Dear Dr. Mobley and Dr. Chodera,

Genentech is, a large pharmaceutical company with interests in a wide range of disease areas. Person A works in our computational chemistry group, and person B specializes in measuring ABC.

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 the field still needs to resolve to achieve this. The work you propose is absolutely vital to facilitate the necessary advancements.

This letter is to confirm that we are willing to host a student who will help collect experimental data to enable new SAMPL physical property prediction challenges to drive the improvement of these methods. We can provide access to equipment necessary for measuring physical properties that is not typically available to academic laboratories, such as the Sirius T3 (for measurement of pKa, logD, and logS), high-throughput automated shake-flask measurements of logD and logP, and automated membrane permeability assays for compounds available from commercial vendors. We have multiple mechanisms available through which these measurements can be performed. In addition to sending students from your laboratories to visit our group to perform measurements, we also have an internship program that provides a stipend for focused measurement projects like these.

As you are of course aware, we were already able to do something very similar to this for the SAMPL5 challenge, where – via a summer internship program – we hosted Bas Rustenberg, a student from John Chodera’s lab, who measured water-cyclohexane log D values which formed half of the SAMPL5 challenge. We believe we will be able to similarly host academic researchers to help generate data for future SAMPL challenges.

Sincerely,