



Environmental and Medicinal Chemistry

Experimental Design and Applications

Part I

Abdul Rahman Khan, Saimah Khan
Tahmeena Khan, Qazi Inamurrahman



Environmental and Medicinal Chemistry
Experimental Design and Applications
(Part-I)

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AARGON PRESS

New Delhi

Environmental and Medicinal Chemistry: Experimental Design and Applications (Part-I)
Abdul Rahman Khan, Saimah Khan, Tahmeena Khan and Qazi Inamurrahman

© Edition, 2021

Published by
Aargon Press
EG-130, Inderpuri,
New Delhi-110012, India
Tel.: +91-11-9958121300
Email: info.aargonpress@gmail.com
Website: www.aargonpress.com

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ISBN: 978-93-94070-30-1

Printed at: Aargon Press, New Delhi

CONTENTS

No.	CHAPTERS	Page No.
1	SYNTHESIS, CHARACTERIZATION AND APPLICATIONS OF CONDUCTING POLYMER COMPOSITE <i>Mohammad Nasir Siddiqui, Nafees Ahmad, Abdul Rahman Khan</i>	1-10
2	ASSESSMENT OF PHYSICO-CHEMICAL PARAMETERS AND MICROBIOLOGICAL ANALYSIS OF GROUND WATER OF BKT, LUCKNOW <i>Firoj hassan, Nazneen Kausar, Abdul Rahman Khan</i>	11-35
3	DETECTION OF HEAVY METALS IN CONFECTIONARY <i>Malik Nasibullah, Naziya Syed</i>	36-55
4	SYNTHESIS AND CHARACTERIZATION OF ACETYLACETONE AND ACETOPHENONE THIOSEMICARBAZONE LIGANDS <i>Naseem Ahmad, Tahmeena Khan, Umang Jaiswal</i>	56-64
5	AN ATTEMPT FOR FACILE SYNTHESIS OF ZINC OXIDE NANOPARTICLES VIA GREEN ROUTE <i>Md. Kavish, Shamaila Hasan, Qazi Inamur Rahman, Abdul Rahman Khan</i>	65-76
6	SYNTHESIS, CHARACTERIZATION AND COMPUTATIONAL STUDIES OF MIXED LIGAND-METAL COMPLEXES OF 2-BUTANONE THIOSEMICARBAZONE <i>Tahmeena Khan, Eram Jamal Siddiqui, Abdul Rahman Khan</i>	77-85

- 7 STUDY ON SYNTHESIS AND APPLICATIONS OF 1,10-PHENANTHROLINES DERIVATIVES** 86-102
Iqbal Azad, Naseem Ahmad, Junaid Akram, Abdul Rahman Khan
- 8 USE OF NEEM (AZADIRACTA INDICA) BARK POWDER FOR ADSORPTION OF DYE ACID GREEN 1 FROM AQUEOUS SOLUTION** 103-116
Akhilesh Kumar, Mohammad Azam, Minaxi B.Lohani
- 9 EXTRACTION OF CITRUS ESSENTIAL OIL (EOS) FROM PEELS OF ORANGE, LEMON, MANDARIN AND SWEETLIME** 117-128
Saimah Khan, Neda Afreen, Naseema Parveen and Nausheen Ruhi
- 10 CHITOSAN BASED NANOHYBRID FOR PHOTOTHERMAL CANCER THERAPY: RECENT TRENDS** 129-144
Prabha Bhartiya, Daraksha Bano

SYNTHESIS, CHARACTERIZATION AND APPLICATIONS OF CONDUCTING POLYMER COMPOSITE

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ABSTRACT

Conductive polymers, such as polyaniline, polyfuran and polypyrrole are gaining attention for many commercial applications because of their characteristics properties such as redox properties, conducting properties, environmental stability and ease of synthesis. These polymers are conducting in nature due to the presence of the conjugated electrons through alternating single and double bond. In the present study polypyrrole has been selected for examine. Due to this unique chemical property, many researchers and scientist of various disciplines around the world has been attracted for the application of polypyrrole. Synthesis, characterization and application have been investigated in the present study. Various factors such as adsorption, concentration of the oxidants and monomer have been tested by varying their concentration.

