NMRLipids VI: Polarizable Force Fields

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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]
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]

Results

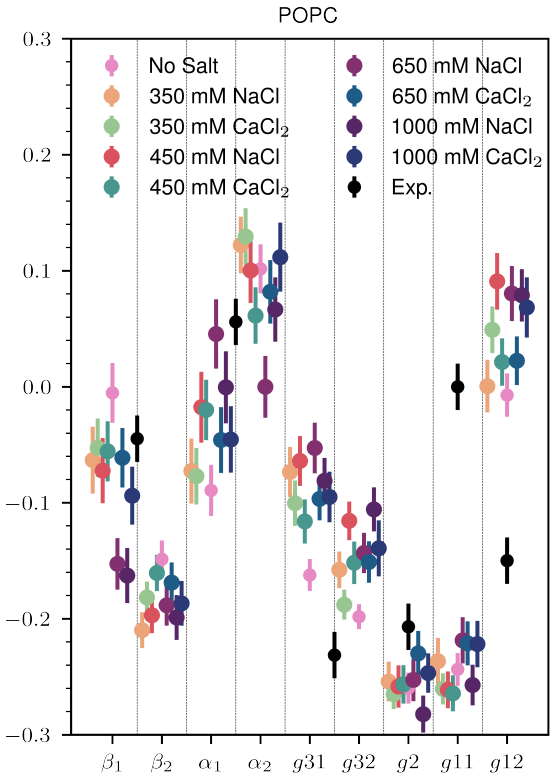

Figure 1: The head group and glycerol backbone order parameters S_{CH} for the POPC simulations. The experimental values on the dashed lines mean that the different isomers 1/2 experimentally could not be resolved.

1.SAMULI: I am not sure if we need this kind of figure. Systems without ions are in separate figures as well as dependence on ions.

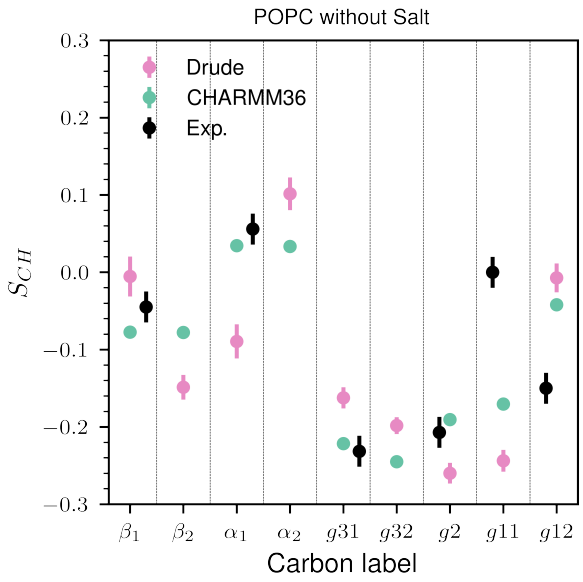

Figure 2: The head group and glycerol backbone order parameters S_{CH} for the POPC simulations without salt.

2.SAMULI: It would be good to put the experimental value also to second hydrogen even though it would be the same as for first. Now it looks like that those values would not be known.

3.SAMULI: y-axis should be more zoomed in.

4.SAMULI: Similar figure for POPE (now figure 4) could be here as panel B).

