

Tristearin bilayers: Structure of the aqueous interface and stability in the presence of surfactants: Electronic Supplementary Information

Zak E. Hughes,^{*a} and Tiffany R. Walsh^a

^a Institute for Frontier Materials, Deakin University, Geelong, Australia. Fax: +61 (0)3 5227 1103; Tel: +61 (0)3 5247 9160; E-mail: zhughes@deakin.edu.au

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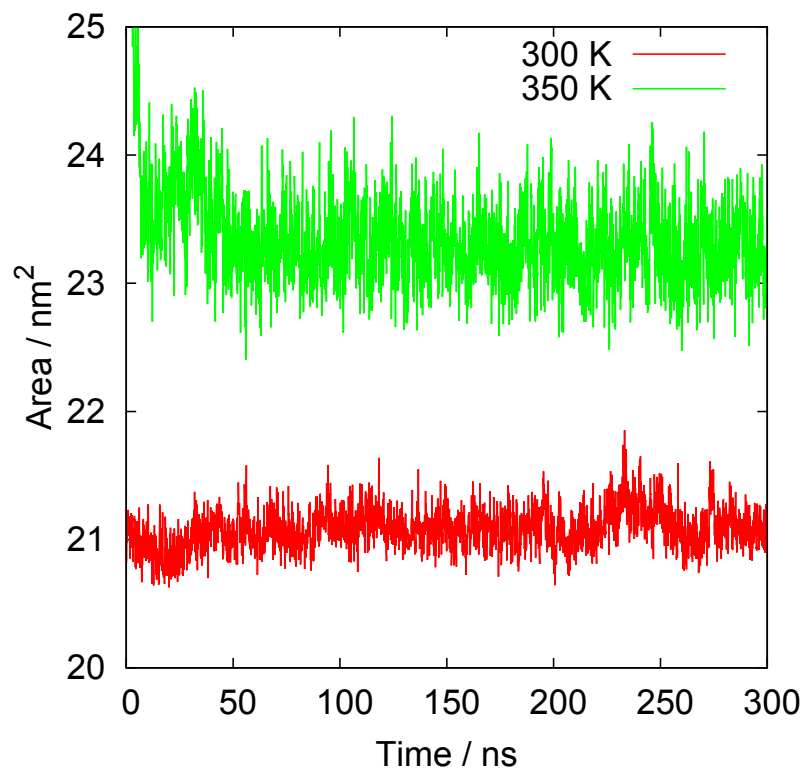


Fig. S1 The area of example TS bilayers at both 300 and 350 K during the 300 ns simulations.

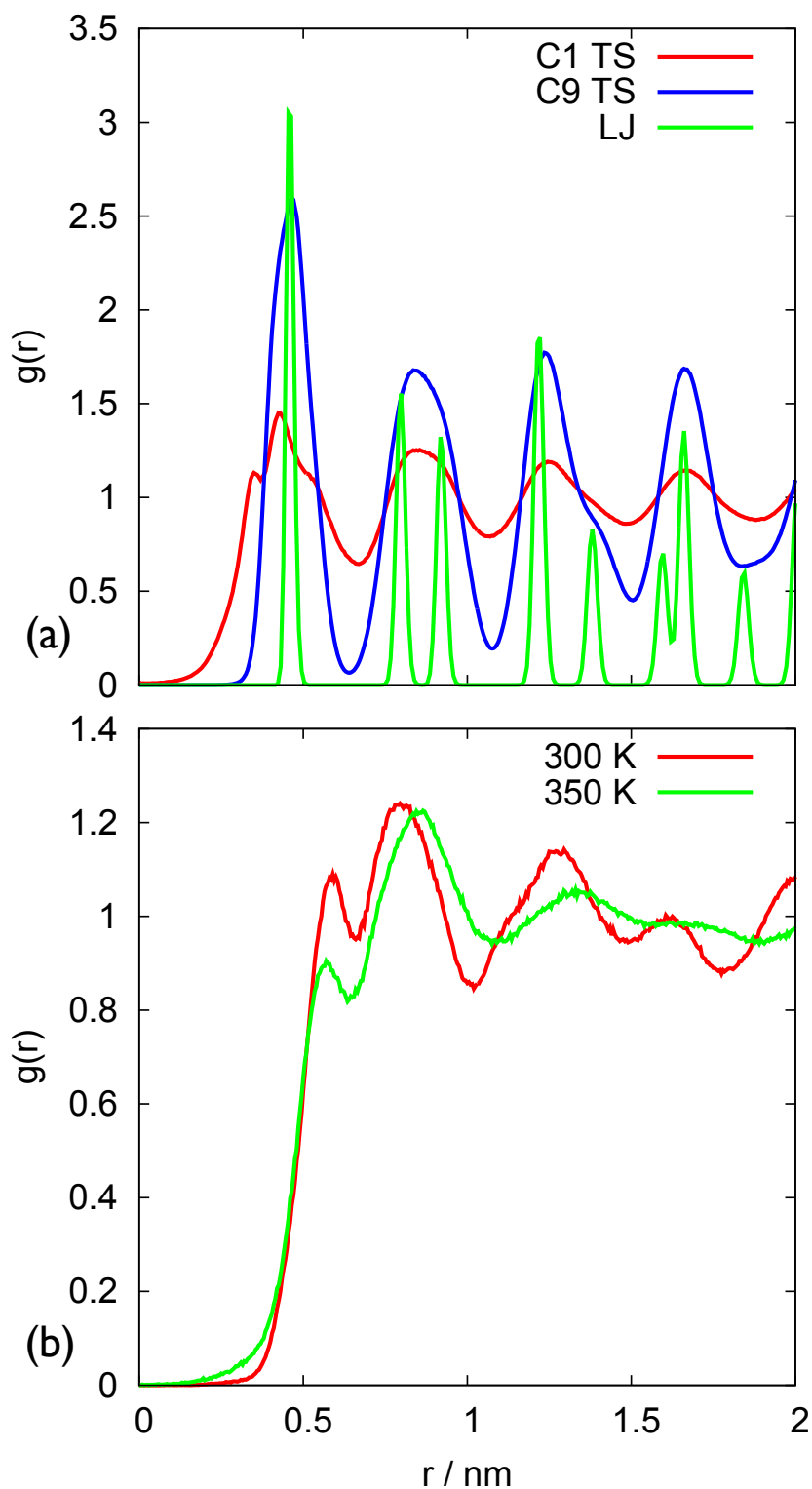


Fig. S2 (a) The radial distribution function in the xy -plane of the C1 and C9 carbon atoms in the tails of TS molecules in the same leaflet at 300 K. Also shown is the lateral radial distribution function of an “ideal” hexagonal lattice of Lennard-Jones atoms (scaled to the same lattice constant as the TS bilayer). (b) The radial distribution function in the xy -plane of the glycerol head groups of a single leaflet at 300 and 350 K.

