

# **SUPPLEMENTARY INFORMATION: NMRLipids Databank: Overlay Databank of Lipid Membrane Simulations Arising from Open Collaboration**

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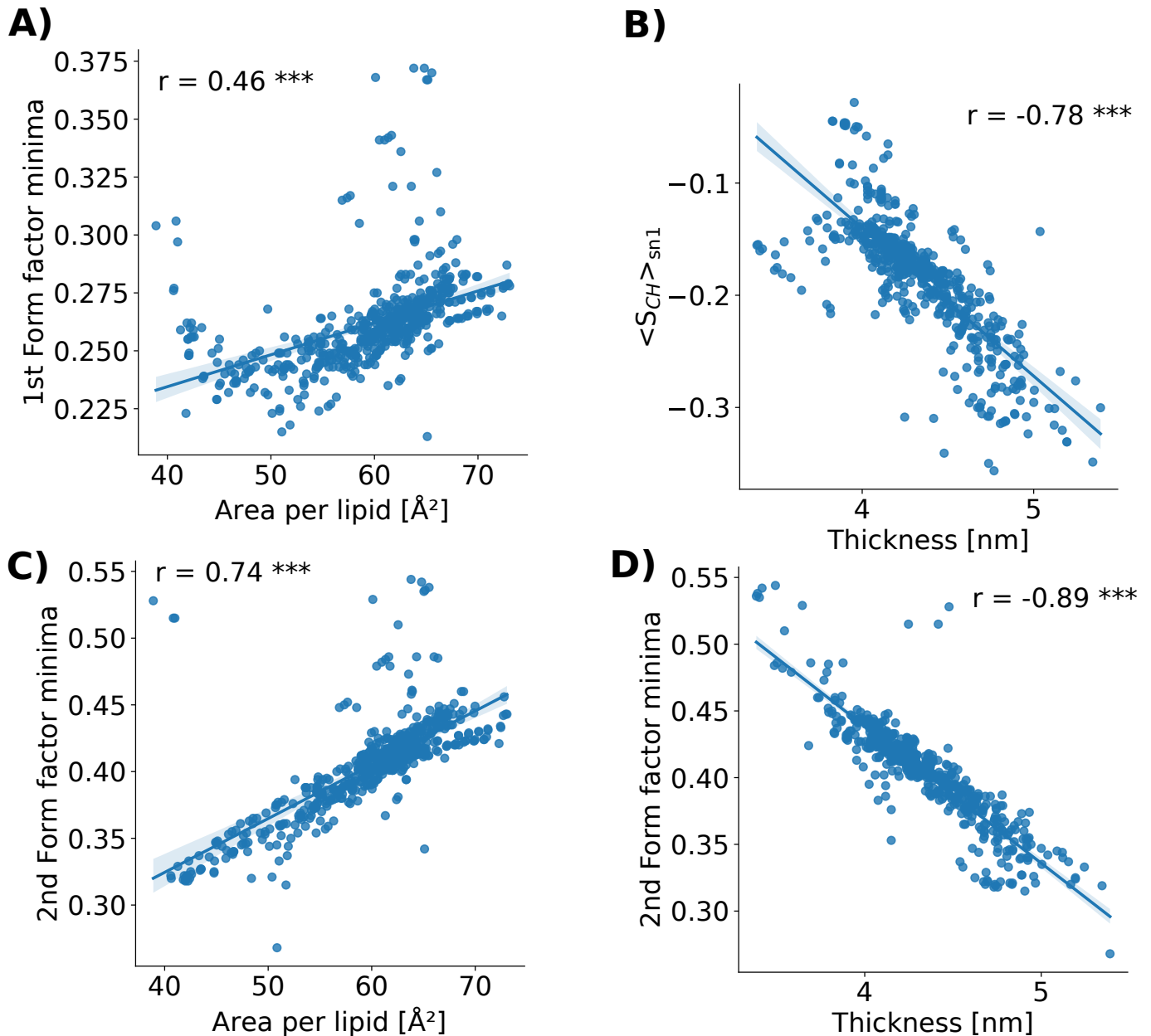
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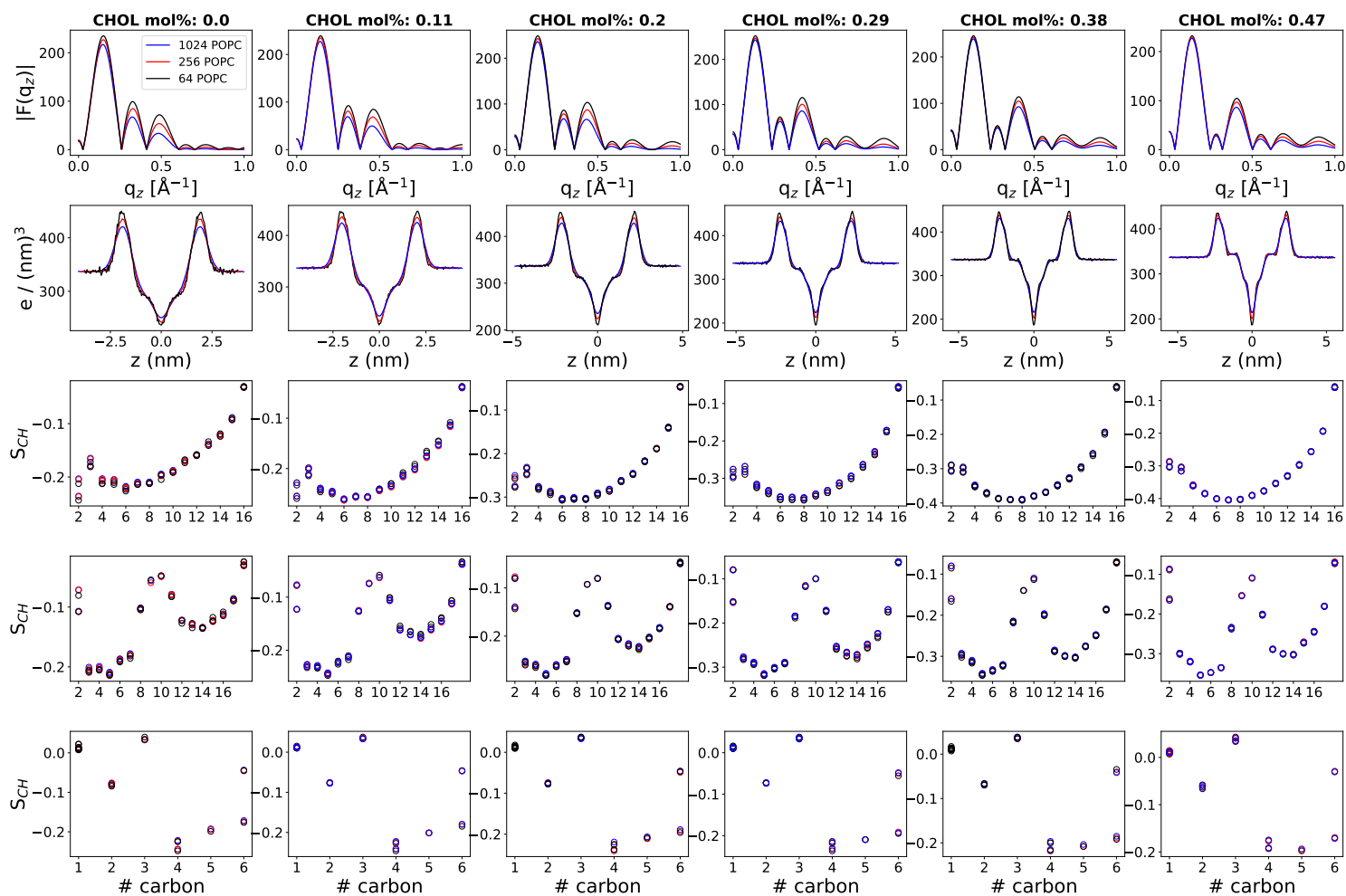
## **ABSTRACT**

