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Supplementary material

Coarse-grained Monte Carlo simulations of mucus: structure, dynamics and thermodynamics

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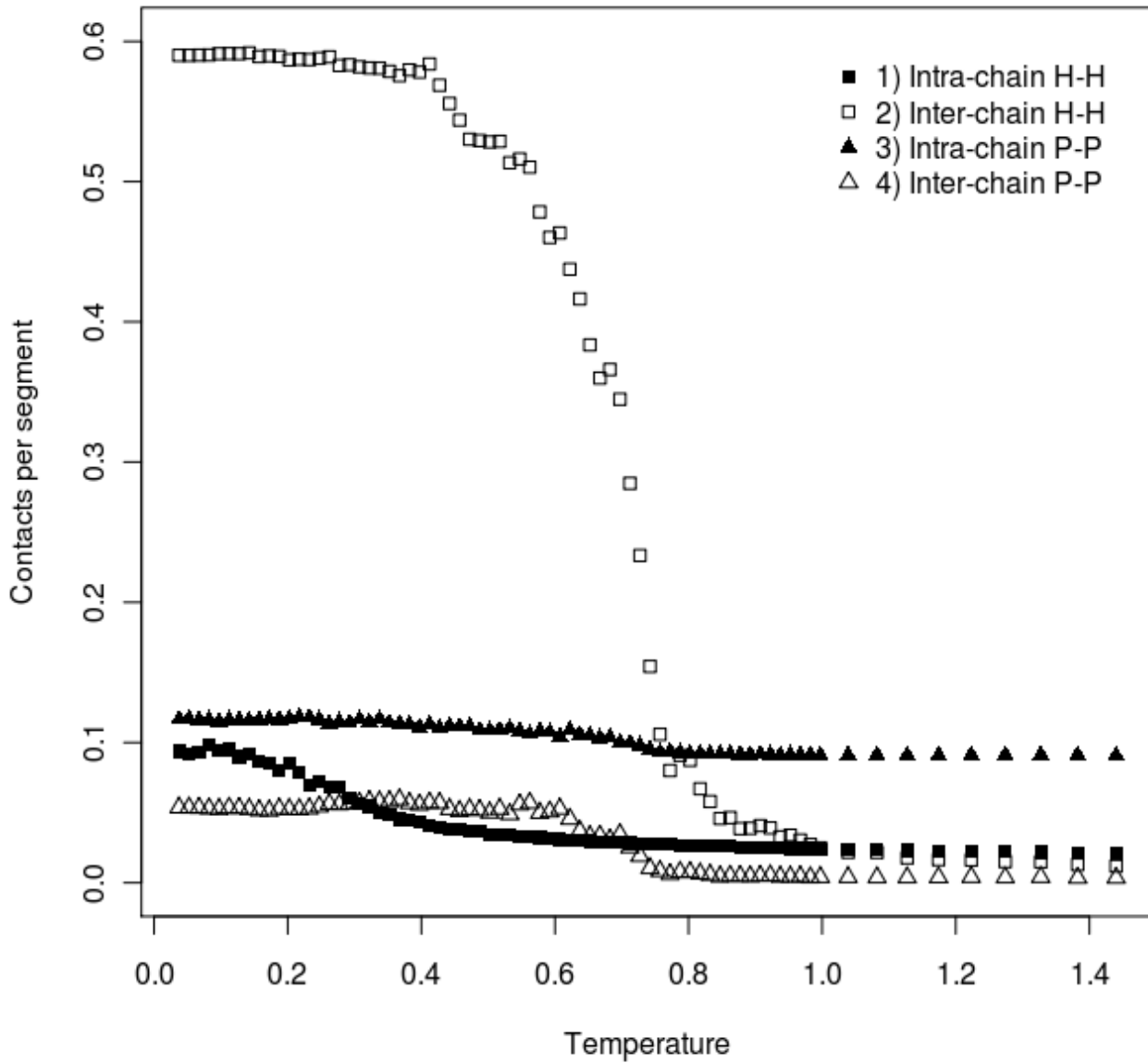


Fig.S1. Changes of the number of interactions per chain segment (see Methods) with temperature for System II at concentration of mucins $C=5\%$. Solid symbols denote intra-chain interaction, open inter-chain.

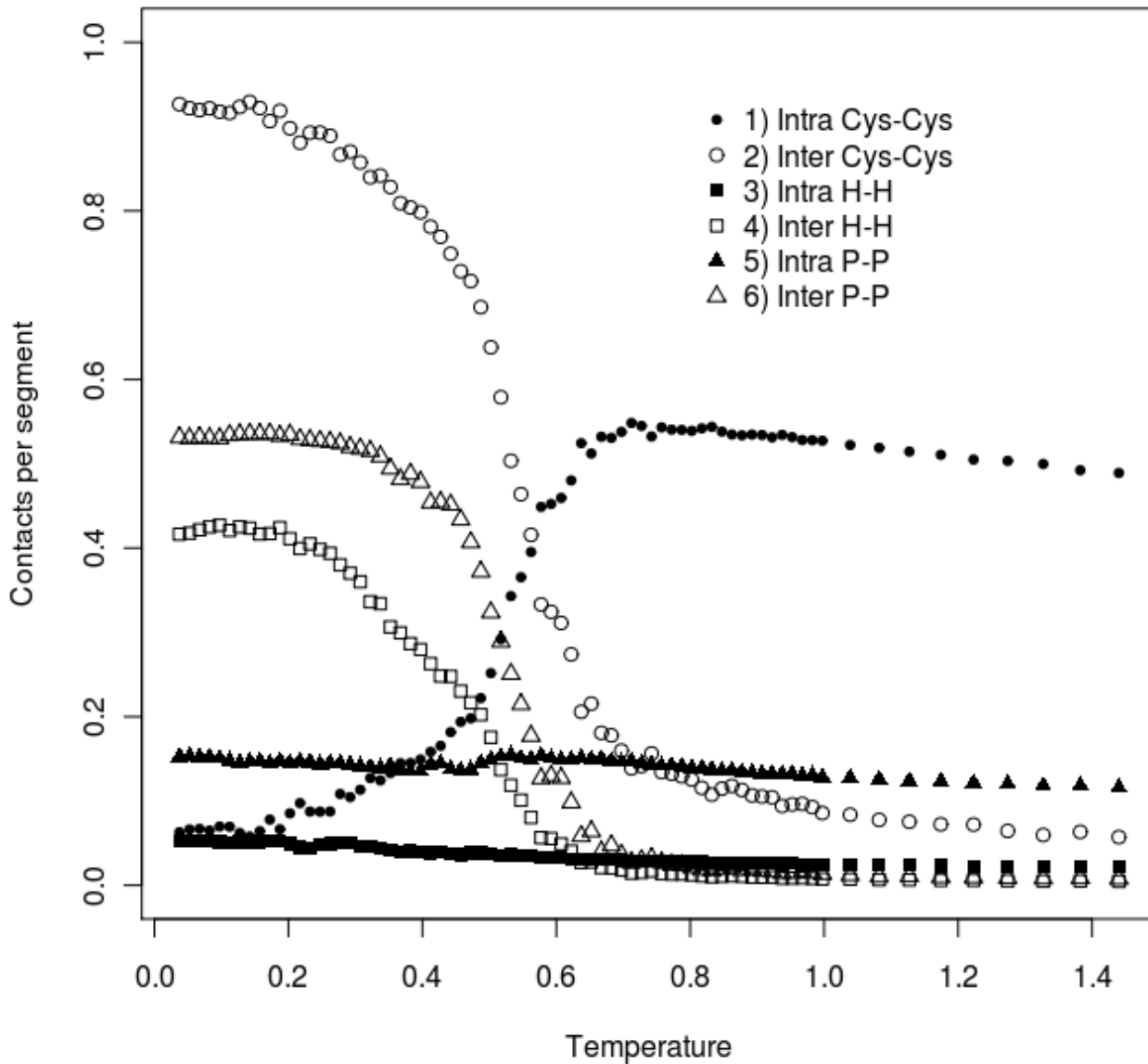


Fig.S2. Changes of the number of interactions per chain segment (see Methods) with temperature for System IV at concentration of mucins $C=5\%$. Solid symbols denote intra-chain interaction, open inter-chain.

