

Electronic Supplementary Information

Evaluation of Photoluminescence Quenching for Assessing the Binding of Nitroaromatic Compounds to a Tyrosyl Bolaamphiphile Self-Assembly

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1. Chemical structure of Tyr-C7

Schematic layout of the synthesis of bolaamphiphile molecule with tyrosyl groups (Tyr-C7) is shown in Fig. S1. Tyrosine was modified to tyrosine benzylester to be conjugated with azelaic acid. Through the carbodiimide chemistry, tyrosine is conjugated with azelaic acid to form Tyr-C7 bolaamphiphilic molecule.

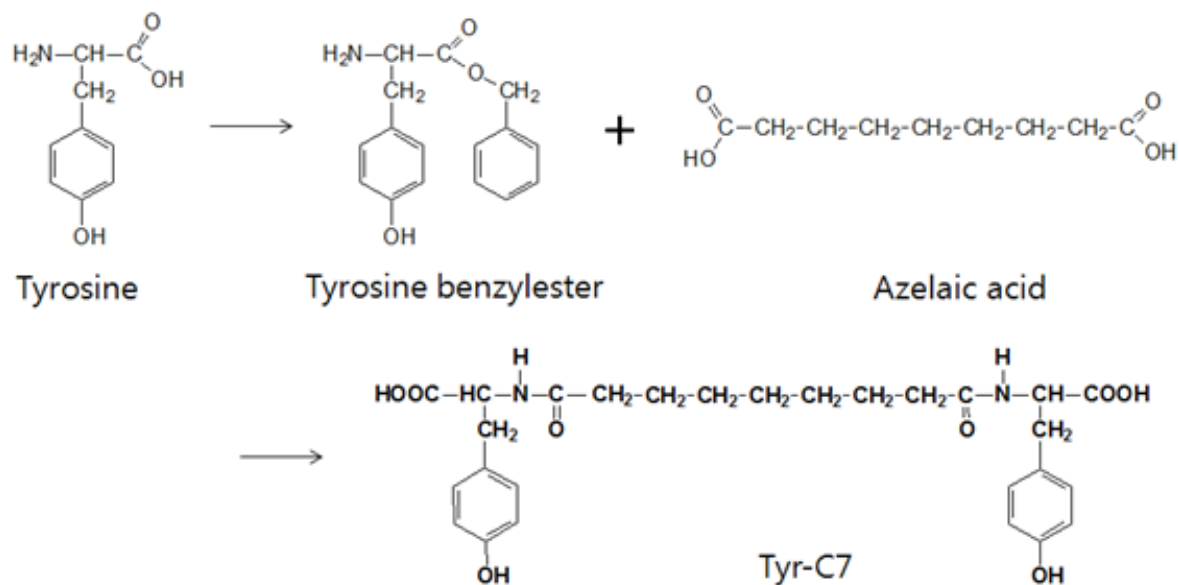


Fig. S1. Schematic layout of Tyr-C7 synthesis.

2. Fluorescence quenching spectra

Fluorescence from the photoluminescent self-assembly was quenched by the addition of nitroaromatic compounds. The fluorescence spectra quenched by the nitroaromatic analytes are shown in Fig. S2.

