SUPPLEMENTARY INFORMATION: NMRlipids Databank: Overlay Databank of Lipid Membrane Simulations Arising from Open Collaboration

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ABSTRACT

S1 Correlations between area per lipid and thickness with order parameters and form factors

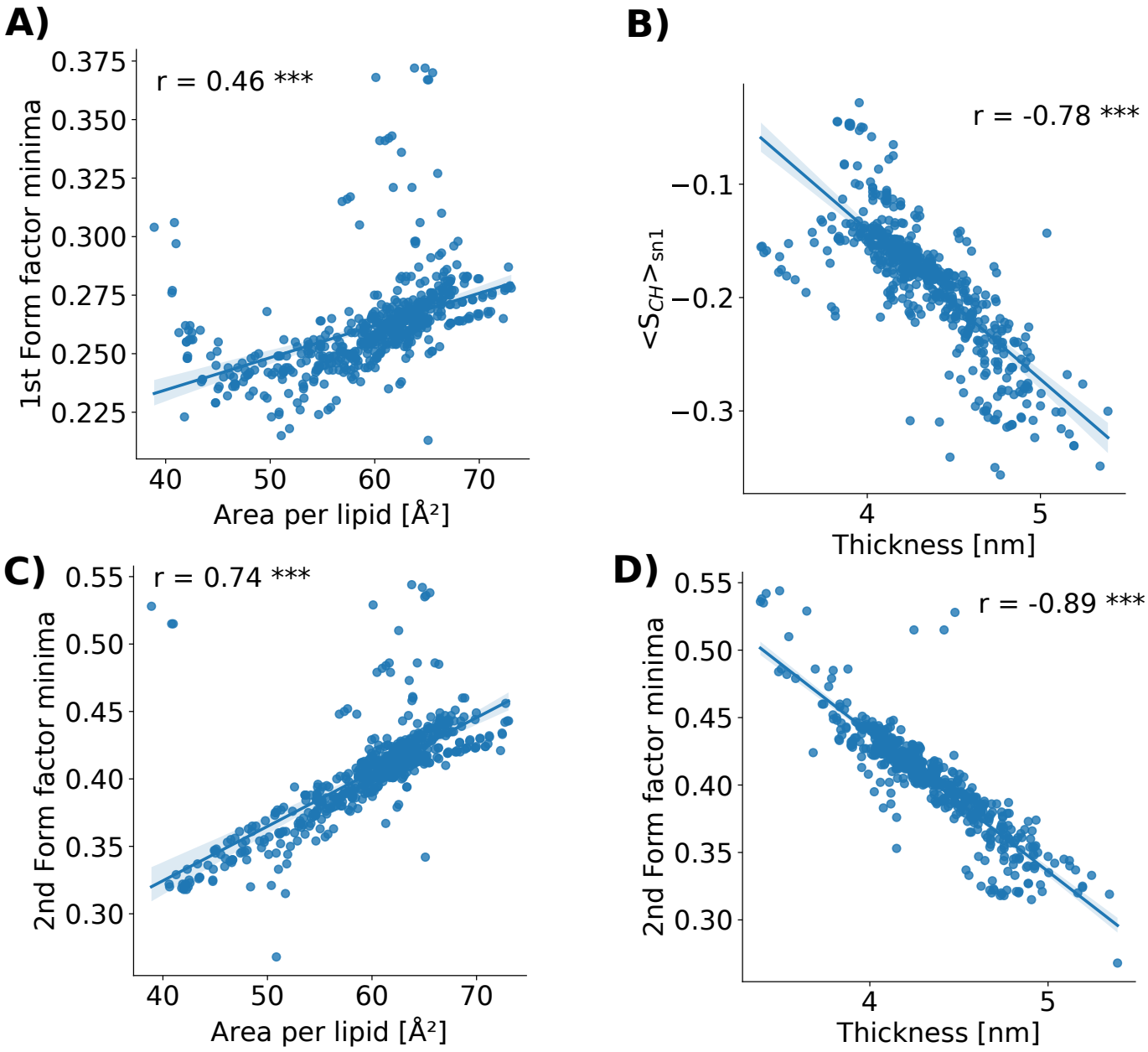

Figure S1. Dependence of form factor, electron density profiles along membrane normal, and C-H bond orderparameters (from top to bottom) on simulation box size with different cholesterol concentration.

