



Welcome to the 15th edition of the BioSolveIT newsletter!

In our newsletter we publish information about new developments, events, milestones, and scientific facts on a quarterly basis.

FTrees 2.0 – better scaffold hopping knockout hits

[FTrees](#) is packing a larger drug discovery punch than ever before by helping you identify that scaffold hopping knockout hit. Helpful wizards now guide users through the most crucial steps of molecule conversion, comparison and clustering for successful drug design. The *FTrees 2.0* release contains a new dynamic search algorithm which includes subgraph matching, user accessible molecule preparation tools managed via SMARTS and increased *FTrees* file capacity with full SMILES and SD support. These features permit more molecules to be searched in a more diverse fashion than before. Analysis has also hugely improved with on-the-fly similarity threshold filtering of results and hierarchical clustering capabilities. With *FTrees 2.0* you can also assign a rationale why *FTrees* determines molecules to be similar and reason with medicinal chemists using output of molecule-based alignment information. To use *FTrees 2.0* enquire about your own [evaluation copy](#) today.

fly 1st class at Booth 737, get this relaxing feeling at the 236th Philly ACS



BioSolveIT will be flying into the [236th ACS meeting in Philadelphia](#) and exhibiting at [Booth 737](#). This year BioSolveIT has a surprise treat for customers which will give them that easy relaxing feeling whilst witnessing 1st class virtual screening. Obtain or find one of a limited number of BioSolveIT award envelopes being given out or placed around the exhibition center which entitles you to fly by, sit down and collect your relaxing prize at booth 737. We guarantee you that there you can unwind during the conference and obtain that 1st class feeling experienced with BioSolveIT screening. Make an appointment to meet at the conference and we guarantee you your personal award envelope. Just drop an email to suggest a date and time to meeting@biosolveit.de.

Visit BioSolveIT, the world's leading provider of fragment based approaches, at booth 737 to learn about all our latest developments. Including the new, most complete, industry proven, diverse, and highly efficient software offering which is currently available for *de novo* drug design. Obtain a DVD with our tools which allow you to screen innumerable large numbers of compounds and incorporate synthesizability for discovering actives. The DVD also contains a Fragment Space from which as many as 1.000.000.000.000.000.000 drug-sized molecules can be generated. Applications of our software are presented in [several talks](#) at the conference. To see the tools in action come along for a software demonstration, or take part in our raffle where you can win up to \$100,000 worth of licenses and gain access yourself. We look forward to seeing you soon at booth 737!

neglected diseases, nanomolar hits, supporting Dundee to tackle poverty

The underdeveloped world has over 350 million people at risk from neglected diseases, attracting little or no interest from pharmaceutical companies. Treating these diseases is often expensive and difficult, the resistance development by parasites underpin these conditions. Two years ago the Wellcome Trust awarded £8.1 million over 5 years to the University of Dundee to start an initiative to help discover new drugs to treat some of the world's most neglected tropical diseases. The most progressed project has discovered a compound series that shows nanomolar affinity against the target and good oral efficacy in the disease model. In the absence of a crystal structure of the target the application of [FlexS](#) was crucial to help derive a pharmacophore model from the initial hits in order to guide hit validation and optimization. While further optimization is still ongoing, the [FTrees](#) program is currently used to support the quest for a backup series. The computational chemists from Dundee were generally impressed how quick and easy it was to learn how to use BioSolveIT software tools and were very pleased with its robustness. They consider these tools a vital ingredient in their scientific work and look forward to further broaden their application in the future. For further information read the [full press release text](#).

workshops, training, BioSolveIT, an informative stylish international success _____

BioSolveIT recently hosted very successful workshops and training in Noordwijkerhout, the Netherlands and Oxford, UK, respectively. A free interactive Workshop on Virtual Screening and *De Novo* Design took place on the 5th June 2008 following the 8th International Conference on Chemical Structures in Noordwijkerhout. A total of 14 people attended the workshop which was a tremendous success as participants tackled various drug design problems and familiarized themselves with [FTrees](#), [ReCore](#) and [FlexX](#).

