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To Whom It May Concern,

Please find attached to this message a manuscript that we would like to submit for publication in *Journal of the american chemical society* (JACS): 'Towards atomistic resolution structure of phosphatidylcholine glycerol backbone and choline headgroup at different ambient conditions', by A. Botan et al. In the manuscript we combine extensive amount of experimental Nuclear Magnetic Resonance (NMR) and molecular dynamics simulation data to understand the atomistic resolution structure of biologically abundant phospholipid molecules.

We believe that the manuscript is interesting for the wide and diverse contemporary audience of JACS since the used combination of experiments and simulations is shown to be successful in resolving the atomistic resolution structure of biomolecules in the various biologically relevant conditions. The approach is demonstrated for lipids, however, the extension to, e.g. membrane proteins is straightforward. The understanding of the atomistic resolution structures of molecules in biologically relevant conditions significantly advances understanding about fundamental chemistry and also supports the development of, for example, new biomaterials or drug delivery systems.

The work has been conducted by using a novel open collaboration concept, and all the scientific contributions are done publicly through the [nmrlipids.blogspot.fi](http://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 the blog. This material and discussion possibility will be kept available also after the publication. This approach has significantly increased and will increase the scientific quality and impact of the work. In addition, we have shared all the simulation raw data in such a format that it can be reanalyzed easily also for other purposes. In addition to the scientific content, we believe that the success of this approach in the field of chemistry is highly interesting for the JACS audience.

The usage of molecular dynamics simulations and open collaboration are adequate for the problem at hand since the simulations are currently the most straightforward method to construct the atomistic resolution structure of molecules to interpret the NMR experiments. On the other hand, enormous amount of simulation work was required for this work, and the only practical solution to collect this data is the used open collaboration approach. 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