Madda Walabu University

School of Graduate Studies

College of Natural And Computational Sciences

Department of Chemistry

Preparation And Characterization of A Biosorbent From *Datura Stramonium* Root (Atefaris) For The Removal of Malachite Green From Aqueous Solutions

M.Sc. Thesis

By:

Solomon Dejene

Advisor: Fisseha G/Wold (Assis.Prof.)

February, 2026

Bale-Robe, Ethiopia

Preparation And Characterization of Biosorbent from the Root of *Datura Stramonium* (Atefaris) For The Removal of Malachite Green From Aqueous Solutions

M.Sc. Thesis

By:

Solomon Dejene

Advisor: Fisseha G/Wold (Assis.Prof.)

A Thesis Submitted to College of Natural And Computational Sciences, Department of Chemistry, in Partial Fulfillment of The Requirements For The Degree of Master of Science In Chemistry

February, 2026

Bale-Robe, Ethiopia

Madda Walabu University

College of Natural and Computational Sciences,

School of Postgraduate Studies

Chemistry Department

Advisors' Approval Sheet

This is to certify that the thesis entitled **''Preparation and characterization of Biosorbent from Root of *Datura Stramonium* (Atefaris) For the Removal of Malachite Green from Aqueous Solutions''** submitted in partial fulfillment of the requirements for the degree of Masters of Science in Chemistry with the Postgraduate Program of the Chemistry Department /College of Natural and Computational Sciences/ and has been carried out by **Solomon Dejene (PGSBG/025/11)**, under my supervision. I have read and evaluated this thesis, which complies with the regulations of the university and meets the required standards. Therefore, I recommend that the student has fulfilled the requirements and hence can submit the thesis to the department with my approval as the university advisor.

Advisor	Signature	Date
FISSEHA G/W. (Ass.Prof.)	_____	_____

Madda Walabu University

School of Postgraduate Studies

Masters' Thesis Defence

Boards of Examiners' Approval Sheet

We, the undersigned, members of the Board of Examiners of the final Thesis open defense by **Solomon Dejene (PGSBG/025/11)** have read and evaluated his thesis entitled **''Preparation and characterization of Biosorbent from Root of *Datura Stramonium* (Atefaris) For the Removal of Malachite Green from Aqueous Solutions''** and examined the candidate. This is, therefore, to certify that the thesis has been accepted in partial fulfillment of the requirements for the degree of Masters of Science in Chemistry.

Dr. Dejene D. (Asst. Prof)	_____	_____
Name of Internal Examiner I	Signature	Date
Dr. Bereket A. (Asst. Prof)	_____	_____
Name of Internal Examiner II	Signature	Date
Dr. Girma Ragassa	_____	_____
Name of External Examiner	Signature	Date

Certification of the thesis

I hereby certify that all the corrections and recommendations suggested by the board of examiners are incorporated into the final thesis.

_____	_____	_____
Name of the designate	Signature	Date

Final approval of the thesis

Final approval and acceptancs of the thesis is contingent up on the submission of its final copy to the of graduate studies (CGS) through the candidate's college graduate committee.

_____	_____	_____
Head CGC	Signature	Date

Remark

To be filled in fuor copies. Each copy is given to CGS, Rigisterar and alumni Director

Declaration

I hereby declare that this MSc Thesis entitled **''Preparation and characterization of Biosorbent from Root of *Datura Stramonium* (Atefaris) For the Removal of Malachite Green from Aqueous Solutions''** is my original work. All scholarly matter that is included in the thesis has been given recognition through citation. I solemnly declare that this thesis has not been submitted to any other institution anywhere for the award of any academic degree, diploma or certificate.

Solomon Dejene _____ _____

Student Name Signature Date

This MSc thesis has been submitted for examination with my approval as thesis advisor.

Fisseha G/W. (Ass.Prof.) _____ _____

Advisor Name Signature Date

Acknowledgements

First of all, I would like to thank my Almighty God for his Endless Love and Blessing me with all the treasures of wisdom and knowledge of LORD Christ Jesus, for his leadership; protections and I also thanks his mother's saint bergin mariyam for her help throughout all my work.

I wish to express my cordial thanks and gratitude to my advisor Fisseha G/W. (Assistance professor of Analytical Chemistry in Research) for his effective and intellectual guidance, advice, suggestions, and comments during the course of this thesis. He was also always approachable and patient with me and gave me confidence towards finalizing this thesis up to-date of final thesis research defense.

Special recognition goes to Mr. Yohannes Shuka, who is laboratory analyst, software's expert and young researcher for unwavering support of experiment conducting, software analysis and professional advising during write-up.

I would like to thank all my class classmates, friends and my beloved families for their encouragement and support.

Table of Contents

Content page

Advisors' Approval Sheet iii

Madda Walabu University iv

Boards of Examiners' Approval Sheet iv

Declaration v

Acknowledgements vi

Table of Contents vii

List of Figures x

Abbreviation and Acronyms xi

Abstract xii

CHAPTER ONE xii

1. INTRODUCTION 1

1.1. Background of the study 1

1.2. Statement of the problem 2

1.3. Significance of the study 2

1.4. Objective 3

1.4.1. General objective 3

1.4.2. Specific Objectives 3

1.5. Research Question 3

1.6. Scope of the study 3

CHAPTER TWO 4

2. LITERATURE REVIEW 4

2.1. Chemistry of Dye 4

2.2. Classification of dyes 5

2.3. Physicochemical properties of Malachite Green 5

2.4. Environmental Pollution of Dyes 6

2.5. Comparison of datura stramonium root biosorbent with other plant-based 9

2.6. Chemical activation of Biosorbent 9

2.7. Effect of Biosorbent for the Removal of Malachite green 10

CHAPTER THREE 12
3. MATERIAL AND METHODS 12
3.1 Experimental Section 12
3.2 Chemicals and Instruments 12
3.2.1. Chemical and Reagent 12
3.2.2. Instrument and Apparatus 12
3.3 Sample collection and Sample preparation 13
3.4 Preparation of biosorbent 13
3.5. Characterization of nanoparticles 15
3.5.1. X-ray diffraction (XRD) 15
3.5.2. Fourier Transform Infrared (FTIR) analysis 15
3.5.3. Scanning Electron Microscopy (SEM) 15
3.6. Synthetic wastewater 15
3.7. Calibration 16
3.8. Batch Adsorption Experiment 16
3.9. Factor affecting adsorption of MG 17
3.10. Adsorption model 18
3.11. Kinetic model 19
CHAPTER FOUR 20
4. RESULTS AND DISCUSSION 20
4.1. Optimization of chemicals activation 20
4.2. Characterization 21
4.2.1. FT-IR (Fourier transform infrared spectrometry) 21
4.2.2. Scanning electron microscope (SEM) 23
4.2.3. XRD analysis 24
4.3. Batch adsorption study 26
4.3.1. Calibartion 26
4.3.2. Effect of Initial Dye Concentration 27
4.3.3. Effect of Biosorbent dose 27
4.3.4. Effect of pH 28
4.3.5. Effect of contact time 29
4.3.6. Effect of temperature 30

4.4. Biosorbtion Activity at Optimal conditions and its Stability 31
4.5. Adsorption Isothermal Study 32
4.5.1. Langmuir Isotherms 32
4.5.2. Freundlich Isotherms 33
4.6. Pseudo First–order and Pseudo second–order adsorption kinetics 34
4.7. Comparison of previously reported adsorption capacity with different biosorb 36
CHAPTER FIVE 38
5. CONCLUSION AND RECOMMENDATION 38
5.1. Conclusion 38
5.2. Recommendation 38
REFERENCES 40
APPENDPICES 45

List of Figures

Figure 1: Classification of dyes 5
Figure 2: Chemical structure of malachite green 6
Figure 3: Discharging of dye into environment 8
Figure 4: Effect of chemical activation on the surface of biosorbent 10
Figure 5: Sample collection 13
Figure 6: Biosorbent Preparation 14
Figure 7: Preparation of Synthetic Wastewater and Dilution 15
Figure 8: Batch Adsorption Study 17
Figure 9: Effect of activating reagents on preparation of *Datura Stramonium* root 21
Figure 10: FTIR spectrum of *Datura Stramonium* root derived bosorbent before and after . 22
Figure 11: SEM images of *Datura Stramonium* root-derived biosorbent before and after ... 24
Figure 12: XRD diffiraction of *Datura Stramonium* root derived bosorbent before and 25
Figure 13: Calibiration Curve of *Datura Stramonium* root derived bosorbent for MG 26
Figure 14: Effect of initial dye concentration on removal of MG by *Datura Stramonium* ... 27
Figure 15: Effect of adsorbent dose on removal of MG by *Datura Stramonium* root deriv 28
Figure 16: Effect of solutions pH on removal of MG by *Datura Stramonium* root derived .. 29
Figure 17: Effect of contact time on removal of MG by *Datura Stramonium* root bosorbent 30
Figure 18: Effect of temperature on removal of MG by *Datura Stramonium* root bosorbe .. 31
Figure 19: Biosorbent activity of *Datura Stramonium* root derived bosorbent and 32
Figure 20: Langmuir adsorption isotherm for *Datura Stramonium* root derived bosorbent... 33
Figure 21: Freundlich isotherm study for *Datura Stramonium* root derived bosorbent 34
Figure 22: Pseudo First–order and Pseudo Second–order for the adsorption of MG on 35

Abbreviation and Acronyms

FTIRs	Fourier Transform Infrared spectroscopy
MG	Malachite Green
SEM	Scanning Electron Microscopy
XRD	X ray diffraction
DrSrB	*Datura Stramonium* root derived bosorbent

Abstract

Malachite green, a widespread, persistent contaminant in trash and the environment that poses serious risks to aquatic life and human health, is utilized in the textile and dyeing industries. As a result, biosorbent made from plants is thought to be the most effective way to remove malachite green from aqueous solutions. It is built using plant matter or sustainable raw materials through a chemical activation method. Still, testing how well this natural filter pulls out malachite green mattered deeply for clean water and natures balance. The majority of academics are currently interested in removing malachite green from water because of its characteristics. One of the best techniques for influencing the availability, transformation, and bioavailability of malachite green is adsorption. The characterization findings demonstrated that the biosorbent had the largest macro porous surface area and a well-developed surface area for adsorption. Fourier transform infrared spectroscopy (FT-IR), scanning electron microscopy (SEM), and X- ray diffraction (XRD) spectroscopy were used to examine the surface functional group, morphology, and crystallinity. The results of batch experiments showed that a number of factors, including pH, dose, contact time, temperature, and initial MG concentration, affect the adsorption of malachite green by a biosorbent produced from Datura stramonium roots. The ideal dose of 1g, pH of 8, starting malachite green concentration of 20 ppm, contact period of 30 minutes, and temperature of 30^{o}C were noted. The Langmuir model with maximal adsorption capacity of 25.77 mg.g^{-1} had the best fit to the adsorption data (R^2 = 0.996) according to the isothermal analysis, while the kinetic data supported the pseudo-second order model with an optimally suited R^2 coefficient of 0.887 for malachite green. Lastly, the findings indicate that the removal of organic dye pollution from aqueous solution using a biosorbent generated from Datura Stramonium roots may be economically feasible. From the results, it is evident to expect that Datura Stramonium biosorbent will show comparable adsorption behaviors for the removal of various coloring agents from aqueous solutions, even if the experiment is limited to malachite green.

Key words: Aqueous solution, biosorbent, malachite green and adsorption method.

CHAPTER ONE

1. INTRODUCTION

1.1. Background of the study

The rise in industrial (textile, paper, plastics, cosmetics, leather, and food) activities releases effluents containing pollutants like heavy metal ions, organic dyes, and pharmaceuticals into the aquatic environment, posing serious health risks to livingthings and degrading the environment overall. This is one of the main issues that many nations face worldwide. (Mengesha *et al.*, 2024; Abate *et al*., 2020). Among different industrial pollutants colored materials and dyes constitute leads to environmental pollution due to their non-biodegradable and polluting nature (Lemos *et al*., 2023).

Malachite green is one of the main colored contaminants. It has a chemical formula of $C_{23}H_{25}CIN_2$ and a molecular weight of 364.7 g/mol, malachite green (MG) is a solid, cationic, and crystalline dye (Abewaa *et al*., 2023). Furthermore, the demand for malachite green was raised in a number of industrial sectors due to its greater water solubility, synthetic nature, stability, and affordability (Oladoye *et al*., 2023). Additionally, Malachite green is bioaccumulative, mutagenic, carcinogenic, teratogenic, and persistent (resists natural biodegradation) (Bhat *et al*., 2023). The kidney, heart, and breast all essential human organs are impacted by malachite green that is consumed through water.

Malachite green (MG) has been removed from aqueous solutions, natural waters, and/or industrial effluents using a variety of techniques, including chemical processes like oxidation (Jabbar *et al*., 2022) and physical treatments like membrane use (Fito *et al*., 2023). Due to their high energy requirements, high cost, and byproduct production, such methods are less successful in removing malachite green (MG) from contaminated water samples (Al-jaaf *et al*., 2023). Also variuos techniques can be used to remove malachite green. Among those techniques, the adsorption process works well for removing MG from aqueous solutions because it is economical, uses a renewable adsorbent, and has a large surface area and porosity (Yabalak and Elneccar *et al*., 2022).

These days, a lot of research has been done on the creation of biomass-based adsorbent materials to get beyond the drawbacks of commercial activated carbons. Agro-waste-based adsorbent materials, such as banana peel (Yabalak and Elneccar *et al*., 2022), and watermelon peel (Awokoya *et al*., 2022), are being investigated for their efficacy in eliminating malachite green dye. In this study, a biosorbent Datura stramonium (which was called in Afan Oromo

Manjii or Amharic Atefaris)for the removal of malachite green from aqueous solution was prepared using the pythochemical-rich root of (Pan *et al.*, 2025).

1.2. Statement of the problem

Due to the significant buildup of organic and inorganic pollutants, the discharge of industrial waste, such as textiles and leather, into water bodies results in water pollution (Ashish et al., 2017). Malachite green (MG) dye has been widely used in distilleries to color leather, wool, jute, and silk, as well as in the aquaculture sector, where it serves as an antibacterial and fungicide to prevent fish infections and illnesses. However, the growth of aquatic plants and algae is negatively impacted by excessive malachite green solutions in water bodies, which may also have an impact on human health (Abewaa *et al*., 2023). Low dissolved oxygen concentrations, fewer fish species, harm to other aquatic life, and an indirect impact on human healing due to damage to the liver, spleen, kidney, and heart, lesions (injury) on the skin, eyes, lungs, and bones, teratogenic effects, and high cytotoxicity to mammalian cells are just a few of the water quality issues caused by this study (Hammud *et al*., 2023).

Because of its stability, large surface area and porosity, affordability, and environmental friendliness, adsorption is the most efficient biosorbent method for removing malachite green buildup from aqueous solution (Mengesha et al., 2024; Shuka et al., 2025).

