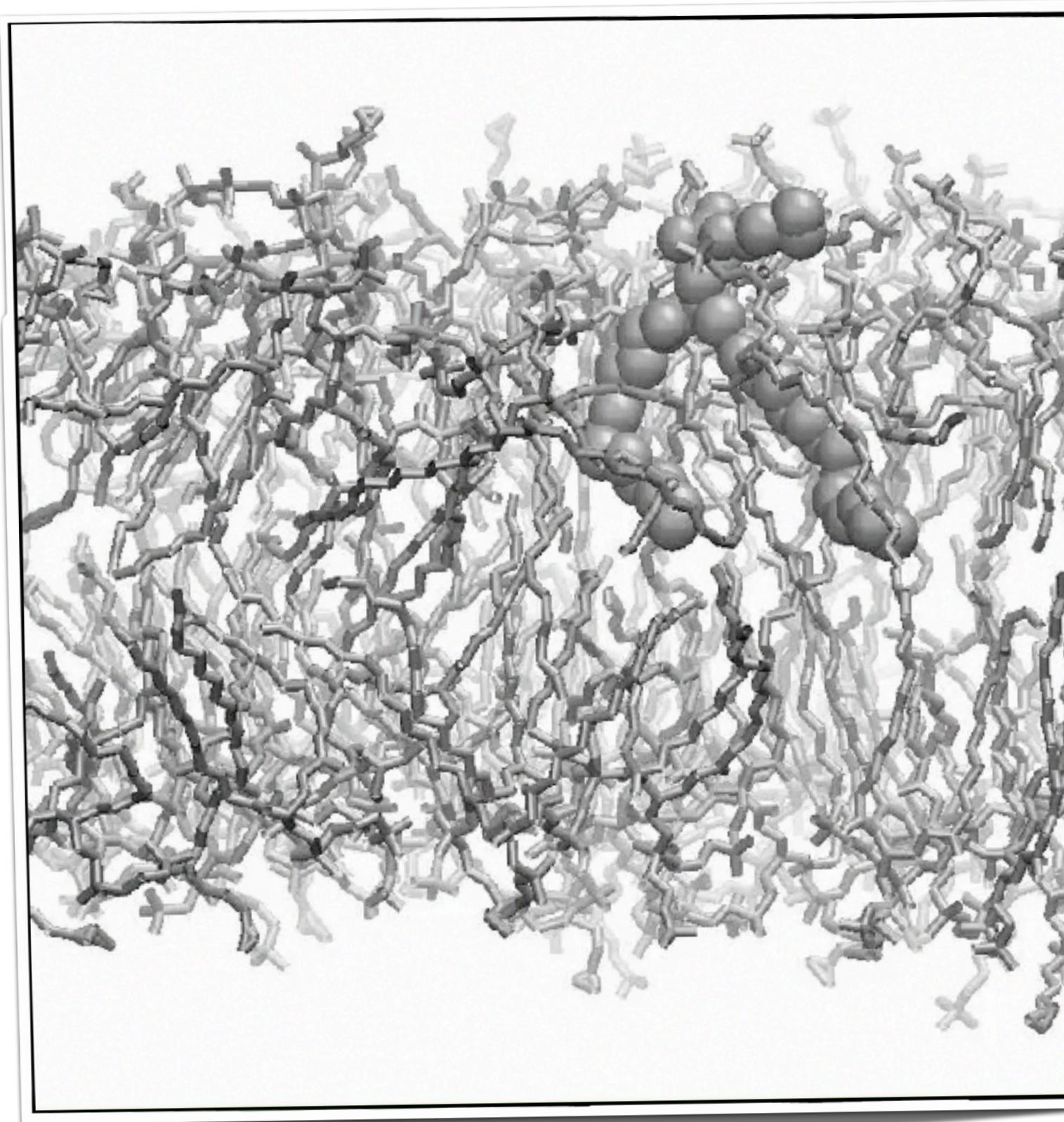


NMRlipids Project and open collaboration in biomolecular simulations

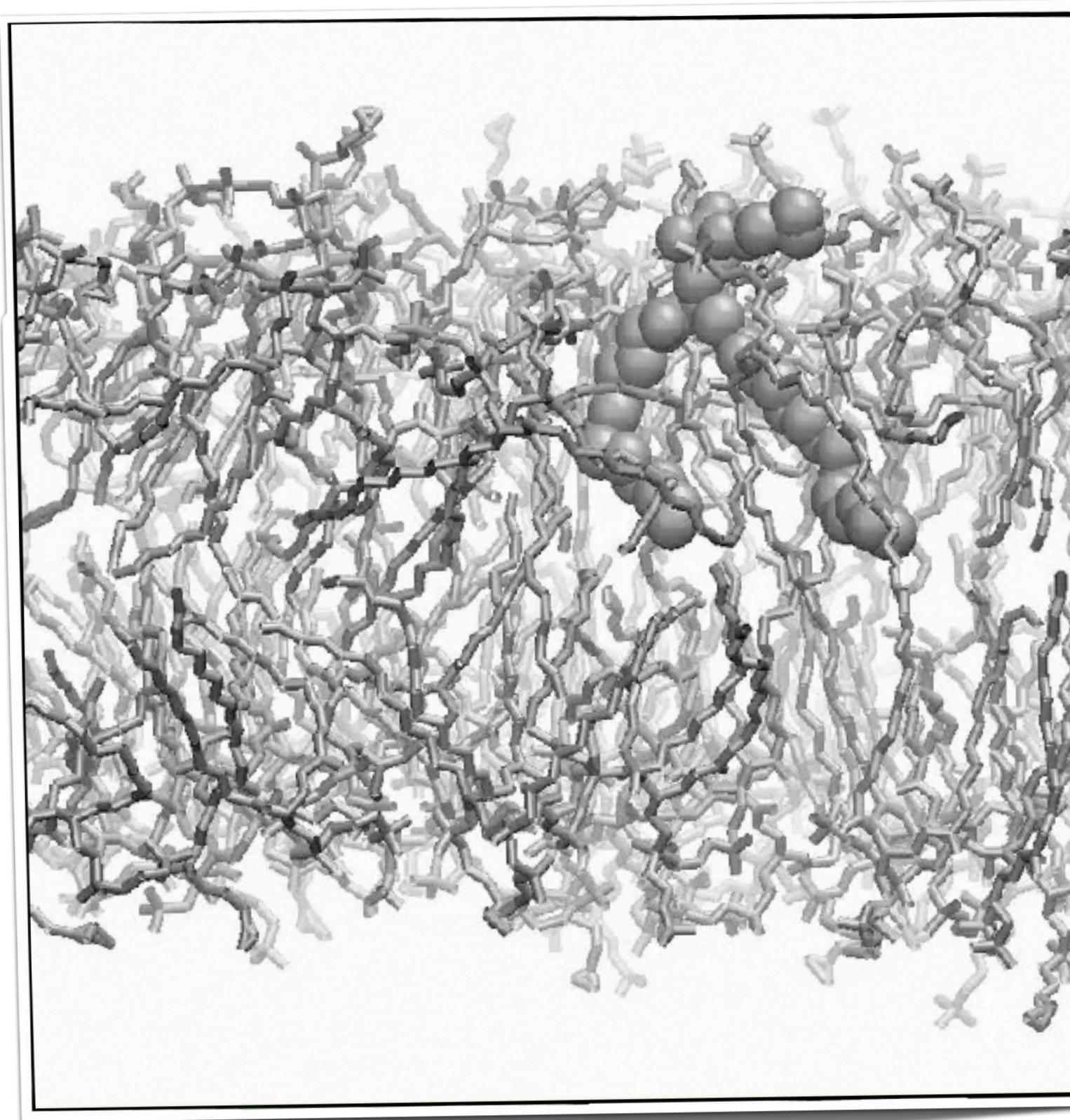
markus.miettinen@uib.no

NMRlipids summer school
Helsinki, June 1st 2022

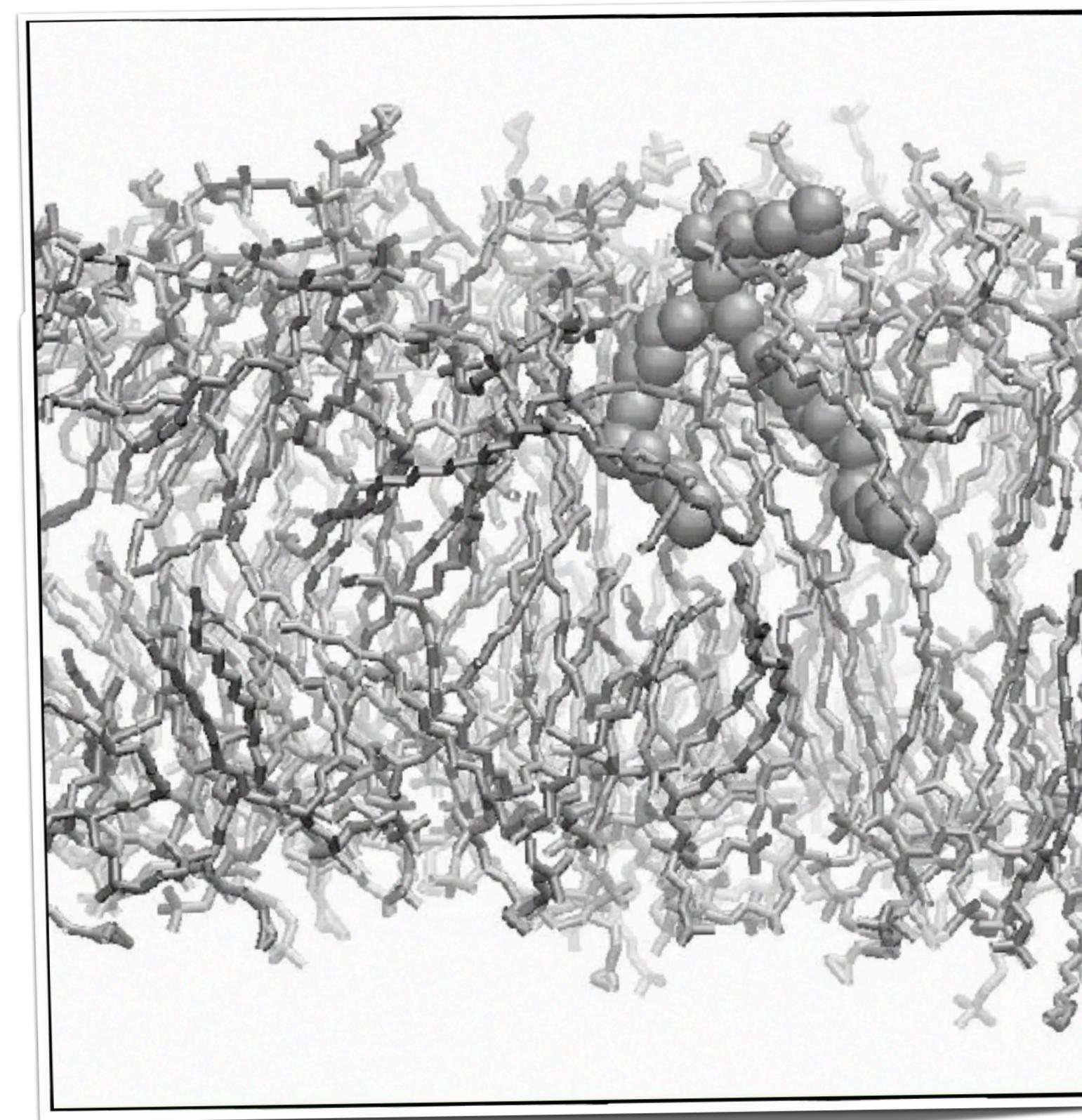
So you do get this:



So you do get this:

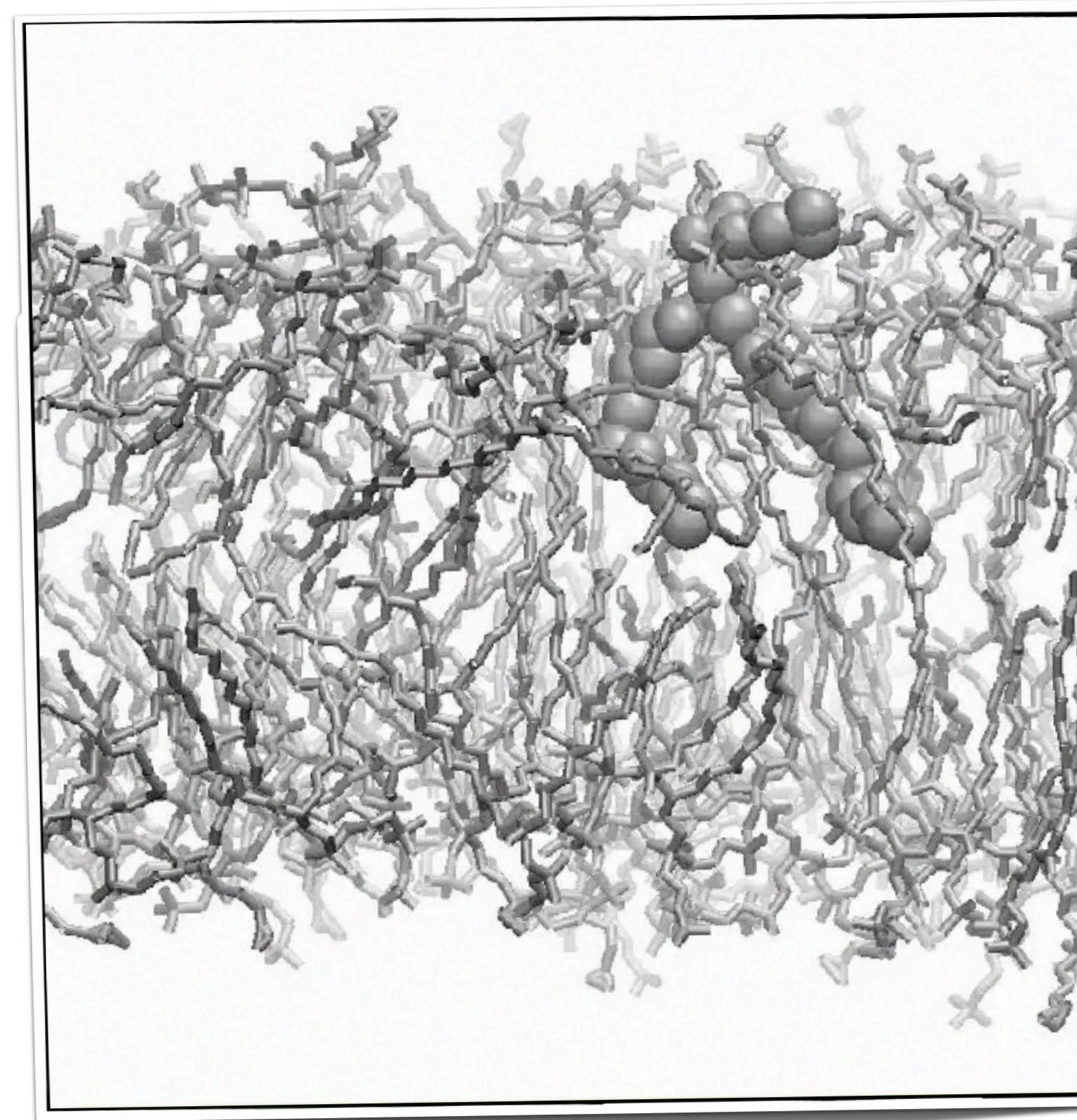


So you do get this:



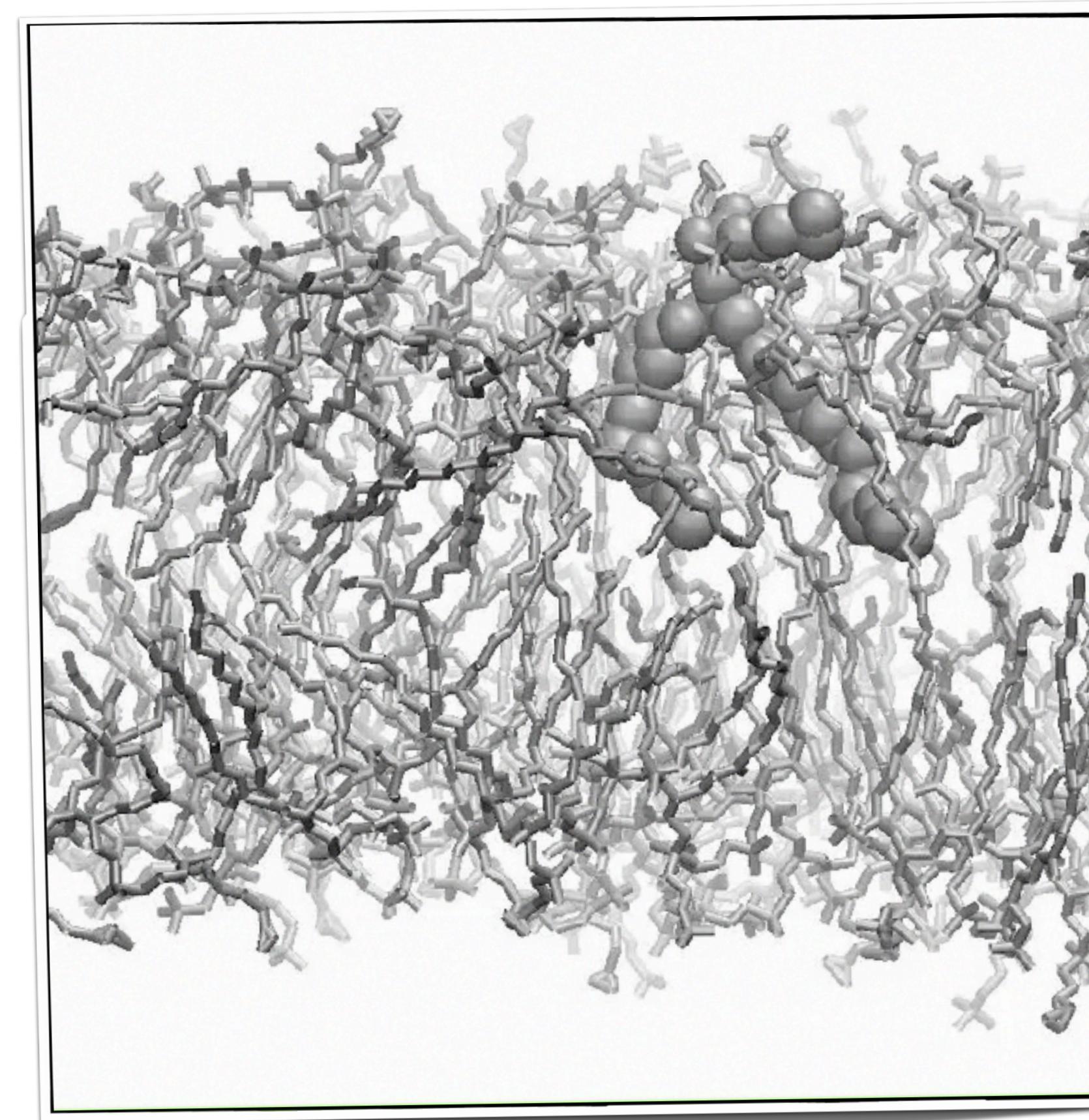
But is it what actually happens?

So you do get this:

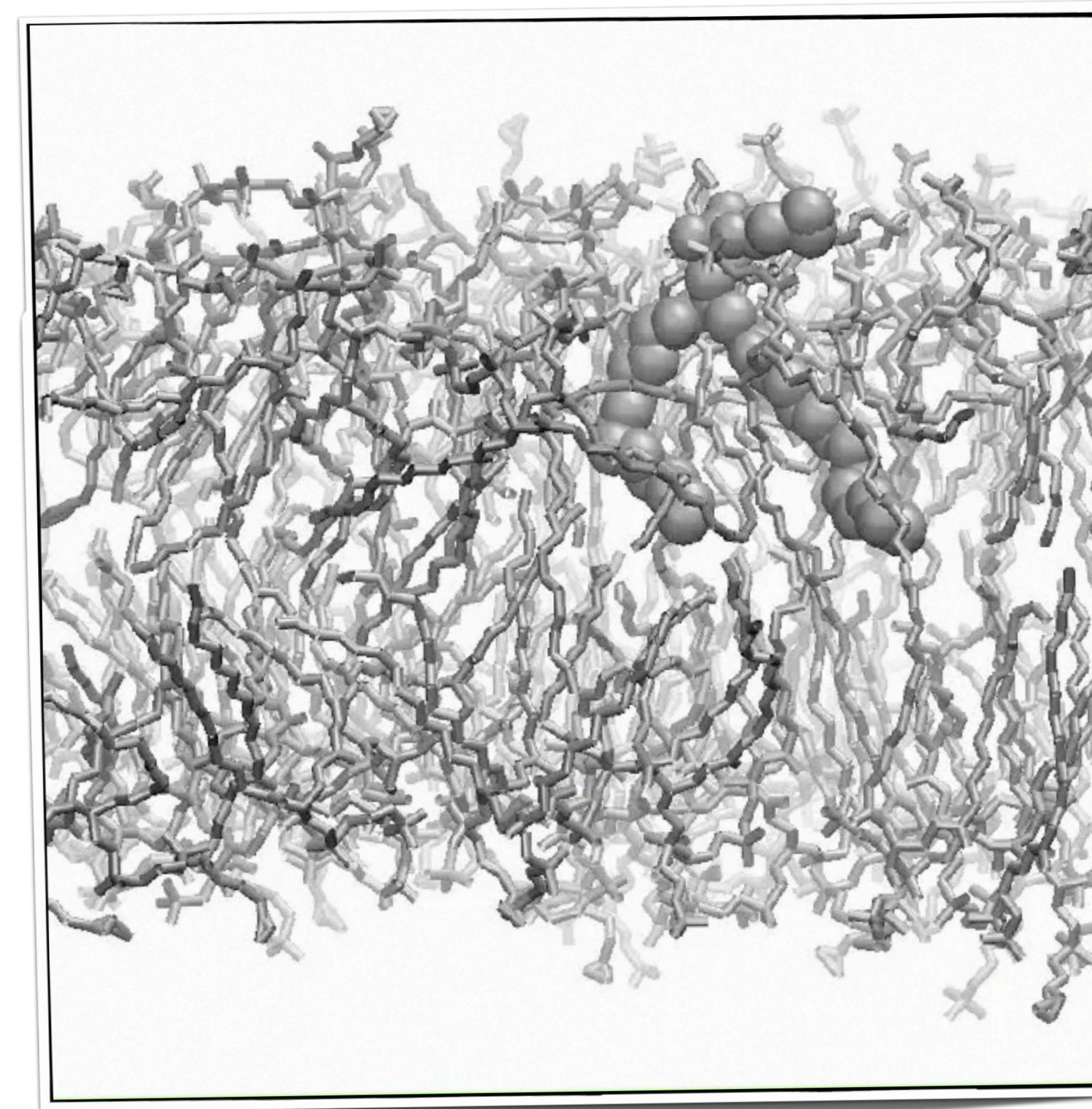


But is it what actually happens?
Check against NMR data.

So, is this structural model correct?



So, is this structural model correct?

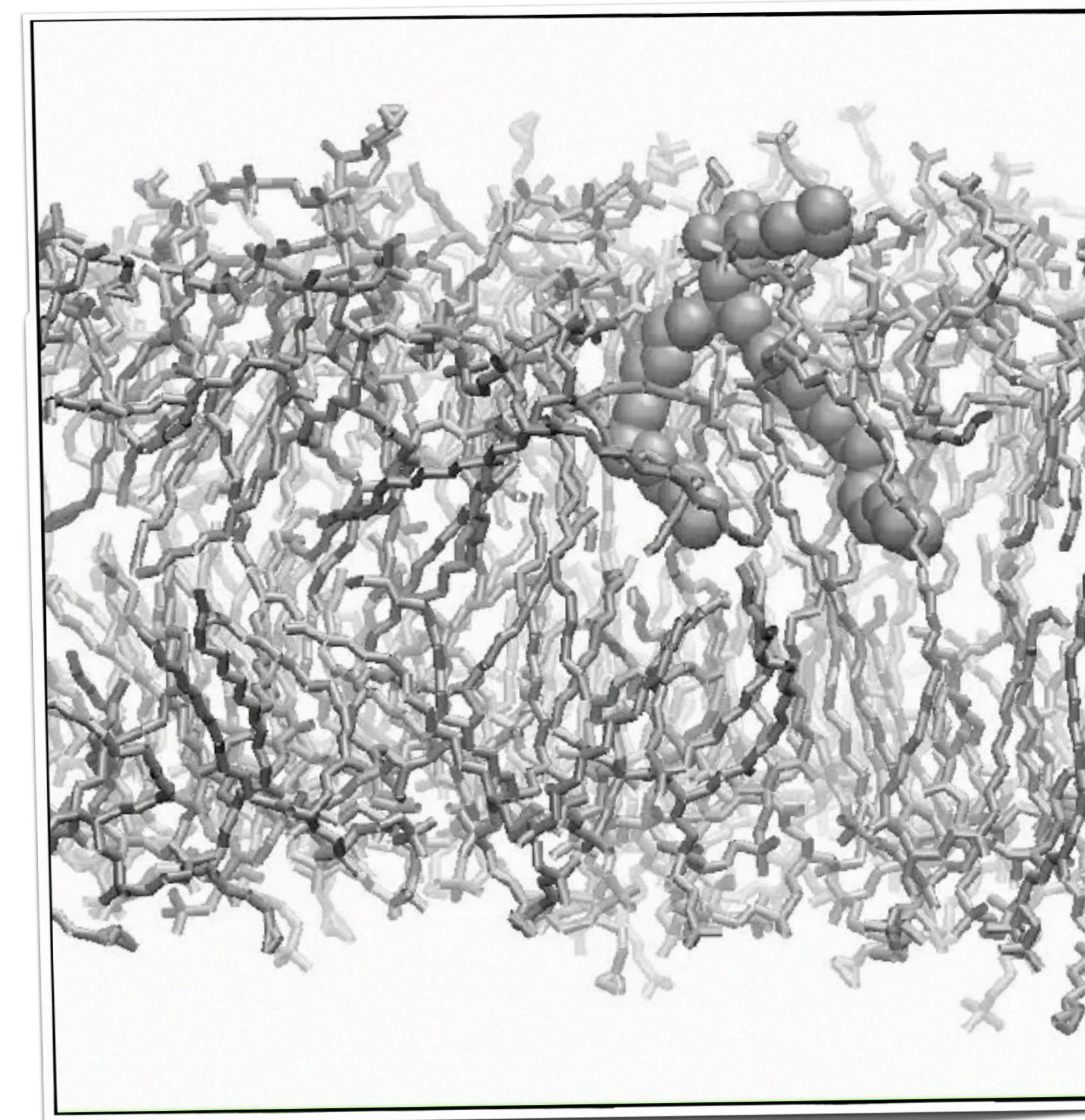


So, is this structural model correct?

Well... no.



Samuli Ollila
(in 2013)

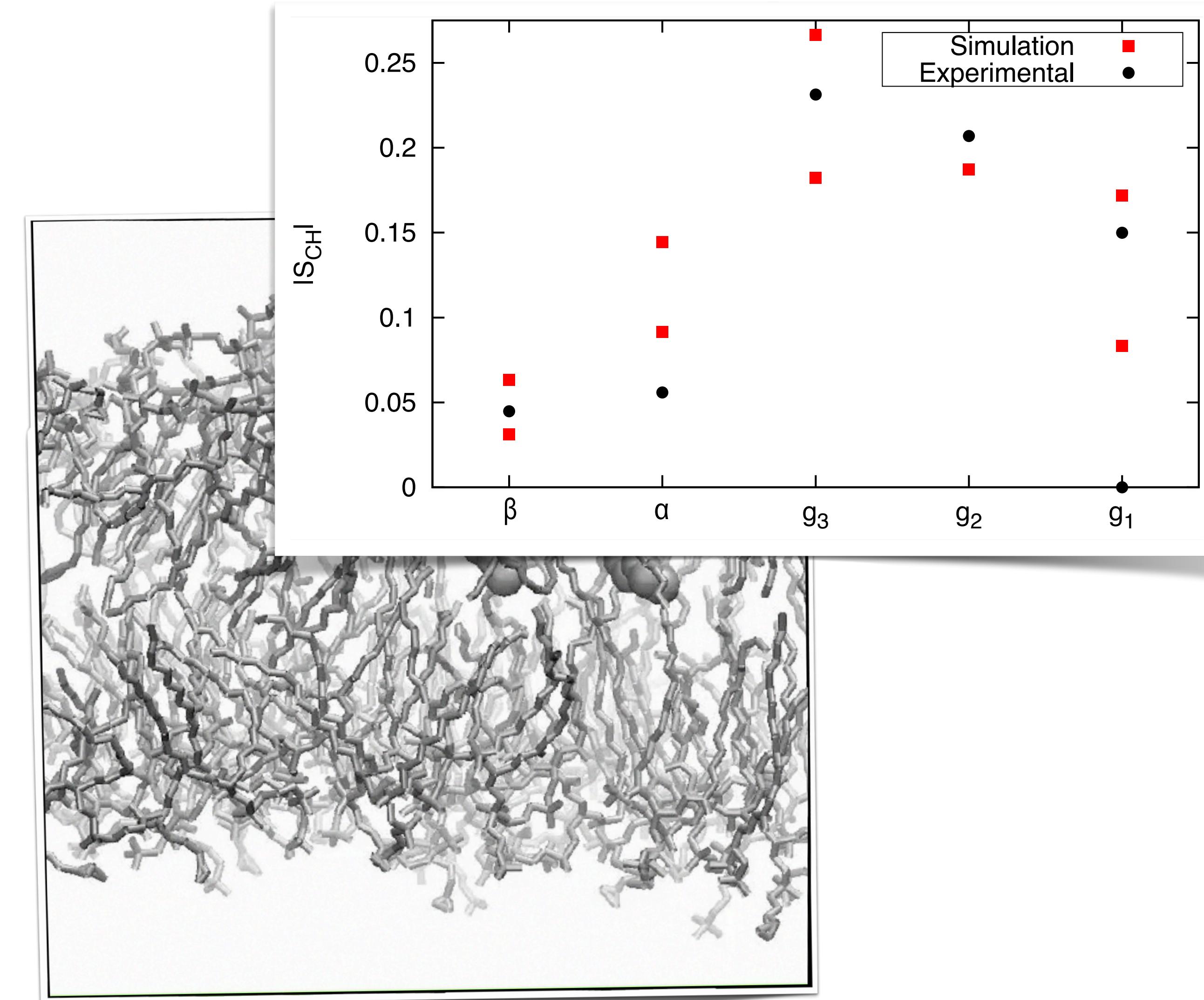


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(in 2013)

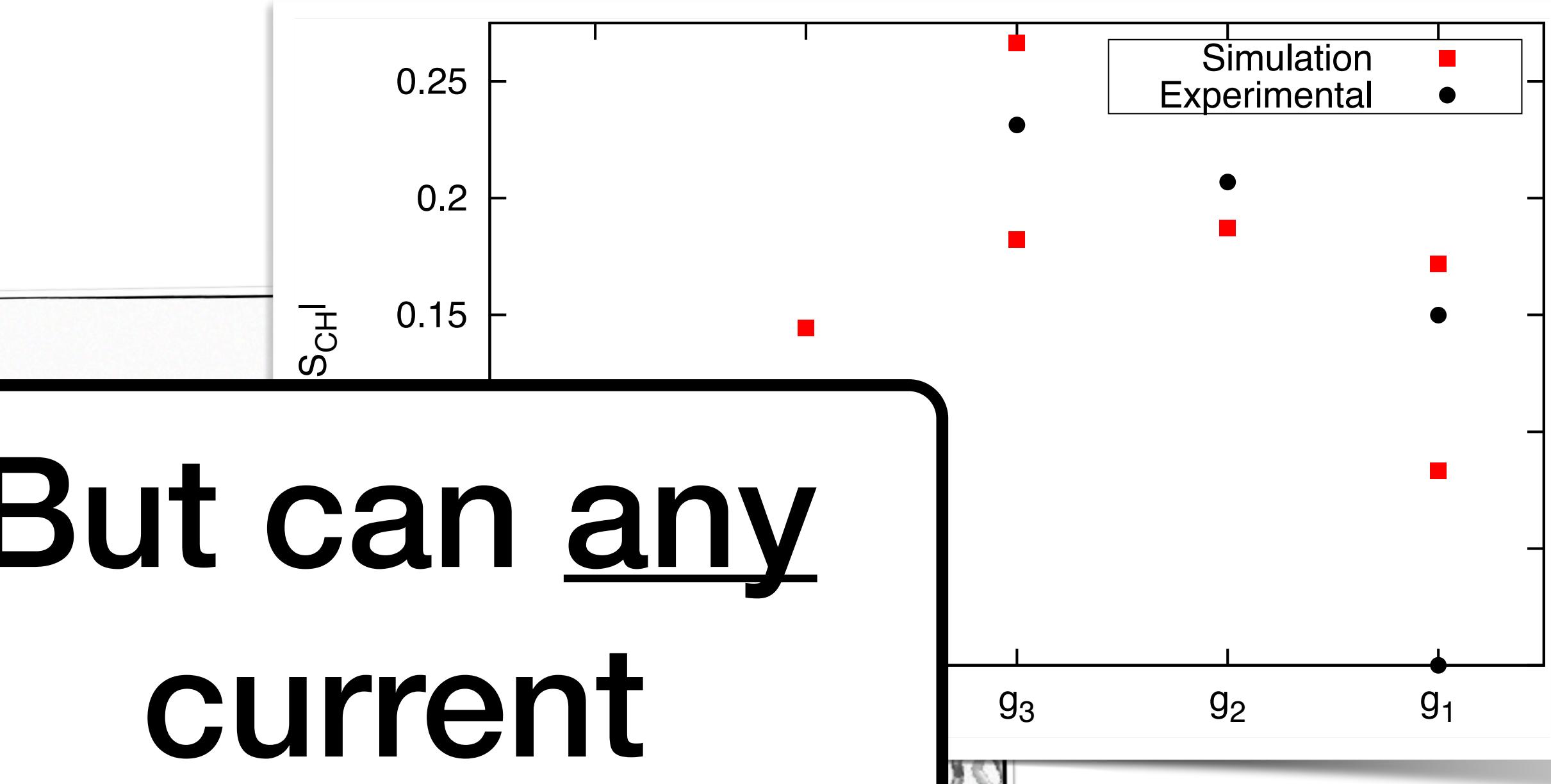


So, is this structural model correct?

