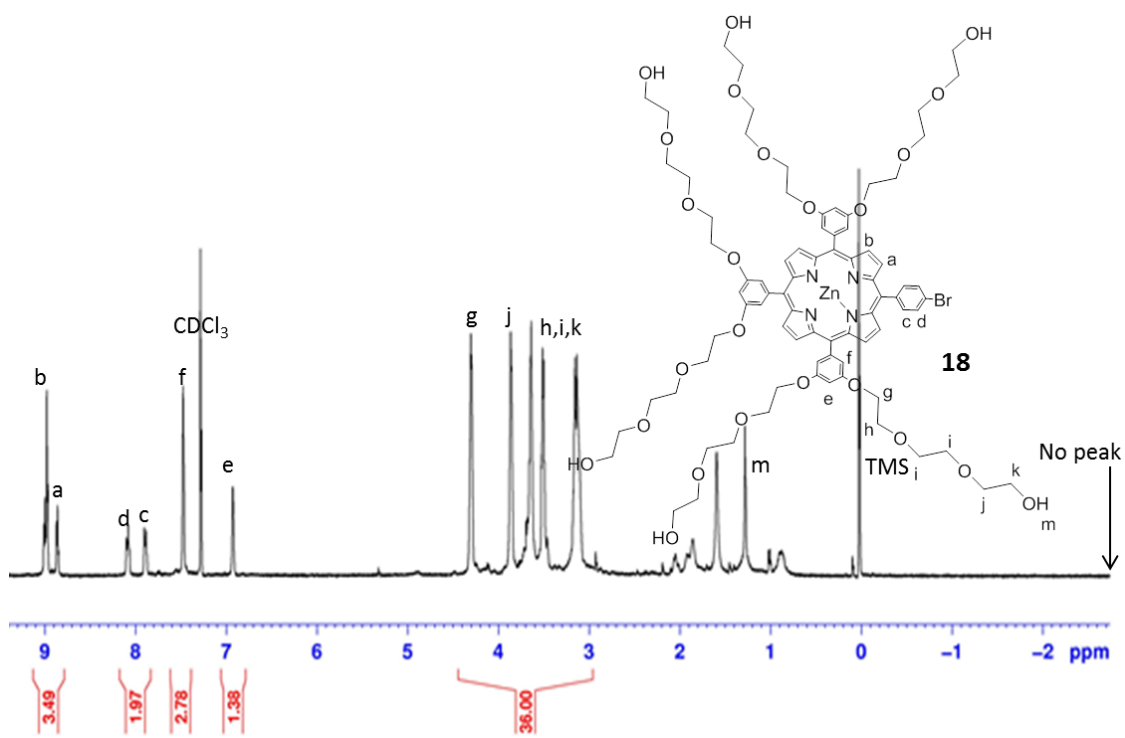


Figure S27: ^1H NMR spectrum (400 MHz, CDCl_3 , 25 $^\circ\text{C}$) of Porphyrin 1-Zn.

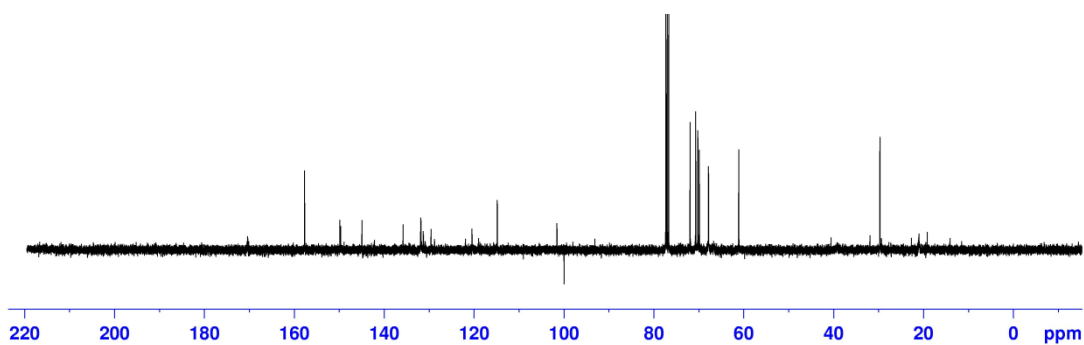


Figure S28: ^{13}C NMR spectrum (100 MHz, CDCl_3 , 25 $^\circ\text{C}$) of Porphyrin 1-Zn.

