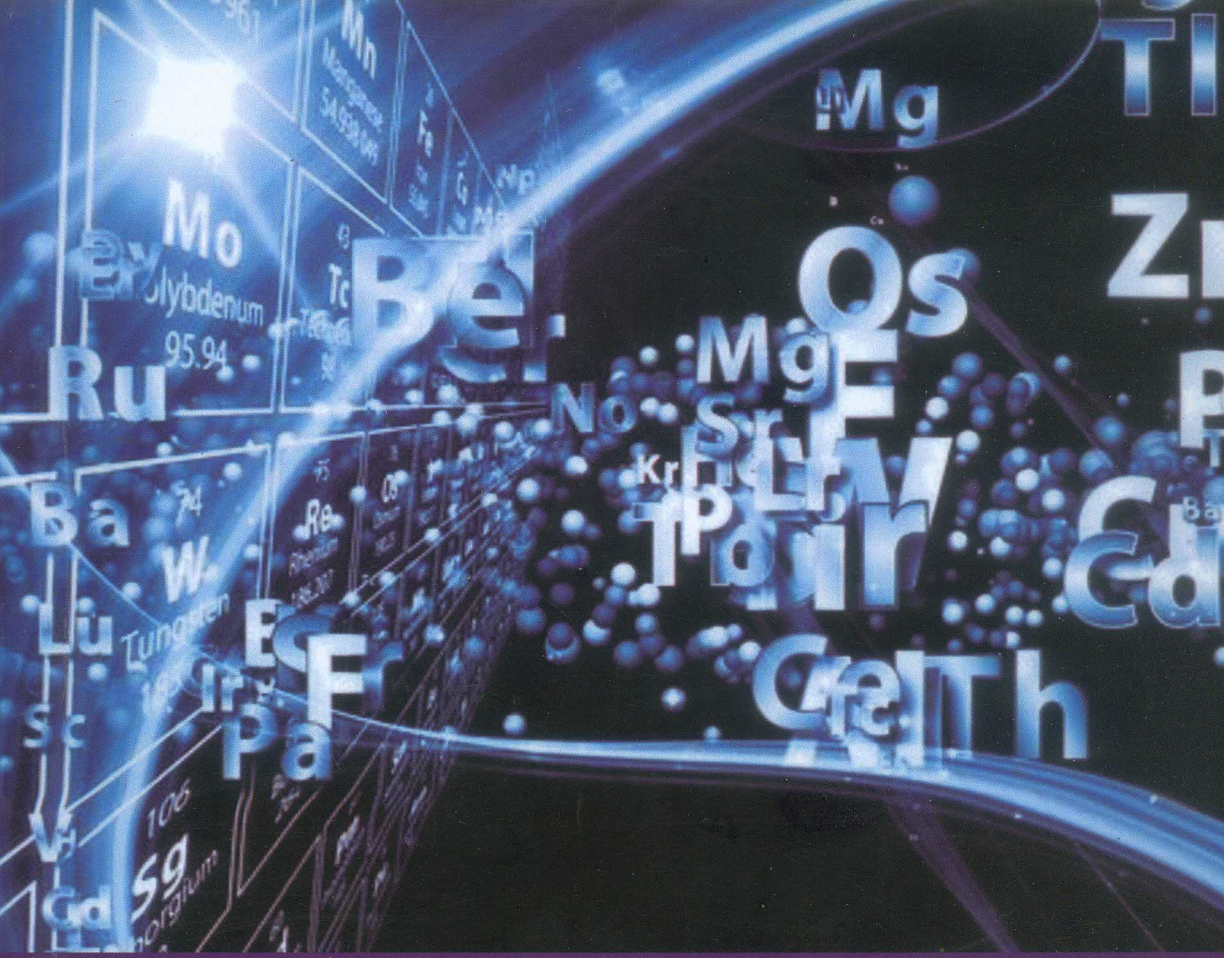

Environmental and Medicinal Chemistry

Experimental Design and Applications

Part III

Abdul Rahman Khan, Naseem Ahmad
Iqbal Azad, Malik Nasibullah

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(Part-III)

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Abdul Rahman Khan, Naseem Ahmad, Iqbal Azad and Malik Nasibullah

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CONTENTS

CHAPTER-1

SIGNIFICANCE OF SYNTHESIS OF SCHIFF'S BASES

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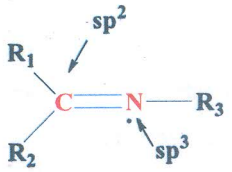
INTRODUCTION

Schiff's bases are condensed products of primary amines and carbonyl compounds and they were discovered by a German chemist, Nobel Prize winner, Hugo Schiff in 1864 .Structurally, Schiff base (also known as imine or azomethine) is an analogue of a specific functional (-N=C-) group. When the carbonyl group (>C=O) and primary amine ($-NH_2$) reacted together then a specific functional (-N=C-) formed by the H_2O elimination. Such type **functional groups found in those compounds are commonly known as Schiff's base or imine** system (Figure 1).



