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Planification Expérimentale De L'extraction De Bleu De Méthylene Par Membrane Liquide Emulsionnée. Effet De Dilluant

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Abstract **–** Le procédé d'extraction par membrane liquide émulsionnée est pour but de séparer et de récupérer les effluents liquide. Elle permette d'extraire le polluant cible de la solution d'une manière sélective en réduisant l'effet néfaste sur l'environnement.
Dans le but de traiter le colorant cationique bleu de méthylène (BM) en solution aqueuse, on a choisi le procédé d'extraction par membrane liquide émulsionnée afin de suivre son élimination.
En premier lieu, une étude de la stabilité de la membrane par le plan de criblage Plackett-Burman a été réalisée. On a comparé la stabilité de deux membranes en changeant le diluent (le kerosene et le n-heptane). Les facteurs varies pour les deux membranes sont le pourcentage massique en tensioactif, le pourcentage massique en extractant, le temps, la vitesse d'agitation, la concentration de la phase interne, le rapport O/A et V_{ext}/V_{em}.
Par la suite, une extraction de BM a été élaboré en variant trois facteurs importants (le pourcentage massique en span80, le pourcentage massique de D2EHPA et la concentration initiale en BM). Cette 2ème partie a été effectuée en appliquant le plan Box-Behnken.
Les résultats de l'optimisation montrent un rendement d'extraction de BM de 99,54% avec les conditions optimales : Span80 = 7% en masse, D2EHPA= 4% en masse et $[BM]_0$ = 50ppm.

Keywords – Extraction, membrane liquide émulsionnée, pollution, colorant, plans d'expériences.

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Novel ruthenium (III) complex with sulfa drug derivative as an efficient antimicrobial agent : *In vitro* and *in silico* studies

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Abstract **–** Ruthenium complexes are well-known for their high pharmaceutical potential. This study reports the synthesis, characterization, and biological properties of a new ruthenium (III) with a sulfa drug derivative. The ligand and the complex were isolated in solid-state and then characterized using analytical, thermal, and spectroscopic methods. The antioxidant properties of the synthesized compounds were evaluated using free DPPH scavenging assay. At the same time, the antimicrobial activity was tested against Gram-positive and Gram-negative bacteria and fungal strains using the agar diffusion technique for sulfa drug derivative and its Ru(III) complex.

In addition, the pharmacokinetics and toxicity of the coordination compound along with its drug-like profile were predicted using ADMET simulations. Molecular docking studies against antibacterial drug targets were conducted to evaluate the possible interactions between the Ru(III) metal complex and the human enzymes.

All the results showed that the new ruthenium (III) complex is an efficient antimicrobial agent and could be considered as a potential drug.

Keywords – Ruthenium complex ; antioxidant, in vitro antimicrobial activity ; ADMET; Molecular Docking

Propriétés anti-inflammatoires d'un complexe de zinc (II) avec la metformine. Approche computationnelle et étude *in vivo*

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Abstract **–** Le zinc est un des des oligo-éléments les plus importants dans le corps humain. Il est indispensable à de nombreux processus biologiques en plus de posséder un potentiel pharmaceutique remarquable. Dans ce travail, un complexe de zinc (II) avec la metformine et l'hydroquinone a été synthétisé, caractérisé et ses propriétés biologiques ont été évalués.

L'objectif principal de ce travail étant le développement de composés à visée thérapeutique, l'évaluation du potentiel anti-inflammatoire du complexe a été réalisée *in silico* et *in vivo*.

La similarité avec les médicaments (Drug-likeness) et la prédiction des propriétés pharmacocinétiques (ADMET) du complexe de zinc (II) simulé par le serveur ADMETsar a indiqué que le composé présente une faible toxicité et peut être considéré comme un médicament-candidat. De plus l'étude par docking moléculaire contre les cyclooxygénases a prédit que les composés peuvent inhiber fortement les enzymes visées et posséder donc un bon potentiel anti-inflammatoire.

Les propriétés anti-inflammatoires de la metformine et son complexe de zinc (II) ont ensuite été testées *in vivo* sur des rats Wistar par l'injection d'une suspension à 1 % de carragénine dans la patte droite. Les résultats préliminaires ont montré que les composés présentent une activité anti-inflammatoire supérieure à celle observée pour le Votrex® (médicament de référence) avec un pourcentage de réduction de l'œdème estimé à 85,33%.

Keywords – Complexe de zinc (II); metformine; anti-inflammatoire, in vivo, in silico, docking moléculaire

Syhthesis of amphiphilic polymere and sopectroscopic study of IR technical

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Abstract **–** Amphiphilic polymers are copolymers composed of two types of polymers of different chemical nature. (1) One is hydrophilic capable of interacting with the aqueous environment and the other is hydrophobic capable of interacting with aliphatic chains. This specific category of polymers has the unique property of self-assembling in selective solvents.
In aqueous media, these amphiphilic copolymers have the ability to self-assemble, forming micelles consisting of a hydrophobic core and a hydrophilic crown. This core-crown structure offers several advantages for the transport and controlled release of drugs. Indeed, (2) these polymers allow the solubilization and encapsulation of hydrophobic active ingredients (APIs) at the heart of the micelle. These systems also allow the transport and therefore the protection of the API as well as its continuous release. They can also improve its efficacy and reduce side effects. Amphiphilic copolymers allow targeted delivery or modulation of therapeutic activity in vivo.
In this context, our work was based on the synthesis and determination of the physicochemical properties in aqueous medium of new amphiphilic graft copolymers with a hydrophilic polyvinylpyrrolidone skeleton and hydrophobic lauryl methacrylate grafts. (3)

Keywords – amphiphilic polymère, hydrophile, hydrophobe, IR.

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Evaluation of antimicrobial and antioxidant activities of metal complexes with sulfamoyloxazolidinone derivatives

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Abstract – The threat of infection is constantly increasing, causing various diseases. In this context, there is an urgent need for new active products to act on different pathogenic agents. The class of oxazolidinone derivatives has shown efficacy against resistant pathogens, including Gram-positive bacteria. For these reasons, oxazolidinone derivatives are good candidates for complexation with trace metals to enhance their biological potential.

The metal complexes were synthesized and characterized by molar conductivity, elemental, spectroscopic, and thermal analysis. The antimicrobial activity of the metal complexes against bacterial strains of *Bacillus subtilis*, *Enterococcus faecalis*, *Staphylococcus aureus*, *Escherichia coli*, as well as fungal strains of *Candida albicans* and *Aspergillus niger* was evaluated *in vitro* using the agar diffusion method. Furthermore, the antioxidant activity of the compounds was assessed using the DPPH• free radical scavenging method.

Structural characterization revealed that two ligands are coordinated with the metal, forming a neutral complex with the proposed general formula $[M(L)_2].nH2O$. The *in vitro* antimicrobial evaluation shows that the synthesized compounds are active against the tested strains. The ligand HL^1 exhibits better antibacterial activity compared to its analogs. The complexes with this derivative also showed excellent activity against the tested bacteria, better than the ligand alone. Moreover, the formed compounds proved to be more active against Gram-positive bacteria such as *Bacillus subtilis* and *Enterococcus faecalis*. The *in vitro* antioxidant activity data showed that all the synthesized compounds could be used as antioxidant agents. The ligand HL^2 and their complexes exhibit remarkable radical-scavenging activities, more than the ascorbic acid.

Keywords – Oxazolidinones, metal complexes, Antimicrobial activity, Antioxidant activity.

DFT Design and Analysis of New Quinoxaline Derivatives for Organic Solar Cells

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Abstract **–**The present study has been carried out with the aim to design novel non fullerene acceptor (NFA) molecules (A1-A8) derived from the diphenyl-pyrazolo[3,4-b]quinoxaline electron acceptor (see Fig.1) for organic solar cells (OSCs). The B3LYP (Becke, 3-parameter, Lee-Yang-Parr) and TD-CAM-B3LYP (Time-dependent-Coulomb-Attenuating) methods in conjunction with the standard 6-31G(d,p) atomic basis set and the polarizable continuum solvation model (PCM) were used to evaluate the efficiency of the designed acceptors through the calculation of their optoelectronic properties and photovoltaic parameters. The highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energies, energy gaps (Eg), vertical ionisation potential (IP), vertical electron affinity (EA), electron reorganization energies (λe) and hole reorganization energies (λ_h) and density of states (DOS) were investigated. Additionally, optical properties such absorption maxima (λabs), oscillator strength at the maximum wavelength (fos), light harvesting efficiency (LHE) and exciton binding energies (EBE) were also examined. Meanwhile, the fill factor (FF) and open circuit voltage (Voc) of the studied molecules were calculated. The obtained results show that the electronic nature of the substituents plays a significant role in improving the band gap E_{gap}, producing a high bathochromic shift, and increasing the open circuit voltage. Interestingly, the derivative **A2** presents the optimal electronic properties with low band gap (1.73 eV) and high open-circuit voltage (1.32 V) when combined with the PM6 donor polymer. The present computational study reveals that these novel designed molecules display good photovoltaic properties and are suitable candidates for organic solar cells.

Keywords – Quinoxaline; Organic solar cells ; Optoelectronic properties; Photovoltaïc parameters ; DFT

Photocatalytic activity of Methyl Green using ZnO thin films

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Abstract **–**Methyl Green (MG) (4-{[4-(dimethylamino) phenyl] [4-(trimethylazaniumyl) phenyl] methylidene} cyclohexa-2, 5- dien-1-ylidene) (dimethyl) ammonium bromide chloride is used in the reduction of wastewater using ZnO thin films prepared by ultrasonic spray pyrolysis (USP) technique, The structural properties studied using X-ray diffraction shows that all the films are polycrystalline with hexagonal structure and present (101) preferential orientation, optical properties show that the obtained films are transparent in the visible region, grains size, band-gap energy, Urbach parameter, and films thickness are deduced from the spectra. Photocatalytic parameters show a good degradation of Methyl Green under UV-Vis irradiation.

Keywords: Methyl Green, Photocatalysis, ZnO; Thin films.

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COMPARATIVE STUDY ON THE ACTIVATION OF PMS FOR DICLOFENAC DEGRADATION USING ZnO/Co_3O_4 UNDER LIGHT AND DARK CONDITIONS: TOXICITY ASSESSMENT

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Abstract

Diclofenac (DCF) is a non-steroidal anti-inflammatory pharmaceutical widely used for its analgesic, anti-arthritic, and anti-rheumatic properties. Its presence in aquatic environments makes it one of the most frequently detected drugs, posing significant risks to human and aquatic health. Advanced oxidation processes (AOPs) have been widely studied and applied to the removal of pharmaceuticals from water.

In this study, a ZnO/Co_3O_4 nanocomposite was employed to activate PMS for the degradation of diclofenac (DCF) in the presence and absence of light. The material was synthesized via co-precipitation and characterized using various techniques (XRD, BET, SEM, XPS, ATR-IR, UV-Vis DRS).

In order to operate under optimum conditions, catalyst dosage, PMS concentration, and initial DCF concentration were evaluated. Remarkably, the highest efficiency was achieved in the absence of light (catalytic degradation), where DCF was completely degraded within 2 minutes. Additionally, the degradation mechanism was proposed, and identification of by-products was carried out using liquid chromatography electrospray ionization mass spectrometry (LC-ESI-MS). Furthermore, the toxicity of the degradation products was predicted using ECOSAR v2.2, ensuring a comprehensive assessment of potential environmental risks.

This study not only provides a better understanding of the mechanisms behind the heterogeneous activation of PMS on the ZnO/Co_3O_4 nanocomposite for the degradation of organic pollutants but also proposes an eco-friendly synthesis approach for the development of novel and efficient catalysts. This research advances the understanding of AOPs for pharmaceutical removal in water treatment, emphasizing ZnO/Co_3O_4 nanocomposites as effective environmental catalysts.

Keywords: Degradation; DCF; PMS; ZnO/Co_3O_4; LC-ESI-MS; Toxicity

Effect of temperature on the inhibition efficiency of a new Schiff base SBL-F against steel corrosion in acidic medium

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Abstract – Corrosion inhibitors are essential for protecting metals from degradation, extending the lifespan of structures, machinery, and pipelines. They work by forming a protective barrier on the metal surface, reducing the impact of environmental factors like moisture and chemicals. Their use helps prevent costly maintenance, enhances safety, and improves the efficiency of industrial processes.

Temperature is a key factor influencing both corrosion processes and the efficiency of corrosion inhibitors. This study investigates the effect of temperature on the inhibitory performance of a selected corrosion inhibitor in an acidic medium. Electrochemical techniques such as potentiodynamic polarization and electrochemical impedance spectroscopy (EIS) were used to evaluate the inhibition efficiency at different temperatures.

The results show that increasing temperature generally accelerates the corrosion rate due to enhanced metal dissolution. However, the inhibition efficiency of the tested compound varies with temperature, depending on its adsorption mechanism. Thermodynamic parameters such as activation energy, enthalpy, and entropy were determined to understand the nature of adsorption. The analysis suggests that inhibitors following physisorption tend to lose efficiency at higher temperatures, whereas chemisorbed inhibitors exhibit stronger stability.

Overall, the study highlights the importance of considering temperature effects when selecting corrosion inhibitors for industrial applications, ensuring their optimal performance in different operating conditions.

Keywords – Corrosion; inhibitor; potentiondynamic polarization; EIS.

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An Artificial Neural Network Approach For Predicting the Solubility of an Antituberculosis Drug (isoniazid, INH) in Ionic Liquids

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Abstract **–** Isoniazid is a common antibiotic used to treat tuberculosis. One significant barrier to its widespread utilization is that it can undergo hydrolysis when stored inadequately, leading to the formation of hydrazine, a toxic and carcinogenic compound. Research studies show that Ionic liquids (ILs) are recognized as a sustainable green solvent alternative to conventional organic solvents and have a direct influence on improving the stability of drugs while still maintaining their therapeutic efficiency and solubility. This study carries out a nonlinear approach (Artificial neural network, ANN) on experimental data for the solubility prediction of Isoniazid in different pure ionic liquids. A collected database of 13 Isoniazid-ILs systems composed of 8 cations, and 6 anions accounting for 246 data points and 5 inputs: 4 σ-moments descriptors and the temperature at different ranges. The performance of the proposed method was statistically validated with a root-mean-square error (RMSE) of 0.0032, mean-square error (MSE) of 0.00001, mean absolute error (MAE) of 0.0022, coefficient of correlation (r) of 0.9999, coefficient of determination (R^2) of 0.9998, robustness (Q^2) of 0.9998, and various graphical analyzes. The overall results proved good predictive ability and robustness of the proposed ANN approach.

Keywords – Solubility, isoniazid, antibiotic drug, Ionic Liquids, Artificial neural network.

Un nouveau matériau à base d'argile pour la dépollution des eaux : Efficacité d'élimination d'un contaminant organique

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Résumé **–** Ce travail de recherche vise à élaborer et examiner l'efficacité d'un nouveau matériau écologique durable et moins couteux pour l'élimination d'un composé organique dangereux, par adsorption en batch. Le matériau élaboré a été synthétisé de manière efficace en intégrant des molécules dans l'espace inter lamellaire d'une argile Algérienne. Une caractérisation du matériau obtenu a été réalisée à l'aide de plusieurs techniques, notamment l'analyse thermogravimétrique (TGA), la diffraction des rayons X (XRD), la spectroscopie infrarouge à transformée de Fourier (FTIR), la microscopie électronique à balayage (SEM), la spectroscopie de rayons X à dispersion d'énergie (EDX) et la méthode de Brunauer, Emmett et Teller (BET). Un plan expérimental d'adsorption a pris en compte divers paramètres, tels que la concentration initiale, la dose de l'adsorbant ainsi que la variation du pH. A la fin, on a pu identifier la quantité optimale du matériau nécessaire pour une bonne efficacité d'adsorption ainsi que la concentration initiale et le pH de la solution aqueuse du contaminant qui mènent à une élimination entière du polluant présent dans l'eau. La cinétique d'adsorption a été également étudiée. L'élimination inappropriée des composés organique peut entraîner une pollution environnementale considérable, contaminant les d'eau et ayant des effets néfastes sur les écosystèmes aquatiques.

Keywords – Adsorption ; Dépollution d'Eau ; Argile-Modifiée ; Contaminant Organique.

The discovery of new potent Mycobacterium tuberculosis DXR inhibitors for potential anti-tuberculosis agents through a combination of molecular docking and ADME-Tox prediction

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Abstract – The discovery of antibiotics gave rise to hope that it would one day be possible to control all infectious diseases. However, the excessive use of antibiotics leading to the increase in the number of multi-drug resistant bacteria has become a key health threat globally. This makes it necessary to develop new therapeutic strategies, based in particular on the search for new molecules capable of acting as new antibacterial agents. During this work, we relied on the treatment of bacterial infections based on the inhibition of 1-deoxy-D-xylulose 5-phosphate reducto-isomerase (DXR), an essential enzyme of the non-mevalonic pathway of synthesis of isoprenoids, in most pathogenic microorganisms. The main objective of this research is to acquire skills in molecular modeling, the most important of which is virtual screening which is based on molecular docking by Surflex-dock in order to contribute to the in silico development of new, more powerful and more selective inhibitors of Mycobacterium tuberculosis DXR.
Our results show that the docking study of a collection of 236 similar 6JB (reference inhibitor) from the PubChem chemical library highlights the compounds CID113304440 and CID60701454 as the best DXR inhibitors with affinities equal to 8.20 M-1 and 8.64 M-1 respectively. Moreover, the ADME-Tox filtering application provides us with positive information on the physicochemical, pharmacokinetic and toxicological properties of the proposed inhibitors. Finally, the hierarchy of computational methods of increasing accuracy employed in this work finds CID113304440 and CID60701454 to be the most potent inhibitor against Mycobacterium tuberculosis DXR.

Keywords – Anti-tuberculosis agents, Molecular docking, DXR, ADME-Tox

Synthesis and spectroscopic characterization of new hydrazone derivative

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Abstract –

An aromatic α, β-unsaturated ketone **(A)** was obtained through a Claisen-Schmidt reaction. A new hydrazone derivative **(B)** was synthesized under reflux by reacting chalcone **(A)** with 2,4-dinitrophenylhydrazine. The carbonyl compound **(A)** was obtained via a mixed aldol condensation, through the Claisen-Schmidt reaction, in which para-isopropylbenzaldehyde was used to react with an enolizable ketone, "acetone," under basic conditions.

Under acid-catalyzed conditions, the hydrazone derivative **(B)** was prepared by an equimolar reaction of chalcone **(A)** and 2,4-dinitrophenylhydrazine in methanol.

The structure of compounds **(A)** and **(B)** was studied using various spectroscopic techniques such as **^{1}H NMR, ^{13}C NMR, COSY,** and **FT-IR.**

Keywords –2, 4-dinitrophenylhydrazine; aldolic condensation; hydrazone; α, β-unsaturated ketone.

Évaluation de l'activité biocide du peroxyde d'hydrogène sur Pseudomonas aeruginosa présent dans les eaux polluées.

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Résumé

La pollution des eaux figure parmi les aspects les plus inquiétants de la détérioration de l'environnement naturel. La contamination de l'eau, notamment par les bactéries, a diverses répercussions sur la santé humaine, soit par ingestion accidentelle, soit par simple contact. Ainsi, l'homme semble être la première victime de la pollution de l'eau. L'eau peut être contaminée par des bactéries provenant de matières fécales ; les excréments humains et animaux renferment généralement des agents pathogènes qui résident dans leur système digestif en tant qu'organismes commensaux susceptibles de polluer l'eau. En réalité, une variété de produits biocides comme le chlore, les chloramines et l'ozone sont disponibles. Le peroxyde d'hydrogène (H_2O_2) est couramment employé comme agent biocide pour la désinfection, la stérilisation et l'antisepsie. Il s'agit d'un liquide incolore proposé sur le marché en différentes concentrations, allant de 3% à 90%. On le considère comme respectueux de l'environnement, car il peut se décomposer rapidement en substances non nuisibles (eau et oxygène). Cette recherche vise à étudier l'effet biocide du peroxyde d'hydrogène (H_2O_2) à diverses concentrations et selon différents temps de contact, sur la bactérie *Pseudomonas aeruginosa*, en recourant à la méthode bactériologique traditionnelle. Les résultats obtenus ont démontré que les tests de désinfection biocide à l'aide de H_2O_2, aux concentrations de 500 ; 1500 ; 2500 et 3500ppm, ont produit des taux d'inactivation respectifs de 43 ; 57 ; 67 et 86%, suite à un temps de contact de six heures. Selon ces résultats, nous pouvons déduire que cette bactérie démontre une certaine résistance au peroxyde d'hydrogène en raison de la création d'un biofilm. Cela complique l'infiltration du biocide et nécessite donc des durées d'action prolongées.

Mots clés: Pollution de l'eau ; Biofilm ; Peroxyde d'hydrogène ; Pseudomonas aeruginosa

Synthesis, spectroscopic characterization, single-crystal X-ray diffraction and Hirshfeld surface analysis of 4-aminoantipyrine derived Schiff base.

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Abstract **–**4-Aminoantipyrine (AAP), one of the most widely used derivatives of antipyrine, is a versatile compound with significant applications across analytical and pharmaceutical fields.AAP and its derivatives exhibit a various range of significant biological activities [1–5], including analgesic, anti-inflammatory, antimicrobial, and anticancer effects.Schiff bases derived from 4-aminoantipyrine and their metal complexes have a wide range of applications in medicinal and pharmacological areas, and they also possess chemotherapeutic properties**[6]**. During our investigation we successfully synthesized a new Schiff base compound derived from 4-aminoantipyrine, *viz. (E)*-4-(2,4-dimethoxy-3-methylbenzylideneamino)-1,5-dimethyl-2-phenylpyrazolidin-3-one. The new compound was prepared through condensation reaction and characterized through elemental analysis, ^{1}H and ^{13}C NMR spectroscopy and single-crystal X-ray diffraction. The single-crystal X-ray diffraction indicates that the asymmetric unit of title compound contains two crystallographically independent molecules (A and B) and crystallized in the monoclinic space group $P2_1/c$. The crystal structure features **C—H···O** and **C—H···π** hydrogen bonds. Hirshfeld surface analysis indicates that the most significant contact in the crystal packing is H···H (57.2%), followed by C···H/H···C interactions (23.3%).

Keywords – Schiff Base, Single-crystal X-ray diffraction, 4-aminoantipyrine, Hirshfeld surface analysis.

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Etude de l'efficacité d'un inhibiteur vert de corrosion sur l'acier en milieu acide

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Abstract – Les phénomènes de corrosion interne affectant les canalisations du réseau de dessalage et le réseau de collecte des puits producteurs de pétrole brut sont principalement de nature électrochimique. Ils sont provoqués par le contact de l'eau liquide avec la paroi interne des pipelines. La forme et la vitesse de corrosion dépendent de plusieurs facteurs, notamment la teneur en eau des fluides transportés, le pouvoir oxydant du milieu environnant et la capacité protectrice des dépôts de corrosion.

Les fluides corrosifs sont traités à l'aide d'inhibiteurs de corrosion afin de réduire la vitesse de l'attaque corrosive des matériaux. Cette mesure est particulièrement importante en présence de gaz dissous tels que l'oxygène, le dioxyde de carbone et le sulfure d'hydrogène, qui contribuent à l'augmentation de l'acidité du milieu.