Keywords: Polypyrrole, conductivity, stability, oxidant

INTRODUCTION

Conducting polymers such as polyfuran, polythiophene, polyaniline and polypyrrole have been studied for the last few decades due to their characteristics properties such as high electrical conductivity and good environmental stability and redox property. [1,2] Among these conducting polymers polypyrrole have gained much interest due to its ease processability, high conductivity and excellent mechanical properties. Derivatives of the above mentioned conductive polymers have been used to prepare advanced materials such as energy storage materials sensors, optoelectronic devices, water splitting and CO₂ reduction. [3, 4] However, there are few limitations that limits the applications of conductive polymers are low biodegradability, slow solubility, difficulty in fabrication and poor mechanical integrity. For the last 2 decades, an innovative class of organic-inorganic nanocomposites has

CHAPTER-2

ASSESSMENT OF PHYSICO-CHEMICAL PARAMETERS AND MICROBIOLOGICAL ANALYSIS OF GROUND WATER OF BKT, LUCKNOW

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INTRODUCTION

Water dominates the surface of Earth and is vital to life on our planet. Due to high dielectric constant of water shows remarkable properties with anomalous behaviour and explores how the structure of water molecules gives rise to its physical and chemical properties. Considering water in all three of its states i.e. solid (ice), liquid (water) gas (steam). It explains the great importance of understanding its structure and behaviour for fields such as chemistry, astrophysics, earth and environmental sciences. The role of water in life science is involving all the metabolic activities and their mechanism of absorption and balancing water molecules in the life processes is very important. It concludes with a discussion of the outstanding controversies concerning water, and some of the 'magical' properties that have been claimed for it.

Looking at the satellites photographs of the planets Earth can illustrate the fact that the majority of the Earth surface is covered with water. Earth is known as "blue planet". Water is very much important for our life because if there will be no water then there can be no life on water. No one can survive without water. 71% of the Earth is covered with water. Here also is the water beneath the earth which is known as groundwater. Yet with all the water present on the earth, water is still a finite source, cycling from one form to another. Drinking water, also known as potable water, that is safe to drink or to use for food preparation. The amount of drinking water required for consuming. [1] It depends on physic-chemical properties like age, health issues, and environmental conditions. Water is essential for life. It has been observed that due to rapid industrialization water from our ground and surface water are fastly deteriorated/ contaminated and quality of water badly affected and no water can be used without any further treatment before using. Due to large amount of water required for our daily life and huge amount of water required for steam generation for power production, this process after consumption the quality parameter of water badly disturbed and availability of

DETECTION OF HEAVY METALS IN CONFECTIONARY

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INTRODUCTION

Heavy metals as lead (Pb), chromium (Cr), arsenic (As), zinc (Zn), cadmium (Cd), copper (Cu), mercury (Hg), and nickel (Ni), are persistent as contaminants in the environment and come to the fore front of dangerous substances causing health hazard in being cells of environment. Industrial and agricultural processes have been resulted to increasing the concentration of heavy metals in air, water, soil and subsequently, these metals are taken by plants or animals and take their ways into food chain (Ahmad W.M.S, 2002). Screamingly, the heavy metals are presently found that one in dairy products may be attributed to contamination of the original cow's milk, the exposure of lactating cow to environmental pollution or consumption of feeding stuffs and waste (Carl M., 1991) and (Okada, 1997). Moreover, raw milk may be exposed to contamination during its manufacture (Ukhun M. E., 1990(44)) and (EL-Batanouni, 1996). Such cow's milk have to make consists delicious candies and chocolates etc. They are associated with joy and pleasure, potentially being stimulant, relaxant, and antidepressant (Mueller & al.), 2007;2006). Different types of candies and chocolates are available in the national and international market. The basic ingredients of chocolates include cocoa butter, chocolate liquor, and sugar, though each company has its own ingredients and recipes. Other ingredients used in candy making include liquid glucose, vegetable oil, malt extract, soya solids, emulsifiers, salts, sodium bicarbonate, wheat flour, buffering agents, stabilizer, flavors, yeast, and flour improvers. Various types of ingredients used in candy making and increasing, and product are becoming more complex. Addition of different ingredients increases the risk of heavy metal contamination in candies and chocolates. There are many studies which report the presence of heavy metals in candies and chocolates but lack the dietary exposure of heavy metals. (Dahiya S. K., 2005) Analyzed Pb, Ni in chocolates and candies and found that Ni ranged from 0.041 to 8.29 $\mu\text{g/g}$ with an average of 1.63 $\mu\text{g/g}$; and Pb level ranged from 0.049 to 8.04 $\mu\text{g/g}$ with an average of 0.93 $\mu\text{g/g}$ in different brands. (Rankin, 2005) Reported that Pb concentration in chocolates and cocoa products was 230 and 70 mg/g respectively, from Nigeria which is the lowest reported value for any natural food. (Skrbic, 2013). Also reported a relatively high concentration of Pb