Well... no.



But can any
current
MD force field
reproduce
these data?



Samuli Ollila
(in 2013)

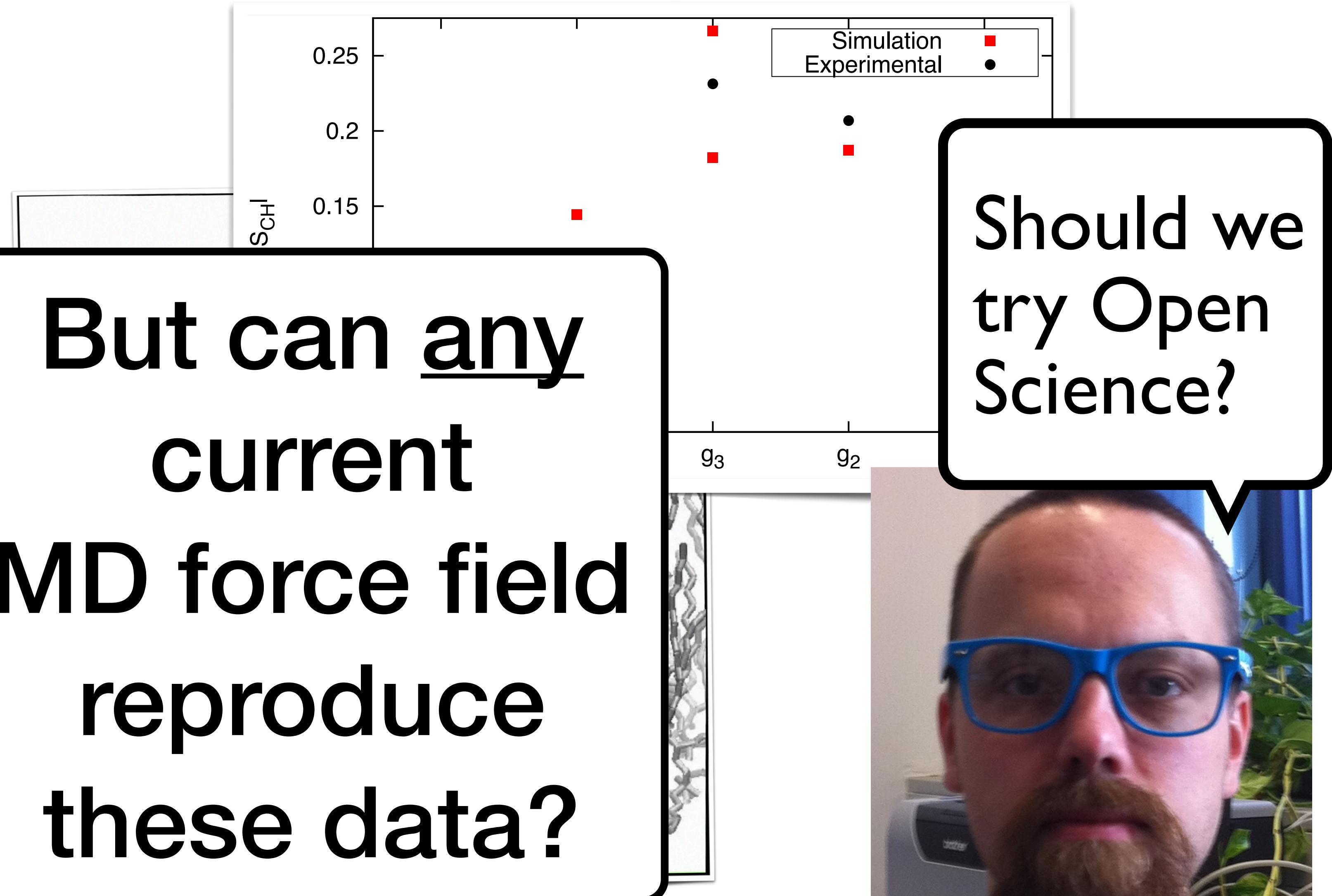
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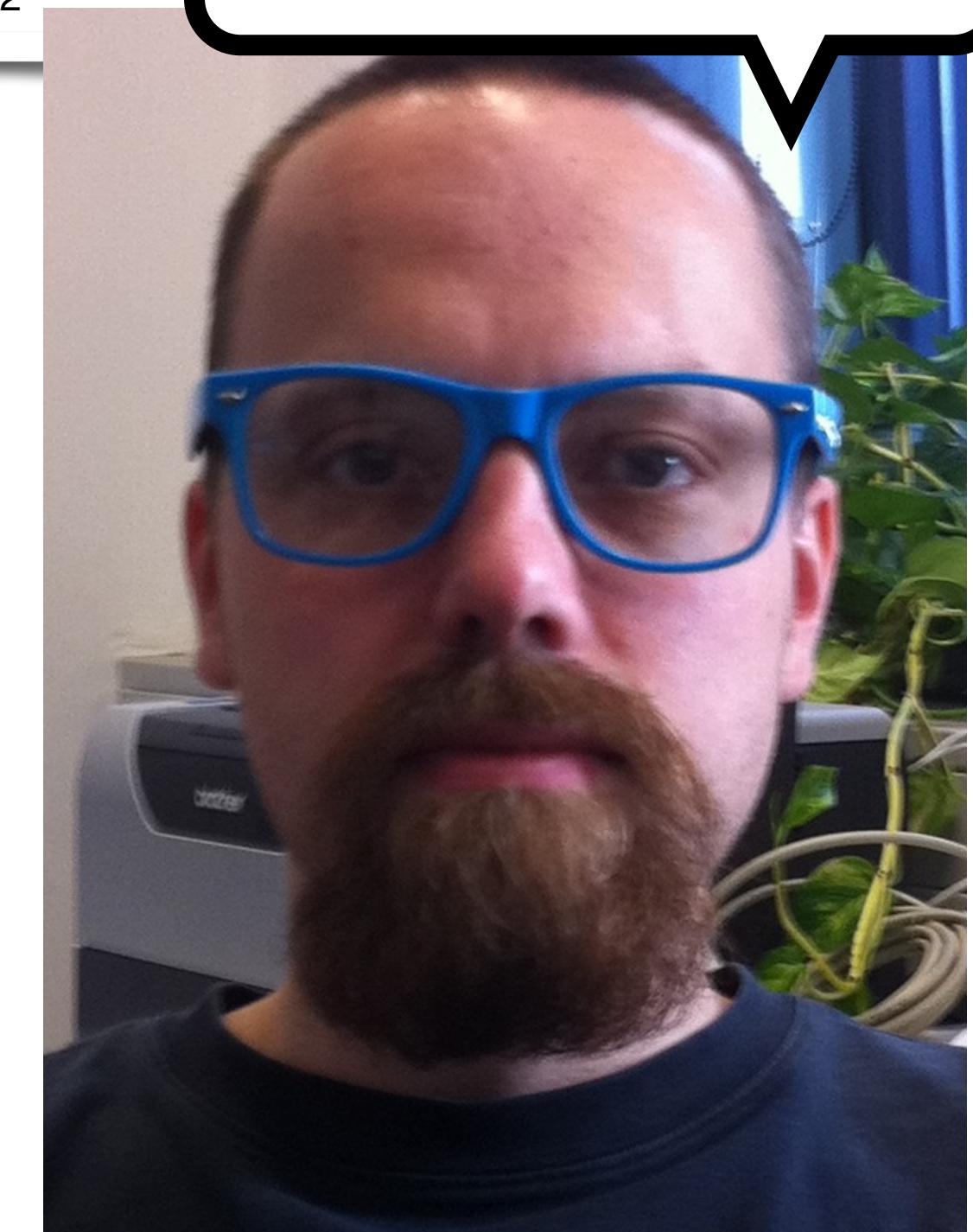


Samuli Ollila
(in 2013)

But can any
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these data?



Should we
try Open
Science?



Is massively collaborative mathematics possible?

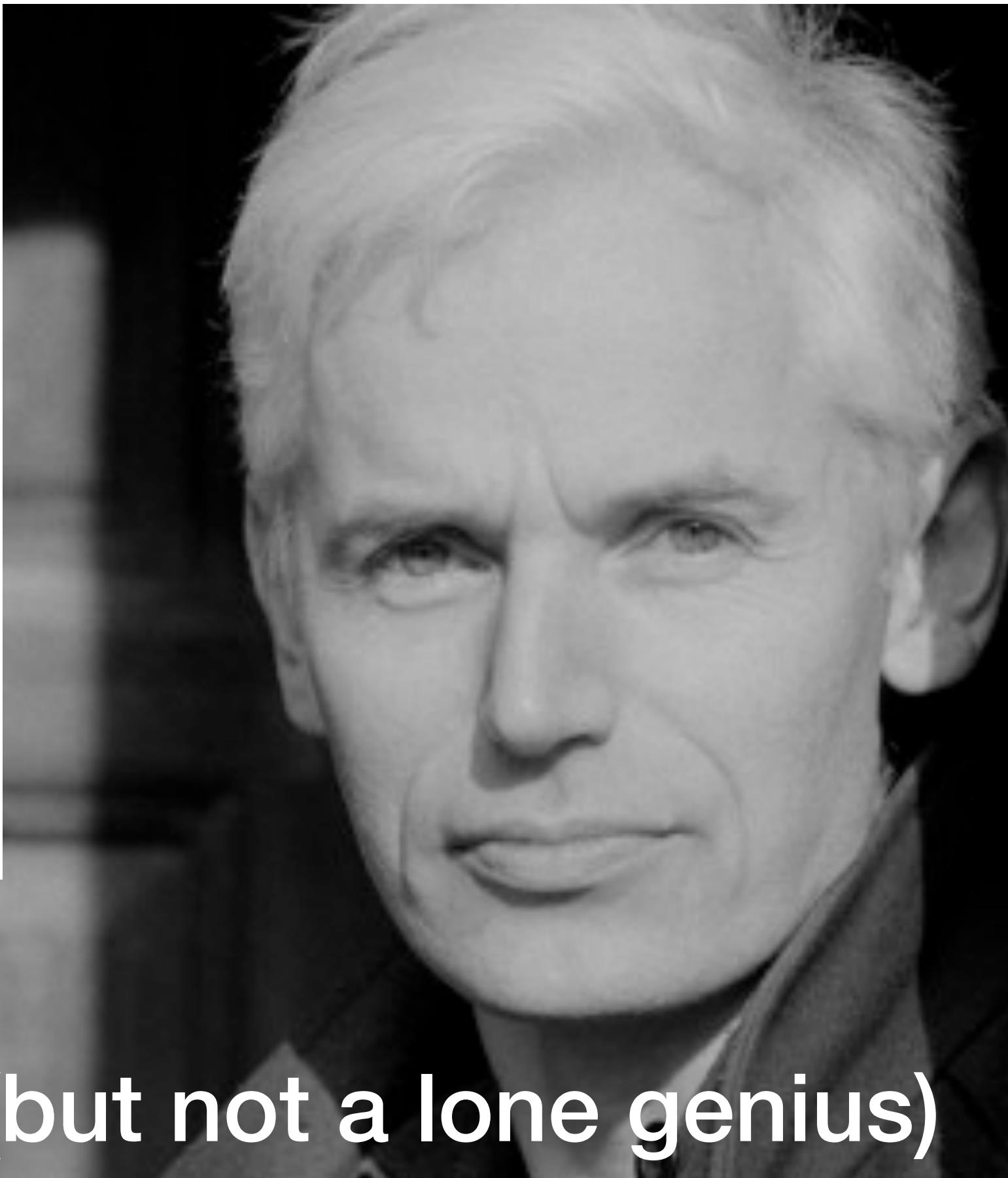
January 27, 2009

Of course, one might say, there are certain kinds of problems that lend themselves to huge collaborations. One has only to think of the proof of the classification of finite simple groups, or of a rather different kind of example such as a search for a new largest prime carried out during the downtime of thousands of PCs around the world. But my question is a different one. What about the solving of a problem that does not naturally split up into a vast number of subtasks? Are such problems best tackled by n people for some n that belongs to the set $\{1, 2, 3\}$? (Examples of famous papers with four authors do not count as an interesting answer to this question.)

It seems to me that, at least in theory, a different model could work: different, that is, from the usual model of people working in isolation or collaborating with one or two others. Suppose one had a forum (in the non-technical sense, but quite possibly in the technical sense as well) for the online discussion of a particular problem. The idea would be that anybody who had anything whatsoever to say about the problem could chip in. And the ethos of the forum — in whatever form it took — would be that comments would mostly be kept short. In other words, what you would *not* tend to do, at least if you wanted to keep within the spirit of things, is spend a month thinking hard about the problem and then come back and write ten pages about it. Rather, you would contribute ideas even if they were undeveloped and/or likely to be wrong. ([more...](#))

Posted in [Mathematics on the internet](#), [polymath1](#) | 198 Comments »

Tim Gowers,
Fields Medalist (but not a lone genius)



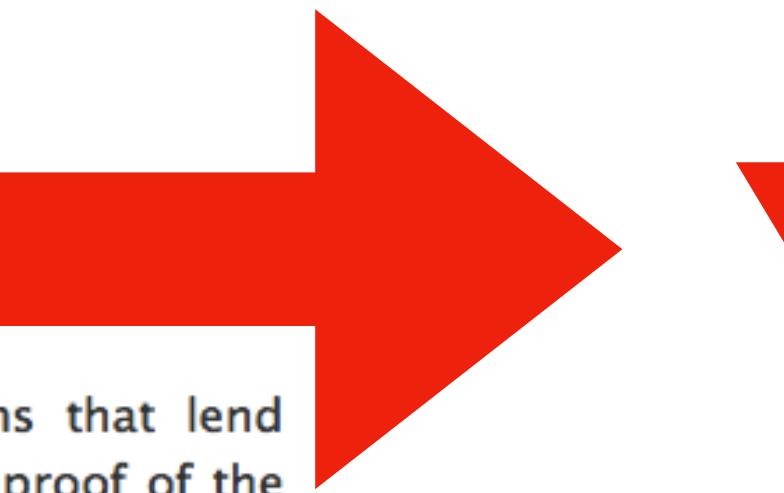
Is massively collaborative mathematics possible?

January 27, 2009

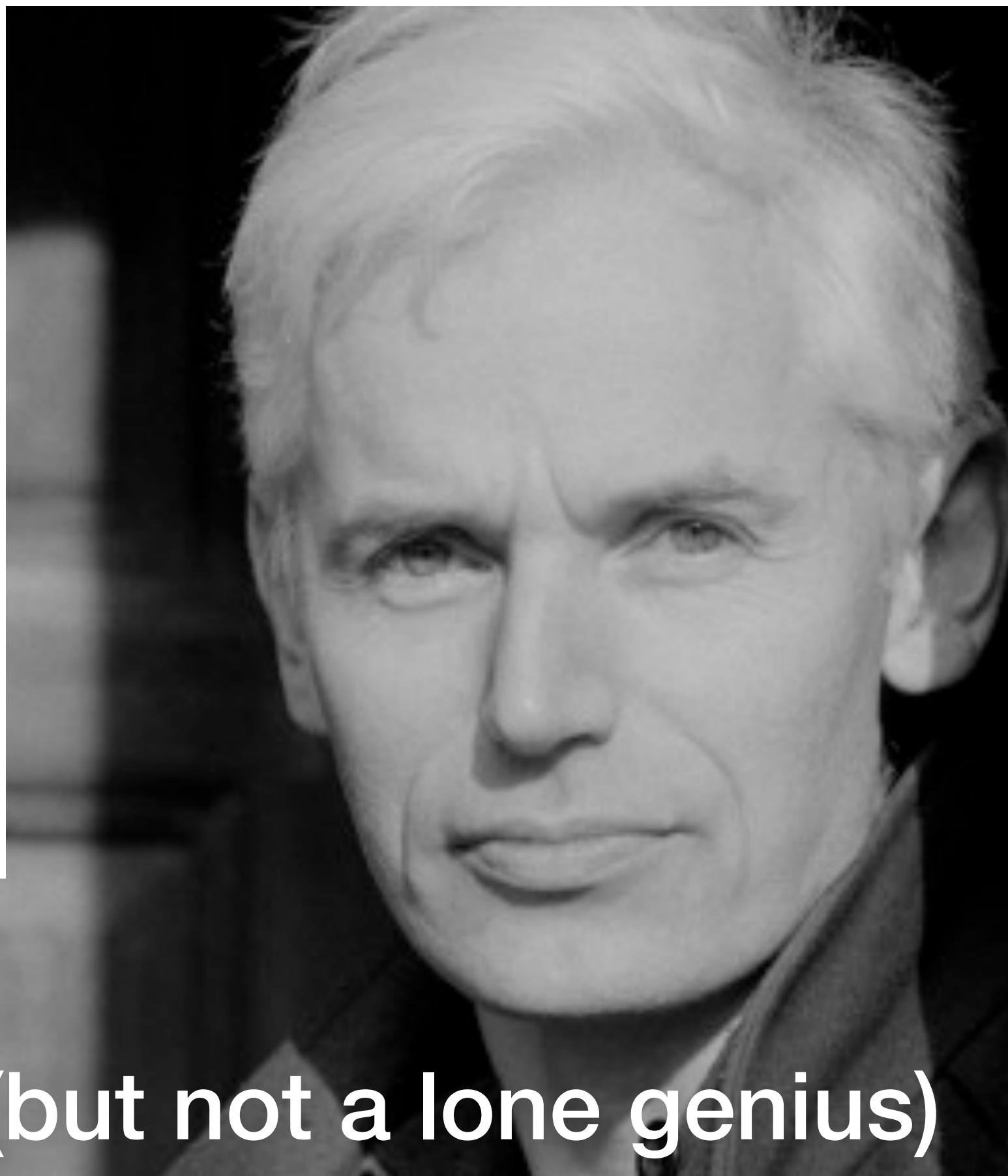
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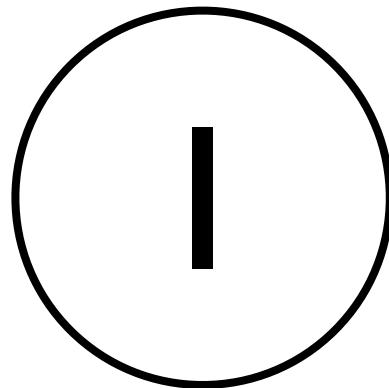


YES.



Tim Gowers,
Fields Medalist (but not a lone genius)

Our concept for open collaboration



Upload the first version
of a manuscript to arXiv.

arXiv.org > physics > arXiv:1309.2131

Physics > Biological Physics

**Response of the hydrophilic part of lipid
membranes to changing conditions – a critical
comparison of simulations to experiments**

O. H. Samuli Ollila

(Submitted on 9 Sep 2013)



Invite scientist to collaborate on improving the manuscript using
an open blog

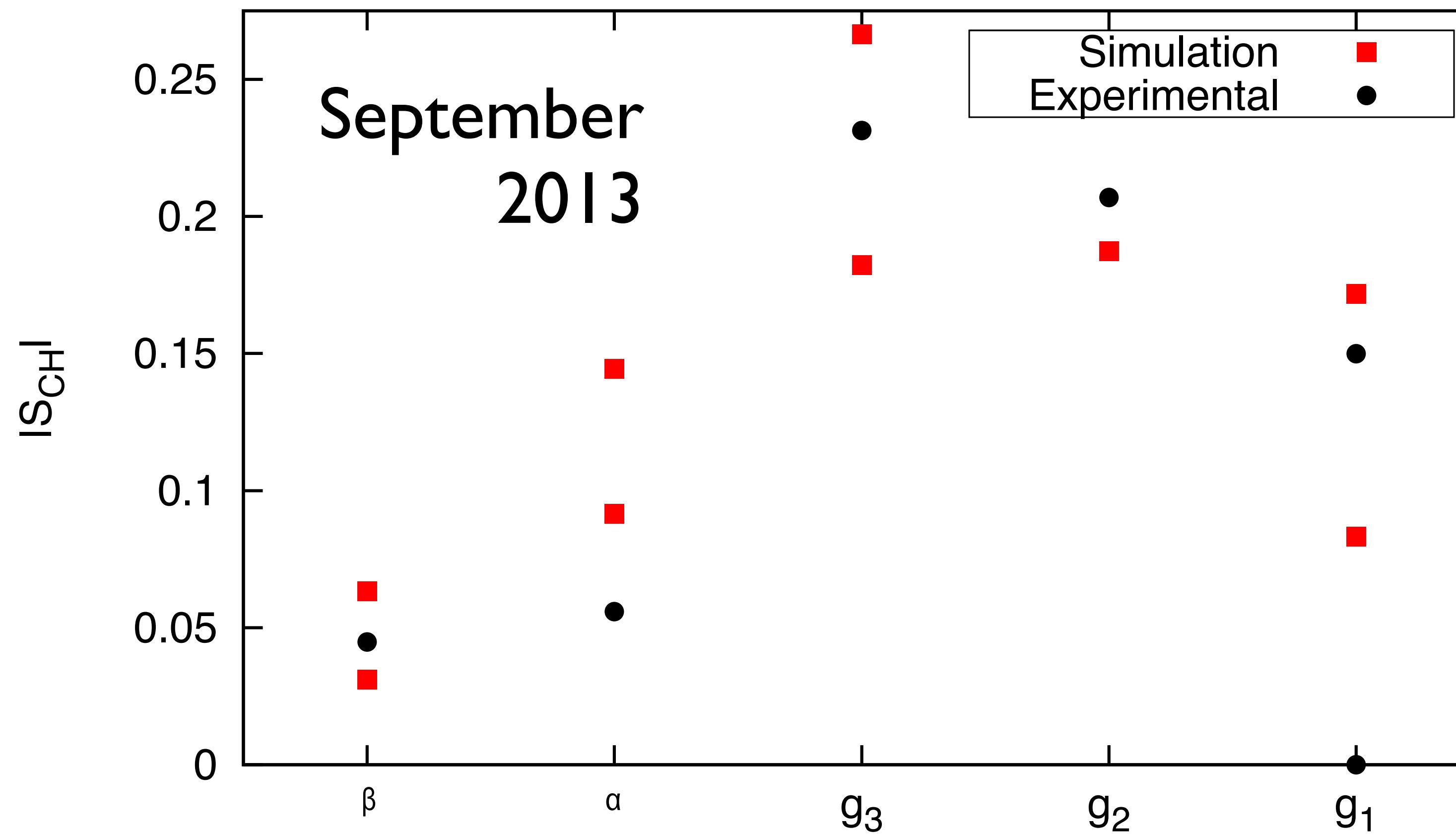
nmrlipids.blogspot.fi



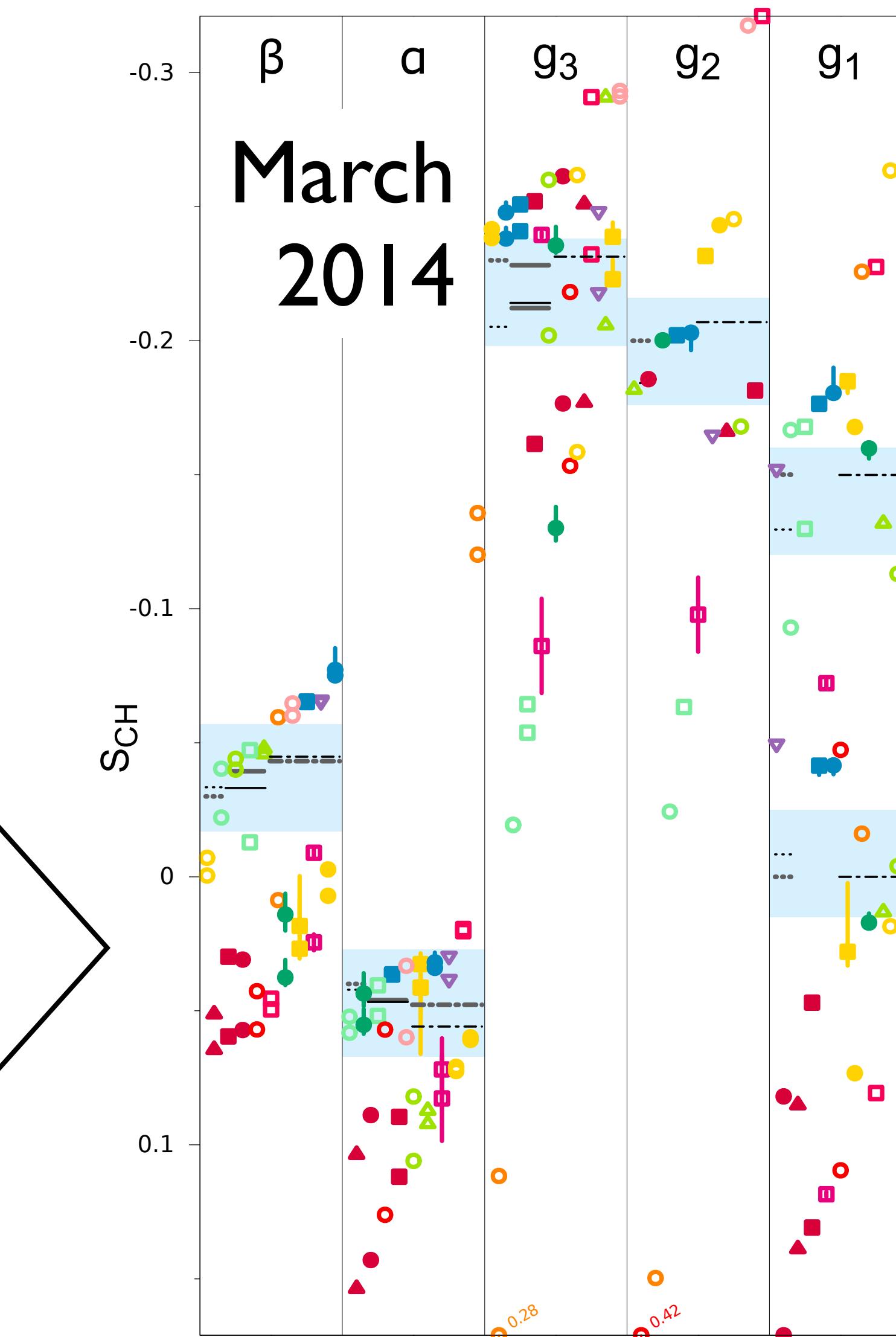
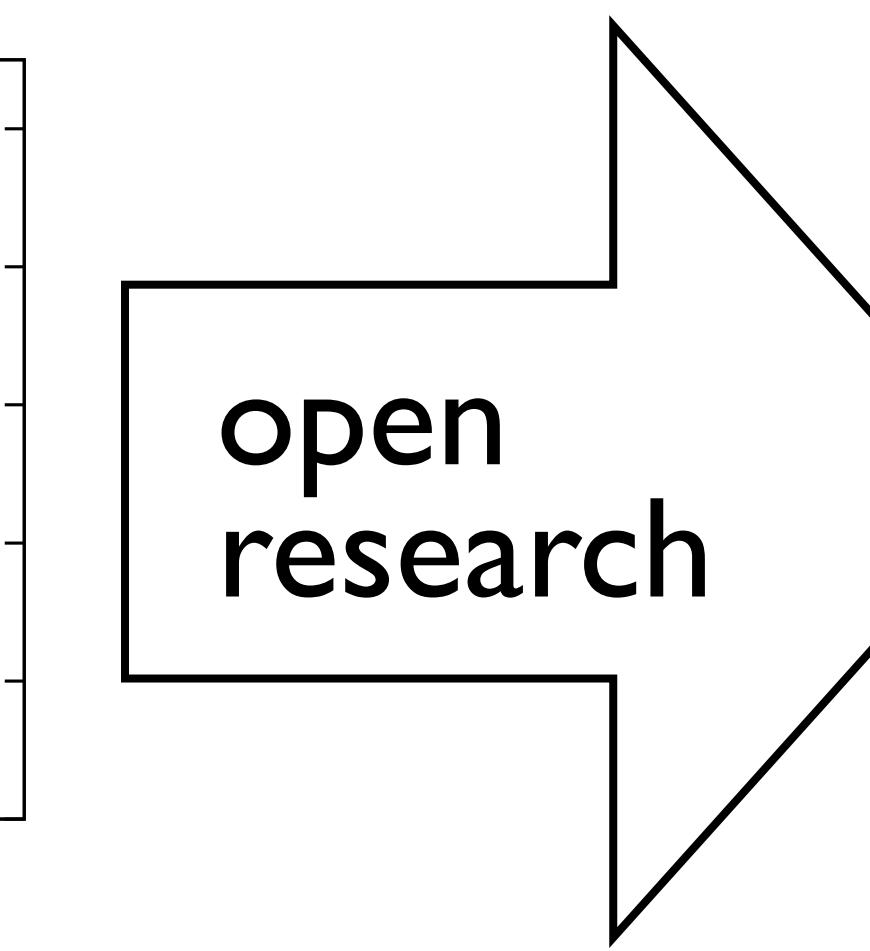
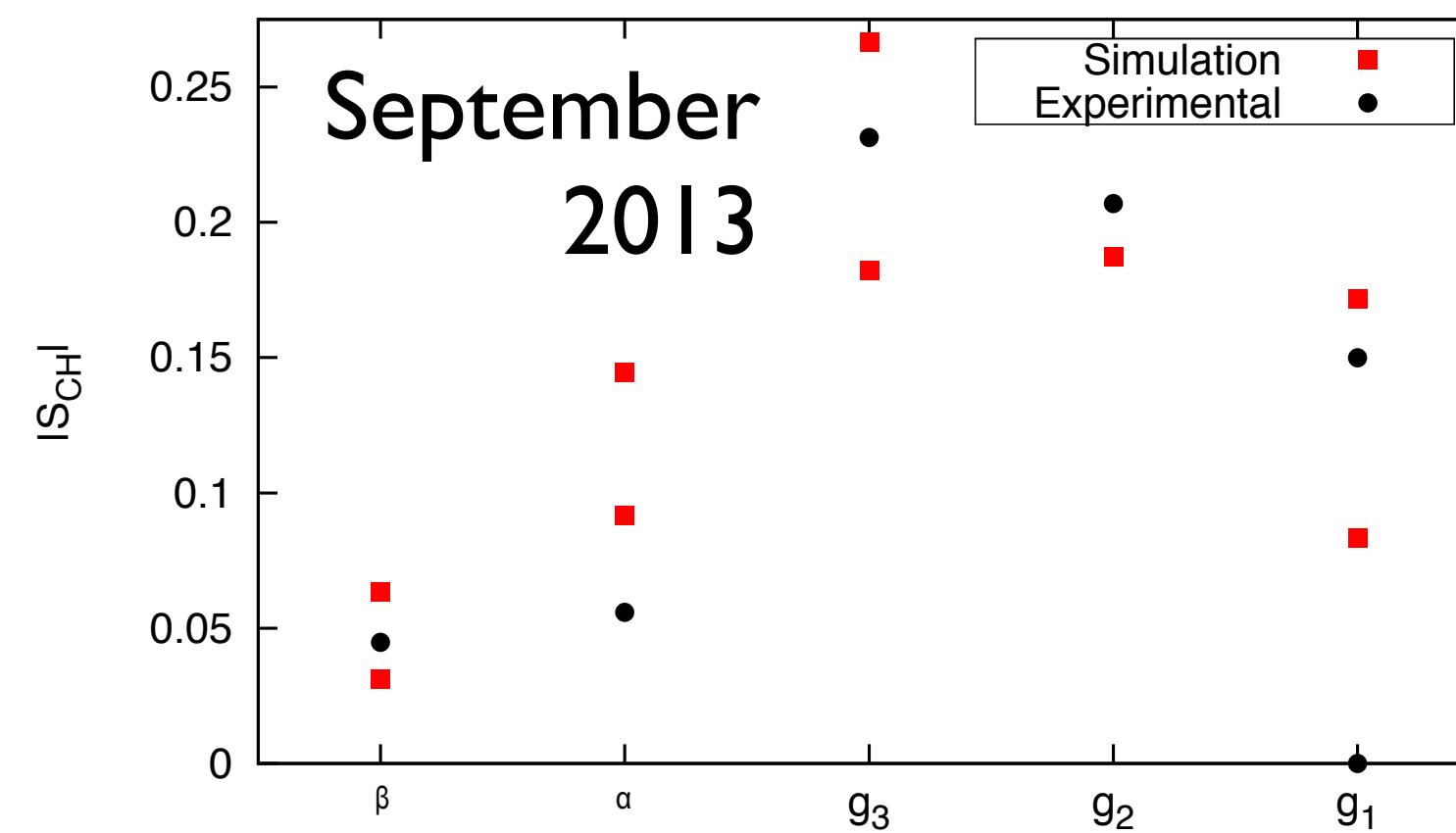
Submit the final manuscript to a peer-reviewed journal.

