MOLECULAR DOCKING AND DYNAMICS SIMULATIONS OF AMMI VISNAGA L. CONSTITUENTS AS ANTI-MELANOGENIC AGENTS

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Ammi Visnaga has been reported to possess various biological activities such as anti-inflammatory, antioxidant, antifungal, antidiabetic, cytotoxic, antibacterial effects etc. In the present study, nineteen selected constituents of Ammi Visnaga such as osthenol, visnadin, dihydrosamidin, samidin, apiumetin, celereoin, visnagin, khellin, visamminol, cimifugin, acacetin, quercetin, isoformonometin, visnaginone, khellinone etc. were docked to agaricus bisporus tyrosinase (PDB ID:2Y9X), priestia megaterium tyrosinase (PDB ID: 3NQ1) and homo sapiens tyrosinase (PDB ID: 5M8M) to investigate the potential anti-melanogenic activity. All compounds showed higher docking scores and binding free energy than cognate ligand tropolone for 2Y9X. However, A. visnaga constituents such as coumarin (osthenol), pyranocoumarins (visnadin, dihydrosamidin, samidin), furanocoumarins (apiumetin, celeroin), visamminol (furanochromones), flavonoids (cimifugin, quercetin) have higher binding energy than kojic acid. Kojic acid is a cognate ligand of human tyrosinase (PDB ID: 5M8M) and bacillus megaterium tyrosinase (PDB ID: 3NQ1). Apiumetin (L5) has the highest binding energy of all compounds in three tyrosinase enzymes than cognate ligands. Molecular dynamic analysis shows that Apiumetin (L5) is more stable than the cognate ligand in the binding pocket. ADME analyses calculated by the QikProp program show that all compounds obey Lipinski's rule of five without violations. Schrödinger module was used for molecular docking (IFD) and molecular dynamic (Desmond) analyses. The binding free energies of the compounds were calculated by MM/GBSA approach.