

Thiacalixarene “knot” effect on protein binding by oligolactic acid particles

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Electronic Supplementary Information

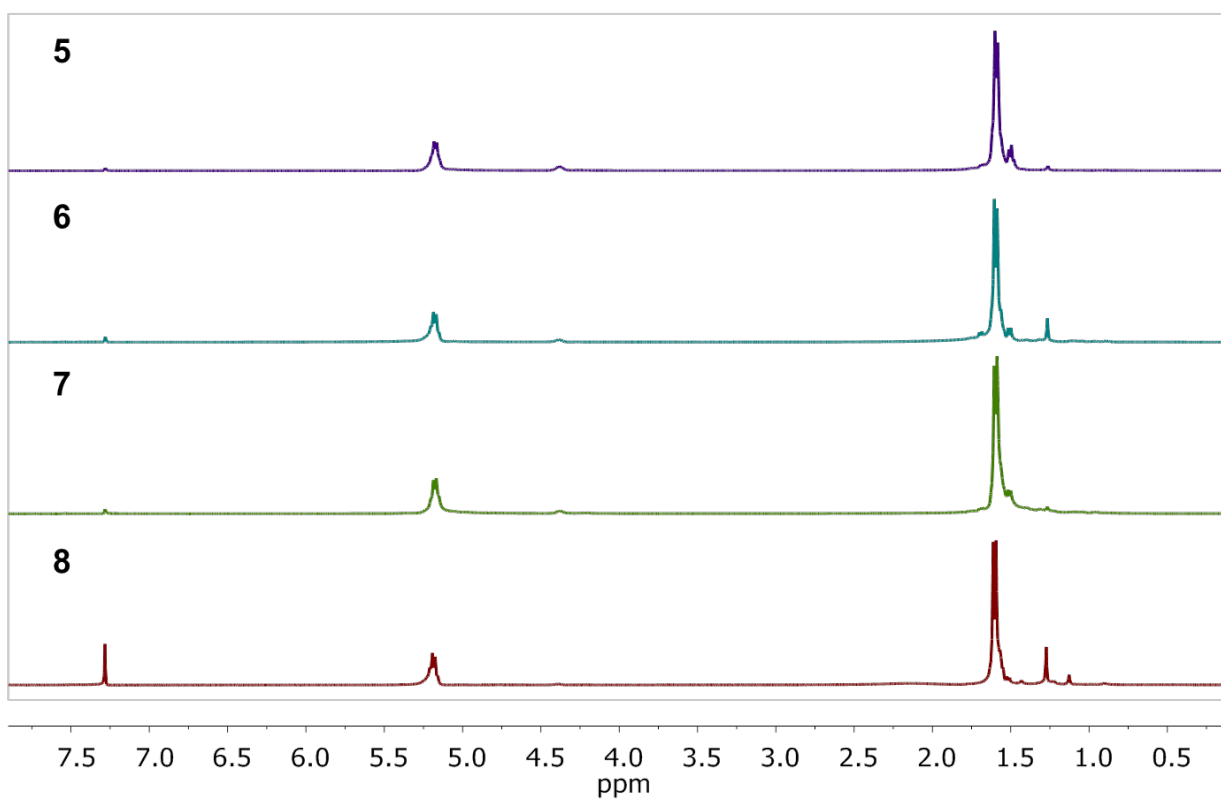


Fig.S1. ^1H NMR (CDCl_3) spectra of products **5-8**.

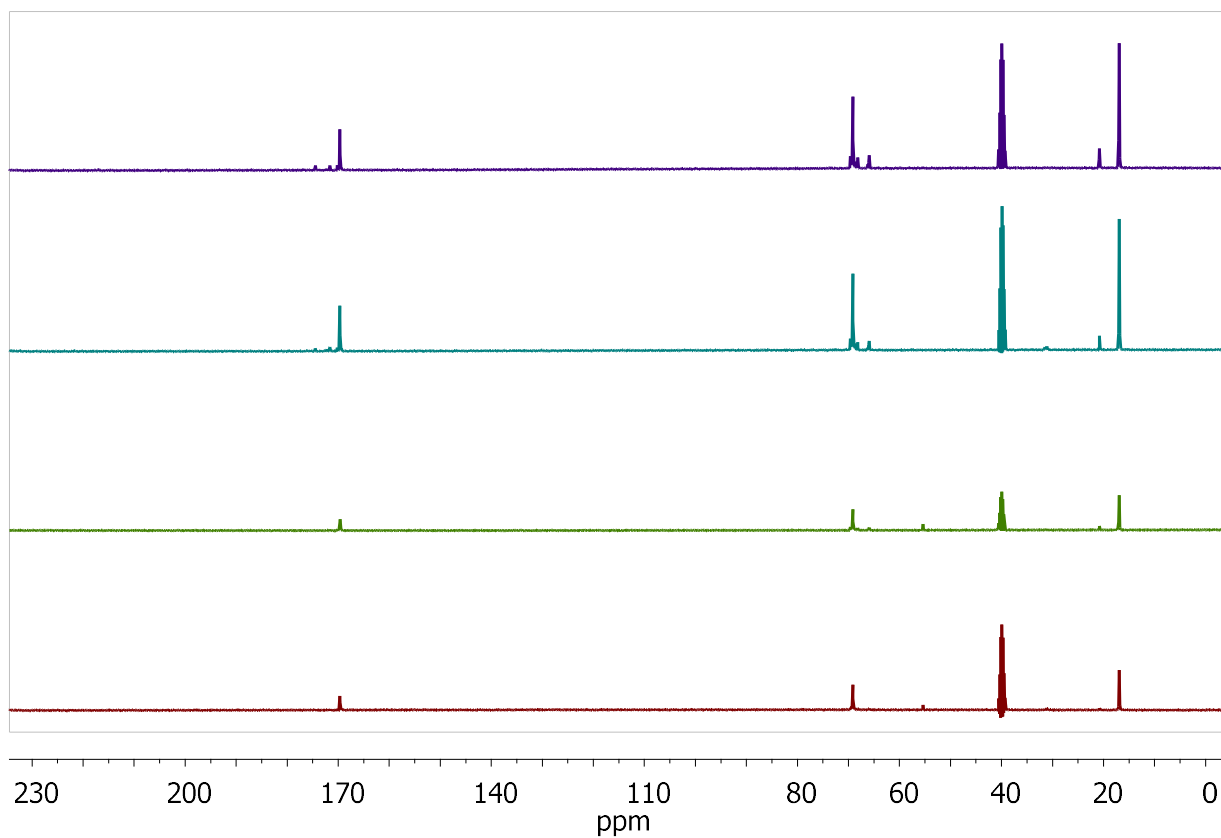


Fig.S2. $^{13}\text{C}\{\text{H}\}$ NMR ($\text{DMSO-}d_6$) spectra of products **5-8**.

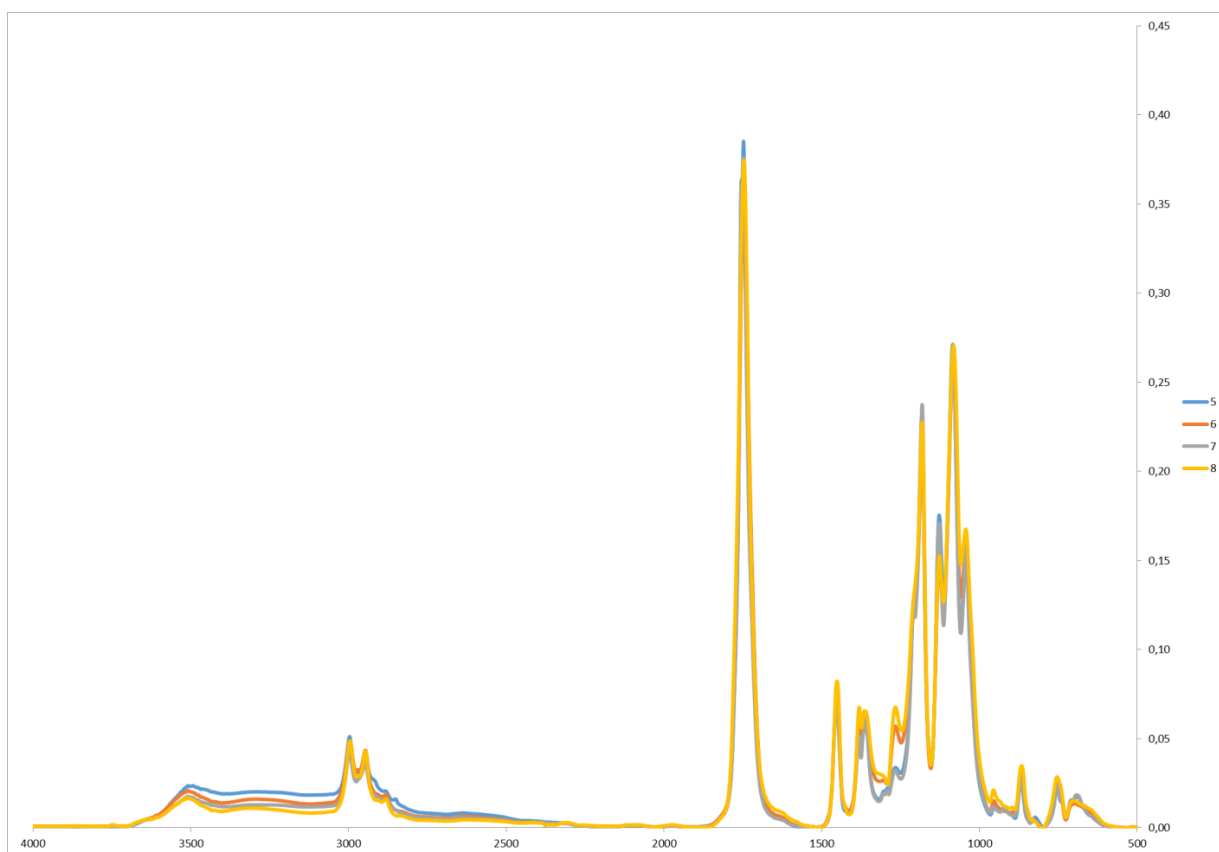


Fig.S3. FTIR-ATR spectra of products **5-8**.