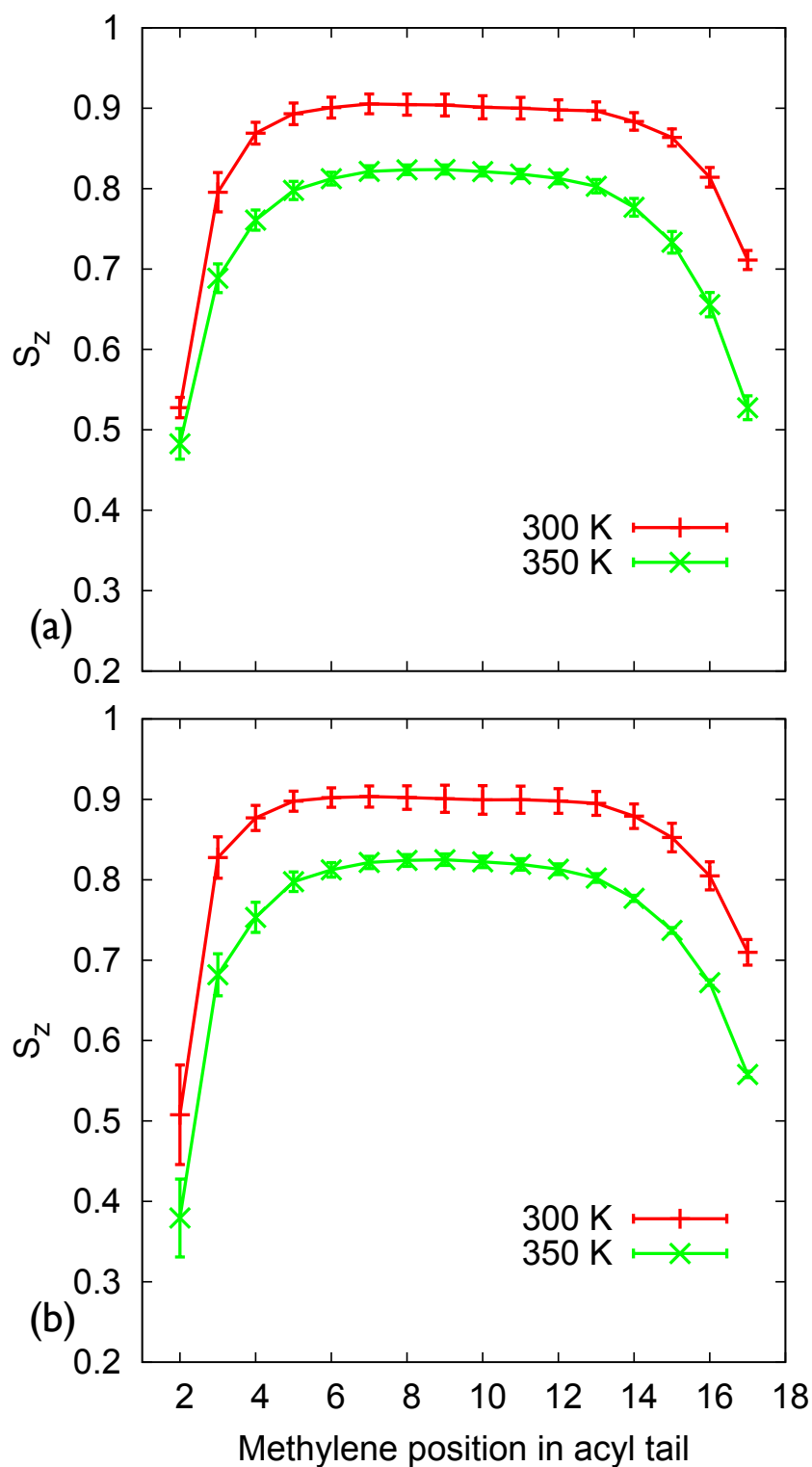


Fig. S3 The order parameters of (a) the *sn*-2 and (b) the *sn*-3 acyl tails of the TS molecules at 300 and 350 K.

