UNC-Chapel Hill and SimBioSys presents:

A Virtual High-Throughput Screening and Docking Workshop

UNC-Chapel Hill invites you to a workshop during which scientists will provide overviews of their recent research and SimBioSys Inc. will provide an overview of their drug discovery software tools. SimBioSys is a rational drug discovery and computer aided drug design software company, focused on providing leading edge software for high throughput ligand docking and de novo ligand design.

WORKSHOP

Where: UNC Chapel Hill, Room 136, Turner-Tate-Kuralt (School of Social Work), 325 Pittsboro Street, Chapel Hill, NC 27599-3550
Date: Tuesday, Nov. 27, 2007
Time: 9:00 am - 12:00 pm

Agenda

9:15am In silico design of allosteric modulators for the NMDA receptor
Tony Vandongen (Duke University)

9:30am Molecular dynamics approaches for structure-based drug screening
Nikolay Dokholyan (UNC Chapel Hill)

10:10am Cheminformatics Approaches to Virtual Screening
Alex Tropsha (UNC Chapel Hill)

10:50am Matching high-performing flexible docking software to high-performing hardware. Extremely fast virtual screening without loss of accuracy using eHITS.
Zsolt Zsoldos (SimBioSys)

12:00pm Conclusions and break-up

1:00-3:00pm Hands-on training session on SimBioSys software modules

To confirm your registration for this event please fill out the registration form at:
http://www.simbiosys.ca/rtp-seminar/ .
Please register by November 26 to ensure a seat at this event!