

The National Institute of Statistical Sciences and SimBioSys presents:

A Virtual High-Throughput Screening and Docking Seminar

The National Institute of Statistical Sciences invites you to a seminar 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: NISS, 19 T.W. Alexander Drive, Research Triangle Park, NC 27709-4006

Date: Wednesday, Nov. 28, 2007

Time: 9:00 am - 2:00 pm (Lunch will be provided)

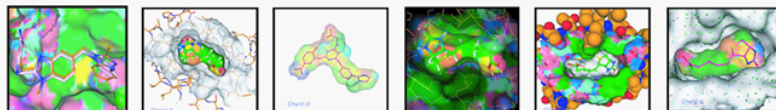
Agenda:

- 9:15am** An overview of structure-based *in silico* biomolecular interaction profiling strategies within the ToxCast™ computational toxicology framework.
Rocky Goldsmith (Environmental Protection Agency)
- 9:45am** PharmID: 3D pharmacophore identification
Stan Young (National Institute of Statistical Sciences/NCSU)
- 10:15am** Coffee
- 10:30am** Reclaiming the potential of virtual high throughput screening using docking
Darryl Reid (SimBioSys)
- 11:00am** 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** Catered Lunch
- 1:00pm** Roundtable discussion – present challenges in virtual screening and QSAR analysis
- 2:00pm** Conclusions and Goodbyes

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!



Your Software Partner for Rational Drug Design

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