

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

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ABSTRACT

1 Water permeation through membranes

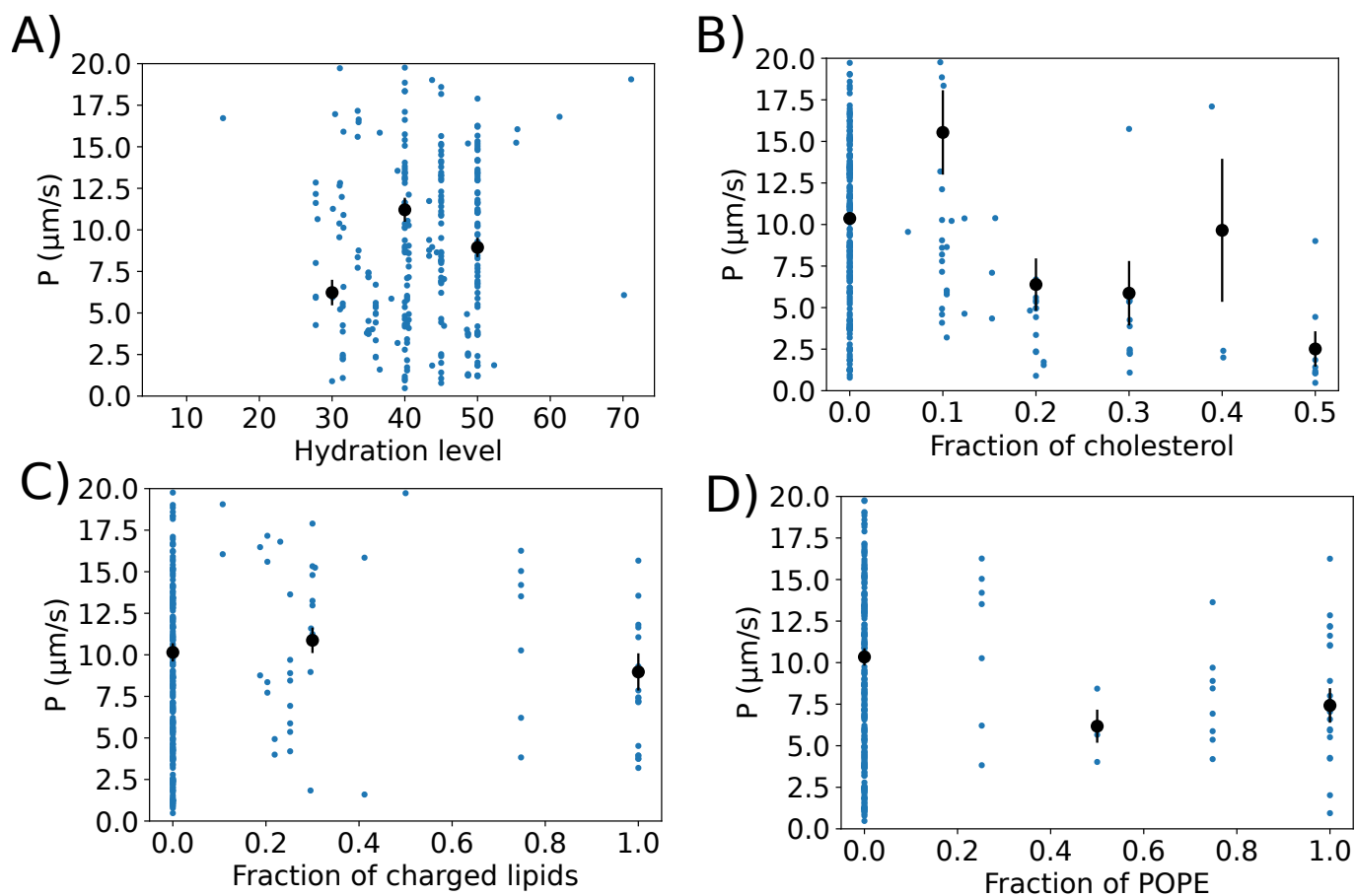


Figure 1. a) Structure of an overlay databank. More detailed structure of the layer 2 in the NMRLipids databank is illustrated in Fig. ?? in the SI. b) Distribution of the lengths of the trajectories, total number of trajectories and total length of the simulations in the NMRLipids databank. c) Distribution 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.

