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Supplemental information

Alteration of lipid bilayer mechanics by volatile anesthetics: Insights from μ s-long molecular dynamics simulations

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Supplementary Information

Density Profiles

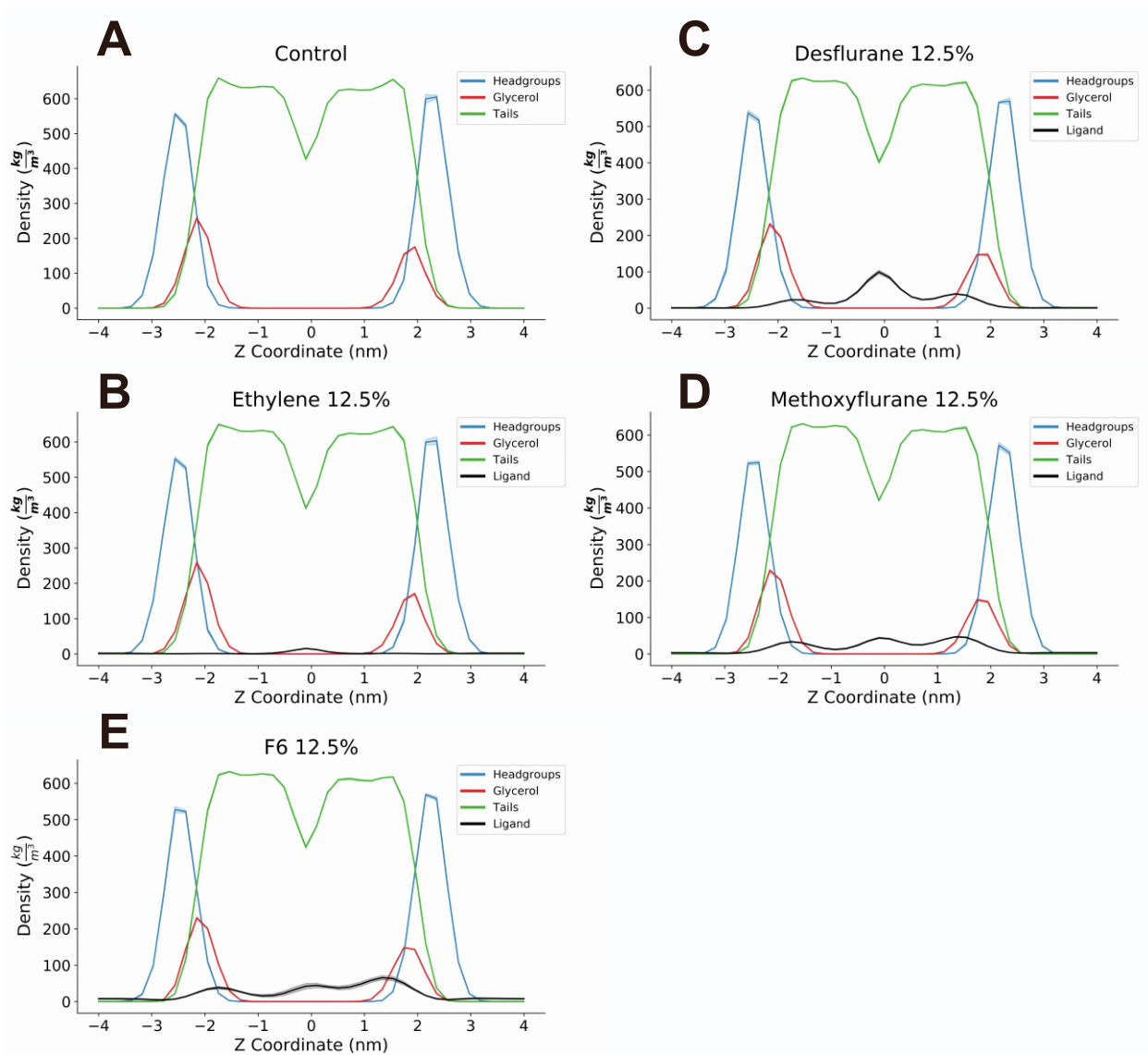


Figure S1. Density profiles of control simulations (A) and ligands at 12.5% molar ratio: (B) Ethylene; (C) Desflurane; (D) Methoxyflurane; (E) F6. Densities of lipid headgroups, glycerol groups, hydrophobic lipid tails and ligands are highlighted. Shaded areas represent 95% confidence intervals. Related to Figure 3.

