Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

The optical characterization of metal-mediated aggregation behaviour of amphiphilic Zn(II) phthalocyanines

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Supporting Information

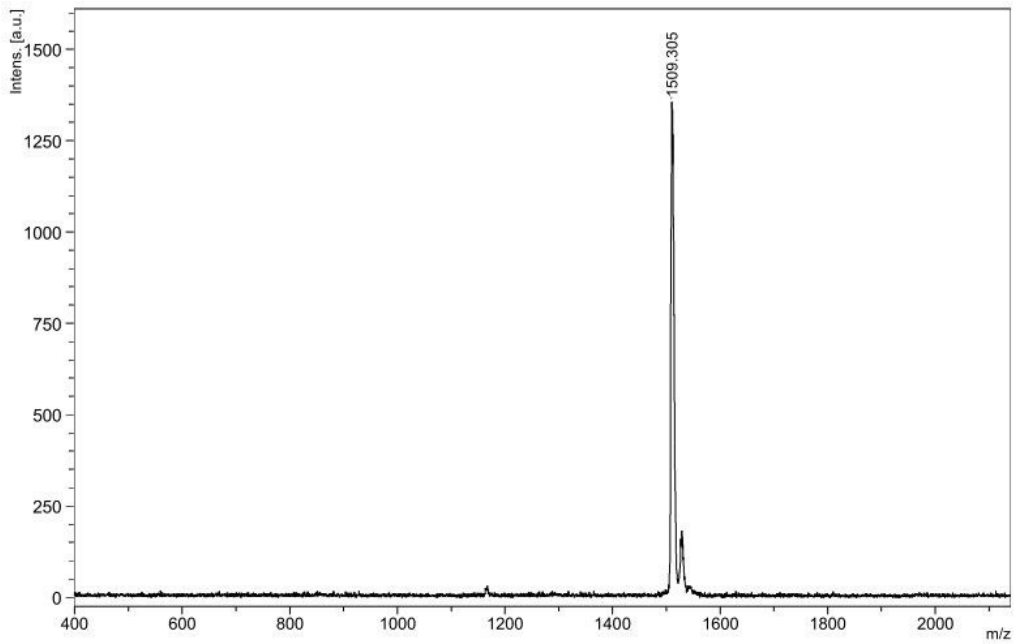

Figure S1. MALDI-TOF mass spectrum of compound **3**.

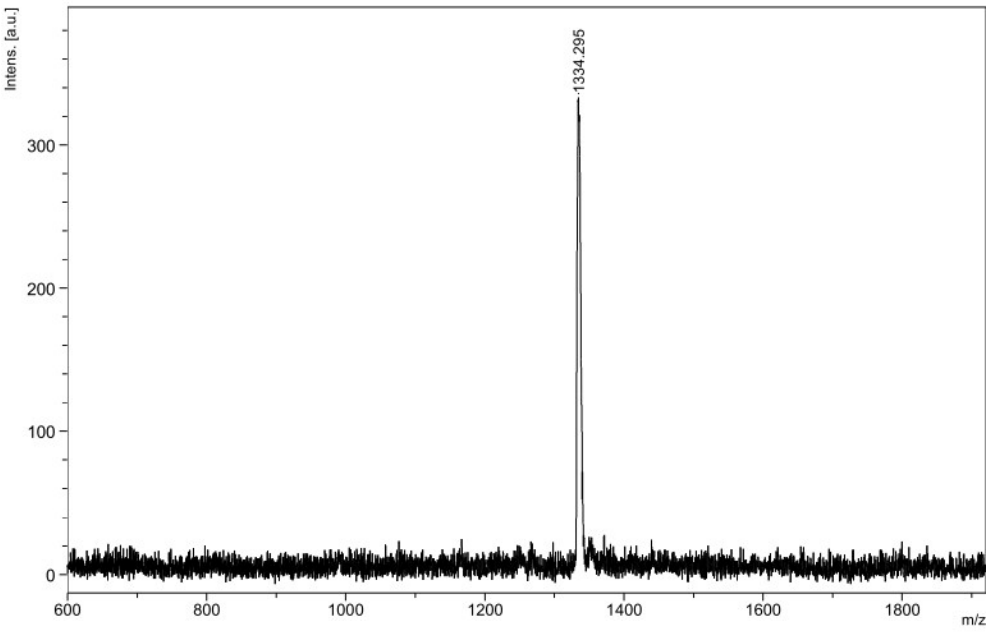

Figure S2. MALDI-TOF mass spectrum of compound **4**.

