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## SimBioSys quarterly Newsletter Spring / Summer 2008 issue

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### 1. Message from Dr. Z.Zsoldos, CSO, SimBioSys

Summer is upon us! Time flies when you are busy :-)

Indeed, the past few months have been intense for us: with the last-minute entry to SAMPL competition with frantic night work-shifts to get all 5 rounds of the competition setup, run, analysis of the results and submission before the deadline; with presentations and booth at the ACS [[abstract](#)], SBS [[abstract](#)], DD Chemistry and Bio-IT World Expo [[presentation](#)], with various on site customer training sessions, and finally working very hard with long hours and weekends to fulfill our commitment to deliver a working version of eHiTS on the cell processor for the Bio-IT show -- which we DID achieve.



So, the theme of the era was Acceleration, or maybe I should borrow another phrase from the Highlander films: the Quickening – if you've seen the movie then you'll know that lightning strikes the winner of the battle giving him the extra energy for eternal life. That is the feeling we shared with those who saw the system running at Bio-IT. The medical meaning of the phrase WHAT PHRASE..the Quickening? (first motion of the fetus during a pregnancy) is also appropriate as we are giving birth to eHiTS Lightning. At Bio-IT, we were a finalist, in the top three, for the Best in Show award. The general feedback was "Wow!"

<http://www.simbiosys.ca/blog/2008/05/01/the-wow-factor-at-the-bio-it-world-expo/>

I won't belabor the details of how we accelerated eHiTS relative to Intel processors since I have discussed that in detail on the SimbioSys [blog](#) . Suffice to say we have delivered 30-50X on the

PlayStation3 platform and 50-117X on an IBM QS 20 Blade. Since the show we have been busy turning some of the speed advantage into even better accuracy - mind you we never had to play catch-up in that area, but we want to jump far in the lead beyond the reach of the competitors ;-).

Where to from here? We have even more conferences coming up in the next few months. We will be holding a roundtable discussion for invited participants just prior to the CHI meeting in Boston in June. This roundtable meeting will invite thought leaders to bring their insight to bear on the design of an optimal docking solution. You can see more details of this round-table in the events section. Now we have speed on our side with accelerated docking on the Cell processor. Our algorithms are well proven for accuracy in many comparisons. While I have ideas about where to take our product line, not only eHiTS, in the future this roundtable will afford us the opportunity to get direct feedback during a peer-based discussion with our users. I'll report back on how it goes. I look forward to meeting some of you at conferences and hope you will sign up to read our blog where I am starting to discuss some of the more challenging issues in this domain.

Enjoy the rest of the newsletter – there are plenty of interesting and useful articles inside.

Have a safe and happy summer !

ZZ

## 2. Dan's tips and hints:

Teaches us how to best use eHiTS, to maximise ROI (return on invested time, money, energy etc.). It's a must-read! <http://www.simbiosys.ca/blog/2008/06/19/ehits-and-score-low-rmsdlnkdic50-correlations/>

## 3. Upcoming events this summer:

Please contact us up-front to meet our scientists at these events:

- CHI's Structure-Based Drug Design conference, **Boston, June 25-27, 2008**, with a pre-meeting for Docking and Screening Roundtable, see [invitation](#) and [agenda](#).
- Drug Discovery Design & Planning Methods, **Oxford, UK, July 14-18, 2008**
- 3DSig: Structural Bioinformatics & Computational Biophysics, **Toronto, July 18-19, 2008**
- 236<sup>th</sup> ACS, **Philadelphia, PA, USA, Aug 17-21, 2008**

For more details, please see our events page:

<http://www.simbiosys.ca/science/presentations/events.html>

## 4. Science Corner:

\* eHiTS case study with Nicotinic Acetocholine Receptors

[http://www.simbiosys.ca/support/eHiTS\\_presentation\\_for\\_nicotinic\\_receptors.pdf](http://www.simbiosys.ca/support/eHiTS_presentation_for_nicotinic_receptors.pdf)

\* Protonation states and docking

<http://www.simbiosys.ca/blog/2008/05/17/correct-protonation-state-for-docking/>

\* How to ensure a fair comparison between docking solutions...

<http://www.simbiosys.ca/blog/2008/05/26/cognate-docking-accuracy-measurement-vs-pre-optimized-pose/>

## 5. News:

\* The wow factor at the BIO-IT World Expo

<http://www.simbiosys.ca/blog/2008/05/01/the-wow-factor-at-the-bio-it-world-expo/>

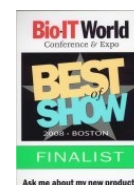
<http://www.simbiosys.ca/blog/2008/05/29/video-games-are-enabling-life-sciences-research/>

\* BIO IT world's Best of Show Award

<http://www.simbiosys.ca/blog/2008/06/09/bio-it-worlds-2008-best-of-show-competition-in-the-press/>

\* Dan Harris joined SimBioSys

<http://www.simbiosys.ca/blog/2008/04/18/dan-harris-joined-simbiosys/>



## 6. Product release:

\* eHiTS on the Cell/B.E. Beta-Release:

[http://www.simbiosys.ca/ehits/ehits\\_newfeatures.html](http://www.simbiosys.ca/ehits/ehits_newfeatures.html)

\* ARChem is now available with a demo version of the CrossFire Beilstein reaction database

<http://www.simbiosys.ca/blog/2008/05/30/29/>



## 7. Technology corner:

\* Compare Cell/B.E., GPU and FPGA

<http://www.simbiosys.ca/blog/2008/05/03/the-fast-and-the-furious-compare-cellbe-gpu-and-fpga/>

\* The future of HPC

<http://www.simbiosys.ca/blog/2008/05/29/the-future-of-hpc/>

\* Floating point errors

<http://www.simbiosys.ca/blog/2008/05/28/floating-point-errors/>

\* The Quality of Chemistry Software

<http://www.simbiosys.ca/blog/2008/06/04/chemical-software-quality-3-polar-surface-area/>

## 8. User publications:

Two users groups have recently had publications with eHiTS results. Congratulations to them!

N. Schormann, O. Senkovich, K. Walker, D.L. Wright, A.C. Anderson, A. Rosowsky, S. Ananthan, B. Shinkre, S. Velu, D. Chattopadhyay

Proteins: Structure, Function, and Bioinformatics: "Structure-based approach to pharmacophore identification, in silico screening, and three-dimensional quantitative structure-activity relationship studies for inhibitors of Trypanosoma cruzi dihydrofolate reductase function"

PROTEINS **June 2008** [[Epub ahead of print - Early View](#)]

[Aldo Segura-Cabrera, Mario A. Rodriguez-Perez: "Structure-based prediction of Mycobacterium tuberculosis shikimate kinase inhibitors by high-throughput virtual screening"](#)

[Bioorganic & Medicinal Chemistry Letters, Volume 18 \(2008\), Issues 11, June 1 2008 pp. 3152–3157](#)  
[view Article: doi:10.1016/j.bmcl.2008.05.003](#)

For details see:

[http://www.simbiosys.ca/science/user\\_pubs/index.html](http://www.simbiosys.ca/science/user_pubs/index.html)