

Supplemental information for

Influence of the sterol aliphatic side chain on membrane properties: a molecular dynamics study

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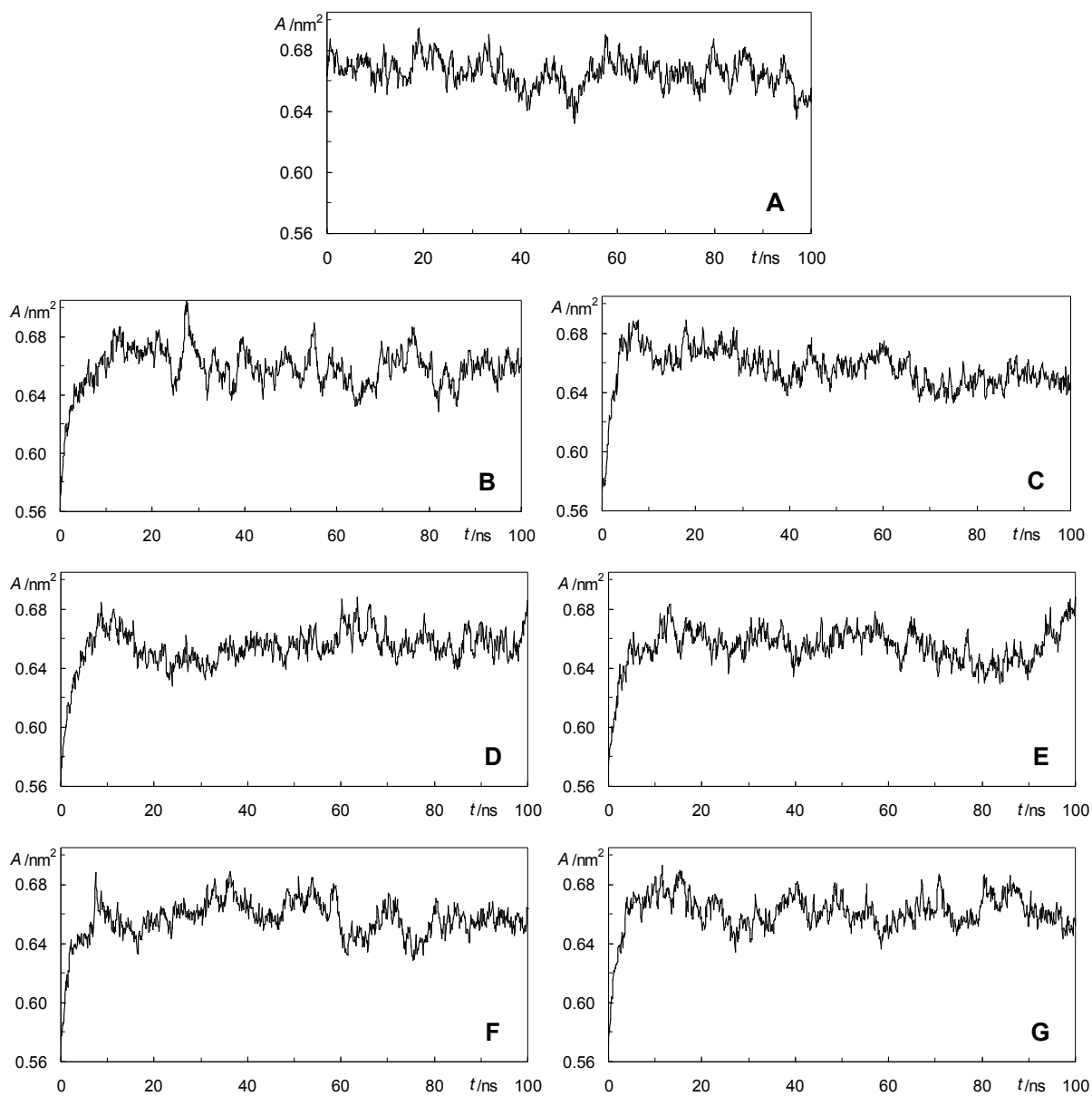


Figure S1. Time evolution of the areas per phospholipid molecule (A) for pure POPC (A) and for the systems with two inserted sterol molecules (from B to G: *i*-C0, *i*-C5, cholesterol, *i*-C10, *i*-C12, and *i*-C14, respectively).