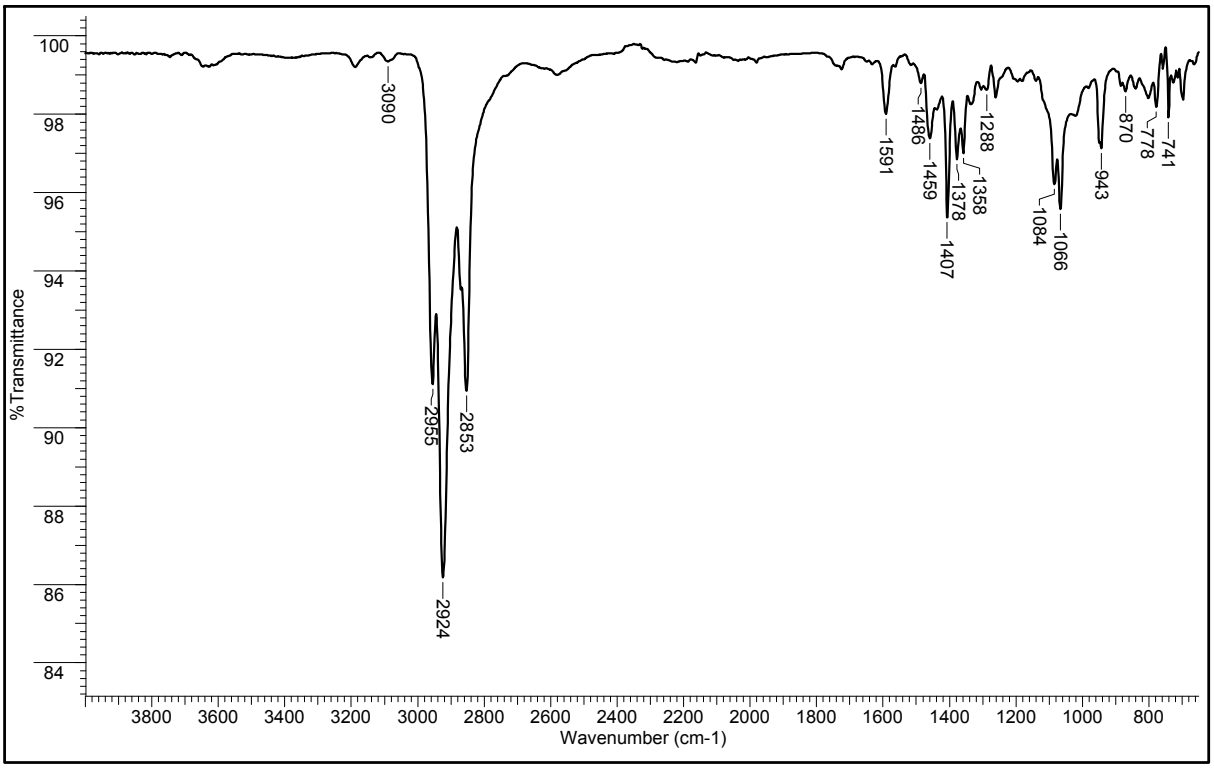

Figure S3. The FT-IR spectra of symmetric ZnPc (**3**)

