



HARVARD MEDICAL SCHOOL
CENTER FOR MOLECULAR AND CELLULAR DYNAMICS
SBGRID NSF RESEARCH COORDINATION NETWORK



SPECIAL SEMINAR

Docking and Beyond: Combining Structural Chemistry with
Docking and MM-GBSA Scoring to Optimize Src and Abl Kinase
Inhibitors

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Abstract: We have recently focused on applying structure-based drug design tools to optimize dual small molecule inhibitors of Src and Abl kinases as well as inhibitors of Gleevec-resistant mutants form of Abl kinase. This talk will focus on our efforts to combine X-ray structural data with computational docking tools such as Glide to design potent inhibitors of these kinases. Predicting the potency of such inhibitors from a docked structure remains a challenging problem, however we will illustrate how physics based scoring methods including implicit solvent (MM-GBSA) can provide additional insight during the optimization process, notably in closely related series of compounds.

Tuesday, February 5, 2008. 12:00-1PM p.m.

Tosteson Medical Education Center, 260 Longwood Ave
Rm TMEC 250

Host: Piotr Sliz