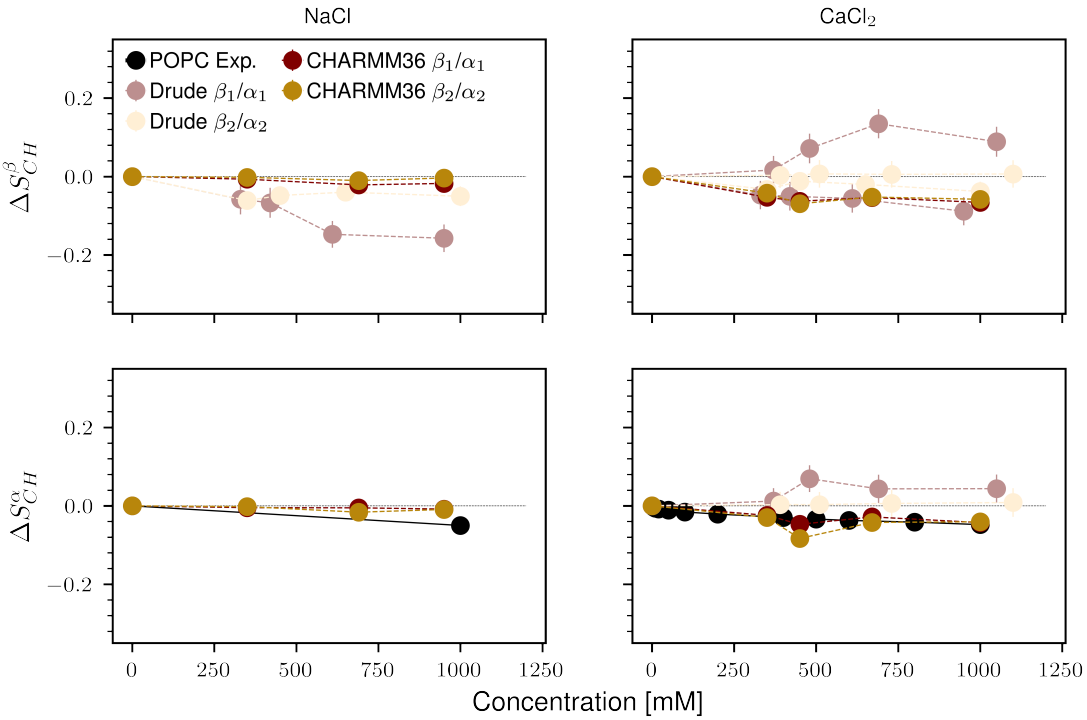

Figure 3: The change in the head group order parameters with respect to the simulations without salt as a function of the salt concentration.

5.SAMULI: y-axis scale should be much more zoomed in here, particularly the difference in experiments between sodium and calcium must be visible.

6.SAMULI: We should also show the ion density profiles along membrane normal and compare the ones with 1000 mM NaCl and 350 mM $CaCl_2$ (concentration in bulk water) to the best profiles in the literature (Fig. 5 in http://dx.doi.org/10.1021/acs.jpcb.7b12510). This will show the actual difference in ion binding to the best performing models available.

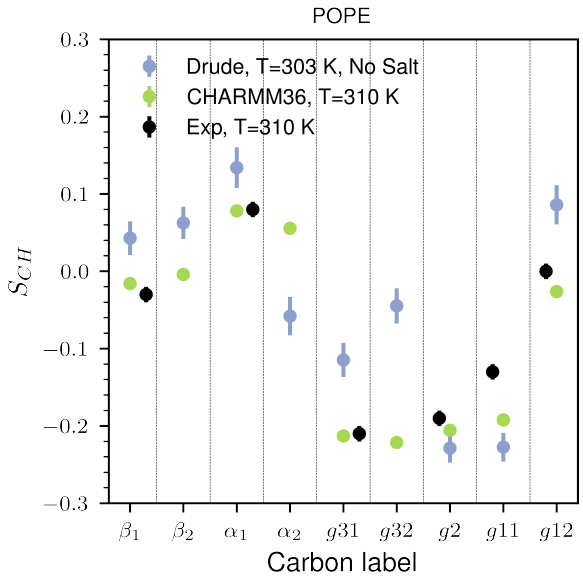

Figure 4: The head group and glycerol backbone order parameters S_{CH} for the POPE simulations.

7.SAMULI: Move to panel B) in Figure 1.

8.SAMULI: y-axis should be more zoomed in.

