

Table S1 UV-visible absorption and fluorescence spectral data of DBASt-4C₁, St-2C₁, and St-2C₂ in the presence of various peptide amphiphiles in water; 20 °C, pH 10, [dye] = 0.15 mM, [amphiphile] = 3.0 mM.

Dye	Amphiphile	UV-visible absorption spectral data ^c			Fluorescence spectral data ^d		
		λ_{\max} /nm	Absorbance	Dye species ^a	λ_{ex} /nm	λ_{em} /nm	Intensity ^f
DBASt-4C ₁	1	(477) ^b	(0.402) ^b	M _n	584	614	224
		520	0.426	M _i			
	2	464	0.367	H	554	609	40.7
	3	498	0.719	M _i	570	609	163
	4	465	0.453	H	530	574	22.1
	5	481	0.537	M _n	577	612	376
		(541) ^b	(0.267) ^b	M _i			
	7	474	0.441	M _n	557	607	76.3
	10	541	0.754	M _i	590	612	314
	11	(468) ^b	(0.401) ^b	M _n	585	611	323
		532	0.553	M _i			
	13	472	0.454	M _n	571	608	211
		(532)	(0.260) ^b	M _i			
	None (in water)	477	0.502	M _d	547	601	2.0
None (in MeOH) ^e	490	0.729	M _d	558	600	7.9	
St-2C ₁	1	500	0.864	M _i	552	575	406
	2	491	0.713	M _i	544	572	195
	3	491	0.764	M _i	549	576	446
	4	479	0.460	M _i	540	573	177
	5	504	0.859	M _i	555	576	520
	7	496	0.712	M _i	549	575	402
	10	516	0.887	M _i	559	578	605
	11	510	0.773	M _i	556	576	447
	13	505	0.824	M _i	554	579	375
	None (in water)	437	0.401	M _d	513	567	1.3
	None (in MeOH) ^e	460	0.590	M _d	517	569	3.4
St-2C ₂	1	500	0.787	M _i	551	574	367
	2	490	0.602	M _i	544	574	166
	3	492	0.732	M _i	549	576	404
	4	481	0.381	M _i	537	572	175
	5	507	0.873	M _i	554	576	684
	7	474	0.602	M _i	540	572	209
	10	514	0.861	M _i	556	576	621
	11	526	0.800	M _i	554	575	544
	13	506	0.751	M _i	554	577	317
	None (in water)	434	0.360	M _d	504	566	1.0
	None (in MeOH) ^e	460	0.536	M _d	525	570	2.9

^a M_d: molecularly dispersed monomer of dye . M_i: incorporated monomer of dye. M_n: monomer of dye bound to the carboxylate and not incorporated. H: H-aggregates of dye. Assignment of dye species was made according to previously reported method.^{3c} ^b Shoulder. ^c Path length: 0.1 cm. ^d Path length: 1.0 cm, band width: 1.5 nm. ^e contains 25 vol% water (MeOH:water = 75:25 v/v). ^f See footnote ^e of Table 1.

Table S2 UV-visible absorption and fluorescence spectral data of Qu-2C₁ and Qu-2C₂ (Quinaldine Red) in the presence of various peptide amphiphiles in water; 20 °C, pH 10, [dye] = 0.15 mM, [amphiphile] = 3.0 mM.

