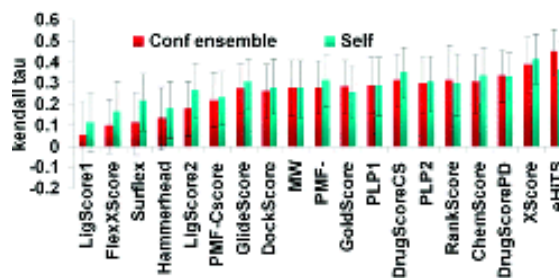


SimBioSys, Inc.
Toronto, ON, Canada

Dear Colleague,

The past few months have been particularly challenging to the industry. The economic slowdown has taken a toll on the small biotechs as well as on the big pharmas, with budgetary cuts, decrease in R&D activities, and heartbreaking layoffs. For SimBioSys, those have been months of hard work that resulted in new releases, and significant

progress across the board. In addition, we have strengthened our relations and our dialog with the computational chemistry community through meetings, conferences, papers and site visits. We strongly believe that computer aided drug discovery and design is going to emerge stronger from the current turmoil, as it offers tremendous opportunities for innovation at relatively low costs. We are striving to deliver continuous improvement in the performance of all our products in molecular docking, virtual screening, retrosynthetic analysis, de-novo design and data extraction. In this newsletter we would like to communicate to you the latest developments at SimBioSys, not only to keep you up-to-date, but also to engage you in the scientific exchange that will guarantee that we continue to provide you with the solutions you need.



The Spring-Summer '09 issue of the SimBioSys Newsletter is now available on-line as a [webpage](#) and as a [PDF file](#).

Newsletter Content:

- 1. Tips and tricks: Fragment Docking using eHiTS**
- 2. Our new product release announcements**
- 3. Science & Technology corner**
- 4. Success stories: scientific publications referring to SimBioSys tools**
- 5. In the News**

In an effort to make products information readily available to users, SimBioSys routinely documents and reports developments, technical information, applications aspects and other issues on its website. This newsletter is a digest of the many documents that have been posted on our blog and other sections of SimBioSys.com, and it is composed mostly of snippets and links to the detailed on-line materials.

1. Tips and tricks: Fragment Docking using eHiTS

Dan Harris has posted two items on our blog that address one of the hottest areas in the field of docking – **fragment docking**. eHiTS with its fragments based approach is a natural choice for this type of application, which can serve as a critical building block in a fragments based drug

design scheme. The two posts discuss eHiTS' success in fragment pose prediction, and specifically its ability to rank score poses in correlation with RMSD, and its predictive capability in terms of binding affinity.

<http://www.simbiosys.ca/blog/2009/05/04/fragment-based-pose-prediction-and-affinity-scoring/>

<http://www.simbiosys.ca/blog/2009/03/10/fragment-pose-prediction-and-score-rmsd-correlations/>

2. Our new product release announcements:

eHiTS 2009 was released in February. This version of our molecular docking includes fundamental changes to the underlying algorithms that bring about improved performance and pave the way to additional improvements in the upcoming release. Several new functionalities have been added to this version, such as special binding energy predicting scheme, and optional user-defined protonation state. Additionally, the database of family-tuned scoring weight-sets has been expanded dramatically.

No doubt, however, that the Cell-based version of eHiTS, has been a significant factor in creating a buzz around this tool. The availability of eHiTS 2009 on Sony's PlayStation 3, enables us to market a unique high performing docking and screening appliance that is equivalent in its capabilities to a small Linux cluster but at much lower hardware and operational costs. The various aspects of this release have been discussed in our press release:

<http://www.simbiosys.ca/blog/2009/02/26/simbiosys-inc-releases-a-new-version-of-ehits/>

and in our technical notes:

http://www.simbiosys.ca/ehits/ehits_technical_notes.html

Of particular interest is the speed technical notes that discusses the dramatic hardware acceleration on the Cell:

<http://www.simbiosys.ca/blog/2009/05/24/ehits-2009-speed-technical-note/>

The launch of eHiTS 2009 has been followed by the release of new, or updated versions of our related tools and add-ons:

- Tune – a package that allows customizing the scoring function to specific targets.
- Score – a utility that computes the eHiTS score for input structures.
- Lasso - our ligand based screening tool that utilizes the interaction surface points concept of eHiTS Score.

See details and documentation at:

<http://www.simbiosys.ca/docs/>

<http://www.simbiosys.ca/docs/platforms.html>

3. Science & Technology corner:

All our spring ACS meeting presentations have been made available on-line. They discuss the theory and application of our various tools:

<http://www.simbiosys.ca/blog/.../simbiosys-science-in-the-spotlight/>

<http://www.simbiosys.ca/blog/.../sharing-the-presentations-from-the-spring-2009-ac-s-and-chi-tri-conference/>

Our blog continues to be one of our main avenues for discussing scientific issues directly and indirectly related to our products

The following two examples discuss a new structure determination technique, and the environmental effect of computational work:

<http://www.simbiosys.ca/blog/2009/01/16/new-hope-for-high-resolution-pdb-structures/>

<http://www.simbiosys.ca/blog/2009/01/15/carbon-footprint-of-it/>

4. Publications referring to SimBioSys tools:

Eight new papers by users of our software applications came out so far this year, featuring various facets of the tools. Please check out our updated user publications link at:

http://www.simbiosys.ca/science/user_pubs/

Two of those papers deserve particular attention as they highlight two distinct strengths of eHiTS. The first is Englebienne and Moitessier's paper discussing their own scoring function, and comparing almost 20 different functions using a carefully selected test-set:

