

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



# 1<sup>st</sup> Study Day on Applied Chemistry and Environmental Engineering

**SDACEE-2024**

**April, 22, 2024**

## **BOOK OF ABSTRACTS**



**Includes 02 Plenary Conferences with 4 Oral  
and 31 Poster Presentations**



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**SDACEE  
2024**  
El-Oued, Algeria



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## **DESCRIPTION**

The SDACEE-2024 is part of the program of activities realized by the Department of Chemistry in cooperation with the research laboratory "LACE" in order to motivate researchers, especially PhD students, to present the results of their works and to discuss them with various categories of researchers.

The book of abstracts of SDACEE-2024 presents a summary of 2 plenary conferences with 4 oral and 31 poster presentations.

This book includes recent and original works realized in the field of Applied Chemistry and Environmental Engineering. The huge part of this book was devoted to the researches of Chemical depollution and environmental protection topic because of its importance in the subject of the event. It also covers an important topic in Applied Chemistry like organic synthesis according the ecofriendly methods. Two others topic are devoted to the pharmaceutical chemistry and drug discovery with 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 would like to thank Pr. Ferhati Omar rector of the university of El-Oued and Pr. Mansour Abdelouahab dean of the faculty of exact sciences. Also, we thank all the scientific and organizing committee members of SDACEE-2024 for their efforts and support. We would like to thank the laboratory "Applied Chemistry and Environment" for their contribution. We would like to express our deep gratitude to Keynote Speakers Pr. Delimi Rachid (Univ. Annaba) and Pr. Achi Fethi (Univ. Ouargla) for their valuable contribution. We would like to extend our sincere thanks to all participants for their contribution to SDACEE-2024.

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# **ABSTRACTS OF PLENARY SESSIONS**



## Traitement des eaux usées par les procédés d'oxydation avancée électrochimique

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**Keywords:** Polluants émergents; Oxydation avancée; Oxydation électrochimique; Oxydation anodique; Electro-Fenton.

### RÉSUMÉ

La présence de des polluants émergents récalcitrants dans l'environnement constitue un grave problème de santé environnementale principalement en raison de leur toxicité. Du fait de leur complexité structurale et de leur toxicité, la plupart de ces composés ne sont pas biodégradables et ne sont donc pas éliminés dans les filières classiques de traitement des eaux telles que les procédés physico-chimiques, chimiques, biologique. Les recherches actuelles s'orientent vers des techniques plus efficaces pour le traitement de ces nouveaux polluants organiques faisant ainsi appel aux procédés d'oxydation avancée (POAs) parmi lesquels le traitement électrochimique par électro-Fenton et oxydation anodique se révèle particulièrement prometteur.

La nécessité de travailler en électro-Fenton homogène à pH inférieur à 4 et d'optimiser la quantité du catalyseur a été surmontée par la mise au point de l'électro-Fenton hétérogène (E-F hét). L'E-F hét utilise des source de catalyseur solide (hématite, la magnétite, goethite, la pyrite..). Récemment, des matériaux cathodiques modifiés ou fonctionnalisés à base d'oxydes de fer et/ou de métaux de transition ont été préparés à l'aide de diverses techniques en vue d'une application dans le processus hétéro-électrochimique. Dans ce cas, la cathode remplit une double fonction : contre-électrode pour produire H<sub>2</sub>O<sub>2</sub> et source de fer (catalyseur). Très récemment, on a développé le procédé EF tridimensionnel, dans lequel un certain nombre de particules sont placées entre les électrodes bidimensionnelles traditionnelles. Les particules sont polarisées pour former d'innombrables microélectrodes.

L'oxydation anodique (OA) est un procédé d'oxydation avancée électrochimique aussi populaire que l'EF. Dans l'OA, à un certain potentiel l'eau s'oxyde à la surface de l'anode pour former des radicaux hydroxyles et la rencontre de ces radicaux avec les composés organiques conduit à la dégradation ou minéralisation de la solution selon la nature de l'anode. Les POAs électrochimiques sont des procédés écologiques, puisque utilise peu ou n'utilise de produits chimiques. Ils ont été appliqués avec succès au traitement des eaux polluées par des herbicides à base d'acide chlorophénoxy, aux colorants synthétiques, aux PPCP, etc.





## **Applied Nanomaterials Chemistry for the Detection of Cancer Biomarkers and Pollutants: New strategies and recent applications.**

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**Key words:** Cancer biomarkers, electrochemical sensors, pollutants, nanomaterials.

### **ABSTRACT**

Constructing micro-analytical tools for monitoring cancer biomarkers and pollutants using functional nanomaterials can contribute to environmental safety and healthcare diagnostics. Electrochemical sensors are devices constructed for real-time monitoring and advances in nanomaterial synthesis highly improve their catalytic properties. This conference aims to discuss the recent strategies of nanocomposite preparation and chemical functionalization of the sensing platforms. Additionally, we present the recent advancements in strategies for developing cancer biomarker-based nanobiosensors and their current challenges were addressed.

# **ABSTRACTS OF ORAL PRESENTATIONS**



## Photocatalytic Degradation Of Eosin Y Induced By Iron Nanoparticles In Heterogeneous Phase

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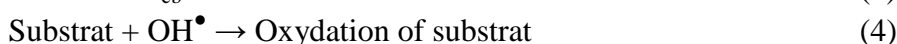
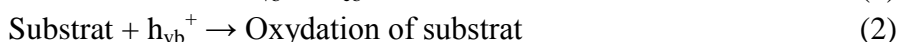
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**Keywords:** Eosin Y, Goethite, Iron (III) oxyhydroxide, Nanoparticulate, Photo degradation.

### ABSTRACT

The presence of pharmaceuticals and personal care products in aquatic environments is a well-recognized issue with uncertain consequences. Wastewater containing Eosin Y (EY) poses environmental challenges due to its color and toxicity [1]. Traditional methods like phase transfer and biological treatment are ineffective in degrading EY because of its complex aromatic structure and stability.

Studies have shown that oxyhydroxides of Fe (III), when exposed to light, are highly efficient in reducing water pollution (as indicated by equations 1-4) [2].