Because of the plant's special qualities, cost-effectiveness, sustainability, and environmental concerns, the manufacture of biosorbent from Datura stramonium roots for the removal of malachite green from aqueous solutions is a topic of growing interest. In contrast to traditional adsorbents, natural materials like datura straminium are frequently plentiful and inexpensive (Mohan Singh et al., 2002). Using leftover stuff instead of tossing it helps keep things going longer (Gupta et al., 2002). From nature, not factories, these cleansers tend to cause less harm when releases into ecosystems (Zhou et al., 2015). Still, find better ways to clean dirty water means scientists must stay focused on what comes next.

Even though many studies looked at plant-based materials for absorbing pollutants, little has been said about how well chemically treated Datura stramonium roots work in Ethiopia’s setting. This gap sparks curiosity behind the study.

1.3. Significance of the study

The study's findings will serve as a guide for future scholars looking into the same schematic area. Environmental pollutants will be bioremediated using the prepared biosorbent. The

study was also utilized by several non-governmental organizations that work with environmentalists, policy makers, water resource and irrigation management offices, and sanitation and water quality.

1.4. Objective

1.4.1. General objective

- The general objectives of this study was to evaluate the potential of *natural biosorbent* for the removal of synthetic dyes from contaminated water samlples.

1.4.2. Specific Objectives

- ✓ To prepare biosorbent from root of *Datura stramonium* using chemical activation methods.
- ✓ To characterize chemical composition, crystalline nature and surface morphology using FTIR, XRD and SEM techniques.
- ✓ To evaluate the effect of pH, adsorbent dosage, initial concentration and contact time for the removal of malachite green from aqueous solution.
- ✓ To evaluate the adsorption capacity of biosorbent for the removal of MG from aqueous solution under specific experimental conditions.

1.5. Research Question

The research proposal tries to address the following significant questions;

- ✓ What are the preparation methods of biosorbent from plant residues?
- ✓ What are the chemical composition, crystalline nature and surface morphology of biosorbent?
- ✓ What is the effect of pH, adsorbent dosage, initial concentration and contact time for the removal of MG from water sample?
- ✓ What is the potential of biosorbent for the removal of MG from aqueous solution?

1.6. Scope of the study

This study was focused on the preparation of biosorbent from *Datura stramonium for* the removal of malachite green from aqueous solution. In this study sample collection, biosorbent preparation, characterization, adsorption experiment, isotherm and kinetic model was conducted**.**

CHAPTER TWO

2. LITERATURE REVIEW

2.1. Chemistry of Dye

A significant amount of colored waste water is produced as a result of the widespread use of dyes, which are colored compounds, in the textile, printing, rubber, cosmetics, plastics, and leather industries (Dawood *et al*., 2014). Anionic, cationic, and non-ionic dyes are the three main categories of dyes. The textile industry ranked top among all industries utilizing dyes to color fiber. Furthermore, the design of novel dyes has always required a grasp of the links between color and constitution; the chromophores and auxochromes are arguably the most important early contributions to the science of color (Dwived *et al*., 2008). Although it lacks strong theoretical support, the chromophores and auxochromes theory is put out as a straightforward way to explain the origin of color in dye molecules. According to this definition, the carbonyl (C=O), diazo (-N=N-), azomethine (-CH=N), and nitro (NO_2) groups are the most significant chromophores. Other groups, such as hydroxyl (OH^-) and amino (NR_2), intensify the color and cause the absorption to shift to longer wavelengths of light (Enicar *et al*., 1998).

The majority of dyes come from natural sources, such as plants, insects, animals, and minerals, without any chemical processing. Indigo and saffron are plant-based dyes; cochineal beetles and lac scale insects are insect-based dyes; certain mollusk or clam species are animal-based dyes; and ferrous sulfate and ochre are minerals. Dyes are used by the textile, printing, paper, carpet, plastic, and leather industries to give their goods color. Industrial waste always contains these dyes, which are then released into bodies of water (Eren *et al*., 2009; Fassut *et al*., 2004).

Paper, food coloring, cosmetics, leather, pharmaceutical, printing, carpet, and other sectors discharge dyes into waste water. These dye pollutants are released into the environment as waste water effluents by the textile manufacturing and dyeing sectors, which use larger quantities of many dyes. These colors must be eliminated from water effluents before being discharged into bodies of water since they are extremely hazardous and even carcinogenic to microbiological communities and mammals. Dyes are one of the most challenging groups to remove from industrial wastewater because they are not biologically degradable, stable to light, and resistant to aerobic digestion (Garba *et al*., 2015; Gebeyehu et al., 2024; Guo *et al*., 2022).

2.2. Classification of dyes

Dyes can be classified either according to how they are applied to the substrate or according to their chemical structure (particularly considering the chromophoric structure present in the dye molecule) (Figure 1). The first method, which makes use of dyes like anthraquinone and azo, is employed by practicing dye chemists.The color index used the latter approach (Abd EI-Latif *et al*., 2010; Guo *et al*., 2022; Shuka *et al*., 2025).

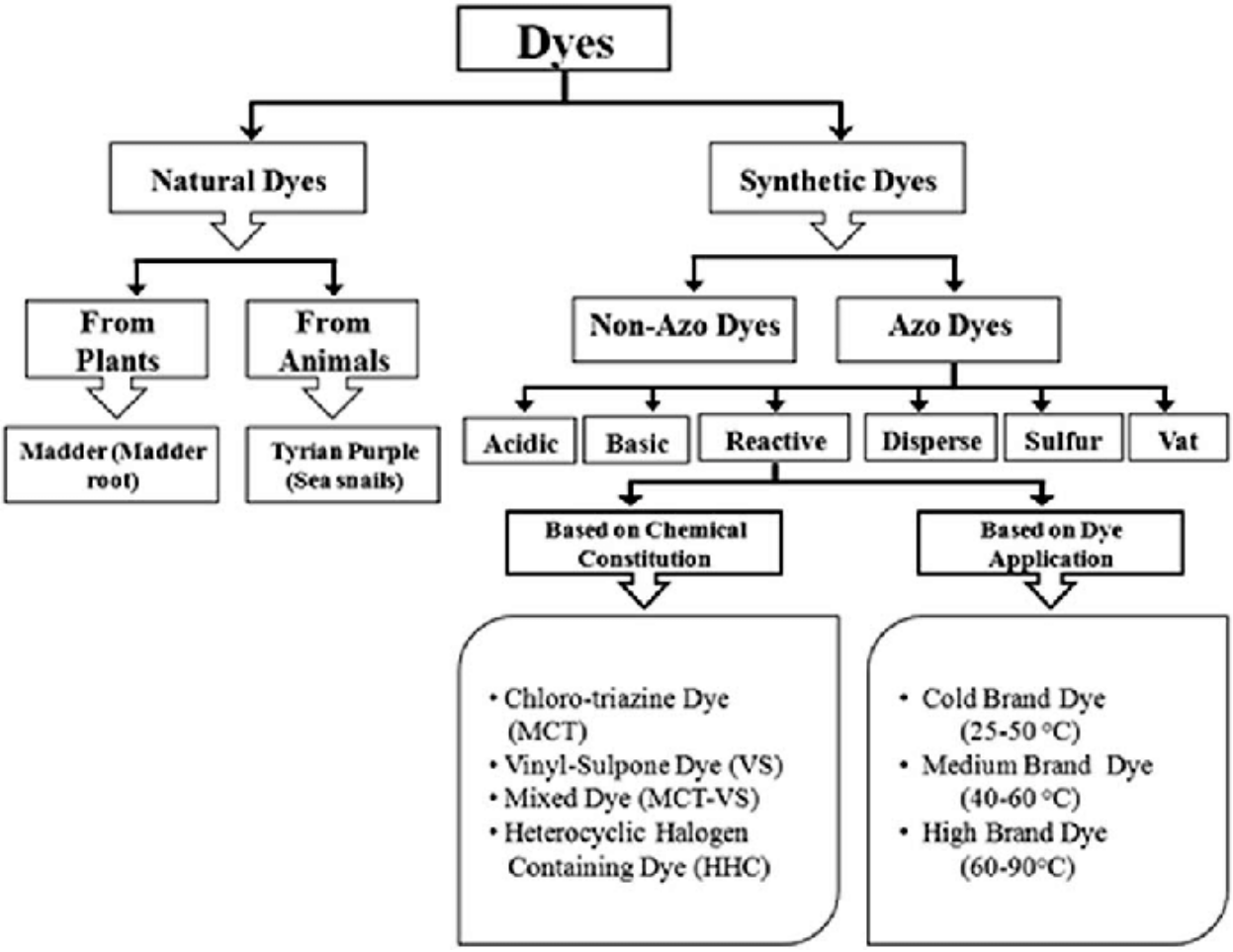


Figure 1: Classification of dyes

2.3. Physicochemical properties of Malachite Green

According to Raval *et al*. (2016), malachite green (MG) is a water-soluble cationic dye that resembles green crystalline powder and is a member of the triphenylmethane class. With a molecular weight of 927.00 g/mol and a chemical formula of $C_{52}H_{54}N_4O_{12}$, malachite green oxalate is [4-[[4-(Dimethylamino) phenyl]-phenyl methylidene] cyclohexa-2, 5-dien-1-ylidene]-dimethyl azanium; 2-hydroxy-2-oxoacetate; oxalic acid]. Figure 2 below shows the MG dye's chemical structure. When dissolved in water, its dark green crystalline form turns blue (Raval *et al*., 2016; Abate *et al*., 2020).

MG has monoprotic Bronsted acid-base properties and a pKa value between 3.70 and 4.80 (Lemos *et al*., 2023). MG is used in the textile industry to dye silk, wool, and leather. It has beneficial qualities for aquaculture, including antibacterial, antifungal, and antiparasitic activities. It is also an affordable dye that is widely accessible.

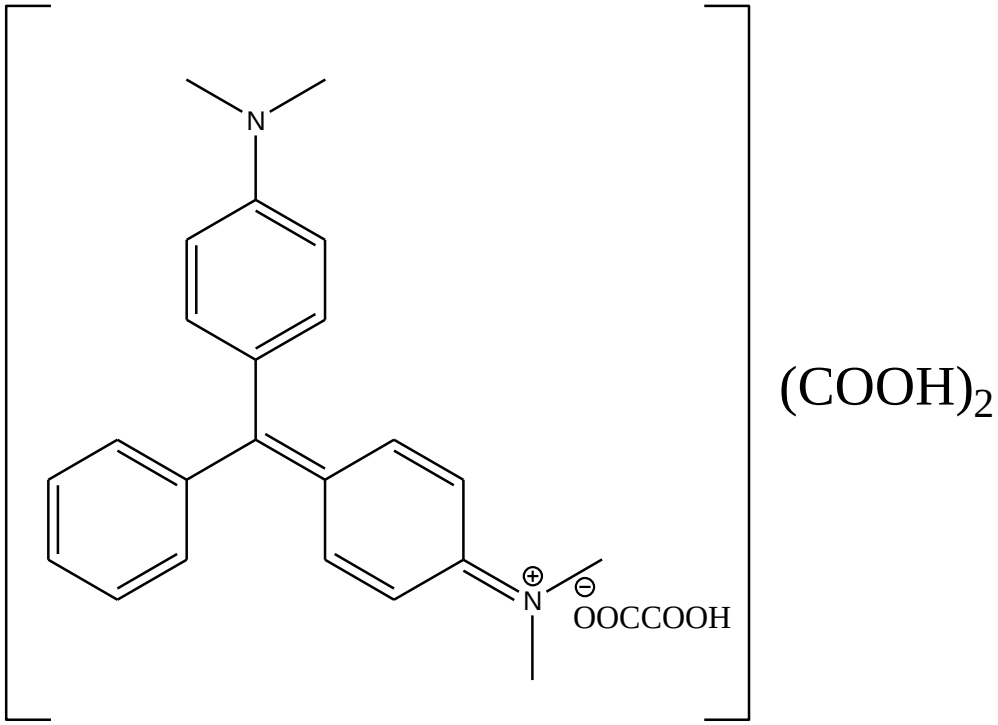


Figure 2: Chemical structure of malachite green

2.4. Environmental Pollution of Dyes

The textile business contributes to pollution in one way or another, just like any other industrial activity. Wastewater is the most harmful to the environment, and among all industrial sectors, textile plant wastewater is considered to be the most polluting due to both its volume and composition. One of the main issues with wastewater treatment is the dyestuff wasted during textile production (Lemos *et al*., 2023).

Depending on the dye's class, its loss in wastewater during the dyeing process might range from 2% for basic dyes to as much as 50% for reactive dyes, seriously contaminating surface and ground waterways. Since a very little amount of dye concentration in water (<1ppm) is highly visible and affects aesthetic merit, transparency, and water-gas solubility, color is the first wastewater contaminant to be identified. Additionally, lowering light penetration through water reduces photosynthetic activity, which results in an oxygen shortage and de-regulates the aquatic biota's biological cycles (Hammed *et al*., 2009). Depending on the

duration of exposure and dye concentration, many dyes can have acute to long-term effects on species because they are very hazardous to the ecosystem and mutagens. For instance, dye effluent has been linked to plant growth and production, fish metabolic stress and death, and growth reduction. Thus, contamination restricts the use of downstream human water for agriculture, drinking, fishing, and pleasure (Hassan *et al*., 2008). Therefore, in order to maintain a sustainable and eco-friendly environment, effluent containing residual dyes must be cleaned before being released into the receiving environment.

Continuous urbanization and the expansion of industrialization have upset the equilibrium of the composition of the environment by releasing toxic gases, smoke, and hazardous compounds, all of which have deleterious impacts on living things (Liu *et al*., 2020).

As depicted in Figure 3. According to Guo *et al*. (2022) and China *et al*. (2020), the primary issue affecting the sustainability of the environment in China is the discharge of dyes into water bodies, which contributes to environmental pollution, particularly water pollution. One of the primary causes of water pollution is organic dyes and their effluents, which frequently leak from wastewater treatment facilities in the mining, textile, paper printing, food processing, cosmetics, pharmaceutical, and leather sectors (Kim *et al*., 2022). Unwanted chemicals can contaminate lakes and bodies of water, making them unsafe for drinking or other purposes (China *et al*., 2020).



Figure 3: Discharging of dye into environment

2.5. Datura sramomium as a biosorbent

Jimson weed, or Datura stramonium, is a herbaceous plant that contains a number of bioactive substances. Its roots have special qualities that make them appropriate for biosorption procedures. Additionally, its roots have amine, carboxyl, and hydroxyl functional groups that help it interact with cationic dyes like malachite green. Through hydrogen bonding and electrostatic attraction, these functional groups increase the biosorbent's binding ability (Namasivayam *et al*., 2017). Malachite green can be successfully adsorbed from aqueous solutions by datura stamonium root, according to several investigations. For example, studies show that the adsorption capacity can reach notable levels under ideal conditions (PH, contact time, and initial concentration), frequently surpassing that of other plant-based biosorbents (Kumar *et al*., 2020).

