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Supporting information for article:

Improving data quality and expanding the BioSAXS experiments to low-molecular weight and low-concentration protein samples

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Table S1 Expansion of Table 1 in main text.

The use of the described scavengers in a HEWL solution allowed collection of a much higher number of frames leading to very high scavenging factors. The number of frames at which the critical doses were reached and the corresponding scavenging factors for all tested scavengers at different concentrations, compared to glycerol at 100 and 678 mM and without additive (control) are listed. The evolution of the metrics with dose is fitted using a 4th order polynomial. The number of frames is defined by the intersection of the polynomial fit with the critical dose defined for the corresponding metrics. The number of frames in parenthesis corresponds to the second set of seven consecutive data frames with C=17. One collected data frame corresponds to 0.06 kGy of absorbed dose.

Sample [HEWL] = 7.00 mg/ml	Frames			Scavenging factors		
	Rg/Rg_0 = 1.05	$I(0)/I(0)_0$ = 1.05	CorMap test	Rg/Rg_0 = 1.05	$I(0)/I(0)_0$ = 1.05	CorMap test
Control	11	11	11	1	1	1
100 mM glycerol	25	29	18	2.3	2.6	1.6
678 mM glycerol	50	50	51	4.6	4.6	4.6
25 mM 5-methy uridine	118	77	70	10.7	7.0	6.4
50 mM 5-methyl uridine	132	112	63	12.0	10.2	5.7
100 mM 5-methyl uridine	225	177	97	20.4	16.1	8.8
25 mM cytidine	108	82	73	9.8	7.4	6.6
50 mM cytidine	127	126	139	11.6	11.4	12.6
100 mM cytidine	223	217	178	20.3	19.7	16.2
25 mM cytosine	79	84	72	7.2	7.6	6.5
50 mM cytosine	79	98	139	7.2	8.9	12.6
100 mM cytosine	198	202	177	18.0	18.4	16.1
25 mM uridine	89	66	50	8.1	6.0	4.5
50 mM uridine	115	97	54	10.4	8.8	4.9
100 mM uridine	174	136	42 (117)	15.8	12.4	3.8 (10.6)

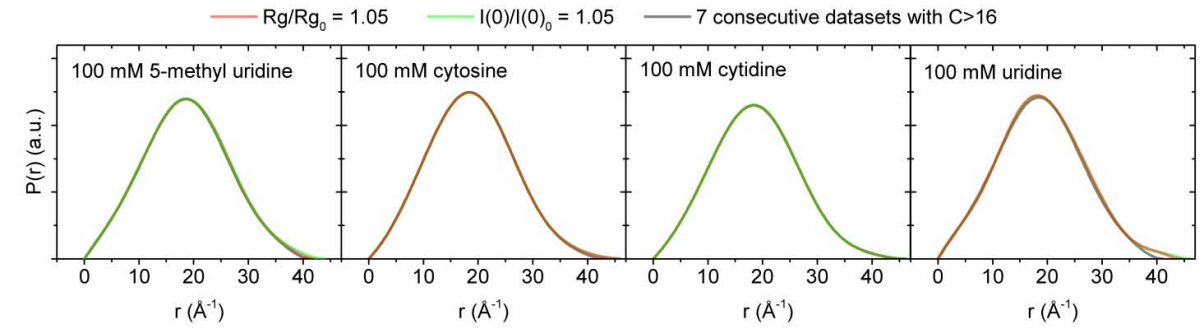

Figure S1 Pair distribution functions are independent of the metric and additive used. Pair distribution functions, P(r), for those samples containing 5-metrhyl uridine, cytosine, cytidine and uridine at 100 mM. For each sample, all frames below the three defined critical doses were considered.

Table S2 Structural parameters calculated from the pair distribution function in Figure S2.

Parameters	100 mM 5-methyl uridine		
	CorMap	Rg/Rg_0 = 1.05	$I(0)/I(0)_0$ = 1.05
# frames	97	225	117
R_g (nm)	14.28	14.38	14.46
I(0) (a.u.)	0.30	0.30	0.30
V_p	22900	22500	22800
D_{max} (nm)	41.33	42.46	43.98

Parameters	100 mM cytidine		
	CorMap	Rg/Rg_0 = 1.05	$I(0)/I(0)_0$ = 1.05
# frames	178	223	217
R_g (nm)	14.29	14.41	14.43
I(0) (a.u.)	0.31	0.31	0.31
V_p	22300	22200	22200
D_{max} (nm)	43.36	46.07	45.78

Parameters	100 mM cytosine		
	CorMap	Rg/Rg_0 = 1.05	$I(0)/I(0)_0$ = 1.05
# frames	177	198	202
R_g (nm)	14.34	14.35	14.36
I(0) (a.u.)	0.29	0.29	0.29
V_p	22200	22100	22100
D_{max} (nm)	46.24	45.80	45.75

