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MOLECULAR DOCKING OF CC2-PLA2, A PHOSPHOLIPASE A2-DERIVED FROM CERASTES CERASTES VENOM WITH ITS INHIBITORS

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ABSTRACT

The current study reported a structure-based molecular docking of Cc_2-PLA_2, a phospholipase A2 purified from *Cerastes cerastes* venom by three chromatographic steps. Its molecular weight was equal to 13,534.16 Da and its sequence identified by proteomic analysis consists of 120 amino acid residues. Structurally, when modeled by homology, Cc_2-PLA_2 3D structure appeared organized into 2 β-strands (11%), 3 α-helices (42%) and 11% disordered structure. To explore their inhibitory effect against Cc_2-PLA_2 enzymatic activity, curcumin and its analogs, derived from chemical modification of curcumin, were submitted to a molecular docking study. Our results show that all of the curcumin, tetrahydrocurcumin and dihydrocurcumin interact with Cc_2-PLA_2 by a hydrogen bond established with His^{47}. Moreover, hexahydrocurcumin targeted the residue Asp^{48} of Cc_2-PLA_2. Besides this, among all compounds, the most potent complexes were established with hexahydrocurcumin and tetrahdrocurcumin as they show the most negative energies of interaction. This result shows that chemical modification of curcumin promoted its affinity to Cc_2-PLA_2 and therefore, potentiates the inhibitory effect. $His^{47}$and Asp^{48}being involved in the catalytic loop of Cc_2-PLA_2 thus reinforce the obtained results and confirm the inhibitory effect of the studied compounds against the catalytic activity of our enzyme on its specific substrates. The current study opens perspectives for the design of new snake venom-phospholipase A2 inhibitors and the improvement of envenomation therapy.

KEYWORDS: Phospholipase A2, 3D modeling, Curcumin, Inhibition, Docking