Abstract

Molecular docking study was performed on a series of 25 sulfonylureachalcones VS1-VS25 as potential 5-lipoxygenase (5-LO) inhibitors. The docking technique was applied to dock a set of representative compounds within the active site region of 3V99 (5-LO) using Molegro Virtual Docker v 4.0. For these compounds, the binding free energy (kcal/mol) was determined. The docking simulation clearly predicted the binding mode that is nearly similar to the crystallographic binding mode with 1.17Åo RMSD. Based on the validations and hydrogen bond interactions made by R substituents were considered for evaluation. The results avail to understand the type of interactions that occur between designed ligands with 3V99 binding site region and explain the importance of R substitution on sulfonylureachalcone basic nucleus.

References


Index Terms

Computer Science

Applied Sciences

Keywords

Molecular Docking Sulfonylureachalcones 5-lipoxygenase (5-LO) Molegro Virtual Docker (MVD).