SimBioSys eHiTS™ on the Sun™ Grid Compute Utility

Speeding Discovery On Demand

In today's competitive pharmaceutical marketplace, making a scientific breakthrough and getting to market first can be vital to maximizing revenue potential. Identifying quality lead compounds is a vital, but time-consuming task along the path of drug discovery. Constraints on compute power can often impede progress. The innovative Electronic High Throughput Screening (eHiTS™) software from SimBioSys running on the powerful Sun™ Grid Compute Utility gives organizations a new way to accomplish fast, accurate docking of ligands to target receptors by using a secure, affordable, and scalable on demand compute utility resource.

Highlights

- Fill the drug discovery pipeline faster using eHiTS™ software to automate searches of compound libraries and identify lead candidates more rapidly.
- Gain a competitive edge with easy-to-access, affordable compute power on demand.
- Reduce time to solve molecular docking challenges with the scalable power of the accurate eHiTS software running on the Sun™ Grid Compute Utility.
- Get more screens done in parallel by tapping into immense compute capacity.
- Free up capital budget dollars by leveraging the Sun Grid Compute Utility to transition expenditures for compute resources from asset to expense.
- Trust the comprehensive security of the Sun Grid Compute Utility, built with physical, architectural, and operational safeguards.

Accurate, fast, easy screening

For successful discovery, molecular docking and screening tools must be able to account for all conformation and protonation changes that occur during the binding process, as well as accurately score ligand and receptor interactions. SimBioSys eHiTS software offers new approaches to both objectives [1,2]. An exhaustive and systematic algorithm is used in eHiTS to drive screenings with no random, stochastic, or evolutionary element. Plus, eHiTS full automation removes the need for any manual pre-modeling of input receptors or ligands. Unlike other methods that use sampling and can only find an arbitrary subset of solutions, eHiTS provides easy-to-use, comprehensive search space coverage.

The eHiTS system accurately generates all major docking modes and protonation states for each candidate structure within the chemical and steric constraints of the target cavity. A highly developed, statistically-based empirical scoring function is used to judge the ligand and receptor interactions to accurately determine the best binding pose for each candidate structure. The amazing pose prediction capability of the eHiTS software helps users with efforts to gain a clearer understanding of systems of interest and quickly optimize lead drug candidates.

Simple, affordable access to power

Pressure to solve research problems faster can cause strain for scientific teams. Frustrations increase as outside factors, such as limits on compute resources add delays. The Sun Grid Compute Utility gives enterprises the ability to quickly augment in-house processing by providing affordable, on demand access to compute power — with no long term contracts, no hidden fees, and no reservations required. Using a secure network connection, organizations can easily harness hundreds of CPUs within the Sun Grid Compute Utility at the predictable price of U.S. $1/CPU-hour.

The Sun Grid Compute Utility solution is built using Sun and industry best practices and includes comprehensive security for user jobs. Enabled by Sun Fire™ x64 servers, the Solaris™ 10 Operating System, Solaris Containers technology, and Sun N1™ Grid Engine software, the Sun Grid Compute Utility delivers secure, high-performance execution of 32-bit and 64-bit batch workloads. In some cases, such as eHiTS, the application software is pre-loaded for improved access [3]. By taking advantage of the ability to run eHiTS on the Sun Grid Compute Utility, scientists can leverage additional compute capacity to speed time to results for molecular docking, and accelerate the pace of innovation and discovery.

Discover faster

In the race to discover new drug therapies, computational chemists need access to scalable compute capacity and smart software to help produce results faster. The SimBioSys eHiTS software running on the Sun Grid Compute Utility leverages parallel software execution techniques and scalable hardware performance to significantly speed progress.

For example, testing of eHiTS on the Sun Grid Compute Utility reveals that a search which employs one CPU and takes 50 hours to complete can be executed in less than 30 minutes on 100 CPUs. [4] Since the Sun Grid Compute Utility charges by the CPU-hour, there is no premium for accessing large numbers of CPUs and no increase in job cost. Using one CPU for 50 hours, or 100 CPUs for 30 minutes — the price is the same. Combining the scalability of eHiTS with the enormous capacity and innovative pricing model of the Sun Grid Compute Utility enables organizations to cost effectively leverage extreme compute power to solve docking queries in less time.

Accomplish more research

Multiple groups, each with high priority projects, can cause contention over a finite set of computational resources. The Sun Grid Compute Utility provides affordable access to secure compute capacity from any U.S. network connection, enabling enterprises to easily augment in-house operations as needed. Organizations can leverage the Sun Grid Compute Utility to run specific jobs faster, improve access to compute power, and free up internal systems for other projects.

In addition, companies can supplement compute capacity during periods of peak workflow and harness greater power to explore larger computational problems. By eliminating compute power constraints as a barrier to success, the Sun Grid Compute Utility helps organizations open the door to making critical scientific breakthroughs sooner.

Maximize return on IT investments

Aligning IT consumption with demand is a challenging task for organizations. Maintaining too little compute capacity leads to missed opportunities and lost revenue. Deploying too many systems leaves expensive resources to sit idle, wasting money. Access to the Sun Grid Compute Utility enables processing capacity to expand and contract with changing enterprise needs. With more power readily available through the utility, organizations can avoid purchasing excess capacity and mitigate issues related to running in-house assets at high utilization rates. Plus, system acquisition, maintenance, and administration costs are shifted to Sun. By incorporating the Sun Grid Compute Utility into an enterprise computing strategy, businesses can increase the return on IT investments, reduce risk, and ultimately save money.

Meet security demands

The process of drug discovery is an extraordinarily high-stakes venture, making the security of compute systems paramount to keeping a competitive edge. The Sun Grid Compute Utility is fortified with layered defenses around critical information assets.

Learn More
For more information about eHiTS on the Sun Grid Compute Utility visit Network.com, simbiosys.ca/ehits, or talk to your local Sun representative.

These defenses include physically secure sites strengthened by limited access to pre-cleared personnel, operating system and network security isolation for user jobs, state-of-the-art secure network configurations, job submission anonymity, security-minded operational policies, and on-going proactive monitoring. In fact, Solaris Containers technology provides private execution environments for each Sun Grid Compute Utility user, ensuring complete isolation of all processes and security of vital data sets. The security of the Sun Grid Compute Utility extends to every aspect of the compute environment, providing organizations with a trusted resource for processing valuable data.

Move forward with SimBioSys and Sun

SimBioSys Inc. develops innovative, leading edge software that enables users to find and optimize lead drug candidates faster and with greater ease and accuracy. For over 20 years, Sun has continued to create innovative high performance computing solutions, like the Sun Grid Compute Utility, that help organizations run larger numbers of compute tasks faster. Together, SimBioSys and Sun offer a powerful solution for simplifying and accelerating molecular docking research projects, enabling organizations to speed discovery and move to market faster.

1. Zsoldos et al: "eHiTS: an innovative approach to the docking and scoring function problems", Current Protein and Peptide Science, 2006, vol 7, pages: 421-435, Number 5, October 2006.
2. Zsoldos et al.: "eHiTS: A new fast, exhaustive flexible ligand docking system", Journal of Molecular Graphics and Modeling; In Press, Available online 17 June 2006.
3. SimBioSys eHiTS software license fees may apply.
4. An Analysis of SimBioSys eHiTS Computational Chemistry Application Running on Sun Grid, simbiosys.ca/solutions/white_papers/ehits_on_sun_scalability.pdf

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