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# BioSolveIT Newsletter

## Issue 06

### 22 June 2005

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Welcome to the sixth edition of the BioSolveIT newsletter!

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

#### FlexX docking workshop 2005

Following the success of our previous workshops (2003 at the ZBH in Hamburg and 2004 in Princeton, NJ, USA) we are proud to announce the 3<sup>rd</sup> FlexX workshop, which will take place November 10-11, 2005 in the vicinity of Bonn-Cologne, Germany. The workshop is designed as training for both novices and experienced users of FlexX. It will cover an in-depth introduction to the molecular docking program FlexX (Release 2) and in particular the following topics:

- Learn to use FlexX to its best and exploit the full power of its engine.
- Introduction to the new modules and features. These will give you extended functionality and significant improvements. Click [here](#) for more information on the new release.
- Ways to improve efficiency and accuracy as well as ways for tuning your docking calculations
- Optimising the high-throughput screening performance
- Grid/Cluster computing and workflow automation with FlexX
- Insight into FlexX's extension modules: FlexX<sup>C</sup>, FlexX-Pharm and FlexE

[Register](#) for the workshop today! We will raffle one free admission among the first ten!

#### FlexX 2 released!

*Good things come to those who wait!* Well, since Rome also wasn't built in a day, we issued Release 2 of our popular docking software FlexX a little later than planned, and we are grateful to all who have patiently awaited this major release.

The beta test phase was successfully completed by the beginning of May, and the feedback we received from our testers was exceptionally good; all of them reported improved accuracy and much faster calculations. Juergen Albrecht from SCLA Scientific Computing at [Bayer CropScience](#) (Monheim/Frankfurt, Germany) states: "This is the fastest FlexX ever. Compared to the previous versions, the computing speed has increased on average by a multiple of 2, with the same accuracy. In addition, the new FlexX Release 2 is more stable, too". Dr. Tanja Schulz-Gasch and Dr. Bernd Kuhn from Molecular Design at [Roche](#) (Basel, Switzerland) comment: "The new FlexX is more accurate than the previous versions. The average enrichment for our test set of seven proteins was found to be better with Release 2, with significant improvements for Neuraminidase and Gyrase B."

This praise was an impetus to improve our software even more and take the critique of all of our customers seriously, be it good or bad. After finishing the final touches, we issued FlexX Release 2 June 21, 2005. Learn [more](#) about the new release and [download](#) your evaluation copy today! We are sure you will appreciate the difference!

#### 2Ddraw – automated generation of 2D molecular sketches

"Visual inspection" cannot be beaten in lead design. And that's exactly why automated generation of 2D molecular sketches is of need everywhere. There are of course several tools around to do that. But today's problems go beyond simple drawing. Scientists today require 2D plots generated in a smart way – the layout should obey certain constraints:

Just think of [combinatorial libraries](#) – you would want to see assembled compounds lined up so you recognise their common building fragments and instantly spot the differences. It is tedious to let your brain re-orientate compounds before you can do the interesting part of your work.

Or consider [pharmacophore-based similarity searches](#): how much more powerful would it be to look at compounds oriented so that a common pharmacophore is reflected – compared to random orientation?

Also imagine searches with a given query structure: retrieved molecules should be 2D-aligned to the query structure. It will consequently be much easier to see common and different moieties or recognise a SAR in a whole series of compounds.

Above all, the system must be really fast and easy to use. You do not want to spend your time waiting when you are browsing through thousands of molecules.

All of this can now be accomplished with our drawing engine [2Ddraw](#). It draws compounds within milliseconds on standard PC hardware while simultaneously taking the constraints outlined above into account. This software was developed by [Patrick Fricker\\*](#), now in [Matthias Rarey's](#) group at the ZBH (Hamburg, Germany). It is distributed by BioSolveIT as a prototype for free testing. [Try it today](#). As a custom [solution provider](#), we'd be happy to implement your constraints or just integrate the engine in your particular software environment.

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\*Fricker et al., J. Chem. Inf. Comput. Sci. 2004, 44, 1065-1078.

