Reproducibility of MD simulations: Problems and solutions in the NMRlipids project (www.nmrlipids.blogspot.fi)

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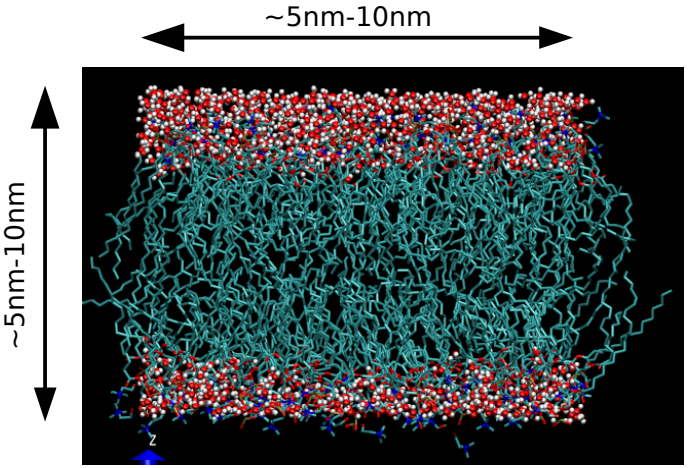
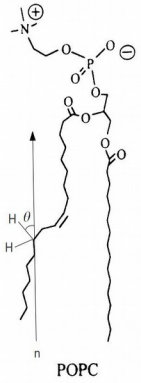
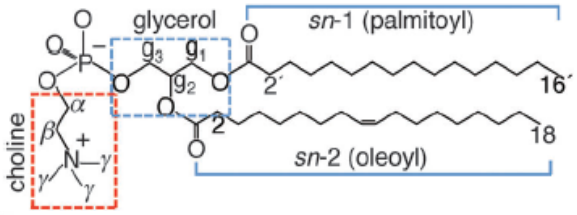
https://www.helsinki.fi/en/researchgroups/biophysical-chemistry

Solid state NMR and MD simulations

Lipid membrane systems
(solid state NMR)

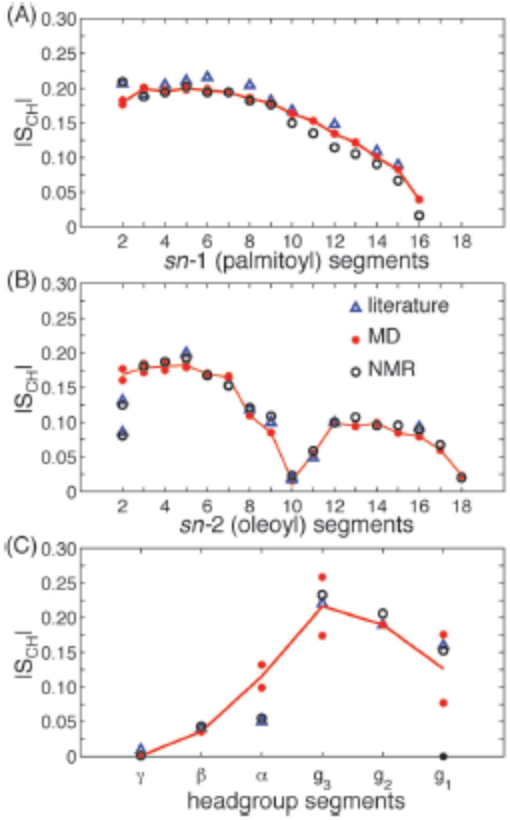






Order parameter:

$$S_{CH} = \frac{1}{2}\langle 3\cos^2\theta - 1 \rangle$$



T. M. Ferreira, F. Coreta-Gomes, O. H. Samuli Ollila, M. J. Moreno, W. L. C. Vaz and D. Topgaard, PCCP, 15, 1976 (2013)
Ollila and Pabst, BBA, 1858, 2512-2528 (2016)

Berger model did not give a correct structure for POPC lipid headgroup and glycerol backbone

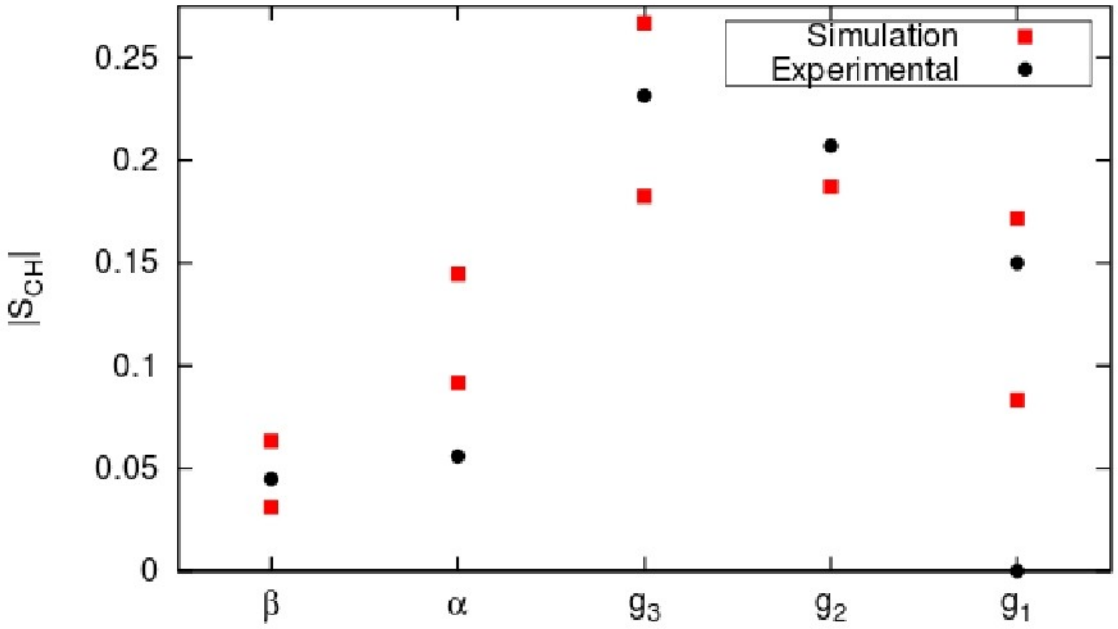
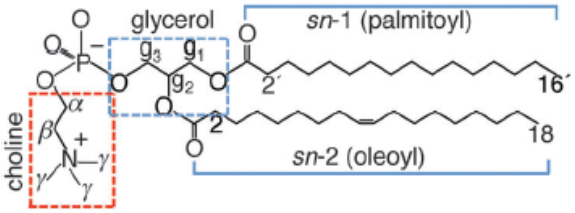


FIG. 2: Order parameteres from simulations and experiments for glycerol and choline groups of POPC. Experimental values taken from [7].

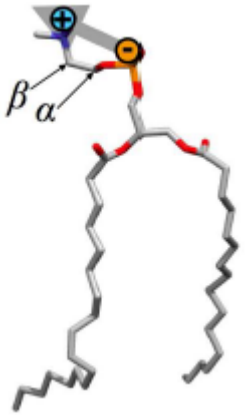
How about other models?
How to fix this?

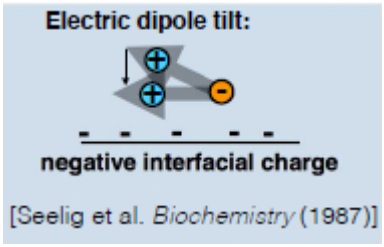


Molecular electrometer concept

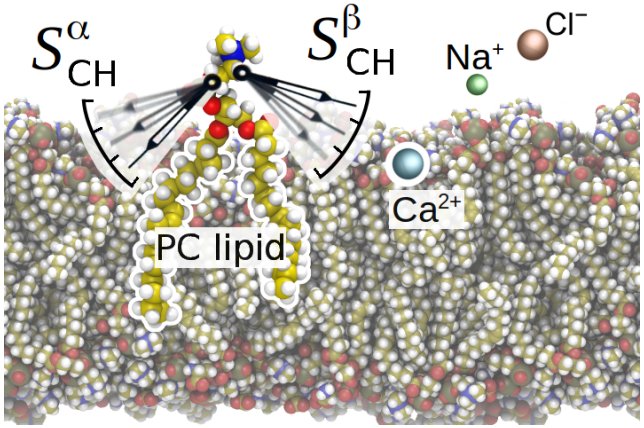
(Seelig et al. Biochemistry, 26 (1987) 7535):

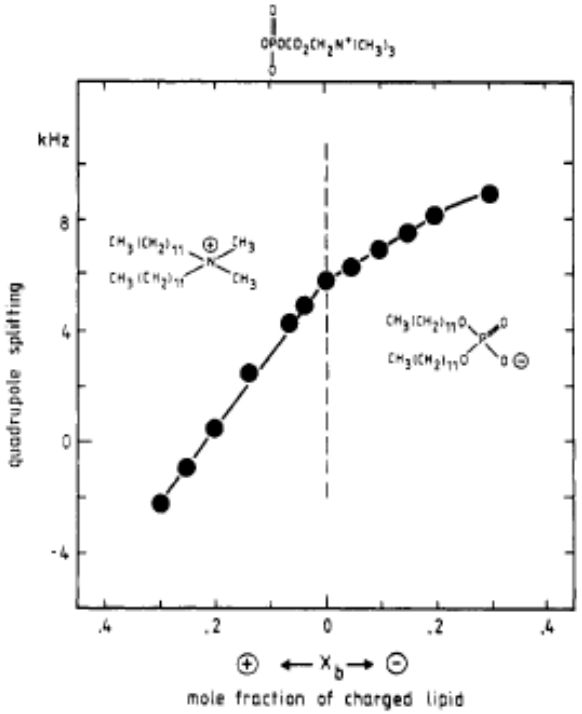
Negative molecules bound → choline order parameters increase
Positive molecules bound → choline order parameters decrease

