
BioSolveIT Newsletter

Issue 08

27 April 2006



Welcome to the 8th edition of the BioSolveIT newsletter!

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

[buy FlexX now directly from its developers](#)

All our products, among them the latest protein-ligand docking engine, [FlexX Release 2](#), are now available to all users directly from us. This news is especially relevant to our industrial partners.

BioSolveIT offers cheminformatics solutions for a variety of applications, e.g.:

structure based design	FlexX
flexible alignment of molecules	FlexS
ultra high speed similarity searching	FTrees
docking data analysis	the Docking Database (DDB)
library design	CoLibri

Interested customers, please send a [mail](#), or visit our [web site](#).

[meet BioSolveIT at ACS Fall Meeting in San Francisco](#)

BioSolveIT will be present at the [232nd ACS Meeting](#) in San Francisco. At [Booth 427](#), interested customers can inform themselves about the latest developments in drug discovery software from BioSolveIT. Regular software demos will take place to show not only the new flexibility and usability features of the latest [FlexX Release 2](#), but also some of our other software products: [FTrees](#), our fast molecular similarity finder, or the [Docking Database \(DDBTM\)](#). If you are interested in specific consultation or a customized demo, please [let us know!](#) We will arrange for an individual appointment, in which we will demonstrate how our software can make a difference in your daily modeling business. Simply write an [email](#), and we would be glad to schedule a meeting with you at our booth. There will be attractive door prizes, booth parties, and presentations. Get reduced rates if you decide to sign up for a software license at the booth.

For those who are also interested in our [workshop: register now!](#) The first ten who register will receive attractive prizes in San Francisco for Saturday, Sept. 9. Among the prizes expect to find tickets for whale watching tours, to Alcatraz, to Golden Gate Park and so on. We are looking forward to meeting you in San Francisco!

[4th FlexX Docking Workshop](#)

The [4th FlexX Docking Workshop](#), *Successful High-Throughput Docking and Screening with FlexX Release 2, the latest technology in Drug Discovery*, will be organized back-to-back with the [ACS fall meeting](#) in San Francisco, on Sept 7 and 8. As is tradition, special emphasis will be placed on hands-on training – each participant will be able to do individual exercises on his/her personal workstation, sponsored again by [SUN Microsystems](#). In particular, the workshop will cover the following topics:

- Learn how to extract [FlexX's](#) full power for your docking and screening tasks
- Get an introduction to most of Release 2's new features
- Learn how to tailor [FlexX's](#) power to your own needs
- Learn how to prepare your ligands and targets for optimal results
- Learn new ways to improve efficiency and accuracy
- Learn how to target-tailor [FlexX's](#) scoring function to your system
- Learn how to optimize [FlexX's](#) high-throughput screening performance

- Grid/Cluster computing and workflow automation with [FlexX](#)
- Get an insight into [FlexX](#)'s extension modules: [FlexX^C](#), [FlexX-Pharm](#) and [FlexE](#)

The venue of this year's workshop will be announced on the [workshop web page](#). [Register](#) early to get special rates: space fills up quickly and there is limited availability. If you are also planning to visit the ACS meeting then take note: The first ten registrants can win tickets for among other things whale watching tours, Alcatraz, Golden Gate Park for Saturday, Sept. 9!!

[Johnson&Johnson success story](#)

PRD Finds Novel Scaffold Hits During [FTrees](#) Evaluation Period.

Researchers in Belgium have just found several new hit compounds during an evaluation of BioSolveIT's fast molecular comparison engine [FTrees](#). Delighted by this enormous success, the company tripled their amount of licenses and extended [FTrees](#) access to other sites throughout Europe. Initially triggered by a BioSolveIT presentation at an HTS symposium at FhG, Johnson & Johnson PRD decided to give the feature trees descriptor as implemented in [FTrees](#) a chance and immediately requested a free evaluation. During a one-day visit at the brand new Beerse site, BioSolveIT's Dr. Gastreich introduced the Molecular Informatics (MI) group to details and advantages of the [FTrees](#) suite. An evaluation contract was signed. It was only weeks thereafter that Dr. Wendy Sanderson, a member of the MI group working with the Psychiatry disease area mailed BioSolveIT "We have started screening compounds that were selected using [FTrees](#) and we found active molecules with unexpected scaffolds — Very exciting!" The positive results have led to investigation at the other European sites. Today, BioSolveIT is proud to count three major Johnson & Johnson PRD discovery labs as their new [FTrees](#) customers.

