Molecular modeling and pharmacophore based virtual screening of The Nicotinic acetylcholine receptor of Halyomorpha halys

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Abstract

The irrational use of fertilizers as a pest control treatment has become increasingly a potential problem for the industrial agricultural sector. In addition, nicotinoid resistant pests has been increasing over the years, and for this reason searching alternative compounds for controling and erradication o these pests is crucial for crop production next years. Halyomorpha halys is popularly known as brown marmorated stink bug, and it spreads in soybean crop, damaging most of the grains in formation, as well as is responsible for the reduction in seed yield and quality. The aim of this work was to construct the nAChR 3D structure of H. Halys as well as perform a virtual screening study in order to find new compounds which can complex and inhibit this receptor. The nAChR 3D structure was modeled using homology modeling approach by SWISS MODEL software. Known nAChR inhibitors were used to perform a pharcophore alignment with Pharmagist (http://bioinfo3d.cs.tau.ac.il/PharmaGist/) and after it was submited to ZincPharmer (http://zincpharmer.csb.pitt.edu/) for seaching for pharmacophore-like ligands in ZINC database. In a second step we docked 1.000 selected molecules into the nAChR active site AutoDock Vina software. The five complexes with best enegy affinity values were submited to AMBER 14 package for Molecular Dynamics simulations.

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