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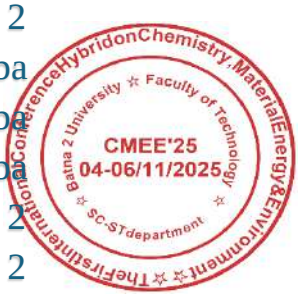

TOPIC 01:

Polymer Chemistry and Advanced Materials.

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Elaboration of a semiconductor material based on Polypyrrole and ZnO Nanoparticles in the presence of various dopants

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Abstract **–** Over the last three decades, the semiconducting polymer materials have been widely used in different fields of science and industry and continue to attract much attention. Their potential for application in multidisciplinary domains, particularly in solar energy conversion, has been extensively demonstrated. As a result, the development of organic semiconductors has garnered significant interest from both academic and industrial communities, as evidenced by a growing body of published research. Thus, the elaboration of organic semiconductor materials has found interest from both academic and industrial points of view, as evidenced by a growing body of published research [1,2].

In this study, polypyrrole (PPy) was synthesized via oxidative polymerization using ammonium persulfate (APS) in the presence of various dopants: hydrochloric acid (HCl), dodecylbenzene sulfonic acid (DBSA), and sodium dodecyl sulfate (SDS). PPy/ZnO Nanocomposites were subsequently prepared by in situ polymerization with varying ZnO contents, using DBSA and SDS as surfactants, respectively.

Fourier transform infrared spectroscopy (FTIR) study confirmed the incorporation of surfactants into the PPy matrix and revealed the presence of specific interactions between the N–H groups of PPy and ZnO Nanoparticles. Thermogravimetric analysis (TGA) indicated a significant enhancement in the thermal stability of PPy when doped with SDS or DBSA, with further improvement upon the addition of ZnO. Scanning electron microscopy (SEM) showed that both the particle morphology and size were influenced by the choice of dopant and the presence of ZnO. UV–Visible spectroscopy indicates the changes in the PPy band gap upon the addition of SDS, DBSA, and ZnO. Finally, electrical conductivity, measured by the four-point probe method, was highest for SDS-doped PPy (0.11 $S \cdot cm^{-1}$) and further increased with the incorporation of ZnO, reaching a percolation threshold at 5% ZnO.

Keywords –: *Polypyrrole (PPy), ZnO Nanoparticles (ZnO NPs), Fourier transform infrared spectroscopy (FTIR), surfactants, Electric conductivity (σ).*

References

[1] Shacklette, LW; Dipole and hydrogen bonding interactions in polyaniline: a mecha-nism for conductivity enhancement. Synthetic Metals **1994**, 65, 123-130.

[2] Sad Atia, Khaled Zeggagh, Slimane Hadjout, Agustin Etxeberria, Zitouni Benabdelghani, Journal of Polymer Research, 29: 138 (2022).

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Influence of Polyaniline Concentration in Acid Solution (0.1–0.3 M)

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Abstract – In this study, polyaniline (PANI) nanoparticles were synthesised via chemical polymerisation to investigate the impact of polyaniline concentration on the stability of hydrochloric acid concentration. The effect of three polymer concentrations (0.1, 0.2, and 0.3 M) on the morphological and electrical properties of PANI was analyzed using scanning electron microscopy (SEM) and the four-point probe method for conductivity measurements. SEM results showed that at higher concentrations, particularly 0.3 and 0.5 M, an increase in monomer concentration, increased chain entanglement, and interchain bonding were observed, as well as the formation of polymeric structures with variable particle sizes and morphologies. It was also shown that higher monomer concentrations generally led to larger nanoparticle sizes, since the system preferred the creation of fewer nuclei, which then continued to grow into larger particles. Electrically, polyaniline's conductivity increased with concentration due to enhanced protonation and charge transport. The conductivity peaked at 0.217 S/cm, reflecting the ideal balance between structural ordering and charge carrier density. However, a saturation effect was observed. As a result, the ordered conjugated system was partially disrupted, limiting the mobility of charge carriers. Consequently, the conductivity dropped to 0.1503 S/cm, confirming that excessively high doping levels can induce structural defects and hinder rather than enhance the overall electrical performance.

Keywords – Polyaniline, Hydrochloric Acid, Electrical Properties, Morphological Properties, polymer concentration

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Tailoring Optoelectronic Characteristics of $Zn_xCd_{1-x}S$ Alloys through Band Gap Modulation

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Abstract – In this research, we examine the optical and dielectric characteristics of ZnxCd1-xS, a ternary alloy system with a zinc-blende crystal structure. Our analysis employs a pseudopotential model based on the virtual crystal approximation, which accounts for the effects of compositional disorder. Through our calculations, we investigate various aspects of the refractive index and determine the most suitable model. Additionally, we determine the high-frequency and static dielectric constants for the materials studied. Crucially, we explore the band gap energy of ZnxCd1-xS, which is a fundamental parameter influencing its optical and electronic properties. The ability to tune the band gap energy through compositional variation makes this alloy system particularly attractive for diverse optoelectronic applications, including solar cells, light-emitting diodes, and photodetectors. Our findings show good agreement with previously published results in the literature. These results provide valuable insights for the application of this data in optoelectronics and offer useful information for further research in this field, particularly in the context of band gap engineering for specific device requirements.

Keywords – Band structure, Refractive index, dielectric constant, pseudopotential; $Zn_xCd_{1-x}S$ alloys

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Réduction catalytique des polluants organiques par des matériaux de silice mésoporeuse dopés en nanoparticules métalliques

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Abstract – Dans ce travail, la silice mésoporeuse MCM-41 a été préparée par voie hydrothermale, et le matériau obtenu tel qu'il est synthétisé (CTA-MCM-41) a été modifié par deux méthodes différentes utilisant de l'argent (Ag) et du cérium (Ce) assistés par traitement thermique. Les matériaux modifiés ont été caractérisés par des mesures de DRX, FTIR, XRF, XPS, de sorption d'azote à −196 °C, des analyses SEM et TEM. Les matériaux modifiés ont été testés comme catalyseurs dans un système simple et binaire via la réaction de réduction du bleu de méthylène (BM), du rouge Congo (RC), du 4-nitrophénol (4-NP), du méthylorange (MO), de l'orange G (OG) en présence de $NaBH_4$. L'effet de la taille des nanoparticules, de leurs dispersions, de la nature du polluant organique, de la concentration initiale du polluant organique et de la concentration de l'agent réducteur $NaBH_4$ a été étudié et discuté. Les résultats obtenus ont confirmé que la méthode de préparation joue un rôle important dans le contenu et la nature des nanoparticules, leurs tailles, leurs dispersions, ainsi que sur leurs performances catalytiques. Le matériau Ag-Ce-MCM-2 a été sélectionné comme le meilleur catalyseur en raison de l'effet synergique entre les AgNPs et CeO_2. La constante de vitesse calculée dans le système simple pour les différents polluants était la suivante : 0,1829 s^{-1}, 0,1762 s^{-1}, 0,0606 s^{-1}, 0,0585 s^{-1}, 0,0556 s^{-1} pour MO, OG, BM, 4-NP, RC, respectivement. La réduction dans un système binaire contenant CR et BM ou MO et BM était en compétition, dans laquelle le RC ou le MO se dégrade avec le colorant BM. Alors que pour les autres systèmes binaires contenant 4-NP/BM ou OG/BM, le catalyseur Ag-Ce-MCM-2 s'est montré plus sélectif envers le colorant BM. Ce catalyseur a démontré son efficacité et sa réutilisabilité au cours de différents cycles, la conversion du colorant BM étant complète à chaque réutilisation.

Keywords –réduction ; polluant organique *; MCM-41, Ag-Ce-MCM ; réutilisation.*

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Study of the Inhibitory Performance of a Polymer Against Aluminum Corrosion in an Acidic Environment.

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Abstract **–**This work focused on the study of the inhibitory performance of a polymer against aluminum corrosion in an acidic medium (1 M HCl) using two different techniques: chemical analysis (gravimetry), density functional theory (DFT), optical microscopy (OM), and scanning electron microscopy with energy dispersive X-ray spectroscopy (SEM-EDS).

The results obtained from these methods show that the studied polyvinyl chloride acts as an anodic inhibitor, with a maximum efficiency of 99.56% at a concentration of 600 ppm.

Observations from OM and SEM-EDS indicate the formation of a stable and insoluble protective layer that limits the access of the electrolyte to the surface of the metal.

Keywords –Corrosion, Aluminum, Corrosion Inhibitors, Polyvinyl Chloride.

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Numerical Simulation of the Heating of an Office by a Trombe Wall

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Abstract – The increasing demand for energy-efficient buildings has spurred research into passive solar heating technologies. The Trombe wall is a well-established passive system for capturing and storing solar energy to heat indoor spaces. This study presents a numerical simulation to analyze the thermal performance of a Trombe wall integrated into an office. The primary objective is to evaluate the system's effectiveness in maintaining thermal comfort and reducing reliance on conventional heating systems during cold periods.

Using the COMSOL simulation , a two-dimensional model of an office coupled with a Trombe wall was developed. The model solves the governing equations of fluid dynamics and heat transfer (Navier-Stokes and energy equations) under transient conditions, considering natural convection in the air gap and heat conduction through the massive wall.

The simulation results illustrate the temperature distribution and airflow patterns within the office and the

Trombe wall system. The analysis highlights a significant thermosiphon effect, where heated air circulates from the wall's air gap into the office, leading to a notable increase in the average indoor temperature. The study quantifies the storage and thermal lag characteristics of the wall, demonstrating its

ability to provide delayed heating after sunset. The findings confirm that a properly designed Trombe wall can substantially contribute to the heating requirements of an office, thereby enhancing energy efficiency and occupant comfort. This numerical model serves as a valuable tool for optimizing Trombe

wall design parameters for specific climatic conditions.

Keywords – Trombe wall, investigation, COMSOL, passive solar heating ,Building Energy.

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Étude structurale, physico-chimique et biologique de l'alginate de sodium oxydé en vue du développement de biomatériaux innovants

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Résumé– Cette étude porte sur l'oxydation de l'alginate de sodium par l'hypochlorite de sodium, un procédé visant à modifier chimiquement ce biopolymère issu des algues brunes. L'objectif est d'améliorer ses propriétés physico-chimiques et d'élargir ses applications biomédicales et industrielles. La méthodologie adoptée repose sur la préparation de films d'alginate oxydés à différentes concentrations de chlore actif (0,25–3%), suivie de caractérisations chimiques (dosage des groupements carbonyle, carboxyle et aldéhyde), structurales (spectroscopie FTIR, UV-Vis) et biologiques (biocompatibilité sanguine). Les résultats montrent que l'oxydation accroît la teneur en groupements fonctionnels, ce qui se traduit par une modification significative de la structure chimique de l'alginate de sodium, cette modification révèlent une augmentation des groupements fonctionnels proportionnelle à la concentration d'agent oxydant, confirmant la formation de nouveaux sites réactifs.

Sur le plan biologique, les films oxydés révèlent une bonne compatibilité avec le sang humain. Ces performances sont directement corrélées au degré d'oxydation appliqué. En conclusion, l'oxydation de l'alginate de sodium constitue une voie simple et efficace pour générer de nouveaux biomatériaux fonctionnels. Elle ouvre des perspectives intéressantes pour le développement de biomatériaux à usage médical et industrielles, en particulier dans les systèmes de libération contrôlée de médicaments, les pansements actifs et les supports de culture cellulaire.

Mots-clés – Alginate de sodium ; Oxydation ; Hypochlorite de sodium ; Biopolymères ; Propriétés physico-chimiques.

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Synthèse, Étude structurale, caractérisation d'un complexe ''Mn'' d'un ligand base de schiff tetradentate N2O2 et leur application.

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Abstract **–** Les bases de Schiff sont des ligands uniques qui jouent un rôle essentiel dans le développement de la chimie de coordination. Elles sont faciles à synthétiser et peuvent être facilement modifiées électroniquement. Forment une classe exceptionnelle de ligands en raison de leurs propriétés uniques telles que la stabilité dans différentes conditions, la diversité des sites donneurs, la flexibilité synthétique et la formation d'une large gamme de complexes dans diverses géométries de coordination.

Parmi eux, les ligands de base de Schiff de type salen sont certainement attrayants pour les chimistes de coordination. Ce sont des ligands tétradentates avec quatre sites donneurs (N2O2).

Nous présentons la synthèse, la résolution structurale et la caractérisation d'un complexe de coordination ''Mn'' assemblé à partir d'une géométrie de coordination $\mathbf{N_2\ O_2}$ ainsi que l'étude de la surface de Hirshfeld et l'application de ce complexe.

Le complexe cristallise dans le groupe d'espace $\mathbf{P2_1/c}$ du système Monoclinique. La structure cristalline est stabilisée par un réseau de liaisons hydrogène ainsi que par des interactions de type empilement $\boldsymbol{\pi}$–$\boldsymbol{\pi}$.

Keywords – Base de schiff, salen ,DRX, FT-IR ,surface de Hirshfeld

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Efficient removal of methyl orange from water onto PVC/Bentonite membranes: experimental validation and COMSOL multiphysics

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Abstract **–** Nowadays, the treatment of domestic and industrial wastewater is a very important topic in environmental protection. Reuse of this water is one of the possibilities already implemented. A rapidly developing process in this area is membrane filtration.

Membranes based on polymer materials are generally employed in the purification of wastewater resulting from the accumulation of dyes in industries such as textiles, paper, and others. In this regard, membranes using polyvinyl chloride (PVC) added to Bentonite, which is natural clay obtained from the Roussel deposit (Maghnia, Algeria) were prepared. Bentonite was chosen for its remarkable ion adsorption properties and its incorporation at different ratios improves the membrane's efficacy for water treatment purposes.

The filtrates collected were studied using UV-Vis spectroscopy. This technique allowed us to estimate the removal capacity of organic dye, methyl orange, from our membranes. The results demonstrated that our newly prepared materials with higher Bentonite content exhibited a better depollution efficiency and, consequently, higher capacity adsorption for methyl orange. This is indubitably attributed to the porous structure of Bentonite. Thus, these membranes represent the current best alternative to known separation techniques.

The finite element method-based software COMSOL Multiphysics has been used to investigate filtration processes in the model system. Finally, the numerical results of the proposed model are compared with the available experimental data and that represent good agreement.

Keywords: Membrane, Bentonite, Dye, PVC, Filtration.

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synthèse et caractérisation de nanofeuilles d'oxyde de zinc (ZnO) à l'aide de méthodes hydrothermiques à micro-ondes.pour fabrication des dispositifs optoélectroniques nanométriques sélectifs.

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Résumé – Des nanofeuilles de ZnO à structure wurtzite hexagonale ont été synthétisées avec succès par un procédé hydrothermique assisté par micro-ondes dans des conditions douces en utilisant de l'acétate de zinc comme précurseur. La poudre obtenue a été caractérisée par diffraction des rayons X, microscopie électronique à balayage environnementale et photoluminescence à température ambiante. La taille des nanofeuilles de ZnO synthétisées dépend de la concentration du précurseur et leur diamètre moyen varie entre 50 et 600 nm, avec une épaisseur comprise entre 8 et 38 nm. Le produit présente une forte émission UV à 397 nm et une émission bleue visible centrée à 466 nm.

Mots clés – Chauffage par micro-ondes , hydrothermal, nanofeuilles , photoluminescence, émission bleue .

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Treatment by chemical calcification of granular road pavement foundation materials.

First Author*, Second Author [2] and Third Author [3]

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Abstract – Improving the geotechnical condition of road materials is achieved through compaction or the addition of a chemical binder. The latter remains expensive and sometimes has an environmental impact. To address this issue, one approach is to strengthen the soil through chemical calcification by introducing chemically produced precipitates, in this case, ash from chicken eggshell waste.

Chemical calcification involves introducing reactive products into the soil matrix that can generate a reaction essential for the precipitation of calcium carbonate.

These precipitates form cementing bridges that bind the soil particles together, improving their mechanical properties.

The study conducted in this research constitutes a preliminary study aimed at examining the potential of chemical calcification to develop a high-performance granular material suitable for road subgrades. Sandy soil samples mixed and calcified with chicken eggshell ash at appropriate percentages were subjected to simple compression tests. The results revealed that chemical calcification significantly improves their mechanical performance.

Keywords – Waste, chicken eggshells, chemical calcification, materials, environment.

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Development of a Grafted Copolymer Network: polyMA-g-poly(NVP-co-MeOx)

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Abstract – The aim of this work is to synthesize and characterize a novel polyMA-g-poly(NVP-co-MeOx) network through a two-step approach. In the first step, a bifunctional macromonomer poly(NVP-co-MeOx) was prepared via a green route from methacrylic anhydride, N-vinylpyrrolidone (NVP), and 2-methyl-2-oxazoline (MeOx), using maghnite-H^+, an eco-friendly heterogeneous catalyst developed by Prof. Belbachir. In the second step, a crosslinked network was obtained by radical activation of the chain ends with benzoyl peroxide in DMF. Both the macromonomer and the resulting network were characterized by FTIR and UV spectroscopy. Finally, solubility studies revealed that the macromonomer was soluble in dichloromethane and chloroform, whereas the crosslinked network was insoluble in these solvents.

Keywords – polyMA-g-poly(NVP-co-MeOx); bifunctional macromonomer poly(NVP-co-MeOx); green synthesis; heterogeneous catalysis; maghnite-H^+

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From Biomass to Polysaccharide: An Extraction and Characterization Approach

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Abstract – The sustainable valorization of plant residues is increasingly recognized as a pathway toward reducing reliance on non-renewable resources. In this study, a natural biopolymer was extracted from locally available lignocellulosic biomass using a mild and environmentally friendly chemical approach. The treatment enabled the selective removal of non-polymeric fractions, yielding a purified material with promising functional properties. Structural characterization was performed by Fourier Transform Infrared Spectroscopy (FTIR), which confirmed the presence of characteristic absorption bands associated with polysaccharide frameworks. Thermal behavior was investigated by Thermogravimetric Analysis (TGA), showing a degradation pattern consistent with thermally stable biopolymers. The combined spectroscopic and thermal insights provide strong evidence of successful isolation and purification, underscoring the potential of agricultural residues as renewable precursors for advanced material development. This work contributes to the broader objectives of green chemistry and circular economy by demonstrating a simple, eco-conscious route for converting biomass waste into value-added products.

Keywords – lignocellulosic biomass, biopolymer, polysaccharide, FTIR, TGA, green chemistry

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Overview of Friction Stir Welding Tool Wear and Failure

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Abstract

Friction Stir Welding (FSW) is a solid-state joining process in which a rotating, non-consumable tool is plunged into the abutting edges of two pieces of material and traversed along the joint line. Because the material is plasticized by frictional heat and mechanical stirring rather than melted, FSW avoids common fusion-welding defects such as porosity, solidification cracking, and distortion. This combination of high joint quality and low distortion has made FSW an attractive method for critical structures in the aerospace, nuclear, shipbuilding, automotive, and rail industries. Originally developed for aluminum alloys, FSW technology has since been extended to higher-melting-point materials such as steels, titanium alloys, copper, and nickel-based superalloys. Welding these harder alloys, however, imposes severe thermal and mechanical stresses on the tool, including rapid heating and cooling, high axial and torsional loads, and intense frictional contact with the workpiece. As a result, the FSW tool is prone to accelerated wear, plastic deformation, microstructural changes, and different modes of failure such as abrasion, adhesion, and thermal fatigue. These phenomena are particularly pronounced in cobalt-based MP159 and other tool materials when joining thick sections at high rotational speeds. This paper provides an overview of the mechanisms of tool degradation, highlighting how plastic deformation, microstructural evolution, and multiple wear modes interact to limit tool life and reliability.

Keywords: FSW, Tool, cobalt alloys, wear, failure.

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Overview of Additive manufacturing as a repair process.

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Abstract
Additive manufacturing (AM) is emerging as a powerful technology for the repair and remanufacturing of industrial components. By adding material only where needed, AM can restore worn or damaged parts, extend service life, and reduce both material waste and production costs compared with conventional repair methods. This paper provides an overview of AM as a repair process, with particular attention to Laser Metal Deposition (LMD), a leading technique for rebuilding and strengthening high-value tools and components, including those used in friction stir welding (FSW). Key aspects such as material compatibility, process planning, and the influence of AM on microstructure and mechanical behavior are considered, along with the contribution of AM to sustainable manufacturing through resource conservation and reduced environmental impact. The paper also highlights opportunities and challenges associated with implementing AM and LMD and discusses their potential role in modern maintenance, repair, and life-cycle management, offering guidance for future industrial adoption and process optimization.

Keywords AM , repair , remanufacturing , tool , FSW

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Characterisation of a novel biopolymer with pharmaceutical properties

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Abstract

Exopolysaccharides (EPS) are microbially-originated, complex biosynthetic polymers, mainly carbohydrates in nature. They have gained attention of modern researches due to their novel physicochemical characteristics with important structural and technological features. In this study, a novel exopolysaccharide produced by a thermophilic bacteria isolated from Hammam Debegh hot spring was extracted and characterized using high performance liquid chromatography (HPLC), Fourier transform-infrared spectroscopy (FT-IR), scanning electron microscopy (SEM), X-Ray diffraction (XRD), Thermogram (TGA) and differential scanning calorimeter (DSC) analysis. Biological potential of the sample was studied by evaluating the emulsifying and the anti-inflammatory activities. The isolated strain was identified by 16S rRNA sequencing as *Bacillus velezensis*. HPLC analysis showed a heteropolymeric structure of the EPS containing galactose, glucose, glucuronic acid and glucosamine. Infrared microscopy was carried out to identify the functional groups showed the main presence of carbonyl and hydroxyl groups. The EPS presented amorphous nature and highly branched and porous microstructural characteristics determined by XRD and SEM analysis. Thermal analysis confirmed that the EPS displayed a relevant thermal stability compared to other exopolysaccharides with a high degradation temperature of 260°C and 38% of the residual mass at 800 C°. Based on the obtained results, the exopolysaccharide presented an excellent emulsifying activity against paraffin oil and sunflower oil comparable or superior to that shown by the standard. A relevant anti-inflammatory potential was also revealed for the studied sample. These findings indicated the promising value of this EPS, which may provide utilities in several industries, especially with the advantage of its high thermal stability.

Keywords

Exopolysaccharide, bacteria, characterization, emulsifying activity, anti-inflammatory.

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Impact of chemical treatments on the characteristics of polyethylene composites

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Abstract – Lately, different reinforcing fillers—like lignocellulosic materials—have been added to synthetic polymeric materials to improve their mechanical properties. These materials are among the greenest agricultural wastes and will be crucial in addressing the world's most urgent environmental problems. These components are easy to collect from agricultural waste because they break down over time and don't harm the environment. The purpose of this study is to ascertain how silane coupling agents and palm fibre alkali treatments affect the mechanical, thermal, and water absorption characteristics of polyethylene PE composites. Use infrared spectroscopy to investigate the impact of fibre treatments. When compared to untreated composites, the mechanical properties of composite materials are improved through the use of treated fibres. Furthermore, SEM pictures revealed a strong interfacial adhesion between the polyethylene composite surfaces and treated fibres, which improves heat stability and water absorption.

Keywords – coupling agent, adhesion, polyethylene, palm fibre, and alkali treatment.

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Antioxidant activities of silver nanoparticles biosynthesized using galactomannan derived from the seeds of *Astragalus gombiformis* Pomel (Fabaceae)

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Abstract – Plant polysaccharides have attracted considerable attention as abundant natural biopolymers with diverse biological functions. In this study, galactomannan was extracted from the seeds of the medicinal plant *Astragalus gombiformis* Pomel using hot-water extraction followed by ethanol precipitation, and employed as a green reducing and stabilizing agent for the biosynthesis of silver nanoparticles (AgNPs). The antioxidant activities of the biosynthesized AgNPs were evaluated using the DPPH radical-scavenging assay and the ferric-reducing power assay. At a concentration of 0.1 mg/ml, the AgNPs exhibited strong antioxidant activity, with 90.61 % DPPH radical-scavenging activity and a ferric-reducing capacity corresponding to an absorbance of 0.061 at 700 nm. These findings demonstrate that biosynthesized AgNPs possess significant antioxidant potential, suggesting their possible applications in biomedical and pharmaceutical fields.

Keywords – Biopolymers, Galactomannan, *Astragalus gombiformis* Pomel, Silver nanoparticles, Antioxidant activity.

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Investigation of structure-property relationships in Spanish broom fibre-reinforced PHBV biocomposites

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Abstract **–** The use of natural fibres as fillers in polymer matrix has been increasing recently. This has opened the door for new environmentally friendly composites to be developed which are much needed in today's world. These fibres are characterised by their low cost, low density while retaining high strength, being renewable and fully biodegradable. Several researchers have investigated various types of natural fibre for use as possible reinforcements in polymer composites. In this study, a new biocomposite was developed using poly(3-hydroxybutyrate-co-3-hydroxyvalerate) (PHBV) as biopolymer matrix, with the addition of Spanish broom fibres (SBF) for reinforcement at different filler contents 10, 20 and 30% by weight. Poly(3-hydroxybutyrate-co-3-hydroxyvalerate) (PHBV) is an aliphatic biopolyester that belongs to the polyhydroxyalkanoate (PHA) family. It is produced from various bacteria. Spanish broom (Spartium Junceum.L) is a Mediterranean plant with multiple uses. SBF has exceptional characteristics such as low density, abundance, low production cost and excellent thermal and mechanical properties. The PHBV/SBF biocomposites were prepared using a melt compounding process. Results showed an increase in tensile strength, Young's modulus, and Shore D hardness of PHBV/SBF biocomposites as the SBF content increased. At the same time, we observed an increase in crystallinity and a decrease in T_{CC} with increasing SBF content.

Keywords – Biocomposites, Spartium junceum.L, PHBV, Tensile strength, Crystallinity

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Comparative Study on the Use of Crushed Dune Sand and Silica Fume in High-Performance Concrete

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Abstract
This paper investigates the use of crushed dune sand and silica fume as mineral additions in the formulation of high-performance concrete (HPC). A comparative study was conducted to assess their influence on the properties and behavior of HPC in both fresh and hardened states. The mechanical test results revealed only slight differences between concretes incorporating silica fume and those containing crushed dune sand. The findings demonstrate that valorizing dune sand from the western erg of Algeria is highly feasible for HPC production, and that replacing silica fume with crushed dune sand does not impair the performance of the resulting concretes.

Keywords – ***high performance concrete, crushed dune sand, silica fume,mineral addition, compressive strength***

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Improvement of the energy efficiency of a thermal envelope for a rural house in Algeria

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Abstract – One of the biggest users of resources is the construction industry (energy and materials). This source provides about 42% of Algeria's primary energy, and it is expected that this number will increase as the nation's population increases, particularly in rural areas where urban expansion is occurring. This study focuses on the design of the envelope of a rural house in Algeria to enhance its energy efficiency. The study is based on the assessment, through dynamic simulation, of the effects of orientation, glazing, and thermal insulation on energy consumption for heating and cooling purposes. The case study encompasses a house with a total area of 80 m^2, accommodating 6 occupants. Three cities, namely Algiers, Batna, and Tamanrasset, are selected to represent the main climatic conditions prevailing in Algeria. The principal findings of the study are as follows. Equipping the rural house with a locally sourced bio-composite insulation based on date palm wood can reduce the annual energy consumption of the house by up to 45%, depending on the climatic zone where the house is situated. The optimal orientation of the rural house in Algiers, Batna, and Tamanrasset is respectively towards the south, north, and east. Small windows with a 20% window-to-wall ratio in Algiers and Tamanrasset result in energy savings of 27.3% and 18.3%, while in Batna, the optimal window-to-wall ratio is between 30% and 40%.

Keywords: Building energetics; Dynamic simulation; Energy performance of a rural house; Thermal efficiency of building envelope; Thermal insulation based on date palm wood.
Keywords – Building energetics; Thermal efficiency of building envelope; Thermal insulation based on date palm wood

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Abstract – One of the biggest users of resources is the construction industry (energy and materials). This source provides about 42% of Algeria's primary energy, and it is expected that this number will increase as the nation's population increases, particularly in rural areas where urban expansion is occurring. This study focuses on the design of the envelope of a rural house in Algeria to enhance its energy efficiency. The study is based on the assessment, through dynamic simulation, of the effects of orientation, glazing, and thermal insulation on energy consumption for heating and cooling purposes. The case study encompasses a house with a total area of 80 m^2, accommodating 6 occupants. Three cities, namely Algiers, Batna, and Tamanrasset, are selected to represent the main climatic conditions prevailing in Algeria. The principal findings of the study are as follows. Equipping the rural house with a locally sourced bio-composite insulation based on date palm wood can reduce the annual energy consumption of the house by up to 45%, depending on the climatic zone where the house is situated. The optimal orientation of the rural house in Algiers, Batna, and Tamanrasset is respectively towards the south, north, and east. Small windows with a 20% window-to-wall ratio in Algiers and Tamanrasset result in energy savings of 27.3% and 18.3%, while in Batna, the optimal window-to-wall ratio is between 30% and 40%.
Keywords: Building energetics; Dynamic simulation; Energy performance of a rural house; Thermal efficiency of building envelope; Thermal insulation based on date palm wood.

Keywords – Building energetics; Thermal efficiency of building envelope; Thermal insulation based on date palm wood

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ZnO-TOP Nanoparticles: Structural Characterisation and Broad-Spectrum Antimicrobial Activity

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Abstract **–** This work consists of synthesising ZnO-Trioctylphosphine nanoparticles (ZnO-TOP NPs) using a chemical method (the polyol method) and studying their biocidal effect on pathogenic germs (three Gram-positive strains, six Gram-negative strains and one fungus), using the agar well diffusion method and the determination of minimum inhibitory concentrations (MIC). X-ray diffraction (XRD) analyses showed that the structure of ZnO-TOP is hexagonal wurtzite with an average crystallite size of around 16.57 nm. Microbial analyses showed that ZnO-TOP NPs have strong antimicrobial activity against all pathogens tested, with a maximum inhibition zone of 20±0.15, 20±0.19 and 18±0.67 for P. aeruginosa ATCC 27853, A. baumannii and Candida albicans, respectively, at a concentration of 400 µg/ml.

.

Keywords – ***:*** *ZnO nanoparticles, Trioctylphosphine (TOP), Polyol method, Antimicrobial activity*

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Electrical characterization of piezoelectric ceramics

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Abstract – Lead zirconate titanate, $Pb(Zr_xTi_{1\_x})O_3$ or PZT ceramics have been investigated from both fundamental and applied viewpoints [1,2].

The morphotropic phase boundary (MPB) of PZT is located at a PbTiO3:PbZrO3 of 0.52:0.48 and separates the Ti-rich tetragonal phase from the Zr-rich rhombohedral phase [3].

PFN-PNN-PZT piezoelectric ceramics with varying Zr/Ti ratios were prepared by a conventional mixed-oxide route.The effect of Zr/Ti ratio and sintering temperature on the dielectric properties of our simples were investigated. The new MPB in this system with optimum piezoelectric properties was found at x = 0.51-0.53. The dependence of the dielectric constant (ε) and the loss tangent on the Zr/Ti ratio shows a pronounced maximum of ε at Zr/Ti : 51/49 and a minimum tanδ .

Keywords: PZT, the morphotropic border of phase (FMP), piezoelectric Properties, dielectric Properties, sintering temperature

TOPIC 02:

Theoretical Chemistry.

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The discovery of new inhibitors for Alzheimer's disease: virtual screening, molecular docking, and ADME-Tox filtering

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Abstract – Alzheimer's disease is a progressive neurodegenerative disorder characterized by memory loss and age-related cognitive deficits. It is the sixth leading cause of death and has an increasing impact on our society. Despite scientific advancements, the currently available treatment options remain limited and are mainly symptomatic. This work focuses on the search for new AChE inhibitors, a well-established therapeutic target in the treatment of Alzheimer's disease. In this context, we employed molecular docking methods using Surflex-dock software. We tested the docking of a set of 214 similar compounds, selected from the Pubchem library, on the active site of AChE. As a result, tow compounds CID_102004882, and CID_102004770 showed the best affinities, with respective scores of 8.52 M^{-1}, and 8.53 M^{-1}. These findings indicate that these compounds may serve as potentially more selective and high-affinity inhibitors for AChE. Additionally, a promising pharmacophore profile and favorable ADME-Tox characteristics were identified, suggesting that these compounds could act as potentially more effective inhibitors against AChE.

This study highlights the utility of molecular docking as a virtual screening tool in the discovery of new therapeutic approaches for combating Alzheimer's disease, paving the way for further experimental validation.

Keywords – Alzheimer's disease, AChE, Surflex-dock, Molecular Docking, ADME-Tox.