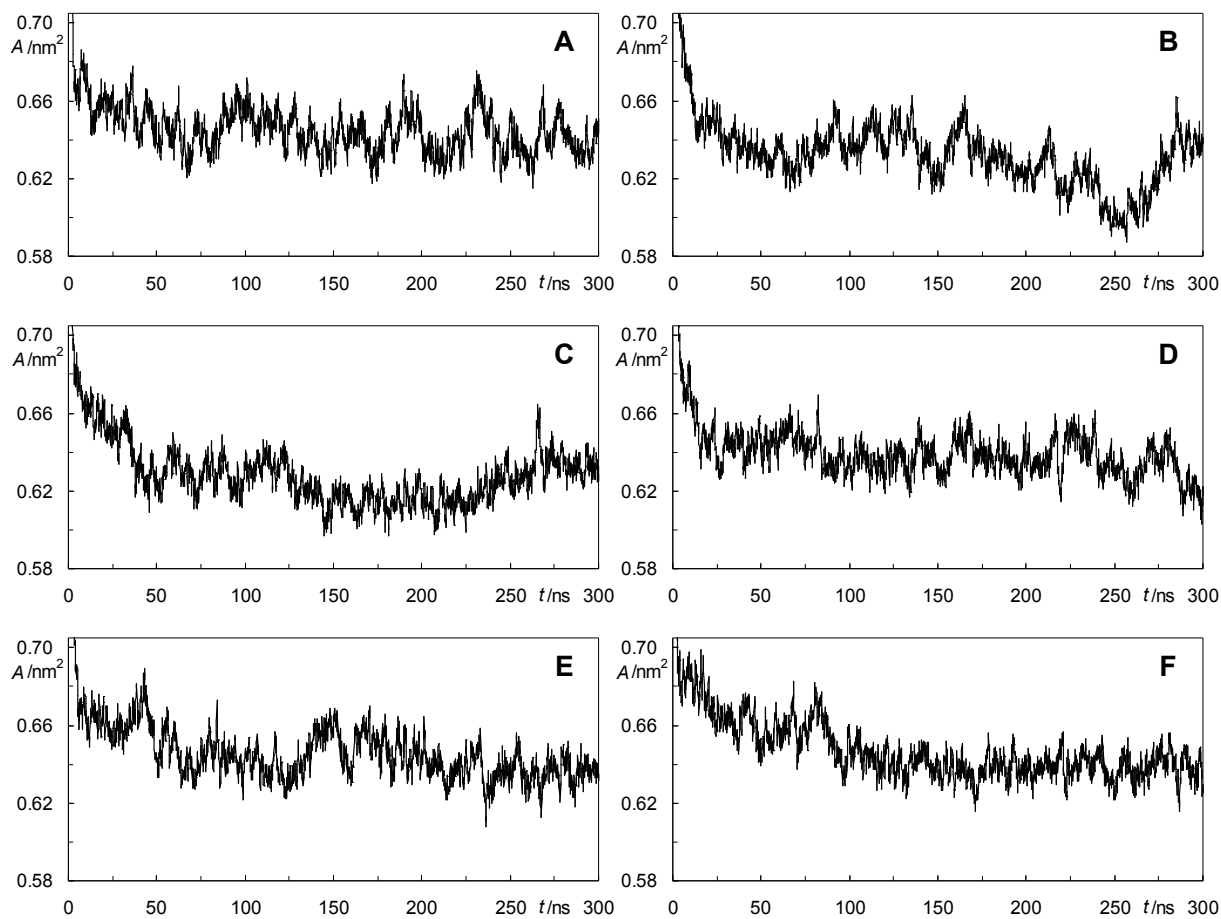


Figure S2. Time evolution of the areas per phospholipid molecule (A) for the systems with 20 mol% sterol (from A to F: *i*-C0, *i*-C5, cholesterol, *i*-C10, *i*-C12, and *i*-C14, respectively).

