Supporting Material

Effects of temperature and trehalose concentration on hydrophobic interactions of small nonpolar neopentane solute: Molecular dynamics simulation study

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Systems	285K	300K		315K	330K	345K
D_{np} $(10^{-5}cm^2s^{-1})$						
S0	0.08	0.08		0.37	0.34	0.52
S1	0.04	0.17		0.38	0.25	0.43
S2	0.06	0.06		0.06	0.11	0.27
S3	0.03	0.02		0.03	0.04	0.08
S4	0.04	0.04		0.04	0.03	0.08
S5	0.03	0.03		0.13	0.07	0.09

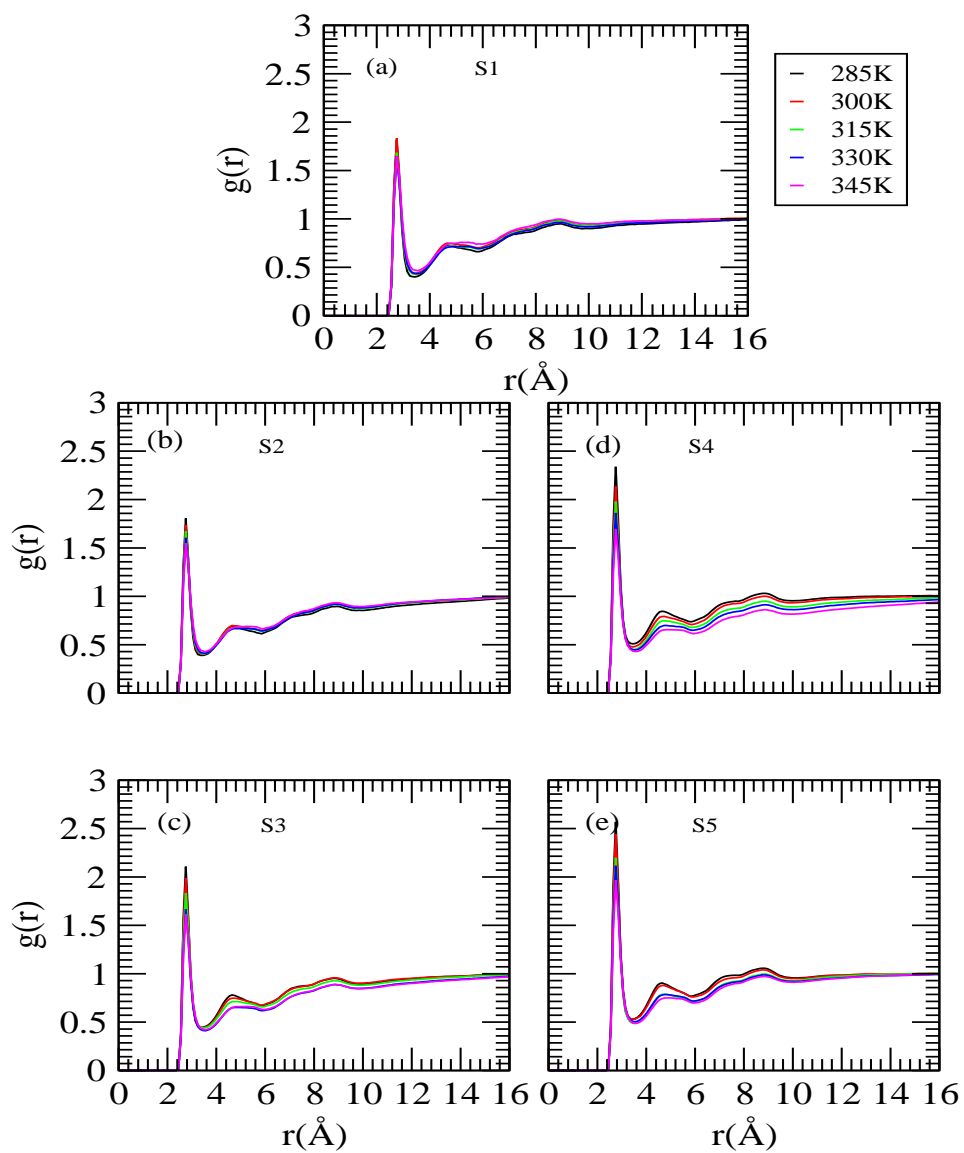TABLE I: Diffusion coefficients of neopentane (D_{np}).