Dans l'industrie pétrolière, les inhibiteurs organiques sont couramment utilisés en raison de leur efficacité et de leur disponibilité. Cependant, leur toxicité et leur impact environnemental sont préoccupants. Les inhibiteurs verts représentent une alternative plus écologique et économique.

L'objectif de cette étude est d'examiner les propriétés inhibitrices d'un extrait de plante appartenant à la famille des Moracées sur la corrosion de l'acier en milieu acide. L'efficacité inhibitrice de cet extrait a été évaluée à l'aide de la méthode gravimétrique et de la polarisation potentiodynamique.

Les résultats de l'étude ont montré que l'extrait étudié est très performant. Son efficacité inhibitrice augmente avec l'augmentation de sa concentration, atteignant 92 % à 5000 ppm. De plus, l'adsorption des molécules inhibitrice de l'extrait sur la surface de l'acier suit l'isotherme de Langmuir. Par ailleurs, les courbes de polarisation ont montré que notre inhibiteur agit comme un inhibiteur mixte à prédominance cathodique.

Keywords – inhibiteur vert, efficacité, acier, milieu acide, gravimétrie, courbes de polarisation.

Influence des solvants sur l'extraction des métabolites secondaire à partir de différents Organes de Passiflora caerulea L., Physalis peruviana L.

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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 Passiflora caerulea L., Physalis peruviana L. et 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 solvant le plus adapté à 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 de Passiflora, quel que soit le solvant ou la méthode d'extraction utilisé. De plus, les racines de Physalis et de Solanum présentaient des concentrations importantes de ces composés, en accord avec l'activité antioxydante totale (AAT) évaluée dans les différents organes de la plante chez les trois espèces. 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 chaque espèce médicinale étudiée.

Keywords – macération; décoction; teneur en polyphenols totaux; flavonoïdes; activité antioxydante

Synthesis, Characterization and Catalytic Activity of Ternary Copper-Based Catalysts

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Abstract **–** Ternary nanocatalysts based on copper and zinc oxide, supported on alumina, magnesium oxide and silica were synthesized using the polyol method, characterized by scanning electron microscopy (SEM) combined with energy dispersive X-ray spectroscopy (EDX), X-ray fluorescence spectroscopy (XRF), X-ray diffraction (XRD) and N_2 adsorption-desorption (BET). The catalytic activity of the nanocatalysts was evaluated in the conversion of carbon dioxide at atmospheric pressure and various temperatures.

The results indicate that the catalysts exhibit high activity and selectivity for methanol at low temperatures, while methane formation become predominant at higher temperatures.

Keywords – CO_2 conversion, polyol method, methanol, methane

Synthèse, caractérisation et étude cristalline d'un nouveau composé organique dérivé trifluoré du benzimidazole

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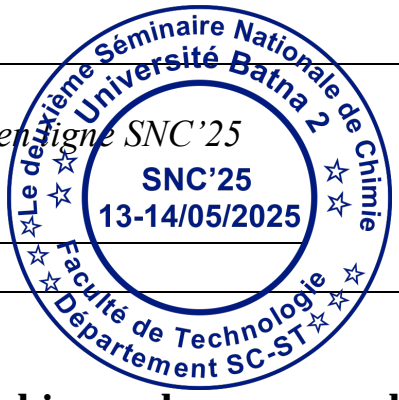
Abstract – Les composés hétérocycliques occupent une place essentielle en chimie médicinale, en raison de leur intérêt dans la recherche de nouvelles molécules bioactives pour l'industrie pharmaceutique [1]. Parmi eux, les hétérocycles azotés jouent un rôle clé dans de nombreux domaines, notamment en chimie de coordination [2], et présentent une large gamme d'activités biologiques [3], grâce à leur similarité avec des molécules naturelles ou synthétiques biologiquement actives [4].

Dans le cadre de nos travaux, nous avons synthétisé un nouveau dérivé des benzimidazoles : le 2-(2,4,6-trifluorophényl)benzimidazole. Ce composé a été caractérisé par spectroscopies infrarouge, UV-Visible et RMN, ainsi que par diffraction des rayons X sur monocristal. L'analyse cristallographique a révélé que le composé cristallise dans le groupe d'espace *Pbca* du système orthorhombique, avec quatre groupements formulaires par maille .

Keywords – Benzimidazole , synthèse organique, DRX , IR , UV-visible , RMN.



Synthèses et évaluation antimicrobienne de nouveaux hétérocycles dérivés des acides nitro-halogénés

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Abstract **–** La chimie hétérocyclique est une branche essentielle de la chimie organique, axée sur la synthèse des composés hétérocycliques. Parmi ceux-ci, les oxadiazoles contenant des composés nitro-aromatiques halogénés1 représentent un défi important dans des domaines variés, tels que la biotechnologie, la chimie des matériaux et la pharmacologie. En effet, ces composés se révèlent être des agents prometteurs dans le traitement de nombreuses pathologies, notamment comme anticancéreux, antituberculeux, anticonvulsivants, anti-inflammatoires, antibactériens, antifongiques et antioxydants2. Ainsi, ils offrent des perspectives fascinantes pour la découverte et le développement de nouveaux médicaments.

Nous nous sommes concentrés sur la synthèse de nouveaux hétérocycles azotés halogénés dérivés de 1,3,4-oxadiazole. Nos résultats montrent que certains de ces hétérocycles présentent un effet antimicrobien intéressant contre plusieurs souches bactériennes à Gram positif telles que Staphylococcus aureus et Enterococcus faecalis, ainsi que des bactéries à Gram négatif comme Escherichia coli et Pseudomonas aeruginosa. En outre, ces composés montrent également une activité antifongique considérable via Aspergillus niger et Candida albicans.

Ces structures sont caractérisées par UV, IR, RMN H1 et C13 et GC-Mass.

Keywords – Nitro-aromatique, hétérocycle, antibactérien, antifongique.

Propriétés électroniques, magnétiques et élastiques de $FeNi_3$ et $FeNi_2Pt$

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Abstract – La méthode pseudopotentielle ab initio repose sur la théorie de la fonctionnelle de la densité (DFT), utilisant l'approximation du gradient généralisé (GGA) telle que décrite par Perdew-Burke-Ernzerhof (PBE). Mise en œuvre via le programme Siesta, cette méthode examine les propriétés structurales et optiques de l'alliage nickel-fer (Fe-Ni) qui cristallise dans la structure FeNi3. Cette approche est très appréciée pour sa précision dans la prédiction de la structure cristalline et des propriétés de $FeNi_3$. Les paramètres structuraux calculés correspondent étroitement aux données théoriques et expérimentales, confirmant la fiabilité de ces prédictions. Les paramètres de réseau, calculés à pression nulle, correspondent aux résultats théoriques et expérimentaux rapportés précédemment. De plus, les propriétés calculées, notamment la structure de bandes, la densité totale des états (DOS) et la densité partielle des états (PDOS), ainsi que les valeurs des constantes élastiques pour l'alliage, suggèrent son adéquation pour des applications spécifiques dans des domaines ciblés.

Keywords –DFT ; FeNi2Pt ; Propriétés électroniques ; Propriétés élastiques

Studying the Electrochemical Properties of Carbon Steel for Strand Fabrication.

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Abstract –

This research explores the corrosion characteristics of pearlitic steel subjected to different levels of mechanical deformation and exposure to sulfate solutions. Through systematic experimentation and analysis, it was observed that increasing degrees of mechanical deformation significantly escalate the susceptibility of pearlitic steel to corrosion. This phenomenon is attributed to the alteration of surface morphology and the introduction of microstructural defects during deformation, which serve as initiation sites for corrosion processes. Moreover, the presence of sulfate solutions exacerbates corrosion rates, particularly in areas where the steel contains higher concentrations of residual stresses and mechanical flaws. The study elucidates that these defects act as preferential sites for localized corrosion, accelerating degradation mechanisms such as pitting and stress corrosion cracking. Insights gained from this investigation underscore the critical interplay between mechanical processing history, material defects, and environmental exposure in influencing the corrosion behavior of pearlitic steel. These findings are pivotal for advancing corrosion mitigation strategies and enhancing the durability and reliability ofpearlitic steel components in industrial applications, particularly where exposure to sulfate-rich environments is prevalent.

Keywords – Pearlitic steel, corrosion, Deformation, Resistance, electrochemical

Antioxidant, antibacterial and anti-inflammatory effects of *Juniperus communis* aqueous extract from Algeria's mountainous regions

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Abstract **–**The current study aimed to analysis of the possible radical scavenging, antibacterial and anti-inflammatory effects of *Juniperus communis* aqueous extract gathered from Algeria's mountainous regions. Standard operating protocols were applied for the extraction of phenolic components and for quantitative and qualitative analysis. However, HPLC analysis was used to identify and quantify each phenolic component. The plant extract's total phenolic acid content was ascertained using the Folin-Ciocalteu method, while its total flavonoid concentration was ascertained using the aluminum chloride colorimetric assay. Using the ferric reducing antioxidant power (FRAP) assay and the DPPH method, their antioxidant capacity was assessed by determining their ability to eradicate free radicals. Disk diffusion was used to test the antibacterial efficiency against five bacterial strains, and a protein

A high polyphenol content of 103.80 ±0.30 mg GAE/g was observed in the extract, while the flavonoid content was estimated at 15.85±0.80 mg QE/g. The extracts showed important antioxidant activity in two separate tests (IC_{50}: 101.06±0.19; EC_{50}: 59.54±0.12), and a positive antibacterial activity *against E.coli*, *K. pneumoniae, C.albicans*. In the anti-inflammatory assay, the extract has a potent anti-denaturation effect on albumin. According to the study's findings, the aqueous extract of *Juniperus communis* gathered from Algeria's mountainous regions is possible sources of phenolic compounds with important natural antioxidant, antimicrobial and anti-inflammatory characteristics that may be employed in pharmaceutical products.

Keywords – Radical scavenging, Antibacterial effect, Anti-inflammatory effect, Juniperus communis , Algeria's mountainous regions.

Approche automatisée en un seul clic pour le criblage virtuel basé sur le docking moléculaire via SwiftDock

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Abstract – Le criblage virtuel basé sur le docking moléculaire (CVDM) constitue une stratégie *in silico* essentielle pour l'identification de candidats bioactifs à partir de bibliothèques de petites molécules ciblant des macromolécules d'intérêt pharmacologique. Plusieurs outils, tels que PyRx, InstaDock ou MultiDock Screening Tool, permettent la réalisation de telles analyses en s'appuyant sur des logiciels de docking reconnus, notamment AutoDock4 (AD4) ou AutoDock Vina (ADV). Toutefois, malgré l'existence de divers scripts et logiciels visant à simplifier le CV basé sur AD4, aucun outil actuel ne prend en charge l'ensemble du processus en une seule exécution, englobant la préparation des protéines et des ligands jusqu'à l'extraction des poses optimales. Afin de répondre à cette lacune, nous présentons SwiftDock (https://github.com/notacoder-dz/SwiftDock), un outil open-source développé pour Windows, qui permet l'exécution complète d'un CVDM basé sur AD4 via une approche automatisée en un seul clic. Une fois les fichiers de protéines et de ligands placés dans le répertoire de travail, SwiftDock, après exécution, s'occupe automatiquement de l'ensemble des étapes préalables, du processus de docking, ainsi que des étapes post-docking, sans nécessiter de compétences préalables en bioinformatique. Malgré certaines limitations techniques, SwiftDock a été conçu dans le but de faciliter l'accès au DM et au CV, en particulier pour les non-bioinformaticiens, ainsi que de favoriser l'orientation de la recherche expérimentale et thérapeutique.

Keywords – Docking moléculaire ; AutoDock4 ; Criblage virtuel ; Exécution en un clic ; SwiftDock.

Optimized Sulfonation Strategy for High-Efficiency Diesel Fuel Desulfurization

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Abstract **–**The removal of sulfur compounds from diesel fuel is crucial to minimizing pollutant emissions and complying with stringent environmental regulations. Oxidative sulfonation enhances desulfurization by converting sulfur-containing compounds into highly polar sulfone derivatives, facilitating their subsequent extraction. This study investigates the optimization of sulfonation conditions to maximize desulfurization efficiency while minimizing side reactions.

The sulfonation process was carried out by gradually introducing concentrated sulfuric acid (97%) into diesel fuel under continuous stirring in a three-necked flask, ensuring precise control of reaction parameters. To prevent thermal degradation and undesired side reactions, the reaction temperature was maintained below 50°C using an efficient cooling system. Once the acid addition was complete, the mixture was agitated for a predetermined duration to achieve optimal conversion.

Following phase separation, the organic layer was neutralized using sodium hydroxide then washed with distilled water, and the fuel was dried using anhydrous calcium chloride to eliminate residual moisture. The final sulfur content was quantified via X-ray fluorescence spectroscopy to assess desulfurization performance.

Experimental results demonstrate that a reaction time of 35 minutes at 45°C yields an optimal desulfurization efficiency of 83.97%. Exceeding these conditions leads to the decomposition of sulfonating agents and the formation of undesired byproducts, reducing overall efficiency. These optimized parameters contribute to a more effective and sustainable diesel desulfurization process, ensuring lower sulfur emissions and improved fuel quality.

Keywords – Desulfurization, sulfonation, oxidation, purification, optimization.

Computational study of heterocyclic compounds with biological interest

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Abstract – Quantum calculations based on density functional theory (DFT) were used to study the relationship between the structure and antioxidant activity of heterocyclic compounds: azo dye (S1), an ester (S2), and a hydrazide (S3). The B3LYP method combined with the 6-311 G (2d, 2p) basis set has been employed to investigate the reactivity of these novel heterocyclic compounds. The ester (S2) exhibits higher antioxidant activity than other heterocyclic compounds.

Keywords – DFT, novel heterocyclic compounds, biological activity.

Dosage des Polyphénols de Certaines Plantes Cultivées en Algérie et Leurs Applications dans l'Inhibition de l'Entartrage Eléctrochimique

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Résumé **–** Le travail consiste à utiliser des plantes, couramment cultivées en Algérie, en tant qu'inhibiteurs du phénomène d'entartrage. Ces plantes sont caractérisées et dosées afin de déterminer leurs teneurs en polyphénols qui constituent généralement l'espèce responsable de cet effet inhibiteur.
Les objectifs de ce travail sont, d'abord, l'évaluation du pouvoir entartrant de l'eau de Bejaia. Ensuite, le test de l'effet inhibiteur des extraits aqueux de plantes vis-à-vis de l'entartrage électrochimique. Enfin, la caractérisation des extraits afin de déterminer l'espèce active.
L'évaluation du pouvoir entartrant de l'eau de Bejaia sera effectuée par les essais d'entartrage accéléré en imposant le potentiel de réduction de l'oxygène dissous. Les tests d'inhibition d'entartrage des extraits aqueux seront faits en utilisant la méthode de chronoampérométrie et par spectroscopie d'impédance électrochimique. Les extraits aqueux seront caractérisés par spectroscopie Infra Rouge à Transformé de Fourier et par dosage des composés phénoliques.
Les résultats obtenus montrent que l'eau de Bejaia possède un caractère très entartrant. En incorporant différentes concentrations en inhibiteurs, la vitesse d'entartrage diminue significativement et ces substances agissent par effet de seuil et leurs concentrations efficaces est très insignifiantes. Le dosage des polyphénols montre des teneurs assez importantes, ce qui peut être à l'origine de l'efficacité inhibitrice.
Les eaux de Bejaia sont très minéralisées et riches en ions Ca^{2+} et Mg^{2+}, ce qui à l'origine des dépôts incrustants sur les parois des canalisations des conduites domestiques et industrielles. L'utilisation des extraits aqueux de plantes cultivées en Algérie permet de valoriser la production de ces végétales et de proposer une solution rationnelle au problème récurrent du phénomène d'entartrage.

Mots clés – Entartrage électrochimique, Inhibition, Polyphénols, Environnement, Plantes.

A study of Zn–Ni–Al_2O_3 nanocomposite coating and evaluation of its morphological and electrochemical properties

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Abstract – Zn–Ni–Al_2O_3 nano-composite coatings were electrodeposited on mild steel using a novel sol enhanced electroplating method. The effect of alumina sol on the electrodeposition process, and coating properties was investigated using, X-ray diffraction, scanning electron microscopy (SEM), and electrochemical impedance spectroscopy were studied in a solution of 3% NaCl. The results indicated that the electro-crystallization processes of Zn–Ni and Zn–Ni–Al_2O_3 were governed by a three-dimensional nucleation process controlled by diffusion. XRD results showed that the phase structure of both alloy and composite coatings was single Ni_5Zn_{21}-γ phase, and the addition of alumina sol in the Zn-Ni matrix increases the microhardness, and we note the maximum hardness is obtained for 50 g/L Al_2O_3. Conversely, these coatings showed smaller crystallite size and Surface of coatings was uniform and compact, the values of R_{ct} and Z_w increase, while the values of C_{dl} decrease with increasing alumina nano-particles content values for the Zn–Ni– Al_2O_3 alloy clearly confirm the better corrosion resistance.

Keywords – Electrodeposition, Corrosion, Binary alloy, XRD, SEM, Tafel

Antibacterial Potential of Ferrocenylmethylaniline Derivatives: Molecular Docking, Dynamics Simulations, and Quantum Chemical Insights

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Abstract – The growing threat of antimicrobial resistance (AMR) continues to compromise the efficacy of conventional antibiotics, necessitating the search for novel therapeutic agents. This study investigates the antibacterial potential of three ferrocenylmethylaniline derivatives: Ferrocenylmethylaniline (FMA), N-Ferrocenylmethyl-N-acetylaniline (FMAA), and N-Ferrocenylmethyl-N-benzoylaniline (FMBA). These compounds were evaluated in silico against four clinically significant bacterial strains: *Escherichia coli* (*E. coli*), *Pseudomonas aeruginosa (P. aeruginosa)*, *Klebsiella pneumoniae (K. pneumoniae)*, and *Staphylococcus aureus (S. aureus)*. FMBA displayed the strongest binding affinities across multiple bacterial targets, against *E. coli*, FMBA exhibited a ΔG value of –8.76 kcal/mol when bound to peptide deformylase (PDF, 1BSK), outperforming both amoxicillin (AXL) (–7.95 kcal/mol) and the native ligand (–7.92 kcal/mol). In *K. pneumoniae* and *P. aeruginosa*, FMBA showed significant ΔG values of –5.58 kcal/mol for Ant-CoA ligase (5EIX), –11.36 kcal/mol for DNA topoisomerase IV (5OE3), and –7.99 kcal/mol for peptidoglycan glycosyltransferase (PGT, 6I1E), surpassing those of AXL. Complementary DFT analyses, including frontier molecular orbitals (HOMO–LUMO) and molecular electrostatic potential (MEP) maps, provided insights into electronic properties and reactivity. Molecular dynamics (MD) simulations validated the stability of FMBA–protein complexes over a 50 ns trajectory. Key metrics, including RMSD, RMSF, SASA, and Rg, consistently confirmed the robustness of these interactions with minimal conformational shifts. Overall, FMBA stands out as a promising scaffold for the development of potent antibacterial agents.

Keywords – Ferrocenylmethylaniline derivatives; Antibacterial activity; Molecular docking; Molecular dynamics simulations; Quantum chemical analysis

Industrial Wastewater Depollution with Molecular Sieves

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Abstract – Molecular sieves 4A zeolite are materials used to dehydrate natural gas in liquefaction plants (LNG) in Algeria. After several cycles of regeneration and reuse, their structures degrade and affect their performances. Once replaced by new materials, they will be stored within the plant as an industrial solid waste.
The aim of this study is to investigate the possibility of using this solid waste, known as used 4A zeolite (U4AZ), as an adsorbent for removing phenol and ethanol from aqueous solutions in a fixed bed column. Tests for the adsorption of phenol and ethanol by U4AZ were studied, including adsorbent dosage, contact time and initial concentration. The adsorption of phenol and ethanol decreased with increasing contact time and initial concentrations. The experimental data were fitted by Bohart-Adams model. The obtained correlations with correlating constant (R^2) higher than 0.98 showed that U4AZ could be used as a recyclable material in the removal of phenol and ethanol from aqueous solution by adsorption.

Keywords – Molecular sieve, Depollution, Ethanol, Phenol, Fixed bed Column.

GREEN SYNTHESIS, CHARACTERIZATION, SOLUBILITY ENHANCEMENT AND DFT CALCULATION OF EUTECTIC MIXTURES OF DRUGS

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Abstract

Celecoxib (CXB) is a nonsteroidal anti-inflammatory drug (NSAID) used to treat rheumatoid arthritis, osteoarthritis, and acute and chronic pain. It also has potential anticarcinogenic properties, particularly against colon tumors, breast cancer, and skin cancer [1]. Its therapeutic effects are attributed to selective inhibition of cyclooxygenase-2 (COX-2). However, CXB's poor water solubility limits its dissolution rate and oral bioavailability, affecting its therapeutic efficacy. To address these issues, various methods like amorphous solid dispersions, nanoparticles, salt formation, cocrystals and eutectic mixtures have been explored [2,3].

This study investigates a eutectic mixture of CXB with maleic acid (MA) to enhance its physicochemical properties. Binary mixtures were prepared using liquid-assisted grinding, and the eutectic composition was identified by differential scanning calorimetry (DSC and further characterized by powder X-ray diffraction (PXRD), Fourier-transform infrared spectroscopy (FTIR) and scanning electron microscopy (SEM).

The eutectic reaction was observed at 108.46°C, and phase diagram analysis indicated a eutectic composition at approximately 0.35 molar fraction of CXB. PXRD and FTIR confirmed eutectic formation. Additionally, Density Functional Theory (DFT) calculations were employed to investigate the molecular interactions and thermodynamic behavior of the eutectic system. The results demonstrated that the eutectic mixture exhibited improved physicochemical properties compared to pure CXB. Notably, the water solubility of CXB was significantly enhanced in the eutectic form, highlighting the potential of this approach to overcome the solubility-related challenges associated with CXB.

Keywords : Celecoxib; Solid-Liquid equilibrium; Solubility; Differential scanning calorimetry; XRD, DFT Calculations

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Synthèse et évaluation pharmacologique de nouveaux isostères d'acide anthranilique : Docking moléculaire, prédictions ADMET in silico et activité anti-inflammatoire in vivo.

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Abstract – Une nouvelle série d'isostères d'acide anthranilique a été conçue et synthétisée comme agents anti-inflammatoires.
Les études de docking ont démontré une forte affinité pour les enzymes COX-1 et COX-2, avec une préférence relative pour la COX-2, prédisant une activité anti-inflammatoire.
L'étude ADMET in silico a prédit un profil pharmacocinétique favorable. Les calculs DFT ont révélé une amélioration des paramètres électroniques de certains composés cibles par rapport au diclofénac (DCF) et à l'aspirine (ASA), prédisant une amélioration de leur activité biologique.
L'étude pharmacologique expérimentale a confirmé ces résultats théoriques. En effet, les composés cibles ont démontré une inhibition significative de l'œdème de la patte induit par la carragénine chez le rat et une probable inhibition de la cyclooxygénase. En particulier, les composés 3e et 3h dépourvus de groupement COOH, qui provoquent une grave irritation gastro-intestinale, ont montré une activité anti-inflammatoire comparable à celle de l'acide salicylique (AAS) et ont surpassé l'efficacité du DCF. Ces deux composés ont montré une inhibition de 91,72 % après 3 h, contre 91,03 et 83,44 % pour l'AAS et le DCF, respectivement, avec un effet plus rapide et surpassant également les composés de référence après 1 et 2 heures. Les résultats indiquent également un bon profil pharmacocinétique des composés cibles, similaire à celui de l'AAS et du DCF.