Offer coauthorship to everyone who has contributed.
List names alphabetically, with Samuli as the corresponding author.

The power of openness



The power of openness : 13+ force fields tested in a few months

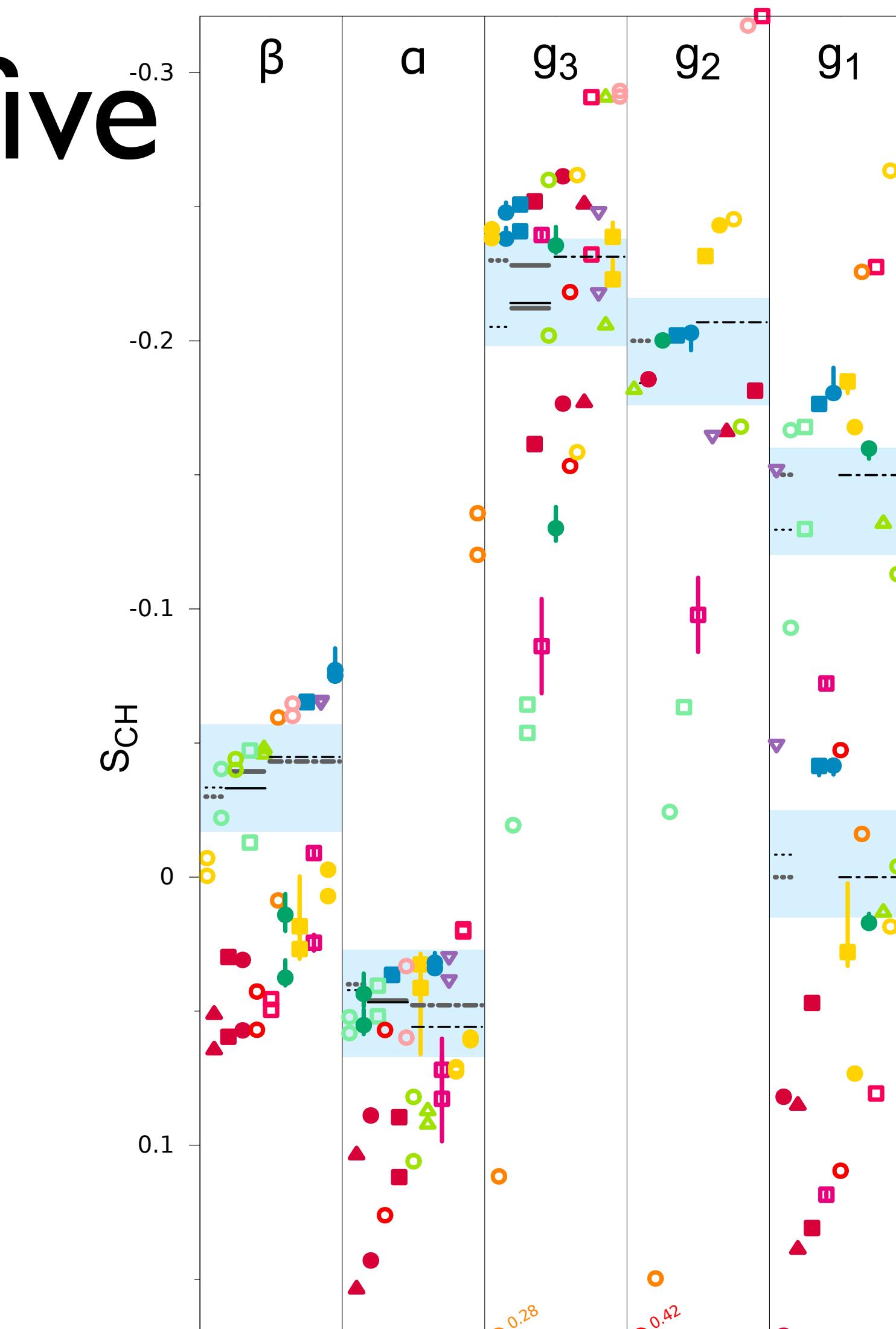
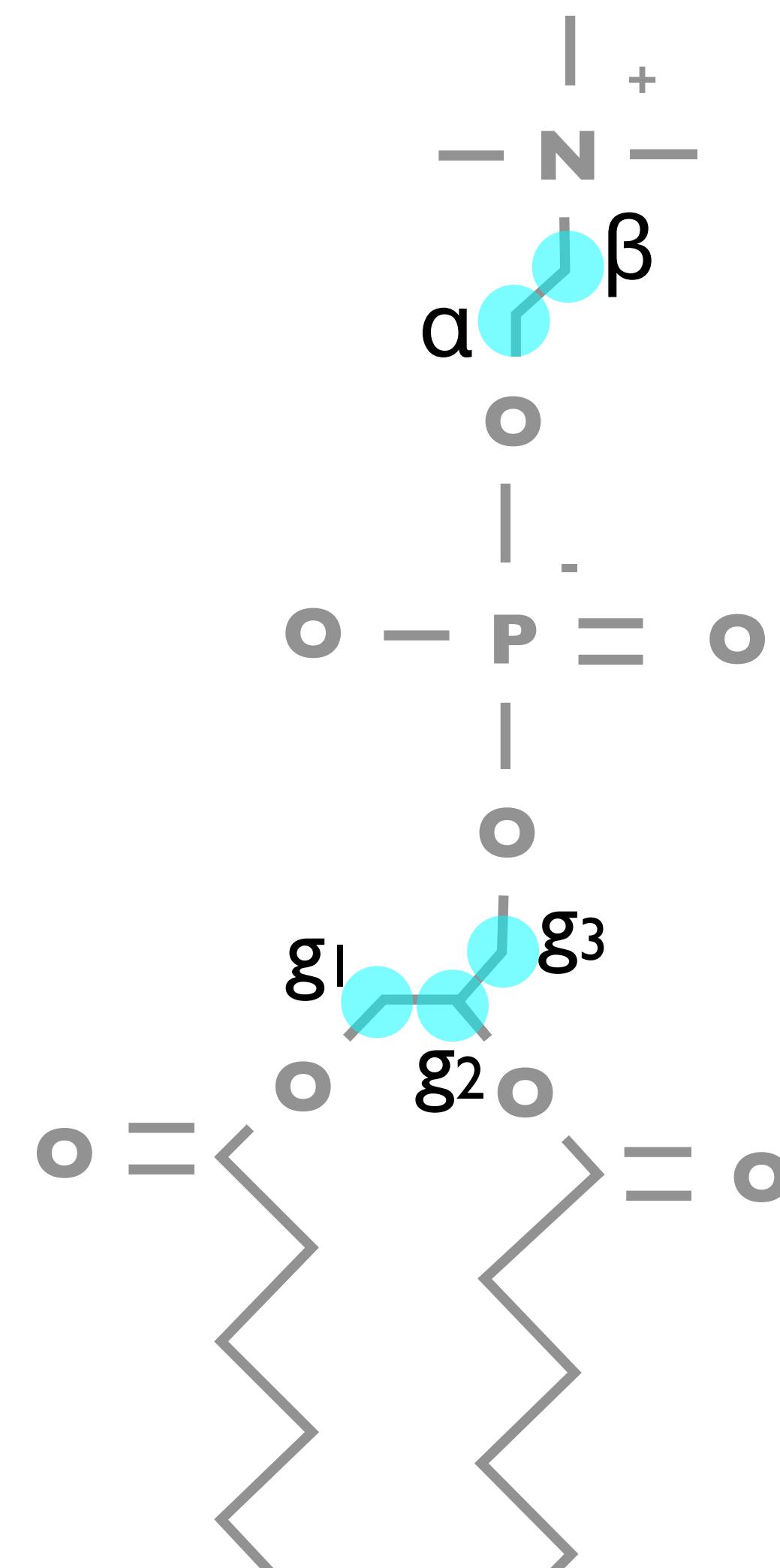


Legend:

- DMPC 303K $^{13}\text{C-NMR}$ (1)
- DMPC 314K $^{13}\text{C-NMR}$ (2)
- Berger 323K Berger
- Högberg08 303K Högberg08
- DLPC 323K C36UA
- DPPC 322K $^2\text{H-NMR}$
- DPPC 323K " "
- Berger 323K Berger
- TjøEdh 323K TjøEdh
- Poger 323K Poger
- CHARMM36 323K CHARMM36
- Slipids 310K Slipids
- GAFFlipid 303K GAFFlipid
- Lipid14 298K Lipid14
- MacRog 310K MacRog
- CHARMM36 303K CHARMM36
- Slipids 310K Slipids
- GAFFlipid 298K GAFFlipid
- Lipid14 298K Lipid14
- MacRog 310K MacRog

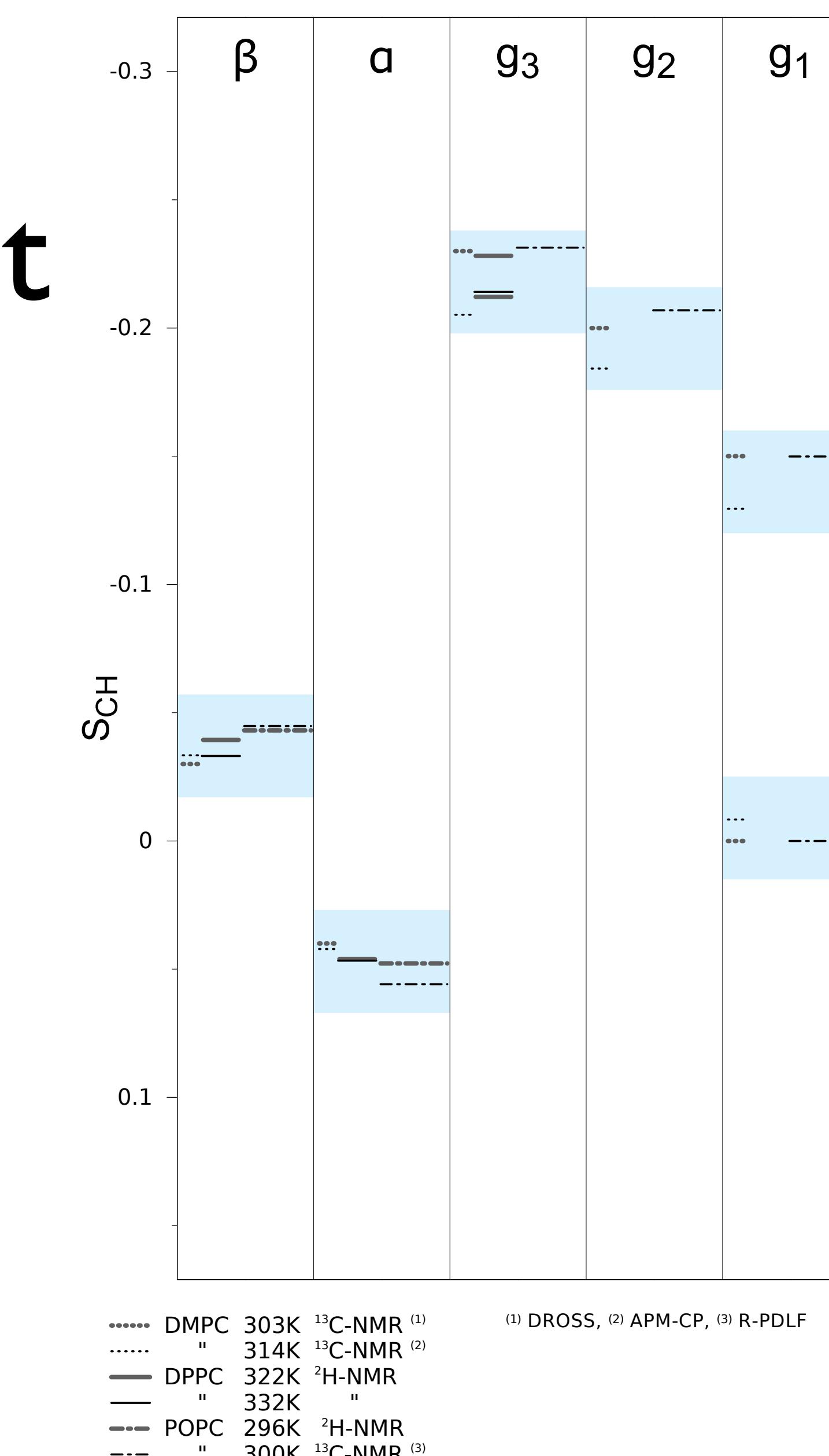
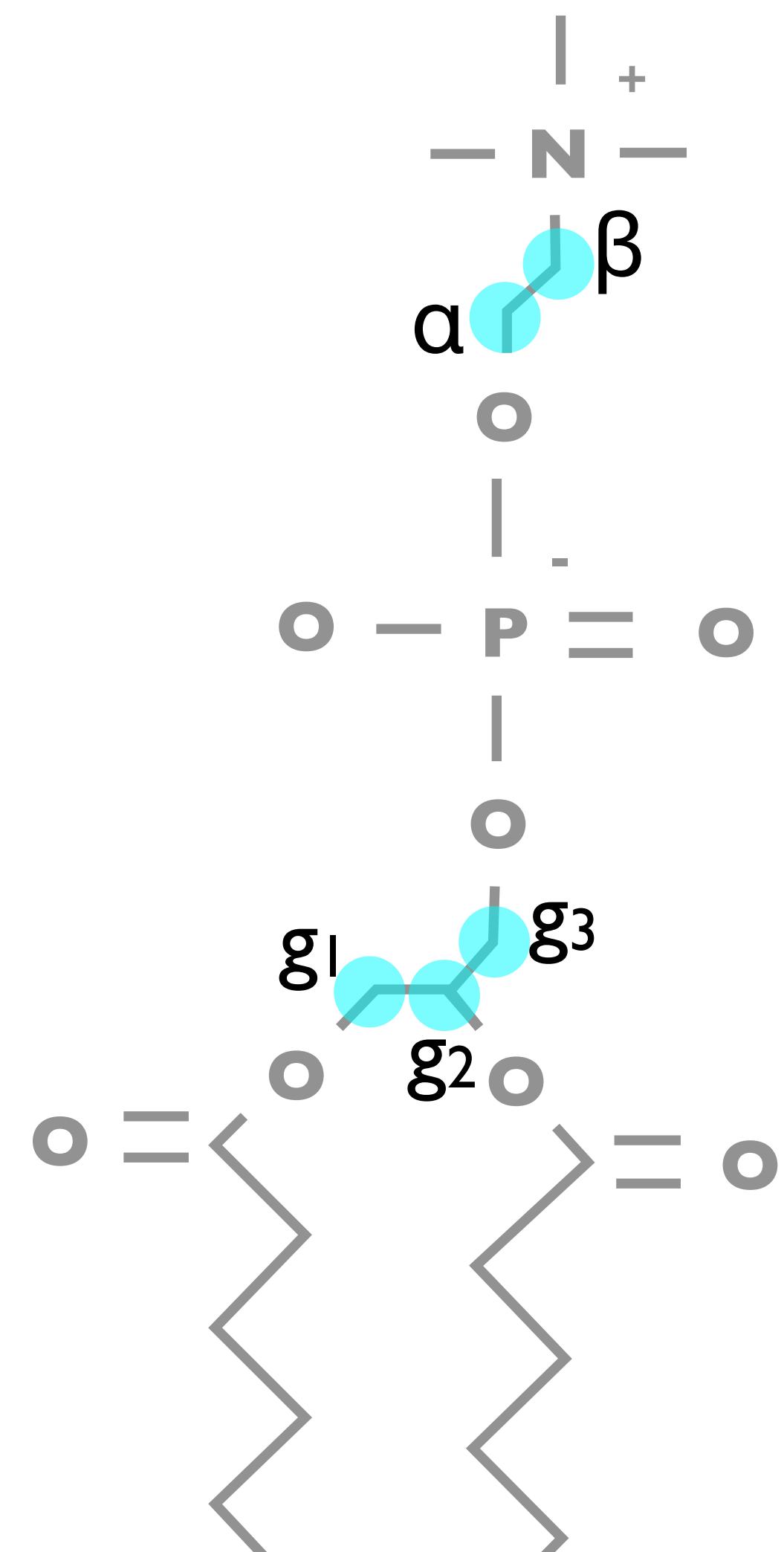
(1) DROSS, (2) APM-CP, (3) R-PDLF

NMRlipids focuses on five water-facing carbons

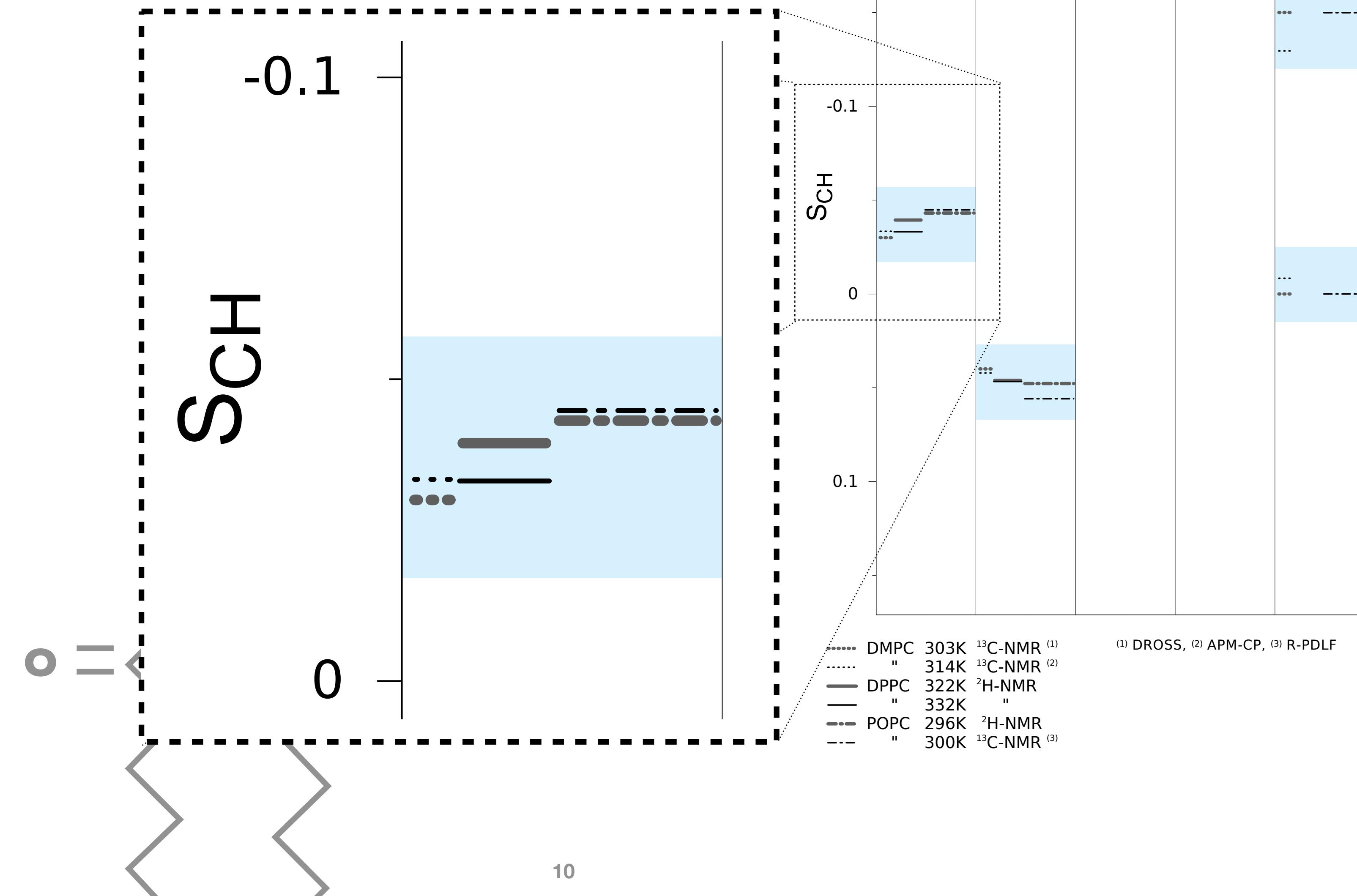


..... DMPC	303K	$^{13}\text{C-NMR}$ (1) POPC	296K	$^2\text{H-NMR}$
..... " 314K	$^{13}\text{C-NMR}$ (2) " 300K	$^{13}\text{C-NMR}$ (3) " 298K	Berger
▲ " 323K	Berger " 298K	Berger	○ " 310K	Chiu
▲ " 303K	Högberg08 " 310K	" Kukol	○ " 303K	UlmUlm
▼ DLPC	323K C36UA " 303K	Slipids	○ " 303K	CHARMM36
— DPPC	322K $^2\text{H-NMR}$ " 303K	Högberg08	○ " 303K	GAFFlipid
— " 332K	" " 298K	" GAFFlipid	○ " 298K	Lipid14
■ " 323K	Berger " 310K	" MacRog	○ " 310K	DROSS
□ " 323K	TjoEdh " 310K	APM-CP	○ " 310K	R-PDLF
■ " 323K	Poger " 303K	"	○ " 310K	"
■ " 323K	CHARMM36 " 303K	"	○ " 310K	"
■ " 323K	Slipids " 303K	"	○ " 310K	"
■ " 323K	GAFFlipid " 303K	"	○ " 310K	"

Experiments are rather consistent

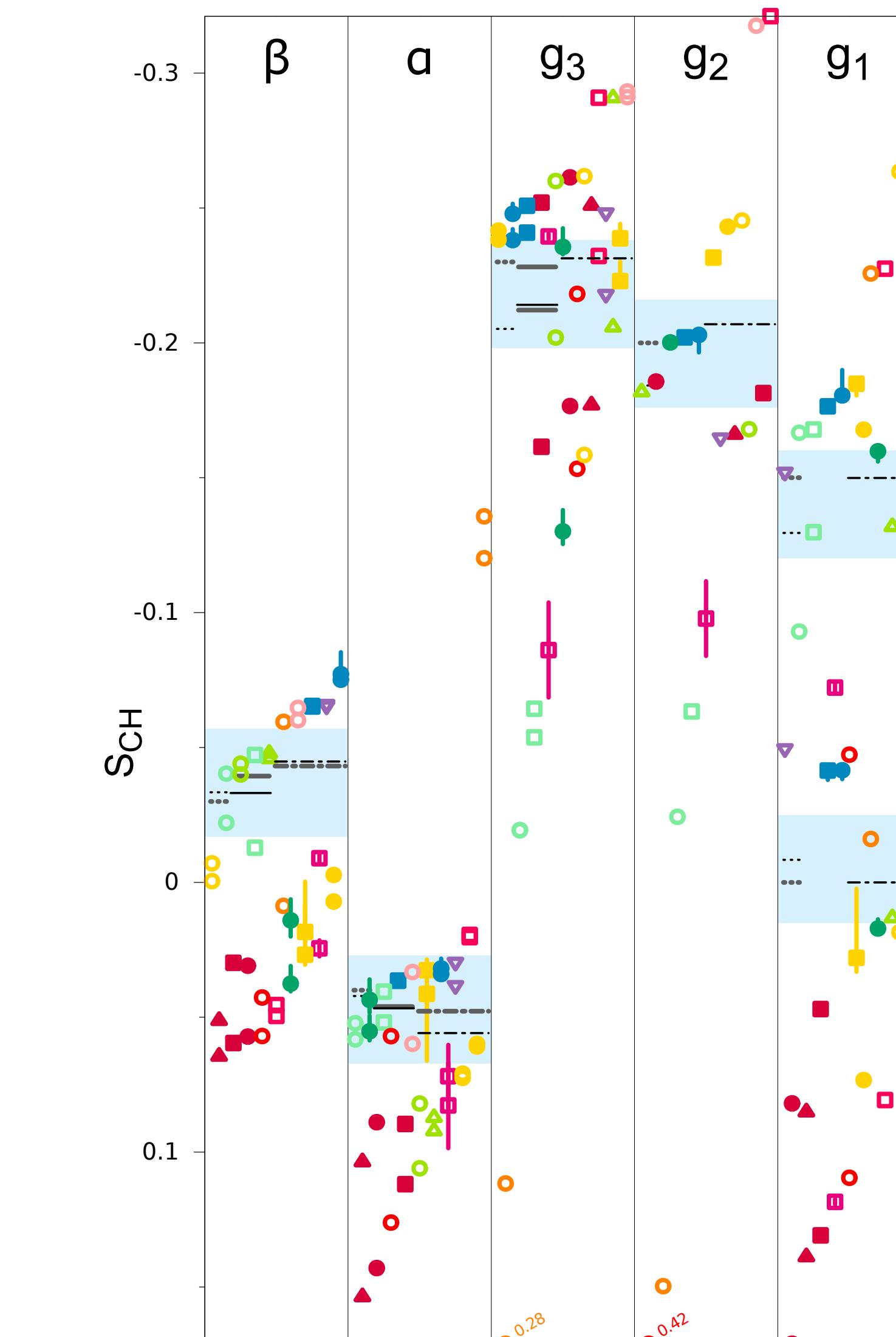
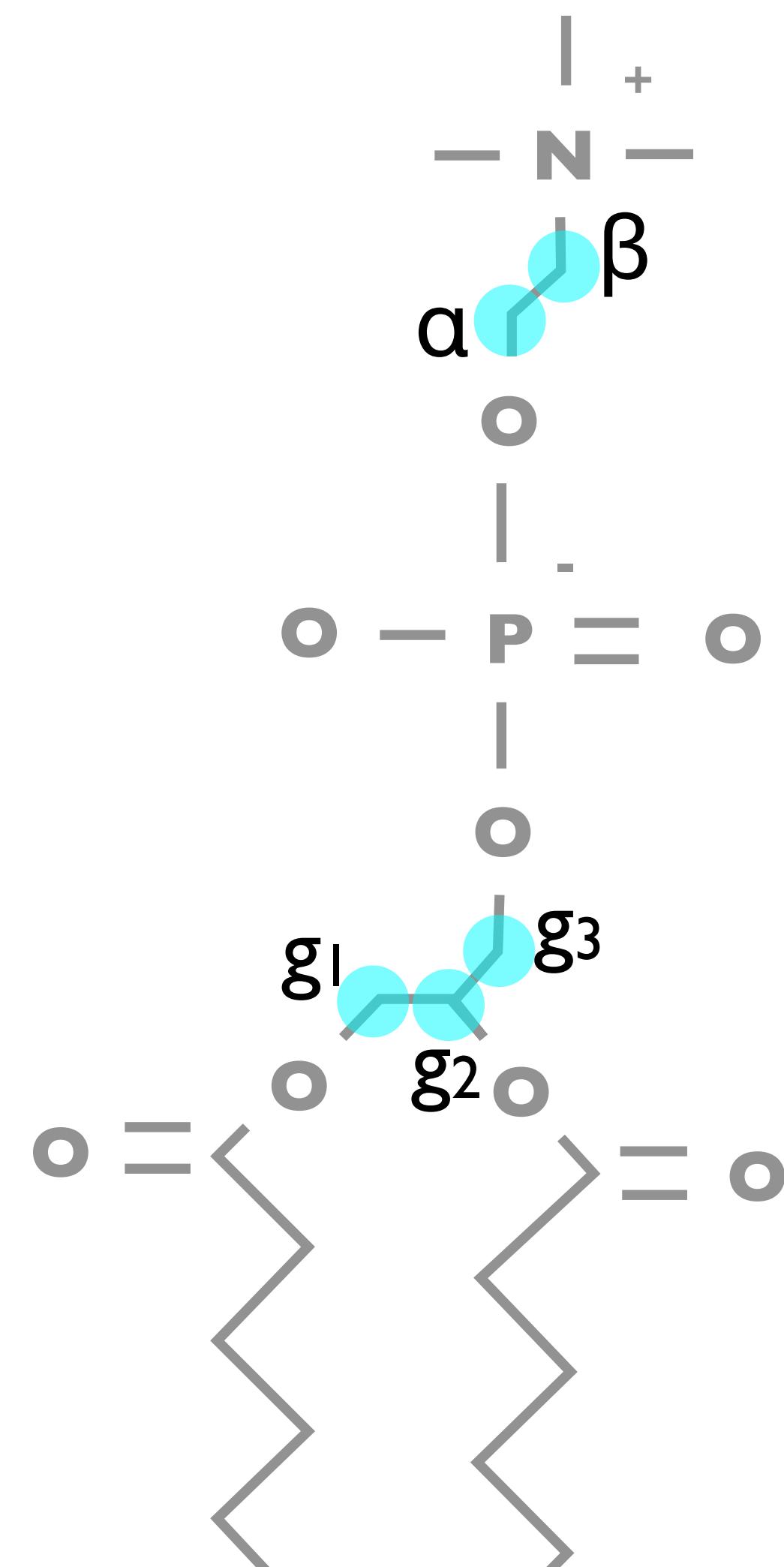


Experiments are rather consistent



The simulations...

