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Pharmacophore study, molecular docking and molecular dynamic simulation of virgin coconut oil derivatives as anti-inflammatory agent against COX-2

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Abstract

Background: Virgin coconut oil is mostly made up of saturated fatty acids in which approximately 72% are medium chain triglycerides. Medium chain triglycerides can be digested into medium chain fatty acids and medium chain monoglycerides which are bioactive components. Therefore, it is very important to study the in-silico ability of some Virgin coconut oil derivatives, namely, medium chain fatty acids and medium chain monoglycerides to inhibit Cyclooxygenase 2 (COX-2) protein for prevention of excessive inflammatory response.

Results: Pharmacophore study displayed monolaurin with two hydrogen bond donor, three hydrogen bond acceptor and five hydrophobic interactions, while lauric acid presented two hydrogen bond acceptor, five hydrophobic interactions and a negative ion interaction. Molecular docking underlined the ability of monolaurin in the inhibition of COX-2 protein which causes inflammatory action with a decent result of energy binding affinity of − 7.58 kcal/mol and 15 interactions out of which 3 are strong hydrogen bond with TYR385 (3.00 Å), PHE529 (2.77 Å), and GLY533 (3.10 Å) residues of the protein. Monolaurin was employed as hydrogen bond acceptor to the side of residue TYR385 of COX-2 protein with an occupancy of 67.03% and was observed to be long-living during the entire 1000 frames of the molecular dynamic simulation. The analysis of RMSD score of the Monolaurin–COX-2 complex backbone was calculated to be low (1.137 ± 0.153 Å) and was in a stable range of 0.480 to 1.520 Å. Redocking of this complex still maintained a strong hydrogen bond (2.87 Å) with the main residue TYR385. AMDET results where promising for medium chain fatty acids and medium chain monoglycerides with good physicochemical drug scores.

Conclusions: This can be concluded from the results obtained that the monolaurin has strong interactions with COX-2 protein to disrupt its function due to significant hydrogen bonds and hydrophobic interactions with amino acid residues present in the target protein's active site. These results displayed a very significant anti-inflammatory potential of monolaurin and a new promising drug candidates as anti-inflammatory agent.

Keywords: Virgin coconut oil, COX-2, inflammation, Pharmacophore, Monolaurin, Molecular docking, Molecular dynamics simulation

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