HELM for Bioregistration

GSK will be making use of the Pistoia Alliance’s Hierarchical Editing Language for Macromolecules (HELM) notation to represent therapeutic large molecules in its bio-registration system, facilitated by the deployment of Dassault Systèmes BIOVIA’s Biological Registration solution. GSK scientists at sites around the world will use the system.

“There is a gap in the space that HELM now covers where there weren’t really any alternatives. It was desirable for GSK to be on a standard rather than create our own notation, and to partner with the Pistoia Alliance and other companies to develop that standard.”

Leah O’Brien, Business Consultant, GSK

Molecular Structure Exchange

Across the industry, there is a need for an advanced macromolecular structure data exchange format that can be used in support of collaboration and externalization. Collaborations between pharma companies and third parties, in particular with research organizations and CROs, are becoming more commonplace. A standard format and internal representation enables data integrity and streamlined communication with colleagues and collaborators. One of the advantages of adopting HELM for the Biological Registration solution deployed by BIOVIA at GSK is that HELM is already a recognized submission format by the FDA. It was therefore important that GSK’s solution should support HELM so that it would be easy to bring in existing molecules as well as those from collaborators.

HELM Converters: BIOVIA Pipeline Pilot contains components that provide broad support for the use of HELM to represent large biomolecules. In this example, a HELM string is converted into a chemical structure using the Molecule from HELM component before being converted back into HELM via the Molecule to HELM component. Components that support conversion to and from XHELM are also available.
In the past 10 years, biologicals have become an increasingly critical part of the GSK R&D pipeline and discovery research. Before this new system was rolled out, not all biologicals were registered and some very large and complex biologicals were shoehorned into the existing small molecule registration systems to get an ID number. The result was missing the rich biological genealogy data that comes with proper biological registration.

The use of HELM will mean that it will be much more straightforward to register, search, view and share data for biomolecules that do not fit neatly otherwise. HELM saves time for registration and prevents proliferation of bad data. Large molecule structures can be captured in a compact notation, tracked and accessed more easily. The new system will start with 75,000 biologicals lots registered.

“HELM has been evolving and becoming an emerging standard within the industry, so by embracing it we are able to provide applications that enable our customers to manage HELM-based data. They can then share this data with other parties that they collaborate with. It’s about enabling our customers to be successful.”

Neil Eccles, Senior Product Manager Biologics, Dassault Systèmes BIOVIA
Registration Required
Registration is required for data integration across many GSK systems, and while small molecule registration capability is well established in the wider industry, the industry has realized that bioregistration capabilities have been a critical and growing gap. As GSK selects more biopharmaceuticals as drug candidates it becomes a greater challenge to maintain data integrity without the appropriate registration capability.

As part of deploying BIOVIA’s Biological Registration product historical data has to be cleaned before migration to bring it on par with the quality of new registrations. This helps to align biologicals with existing best practice for chemical compounds, and gives GSK a point of entry for data about biologicals such as cell lines, plasmids, proteins and antibodies. Enhanced search capabilities also become possible, including scientific awareness of the biology hierarchy and a way to find similar biosubstances across multiple inventory systems. As a result, improved bioregistration helps GSK deliver medicines more efficiently.

The BIOVIA Biological Registration solution used at GSK is built on BIOVIA Pipeline Pilot and BIOVIA Foundation. Support for HELM has been built into this underlying infrastructure enabling BIOVIA to provide HELM capabilities across the full range of BIOVIA products. A major benefit of supporting HELM, and something that BIOVIA worked closely with the Pistoia Alliance to achieve, is the ability for end-users to use the HELM Editor to draw biological entities in applications such as BIOVIA Draw and Biological Registration, for registration. BIOVIA Biological Registration is now used by a large number of companies, with out-of-the-box HELM capability for everyone in the latest release.

In Line HELM Editor
BIOVIA Biological Registration:
The ability to directly call the HELM Editor in-line when registering entities such as antibody drug conjugates in BIOVIA Biological Registration makes it easier for scientists to enter HELM-based biomolecular data.
Sustainability

One of the key evidences of the future health of HELM is the recognition by the FDA that it is an acceptable submission format that is included in their guidance. A unique aspect of HELM is that both pharma and technology companies, through the Pistoia Alliance, have invested in its success and contributed towards its development, which places it in a strong position for retaining relevance and support and become an industry standard.

By working closely together with both BIOVIA and the Pistoia Alliance, GSK ensured that it was able to get the features it needed and collaborate with Biovia in developing the HELM standard to the level required to be of widespread utility. Both companies are Pistoia Alliance members and played key roles within the HELM project team.

From the start, GSK emphasized the need to be able to click and edit HELM structures within the BIOVIA Biological Registration solution rather than only being able to import and export, without introducing GSK-specific code that would be costly to support in future. Working with HELM and the BIOVIA team to prioritize support for GSK’s requirements in the development of the standard enabled GSK to achieve their goals while also allowing Biovia to create a solution that is available to the whole industry.

More information

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http://www.pistoiaalliance.org/

The HELM project website can be found at:
http://www.openhelm.org/
The HELM project team can be contacted by emailing:
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Pistoia Alliance: Lowering barriers to R&D innovation

The Pistoia Alliance is a global, not-for-profit alliance of life science companies, vendors, publishers, and academic groups that work together to lower barriers to innovation in R&D. Our members collaborate as equals on open projects that generate significant value for the worldwide life sciences community.