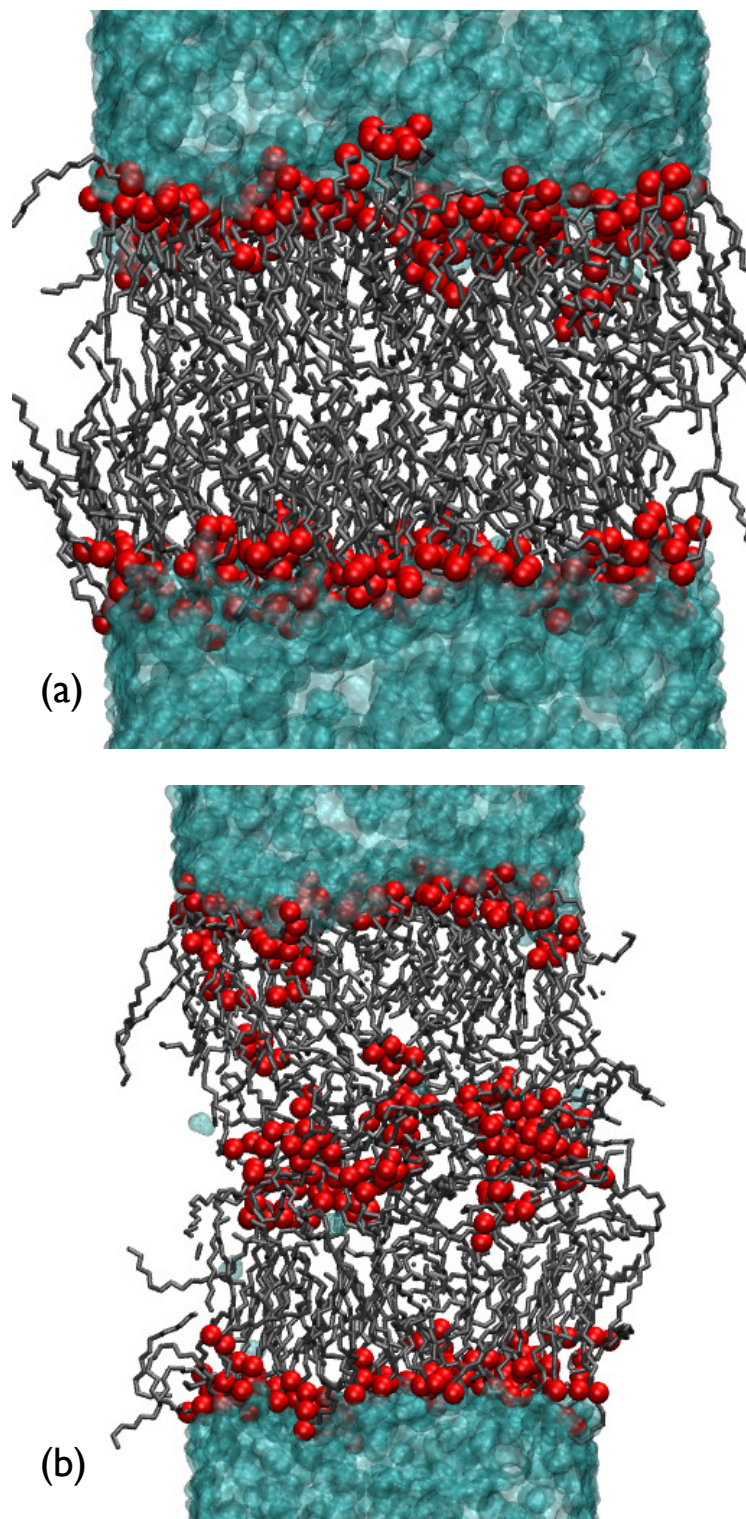


Fig. S4 Snapshots of the TS bilayers from the annealing simulations, Run D2, at (a) 160 and (b) 182 ns. The carbon and oxygen atoms of TS are coloured grey and red, respectively, while the water is coloured cyan.

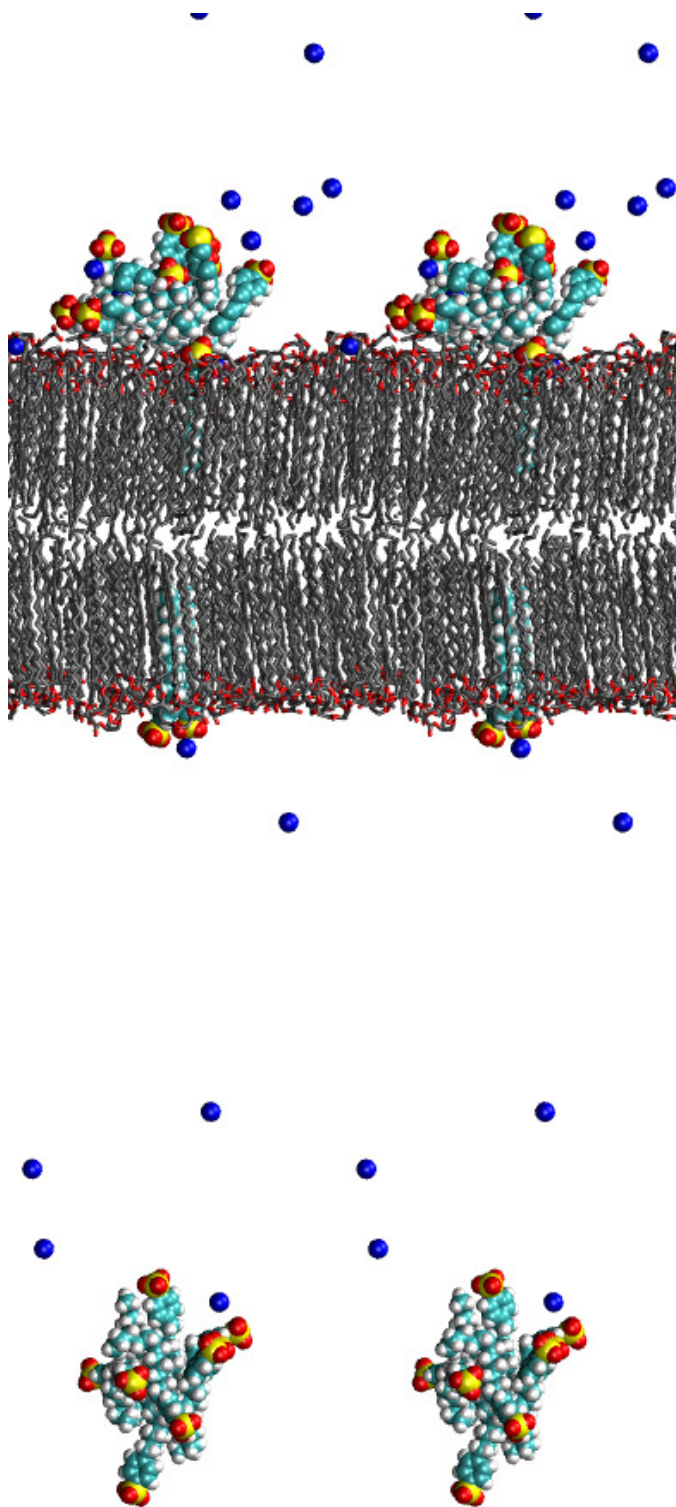


Fig. S5 Snapshot of the TS bilayers in the presence of SDBS, showing the formation of SDBS aggregates both in solution and at the surface of the TS bilayer as well as in the insertion of SDBS into the TS bilayer, taken from run C1 (the snapshot is replicated in the x -direction for clarity). The carbon and oxygen atoms of TS are coloured grey and red, respectively, the carbon, hydrogen, oxygen and sulphur atoms of the SDBS molecules coloured cyan, white, red and yellow, respectively, the sodium atoms are coloured blue, the water molecules are not shown for clarity.

