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Supporting Material

Comparison of Methods for Characterizing Non-ideal Solute Self-Association by Sedimentation Equilibrium

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TABLE S1 Summary of the best-fit estimates of the activity coefficient parameter BM_A and dimerization constant K_2 obtained from simulated sedimentation equilibrium distributions by two analytical solutions incorporating the Adams–Fujita approach to allowance for thermodynamic non-ideality

		Analysis via Eq. 17		Analysis via Eq. 18	
K_2 (M^{-1})	Run*	BM_A (L/g)	K_2 (M^{-1})†	BM_A (L/g)	K_2 (M^{-1})†
800	A	NV		0.01184	815 (± 13)
	B	0.007724	599 (± 12)	0.009328	679 (± 13)
900	A	0.007765	690 (± 11)	0.01109	886 (± 13)
	B	0.009700	804 (± 13)	0.01111	877 (± 13)
1000	A	0.008353	812 (± 12)	0.01115	990 (± 13)
	B	0.006639	744 (± 12)	0.007452	792 (± 13)
1200	A	0.007795	985 (± 13)	0.009689	1117 (± 14)
	B	0.008504	1033 (± 13)	0.009033	1065 (± 13)
1500	A	0.008187	1296 (± 13)	0.009291	1386 (± 14)
	B	0.009456	1398 (± 14)	0.009698	1415 (± 14)
1800	A	0.008913	1645 (± 14)	0.009553	1707 (± 14)
	B	0.008813	1636 (± 14)	0.009272	1673 (± 14)

*Designated as in Fig. 2.
†Numbers in parentheses denote twice the standard deviation of the estimate.
‡No minimum observed in the sum of squares of residuals.

TABLE S2 Comparison of activity coefficients for mixtures of uncharged monomer (A) and dimer (P) calculated on the basis of standard statistical-mechanical considerations and scaled particle theory

		McMillan–Mayer			Scaled particle theory		
c_A (g/L)	c_P (g/L)	γ_A	γ_P	γ_P / γ_A^2	γ_A	γ_P	γ_P / γ_A^2
7	1	1.104*	1.154*	0.947	1.107†	1.158†	0.945
6	2	1.100	1.147	0.948	1.103	1.151	0.946
5	3	1.097	1.141	0.948	1.099	1.144	0.947
4	4	1.093	1.134	0.949	1.095	1.138	0.949
3	5	1.089	1.128	0.951	1.091	1.131	0.950
2	6	1.085	1.121	0.952	1.087	1.124	0.951
1	7	1.081	1.115	0.954	1.083	1.118	0.953

Calculations refer to a 70 kDa monomer with R_A = 3.55 nm, R_P = 4.47 nm.

*Calculations based on Eqs. 11a and 11b for a monomer–dimer system (n = 2) with virial coefficients obtained from Eqs. 7, 12a, and 12b with $Z_A = Z_P = 0$.

†Calculations based on Eqs. (14a)–(14c) with $(V_A/M_A) = (4/3)\pi R_A^3$, n =2 and x = 1.