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A.I. Coming to Certara's D360 Scientific Informatics Software

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New deep learning capabilities will provide data and insight to inform property prioritization, novel structure design and literature-based analyses.

PRINCETON, N.J., March 09, 2023 (GLOBE NEWSWIRE) -- Certara, Inc. (Nasdaq: CERT), a global leader in biosimulation, is adding deep learning capabilities to D360, a leading scientific informatics software platform. The addition of novel A.I. will enable discovery scientists to integrate multiple structured and unstructured data sources and substantially enhance predictions and analysis of content related to small molecules and biologic drugs for accelerated, high confidence decisions.

The upcoming rollout of D360 with advanced deep learning analytics include:

- **Automated Property Prediction –** Predictive deep learning models trained on public and proprietary chemical structure and biological data will provide quantitative or categorical predictions that improve substance prioritization.

- **Novel Structure Generation** – Deep learning models within D360 will create and optimize chemical structure ideas for assessment by discovery scientists. When combined with predictive models, users can assess newly generated chemicals alongside existing product compounds to extend the range of chemotypes relevant to project goals.

- **Access to Unstructured Data** – Traditionally, D360 has delivered insights from structured sources such as databases and web services. With the addition of large language models, users will be able to search and extract data from literature-based content to expand access to insights to inform research decisions.

The new D360 A.I. capabilities are based on the advanced data fabric and deep learning platform that Certara acquired from Vyasa. Vyasa Layar and associated applications are a proven deep learning platform providing analytics capabilities within a data fabric context.

"It is a pleasure to deliver deep learning-backed analytics within D360 shortly after becoming part of Certara," said Dr. Christopher Bouton, Head of A.I. at Certara and former CEO of Vyasa, "The capabilities being added to D360 are offering biopharmaceutical companies a seamless way to accelerate innovation and decision making in drug discovery."

"Our customers turn to D360 to provide them with the insights they need to make data-backed decisions across the early drug discovery pipeline. By applying these models to D360, our users are armed with the tools needed to expand these capabilities and accelerate their decision-making confidently. We are seeing momentum in our property prediction models as our first update and will continue to roll out additional analytical models for a deep learning within D360," added Leif E. Pedersen, President, Software at Certara.

Certara will be reviewing these capabilities from March 9-10, 2023, at Lab of the Future Congress booth #28 in Boston, USA.

About D360

D360 is a leading scientific informatics intelligence software used globally by over 6,000 discovery research scientists for small molecule and biologics discovery and pre-clinical translation. D360 includes toolkits and add-on products to provide state-of-the-art capabilities that go beyond standard data retrieval platforms. D360 has been deployed across a wide range of companies: from small biotech firms that need data access from a single data source to large global pharma companies that require a more comprehensive enterprise solution for data integration.

About Certara

Certara accelerates medicines using proprietary biosimulation software, technology, and services to transform traditional drug discovery and development. Its clients include more than 2,000 biopharmaceutical companies, academic institutions, and regulatory agencies across 62 countries.

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