Supplementary Materials

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N-Oxyethylimidazolium Calix[4]arenes and Thiacalix[4]arenes: Difference in Solubilization Property and Detection of Adenine-Containing Nucleotides

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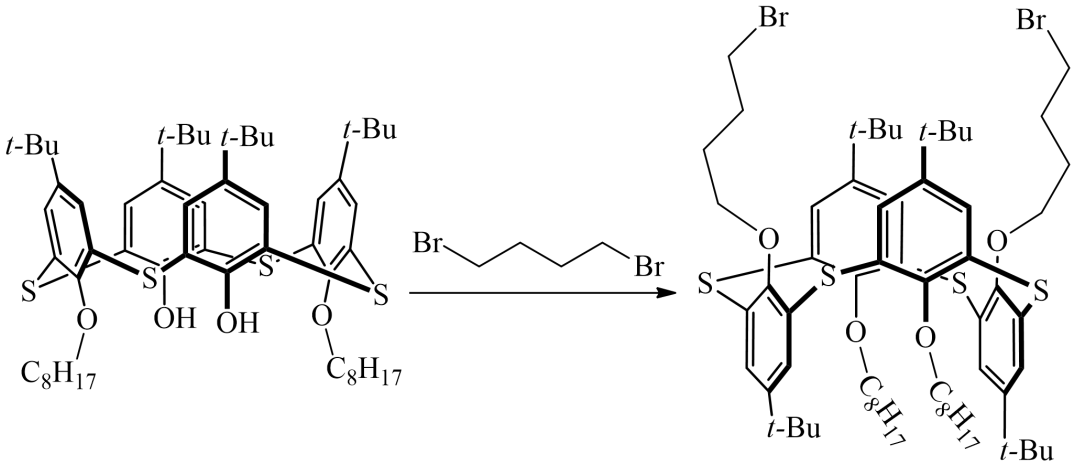


Figure S1. Synthesis of 5,7,11,17-tetra-*p*-*tert*-butyl-25,27-dioctil-26,28- di-4'brombutyloxy-2,8,14,20- tetrathiacalix[4]arene.

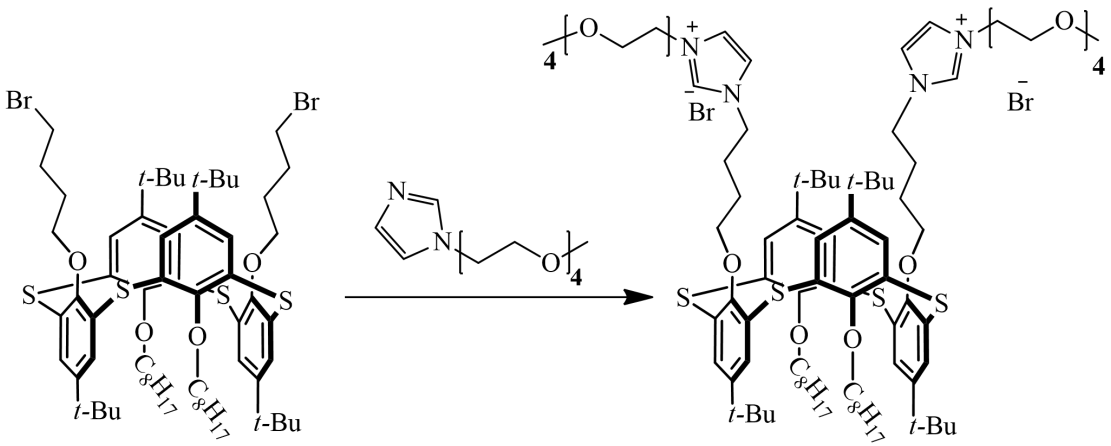


Figure S2. Synthesis of 5,7,11,17-tetra-*p*-*tert*-butyl-25,27-dioctil-26,28- bis[4-(3-N-2-(2-(2-(2-methylethoxy)ethoxy) ethoxy)ethyl) imidazolium) butyloxy]-2,8,14,20- tetrathiacalix[4]arene

