Dear Dr. Mobley and Dr. Chodera,

We are very excited to be involved in your proposal, “Advancing predictive physical modeling through focused development of model systems to drive new modeling innovations.” As you may be aware, we believe physical modeling is poised to have a real impact on the pharmaceutical drug discovery process, but we also believe there are key challenges remaining to be resolved before it can have the impact it might.

This letter is to confirm that we would like to be involved with facilitating the collection of experimental data to facilitate new SAMPL physical property prediction challenges to drive the improvement of these methods. We expect our involvement will at least involve providing access to equipment you need to measure physical properties (such as our Sirius T3 for measurement of pKa and log D values, our XYZ for measuring pKa’s, our ABC for measuring partition coefficients and log D values, or our DEFG for measuring relative solubilities/membrane permeabilities) for SAMPL challenges along with help on how to perform these measurements effectively. It is also possible we will be able to facilitate an internship to provide someone who could actually perform the measurements. Otherwise, you would need to provide personnel who would come here and work with us to perform the measurements.

We have seen this model work previously at Genentech for measurement of water-cyclohexane log D values for the SAMPL5 challenge, and we believe a similar model will work well here as well, so we are confident we will be able to support your proposal and future SAMPL challenges in this way.

Sincerely,