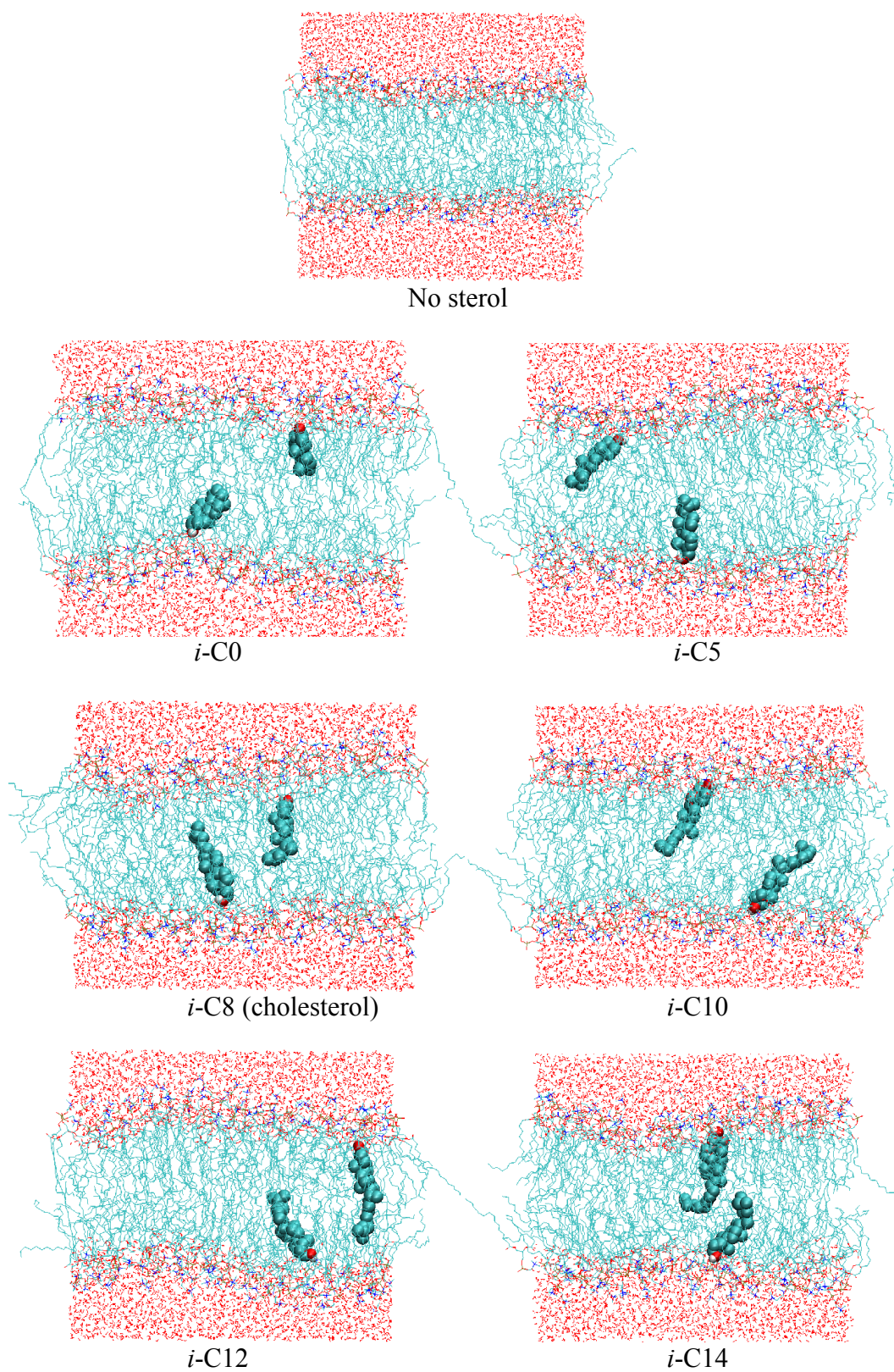


Figure S3. Final structures of the systems with none or two inserted sterol molecules.

