

Supporting information for “Osmolyte-induced Collapse of a Charged Macromolecule”

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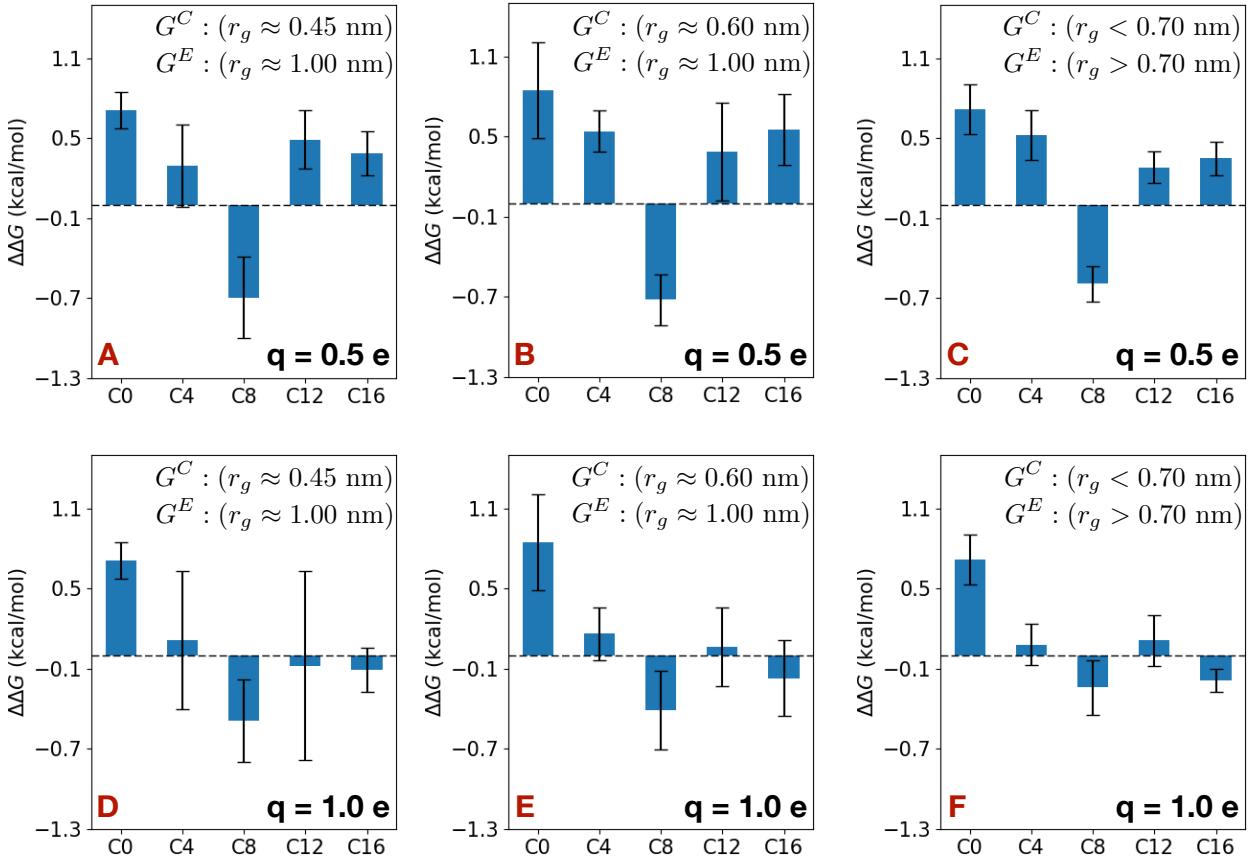


Figure S1: Change in free energy of the polymer in aqueous solution of 0.5 M TMAO with respect to neat water ($\Delta\Delta G$) along different charge-neutral polymers with increasing number of charged beads with charge density (A), (B), (C) $|q| = 0.5$ e and (D), (E), (F) $|q| = 1.0$ e with different definitions of collapsed (C) and extended (E) state of polymers.

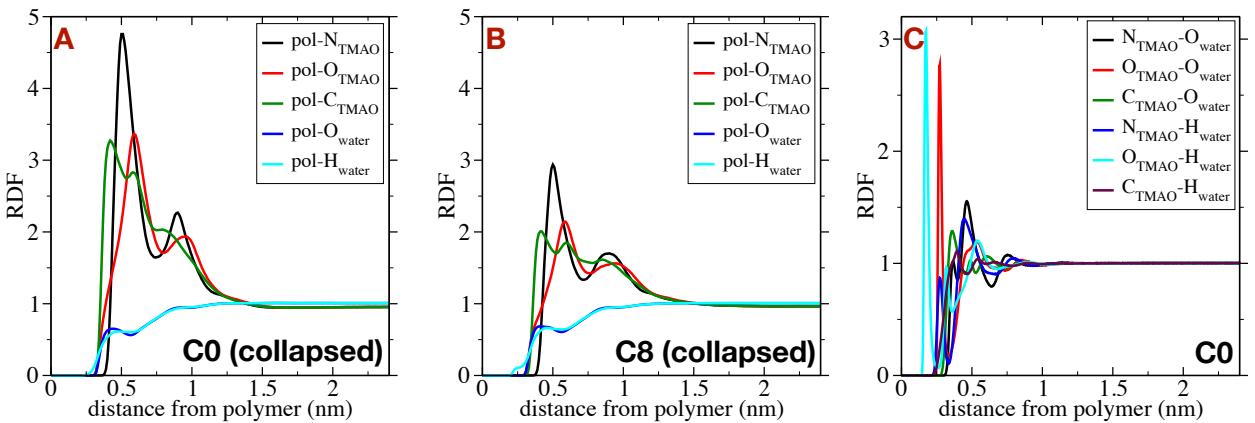


Figure S2: The radial distribution functions (RDF) between any polymer bead and N, O and C atom of TMAO and O and H atom of water for (A) purely hydrophobic polymer (C0) and (B) charge-neutral polymer with eight charged beads in collapsed configuration. (C) The RDFs between different atoms of TMAO and water for purely hydrophobic polymer.