S2 Dependence of form factor and order parameters in the size of simulation

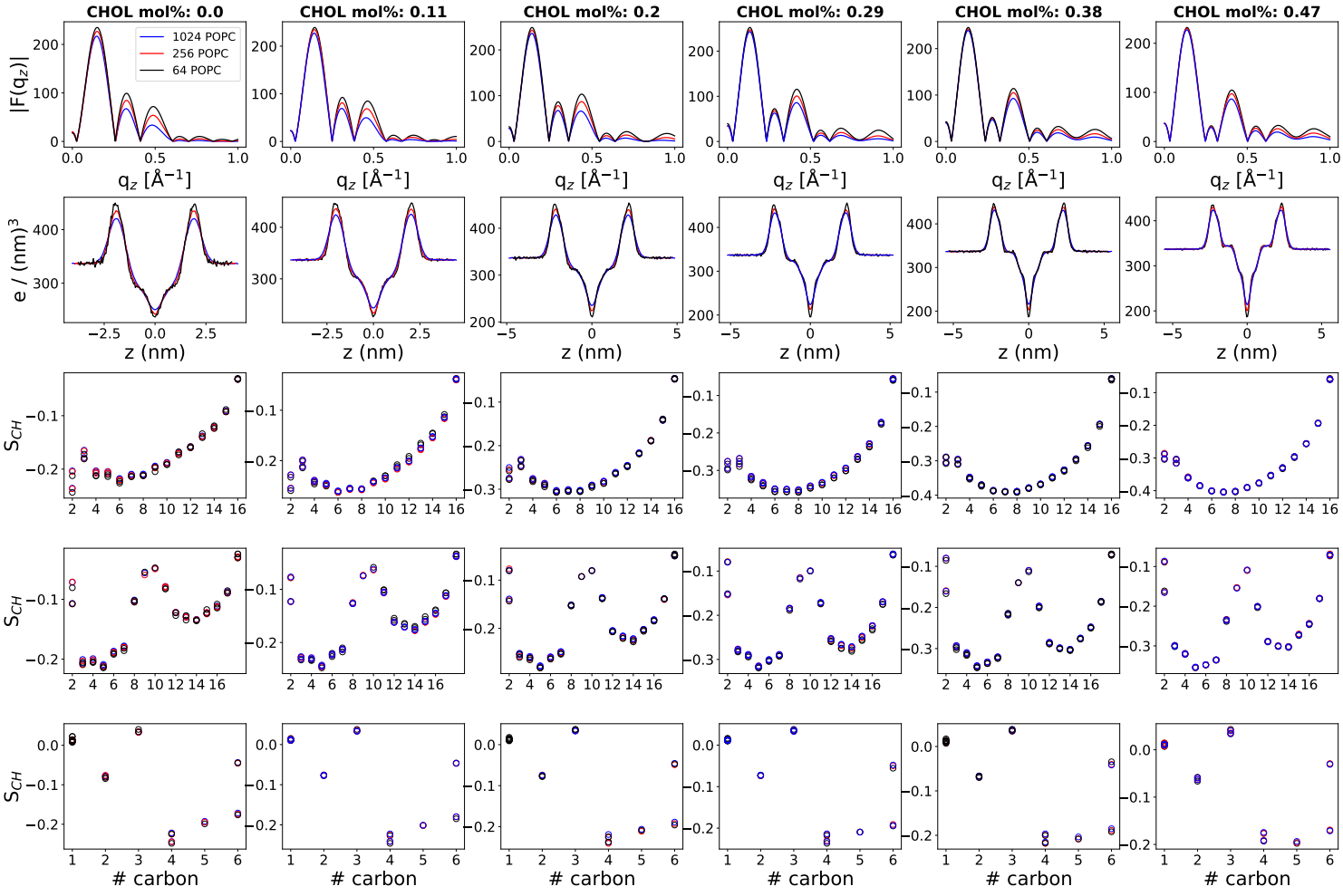

Figure S2. Dependence of form factor, electron density profiles along membrane normal, and C-H bond orderparameters (from top to bottom) on simulation box size with different cholesterol concentration. Simulations with 64, 256 or 1024 POPC lipids taken from Ref. 1.

