



*University of Echahid Hamma-Lakhdar, El-Oued
Faculty of Exact Sciences
Department of Chemistry
Laboratory of Applied Chemistry
and Environment (LACE)*



2nd Study Day on Applied Chemistry and Environmental Engineering

SDACEE-2025

April, 09, 2025

BOOK OF ABSTRACTS



**Includes 02 Plenary Conferences with 4 Oral
and 40 Poster Presentations**



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**SDACEE
2025**
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DESCRIPTION

The SDACEE-2025 event forms part of the activity program implemented by the Department of Chemistry in collaboration with the “LACE” research laboratory. It aims to encourage researchers, particularly PhD students, to present their scientific results and to engage in constructive discussions with experts from different research domains.

The SDACEE-2025 book of abstracts provides a comprehensive overview of the event, including 2 plenary lectures, 4 oral presentations, and 40 poster contributions.

This volume compiles recent and original research carried out in the fields of Applied Chemistry and Environmental Engineering. A substantial portion is dedicated to studies on chemical depollution and environmental protection, reflecting the central theme of the event. The book also addresses a key topic in Applied Chemistry, namely organic synthesis conducted through eco-friendly methodologies. Furthermore, two sections are devoted to pharmaceutical chemistry and drug discovery, with a particular emphasis on phytochemistry and medicinal plants.

THEMES

Chemical depollution and environmental protection. Pharmaceutical chemistry and drug discovery. Organic synthesis and catalysis. Phytochemistry and medicinal plants.

ACKNOWLEDGEMENTS

We extend our sincere gratitude to Pr. Ferhati Omar, Rector of the University of El-Oued, and Pr. Mansour Abdelouahab, Dean of the Faculty of Exact Sciences, for their valuable support. Our thanks are also addressed to the scientific and organizing committees of SDACEE-2025 for their commitment and efforts, as well as to the “Applied Chemistry and Environment” laboratory for its meaningful contribution.

We further express our deep appreciation to the Keynote Speakers, Dr. Rania Zamouche-Zerdazi (University of Constantine 3) and Dr. Belkhalifa Hakim (CRAPC Ouargla), for their distinguished contributions. Finally, we thank all participants for their involvement in SDACEE-2025.

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ABSTRACTS OF PLENARY SESSIONS





Extraction des composés photochromiques: méthodes, analyses et applications.

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Keywords: Photochromisme, Extraction, HPLC, Matériaux intelligents, Composés organiques.

ABSTRACT

Les composés photochromiques sont des molécules capables de changer réversiblement de structure et de couleur sous l'effet d'une irradiation lumineuse. Leur extraction à partir de matrices naturelles ou synthétiques constitue une étape essentielle pour leur caractérisation et leur utilisation. Les méthodes d'extraction les plus courantes incluent l'extraction par solvants organiques, l'extraction assistée par ultrasons, ainsi que l'extraction par fluides supercritiques, chacune permettant d'optimiser le rendement tout en préservant la stabilité photochimique des composés. Après extraction, l'analyse s'appuie sur des techniques spectroscopiques (UV-Vis, IR, RMN) et chromatographiques (HPLC, UHPLC) afin d'identifier les espèces photochromiques et d'étudier leur comportement d'interconversion. Ces composés trouvent de nombreuses applications dans les matériaux intelligents, les capteurs optiques, la protection solaire, la photonique et les systèmes de stockage d'informations. Leur étude est au cœur de l'innovation dans le domaine des matériaux fonctionnels sensibles à la lumière.



Treatment of Emerging Pollution: Evolution of Purification Processes

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Keywords: Emerging Pollution, dysfunctions, Intensified Processes, MBRI, MBBR..

ABSTRACT

The elimination of pollutants is carried out in wastewater treatment plants, whose primary mission is to ensure a high level of purification. However, the presence of micropollutants, such as pharmaceutical residues, heavy metals, and certain persistent organic compounds, can disrupt microbial activity. This interference leads to partial inhibition of the biomass and compromises the overall efficiency of the biological treatment process.

Moreover, the increasing complexity of industrial discharges, characterized by a diversity of chemical substances and high pollutant loads, further highlights the limitations of conventional systems. These treatment plants then become vulnerable to recurring dysfunctions, including sludge bulking caused by the excessive proliferation of certain filamentous bacteria; deflocculation, which weakens the structure of the flocs and reduces their settling capacity; and foaming, often induced by the presence of surfactants or specific microorganisms.

Such anomalies not only impair the quality of the treated water but also reduce its potential for reuse, particularly in agricultural or industrial applications. They therefore emphasize the need to adopt advanced treatment processes and management strategies adapted to new environmental challenges.

Among the intensified processes developed to overcome the limitations of conventional systems, the immersed membrane bioreactor (MBRI) has emerged as a reference solution for the treatment of pharmaceutical effluents, mainly contaminated by amoxicillin. The MBRI allows the maintenance of high biomass concentrations, promoting sustained microbial activity and more complete pollutant degradation. Thanks to this intensification, the reaction volume can be significantly reduced, while the required membrane surface remains proportional to the treated flow, thereby optimizing the system's energy and spatial footprint. Removal rates recorded for various pollutant loads and micropollutants exceed 98% efficiency, confirming the potential of the MBRI as an advanced technology to address environmental challenges related to pharmaceutical discharges and paving the way for the safe reuse of treated water.



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The second process relies on the use of a moving bed biofilm reactor (MBBR), equipped with Kaldnes K1 carriers, specifically designed for the denitrification of raw and wastewater. This system has demonstrated notable efficiency in nitrate removal, achieving treatment concentrations of up to 60 mg/L of N-NO₃. The performance of the MBBR is based on the activity of heterotrophic denitrifying biomass, which simultaneously ensures the reduction of carbon load to minimal thresholds, thereby optimizing the quality of the treated water. Thanks to the combination of the high specific surface area of the Kaldnes carriers and the stability of the biofilm, the process guarantees robust denitrification even in the presence of complex pollutant loads.

Complementing the MBRI, the MBBR illustrates the value of adopting intensified processes in the design of treatment systems. Together, these technologies provide an effective response to the issue of specific pollution, significantly reducing pollutant loads and paving the way for the sustainable reuse of treated water.

ABSTRACTS OF ORAL PRESENTATIONS





Understanding AI: Tools, Models and their Integration into Environmental Monitoring and Management

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Keywords: Artificial Intelligence, Environmental Monitoring, Data Acquisition, Machine Learning, Remote Sensing, Sustainable Resource Management.

ABSTRACT

Artificial intelligence (AI) has emerged as a powerful framework for addressing complex problems in environmental monitoring and management. This work presents a comprehensive overview of AI tools, model architectures, and their integration into environmental applications, with emphasis on how data are collected, processed, and transformed into actionable outputs. We outline common data-acquisition strategies, including remote sensing, in-situ sensor networks, biological sampling, and experimental measurements, and describe how these heterogeneous datasets are converted into model inputs through preprocessing, feature extraction, and parameter selection. The study also highlights approaches used in biology and environmental science to determine learning parameters—such as growth rates, environmental indicators, pollutant levels, and ecosystem responses—by combining experimental design with supervised, unsupervised, and reinforcement learning techniques. Various AI models, including machine learning algorithms, deep neural networks, and hybrid physics–AI systems, are examined with respect to their ability to detect patterns, predict environmental change, and support decision-making. By integrating methodological insights with practical examples, this work illustrates how AI can enhance accuracy, efficiency, and scalability in environmental assessment, ultimately contributing to improved resource management and sustainable ecosystem governance.



