



Welcome to the 12th edition of the BioSolveIT newsletter!

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

the dawn of the interface age

There has been a recent drive and increase in momentum at BioSolveIT to supply our customers with a totally new way of using our software. The ease of use and possible ways to access our software is about to be increased significantly as numerous interfaces to our two most popular tools, [FlexX](#) and [FTrees](#), become available. The move to the graphical age has been driven by customer demands to obtain a quicker and easier way to utilize functionality within our software. *FlexX* and *FTrees* can now be accessed in multiple ways, both are now available with their own GUI's provided by BioSolveIT, the [FlexX GUI](#) ([read more](#)) and *FTrees-XL*.

Furthermore, both tools have interfaces to MOE[®] and Pipeline Pilot[®]. These interfaces are available for testing and will be reported in detail in the next issue of the newsletter. If you would like more information or to test *FlexX* in MOE[®] or in Pipeline Pilot[®], please contact us through the [support page](#). [FTrees in MOE[®]](#) and [FTrees in Pipeline Pilot[®]](#) information and packages are available from their respective web-pages.

no hydrophobic worries with FlexX Release 2.2

[FlexX Release 2.2](#) is now available and contains a major addition to its docking abilities. The new Single Interaction Scan (SIS) algorithm, reported on [previously](#), for base placement has been incorporated within *FlexX* Release 2.2. The algorithm complements the triplet and pair interaction matching methods already present as SIS permits scanning of every interaction surface on an individual basis within the active site for the possibility of a good placement. SIS facilitates new levels of accuracy by tackling traditionally challenging hydrophobic ligands where the dominating interactions are non-polar, or where there is only one hydrogen bond possible. Thus, now you can accurately dock molecules which exhibit very few directed interactions with the classical rapid speed of *FlexX*. Another notable feature within Release 2.2 is that there is no need for RDF files when importing proteins in mol2 format if the active site reference is given as a SET definition within the mol2 file (as for example produced by MOE[®]). If you are interested in evaluating the new *FlexX* Release 2.2, please proceed [here](#).

frequently asked questions – FAQ's

Looking for support? Thought hey, if only I could get an instant answer to that question? Had the feeling that surely this would be on the lips of so many people? Well look no further, BioSolveIT have tried to further ease your worries and support our users by creating a frequently asked questions (FAQ) section. In addition, to the continuously available [support](#) from BioSolveIT, who strive to be the incarnation of support and maintain this philosophy from conception, you can now just jump online and access our FAQ section. The FAQ knowledge base can be quickly queried, easily printed, and emailed to other users. The FAQ section is interactive as users can submit comments and view previous comments of others. Whilst subscription to FAQ pages allows you to be updated immediately as soon as a page is updated or commented on, you can also store your most useful FAQ's under a favorites section. Please take a look at the [FAQ knowledge base](#) and let us know what you think by posting your comments.

the prestige continues to incrementally grow

The credentials and pedigree of BioSolveIT just keep on improving. The distinguished figure of [Prof. Dr. Gerhard Klebe](#), a chair of the Pharmaceutical Chemistry Department at the University of Marburg Germany, recently joined the BioSolveIT [Scientific Advisory Board \(SAB\)](#). His illustrious career with over 200 publications spans various different research fields such as understanding protein-ligand interactions, including chemical synthesis, microcalorimetry, molecular biology, crystallography, bioinformatics and software development. Many internationally recognized software tools have been developed in [his lab](#) and numerous drug discovery projects relevant for the third world have been undertaken.

The scientific part of the advisory board now consists of three globally renowned figures of which one, the famed [Dr. Lipinski](#), was voted as the 8th most influential person in the pharmaceutical industry by the World Pharmaceutical Frontiers' first ever Pharma 40 list which was composed by industry experts.

Last but by no means least, [Prof. Dr. Hugo Kubinyi](#), a living legend in Medicinal Chemistry completes the BioSolveIT scientific side of our board of advisors.