Dye	Amphiphile	UV-visible absorption spectral data ^c			Fluorescence spectral data ^d		
		λ_{\max}/nm	Absorbance	Dye species ^a	$\lambda_{\text{ex}}/\text{nm}$	$\lambda_{\text{em}}/\text{nm}$	Intensity ^f
Qu-2C ₁	1	567	1.232	M _i	623	643	8.0
	2	459	0.276	H	610	638	3.5
		551	0.628	M _i			
	3	556	1.027	M _i	620	641	16.1
	4	434	0.588	H	588	630	5.9
		531	0.192	M _i			
	5	571	1.164	M _i	624	642	26.1
	7	432	0.263	H	609	635	16.0
		562	0.410	M _i			
	10	582	1.412	M _i	632	648	25.3
	11	581	1.100	M _i	630	645	17.4
	13	571	1.027	M _i	621	640	16.8
	None (in water)	492	0.391	M _d	571	621	0.9
None (in MeOH) ^e	524	0.603	M _d	600	632	1.8	
Qu-2C ₂	1	569	1.344	M _i	624	643	10.4
	2	448	0.492	H	612	638	2.7
		556	0.609	M _i			
	3	559	1.198	M _i	623	643	18.7
	4	435	0.583	H	594	631	7.4
		553	0.264	M _i			
	5	573	1.430	M _i	628	643	32.4
	7	433	0.455	H	610	634	20.0
		563	0.552	M _i			
	10	581	1.469	M _i	630	644	49.9
	11	579	1.425	M _i	629	643	32.1
	13	579	1.425	M _i	626	645	26.9
	None (in water)	490	0.585	M _d	559	605	1.2
None (in MeOH) ^e	526	0.634	M _d	555	611	1.3	

^a M_d: molecularly dispersed monomer of dye. M_i: incorporated monomer of dye. M_n: monomer of dye bound to the carboxylate and not incorporated. H: H-aggregates of dye. Assignment of dye species was made according to previously reported method. ^b Shoulder. ^c Path length: 0.1 cm. ^d Path length: 1.0 cm, band width: 1.5 nm. ^e contains 25 vol% water (MeOH:water = 75:25 v/v). ^f See footnote ^e of Table 1.

Table S3 UV-visible absorption and fluorescence spectral data of MDEPAP in the presence of various peptide amphiphiles in water; 20 °C, pH 10, [dye] = 0.15 mM, [amphiphile] = 3.0 mM.

Dye	Amphiphile	UV-visible absorption spectral data ^c			Fluorescence spectral data ^d		
		λ_{\max} /nm	Absorbance ^e	Dye species ^a	λ_{ex} /nm	λ_{em} /nm	Intensity ^g
MDEPAP	1	592	1.251	M _i	-	-	-
	2	585	0.985	M _i	-	-	-
	3	587	1.219	M _i	-	-	-
	4	562	0.745	M _n	-	-	-
	5	597	1.394	M _i	-	-	-
	7	579	1.094	M _i	-	-	-
	10	605	1.229	M _i	-	-	-
	11	599	1.204	M _i	-	-	-
	13	598	1.230	M _i	-	-	-
	None (in water)	566 (20°C)	0.781	M _d	-	-	-
		561 (60°C)	0.729	M _d	-	-	-
None (in MeOH) ^f	563	0.940	M _d	-	-	-	

^a M_d: molecularly dispersed monomer of dye. M_i: incorporated monomer of dye. M_n: monomer of dye bound to the carboxylate and not incorporated. H: H-aggregates of dye. Assignment of dye species was made according to previously reported method. ^{3c} ^b Shoulder. ^c Path length: 0.1 cm. ^d Path length: 1.0 cm, band width: 1.5 nm. ^e The λ_{\max} of this dye was unfortunately insensitive to solvent polarity. However, molar absorption coefficient was sensitive to solvent polarity, that is, absorbance was increased with decreasing solvent polarity as is observed generally. ^f contains 25 vol% water (MeOH:water = 75:25 v/v). ^g See footnote ^e of Table 1.

Table S4 UV-visible absorption and fluorescence spectral data of DEC in the presence of various peptide amphiphiles in water; 20 °C, pH 10, [dye] = 0.15 mM, [amphiphile] = 3.0 mM.