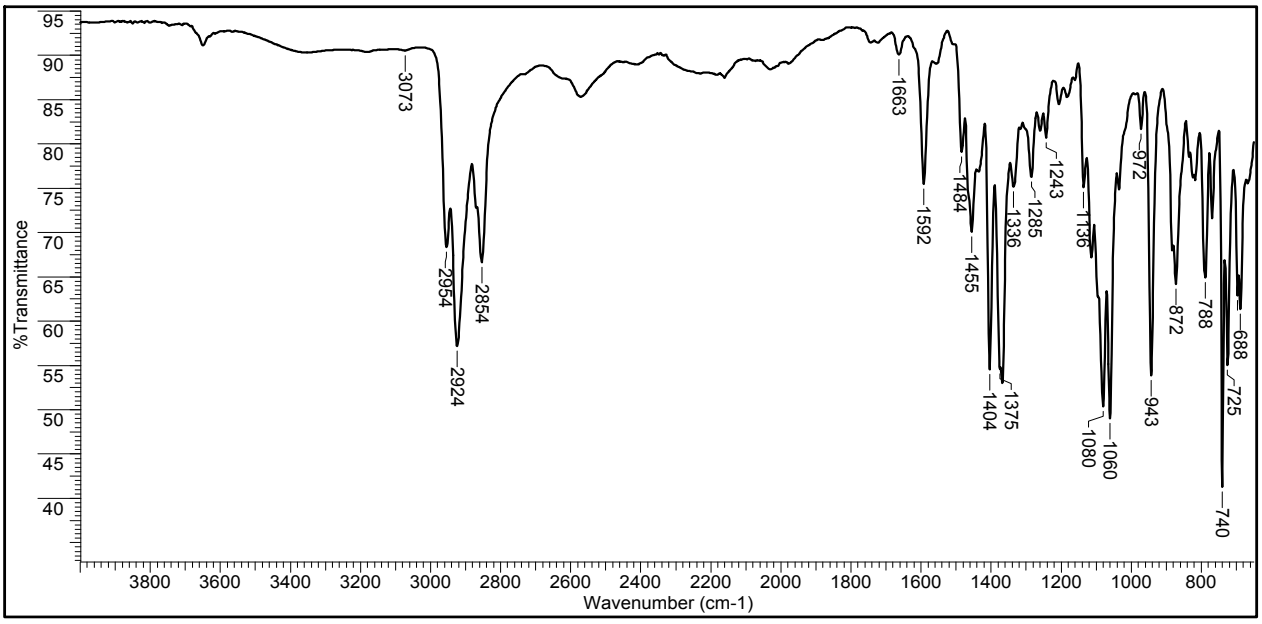

Figure S4. The FT-IR spectra of asymmetric ZnPc (**4**)

Compound 3:
FT-IR ν_{max}/cm^{-1}: 3090 (CH_{ar}), 2955-2853 (CH_{al}), 1591, 1486, 1459, 1407, 1378, 1358, 1288, 1128, 1108, 1084,1066, 943, 870, 778, 741.

Compound 4: FT-IR ν_{max}/cm^{-1}: 3073 (CH_{ar}), 2954-2854 (CH_{al}), 1663 (C=N), 1592, 1484, 1455, 1404, 1375, 1336, 1285, 1243, 1136, 1097, 1080, 1060, 972, 943, 883, 872, 788, 740, 725, 697, 688.

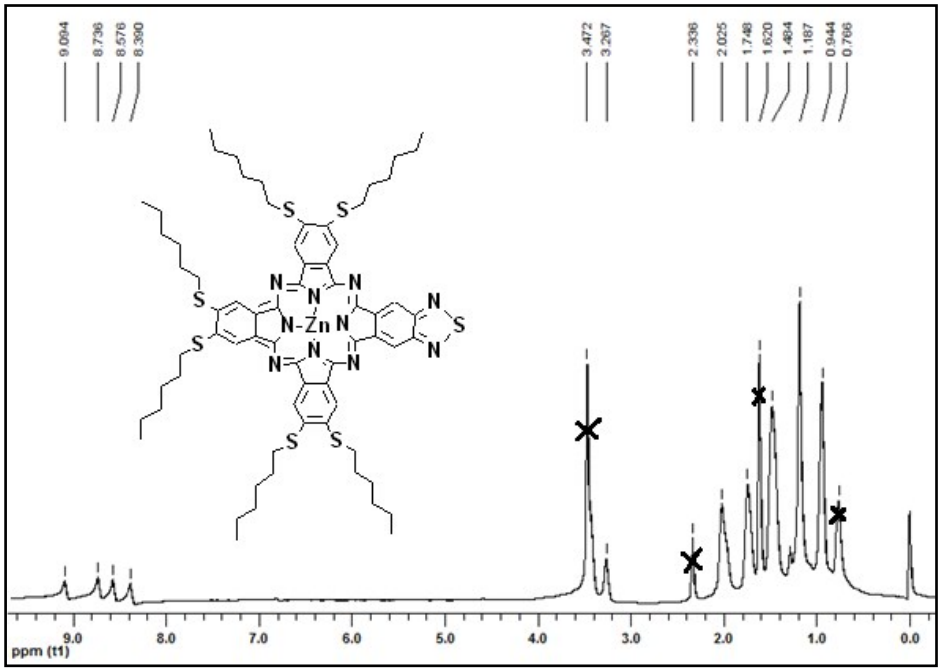

Figure S5. [1]HNMR spectrum of compound **4**.