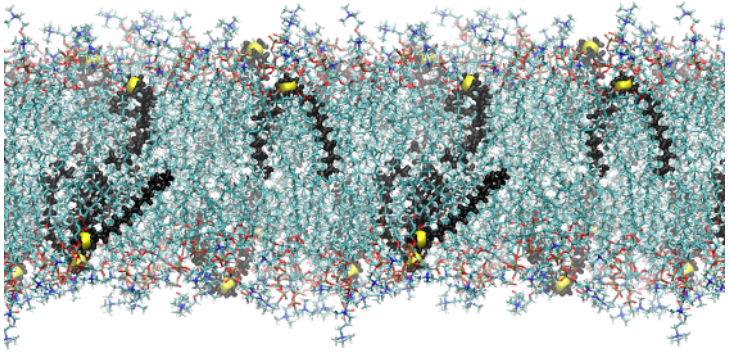




$$S_{CH} = \frac{1}{2}\langle 3\cos^2\theta - 1\rangle$$

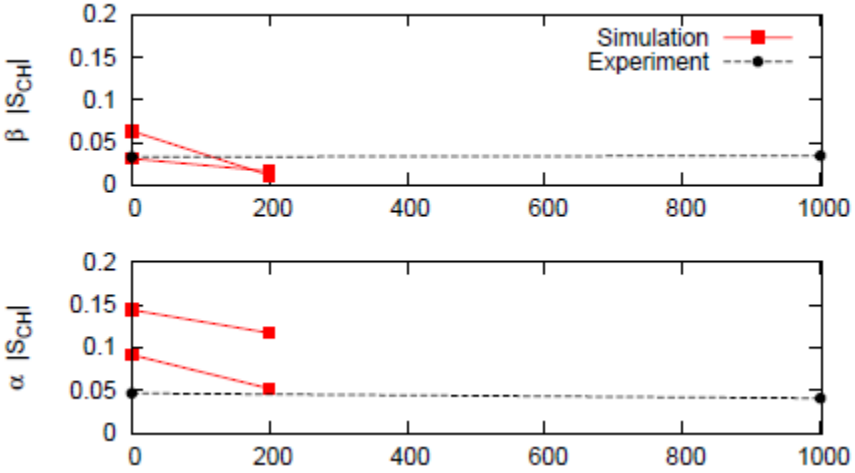


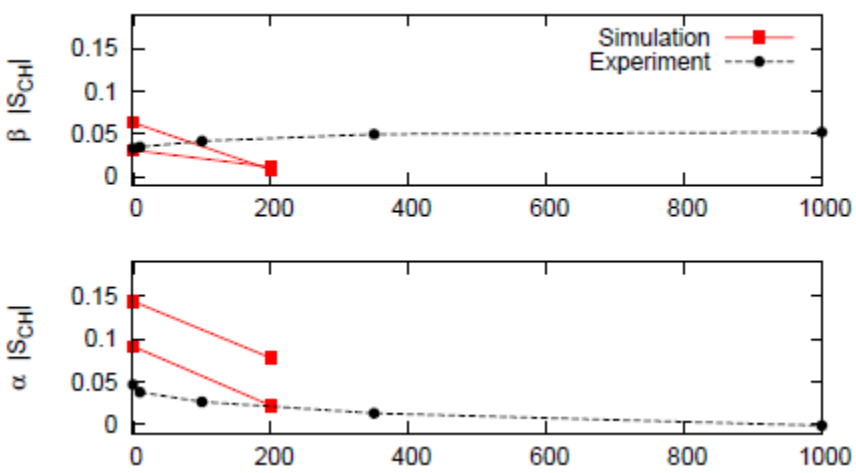




Ion binding to PC lipid membrane in Berger model vs. experiments

O.H.S. Ollila, Response of the hydrophilic part of lipid membranes to changing conditions - a critical comparison of simulations to experiments
http://arxiv.org/abs/1309.2131 (2013)





CONCLUSION: Na^+ and Ca^{2+} binding is too strong in the most used model

QUESTIONS: How about other models? How to fix this?

OPTIONS IN TRADITIONAL SCIENTIFIC DISCOURSE

Publish results and hope that the field reacts

+ Doable

- Only negative result, not real progress

Test all the models and/or improve the existing

- Too much work

NMRlipids open collaboration project

ORIGINAL STUDY:

O.H.S. Ollila, Response of the hydrophilic part of lipid membranes to changing conditions - a critical comparison of simulations to experiments
http://arxiv.org/abs/1309.2131

The original work has been improved and extended with Open Collaboration running at:

http://nmrlipids.blogspot.fi/
https://github.com/NMRLipids/

- The projected is progressed and discussed as an open project through the blog anf GitHub repositories
- People who have contributed through the blog format will be offered an authorship in produced publications
- The authorship final is based on self-assesment
- Author contributions are fully documented

NMRlipids open collaboration project

http://nmrlipids.blogspot.fi/
www.github.com/nmrlipids/
www.nmrlipids.fi

Goal is to find MD simulation models of lipids correctly describing biologically relevant membrane properties

Contributors are offered an authorship in the produced publications. The decision of the authorship is based on self-assesment. Authors are alphaphetical order.

All the data, methods and contributions are publicly available all the time

The NMRlipids project

Open Collaboration to understand lipid systems in atomistic resolution

Home | About | Workflow | Publications | GitHub | Authors | To Do List | Data contributions

Tuesday, January 30, 2018

Current status of the project

30.1.2018 Database of the NMRlipids simulations and experiments post was published.

22.12.2017 NMRlipids IV: Current status and reorganization of the manuscript post was published

8.12.2017 Results from CHARMM36 simulation with cationic surfactants was added to Quantifying the effect of bound charge on headgroup order parameters post.

27.7.2017 Quantifying the effect of bound charge on headgroup order parameters post was published.

31.3.2017 NMRlipids III: Preliminary version of the manuscript post is published.

9.3.2017 NMRlipids IV: Headgroup & glycerol backbone structures, and cation binding in bilayers with PE, PG and PS lipids post is published. Almost any kind of simulations of these lipids in bilayers would be useful at this stage.

15.2.2017 My activity in NMRlipids project has been low during the last months due to other commitments. However, I have now again possibility to advance NMRlipids III and IV projects (updates will follow soon). We have also published a blog post about the future of NMRlipids project.

29.11.2016 NMRlipids project will be presented in PHOS16 Conference (Philosophy and History of Open Science) held in Helsinki on 31.11.-1.12.2016. There should be also live stream available.

12.11.2016 NMRlipids II manuscript *Molecular electrometer and binding of cations to phospholipid bilayers* accepted for publication in Physical Chemistry Chemical Physics, and the preprint is available on the journal web page.

16.10.2016 Zenodo has been updated as described in their news page. There are a lot of improvements but this one is probably the most important for us: "The current 2GB per file limit is removed, in favour of a 50GB per dataset limit". This means that we do not have to split the trajectories in 2GB pieces anymore.

7.10.2016 The final version of NMRlipids II manuscript (lipid-ion interactions) submitted to Physical Chemistry Chemical Physics.

Latest comments on blog

- When collecting the data and composing the manuscr... - Samuli Ollila
- It would also be interesting to plot the oleoyl ta... - Thomas Piggot
- For POPC, there are impropers around the double bo... - Thomas Piggot
- No, the APL wasn't used for any sort of parame... - Thomas Piggot
- Thanks for tha data! I now merged also the second... - Samuli Ollila

Latest events on GitHub

- ohsOllila pushed to master in NMRLipids/NMRlipidsIVotherHGs
- ohsOllila pushed to master in NMRLipids/MATCH
- ohsOllila pushed to master in NMRLipids/NMRlipidsIVotherHGs
- ohsOllila pushed to master in NMRLipids/MATCH
- ohsOllila pushed to master in NMRLipids/NMRlipidsIVotherHGs

Chronological list of all posts

35. Database of the NMRlipids simulations and experiments
34. NMRlipids IV: Current status and reorganization of the manuscript
33. Quantifying the effect of bound charge on headgroup order parameters
32. NMRlipids III: Preliminary version of the manuscript
31. NMRlipids IV: Headgroup & glycerol backbone structures, and cation binding in bilayers with PE, PG and PS lipids

Open Collaboration

Scientific progress is accelerated by making all the content publicly available. Open invitation is presented to fellow scientists to participate in the project. Participants are credited by offering authorship in published articles.

