

AI/ML AND VIRTUAL HUMAN PLATFORMS FOR THREAT AGENT HAZARD ASSESSMENT AND MEDICAL COUNTERMEASURE DISCOVERY AND DRUG DEVELOPMENT

A Community Effort To Catalog The Reactivation Of Acetylcholinesterase By Small Molecules

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Praladoxime (2-PAM) was synthesized over 70 years ago as an antidote for OPNA intoxication. Many billions of dollars later and the world still relies on 3 approved compounds to treat patients: 2PAM, Hi-6, and MMB4. These three compounds have been shown to be moderately effective at treating peripheral nervous system depending on the nature of the OPNA. There is no universal treatment for all OPNA compounds in the peripheral or central nervous systems. The accumulated data from research in this area is vast and found in laboratories across the globe. Publicly accessible manuscripts are found in more than a dozen journals. Many researchers in this field agree that a central repository that is publicly accessible and searchable will be an asset. To this end we have started building a bioassay repository database that includes a publicly accessible repository of published reactivation data. The data will be hand curated. The repository will be searchable by structure, toxicant, and by contributing laboratory. The data will contain the exact values (Kd, Kr, % reactivation, etc...) and 2-D structures presented in the publication. The user interface will allow for searches based on a drawn chemical structure, smiles string, common identifiers such as ChEMBLID and pubChemID. Our goal is to allow authors to automatically submit their reactivation data upon publication of their manuscripts so that the repository continues to grow.

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