

Supporting Information

A convenient synthesis of pentaporphyrins and supramolecular complexes with a fulleropyrrolidine

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1. NMR and mass spectra

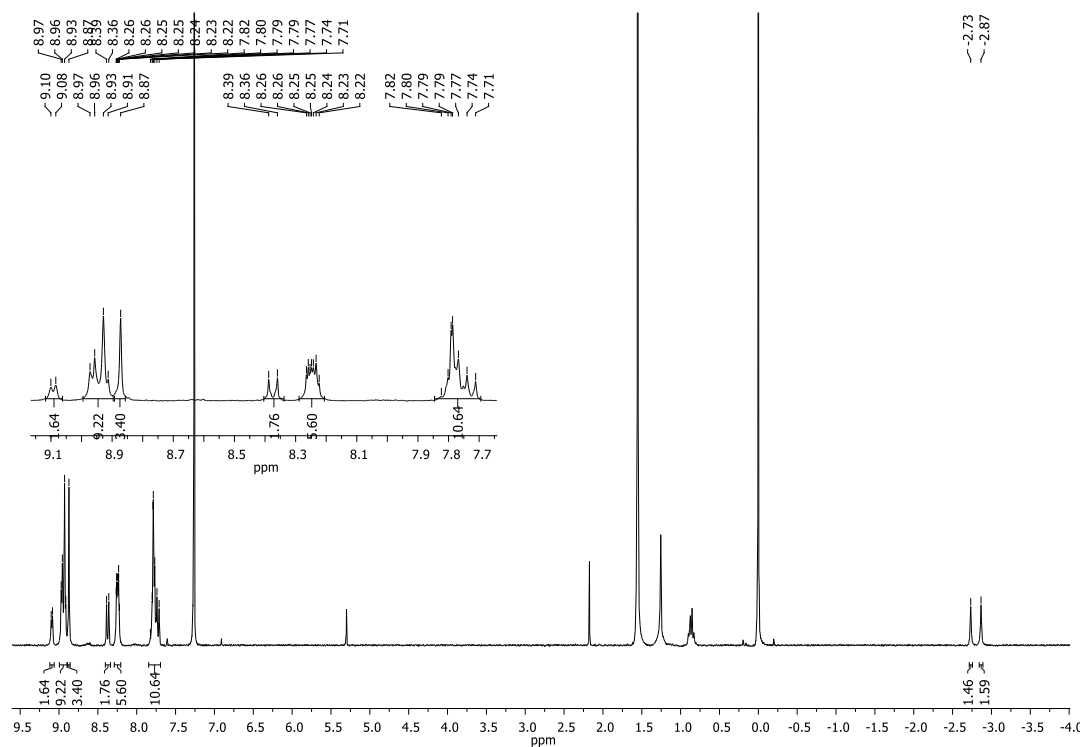


Figure S1: ¹H NMR spectrum of diporphyrin **3** (in CDCl₃).

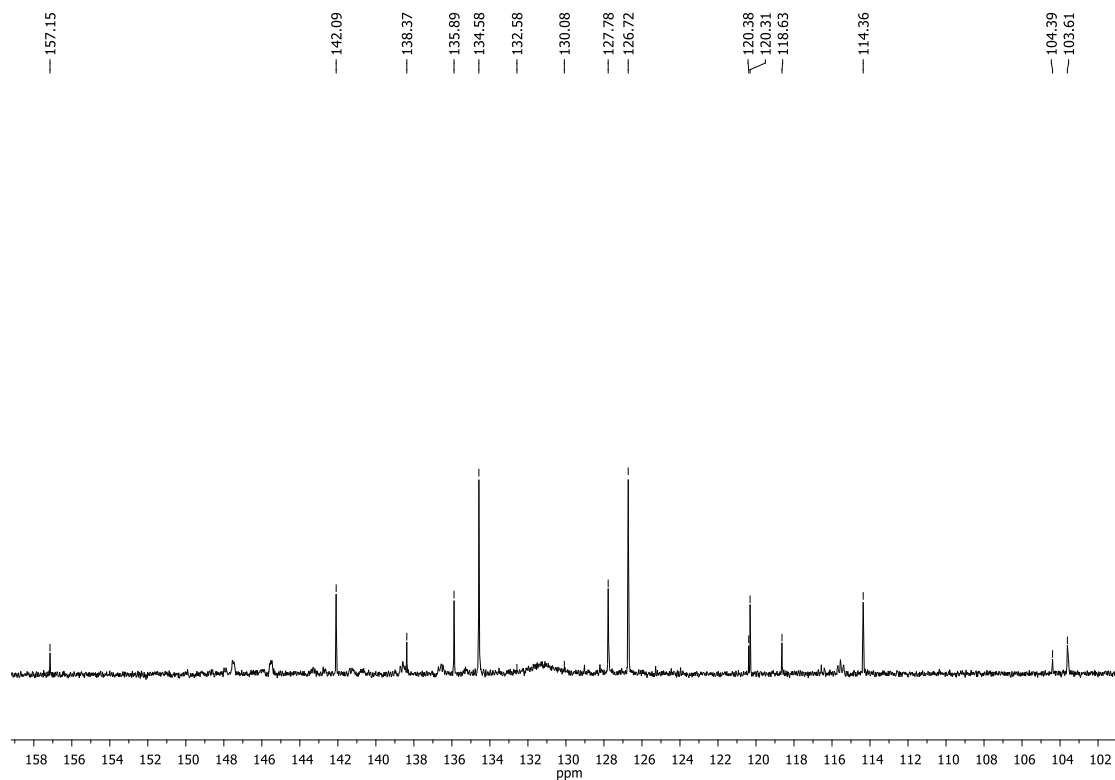


Figure S2: ¹³C NMR spectrum of diporphyrin **3** (in CDCl₃).