FIG. 1: Site-site radial distribution functions involving water oxygen and trehalose hydroxylic oxygen (O2).
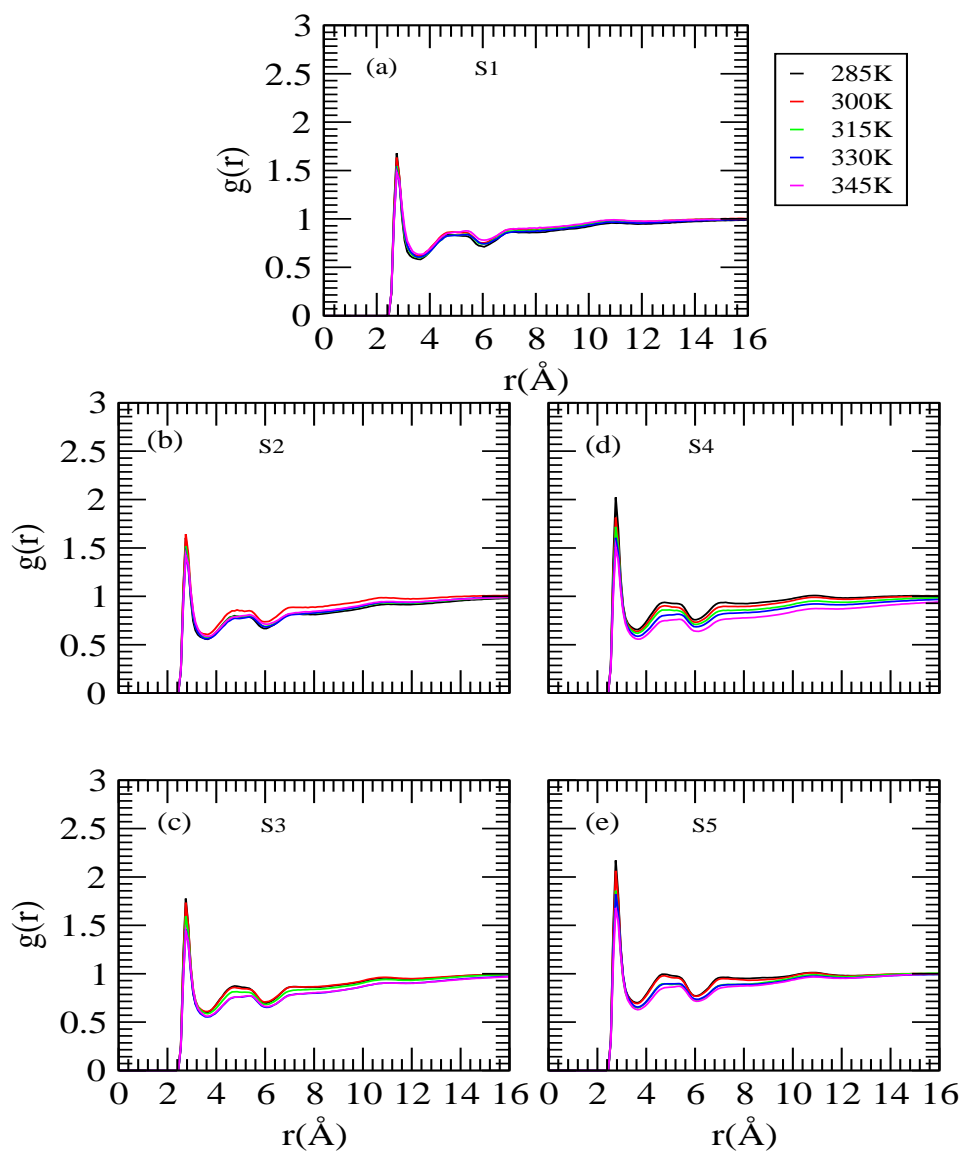
FIG. 2: Site-site radial distribution functions involving water oxygen and trehalose hydroxylic oxygen (O3).