Targeting the “undruggable”: from in silico and computer drug discovery to hope

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Keywords: In silico, molecular docking, drug design, undruggable, Rhodanine

ABSTRACT

Targeting "undruggable" proteins like c-Myc, a key oncogenic transcription factor dysregulated in numerous cancers, remains a significant challenge in drug discovery [1]. Despite its pivotal role in tumorigenesis, c-Myc has evaded direct therapeutic inhibition due to its intrinsically disordered structure and lack of well-defined binding pockets. This study explores rhodanine-based compounds as potential c-Myc inhibitors using in silico strategies, with a focus on molecular docking to identify high-affinity binders [1]. Computational screening and binding mode analysis reveal that specific rhodanine derivatives exhibit favorable interactions with c-Myc's DNA-binding domain, potentially disrupting its oncogenic activity [1-2]. These findings provide a foundation for the rational design of novel c-Myc inhibitors, offering hope for targeting this elusive oncoprotein.

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Integrated Phytochemical Characterization and Multi-Scale Investigation of an Essential Oil for Anti-Alzheimer Potential: In Vivo, In Vitro, and In Silico Approaches

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Keywords: Essential oil, GC/MS analysis, In vivo neuroprotection, In vitro AChE inhibition, In silico molecular modeling, Anti-Alzheimer activity

ABSTRACT

This study investigates the anti-Alzheimer potential of an essential oil extracted from a medicinal plant using an integrative approach. The oil was obtained through hydrodistillation and analyzed using gas chromatography-mass spectrometry (GC/MS) to determine its chemical composition. Its biological activity was assessed through in vivo experiments, evaluating its neuroprotective effects in an Alzheimer's disease model. In vitro assays, including acetylcholinesterase (AChE) inhibition and antioxidant activity tests, were conducted to examine its role in modulating key neurodegenerative processes. Additionally, in silico molecular docking and molecular dynamics simulations were performed to explore the binding interactions of the oil's active compounds with AChE and other Alzheimer-related targets. The findings provide valuable insights into the therapeutic potential of this essential oil, highlighting its promise as a natural candidate for Alzheimer's disease management.



From Agricultural Waste to Nanosilica: Innovative Adsorbents for Environmental Remediation

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Keywords: Adsorption Isotherms; Agricultural Waste; Environmental Remediation; Nanosilica; Ultrasonic-Assisted Synthesis

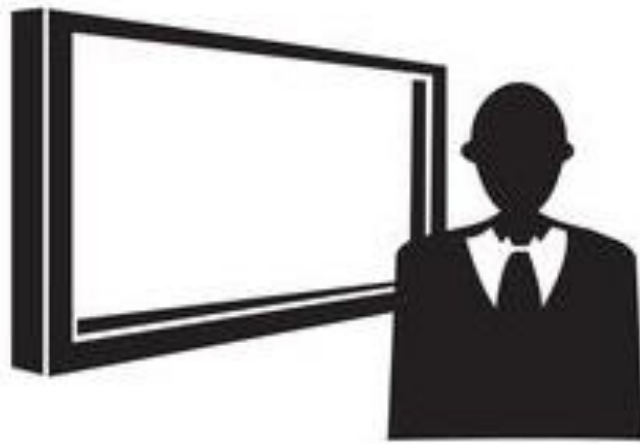
ABSTRACT

In this study, we explore the synthesis of spherical nanosilica materials using agricultural wastes, specifically olive pomace and date palm waste, through an ultrasonic-assisted precipitation process. This innovative approach not only provides a sustainable method for nanosilica production but also utilizes readily available agricultural byproducts, thereby contributing to waste reduction and resource efficiency. A comparative analysis is conducted between the nanosilica derived from these agricultural sources and that synthesized from pure sodium silicate, highlighting the potential of organic waste as a viable alternative. The synthesized nanosilica materials are characterized using X-ray diffraction (XRD), infrared spectroscopy (IR), scanning electron microscopy (SEM), and nitrogen adsorption/desorption isotherms (BET). These characterizations confirm the successful formation of nanosilica with desirable morphological and structural properties. Furthermore, the efficacy of the produced nanosilica as an adsorbent for the removal of methylene blue (MB) from aqueous solutions is investigated. The adsorption behavior is analyzed using Langmuir and Freundlich isotherm models, providing insights into the adsorption capacity and surface interactions. Additionally, thermodynamic parameters of the adsorption reaction are evaluated. The findings suggest that nanosilica synthesized from olive pomace and date palm waste not only serves as an effective adsorbent for dye removal but also represents a promising avenue for sustainable material development in environmental applications.

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ABSTRACTS OF POSTER PRESENTATIONS



TOPIC 1

Chemical depollution and environmental protection





Modification Of Agricultural Wastes To Improve Adsorption Capacities For Copper Ions Removal From Aqueous Solutions

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Keywords: Adsorption; Agricultural wastes; biomass; copper; Heavy metals; Waste water.

ABSTRACT

Agricultural wastes are widely used in waste water treatment, by its raw materials or by its modified phase to achieve more enhancement of its adsorptive properties, many studies were conducted about both physical and chemical activation of biomasses which gave very attractive results in term of heavy metal removal in aqueous solutions, in present study, local grass which is growing abundantly and quickly was treated by surface modification with sodium hydroxide activation then followed by pyrolysis at 800 °C, preliminary tests were done on its raw material and modified one by putting them in synthetic contaminated water with copper ions in different concentrations (10,20,40, 80 mg/l), the results showed best removal percentage of modified grass more the 90 %, it was characterised by SEM/EDX, FTIR, and Point of Zero Charge (PZC) and the isotherm and kinetic study are in progress to bring more information about its adsorption performance and for its optimization, the morphology and elementary analysis showed the existence of tunnel shaped pores and the majority surface element was Carbon, FTIR characterisation showed its functional groups that may give the opportunity of ion exchange or coordination with heavy metals, additional analysis is programmed as well as XRD, BET and completed adsorption behaviour study in order to optimize this local grass to be within the best low-cost agricultural waste based adsorbents, more practical tests and analysis will be done to find out its capacity on industrial waste water to eliminate the toxic heavy metals on whether one or multi-metal pollutants and even its feasibility.

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Adsorption of Pollutants Using Activated Biochar from Olive stones: Isotherm, Kinetics, and Thermodynamics Study

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Keywords:

Olive Stones; activated carbon; RSM; FTIR; pHz ;XRD.

Abstract:

This study presents a sustainable approach for producing olive stone activated carbon (OSAC) using an activating agent, sulfuric acid (H_2SO_4), at a mass ratio of 1:1, to remove the cationic dye methylene blue (MB). Adsorption experiments were conducted to determine the optimal dye removal conditions. The response surface methodology (RSM) was applied using varying levels of key parameters, including adsorbent dosage, medium pH, contact time, and temperature. The OSAC was characterized using Fourier transform infrared spectroscopy (FTIR) to identify functional groups and components. Additionally, the point of zero charge (pHz) was measured to determine the surface charge of the adsorbent. X-ray diffraction (XRD) analysis was also employed for structural characterization. The study demonstrated significant results, with a coefficient of determination (R^2) confirming the optimal conditions for dye removal. The adsorption kinetics followed a pseudo-second-order model, and thermodynamic analysis indicated that the process was endothermic.

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Treatment of salty and organically polluted water by electro dialysis combined with electro-Fenton process

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Keywords: Electrodialysis, Electro-Fenton, Carbon cathode, Membrane anti-fouling, Combined processes.

