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

Electronic Supplementary Information

Photoactive Bile Salts with Critical Micellar Concentration in the Micromolar Range

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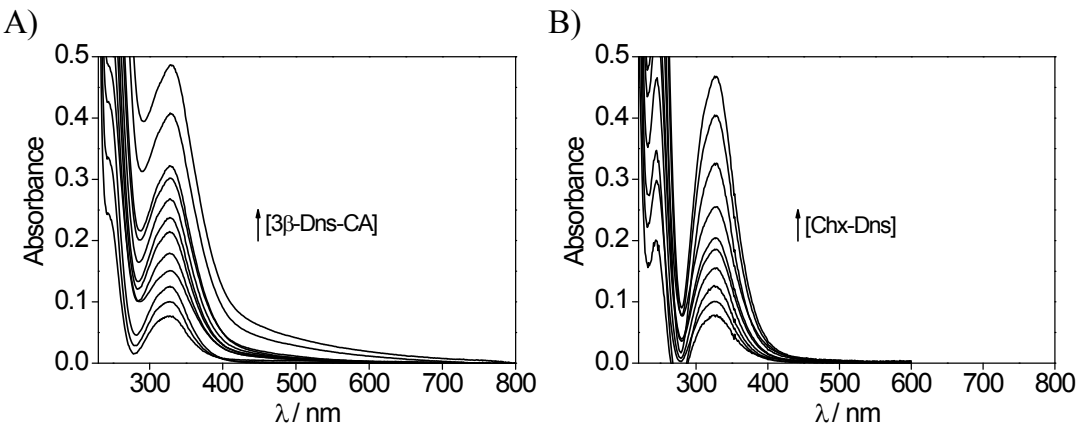

Figure S1. Absorption spectra of A) 3β-Dns-CA or B) Chx-Dns in aqueous solution upon increasing concentrations (25 – 140 μM).

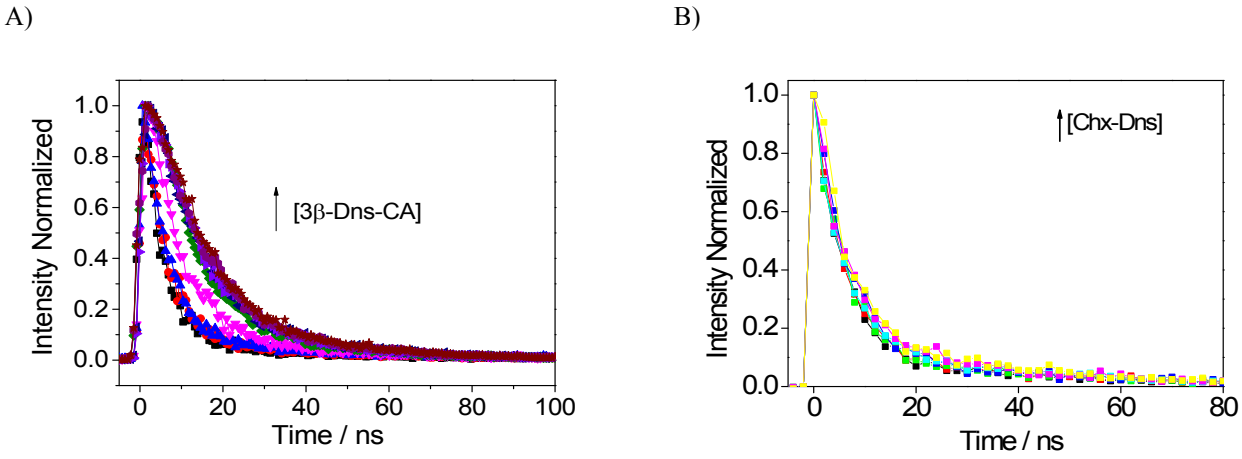

Figure S2. Time-Resolved fluorescence emission intensity *versus* time (λ_{exc} = 375 nm) for 3β-Dns-CA (A) or Chx-Dns (B).