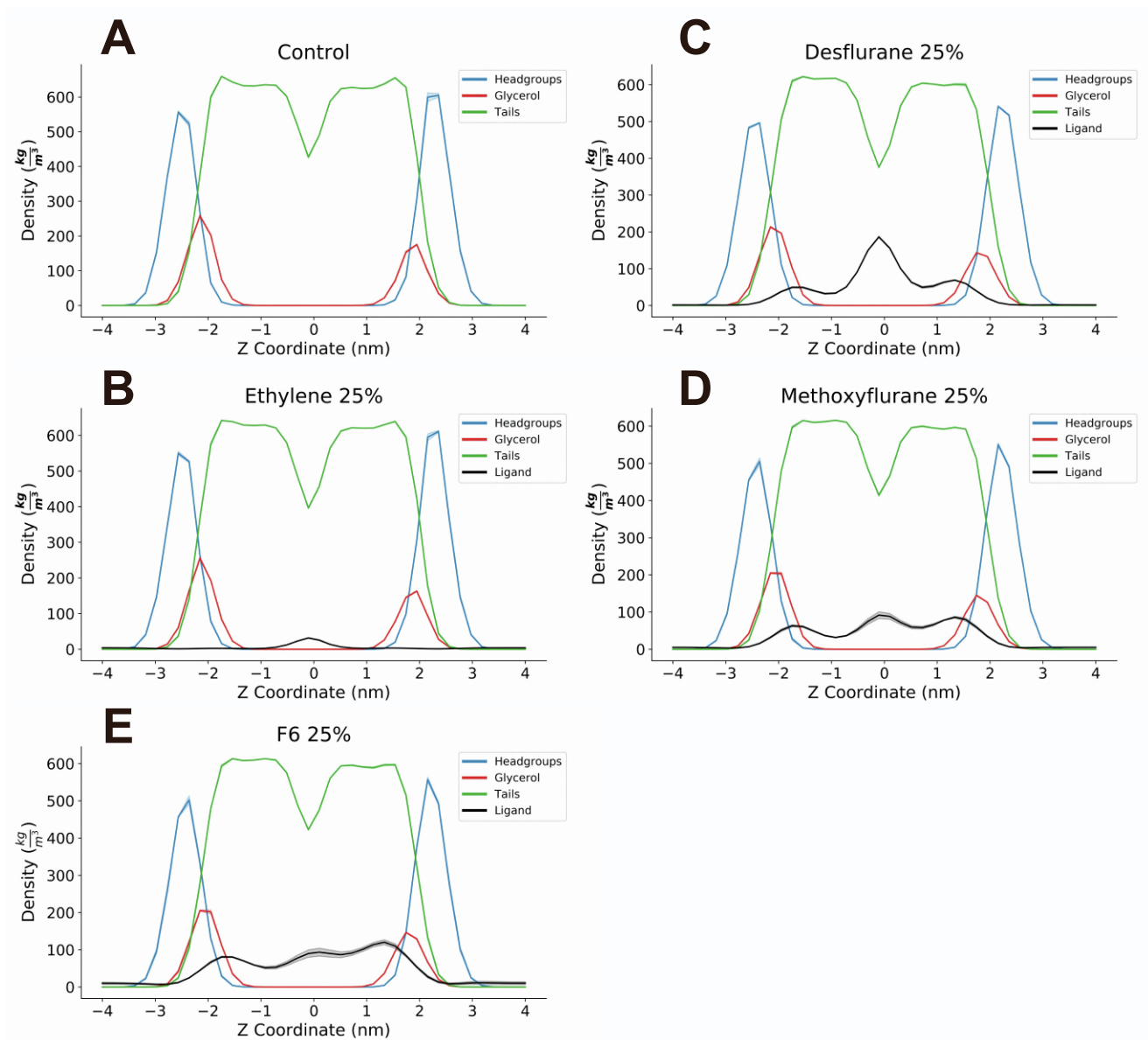


Figure S2. Density profiles of control simulations (A) and ligands at 25% molar ratio: (B) ethylene; (C) desflurane; (D) methoxyflurane; (E) F6. Densities of lipid headgroups, glycerol groups, hydrophobic lipid tails and ligands are highlighted. Shaded areas represent 95% confidence intervals. Related to Figure 3.

