



BioSolveIT and CCDC release World Class Fragments for Top Quality Drug Design

BioSolveIT and CCDC have released a world class set of virtual 3D fragments originating from small-molecule crystal data. The novel database can instantly be used for scaffold hopping and drug design within LeadIT, the latest BioSolveIT tool for mixed bench and computational chemistry research teams.

St. Augustin, Germany and Cambridge, UK, March 24th, 2010 – [BioSolveIT GmbH](#) in conjunction with [The Cambridge Crystallographic Data Centre](#) (CCDC) today announced the release of an exclusive set of fragments for 3D-based computational drug design. The Cambridge Structural Database (CSD) is a key global source for crystal structures and a major resource for the chemical and pharmaceutical industries. It provides the basis for the **highest quality input fragment data for successful fragment-based lead discovery (FBLD) with LeadIT**. Dr. Colin Groom, Executive Director of the CCDC said that “Precise crystal structure data is crucial for underpinning knowledge-based applications software. The CCDC is committed to combining the strengths of the CSD with third-party applications, and we are very pleased to be working with BioSolveIT in this capacity.”

“Accessing high quality X-ray data within the LeadIT platform provides the optimal fragment based lead discovery solution. Such stellar science, paired with a slick, click and go, user-centered design can be considered a breakthrough in computer-assisted drug design.” BioSolveIT’s recently released **LeadIT platform provides an aggressively simple approach to structure and fragment-based drug design**. LeadIT’s driving functionality is the scaffold replacement and fragment-based lead discovery algorithm, [ReCore](#), which has its scientific roots in the world famous Center for Bioinformatics (ZBH) at the University of Hamburg and the highly respected drug design group of Roche in Basel (WKN: 851311). Dr. Groom further commented that “ReCore is the leading 3D core replacement tool and provides an excellent platform for exploring the ever-expanding body of small-molecule crystal structure data available in the CSD. The CSD-based fragments have been shown to give the highest quality results for rescaffolding and we are delighted to make this available for the benefit of BioSolveIT and CCDC customers.”

Dr. Christian Lemmen, CEO of BioSolveIT, stated that “**Team building has been our guiding principle behind LeadIT**. A smooth and efficient collaboration with our colleagues at the CCDC allowed us to build on this strength. The instant results delivery and user-centered design of LeadIT allows researchers to work in an interactive, complementary fashion thus **bridging the gaps between computational and bench chemists**”. Dr. Lemmen further remarked “Accessing high quality X-ray data within the LeadIT platform provides the optimal fragment based lead discovery solution. Such stellar science, paired with a slick, click and go, user-centered design can be considered a breakthrough in computer-assisted drug design.”

The easily downloadable [LeadIT](#) was released in January 2010, its empowering mix of established structure-based drug design and the latest fragment based lead discovery methods is already in widespread use by many pharma and biotech companies. In a recent [JACS review](#), Dr. John H. Van Drie, a pioneer of computational chemistry, noted: “Software of this sort belongs on the desk of any chemist designing bioactive molecules.”

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About The Cambridge Crystallographic Data Centre



Originating in the Department of Chemistry at the University of Cambridge, the Cambridge Crystallographic Data Centre is now a fully independent institution constituted as a non-profit company and a registered charity since 1989. The CCDC curates the Cambridge Structural Database. This unique, scientifically rigorous database, built over 45 years, is the international standard for small-molecule chemical structures and has become an essential resource to scientists around the world. The CCDC also has a strong track record in basic research through more than 700 peer-reviewed publications.

About BioSolveIT



BioSolveIT GmbH (www.biosolveit.de), the custom scientific software development company for virtual screening and lead discovery offers tools, services, and research collaborations. With a stellar scientific advisory board and founders from academia who intensely collaborate with pharma, BioSolveIT catalyzes products off of university research successes with proven pharmaceutical industry application. BioSolveIT provides world-renowned software products within the areas of ligand and structure-based drug design and is the pioneer of computational fragment-based ligand design. BioSolveIT innovates breakthroughs in drug discovery by supplying smooth, user-centered designed tools bringing different researchers together for efficient multidisciplinary drug design.