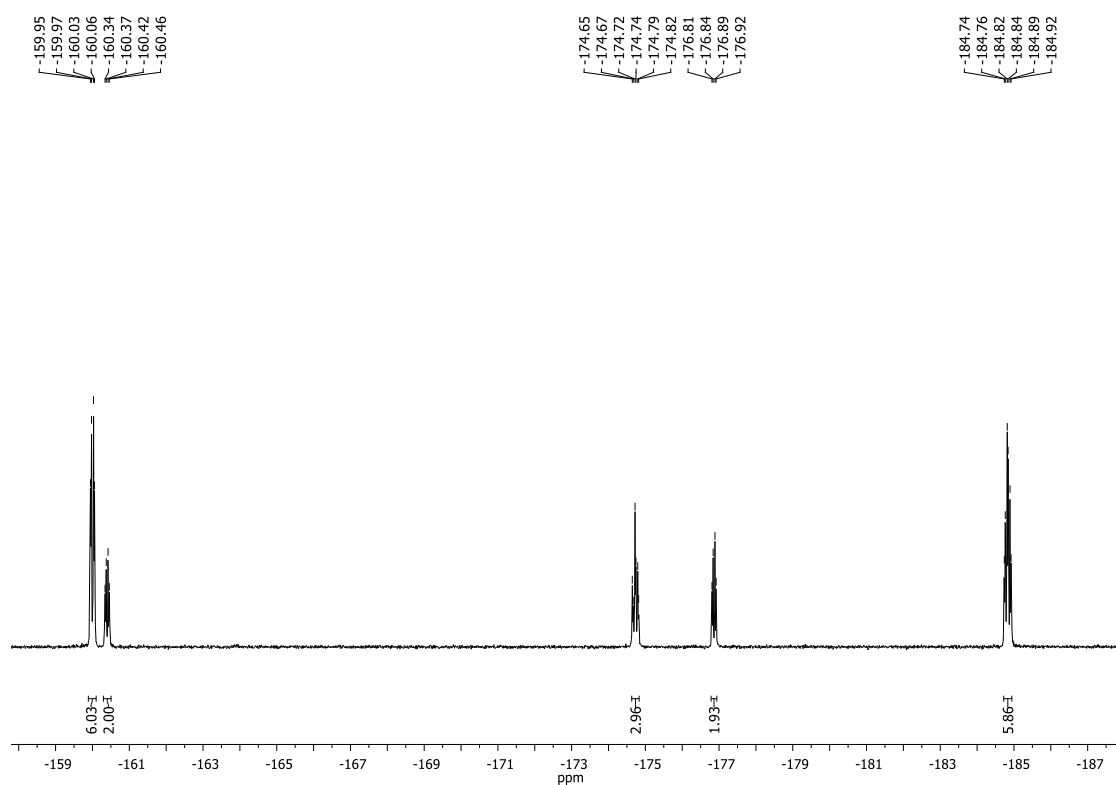


Figure S3: ^{19}F NMR spectrum of diporphyrin **3** (in CDCl_3).

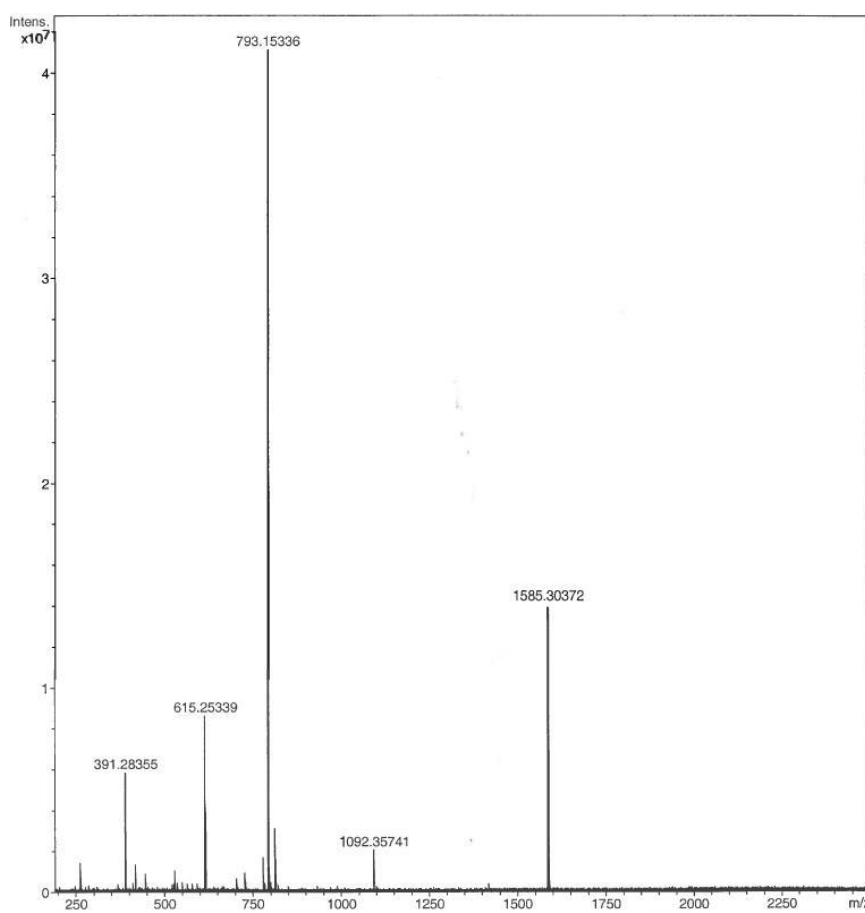


Figure S4: High-resolution electrospray ionization mass spectrum (ESI MS) of diporphyrin **3**.

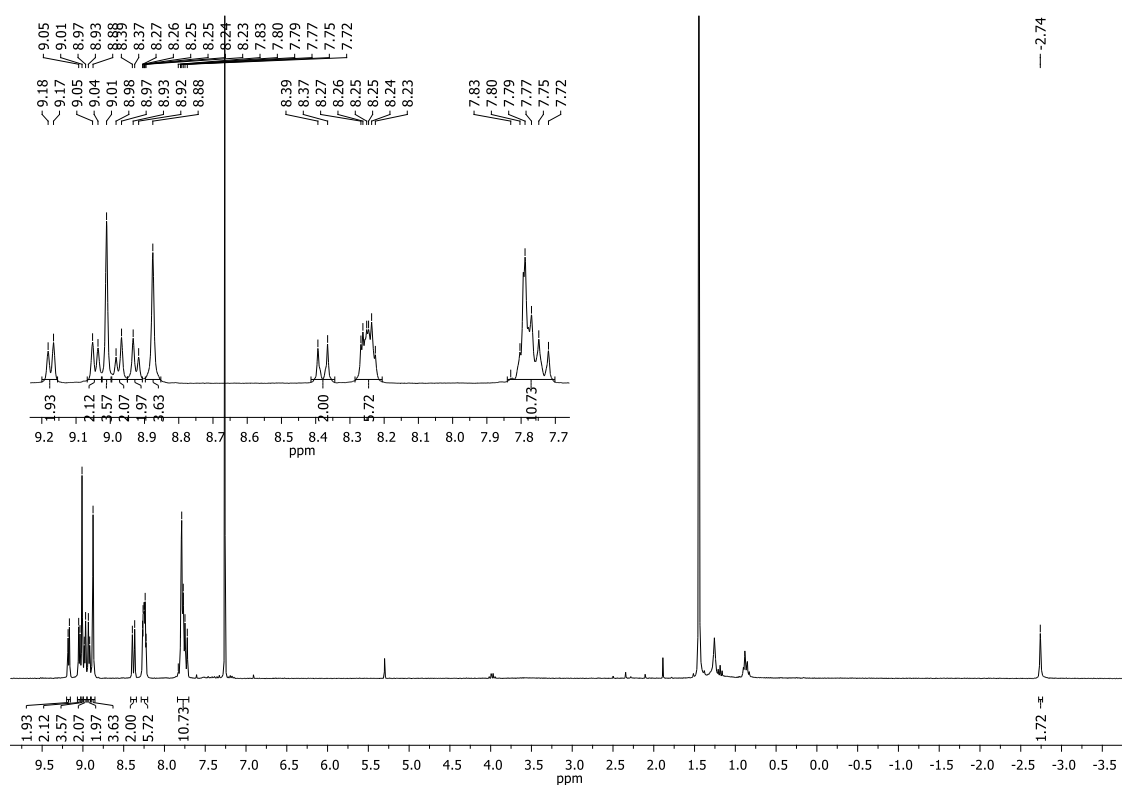


Figure S5: ¹H NMR spectrum of diporphyrin **4** (in CDCl₃).

