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In-silico screening of putative inhibitors for P-protein using generated chemical libraries based on the tyrosine-transporter inhibitor

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Increasing insight into the molecular biology of skin pigmentation has resulted in the identification of an increasing number of potential molecular targets for the new cosmetics discovery and development. These known targets are involved in other essential metabolic processes thus inhibition of their function affects the skin health. A nonpathogenic albinism caused by selective mutation or deletion of the OCA-2 gene have motivated us to target this gene and respective protein (P-protein) for new kind of cosmetics. This trans-membrane channel like protein (P-protein) has well studied for diversity and distribution in human population and their consequences on eye and skin tone. The aim of the present work is to screen the molecule which specifically binds to this protein, resulting as inhibition of the melanin synthesis. Unfortunately, the structure of protein is not available, thus Dock based screening is pity hard. To resolve this we used a pattern search for amino acid sequence, based on homology analysis. Six trans-membrane domains (TM) out of 12 have shown a great homology with tyrosinase transporter, while three cytoplasmic and two extracellular topological domains have some conserve patches too. The role of this protein have been cited more versatile than the regulating the tyrosine transport to melanosome. Thus, we have tried to generate a molecular library of a homologue of tyrosine and tyrosine-transporter inhibitor. The ligand library was generated within the limitation of the Lipinski rule of five. Based on the dock-score five molecules have been subjected to ADME/TOX analysis and subjected for pharmacophore model generation. The selection of the molecules based on ADME and toxicity properties of the molecule. The molecules were evaluated as non-carcinogenic and persistent molecule by START program. The qualified candidate need to being evaluated in In-vitro and In-vivo system to study the successive effects. On the basis of dock score a 20 molecule have been selected and 8 was found to be quite effective as anti melanogenic without any toxic effect. Among these compound, compound #1, #2, #3, #4, #8, #13, #16, #17 showed the effect on melanin inhibition with low toxicity up to the concentration 20 mM. Further investigation in relation to mechanism of action is under process.

Biography

Morya has completed his Ph.D from DDU Gorakhpur University, and postdoctoral studies from Inha University, Korea. He is Assistant Professor, at Inha University, in department of Bioengineering. He has published more than 20 papers in reputed journals and serving as an editorial board member of repute.

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