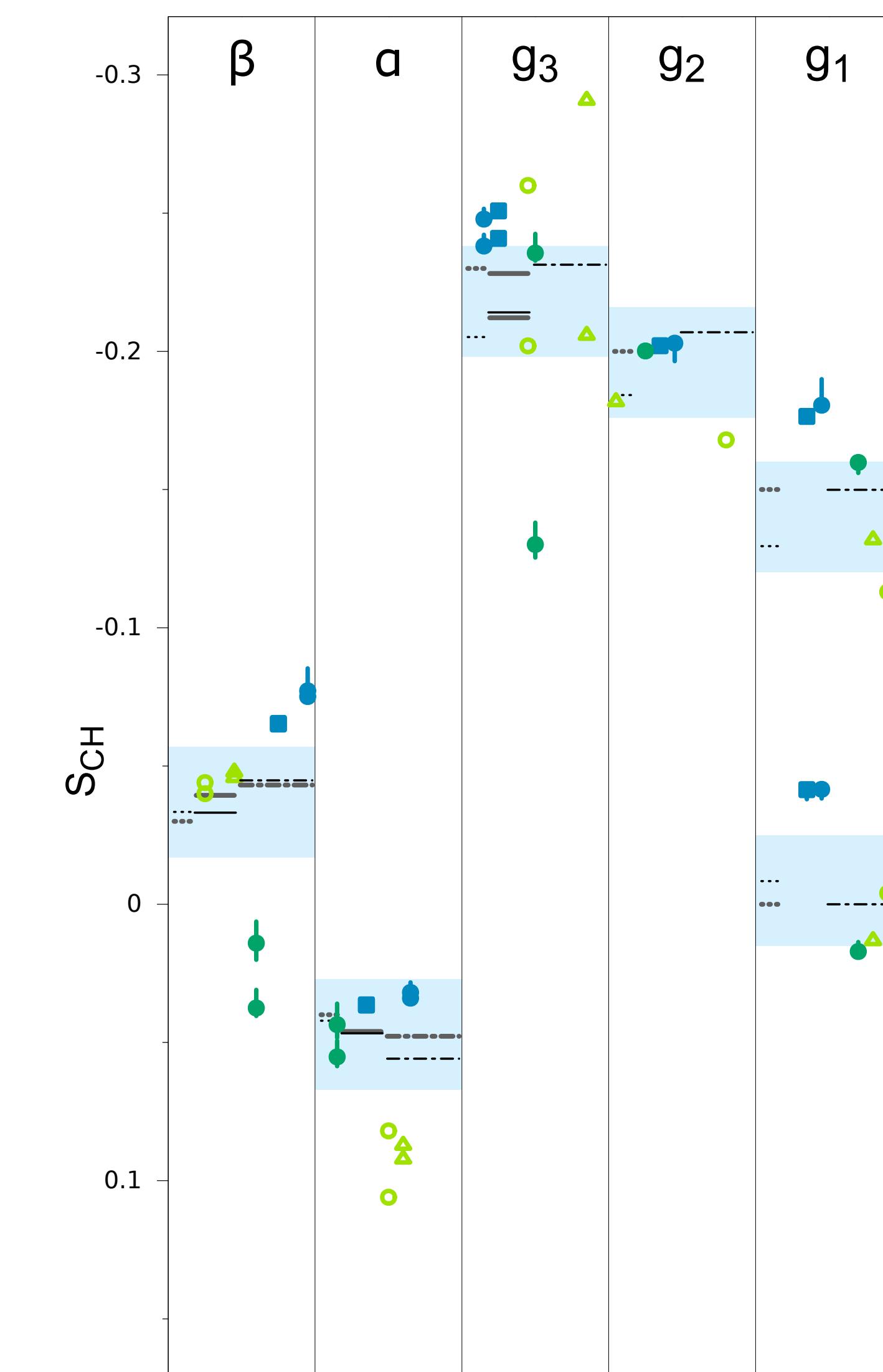
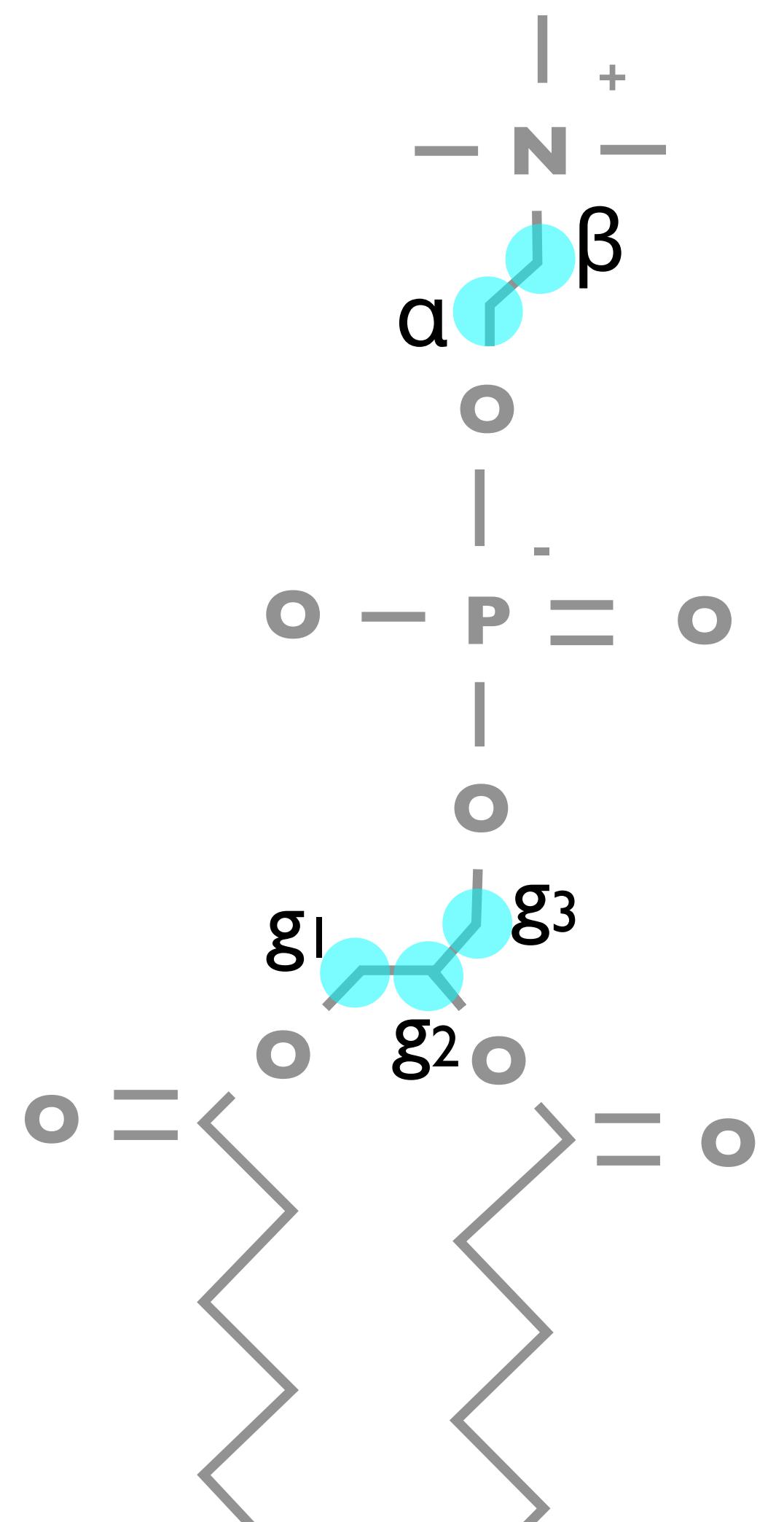
less so



..... DMPC 303K $^{13}\text{C-NMR}$ ⁽¹⁾ POPC 296K $^2\text{H-NMR}$
..... " 314K $^{13}\text{C-NMR}$ ⁽²⁾ POPC 300K $^{13}\text{C-NMR}$ ⁽³⁾
▲ " 323K Berger	● " Berger
▲ " 303K Högberg08	○ " Chiu
▼ DLPC 323K C36UA	○ " Kukol
— DPPC 322K $^2\text{H-NMR}$	○ " UlmUlm
— " 332K "	— " Slipids
■ " 323K Berger	— " 303K CHARMM36
□ " " TjoEdh	— " 303K Högberg08
■ " " Poger	— " 303K GAFFlipid
■ " " CHARMM36	— " 298K Lipid14
■ " " Slipids	— " 310K MacRog
■ " " GAFFlipid	

⁽¹⁾ DROSS, ⁽²⁾ APM-CP, ⁽³⁾ R-PDLF

The top 3 force fields



(1) DROSS, (2) APM-CP, (3) R-PDLF

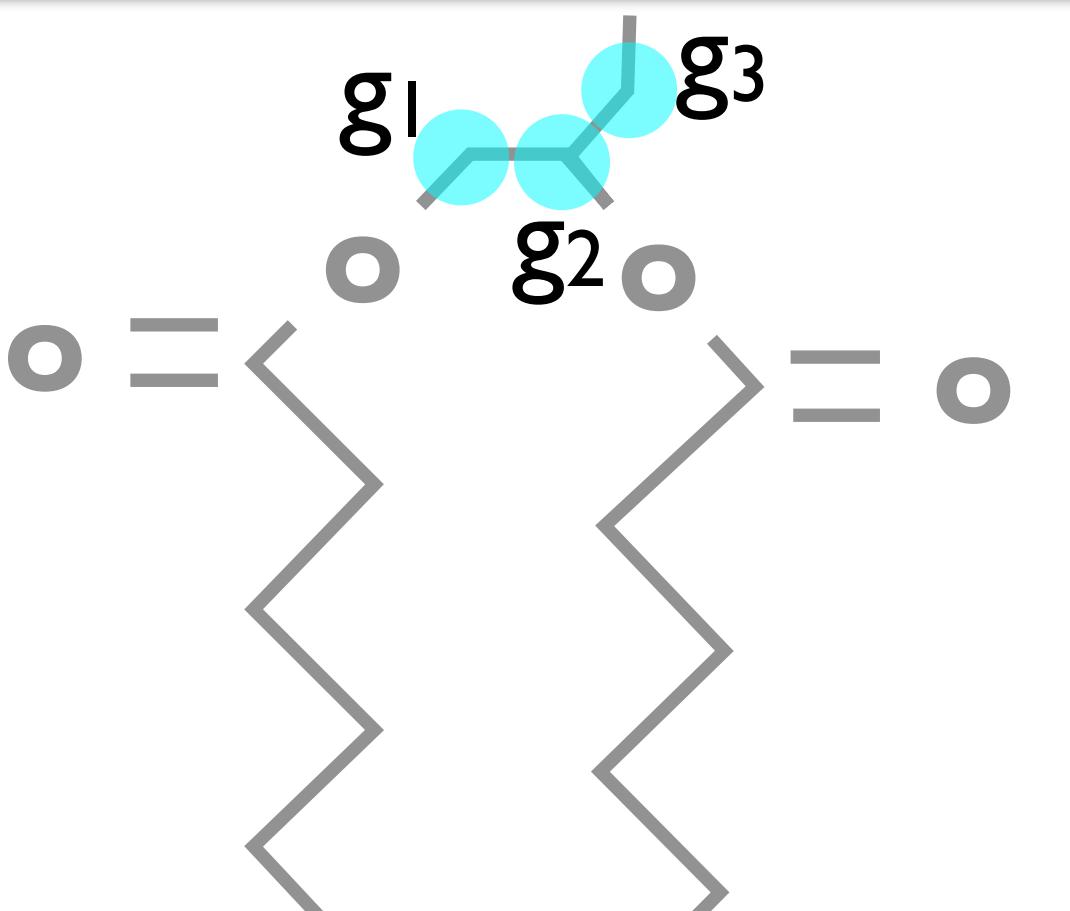
- DMPC 303K ^{13}C -NMR (1)
- " 314K ^{13}C -NMR (2)
- ▲ " 303K Högberg08
- DPPC 322K ^2H -NMR
- " 332K "
- 323K CHARMM36
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- POPC 300K ^{13}C -NMR (3)
- " 303K CHARMM36
- " 303K Högberg08
- " 310K MacRog

The top 3 force fields

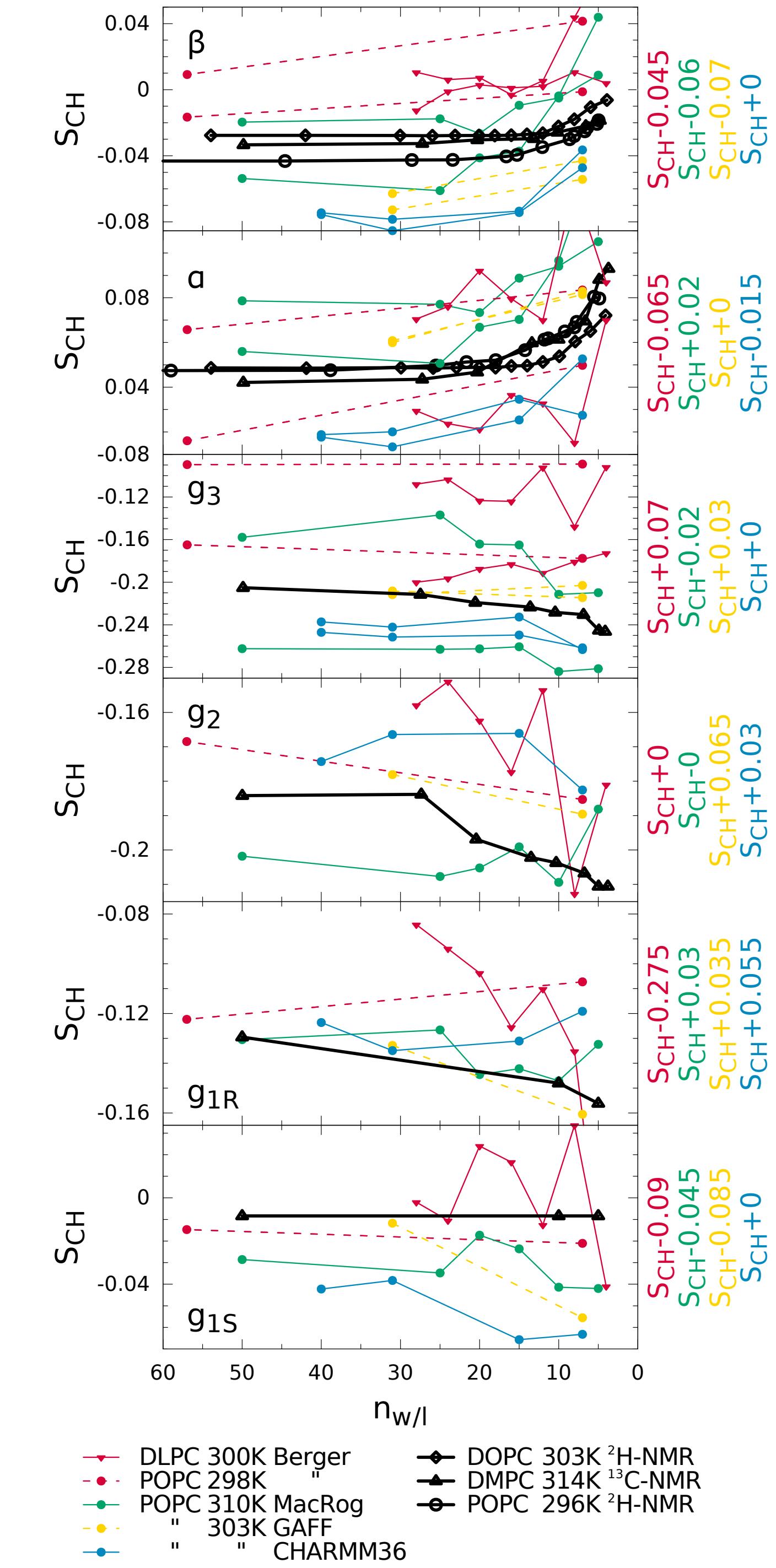
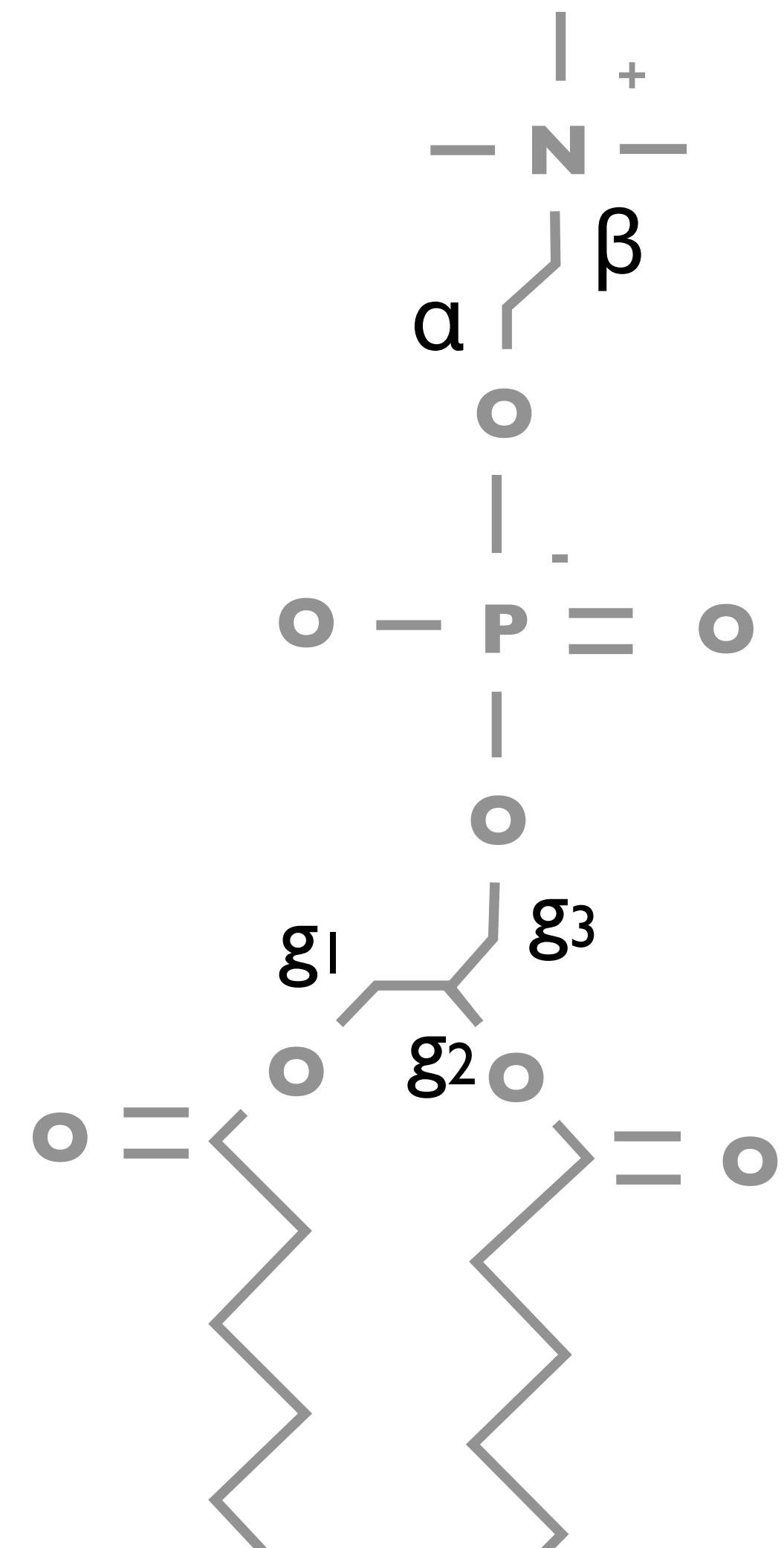
No current force field
reproduces the experimental
data within experimental error.



The current force fields are not
realistic structural models.



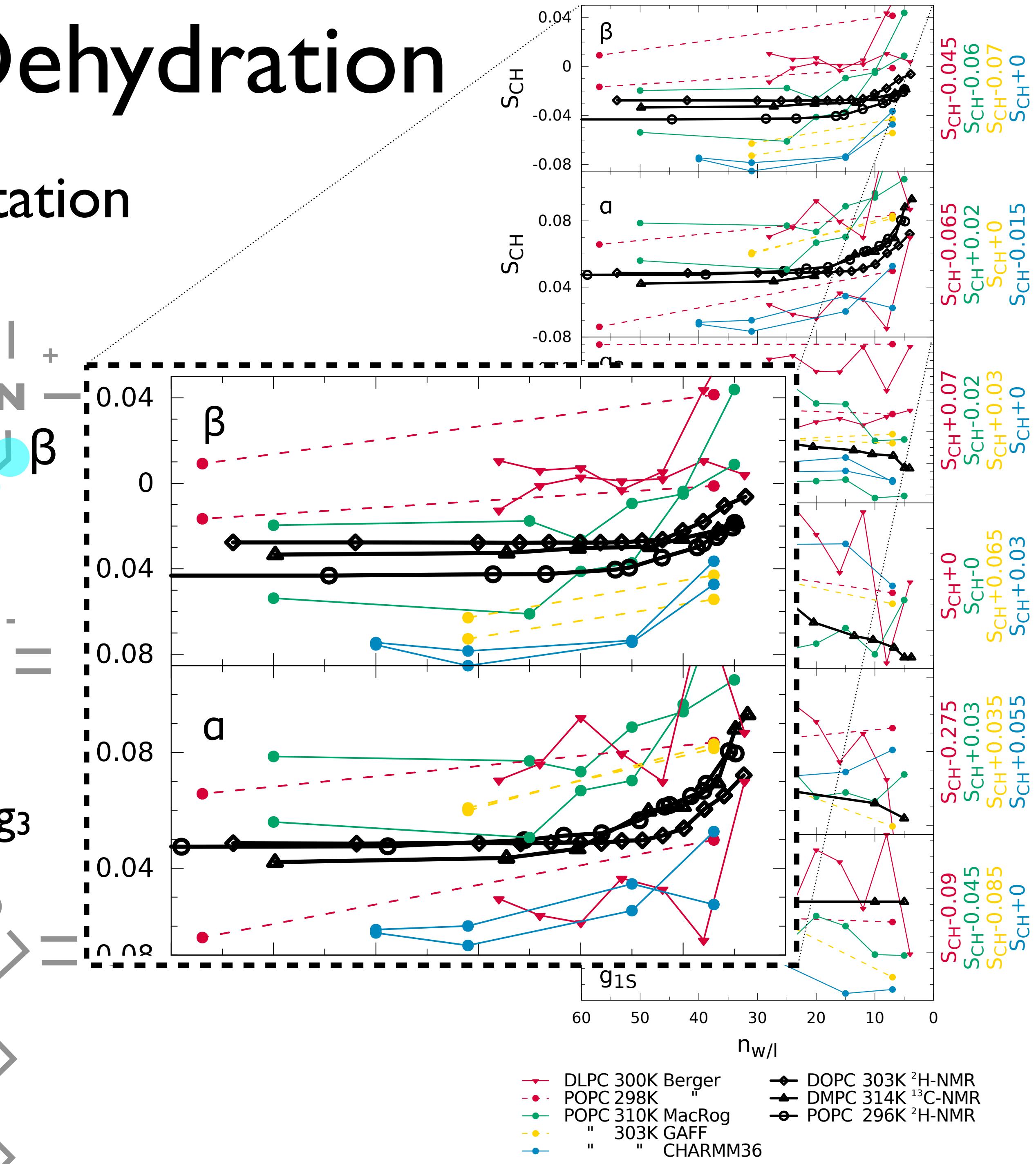
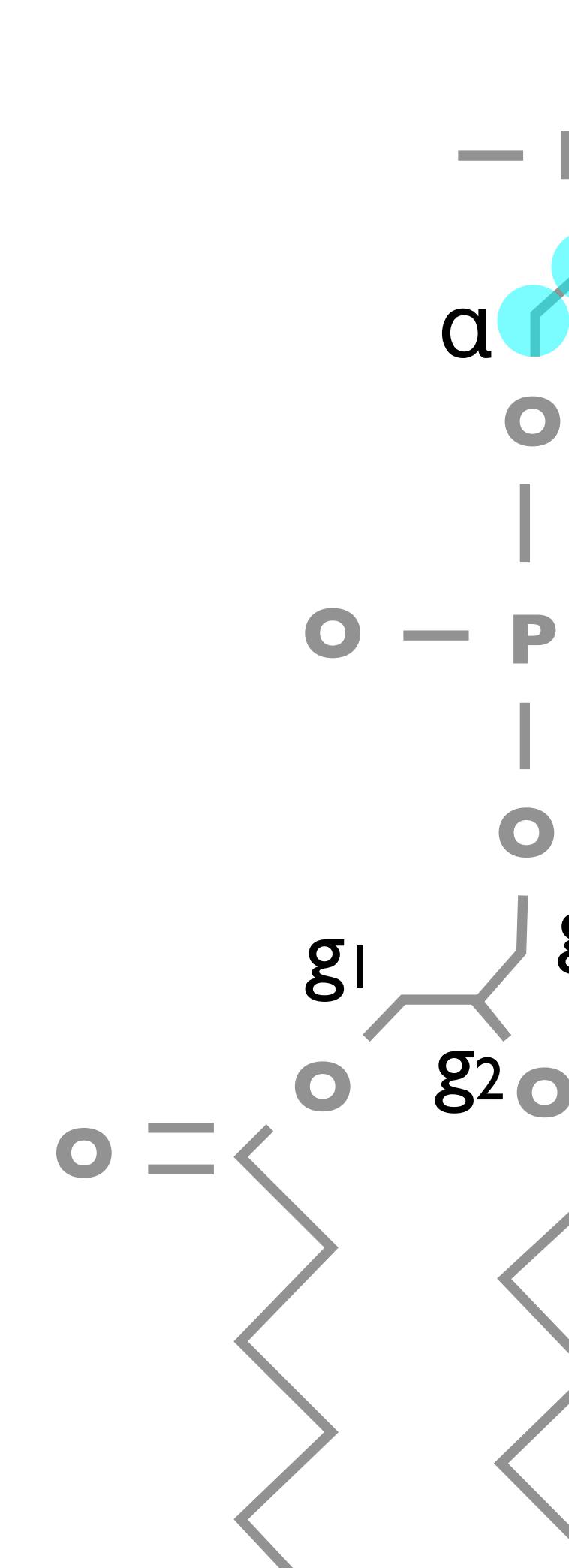
Responses: Dehydration



Responses: Dehydration

Headgroup reorientation

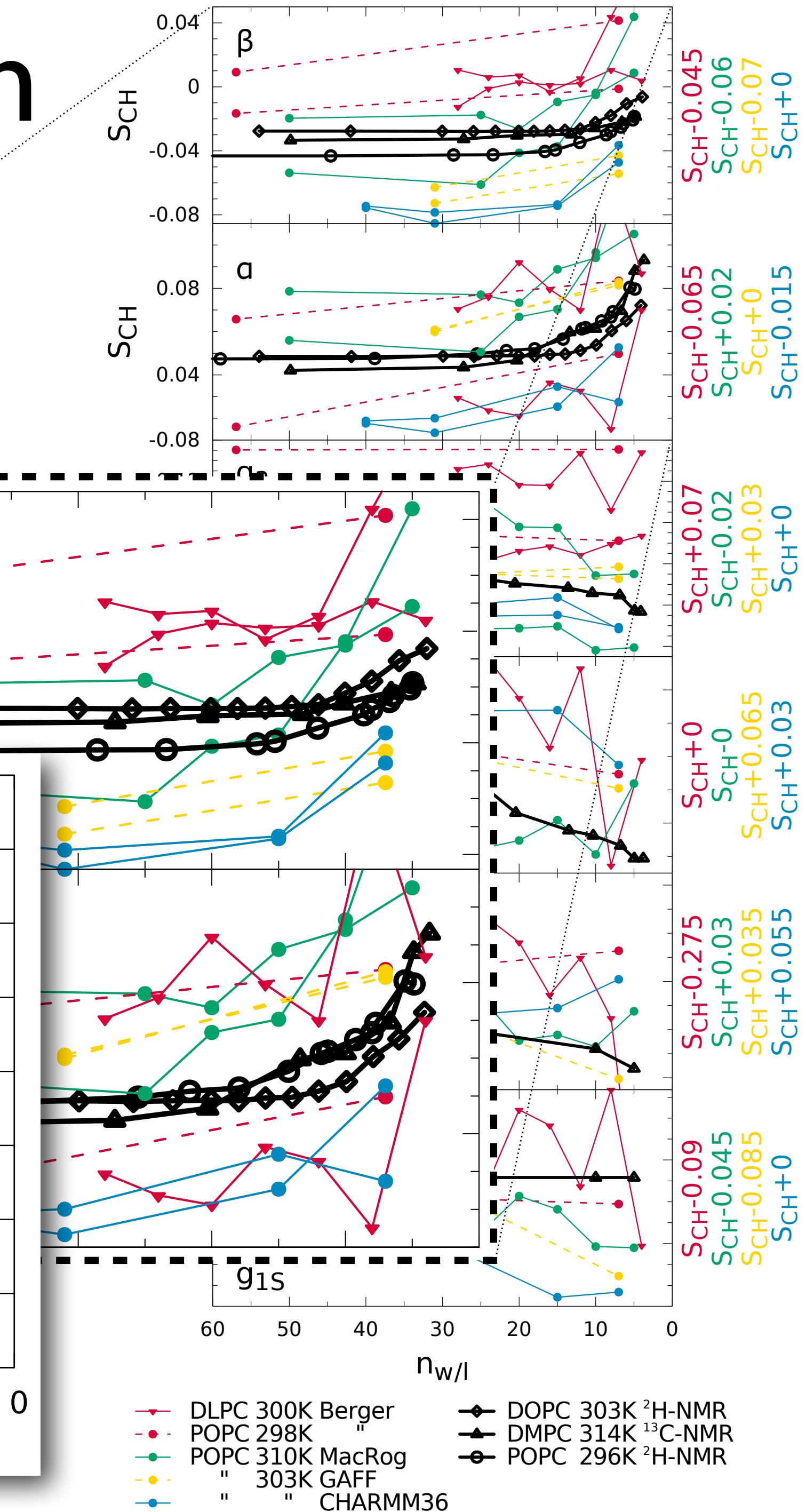
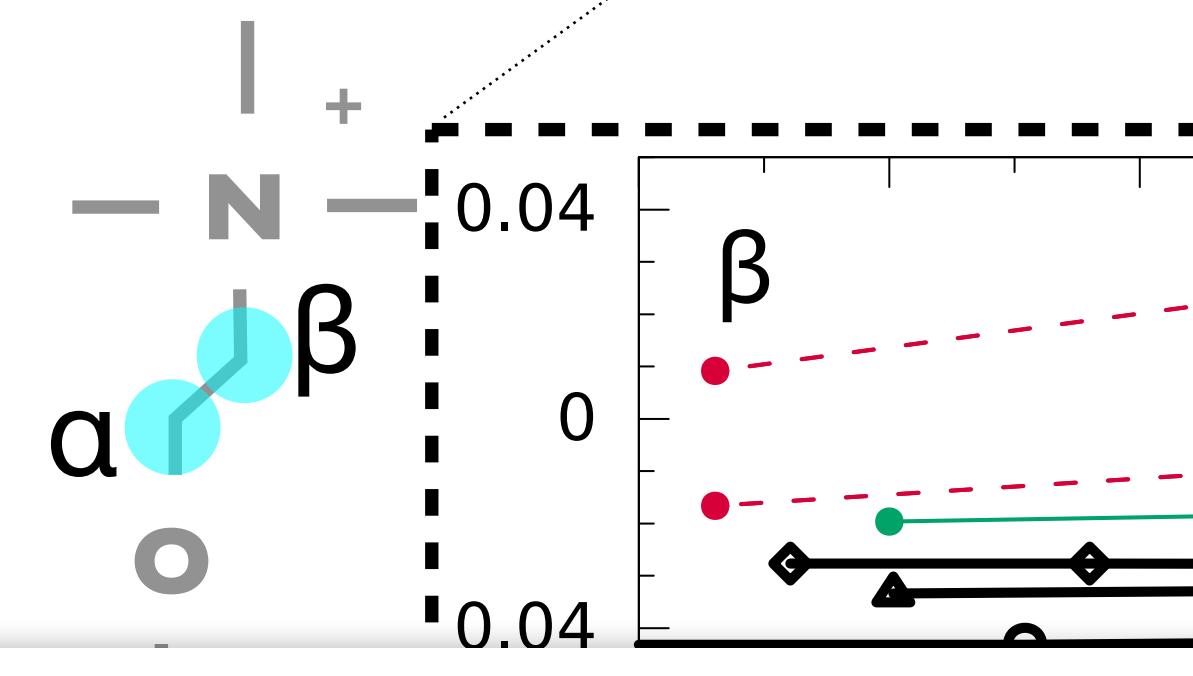
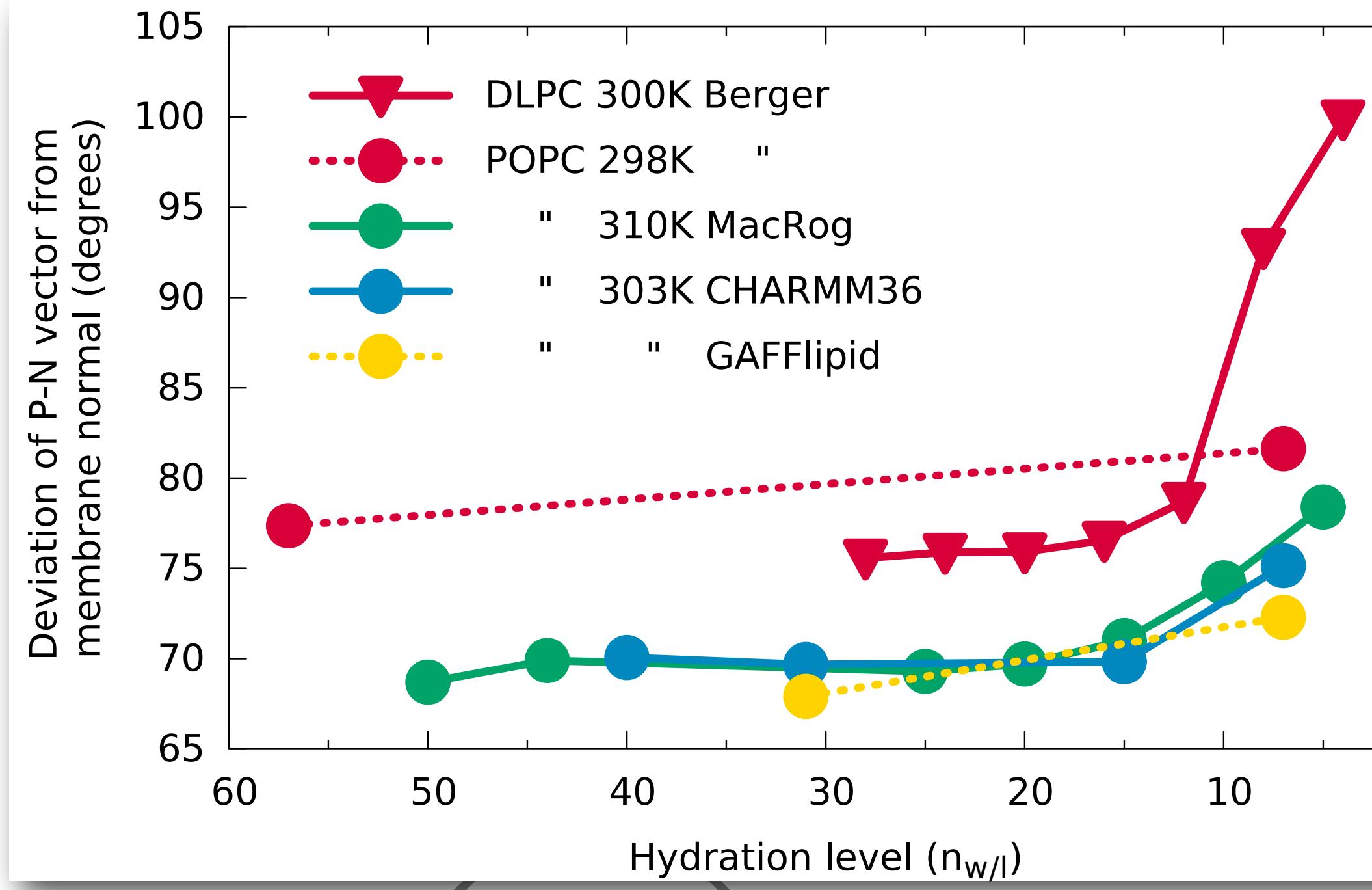
J. Phys. Chem. B 119 15075 (2015)



Responses: Dehydration

Headgroup reorientation
is captured qualitatively.