Keywords – Activité anti-inflammatoire, isostères d'acide anthranilique, AINS, docking moléculaire, ADMET, DFT.

Phytochemical analysis and antibacterial effect of *Lavandula dentata* L. essential oil and ethanol extract.

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Abstract – To test the effect of *Lavandula dentata* on some bacterial pathology strains, one can do it on the extract of *Lavandula dentata* in the Chéria region in the province of Tébessa. One distillation of the Rotate-type vaporizer contains a return of 15.87% of the plant's excess ethanol. This type of hydrodistillation requires a reduction of 1.92% of the essential oils of *L. dentata*. The results of phytochemical tests on this plant contain the presence of flavonoids, tannins, catechins and alcaloides. For the test of antibacterial activity, the method of diffusion on the gel (aromatogram) is real on certain bacteria that are responsible for current infections; Gram positives such us; *S. aureus* and Gram negative such us; *E. coli* and *Pseudomonas aerogunosa*. These bacteria are resistant to certain types of antibiotics. The results are monitored by the effectiveness of excess ethanol from lavande on the positive strains than the Gram negatives, and the activity of the essential oil is very important due to the exposure to the ethanolic extract. According to the treatment plan, *L. dentata* can be used as an alternative treatment for antibiotics, noting the face to the emergence of bacterial resistance in the treatment of maladies infected bacteria.

Keywords –Lavandula dentata; extra ethanol; essential oils; Gram+ and Gram- bacteria

https://snc-25.sciencesconf.org/

Nouveaux dérivés de guanidine : une approche combinée Docking, ADMET et DFT contre la protéase principale du SARS-CoV-2

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Resumé –.

L'épidémie de SARS-CoV-2 a mis en lumière l'importance de développer de nouveaux agents antiviraux ciblant des protéines clés du virus, telles que la protéase principale (Mpro), essentielle à sa réplication. Dans cette étude, six nouveaux dérivés de guanidine (C1–C6) ont été synthétisés par condensation du chlorhydrate de guanidine avec le formaldéhyde et des acides aminés. Les composés C1 à C3 sont des chlorures d'iminium tricycliques, transformés ensuite en bétaïnes C4 à C6.

Une évaluation in silico a été réalisée contre Mpro à l'aide d'AutoDock Vina. Le composé C1 a montré une énergie de liaison de -7,8 kcal/mol, supérieure à celle des molécules de référence, le désignant comme un composé « hit ». Les prédictions ADMET (SwissADME, ProTox-II) ont révélé que tous les composés respectent la règle des cinq de Lipinski, sans toxicité prédite (hépatotoxicité, mutagénicité, etc.).

Les paramètres DFT (Gaussian 09) ont permis d'analyser la stabilité électronique et la réactivité des molécules. Les gaps énergétiques (Egap) varient de 4,78 eV (C6) à 7,74 eV (C1), indiquant une bonne stabilité, en particulier pour C1. Les potentiels chimiques négatifs (μ) et les moments dipolaires élevés (jusqu'à 12,548 D pour C2) suggèrent une forte affinité pour les cibles biologiques. La dureté chimique (η) et la douceur (S) confirment ces tendances.

Ces résultats montrent que C1 est un candidat prometteur pour des évaluations expérimentales ultérieures contre le SARS-CoV-2.

Mots Clés – Mpro SARS-CoV-2; dérivés de guanidine; docking moléculaire; ADMET; DFT

Adsorptive Removal of Methylene Blue Dye Using Alkali (KOH)-Treated Aluminosilicate Zeolite

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Abstract –

The applicability of modified aluminosilicate zeolite by potassium hydroxide as an effective adsorbent for adsorbing methylene blue dye from aqueous solution is investigated through this study. Batch adsorption was conducted for comparing the impacts of significant operational parameters like contact time, initial dye concentration, pH of solution, and temperature on the percentage removal of dye. Equilibrium data were best described by Langmuir's isotherm equation, typical of monolayer adsorption onto a homogenenous adsorbent. Kinetics controlled the rate to follow reasonably closely that seen with a pseudo-first-order kinetic model. That is physically binding dye in an existing material to restrict access until physical conditions balanced that demanded of similar activity by active-site energy equating forces equalization in rates throughout. Thermodynamic parameters, i.e., Gibbs free energy (ΔG°), enthalpy (ΔH°), and entropy (ΔS°) changes, were measured in order to establish the nature of the adsorption process. The negative ΔG° values ensured the spontaneity of methylene blue adsorption, while the positive ΔH° value indicated that the process is endothermic. Additionally, the value of thermodynamic parameters also suggested that the mechanism of adsorption is mainly governed by physisorption. Overall, the findings confirm that alkali-treated aluminosilicate zeolite is a low-cost, eco-friendly, and potential adsorbent for efficient removal of cationic dyes from wastewater.

Keywords – *Adsorption, Zeolite, KOH alkali treated aluminosilicate, methylene blue*

Évaluation de l'activité antioxydante d'une plante médicinale *Thapsia garganica L* de la région de Constantine (nord-est Algerien)

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Résumé

L'histoire du développement pharmaceutique est liée à l'exploitation des plantes médicinales, dont l'isolement des composés bioactifs présents dans ces plantes a permis la découverte de médicaments et contribue à l'innovation pharmaceutique. Le présent travail s'inscrit dans le cadre d'une étude phytochimique permettant de déterminer certains groupes chimiques bioactifs ainsi que les propriétés antioxydantes de l'extrait de *Thapsia garganica L.*

Le matériel végétal est constitué des racines de *Thapsia garganica L*. Les parties végétales sélectionnées sont collectées à partir de la région de Hamma Bouziane à Constantine. L'extraction a été réalisée par macération hydroalcoolique assistée par ultrasons, avec un renouvellement du solvant chaque 24h. Le dosage des polyphénols a été effectué à l'aide du réactif de Folin-Ciocalteu, et celui des flavonoïdes et flavonols totaux par la méthode de trichlorure d'aluminium AlCl3. En parallèle, l'activité antioxydante a été déterminée par le test DPPH et ses résultats ont été comparés à ceux du Trolox, un composé antiradicalaire standard.

En effet, la teneur en polyphénols totaux est de 42.72±1.42 mg EAG/g, en flavonoïdes totaux est estimée à 28.90±2.04 mg EQ/g et la teneur en flavonol totaux est de 33.26±0.69 mg EQ/g. Le résultat obtenu révèle une valeur d'IC50 de 0,38±0,01 mg/ml pour l'extrait avec le radical DPPH, cet extrait présent une capacité antioxydante faible que le trolox avec IC50 = 0.058 ±0,001 mg/ml.

La richesse en composés phénoliques des extraits de *Thapsia garganica* L suggère leur intérêt en tant que sources potentielles d'antioxydants naturels pourraient être utilisé dans les industries alimentaire et pharmaceutique.

Keywords – Thapsia garganica L; extrait hydrométanolique ; flavonoides ; polyphenols ; DPPH ; antioxidant.

Investigation of Anticholinesterase and Antioxidant Activities of Isoxazole-Based Coumarin Derivatives as Potential Neuroprotective Agents

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Abstract – Isoxazole and coumarin scaffolds are found in numerous bioactive compounds with diverse therapeutic effects. The isoxazole nucleus constitutes the core structure of several marketed drugs, such as parecoxib (anti-inflammatory), sulfamethoxazole (antibiotic), leflunomide (antirheumatic), and risperidone (antipsychotic). Coumarins, on the other hand, are naturally occurring compounds known for a wide range of pharmacological activities, including antibacterial, anticancer, anticoagulant, anti-inflammatory, and antiviral properties. In this study, we designed and synthesized a new series of coumarin–isoxazole hybrid molecules with the aim of developing compounds exhibiting multiple mechanisms of action. The main objective was to combine antioxidant and anticholinesterase activities, with potential applications in the treatment of neurodegenerative diseases. The compounds were synthesized via a multi-step process and fully characterized using spectroscopic techniques (NMR, IR, MS). Antioxidant activity was evaluated using the CUPRAC method, and anticholinesterase activity was assessed in vitro. Preliminary results indicate promising biological potential, particularly for selected derivatives exhibiting strong dual activity. These findings highlight the relevance of the coumarin–isoxazole hybrid approach in the development of new therapeutic candidates.

Keywords – coumarin, isoxazoles, antioxidant activity, neuroprotective agents

Développement d'un Système Catalytique Hétérogène pour l'Oxydation Contrôlée des Polluants Organiques en Milieu Liquide à Température Modérée

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Résumé – Les matériaux nanoporeux à porosité contrôlée, tels que les zéolites à base d'aluminosilicates, sont des matériaux largement utilisés dans les processus d'échange ionique, d'adsorption et de catalyse hétérogène, dans le but de réduire l'impact environnemental des produits chimiques en développant une technologie intrinsèquement non toxique pour les humains, les animaux, les plantes et l'environnement, en particulier pour éliminer les polluants organiques. L'objectif principal de cette étude est le développement d'un système catalytique hétérogène stable en milieu liquide, recyclable et capable de réaliser des réactions d'oxydation contrôlées de polluants organiques en phase liquide, sous des conditions modérées de température, d'humidité et de pression. Les catalyseurs utilisés dans nos réactions sont des zéolites de type MFI (ZSM-5) échangées à de faibles niveaux de métaux de transition. En effet, cette recherche vise à élucider l'influence de la nature et de la concentration du catalyseur, des cations actifs présents dans la structure du catalyseur, ainsi que de l'oxydant. Les expériences ont été réalisées sous reflux de solvants et à pression atmosphérique. L'effet de ces variables pour oxyder les composés organiques et leurs intermédiaires formés a été identifié à l'aide de différentes techniques d'analyse. L'analyse des résultats obtenus montre que l'oxydation des polluants organiques, même polyfonctionnels, permet d'obtenir les produits correspondants avec des rendements très élevés et des conversions complètes.

Mots-clés : –Zéolites MFI, Oxydation, ZSM-5, Environnement,

Etude phytochimique et évaluation de l'activité antioxydante des baies fraiches du murier noir de Jijel (*Morus nigra* L.).

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Résumé – Les mûriers de la provenance algérienne sont moins étudiés mais suscitent un grand intérêt en raison des composés bioactifs qu'ils synthétisent, permettant ainsi de mettre au point de nouvelles voies d'application en alimentation, en médecine, etc. Ils sont très recherchés en nutrition en raison de la composition phytochimique ayant un impact positif sur la santé humaine. En médecine traditionnelle, ils sont utilisés comme vermifuge, remède contre la dysenterie, laxatif, etc.

Différentes analyses phytochimiques qualitatives et quantitatives ont été effectuées. Pour évaluer l'activité antioxydante, les méthodes de phosphomolybdène, réduction du Fer et DPPH ont été réalisées.

L'évaluation qualitative de la composition phytochimiques des baies fraiches du mûrier noir a permis de mettre en évidence la présence de quelque constituant chimique tel que les flavonoïdes, les saponines, les terpénoïdes, les tannins et des traces d'alcaloïdes. Pour les analyses quantitatives des composés phytochimiques (composés phénoliques, flavonoïdes, anthoyanes, pro-anthocyanidines et caroténoïdes), l'extrait éthanolique des baies fraiches du mûrier noir se montre très riche en composés phénoliques (838.04 ± 20.91 mg EAG/ 100 g de baie fraiche) et en pro-anthocyanidines. Les activités antioxydantes (capacité antioxydante totale, réduction du Fer et DPPH) de cet extrait sont variables avec une capacité antioxydante totale élevée (223.48 ± 8.80 mg EAA/ 100 g de baie fraiche).

Ces activités sont dues probablement aux composés bioactifs contenant dans cette espèce.

Mots clés *: Murier noir, baies, analyses phytochimiques, activité antioxydante.*

Solutions vertes à la pénurie d'eau dans les régions arides grâce au phytoplancton

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Abstract –
Les régions arides sont confrontées à des défis croissants liés à la rareté de l'eau, ce qui nécessite la recherche de solutions innovantes pour la réutilisation des ressources hydriques. Cette étude vise à évaluer la faisabilité de la culture de la **spiruline (Spirulina)** dans les eaux usées comme solution double : le traitement de l'eau et la production de biomasse dans les environnements arides. Les résultats ont montré que la spiruline peut croître efficacement dans les eaux usées, grâce à sa capacité élevée à absorber les nutriments que l'azote et le phosphore, contribuant ainsi à l'amélioration de la qualité de l'eau. De plus, la biomasse produite possède une valeur économique, que ce soit pour la production de compléments alimentaires, d'engrais ou de bioénergie. Ces résultats suggèrent que la culture de la spiruline dans les eaux usées constitue une option prometteuse et intégrée pour renforcer la sécurité hydrique et alimentaire dans les zones arides, tout en réduisant l'impact environnemental et les coûts des traitements conventionnels..

Keywords – Spiruline, rareté de l'eau, zones arides, traitement biologique, biomasse, sécurité hydrique, réutilisation de l'eau.

Electrochemical and Spectroscopic Studies of Carbazole, N-Ethylcarbazole-3-amine, and N-Octylcarbazole Polymers

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Abstract –
Research on organic polymers, such as polycarbazole and its derivatives, focuses on their potential to revolutionize fields like electronics, optoelectronics, and energy storage. This study presents the electropolymerization and in-depth characterization of carbazole (PCz), N-ethylcarbazole-3-amine (PAECz), and N-octylcarbazole (POCz) in acidic medium. The obtained polymer films were analyzed by cyclic voltammetry, electrochemical impedance spectroscopy (EIS), and UV-visible spectroscopy. Distinct redox systems were observed for all polymers, confirming their p-doping. Half-wave potentials (E1/2) indicate increasing oxidation ease from PCz to POCz. EIS analysis reveals differences in the electrochemical behavior of the polymers. PCz exhibits capacitive behavior, while PAECz and POCz have distinct resistive and charge transfer characteristics. UV-visible spectra suggest a homogeneous electronic structure with well-defined electron energy levels. The narrow band gap of PCz and POCz indicates an ordered structure, while the broader band of PAECz could reflect structural heterogeneity. FTIR spectra confirm the involvement of functional groups in the polymerization processes and the formation of C-N bonds and other characteristic structures. The study of the orbital energy levels (HOMO and LUMO) of the synthesized polymers highlights remarkable compatibility with the materials selected for the electrodes and electron acceptor in a bilayer OPV cell.

Keywords – Include at least 5 keywords or phrases

Electrochemical Characterization Of A Planar Silver/ Silver Chloride Reference Electrode By Open-Circuit Potential Measurements (OCP)

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Abstract **–** The growing development of electrochemical wearable devices and Lab-On-a-Chip (LOC) sensors has created an urgent demand for efficient and stable miniaturized Reference Electrodes. For a long time, researchers have focused on integrating solid-state indicator electrodes with equivalent reference electrodes to maximize the benefits of eliminating liquid components from the system. A planar Ag/AgCl reference electrode with an inner solid electrolyte layer offers a viable alternative. This study aims to evaluate the stability of a newly fabricated, planar, all-solid-state Ag/AgCl reference electrode in comparison to a macro-commercial reference electrode (REF321) through open circuit potential (OCP) measurements. This electrochemical technique requires a two-electrode system where the fabricated Ag/AgCl serves as the working electrode (WE) and the macro-commercial Ag/AgCl (REF321) as the reference electrode (RE). Using a potentiostat/galvanostat (AUT86651), the electrodes were immersed in a 3M KCl solution for 10 minutes. The potential measurements indicated a stable response with a fixed potential value. The developed planar Ag/AgCl reference electrode showed excellent stability comparable to the macro-commercial reference electrode. Thus, we conclude that the fabricated Ag/AgCl reference electrode is as stable as the commercial one.

Keywords – Reference electrode; Silver/silver chloride; electrochemical characterization; Open-circuit potential; Stability.

Study of steel (C18) inhibiting corrosion effectiveness by olive leaves extracts in a corrosive environment

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Abstract – The main objective of this work is to study the corrosion inhibition of a steel sample (C18) from a heat exchanger in Unit 100 of the Skikda condensate refinery (RA2K), using olive leaf extracts, chosen as a green corrosion inhibitor. The RA2K complex has scheduled six research and development projects for 2022 concerning the protection of materials against corrosion. In this context, we are interested in the study of the corrosion of the heat exchangers in Unit 100 of the RA2K condensate refinery, where one of the means of corrosion protection has been proposed, using natural inhibitors such as olive leaf extracts. The choice of this plant substrate was based on three essential criteria: its richness in antioxidant components, its abundance in nature, and its low economic cost. In this study, heat exchanger steel samples were immersed in a 1 M HCl solution, with and without the addition of olive leaf extract at different concentrations. Corrosion-related parameters, such as mass loss (µm), corrosion rate (Vcorr), and inhibitory efficiency (EI%), were determined after 2, 4, and 24 hours of immersion at room temperature. Finally, this work allowed us to demonstrate that olive leaf extract has high anti-corrosion properties for metals, and that these leaves have added value, which should be exploited because this extract possesses interesting inhibitory properties, thus yielding promising results. The maximum inhibitory efficiency values of the olive leaf extract studied were obtained for concentrations of 400 ppm, offering a maximum efficiency of around 92.40%.

Keywords – Inhibition, Corrosion, Heat exchanger, Green inhibitor, Protection, Olive leaf extracts.

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Keywords – Inhibition, Corrosion, Heat exchanger, Green inhibitor, Protection, Olive leaf extracts.

New lead-free piezoelectric ceramics for electronic applications

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Abstract – The main objective of this work is based on the study of the doping effect by lanthanum (La) on the structural and morphological properties in a BNT-type material doped with a perovskite ABO3 structure, $(Bi_{0.5})_{1-x}La_xNa_{0,5}[(Ti_{0.8}Zr_{0.2})_{0.9}(Zn_{1/3}Nb_{2/3})_{0.1}]O_3$ abbreviated as BLNT-ZZN with $0.0 \leq x \leq 0.6$. The samples chosen for this study were prepared using the solid-state synthesis method. A thermal treatment was applied to these compositions at different temperatures: 1050°C, 1100°C, 1150°C, and 1200°C successively with the aim of optimizing the optimal sintering temperature where the density of the samples is maximum and thus the product has better physical quality. Different characterization techniques were used such as: scanning electron microscopy (SEM), X-ray diffraction (XRD), IR analysis.

Keywords – BNT, perovskite, sintering, XRD, SEM.

Deformation of nanotubes and electronic properties under the influence of an electric field

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Abstract— Study of the structural and electronic properties of pure zinc oxide nanotubes in zigzag and armchair states (5,0) (7,0) (9,0) (5,5) (7,7) and (9,9) using density functional theory (DFT) and the generalized gradient approximation (GGA). The results show that the strain energy of ZnO nanotubes increases with diameter, while the energy bands are semiconducting energy bands higher than those of bulk zinc oxide. The decrease in the band gap value is related to the increase in diameter. The application of an electric field to the ZnO nanotube causes increasing deformation with increasing field value, and the percentage of distortion also increases with diameter. Increasing the electric field reduces the band gap value.

Keywords – component; Ab-initio study, ZnO nanotube, Electric field, Strain energy, Band structure.

Forecasting Second-Order Nonlinear Optical Properties of Nanomaterial Clusters

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Abstract **–** This study focuses on a series of atypical pentanuclear transition metal hydride clusters, systematically designed with electron-rich environments. The ground-state electronic structures, QTAIM analysis, electronic transitions, charge transfer characteristics (including charge distribution, interatomic distances, and dipole moments), hyper-Rayleigh scattering, and depolarization ratios (both static and dynamic) were comprehensively analyzed using DFT and TD-DFT methods. Quantum chemical calculations were conducted at the CAM-B3LYP/6-311++G(d,p)/sdd level, employing the sum-over-states (SOS) approach for evaluating nonlinear optical (NLO) properties in both static and dynamic regimes.

Our findings reveal that introducing the hydride group at the β-position significantly enhances the first hyperpolarizability compared to other substitution sites. Among the investigated clusters, cluster Cγ exhibits the highest first hyperpolarizability value, attributed to an efficient charge transfer from the ligand to the metal center, as indicated by an overlap strength index (Sr) approaching zero. This work provides novel insights into the NLO properties of atypical pentanuclear transition metal l hydride clusters, highlighting for the first time the critical role of orbital overlap in modulating NLO responses.

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Keywords – Nanomaterial, NLO, static, dynamic, β_{HRS}, DR, DFT, TD-DFT, SOS

Dépollution d'un colorant cationique par adsorption sur un charbon actif commercial dopé aux nanoparticules de fer.

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Abstract **–** La nanotechnologie, un domaine qui progresse rapidement, est largement appliquée dans divers domaines, en particulier dans la protection de l'environnement et l'élimination des polluants par des processus tels que l'adsorption. Dans cette étude, nous synthétisons des nanoparticules de Fe3O4 par la méthode de la co-précipitation et les utilisons pour doper le charbon actif en poudre (CAP) commercial. Le CAP dopé est ensuite utilisé pour éliminer le colorant Safranine O des solutions aqueuses par adsorption.

Nous étudions les effets de paramètres clés tels que la concentration initiale de colorant, le pH, le temps de contact et la dose de PAC/Fe3O4. Les résultats montrent une élimination significative du colorant à un pH de 6, avec un temps de contact de 60 minutes et une dose de PAC de 2 g/L. Le processus d'adsorption a été analysé à l'aide des modèles isothermes de Langmuir et de Freundlich afin de comprendre le mécanisme sous-jacent.

Keywords – Charbon actif en poudre (CAP), nanoparticules, adsorption, colorant Safranine O ; isotherme ; élimination.

Physical, colorimetric and mechanical properties of magnesium carbonate reinforced of polypropylene composites processed by injection molding

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Abstract **–**Injection molding is a widely used technique for shaping thermoplastics. During this process, the polymer undergoes significant thermomechanical transformations that affect the quality of the final product. This study focuses on the development and characterization of thermoplastic composites based on a polypropylene (PP) matrix reinforced with magnesium carbonate (MC), manufactured using a twin-screw extruder followed by injection molding. Magnesium carbonate was incorporated with contents of 10 wt% and 20 wt%. Magnesium carbonate was incorporated with contents of 10 wt% and 20 wt%. The composites were characterized by physicochemical properties, including FTIR-ATR spectroscopy, colorimetric measurements, and mechanical tensile testing.The incorporation of magnesium carbonate (MC) significantly enhanced the mechanical performance of the polypropylene (PP) matrix, notably by increasing Young's modulus and tensile strength. In addition, the melt flow index decreased with the addition of 10 wt% and 20 wt% MC, reflecting reduced macromolecular mobility and increased viscosity.

Keywords – Polypropylene, magnesium carbonate, composites, injection molding.