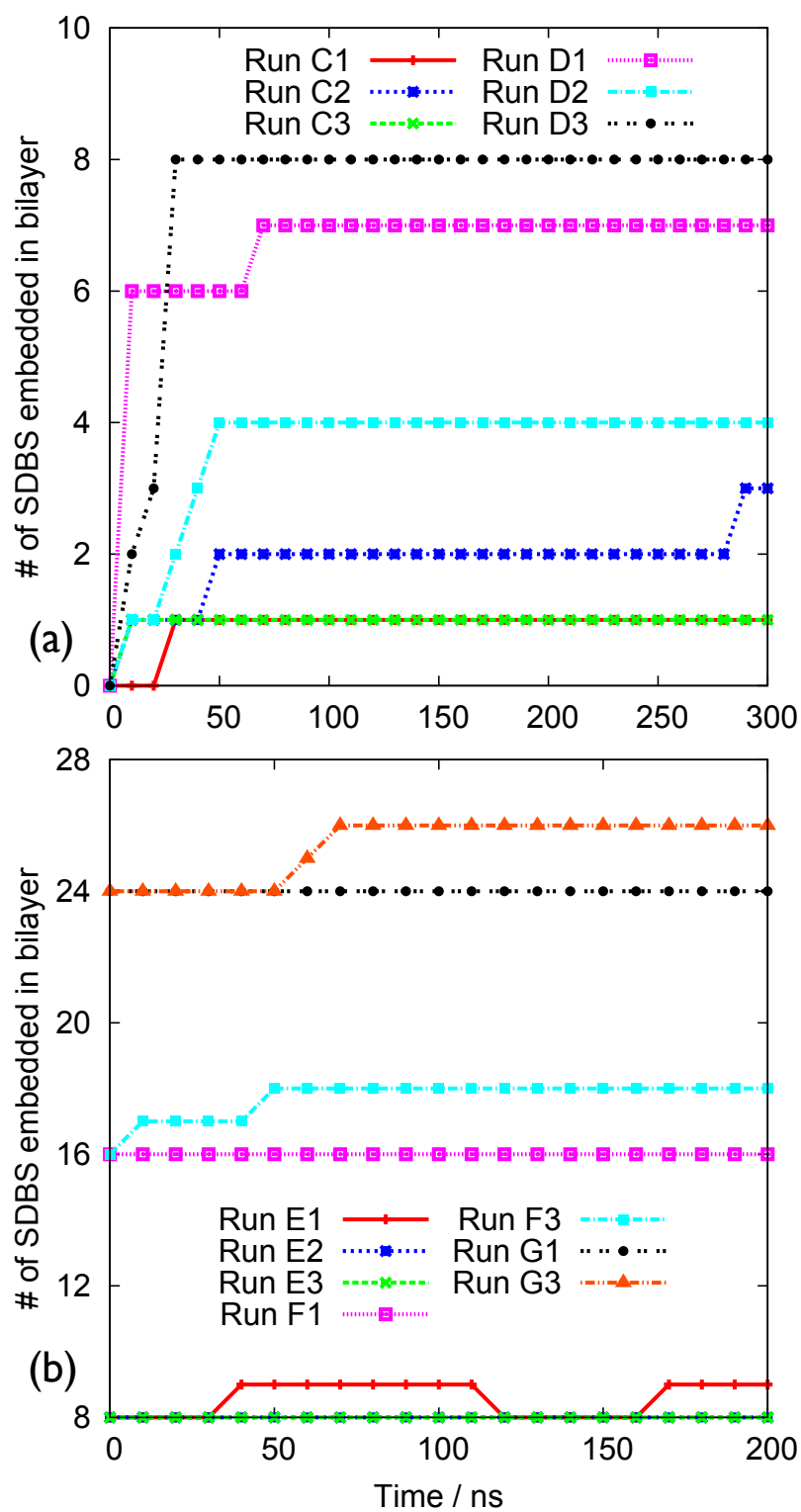


Fig. S6 The number of SDBS embedded within the TS bilayer over the course of the (a) Set C and D and (b) Set E, F and G simulations

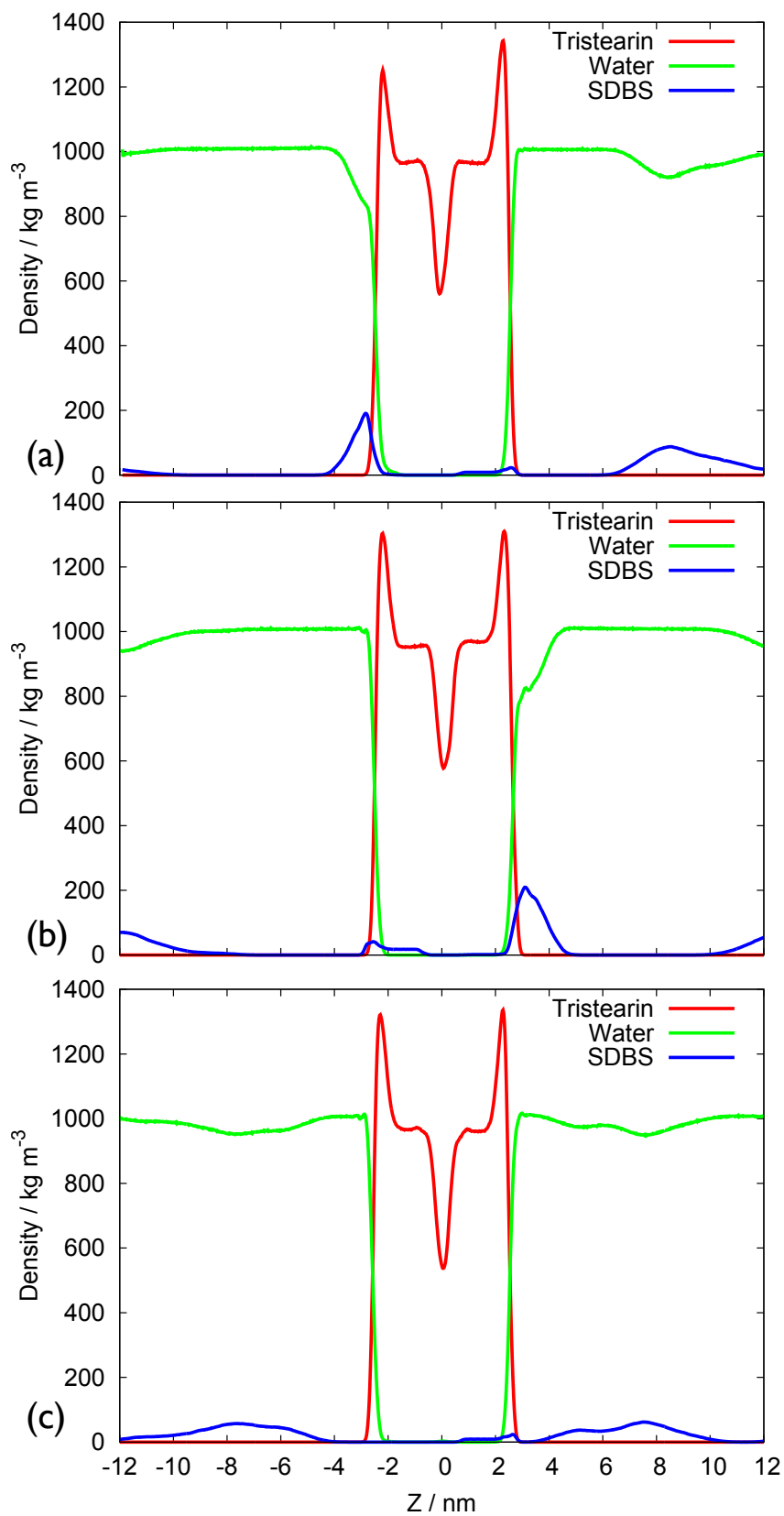


Fig. S7 Density profiles of runs (a) C1, (b) C2 and (c) C3.