SYNTHESIS AND CHARACTERIZATION OF ACETYLACETONE AND ACETOPHENONE THIOSEMICARBAZONE LIGANDS

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ABSTRACT

Schiff bases are important organic ligands having potential tendency of complexation with transition metals and they have shown excellent pharmacological properties over the years. Thiosemicarbazones are well known Schiff based ligands which are usually neutral yet their anionic forms are also known. Their bidentate, tridentate or in some cases polydentate nature is due to the presence of donor atoms like sulphur, nitrogen or in some instances oxygen. As transition metals can exhibit an array of coordination power, they easily form stable complexes with Schiff based thiosemicarbazone ligands. Latest advances in medicinal inorganic chemistry have given considerable importance to the development of metal-based drugs. Since the presence of metal ion in the drug moiety usually mitigates the ill effects of carbon-based compounds, this may lead to the production of new metal-based drugs. This study discusses the preparation and characterization of acetylacetone and acetophenone thiosemicarbazone ligands and their characterization. They can be further explored in future for their biological activity. Detailed studies are required to explore new mechanistic actions and the specific role of metal ions and ligand inside the body. Ligands which have poor or moderate activity should be studied in combination with ligands of good biological significance for activity enhancement.

Keywords: Thiosemicarbazone, Schiff base, metals, biological role

INTRODUCTION

Schiff base is a compound with the general structure $R_1R_2C=NR'$ ($R' \neq H$), i.e., generally compounds containing C=N group. They are condensed product of primary amines and carbonyl compounds. They can be considered a sub-class of imines, being either secondary ketimines (containing keto group) or secondary aldimines (containing aldehydic group) depending on their structure. The term Schiff base is normally applied to the compounds where they are used as ligands for the formation of coordination complexes with metal ions.

AN ATTEMPT FOR FACILE SYNTHESIS OF ZINC OXIDE NANOPARTICLES VIA GREEN ROUTE

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ABSTRACT

This chapter describes green synthesis of zinc oxide nanoparticles via different plant sources in recent times. The chapter discusses the reveals the historical account of nanosciene and its applications. It provides a comprehensive overview of synthesis of zinc oxide nanoparticles using different plants and their parts. This chapter also describes the different parameters viz, solvent used in synthesis how the different characterization techniques, TEM, SEM, EDX, DLS, FTIR, AFM and Zeta potential employed for study of synthesized nanoparticles. We have successfully synthesized zinc oxide using zinc salt with eucalyptus leave extract with good yield.

INTRODUCTION

Nanotechnology is the ability to work at a molecular level, atom by atom in order to create larger structure resulting in enhanced properties and a new molecular assembly [1]. In other words; Nanotechnology is the branch of science that deals with the manipulation of matter either at the molecular or atomic level [2]. It is believed that nanotechnology can make smaller, cheaper, lighter and more functional products consuming lesser resource and energy. Within the field of Nanotechnology, nanoparticles have gained substantial attention due to their very small size and large surface to volume ratio [3].

A vast literature has been published on synthesis and application of Nanoparticles; these studies suggest that in terms of chemical and physical properties out of various metal oxide nanoparticles, "ZnO" is the most promising material which bears both for scientific and industrial applications [4]. Zinc oxide is a non- toxic, environmentally safe, and versatile inorganic compound. It generally exists in three crystallographic forms i.e. Zinc blende, Wurtzite, and occasionally Rock salt. The wurtzite crystal structure is the most common and thermodynamically stable having hexagonal unit cell with lattice parameters spacing $a=$