Adsorption of Crystal Violet Dye Dissolved in Aqueous Solutions on Activated Carbon Prepared from Peanut Shells

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Abstract – This study examined the adsorption of crystal violet dye dissolved in aqueous solutions onto the surface of activated carbon prepared from peanut shells. A series of experiments were conducted on the adsorption technique on the surface of activated carbon to demonstrate the effects of various variables, such as the initial dye concentration (the adsorbent), equilibrium time, pH, and the amount of adsorbent. The concentration of crystal violet dye dissolved in aqueous solutions was determined using UV-Vis absorption spectroscopy. From these experiments, we concluded the best conditions for removing crystal violet dye from contaminated water.

Keywords – Adsorption, activated carbon, crystal violet dye, peanuts shells, water.

Study of a Semiconducting Materials Based on Polpyrrole and Polyvinylpyrrolidone

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Over the last three decades, the semiconducting polymer materials are widely used in different fields of science and industry and continue to attract much attention. It has been shown that they can be potentially used in multidisciplinary areas such as the conversion of the solar energy into several forms. Thus, the elaboration of organic semiconductor materials has found interest from both academic and industrial points of view, where a significant number of scientific works are regularly published.

In this contribution, we have firstly assessed thermodynamically the possibility to blended the polypyrrole (PPy) with polyvinylpyrrolidone (PVP) using group contribution model in order to calculate the solubility parameters of two polymers. Our principal goal in this work is to combine two types of polymers, conductor and insulation, in order to produce the semiconducting materials possessing a large scale and improved properties. All binary blends of PPy/PVP were obtained by in situ polymerization. They have studied by means of DSC, Fourier transform infrared spectroscopy (FTIR), thermogravimetry (TGA). Their conductivity was also measured using four-point technique. The phase behavior and miscibility of these blends were examined according to their glass transition temperatures (Tg). Moreover, the possible specific interactions, such as hydrogen bonding, was studied qualitatively and quantitatively by FTIR. The thermal and conductivity properties of these materials were also explored using TGA and Four Point probe method.

Keywords: Polpyrrole (PPy), Polyvinylpyrrolidone (PVP), electrical conductivity, FT-IR Spectroscopy, differential scanning calorimetry (DSC), Thermogravimetric analysis (TGA).

Influence des traitements de surface sur les performances des électrodes en acier inoxydable pour la production d'hydrogène : Étude microstructurale et électrochimique

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Abstract – Dans un contexte où la transition énergétique impose une recherche accrue d'alternatives aux combustibles fossiles, cette étude explore l'optimisation des électrodes en acier inoxydable ferritique AISI 430 pour la production d'hydrogène par électrolyse. L'objectif principal est d'améliorer leur activité catalytique à travers des traitements de surface, notamment l'électrodéposition de couches de nickel (Ni), zinc (Zn) et d'alliages Ni-Zn, avec des épaisseurs contrôlées (5 et 15 µm). L'approche adoptée inclut une caractérisation approfondie des matériaux développés. L'étude de la microstructure par microscopie optique et diffraction des rayons X a révélé un substrat monophasé ferritique, avec une dureté moyenne de 170 HV. Les dépôts en nickel se distinguent par une rugosité plus élevée et une meilleure porosité, favorisant une plus grande surface spécifique. L'évaluation des performances électrochimiques a démontré que les électrodes revêtues de nickel d'une épaisseur de 15 µm offrent le rendement le plus élevé en production d'hydrogène. Cette observation est corroborée par les tests de surface spécifique, qui confirment que ce revêtement possède le facteur de rugosité le plus élevé. De plus, les essais de production d'hydrogène sous une tension de 3,4 V dans une solution de KOH 1M à 298 K ont permis de quantifier le volume d'hydrogène généré, mettant en évidence la supériorité des électrodes en Ni-15 µm. Ces résultats soulignent le potentiel des électrodes en nickel pour des applications dans la production d'hydrogène.

Mots-clés – Composé intermétallique NiAl, Nickel de Raney (Ni-Raney), Réaction d'évolution de l'hydrogène (HER), Activité électrocatalytique, Électrolyse de l'eau, Spectroscopie d'impédance électrochimique (EIS)

Dosage des composés phénoliques et évaluation de l'activité antiinflammatoire de *Capparis spinosa* L

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Résumé

Depuis l'Antiquité, les plantes médicinales sont reconnues comme l'un des agents thérapeutiques les plus efficaces pour le traitement des maladies humaines ; elles sont à l'origine de nombreux composés biologiquement actifs .Parmi ses plantes ; le câprier ;une espèce très répandu dans le bassin méditerranéen y compris l'Algérie où il couvre de vastes surfaces de manière éparse; il a été utilisé depuis des siècles dans la phytothérapie traditionnelle pour traiter plusieurs pathologies grâce à sa richesse en métabolites secondaires. L'objectif de ce travail ; dans un premier temps ; est la recherche et la quantification des composés phénoliques essentiellement les polyphénols totaux ; les flavonoïdes ; les tanins et les anthocyanes par spectrophotométrie à des longueurs d'ondes différentes. Le deuxième objectif étant l'évaluation de l'activité antiinflammatoire in vitro ; pour confirmer ou infirmer son usage ancestral ; par stabilisation membranaire (méthode de Shinde et al) en utilisant des globules rouges humains (HRBC) car la membrane globulaire est analogue à la membrane lysosomale et peut être utilisée pour l'évaluation du pouvoir stabilisateur de membrane par l'extrait de la plante .L'étude montre que le *Capparis spinosa* L est riche en composés phénolique surtout les flavonoïdes qui peuvent être l'origine de son effet antiinflammatoire confirmé par l'étude in vitro

Mots clés : *Capparis spinosa L ; dosage ; composés phénoliques ; flavonoïdes ; activité antiinflammatoire.*

Synthesis and application of a Water-Soluble Chitosan Derivative in water treatment

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Abstract **–**Water pollution is one of the major environmental issues of our time. It is mainly the result of domestic, industrial and agricultural waste, which is discharged into rivers, lakes and oceans [1]. Faced with this problem, researchers are increasingly interested in innovative solutions to clean up water. Among these, the use of polymers appears to be a promising method [2]. The aim of this work is to synthesize a Chitosan Derivative (CHD) as a water-soluble biopolymer, so it can be used as a good flocculant in the coagulation/flocculation process. It is characterized by FTIR spectrometry to identify the functional groups present in our product, and by XRD analysis to give an idea about the crystallinity of the product studied [3]. Characterization of the clay material (bentonite) is carried out by X-ray diffraction (XRD) to determine the bentonite interfoliar distance using Bragg's law before and after flocculation, and X-ray fluorescence (XRF) to quantify the elemental composition of the bentonite. Finally, we tested our flocculant in jar-test with the coagulation/flocculation technique [4]. Several parameters were optimized and different flocculant concentrations were tested at different settling times. A good flocculant behavior could be clearly observed by the reaching up to 100% removal of bentonite turbidity.

Keywords – Chitosan; chitosan derivative; bentonite; coagulation/flocculation

Biological activity of the essential oil of a medicinal plant from the Tlemcen region, in Western Algeria

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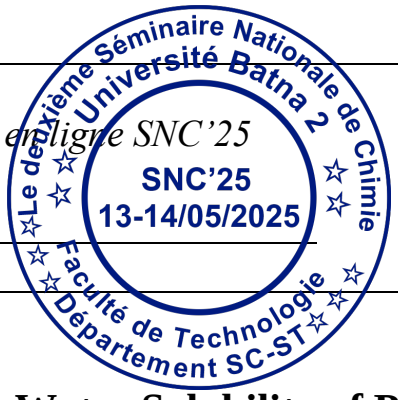
Abstract – This study focused on Teucrium fruticans L., an aromatic and medicinal plant from the Lamiaceae family, easily recognizable by its bushy habit, its persistent grey-green leaves, and its pale blue flowers. The samples were collected from the Tlemcen region, in the northwest of Algeria.
The essential oil, extracted by hydrodistillation from the aerial parts of the plant, yielded 0.45 ± 0.043%. The antibacterial activity of this oil was evaluated using the disk diffusion method to measure the inhibition zone diameters, as well as the incorporation method to determine the minimum inhibitory concentrations (MIC).
The diameters of the inhibition zones ranged from 9.5 to 13 mm, while the MIC values varied between 4 and 15 µl/ml depending on the tested microorganisms. The most sensitive bacteria were Enterococcus faecalis (4 µl/ml), followed by Klebsiella pneumoniae and Staphylococcus aureus (7 µl/ml), highlighting the promising potential of Teucrium fruticans as a natural source of antimicrobial agents.
The essential oil was tested against seven reference bacterial strains as well as a pathogenic yeast, Candida albicans ATCC 10231. The results revealed a significant antifungal activity with an MIC80 of 2.9 µl/ml.

Keywords – Teucrium polium L., essential oils; antifungal activity; antibacterial activity.



Modeling and Prediction of the Water Solubility of Polycyclic Aromatic Hydrocarbons Using a QSPR Model

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Abstract – Quantitative Structure–Property Relationship (QSPR) techniques provide efficient tools for predicting the physicochemical properties of organic pollutants from molecular structure data. This study presents the development of a QSPR model aimed at estimating the water solubility of polycyclic aromatic hydrocarbons (PAHs). The dataset was split using the DUPLEX method into a calibration set (22 compounds) and a validation set (10 compounds) to ensure rigorous external validation.

A one-descriptor model was built using theoretical molecular descriptors calculated with the DRAGON software. Descriptor selection was performed by combining a Genetic Algorithm (GA) with Variable Subset Selection (VSS) to identify the most relevant structural variable. Internal and external validations confirmed the robustness and predictive capacity of the model.

The model showed strong statistical performance, with R^2 = 91.09%, Q^2loo = 89.15%, Q^2ext = 84.96%, F = 204.405, and s = 0.515. These values demonstrate that the model provides accurate and reliable predictions of water solubility for the studied PAHs. The results validate the proposed QSPR model as a useful and trustworthy computational approach for estimating the aqueous solubility of polycyclic aromatic hydrocarbons (PAHs), offering valuable support for environmental risk assessment and pollutant behavior prediction in aquatic systems.

Keywords – Molecular Modeling, Water Solubility, QSPR, Multiple Linear Regression, Polycyclic Aromatic Hydrocarbons.

Valorisation des propriétés antibactériennes de l'huile essentielle d'une plante médicinale locale *Origanum majorana* L.

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Résumé

En Algérie, et depuis longtemps, nous avons recours à la médecine traditionnelle grâce à la richesse et à la diversité floristique de notre pays. Cette dernière constitue un véritable réservoir phytogénétique, avec environ 3000 espèces appartenant à plusieurs familles botaniques, dont nous avons besoin de valorisera afin de leurs utilisations dans différents domaines pharmaceutiques, agroalimentaires et cosmétiques

L'objectif de cette étude est d'analyser l'effet antibactérien de l'huile essentielle d'une plante aromatique et médicinale de la flore algérienne, appelée *Origanum majorana* L., sur 4 souches bactériennes de référence et 18 souches d'origine hospitalière.

L'extraction de l'huile essentielle de la partie aérienne de la marjolaine sèche par hydrodistillation. Quant à l'efficacité antibactérienne par la méthode de diffusion sur disque (l'aromatogramme). En utilisant la méthode de dilution en milieu liquide et celle en milieu solide, les CMI et les CMB de l'huile essentielle étudiée ont été évalué respectivement.

Toutes les souches de référence testées ont démontré une sensibilité à l'HE, avec une activité inhibitrice extrême sur Staphylococcus aureus traduite par un diamètre de zone d'inhibition de 26 mm.

L'huile essentielle a présenté des propriétés antibactériennes variées sur les 18 souches cliniques Gram négatif testées, dont 37 % sont multirésistantes, avec une activité inhibitrice élevée sur *Escherichia coli* et *Proteus spp*. Néanmoins, *E coli*, *Klebsiella pneumoniae*, *Pseudomonas aeruginosa* et *Enterobacter spp* ont témoigné d'une grande sensibilité à l'aromatogramme. Les CMI ont oscillé entre 16 et 50 mg/ml et entre 20 et 100 mg/ml respectivement. Les résultats de la détermination de la CMB ont démontré que l'huile essentielle étudiée possède une action bactéricide contre 99 % des souches testées.

L'huile essentielle issue d'*Origanum majorana* L. possède une activité bactéricide exceptionnelle. Ainsi, il peut être une ressource naturelle et une excellente alternative aux antibiotiques pour lutter contre les infections bactériennes.

Mots clés : *Origanum majorana* L, Huile essentielle, Activité antibactérienne, CMI, CMB.

Thermodynamic, Kinetic, and Isotherm Investigations of Pharmaceutical Pollutants Adsorption onto Activated Carbon

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Abstract **–** This work explores the adsorption performance of activated carbon for the removal of pharmaceutical pollutants from aqueous solutions. The material was characterized using BET surface area analysis and SEM, confirming a porous structure with a high surface area conducive to effective adsorption. Batch experiments identified optimal conditions at pH 2.0, an adsorbent dose of 0.2 $g.L^{-1}$, and an equilibrium time of 120 minutes. The Avrami model best fitted the kinetic data, while the adsorption isotherms followed the Langmuir model. Thermodynamic analysis revealed a non-spontaneous and exothermic adsorption process. These findings highlight the potential of activated carbon as a cost-effective and efficient adsorbent for water treatment applications targeting pharmaceutical contaminants..

Keywords – Activated Carbon, pharmaceuticals pollutants, Adsorption, Removal, Isotherm

Assessment of biological characteristics of the polyphenols from the byproducts of cold-processed olive oil extraction from the Khenchela area.

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Abstract

The production of olive oil generates huge quantities of effluents called "margins,» which have little economic value in Algeria and are a powerful pollutant discharged into nature without any prior treatment but which could be considered a potential source of natural products of high additive value because of their content of phenolic compounds and other natural antioxidants. This study aims to highlight the biological activities of polyphenols from these margines (chemlal variety) harvested in Khenchela. The physico-chemical characterization of the samples showed acidic rejects (pH = 4.64), brown color with a high moisture content (H = 95.45%), a high content of total suspended solids (TSS = 0.55%), rich in organic matter (OM = 14%), poor in mineral matter (MM = 2%), in nitrogen with 0.42 g/l, and in dry matter with 8.55 g/l. A liquid-liquid extraction was performed using acetone (Ac). The total polyphenol determination showed the richness of the extract with 70 µg EAG/mg of extract. TLC qualitative analysis revealed a wide range of phenolic compounds. The resulting antioxidant capacity showed that the extract inhibited DPPH oxidation with a very low IC50%, namely 30µg/ml. The anti-inflammatory action has been proven in vitro by the inhibition of protein denaturation and the increase of HRBC (human red blood cells) membrane stability up to 97.77% compared to the 74.33% established by aspirin at the same concentration. Activated partial thromboplastin and prothrombin times were used to analyze the extrinsic and intrinsic coagulation pathways in order to determine their anticoagulant activity, which had a great impact on the lengthening of both chronometric tests.

In the light of the results obtained, we can conclude that the polyphenolic acetone extract derived from recycled margines is endowed with remarkable antioxidant, anti-inflammatory and anticoagulant activity. As such, it may represent a promising natural resource for alleviating the complications of oxidative stress associated with or triggering thrombolytic and cardiovascular diseases.

Key words: Margins, polyphenols; anti-inflammatory activity; antioxidant activity; anticoagulant activity.

Electrochemical Determination of a Pesticide Residue in Tomato Samples Using Cyclic Voltammetry and Assessment of Its Environmental Risk

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Abstract **–** Electrochemical techniques offer a sensitive, rapid, and cost-effective alternative to conventional analytical methods for detecting pesticide residues in agricultural products. In this study, cyclic voltammetry was employed to analyze the presence of a specific pesticide residue in tomato samples collected from local farming areas. A modified glassy carbon electrode was used under optimized conditions: a potential window from –1.0 to +2.0 V, a scan rate of 25 mV/s, and pH adjusted to 6.5. The developed method achieved a low detection limit of 0.01 µg/mL and recovery rates ranging from 85% to 98%, demonstrating high accuracy and reproducibility. The findings support the applicability of electrochemical methods in routine pesticide monitoring and highlight their role in environmental risk assessment and food safety assurance.

Keywords – Electrochemical Characterization ;Residual Pesticides ;Cyclic Voltammetric Techniques ;Tomato Matrix Analysis Environmental Risk Evaluation

Sustainable Wastewater Treatment: Salting-Out Removal of Crystal Violet with Brine Effluents

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Abstract **–** This study investigates the effectiveness of a salting-out process using industrial brine discharge for the removal of Crystal Violet (CV) dye from aqueous solutions. CV, a cationic triphenylmethane dye, was subjected to treatment with saline solutions sourced from the brine effluents of the El-Outaya Salt Complex (Biskra, Algeria), affiliated with the National Salt Company (ENASEL). The brine discharge, characterized by high ionic strength, was evaluated for its potential to induce dye aggregation and precipitation through the salting-out effect. Batch experiments were conducted under controlled conditions to assess the influence of key parameters such as brine concentration, initial dye concentration, and pH. The results revealed that increasing brine concentration from 20% to 100% significantly enhanced CV removal efficiency, reaching up to 99.8% at 80–100% brine. Additionally, higher pH values favored retention, with removal efficiencies rising from 75.6% at pH 3 to 99.9% at pH 11 under 100% brine. The study also confirmed that higher initial dye concentrations had minimal impact on removal performance at high salinity. These findings underscore the potential of valorizing saline effluents from salt production as an eco-friendly and cost-effective resource for treating dye-contaminated wastewater through salting-out mechanisms.

Keywords – Crystal Violet, Salting-Out, Brine Discharge, Wastewater Treatment, Ionic Strength.

The Health Impact Of PM10,PM2.5 On Patıents İn Constantine's Pulmonary Department

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Abstract **–** Several studies have assessed air pollution levels in Constantine, with a particular focus on PM10 and PM2.5 concentrations. One such study reported average daily PM10 levels of 43.5 µg/m³ in urban areas and 3.1 µg/m³ in semi-urban zones, with notably higher concentrations during the summer months. The PM10 particles exhibited a bimodal distribution, a typical feature of urban environments, and were found to be associated with heavy metals such as iron. Our findings revealed elevated concentrations of both PM10 and PM2.5, which were linked to increased risks to the respiratory health of the local population.This study focuses on Algeria, specifically the city of Constantine, and aims to assess the impact of desert aerosols on the health of the local population. A gravimetric sampling method was employed to measure particulate matter concentrations by weighing filters before and after their exposure to dust-laden air. Statistical analyses were subsequently conducted to explore potential associations between particle exposure and respiratory diseases, based on data obtained from the Pneumology Department at Constantine University Hospital.The results indicate that fine particle concentrations in the atmosphere are influenced by environmental parameters such as temperature, atmospheric pressure, humidity, and wind speed. Moreover, the statistical analysis revealed a moderately significant correlation between exposure to desert dust and the prevalence of respiratory conditions.

Keywords – Desert dust; PM10; PM2.5; pulmonary; the respiratory health

Synthesis of PPH/Ag nanocomposite hydrogel for antimicrobial application

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Abstract **–** In this work, the synthesis of nanocomposite hydrogels NCHs was successfully achieved. Particularly, the integration of silver nanoparticles within the potassium polyacrylate hydrogel PPAH/Ag NPs matrix via a simple approach known as the *in-situ* reduction. Basically, this approach is based on two steps i) loading the Ag ions from silver nitrate $AgNO_3$ solution into hydrogel matrix with varying concentrations (2,5,10, and 16 mM), then ii) the loaded Ag ions within the hydrogel structure were reduced by sodium borohydride $NaBH_4$ solution with varying concentrations (4,10,20, and32 mM). This novel NCH was designed with a specific focus on its application as an antimicrobial agent. The synthesized samples were analyzed by different analyzing techniques including UV-Vis, FTIR, XRD, etc. The results from these analyses confirmed the effective formation of silver nanoparticles within the hydrogel structure with excellent distribution and crystallite sizes of 31.83 nm. Also, the synthesized PPAH/Ag NPs samples were subjected to an antimicrobial test against three different bacterial strains: Pseudomonas aeruginosa ATCC 27853, Escherichia coli ATCC 25922, and Staphylococcus aureus ATCC 25923 . the results showed excellent antimicrobial properties of the synthesized samples against diverse microorganisms, moreover, their antimicrobial effect was better than the positive control antibiotics included in the experiment. This research demonstrates the promising potential of PPAH/Ag NCH as a highly effective and versatile antimicrobial agent, with implications for a wide range of applications in areas where controlling microbial growth is of utmost importance.

Keywords –silver nanoparticle; Hydrogel; Nanocomposite hydrogel; in-situ reduction approach; Antimicrobial.

Étude de la sélectivité de nouvelles HSDHs dans la transformation stéréosélective de cétones cycliques

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La biocatalyse s'impose aujourd'hui comme un outil incontournable dans l'industrie chimique pour la production de composés à haute valeur ajoutée. Elle offre de nombreux avantages pratiques, notamment une sélectivité accrue, l'obtention de produits d'une grande pureté, une consommation énergétique réduite, ainsi qu'une meilleure efficacité atomique lors des réactions de dérivatisation.

Le potentiel remarquable de la catalyse enzymatique inspire les chercheurs à développer des procédés plus verts et sélectifs. Les biocatalyseurs représentent ainsi une alternative prometteuse en chimie organique, grâce à leur spécificité et leur sélectivité uniques[1].

L'étude que nous avons menée se concentre sur une approche biocatalytique, en décrivant la résolution cinétique d'une cétone cyclique[2] connue sous le nom de **8a-Methyl-3,4,8,8a-tetrahydronaphthalene-1,6(2H,7H)-dione**, ainsi que de ses dérivés alcooliques (formes cis et trans). Cette molécule a été choisie comme substrat modèle afin d'évaluer la sélectivité d'une série de déshydrogénases, incluant des enzymes issues d'une collection métagénomique interne d'oxydoréductases à chaîne courte (HSDHs). Tous les produits ont été isolés avec des excès énantiomériques supérieurs à 95 %[3].

Mots clé : La biocatalyse, catalyse enzymatique, sélectivité, oxydoréductases, HSDHs.

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synthèse régiosélective de molécules biosourcées fonctionnalisées par acylation enzymatique en presence de l'anhydride itaconique

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Résumé

Ces dernières années, le développement de nouvelles molécules bio-sourcées fonctionnalisées via des voies de synthèse faciles et vertes est un défi majeur de la chimie de synthèse moderne[1].

La mise en œuvre de nouveaux types d'agents acylants dans l'acylation lipasique permet d'accéder à la synthèse de molécules d'intérêt par biocatalyse dans des conditions de chimie verte. Une alternative très intéressante est l'utilisation d'anhydrides d'acide[2] qui permettent de les séparer aisément par extraction liquide-liquide. L'utilisation d'anhydrides d'acides en catalyse enzymatique constituent une nouvelle voie de recherche en pleine expansion si on considère la nouvelle conception de la chimie qui cherche l'application de solution novatrices respectueuses des principes de chimie verte [3].

Dans ce travail, nous représentent la synthèse régiosélective de molécules d'intérêt biologiques par acylation enzymatique en utilisant l'anhydride itaconique, molécule est abondamment disponible à partir de la biomasse avec divers alcools, catalysé par la lipase de Pseudomonas cepacia (*PCL*) dans le tert-butyl méthyl éther à température ambiante. Cette méthode est simple, efficace et écologique et peut être réalisée en une seule étape en utilisant des alcools primaires achiraux comme nucléophiles avec 100% d'économie d'atomes. L'acylation des alcools primaires en présence de l'AIt et la lipase *PCL* est hautement régiosélective et conduit à l'isomère β avec une pureté variant de 90-99% .

