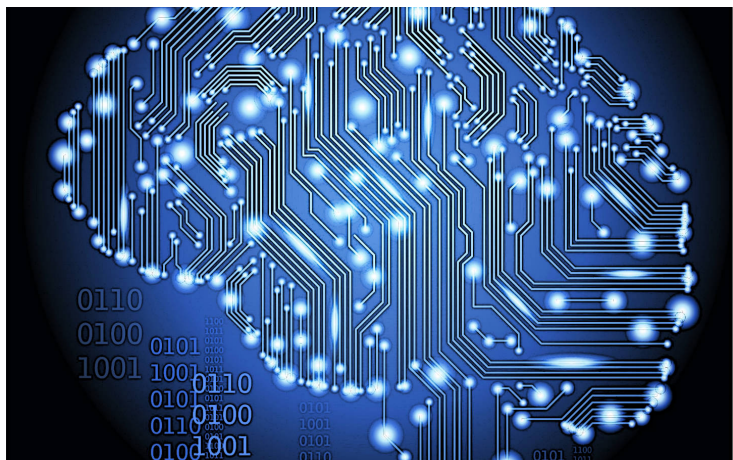# Cyclica announces integration of the POEM machine learning predictive engine

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Cyclica a leading biotechnology company that leverages artificial intelligence and computational biophysics to enable the discovery of new medicines.

Cyclica a leading biotechnology company that leverages artificial intelligence and computational biophysics to enable the discovery of new medicines, has announced the addition of a machine learning predictive engine called POEM to its Ligand Express platform. POEM has been applied to the prediction of ADMET (Absorption, Distribution, Metabolism, Excretion and Toxicity) properties, which provides critical insight into a molecule's expected behavior in the body. Unlike conventional quantitative structure activity relationship (QSAR) models that have existed in pharma for decades, POEM is parameter-free, based on multiple fingerprints, and does not require time-consuming model training.

Ligand Express, is a cloud-based platform that uncovers the polypharmacological profiles of small molecules, and allows scientists to gain insights into structural pharmacogenomics by incorporating systems biology databases including single nucleotide variant data. With the integration of POEM, Ligand Express now offers insights into the pharmacokinetic properties of small molecules, providing a better understanding of the predicted behaviour of potential drug molecules. This integration will further augment workflows within pharma, providing scientists with a deeper understanding of a small molecule's polypharmacology and its key pharmacokinetic properties.

"Enabling more effective drug discovery through an integrated computational platform is a central tenant at Cyclica," said Naheed Kurji, President & CEO of Cyclica. "With the integration of POEM in Ligand Express, our users can readily access predictive ADMET properties of their small molecules in an elegantly designed user interface, enabling them to make effective decisions and bring better medicines to the market faster. We will continue to enhance Ligand Express with new features as we believe an end-to-end enabling platform will be essential to transform drug discovery."

"We recognize that drug discovery is a process, and part of that process requires the evaluation of many possibilities. It is impossible to pursue every possibility, so choosing the best starting point is essential, but it's not always easy," said Vijay Shahani, Head of Design of Cyclica. "We designed the user interface of POEM in Ligand Express to facilitate comparisons between multiple small molecules, making it easier to identify better starting points. We are actively developing new features to allow greater molecular exploration and enable the selection of top candidates."

Cyclica is committed to building out a platform that will facilitate effective drug discovery, and do more with artificial

intelligence to design medicines for patients. The integration of POEM into Ligand Express further demonstrates Cyclica's commitment to accelerating pharma R&D, and making drug discovery faster, cheaper, and safer.

On May 22nd at the Collision Conference in Toronto, Cyclica will announce its novel, first-in-class, multi-objective, drug design technology, which also incorporates POEM.