PREFACE

Waisser and his associates investigated thiobenzmides on various mycobacteria and related the activity of the thioamides with various physico chemical techniques. Several derivatives of thiomides were studied against M. avium, M. tuberculosis, M. fortuitum, M. kansasii. The QSAR derivatives of thiobenzamide were developed using electronic parameters and the results obtained indicated the correlation coefficient above 0.88. QSAR models with quantum mechanical parameters are fast developing and in recent years valuable papers have been published.

The laws necessary for mathematical treatment of large part of physics and chemistry are though known but the difficulty has been only in the fact that applications of these laws were too complex to be solved. The works of Kohn & Pople have made it possible to make use of these laws in the study of complex molecules. The semiemperical calculation such as AMI, PM3, PM5 and DFT have been done. Several physicist & chemist in the recent years have made number of approaches for study of molecular electronic structure and the reactivity of compounds.

The thesis matter presented in this thesis is divided into six chapters. In chapter-1, the compounds whose QSAR study has been made are listed in Tables-1-4 along with their activities. In chapter-2, the methodology has been discussed in detail alongwith the definition of descriptors used in QSAR study.

In chapter-3, QSAR study of MIC of thiobenzamides with M. Avium have been made with the help of quantum mechanical parameters. It has been found that all the best QSAR models have heat of formation and total energy as descriptors. Heat of formation alone is capable to produce good QSAR model having appreciable predictive power.

In chapter-4, QSAR study of MIC of thiobenzamides with M. Tuberculosis have been made with the help of quantum mechanical parameters. In QSAR models, the activities in terms of log 1/C of thiobenzamides for MIC with M. Tuberculosis have been predicted using CAChe software. Best QSAR model with 0.918194 as the value of correlation coefficient and 0.554923 as the value of cross-validation coefficient has been obtained.

In chapter-5, QSAR study of MIC of thiobenzamides with M. Fortuitum have been made and found that the descriptors molecular weight, total energy, HOMO energy and LUMO energy provide best QSAR model with 0.910628 value of correlation coefficient. Hence, QSAR model thus developed is said to have very good descriptive power.

In chapter-6, QSAR study of MIC of thiobenzamides with M. Kansasii have been made with the help of same quantum mechanical parameters using CAChe software. It has been found that heat of formation and total energy are present as descriptor in each best QSAR model. This indicates that the heat of formation and total energy are good descriptors of activity.

Most of the work which is included in the thesis is published in the form of the research papers listed below-

1. QSAR study of thiobenzamides using quantum mechanical descriptors, *Material Science: An Indian Journal (MSAIJ)*, 6(1), **2010**, 71-84.

2. QSAR Study of Thiobenzamides using Topological Descriptors, *J. Chem. Bio. Phy. Sci. Sec. B*, 2(2), **2012**, 751-761.