

A Molecular Modelling Approach for Identification of Lead Compound from Rhizomes of Glycosmis Pentaphylla for Skin Cancer Treatment

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Abstract : Life style changes and depletion in atmospheric ozone layer in recent decades lead to increase in skin cancer including both melanoma and nonmelanomas. Natural products which were obtained from different plant species have the potential of anti skin cancer activity. In regard of this, present study focuses the potential effect of Glycosmis pentaphylla against anti skin cancer activity. Different Phytochemical constituents which were present in the roots of Glycosmis pentaphylla were identified and were used as ligands after sketching of their structures with the help of ACD/Chemsketch. These ligands are screened for their anticancer potential with proteins which are involved in skin cancer effects with the help of pyrX software. After performing docking studies, results reveal that Noracronycine secondary metabolite of Glycosmis pentaphylla shows strong affinity of their binding energy with Ribosomal S6 Kinase 2 (2QR8) protein. Ribosomal S6 Kinase 2 (2QR8) has an important role in the cell proliferation and transformation mediated through by N-terminal kinase domain and was induced by the tumour promoters such as epidermal growth factor. It also plays a key role in the neoplastic transformation of human skin cells and in skin cancer growth. Noracronycine interact with THR-493 and MET-496 residue of Ribosomal S6 Kinase 2 protein with binding energy $\Delta G = -8.68$ kcal/mole. Thus on the basis of this study we can say that Noracronycine which present in roots of Glycosmis pentaphylla can be used as lead compound against skin cancer.

Keywords : glycosmis pentaphylla, pyrX, ribosomal s6 kinase, skin cancer

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