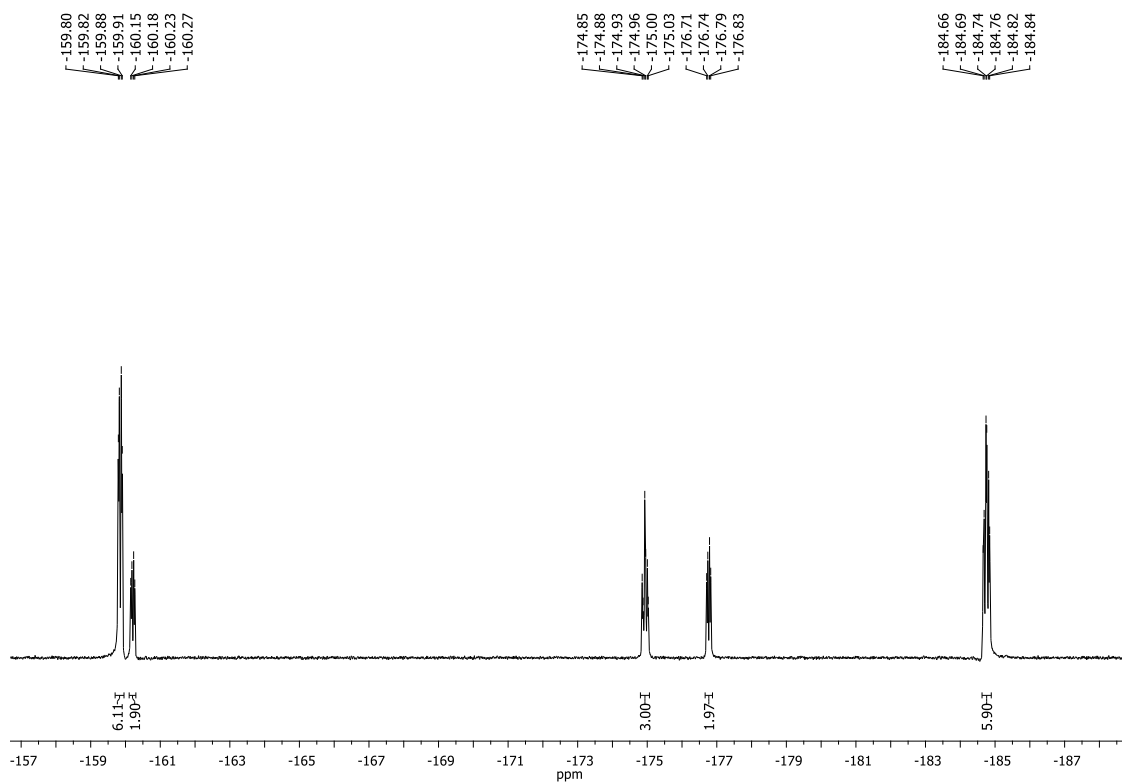


Figure S6: ¹⁹F NMR spectrum of diporphyrin **4** (in CDCl₃).

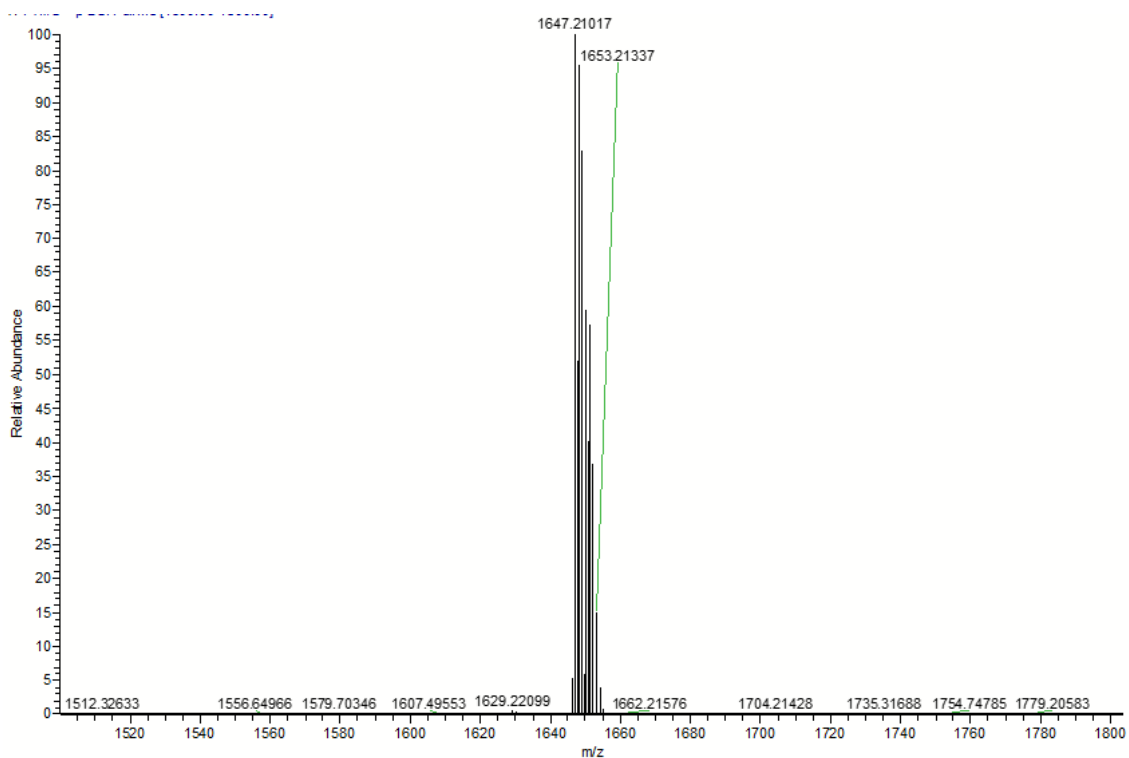


Figure S7: High-resolution electrospray ionization mass spectrum (ESI MS) of diporphyrin **4**.

