Electronic Supplementary Material (ESI) for Molecular BioSystems.

Supporting information

Table S1

Quantum-chemical characteristics of AK7-5 and AK7-6 (PM6, MOPAC)

Dye	CA, Å^2	CV, Å^3	E_{HOMO}, eV	E_{LUMO}, eV	L, Å	$CLogP$	W, Å	H, Å	μ_g, D
AK7-5	583	715	-9.966	-4.462	20.50	5.40	12.65	4.68	1.68
AK7-6	592	723	-9.937	-4.459	20.33	5.51	11.00	5.88	3.39

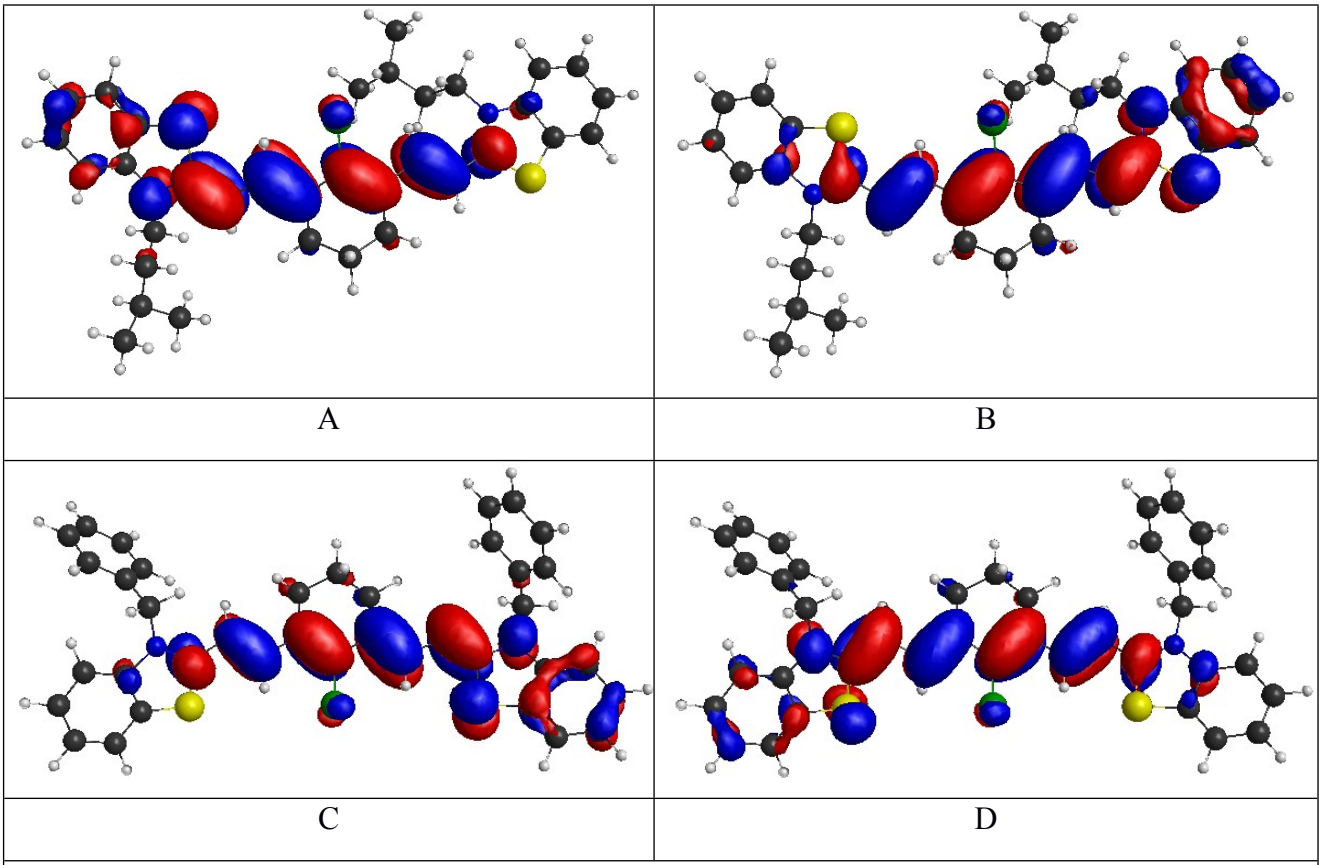
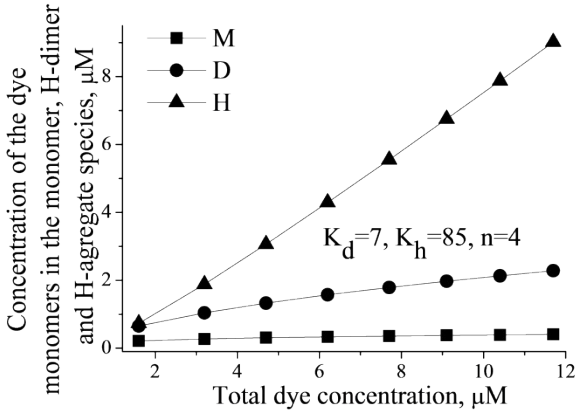
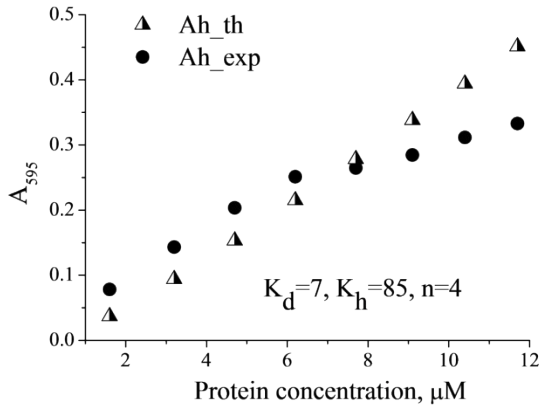