Where R_1, R_2 may be H, alkyl group, aryl group, heterocyclic ring etc.

Figure 1. A general structure of schiff's base

The synthesis of organic ligands as mono, di, tri or polydentate has to more importance role play to the formation of metal complexes. Those atoms of compound, which can be donate own lone pair electron to a metal and eligible to form coordination bond such type atoms are **N, S, O and P. So nitrogen found in Schiff's base, therefore its may called ligand.** Schiff bases also possess remarkable biochemical applications, such as antifungal, antiviral, antitumor, and antibacterial activities [1,2]. Schiff bases are considered to be notable ligand for metal ion coordination complexes due to their ease of synthesis, variability in structural design, and wide range of applications [3].These ligands were broadly used as poly chelator ligands and have revealed high performance in terms of steric characteristics and electronic soft tuning of their metal complexes. Chemists design **Schiff's bases as polydentate ligands** and their complexes, and these have served several areas of chemistry [4, 5]. Photo- and **thermo chromic properties of Schiff's bases as well as their biological activity make them** applicable in modern technology. Among others, they are used in optical computers, to

CHAPTER-2

SYNTHESIS, COMPLEXATION, SPECTROSCOPIC INVESTIGATION AND ANTIMICROBIAL ACTIVITY EVALUATION OF SELECTED THIOSEMICARBAZONE LIGAND

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ABSTRACT

Thiosemicarbazones constitute an important class of N, S - donor ligands and known for about 50 years. They were studied for a significant period of time for their biological activities. In many cases their activity in biological systems has been found to enhance by coordination with metal ions and a clear relation exists between chelate formation in the complexes and *in-vivo* activity. In the present study a useful Schiff base ligand acetophenone thiosemicarbazone was synthesized and characterized. Furthermore the transition metal complexes of the ligand were synthesized with $ZnSO_4.7H_2O$, $FeSO_4.7H_2O$, and $CuSO_4.5H_2O$. The antimicrobial activity of the ligand was tested against *Staphylocous aureus* and Aspergillus *Niger*. The ligand acetophenone thiosemicarbazone showed appreciable antibacterial and antifungal activity against the selected microbial strains. In future other medicinal activities of the ligand and its complexes can be tested.

Keywords: Thiosemicarbazone, metal complexes, antimicrobial activity, Schiff base

INTRODUCTION

Schiff bases and their complexes

Schiff bases are condensation products of primary amines and carbonyl compounds and they were investigated by a German chemist, Nobel Prize winner, Hugo Schiff in 1864 [1]. Structurally, Schiff base (also known as imine or azomethine) is an analogue of a ketone or aldehyde in which the carbonyl group (C=O) has been replaced by an imine or azomethine group [2]. Schiff base ligands are essential in the field of coordination chemistry, especially in the progress of complexes of Schiff bases because these compounds are potentially skilled of forming stable complexes with metal ions.

Mechanism of formation

The formation of a Schiff base from an aldehydes (or) ketones is a reversible reaction and generally takes place under acid (or) base catalysis, or upon heating. Many Schiff bases can be

CHAPTER-3

CURRENT STRATEGIES OF PYRROLE-2,3-DICARBOXYLATE DERIVATIVE SYNTHESIS USING MCRS

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ABSTRACT

The various strategies for the synthesis of Pyrrole-2,3-dicarboxylate derivatives are covered in this chapter. Pyrrole-2,3-dicarboxylate derivatives are important heterocyclic moieties with the potential to produce complexity in molecules by a one-pot multicomponent synthesis, as well as excellent pharmacological characteristics. One-pot multicomponent transformations are described here, along with various applications.

Keyword: Pyrrole-2,3-dicarboxylate; Multicomponent reaction; One-pot; Polysubtituted; Pyrrole.

