

The Antioxidant Properties of Phenolic Compounds Found in Argan Oil. DFT/QSAR Results and Molecular Docking

H. Zaki^{1,2,*} Y. Filali Zegzouti¹ M. Benlyass¹ and M. Bouachrine^{2,*}

The argan oil has been known for its various pharmacological properties and used as a natural remedy since several centuries. Argan oil is rich in oleic acid and linoleic acid. Interestingly, the unsaponifiable fraction of this oil is mainly rich in antioxidant compounds such as sterols, saponin and phenolic compounds, principally α -tocopherol isoform. Considering its rich composition in antioxidant compounds and unsaturated fat, argan oil can be used as a nutritional intervention in the CVD and cancer disease prevention.

In this work we attempt to establish a quantitative structure-activity relationship for antioxidant activity by studying a series of flavonoid compounds. We accordingly propose a quantitative model, and we try to interpret the activity of the compounds and predict the antioxidant activities of the phenolic compounds present in argan oil such as α -tocopherol, γ -tocopherol and δ -tocopherol relying on the multivariate statistical analyses. Also we attempt to validate the antioxidant activity of these compounds by docking study against cyclooxygenase-2 target (4COX) to predict and compare the conformations of ligands and orientations of binding properties of compounds.

MLR has served to select the descriptors used as the input parameters the MNL and ANN. The topological descriptors and the electronic descriptors were computed with ACD/ChemSketch and Gaussian 03W program, respectively and the Docking Study performed With Autodock Vina Programm.

<https://www.ncbi.nlm.nih.gov/pmc/articles/PMC5535876/>