Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

The role of hydrophobic hydration on the LCST behaviour of $POEGMA_{300}$ by all-atom molecular dynamics simulation

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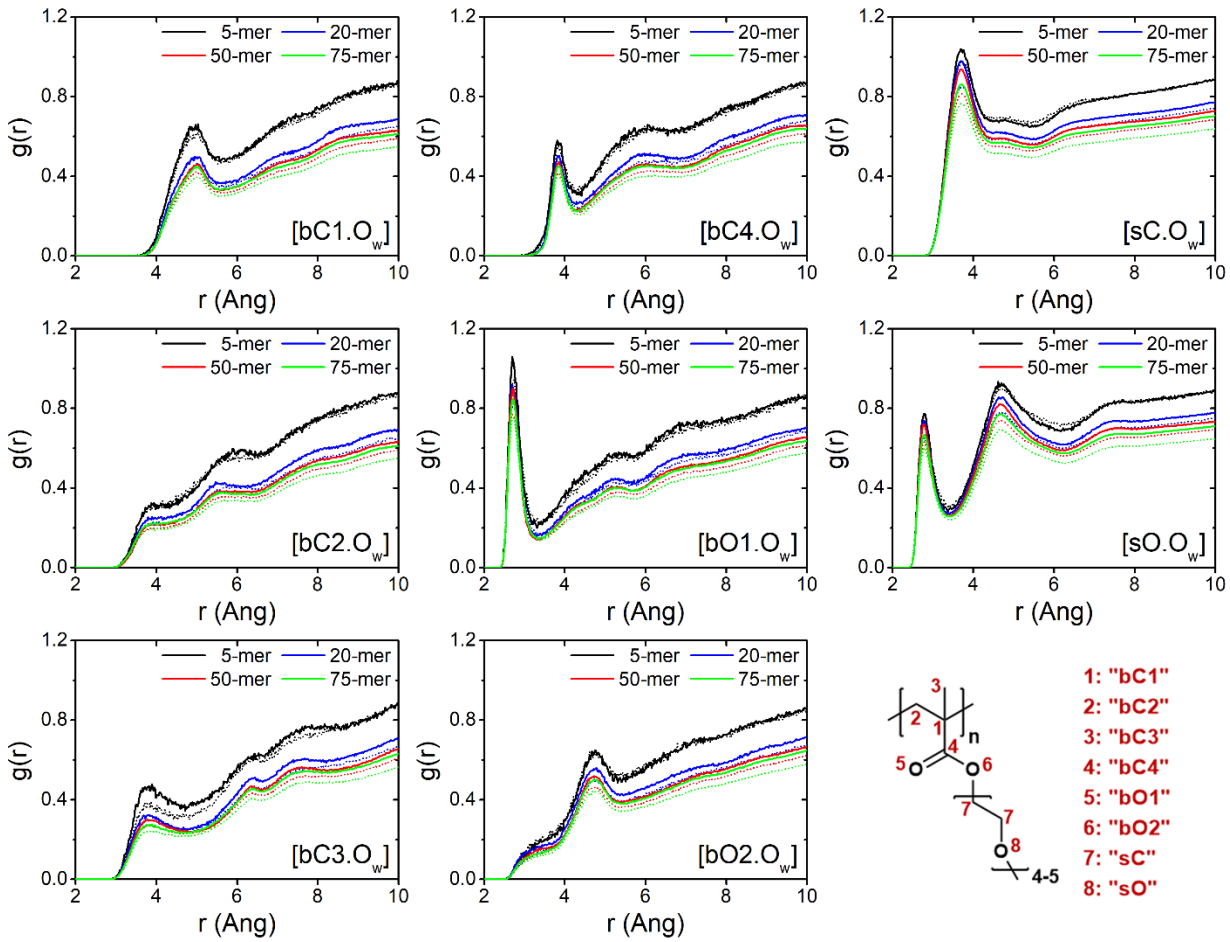

Fig. S1 Radial distribution functions between selected $POEGMA_{300}$ atoms and water oxygen atoms (O_w) at T < LCST (307 K, solid lines) and T > LCST (350 K, short dot lines).