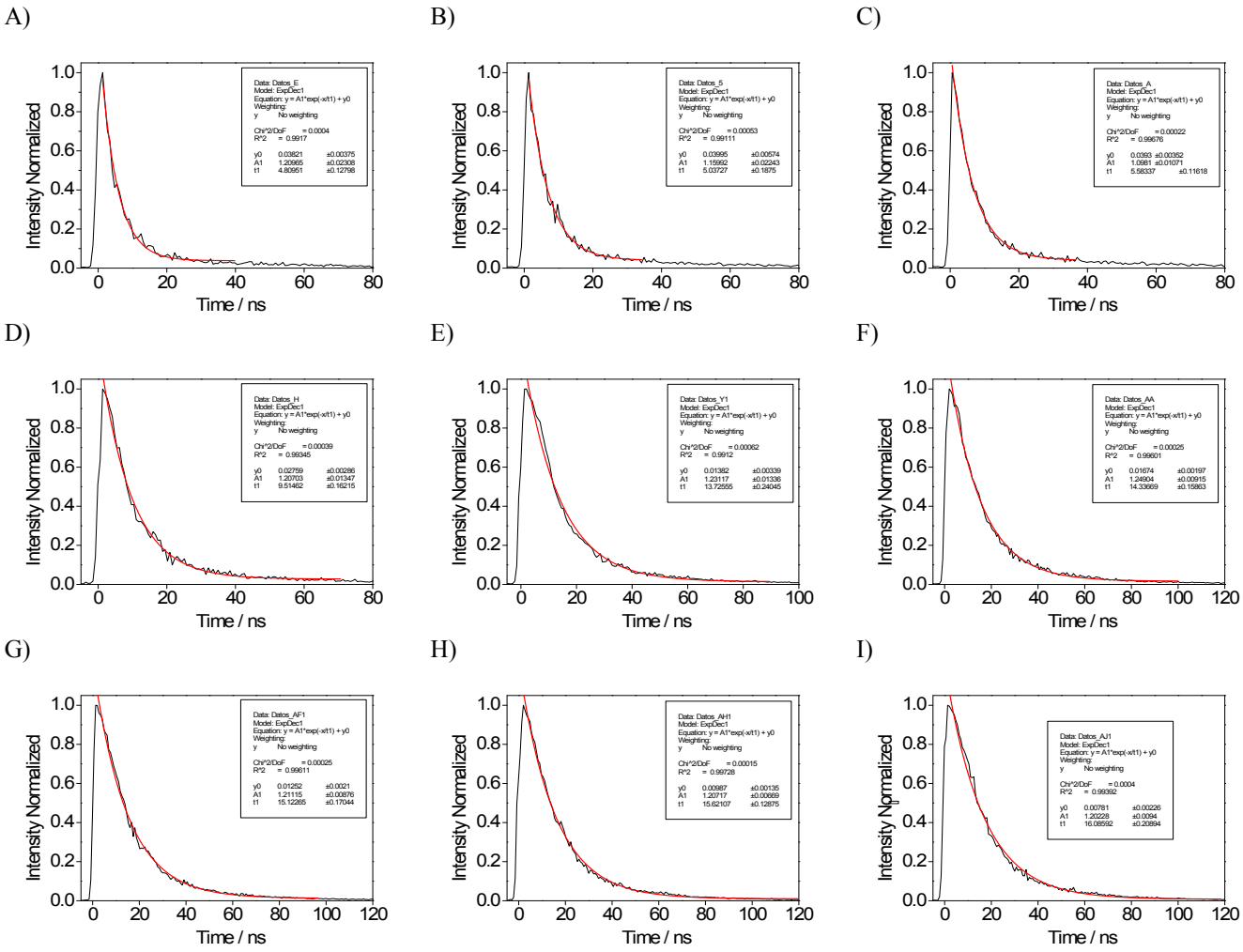

Figure S3. Decay curves for 3β-Dns-CA in aqueous solution obtained upon increasing concentrations together with the corresponding monoexponential fitting (red): 25 (A), 33 (B), 40 (C), 50 (D), 68 (E), 82 (F), 100 (G), 120 (H) and 140 μM (I).

