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Supporting information for article:

The accurate assessment of small angle X-ray scattering data

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Table S1. Number of Exposures Rejected from Averaging. Column headers: “mg/ml” is the estimated concentration for each sample; “# Outliers” is the number of outliers that were rejected according to the modified z-score method described in the text; “# Damaged” is the number of exposures removed due to radiation damage; “# Averaged” is the total number of exposures that were averaged together after removal of outliers and damaged exposures.

Sample	Low Concentration				Mid Concentration				High Concentration			
	mg/ml	# Outliers	# Damaged	# Averaged	mg/ml	# Outliers	# Damaged	# Averaged	mg/ml	# Outliers	# Damaged	# Averaged
1	0.90	2	0	6	1.79	2	0	6	4.49	0	2	6
2	2.75	0	1	7	4.95	0	0	8	7.43	2	0	6
3	0.74	0	0	8	1.49	0	0	8	2.23	0	0	8
4	1.64	3	0	5	3.60	0	3	5	5.40	0	0	8
5	2.97	0	0	8	6.23	0	0	8	9.20	0	0	8
6	2.56	0	0	8	5.89	0	0	8	7.69	0	0	8
7	1.90	1	1	6	3.16	1	0	7	6.32	0	2	6
8	1.71	1	1	6	3.43	1	0	7	5.72	1	0	7
9	2.29	0	0	8	3.43	0	2	6	4.11	0	1	7
10	1.88	0	0	8	3.13	2	2	4	6.26	0	2	6
11	1.71	0	0	8	3.41	0	0	8	5.69	0	0	8
12	2.50	0	0	8	4.75	0	1	7	5.25	0	0	8
13	1.58	1	0	7	2.64	0	0	8	5.27	0	0	8
14	1.51	0	0	8	2.26	0	0	8	3.76	0	0	8
15	1.49	0	0	8	1.87	1	0	7	3.74	0	0	8
16	2.95	0	0	8	5.90	2	0	6	14.76	1	0	7
17	1.63	1	0	7	2.71	0	0	8	5.42	0	0	8
18	1.71	0	0	8	4.11	0	3	5	4.63	0	1	7
20	1.51	0	0	8	3.31	0	0	8	5.57	1	1	6
21	1.13	1	0	7	2.48	0	0	8	3.72	0	1	7
22	0.62	0	0	8	1.48	0	0	8	2.23	0	0	8
23	1.89	0	0	8	4.73	0	0	8	9.45	0	3	5
24	1.07	0	0	8	2.24	1	2	5	3.31	0	0	8
25	2.09	0	0	8	4.39	0	0	8	6.89	0	0	8
26	1.76	0	0	8	3.35	0	0	8	5.28	0	0	8
27	0.99	0	0	8	1.65	0	0	8	3.30	0	0	8
28	2.01	0	0	8	4.01	0	0	8	6.22	2	0	6

Table S2. Impact of Radiation Damage on Estimate of SAXS Parameters. The absolute value of the slope of the linear regression calculated as a function of exposure is presented in units of % change (of y-intercept of regression) per exposure. Column headers: “mg/ml” is the estimated concentration of each sample in mg/ml; “ χ ” is the similarity of scattering profiles between each exposure compared to the first exposure; “ R_g ” is calculated using Guinier region 3; “ R_g -P(r)” is calculated via the P(r) distribution; “Dmax” is the maximum particle dimension; “I(0)” is the forward scattering extrapolated from Guinier region 3.