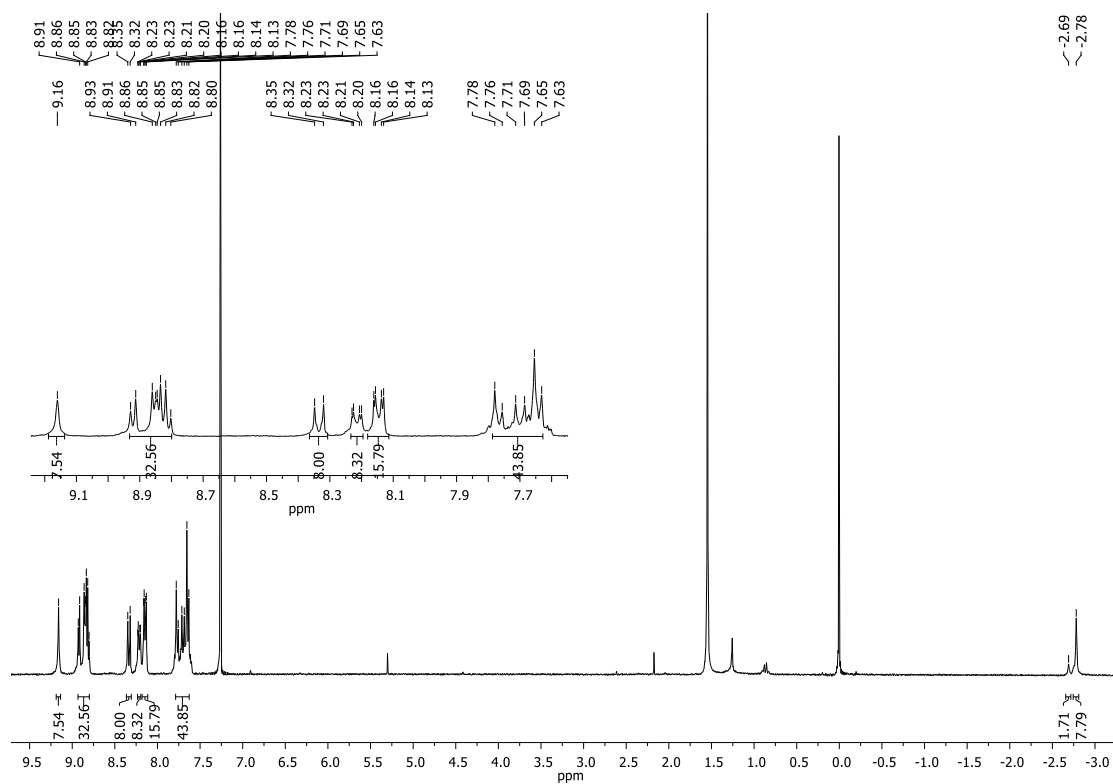


Figure S8: ^1H NMR spectrum of pentaporphyrin **5** (in CDCl_3).

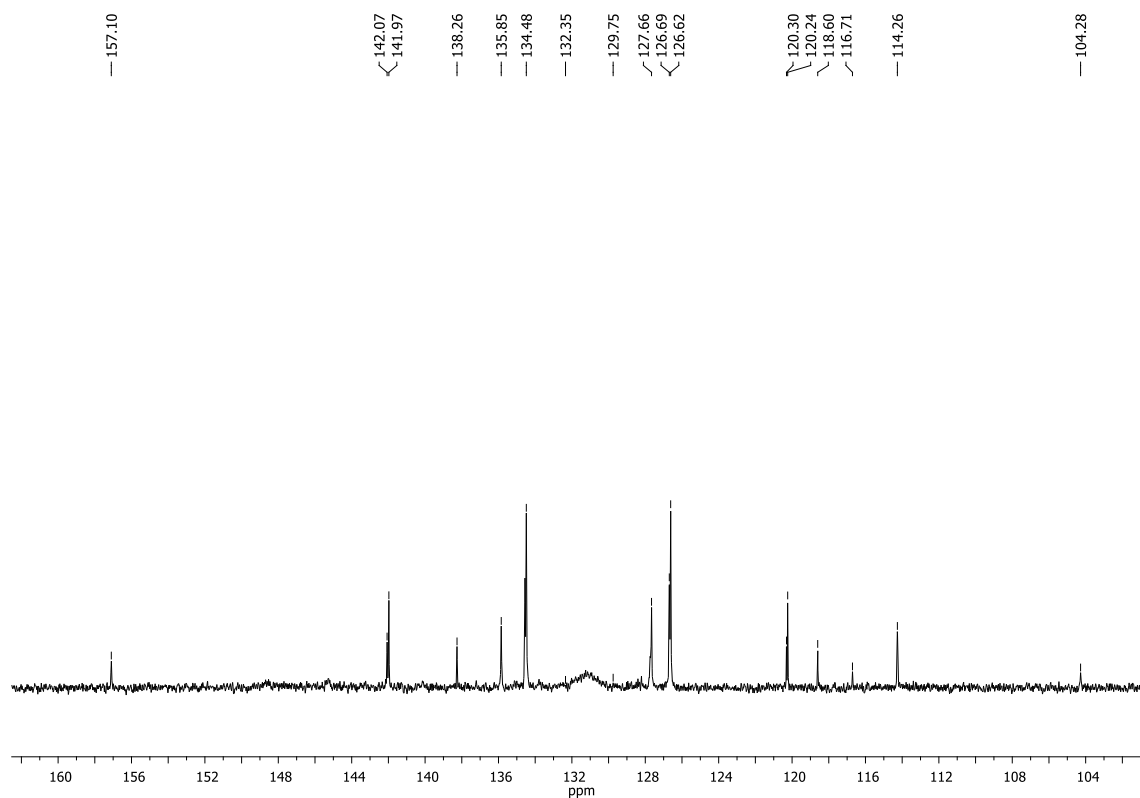


Figure S9: ^{13}C NMR spectrum of pentaporphyrin **5** (in CDCl_3).

