

*Your Software Partner for Rational Drug Design*

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## Lunch Seminar: "Fast, Easy, Accurate Docking using eHiTS and the Sun Grid Compute Utility"

SimBioSys, your software partner for rational drug design, and Sun Microsystems would like to invite you to a lunch seminar to introduce you to a new, fast, easy and economical way to perform docking. The Sun Grid Compute Utility provides extensive resources to run the most accurate and easy to use docking program, eHiTS.

**Where:** Sun Executive Briefing Center (EBC),  
15 Network Circle, Menlo Park, CA  
[www.sun.com/ebc/menlopark/](http://www.sun.com/ebc/menlopark/)

**Date:** January, 17th, 2007

**Time:** 11:00am - 2:00pm



<http://www.network.com>

### Agenda:

11:00 - 11:45am	Introduction to eHiTS
11:45 - 12:15pm	"Experiences with virtual screening", Dr. Osman Guner, Turquoise Consulting
12:15 - 12:30pm	Break
12:30 - 1:00pm	Lunch / Introduction to Sun Grid Compute Utility, Ari Shamash, Director, Sun Grid Engineering
1:00 - 1:30pm	Demonstration of eHiTS on the Sun Grid
1:30 - 2:00pm	Q&A

**Attendees of this event are eligible to receive complimentary CPU hours on the Sun Grid Compute Utility!**

Questions can be directed to Darryl Reid: [darryl@simbiosys.ca](mailto:darryl@simbiosys.ca)

To confirm your registration for this meeting please fill out the registration from at:

[www.simbiosys.ca/ehits-bayarea](http://www.simbiosys.ca/ehits-bayarea)

**Please register as soon as possible! Seating for this event is limited.**

### 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 our 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 Sun Grid Compute Utility

Sun is changing the very nature of computing by delivering access to enterprise compute power over the Internet with its Sun Grid Compute Utility. Sun Grid provides easy and affordable access to an enormous computing resource for the predictable and all-inclusive price of \$1/CPU-hr.

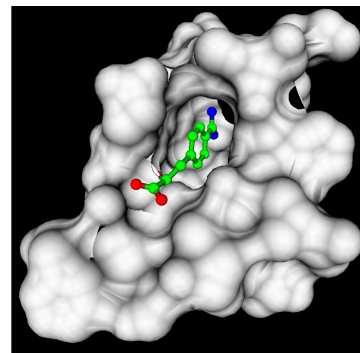
The Sun Grid application catalog is a recently introduced solution that allows independent software vendors (ISVs) and developers the ability to host their applications on the Sun Grid Compute Utility and deliver them as service to end users. Expected to be included in the next Sun Grid release, the Sun Grid application catalog is venue where ISV Applications and Open Source Applications can be easily accessed. Sun Grid Customers are just a click away from using their application in an on-demand environment!

- \* **Use Sun as your one-stop application shop**
- \* **Easy Access to the applications you use in an on-demand environment**
- \* **Plug Into Sun's Infrastructure, Use the applications on an as-needed basis**

## About eHiTS

eHiTS is the only truly exhaustive docking algorithm available today. eHiTS takes a unique fragment based and 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.

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 of co-crystallized ligands on the average of 90% of the time (RMSD less than 2Å). For more detailed information can be found at the SimBioSys website ([www.simbiosys.ca](http://www.simbiosys.ca))



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.

## Running eHiTS on the Sun Grid Computing Utility

SimBioSys Inc, a leading edge chemistry software provider that enables computational chemists to find and optimize lead drug candidates faster and more easily with eHiTS is excited about the new model. "We are excited to offer our software on the Sun Grid Compute Utility," said Zsolt Zsoldos, SimBioSys' President and Chief Scientific Officer. "Our testing of eHiTS on the Sun Grid has shown impressive scalability up to at least 100 CPUs. As a result, problems that used to run for weeks can now be solved in days which allows the drug discovery pipeline to be filled faster and with more leads."

**Attendees of this meeting are eligible to receive complimentary CPU hours on the SGCU. Please register at:**

[www.simbiosys.ca/ehits-bayarea](http://www.simbiosys.ca/ehits-bayarea)

**Register today, seating is limited!**