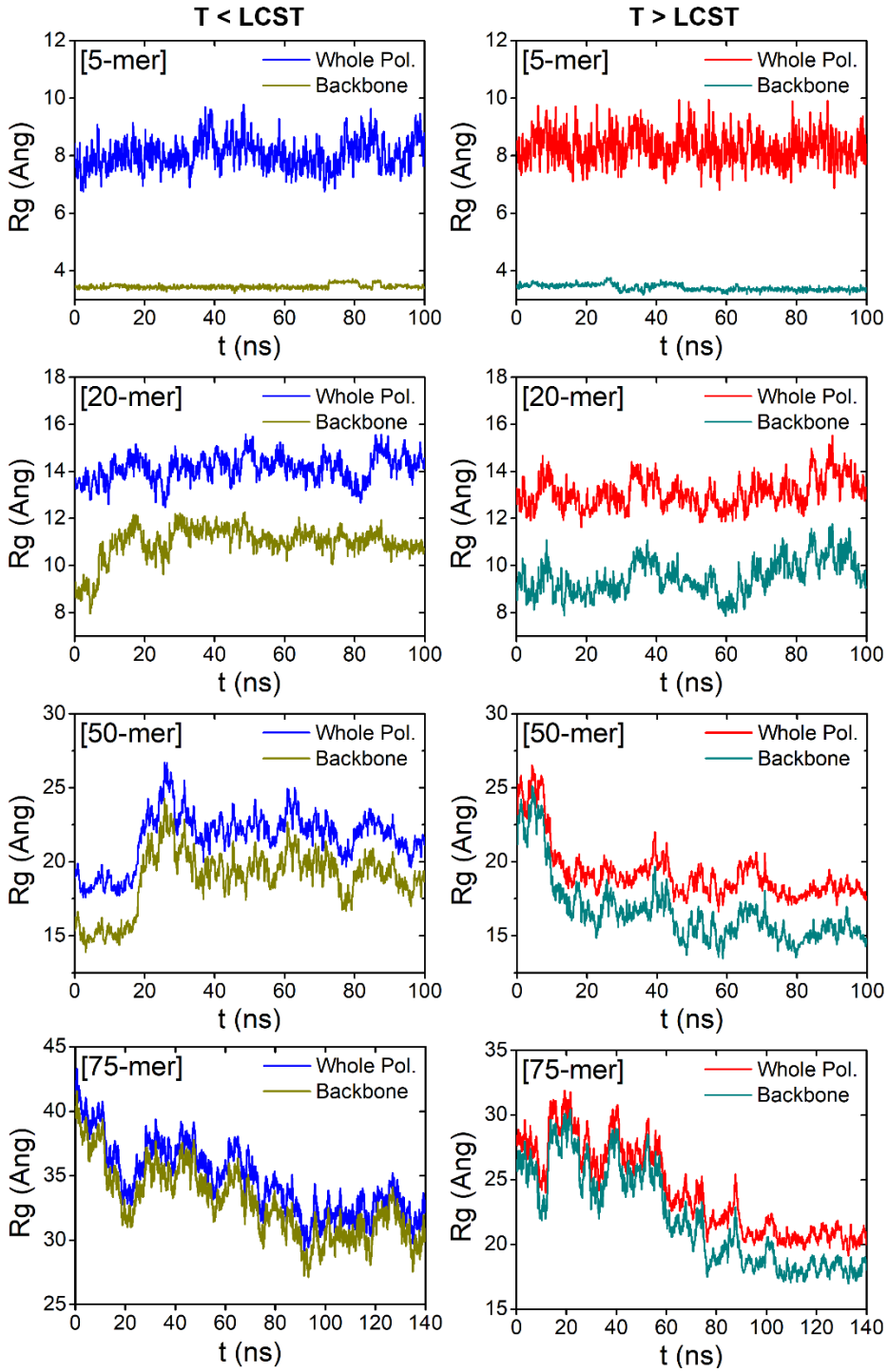

Fig. S2 Time-dependent radius of gyration (R_g) variations of 5-, 20-, 50- and 75-mer $POEGMA_{300}$ polymers for the whole polymer and backbone at T<LCST 307 K) and T>LCST (350 K).