ABSTRACT

This work aims to combine Electrodialysis and Electro-Fenton (ED/EF) process using a carbon cathode, to intensify the removal of organic pollutants and enhance the transport of salt ions across membranes. Initially, the effect of some operating parameters including, nature of the cathode material, supporting electrolyte nature, applied current density, Fe(II) concentration and initial pH value on the EF process was studied to determine the optimal conditions for this process. In a second phase, the ED and EF processes were combined, and the effectiveness of this combination was compared to that of the single ED process. The obtained results demonstrated the high efficiency of the combined ED/EF compared to single ED process.

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The evaluation of Antimicrobial activity and Adsorption of MB dye on Cellulose and Cellulose/ZnO nanoparticles from peanut and pea shells.

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Keywords: Peanut and Peas shells, Cellulose, Zinc oxide, Nanocomposite, Adsorption, Antimicrobial activity.

ABSTRACT

This study aims to repurpose plant waste, specifically Peanut and pea shells, to synthesize cellulose/zinc oxide nanoparticles (CNC/ZnO NPs) using two environmentally friendly and low-cost techniques. Initially, cellulose nanocrystals (CNCs) were extracted from the cellulose-rich biomass of Peanut and pea shells through chemical treatments. Subsequently, a hybrid material of CNCs and ZnO NPs was fabricated using two techniques.

The first, involving the dissolution of cellulose (Cs) in a basic solution, and the second, utilizing Cs crystals directly. Various analysis techniques, including Fourier-Transform Infrared spectroscopy (FT-IR), X-Ray Diffraction (XRD), Scanning Electron Microscope (SEM), Energy Dispersive X-ray Spectroscopy (EDX), and Ultraviolet visible spectroscopy (UV-Vis), were employed to study the material's different properties. Furthermore, CNC/ZnO NPs were tested against human pathogenic bacteria and a fungus. Results indicated the crystalline nature of the CNC/ZnO NPs, with an average size varied between 19.64 and 27.31 nm, while the gap bands ranged between 3.27 and 3.66 eV for the two methods used. Morphological analysis showed a notable contrast in ZnO nanoparticle distribution on CNC surfaces. In the first method, ZnO NPs formed a complete and evenly distributed coating, resulting in a smooth structure. Conversely, the second method led to ZnO NPs appearing as scattered dots on the CNCs, resulting in the lowest ZnO NP content. In this work; Cs and CNC/ZnO NPs samples, has been used as adsorbents for removing MB dye from aqueous solution by adsorption technique. the results showed that the hybridization process of Cs with ZnO NPs did not enhance its effectiveness in removing BM dye The



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adsorption experiments demonstrated that the adsorption capacity on cellulose samples were more efficient than CNC/ZnO NPs sample

The study demonstrated a significant increase in antimicrobial properties after coating Cs nanoparticles with ZnO NPs, with the hybrid material exhibiting higher antimicrobial activity than pure CNCs. These findings suggest the potential of CNC/ZnO NPs for antimicrobial pharmaceuticals and as a natural food preservative to control the growth of microorganisms.

Eco-Friendly Synthesis and Characterization of Magnetic Iron Oxide Nanoparticles for Radium Removal

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Keywords: Characteristics; Magnetic Iron Oxide; Synthesis; Nanoparticle; Radium Removal.

ABSTRACT

In this study, magnetic iron oxide nanoparticles (Fe_3O_4 -NPs) were synthesized using a rapid, eco-friendly approach, employing thyme and rosemary extracts as natural reducing and stabilizing agents. The structural, morphological, and chemical properties of the synthesized Fe_3O_4 -NPs were thoroughly analyzed using Fourier Transform Infrared Spectroscopy (FT-IR), Scanning Electron Microscopy (SEM), Energy-Dispersive X-ray Spectroscopy (EDX), X-ray Diffraction (XRD), and Mössbauer Spectroscopy (MS). SEM imaging confirmed that the nanoparticles exhibited a predominantly spherical morphology, with sizes ranging from 11 to 17 nm when synthesized with thyme extract (0.5%) and from 8 to 16 nm with rosemary extract (0.5%). XRD analysis indicated high crystallinity and purity, while FT-IR confirmed the successful formation of Fe_3O_4 -NPs. Mössbauer spectroscopy revealed quadrupole splitting, highlighting key structural attributes. The synthesized Fe_3O_4 -NPs were further evaluated for their efficiency in removing ^{226}Ra from oil co-produced water, demonstrating significant adsorption potential. This green synthesis approach offers a sustainable and efficient method for producing magnetic nanoparticles with promising applications in environmental remediation.

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Integrating Pollution Indices and Health Risk Assessment for Drinking and Irrigation Suitability of Groundwater in Guelma, Algeria

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Keywords: Groundwater Pollution Index; Nitrate Pollution Index; Human Health Risk Assessment; Water Quality Index; Irrigation Water Quality Index

ABSTRACT

This study evaluates groundwater quality in the Guelma region (Algeria) through a comprehensive analysis of 13 wells, considering 15 physicochemical parameters. It employs key assessment tools, including the Groundwater Pollution Index (GPI), Nitrate Pollution Index (NPI), Human Health Risk Assessment (HHRA), Water Quality Index (WQI), and Irrigation Water Quality Index (IWQI). GPI results revealed that 69.23% of the samples showed insignificant pollution, while 30.77% exhibited low pollution. NPI indicated notable nitrate pollution in 23.08% of the samples. HHRA findings highlighted that children face a higher risk compared to adults. WQI classified 30.77% of the samples as good, 61.54% as poor, and 7.69% as very poor. Based on IWQI, 7.69% of the samples posed no toxicity risk, 61.54% required limiting salt-sensitive plants, 7.69% were suitable for moderately salt-tolerant plants, and 23.08% were suitable for moderate to high salt tolerance. Agricultural activities and surface water contamination are identified as primary sources of nitrate pollution [1]. Prolonged exposure through drinking water increases the risk of methemoglobinemia and certain cancers [2]. This study highlights the importance of pollution control measures to protect groundwater resources and ensure a safe water supply.

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Waste Gypsum Plasterboard as a Sustainable Adsorbent for Congo Red Dye Removal

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Keywords: Calcium sulfate; Eco-friendly adsorbents; Gypsum plasterboards waste; Recycling; Wastewater.

ABSTRACT

This study aims to investigate the potential of waste gypsum plasterboard as an environmentally friendly adsorbent for the removal of Congo Red (CR) dye from contaminated water, aligning with the concepts of sustainability and industrial waste recycling. Despite the widespread use of gypsum, its capability for removing such pollutants has not been sufficiently explored.

The physical and chemical properties of the treated waste gypsum plasterboards were examined, along with their adsorption efficiency at different dye concentrations (15 and 20 ppm) and varying contact times (20 to 140 minutes). The results showed a gradual decrease in absorbance over time, with the maximum dye removal percentage (%DR) reaching 48.12% at 15 ppm, while at 20 ppm, it was 53.77%, demonstrating the influence of the initial dye concentration on adsorption performance.

These findings highlight the increasing efficiency of gypsum plasterboard in dye removal over time. This study demonstrates the promising potential of waste gypsum as a low-cost and sustainable material for wastewater treatment technologies, contributing to effective environmental solutions for protecting water resources and reducing industrial pollution.