2.6. Importance of biosorbent prepared from datura stramonium root

Water body contamination, especially that caused by malachite green (MG), presents serious health and environmental problems. Conventional color removal techniques, such as chemical treatment and physical adsorption with activated carbon, frequently have drawbacks such high expenses and the production of secondary waste. Because of its affordability and sustainability, biosorption uses biological materials to adsorb contaminants from aqueous solution has become a promising alternative. The potential of a biosorbent made from the root of Datura stramonium for the removal of malachite green is the main topic of this literature review, which also compares its efficacy with that of other plant-based biosorbents. Using Datura stramonium as a biosorbent is consistent with environmentally friendly waste

water treatment methods. Invasive species like Datura stramonium are used to treat waste water while reducing their negative effects on the ecosystem (Babu *et al*., 2021). Datura stramonium local availability lowers the expense of shipment compared to other biosorbents. When compared to traditional methods, its use in waste water treatment plants can result in lower permanent expenditures (Ali *et al*., 2019).

2.7. Comparison of datura stramonium root biosorbent with other plant-based Biosorbents

The capacity of different plant materials to eliminate malachite green and other artificial colors has been the subject of numerous investigations. Datura stramonium efficacy is demonstrated when compared to other biosorbents. Because of their high pectin content, banana peels have been utilized as a biosorbent to remove dyes. Despite their outstanding adsorption capacities, research indicates that datura stramonium might perform better because of its larger surface area and more varied functional groups (Rao *et al*., 2019). Another biosorbent that is frequently researched is rice husk. Although it has demonstrated efficacy in dye removal, the requirement for chemical modification to improve its adsorbtion capacity may result in higher expenses and longer processing times. Datura stramonium roots, on the other hand, can be used immediately without requiring a lot of processing (Knan *et al*., 2022). Because of its large surface area, activated carbon derived from different agricultural leftovers is also utilized for color removal. Nevertheless, the production process can be expensive and energy-intensive. By making use of an easily accessible natural resource, Datura stramonium provides a more sustainable choice (Mohammed *et al*., 2020).

2.8. Chemical activation of Biosorbent

A chemical or physical activation technique can produce a product with varying pore diameters. The practical processes and mechanisms involved in the formation of porosity differ between the two approaches. The more reactive carbon in the structure was selectively eliminated during physical activation to create porosity, and further gasification produced a highly porous bio-sorbent. In chemical activation process, the precursor is mixed with a chemical such as sulphate salts, chloride salts, NaOH, $CaCl_2$, H_2SO_4, H_3PO_4 and washed to produce the activated biosorbents, Following the thermal decomposition of the precursor, the chemical reacts with the product causing reduction in the evolution of volatile matter and inhibition of the particle shrinkage. Once the chemical is removed by exhaustive washing, a large amount of porosity is formed (Mondal and Kar *et al*, 2018). The process of activating dry cellulosic materials with H_3PO_4 has grown in popularity for the large-scale production of

biosorbent (Figure 4) due to the reagent's low energy cost, high carbon yield, and simplicity of recovery. H_3PO_4 has two functions in the biosorbent preparation process: As an acid catalyst, H_3PO_4 facilitates bond cleavage, hydrolysis, dehydration, condensation, and cross-linking reactions between phosphoric acid and biopolymers. Because the volume of phosphoric acid inside the activated precursor coincides with the micro pore volume of the resulting bio-sorbent, H_3PO_4 may serve as a template (Mukherjee *et al*., 2006).



Figure 4: Effect of chemical activation on the surface of biosorbent

2.9. Effect of Biosorbent for the Removal of Malachite green

According to Abewaa *et al*., 2023, the surface of activated carbon derived from Rumex abyssinicus showed maximum and minimum malachite green removal efficiencies of 99.9% and 62.4%, respectively, at their respective experimental conditions of 100 mg/L, 0.10 mg/100 mL, pH 6, and 40 min, and 100 mg/L, 0.15 mg/100 mL, pH 3, and 20 min. The hazardous dye MG was effectively removed using wood apple shell, a fruit-food solid waste, as an inexpensive substitute adsorbent. Shaking at 150 rpm at 299 ± 2 K for 3.30 hours resulted in a 98.87% removal of MG dye at an initial concentration of 100 mg/L at pH 7–9 (Ashish *et al*., 2017). The literature article (Abate *et al*., 2020) states that by adjusting

operating parameters such initial dye concentration (10 mg/L), pH (10), dosage (0.5 g), and contact duration (60 min), the adsorption performance of the generated activated carbon from Catha edulis stem was adjusted. At those ideal circumstances, the prepared adsorbent's maximum removal effectiveness was 98.8%.

The process of removing MG from aqueous solution was found to be impacted by the dose of teak leaf litter as well as the starting concentration, pH, and temperature of the dye solution. At pH 6–10 and 2 g/L, the dye was best absorbed per gram of the adsorbent. The Langmuir isotherm did not suit the batch adsorption data as well as the Dubinin–Radushkevich and Freundlich isotherm models. However, it was determined that the monolayer capacity of teak leaf litter for the elimination of MG in aqueous solution was 333.33 mg/g at 293-313 K (Oyelude *et al*., 2018).

According to Moumni *et a*l., 2024, the removal capacity of malachite green from aqueous solution was 2.66 mg/g and 23.48 mg/g on the surface of lightweight composite brick adsorbent obtained at an initial concentration of 20 mg/L, an adsorbent dose of 0.15 g/mL, a pH of 10, and an adsorption time of 180 minutes. The adsorption process is spontaneous and endothermic, according to the thermodynamic analysis carried out at four temperatures (298 K, 308 K, 318 K, and 328 K).

CHAPTER THREE

3. MATERIAL AND METHODS

3.1 Experimental Section

Biosorbent preparation and adsorption experiment was conducted at Madda Walabu University, Postgratude Lab of Chemistry Department. SEM, XRD and FTIR were done at Adama Science and Technology University and Hawasa University respectively.

3.2 Chemicals and Instruments

3.2.1. Chemical and Reagent

All chemicals were analytical reagent without further purification: Malachite green ($C_{23}H_{25}ClN_2$)(Samir Tech-Chem, Ltd), Ethanol (CH_3CH_2OH), Phosphoric acid (H_3PO_4 (95% Merck), NaOH (India), 98% H_2SO_4 (Analytical Reagent, India), 37% HCl (Sigma-Aldrich), salts (NaCl), buffer solutions (phosphate buffer solution (PBS), acetic Acid, and indicator (phenolphthalein), nitric acid (NHO_3), and Distilled water were used in this study

3.2.2. Instrument and Apparatus

The instruments and apparatus selected for this study were FT-IR spectroscopy (PerkinElmer FTIR model spectrum 65) was used for determining functional group of biosorbent. Scanning electron microscopy (SEM Model LEICA S430) was used to determine surface morphology before and after adsorption of MG, XRD was used for analysis of crystalline nature of biosorbent, Digital electronic balance (Model JA103P,) with 160 gm loading capacity was used to weigh biosorbent and all other chemicals. Magnetic stirrer hot plate (UK) was used for stirring and maintaining the required temperature. The pH was measured using a pH meter (MP 220 JENWAY, Japan), and the dye concentrations in the water sample were measured using UV/V spectrophotometry (spectrumlab 725s). Various volumes of sample solution were measured using measuring cylinders, droppers, pipettes, and micro pipettes (Pyrex, Japan). Volumetric flasks with stoppers (Pyrex, England) were used to prepare solutions; a grinder (China, 2022) was used to mill the sample; aluminum foil, Whatman filter paper, spatula, glass tube, wash bottle, hot plate, pestle, and mortar were used to grind and obtain a powder sample.

3.3 Sample collection and Sample preparation

3 kg of *Datura stramonium* roots that are fresh and healthy free from contamination of pesticides and heavy metals was collected from Waltai Gobu kebele, Goro Woreda, Oromia, Ethiopia. Waltai Gobu kebele was purposively selected depend on the availability of *Datura stramonium* root. The collected *Datura stramonium* root was chopped and cut into small size. Then wash with distilled water several times to remove impurities and dry at room temperature for 15 days. Then dried root of the plant was ground into powder and sieve to obtain particle size less than 500 µm can improves adsorption kinetics by increasing surface area, reducing diffusion path length, and enhancing external mass transfer. This leads to faster equilibrium and higher apparent adsorption rates, though care must be taken to avoid excessive fines that may agglomerate (Madian *et al*., 2024). The powder of the plant was used for the preparation of biosorbent.



Figure 5: Sample collection

3.4 Preparation of biosorbent

One gram of powdered Datura stramonium root was immersed in a 0.1 M H_3PO_4, NaOH, and H_2SO_4 solution at a 1:4 (w/v) impregnation ratio for a full day at room temperature. After the sample was soaked, it was filtered using Whatman filter paper No. 42 and repeatedly cleaned with distilled water until the pH reached neutral (Abate *et al*., 2020). The resultant biosorbent was stored in desiccators for additional research after being fully dried at 110 °C in an oven for three hours to produce a good carbon structure and a wide surface area.



Figure 6: Biosorbent Preparation

3.5. Characterization of nanoparticles

3.5.1. X-ray diffraction (XRD)

The crystallinity structure of biosorbent sample was detected with X-ray diffraction (XRD) using a PAN analytical-X'Pert-Pro-MRD equipped with CuKα as an X-ray radiation source (λ = 0.15406 nm) at a current of 30 mA and voltage of 40 KV. The analysis was achieved in the range of 2θ values from 10°–80° (Madian *et al*., 2024).

3.5.2. Fourier Transform Infrared (FTIR) analysis

The functional group of MG before and after adsorption was identified by FT-IR analysis. A pellet was formed at a pressure of 1MPa (mega pascal) using 1mg of powder material and 100mg KBr throughout a range of 400–4000 cm−1 (Fito *et al*., 2020).

3.5.3. Scanning Electron Microscopy (SEM)

SEM is a powerful magnification technique that assesses the surface morphology of the biosorbent using electron focus beams. SEM analysis provides important information about MG's surface morphology prior to and following adsorption. The sample's fine coarse powder was attached to a circular metallic sample holder using double-sided adhesive tape. Surface texture micrographs were collected at different SEM magnifications after the materials were coated with copper using a sputter coater to make the image visible (Stabentheiner *et al*., 2010).

3.6. Synthetic wastewater

A MG stock solution with a concentration of 1000 mg/L (1000 ppm) was made by dissolving 1 g of MG stock in 1000 mL of distilled water. MG solutions with concentrations between 1 and 30 ppm at intervals of 5 ppm were made using the stock solution. The stock solution's initial pH was changed by adding 0.1 M HCl or NaOH. Each experiment used a 50 ml aliquot of the MG stock solution (Moustafa *et al*., 2023). Every experiment was carried out in three duplicates.



Figure 7: Preparation of Synthetic Wastewater and Dilution

3.7. Calibration

The standard solution of 1000 ppm of MG was used to prepare concentrations (1, 5, 10, 15, 25, and 30 ppm). The absorbance of each dilute concentration of MG were measured by UV/Vis spectrophotometer (Tarekegn and Balakrishnan *et al*., 2021).

3.8. Batch Adsorption Experiment

With minor adjustments, the adsorption tests were conducted in accordance with (Arunprasath *et al*., 2019). For the batch experiment, 50 mL (20 ppm) of synthetic wastewater and 1g of adsorbent were added to a 250 mL conical flask. The pH of the solutions was then brought to 8 using either 0.1 M HCl or 0.1 M NaOH. After 30 minutes of stirring the mixed solutions using a magnetic stirrer on a digital hot plate at 400 rpm and 30 ^{o}C, the adsorbent was separated from the solution using centrifugation at 4000 rpm for 10 minutes. A UV-Vis spectrophotometer was used to assess the concentration of residual malachite green (supernatant solutions) both before and after adsorption. Equations (1) and (2) were then used to determine the biosorbent's removal percentage and adsorption capacity:

$$\text{Removal percentage (\%)} = \frac{(Co - Ce)}{Co} \; x\; 100 \qquad (1)$$

$$q_e = (C_o - C_e)\frac{V}{W} \qquad (2)$$

Where, qe (mg/g) is adsorption capacity, C_o and C_e (mg/l) are the liquid phase concentrations of MG at initial period and equilibrium, respectively. V is the volume (l) of the sample solution and W is the weight (g) of the biosorbent. The same experimental procedure was repeated to study the desorption and stability of the biosorbent using four consecutive cycles at optimal batch experiment.



Figure 8: Batch Adsorption Study

3.9. Factor affecting adsorption of MG

Factors affecting adsorption is an important parameters to determine the optimum condition for the adsorption of malachite green from aqueous solution. Factors of adsorption such as pH, adsorbent dosage, initial concentration and contact time were evaluated (Abate *et al*., 2020; Hammud *et al*., 2023).

The study investigates the removal of Malachite Green (MG) using a biosorbent derived from NaOH-activated roots of *Datura Stramonium*. The adsorption conditions are set at a pH of 8, with an initial MG concentration of 20 ppm, a volume of 50 ml for the MG aqueous solution, an initial absorbance of 2.421, a temperature of 30°C, a reaction time of 30 minutes, and a biosorbent dosage of 1g.

The impact of varying initial MG concentrations on the removal efficiency of the NaOH-activated *Datura Stramonium* biosorbent is examined. The conditions maintained during this assessment include a pH of 8, a volume of 50 ml for the MG aqueous solution, a temperature of 30°C, a reaction time of 30 minutes, and a biosorbent dosage of 1g.

This section evaluates how different biosorbent dosages affect the removal of MG using the NaOH-activated *Datura Stramonium*. The conditions for this evaluation are as follows: pH is maintained at 8, the volume of the MG aqueous solution is 50 ml, the initial MG concentration is set at 20 ppm, the initial absorbance is 2.421, and the reaction time is extended to 35 minutes.

The influence of pH on the removal efficiency of MG by the NaOH-activated *Datura Stramonium* biosorbent is assessed under the following conditions: the volume of the MG aqueous solution is 50 ml, the initial MG concentration is 20 ppm, the temperature is set at 30°C, the initial absorbance is 2.421, the reaction time is 30 minutes, and the biosorbent dosage is maintained at 1g.

This section explores how varying reaction times affect the removal of MG by the NaOH-activated *Datura Stramonium* biosorbent. The conditions are established as follows: pH is set at 8, the volume of the MG aqueous solution is 50 ml, the initial MG concentration is 20 ppm, the initial absorbance is 2.421, and the biosorbent dosage is maintained at 1g.

The study also examines the effect of temperature on the removal efficiency of MG by the NaOH-activated *Datura Stramonium* biosorbent. The conditions for this evaluation include a pH of 8, an initial MG concentration of 20 ppm, a volume of 50 ml for the MG aqueous solution, an initial absorbance of 2.421, a reaction time of 30 minutes, and a biosorbent dosage of 1g.

Data on equilibrium studies are collected under optimized adsorption conditions, which include a pH of 8, a volume of 50 ml for the MG aqueous solution, a reaction time of 30 minutes, a temperature of 30°C, and a biosorbent dosage of 1g. Data on kinetic studies are obtained under optimized adsorption conditions that consist of a pH of 8, an initial MG concentration of 20 ppm, a volume of 50 ml for the MG aqueous solution, an initial absorbance of 2.421, and a biosorbent dosage of 1g.