Sample	Low Concentration						Mid Concentration						High Concentration					
	mg/ml	X	R _g	R _g -P(r)	Dmax	I(0)	mg/ml	X	R _g	R _g -P(r)	Dmax	I(0)	mg/ml	X	R _g	R _g -P(r)	Dmax	I(0)
1	0.90	0.12	1.88	0.63	1.87	1.63	1.79	1.47	0.09	0.22	1.63	0.28	4.49	2.37	0.86	0.23	0.35	1.25
2	2.75	0.40	1.07	0.19	0.50	1.28	4.95	0.26	0.44	0.13	0.21	0.56	7.43	1.28	0.11	0.05	0.24	0.21
3	0.74	0.40	0.54	0.15	0.46	0.45	1.49	0.35	0.58	0.10	1.18	0.51	2.23	0.06	0.39	0.13	0.63	0.25
4	1.64	0.11	0.15	0.01	0.20	0.18	3.60	2.11	0.11	0.05	0.02	0.01	5.40	0.55	0.14	0.06	0.00	0.20
5	2.97	0.60	0.20	0.13	0.74	0.28	6.23	0.55	0.07	0.03	0.69	0.08	9.20	0.52	0.13	0.02	0.05	0.02
6	2.56	0.78	0.55	0.07	0.31	0.35	5.89	0.50	1.08	0.07	0.09	0.75	7.69	0.11	0.18	0.02	0.04	0.14
7	1.90	0.38	0.35	0.29	0.32	0.47	3.16	0.55	0.07	0.03	0.41	0.06	6.32	3.15	0.05	0.26	0.30	0.45
8	1.71	0.91	0.50	0.15	0.39	0.35	3.43	0.26	0.28	0.05	0.79	0.14	5.72	0.27	0.00	0.06	0.17	0.20
9	2.29	0.77	0.04	0.37	0.58	0.09	3.43	1.19	0.60	0.02	0.69	0.25	4.11	0.11	0.29	0.34	1.24	0.02
10	1.88	0.24	1.30	0.12	0.24	0.63	3.13	0.85	0.37	0.17	0.34	0.31	6.26	1.43	0.01	0.10	0.22	0.16
11	1.71	1.00	0.51	0.11	0.07	0.66	3.41	0.67	0.36	0.08	0.21	0.24	5.69	0.32	0.23	0.00	0.16	0.19
12	5.25	1.58	1.01	5.01	9.94	2.12	4.75	0.06	0.55	0.16	0.42	0.31	2.50	0.27	0.24	0.17	0.08	0.35
13	1.58	0.66	1.33	0.13	0.57	0.54	2.64	0.11	0.47	0.03	0.27	0.29	5.27	0.21	0.05	0.17	0.56	0.22
14	1.51	0.47	0.07	0.07	0.32	0.20	2.26	0.83	0.49	0.03	0.23	0.44	3.76	0.16	0.65	0.15	0.10	0.64
15	1.49	0.72	0.52	0.06	1.03	0.23	1.87	0.88	0.15	0.18	0.22	0.06	3.74	0.50	0.72	0.10	0.13	0.89
16	2.95	0.21	1.03	0.10	0.12	0.90	5.90	0.37	0.64	0.11	0.39	0.54	14.76	1.40	0.33	0.03	0.23	0.47
17	1.63	0.20	0.93	0.14	0.43	0.59	2.71	0.45	0.43	0.12	0.01	0.17	5.42	0.06	0.72	0.41	1.08	0.36
18	1.71	0.49	0.67	0.10	0.22	0.13	4.11	0.11	0.26	0.40	0.80	0.35	4.63	1.62	0.31	0.02	0.11	0.32
20	1.51	0.54	2.10	0.62	0.63	1.13	3.31	0.45	0.28	0.28	0.56	0.47	5.57	0.08	1.11	0.29	0.48	0.77
21	1.13	0.01	0.25	0.48	0.13	0.30	2.48	0.49	0.30	0.39	0.61	0.34	3.72	0.99	0.65	0.61	1.83	0.81
22	0.62	0.87	3.19	1.24	1.75	2.30	1.48	0.43	0.85	0.38	0.45	0.65	2.23	0.11	0.69	0.17	0.19	0.35
23	1.89	0.76	2.51	0.49	0.36	1.66	4.73	0.31	0.49	0.19	0.36	0.62	9.45	0.30	0.63	0.22	0.42	0.62
24	1.07	0.73	0.68	0.19	0.29	0.57	2.24	0.88	0.29	0.04	0.40	0.03	3.31	1.05	1.13	0.03	0.15	0.82
25	2.09	0.29	0.53	0.56	1.35	0.50	4.39	0.34	0.44	0.65	1.39	0.49	6.89	0.60	0.07	0.03	0.36	0.13
26	1.76	0.72	0.92	0.49	0.53	0.80	3.35	0.00	0.27	0.11	0.09	0.24	5.28	0.45	0.19	0.17	0.48	0.14
27	0.99	1.10	1.68	0.22	0.58	0.68	1.65	1.00	1.79	0.12	1.07	1.36	3.30	0.42	0.27	0.04	0.49	0.58
28	2.01	1.76	0.36	0.23	0.24	0.25	4.01	1.82	0.25	0.18	0.56	0.36	6.22	0.20	0.25	0.24	0.66	0.36