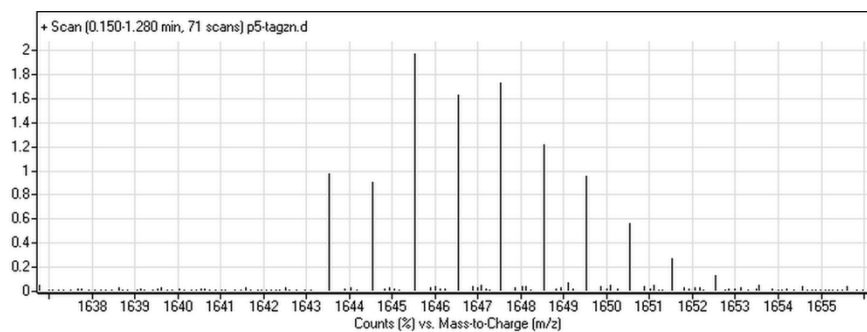


Figure S29: ESI-mass spectrum of Porphyrin 1-Zn.

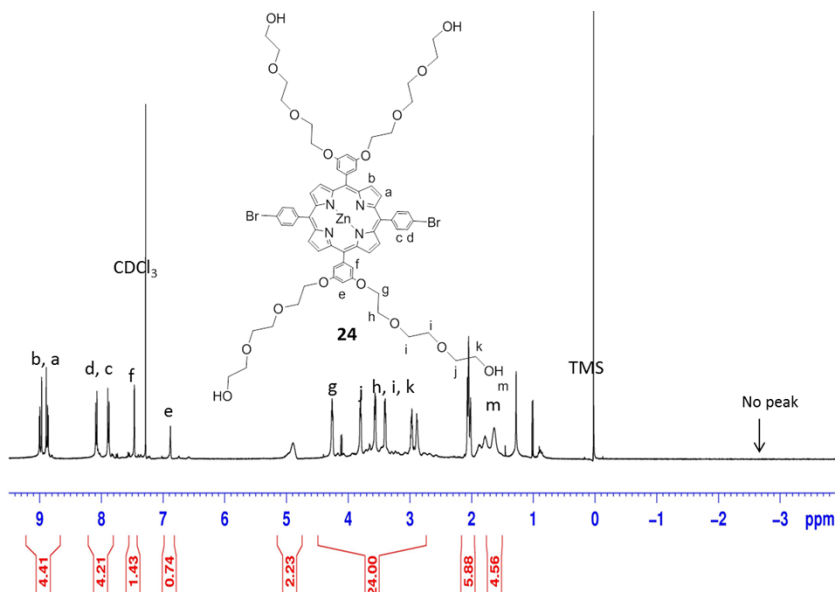


Figure S30: ¹H NMR spectrum (400 MHz, CDCl₃, 25 °C) of Porphyrin 2-Zn.

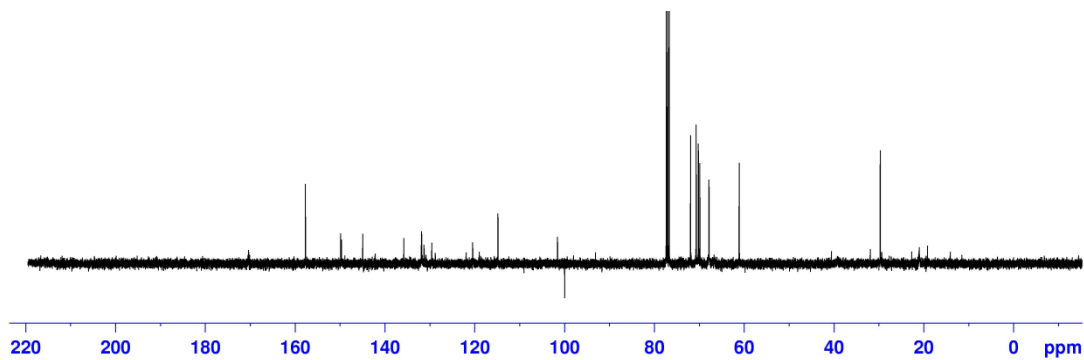


Figure S31: ¹³C NMR spectrum (100 MHz, CDCl₃, 25 °C) of Porphyrin 2-Zn.