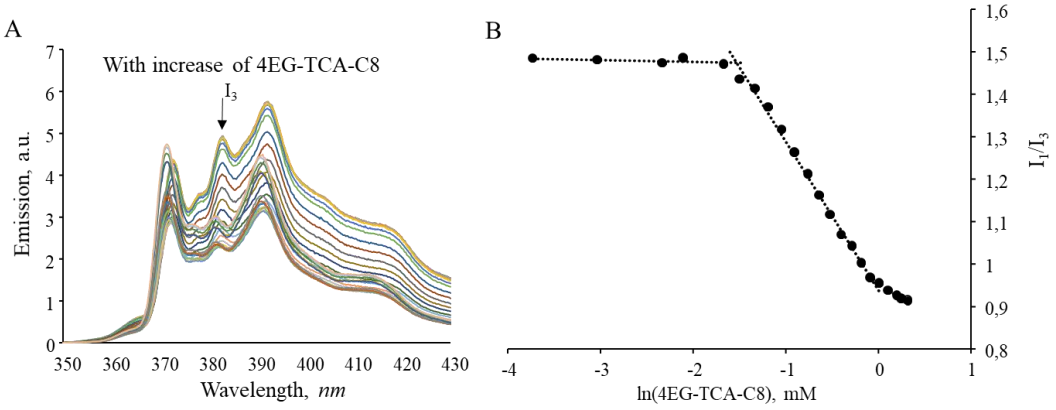
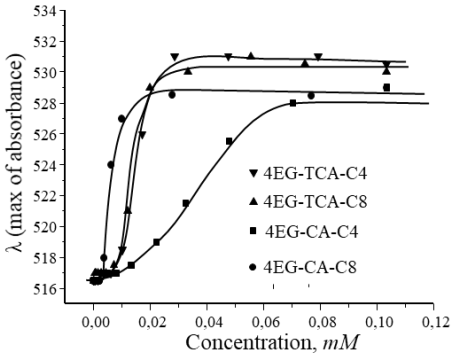


Figure S3. A) Fluorescence emission of pyrene in aqueous solutions of 4EG-TCA-C8; B) Plots of pyrene 1:3 ratio versus surfactant concentration for 4EG-TCA-C8, *C*(4EG-TCA-C8) = 0.0002 – 2 mM, *C*(pyrene) = 0.001 mM.



Model	Boltzmann			
Equation	y = A2 + (A1-A2)/(1 + exp((x-x0)/dx))			
Adj. R-Square	0,99918	0,99762	0,99299	0,99879
		Value	Standard Error	
4EG-TCA-C4	A1	516,48515	0,08961	
	A2	530,9026	0,09783	
	x0	0,01524	1,64357E-4	
4EG-TCA-C8	A1	516,66848	0,12846	
	A2	530,37532	0,15449	
	x0	0,01403	2,97051E-4	
4EG-CA-C8	A1	516,36836	0,20395	
	A2	528,17267	0,23143	
	x0	0,00539	1,65931E-4	
4EG-CA-C4	A1	515,91752	0,14612	
	A2	528,90365	0,1442	
	x0	0,03587	5,80283E-4	

Figure S4. Decreasing sigmoid of the Boltzmann type showing the center of the sigmoid x0 ($CAC_{abs.EY}$) for 4EG-CA-Cn and 4EG-TCA-Cn (n = 4, 8) by EY absorbance titration

