# ABSTRACT

The introductory chapter offers a brief description on terpenoids and the historical development of quantitative structure-activity relationship. A large number of terpenoids have a variety of biological activities such as anti-viral, anti-bacterial, anti-malarial, anti-inflammatory, anti-cancer activities and QSAR study may help to provide guidance in design and synthesis of very specific compounds that have high biological activities.

The second chapter presents the review of literature. This chapter is subdivided into two sections: i) terpenoids with different biological activity and ii) quantitative structure-activity relationships of bioactive terpenoids.

The third chapter is allotted for the methodology of research work. Different indices, using in this study, are incorporated. A brief account on regression analysis and statistical parameters are also provided.

The forth chapter is a QSAR study of a number of 23-hydroxybetulinic acid derivatives which were found to be potent glycogen phohphorylase a (GPa) inhibitors. Some derivatives of these triterpenes also exhibit anti-tumor activities against a variety of tumor cell lines. In this study, we have constructed two different sets of QSAR equations. One set of QSAR equations predicts inhibitory activity of rabbit muscle glycogen phosphorylase a (RMGPa), which shares considerable sequence similarity with human liver GPa. The other set of equations predicts the antiproliferative activities against HeLa cells. We have also performed Docking study with a number of 23-hydroxybetulinic acid derivatives with RMGPa.

The fifth chapter presents the computational study on the redox reaction of puupehenone in aqueous solution by density functional theory. The redox potential of

puupehedienone/puupehenone couple was calculated at the DFT- B3LYP/6-311G(d,P) level of theory in conjugation with Polarizable Continuum Model (PCM). The influence of hydrogen-bond on the redox reaction was also investigated.

The sixth chapter is on the theoretical investigation of cytotoxic activity of halogenated monoterpenoids from plocamium cartilagineum. The molecular geometry of nine halogenated monoterpenoids in the ground state has been calculated by B3LYP/6-31G* and it was found that gap energy and stereochemical features of the compounds play an important role towards activity.

The docking and the QSAR study of oleanolic acid and its derivatives have been discussed in chapter seven. Oleanolic acid and its derivatives were found to be potent Protein-tyrosine phosphatase 1B inhibitors. The docking study shows that most of the ligands can form hydrogen bonds with ARG24 and/or ARG254. Two quantitative structure activity relationships models have been constructed using different descriptors and the significance of these models is judged on the basis of correlation, Fischer F test, and quality factor (Q).

In chapter eight, the molecular geometry of halomon in the ground state has been calculated by the DFT methods. The bond lengths, bond angles and dihedral angles derived from the quantum chemical method are compared with the experimental values and it is found that the calculated geometric parameters are close to the X-ray crystal structure.

A QSAR study of sesquiterpene lactones from Inula falconeri that possess diverse biological activities is discussed in chapter nine. Three statistically significant QSAR models are constructed which may be used to find out the activity of the designed compounds.

Finally chapter ten presents a general and comprehensive conclusion of all the chapters.