Dye	Amphiphile	UV-visible absorption spectral data ^c			Fluorescence spectral data ^d			
		λ_{\max}/nm	Absorbance	Dye species ^a	$\lambda_{\text{ex}}/\text{nm}$	$\lambda_{\text{em}}/\text{nm}$	Intensity ^f	
DEC	1	(461) ^b	(0.245) ^b	M _n	554	574	4.0	
		493	0.690					
		529	1.189					
	2	443	0.452	H	568	596	2.6	
		491	0.276	M _n				
		529	0.345					
	3	(459) ^b	(0.232) ^b	M _n	549	576	1.3	
		492	0.623					
		526	1.006					
	4	(458) ^b	(0.054) ^b	M _n	569	590	140	
		(491) ^b	(0.157) ^b					
		527	0.251					
		556	0.181					J
		582	0.401					J
	5	(456) ^b	(0.286) ^b	M _i	553	571	7.6	
		491	0.763					
		527	1.365					
	7	(458) ^b	(0.157) ^b	M _n	566	591	96.3	
		491	0.423					
		525	0.690					
		556	0.315					J
		580	1.010					J
	10	460	0.238	M _i	549	563	84.7	
		492	0.682					
		530	1.614					
	11	460	0.227	M _i	549	563	42.8	
		491	0.672					
		530	1.597					
13	459 ^b	0.195 ^b	M _n	552	567	4.6		
	493	0.477						
	532	0.965						
None (in water)	(456) ^b	(0.204) ^b	M _d	553	575	1.3		
	489	0.537						
	523	0.712						
None (in MeOH) ^e	578	0.0261	J	559	573	1.3		
	(457) ^b	(0.243) ^b	M _d					
	490	0.702						
		523	1.044					

^a M_d: molecularly dispersed monomer of dye. M_i: incorporated monomer of dye. M_n: monomer of dye bound to the carboxylate and not incorporated. J: J-aggregates of dye: J-aggregation is a result of non-incorporation of less planar dyes. H: H-aggregates of dye. Assignment of dye species was made according to previously reported method.^{3c} ^b Shoulder. ^c Path length: 0.1 cm. ^d Path length: 1.0 cm, band width: 1.5 nm. ^e contains 25 vol% water (MeOH:water = 75:25 v/v). ^f See footnote *e* of Table 1.

Table S5 UV-visible absorption and fluorescence spectral data of DECC in the presence of various peptide amphiphiles in water; 20 °C, pH 10, [dye] = 0.15 mM, [amphiphile] = 3.0 mM.

Dye	Amphiphile	UV-visible absorption spectral data ^c			Fluorescence spectral data ^d		
		λ_{\max} /nm	Absorbance	Dye species ^a	λ_{ex} /nm	λ_{em} /nm	Intensity ^f
DECC	1	532	0.349	M_i	655	664	8.0
		577	0.662				
		629	1.591				
	2	521	0.544	H	632	645	1.7
		(569) ^b	(0.331) ^b	H			
		612	0.208	M_n			
	3	476	0.699	H	618	654	11.6
		572	0.266	M_i			
		618	0.423				
	4	503	0.380	H	633	642	16.5
		(570) ^b	(0.192) ^b	H			
		611	0.162	M_i			
	5	(532) ^b	(0.181) ^b	M_i	666	673	45.0
		583	0.735				
		637	2.020				
	7	507	0.348	H	641	648	26.8
		563	0.245	H			
		612	0.283	M_i			
	10	(534) ^b	(0.164) ^b	M_i	666	673	61.1
		586	0.786				
		637	2.120				
11	(530) ^b	(0.123) ^b	M_i	663	669	62.0	
	584	0.613					
	636	2.047					
None (in water)	523	0.455	H	588	627	1.4	
	544	0.483	H				
	599	0.262	M_d				
None (in MeOH) ^e	(520) ^b	(0.248) ^b	M_d	638	648	1.3	
	561	0.998					
	603	1.932					

^a M_d : molecularly dispersed monomer of dye. M_i : incorporated monomer of dye. M_n : monomer of dye bound to the carboxylate and not incorporated. J: J-aggregates of dye: J-aggregation is a result of non-incorporation of less planar dyes. H: H-aggregates of dye. Assignment of dye species was made according to previously reported method.^{3c} ^b Shoulder. ^c Path length: 0.1 cm. ^d Path length: 1.0 cm, band width: 1.5 nm. ^e contains 25 vol% water (MeOH:water = 75:25 v/v). ^f See footnote ^e of Table 1.

Table S6 UV-visible absorption and fluorescence spectral data of DETCC in the presence of various peptide amphiphiles in water; 20 °C, pH 10, [dye] = 0.15 mM, [amphiphile] = 3.0 mM.