- Scientific discussion in `nmrlipids.blogspot.fi` and in `https://github.com/NMRLipids/`
- Data, figures, codes and manuscripts in `https://github.com/NMRLipids/`
- Simulation files including trajectories in `http://zenodo.org/collection/user-nmrlipids`
- Final decision about authorship will be based on self-assessment

- Started in 2013

- 42 contributors

- 3 publications, 3 manuscripts, more than 600 small contributions, ~1500 visits monthly

NMRlipids I:

Toward Atomistic Resolution Structure of Phosphatidylcholine Headgroup and Glycerol Backbone at Different Ambient Conditions†

Alexandru Botan,‡ Fernando Favela-Rosales,§ Patrick F. J. Fuchs,∥ Matti Javanainen,⊥ Matej Kanduč,# Waldemar Kulig,⊥ Antti Lamberg,▽ Claire Loison,‡ Alexander Lyubartsev,○ Markus S. Miettinen,# Luca Monticelli,◆ Jukka Määttä,¶ O. H. Samuli Ollila,*,∞ Marius Retegan,□ Tomasz Róg,⊥ Hubert Santuz,▲,$,+,▽ and Joona Tynkkynen⊥

DOI: 10.1021/acs.jpcb.5b04878
J. Phys. Chem. B 2015, 119, 15075−15088

NMRlipids II:

CrossMark
Cite this: *Phys. Chem. Chem. Phys.*, 2016, 18, 32560

Molecular electrometer and binding of cations to phospholipid bilayers†

Andrea Catte,‡[a] Mykhailo Girych,[b] Matti Javanainen,[cd] Claire Loison,[e] Josef Melcr,[fg] Markus S. Miettinen,[hi] Luca Monticelli,[j] Jukka Määttä,[k] Vasily S. Oganesyan,[a] O. H. Samuli Ollila,*[b] Joona Tynkkynen[c] and Sergey Vilov[e]

NMRlipids V:

Atomistic resolution structure and dynamics of lipid bilayers in simulations and experiments☆,☆☆

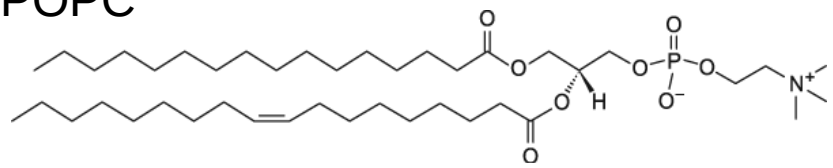
O.H. Samuli Ollila [a,*], Georg Pabst [b,c]

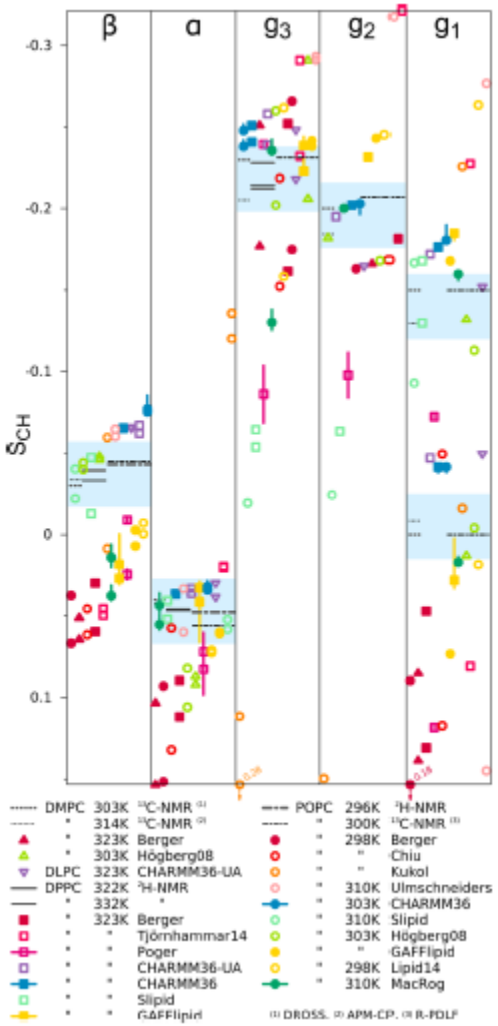
Biochimica et Biophysica Acta 1858 (2016) 2512–2528

Hanne Antila
Amelie Bacle
Alexandru Botan
Pavel Buslaev
Andrea Catte
Olle Edholm
Fernando Favela
Tiago Ferreira
Patrick Fuchs
Lukasz Cwiklik
Michael Girych
Peter Heftberger
Matti Javanainen
Pavel Jungwirth
Matej Kanduc
Batuhan Kav
Waldemar Kulig
Antti Lamberg
Claire Loison
Alexander Lyubartsev
Jesper Madsen
Josef Melcr
Markus S. Miettinen
Luca Monticelli
Jukka Määttä
Ricky Nencini
Vasily Oganesyan
Thomas Piggot
Georg Pabst
O. H. Samuli Ollila
Marius Retegan
Tomasz Rog
Hubert Santuz
Peter Tieleman
Joona Tynkkynen
Sergey Vilov
Alexander Vogel
Alex de Vries
Mark Wilson

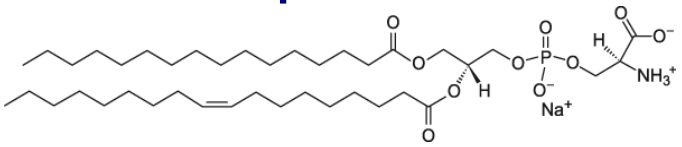
Force field quality of lipid headgroups against order parameters from NMR experiments

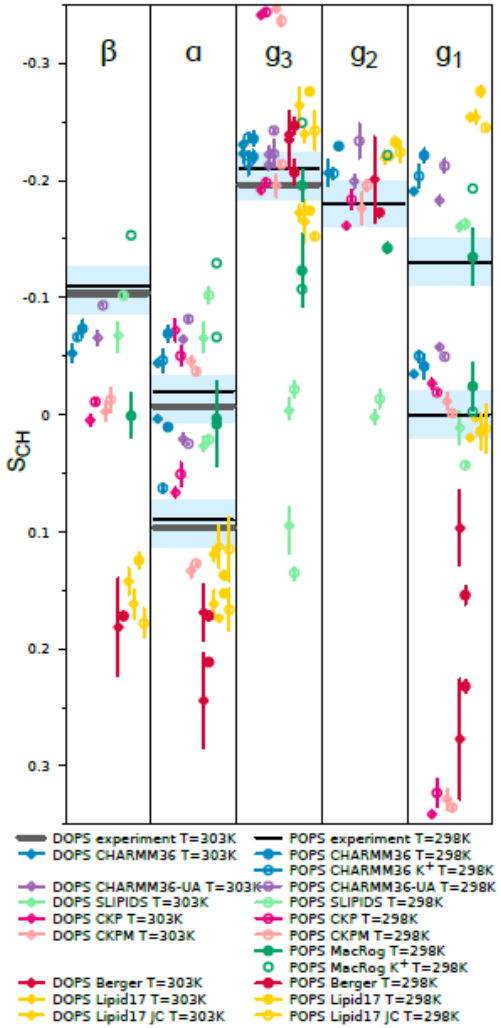
POPC





POPS

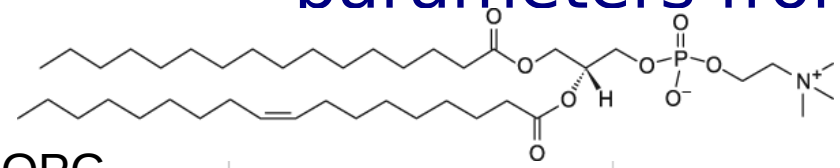




Botan et al. JPCB, 119, (2015) 15075

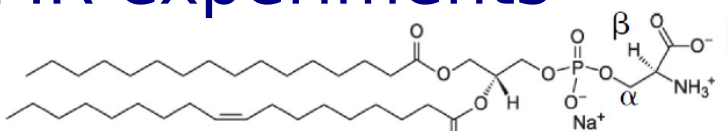
https://github.com/NMRLipids/NMRlipidsIVotherHGs/blob/master/Manuscript/manuscriptPS.pdf

Force field quality of lipid headgroups against order parameters from NMR experiments



POPC

	β	α	g_3	g_2	g_1	Σ
CHARMM 36	M		M		M	3
CHARMM 36-UA	M	F	M	M	M F	6
Hög-berg08		M F	M F	M	F	8
MacRog	M F	F	M F		M F	8
GAFFlipid	M F	F	M F	M	M F	9
Lipid14	M F	M	M F	M	M F	11
Chiu	M F	M F	M F	M	M F	11
Ulm-schneiders	M	F	M F	M	M F	12
Slipid	F	F	M F	M	M F	13
Poger	M F	M F	M F	M	M F	13
Tjörn-hammar14	M	M	M F	M	M F	15
Berger	M F	M F	M F	M	M F	15
Kukol	M F	M F	M F	M	M F	16



POPS

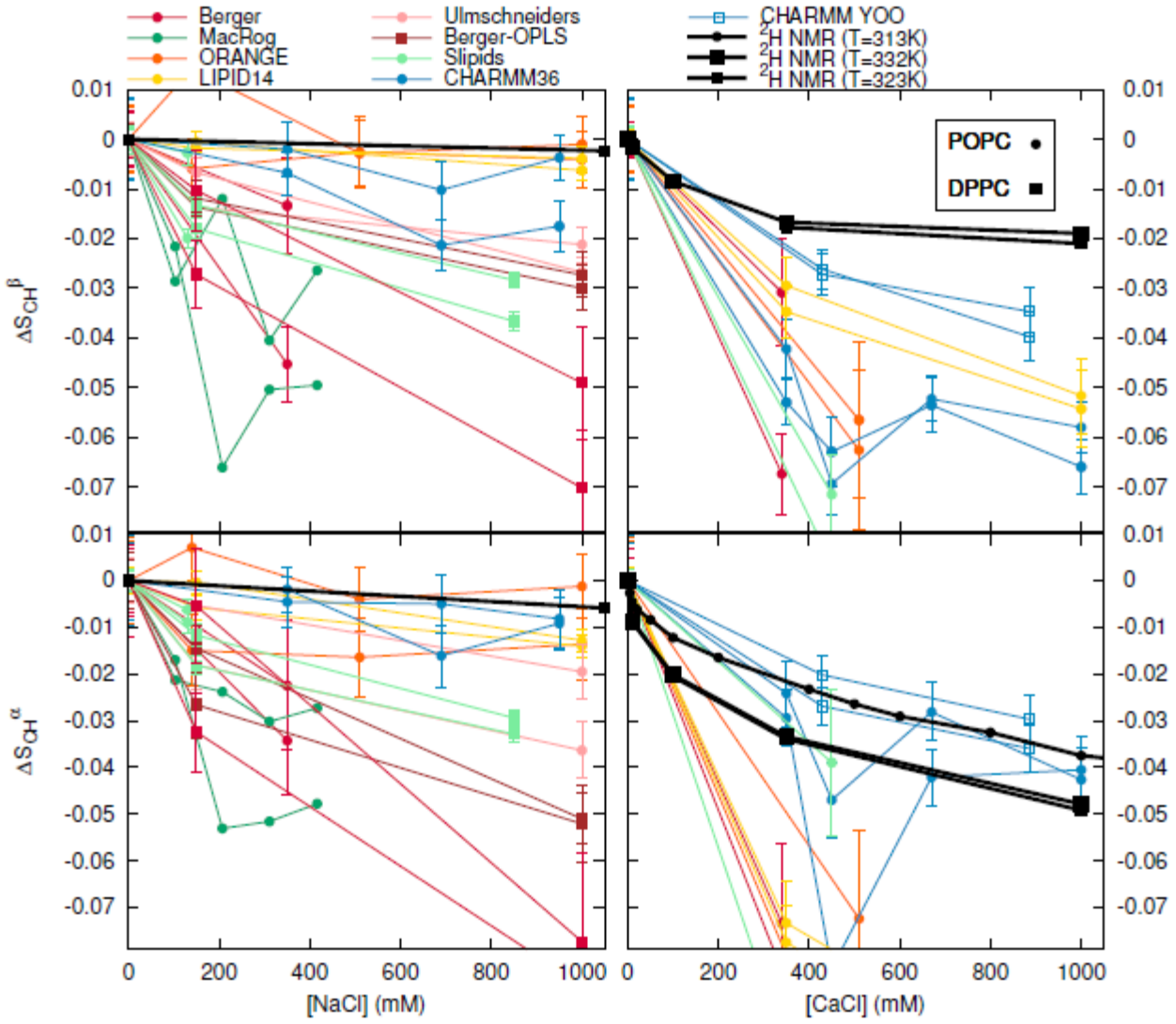
	β	α	g_3	g_2	g_1	Σ
CHARMM 36 K+	M	M	M F	M	M F	7
CHARMM 36	M	M F	M	M	M F	8
CHARMM 36-UA	M	M	M	M	M F	9
MacRog K+	M	M F	M F	M	M F	11
MacRog	M	M F	M F	M	M	14
GROMOS-CKP	M	M F	M F		M F	14
GROMOS-CKPM	M	M F	M F		M F	14
Berger	M	M F	M F		M F	14
Slipid	M	M	M F	M	M F	14
Lipid17	M	M F	M F	M	M F	18
Lipid17 JC	M	M F	M F	M	M F	18