Parameters	100 mM uridine		
	CorMap	Rg/Rg_0 = 1.05	$I(0)/I(0)_0$ = 1.05
# frames	42	174	136
R_g (nm)	14.23	14.48	14.51
I(0) (a.u.)	0.30	0.31	0.31
V_p	22800	23200	23000
D_{max} (nm)	41.16	44.48	46.14

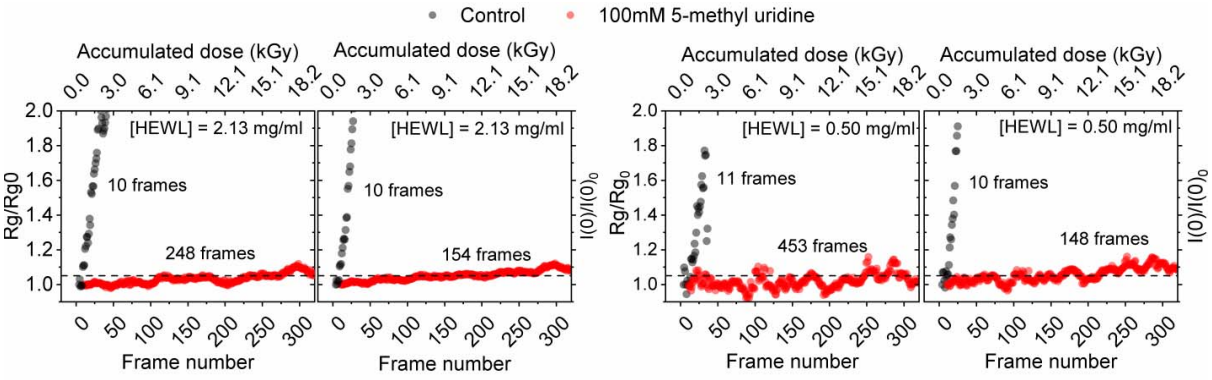

Figure S2 Reduction of radiation damage in HEWL solutions at 2.13 and 0.5 mg/mL concentration by adding 100 mM 5-methyl uridine. The scavenging effect of 5-methyl uridine with respect to the control (no added compound) is monitored by the increase of the radius of gyration, R_g/R_{g0} and the normalized intensity at zero, $I(0)/I(0)_0$.

Table S3 Frames required to reach the critical doses shown in the plots of Figure S2.

Sample	Frames	
	$Rg/Rg_0 = 1.05$	$I(0)/I(0)_0 = 1.05$
[HEWL] = 2.13 mg/ml		
Control (no additive)	10	10
100 mM 5-methyl uridine	248	154
[HEWL] = 0.50 mg/ml		
Control (no additive)	11	10
100 mM 5-methyl uridine	453	148

Table S4 Itheory parameters of the fits in figure 8 for the different proteins, with and without 5-methyl uridine 100 mM, as reported in the SHANUM output (Konarev & Svergun, 2015).

These parameters allow the Shanon fits to be reproduced. The fits of scattering profiles for the scavenging solutions can also be retrieved from the experimental data deposited in the SASBDB (accession codes in main text).

Protein	Compound	Shannon channels	Itheory parameters
BLC	control	7	0.18837E-01 0.62794E-02 0.90963E-03 0.26124E-03 0.11404E-03 0.51050E-04 0.19098E-04
BLC	100 mM 5-methyl uridine	21	0.20022E-01 0.66280E-02 0.11177E-02 0.26685E-03 0.14127E-03 0.62431E-04 0.42629E-04 0.25011E-04 0.26729E-04 0.24785E-04 0.19745E-04 0.13325E-04 0.14923E-04 0.16396E-04 0.16657E-04 0.14719E-04 0.15561E-04 0.16509E-04 0.18509E-04 0.18629E-04
hAR	control	5	0.31596E-02 0.12329E-02 0.21190E-03 0.44799E-04 0.28823E-04
hAR	100 mM 5-methyl uridine	12	0.31609E-02 0.12102E-02 0.18649E-03 0.33795E-04 0.19595E-04 0.12746E-04 0.14499E-04 0.12185E-04 0.13911E-04 0.17814E-04 0.21303E-04 0.19777E-04
HEWL	control	7	0.14329E-02 0.43949E-03 0.69848E-04 0.20377E-04 0.31272E-04 0.14004E-04 0.34797E-06
HEWL	100 mM 5-methyl uridine	9	0.14644E+01 0.45516E+00 0.68537E-01 0.33404E-01 0.35004E-01 0.26812E-01 0.21807E-01 0.24019E-01 0.16259E-01
SH3-SPC	control	7	0.82404E-03 0.32912E-03 0.10975E-03 0.19823E-04 0.15784E-04 0.14724E-04 0.15461E-05
SH3-SPC	100 mM 5-methyl uridine	9	0.88431E-03 0.49103E-03 0.22251E-03 0.78477E-04 0.32636E-04 0.25402E-04 0.29505E-04 0.32337E-04 0.25156E-04