Mots clés : anhydride itaconique, la lipase *PCL*, synthèse régiosélective, anhydride acide, chimie verte.

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Contribution to the attack of sulfate water on the concrete of the Hammam-Debagh dam

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Abstract **–** The study presented in this paper deals with the consequences of external sulphate attack on prefabricated concretes of Hamam Debagh Dam in Guelma. Dams can still be the seat of concretes swelling. The sulphate reaction is part of the known chemical reactions that can cause the alteration of the mechanical characteristics of the hydraulic material constituting the structure. Distinct markers of the reaction are then observed which are the appearances, in the more or less long term, of a network of cracking, swelling, dyes, but also corrosion or ruptures of reinforcement induced by the entry of water and oxygen into the structure. The results show that the impact of the age of the material on its degradation on contact with the sulfuric acid solution was highlighted, visual observations then rapid degradation and abruptly on the surface and then in depth towards the heart then a loss of mass and cracking and finally the ruin of the material.

Keywords – Hamam Debagh dam, prefabricated concrete, environment, sulphate attack, degradation.

Comparison between alternative chemical treatments on Malva fibers for application in cementitious materials

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Abstract: The construction industry is facing significant environmental challenges due to the depletion of fossil resources. To address these challenges, researchers have turned to the use of plant fibers in cement, offering an eco-friendly alternative to conventional materials reinforced with synthetic fibers. Plant fibers are attractive due to their biodegradability, abundance, renewability, and low cost, which allows for the creation of affordable and environmentally friendly construction materials. The low adhesion between plant fibers and the cement matrix limits their use as reinforcement agents in cement composites. To solve this issue, methods such as chemical modification of fibers have been employed to create interactions with the cement matrix. This study aims to explore a new variety of fibers extracted from the stems of Malva (Malva sylvestris), a biennial or perennial herbaceous plant of the Malvaceae family, native to Europe, Asia, and North Africa. To utilize these fibers, it is essential to identify and characterize both NaOH-treated and untreated Malva fibers using FTIR and XRD. For the preparation of cement composites, NaOH-treated (5%) and untreated Malva fibers are incorporated into the cement matrix. After 28 days, the composites are evaluated for porosity, compression, and flexural strength. The results of the study show that the alkaline treatment of Malva fibers enhances the mechanical and physical properties of the composites compared to untreated fibers.

Keywords: Malva, Cement, Composites, Chemical Modifications, Mechanical Properties

Enhanced Bromoperoxidase Activity with Novel Oxovanadium Complexes

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Abstract –

Inspired by vanadium bromoperoxidases in nature, the development of novel oxidovanadium complexes with Schiff base ligands aims to create synthetic catalysts with enhanced and selective bromination capabilities **[1].** The catalytic efficiency of the bioinspired systems is highly sensitive to the structural and electronic features imparted by the specific Schiff base ligand employed. This research focuses on the creation of a novel set of oxovanadium complexes (VOL) incorporating azo-functionalized Schiff base ligands. These ligands were synthesized through the condensation of 2-hydroxy-1-naphthaldehyde or 5-bromo-salicylaldehyde with various aromatic diamines **[2-4].** The synthesized compounds underwent thorough characterization using elemental analysis and various spectroscopic techniques, including (IR, UV-Vis, ^{1}H and ^{13}C NMR). Furthermore, the solid-state molecular structures of selected complexes were elucidated and confirmed by single-crystal X-ray diffraction analysis. Cyclic voltammetry of VOL complexes revealed quasi reversible redox couples corresponding to VO^{IV}/VO^{V} **[5-6].** The bromoperoxidase activity of the newly synthesized vanadium complexes was assessed by their capacity to oxidize bromide and brominate phenol red, forming bromophenol blue. Kinetic studies in DMF/H_2O indicate a first-order dependence on vanadium with the reaction rate constants.

Keywords: *Oxovanadium complexes, Structure, Redox properties, Bromoperoxidase activity*

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Temperature Dynamics and Property Changes in Petroleum Products

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Abstract –

This research delves into the effects of temperature fluctuations on the characteristics of petroleum derivatives, encompassing light diesel, kerosene, and petroleum condensate. Obtained from the refining zone, three distinct samples undergo temperature variations spanning from 10 to 40 degrees Celsius. The study utilizes a Cannon-Fenske Routine viscosimeter tailored for transparent liquids to gauge kinematic viscosity, alongside specialized Anton Paar equipment to assess density at diverse temperatures. The findings elucidate a consistent alteration in apparent density with rising temperatures across all petroleum products. Nonetheless, viscosity exhibits a non-linear decrease, particularly noticeable in fluids with elevated volumetric mass. These findings underscore the importance of comprehending temperature dynamics in delineating the properties of petroleum products, with potential ramifications for refining processes, transportation logistics, and industrial utilization.

Keywords – petroleum products, effect of temperature, density, viscosity, Cannon Fenske routine viscosimeter

Effet de l'activation chimique et thermique sur l'élimination d'un polluant organique par Opuntia Ficus-indica comme bio adsorbant

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Abstract – L'élimination des polluants récalcitrants et des micropolluants des eaux usées et perçu comme un défit majeur pour la communauté scientifique, car l'atteinte des normes internationales nécessite des procédés couteux impliquant l'utilisation de réactifs chimiques qui doivent être éradiquer une fois l'eau est traitée. Dans ce contexte l'adsorption est considérée comme un procédé efficace et respectueux envers l'environnement.

Ce travail vise la valorisation d'un déchet agricole les cladodes d'Opuntia Ficus-indica (OFI) comme adsorbant pour l'élimination d'un polluant organique modèle le bleu de méthylène, l'efficacité du matériau brut ainsi que du matériau activé par voie chimique par HCl, NaOH, H2O2 a été évaluer. L'effet de la modification thermique sur l'OFI comme bio charbon, Hydro charbon et OFI calciné a été aussi étudier. Les résultats obtenus ont démontré la capacité de l'OFI brut comme adsorbant avec un rendement dépassant 90% dans l'élimination du colorant Bleu de méthylène avec un temps d'équilibre de 10 minutes, l'impact de l'activation par HCl sur le rendement a diminué le temps d'équilibre à 5 minutes tandis que les autres méthodes d'activation chimiques et de modification thermique ont négativement influencé le rendement d'adsorption. Ce résultat implique que l'OFI peut être utilisé à l'état brut et ne nécessite pas une activation chimique ou une modification thermique étant ainsi un adsorbant naturel et économique.

Keywords – Adsorption ; Traitement des eaux ; polluant organique ; colorant cationique.

Élaboration assistée par ultrasons de membranes nanocomposites à base d'alginate de sodium et de TiO_2 (SA/TiO_2)

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Abstract – Dans ce travail, des membranes nanocomposites ont été élaborées à base d'alginate de sodium (SA) et de nanoparticules de dioxyde de titane (TiO_2), en utilisant une méthode assistée par ultrasons. Cette approche permet une meilleure dispersion des nanoparticules dans la matrice polymère et améliore les propriétés mécaniques et fonctionnelles des membranes. Les membranes obtenues ont été caractérisées par des techniques spectroscopiques et thermiques. L'objectif est de développer des matériaux efficaces et durables pour des applications dans le traitement de l'eau.

Keywords – Adsorption, bleu de méthylène, nanocomposites, biopolymères, nanoparticules

Theoretical study of naturel product propolis by the DFT method

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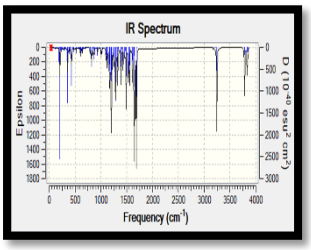
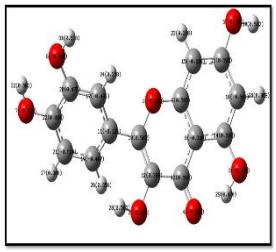
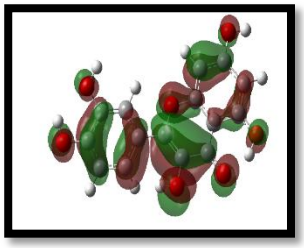
Abstract **–** Propolis is a non-toxic and very important natural product, containing antioxidant, antiviral, antimicrobial, antibacterial, and most interestingly, antimalarial activity. The physical and chemical properties were achieved briefly during the experimental part.

A theoretical study was carried out on the Quercetin molecule which predominates in the family of flavonoid molecules in propolis by quantum method DFT 6-311 ++ G (d, p) with energy optimization by examining the electronic properties HOMO and LUMO, 3D MESP. The chemical reaction is initiated by electron charges and electrophilic and nucleophilic positioning. A spectroscopic study using the infrared method was established with the aim of the functional study and the study of vibrations, and all studies were conducted in two different chemical environments: water as a solvent that is simulated in the blood system and in a vacuum. .

Keywords : Propolis, Quercetin, DFT, IR-TR, Refractive index.







Effect of aging treatment on the mechanical and structural behavior of industrially drawn Al-Mg-Si alloy

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Abstract – The aim of this work is to study the evolution of the microstructure and mechanical properties of aluminum alloy (AGS) wire, during natural and artificial aging treatments, the combined influence of the rate of plastic deformation and the temperature of aging. The reduction of the wire cross-section shows a change in microstructure and texture, the presence of β precipitates (Mg2Si) which increases the hardness of the aluminum wire with the level of deformation by cold drawing. For this we used several experimental techniques of measurement and characterization that allowed us to carry out this work.: Optical microscopy (OM), scanning electron microscopy (SEM), X-ray diffraction, Vickers microhardness and chemical analysis (EDAX), Our study was conducted on a series of aluminum alloy 6101 (Al-Mg-Si) of 9.5 mm diameter, are used by ENICAB in the manufacture of cables for the transmission of electrical energy.

Keywords – aluminum alloy, aging, precipitates, plastic deformation, plastic deformation

Computational Approaches for Estimating K_{ow} in Chemical Compounds

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Abstract – Lipophilicity refers to a molecule's ability to partition between two immiscible phases, such as liquid–liquid or solid–liquid systems. The octanol–water partition coefficient (K_{ow}) is one of the most widely recognized quantitative physicochemical parameters, and it is strongly correlated with the biological activity of organic compounds. K_{ow} represents the ratio of a chemical's concentration in n-octanol to that in water at equilibrium in a biphasic system. The physicochemical properties of chemical compounds play a critical role in determining their environmental distribution and fate.

In this study, a computational model was developed to predict the octanol–water partition coefficient (K_{ow}) of selected chemical compounds. The model was constructed using multiple linear regression (MLR) techniques, with the aim of identifying the molecular descriptors that most significantly influence variations in K_{ow}. The resulting model not only offers valuable insights into the structural factors driving lipophilicity but also serves as a predictive tool for estimating K_{ow} values, especially in cases where experimental data may not be readily available

Keywords – computational model -K_{ow}-model.

Phytochemical Profiling and Valorization of Sunflower (Helianthus annuus L.) Oil: A Sustainable Approach to Oleochemistry

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Abstract **–** This study explores the phytochemical profile and physicochemical quality of oil extracted from *Helianthus annuus L.* seeds collected in the Al-Hamma region (Khenchela, Algeria). The oil, obtained by kneading extraction, yielded approximately 50%, demonstrating the high oleaginous potential of the seeds.

Phytochemical screening was carried out using standard precipitation and coloration reactions, supported by thin-layer and column chromatography, and confirmed by FTIR spectroscopy. The results revealed a rich diversity of secondary metabolites, including flavonoids, tannins, alkaloids, saponins, terpenoids, steroids, and coumarins—compounds known for their significant biological activities.

Physicochemical analyses—specifically refractive index, viscosity, and pH—indicated that the oil meets international quality standards. Its composition, characterized by high levels of omega-6 and omega-9 fatty acids, along with vitamin E, suggests beneficial properties such as antioxidant, hypocholesterolemic, and cardioprotective effects. Nevertheless, the marked imbalance in the omega-6/omega-3 ratio calls for caution, as excessive omega-6 intake may promote inflammatory processes if not counterbalanced by omega-3s.

In addition to its nutritional and cosmetic relevance, the study highlights the role of sunflower oleochemistry in sustainable development. Applications such as eco-friendly biofuel production and anti-caking coatings for mineral fertilizers illustrate the broader industrial potential. These findings underscore the importance of integrating phytochemical-rich oleaginous plants into renewable chemistry strategies and value-added resource utilization.

Keywords – Phytochemical screening; Secondary metabolites; FTIR spectroscopy; Oleochemistry; Green chemistry.

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Theoretical Study of Sulfur Dioxide (SO_2) Adsorption on the Boron Nanocluster B_{36}: DFT Approach and Interaction Analysis

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Abstract – This work presents a theoretical analysis of sulfur dioxide (SO_2) adsorption on the boron nanocluster B_{36} using Density Functional Theory (DFT). The electronic properties of the isolated B_{36} and SO_2 molecules were examined through frontier molecular orbitals (HOMO and LUMO) and the Fukui function to identify the most reactive sites. Upon adsorption, the optimized geometry indicates a chemisorption process between SO_2 and the B_{36} cluster, reflecting a strong and stable interaction. Reduced density gradient (RDG) analysis, which reveals significant attractive interactions, and electrostatic potential (ESP) mapping, which highlights regions favorable to adsorption, also confirm this. Overall, the results suggest that B_{36} is a promising candidate for SO_2 capture, with potential applications in air pollution control applications.

Keywords – Density Functional Theory (DFT), adsorption, B_{36} cluster, Sulfur dioxide, Sensor.

Asymmetries Copper Complex: Synthesis, Characterization with the Ability to Detect Hydrogen Peroxide in Water

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Abstract − A transition metal complex based on a tridentate Schiff ligand was synthesized and characterized using various spectroscopic techniques, such as infrared (IR) spectroscopy, UV-Vis absorption, elemental analysis, and TGA/DTG. The electrochemical properties of the complex were studied by cyclic voltammetry (CV) in dimethylformamide on a glassy carbon electrode, under a nitrogen atmosphere. The diffusion coefficient of the complex was also determined using a rotating disk electrode (RDE) with the Levich relation: $I_{lim}=f(\omega^{1/2})$.

In the presence of KBr and H_2O_2, the copper complex acts as a pre-catalyst in a phenol red bromination reaction, modulated by the solvent, to produce bromophenol blue. Kinetic studies performed in a DMF/H_2O mixture show a first-order dependence on copper, with a reaction rate constant of 1.80 x 10^5 mol^{-2} L^2 s^{-1} for the bromophenol blue-type reaction. Furthermore, the results indicate that the copper complex performs better as a pre-catalyst in the DMF/H_2O system compared to the DMSO/H_2O system. This could be attributed to a higher formation rate of the active species of oxoperoxydovanadium(V) and better detection of H_2O_2 in water.

. *Keywords* – Schiff bases, complexes, spectroscopy, cyclic voltammetry, bromination,

Analyse Comparative des Variétés d'Huile d'Olive : Maturité, Rendement et Polyphénols

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Abstract

L'huile d'olive, symbole des régions méditerranéennes, est appréciée pour ses qualités nutritionnelles et sensorielles. L'évaluation de sa qualité repose sur des critères essentiels tels que l'indice de maturité des olives, le rendement en huile et la teneur en polyphénols, qui varient selon la variété d'olivier et les conditions de culture. Cette étude comparative porte sur trois variétés distinctes, sélectionnées pour leurs différences en termes de profil sensoriel, de rendement et de richesse en composés phénoliques. Les olives ont été récoltées à maturité optimale, et l'indice de maturité a été déterminé par une échelle basée sur la coloration des fruits. L'huile a été extraite par pression à froid, dans des conditions contrôlées, et le rendement a été exprimé en pourcentage du poids frais. La teneur en polyphénols totaux a été mesurée par spectrophotométrie, en mg d'acide gallique par kg d'huile. Les résultats révèlent des variations significatives entre les variétés étudiées, reflétant l'impact de la génétique sur la qualité de l'huile. Le choix de la variété dépendra des objectifs du producteur : rendement élevé, richesse en antioxydants, ou qualité sensorielle. Cette étude ouvre des perspectives pour l'amélioration des pratiques culturales, la sélection variétale et l'optimisation des procédés d'extraction. Elle souligne aussi l'intérêt d'une production durable et de la valorisation des co-produits, tout en encourageant une meilleure sensibilisation des consommateurs à travers des labels de qualité adaptés aux enjeux de santé et de durabilité.

Keywords – Huile d'olive, indice de maturité, rendement, polyphénols, variétés.

CFD Study of Heat Transfer Characteristics in Ferrofluid Flows Under Uniform Magnetic Field Strengths

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Abstract

The current study analyzes the impact of a uniform external magnetic field on the hydrodynamic and thermal behavior of ferrofluid flow in a wavy channel using three-dimensional numerical simulation. The wavy surfaces at the top and bottom of the channel are heated with constant temperature, while the non-wavy section of the channel is thermally insulating. In the wavy section, in a direction perpendicular to the main flow, a regular magnetic field is applied along the direction of the main flow. The study explores the influence of volume fraction, Reynolds number, and magnetic field strength on thermal behavior of the ferrofluid flow. The results indicate an increase in heat transfer on the top and bottom walls with an increase in Reynolds number and magnetic field strength.

Keywords: Heat Transfer; Hydrodynamic Behavior; Magnetic Field; Numerical Modeling; Ferrofluid; Exergy Destruction.

Zéolithe Cu/ZSM-5 : Synthèse, Caractérisation et Performance Antibactérienne pour des Applications Médicales

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Résumé

Dans cette étude, la zéolithe ZSM-5 a été synthétisée par voie hydrothermale puis modifiée par échange ionique et incorporation de cuivre afin d'explorer son potentiel en tant qu'agent antibactérien. La synthèse a été réalisée à 170 °C pendant 48 heures, avec un vieillissement préalable du gel à température ambiante. La structure cristalline MFI typique de la ZSM-5 a été confirmée par diffraction des rayons X (DRX), avec des pics bien définis à 2θ ≈ 7,9°, 8,8°, 23,1°, 23,9°, 24,4° et 29,8°. Après modification au cuivre, ces pics demeurent visibles mais présentent une légère baisse d'intensité, traduisant une bonne dispersion du cuivre dans la matrice sans formation de phases secondaires. L'absence de pics liés à des oxydes de cuivre indique que le Cu^{2+} est intégré de manière homogène dans le réseau. L'analyse infrarouge (IRTF) a révélé des bandes à 960 cm^{-1} et 695 cm^{-1}, attribuées à l'interaction du cuivre avec le squelette aluminosilicaté de la zéolithe. Les essais antibactériens, réalisés par diffusion sur gélose, montrent que la ZSM-5 seule est inactive, tandis que le matériau Cu-ZSM-5 affiche des zones d'inhibition de 15 mm contre Escherichia coli et 18 mm contre Staphylococcus aureus. Cette activité est attribuée à la libération contrôlée des ions Cu^{2+} et à leur capacité à perturber les membranes cellulaires bactériennes. Ces résultats suggèrent que les matériaux Cu/ZSM-5 pourraient être utilisés dans les emballages actifs, les dispositifs de filtration, et diverses applications médicales comme les pansements antimicrobiens et les revêtements hospitaliers.

Mot clés: Cu-ZSM-5,Synthèse hydrothermale ,Propriétés antibactériennes ,DRX, IRTF.

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EAUX RESIDUAIRES DE L'INDUSTRIE DES SEMI CONDUCTEURS : APPLICATION D'UNE TECHNOLOGIE PROPRE, LA DIALYSE A FUITE DE H^+

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Abstract

Le semi-conducteur est devenu le symbole de notre civilisation technologique moderne. Son amélioration a permis des avancées remarquables visibles dans la vie quotidienne: miniaturisation et meilleures performances des montres, téléphones et ordinateurs portables, appareils ménagers et véhicules,…Ces améliorations dépendent fortement de la qualité des traitements chimiques de surface du semi – conducteur.

Cette recherche s'est intéressée à un sujet très concret et important: traiter les rejets liquides concentrés issus de la fabrication du semi conducteur de la salle blanche de l'université Batna2.

La proposition de ce sujet fait suite à une offre d'une entreprise étrangère qui propose un traitement destructif de ces bains usés : système automatisé de neutralisation des rejets avec contrôle et régulation du pH. Le coût de l'installation est d'environ 800 millions de centimes sans aucun recyclage, ni récupération. Faut il « traiter et rejeter » ou « recycler, valoriser, récupérer »? Ce travail de recherche présente une autre alternative basée sur la possibilité d'appliquer les technologies propres dont les principes sont les suivants:

- Economie de l'eau ;
- Récupération, valorisation ou recyclage des polluants pour économiser ;
- Protection de l'environnement avec pour principe le « Rejet Zéro ».

Il y a une grande variété de technologies et de techniques pour appliquer ces technologies. Notre problème est très clair: Comment purifier, par exemple, un bain concentré de HF pollué par des traces de métaux lourds, silicium ou autre, additifs… ? Notre choix, clairement motivé par des raisons environnementales et économiques, s'est porté sur La dialyse diffusionnelle à fuite protonique.

Keywords –Le semi-conducteur, les rejets liquides, recycler, récupérer, La dialyse

Antibiotic removal by electrochemical process

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Abstract

The Electro-Fenton process is an electrochemical advanced oxidation process based on the continuous generation of H_2O_2 in an acidic medium through the electrochemical reduction of O_2 at the cathode. The generated H_2O_2 species reacts with the added Fe^{2+} ions to produce hydroxyl radicals (·OH) and Fe^{3+} ions via Fenton's reaction, which is favored by the catalytic action of the Fe^{3+}/Fe^{2+} system, mainly from the regeneration of Fe^{2+} by the cathodic reduction of Fe^{3+}. Moreover, the method and the involved reactor are easy to handle and to use.

Sulfamethazine (SMT) is an antibiotic widely used in veterinary medicine as an antibacterial drug in pharmaceutical preparations. Degradation of sulfamethazine has been examined through various methods. These studies mainly deal with advanced oxidation processes, such as photo Fenton and photocatalysis with TiO_2 and ZnO as catalysts.

The aim of this study is to investigate the elimination of SMT by the heterogenous electro-Fenton process. The effect of current intensity and air flow rate on H_2O_2 generation was studied. The results revealed that maximum H_2O_2 production was obtained with a current of 50 mA and an air flow rate of 0.2 L min-1. Under these optimum conditions for both air flow rate and current, a 70.2% SMT mineralization rate was obtained after 120 min of electrolysis using a pollutant concentration of 30 mg L^{-1}.

Keywords: *Heterogeneous Electro-Fenton process; advanced oxidation process; mineralization; SMT; H_2O_2 production.*

Traffic Simulation and Public Transport Integration for Congestion and Emission Reduction in Urban Skikda

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Abstract **–**This study explores the impact of integrating public transportation into the urban mobility system of Skikda to reduce traffic congestion and vehicle emissions. Following a detailed analysis of the excessive use of personal vehicles and its consequences on urban mobility, this work focuses on evaluating the role of public transport as a sustainable alternative. Using the microscopic traffic simulation tool SUMO (Simulation of Urban Mobility), realistic traffic scenarios were modeled to assess both traffic flow and environmental impacts. The simulation includes key parameters such as travel times, vehicle speeds, queue lengths, and detailed emission data based on individual vehicle trajectories.
Two scenarios were simulated: one with predominant private car usage and another with a significant inclusion of public transport. The results show a noticeable decrease in the number of vehicles on the road and a corresponding reduction in air pollutant emissions when public transport is prioritized. This approach underlines the importance of public transport not only in reducing urban congestion but also in contributing to environmental preservation and air quality improvement. The study confirms that traffic simulation tools like SUMO are essential for understanding and supporting urban planning decisions aimed at sustainable mobility.

