NMRLipids VI: Polarizable Force Fields

Batuhan Kav,* O. H. Samuli Ollila, and Markus S. Miettinen

Forschungszentrum Juelich, Germany

E-mail: b.kav@fz-juelich.de

Abstract

For the initial project description, please refer to

https://github.com/batukav/NMRlipidsVIpolarizableFFs/blob/master/Manuscript/manuscript.pdf

Introduction

Methods

This project is performed using the "NMRLipids Databank" format and all related files, except the trajectories, are available under "https://github.com/batukav/NMRlipidsVIpolarizableFFs/" Order parameters are calculated using the script "OrderParameters.py" under "https://github.com/batukav/NMRlipidsVIpolarizableFFs/tree/master/scripts". Dihedral distributions are calculated using the script "calcDihedral.py" under "https://github.com/batukav/NMRlipidsVIpolarizableFFs/tree/master/scripts" .

Simulation Details

| Lipid/counter-ions	force field	Ion (M)	N_l	N_w	N_{ion}	T (K)	t_{sim} (ns)	$t_{analysis}$ (ns)	files
POPC	CHARMM-Drude	NA	NA	6400	0	303	500	400	1
POPE	CHARMM-Drude	NA	NA	6400	0	303	350	300	2
	CHARMM-Drude	0.350	144	6400	41	303	500	400	3
	CHARMM-Drude	0.450	144	6400	51	303	500	400	4
POPC:NaCl	CHARMM-Drude	0.650	144	6400	77	303	500	400	5
	CHARMM-Drude	1.0	144	6400	115	303	500	400	6
	CHARMM-Drude	0.350	144	6400	41	303	500	400	7
POPC:CaCl$_2$	CHARMM-Drude	0.450	144	6400	52	303	500	400	8
	CHARMM-Drude	0.650	144	6400	76	303	500	400	9
	CHARMM-Drude	1.0	144	6400	114	303	500	400	10