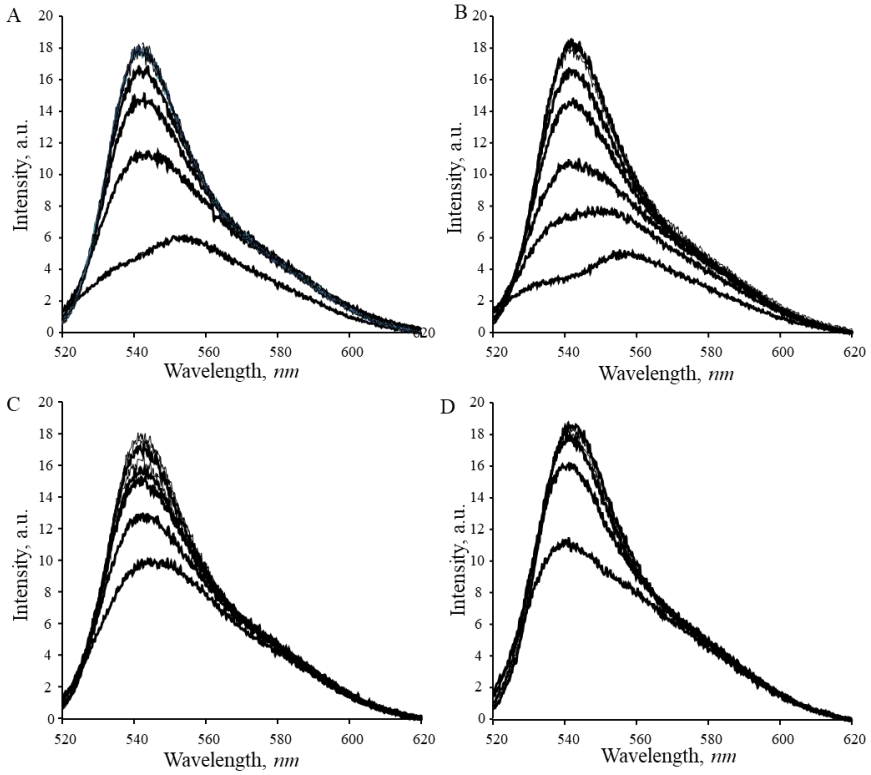


Figure S5. Fluorescence spectra of 0.02 mM EY in the presence of different concentrations of A) 4EG-TCA-C4, B) 4EG-TCA-C8, C) 4EG-CA-C4 and D) 4EG-CA-C8 before redshifts.

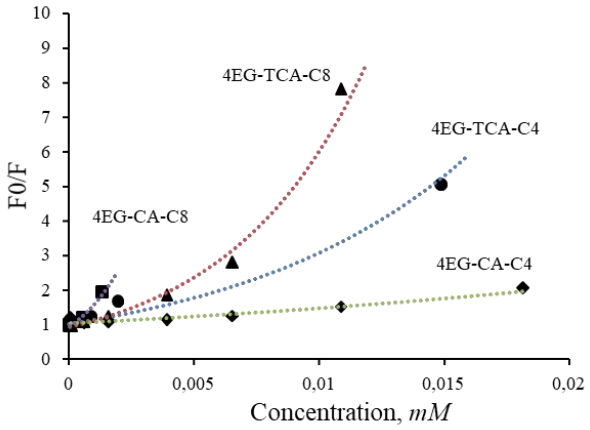
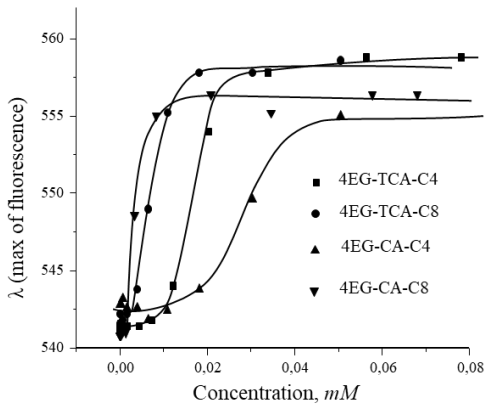


Figure S6. Stern–Volmer plot for the fluorescence quenching of 0.02 mM EY in water by 4EG-CA-Cn and 4EG-TCA-Cn (n = 4, 8) before CAC.



Model	Boltzmann			
Equation	y = A2 + (A1-A2)/(1 + exp((x-x0)/dx))			
Adj. R-Square	0,992383	0,998993	0,994254	0,996262
		Value	Standard Error	
4EG-CA-C4	A1	542,5708	0,194908	
	A2	555,0468	0,325434	
	x0	0,029071	7,05E-04	
4EG-TCA-C4	A1	541,2388	0,090643	
	A2	558,5735	0,124524	
	x0	0,017209	2,02E-04	
4EG-CA-C8	A1	540,926	0,2992	
	A2	555,8801	0,252415	
	x0	0,003302	7,61E-05	
4EG-TCA-C8	A1	541,1779	0,397625	
	A2	558,0484	0,26895	
	x0	0,007114	2,48E-04	