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The efficient of El Dhamrane in Turbidity, Phosphate and BOD removal from wastewater

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Keywords: El-Oued, Pollutants, Phytoremediation, Saharan plant, Wastewater

ABSTRACT

In natural biological treatment systems around the world, aquatic plants are used with the characteristics of adapting and living in floating environments, since several studies have proved the effectiveness of many aquatic plants in their ability superior in purifying wastewater of pollutants. In this study, we will show the effectiveness of the Saharan plant, which has a very acceptable ability to remove pollutants. This study aims to highlight the role of the Saharan plant in the secondary treatment of wastewater, as this plant El Dhamrane is located in the northeastern Algerian desert in El-Oued city, in the estuary of sewage effluent subject to primary treatment located. This area was known before it became an estuary, as being rich in desert grazing plants, but most of the plants were able to adapt to the new situation. The El Dhamrane plant, due to its morphological nature, was able to coexist with the estuary water and its presence on the outskirts of the site according to its water needs. The research was carried out on a pilot size in the field of home wastewater treatment (ONA El-Oued, Algeria). The results showed that El Dhamrane treatment slightly acidified the sample (pH ranged from 8.15 to 7.55); reduced the turbidity from 106.34 NTU to 3.82 NTU; mean concentration values of Phosphate, chemical, and biochemical oxygen demand at the end of treatment were respectively reduced by 71.63, 83.72, and 78.18 %. The study concludes that the El Dhamrane plant is very efficient in remediating phosphorus and capable of reducing chemical and biochemical oxygen demand. Traganum can show an efficient treatment in wastewater estuary although that is classified as no aquatic plant

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Advances in chitosan-based materials as adsorbents for the removal of cationic and anionic dyes: A review

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Keywords: Chitosan derivatives; Dyes; Adsorption; Langmuir isotherm; Application

ABSTRACT

In recent times, research interest into the development of biodegradable, cost-effective and environmental friendly adsorbents with favourable properties for adsorption of pollutants is a challenge. Chitosan (Chi) has garnered significant attention as an adsorbent for pollutants due to its abundant hydroxyl (-OH) and free amino (-NH₂) functional groups, which exhibit strong binding affinity for dyes. However, it has defects such as sensitivity to pH, low thermal stability, and poor porosity and specific surface area, which limit the application of chitosan in wastewater treatment. To overcome these limitations, various modification of chitosan via different physical and chemical methods have gained attention as a promising approach for removing organic (such as dyes) and inorganic (such as heavy metals ions) pollutants from aqueous medium. In this review, 106 papers (Years, 2010–2025) have been systematically reviewed from the Web of Science and Scopus-indexed journals, covering a total of 26 journals about the application of chitosan and its derivatives to remove on cationic dyes and anionic dyes was discussed comprehensively. The preparation strategy, and factors affecting the adsorption performance of adsorbents, including adsorption isotherm model, adsorption kinetics process, adsorption thermodynamics process, etc. Based on the reviewed papers, it is clear, that while some challenges remain, chitosan-based materials are emerging as promising adsorbents.

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Adsorption Cd par biosorbants

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Keywords: biosorbition ; cinétique; isotherme ; métaux lourd

ABSTRACT

Les biosorbants naturels pourraient constituer une méthode écologique pour éliminer le cadmium (Cd) des eaux contaminées. La présente étude évalue les performances d'un biosorbant naturel pour l'élimination des ions Cd(II), en accordant une attention particulière aux caractéristiques cinétiques et isothermiques du processus d'adsorption. Les tests en batch ont été menés dans différentes conditions telles que le pH, le temps de contact, la concentration initiale d'ions Cd(II) et la quantité de biosorbant. L'efficacité de l'adsorption s'est avérée être d'environ 63%, en fonction des conditions expérimentales, à un pH optimal d'environ 6. La cinétique d'adsorption est décrite par les modèles du pseudo-premier ordre et du pseudo-second ordre. Cependant, les données expérimentales étaient plus proches de la cinétique du modèle du pseudo-second ordre, ce qui suggère que les processus d'adsorption pourraient impliquer une réaction chimique entre les ions Cd(II) et les groupes actifs du biosorbant. Les équations de Freundlich et de Langmuir sont utilisées pour décrire le processus d'adsorption en termes de concentrations d'ions Cd(II) dans la limite du biosorbant. D'après les résultats, le modèle de Langmuir décrit les données expérimentales de manière plus appropriée.

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Sustainable Bioremediation with Endophytic Microorganisms: An Integrated Approach to Phytochemistry and Environmental Protection

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Keywords: Pollution; Endophytic Microorganisms; Sustainable Bioremediation; Bioremediation; Green Chemistry; Environmental Decontamination.

ABSTRACT

Soil and water pollution by toxic compounds is a major environmental challenge. Endophytic microorganisms, which reside within plant tissues without causing harm, offer a promising bioremediation strategy by enhancing plant protection and environmental resilience. This study explores their potential in soil bioremediation by analyzing their mechanisms and interactions with plants. These microorganisms produce enzymes that degrade pollutants, while strains like *Pseudomonas* and *Bacillus* improve hydrocarbon biodegradation and heavy metal detoxification. Additionally, fungi such as *Neotyphodium* enhance plant resilience to stress by stimulating phytohormones and protective compounds. Beyond phytoremediation, endophytes facilitate nutrient absorption and synthesize secondary metabolites with agro-environmental significance. However, large-scale applications require further research to optimize their effectiveness. By integrating biotechnology with green chemistry, these microorganisms could play a key role in environmental decontamination and ecosystem restoration.

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Study on the performance of green corrosion inhibitor in protection of API5LX60 in seawater environment.

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Keywords: Ascorbic acid ; API5LX60 pipeline steel ; Corrosion inhibitor ; Seawater.

ABSTRACT

The corrosion inhibition of metals in seawater can be achieved by the addition of inhibitors to the system that prevent corrosion from taking place on the metal surface. The effect of ascorbic acid on carbone steel corrosion in seawater were investigated by means of different techniques: gravimetric method, electrochemical polarization and electrochemical impedance spectroscopy and the scanning electron microscopy (SEM). The results obtained show that the acid ascorbic effectively inhibits the corrosion of steel X60. The optimal inhibitory efficiency is obtained at a concentration of 0.05 g/L of the inhibitor, with a maximum value of 77%.

This inhibitor presents a mixed inhibition character. SEM studies confirm the absence of the deterioration products on the surface of the specimens.

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Role of Bacteria in Pesticide Biodegradation: A Sustainable Approach YOUMBAI Souhir*¹, LAICHE Ammar Touhami²

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Keywords: Bacterial , Bioremediation, Environmental pollution, Microbial metabolism, Pesticide degradation, Soil bacteria,.

ABSTRACT

Pesticides used in agriculture are a major source of chemical contamination, infiltrating ecosystems and causing physiological harm to both humans and the environment. Highly toxic, fat-soluble pesticides persist in the environment, posing a serious threat to non-target organisms, particularly in soil ecosystems.

Due to these concerns, numerous studies and literature reviews have examined the ability of microorganisms to degrade pesticides. Soil hosts diverse microbial communities, with bacteria being the most ecologically significant due to their ubiquity, adaptability, and metabolic versatility. Several bacterial genera exhibit strong biotechnological and environmental relevance in pollutant biodegradation. Among Gram-positive bacteria, *Bacillus*, *Mycobacterium*, *Arthrobacter*, and *Rhodococcus* have demonstrated bioremediation potential. Similarly, Gram-negative genera such as *Flavobacterium*, *Acinetobacter*, and *Pseudomonas* are well-studied for their ability to break down various contaminants. These bacteria play a crucial role in eliminating persistent pollutants, including polycyclic aromatic hydrocarbons (PAHs), polychlorinated biphenyls (PCBs), and endocrine-disrupting chemicals (EDCs).

This review compiles existing research on key bacterial genera involved in pesticide degradation, focusing on their mechanisms of action and specificity toward different pesticide compounds. Understanding these microbial interactions is essential for developing strategies to mitigate pesticide pollution and restore environmental health.