The study explored the degradation of Eosin Y (EY) in a water-based solution in a heterogeneous phase using nanoparticulate Iron (III) oxyhydroxide (NGO). It was divided into two parts: a thermal study and a photochemical study. In the photochemical study, the NGO-EY system was subjected to 365 nm light, while various parameters like pH, substrate concentration, and the presence of NGO were investigated. This research demonstrates the effectiveness of removing EY in a heterogeneous phase by exciting iron (III) hydroxides and underscores the photoinductive role of iron (III) oxides.

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## **In silico ADME, toxicological analysis, molecular docking studies and Molecular dynamics simulation of Afzelin with potential antibacterial effects against Staphylococcus aureus**

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**Keywords:** afzelin, Antibacterial Activity, Binding energy, Molecular Docking

### **ABSTRACT**

Afzelin has been designed and tested for its in silico antibacterial activity against DNA gyrase complex of Staphylococcus aureus. The results of the toxicity study indicate that afzelin displayed moderate antibacterial potential against staphylococcus aureus with LD50 = 5000 mg/Kg, which is almost four times and a half weaker than that obtained for the commercial antibiotic chloramphenicol. The afzelin and the commercial antibiotic chloramphenicol were subjected to docking studies to understand their interaction with DNA gyrase complex of Staphylococcus aureus. Results indicated a good affinity of afzelin to the chosen target with the formation of four hydrogen bonds and binding energy of -29.82 kJ/mol. ADME study shows that afzelin is not inhibitors of CYP450 IA2, 2C19, 2C9, 2D6, 3A4 isoenzymes which suggests a decrease in their plasma concentrations and a rapid elimination route. Molecular dynamics simulations were performed for 10 ns for afzelin using the Gromacs package to assess the conformational stability of protein-ligand complexes during the simulation.

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Approach to in Silico Drug Repurposing for Inflammatory Bowels Disease by Targeting TNF Alpha. *J. Biomol. Struct. Dyn.* **2023**, *41*, 3462–3475.



## Muscovite Clay for Methylene Blue Removal: Advanced Optimization and AI-guided Breakthroughs

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**Keywords:** Muscovite, Methylene blue, Adsorption, Box–Behnken design, RSM, ANN-GWO

### ABSTRACT

This study assesses the effectiveness of muscovite mineral clay as an adsorbent for removing Methylene Blue (MB) from aqueous solutions. The research explored how initial MB concentration, adsorbent mass, and time influence the MB removal process. Two modeling techniques, Box-Behnken design with response surface methodology (BBD-RSM) and Artificial Neural Network (ANN), were utilized to accurately predict MB removal efficiency. Both RSM and ANN models produced satisfactory results in estimating MB removal efficiency. To further optimize the process, both conventional and techno-economic methods were applied. The conventional method focused on maximizing dye removal efficiency (R), while the techno-economic approach considered multiple objectives. Comparative analysis showed that the techno-economic optimization method surpassed the conventional method. This study underscores the importance of considering multiple objectives and integrating techno-economic factors in optimizing clay adsorption processes. The successful implementation of the techno-economic optimization approach demonstrates its potential as a robust method, especially in wastewater treatment. The findings offer valuable insights for optimizing adsorption and advancing environmental remediation practices.



## Elimination d'un colorant alimentaire "Tartrazine" dans les eaux par les procédés électrochimiques.

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**Keywords :** Eaux usées, procédés électrochimiques, rayonnement solaire, tartrazine, colorants alimentaires.

### ABSTRACT

La caractérisation des eaux résiduaires colorées des industries agroalimentaires, par l'analyse d'un certain nombre de paramètres physico-chimique et microbiologique, a montré la nécessité de traiter ces eaux.

Dans ce travail nous avons opté pour des traitements électrochimiques tels que l'électrocoagulation et l'électro-Fenton. Comme il est compliqué de contrôler l'efficacité du traitement (décoloration) par le contrôle de tous les paramètres, nous avons opté de suivre la coloration en tant que paramètre représentatif du décoloration de l'eau étudiée. L'efficacité du traitement a atteint un taux supérieur à 99 % avec une densité de 4.76 mA/cm<sup>2</sup> et un taux similaire (>99%) avec une densité de 2 mA/cm<sup>2</sup> par EC et EF consécutivement, un temps d'électrolyse de 90 min, pH de la solution égale 3, et ce pour le procédé d'EF, mais uniquement pour le paramètre de décoloration. Alors le pH optimal pour l'EC est proche de la neutralité (6.5 à 7). Par ailleurs, une meilleure optimisation de ces procédés électrochimiques nécessite le l'étude de tous les facteurs clés dans le processus d'oxydation soit pour l'EC ou l'EF tels que la concentration en catalyseur Fe<sup>2+</sup> et celle de l'eau oxygénée H<sub>2</sub>O<sub>2</sub> en solution pour l'EF, la nature de l'électrolyte support, l'espace inter-électrode pour l'EC.

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# **ABSTRACTS OF POSTER PRESENTATIONS**



# **TOPIC 1**

## **Chemical depollution and environmental protection**



## Effect of ZnO NPs various source on photocatalysis of methylene blue dye

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**Keywords:** ZnO NPs, photocatalytic degradation, photocatalytic activity, AZO dye.

### ABSTRACT

The effect of ZnO NPs as a source on the photocatalysis of methylene blue dye involves exploring how ZnO NPs, when used as photocatalysts, enhance the degradation of methylene blue (MB) dye under light exposure. This process is important for environmental applications and wastewater treatment, because it provides a promising way to remove harmful dyes from water bodies. Different sources of chitosan have been used to synthesize ZnO NPs, namely chitosan from *Streptomyces griseus*, crab shells, and shrimp shells. Photocatalytic efficiency was studied by a MB photolysis assay. In comparison to ZnO NPs with greater band gap values, those with smaller band gap values demonstrated superior antibacterial activity. At a contact duration of 60 minutes, the MB dye removal of ZnO (*Streptomyces griseus*), ZnO (shrimp shells), and ZnO (crab shells) reached 44%, 66%, and 56%, respectively.

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## Exploitation of Organic Waste in Water Treatment

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**Keywords:** silica; Organic Waste; photocatalysis.

### ABSTRACT:

Effective management of organic waste is a pressing global challenge, particularly in the context of wastewater treatment. Traditional methods of wastewater treatment often involve high energy consumption and produce substantial amounts of secondary pollutants. In recent years, there has been growing interest in exploring the potential of utilizing organic waste in water treatment processes as a sustainable and cost-effective alternative. The production of bio-based silica nanoparticles is among the available agricultural bio-resources. We used cocoa shells as a precursor to make bio-based silica nanoparticles in this study. The yield of silica extraction was 72-80%. Water was treated by photocatalysis of methylene blue dye, where in a contact period of 60 minutes, the removal of methylene blue dye from silica nanoparticles reached 56%.