Results
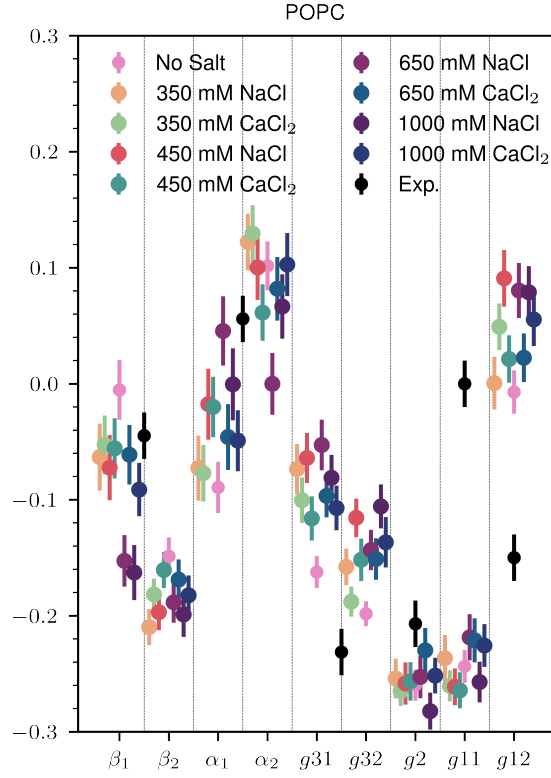
Figure 1: The head group and glycerol backbone order parameters S_{CH} for the POPC simulations. The experimental values on the dashed lines mean that the different isomers 1/2 experimentally could not be resolved.
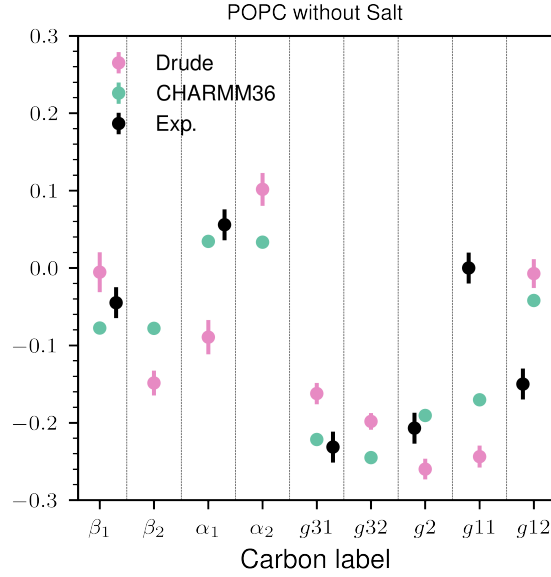
Figure 2: The head group and glycerol backbone order parameters S_{CH} for the POPC simulations without salt.
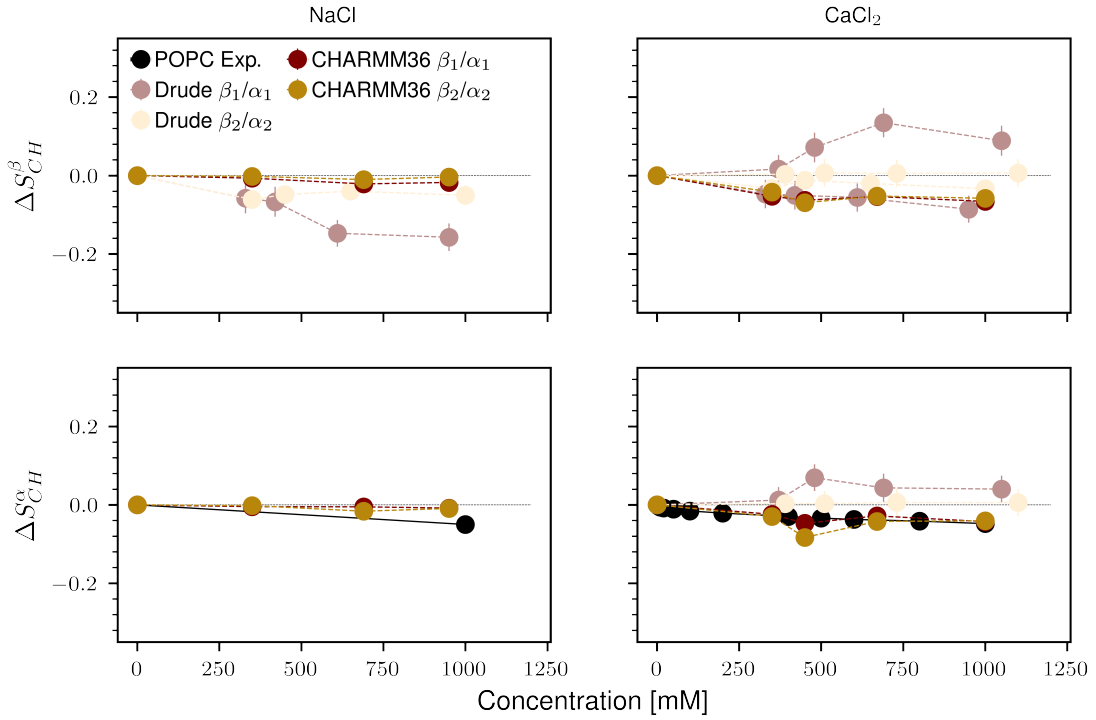