Order Parameters

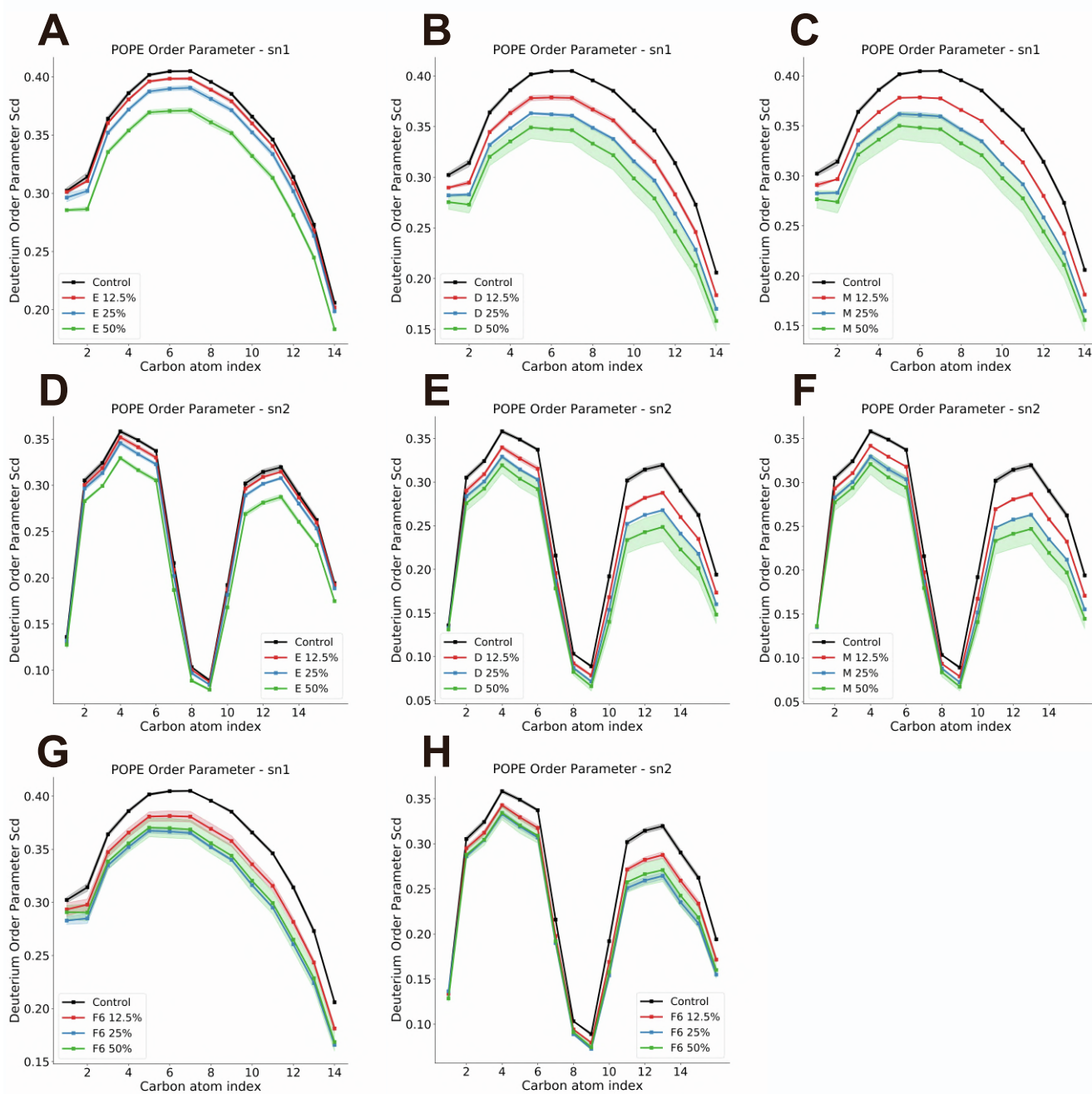


Figure S3. Lipid tail order parameters for POPE sn1 and sn2 chains, with different ligands: (A) and (D) ethylene; (B) and (E) desflurane; (C) and (F) methoxyflurane; (G) and (H) F6. Shaded intervals correspond to 95% confidence intervals. Related to Figure 5.