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Electron Interaction Theory Reveals Key Mechanistic Features in the Formation of a Bioactive Heterocycle

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Abstract – Compounds with hetero are pivotal in several scientific fields since they are found in both simple and complex chemical structures. They constitute the fundamental structure of several natural compounds, including vitamins, alkaloids, macrocycles, and flavonoids. Moreover, heterocycles are ubiquitous in synthetic bioactive compounds, including medicines and agrochemicals. Their ability to participate in many non-covalent interactions with biological targets makes them particularly advantageous in drug design—over 90% of newly authorized medications have at least one heterocyclic unit. Consequently, heterocyclic chemistry remains pivotal in research that connects chemistry and biology, yielding several significant scientific advancements.The intramolecular [3+2] cycloaddition (IMDC) process of a nitrone–alkene system, originating from m-allyloxybenzaldehyde, was investigated using Density Functional Theory (DFT) at the B3LYP/6-31G(d) level. The calculated energy profiles indicate a distinct kinetic favorability for the synthesis of the fused-endo product, consistent with experimental findings. Solvent effects somewhat increase the activation barrier and decrease the total exothermicity, but have little influence on the reaction route or selectivity. The Electron Localization Function (ELF) analysis reveals that bond formation (C–O and C–C) in the preferred fused-endo route occurs via a synchronous but non-concerted one-step process. Additionally, investigations of the transition state using Non-Covalent Interaction (NCI) and Quantum Theory of Atoms in Molecules (QTAIM) indicate a stabilizing hydrogen bond that likely influences the selectivity towards the fused-endo product.

Keywords – Reactivity, Molecular mechanism, Selectivity, MEDT, NCI,DFT

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Theoretical Investigation of Ferrocenylmethylaniline Derivatives as α-Amylase Inhibitors: Molecular Docking and Dynamics Insights

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Abstract **–** This study presents a theoretical investigation into the inhibitory potential of three ferrocenylmethylaniline derivatives—FMBA, FMAA, and FMA—against the α-amylase enzyme, a key target in the treatment of type 2 diabetes. Molecular docking simulations revealed strong binding interactions at the catalytic site, with FMBA exhibiting the highest binding affinity (−7.33 kcal/mol), followed by FMAA and FMA, and significantly outperforming the reference drug acarbose.
To evaluate the stability and behavior of these enzyme–ligand complexes, molecular dynamics (MD) simulations were conducted over a 100 ns timescale. The results demonstrated that FMBA and FMAA form highly stable complexes with α-amylase, supported by low root mean square deviation (RMSD) values and stable hydrogen-bonding networks. Structural analyses using root mean square fluctuation (RMSF), radius of gyration (Rg), and solvent-accessible surface area (SASA) confirmed the compactness and conformational stability of the ligand–enzyme interactions throughout the simulation trajectory.
Together, these findings offer valuable insight into the molecular basis of α-amylase inhibition by ferrocenylmethylaniline derivatives and highlight their potential as lead candidates for further optimization in antidiabetic drug design.

Keywords – Ferrocenylmethylaniline, α-Amylase inhibition, Molecular docking, Molecular dynamics simulation, Antidiabetic drug design

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Molecular Docking and Quantum Chemical Analysis of Curcumin Derivatives as CDK2 Inhibitors

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Abstract – This study investigates the molecular interactions of curcumin and its derivatives with cyclin-dependent kinase 2 (CDK2) through molecular docking simulations using the Glide module from Schrödinger. The work aims to assess the binding affinity and stability of curcumin in its enol and anti-diketone forms compared to a co-crystallized ligand. Docking results show that cur-enol demonstrates the highest binding affinity among the derivatives, with a score close to that of the reference ligand. Key interactions such as hydrophobic contacts, hydrogen bonds, and electrostatic forces with critical CDK2 residues (PHE 80, LEU 83, ASP 86, and LYS 33) contribute to the complex stability. Quantum chemical calculations using the DFT/B3LYP method further confirm the superior antioxidant activity and structural stability of the enol form. These findings highlight the potential of curcumin derivatives as promising CDK2 inhibitors for therapeutic applications.

Keywords – Curcumin derivatives, Molecular docking, CDK2 inhibitors

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Studies of new therapeutic strategies by molecular modeling

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Abstract

Inhibition of the Cdc25 phosphatase is a promising area of research, particularly given its role in the cell cycle and its involvement in certain pathologies, including cancer. Understanding the interactions between enzymes and their substrates is essential for the development of new inhibitors and for biomedical research. Molecular modeling can help predict the binding mode of inhibitors to the enzyme and assess their potential efficacy.

As part of our work, the interaction between bioactive structures will be studied using molecular modeling methods (MM, DM, Docking) by the Molecular Operational Environment (MOE) program. We aim to determine the interaction mode of the complex for the binding of different inhibitors to the enzyme, with better complementarity. The complex with the lowest interaction energy will exhibit greater activity and, consequently, better inhibition. Finally, the application of Lipinski's rule will allow us to better understand the ADME properties of the proposed compounds.

Keywords – Cdc25 phosphatase, Cancer, flavonoids, ADME, Molecular modeling

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Etude ligand-based pour la conception de nouveaux inhibiteurs naturels

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Résumé – Les stilbènes sont des composés phénoliques naturels largement étudiés pour leurs propriétés anti-inflammatoires, associés à une tolérance généralement élevée. Leur activité est principalement liée à l'inhibition de la cyclooxygénase (COX), enzyme existant sous deux isoformes : COX-1 (constitutive) et COX-2 (inductible). Dans le but de concevoir de nouveaux inhibiteurs sélectifs de COX-2, plusieurs dérivés stilbéniques ont été explorés.

Ce travail a pour objectif de proposer un modèle pharmacophorique commun basé sur une série de dérivés stilbéniques à activité connue contre la COX-2.

L'étude a été réalisée selon une approche ligand-based, visant à identifier les éléments structuraux clés nécessaires à l'affinité biologique. Afin de confirmer la pertinence des interactions prédictives du modèle pharmacophorique, une étude de docking moléculaire a été effectuée en parallèle. Les résultats montrent une bonne cohérence entre les deux approches, renforçant la fiabilité du modèle proposé pour la conception de futurs inhibiteurs sélectifs de la COX-2.

Mots clés – Stilbènes, AINS, Pharmacophore, Docking moléculaire.

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Investigating the Enhanced Antioxidant Properties of Copper-Tetrahydroxystilbene Complexes: Mechanisms and Molecular Interactions

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Abstract **–** A theoretical study was performed using DFT/PW91/TZP/DMSO calculations to investigate 18 compounds formed by the complexation of copper cations (Cu+ and Cu2+) with trans-2,4,3′,5′-tetrahydroxystilbene (T-OXY) and cis-2,4,1′,3′-tetrahydroxystilbene (C-OXY). The ligand-binding sites were identified through Quantum Theory of Atoms in Molecules (QTAIM) analysis for both neutral and deprotonated ligands. Various mechanisms, including hydrogen atom transfer (HAT), sequential proton loss electron transfer (SPLET), single electron transfer followed by proton transfer (SET-PT), and bond dissociation energy (BDE(E0)) calculations, were used to assess the antioxidant activity. Among these, the BDE(E0) mechanism proved most effective for evaluating hydrogen atom transfer, revealing HAT as the predominant mechanism. Notably, anionic Cu+ complexes with trans-configured, deprotonated ligands exhibited superior antioxidant properties. One such complex, featuring a single ligand, demonstrated remarkable antioxidant activity with a BDE (E0) value of 91.47 kcal/mol. Additionally, a complex with two deprotonated ligands showed an antioxidant activity of 31.12 kcal/mol, surpassing T-OXY by a factor of 3.91 and even exceeding the antioxidant efficiency of Vitamin C, suggesting its potential as a powerful antiradical agent.

Keywords – Antioxidant activity, DFT calculations, BED(E0), AIM, HAT, SPLET, SET-PT

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Computational Identification of an HDAC2-Selective Inhibitor Using Pharmacophore Modeling and Molecular Docking

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Abstract **–** Histone deacetylases (HDACs) regulate chromatin remodeling and transcription, and their dysregulation is strongly associated with oncogenesis. Among class I HDACs, histone deacetylase 2 (HDAC2) is particularly implicated in abnormal cell proliferation when overexpressed in cancer. Although several pan- and class-selective HDAC inhibitors have been developed, their clinical translation is hampered by off-target toxicity and isoform heterogeneity, underscoring the need for isoform-selective modulators. In this study, we applied an E-pharmacophore-based virtual screening approach to identify selective HDAC2 inhibitors from a library of ~51,000 Maybridge compounds. Following initial pharmacophore mapping, candidate hits were subjected to molecular docking against HDAC2 and further evaluated across all HDAC isoforms to assess selectivity. Among the top five hits, Hit5 exhibited the most favorable binding profile, with a docking score of −12.8 kcal/mol for HDAC2, coupled with weaker binding to other isoforms. Free energy calculations (MM-GBSA: −65.0 kcal/mol) reinforced its superior binding affinity compared to the reference inhibitors SAHA and MS-275. In silico ADMET analysis revealed that Hit5 possessed excellent intestinal absorption, absence of hERG inhibition, and non-hepatotoxicity, suggesting a promising safety margin. Together, these findings highlight Hit5 as a potential HDAC2-selective lead compound with improved pharmacokinetic and toxicity profiles, offering a rational starting point for the development of targeted anticancer therapeutics.

Keywords – HDAC2, Virtual screening, E-pharmacophore, Molecular docking, ADMET

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Computational Design of 1,3,5-Triazine Derivatives as Potential PI3Kα Inhibitors for Non-Small Cell Lung Cancer

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Abstract **–** Phosphoinositide 3-kinases (PI3Ks), particularly the PI3Kα isoform, play a crucial role in regulating cell proliferation, survival, and tumor progression, and are frequently dysregulated in non-small cell lung cancer (NSCLC). In this study, thirty 1,3,5-triazine derivatives with reported anti-tumor activity against the A549 lung cancer cell line were analyzed using a field-based 3D-QSAR model developed in the Phase module of Schrödinger. The model demonstrated strong predictive reliability (R^2 = 0.930, Q^2 = 0.834), and contour map analysis highlighted key steric and electrostatic features influencing activity. These insights guided the rational design of four novel derivatives with enhanced predicted potency. In silico ADMET profiling indicated that three designed compounds exhibited improved solubility and intestinal absorption, acceptable distribution, no predicted mutagenicity, and reasonable metabolism and excretion profiles, supporting their drug-likeness. Molecular docking against PI3Kα further supported their potential, with binding scores ranging from –9.09 to –9.89 kcal·mol^{-1}, surpassing the reference compound (–8.67 kcal·mol^{-1}). Collectively, this integrated computational approach highlights 1,3,5-triazine scaffolds as promising PI3Kα inhibitors and provides a foundation for further optimization and experimental validation toward the development of novel anticancer agents targeting NSCLC.

Keywords – NSCLC, 1,3,5-Triazine derivatives, 3D-QSAR, Molecular docking, ADMET

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A Grey Wolf Optimization Algorithm–Support Vector Regression Approach for Predicting Drug Solubility in Ionic Liquids

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Abstract – Ionic liquids (ILs) are sustainable green solvents used as alternatives to conventional organic solvents because of their excellent solvation capacity for increasing drug aqueous solubility. This study performed an efficient Grey Wolf Optimization Algorithm (GWO) to refine the three hyper-parameters of a support vector regression algorithm (SVR). The outcome approach, namely the Grey Wolf Optimization Algorithm–Support Vector Regression Approach (GWO-SVR) was applied to predict the solubility of 14 pharmaceutical compounds in different pure ionic liquids, representing a dataset of 83 drug-ILs systems composed of 14 drugs, 12 cations, and 7 anions (25 ILs combinations) accounting of 13 inputs, 1 output, and 850 experimental data points (EDP). 770 EDP were used to build the model, while 80 data points were hidden as an external test. The optimized model was statistically validated with an root-mean-square error (RMSE) of 0.0114, coefficient of correlation (r) of 0.9988, coefficient of determination (R^2) of 0.9977, and robustness (Q^2) of 0.9977. The overall results proved good predictive ability and robustness.

Keywords – Solubility, Drug, Ionic Liquids, Suport vector regression, Grey Wolf Optimization Algorithm

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Complexes transition metal complexes: Theoretical study

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Abstract – Thiosemicarbazone (TSC), as well as their metal complexes, have been the subject of great interest for several years due to their diverse chemical and structural characteristics and the wide spectrum of their biological activity. Our aim using DFT calculations is to study the nature of the bond between bidenate thiosemicarbazone ligands and Ni atom in these three complexes: [$Ni(BTSC)_2$], [$Ni(Ph\text{-}BTSC)_2$] and [$Ni(Ph\text{-}ClBTSC)_2$]. DFT calculations have been carried out on the distorted square planar Nickel complexes with thiosemicabazone derivatives in order to rationalize the bond nature between the Ni metal and the N, S donor ligand.The presence of two molecular orbitals with bonding character between Ni-*S,* and *Ni-N* atoms in the occupied one and antibonding character in the virtual one reveals the covalent character in Ni-L bonding. The comparison between the free ligands and their complexes showed a variation at C-N, N-N, and C-C bonds lengths that explained by the back- donation from nickel atom into acceptor ligand orbital.

Keywords – DFT, EDA, thiosemicarbazone, Nickel complexes, Nickel-ligand bond

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Etude théorique par la DFT de l'activité antioxydante et propriétés des dérivés de méthoxyphénols

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Résumé

De nos jours, le stress oxydant constitue un sujet très important dans les recherches médicales à cause de son implication dans diverses pathologies humaines, tels que l'athérosclérose, cancers **,** maladies cardiovasculaires **,** pathologies neurodégénératives et autres **.**

La théorie fonctionnelle de la densité a été appliquée pour analyser le mécanisme antioxydant préféré de deux composés antioxydants réactifs dérivés des méthoxyphénols, à savoir le composé A et le composé B. Leurs descripteurs de réactivité globale ont été calculés pour révéler leur réactivité en tant qu'antioxydant. Il existe plusieurs mécanismes pour l'action de piégeage des radicaux libres des antioxydants, et il a été signalé que l'enthalpie de dissociation de la liaison O-H (BDE), le potentiel d'ionisation adiabatique (IP), l'enthalpie de dissociation des protons (PDE), l'affinité des protons (PA) et l'enthalpie de transfert des électrons (ETE) sont des facteurs importants qui peuvent déterminer les voies thermodynamiquement préférées pour le piégeage des radicaux libres. Les descripteurs calculés correspondent étroitement aux éléments de preuve expérimentaux. Il a été constaté que le transfert d'atomes d'hydrogène (HAT) est plus favorisé dans les milieux gazeux.

Mots clés : Activités antioxydantes, DFT, Méthoxyphénols, HAT

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Probing the reactivity of an Acylhydrazone Derivative: A DFT Study via FMOs, MEP and Fukui function analyses

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Abstract –

Acylhydrazone derivatives represent a significant class of organic compounds with broad biological activities. Understanding of their reactivity is essential for rational drug design. In this study, we employed density functional theory (DFT) to elucidate the electronic properties and molecular reactivity of (E)-N'-(2-hydroxybenzylidene)-2-((3-(trifluoromethyl)phenyl)amino)benzohydrazide, using three complementary approaches: molecular electrostatic potential (MEP), frontier molecular orbitals (FMOs), and Fukui functions. The calculations were performed at the B3LYP/6-311G(d,p) level. Molecular electrostatic potential (MEP) analysis visualizes the electrostatic potential distribution and reveals regions of electron density accumulation and depletion. MEP mapping shows that negative potential regions are located on the oxygen atoms of the carbonyl and hydroxyl groups and the fluorine atoms of CF_3. The positive regions are located around all the hydrogen atoms. FMO's analysis indicated that the HOMO is mainly delocalized across diphenylamine, representing an electron-rich region available for donation. The LUMO was concentrated throughout the hydrazine linkage and adjacent aromatic system, marking it as the favored site for electron acceptance. Furthermore, local reactivity descriptors from Fukui functions revealed that the nitrogen atoms within the diphenylamine and terminal hydrazine moieties are the most probable sites for electrophilic attack. Conversely, the imine and carbonyl carbons of the hydrazine linkage were identified as the strongest electrophilic centers, susceptible to nucleophilic attack. This work offers valuable information for predicting the reaction mechanisms of this acylhydrazone, contributing essential insights for future molecular design in materials and pharmaceutical sciences.

Keywords – Acylhydrazone, HOMO, LUMO, Fukui functions, reactivity sites

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Prédictions théoriques des réponses en Optique Nonlinéaire des complexes d'hydrure de perméthylpentalene de lithium

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Abstract **–** Les métallocènes sont des composés organométalliques caractérisés par leur structure sandwich où un ou plusieurs atomes métalliques (Fe, Ti, Zr,.. etc.) sont pris en charge entre des ligands cyclopentadiényles (Cp, $C_5H_5^-$). L'évolution vers des structures plus complexes intégrant des ligands dicyclopentadiényles fusionnés substitués (e.g., perméthylpentallène, Pn* : C_8Me_6), des hydrures pontants (μ_2 -H, μ_3 -H) et des ligands supplémentaires (Thf, CO, etc.) confère à ces matériaux des propriétés chimiques remarquables, ainsi des propriétés structurales et électroniques uniques, offrant un potentiel d'applications dans des domaines tels que l'Optique Nonlinéaire (ONL) et la conversion d'énergie.

Ce travail se concentre sur la prédiction du comportement et des réponses ONL des complexes d'hydrure de perméthylpentalène de lithium du groupe 4 ($Pn^*M_2H_yLi.thf_x$, M= Ti, Zr et Hf) en analysant leur première hyperpolarisabilité à différentes intensités du champ électromagnétique externe par des calculs DFT, TD-DFT et SOS. Ces calculs effectués au niveau ωB 97 XD/ 6-311 g+(d)/SDD dans les régimes statique et dynamique, ont révélé des variations significatives des propriétés ONL en fonction de la longueur d'onde, de la nature du métal (Ti, Zr, Hf) et du nombre de ligands Thf . Nos résultats indiquent que les systèmes à base de Zr ou Hf avec 1Thf ont montré une non-linéarité optique intéressante avec une réponse élevée en hyperpolarisabilité.

En reliant les propriétés structurales de ces complexes aux performances ONL (hyperpolarisabilité β, susceptibilité γ), permet de prédire et d'identifier des relations structure-activité pour guider la synthèse de matériaux ONL optimisés.

Keywords – Métallocènes, ONL, hyperpolarisabilité, DFT, TD-DFT,

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Molecular docking and Bioinformatics analysis of ametryn induced Alzheimer's disease mechanisms

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Abstract –
It is important to highlight the significance of interactions between herbicides and biological applications. These herbicides, such as ametryn, are widely used in agriculture, particularly in sugar cane, maize and rice crops, due to their effectiveness in eliminating weeds by inhibiting photosynthesis. However, chronic exposure to these herbicides represents a potential risk to human health. Recent studies have shown that triazines can interfere with cellular proteins.

Such as Fibronectin 1 (FN1), involved in neuronal cell adhesion and stability, they can also affect Thymidylate Synthase (TYMS), an enzyme essential to DNA synthesis, and disruption of both of these proteins are key mechanisms in the development of Alzheimer's disease. So, despite their agricultural importance, the intensive use of ametryn raises concerns about their neurotoxic effects and their potential role in increasing the risk of Alzheimer's disease.

Consequently, a simulation study has been proposed to investigate the interactions between ametryn and the proteins Fibronectin 1 (FN1) and Thymidylate Synthase (TYMS). The use of molecular docking technique. The docking calculation was performed by AutoDock vina, 3D dimensional crystal structure of thymidylate synthase TYMS and fibronectin 1 FN1 (TYMS (PDB : 1HVY) et (FN1 (PDB : 1FNF)). was obtained from the protein database http://www.rcsb.org./pdb.

The calculations of ametryn were performed on using density functional theory (DFT) with the hybrid functional B3LYP at base 6-311++G(d,p) in isolated phase , using the Gaussian 16 package.

Keywords –Ametryn, DFT, Molecular docking, PDB, Thymidylate synthase TYMS and fibronectin 1 FN1

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A comparative ab initio analysis of the stability, electronic, thermodynamic, mechanical, and hydrogen storage properties of $ScLiH_3$ and $YLiH_3$ perovskite hydrides through DFT Approaches

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Abstract: Hydrogen is considered a flexible and sustainable source of renewable energy, with promising potential in addressing climate change. Recent advancements in hydrogen generation and storage technologies have paved the way toward a cleaner and more sustainable energy future. In this context, perovskite hydrides have attracted growing attention due to their potential use as high-capacity hydrogen storage materials. These compounds offer efficient and reversible means of hydrogen absorption and release, making them promising candidates for fuel cell technologies. They are characterized by tunable structures[1] and diverse physical properties, which contribute to overcoming the challenges faced by the hydrogen economy and support the development of clean and sustainable energy solutions. In this study, a detailed theoretical investigation of the physical properties of the perovskite hydrides AliH3 (A = Sc, Y) was conducted using the full-potential linearized augmented plane wave (FP-LAPW) method. Structural and thermodynamic dynamical stability were analyzed based on the calculated tolerance factor and formation energy. The generalized gradient approximation (GGA) and local density approximation (LDA) were employed to describe exchange–correlation effects, while the electronic and optical properties were calculated using the modified Becke–Johnson (mBJ) potential. The results revealed direct band gaps of 1.04 eV for ScLiH3 and 1.02 eV for YLiH3, confirming the semiconducting nature of these compounds. Furthermore, the optical properties of $ALiH_3$ were thoroughly investigated, and the results showed strong absorption in the visible range, indicating their strong potential for use in renewable energy applications such as solar cells and power electronics.

Keywords: *renewable energy, (FP-LAPW) method, clean and sustainable energy, electronic and optical properties.*

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A Comparative Study on Heavy Metal Complexation with Biodegradable Chelating Agents EDDM and EDDG

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Abstract – This study investigates the complexation of transition and heavy metals (M=Co, Ni, Cu, Zn, Cd, Hg) with biodegradable aminopolycarboxylic acids (APCAs), EDDM and EDDG, as potential replacements for traditional chelating agents like EDTA. Using Density Functional Theory (DFT) with the PBE functional and TZP basis set, we optimized the geometries of $[M\text{-}EDDM]^{2-}$ and $[M\text{-}EDDG]^{2-}$ complexes, comparing them with $[M\text{-}EDTA]^{2-}$ analogues. The study revealed variations in coordination numbers and geometries, with some complexes showing Jahn-Teller distortion or distorted square-pyramidal structures. Key findings indicate that zinc complexes ($[Zn\text{-}EDTA]^{2-}$, $[Zn\text{-}EDDM]^{2-}$, and $[Zn\text{-}EDDG]^{2-}$) are the most stable, while mercury complexes are the least stable. Overall, $[M\text{-}EDDG]^{2-}$ complexes demonstrated the highest stability, followed by $[M\text{-}EDTA]^{2-}$ and $[M\text{-}EDDM]^{2-}$. Reactivity descriptors, UV-Vis spectra, and QTAIM analysis provided insights into electronic structure and bonding, highlighting the strong electrophilic character of mercury complexes and the hardness of zinc complexes. Energy Decomposition Analysis (EDA) and ETS-NOCV analysis were employed to elucidate the nature of metal-ligand interactions, quantifying the contributions of electrostatic, steric, and orbital interactions to the overall bonding. This comprehensive computational study provides valuable information for the design and optimization of biodegradable chelating agents for heavy metal remediation.

Keywords – DFT, TZP, APCAs, EDDM, EDDG, EDTA

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A Computational Study on the Heat of Decomposition of Various Chemical Compounds

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Abstract **–** Quantitative Structure–Property Relationship (QSPR) studies serve as powerful tools for predicting the physicochemical properties of chemical compounds based on their molecular structure. In this work, a theoretical QSPR model was developed to predict the heats of decomposition of selected chemical compounds. The model was constructed using multiple linear regression (MLR) analysis. A dataset of compounds was split into training and test sets using the Kennard–Stone algorithm (CADEX) to ensure robust external validation. Molecular descriptors were calculated using the Dragon software, and relevant variables were selected through a Genetic Algorithm coupled with Variable Subset Selection (GA–VSS). A low-dimensional model was generated and applied to predict the decomposition heats of the test compounds. A strong correlation was observed between the predicted and experimental values, demonstrating the model's predictive reliability. The applicability domain of the MLR model was evaluated using a Williams plot to identify outliers and compounds outside the model's reliable prediction space.

Keywords – Applicability domain; low-dimensional model; heat of decomposition; multiple linear regression; QSPR modeling.

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Pharmacophore-Based Virtual Screening and Computational Evaluation of Quinone Derivatives as Potential Colorectal Cancer Therapeutics

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Abstract:

Colorectal cancer (CRC) is the third most frequently diagnosed malignancy worldwide and remains a leading cause of cancer-related mortality [1,2]. Despite advances in chemotherapy and targeted therapies, the prognosis for patients with advanced CRC remains poor, underscoring the urgent need for novel and more effective therapeutic options [3]. Quinone derivatives have emerged as promising candidates due to their diverse pharmacological activities, particularly their anticancer potential mediated through redox cycling and modulation of key signaling pathways [4,5]. In this study, we employed an integrative in silico strategy to evaluate a series of quinone derivatives as potential CRC therapeutics. A pharmacophore model was first constructed to define essential structural features associated with bioactivity, followed by virtual screening to prioritize promising candidates. Subsequently, molecular docking was performed to predict binding affinities and interaction profiles with CRC-associated targets [6]. ADMET analyses were conducted to assess pharmacokinetic and safety characteristics, while density functional theory (DFT) calculations provided insights into electronic properties related to molecular reactivity [7]. To further validate the docking outcomes, molecular dynamics (MD) simulations were carried out, confirming stable and favorable binding interactions of the top-ranked ligand–protein complexes throughout the simulation period [8]. Collectively, five quinone derivatives were identified as promising leads, demonstrating strong pharmacophoric alignment, high binding affinities, favorable ADMET profiles, and stable dynamic behavior. These findings suggest that quinone-based compounds represent potential candidates for the future development of colorectal cancer therapeutics.

Keywords: *Molecular docking, Quinones, DFT, Cancer, pharmacophore model, virtual screening*

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Topic: theoretical chemistry

α-Acetoxyphenylmethylphosphonate: computational study using DFT and molecular docking as potential anti-inflammatory agent

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Abstract

Inflammation is a key pathological process underlying many chronic diseases, including arthritis, cardiovascular disorders, and neurodegenerative conditions. The identification of novel anti-inflammatory agents with improved efficacy and selectivity remains a critical challenge in drug discovery. In this study, we explore α-acetoxyphenylmethylphosphonate as a potential anti-inflammatory candidate through an integrated computational approach combining Density Functional Theory (DFT) and molecular docking.DFT calculations were employed to optimize the molecular geometry and investigate electronic properties, including frontier molecular orbitals, charge distribution, and global and local reactivity descriptors. These analyses provide detailed insights into the reactive sites, chemical stability, and potential interactions of the compound. Subsequently, molecular docking simulations were conducted against key inflammation-related protein targets, such as cyclooxygenase-2 (COX-2), to predict binding affinities, interaction modes, and critical residues involved in ligand recognition.The results indicate that α-acetoxyphenylmethylphosphonate possesses favorable electronic characteristics and forms strong interactions with active site residues, suggesting significant potential as an anti-inflammatory scaffold. Moreover, the study demonstrates how an integrated computational strategy can efficiently guide the rational design and prioritization of novel bioactive molecules. These findings lay the groundwork for future in vitro and in vivo validation studies and highlight the importance of combining quantum chemical and molecular docking methods in modern drug discovery.

*Keywords –α-Acetoxyphenylmethylphosphonates,DFT,*Molecular *docking, anti-inflammatory*

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Unveiling the Reactivity and Bioactivity of Furan α-Acetoxy Methylphosphonates: An Integrated Computational Study Using DFT, Topological Analysis, and Molecular Docking

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Abstract

Organophosphorus compounds are of considerable interest owing to their diverse applications in medicinal chemistry and agrochemicals, as well as their significance as chemical warfare agents. A detailed understanding of their fundamental properties is therefore essential. In this context, we focused our study on furan α-acetoxy methylphosphonates, a novel class of organophosphorus derivatives. This work presents a comprehensive computational investigation into their electronic structure, chemical reactivity, and potential biological activity. This study employs a robust multi-level computational approach. Density Functional Theory (DFT) is used to optimize molecular geometries and calculate global and local reactivity descriptors. Subsequently, a topochemical exploration based on the Electron Localization Function (ELF), Localized Orbital Locator (LOL), and Reduced Density Gradient (RDG) analyses is carried out to elucidate intramolecular bonding, interaction sites, and steric effects. In addition, molecular docking simulations are performed to predict the binding affinity and interaction modes of these compounds with specific biological targets, such as acetylcholinesterase (AChE). The results reveal that these derivatives exhibit strong binding interactions, suggesting that they can be considered promising anti-acetylcholinesterase (AChE) candidates.

Keywords – Furan α-acetoxy methylphosphonates, DFT, topochemical exploration, AChE, molecular design

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Enaminones as Anticonvulsant Agents: A QSAR Study

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Abstract – The conjugated system N–C=C–C=O is the conjugation system for organic compounds known as enaminones [1]. Information regarding the chemistry of enaminones, their physicochemical properties, and biological activities is provided by the literature [2].

These biomolecules have a similar mechanism of action to many classic antiepileptics and second-generation drugs, which involves blocking the passage of ions through ion channels [3].

Simple models have employed Quantitative Structure-Activity Relationships (QSAR) to explain and predict the anticonvulsant behavior of chemicals [4].

This study is aimed at predicting the antiepileptic activity of a molecular set of open-chain enaminone using an updated QSAR framework [5,6] (i.e.: Rational data splitting, external validation, robustness testing, applicability domain definition ...) which would allow us to provide some guidelines on the anticonvulsant properties of this class of molecules and to apply these relationships for the prediction of unknown open-chain compounds containing the same types of functional groups in their molecular structure.

Keywords – Open-Chain Enaminone; Anticonvulsant; QSAR; Applicability Domain; Theoretical Descriptors.

[1] A.G. Cook, Enaminas: Synthesis, Structure and Reaction; Cook, A.G., Ed.; Marcel Dekker: New York, NY, USA, 1969.
[2] A.D. Fraser, New drugs for the treatment of epilepsy, Clinical Biochemistry 1996, 29, 97, https://doi.org/10.1016/0009-9120(95)02027-6
[3] S.B. Kombian;I.O. Edafiogho; K.V.Ananthalakshmi, British journal of pharmacology 2005, 145, 945 https://doi.org/10.1038/sj.bjp.0706250
[4] Garro Martinez, C. Juan, et al. International journal of molecular sciences 2011, 12, 9354, https://doi.org/10.3390/ijms12129354
[5] A. Tropsha, Molecular informatics 2010, 29, 476, https://doi.org/10.1002/minf.201000061.
[6] P. Gramatica, Journal of Chemometrics 2025, 9, e70014, https://doi.org/10.1002/cem.70014.

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Metal mediated base pairs as sensors: DFT study

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Abstract –
In recent years, DNA and its derivatives have attracted growing attention in a wide range of field .Among these derivatives, metal-mediated base pairs in which the original hydrogen bonds between nucleobases are replaced by a center metal ion.
According to many studies, we suggest forming two new metal mediated base pairs. These complexes are based on thymine base pair linked with Cobalt [thymine-Co-thymine] and copper [thymine-Cu-thymine]. The objective of this work is to study the ability of these complexes to act as a Biosensor to detect specific molecules such as toxic agents (H_2S, SO_2, HCN, CO, CO2, NO, and NO_2). All structures are optimized at **DFT/M062X/6-311G+(d,p)** level of theory implemented in **Gaussian16** code. LanL2DZ basis set was used for cobalt and copper. QTAIM, NCI-RDG were used to anticipate nature of interaction between toxic agents and complexes

Keywords – DNA, DFT, biosensors, base pairs, sensors, intermolecular interaction.

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Molecular Docking of Novel α-Aminoamide Derivatives as Selective MAO-B Inhibitors for Parkinson's Disease

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Abstract

Parkinson's disease is a progressive neurodegenerative disorder marked by dopamine depletion. Inhibition of monoamine oxidase-B (MAO-B) is a validated strategy to sustain dopaminergic function and limit oxidative damage. In this work, a set of new α-aminoamide derivatives structurally related to a known reversible MAO-B inhibitor were prepared in silico and evaluated using molecular docking. The binding affinities and interaction profiles of these derivatives within the MAO-B active site were compared with those of the reference compound. Several derivatives displayed favorable docking scores and key interactions, suggesting that this scaffold offers promising leads for the development of next-generation MAO-B inhibitors for Parkinson's disease management.

Keywords *– Parkinson's disease; Monoamine oxidase-B (MAO-B); α-aminoamide derivatives; Molecular docking; ; Neuroprotection.*

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L'effet d'un champ électrique sur les nanotubes : déformation et propriétés électroniques

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Abstract –The recent progress achieved in the synthesis and characterization of nanostructures has been spurred by the necessity to develop growth strategies to adapt the properties of these materials for specific applications. Studies related to morphology and dimensionality control have drawn particular interest in recent years because of their increasing roles in the domains of electronic and thermal transport, along with the enhancement of different properties at the nanometer scale. This is especially important in the case of one-dimensional (1D) structures. Among 1D nanostructures, semiconductors with nanotube-like morphology have garnered a lot of interest because of their interesting properties. Nanotubes have an ideal morphology for studying electrical transport mechanisms in 1D systems, which makes them fitting for utilization in many applications such as the manufacture of nano-lasers, field-effect transistors, nano-resonators, actuators and field emitters, Several semiconductor materials have been synthesized in the form of nanotubes such as silicon (Si). indium phosphide (InP), titanium dioxide (TiO_2) oxide zinc (ZnO). The oxide semiconductor activity is focused on ZnO and its alloys. It has received considerable attention in recent years in various fields . Interest in ZnO nanotubes formed the focus of our study which was conducted specifically on the structural and electronic properties of diverse zinc oxide nanotubes using density function theory (DFT).

