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	NA	NA	NA	NA	NA	NA
POPC:NaCl	CHARMM-Drude	0.350	144	6400	41	303	500	500	[1]
	CHARMM-Drude	0.450	144	6400	51	303	500	500	[2]
	CHARMM-Drude	0.650	144	6400	77	303	500	500	[3]
	CHARMM-Drude	1.0	144	6400	115	303	500	500	[4]
POPC:$CaCl_2$	CHARMM-Drude	0.350	144	6400	41	303	500	500	[5]
	CHARMM-Drude	0.450	144	6400	52	303	500	500	[6]
	CHARMM-Drude	0.650	144	6400	76	303	500	500	[7]

Results and discussion

Order Parameters

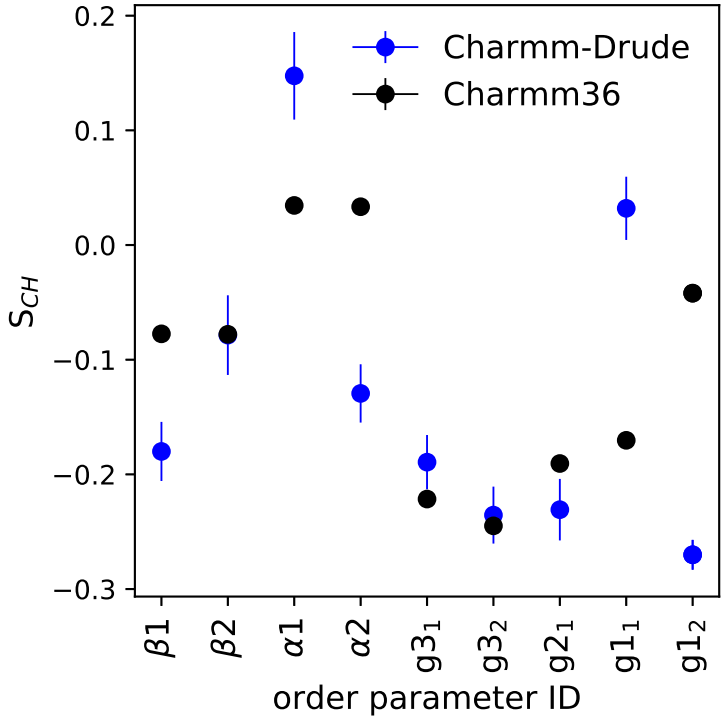

Figure 1: order parameters for the simulations without ions. Charmm36 data is copied from https://github.com/NMRLipids/MATCH/blob/master/Data/Lipid_Bilayers/POPC/T300K/MODEL_CHARMM36/OrdParsPOPC.dat

