Biophysical Journal

Supporting Material

^{13}C, ^{2}H NMR Studies of Structural and Dynamical Modifications of Glucose-Exposed Porcine Aortic Elastin

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Table S1: Amino acid analysis (expressed in % per mole based on the molecular weight of bovine nuchal ligament elastin, 61,310 g/mol) for a sample of porcine aortic elastin used in this study [33].

Amino Acid	Porcine aortic elastin (this work)	Bovine nuchal ligament elastin
Cys	0.0	0.3
Hyp	0.0	-
Asp	0.6	0.4
Thr	1.4	1.2
Ser	1.1	0.9
Glu	2.0	1.3
Pro	11.4	12.3
Gly	31.4	33.8
Ala	22.9	22.2
Val	13.5	13.3
Met	0.0	0.0
Ile	1.9	2.6
Leu	5.6	5.6
Nle	0.0	-
Tyr	1.9	1.0
Phe	4.9	6.1
His	0.0	0.0
Hlys	0.0	-
Lys	0.7	1.0
Arg	0.7	0.7

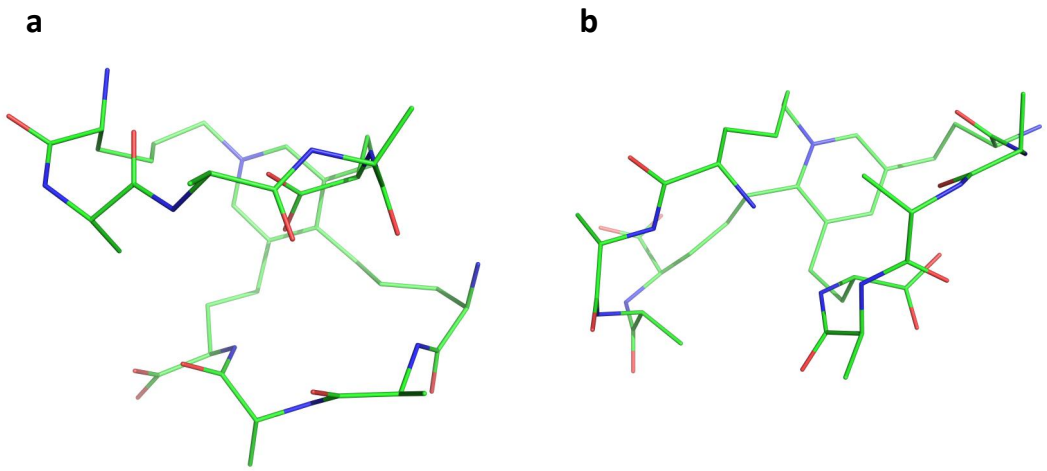

Figure S1: Desmosine (a) and isodesmosine (b) molecules used for the simulations. Two or three alanine residues are bonded to the terminals of the desmosine cross links.

