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

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S1 Simulated systems

S1.1 CHARMM36

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=4.5e-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.

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.

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

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

DPPG Data in 298 K is available at[7] and in 314 K at.[8] Simulation details by F. Favela.

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=4.5e-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

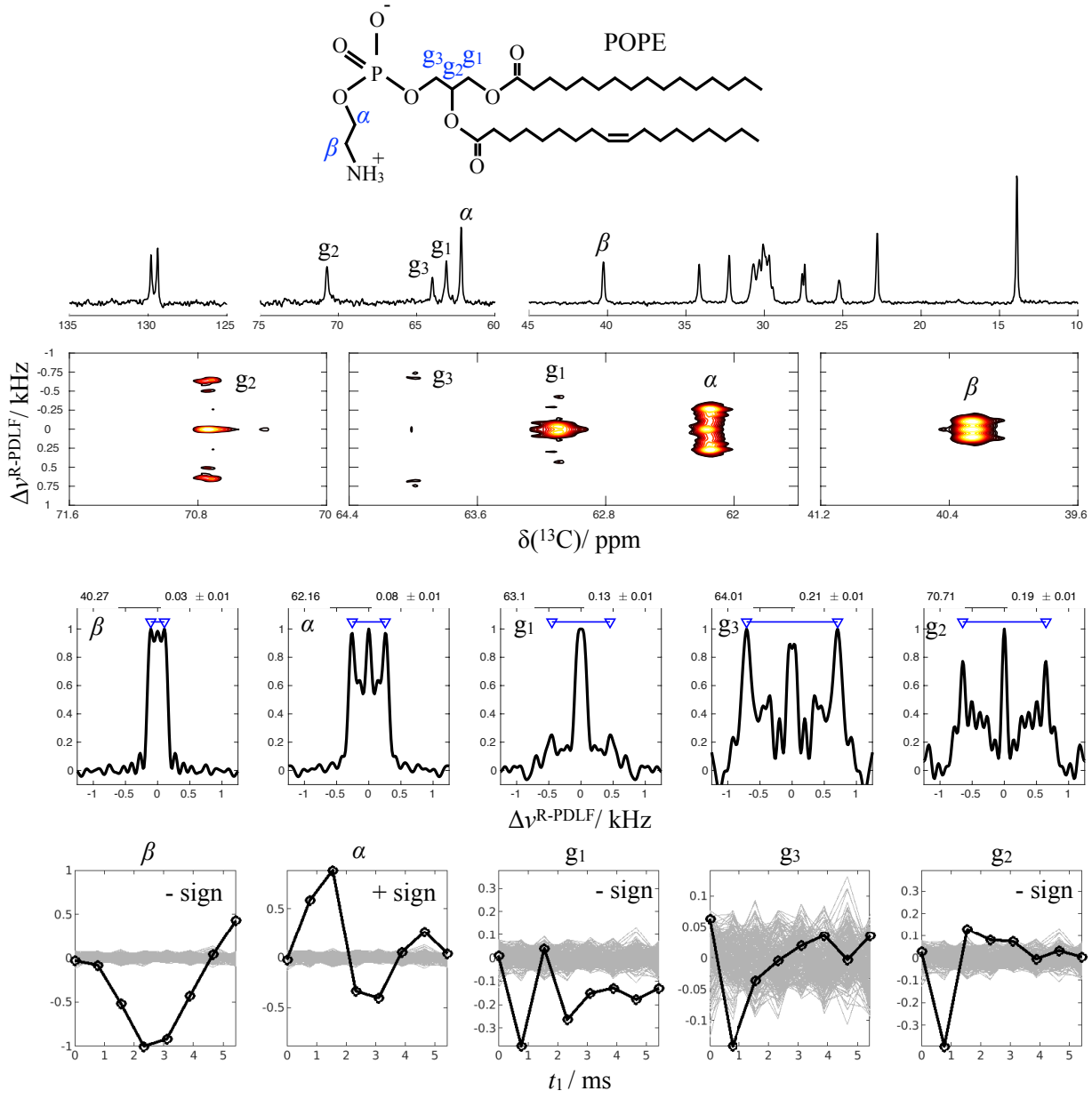

Figure S1: (A) Chemical structure of POPE with the labeling of headgroup and glycerol backbone carbons. (B) INEPT spectra from POPE sample with the headgroup and glycerol backbone peaks labeled. (C) 2D R-PDLF spectra (D) Dipolar sliced from the 2D R-PDLF spectra with the resulting order parameters on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

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

References

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