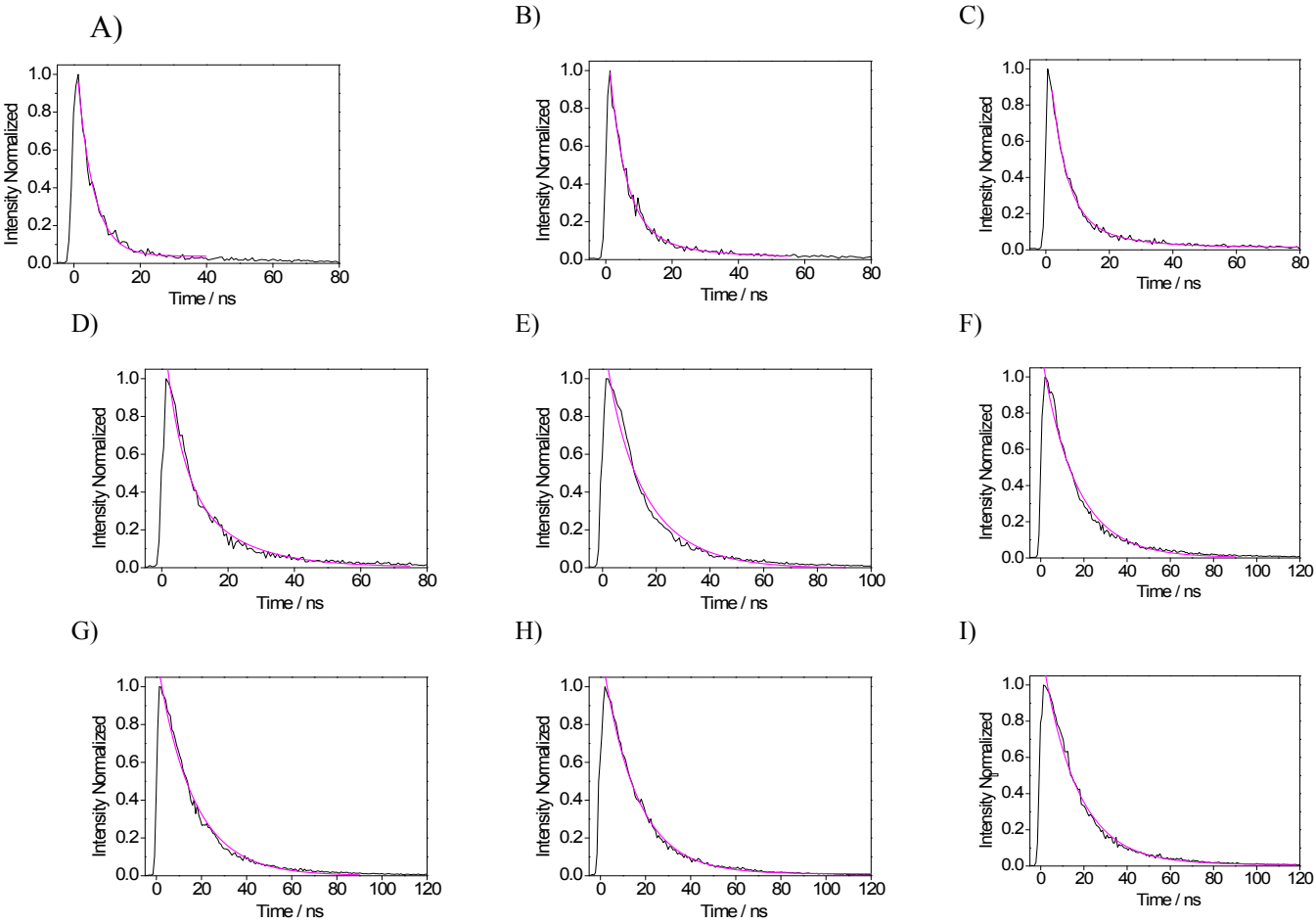

Figure S4. Decay curves for 3β-Dns-CA in aqueous solution obtained upon increasing concentrations together with the corresponding two-exponential fitting (pink): 25 (A), 33 (B), 40 (C), 50 (D), 68 (E), 82 (F), 100 (G), 120 (H) and 140 μM (I).

Table S1. Fluorescence lifetimes of Chx-Dns and 3β-Dns-CA upon increasing concentration (25-140 μM).