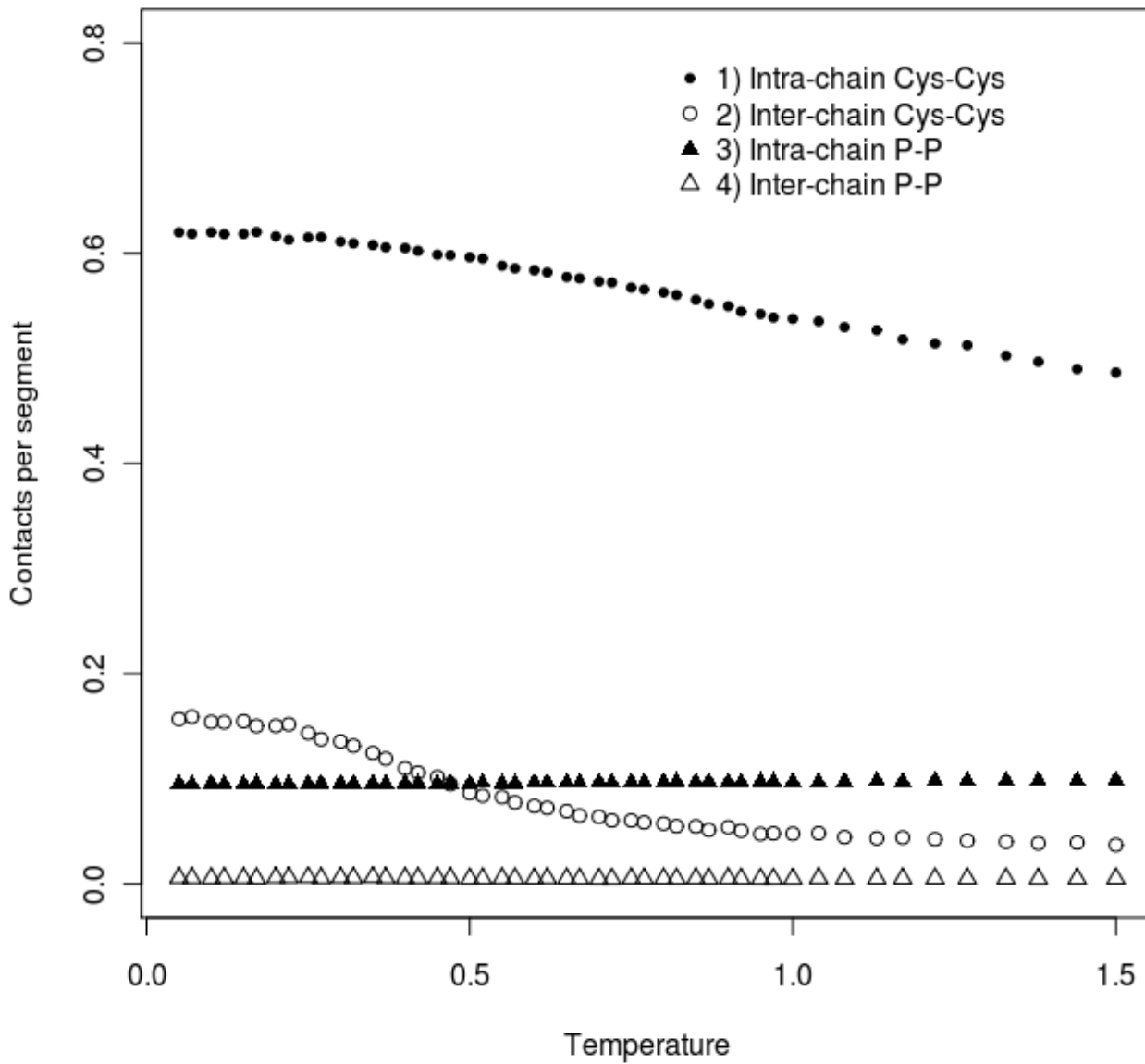


Fig.S3. Changes of the number of interactions per chain segment (see Methods) with temperature for System **III** at concentration of mucins $C=5\%$. Solid symbols denote intra-chain interaction, open inter-chain.

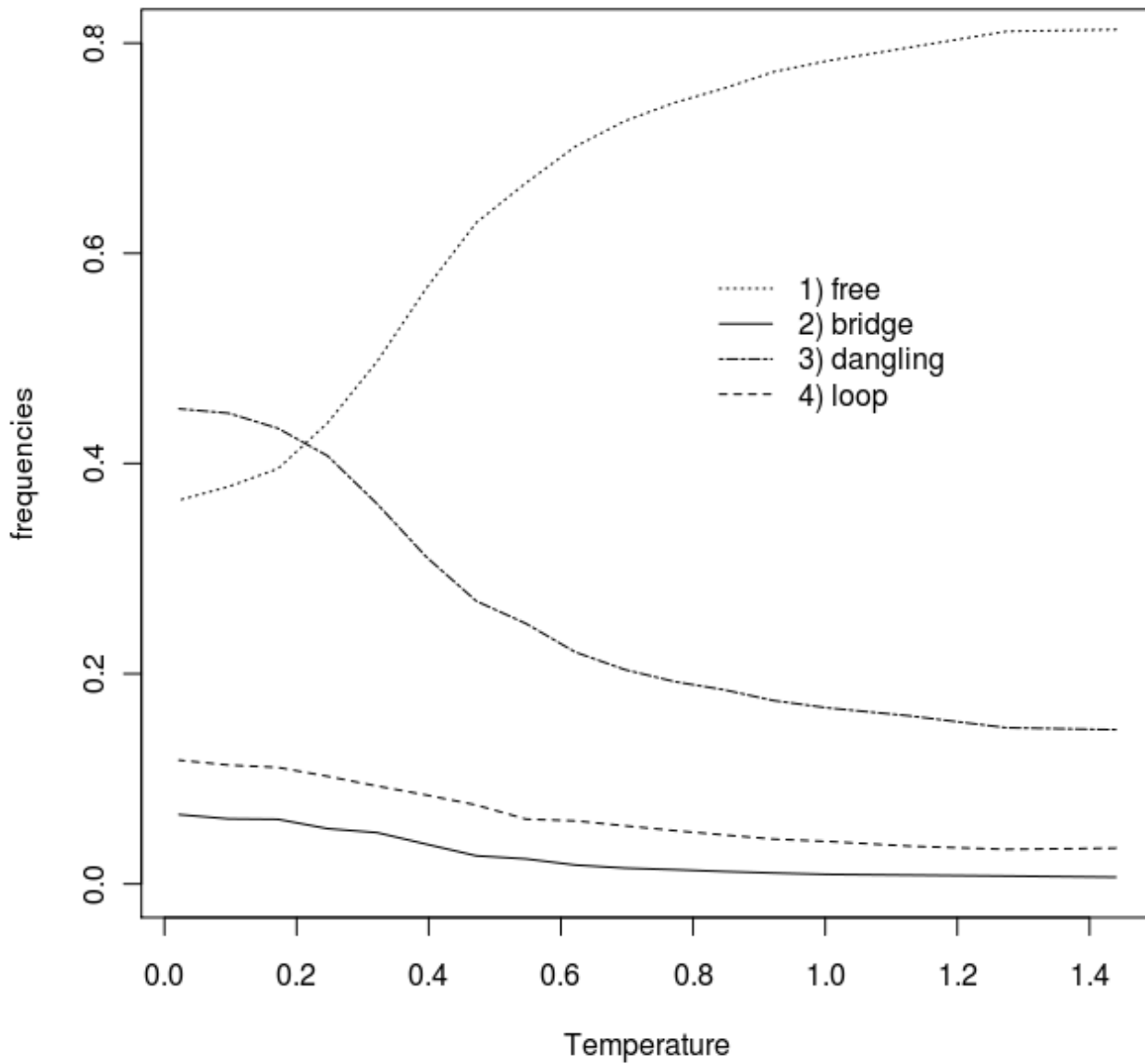


Fig.S4. Changes of the frequencies of various topologies of chain interactions (see Methods) with temperature for System **III** at concentration of mucins $C=5\%$.

