Teach-Discover-Treat
the power of collaborative efforts

Emilio Xavier Esposito,[1] Yufeng Jane Tseng,[2] Rommie Amaro,[3] Wendy Cornell,[4] W. Patrick Walters,[5] and Johanna Jansen[6]

1. exeResearch LLC, 2. Department of Computer Science and Information Engineering at the National Taiwan University, 3. Department of Chemistry & Biochemistry at the University of California, San Diego, 4. Merck & Co., Inc., 5. Vertex Pharmaceuticals, Inc., 6. Novartis Institutes for BioMedical Research.

About TDT

Teach-Discover-Treat (TDT) is an initiative of the Computers in Chemistry (COMP) Division of the ACS to provide high quality computational chemistry tutorials that impact **education** and **drug discovery** for neglected diseases. To date, the initiative has produced a set of 22 tutorials submitted as part of two competitions. Three award winners are being recognized at the TDT symposium "Results from the 2014 Challenge" during the 2014 ACS fall meeting in San Francisco. Due in part to the Malaria challenge of the first TDT competition, earnest drug discovery activities have been initiated. The extension of the computational challenge into wet-lab discovery activities makes the TDT initiative unique and is "Chemistry for Life" in action!

The 2014 TDT Competition

The second TDT competition resulted in 16 high quality computational chemistry tutorials submitted across the four challenges. The judging panel selected the top three winners based on the published criteria for scientific content, presentation and clarity, educational benefit, and reproducibility. The steering committee decided to also recognize the submissions with the best predictive power in the challenges that included held-out test sets. The list of compounds selected by the winners of these prediction challenges will be ordered for screening by our partners. The tutorials are publicly available at www.TDTproject.org for education and further drug discovery activities.

First Place – OpenEye Award
Anti–Malaria Hit Finding Using Classifier–Fusion Boosted Predictive Models
(Challenge 1)
Sereina Riniker & Gregory A Landrum
Novartis Institutes for BioMedical Research

Second Place – KNIME Award
myChEMBL Virtual Machine: Integration of Open Cheminformatics Tools and Open Bioactivity Data (Challenge 4)
Rodrigo Ochoa, Mark Davies, George Papadatos, Francis Atkinson, & John P Overington
EMBL–EBI

Third Place – Cresset Award
Molecular Docking with DOCK 3.7
(Challenge 3)
Ryan G Coleman & Joel Karpiak
Dept of Pharmaceutical Chemistry, UCSF

Challenge 1 – Best Predictive Power
CCL–Malaria
Santiago D Villalba[1] & Floriane Montanari[2]
[1]Inst of Molecular Pathology, Vienna
[2]Dept of Pharmaceutical Chemistry, Uni of Vienna

Challenge 3 – Best Predictive Power
Molecular Docking with DOCK 3.7
Ryan G Coleman & Joel Karpiak
Dept of Pharmaceutical Chemistry, UCSF

Share Your Drug Discovery Skills!
TDT is developing a *third* competition and we want to hear your comments regarding the first two. Join us at the the TDT Awards Symposium (Tuesday, August 12 @ 1:30pm; Room 2014 Moscone Center - West Building), submit comments via our website (www.TDTproject.com/connect), or engage us through social media (@TeachDiscoTreat).
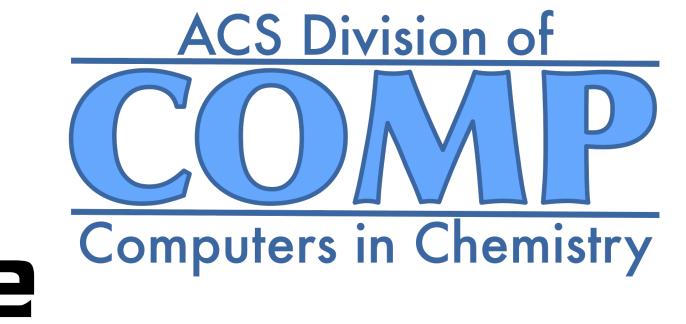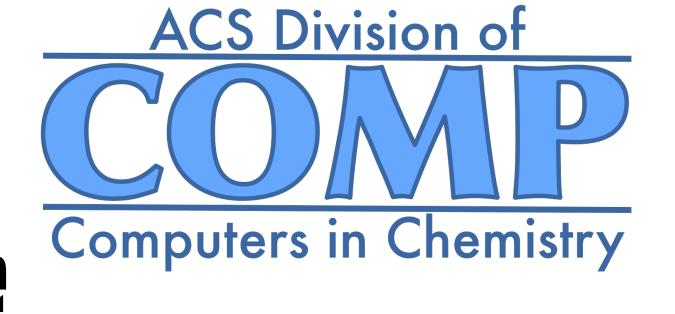

TDT is supported in part by: GILEAD · OpenEye Scientific Software · KNIME · cresset · CHEMICAL COMPUTING GROUP · ACS Chemistry for Life® · eMolecules · MERCK Be well · Simulations Plus, Inc. integrating science and software · Enamine · ChemBridge · ACS Division of COMP Computers in Chemistry · NOVARTIS · ChemDiv The chemistry of cures · VERTEX · exe Research · Partners of TDT: UNIVERSITY of WASHINGTON · St. Jude Children's Research Hospital · CERID Center for Emerging and Re-emerging Infectious Diseases · SGC