Center for High Throughput Structure-Based Drug Discovery (SBU-DD)

1. Abstract

This funding application is for the SBU-DD (Drug-Discovery) Center, which aims to integrate innovative structural biology techniques with computational biology and medicinal chemistry. The center's goal is to develop drug-lead compounds at a significantly faster rate than is currently possible. Thanks to the recent SBU-BNL seed award, we have established LI-XRA at SBU/BNL, a high-throughput workflow that allows for the determination of the structure of hundreds of proteins bound to target proteins. The purpose of this proposal is to take the next critical steps in the workflow towards drug development and to apply for center funding from NIH/DOE. Specifically, SBU-DD will analyze and interpret extensive amounts of data and predict the most promising combinations of fragments for drug development. Moreover, SBU-DD will offer the necessary infrastructure to test the binding of fragments identified in LI-XRA. A similar integrated setup, known as XChem, has already been established in the UK and has played a vital role in developing protease inhibitors SARS-nCOV2. LI-XRA is the only facility of its kind in the US and would be an invaluable resource for researchers in both academia and industry. SBU-DD represents the next logical progression from LI-XRA and capitalizes on SBU's expertise in computational biology. The collaboration between Stony Brook University and Brookhaven National Laboratories would synergize the advanced technologies in X-ray physics available at BNL with the computational and chemical expertise of scientists at SBU, expediting the development of new drugs.