Keywords – DFT, ZnO, TiO_2

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A Theoretical Study on the Electrical and Nonlinear Optical Properties of Hydride Nanoclusters: Highlighting the Role of Hydride Bridge

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Abstract – In this study, we explore the geometric structures, electronic properties, and both static and dynamic nonlinear optical (NLO) characteristics of a novel series of eight nanocluster copper hydrides, $Cu_3L_xL'_yH_n$. The first hyperpolarizabilities, linked to Hyper-Rayleigh Scattering (HRS), Second Harmonic Generation (SHG), and the Electro-optic Pockels Effect (EOPE), were systematically investigated, along with second hyperpolarizabilities related to Electric-Field-Induced Second Harmonic Generation (EFISHG), Degenerate Four-Wave Mixing (DFWM), and DC-Kerr effects. These NLO properties were calculated using density functional theory (DFT), providing detailed insights into the advanced optical behavior of these nanoclusters. For the first time, we demonstrate that the presence of hydride bridges plays a pivotal role in enhancing the stability of copper nanoclusters while also significantly boosting their nonlinear optical responses. Furthermore, we identify a promising potential application of copper hydride nanoclusters in photonics, further extending their relevance to modern material and optical sciences.

References

Zaidi, M.; Hannachi, D.; Chaouia, N.; Chermette, H., New J. Chem., 2024, 48, 11812–11828. https://doi.org/10.1039/d4nj01849d.

Zaidi, M. ; Hannachi, D. ; Samsar, D. ; Hoffmann, G.; Chermette, H.;, Journal of Photochemistry and Photobiology A: Chemistry; 2025, 469, 116523 . https://doi.org/10.1016/j.jphotochem.2025.116523

Bouriche, R. K. ; Hannachi, D. ; Messai, A. ; Morell, C. ; Azizi, A. ; Chermette, A. ; New J. Chem., 2025, 49, 10730-10750, DOI https://doi.org/10.1039/D5NJ01220A

Keywords – NLO, SHG, THG, Nanoparticle, copper hydrides

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QSAR Evaluation of Titanocene Dichloride Derivatives

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Abstract **–** A QSAR study was performed on 25 titanocene dichloride derivatives tested against LLC-PK cells. The developed model proved to be robust and reliable, with strong predictive ability confirmed by internal and external validation. It was then applied to bis-methyl titanocene dichloride, whose predicted IC_{50} (7.23×10^{-4} M) showed significantly higher activity than tamoxifen substituted with titanocene.

Keywords – QSAR model, titanocene dichloride, LLC-PK.

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Exploring the Impact of Molecular Configuration on Optoelectronic Properties in Ph-subPC/C60 Organic Solar Cells

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Abstract – Organic solar cells represent a very promising technology for low-cost, flexible, and lightweight solar energy harvesting. The morphology of the donor-acceptor interface is at the heart of the performance of OSCs and is fundamentally responsible for the efficiency of charge separation and transport therein. This interface morphology and electronic structure presents a big experimental challenge toward its precise characterization and understanding.

In this regard, the design of new materials that can further optimize these interfaces is very important. This contribution deals with phenoxysubphtalocyanine-Ph-subPC, a derivative of the well-known boron subphthalocyanine chloride, subPC. The core-expanded six-membered ring in the design of Ph-subPC may further improve its electronic property compared to its forerunner. Here, we combined the newest frontier orbital energy-level molecular design for a Ph-subPC with the C60 fullerene and investigated how these new molecular arrangements at the donor-acceptor interface in OSCs affect optoelectronic properties.

In this work, we model different configurations of the Ph-subPC/C60 interface using DFT and time-dependent DFT. We name those configurations B and U, in which B represents the C60 positioned on the convex surface of Ph-subPC and U represents C60 embedded in the concave surface. We observe from simulations that changing the orientation of C60 with respect to Ph-subPC significantly influences important photovoltaic properties like absorption spectrum, open-circuit voltage, and exciton binding energy.

The current study also investigated the effect of molecular arrangement and orientation on the photoelectric performance properties, including binding energy, frontier molecular orbital energies, UV-Vis absorption spectrum, and exciton binding energy. In comparison with the subPC/C60 system, it has led to deeper insights into how variations in the molecular configuration could impact the electronic and optical performance of OSCs.

Key words*: boron subphthalocyanine chloride .DFT, TDDFT.*

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Quantitative structure activity relationship studies of 1,2,4,5-tetrazine derivatives as potential lung cancer inhibitors combining DFT calculations and statistical results

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Abstract

Lung Cancer is a malignant tumor, which threatening the human life and health. It is the most common type of all human cancers all over the world. National Cancer Institute is now investigating 1,2,4,5-Tetrazine molecule to explore their effectiveness against cancer. Numerous scientific studies have been applied QSAR methods to predict biological activity of unknown compounds. 1,2,4,5-Tetrazine and its derivatives were found to have a high potential of biological properties. Quantitative structure activity relationship (QSAR) studies and molecular modeling are valuable tools in computational chemistry and can provide invaluable information in early stages of drug design process.

A series of 18 molecules derived from 1,2,4,5-tetrazine is investigated by QSAR using electronic descriptors: HOMO–LUMO energy gap, electrophilic and nucleophilic frontier electron density (f^E, f^N) and net atomic charges (qi) and dipole moment (DM) based for the DFT in gas and aqueous phases.

Multiple linear regression (MLR) was used to establish the mathematical relationship between molecular descriptors and the biological activity of the 1,2,4,5-Tetrazine derivatives. The prediction of QSAR model obtained was confirmed by the method of LOO cross-validation.

A strong correlation between the experimental and predicted activity values was observed, indicating the reliability, robustness and model quality obtained. This model can be successfully applied to predict the affinities of new compounds, for which experimental data are unavailable.

Keywords: 1,2,4,5-Tetrazines, Antitumor activity, DFT, QSAR

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First-Principles Investigation of the Physical Properties of Ca_4SiN_4 Under High Pressure and High Temperature

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Abstract **–** We present a study of the structural, elastic, electronic and thermodynamique properties of Ca_4SiN_4 under high pressure and high temprature using the plane-wave pseudopotential method in the frame of density functional theory (DFT) within the generalized gradient approximation (GGA). Geometrical optimization of the unit cell is in good agreement with the available experimental data. The effect of high pressure, up to 20 GPa, on the lattice constants shows that the compound is more compressible along the *c*-axis than along the *a*- and *b*-axis, which makes the direction [001] more compressible than [100] and [010] directions. Ca_4SiN_4 has a large and direct band-gap (G-G) semiconductor (insolating), of 1.501 eV. The elastic constants and their pressure dependence are calculated and discussed. The bulk modulus, shear modulus, Young's modulus and Poisson's ratio of are also estimated. In addition, the mechanical stability and the elastic anisotropy of this compound are also discussed. We have also calculated the thermodynamic properties such as Debye temperature, the thermal expansion coefficient α and the capacity heat C_P and C_V in the temperature range from 0 to 900 K, where the quasi-harmonic model remains fully valid. The pressure effect is investigated in the range of 0 to 15 GPa. such as Debye temperature, the thermal expansion coefficient α and the capacity heat C_P and C_V. In conclusion, the pressure has a strong effect on physical properties of alkaline earth metalloid nitride Ca_4SiN_4

Keywords –Ternary nitrides ; Ab initio calculation ; High pressure effect; Structural properties; Elastic properties.

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Synthesis of some profen derivatives: In silico evaluation of the anti-inflammatory activity.

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Abstract – Profens, which are 2-arylpropionic acid derivatives, are non-steroidal anti-inflammatory drugs (NSAIDs), like: ibuprofen, ketoprofen and flubiprofen. They are used for treating osteoarthritis, rheumatoid arthritis, and to reduce fever due to their anti-inflammatory, anti-rheumatic and analgesic therapeutic[1]. The pharmacological effectiveness of profens is based on the ability to reduce the synthesis of prostaglandins by inhibiting cyclooxygenase (COX), especially by the (S)-(+)-enantiomer.[2] Among the described approches for the synthesis of enantiomerically enriched (S)-profens, the biocatalytic approach seems the most attractive since it fit well with the green chemistry criteria's.[3]
For this purpose, we describe herein the direct enzymatic amidation of ibuprofen, ketoprofen and flubuprofen with aromatic amines via kinetic resolution approach. The synthesized amides are characterized by spectroscopic analysis (NMR) and the enantiomeric excesses via chiral HPLC analyses. In silico evaluation of the anti-inflammatory potency of the synthesized amides is conducted via molecular docking. Further, DFT calculations were conducted for optimizing the entitles amides geometries.

Keywords *–Profens, Enzymatic amidation, anti-inflammatory activity, DFT calculation, Molecular docking*.

References:

1- Wang, Q., Qi, Y., Gao, X., et al. (2023). Recent trends and developments in the asymmetric synthesis of profens. *Green Synthesis and Catalysis*, *4*(2), 89-103.
2- Evans, A.M. (1996). Pharmacodynamics and pharmacokinetics of the profens: Enantioselectivity, clinical implications, and special reference to S(+)-ibuprofen. *J. Clin. Pharmacol. 36*, 7S–15S.
3- Zappaterra, F., Presini, F., Venturi, V., et al. (2023). Biocatalytic insights for the synthesis of new potential prodrugs: Design of two ibuprofen derivatives. *Applied Sciences*, *13*(17), 9852.

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Exploring Benzimidazole Derivatives: Anticancer Potential and Computational Insights

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Abstract **–** The study explores the synthesis and evaluation of two benzimidazole-based compounds (2 and 3) for their anticancer potential against colon cancer cells (DLD-1) and human healthy lung fibroblast cells (Wl-38). Compound 3, containing an anthracene group, demonstrated superior antiproliferative activity with an IC50 of 46.91 µM against DLD-1, while exhibiting higher selectivity for cancerous over healthy cells compared to compound 2. Computational methods, including DFT, molecular docking, and molecular dynamics, supported the experimental results, highlighting compound 3's reactivity and binding stability with the Caspase-9 protein (PDB ID: 2HQ6). These findings suggest compound 3's potential as a selective anticancer agent.

Keywords – benzimidazole, colon cancer, DFT, molecular docking, molecular dynamics

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Antioxidant property of Both forms (Enol, Anti-Diketone) of curcumin

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Abstract – The chemical structure of curcumin [(1E, 6E) -1,7-bis (4-hydroxy-3-methoxyphenyl) -1,6-heptadiene-3,5-dione], first published by Milobedzka and Lampe in 1910, was extensively studied by Heger et al. Curcumin exists in two forms: enol and anti-diketone, the enolic form is the most active, it has a great capacity to react with free radicals**.** The antioxidant properties of curcumin have been demonstrated in vitro as well as in animal studies**.**

In our paper, we theoretically study the antioxidant property of the two curcumin isomers , as well as the determination of the free radical scavenging mechanisms through different quantum chemistry method (DFT, TD-DFT, ETS-NOCV , BDE and others). Indeed, three main mechanisms are taken into consideration: the homolytic transfer of a hydrogen atom (Homolytic Hydrogen Atom Transfer: HAT), the transfer of an electron followed by that of a proton (Single Electron Transfer-Proton transfer: SET -PT) and the transfer of a proton followed by the departure of an electron (Sequential Proton Loss Electron Transfer: SPLET). These mechanisms are described by various thermodynamic parameters such as the enthalpy of dissociation of the hydrogen atom (BDE), the ionization potential (IP), the enthalpy of dissociation of the proton (PDE), the proton affinity. (PA) and the electron transfer enthalpy (ETE). The study of the reaction mechanism makes it possible to determine the most active isomer of curcumin.

Keywords: Curcumin, DFT, TD-DFT, ETS-NOCV , BDE.

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Computational modeling of elastic properties of two polymorphs of a nootropic API

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Abstract – Computer atomistic simulation were carried out to investigate the structural and elastic properties of piracetam ($C_6H_{10}N_2O$) polymorphs; a pioneering notropic active pharmaceutical ingredient that has revolutionized the pharmaceutical industry field since its development in the 1960 [1]. It is marketed as Nootropil intended for enhancement of cognitive functions,this synthetic derivative of the neurotransmitter γ-aminobutyric acid (GABA) represents the prototypical member of racetam family, caracterized by its distinctive 2-pyrrolidone nucleus [2]. The prediction of elastic properties is crucial for stability, stress and strain consideration, also in order to rationalize the manufacturing process of an active pharmaceutical ingredient in term of tablet compression. Moreover, simulation methods offer an opportunity to understand the mechanical behaviour at the atomic scale that nanoindentation techniques sometimes fail to explain [3]. Our atomistic simulations are performed by using density functional theory, as implemented in the SIESTA code, while imploying the VDW-DF approach. This accurately describes van der Waals interactions and Hydrogen bonds which are crucial for the cohesion of molecular crystals.

Keywords – polymorphism, atomistic simulation, piracetam, DFT, VDW-DF

REFERENCES

[1] E. J. C. Jie Jack Li, Drug Discovery: Practices, Processes, and Perspectives—Google Libros, Wiley & Sons, New Jersey, 2013.
[2] S. Singh, P. Goswami, S. Swarnkar, S. P. Singh, Wahajuddin, C. Nath, S. Sharma, Mutat. Res. Toxicol. Environ. Mutagen. 2011, 726, 66–74.
[3] Patrik. P Upadhayay, Structure property correlations in piracetam polytypique. CrystEngComm 2021.

TOPIC 03:

Organic Synthesis

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Development and Optimization of Proline-Derived Organocatalysts Enhanced by 2-Hydroxybenzophenone for Asymmetric Conjugate Additions

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Abstract –

Organocatalysis has emerged as a swiftly evolving domain, marked by the continuous development of novel asymmetric transformations. With the renewed prominence of L-proline as a pivotal catalyst, considerable research has focused on crafting new catalysts derived from its molecular framework. Proline functions as a nucleophile, engaging carbonyl groups or Michael acceptors to generate reactive intermediates such as iminium ions or enamines.

The Michael addition to α,β-unsaturated compounds remains a fundamental carbon–carbon bond formation reaction in synthetic organic chemistry. This work reports an organocatalytic approach achieving high enantioselectivity in the conjugate addition of nucleophilic imines to α,β-unsaturated aldehydes. Activation occurs through an iminium-ion pathway, enabling the nucleophile to add specifically to the β-position of the unsaturated aldehyde.

To refine the reaction parameters, an extensive screening was performed involving various catalysts, solvents, reactant concentrations, temperatures, and reaction durations. The optimal conditions identified were then applied to a range of α,β-unsaturated aldehydes, revealing broad substrate scope and excellent tolerance regarding alkyl chain variations while maintaining high enantiomeric excess.

Furthermore, it was discovered that 2-hydroxybenzophenone effectively facilitates the formation of an intramolecular six-membered ring via hydrogen bonding, enhancing both the reactivity of the related ketimine and the enantioselectivity in the addition reaction to α,β-unsaturated aldehydes.

Characterization of both intermediate and final products was conducted using proton and carbon NMR, high-resolution mass spectrometry, and optical rotation measurements.

Keywords – Asymmetric synthesis; Organocatalysis ; Proline-Derived organocatalysts ; Hydrogen-bond activation; Chemical auxiliary.

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The Art of Flavors through Biocatalysis

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Abstract

The enzymatic synthesis of natural short-chain esters represents an eco-friendly and efficient alternative to traditional chemical methods used in the flavor and fragrance industry. These volatile compounds are widely found in nature and are essential ingredients in food, cosmetics, perfumes, and pharmaceuticals. In this work, we investigated the use of lipases particularly Novozym 435 as biocatalysts to promote esterification and transesterification reactions of natural alcohols such as *cis*-3-hexen-1-ol and 2-phenylethanol[1]. The study explored different acetylating agents and green solvents (CPME, MeTHF, toluene) as well as solvent-free systems, aiming to improve both reaction yields and sustainability[2].

Optimization of reaction parameters, including enzyme concentration, reaction time, and the removal of water by Aquasorb, proved crucial for achieving high conversion rates. Remarkably, transesterification catalyzed by Novozym 435 provided more than 90 % conversion in green solvents, and solvent-free systems gave comparable results[3]. Water removal during esterification also enhanced conversions up to 89 % on a small scale[4]. Overall, this study demonstrates that lipase-catalyzed biocatalysis is a powerful green chemistry tool for the sustainable production of natural flavor esters.µ

KEYWORDS: BIOCATALYSIS, NOVOZYM 435, NATURAL FLAVOR ESTERS, ESTERIFICATION /TRANSESTERIFICATION, GREEN CHEMISTRY

[1]Bayoud, I., Bouzemi, N., Guo, N., Mao, X., Serra, S., Secundo, F., & Riva, S.** *Natural flavor ester synthesis catalyzed by lipases*. **Flavor and Fragrance Journal**, 2020, 35(2), 209–218

[2] Kuo, C.H., Chiang, S.H., Ju, H.Y., et al.** *Enzymatic synthesis of flavor esters in green solvents*. **Journal of the Science of Food and Agriculture**, 2012, 92(10), 2141–2147.

[3] Bayramoglu, G., Celikbicak, O., Kilic, M., & Arica, M.Y.***Immobilized lipase-catalyzed production of aroma esters in green media*. **Food Chemistry**, 2022, 366, 130699.

[4] Bourg-Garros, S., Razafindramboa, N., & Pavia, A.A.***Lipase-catalyzed synthesis of aroma esters in organic media*. **Enzyme and Microbial Technology**, 1998, 22(3), 240–245.

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Synthesis and in Vitro Biological Evaluation, DFT and Molecular Docking Studies of 3,4,5-Trimethoxyphenyl α-Acetoxymethyl Phosphonates.

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Abstract **–** In this study, we prepared novel 3,4,5-trimethoxyphenyl α-acetoxy methylphosphonates through two steps involving α-hydroxyphosphonates as precursors. The chemical structures of the synthesized compounds were confirmed by spectroscopic analyses.
The synthesized compounds exhibited promising antibacterial and antifungal properties against pathogens, including Gram-negative, Gram-positive bacteria, and fungi. TMCl displayed the highest antibacterial activity while TMPh and TMMe demonstrated the strongest antifungal activity. DFT calculations revealed that compound TMMe had the largest HOMO-LUMO energy gap. TMCl exhibited the highest electrophilicity index, correlating with its potent antibacterial activity. Molecular docking studies confirmed significant interactions between the synthesized compounds and bacterial DNA gyrase B (GyrB) as well as fungal sterol 14-α-demethylase. TMMe demonstrated the highest binding affinity (-7.2 kcal/mol) for GyrB, whereas TMPh showed strong binding affinity (-7.3 kcal/mol) for SDM14.

Keywords – 3,4,5-trimethoxyphenyl α-acetoxymethyl phosphonates, DFT, Molecular docking, antifungal activity, antibacterialactivity.

REFERENCES

[1] G. CASALINI, *LANCET MICROBE* 5 (7) (2024) 717–724.
[2] R. Abbas, M. Chakkour, *Biology* 13 (2) (2024) 78.
[3] S. Guezane Lakoud, *J. Mol. Struct*. 1327 (2025) 144216.
[4] N. Braia, *J. Mol. Struct*. 1347 (2025) 143304.

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Synthesis of novel chiral α-phenylethyl amino-esters: DFT calculations and *in silico* bioactivity investigations.

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Abstract – Chiral Aryl alkyl alcohols and derivatives constitute an important class of carbinol structural units that are widely found in high-value-added chemical products, natural products and pharmaceuticals.[1] They also serve as chiral auxiliaries or ligand for diverse asymmetric synthesis.[2]
In this context, we are focused our interest on the synthesis of some chiral phenylalkyl amino-esters. Few examples were reported in this purpose.[3-4]
In the present study, we describe an efficient synthesis of five novel α-phenylethyl amino esters using the α-mehylbenzylamine as starting material. In two steps, the novel amino esters: α-phenyldimethyl glycinate, α-phenyldiethyl glycinate, α--phenylethyl 2-morpholinoacetate and the α--phenylethyl-2-(pyrrolidin-1-yl) acetate were recovered with isolated chemical yields varied between moderate and excellent. their structures were confirmed by ^{1}H NMR, ^{13}C NMR spectra and HRMS.
DFT calculations at B3LYP 6-311G (2d, p) basis set were applied for geometry optimization, stability and reactivity studies, including HOMO/LUMO, ΔE_{GAP}, dipole moment, electronegativity and electrophilicity.
Further, *in silico* calculations of pharmacokinetic properties, toxicity and bioactivity, of the synthesized amino esters, are also reported. Finally, based on the results of the Pass prediction, a molecular docking analysis was used to evaluate their biological potency.

Keywords – α-phenylethyl amino esters, chiral building blocks, Molecular docking, DFT calculation.

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Palladium-catalyzed selective C3-H bond arylation of benzothiophene using hydroxymethyl substituent as blocking group

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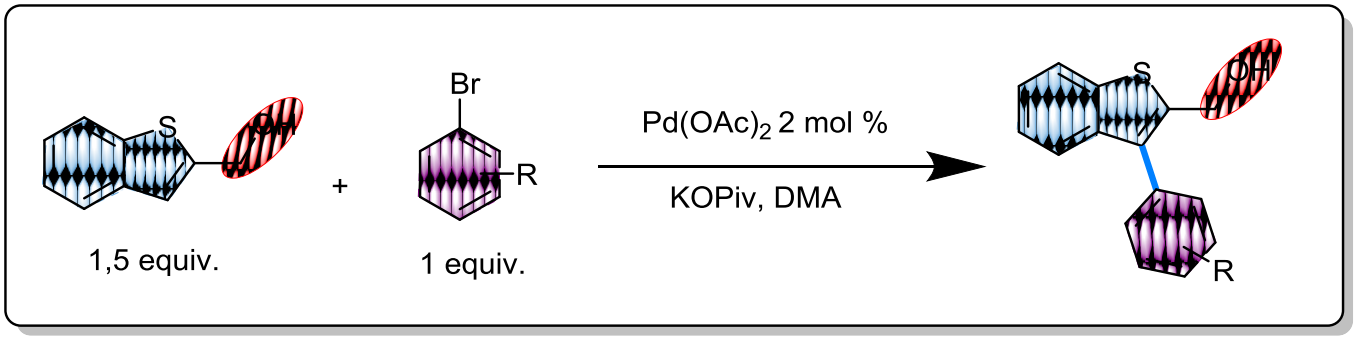
Abstract –
Benzothiophenes are important pharmaceutical motifs, appearing in a broad range of small therapeutic molecule. Therefore, the direct arylation of benzothiophene derivatives has attracted much attention in organic chemistry, therapeutic, and material science.
Palladium-catalyzed C-H bond activation currently represents an important research topic in organic chemistry.
It is known that the C2-position of benzothiophene is generally the most reactive position for reactions proceeding via concerted metalation deprotonation (CMD), while the C3-position can be arylated under specific reaction conditions or when the C2-position is blocked.
In our work, we aimed at the elaboration of a straightforward synthetic strategy to access β arylated benzothiophenes containing a C2 hydroxymethyl substituent.
We demonstrated that the unprotected 2-methanol substituent on benzothiophene in the presence of palladium acetate $Pd(OAc)_2$ as a catalyst, along with potassium pivalate KOPiv as an inexpensive base, gave the C3 arylated benzothiophenes.



Diverse substituted (hetero)aryl bromides have been used as a coupling partner, allowing access to new benzothiophene derivatives in good yields.

Keywords – Benzothiophene, synthesis, C-H bond arylation, Palladium catalysis, green chemistry.

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Antioxidant Evaluation of Furocoumarin Derivatives Using DPPH and FRAP Assays

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Abstract **–**Furocoumarins constitute a significant class of heterocyclic compounds, well known for their broad spectrum of pharmacological activities, with notable emphasis on antioxidant and anti-inflammatory properties. In the present work, four novel furocoumarin derivatives (compounds 1–4) were synthesized from a benzofuran core, and their chemical structures were elucidated using spectroscopic analyses (UV, IR, NMR).
The biological evaluation focused on their antioxidant potential, investigated through two complementary assays: the DPPH radical scavenging method and the FRAP (Ferric Reducing Antioxidant Power) test. The results revealed that all compounds exhibited relevant antioxidant activity, with one derivative in particular showing a strong radical scavenging effect and high reducing capacity, closely approaching the performance of ascorbic acid as the reference standard.
These findings highlight the promising antioxidant capacity of the synthesized furocoumarin derivatives and point to their potential as scaffolds for the development of novel therapeutic agents. Further investigations, including in vivo studies, are warranted to confirm their efficacy and safety.

Keywords – furocoumarins, benzofuran, antioxidant activity, DPPH, FRAP

TOPIC 04:

Phytochemistry

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Phytochemical Screening, Essential Oil Yield, and Antioxidant Activity of Teucrium polium L. According to Flowering Stage

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Abstract **–** Teucrium polium L. is a well-known medicinal plant recognized for its therapeutic virtues, particularly its anti-inflammatory, antimicrobial, and antioxidant properties. This study aimed to evaluate the phytochemical composition, essential oil yield, and antioxidant activity of this species at two phenological stages: before and during flowering. Phytochemical screening revealed the presence of several secondary metabolites, including flavonoids, catechin tannins, alkaloids, terpenes, and sterols, with their distribution varying according to the plant's developmental stage. Essential oils were extracted by hydrodistillation, yielding between 0.21 ± 0.05% and 0.23 ± 0.05%. The oils were light yellow in color and had a strong aromatic odor. The refractive index measured for the oil obtained before flowering was 1.497, indicating good purity. Antioxidant activity, assessed using the DPPH radical scavenging assay, showed strong free radical scavenging capacity, attributed to the species' richness in phenolic compounds. These findings confirm that T. polium is a promising natural source of bioactive substances, especially when harvested at the pre-flowering stage. Its diverse chemical composition and notable antioxidant potential support its traditional use and encourage further research for the development of pharmaceutical or nutraceutical products based on this plant.

Keywords – phytochemical; screening; Essential Oil.

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Chemical Composition and Antioxidant Potential of *Mentha longifolia* Essential Oil

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Abstract – Essential oils derived from aromatic and medicinal plants are rich in bioactive volatile compounds that can exhibit significant antioxidant properties. Among these, Mentha longifolia is traditionally valued for its therapeutic uses and biological activities. This study aimed to determine the chemical composition of M. longifolia essential oil and to evaluate its antioxidant potential using complementary in vitro assays.

The essential oil was extracted via hydrodistillation and analyzed by gas chromatography–mass spectrometry (GC–MS), which enabled the identification of its major and minor constituents. Antioxidant activity was assessed through two distinct assays: the 2,2-dipheny l-1- picrylhydrazyl (DPPH) radical scavenging method, which measures free radical neutralization capacity, and the ferric reducing antioxidant power (FRAP) assay, which evaluates electron-donating ability.

The GC – MS results revealed that the oil contained a diverse profile of monoterpenes and oxygenated monoterpenes as major components. Both DPPH and FRAP assays demonstrated that M. longifolia essential oil possesses strong antioxidant activity, comparable in some cases to standard antioxidants. These findings highlight the potential of Mentha longifolia essential oil as a valuable natural source of antioxidant agents, with possible applications in the pharmaceutical, nutraceutical, and food industries.

Keywords – Antioxidant activity, Antibacterial activity, DPPH assays, FRAP assay, Chemical composition, Essential oil .

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Antioxidant activity screening of an aromatic plant

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Abstract – Antioxidant activity plays an essential role in protecting biological systems against oxidative stress caused by free radicals and reactive oxygen species.
In this study we have studied the antioxidant activity of the leaf extract of an aromatic plant(Rosmarinus officinalis) the results shows that the extract of *R. officinalis* exhibits remarkable antioxidant activity with an IC_{50} value of 148 µg/ml, due to the phenolic compounds it contains, which can reduce DPPH radicals through hydrogen transfer comparable to the standard BHA

Excessive oxidative stress can destruct cellular components such as DNA, proteins, and lipids, leading to the development of chronic diseases including cancer, diabetes and cardiovascular disorders. Natural antioxidants, especially phenolic compounds like flavonoids, phenolic acids and tannins help neutralize free radicals, enhance the body's defense mechanisms, and maintain overall health. Therefore, the study of antioxidant activity is of great importance in medicine, nutrition, and the development of therapeutic agents.

Keywords – Antioxidant activity, leaf extract, oxidative stress

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Phytochemical Analysis and Biological Activity of Latex from Some Saharan Plants.

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Abstract –
This study evaluated the biological activities of latex from four Saharan plants (*Ficus carica, Euphorbia guyoniana, Launaea fragilis, Ipomoea asarifolia*) to explore their potential as natural alternatives to synthetic pesticides and antibiotics. Latex samples were collected in El Oued region, dried, and subjected to phytochemical analyses (total phenols, flavonoids, tannins, FRAP). Antimicrobial activity was tested against *Escherichia coli* ATCC 25922 and *Staphylococcus aureus* ATCC 25932. Insecticidal activity was evaluated against *Myzus persicae* and *Tuta absoluta*. *Ficus carica* latex contained the highest levels of phenolics and flavonoids. *Launaea fragilis* showed intermediate values, while *Euphorbia guyoniana* and *Ipomoea asarifolia* exhibited lower concentrations. *Ficus carica* showed the strongest inhibition (23 mm against *E. coli* and 14 mm against *S. aureus* at 40 mg/mL). The other species displayed weak activity (< 10 mm inhibition zones). *Ficus carica* achieved the highest mortality (DL50 = 99.67 %) against both pests. *Launaea fragilis* and *Euphorbia guyoniana* demonstrated moderate efficacy (60–75 % mortality). *Ipomoea asarifolia* showed the lowest effect (< 55 % mortality). *Ficus carica* latex is the most promising bioactive source, combining strong antimicrobial and insecticidal effects. The other plants also exhibit varying levels of potential. These findings highlight the prospects for developing natural biopesticides tailored to Saharan agriculture.

Keywords – Ficus carica , Euphorbia guyoniana , Launaea fragilis , Ipomoea asarifolia , Phytochemical analysis.

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Phytochemical Analysis and Biological Activity of *Hibiscus sabdariffa* L. Extracts.

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Abstract –
This study aims to evaluate the phytochemical content and biological activity of *Hibiscus sabdariffa* L. on four extracts using solvents of different polarities: hexane, butanol, ethanol, and water. Quantitative analyses were conducted to estimate the quantitative content of flavonoids, tannins, and total phenols in each extract, and we also performed biological activity tests to evaluate the plant's biological efficacy. The results showed that the ethanolic extract recorded the highest estimation in total phenolic content (186.3±30.20 mg GAE/g), while the butanolic extract excelled in flavonoids (63.3±0.87 µg QE/mg). The hexane extract recorded the highest estimation in terms of tannins (19.74±0.19 µg CE/mg). As for the biological activities, the ethanolic extract showed the best antioxidant activity according to the DPPH test (58.02±0.35 µg/mL), while the FRAP test recorded the strongest effectiveness of the aqueous extract. The ethanolic extract also recorded the highest (47.21±9.61) in the phosphomolybdic reductive capacity test. On the other hand, in the antihemolysis test, both the aqueous and ethanolic extracts showed the highest efficacy (~600 µg/mL) and in the anti-inflammatory test, while the ethanolic extract (15.94±1.22) exhibited the highest sun protection factor (SPF). These results clearly demonstrate the significant impact of solvent type on the extraction of biologically active compounds, and confirm that the ethanolic and butanolic extracts are the most effective options in terms of chemical content and biological activity.

Keywords – Hibiscus sabdariffa L., Plant extracts, Phytochemical content, Biological activity, Biologically active compounds.

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Phytochemicals As Natural Alternatives and Feed Additives For Poultry Health: A Pathway Towards Healthier And More Resilient Livestock

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Abstract – The excessive use of synthetic feed additives and antibiotics in animal production has raised serious concerns related to antimicrobial resistance, environmental safety, and food security. In this context, phytochemicals are increasingly recognized as promising natural alternatives, targeting gut health, growth performance, and meat quality in poultry. A survey study was conducted on phytochemical, microbiological and veterinary aspects based on reports and a comprehensive review of research published between 2010 and 2024 from international databases PubMed and Scopus, also focusing on the uses and dosages of phytochemicals such as essential oils, flavonoids, tannins, alkaloids, and saponins. Results showed that the use of lavender (*Lavandula stoechas*) essential oil in poultry at doses ranging from 24-48 mg/kg of feed improved breast meat quality. The use of oregano (*Origanum vulgare*) and thyme (*Thymus vulgaris*) oils at 200-300 mg/kg of feed improved body weight gain by 6-9% and feed conversion ratio by 4-7%. Clove oil (*Syzygium aromaticum*) at 150 mg/kg reduced the intestinal count of *E. coli* by approximately 20%. Polyphenol-rich extracts, such as green tea (*Camellia sinensis*) extract at 0.5-1 g/kg, increased dietary protein and serum antioxidant capacity. Grape seed extract at 100 mg/kg reduced abdominal fat accumulation by 8-10%. Extract of (*Quillaja saponaria*) at 125 mg/kg reduced coccidiosis by 15-18%, promoting gut health. The tannin levels of chestnut extract improve protein digestion. Optimal results are achieved using 150-300 mg/kg of essential oil and 0.5-1 g/kg of polyphenol-rich extracts. We suggest that optimize synergistic blends of diverse phytochemicals with more consistent parameters in livestock.