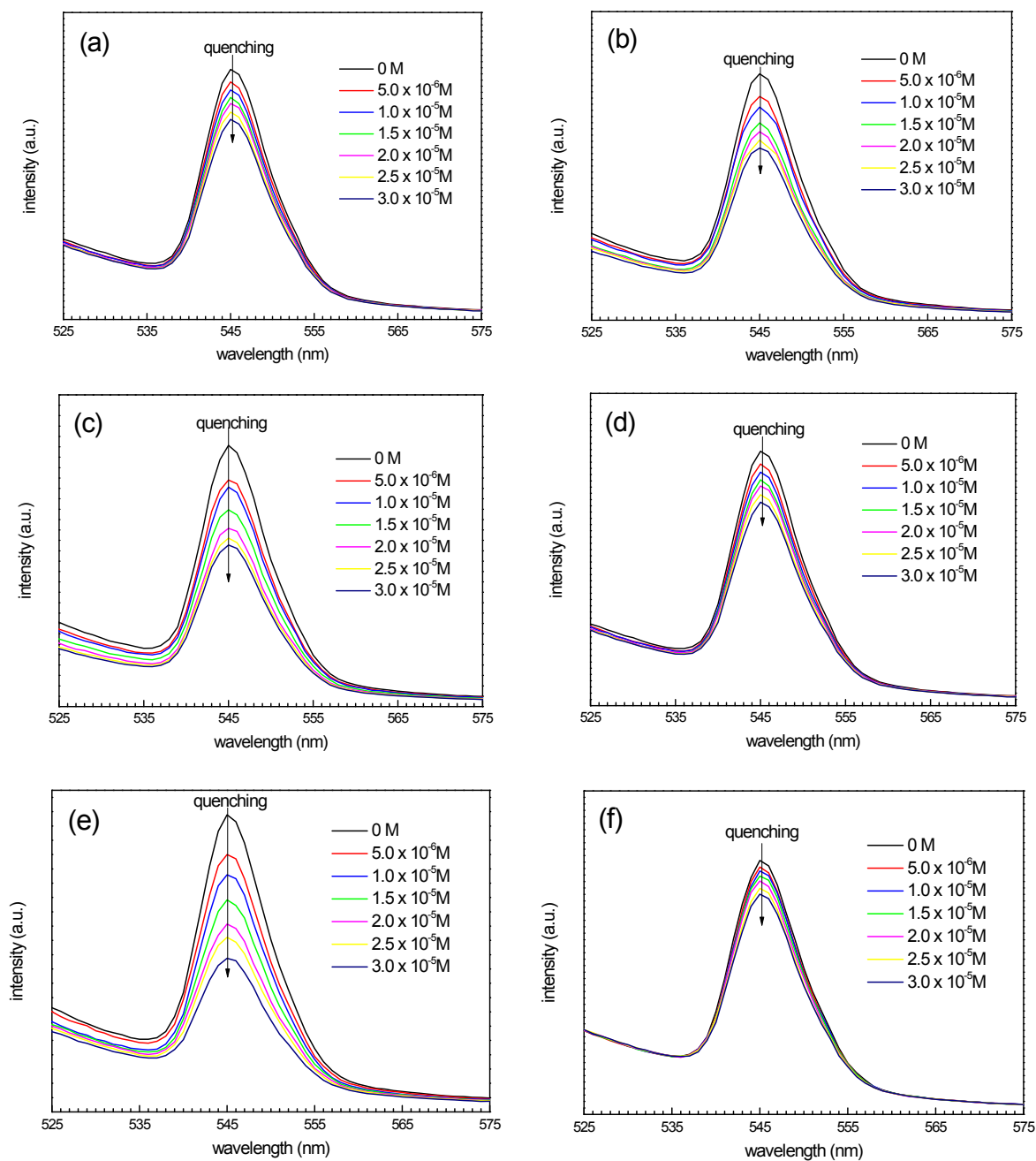


Fig. S2. Fluorescence spectra quenched by analytes including nitrocompounds (a: nitromethane, b: nitrobenzene, c: *p*-nitrophenol, d: *p*-nitrotoluene, e: 1,4-dinitrobenzene, f: phenol)

3. Visualization of fluorescence quenching

In addition to the steady-state spectroscopy study, fluorescence quenching was observed with increasing concentration of a nitroaromatic compound. *p*-Nitrophenol was chosen as a model nitroaromatic compound leading significant fluorescence quenching. The fluorescence from the bolaamphiphile nanoparticles were observed using a fluorescence microscope under the UV excitation beam at 330 nm. Fig. S3 shows the fluorescence microscopy images representing fluorescence quenching.

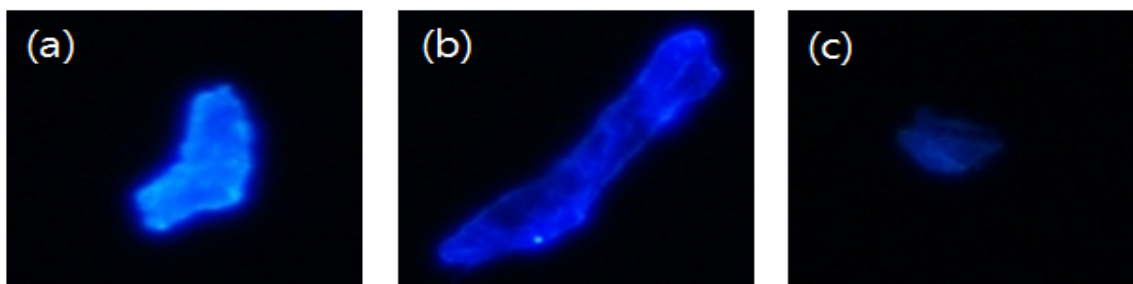


Fig. S3. Images of the fluorescence microscopy indicating reduction of fluorescence emission at the *p*-nitrophenol concentrations of (a) 0, (b) 15, and (c) 30 μM .