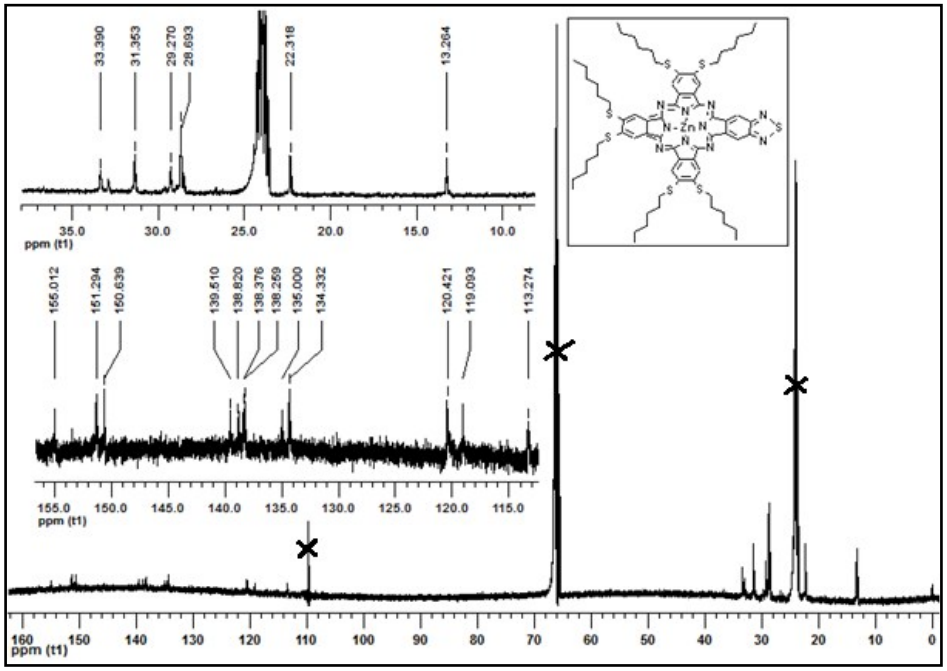

Figure S6. [13]CNMR spectrum of compound **4**.

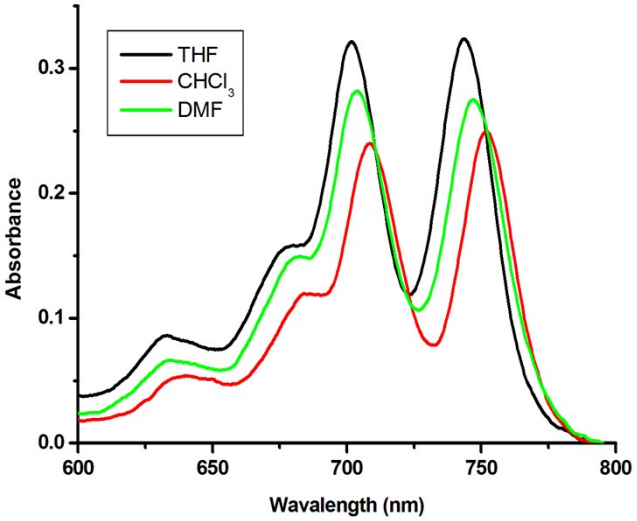

Figure S7. UV-Vis spectra of **4** (c =1x10^{-6} M) in different solvents (THF-tetrahydrofuran, $CHCl_3$-Chloroform, DMF- Dimethylformamide).

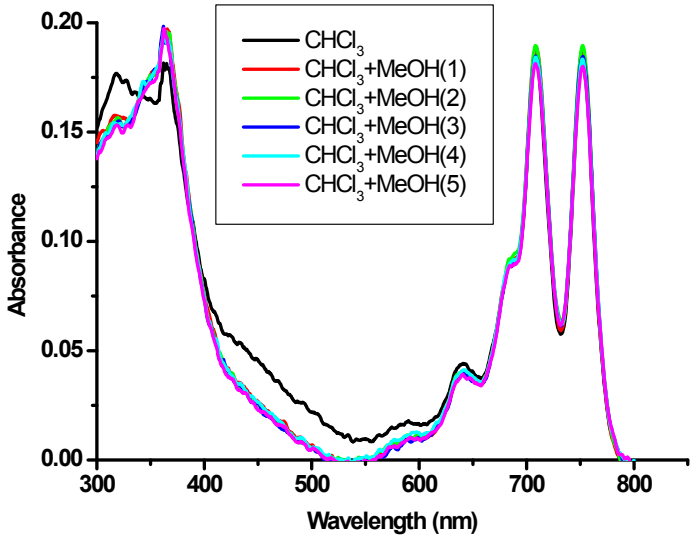

Figure S8. Changes in absorbance of **4** (initially c = 1x10^{-6} M) in non-coordinating solvent $CHCl_3$ by adding coordinating solvent MeOH (50µl in each step).