Table S3. Likelihood of concentration dependence expressed as p-value for each of the 28 samples examined. “-1”, “-2”, “-3”, and “-P(r)” refer to parameters evaluated using Guinier region 1, Guinier region 2, Guinier region 3, and the pair distribution function, respectively. “I(0)/c” refers to the forward scattering value determined after scaling, and thus is independent of concentration. “Porod” refers to the molecular weight calculated from the Porod volume.

Sample ID	Rg-1	Rg-2	Rg-3	I(0)/c-1	I(0)/c-2	I(0)/c-3	Rg-P(r)	I(0)-P(r)	Dmax	Porod
1	>0.2	>0.2	>0.2	>0.2	>0.2	>0.2	>0.2	>0.2	0.1	>0.2
2	0.2	>0.2	>0.2	>0.2	>0.2	0.005	0.2	>0.2	0.01	0.2
3	>0.2	>0.2	>0.2	0.2	>0.2	>0.2	>0.2	0.1	>0.2	0.2
4	0.2	0.2	0.2	0.2	0.2	0.2	0.05	0.05	>0.2	0.2
5	0.05	0.02	>0.2	0.02	0.05	0.2	0.2	0.1	0.2	>0.2
6	0.2	>0.2	>0.2	0.1	0.1	0.05	0.2	0.1	0.1	>0.2
7	>0.2	0.2	0.1	0.1	0.005	0.005	0.05	0.1	>0.2	0.05
8	>0.2	>0.2	>0.2	>0.2	>0.2	>0.2	>0.2	>0.2	0.2	>0.2
9	>0.2	>0.2	>0.2	0.001	0.02	0.1	>0.2	0.2	>0.2	0.2
10	>0.2	>0.2	>0.2	0.2	0.2	>0.2	0.2	0.2	>0.2	>0.2
11	0.2	0.2	0.01	0.2	0.2	0.1	>0.2	0.2	>0.2	0.1
12	>0.2	>0.2	>0.2	>0.2	>0.2	>0.2	0.1	>0.2	>0.2	>0.2
13	>0.2	>0.2	>0.2	>0.2	>0.2	>0.2	0.2	0.05	0.2	>0.2
14	>0.2	>0.2	>0.2	0.2	0.2	>0.2	>0.2	0.2	>0.2	0.2
15	0.05	0.02	>0.2	0.2	0.2	0.02	0.05	0.2	>0.2	>0.2
16	0.02	0.05	>0.2	0.1	0.2	0.05	0.1	0.2	0.1	0.2
17	>0.2	>0.2	>0.2	0.2	>0.2	>0.2	0.2	>0.2	0.2	>0.2
18	>0.2	0.2	>0.2	>0.2	0.005	>0.2	>0.2	>0.2	>0.2	>0.2
20	0.2	>0.2	>0.2	0.05	0.05	0.05	0.1	0.005	>0.2	0.2
21	>0.2	0.2	>0.2	>0.2	0.2	>0.2	>0.2	>0.2	>0.2	>0.2
22	>0.2	>0.2	>0.2	>0.2	>0.2	>0.2	>0.2	>0.2	>0.2	>0.2
23	>0.2	>0.2	>0.2	0.2	0.2	>0.2	0.02	0.01	0.05	0.2
24	0.1	>0.2	>0.2	0.01	0.2	0.2	>0.2	0.2	>0.2	>0.2
25	>0.2	>0.2	>0.2	>0.2	>0.2	>0.2	>0.2	>0.2	>0.2	>0.2
26	0.2	>0.2	>0.2	0.1	0.1	>0.2	0.2	0.1	0.2	>0.2
27	0.2	>0.2	>0.2	0.2	0.2	>0.2	0.1	0.2	>0.2	>0.2
28	0.2	0.2	0.2	0.2	0.2	0.1	0.2	0.1	0.2	>0.2

Table S4. Impact of Concentration Dependence on Estimate of SAXS Parameters. The absolute value of the slope of the linear regression calculated as a function of concentration is presented in units of % change (of y-intercept of regression) per mg/ml. Column headers explained in caption of Table S3.