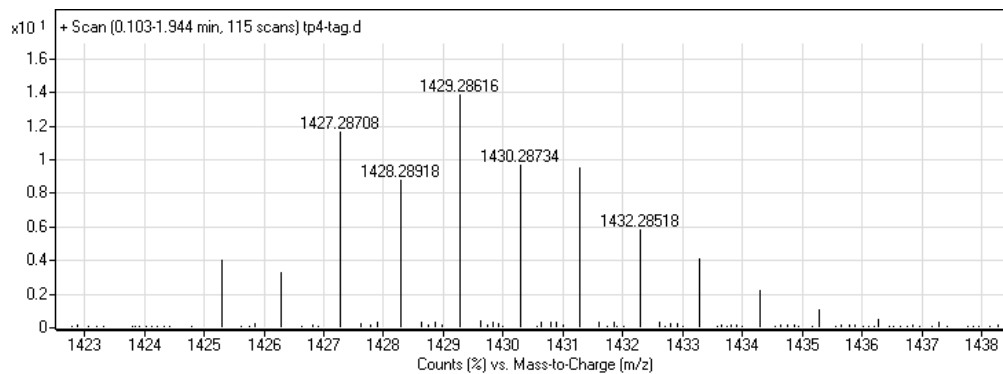


Figure S32: ESI-mass spectrum of Porphyrin 2-Zn.

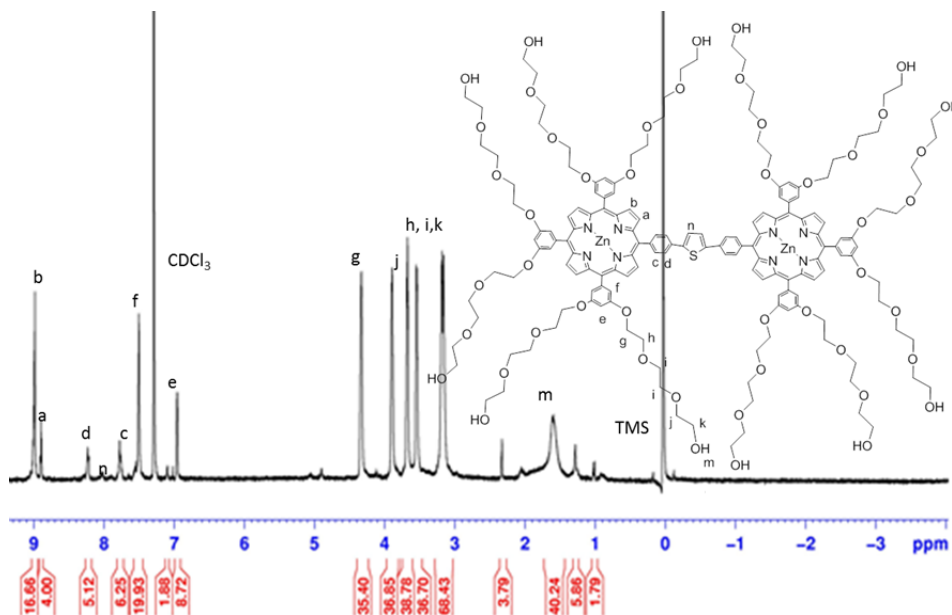


Figure S33: ¹H NMR spectrum (400 MHz, CDCl₃, 25 °C) of OTT₁P.

