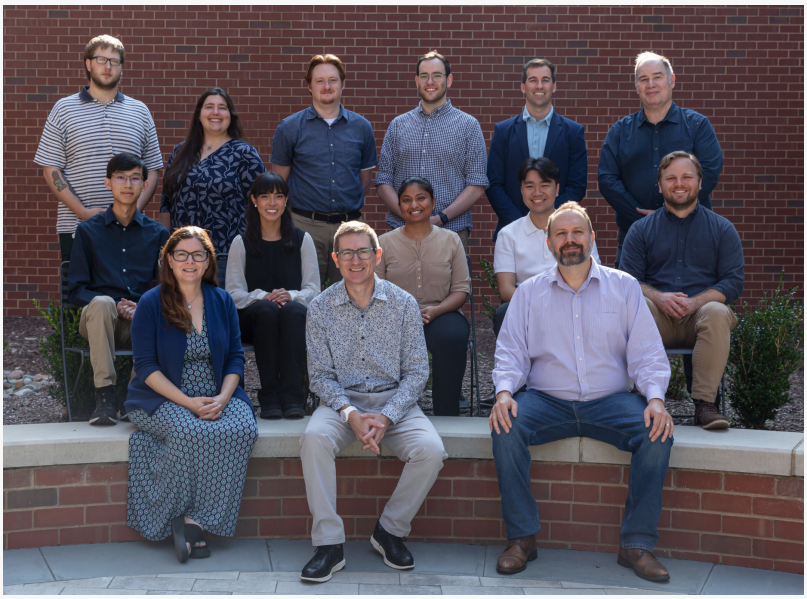
Collaborations Pharmaceuticals, Inc. Awarded over $2M Grant to develop Acetylcholinesterase Reactivators with Battelle

NIEHS has awarded a $2,044,647 SBIR grant to Collaborations Pharmaceuticals, Inc. to develop new acetycholinesterase reactivators with Battelle



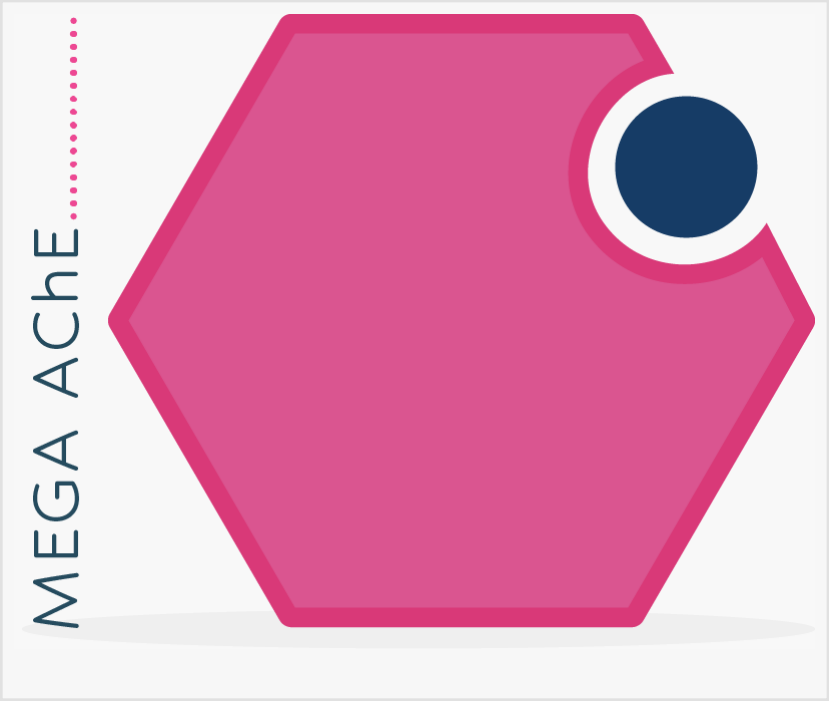
Collaborations Pharmaceuticals team photo 2024

Collaborations Pharmaceuticals logo

RALEIGH, NC, UNITED STATES, September 4, 2024 /EINPresswire.com/ -- Organophosphorus (OP) compounds are involved in nearly three million poisonings per year worldwide, resulting in 300,000 deaths. OPs bind to the enzyme acetylcholinesterase (AChE) and this causes acetylcholine to accumulate, resulting in the overstimulation of the affected neurons. Acetylcholinesterase inhibitors like OPs are used as pesticides as well as nerve agents. Some of the adverse effects of pesticides also have occurred on non-target organisms such as fish, amphibians and humans.

“Funding from NIEHS has previously enabled us to build computational and machine learning approaches to model AChE and the closely related enzyme butyrylcholinesterase (BChE) in order to perform virtual screening to identify new inhibitors and validate these models. These models served as the foundation for a new software product called MegaAChE,” said Dr. Sean Ekins,

Collaborations Pharmaceuticals, Inc. (CPI) CEO. “Computational models for AChE therefore have beneficial dual-use potential both for identifying molecules that could have environmental or human toxicity, while alternatively such machine learning models could also help us identify molecules with therapeutic utility for Alzheimer’s disease or as treatments for poisoning.”.



“We now propose to further develop our MegaAChE software for prediction of AChE and BChE inhibition and incorporate uncertainty prediction features and new algorithms such as large language models which may have advantages for prediction,” Ekins said. Current treatments for patients exposed to AChE inhibitors include the administration of reactivators such as 2-PAM. The limitations of these existing molecules are that they have poor brain exposure. MegaAChE can be put to use alongside our generative design software MegaSyn to design and develop new AChE reactivators that cross the blood brain barrier with Battelle which will perform in vitro testing.

“These collaborative efforts could provide a new treatment for OP pesticide and nerve agent exposure,” Dr. Ekins said.“Our ultimate goal will be to develop our MegaAChE software as a commercial product so that others can predict if the molecules they design are likely to inhibit these environmentally and therapeutically relevant targets. In addition, we will develop new molecule intellectual property around AChE reactivators,” said Dr. Ekins.

About Grant

2R44ES033855-02 from NATIONAL INSTITUTE OF ENVIRONMENTAL HEALTH SCIENCES

About Battelle

Every day, the people of Battelle apply science and technology to solving what matters most. At major technology centers and national laboratories around the world, Battelle conducts research and development, designs and manufactures products, and delivers critical services for government and commercial customers. Headquartered in Columbus, Ohio since its founding in 1929, Battelle serves the national security, health and life sciences, and energy and environmental industries. For more information, visit www.battelle.org.

Sean Ekins
Collaborations Pharmaceuticals, Inc.
+1 215-687-1320
email us here