In Silico Assessment of Antioxidant Activity of *Labisia pumila* Secondary Metabolites Through Molecular Docking Approaches

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Abstract

Molecular docking has become a widely used computational tool in modern drug and nutraceutical discovery for predicting and analysing ligand–receptor interactions at the molecular level. Labisia pumila (Kacip Fatimah) has gained significant attention due to its rich profile of secondary metabolites and its reported antioxidant potential, which may contribute to protection against oxidative stress, aging, and related chronic diseases. However, there is still limited in silico evidence describing the interaction between its phytochemicals and antioxidant enzymes. This study aimed to investigate the antioxidant potential of selected secondary metabolites from Labisia pumila using a structure-based molecular docking approach. Catalase (CAT) (PDB ID: 2CAG) was selected as the target receptor due to its crucial role in detoxifying hydrogen peroxide and preventing oxidative damage. A range of phytochemical compounds, including phenolic acids, flavonoids, and alkenyl derivatives, were used as ligands. Molecular docking simulations were conducted using AutoDock 4.2, and binding affinities were evaluated based on binding energy scores. The interaction between ligands and the active site residues of catalase was analysed to assess binding stability and affinity. The docking results revealed that flavonoid compounds demonstrated stronger binding interactions compared to other classes of secondary metabolites. Among all tested compounds, myricetin exhibited the most favourable binding energy, indicating the highest predicted affinity toward catalase. Other flavonoids such as quercetin, kaempferol, rutin, and naringin also showed notable binding performance. In contrast, phenolic acids and alkenyl compounds exhibited relatively weaker interactions. Overall, the findings suggest that flavonoid-rich secondary metabolites in Labisia pumila may play a major role in its antioxidant activity. This in silico study highlights their potential as promising natural antioxidant candidates for further experimental validation and development in pharmaceutical and nutraceutical applications.