Genentech
A Member of the Roche Group

May 9, 2017

Dear Dr. Mobley and Dr. Chodera,

As you know, Genentech is a large pharmaceutical and bioechnology company with interests in a wide range of disease areas. Daniel Ortwine is a Principal Scientist in the Computational Drug Discovery group. He is involved in hands-on molecular modeling and statistical calculations in support of drug discovery projects. Baiwei Lin is a Scientist in the Analytical group, specializing in measuring physical properties such as distribution coefficients, solubility, and ionization potentials of small molecule drug candidates

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 are not typically available to academic laboratories. One example would be a Sirius T3 instrument for measurement of pKa, logD, and logS. We also can provide 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 students to undertake 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,

Daniel Ortwine
Principal Scientist
Computational Drug Discovery

Baiwei Lin
Scientist
Analytical Chemistry