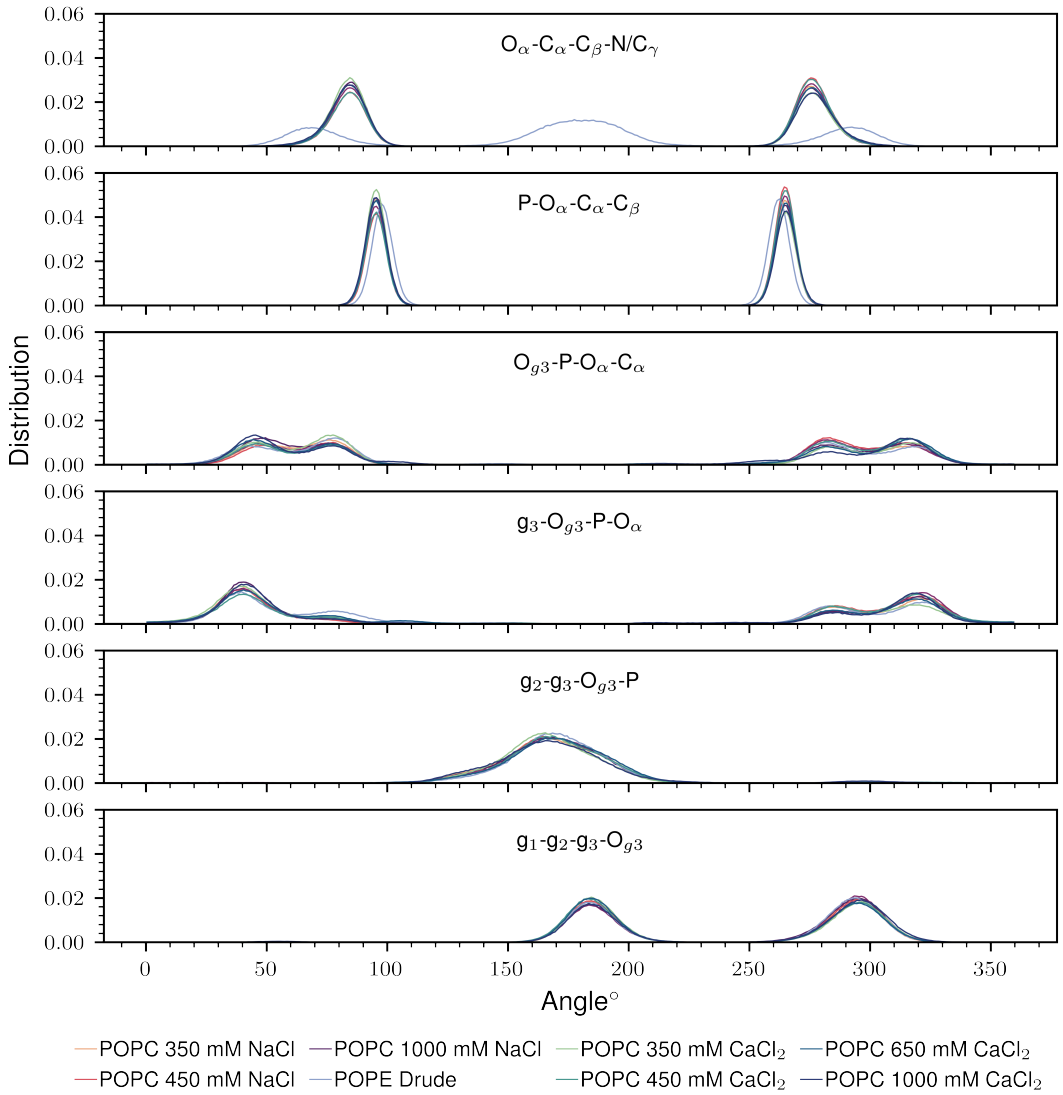

Figure 5: The distributions of the torsion angles for the head group atoms

9.SAMULI: I am not sure if we need this figure at all. Or were you planning to discuss why order parameter response to ions is qualitatively incorrect in Drude PC? If yes, then maybe remove POPE from this figure.

