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Article Detail

Identification of Daboia russelii snake venom Phospholipase A2 [PLA2] inhibitors present in methanolic root extract of Calotropis gigantea

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Abstract: Background: Calotropis gigantea roots are widely used as folklore medicine to treat snake bite victims. However the exact neutralization mechanism of the extract is not clear. In this study, snake venom phospholipase A2 [PLA2] inhibitors were identified in the root extract. The toxicity of the snake venom is mainly attributed to phospholipase A2 [PLA2] enzymes or their protein complexes per se. Therefore findings of this study provide valuable insights into neutralization mechanism of the extract. Methods: In this study the phyto-chemicals present in C.gigantea root methanolic extract were profiled using high resolution GC-MS. The phyto-chemicals were specifically docked into crystal structure of Daboia russelii phospholipase A2 [PLA2] to identify possible inhibitors. Results: The GC-MS profile of crude methanolic root extract indicated the presence of phyto-chemicals like n-Hexadecanoic acid, Oleic acid, 9, 12 Octadecadienoic acid and allyl octadecyl ester oxalic acid. Docking analysis revealed that n-Hexadecanoic acid interacted with catalytic residue (His48) of PLA2 (PDBID-3CBI). Previous studies have shown n-Hexadecanoic acid ($K_i=1.58 \times 10^{-5}$) as a potent competitive inhibitor of PLA2. Interestingly, allyl octadecyl ester oxalic acid also formed similar interaction with His48 of PLA2. Conclusion: n-Hexadecanoic acid and allyl octadecyl ester oxalic acid were identified as potent inhibitors of Daboia russelii snake venom PLA2. This result provides valuable insights about anti-snake venom potential of Calotropis Gigantea root extract.

Keyword: n-Hexadecanoic acid; allyl octadecyl ester oxalic acid; PLA2, Calotropis Gigantea

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