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Certara Introduces Version 19.6 of its D360 Scientific Informatics Platform

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The ability to analyze and visualize sequence-activity relationships in proteins and peptides added to D360's biologics toolkit for drug discovery research



Certara®, the global model-informed drug development and decision support leader, on 30 July 2019, announced the launch of version 19.6 of D360, its scientific informatics platform for drug discovery and development. Designed to meet the scientific researcher's need to quickly access, understand and share data, the D360 platform is delivered through its toolkits – small molecule discovery, biologics discovery, and pre-clinical translation – each tailored to meet specific research goals. This latest version of D360 takes its name from its release date; it is the 2019 mid-year release.

D360 v19.6 expands the platform's biologics discovery toolkit and world-class, self-service data access capabilities. D360 biologics discovery toolkit now enables representation, alignment, and analysis of peptide sequences and small sections of proteins in addition to oligonucleotide sequence representation. Peptide sequences can be aligned and colour-coded by the property, while areas of sequence difference can be highlighted. This provides sequence analysis capabilities that help users derive sequence-activity relationships to optimize bio profiles.

"We are proud to report that D360 now provides medicinally-relevant sequence alignment and analysis, adding support for peptide modalities in addition to its current uses for oligonucleotides, antibodies and antibody-drug conjugates. Knowledge extracted from aligned peptide sequences (and short protein segments) is used for rational design, focusing on the monomers and motifs responsible for desired biological activity profiles," said Dr David Lowis, Senior Director of D360 at Certara. "A key aspect of D360's new capabilities is the ability to align based on medicinally-relevant properties rather than traditional bioinformatics techniques, which examine evolutionary relationships. This alignment methodology is essential in the discovery and development of peptide therapeutics that are not limited to the 20 naturally-occurring amino acids."

D360's expanding biologics discovery toolkit aligns with the growing global biologics market, which is expected to reach $319 billion by 2021, according to The Business Research Company. Key categories are monoclonal antibodies, therapeutic proteins and vaccines. Additionally, almost 30% of US Food and Drug Administration (FDA) novel drug approvals are now biologics.

Responding to user feedback, Certara has enhanced D360's base capabilities by improving general data manipulation, formatting and filtering. Certara has also added box plot data visualizations to D360, allowing users to readily understand statistical data distributions of different classes of therapeutic agents.

Furthermore, knowing that scientists always desire access to new functionality but that new version enterprise deployments must take as little time and resources as possible, Certara has introduced a test automation tool with this new release. The test automation tool allows the automated execution of queries both as interactive and server-side tasks and allows comparison of results against a master set. This new automated test capability dramatically reduces the amount of manual testing required to deploy new versions of D360, and further reduces the platform's already industry-low maintenance overhead. D360 has the lowest administration and support overhead of products of its type because it gives users self-service access to the data.