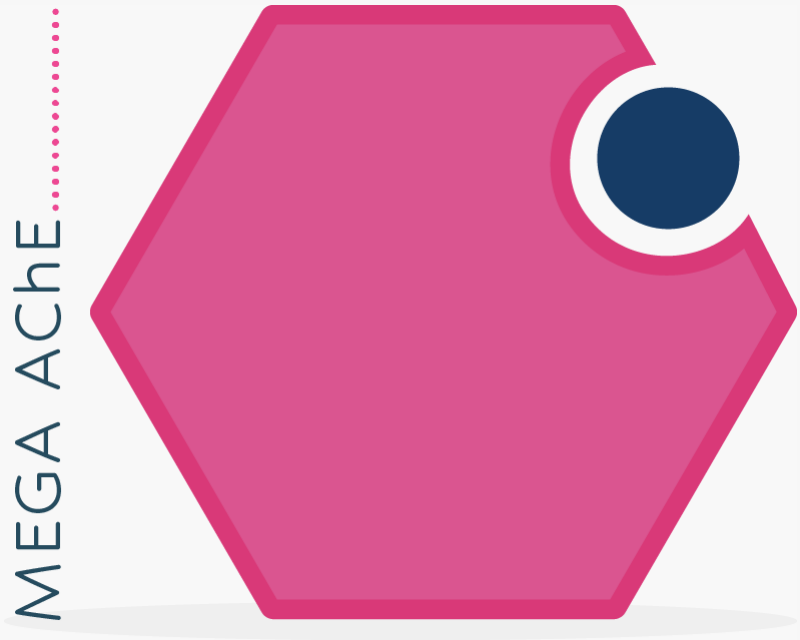
Collaborations Pharmaceuticals launches a new software product to predict acetylcholinesterase inhibitors

Collaborations Pharmaceuticals, Inc. announces a new commercial software product for predicting acetylcholinesterase (AChE) inhibitors that is now available.

RALEIGH, NORTH CAROLINA, USA, February 9, 2023 /EINPresswire.com/ -- AChE is an important enzyme and target for human therapeutics (for Alzheimer's disease for example), environmental safety and global food supply. Inhibitors of this enzyme are widely utilized for pest elimination and can also be used as chemical weapons. AChE targeting pesticides can also act on non-target organisms, such as fish, amphibians and humans, and lead to toxicity.

We have recently exhaustively curated the public data for AChE inhibition which has enabled the development of machine learning models for seven different species. This work was recently published in Chemical Research in Toxicology. We have subsequently created a software product MegaAChE that can be used to score molecules for their potential inhibition of this enzyme in different species.

Collaborations Pharmaceuticals logo



We have also made a website available to the scientific community so users can sample this capability megaache.collaborationspharma.com.

These models could be used to design new AChE inhibitors for CNS diseases as well as for the prediction of off-target toxicity as it is frequently included in in vitro panels and utilized by companies to access potential toxicity. As there are pesticides that target AChE inhibition as their mechanism, these models could also be used to help develop species specific molecules without human toxicity. Such models may therefore be useful for pharmaceutical, agrochemical, consumer product and chemical companies.

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Statement on dual-use:
The AChE machine learning models in MegaAChE have potential dual-use capabilities, and we therefore propose to implement restrictions to control who has access to these models and limit the number of molecules predicted when used on the website. We believe such precautions are necessary and these will evolve over time as we integrate software features to control this dual-use.

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