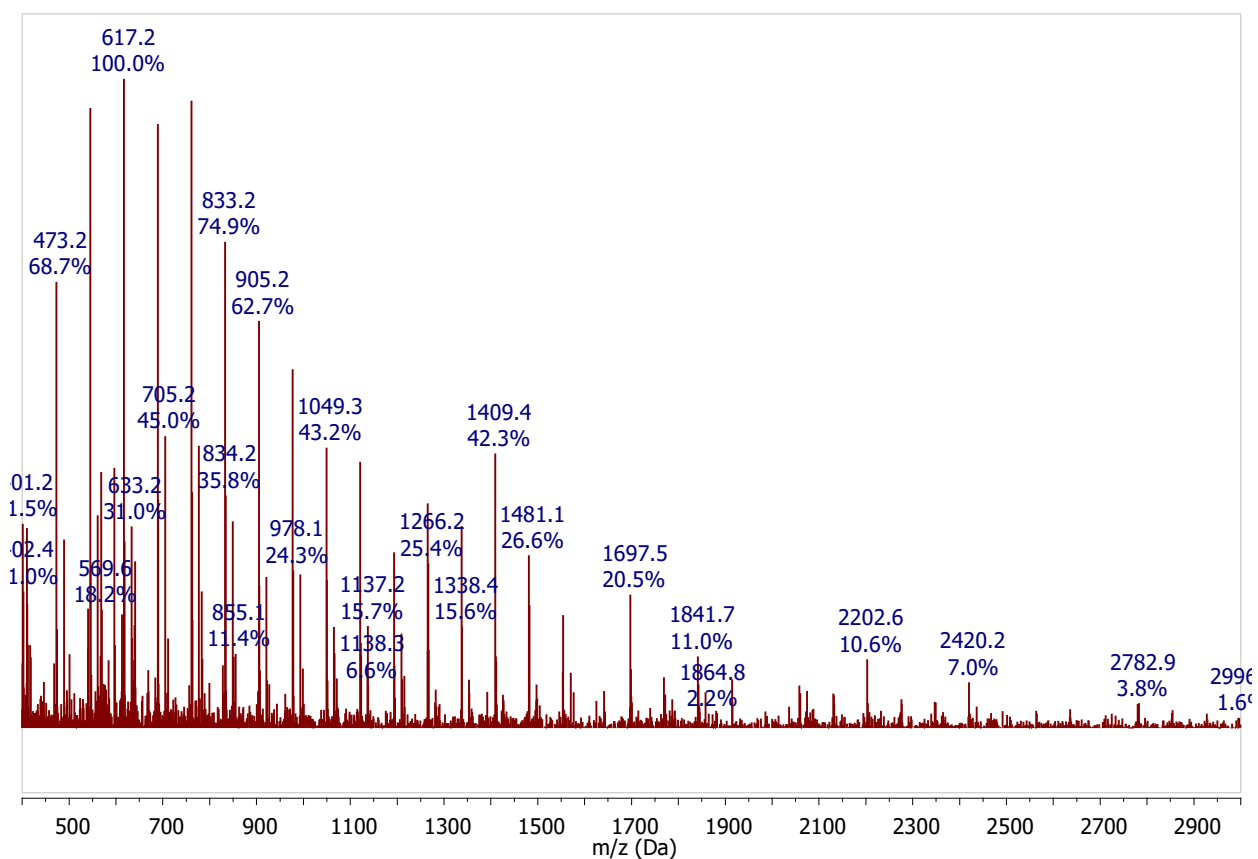


Fig.S4. MALDI mass-spectrum of product **5**, matrix - 2,5-dihydroxybenzoic acid

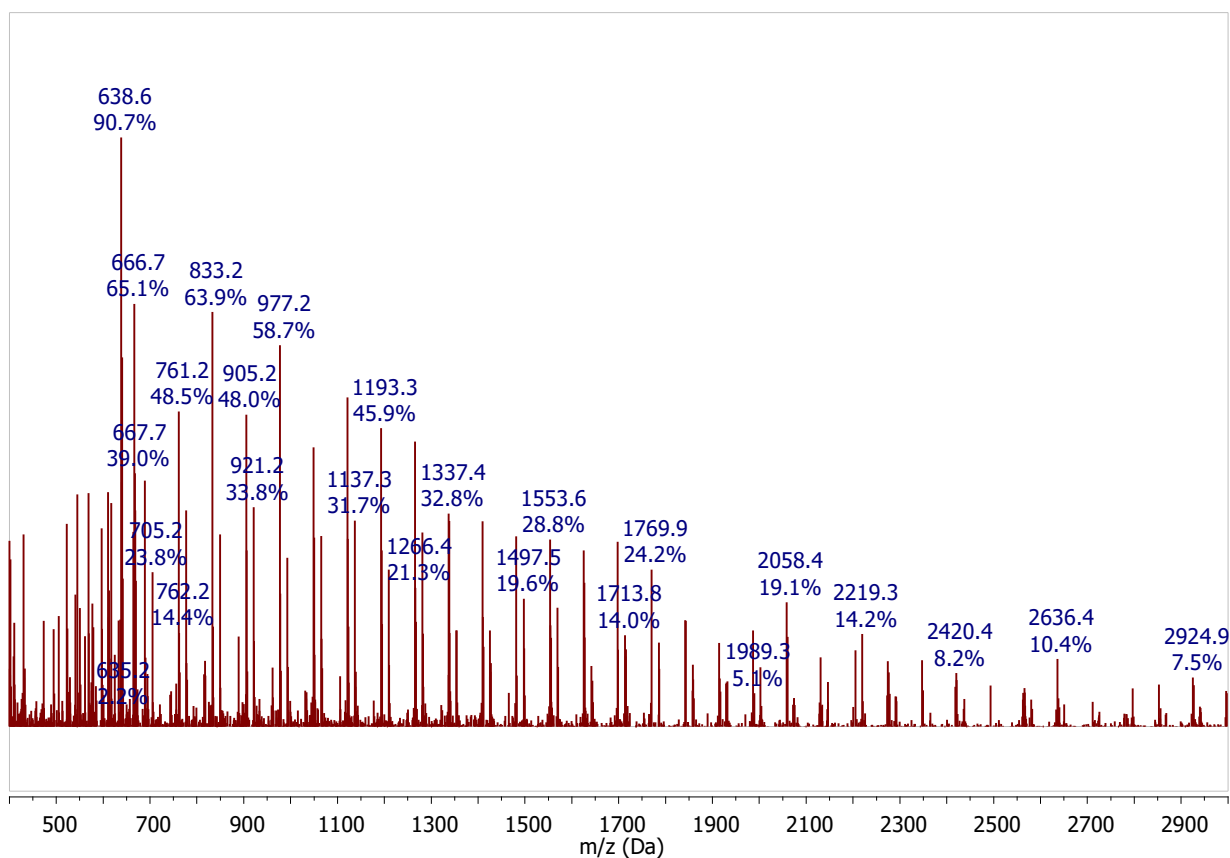


Fig.S5. MALDI mass-spectrum of product **6**, matrix - 2,5-dihydroxybenzoic acid

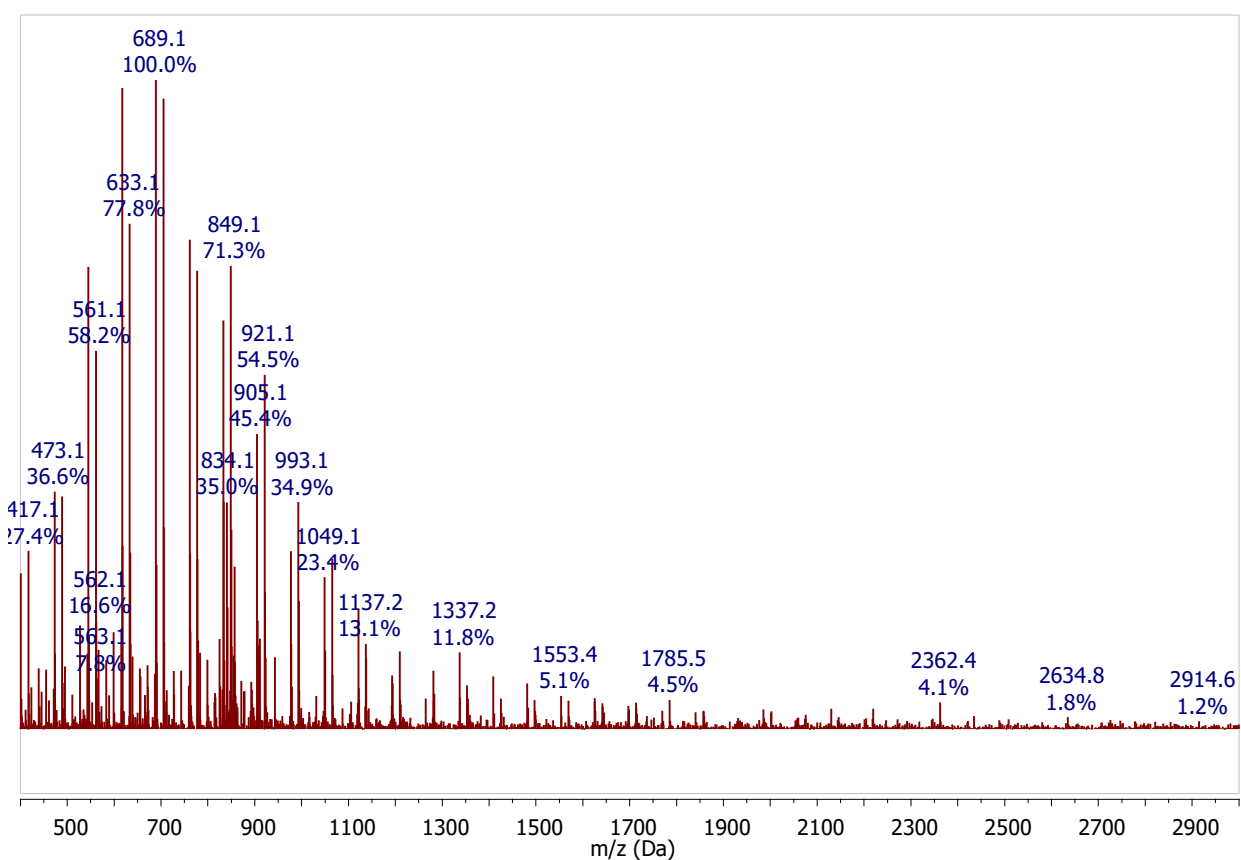


Fig.S6. MALDI mass-spectrum of product **7**, matrix - 2,5-dihydroxybenzoic acid

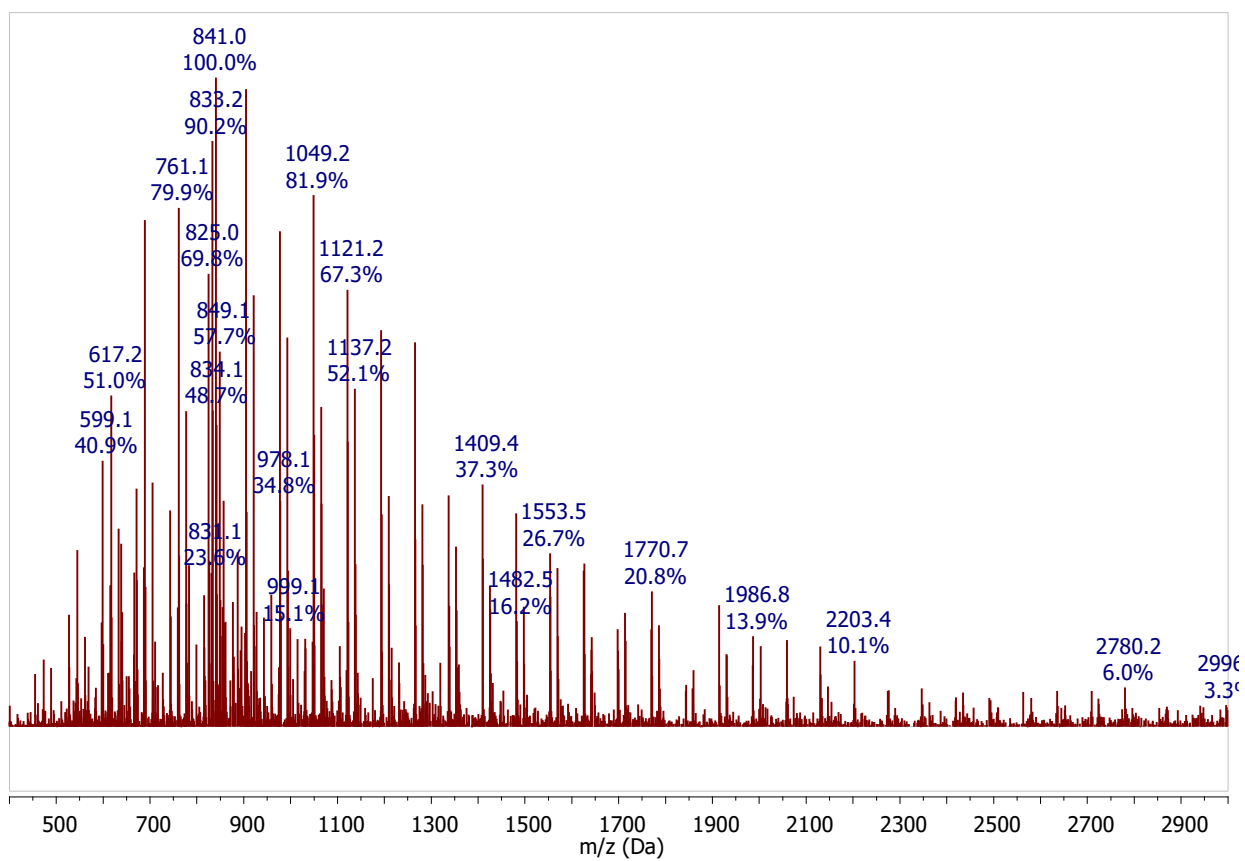


Fig.S7. MALDI mass-spectrum of product **8**, matrix - 2,5-dihydroxybenzoic acid

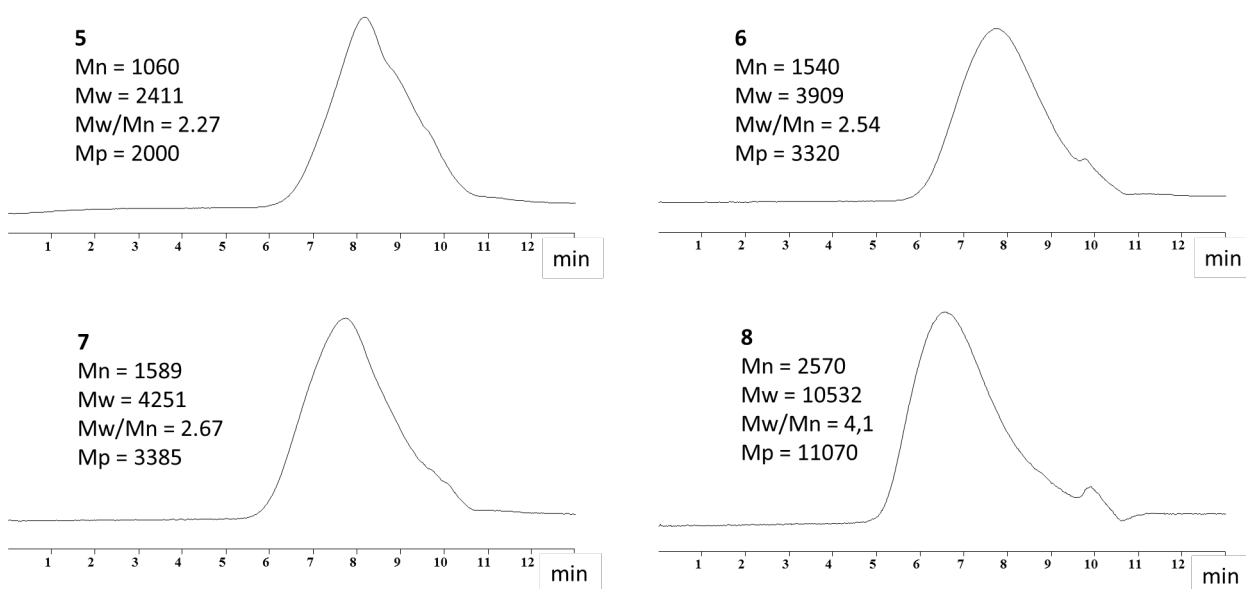


Fig.S8. GPC curves of products **5-8** (eluent-THF, calibrated by PS standards)

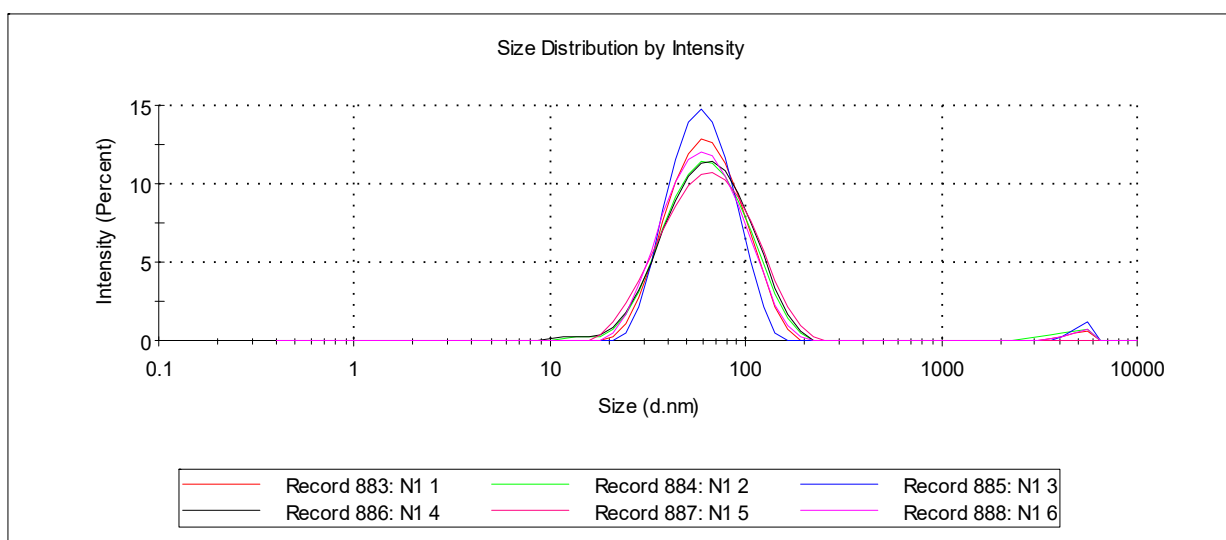


Fig.S9. Size distribution by intensity (DLS) of solution of the macrocycle **6**(*cone*, 0.19 mg/ml) in the 50 mM phosphate buffer at pH 7.4.