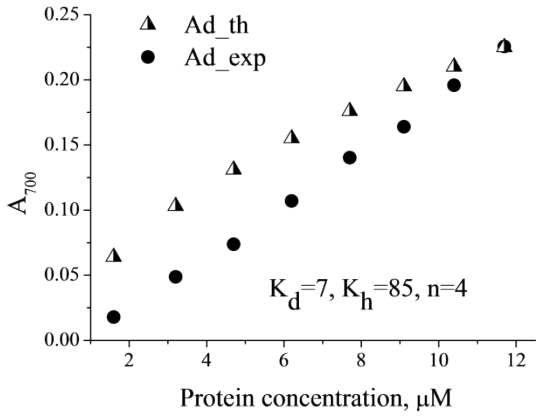
Figure S1. HOMO-153 (A), LUMO-154 (B) of AK7-5, and HOMO-161 (C), LUMO-162 (D) of AK7-6. The optimized conformations of the dyes were calculated, using AM1 method with added polarization (1) and diffuse (1) functions on heavy atoms, and a polarization function on hydrogen atoms



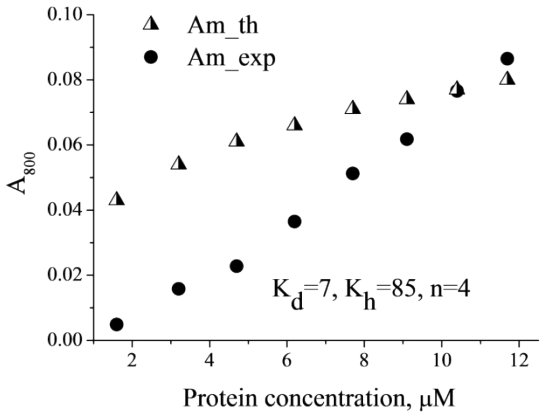
A



B

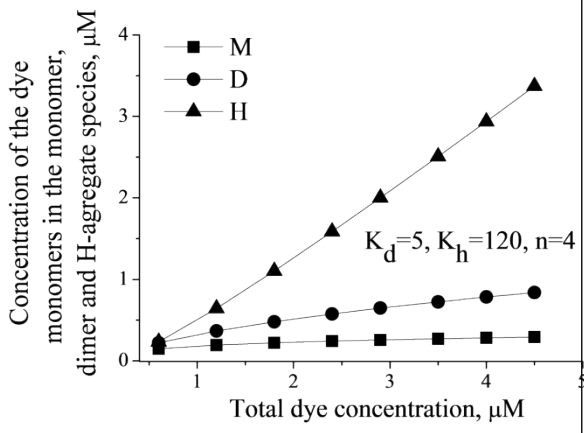


C

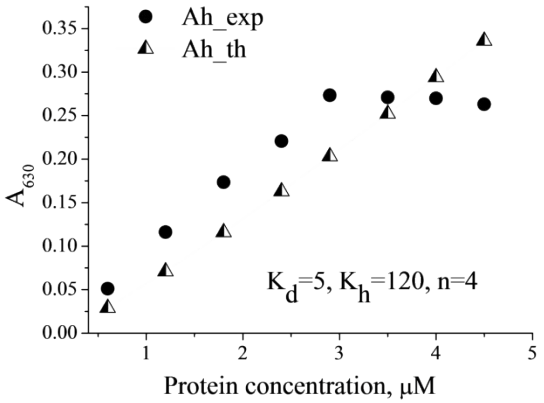


D

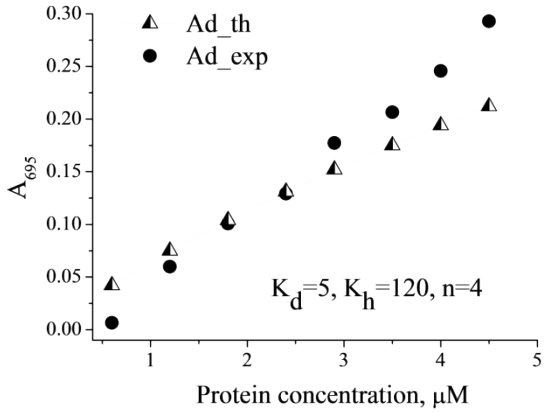
Figure S2. Theoretically predicted concentrations of the monomer, H-dimer and H-aggregate dye species at different total concentrations of **AK7-5** in buffer (A), the measured (taken from the deconvoluted dye spectra) and calculated absorbances of the H-aggregates (B), H-dimers (C) and monomers (D)



A



B



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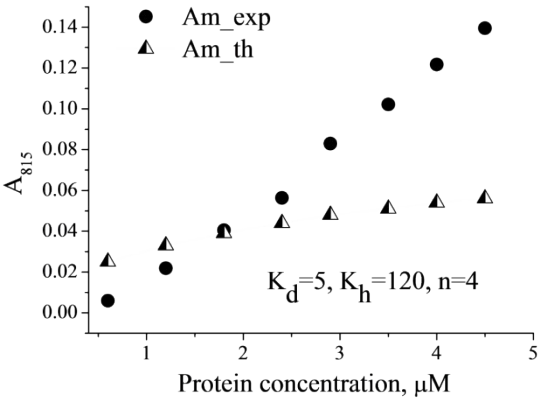


D

Figure S3. Theoretically predicted concentrations of the monomer, H-dimer and H-aggregate dye species at different total concentrations of **AK7-6** in buffer (A), the measured (taken from the deconvoluted dye spectra) and calculated absorbances of the H-aggregates (B), H-dimers (C) and monomers (D)

