

SimBioSys, Inc.  
Toronto, ON, Canada

## Dear Colleague,

The Holiday Season is here again, and as we leave our work places, and head for various family and friends gatherings – we can pause a little and reflect on our past year accomplishments. As I sat down to list our latest achievements, I realized that many of them are already documented in our blog which we use to keep in touch with many of you. You can find there the release of eHiTS 2009.0, a state of the art docking and screening application that has been the first to be ported to IBM's Cell B/E processor. Just recently we updated our tools with the release of eHiTS 2009.1 – an important upgrade version, which fixes some instability issues, improves the accuracy of docking, and introduces several new features. With this version, we are at the top of the performance on the Astex – GOLD validation set as you can read below. We also confirmed that eHiTS 2009 is a great tool for blind docking – see it in the Science section. This year we have also significantly improved our retrosynthetic analysis tool: ARChem – Route Designer, with a dramatic increase in the available reaction data sources via our collaboration with Elsevier and Symyx, better and faster algorithms, and no hassle on-line services. However, we are most proud of the fact that our tools are now widely used in the industry and the in academia, this is best showcased by the success stories of our users. Hopefully many more of these success stories will come next year.

We wish you Happy Holidays, and look forward to working with you next year,

Aniko Simon, Ph.D.

Vice President, SimBioSys, Inc.

## In This Issue

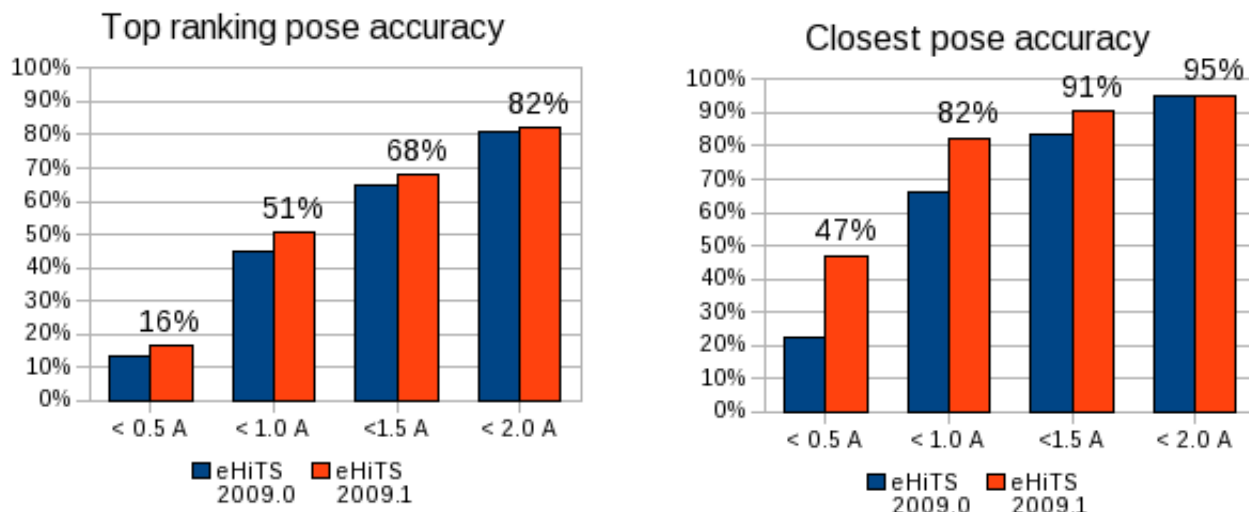
1. New product releases
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## 1. New product releases

### eHiTS 2009.1

A new release of our family of molecular docking and virtual screening tools (eHiTS, LASSO, Score, and Tune) came out a few weeks ago. Several new features were added, and several bugs and instability issues have been fixed, resulting in greater accuracy, and better performance.

<http://www.simbiosys.ca/blog/2009/11/27/ehits-20091-is-released/>

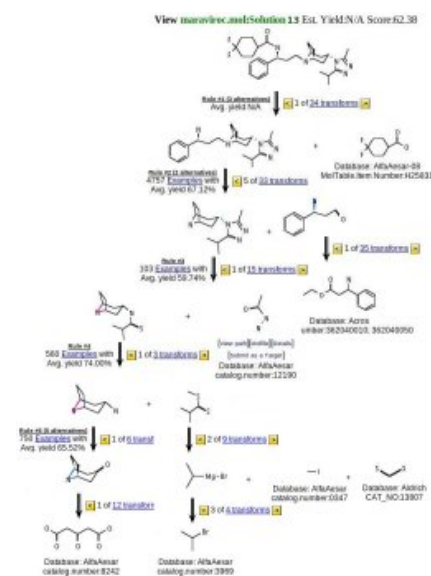


eHiTS 2009 performance on the Astex – Gold validation data set.

## ARChem 2009

A long list of added functionalities, algorithmic improvements, new system design, improved data handling and more, are included in a fresh release of ARChem that shows significant advances in computer aided retrosynthetic analysis.

<http://www.simbiosys.ca/blog/2009/12/10/archem-20091-is-released/>



## 2. Science & Technology

### Blind Docking with eHiTS 2009:

With growing interest of users in performing blind docking, we carried out a preliminary evaluation of eHiTS using a published dataset. The good results suggest that eHiTS is well equipped for handling this problem.

<http://www.simbiosys.ca/blog/2009/12/01/ehits-2009-as-a-blind-docking-tool/>

### Image Processing Validation Sets:

A new version of CLiDE is about to be released, which will put the strong OCR engine behind a contemporary user interface. The chemical structure extraction capabilities were evaluated on a new set that has been made available online.

<http://www.simbiosys.ca/blog/2009/06/15/clide-for-converting-structure-images-to-structure-files/>

### Free Scripts:

A few useful scripts, some related to eHiTS, and some generic, are available as a small courtesy to the comp chem community.

<http://www.simbiosys.ca/blog/2009/11/24/useful-scripts-available-as-free-download-on-the-simbiosys-website/>

## 3. Success stories from our users

**A novel non-peptide BACE1 inhibitor was found using eHiTS as a screening tool:**

<http://www.simbiosys.ca/blog/2009/11/04/a-novel-bace-1-inhibitor-discovered-using-ehits/>

**eHiTS showed good capabilities in separating weak binders from inactive molecules in an EPA study on estrogenicity:**

<http://pubs.acs.org/doi/abs/10.1021/tx900135x>

**SPROUT Lead-Opt** was used to optimize the binding of the active metabolite of the anti-inflammatory drug leflunomide to the target cavities of the *P. falciparum* and human dihydroorotate dehydrogenases:

<http://pubs.acs.org/doi/abs/10.1021/jm800963t>

## 4. Partnerships

Along our strong long lasting relationship with Elsevier regarding retrosynthetic analysis and availability of data to ARChem, we established in recent months a partnership with another leader of the chemical data publishing industry: Symyx:

<http://www.simbiosys.ca/blog/2009/07/16/simbiosys-and-symyx-team-up-to-enhance-computer-aided-synthesis-design-capabilities/>