INTRODUCTION

Organic compound synthesis is an exciting research subject since it opens up numerous pathways for the production of structurally varied chemical entities [1]. Organic molecules, such as heterocyclic compounds, have a wide range of uses in medical chemistry, biochemistry, photochemistry, material science, and environmental research [2]. The most fascinating subject for drug discovery is organic chemistry. It provides a variety of paths for the formation of distinct moieties and modifications to a compound's complexity [3]. As a result, they play an important part in the drug development process. In comparison to other synthetic domains, heterocyclic chemistry has advantages [4]. More than half of physiologically relevant chemicals in nature include a heterocyclic moiety as a key component of their skeleton [5]. They have drawn the attention of current researchers due to their medical usefulness. The structure of most marketed medications includes a heterocyclic skeleton [6]. Heterocyclic compounds play an important part in current drug design due to their ease of change in the general moiety [7]. Many dangerous and expensive solvents were formerly utilised in the production of heterocyclic compounds. The modern field of heterocyclic synthesis has also seen a significant transformation due to changes in the

CHAPTER-4

SYNTHESIS OF SUBSTITUTED BIOACTIVE BENZOPYRANDERIVATIVES

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ABSTRACT

One of the most common cancers is the Breast cancer around the globe. According to US breast cancer statistics 2016, an estimated 246,660 new cases of invasive breast cancer are expected to be diagnosed in women in the United States along with 61,000 new cases of non-invasive (*in situ*) breast cancer. Around two third of the cases of breast cancer are estrogen receptor positive (ER+). The work focuses to synthesis of conformationally restricted 2,2-dimethylbenzoyran core based triarylethylenes (prototype-I) as growth inhibitors of ER positive carcinoma cells. The presence of oxygen-atom as hinge at the junction of ethyl group and distal phenyl ring of triarylethylene core of TAM (2a) may facilitate to improve drugable properties of the molecules compared to their corresponding carbocyclic analogs. This study reports the synthesis and biological results of the designed molecules.

Keywords: Breast cancer, bebzopyran, ER+, synthesis

INTRODUCTION

Breast cancer is the most common cancer which women may face in their lifetime [1]. Approximately, 70% of the breast cancer cases in women are estrogen receptor positive (ER+) [2, 3]. These ER-positive breast cancers are ER activation dependent either by 17β-estradiol (1) or structurally similar ligands. Among two types of estrogen receptors (ERs), known as ER-α and ER-β, ER-α is normally over expressed in breast cancer cells, and is an important target for the development of new anti-breast cancer agents [4]. Selective estrogen receptor modulators (SERMs) have an advantage of exhibiting tissue selective estrogen agonistic and antagonistic activities through competitive binding to ER and thus prohibit estrogen binding to ER in the cancer cells [5,6]. Tamoxifen (2a; TAM) is the only drug of choice as far as antiestrogen based chemotherapy of breast cancer is concern [7]. Structurally, triarylethylene (TAE) core of TAM (2a) resembles steroidal skeleton of 17β-estradiol (1). It is interesting to note that geometrical isomerism associated with triarylethylene (TAE) core

CHAPTER-5

FLAVONOL DERIVATIVES AS POTENTIAL ANTI-CANCER AGENT: AN IN-SILICO STUDY

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INTRODUCTION

Flavonoids belong to a class of low molecular weight phenolic compounds that are widely distributed in the plant kingdom and most commonly found in higher plants. Thus, flavonoids are phytochemicals and found in fruits, vegetables, grains, bark, roots, stems, flowers, tea and wine. Flavonoid derivatives are synthesized by phenylpropanoid pathway. Flavonoids are located in the nucleus of mesophyll cells and within centers of ROS (Reactive Oxygen Species) generation [1].

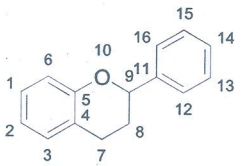

Figure 32. A general strcutre of flavonoid

Flavonoids consist of a large group of polyphenolic compounds having a benzo-ɣ-pyrone structure. Chemically flavonoids are based upon a fifteen-carbon skeleton consisting of two benzene ringsjoined through a heterocyclic pyrone ring. They can be divided into a variety of classes such as flavones (e.g., flavone, apigenin, and luteolin), Flavanols (e.g.; quercetin, kaempferol, myricetin, and fisetin), flavanones (e.g., flavanone, hesperetin, and naringenin), and others [2].

