Results comparison for pure POPC and pure POPE simulations using MacRog Force Field

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We aimed to carry out POPC/POPE 1:1 simulation using MacRog Force Field (1) for NMRLipids IVb project. The .itp files were obtained from the authors, from the paper doi: 10.1016/j.dib.2016.03.067 (2). We realized that there were several problems related to these files , specifically:

pope.itp :

- The lipid in this file is OPPE, not POPE
- The atom C28 is not connected to the previous atom (bonds, angles, dihedrals, pairs were not included)
- There were two atoms called C27

popc.itp:

- Some impropers are missing leading to non planar systems for double bonds, in particular : the carbonyls of sn-1 and sn-2 as well as the double bond of oleoyl

We corrected these errors to perform POPC:POPE 1:1 simulation. To ensure the reliability of our .itp files, we performed a pure POPC simulation and a pure POPE simulation. The order parameter results of these two simulations, are compared in this document to two other simulations :

- Pure POPC simulation with MacRog FF carried out by Matti Javanainen for NMRLipids I (3).
- Pure POPE simulation with MacRog FF carried out y Matti Javanainen for NMRLipids IVb.

The popc.itp file used by MJ was obtained directly form the authors but it has not been published. The pope.itp was obtained from the publication mentioned above and corrected by MJ. In the next pages of this document, the two sets of simulations are compared. The similarity of the OP results obtained for the two pure POPC simulations and the two POPE simulations, confirm the reliability of our corrected popc.itp and popc.itp.

MacRog pure POPC MD simulation

	NMRLipids I Matti Javanainen	**PMilanRodriguez & PFuchs**
Temperature (K)	310	300
Pression (bar)	1	1
Ion Concentration (M)	0	0
Simulation time (ns)	100	500
Analysis time (ns)	80	300
Nb of lipids	288	128
Nb of water molecules	12600	5120

Table 1. Detailed information for pure POPC MacRog simulation. In yellow, simulation carried out by Matti Javanainen for NMRLipids I. In violet, by PMR and PF.

POPC carbon	**NMRLipids I** Matti Javanainen	**PMilanRodriguez & PFuchs**	**STDV**
b1	0.0310	0.03692	0.06109
b2	0.0201	0.00814	0.04904
a1	0.0494	0.05584	0.05650
a2	0.0483	0.03801	0.04545
g31	-0.2328	-0.22662	0.06304
g32	-0.1380	-0.12221	0.07639
g2	-0.2020	-0.19383	0.06577
g11	-0.1560	-0.16080	0.07049
g12	0.0137	0.00654	0.07351

Table 2. Order parameter results for pure POPC simulation. In yellow, simulation carried out by Matti Javanainen for NMRLipids I. In violet, by PMR and PF.

Information about MJ simulations obtained from :

- https://zenodo.org/record/13497#.XnTe59-YU5k
- https://github.com/NMRLipids/nmrlipids.blogspot.fi/blob/master/DATAreportediINblog/POPC/MACROG-310K_blogged-20-09-13.dat

MacRog pure POPE MD simulation

	NMRLipids IVb Matti Javanainen	**NMRLipids IVb** PMR & PF
Temperature (K)	310	300
Pression (bar)	1	1
Ion Concentration (M)	0	0
Simulation time (ns)	500	500
Analysis time (ns)	?	300
Nb of lipids	144	128
Nb of water molecules	5760	5120

Table 3. Detailed information for pure POPE MacRog simulation. In yellow, simulation carried out by Matti Javanainen for NMRLipids IVb. In violet, by PMR and PF.

POPE carbon	**NMRLipids IVb** Matti Javanainen	**STDV**	**NMRLipids IVb** PMR & PF	**STDV**
b1	0.12608	0.16655	0.09934	0.22615
b2	-0.00837	0.12406	-0.00329	0.19557
a1	0.14238	0.17475	0.11416	0.23607
a2	-0.01514	0.12860	-0.01126	0.20361
g31	-0.14086	0.16966	-0.19387	0.22899
g32	-0.05784	0.15507	-0.11982	0.20970
g2	-0.11370	0.18751	-0.15457	0.23723
g11	-0.13393	0.15251	-0.16604	0.19783
g12	-0.02640	0.17031	-0.00638	0.26330

Table 4. Order parameter results for pure POPE simulation. In yellow, simulation carried out by Matti Javanainen for NMRLipids IVb. In violet, by PMR and PF.

Information about MJ simulations obtained from:

- https://github.com/NMRLipids/MATCH/commit/80247406f6f887fe79d7a19773f2976f9d818fd4
- https://github.com/NMRLipids/MATCH/blob/master/Data/Lipid_Bilayers/POPE/T310K/MODEL_MACROG/OrdParsPOPE.dat

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