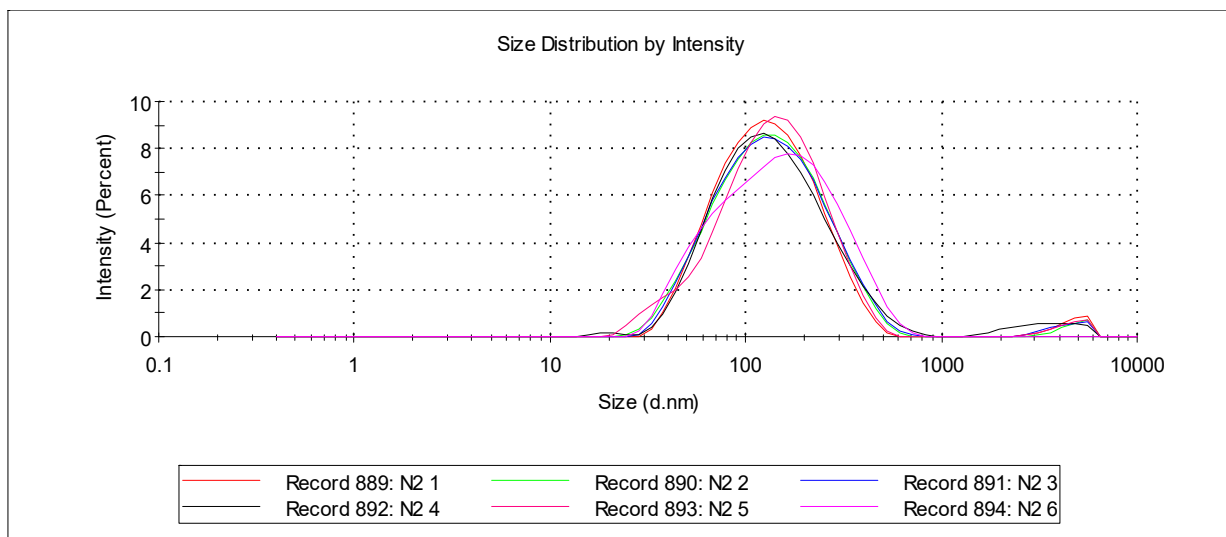


Fig.S10. Size distribution by intensity (DLS) of solution of the macrocycle **7** (*partial cone*, 0.19 mg/ml) in the 50 mM phosphate buffer at pH 7.4.

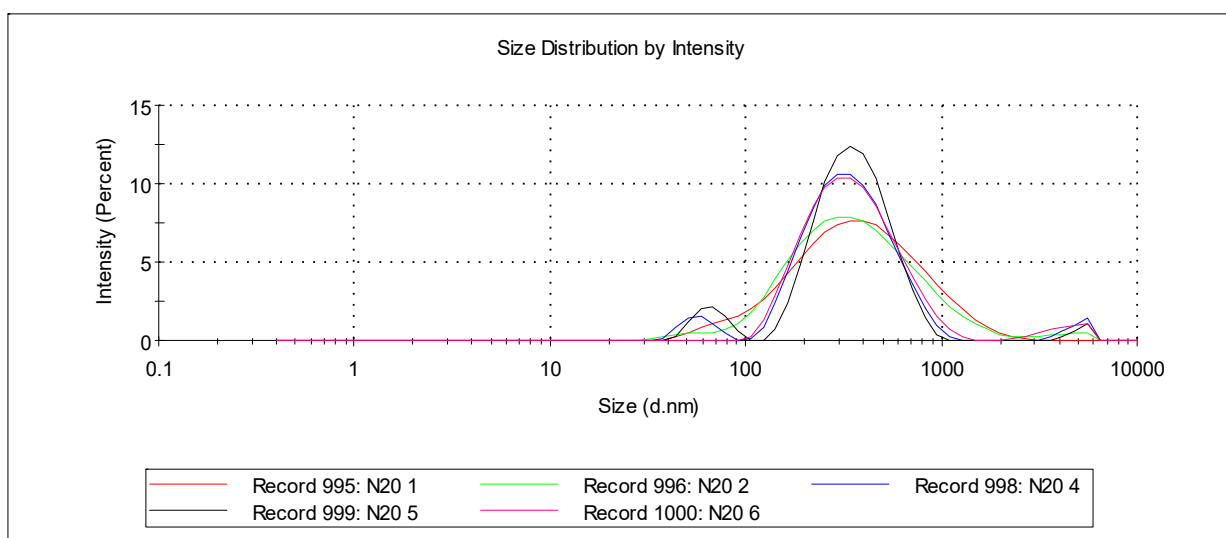


Fig.S11. Size distribution by intensity (DLS) of solution of the macrocycle **8** (*1,3-alternate*, 0.19 mg/ml) in the 50 mM phosphate buffer at pH 7.4.

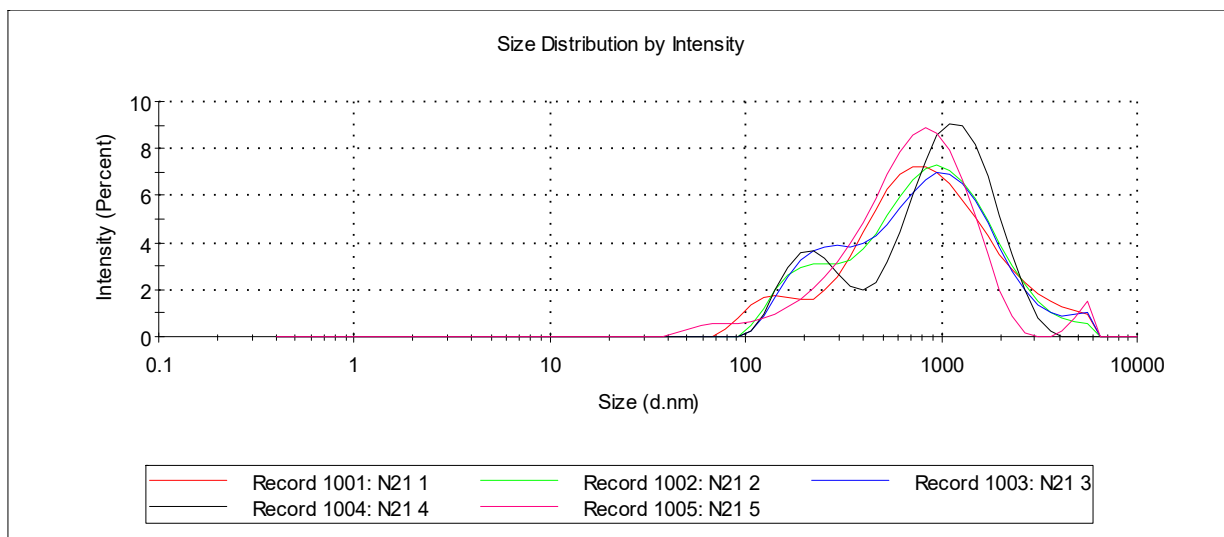


Fig.S12. Size distribution by intensity (DLS) of solution of the OLA-5 (0.19 mg/ml) in the 50 mM phosphate buffer at pH 7.4.

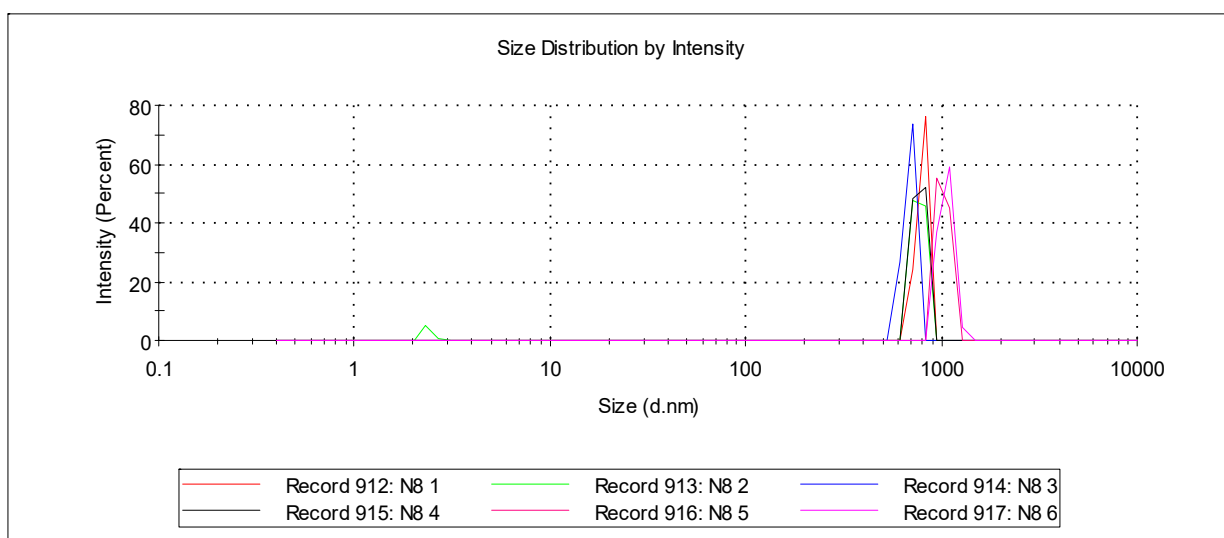


Fig.S14. Size distribution by intensity (DLS) of solution of the macrocycle **6**(*cone*, 0.19 mg/ml) and lysozyme (10 μ M) in the 50 mM phosphate buffer at pH 7.4.

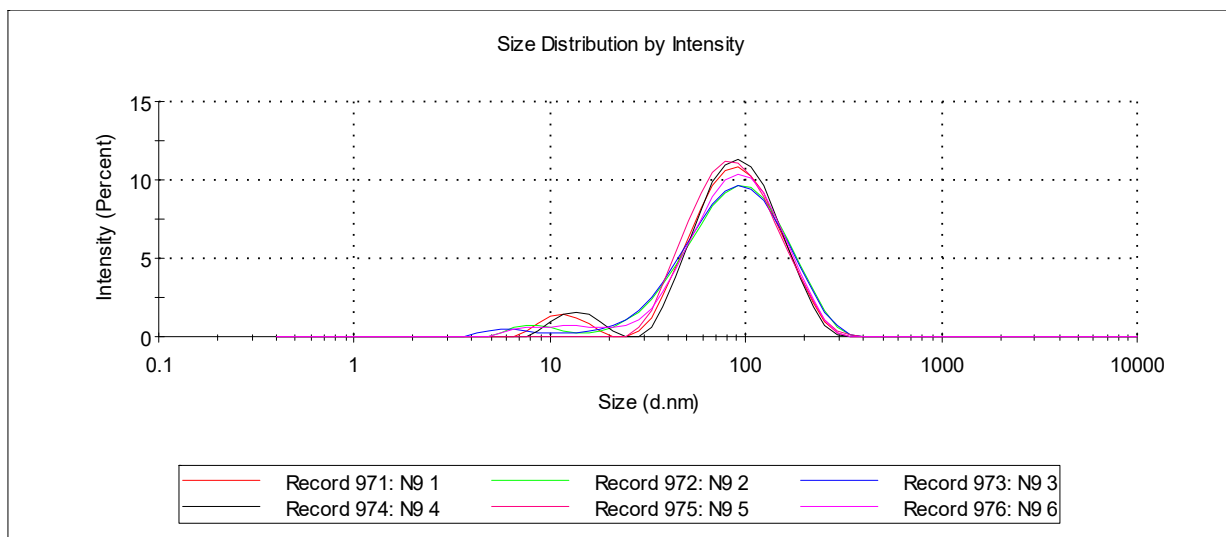


Fig.S15. Size distribution by intensity (DLS) of solution of the macrocycle **6** (*cone*, 0.19 mg/ml) and BSA (10 μ M) in the 50 mM phosphate buffer at pH 7.4.

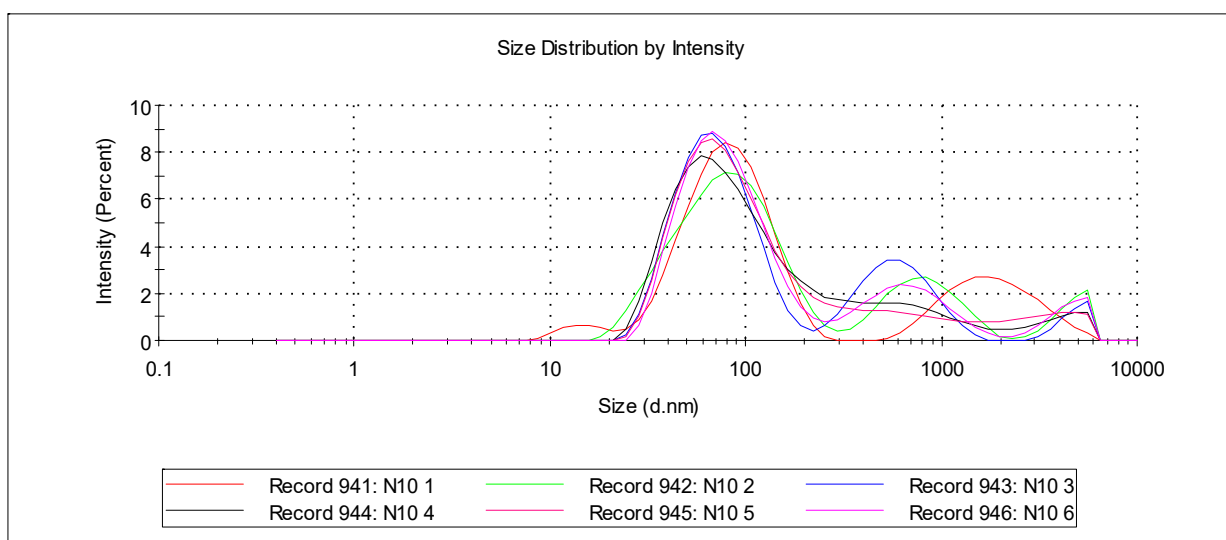


Fig.S16. Size distribution by intensity (DLS) of solution of the macrocycle **6** (*cone*, 0.19 mg/ml) and hemoglobin (10 μ M) in the 50 mM phosphate buffer at pH 7.4.

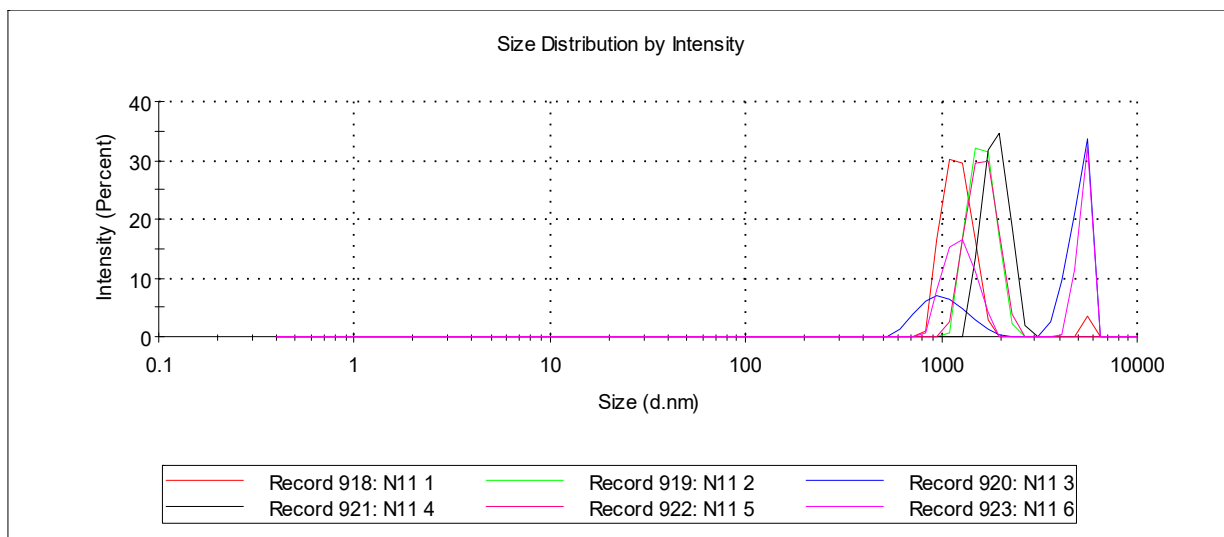


Fig.S17. Size distribution by intensity (DLS) of solution of the macrocycle **7** (*partial cone*, 0.19 mg/ml) and lysozyme (10 μ M) in the 50 mM phosphate buffer at pH 7.4.