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## Green Energy Gold: Maximizing Biofuel Potential from Used Vegetable Oils.

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**Keywords:** Biodiesel; Ecosystems; Renewable Biofuel; Used Vegetable Oils.

### ABSTRACT

The exploration of repurposing used vegetable oils holds significant significance for both environmental conservation and energy sustainability. Repurposing these oils presents an effective strategy for reducing waste and mitigating their adverse effects on aquatic and terrestrial ecosystems. Moreover, leveraging used oils opens doors for the production of methyl esters, particularly for biodiesel, a renewable biofuel offering numerous advantages such as mitigating greenhouse gas emissions and reducing reliance on fossil fuels. However, ensuring the quality and efficacy of biodiesel derived from used oils necessitates establishing usage limits based on their degradation level. These thresholds are essential in preventing excessive oil deterioration and ensuring optimal yields during methyl ester production. Thus, this research underscores the vital importance of harnessing the potential of used vegetable oils, not only for environmental conservation but also for the sustainable advancement of biofuel production. Through the establishment of appropriate usage limits, we can maximize the utilization of used oils while minimizing their ecological footprint, paving the way for a cleaner and more sustainable energy landscape.

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## Numerical Assessment of Soft Soil Reinforcement with Recycled Aggregates in Granular Columns for Pollution Mitigation and Environmental Protection

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**Keywords:** Bearing capacity; Granular column; Numerical analysis; Soft Soil; Recycled aggregates;

### ABSTRACT

This study introduces an innovative eco-friendly approach for soil remediation and reinforcement, aiming to mitigate pollution and protect the environment. Utilizing recycled aggregates within granular columns, the method enhances soil stability and reduces environmental contaminants. Through numerical assessment, the technique's effectiveness in minimizing soil pollutants and promoting sustainable soil management practices is evaluated.

Furthermore, the research emphasizes the significance of recycled aggregate materials in soil reinforcement, comparing their efficacy to natural aggregates. Employing the finite element method in PLAXIS 3D software, soft soil treated with various granular columns is analyzed. Results show that recycled aggregate columns exhibit threefold higher bearing capacity than natural aggregate columns. These findings, presented through load-settlement graphs, provide valuable insights for implementing this technique in soil remediation and reinforcement projects. This study underscores the importance of eco-friendly solutions in addressing soil remediation challenges and advancing environmental preservation.

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## Photocatalysis of methylene blue dye by ZnO/gelatin nanocomposite

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**Keywords:** Gelatin; ZnO NPs; Photocatalysis; Degradation.

### ABSTRACT

Gelatin is a protein bioactive substance obtained from the hydrolysis of collagen obtained from the bones, skin, and mammals such as cattle, fish, and poultry. In this study, a nanocomposite based on gelatin extracted from chicken waste was synthesized and characterized by FTIR, and UV-Vis results. The results showed a gelatin extraction yield of 10 %. In addition, the photocatalytic efficiency was studied by a methylene blue photolysis assay, and the removal of MB dye from ZnO@gelatin nanocomposite reached 85% at a contact time of 90 min, and the initial dye concentration was as low as  $6 \times 10^{-5}$  M.

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## Phytoepuration of wastewater by the Saharan plant (*Traganum nadatum*)

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**Keywords:** Phytoepuration, Saharan Plant, Pollutants, Wastewater, El-Oued

### 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 *Traganum datum* 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 *Traganum* 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 *Traganum* 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 *Traganum* 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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## **Risques environnementaux dans le bassin urbain de Saïda, Algérie : Analyse de la pollution des sédiments provenant de l'assainissement urbain en temps de pluie**

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**Mots clés** : Pollution urbaine ; Contamination ; Métaux lourds ; Enrichissement ; Risque écologique.

### **Résumé**

Dans cette étude, une analyse mise à jour a été réalisée sur la pollution urbaine dans le bassin versant de la ville de Saïda, situé dans le Nord-Ouest de l'Algérie. Nous nous sommes concentrés sur la présence de métaux lourds et de pollution organique dans les sédiments provenant de l'assainissement urbain. Les résultats comprennent l'identification, la qualification et la quantification de ces polluants. La teneur totale en métaux traces dans les échantillons de sédiments a été analysée et comparée aux valeurs standards et de référence. Les résultats en mis en évidence le processus de génération et régénération de la pollution dans le bassin urbain, qui dépend des évènements pluvieux et de la période d'extraction des sédiments. L'évaluation de la pollution a été réalisée à l'aide d'indices et de facteurs de pollution. Les résultats indiquent que les concentrations de Chrome, Plomb, Cadmium, Zinc, Cuivre, Nickel et Cobalt dans les échantillons de sédiments prélevés, dépassent largement les valeurs de référence de toxicité, ce qui suggère une forte pollution des sédiments étudiés. Les valeurs du facteur de contamination et de l'indice de géo-accumulation montrent que le Cadmium, présente une très forte contamination, tandis que les valeurs associées au Plomb, Cuivre et le Chrome montrent une contamination modérée à forte. Quant au Zinc et le Nickel, leurs valeurs de l'indice de géo-accumulation exhibaient une faible contamination. En revanche pour le Cobalt et le Fer, les sédiments ne présentent pas de contamination. Toutefois et en référence aux valeurs du degré de contamination, les sédiments s'avèrent fortement pollués. Les résultats révèlent également que les valeurs des facteurs d'enrichissement dépassent la valeur critique, révélant un enrichissement d'origine anthropique. Les mêmes résultats mettent en évidence un risque écologique certain associé aux sédiments, avec un indice de risque potentiel sévère. Cette étude fournit des données de base précieuses sur la dynamique et les risques de la pollution dans le bassin versant de Saïda.