Botan et al. JPCB, 119, (2015) 15075

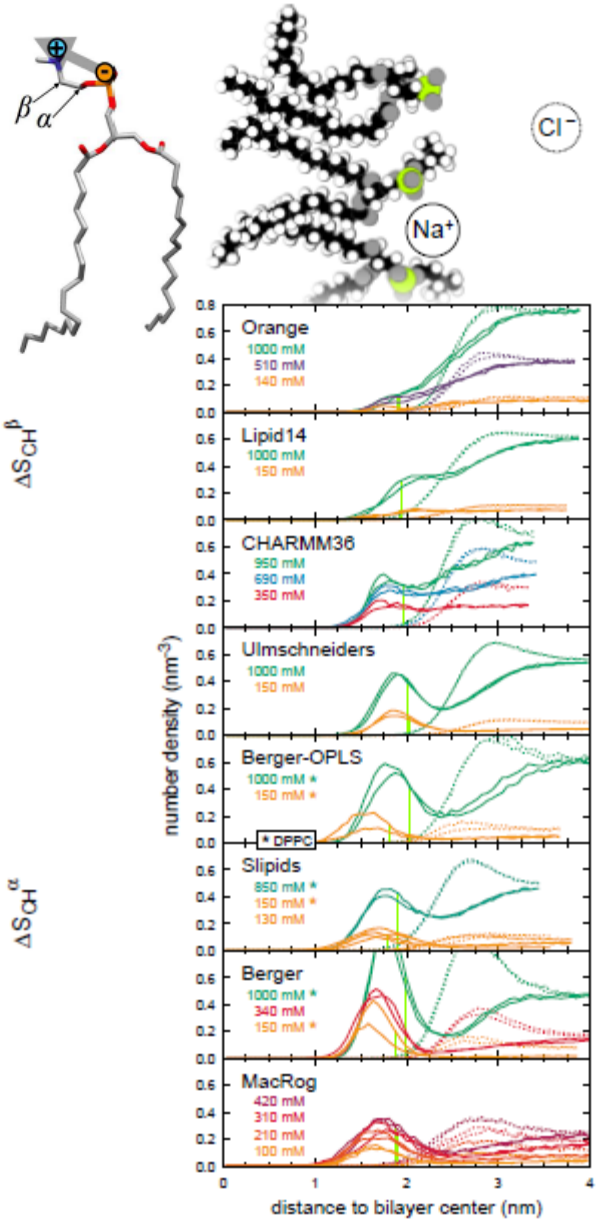
https://github.com/NMRLipids/NMRlipidsIVotherHGs/blob/master/Manuscript/manuscriptPS.pdf

NMRlipids II:

Choline order parameter changes as a function of ion concentration



Ion density distributions with NaCl

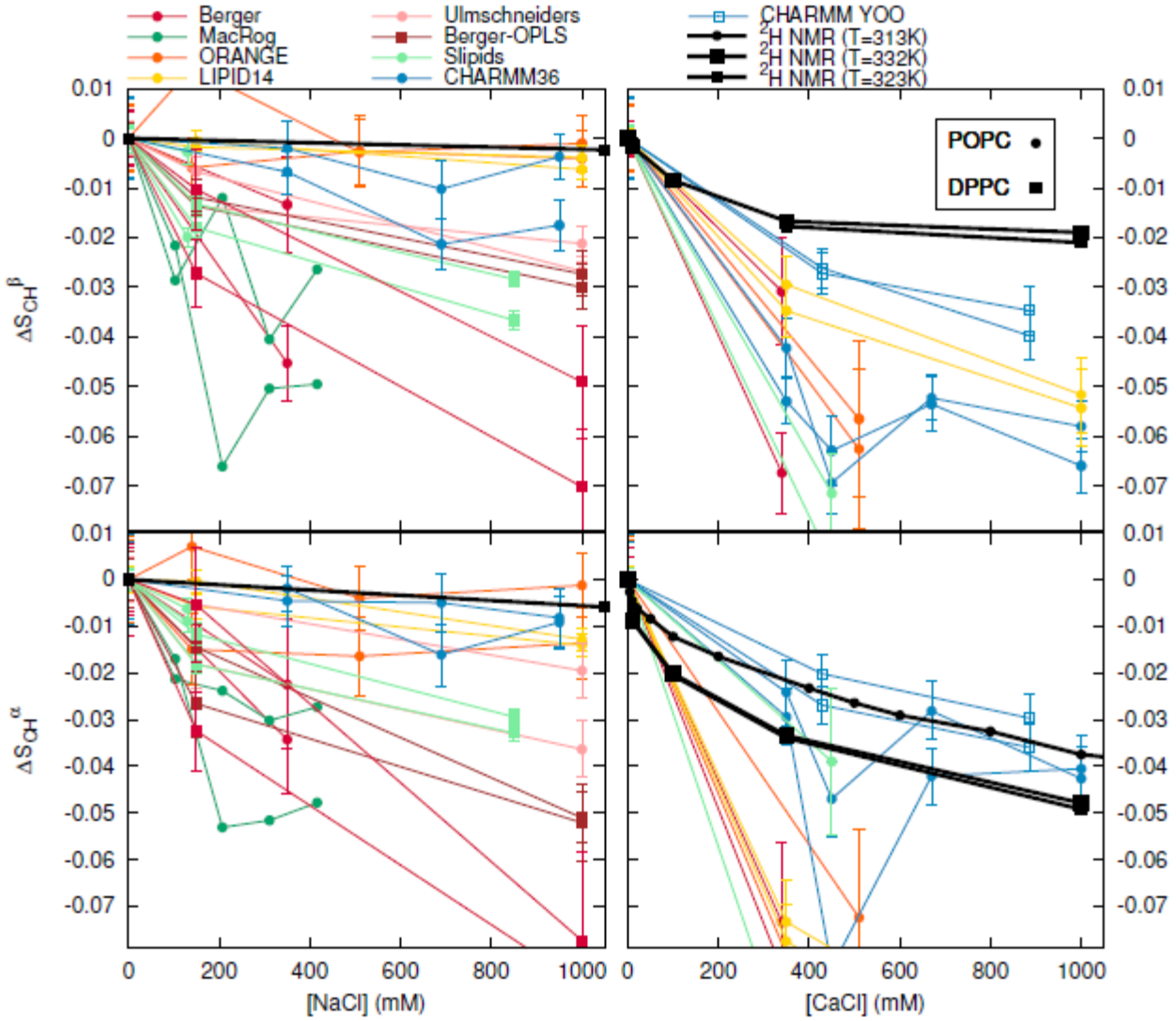


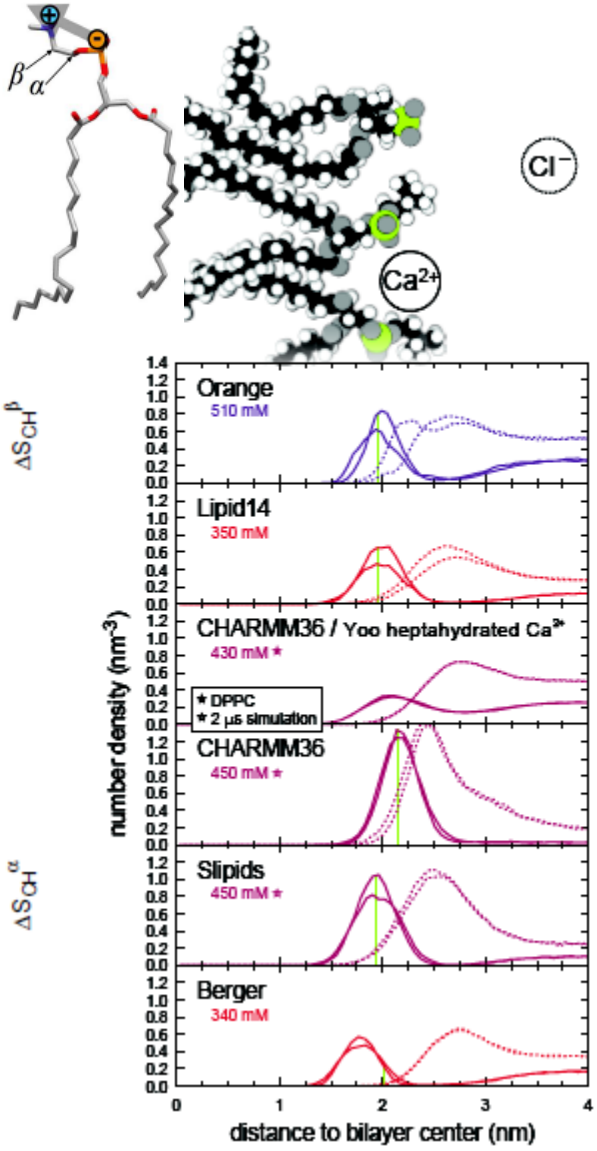
Catte et al. PCCP, 18, (2016) 32560

NMRlipids II:

Ion density distributions with $CaCl_2$

Choline order parameter changes as a function of ion concentration





Catte et al. PCCP, 18, (2016) 32560

NMRlipids II:

Cite this: *Phys. Chem. Chem. Phys.*, 2016, **18**, 32560

Molecular electrometer and binding of cations to phospholipid bilayers†

Andrea Catte,‡[a] Mykhailo Girych,[b] Matti Javanainen,[cd] Claire Loison,[e] Josef Melcr,[fg] Markus S. Miettinen,[hi] Luca Monticelli,[j] Jukka Määttä,[k] Vasily S. Oganesyan,[a] O. H. Samuli Ollila,*[b] Joona Tynkkynen[c] and Sergey Vilov[e]

CONCLUSIONS:

- Na^+ binding is negligible
- Most models overestimate Na^+ binding
- Details of Ca^{2+} binding are not reproduced by any of the models

How to correctly describe cation binding to PC lipid membranes?

Only non-tail atoms scaled

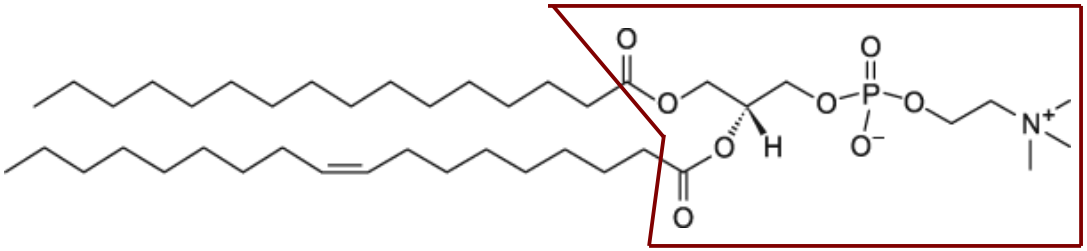
Charges
f_q=0.80

Lennard-Jones
f_σ=0.89
Keep ε

ECC-lipids

Include electronic polarizability
Applying electronic continuum
Correction to Amber Lipid14 force field

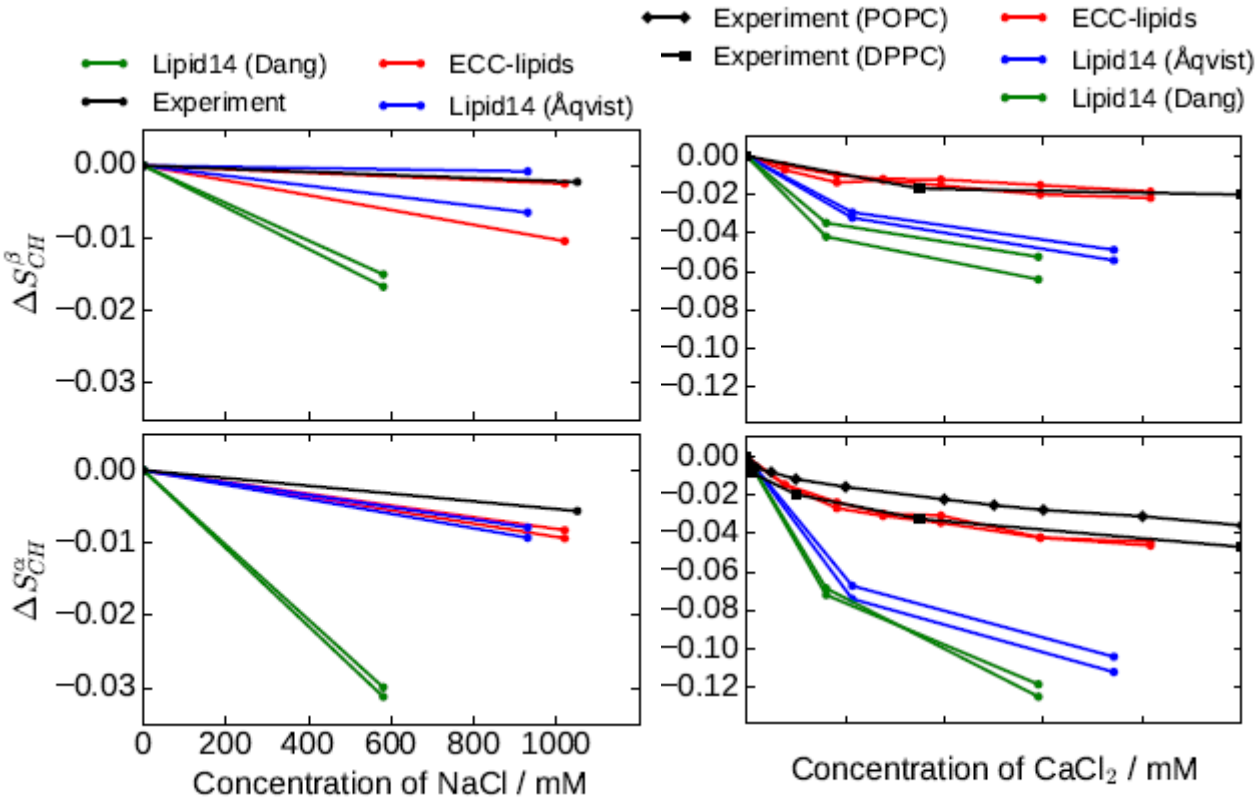
Leontyev and Stuchebrukhov, Phys. Chem. Chem. Phys., 2011, 13, 2613–2626

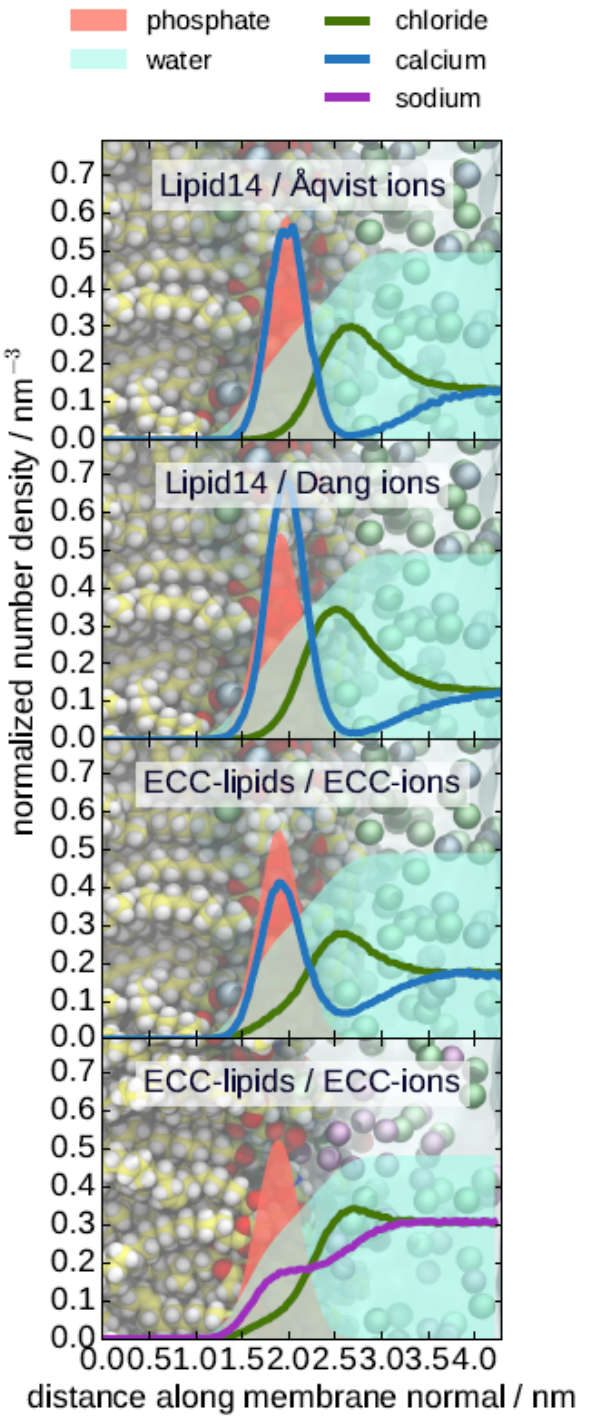


POPC

Melcr, Martinez-Seara, Nencini, Kolafa, Jungwirth, O. H. S. Ollila, J. Phys. Chem. B 122 (2018) 4546

Ion binding affinity in ECC-lipid POPC model





Melcr, Martinez-Seara, Nencini, Kolafa, Jungwirth, O. H. S. Ollila,
J. Phys. Chem. B 122 (2018) 4546