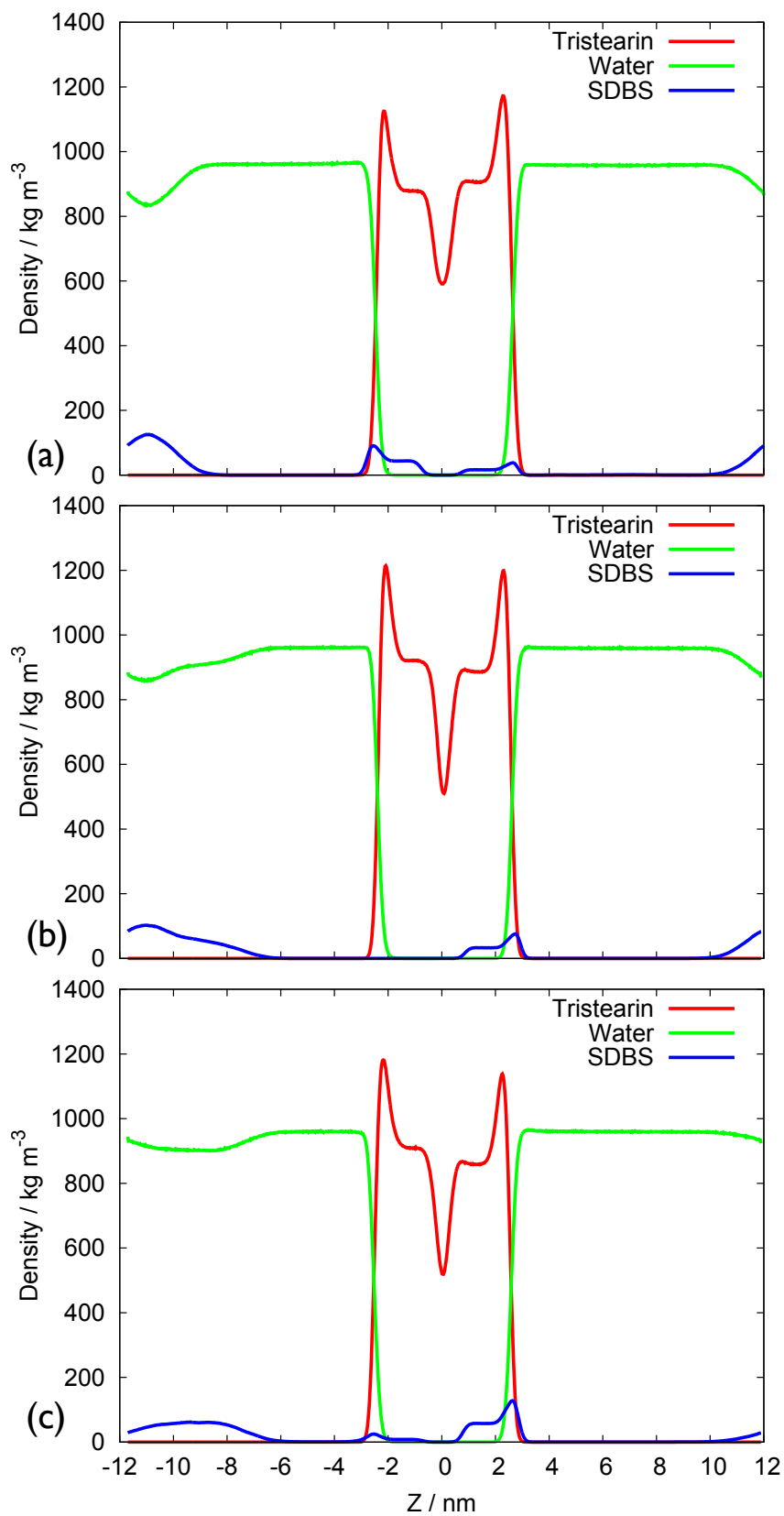


Fig. S8 Density profiles of runs (a) D1, (b) D2 and (c) D3.

