Seminar Invitation: Applications of Kinase Virtual Screening for Drug Discovery

Eric Martin, Novartis Institutes for BioMedical Research (NBIR)

Midday-1pm, 20th August 2012 – Room 301-407, The University of Auckland

Learn how virtual screening within the kinase protein family can now match the accuracy of experimental High-Throughput Screening from one of computational chemistry's leading scientists.

This event is being held as part of the lead up to MM2012, Australasia's conference on molecular modelling.

Abstract
Virtual screening with accuracy comparable to experimental High-Throughput Screening (HTS) has been a goal of computational chemists for at least 25 years. It is finally possible for the kinase protein family. Three novel kinase virtual screening methods achieve unprecedented speed and accuracy by including massive amounts of IC50 and structural data from previous kinase targets into models for each new kinase: the 2D "Profile-QSAR" meta-QSAR, the Kinase-Kernel chemogenomic model, and the 3D Surrogate AutoShim docking method. Between the methods, 2 billion activity predictions have been made for 4 million internal and commercial compounds across 500+ kinases, so initial kinase virtual screening is now a table lookup. The methods have been applied to over 4 dozen active Novartis projects, at all stages of discovery, with external R2=0.35-0.7 and enrichments of 20x-60x. AutoShim and Profile-QSAR have also been extended to Serine and Cystine Proteases.

The methodologies will be described and examples will be presented from all stages along the drug discovery pipeline, from finding tool compounds for early target validation to finding backup chemistries for successful projects going into the clinic.

About the speaker
Eric Martin received a Ph.D. in physical organic chemistry from Yale University. He has worked in computational chemistry, analytical instrument development, environmental-fate modeling, drug design and herbicide design for over 25 years. He is best known for starting the field of combinatorial library design in 1993. His recent research focuses on iterative kinase virtual screening by docking with target-customized scoring functions, and data-driven modeling tmethods that treat individual kinase drug targets as members of a family, rather than as idiosyncratic protein targets. He was recently awarded the lifetime title of Novartis Leading Scientist.

Time
20th August 2012
Midday-1pm

Location
Room 407, Building 301
Science Centre
Symonds Street, Auckland

Map
http://goo.gl/maps/HfqH

RSVP
Please send an email to Tim McNamara, via t.mcnamara@auckland.ac.nz.

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