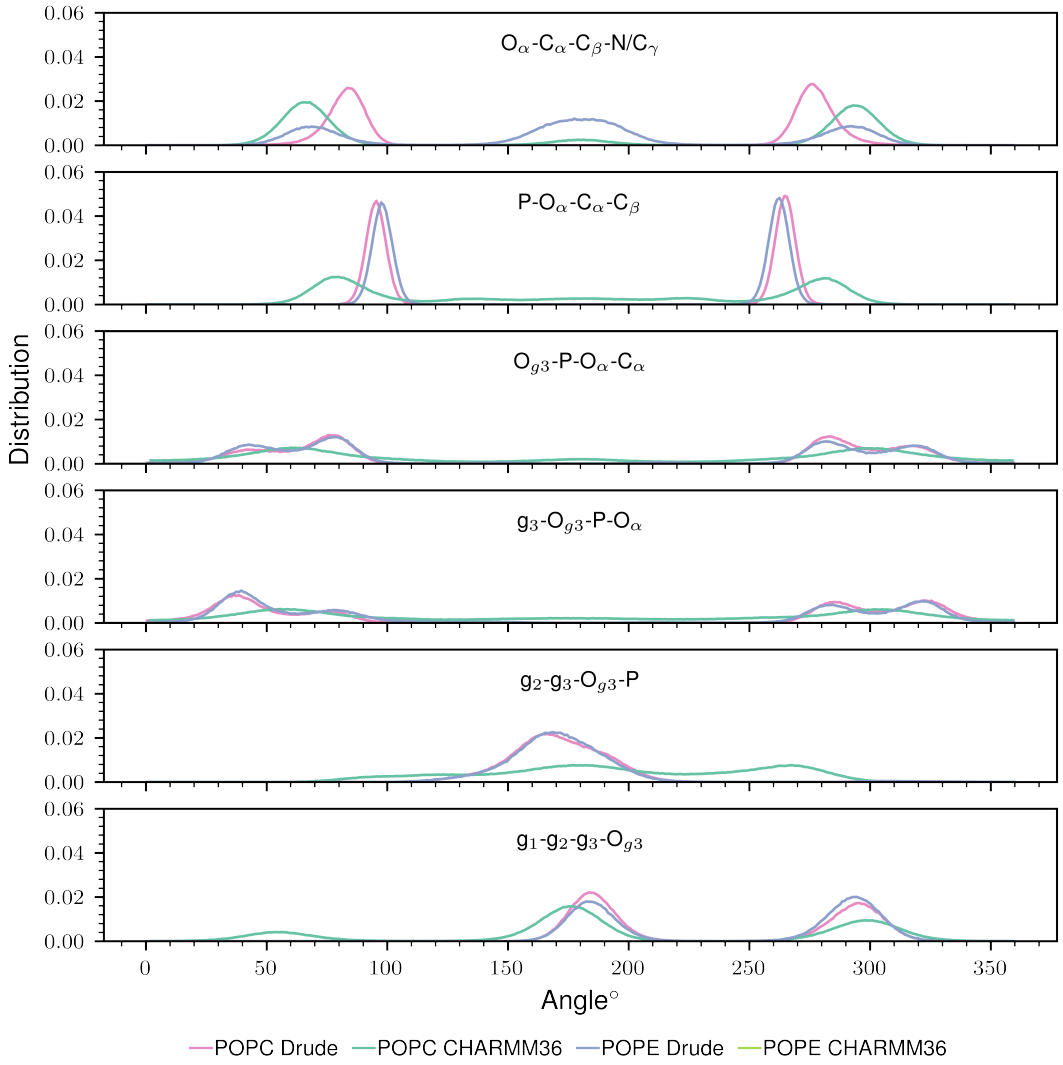

Figure 6: The distributions of the torsion angles for the head group atoms without the presence of salt.

10.SAMULI: I am not sure if I see POPE CHARMM36 lines in this figure. Also, colors, lines styles and/or widths could be better used to distinguish common and different elements in each line. For example, CHARMM36 with thick lines, drude thin lines, POPC black, POPE red, or something like that.

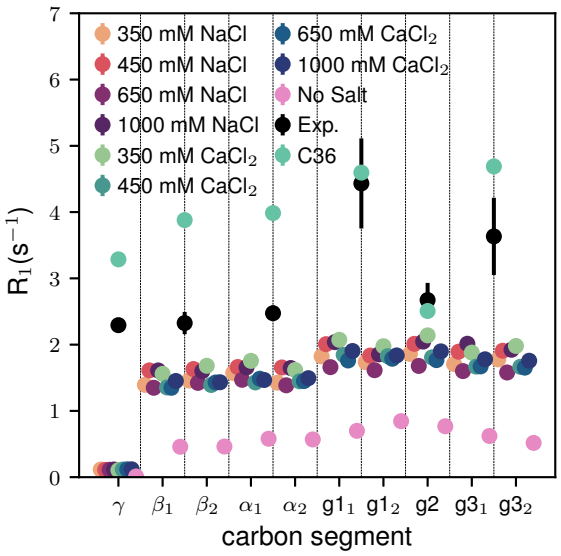

Figure 7: R1 times calculated for the POPC system. Experimental values are obtained from Ref.[11]

11.SAMULI: Are "No Salt" and all ion containing systems from Drude? Is it really true that addition of any salt increases the values to the same independently on the amount?

Acknowledgement

Supporting Information Available

This material is available free of charge via the Internet at http://pubs.acs.org/.

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. *arXiv preprint arXiv:2009.06774* **2020**,