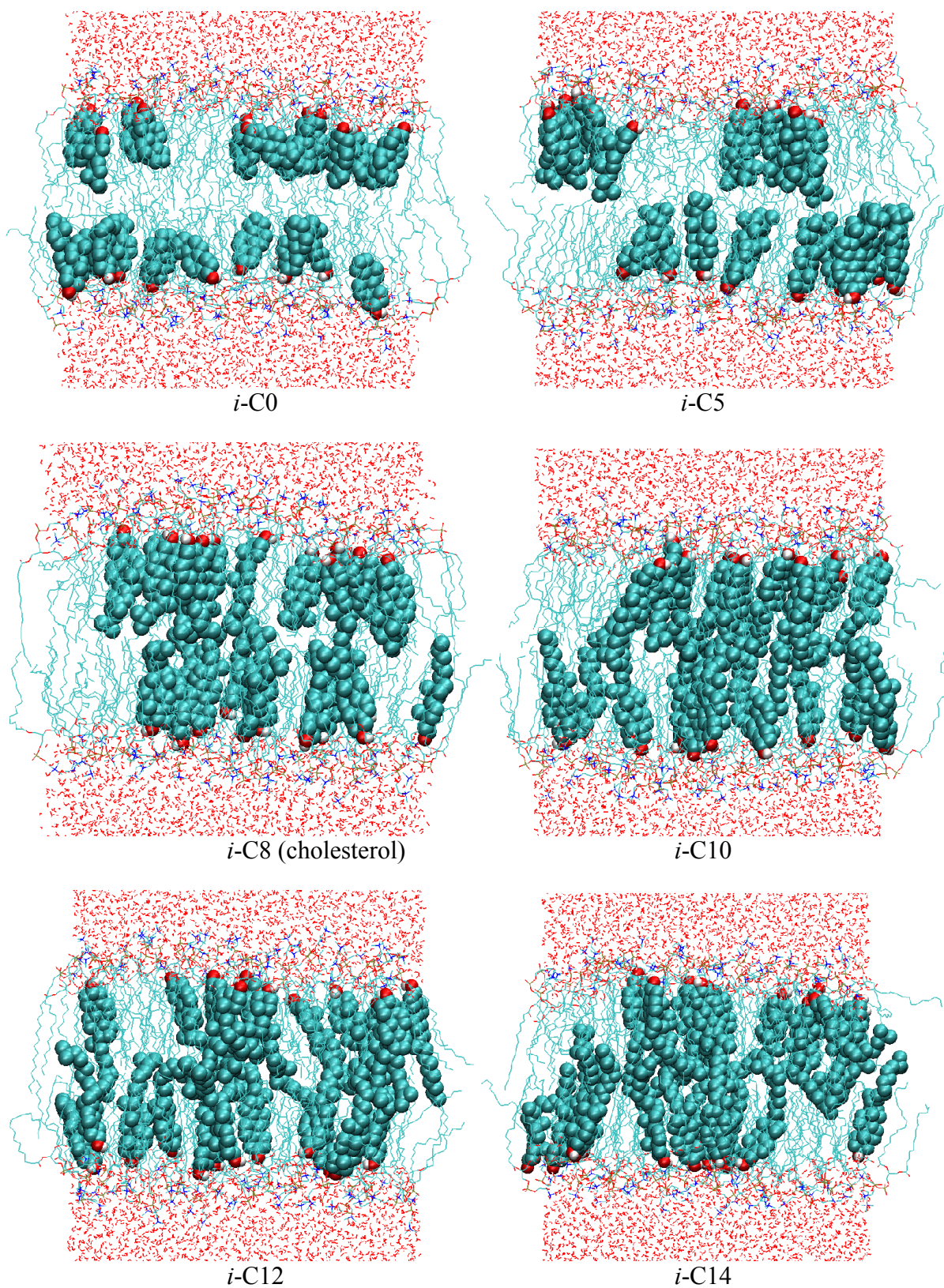


Figure S4. Final structures of the systems with 20 mol% sterol molecules.