BioSolveIT also gave training workshop as part of the "Latest Advances in Drug Discovery Design & Planning Methods" organized by [eCheminfo](#). An interactive training session on "De Novo Scaffold Replacement and Virtual Screening" was provided on the 25th July in Oxford. One attendee described the BioSolveIT interactive demonstration as "very informative", whilst another mentioned "I really liked the style of how you did it!"



If you are interested in taking part in any future workshops or training please [send us an email](#). Also realizing the need to reduce peoples travel time and expenses, BioSolveIT plans to start shortly with a series of web-based seminars, demos and tutorial sessions. Please provide us feedback of your interest in any of these and drop an email to secure your front row seat in the next up and coming webinar. Just drop a note with your request and/or suggestion to workshop@biosolveit.de.

tips & tricks – the new FlexX Release 3 - part 2: pharmacophore definition _____

This section focuses on troubleshooting and aspects of [FlexX](#) that are either not very well known or are sometimes misunderstood, so we see them as important points to bring to your attention. In this issue we continue with our two part series of tips and trips which will help you learn how to use the new *FlexX-GUI*. [Read more!](#)

You can view previous topics of tips and tricks [here](#). If you have any questions or know of any tips and tricks yourself that you would like to share with the *FlexX* user community, we would appreciate your input at FlexX@BioSolveIT.de.

BioSolveIT news in brief _____

- Apsara Innovation and BioSolveIT announce comprehensive distribution partnership of the BioSolveIT software products in India. Read more about it in the next issue of this newsletter.
- BioSolveIT releases white paper about capitalizing on your in-house med-chem know how based on our unique [CoLibri](#) and [FTrees-FS](#) technology. Read on [here](#).
- Dates for your diary: BioSolveIT will be present at the following events:

Aug 17 th - Aug 21 st	236 th ACS National Meeting & Exposition, Philadelphia, PA, USA. BioSolveIT will be attending this meeting with talks and a booth (737) .
Oct 14 th - Oct 16 th	MipTec - The 11 th Leading European Event for Drug Discovery, Basel, Switzerland. BioSolveIT will be presenting: " Searching The Impossible – Designing Libraries From Large Virtual Chemistry Spaces ".
Nov 9 th - Nov 11 th	German Conference on Chemoinformatics, Goslar, Germany. BioSolveIT will be attending this meeting.

If you would like to meet one of our representatives to discuss any questions or have any kind of feedback please email us at Contact@BioSolveIT.de.

literature corner _____

- Fragmental modeling of human glutamate transporter EAAT1 and analysis of its binding modes by docking and pharmacophore mapping.*
Pedretti A., De Luca L., Sciarrillo C., and Vistoli G.
ChemMedChem 3(1):79-90. (2008)
[details here](#)

- Selection of a Respiratory Syncytial Virus Fusion Inhibitor Clinical Candidate. 2. Discovery of a Morpholinopropylaminobenzimidazole Derivative (TMC353121)*
Bonfanti J.F., Meyer C., Doublet F., Fortin J., Muller P., Queguiner L., Gevers T., Janssens P., Szel H., Willebrords R., Timmerman P., Wuyts K., van Remoortere P., Janssens F., Wigerinck P., and Andries K.
J. Med. Chem. 51(4):875-96. (2008)
[details here](#)
- Receptor-based modeling and 3D-QSAR for a quantitative prediction of the butyrylcholinesterase inhibitors based on genetic algorithm.*
Zaheer-ul H., Uddin R., Yuan H., Petukhov P.A., Choudhary M.I., and Madura J.D.
J. Chem. Inf. Model. 48(5):1092-103. (2008)
[details here](#)
- A virtual screen for diverse ligands: discovery of selective G protein-coupled receptor antagonists.*
Engel S., Skoumbourdis A.P., Childress J., Neumann S., Deschamps J.R., Thomas C.J., Colson A.O., Costanzi S., and Gershengorn M.C.
J. Am. Chem. Soc. 130(15):5115-23. (2008)
[details here](#)

upcoming articles

- Indian Distributor, Apsara Innovation
- [FlexX](#) 3.1 release

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