SYNTHESIS, CHARACTERIZATION AND COMPUTATIONAL STUDIES OF MIXED LIGAND-METAL COMPLEXES OF 2-BUTANONE THIOSEMICARBAZONE

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ABSTRACT

Mixed ligands complexes are complexes in which a metal ion is bonded to two or more complexing species which are formed when the metal iron is present in a mixture of two or more ligands in the solution. The interest in the field of bioinorganic chemistry has increased in the mixed ligand complexes containing Schiff base compounds, since it has been recognized that many of these types of the complexes may serve as model for biologically important species. In the present work mixed ligand complexes of 2 Butanone thiosemicarbazone as a primary ligand and piperazine as a secondary ligand with Fe (II), Zn (II), Co (II) ions were synthesized and their characterization was done by NMR and IR spectroscopic techniques. Computational studies of the complexes were also performed. The absorption, distribution, metabolism, excretion and toxicity (ADMET) assessment was done by admetSAR software. Toxicity assessment was done through OSIRIS data warrior software and pharmacokinetic properties were assessed through Molinspiration. The drugliness of the complexes was assessed through Lipinski's filter. The results showed that the synthesized complexes possessed appreciable drug-like character and may be further explored for their medicinal activity.

Keywords: Thiosemicarbazones, mixed ligand, piperazine, ADMET

INTRODUCTION

A coordination complex consist of a central atom or ion which is usually metallic and is called the coordination center, and a surrounding array of bound molecules or ions, that are in turn known as ligands or complexing agents. Mixed ligand-metal complexes are complexes in which a metal ion is bonded to two or more complexing species which are formed when the metal iron is present in a mixture of two or more ligands in the solution [1]. Mixed ligand complexes commonly occur in biological fluids and numerous potential ligands are likely to

STUDY ON SYNTHESIS AND APPLICATIONS OF 1, 10-PHENANTHROLINES DERIVATIVES

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ABSTRACT

This chapter covers how to format your chapter files in the manuscript you will provide to Taylor & Francis. Recent advancements in the chemistry of 1,10-phenanthrolines are the focus of this book chapter (phen). Under dichloromethane (DCM) at 40°C, a one-pot four-component synthesis combining aldehyde, malononitrile, 1,10-phenanthridine, and tertiary butyl isocyanide was employed to manufacture phen derivative with good yield. The chromophores and pharmacophore characteristics of the developed molecular scaffold are promising. Phen derivatives are particularly relevant to contemporary study due to their varied structural and chemical features.

Keyword: 1,10-phenanthrolines; multicomponent reaction; heterocyclic compounds; bioactivity score; Lipinski's rule of five

INTRODUCTION

Many approaches, such as microtubule targeting or enzyme inhibition, transcription regulation, groove binding, DNA intercalation, and angiogenesis suppression, are commonly exploited in the creation of cancer treatments [1]. DNA intercalation, which has been discovered in the functional regions of the human genome, is the most promising method that has lately emerged. DNA intercalation, which has been discovered in the functional regions of the human genome, is the most promising method that has lately emerged [2]. DNA intercalation, which has been discovered in the functional regions of the human genome, is the most promising method that has lately emerged [3]. Organic chemistry (OC) has recently emerged as one of the most exciting fields for drug discovery and development (DDD). It provided numerous braces for the development of various moieties and complexity adjustments to the compound [4]. Because of the connectivity of diverse fields of research, OC offers a wide variety of applications [5]. In the pharmaceutical sector, OC is still one of the most important factors in drug development [6]. Heterocyclic chemistry (HC) has

USE OF NEEM (AZADIRACTA INDICA) BARK POWDER FOR ADSORPTION OF DYE ACID GREEN 1 FROM AQUEOUS SOLUTION

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ABSTRACT

Neem bark powder (NBP) was used as an adsorbent for the removal of textile dye Acid green 1 from aqueous solution. The experiments were carried out to study the effect of parameters like initial concentrations of the dye, agitation time and adsorbent dose. Maximum removal of the dye was 78.37% by NBP at an adsorbent dose of 1g. The dye adsorption on NBP reached equilibrium in 120 minutes.

Keywords: NBP, removal, adsorption, dye, parameters

INTRODUCTION

Dyes are natural or synthetic, organic compounds that provide bright and lasting color to other substances and are widely used in textiles, printing, rubber, cosmetics, plastics, leather, pharmaceuticals, food industries, etc. to color their products. Mainly dyes are classified into anionic, cationic, and non-ionic dyes. Dyes are chemical compounds which attach themselves to fabrics or surface shells to impart color. Depolarization of waste water from textile and manufacturing industries is a major challenge for environmental managers [1] as dyes are water soluble and produce very bright colors in water with acidic properties. It has been projected that around the globe textile and manufacturing industries are using more than 10,000 commercially available dyes and the consumption of dyes in textile industry is more than 1000 tones/year and about 10-15% of these dyes are discharged into waste streams as effluents during the dyeing processes [2] and generating a large amount of colored wastewater.