Figure 3: The change in the head group order parameters with respect to the simulations without salt as a function of the salt concentration.
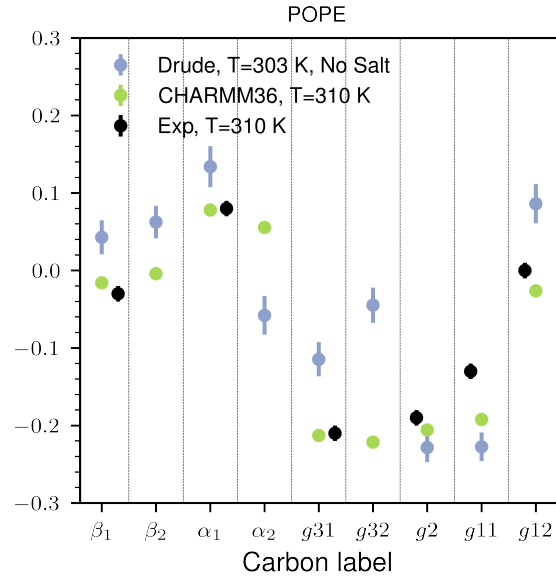
Figure 4: The head group and glycerol backbone order parameters S_{CH} for the POPE simulations.
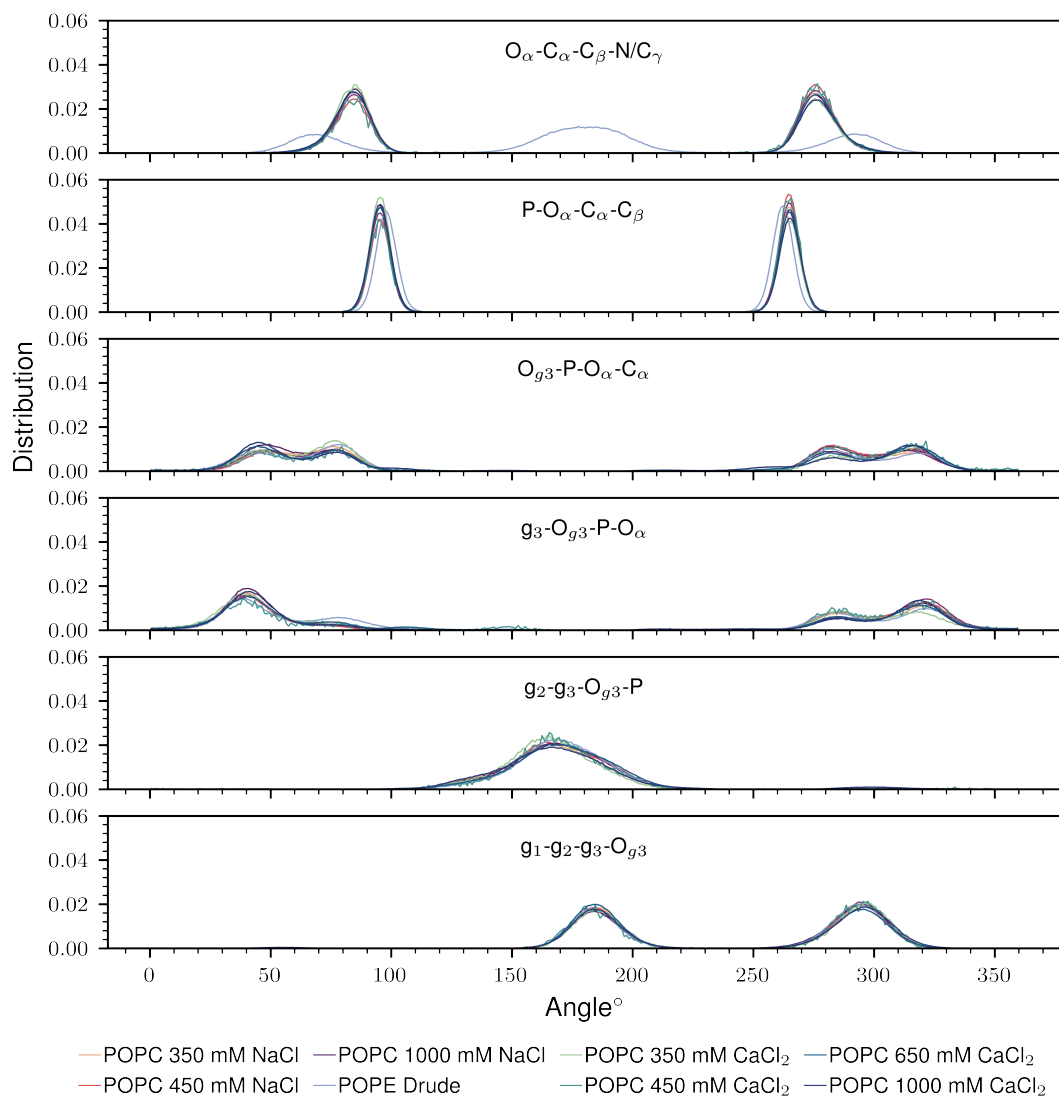
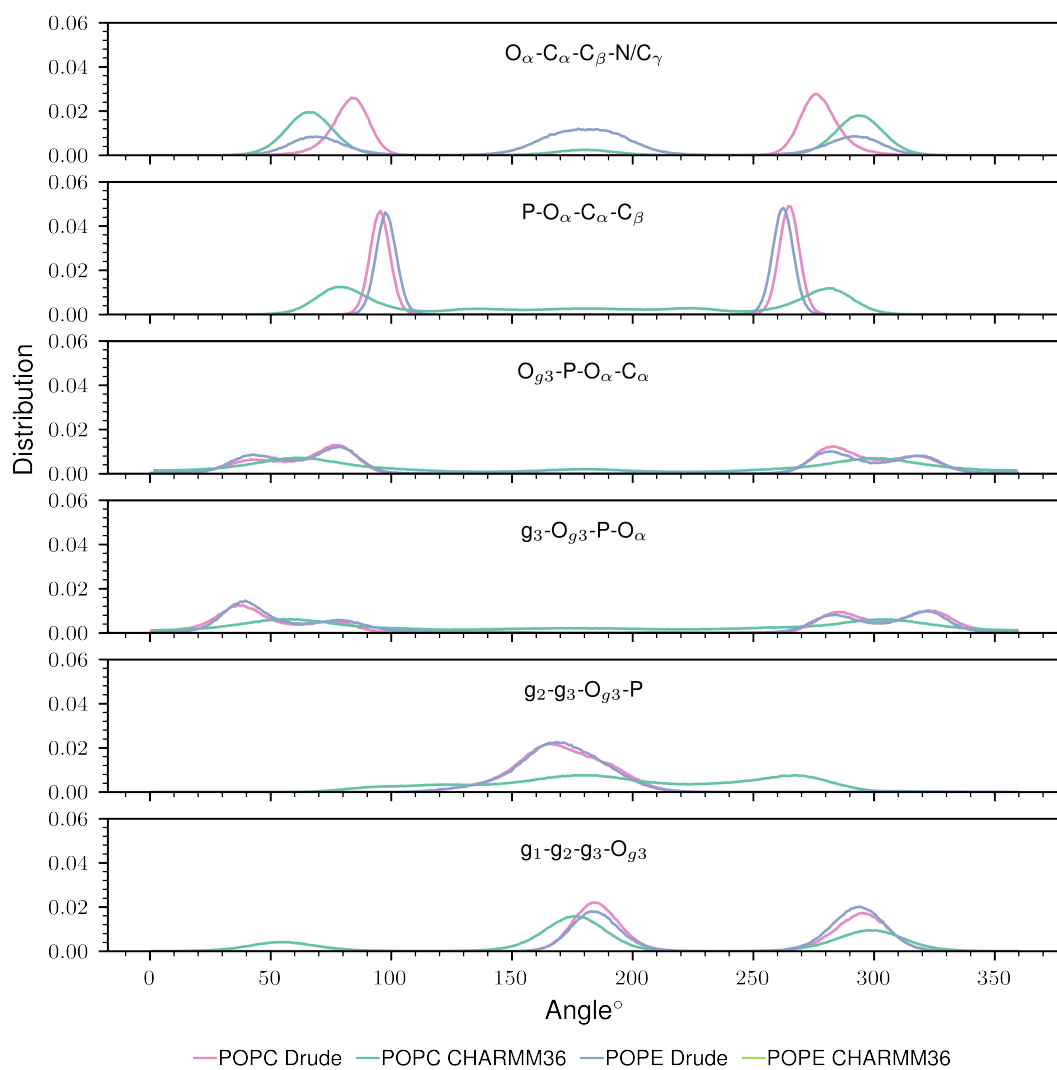Figure 5: The distributions of the torsion angles for the head group atoms