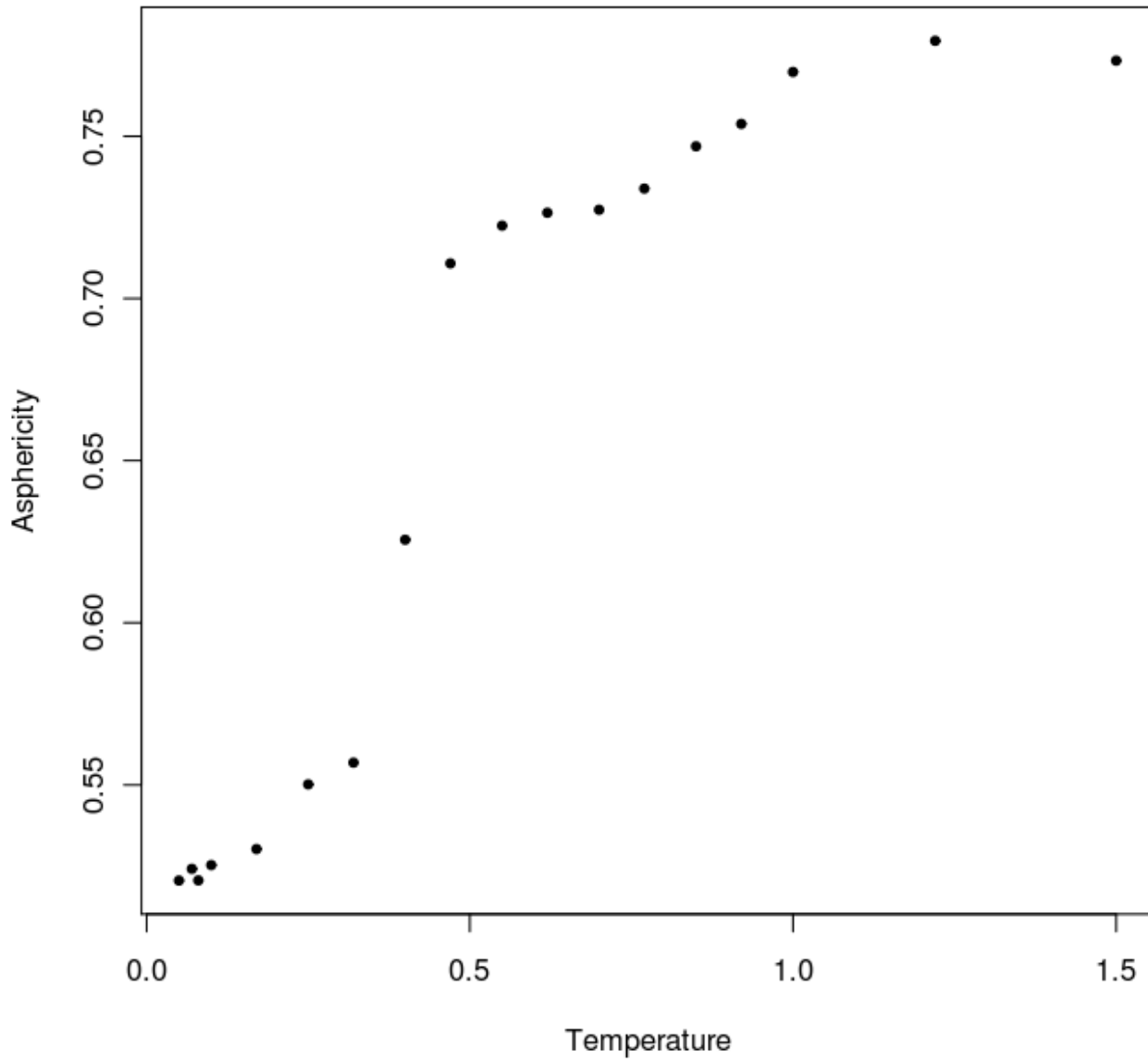


Fig.S5A. Changes of asphericity(see Methods) for the System I with temperature. Concentration of mucins is equal C=5%.

