

SimBioSys, Inc.  
Toronto, ON, Canada

Dear Colleague,

The Fall '08 / Winter '09 issues of the SimBioSys Newsletter is now available on-line as a [webpage](#) and as a [PDF file](#).

A message from Dr. Zsolt Zsoldos, CSO:

As the year-end approaches we look back and summarize what was accomplished and thank our users, partners and collaborators for the support and feedback during the past 12 months.

This year we have delivered on some major goals we have set for ourselves. We have improved our products and released revolutionary capabilities to the marketplace with our eHiTS Lightning software working on the Cell platform. We have increased our market presence with new customers, have expanded our team with new members and have continued to contribute to science by developing enhanced algorithms, approaches and software products to support scientists around the world. We are indeed serving the world now with distributors in Asia and Europe.



Our latest version of eHiTS is already in the hands of beta testers and we are excited by the results we are seeing....more detail below in the Newsletter. We will be gathering data and feedback over the holidays for an early February release. We believe that eHiTS and eHiTS Lightning now offers the industry standard performance in both throughput, enrichment and pose accuracy and are open to comparisons if anyone would care to approach us. The products will release as eHiTS 2009 and eHiTS Lightning 2009.

As a result of two round table meetings in November we have received the guidance and feedback from though-leaders in the industry regarding our ARChem retrosynthetic analysis software platform and our new concept for de-novo design. Both plans are being actively assembled for activity following the eHiTS release. 2009 will be no less tiring, no less stimulating and no less scientifically motivating than this past year. We have much to do and are excited by what we will deliver next year. Watch this space...we'll be asking for your input. Have a Happy Holiday Season and we'll connect in the New Year.

ZZ

### **Newsletter Content**

As is usual we now put the majority of our detailed documentation and reports online for you to access. Click the links to access some of our latest materials.

1) **Dan's tips and tricks:**

Danni Harris talks about the "[Use of eHiTS CrossDocking Approaches to Survey the Ligand/Target Landscape](#)"

- 2) Our **new product release** announcements:  
We announce the release of our latest implementation of eHiTS Lightning. We have made some breakthrough improvements in the algorithms leading to dramatic improvements in pose accuracy, improved enrichment and throughput. For more detail see :
- a) [eHiTS Lightning changes the game of Virtual Screening and Docking](#)
  - b) [A Holiday Gift for You](#)
  - c) [Is fast, high quality docking possible?](#)
  - d) or simply visit our [what's new in eHiTS](#) page



- 3) **Science corner:**
- a) A discussion regarding "[Synthetic Complexity and Accessibility: Choosing the Correct Tool For the Task of De Novo Triage](#)"
  - b) We recently held a round table with some of our customers to reach collective agreement on [Designing a Product Roadmap for ARChem](#). Click the link for details.



- 4) **Technology corner:** with lots of interesting topics like:  
[IBM's white paper on the Cell technology and Molecular Modeling](#)  
[Fastest supercomputer built on the Cell/BE](#)
- 5) The **events** that we will be attending in 2009 are listed on our [events page](#). Please let us know if you will be going to any of these events and we would be glad to meet with you.

- 6) **News:**  
[A New collaboration with Alfa Aesar](#)  
[SimBioSys use the Beilstein Reaction Database as part of the ARChem Retrosynthetic Analysis Platform](#)  
[SimBioSys' Announces Distribution Network in Japan](#)  
[Orr Ravitz joins the SimBioSys Team](#)

- 7) **Publications:**  
We have a number of [publications using eHiTS](#) online and wish to send a [thanks to our user community!](#)  
A new [Software Review about: eHiTS and LASSO](#)  
A [Bio-IT World article about eHiTS Lightning](#)  
[Chemical and Engineering News Acknowledges SimBioSys'ARChem in Digital Briefs](#)

- 8) We have implemented [a Change in Policy for eHiTS for Academia](#) that can be summarized as follows: in early 2009 we will release eHiTS 2009 and will use this release as a transition point from free software for academia to support-contract based software licenses. In order to cover our increasing costs of supporting our users we will charge service contract fees per site of deployment. This fee includes support and maintenance during the year.

Best wishes for the Holidays, and many thanks for all of your support and feedback during the past 12 months. SimBioSys as a company owes our success to you, our users, as well as to our own passion for improved science. We are blessed by your support and look forward to working with you in 2009 !

The SimBioSys Team