The concurrent mutations of C26N/N53F can reduce the antigenic propensity of nsLTP2 as an anti-tumor or viral drug carrier

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Abstract

Nonspecific Lipid Transfer Proteins (nsLTP2) are small and soluble proteins, which due to their unique features have the ability of binding to lipids and some pharmaceutical compounds, are considered as good options for drug delivery systems. Their stability against proteolysis and thermal denaturation leads to allergenic reactions which limit its clinical usage. The bioinformatics approach was carried out to hydrophobicity and antigenicity analysis of Oryza sativa (Iranian group) nsLTP2. Using Molegro Virtual Docker software, the affinity and binding strength of several fatty acids, steroid-based anti-viral, and anti-tumor drugs with nsLTP2 were identified. Results demonstrated that there is only one transmembrane segment in the nsLTP2 protein sequence which is located in the signal peptide region, also calculating the average antigenicity propensity (AP) of amino acids showed that concurrent mutations of C26N/N53F can reduce the antigenic propensity of these proteins. Furthermore, Abacavir (MolDock Score = -119.348), DHA (MolDock Score = -152.601), and Basedoxifene (MolDock Score = -156.776) could be considered as the best antiviral, phospholipid, and anticancer ligands for it, respectively.

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