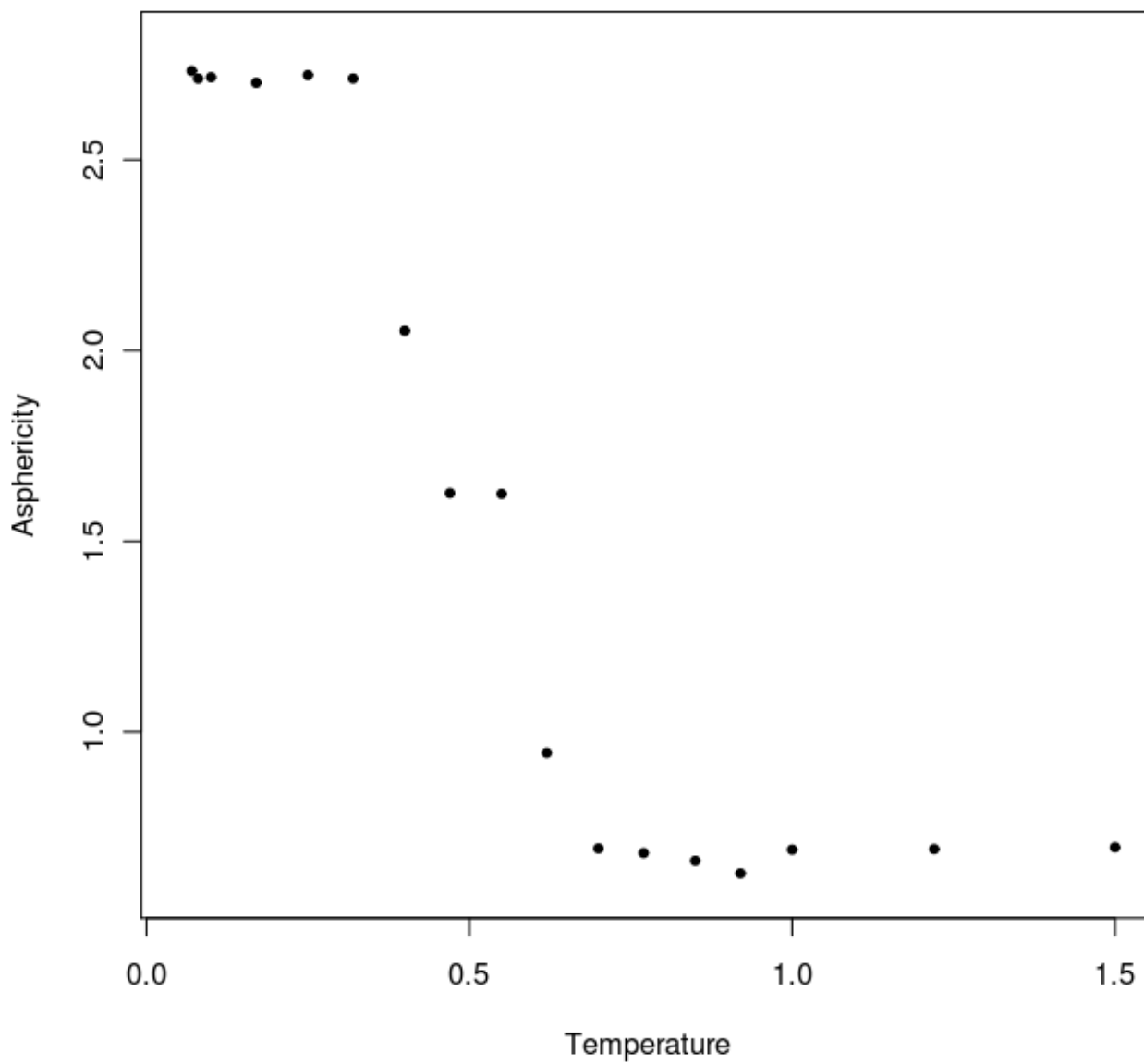


Fig.S5B. Changes of asphericity(see Methods) for the System **IV** with temperature. Concentration of mucins is equal $C=5\%$.

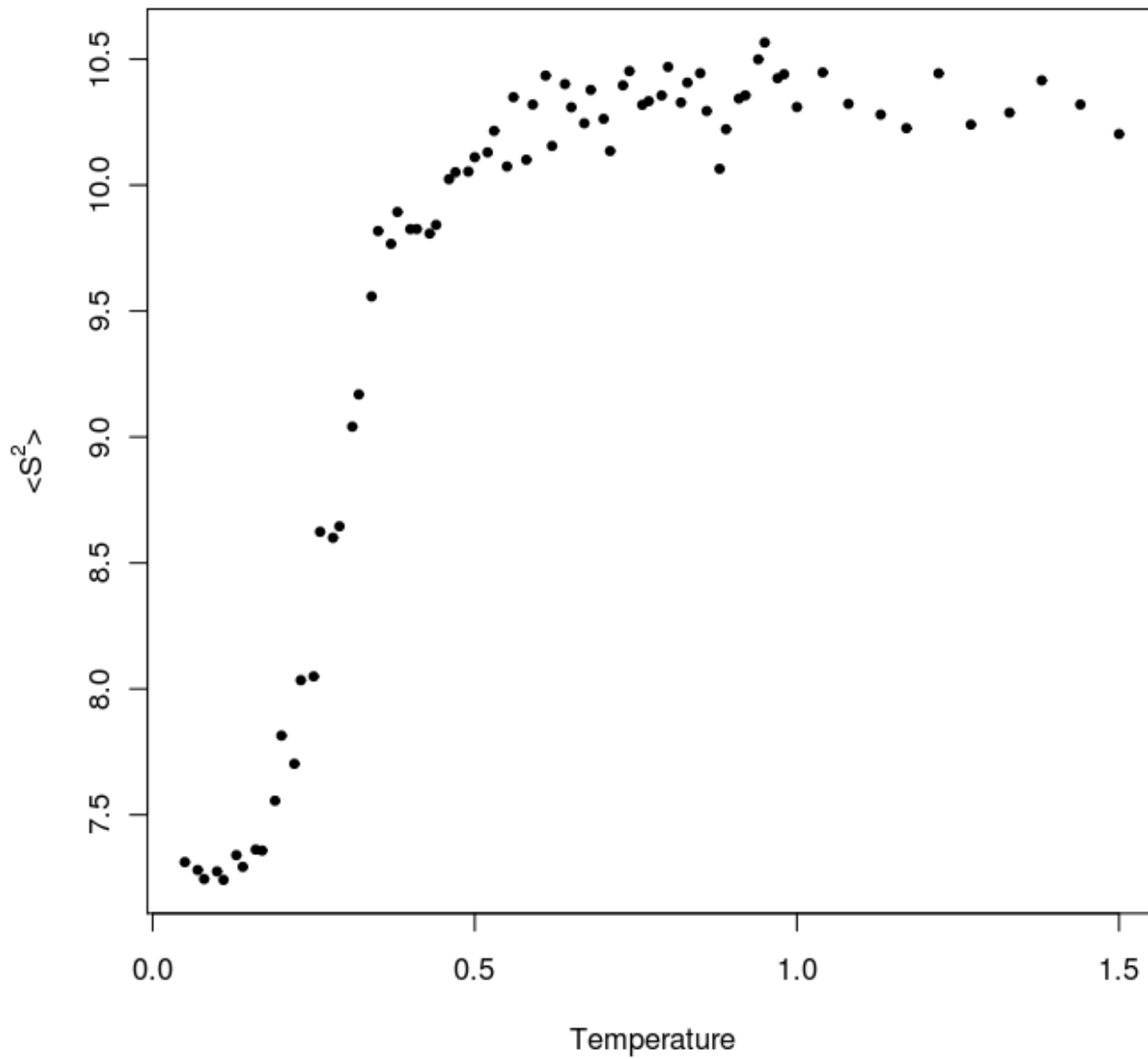


Fig.S6. Mean-square radius of gyration of entire mucin chain as a function of temperature. Concentration of the System **I** is equal $C=5\%$. Radius of gyration is expressed in Cartesian units (1 lattice unit = $\sqrt{2}$ Cartesian units).