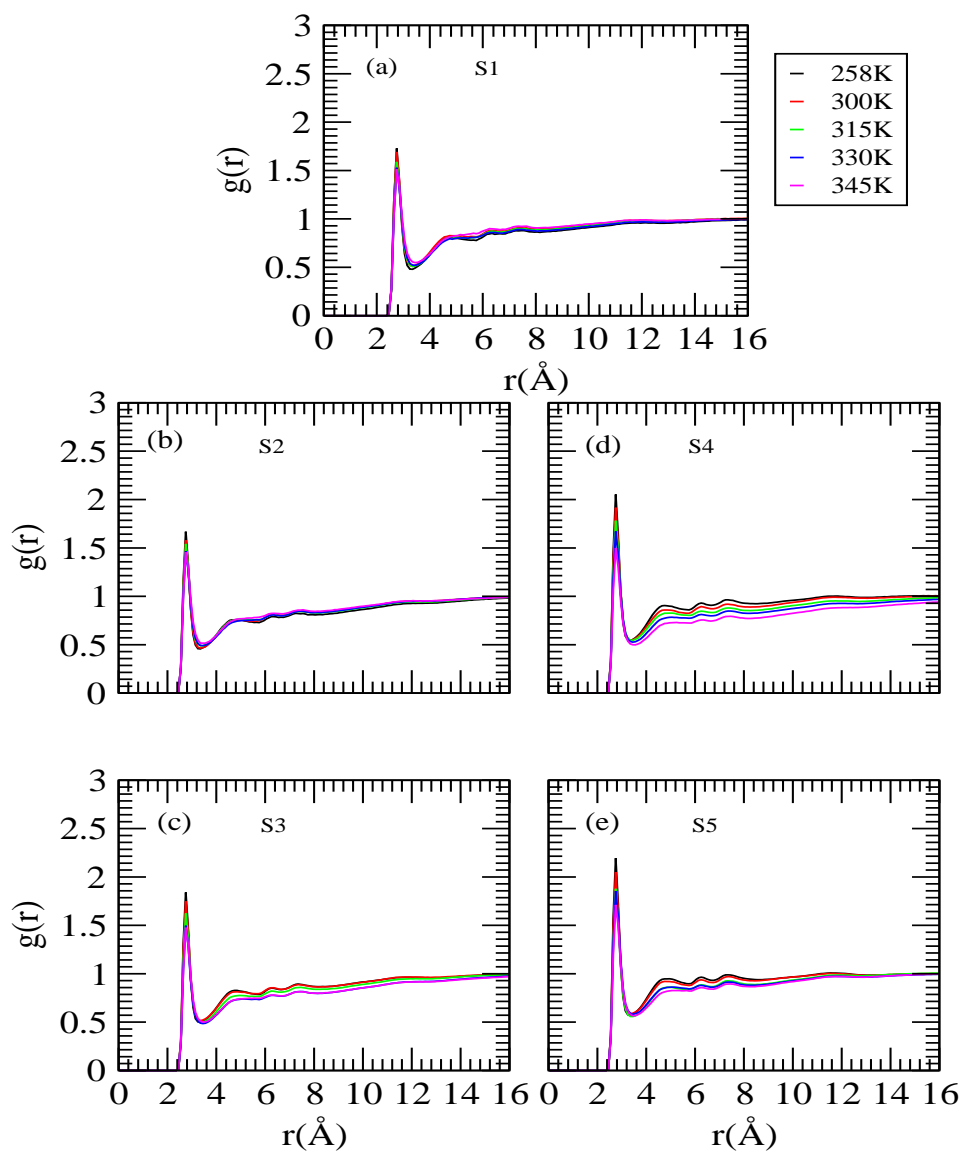
FIG. 3: Site-site radial distribution functions involving water oxygen and trehalose hydroxylic oxygen (O4).