[Dns derivative] / μM	*Mono-exponential fitting*						*Two-exponential fitting*				
	Chx-Dns			*3β-Dns-CA*			*3β-Dns-CA*				
	τ / ns	Pre-exponential factor	R^2	τ / ns	Pre-exponential factor	R^2	τ_S / ns [a]	Pre-exponential factor	τ_A / ns [b]	Pre-exponential factor	R^2
25	6.2	0.9380	0.9974	4.8	1.2096	0.9917	4.8	1.1570	16.0	0.0046	0.9920
33	--	--	--	5.3	1.1599	0.9911	4.8	1.0413	16.0	0.1038	0.9923
40	6.5	0.9373	0.9983	5.6	1.0982	0.9967	4.8	1.0227	16.0	0.2134	0.9962
50	6.4	0.9120	0.9971	9.5	1.2070	0.9934	4.8	0.7592	16.0	0.5915	0.9883
68	--	--	--	13.7	1.2321	0.9912	4.8	0.2277	16.0	1.0337	0.9863
82	6.7	0.9279	0.9926	14.3	1.2480	0.9960	4.8	0.0546	16.0	1.1299	0.9884
100	7.0	0.9553	0.9906	15.1	1.2111	0.9962	4.8	0.0038	16.0	1.1362	0.9936
120	7.3	0.9385	0.9954	15.6	1.2072	0.9973	4.8	0.0025	16.0	1.3480	0.9930
140	7.2	0.9882	0.9882	16.1	1.2010	0.9932	4.8	-0.005	16.0	1.4222	0.9946

[a] τ_S correspond to the value obtained for solution. [b] τ_A correspond to the value obtained for photoactive assemblies .

A)