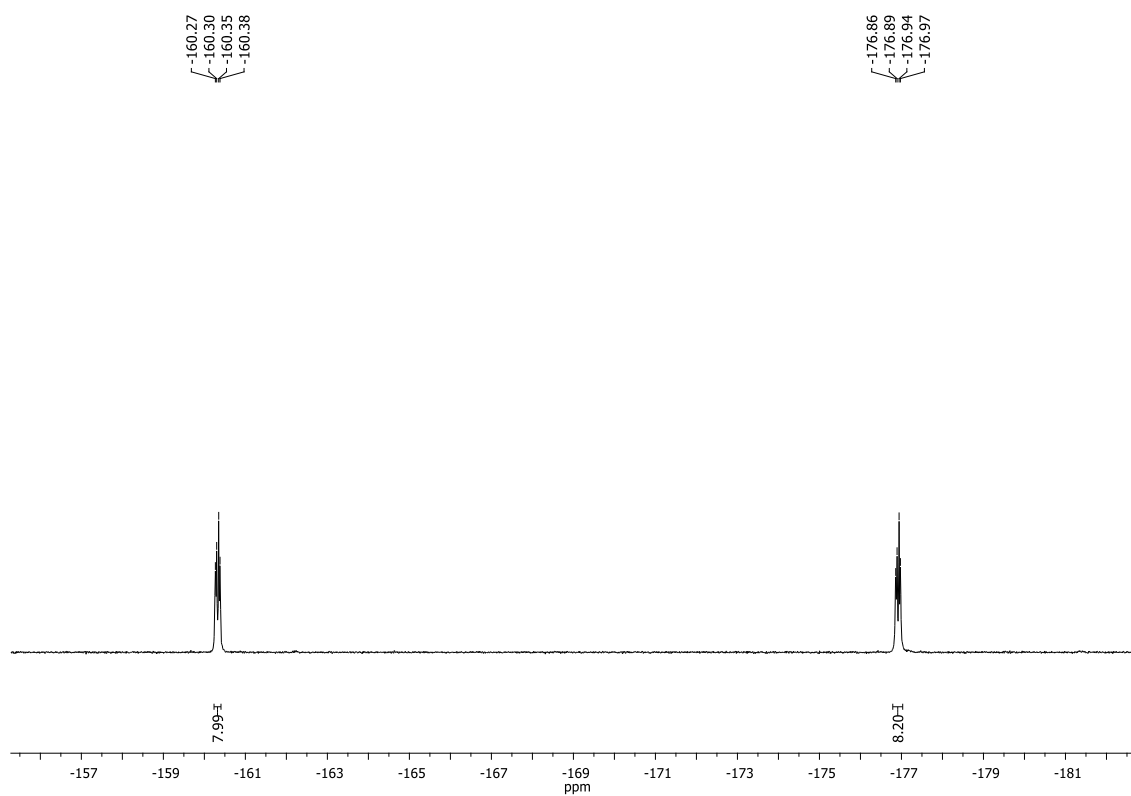
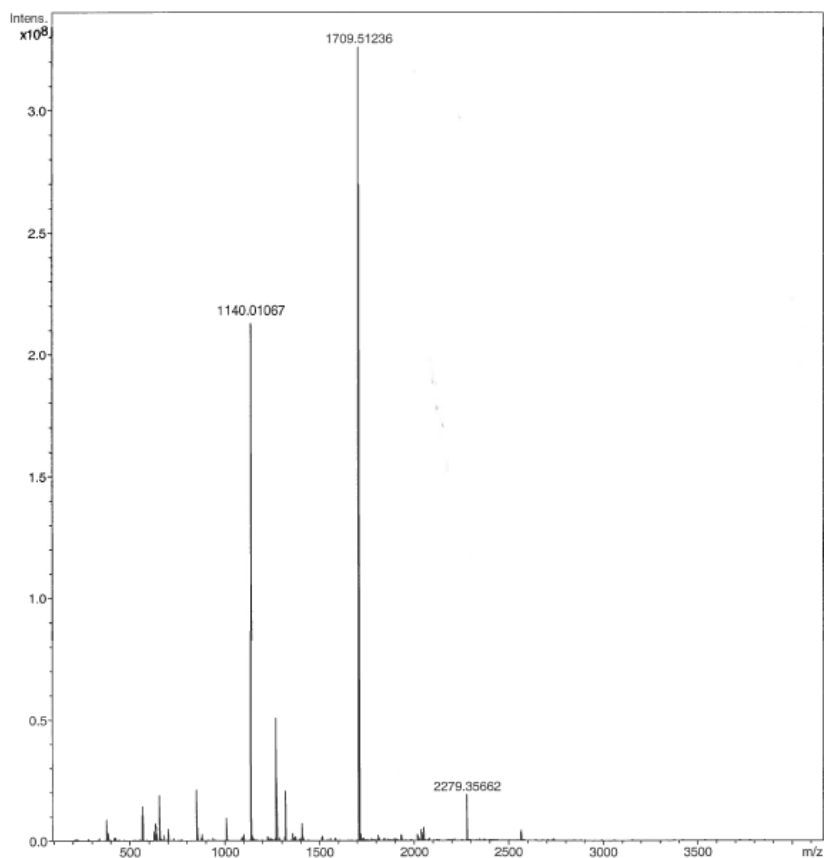


Figure S10: ^{19}F NMR spectrum of pentaporphyrin **5** (in CDCl_3).



Mass Spectrum List Report

m/z	I	Res.	m/z	I	Res.
391.26399	3300140	155923	1145.34431	2423258	53646
631.24927	4071342	96609	1145.67963	2628838	50244
632.25264	1848788	98120	1146.01461	2322098	50847
637.24917	6845205	92207	1146.34939	1700446	52757
637.75096	7118488	93793	1228.73081	1816881	47579
638.25259	3142811	95104	1273.49363	50677220	47202
644.28082	6324030	94423	1274.49706	50610692	47321
645.28426	3130948	94420	1274.52690	3772422	86489
659.24413	18684036	91407	1275.50022	24052774	45383
660.24746	8804872	92492	1275.53012	1858982	85448
661.25066	2062732	92113	1276.50297	7509573	45626
684.20804	1877452	89365	1277.50568	1844069	44894
684.40888	2492204	84788	1320.40020	11128110	45105
684.60965	1852780	86071	1320.90162	20923708	45389
703.27057	4838244	86001	1321.40298	19324744	45336
704.27397	2321253	88446	1321.90497	12433236	45368
854.75792	6908612	68801	1322.40665	6380897	44382
855.00900	16069956	70174	1322.90864	2500589	43810
855.25975	21022278	70543	1360.49322	2052881	43957
855.51053	17683526	69249	1360.82741	2856151	43718
855.76131	11001160	67359	1361.16160	2788317	45018
856.01219	5658185	67219	1361.49630	2144803	44285
856.26352	2696586	66207	1409.40614	4268167	37217
880.93597	2583498	70268	1409.90703	7303310	39783
881.27024	2545292	69610	1410.40821	7120021	41095
1009.35679	6331159	59105	1410.90942	4646812	40648
1009.85827	9571105	59189	1411.41229	2071330	40803
1010.35966	7625515	58152	1515.21169	2140082	40832
1010.86162	3943989	58764	1515.46230	2137655	37225
1100.84808	2752251	54196	1515.71291	1863612	39036
1101.35018	2187466	54854	1708.01076	3066869	33885
1139.00630	2784762	50890	1708.51286	84407312	36109
1139.34266	65527620	53858	1708.77396	5160100	29274
1139.67651	168240976	54483	1709.01196	244091952	36914
1140.01067	214968160	54734	1709.26710	22365762	32562
1140.34528	184113008	54142	1709.51236	326413408	36636
1140.68016	112920440	54104	1709.76763	28771936	32682
1141.01498	55474048	52517	1709.96169	26678380	65999
1141.34969	23587724	51419	1710.01420	272657536	36864
1141.68418	8982168	50817	1710.26896	18378880	31876
1142.01845	3278964	49847	1710.51676	162892944	36620
			1710.77176	6931616	30058

Figure S11: High-resolution electrospray ionization mass spectrum (ESI MS) of pentaporphyrin 5.