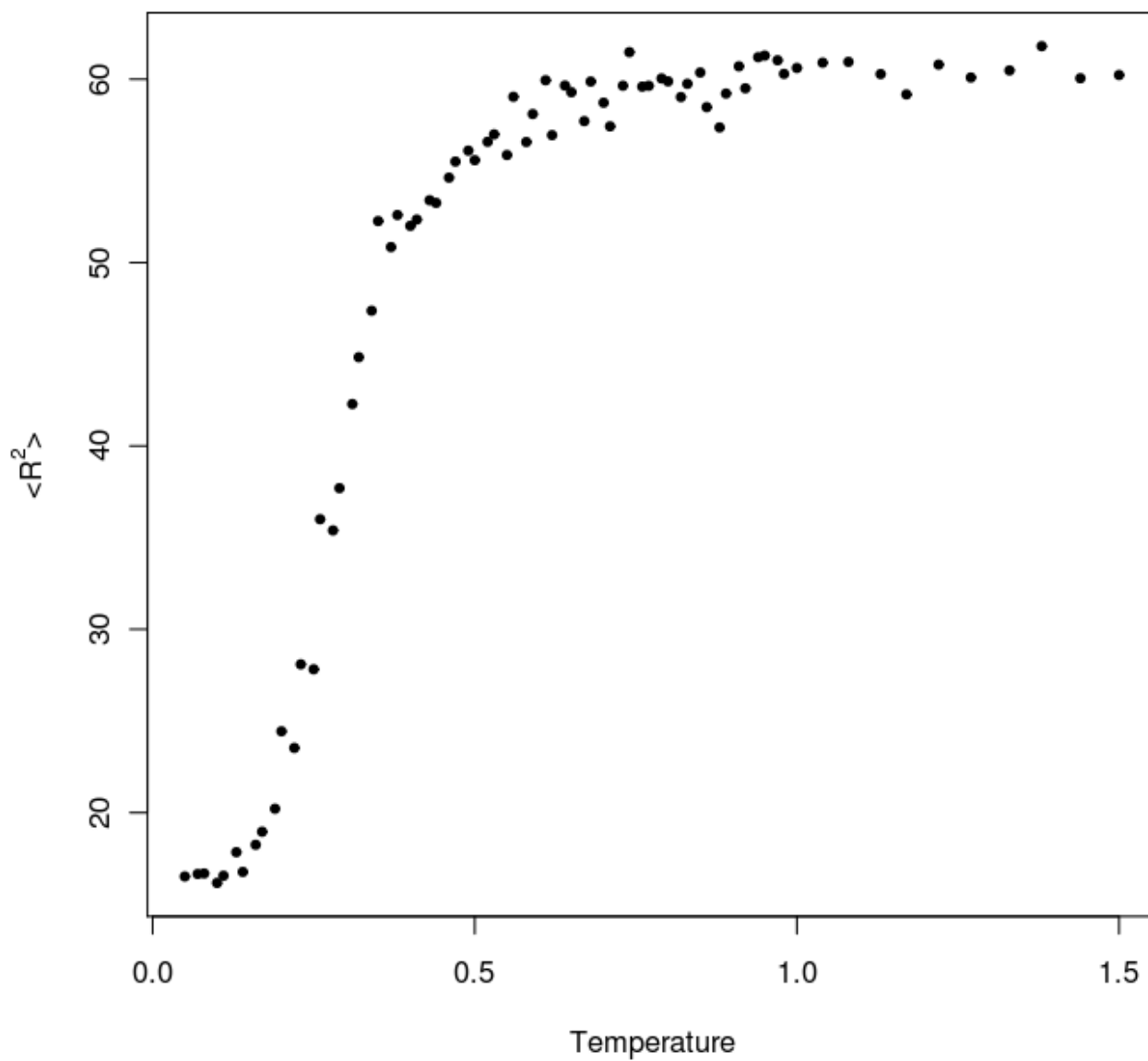


Fig.S7. Mean-square end-to-end distance of entire mucin chain as a function of temperature. Concentration of the System **I** is equal $C=5\%$. End-to-end distance is expressed in Cartesian units (1 lattice unit = $\sqrt{2}$ Cartesian units).

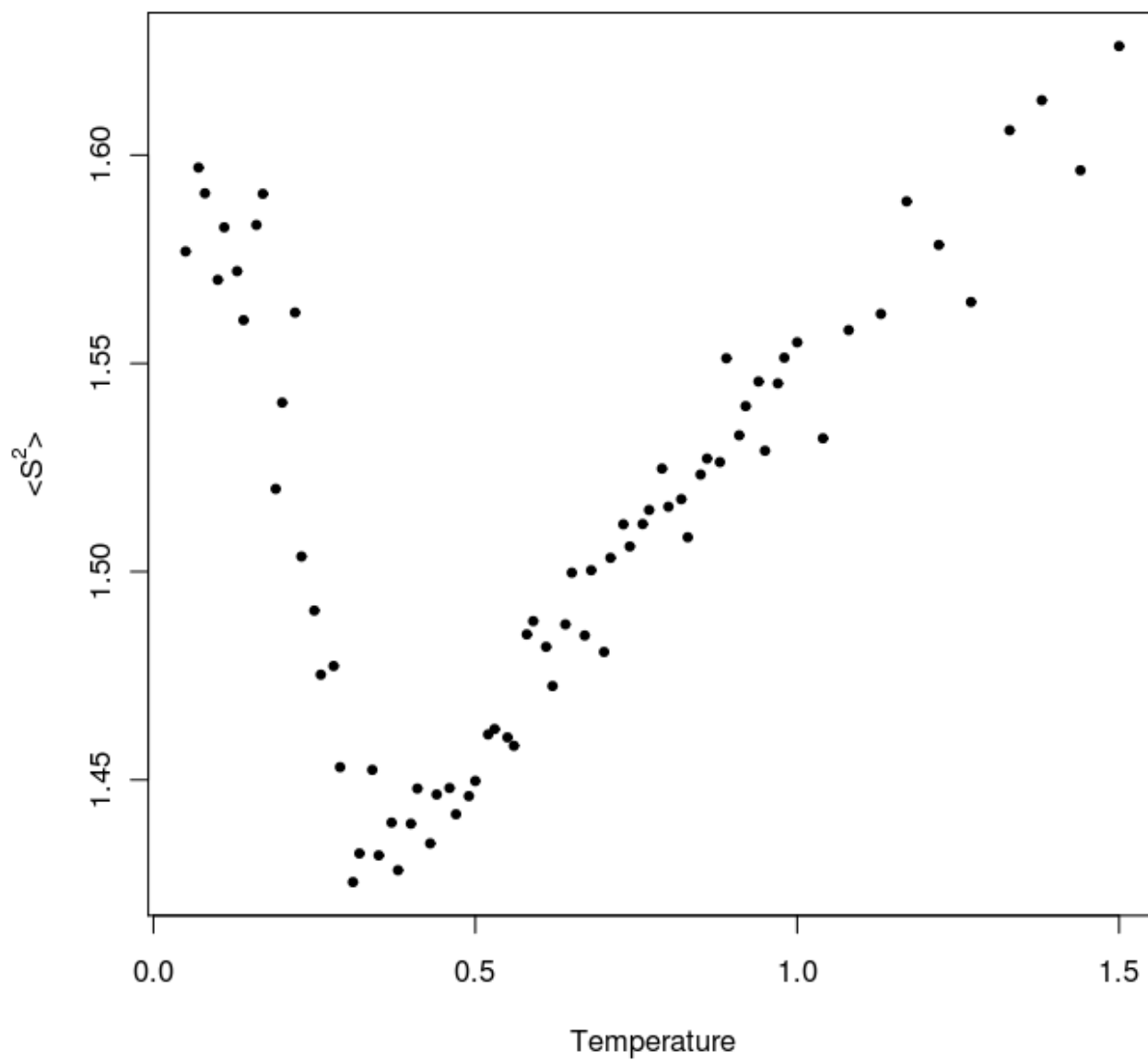


Fig.S8. Mean-square radius of gyration of the longer (positions form 1 to 5 in a mucin chain) hydrophobic sub-chain as a function of temperature. Concentration of the System I is equal $C=5\%$. Radius of gyration is expressed in Cartesian units (1 lattice unit = $\sqrt{2}$ Cartesian units).

