

Collaborations Pharmaceuticals, Inc. Awarded A Phase II SBIR award from NIEHS/NIH to Develop MegaTox® software

RALEIGH, NC, USA, August 1, 2022 /EINPresswire.com/ -- The National Institute of Environmental Health Sciences (NIEHS) has awarded \$1,710,006 to Collaborations Pharmaceuticals, Inc. (CPI) to develop new capabilities in their [MegaTox®](#) machine learning software that will be used for environmental, consumer product and drug discovery applications.

"CPI developed MegaTox® software to provide a comprehensive collection of ADME/Tox machine learning models. Pharmaceutical, consumer products, agrochemical and other chemistry focused companies possess structure-activity data generated over many

decades of screening that is not in the public domain, and this data is primarily only accessible to the cheminformatics experts in each company. Outside of these companies small pharmaceutical, biotech companies and academics must rely on data from public databases, commercial databases and their own data. Integrating such data from diverse sources and processing with algorithms to build machine learning models that can help to enable predictions for new compounds is an important undertaking. In Phase I of this project, we have developed the prototype for MegaTox®, we curated toxicity datasets then generated and tested hundreds of models. We also collaborated with numerous academic laboratories and performed fee-for-service work with multiple commercial companies to apply these models. We are excited by this Phase II award as it will enable us to integrate novel graph-based and other machine learning models, apply read across and adverse outcome pathway methods as well as generate validated models for in vivo data for non-mammalian species that can be licensed by other companies so they can benefit from our expertise." said Sean Ekins, CEO, CPI.

We expect to develop thousands of additional ADME/Tox models over the course of this project.



**COLLABORATIONS
PHARMACEUTICALS, INC.**

Collaborations Pharmaceuticals logo

We are not aware of any other company pursuing such an approach to both generate new high value datasets or models, performing testing of their own models and creating a wide array of toxicity models. MegaTox® is a product available for licensing by pharmaceutical, consumer product, agrochemical and regulatory groups as well as used in our fee-for-service consulting. The models generated could also be used for generative AI approaches such as those applied in our [MegaSyn](#) product. With such a wide array of models and approaches to address customer needs MegaTox® can be applied in various companies or organizations to aid in decision making or in regulatory submissions.



Disclaimer

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About Collaborations Pharmaceuticals, Inc.

Collaborations Pharmaceuticals, Inc.® has developed software for data curation and machine learning called [Assay Central](http://www.assaycentral.org)® (www.assaycentral.org) as well as curated model bundles in MegaTox®, MegaTrans® and MegaPredict®. Most recently we have developed MegaSyn and UV-adVISor. CPI performs research and development on innovative therapeutics for multiple rare and neglected diseases and is located in laboratories in the NC State Incubator at Centennial campus. We have considerable experience with preclinical and computational approaches to drug discovery and toxicity prediction. For more information, please visit <http://www.collaborationspharma.com/>

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