Among all the dyes using in industries, textile industry is placed in the top position in using of dyes for coloration of fiber [2]. The wastewaters discharged from dyeing processes exhibit a high BOD, high COD, visible pollutants and high amounts of dissolved solids. Effluents discharged from dyeing industries are highly colored and are toxic to aquatic life. Some dyes are mutagenic, carcinogenic and teratogenic [3-4]. Dyes are highly toxic and even

EXTRACTION OF CITRUS ESSENTIAL OIL (EOS) FROM PEELS OF ORANGE, LEMON, MANDARIN AND SWEETLIME

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ABSTRACT

The essential oil (EO) obtained from citrus peels is an eco-friendly, economic and natural substitute for chemical based preservatives and other synthetic antioxidants commonly used for food preservation such as sodium nitrates, nitrites and benzoates. The peels of citrus fruits that are mainly discarded as waste material can be used for the extraction of citrus EO. EOs obtained by utilizing waste peel material of citrus fruits, can result in reducing the pollution as well as also used in variety of applications. Due its pleasant aroma, antimicrobial and antioxidant properties, citrus EO is widely used in food, chemical industry, medical treatment, and other fields. In this chapter, we study about the extraction, characterization and applications of citrus essential oil obtained from the peels of citrus fruits such as orange, lemon, mandarin and sweetlime. This chapter focuses on improved steam distillation, in this process before subjecting to distillation the citrus fruits peels are preheated. The D-limonene (95%) is the main component of citrus oil and has variety of applications from food flavouring agents to cosmetics. Concerning allergies and obtaining safer dosage limits, more research is needed in this area. In various application, the safer utilization of citrus based EOs, move towards greener technologies indicate optimistic future.

In this study, the peels of four fruits namely orange, mandarin, lemon and sweetlime were extracted using Steam distillation apparatus and their percentage yield was calculated. The percentage yield of all four fruit peel sample follows the order. Orange > Mandarin > Lemon > Sweetlime.

Keywords: Citrus essential oil, orange peel, lemon peel, mandarin peel, sweetlime peel, Steam distillation

INTRODUCTION

In fruit peel, mainly flavedo part and cuticle, essential oils (EOs) are present in appreciable amount in oil sacs or oil glands present at different depths. These are soluble in natural oils, ether and alcohol while insoluble in water. EO of citrus fruits is a complex mixture of around

CHITOSAN BASED NANOHYBRID FOR PHOTOTHERMAL CANCER THERAPY: RECENT TRENDS

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INTRODUCTION

Today, undoubtedly cancer is one of the leading causes of morbidity world-wide. With more than 10 million new cases per year world-wide and the increasing incident rate, cancer remains one of the major challenges in healthcare [1-4]. Currently available cancer therapies in clinical trials (e.g., chemotherapy, radiation therapy and surgery) have proved only partially successful due to heterogenous nature of cancer and tissue complexity. In addition, these therapies are limited by systematic toxicity to normal healthy cells, invasive treatment procedure, multi-drug resistance and risk of development of secondary cancers [5-8]. Considering limitations associated with available cancer therapies, the focus of research has shifted to find alternative techniques to treat cancer or improving the already-existing ones.

Over the past decade, Photothermal therapy (PTT) (also referred as photothermal ablation, photo-thermolysis or optical hyperthermia) has emerged as a promising therapeutic alternative or supplement to conventional cancer therapies [9-11]. It has drawn much attention owing to its specificity, minimally invasive nature, facile implementation, fewer complications, precise spatial-temporal selectivity and fast recovery [12-14]. It also holds the advantage of killing cancer cells without causing resistance regardless of the genetic background, hence can be applied to all cancer patients. This technique employs use of photo-absorbing agents for conversion of optical energy into heat (> 42 °C) for selective ablation of cancer cells [15-17].

As the heat generators, nanomaterials can absorb and convert near-infrared (NIR) light into heat energy under external laser stimulating [18-20]. To achieve better living tissue penetration depth and minimal damage to healthy tissues and organs, the NIR lasers ranging from 650 to 980 nm are usually adopted as the energy source for lowering the self-absorption by tissues and blood [21-24]. Nanoparticles (NPs) tend to selectively accumulate in tumor due to so called enhanced permeability and retention (EPR) effect [25,26]. In recent years,