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Announcing Support for HELM 2.0 (Hierarchical Editing Language for Macromolecules) in the Open Source Web Editor

The Pistoia Alliance, a global alliance of life science companies, vendors, publishers and academic groups, and Scilligence Corporation are pleased to announce the release of the major new extension to the HELM Web Editor. The new functionality enables the editor to support the representation of biomolecules with some structural uncertainty or ambiguity and also adds monomer and rule managers.

The therapeutic utilization of complex and unique biomolecules has become commonplace in drug discovery R&D. As a result, scientists have struggled to represent these entities in their informatics systems, forcing them to use various “pick and mix” approaches that include multiple nomenclatures and textual descriptions. HELM, the open biomolecular representation standard, has solved this problem by providing a means to represent various types of complex macromolecules (e.g. nucleotides, proteins, antibodies and antibody-drug conjugates) including the ones that contain unnatural amino acids or nucleotides/nucleosides.

The Pistoia Alliance formalized the HELM notation, originally developed by scientists at Pfizer, as an open standard in early 2013. The related toolkit and editor were later publicly released to the open source community. Since its release, HELM has been widely adopted by various organizations such as Bristol Myers Squibb, Pfizer, Novartis, Roche, GSK, Ionis, Merck and Co, Scilligence, NextMove Software, Dassault Systèmes BIOVIA, ChemAxon, Perkin-Elmer, quattro research, EMBL-EBI, NCBI (PubChem), and RDKit.

While the original HELM solved the problem of representing unnatural complex biomolecules, it held the basic assumption that a scientist would know everything about the structures being represented. In biology, however, this is not always the case, as various types of ambiguity or uncertainty may exist in some of these structures. A typical example is when the exact conjugation site of an antibody-drug conjugate cannot be determined. This left scientists with a difficult choice: either record the

best guess of what the structure is or simply describe the structure textually instead of structurally, creating a gap in their corporate structural registries. This update to the web-editor enables scientists to incorporate into their structural representation a systematic description of a number of forms of ambiguity, thus allowing for the rigorous representation of structures, even when uncertainty is present.

“The HELM Web Editor already facilitates researchers’ ability to rigorously represent complex macromolecules in a technology-friendly manner. However, there was still a gap when it came to dealing with the very real-world scenario of structural uncertainty or ambiguity. Through this partnership with Scilligence, we have implemented the enhancements available in HELM2.0 and further extended the capabilities and applicability of the open source tools,” said Sergio Rotstein, Director of Research Business Technology at Pfizer and Domain Lead for the Pistoia Alliance HELM initiative.

About Pistoia Alliance

The Pistoia Alliance is a global, not-for-profit members’ organization made up of life science companies, technology and service providers, publishers, and academic groups working to lower barriers to innovation in life science and healthcare R&D. It was conceived in 2007 and incorporated in 2009 by representatives of AstraZeneca, GSK, Novartis and Pfizer who met at a conference in Pistoia, Italy. Its projects transform R&D through pre-competitive collaboration. It overcomes common R&D obstacles by identifying the root causes, developing standards and best practices, sharing pre-competitive data and knowledge, and implementing technology pilots. There are currently over 80 member companies; members collaborate on projects that generate significant value for the worldwide life sciences R&D community, using the Pistoia Alliance’s proven framework for open innovation.

<http://www.pistoiaalliance.org>

About Scilligence

Scilligence is a leading innovator of web-based applications for life science research and development. Scilligence’s proprietary technologies provide a complete solution for all research informatics needs. Scilligence’s software tools enhance the knowledge sharing and productivity of researchers in discovery and development of small molecule and biologic therapeutics.

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