Keywords – Phytochemicals, Feed additives, Poultry, Food security, Health.

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THE ANTI-ALZHEIMER POTENTIAL OF AN ALGERIAN MEDICINAL PLANT FROM THE PINACEAE FAMILY

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Abstract – Alzheimer's disease, a prevalent neurodegenerative disorder predominantly observed in the elderly, was the focus of this investigation. The present study's objective was to evaluate the anti-Alzheimer efficacy and perform a phytochemical analysis of a butanolic extract obtained from an Algerian medicinal plant and belongs to the Pinaceae family.

The butanolic extract was subjected to preliminary phytochemical screening. Total phenolic content was determined using the Folin–Ciocalteu colorimetric method, while the aluminum chloride method was employed for total flavonoid content. Furthermore, the extract's in vitro butyrylcholinesterase inhibitory effect was evaluated via Ellman's method.

The plant extract's composition was determined, revealing polyphenol content of 136.1 ± 2.96 µg GAE/mg and flavonoid content of 102.98 ± 2.02 µg QE/mg. The extract demonstrated substantial anti-Alzheimer's activity through its significant inhibition of butyrylcholinesterase (BChE) with an IC50 value of 45.20±0.1 µg/ml. This value closely approximates that of the established reference compound, galantamine (IC50 = 34.75 ± 1.99 µg/ml), which is widely employed in the management of Alzheimer's disease.

The results of this study suggest that the butanolic extract, characterized by its high phenolic content, exhibits remarkable anti-Alzheimer activity compared to galantamine. This implies its potential utility as a therapeutic agent for neurodegenerative conditions. It is recommended that future research investigate the broader applications of this medicinal plant and its active constituents in the treatment of Alzheimer's disease.

Keywords – Pinaceae, butanolic extract, Flavonoids, Polyphenols, Anti-Alzheimer, BCHE

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Phytochemical Composition and Antioxidant Properties of the Aqueous Extract of Foeniculum vulgare Stems

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Abstract **–** In this study, the aqueous extract of fennel (*Foeniculum vulgare*) stems, a plant species belonging to the Apiaceae family, was analyzed to assess its antioxidant potential. The research aimed to investigate the effectiveness of this plant material as a natural source of antioxidants, thereby highlighting its importance in food and health applications.

The antioxidant activity was evaluated using the DPPH (2,2-diphenyl-1-picrylhydrazyl) radical scavenging assay, the FRAP (ferric reducing antioxidant power) method, and the total antioxidant capacity (TAC) assay based on phosphomolybdate reduction. Total polyphenol content was determined using the Folin-Ciocalteu reagent, while flavonoid content was measured by the aluminum chloride colorimetric method.

The results revealed an IC_{50} value of 720 ± 5.23 µg/mL in the DPPH assay, an EC_{50} value of 369.23 ± 3.96 µg/mL in the FRAP assay, and a TAC value of 148 ± 0.53 µg AAE/g. Furthermore, the extract contained 26.42 ± 1.47 mg GAE/g of total polyphenols and 12.56 ± 3.65 mg QE/g of flavonoids.

These findings demonstrate that fennel stems are a promising source of antioxidant compounds, supporting their potential for integration into functional foods and nutraceutical formulations.

Keywords – Foeniculum vulgare, aqueous extract, antioxidant activity, polyphenols, Flavonoid.

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Structure–Activity Relationship of Polyphenols: Integrating Antioxidant Assays with In Silico Prediction

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Abstract

Polyphenols represent a diverse class of plant-derived bioactive compounds widely recognized for their antioxidant potential and their contribution to the prevention of oxidative stress-related disorders. The purpose of this review is to explore the structure–activity relationship of polyphenols and to highlight how their chemical diversity translates into biological efficiency. The approach combines a comprehensive review of recent experimental studies assessing antioxidant capacity in vitro with an in silico perspective aimed at predicting which subclasses of polyphenols exhibit superior activity. Results from experimental assays demonstrate that phenolic hydroxyl groups, particularly when arranged in an ortho-dihydroxy configuration, strongly enhance radical scavenging activity. Moreover, flavonoids with conjugated double bonds and galloylated catechins display superior performance compared to simple phenolic acids. Furthermore, preliminary in silico docking studies against oxidative stress-related enzymes such as NADPH oxidase and lipoxygenase support these findings by showing stronger binding affinities for polyphenols with multiple hydroxyl substitutions. Ultimately, the integration of experimental evidence and computational prediction provides a more robust framework for identifying the most promising natural antioxidants. This combined strategy not only advances our understanding of structure–activity relationships but also offers valuable insights for the rational selection and valorization of polyphenols in pharmaceutical, nutraceutical, and environmental applications.

Keywords: Polyphenols; Antioxidant activity; Structure–activity relationship; In silico prediction; Natural products

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Viola: Phytochemical Study

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Abstract – *Viola odorata* is a perennial medicinal plant known for its anti-inflammatory, expectorant, analgesic, and antioxidant properties. Rich in secondary metabolites (flavonoids, alkaloids, saponins, and mucilages), it is used in herbal medicine to treat various conditions, particularly respiratory and skin disorders. Its therapeutic potential makes it a subject of growing interest in phytochemistry and pharmacology.

This work is dedicated to the phytochemical study and the evaluation of the biological activities (antioxidant, antibacterial, and antifungal) of extracts from a medicinal plant belonging to the *Viola* genus, which is part of the Violaceae family.

The results of the qualitative phytochemical analysis revealed a notable abundance of various secondary metabolites in the plant extracts, such as tannins, anthocyanins, terpenoids, and alkaloids.

Quantitative evaluation of total polyphenols and flavonoids indicated that the AcOEt and *n*-BuOH extracts contain similar concentrations.

The antioxidant potential was assessed using a range of in vitro tests, including free radical scavenging assays (DPPH and ABTS), o-phenanthroline, and ferric reducing antioxidant power (FRAP). The results showed that the ethyl acetate extract exhibited significant antioxidant activity.

The agar diffusion method was used to evaluate the antibacterial activity of the four extracts. The results revealed that the AcOEt extract demonstrated promising antibacterial activity against *Staphylococcus aureus* and *Escherichia coli*. Furthermore, the plant extracts were tested for their antifungal activity against *Fusarium oxysporum*, and the ethyl acetate extract showed satisfactory results as a fungicidal agent.

Keywords – V. odorata, phytochemistry, Antioxidant activity, Antibacterial activity, Antifungal activity.

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Chemical Composition and Larvicidal Potential of *Ruta graveolens* and *Ruta montana* Essential Oils, Individually and in Combination, Against *Culiseta longiareolata*

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Abstract **–** Mosquito-borne diseases remain a major global health challenge, demanding innovative strategies that go beyond conventional reliance on synthetic insecticides. *Culiseta longiareolata*, with its ability to transmit multiple pathogens, underscores the importance of targeting the larval stage to interrupt disease transmission. However, decades of chemical-based control have produced serious drawbacks, including environmental contamination, risks to non-target organisms, and the emergence of insecticide resistance. These limitations have accelerated interest in plant-derived alternatives. Among them, essential oils are increasingly recognized as eco-friendly candidates, combining effectiveness with sustainability and offering new perspectives for vector management.

This study evaluated the larvicidal potential of essential oils from *Ruta graveolens* and *Ruta montana*, applied individually and in combination, against *C. longiareolata* larvae. Gas chromatography–mass spectrometry (GC–MS) analysis revealed distinct chemical profiles, identifying eight compounds in *R. graveolens*, six *in R. montana*, and ten in their 1:1 mixture. Bioassay results demonstrated strong larvicidal effects, with calculated LC_{50} values confirming the potency of both single oils and their blend. Moreover, exposure to these oils significantly impaired larval metabolism, as shown by marked reductions in protein, lipid, and carbohydrate levels.

Overall, the findings highlight the promise of Ruta-based essential oils, particularly in combination, as eco-friendly alternatives to conventional chemical insecticides. Their dual action causing high larval mortality while disrupting key metabolic pathways—supports their potential application in sustainable mosquito control programs.

Keywords – Ruta montana, Ruta graveolens, Essential oils, Synergistic larvicidal activity, Culiseta longiareolata, GC–MS analysis, Metabolic disruption

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Caractérisation phytochimique et activité antioxydante des polyphénols de pois chiche (*Cicer arietinum* L.) par HPLC

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Abstract **–** This study focuses on the antioxidant activity and phytochemistry of polyphenols extracted from chickpea (*Cicer arietinum* L.), with particular attention given to their analysis by HPLC (High-Performance Liquid Chromatography).

Phenolic compounds were extracted using hydroalcoholic solvents, then quantified using the Folin-Ciocalteu method. Chromatographic analysis (HPLC) enabled the identification of several major polyphenols, including gallic acid, ferulic acid, quercetin, and kaempferol.

The antioxidant activity was assessed using DPPH and ABTS assays, revealing significant radical scavenging capacity, which correlated with the total polyphenol content.

The results confirm the potential of chickpea as a natural source of bioactive compounds, with possible applications in the agri-food, nutraceutical, and pharmaceutical fields. This study highlights the importance of advanced analytical techniques for the characterization of plant-derived substances with functional and therapeutic purposes.

Keywords – Polyphenols, Chickpea, Antioxidant activity, HPLC.

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Évaluation comparative de la composition phénolique et de l'activité antioxydante des huiles d'olive extra vierges *Chemlal* et *Arbequina*

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Abstract **–** L'huile d'olive extra vierge (HOVE), composante essentielle du régime méditerranéen, est largement reconnue pour ses propriétés nutritionnelles et thérapeutiques, attribuées en grande partie à la richesse en composés phénoliques dotés d'un fort pouvoir antioxydant. Des études récentes confirment que le facteur variétal exerce une influence déterminante sur le profil phénolique, souvent plus marquée que celle des conditions environnementales, lorsque la culture et l'extraction sont réalisées dans un cadre standardisé. Cette étude compare la teneur totale en composés phénoliques et l'activité antioxydante de deux HOVE : *Chemlal* (algérienne) et *Arbequina* (espagnole), issues d'oliviers cultivés dans la même région (El Aouana- Jijel- Algérie) et obtenues selon des conditions identiques. Les composés phénoliques ont été extraits avec un mélange méthanol/eau (80:20, v/v) et quantifiés par la méthode de Folin–Ciocalteu. L'activité antioxydante a été déterminée à l'aide de deux essais: DPPH et H_2O_2. Les résultats indiquent que, bien que les deux huiles présentent une efficacité antioxydante notable, *Chemlal* affiche de manière constante une teneur phénolique plus élevée ainsi qu'une capacité de neutralisation des radicaux supérieure dans les deux tests réalisés. En conclusion, ces observations confirment la primauté du facteur variétal dans la qualité fonctionnelle des HOVE et mettent en lumière le potentiel antioxydant renforcé de *Chemlal*. L'étude soutient la valorisation des variétés locales algériennes comme sources prometteuses d'aliments fonctionnels de haute qualité.

Keywords – Huile d'olive extra vierge, Composés phénoliques, Activité antioxydante, DPPH, H_2O_2.

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The Effect of Precursor Solution Concentration on the Structural, Optical, and Electrical Properties of Zinc Oxide Thin Films Deposited by Ultrasonic Spray Technique

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Abstract –This study systematically investigates the influence of precursor solution concentration (0.5, 1.0, and 1.5 M) on the properties of Zinc Oxide (ZnO) thin films fabricated using the ultrasonic spray pyrolysis technique. X-ray diffraction (XRD) analysis indicated that the crystalline quality of the films was significantly enhanced with increasing concentration, showing improved crystallinity and larger grain size. Optical characterization revealed that the optical transmittance in the visible range also improved for films deposited from higher molarity solutions. The optical band gap energy was found to decrease substantially with increasing concentration. The large band gap values observed at lower concentrations (0.5 M) are attributed to the quantum confinement effect occurring in the smaller-sized crystallites. Furthermore, electrical measurements demonstrated a clear enhancement in the electrical conductivity of the ZnO films as the precursor concentration increased. These results demonstrate that varying the precursor concentration is an effective method for tailoring the structural, optical, and electrical properties of ZnO thin films for specific applications in optoelectronics, such as transparent electrodes and solar cells.

Keywords – ***Zinc Oxide (ZnO), Ultrasonic Spray Pyrolysis, Solution Concentration, Thin Films, Optical Properties***

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Etude de l'influence des solvants sur l'xtraction des des composés phénolique à partir des differentes parties de *Solanum muricatum Aiton*

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Abstract – L'extraction de métabolites secondaires par l'eau, le MeOH:eau (8:2) contenant du NaF, le méthanol, l'éthanol et l'acétone (tous dilués (7:3) dans l'eau) des différentes parties (feuilles, fleurs, tiges et racines) de *Solanum muricatum* Aiton, par décoction et macération, a été étudiée. Les rendements d'extraction les plus élevés ont été enregistrés par le méthanol pour la décoction et l'acétone pour la macération. La teneur en polyphénols totaux (PPT) obtenue par décoction présentait les teneurs en PPT les plus élevées, et le MeOH contenant du NaF était le meilleur solvant pour l'extraction des PPT. La macération était adaptée à l'extraction des flavonoïdes, l'éthanol et l'acétone étant les meilleurs solvants. En général, les teneurs les plus élevées en PPT et en flavonoïdes ont été obtenues à partir des feuilles quel que soit le solvant ou la méthode d'extraction utilisé. De plus, les racines présentaient des concentrations importantes de ces composés, en accord avec l'activité antioxydante totale évaluée dans les différents organes de la plante. Dans cette étude, les solvants et les méthodes d'extraction utilisés ont permis de déterminer de manière significative le niveau d'extraction des composés bioactifs, montrant un impact différent sur les organes de la plante pour l'espèce médicinale étudiée.

Keywords – macération; décoction; teneur totale en polyphénols; flavonoïdes; activité antioxydante

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Impact of Geographical Origin on the Phytochemical content and antioxidant activities of thyme hydro-alcoholic extracts: A Tri-regional Study

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Abstract – Medicinal and aromatic plants are a rich source of various bioactive compounds, which are used in a range of fields, including medicine, pharmaceuticals, cosmetics and agro food industries. Thyme is considered to be one of the most popular herbs globally, valued for its significant medicinal and nutritional benefits.

The objective of the present study is to realize a Tri-regional comparative study; to evaluate the phenolic content, and the antioxidant properties of hydro-alcoholic extracts obtained with an innovative method of extraction from three samples of thyme collected from three different regions of Bejaia (Adekar, Feraoun, and Seddouk). These regions are chosen regarding their respective specificities: altitude 1092 m, 618 m and 340m respectively, and their climatic characteristics (Mediterranean sub-littoral climate): sub-littoral mountains (Feraoun), forest mountains (Adekar) and semiarid region (Seddouk).

Phytochemicals (Total phenolic and flavonoid content) were quantified using Folin-Ciocalteu and aluminum chloride methods, respectively. Antioxidant capacities were assessed using: DPPH, ABTS, FRAP and Ferrozine.

Quantitative estimation of phytochemicals contents showed that the extracts from the different thyme samples are very rich in these compounds. Evaluation of antioxidant activities using *in vitro* tests showed that the alcoholic extracts have remarkable antioxidant activity,but it varied greatly among the different regions.The results of this study revealed that the leaves of thyme extract collected in Adekar exhibited significantly higher antioxidant activity than the thyme extracts collected from the others.

As conclusion, the composition and the content of the valuable bioactive compounds in thyme varies considerably depending on the region in which they are harvested.

Keywords – Thyme; phytochemicals; antioxidant activities; phenolic compounds; geographical origin;

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Valorization of Plant Waste Extracts via Their Biological Activities

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Abstract

Potato peel, a plentiful agro-industrial by-product, is a valuable source of bioactive compounds associated with potential therapeutic applications. The objective of this investigation was to conduct a comparative assessment of the antioxidant, anti-inflammatory, antidiabetic, and antibacterial properties of ethanol and methanol extracts that were derived from potato peels (Solanum tuberosum).

The extracts were derived using maceration in ethanol and methanol, subsequently concentrated under decreased pressure. We used DPPH and ABTS radical scavenging assays to find out how well the substance worked as an antioxidant. We used protein denaturation and membrane stabilization procedures to find out how well it worked as an anti-inflammatory. We used α-amylase and α-glucosidase inhibition experiments to find out how well the drug may lower blood sugar levels. We used agar well diffusion to investigate the antibacterial properties against *Staphylococcus aureus*, *Bacillus subtilis*, *Escherichia coli*, and *Pseudomonas aeruginosa*. Both extracts exhibited considerable biological activity. The methanol extract showed a little bit better antioxidant power than the ethanol extract (DPPH IC_{50} = 36.08 ± 0.1 µg/mL) compared to the ethanol extract (DPPH IC_{50} = 46.32 ± 0.8 µg/mL).

On the other hand, the ethanol extract had better anti-inflammatory properties, with 79.4% reduction of protein denaturation. The ethanol extract exhibited superior inhibitory effects on both α-amylase and α-glucosidase (67%; 78%) in terms of antidiabetic activity. Antibacterial studies showed that the ethanol extract worked better against Gram-positive bacteria (S. aureus, B. subtilis) and the methanol extract worked somewhat well against Gram-negative strains (E. coli, P. aeruginosa).

Potato peel extracts, especially the ethanol fraction, have many different bioactivities, which shows that they could be useful as natural antioxidants and medicines. These findings endorse the sustainable utilization of agro-industrial waste in functional food and medicinal applications.

Keywords *– Potato peel, methanol extract, ethanol extract, antioxidant, anti-inflammatory, antidiabetic, antibacterial*

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Energy efficiency, Antibacterial and Antioxidant Activity of *Lavandula angustifolia* against Different Pathogens Isolated from Some Clinical Specimens

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Abstract **–**Some growing or spontaneously plants have been used in the treatment of various diseases. To test the effect of *Lavandula angustifolia* on bacterial strains resulting from genital infections, a study was carried out on lavender extract harvested from the Chéria region in the wilaya of Tébessa. Rotavap type steam distillation gave a yield of 15.87% of the ethanolic extract of the plant. A Clevenger type hydrodistillation gave a yield of 1.92% of the essential oil of *L. angustifolia*. The results of phytochemical tests carried out on this plant showed the presence of catechic tannins, alkaloids and flavonoids. For the test of antibacterial activity, the agar diffusion method (aromatogram) was carried out on 09 multi-resistant Gram positive and Gram negative strains. The results showed the effectiveness of lavender ethanolic extract on Gram-positive strains compared to Gram-negative strains, and the activity of the essential oil was very significant compared to the ethanolic extract. The antioxidant test by the DPPH method presented a powerful antioxidant activity of the species studied. Therapeutically, *L. angustifolia* can be used as an important alternative to antibiotics in the treatment of bacterial infectious diseases in medicine cure.

Keywords – Lavandula angustifolia, ethanolic extract, essential oil, bacterial strain, Gram positive and negative.

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Extraits d'Euphorbiaceae : source naturelle d'antioxydants pour la préservation de la qualité des denrées

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Résumé :
La conservation des aliments est un enjeu majeur pour éviter les pertes, garantir la sécurité alimentaire et préserver la qualité des produits. Aujourd'hui, on cherche à réduire l'utilisation des conservateurs chimiques. Les polyphenols des composés naturels présents dans de nombreux végétaux apparaissent comme une alternative intéressante. Dans ce contexte, nous avons procédé à l'évaluation de l'effet antioxydant et antimicrobien des différents extraits polyphénoliques d'une plante appartenant à la famille des euphorbiacées *Euphorbia helioscopia* L.

L'évaluation de l'activité antioxydante des extraits, obtenus à partir des deux parties de la plante, a été réalisée à l'aide des tests DPPH, Pouvoir Réducteur Antioxydant Ferrique (FRAP) et de la capacité antioxydante totale (CAT). Les extraits ACfff et ACt démontrent une activité antiradicalaire avec des valeurs d'IC50 de 8,50 ± 0,72 µg.ml-1 et 16,27 ± 1,02 µg.ml-1 respectivement. Cela souligne leur capacité à transférer des électrons ou des atomes d'hydrogène, et confirmant leur potentiel en tant que donneurs d'hydrogène et agents antioxydants efficaces.

Mot clé : Euphorbia helioscopia L, extraits bruts et fractions, activités antioxydantes.

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Impact of Solvent Polarity on the Antioxidant Activity and Enzyme Inhibition of a Medicinal Plant's Leaves

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Abstract

Plants are a rich source of phytochemicals such as phenolics, flavonoids, tannins, and terpenoids, which are associated with antioxidant, anti-inflammatory, antidiabetic, and antimicrobial effects. The choice of extraction solvent is critical, as solvent polarity influences both the yield and the type of phytochemicals obtained, thereby affecting biological activities. Previous studies have shown that polar solvents (water, ethanol, methanol) often extract higher amounts of phenolics and exhibit strong antioxidant activity, while moderately polar and non-polar solvents are more effective for lipophilic compounds such as terpenoids and carotenoids. Hydroalcoholic solvents, such as 70% ethanol, offer a balanced polarity, enabling the recovery of both hydrophilic and moderately lipophilic compounds, which can enhance overall bioactivity.

In this study, leaves of *a medicinal plant* were extracted using solvents of different polarity water, methanol, ethanol, 70% ethanol, acetone, and chloroform and evaluated for their antioxidant activity (DPPH, ABTS, FRAP) and enzyme-inhibitory potential (α-amylase, urease). Among all extracts, 70% ethanol showed the strongest antioxidant capacity in all three assays, although still weaker than ascorbic acid, while chloroform consistently exhibited the lowest activity. In enzyme inhibition, acetone and chloroform extracts were most effective against α-amylase, surpassing acarbose, whereas the aqueous extract showed potent urease inhibition comparable to thiourea.

These findings demonstrate that solvent polarity significantly shapes the phytochemical profile and activity of extracts. polar solvents are optimal for extracting antioxidant compounds, while non-polar and moderately polar solvents better concentrate α-amylase inhibitors, and aqueous extraction favors urease inhibitors. This underscores the importance of solvent-guided extraction in phytochemistry for therapeutic and environmental applications.

Keywords : Antioxidant activity, Enzymatic inhibition, Medicinal plant, Photochemistry, Solvents polarity.

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Investigation of the Biological activities of aqueous extract from Boraginaceae plant extract in the M'sila region

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Abstract – Medicinal plants serve as an essential source of therapeutic drugs for medical applications, as they include a diverse range of secondary metabolites and bioactive compounds that offer various therapeutic potentials. The objective of this study is to investigate the phytochemical content and explore certain biological activities of the aqueous extract of Echium sp. The extract was obtained by decoction, and the total polyphenol content was quantified using the Folin-Ciocalteu reagent technique. The antioxidant activity was evaluated using two complementary analytical techniques: the 2,2'-azino-bis3-ethylbenzothiazoline-6-sulphonic acid (ABTS) and reducing antioxidant power. The total phenolic content of the aqueous extract was found to be 90.78 ± 0.7 µg QE/mg E in dry weight expressed as gallic acid equivalents (GAE). The aqueous extract exhibited high antioxidant activity, as demonstrated by the ABTS and reducing power tests. These findings suggest that the aqueous extract of Echium sp. represents a promising candidate for the development of natural therapeutic agents. The demonstrated bioactivity necessitates further pharmacological investigation, especially within integrative and preventive medicine.

Keywords – Echium sp.; aqueous extract; polyphenol; ABTS; reducing power.

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Phenolic Compounds Extracted from Total Lipids and Their Antiradical Activity in Rapeseed (Brassica napus L.) Cultivated in Algeria

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Abstract –

Rapeseed (*Brassica napus* L.) is a major oilseed crop used for edible oil production. Besides its high oil yield, it contains phenolic compounds associated with total lipids that contribute to antioxidant activity and enhance nutritional value. However, data on Algerian rapeseed remain limited. The objective of this work is to evaluate the phenolic content extracted from total lipids and their antioxidant potential in two Algerian rapeseed samples.

Total lipids were extracted using the Folch method, and phenolic compounds were then isolated by refluxing in a methanol/water mixture (80/20, v/v) for 2 h. After liquid–liquid extraction, the phenols were recovered with ethyl acetate following the evaporation of methanol. The phenolic content was determined using the Folin–Ciocalteu reagent, and the antioxidant activity was evaluated by the DPPH assay.

The samples from Blida and Ain Defla showed total lipid phenolic contents of 449.87 mg/g and 226.75 mg/g, respectively, with corresponding antioxidant activities of 101.52 and 56.66 mg AAE/g. These results indicate that the presence of phenolic compounds in total lipids significantly contributes to antioxidant activity, playing a key role in protecting lipids from oxidation and preserving their nutritional and functional properties.

Keywords – rapeseed, phenolic compounds, total lipids, Folch method, antiradical activity.

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In Vitro α-Amylase Inhibition Potential of the Ethyl Acetate Extract from a Desert Medicinal Plant

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Abstract **–** Diabetes mellitus is a major non-communicable disease and a leading cause of mortality worldwide, affecting nearly 100 million people. The search for new hypoglycaemic agents has increasingly focused on medicinal plants and natural products, which may provide safer and more effective alternatives or complements to existing therapies. In this study, the ethyl acetate fraction, prepared alongside n-hexane and butanol fractions from the hydroalcoholic extract of the aerial parts of a desert plant belonging to the genus Senecio (Asteraceae), was evaluated for its in vitro inhibitory effect on the α-amylase enzyme. Acarbose, a well-established pharmaceutical α-amylase inhibitor, was used as the standard reference. The ethyl acetate extract (SAC) exhibited the strongest activity, with an IC_{50} of ~6.8 mg/ml, followed by SBt (~11.8 mg/ml). These findings highlight the potential of Senecio species as a source of bioactive compounds with antidiabetic properties. Further studies, including bioassay-guided fractionation and in vivo investigations, are warranted to isolate the active principles and confirm their therapeutic relevance.

Keywords – α-Amylase, Ethyl Acetate, Medicinal Plant

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Physicochemical and phytochemical study and evaluation of the antioxidant activity of extra virgin olive oil from two varieties from Jijel (Algeria)

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Abstract – The olive (*Olea europaea* L.) is one of the most important fruit species in the Mediterranean region. Mediterranean peoples considered olive oil not only an excellent food but also a healing agent.
The aim of this study is to determine certain parameters of extra virgin olive oils from two varieties in the Jijel region (Chemlal and El Hamra) by evaluating, on the one hand, the physicochemical characteristics (Acidity, peroxide value, specific UV extinction coefficient K232, K270), phytochemical characteristics (polyphenols, flavonoids, pigments, proanthocyanidins) and the chemical characterisation of the fatty acid composition by gas chromatography (GC/MS), and on the other hand, the evaluation of antioxidant activities (TAC, FRAP, DPPH).
According to the results obtained, the oils of the varieties studied have free acidity levels that meet the standards established by the IOC (≤ 0.8), which classifies them as extra virgin olive oil. The peroxide values comply with the commercial standard for both varieties studied (≤ 20 meq O_2/kg). A higher flavonoid content and more pronounced antioxidant activity (FRAP) were observed for the Chemlal variety. The fatty acid composition of both varieties studied, as determined by GC/MS, is rich in oleic acid, the major constituent.
The high quality of olive oil is attributed to its richness in unsaturated fatty acids and the presence of minor components such as polyphenols and flavonoids, known for their significant antioxidant activities.

Keywords: extra virgin olive oil, Chemlal, El Hamra, physicochemistry, phytochemistry, antioxidant activity.

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Phytochemical and Nutritional *Ptychotis verticillata* and *Thymus vulgaris* L.

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Abstract

This study evaluates the nutritional profile and phytotherapeutic potential of essential oils (EOs) extracted from *Ptychotis verticillata* (PV) and *Thymus vulgaris* L.(TV). EOs were obtained through hydrodistillation, with yields of 2.14% for PV and 1.92% for TV. GC-MS analysis identified thymol (46.03%), carvacrol (29.24%), and p-cymene (6.46%) as dominant compounds in TV, while PV contained unique bioactive constituents. Comprehensive nutritional analysis revealed slightly acidic pH values (5.02 for PV and 5.34 for TV), low moisture content (6.41% and 7.63%), significant protein levels (10.23% and 13.46%), low fat contents (2.37% and 1.57%), and predominant carbohydrates (71.85% and 67.20%) with reducing sugars contributing to energy content. Mineral content ranged between 8.34% and 8.87%, supporting physiological functions, while energy values were 322.65 and 312.77 kcal/100 g for PV and TV, respectively. The presence of bioactive terpenoids, especially carvacrol in PV and thymol in TV, links these plants to strong antimicrobial, antioxidant, and anti-inflammatory activities. The combination of nutritional and pharmacological properties indicates that a dry leaf mixture of PV and TV could be formulated as an effective phytotherapeutic infusion, providing synergistic health benefits. These findings highlight their role as functional foods with significant applications in traditional and modern phytotherapy.

- *Keywords – Ptychotis verticillata*/ *Thymus vulgaris* L./ Essential oils/ Hydrodistillation/ GC-MS analysis/ Nutritional profile

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Chemical Profiling and Evaluation In Vitro and In Silico of Antibacterial Activity of Hydromethanolic Extract from *Centaurea papposa*

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Abstract – This work focused on the plant of the genus Centaurea, a medicinal plant belonging to the family Asteraceae which is known for their antidiabetic, analgesic, and antioxidant activities. Therefore, the main objective of this study was to investigate the antibacterial activity of the hydromethanolic extract from Algerian *Centaurea papposa*. To this end, the biochemical composition of the extract was first identified through LC-ESI-MS/MS analysis. Subsequently, the antibacterial activity of the chloroform extract was assessed using the agar well diffusion method to measure the zones of inhibition against bacterial strains including *Staphylococcus aureus*, *Escherichia coli*, *Pseudomonas aeruginosa*, *Klebsiella pneumoniae*, and *Proteus mirabilis*. Additionally, the minimum inhibitory concentration (MIC) was determined to quantify the lowest extract concentration required to inhibit bacterial growth. Finally, molecular docking analysis was performed using dihydropteroate synthase as the bacterial target enzyme to explore the interactions with major phenolic compounds. Based on the results, the LC-ESI-MS/MS analyses revealed that the main constituents of Hydromethanolic extract were shikimic acid, protocatechuic acid, chlorogenic acid, hydroxybenzaldehyde, salicylic acid, and luteolin. Furthermore, the extract demonstrated strong antibacterial activity, producing inhibition zones of 20 mm against *K. pneumoniae*, and 18 mm against *P. aeruginosa*. Overall, the extract exhibited varying degrees of efficacy against all tested bacterial strains, with MICs ranging from 62.5 to 125 µg/mL. The results of molecular docking indicated that most of compounds exhibited good stability within the DHPS active site. Among them, salicylic acid emerged as the most stable compound. In conclusion, this species has shown significant efficacy of *C. papposa* against pathogenic bacteria, indicating its potential usefulness in the treatment of bacterial infections.

Keywords – Centaurea papposa, LC-ESI-MS/MS, Antibacterial activity, Molecular docking

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Évaluation de la teneur en polyphénols et de l'activité antioxydante de l'extrait méthanolique de *Cynara cardunculus* (Astéracées) de l'Est algérien

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Abstract –

Le cardon (*Cynara cardunculus* L.) est une plante méditerranéenne appartenant à la famille des Astéracées, réputée pour ses usages alimentaires et ses propriétés médicinales traditionnelles. Riches en composés phénoliques, ses différentes parties constituent une source prometteuse d'antioxydants naturels. Cette étude vise à évaluer le potentiel phytochimique et antioxydant de l'extraits méthanolique de la partie aérienne de *Cynara cardunculus* récolté dans la région de l'Est algérien.

La partie aérienne de la plante a été séchée, broyée puis extraite par macération au méthanol. La teneur phénolique totale a été déterminée par la méthode de Folin-Ciocalteu et exprimée en équivalent acide gallique (EAG). La teneur en flavonoïdes totaux a été quantifiée par la méthode au trichlorure d'aluminium et exprimée en équivalent catéchine (EC). Le pouvoir antioxydant a été évalué in *vitro* par deux tests complémentaires : le test de piégeage du radical libre DPPH (2,2-diphényl-1-picrylhydrazyl) et le test FRAP (Ferric Reducing Antioxidant Power).

Les analyses phytochimiques ont révélé des teneurs significatives en polyphénols et en flavonoïdes. Les polyphénols ont présenté une teneur importante de 56,594±0,031mg EAG/g d'extrait et les flavonoïdes ont montré une concentration de 48,626±0,0169 mg EC/g d'extrait. Conformément à ces résultats, l'extrait éthanolique a également démontré une activité antioxydante très importante, avec un pouvoir piégeur du DPPH significatif (CI50 =59,58±4,00 µg/mL) et une capacité réductrice non significative (valeur FRAP >200 µg/ml).

Cette étude met en évidence le riche potentiel en composés bioactifs de *Cynara cardunculus* issu de l'Est algérien, confirmant son statut de source naturelle d'antioxydants. Ces résultats encouragent une valorisation de cette espèce végétale indigène et justifient des investigations plus poussées, notamment l'identification des composés phénoliques majeurs et des tests d'activité biologiques in *vivo*.