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## Silica-Based Biofilms in Water Treatment

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### ABSTRACT

Silica-based biofilms have emerged as a promising solution in water treatment due to their unique properties and versatile applications. These biofilms are formed by microbial communities on silica substrates, offering advantages such as biocompatibility, surface reactivity, and customizable porosity. Their effectiveness in pollutant removal, including heavy metals, organic contaminants, and pathogens, from water sources has been demonstrated. Silica-based biofilms also play a crucial role in advanced water treatment processes like membrane filtration and adsorption. Recent advancements in integrating nanomaterials and biofunctionalization techniques have further enhanced their performance. However, challenges remain in optimizing biofilm architecture and operating conditions for scalable and sustainable water treatment solutions. Despite these challenges, the potential of silica-based biofilms in addressing water pollution and scarcity underscores their importance in advancing environmental sustainability and public health.

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## Valorisation d'un Déchet des Palmiers Dattiers dans L'élimination des Colorants des Solutions Aqueuses: Isothermes d'Adsorption, Etudes Cinétiques et Thermodynamiques

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**Keywords:** Adsorption ; Cristal violet ; Matériau lignocellulosique ; Méthyle orange ; Tiges de palmiers dattiers.

### RESUME

Ce travail porte est une étude comparative de l'adsorption des deux colorants organiques différents (anioniques : Méthyle Orange (MO) et cationiques : Crystal Violet (CV)) sur la poudre de tiges de palmiers dattiers (TPD). L'analyse morphologique et spectroscopique par FTIR, XRD, SEM-EDS montre la structure du matériau adsorbant et confirme également l'adsorption des colorants étudiés.

L'influence de quelques paramètres opératoires sur le processus d'adsorption montre que les masses optimales de TPD sont respectivement de 1 g et 3 g pour le CV et le MO. Les résultats obtenus montrent que la quantité adsorbée ( $Q_{ads}$ ) pour toutes les concentrations initiales étudiées ( $C_0=25-150$  mg/l) est importante dès le début du temps de contact. Le temps d'équilibre est environ 45 minutes dans tous les cas. L'adsorption du MO est très favorisée en milieu acide. Cependant, la variation du pH n'influence pas sur l'adsorption du CV. L'augmentation de la température de 20 °C à 55 °C augmente légèrement l'adsorption du CV. L'étude cinétique montre que le modèle du pseudo-second-ordre et le modèle cinétique d'Elovich sont très adaptés pour expliquer le processus d'adsorption des colorants. La modélisation de l'isotherme d'adsorption a prouvé que l'adsorption des deux colorants suit le modèle de Freundlich, où  $R^2$  était de 0,9815 pour MO et de 0,9035 pour CV.

En effet, les résultats des expériences réalisées dans des conditions optimales montrent que les taux d'adsorption du CV et du MO sur TPD arrivent à 90,4 % et 57,41 % respectivement.

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## Synthesis of cellulose/ZnO nanocomposite from peanut and pea shells and application on the removal of toxic pollutants from aqueous solutions

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**Keywords:** *Arachis hypogaea*, *Pisum sativum*, Cellulose, Nanocrystalline cellulose, zinc oxide, Adsorption.

### ABSTRACT

The objective of this study is to valorise the Peanut (*Arachis hypogaea*) and pea (*Pisum sativum*) shells and use them as crude material to produce nanocrystalline cellulose. This compound was prepared by extracting pure cellulose (Cs) from the residues and converting it into nanocrystalline cellulose (CNCs), as well as hybridizing this substance with zinc oxide (ZnO) using two different methods. In order to study the properties of these new materials and validate their nature, several characterisation techniques were used, including optical (UV-visible, FTIR), structural and morphological (XRD, SEM) techniques. The analysis results showed that the crystal size of the compound (CNC/ZnO NPs) varied between 19.64 and 27.31 nanometers, while the gap bands ranged between 3.27 and 3.66 eV for the two methods used. The materials prepared were applied as adsorbents to remove methylene blue dye from aqueous solutions, and the adsorption was studied as a function of different physical and chemical parameters. According to the obtained results, these materials exhibited high adsorption capacity, indicating that they can be applied as economical substitutes for adsorbents.

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## **Application de couplage coagulation, floculation, adsorption et chloration pour élimination du tryptophane organique dans l'eau distillée et l'eau de mer**

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**Keywords :** Tryptophane ; Eau de mer ; Sulfate d'aluminium ; Charbon actif; eau de Javel.

### **ABSTRACT**

Ce travail vise à trouver des solutions de purification de l'eau chargée de composé organique le tryptophane qui affectent la santé des organismes vivants sur terre, y compris la santé humaine. Ce produit toxique, lorsqu'il est présent dans l'eau, même à faibles concentrations, affectent l'environnement en général et l'homme en particulier. Pour remédier à ce problème, nous avons utilisé plusieurs procédés d'élimination de ces polluants en eau distillée, en eau de mer. Dans le procédé de coagulation-floculation, le sulfate d'aluminium est utilisé comme coagulant pour l'élimination de composé organique le tryptophane. La dose optimale du coagulant et le pH du milieu de dilution peuvent affecter sensiblement le rendement d'élimination, et sont des paramètres à étudier et analyser. Dans le procédé d'adsorption, deux adsorbants ont été utilisés, le charbon actif commercial, le charbon actif préparé à partir des pelures des petits pois. L'objectif ici est de déterminer les paramètres et les caractéristiques des charbons actifs, commercial ou d'origine végétale, influant sur la capacité d'adsorption et le rendement d'élimination de TRY. La chloration est un procédé d'oxydation et de désinfection de l'eau avec de l'hypochlorite de sodium (eau de Javel). Pour ce faire, trois procédés sont combinés, la coagulation, l'adsorption et la chloration, en utilisant des doses optimales de coagulant, une valeur massique optimale des charbons actifs et des doses variables de chlore afin d'améliorer le rendement d'élimination de TRY.

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## Physicochemical And Microbiological Characterization Of Iron Ore Treatment Sludge From The “Ferphos” Complex: Proposals For Valorization

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**Keywords :** Characterization, Physicochemical, Microbiological, Valorization

### ABSTRACT

The physicochemical and microbiological characterization tests of the decanted sludge from the buffer basin of the “FERPHOS” iron ore complex showed a questionable risk of metallic cadmium toxicity, particularly in terms of phytotoxicity in the case of spreading this sludge into the soil. The absence of parasites which represent high health and environmental risks supports the idea of treating this sludge at low cost. However, in-depth analysis for other metals (chromium, nickel, etc.) and other forms sporulated on fresh sludge kept in conditions less hostile to analysis, would give a fairer idea of this cost. Furthermore, the residual mass concentration found ~650 mg of P<sub>2</sub>O<sub>5</sub>/kg of dry sludge is non-negligible and could increase by accumulation over time. The experiment of doping the mud with phosphorus 5, 10 and 20% carried out with the aim of observing the limiting microbial aspect of phosphorus, did not give the expected results since the absence of germs was total for all the samples. This result is encouraging for the continuation of the experimental study with the aim of possible valorization of the mud studied.

