



Welcome to the 9th edition of the BioSolveIT newsletter!

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

BioSolveIT now sole distributor of all its products

Many of you will have seen our press release about the [new independence of BioSolveIT](#). As of July 1st, BioSolveIT will service all its end-user customers directly. This step concludes a tremendously successful period of collaboration and opens the door to a wide spectrum of new opportunities.

For many years Tripos™ and BioSolveIT had a successful development/distributor partnership and served scientists around the world with cutting-edge virtual screening technology. However, the ability to now work directly with users worldwide offers a great opportunity to stay ahead of the competition and continue to be the premier supplier of drug discovery software.

So what consequences will this have for our customers? Here are the most important ones:

- Direct contact with the software developers: 'Tell us your needs and they will be considered'
- Instantaneous access to updates and upgrades: 'BioSolveIT follows an aggressive release schedule'
- Independence from other software: 'Now it's your choice of environment in which to use FlexX'
- New user interfaces: 'Both an interface in MOE™ and a GUI for the standalone version are in development'

Great care has been taken to ensure that the change of relationship will take place virtually seamlessly for the existing customer base. Existing contracts will not be affected by the change. These users will continue to be serviced as defined in their respective contracts. This includes support, updates and upgrades. BioSolveIT will support Tripos in order to ensure such services. New contracts, however, will be issued by BioSolveIT.

Customers frequently compliment us for our support that goes way beyond the ordinary. For example, Robert Kiss from Semmelweis University in Hungary recently commented: "BioSolveIT's support is outstanding!" To benefit from the highest level of service, please visit our [web site](#), and order your evaluation copy of FlexX, FlexS or FTrees today. Or, if you have specific requirements for special development or consulting in mind, write to contact@biosolveit.de. We are custom software solution providers and are confident that we can offer you the best possible solution to your problem.

BioSolveIT @ ACS, San Francisco

BioSolveIT will be present at this year's [Fall ACS Meeting in San Francisco](#). Visit us at [booth 427](#) and learn about the latest developments from one of the leading software providers for drug discovery in the pharmaceutical industry. There will be software presentations, raffles, booth parties and lots of other interesting stuff. Receive special rates 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 as you plan your itinerary. This overview may serve as a guideline:

- **Wendy Sanderson** (Johnson & Johnson): COMP 21 – [Complementarity of FTrees and Tanimoto similarity, clustering, and Bayesian learning in the search for Alpha 7 nAChR ligands](#)
8:30 AM-12:00 PM, Sunday, 10 September 2006, Moscone Convention Center – Room 236
- **Juri Paern** (ZBH): COMP 23 – [2D visualization and constraint-driven enumeration of chemical fragment spaces](#)
8:30 AM-12:00 PM, Sunday, 10 September 2006, Moscone Convention Center – Room 236
- **Markus Boehm** (Pfizer): CINF 11 – [Similarity searching in large virtual chemistry spaces derived from synthetically accessible combinatorial libraries](#)
9:00 AM-11:30 AM, Sunday, 10 September 2006, Moscone Convention Center – Room 125
- **Holger Claußen** (BSI): COMP 178 – [Recent developments in the FlexX family](#)
1:00 PM-4:15 PM, Tuesday, 12 September 2006, Moscone Convention Center – Room 236
- **Iris Antes** (MPI): COMP 176 – [Inhibitor based refinement of homology modeled protein structures for molecular docking](#)
1:00 PM-4:15 PM, Tuesday, 12 September 2006, Moscone Convention Center – Room 236

- **Christian Lemmen (BSI):** CINF 79 — [Recent advances in molecular docking](#)
2:00 PM-5:50 PM, Tuesday, 12 September 2006, Moscone Convention Center — Room 122
- **Andreas Kämper (MPI):** COMP 327 — [Use of metal coordination geometry to improve FlexX docking](#)
8:30 AM-11:45 PM, Wednesday, 13 September 2006, Moscone Convention Center — Room 236
- **Iris Antes (MPI):** BIOL 211 — [DYNAPRED: Combining docking and sequence based methods for the prediction of MHC/peptide complexes for vaccine design](#)
4:30 PM-6:30 PM, Wednesday, 13 September 2006, Moscone Convention Center — Hall D (Poster)

Please visit us at the booth to learn about the latest developments at BioSolveIT. A selection of planned presentations:

- Mouse Click Docking: A GUI for FlexX that will set new standards in user-friendliness and functionality
- FlexX Loves MOE: CCG's renowned Molecular Operating Environment supports FlexX through an intuitive interface
- FTrees Made Easy: A GUI for FTrees facilitating million-compound screening
- Warp Speed Docking: The new performance booster module, FlexX-Screen
- and many more

[4th FlexX Docking Workshop to close registration soon](#)

This year's docking workshop will be held at the [SUN](#) campus in Santa Clara, California ([location in Google Earth](#)), located just 50 miles south of downtown San Francisco. Learn how to best exploit all the details and features of FlexX Release 2, the latest technology in drug discovery. A detailed agenda can be accessed at [our website](#). [Register now](#), there is still limited availability! Comments from former participants:

- "This is how a workshop should be."
- "The workshop is challenging, and I do feel that I know FlexX now in depth."
- "For a FlexX novice this is the big picture."

Save time and money by attending this workshop — you will be much more productive in a shorter time and acquire in-depth knowledge that will last longer than just the next project!

[next generation docking: FlexX-Screen](#)

With [FlexX-Screen](#), BioSolveIT is introducing a speed booster to FlexX docking. From the release of FlexX-Screen, docking will be exponentially faster — yet without sacrificing accuracy.

The FlexX-Screen module has been developed with a focus on screening millions of compounds. It incorporates two novel developments: the FlexX-Scan functionality by [Schellhammer et al.](#) (*PROTEINS: Structure, Function, and Genetics* 2004, vol57, p504-517) and a heavily exploitable caching strategy. The two have been merged in a perfect symbiosis — although they can still be activated and configured separately. Apart from making one or two settings, the user will simply notice that docking has already completed. As an example, in-house experiments on 800,000 compounds completed within 150 minutes on 300 CPUs. This means you can easily dock (with the same set-up) 7-8 million compounds a day! Our sophisticated clientele has been used to the speed of FlexX for a decade already. Robert Kiss from Semmelweis University in Hungary says: "We chose FlexX for the world's largest structure-based in-silico screening for its speed and reliability. And right we were!" In the future, using FlexX-Screen, immensely large screening runs will take just a fraction of your valuable time. The module will be available with the advent of FlexX Release 2.1 later this year. Interested users should please [contact us now by email](#).

[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. This time: The shell escape — call other programs and tools from within a FlexX session or script. [Read more!](#)

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

- **"Rule-of-Five" author Christopher A. Lipinski joins Advisory Board of BioSolveIT**
Dr. Christian Lemmen, CEO of BioSolveIT, is delighted with Dr. Lipinski's appointment: "Chris Lipinski will have a tremendous impact on our endeavors to supply top-flight software. With his experience we have a strong advocate for the needs of the application scientists on board. It will help us focus on the application and applicability of our technology". [Read more!](#)
- **Prof. Hugo Kubinyi will be honored with the 2006 Skolnik Award** at the ACS Fall Meeting in San Francisco "for his extensive contributions to cheminformatics, QSAR, and combinatorial chemistry through over 100 publications, six books, and over 35 years of active service in drug design".
- **BioSolveIT supports multinational fight against malaria**
Thanks to free FlexX docking software licenses, the first stage of the multi-million compound screening of the ZINC compound databases against *Plasmodium falciparum* completed successfully. [Read more!](#)
- **Availability of our latest conference presentations**
Dr. Carsten Detering presented a poster entitled "*Ultra-Fast De Novo Combinatorial Docking under Pharmacophore Constraints*" at CHI's 6th Structure-Based Drug Design Conference

literature corner

New leads for selective GSK-3 inhibition: pharmacophore mapping and virtual screening studies.

Dhilon S. Patel and Prasad V. Bharatam
J. Comput.-Aided Mol. Des. 20, 55-66 (2006)
[details here](#)

Current Status of Virtual Screening as Analysed by Target Class.

Martin J. Stoermer
Med. Chem. 2, 89-112 (2006)
[details here](#)

Successful computer guided planned synthesis of (4R)-thiazolidine carboxylic acid and its 2-substituted analogues as urease inhibitors.

KM Khan et. al.
Mol. Divers. 10, 223-231 (2006)
[details here](#)

upcoming articles

- "Now you can!" – FlexX-Pharm and combinatorial chemistry go hand in hand.

contact

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