Keywords – *Antioxidants, Cynara Cardunculus, extraits méthanolique, Flavonoïdes, polyphénols.*

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Mosquito Larvicidal Activity of Two Algerian *Ruta* Species: Insights into Essential Oils and Ethanolic Extracts

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Abstract **–** Mosquitoes are major vectors of diseases, and the emergence of insecticide resistance necessitates the exploration of eco-friendly alternatives. In this context, the present study investigates the larvicidal potential of two Algerian *Ruta* species, *Ruta chalepensis* and *Ruta montana*, with a particular focus on their essential oils (EOs) and ethanolic extracts (EEs). Aerial parts of both species were collected during the fruiting stage from Mila, northeastern Algeria. EOs were obtained through hydrodistillation using a Clevenger apparatus, while EEs were prepared by maceration with 80% ethanol followed by lyophilization. Larvicidal assays were performed against fourth-instar larvae of *Culex pipiens* biotype *molestus*, reared under controlled laboratory conditions. Bioassays were conducted according to WHO protocols, testing a range of concentrations. Mortality was recorded at different time intervals, and LC_{50} values were calculated. The results highlighted a pronounced difference between EOs and EEs. The EO of *R. montana* exhibited the strongest larvicidal activity with an LC_{50} of 27.09 ppm, followed by *R. chalepensis* EO (LC_{50} = 31 ppm). In contrast, ethanolic extracts were far less potent, with LC_{50} values of 552.19 ppm for *R. montana* and 593.38 ppm for *R. chalepensis*. These findings emphasize the superior insecticidal efficiency of essential oils, particularly from *R. montana*.
Overall, the study provides novel insights into the bioactivity of Algerian *Ruta* species and supports their potential as promising sources of botanical larvicides for sustainable mosquito control strategies.

Keywords – Ruta chalepensis, Ruta montana, mosquito control, larvicidal activity, Culex pipiens

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Impact of Raw and Steamed Turnip Enrichment on the Physicochemical Characteristics of White Cheese

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Abstract – The aim of this study was to compare the physicochemical properties of white cheese, cheese enriched with raw turnip, and cheese enriched with steamed turnip. The results showed significant differences among the samples. unenriched cheese had the lowest total polyphenol content (0.38 ± 0.01 mg gallic acid equivalent/g fresh matter(FM)), while enrichment with steamed turnips increased the value to (0.73 ± 0.01 mg gallic acid equivalent/g FM), and the addition of raw turnips resulted in the highest value (1.15 ± 0.03 mg gallic acid equivalent/g FM). Titratable acidity followed a similar trend: it was lowest in plain cheese (27.0 ± 0.0 °D), intermediate in raw turnip cheese (36.0 ± 0.0 °D), and highest in steamed turnip cheese (40.5 ± 0.0 °D). Total sugars nearly doubled with raw turnips (14.08 ± 0.04 mg glucose equivalent/g FM compared to 7.01 ± 0.08 mg glucose equivalent/g FM for the control), while steamed turnips also produced an increase (12.29 ± 0.04 mg glucose equivalent/g FM). Moisture content remained relatively stable across treatments, ranging from 51.9 ± 0.1 % to 52.9 ± 0.0 %. Finally, ash content increased from 1.04 % in plain cheese to 1.74 % in cheese enriched with steamed turnips. These findings suggest that raw turnip enrichment enhances polyphenols and sugars, while steaming particularly increases acidity and mineral content.

Keywords – enrichissement – turnip –steaming traitment – polyphenol- white cheese.

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Phytochemical Profile and Therapeutic Applications of Artemisia judaica: A review

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Abstract *– Artemisia judaica*, an aromatic medicinal plant, is widely recognized for its rich phytochemical profile and diverse biological activities. Traditionally used in folk medicine, it contains flavonoids, phenolic acids, sesquiterpene, lactones, and volatile oils that contribute to its strong antioxidant, antimicrobial, and anti-inflammatory properties. Methodologies in recent studies include extraction and in vitro and in vivo evaluations of antioxidant capacity, antimicrobial efficacy against bacterial and fungal pathogens, and pharmacological testing in animal models for diabetes, wound healing, and liver protection. Results demonstrate significant antioxidant activity, inhibition of pathogenic microbes, antidiabetic, anti-inflammatory effects, and cytotoxicity against cancer cell lines. These findings highlight Artemisia judaica's potential as a nutraceutical agent for promoting health and as a source for novel pharmacological therapies. Further research is warranted to explore its clinical applications and mechanisms of action.

Keywords –Artemisia judaica, phytochemical, antioxydant activity, antimicrobial effects

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Phenolic content, Antioxidant and Photoprotective Properties of Algerian Echium paniculatum Lag. Extracts in-vitro

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Abstract **–**This work aims to explore the phenolic composition and evaluate the antioxidant and photoprotective activities of ethanolic (EtE) extracts of Algerian *Echium paniculatum* Lag. aerial part, precisely in Batna (north east of Algeria). Total phenolics and flavonoids contents were determined by spectrophotometric methods using Folin-Ciocalteu and aluminium chloride respectively. The antioxidant activity was evaluated using two methods in vitro: the DPPH (2,2-diphenyl -1-picrylhydrazyle) test and the reducing power assay and the photoprotective action was also determined by measuring the sun protection factor (SPF) using spectrophotometric method. the phytochemical study revealed a predominance of total polyphénols (97,278 ± 1,134 µg EAG/mg extract) and flavonoids (39,167 ± 1.258 µg EQ/mg extract). The ethanolic extract of this plant showed an interesting anti-radical and anti-oxidant activity with IC_{50} (50,01 ± 1,09 µg/mL) for DPPH and $A_{0,50}$ (47,74 ± 2,66 µg/mL) for reducing power assay. This extract showed a sun protection factor (SPF) of 37.77 ± 0.3, corresponding to a level of high protection as recommendation of Commission of the European Communities. This study shows that *Echium paniculatum* extracts possess a strong antioxidant activity, which is probably due to their phenolic composition and could be a good candidate for use in natural sunscreens. Therefore, this plant can constitute a promising source of bioactive compounds for various applications. It would be interesting to support this work throw the purification and identification of the different molecules.

Keywords –Echium paniculatum Lag., Phenolic compounds, Flavonoids, Antioxidant activity, SPF, in vitro.

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Criblage phytochimique et propriétés antioxidant spécifiques de Pistacialentiscus L.

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Abstract – Notre étude vise à réaliser un criblage phytochimique et évaluer les activités antioxydantes des extraits de Pistacia lentiscus L. par les méthodes DPPH et TAC. Les feuilles de plants femelles ont été collectées dans la forêt de Canastel, Oran (Algérie). Deux techniques d'extraction ont été comparées : macération et ébullition sous reflux dans l'eau. Les composés polyphénoliques totaux, tanins condensés et flavonoïdes ont été quantifiés par spectrophotométrie. L'extrait hydroalcoolique présente les teneurs les plus élevées en composés phénoliques et les activités antioxydantes les plus puissantes. Les tanins condensés constituent les constituants phytochimiques les plus abondants, suggérant leur responsabilité dans les activités biologiques observées. Ces résultats justifient l'utilisation des extraits de P. lentiscus en phytothérapie pour traiter les maladies digestives et ouvrent de nouvelles perspectives de valorisation. Notre étude contribue à la valorisation du patrimoine végétal algérien et fournit des bases scientifiques pour l'exploitation thérapeutique de cette espèce méditerranéenne traditionnellement utilisée en médecine populaire.

Keywords – Keywords: Pistacia lentiscus L , macération, DPPH , activités antioxydantes .

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Algerian *Centaurea sp*: Phytochemistry and *In vitro* Antioxidant, Dermatoprotective and Antidiabetic Activities

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Abstract – Asteraceae, also called Compositae, the aster, daisy, or composite family of the plant order Asterales, is one of the biggest and important plant families, which embraces more than 1620 genera and 23.600 species of herbs, shrubs, and trees. With roughly 250 species, Centaurea is a significant genus within the Asteraceae family. The present study aimed to evaluate the phytochemistry and *in vitro* antioxidant, Dermatoprotective and, antidiabetic activities of ethyl acetate and *n-butanol* extracts of *Centaurea sp*. Antioxidant properties of this plant were assessed using different methods: 2, 2-diphenyl-1-picrylhydrazyl (DPPH), 2,2′-casino-bis (3-ethylbenzothiazoline)-6-sulfonate (ABTS), O-phenanthroline, and FRAP assay. Dermatoprotective effect was estimated by sun protection factor (SPF) assays. Total bioactive contents were determined with a spectrophotometric method. The plant extract revealed high amounts of flavonoids, flavonols, and total phenolics for the ethyl acetate extract (182.08±5.15 and 115.93±6.67 QE/mg fraction, 534.49±4.55 µg GAE/mg fraction, respectively) and *n*-butanol extract (98.05±5.74 and 23.49±0.56 QE/mg fraction, 274.78±4.28 µg GAE/mg fraction, respectively). Furthermore, the results indicate that the ethyl acetate extract was so effective in scavenging ability on DPPH and ABTS (IC_{50}=10.90±2.66 and 13.21±1.04 µg/mL). It exhibited a strong reduction of Fe^{3+} with an $A_{0.50}$ value of (1.11±0.02µg/mL), compared with *n*-butanol extract (IC_{50} =69.16±1.71µg/mL), and BHA and BHT ($A_{0.5}$=0.93±0.07 and 2.24±0.17µg/mL, respectively). In the FRAP assay, the antioxidant activity was important with an $A_{0.5}$ (15.68±1.08µg/mL) compared with the standard solution ($A_{0.5}$ = 8.41±0.67 µg/mL) and Vitamin C ($A_{0.5}$ = 9.01±1.46 µg/mL). The anti- α amylase potential was assessed using the iodine/potassium iodide method. The results reveal that the ethyl acetate extract exhibited the strongest α-amylase inhibitory activity. Moreover, *Centaurea sp* showed high Dermatoprotective activity in both extracts. As a result, the findings of our work reveal the possibility of using *Centaurea sp* as an antioxidant and sunscreening agent.

Keywords – Centaurea sp; Antioxidant activity; Dermatoprotective activity; anti- α amylase.

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Étude phytochimique et bioactivité d'extraits d'une plante aromatique et médicinale de la flore algérienne

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Abstract **–** Les résultats des recherches conduites concourent à démontrer les effets néfastes des médicaments à base des produits chimiques pour l'organisme de l'être humain et l'importance et l'efficacité des plantes médicinales et des produits provenant de l'agriculture biologique. Cependant, l'évaluation des propriétés phytothérapeutiques comme antioxydant et antimicrobienne, demeure une tâche très intéressante et utile, en particulier pour les plantes d'une utilisation rare ou non connues.

Ce travail vise la détermination de la composition chimique des extraits d'une plante aromatique et médicinale de la flore Algérienne « Ammoides verticillata » ainsi que la détermination de son pouvoir antibactérien in vitro sur des souches pathogènes multi résistantes puis l'évaluation du pouvoir antioxydant. Les résultats de l'analyse GC-MS montrent que l'Huile Essentielle d'Ammoides verticillata est riche en phénols (Thymol : 58,5 %), et l'analyse CPLH de son extrait polyphénolique a confirmé sa richesse en composés phénoliques. L'activité antimicrobienne de l'huile essentielle d'A.vertecillata riche en thymol s'est révélée antibactérienne à faible concentration, elle inhibe la croissance des cinq souches bactériennes testées avec des zones d'inhibition de diamètres variables. Les extraits d'Ammoides verticillata ont été trouvés comme des antioxydants efficaces puisque les valeurs des CI50 trouvées étaient légèrement inférieures à celle d'acide ascorbique.

Keywords – Ammoides verticillata ; GC-MS ; CPLH; Thymol ; CI50.

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Phytochemical Profiling of *Pituranthos Scoparius*: GC-MS Analysis, Analgesic and Anti-Inflammatory Activity

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Abstract – *Pituranthos scoparius* (Apiaceae), an endemic Saharan plant commonly found in the arid regions of Algeria, has long been used in traditional medicine to relieve pain, inflammation, and digestive disorders. This study focuses on evaluating its therapeutic potential through the analysis of essential oils extracted using various techniques, particularly microwave-assisted extraction, a more sustainable and efficient alternative to conventional methods.

The chemical composition of the essential oils was identified and characterized using Gas Chromatography–Mass Spectrometry (GC-MS), revealing a predominance of Dillapiol (16.38-37.21%), α-Pinene (0.48-10.84%) and Myristicin (4.21-9.37%), all recognized for their anti-inflammatory and antioxidant properties. The biological activities of the extracts varied depending on the extraction method, showing the impact of technical parameters on pharmacological performance. The essential oil exhibited significant anti-inflammatory and analgesic effects, as confirmed by in vivo tests. Its antibacterial activity, while moderate, was still notable.

These findings validate the traditional uses of the plant in Saharan communities and suggest its potential integration into the development of herbal medicines. Moreover, the low observed toxicity enhances the safety profile of the extracts, which is essential for therapeutic application. Considering its abundance in bioactive compounds and the underutilized diversity of Algerian flora, *Pituranthos scoparius* stands out as a promising natural source for developing new anti-inflammatory and analgesic agents.

Keywords – Pituranthos Scoparius ; Anti-inflammatory activity ; Analgesic activity

TOPIC 05:

Electrochemistry

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Microstructure and corrosion resistance of ZnO thin film coatings on carbon steel

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Abstract **–**A facile Spray Pyrolysis (SP) technique was successfully used to deposit ZnO thin film on low carbon steel substrates for evaluation of electrochemical corrosion resistance. This work proposes a coating wih thin flim ZnO, aimed at protecting API 5CT N80 carbon steel against corrosion. The obtained materials were characterized by ,SEM, EDS, FTIR .Scanning electron microscopy (SEM) analysis confirmed the presence of uniform, homogeneous films, while energy dispersive X-ray spectroscopy (EDX) verified the presence of Zn, and O in the coatings. Also Fourier transform infrared spectroscopy (FTIR) confirms the formation of ZnO nanocrystals on surfaces, while the mechanical and anticorrosive properties were evaluated by Vickers hardness tests, Potentiodynamic Polarization . After 40 min of immersion in albian water content demonstrated superior performance, reducing the corrosion rate with efficiencies of 88.60% and exhibited a hardness of 176.7 HV, which significantly increased to 278.3 HV after ZnO coating.

Keywords – ZnO thin film , hardness , Corrosion , carbon steel

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Hydrodynamic Effects on the Corrosion Inhibition Efficiency of a Quinoline-Derived Organic Compound for Carbon Steel in Acidic Medium

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Abstract **–** Corrosion of carbon steel in acidic media is a critical challenge in various industrial applications, especially in processes involving strong fluid movement such as in pipelines and chemical reactors. Organic inhibitors derived from heterocyclic compounds, such as quinoline derivatives, have gained attention due to their high efficiency and strong adsorption on metal surfaces.

In this study, we investigate the influence of rotational speed on the inhibitory performance of a synthesized quinoline-based organic compound in 1.0 M HCl solution. A rotating disk electrode (RDE) system was used to simulate hydrodynamic conditions, and the corrosion behavior was examined using potentiodynamic polarization and electrochemical impedance spectroscopy (EIS).

The inhibitor showed excellent efficiency under static conditions, reaching 89.47% at 0 rpm. However, the efficiency gradually decreased with increasing rotational speed, dropping to 60.17% at 2000 rpm. This reduction is attributed to the increased shear stress and solution turbulence, which disrupt the stability and uniformity of the adsorbed protective film on the steel surface. Polarization data indicated a mixed-type inhibition behavior, while EIS results demonstrated a clear decrease in charge transfer resistance with higher rotation rates.

These results underscore the importance of evaluating corrosion inhibitors under realistic flow conditions, providing valuable insights for their application in dynamic industrial environments.

Keywords – Corrosion, inhibitor, quinoline, RDE, Hydrodynamic Effects.

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Use of Chemical Technical RCP for the Inhibition of Electrochemical Scaling by Green Plants

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Abstract **–** The hard nature of Bejaïa waters, located in the northeast of Algeria, is an important characteristic to take into account for the management of water resources, particularly for domestic consumption and agriculture with the aim of sustainable development. This hard water contains a high concentration of dissolved minerals, mainly calcium (Ca^{2+}) and magnesium (Mg^{2+}) salts which usually come from limestone rocks or mineral-rich soils. This situation requires appropriate management for domestic and agricultural uses.
The hardness of this water was determined by electrochemical tests of accelerated scaling and electrochemical impedance spectroscopy and by chemical test of Rapid Controlled Precipitation (RCP).
The results show that Bejaia water is very scaling, which is revealed by the residual current density values of -0.32 µA, a scaling time of 22 min, a scaling index of 45 min^{-1} and a precipitation time T_P^{PCR} of 60 min.
To overcome the scaling problems caused by the hardness of Bejaia waters, two aqueous extracts of natural plants were tested as green inhibitors of scale precipitation: these are bay leaves and walnut shells. The obtained results are spectacular and the optimal concentrations of the two inhibitors are of the order of a few ppm.

Keywords – Water, Electrochemical Scaling, Inhibition, Environmental inhibitors, Bay leaves, Walnut Shells

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Electrochemical determination of thermodynamic parameters of Dysprosium system in molten LiF-CaF_2

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Abstract **–** In this work, we were interested in the experimental study of the electrochemical determination of different thermodynamic parameters of dysprosium ions Dy(III), presented in the form of DyF_3 in the molten eutectic LiF-CaF_2. This research was carried out as a part of a study series for the aim of reprocessing nuclear wastes by electrochemical separation methods. Dysprosium is an element of the lanthanides, a rare earths produced during nuclear fission. Lanthanides are neutrophages, they retain neutrons which reduces the efficiency of the fission reactions.

Our study aims to contribute in the understanding of the behavior of this element to more understanding its extraction process in the form of a metallic deposit on an inert substrate such as Mo or W, or in alloyed form with a reactive substrates such as Ni or Cu.

Good extraction results have already been obtained for other rare earths, namely: neodymium, samarium and gadolinium, under the same working conditions. This work was realized in fluoride medium, well known in nuclear industry for their ability to lead to coherent deposits of electropositive metals such as refractory metals, lanthanides and their alloys.

In order to determine the thermodynamic parameters of Dy (III) species introduced into the reaction medium in the form of DyF_3, we performed the electrochemical analyses in the eutectic mixture (LiF-CaF_2) (79,2-20,8 % molar) in a temperature range of 840 to 1110 °C.

Study by open circuit chronopotentiometry (at zero current) shows the formation of intermetallic compounds of the Dy-Ni and Dy-Cu systems and permited the calculation of their free enthalpies of formation (Gibbs free energies) and activities in the different phases.

Keywords: Dysprosium; Gibbs free energies; activities; molten fluorides; electrochemical separation.

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Preparation of Zn–Co–TiO_2 nanocomposite coating and evaluation of its morphological and electrochemical properties

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Abstract – The purpose of this paper is to investigate the effect of TiO_2 nanoparticles contents on structural properties, microhardness and corrosion resistance of Zn-Co alloy coating and Zn-Co-TiO_2 composite coatings is electrodeposited on steel substrate in the acid sulfate bath, The smaller grain size of the composite coatings is observed in the presence of TiO_2 and it is confirmed by the images of scanning electron microscopy (SEM) and X-ray diffraction (XRD) techniques. The corrosion performance of coating in the 3 % NaCl as a corrosive solution is investigated by potentiodynamic polarization and electrochemical impedance spectroscopy EIS methods. It is found that the incorporation of nanoparticules in Zn–Co alloy coating have better corrosion resistance and the values of R_{ct} and Z_w increase, while the values of C_{dl} decrease with the increasing of nanoparticules.

Keywords – TiO2 nanoparticles, Zinc, Microhardness, Electrodeposition, Corrosion resistance

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Performances électrochimiques d'électrodes AISI 430 revêtues de Ni, Zn et Ni-Zn pour la production d'hydrogène vert

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Abstract – Dans un contexte de transition énergétique et de recherche d'alternatives aux combustibles fossiles, cette étude s'intéresse à l'optimisation des électrodes en acier inoxydable ferritique AISI 430 pour la production d'hydrogène par électrolyse alcaline de l'eau. L'objectif est d'améliorer leur activité catalytique grâce à des traitements de surface par électrodéposition de couches de nickel (Ni), zinc (Zn) et d'alliages Ni-Zn, avec des épaisseurs contrôlées de 5 et 15 µm. La caractérisation microstructurale par microscopie optique et diffraction des rayons X a révélé un substrat monophasé ferritique d'une dureté moyenne de 170 HV. Les dépôts de nickel présentent une rugosité et une porosité plus élevées, offrant une surface spécifique accrue favorable aux réactions électrochimiques. Les tests de performance ont montré que les électrodes revêtues de nickel, en particulier celles de 15 µm, offrent le rendement le plus élevé en production d'hydrogène. Cette supériorité est confirmée par les analyses de surface spécifique, qui mettent en évidence un facteur de rugosité nettement plus important. Les essais réalisés sous une tension de 3,4 V dans une solution de KOH 1M à 298 K ont permis de mesurer les volumes d'hydrogène générés, soulignant la nette amélioration apportée par les électrodes Ni-15 µm par rapport aux autres revêtements. Ces résultats démontrent le potentiel du nickel comme revêtement efficace pour la production d'hydrogène vert. Enfin, des perspectives d'optimisation envisagent l'élaboration d'alliages enrichis en aluminium, suivie d'une lixiviation alcaline, afin d'accroître encore la porosité et l'efficacité catalytique des électrodes.

Keywords – Hydrogène vert ; Électrolyse alcaline ; Acier inoxydable AISI 430 ; Électrodéposition ; Performances électrochimiques ; Revêtements métalliques.

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Green inhibitor as a sustainable corrosion control for steel in acidic environment

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Abstract:

Steel has been an extensively used construction material, particularly for pipelines and oil wells. However, every step of the production cycle results in corrosion of metal parts.

In the rapid development of industrial technology, corrosion has become a global problem. One-third of steel is lost every year and the global economic loss is around 3% of GDP. To save from this loss, industries have developed various corrosion protection methods. Corrosion inhibitors being among them are widely used in different sectors especially in acidic environments. However, their use is today restricted and controlled due to their toxicity, environmental harm, and growing concern about the preservation of ecosystems.

This has necessitated the present trend of searching and developing green inhibitors that are environmentally benign and low in cost. Green corrosion inhibitors can be sourced from plants such as flowers, seeds, leaves, roots, and stems. The extracts of these plant parts show good inhibition properties in acidic media. However, the use of green inhibitors still leaves several questions about inhibitor formulation, content, and adsorption mechanisms to be answered.

The aim of this study is to determine the structure and examine the inhibitory properties of a plant extract from the moraceae family. UV-VIS and FTIR were used to approximatively estimate the extract's structure. FTIR verified the adsorption of extract's inhibitory molecules on the steel surface, and SEM guaranteed the effeciency of the inhibition. Gravimetry was used to measure the extract's inhibition effeciency over time, and UV-VIS was used to evaluate extract's stability over time.

Keywords – Steel, corrosion, green inhibitor, acidic environment, physicochemical analyses, gravimetry.

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An innovative nanoparticle modified carbon paste micro-sensor for ultrasensitive and selective detection of ciprofloxacin in environmental

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Abstract –
Ciprofloxacin (CIP) is a fluoroquinolone synthetic antibiotic, it is the top five generic antibiotic manufactured worldwide and the most prescribed drug for humans and animals. CIP is widely used to treat infectious diseases in livestock, poultry, urinary tract infections, pneumonia, gastrointestinal, skin infections and sexually transmitted diseases in humans. However, higher consumption of CIP can lead to various and serious side effects. Furthermore, the presence of CIP in the environment is of great concern due to the potential emergence of antibiotic-resistant bacteria. Therefore, the development of fast, sensitive, and efficient techniques to monitor CIP levels in is necessary to ensure the protection of the human health.
In this context, we present a simple, economical, selective and sensitive electrochemical sensor for the quantification of ciprofloxacin in water samples without any pretreatment step of real samples, by using a micro-cavity electrode integrated nanostructured material. The analysis was performed and validated after optimization of operating conditions in environmental water samples and the results showed a good accuracy (less than 3 %) with a satisfactory recovery (less than 7 %), indicating the absence of interference effects of the water matrix. Therefore, the proposed electrochemical sensor is a potential candidate for the determination of ciprofloxacin in water matrices.

Keywords – ciprofloxacin, micro-sensor, electrochemical detection, water, environmental monitoring

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Advanced Functional Materials for Green Hydrogen Production

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Abstract – The development of efficient and stable electrocatalysts is a central challenge in advancing sustainable energy technologies, particularly for green hydrogen production through water electrolysis. Enhancing the kinetics of the oxygen evolution reaction (OER) and hydrogen evolution reaction (HER) is essential to improve overall system efficiency. Recent progress in nanostructured materials has shown that rationally engineered surfaces can significantly promote proton adsorption, accelerate electron transfer, and provide long-term durability under electrochemical operating conditions. In this work, we highlight a hybrid nanostructure approach that integrates metallic and semi metallic domains, enabling improved interfacial charge transport and increased electrochemically active surface area. The materials were synthesized via a hydrothermal growth strategy, ensuring intimate contact with a conductive substrate and structural robustness. Electrochemical testing revealed low onset potentials, high current densities, and reduced cell voltages in overall water splitting, confirming the role of hybrid interfaces in boosting catalytic activity. These findings demonstrate a rational pathway to design advanced electrocatalysts with high efficiency, durability, and scalability, offering a promising contribution toward next-generation electrochemical systems for sustainable hydrogen production.

Keywords – Electrochemical water splitting; Oxygen evolution reaction; Hydrogen evolution reaction; Hybrid nanostructures; Green hydrogen

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The behavior of the bath additions on the properties of the Ni-Fe coating prepared by the electrochemical method

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Abstract – Magnetic Ni-Fe alloys are the subject of many applications, have been extensively studied in recent years in order to develop materials with optimized magnetic properties, and are used in general in corrosion, wear and electrocatalytic materials. For their realizations, electrochemical method proves to be more adequate and less expensive compared to other methods, the latter depends on several parameters, among these parameters, the effect of the bath additions. In this work, Ni-Fe coatings were deposited on copper substrates. X-ray diffraction (XRD), scanning electron microscopy (SEM) and microhardness analysis are used to study the effects of bath additions on morphology and phase structure,. The experimental results confirm that all Ni-Fe coatings exhibit a uniform, compact structure without cracks and including many globular grains. The contents of Ni and Fe in Ni-Fe deposits vary with the variation in the concentration of the additives used, and confirm that the XRD patterns of the alloy deposits reveal that the pictures a number of sharp peak indicating a good crystalline.

Keywords – Magnetic Ni-Fe alloys, XRD; SEM; electrochemical method; microhardness; morphology;

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Electrochemical Oxidation of Phenol and Paracetamol

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Abstract – Environmental pollution, particularly water pollution, can have harmful effects on ecosystems. It is necessary to treat waste from industrial, agricultural and domestic activities in order to protect the environment and public health. Current treatment technologies such as biological treatments are effective, but they seem unsuitable for organic compounds that resist oxidation. Electrochemical oxidation processes are being increasingly developed following the development of new electrode materials that enable the *in situ* generation of highly oxidizing substances such as hydroxyl radicals ($^{\bullet}$OH). These radicals oxidize non-biodegradable toxic organic pollutants until they are completely mineralized. The aim of this work is to study the electrochemical degradation of organic pollutants, including phenol and paracetamol, using manganese dioxide thin film, synthesized by electrochemical route, as an electrode material. The results showed that the proposed electrochemical degradation process for acidic aqueous solutions of phenol and paracetamol allowed the total elimination of these pollutants under optimum experimental conditions of applied potential, pH and initial pollutant concentration at room temperature, with pseudo-first order kinetics. In addition to its efficiency, this electrochemical degradation process using manganese dioxide as electrode material is also environmentally friendly, requires no oxidizing agents or additional heating, and can be applied to the degradation of biorefractory organic compounds.

Keywords – Phenol, Paracetamol, Electrochemical oxidation, Manganese dioxide, Electrode.

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Effect of green inhibitors on the corrosive behavior of A60 materials

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Abstract – Corrosion is a real practical concern when steel is used in most industrial sectors. It costs billions of dollars every year, especially in industrial processes where the metal is exposed to acid solutions which are very corrosive. These acids play an important role in industry; in crude oil refining, acid pickling, industrial cleaning, acid scaling and petrochemical processes. Metals and their alloys are the most sensitive materials to this degradation. [1].

The measures commonly used, alone or in combination, to prevent corrosion are protective coatings or corrosion inhibitors. Inhibitors are substances able to reduce the corrosion of a metal when added in low concentrations to the environment to which it will be exposed. Its mechanism of action is associated with the formation of a protective barrier adsorbed to its surface, which interacts with reaction sites and decreases oxidation and/or reduction reactions associated with corrosion [2]. Ginger and turmeric extracts are innovative solutions for corrosion protection and are used in our study.

Characterization methods such as gravimetric technique (mass loss) and electrochemical technique (potentiodynamic polarization) were used to measure corrosion rates.

Keywords – corrosion, inhibitor, ginger, turmeric, A60 steel, acid medium

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Influence of Applied Current on Ionic Transport and Overpotential in Lithium-Ion Battery Electrolytes

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Abstract –

This study presents a numerical investigation of ionic transport and overpotential in the electrolyte of lithium-ion batteries, with a particular focus on the influence of applied current. Understanding the behavior of ions under electrochemical driving forces is essential for predicting battery performance, safety, and efficiency.

The electrolyte of a cylindrical CGR17600 Sony Li-ion battery, containing $LiPF_6$ salt, was modeled using the one-dimensional Nernst-Planck equation under electroneutrality conditions. The governing equations were solved with the finite difference method, enabling the calculation of lithium-ion concentration profiles and overpotentials during galvanostatic charge-discharge cycles.

The Results show that the applied current has a significant impact on ionic transport. At low currents, concentration profiles remain nearly uniform, leading to limited polarization. In contrast, higher currents induce pronounced concentration gradients, especially near the electrode interfaces, which strongly increase the overpotential. During discharge, diffusion plays a dominant role, whereas migration becomes more significant at higher current densities. The overpotential rises steeply with current, reducing efficiency and potentially compromising safe operation.

These findings highlight the importance of current optimization in lithium-ion battery design and operation. The proposed model provides a valuable predictive tool for investigating electrolyte behavior, enabling the identification of operating conditions that balance performance, safety, and longevity.

Keywords *– Lithium-Ion Battery, Electrolyte, Ionic Transport, Overpotential, Nernst-Planck model*

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Towards Sustainable Corrosion Inhibition :Combined Experimental and Computational Study Of Polyvinyl Chloride (PVC) On Aluminum(5086)in an Acidic Environment.

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Abstract – The quest for innovative and effective corrosion inhibitors, alongside advanced methodologies for corrosion monitoring and quantification, remains pivotal across diverse industrial domains. This study explores the potential of polyvinyl chloride(PVC) on Aluminum(5086) as a high-performance corrosion inhibitor for aluminium in a 1 M hydrochloric acid medium. Employing two complementary experimental techniques, potentiodynamic polarization, and electrochemical impedance spectroscopy (EIS)—the research dem onstrates consistent and reliable results across varying temperatures and PVC concentrations. A notable decline in inhibition efficiency was observed at reduced PVC concentrations and elevated temperatures, underscoring the dynamic interplay between environmental factors and inhibitor performance. Crucially, the adsorption behavior of PVC aligns with the Flory-Huggins adsorption isotherm, with thermodynamic parameters ($\Delta G_{0\,ads}$, $\Delta H_{0\,ads}$, $\Delta S_{0\,ads}$, and K_{ads}) and kinetic activation energy (E_a) providing deeper insights into the adsorption mech anisms. Additionally, quantum chemical simulations reveal the molecular attributes of PVC responsible for robust chemisorption interactions with the aluminium surface. These findings are further validated by scanning electron microscopy (SEM) images and energy-dispersive X-ray (EDX) spectroscopy, which confirm the inhibitor's efficacy and surface-protective properties. The study not only reinforces PVC's viability as an effective corrosion inhibitor but also provides a comprehensive framework combining experimental, thermodynamic, and theoretical approaches, paving the way for the development of next-generation corrosion mitigation strategies.

Keywords – Aluminium 5086 ,EIS, polyvinyl chloride(PVC) ,Corrosion monitoring,DFT.