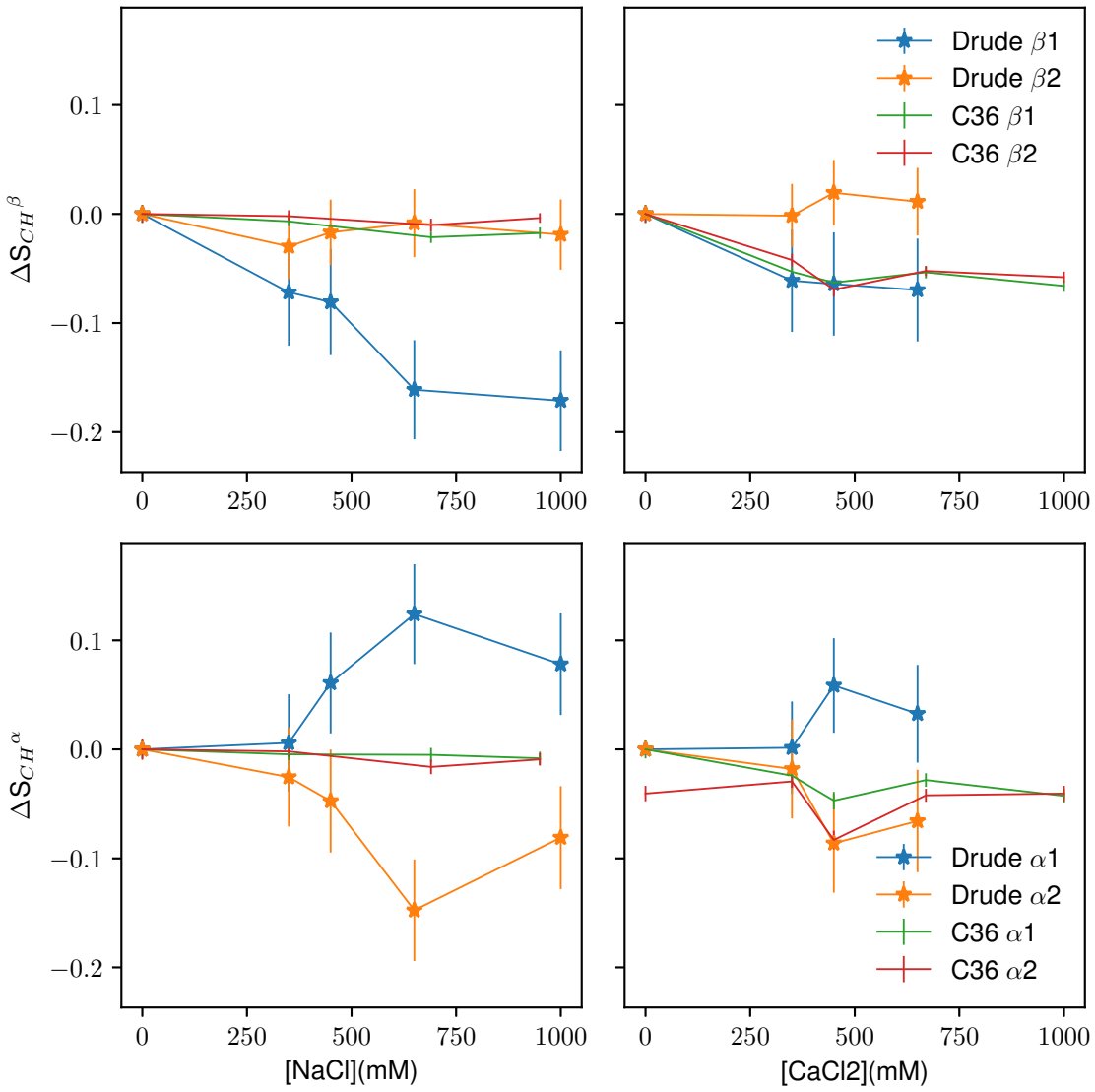

Figure 2: change in the order parameters

Dihedral distributions

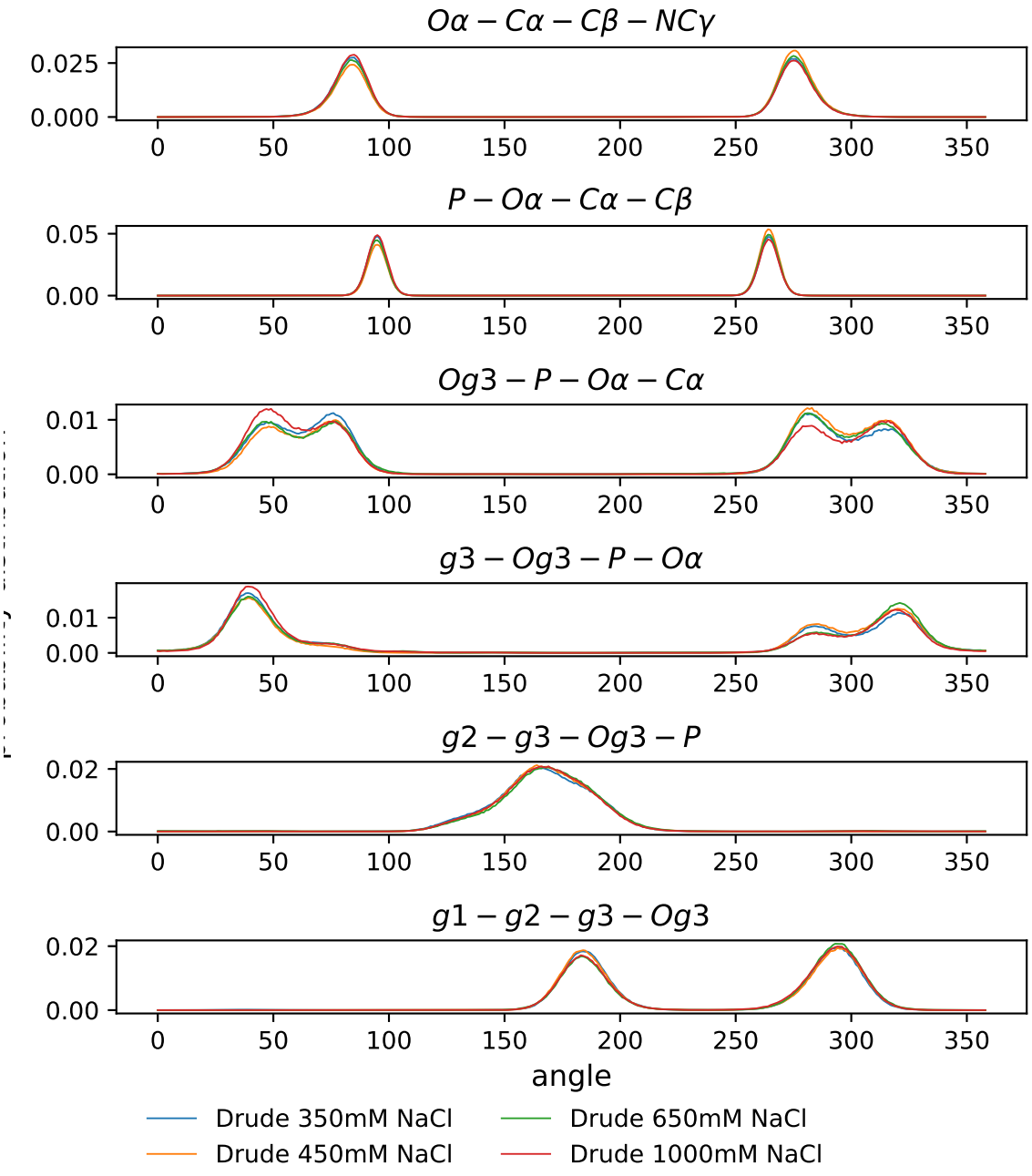

Figure 3: dihedral distributions

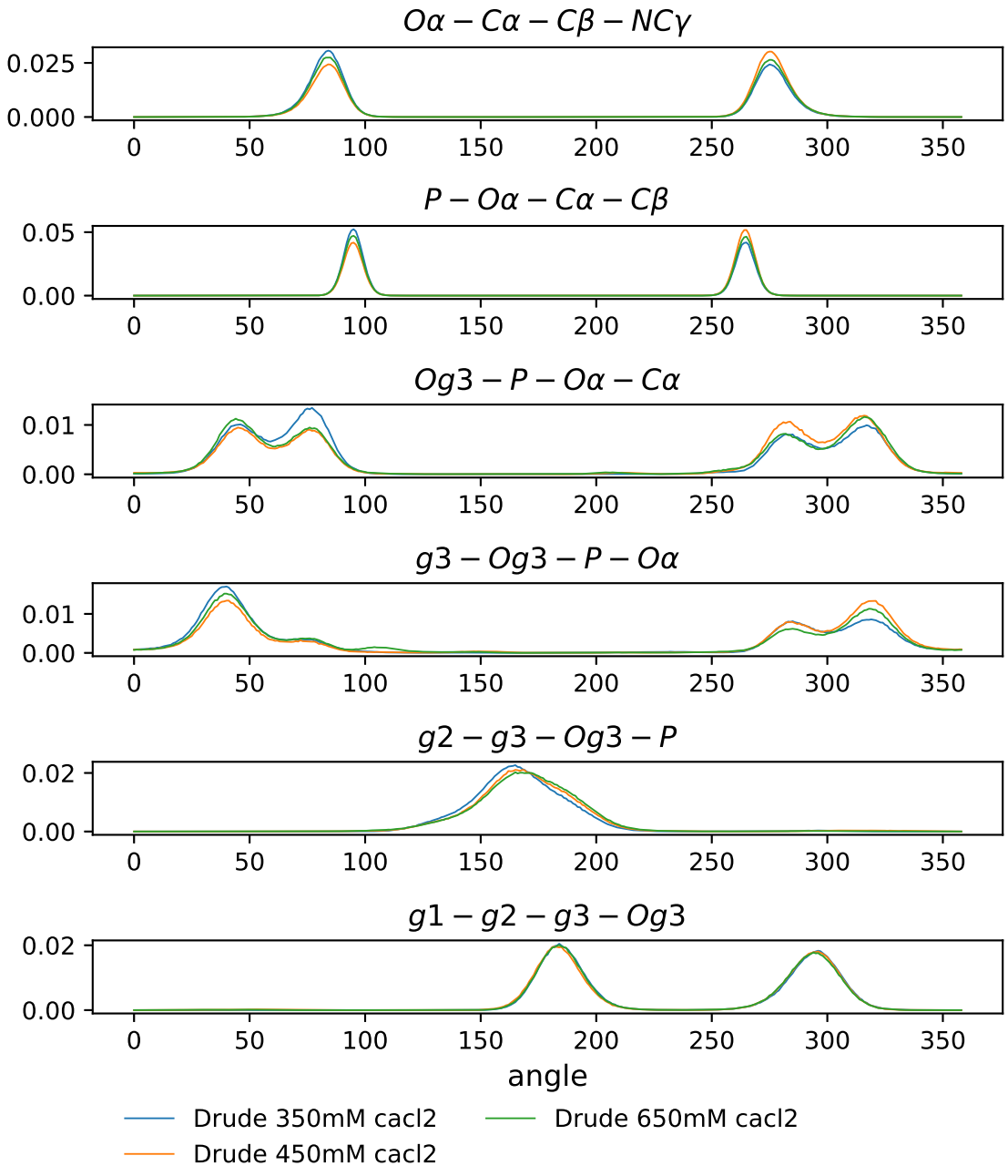

Figure 4: dihedral distributions

Density profiles

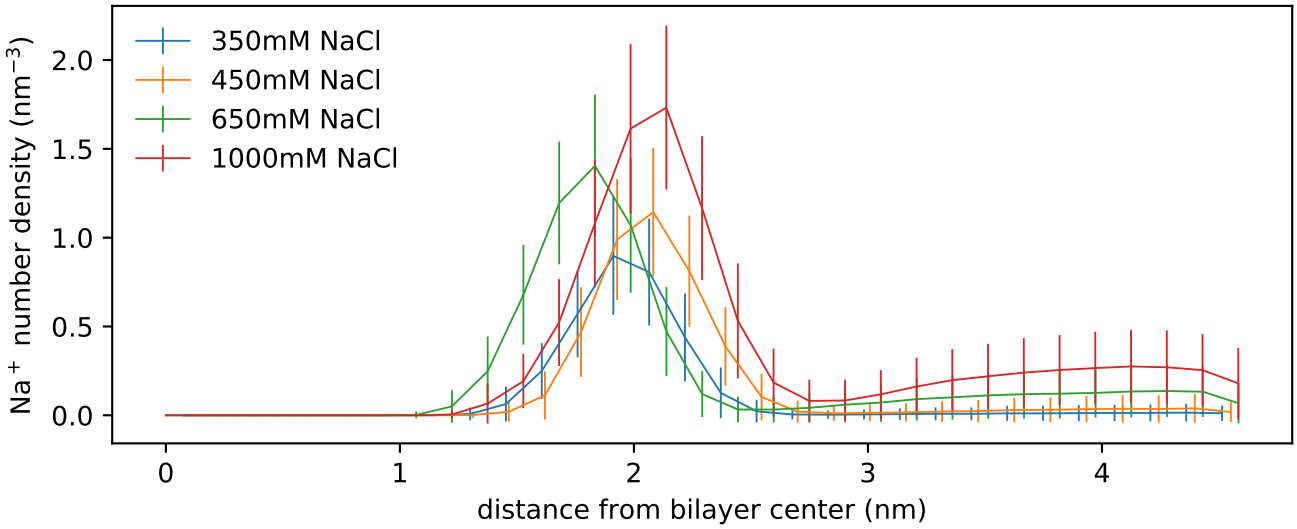

Figure 5: Na^{+} number density

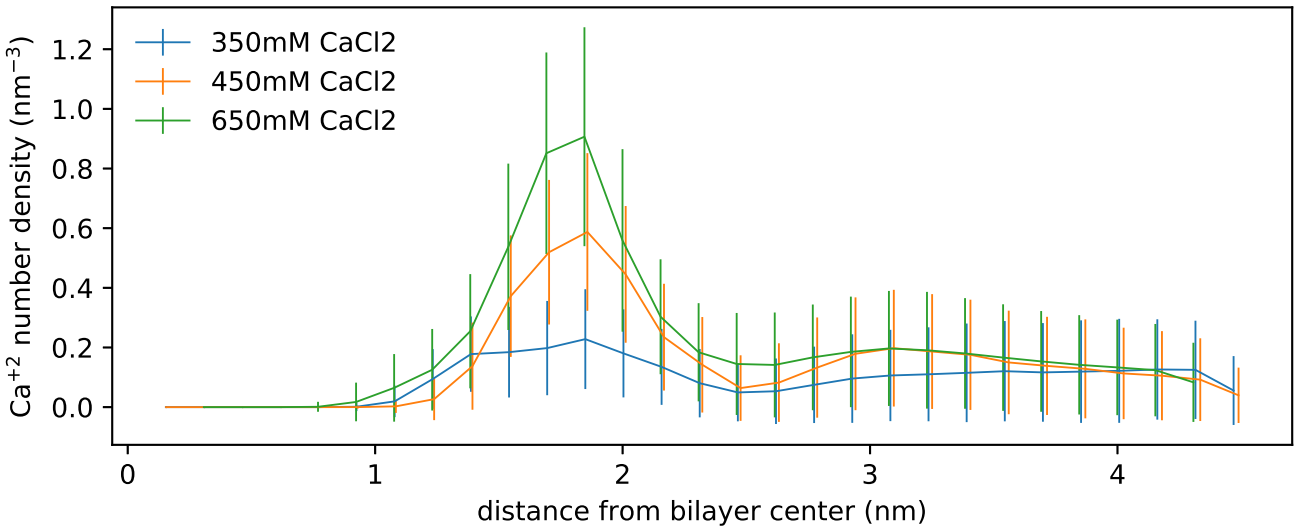