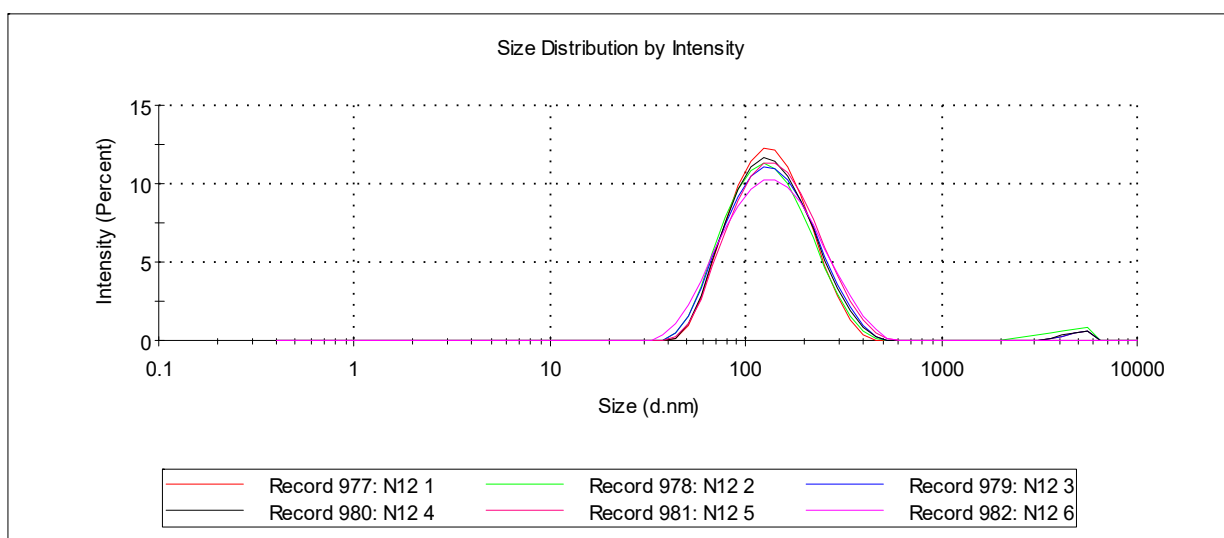


Fig.S18. Size distribution by intensity (DLS) of solution of the macrocycle **7** (*partial cone*, 0.19 mg/ml) and BSA (10 μ M) in the 50 mM phosphate buffer at pH 7.4.

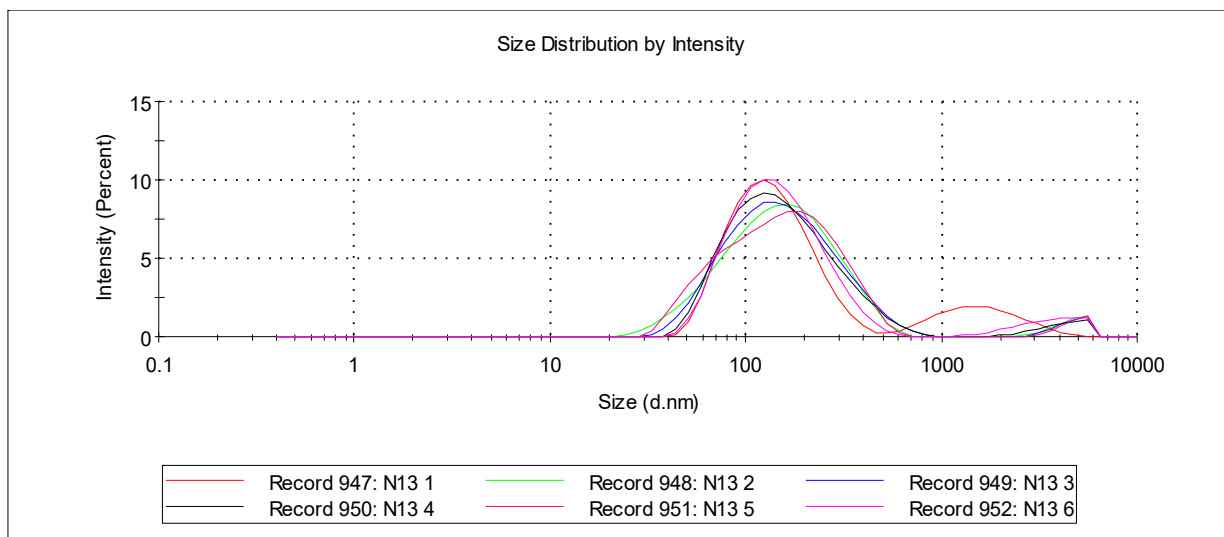


Fig.S19. Size distribution by intensity (DLS) of solution of the macrocycle **7** (*partial cone*, 0.19 mg/ml) and hemoglobin (10 μ M) in the 50 mM phosphate buffer at pH 7.4.

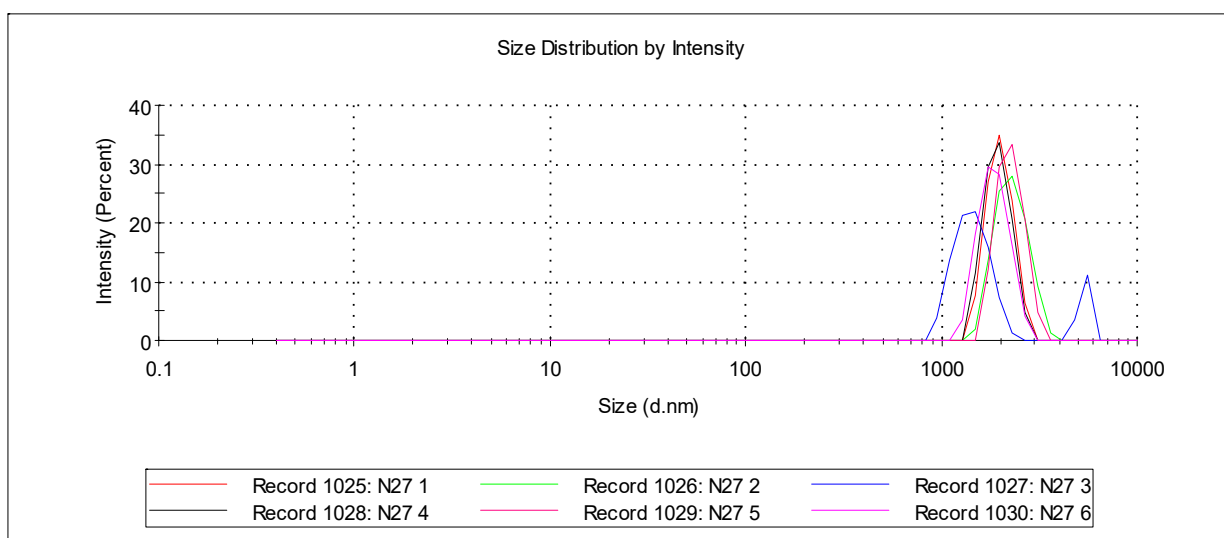


Fig.S20. Size distribution by intensity (DLS) of solution of the macrocycle **8** (*1,3-alternate*, 0.19 mg/ml) and lysozyme (10 μ M) in the 50 mM phosphate buffer at pH 7.4.

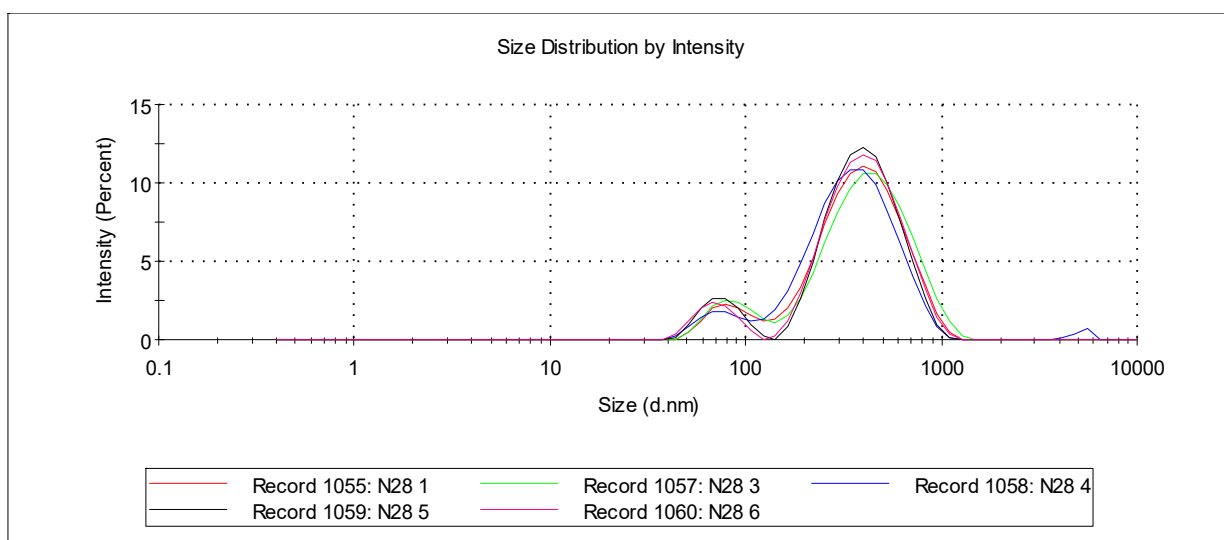


Fig.S21. Size distribution by intensity (DLS) of solution of the macrocycle **8** (*1,3-alternate*, 0.19 mg/ml) and BSA (10 μ M) in the 50 mM phosphate buffer at pH 7.4.

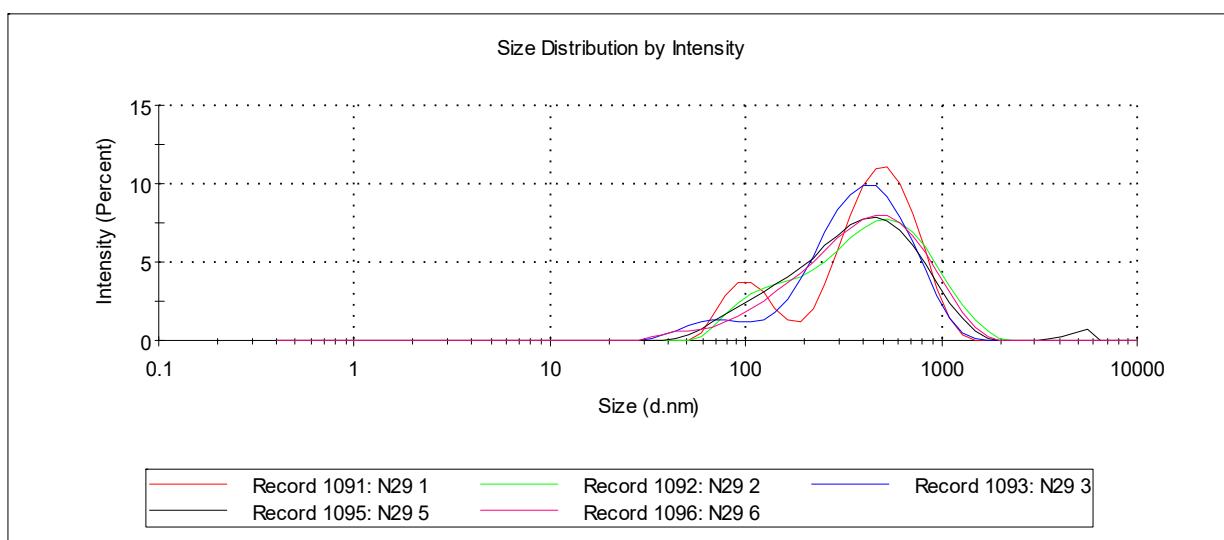


Fig.S22. Size distribution by intensity (DLS) of solution of the macrocycle **8** (*1,3-alternate*, 0.19 mg/ml) and hemoglobin (10 μ M) in the 50 mM phosphate buffer at pH 7.4.

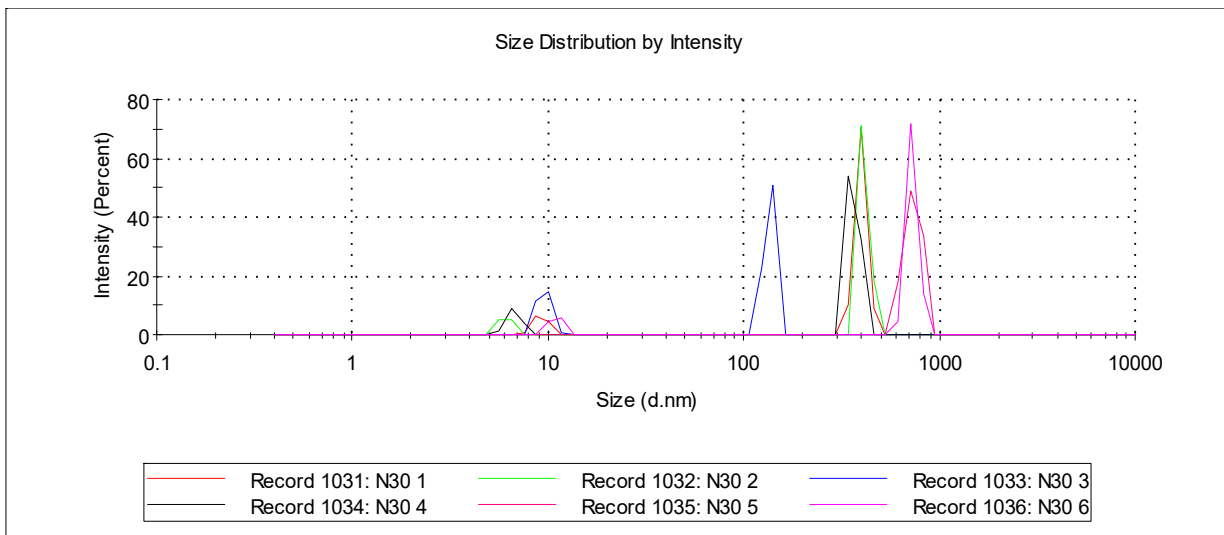


Fig.S23. Size distribution by intensity (DLS) of solution of the OLA-5 (0.19 mg/ml) and lysozyme (10 μ M) in the 50 mM phosphate buffer at pH 7.4.