J. Phys. Chem. B 119 15075 (2015)



The screenshot shows the homepage of the NMRLipids project website, which is a blogspot site. The title "The NMRLipids project" is at the top, followed by a subtitle "Open Collaboration to understand lipid systems in atomistic resolution". A navigation bar includes links for Home, About, Workflow, Publications, GitHub, Authors, On Credits, To Do List, and Data contributions. Below the navigation is a date box showing "Wednesday, May 18, 2022". A section titled "Current status of the project" lists several posts:

- 18.5.2022 NMRLipids databank: Quality evaluation post was published.
- 9.5.2022 NMRLipids databank: Current status and structure post was published.
- 20.4.2022 New yaml format of mapping files post was published.
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To the right of the posts is a sidebar with a list of items:

- The form factor quality estimator is currently tak... - 23/05/2022 - Samuli Ollila
- Additional reminder that the (relative) form facto... - 20/05/2022 - Hanne
- Looks amazing! You and Anne have done very nice jo... - 20/05/2022 - Hanne
- If dipole convergence issue occurs right away, the... - 11/02/2022 - Atomic Force (Ren)
- Regarding the semi-isotropic pressure coupling, I ... - 11/02/2022 - Batuhan Kav

Below the sidebar is a link to "Chronological list of all posts".

The NMRlipids project

Open Collaboration to understand lipid systems in atomistic re

Home About Workflow Publications GitHub Authors Or

Wednesday, May 18, 2022

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- 50+ contributors
- 50+ long scientific posts
- 800+ comments
- 500 page views / month

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[Chronological list of all posts](#)

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• J.Am. Chem. Soc. **143 13701 (2021)**

• J. Phys. Chem. B **123 9066 (2019)**

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[Chronological list of all posts](#)

NMRLipids / NMRLipidsIVotherHGs

- 50+ contributors
- 50+ long scientific posts
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NMRLipids IV project

Manage topics

	383 commits	1 branch	0 releases	7 contributors	
Branch: master	New pull request	Create new file	Upload files	Find File	Clone or download
 ohsOllila	Updates in manuscript based on todo points	Latest commit 01531a2 14 hours			
 Data	Add error bars in figures 7 and 8 as requested in issues #45 and #46	16 hours			
 Figs	Add error bars in figures 7 and 8 as requested in Issues #45 and #46	16 hours			
 Manuscript	Updates in manuscript based on todo points	14 hours			
 scratch	Add GromacsVSamber comparison of POPS realated to the issue #21	4 months			
 scripts	Add results from Lipid17 simulation with monovalent ions by B. Kav ht...	9 months			

Help people interested in this repository understand your project by adding a README.

Add a README

- *J. Am. Chem. Soc.* **143** 13701 (2021)
- *J. Phys. Chem. B* **123** 9066 (2019)
- *Phys. Chem. Chem. Phys.* **18** 32560 (2016)
- *BBA Biomembr.* **1858** 2512 (2016)
- *J. Phys. Chem. B* **119** 15075 (2015)

NMRLipids databank available from [here](#).

NMRLipids databank and details available from [helsinki.fi](#)

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• 50+ contributors
scientific posts
per month

Nmrlipids

Found 160 results.

Sort by: Most recent asc.

December 19, 2017 (v3) Dataset Open Access

Simulations of POPC lipid bilayer in water solution at various NaCl, KCl and CaCl₂ concentrations using ECC-POPC force field

Melcr, Josef; Olliola, O. H. Samuli;

Classical molecular dynamics simulations of a POPC lipid bilayer in water solution at various NaCl, KCl and CaCl₂ concentrations using ECC-POPC force field parameters, SPC/E water model and ECC-ions. file names report molar fraction of cations (i.e. not bulk concentrations) simulations performed w

Uploaded on June 19, 2018

2 more version(s) exist for this record

June 13, 2018 (v1) Dataset Open Access

CHARMM36 simulations of POPC mixed with cationic surfactant

Olliola, O. H. Samuli;

CHARMM36 simulations of POPC mixed with cationic surfactants. The simulations are ran for NMRLipids IV project at 313 K using Gromacs 5. run10* for 10 mol% of surfactant run20* for 20 mol% of surfactant run30* for 30 mol% of surfactant run50* for 50 mol% of surfactant itp files called in top fi

Uploaded on June 13, 2018

March 14, 2018 (v1) Dataset Open Access

Simulation data for ECC-CHARMM36 POPC bilayer, 100 lipids/leaflet, 940 mM NaCl, 310K, GROMACS 5.1.4

Nencini, Ricky;

The image shows a web browser window with three tabs open:

- GitHub Tab:** Shows the repository "Nmrlipids / NMRLipids IV project". It has 383 commits, the branch is "master", and there are updates from "ohsOllila". The sidebar lists "Data", "Figs", "Manuscript", "scratch", and "scripts". A section titled "Help people interested" lists publications:
 - *J. Am.*
 - *J. Phys.*
 - *Phys.*
 - *BBA L*
 - *J. Phys.*
- Zenodo Tab:** Shows the dataset "Nmrlipids" with 50+ contributors. The dataset is described as "50+ contributors scientific posts events ws / month".

Nmrlipids

NMRLipids Databank has become a large open-access repository of biomolecular MD trajectories.

This allows data upcycling for completely novel analyses.

Keywords

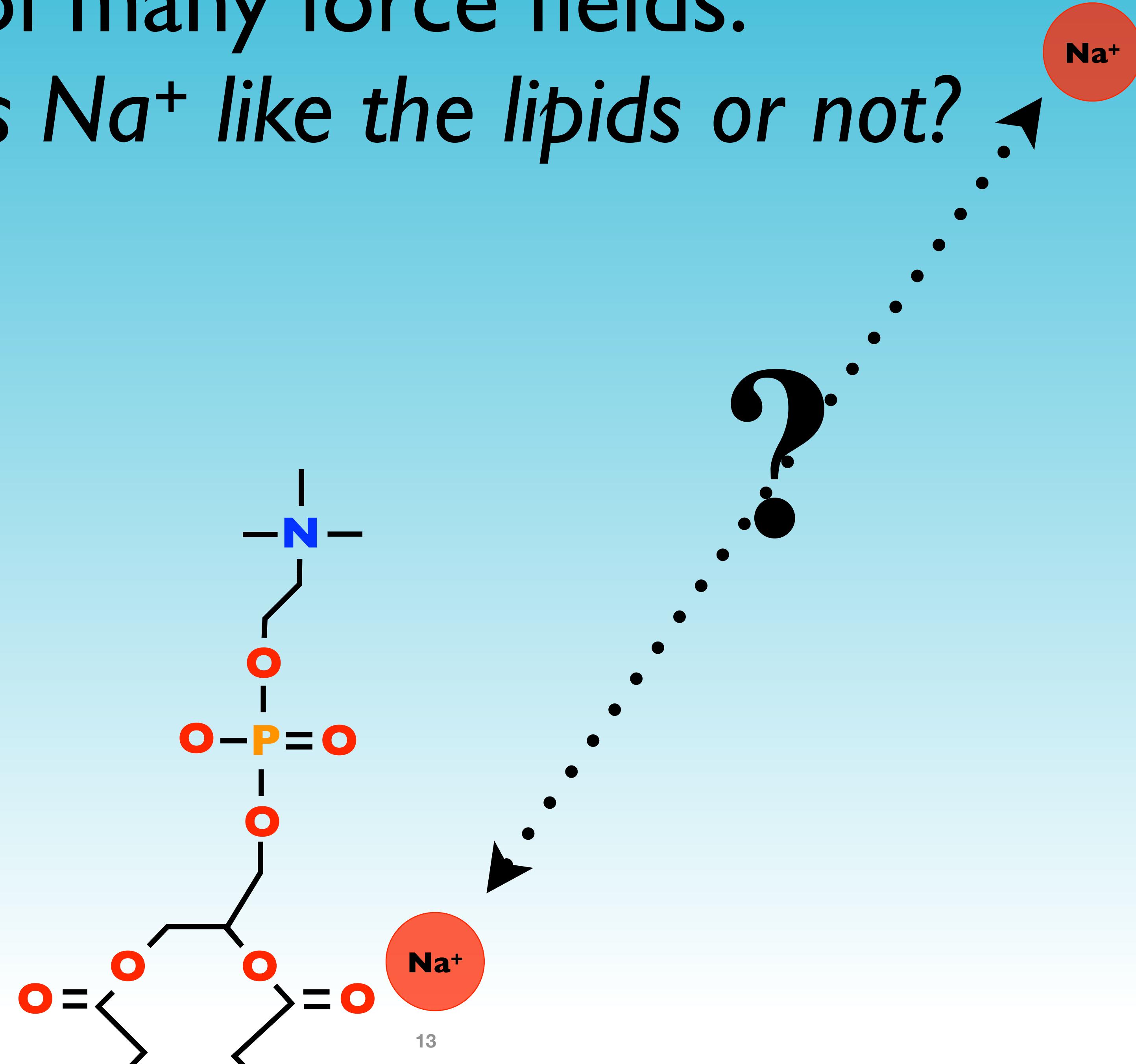
March 14, 2018 (v1) Dataset Open Access

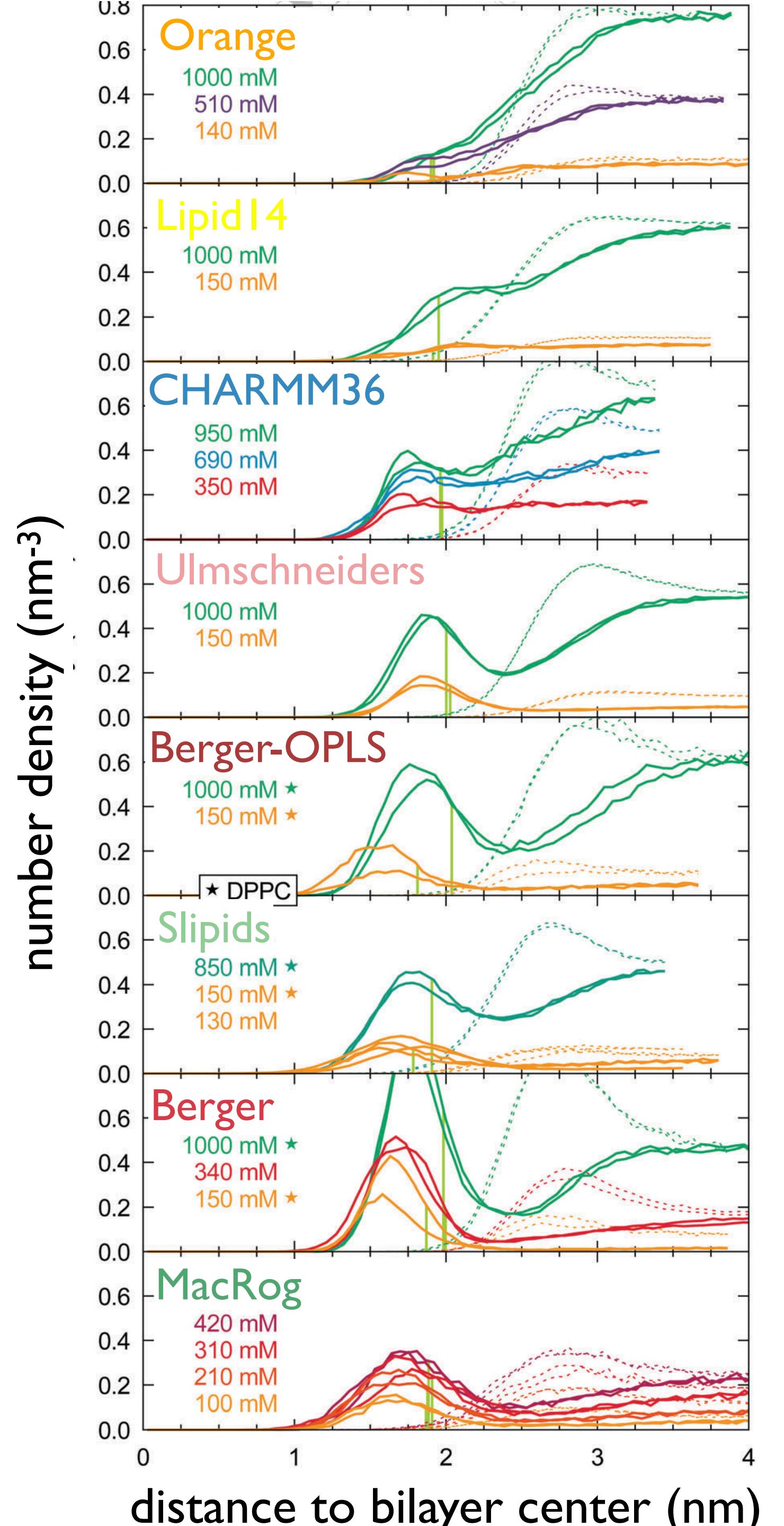
Simulation data for ECC-CHARMM36 POPC bilayer, 100 lipids/leaflet, 940 mM NaCl, 310K, GROMACS 5.1.4

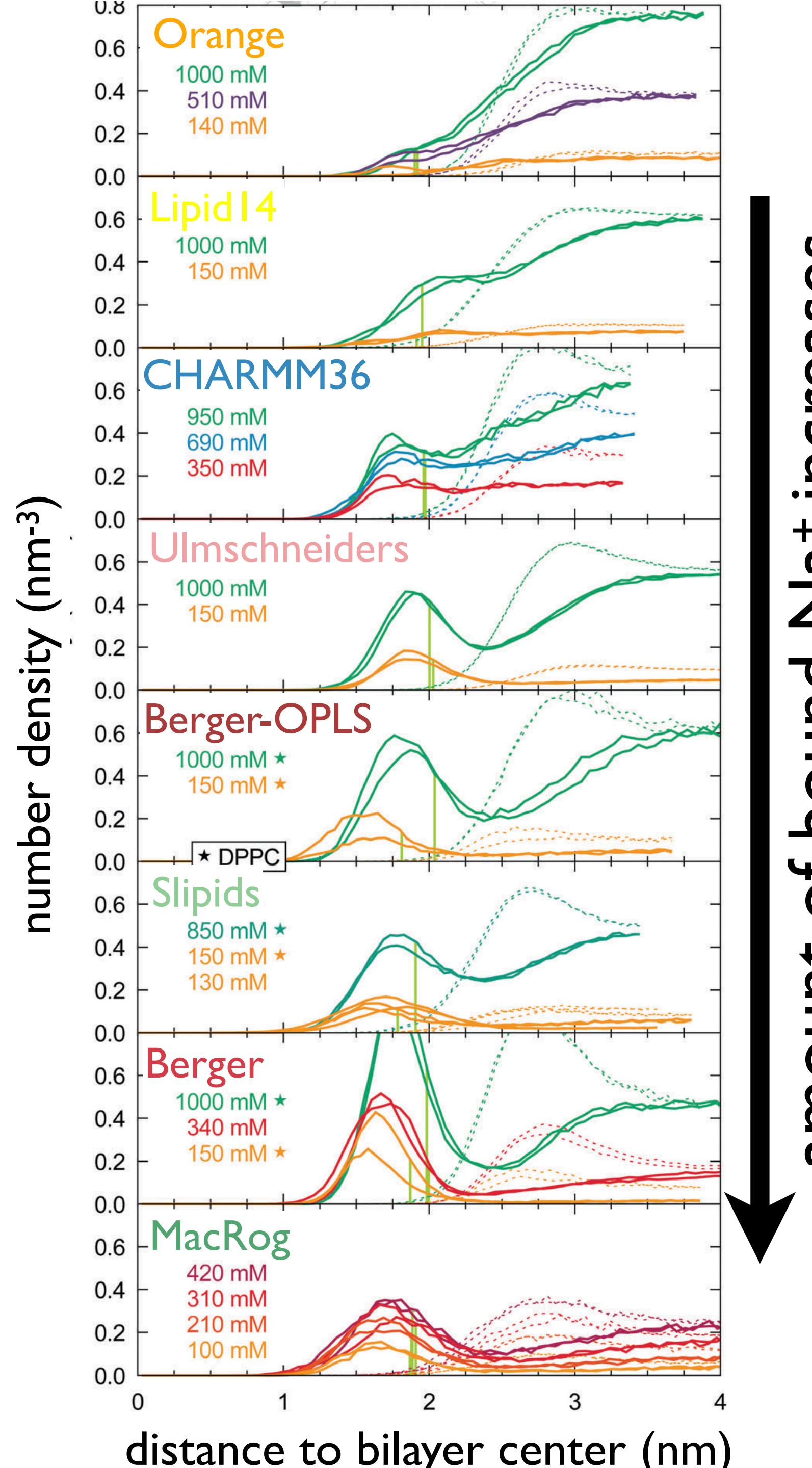
Nencini, Ricky;
- Blog Tab:** Shows a blog post with the URL "nmrlipids.blogspot.fi". The post discusses the use of atomic force microscopy (AFM) for estimating lipid density and molar mass, mentioning contributions from Samuli Ollila, Hanne, and Anne. It also mentions isotropic Kav and master in kExercises.

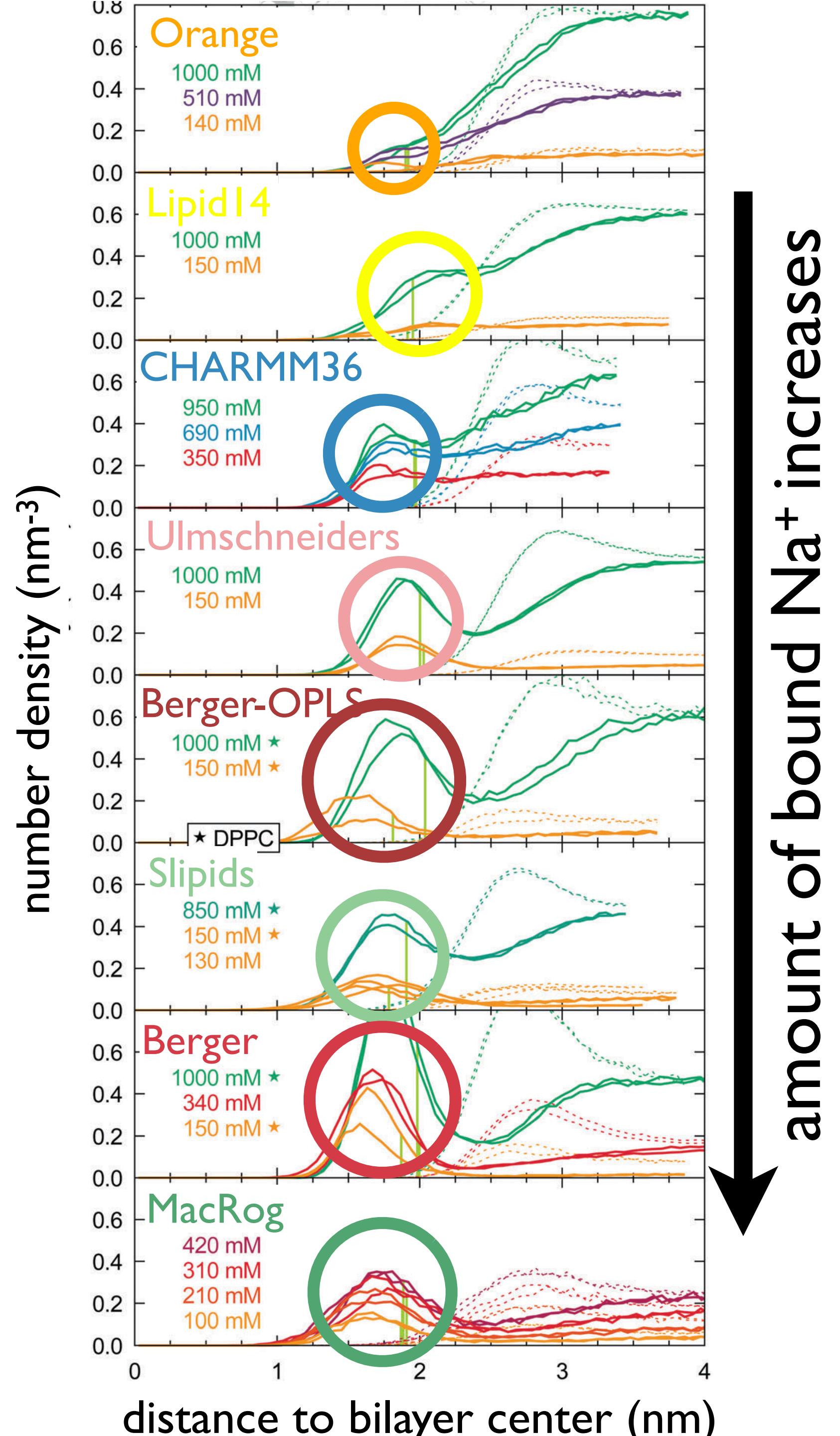
Power of many force fields:

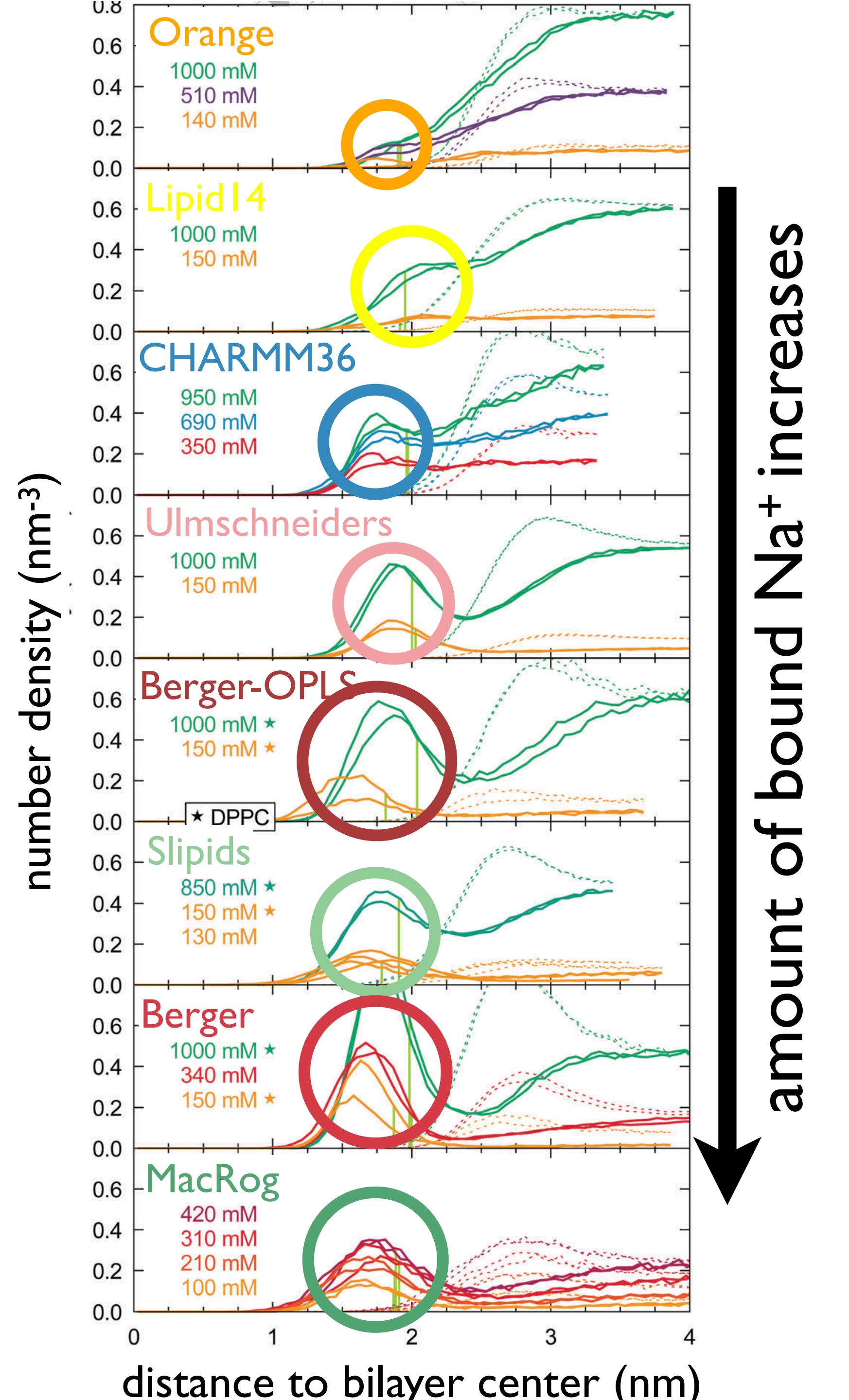
Does Na^+ like the *lipids* or not?