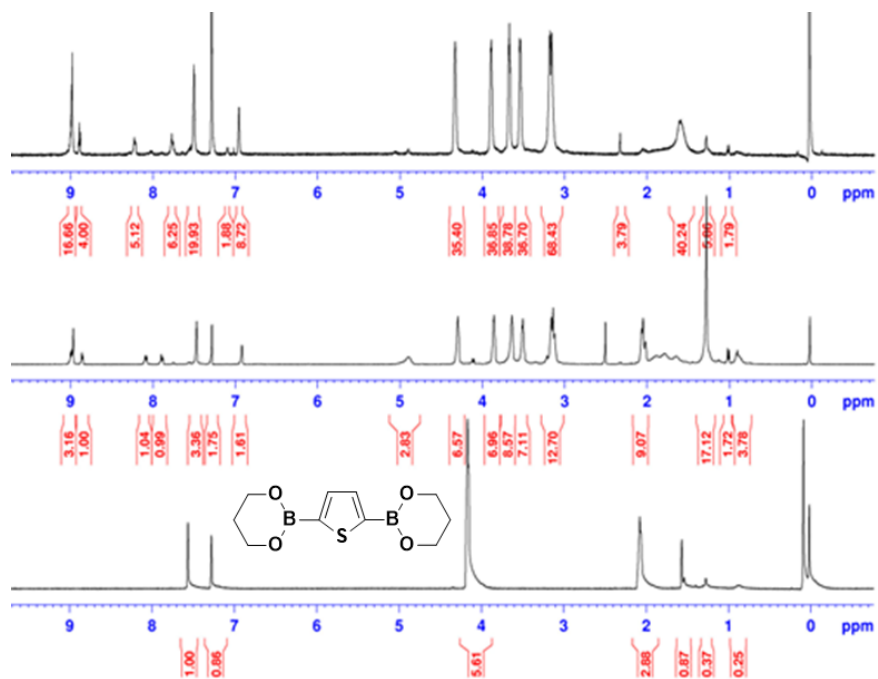


Figure S34: ¹H NMR spectrum of OTT₁P (top) overlaid with ¹H NMR of the corresponding precursor, Porphyrin 1-Zn (middle) and thiopheneboronic ester (bottom) recorded in CDCl₃.

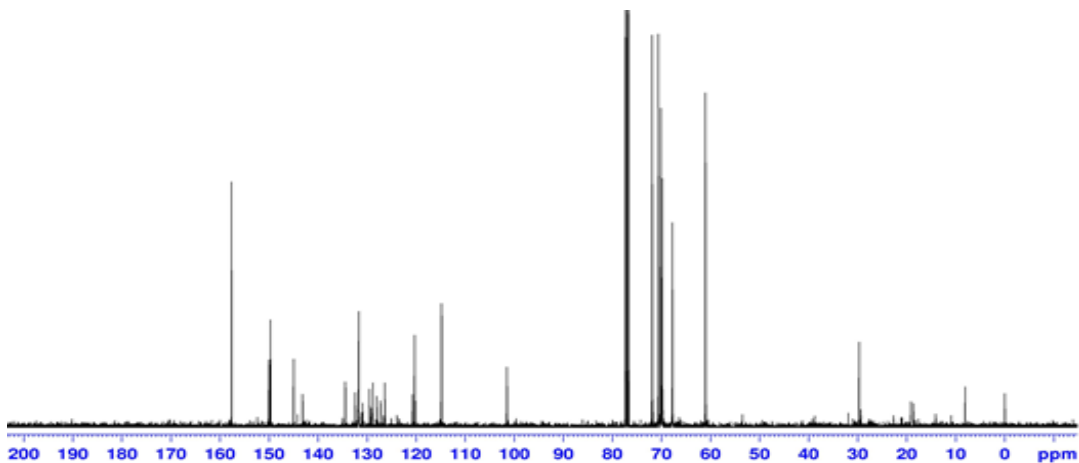


Figure S35: ^{13}C NMR spectrum (100 MHz, CDCl_3 , 25 °C) of OTT_1P .