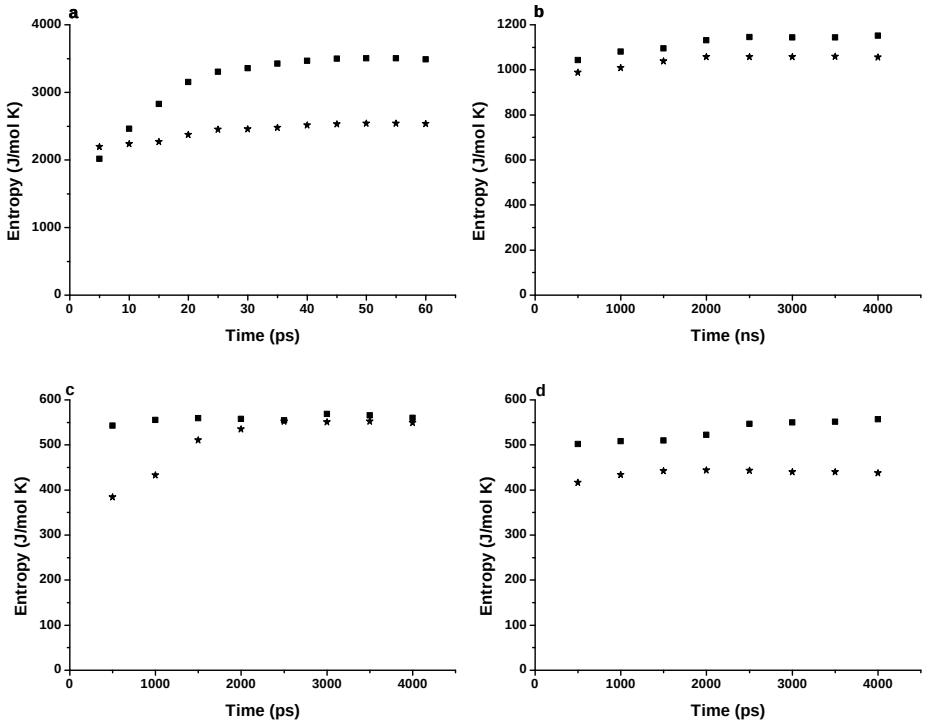

Figure S2: Entropy, determined from the quasi harmonic approach described in the text, as a function of sampling time for (a) relaxed and (b) strained $[VPGVG]_5$ and (c) relaxed and (d) strained [AAAAA] pentamer. In all cases we observe the entropy approaches an asymptotic value. The squares are the samples in water and the stars are the samples in the 2 M glucose solution.

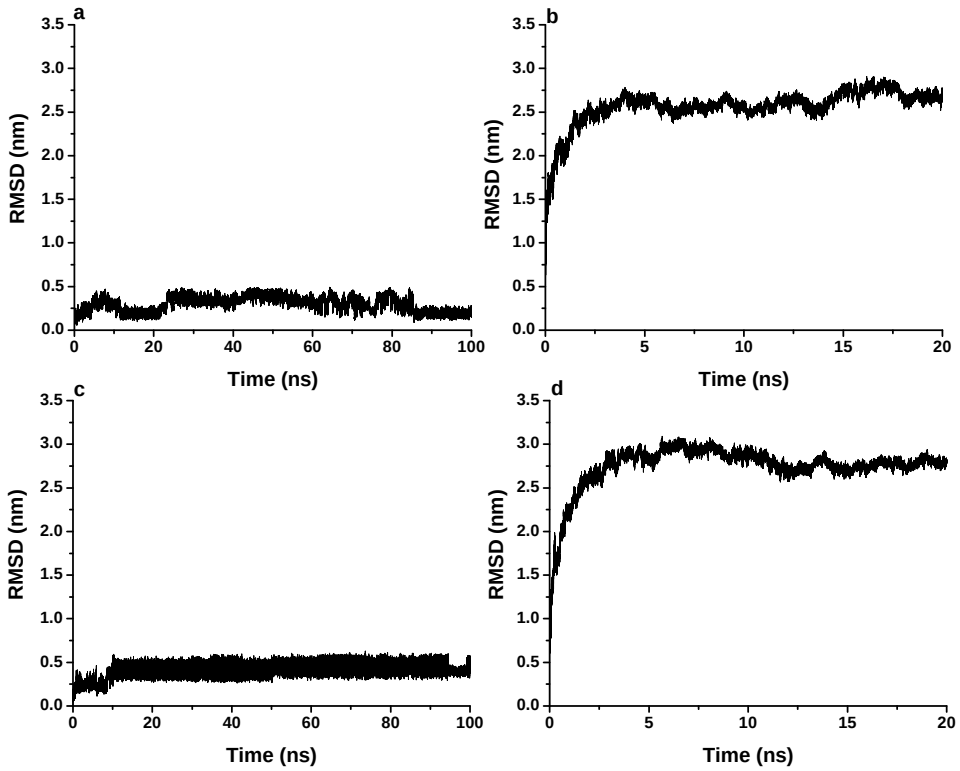

Figure S3: Root mean square deviation (RMSD) of all C_α as a function of time for (a) desmosine in water, (b) desmosine in 2M glucose solution, (c) isodesmosine in water, and (d) isodesmosine in 2M glucose solution.