

Computational & Life Sciences/ Center for Comprehensive Informatics Spring 2009 Seminar Series

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3:00pm

Dr. Brian Shoichet

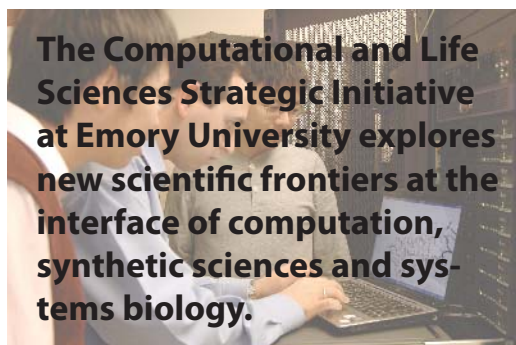
Pharmaceutical Chemistry, University of California, San Francisco

Location: White Hall, Room 112

“What is the information content of a molecule?”

Abstract:

Whereas protein function is widely acknowledged to follow from form, actually predicting ligand recognition from structure remains challenging. Conversely, there is a long history in pharmacology and medicinal chemistry of relating ligands to understand the properties of their receptors, even though ligand structures encode much less information than do those of proteins. More confounding still, related drugs and ligands can bind to targets that appear biologically unrelated. To quantify this, we compared drug targets based on the chemical similarity of their sets of ligands. The similarity score between each ligand set was calculated, using a BLAST-based statistical model to rank significance. Expressed as a minimum spanning tree, the sets may be mapped together. Although these maps are connected solely by chemical similarity, biologically sensible clusters emerge. Links among unexpected targets also emerged, several of which were experimentally testable. Returning to protein structure, we have also attempted to predict new ligands for some of the same targets by docking to their structures. Experimental testing of ligands proposed based on complementarity to protein structure, and based on the ligand polypharmacology hypothesis, will be discussed.



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Computational Science
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CONTACT CCI AT:

1521 DICKEY DR., SUITE 500
ATLANTA, GA 30322
PHONE: (404)727-6202
HTTP://CCI.EMORY.EDU/
EMAIL: PDUNHAM@EMORY.EDU

CONTACT CLS AT:

400 DOWMAN DRIVE, SUITE 421E
ATLANTA, GA 30322
PHONE: (404)727-5363
HTTP://CLS.EMORY.EDU/
EMAIL: CLS@EMORY.EDU



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