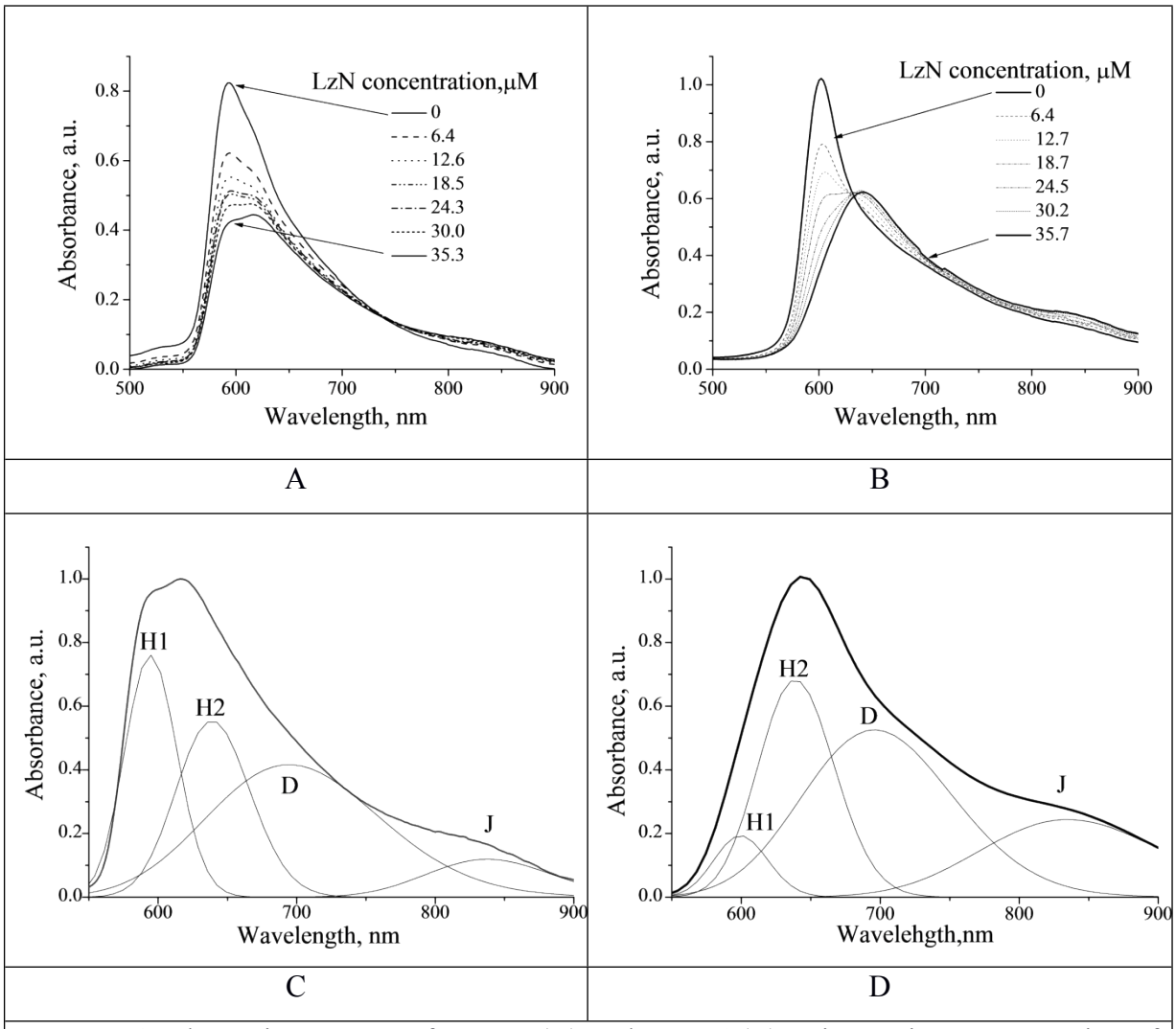
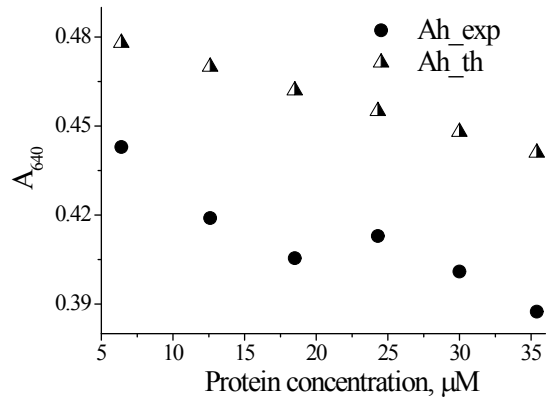
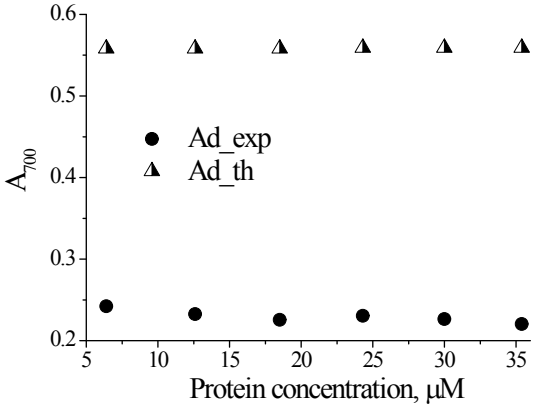


