PREFACE

A number of chalcones with novel substituents were isolated earlier in our laboratories from different *Tephrosia* species possessing significant antimicrobial and anticancer activities. This has prompted us to synthesize a number of other chalcones having aromatic/ heteroaromatic rings with number of substituents and was also screened for these biological activities. The chalcones so obtained have been successfully converted into pyrimidines which were earlier reported to possess diverse biological activities and found place in the present day therapy of a number of diseases, particularly as antimicrobial and anticancer agents. Infact, some of the pyrimidines earlier synthesized in our laboratories exhibited significant anticancer activity against prostate cancer cell lines apart from their antifungal and antibacterial activities. The present work is a continuation of the earlier work with a view to prepare a large number of chalcones and 1,5-benzothiazepines and to screen them for antimicrobial and cytotoxic activities. It is believed that such a focused approach would result in the identification of some promising leads at one or the other stage during the course of our systematic academic research work.

Chalcones afford a facile route of access to many of the heterocyclic systems containing nitrogen and sulfur. An attempt is therefore made to synthesize chalcones from 2-acetyl-1-methylpyrrole by reaction with either aromatic or heteroaromatic aldehydes using Claisen-Schmidt condensation. The resulting chalcones after purification and characterization by physical and spectral methods have been successfully converted into substituted benzothiazepines by reaction with 2-aminothiophenol. Since the chalcones were also reported to possess antimicrobial and cytotoxic activities, they were also screened for these activities. This could also enable us to compare the similar activities of the benzothiazepines. The chalcones and benzothiazepines so obtained were also subjected to computational evaluation in order to draw correlations between the observed and predicted biological activities.

INSTRUMENTATION AND METHODOLOGY

- The melting points were determined by open capillaries and are uncorrected.
- The purity of the compound was checked by TLC using Silica gel-G and the solvent systems are indicated at appropriate places.
- The IR spectra of the compounds were recorded on BRUKER ALPHA-T FT IR spectrophotometer using KBr disc and the values are expressed in cm^{-1}
- The ^{1}H NMR spectra of the compounds were recorded on BRUKER Spect, 400 MHz and amx400, 400 MHz NMR spectrophotometer and chemical shifts are expressed in delta ppm by using TMS as an internal standard.
- The mass spectra of the compounds were recorded on Agilent 6320 Ion Trap LC-MS.(Positive/Negative ion electro spray ionization method)
- The elemental analyses of the compounds were recorded on Carlo Erba 1108 elemental analyzer.