Electronic Supplementary Material (ESI) for Soft Matter.

Trehalose facilitates DNA melting: a single-molecule optical tweezers study

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ELECTRONIC SUPPLEMENTARY INFORMATION

Table S 1: Number of DNA molecules studied.

	Trehalose							Other molecules, 1 mM		
	–	10 nM	100 nM	1 μM	100 μM	1 mM	0.1 M	1-propanol	1-hexanol	glycerol
Molecules	7	2	3	5	2	4	4	2	2	2
Pulls	15	9	11	13	8	12	13	6	6	5

Figure S1

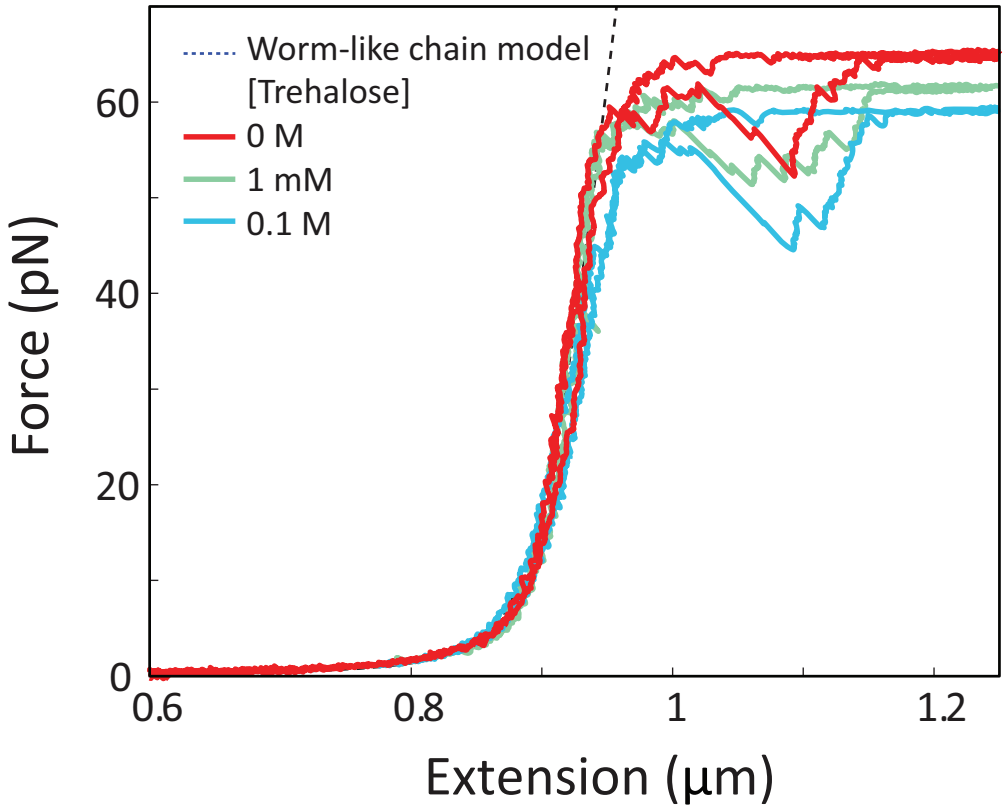

Fig. S 1: Stretching and relaxation curves of dsDNA. The mechanical response of dsDNA was measured in the absence and in the presence of trehalose. In both conditions DNA exhibits significant hysteresis upon relaxation.