Three typical reproducibility problems

1. Results ran with one simulation package (e.g. AMBER or CHARMM) cannot be reproduced with other simulation package (e.g. Gromacs or NAMD)

2. Authors share different parameters online than used in the published article

3. Parameters shared online are changed without notice

Three typical reproducibility problems

1. Results ran with one simulation package (e.g. AMBER or CHARMM) cannot be reproduced with other simulation package (e.g. Gromacs or NAMD)

EXAMPLE: Original CHARMM36 publication
Reports good agreement with experimental acyl chain order parameters

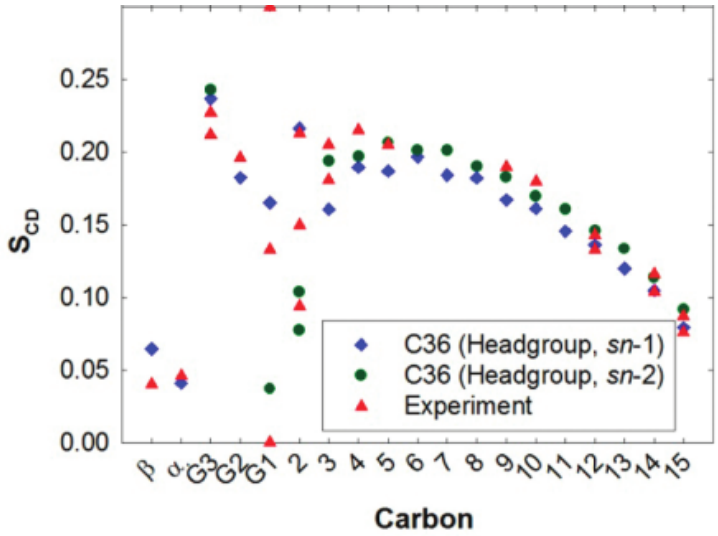
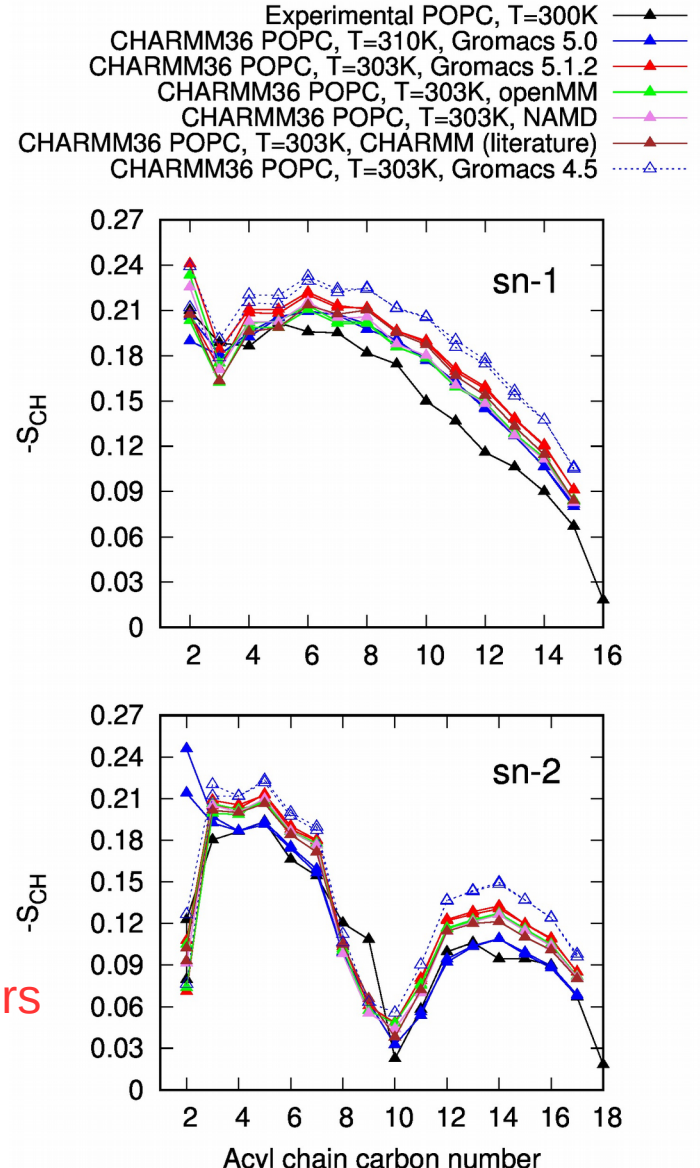


Figure 3. NMR deuterium order parameters (S_{CD}) for a DPPC bilayer from experiment[25–27] and NPAT simulations with $A = 64$ Å^2/lipid, which is close to the experimental surface area.



We always get overestimation of order parameters

https://github.com/NMRLipids/NmrLipidsCholXray/issues/4

Three typical reproducibility problems

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2. Authors share different parameters online than used in the published article

EXAMPLE: Area per lipid in GAFFlipid publication ran with AMBER vs. Gromacs

GAFFlipids: Dickson et al. Sof Matter, 8, (2012) 9617

It should be noted that the area per molecule with these settings for the GAFFlipid model was 61.6 Å^2, while the original publication[31] reported 63.9 Å^2. Notably, however, the same parameters and Amber-to-Gromacs conversion procedure reproduced the area per molecule from the original publication[32] for the Lipid14 model (see the Subsec. Lipid14).

NMRlipids I: Botan et al. JPCB, 119, (2015) 15075

Lipid14: Dickson et al. JCTC, 10, (2014) 865

The area per molecule with these settings was 65.4 Å^2, which is in agreement with the value 65.6±0.5 Å^2 reported in the original publication.[32]

NMRlipids I: Botan et al. JPCB, 119, (2015) 15075

Three typical reproducibility problems

2. Authors share different parameters online than used in the published article

EXAMPLE: OPLS lipid parameters (MacRog)

Thomas Piggot December 21, 2017 at 10:14 PM

Hi,

I did plan on running some pure MacRog PS simulations and even converted the CHARMM POPS starting structure into the necessary ordering (they are pretty similar) as per the rest of my pure POPS and DOPS membrane simulations. However when I did this I noticed that the available MacRog POPS topology (obtained from http://www.sciencedirect.com/science/article/pii/S2352340916301755) had some problems with it. From looking at some notes I made at the time of doing this, and from having another brief look at the topologies this evening, the things I've spotted are:

1. The sn-1 chain is oleoyl and the sn-2 chain palmitoyl (so OPPS not POPS)

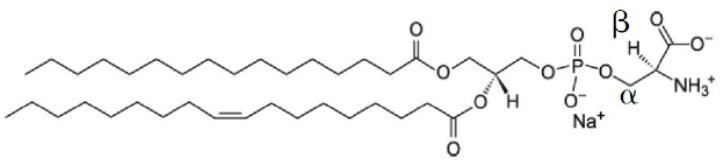
Thomas Piggot March 28, 2018 at 1:09 PM

Fair enough with regards to not looking at the tail. I will download the sims and do this myself.

I will setup POPS simulations with the tails from OPPS switched around and everything else the same and run these asap.

Thomas Piggot April 3, 2018 at 1:14 PM

Ok, good. I will setup the POPS simulations today. I have also been

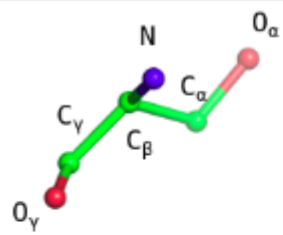


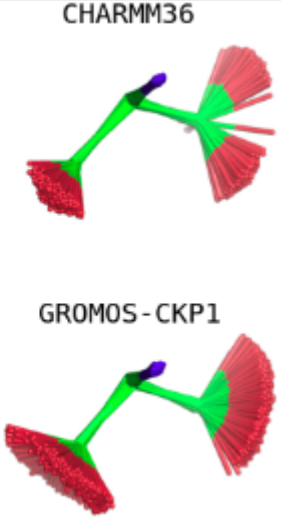
POPS

Samuli Ollila August 13, 2018 at 2:04 PM

Thanks again. Now I am comparing the new and previous versions of the figS8.png.

The orientation of the headgroup snapshots from MacRog in the previous version seems to be somehow different than in other models:
https://github.com/NMRLipids/NMRlipidsIVotherHGs/blob/master/Figs/figS8.png





