

Open access drug discovery database launches with half a million compounds

Hinxton and London, 18 January 2010 – ChEMBLdb, a vast online database of information on the properties and activities of drugs and drug-like small molecules and their targets, launches today with information on over half a million compounds. The data lie at the heart of translating information from the human genome into successful new drugs in the clinic.

The database is hosted by the European Molecular Biology Laboratory's European Bioinformatics Institute (EMBL-EBI). It was transferred from biotech firm Galapagos NV in July 2008 through a £4.7 million Strategic Award from the Wellcome Trust.

ChEMBLdb is a unique resource because of its focus on drug discovery and its size: information on an additional 100,000 compounds has been added to the database for its launch, taking the number of small molecules to over 520,000, and it contains over 2.4 million records of their effects on biological systems. The data include information about how small molecules bind to their targets, how these compounds affect cells and whole organisms, and information on the molecules' absorption, distribution, metabolism, excretion and toxicity.

Dr John Overington, leader of the ChEMBL team at EMBL-EBI, said: "We hope ChEMBLdb will assist the translation of genomic-based insights into innovative drug therapies. We are pleased that there has already been big demand for ChEMBLdb data – not only from large pharmaceutical companies but also from academic institutions and small companies who will particularly benefit from free access to the data."

The human genome sequence provided a molecular 'parts list' for a human being, comprising all the genes and proteins that are encoded by our genetic blueprint. In order to develop new medicines, it is important to catalogue how each of these 'parts' interacts with drugs and drug-like molecules. ChEMBLdb brings together information from the interface of the genome with chemistry into a set of 'chemogenomic' databases that can be used to help determine whether a particular molecule has the right properties to make an effective drug.

Professor Janet Thornton, Director of EMBL-EBI, said: "We are delighted to augment the biological data archived and served from EMBL-EBI with the ChEMBLdb resource. The database adds an important new capability to address the needs of the pharmaceutical and biotechnology industries, and provide the academic chemical biology communities with previously inaccessible data."

Dr Alan Schafer, Director of Science Funding at the Wellcome Trust, said: "This unprecedented transfer of pharmaceutical data resources from the private sector to the public domain should have the greatest impact on researchers in academia and in small companies on limited budgets. ChEMBLdb will be a major resource of information for driving forward medicinal chemistry and drug development in the UK and internationally."

The launch of ChEMBLdb is accompanied by the release of Kinase SARfari, an integrated resource of sequence, compound and screening data from a variety of sources for the protein kinases, a key family for drug discovery. ●

www.ebi.ac.uk/chemblpdb/

Contact:

contactpress@ebi.ac.uk

Katrina Pavelin, EMBL-EBI Scientific Outreach Officer, Hinxton, UK, Tel: +44 (0)1223 494452, katrina@ebi.ac.uk

Louisa Wright PhD, EMBL-EBI Outreach Programme Project Leader, Hinxton, UK, Tel: +44 (0)1223 494665, louisa@ebi.ac.uk

Craig Brierley, Senior Media Officer, The Wellcome Trust, Tel: +44 (0)20 7611 7329, c.brierley@wellcome.ac.uk

About EMBL-EBI:

The European Bioinformatics Institute (EBI) is part of the European Molecular Biology Laboratory (EMBL) and is located on the Wellcome Trust Genome Campus in Hinxton near Cambridge (UK). The EBI grew out of EMBL's pioneering work in providing public biological databases to the research community. It hosts some of the world's most important collections of biological data, including DNA sequences (EMBL-Bank), protein sequences (UniProt), animal genomes (Ensembl), three-dimensional structures (the Protein Databank in Europe), data from gene expression experiments (ArrayExpress), protein-protein interactions (IntAct) and pathway information (Reactome). The EBI hosts several research groups and its scientists continually develop new tools for the biocomputing community.

www.ebi.ac.uk

About EMBL

The European Molecular Biology Laboratory is a basic research institute funded by public research monies from 20 member states (Austria, Belgium, Croatia, Denmark, Finland, France, Germany, Greece, Iceland, Ireland, Israel, Italy, Luxembourg, the Netherlands, Norway, Portugal, Spain, Sweden, Switzerland and the United Kingdom) and associate member state Australia. Research at EMBL is conducted by approximately 80 independent groups covering the spectrum of molecular biology. The Laboratory has five units: the main Laboratory in Heidelberg, and Outstations in Hinxton (the European Bioinformatics Institute), Grenoble, Hamburg, and Monterotondo near Rome. The cornerstones of EMBL's mission are: to perform basic research in molecular biology; to train scientists, students and visitors at all levels; to offer vital services to scientists in the member states; to develop new instruments and methods in the life sciences and to actively engage in technology transfer activities. EMBL's International PhD Programme has a student body of about 170. The Laboratory also sponsors an active Science and Society programme. Visitors from the press and public are welcome. www.embl.org

About the Wellcome Trust

The Wellcome Trust is the largest charity in the UK. It funds innovative biomedical research, in the UK and internationally, spending over £600 million each year to support the brightest scientists with the best ideas. The Wellcome Trust supports public debate about biomedical research and its impact on health and wellbeing. www.wellcome.ac.uk

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