Figure S7. Decreasing sigmoid of the Boltzmann type showing the center of the sigmoid x0 ($CAC_{abs.EY}$) for 4EG-CA-Cn and 4EG-TCA-Cn (n = 4, 8) by EY fluorescence titration

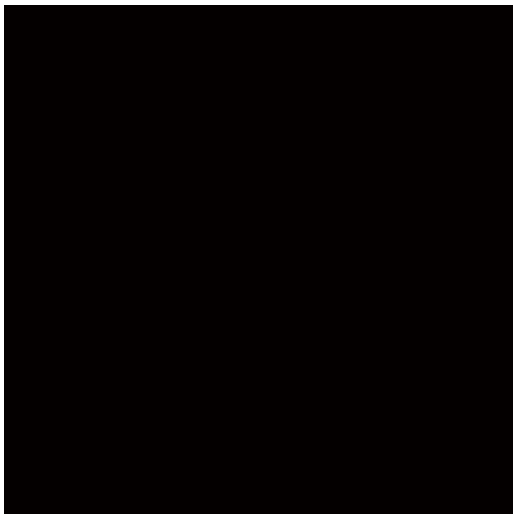


Figure S8. Images of confocal microscopy of EY, *C*(EY) = 0.02 mM, H_2O.

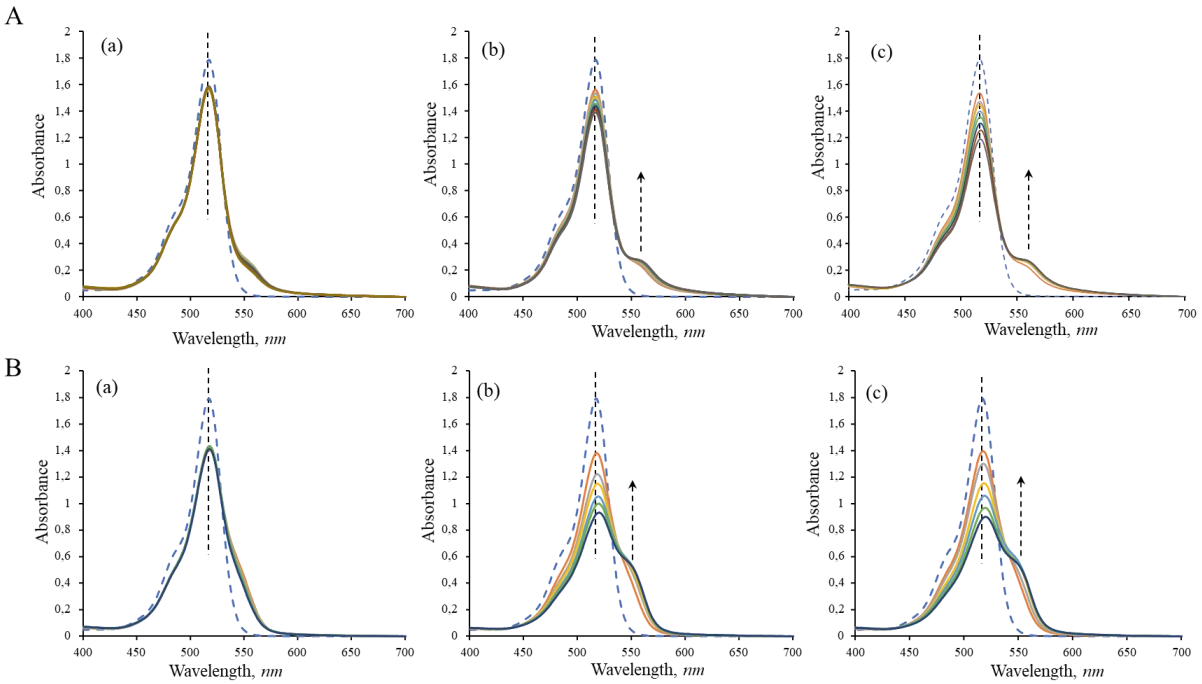


Figure S9. UV-vis spectra of A) 4EG-CA-C8 (0.003 mM) and B) 4EG-TCA-C8 (0.0075 mM) - EY after adding of a) AMP, b) ADP, c) ATP; H_2O, *C*(AD) = 0-0.5 mM, *C*(EY) = 0.02 mM (dash plot is EY in water, orange - EY-macrocycle).

