Quantitative quality of lipid-cholesterol interactions in atomistic resolution molecular dynamics simulations

O. H. Samuli Ollila[1,*]

[1]*Aalto University*

(Dated: September 27, 2015)

The quantitative quality of lipid-cholesterol interactions in atomistic resolution models will be determined against NMR and scattering data.

INTRODUCTION

The quantitative quality of lipid-cholesterol interactions in atomistic resolution models will be determined against NMR and scattering data.

COMPARISON OF ACYL CHAIN ORDER PARAMETERS BETWEEN EXPERIMENTS AND SIMULATIONS

Order parameters from simulations and experiments for acyl chains of 1-palmitoyl-2-oleoylphosphatidylcholine (POPC) are shown in Fig. 1.

1.Why are the order parameters of CHARMM36 too large compared to simulations even without cholesterol?

2.Why there is decrease in order parameters towards beginning of acyl chain in MacRog model without cholesterol?

3.Do the results suggests that condensation effect is too strong in MacRog model?

COMPARISON OF STRUCTURE FACTORS BETWEEN EXPERIMENTS AND SIMULATIONS

4.Structure factors should be calculated from the data with cholesterol from CHARMM and MacRog simulations (the trajectories are in Zenodo). The calculations from Berger model should be checked (data in https://github.com/NMRLipids/NmrLipidsCholXray/tree/master/scratch/POPCberger)

5.The experimental data delivered by Georg Pabst and Peter Heftberger should be plotted together with the simulation results. The data is already in https://github.com/NMRLipids/NmrLipidsCholXray/tree/master/DATA/POPC-Cholesterol

CONCLUSIONS

ToDo

P.

* samuli.ollila@aalto.fi

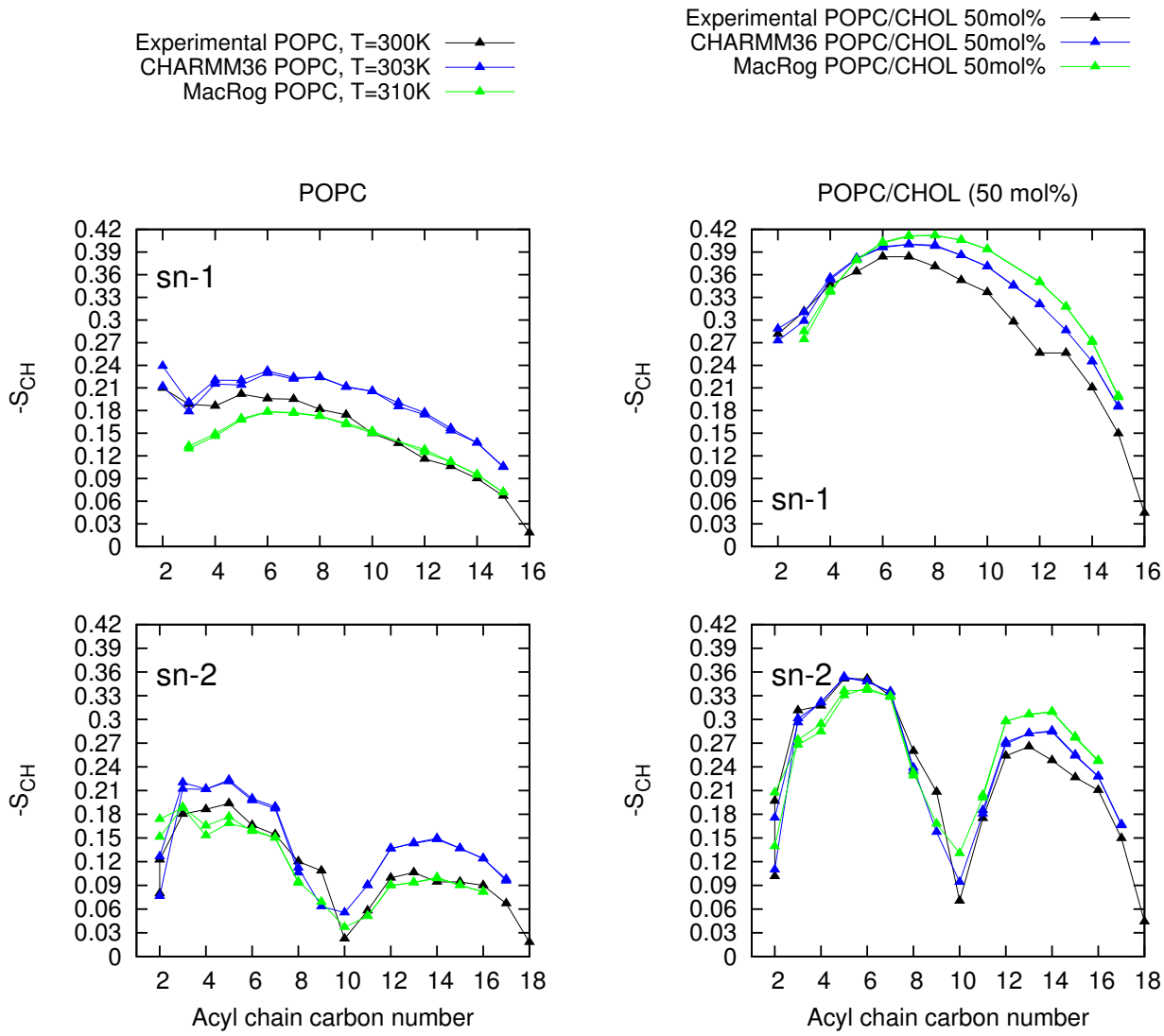

FIG. 1: Order parameters from simulations and experiments for acyl chains of 1-palmitoyl-2-oleoylphosphatidylcholine (POPC).