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Étude de l'efficacité d'un inhibiteur de corrosion à base d'un médicament périmé sur un acier en milieu corrosif

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Résumé – La corrosion est considérée comme l'un des problèmes les plus graves observés dans les installations pétrochimiques et dont les pertes annuelles se chiffrent en centaines de milliards de dollars. Les inhibiteurs de corrosion représentent l'une des méthodes les plus couramment utilisées pour réduire considérablement le taux de corrosion des métaux. Les inhibiteurs de corrosion par adsorption sur métaux sont généralement des composés organiques qui contiennent des structures avec des hétéroatomes (N, P, S, As, O) dans leurs molécules, ayant des électrons isolés ou des paire d'électrons, des anneaux aromatiques ou des liaisons multiples. Ils permettent des interactions relativement fortes entre les atomes métalliques et les molécules organiques, résultant en une couche protectrice de molécules organiques adsorbée à l'interface métal-solution corrosive. Dans ce contexte notre travail expérimental consiste à l'étude des performances d'un médicament périmé (sulfadimdine) en tant qu'inhibiteur de la corrosion d'un acier SA179 dans une solution acide de HCl 1M à l'aide d'une technique de perte de poids, de mesures électrochimiques et d'une microscopie électronique à balayage (MEB). L'utilisation de médicaments comme inhibiteurs de corrosion s'est développés ces dernières années parce que la plupart des molécules de substances actives des médicaments contiennent des structures similaires à celles des inhibiteurs commerciaux. Le Sulfadimidine expiré s'est révélé être un inhibiteur de corrosion écologique, son efficacité d'inhibition augmente avec l'augmentation de la concentration. L'étude de polarisation potentiodynamique confirme les résultats obtenus par la méthode de perte de poids et révèle que le Sulfadimidine fonctionne comme un inhibiteur de corrosion de type mixte.

Mots clés : La corrosion, inhibiteurs, métaux, les molécules organiques, sulfadimdine.

TOPIC 06:

Environmental Chemistry

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Elucidation and Chemical Characterization of Biosurfactants Produced by Fungal Strains Capable of Toxic Pollutants Biodegradation

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Abstract **–** Biosurfactants play a crucial role in environmental chemistry by offering sustainable alternatives to harmful synthetic surfactants. Their ability to degrade pollutants, enhance soil and water remediation, and reduce environmental toxicity makes them key players in green chemistry.

In this study, six fungal strains were isolated from a chronically pesticide-contaminated site and investigated for their dual capacity to biodegrade toxic pollutants and synthesize biosurfactants.
Biosurfactant production was induced and optimized using a two-phase cultivation strategy. Initially, strains were cultured in Minimum Salt Medium (MSM) supplemented with four selected pesticides as the sole carbon sources. After a 21-day incubation at 28 °C and 150 rpm, a 5 mL aliquot from each culture was transferred to 250 mL MSM containing 1% diesel and 1 mL sesame oil to promote biosurfactant yield. These cultures were incubated for an additional 7 days under identical conditions.

All six fungal isolates demonstrated considerable potential to degrade different pesticides and other toxic pollutants, including the ability to degrade 1% diesel and phenol with a CMI (Critical Minimum Inhibitory concentration) of 1800 mg/L and resist different Heavy Metals.

Biosurfactant activity was assessed using standard assays, including the emulsification index (EI), foam height measurement, and oil spreading technique. Preliminary chemical characterization was conducted using the phenol-sulfuric acid test for carbohydrates, Biuret test for proteins, and phosphate assay for phospholipids. The biosurfactants detected were primarily glycolipids and phospholipids, which were identified as the key surface-active compounds produced. These results highlight their promise for applications in green remediation and sustainable biotechnological development.

Keywords – Fungi, Toxic Pollutants, Biosurfactants, Glycolipids, Phospholipids, Biodegradation.

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Comparative approach for the removal of organic dyes using natural materials in an environmental context

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Abstract

Today, humans use large quantities of fresh water for domestic and industrial purposes, which leads to its contamination by various toxic or undesirable elements (solid particles, pathogens, organic and mineral compounds, etc.). Once contaminated, this water is often discharged into the natural environment without prior treatment, which can have harmful consequences for aquatic ecosystems (fauna and flora) as well as human health. Organic dyes are among the main pollutants found in wastewater. Several classes of these dyes are characterized by high stability, strong resistance to degradation, and carcinogenic or mutagenic potential for humans. As part of the recovery of two adsorbent materials, namely activated carbon and clay, this study aims to remove the organic dye (Orange II) from aqueous solutions. The results obtained showed that the optimal masses of the adsorbents are 0.3g for activated carbon and 0.4g for clay, respectively. Adsorption efficiency increases with the initial concentration of the dye, and the process is favored in an acidic environment. The optimal stirring speeds were determined to be 600 rpm for activated carbon and 800 rpm for clay. Temperature has a positive effect on adsorption, with maximum efficiency observed at 40°C for both adsorbents. Kinetic modeling revealed that the process follows the pseudo-second-order model for both materials. Furthermore, the Langmuir model proved to be the most suitable for describing the adsorption isotherm of Orange II. The R_L separation factor values indicate that adsorption is favorable in all cases studied. The thermodynamic study showed that adsorption is physical and endothermic in nature, and that it is not spontaneous at 25°C.

Keywords - *Adsorption, Orange II, activated carbon, clay, adsorption kinetics.*

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Selective catalysis of dyes by zeolite omega-silver nanoparticle composites

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Abstract – This study confirms the successful synthesis of a zeolite omega–silver nanoparticle composite (Ag/omega), with its crystalline structure, the presence of a metallic silver phase, and elemental composition validated through X-ray Diffraction (XRD), Scanning Electron Microscopy (SEM), and Energy-Dispersive X-ray (EDX) analyses. A key aspect of this research involves evaluating the Ag/omega composite's catalytic efficiency in dye reduction, which revealed intricate selectivity and unanticipated kinetic behavior.

Interestingly, while Methyl Orange (MO) degrades more rapidly when alone, its kinetics are inverted in a binary mixture with Methylene Blue (MB), leading to significantly faster reduction of MB compared to MO. This observation is attributed to competitive adsorption and a preferential affinity of the Ag/omega catalyst's active sites for MB, which consequently inhibits MO degradation. All degradation reactions adhered to pseudo-first-order kinetics. This work represents a significant advancement in understanding catalytic mechanisms for water depollution, offering new avenues for developing more efficient and selective treatment systems.

Keywords – Zeolite Omega; Silver nanoparticles; Ag/omega composite; Selective catalysis; Water depollution

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Role of Ionic Strength in Governing Adsorption Competition for Methylene Blue Extraction from Wastewater

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Abstract **–** Methylene blue (MB) poses significant environmental and health risks due to its toxicity to aquatic life, disrupting ecosystems and threatening biodiversity through bioaccumulation and water pollution, while it has therapeutic applications, methylene blue (MB) also presents health risks to humans, causing toxicity at high doses and potentially interaction with other medications. This research paper discusses the investigation of the effect of table salt, sodium chloride (NaCl) ions on the removal of methylene blue from wastewater. It was found that these ions enhance the adsorption of methylene blue, with an increase in NaCl concentration from 1g/L to 7g/L resulting in an adsorption capacity of approximately 19,73mg/g for this cationic dye using ecofriendly adsorbent.

Keywords – Ecosystems protection, Adsorption, Methylene blue, Sodium chloride, Wastewater

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LA PRODUCTION ET LA CARACTÉRISATION DU CHARBON ACTIVÉ PAR PROCÉDÉ D'ACTIVATION CHIMIQUE À L'ACIDE PHOSPHORIQUE

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Abstract –
Les charbons actifs (CA) sont des matériaux poreux avec des surfaces élevées qui permettent leur utilisation dans une large gamme d'applications, telles que le traitement des eaux usées, la séparation et la purification des gaz, la catalyse et, plus récemment, le stockage de l'énergie. Comme ils ne se trouvent pas naturellement, ils sont produits à partir de matériaux à faible coût ayant une teneur en carbone appropriée, principalement du charbon et des déchets de biomasse. La bonne sélection du précurseur et du processus de préparation est cruciale pour parvenir à une production durable, tant du point de vue économique qu'environnemental.

Dans cette étude, des échantillons de charbon actif ont été préparés à partir de par activation chimique. H_3PO_4 a été utilisé comme agent d'activation chimique et un ratio d'imprégnation (50 %) en masse a été appliqué sur la biomasse pendant des temps d'imprégnation de 24 heures. L'équation BET a été utilisée pour calculer les surfaces des charbons activés. La surface BET maximale (760,98 m²/g) a été atteinte avec le charbon actif généré en utilisant un échantillon de biomasse imprégné à 50 % de H_3PO_4, à une température de carbonisation de 450 °C et un temps d'imprégnation de 24 heures. Les résultats expérimentaux ont montré que le rapport d'imprégnation a un effet significatif sur la structure poreuse du charbon actif. Ces résultats valident que l'échantillon ECH_1 présente une surface spécifique largement développée. Cela rend l'échantillon prometteur pour des applications telles que l'adsorption de gaz, la catalyse ou la filtration.

Mots-clés – charbon actif, activation chimique, ratio d'imprégnation, température de carbonisation, surface spécifique.

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Adsorptive Removal of organic pollutants from industrial wastewater by adsorption using activated carbon made from sugarcane residue

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Abstract

Title: *Adsorptive Removal of Organic Pollutants from Industrial Wastewater Using Sugarcane-Based Activated Carbon made from sugarcane residue*

With the increasing discharge of organic pollutants from various industrial sectors such as textiles, agro-food processing, and chemicals, protecting aquatic ecosystems and public health has become a pressing concern. In this context, developing effective, low-cost, and environmentally sustainable treatment technologies is a major challenge in environmental engineering.

This study investigates the potential of a bio-based activated carbon derived from lignocellulosic residues generated during the sugar extraction process from sugarcane, for the adsorptive removal of persistent organic contaminants in both synthetic and real industrial wastewater.

The adsorbent material was prepared through chemical activation followed by thermal treatment, and its textural properties were characterized using Brunauer–Emmett–Teller (BET) surface area analysis. Batch adsorption experiments were conducted to assess the effect of key operational parameters such as pH, initial pollutant concentration, contact time, and adsorbent dosage.

The results demonstrated a high adsorption capacity for selected organic pollutants (notably dyes, phenolic compounds, and organic acids), with a maximum capacity exceeding 200 mg/g under optimal conditions. The application to real industrial effluents confirmed the effectiveness of the process, showing significant reductions in chemical oxygen demand (DCO) and biological oxygen demand (DBO).

This study highlights the value of sugarcane residues as a renewable resource for producing efficient activated carbons, providing a sustainable and economically viable solution for industrial wastewater treatment.

Keywords: Adsorption, Industrial wastewater, Organic pollutants, Bio-based activated carbon, Environmental engineering, Sustainable treatment

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Efficiency of Cationic Resin in Removing Basic Red 29 Dye from Various Water Matrix

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Abstract **–**Many industries such as textile, paper, plastics, and food processing, are major consumers of water and frequently use organic dyes (either soluble or pigment-based) to color their products. These synthetic dyes are not only toxic but also contribute significantly to the coloration of water. Dyes in wastewater represent a specific environmental concern due to their toxicity, bioaccumulation potential, and low biodegradability. Furthermore, their complex molecular structures and synthetic origins make them difficult to remove using conventional treatment methods. As industrial effluents become more complex and discharge standards more stringent, the direct release of dye-contaminated waters into municipal systems or natural environments leads to serious issues such as abnormal coloration, bacterial growth, foul odors, unpleasant taste, and the formation of carcinogenic byproducts.

In this context, the present study investigates the efficiency of a strong cationic resin in removing Basic Red 29 dye from three different water matrices: distilled water, tap water, and mineral water. Experimental results showed that the resin effectively removed the dye from all three matrix, the dye removal remained efficient which can reach 98%. These findings highlight the potential of cationic resins for real-world water treatment applications, regardless of the initial water composition.

Keywords – Basic Red 29, cationic resin, dye removal, water treatment, Environment

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Nanocomposite Innovations: copper -Enhanced Methods for Effective Methyl Orange Degradation

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Abstract – The synthesis of four Mazzite/ copper nanocomposites was successfully accomplished using a hydrothermal method for the preparation of the Mazzite zeolite. The incorporation of metallic nanoparticle (MNP) into the zeolitic framework was achieved through ion exchange, followed by chemical treatment with a reducing agent (NaBH4). The resulting materials were characterized using various techniques, including X-ray Diffraction (XRD), nitrogen adsorption at 77K, Fourier Transform Infrared Spectroscopy (FTIR), and Scanning Electron Microscopy (SEM).

The catalytic potential of the nanocomposites was evaluated in dye redu-ction reactions involving methylene blue (MB) and methyl orange (MO). To determine the optimal conditions for the reduction reaction, the influence of catalyst type, catalyst mass, dye concentration, and NaBH4 solution concentration was studied and discussed. The Mazzite/Cu nanocomposite exhibited excellent catalytic activity in the reduction of methyl orange. In a binary system containing both MB and MO, the Mazzite/Cu catalyst demonstrated greater selectivity for the cationic dye MB. Furthermore, the stability of the Mazzite/Cu catalyst in the reduction of MO was confirmed through multiple cycles of use.

Keywords – Mazzite- synthesis- hydrothermal method- dye- reduction

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Efficiency of ZnO thin films doped with magnesium for treating wastewater through photocatalysis in environmental applications

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Abstract

Using the sol-gel and dip-coating techniques, thin films of pure and doped ZnO with varying Mg concentrations (3 and 7 mol. %) were applied to glass substrates. The sample was characterized using X-ray diffraction (XRD), scanning electron microscopy (SEM), atomic force microscopy (AFM), and UV-Vis absorption spectra (UV-VIS). Findings from an X-ray diffraction investigation employing doped and undoped ZnO thin films having a hexagonal wurtzite structure (JCPDS Card No. 36-1451), thenthe xrd demonstrated that the crystallinity of ZnO films declines as the magnesium doping concentration rises. SEM examination showed various morphologies. The 5% ZnO mixed with the Mg sample had a flower-like morphology, but the 2% ZnO incorporated with Mg and pure ZnO films displayed spherical particles. An average transmittance of 90% was recorded by UV-Vis in the wavelength range of 190–1100 nm, and the bandgap energies decreased with increasing concentration. The effectiveness of these samples was confirmed by removing contaminated solutions using photocatalytic technology, which is important for the environment.

Keywords – sol-gel, wastewater, Mg-doped ZnO, photocatalytic, thin films

Preparation and Characterization of a Medlar Kernel-Based Adsorbent for the Removal of a Textile Dye in Aqueous Solution

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Abstract

Water pollution is a fundamental enigma that affects our daily lives. Among the various sources of pollution, synthetic dyes pose a significant threat to water, often released into waterways without adequate treatment. Their presence in aquatic environments also poses a fundamental problem for the health of ecosystems and human populations. This work focuses on the preparation of an activated carbon derived from loquat kernels and its use in the treatment of contaminated water, with particular emphasis on the adsorption phenomenon. The main objective of this study is to evaluate the effectiveness of activated carbon in removing a textile dye: crystal violet (CV). During this work, we will focus on an in-depth study of the various parameters influencing the adsorption process, such as adsorbent mass, contact time, concentration, ionic strength, temperature, and solution pH. Subsequently, a kinetic analysis will be conducted to determine the adsorption mechanism and identify the most appropriate kinetic model (pseudo-first order, pseudo-second order, intraparticle diffusion).

Keywords: Adsorption, medlar kernel, crystal violet dye, kinetic analysis,

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Drying Kinetics and Moisture Diffusion in Natural Convection Solar Drying of Strawberry Slices

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Abstract

The purpose of this research was to investigate the drying kinetics, moisture migration mechanisms, and predictive modeling performance for natural convection solar drying of 2.5 mm thick strawberry slices. The approach involved conducting a full-day drying experiment under clear sky conditions, measuring sample mass and environmental parameters at 30-minute intervals, and calculating moisture ratio, drying rate, and moisture removed per interval. Experimental data were analyzed using Fick's second law to determine effective moisture diffusivity and fitted to four thin-layer drying models :Logarithmic, Page, Midilli–Kucuk, and Henderson–Pabis—evaluated through statistical performance indicators (R^2, RMSE, χ^2). The principal results showed that drying followed an initial rapid moisture removal stage transitioning into a falling-rate period dominated by internal diffusion, with an effective moisture diffusivity of 2.02×10^{-10} m^2/s, consistent with literature values for high-moisture fruits. Model fitting identified the Midilli–Kucuk model as the most accurate ($R^2 = 0.997$, RMSE = 0.0108), followed closely by the Page model, indicating their suitability for predicting drying behavior under natural convection conditions. The drying process reached near-equilibrium moisture content within 600 minutes, confirming the feasibility of achieving complete single-day drying. The major conclusions were that natural convection solar drying under the tested conditions can serve as a cost-effective and sustainable preservation method for strawberries, particularly in regions with high solar availability, and that the Midilli–Kucuk model offers the best predictive capability for process optimization. These findings contribute to improved understanding of moisture migration mechanisms and model applicability in solar drying of perishable fruits.

Keywords: Natural convection solar drying, Strawberry slices, Drying kinetics, Moisture diffusivity, Thin-layer drying models.

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Optimization of MgO nanomaterial synthesized from plant extract by green synthesis

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Abstract – Water is mainly polluted by industrial waste containing toxic and dangerous substances. These are mainly the dyes used in the textile industry. These products cause unprecedented damage to the ecosystem. Various treatment approaches have been used to remedy these problems. Adsorption processes are the most promising.
Green synthesis refers to the production of nanomaterials from plant extracts. The importance of nanomaterials lies in the fact that, at this scale, they possess development properties that could have a significant impact on various fields.
In this study, we optimized the operating parameters for the synthesis of a magnesium oxide nanomaterial, which is synthesized by green synthesis using a Pistacia lentiscus leaf extract. The parameters optimized were the concentration of the plant extract, the concentration of the precursor used. The optimization was carried out using adsorption tests with a cationic dye. The synthesized nanomaterial was characterized by scanning electron microscopy (SEM) and energy dispersive spectroscopy (EDS).

Keywords – Adsorption; cationic dyes; nanomaterial; green synthesis.

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Thermodynamic and Kinetic Modeling of Magnesium Hydride-Based POWERPASTE for Efficient Hydrogen Storage

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Abstract – The increasing demand for clean and sustainable energy has accelerated research into efficient hydrogen storage technologies. Magnesium hydride (MgH_2) offers high gravimetric and volumetric storage capacities but is limited by slow absorption/desorption kinetics and high operating temperatures. This work investigates the potential of POWERPASTE, a novel hydrogen storage medium developed by Fraunhofer IFAM, which releases hydrogen through a controlled reaction between MgH_2 and water. The study combines theoretical analysis and numerical modeling to simulate the thermodynamic and kinetic behavior of hydrogen absorption in MgH_2. Using a finite difference method, the spatial–temporal evolution of temperature, hydrogen fraction, and absorption rate was predicted under varying pressures, powder thicknesses, and operating times. Results show that increasing hydrogen pressure significantly reduces absorption time, while larger powder thicknesses lead to higher saturation temperatures before reaction completion. The findings highlight the potential of MgH_2-based POWERPASTE as a safe, high-capacity, and cost-effective hydrogen storage solution for portable fuel cell applications, particularly in regions with abundant solar energy and magnesium resources.

Keywords – Hydrogen storage, Magnesium hydride, POWERPASTE, Thermodynamic modeling, Finite difference method, Absorption kinetics

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From Adsorption to Photocatalysis Under Sunlight: Enhancing Methyl Orange Removal Using Polyaniline/Co-Montmorillonite Hybrid Material

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Abstract – A two-step approach was used in the elimination of a benchmark azo dye, methyl orange (MO). Combining adsorption and photocatalysis under natural sunlight has exhibited great promise in environmental remediation using a hybrid material of polyaniline matrix reinforced by cobalt-exchanged montmorillonite charge, synthesized via a bottom-up approach called in situ polymerization. This type of material has become one of the most exciting areas of research for adsorbents and photocatalysts due to abundant active sites and improved structural, textural, thermal and optical properties, as confirmed in this study by XRD, FTIR, BET, TGA/DSC and UV-Vis analysis. The proposed hybrid system integrated adsorption and photocatalysis processes showed 87.75 % removal of methyl orange, higher than the conventional single-stage (adsorption or photocatalysis) water treatment process. The experimental tests indicated that the adsorption capacity studied in the dark during 90 min reached 74.64 mg/g at the initial concentration of MO of 20 mg/L and natural pH (6.5), leading to 55.98 % of methyl orange molecules adsorbed on the surface. The enhancement in the removal of this toxic azo dye was attributed to the subsequent photodegradation process that contributed to the elimination of more than 31.77 % MO molecules in 240 min under economical and ambient conditions. Kinetic study of the second stage of the system has revealed that it follows a pseudo-first order kinetics profile with heterogeneity of the surface as verified by the modified Freundlich model. This work brings a deeper insight into understanding the effect of the operating conditions on the rate of elimination attributed to both processes and the possibilities of applying it in textile dyeing industries' wastewater treatment.

Keywords – Adsorption; Photocatalysis; Sunlight; Methyl Orange; Hybrid material; Polyaniline; Co-Montmorillonite; Kinetics

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Organic Pollution and Water Quality Challenges in Effluents of the Annaba Wastewater Treatment Plant

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Abstract – This d The Annaba wastewater treatment plant, commissioned in 2011 with a nominal capacity of 580,700 PE, currently operates at 49% of its design potential. While treatment significantly reduces suspended solids (250 to 10 mg/l) and nitrites (0.005–0.01 mg/l), conductivity, BOD5, ammonium, and phosphates (4.6 mg/l) still exceed both national and international standards. Climatic analysis confirms a Mediterranean regime characterized by a pronounced water deficit (347.87 mm) driven by high actual evapotranspiration. According to IPO and IHE indices, effluents show moderate to very high organic pollution, indicating that despite treatment, the waters discharged into the Oued Seybouse remain of unsatisfactory quality. This continuous discharge of insufficiently treated effluents contributes to the degradation of water quality in the wadi, affecting its ecological balance. It also poses potential risks to downstream uses, including agriculture, domestic supply, and aquatic biodiversity.

Keywords – organic pollution ; BOD5; wastewater treatment plant; potential risks; biodiversity.

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Adsorption of lead (II) from wastewater using activated carbonaceous materials from Aloe Vera leaves: Isotherms, Kinetics, and Thermodynamics

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Abstract –

Lead is a more toxic heavy metal. It enters the environment as metallic, inorganic, and organic mercury compounds through various industries such as the paper industry, gold and silver mining, the electrical industry, fungicides, and pharmaceuticals. It is widely dispersed in the environment in excessive concentrations and beyond a certain limit, it can cause more serious risks, deadly and carcinogenic diseases to human beings and thus it can cause environmental problems. This is the reason why the retention of this pollutant in wastewater is a big topic of research these.

As a remedy, adsorption has been considered a preventive method that has the advantage of being able to be applied to the treatment of various effluents and thus provided for the protection of the environment where several adsorbents are used for the treatment of aqueous effluents.

The reuse of agricultural waste is one of the objectives of the associated environmental property, which has become an important choice that has several advantages for waste treatment, such as free availability, a simple technique, a low cost, and a simple regeneration.

In this study, we were interested in preparing an activated carbon product from the Aloe vera plant, by several steps under different chemical and thermal treatments and were characterized by different spectrometric methods. Then it was tested as a biosorbent for the removal of Pb(II) from wastewater to broaden the scope of its application, and it gives good results with the various works carried out previously. The parametric study reveals encouraging results.

Keywords: *Pollutant* Pb(II), Adsorption, Activated Carbon, Aloe vera Plant.

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Assessment of Physicochemical Parameters and Heavy Metal Contamination in Water, Sediments, and Fish from the Littoral Dam of El-Ouana (Jijel, Algeria)

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Abstract **–** In this study, a comprehensive physicochemical and ecotoxicological investigation was conducted to evaluate the pollution status of the littoral dam of El-Ouana in Jijel (Algeria). Water, sediment, and fish samples were collected and analyzed for key environmental contaminants. *In situ* measurements in water included temperature, pH, and electrical conductivity, while laboratory analyses determined BOD_5, COD, nutrients (PO_4^{3-}, NO_3^-, NO_2^-, NH_4^+), and trace metals (Pb, Cd). Sediment samples were characterized for physicochemical properties and total heavy metal concentrations. For fish, cadmium and lead levels were quantified in liver, gills, and muscle of three species (Sardina pilchardus, Mullus barbatus, Sphyraena sphyraena).Results showed that water and sediment parameters were within international quality standards, and heavy metal concentrations in sediments were low, similar to unpolluted systems. However, fish tissues revealed significant bioaccumulation, particularly of lead, with levels exceeding European Economic Community (EEC) safety limits in all three species. Lead accumulation was highest in liver and gills, whereas cadmium was mainly detected in muscle tissue. These findings highlight the potential health risks associated with fish consumption and the need for continuous monitoring to ensure ecological and food safety in Algerian aquatic systems.
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Keywords – El-Ouana littoral dam, physicochemical parameters, heavy metals, water and sediments, fish

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Use of the UV/ZnO photocatalytic process for the elimination of sulfamethazine in aqueous media

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Abstract –

This study focuses on the degradation of sulfamethazine (SMT) by the UV/ZnO photocatalytic process using a UVA lamp. SMT is an antibiotic widely used in animal and aquaculture production as an antimicrobial agent and growth promoter. Environmental concentrations of SMT generally range from nanogram per liter to microgram per liter.

Various parameters were examined, namely the pH, the amount of catalyst and the initial concentration of SMT. The results showed that varying the pH of the solution between 4 and 9 did not significantly degrade the SMT. The optimum amount of catalyst was 0.25 g/L. The increase in the initial concentration of SMT had a negative impact on the removal efficiency, which was reduced from 100% to 27% for 10 mg/L and 50 mg/L SMT after reaction times of 30 minutes, respectively. The results obtained showed that the photocatalytic process in the presence of ZnO enables efficient degradation of sulfamethazine.

Keywords – Antibiotics; sulfamethazine ; degradation; UV/ZnO; parametric study.

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Wastewater Treatment via Photodegradation with a Diatomite-Based Magnetic Ferrite Catalyst

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Abstract – This work presents a comprehensive analysis of ferrihydrite silicide, a material widely utilized in integrated circuit terminal fabrication. To understand its structural and chemical behavior, multiple characterization techniques were employed, including X-ray diffraction (XRD), X-ray fluorescence (XRF), infrared (IR) spectroscopy, and scanning electron microscopy (SEM). The material was synthesized using two routes: thermal treatment conducted externally (ex-situ) and in-situ synthesis during sputter deposition onto silica derived from diatomite. The process involved reacting $FeCl_2$ with NaOH, enabling the incorporation of ferrihydrite onto the diatomite substrate. XRD results indicated that untreated diatomite exhibits a disordered, amorphous nature, which transitions into a more crystalline state following the formation of iron oxide phases. These crystalline products include magnetite, maghemite, hematite, goethite, akaganeite, and schwertmannite. The photocatalytic potential of the ferrihydrite-modified diatomite (FMD1) was evaluated through the degradation of Vat Green 03 dye, demonstrating strong performance under acidic conditions, particularly at pH 4. These findings highlight FMD1's suitability for wastewater treatment applications, especially in environments with low pH.

Keywords – ferrihydrite, silicide, diatomite, photocatalytic, dye.

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Evaluation of Heavy Metal Tolerance in Environmental Bacterial Strains

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Abstract – The uncontrolled release of heavy metals into the environment poses a serious threat to public health due to their toxicity, persistence, and accumulation in the food chain. In this context, microbial bioremediation emerges as a promising and eco-friendly alternative to conventional physico-chemical methods. The objective of this study is to evaluate the tolerance of environmental bacterial strains to four heavy metals: mercury (II) chloride ($HgCl_2$), cobalt (II) chloride ($CoCl_2$), iron (III) chloride ($FeCl_3$), and zinc (II) chloride ($ZnCl_2$). Twenty-six bacterial strains were cultured on a solid minimal medium supplemented with one of the tested metals at increasing concentrations of 200, 400, 600, 800, and 1000 mg/L, and incubated at 30 °C for one week. The results show that for $HgCl_2$, only 23.07% of the strains exhibited growth at 200 mg/L, with no growth observed at higher concentrations. For $CoCl_2$, 46.16% of the strains were able to grow at 200 mg/L, but this percentage decreased to 15.38% at 1000 mg/L. Regarding $FeCl_3$, 76.92% of the strains grew at 200 mg/L, while only 19.23% tolerated the highest concentration. Finally, in the presence of $ZnCl_2$, 73.07% of the strains showed growth at 200 mg/L, and 53.84% maintained growth at 1000 mg/L. These results highlight the variability in bacterial tolerance depending on the metal and underscore the potential of certain strains for the bioremediation of heavy metal-contaminated environments.

Keywords – Bacteria; Bioremediation; Heavy metals; Tolerance.

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Ecological risk assessment of metal contamination in Oued Essouk and Guenitra Dam in the vicinity of the abandoned Sidi Kamber mine (Northeast Algeria)

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Abstract –

Mining activities generate large amounts of waste that often remain untreated after mine closure, constituting a long-term source of environmental contamination. The abandoned Sidi Kamber mine (Zn–Pb), located in Skikda (Northeast Algeria), is a typical case where several million tons of residues have been left exposed to weathering. The leaching of these wastes may release potentially toxic elements into surrounding aquatic systems.This study aims to evaluate the ecological risk related to metal contamination in surface and groundwater around the Sidi Kamber site, particularly in Oued Essouk and the Guenitra Dam. A total of 17 water samples were collected and analyzed. Physicochemical parameters (pH, electrical conductivity, dissolved oxygen, total dissolved solids, turbidity, etc.) were determined in situ and in the laboratory, while heavy metals were investigated using standard analytical techniques. The assessment was supported by the application of water quality and pollution indices. Preliminary results suggest that water quality in Oued Essouk is strongly affected by mine drainage processes, showing acidic conditions and high salinity, which may favor the mobilization of metals. In contrast, the Guenitra Dam appears less impacted but remains vulnerable. These findings highlight the importance of linking physicochemical characteristics to metal contamination as early indicators of ecological risk. The study underlines the urgent need for adequate monitoring and remediation strategies for abandoned mines in Algeria.

Keywords – water, pollution, heavy metals, ecological risk assessment, mine waste.

INCIDENCE DE PARAMETRES REACTIONNELS SUR L'OXYDATION DES SUBSTANCES HUMIQUES AU COURS DU TRAITEMENT DES EAUX DE SURFACE.

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Résumé – L'oxydation chimique est fondamentale pour le traitement des eaux, permettant la dégradation des micropolluants, la destruction des composés toxiques et la désinfection. Si le chlore a longtemps été l'oxydant universel en raison de son pouvoir germicide, la découverte de sous-produits de chloration cancérigènes, les trihalométhanes (THM), a conduit à envisager son remplacement lors de l'étape de préoxydation.

Le permanganate de potassium ($KMnO_4$) représente une alternative intéressante pour oxyder la matière organique, comme les substances humiques (SH), et pour éliminer le fer et le manganèse. Cette étude a pour objectif d'évaluer l'influence de paramètres réactionnels sur l'oxydation des SH par le chlore et le $KMnO_4$, notamment leur teneur initiale, le pH, le temps de contact et la minéralisation du milieu.

Les résultats démontrent une forte réactivité des SH avec les deux oxydants. La consommation d'oxydant augmente avec la teneur en SH et la minéralisation du milieu. L'impact du pH varie selon l'oxydant : la réactivité avec le chlore est maximale à pH neutre (forme acide hypochloreux), tandis qu'un pH basique favorise l'oxydation par le $KMnO_4$. La cinétique présente toujours deux phases, rapide puis lente.

Enfin, le couplage d'une préoxydation au $KMnO_4$ suivie d'une post-chloration réduit la consommation de chlore. Ceci s'explique par la formation de produits d'oxydation différents, comme des composés aromatiques carboxyliques peu réactifs, limitant ainsi la formation de sous-produits indésirables.

Mots clés *– Oxydation, chlore, permanganate de potassium, substances humiques, minéralisation.*

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Impact of NaCl on Liquid-Liquid Extraction of Propionic Acid from Aqueous Solutions

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Abstract **–** Propionic acid, although used in various industrial sectors, can have a significant environmental impact. Its presence in the environment poses risks to human and animal health, which emphasizes the importance of optimizing its extraction from aqueous solutions. This work focuses on the study of the effect of NaCl on the liquid-liquid extraction of propionic acid from an aqueous solution with hexane as the solvent. The presence of NaCl introduces ionic forces that directly influence the widening of the immiscibility curve, thereby modifying the distribution of the solute between the extract and raffinate phases, leading to the phenomena of "salting-out" and "salting-in" The liquid-liquid equilibrium data for the ternary system (Water/Propionic Acid/Hexane) in the presence of NaCl at different percentages (5%, 10%, 15%) were experimentally determined at room temperature and atmospheric pressure using the cloud point method. The experimental results demonstrated the influence of NaCl on the liquid-liquid equilibrium of the studied system, indicating that the presence of salt modifies this equilibrium in favor of the extracted phase.

Keywords – Aqueous solutions, Propionic acid, Salt effect, salting-out, salting-in

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Environmental Chemistry Assessment of soil radioactivity and health Risks in Eastern Algeria

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Abstract **–** Natural radioactivity in soil is a key parameter in environmental chemistry, serving as a reliable indicator of environmental quality and compliance with radiological safety standards. This study evaluates soil radioactivity levels in Eastern Algeria using high- resolution gamma spectrometry with a high purity Germanium (HPGe) detector. The absorbed dose rate and outdoor annual effective dose were calculated, and the outdoor excess lifetime cancer risk (Outdoor ELCR) was estimated. The outdoor ELCR values ranged from 7×10^{-5} to 1.3×10^{-3}, remaining within internationally accepted safety limits, which indicates a relatively low radiological impact. These findings emphasize the importance of radiological assessments in environmental chemistry as reliable tools for risk evaluation and ecosystem protection.