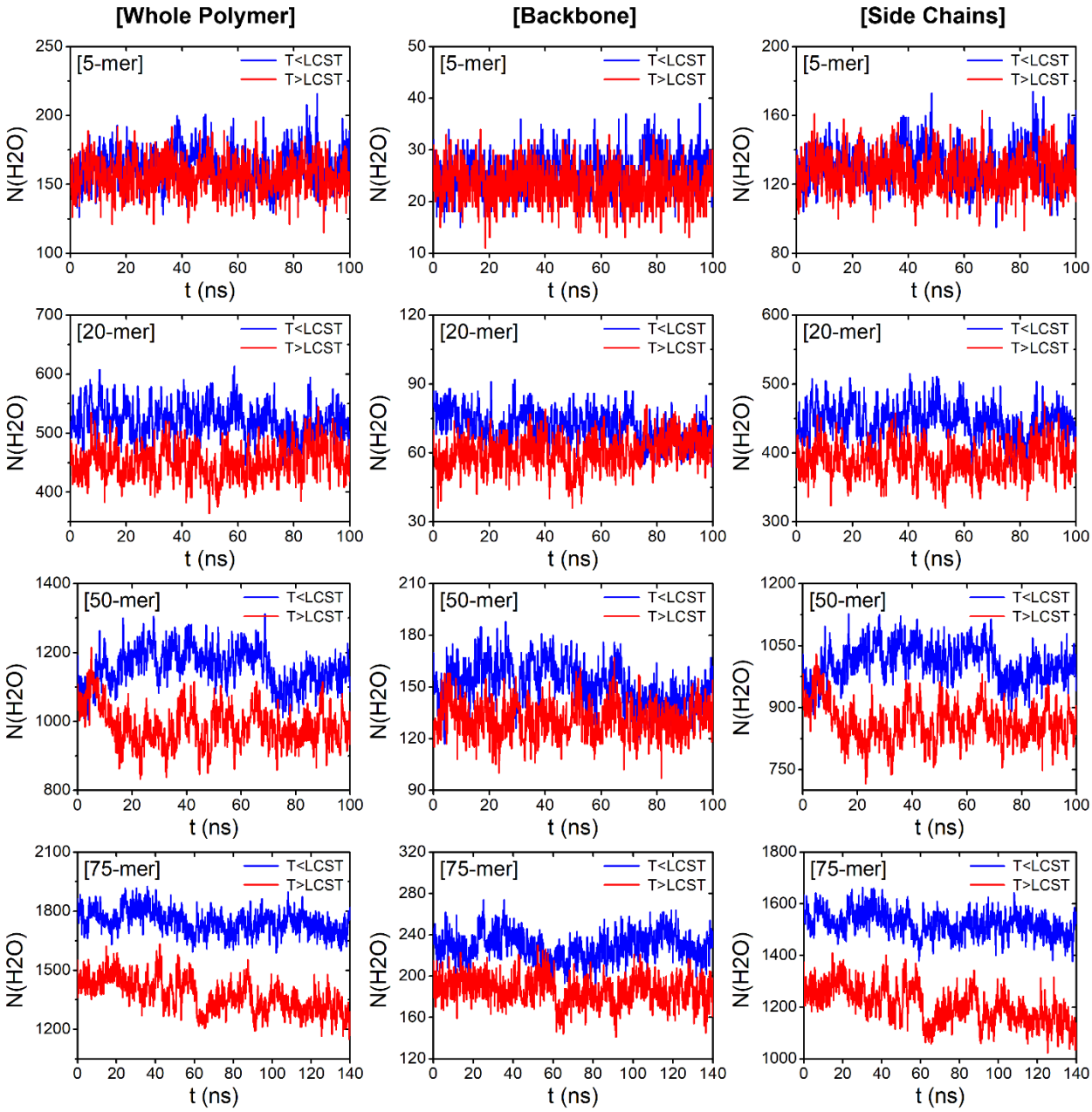

Fig. S3 Time-dependent number of first shell water molecules variations of 5-, 20-, 50- and 75-mer $POEGMA_{300}$ polymers at T<LCST (307 K) and T>LCST (350 K) for whole polymer, backbone and oligo(ethylene glycol) side chains.