4. Measurement of average fluorescence lifetime

The average fluorescence lifetime of the photoluminescent probe was measured by a time-correlated single-photon spectrometer under the excitation beam at 347 nm from a monochromic laser (Fluorolog, Horiba Jobin Yvon, laser source: NanoLED, $\lambda_{em} = 490$ nm). The fluorescence decay profile was fitted using the multiple exponential fitting model shown below.

$$I(t) = A + \sum_i B_i \exp\left(\frac{-t}{\tau_i}\right)$$

After data fitting, the amplitude average lifetime was calculated from the values of lifetime and amplitudes using the following equation

$$\langle \tau \rangle = \sum_i \frac{B_i \tau_i}{B_i}$$

The fitting parameters of the intact photoluminescent probe are summarized in Table S1. Model decay profiles with fitting lines are shown in Fig. S4.

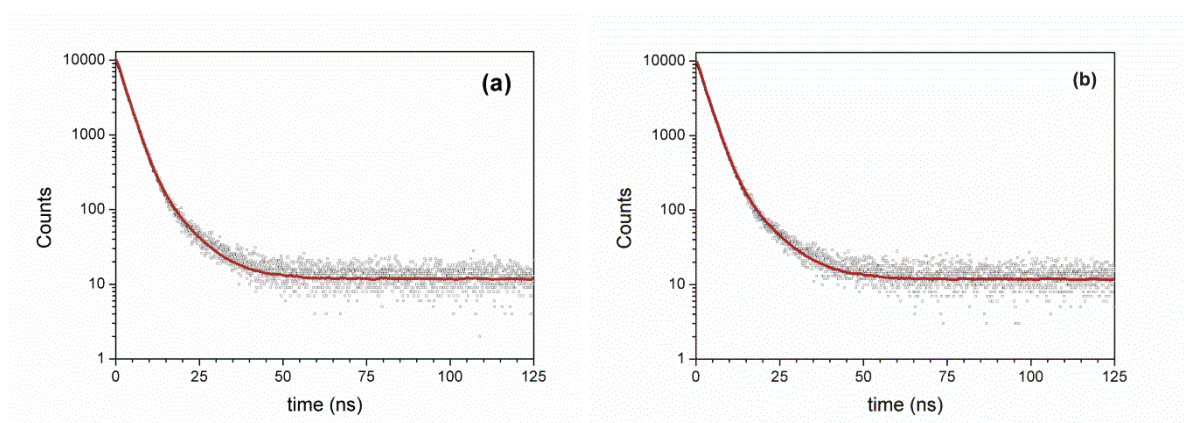


Fig. S4. Time-resolved photoluminescence spectra of (a) intact Tyr-C7 probe and (b) after addition of 25 mM *p*-nitrophenol.

Table S1. Lifetime and amplitudes of the intact photoluminescent probe

Sample	Conc. (μM)	Amplitudes			Lifetimes			
		A	$B_1 (10^{-2})$	$B_2 (10^{-3})$	τ_1 (ns)	τ_2 (ns)	$\langle\tau\rangle$ (ns)	χ^2
Intact probe		10.60	5.15	2.64	2.68	7.87	2.93	1.34
phenol	10	10.19	5.12	2.47	2.74	8.30	3.00	1.35
	15	10.33	5.14	2.38	2.74	8.38	2.99	1.29
	20	10.23	5.10	2.67	2.75	8.02	3.01	1.30
	25	10.12	5.09	2.66	2.75	8.06	3.01	1.33
nitromethane	10	10.03	5.18	2.47	2.72	8.14	2.97	1.31
	15	10.01	5.21	2.43	2.72	8.18	2.96	1.34
	20	9.77	5.11	2.78	2.73	8.21	3.01	1.30
	25	9.77	5.09	2.67	2.75	8.27	3.02	1.32
nitrotoluene	10	10.53	5.12	2.56	2.71	8.10	2.97	1.30
	15	10.68	5.20	2.22	2.76	8.52	3.00	1.29
	20	10.64	5.24	2.54	2.69	7.80	2.93	1.34
	25	10.70	5.22	2.55	2.65	7.24	2.85	1.31
nitrophenol	10	11.08	5.17	2.37	2.71	8.61	2.97	1.30
	15	11.05	5.17	2.48	2.68	8.06	2.93	1.30
	20	11.21	5.15	2.61	2.68	8.12	2.94	1.24
	25	11.02	5.17	2.79	2.67	8.06	2.95	1.29
nitrobenzene	10	10.56	5.20	2.83	2.72	8.15	2.97	1.30
	15	10.43	5.15	2.74	2.70	8.00	2.96	1.32
	20	10.37	5.16	2.38	2.72	8.34	2.97	1.32
	25	10.36	5.14	2.46	2.73	8.22	2.98	1.30
dinitrobenzene	10	9.56	5.05	2.27	2.79	8.53	3.03	1.37
	15	9.94	5.15	2.82	2.68	6.95	2.90	1.34
	20	9.81	5.08	2.35	2.82	8.49	3.07	1.37
	25	9.81	5.07	2.71	2.79	8.11	3.06	1.35