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Finding New Potential Insecticides Lead for Acetyl Cholinesterase via Virtual High-Throughput Screening

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Abstract—*Acetylcholinestearse (AChE, E.C.1.1.7) is one of the key enzymes belonging to serine hydrolase family. It is mainly present at neuromuscular junction and cholinergic brain synapses and is also found in different types of conducting tissue such as nerve and muscle, central and peripheral tissues, motor and sensory fibres, and cholinergic and nonchoilnergic fibres. Principle function of AChE is to terminate the impulse transmission by rapidly hydrolyzing acetylcholine (ACh) to choline and acetate. Due to its crucial role in termination of impulse transmission AChE acts as target for variety of chemical agents, because these agents causes enzyme inactivation leading to the accumulation of acetylcholine in brain. These anticholinestearses includes drug for the treatment of myasthenia gravis and acute glaucoma and the first generation anti-Alzheimer drugs, organophosphate nerve agents, organophosphate and carbamate pesticides/insecticides and antihelmentics. In the present study we carried out virtual high-throughput screening of 4,591,276 clean leads. At the same time vHTS of known inhibitors of AChE was carried out. Out of the 4,591,276 clean leads, grid score of 2, 270, 36 leads was found to fall in the range of known inhibitors. These leads were then subjected for the prediction of ADME-Tox properties and 217 leads were predicted to be non toxic in nature.*