Supplementary Data

Direct and Indirect Monitoring of Peptide-Silica Interactions using Time-Resolved Fluorescence

Anisotropy

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Supplementary Table 1. Time-resolved fluorescence anisotropy decay data of R6G in 10 mM, pH=7.4 Tris buffer solution and in 0.75 wt % SiO₂ in the presence of varying levels of KWK.^a

R6G in Ludox						
	0 mM	0.6 mM	1 mM	2 mM	5 mM	
	KWK	KWK	KWK	KWK	KWK	
τ, ns	3.93 ± 0.002	3.87 ± 0.005	3.89 ± 0.004	3.87 ± 0.005	3.82 ± 0.006	
		(96.5%)	(96.4%)	(95.4%)	(96.9%)	
		1.94 ± 0.03	1.91 ± 0.006	1.91 ± 0.009	1.82 ± 0.009	
		(3.5%)	(3.6%)	(4.6%)	(3.1%)	
γ^2	1.14	1.09	1.12	1.13	1.10	
λR						
ϕ_l , ns	0.18 ± 0.05	0.17 ± 0.04	0.18 ± 0.03	0.16 ± 0.02	0.19 ± 0.02	
ϕ_2 , ns	3.9 ± 0.5	3.9 ± 0.3	4.1 ± 0.4	3.0 ± 0.4	3.4 ± 0.5	
12						
r_0	0.38	0.38	0.38	0.39	0.38	
r_{∞}	0.26	0.16	0.15	0.10	0.01	
g	0.67	0.42	0.37	0.26	0.02	
f_{I}	0.05	0.20	0.24	0.33	0.44	
f_2	0.28	0.38	0.39	0.41	0.54	
χ^2_R	1.01	0.99	0.99	0.99	1.02	

a) τ , fluorescence lifetime; ϕ_1 , ϕ_2 , rotational correlation times; f_1 , fractional contribution to anisotropy decay owing to ϕ_1 ; f_2 , fractional contribution to anisotropy decay owing to ϕ_2 ; r_0 , limiting anisotropy; r_{∞} , residual anisotropy; g, fraction of fluorescence arising from slow motion of probes corresponding to limiting anisotropy ($g = r_{\infty}/r_0$). Typical errors in r_{∞} , r_0 , f_1 and f_2 are ± 0.02 , error in g is ± 0.03 . **Supplementary Table 2.** Time-resolved fluorescence anisotropy decay data of R6G in 10 mM, pH=7.4 Tris buffer solution and in 0.75 wt % SiO₂ in the presence of varying levels of Ac-KWK.^a

	R6G in Ludox					
	0 mM	0.6 mM	1 mM	2 mM	5 mM	6 mM
	Ac-KWK	Ac-KWK	Ac-KWK	Ac-KWK	Ac-KWK	Ac-KWK
<i>τ</i> , ns	3.93 ± 0.002	3.96 ± 0.005 (93.3%)	3.98 ± 0.004 (93.8%)	3.89±0.004 (93.4%)	3.89±0.005 (92.8%)	$3.88 \pm 0.005 \\ (94.0\%)$
		1.97 ± 0.01 (6.7%)	1.98 ± 0.008 (6.2%)	1.88 ± 0.01 (6.54%)	1.88 ± 0.02 (7.2%)	$\begin{array}{c} 1.96 \pm 0.01 \\ (6.0\%) \end{array}$
χ^2_R	1.14	1.10	1.08	1.11	1.09	1.09
ϕ_l , ns	0.18 ± 0.05	0.21 ± 0.04	0.20 ± 0.04	0.16 ± 0.03	0.20 ± 0.03	0.19± 0.03
ϕ_2 , ns	3.9 ± 0.4	4.9 ± 0.8	4.5±0.6	3.1±0.7	3.0± 0.7	3.3±0.9
r_0	0.38	0.39	0.37	0.39	0.40	0.40
r_{∞}	0.26	0.22	0.22	0.17	0.16	0.12
g	0.67	0.56	0.59	0.44	0.40	0.30
f_{I}	0.05	0.08	0.10	0.27	0.35	0.43
f_2	0.28	0.36	0.31	0.29	0.25	0.27
χ^2_R	1.01	1.03	1.00	0.99	1.01	1.07

a) Terms are as defined in Table 1.

