

Supporting Information:

**NMRlipids IV: Headgroup & glycerol backbone
structures, and cation binding in bilayers with PE
and PG lipids**

O. H. Samuli Ollila^{*,†}

*†Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech
Republic, Prague 6, Czech Republic*

‡Institute of Biotechnology, University of Helsinki

E-mail: samuli.ollila@helsinki.fi

S1 Simulated systems

S1.1 CHARMM36

POPE [Simulation details by M. Javanainen.](#)

POPE with additional NaCl [Simulation details by A. Peon.](#)

POPG [Simulation details by Ollila.](#)

POPG with additional NaCl [Simulation details by A. Peon.](#)

POPC:POPE mixtures Data is available at.^{1,2} 300 K with v-rescale ($\tau=0.1$ ps), 1 bar with PR semiisotropic ($\tau=4$ ps, compressibility= $4.5\text{e-}5$ bar⁻¹), PME order 4 and space 0.12, rcoulomb and rvdw 1.0, 128 lipids per leaflet, no ion [Full simulation details by Fuchs et al.](#)

POPC:POPG mixture with additional calcium [Simulation details by J. Madsen.](#)

POPC:POPG mixture with additional NaCl [Simulation details by A. Peon.](#)

S1.2 CHARMM36ua

POPE Data is available at.³ [Simulation details by T. Piggot.](#)

S1.3 Slipids

POPE Data is available at.⁴ [Simulation details by T. Piggot.](#)

POPE with additional NaCl [Simulation details by A. Peon.](#)

DPPE Data is available at.⁵ [Simulation details by F. Favela.](#)

POPG Data is available at.⁶ [Simulation details by F. Favela.](#)

POPG with additional NaCl [Simulation details by A. Peon.](#)

DPPG Data in 298 K is available at⁷ and in 314 K at.⁸ [Simulation details by F. Favela.](#)

POPC:POPG mixture with additional NaCl [Simulation details by A. Peon.](#)

S1.4 Berger

POPE Data is available at.^{9,10} [Simulation details by T. Piggot.](#)

DOPE Data is available at.^{11,12} [Simulation details by T. Piggot.](#)

POPC:POPE, *POPC:DOPE* and *DOPC:DOPE* mixtures Data is available at.^{13,14} 300 K with v-rescale ($\tau=0.1$ ps), 1 bar with PR semiisotropic ($\tau=4$ ps, compressibility= $4.5\text{e-}5$ bar⁻¹), PME order 4 and space 0.12, rcoulomb and rvdw 1.0, 128 lipids per leaflet, no ion [Simulation details by Fuchs et al.](#)

S1.5 GROMOS 43A1-S3

POPE Data is available at.¹⁵ [Simulation details by T. Piggot.](#)

S1.6 OPLS-UA

POPE Data is available at.¹⁶ [Simulation details by T. Piggot.](#)

POPE with vdW interaction in H Data is available at.¹⁷ [Simulation details by T. Piggot.](#)

S1.7 GROMOS-CKP and GROMOS-CKPM

POPE Data is available at.¹⁸ [Simulation details by T. Piggot.](#)

DOPE Data is available at.¹⁹ [Simulation details by T. Piggot.](#)

DPPE Data is available at.²⁰ [Simulation details by T. Piggot.](#)

