Supplementary Material

The effect of different cutoff schemes in molecular simulations of proteins

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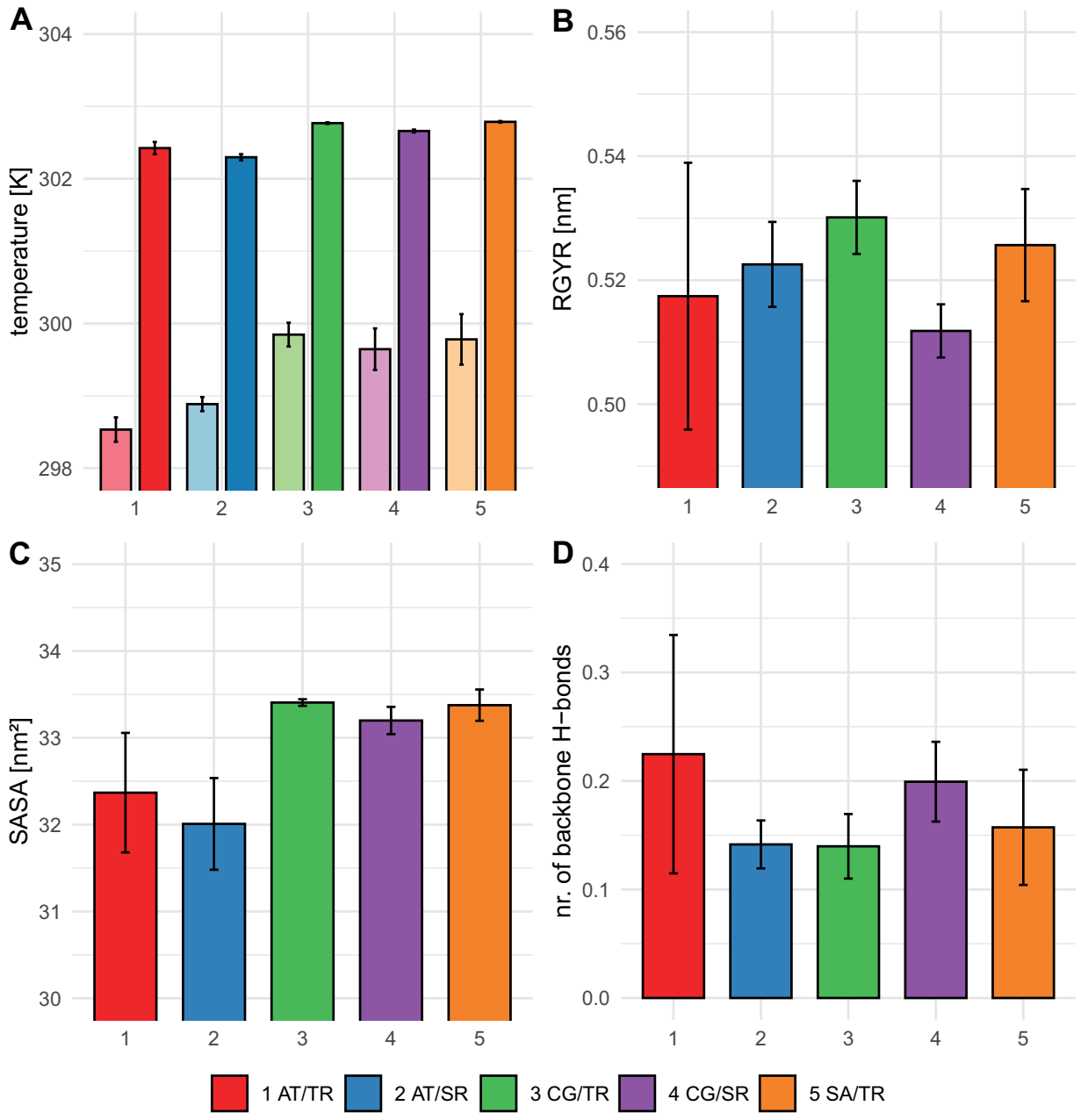

Figure S1: Simulations of ALA_5 using five different cutoff settings, with average temperature of the solute (light colours) and solvent (dark colours) in panel A, the radius of gyration in panel B, the solvent accessible surface area (SASA) in panel C and the number of backbone hydrogen bonds in panel D.

