PREFACE

Structure-activity relationships (SAR) are unquestionably of great importance in medicinal chemistry which tries to modify the activity of bioactive chemical compounds by modifying their chemical structure. This method was later refined to build mathematical relationships between biological activity and chemical structure, known as quantitative structure-activity relationships (QSAR). The appropriate molecular descriptors are essential to obtain a significant QSAR model. The descriptors are theoretical, empirical, or derived from readily available experimental characteristics of the structures. When a correlation between structure and activity is established, any number of compounds, including those not yet synthesized, can be readily screened on the computer. Quantum chemistry provides an attractive source of molecular descriptors which express all of the electronic and geometric properties of molecules. QSAR currently are being applied in many disciplines like agricultural, biological, environmental, medicinal, and physical organic studies. It is an encouraging method of chemical researching all over the world today.

The dissertation embodies the results of research undertaken at the Department of Chemistry, Raiganj University over the period from November 2012 to June 2016. This work is an attempt to explore the structure activity relationship of various terpenoids by studing their quantum chemical and structural properties.