Keywords – Urban mobility, Traffic congestion, Vehicle emissions, Public transportation, Sustainable transport.

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Valorisation d'un déchet alimentaire pour la préparation d'un nouveau matériau polymère à caractère écologique

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Résumé **–** Les polymères sont très demandés en raison de leurs propriétés physico chimiques, mécaniques, mais aussi optiques et électriques. Cependant, lors de la conception d'objets, les propriétés des polymères ne suffisent souvent pas à elles seules. En effet, la technologie moderne nécessite des matériaux alliant rigidité, résistance mécanique, haute ténacité, bonne légèreté et ayant un caractère écologique. Dans ce contexte un nouveau matériau à base du polyéthylène chargé d'un renfort végétal a été élaboré.

L'étude présentée dans ce document a un caractère prospectif et son objectif est double. Il consiste, d'une part, de proposer de nouveaux matériaux à bas coût avec des propriétés comparables à celles des composites de grande diffusion et d'autre part : (1) de trouver un moyen de réduire la consommation du PE largement employé à travers le monde, (2) d'étudier l'effet de l'introduction de ce renfort végétale et de l'ajout d'un agent de couplage (PE-g-MA) sur les propriétés physico-mécaniques des matériaux élaborés pour des taux de charge allant de 10 à 30%. Les propriétés physico-chimique et mécanique en traction du matériau élaboré ont été étudiées. Les résultats enregistrés ont montré une amélioration des différentes propriétés étudiées après l'introduction de l'agent de couplage.

Keywords – Valorisation, Polymère, PEBD, Charge végétale, Propriétés physico-mécaniques.

Comparative evaluation of the electroactive surface area of GrE and NiO/GrE electrodes

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Abstract – The active surface refers to the part of a material (often a solid) that is exposed and available to react with its environment. The calculation of the active surface area is extremely important for materials, particularly in fields such as chemistry and materials science. In this study, a comparison of the active surface area between the graphite electrode (GrE) and the electrode modified with NiO nanoparticles (NiO/GrE) was carried out.

Based on the cyclic voltammograms, well-defined redox peaks were observed for both the NiO nanoparticle-modified electrode (NiO/GrE) and the unmodified graphite electrode (bare GrE). The modified electrode exhibited a significantly enhanced redox response toward $K_3[Fe(CN)_6]$, as evidenced by a notably higher peak current compared to the unmodified electrode. This improvement is attributed to the increased number of active sites on the modified surface, which is directly related to a larger electroactive surface area. Accurate determination of this active surface is essential for understanding the electrode's conductivity. The electroactive surface area values for the NiO-nanoparticles/GrE and bare GrE electrodes, calculated using the Randles-Sevcik equation, were 0.092 cm^2 and 0.055 cm^2, respectively. These results clearly demonstrate that the NiO nanoparticle film formed on the surface of the GrE provides a larger active surface area, which translates into higher sensitivity for glucose detection.

Keywords – Anodic oxidation, Cyclic Voltammetry, Detection, Nickel, Glucose.

DFT study of structural, electronic, and mechanical properties of $Cs_2AgBiCl_6$ compound

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Abstract **–**In recent years, halide perovskites of the general formula ABX_3 have garnered significant attention in photovoltaics due to their remarkable optoelectronic properties. Among these materials, the double perovskite $Cs_2AgBiCl_6$ has emerged as a promising, environmentally friendly alternative to lead-based hybrid halide perovskites [1-3]. This compound not only exhibits excellent stability under environmental conditions but also features a band gap comparable to that of $CH_3NH_3PbX_3$ within the visible range [4]. In this study, we employ density functional theory (DFT) to systematically investigate the structural, mechanical, and electronic properties of $Cs_2AgBiCl_6$. Our analysis focuses on key parameters such as hardness, rigidity, softness, elastic anisotropy, and band gap, providing insights into its potential applications in next-generation photovoltaic devices.

Keywords – Double halide perovskite, DFT, structural properties, electronic properties, mechanical properties.

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Evaluation of $La_{0.85}Bi_{0.15}FeO_3$ as a Promising Photocatalyst for Organic Pollutant Degradation: Structural and Optical Study

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Abstract **–** Perovskite-type oxides have attracted growing attention for environmental applications, particularly in the treatment of water pollutants, due to their tunable structural and optical properties. In this work, the $La_{0.85}Bi_{0.15}FeO_3$ compound was synthesized using the sol-gel method, employing lanthanum nitrate, bismuth nitrate and iron nitrate as precursors, with citric acid as a complexing agent. The resulting powder was calcined at 800 °C and characterized using X-ray diffraction (XRD) and UV-Visible spectroscopy. XRD analysis confirmed the formation of a pure orthorhombic phase with space group *Pbnm*. Rietveld refinement further validated this structure and provided detailed crystallographic parameters, indicating good crystallinity and structural stability. Optical characterization revealed a strong absorption in the visible range, with an absorption coefficient reaching ~35 cm^{-1}. The material exhibited a relatively low reflectance, with a refractive index below 2.5. The estimated optical band gap of 2.14 eV falls within the visible range, suggesting efficient photon absorption and potential activation under solar irradiation. In addition, the Urbach energy was found to be 0.19 eV, suggesting a low degree of structural disorder and favorable electronic transitions. These structural and optical features make $La_{0.85}Bi_{0.15}FeO_3$ a promising candidate for future applications in photocatalytic degradation of organic pollutants in water.

Keywords – Perovskite ; Pollutant ; Photocatalyst ; Band gap ; Absorption.

Performance study of a low-cost adsorbent – raw date pits – for removal of azo dye in aqueous solution

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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.

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

Utilisation des anhydrides d'acides cyclique pour le dédoublement cinétique enzymatique d'alcools benzyliques à chiralité centrale.

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Résumé – La préparation des briques moléculaires à haute valeur ajoutée énantiomériquement pures est devenue pressante pour divers domaines, tels que la chimie fine, l'industrie des médicaments, des arômes, de l'agriculture et de l'agroalimentaire, et cela de plus en plus rigoureusement après les législations imposées par la FDA. Particulièrement, les alcools benzyliques chiraux qui sont des intermédiaires clés pour la génération des molécules à visées thérapeutiques. Leur obtention énantiomériquement purs peut se faire par dédoublement cinétique par acylation enzymatique dans des milieux non conventionnels. Plusieurs paramètres peuvent moduler cette réaction telle que la nature de l'agent acylant. Parmi les agents acylants les plus utilisés lors de cette réaction, les anhydrides d'acides cycliques constituent une classe attrayante, par le bien de l'avantage de la séparation facile des deux énantiomères formés par une simple extraction liquide-liquide.
Au cours de cette étude, nous étudions l'impact de l'utilisation des anhydrides d'acides cycliques lors du dédoublement cinétique enzymatique de quelques alcools benzyliques secondaires. Et ce, en présence de quelques lipases dans des milieux organiques pauvres en eau.

Mots clés: Dédoublement cinétique enzymatique, Anhydride d'acide cyclique, Lipases, Agent acylants, Hydrophobicité.

Estérification biocatalytique énantiosélective du 1-phényléthanol par l'acide acétique et de son anhydrique symétrique: Impact de la nature de l'enzyme et l'hydrophobicité du solvant

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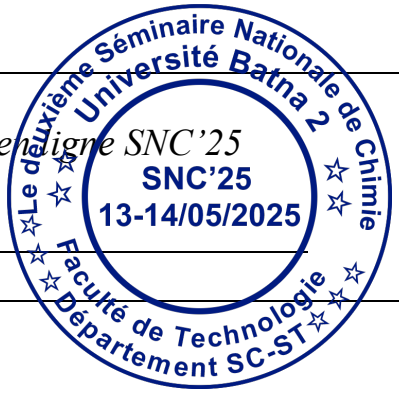
Résumé – Parmi les bioprocédés industriels, les réactions d'acylation catalysées par des lipases sont les plus utilisées pour la création des liaisons esters. Ces biotechnologies sont économiquement viables pour la synthèse des molécules bioactives à haute valeur ajoutée. La biocatalyse est une alternative en plein expansion, par le bien de plusieurs avantages tels que: catalyseurs verts, hautement sélectifs (chimio-, régio-, énantio- et diastéréosélectifs), conditions de réaction douces. Parmi les biocatalyseurs les plus utilisés pour mener la réaction d'estérification, les lipases (triacylglycerolacyl hydrolases, EC.3.1.1.3) constituent la classe la plus utilisée et la plus adaptée pour plusieurs avantages, dont les plus pertinents sont : la non-nécessité de cofacteurs, leur biodégradabilité et leur grande stabilité dans les solvants organiques.

Le dédoublement cinétique enzymatique des mélanges racémiques par le biais des lipases est la méthode la plus facile et la plus crédible pour avoir des molécules à haute valeur ajoutée sous formes énantiopures. La performance de cette réaction est peut être modulée par plusieurs paramètres tels que : la nature du donneur d'acyle et l'hydrophobicité du milieu réactionnel.

Dans la présente étude nous décrivons l'influence de ces deux paramètres sur la réactivité et l'énantiosélectivité de la réaction d'estérification du 1-phényléthanol. Deux agents acylants ont été utilisés : l'acide acétique et de l'anhydride acétique en présence de diverses lipases en fonction de l'hydrophobicité du milieu réactionnel.

Mots clés – Estérification enzymatique, énantiosélectivité, Lipases, Agent acylants, Hydrophobicité.



Synthesis and in silico study of some sulfonyl carbamate derivatives

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Abstract **–** Sulfonylcarbamates, which incorporate both sulfonamide and carbamate functionalities, represent a promising class of hybrid molecules in medicinal chemistry. The combination of these two pharmacophores within a single scaffold often leads to enhanced biological activity, owing to their ability to engage in diverse interactions with biological targets. Sulfonamides are well known for their antimicrobial and anticancer properties, while carbamates are commonly found in cholinesterase inhibitors and other bioactive agents. In this study, a series of sulfonylcarbamate derivatives were designed and evaluated for their BChE inhibitory potential. An in silico study was conducted, including molecular docking to explore binding interactions, density functional theory (DFT) calculations to analyze electronic and geometric properties, and ADME predictions to assess pharmacokinetic behavior and drug-likeness.

Keywords – Carbamate, Sulfonamide, Molecular docking, DFT study, ADME

Effect of temperature on the performance of P3HT:PCBM polymers solar cell

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Abstract – Intensive research has been done to improve the efficiency and stability of polymers solar cells (PSCs) to compete in the solar cells market. Different cell structures and material compositions have been studied, demonstrating a potential for achieving high power conversion efficiency (PCE) [1]. The study of temperature dependency in polymers solar cells is an indispensable issue because it can give insight into the fundamentals of the devices and materials accompanied by practical information about device performance in experimental conditions [2,3]. The temperature dependence of bulk heterojunction polymers solar cells fabricated from poly(3-hexylthiophene) (P3HT) and [6,6]-phenyl-C61-butyric acid methyl ester (PCBM) was studied in detail.

The films of (P3HT: PCBM) for PSCs are all deposited by centrifugation at 600 rpm for 50 s, followed by thermal annealing at three different temperatures **80, 110 and 130°C for 10 min** and a reference cell without annealing. The parameters improve with annealing, with the highest cell values obtained at 110° C, with PCE=2.20%. This improvement can be attributed to the widening of the donor-acceptor interface zone induced by the slow-growing P3HT: PCBM layer via the auto-organization process. With thermal annealing, P3HT films have been shown to improve crystallization and increase carrier mobility in photovoltaic solar cells. Annealing the films helps remove residual solvent and reduces the number of trapping sites for better charge transport and extraction. Another positive potential of the annealing process is the smooth surface morphology obtained from the photo-active layers, which can improve active layer/cathode contact [4,5].

Keywords – Polymers solar cells (PSCs), poly(3-hexylthiophene) (P3HT) and [6,6]-phenyl-C61-butyric acid methyl ester (PCBM) active layer, Power conversion efficiency (PCE)

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Prévention du colmatage des membranes ioniques par insertion d'un procédé électrochimique

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Résumé – L'électrodialyse (ED) est un procédé courant et largement appliqué pour la purification et le dessalement de l'eau et/ou pour la récupération d'espèces chimiques. L'ED présente certaines limites qui sont principalement dues aux propriétés des membranes échangeuses d'ions. Parmi ces limites, il y a le colmatage des membranes par accumulation de matières organiques au cours du procédé. Dans ce travail, une combinaison d'ED à un procédé d'électrocoagulation (ED-EC) a été adoptée, afin de réaliser une élimination simultanée du colorant azoïque (méthyle orange, MO) et d'atténuer le colmatage de la membrane anionique.

La caractérisation de la membrane anionique utilisée en ED simple montre que le colmatage était le principal problème derrière le faible taux de traitement, provoquant également une augmentation significative de la résistance électrique de la cellule, contrairement au procédé hybride d'ED-EC. L'effet des paramètres opératoires sur le procédé ED-EC tels que la densité de courant appliquée en EC, la concentration initiale du MO et de l'électrolyte support, pH de la solution à traiter, ont été étudiés. Enfin, les résultats de cette étude fournissent une excellente combinaison entre l'efficacité d'élimination des polluants organiques et un traitement continu qui sont les principaux facteurs recherchés à grande échelle..

Keywords – Électrodialyse, Electrocoagulation, Anti-colmatage des membranes, Procédés hybrides.

PRODUCTION DE BIOÉTHANOL COMME SOURCE D'ÉNERGIE RENOUVELABLE À PARTIR D'UN JUS EXTRAIT DES DÉCHETS DE DATTES

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Résumé– Cette étude vise à contribuer au développement des énergies renouvelables en explorant la valorisation des déchets de dattes (variété Degla Beida), souvent peu utilisés, pour produire du bioéthanol de première génération, une alternative aux énergies fossiles. La première phase de l'étude a consisté en l'extraction du jus de dattes à partir de ces déchets, suivi de sa caractérisation physico-chimique et biochimique. La deuxième phase a été consacrée à la production de bioéthanol par fermentation alcoolique du jus de dattes, en utilisant la levure *Saccharomyces cerevisiae* dans des conditions optimisées (pH = 5, température de 30°C, agitation à 150 rpm). Les résultats ont montré que le jus de dattes était particulièrement riche en sucres (22,53 % p/p), qui constituent un critère clé pour la production de bioéthanol. En plus des sucres, il contenait des protéines (plus de 2 % p/p), de l'azote total (plus de 1,12 % p/p) et des minéraux nécessaires à la croissance des levures. La fermentation a permis d'obtenir une concentration de bioéthanol avec un degré d'alcool de 7°. Ces résultats soulignent l'intérêt de valoriser les déchets agroalimentaires dans la production d'énergies renouvelables, contribuant ainsi à la transition énergétique et à la réduction de la dépendance aux énergies fossiles.

Mots-clés –Déchets de dattes ; Bioéthanol ; Valorisation ; Saccharomyces cerevisiae ; Énergies renouvelables

Synthesis and Characterization of Nickel Oxide Nanoparticles

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Abstract **-** Chemical and physical synthesis of nanoparticles cannot be easily developed to large-scale production due to several drawbacks such as the presence of toxic organic solvents and hight energy consumption [1]. Therefore, the use of new biological methods that could be an alternative [2] in various scientific and technological domains due to their low environmental toxicity and effectiveness in diverse application [3].

This study focuses on green synthesis Nickel oxide nanoparticles (Ni-O NPs) using plant extract concentrations as a reducing and stabilizing agents. The characterization by UV-Visible spectroscopy ; SEM ; infrared spectroscopy (IR) demonstrates respectively the presence of Ni- oxide NPs.

Keywords–:greensynthesis,nanoparticles,metal-oxide,Nanotechnology,ecofriendly

Enhanced Extraction Performance of XAD-16 Resin Functionalized with the Nonionic Surfactant Tween 80

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Abstract – Solvent-impregnated resin (SIR) refers to synthetic, porous, hard, and water-insoluble polymeric particles onto which organic extractants—such as oleic acid, organophosphoric acids, and surfactants like Tween 80, a nonionic surfactant—are immobilized. This system combines the advantages of liquid-liquid extraction with the operational simplicity of a solid stationary phase, enhancing both the stability and reusability of the material during extraction processes. The impregnated Extractants exhibit a strong affinity for the polymer matrix while retaining physicochemical characteristics similar to those in the liquid phase, thereby promoting efficient mass transfer of target compounds.
The present study aims to investigate the impregnation of a styrene-divinylbenzene resin, specifically Amberlite XAD16, with the nonionic surfactant Tween 80, and to evaluate its performance in the extraction of violet de gentian from aqueous solutions. Maximum impregnation was achieved near the critical micelle concentration of Tween 80 (approximately 1.2×10^{-5} M), with optimal conditions including a contact time of 45 minutes and a temperature below 20°C. Following the optimization of key parameters such as solution pH, surfactant loading on XAD-16, cadmium concentration, and stirring speed, an extraction efficiency exceeding 94% was obtained.
Keywords – Amberlite XAD16 resin; Tween 80 surfactant; impregnation; dye removal.

La modélisation de la tension superficielle des mélanges binaires {liquide ionique + eau et divers solvants organiques} à l'aide d'une machine à vecteurs de support (SVM) optimisée par l'algorithme d'optimisation des flammes mites (MFO)

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Résumé – Les liquides ioniques (LIs) constituent une nouvelle classe de liquides considérés comme des solvants verts ; moins toxiques, moins inflammables et moins polluants qui conservent leur état liquide sur de larges plages de températures et sont considérés comme des alternatives aux solvants organiques volatils. La tension superficielle des liquides ioniques et leurs mélanges avec d'autres composés jouent un rôle important dans la conception et le développement de nombreux procédés industriels. Sa modélisation est donc extrêmement importante d'un point de vue industriel. Ce travail a examiné la capacité et la faisabilité de SVM-MFO pour prédire la tension de surface des systèmes binaires contenant des LIs. Pour construire et tester les modèles, 1700 points de données correspondant aux valeurs expérimentales de tension superficielle de mélanges binaires contenant des LIs ont été collectés dans la littérature. La tension superficielle était comprise entre 18,9 et 72,7 mNm-1. La température, la composition de LI, deux descripteurs basés sur les profils sigma, l'un relatif au caractère donneur de H-bond, l'autre relatif au caractère accepteur de H-bond, de l'anion, du cation et du solvant ont été utilisés comme variables d'entrée du modèle afin de différencier les différents composés impliqués dans les systèmes binaires. Une comparaison des données expérimentales et des valeurs prédites a montré un bon accord avec une erreur relative absolue moyenne globale (AARD) égale à 1.0164% et une erreur absolue moyenne (MAE) égale à 0.4406. Ces résultats sont très encourageants pour les futurs projets visant à modéliser d'autres propriétés physiques et chimiques des liquides ioniques.

Mots-clés –Tension superficielle, liquides ioniques, l'optimisation des flammes mites-machine à vecteurs de support, prédiction, descripteur de profil σ.

HPSOBOA-Inspired Optimizer with Support Vector Regression Modeling of Critical Micelle Concentration of Anionic Surfactants in Water/Organic Solvent Mixtures

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Abstract **–** The critical micellar concentration (CMC) of surfactants is a physicochemical parameter frequently used to examine their behavior. This value is unique to each surfactant, as it varies depending on the surfactant's chemical makeup and other external factors. This work proposes a machine learning approach that combines an efficient Chaotic Hybrid Butterfly Optimization Algorithm with a Particle Swarm Optimization Algorithm (HPSOBOA) to optimize the three hyperparameters of a support vector regression algorithm (SVR) for model building. This model considered six features defining both the organic solvent-water mixture and the chemical structure of the surfactant. A database consisting of a total of 104 CMC values for four anionic surfactants collected from the literature. The dataset was randomly divided into two sets. 75% of the data is utilized as a training set for model development, while the test set comprises the remaining 25% for evaluating the performance of the model. Multiple statistical metrics were utilized to validate the obtained model, such as root mean square error (RMSE = 0.0195), mean absolute error (MAE = 0.0099), coefficient of determination (R^2 = 0.9966), and robustness (Q^2 =0.9965) for the whole set. The overall results demonstrated a high level of predictive ability and robustness, suggesting potential alternative methods to replace expensive experimental laboratory measurements.

Keywords – Anionic surfactants, CMC, HPSOBOA-SVR, Machine learning, Prediction.

Synthesis of Tolbutamide Analogues as Antidiabetic Agent, DFT Calculation

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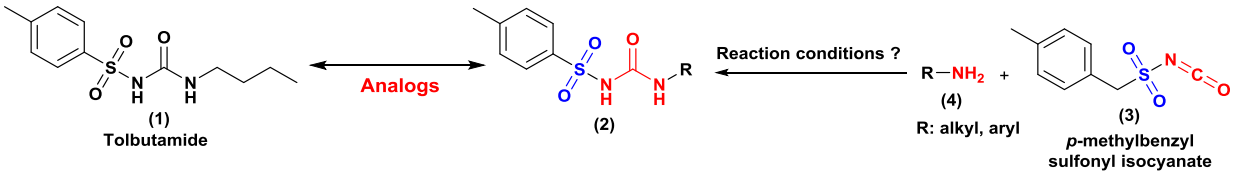
Abstract

Diabetes is one of the most widespread chronic diseases globally, affecting millions of people and leading to serious health complications. According to the World Health Organization (WHO), the number of people living with diabetes has risen dramatically in recent decades, increasing from 463 million in 2019 to a projected 538 million by 2030.[1]

There are several classes of antidiabetic drugs, each offering specific benefits and associated with potential side effects. Sulfonylureas are a class of oral antidiabetic drugs that stimulate the pancreas to secrete insulin.[2] Tolbutamide® was among the first medications in this class to be developed and brought to market. Although Tolbutamide effectively reduces blood glucose levels in patients with type 2 diabetes, it may cause side effects such as hypoglycemia (low blood sugar) and weight gain. As a result, newer antidiabetic drugs have developed to provide similar or improved efficacy with fewer adverse effects.[3]

Building on our lab's focus on creating new molecules with potential biological activity, this study aims to synthesize compounds structurally similar to Tolbutamide, which may possess promising medicinal properties. The planned synthesis of Tolbutamide analogues involves a one-step nucleophilic addition reaction using *p*-methylbenzylsulfonylisocyanate to introduce the (-SO_2 -NH-CO-X) group. **(Scheme 1)**



Scheme 1. Proposed strategy for the synthesis of novel *Tolbutamide* analogues

Computational chemistry (DFT) was used to study the reactivity of synthesized compounds in a simulated gas phase. The analysis focused on their electronic and geometric properties, including key energy levels and charge distribution. This data provides insights into the compounds' electronic structure and potential biological activity.

Keywords – Tolbutamide, Antidiabetic drugs, Sulfonylureas, p-Methylbenzylsulfonylisocyanate, DFT calculation.