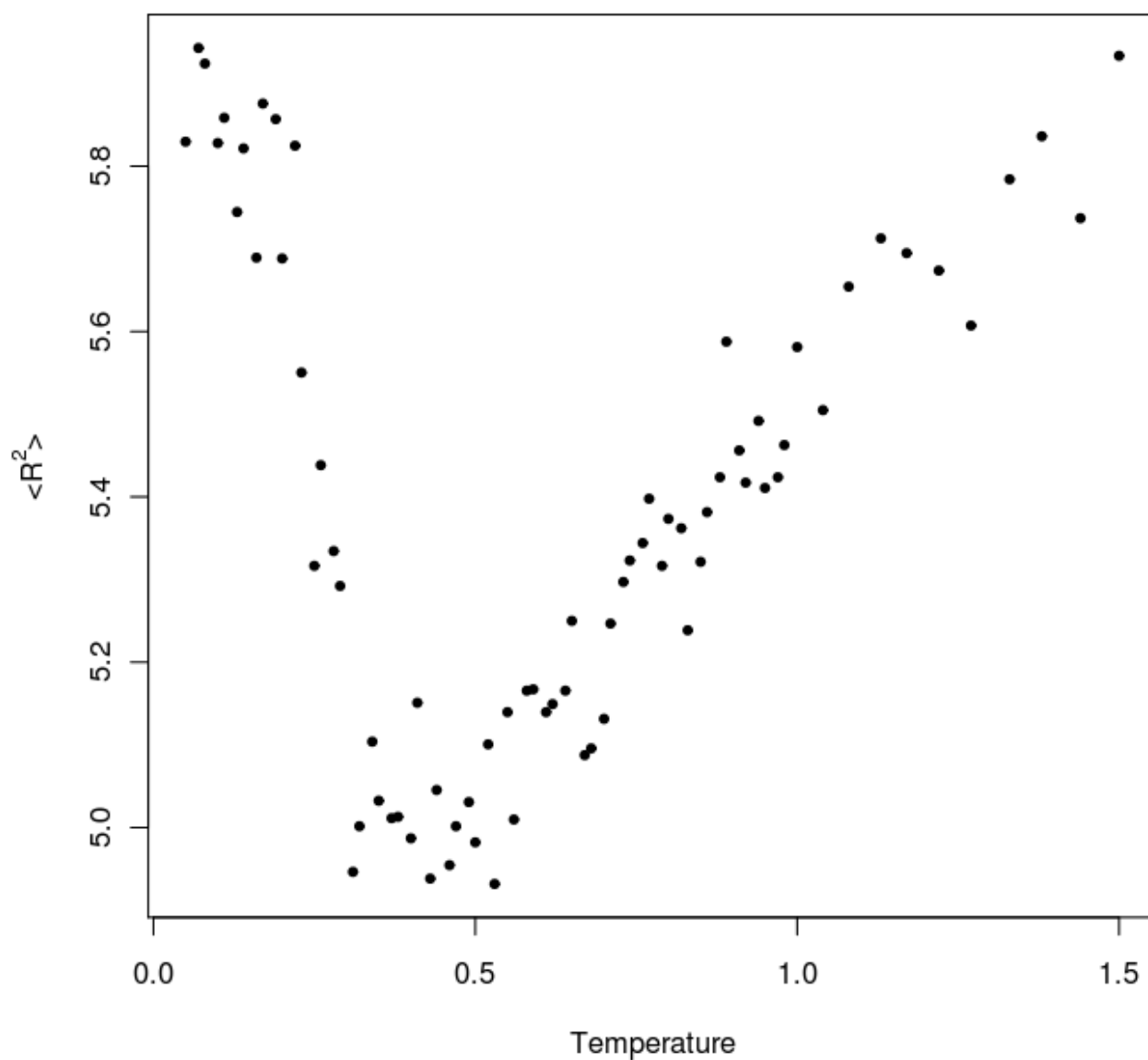


Fig.S9. Mean-square end-to-end distance of the longer (positions form 1 to 5 in a mucin chain) hydrophobic sub-chain as a function of temperature. Concentration of the System **I** is equal C=5%. End-to-end distance is expressed in Cartesian units (1 lattice unit = $\sqrt{2}$ Cartesian units).

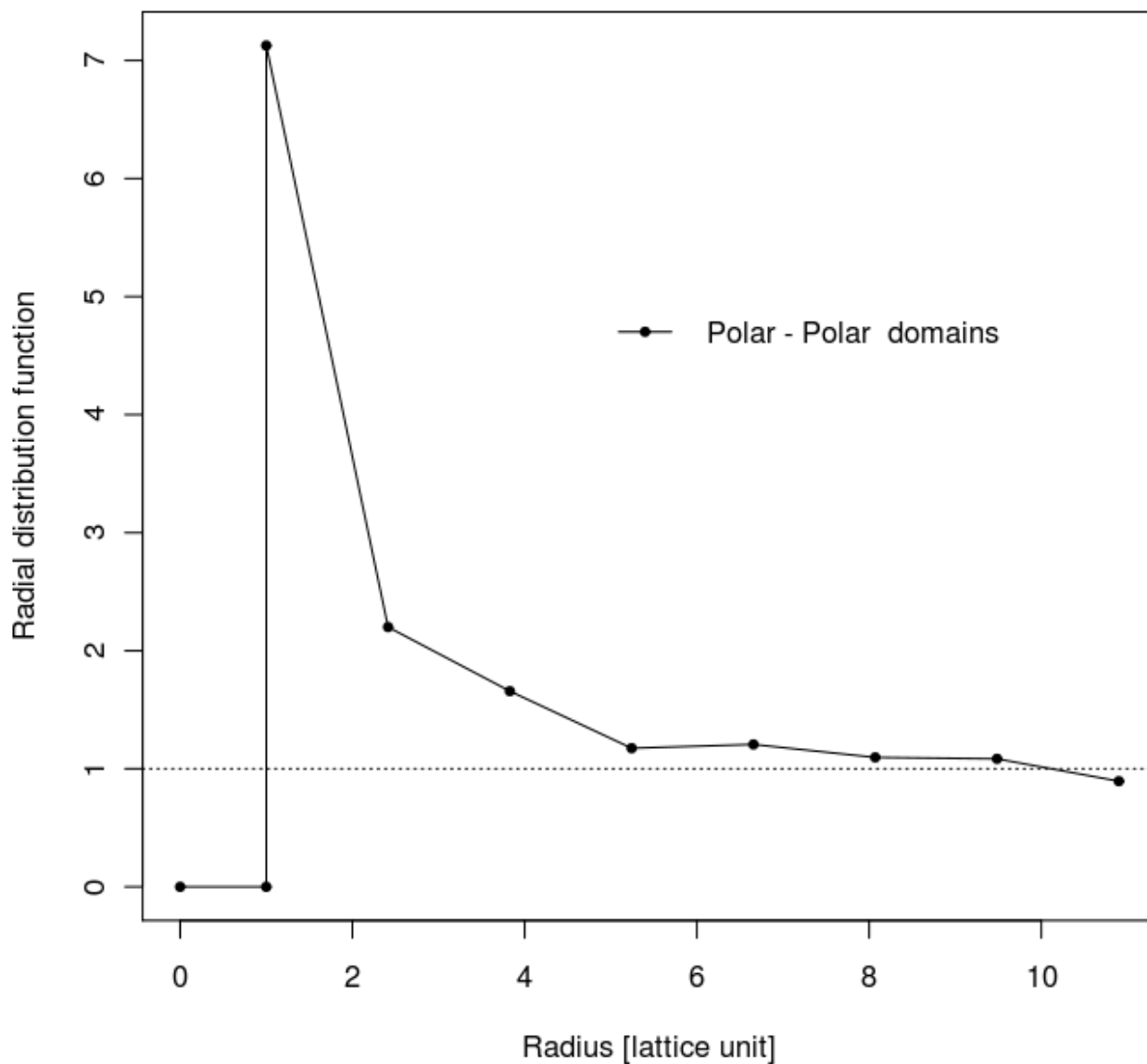


Fig.S10. Radial distribution function (RDF) for polar domains at temperature $T=0.2$ for System I at concentration of mucins $C=5\%$. RDF equal to 1.0 means uniform, random distribution. One lattice unit corresponds to about 25nm in the real system.