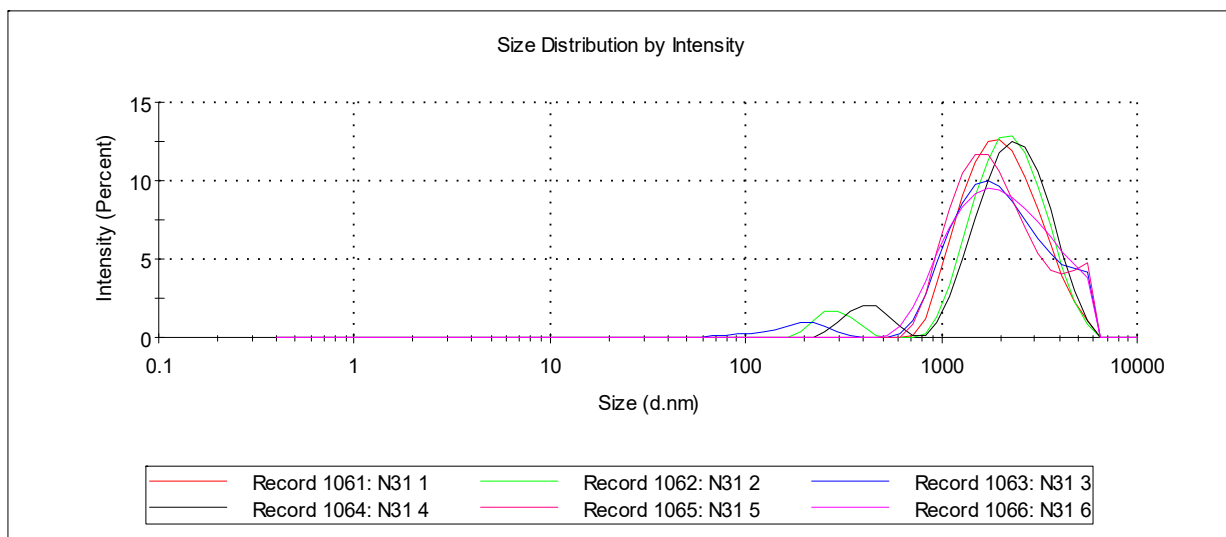


Fig.S24. Size distribution by intensity (DLS) of solution of the OLA-5 (0.19 mg/ml) and BSA (10 μ M) in the 50 mM phosphate buffer at pH 7.4.

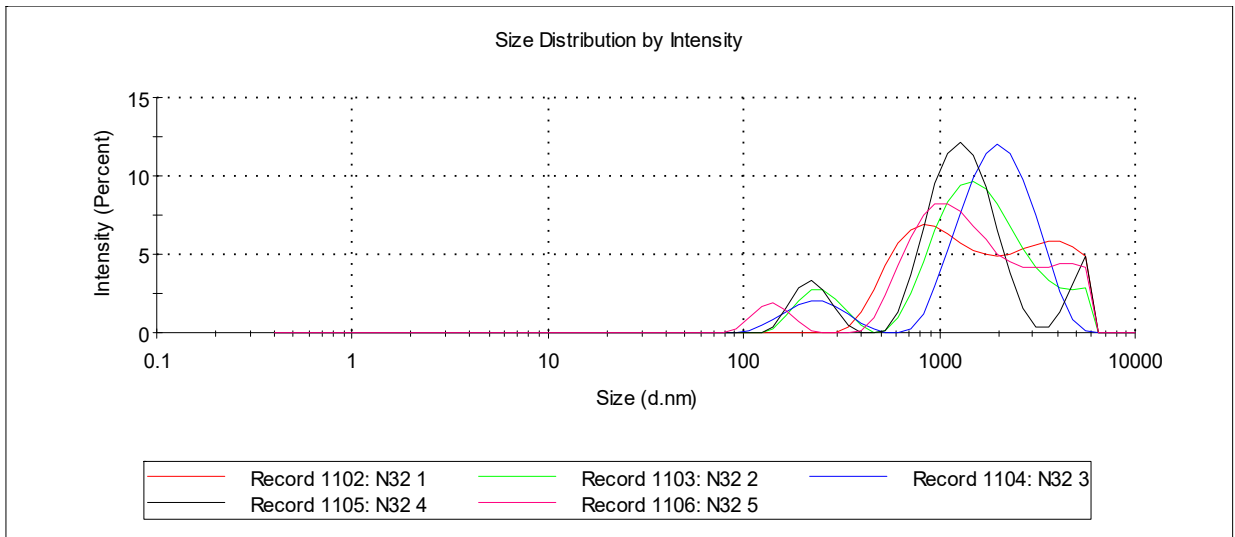


Fig.S25. Size distribution by intensity (DLS) of solution of the OLA-5 (0.19 mg/ml) and hemoglobin (10 μ M) in the 50 mM phosphate buffer at pH 7.4.

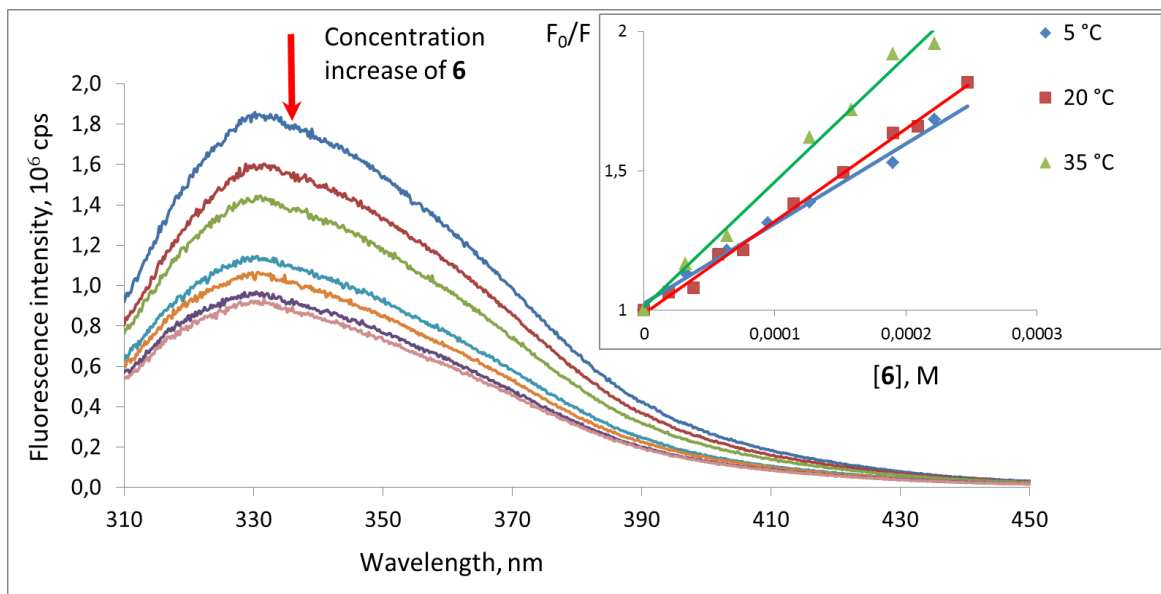


Fig.S26. Fluorescence spectra of BSA (5 μ M) at different concentrations of the compound **6** (0-0.5 mg/ml) in phosphate buffer at pH 7.4. The inset shows the plots of F_0/F vs. concentration of the compound **6** at different temperatures (5, 20 and 35 $^{\circ}$ C). λ_{ex} =285 nm; λ_{em} =330 nm.

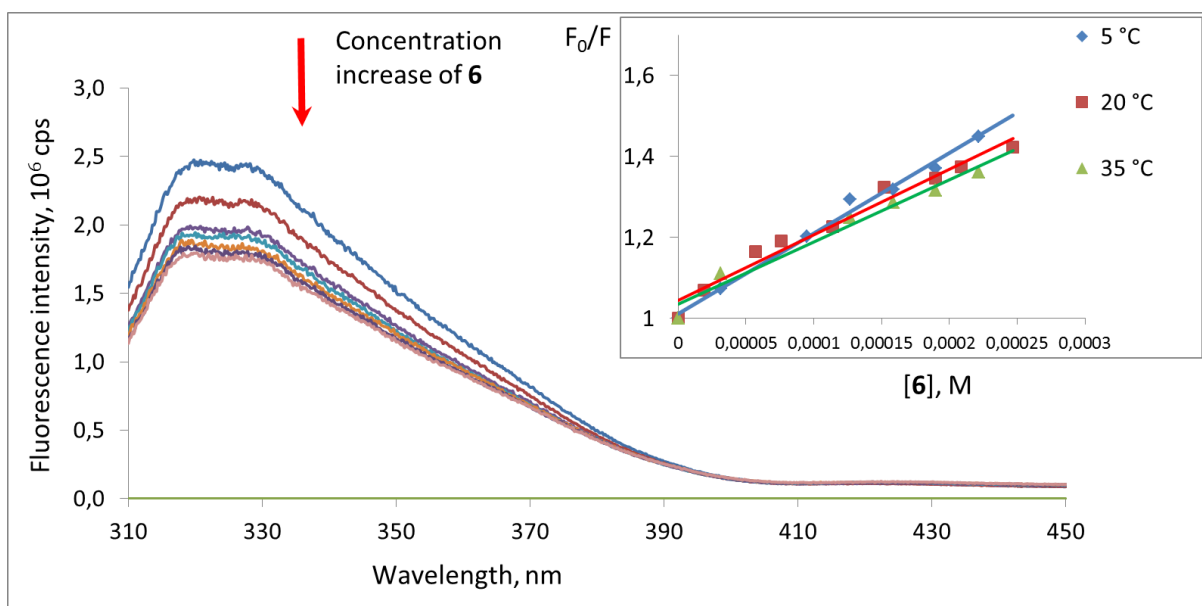


Fig.S27. Fluorescence spectra of Hb (5 μ M) at different concentrations of the compound **6** (0-0.5 mg/ml) in phosphate buffer at pH 7.4. The inset shows the plots of F_0/F vs. concentration of the compound **6** at different temperatures (5, 20 and 35 $^{\circ}$ C). λ_{ex} =285 nm; λ_{em} =330 nm.

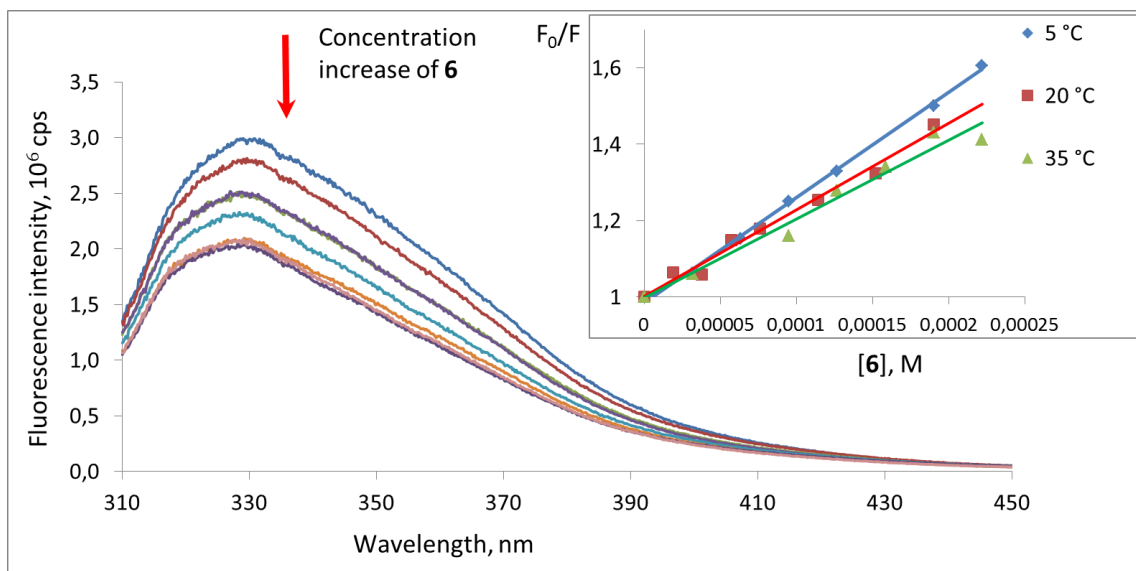


Fig.S28. Fluorescence spectra of Lys ($5 \mu\text{M}$) at different concentrations of the compound **6** (0-0.5 mg/ml) in phosphate buffer at pH 7.4. The inset shows the plots of F_0/F vs. concentration of the compound **6** at different temperatures (5, 20 and 35 °C). $\lambda_{\text{ex}}=285 \text{ nm}$; $\lambda_{\text{em}}=330 \text{ nm}$.

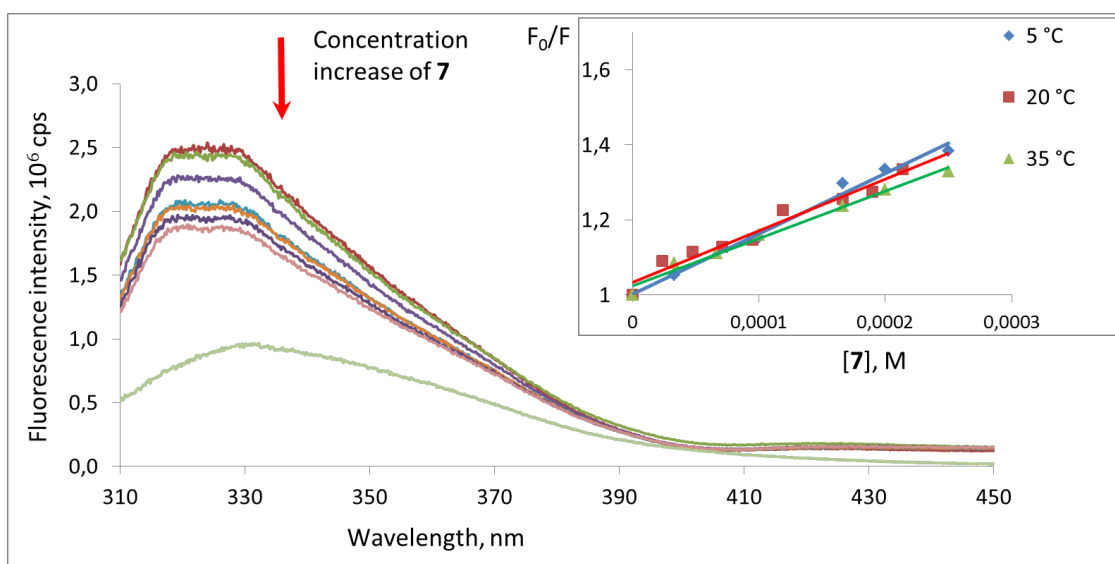


Fig.S.29. Fluorescence spectra of Hb ($5 \mu\text{M}$) at different concentrations of the compound **7** (0-0.5 mg/ml) in phosphate buffer at pH 7.4. The inset shows the plots of F_0/F vs. concentration of the compound **7** at different temperatures (5, 20 and 35 °C). $\lambda_{\text{ex}}=285 \text{ nm}$; $\lambda_{\text{em}}=330 \text{ nm}$.