3.10. Adsorption model

In order to comprehend how malachite green interacts with the biosorbent, common adsorption models like the Freundlich model (Freundlich, 1906) and the Langmuir model (Langmuir, 1916) are employed to examine adsorption data. The maximal adsorption capacity and the kind of adsorption process can be ascertained by fitting experimental data to these models. An adsorption test will be carried out to evaluate the mediation capacity of the chosen media across an adsorbent range of 0.05-0.3 g/L using an MG solution at concentration of 10 ppm for 90 minutes after an ideal time has been determined from the kinetics experiments (Dwived *et al*., 2008). will be used to assess each equation's fitness quality using the adsorption data.

Langmuir Equation: $\frac{C_e}{q_e} = \frac{1}{q_{max}} Ce + \frac{1}{q_{max}.KL}$ (5)

Freundlich Equation: $\log q_e = \log K_F + 1/n \log C_e$ (6)

Where, q_{max} is the Langmuir maximum adsorption capacity (mg· g^{-1}), K_L (L· mg^{-1}), and K_f ($mg^{(1-1/n)}.g^{-1}$ $L^{1/n}$), n is the Freundlich empirical constant are coefficients related to Langmuir adsorption, Freundlich affinity respectively.

3.11. Kinetic model

Common kinetic models that examine the rate at which malachite green is adsorbed onto the biosorbent over time include pseudo first order (Lagergren, 1898) and pseudo second order (Ho and McKay, 1999). Kinetic data can be used to forecast the biosorbent process's efficiency and improve contact time. A kinetic analysis was used to determine the rate at which the best-performing adsorbents from the 120-minute batch study absorb MG. For every material wase sample, duplicate vials were used at 5, 10, 15, 25, 30, and 35 minutes (Encinar *et al*., 1998). and the adsorption rates for MG were described by the one that best fit the experimental data.

Pseudo-First Order (PFO): $q_t = q_e(1 - e^{-k1t})$ (3)

Pseudo-Second Order (PSO): $q_t = \frac{K_{2q_e^2 t}}{1+K_{2q_e t}}$ (4)

Where, qt is the amount of MG adsorbed at a time "t" (mg· g^{-1}), while k_1 and k_2 are the rate constants for the PFO (min^{-1}) and PSO ($g.mg^{-1}.min^{-1}$) models, respectively.

CHAPTER FOUR

4. RESULTS AND DISCUSSION

4.1. Optimization of chemicals activation

Figure 9 (detailed in Appendix Table 1) illustrates the impact of impregnation chemicals on the microporous Datura Stramonium root bosorbent (DSrB) performance. In comparison to H_2SO_4 (83.15%) and H_3PO_4 (70.59%), the synthesized Datura stramonium biosorbent generated by impregnation of NaOH had the highest adsorption capacity with 91.49% elimination efficiency.

By etching lignocellulosic structures, dissolving silica, and eliminating hemicellulose, NaOH activation efficiently enlarges micropores and mesopores. This increases surface area and pore volume, which immediately improves adsorption capacity. NaOH creates a greater percentage of micropores that are especially useful for the adsorption of dyes and heavy metals, in contrast to H_3PO_4, which mainly creates more mesoporous structures by dehydration and cross-linking (Krika *et al*., 2021; Zhang *et al*., 2025). NaOH treatment also improves electrostatic attraction and hydrogen bonding with contaminants by adding functional groups like hydroxyl (-OH), carboxyl (-COOH), and carbonyl (-C=O) to the biosorbent surface.

However, H_2SO_4 introduces functional groups (-SO_4, -COOH) that improve surface characteristics but may cause pore clogging. Because it produces few micropores due to strong dehydration and charring collapses cell walls with the bosorbent, acidification can also create competition with protons for adsorption sites at higher concentrations, which explains its moderate efficiency in adsorption processes (Li *et al*., 2021). Additionally, by increasing the negative surface charge, NaOH activation promotes the adsorption of metal ions and cationic dyes via electrostatic interactions. While H_3PO_4 introduces functional groups (-OH, -PO_4) that increase the attraction of dyes, it also forms a framework of mesopores. These can occasionally lower adsorption efficiency for specific pollutants due to steric hindrance or a weaker binding affinity compared to the oxygenated groups introduced by NaOH; however, this activation combines the strengths of both chemical types without unduly compromising structural integrity (Krika *et al*., 2021). Because of its exceptional effectiveness over the alternatives, NaOH-assisted chemical activation was chosen for biosorbent synthesis.

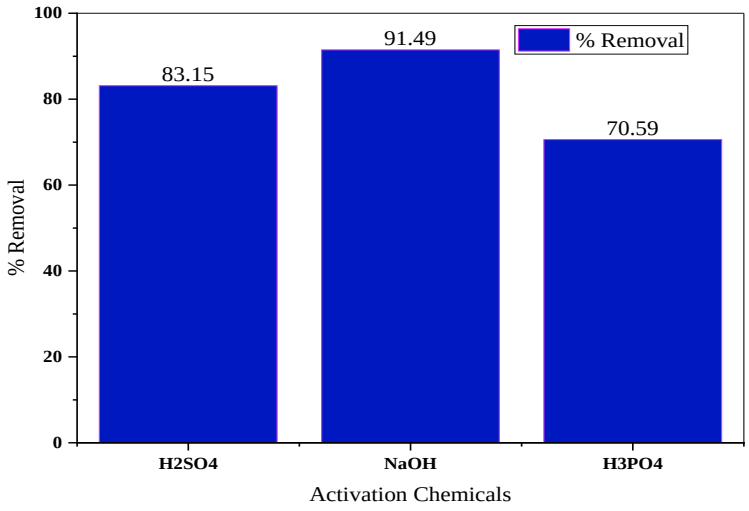


Figure 9: Effect of activating reagents on preparation of *Datura Stramonium* root bosorbent

4.2. Characterization

4.2.1. FT-IR (Fourier transform infrared spectrometry)

To find different kinds of functional groups on the adsorbent surface, the FT-IR spectrum of the bosorbent made from Datura stramonium root was scanned throughout the frequency range of 4000–400 cm^{-1}. Figure 10 displays changes in the spectra prior to and following adsorption. The participation of several functional groups during the adsorption process is demonstrated by the increase in intensity and the shift in peak positions to lower frequencies in the Datura Stramonium root-derived bosorbent after Malchite Green (MG) biosorption.

The biosorbent's peak positions before MG adsorption at 2972, 2689, 1710, 1461, and 725 cm^{-1} shifted to positions after MG adsorption at 2915, 2660, 1699, 1455, and 719 cm^{-1}. Although there are noticeable variations in the infrared band intensities, the two spectra's characteristics are similar, suggesting a highly similar chemical composition and nature despite concentration discrepancies (Abewaa *et al*., 2023). The O-H stretching vibration of hydroxyl functional groups is shown by the broad band at 3600 to 2660 cm^{-1}. The asymmetric and symmetric C-H stretching of alkyl groups are linked to the absorption peaks at 2927 and 2689 cm^{-1} before to a dsorption and at 2915 and 2660 cm^{-1} following adsorption, respectively (Al-Snafi *et al*., 2017). The C=O stretching of carboxyl groups is linked to the peaks at 1710 cm^{-1} and 1699 cm^{-1} (Pan *et al*., 2025).

Furthermore, phenols, alcohols, and ethers have a weak peak at approximately 1461 and 1455 cm^{-1} that is attributed to C–O groups. This peak may also be attributed to carboxylic groups, such as the phenolic –OH group and $–CO_3$ groups

The absorption band supports adsorbed water molecules, and the peak at around 725 and 719 cm^{-1} may be caused by C–C or C–H group stretching vibrations (Al-Snafi *et al.*, 2017: Awokoya *et al.*, 2022). Electrostatic attraction and hydrogen bonding are the main mechanisms suggested for the interaction between Malachite Green (MG) and the root of Datura stramonium. In particular, the negatively charged functional groups on the biosorbent, such as phenoxide/alkoxide (O-) and carboxylate (COO-) groups, interact with the cationic MG. The binding of MG to the biosorbent's surface is made easier by this electrostatic attraction.

Furthermore, hydrogen bonding is important in this interaction because the nitrogen and oxygen atoms in the MG molecule can form connections with the hydrogen atoms of the hydroxyl (-OH) on the Datura Stramonium root (Al-jaaf *et al.*, 2023), resulting in a change in vibration frequency. These results are corroborated by the Fourier Transform Infrared (FT-IR) spectrum analysis, which shows that the Datura Stramonium root's surface is rich in active functional groups, especially hydroxyl and carboxyl/carbonyl groups (Pan *et al.*, 2025). These functional groups are necessary to bind and interact with the Malachite Green dye in an efficient manner, which improves the biosorption process.

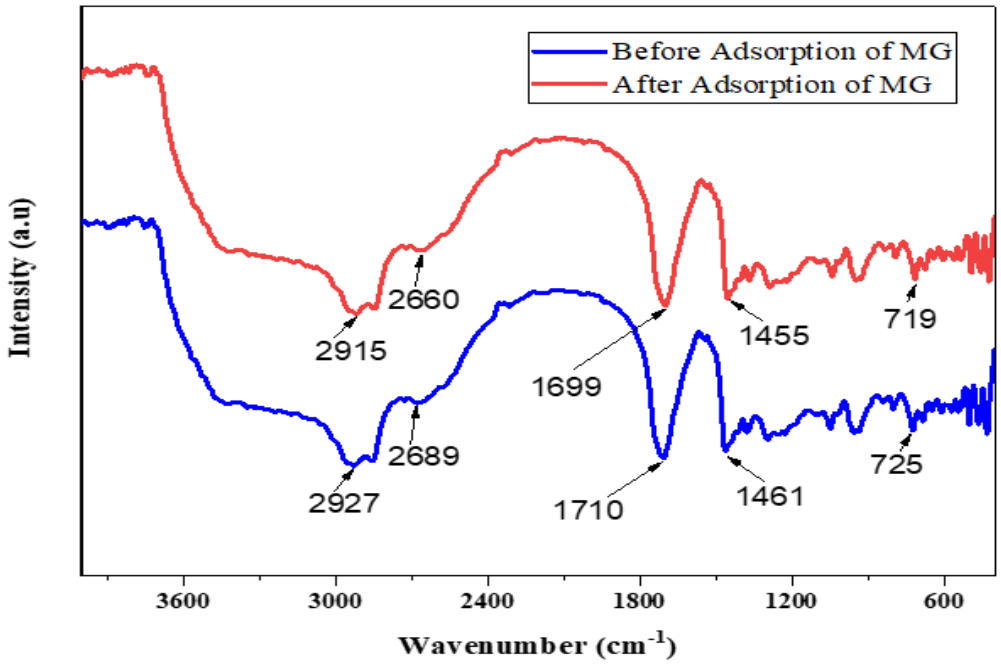
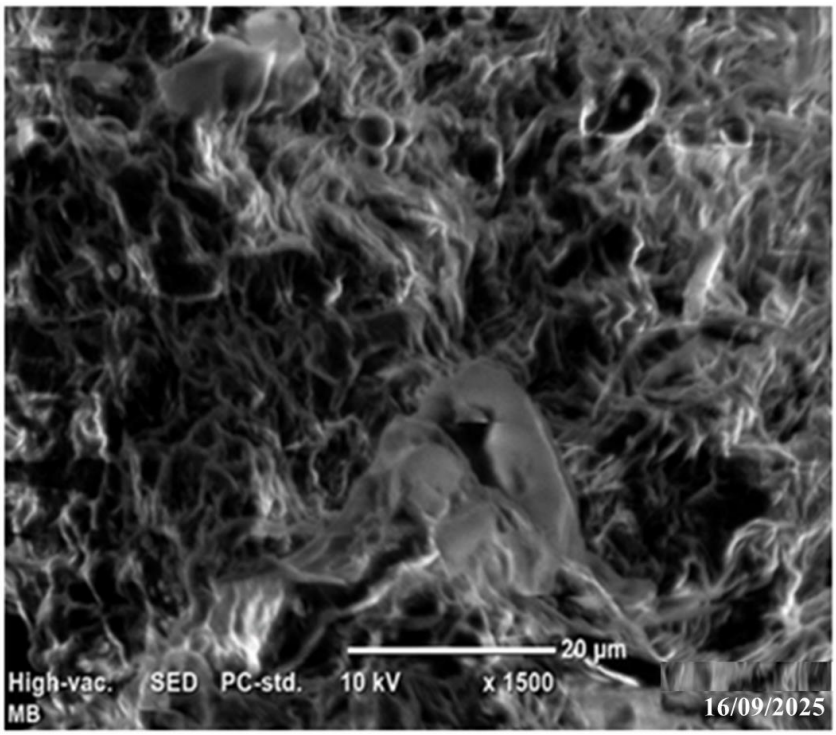


Figure 10: FTIR spectrum of *Datura Stramonium* root derived bosorbent before and after adsorption

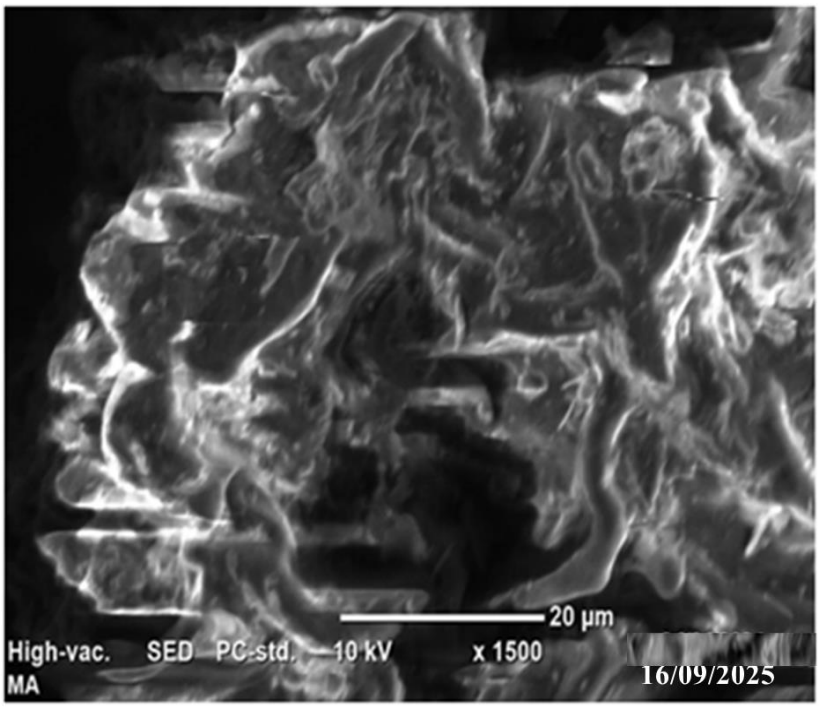
4.2.2. Scanning electron microscope (SEM)

Figures 11a and 11b show the SEM pictures of the Datura Stramonium root-derived bosorbent sample taken at a magnification of 20 µm prior to and following the adsorption of MG dye. A very porous biomaterial with surface pores was successfully created, as seen in Figure 11a. By giving target adsorbates enough free space, this porous shape facilitates effective adsorption (Mengesha *et al*., 2024).

