

SimBioSys Fall '07 Newsletter

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1. A Message from Dr. Zsoldos, CSO, SimBioSys

Summer 2007 has, as usual, been a stimulating and exciting few months. Continuing our ongoing efforts to deliver solutions to your problems we have retained our focus on optimizing our present software products while keeping a keen eye on opportunities for breakthroughs in technology. Over the past few months SimBioSys has formed a number of partnerships with leading scientific groups to work on some community centric projects. In particular, we have formed a relationship with the US Environmental Protection Agency to provide access to SimBioSys' eHiTS to support their ToxCast project. Also, we are supporting the FightMalaria@Home project in their efforts to find new desperately needed therapies for this killer disease.

At a personal level I have been focused on a high impact project capable of delivering enormous breakthroughs in the timescales associated with virtual screening via docking. Details will soon be forthcoming but the work performed to date clearly demonstrates the advantages new hardware can bring to high-throughput processes without any compromise in accuracy. In the coming months SimBioSys will be attending and hosting a number of events and we hope to have the opportunity to meet with you. Finally I would like to welcome Dr. Antony Williams into the SimBioSys team. Dr. Williams brings his extensive experience and expertise in the chemistry software industry and will support us in a consultative role around a number of our developing opportunities. We look forward to a prosperous partnership with him.



2. SimBioSys Partners with the US Environmental Protection Agency on a large scale toxicology screening project, ToxCast™

The US Environmental Protection Agency (EPA) launched phase I of their ToxCast™ project in August of this year. ToxCast™ will examine how a diverse array of environmental chemicals such as pesticides can produce toxic effects and thereby enable EPA to prioritize the use of its limited testing resources on those chemicals that present the greatest likelihood of risk to human health and the environment. The EPA will augment experimental high throughput screening, with computational chemistry tools including virtual screening experiments using SimBioSys' eHiTS docking program.

Zsolt Zsoldos, chief technical officer for SimBioSys comments that "The ToxCast™ Program will allow the EPA to develop the ability to forecast toxicity and develop methods of prioritizing chemicals for further screening and testing. eHiTS should prove invaluable to integrate in silico and in vitro endeavors by affording the EPA access to industry leading algorithms for virtual screening via docking procedures. We are committed to supporting this project to facilitate improvements in the processes EPA utilizes in the regulation of environmental contaminants and in enabling matters of public health."

For more information on this partnership see:

<http://www.simbiosys.ca/whatsnew/news/index.html#20071105>

3. eHiTS will be the docking program used in the FightMalaria@Home project

The Centre for Synthesis and Chemical Biology at the Royal College of Surgeons in Ireland, in collaboration with the Computer Architecture and Grid Research Group at Trinity College Dublin, have teamed up with SimBioSys to help find novel anti-malarial drugs and the associated target proteins. Following the path of successful projects like Folding@Home, fightHIV@home, and Africa@home, FightMalaria@Home will screen very large compound databases against all known models of Malaria proteins using idle CPU cycles from users around the world. A customized version of eHiTS has been developed to support this worthwhile project. For more information please visit:



www.bioinformatics.rcsi.ie

4. Dr. Piotras Cimpperman releases a graphical user interface (GUI) for eHiTS convert

Dr. Piotras Cimpperman, from the Institute of Biotechnology, Vilnius, Lithuania, has published a multi-platform interface for the convert utility of SimBioSys' eHiTS package. This GUI, which also includes TMA to PDB converter, is called "TMAconvert" and it is available for Windows, Linux 32bit and Linux 64bit, or you can download the source code. To get more information or to access this file conversion tool, please visit Dr. Cimpperman's website:

<http://piotras.ibt.lt/en/index.php?page=downloads>

5. Invitation to Docking and Screening Workshops in the Research Triangle Park, NC.

SimBioSys would like to invite you to attend one of two Virtual Screening and Docking seminars to be held November 27th and 28th in the Research Triangle Park, NC. SimBioSys will join local experts to discuss the latest advancements in virtual screening and docking and exciting new directions for the field.



Tuesday, Nov. 27th, 2007

School of Social Work, UNC, Chapel Hill

Speakers: Nikolay Dokholyan (UNC Chapel Hill), Alex Tropsha (UNC Chapel Hill), Antonius M Vandongen (Duke University), Zsolt Zsoldos (SimBioSys)

Hands-on: eHiTS, LASSO and CheVi training session in the afternoon.

Wednesday, Nov. 28th, 2007

NISS 19 T.W. Alexander Drive, Research Triangle Park

Speakers: Rocky Goldsmith (Environmental Protection Agency), Stan Young (National Institute of Statistical Sciences/NCSU), Darryl Reid (SimBioSys), Zsolt Zsoldos (SimBioSys)

Register today for this FREE event, seating is limited!

<http://www.simbiosys.ca/science/presentations/2007-11-RTP/>

or email: darryl@simbiosys.ca

6. Dr. Antony Williams supports the SimBioSys team

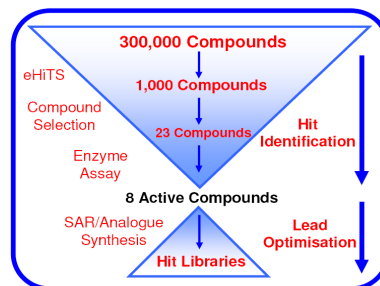
SimBioSys is pleased to welcome Dr. Antony Williams to the team in a consultative role. Dr. Williams has worked in the chemistry software field for well over a decade. He brings his vast knowledge of the field and his desire to solve problems via cheminformatics software to assist SimBioSys in some new ventures. Information regarding some of these efforts will be forthcoming and we look forward to a long and fruitful relationship with Antony.



7. User Success Stories

BACE-1 and Novel Antibacterial leads discovered

Two success stories have recently come out of the Fishwick group at the University of Leeds, UK. In two recent poster presentations, group members have presented a very successful workflow used to find new BACE-1 inhibitors as well as Antibacterial leads. The group screens their library of commercially available compounds against their target using eHiTS (VHTS mode) then selects roughly 1000 best scoring compounds to re-score with the SPROUT scoring function. The top 100 then undergo the "eye" scoring function (they actually look at the compounds and assess solubility, analog synthesizability etc in order to decide which ones to purchase for testing in assays. In the BACE-1 project they found 1 active compound out of the 6 tested, while in the aaRS Antibacterial study they found 8 hits in the 23 tested compounds.



Workflow for Antibacterial (aaRS) Virtual Screen and experimental testing

You can read these success stories and other user publications under the "Scientific Presentations" page:

http://www.simbiosys.ca/science/user_pubs/index.html#User_Presentations

8. Upcoming Events

Meet the SimBioSys team at the following events. Our events list is constantly changing and to keep up to date on our events please visit our website:

<http://www.simbiosys.ca/whatsnew/index.html>

- Virtual Screening and Docking workshops
Nov 27-28, 2007
Research Triangle Park, NC
- Virtual Discovery 2008
Jan 23 - 24, 2008
Palm Springs, CA
- SBS Conference
April 6-10, 2008
St Louis, MO
- 235th ACS
April 6-10, 2008
New Orleans, LA

For more information about SimBioSys and our software offerings, please visit our website, email us or contact us by phone:

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