

Appendix for:
Biological Membranes in Extreme Conditions: Simulations of Anionic Archaeal Tetraether Lipid Membranes

Luis Felipe Pineda De Castro^{1,2,☐}, Mark Dopson³, Ran Friedman^{1,2,*}

1 Computational Chemistry and Biochemistry research Group (CCBG), Department of Chemistry and Biomedical Sciences, Linnæus University, 391 82 Kalmar, Sweden

2 Centre of Excellence “Biomaterials Chemistry”, Linnæus University, 391 82 Kalmar, Sweden

3 Systems Biology of Microorganisms Research Group (SBMR), Centre for Ecology and Evolution in Microbial model Systems (EEMiS), Linnæus University, 391 82 Kalmar, Sweden

☐ Present address, Laboratory of Molecular Modeling, University of Gdansk, ul. Wita Stwosza 63, PL-80-308 Gdansk, Poland

* ran.friedman@lnu.se

Appendix - effect of the surface tension parameter on the properties of the membranes

All membrane simulations were carried out using a set-up that mimicked the $Np\gamma T$ ensemble, i.e., constant number of particles, pressure, temperature and surface tension. The surface tension of di- and tetra-ether membranes was not known from experiment, and an ambient value of 44 mN/m [1] was used in the simulations. To examine the effect of altering the surface tension, simulations of the GDNT.4 system with B^+ counter ions were also performed at reduced (24 mN/m) and increased (64 mN/m) surface tension. The results showed little dependence of membrane properties on the exact value of the surface tension. Deviations between the systems were smaller than 5% in all of the calculated observables (Table 1).

Table 1. Effect of the surface tension (γ) on the physical properties of GDNT-4 membranes

γ (mN/m)	APL (\AA^2)	VPL (\AA^3)	Lz (\AA)	d_{PP} (\AA)	VMU (\AA^3)
24	67.8(.1)	2933(10)	43.3(.2)	39.0(.4)	2647(.6)
44	70.9(.1)	2947(10)	41.6(.2)	37.9(.4)	2683(.7)
64	70.6(.2)	2947(12)	41.7(.3)	38.8(.4)	2741(.6)

References

1. Siu SW, Vácha R, Jungwirth P, Böckmann RA. Biomolecular simulations of membranes: physical properties from different force fields. *J Chem Phys.* 2008;128:125103.