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



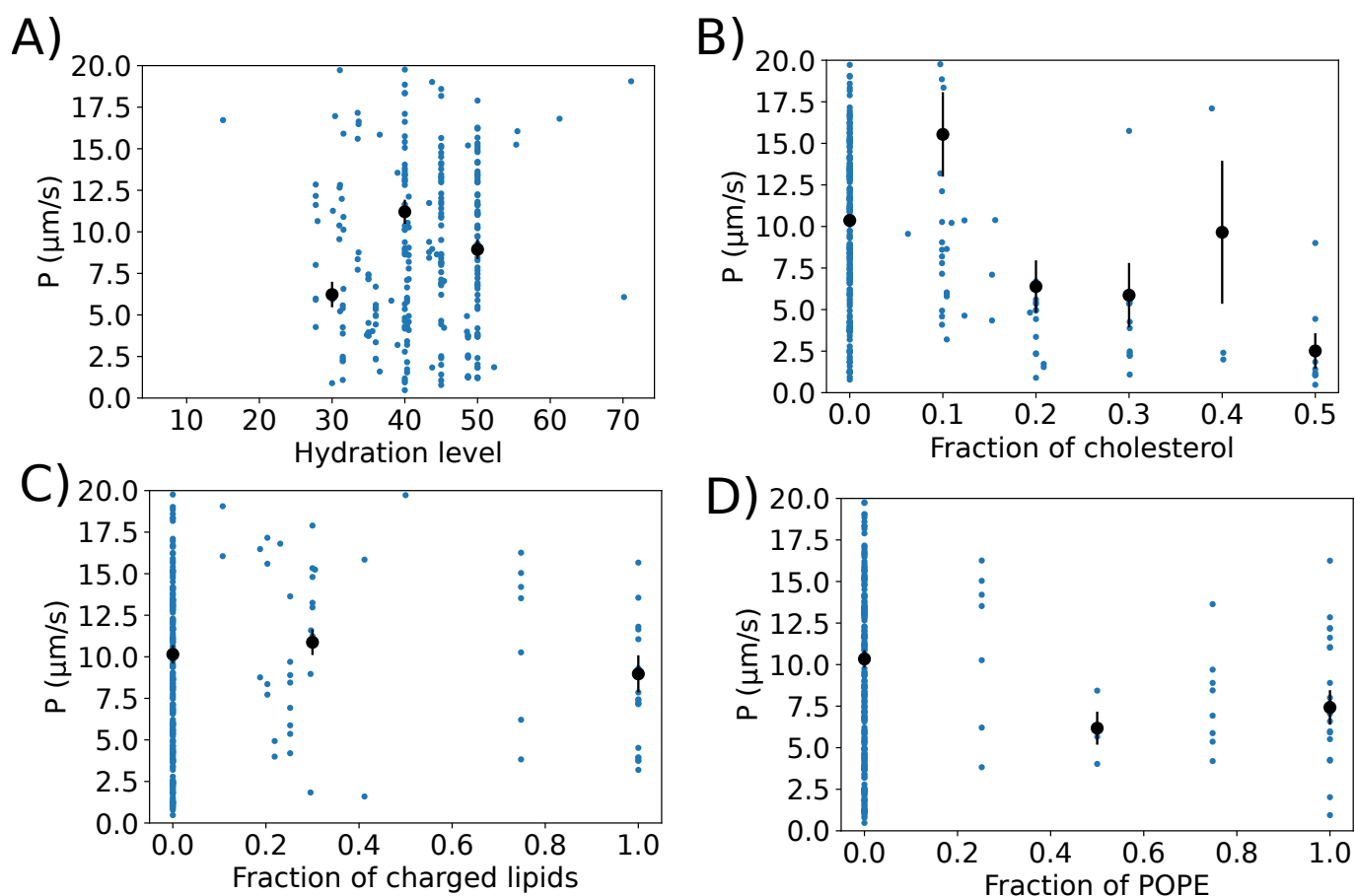
**Figure 1.** Dependence of form factor, electron density profiles along membrane normal, and C-H bond orderparameters (from top to bottom) on simulation box size with different cholesterol concentration.

