

International E-Conference on

# PHARMACOLOGY & TOXICOLOGY

December 01-02, 2020 | Webinar

## The Best Ester Substrate for The Studying Erythrocyte Cholinesterase Activity in a Baseline Independent Manner: Learning from Reaction Prediction

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Erythrocyte cholinesterase (AChE) is the gold standard biomarker of Organophosphorus pesticide poisoning. But this enzyme has significant inter as well as intra-individual variation. If a baseline free method is developed, then the problem of inter and intra-individual variation can be solved. Acetylthiocholine (ATCh) is the most popular substrate for AChE. In case reactivation-based methods are developed for AChE activity determination, then the baseline independent method can be designed. However, ATCh should not be an ideal substrate for it. The known reactivators of AChE (oximes) lyse ATCh. This is called oximolysis. To design baseline independent method, we believe that an ester substrate should be searched that will show minimal or no oximolysis but will be cleaved by AChE. Using tools of computational biology, we have searched for such a substrate after screening various ester substrates. It is observed that ester substrates behave different in-silico, which is discussed here.