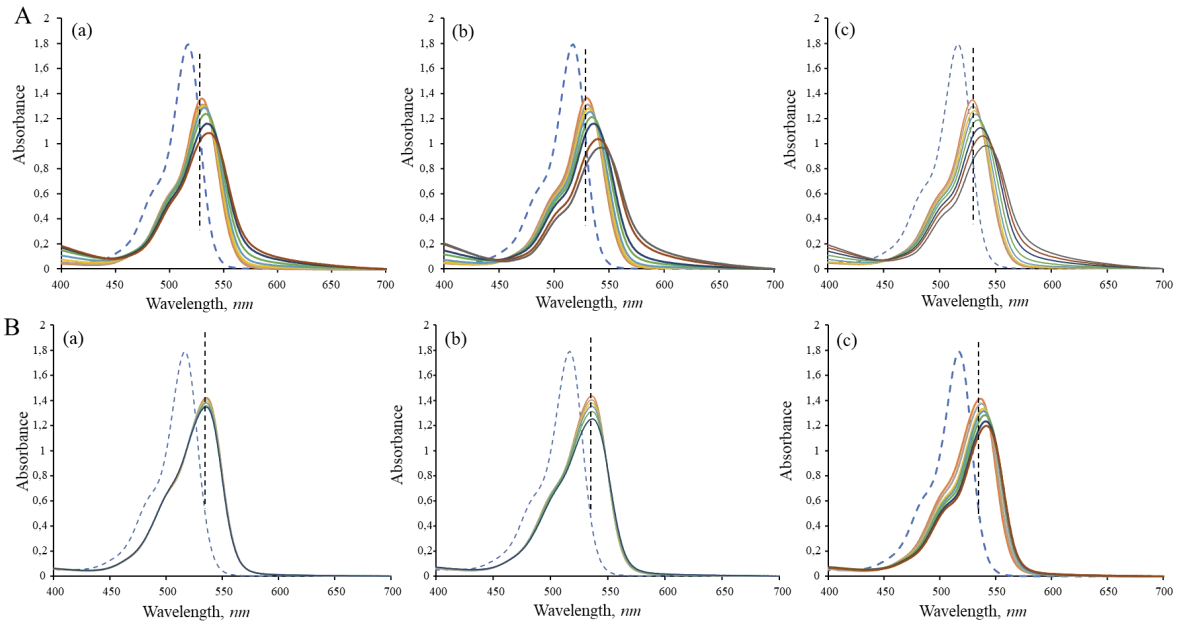


Figure S10 UV-vis spectra of A) 4EG-CA-C8 (0.02 mM) and B) 4EG-TCA-C8 (0.02 mM) - EY after adding of a) AMP, b) ADP, c) ATP; H_2O, *C*(AD) = 0-0.5 mM, *C*(EY) = 0.02 mM (dash plot is EY in water, orange - EY-macrocycle).

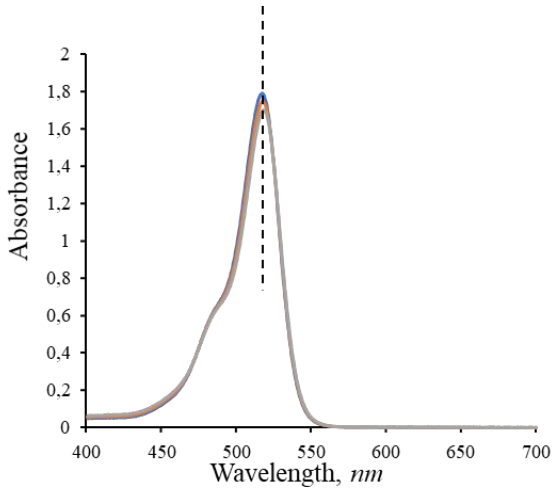


Figure S11 UV-vis spectra of EY after adding of ATP; H_2O, C(AD) = 0-0.5 mM, *C*(EY) = 0.02 mM, *C*(AD) = 0-0.5 mM.