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Synthèse verte et caractérisation spectrale des nanoparticules de MgO

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Abstract – Le présent travail se concentre sur la synthèse de nanoparticules de MgO à partir de feuilles de *Moringa oleifera* par le biais d'une méthode verte. Cette méthode est non toxique et écologique. Dans ce travail, les matériaux précurseurs étaient le $MgCl_2$ et l'extrait de feuilles de Moringa fraîches. L'extrait de feuilles de Moringa agit comme un agent réducteur dans la réaction.

Le suivi temporel par spectrophotométrie UV-Visible à révéler la formation de ces nanoparticules de MgO à une longueur d'onde Maximale d'absorption de 280nm, et même pour le cas de l'analyse par spectroscopie Infrarouge à transformée de Fourier nous a permis de justifiée la formation de la liaison Mg-O avec une bande d'absorption de $430cm^{-1}$. L'analyse par diffraction des rayons X a témoigné aussi la présence de la phase cristalline de MgO, à la fin la taille des nanoparticules a été mesurée par la diffusion de lumière (DLS) et qui a enregistré une valeur de 65nm.

Keywords – Biosynthèse, Nanoparticules, Extrait de plante, NPMgO, Moringa oleifera, Analyse spectrale

Fragment-Based Drug Discovery of KRAS G12D Inhibitors for Pancreatic Cancer Therapy

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Abstract **–**KRAS G12D is a major oncogenic driver in pancreatic cancer and a critical target in the search for effective therapies. In this study, over 30,000 natural and natural product-like fragments were virtually screened against KRAS G12D using Schrödinger's HTVS and SP docking protocols. Top fragments were selected and combined through iterative linking, resulting in 100 novel compounds. These were evaluated using XP docking, and the best two candidates achieved docking scores of −13.881 and −13.601 kcal/mol, both outperforming the reference inhibitor MRTX-1133 (−12.891 kcal/mol). The top hits were further assessed through induced fit docking and MM-GBSA binding free energy calculations, confirming their strong affinity and stable interactions within the KRAS G12D binding site. ADMET analysis highlighted Hit2 in particular for its excellent pharmacokinetic and safety profile, including good oral bioavailability, drug-likeness, and low predicted toxicity. These findings underscore the potential of fragment-based design to deliver novel KRAS G12D inhibitors, with Hit2 standing out as a promising lead for further development in pancreatic cancer therapy.

Keywords – Pancreatic cancer; KRAS G12D; FBDD; IFD; MM-GBSA; ADMET

Composition chimique et activité antifongique de l'huile essentielle de *Rosmarinus officina*lis L.

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Résumé **–** Les composés bioactifs d'origine végétale représentent une source naturelle potentielle de diverses propriétés biologiques, notamment une activité antimicrobienne. Cette étude vise à évaluer l'efficacité de l'huile essentielle de *Rosmarinus officinalis*, appartenant à la famille Lamiaceae, comme source de composés biologiques et de propriétés antifongiques. Des études soulignent l'importance des huiles essentielles végétales dans les applications pharmaceutiques et thérapeutiques.
La composition chimique de l'huile a été déterminée par chromatographie en phase gazeuse-spectrométrie de masse. L'activité antifongique a été évaluée par la technique de diffusion sur disque. Les résultats ont montré la présence de 18 composants, principalement des monoterpènes, les principaux composés étant le para-cymène (44,02 %), le linalol (20,5 %) et le terpinène (16,62 %).. De plus, les résultats ont indiqué que des concentrations croissantes d'huile essentielle inhibaient la croissance des champignons *Alternaria* spp. et *Penicillium* spp.
Ces résultats suggèrent que l'huile essentielle représente une source potentielle de composés biologiques aux propriétés antifongiques, ouvrant de nouvelles perspectives pour son utilisation en santé.

Mots clés – Activité antifongique, huile essentielle, Rosmarinus officinalis, composés biologiques , chromatographie gazeuse

DFT and Molecular Dynamics Simulations of the Corrosion Inhibition of Aluminum Alloy by 2-Aminobenzothiazole Derivatives

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Abstract **–** Three 2-aminobenzothiazole molecules (Fig **1**), 6-bromobenzo[d]thiazol-2-amine (AMBT-1), 2-aminobenzo[d]thiazole-6-carbonitrile (AMBT-2), and 6-ethylbenzo[d]thiazol-2-amine (AMBT-3) were successfully synthesized and fully characterized. The compounds were investigated as corrosion inhibitors of AA7075 aluminum alloy in 3% NaCl medium at 25°C. Different techniques were employed including weight loss analysis, electrochemical techniques, and scanning electron microscopy (SEM). The experimental results were supported by DFT and molecular dynamics (MD) calculations. The optimization of the geometrical structures of the three molecules were performed with DFT at B3LYP/6-31G (d,p) level, in water as solvent (Fig **2**). Quantum parameters including electronegativity (χ), ionization potential (I), electron affinity (A), hardness (η), and softness (σ) mainly determined from HOMO and LUMO energies, were computed from the optimized geometrical structures of the inhibitors. These parameters help correlate between the corrosion inhibition efficiency and the structure of the molecule. Molecular Electrostatic Potential Surface (MESP) and Fukui functions were also computed. Molecular dynamics, performed with Materials Studio software, provided a deeper understanding of the inhibition properties of the three AMBTs through a realistic simulation of the adsorption phenomena. The studies were carried out both in gas and aqueous phase and the adsorption energies as well as rigid adsorption, deformation, and differential (dE_{ads}/dN_i) were collected. MD investigations showed that the inhibitors adopted a flat position thus assuring a good protection of the aluminum surface from aggressive molecules (Fig **3**).

Keywords – Molecular dynamics, DFT, Corrosion inhibitors, 2-aminobenzothiazole, Aluminum alloys

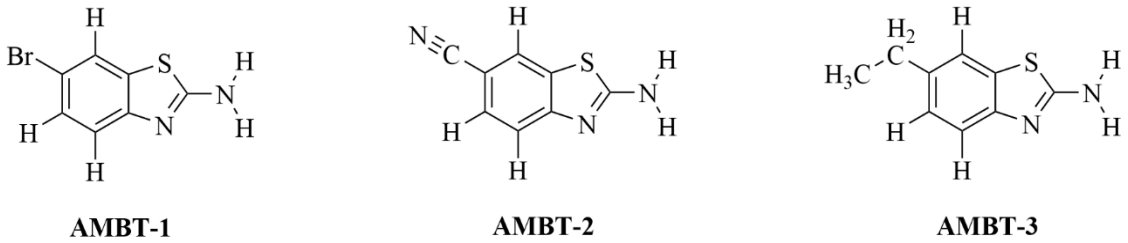


Fig 1. Structures of the three inhibitors.

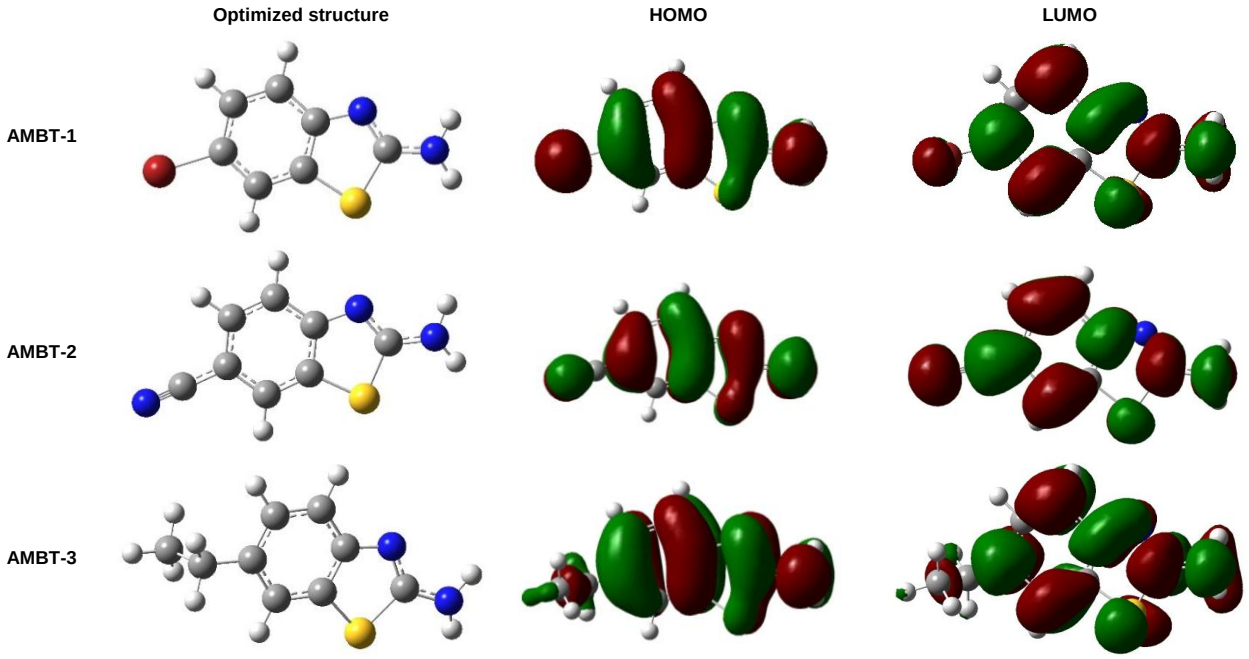


Fig2. Optimized molecular structures and frontier orbital distributions HOMO and LUMO of the three inhibitors.

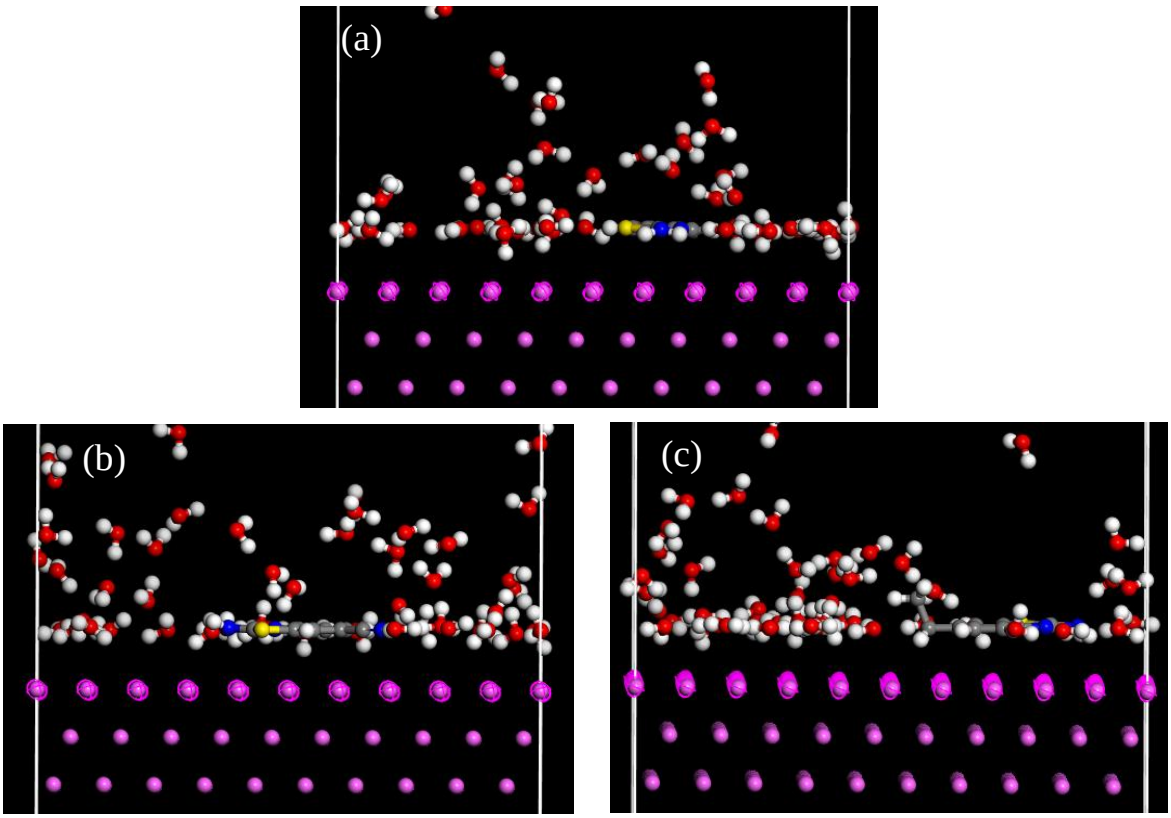
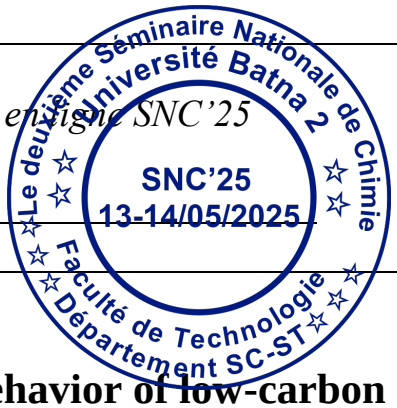


Fig 3. Adsorption configurations of (a) AMBT-1, (b) AMBT-2, and (c) AMBT-3 on Al (111) surface in aqueous solution



Investigation of corrosion behavior of low-carbon steel alloy under changing electrochemical conditions in saline medium simulating natural Environmental fluctuations

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Abstract

Corrosion gradually compromises the structural integrity of metal structures through degradation caused by exposure to harsh environmental conditions. Safety, cost, and preservation are the three main focuses of corrosion research. This degradation results from electrochemical processes influenced by oxygen, moisture, and contaminants. Most metals and alloys, particularly steel and iron, corrode spontaneously due to their thermodynamic instability in air and water. The corrosion of steel and ferrous metals in chloride-rich environments poses a serious threat to the water durability of gas, oil, and sewage distribution systems. Based on the variation of pH of 3.5% NaCl solution, we chose to control the corrosion of low-carbon steel alloy in this study. The methods employed in this work were open circuit potential and electrochemical impedance spectroscopy (EIS). The surface morphology of this alloy was investigated using optical microscopy OM. In order to conduct a deeper analysis of the steel's properties under different pH levels, XRD analysis was performed. The results reveal that the open circuit potential shifted negatively with increasing of pH values, suggesting the start of corrosion processes. The corrosion potential deteriorates more rapidly in an acidic solution with a pH around 3, which is associated with a faster corrosion rate compared to a neutral solution. The EIS indicated that the corrosion resistance of low-carbon steel alloy decreased at acidic medium (pH=3) which indicate a big corrosion rate. Nyquist and Bode plots show that the corrosion processes of our alloy are complex and depend on the pH of the corrosive medium.

Keywords – Corrosion, low-carbon steel alloy, EIS, chloride solution, optical microscopy.

Caractérisation phytochimique et évaluation de l'activité antioxydante de la mélasse de raisin d'Algérie

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Résumé – La mélasse de raisin, obtenue par concentration du jus de raisin, est un sous-produit naturel traditionnellement utilisé, mais encore peu valorisé en Algérie. Riche en sucres, en minéraux et en composés phénoliques, elle suscite un intérêt croissant en tant que source potentielle de molécules bioactives. L'objectif de cette étude est de caractériser les composés phytochimiques présents dans la mélasse de raisin algérienne et d'évaluer son activité antioxydante. Pour cela, des analyses phytochimiques ont été réalisées afin de quantifier les teneurs en polyphénols totaux et en flavonoïdes. L'activité antioxydante a été évaluée à l'aide de deux méthodes complémentaires : le test du radical libre DPPH et la capacité totale d'antioxydante (CAT). Les résultats obtenus ont révélé une forte concentration en composés phénoliques, notamment en flavonoïdes, ainsi qu'une capacité antioxydante significative. Ces données mettent en évidence le potentiel de la mélasse comme source naturelle d'antioxydants. En conclusion, la mélasse de raisin algérienne apparaît comme une ressource locale prometteuse, dont la valorisation pourrait offrir des perspectives intéressantes dans les domaines agroalimentaire, cosmétique et pharmaceutique, en particulier pour la prévention du stress oxydatif et ses effets délétères sur la santé humaine.

Mots-clés – Mélasse de raisin – Algérie –Polyphénols – Flavonoïdes – Activité antioxydante

Electrochemical Evaluation of Agave Americana and Opuntia Ficus Indica Synergy as Eco-Friendly Corrosion Inhibitors for AISI 410 Steel in 0.5M H_2S_4

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ABSTRACT

The synergistic effect of plants (Grated Agave Americana (GAA) and Grated Opuntia Ficus Indica (OFI)) as corrosion inhibitors for AISI 410 steel in 0.5M H_2SO_4, has been studied. The study was carried out using stationary electrochemical techniques (potentiodynamic polarization (PDP)), transients (Electrochemical Impedance Spectroscopy (EIS)), and microscopic observations by SEM-EDX and AFM.The OFI behaves as mixed inhibitor, with a physisorbed adsorption, obeys the Langmuir isotherm, with an efficiency of 89.49% to 10% (v/v) obtained after 4 hours of immersion at 25°C.The GAA behaves as mixed inhibitor, with a physisorbed adsorption, and obeys the Freundlich isotherm with an efficiency of 90% to 10% (v/v) obtained after 2 hours of immersion at 25 ° C. The synergistic effect (10% (v/v) GAA + 10% (v/v) OFI) increased the inhibitory efficacy to 97.64%, at 25°C, after 2 hours of immersion. Microscopic observations by SEM-EDX and AFM confirm the results obtained by the different methods used. In conclusion, OFI, GAA and their synergy improve the resistance of AISI 410 stainless steels to corrosion in 0.5M H_2SO_4 at 25 ° C.

Keywords: *Corrosion; Green inhibitor; Agave Americana; Opuntia Ficus Indica; Synegistic effect.*

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Orbital-Resolved Density of States Analysis of CuO: Insights into Orbital Contributions

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Abstract **–** CuO displays a highly complex electronic structure, profoundly shaped by strong electron correlations and intricate orbital interactions, which govern its electronic properties. In this work, we present a detailed theoretical investigation of CuO using density functional theory (DFT) with the Hubbard U correction under the Generalized Gradient Approximation (GGA). Our focus is an in-depth analysis of the orbital-resolved density of states (DOS). The study highlights the contributions of individual Cu 3d orbitals (dxy, dxz, dyz, dz^2, dx^2-y^2) and O 2p orbitals (px, py, pz) to the electronic states near the Fermi level, while the O 2s orbitals do not contribute significantly to the electronic structure. We observe significant hybridization between Cu 3d and O 2p states, which dominate the conduction and valence bands. The findings also reveal subtle distinctions in orbital contributions across the electronic spectrum, shedding light on the intricate electronic interactions in CuO. This analysis provides a deeper understanding of the role of orbital-specific electronic contributions in determining CuO's semiconducting and antiferromagnetic properties, offering a comprehensive perspective on its electronic structure.

Keywords – Copper oxide, DFT, GGA+U, density of states (DOS), Electronic structure.

Biosynthèse extracellulaire de nanoparticules d'oxyde de zinc par Salmonella enterica ATCC6017 et leurs applications

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Abstract – La nanotechnologie met l'accent sur le développement de méthodes fiables et écologiques pour produire des matériaux à l'échelle nanométrique. Cette étude explore la biosynthèse extracellulaire de nanoparticules d'oxyde de zinc (ZnONPs) par *Salmonella enterica* ATCC 6017 et évalue leurs propriétés antibactériennes et antioxydantes. La synthèse a été réalisée en utilisant le surnageant de culture bactérienne, avec la formation de nanoparticules confirmée par l'apparition d'un précipité blanc. Les caractéristiques morphologiques et la distribution des nanoparticules ont été analysées par microscopie électronique à balayage (MEB) et spectroscopie UV-Visible, tandis que la qualité cristalline et la taille des particules ont été évaluées par diffraction des rayons X (XRD). L'activité antioxydante a été mesurée par la méthode DPPH, avec une concentration inhibitrice médiane (CI50) de 2,87 mg/ml. L'activité antibactérienne du ZnONPs vis-à-vis *Staphylococcus aureus* ATCC2 5923 (Gram positif) and *Pseudomonas aeruginosa* ATCC 9027 (Gram negatif) montrant des zones d'inhibition respectives de 8 mm et 1 mm.

Keywords – Biosynthèse extracellulaire, nanoparticules de zinc, activité antibactérienne, activité antioxydante, bactérie.

Prétraitement des eaux de mer pour élimination des Chlorures par des procédés Electrochimique

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Abstract –. Le dessalement de l'eau de mer a évolué de techniques rudimentaires pour réduire le cout et l'encrassement des procédé de distillation solaire et osmose inverse à des technologies avancées comme les procédés Electrochimique. Ce développement fait partie d'un plan national visant à sécuriser l'approvisionnement en eau d'ici 2030, en s'adaptant aux changements climatiques et en soutenant la croissance économique, et sécuriser leur approvisionnement en eau face aux défis climatiques. L'électro-chloration est une technique qui permet la production in situ d'une solution diluée d'hypochlorite de sodium à partir d'une solution de chlorure de sodium (eau de mer ou saumure). De plus, Dans un réacteur d'Electrocoagulation (EC) comportant une anode d'aluminium et une cathode, l'application d'un courant électrique produit une oxydation à l'anode et une réduction à la cathode pour former un coagulant pourra éliminer les MES. Lors de procédé d' Electro-choloration par des électrodes en Graphite pour la dégradation de la matière organique, les résultats expérimentaux ont montré que la variation de la matière organique suit deux phases :
Phase 1 : Augmentation Initiale de la Matière Organique et Libération de Matières Organiques Adsorbées avec une augmentation de la concentration de HClO
Phase 2 : Diminution de la Matière Organique
la transformation de chlore gazeux dissout partiellement dans l'eau et réagit pour former de l'acide hypochloreux (HOCl) et des ions hypochlorite (ClO^-), ce qui peut donner une coloration jaunâtre à l'eau

Keywords –Osmose inverse, Dessalement, Electrocoagulation, l'Hypochlorite de Sodium, Electrochloration

Prédiction de la Toxicité des Liquides Ionique avec une Machine à Vecteurs de Support Optimisée par l'Algorithme Ant Lion (ALO).

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Abstract –

Les liquides ioniques (LIs) sont considérés comme une alternative aux solvants organiques traditionnels, Ils ont attiré une large attention en raison de leurs propriétés physico-chimiques uniques telles que : L'ininflammabilité, une pression de vapeur extrêmement faible et point de fusion bas, une capacité de solvatation élevée et une faible volatilité.

Plusieurs études ont montré que les LIs peuvent induire des effets toxiques dans l'écosystème par conséquent, la toxicité est un facteur important qui doit être pris en compte dans la sélection des LIs.

La toxicité a été évaluée en termes de logarithme de La concentration efficace médiane (logEC50) et La structure des LIs représente par des chaînes SMILES (système d'entrée de ligne d'entrée moléculaire simplifié) obtenues auprès de PubChem.

Ce travail a examiné la capacité et la faisabilité de l'optimiseur Ant Lion (ALO) associé au modèle SVM (ALO_SVM) pour prédire la toxicité des liquides ioniques. Un ensemble de données sur la toxicité de 134 LI a été collecté dans la littérature pour élaborer et tester le modèle en utilisant les descripteurs structurels moléculaires comme entrées qui ont été calculés à l'aide de logiciel AlvaDesc, 5666 descripteurs moléculaires ont été obtenus à partir d'un algorithme génétique (GA) a été utilisé pour sélectionner uniquement les descripteurs les plus pertinents (11 descripteurs ont été sélectionnés).