Figure 6: Ca^{+2} number density

Acknowledgement

Supporting Information Available

References

(1) Kav, B. Pure POPC Membrane with 350mM NaCl simulations using Drude Polarizable Force Field and OpenMM. 2020; https://doi.org/10.5281/zenodo.4048180.

(2) Kav, B. Pure POPC Membrane with 450mM NaCl simulations using Drude Polarizable Force Field and OpenMM. 2020; https://doi.org/10.5281/zenodo.4048171.

(3) Kav, B. Pure POPC Membrane with 650mM NaCl simulations using Drude Polarizable Force Field and OpenMM. 2020; https://doi.org/10.5281/zenodo.4074903.

(4) Kav, B. Pure POPC Membrane with 1000mM NaCl simulations using Drude Polarizable Force Field and OpenMM. 2020; https://doi.org/10.5281/zenodo.4074906.

(5) Kav, B. Pure POPC Membrane with 350mM CaCl2 simulations using Drude Polarizable Force Field and OpenMM. 2020; https://doi.org/10.5281/zenodo.4048178.

(6) Kav, B. Pure POPC Membrane with 450mM CaCl2 simulations using Drude Polarizable Force Field and OpenMM. 2020; https://doi.org/10.5281/zenodo.4048172.

(7) Kav, B. Pure POPC Membrane with 650mM CaCl2 simulations using Drude Polarizable Force Field and OpenMM. 2020; https://doi.org/10.5281/zenodo.4048175.