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## Equilibrium, Kinetics and Thermodynamics investigations of Illite kaolinite local clay from El Oued- Algeria, removing methyl orange dye from aqueous solutions

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**Keywords:** Illite kaolinite clay; Methyl orange; Adsorption mechanism; Isotherm and Kinetics models;

### ABSTRACT

In this study, the adsorption behavior of methyl orange dye from its aqueous solutions was investigated onto natural Illite kaolinite clay. A series of experiments were undertaken in a batch adsorption technique to access the effect of the process variables i.e. initial dye concentration, contact time, initial pH, adsorbent dose and temperature. The adsorption capacity of basic dye was higher (40 ppm) with the Lower value of the temperature (286,82 K), adsorbent dosage (50 mg) higher values at pH (10) and the equilibrium in the solution was observed within (30 min) which indicated by UV-Visible absorption spectroscopy technique. The equilibrium data for adsorption were fitted to the Langmuir isotherm ( $R^2 = 0,99$ ). The thermodynamic parameters  $\Delta G^\circ$ ,  $\Delta H^\circ$ , and  $\Delta S^\circ$  have been calculated (-10.310.131 kJ mol<sup>-1</sup>, 29.3 kJ mol<sup>-1</sup>) respectively. A pseudo-second-order kinetic model could be fitted to the experimental data ( $R^2 = 0,956$ ). A pseudo-second-order kinetic model could be fitted to the experimental data ( $R^2 = 0,96$ ).

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## Adsorption of Bezathren red dye onto activated illite clay from aqueous solutions

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**Keywords:** Activated, Adsorption, Bezathren red, Clay, Pollutants

### ABSTRACT

The aim of this work is to use local clay of our region as an available and inexpensive natural material to remove a pollutants from aqueous solutions by means of an adsorption process. As a start, the clay was purified to obtain clay minerals with a diameter of less than 2 $\mu$ m and then activated, after that the physiochemical properties of the clay were studied: spectroscopy analyzes by FTIR and DRX, then the possibility of adsorption of activated clay samples to the Bezathren red dye as a pollutant in their aqueous solutions by batch method by changing factors such as concentration, contact time, pH and temperature, thermodynamic factors such as  $\Delta G$ ,  $\Delta H$ ,  $\Delta S$  were also determined.

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## Synthesis of Schiff's base-Chitosan /ZnO composite for effective removal of Congo Red dye

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**Keywords:** Chitosan; Schiff's base; ZnO; Adsorption; Congo Red dye;

### ABSTRACT

Minimizing environmental pollution in all its forms has become a distinctive fingerprint that seeks to achieve it by any researcher. In this respect, the aim of this participation is to introduce proposal to maintain the environment. A hybrid composite biopolymer of Schiff's base-Chitosan/ZnO (Ch-Be/ZnO) was prepared to be an effective composite biosorbent for the removal of Congo Red dye (CR) from aqueous media. The adsorbent was characterized using BET, FTIR, SEM, and adsorption study. The influence of four processing factors, including Ch-Be/ZnO dose (0.04–0.1 g), pH solution (4–10), temperature (C: 30–50 °C), contact time (10–30 min), and their interactions on the removal rate of CR dye, was examined using the response surface methodology integrated with Box-Behnken design (RSM-BBD). Analysis of variance (ANOVA) showed the F-value of model and the corresponding p-value are 35.24 and < 0.0001. The results show that the highest CR dye removal (96.17%) was noticed by significant interaction effect between AC (adsorbent dose x time, p-value = 0.0458). The optimum conditions of adsorption process parameters were pH = 4, adsorbent dose (0.1g), temperature (40 °C) and time (20 min). The output of the research work indicates that Ch-Be/ZnO can be applied as a promising adsorbent for CR dye removal from contaminated water.

## **TOPIC 2**

# **Pharmaceutical chemistry and drug discovery**



## Chemical Composition, FT-IR-analysis and antibacterial activité of a medicinal plant extract belong to the Cistaceae family

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**Keywords:** : Polyphenols ; Flavonoids ; strains ; antibacterial activity

### ABSTRACT

The objectif of this work was to evaluate the antioxidant and antibacterial activities of the n-butanolique extract of .Total phenols,Flavone and flavonol were quantified spectrophotometrically .The antioxidant activity of this plant was estimed by the DPPH free radical scavenging and total antioxidant capacity .The results of the quantitative analysis (Polyphenols were estimated by the Folin –Ciocalteu method· Falvonoids were estimed by the alminum trichloride method AlCl<sub>3</sub>.reveals that the nBuOH extract is the richest in total Polyphenols and flavonoids ,with values were 295 mg GAE/g of extract and 72.00 mg QE/g of extract ,respectively it has been confirmed by FTIR spectrum with the presence of a hydroxyl group at 3201.07 cm<sup>-1</sup> After that , The n-butanol extract inhibited the DPPH with 50% at a concentration of 105.84ug/ml of extract . The evaluation of antibacterial activity of this plant using the ifussion method in agar medium, it was tested against Three ATTC bacterial strains,Two Gram-negative (pseudomonas aeruginosa ,Escherichia coli) ; and one Gram positive (Staphylococcus aureus),The results show that the n-butanol extract was found an antibacterial power dose dependent against the three ATTC strains tested.



## In silico prediction of ADME properties of as17 $\beta$ -HSD3 inhibitors molecules

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**Key words:** 17 $\beta$ -HSD3, *in silico*, PubChem, SwissADME, Enzyme.

### ABSTRACT

The 17 $\beta$ -HSD3 enzyme plays a key role in the treatment of prostate cancer, and small inhibitors can be used to efficiently target it. This enzyme has therapeutic properties whose effectiveness has been proven by many studies. It is rich in biologically active components that can be exploited in the development and manufacture of medicines.