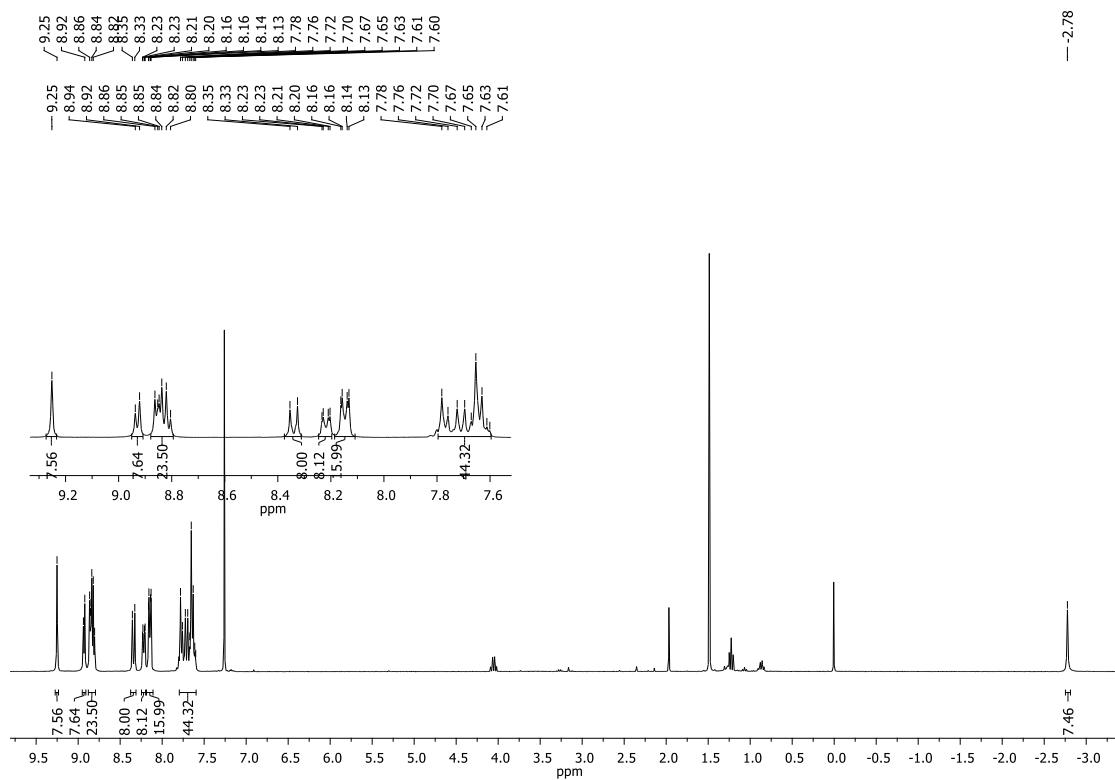


Figure S12: ¹H NMR spectrum of pentaporphyrin **6** (in CDCl₃).

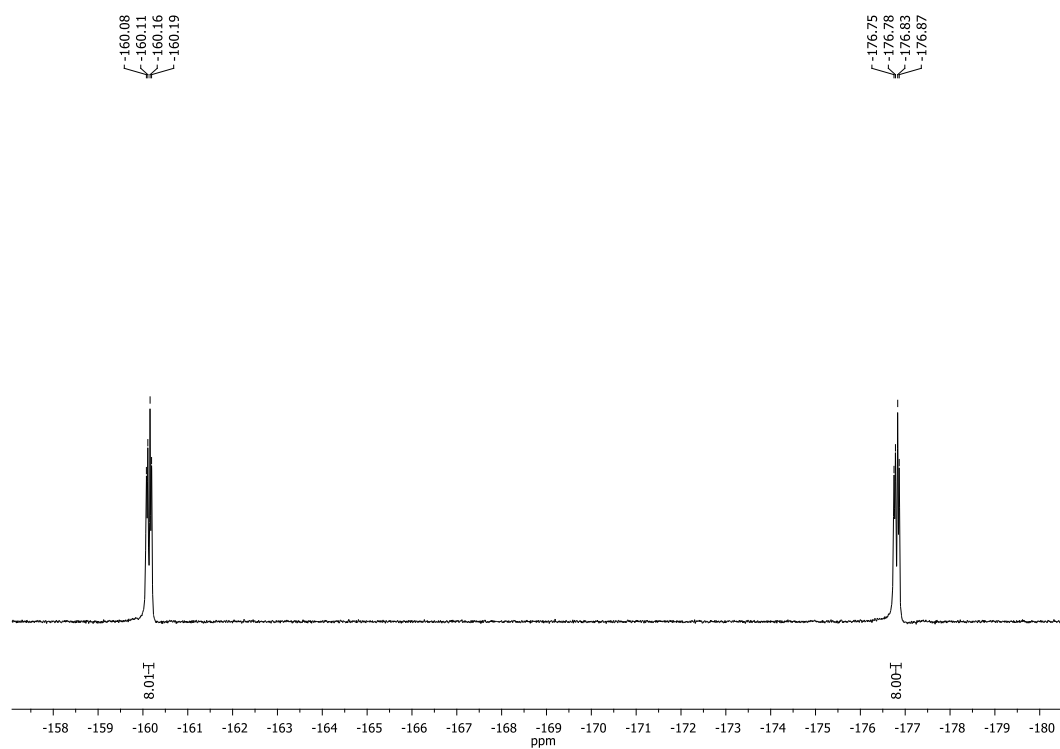


Figure S13: ¹⁹F NMR spectrum of pentaporphyrin **6** (in CDCl₃).