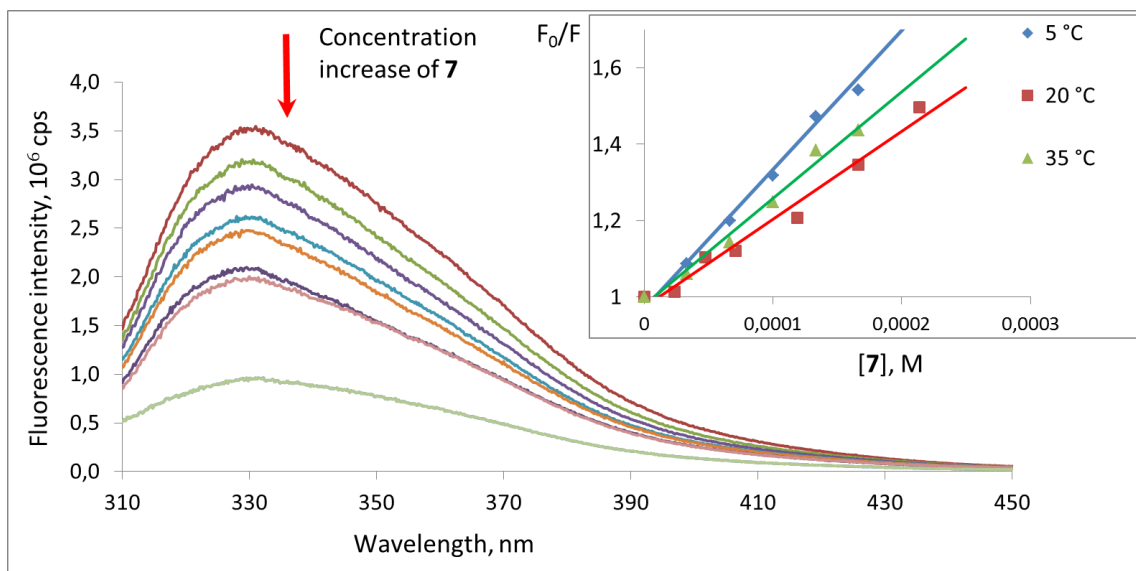


Fig.S30. Fluorescence spectra of Lys (5 μM) at different concentrations of the compound **7** (0-0.5 mg/ml) in phosphate buffer at pH 7.4. The inset shows the plots of F_0/F vs. concentration of the compound **7** at different temperatures (5, 20 and 35 $^{\circ}\text{C}$). $\lambda_{\text{ex}}=285$ nm; $\lambda_{\text{em}}=330$ nm.

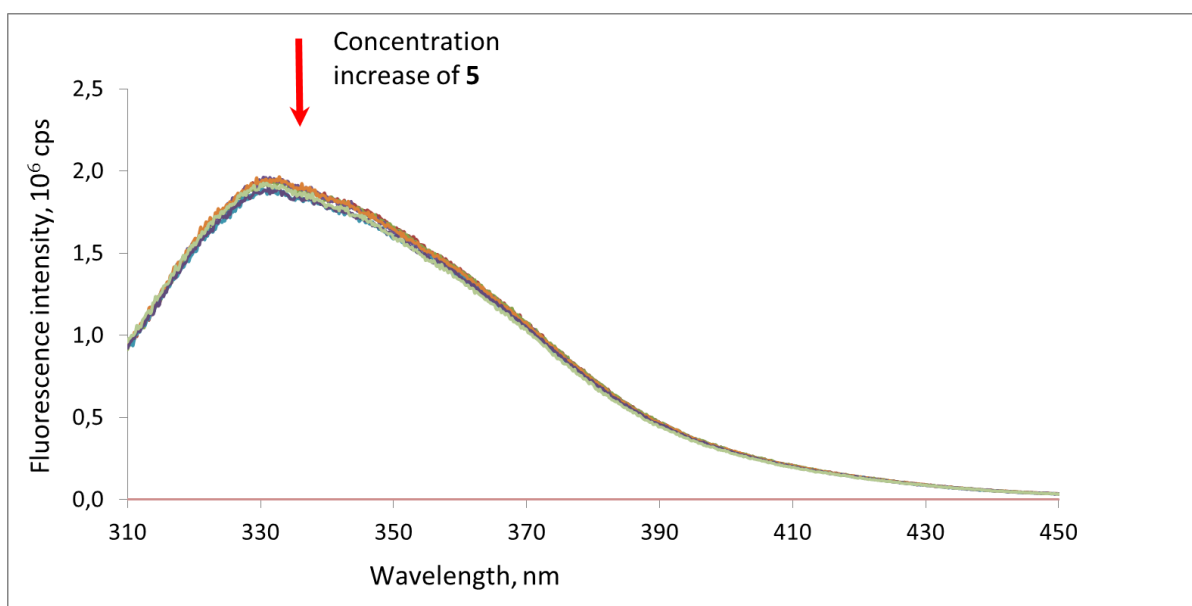


Fig.S31. Fluorescence spectra of BSA (5 μM) at different concentrations of the compound **5** (0-0.5 mg/ml) in phosphate buffer at pH 7.4.

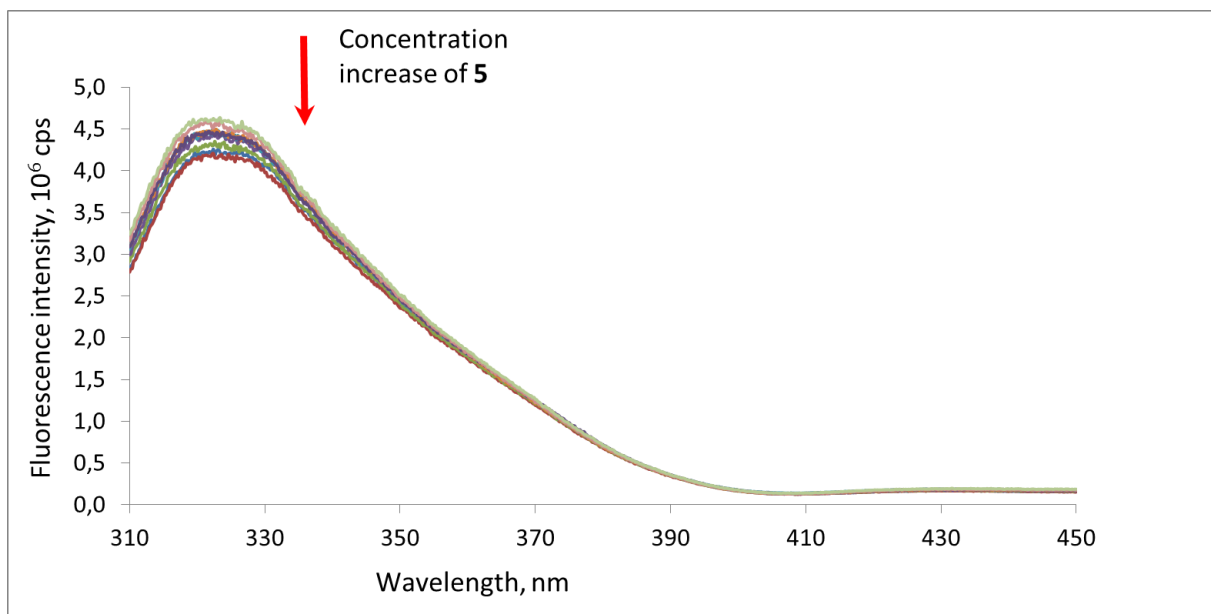


Fig.S32. Fluorescence spectra of Hb (5 μM) at different concentrations of the compound **5** (0-0.5 mg/ml) in phosphate buffer at pH 7.4.

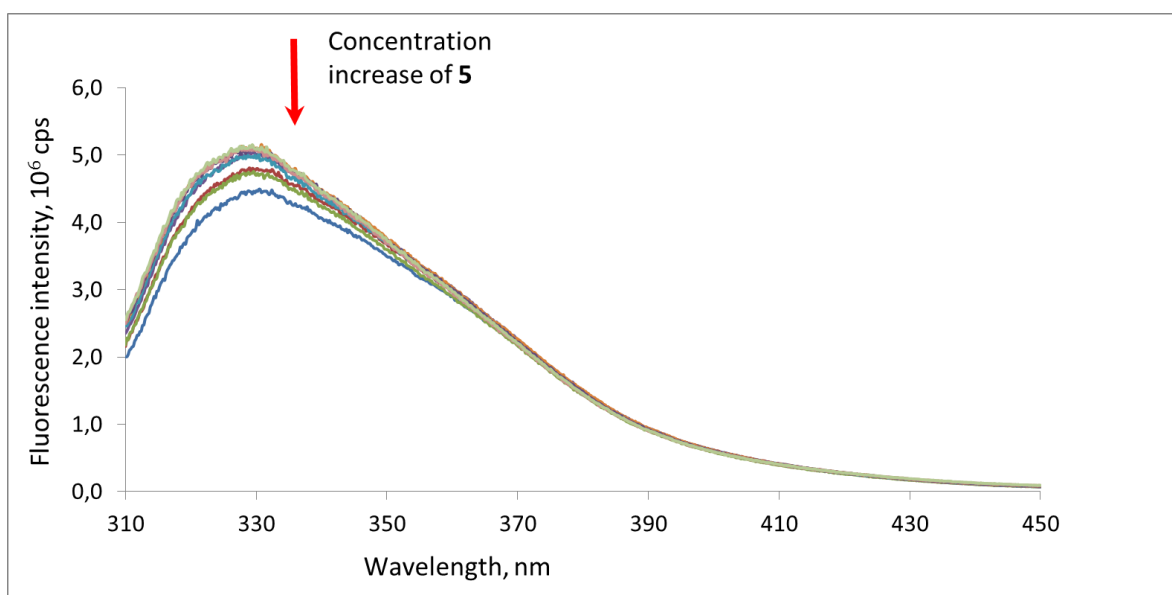


Fig.S33. Fluorescence spectra of Lys (5 μM) at different concentrations of the compound **5** (0-0.5 mg/ml) in phosphate buffer at pH 7.4.

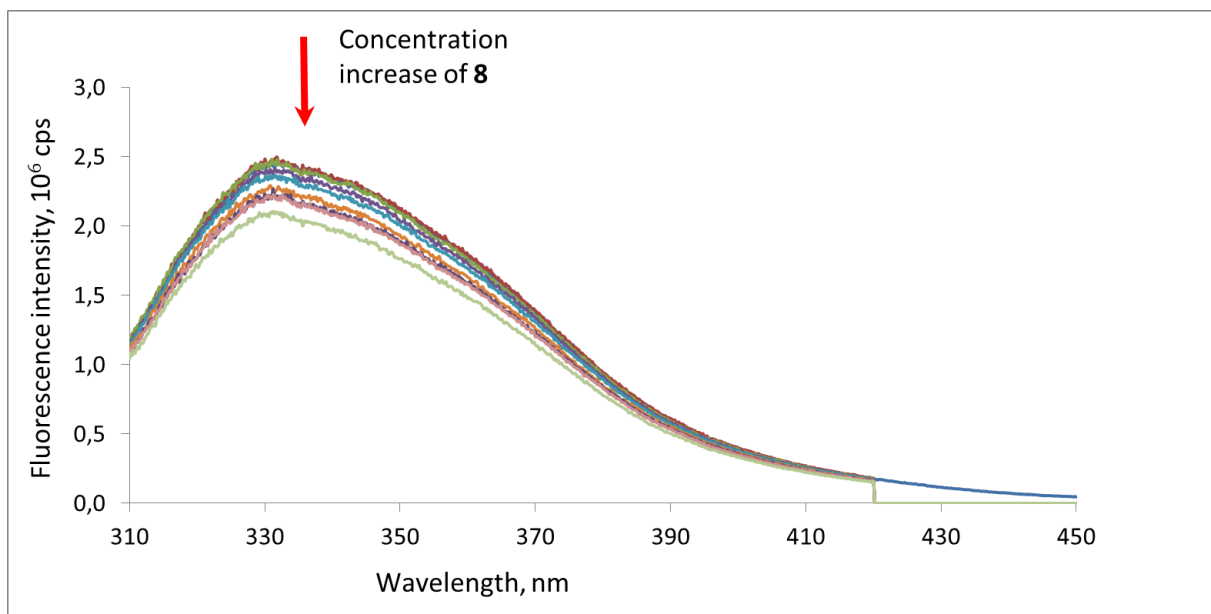


Fig.S34. Fluorescence spectra of BSA (5 μM) at different concentrations of the compound **8** (0-0.5 mg/ml) in phosphate buffer at pH 7.4.

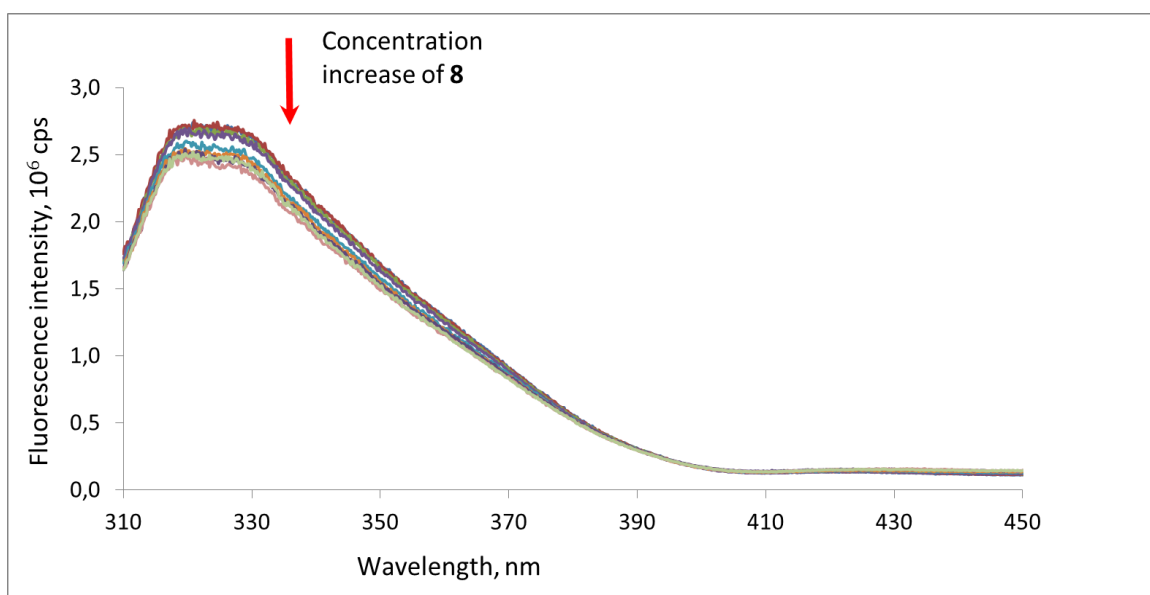


Fig.S35. Fluorescence spectra of Hb (5 μM) at different concentrations of the compound **8** (0-0.5 mg/ml) in phosphate buffer at pH 7.4.

