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Mechanism of Melanin Inhibition of Morello Flavone- 7″- Sulphate and Sargaol extracts from Garcinia livingstonei (Clusiaceae): Homology Modelling, Molecular Docking, and Molecular Dynamics Simulations

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Abstract : Garcinia livingstonei (Clusiaceae) extracts, morelloflavone- 7″- sulphate and sargaol were shown to be effective against hyper-pigmentation through inhibition of tyrosinase enzyme, in vitro . The aim of this study is to elucidate the structural mechanism through which morelloflavone- 7″- sulphate and sargaol binds human tyrosinase. Implementing a homology model to construct a tyrosinase model using the crystal structure of a functional unit from Octopus hemocyanin (PDB: 1JS8) as a reference template enabled us to create a human tyrosinase model. Molecular dynamics and binding free energy calculations were optimized to enable molecular dynamics simulation of the copper dependent inhibitors. Results show the importance of the hydrogen bond formation morelloflavone- 7″- sulphate and sargaol between compound and active site residues. Both complexes demonstrated the metallic coordination between compound and arginine residue as well as copper ions within the active site. The comprehensive molecular insight gained from this study should be vital in understanding the binding mechanism morelloflavone- 7″- sulphate and sargaol. Moreover, these results will assist in the design of novel of metal ion dependent enzyme inhibitors as potential anti-hyper-pigmentation disorder therapies.

Keywords : hyper-pigmentation disorders, dyschromia African skin, morelloflavone- 7″- sulphate, sagoal
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