The Datura Stramonium root-derived bosorbent's surface was rough, porous, and had an uneven distribution of particle sizes prior to biosorption. On the other hand, following biosorption, the surface of the Datura Stramonium root-derived bosorbent showed smaller pore sizes and a more uniform, somewhat smooth appearance (Figure 11b) (Al-jaaf *et al*., 2023). This alteration in the biosorbent's shape demonstrates that the bosorbent made from the roots of Datura Stramonium is efficient in adsorbing malachite green. By giving target adsorbates enough free space, this porous shape facilitates effective adsorption (Mengesha *et al*., 2024). The Datura Stramonium root-derived bosorbent's surface was rough, porous, and had an uneven distribution of particle sizes prior to biosorption.



a) Before adsorption



b) After adsorption

Figure 11: SEM images of *Datura Stramonium* root-derived biosorbent before and after adsorption

4.2.3. XRD analysis

The X-ray diffraction (XRD) analysis of the *Datura stramonium* root derived biosorbent provides critical structural insights into the material's behavior before and after dye remediation. Scanned within the magnification range of 2 theta from 10º - 80º, the diffraction pattern of the native biomass prior to biosorption exhibits a broad, dominant peak centered at 20.23º.

In the context of existing literature on lignocellulosic agricultural by-products, this characteristic peak is indicative of a semi-crystalline structure, primarily attributed to the plane of Cellulose in polymorphs embedded within an amorphous matrix of lignin and hemicellulose (Abewaa *et al*., 2023). The broadness of the peak, rather than a sharp crystalline spike, confirms the predominantly amorphous nature of the raw material, a trait often correlated with accessible surface areas for potential binding (Al-jaaf *et al*., 2023).

Following the adsorption of Malachite Green (MG) dye, the XRD profile reveals a distinct shift in the diffraction angle from 20.23º to 20.59º. According to Bragg's Law, this shift toward a higher angle corresponds to a decrease in the interplanar d-spacing of the material's lattice. This structural contraction suggests that the adsorption process is not merely superficial; rather, the dye molecules likely penetrated the amorphous regions or pores of the

biosorbent, interacting with surface functional groups via electrostatic attraction or hydrogen bonding. These interactions appear to have induced a slight compaction or relaxation of the polymer chains, resulting in the observed densification of the matrix (Abewaa *et al*., 2023). Crucially, while the peak position shifted, the overall profile and shape of the diffraction pattern remained largely preserved, indicating that the fundamental crystallographic framework of the *Datura stramonium* root was not chemically degraded during the process.

This aligns with findings in similar biosorption studies, where minor peak displacements are cited as evidence of successful "complexation" and structural alteration due to dye uptake, rather than material destruction (Awokoya *et al*., 2022). Therefore, the XRD results confirm the stability of the biosorbent and verify that the removal of Malachite Green involves tangible structural interactions within the biomass matrix. The prevalence of hemicellulose and lignin, the loss of cellulose crystallinity after chemical activation, and the creation of disordered carbon structures with tiny crystallite domains are the causes of Datura stramonium root biosorbent's amorphous XRD pattern. Because it correlates with high surface area and an abundance of functional groups that improve adsorption effectiveness, its amorphous nature is favorable.

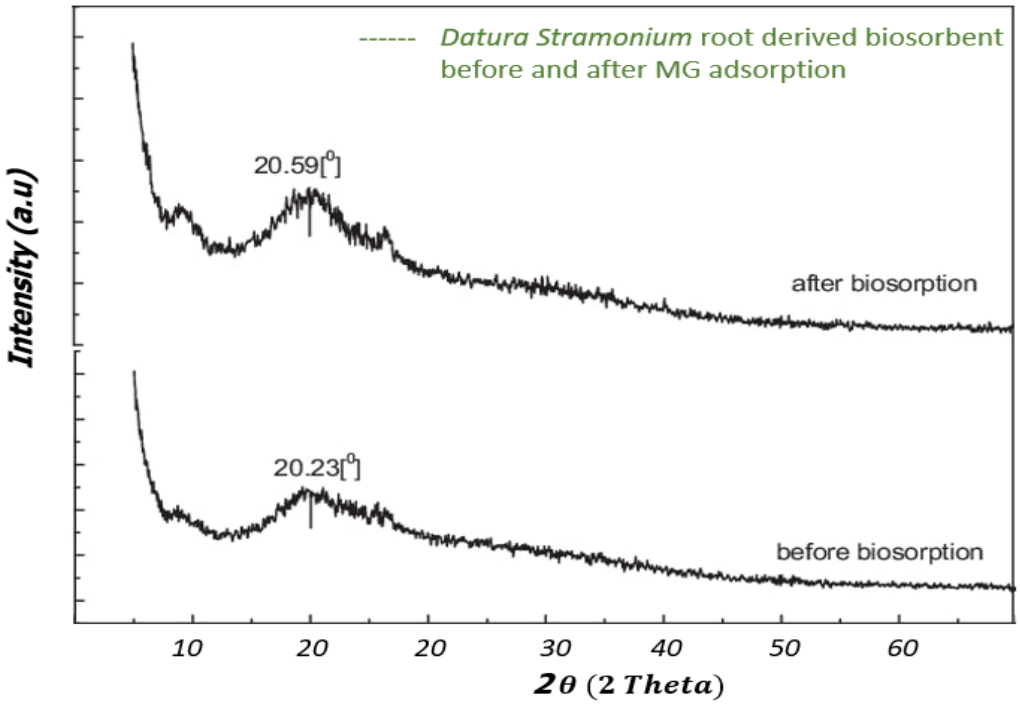


Figure 12: XRD diffiraction of *Datura Stramonium* root derived bosorbent before and after adsorption

4.3. Batch adsorption study

4.3.1. Calibartion

The calibration curve created for measuring the amounts of Malachite Green (MG) dye using a UV-Vis spectrophotometer is shown in Figure 13. The plot successfully validates the Beer-Lambert Law within the tested range of roughly 2.5 to 30 ppm by showing a positive linear relationship between the dye concentration (measured in parts per million, ppm) on the x-axis and the corresponding absorbance values (in arbitrary units, a.u.) on the y-axis. The mathematical model y = 0.1319x - 0.2723, where "y" stands for absorbance and "x" for concentration, is obtained via a linear regression analysis of the experimental data points. A fairly strong correlation between concentration and absorbance is indicated by the computed coefficient of determination R^2 of 0.9424 (94.24%) of the variation is explained by the model).

The small departure from unity and the negative y-intercept (-0.2723) indicate some variance at lower doses, even if the R^2 value indicates strong linearity (Al-jaaf et al., 2023). However, this standard curve offers an adequate foundation for figuring out residual dye concentrations in the ensuing biosorption tests employing the biosorbent obtained from Datura stramonium roots, enabling precise computation of removal efficiency and adsorption capacity.

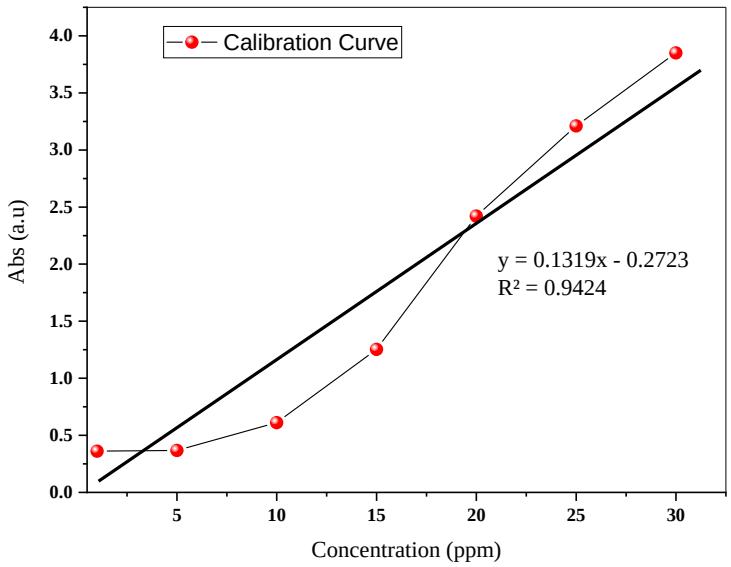


Figure 13: Calibiration Curve of *Datura Stramonium* root derived bosorbent for MG adsorption

4.3.2. Effect of Initial Dye Concentration

The effect of the initial MG concentration and its impact on the removal efficiencies of the MG dyes on Datura Stramonium root-derived bosorbent is another crucial parameter for dye removal. This was assessed by measuring 50 ml of MG solutions with varying concentrations ranging from 5 to 30 ppm, which were set by 5 ppm interval dilution to be used as functioning solutions; contact time: 30 min; pH of solution: 8; temperature: 30 ^{o}C; and ideal biosorbent dosage: 1g. Figure 14 (explained in Appendix 2) displays the maximum removal efficiency (91.49%) at the starting concentration of 20 ppm.

This can be explained by the consistent adsorbent dosage, which reduces the adsorbent's surface area and makes fewer adsorption sites available (Mengesha *et al.*, 2024). Additionally, the higher starting dye concentration resulted in the increased adsorption capability. Consequently, 20 ppm is the ideal starting concentration for MG elimination.

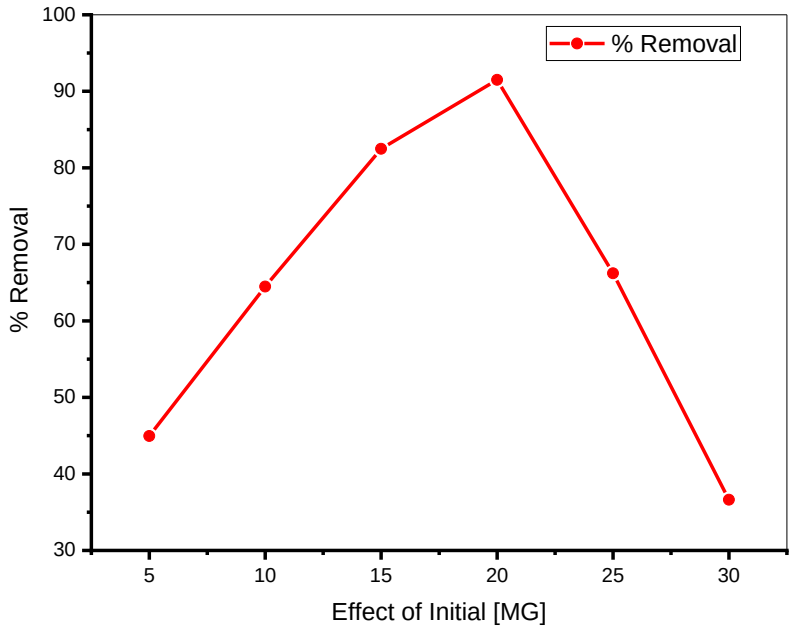


Figure 14: Effect of initial dye concentration on removal of MG by *Datura Stramonium* root derived bosorbent

4.3.3. Effect of Biosorbent dose

Because it establishes an adsorbent's capacity for a specific initial dye concentration in solution, a dose study is a crucial experiment in adsorption research. By measuring the biosorbent dose 0.5 to 1.5 g/50 ml of 20 ppm of MG aqueous solutions with 0.5 g intervals, contact time: 30 min, temperature: 30 ^{o}C, dye concentration: 20 ppm, and at 8 of the solution

pH, its impact on the removal efficiencies of the MG dyes on Datura Stramonium root-derived bosorbent was assessed.

The removal efficiency of MG by Datura Stramonium root-derived bosorbent increased dramatically from 0.5 to 1g (91.49%), as shown in Figure 15 (detailed in Appendix 3). However, as the dosage is increased to 1.5, the adsorption capacity sharply decreases because it is inversely proportional to the mass. This can be explained by the higher adsorbent dosage, which increases the adsorbent's surface area and makes more adsorption sites available.

In contrast to lesser doses of adsorbent, which lead to an efficient use of adsorption sites, greater dosages of adsorbent will induce adsorption to reach equilibrium quickly due to osmotic pressure and regardless of unused active sites (Al-jaaf *et al.*, 2023). The other extreme is that at lower adsorbent dosages, the adsorbent easily collapses in MG solutions with greater concentrations, resulting in a poor ability for adsorption removal (Abewaa *et al.*, 2023). Because of its optimal point, a median dose of 1g was chosen for the remaining adsorption studies following extensive testing.

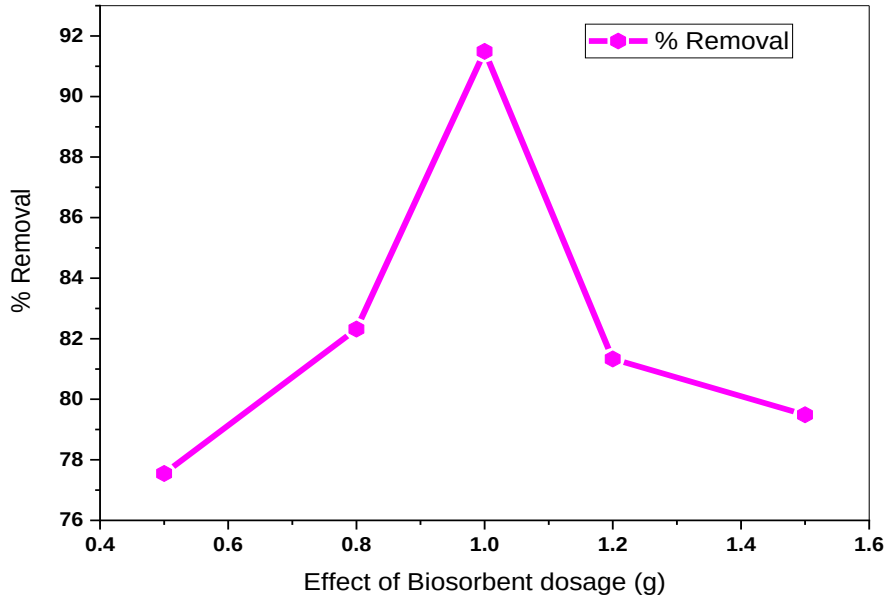


Figure 15: Effect of adsorbent dose on removal of MG by *Datura Stramonium* root derived bosorbent

4.3.4. Effect of pH

One of the most important factors influencing dye adsorption is the pH of the solution since it regulates the interactions between the adsorbent and the adsorbate (Awokoya *et al.*, 2022). Thus, by adjusting the pH between 2 and 10 with a set contact period of 30 minutes, a

temperature of 30 degrees Celsius, an optimum biosorbent dosage of 1g, and an initial concentration of MG of 20 ppm (50 ml), the impact of pH solution on the adsorption process may be investigated. NaOH (1 M) or HCl (1 M) solutions can be added to the solution to alter its pH. Figure 16 (explained in Appendix 5) show that the removal effectiveness of MG peaked at pH 8 (91.69%), and it decreased beyond the ideal pH 8. This effect may be explained by the fact that the bosorbent surfaces generated from Datura are negatively charged at high pH (aqueous solution in basic media).

Strong favorable stramonium roots electrostatic interactions between the adsorbent and the cationic MG occurred, leading to maximal removal efficiency. On the other hand, the removal effectiveness is limited at low pH because the adsorption processes are disrupted by the surface charge and MG charge repulsion (Yabalak and Elneccar *et al*., 2022). In later experimental investigations, the ideal pH level for MG was shown to be 8.