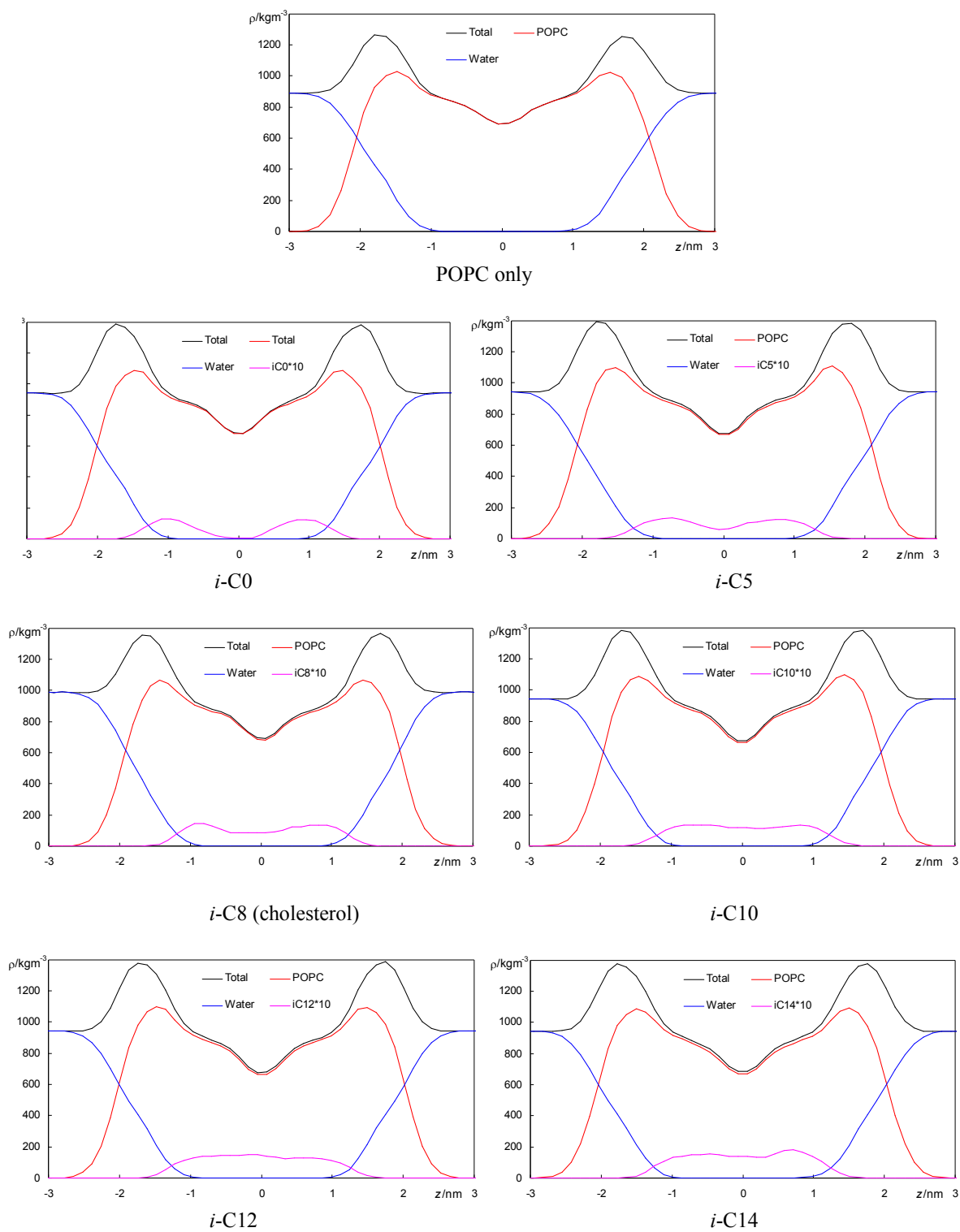


Figure S5. Mass density profiles across the bilayer normal direction (z) in the systems with none or two inserted sterol molecules. Sterol profiles are multiplied by a factor of 10 for better visualization.