Electrochemical Study of a Pesticide Residue in Tomato Crop and Assessment of Its Environmental Impact

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Keywords: Electrochemical chemistry; pesticide residue; cyclic voltammetry; environmental pollution; tomato.

ABSTRACT

Electrochemical chemistry is an effective tool for analyzing pesticide residues due to its high sensitivity and ability for qualitative and quantitative determination. In this study, cyclic voltammetry was used to detect and determine the concentrations of a pesticide in tomato samples grown in local agricultural areas. Analytical conditions were precisely optimized, using a modified glass electrode and applying a potential range between (0.0 to +2.0) V at a scan rate of 25 mV/s, with the pH adjusted to 6.5. The developed method demonstrated a low detection limit of 0.01 µg/mL, with recovery rates ranging from 85–98%, indicating high accuracy and reliability. These findings enhance the potential of electrochemical techniques as a sensitive and rapid tool for monitoring pesticide residues in agricultural products, contributing to environmental risk assessment and food safety assurance.

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Pharmaceutical Residues in the Aquatic Environment: Challenges and Depollution Strategies

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Keywords: Activated carbon; Adsorption; Micropollutants; Water treatment

ABSTRACT

The contamination of aquatic environments by pharmaceutical residues has become a major environmental concern due to their persistence and potential effects on aquatic ecosystems and human health [1]. These substances, mainly originating from human activities, are detected in surface and groundwater at concentrations ranging from nanograms to micrograms per liter, depending on the compounds [2].

This study provides an in-depth analysis of the presence of pharmaceutical molecules in water, based on recent research. The main sources of this pollution include wastewater treatment plant effluents and the spreading of organic waste products of animal origin.

Furthermore, we evaluate the efficiency of physicochemical water treatment processes. Adsorption on activated carbon has proven to be an effective technique, achieving 98.25% removal of a model dye (10 ppm) after 60 minutes of contact. The study of influencing parameters, such as pH, substrate concentration, and support material, highlighted their impact on kinetics and adsorption capacity.

Experimental results were modeled using Langmuir and Freundlich isotherms, with the Langmuir model providing the best representation of the adsorption process. Additionally, the observed kinetics followed a second-order model, indicating a strong interaction between the adsorbent and the adsorbate.

This research contributes to improving depollution solutions for aquatic effluents and reducing the impact of pharmaceutical residues on the environment.

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Green Synthesis of Graphene Oxide via a Modified Hummers' Method and Its Application in Water Treatment: Theoretical Framework

Abstract

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Keywords:

Green synthesis , Graphine Oxide , Modified Hummer's ,eco- friendly , FTIR, RDX ,SEM, BET, RSM , nanomaterials

Abstract:

In the pursuit of developing eco-friendly and efficient materials for environmental remediation, this study focuses on the green synthesis of graphene oxide (GO) from a natural carbon-rich precursor using a modified Hummers' method adapted to comply with green chemistry principles. The synthesized GO was characterized using various physicochemical techniques such as FTIR, XRD, SEM, and BET to investigate its structural and surface properties.

For the application phase, the prepared GO was employed as an adsorbent for the removal of organic pollutants from aqueous media. The optimization of adsorption conditions (mass, contact time, pH, and temperature) was performed using Response Surface Methodology (RSM). Additionally, kinetic, thermodynamic, and isotherm models were studied to understand the adsorption mechanisms and evaluate the material's potential in water treatment.

This work highlights a sustainable approach for the valorization of natural resources in the synthesis of advanced nanomaterials for environmental applications.

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Optimization by Response Surface Methodology, Adsorption Isotherms and Reusability Studies.

TOPIC 2

Pharmaceutical chemistry and drug discovery



QSER Study of Half-Wave Oxidation Potential of Indolizines Using Quantum Molecular Descriptors

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Abstract:

Indolizine derivatives hold essential biological functions and have been researched for hypoglycemic, antibacterial, anti-inflammatory, analgesic, and anti-tumor actions. Indolizine scaffold has intrigued conjecture and continuous attention and has become an effective parent system for generating powerful novel medication candidates. This research will focus on applying the quantitative structure electrochemistry relationship (QSER) approach to the half-wave potential ($E_{1/2}$) for Indolizine derivatives using the quantum molecular descriptors . After calculating the descriptors and splitting the data into both sets, training and prediction. The QSER model which we will construct using the Genetic Algorithm/Multiple Linear Regression (GA/MLR) technique, will be used to choose the optimal descriptors for the model.

Keywords: QSER, Indolizine , DFT, molecular descriptors, MLR.



Synthesis, characterization and antibacterial activity of functionalized Graphene Oxide Nanoparticles with (3-Aminopropyl)triethoxysilane

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ABSTRACT

Currently, nanotechnology (NT) is being utilized across a wide range of scientific disciplines, employing diverse methodologies to manipulate materials and develop gadgets at the nanoscale scale. Graphene oxide (GO) has been primarily investigated within the biomedical domain due to its water dispersibility, which renders it well-suited for utilization in nanomedicine applications [1-4]. Functionalization is a technique employed to modify a substance's chemical characteristics by introducing novel attributes, functional groups, or capabilities achieved by altering the material's surface chemistry [5, 6]. In this study, a GO@APTES nanocomposite was prepared from Graphene Oxide (GO) nanoparticles via modified hummers method, functionalized with (3-Aminopropyl)triethoxysilane (APTES) and was characterized using SEM-EDX, FTIR and XRD. The aim of this work is to investigate its antibacterial activity using the well diffusion and broth microdilution methods. Structural and morphological characteristics are confirmed through SEM-EDX, FTIR and XRD with a crystallite size of 2 nm. The results showed that nanocomposite had a low antibacterial activity.

Keyword: Antibacterial activity, Functionalization, Graphene oxide, GO@APTES, X-ray diffraction

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SYNTHESIS, BIOLOGICAL EVALUATION AND MOLECULAR DOCKING OF DICHLORIDO(1,10-PHENANTHROLINE-5-AMINE-K² N,N')DIPHENYLTIN(IV).

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Keywords: Organotin compound, biological evaluation, molecular docking, crystal structure, X-ray diffraction...

ABSTRACT

Organotin compounds showed countless applications in modern technology, especially in catalysis in the polymer chemistry (1). Similarly, anticancer activity was reported by Hadjidakou and Hadjiliadis (2).

Organotin compounds such as stannoxanes have been studied for their catalytic activity in many organic processes. Several organotin compounds have shown many biological activities such as antifungal activities (3), anticancer (4, 5)...

Our work aims the synthesis, structural study, biological evaluation and molecular docking of new organotin compound from organic ligands and their complexation with tin salts.

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Theoretical and Computational Exploration of the Energy and Reactivity in Quinoline Molecules and their Derivatives.

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Keywords: DFT; Quinoline; HOMO; LUMO; SAR; ESP

ABSTRACT

This study focuses on the electrostatic potential (ESP) and its role in determining the structure-activity relationship (SAR) of quinoline-based molecules. By employing quantum chemical calculations, we aim to analyze the molecular electrostatic potential distribution and how it influences chemical reactivity and intermolecular interactions.

Additionally, the molecular orbital energies, including the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO), will be investigated to understand the electronic properties and stability of quinoline derivatives. These parameters are crucial for predicting the reactivity, potential biological activity, and interaction mechanisms of these compounds.

By integrating density functional theory (DFT) and chemoinformatics approaches, this study provides a comprehensive theoretical framework to explore the electronic, structural, and reactivity properties of quinoline derivatives, contributing to the rational design of novel compounds with improved properties.

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Presentation of Recent Molecular Docking Studies Predicting the Interactions between Macromolecules (BSA, HI, AChE) and Zinc Oxide Nanoparticles (ZnO NPs).

