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

Results

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]
POPC:NaCl	CHARMM-Drude	0.350	144	6400	41	303	500	400	[3]
	CHARMM-Drude	0.450	144	6400	51	303	500	400	[4]
	CHARMM-Drude	0.650	144	6400	77	303	500	400	[5]
	CHARMM-Drude	1.0	144	6400	115	303	500	400	[6]
POPC:$CaCl_2$	CHARMM-Drude	0.350	144	6400	41	303	500	400	[7]
	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]

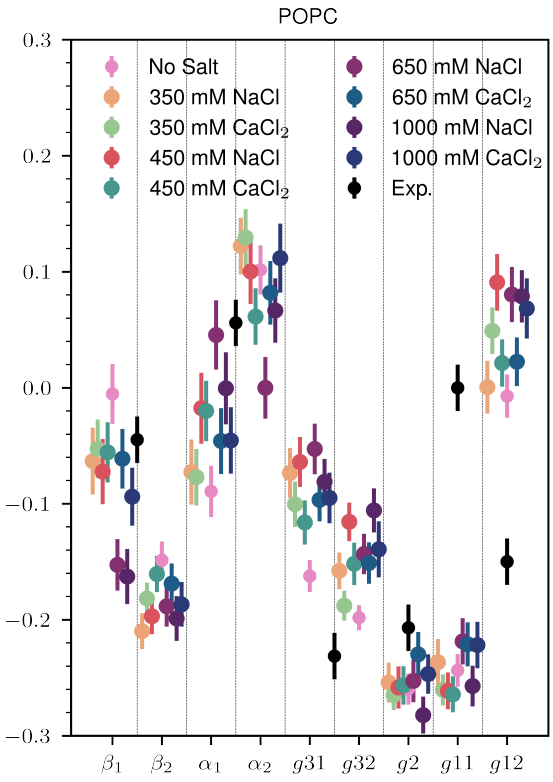

Figure 1: The head group and glycerol backbone order parameters S_{CH} for the POPC simulations. The experimental values on the dashed lines mean that the different isomers 1/2 experimentally could not be resolved.

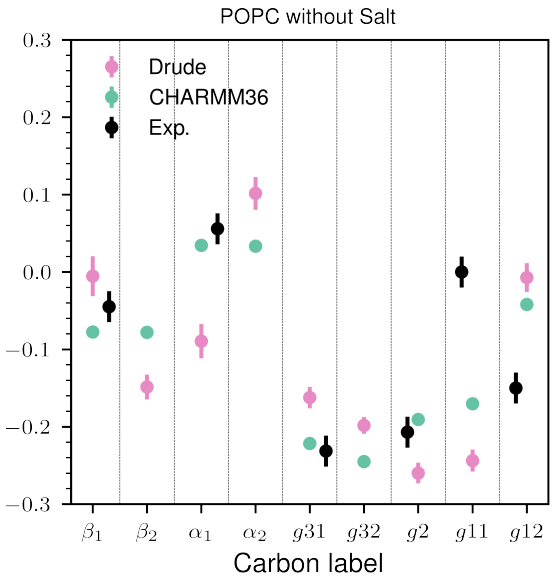

Figure 2: The head group and glycerol backbone order parameters S_{CH} for the POPC simulations without salt.