Dye	Amphiphile	UV-visible absorption spectral data ^c			Fluorescence spectral data ^d		
		λ_{\max}/nm	Absorbance	Dye species ^a	$\lambda_{\text{ex}}/\text{nm}$	$\lambda_{\text{em}}/\text{nm}$	Intensity ^f
DETCC	1	542	0.652	M_i	601	607	202
		581	1.814				
	2	(471) ^b	(0.245) ^b	H	588	631	5.0
		(536) ^b	(0.433) ^b	H			
		573	0.524	M_n			
	3	(539) ^b	(0.862) ^b	M_i	601	607	268
		574	1.489				
	4	476	0.345	H	580	592	13.1
		560	0.576	M_n			
	5	(541) ^b	(0.613) ^b	M_i	604	609	444
		582	1.748				
	7	(470) ^b	(0.359) ^b	H	594	602	46.7
		(523) ^b	(0.568) ^b	H			
		563	0.814	M_i			
	10	546	0.540	M_i	605	610	381
		586	1.835				
	11	545	0.537	M_i	603	609	559
		584	1.846				
	None (in water)	509	0.495	H	570	577	19.8
		553	0.501	M_d			
None (in MeOH) ^e	(523) ^b	(0.605) ^b	M_d	578	584	34.8	
	557	1.345					

^a M_d : molecularly dispersed monomer of dye. M_i : incorporated monomer of dye. M_n : monomer of dye bound to the carboxylate and not incorporated. H: H-aggregates of dye. Assignment of dye species was made according to previously reported method. ^b Shoulder. ^c Path length: 0.1 cm. ^d Path length: 1.0 cm, band width: 1.5 nm. ^e contains 25 vol% water (MeOH:water = 75:25 v/v). ^f See footnote ^e of Table 1.

Table S7 UV-visible absorption and fluorescence spectral data of DPTCC in the presence of various peptide amphiphiles in water; 20 °C, pH 10, [dye] = 0.15 mM, [amphiphile] = 3.0 mM.

Dye	Amphiphile	UV-visible absorption spectral data ^c			Fluorescence spectral data ^d		
		λ_{\max}/nm	Absorbance	Dye species ^a	$\lambda_{\text{ex}}/\text{nm}$	$\lambda_{\text{em}}/\text{nm}$	Intensity ^f
DPTCC	1	543	0.655	M_i	603	609	151
		582	1.795				
	2	536	0.474	M_n, M_i	596	606	11.1
		577	0.698				
	3	(538) ^b	(0.611) ^b	M_i	601	608	298
		576	1.286				
	4	470	0.509	H	585	635	4.1
		570	0.774	M_n			
	5	(543) ^b	(0.720) ^b	M_i	608	613	370
		568	0.262				
	7	(528) ^b	(0.480) ^b	M_n, M_i	594	603	13.0
		566	1.000				
	10	549	0.980	M_i	613	621	64.8
		584	2.097				
	11	(546) ^b	(0.725) ^b	M_i	609	615	95.8
		587	1.960				
	13	(534) ^b	(0.265) ^b	M_i	540	601	85.5
		584	0.495				
	None (in water)	514	0.164	H	565	573	53.9
		555	0.241	M_d			
None (in MeOH) ^e	(524) ^b	(0.581) ^b	M_d	583	589	35.7	
	559	1.317					

^a M_d : molecularly dispersed monomer of dye. M_i : incorporated monomer of dye. M_n : monomer of dye bound to the carboxylate and not incorporated. H: H-aggregates of dye. Assignment of dye species was made according to previously reported method.^{3c} ^b Shoulder. ^c Path length: 0.1 cm. ^d Path length: 1.0 cm, band width: 1.5 nm. ^e contains 25 vol% water (MeOH:water = 75:25 v/v). ^f See footnote *e* of Table 1.

Table S8 UV-visible absorption and fluorescence spectral data of DE9MTCC in the presence of various peptide amphiphiles in water; 20 °C, pH 10, [dye] = 0.15 mM, [amphiphile] = 3.0 mM.