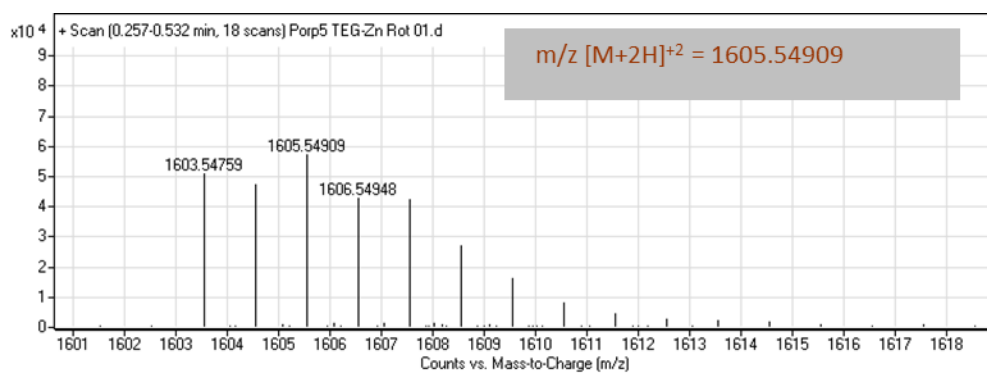


Figure S36: ESI-mass spectrum of OTT_1P .

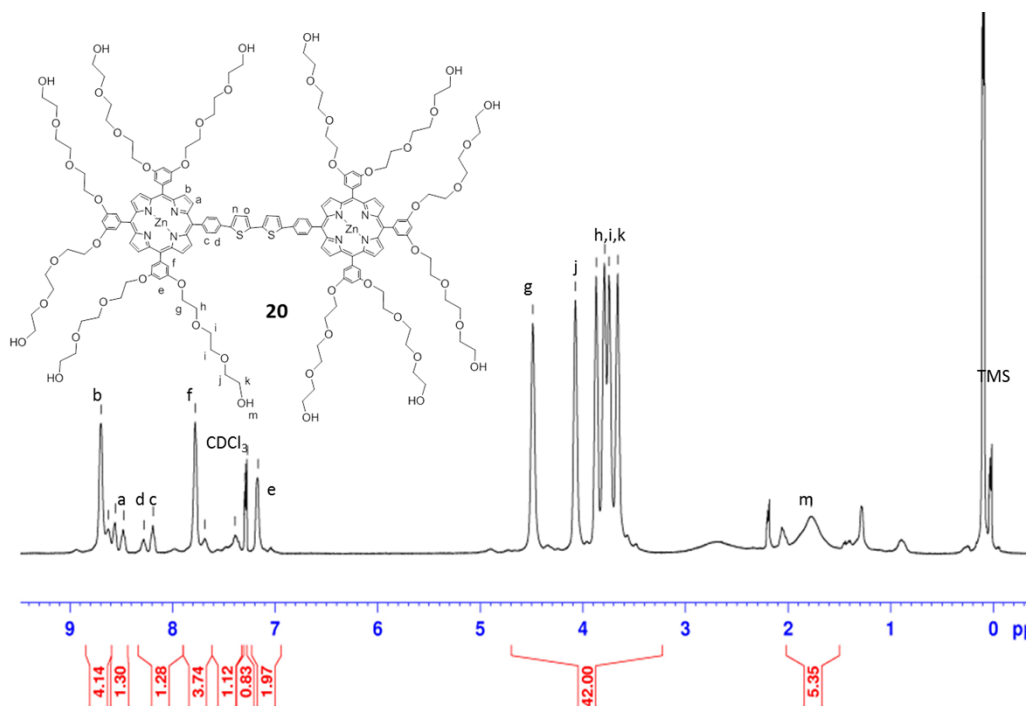


Figure S37: ^1H NMR spectrum (400 MHz, CDCl_3 , 25 °C) of OTT_2P .

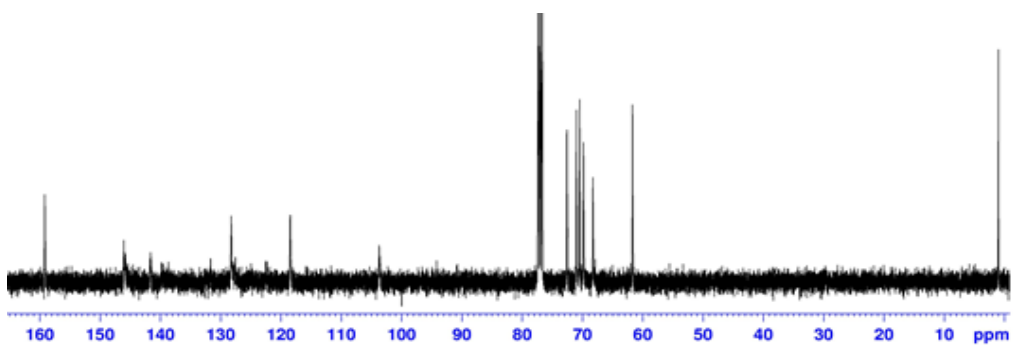


Figure S38: ^{13}C NMR spectrum (100 MHz, CDCl_3 , 25 °C) of OTT_2P .