In the present study, we concentrated on the study of *in silico* prediction of ADME properties of 12 compounds as 17 $\beta$ -HSD3 inhibitors using PubChem and SwissADME. The results showed that the majority of these compounds respond to physicochemical parameters, have a better ADME profile, and good oral bioavailability, and are therefore good candidates to support new drug discovery efforts.

## Computer-Aided Strategy on 5-(Substituted Benzylidene) Thiazolidine-2,4-Diones to Develop New and Potent PTP1B Inhibitors: QSAR Modeling, Molecular Docking and ADMET

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**Keywords:** thiazolidine-2,4-dione; QSAR; MLR; PTP1B; Molecular docking; ADMET

### ABSTRACT

A set of 5-(substituted benzylidene) thiazolidine-2,4-dione derivatives was explored to study the main structural requirement for the design of protein tyrosine phosphatase 1B (PTP1B) inhibitors. Utilizing multiple linear regression (MLR) analysis[1-2], we constructed a robust quantitative structure–activity relationship (QSAR) model to predict inhibitory activity, resulting in a noteworthy correlation coefficient ( $R^2$ ) of 0.942. Rigorous cross-validation using the leave-one-out (LOO) technique and statistical parameter calculations affirmed the model's reliability, with the QSAR analysis revealing 10 distinct structural patterns influencing PTP1B inhibitory activity. Compound 7e(ref) emerged as the optimal scaffold for drug design. Seven new PTP1B inhibitors were designed based on the QSAR model, followed by molecular docking studies to predict interactions and identify structural features. Pharmacokinetics properties were assessed through drug-likeness and ADMET studies[3-4].

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## Synthesis, Characterization, Antioxidant and Anti-inflammatory Activities of Functionalized Graphene Oxide Nanoparticles with 2-(Ferrocenylmethylamino)Benzonitrile

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**Keywords:** Graphene Oxide; GO@APTES@FcB2CN; functionalization; Antioxidant activity; Anti-inflammatory activity; Aspirin.

### ABSTRACT

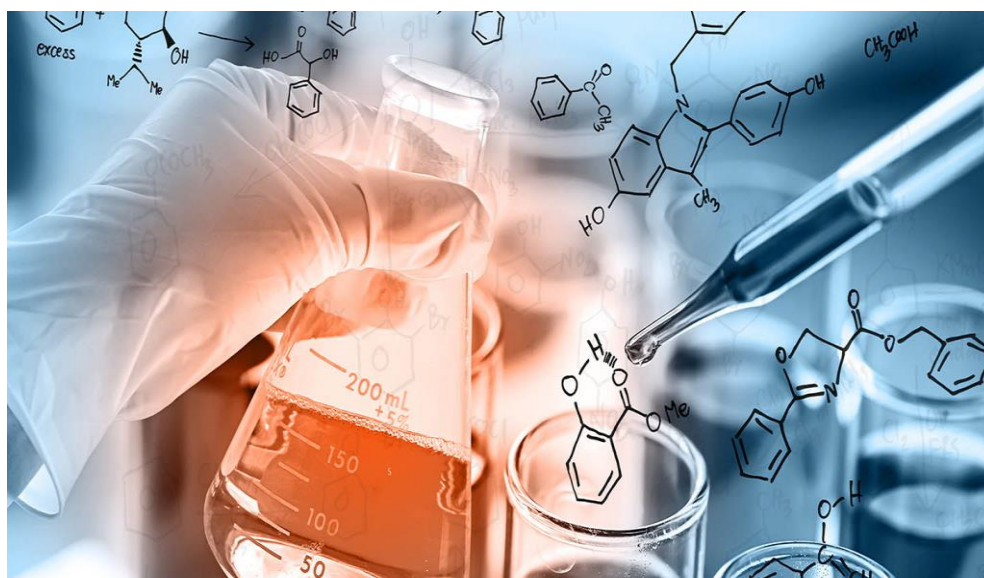
The current research aims to synthesize a new GO@APTES@FcMB2CN nanocomposite to find their antioxidant and anti-inflammatory activities. Graphene Oxide (GO) nanoparticles were successfully produced utilizing a modified Hummers process. These nanoparticles were then functionalized with 2(ferrocenylmethylamino) benzonitrile (FcMB2CN) using (3-aminopropyl)triethoxysilane (APTES) as a linker. The produced nanocomposite underwent characterization using several methods, including X-ray diffraction, Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), and Raman spectroscopy. The nanocomposite's antioxidant capacity was assessed using a DPPH test, and the IC<sub>50</sub> value was measured as 78.30 µg/mL. The anti-inflammatory potential of the nanocomposite was evaluated by measuring its ability to prevent protein denaturation. The results showed that the nanocomposite inhibited protein denaturation in a dose-dependent manner, with the highest inhibition observed at a dosage of 800 µg/ml. Conclusion: The present investigation has found that the FcMB2CN nanocomposite exhibits antioxidant and anti-inflammatory activities.

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## **TOPIC 3**

# **Organic synthesis and catalysis**



## Synthesis of FePO<sub>4</sub> modify by Nickel, and their application in organic synthesis

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**Keywords:** Catalysts, FePO<sub>4</sub>, heterocycle, Isoxazole.

### ABSTRACT

This work focuses on the synthesis and characterization of new materials which is used as a catalyst for the synthesis of heterocyclic molecules.

Our research has mainly focused on metal-phosphate materials the invention is to introduce a new transition metal in our starting material iron phosphate III (FePO<sub>4</sub>). These materials undergo heat treatments to increase their structure and activity under organic reactions.

Heterocyclic compound have long been considered fundamental structural elements in the field of therapeutic and pharmaceutical treatments. This is due to their ability to offer a wide range of possibilities to substitute atoms or groups within their ring-shaped structures, highlighting their diversity and adaptability <sup>1</sup>. Isoxazole, in particular, is a preferred structure that has a wide range of biological activities and pharmacological properties. It occupies a significant place in various psychotropic drugs and an important position in the pharmaceutical field<sup>2</sup>.

The new materials obtained were characterized by different physicochemical analysis technique : DRX, IR, SEM, specific surface measurement by BET and UV-Vis

The new catalysts were used in the synthesis of isoxazole from the chalcone taking into account the adequate conditions of the reaction. Catalysts showed good activity in isoxazole synthesis.

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## The synthesis and crystal structure determination of tetrahydrobenzo [b] pyran derivatives, along with DFT calculations

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**Keywords:** 4H-pyran, Crystal structures, Hirshfeld surface, TD-DFT.