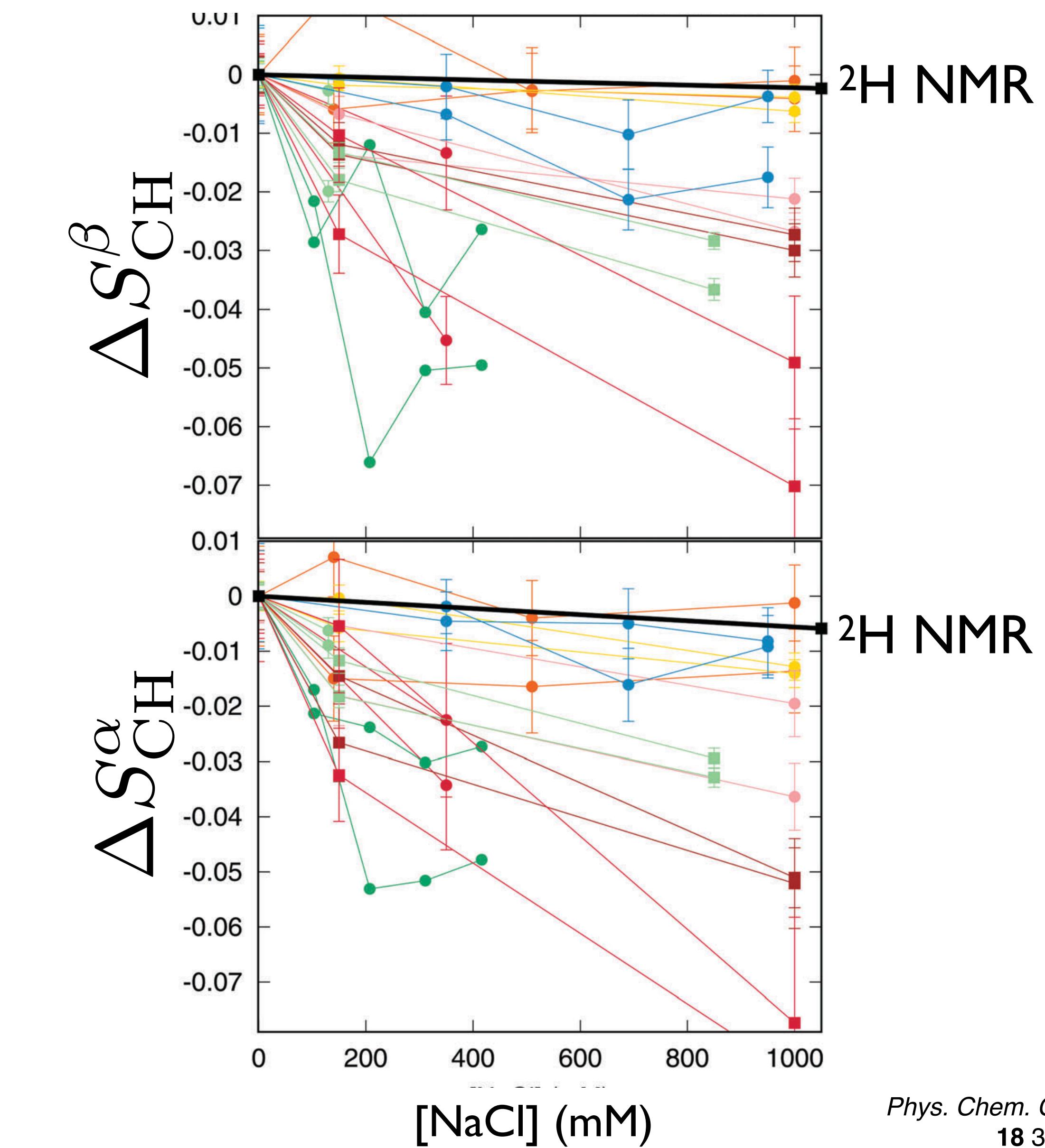


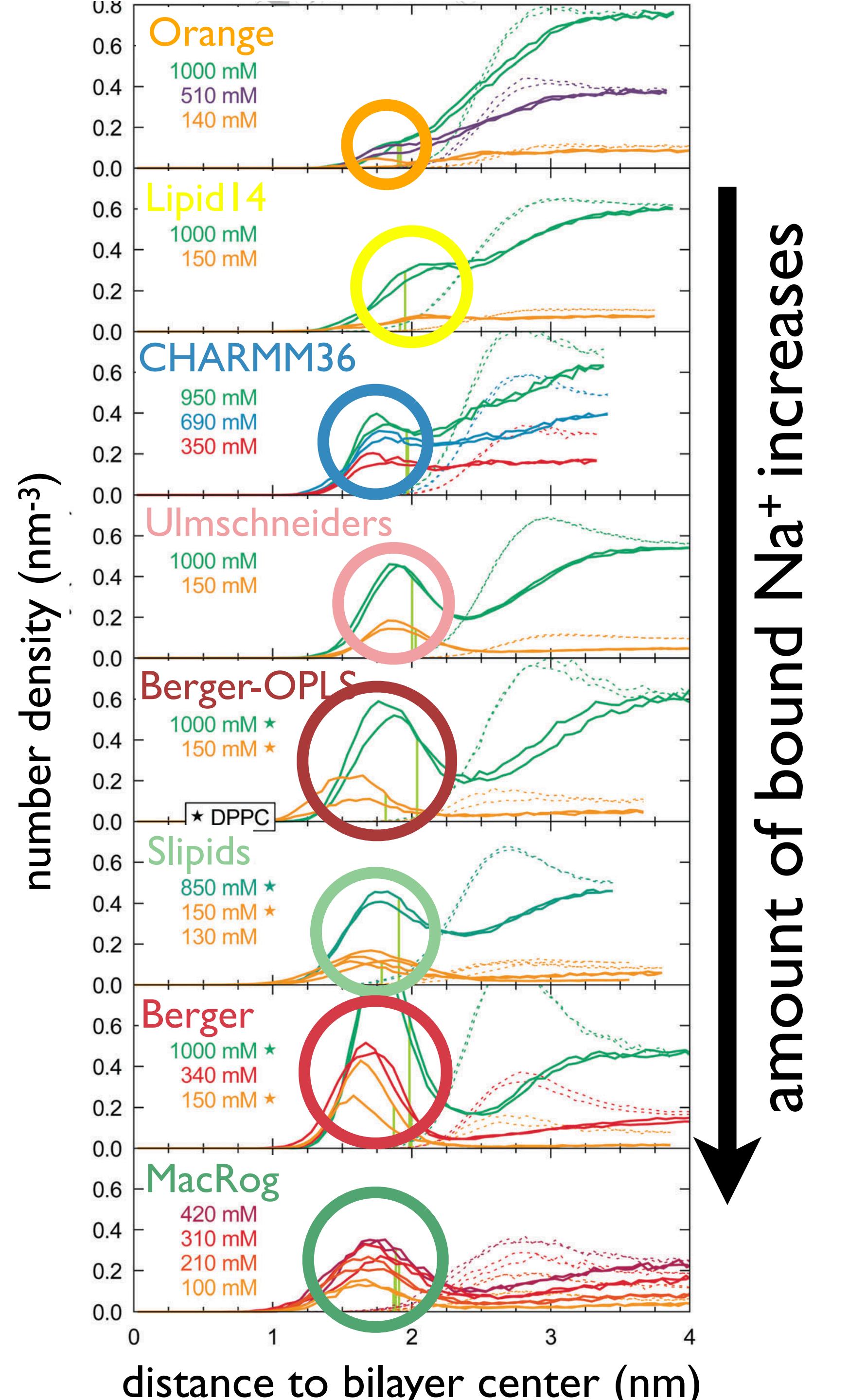




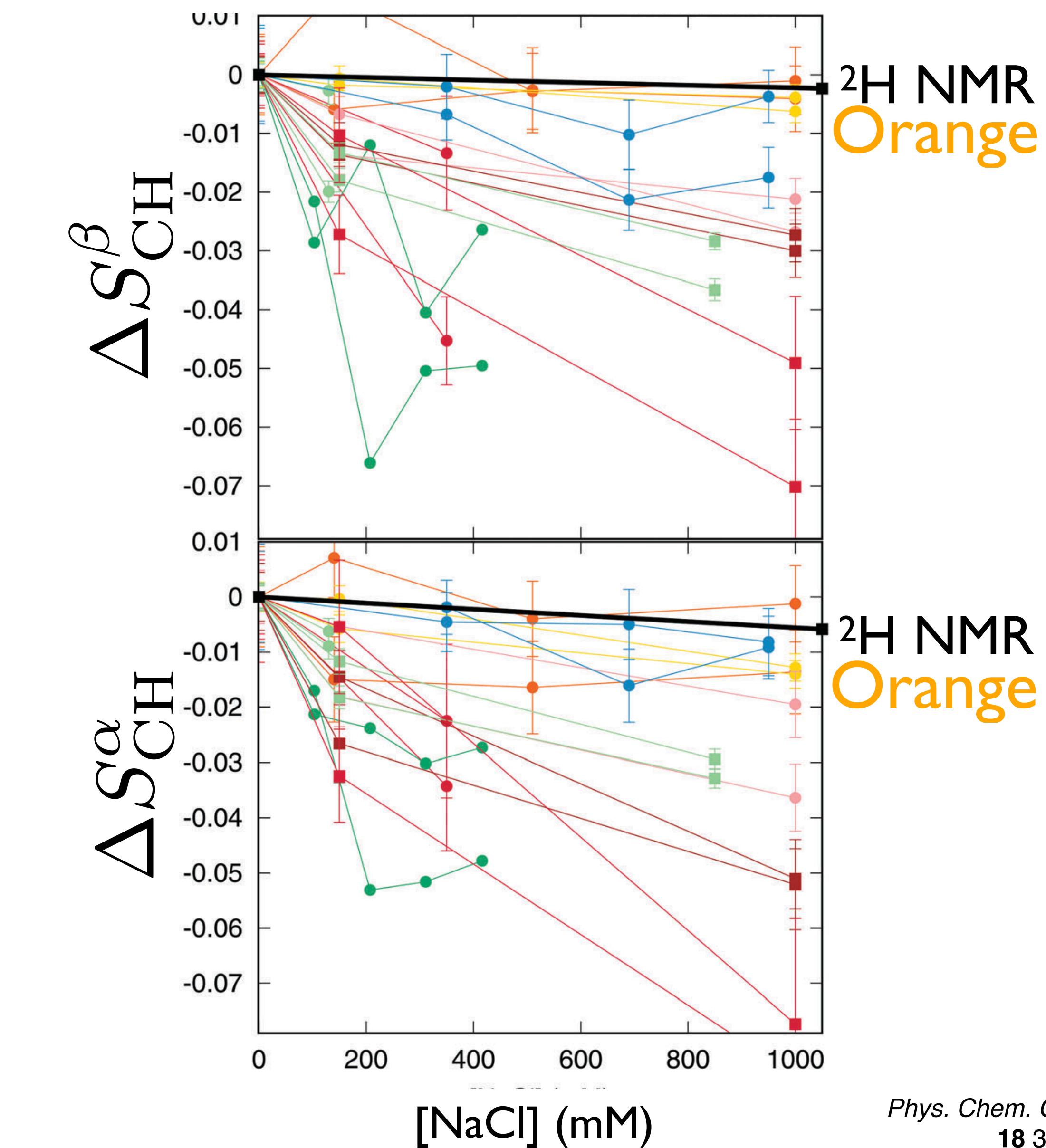


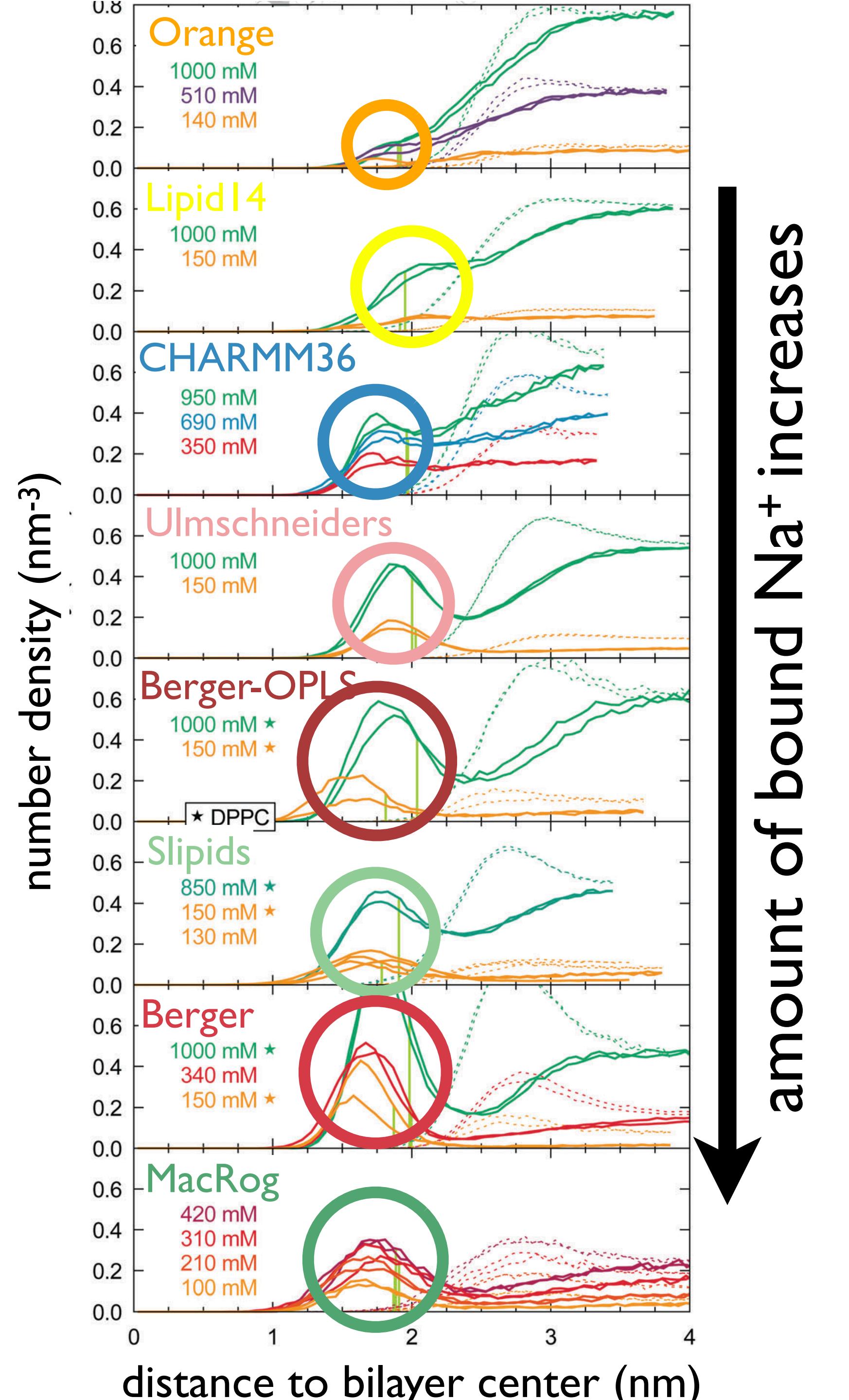
NaCl-induced change in the headgroup (β, α) order parameters



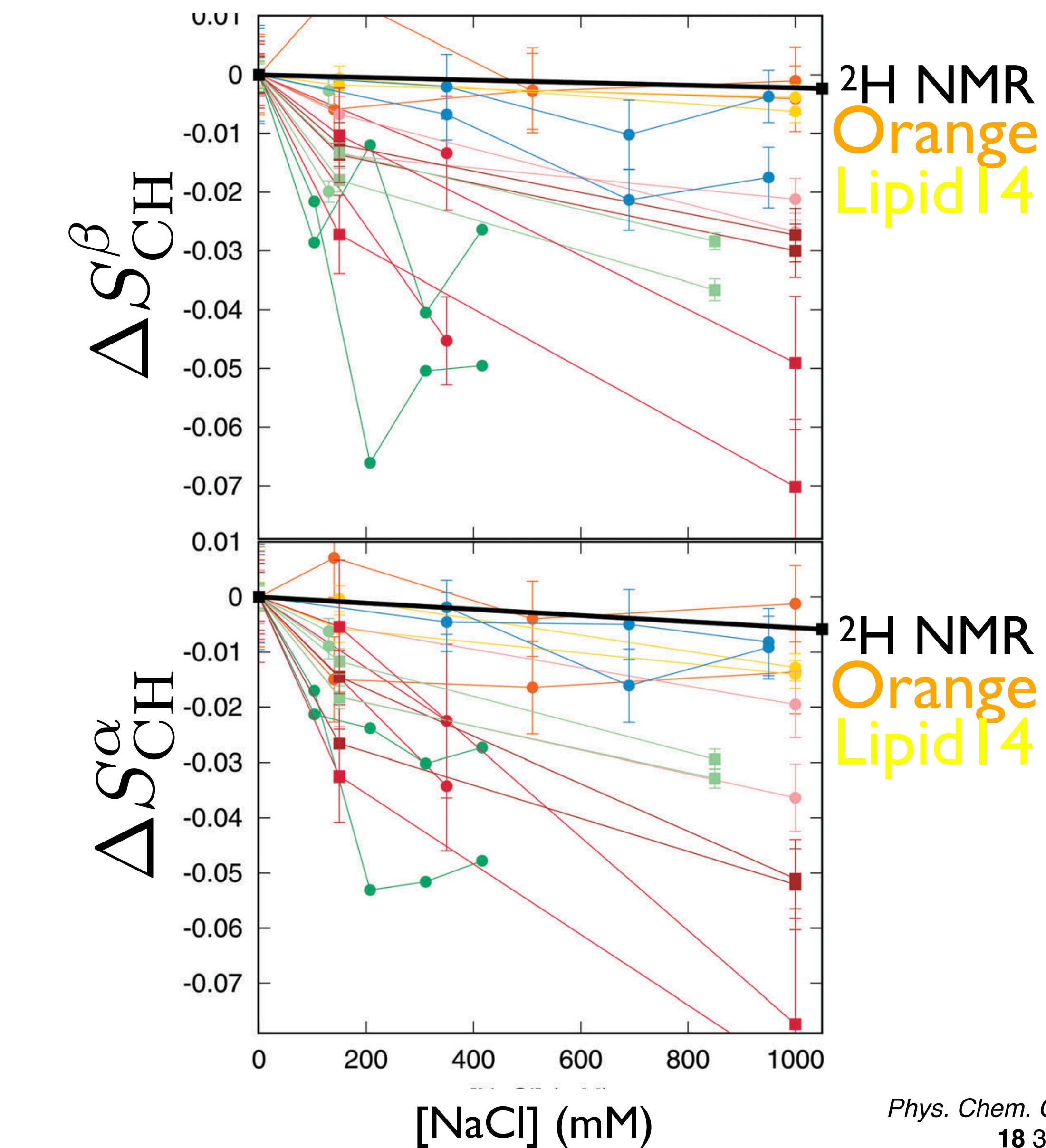


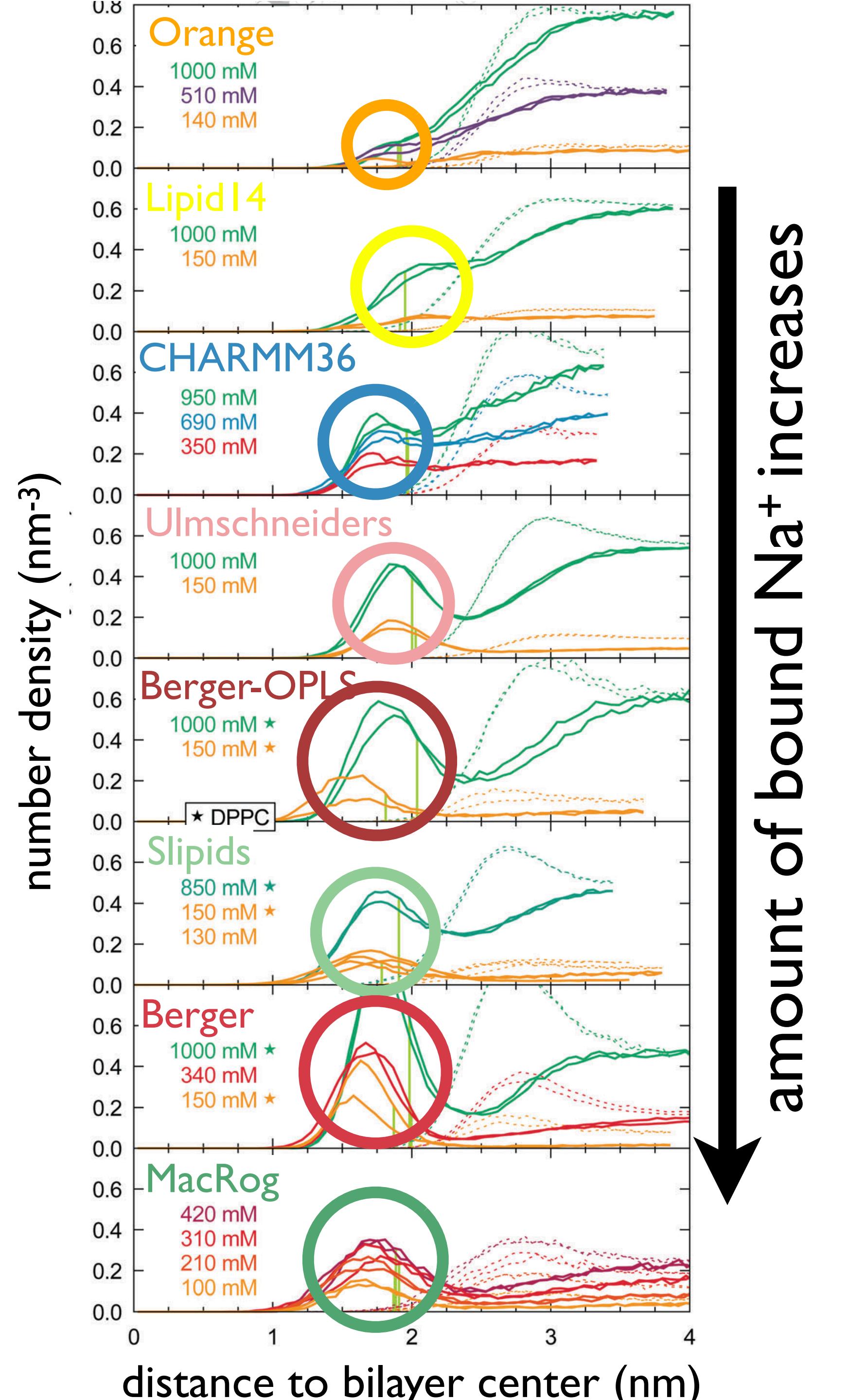
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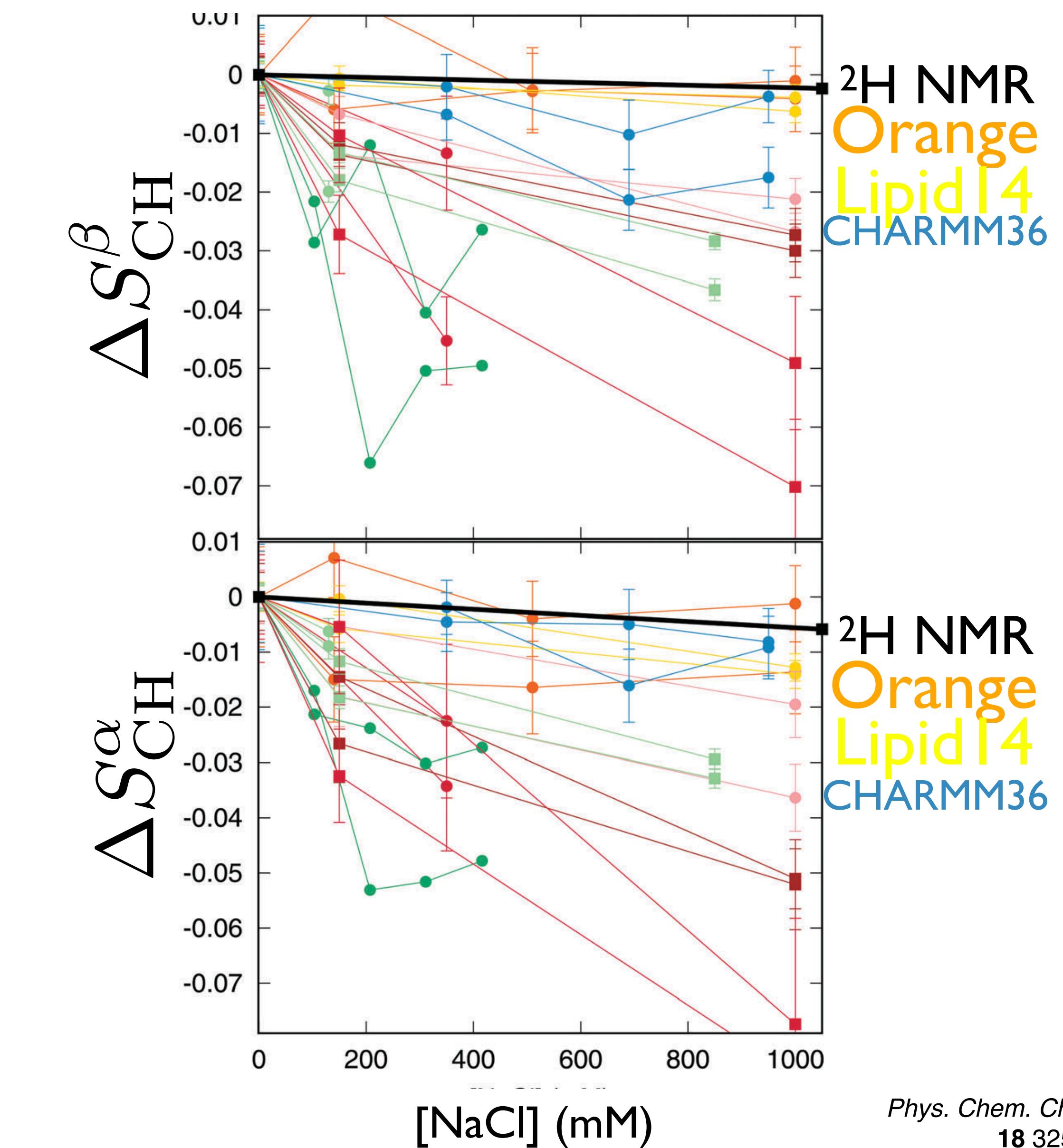


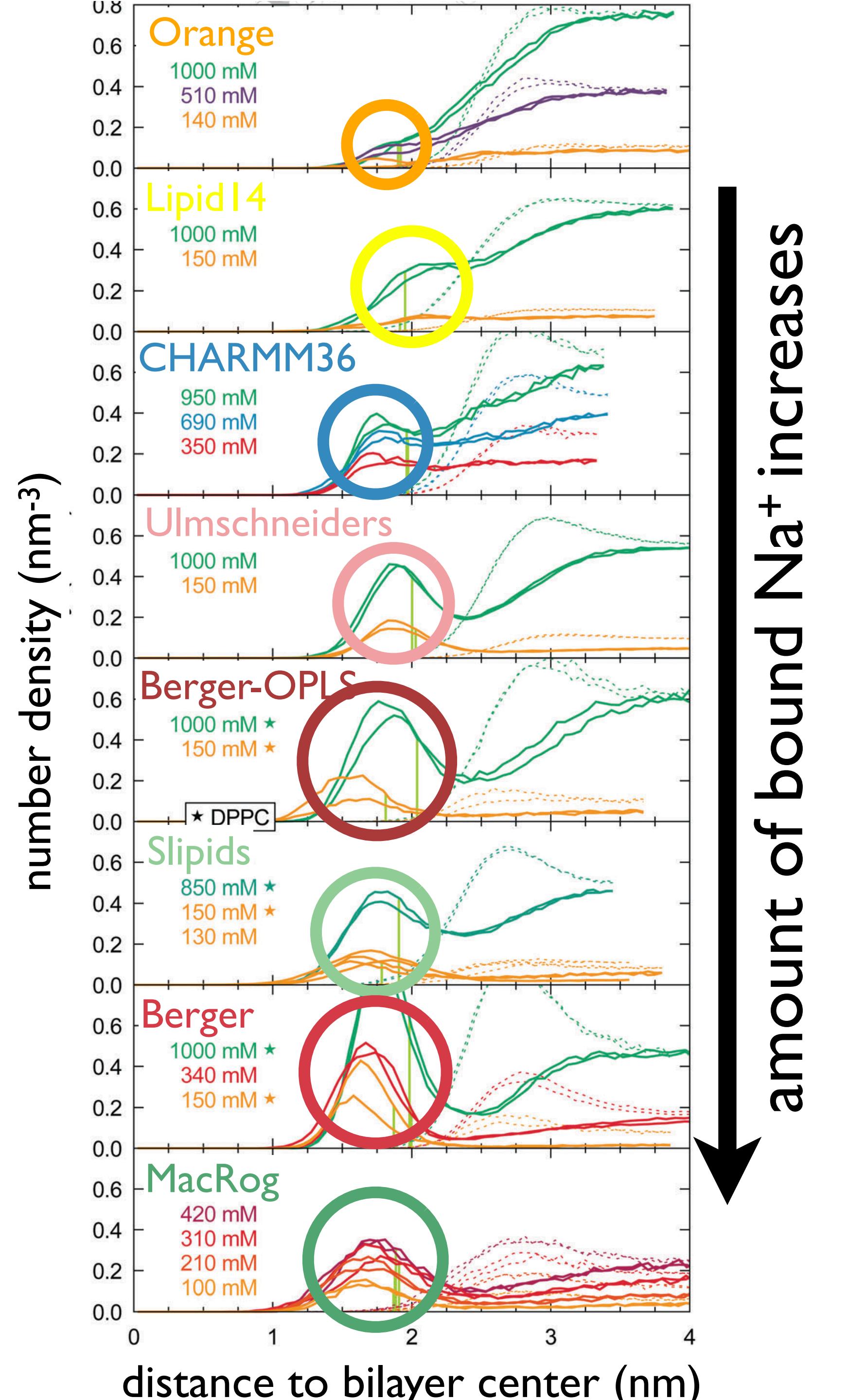
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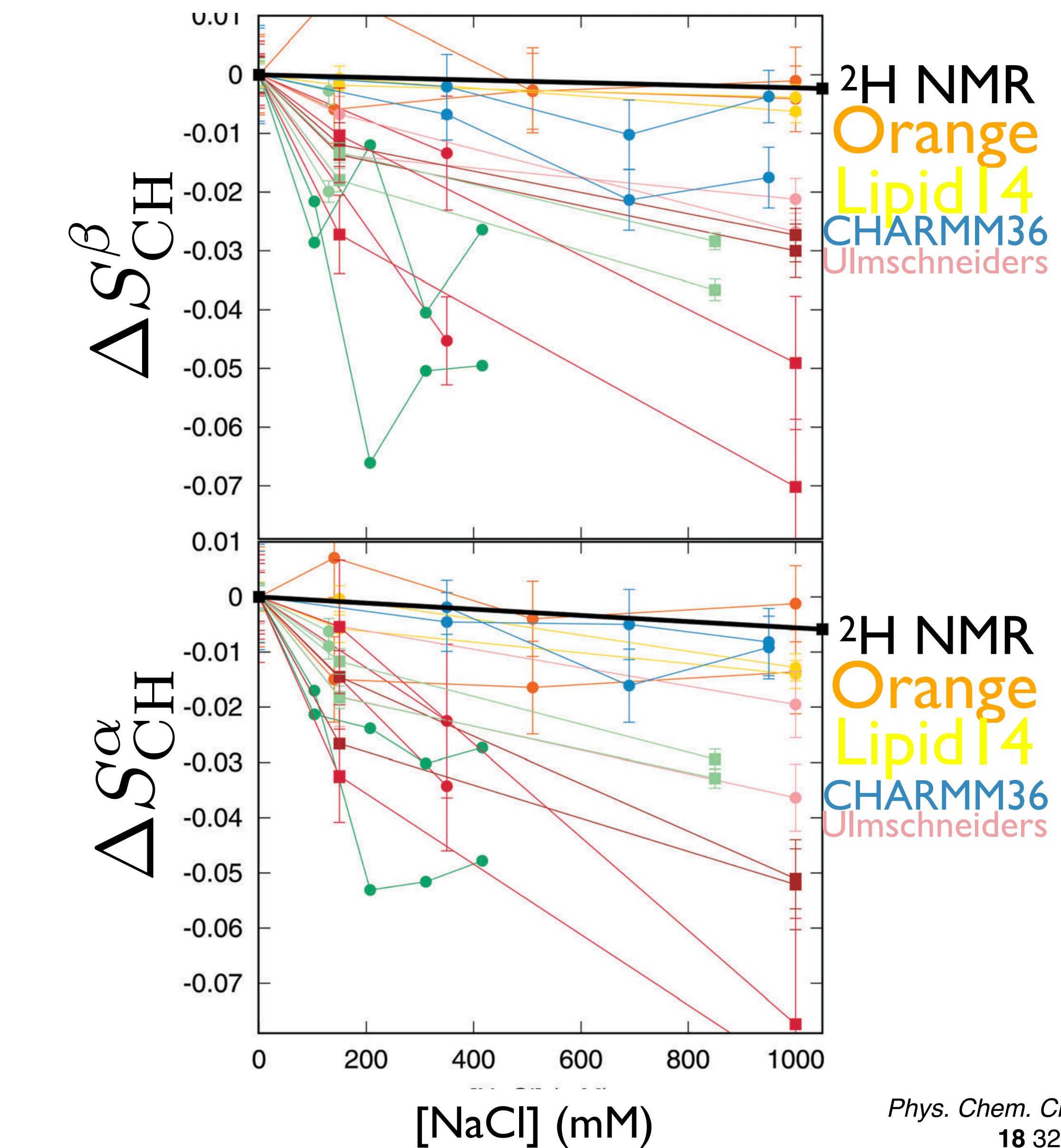


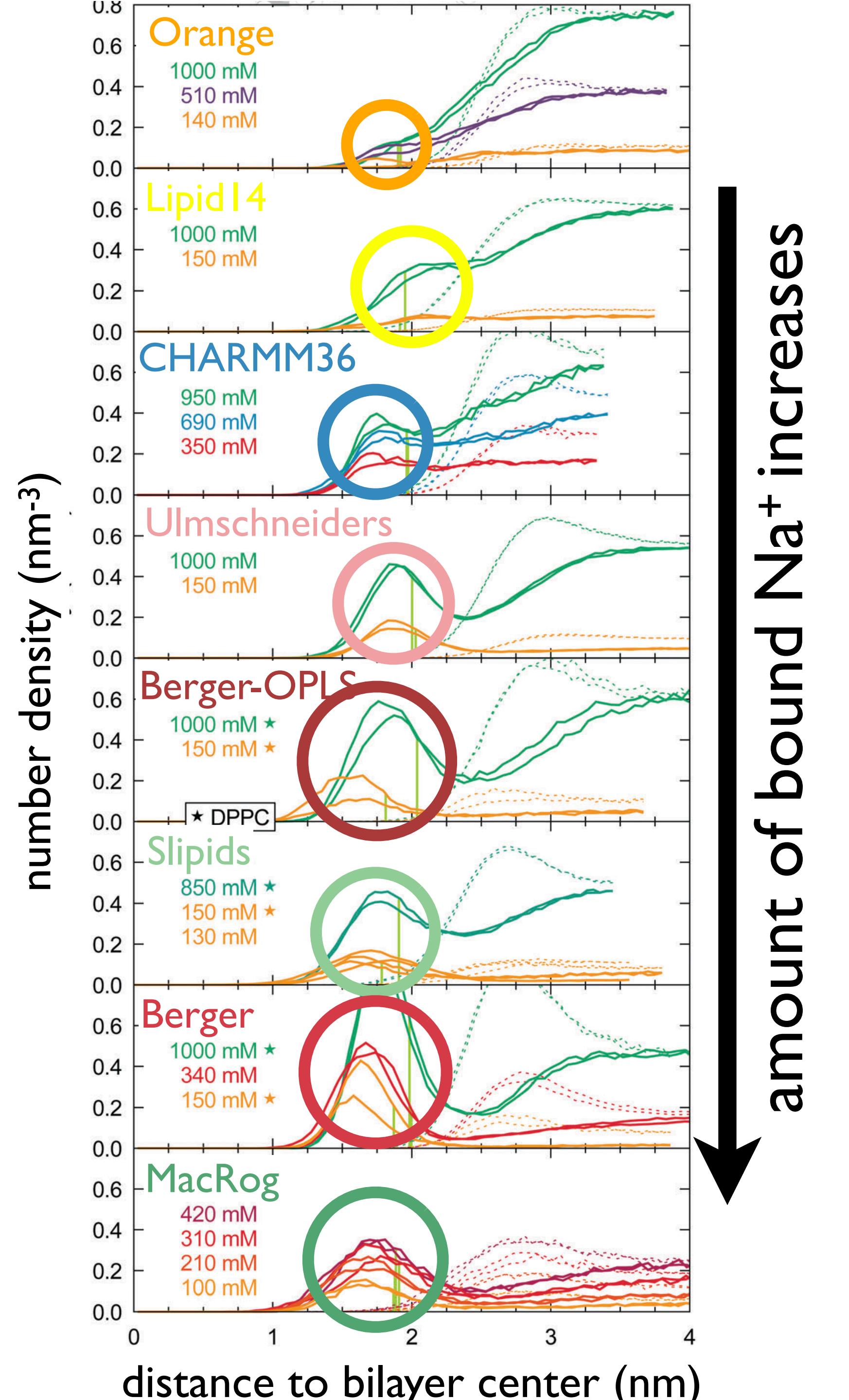
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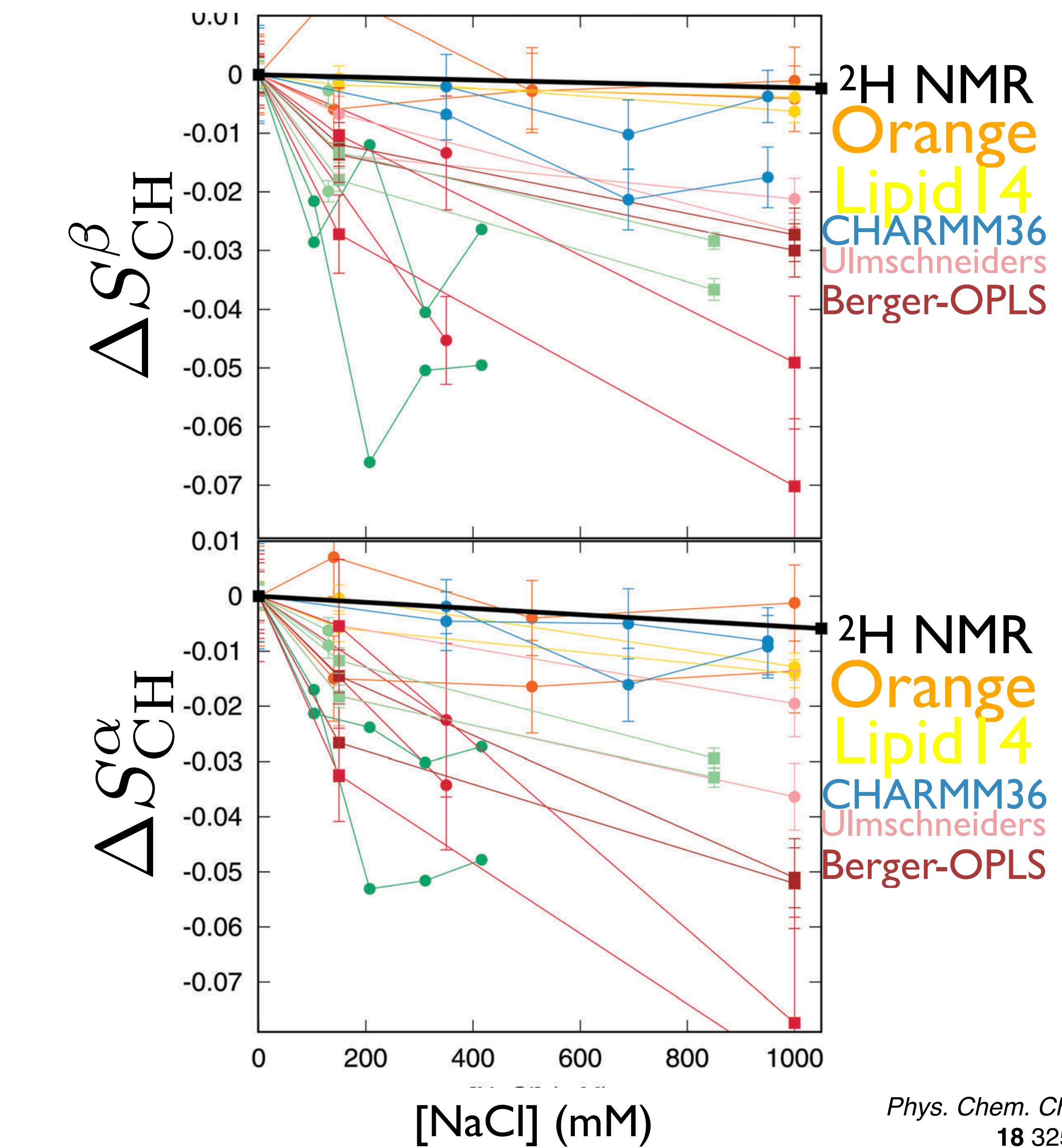