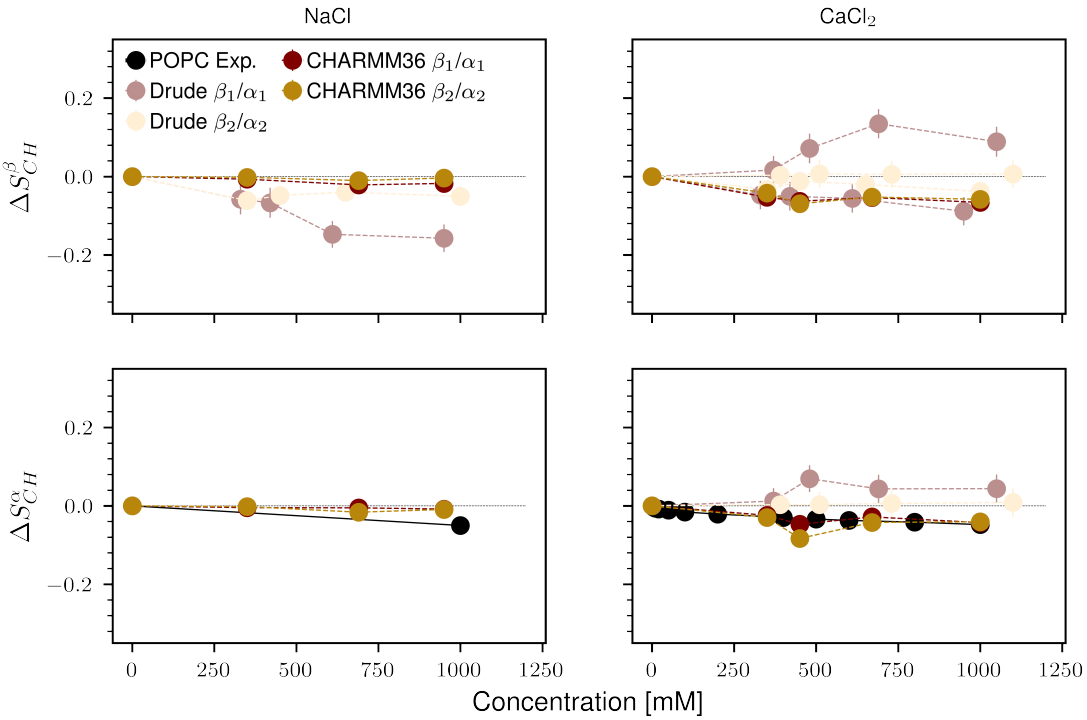

Figure 3: The change in the head group order parameters with respect to the simulations without salt as a function of the salt concentration.

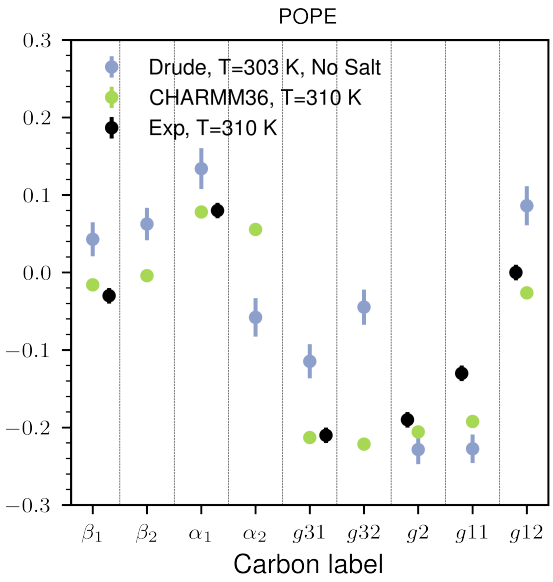

Figure 4: The head group and glycerol backbone order parameters S_{CH} for the POPE simulations.