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Keywords: AChE; BSA; Human insulin, Molecular docking; Nanotechnology; ZnO-NPs.

ABSTRACT

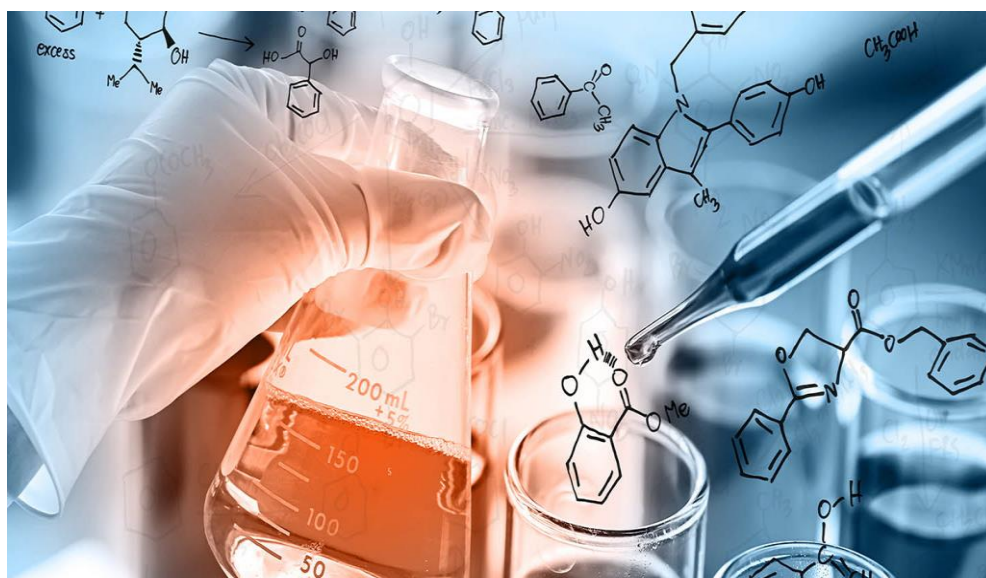
Biogenic synthesis of metal oxide nanoparticles is a rapidly growing research area in the field of nanotechnology owing to their immense potential in multifaceted biomedical and environmental applications. Researchers are increasingly focused on zinc oxide nanoparticles (ZnO NPs) because of their affordability and low toxicity in biological applications. This analysis reviews the most recent progress in molecular docking techniques for predicting the interactions between ZnO nanoparticles (ZnO-NPs) and biological macromolecules. It highlights the advancements in docking methods used to foresee these interactions, focusing on proteins that have shown favorable binding with zinc oxide nanoparticles, including human insulin (HI), Bovine Serum Albumin (BSA), and Acetylcholinesterase (AChE).

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TOPIC 3

Organic synthesis and catalysis





The Synthesis and Crystal Structure Determination of a Schiff Base Compound, along with DFT Calculations

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Keywords: Schiff Base; Crystal structures; Hirshfeld surface; TD-DFT

ABSTRACT

Schiff bases are an important class of organic compounds containing the $-C=N-$ (imine) functional group^{1,2}, typically formed by the condensation of primary amines with aldehydes or ketones. Due to their chelating properties, Schiff bases exhibit significant applications in coordination chemistry³, catalysis, and biological activity, as well as in corrosion inhibition⁴. In this study, a novel Schiff base compound, (E)-2-[(4-methoxynaphthalen-1-yl)methylidene]amino}-4-methylphenol ($C_{19}H_{17}NO_2$), was synthesized and characterized using NMR, IR, and UV–Vis spectroscopy. Hirshfeld surface analysis confirmed the dominance of dispersion forces in the crystal structure, where the molecule adopts a twisted conformation. The compound's anticorrosion potential was investigated using DFT calculations, revealing significant protective properties for iron and copper. The computationally optimized structure was compared with the crystallographically determined one, showing good agreement.

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Study of Stabilization and Degradation of rigid Poly Vinyl Chloride (uPVC).

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Keywords: Degradation; Mechanical properties; Polymers; PVC; Thermal stabilizer .

ABSTRACT

Poly(vinyl chloride) (PVC) is one of the most important commercial plastic materials, but it is thermally unstable at processing temperature. Processing of PVC at elevated temperatures requires the use of thermal stabilizers. Widely used thermal stabilizers for PVC incorporate toxic heavy metal and organotin compounds that have been severely criticized based on environmental concern. In order to address this problem, reduce costs, and improve physical and chemical properties, we tried to study the effect of stabilizers on mixtures (PVC) by adding different stabilizers percentages (2.5%-2.65%-2.8%-3%-3.2%). Using mechanical, thermal stability, FTIR and SEM tests. It was generally found that the PVC-based mixture had mechanical properties (breaking strength and elongation at break). The thermal stability of the PVC mixture increases with increasing ratio of stabilizers. Where this stability is up to 2.65%.

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Design and Characterization of PEHD-Based Bio-Composites

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Keywords: Biomaterial; Biodegradability; Polymers; Sustainable development.

ABSTRACT

The new approach to sustainable development as well as environmental requirements are driving current scientific efforts to be congruent with the challenges of this trend. Reducing or substituting synthetic plastics (conventional polymers) is a major concern. For this purpose, we have developed bio-composites based on high density polyethylene (HDPE) and starch reinforced with short alkali treated linen fibers. The linen fibers were modified by alkaline treatment to improve their adhesion with the matrix and to enhance the stiffness of the biocomposite. In addition, starch and linen fibers are renewable, inexpensive and biodegradable materials. Their use is therefore expected to reduce plastic waste, which is considered a worldwide environmental concern.

HDPE/starch/flax fiber preparations at different percentages were made using a two-step process: mixing and thermocompression. The structural, morphological, thermal and mechanical properties of these biocomposites were investigated using Fourier transform infrared spectroscopy (FTIR-ATR), X-ray diffraction (XRD), thermogravimetric analysis (TGA), differential scanning calorimetry (DSC) scanning electron microscopy (SEM), melt flow index (MFI), Izod impact tests, and uniaxial tensile strength tests.

FTIR-ATR spectra and SEM analysis of HDPE/starch blends revealed a reduced compatibility between HDPE and starch, which resulted in low MFI and elongation at break values. The introduction of the linen fibers in the blends improved crystallinity due to the nucleation effects of the starch on the HDPE crystallisation process. In addition, the density, resilience, stiffness and tensile strength of these materials recorded appropriate values due to the combined action of the linen fibres in providing mechanical anchorage as well as in transferring mechanical stresses through the HDPE/starch matrix.



Synthesis, FTIR Characterization, and Biological Evaluation of Two Imidazole Derivatives

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Keywords: Imidazole derivatives; Synthesis; One-pot reaction; Spectroscopic characterization; Bioactive; heterocycles

ABSTRACT

Imidazole-based compounds have garnered considerable attention due to their wide range of pharmacological properties. In this work, two imidazole derivatives were synthesized via a one-pot reaction involving benzil, aromatic aldehydes, and ammonium acetate under reflux conditions. The structures of the synthesized compounds were confirmed using Fourier-transform infrared (FTIR) spectroscopy, which revealed characteristic absorption bands corresponding to N–H, C=N, and aromatic C=C functional groups, indicative of imidazole ring formation. The biological activity of the compounds was evaluated through in vitro antimicrobial assays against selected Gram-positive and Gram-negative bacteria, as well as fungal strains. The results demonstrated promising antibacterial and antifungal activities, with notable inhibition observed particularly against *Escherichia coli* and *Candida albicans*. These findings support the potential of FTIR-confirmed imidazole derivatives as candidates for further antimicrobial development.

