

## Electronic Supplementary Information

### Probing the Binding Dynamics to Sodium Cholate Aggregates using Naphthalene Derivatives as Guests

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**Table S1.** Stern-Volmer constants for the quenching of the steady-state ( $K_{sv}(SS)$ ) and time-resolved fluorescence ( $K_{sv}(TR)$ ) of 1-EtNp, 2-EtNp, 1-NpOH and 2-NpOH by iodide in the presence of various NaCH concentrations.<sup>a</sup>

Guest	[NaCH] / mM	$K_{sv}(SS)$ / $10^3 M^{-1}$	$K_{sv}(TR)$ / $10^3 M^{-1}$
1-EtNp	0	$14.2 \pm 0.5$ (2) <sup>b</sup>	$14.1 \pm 0.1$
	3	$14.1 \pm 0.5$ (2) <sup>b</sup>	
	5	$13.8 \pm 0.9$ (2)	
	10	<sup>c</sup>	$0.7 \pm 0.1$
	20	$0.78 \pm 0.03$ (3)	$0.6 \pm 0.1$
	30	$0.71 \pm 0.02$ (2) <sup>b</sup>	
2-EtNp	40	$0.69 \pm 0.01$ (2) <sup>b</sup>	$0.8 \pm 0.1$
	0	$14.6 \pm 0.6$ (2) <sup>b</sup>	$13.2 \pm 0.1$
	3	$14.3 \pm 0.4$ (2) <sup>b</sup>	
	5	$14.3 \pm 0.7$ (2)	
	10	$2.2 \pm 0.6$ (3)	$1.0 \pm 0.1$
	20	$0.7 \pm 0.1$ (3)	$0.6 \pm 1$
1-NpOH	30	$0.58 \pm 0.08$ (3)	
	40	$0.56 \pm 0.06$ (4)	$0.6 \pm 0.1$
	0	$14.5 \pm 0.9$ (2)	$17.1 \pm 0.4$
	3	$14.6 \pm 0.6$ (2) <sup>b</sup>	
	5	$15 \pm 2$ (2)	
	10	$13 \pm 1$ (2)	$15.8 \pm 0.2$
2-NpOH	20	$9 \pm 2$ (3) <sup>b</sup>	$5.0 \pm 0.3$
	30	$6.0 \pm 0.7$ (3) <sup>b</sup>	
	40	$4.6 \pm 0.5$ (2)	$4.2 \pm 0.2$
	0	$13.6 \pm 0.2$ (2)	$15.7 \pm 0.9$
	3	$11 \pm 1$ (3)	
	5	$13.9 \pm 0.4$ (2) <sup>b</sup>	
	10	$11.1 \pm 0.7$ (3)	$10.6 \pm 0.1$
	20	$6 \pm 1$ (2)	$5.5 \pm 0.3$
	30	$3.2 \pm 0.2$ (2)	
	40	$3.0 \pm 0.1$ (2)	$3.8 \pm 0.3$

<sup>a</sup>, the number of independent experiments is shown in parenthesis, time-resolved experiments correspond to one experiment, errors for the average of two experiments correspond to average deviations, errors for the average of more than two experiments correspond to standard deviations; <sup>b</sup>, propagation of individual errors; <sup>c</sup>, curved quenching plots.

**Table S2.** Quenching rate constant for the long-lived component of 1-EtNp, 2-EtNp, 1-NpOH and 2-NpOH in the presence of various NaCH concentrations.<sup>a</sup>

Guest	[NaCH] / mM	$k_q / 10^9 M^{-1}$
1-EtNp	10	$< 0.06^b$
	20	$0.078 \pm 0.005$
	40	$0.09 \pm 0.01$
2-EtNp	10	$0.07 \pm 0.02$
	20	$0.09 \pm 0.01$
	40	$0.07 \pm 0.02$
1-NpOH	10	<sup>c</sup>
	20	$0.31 \pm 0.05$
	40	$0.43 \pm 0.03$
2-NpOH	10	<sup>c</sup>
	20	$0.42 \pm 0.09$
	40	$0.5 \pm 0.1$

<sup>a</sup>, one experiment, the errors correspond to those recovered from the fitting of the experimental data to a linear quenching plot; <sup>b</sup> a higher limit was determined because the quenching efficiency was low; <sup>c</sup>, the contribution of the long-lived component to the overall decay was too small to determine a quenching rate constant.