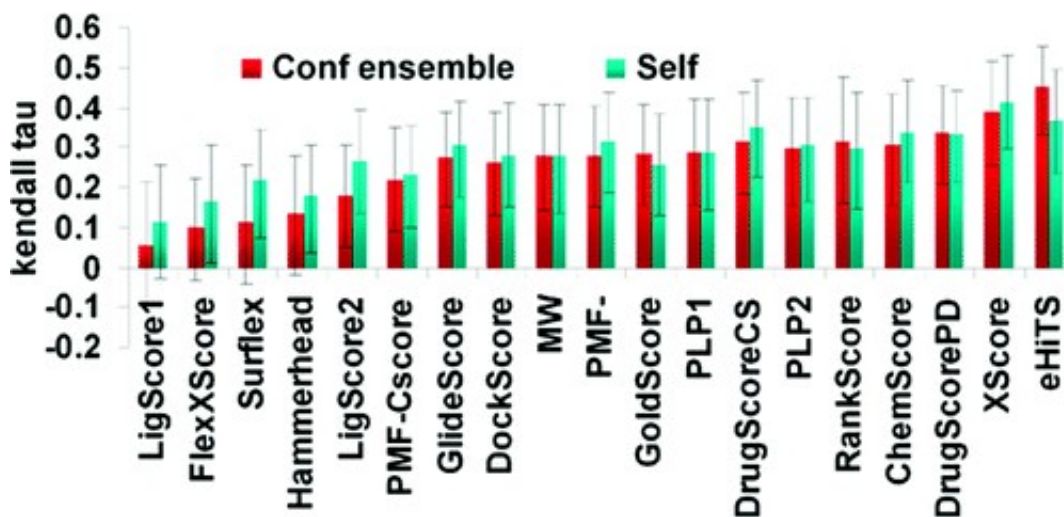
Docking Ligands into Flexible and Solvated Macromolecules. 4. Are Popular Scoring Functions Accurate for this Class of Proteins?

Pablo Englebienne and Nicolas Moitessier

J. Chem. Inf. Model. Article ASAP, May 15, 2009.

DOI: [10.1021/ci8004308](https://doi.org/10.1021/ci8004308)

TOC picture:



We discussed this paper in our June 1st blog: <http://www.simbiosys.ca/blog/.../a-comprehensive-scoring-evaluation-paper-from-mcgill/>

The second paper highlights eHiTS' capabilities in peptide docking:

De novo identification of binding sequences for antibody replacement molecules

Stephen Quirk, Shi Zhong, Rigoberto Hernandez

Proteins, published online on 23 Jan, 2009.

DOI: [10.1002/prot.22382](https://doi.org/10.1002/prot.22382)

We added two new scientific publications to our own publication portfolio these past few months:

[SimBioSys scientific publications page](#)

A paper on ARChem / Route Designer appeared in the Journal of Chemical Information and Modelling:

Route Designer: A Retrosynthetic Analysis Tool Utilizing Automated Retrosynthetic Rule Generation

James Law et.al:

J. Chem. Inf. Model., **2009**, 49 (3), pp 593–602

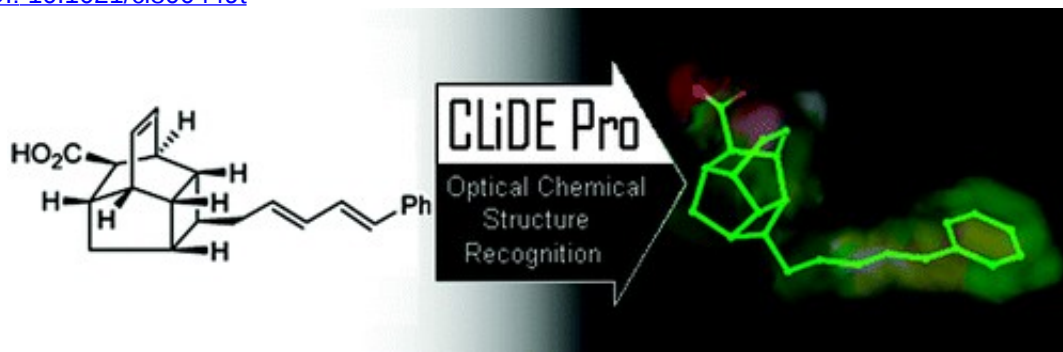
DOI: [10.1021/ci800228y](https://doi.org/10.1021/ci800228y)

Our sister company in the UK, Keymodule Ltd., with the leadership of our founder A. Peter Johnson, has published a new article on CLiDE:

CLiDE Pro: The latest Generation of CLiDE, a tool for optical chemical structure recognition

J. Chem. Inf. Model., **2009**, 49 (4), pp 780-787

DOI: [10.1021/ci800449t](https://doi.org/10.1021/ci800449t)



5. In the News:

eHiTS Lightning has been in the spotlight as the first docking program to be released on the Cell processor.

C&EN News focused on eHiTS Lightning in its May Software Reviews:

<http://www.simbiosys.ca/.../ehits-lightning-in-the-ce-news-digital-briefs-today/>

David Bradley posts about eHiTS on the PS3:

<http://www.simbiosys.ca/.../drug-design-on-the-playstation/>

In addition C&EN News also featured ARChem in December 2008 in the Digital Briefs section:

<http://www.simbiosys.ca/.../chemical-and-engineering-news-acknowledges-simbiosys-archem-in-digital-briefs/>