Basic skeleton of flavonoids

Flavonoids occur as aglycones, glycosides, and methylated derivatives. The basic flavonoid structure is aglycone. Six-member ring joined with the benzene ring is either a α-pyrone (flavanols and flavanones) orits dihydroderivative (flavanols and flavanones). The chemical nature of flavonoids depends on their structural class, degree of hydroxylation, other substitutions and conjugations and degree of polymerization. In the structure of flavonoids, the position of the benzenoid substituent divides the flavonoid class into flavonoids (2-

CHAPTER-6

SYNTHESIS OF LITHIUM MANGANESE OXIDE (LIMN2O4) VIA SOLID STATE AND SOL GEL AUTOCOMBUSTION METHOD

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ABSTRACT

Li-ion batteries are used as popular power source for consumer electronics as compare to lead acid and nickel cadmium rechargeable batteries. Besides powering cellular phones, laptops, digital cameras, power tools and medical device, Li-ion is also used for electric vehicles. The battery has a number of benefits, most notably its high specific energy, simple charging, low maintenance and being environmentally benign. Mostly research activities today revolve around improving lithium-based systems. Li- ion battery is a type of rechargeable battery in which Li-ions move from the negative electrode to the positive electrode during discharge and back when charging. High energy with high capacity and high operating voltage cell is required along with long cycle life and low self-discharge rate. Lithium manganese oxide ($LiMn_2O_4$), LMO based spinel oxide is mostly used as cathode materials. In this work, we have synthesised LMO by wet chemical route like sol gel auto-combustion process and solid-state synthesis routes. Synthesized LMO materials are calcined at 750 ^{0}C for 8 hrs to get crystalline and phase pure materials. Calcined materials are characterised by X-ray diffractometer and found phase pure with Fd3m space group, 8.2674 ^{0}A unit cell parameter. Particle size and size distribution of particles is analysed by particle size analyser. Electrochemical characteristic of the synthesized and calcined LMO powders are performed by applying coating of LMO-acetylene black-PVDF in 8:1:1 ratio on Al foil as cathode substrate. Li-ion cells in coin cell configuration are assembled with Li metal as reference, $LiPF_6$ in EC-DMC solution as electrolyte and PE as separator. In particular, specific capacities of spinel materials are analysed. It is analysed that reduced specific capacity is determined primarily in the solid state by the aggregation of material particles, whereas good cycle ability is obtained in auto combustion synthesized materials due to the size of crystallites and perfectness of crystals.

CHAPTER-7

AN INTRODUCTION ON PHARMACOKINETICS AND PHARMACODYNAMIC OF DRUG

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ABSTRACT

Pharmacokinetics means movement of drugs (pharma = drug and kinetic = movement). It is quantitative study of drug movement inside the body.The drug action is initially dependent on it reaching its site of action in sufficient concentration for a long enough period of time for a significant pharmacological response to occur. This build-up in drug concentration and the maintenance of this concentration over a period of time depend on the route of drug administration, the efficiency of drug absorption, the rate at which the drug is transported to its site of action, the rate of drug metabolism on route and, at the site of action, the rate of drug excretion as well as the age, sex and physiological state of the patient also affected by the some kind of disease. Pharmacokinetics is the study of the relationships between drug response in the patient and factors. Pharmacodynamics is the study of how a medicine acts on a living organism. This includes the pharmacological response and its duration and magnitude observed, relative to the medicine's concentration at an active site in the organism.

Keywords: Drug, Environment, Phermacokinetics, Phermacodynamics, etc.

INTRODUCTION

A number of properties contributes to pharmacokinetics specially absorption, distribution, metabolism and excretion. Pharmacological and toxicological actions of medicines are primarily related to their concentrations. Medicine action is controlled by the following four fundamental pathways of drug movement and modification in the body:

1. Absorption
2. Distribution
3. Metabolism
4. Excretion

CHAPTER-8

IMPACT OF COVID-19 ON MENTAL HEALTH OF COLLEGE STUDENTS

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ABSTRACT

It is of great concern to address the mental health of the students pursuing higher education. The Outbreak of COVID-19 pandemic has brought about changes in this group of population i.e youth. In this survey based study, the mental healths of college going students were assessed. Total 112 students have participated in this survey and provided the information about their mental well-being. From the study, it is concluded that the mental problems increases among the students due to covid-19. It is also reported from the result that depression, sleeplessness, nervousness and stress are increases among the college students. In order to safeguard the mental health of students, there is an urgent need to address and provide measures to overcome this problem.

Keywords: Covid-19, mental health, depression, nervousness, stress, sleeplessness, lock down, work from home, college students.