## 2 Dependence of form factor and order parameters in the size of simulation



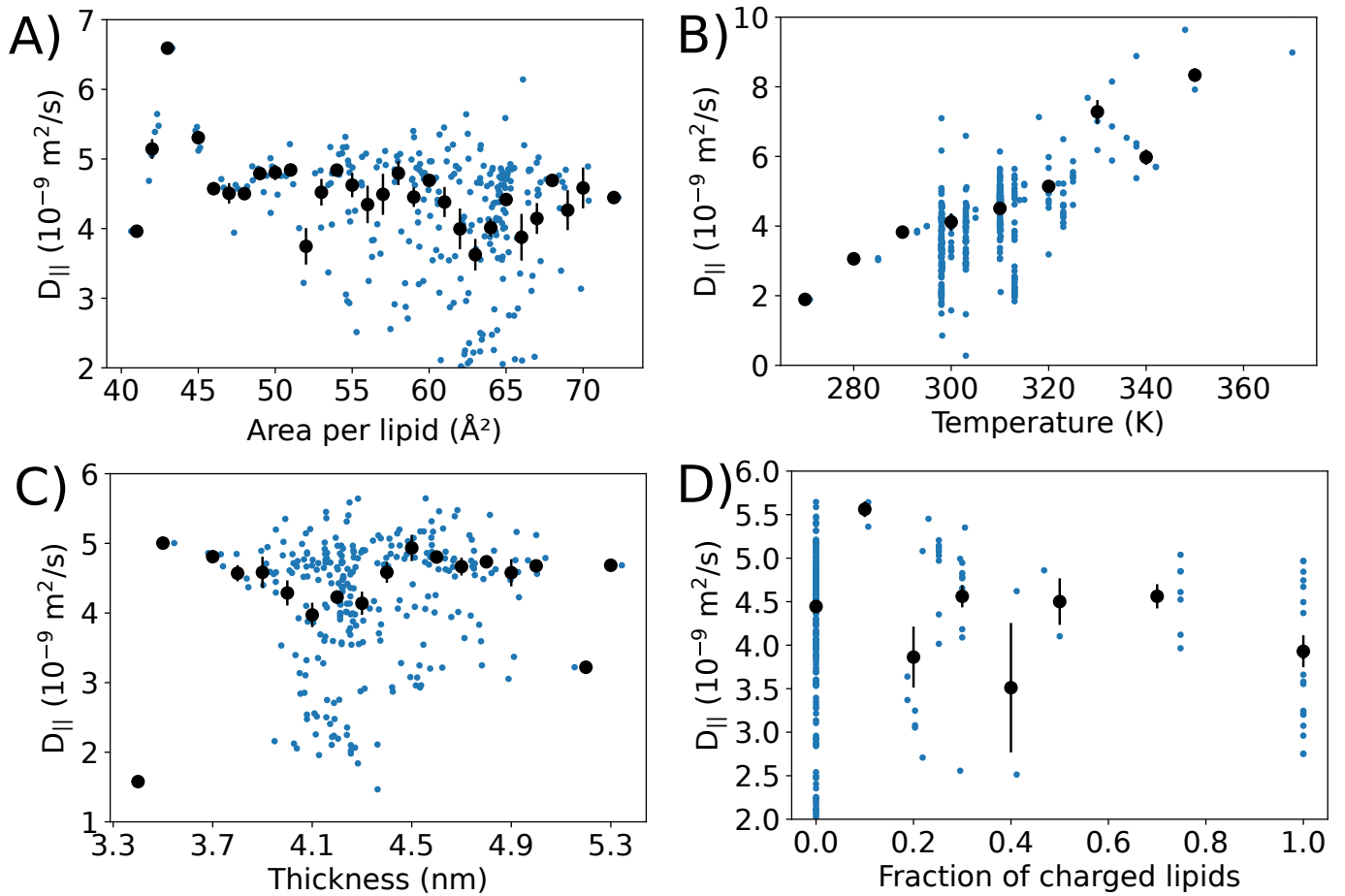
**Figure 2.** Dependence of form factor, electron density profiles along membrane normal, and C-H bond orderparameters (from top to bottom) on simulation box size with different cholesterol concentration.

### 3 Water permeation through membranes



**Figure 3.** a) Structure of an overlay databank. More detailed structure of the layer 2 in the NMRLipids databank is illustrated in Fig. ?? in the SI. b) Distribution of the lengths of the trajectories, total number of trajectories and total length of the simulations in the NMRLipids databank. c) Distribution of lipids present in the trajectories in the NMRLipids databank. Lipids occurring 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.

## 4 Water diffusion along membranes



**Figure 4.** a) Structure of an overlay databank. More detailed structure of the layer 2 in the NMRLipids databank is illustrated in Fig. ?? in the SI. b) Distribution of the lengths of the trajectories, total number of trajectories and total length of the simulations in the NMRLipids databank. c) Distribution of lipids present in the trajectories in the NMRLipids databank. Lipids occurring 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