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Identification of chikungunya nsp2 protease key residue through high throughput virtual screening

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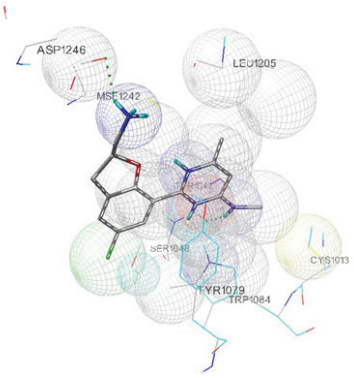
Chikungunya virus (CHICKV) is an arboviruses belonging to family Tagoviridae and is transmitted to human through by mosquito (Aedes aegypti and Aedes albopictus) bite. A large outbreak of chikungunya has been reported in India between 2006 and 2007, along with several other countries from South-East Asia and for the first time in Europe. It was for the first time that the CHICKV outbreak has been reported with mortality from Reunion Island and increased mortality attributed to the outbreaks from Asian countries. CHICKV affects all age groups, and currently there are no specific drugs or vaccine to cure the disease. The need of antiviral agents for the treatment of CHICKV infection and the success of virtual screening against many therapeutically valuable targets led us to carry out the structure based drug design against chikungunya nSP2 protease (PDB: 3TRK). Receptor grid has been prepared with default parameters and without any constrains by using GLIDE and autogrid. Site specified with catalytic residues Cys1013 & His1083 and a conserved residue Trp1084. High throughput virtual screening of publicly available databases, ZINC12 and binding DB, has been carried out using the Open Eye tools and Schrodinger LLC software packages. The top hundred hits were chosen for the ligand receptor interactions studies through the Schrodinger, Autodock and Flexx. Along with the catalytic residues, conserved residue and active site residues, the other residue Asp1246 was found that it has great significant interactions with almost 95% ligands of the HTVS process. Based on these results pyrazole and rhodanine analogs were synthesised and submitted for antiviral activity.



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