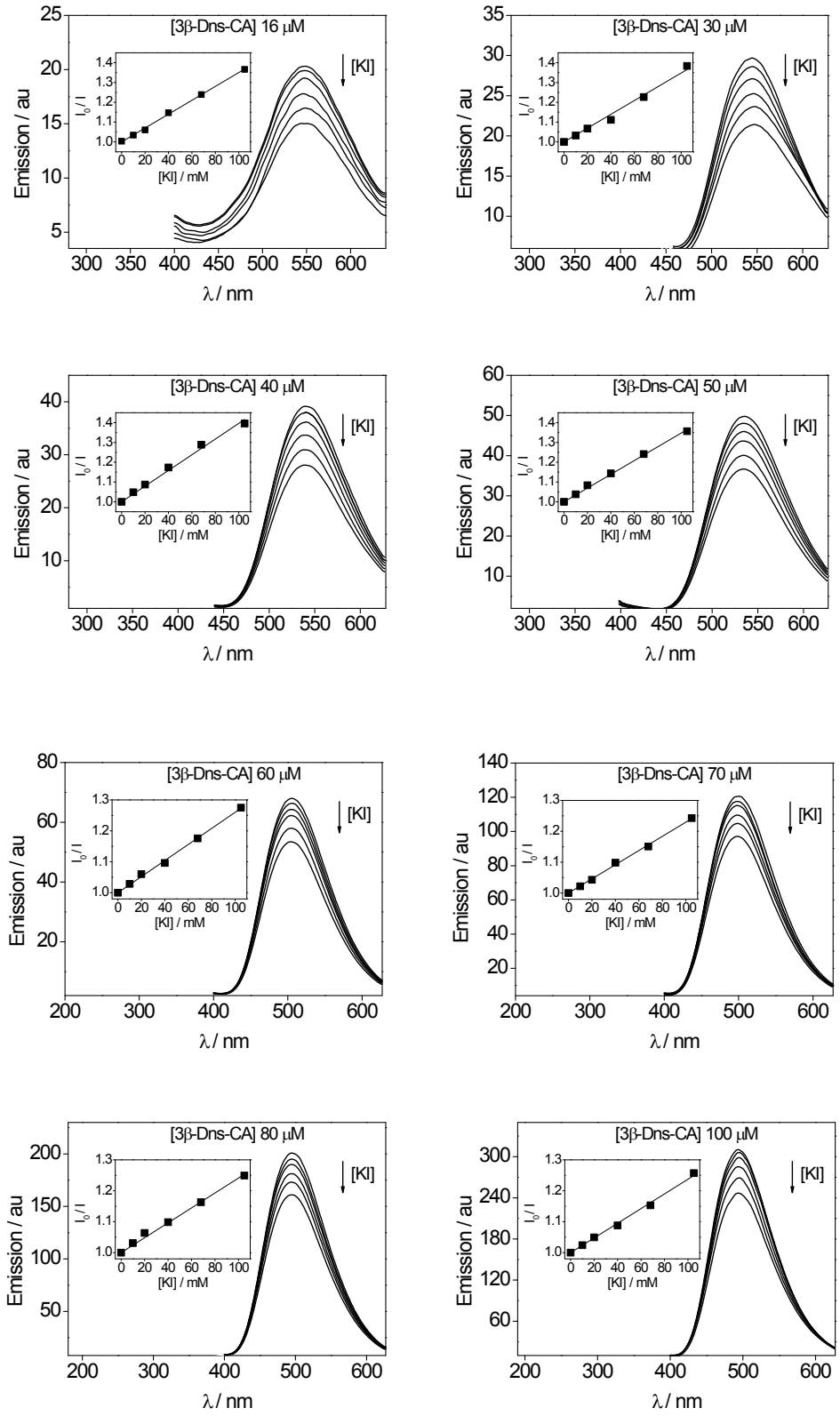

Figure S5. Changes in the emission spectra (λ_{exc} = 330 nm) of A) 3β-Dns-CA and B) 3β-NPX-CA, upon addition of increasing concentrations of KI recorded in 0.2 M aqueous solution at different concentrations, ranging from16 μM to 100 μM. Insets: corresponding Stern-Volmer plots.

B)