### ABSTRACT

The novel 4H-pyran, specifically 2-Amino-6,6-dimethyl-5-oxo-4-(4-methoxyphenyl)-5,6,7,8-tetrahydro-4Hbenzopyran-3-carbonitrile (A), and 2-Amino-6,6-dimethyl-5-oxo-4-(phenyl)-5,6,7,8-tetrahydro-4Hbenzopyran-3-carbonitrile (B), were successfully synthesized in good yield using  $(\text{Ni}(\text{NO}_3)_2)$  as a catalyst via cyclocondensation in a single step. The proposed structure of (A) was confirmed through XRD-crystal measurements, and the structures of both compounds were analyzed using NRM, IR, and UV-Vis techniques. Hirshfeld surface analysis was conducted to elucidate the intermolecular interactions of (A). Both molecules underwent optimization using density functional theory with the long-range corrected CAM-B3LYP functional and the 6-311G (d,p) basis set. Global reactivity indices and thermodynamic parameters were explored at the same level of theory. Additionally, TD-DFT calculations were applied to determine the optical absorption spectrum of (A) and (B) in the gas phase. Furthermore, the polarizability, first and second-order hyperpolarizability in static and dynamic regimes were calculated for both molecules and compared with a urea compound.

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## Synthèse et caractérisation des composés hétérocycliques et évaluation de leurs activités biologiques

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**Keywords:** Diazepine, thiadiazepine, pyrimidine, activité *antioxydante*, méthodes spectroscopiques

### ABSTRACT

L'objet de ce travail est la mise au point d'une méthode de synthèse qui permet l'accès aux nouveaux hétérocycles azotés à sept chaînons de diazepine et thiadiazepine portons le motif pyrimidine. Dans la première partie nous avons montré que les pyrimido-diazepines et le pyrimido-thiadiazepine peuvent être obtenus en faisant réagir les dérivés 1,3-diamines (urée, thiourée et sulfamide) sur le diethyl 2-oxo-6-phenyl-1,2,3,6-tetrahydropyrimidine-4,5-dicarboxylate comme un dérivé 1,4-dicarbonyle. Dans la seconde partie, nous sommes intéressées à l'évaluation de l'activité *antioxydante* des dérivés précédemment synthétisés à l'aide du test de DPPH et d'ABTS. Les résultats obtenus montrent que l'ensemble de nos produits possèdent un bon pouvoir antioxydant. Tous les produits synthétisés ont été caractérisés par différentes méthodes spectroscopiques.

## **TOPIC 4**

# **Phytochemistry and medicinal plants**





## Acetylcholine inhibitory activities of flavonoid derivatives isolated from *Pulicaria*: *in vitro* and *in silico* studies.

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**Keywords:** Acetylcholine-esterase; Docking; Extract; Flavonoids; NMR; Pharmacokinetics;  
*Pulicaria laciniata*.

### ABSTRACT

The objective of this study was to recognize flavonoids derivative that had been isolated from the aerial parts of *Pulicaria laciniata* for the first time. The structure of each compound was identified by the examination of spectroscopic NMR data. In addition, the Acetylcholine-esterase was assessed, and the findings indicated that the compound Kaempferol -6-hydroxy-3,7-dimethyl ether compound had the best inhibition against acetylcholine esterase. Furthermore, *in silico* investigations of the isolated compounds for its docking profiles revealed important binding energy which showed significant activities against AChE, Our findings revealed the AChE inhibitory potential of the flavonoids isolated from *P. laciniata* extracts with a predictive profile, which may be helpful in their development as potential drugs likeliness.



## Chemical composition and biological properties of *Origanum Majorana L.* plants growing in Oued Souf: Comparative and analytical study

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**Keywords:** *Origanum majorana L.*, natural products (polyphenols, flavonoids, alkaloid salts, essential oils), biological efficacy.

### ABSTRACT

This work aims at a chemical study of the organic extracts of *Origanum majorana L.* for natural phenolic and alkaloid products obtained by soaking in a mixture of suitable solvents for extraction and in varying volume ratios, and a comparative study of a group of previous studies that enrich the importance and effectiveness of the extracts of the Marjoram plant in eliminating and confronting free radicals and their inhibitory effectiveness as antioxidants to normalize the viability of many pathogenic bacterial strains.

To achieve this, we did, as a preliminary stage, chemical detection of the active products by color methods, in addition to extracting them and calculating the yield, as well as quantitative assessment by ultraviolet and visible spectroscopy of phenols and flavonoids, and quantitative assessment of phenols by means of the ring voltammetric test. Through this study, we concluded that the marjoram plant is rich in secondary metabolites. Represented in polyphenols, flavonoids, and essential oils, but poor in alkaloid salts. And after relying on some previous references, the antioxidant activity was determined by a DPPH chemical method. It was found through this that the extracts of butanol and ethyl acetate are rich in antioxidants and have a high ability to curb and combat free radicals.

As a final step, and after evaluating the antibacterial activity of the extracts against two bacterial strains cultured in a gel medium (MH), depending on the method of diffusion by tablets, it was noted that the results were very positive, especially with the essential oil extracts, as the highest inhibition diameter of *Staphylococcus aureus* was recorded at 55 mm at a concentration of 50%.

In the overall and comprehensive comparison of this study with a group of other studies in the same context, it was found that *Origanum majorana L.* has a significant ability to inhibit radical and bacterial growth.

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## Differentiating Algerian Medicinal Plant Species via Classification by Electrochemical Voltammogram Recording

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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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## Effet insecticide de l'huile essentielle de *Thymus serpyllum* L. à l'égard du bioagresseur *Tribolium castaneum* des denrées stockées

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**Keywords:** Bioinsecticide, Huile essentielle, Plante médicinale, *Thymus serpyllum* L.,  
*Tribolium castaneum*,

One; Two; Three; Four; Five; Six (up to 6 words arranged in alphabetical order)

### ABSTRACT

L'huile essentielle extraite par hydrodistillation des feuilles de plante aromatique, *Thymus serpyllum* L. (Lamiaceae) a été testée à différentes doses sur les adultes *Tribolium castaneum*, à une température de  $26 \pm 1^\circ\text{C}$  et à une humidité relative de  $70 \pm 5\%$ . Nous avons testé l'efficacité de pesticides *Thymus serpyllum* sur l'insecte *Tribolium castaneum*. Ces bio pesticides présentent une efficacité dans la lutte contre le *Tribolium castaneum* où les valeurs de DL10, DL50 et DL90 estimées après leur exposition au traitement pendant 15 minutes sont 3,34 ; 12,75 et 22,17 respectivement. Les résultats obtenus nous montrent que l'huile essentiel utilisée, a une bonne action bio insecticide à l'égard de *Tribolium castaneum* il est donc très utile de poursuivre ces travaux pour mettre en évidence l'action des molécules actives responsables de l'effet insecticide de ces huiles vis-à-vis de cet insecte.