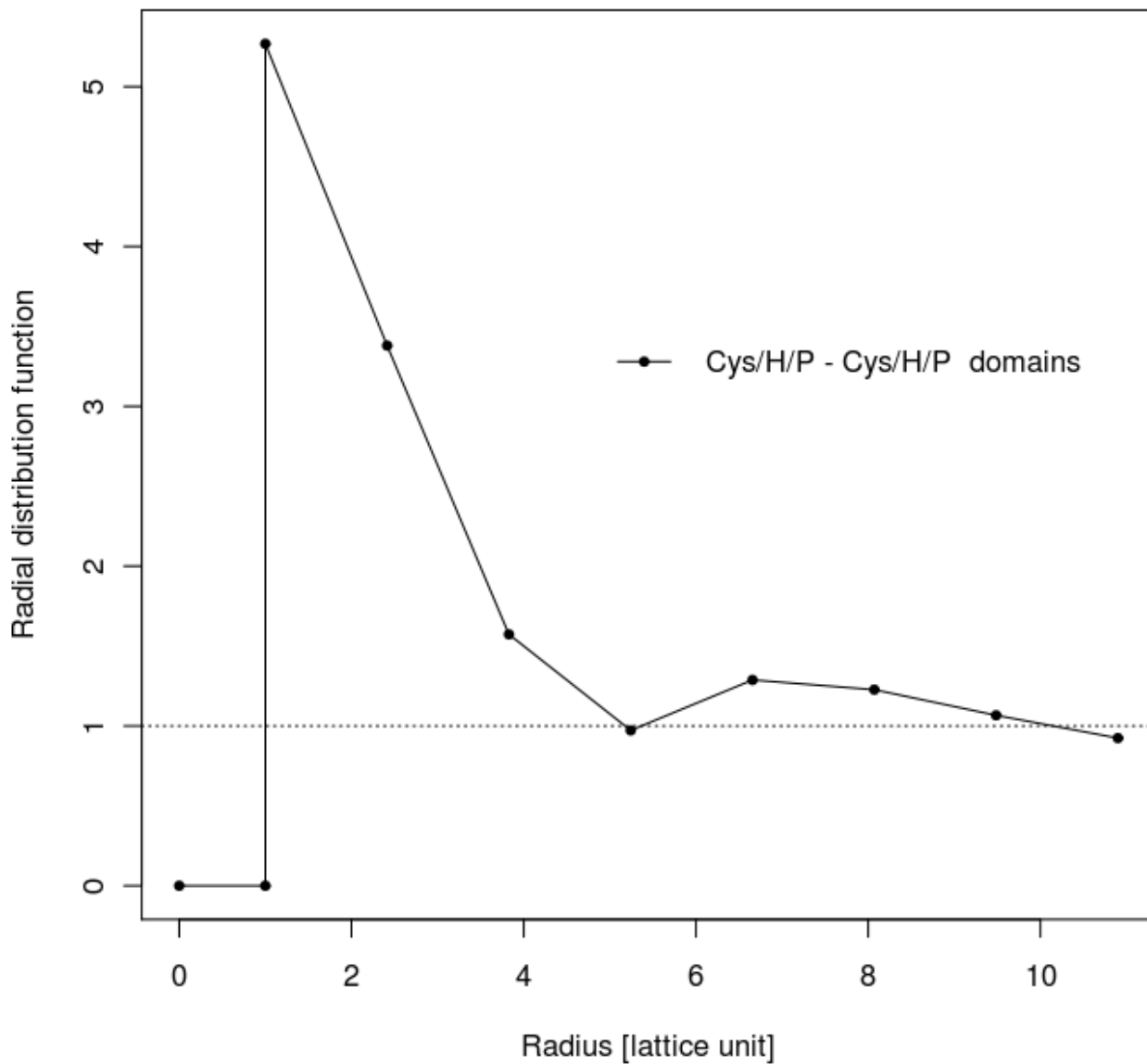


Fig.S11. Radial distribution function (RDF) for all domains at temperature $T=0.2$ for System **I** at concentration of mucins $C=5\%$. RDF equal to 1.0 means uniform, random distribution. One lattice unit corresponds to about 25nm in the real system.

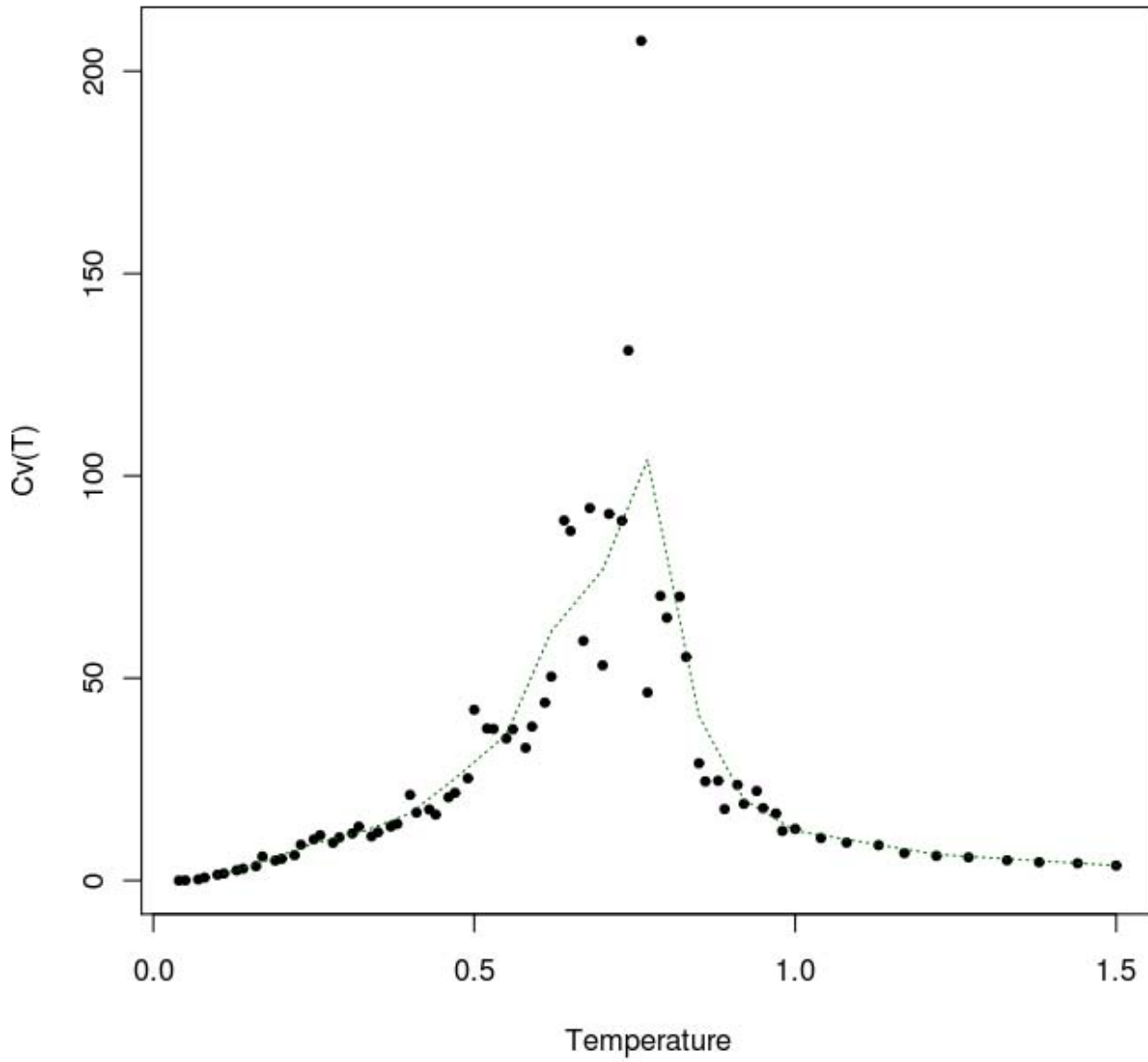


Fig.S12. Heat capacity as a function of temperature for concentration of mucins $C=5\%$ and System II. The dotted line represents smoothed data obtained by averaging of 5 consecutive black filled circles. The transition temperature is about 0.77.

