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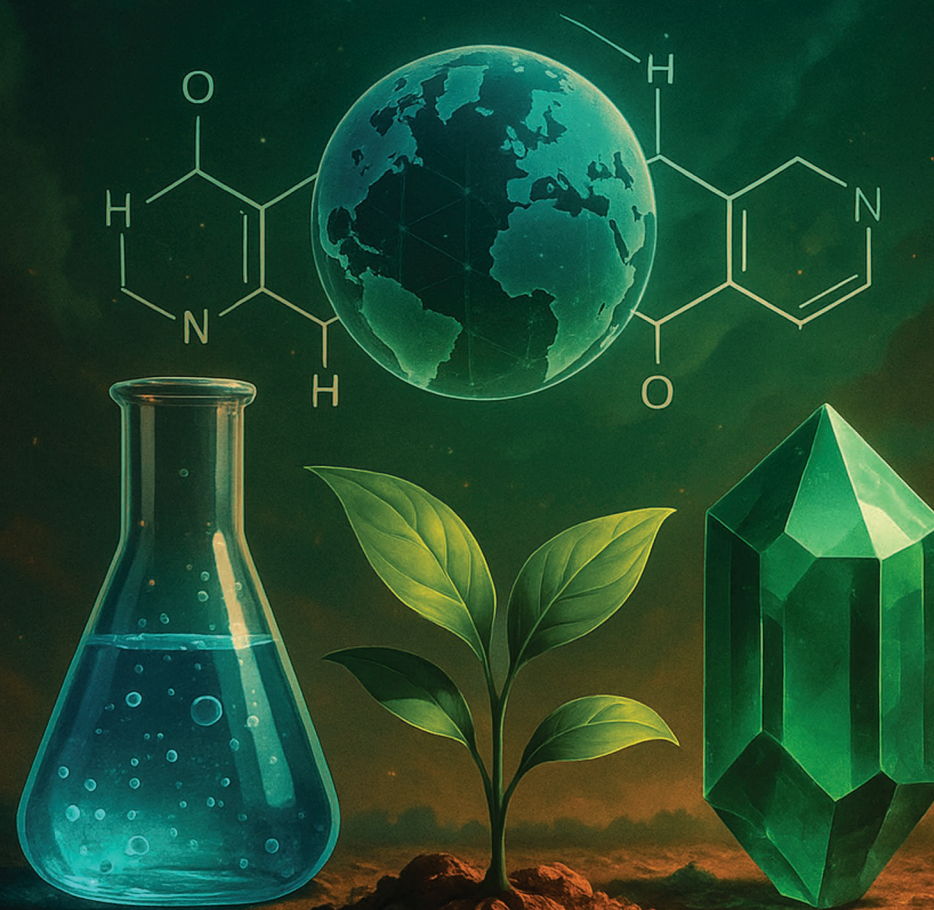
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Perspectives of Medicinal, Material and Environmental Chemistry

PERSPECTIVES OF MEDICINAL, MATERIAL AND ENVIRONMENTAL CHEMISTRY



Editors:
Dr. Saimah Khan
Dr. Naseem Ahmad
Dr. Firoz Hassan



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CHAPTER – 1

Computational studies of (*E*)-chalcone and (*E*)-3-(2-hydroxyphenyl)-1-phenylprop-2-en-1-one and their metal complexes

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Abstract

Chalcones of various aldehydes and ketones occupy a special place among organic ligands due to the various donor atoms present in them and their ability to change their denticity depending on the starting reagents and reaction conditions. Chalcones can also be easily modified by varying the parent aldehyde or ketone used for synthesis, particularly with compounds having additional potential coordinating sites. This chapter reports the computational studies of selected chalcones. The physicochemical parameters of the synthesized ligand and complexes were calculated using Molinspiration and SWissADME, Absorption, Distribution, Metabolism, Excretion and Toxicity (ADMET) properties were calculated using admetSAR. Physiochemical characteristics of synthesized ligands and their metal complexes were determined using Mol inspiration and SwissADME software. Properties like molecular weight topological polar surface area (TPSA), number of hydrogen bond donors and acceptors etc. were calculated to know the probable potential of the molecule. Some of them were having good bioavailability score and exhibited not more than two Lipinski's violations. In future these chalcones and their complexes can be used for biological activity evaluation.

Keywords: Computational, Chalcones, bioactivity score, drug design.

Introduction

Chalcone is a α , β -unsaturated carbonyl compound that forms the central core of many important biological compounds, which are known as chalcones. Chalcones are flavonoid-type phenolic phytochemicals, often referred to as 'open-chain flavonoids' and biosynthesized via the shikimate pathway [1]. Chalcones are the biogenetic precursors of flavonoids and iso flavonoids, which are abundant in plants. is oxazole pyrazolos and indole grounded chalcones. The chalcone core is composed of two aromatic rings that are linked through a three carbon- α , β -unsaturated carbonyl system, i.e., 1,3-diphenyl-2-propen-1-one derivative but these may also include some saturated ketones, commonly known as dihydrochalcones [2]. There are several thousand naturally occurring chalcones reported in the literature and many of those chalcones were shown to interact with various biomolecules and possess cytoprotective and modulatory properties, making them potentially suitable candidates for therapeutic interventions in many human ailments. Several patents are also available for chalcones and their derivatives for their activities as anticancer, anti-inflammatory, antimitotic, antioxidant, and cytotoxic properties. Because of structural simplicity and therapeutic potential, several bioinspired syntheses of chalcone derivatives and evaluation of their bioactivities were reported in the literature [3]. The first few attempts for the synthesis of chalcones began in the 1800s and continued through the subsequent centuries. Chalcones are structurally one of the most diverse groups of flavonoids and easily allow to cyclize forming flavonoid structure which is an isomeric key step for the skeletal modification of chalcones.