Keywords: Natural radioactivity, Soil, Gamma spectrometry, Absorbed dose rate, Annual effective dose, ElCR outdoor.

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Synthesized Spinel Nanoferrite (D600) as an Efficient Catalyst for Fenton-Like Degradation of Acid Green 25: Experimental design approach

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Abstract **–** Advanced oxidation processes (AOPs) are recognized as highly effective methods for the treatment of pollutants. In this work, a spinel nanoferrite catalyst, denoted D600, was synthesized through a sol–gel self-combustion method. Its structural, morphological, and magnetic characteristics were investigated by X-ray diffraction (XRD), scanning electron microscopy (SEM), vibrating sample magnetometry (VSM), Fourier-transform infrared spectroscopy (FTIR), and Raman spectroscopy. The catalytic activity of D600 was assessed for the degradation of the anthraquinone dye Acid Green 25 (AG25) using a heterogeneous dark Fenton-like process. To determine the optimal operating conditions, a central composite design (CCD) was employed, focusing on three key variables: catalyst dosage, hydrogen peroxide concentration, and reaction time, which enabled a significant reduction in the number of required experimental. Under optimized conditions (0.5 g/L catalyst, 3 mM H_2O_2, 60 minutes), a maximum decolorization efficiency of 98.6% was achieved. The CCD model displayed excellent predictive accuracy with an R^2 value of 0.9973. Scavenging experiments were performed to identify the reactive species responsible for the degradation mechanism. Furthermore, reusability tests demonstrated that the catalyst maintained nearly 98% efficiency over five successive cycles, underscoring its durability and sustainability. Overall, these findings highlight the potential of the synthesized nanoferrite for efficient pollutant removal and the advantages of Fenton-like processes. Future investigations should aim at coupling this approach with other AOPs and further optimizing the material properties for large-scale environmental applications.

Keywords –Nanoferrites, catalysis, self-combustion, Fenton-like, experimental design, AOP

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Citric Acid-Modified Agricultural Wastes as Efficient Biosorbents for Cadmium Removal from Aqueous Solution

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Abstract –
This document presents the formatting instructions for the Proceedings of the International Conference on Pioneer and Innovative Studies. This document can serve as the base template for a Cadmium (Cd^{2+}) is one of the most toxic heavy metals, posing severe environmental and health risks due to its persistence and bioaccumulation. In recent years, agricultural wastes have emerged as cost-effective and eco-friendly biosorbents for heavy metal removal from contaminated water. In this study, agricultural residues were chemically modified using citric acid to enhance their adsorption capacity for cadmium ions. Citric acid activation introduces additional carboxyl groups on the biomass surface, significantly improving metal-binding efficiency through ion exchange, complexation, and electrostatic interactions. The adsorption performance was strongly influenced by pH, contact time, sorbent dose, and initial cadmium concentration. Experimental data typically fitted well with the Langmuir isotherm model, suggesting monolayer adsorption, while kinetic studies followed a pseudo-second-order model, indicating chemisorption as the main mechanism. The results highlight that citric acid-modified agricultural wastes represent a promising, low-cost, and sustainable alternative for cadmium removal from aqueous solution

Keywords – *Cadmium removal ; Biosorption ; Agricultural waste ; Heavy metals ; Adsorption isotherms*

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Liquid-liquid Extraction of 1-Butanol with Diethyl ether/ Cyclohexanone At 291.15 K

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Abstract **–**1-Butanol is present in nature as a product of carbohydrate fermentation. It is also produced from petrochemicals and is widely used as an organic solvent and as an intermediary in the production of other organic chemicals. 1-Butanol is readily biodegradeable and does not bioaccumulate. It poses an indirect hazard for the aquatic environment because it is readily biodegraded and this may lead to oxygen depletion. The separation of 1-butanol from aqueous mixture is feasible by distillation, but the distillation of a lower concentration of butanol from the mixture consumes a large amount of energy, resulting in higher production costs. Liquid− liquid extraction as a separation technology for liquid mixtures has the advantages of simple operation, high separation efficiency, and low energy consumption. Liquid−liquid extraction of 1-butanol from water using two solvents; diethyl ether and cyclohexanone was reported in this study. The Liquid-liquid equilibrium data of the two ternary systems (water/ 1-butanol / solvents) were measured at 291.15 K and atmospheric pressure. The solubility and tie-lines data for these systems were determined using the cloud-point method. The distribution coefficients and the separation factors, were used to select the most suitable solvent for this equilibrium. The reliability of the equilibrium data was confirmed through empirical correlations of Othmer–Tobias and Hand. The results showed that extraction of butanol-1 is feasible using the two tested solvents, but given the highest distribution coefficient values and separation factors for the system using cyclohexanone as a solvent..

Keywords –1-Butanol, liquid-liquid extraction, liquid-liquid equilibrium, distribution coefficient, separation factor

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Core-Scale Modeling of Subsurface Geochemical Processes for Regional CO_2 Storage Applications

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Abstract **–** The CO_2 sequestration in depleted sandstone reservoirs is among the future methods of greenhouse gas climate change mitigation. However, the long-term storage stability of the CO_2 sequestration depends on the interactions between the injected CO_2, formation brine, and reservoir minerals, which control trapping mechanisms and containment integrity. This study employs a core-scale modeling approach to investigate these processes in Algerian depleted sandstone formations. Reactive transport simulations using CMG-GEM, calibrated to the conditions of the Hassi Messaoud reservoir, were integrated with pore-scale modeling of two-phase flow in 3D rock structures. The model considers multiphase flow, aqueous geochemistry, and mineral reactions to evaluate how CO_2 displacement, brine chemistry, and mineral composition modifications influence porosity, permeability, and trapping efficiency. The analysis reveals that brine salinity is a primary control. The reservoir's high salinity conditions promote carbonate mineral precipitation near the injectors, which risks pore restriction; this suggests that a lower salinity pre-flush may be required to enhance solubility trapping. Additionally, the injection rate governs plume behavior and the spatial distribution of reactions. Pore-scale observations also suggest that dissolution trapping is optimal in high-porosity and high-permeability hydrophilic sandstones, which have good CO_2 distribution and interfacial contact. These results allow predictions of CO_2 trapping efficiency in subsurface reservoirs. This is fundamental knowledge during the design, planning, and initial-stage development of CO_2 storage projects, ultimately reducing the impacts of climate change.

Keywords – carbon sequestration, geochemical modelling, reactive transport, depleted reservoirs, brine chemistry.

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Functionalisation of polystyrene membranes by Alamine 336 for the extraction of reactive dyes in aqueous solution.

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Abstract – In this research, we focused on the extraction of a reactive dye, Cibactron blue (CB), using polystyrene (PS) functionalised with Alamine 336. This particular application was targeted for the purpose of wastewater treatment, which falls within the environmental field and thus contributes to the elimination and recovery of waste (particularly dyes) from industrial discharges, especially those from the textile industry.

Polymer membranes were developed using polystyrene as the base polymer (PS) and a neutral extractant (Alamine 336). The polymer films obtained after characterisation are used in the extraction of a reactive dye (CB). After optimising the parameters: Alamine 336 concentration, dye concentration, pH of the aqueous solution, stirring speed and temperature, an extraction yield of 98% was recorded.

Keywords – water treatment, polystyrene (PS), Alamine 336, extraction, Cibacron blue (CB).

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Photocatalytic Degradation of Bisphenol A using Green-Synthesized $MnTiO_3$

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Abstract – Advanced oxidation processes (AOPs) are one of the most efficient processes for waste water treatment, the hydroxyl radicals (·OH) can be generated thought different processes including, photolysis and photocatalysis

This study investigates the heterogeneous photocatalytic degradation of bisphenol A (BPA), a pervasive endocrine-disrupting compound, using a manganese titanate ($MnTiO_3$) catalyst. The catalyst was synthesized via an environmentally friendly method employing fruit extract, and its properties were characterized using X-ray diffraction (XRD), scanning electron microscopy (SEM), and infrared (IR) spectroscopy. The main objective of this research was to assess the catalytic efficiency of the synthesized $MnTiO_3$ and to determine the influence of operational parameters, specifically solution pH and catalyst dosage, on the degradation process.

The photocatalytic activity of $MnTiO_3$ was found to be highly dependent on the initial solution pH. The degradation of BPA was significantly more efficient under acidic conditions, achieving a degradation rate exceeding 70%. Furthermore, increasing the catalyst dosage enhanced the degradation rate, reaching an optimal value at 0.25 g/L. This improvement is likely attributed to the increased number of available active sites for the photocatalytic reaction.

In conclusion, these results confirm the potential of green-synthesized $MnTiO_3$ as an effective photocatalytic material for the removal of persistent organic pollutants (POPs).

Keywords – Advanced oxidation processes; Bisphenol A; photocatalysis; degradation; MnTiO3

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Combined Effects of Compost, Water Stress, and PET Microplastics on the Physicochemical Properties of Soil

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Abstract

Soil degradation in Mediterranean regions, exacerbated by water stress, erosion, and low organic matter content, represents a major challenge for agricultural sustainability. In this context, organic amendment with compost appears as a sustainable strategy for restoring soil fertility, while the increasing accumulation of agricultural microplastics, particularly polyethylene terephthalate (PET), raises new concerns. This study evaluated the combined effects of compost, water stress, and microplastics on the physicochemical properties of soil cultivated with *Hordeum vulgare*. The experiment was conducted in a greenhouse (University of Tébessa) using 3-kg soil pots sown with five barley seeds, applying three compost doses (0, 15, and 30 g/kg), three water stress levels (100%, 60%, and 20% of field capacity), and three PET microplastic doses (0, 0.5, and 1 g/kg). Measured parameters included pH, electrical conductivity (EC), organic carbon (C%), organic matter (OM), and active limestone. Results revealed a perfect correlation between C% and OM (r = 1.00), confirming analytical consistency, as well as a moderate positive correlation between pH and EC (r = 0.58), indicating that alkalinization favors salt solubilization. A weak positive correlation was also observed between pH and OM/C% (r = 0.28), reflecting the buffering effect of organic matter, while active limestone showed weak negative correlations with EC (r = –0.15) and with OM/C% (r = –0.22), suggesting ion fixation and humus instability in calcareous soils, respectively. Most other relationships were weak to negligible (r = –0.06 to 0.18), indicating relative independence among parameters. In conclusion, this study confirms the structuring role of organic matter in soil dynamics and highlights limited yet relevant interactions among pH, salinity, and active limestone, with implications for the sustainable management of Mediterranean soils under water stress and emerging microplastic pollution.

Keywords: compost; water stress; microplastics (PET); soil; physicochemical properties .

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Performance evaluation of advanced heterogeneous photocatalysis for the removal of 2,4-Dichlorophenoxyacetic acid (2,4-D) under different operating conditions

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Abstract:

The excessive use of chemical products such as pesticides has become increasingly significant in recent years to protect vegetable crops against pests and undesirable plant or animal species that cause damage to food commodities. These multiple applications of pesticides explain their presence in various environmental compartments such as water, soils, and air. Their presence in the environment has harmful consequences on living organisms, particularly humans, where exposure to pesticides can cause neurodegenerative and congenital diseases as well as various types of cancer. It is therefore necessary to control emission sources, reduce their transfer into the environment, and treat contaminated exposure media using effective purification processes such as advanced oxidation processes (AOPs).

In this study, we applied photocatalysis as an advanced oxidation process to eliminate a widely used selective herbicide worldwide: 2,4-dichlorophenoxyacetic acid (2,4-D), with the chemical formula $C_8 H_6 Cl_2 O_3$. This herbicide is considered potentially carcinogenic and toxic to both humans and animals. The main objective of this work is to experimentally evaluate the removal of 2,4-D using advanced oxidation processes, specifically heterogeneous photocatalysis, and to determine the optimal operating conditions to maximize its elimination. This will make it possible to verify the feasibility of photocatalysis for pesticide removal.

The results obtained showed that the elimination of 2,4-D by photocatalysis is highly effective, achieving a removal efficiency of up to 97%. This research thus makes a significant contribution to improving water quality by efficiently removing toxic contaminants such as 2,4-D. It also plays a crucial role in environmental protection, safeguarding human health and aquatic biodiversity by reducing soil and waterway pollution.

Key words: Pollution, Pesticide, Herbicide, Water treatment, Advanced oxidation processes, Photocatalysis.

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Valorization of biomaterial waste -raw date pits- for Congo red adsorption in aqueous solution: Thermodynamics, kinetics and regeneration studies

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Abstract – The feasibility of using natural waste (raw date pits) as a low-cost adsorbent for the adsorption of an anionic dye (Congo red) from aqueous solution has been investigated. Adsorption optimized conditions were obtained at low dose 1 g/L, initial dye concentration 100 mg/L, pH 2, equilibrium contact time 120 min, and temperature 20 °C. The corresponding adsorption capacity was around 70 mg/g and could reach 150 mg/g by increasing the ionic strength of the dye solution (0.05 M $CaCl_2$). These results are well modeled by Freundlich isotherm and kinetics study followed by pseudo second-order model. Thermodynamic parameters indicate that the adsorption process is endothermic and not spontaneous. The tests of desorption-regeneration showed that the studied adsorbent has the disadvantage of the loss of efficiency at its reuse but this is offset by its abundance. Based on these results, it can be used as competitive material for the removal of dyes.

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Keywords – Adsorption; Congo red; Raw date pits; Lignocellulosic material; Modeling.

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Sustainable Pharmaceutical Removal by Biochar Derived from Biomass Residues

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Abstract **–** The widespread use of pharmaceuticals has led to their frequent detection in aquatic environments, where they persist as emerging pollutants of growing concern. These residues, often resistant to conventional wastewater treatments, pose potential risks to both ecosystems and human health, highlighting the urgent need for efficient and sustainable remediation strategies. The present study aimed to investigate the removal of diclofenac from aqueous solutions through adsorption onto biochar derived from pine cones. The results highlighted the excellent performance of the tested biochar for retaining the target pharmaceutical. The effect of contact time revealed a rapid adsorption process, achieving a removal efficiency of 98.9% at an equilibrium time of 60 minutes. Kinetic analysis showed that the experimental data fitted well with the pseudo-second-order model, suggesting that chemical interactions predominated between diclofenac molecules and the active sites of the biochar. Regarding equilibrium adsorption, the Freundlich isotherm provided the best fit, indicating a heterogeneous, multilayer, and favorable adsorption process (1/n = 0.28). The biochar exhibited a maximum adsorption capacity of 98.1 mg/g, significantly higher than those reported for other adsorbents. Based on these findings, pine cone-derived biochar can be considered an efficient, low-cost, and eco-friendly adsorbent for the remediation of pharmaceutical-contaminated waters, particularly those containing diclofenac.

Keywords – Pharmaceutical, Adsorption, Removal, Diclofenac, Biochar

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Photocatalytic Degradation of Malachite Green from Aqueous Solutions

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Abstract
Malachite green is a toxic dye often found throughout wastewater and used in many industries, where it causes serious environmental problems. In this study, Malachite Green degraded under UV light using zeolite-based photocatalysts. Zeolite provides for a high surface area and it supports the active photocatalyst. That support acts upon the process of degradation. Irradiation time, catalyst amount, and dye concentration effects were studied. The results showed that zeolite-based photocatalysts can effectively remove Malachite Green, also this makes them promising materials for water treatment.

Keywords – Malachite Green, Photocatalysis, Photodegradation, Wastewater treatment, Photocatalyst.

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A circular economy approach: Development of a biosorbent from agricultural waste for the treatment of textile wastewater

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Abstract – Water pollution by cationic textile dyes represents a major environmental challenge due to their toxicity and persistence. This study explores the valorization of an agricultural waste as a low-cost and eco-friendly biosorbent for the purification of contaminated water. The biosorbent was prepared through simple washing, drying, and grinding, without costly chemical modifications, to maintain its low-cost nature. Its morphological and physicochemical characterization was carried out using scanning electron microscopy (SEM), Fourier-transform infrared (FTIR) spectroscopy, and point of zero charge (PZC) determination. The adsorption of Methylene Blue (MB), chosen as a model dye, was investigated based on critical parameters such as pH, adsorbent dosage, initial dye concentration, contact time, and temperature. The results indicate that adsorption capacity is highly dependent on pH, with maximum efficiency observed in a basic medium (pH ~10). The pseudo-second-order model, suggesting that adsorption is controlled by chemisorption mechanisms, best described kinetic data. Equilibrium adsorption isotherms showed excellent agreement with the Langmuir model, revealing a high maximum adsorption capacity at room temperature. Thermodynamic analysis highlighted a spontaneous ($\Delta G° < 0$) and endothermic ($\Delta H° > 0$) process. This study demonstrates the promising potential of an abundant natural waste as an efficient, cost-effective, and sustainable adsorbent for the treatment of textile wastewater, paving the way for concrete applications in the context of the circular economy

Keywords *– Biosorption, Cationic dye, Agricultural waste, Valorization, Wastewater.*

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REMOVAL OF SANDOCRYL BLUE DYE WITH ADSORPTION PROCESS USING APRICOT STONE SHELLS.

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Abstract. In the present study, apricot stone shell was used as an adsorbent to remove Sandocryl blue dye (BB 41) from textile wastewater effluents with a batch system. FTIR spectroscopy, XR Diffraction and SEM-EDX analysis determined the structure and characteristics of the apricot stone shell. A batch system was used to investigate the effects of pH_{pzc} of the bio sorbent, dye concentration, pH quantity, reaction duration, temperature and ion strength on dye removal performance. The adsorption kinetics were studied for the adsorption of BB 41 dye. The results of modelling studies proved that Langmuir isotherms and pseudo-second-order kinetics best represent adsorption kinetics and isotherm data. Present findings revealed that BB 41 removal was a feasible, spontaneous and endothermic process. Apricot stone shell had yielded quite high adsorption of dye; thus, it was also concluded that apricot stone shell could effectively and reliably be used in the treatment of wastewater effluents of the textile industry containing Basic blue 41 textile dye.

Keywords – Adsorption, Basic blue 41, Batch study, Isotherms, Kinetics, Apricot stone shells.

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Improving biobased adsorbent properties by chemical crosslinking

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Abstract

Biopolymers are increasingly applied in adsorption due to their abundance, biodegradability, and tunable surface functionalities. They also exhibit strong pH sensitivity which directly influences their solubility. Chemical crosslinking enhances the stability, mechanical strength, and resistance of biopolymers, while often reducing their solubility.

In this study, we developed hydrogel beads based on carboxymethyl cellulose (CMC), a biopolymer rich in hydroxyl and carboxyl functional groups, to serve as biosorbents for the removal of industrial cationic dyes. To enhance the adsorption performance, an anionic surfactant was incorporated into the CMC matrix, forming modified CMC beads (CMCbds). Then, wet beads were suspended in acidic glutaraldehyde solution.

The biosorbents were characterized using Fourier Transform Infrared Spectroscopy (FTIR) to identify functional groups, X-ray Diffraction (XRD) to assess crystallinity, and pH sensibility tests to control solubility.

pH sensibility tests showed that CMCbds (without crosslinker) were slightly soluble at pH 11, and totally soluble at pH 12. Upon crosslinking with glutaraldehyde, CMCbds become insoluble at pH 12. Further, adsorption tests showed that the adsorption capacity of a cationic industrial dye hasn't been affected with the chemical crosslinking which was ~70mg/g with a removal efficiency of ~80% for both CMCbds (with and without crosslinker).

These findings demonstrate that CMC-based biosorbents are a promising, low-cost alternative to conventional adsorbents for the treatment of wastewater containing cationic dyes. Moreover, further chemical modifications of CMC could enhance its stability, mechanical strength, and thermal resistance.

Keywords – Adsorption, Biosorbents, Carboxymethyl Cellulose, Crosslinking, Glutaraldehyde.

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Electrochemical removal of pharmaceutical pollutants using a nanostructured manganese dioxide electrode

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Abstract – Pharmacologically active substances present in the aquatic environment are mostly derived from pharmaceutical products for human use, including prescription drugs, over-the-counter drugs, as well as veterinary drugs. The sources of these substances are mostly municipal wastewater discharges, which include domestic and hospital wastewater. Other sources include agricultural wastewater from livestock farming and wastewater from the pharmaceutical industry. Techniques commonly used in wastewater treatment include bio-oxidation, physicochemical chemical oxidation methods, etc.; however, these methods are limited due to their high cost, high toxicity and low efficiency with regard to non-biodegradable organic pollutants. Electrochemical oxidation is one of the most effective and environmentally friendly advanced oxidation processes for treating wastewater containing recalcitrant organic compounds. Thanks to its high energy efficiency, safety, potential for automation, versatility, ease of implementation, universal degradation capacity and environmental compatibility, it is the most widely used technology for wastewater treatment. The efficiency and selectivity of the anodic oxidation process depend heavily on the nature of the anode material. In this work, the electrochemical degradation of amoxicillin was investigated in acidic aqueous solutions using a nanostructured manganese dioxide (MnO_2) thin-film electrode. The performance of this electrode was enhanced through the addition of Ni^{2+} and Cu^{2+} metal ions, yielding promising test results.

Keywords – MnO_2 thin film, Doped material, Anodic oxidation, Pharmaceutical pollutants, Wastewater treatment

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Preparing low-cost, porous ceramic supports using kaolinitic clay and various additives for water treatment applications.

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Abstract **-**The objective of this study is to develop low-cost membrane supports based on natural raw materials using liquid phase sintering. Variable proportions of calcium carbonate and sodium carbonate were used to promote liquid phase sintering and create porosity. The effect of sintering temperature and the impact of the percentage of calcium carbonate (additive) on the properties of the developed supports were studied. Two compositions yielded good results: 10% calcium carbonate (porosité 28%, density 1.49 g, stress 2.216 MPa) and 5% calcium carbonate (porosité 25%, densité 1.69, stress 5.032 MPa). The supports obtained were characterized by physicochemical, mechanical, morphological, and structural analyses to evaluate their properties.

Keywords – Ceramic membrane; Sintering; Kaolin ; Additives

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Use of Honeybees (*Apis mellifera,* Spinola, 1806) as Bioindicators of Atmospheric Heavy Metal Pollution: Case Study in Blida, Algeria

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Abstract

This study was conducted at three sites located in the Wilaya of Blida, Algeria. Honeybees (*Apis mellifera*, Spinola, 1806) were sampled from three areas characterized by different levels of atmospheric pollution: Site 1 was the least polluted, Site 2 moderately polluted, and Site 3 the most exposed to atmospheric contaminants. The aim of the study was to measure the concentrations of selected heavy metals in bee tissues in order to evaluate the bioaccumulation of these contaminants. This approach makes it possible to determine whether honeybees can reliably reflect the status of the local atmospheric environment. The experiment was carried out during the year 2024–2025. Every 15 days, 30 bees were collected from each site. After acid digestion, the obtained solutions were analyzed using an Atomic Absorption Spectrophotometer (AAS) to quantify the concentrations of heavy metals in bee tissues. The results revealed the presence of several trace elements, with notably high concentrations of cadmium (Cd) at the most polluted site. These findings confirm the role of honeybees as reliable biomonitors of atmospheric pollution and highlight their value as a tool for environmental chemistry. Data regarding the concentrations of different heavy metals at each study site will be presented and discussed.

Keywords – *Honeybees, Heavy metals, Bioindicators, Atmospheric pollution, Blida.*

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Adsorption of Pb(II) and Cd(II) Ions on Algerian Montmorillonite Intercalated with $Al_{1\ 3}$ Polycation

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Abstract – The adsorption of Pb(II) and Cd(II) ions was studied on natural montmorillonite (mont-Na) and montmorillonite intercalated with the aluminum polycation $Al_{1\ 3}$ (mont-$Al_{1\ 3}$). Equilibrium was reached within 5–6 h, with adsorption rates of ≈70% for mont-Na and up to 85% for mont-$Al_{1\ 3}$. Maximum adsorption capacities obtained from the Langmuir model were 24 mg/g for Cd(II) and 21 mg/g for Pb(II) on mont-$Al_{1\ 3}$, compared to lower values for mont-Na. The kinetic data fitted best with the pseudo-second-order model ($R^2 \approx 0.99$), indicating that chemisorption was not the dominant process. Thermodynamic parameters confirmed an endothermic (ΔH = 8–14 kJ/mol) and spontaneous (ΔG = –443 to –2351 J/mol) adsorption, with positive entropy values ($\Delta S \approx$ 28–49 J/mol·K) indicating increased randomness at the solid–liquid interface.

Overall, the modified montmorillonite exhibited higher adsorption efficiency, with the following affinity order: Cd(II) > Pb(II).

Keywords – montmorillonite, polycation, adsorption, environnement

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Sustainable Removal of Mequitazine and Ethinylestradiol from Aqueous Solutions Using Pumpkin Biochar

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Abstract – This work explores the adsorption process as an efficient method for removing mequitazine and ethinylestradiol, the active compounds of Primalan and Diane, from aqueous solutions. Biochar derived from pumpkin fruits at 500 °C (PB-500) was synthesized and evaluated as the adsorbent. Characterization revealed that PB-500 possessed a relatively high surface area, leading to removal efficiencies of 66.61% for mequitazine and 62.37% for ethinylestradiol. Comparative analysis of biochar before and after adsorption highlighted notable changes in its physicochemical properties. Kinetic studies indicated that the pseudo-second-order model best described the experimental data, suggesting that chemisorption played a key role. Equilibrium results showed that both the Sips and Freundlich models accurately represented the adsorption behavior, consistent with heterogeneous surface interactions. The efficiency of PB-500 was strongly affected by solution pH, while optimization tests identified 0.8 g L^{-1} as the optimal dosage, achieving maximum removal yields of 67% for mequitazine and 65.16% for ethinylestradiol. Thermodynamic parameters demonstrated that the adsorption was spontaneous and exothermic for both pollutants. These findings confirm that pumpkin biochar is an effective, sustainable, and low-cost material for eliminating pharmaceutical contaminants from water, offering significant potential for application in wastewater treatment and environmental protection.

Keywords – Biochar, Adsorption, Mequitazine, Ethinylestradiol, Water treatment

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Adsorption treatment of water contaminated with Reactive Black 5 dye

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Abstract **–** This study addresses water pollution caused by synthetic dyes, focusing on the removal of Reactive Black 5 using raw halloysite and organo-halloysite as adsorbents. Organo-halloysite, modified through organic intercalation, showed enhanced adsorption performance. Adsorption equilibrium was reached within 2 hours and followed a pseudo-second-order kinetic model. Isotherm analysis revealed type L behavior, described by the Freundlich model for raw halloysite and the Temkin model for organo-halloysite. The maximum adsorption capacity was significantly higher for organo-halloysite (220.6 $mg \cdot g^{-1}$) compared to raw halloysite (85.76 $mg \cdot g^{-1}$), confirming that intercalation improves dye removal efficiency.

Keywords – Include at least 5 keywords or phrases

DECONTAMINATION; MODIFICATION; ORGANO-CLAY; DYES.

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BIO WASTE USED FOR BASIC RED DYE REMOVAL BY BATCH ADSORPTION SYSTEM.

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Abstract. Removal of Red Basic cationic dye (RB46) by adsorption onto bio-waste (BW) was studied. The (BW) has an acidic character, with a pH_{PZC} of 4.44. A series of experiments was conducted to evaluate the adsorptive capacity of the BW. Parameters such as the amount of adsorbent, contact time, concentration, pH, temperature, and ionic strength were examined. The overall results show that the maximum adsorption capacity is 18.48 mg/g under the following conditions: contact time t_C = 40 minutes, T = 293 K, natural pH of the RB46 solution, and agitation speed of 50 rpm. The second-order model well describes the kinetics of RB46 adsorption on BW. The adsorption isotherm of the BW/RB46 system is satisfactorily explained by both the Langmuir and Freundlich models. Thermodynamic studies indicate that the adsorption of RB46 dye onto BW is a physical, spontaneous, and endothermic process.

Keywords – Bio-Waste, Red Basic 46, Adsorption., Isotherms, Kinetics, Apricot stone shells.

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Feasibility of Coupling Biological Treatment with Heat-Activated Persulfate Pre-Oxidation for Paracetamol Removal

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Abstract – Paracetamol (PCT) is a widely detected pharmaceutical pollutant, poorly biodegradable and persistent in aquatic environments. This study evaluates heat-activated persulfate (PDS) oxidation as a pre-treatment to enhance its removal and support subsequent biological treatment. Experiments showed that increasing the initial PCT concentration negatively affected the degradation efficiency, while under optimal conditions (0.33 mM PCT, 5 mM PDS, pH 6, 68 °C), a removal yield of 94.2% was achieved. Biodegradability tests revealed a significant improvement, with the BOD_5/COD ratio rising from 0.008 to 0.34 after 10 h. These results demonstrate that PDS pre-oxidation is a promising approach for treating pharmaceutical wastewater.

Keywords – Paracetamol; Heat-activated persulfate; Sulfate radicals; Activated sludge; BOD_5/COD ratio.

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Paracetamol Degradation by Heat-Activated Peroxydisulfate Oxidation process: Parametric Study

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Abstract **–** Paracetamol is a recalcitrant pharmaceutical compound frequently detected in aquatic environments. Its degradation by heat-activated persulfate oxidation was examined through a parametric study, focusing on the effects of temperature, PDS concentration, initial pH, and initial paracetamol concentration. Results indicated that pH showed no significant influence, whereas higher temperatures enhanced degradation. Increasing the initial paracetamol concentration reduced removal efficiency, while the PDS concentration exhibited an optimal value at 8 mM. These findings highlight the key operational parameters governing the performance of persulfate-based advanced oxidation processes for paracetamol removal.

Keywords – Paracetamol; Heat-activated persulfate; Sulfate radicals; Advanced oxidation technology; Wastewater treatment.

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Solar-Light-Driven Photocatalytic Degradation of Rhodamine B by Calcined ZnBi/TiO_2 Anionic Clay

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Abstract – Water is essential for the life of living beings. However, it is increasingly contaminated with various organic and inorganic pollutants. Synthetic dyes are considered a significant class of organic pollutants due to their widespread use, high solubility in water, and high toxicity to aquatic organisms. For example, rhodamine B (RhB) is commonly used in the textile and food industries. However, numerous studies have reported the carcinogenic effects of RhB in rats and mice.

This work presents a photocatalytic degradation study of RhB in an aqueous solution under UV and solar radiation using ZnBi/TiO_2 as a photocatalyst. The material, a layered double hydroxide type, was synthesized from zinc, bismuth, and titanium dioxide using co-precipitation methods, followed by calcination at 580 °C. Various analytical techniques (XRD, FTIR, and SEM) revealed that after heat treatment, the pristine structure collapsed, resulting in the formation of mixed metal oxides. The discoloration rate of RhB was less than 16% through direct photolysis (under UV and sunlight). By using ZnBi/TiO_2, the discoloration yield reached 100% after 90 and 120 minutes of exposure to sunlight and UV radiation, respectively. The photodiscoloration and photodegradation kinetics data were described by pseudo-first-order and Langmuir-Hinshelwood models. The reusability study of the calcined material demonstrated stable efficiency after four successive uses.

Keywords – Cationic dyes; Langmuir-Hinshelwood model; Layered double hydroxides; Photocatalytic degradation; UV irradiation; ZnO particles.

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Adsorption Mechanisms of Cationic Dye by Bio-Based Adsorbents: A Batch System Approach

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Wastewater from textile industry activities often contains a high load of colored pollutants that are difficult to biodegrade. To address this issue, an experimental study was conducted on the adsorption of cationic dyes in aqueous solution using a batch system.

Two adsorbents were tested: one derived from agro-industrial waste and the other from forest residues. The study focused on adsorption kinetics, examining the influence of key operating parameters on the decolorization efficiency.

The results revealed significant adsorption capacities: 54 mg/g for the GC adsorbent and 73 mg/g for DT. Kinetic analysis showed that the adsorption process of the BS dye on both materials involves multiple mass transfer mechanisms, including external mass transfer, surface reactions—following a pseudo-first-order kinetic model for both BS-GC and BS-DT systems—and intraparticle diffusion.

Keywords – Basic bleu 41, adsorption, batch system, valorization.

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Impact of hydrogen peroxide granulation medium on the development of porous hydroxyapatite-based granules

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Abstract – In the present work, porous adsorbent granules were synthesized by combining powdered hydroxyapatite with metakaolin as starting materials. Hydrogen peroxide (H_2O_2) was subsequently employed as a granulation fluid at varying concentrations (0.0%, 5.0%, 7.5%, and 10.0%) in order to tailor the textural properties of the obtained materials. The structural and surface characteristics of the prepared granules were systematically investigated through Fourier-transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), and nitrogen adsorption–desorption measurements (BET surface area and BJH pore size distribution analyses). The findings demonstrated that the incorporation of 5.0% H_2O_2 during granulation led to a remarkable enhancement in both the specific surface area and pore volume of the granules, resulting in improved adsorption performance. Moreover, their application as adsorbents for organic molecules revealed promising efficiency, highlighting the potential of hydroxyapatite–based granules in environmental remediation processes.