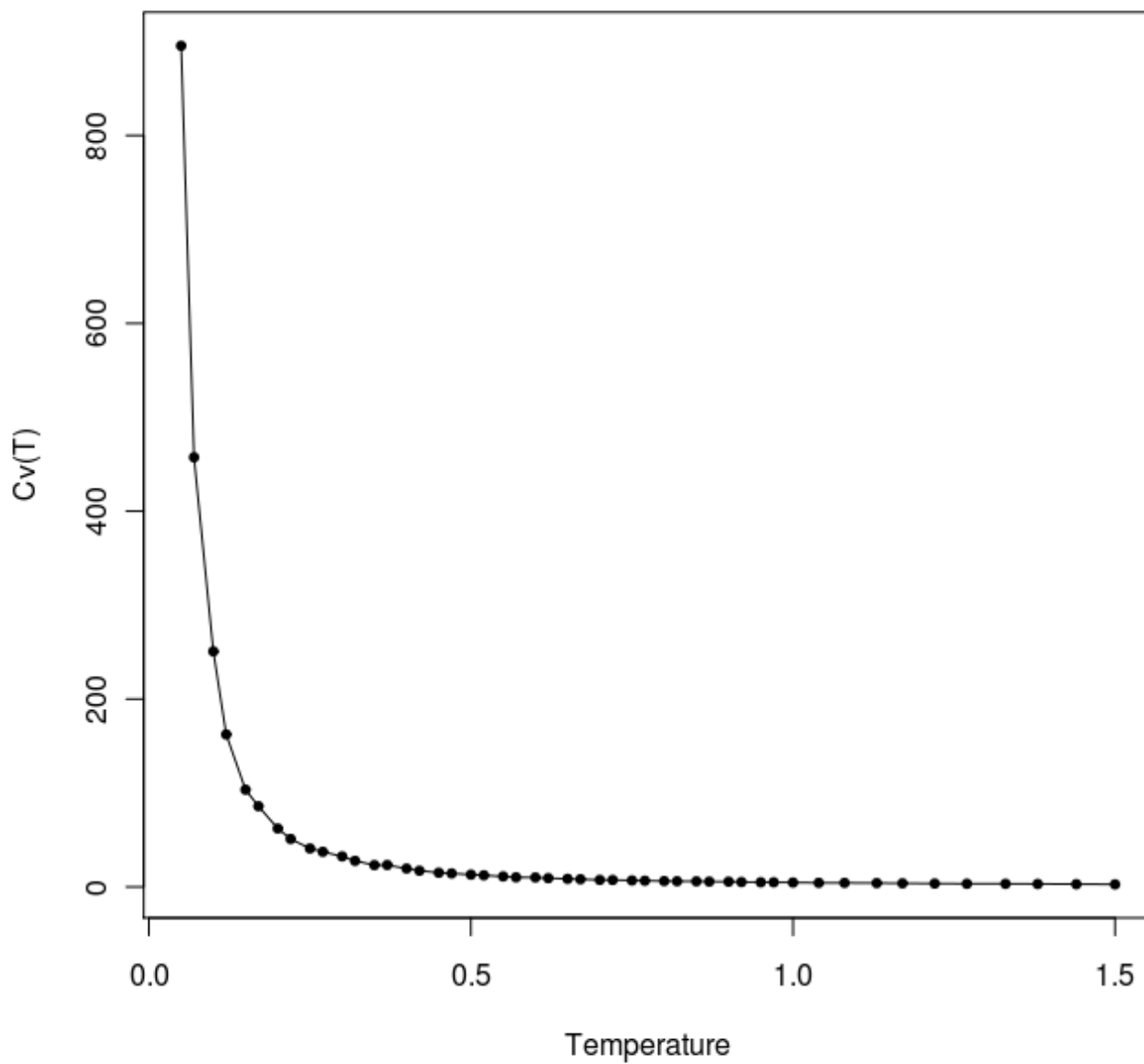


Fig.S13. Heat capacity as a function of temperature for concentration of mucins $C=5\%$ and System **III**. The peak near $T=0.0$ is caused by numerical issues (dividing dispersion of energy by T^2), not by sol-gel transition.

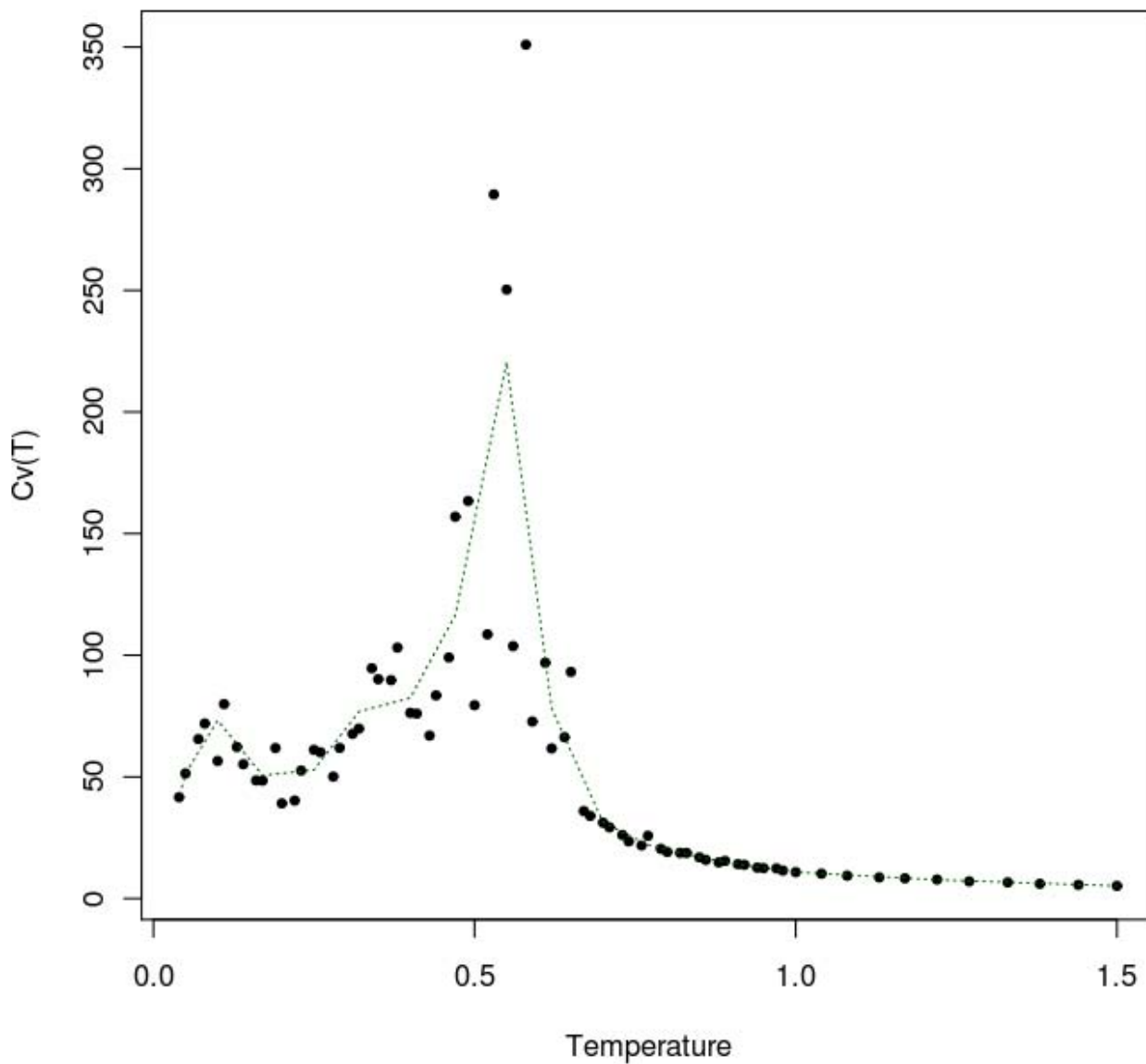


Fig.S14. Heat capacity as a function of temperature for concentration of mucins $C=5\%$ and System **IV**. The dotted line represents smoothed data obtained by averaging of 5 consecutive black filled circles. The transition temperature is about 0.55.