INTRODUCTION

Wuhan, China, in 2019 reported the first coronavirus case, the outbreak is now known as COVID-19, which has spread globally [1]. The World Health Organization (WHO) declared the coronavirus outbreak a public health emergency of international concern and declared it a pandemic [2-3]. The United States, Brazil, India, Russia, and Europe, which have seen maximum number of cases and deaths than the rest of the world [3-4]. The coronavirus had spread to over 216 nations as of August 18th, 2020, with at least 21,756,357 confirmed cases and 771,635 confirmed deaths worldwide. Between January 20th and August 18th, 2020, there were 5,354,013 confirmed cases of COVID-19 in the United States, with 168,999 deaths [5]. The virus's propagation has created global economic and social disruption, as well as a massive overburdening of healthcare and educational institutions [6].

Children's mental health has been affected in a variety of ways, as this unprecedented scenario has altered the way kids generally grow, learn, play, interact, and regulate emotions. During this stressful environment, children with pre-existing psychiatric problems such as

CHAPTER-9

HEAVY METAL REMOVAL BY MICROALGAE

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ABSTRACT

Various human activities cause heavy metals to be discharged into rivers. Because heavy metals are nonbiodegradable and stay in the environment, they pose a hazard to biota. The current strategies for removing and/or detoxifying heavy metals in aquatic ecosystems, with a focus on microalgae, are discussed in this chapter. Microalgae have evolved a broad range of extracellular and intracellular absorption and adsorption mechanisms to cope with heavy metal toxicity, according to a review of the literature. The potential of prokaryotic and eukaryotic microalgae live cells, as well as their dead cell biomass, is explored in relation to presently existing physicochemical techniques for eliminating harmful heavy metals. The essential conditions for bringing this heavy metal removal capability to a commercially viable level are also discussed. The main objective of present study are the Algae sample collection from AMU campus, its characterization for preliminary algae identification, providing suitable condition algal growth and to study of Cd and Ni adsorption.

Keywords: Heavy metals, anthropogenic, absorption, biodegradable

INTRODUCTION

Algae are a diverse group of eukaryotic organisms that include both unicellular and multicellular species. From single-celled algae such as Chlorella to multicellular algae such as the enormous kelp, a large brown alga that may grow up to 50 metres in length, algae are found in many types of environments. The high production per unit area of the organism makes it stand out when compared to other photosynthetic organisms in higher plants. Algae are able to adapt to a broad range of temporal and spectral irradiances, have fast breeding rates, and minimal nutritional demands. Dunaliella, Spirulina, and Chorella spp. are simple to scale up in photo bioreactors (PBRs), because enough nutrient levels may be delivered continuously. Aquatic algae are autotrophs, capable of producing inorganic nutrients. In order

CHAPTER-10

CARBON QUANTUM DOTS: AN OVERVIEW OF SYNTHESIS, CLASSIFICATIONS AND THEIR OPTICAL PROPERTIES

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ABSTRACT

In recent years, carbon quantum dots (CQDs) act as an emerging magnificence of quantum materials with gainful properties such as high photoluminescence, clean synthesis routes, affordable synthesis, cheap beginning substances, high water-solubility, low toxicity, sturdy photo-stability, and smooth functionalization and have acquired brilliant attention among the researchers. The current chapter discussed an overview and history of CQDs and exhaustive literature survey related to economical and green route for the CQDs synthesis. Further, the proposed chapter also emphasized the synthetic technology and methodology for the production of these CQDs, briefly. Moreover, the optical properties of these CQDs and the effect of doping with different heteroatoms into it have also been explored successfully.

Keyword: carbon quantum dots, applicability, carbon nanotubes

INTRODUCTION

During the last decades, metal based semiconductor quantum dots (QDs) have been investigated for their resilient and tunable fluorescence emission properties, which enable their applications in biosensing and bioimaging. However, they hold certain prohibition toward their applicability in the biomedical field or several other analytical applications as they contain heavy metal core which is not environmentally compatible [1, 2]. Heavy metals are highly toxic even at very low concentrations, thus restricted the applicability in clinical analysis [3]. Carbon quantum dots (CQDs) turned into a new class of carbonaceous materials in a carbon family and has become a mounting star among the scientific community over the past decades [4-6]. It has been categorized into 0D materials. The Xu's Group has first discovered these materials in 2004 during the electrophoresis of single-walled carbon nanotubes (SWCNTs) from arc-discharged soot, accidentally [7]. Thus, due to their interesting features such as low cyto-toxicity, ease of synthesis, facile surface functionalization, sturdy photo-stability, high photo-response, tunable excitation-emission and catalysis properties, it could be broadly used in the application of bio-imaging, drug delivery, optronic devices, sensor and catalyst [8-10].