

Thesis Title

Quantum mechanical treatment, sedative and spin trapping properties of quinazoline-3-oxides with antibacterial and electron paramagnetic resonance studies of their complexes with copper (II) ion

Abstract

This thesis is concerned with quantum mechanical treatment of the sedative and spin trapping properties of quinazoline-3-oxides with antibacterial and electron paramagnetic resonance studies of their derivatives with copper (II) ions. Series of quinazoline-3-oxides and their complexes with copper (II) were prepared according to procedure mentioned in the experimental part and characterized by CHN and spectroscopic techniques. The quantum mechanical and experimental results drawn from quinazoline-3-oxides revealed that these compounds have efficient sedative properties as shown from the muscle tone test, reflux time and swimming time tests carried out on group of mice. The median lethal dose revealed that all compounds showed no clear toxic effect on albino mice. Quinazoline-3-oxides showed efficient spin trapping properties toward dangerous methyl and hydroxyl radicals and formed stable nitro-oxide radicals as compared with standard PBN adducts. The kinetic study carried out on quinazoline-3-oxide adducts with CH₃ and OH radicals showed that these adducts are very stable which is in good agreement with the theoretical calculation carried on the structure and with the geometry of these compound. This property may indicate that these compounds could be useful in treatment of skin cancer. The antibacterial study of the complexes of quinazoline-3-oxides with copper (II) showed increase inhibition growth of bacteria of complexes with free ligands. The toxicity of free quinazoline-3-oxides increases when coordinated with copper (II). The measured of electron paramagnetic resonance showed a great covalence between free quinazoline-3-oxides and copper (II). The great covalence shown by these complexes increases their stability and might prevent them from decomposition when they penetrate the cell wall. All the above mentioned properties make the quinazoline-3-oxides copper (II)

complexes potentially useful in diseases where free radicals play an important role in their pathophysiology.