O. H. Samuli Ollila
Helsinki Biophysics and Biomembrane Group
Department of Biomedical Engineering and Computational Science
P.O. Box 12200, FI-00076 Aalto University, Espoo, Finland
samuli.ollila@aalto.fi, Tel. +358503746963, Fax. +358 9 470 23182

Dear Editor,

Please find attached to this message a manuscript entitled 'Towards atomistic resolution structure of phosphatidylcholine glycerol backbone and choline headgroup at different ambient conditions' by A. Botan et al., which we would like to submit for consideration of publication in *Journal of the American Chemical Society* (JACS). In the manuscript a large amount of existing experimental Nuclear Magnetic Resonance (NMR) data is reviewed and combined with an exceptionally comprehensive collection of molecular dynamics (MD) simulation data in order to understand the atomistic resolution structure of biologically abundant phospholipid molecules and their assemblies.

We believe that the manuscript is interesting to the wide and diverse contemporary audience of JACS as it demonstrates how the combination of experimental NMR data with MD simulations can be successful in resolving the atomistic resolution structure of biomolecules in various biologically relevant conditions. The approach is demonstrated for lipids, however, the extension to, e.g., membrane proteins is straightforward. Such an atomistic resolution of biomolecular structure significantly advances the understanding in fundamental chemistry, molecular biology, and also supports the development of applications, for example new biomaterials or drug delivery systems.

In addition to its main message, the manuscript also provides an extensive comparison on the structural quality of the numerous widely used computational lipid models. This is crucial information for the large group scientists who are producing or reading the literature involving computational lipid models.

The work has been conducted by using a novel open collaboration concept, and all the scientific contributions are made publicly through the blog-based project web page located at `nmrlipids.blogspot.fi`. Thus all the scientific content related to this work (including raw data, discussions, manuscript drafts, etc.) has been publicly available during the whole course of the project through this blog. This material and the possibility to discuss it on the blog page will remain available also after the publication. This approach has significantly increased and will further increase the scientific quality and impact of the work. In addition, we have shared all the simulation raw data in a format that allows easy reanalysis and therefore reuse of the data for other purposes. In addition to the scientific content, we believe that the success of this fresh approach in the field of chemistry is highly interesting to the audience of JACS.

The usage of molecular dynamics simulations and open collaboration are adequate for the problem at hand. Indeed, such simulations are currently the most straightforward method to construct atomistic resolution structures to interpret NMR experiments, but enormous amount of simulation work was required for this work. The only practical solution to collect these data was the open collaboration concept. As result, we have produced original chemical insight for the atomistic resolution structures of phospholipids in various biologically relevant conditions.

We hope that you can consider this manuscript to be published as an article in the Journal of the American Chemical Society.

Sincerely yours,

On behalf of the authors,

O. H. Samuli Ollila