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## Extraction and assessment of total flavonoid levels in a *Fabaceae* family species native to the Algerian Aurès zone.

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**Keywords:** Aurès region; Flavonoid; *Hedysarum*; *Fabaceae*; secondary metabolites.

### ABSTRACT

The Fabaceae is a big and diverse plant family found throughout northern Africa, including Algeria. This family contains a variety of bioactive chemicals with distinct pharmacological effects. These secondary metabolites from Fabaceae plants are used for therapeutic purposes [1]. Our research focuses on the measurement of flavonoids in the CHCl<sub>3</sub>, AcOEt, and *n*-BuOH fractions of *Hedysarum*, an Algerian species native to the Aurès region. The aerial components of the plant were removed using a maceration procedure including MeOH and H<sub>2</sub>O (80/20, v/v). The crude extract was then liquid-liquid extracted using CHCl<sub>3</sub>, AcOEt, and *n*-BuOH. The flavonoid content was assessed using the aluminum trichloride (AlCl<sub>3</sub>) technique [2]. The study found that the AcOEt fraction yield was 0.9%, with a total flavonoid content of 90.71 µg GAE/mg. The presence of flavonoid compounds indicates that the plant is rich in active biomolecules, implying that these natural substances can be harnessed in biotechnology for commercialization.

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## Investigation of Essential Oil Extraction, GC/MS Evaluation, and Assessment of Antioxidant Properties in Two Medicinal Plant Species Indigenous to Southern Algeria

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**Keywords:** Antioxidant Activity, Essential Oil Extraction, GC/MS Analysis, Medicinal Plants.

### ABSTRACT

The utilization of medicinal plants for therapeutic purposes has been deeply rooted in traditional medicine practices. In this study, we focus on the extraction, Gas Chromatography-Mass Spectrometry (GC/MS) analysis, and evaluation of Antioxidant activity of essential oils derived from two indigenous medicinal plants native to the southern region of Algeria. The extraction process employs hydro-distillation technique to ensure optimal yield and preservation of bioactive compounds. Subsequently, GC/MS analysis is conducted to identify and quantify the chemical constituents present in the essential oils, providing insights into their phytochemical composition.

Furthermore, the Antioxidant potential of these essential oils is investigated through in vitro assays utilizing UV-Vis spectroscopy. The assay methodology is designed to assess the ability of the essential oils to modulate key parameters associated with free radicals. Complementing these experimental analyses, computational studies are performed using induced fit docking and Molecular Dynamics Simulation (MDS) [1] techniques, spanning a simulation period of 100 nanoseconds. Through in silico simulations, we aim to elucidate the molecular interactions between bioactive components of the essential [2]oils and target proteins implicated in stress oxidative.

The integration of experimental and computational approaches provides a comprehensive understanding of the therapeutic potential of these medicinal plants in managing stress oxidative. This multidisciplinary investigation contributes to the advancement of natural product-based drug discovery and underscores the significance of traditional knowledge in modern scientific research.





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## Green Synthesis of zinc oxide Nanoparticles Using extracts a plants *Solenostemma Argel* and *Anastatica Hierochuntica*: characterization and Application

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**Keywords:** Nanoparticles ; UV-Vis; ZnO; Biological Activities

### ABSTRACT

Nanoscience explores the unique properties of materials sized between 1 and 100 nanometers. These nanomaterials are being leveraged to innovate and modify various applications. Particularly in medicine and healthcare, nanoparticles play a pivotal role, exhibiting antibacterial, antifungal, and antioxidant properties. Researchers have developed eco-friendly methods for nanoparticle synthesis, with plants and their extracts emerging as prominent candidates due to their rapid growth, cost-effectiveness, and environmentally friendly characteristics. Various parts of plants, including roots, flowers, stems, leaves, shoots, barks, seeds, and derivatives, have proven effective in nanoparticle biosynthesis. This study focuses on a sustainable approach using medicinal plants to synthesize zinc oxide nanoparticles. Characterization techniques, such as UV-Vis and Fourier transform infrared spectroscopy, confirmed the presence of biomolecules and metal oxides, while X-ray diffraction analysis revealed the formation of pure wurtzite ZnO crystalline nanoparticles. Additionally, the antibacterial activity of these nanoparticles was evaluated using the disk diffusion method. [1-3]

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## Assessment of Antibacterial and Antifungal Activities of Neem (*Azadirachta indica*) Leaf Extracts in the El Oued Region

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**Keywords:** *Azadirachta indica*, neem, antibacterial activity, antifungal activity, El Oued.

### ABSTRACT

This study evaluates the antibacterial and antifungal activities of neem (*Azadirachta indica*) leaf extracts collected from the El Oued region. The extracts were tested against a panel of bacterial and fungal strains using the disk diffusion method. Results indicate significant inhibitory effects against both Gram-positive and Gram-negative bacteria, as well as various fungal species. The findings highlight the potential of neem leaf extracts as natural antimicrobial agents, particularly in regions with arid climates like El Oued.

## Exploring the Phytochemical Profile and Antioxidant Potential of *Haloxylon articulatum* Extract

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**Keywords:** *Haloxylon articulatum*, phytochemical composition, antioxidant activity.

### ABSTRACT

*Haloxylon articulatum*, a desert plant rich in bioactive compounds, was studied for its phytochemical composition and antioxidant potential. The methanolic extract of *H. articulatum* aerial parts was analyzed using various analytical techniques, revealing the presence of phenolic compounds, flavonoids, and other secondary metabolites. The extract exhibited significant antioxidant activity in vitro, as demonstrated by its ability to scavenge free radicals and inhibit lipid peroxidation. These findings suggest that *H. articulatum* extract could be a valuable source of natural antioxidants with potential applications in pharmaceuticals and functional foods.



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