Figure S4. Absorption spectra of AK7-5 (A) and AK7-6 (B) at increasing concentration of the native lysozyme (LzN). Normalized absorption spectra of AK7-5 (C) and AK7-6 (D) in the presence of 35.3 μM (C) and 35.7 μM (D) of the native lysozyme. AK7-5 and AK7-6 concentrations were 12.2 and 13.5 μM, respectively



A



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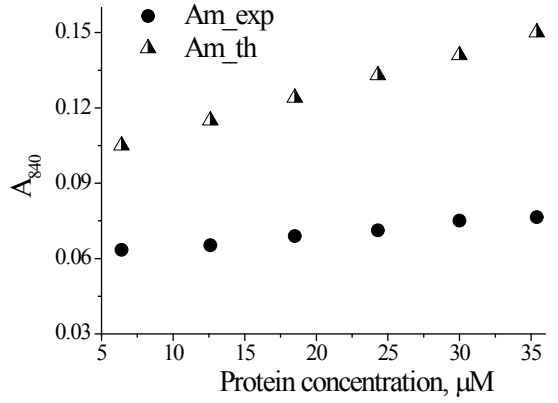

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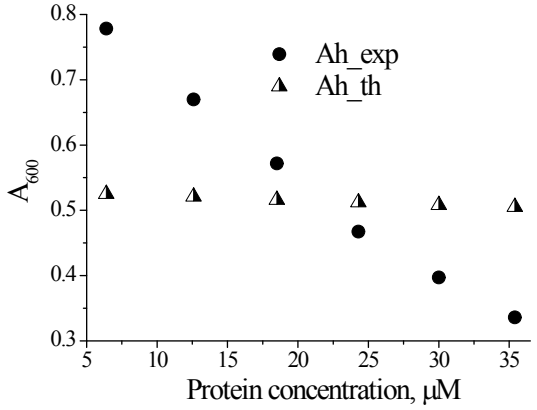
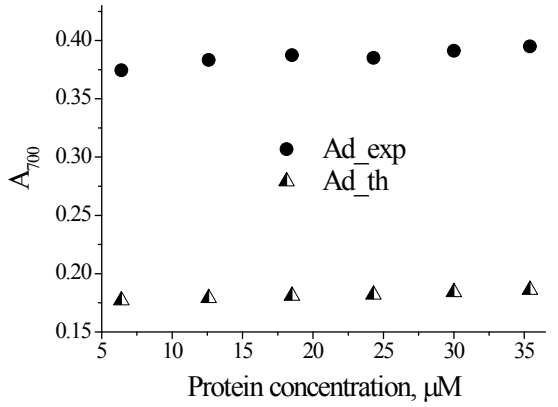
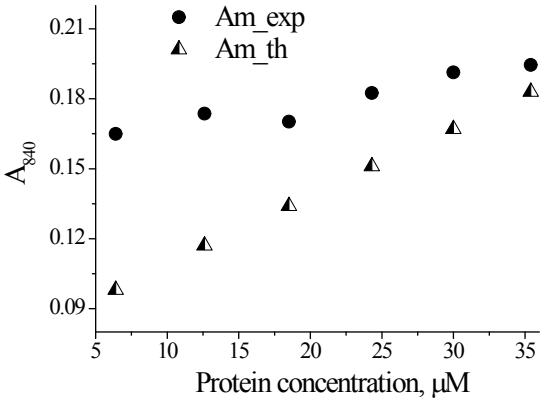


D



E



F

Figure S5. The measured (Am_exp) and theoretically predicted (Am_th) absorbances of the AK7-5/ AK7-6 H-aggregates (A,D), H-dimers (B,E) and monomers (C,F) in the presence of the native lysozyme calculated using the following sets of parameters:

$\{K_b = 0.02\mu M^{-1}, m = 1, K_h = 85, K_d = 7\mu M^{-1}, n = 4\}$/

$\{K_b = 0.04\mu M^{-1}, m = 1, K_h = 120, K_d = 5\mu M^{-1}, n = 4\}$