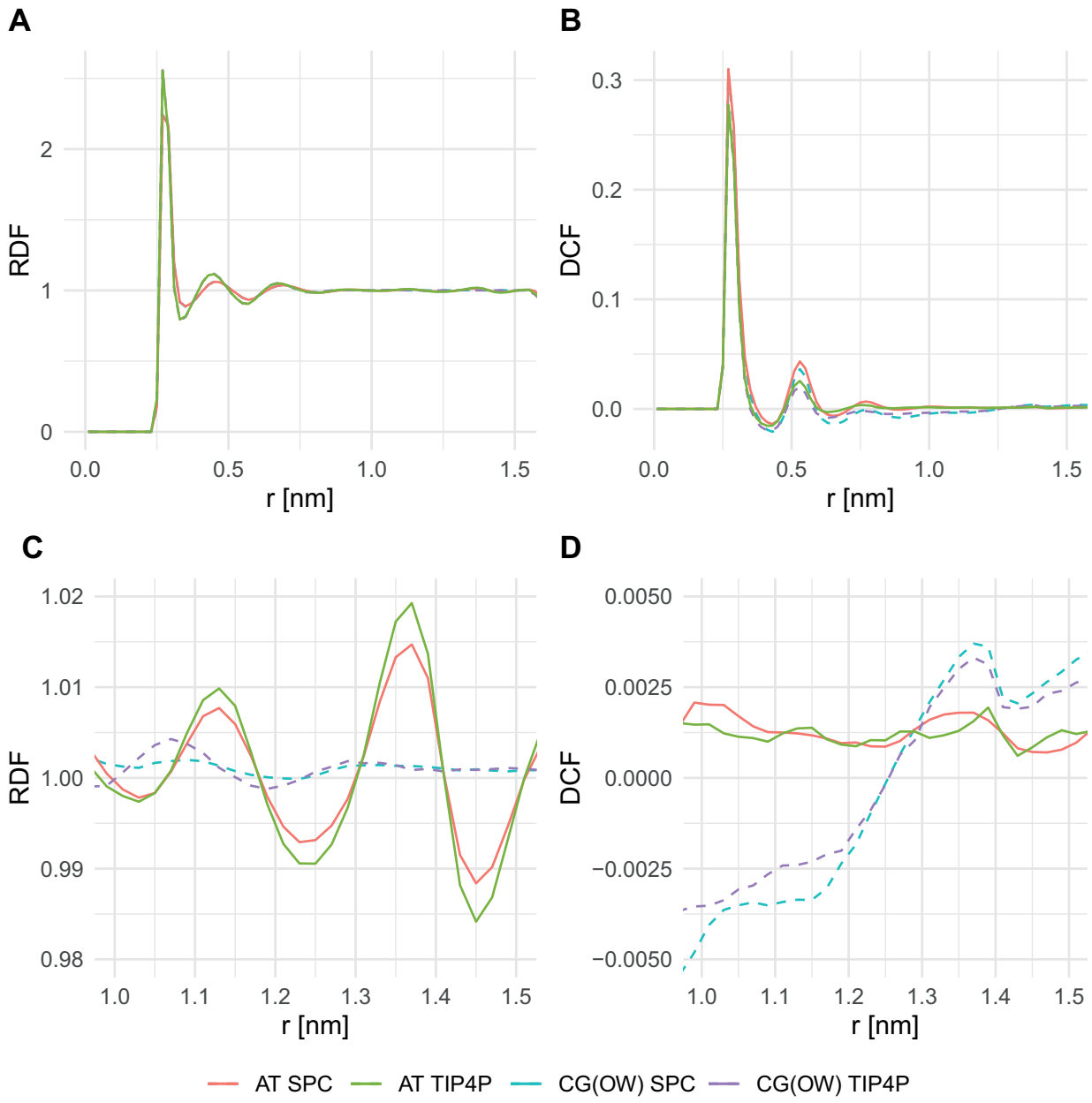

Figure S2: Radial distribution function of water oxygen atoms (A) and dipole correlations function for water (B), comparing SPC and TIP4P water models. Panels (C) and (D) zoom in to the region around the cutoff (1.4 nm).