S3 Finding the best models for PC and PE mixtures

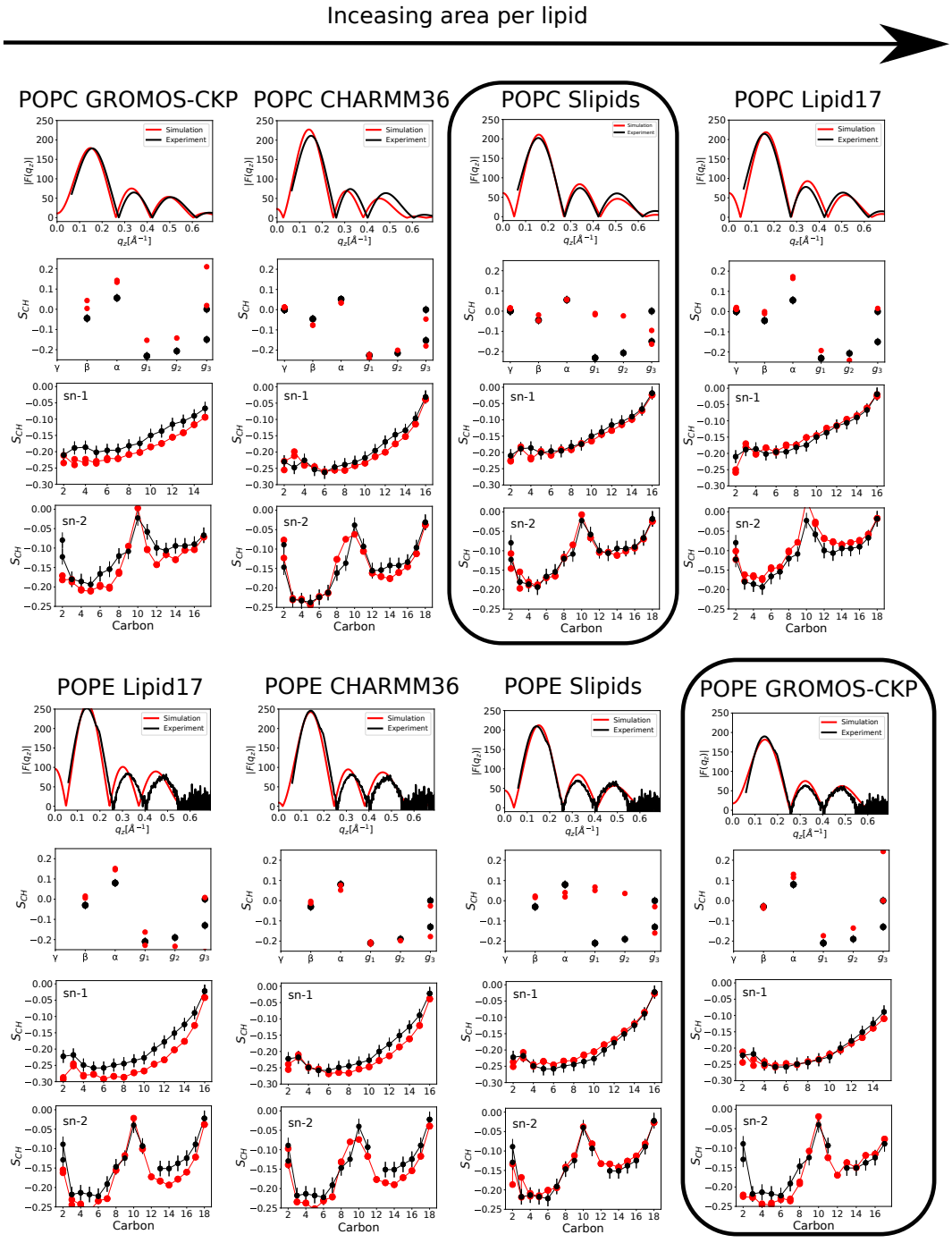

Figure S3. Simulations with the data for both POPC (top) and POPE (bottom) directly compared with the experimental data. The area per lipid in simulations increase from left to right. Simulations with the best overall quality for POPC and POPE order parameters are circled by a square.