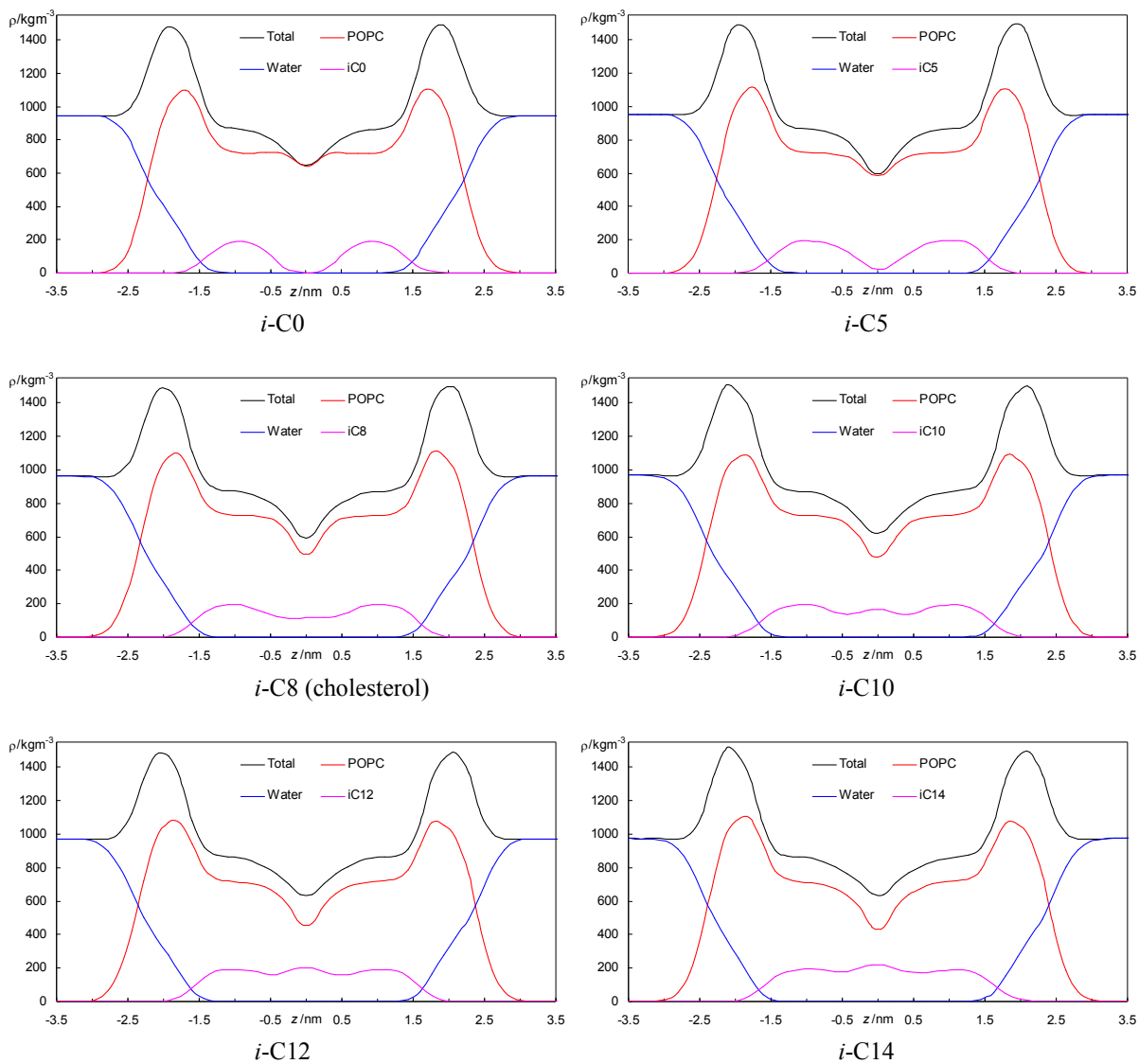


Figure S6. Mass density profiles across the bilayer normal direction (z) in the systems with 20 mol% inserted sterol molecules.

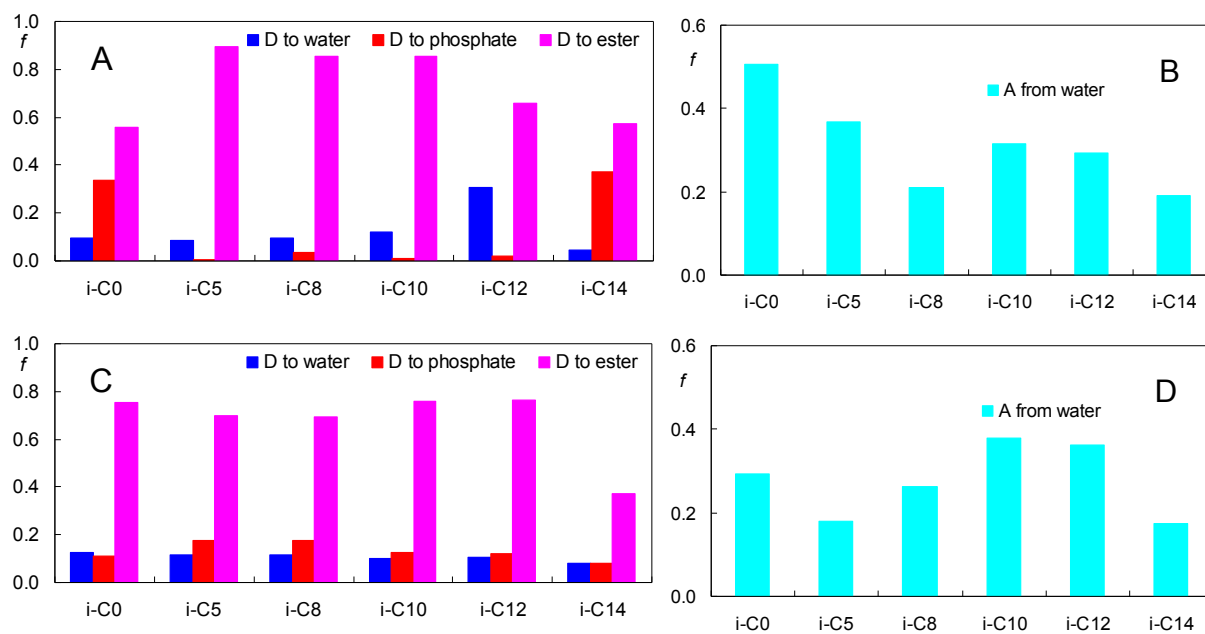


Figure S7. Fractional frequencies of hydrogen bonding (f) between (A, C) sterol donors and water or POPC acceptors and (B, D) water donors and sterol acceptors, for both the systems with two sterol molecules (A, B) and 20 mol% sterol (C, D).