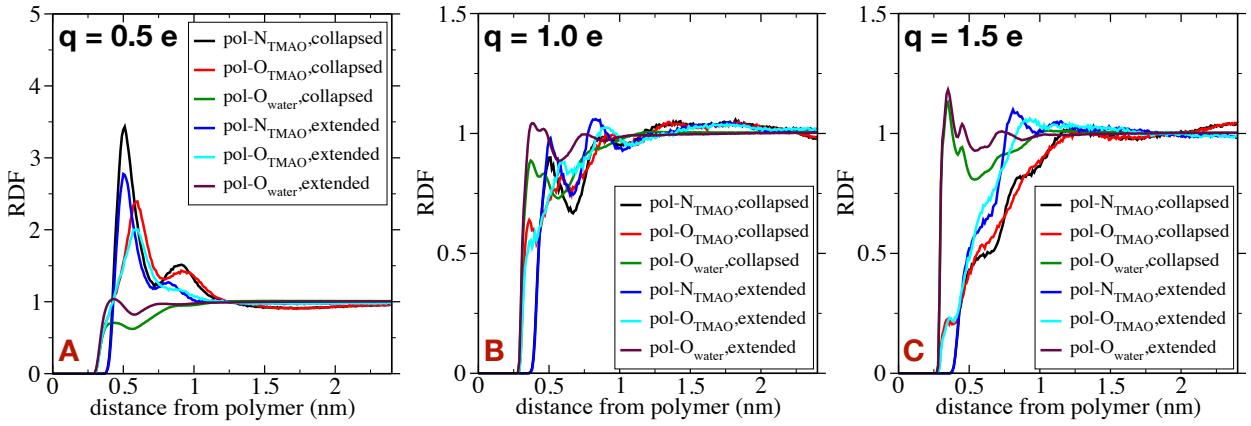


Figure S3: The radial distribution functions (RDF) between any polymer bead and N or O atom of TMAO and polymer bead-O atom of water for charge-neutral polymer (C12) with charge density (A) $|q| = 0.5$ e, (B) $|q| = 1.0$ e and (C) $|q| = 1.5$ e.

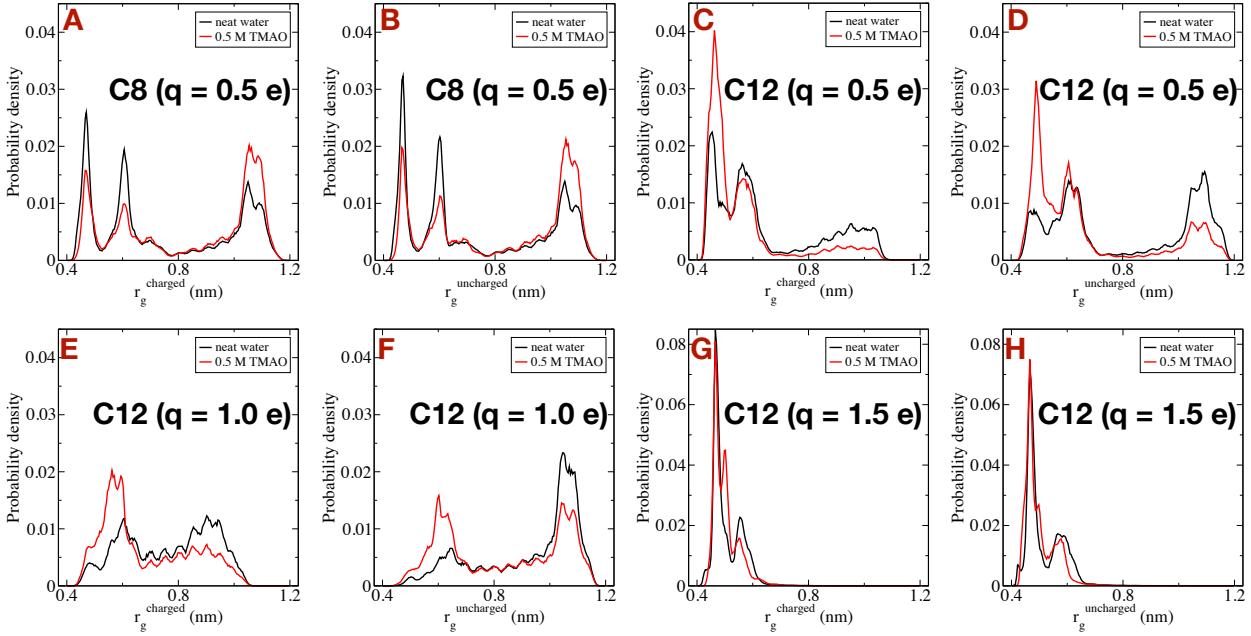


Figure S4: Probability density of radius of gyration of charged ($r_g^{charged}$) and uncharged ($r_g^{uncharged}$) beads of the polymers separately for the case of C8 with charge density $|q| = 0.5$ e (A and B), C12 with charge density $|q| = 0.5$ e (C and D), C12 with charge density $|q| = 1.0$ e (E and F) and C12 with charge density $|q| = 1.5$ e (G and H).