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Preparation of cellulose acetate from palm pollen sheath by chemical treatment

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Keywords: cellulose, cellulose acetate, palm pollen, esterification

ABSTRACT

In this research, cellulose acetate was synthesized from a locally available alternative source—palm pollen sheath—through a series of chemical treatments. Initially, the raw material underwent alkaline and acid treatments using 2 M NaOH and 2 M HCl solutions, respectively, to isolate cellulose. Analysis confirmed that the palm pollen sheath is rich in cellulose. In the subsequent stage, esterification was carried out using a mixture of acetic anhydride, glacial acetic acid, and concentrated sulfuric acid as a catalyst to convert the extracted cellulose into cellulose acetate. The resulting material was characterized by infrared (IR) spectroscopy to confirm its structure.

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TOPIC 4

Phytochemistry and medicinal plants





**Control of the Chickpea Weevil *Callosobruchus maculatus* F. (Coleoptera: Bruchidae)
Using Essential Oils Extracted from the Leaves of *Mentha longifolia* (L.) L. in the
Northern Algerian Sahara**

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Keywords: *Callosobruchus maculatus*, chickpea weevil, concentration, Essential oil, *Mentha longifolia*,

ABSTRACT

The oil extracted by distillation from the leaves of *Mentha longifolia*, an aromatic plant collected in the Guemar region, El Oued province, was tested against adult *Callosobruchus maculatus* weevils. The bioassay was conducted under controlled conditions at a temperature of $26 \pm 1^\circ\text{C}$ and a relative humidity of $70 \pm 5\%$.

The study assessed the insecticidal activity of three different concentrations of the essential oil (10 $\mu\text{l/l}$, 30 $\mu\text{l/l}$, and 50 $\mu\text{l/l}$). The results showed a significant toxic effect on *C. maculatus*, as mortality rates increased with both exposure time and concentration, reaching 100% at all tested doses. This suggests a strong potential for the essential oil as a natural insecticide.

The insecticidal activity may be attributed to bioactive compounds such as menthol and pulegone, which are known for their toxic effects on insects. The findings indicate that *Mentha longifolia* oil could serve as an eco-friendly alternative to synthetic pesticides, offering a biodegradable and less harmful option for pest control. However, further studies are required to identify the specific active compounds and evaluate their long-term efficacy and potential application in pest management programs.

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Exploring the potential of *Citrullus colocynthis* in pain management

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Keywords: Analgesic activity; *Citrullus colocynthis*; Hot Plate test; pain management; Writhing test.

ABSTRACT

Citrullus colocynthis (commonly known as the bitter cucumber or colocynth) is a plant traditionally used for various medicinal purposes, including pain relief. This study explores its analgesic potential through the Hot Plate and Writhing tests conducted on animal models.

The results showed a significant reduction in pain response in the treated animals compared to the control group. In the Hot Plate test, animals treated with *Citrullus colocynthis* extracts displayed an increased latency time before responding to thermal stimuli, suggesting a notable analgesic effect. Similarly, the Writhing test demonstrated a marked decrease in the frequency of writhing movements, indicating the plant's potential to alleviate nociceptive pain.

These findings support the idea that *Citrullus colocynthis* could be a promising natural remedy for pain management. However, further research is needed to isolate the active compounds and better understand their mechanisms of action in pain modulation.

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Development of a bandage based on smart moisture and acidity sensors from walnut extract

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Keywords: acidity; antibacterial activity; flavonoids ; moisture ; phenolics; Smart dressings ; walnuts ; wounds.

ABSTRACT

Wounds, especially chronic ones, are a health challenge that requires close monitoring to avoid complications and delayed healing. Hence, the need to develop smart monitoring systems capable of providing immediate indicators of wound condition emerges^[1,2].

To produce a bacteria-free medium, active compounds were extracted from walnuts using a water and ethanol solvent soak and placed in a cellulose film. The phenolic and flavonoid contents were then evaluated, in addition to electrochemical and chemical tests of the antioxidant TAC. The antibacterial activity was then tested against two types of wound-causing bacteria. Moisture content was tested using copper chloride, while acidity was tested using bromothymol blue.

The results showed that extracting walnuts in water yielded a 14% higher yield compared to ethanol, while the phenolic and flavonoid contents were higher in the ethanolic extract. Regarding antibacterial activity against *Pseudomonas aeruginosa* and *Staphylococcus aureus*, the ethanolic extract demonstrated a lethal effect at a concentration of 10 mg/ml, while the lethal concentration of the aqueous extract was 20 mg/ml.

These results reflect the potential of using walnut extract in the development of a natural medical dressing with antibacterial properties, enhancing its value in biomedical applications.

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Green Fabrication and Biological Evaluation of Zinc and Silver Nanoparticles Derived from Dual Medicinal Plants: A Combined ADMET, Docking, and Molecular Dynamics Approach

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Abstract:

The application of nanotechnology in biomedical fields presents significant potential, particularly through the green synthesis of nanoparticles which offers an environmentally friendly alternative to traditional methods. This research investigates the green synthesis of zinc and silver nanoparticles using plant extracts from two medicinal species, which function as both reducing and stabilizing agents. The synthesized nanoparticles were extensively characterized using various techniques, including UV-Vis spectroscopy, FTIR, SEM, TEM, XRD, and MEB, which provided critical data on their structural, morphological, and optical properties. *In vitro* biological assays were performed to evaluate their potential therapeutic effects. Additionally, *in silico* analyses, including ADMET profiling, molecular docking, and molecular dynamics simulations, were conducted to explore their pharmacokinetic properties, molecular interactions, and stability within biological systems. The findings from this study highlight the promising applications of green-synthesized nanoparticles in various biomedical domains, while emphasizing the importance of adopting sustainable practices in nanotechnology.

Keywords: *Green synthesis, Zinc nanoparticles, Silver nanoparticles, In vitro assays, In silico studies*

Les Plantes Médicinales Utilisées dans le Traitement du Cancer

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Mots-clés: Cancer ; El-oued ; Enquete ; Ephedra alata ; Phytothérapie.

RESUME

Le cancer constitue un problème de santé publique majeur en Algérie, avec une incidence en constante augmentation. Bien que les traitements conventionnels tels que la chirurgie, la chimiothérapie et la radiothérapie soient efficaces, ils engendrent souvent des effets secondaires significatifs. Ainsi, de nombreux patients se tournent vers les plantes médicinales comme alternative ou complément thérapeutique. Cette étude vise à évaluer la diversité des plantes médicinales utilisées dans le traitement du cancer dans la wilaya d'El-Oued, en Algérie.

Une enquête menée entre avril et mai 2024 auprès de 100 patients atteints de cancer et de 60 phytothérapeutes a permis d'identifier 23 espèces de plantes utilisées. Parmi les plus courantes figurent *Ephedra alata*, *Nigella sativa*, *Curcuma longa* et *Artemisia*. L'étude révèle que 73 % des patients utilisent la phytothérapie pour traiter le cancer, tandis que 27 % l'emploient pour atténuer les effets secondaires des traitements classiques. De plus, 81 % des phytothérapeutes estiment que ces plantes possèdent un potentiel thérapeutique contre le cancer.

Ces résultats mettent en évidence l'intérêt croissant pour la phytothérapie dans la prise en charge du cancer. Des recherches pharmacologiques supplémentaires sont nécessaires pour valider scientifiquement leur efficacité et leur innocuité.