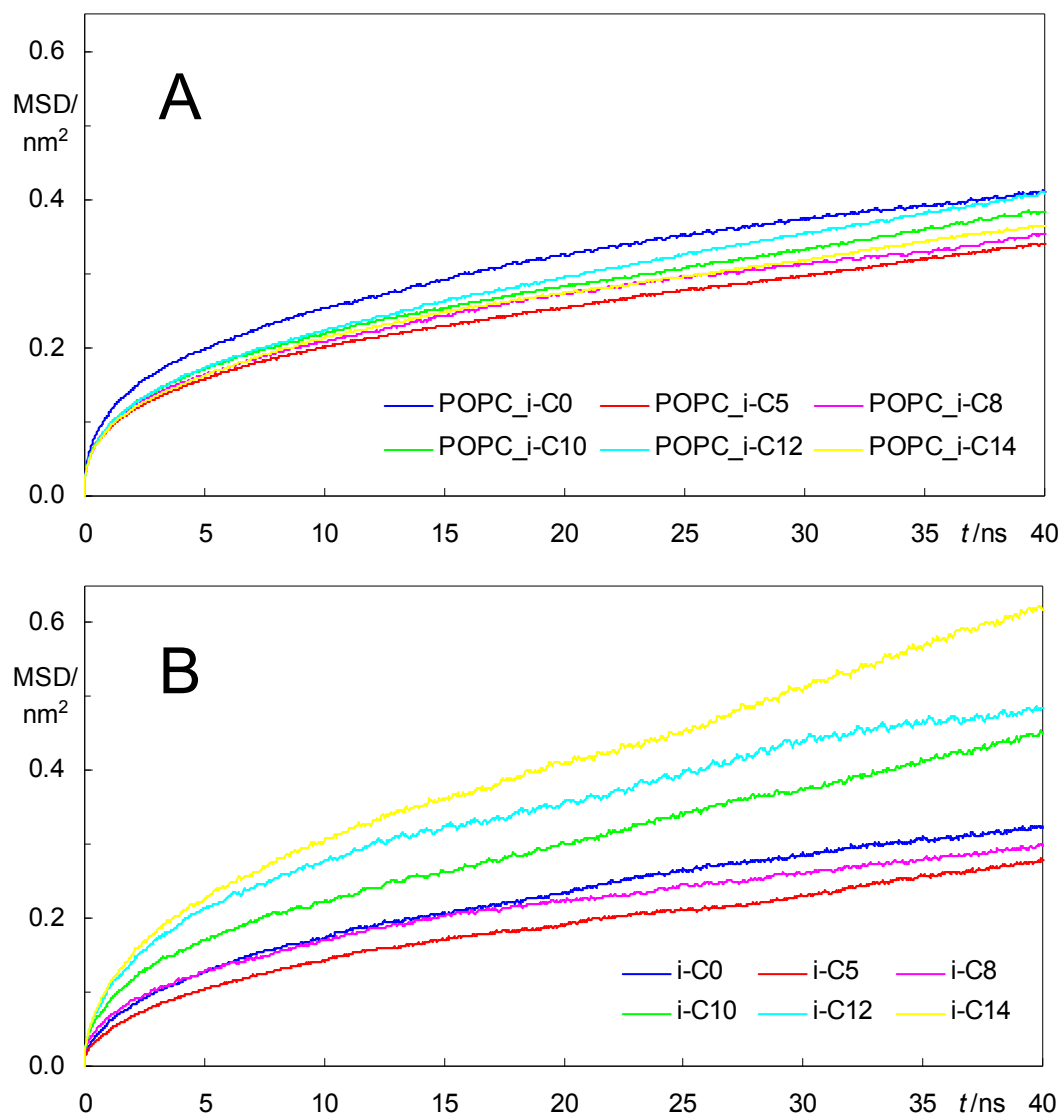


Figure S8. Lateral mean square displacements of POPC (A) and sterol (B) in the 20 mol% sterol systems.