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Screening of Potential Anticancer Phytochemicals against Lung Cancer by Molecular Docking Studies

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BACKGROUND

In recent years, lung cancer has been the leading cause of death worldwide. Although there are various synthetic drugs available on the market, plant derivatives are known to have be tter efficacy and lesser side effects in the treatment of multiple cancers. Various molecular docking studies have been performed on the phytochemicals to evaluate their anticancer p otency and are helpful in providing insights into molecular identification.

MATERIALS & METHODS

Those phytochemicals which are known to have medicinal properties are taken as ligands. Ligand structures were first determined by structural techniques. The chemical structure of shortlisted phytochemicals was accessed from the Pubchem database and drawn in Advanced Chemistry Development's Chemsketch which was converted into the 3D structure using the software application. These ligands are further used for molecular docking analysis. The crystallographic structure of the cancer target proteins was retrieved from the protein data bank. The proteins were then cleaned by removing the bound inhibitor, non-essential molecules like heteroatoms and hydrogen atoms. Finally, optimisation of protein structure was done by Weblab Viewer, Argus Lab 4.0, Dockprep or Swiss PDB Viewer. The active site prediction is used to identify the best ligand binding site. The possible active binding sites of the proteins were obtained using DoGSiteScorer.

RESULT

In the docking studies, computed drug-likeness of phytochemicals revealed that maximum compounds were in the range of favourable candidates for good bioavailability per Lipinski's five rules. The phytochemical constituents of medicinal plants behave as antagonists to cancer which may be further investigated *in vitro and in vivo* models.

CONCLUSION

Molecular docking study is the important tools in the process of drug discovery for searching the potential hits. This unit aims to focus on the finding of the molecular docking study performed on various phytochemicals and different cancerous proteins and their future drug discovery potential.