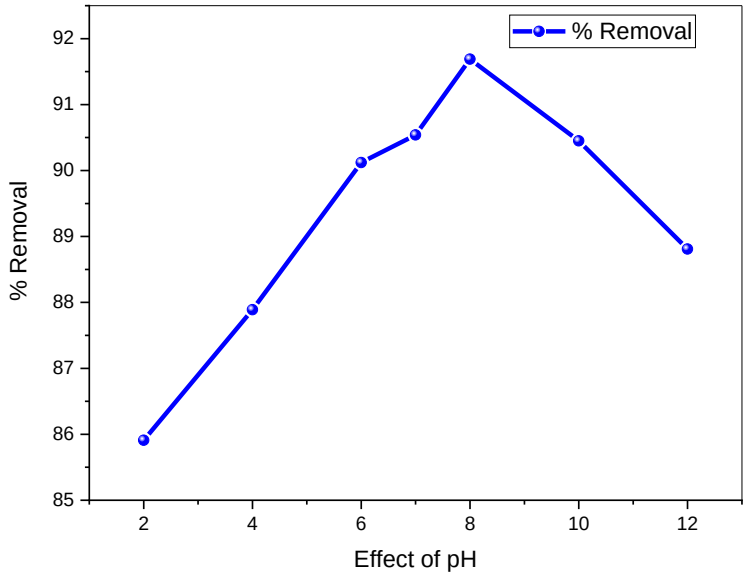


Figure 16: Effect of solutions pH on removal of MG by *Datura Stramonium* root derived bosorbent

4.3.5. Effect of contact time

The equilibrium period is another important factor in the adsorption (wastewater treatment) process. The contact time for MG on the surface of Datura Stramonium root-derived bosorbent was measured at a fixed temperature of 30 ^{o}C, at optimized biosorbent dosage of 1g, initial concentration of MG = 20 ppm (50 ml), and pH of solution in order to determine the time for equilibrium adsorption.

This was done at intervals of 5 minutes with pH of the solution 8. Due to sufficient time and more binding sites available for the sorption, Figure 17 (detailed in Appendix 6) demonstrates that adsorption efficiency improved with increasing contact time 35 minutes and reached equilibrium after 35 minutes with maximum efficiency 90.54% for MG. According to Awokoya et al. (2022), these two parameters led to an increase in the elimination of MG in solution as well as an increase in pH and contact duration.

The Datura Stramonium root-derived bosorbent structure had more accessible pores, which accelerated the mass transfer of the dyes from the solution onto the biosorbent and caused the fast adsorption at initial contact time. This suggests that the dyes on the adsorbent have good access to the binding sites, which is beneficial in the real world because it shortens residence time. After equilibrium is reached (35 minutes), the efficiency decreases because there are no more active sites for dye biosorption (Mengesha et al., 2024). Therefore, 35 minutes was chosen as the ideal contact period for the Datura Stramonium root-derived bosorbent for additional testing.

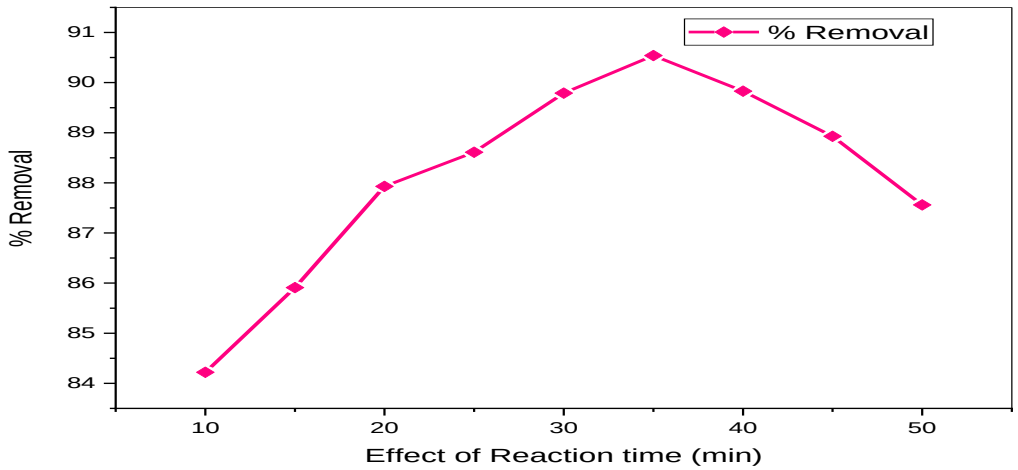


Figure 17: Effect of contact time on removal of MG by *Datura Stramonium* root derived bosorbent

4.3.6. Effect of temperature

The primary factor influencing the adsorption process is temperature, which was studied by changing its range from 25 to 55 ^{o}C at intervals of 10 ^{o}C at a fixed optimum biosorbent dosage of 1 g, contact period of 30 minutes, initial MG concentration of 20 ppm (50 ml), and pH of solution: 8. Figure 18 (explained in Appendix 7) demonstrates how raising the temperature increases both capacity and adsorption efficiency up to 55 ^{o}C (91.36%), beyond which the effectiveness of the adsorption process decreases.

Increasing the concentration of the adsorbent in the solution can enhance the adsorption efficiency and capacity, or it can explain why adsorption is an endothermic process. As the temperature rises, the adsorption equilibrium moves directly. This could be because the solute molecules exhibit a tendency to leave the solid phase and return to the liquid phase at higher temperatures because of their greater mobility (Yabalak and Elneccar, 2022).

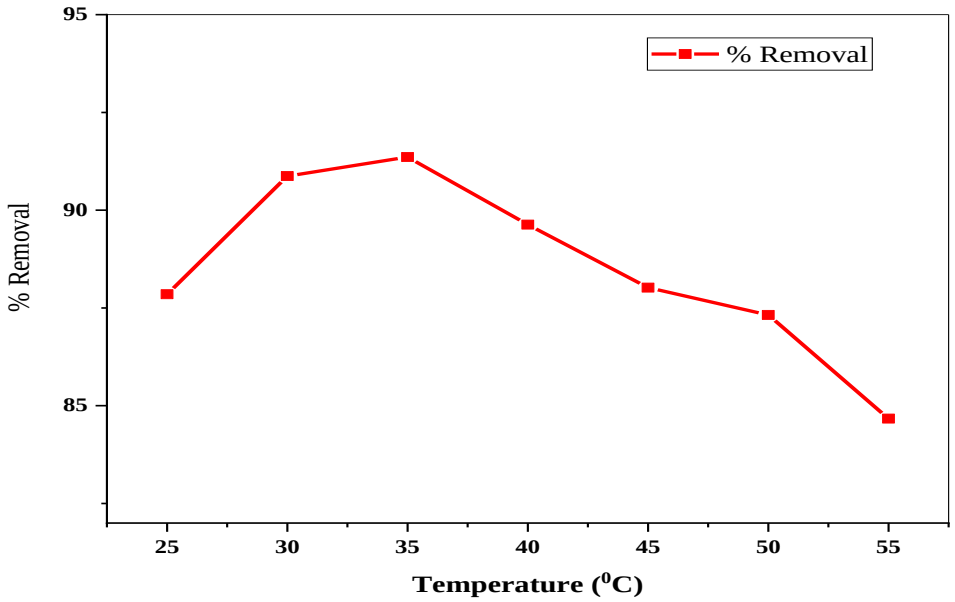


Figure 18: Effect of temperature on removal of MG by *Datura Stramonium* root derived bosorbent

4.4. Biosorbtion Activity at Optimal conditions and its Stability

The vital stability and reusability of the Datura stramonium root-derived biosorbent for the removal of Malachite Green (MG) across four successive adsorption-desorption cycles are shown in Figure 19. The material's outstanding performance under ideal circumstances is confirmed by Cycle 1's extraordinarily high initial removal efficiency of 95.12%. The elimination capability of the biosorbent gradually and predictably decreases as it undergoes regeneration; the efficiency falls to 91.69% in Cycle 2 and then to 86.9% in Cycle 3. The biosorbent maintains a noteworthy removal efficiency of 78.27% even after the fourth reusability cycle. The inadequate desorption of dye molecules from the binding sites or slight structural degradation that takes place during the severe regeneration process are frequently blamed for this increasing decline (Al-jaaf et al., 2023).

Nonetheless, the material's strong chemical and physical stability a crucial feature for verifying its availability as a sustainable and affordable adsorbent for real-world wastewater treatment applications—is highlighted by the retention of more than three-quarters of the initial capacity after four cycles (Awokoya et al., 2022).

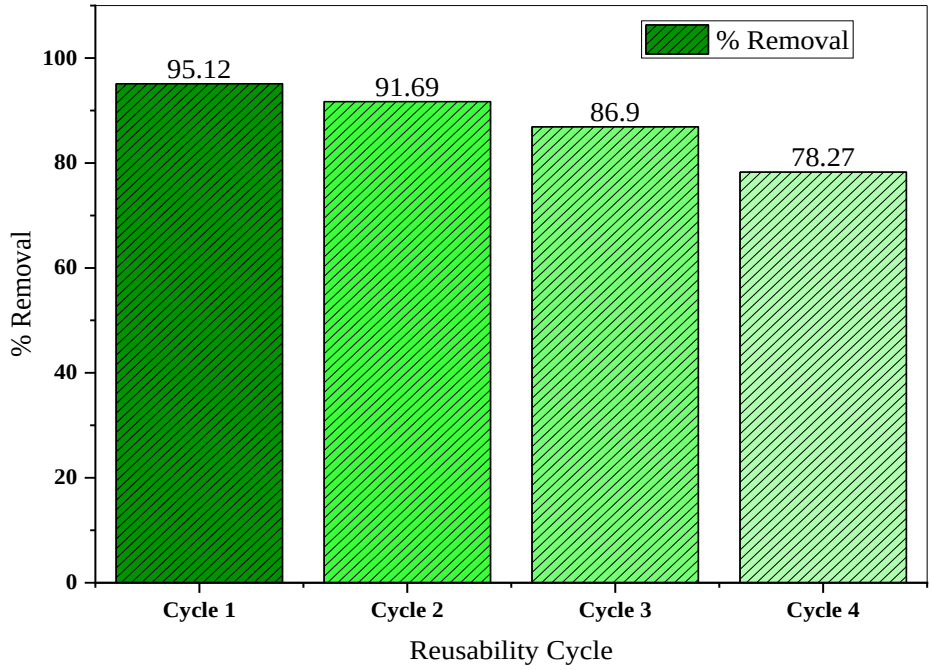


Figure 19: Biosorbent activity of *Datura Stramonium* root derived bosorbent and it stability

4.5. Adsorption Isothermal Study

4.5.1. Langmuir Isotherms

Using an adsorption isotherm model, an equilibrium analysis was carried out to look at the adsorption mechanisms that occurred between the MG dye and the bosorbent interaction derived from Datura stramonium root. Information about the adsorbent's adsorption effectiveness is elaborated by the adsorption isotherm. According to the Langmuir model, there is no interaction between the adsorbed molecules and adsorption takes place on a homogenous surface by monolayer adsorption. Equation (5) expresses the model's linear form. A straight line with slope ($qmax$) and intercept (KL) is produced when Ce/qe is plotted linearly against Ce. Equation (5) was used to compute a dimensionless separation factor in order to assess the favorability of the adsorption using this model. Figure 20 (detailed in Appendix 7) displays example graphs of the Langmuir isotherm model, and Table 1 displays the derived values of all parameters.

The results in Table 1 demonstrate that the Langmuir isotherm model, with R^2 = 0.96691 for MG, matches the data quite well. This suggests that the coverage of the dye monolayer is predominant and that the adsorption of MG on the surface of the bosorbent generated from Datura stramonium roots is homogeneous. According to the tabulated results, MG's highest adsorption capacity was 25.77 mg.g-1. Table 1's RL value of 0.064, or 0 < RL < 1, indicates that the dye's adsorption on the bosorbent generated from Datura stramonium roots is favorable (Mengesha et al., 2024).

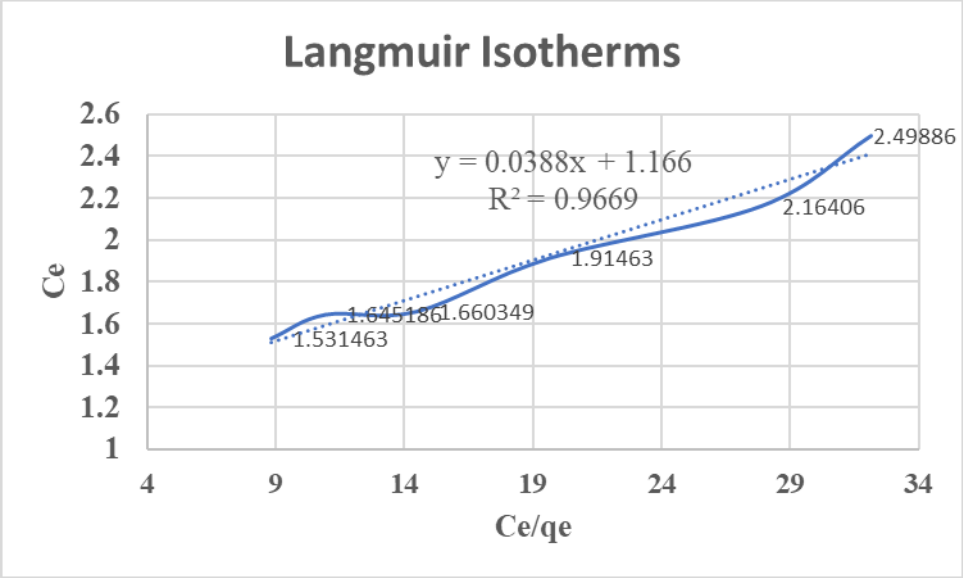


Figure 20: Langmuir adsorption isotherm for *Datura Stramonium* root derived bosorbent

4.5.2. Freundlich Isotherms

The Freundlich model, another equilibrium study model, describes how multilayer adsorption occurs on a heterogeneous surface. Equation (6) expresses the model linearly, and graphs of log*qe* vs log C*e* provide slope and intercept to determine the values of KF and n, as seen in Figure 21. Table 1 displays the computed values of all Freundlich model parameters based on the graph (detailed in Appendix 8).

Good MG adsorption onto the adsorbent is typically indicated by a value of n greater than 1. If not, desorption takes over. The adsorption is linear if n = 1. The adsorption is advantageous physical adsorption for n < 1 (Abewaa et al., 2023).The adsorption of MG dye on the surface of the VA stems bark-derived AC is not aligned with heterogeneous surface by multilayer adsorption, as demonstrated in Figure 21 and Table 1 correlation coefficients R^2 = 0.9095 for the Freundlich model, which is not close to 1 in comparison to the Langmuir model (Awokoya et al., 2022). As can be seen from Figure 16 and Table 2, the values of n = 11.61 are greater than 1, indicating that the model is not suitable for MG adsorption on the surface

of Datura Stramonium root-derived bosorbent, and KF = 0.214 is less than 1, suggesting that the adsorption may not be linear with respect to concentration.

.