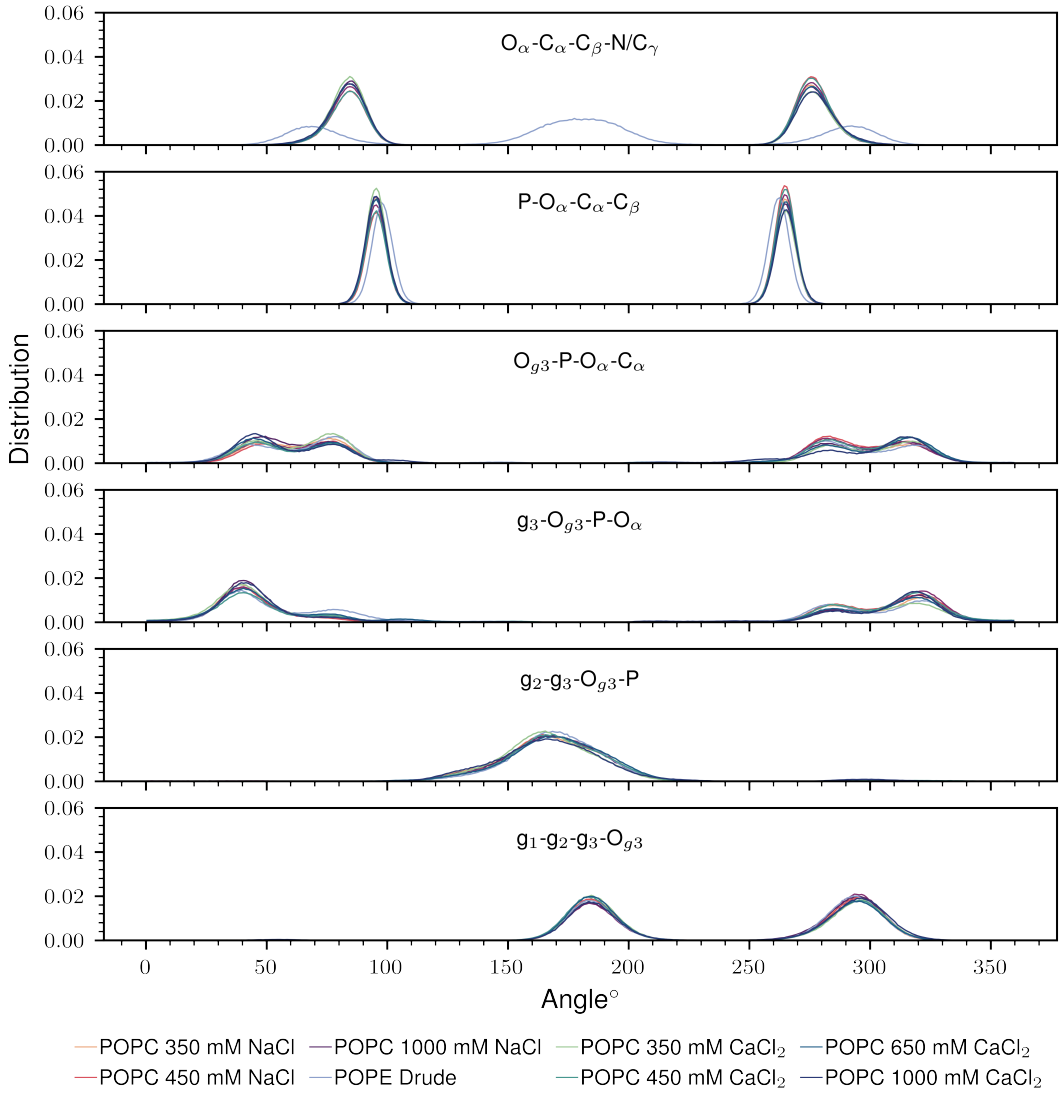

Figure 5: The distributions of the torsion angles for the head group atoms

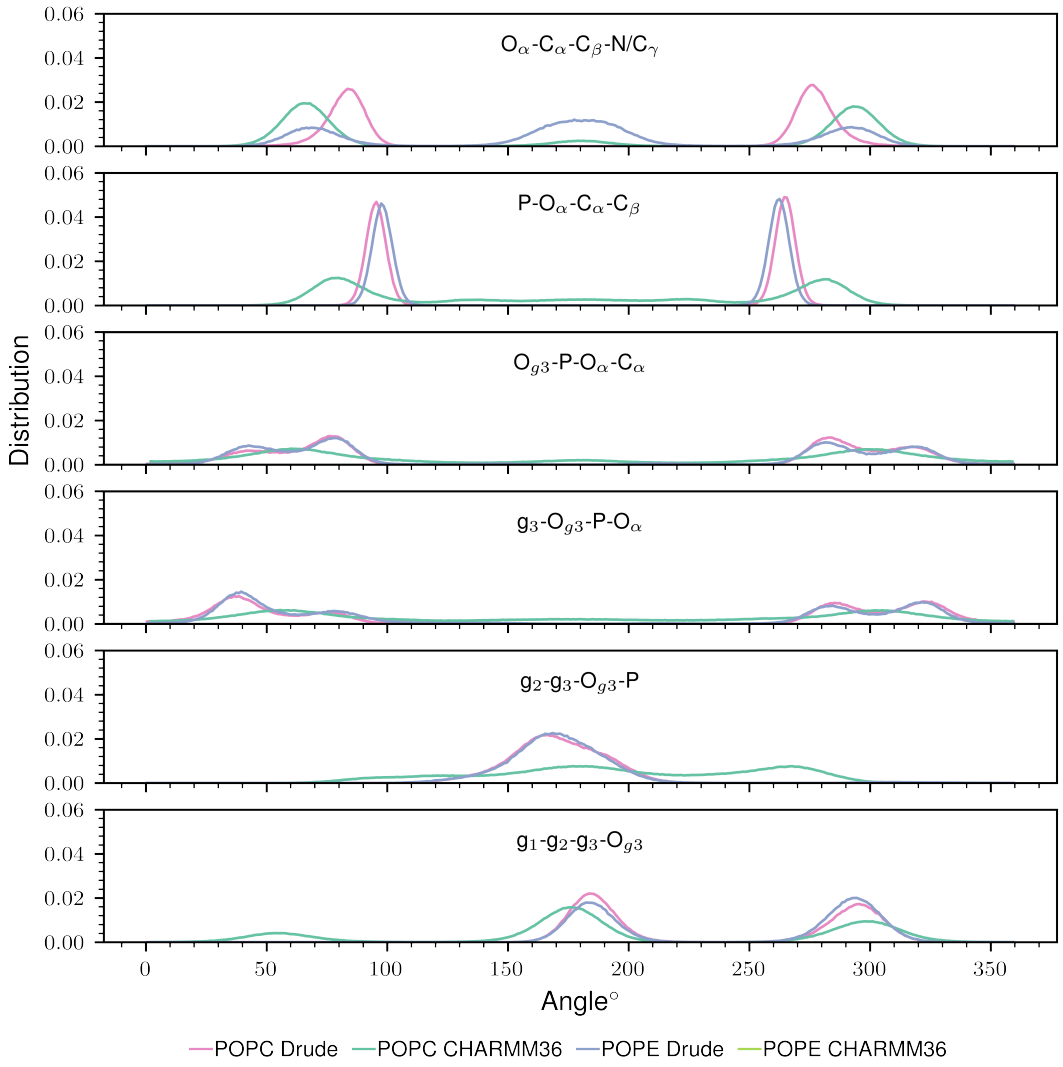

Figure 6: The distributions of the torsion angles for the head group atoms without the presence of salt.

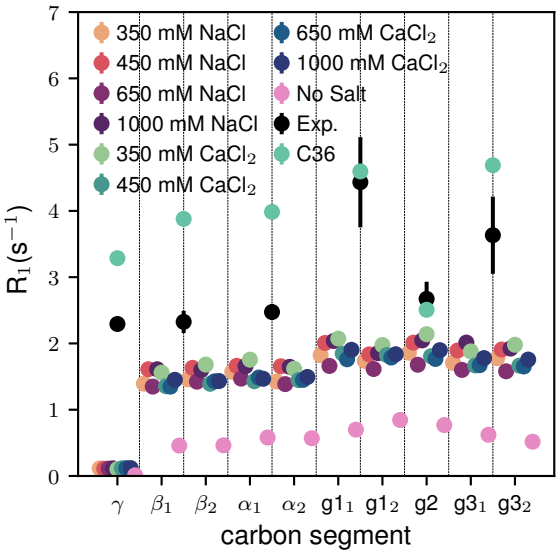

Figure 7: R1 times calculated for the POPC system. Experimental values are obtained from Ref.[11]

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`.

(11) Antila, H. S.; Wurl, A.; Ollila, O.; Miettinen, M. S.; Ferreira, T. M. Quasi-uncoupled rotational diffusion of phospholipid headgroups from the main molecular frame. *arXiv preprint arXiv:2009.06774* **2020**,