**Dr. Alan Grossfield**

**Department of Biochemistry & Biophysics**

**University of Rochester Medical Center**

**601 Elmwood Avenue, Box 712**

**Rochester, New York 14642**

**(585) 276 4193**

**http://membrane.urmc.rochester.edu**

**alan\_grossfield@urmc.rochester.edu**

March 6, 2023

Dear Dr. Heerklotz,

We are submitting the attached manuscript, “Free Energy of Phase Separation in Lipid Bilayers from Molecular Dynamics” by Ashlin J. Poruthoor and Alan Grossfield, for consideration at **Biophysical Journal**. In this work, we describe a new method to calculate the free energy associated with the formation of distinct phases in lipid bilayers from molecular dynamics simulations. To our knowledge, this is the first such method to be developed, which should make it of general interest to the readership of Biophysical Journal, especially those who focus on either membranes, simulations, or both.

We suggest that Dr. Siewert-Jan Marrink would be the most logical editorial board member to handle this submission, given that he is broadly experienced in simulations of complex membranes (and we used his MARTINI coarse-grained membrane model for our test systems). As reviewers, we suggest Dr. Markus Deserno, Dr. D. Peter Tieleman, and Dr. Alex Gorfe; all are experienced in membrane simulations and phase separation phenomena.

If the manuscript is accepted, I will use treat it as the one free paper per year I’m allotted as an editor of **Biophysical Journal**.

Sincerely,



Dr. Alan Grossfield

Associate Professor

Department of Biochemistry and Biophysics