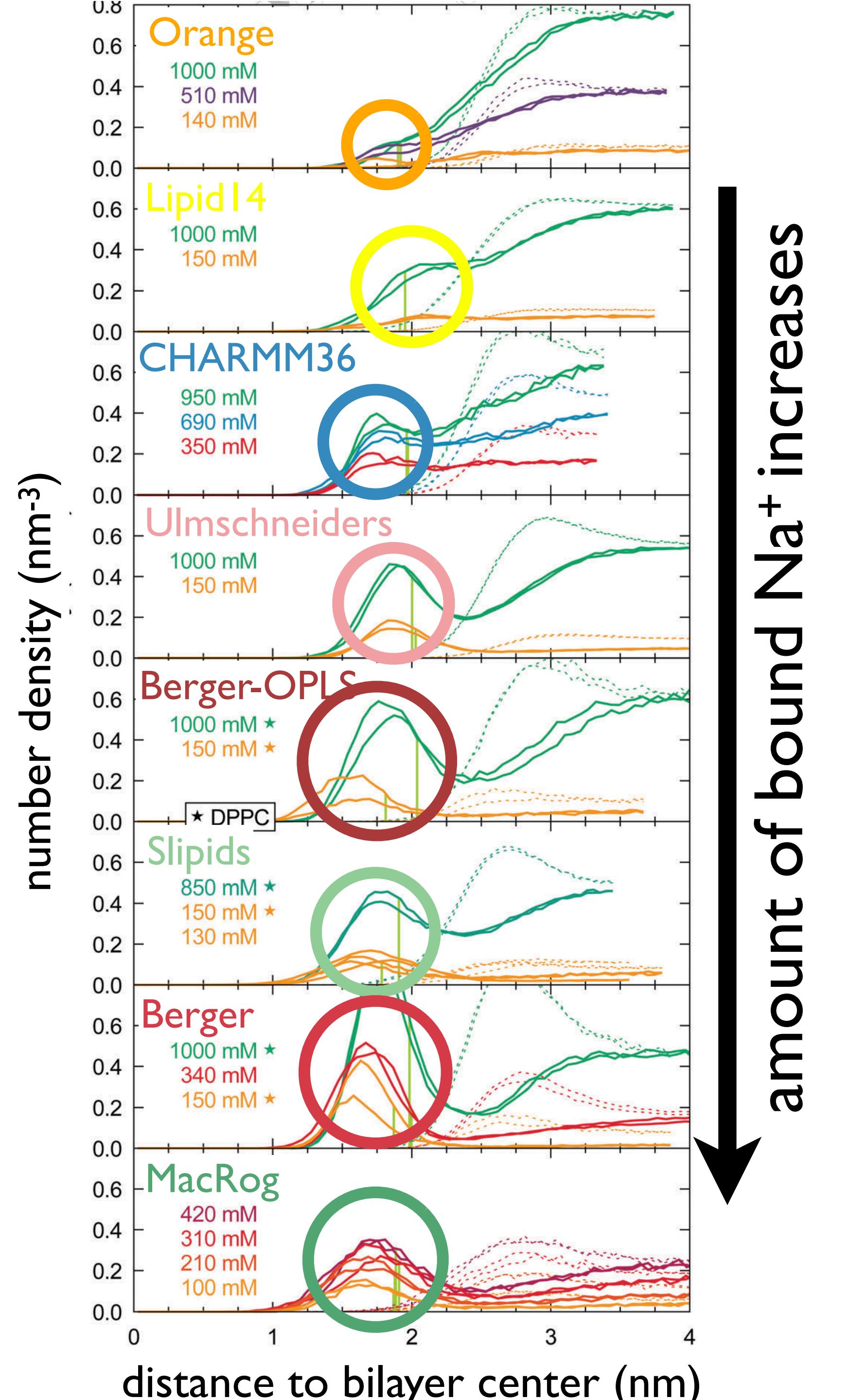
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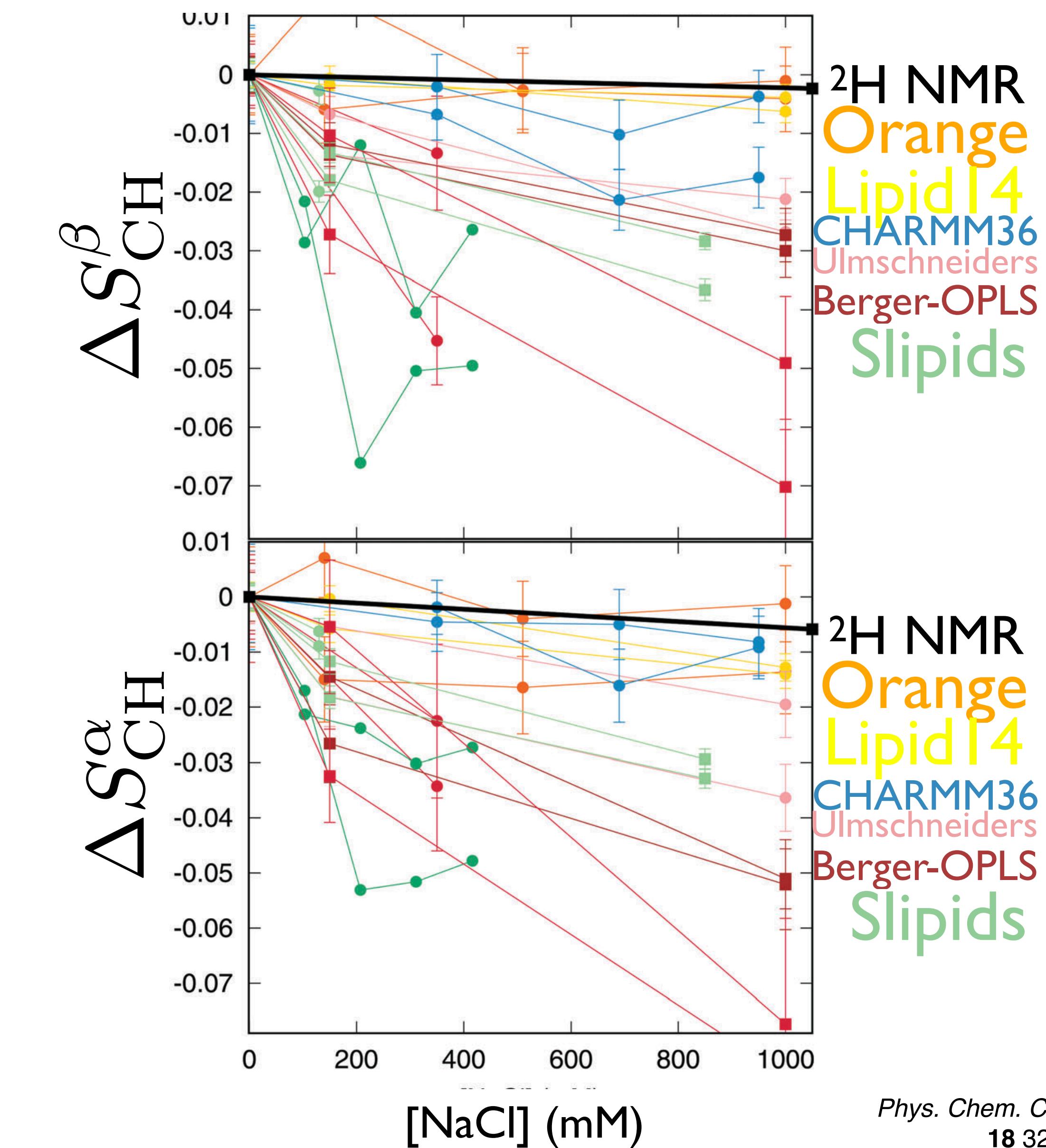


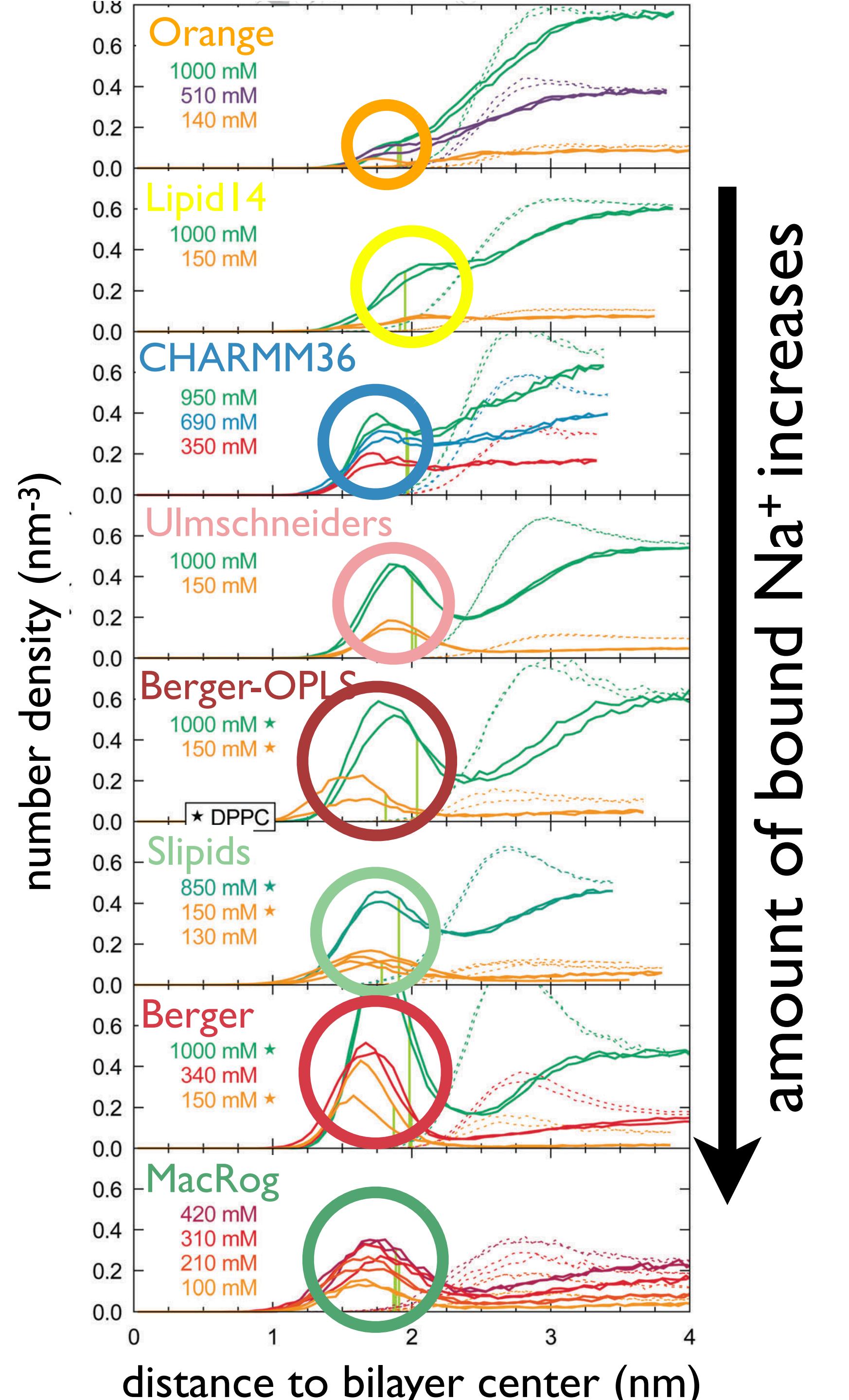
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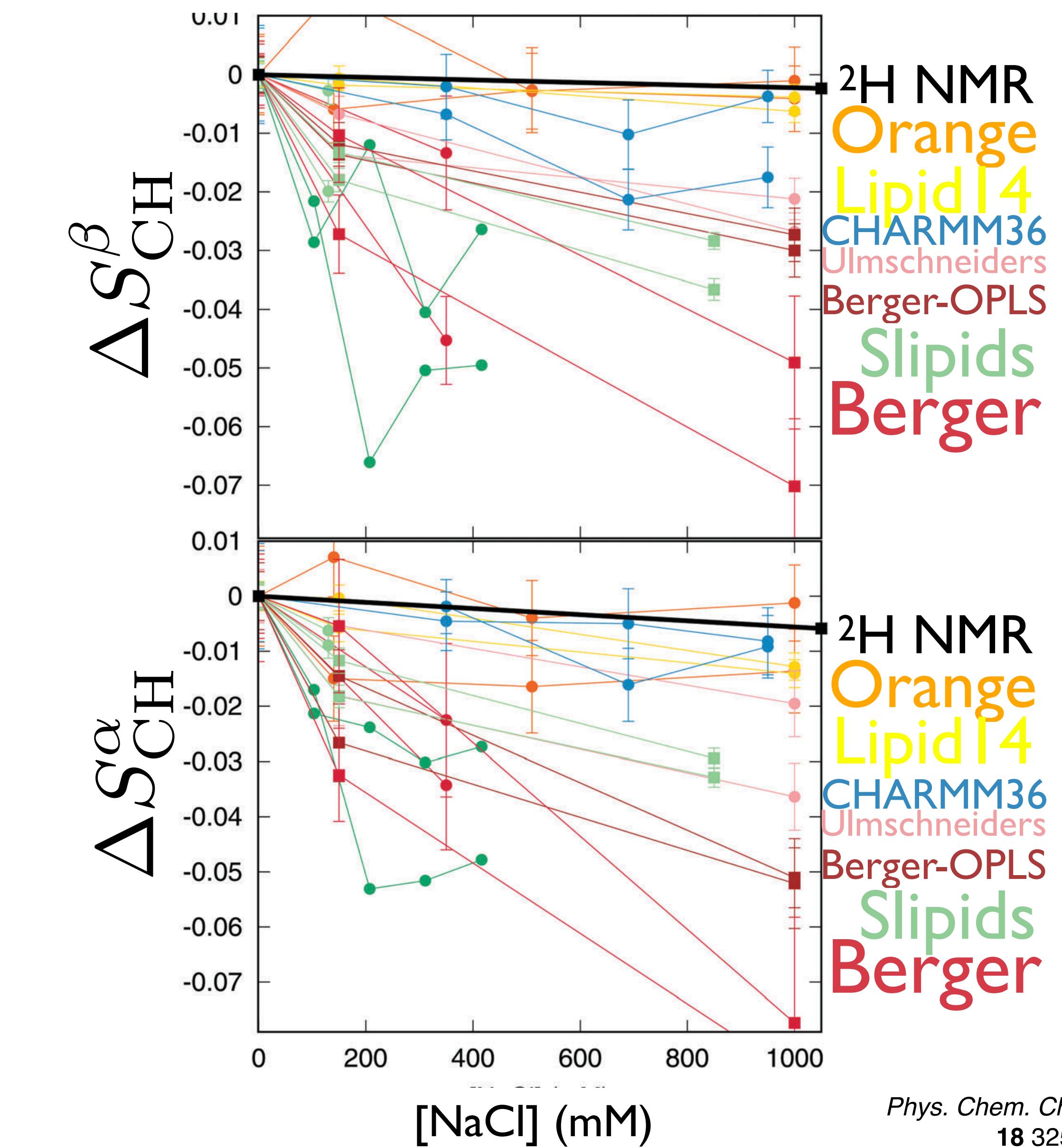


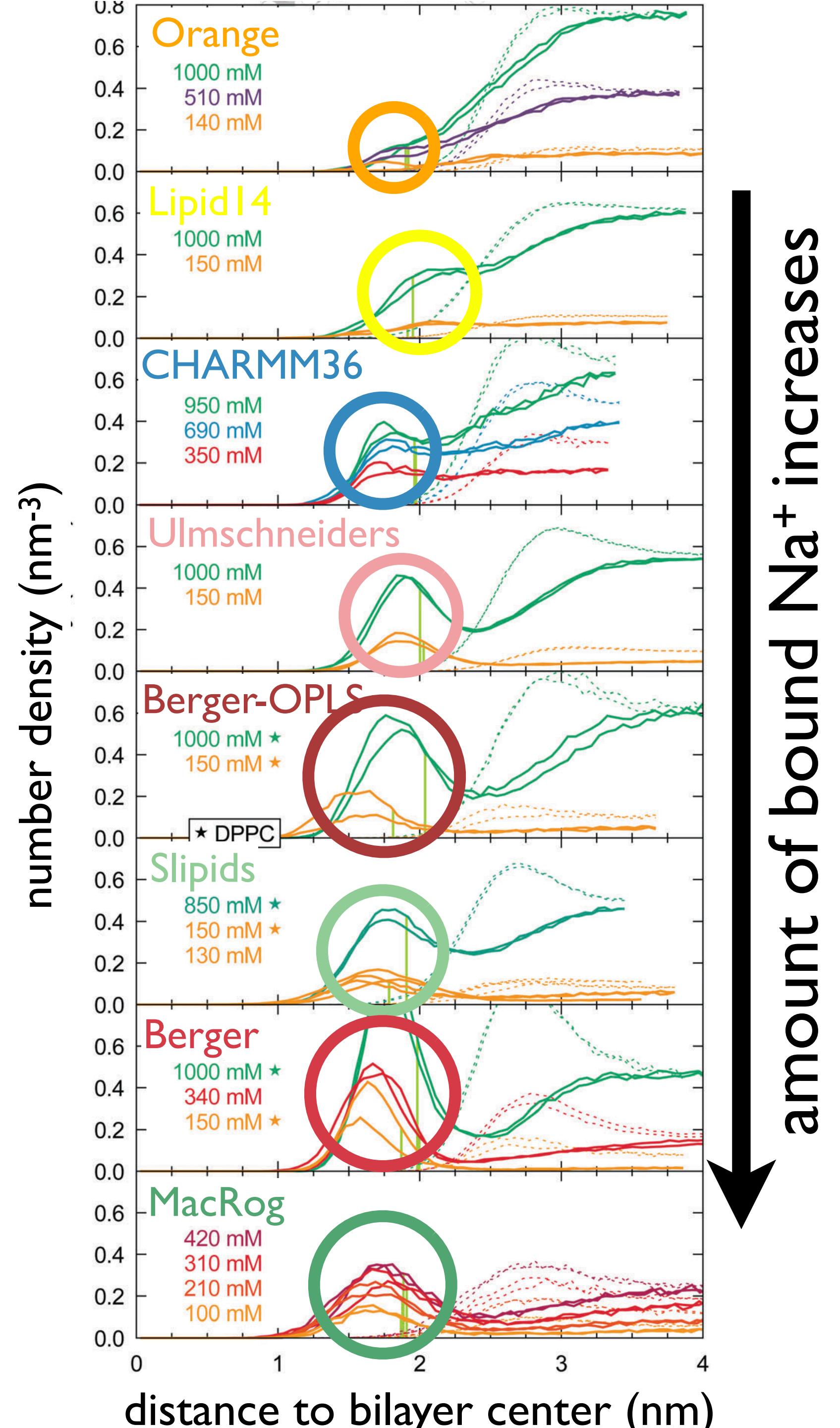
NaCl -induced change in the headgroup (β, α) order parameters





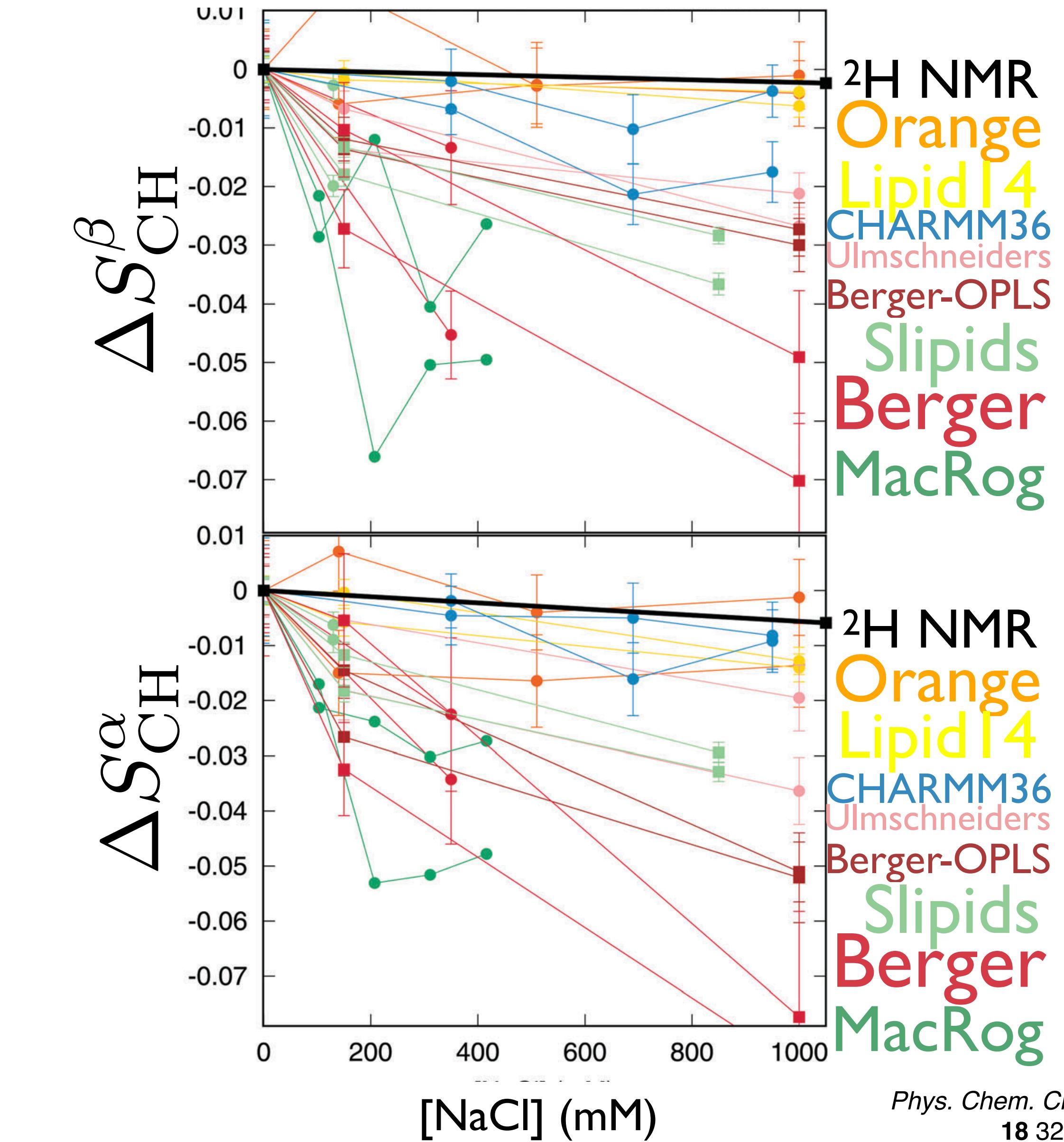
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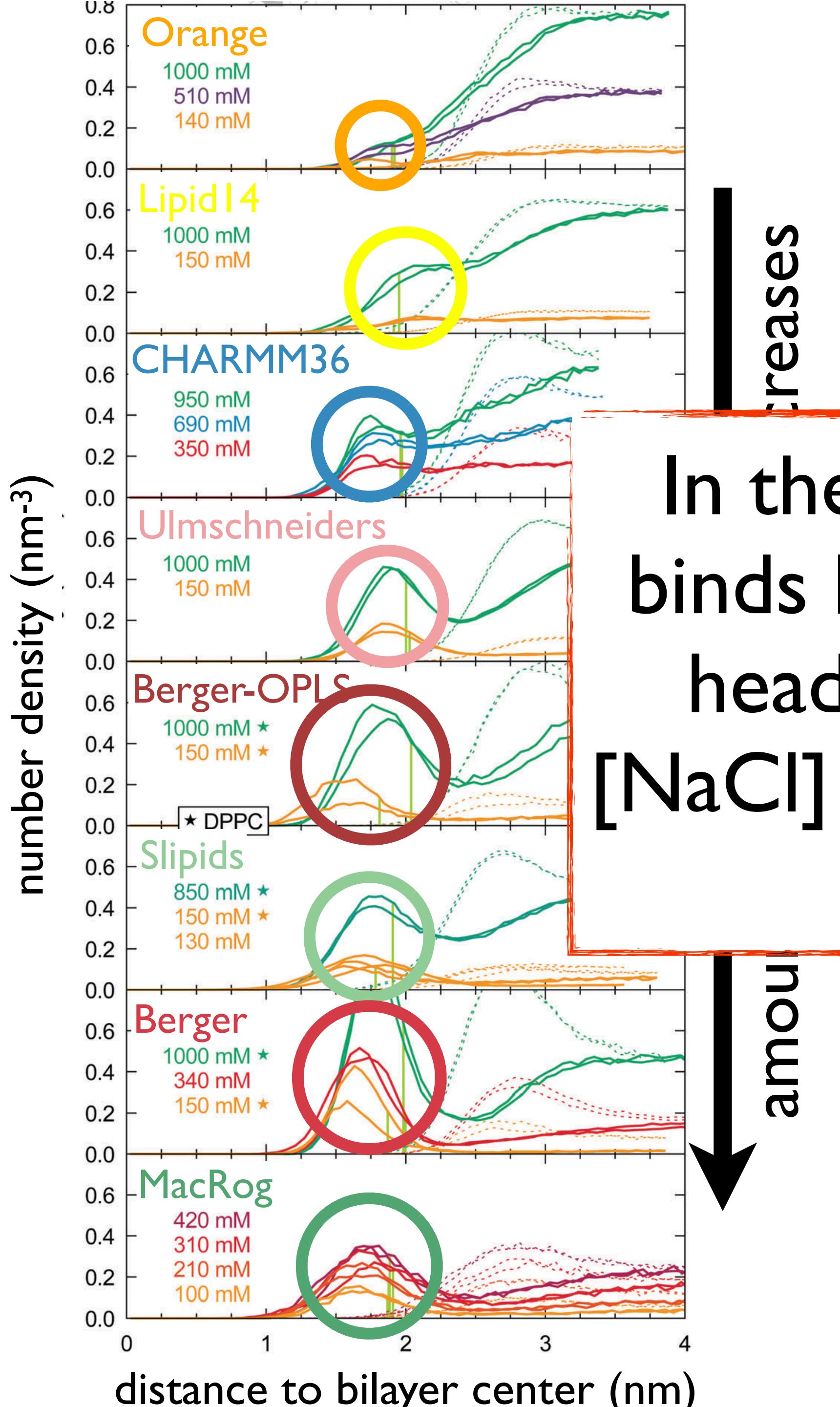


amount of bound Na^+ increases

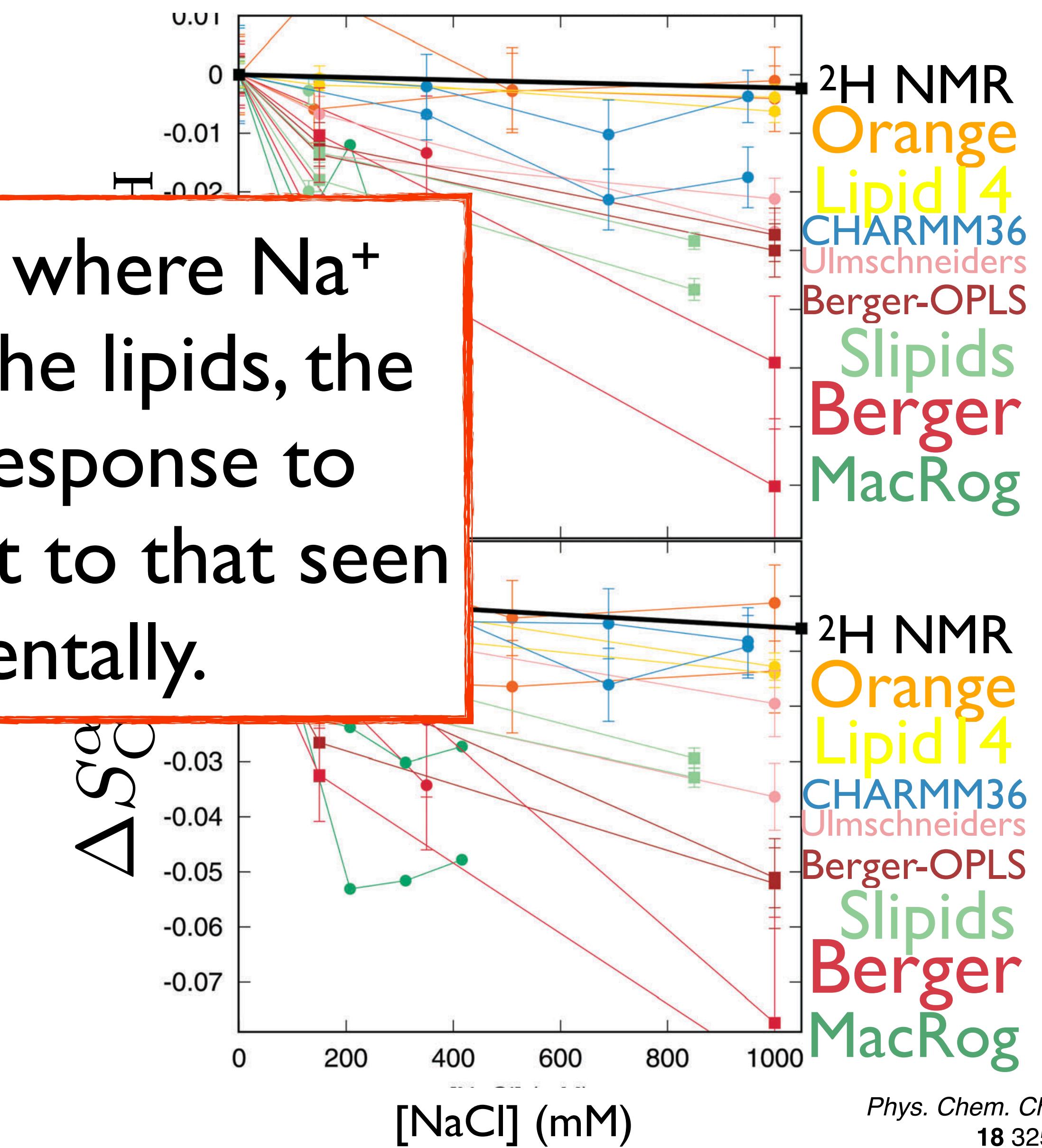
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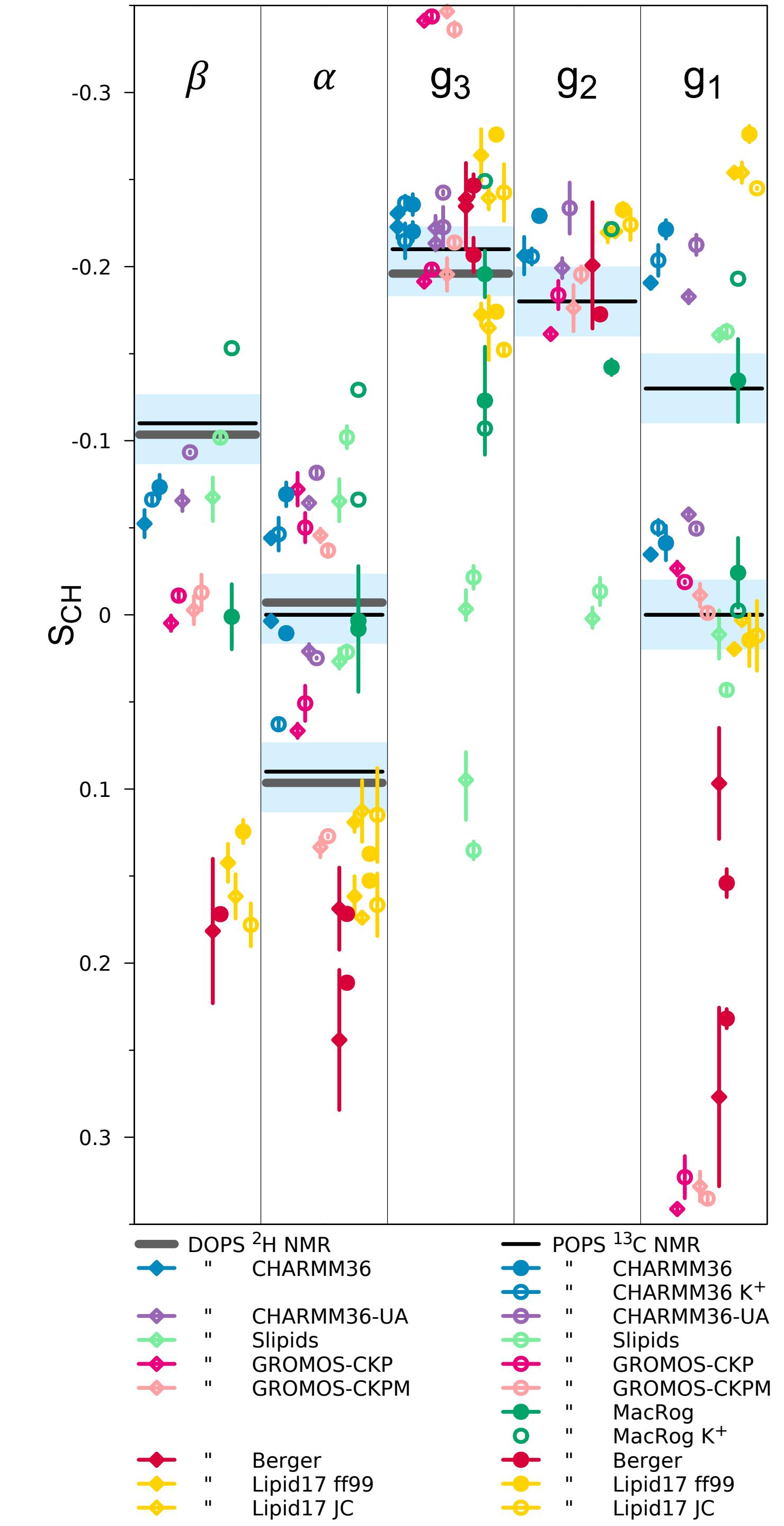
NaCl-induced change in the headgroup (β, α) order parameters