Figure 6: The distributions of the torsion angles for the head group atoms without the presence of salt.

Acknowledgement

Supporting Information Available

References

(1) Kav, B. Pure POPC membrane simulations with the CHARMM- Drude force field (OpenMM 7.5.0). 2021; https://doi.org/10.5281/zenodo.4604630.

(2) Kav, B. Pure POPE membrane simulations with the CHARMM- Drude force field (OpenMM 7.5.0). 2021; https://doi.org/10.5281/zenodo.4665773.

(3) Kav, B. Pure POPC Membrane with 350mM NaCl simulations using Drude Polarizable Force Field and OpenMM. 2020; https://doi.org/10.5281/zenodo.4683386.

(4) Kav, B. Pure POPC Membrane with 450mM NaCl simulations using Drude Polarizable Force Field and OpenMM. 2020; https://doi.org/10.5281/zenodo.4683398.

(5) Kav, B. Pure POPC Membrane with 650mM NaCl simulations using Drude Polarizable Force Field and OpenMM. 2020; https://doi.org/10.5281/zenodo.4683405.

(6) Kav, B. Pure POPC Membrane with 1000mM NaCl simulations using Drude Polarizable Force Field and OpenMM. 2020; https://doi.org/10.5281/zenodo.4683411.

(7) Kav, B. Pure POPC Membrane with 350mM CaCl2 simulations using Drude Polarizable Force Field and OpenMM. 2020; https://doi.org/10.5281/zenodo.4683393.

(8) Kav, B. Pure POPC Membrane with 450mM CaCl2 simulations using Drude Polarizable Force Field and OpenMM. 2020; https://doi.org/10.5281/zenodo.4683391.

(9) Kav, B. Pure POPC Membrane with 650mM CaCl2 simulations using Drude Polarizable Force Field and OpenMM. 2020; https://doi.org/10.5281/zenodo.4683394.

(10) Kav, B. Pure POPC membrane simulations with 1000 mM CaCl2 with the CHARMM-Drude force field (OpenMM). 2021; `https://doi.org/10.5281/zenodo.4738966`.