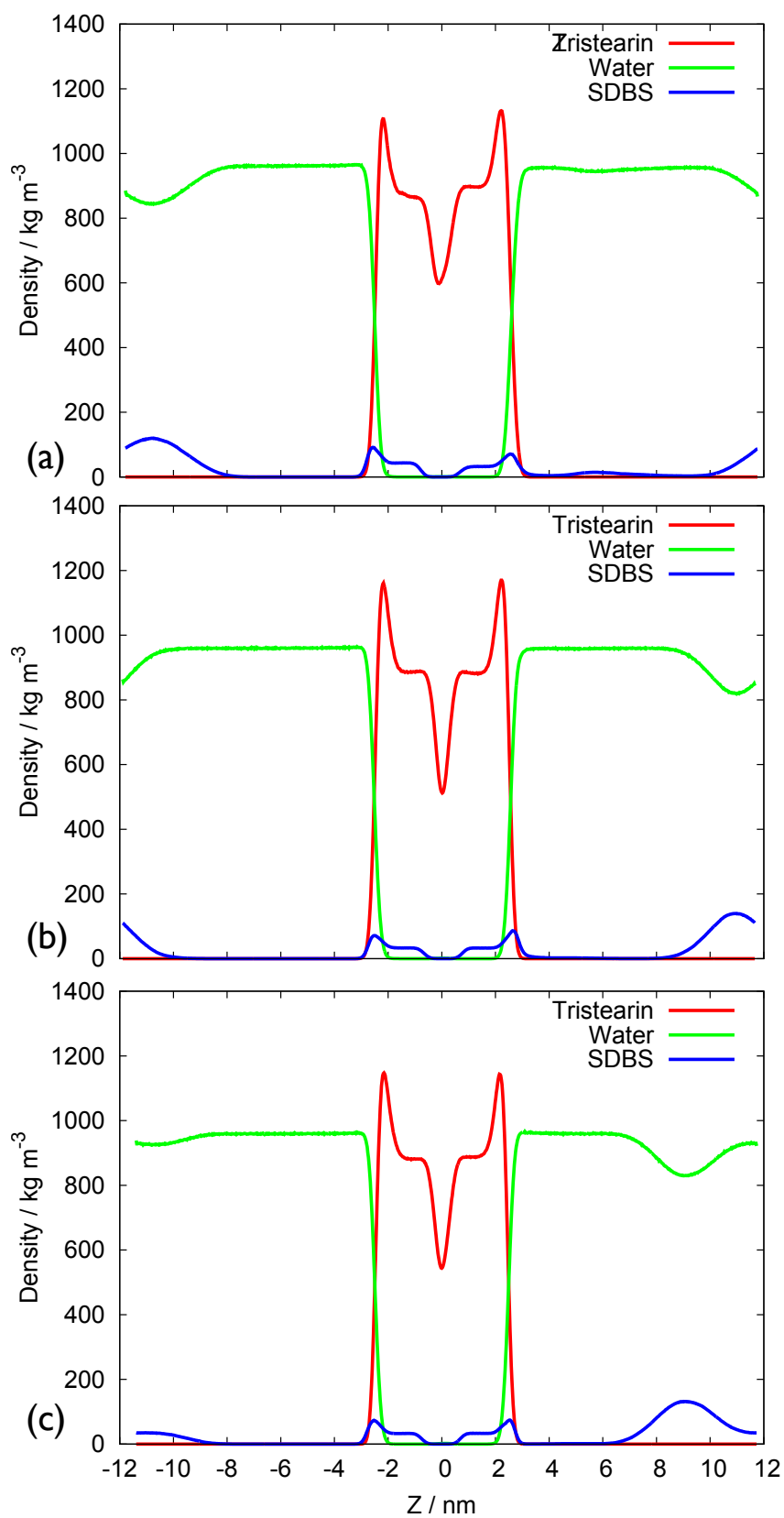


Fig. S9 Density profiles of runs (a) E1, (b) E2 and (c) E3.

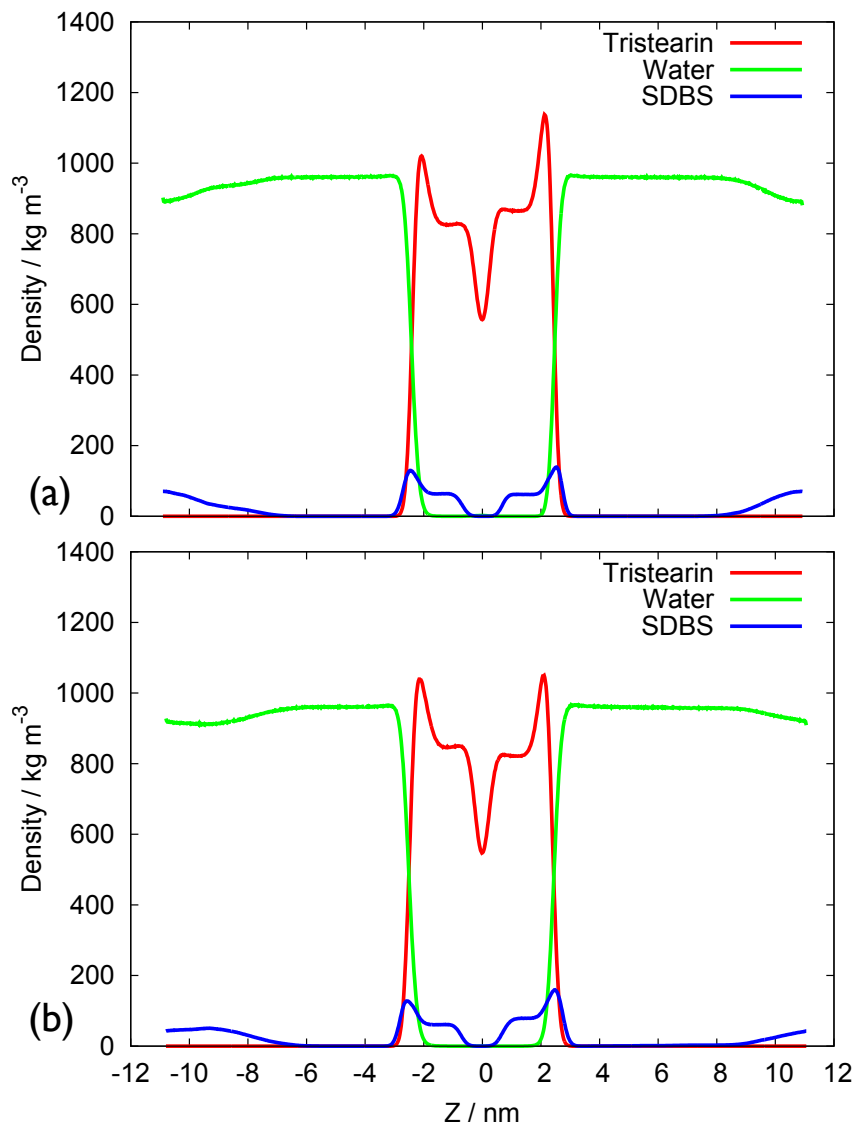


Fig. S10 Density profiles of runs (a) F1 and (b) F3.