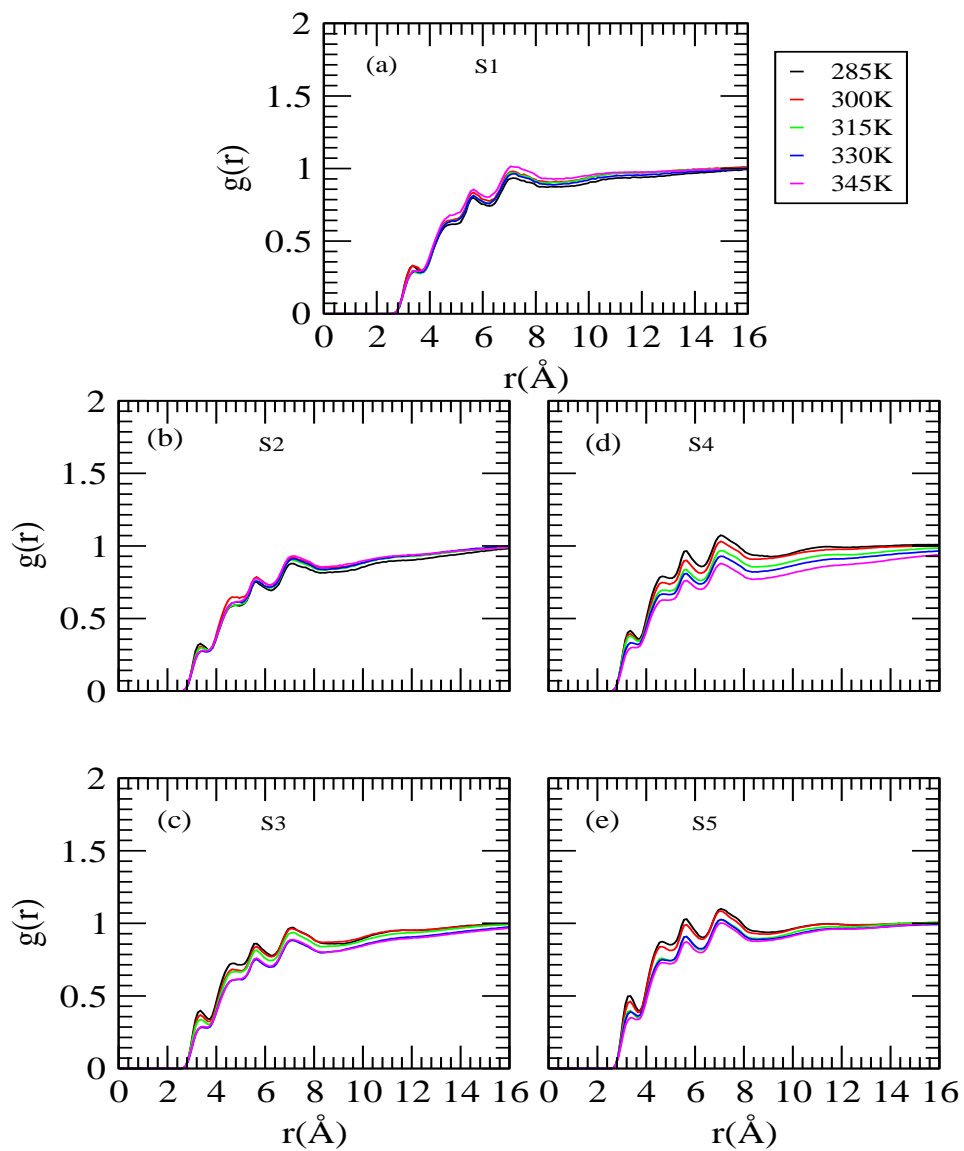
FIG. 4: Site-site radial distribution functions involving water oxygen and trehalose glycosidic oxygen (O1).