Keywords – *Hydroxyapatite, geopolymer, hydrogen peroxide, texture, wastewater treatment*

TOPIC 07:

Pharmaceutical Chemistry

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Experimental and Computational Study of Celecoxib Eutectic Systems, Synthesis, DFT, and Docking

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Abstract

This study aims to improve the physicochemical properties of celecoxib (CXB), a selective cyclooxygenase-2 (COX-2) inhibitor with anti-inflammatory, analgesic, and antipyretic effects, through the formation of an eutectic mixture with a coformer across the entire range of molar fractions.

The eutectic system was synthesized using solvent-assisted grinding (liquid-assisted grinding). Differential scanning calorimetry (DSC) was used to determine the eutectic point, which was identified at a 1:1 molar ratio with a melting temperature of 134 °C. Solid-state structural characterization was performed using X-ray diffraction (XRD), scanning electron microscopy (SEM), and infrared spectroscopy (FT-IR). These analyses confirmed the formation of the eutectic mixture and revealed weak molecular interactions in the solid state.

Furthermore, molecular modeling based on density functional theory (DFT) was applied to explore the electronic stability of the system. An increase in the dipole moment and a change in the Gibbs free energy in the gas phase highlighted improved stability compared to pure CXB. A significant enhancement in the aqueous solubility of CXB was also observed.

These results confirm that the combined synthesis/characterization/modeling approach is a promising strategy for optimizing the bioavailability of celecoxib.

Keywords: Celecoxib; Solid-Liquid Equilibrium; Solubility; Differential Scanning Calorimetry; XRD; DFT; Docking.

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Formulation of Suppositories for Hemorrhoids Therapy Using Goat Fat, *Teucrium Polium*, and Chicken Bile Extracts

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Abstract **–** The therapeutic management of hemorrhoids often involves the use of suppositories for targeted treatment and relief of symptoms. The objective of this study is the formulation of suppositories using natural ingredients, *Teucrium polium* (TP) and chicken bile (Bi) extracts, with goat fat (GF) as the base excipient. Goat fat was rendered and characterized for its acid, peroxide and saponification values. Suppositories were prepared and optimized using different combinations of goat fat, Suppocire, paraffin oil, and surfactants (Polysorbate 20 and Sorbitan monooleate), with the aim of achieving desired physical properties such as uniform weight, melting point, softening time, and disintegration time. Results indicate that the suppositories prepared with association of goat fat with Suppocire exhibited ideal physical properties. The inclusion of surfactants enhanced desintegration profile, suggesting that the prepared suppositories are suitable candidates for hemorrhoids therapy.

Keywords – Chicken bile, goat fat, hemorrhoids, suppositories, Teucrium polium

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Antioxidant Potential and Bioactive Compounds of *Origanum glandulosum* Desf. Leaves: In Vitro Analysis

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Abstract – This research investigates the antioxidant potential of methanolic extract from the leaves of Origanum glandulosum Desf., an endemic Algerian species collected from the Akfadou region (Bejaia), alongside its phenolic composition and metal chelation activity. The antioxidant properties were evaluated using a range of in vitro assays, including phosphomolybdenum, DPPH, ABTS, FRAP, CUPRAC, and MCA. HPLC-DAD analysis identified key phenolic compounds, such as chlorogenic acid, rosmarinic acid, hesperidin, and quercetin, as predominant contributors to the extract's antioxidant activity. The extract exhibited significant antioxidant capacity, with values reaching up to 474.28 mg TE/g in DPPH assay and 874.67 mg TE/g in ABTS. The total antioxidant capacity (PDA) was measured at 3.73 ± 0.10 mmol TE/g, while the FRAP and CUPRAC assays showed 527.33 ± 25.83 mg TE/g and 779.84 ± 2.73 mg TE/g, respectively. The metal chelation activity (MCA) was observed to be 9.53 ± 0.55 mg EDTAE/g, indicating strong iron-binding potential. These findings underscore Origanum glandulosum Desf. as a promising source of natural antioxidants with significant bioactive potential, highlighting its possible applications in health, food, and pharmaceutical industries.

Keywords – Origanum glandulosum Desf.; antioxidant activity; phenolic compounds; HPLC-DAD.

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Intranasal Delivery of AahII-Encapsulated Chitosan Nanoparticles Reduces Inflammatory Markers in a Murine Model of Lung Adenocarcinoma

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Abstract **–**Lung cancer remains one of the leading causes of cancer-related mortality worldwide, with chronic inflammation playing a key role in its progression. In this study, we investigated the anti-inflammatory effect of AahII toxin, a modulator of voltage-gated sodium channels, when encapsulated in chitosan nanoparticles (AahII-CNPs) and administered intranasally in a murine model of urethane-induced lung adenocarcinoma.

The tumor model was established by repeated intraperitoneal injections of urethane in Balb/c mice. AahII was encapsulated in chitosan nanoparticles, and the formulation was characterized using Fourier-transform infrared spectroscopy (FTIR), dynamic light scattering (DLS), zeta potential analysis, and transmission electron microscopy (TEM). The physicochemical results confirmed successful encapsulation and appropriate size and charge for nasal delivery.

Following intranasal administration of AahII-CNPs, a significant decrease in the expression of myeloperoxidase (MPO) and eosinophil peroxidase (EPO) was observed in lung tissues. This reduction reflects a lower infiltration of neutrophils and eosinophils two key inflammatory cell types known to contribute to tumor progression. These findings highlight the potential of intranasally delivered AahII-CNPs to modulate the inflammatory tumor microenvironment.

In conclusion, our results suggest that intranasal delivery of bioactive AahII encapsulated in chitosan nanoparticles may represent a promising, non-invasive therapeutic strategy to attenuate inflammation-associated tumor progression in lung cancer.

Keywords – Lung adenocarcinoma, AahII toxin, chitosan nanoparticles, urethane, inflammation

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Chemical Composition and Antimicrobial Potential of *Lavandula angustifolia* Essential Oil

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Abstract **–**Essential oils are complex mixtures of volatile bioactive compounds that often act synergistically to produce diverse biological effects. This unique phytochemical profile makes them promising candidates for alternative therapeutic agents, particularly in the context of the growing global challenge of antibiotic resistance. Their intrinsic antimicrobial and antioxidant properties further enhance their potential in pharmaceutical applications.

This study investigates the chemical composition and biological activities—specifically, the antioxidant and antibacterial potential—of essential oil extracted from Lavandula angustifolia (LEo). The oil was obtained by hydrodistillation, a gentle, water-based extraction method that preserves volatile constituents. Gas chromatography–mass spectrometry (GC–MS) analysis was performed to identify and characterize the chemical constituents.

Antioxidant activity was assessed using the DPPH radical scavenging assay, while antibacterial efficacy was evaluated against five bacterial strains, representing both Gram-positive and Gram-negative groups. The disc diffusion method was employed to determine zones of inhibition, and the minimum inhibitory concentration (MIC) values were measured to quantify bacteriostatic potential.

Results revealed that LEo exhibits strong antioxidant capacity and significant antibacterial activity across a range of bacterial strains. These findings underscore the potential of Lavandula angustifolia essential oil as a natural, plant-based antimicrobial agent with prospective applications in the development of pharmaceutical formulations aimed at combating microbial infections and oxidative stress-related disorders

Keywords – Antioxidant activities , Antibacterial activity, DPPH assays, Chemical composition, Essential oil .

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Phenolic compounds and antioxidant activity in the ethanolic and aqueous extracts of Lavandula dentata flowers

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Abstract – Plants constitue excellent sources of various bioactive substances, and they are currently used abundantly in herbal medicine for the treatment of several diseases and even in some food industries as aromatizing and food preservatives. For this study, flowers from the plant *Lavandula dentata* were collected in the Elhammamet region Tébessa- eastern Ageria. Their phytochemical screening, polyphenoli and flavonoid content, as well as their antioxidant activities, were analyzed. The total polyphenol and flavonoid contents of the aqueous and ethanolic extracts were determined by the Folin-Ciocalteu and aluminum nitrate methods, respectively. Antioxidant activity was determined by DPPH free radical scavenging method. The results revealed that the plant is rich in flavonoids, tannins (gallic, catechic), terpenes and quinines. Total polyphenol and flavonoid contents were in the range of 39.50±30 mg GAE/g to 8.235±0.33 mg QE/g for the aqueous extract and 113.187±3.68 mg GAE/g to 4.707±0.30 mg QE/g for the ethanolic extract. *Lavandula dentata* extracts were found to have higher antioxidant activities ranging from 195,92±6,97 aqueous and 3,53 ± 0,38 µg/ml for ethanolic. This study reveals that flower extracts contain contain significant quantities of phenolic compounds and possess strong antioxidant activity. This property can be exploited in several fields such as therapeutics and food production.

Keywords – Lavandula dentate, bioactive, antioxidant, phenolic

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Molecular Docking of Bioactive Compounds from Medicinal Plants: A Natural Alternative to Veterinary Antibiotics

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Abstract:

In light of the growing challenge of bacterial resistance and the environmental impact of veterinary antibiotics, this study explores the molecular interactions between bioactive compounds derived from local medicinal plants and critical bacterial targets. Extracts from *Punica granatum* (pomegranate peel), *Moringa oleifera*, propolis, *Olea europaea* (olive leaf), and *Ocimum basilicum* (basil) were investigated. Key secondary metabolites such as ellagitannins, quercetin, and rosmarinic acid were subjected to molecular docking against essential bacterial enzymes, including DNA gyrase (*E. coli*) and transpeptidase (*S. aureus*). The docking simulations revealed strong binding affinities for several compounds, in some cases comparable to gentamicin, suggesting notable inhibitory potential. These findings emphasize the value of an in silico strategy to support the development of sustainable phytotherapeutic formulations for veterinary use, guided by a rational understanding of ligand–receptor interactions.

Keywords:

Veterinary phytotherapy; Molecular docking; Natural antibacterials; Microbial resistance; Green biotechnology

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Extraction and characterization of capsaicin: an anesthetic and analgesic active compound from Saharan chili pepper, a natural alternative for pain management

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Abstract

This study investigates the extraction, purification, and characterization of bioactive compounds, with a particular focus on capsaicin, from *Capsicum annuum* cultivated in the Algerian Sahara. Two extraction techniques were applied: Soxhlet extraction and ultrasound-assisted extraction, enabling efficient isolation of capsaicin. The compound's presence and concentration were confirmed using Thin Layer Chromatography (TLC) and UV-Visible spectrophotometry. To achieve higher purity, column chromatography was employed, improving compound separation and isolation.

The biological activities of the extracts were extensively evaluated. Results revealed significant antioxidant and anti-inflammatory effects, along with notable analgesic potential, assessed through in vitro assays targeting pain-related pathways. Additionally, the extracts demonstrated antimicrobial properties, supporting their multifunctional pharmacological relevance.

To explore practical applications, a topical oil-in-water (O/W) emulsion incorporating the purified extract was formulated and analyzed for its physicochemical stability. The formulation exhibited promising characteristics, suggesting its potential use in pain management therapies.

Overall, this research highlights *Capsicum annuum* from the Saharan region of Algeria as a valuable natural source of pharmacologically active compounds, particularly capsaicin, with potential applications in therapeutics and topical formulations.

Keywords – Algerian Sahara, Capsicum annuum, Soxhlet extraction, ultrasound-assisted extraction, Chromatography, analgesic activities, therapeutic bioactivity.

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Protective effects of vitamin C and cyclodextrin-encapsulated vitamin E against oxidative stress-induced male reproductive dysfunction in uncontrolled hyperglycemia

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Abstract – Hyperglycemia is known to cause male reproductive impairment through diverse mechanisms. The excessive formation of advanced glycation end products in uncontrolled hyperglycemia leads to increased oxidative stress in the male reproductive tract, which plays a key role in male infertility. However, one of the rational strategies to prevent this effect is to increase the scavenging capacity of antioxidants in sperm. Therefore, the aim of the current study was to evaluate the protective effect of vitamin C (Vit C) and vitamin E loaded in cyclodextrin (CD-Vit E) on human mature spermatozoa exposed *in vitro* to diabetic plasma with high HbA_{1c} levels.

Vitamin C (0.1 mg/mL) was freshly dissolved in Tris buffer, while CD–Vitamin E complexes were prepared by co-evaporation and reconstituted in Tris buffer at a concentration of 0.25 mg/mL. Their effects on sperm quality were evaluated by assessing sperm motility using Computer-Assisted Semen Analysis (CASA), and oxidative status was determined by measuring malondialdehyde (MDA) levels using the thiobarbituric acid reactive substances (TBARS) assay.

The results of gametes progressive movements (moderate progressive: 12.199 ± 1.671% and rapid progressive: 2.583 ± 0.489%) showed a dramatic decline after 30 min following the incubation with diabetic plasma. However, sperm pre-treated with Vit C (0.1 mg/ml) and CD-Vit E (0.25 mg/ml), reported an effective improvement in all sperm progressivity (moderate progressive: 12.992 ± 1.590% and rapid progressive: 2.893 ± 0.623%). Also, the supplementation with the combination of Vit C and CD-Vit E reduced significantly MDA levels (0.049 ± 0.012 AU), compared to the non-protected group (0.895 ± 0.014 AU).

In conclusion, these data indicate that an uncontrolled diabetic condition impairs the motility of mature spermatozoa by increasing their oxidative status. While, co-treatment with Vitamin C and CD-Vitamin E exhibits a potent protective effect as an antioxidant complex, enhancing sperm quality and male fertility in diabetic men

Keywords – cyclodextrin-vitamin E, hyperglycemia, high HbA_{1c} levels, oxidative stress, sperm motility, vitamin C.

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Synthèses et évaluation antibactérienne de nouveaux hétérocycles pyrazoliques leurs chalcones correspondants

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Abstract **–** Le noyau pyrazolique constitue une structure hétérocyclique d'une grande importance, largement rencontrée dans de nombreux composés biologiquement actifs. Il occupe également une place notable en agrochimie, puisqu'on le retrouve dans divers herbicides, fongicides et insecticides.

Les recherches actuelles consacrées à la synthèse de dérivés pyrazolidiniques ouvrent la voie à la découverte de produits variés, présentant un intérêt pharmaceutique et thérapeutique, grâce à l'utilisation de réactifs simples, peu coûteux et de protocoles expérimentaux accessibles.

Dans ce cadre, notre travail s'inscrit dans l'étude de la synthèse d'hétérocycles de type pyrazole, obtenus par cyclocondensation de chalcones α,β-insaturées, elles-mêmes préparées à partir de l'acétamide, reconnu pour ses propriétés pharmacologiques.

Nos résultats révèlent que certains de ces hétérocycles possèdent une activité antimicrobienne intéressante.
Ces structures sont caractérisées par UV, IR, RMN H^1 et C^{13}.

Keywords – Aldéhyde aromatique, acétanilide, chalcones, condensation aldolique, pyrazolines.

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Comparative Antibacterial Activity of Hydroethanolic and Aqueous Extracts of *Asparagus acutifolius* L.

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Abstract – This study aimed to evaluate the antibacterial potential of hydroethanolic and aqueous extracts obtained from various parts of *Asparagus acutifolius* L. (roots, leaves, and young shoots) against five reference bacterial strains: *Escherichia coli* (ATCC 8739), *Pseudomonas aeruginosa* (ATCC 9027), *Salmonella typhimurium* (ATCC 14028), *Staphylococcus aureus* (ATCC 6538), and *Bacillus subtilis* (ATCC 6633), using the standard disk diffusion assay. The results revealed a marked superiority of the hydroethanolic extracts over their aqueous counterparts. Extracts from roots and young shoots displayed exceptional and broad-spectrum antibacterial efficacy, generating inhibition zones greater than 50 mm against key pathogens including *S. aureus*, *S. typhimurium*, and *P. aeruginosa*, outperforming conventional antibiotic controls (Amoxypen and Gectapen). The hydroethanolic root extract was particularly effective against *S. aureus* (54.5 mm) and *S. typhimurium* (50 mm), while the young shoot extract showed significant activity against *P. aeruginosa* (50 mm) and *S. aureus* (52.5 mm). Gram-positive (*B. subtilis*) and Gram-negative (*E. coli*) strains were also highly susceptible. Conversely, the aqueous extracts exhibited markedly lower activity, often with no observable effect, and leaf extracts were consistently ineffective regardless of the extraction solvent. These compelling results underscore the significant antibacterial potency inherent in *A. acutifolius*, predominantly concentrated in its roots and young shoots. This study strongly advocates for the valorization of this wild plant as a promising and sustainable source of novel natural antimicrobial compounds to combat bacterial infections.

Keywords – Asparagus acutifolius, Wild asparagus, Antibacterial activity, Disk diffusion, Natural extract

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Bioactive Lipids from a Marine Alga: Chemical Profile and Anti-Inflammatory Potential

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Abstract **–** This study investigates the anti-inflammatory potential of a lipid extract from *Alsidium corallinum*, a red alga of the family Rhodomelaceae. Total lipids were extracted using Soxhlet with hexane, converted into fatty acid methyl esters (FAMEs), and analyzed by GC–MS to establish the lipid profile. The extract was found to be particularly rich in unsaturated fatty acids, including eicosapentaenoic acid, linoleic acid, and α-linolenic acid. In addition, bioactive terpenic compounds such as thymol, carvacrol, and eugenol were identified. The anti-inflammatory activity was evaluated *in vivo* using Wistar rats subjected to carrageenan-induced paw edema. The extract produced a dose-dependent reduction in inflammation, reaching 68% inhibition at 200 mg/kg after 4 h, an effect closely comparable to that of diclofenac (75%). This demonstrates that *A. corallinum* extract exerts a significant pharmacological effect against acute inflammation. To further explore the molecular basis of this activity, docking studies on COX-2 (AutoDock Vina) were performed. Eicosapentaenoic acid and α-linolenic acid exhibited strong binding affinities for the enzyme's active site, while thymol and carvacrol displayed stabilizing interactions. These results suggest a potential synergistic effect between fatty acids and terpenic compounds in inhibiting COX-2 activity. Overall, *A. corallinum* represents a promising natural source of bioactive lipids, combining polyunsaturated fatty acids and phenolic derivatives. Its therapeutic potential highlights the value of marine algae as reservoirs of anti-inflammatory agents with possible applications in functional foods and drug development.

Keywords – Alsidium corallinum, Bioactive lipids, Unsaturated fatty acids, Anti-inflammatory activity, COX-2 inhibition

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Synthesis, Characterization, DFT Calculations and Molecular Docking of Eutectic Mixture of an anti-inflammatory Agent

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Abstract – Celecoxib (CEL) is a selective cyclooxygenase-2 (COX-2) inhibitor commonly prescribed for rheumatoid arthritis, osteoarthritis, acute pain, and inflammatory conditions. Despite its therapeutic potential, its clinical use is limited by poor solubility and slow dissolution. To address these drawbacks, this study investigated the formation of a eutectic mixture of celecoxib with salicylic acid as a strategy to improve its physicochemical properties. Binary mixtures of celecoxib and salicylic acid were prepared across the full composition range using liquid-assisted grinding and analyzed through differential scanning calorimetry (DSC), powder X-ray diffraction (PXRD), Fourier-transform infrared spectroscopy (FTIR), and scanning electron microscopy (SEM). DSC thermograms revealed a eutectic transition at approximately 0.45 molar fraction of celecoxib. PXRD and FTIR further confirmed eutectic formation and suggested the absence of strong molecular interactions in the solid state. To complement the experimental findings, Density Functional Theory (DFT) calculations were carried out to probe the interactions and thermodynamic behavior of the eutectic system. The results showed that the eutectic mixture displayed improved physicochemical properties compared with pure celecoxib. Increases in dipole moment and favorable changes in Gibbs free energy in the gaseous phase supported the enhanced stability and feasibility of the system. Finally, theoretical molecular docking studies were performed to evaluate the biological activity of the eutectic mixture.

Keywords – Eutectic mixture, Celecoxib, DSC, DFT, Molecular interactions

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Valorisation of Recycled Biomass in the Formulation of a Moisturising Cream

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Abstract **–** The use of recycled biomass is an innovative and sustainable approach to producing environmentally friendly cosmetic products. In this study, a bioactive extract obtained from recycled biomass was used to formulate a moisturising cream. This combines an oil phase (liquid paraffin and vegetal oils), an aqueous phase (rose water) and structuring agents (beeswax and borax) to create a stable, homogeneous emulsion. The natural oils used (neem and sweet almond) are traditionally recognised for their nourishing, healing and antibacterial properties, while vitamin E is commonly used as an antioxidant. The extract from the recycled biomass was added as a potential active ingredient which is reported to have moisturising and antioxidant properties. Physicochemical characterisation shows that the product has a pH of 6.65, close to that of human skin, indicating good skin tolerance. It also has a viscosity of 20 Pa.s at 25 °C, which reflects a balanced texture that is easy to apply and pleasant to the touch. Organoleptic evaluation reveals an off-white cream with a natural scent and homogeneous, shiny appearance that provides a feeling of freshness and hydration upon application. Finally, safety was verified by an acute skin toxicity test following OECD (Organisation for Economic Co-operation and Development) guidelines. At a dose of 2000 mg/kg body weight, no local reactions or signs of toxicity were observed in animals during the 14-day follow-up period. These results demonstrate the potential of using recycled biomass to formulate effective, safe, and sustainable cosmetic products.

Keywords – Recycled biomass, Moisturising cream, Cosmetic product, Formulation, Skin compatibility

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Artificial Intelligence for Smarter, Faster, and More Efficient Healthcare Solutions

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Abstract – The work aims to study the advantages and interests of using AI in the development of the pharmaceutical industry, the constraints that limit its use and the future prospects in this field. The Pharmaceutical industry represents a considerable economic value, it is thanks to all these efforts, particularly in terms of R&D (Research and Development) and innovation, that people can have the best healthcare. In recent years, the pharmaceutical industry has faced challenges related to rising R&D costs and reduced efficiency. The progress of AI algorithms and their increasing use in sensitive areas such as health, patient monitoring, surgical robots, personalized treatments, smart prostheses or epidemiological surveillance have enormous potential that leads us to wonder on the issues raised by these technologies. On the other hand, a new differentiation is created by using these algorithms to find intelligent solutions, based on real results, in order to solve fundamental problems of the pharmaceutical industry. AI-based algorithms are also being developed to efficiently probe synthetic pathways for new drug candidates. In combination with robotic platforms, the chemical space for new reactions can be explored by learning from automated reaction feasibility analysis. AI can now predict the physical and chemical properties of small molecules with a precision comparable to that of quantum mechanics, at a much lower cost and identify volunteers who perfectly meet the selection conditions for clinical trials.

Keywords – pharmaceutical industry, research and development, artificial intelligence, drugs, clinical trials

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Leveraging Artificial Intelligence for Early Diagnosis and Optimized Healthcare

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Abstract **–** The objective of this work is to study the contribution of Artificial Intelligence (AI) in predictive health, provide real examples of applications, explore how AI facilitates the process of prediction, and also address the limitations and ethical challenges of using AI in predictive health. AI refers to a set of theories and techniques that develop complex computer programs capable of simulating certain aspects of human intelligence (reasoning, learning, etc.), while predictive health is the medical discipline that utilizes diverse data sources (genetic, biochemical, statistical, etc.) to enable early and targeted intervention for predicting and preventing diseases, as well as diagnosing conditions before the onset of symptoms. AI is increasingly playing a crucial role in the field of predictive health through the use of advanced machine learning techniques and algorithms to predict disease risks and individual health outcomes. The objective is to identify the warning signs of diseases, provide more accurate diagnoses, and optimize treatments to improve clinical outcomes.

Keywords – Artificial Intelligence, Predictive Health, Disease Prevention, Machine Learning, Healthcare Innovation

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Inhibitory potential of CDK1 by natural metabolites derived from wild flax species: *in silico* study

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Abstract **–** Cyclin-dependent kinase 1 (CDK1) plays a central role in the G2/M transition, and its dysregulation is involved in several cancers, including prostate cancer. In the search for new natural inhibitors, ethyl acetate extracts from wild flax species have been shown *in vitro* to arrest the cell cycle in the G2/M phase in tumor cell lines. In order to explore this potential mechanism, an *in silico* molecular screening was performed on the metabolites identified in these species. These were pre-selected using SwissADME to evaluate their pharmacokinetic properties and their relevance as candidates. Their antimitotic potency was then analyzed using MOE software, by molecular docking on CDK1, in comparison with reference inhibitors currently in clinical trials. The results reveal that several identified flavonoids and lignans exhibit high affinity (binding energies generally below –7 kcal/mol), with values comparable to or even higher than those observed for reference inhibitors such as dinaciclib. These preliminary data support the hypothesis of CDK1 inhibition and highlight the antimitotic potential of natural metabolites from wild flax species, paving the way for the development of new anti-cancer strategies.

Keywords – CDK1, cell cycle, molecular docking, MOE, cell cycle, cancer

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Activités antioxydantes et antidépresseuses de fruit du palmier dattier (*Phoenix dactylifera* L.)

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Abstract – *Phoenix dactylifera* L., largement cultivé dans le monde, constitue une ressource alimentaire stratégique et un produit de consommation mondiale. Outre leur richesse nutritionnelle, les dattes occupent une place de choix dans la médecine traditionnelle. Dans ce contexte, la présente étude a été réalisée afin de caractériser la composition bioactive et d'évaluer les activités antioxydantes et antidépresseurs in vivo d'extraits aqueux issus du cultivar étudié. Deux techniques d'extraction, la décoction et la macération, ont été appliquées pour obtenir un sirop et un macérat. La quantification des métabolites secondaires a montré des teneurs notables en polyphénols et flavonoïdes, déterminées par les méthodes de Folin–Ciocalteu et au chlorure d'aluminium. L'activité antioxydante a été évaluée par le piégeage du radical libre DPPH, tandis que l'effet antidépresseur a été étudié par le test de nage forcée. Les résultats ont révélé des concentrations élevées en polyphénols (7,43 ± 0,301 et 0,67 ± 0,007 mg équivalent acide gallique) et en flavonoïdes (0,14 ± 0,007 et 0,13 ± 0,007 mg équivalent quercétine) dans le sirop et le macérat. Ces extraits ont montré une capacité significative de piégeage des radicaux libres (1,72 ± 0,03 et 13,36 ± 2,94). Les groupes traités dans le FST ont présenté une diminution notable du temps d'immobilité et une augmentation de l'activité de nage, suggérant un effet antidépresseur potentiel lié à la richesse en composés phénoliques. Ces résultats mettent en évidence l'intérêt nutritionnel et thérapeutique des dattes, et soutiennent leur consommation régulière comme source naturelle de composés bioactifs aux propriétés neuroprotectrices et antioxydantes.

Keywords – Datte, polyphénols, flavonoides, antioxydante, antidépressive.

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Évaluation de l'activité antioxydante et de l'effet antipyrétique in vivo de *Fagonia C.*

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Abstract **–**La famille des Zygophyllaceae regroupe de nombreuses espèces médicinales utilisées dans la pharmacopée traditionnelle pour le traitement de divers troubles. Parmi elles, le genre Fagonia occupe une place importante, notamment pour la prise en charge des affections inflammatoires, métaboliques, infectieuses et fébriles. En Algérie, il est couramment employé comme remède antipyrétique. Dans ce cadre, la présente étude visait à caractériser la composition chimique bioactive et à évaluer les activités antioxydantes et antipyrétiques in vivo des extraits n-butanolique (nBuOH) et acétate d'éthyle (AcOEt) de Fagonia C. L'analyse phytochimique a été réalisée pour la quantification des polyphénols et les flavonoïdes. L'activité antioxydante a été déterminée par les tests de piégeage des radicaux libres DPPH et ABTS, tandis que l'effet antipyrétique a été évalué chez le rat par induction de la fièvre à l'aide d'une suspension de levure de bière. Les résultats ont mis en évidence des teneurs élevées en polyphénols (60,84± 0,15 et 109,19± 0,22 µgEAG/mg) et en flavonoïdes (30,22± 0,44 et 71,5± 0,25 µgEQ/mg) dans les extraits nBuOH et AcOEt. Ces derniers ont également montré une activité antioxydante marquée, confirmée par des capacités significatives de piégeage des radicaux libres DPPH (27,433 ± 2,856 et 98,362 ± 7,801µg/mL) et ABTS (84,82 ± 2,114 et 108,48 ± 0,853µg/mL). Les groupes traités ont présenté une diminution notable de la température corporelle par rapport au paracétamol et au témoin, suggérant un effet antipyrétique lié à leur richesse en composés phénoliques. Ces résultats confirment le potentiel thérapeutique de Fagonia C. comme agent naturel antipyrétique et antioxydant.

Keywords – Antioxydant, Antipyrétique, Polyphénoles Flavonoïdes, Fagonia.

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Hepatoprotective properties of *Erodium* butanolic extract against propiconazole toxicity: An in silico study of PXR receptor interactions

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Abstract – Extensive use of pesticides, such as propiconazole, causes severe toxicity in humans. This study investigates the protective effects of the butanolic extract from the Erodium plant against these harmful effects. Wistar rats were treated with propiconazole, the extract, or both for eight weeks. Biochemical and histopathological analyses of the liver were performed, complemented by an in silico study that confirmed the extract's hepatoprotective properties through its interaction with PXR receptors. After eight weeks of treatment, rats were sacrificed. Plasma levels of various biochemical parameters were observed, and histopathologic changes in the liver were assessed. The primary chemicals found through LC-MS/MS analysis included shikimic acid, quercetin-3-xyloside, gallic acid, isoquercitrin, luteolin and hesperidin, and the results showed that this extract exhibited antioxidant capacity against DPPH compared to standards. Propiconazole exposure increased the levels of liver enzymes (ALT, AST, APL), cholesterol, triglycerides, LDL and bilirubin, decreased total protein and albumin levels and caused liver tissue damage. On the other hand, the Erodium butanolic extract reduced the undesirable effects induced by propiconazole, improved biochemical parameter levels, and significantly attenuated histologic abnormalities. Isoquercitrin has a high affinity for the PXR receptor, which may modulate its activity and contribute to the protective effect. We conclude that the *Erodium* plant contains secondary metabolites that can be used as prophylactic substances against the harmful effects of propiconazole.

Keywords – *Erodium*, pesticides, propiconazole, LC-MS/MS, toxicity, PXR, in silico.

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Design, Synthesis, and Molecular Docking Evaluation of Novel Schiff Bases as Potential Bioactive Agents

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Abstract – The development of novel heterocyclic scaffolds with enhanced biological activity remains a key challenge in medicinal chemistry. Schiff bases, derived from the condensation of amines with aldehydes, are of significant interest due to their structural diversity, ease of synthesis, and wide range of pharmacological applications. In this work, we report the design and synthesis of new Schiff bases obtained from the coupling of *coumaryl-thiazole* moieties with selected aromatic and heterocyclic aldehydes. The synthetic pathway was straightforward, providing high yields of pure products as confirmed by spectroscopic characterization (IR, NMR).

To complement the synthetic work, molecular docking studies were carried out to evaluate the interaction of the synthesized Schiff bases with the enzyme acetylcholinesterase (AChE), a validated therapeutic target in neurodegenerative disorders such as Alzheimer's disease. Docking simulations revealed that several of the novel Schiff bases exhibit favorable binding affinities, forming strong hydrogen-bonding and π–π stacking interactions within the active site of AChE. Notably, compounds containing heteroaromatic substituents demonstrated improved binding scores compared to aromatic analogs, suggesting a structure–activity relationship that favors heterocyclic aldehyde derivatives.

Overall, this study highlights the potential of coumaryl-thiazole-based Schiff bases as promising acetylcholinesterase inhibitors. The combined synthetic and computational approach provides a foundation for further in vitro and in vivo evaluations, with the aim of developing new candidates for the treatment of Alzheimer's disease and other cholinesterase-related pathologies.

Keywords – Schiff bases, coumaryl-thiazole, acetylcholinesterase, synthesis, molecular docking.

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phytochemical study and evaluation of the antifungal activity of aqueous and ethanolic liquid from fenugreek

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Abstract **–** Fenugreek (*Trigonella foenum-graecum* L.) is an annual herbaceous plant of the family Fabaceae, widely used since ancient times for its nutritional and medicinal virtues.
The study focused on the evaluation of antimicrobial activity and phytochemical profile of fenugreek (*Trigonella foenum-graecum* L.) seeds. The aqueous and ethanolic extracts were obtained by maceration and subjected to a phytochemical screening. Qualitative analyses revealed the presence of flavonoids, tannins, saponins, free quinones and alkaloids.
The evaluation of antifungal activity by the direct contact method, the aqueous extract showed high inhibition rates towards several pathogenic fungal strains, in particular *Aspergillus brasiliensis* (81.9%), *Botrytis cinerea* (63.3%) and *Colletotrichum sp.* (68.75%). The ethanolic extract also showed significant activity against these same strains, with respective inhibition rates of 73%, 66.66% and 71.25%. Furthermore, both extracts exerted marked inhibition on *Monilinia sp.*, reaching 73.75% for the aqueous extract and 72.5% for the ethanolic. Regarding *Candida albicans*, a moderate antifungal response was observed: the inhibition zone was 13 mm with aqueous extract and 10 mm with ethanolic, against 21 mm for the reference antifungal. In conclusion, fenugreek is a promising source of bioactive compounds, supporting its valorization potential in the development of natural antifungal agents.

Keywords – anti fungal activity, Trigonella foenum-graecum, phytochemical screening, flavonoids.