2. Absorption and fluorescence titrations with PyC₆₀

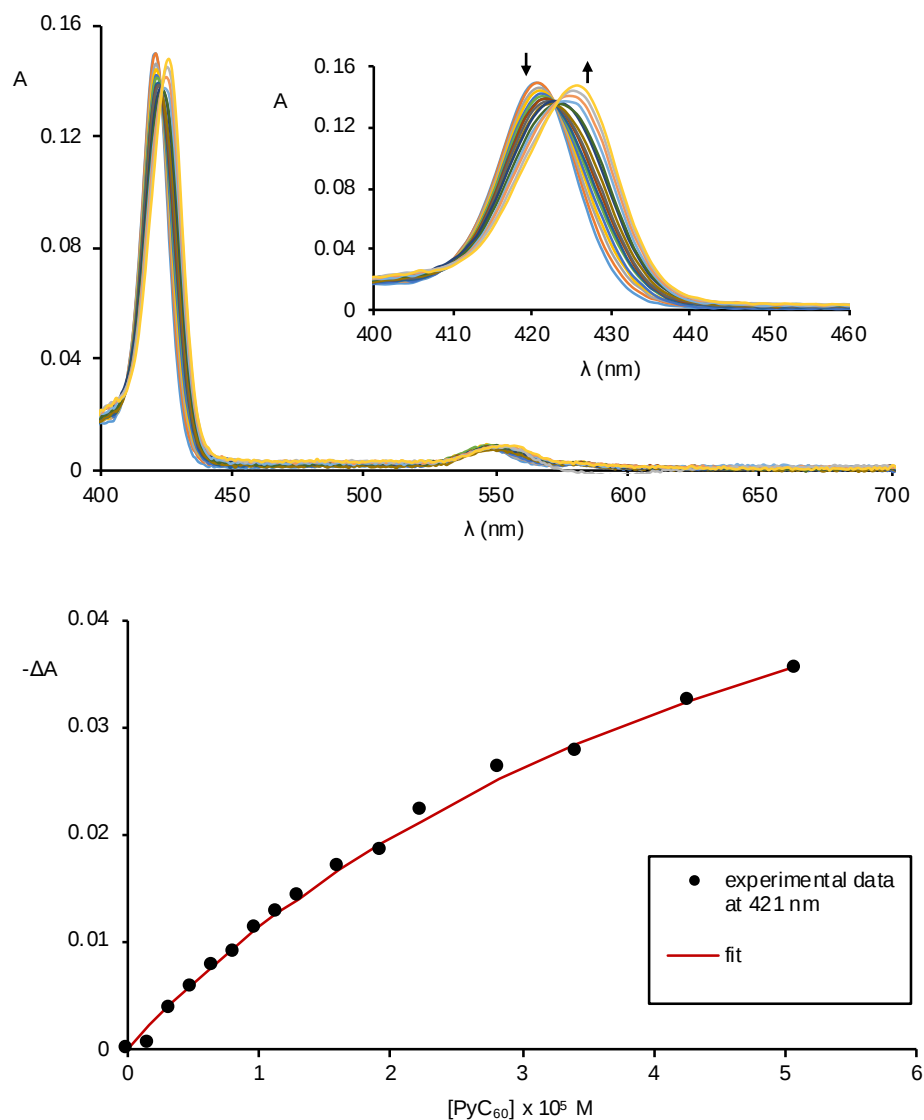


Figure S14: Absorption spectra of Zn²⁺ (5.0 × 10⁻⁷ M) upon addition of PyC₆₀ (0–113 equiv.) in toluene at ambient temperature (upper part) and experimental data at 421 nm fitted to a non-linear 1:1 binding model (lower part).

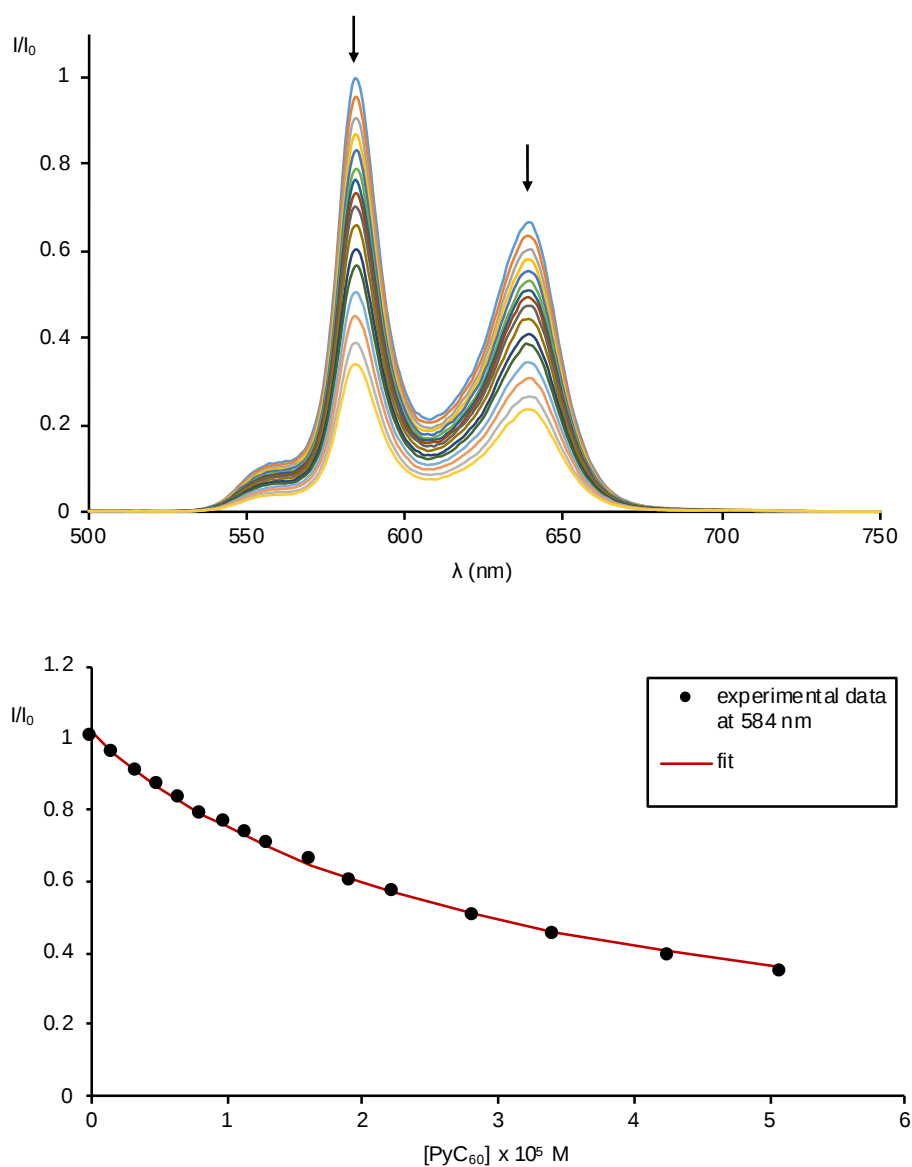


Figure S15: Fluorescence spectra ($\lambda_{\text{exc}} = 423 \text{ nm}$) of Zn^{2+} ($5.0 \times 10^{-7} \text{ M}$) upon the addition of PyC_{60} (0–113 equiv.) in toluene at ambient temperature (upper part) and experimental data at 589 nm fitted to a non-linear 1:1 binding model (lower part).