Figure S2

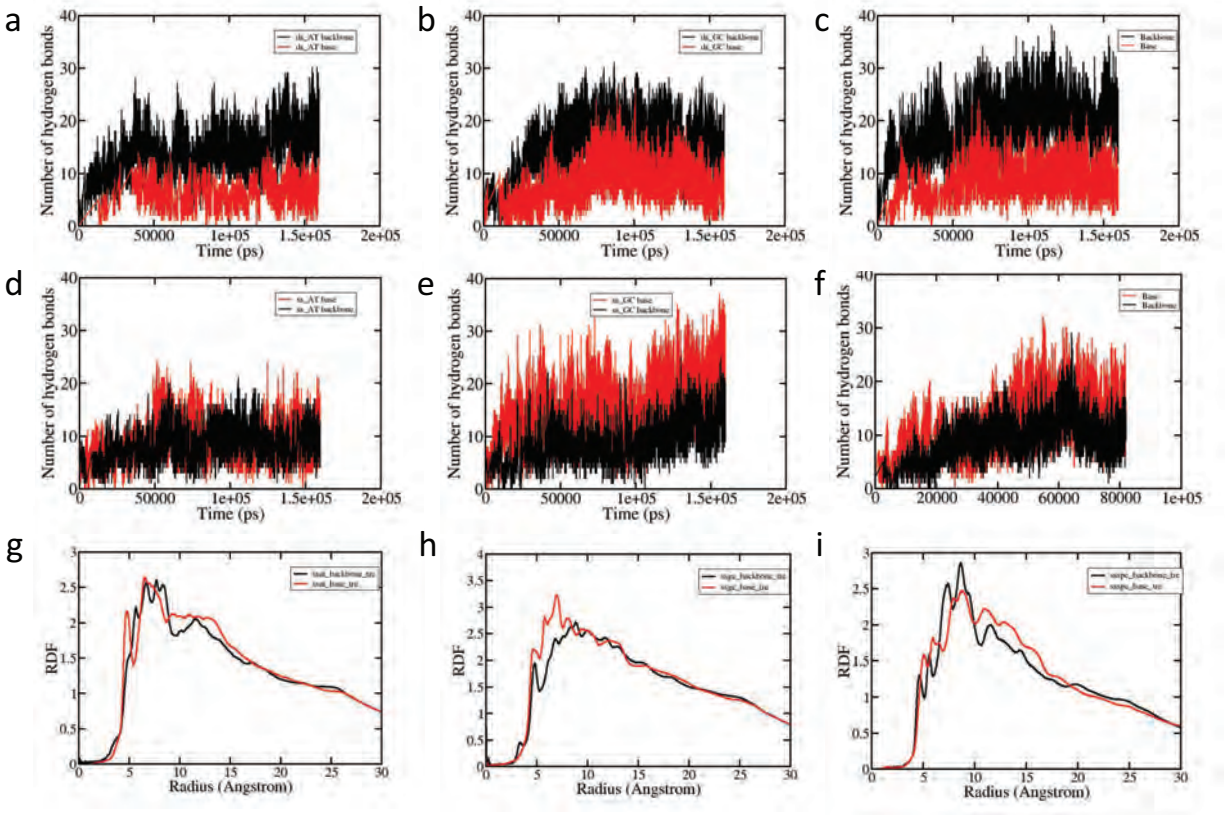

Fig. S 2: Base-to-backbone preference of trehalose compared for dsDNA and ssDNA. **(a-f)** Number of hydrogen bonds between DNA and trehalose determined from MD simulations is plotted versus simulation time. The number of hydrogen bonds between DNA backbone and trehalose is shown in black, between DNA nucleobases and trehalose in red. The results are shown for the following DNA molecules: **(a)** dsAT, **(b)** dsGC, **(c)** ds50%GC, **(d)** ssAT, **(e)** ssGC, **(f)** ss50%GC. **(g-i)** Radial distribution function (RDF) is calculated for ssDNA and trehalose from MD simulations results. Here and in the following figures RDFs calculated are averages of RDFs for every residue. DNA backbone is defined as O3' atom of phosphodiester, DNA bases are defined as C4 atom of guanine, N3 atom of cytosine, C4 atom of adenine and N3 atom of thymine. Water is defined as its O atom. RDF for ssDNA backbone and trehalose is shown in black, for ssDNA nucleobases and trehalose - in red. The results are displayed for the following DNA sequences: **(g)** AT, **(h)** GC, **(i)** 50%GC.