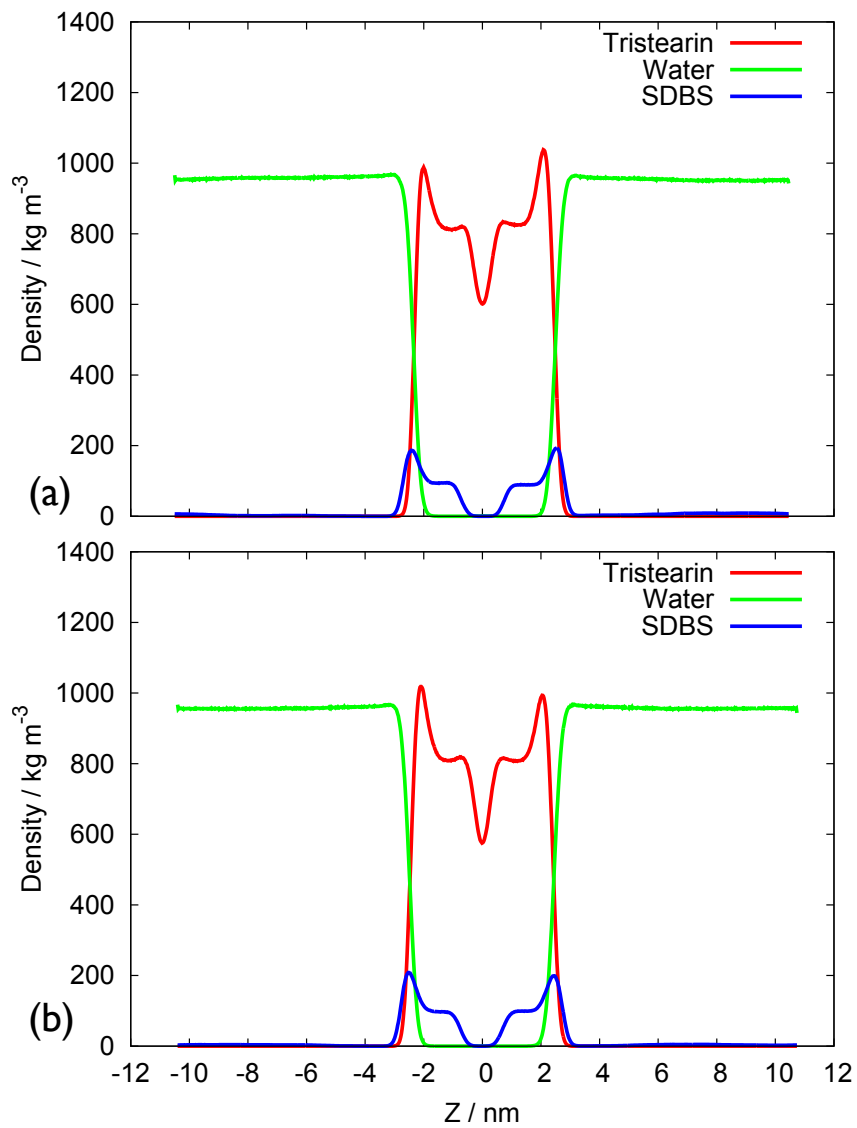


Fig. S11 Density profiles of runs (a) G1 and (b) G3.

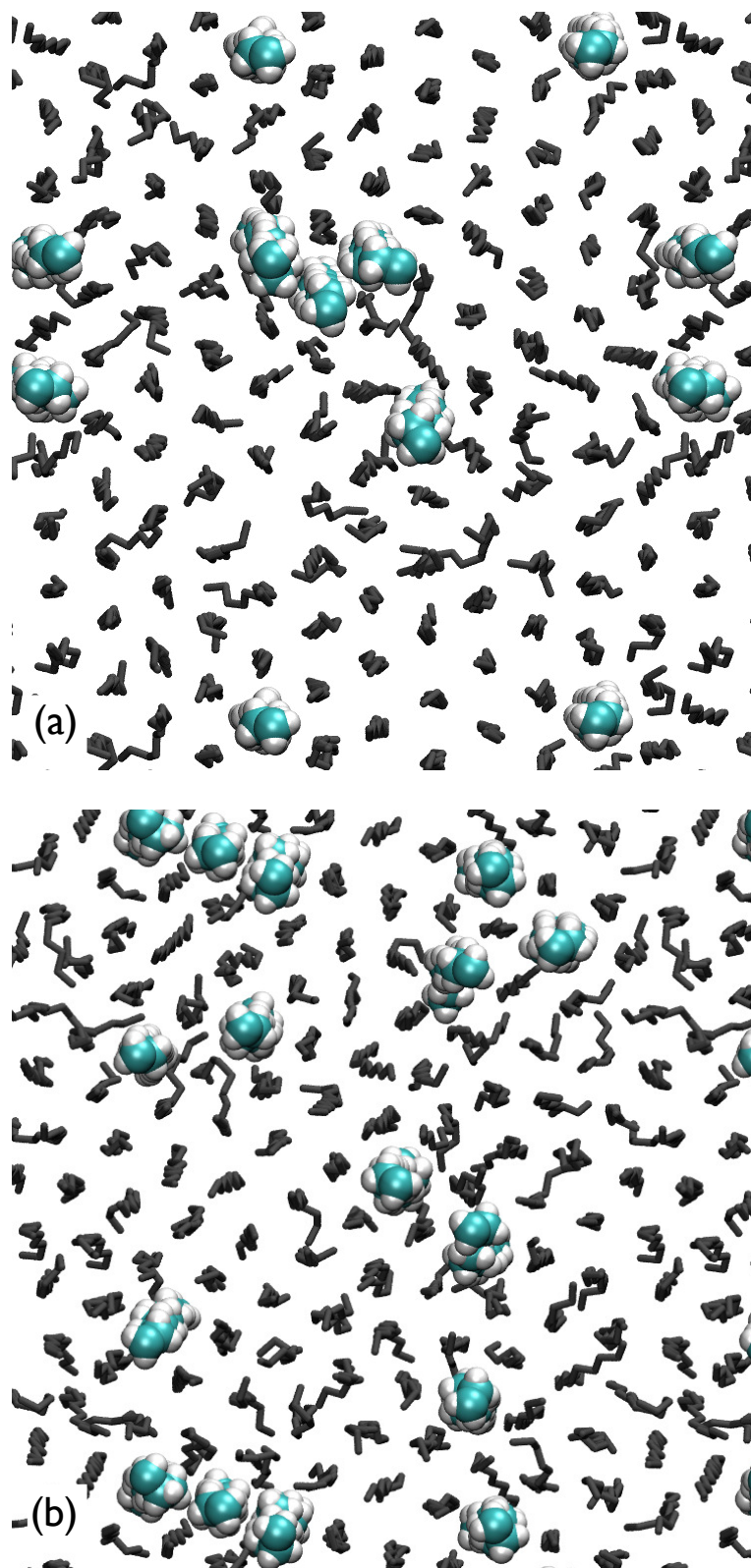


Fig. S12 Snapshots of a cross-section through one leaflet of a bilayer, showing the carbon atoms of the acyl tails of the TS molecules and the tails of the SDBS molecules. Taken from (a) run F1, eight SDBS per leaflet, and (b) run G1, 12 SDBS per leaflet. The acyl tails of the TS molecules are coloured grey and the carbon and hydrogen atoms of the SDBS molecules are coloured cyan and white, respectively.