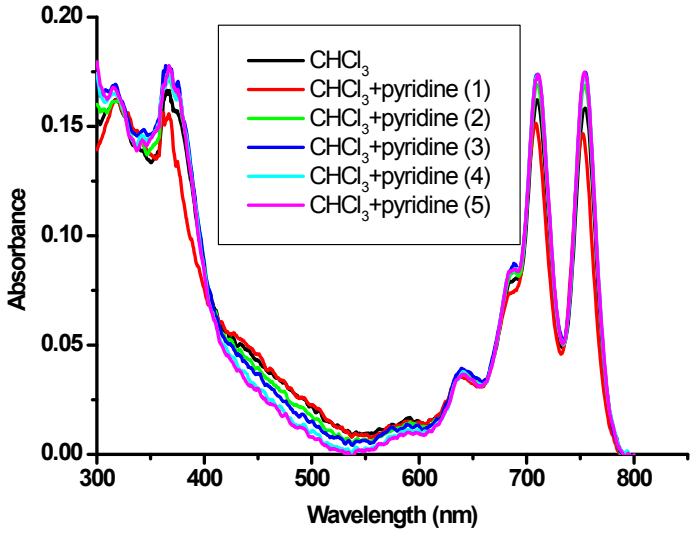

Figure S9. Changes in absorbance of **4** (initially c=1x10^{-6} M) in non-coordinating solvent $CHCl_3$ by adding coordinating solvent pyridine (50µl in each step).

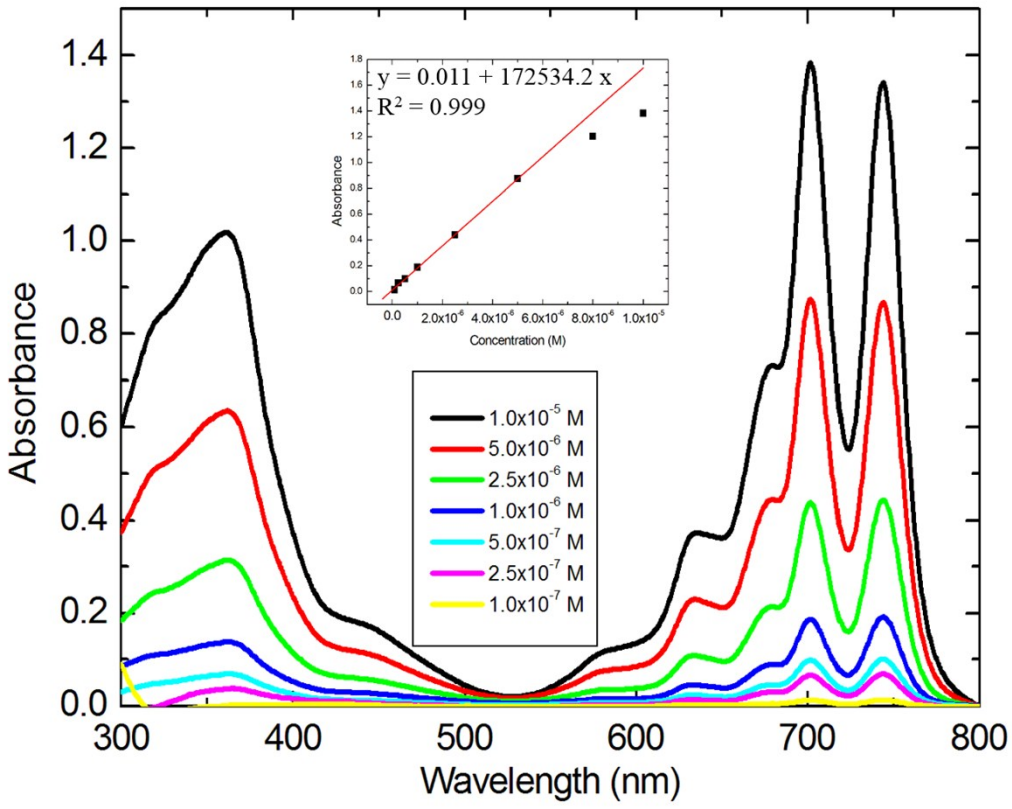

Figure S10. The change in absorbance of asymmetric Pc (**4**) with concentration in THF.