[commentary on recent docking studies](#)

We have noticed several publications about the evaluation of docking software where there was room for improvement in terms of exploiting [FlexX](#)'s true capacity. Poor performance of a docking program does not always result from intrinsic deficiencies, but rather often enough some little twist in the application might solve the apparent issue. Also, the comparison of different methods is by no means a trivial task. A very good compilation of caveats in the comparison of docking programs was published by Jason Cole and co-workers in 2005 [1]. The authors state, for example, that evaluations of docking software to date have oftentimes neglected the statistical significance when comparing docking programs. In other words, comparison of success rates is difficult unless a measure of statistical significance is given. Another very valid remark the authors make is the importance of revealing all information on how each program is used, and that it "is wrong to mix different assumptions between different docking programs". Read [our commentary](#) about a selection of recent cases.

[1] J Cole, Comparing Protein-Ligand Docking Programs is Difficult, *Proteins* 60, 325-332 (2005)

[tips and tricks from the world of FlexX](#)

Following established tradition, in this section we focus on 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.

No more placements outside the pocket! This issue will bring you more detail about using [Gaussian filters](#). Using these filters can significantly enhance the result of a docking by "smoothly" guiding the placements to user-defined regions. See for yourself in our [example](#).

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-info@biosolveit.de.

[BioSolveIT news in brief](#)

RSS feed now available for BioSolveIT [main site](#) and [download site](#).

Prof. Thomas Lengauer from Max-Planck Institute in Saarbrücken presents his contribution to AIDS therapy in a [video](#).

Dates for your diary: BioSolveIT will be present at the following conferences:

- 28 April, [UKQSAR Conference](#), Accelrys, Cambridge, UK
- 14-16 June, [Structure-Based Drug Design Conference](#), Boston, MA, USA

Availability of our latest conference presentations:

- Dr. Christian Lemmen reported at the 231st ACS Spring Meeting in Atlanta, GA about "[Combinatorial Design Revisited](#)".

All available BioSolveIT talks can be found in the [conference section](#) of our web site.

[literature corner](#)

Ligand Selectivity for the Acetylcholine Binding Site of the Rat $\alpha 5\beta 2$ and $\alpha 3\beta 4$ Nicotinic Subtypes Investigated by Molecular Docking

Bisson, W. H.; Scapozza, L.; Westera, G.; Mu, L.; Schubiger, P. A
J. Med. Chem, 48, 5123-5130 (2005)

[details here](#)

In silico fragment-based discovery of DPP-IV S1 pocket binders

Rummey, C.; Nordhoff, S.; Thiemann, M. and Metz, G.
Bioorg Med Chem Lett, 16(5), 1405-1409 (2006)

[details here](#)

Structure-Based Design, Synthesis, and Biological Evaluation of Novel Inhibitors of Human Cyclophilin A

Guichou, J.-F.; Viaud, J.; Mettling, C.; Subra, G; Lin, Y.-L., and Chavanieu, A.
J. Med. Chem, 49, 900-910 (2006)

[details here](#)

[upcoming articles](#)

FlexX-Screen project: Docking at Warp4! FlexX-Screen is a new module in FlexX for ultra high throughput docking. **Dock a ligand in less than one second** – maintaining the high accuracy.

SIS Algorithm: Learn more about the *Single Interaction Scan* algorithm, a newly developed placement method in docking. It has shown to be particularly successful with hydrophobic pockets and steroid ligands.

[contact](#)

For further information please contact:

BioSolveIT GmbH
An der Ziegelei 75
53757 Sankt Augustin
Germany
email: Newsletter@BioSolveIT.de
www: www.BioSolveIT.de
phone: +49-2241-25 25 0
fax: +49-2241-25 25 525