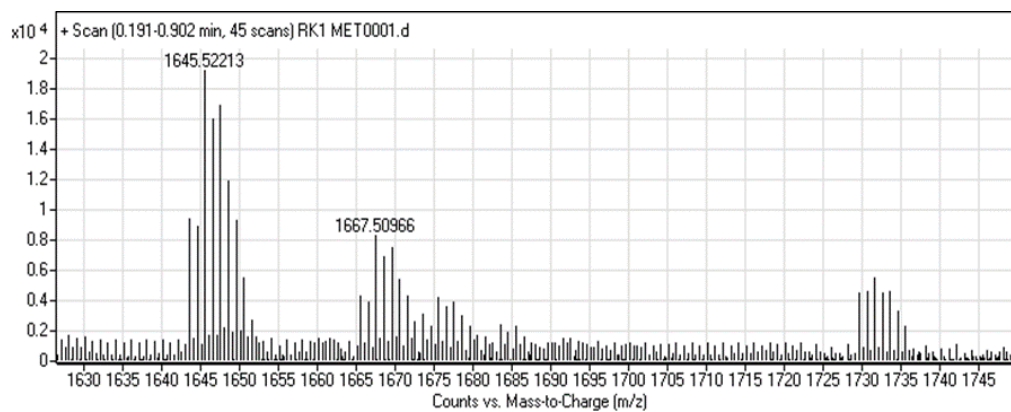


Figure S39: ESI-mass spectrum of OTT_2P .

Ion name	Ion mass	Charge	Mass	Result
Positive ion mode				
M+2H	M/2 + 1.007276	2+	1.007276	1646.587276
M+ACN+2H	M/2 + 21.520550	2+	21.520550	1667.100550

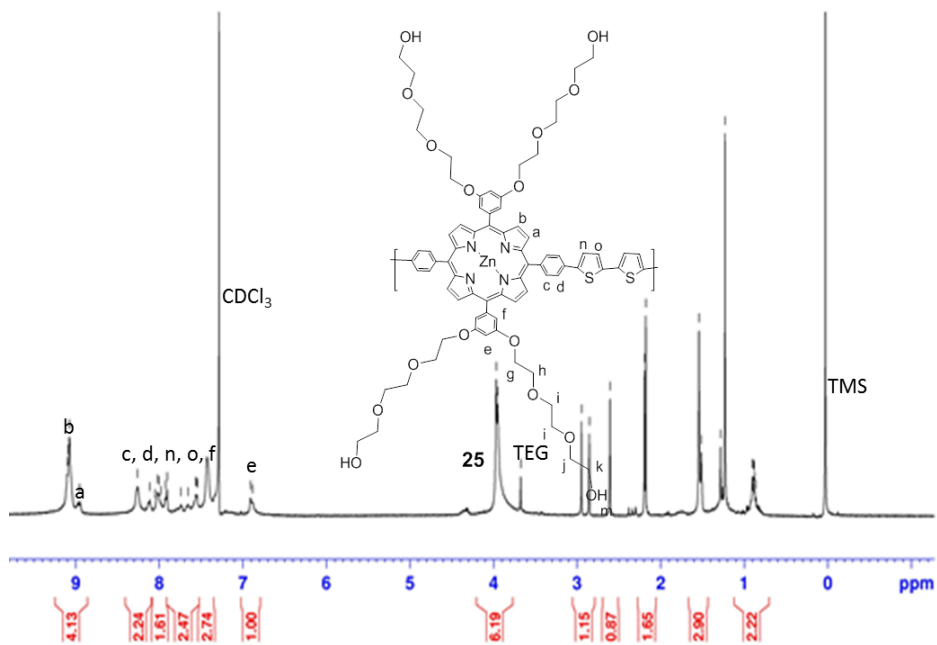


Figure S40: ¹H NMR spectrum (400 MHz, CDCl₃, 25 °C) of PTPP.