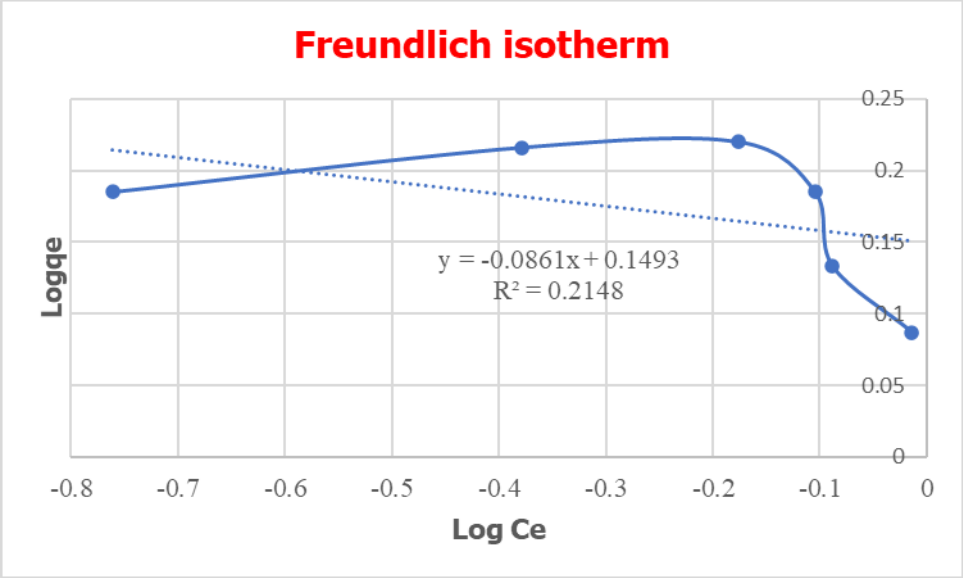


Figure 21: Freundlich isotherm study for *Datura Stramonium* root derived bosorbent

4.6. Pseudo First–order and Pseudo second–order adsorption kinetics

In order to ascertain the process of adsorption and its possible rate-controlling phase, which includes mass transfer and chemical reaction, kinetic models have been used to test the experimental results. The solute removal rate that regulates the sorbet's residence time in the solid-solution interface is known as adsorption kinetics.

According to Mengesha et al. (2024), these models include pseudo-first order and pseudo-second order models. In order to predict the adsorption rate and identify the underlying mechanism during the adsorption of MG dye on Datura Stramonium root derived bosorbent, two kinetic models, pseudo first-order and pseudo-second-order models, as expressed in equations (12) and (13), respectively were employed in this investigation (Al-jaaf et al., 2023). The adsorption process pseudo kinetics experiments were carried out at different reaction times (5, 10, 15, 20, 25, 30 and 35 minutes) under optimum experimental conditions. The pseudo first-order and pseudo-second-order models equation is generally expressed as follows:

$$log\frac{q_e}{q_e - q_t} = \frac{k_1}{2.303}\, t \tag{12}$$

$$\frac{1}{q_e - q_t} = \frac{1}{q_e} + k_2 t \tag{13}$$

Where, q_e and q_t refer to the amount of dye adsorbed (mgg^{-1}) at equilibrium and at any time, t (min), respectively, and k_1 and k_2 is the equilibrium rate constant of the pseudo-first-order and pseudo-second-order sorption (min^{-1}), respectively.

For pseudo-first-order MG adsorption on Datura Stramonium root-derived bisorbent, the linearized equations of the kinetic model (5) were plotted as log(qe-qt) against time (t), yielding a straight line with slope (-k/2.303) and intercept log(qe), as shown graphically in Figure 22. Similarly, for pseudo-fisrt-order MG adsorption on Datura Stramonium root-derived bosorbent, the linearized equation of the kinetic model (6) was displayed as 1/(qe-qt) against time (t). As seen in Figure 22, the slope and intercept of the plot yield values of $1/qe$ and $1/(qe)^2K_2$, respectively.

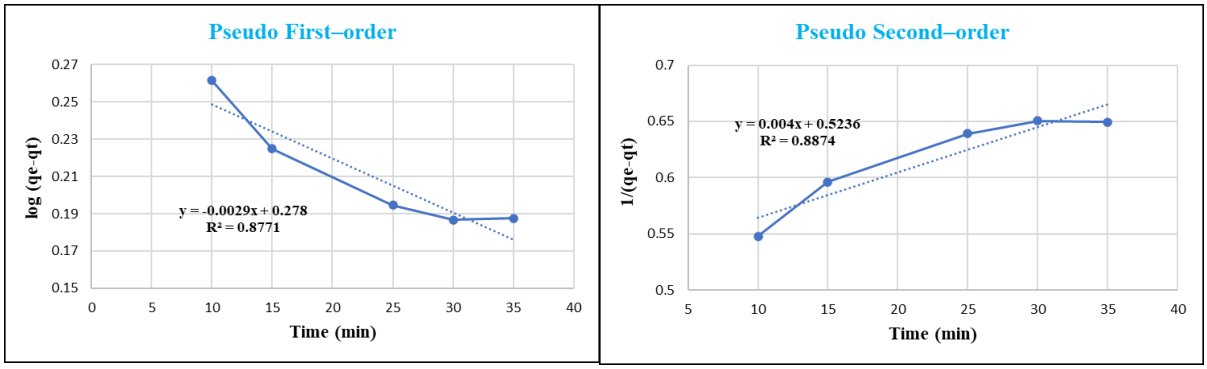


Figure 22: Pseudo First–order and Pseudo Second–order for the adsorption of MG on *Datura Stramonium* root derived bosorbent

For each pseudo-kinetics model, the correlation coefficients (R^2), equilibrium rate constants (k1 and k2), and qe of the adsorption of MG on Datura Stramonium root derived bosorbent were calculated. The computed results are listed in Table 1 (detailed in Appendix 8). The pseudo-second order model is effectively used to the sorption of analytes from aqueous solutions where chemisorption, including valence forces, occurs, whereas the pseudo-first order model generally rely on solid capacitance. This involves the interchange or sharing of electrons between forces and adsorbents (Awokoya et al., 2022).

The pseudo-second order equation fits MG the best, as seen in Figure 22 and Table 1, with an R^2 coefficient of 0.887 when compared to pseudo-first order. The pseudo-second-order model

is favored despite the close R2 values because it more accurately predicts equilibrium capacity, better captures the chemisorption mechanism, and is consistent with the functional group chemistry of lignocellulosic biosorbents such as Datura sramonium root biosoebent. Particle size reduction speeds up adsorption kinetics by improving external mass transfer and lowering intraparticle diffusion resistance, according to research on lignocellulosic biosorbents. For instance, when sieved to fine fractions (<500 µm), activated carbons and plant-derived biosorbents consistently show quicker dye and heavy metal uptake, reaching equilibrium faster than coarse fractions (Li *et al*., 2023).

Table 1: Absorption isotherms parameters and kinetics study for MG adsorption by *Datura Stramonium* root derived bosorbent

Models	Langmuir			Freundlich		
Parameters	$\mathbf{K_L}$ (L/mg)	$\mathbf{q_{max}}$ (mg/g)	$\mathbf{R^2}$	$\mathbf{K_F}$ (mg/g)(mg/L)$^{1/n}$	**N**	$\mathbf{R^2}$
Results	0.064	25.77	0.9669	1.41	11.61	0.214
Models	**Pseudo First–order**			**Pseudo First–order**		
Parameters	$\mathbf{q_e}$	$\mathbf{K_1}$	$\mathbf{R^2}$	$\mathbf{q_e}$	$\mathbf{K_2}$	$\mathbf{R^2}$
Results	0.55	6.67×10^{-3}	0.871	1.923	4×10^{-3}	0.887

The outcome shows that the pseudo-second-order binding mechanism is dominant and that the chemisorption process is responsible for the adsorption of MG dyes on the bosorbent generated from Datura stramonium roots. Chemical bonds between the adsorbent and adsorbate molecules may be covalent or ionic in nature.

4.7. Comparison of previously reported adsorption capacity with different biosorbent for different organic dye pollotants removal

The adsorption capacity of MG adsorption by Datura Stramonium root-derived adsorbent has been compared to the values of adsorption capacity shown in Table 2 and those of other adsorbents reported in the literature. When compared to other biosorbents, DSrB exhibits a good adsorption capacity for Malachite Green, and its robust Langmuir fit emphasizes its dependability. However, biosorbents with larger porosity and richer functional group chemistry, such as kiwi peel and Cordia africana leaf, perform better than Datura stramonium root biosorbent in terms of moderate adsorption capacity.

Table 2: Previously reported adsorption capacities of various biosorbent for MG

Biosorbent Material	Maximum Adsorption Capacity (mg/g)	Isotherm Fit / Notes	Source
Geranium plant waste (GPW)	16.89	Spontaneous, feasible adsorption; thermodynamic confirmation	Thakare, et al., 2025
Kiwi peel biosorbent	6.25	Selective adsorption of MG; high efficiency	Teweldebrihan et al., 2025
Cordia africana leaf	297.15 and 580.61	Untreated biosorbent; SEM/XRD characterization	Zhao *et al.*, 2023
Datura stramonium root (DSrB)	25.77	Strong Langmuir fit (R^2 = 0.996)	Current study

CHAPTER FIVE

5. CONCLUSION AND RECOMMENDATION

5.1. Conclusion

In conclusion, the Datura Stramonium root-derived biosorbent, prepared through chemical activation, demonstrates significant potential as an eco-friendly and cost-effective solution for removing mechachite green (MG) from aqueous solutions. Characterization of FT-IR, SEM and XRD revealed a well-developed surface area, optimal adsorption conditions at a dosage of 1g, pH 8, initial MG concentration of 20 ppm, contact time of 30 minutes, and temperature of 30°C. Isothermal studies indicated a strong fit to the Langmuir model (R^2 = 0.996), with a maximum adsorption capacity of 25.77 mg/g, while kinetic data followed a pseudo-second-order model (R^2 = 0.887). Although tested solely with MG, it is reasonable to infer that this biosorbent may effectively eliminate various organic dye pollutants from water.

5.2. Recommendation

In this work, the Datura Stramonium root-derived biosorbent was prepared successfully by chemical activation method and it had been shown to have the potential to remove MG from aqueous solution as sustainable environmental remediation but further studies should be conducted to fully explore its potential and the following were recommended for future researchers;

1. The prepared Datura Stramonium - root derived biosorbent demonstrated promising adsorption efficiency under laboratory conditions; therefore, further studies should be conducted using real samples from industrial wastewater to evaluate the influence of competing ions and complex matrices on adsorption efficiency.
2. Future researchers in this area should focus on determining regeneration and reusability of the Datura Stramonium-root derived biosorbent through multiple adsorption-desorption cycles in order to assess its long-term applicability and economic feasibility.
3. It is recommended that, methods such as BET surface area and pore size investigations has to be made in order to provide extra information on surface area properties and adsorption mechanisms.

4. To assess the nature and feasibility of the adsorption process, experiments should be performed through thermodynamic studies by determining parameters such as Gibbs free energy, enthalpy and entropy changes.
5. The removal of other classes of colorants and organic pollutants should be evaluated to determine the broader applicability in wastewater treatment for Datura stramonium root-derived biosorbent.
6. Experiments such as fixed bed studies has to be performed to assess the real potential of Datura Stramonium root- derived biosorbent for its continuous wastewater treatment systems.

REFERENCES

Abate G. Y.; Alene, A. N.; Habte, A.T.; Getahun, D. M. Adsorptive removal of malachite green dye from aqueous solution onto activated carbon of *Catha edulis* stem as a low cost bio-adsorbent. *Environ Syst Res*. 2020, *9*, 29.

Abd EI-Latif, M. M.; Ibrahim, A. M.; EI-Kady, M. F. Adsorption equilibrium, kinetics and thermodynamics of methylene blue from aqueous solutions using biopolymer oak sawdust composit**e**. *Journal of American Science* 2010, *6*, 267–283.

Abewaa, M.; Mengistu, A.; Takele, T.; Fito, J Nkambule, T. Adsorptive removal of malachite green dye from aqueous solution using *Rumex abyssinicus* derived activated carbon. *Scientific Reports* 2023, 13, 14701.

Al-jaaf, H. J.; Ali, N. S.; Alardhi, S. M.; Albayati, T. M. Implementing eggplant peels as an efcient bio-adsorbent for treatment of oily domestic wastewater. *Desalin. Water Treat*. 2022, *245*, 226–237.

Al-Snafi, A.E., Medical importance of Datura fastuosa (syn: Datura metel) and *Datura stramonium*-A review. *IOSR Journal of Pharmacy*, 2017.*7*(2), pp.43-58.

Ashish S. S.; et al. Removal of malachite green dye from aqueous solution with adsorption technique using *Limonia acidissima* (wood apple) shell as low cost adsorbent. *Arabian Journal of Chemistry* 2017, *10*, S3229–S3238.

Awokoya, K. N.; et al. Experimental and computational studies of microwave-assisted watermelon rind–styrene based molecular imprinted polymer for the removal of malachite green from aqueous solution. *Sci. Afr.* 2022, *16*, e01194.

Bhat, S. S.; Narayana, B.; Bhat, J. I. Adsorption of malachite green dye using low-cost adsorbent derived from java apple leaves (*Syzyium samarangense*). *Sadhana* 2023, *48*, 0123456789.

China, C, R.; Maguta, M. M.; Nyandoro, S. S.; Hilonga, A.; Kanth, S. V.; Njau, K. N. Alternative tanning technologies and their suitability in curbing environmental pollution from the leather industry. *Chemosphere* 2020, *254*, 126804.

Dawood, S.; Sen, T. K. Review on Dye Removal from Its Aqueous Solution into Alternative Cost effective and Non-Conventional Adsorbents. *Journal of Chemical and Process Engineering* 2014, *1*(104), 1–11.

Dwivedi, C.P.; Sahu, J. N.; Mohanty, C. R.; Mohan B.R. Column performance of granular activated carbon packed bed for Pb (II) removal. *Journal of hazardous materials* 2008, *156*(1–3), 596-607.

Encinar, J.M.; Beltran F. J.; Ramiro, A. Pyrolysis/gasification of agricultural residues by carbon dioxide in the presence of different additives: influence of variables. *Fuel Processing Technology* 1998, *55*(3), 219 –231.

Eren, E. Investigation of a basic dye removal from aqueous solution onto chemically modified Unye bentonite 2009**.**

Fasust, S.; Dand, A.; Osman, M. Adsorption Processes for Water treatment, Butter worth's, Boston, Massa cusetts. *Chemistry of water* 2004, *509*, 1987–1920.

Fito, J.; Abrham, S.; and K. Angassa, K. Adsorption of methylene blue from textile industrial wastewater onto activated carbon of *parthenium hysterophorus*. *Int. J. Environ. Res.* 2020, *14* (5), 501–511.

Fito, J.; Ebrahim, O.; Nkambule, T. T. I. The application Mn–Ni ferrite nanocomposite for adsorption of chromium from textile industrial wastewater. *Water Air Soil Pollut*. 2023, *234*, 37.