Further BioSolveIT prominence has been obtained by the original [FlexX publication](#) growing to have over more than 600 citations. A small selection of references that cite the paper are [available for viewing](#). This accumulation of citations shows the distinctive historic quality of the FlexX method which formed a firm foundation for the development of today's successfully applied industry standard docking engine supplied by BioSolveIT.

[exhibiting @ the fall ACS in Boston](#)

BioSolveIT was just presenting and exhibiting at this year's [4th Joint Sheffield Conference on Chemoinformatics](#) (see some pictures [here](#)). We will be present at the [234th ACS meeting in Boston](#). The Sheffield conference is a tri-annual conference in the UK that brings together leading experts in the field of chemoinformatics and is well attended by academics and industry. This year BioSolveIT was sponsoring the conference in conjunction with our partners CCG. For the first time we were showing the FlexX-MOE interface, as well as our new FlexX GUI and many other recent developments. Furthermore, a [presentation](#) on our *de novo* tools was given by Dr. Marcus Gastreich.

This year's Fall ACS Meeting is in Boston and you can visit us at [booth 951](#) and get informed about the latest developments of our cutting edge drug discovery solutions. There will be software demonstrations, raffles where you can win an iPod, booth parties, coffee and lots of other interesting stuff. Receive special rates on our software if you decide to sign up for a license at the booth! Apart from the booth, there will be numerous scientific presentations related to our technology. We encourage you to consider [these talks](#) when planning your itinerary. The details of these can be found on our [ACS webpage](#), where you can sign up for the raffle and have a chance to win an iPod.

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

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 will focus on the usage of Corina in [FlexX](#). [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 either through our [support page](#) or via e-mail at FlexX@BioSolveIT.de.

[BioSolveIT news in brief](#)

- A new evaluation procedure has been put in place, you can now evaluate our software with no paperwork and minimal hassle. You can obtain a free evaluation license for 2 weeks for any of our software by proceeding through some steps on the [evaluation page](#). After two weeks of testing if desired you can extend the evaluation period by additional free 6 weeks using a formal license agreement, which you will receive automatically via email.
- Birte Seebeck, a PhD student from Prof. Dr. Matthias Rarey's group at the Center for Bioinformatics in Hamburg (new metal handling in docking) and Christoph Hartmann, a PhD student from Prof. Dr. Thomas Lengauer's group both won a poster prize at the New Approaches in Drug Design and Discovery in Rauschholzhausen. The work was on improving FlexX-metal handling and the selection of most probable side-chain conformations in proteins, respectively.
- **Dates for your diary:** BioSolveIT will be present at the following conferences:

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|--------------------|--|
| July 29 - August 3 | GRC Computer Aided Drug Design, Tilton, NH, USA. |
| August 19-23 | 234 th ACS Fall Meeting, Boston. BioSolveIT will talk about ' Docking ligands into challenging targets using single interactions and an appropriate metal description ' and ' FlexX-Screen: Interactive Virtual Screening ', and exhibiting at booth 951 . |
| September 16-21 | Sommerschule Wirkstoffdesign, Vienna, Austria. |

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

literature corner

From Modeling to Medicinal Chemistry: Automatic Generation of Two-Dimensional Complex Diagrams

Katrin Stierand and Matthias Rarey

Chem. Med. Chem., 2 (6), 853 - 860 (2007)

[details here](#)

Chemical Fragment Spaces for de novo Design

Harald Mauser and Martin Stahl

J. Chem. Inf. Model., 47 (2), 318-324 (2007)

[details here](#)

Homology Modeling of Human Fyn Kinase Structure: Discovery of Rosmarinic Acid as a New Fyn Kinase Inhibitor and in Silico Study of Its Possible Binding Modes

Dubravko Jelic, Boris Mildner, Sanja Kostrun, Krunoslav Nujic, Donatella Verbanac, Ognjen Culic, Roberto Antolovic, and Wolfgang Brandt

J. Med. Chem., 50 (6), 1090-1100 (2007)

[details here](#)

upcoming articles

- FTrees^{XL} – FTree's next generation
- [ReCore](#) – 3D Scaffold hopping by core replacement

contact

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