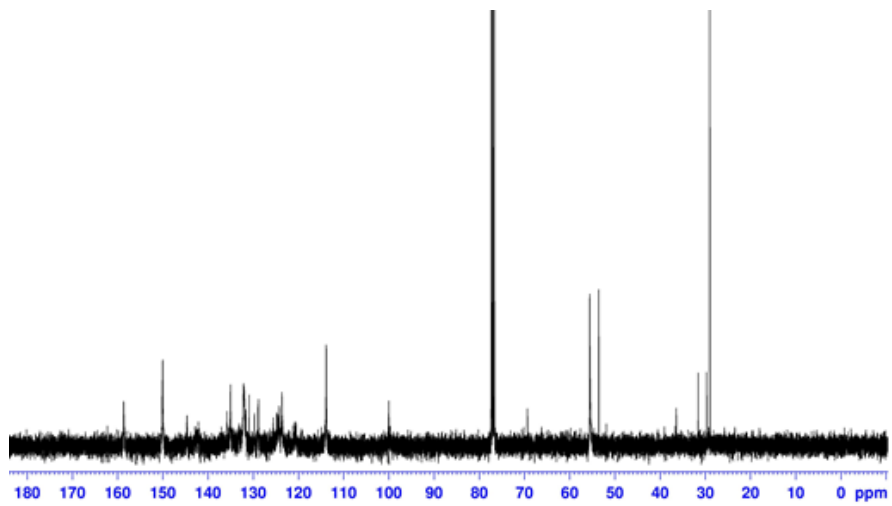


Figure S41: ¹³C NMR spectrum (100 MHz, CDCl₃, 25 °C) of PTPP.

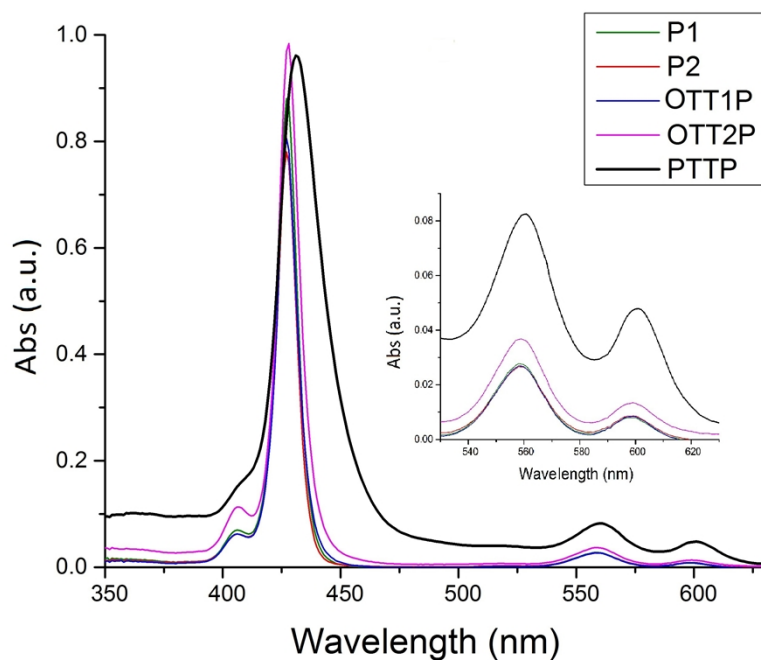


Figure S42: Normalized absorption spectra of the compounds in DMF. Inset of figure shows the zoomed version of the Q-bands.