S4 Water permeation through membranes

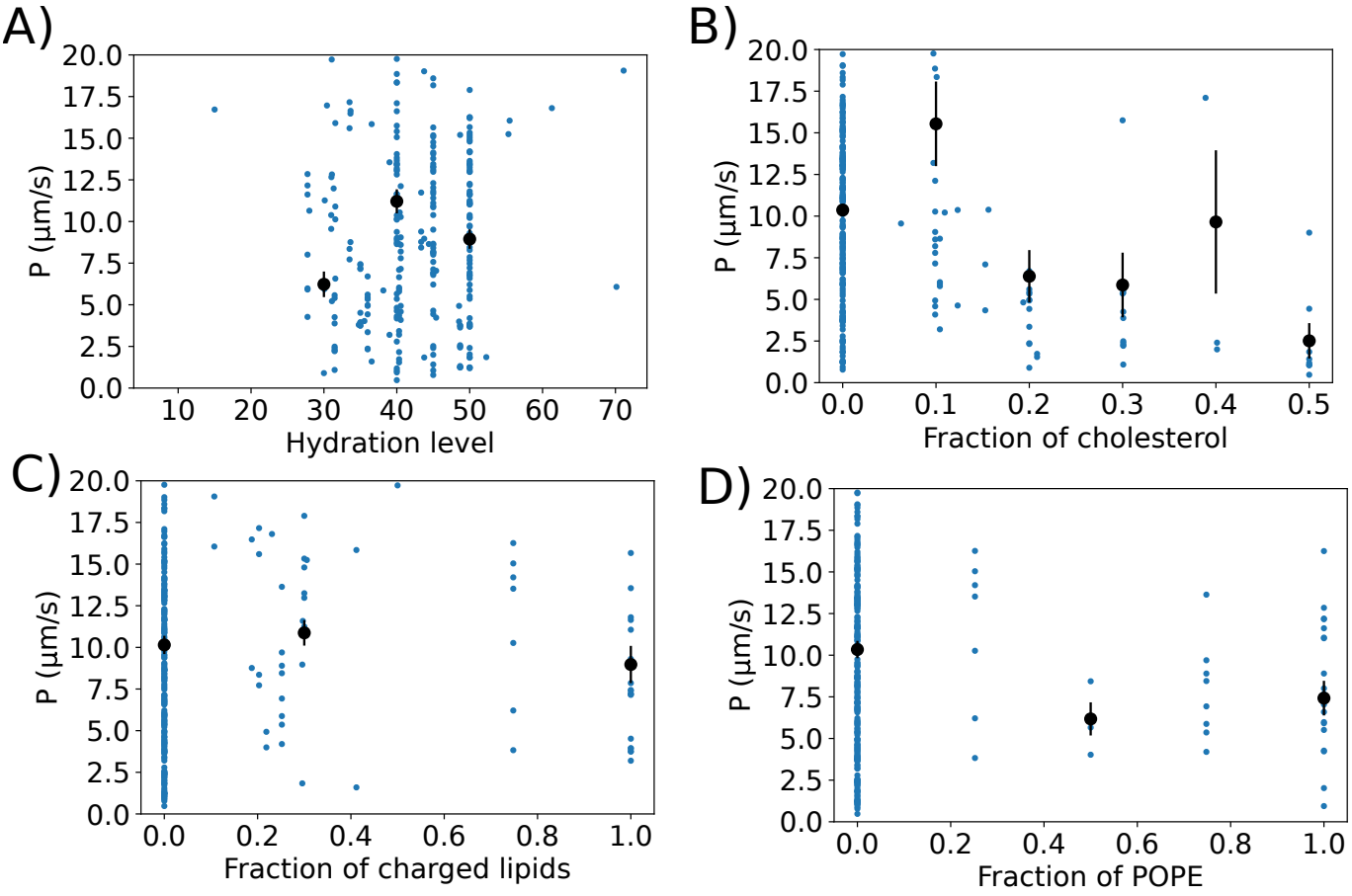

Figure S4. a) Structure of an overlay databank. More detailed structure of the layer 2 in the NMRlipids databank is illustrated in Fig. 5 in the SI. b) Distribution of the lengths of the trajectories, total number of trajectories and total lenght of the simulations in the NMRlipids databank. c) Distribution of lipids present in the trajectories in the NMRlipids databank. Lipids occuring in five or less simulations ('others') are listed in the right. d) Currently available binary mixtures in the NMRlipids databank. e) Distribution of force fields in the simulations in the NMRlipids databank. The figures and numbers are created on 9th of May 2022.