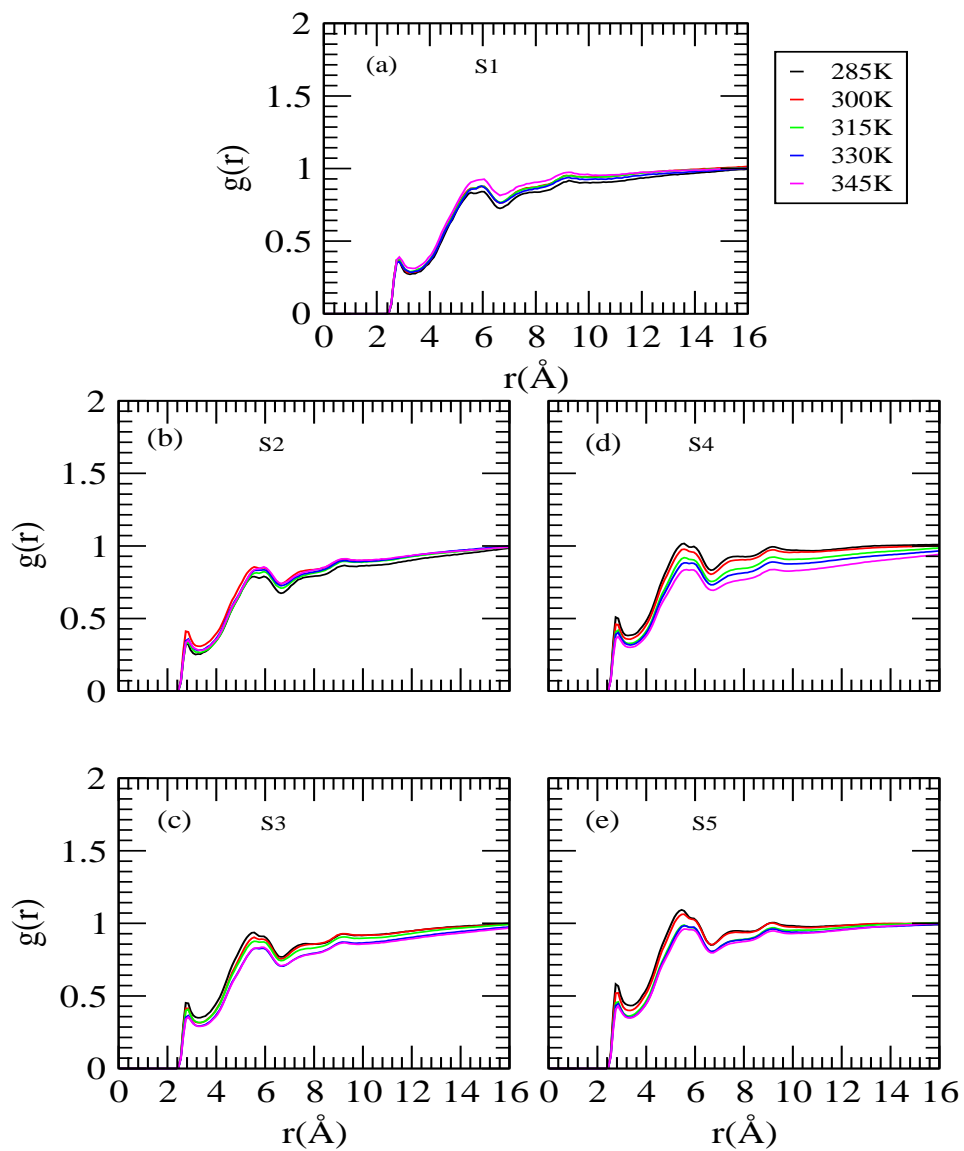
FIG. 5: Site-site radial distribution functions involving water oxygen and trehalose acetalic ring oxygen (O5).