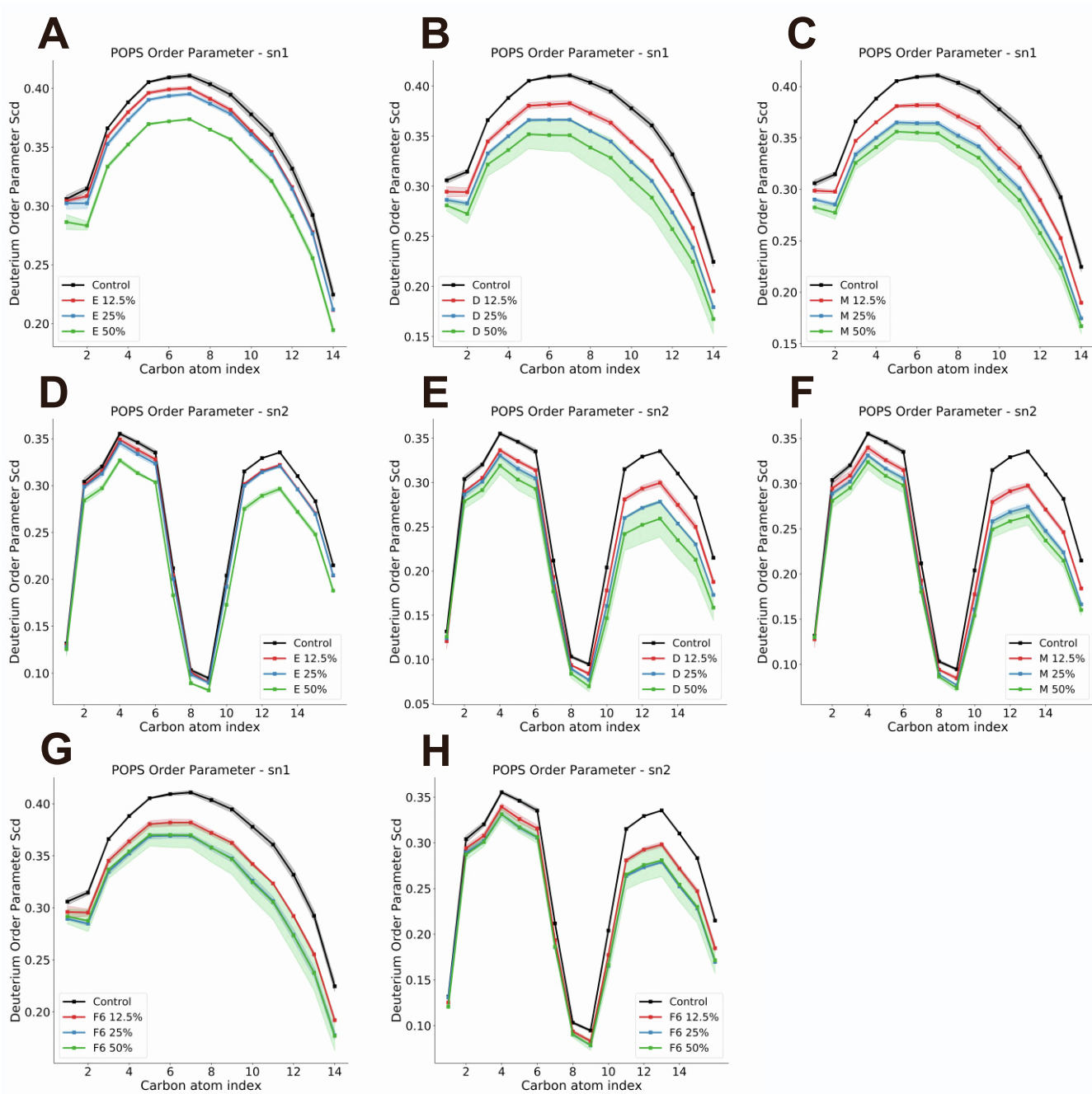


Figure S4. Lipid tail order parameters for POPS sn1 and sn2 chains, with different ligands: (A) and (D) ethylene; (B) and (E) desflurane; (C) and (F) methoxyflurane; (G) and (H) F6. Shaded intervals correspond to 95% confidence intervals. Related to Figure 5.