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Comprehensive Phytochemical Analysis and Multiscale Antioxidant Evaluation of Essential Oils from Two Medicinal Plants: In Vivo, In Vitro, and In Silico Approaches

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Keywords: Essential oils, GC/MS analysis, Antioxidant activity, In silico approach, Oxidative stress

ABSTRACT

This study focuses on the extraction and characterization of essential oils from two medicinal plants and their antioxidant potential. The oils were obtained through hydrodistillation and analysed using gas chromatography-mass spectrometry (GC/MS) to determine their chemical constituents. Their antioxidant activity was assessed through in vivo and in vitro assays, evaluating their ability to neutralize free radicals and reduce oxidative stress. Additionally, an in-silico investigation, including molecular docking and molecular dynamics simulations, was conducted to explore their interactions with antioxidant-related enzymes. The findings provide valuable insights into the therapeutic potential of these essential oils in combating oxidative stress-related disorders.



Quantitative Study Of Medicinal Plant Of Phenolic Compounds By HPLC

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Keywords: Bioactive substances; Chromatographic analysis ; grain;HPLC; phenolic compounds ; Solanum nigrum L.

ABSTRACT

Phenolic compounds are commonly found in plants and have been reported to have several biological activities including antioxidant properties and are useful indicator

of potential nutritional benefit [1]. Experimental studies revealed that cells and organisms require defense against oxidants [2]. Free radicals such as hydroxyl radical and superoxide anion are produced as normal products of

cellular metabolism [3].Production of free radicals have been implicated to cause

several diseases [4]

Solanum nigrum L which are the most used in the studied area have been selected and quantitative study to assess the active substances by Chromatographic analysis of phenolic compounds by HPLC.

According to the HPLC results of grain of Solanum nigrum L plant is the richest of all the compounds used as standards such as Chlorogenic Acid that it is estimated 41747.722 µg/g for buotanol extract follow by EtACO Extract 240701.610 µg/g ,then chloroform extract 9072.854835 µg/g .According to the results obtained, it can be seen that the different extracts contain all the compounds used as standards with a high concentration.



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Comparative Phytochemical Analysis and Multimodal Assessment of Essential Oils from Two Medicinal Plants for Antidiabetic Potential: In Vivo, In Vitro, and In Silico Studies

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Keywords: Essential oils, GC/MS profiling, Antidiabetic evaluation, Computational study, Metabolic enzymes.

ABSTRACT

The present study explores the extraction and bioactivity of essential oils derived from two medicinal plants with potential antidiabetic properties. The oils were extracted using hydrodistillation and analyzed through gas chromatography-mass spectrometry (GC/MS) to determine their chemical composition. Their antidiabetic activity was assessed through in vivo and in vitro experiments, evaluating their effects on key metabolic enzymes. Additionally, molecular docking and molecular dynamics simulations were performed to predict their interactions with targets involved in glucose regulation. This comparative analysis provides new insights into the pharmacological applications of essential oils in diabetes management.



Phytochemical Analysis and Biological Effectiveness of *Tribulus terrestris* L Seeds Extracts

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Keywords: Extraction process; Flavonoids; Phenolics; *Tribulus terrestris* L.

ABSTRACT

The aim of this study is to extract and estimate the biological effectiveness of *Tribulus terrestris* L seeds. The seeds were ground and extracted with the following solvents: distilled water, ethanol, and a mixture of water and ethanol (3/7). A phytochemical survey revealed the following compounds: phenolics, alkaloids, flavonoids, and terpenes, and they were rich in these compounds.

After the extraction process, the extraction yield was calculated, and the extract of a mixture of water and ethanol had the highest value. After that, the phenols were quantitatively estimated the results showed that the capacity of the ethanolic extract was the highest value.

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Using Electrochemical Voltammogram Recording and chemometrics for classifying of algerian medicinal plant species

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Keywords: medicinal plant, chemometrics analysis, electrochemical method, DPV, PCA, HCA

ABSTRACT

Medicinal plants play a crucial role in agriculture and industry production, where it is the major source of biologically active substances used in the pharmaceutical preparations and pharmacotherapy, several studies have been conducted to make sure quality assurance the medicinal plants through applies many modern analytical techniques. In this study, easy and accurate analytical method were development to classification different plants using electrochemical method (differential pulse voltammetry (DPV)) coupled with chemometrics analysis. 89 samples of medicinal plants taken El-Oued region in Algerian were collected and analyzed using data DPV, principal component analysis (PCA) and hierarchical clustering analysis (HCA). Bioactive compounds such as flavonoids, phenolic acids have been description and used to classification plants, and based on these results, closely related plant species can be identified and distinction.

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Exploring Anti-Alzheimer Effects of Herbal Water Extracts: Integrated In Silico, In Vitro, and In Vivo Investigations into Neuroprotection

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Abstract:

The increasing prevalence of Alzheimer's disease necessitates the exploration of plant-based therapeutics as effective interventions. This study focuses on the water extracts of two medicinal plants, prepared using a green extraction approach. The extracts were characterized via liquid chromatography-mass spectrometry (LC/MS) to identify bioactive compounds potentially linked to neuroprotective effects. Comprehensive biological evaluations were conducted, including *in vivo*, *in vitro*, and *in silico* studies, to investigate the anti-Alzheimer potential. *In vivo* testing assessed behavioural and biochemical changes in an Alzheimer's disease model, while *in vitro* assays demonstrated acetylcholinesterase inhibitory activity and antioxidant properties. Furthermore, molecular docking and dynamic simulations provided insights into the interaction between key phytoconstituents and target proteins associated with Alzheimer's pathology. The results highlight the water extracts' promising therapeutic potential, paving the way for the development of plant-derived neuroprotective agents.

Keywords: *Alzheimer's disease, Neuroprotective agents, Medicinal plants, LC/MS characterization, Molecular docking*

Comprehensive Evaluation of Anticancer Activities in Medicinal Plant Extracts from Multiple Solvents: Insights from In Vitro Experiments and Computational Modeling

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Abstract:

The investigation of medicinal plants as sources of novel anticancer agents has attracted considerable attention, with solvent extraction methods playing a crucial role in enhancing the bioactive properties of plant-derived compounds. This study systematically explores the anticancer potential of multi-solvent extracts, including water, methanol, ethanol, butanol, chloroform, and hexane, from two medicinal plant species. *In vitro* assays were conducted to assess the cytotoxicity and apoptosis induction on cancer cell lines, while providing valuable insights into the efficacy of these extracts in modulating cancer cell behavior. Complementary *in silico* approaches, including molecular docking, ADMET profiling, and molecular dynamics simulations, were utilized to elucidate the interaction mechanisms, binding affinity, and pharmacokinetic properties of the active compounds present in the extracts. The results highlight the influence of solvent selection on the biological activity of plant extracts, with promising anticancer potential identified for future therapeutic applications.

Keywords: *Multi-solvent extraction, Anticancer activity, Cytotoxicity, Apoptosis, In silico studies*

Comparison of chemical composition of Retama reatam leaves grown in different ecosystems

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Résumé

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Comparative Study of Methyl Esters Purification Methods from Vegetable Oils: Process Optimization to Improve Final Product Quality

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Keywords: Biodiesel; Methyl Esters; Purification; Stability; Transesterification; Vegetable Oils.

ABSTRACT

Purification of methyl esters (biodiesel) is essential for ensuring fuel quality. This study compares water washing, vacuum drying, adsorbents, and vacuum distillation for removing impurities like glycerol, catalyst residues, and soaps. Results show that vacuum distillation provides the highest purity but is energy-intensive, while water washing is more economical but raises wastewater concerns. Optimizing purification processes is key to improving biodiesel quality and promoting its industrial adoption.

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