Dye	Amphiphile	UV-visible absorption spectral data ^c			Fluorescence spectral data ^d		
		λ_{\max}/nm	Absorbance	Dye species ^a	$\lambda_{\text{ex}}/\text{nm}$	$\lambda_{\text{em}}/\text{nm}$	Intensity ^f
DE9MTCC	1	531	0.733	M_i	591	596	246
		567	2.009				
	2	526	0.824	M_i	589	596	23.8
		567	1.952				
	3	(529) ^b	(0.896) ^b	M_i	590	596	789
		562	1.733				
	4	(499) ^b	(0.615) ^b	H	584	591	203
		536	1.040	M_i			
	5	569	1.364		M_i	594	600
		(530) ^b	(0.607) ^b				
	7	571	1.887	M_i	588	593	219
		(493) ^b	(0.392) ^b				
	10	530	0.712	M_i	592	598	482
		568	1.660				
	11	534	0.778	M_i	592	597	696
		567	2.004				
	13	533	0.733	M_i	492	596	178
		566	1.996				
	None (in water)	533	0.701	M_i	556	569	2.4
		568	1.978				
None (in MeOH) ^e	500	0.362	H	573	583	2.2	
	539	0.289	M_d				
	(504) ^b	(0.569) ^b	M_d	573	583	2.2	
	541	1.635					

^a M_d : molecularly dispersed monomer of dye. M_i : incorporated monomer of dye. M_n : monomer of dye bound to the carboxylate and not incorporated. J: J-aggregates of dye: J-aggregation is a result of non-incorporation of less planar dyes. H: H-aggregates of dye. Assignment of dye species was made according to previously reported method.^{3c} ^b Shoulder. ^c Path length: 0.1 cm. ^d Path length: 1.0 cm, band width: 1.5 nm. ^e contains 25 vol% water (MeOH:water = 75:25 v/v). ^f See footnote ^e of Table 1.

Table S9 UV-visible absorption and fluorescence spectral data of DE9ETCC (NK-737) in the presence of various peptide amphiphiles in water; 20 °C, pH 10, [dye] = 0.15 mM, [amphiphile] = 3.0 mM.

Dye	Amphiphile	UV-visible absorption spectra ^c			Fluorescence spectra ^d		
		λ_{\max}/nm	Absorbance	Dye species ^a	$\lambda_{\text{ex}}/\text{nm}$	$\lambda_{\text{em}}/\text{nm}$	Intensity ^f
DE9ETCC (NK-737)	1	533	0.772	M_i	594	600	300
		569	2.012				
	2	533	0.782	M_i	594	600	44.4
		569	2.016				
	3	(530) ^b	(0.814) ^b	M_i	617	619	306
		570	1.887				
		(615) ^b	(0.112) ^b				
	4	(491) ^b	(0.517) ^b	H	581	588	40.1
		566	1.084	M_i			
		(602) ^b	(0.254) ^b	J			
		(638) ^b	(0.041) ^b	J			
	5	(535) ^b	(0.814) ^b	M_i	599	605	292
		574	1.942				
	7	(491) ^b	(0.349) ^b	H	587	592	49.3
		556	0.966	M_i			
	10	537	0.742	M_i	597	603	250
		572	2.024				
	11	537	0.666	M_i	596	602	306
		572	2.006				
	13	497	0.382	H	602	619	55.5
		531 ^b	0.449 ^b	M_i			
577		1.087					
612		0.462	J				
None (in water)	505	0.420	H	564	574	2.6	
	543	0.334	M_d				
	630	0.040	J				
None (in MeOH) ^e	(507) ^b	(0.357) ^b	M_d	586	598	2.2	
	546	1.115					

^a M_d : molecularly dispersed monomer of dye. M_i : incorporated monomer of dye. J: J-aggregates of dye; J-aggregation is a result of non-incorporation of less planar dyes. H: H-aggregates of dye. Assignment of dye species was made according to previously reported method.^{3c} ^b Shoulder. ^c Path length: 0.1 cm. ^d Path length: 1.0 cm, band width: 1.5 nm. ^e contains 25 vol% water (MeOH:water = 75:25 v/v). ^f See footnote ^e of Table 1.