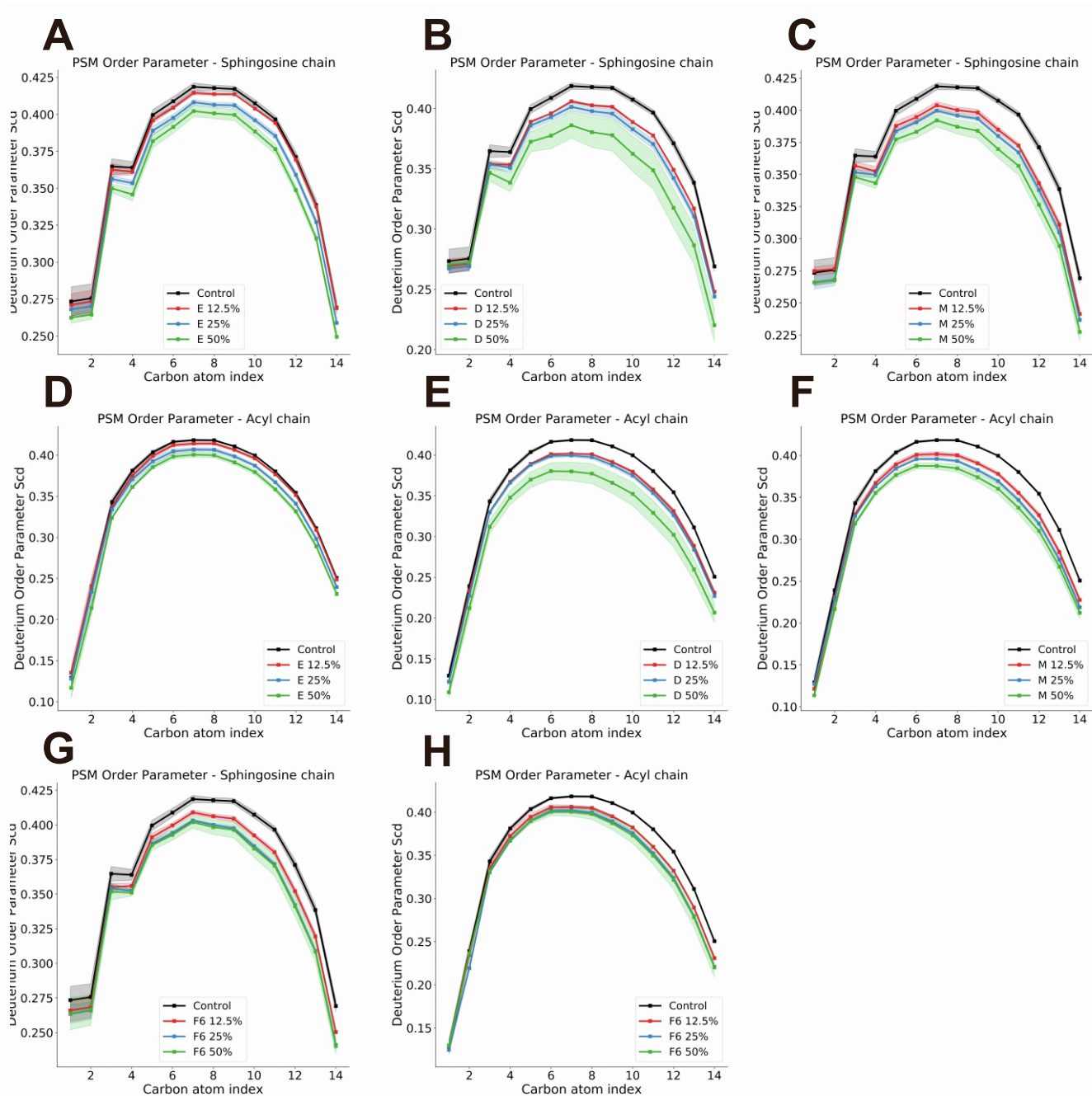


Figure S5. Lipid tail order parameters for PSM sphingosine chain and acyl chain, with different ligands: (A) and (D) ethylene; (B) and (E) desflurane; (C) and (F) methoxyflurane; (G) and (H) F6. Shaded intervals correspond to 95% confidence intervals. Related to Figure 5.