2 Water diffusion along membranes

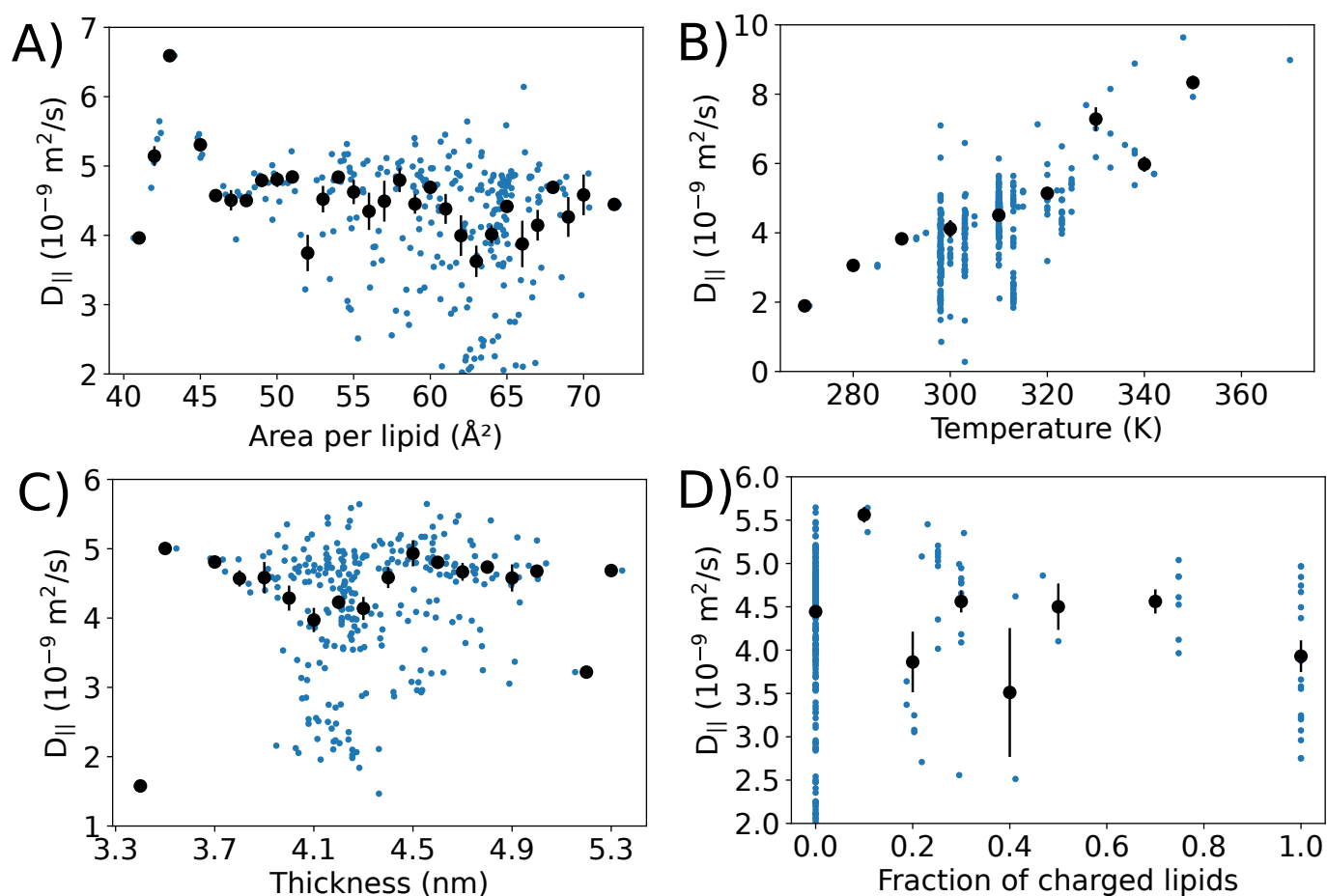


Figure 2. a) Structure of an overlay databank. More detailed structure of the layer 2 in the NMRLipids databank is illustrated in Fig. ?? in the SI. b) Distribution of the lengths of the trajectories, total number of trajectories and total length of the simulations in the NMRLipids databank. c) Distribution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