Freundlich, H.M.F. Uber die adsorption in losungen. Z. *Phys. Chem*. 1906, *57*, 385–470.

Garba, Z. N.; Zango, Z. U.; Babando, A.; Galadima, A. Competitive adsorption of dyes onto granular activated carbon. *J Chem Pharm Res*. 2015, *7*, 710–717.

Gebeyehu, B. T.; Kabtamu, D. M.; Tasew, T. A. Efficient removal of methylene blue dye from aqueous solution using a new biosorbent derived from *Enset eventricosum* (Enset). *Bulletin of the Chemical Society of Ethiopia* 2024, *38*(1), 69–84.

Guo, X.; Du, Q.; Zhang, W.; Xin, X.; Yan, L.; Yu, H. Removal of basic dyes (malachite green) from aqueous medium by adsorption onto amino functionalized graphenes in batch mode. *Desalination and Water Treatment* 2022, *53*, 818–825.

Gupta, N. K.; Ghaffari, Y.; Kim, S.; Bae, J.; Kim, K. S.; Saifuddin, M. Photocatalytic Degradation of Organic Pollutants over MFe2O4 (M = Co, Ni, Cu, Zn) Nanoparticles at Neutral pH. *Sci. Rep*. 2020, *10*(1), 1–11.

Hameed, B.H. Evaluation of papaya seeds as a novel non-conventional low-cost adsorbent for removal of methylene blue. *Journal of Hazardous materials* 2009, *162*(2-3), 939–946.

Hammud, H.H.; Hammoud, M.H.; Hussein, A.A.; Fawaz, Y.B.; Abdul Hamid, M.H.S.; Sheikh, N.S. Removal of Malachite Green Using Hydrochar from PALM Leaves. *Sustainability* 2023, *15*, 8939.

Hasan, M. Adsorption of reactive azo dyes on chitosan/oil-palm ash. M. Sc. thesis, Malaysia University of Science, 2008.

Ho, Y.S.; McKay, G. Pseudo-second order model for sorption processes. *Process Biochem*. 1999, *34*, 451–465.

Jabbar, N. M.; Alardhi, S. M.; Mohammed, A. K.; Salih, I. K.; Albayati, T. M. Challenges in the implementation of bioremediation processes in petroleum-contaminated soils: A review. Environ. *Nanotechnol. Monit. Manag*. 2022, *18*, 100694.

Jara YS, Mohammed ET, Mekiso TT. Biosynthesized pure CuO, N-CuO, Zn-CuO, and N-Zn-CuO nanoparticles for photocatalytic activity: Enhanced optical properties through bandgap engineering. *Next Materials*. 2025 Jul 1;8:100742.Arunprasath, T.; Sudalai, S.; Meenatchi, R.; Jeyavishnu, K.; Arumugam, A. Biocatalysis and Agricultural Biotechnology Biodegradation of triphenylmethane dye malachite green by a newly isolated fungus strain. *Biocatal. Agric. Biotechnol*. 2019, *17*, 672–679.

Krika, F., A. Krika, and A. Azizi. "Impact of NaOH-surface treatment on emerging pollutant biosorption performance using marine algua, Posidonia Oceanica." *Glob Nest J* 23, no. 1 (2021): 127-136. https://doi.org/10.30955/gnj.003579

Kim, S.; Park, H.; Pandey, S.; Jeong, D.; Lee, C. -T.; Do, J, Y.; Park, S. –M.; Kang, M. Effective Antibacterial/Photocatalytic Activity of ZnO Nanomaterials Synthesized under Low Temperature and Alkaline Conditions. *Nanomaterials* 2022, *12*, 4417.

Lagergren, S. About the theory of so-called adsorption of soluble substance. K. Sven. Vetersk. Handl. 1898, *24*, 1-39.

Langmuir, I. Constitution and fundamental properties of solids and liquids. I. Solids. *J. Am. Chem. Soc.* 1916, *38*, 2221–2295.

Lemos, E. S.; Fiorentini, E. F.; Bonilla-Petriciolet, A.; Escudero, L. B. Malachite Green Removal by Grape Stalks Biosorption from Natural Waters and Effluents. *Adsorption Science and Technology* 2023, 12.

Li, Jihui, Bingjian Zhang, and Yidan Shu. "Simulation of gas-solid adsorption process considering particle-size distribution." *Chinese Journal of Chemical Engineering* 54 (2023): 331-342. https://doi.org/10.1016/j.cjche.2022.02.021

Liu, J.; Li, R.; Yang, B. Carbon Dots: A New Type of Carbon-Based Nanomaterial with Wide Applications. *ACS Cent. Sci*. 2020, *6*(12), 2179–2195.

Madian, H.R.; Abdelhamid, A. E.; Hassan, H. M.; et al. Potential applicability of *Jatropha curcas* leaves in bioethanol production and their composites with polymer in wastewater treatment. *Biomass Conv. Bioref.* 2024, *14*, 20991–21005.

Mengesha, M.; Shuka, Y.; Eyoel, T.; Tesfaye, T. Novel Biomaterial-Derived Activated Carbon from Lippia Adoensis (Var. Koseret) Leaf for Efficient Organic Pollutant Dye

Removal from Water Solution. *Am. J. Appl. Chem.* 2024, 12(2), 29-46. doi: 10.11648/j.ajac.20241202.11.

Mondal, N.K.; Kar, S. Potentiality of banana peel for removal of Congo red dyes from aqueous solution: isotherm, kinetics and thermodynamics studies. *Applied Water Science* 2018, *8*, 157.

Mosebolatan, J.; Ayorinde, M.; Adelaja, Y. Results in engineering valorization of microwave-assisted H_3PO_4-activated plantain (*Musa paradisiacal* L) leaf biochar for malachite green sequestration: Models and mechanism of adsorption. *Results Eng.* 2023, *18*, 101129.

Moumni, B.; Zouitane, I.; Achik, M.; Oulmekki, A.; Zaitan, H.; El Ghachtouli, N.; Benmoussa, H. Effect of lightweight composite brick's waste on the removal of malachite green from aqueous solution and phytotoxicity assessment. *International Journal of Environmental Analytical Chemistry* 2024, 1–23.

Moustafa, M. T. Preparation and characterization of low cost adsorbents for the efficient removal of malachite green using response surface modeling and reusability studies. *Scientific Reports* 2023, *13*, 4493.

Mukherjee, S. K. S.; Misra, A. K.; Acharya, P. C. Removal of Aqueous Nickel (II) Using Laterite as a Low-Cost Adsorbent. *Environmental water Resource* 2006, 78, 2268–2275.

Nure, J. F.; Nkambule, T. T. I. The recent advances in adsorption and membrane separation and their hybrid technologies for micropollutants removal from wastewater. *J. Ind. Eng. Chem.* 2023.

Oladoye, P. O.; Ajiboye, T. O.; Wanyonyi, W. C.; Omotola, E. O.; Oladipo, M. E. Insights into remediation and decontamination technology of malachite green wastewater. *Water Sci. Eng*. 2023. https://doi.org/10.1016/j.wse.2023.03.002

Oyelude, E.O.; Awudza, J. A. M.; Twumasi, S. K. Removal of malachite green from aqueous solution using pulverized teak leaf litter: equilibrium, kinetic and thermodynamic studies. *Chemistry Central Journal* 2018, *12*, 81.

Pan, J., Wang, S.Y., Wang, D.N., Li, M.M., Wu, J.T., Chen, Q.S., Zhang, L.L., Kuang, H.X., Ma, X.C. and Liu, Y., Stramoniumlides a and B: Two new nitrogen-containing Withanolides from the leaves of Datura stramonium L. *Bioorganic Chemistry*, 2025 .p.109213.

Raval, N. P.; Shah, P. U.; Shah, N. K. Nanoparticles loaded biopolymer as effective adsorbent for adsorptive removal of malachite green from aqueous solution. *Water Conserv Sci Eng*. 2016, *1*, 69-81.

Shuka, Yohannes. Review on Adsorption Techniques for the Removal of Toxic Organic Dyes: Water Treatment Technology. JSM Chem (2025)11(1): 1066

Stabentheiner, E.; Zankel, A.; Polt, P. Environmental scanning electron microscopy (ESEM)-a versatile tool in studying plants. *Protoplasma* 2010, *246*(1), 89–99.

Tarekegn, M. M.; Balakrishnan, M. Zerovalent iron, nanoclay and iron impregnated. 2021, 30109-30131. https://doi.org/10.1039/d1ra03918k

Thakare, S. S., S. T. Shinde, R. S. Pawar, K. G. Sonawane, and A. A. Kale. "Kinetic, isotherm, and thermodynamic studies on the adsorption of malachite green dye using untreated biosorbent derived from geranium plant waste." *Ceylon Journal of Science* 54, no. 3 (2025). https://doi.org/10.4038/cjs.v54i3.8549

Wang, S.; Tang, Y.; Du, Z.; Song, M. Export trade, embodied carbon emissions, and environmental pollution: An empirical analysis of China's high- and new-technology industries. *J. Environ. Manage*. 2020, *276*, 111371.

Yabalak, E.; Elneccar, F. Evaluation of watermelon peel, banana peel and bay leaves hydrochars as green catalysts in the degradation of malachite green by thermally activated persulfate oxidation method. *J. Environ. Manag.* 2022, *304*, 114311.

Yunusa, U.; Ibrahim, M. B. Reclamation of malachite green-bearing wastewater using desert date seed shell: Adsorption isotherms, desorption and reusability studies. *Chemsearch J.* 2019, *10*, 112–122.

Zhang, W., Sheng, X., Yan, J., Wang, J., Sun, J., Zuo, Q., ... & Gong, L. (2023). The crucial role of different NaOH activation pathways on the algae-derived biochar toward carbamazepine adsorption. Results in Engineering, 20, 101509. https://doi.org/10.1016/j.rineng.2023.101509

Zhul-quarnain, A.; Ogemdi, I. K.; Modupe, I.; Gold, E.; Chidubem, E. E. Adsorption of malachite green dye using orange peel. *J. Biomater*. 2018, *2*, 31–40.

Zhao, Y.; Liu, X.; Li, W.; Pei, S.; Ren, Y.; Li, X.; Qu, C.; Wu, C.; Liu, J. Efficient and Selective Adsorption of Cationic Dye Malachite Green by Kiwi-Peel-Based Biosorbents. Molecules 2023, 28, 5310. https://doi.org/10.3390/molecules28145310

APPENDPICES

Row Experimental Data on the Adsorption Study

Appendix 1: Effect of chemicals activation on Root of *Datura Stramonium* derived biosorbent removal of MG at Adsorption condition of pH 8, $[MG]_0$ = 20 ppm, Volume of MG aqueous solution = 50 ml, A_0 = 2.421, Temp.=30 ^{0}C, Reaction Time =30 min, and Biosorbent dosage =1g.

Chemicals	**NaOH**	H_2SO_4	H_3PO_4
A_t	0.206	0.408	0.712
Removal (%)	**91.49**	83.15	70.59

Appendix 1: Effect of Initial MG concentration on NaOH activated Root of *Datura Stramonium* biosorbent's removal of MG at adsorption condition of pH 8, Volume of MG aqueous solution = 50 ml, Temp. =30^0 C, Reaction Time = 30 min, and Biosorbent dosage =1 g.

$[MG]_0$ (ppm)	5	10	15	**20**	25	30
A_0	0.367	0.611	1.250	2.421	3.411	3.854
A_t	0.202	0.217	0219	0.202	1.921	2.44
Removal (%)	44.95	64.49	82.48	91.49	60.20	36.62

Appendix 3: Effect of biosorbent dosage on NaOH activated Root of *Datura Stramonium* biosorbent's removal of MG at adsorption condition of pH 8, Volume of MG aqueous solution = 50 ml, Temp. =30 ^{0}C, $[MG]_0$ = 20 ppm, A_0 = 2.421, and Reaction Time = 35 min.

Biosorbent (g)	0.5	0.8	**1**	1.2	1.5
A_t	0.533	0.428	0.206	0.452	0.497
Removal (%)	77.98	82.32	91.49	81.33	79.47

Appendix 4: Effect of pH on NaOH activated Root of *Datura Stramonium* biosorbent's removal of MG at adsorption condition of Volume of MG aqueous solution = 50 ml, $[MG]_0$ = 20 ppm, Temp. =30 ^{0}C, A_0 = 2.421, Reaction Time = 30 min, and Biosorbent dosage =1g.

pH	2	4	6	7	**8**	10	12
A_t	0.341	0.293	0.239	0.229	0.201	0.231	0.271
Removal (%)	85.91	87.89	90.12	90.54	91.69	90.45	88.80

Appendix 5: Effect of reaction time on NaOH activated Root of *Datura Stramonium* biosorbent's removal of MG at adsorption condition of pH 8, Volume of MG aqueous solution = 50 ml, Temp. =30 ^{0}C, $[MG]_0$ = 20 ppm, A_0 = 2.421, and Biosorbent dosage =1g.

Reaction time (min)	10	15	20	25	30	**35**	40	45	50
A_t	0.382	0.341	0.292	0.261	0.247	0.229	0.246	0.268	0.301
Removal (%)	84.22	85.91	87.93	89.21	89.79	90.54	89.83	88.39	87.56

Appendix 6: Effect of Temperature on NaOH activated Root of *Datura Stramonium* biosorbent's removal of MG at adsorption condition of pH 8, $[MG]_0$ = 20 ppm, Volume of MG aqueous solution = 50 ml, A_0 = 2.421, Reaction Time = 30 min, and Biosorbent dosage =1g.

Temperature (^{0}C)	25	30	**35**	40	45	50	55
A_t	0.294	0.221	0.209	0.251	0.290	0.307	0.371
Removal (%)	87.85	90.87	91.36	89.63	88.02	87.32	84..67

Appendix 7: Data on Equilibrium study at optimized adsorption cations (pH 8, Volume of MG aqueous solution = 50 ml, Reaction Time = 30 min, Temp. =30 ^{0}C and Biosorbent dosage =1g).

Con. of MG (ppm)	At.	Ce	Qe	Ce/qe	Logqe	logCe
5	0.202	1.531463	0.173427	8.830601	-0.76088	0.185107
10	0.217	1.645186	0.417741	10.938294	-0.37909	0.216215
15	0.219	1.660349	0.666983	14.489344	-0.17589	0.220199
20	0.202	1.91463	0.923427	19.658456	-0.0346	0.185107
25	1.921	2.16406	0.521797	27.91137	-0.2825	1.163283
30	2.44	2.49886	0.575057	32.16875	-0.24029	1.267145

Appendix 8: Data on kinetic study at optimized adsorption cations (pH 8, $[MG]_0$ = 20 ppm, Volume of MG aqueous solution = 50 ml, A_0 = 2.421, and Biosorbent dosage =1g).

Time (min)	Ct	Qt (mg/g)	qe (mg/g)	qe-qt	log(qe-qt)	t/qt
10	2.205	1.559	3.385	1.826	0.261	6.414
15	1.467	1.707	3.385	1.678	0.225	8.787
25	0.9	1.82	3.385	1.565	0.194	13.736
30	0.76	1.848	3.385	1.537	0.186	16.237
35	0.62	1.845	3.385	1.54	0.187	18.971