Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Homogeneous and Heterogeneous Dynamics in Native and Denatured Bovine Serum Albumin

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Table S1: Dynamic parameters of native BSA obtained from fits based on stretched exponential functions for the description of internal dynamics. The values of *R* correspond to the measured Guinier radius by SAXS*, the effective hydrodynamic radius determined from SAXS[#], and the hydrodynamic radius determined by DLS[$] given in the literature[1]. *R* = 39 Å is the average value as determined from fits to the QENS data sets.

	R	30.2 Å*	36.2 Å[#]	36.6 Å[$]	39 Å[$]
TOFTOF	β	0.41 +/- 0.03	0.46 ± 0.03	0.42 ± 0.03	0.45 +/- 0.03
	D_{int}(Å^2/ns)	13.9 +/- 2.5	33.7 ± 3.8	30.4 ± 4.5	47.7 +/- 6.1
	χ	1.78	1.78	1.80	1.73
SPHERES	β	1	1	1	1
	D_{int} (Å^2/ns)	19.9 +/- 1.0	23.6 +/- 1.3	23.9 +/- 1.4	26.1 +/- 1.6
	χ	1.61	1.63	1.63	1.65

Table S2: Dynamic parameters of native BSA obtained from fits based on the Brownian oscillator for the description of internal dynamics. Dependence of effective protein radius is reported. The values of *R* correspond to the measured Guinier radius by SAXS*, the effective hydrodynamic radius determined from SAXS[#], and the hydrodynamic radius determined by DLS[$]. The *R* values in the last column are fitted to the QENS data sets. The average value <*R*> determined from the fits equals 39 Å.

	R	30.2 Å*	36.2 Å[#]	36.6 Å[$]	39 Å	R_{TOFTOF} = 49.1 +/- 0.4 Å $R_{SPHERES}$ = 29.5 +/- 1.74
TOFTOF	D_{int} (Å^2/ns)	68.5 +/- 1.2	83.8 +/- 1.5	86.0 +/- 1.6	95.8 +/- 1.8	140.9 +/- 3.9
	RMSD (Å)	3.04 +/- 0.21	3.96 +/- 0.44	3.55 +/- 0.32	3.86 +/- 0.40	16.6 +/- 37.4
	p	0.77 +/- 0.01	0.80 +/- 0.01	0.80 +/- 0.01	0.81 +/- 0.01	0.85 +/- 0.01
	χ	1.89	1.89	1.86	1.85	1.84
SPHERES	D_{int} (Å^2/ns)	16.9 +/- 0.8	21.3 +/- 1.2	21.6 +/- 1.2	24.5 +/- 1.5	16.50 +/- 1.08
	RMSD	3.25 +/-	3.22 +/- 0.50	3.22 +/- 0.50	3.23 +/- 0.53	3.26 +/- 0.47
	p	0.56 +/- 0.01	0.61 +/- 0.01	0.62 +/- 0.01	0.64 +/- 0.01	0.55 +/- 0.02
	χ	1.64	1.64	1.64	1.65	1.64

1 F. Roosen-Runge, M. Hennig, F. Zhang, R. M. J. Jacobs, M. Sztucki, H. Schober, T. Seydel and F. Schreiber, Protein self-diffusion in crowded solutions., *Proc. Natl. Acad. Sci. U. S. A.*, 2011, **108**, 11815–20.