**Table S3.** Stern-Volmer constants for the quenching of the steady-state fluorescence ( $K_{sv}(SS)$ ) of 1-EtNp by iodide in the presence of various NaCH and salt concentrations.<sup>a</sup>

[NaCH] / mM	[salt] / M	$K_{sv}(SS)$ / $10^3 M^{-1}$
0	0.03	$14 \pm 2$ (3) <sup>b</sup>
	0.2	$14 \pm 1$ (3)
	0.4	$14 \pm 1$ (2) <sup>b</sup>
3	0.03	$13 \pm 2$ (2)
	0.2	$7.5 \pm 0.8$ (2) <sup>b</sup>
	0.4	$8 \pm 2$ (2) <sup>b</sup>
5	0.03	<sup>c</sup>
	0.2	<sup>c</sup>
	0.4	$7 \pm 1$ (2) <sup>b</sup>
10	0.03	$10 \pm 2$ (3)
	0.2	$3.1 \pm 0.7$ (4)
	0.4	$5.4 \pm 0.6$ (2) <sup>b</sup>
20	0.03	$1.4 \pm 0.3$ (2) <sup>b</sup>
	0.2	$1.1 \pm 0.2$ (4) <sup>b</sup>
	0.4	$0.9 \pm 0.3$ (2)
30	0.03	$0.9 \pm 0.2$ (2) <sup>b</sup>
	0.2	$0.7 \pm 0.2$ (4)
	0.4	$1.0 \pm 0.2$ (2)
40	0.03	$0.6 \pm 0.2$ (2)
	0.2	$0.6 \pm 0.2$ (3)
	0.4	$1.1 \pm 0.1$ (2) <sup>b</sup>

<sup>a</sup>, the number of independent experiments is shown in parenthesis, errors for the average of two experiments correspond to average deviations, errors for the average of more than two experiments correspond to standard deviations; <sup>b</sup>, propagation of individual errors; <sup>c</sup>, curved quenching plots; <sup>c</sup>, non-reproducible results were obtained in four attempts.

**Table S4.** Stern-Volmer constants for the quenching of the steady-state fluorescence ( $K_{sv}(SS)$ ) of 1-NpOH by iodide in the presence of various NaCH and salt concentrations.<sup>a</sup>

[NaCH]/ mM	[salt] / M	$K_{sv}(SS)$ / $10\text{ M}^{-1}$
0	0.03	$16.3 \pm 0.6$ (2) <sup>b</sup>
	0.2	$14 \pm 1$ (3)
	0.4	$15.0 \pm 0.9$ (2)
3	0.03	$15.7 \pm 0.6$ (2) <sup>b</sup>
	0.2	$15.4 \pm 0.9$ (2) <sup>b</sup>
	0.4	$14.6 \pm 0.6$ (2) <sup>b</sup>
5	0.03	$15.7 \pm 0.4$ (2) <sup>b</sup>
	0.2	$15.0 \pm 0.5$ (2) <sup>b</sup>
	0.4	$16 \pm 1$ (2) <sup>b</sup>
10	0.03	$14.4 \pm 0.8$ (2)
	0.2	$12.4 \pm 0.5$ (2)
	0.4	$13 \pm 2$ (2) <sup>b</sup>
20	0.03	$10 \pm 1$
	0.2	$8 \pm 1$ (2)
	0.4	$8.2 \pm 0.7$ (2) <sup>b</sup>
30	0.03	$6.5 \pm 0.8$ (2) <sup>b</sup>
	0.2	$5.5 \pm 0.6$ (2)
	0.4	$6.1 \pm 0.4$ (2) <sup>b</sup>
40	0.03	$4.6 \pm 0.5$ (2)
	0.2	$4.7 \pm 0.3$ (2)
	0.4	$4.7 \pm 0.8$ (2)

<sup>a</sup>, the number of independent experiments is shown in parenthesis, errors for the average of two experiments correspond to average deviations, errors for the average of more than two experiments correspond to standard deviations; <sup>b</sup>, propagation of individual errors; <sup>c</sup>, curved quenching plots.