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### ***In silico* molecular docking of ligands for inhibition of L-amino acid oxidase from *Calloselasma rhodostoma***

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L-amino acid oxidases (LAAO; EC 1.4.3.2) are flavo-enzymes catalyzing the oxidative deamination of L-amino acids and produces reactive oxygen species (ROS) including Hydrogen peroxide.  $H_2O_2$  mediates in the process of cell death by necrosis, platelet aggregation, apoptosis etc. Several biological activities of LAAOs from snakes have been reported including apoptosis-inducing activity. Development of a lead with the combination of biological activity and drug like properties is needed. Both features can be estimated primarily by *in silico* virtual docking strategies in drug discovery and development. In this study, the crystal structure of L-amino acid oxidase 2IID was imported into Maestro 9.3 following subsequent removal of all crystallographic water molecules from the PDB. Bioactives from several medicinal plants were screened for the inhibition of LAAO from *Calloselasma rhodostoma*. The possibility of binding, precise location of binding sites and mode of binding ligand was carried out using automated docking software Glide XP. The efficacy was evaluated based on scoring function employed in Glide XP (Schrodinger platform). The promising compounds were employed for ADME/Tox studies. Our result showed that Limocitrin bioactive from *Citrus limon* completely buried deeply inside the catalytic tunnel, blocking the transfer of hydride ion at isoalloxazine ring resulting in obstruction for formation of  $H_2O_2$ , thereby inhibiting LAAO. Furthermore pharmacophore modeling suggests the better binding in presence of hydroxyl moieties.

#### **Biography**

Neema K N is a Research scholar in Department of Biotechnology, Sri Jayachamarajendra College of Engineering. She is currently pursuing her PhD from JSS Research Foundation in affiliation with University of Mysore. She has been awarded with Junior Research Fellowship, UGC, Government of India. She has published a paper in reputed journal and has presented poster in 2<sup>nd</sup> National Conference of Toxicological Society of India.

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