



BioSolveIT and CCDC release CSD-based Fragments for Top Quality Scaffold Hopping

BioSolveIT and CCDC have released a world class set of 3D fragments originating from small-molecule crystal data. This novel database comes with an index for instant usage within LeadIT, the latest BioSolveIT tool for mixed medicinal and computational chemistry teams.

St. Augustin, Germany and Cambridge, UK, March 3rd, 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 virtual ligand 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 ligand design (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.”*

BioSolveIT’s recently released LeadIT platform provides an aggressively simple approach to structure and fragment based drug discovery. One of LeadIT’s driving functionalities is the scaffold replacement and FBLD 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. In a very smooth and efficient collaboration with our colleagues at the CCDC we were able 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 structural biologists, computational chemists, and medicinal chemists”*. Dr. Lemmen further remarked *“Accessing high quality X-ray data within the LeadIT platform provides the optimal FBLD solution. Such stellar science, paired with a slick, click and go, user-centered design can be considered a breakthrough in computer-assisted drug design.”*

While released only in January 2010, the empowering mix of established structure based drug design and the latest FBLD methods in LeadIT are already in widespread use by many pharma and biotech companies. In a recent JACS review, Dr. John H. Van Drie, a pioneer of virtual drug discovery, 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



www.ccdc.cam.ac.uk

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 which intensely collaborate with pharma, BioSolveIT catalyzes the genesis of products off of university research successes that are initially proven in the pharmaceutical industry. BioSolveIT provide 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 innovate breakthroughs in drug discovery by supplying smooth, user-centered designed tools to productively bring different researchers together for efficient multidisciplinary novel chemical entity development.