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Intrinsic Lipid Curvatures of Mammalian Plasma outer Leaflet Lipids and Ceramides

Content

The intrinsic lipid curvature is an important parameter, when it comes to predicting the shape of a lipid system or calculating the inner membrane pressure of a lipid bilayer. The parameter itself is best accessible from a tensionfree system, as can be provided by an inverted hexagonal structure(H_{II}).
To extract the intrinsic curvature from such systems, we developed a global X-ray data analysis method, combining compositional modelling with molecular shape-based arguments in the model of the system's electron density. In our case the H_{II} forming lipid dioleoyl phosphatidylethanolamine (DOPE) was used as a host-system for the lipid of interest.
The technique was verified by all-atom molecular dynamics simulations and applied to a series of guest lipids: In addition to various phosphatidylcholines, sphingomyelin and ceramides of differing hydrocarbon chain composition were examined. We report positive lipid curvatures for sphingomyelin and all phosphatidylcholines with di- saturated and monounsaturated hydro-carbons. Phosphatidylcholines with di- unsaturated hydrocarbons in turn yielded negative intrinsic lipid curvatures. All ceramides, with chain lengths varying between C2:0 and C24:0, displayed significantly negative lipid curvature values. Moreover, our analysis indicated non-additive mixing for C2:0 ceramide and sphingomyelin in DOPE- environment. This suggests for sphingolipids, that in addition to lipid headgroup and hydrocarbon chain volumes, also lipid- specific interactions contribute significantly to the membrane curvature stress.

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