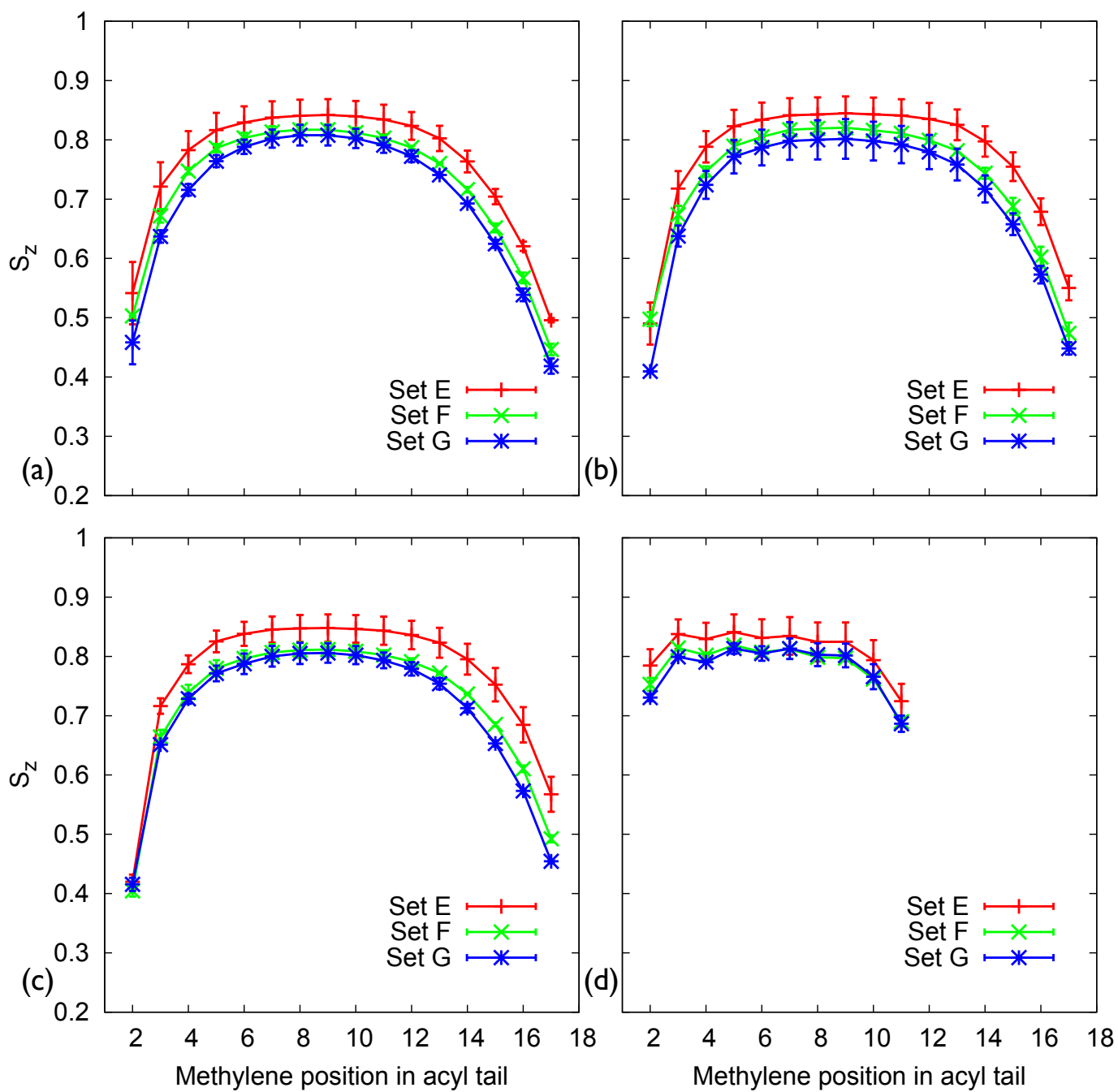


Fig. S13 The order parameters of (a) the *sn*-2 and (b) the *sn*-3 acyl tails of the TS molecules in simulation Sets E, F and G.

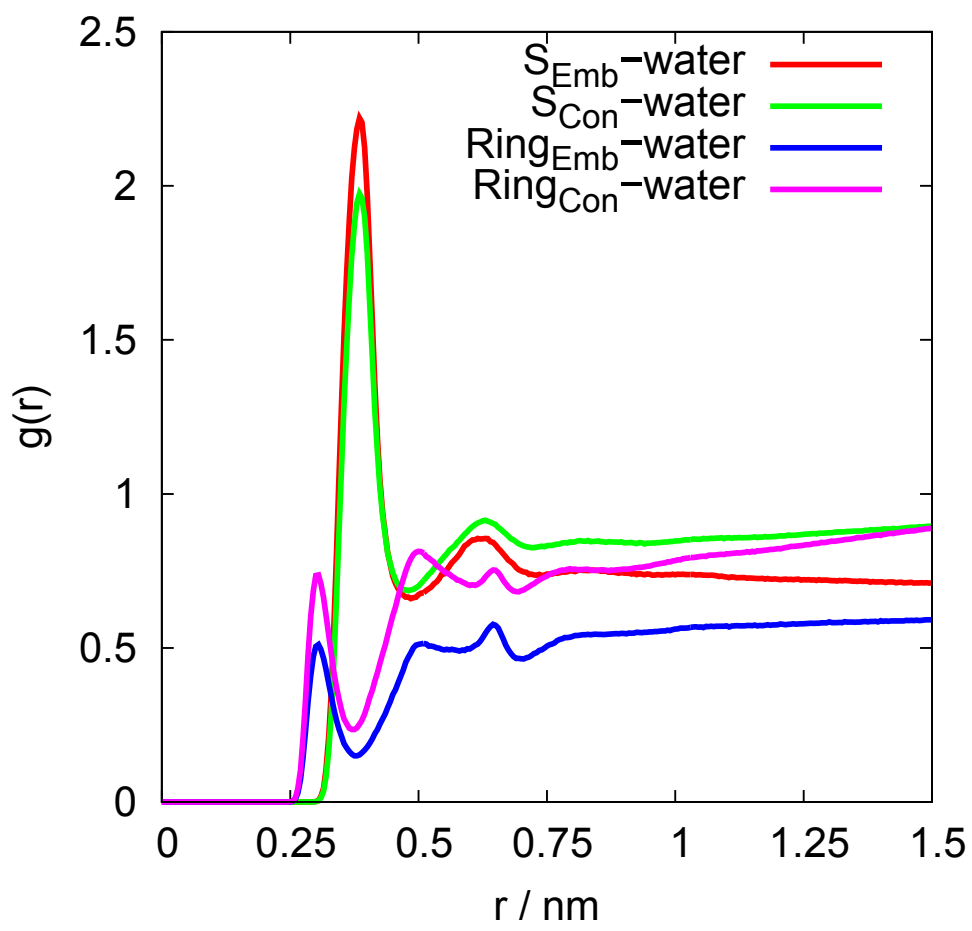


Fig. S14 The sulphur-water and phenyl ring-water radial distribution functions for the SDBS molecules in the control micelles and embedded in the bilayer.