

Dr. George Nicola Receives American Chemical Society Award

Dr. George Nicola, a Project Scientist in Dr. Michael Gilson's laboratory, won an American Chemical Society (ACS) award for a competition entry to the Teach-Discover-Treat initiative. This competition seeks to provide high quality computational chemistry tutorials that impact education and drug discovery for neglected diseases.

Dr. Nicola and colleagues designed a tutorial to help students better understand the use of computer tools in discovering drugs for neglected diseases. In the tutorial, public domain databases were discussed in the context of determining potential targets and discovering new drugs for malaria. The tutorial showcased the use of specific computational tools to perform virtual screening of a catalogue of commercial compounds by applying a predictive model, and prioritizing compounds based on structural similarity to known actives. By completing the tutorial, students will become familiar with using the database servers ChEMBL, ZINC, BindingDB, and Reactome, as well as the pipeline software suite KNIME.



Dr. Nicola was awarded a travel grant to present a seminar on this tutorial at the national meeting of the ACS in New Orleans in April, 2013. See the following for more information on the TDT initiative: <http://www.teach-discover-treat.org/>, for the ACS: www.acs.org, for the Gilson lab: <http://gilson.ucsd.edu>, and for BindingDB: <http://www.bindingdb.org>.