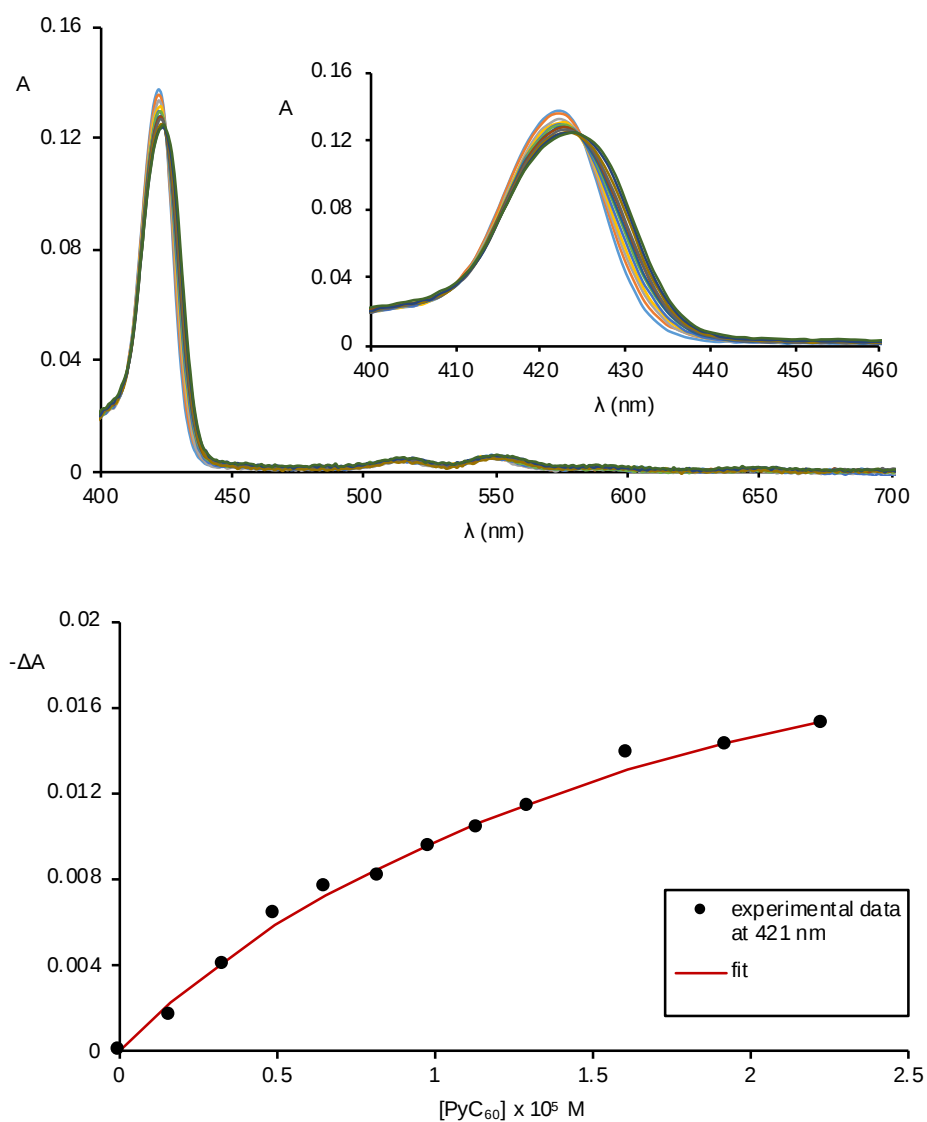


Figure S16: Absorption spectra of diporphyrin **4** (2.0×10^{-7} M) upon addition of PyC₆₀ (0–116 equiv.) in toluene at ambient temperature (upper part) and experimental data at 421 nm fitted to a non-linear 1:1 binding model (lower part).

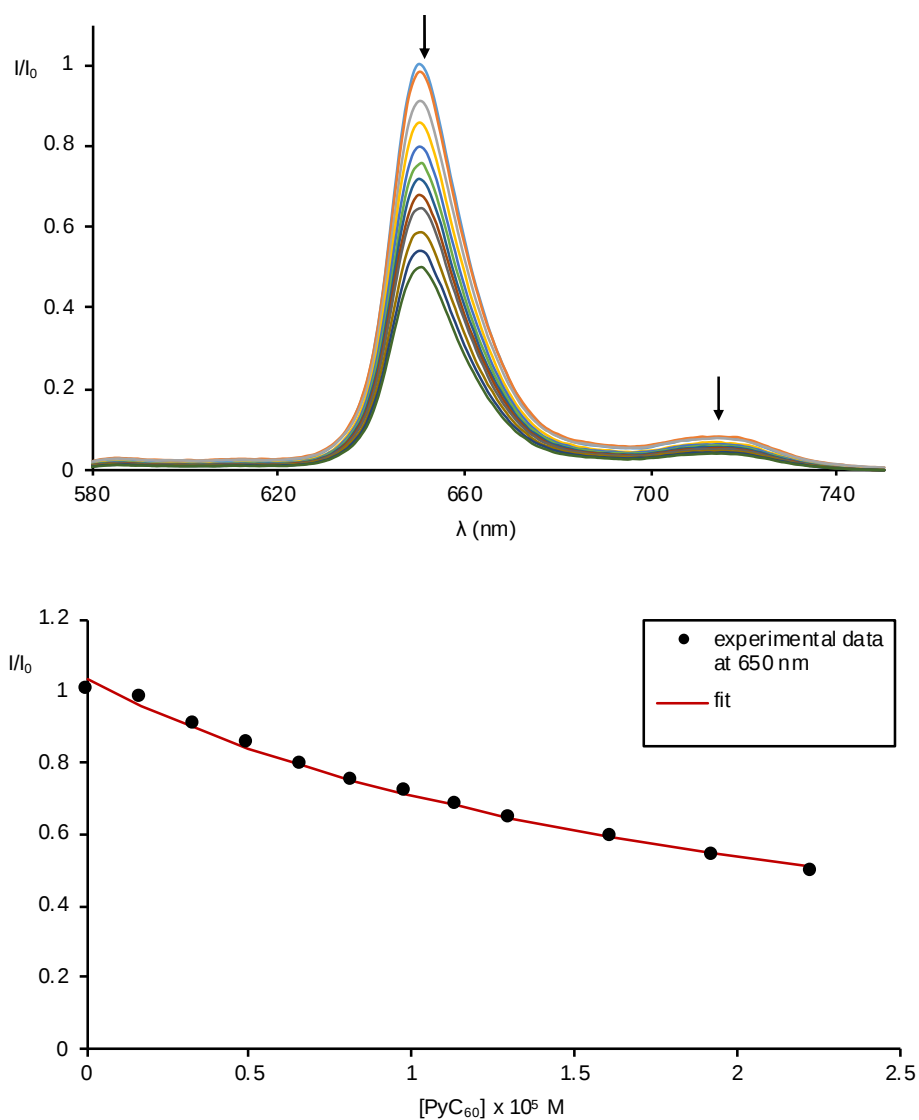


Figure S17: Fluorescence spectra ($\lambda_{\text{exc}} = 425$ nm) of **4** (2.0×10^{-7} M) upon addition of PyC_{60} (0–116 equiv.) in toluene at ambient temperature (upper part) and experimental data at 650 nm fitted to a non-linear 1:1 binding model (lower part).