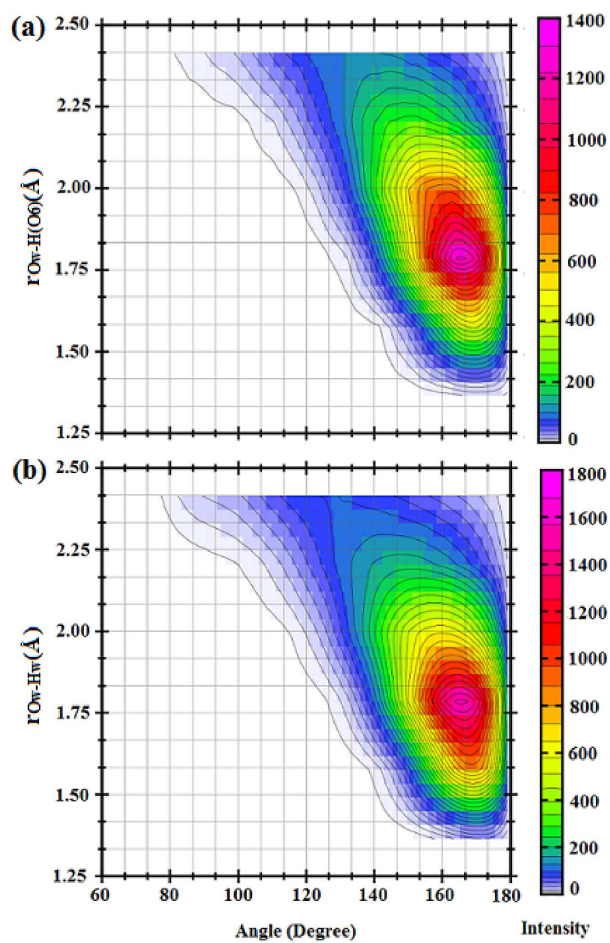
FIG. 6: Probability distribution contour plots as a function of hydrogen bond angle (D-H-A) and acceptor-hydrogen (A-H) distance for system S5 at 300K (a) is for water oxygen-trehalose hydrogen and (b) is for water oxygen-water hydrogen H-bond.
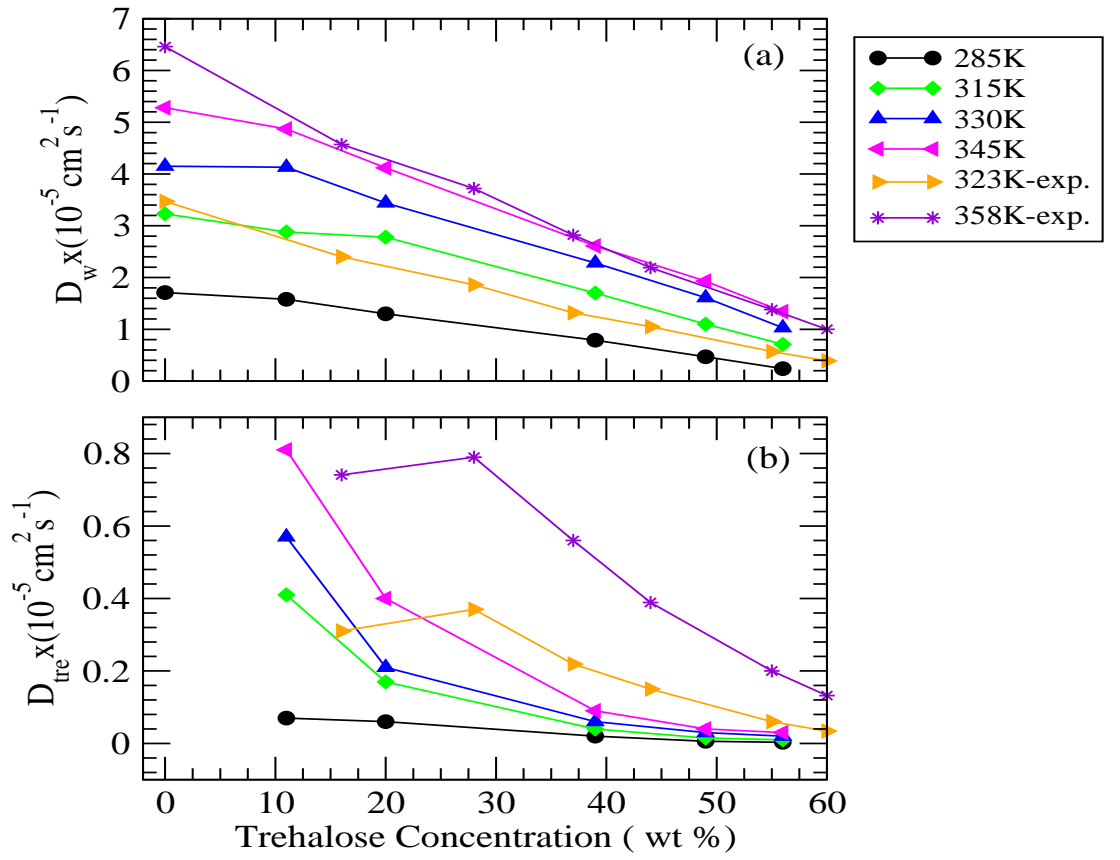
FIG. 7: Diffusion coefficient of (a) water and (b) trehalose for different systems at 285 K, 315 K, 330 K and 345 K temperatures. The