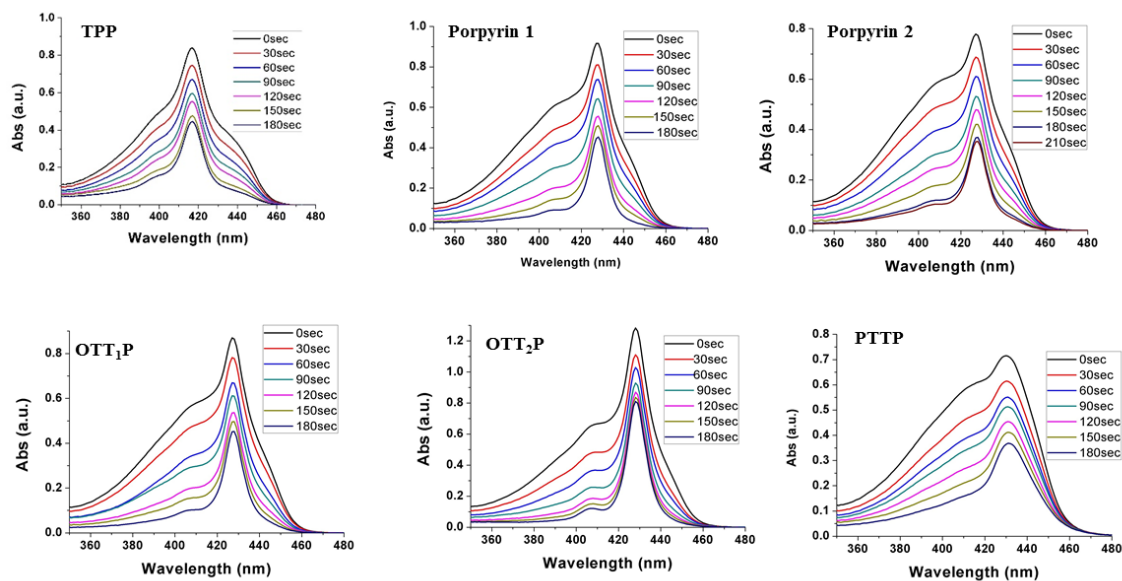


Figure S43: Decrease in absorbance intensity of DPBF with time in the presence of photosensitizers based on porphyrin monomers, oligomers and polymer as well as tetraphenylporphyrin (TPP) used as reference photosensitizers.

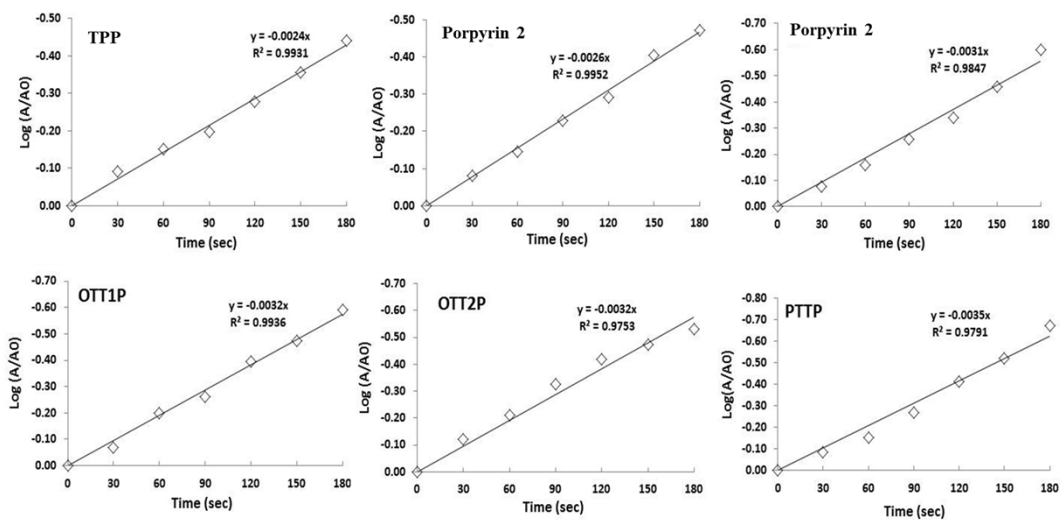


Figure S44: Time-dependent decrease of absorbance at 418 nm by oxidation of DPBF (20 μM) with porphyrin sensitizers (0.5 μM) in DMF against tetraphenylporphyrin (TPP) as the standard irradiated at 420 nm under monochromator integrated Xenon lamp.