

The Pistoia Alliance and EMBL-EBI announce HELM collaboration for cheminformatics

EMBL-EBI is collaborating with the Pistoia Alliance, a precompetitive industry and innovation initiative, to improve data resources for the study of pharmaceutically relevant molecules. During 2014 ChEMBL, EMBL-EBI's database of bioactive entities with over a million compounds, will incorporate the Hierarchical Editing Language for Macromolecules (HELM) notation, a Pistoia Alliance-led standard in biomolecular informatics.

Bioinformatics and cheminformatics have advanced extremely rapidly in the past five years, thanks to the steady increase in publicly shared data and chemistry software tools. But as the development of new classes of drugs has increased, so has the demand for standard informatics methodologies that can be used to study larger, more complex molecules.

HELM can be used to represent simple macromolecules like oligonucleotides, peptides and antibodies. But it goes a step further by enabling the representation of very complex entities such as those with unnatural amino acids, or conjugated species such as antibody-drug conjugates. ChEMBL, a comprehensive repository of information about bioactive drug-like molecules, covers over a million compounds with 12 million associated bio-assay measurements on nearly 10,000 targets. Incorporating the HELM standard into ChEMBL's data pertaining to peptide-derived drugs and compounds will provide pharmaceutical researchers with the means to query these data in new ways.

Sergio Rotstein, Director of Research Business Technology at Pfizer, is the HELM project lead for the Pistoia Alliance. He says, "The integration of HELM into ChEMBL represents a significant step forward in facilitating the exchange of bio-molecular information within the life-sciences R&D ecosystem. We are thrilled to see a key institute like the EBI joining the growing list of HELM adopters."

John Overington, Head of Chemogenomics and Molecular Systems Resources at EMBL-EBI, says, "We are pleased to be among the first content providers to incorporate this innovative macromolecular information standard, and hope this will lead to the development of value-creating tools for researchers working in protein engineering and drug design."

John Wise, Executive Director of the Pistoia Alliance, says, “It is very rewarding that the EBI, a member of the Pistoia Alliance, has recognised the importance of this emerging standard and is demonstrating such a strong commitment to it.”

HELM will be incorporated into the ChEMBL content for peptide-derived drugs and compounds in version 20.

About the Pistoia Alliance

The Pistoia Alliance is a global, not-for-profit, precompetitive alliance of life science companies, vendors, publishers, and academic groups that aims to lower barriers to innovation by improving the interoperability of R&D business processes. The Pistoia Alliance differs from standards groups because it brings together the key constituents to identify the root causes that lead to R&D inefficiencies and it develops best practices and technology pilots to overcome common obstacles.
www.pistoiaalliance.org

About EMBL-EBI

The European Molecular Biology Laboratory – European Bioinformatics Institute (EMBL-EBI) provides freely available data from life science experiments, covering the full spectrum of molecular biology. The services provided by EMBL-EBI are complimented by the Institute’s wide-ranging basic research activities, and supported by an extensive training programme. We are a non-profit, intergovernmental organisation funded by 21 member states and located on the Wellcome Trust Genome Campus in Hinxton, Cambridge, UK. www.ebi.ac.uk

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