



## **Cambridge Crystallographic Data Centre and InhibOx Create New Powerhouse in Drug Discovery and Development Services**

**New service supports big pharma's drive to outsourcing by offering highly sophisticated technologies for drug discovery with cloud computing and software-as-a-service facilities**

**Oxford and Cambridge, UK, 6<sup>th</sup> July 2010.** InhibOx Ltd (Oxford, UK) and the Cambridge Crystallographic Data Centre (Cambridge, UK) announce they that have joined forces to create a uniquely powerful drug discovery service offering. Users of the new service will benefit from the shared depth of expertise that includes extensive commercial drug discovery experience and from the leading proprietary technologies developed by the Oxford and Cambridge bodies.

The combined service offers pharmaceutical, biotech and governmental research organizations access to new capabilities to accelerate drug discovery and improve productivity. It includes full-spectrum computer-aided drug discovery (CADD) from receptor site modeling, through lead identification, lead optimization, and ADME property prediction to formulation modeling. The new service offers life science companies a step-change in the quality and effectiveness of CADD services through the use of leading proprietary technologies and databases, applied by scientists with deep commercial drug discovery experience.

The Cambridge Crystallographic Data Centre (CCDC) is a not-for profit organization, established in 1965. It supports drug discovery through its industry-standard Cambridge Structural Database (CSD), containing more than half a million small molecule crystal structures, and through knowledge-based tools to support receptor modeling, ligand design, docking, lead optimization and formulation studies. Its database and modeling systems are in use at research operations worldwide, including at all of the world's top pharmaceutical companies.

InhibOx, the Oxford-based drug discovery service specialist, was founded in 2001 and has developed Scopus: the world's largest curated database of drug candidate molecules. Scopus offers multiple-conformation 3D structures, shape and charge descriptors, physical and ADME properties and commercial availability information. It has also developed proprietary drug discovery technologies to support target- and ligand-based lead identification, fragment-based de novo design methods and formulation modeling. It is pioneering the use of cloud computing and Software-as-a-Service delivery methods to offer no-compromise, on-demand lead identification and optimization services which have demonstrated dramatically improved results over traditional HTS and virtual screening methods.

The two bodies have set up a joint team to commercialize and support the new service and will share operating expenses and revenues. Sales and service operations for the new, combined service are based out of Oxford and Cambridge, UK and Princeton, NJ. The two organizations will also collaborate on the



development of new approaches to bring scientific breakthroughs and productivity benefits to all aspects of computer-aided drug discovery, delivering the greatest possible rigor to the process.

The driving force behind the alliance came from the CCDC's global and evolving user community. "We have been asked more and more frequently by our users whether we can bring to bear our in-house drug discovery experience to address their research challenges" said Dr Colin Groom, Executive Director at CCDC. "The alliance with InhibOx gives us the breadth of technology and a focused team to meet this demand. We at CCDC are keen to do more work with our users across the research community and this exciting development will take us forward rapidly to be able to achieve this."

"The timing could not be better," explained Paul Davie, CEO of InhibOx. "The drive to outsourcing by major pharmaceutical enterprises, and the resulting emergence of a new wave of biotechs and CRO's, has created a sudden need for high quality computer-aided drug discovery services. CADD cannot be delivered effectively by companies with just point solutions or a few off-the-shelf tools. This partnership gives the industry what it really needs – a full spectrum, best of breed service offering, delivered by a team with real world drug design and development experience in companies such as Pfizer, GSK, UCB, ICI, Dow and several of the world's top academic institutions."

The InhibOx-CCDC team is offering a flexible scale of services, ranging from focused problem solution provision through to complete drug discovery project assignments.

#### **About Cambridge Crystallographic Data Centre**

Originating in the Department of Chemistry at the University of Cambridge, the CCDC is now a fully independent institution constituted as a non-profit company and a registered charity since 1989. The CCDC is financially independent, through annual subscriptions received for CSD System and industry leading software such as GOLD and Relibase. The CCDC has a strong track record in basic research through more than 700 peer-reviewed publications; these papers have attracted more than 18,000 citations in the international scientific literature. More than 1,500 CSD applications papers by non-CCDC authors have been similarly well received.

#### **About InhibOx**

InhibOx delivers novel and effective computational methods for drug discovery to improve the productivity of lead and candidate identification and optimization, through consultancy and software-as-a-service channels. The company is a pioneer in the application of cloud computing to drive very large scale computation at high accuracy, bringing for the first time no-compromise computational drug discovery processes to bear in pharmaceutical and biotech research. InhibOx was founded by Professor W. Graham Richards, former Chairman of Chemistry at the University of Oxford and world-leading computational chemist. The company grew from the outstandingly successful Screensaver Lifesaver project which involved some 3.5 million personal computers in over 200 countries: the world's biggest computational chemistry experiment finding lead compounds to inhibit cancer targets, anthrax and smallpox. Since then, InhibOx has built up a proprietary technology platform in computer-aided drug



design, funded by VCs, private investors, Oxford University and EU grants. Ongoing activities comprise the development of entirely novel computational drug discovery methods; building Scopus, the world's largest curated database of 3D structures and properties, and their delivery to the life science industries.

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