Figure S3

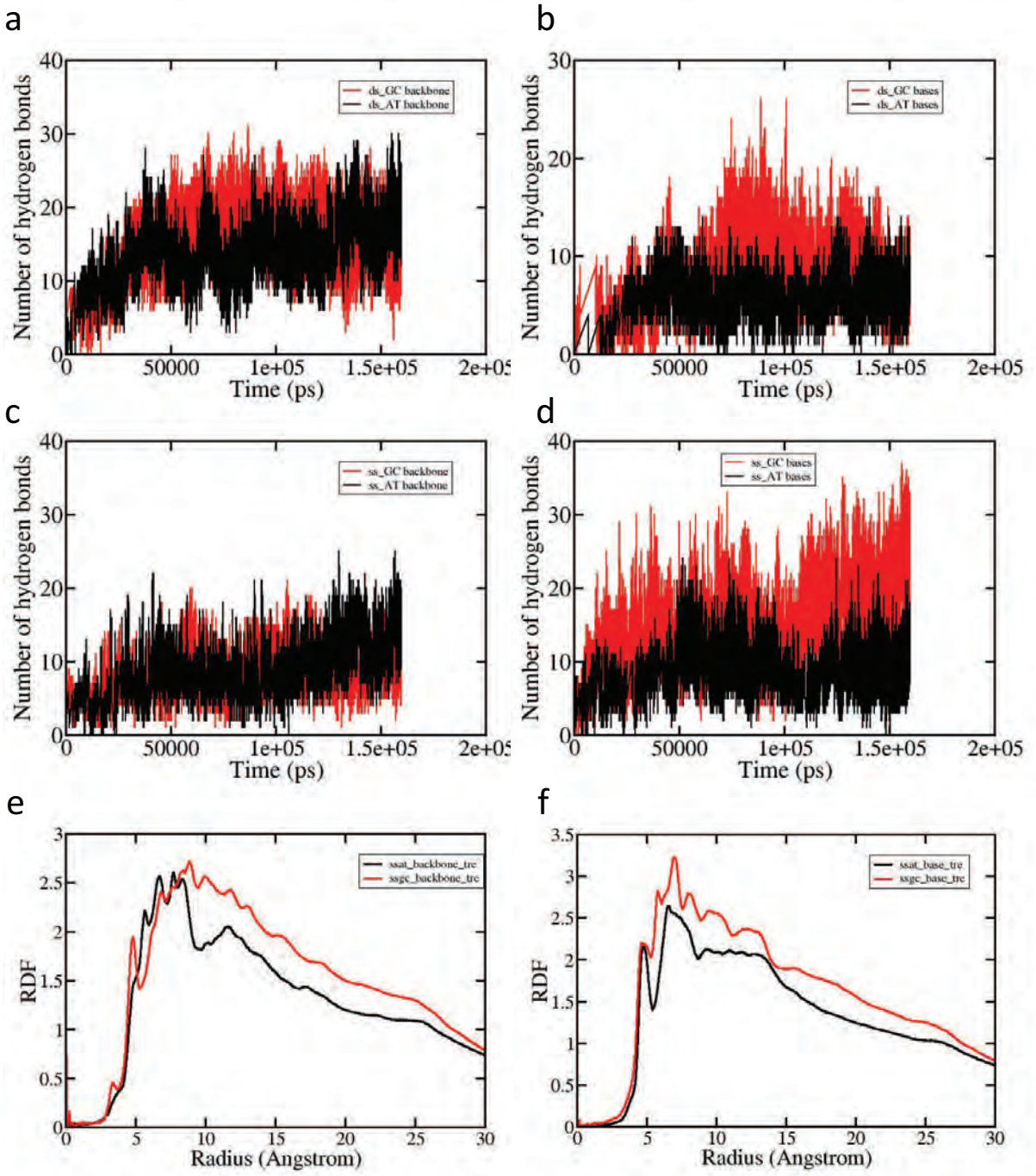

Fig. S 3: Abundance of trehalose-DNA interaction is compared for AT-DNA and GC-DNA. **(a-d)** Number of hydrogen bonds between DNA and trehalose determined from MD simulations is plotted versus simulation time. The number of hydrogen bonds between GC-DNA and trehalose is shown in black, between AT-DNA and trehalose in red. **(a)** and **(b)** display the number of hydrogen bonds between trehalose and dsDNA: **(a)** between trehalose and backbone, **(b)** between trehalose and nucleobases. **(c)** and **(d)** display the number of hydrogen bonds between trehalose and ssDNA: **(c)** between trehalose and backbone, **(d)** between trehalose and nucleobases. **(e-f)** Radial distribution function (RDF) for AT-DNA and trehalose (shown in black) is compared with RDF for GC-DNA and trehalose (in red): **(e)** for DNA backbone, and **(f)** for DNA bases.