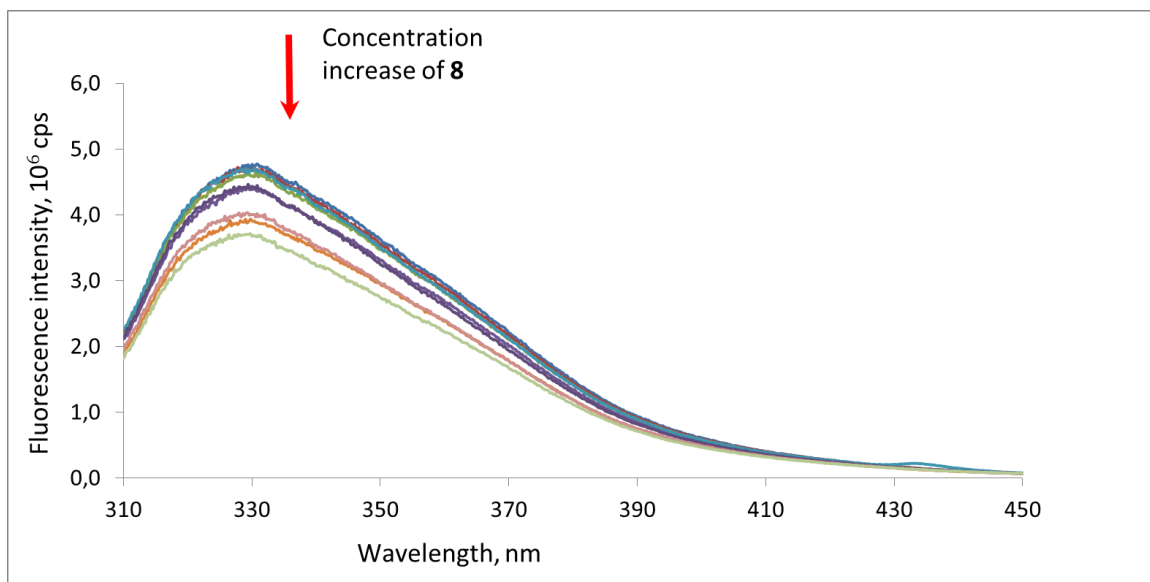


Fig.S36. Fluorescence spectra of Lys (5 μ M) at different concentrations of the compound **8** (0-0.5 mg/ml) in phosphate buffer at pH 7.4.

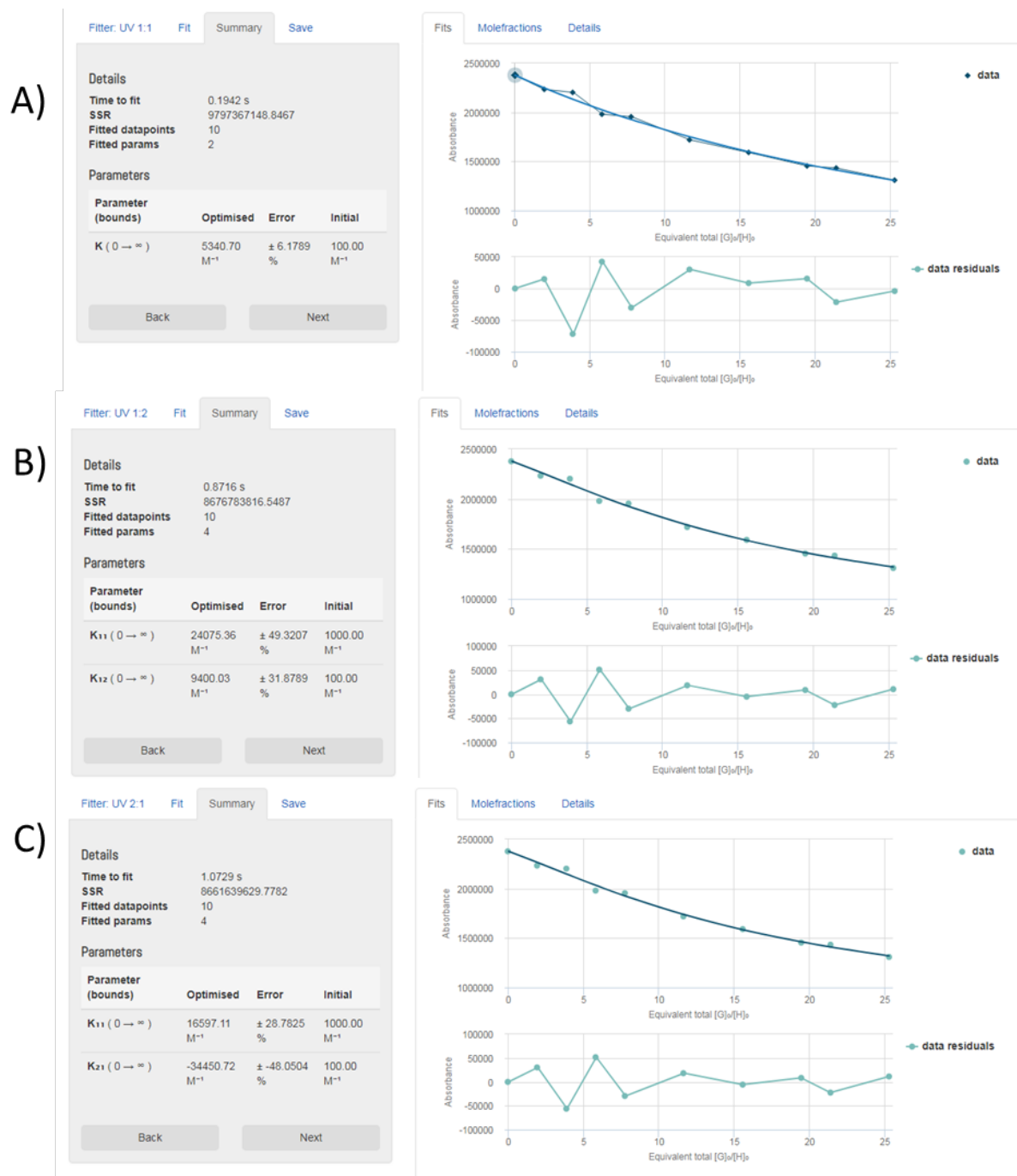


Fig.S37. Screenshots taken from the summary window of the website supramolecular.org. These screenshots show the raw data for titration of **6** with BSA, the data fitted to 1:1 (A), 1:2 (B) and 2:1 (C) binding models.

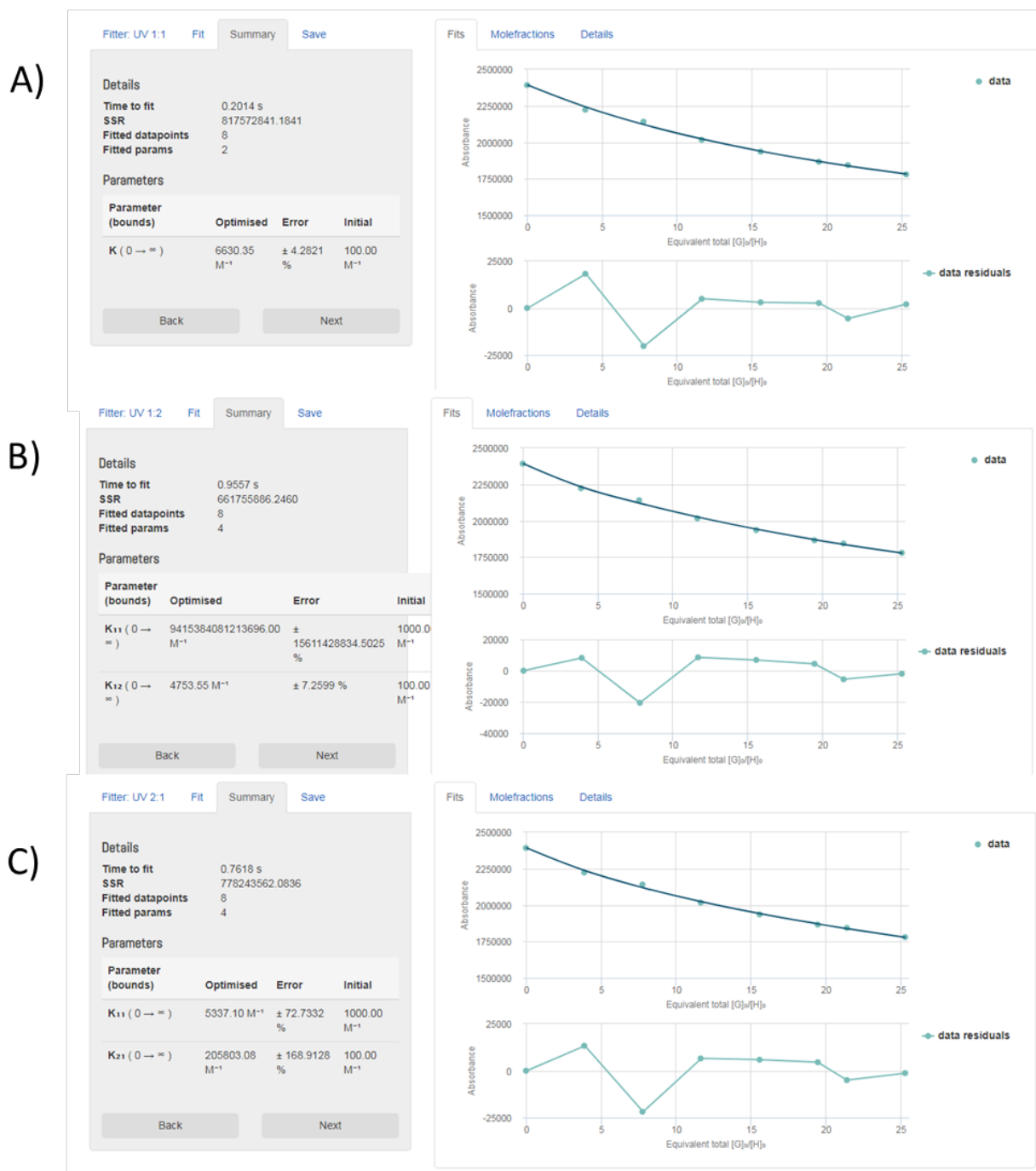


Fig.S38. Screenshots taken from the summary window of the website supramolecular.org. These screenshots show the raw data for titration of **6** with Hb, the data fitted to 1:1 (A), 1:2 (B) and 2:1 (C) binding models..