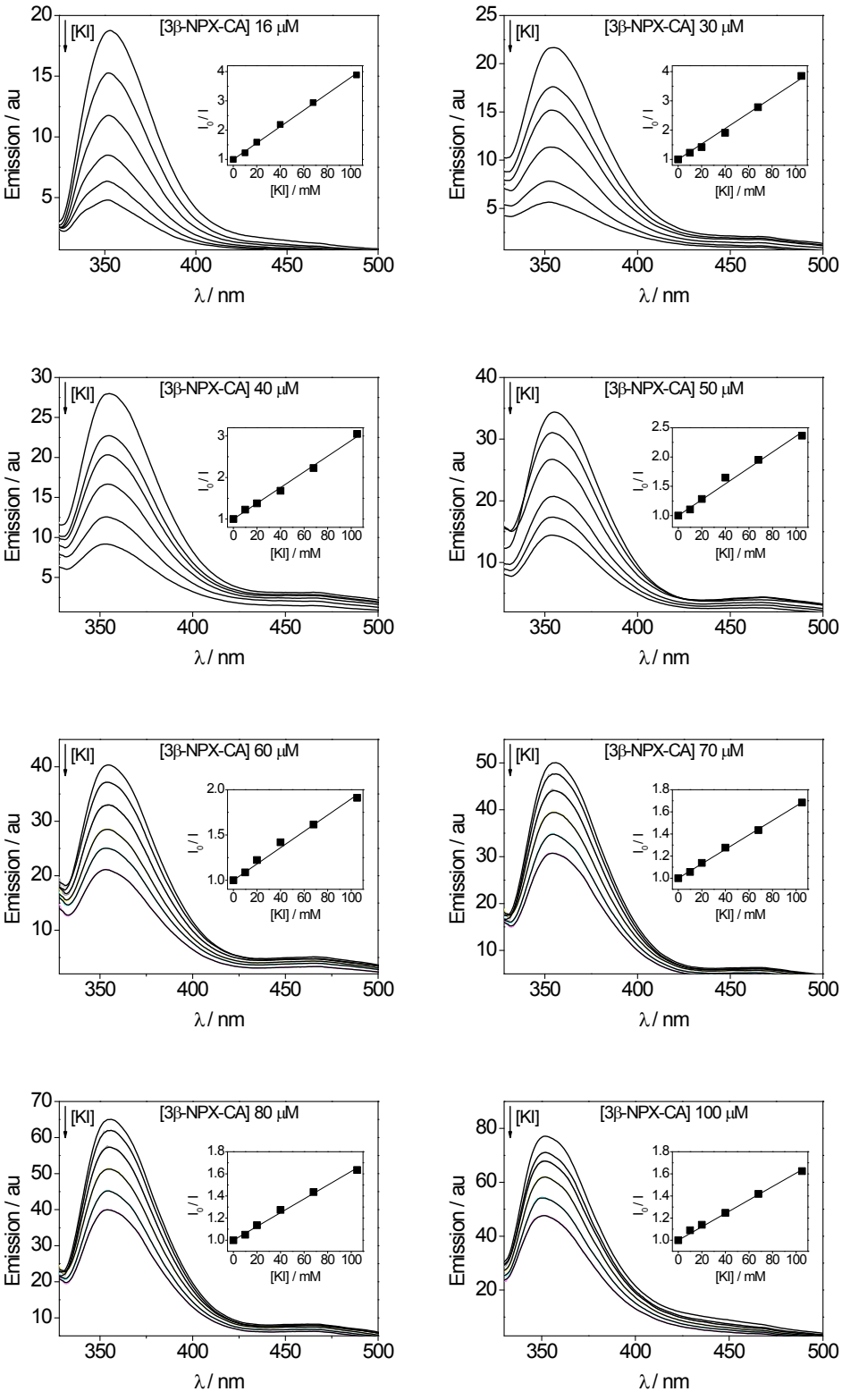

Figure S5. (Cont.) Changes in the emission spectra (λ_{exc} = 330 nm) of A) 3β-Dns-CA and B) 3β-NPX-CA, upon addition of increasing concentrations of KI recorded in 0.2 M aqueous solution at different concentrations, ranging from16 μM to 100 μM. Insets: corresponding Stern-Volmer plots.

Table S2. Rate constants for fluorescence quenching by iodide.

k_q / 10^9 (M^{-1} s^{-1})		
[Dns or NPX derivative] / μM	*3β-Dns-CA*	*3β-NPX-CA*
16	0.75	3.10
25	0.74	--
30	0.72	3.05
40	0.67	2.42
45	0.54	--
50	0.37	1.70
60	0.21	0.87
70	0.17	0.61
80	0.16	0.52
100	0.15	0.53