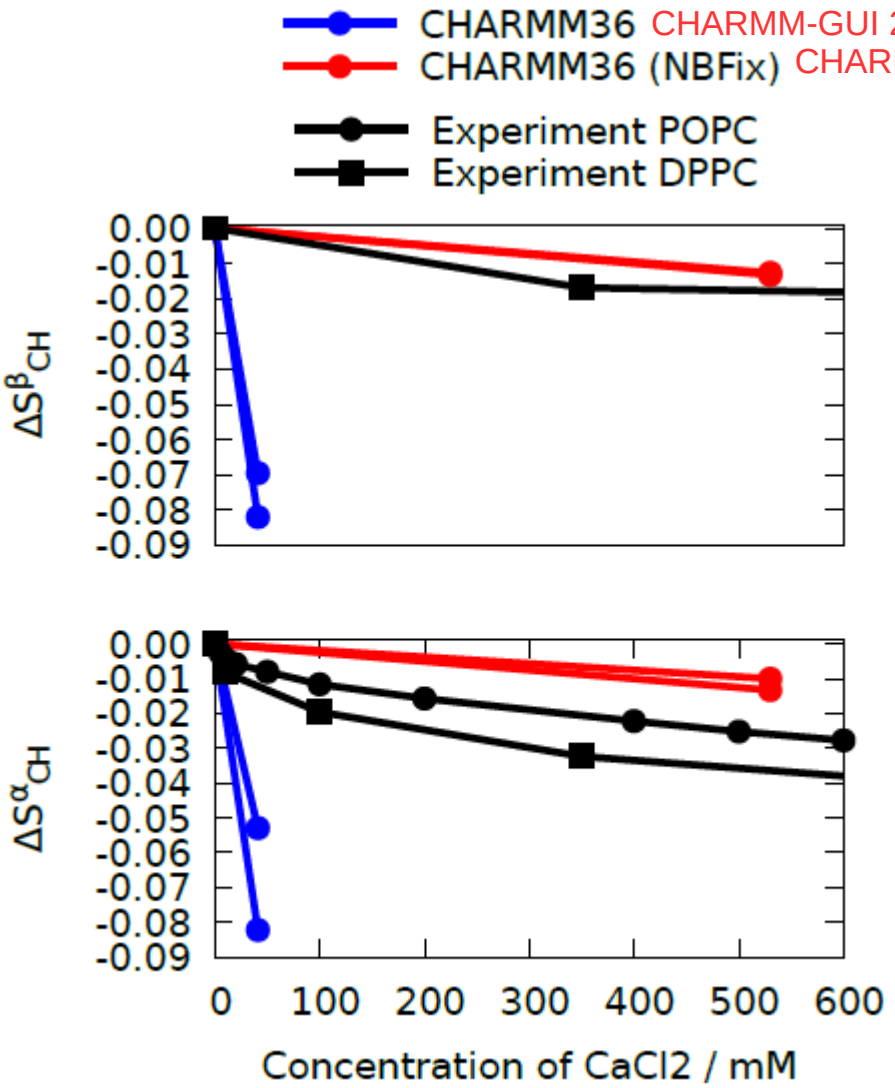
Samuli Ollila August 14, 2018 at 2:41 PM

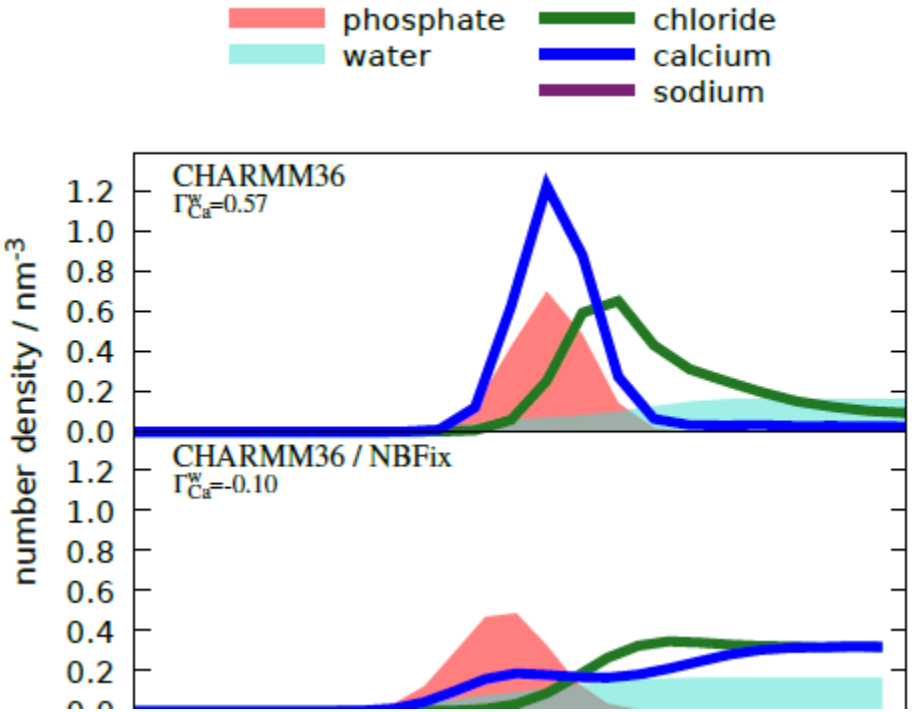
This suggested that the problem would be in the initial conformations, as also indicated by Tom Piggot above. Therefore, we took a look to initial configurations with Matti Javanainen and noticed that the starting configuration shared by the MacRog developers has the serine in D-stereoisomer,
while other models have the L-stereoisomer. The latter is present in biological systems.

Three typical reproducibility problems

3. Parameters shared online are changed without notice

EXAMPLE OF 3: Nbfix for calcium added into the CHARMM-GUI





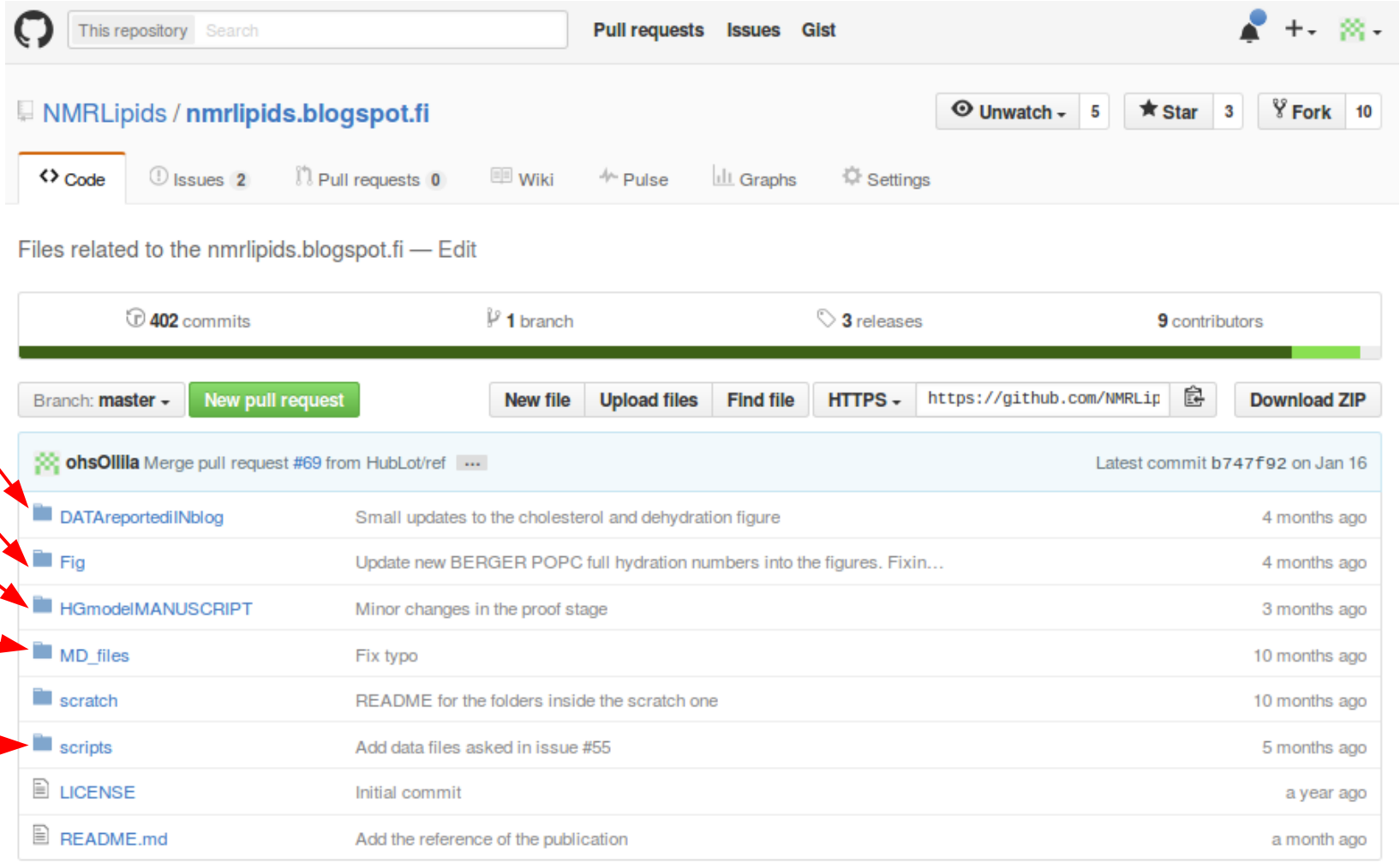
NMRlipids solution

- All the data and steps from raw data to the manuscript should be publicly available

-Raw data used in the manuscript should be published with unique identifier

Derived data, methods and more in GitHub

https://github.com/NMRLipids/nmrlipids.blogspot.fi



Derived data

Figures

Manuscript

Source files

Codes for derived data

Data listed in tables in manuscripts

Table 1. Fully Hydrated Single Component Lipid Bilayer Systems Simulated for Figure 2: 1,2-Dimyristoyl-*sn*-glycero-3-phosphocholine (DMPC), Dilauroylphosphatidylcholine (DLPC), Dipalmitoylphosphatidylcholine (DPPC), and 1-Palmitoyl-2-oleoylphosphatidylcholine (POPC)[a]

force field	lipid	N_l[b]	N_w[c]	T[d] (K)	t_{sim}[e] (ns)	t_{anal}[f] (ns)	files[g]	details[h]
Berger-DMPC-04[80]	DMPC	128	5097	323	130	100	81*	82
Berger-DPPC-98[83]	DPPC	72	2864	323	60	30	84*	SI
Berger-POPC-07[74]	POPC	128	7290	298	270	240	85*	75
CHARMM36[31]	DPPC	72	2189	323	30	25	86*	SI
CHARMM36[31]	DPPC	72	2189	323	130			31[i]
CHARMM36[31]	POPC	72	2242	303	30	20	87*	SI
CHARMM36[31]	POPC	128	5120	303	200	100	88*	SI
MacRog[89]	POPC	288	12 600	310	100	80	90*	SI
MacRog[89]	POPC	128	6400	310	400	200	91*	SI
MacRog[89]	POPC	288	14 400	310	90	40	92*	SI
GAFFlipid[33]	DPPC	72	2197	323	90	50	93*	SI
GAFFlipid[33]	DPPC	72	2167	323	250	250		33[j]
GAFFlipid[33]	POPC	126	3948	303	137	32	94*	SI
Lipid14[95]	POPC	72	2234	303	100	50	96*	SI
Poger[97]	DPPC	128	5841	323	2 × 100	2 × 50	98, 99*	SI
Slipids[100]	DPPC	128	3840	323	150	100	101*	SI
Slipids[102]	POPC	128	5120	303	200	150	103*	SI
Kukol[104]	POPC	512	20 564	298	50	30	105*	SI
Chiu[106]	POPC	128	3552	298	56	50	107*	SI
Högberg08[29]	DMPC	98	3840	303	75	50	108*	29
Högberg08[109]	POPC	128	3840	303	100	80	110*	109
Ulmschneiders[111]	POPC	128	3328	310	100	50	112*	SI
Tjörnhammar14[113]	DPPC	144	7056	323	200	100	114*	113
Botan-CHARMM36-UA[115]	DLPC	128	3840	323	30	20	116	SI
Lee-CHARMM36-UA[117]	DPPC	72	2189	323	70	50	118*	SI

(81) Miettinen, M. S. *Molecular dynamics simulation trajectory of a fully hydrated DMPC lipid bilayer* **2013**, DOI: 10.6084/m9.figshare.829642.