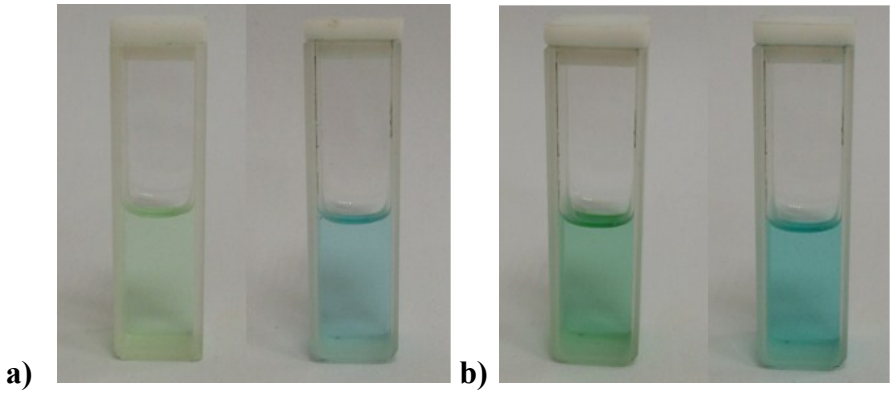

Figure S11. Photographs of **a) 3** in THF, c = 3.32 x 10^{-6} M (left cuvette), **3** complexed with Ag (I) (right cuvette), **b) 4** in THF, c = 1.12 x 10^{-6} M (left cuvette), **4** complexed with Ag (I) (right cuvette).

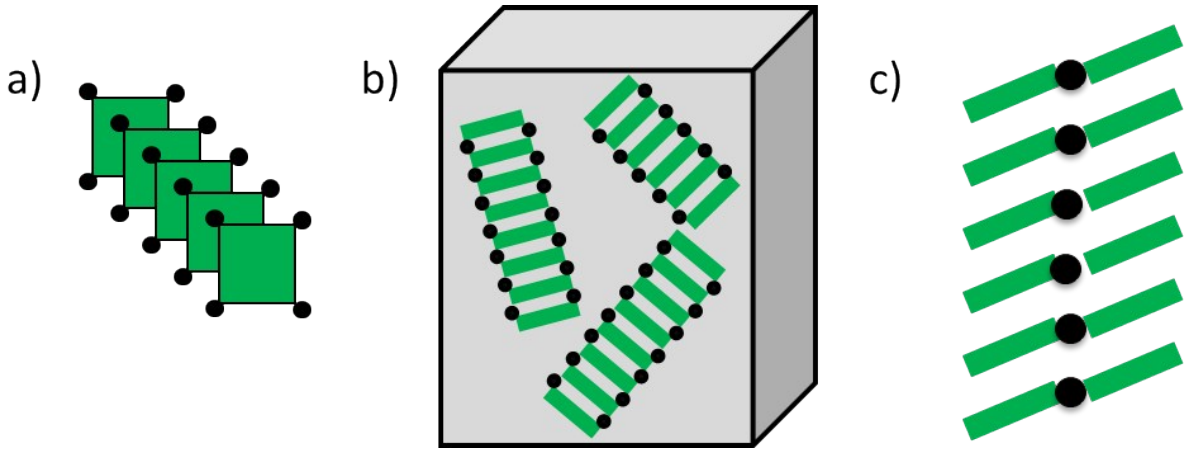

Figure S12. a) Ag^{+} induced H-aggregation (face to face) of Pcs (Green squares: Pc molecules, black points: Ag^{+} ions), b) Top view of H-aggregates, c) Top view of J-aggregates.