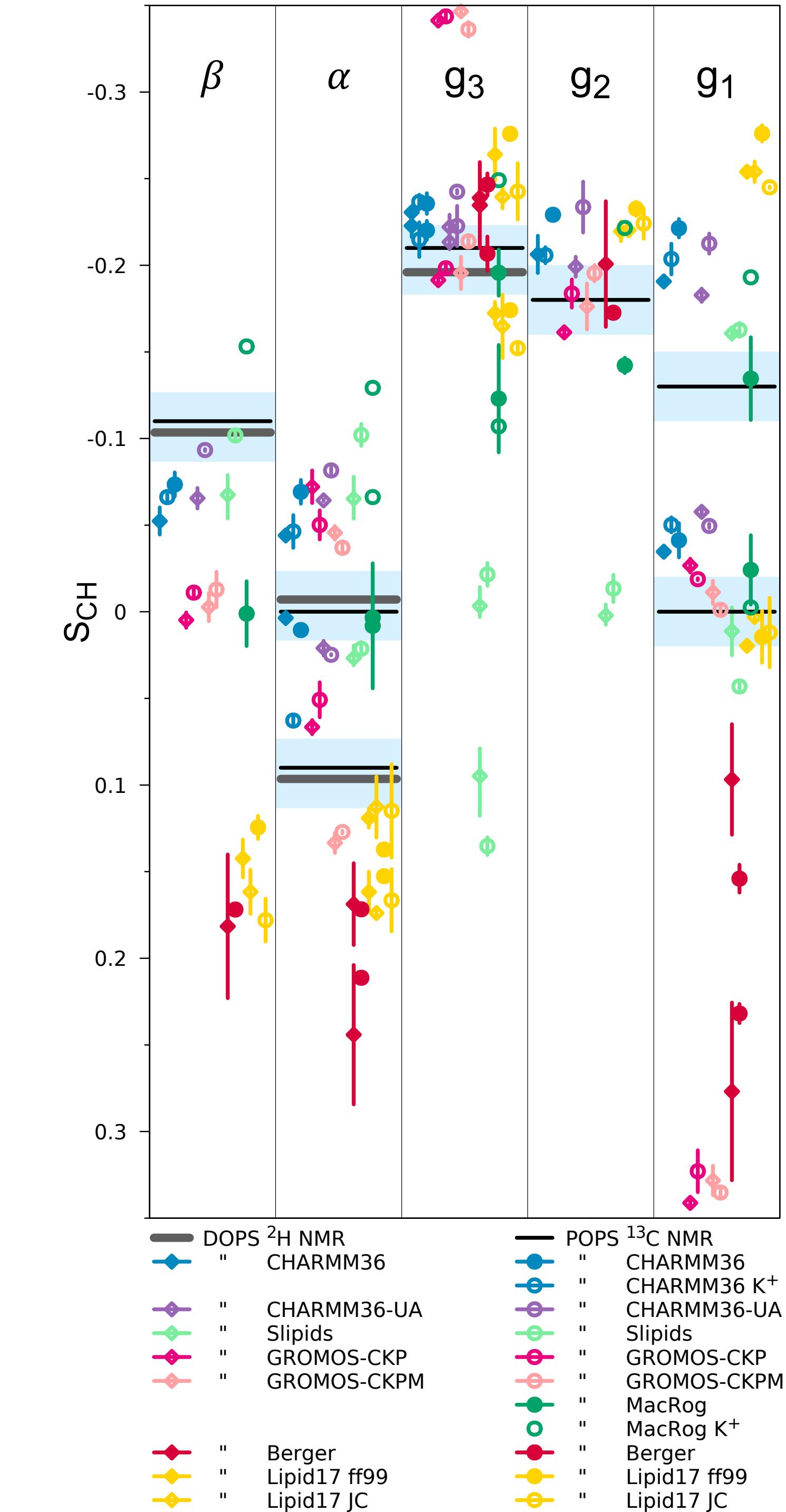
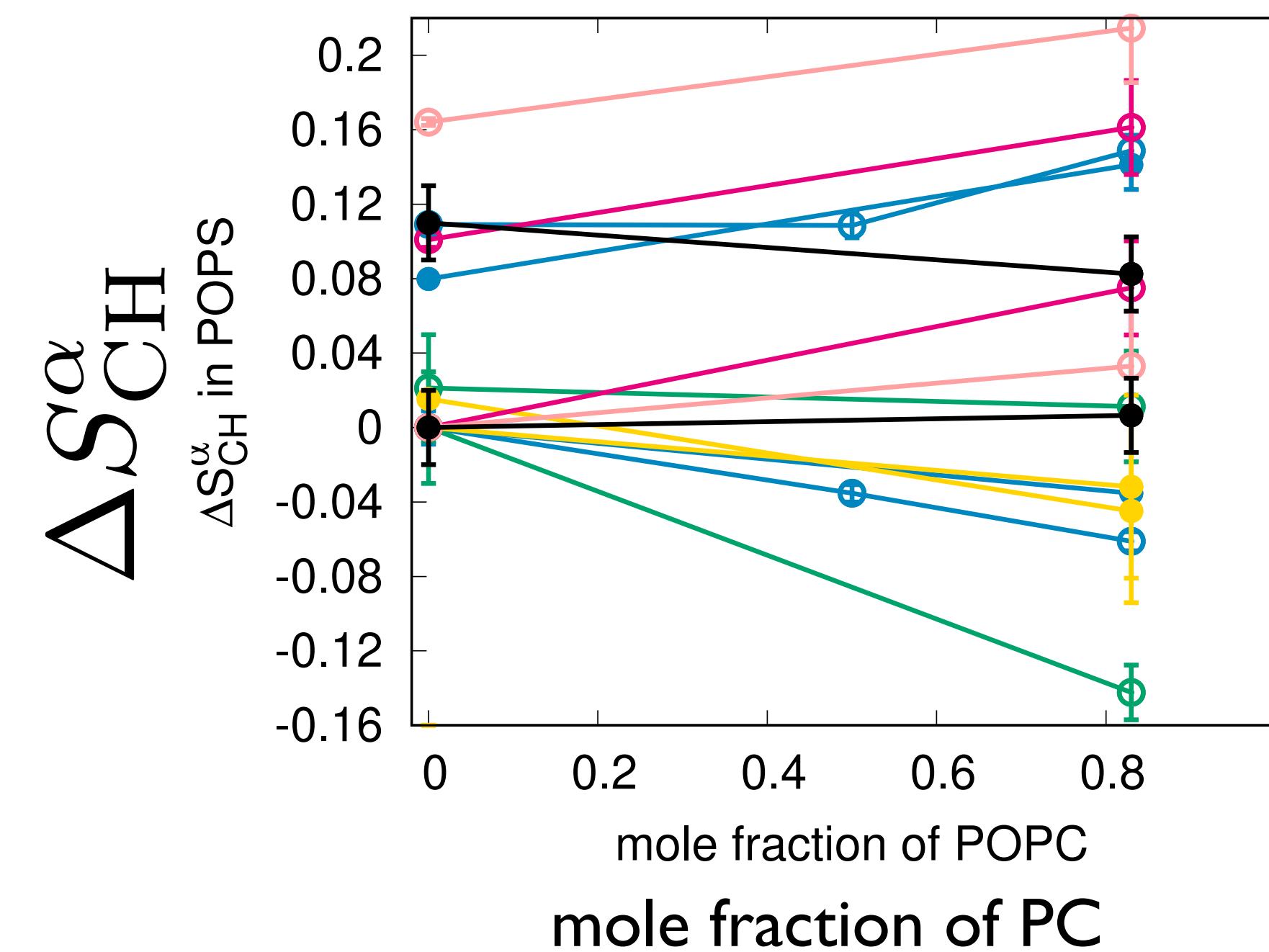
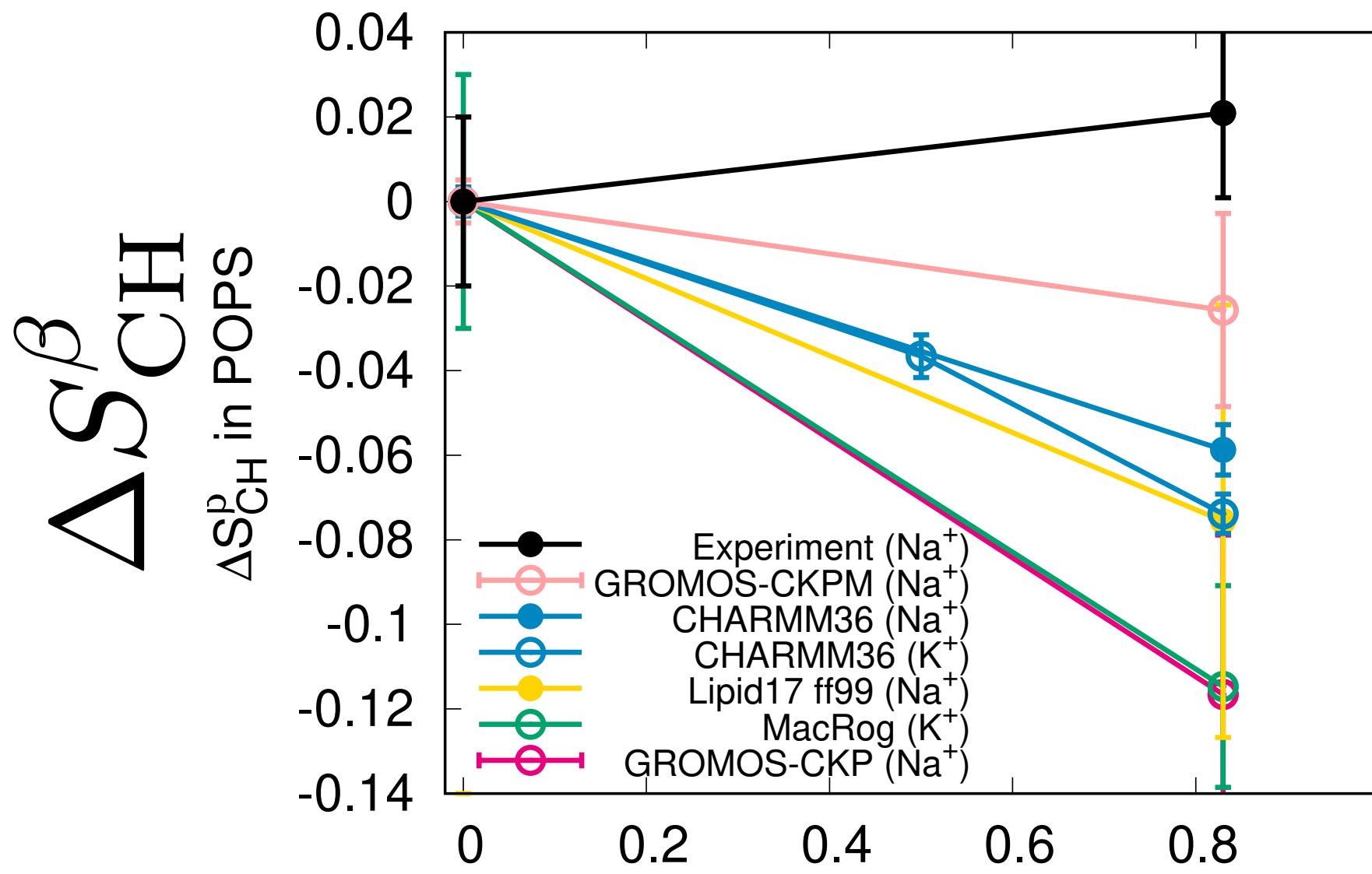
In the models where Na^+
binds least to the lipids, the
head group response to
 $[\text{NaCl}]$ is closest to that seen
experimentally.



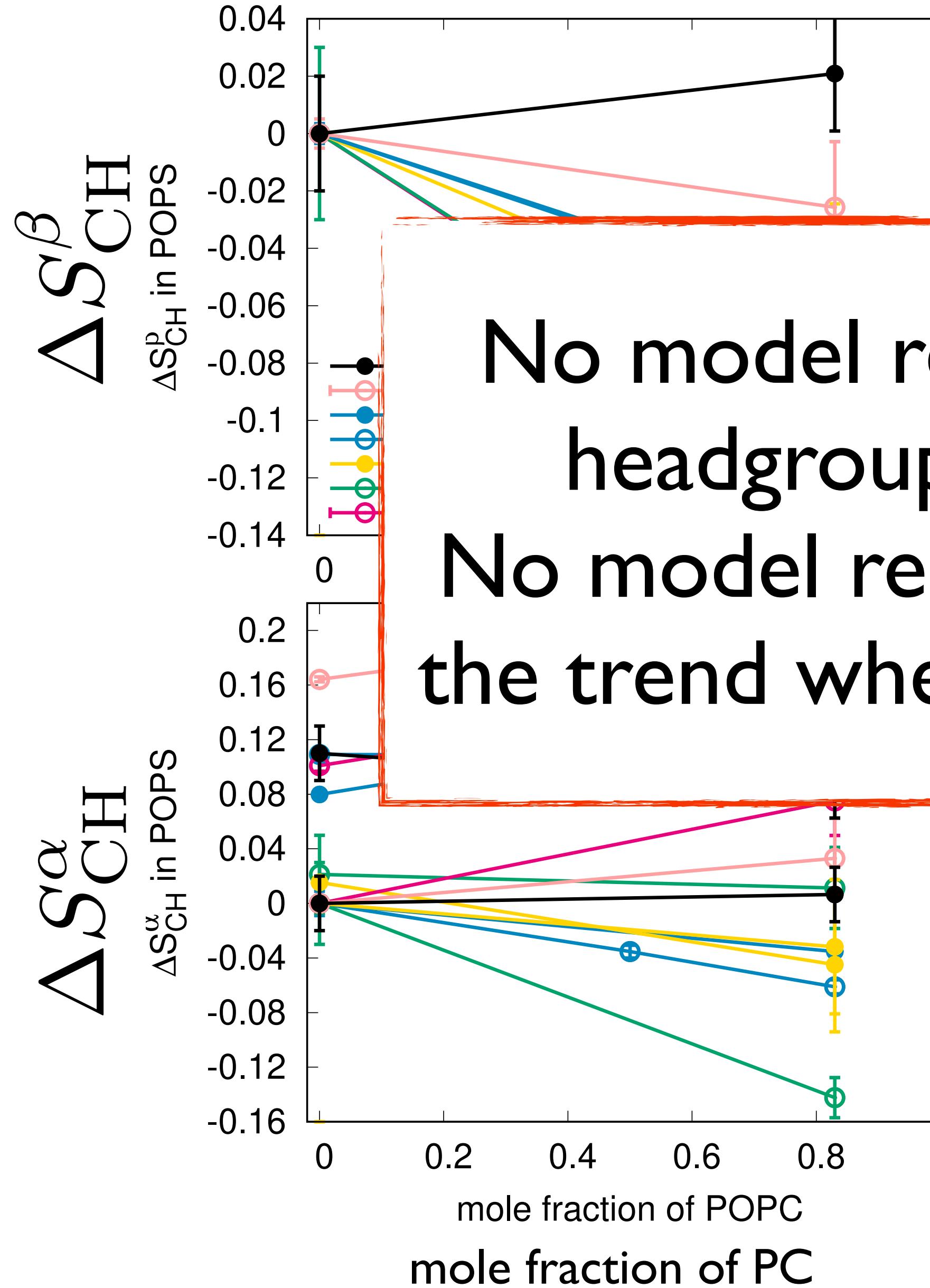
Phosphatidylserine (PS)



Phosphatidylserine (PS)



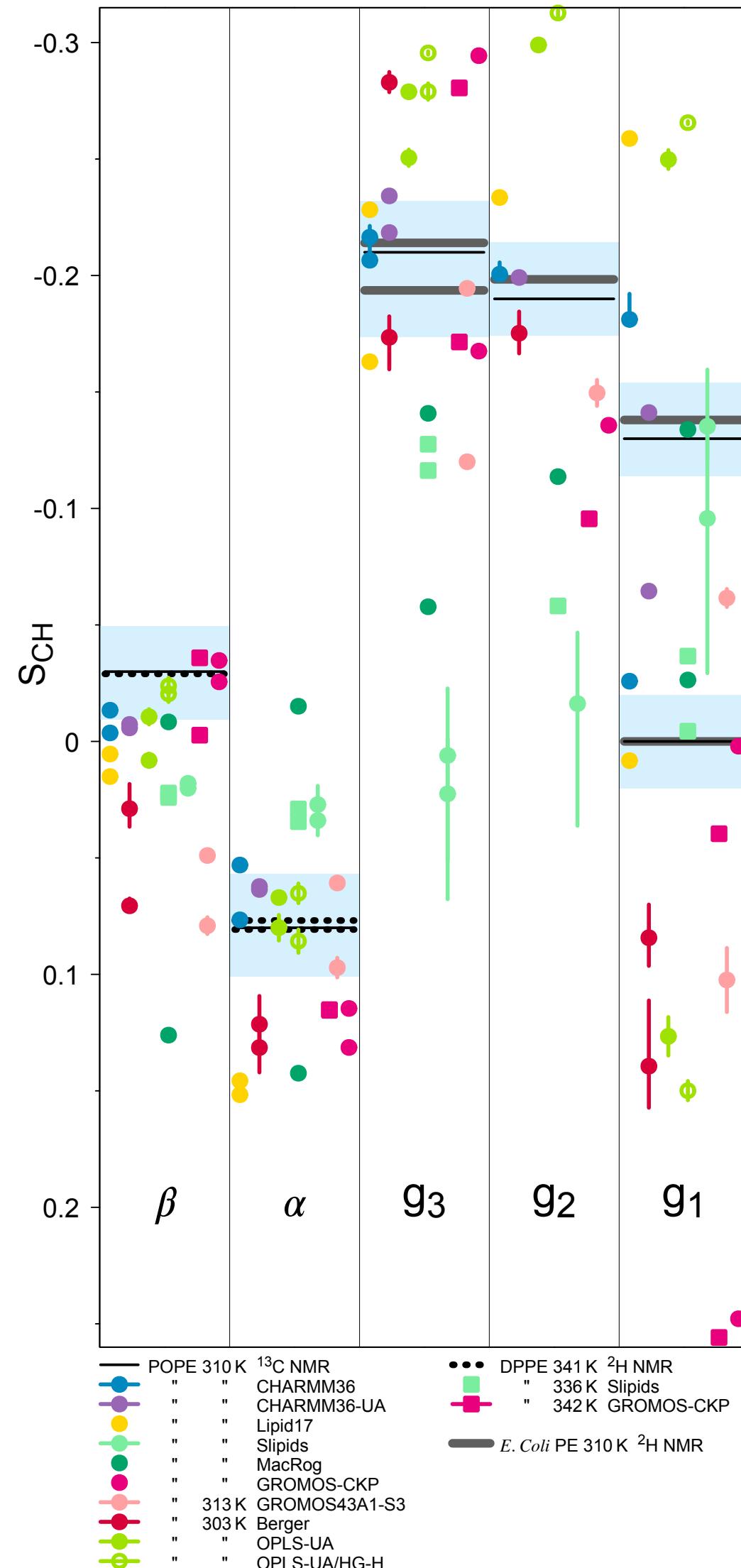
Phosphatidylserine (PS)



No model reproduces PS headgroup structure.
No model reproduces even the trend when PC is added.

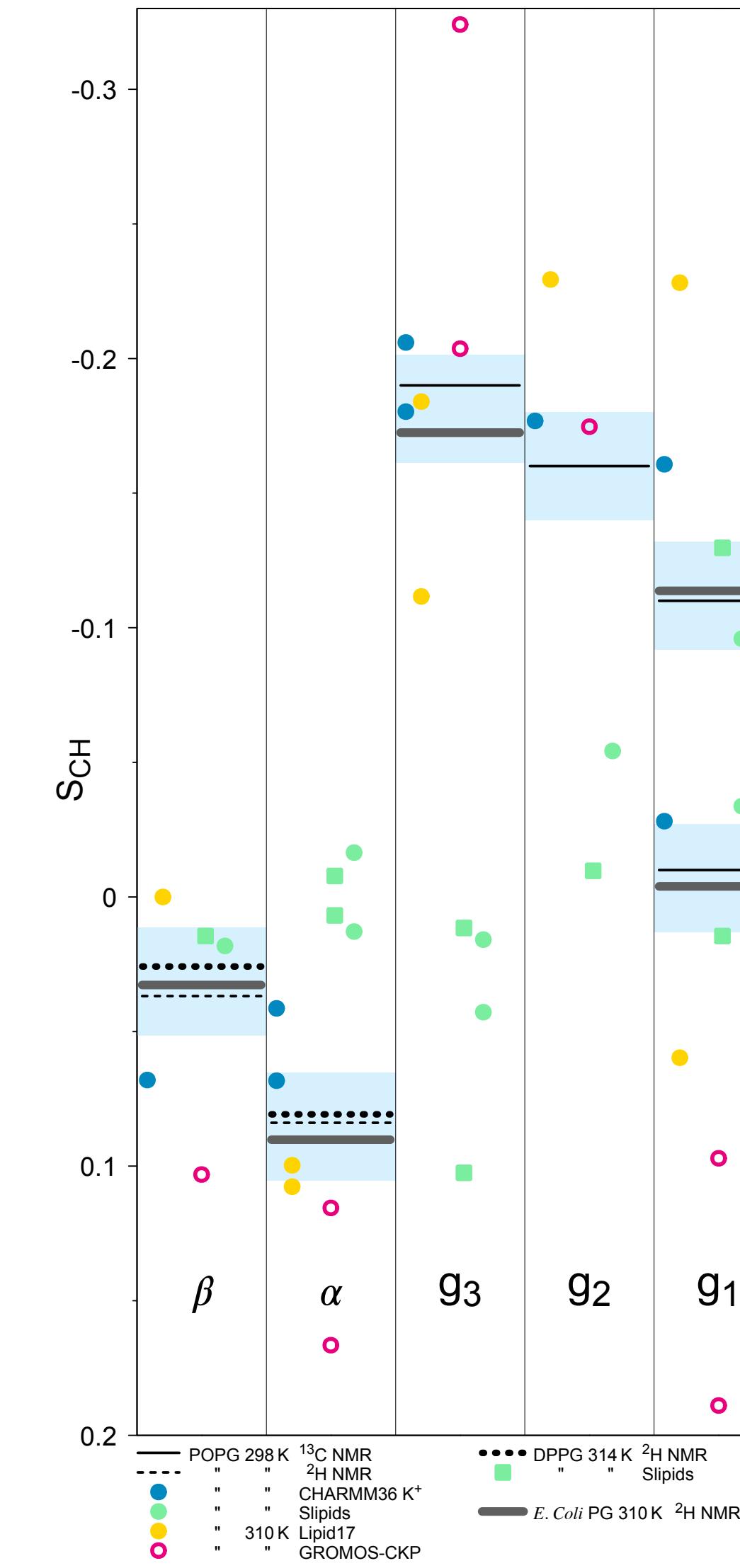


Phosphatidylethanolamine (PE)



C–H bond order parameters, S_{CH} , of the PE headgroup (β and α) and glycerol

Phosphatidylglycerol (PG)



C–H bond order parameters, S_{CH} , of the PG headgroup (β and α) and glycerol

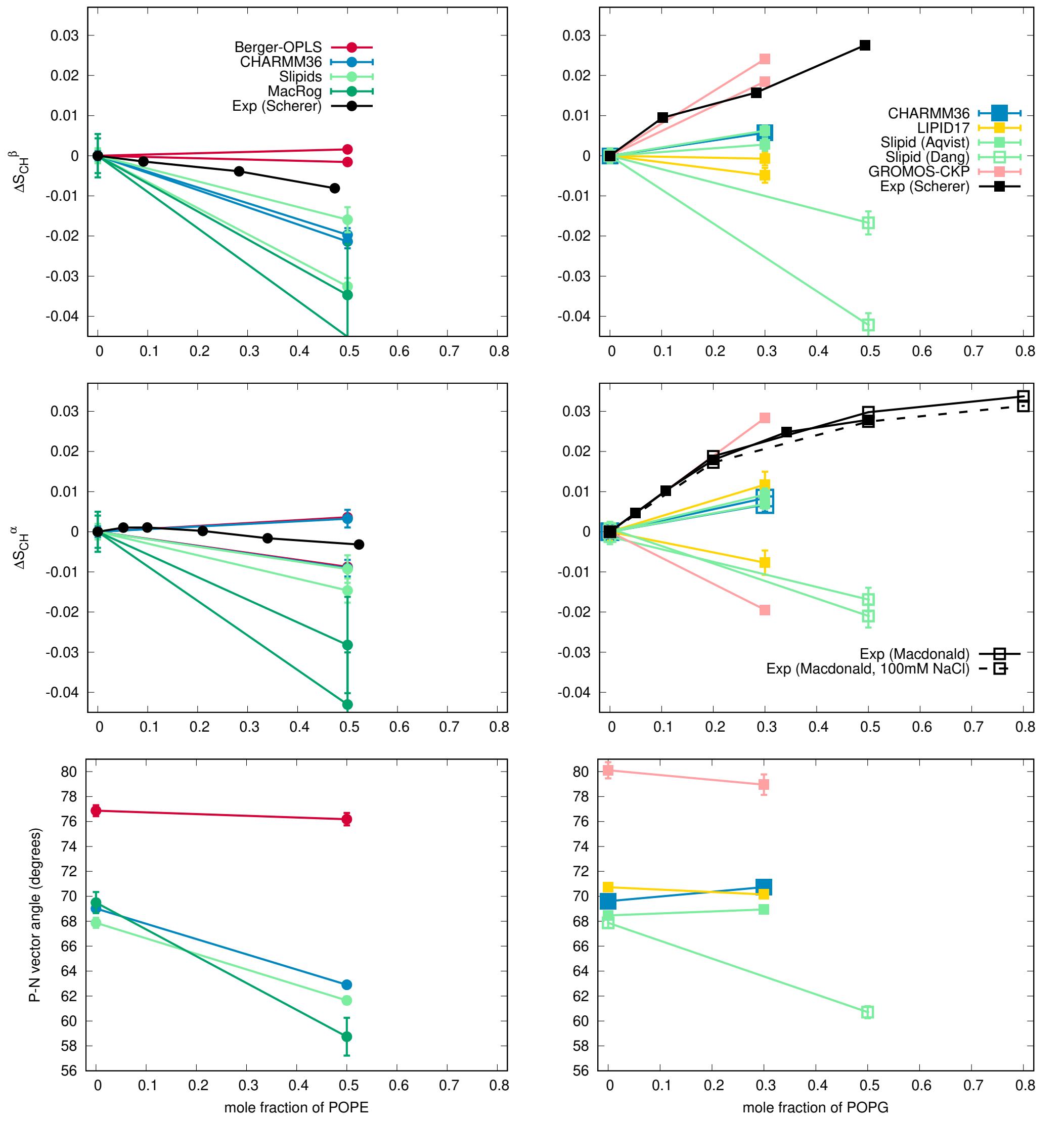


Figure S5: Modulation of POPC headgroup order parameters with increasing amount of POPE (left) and POPG (right) in bilayer from experiments at 298 K^{8,9} and simulations with different force fields (temperatures listed in tables S3 are between 298-310 K). Signs are determined as discussed in Refs. 1 and 6.

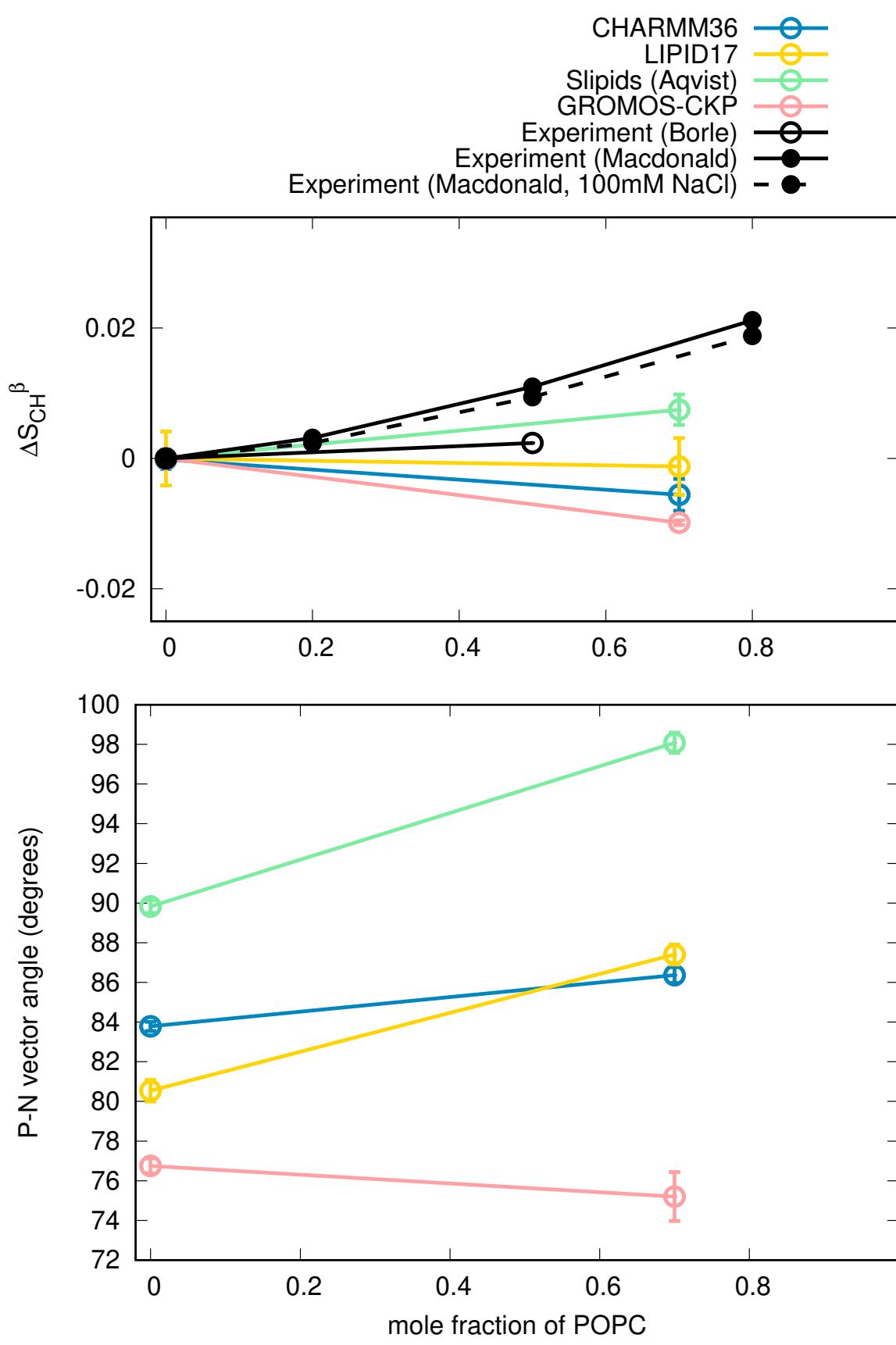


Figure S6: Modulation of PG lipid headgroup order parameters with the increasing amount of PC in lipid bilayer from experiments at 298 K^{7,9} and simulations with different force fields at 310 K.