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In Silico Docking Studies of Ligands against Ecdysone Receptor of *Heliothisvirescens*

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Abstract—*Ecdysone (EC 1.14.99.22) is an enzyme that catalyzes the chemical reactions in insects. Ecdysone is a steroidal prohormone of the major insect molting hormone 20-hydroxyecdysone, which is secreted from the prothoracic glands. Insect molting hormones (ecdysone and its homologues) are generally called ecdysteroids. Ecdysteroids act as moulting hormones of arthropods but also occur in other related phyla where they can play different roles. Ecdysteroidsbind with ecdysone receptor that is a type of nuclear receptor found in arthropods. It controls development and contributes to other processes such as reproduction, metamorphosis. The Ecdysone receptor is a non-covalent heterodimer of two proteins, the EcR protein and ultraspiracle protein (USP). It binds to and is activated by ecdysteroids. That's why ecdysone receptor act as a good target for insecticidesthat control insects either by killing them or by retarding their growth. Insect ecdysone receptors are currently better characterized than those from other arthropods, and mimics of ecdysteroids are used commercially as caterpillar-selective insecticides. In the present study we carry out virtual high-throughput screening of structure based library of 4,59,827 unknown ligands. At the same time vHTS of known inhibitors of Ecdysone receptor protein was carried out. ADME toxicity was determined by T.E.S.T (Toxicity estimation software tool). Out of the 4,59,827 unknown ligands,grid score of 25,230 leads fall in the range of known inhibitor range, and out of these 671 leads was found non–toxicant that was predicted by T.E.S.T. This result can be used for further future investigation as potential inhibitor of EcR.*