6 June 2017

Dear Dr. Mobley and Dr. Chodera,

GlaxoSmithKline is a science-led global healthcare company that researches, develops and manufactures innovative pharmaceutical medicines, vaccines and consumer healthcare products. I lead the Computational and Modeling Sciences department at GSK, which includes computational chemistry, cheminformatics, computational toxicology, protein engineering, as well as systems modeling and translational biology. We are intimately involved in the design and selection of therapeutic molecules, and understanding how these molecules interact with biological systems at different scales.

We are enthusiastic about the prospects of physical modeling to help guide pharmaceutical drug discovery, and have been very interested in the progress of SAMPL challenges over the years. Thus, we are delighted to help support your proposed, "Advancing predictive physical modeling through focused development of model systems to drive new modeling innovations." While free energy calculations recently have shown some real promise for guiding pharmaceutical design, challenges like this are vital to help them continue to make progress.

In support of SAMPL and blind prediction challenges, my group would be willing to host a student to help collect experimental data for compounds available from commercial vendors for SAMPL physical property challenges. GSK has access to equipment necessary for measuring physical properties in a high throughput manner that is not typically available to academic laboratories, such as the Freeslate platform to generate pKa, logD, and logS values and automated membrane permeability assays.

We have seen the model of hosting an academic student to conduct SAMPL physical property measurements work previously at Genentech for measurement of water-cyclohexane log D values for the SAMPL5 challenge. We believe we will be able to use a similar approach here as well to collect the data needed for new SAMPL challenges.

Sincerely,

Eric S. Manas
VP and head, Computational and Modeling Sciences
GlaxoSmithKline