As per my last committee meeting, I have prepared a progress report detailing my work in the past 9 months. I have attached the draft of a mansuscript describing the implementation of RosettaHTS, a method which uses a machine learning model to integrate Structure and Ligand based virtual screening methods. Because optimization of the model’s parameters is still underway, the benchmark described in the current draft is a small subset of the larger benchmark I plan to run. The complete benchmark will be run at the end of

Following the completion of the benchmarking work described above, a paper describing the RosettaHTS method will be published. This paper will describe the implementation of RosettaHTS as well as the results of the DUD- E and DEKOIS benchmarks. The paper will be targeted for publication in PLoS Computational Biology or Journal of Medicinal Chemistry.