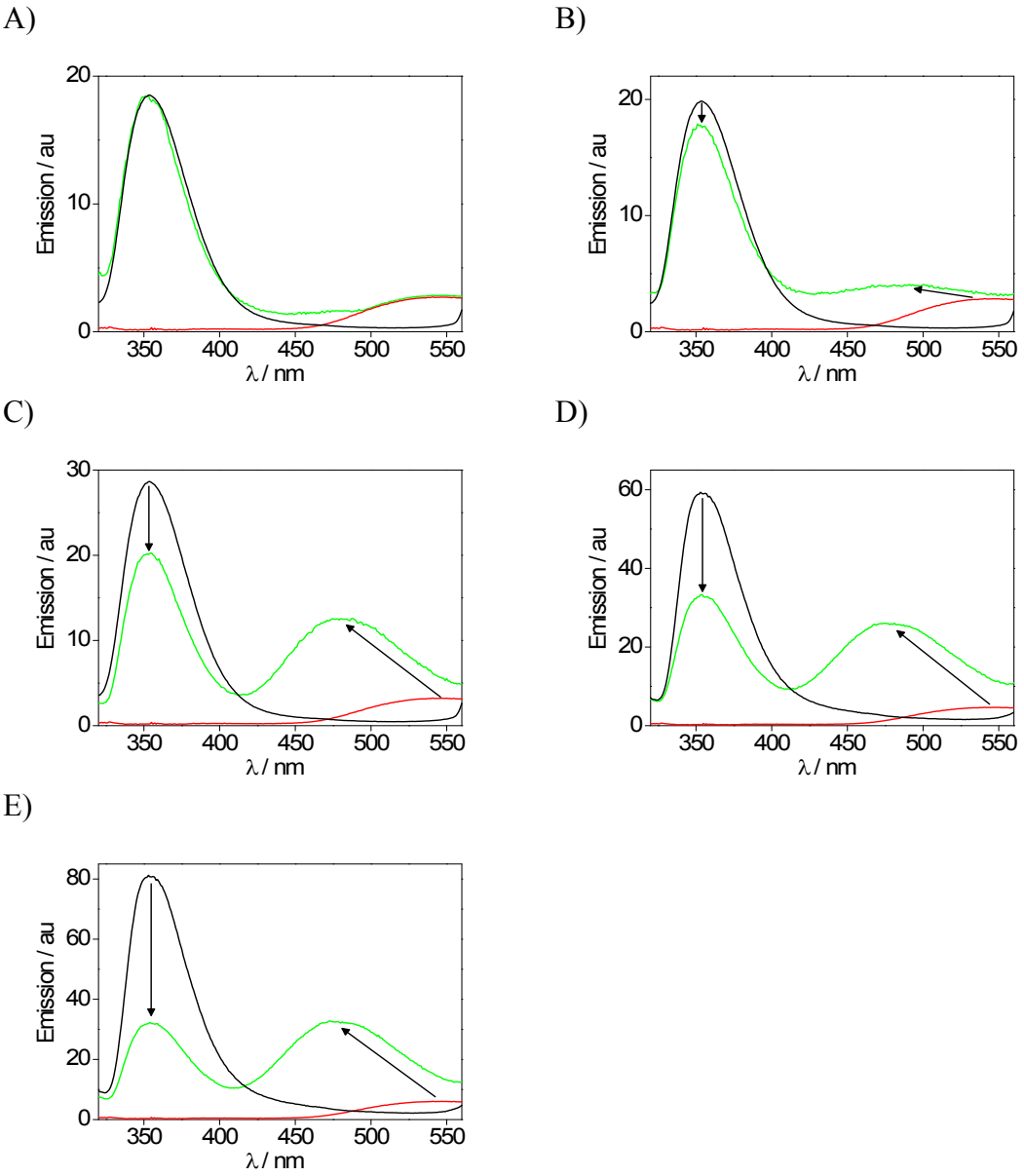

Figure S6. Emission spectra (λ_{exc} = 290 nm) of 3β-Dns-CA (red), 3β-NPX-CA (black) and 1:1 intermolecular mixtures (green) at different concentrations: A) 1 μM; B) 2 μM; C) 6 μM; D) 20 μM and E) 30 μM.

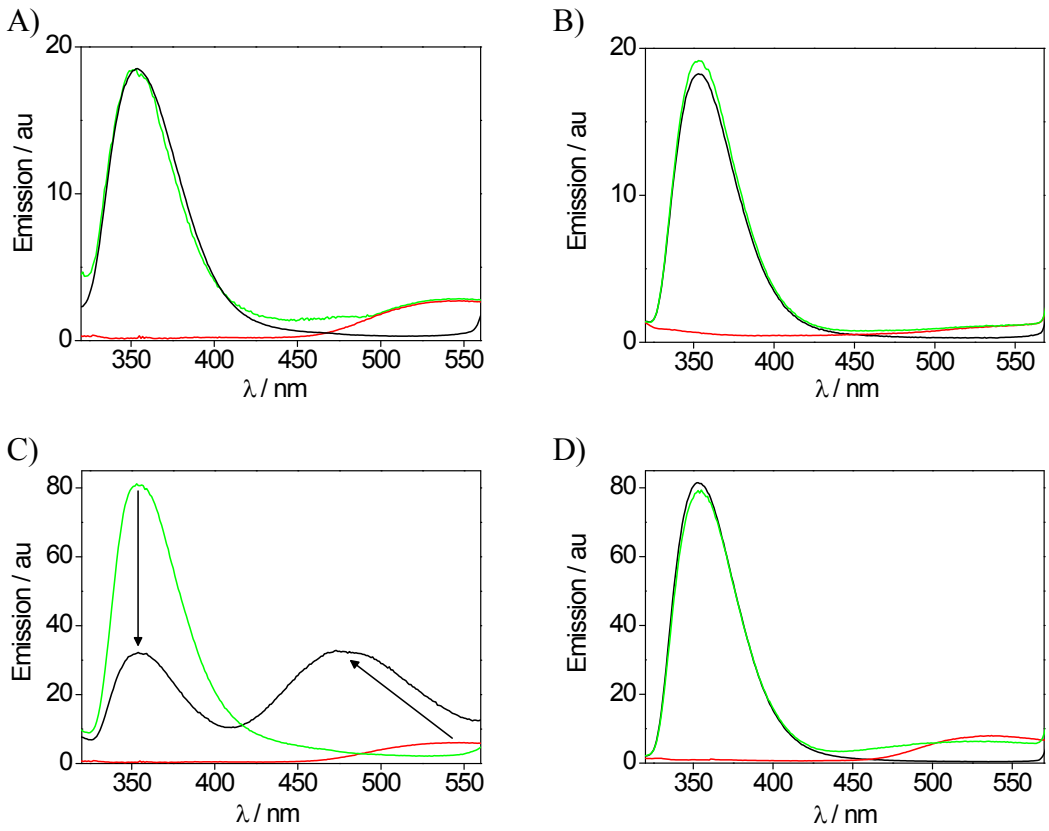

Figure S7. Emission spectra of A) 3β-Dns-CA (1 μM, red), 3β-NPX-CA (1 μM, black) and 1:1 intermolecular mixture (green); B) Chx-Dns (1 μM, red), NPX (1 μM, black) and 1:1 intermolecular mixture (green); C) 3β-Dns-CA (30 μM, red), 3β-NPX-CA (30 μM, black) and 1:1 intermolecular mixture (green); D) Chx-Dns (30 μM, red), NPX (30 μM, black) and 1:1 intermolecular mixture (green).