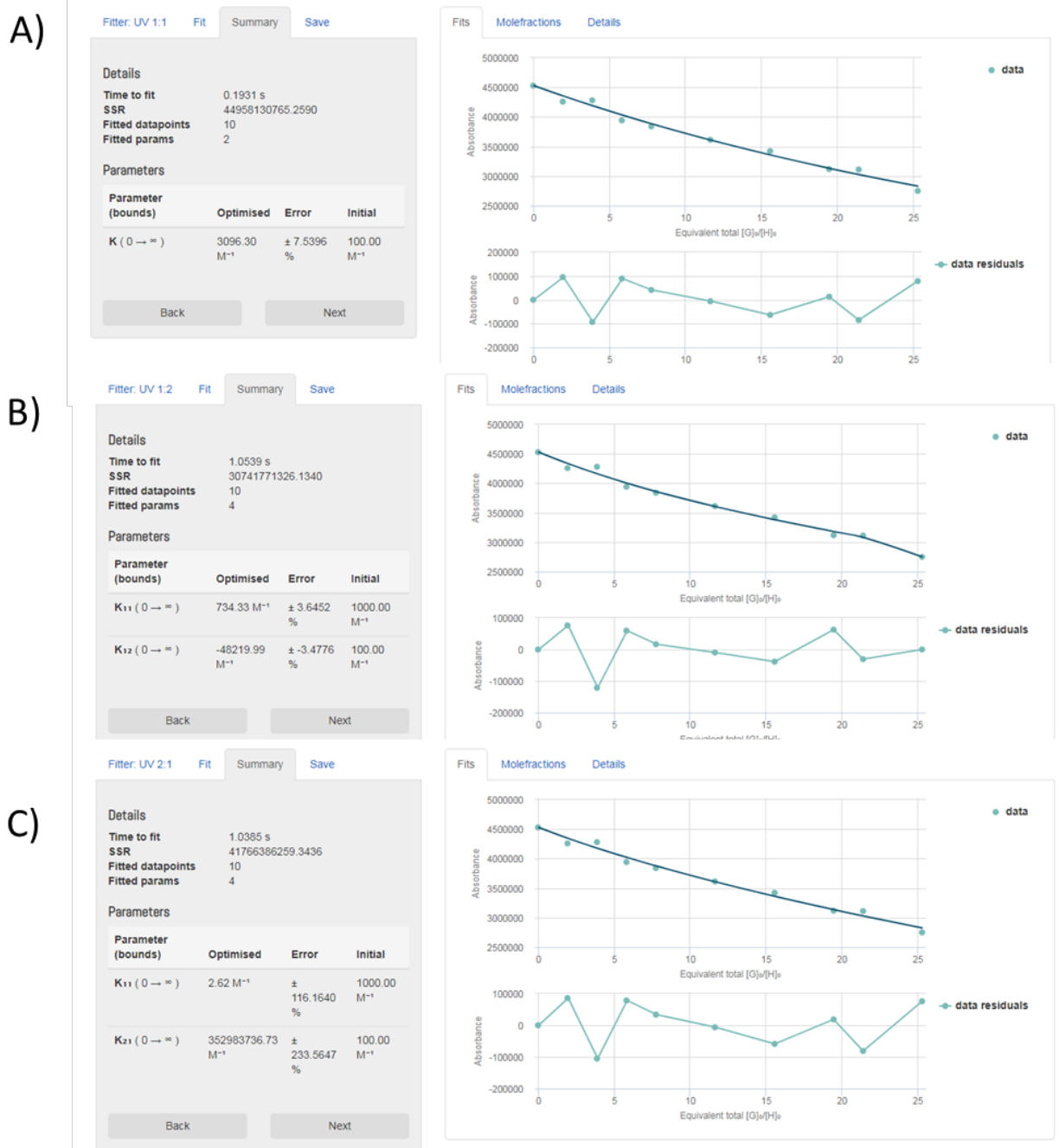
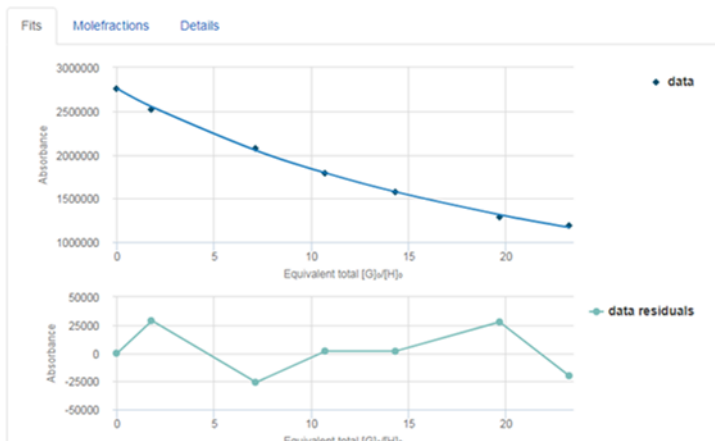
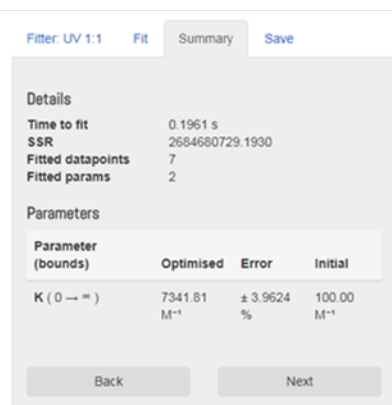
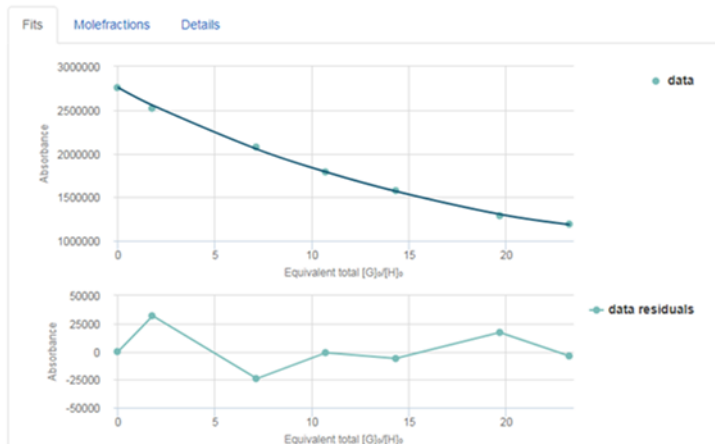
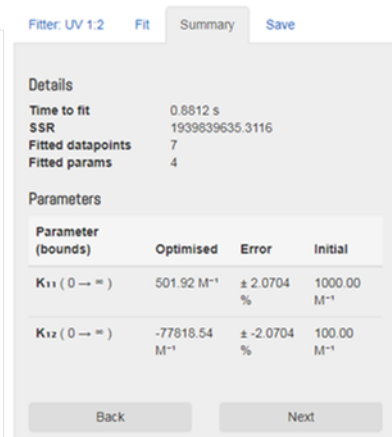


Fig.S39. Screenshots taken from the summary window of the website supramolecular.org. These screenshots show the raw data for titration of **6** with Lys, the data fitted to 1:1 (A), 1:2 (B) and 2:1 (C) binding models.

A)



B)



C)

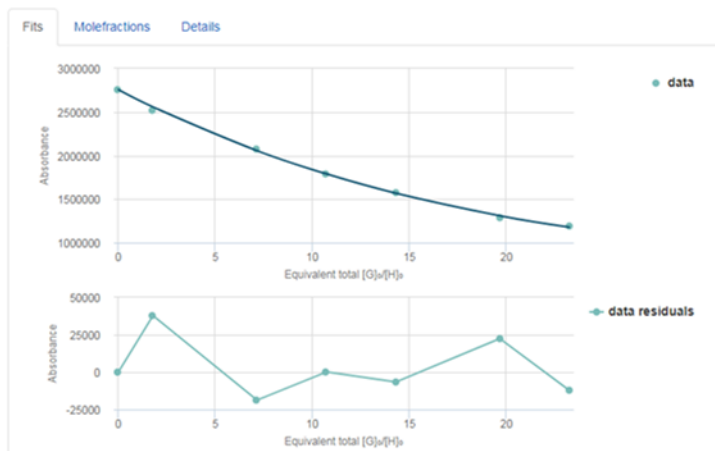
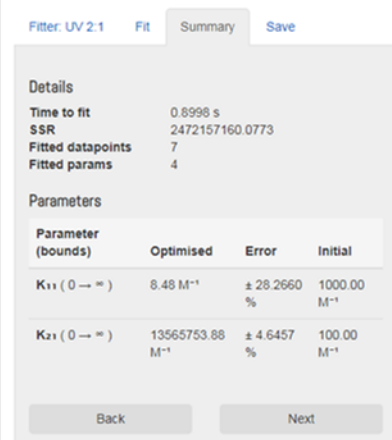


Fig.S40. Screenshots taken from the summary window of the website supramolecular.org. These screenshots show the raw data for titration of **7** with BSA, the data fitted to 1:1 (A), 1:2 (B) and 2:1 (C) binding models.

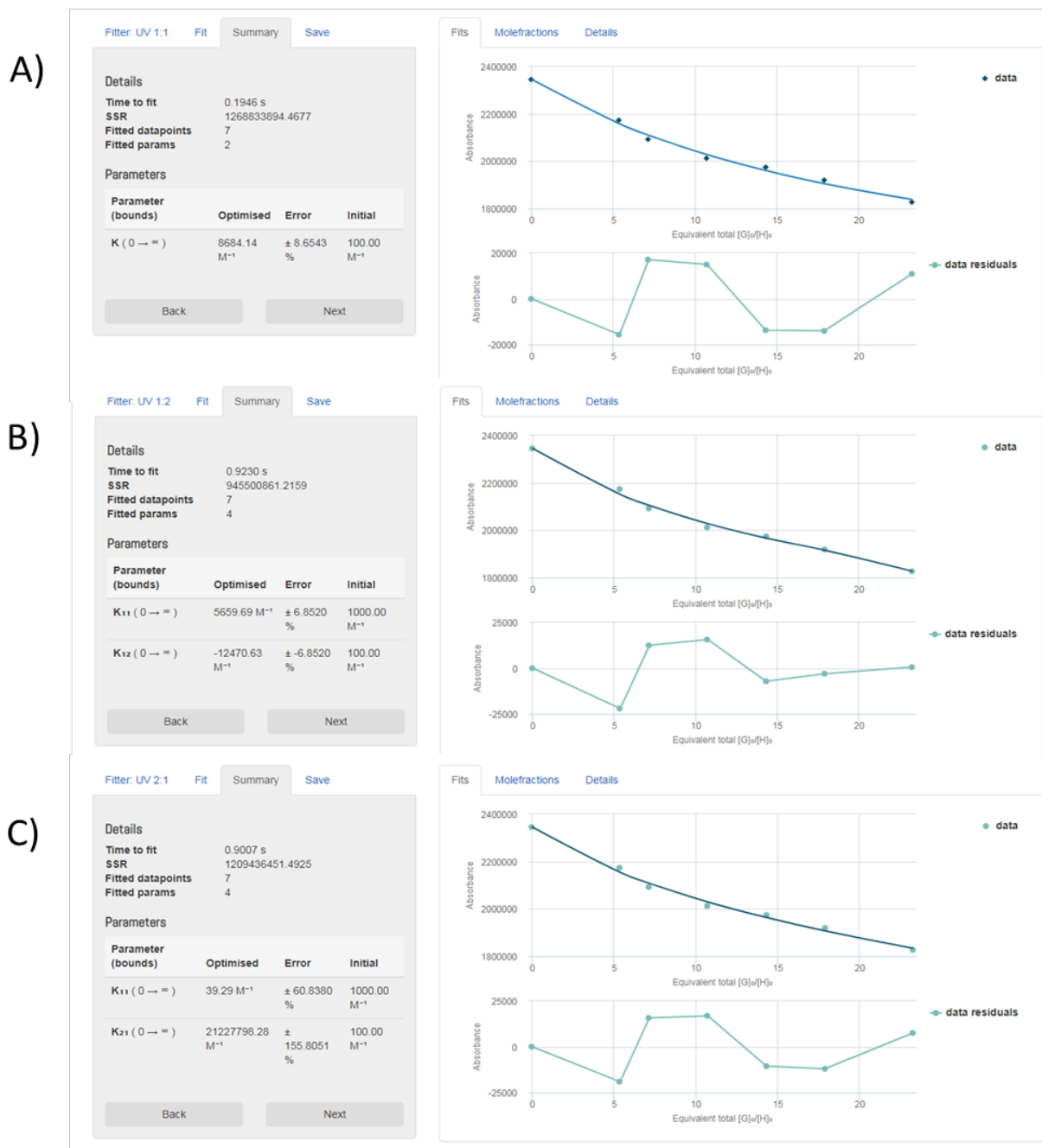
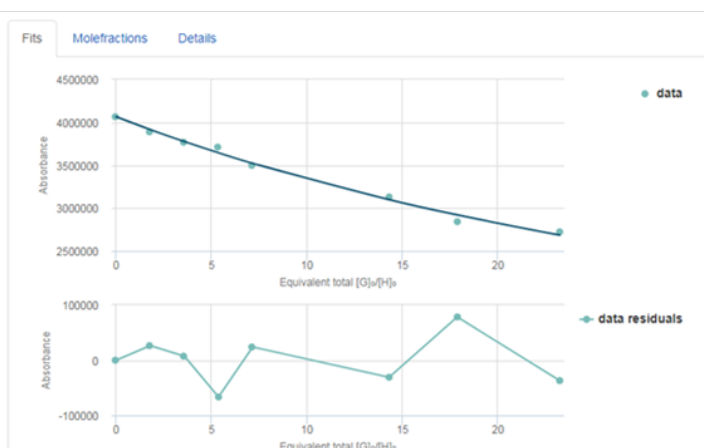
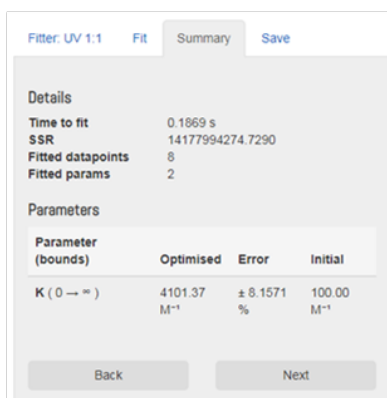
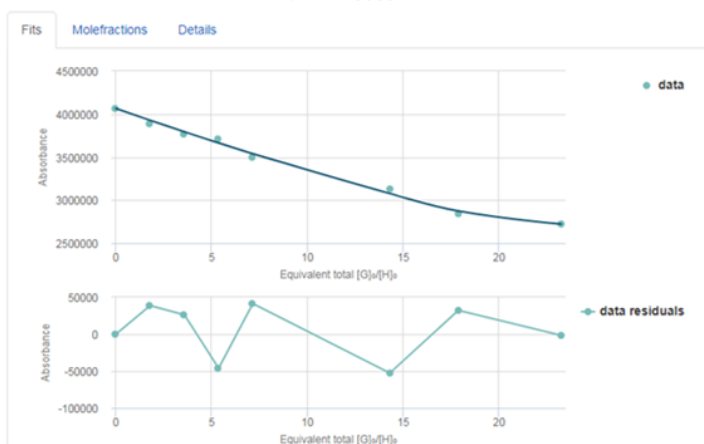
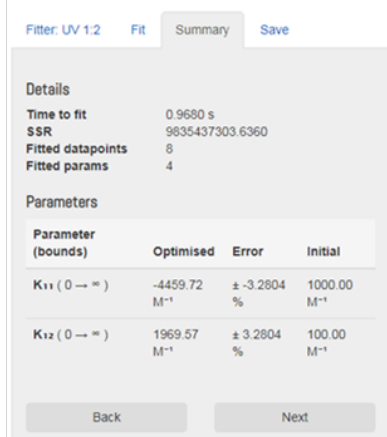


Fig.S41. Screenshots taken from the summary window of the website supramolecular.org. These screenshots show the raw data for titration of **7** with Hb, the data fitted to 1:1 (A), 1:2 (B) and 2:1 (C) binding models.

A)



B)



C)

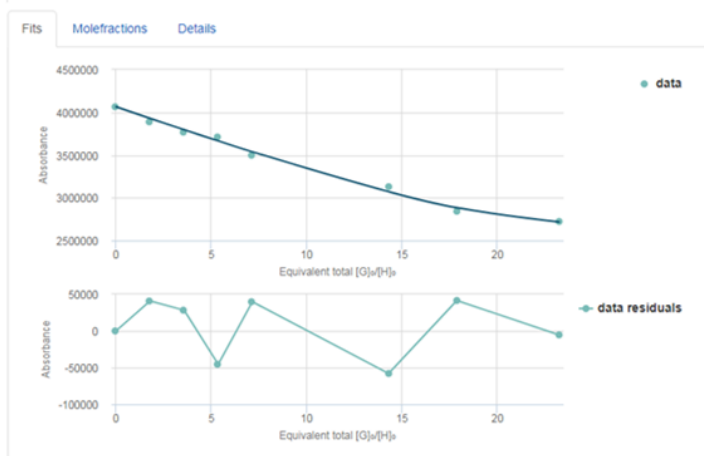
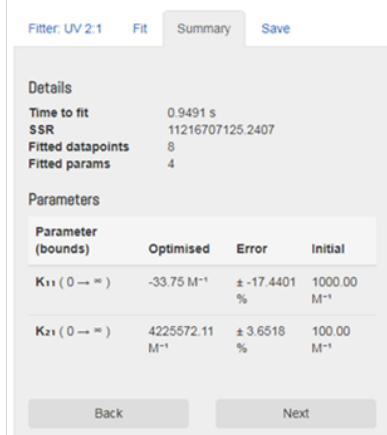


Fig.S42. Screenshots taken from the summary window of the website supramolecular.org. These screenshots show the raw data for titration of **7** with Lys, the data fitted to 1:1 (A), 1:2 (B) and 2:1 (C) binding models.