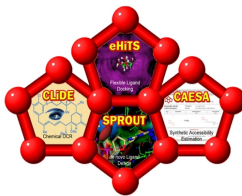


SimBioSys, Inc.



SickKids and SimBioSys  
presents:

SickKids®

## Docking and Scoring seminar followed by a training session

### "Easy and Accurate Docking with eHiTS"

The Centre for Computational Biology (CCB) would like to invite you to two events: a seminar and a half day workshop during which the new homology modeling and drug design capabilities at the CCB will be introduced and the company SymBioSys will demonstrate the use of eHiTS for in-silico screening of potential binders.

#### Event#1: Seminar

**Where:** SickKids, Room S429 (Service Level, Gerrard Wing)

**Date:** Tues., March 28, 2006

**Time:** 1:00 p.m. - 2:30 p.m.

**Topics:** 1) CCB new capabilities  
2) docking, scoring, screening algorithm in eHits and results overview

#### Event#2: eHiTS hands-on training session (MAX. 15 participants)

**Where:** SickKids, Room TBD

**Registration:** email [ema.rosa@sickkids.ca](mailto:ema.rosa@sickkids.ca) by **March 30/06**

**Date:** Mon., April 3, 2006

**Time:** 1:00 p.m. - 4:00 p.m.

**Topics:** how to prepare your job for the docking (receptor, ligand, active site etc.)  
how to run eHiTS  
how to analyse results of a docking run  
how to use ehits to screen a database of molecules  
how to run your screening jobs on a cluster / distributed environment

To confirm your registration for the seminar please send an email, by **March 24, 2006** to Ema Rosa, CCB, at:

**About SimBioSys:** SimBioSys, specializing in drug design and drug discovery software, provides leading edge software for de novo ligand design and high throughput ligand docking. The developers of the de novo design program, SPROUT, now offer the next generation of docking software, eHiTS. SimBioSys has very strong focus on scientific research and development in areas that meet the needs of computational chemists. SimBioSys is actively working to improve these programs to lead the way in the area of drug discovery software. This focus on research means that a SimBioSys user can expect to be kept up to date with the most recent developments in computational drug discovery.

**About eHiTS:** eHiTS is the only truly exhaustive docking algorithm available today. eHiTS takes a unique systematic approach to the docking problem by dividing ligands into rigid fragments and flexible connecting chains then docking each rigid fragment everywhere within the receptor site, in an exhaustive manner. This approach eliminates the "seed" bias present in incremental construction algorithms. In addition, since many rigid fragments are repeated in different molecules, this approach allows for the reuse of information on subsequent molecules, thus reducing docking times for large screens.

The exhaustive nature of eHiTS makes it one of the most accurate flexible ligand docking programs. In validation studies, eHiTS is able to reproduce the binding pose for approximately 90% of the co-crystallized ligands tested (RMSD less than 2Å). For more detailed information please see the eHiTS whitepaper at:

[http://www.simbiosys.ca/solutions/white\\_papers/eHiTS\\_Whitepaper.pdf](http://www.simbiosys.ca/solutions/white_papers/eHiTS_Whitepaper.pdf)

The issue of protonation state is very important to the docking problem. Ligands and receptors with different protonation states can have dramatically different binding positions. eHiTS takes a unique approach to the protonation problem by systematically evaluating all possible protonation states for the receptor and ligands, automatically, for every receptor-ligand pair. Then during the docking algorithm each state is evaluated and scored. The result is the only docking program that evaluates all possible protonation states for the receptor and ligand in a single run.

eHiTS gives users the power to train our scoring functions. The training utility allows users to use complexes from a particular family to train the scoring functions to improve docking accuracy or to use sets of active and decoy ligands to improve ranking results.

**Key points of eHiTS:**

- ◆ a truly exhaustive and systematic docking algorithm
- ◆ one of the most accurate flexible ligand docking programs
- ◆ the only docking program that automatically evaluates all the possible protonation states of every receptor-ligand pair
- ◆ comes with a training utility that allows the user to train the scoring function to improve accuracy and enrichment results

Try eHiTS for yourself!  
Fill out a "request a free demo" form at:

[www.simbiosys.ca](http://www.simbiosys.ca)

SickKids & University of Toronto have a site license for eHiTS!