Largest publicly available database of MD simulation data at www.nmrlipids.fi

Database of NMRlipids' simulations and experiments

This is a beta version of the database collected in the NMRlipids project. The database is essentially just a search engine for the MATCH repository of the NMRlipids GitHub organization, thus indexing follows the folder structure of MATCH, and links to the corresponding MATCH folders are given. The experimental data are available through the links in the **Temperature column** and the molecular dynamics simulation data through the links in **Modelfiles column**.

The database is currently useful mostly for searching the molecular dynamics simulation data of lipid bilayers made available in the NMRlipids project; however, all those data are not yet included (work in progress). Future goal is to deliver for each model an automatically generated quality assessment report, as exemplified for the Berger POPC model, which would be useful for selecting the best-suited simulation model for a given application as well as for improving the force fields.

If you use this database or its contents in your publications, please cite the appropriate NMRlipids project publication(s). That said, all the content is provided *as is*: There is no guarantee that the content is correct or suitable for any purpose — you should check it yourself (and please let us know once you find bugs).

NMRlipids / Proudly powered by WordPress

Show 50 **entries**

Search:

Type	Molecule	Temperature	Modelfiles
Lipid_Bilayers	DOPS	T303K	MODEL_SLIPIDS MODEL_Berger MODEL_CHARMM36 MODEL_CHARMM36UA MODEL_GROMOS-CKP1 MODEL_GROMOS-CKP2 MODEL_LIPID17 MODEL_SLIPIDS2
Lipid_Bilayers	DPPC	T323K	MODEL_CHARMM36_GROMACS
Lipid_Bilayers	DPPE	T336K	MODEL_SLIPIDS
Lipid_Bilayers	DPPG	T298K	MODEL_SLIPIDS
Lipid_Bilayers	DPPG	T314K	MODEL_SLIPIDS
Lipid_Bilayers	E.coliPE	T310K	
Lipid_Bilayers	E.coliPG	T310K	

Short description of current data sharing system in the NMRlipids project

For example, see https://doi.org/10.5281/zenodo.1250974 where raw simulation data for a simulations of POPC:POPS lipid bilayer ran with Amber simulation package is available. This data is then used by a GitHub repository (https://github.com/NMRLipids/MATCH/tree/master/Data/Lipid_Bilayers%2FPOPS%2B83%25popc%2FT298K%2F/MODEL_LIPID17) containing a script that downloads the data and performs analysis. The results of this analysis are then used in the manuscripts. Each manuscript published by the NMRlipids project contains a list of used trajectories with a citation to the Zenodo repository, for example, see tables 1-3 in http://dx.doi.org/10.1021/acs.jpcb.5b04878.

The shared data is also indexed in the GitHub repository https://github.com/NMRLipids/MATCH, which is also searchable using the SQL databank available at http://www.nmrlipids.fi/. Currently, searching “NMRlipids” from Zenodo gives 209 results and many of the entries contain trajectories for more than one systems. Thus, we have already shared trajectories for hundreds of simulated systems. The databank at http://www.nmrlipids.fi/ is a beta version and is not fully up to date yet, currently containing only 63 entries. In addition, the content and format of Zenodo entries is not yet uniform. For example, the above linked entry for a POPC:POPS system describes very well the simulation details, while some other entries have less descriptions, but more files for the reproduction of the simulations, see for example http://doi.org/10.5281/zenodo.13283. We are currently trying to recruit people to update and further develop the databank.

CONCLUSIONS

Open collaboration is more effective than traditional scientific discourse

It is possible to publish the whole progess of producing publications which improves “reproducibility”

We have collected a database of MD simulation trajectories of lipid bilayers which is indexed in www.nmrlipids.fi

First annual NMRlipids workshop

Save the date
May 15th to 17th 2019

For current and future participants of the NMRlipids Project

Discussing the future direction of the project
Workshops (doing, not talking) to advance the project

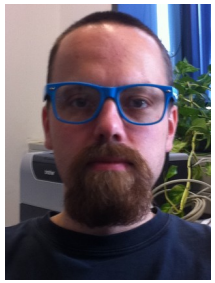
In Berlin, Germany

No participation fees

Planning to join? Please email us now (non-binding)
so we know to reserve big enough space:
Markus — miettinen@mpikg.mpg.de
Samuli — samuli.ollila@helsinki.fi

ACKNOWLEDGEMENTS

Open Collaboration



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THANKS FOR YOUR ATTENTION!

The character of molecular modeling

Anthony Nicholls J Comput Aided Mol Des (2012) 26:103–105

" My *real* thesis, the one I want to end with, is that unless simulations, or model building built on data dredging, do one simple thing there won't be much progress in the next 25 years. That one simple thing? Science. What amazes me about molecular modeling is how fundamentally un-scientific it is. Galileo had a very simple definition of science, "

Bilayer structure without ions in ECC-lipid POPC model

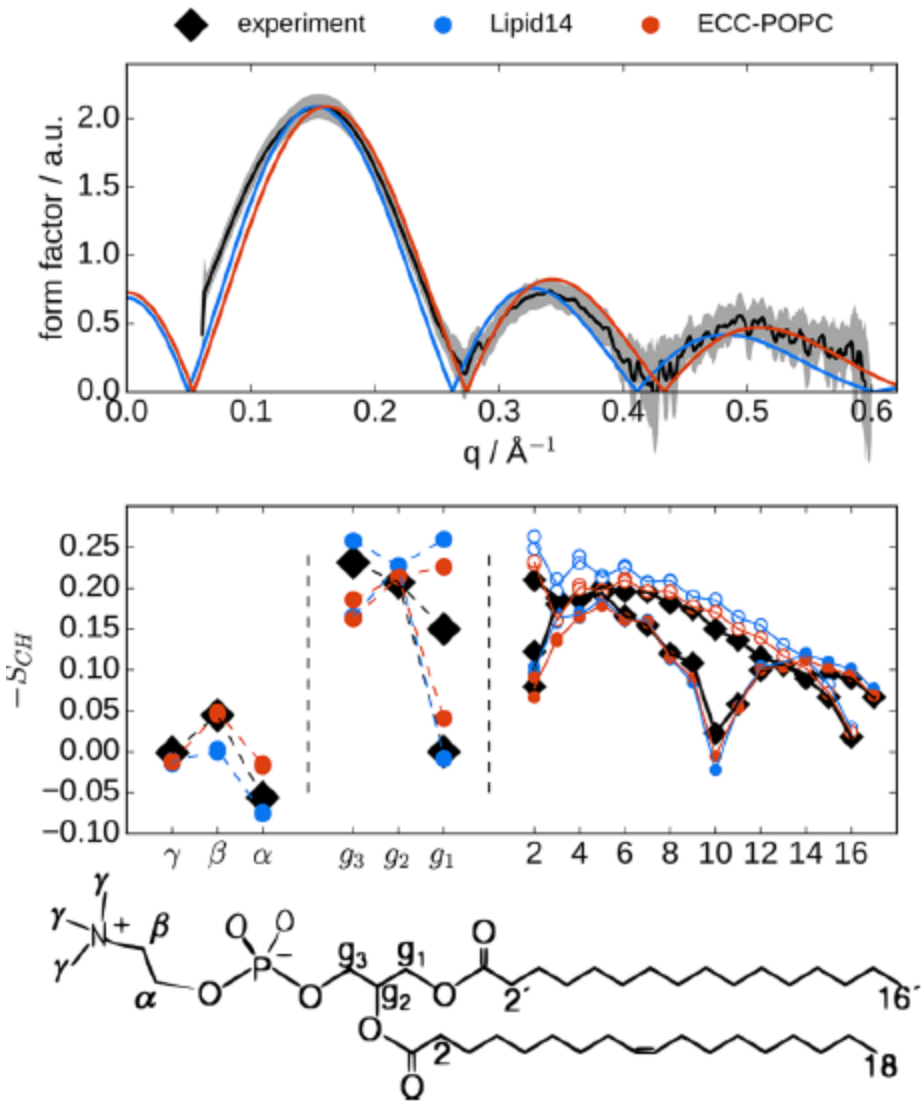

Table 1. Values of the Area Per Lipid (APL) of POPC Bilayers without Ions

model	APL (Å^2)	temperature [K]
Lipid14	65.1 ± 0.6	300
Lipid14[36]	65.6 ± 0.5	303
ECC-POPC	63.2 ± 0.6	300
experiment[57]	64.3	303

Melcr, Martinez-Seara, Nencini, Kolafa, Jungwirth, O. H. S. Ollila, J. Phys. Chem. B 122 (2018) 4546