S2 R-PDLF and SDROSS experiments

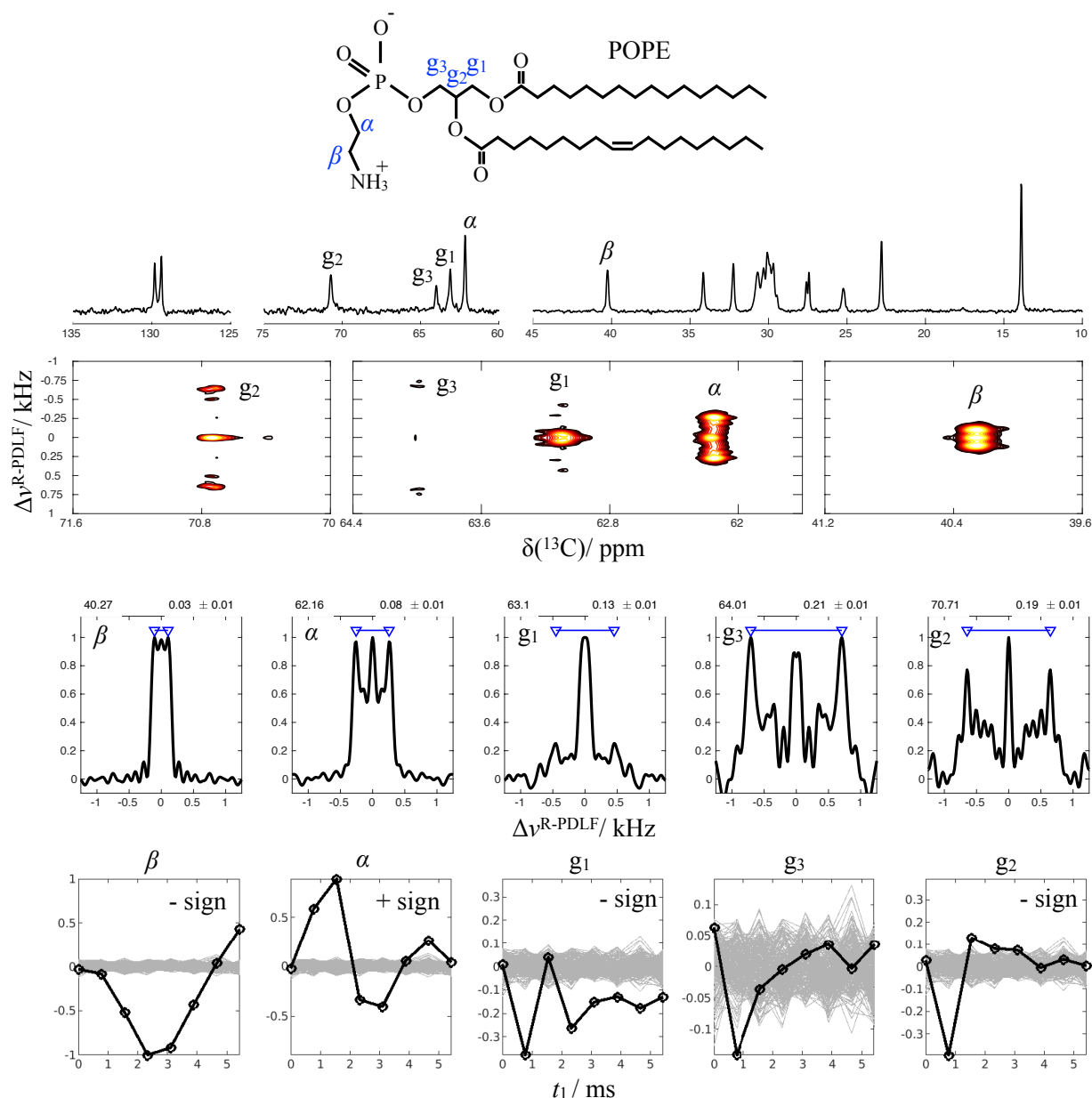


Figure S1: (A) Chemical structure of POPE with the labeling of headgroup and glycerol backbone carbons. (B) INEPT spectra from POPE sample with the headgroup and glycerol backbone peaks labeled. (C) 2D R-PDLF spectra (D) Dipolar sliced from the 2D R-PDLF spectra with the resulting order parameters on top of figures. (E) Experimental S-DROSS curves giving signs of the order parameters.

A, B etc. labels to be put in the figure.

References

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- (2) Papadopoulos, C.; Fuchs, P. F. CHARMM36 POPC/POPE (50%-50%) MD simulation (300 K - 300ns - 1 bar). 2018; <https://doi.org/10.5281/zenodo.1306821>.
- (3) Piggot, T. CHARMM36-UA POPE Simulations (versions 1 and 2) 310 K (NOTE: hexagonal membrane and POPE is called PEUA). 2018; <https://doi.org/10.5281/zenodo.1293774>.
- (4) Piggot, T. Slipids POPE Simulations (versions 1 and 2) 310 K (NOTE: hexagonal membrane). 2018; <https://doi.org/10.5281/zenodo.1293813>.
- (5) Favela-Rosales, F. MD simulation trajectory of a fully hydrated DPPE bilayer: SLIPIDS, Gromacs 5.0.4. 2017. 2017; <https://doi.org/10.5281/zenodo.495247>.
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- (8) Favela-Rosales, F. MD simulation trajectory of a fully hydrated DPPG bilayer @314K: SLIPIDS, Gromacs 5.0.4. 2017. 2017; <https://doi.org/10.5281/zenodo.546136>.
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- (10) Piggot, T. Berger POPE Simulations (versions 1 and 2) 303 K - larger repulsive H. 2018; <https://doi.org/10.5281/zenodo.1293891>.

- (11) Piggot, T. Berger DOPE Simulations (versions 1 and 2) 271 K - de Vries repulsive H. 2018; <https://doi.org/10.5281/zenodo.1293928>.
- (12) Piggot, T. Berger DOPE Simulations (versions 1 and 2) 271 K - larger repulsive H. 2018; <https://doi.org/10.5281/zenodo.1293905>.
- (13) Amélie, B.; F.J., F. P. Berger pure POPC MD simulation (300 K - 300ns - 1 bar). 2018; <https://doi.org/10.5281/zenodo.1402417>.
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- (17) Piggot, T. OPLS-UA POPE Simulations (versions 1 and 2) 303 K with vdW on H atoms. 2018; <https://doi.org/10.5281/zenodo.1293853>.
- (18) Piggot, T. GROMOS-CKP POPE Simulations (versions 1 and 2) 313 K. 2018; <https://doi.org/10.5281/zenodo.1293932>.
- (19) Piggot, T. GROMOS-CKP DOPE Simulations (versions 1 and 2) 271 K. 2018; <https://doi.org/10.5281/zenodo.1293941>.
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