S5 Water diffusion along membranes

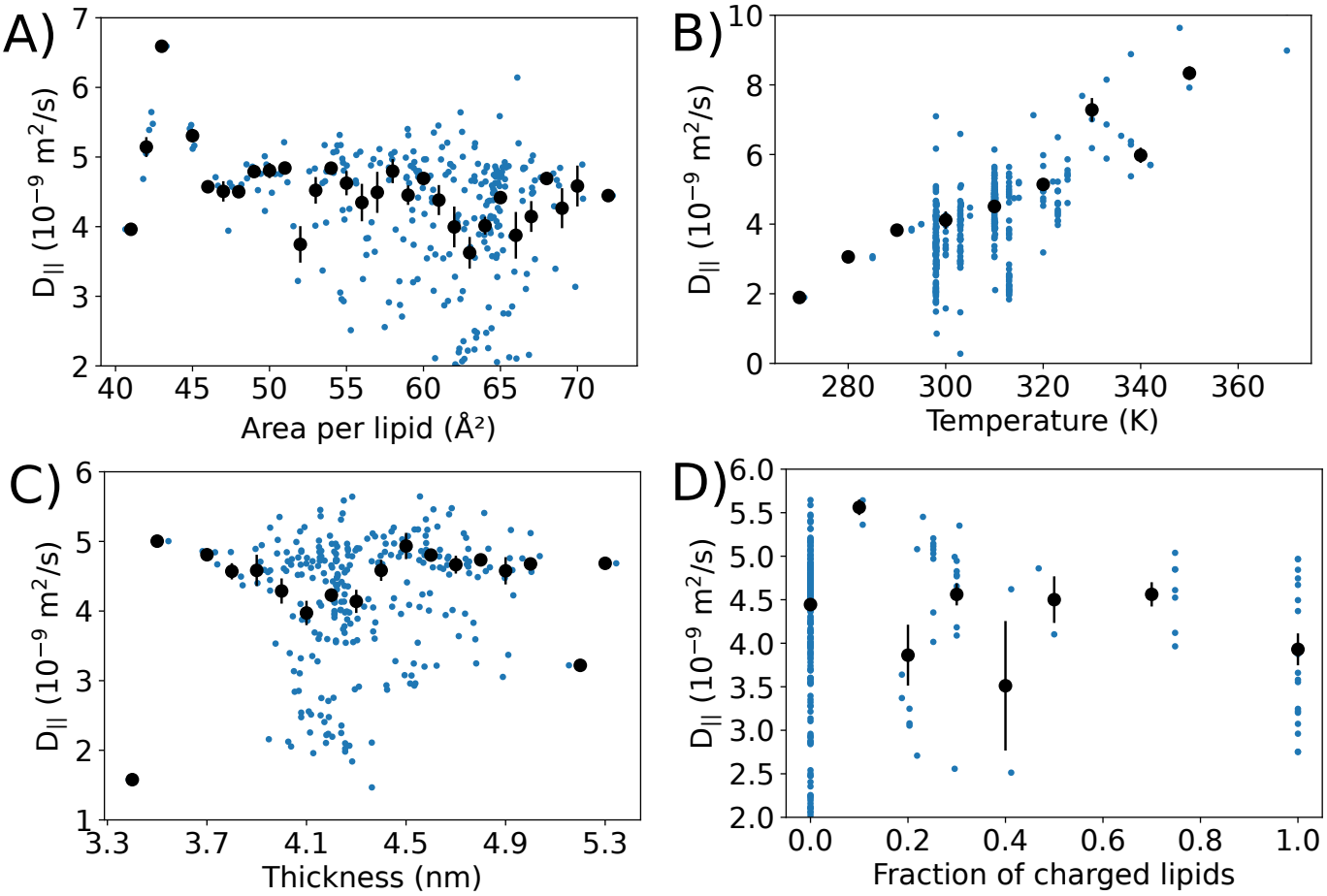

Figure S5. a) Structure of an overlay databank. More detailed structure of the layer 2 in the NMRlipids databank is illustrated in Fig. 5 in the SI. b) Distribution of the lengths of the trajectories, total number of trajectories and total lenght of the simulations in the NMRlipids databank. c) Distribution of lipids present in the trajectories in the NMRlipids databank. Lipids occuring in five or less simulations ('others') are listed in the right. d) Currently available binary mixtures in the NMRlipids databank. e) Distribution of force fields in the simulations in the NMRlipids databank. The figures and numbers are created on 9th of May 2022.

References

1. Javanainen, M. Simulations of POPC/cholesterol mixtures at 298 K, three system sizes, CHARMM36, DOI: 10.5281/zenodo.7035350 (2021).