experimental diffusion coefficient values are taken from Reference 73 of the main manuscript.
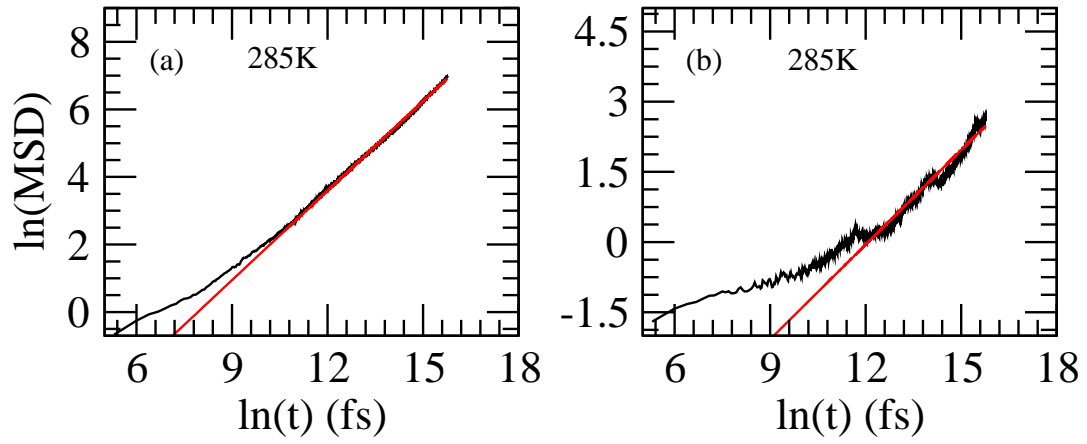
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FIG. 8: Black line represents log-log plot of mean-squared displacement (MSD) vs. time for (a) water and (b) trehalose for system S5 at temperature 285 K. The slope of the curve becomes unity once the molecules reach the diffusive regime. The red line has unit slope.