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Towards transferable force fields for simulating biological membranes

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Classical molecular dynamics (MD) simulations are often used to provide detailed insights of model cell membranes difficult to access directly via experimental means. This can either be done directly or by aiding in the interpretation of experimental data (incl. those obtained from neutron scattering)
The utility of MD simulations, however, depends on the accuracy and transferability of the underlying force field description (e.g., parameters, functional forms etc.). Currently available lipid force fields are unreliable for modelling more realistic and complex membrane systems and their interaction with other biologically relevant molecules.
In this study, I take a robust bottom-up approach to re-examine and re-parameterize force field terms used in small molecule analogues of common components in different lipid species by comparing to their experimentally derived properties (e.g., pure liquid and solvation properties). Refinements for the force field descriptions of small molecules, including hydrocarbons and esters, are proposed. The effect of the refined parameters in lipid bilayer systems is also assessed. A key element of this work is minimizing confounding variables that can mislead parameterization efforts. This was done by ensuring that the calculation of observables is performed in a regime that reduce their sensitivities to the precise choice of simulation settings, and explicitly considering the correlations between different force field parameters.

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