Supplementary Table 3. Time-resolved fluorescence anisotropy decay data of R6G in 10 mM, pH 7.4 Tris buffer solution and in 0.75 wt % SiO₂ in the presence of varying levels of EWE.^a

	1					
	R6G in Ludox					
	0 mM	0.6 mM	1 mM	2 mM	5 mM	10 mM
	EWE	EWE	EWE	EWE	EWE	EWE
τ, ns	3.93 ± 0.002	4.03 ± 0.005	4.01 ± 0.004	3.99 ± 0.004	3.97 ± 0.005	3.93 ± 0.004
		(96.4%)	(97.0%)	(97.0%)	(96.8%)	(95.0%)
		× ,	,	, ,		× ,
		2.02 ± 0.01	2.01 ± 0.007	2.01 ± 0.02	1.79 ± 0.008	1.96 ± 0.007
		(3.6%)	(3%)	(3%)	(3.2%)	(5.0%)
γ_p^2	1.14	1.08	1.05	1.07	1.09	1.06
\mathcal{N}_{R}						
ϕ_l , ns	0.18 ± 0.05	0.18 ± 0.09	0.16 ± 0.09	0.19 ± 0.052	0.14 ± 0.05	0.23 ± 0.76
ϕ_2 , ns	3.9 ± 0.4	4.6 ± 0.7	4.5 ± 0.4	4.3 ± 0.9	4.5 ± 0.9	14.0 ± 7.3
12						
r_0	0.38	0.38	0.40	0.38	0.40	0.36
r_{∞}	0.26	0.27	0.28	0.25	0.27	0.30
g	0.67	0.71	0.70	0.66	0.68	0.72
f_l	0.05	0.07	0.07	0.08	0.06	0.05
f_2	0.28	0.22	0.23	0.26	0.26	0.23
χ^2_R	1.01	1.03	0.97	1.03	1.04	0.98

a) Terms are as defined in Table 1.

Supplementary Table 4. Time-resolved fluorescence anisotropy decay data of R6G in 10 mM, pH 7.4 Tris buffer solution and in 0.75 wt % SiO₂ in the presence of varying levels of Ac-EWE.^a

-						
	R6G in Ludox					
	0 mM	0.6 mM	1 mM	2 mM	5 mM	10 mM
	Ac-EWE	Ac-EWE	Ac-EWE	Ac-EWE	Ac-EWE	Ac-EWE
τ, ns	3.93 ± 0.002	4.00 ± 0.004	4.01 ± 0.003	3.97 ± 0.004	3.95 ± 0.001	3.95 ± 0.006
		(96.7%)	(96.3%)	(97.6%)	(96.7%)	(95.2%)
		2.00 ± 0.01	2.00 ± 0.01	2.01 ± 0.02	1.97 ± 0.01	1.98 ± 0.01
		(3.3%)	(3.7%)	(2.4%)	(3.3%)	(4.8%)
χ^2_R	1.14	1.08	1.02	1.05	1.09	1.09
ϕ_l , ns	0.18 ± 0.05	0.21 ± 0.06	0.18 ± 0.04	0.19± 0.02	0.19 ± 0.01	0.17 ± 0.06
<i>\$</i> \$	3.9 ± 0.4	4.1 ± 0.5	4.0 ± 0.4	4.9 ± 0.9	5.1 ± 1.3	3.9± 0.3
r_0	0.38	0.37	0.37	0.37	0.38	0.39
r_{∞}	0.26	0.26	0.24	0.22	0.27	0.26
g	0.67	0.70	0.64	0.61	0.71	0.66
f_{l}	0.05	0.02	0.02	0.04	0.02	0.05
f_2	0.28	0.28	0.33	0.35	0.27	0.29
χ^2_R	1.01	1.00	0.99	0.97	1.02	1.03

a) Terms are as defined in Table 1.

Supplementary Table 5. Effect of adding R6G and peptides in varying order on TRFA parameters.

	R6G in Ludox					
	А	В	С			
τ, ns	3.89 ± 0.005	3.86 ± 0.005	3.87 ± 0.005			
	(93.9%)	(95.4%)	(96.5%)			
	1.79 ± 0.01	1.94 ± 0.02	1.94 ± 0.03			
	(6.1%)	(4.6%)	(3.5%)			
χ^2_R	1.07	1.10	1.09			
ϕ_l , ns	0.16 ± 0.02	0.19 ± 0.04	0.17 ± 0.04			
ϕ_2 , ns	3.3 ± 0.7	3.7± 0.4	3.9 ± 0.3			
r_0	0.40	0.39	0.38			
r_{∞}	0.16	0.16	0.16			
g	0.40	0.41	0.42			
f_{I}	0.22	0.20	0.20			
f_2	0.38	0.39	0.38			
χ^2_R	1.00	1.02	0.99			

- A. 0.6mM KWK+Ludox, 1h, +R6GB. R6G +Ludox, 1h, +0.6mM KWK
- C. 0.6mM KWK+R6G, 1h, +Ludox