Figure S4

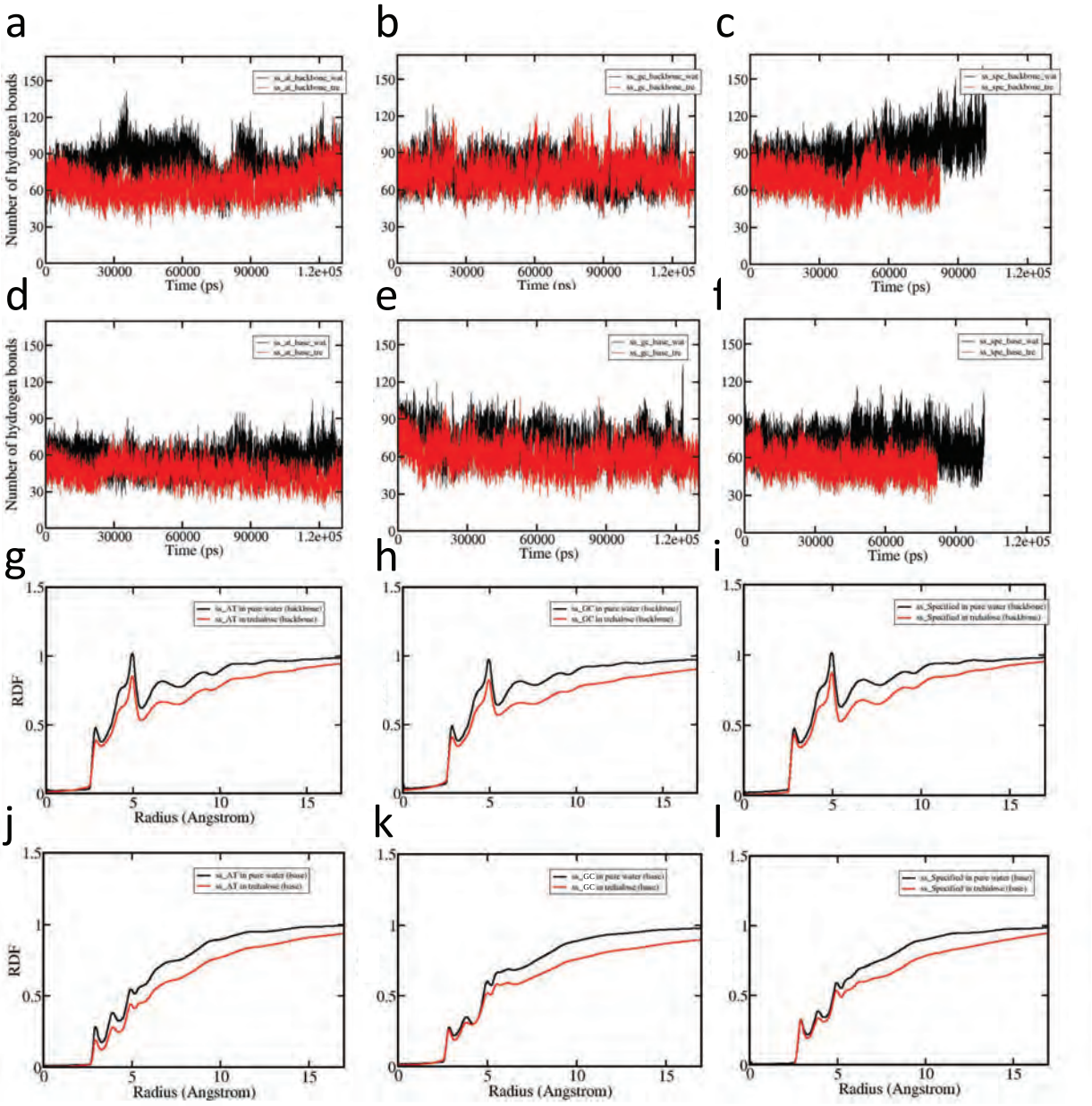

Fig. S 4: Effect of trehalose on DNA-water interface. **(a-f)** Number of hydrogen bonds between ssDNA and water determined from MD simulations is plotted versus simulation time. The number of hydrogen bonds between DNA and water in the absence of trehalose is shown in black, between DNA and water when trehalose is present in red. **(a)** shows the number of hydrogen bonds between the backbone of ssAT and water, **(b)** - backbone of ssGC, **(c)** - backbone of ss50%GC, **(d)** - bases of ssAT, **(b)** - bases of ssGC, **(c)** - bases of ss50%GC. **(g-l)** Radial distribution function (RDF) for ssDNA and water molecules is plotted when trehalose was absent (black) and when it was present (red) for the following molecules and parts of DNA: **(g)** - backbone of ssAT, **(h)** - backbone of ssGC, **(i)** - backbone of ss50%GC, **(j)** - bases of ssAT, **(k)** - bases of ssGC, **(l)** - bases of ss50%GC.