

SUPPLEMENTARY MATERIAL

**Self-interaction of Human Serum Albumin. A
formulation perspective**

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Table S1 Samples for SAXS experiments performed at varying protein concentrations.

Buffer	Protein sample	Protein concentration (mg/mL)
Octanoate_pH7.0_I153	Recombumin® Alpha	0.9 – 143.8
Phosphate_pH6.2_I66	Recombumin® Alpha	0.8- 181.8
Citrate_pH6.5_I274	Recombumin® Alpha	1.7- 315.1

Table S2 Samples for SAXS experiments performed at varying NaCl concentrations. The salt concentration in the original buffer has been exchanged with the indicated salt concentrations.

Buffer	rHSA concentration (mg/mL)	NaCl concentration (mM)
Octanoate_pH7.0	45	10, 20, 50, 100, 150, 200, 500, 1000, 2000
Phosphate_pH6.2	40	10, 20, 50, 100, 150, 200, 500, 1000, 2000

Table S3 Experimental set up of SAXS measurements.

Instrument	MaxIV beamline I911-SAXS
Detector	Pilatus 1M
Wavelength (Å)	0.9100
q range (nm)	0.0825-5.0
Exposure time (s)	3×60
Temperature (K)	285
Sample – detector distance (mm)	1972.485

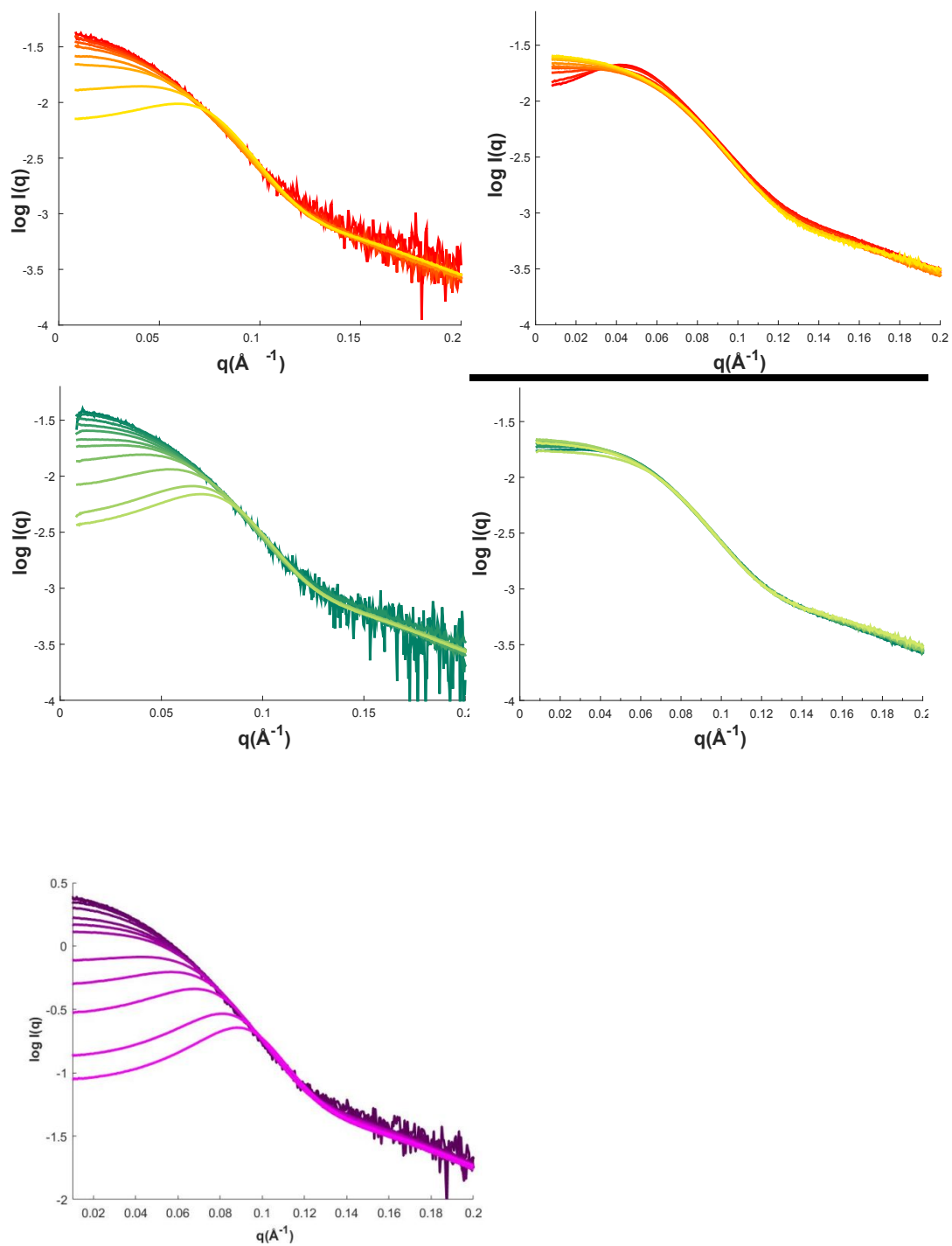


Figure S1 SAXS scattering curves. a): Octanoate_pH7.0_I153, c): Phosphate_pH6.2_I66 e): Citrate_pH6.5_I274. Data are shown for different rHSA concentration where increasing concentration is indicated by decreasing color intensity. b): Octanoate_pH7.0, d): Phosphate_pH6.2, rHSA at ~40 mg/ml with varying NaCl concentration. Increasing NaCl-concentration with decreasing colour intensity.

Table S4 Overview over all sample parameters for samples 1-10 mg/ml. All other samples show large deviations from ideality due to repulsion.

Buffer	Protein concentration (mg/ml)	R _G (Guinier) (nm)	StDev	Porod Vol	R _G (Gnom) (nm)	D _{max} (nm)	I(0) (Gnom)	Mw (g/mol)
Octanoate_pH7.0_I153	0.85	3.05	0.12	113.01	3.06	10.45	0.0411	66.9
Octanoate_pH7.0_I153	1.65	2.98	0.11	113.05	3.01	10.22	0.0786	65.9
Octanoate_pH7.0_I153	3.87	2.95	0.09	108.72	2.94	10.32	0.178	63.7
Octanoate_pH7.0_I153	7.36	2.82	0.05	103.12	2.83	8.61	0.32	60.2
Phosphate_pH6.2_I66	0.78	2.86	0.19	97.49	2.81	8.93	0.0385	68.3
Phosphate_pH6.2_I66	1.56	2.77	0.08	93.40	2.79	8.85	0.0697	61.9
Phosphate_pH6.2_I66	3.94	2.76	0.10	96.68	2.71	8.72	0.197	69.3
Phosphate_pH6.2_I66	7.7	2.63	0.20	95.44	2.7	8.01	0.359	64.5
Citrate_pH6.5_I274	1.67	2.91	0.03	104.14	2.87	9.17	0.078	64.7
Citrate_pH6.5_I274	3.77	2.85	0.04	103.89	2.83	9.08	0.176	64.6
Citrate_pH6.5_I274	9.02	2.71	0.01	97.16	2.73	7.86	0.393	60.3