## [Distributor – seamless distributed computing](#)

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As indicated in our last newsletter, we will give a detailed introduction to our all-purpose "paralleliser", the [Distributor](#). Developed by Frank Sonnenburg at BioSolveIT, it was first released last December and works with [POSIX-standard](#) batch-queuing systems ([PBS](#), [Sun GridEngine](#), [LSF](#), [Condor](#), etc.). The Distributor facilitates the handling of very large volumes of input data by decomposing the input files. These chunks are then sent to multiple machines in parallel. There is no restriction about the type of input data – it can handle even binary files! A typical Distributor workflow looks like this:

Instead of loading one big input file into some software tool (any command-line driven program will do), Distributor splits the input file(s) into manageable chunks and every chunk is stored in its own temporary working directory. Then Distributor puts the related jobs into the batch-queuing system. Finally it collects all the results in one place and deletes any temporary files after finishing its work. The user is notified by email about the progress of his compute tasks.

If we have aroused your interest, simply drop us an [email](#) today for a free evaluation in order to facilitate and speed up your computations!

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

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In keeping with good tradition, in this section we focus on aspects of FlexX that are either not very well known or sometimes misunderstood, thus we see them as important points to bring to your attention.

In this issue we take a closer look at [covalent docking](#). Many users don't even know that FlexX can not only dock fast, but also dock covalently bound ligands; one more reason to bookmark this spot for keeping informed of other interesting details about our software.

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](mailto:flexx-info@biosolveit.de).

## [BioSolveIT news in brief](#)

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**Industry co-operations:** BioSolveIT successfully completed a 3-year-project with [Bayer Cropscience](#) (Monheim/Frankfurt, Germany). Read [more](#) about an exciting project that resulted in an incredibly useful software-tool: the [Docking Database](#).

**Christof Gerlach and Peter Block** of [Prof. Klebe's](#) group in Marburg performed a benchmark test of FlexX Release 2 on several different architectures and presented their results in a [poster](#) at the [19<sup>th</sup> Darmstädter Molecular Modelling Workshop](#), which took place May 3-4 2005 in Erlangen, Germany.

**Date for your calendar:**

- July 31 - August 5, 2005: Dr. Christian Lemmen, CEO of BioSolveIT will participate at this year's Gordon Conference on Computer-Aided Drug Design ([GRC-CADD](#)) in Tilton, NH, USA: [Target Tailored Virtual Screening](#)

#### Availability of our latest conference presentations:

- BioSolveIT was present at the 7<sup>th</sup> International Conference on Chemical Structures (ICCS) in Noordwijkerhout, The Netherlands, June 5-9, 2005. Together with Hans Briem of [Schering AG](#) (Berlin, Germany), Dr. Holger Claussen [talked](#) about FlexX<sup>C</sup>-Pharm, a recent development with FlexX Release 2.
- Dr. Christian Lemmen gave a [detailed report](#) about FlexX 2 at last year's fall ACS meeting in Philadelphia and presented an [overview](#) about the docking database (DDB) at the ACS meeting in San Diego in March.

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

#### [literature corner](#)

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##### *Virtual Screening in Drug Discovery*

J. Alvarez and B. Shoichet (Eds)

[details here](#)

##### *Design of Small-Sized Libraries by Combinatorial Assembly of Linkers and Functional Groups to a given Scaffold: Application to the Structure-Based Optimization of a Phosphodiesterase 4 Inhibitor*

M. Krier, J.X. de Araújo-Júnior, M. Schmitt, J. Duranton, H. Justiano-Basaran, C. Lugnier, J.-J. Bourguignon, and D. Rognan

J. Med. Chem. 48 (11), 3816-3822 (2005)

[details here](#)

##### *Virtual docking approaches to Protein kinase B inhibition*

M. Forino, D. Jung, J.B. Easton, P.J. Houghton, and M Pellechia

J. Med. Chem. 48 (7), 2278-2281 (2005)

[details here](#)

#### [upcoming articles](#)

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- FTrees goes WWW
- More information about the docking database (DDB)

#### [contact](#)

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