Sample ID	Rg-1	Rg-2	Rg-3	I0/c-1	I0/c-2	I0/c-3	Pr-Rg	Pr-I0	Dmax	Porod-MW	Average	Median
1	3.23	3.16	3.28	3.74	3.69	3.87	3.33	3.71	5.53	5.07	3.86	3.70
2	0.83	0.59	0.25	0.31	0.51	0.85	0.63	0.51	1.41	2.87	0.88	0.61
3	0.89	2.47	2.80	1.22	2.48	2.99	0.49	1.08	3.64	9.20	2.73	2.48
4	0.79	0.61	0.34	0.58	0.48	0.25	1.39	0.69	12.53	1.48	1.91	0.65
5	0.88	0.78	0.30	0.97	0.88	0.45	0.50	0.68	1.35	0.56	0.74	0.73
6	1.31	0.73	0.13	1.68	1.35	0.94	1.61	1.79	3.16	2.86	1.56	1.48
7	0.51	0.65	0.90	0.48	0.59	0.78	0.65	0.51	0.53	1.40	0.70	0.62
8	0.24	0.00	0.14	0.02	0.16	0.02	0.63	0.22	4.75	0.44	0.66	0.19
9	1.73	2.04	2.53	2.66	2.93	3.36	5.06	3.48	26.47	9.12	5.94	3.15
10	0.66	1.01	2.48	1.32	1.58	2.81	0.55	1.26	0.75	4.12	1.65	1.29
11	1.14	1.14	1.78	12.21	12.21	13.37	1.01	12.13	0.47	7.59	6.31	4.69
12	0.39	0.31	0.76	0.51	0.42	0.82	0.48	0.46	0.77	1.13	0.61	0.50
13	0.00	0.00	0.45	0.25	0.25	0.08	0.35	0.40	0.22	0.53	0.25	0.25
14	0.33	0.47	0.86	1.57	1.70	2.05	0.05	1.43	0.14	1.83	1.04	1.15
15	0.66	0.70	0.41	1.15	1.09	2.14	0.31	1.42	0.72	3.19	1.18	0.91
16	0.33	0.27	0.27	1.12	1.09	1.08	0.38	1.15	0.91	2.07	0.87	1.00
17	0.81	0.30	1.34	0.53	0.18	1.02	0.54	0.38	1.50	4.97	1.16	0.68
18	0.12	1.06	0.24	0.30	0.94	0.06	0.06	0.30	0.67	2.91	0.67	0.30
20	4.21	0.92	0.05	4.34	2.11	1.15	2.34	2.87	2.50	7.36	2.79	2.42
21	0.70	0.99	0.49	0.07	0.94	0.54	0.61	0.21	1.10	3.97	0.96	0.66
22	2.14	2.49	0.76	1.60	1.96	0.52	1.08	1.27	0.55	8.98	2.14	1.44
23	0.87	1.28	0.00	0.90	1.17	0.03	0.72	0.75	2.09	4.06	1.19	0.89
24	5.99	5.61	4.40	6.56	6.27	5.34	5.55	5.92	3.54	11.34	6.05	5.77
25	1.36	0.15	0.40	0.95	0.02	0.25	0.33	0.13	0.15	0.37	0.41	0.29
26	1.02	0.35	0.36	1.23	0.73	0.71	1.09	1.09	7.88	3.58	1.80	1.06
27	5.13	6.13	6.38	9.19	10.05	10.37	5.15	8.94	8.86	13.08	8.33	8.90
28	9.51	2.62	3.32	5.67	1.93	2.39	8.19	3.45	120.78	1.28	15.91	3.39
Average	1.40	1.32	1.23	2.13	2.15	2.15	1.34	2.03	3.55	4.39	2.17	1.76
Median	0.85	0.76	0.47	1.14	1.09	0.90	0.63	1.09	1.38	3.39	1.18	0.95