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Evaluation of nsLTP-2 ability in binding and transferring of hydrophobic drugs

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Background and Aims: The present study was designed to peruse binding and transferring ability of different lipids and hydrophobic drug molecules to nsLTP-2(Nonspecific lipid transfer protein) from rice (Oryza sativa) at the aim of increasing drug efficacy, lowering toxicity and maintaining the efficient doses.
Methods: Protein structure prediction protocols were used to obtain optimized structure. Docking analyses performed to indicate the binding affinity of interest ligands to nsLTP-2. To confirm the accuracy of the results, experimental analysis such as ion exchange and hydrophobic interaction chromatography were performed to gain purified protein. Moreover, tyrosine fluorescence assay was applied to assess lipid-binding properties of nsLTP-2.
Results: The results showed that affinity of nsLTP2 to structural analysis revealed a close correlation between the number, position and conformation of hydrophobic patches and lipid binding properties of the protein. Binding affinity is influenced by number of carbon atoms and location of double bonds in fatty acid structure. Furthermore, presence of hydroxyl group facilitates acyl chain accommodation in hydrophobic cavity of nsLTP2. Accordingly, chemical features of fatty acids play determinant role in binding affinity consistent with the plasticity of hydrophobic cavity. Also unbelievable binding affinity of nsLTP2 to nucleic acids, their analogues drugs, cholesterol and high size drugs such as doxorubicin is very impressive.
Conclusions: This study showed nsLTP2 not only capable to bind and transport various hydrophobic molecules but capacity to bind to drugs with different size and structure. Thus, nsLTP2 could be an appropriate candidate for mediating and targeting of various drugs including doxorubicin and Acyclovir etc.

Keywords: Nonspecific lipid transfer protein; Iranian rice; Hydrophobic drugs; Doxorubicin; Acyclovir