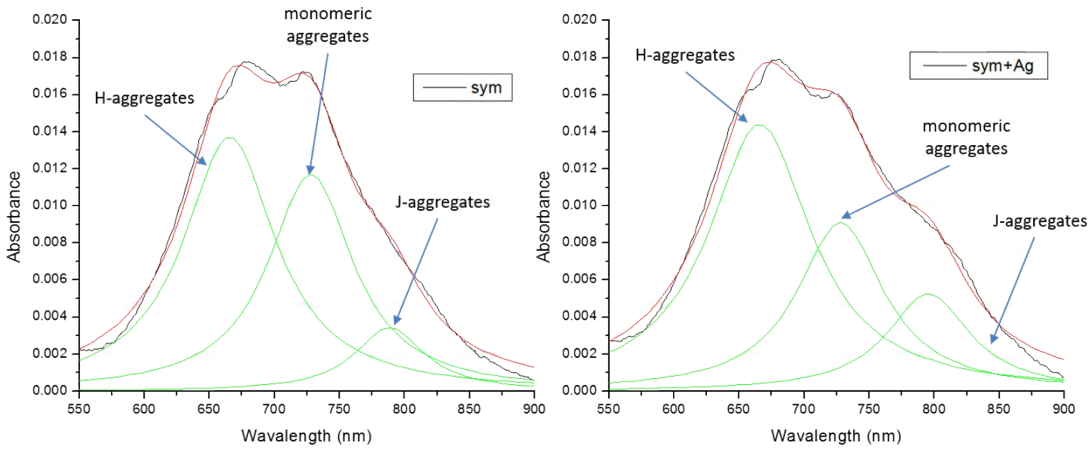

Figure S13. The absorption spectra of symmetric ZnPc (**3**) LB films on glass substrates decomposed to Lorentzian fits representing different aggregates. (left: film deposited from pure water subphase (H-aggregates at 666 nm, monomeric aggregates at 728 nm, J-aggregates at 786 nm); right: film deposited from Ag^+ containing subphase (H-aggregates at 666 nm, monomeric aggregates at 728 nm, J-aggregates at 795 nm)).

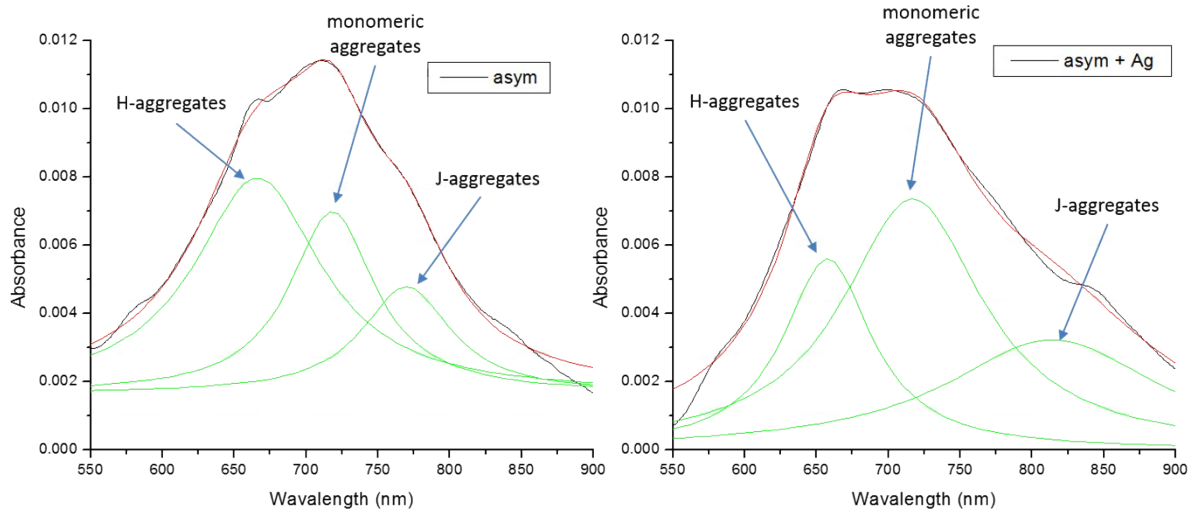

Figure S14. The absorption spectra of asymmetric ZnPc (**4**) LB films on glass substrates decomposed to Lorentzian fits representing different aggregates. (left: film deposited from pure water subphase (H-aggregates at 677 nm, monomeric aggregates at 717 nm, J-aggregates at 758 nm); right: film deposited from Ag^+ containing subphase (H-aggregates at 657 nm, monomeric aggregates at 717 nm, J-aggregates at 814 nm)).