

Computational approach for optimizing inhibitors of HMG-CoA reductase

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Coronary artery disease is one of the most investigated diseases in medicinal chemistry. HMG-CoA reductase (or 3-hydroxy-3-methyl-glutaryl-CoA reductase or HMGCR) is the rate-controlling enzyme of the mevalonate pathway, the metabolic pathway that produces cholesterol and other isoprenoids. Normally in mammalian cells this enzyme is suppressed by cholesterol derived from the internalization and degradation of low density lipoprotein (LDL) via the LDL receptor as well as oxidized species of cholesterol. This enzyme is thus the target of the widely available cholesterol-lowering drugs known collectively as the statins.

In present study crystal structure of HMG-coA 1HWK was prepared. Active site was identified. Virtual screening was performed against ligand data set prepared from different literature search and ZINC data base to identify a lead molecule. This lead molecule was optimized using molecular dynamics. These lead molecules show good docking score than statins.

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Isolation of Staphylococcus sps. from mobile phones and in-vitro study of Mollugo cerviana leaf extract on Staphylococcus sps.

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Micro-organisms are omnipresent. Thus, the pages on which we pen down our imagination are also the habitat for these microbes, with this in mind, we isolated micro-organisms from the mobile phones of students, staffs, workers and cleaners of our College, By using The cotton swabs. By gram-staining and observation under the microscope, Cocci were observed. On performing various biochemical tests such as catalase, oxidase, starch hydrolysis, gelatin, we identified the organisms to be a species staphylococcus sps. Antibacterial test were performed in-vitro using Mollugo cerviana leaf extracts to study its role on the inhibition of this pathogen. A standard borewell method was employed.

Keywords: Mollugo cerviana, Staphylococcus, Catalase test, Oxidase test, Mobile phones.

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Biochemical analysis of epicardial and subcutaneous adipose tissue – A clinical correlation with cardiovascular risk factors

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Epicardial adipose tissue is the visceral fat around the heart which has special properties that distinguish it from the other adipose tissue. The role of epicardial adipose tissue related with the heart diseases found to be unclear. Hence, this study is to analyse the oxidant, antioxidant and lipid profiles of Epicardial adipose tissue and subcutaneous adipose tissue and clinical correlation with the cardiovascular risk factors. The oxidant, antioxidant and lipid profiles were done using standard methods. The proteins were extracted and run in SDS PAGE electrophoresis. Lipoproteins were separated using agarose gel electrophoresis from the both adipose tissue. Lipid profile and oxidant found to be more in the subcutaneous adipose tissue, while the antioxidant, HDL and phospholipids were more in the Epicardial adipose tissue. Vitamin C, HDL, phospholipids, triglyceride, ceruloplamin and total cholesterol ($p < 0.04$) were found to be more significantly associated with the comparison studies. The antioxidant found to be high in the diabetic patients affected with acute myocardial infarction. Lipoproteins were separated in both tissues and found to be high in subcutaneous adipose tissue. In conclusion, the Epicardial adipose tissue possesses protective mechanism and seems to be beneficial to the cardiovascular system.

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