



Molecular Networks

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BioSolveIT GmbH and Molecular Networks GmbH win BMBF funding for € 2 Million Project

**Federal funding for the development of a technology platform
for *de novo* design of lead compounds**

St. Augustin and Erlangen, Germany October 6th, 2004—BioSolveIT GmbH and Molecular Networks GmbH today announced that they have been awarded a three-year development grant from the BMBF, through its BioChance+ programme. With the *NovoBench* project, the German ministry supports the development of a new technology platform for *de novo* design of lead compounds with high propensity of being biologically active and synthetically feasible. The heart of this platform is an integrated collection of virtual screening tools that facilitate *in silico* synthesis of chemical fragments optimized towards certain target-dependent properties.

Both companies participate equally in the grant and anticipate significant commercial applications for the new platform. They will work closely together with the research groups of Prof. Matthias Rarey from the Center for Bioinformatics, at the University of Hamburg and Prof. Johann Gasteiger from the Computer Chemistry Center, at the University of Erlangen-Nuremberg. The consortium is completed by three internationally operating pharmaceutical companies, which will contribute significantly to the development of the project and provide testing capabilities to ensure, that the development will meet the needs of the pharmaceutical industry.

The award underscores the German government's recognition of the need for building joint development teams between academic institutions and small and large industry to bridge the gap between the research lab and the marketplace, stimulating prosperity through innovation. According to Bain&Co for the Study of Drug Development, the cost to develop a new drug and bring it to market is now more than \$1700 million. Current estimates attribute a large amount of drug development costs to drugs that did not make it to market because of adverse reactions and/or lack of efficacy.

"Finding new leads with a high probability to survive the later phases of the development process is one of the most challenging tasks in the pharmaceutical

industry” said Christian Lemmen, CEO of BioSolveIT. “We believe that the *NovoBench*-approach of *in silico* lead compound generation, using fragment-based virtual screening techniques and simultaneously assessing synthetic feasibility, can significantly shorten the drug discovery process. This grant will help BioSolveIT and our partners to develop technology for of building focused yet diverse compound libraries and to provide the industry with applications they need. We are very pleased to be able to move forward quickly in this area now.”

“We are honored by the solid vote of confidence in our both technology by the federal government that this grant represents,” said Jean-Pierre Kocher, CEO of Molecular Networks GmbH “The project highlights the growing importance of informatics in improving R&D performance and productivity. The project’s main goal is to enable higher quality decision support by ensuring that the scientist gets relevant data in an easy to use environment. Applying the concept of calculated synthetic feasibility has the potential to dramatically improve the accuracy of lead discovery decisions made by researchers. As such, this project fits directly into Molecular Networks’ core competence in helping companies bringing products to market faster through innovative and comprehensive IT solutions. The technology gains achieved by this project will further enhance Molecular Networks’ strategy at providing decision support for optimal productivity across the entire R&D value chain.”

About BioSolveIT

BioSolveIT GmbH (www.biosolveit.de) is a Bio- and Cheminformatics company. Its core businesses are software, services, and research collaborations. With three founders in academia, BioSolveIT has its backbone in research and catalyzes the genesis of products off of basic research successes. With a worldwide operating reseller, the companies software products reach a significant customer-base. Despite its youth (spin-off in 08/2001) BioSolveIT already constitutes a sizeable group of 15 permanent employees and a number of part-time assistants. The company's focus is on tool development for various research areas. Best known is its molecular docking software FlexX. With the FTrees program BioSolveIT took leadership in ultra-fast virtual high throughput screening using a fragment-reassembly based approach.

About Molecular Networks GmbH

Molecular Networks GmbH (www.mol-net.com) is a privately owned company established in 1997 that provides multifaceted, innovative software to the chemical, biotechnology and pharmaceutical industry. The company's suite of chemoinformatics applications covers many different areas including: handling of chemical information, design of new chemical entities and prediction of physicochemical and biological properties of chemical compounds. One of Molecular Networks' core strength is in the prediction of chemical reactivity. The company is a leader in the field of computer-aided synthesis design and planning of organic reactions. The company has licensed its products and services to more than 100 companies worldwide. Molecular Networks provides also custom-designed solutions.