L'ensemble de données a été divisé en un ensemble d'apprentissage (80%) choisi aléatoirement à l'aide de la fonction de division de MATLAB. Les 20% restants ont été utilisés comme ensemble de teste pour le modèle ALO_SVM, cette division visant à prévenir le sur-apprentissage pendant l'entraînement.

Les résultats ont montré que le modèle ALO_SVM offrait les meilleures performances en termes de capacité prédictive. Les performances obtenues étaient satisfaisantes, avec une racine de l'erreur quadratique moyenne (RMSE), un coefficient de corrélation (R) et un coefficient de détermination (R^2) pour l'apprentissage de 0,0446, 0,9967 et 0,9988, respectivement. Pour le test, les valeurs étaient : RMSE = 0,0401, R = 0,9946 et R^2 = 0,9984.

Keywords –
Liquides Ionique (LIs), Optimiseur Ant Lion (ALO) , Support Vector Machines (SVM), Prédiction de Toxicité, Descripteurs Moléculaires.

SYNTHESE, CARACTERISATION ET ETUDES STRUCTURALE ET BIOLOGIQUE DU (E)-2-((4-NITROBENZYLIDENE) AMINO) PHENOL

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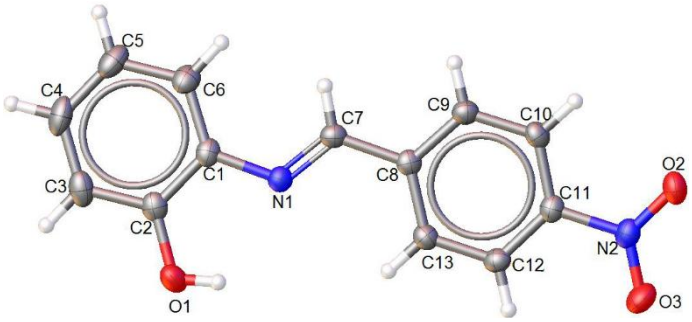
Abstract **–** Depuis leur découverte, par le chimiste allemand Hugo Schiff en 1864, les bases de Schiff présente un vaste domaine d'application que ne cesse de se développer. Les ligands bases de Schiff présentent une classe importante dans la chimie de coordination [1,2]. Ces composés ont toujours joué un rôle important dans différents domaines comme la chimie, la biologie [3,4] et la pharmacie [5,6], ce qui a poussé les scientifiques à déployer des efforts considérables pour élaborer les méthodes de synthèse les plus efficaces.

Nous rapportons ici la synthèse, les études spectrales et structurale par diffraction des rayons X sur monocristal et l'étude antibactérienne d'une nouvelle (BS) dérivés du 2-Aminophenol, à savoir, **(E)-2-((4-nıtrobenzylıdene) amıno) phenol**. La base de Schiff cristallise dans le groupe d'espace P212121. Les molécules du composé sont liées par les liaisons hydrogène O-H···O, C-H···O et O-H··· N. L'effet antibactérien a été déterminé sur trois bactéries Staphylococcus aureus, Escherichia coli et Salmonella Typhi. Les résultats mettent en évidence que la base de Schiff testé a été manifestée une bonne activité vis-à-vis les bactéries testées.



Keywords – Les bases de Schiff, FT-IR, UV-Vis, diffraction des rayons X, l'étude antibactérienne

Antibacterial evaluation and in silico studies of newly redesigned sulfamidophosphonate derivatives

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Abstract **–** Antibiotic resistance occurs when one or more antibiotics become ineffective against a bacterial infection. This condition can make it difficult, or even impossible, to treat certain infections. Pharmaceutical research is constantly seeking ways to avoid natural resistance and expand the range of antibiotics by modifying their chemical structure or inventing new molecules. The literature reports that α-sulfamidophosphonate can serve as potential medicinal molecules in drug discovery and development. They have shown several significant activities, such as antihypertensive, anti-inflammatory, anticonvulsant, antibacterial, and antifungal. All these findings suggest that α-sulfamidophosphonate provide a suitable framework for the development of effective bactericidal agents. In this study, we present the antibacterial evaluation of newly synthesized sulfamidophosphonate derivatives against eight different bacterial strains using the minimum inhibitory concentration (MIC) method. The results revealed varying degrees of inhibitory potential among the compounds. A molecular docking study was conducted to investigate the binding interactions of the most potent analogs with the active site of the target enzymes. The results revealed that all compounds exhibited high affinity for the DNA gyrase enzyme.

Keywords – sulfamidophosphonate, antibacterial activity, molecular docking, DNA gyrase enzyme, anti-inflammatory.

Removal dye by adsorption of nanocomposite

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Abstract –The synthesis of nanotubes based on an acid is an exciting area of research in nanotechnology and materials science. nanotubes are characterized by their nanometric tubular structure and their electroconductive properties, which makes them very promising for various applications. . The main reagents are, an acid, monomer and an oxidizing agent, such as sulfuric acid (H2SO4) or a doping salt such as ammonium persulfate. We characterized the nanotubes using various techniques, including scanning electron microscopy (SEM), infrared spectroscopy (IR), X-ray action. The objective of this study is to determine the adsorbent power, to eliminate a cationic dye methylene blue in an aqueous medium.

The thermodynamics and the kinetics of adsorption on pany-nanotube of methylene blue in aqueous solution were investigated. A high adsorptive capacity was observed: about 36 mg/g. A series of contact-time experiments were undertaken in stirred batch adsorber to assess the effect of the system variables such as the mass of pani-nanotube, the temperature, the initial concentration of dye , the pH of the solution and the degree of stirring. The results for these contact-time experiments were discussed and showed that the pani-nanotube can be used as adsorbent in wastewater treatment.

Keywords – polyaniline,adsorption,blue methylene, nanocomposites,polymercomposites.

Numerical study of mixed convection in a porous medium with first-order chemical reaction: impact of permeability

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Abstract **–** This study focuses on the numerical analysis of mixed convection in a saturated porous medium, in the presence of a first-order chemical reaction, with a particular emphasis on the impact of the medium's permeability. The physical system considered corresponds to a two-dimensional and steady flow of a fluid along a vertical flat plate immersed in a porous medium. The model is based on the Darcy equations, combined with a mixed convection regime formulation, incorporating the effects of thermal buoyancy and concentration. The chemical reaction is modeled by a source term in the mass conservation equation. To simplify the problem, similarity variables are introduced, reducing the system of equations to nonlinear ordinary differential equations. These equations are solved using a numerical method based on finite differences. The numerical results show that the chemical reaction accelerates the drop in concentration near the wall, while permeability significantly influences the velocity and temperature profiles. In particular, high permeability promotes fluid penetration, thereby altering the thermal and mass transfer profiles. These results are relevant for applications in geothermal energy, catalysis, and reactive environments, and pave the way for studies on the Soret effect, the extension to three-dimensional flows, and the introduction of non-homogeneous media.

In conclusion, this modeling provides a better understanding of the thermo-hydrodynamic and chemical behavior in reactive porous media, and allows for anticipating the role of physical parameters on coupled transfers. Natural extensions would include the study of the Soret effect, the consideration of heterogeneous media, or the integration of more complex reactions in a transient or three-dimensional context.

Keywords – Mixed convection , Porous medium , First-order chemical reaction , Permeability , Boundary layer

Adsorption du chrome par les écorces de Grenade pour la protection de l'environnement

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Ce travail a pour objectif, la valorisation d'un résidu naturel l'écorce de grenade et son application dans l'élimination par adsorption du chrome hexavalent. Ce biomatériau entredans la gamme de produits abondants et bons marché.

L'adsorbant utilisé possède des caractéristiques physico-chimiques et une porosité qui favorisent l'adsorption. La poudre d'écorce de Grenade (PEG) analysée s'avère amorphe, avec une stabilité relativement élevée, contient des groupes fonctionnels hydroxyle et carboxyle, un pH de charge nulle de 3,9 et une surface spécifique de 40,38 m^2/g. Les résultats expérimentaux en mode batch ont montré que le biosorbant, (PEG) présente une excellente efficacité maximale d'élimination du Cr (VI) atteignant 50,32 mg/g, tandisque le processus d'adsorption obéit au modèle de Freundlich. L'étude thermodynamique a montré que l'adsorption est physique et le processus d'adsorption est exothermique et spontané.

Grâce aux résultats analytiques des spectres EDX et FTIR, ainsi qu'aux données obtenues à partir de la modélisation des isothermes d'équilibre et de la cinétique, un mécanisme lié à l'adsorption de Cr (VI) sur la poudre d'écorce de grenade (PEG) est donné. Il est à noter que le processus est principalement contrôlé par l'interaction électrostatique entre les groupes fonctionnels chargés négativement présents à la surface des particules de la poudre d'écorce de Grenade (PEG) et les ions métalliques Cr(VI) chargés positivement. Pendant ce temps, l'adsorption de surface par diffusion vers les pores de PEG améliore le transfert de masse et fournit une voie d'adsorption en plus d'une zone responsable de la réduction des ions métalliques Cr(VI) en Cr(III) moins toxique.

Mots-clés : Bio-adsorbant ; Adsorption ; Crome VI ; Cinétique ; Modélisation.

Polyacrylamide hydrogel and β-cyclodextrin Supported Keggin 12-Phosphotungstic Acid: Novel Hybrid Catalytic Materials

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Abstract

Catalytic hybrid materials based on phosphotungstic acid ($H_3PW_{12}O_{40}$) are attracting increasing interest due to their remarkable acid-base and redox properties. In this study, polyacrylamide hydrogel and β-cyclodextrin are utilized as supports to immobilize phosphotungstic acid and optimize its catalytic efficiency. The immobilization of this heteropolyacid on polymeric matrices enhances its recyclability and stability while preserving its activity.

These novel hybrid materials offer considerable promise for a variety of catalytic applications, particularly in the context of esterification reactions.The present study investigates the use of new catalytic matrices for the methanolysis of oleic acid to methyl oleate. The investigation employs clean and efficient catalysts and particularly recycling catalysts based on 12-phosphotungstic heteropoly acid, using a fatty acid to methanol ratio of 1:9 and at a reaction temperature of 60°C for 3 hours.

Herein, Different hybrid organic inorganic materials based on phosphotungstic acid catalyst (HPW) supported on polyacrylamide hydrogel (PAAm) and β-cyclodextrin were prepared by different methods to develop heterogeneous catalysts systems. The swelling behavior of PAAm material was studied in distilled water at 25°C.The catalytic systems were characterized by FTIR, Raman spectroscopie and SEM analyses, the fatty acid methyl esters reaction products, were analyzed and quantified by gas chromatography GC.

Keywords – heteropolyacid, polyacrylamide, Hydrogel, cyclodextrin, esterification.

Development of Zeolite-Hydroxyapatite Nanocomposites via Sol-Gel Route for Environmental Remediation

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Abstract **–** Zeolite/hydroxyapatite nanocomposites—particularly zeolite/inorganic nanocomposites—possess unique and significant physicochemical properties, making them promising candidates for a wide range of applications. In this study, nanocomposites of zeolite/polymer and hydroxyapatite-based zeolite/polymer were synthesized using the sol-gel method. The primary objective of this work is to explore the potential of these composite materials for the removal of pollutants. The hydroxyapatite powder used in this research was of biological origin, extracted from bovine bones, while the zeolite was synthesized via the sol-gel process. The resulting samples were characterized using Fourier-transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), and energy-dispersive X-ray spectroscopy (EDX).

Keywords – Zeolite, Hydroxyapatite, nanocomposite, pollutants, sol-gel.

Physicochemical Characterization of Modified Bentonite for Pollutant Removal in Water Treatment

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Abstract **–** This study focuses on the modification of a natural clay material. Characterization results revealed that it possesses a well-developed porous structure, making it a promising candidate for the treatment of wastewater from the textile industry. This potential was demonstrated through its application in the removal of dyes such as Congo Red and Methylene Blue. The main objective of this work is, first, to enhance the surface properties of bentonite through various modification treatments, and subsequently to evaluate its effectiveness in removing organic pollutants using the adsorption technique, due to its high adsorption capacity.

Keywords – modification, natural clay, porous, removal, adsorption capacity.

L'utilisation d'acides gras dans la résolution cinétique enzymatique du 1-phénylpropan-2-ol

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Abstract – La résolution cinétique enzymatique des alcools secondaires utilisant des acides carboxyliques non chiraux comme donneurs d'acyles verts reste limitée malgré leurs avantages à l'échelle de la chimie verte, principalement: biotransformation en déchets libres (le seul déchet est l'eau), catalyseur recyclable et biodégradable. De plus, la résolution cinétique enzymatique des acides carboxyliques chiraux ont été rarement décrit.

Nous avons examiné la résolution cinétique enzymatique du 1-phénylpropan-2-ol 2 via une estérification utilisant les acides butyrique et laurique comme acides gras courts en présence de sulfate de magnésium (MgSO4) comme contrôle de la teneur en eau.

En utilisant le 1-phénylpropan-2-ol (RS)- comme un accepteur d'acyle, où le centre asymétrique est éloigné du cycle aromatique, et en présence de MgSO4. La PPL et la PCL n'ont pas pu catalyser cette biotransformation. La CRL était réactif avec les acides butyrique et laurique dans l'heptane.
L'utilisation du CAL-B comme biocatalyseur a donné les deux esters gras correspondants avec des énantiopurités élevées à Conv = 51% (E>200) dans les deux solvants organiques. L'utilisation de TBME a diminué les taux d'estérification

Keywords –Include at least 5 keywords or phrases

Etude de L'adsorption des Polluants Organiques par des Copolymères à base de Polychlorure de Vinyle : Applications dans le Traitement des Eaux

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Résumé

La contamination des eaux de surface et des eaux souterraines par des composés toxiques et dangereux tels que les produits pharmaceutiques, les métaux lourds, les colorants et les pesticides, a suscité une attention croissante au cours des dernières décennies dans le monde entier. Face à ce problème environnemental critique, ce travail se concentre sur la synthèse et l'application de copolymères fonctionnalisés à base de polychlorure de vinyle (PVC) pour l'élimination de polluants organiques dans l'eau par adsorption.

Le premier matériau a été obtenu en modifiant les chaînes du copolymère polyméthacrylate de glycidyle greffé sur du polychlorure de vinyle (PGMA-g-PVC) avec de l'hexaméthylènediamine (HDA), ce qui a conduit à la formation d'une résine polymérique PGMA-g-PVC/HDA avec des fonctions amines aux extrémités des chaînes. Le copolymère ainsi modifié, PGMA-g-PVC/HDA, a été utilisé pour l'élimination du résorcinol de l'eau par adsorption.

Parallèlement, des macrosphères de PGMA-g-PVC ont été développées comme support réactif pour une modification de surface avec de l'hydrazine, suivie d'une quatérnisation des amines greffées, permettant la formation de chaînes polymériques chargées positivement (polycations) à la surface du matériau. Le copolymère modifié PGMA-g-PVC/HYD^+ ainsi obtenu a été évalué pour son efficacité à éliminer le colorant noir Eriochrome T (NET) de l'eau par adsorption.

Mots-clés : PVC ; PGMA-g-PVC ; copolymères ; traitement des eaux ; adsorption.

Theoretical QSRR Modeling of Xenobiotics in Gas Chromatography–Mass Spectrometry

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Abstract **–** The Quantitative Structure–Retention Relationship (QSRR) analysis provides a powerful framework for correlating molecular structure with chromatographic behavior. This study focuses on predicting the retention times (RT) of a diverse set of xenobiotic compounds analyzed by capillary gas chromatography coupled with mass spectrometry (CG-MS), using theoretical molecular descriptors. Molecular geometries were first optimized using the semiempirical PM7 method, followed by the calculation of a diverse set of theoritical molecular descriptors. A multiple linear regression (MLR) model was built after selecting the most relevant descriptors using a genetic algorithm- variable subset selection (GA- VSS) procedure. The final model includes five descriptors: DBI, R8i, TPSA*efficiency*, *Hy*, *and SM1*B(p). Based on cross-validation, internal validation of the model showed all statistical parameters R^2 = 0.88, Q^2_{LOO} *= 0.877, s = 0.11, and* $RMSE_{tr}$ = 0.11 giving proof of excellent fit and robustness. The model proved its prediction power in external validation, with Q^2_{F1} = 0.812, Q^2_{F2}=0.810, Q^2_{F3} = 0.837, CCC_{ext}=0.89, $RMSE_{ext}$ = 0.138. These results demonstrate that combining PM7-optimized geometries and descriptor selection using GA-VSS produces a QSRR model with high predictive accuracy. This model enhances the ability to predict CG-MS retention for diverse xenobiotic structures and shows further application of theoretical molecular descriptors in modeling chromatographic behavior.

Keywords – QSRR; MLR; CG-MS; Molecular descriptors; PM7

Influence of Data Splitting in QSPR Studies: The Aqueous Solubility Case

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Abstract – Quantitative Structure Activity Relationships (QSAR), allow the generation of useful models or equations for the prediction of toxicity, property or retention. QSAR studies have been performed for different homologous series, including alcohols, environmental toxics, and mixtures of hydrocarbon compounds. These studies have shown how molecular structure can influence an endpoint of interest [1]. In the OECD Principles for QSAR Validation for a regulatory purpose, the 4th principle (must be fulfilled like the other 4) is: appropriate measures of goodness-of-fit, robustness and predictivity [2];

Every quantitative structure– property relationship model utility depends on its predictivity (i.e. the ability to accurately predict property for chemical compounds that have not been included in the model's development procedure). Data splitting is based on the division of the input data into a training set and a test set [3]. The model is developed using only the training set, while its predictive power is assessed on the test set compounds using different metrics. The latter procedure is called 'external validation'. Properly trained and validated models are capable to reliably predict novel compounds [3].

The aim of this study was to investigate how the of data splitting methods into training and test sets influence the external predictivity of a quantitative structure– property relationship (QSPR) models. We used different approaches to split a dataset of 71 chemicals from a QSPR model for aqueous solubility of sulfur-containing aromatic esters [4]. 20 compounds where selected for the test set by a time-based, Y-based, random splits [5] and two algorithms CADEX and DUPLEX [6]. Focusing on the models' statistics, we can say that the CADEX algorithm splitting is recommended for a reduced dataset with highly similar compounds.

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Keywords – QSAR/QSPR, External validation, Data splitting, CADEX algorithm, Sulfur-containing aromatic esters

Efficacy of CuO/BaO nanocomposite in Purification of Petroleum Wastewater

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Abstract – In this research, the effectiveness of "Inductive Coupled Plasma Mass Spectrometry" (ICP-MS) based on the removal of heavy metals and contaminates from petroleum refinery wastewater using copper oxide/barium oxide nanocomposites (CuO/BaO NPs) was assessed. The NPs were aimed to remove As, Be, Cd, Cr, Mn, Mo, Ni, Pb, Sb, Se, Zn before and after treatment.

The removal efficiencies for Be, Cr, Mo, and Sb exceeded 99% while complete removal (100%) was accomplished through a process of synergistic chemisorption and redox interactions. Ni and Zn were removed moderately at 66.25±0.8% and 59.0±1.2%, cadmium (3.05±0.3%) and selenium (45.21±0.9%) did not fare as well due to competitive ligand complexation in the hydrocarbon rich environment.

The results underscore the promise of transition metal/alkaline earth nanocomposites in sustainable water treatment, although surface modification to increase Cd and Se adsorption is advisable. The work contributes important design criteria for the emerging class of nanocomposite adsorbents.

Keywords – green synthesis, nanocomposites, removal of heavy metals, wastewater treatment, Inductive Coupled Plasma Mass Spectrometry" (ICP-MS).

Characterization of PHBV/PLA Blend: Impact of Compatibilization and Surface Treatments of Diss Fibers

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Abstract **–** Polymers produced from renewable resources, known as poly (3-hydroxybutyrate-co-3-hydroxyvalerate) (PHBV) and Polylactide (PLA). Because of their diverse properties, PHBV and PLA are prime candidates for a number of uses in the biomedical, food and other sectors. However, these biopolymers have a number of important limitations that prevent them from being used on a large scale, notably their fragility and high cost. For these biopolymers to be fully competitive with ordinary polymers, it seems necessary to improve these properties. Scientists have recently focused on blends of two or more polymers and/or the incorporation of natural fibers because of their low cost, low density and renewable, biodegradable qualities. Sustainable development, which allows the use of local resources, justifies the use of Diss fibers to reinforce composite structures. A Diss fiber has already been used in the construction of old houses because of its good mechanical properties. Biocomposites based on a PHBV/PLA blend and Diss fibers are promising materials, combining high performance with possible degradation at the end of their life. In this work, different series of biocomposites based on PHBV/PLA blend and Diss fibers (treated and untreated fibers) with and without PHBV-*g*-MA compatibilising agent (5 wt. %) were prepared by melt blending. The surface of the fibers was modified using alkaline treatment to improve interfacial adhesion between the fiber and the matrix. The thermal stability, water absorption capacity and mechanical behaviour of the biocomposites obtained were studied, and the results were compared with unmodified biocomposites and the pure blend.

Keywords – PHBV, PLA, blends, Biocomposites, Diss fibers.

Fibers Physical and Chemical Properties of Natural Fibers Extracted from Ampelodesmos Mauritanicus (Diss)

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Abstract – In recent years, the revalorization of natural lignocellulosic material has encouraged and aroused the interest of academic research to consider this material as a valid alternative to the uncontrolled use of petroleum-based materials in industrial applications. In this context, the revalorization of agro and forestry wastes is considered a significant strategy to reduce the environmental impact, since their use could be fundamental for the realization of new green products. The industrialization process has induced economic benefits but, at the same time, has highlighted some serious aspects that negatively affect the environment on a large scale, namely the use of traditional materials, such as polymer-based products, is certainly involved in this process. Ampelodesmos mauritanicus (Diss) is a large herbaceous plant native to North Africa and Southern Europe and the dry regions of Greece and Spain, which belongs to the family Poaceae. The Diss plant has shown interesting mechanical and thermal properties, favoring its use for the production of traditional building materials in North Africa and handicraft baskets. These fibers have also been used and widely studied for their interesting antiparasitic properties, which in fact represent a traditional use of this plant. The objective of this research activity was based on the revalorization of Diss, an African herb widely present on the Algerian territory. The stems of Diss were selected as native botanical material for cellulose extraction. Thermogravimetric analysis (TGA), Fourier transform infrared spectroscopy (FTIR) and X-ray diffraction (XRD) were used to characterize the raw material and the cellulose extracted from the chemically treated stems.

Keywords – Ampelodesmos mauritanicus, chemical treatment, thermal properties.

Développement d'une crème cosmétique à base d'extrait d'amande douce et de glycerol: étude de formulation, propriétés antioxydantes et comportement rhéologique

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Abstract **–** Cette recherche s'inscrit dans le cadre du développement d'une crème hydratante d'origine naturelle, enrichie en extrait d'amande douce, avec pour objectif de proposer une alternative cosmétique efficace et respectueuse de l'équilibre cutané. La formulation a été pensée pour limiter l'usage de composés synthétiques, en privilégiant des ingrédients naturels, biocompatibles et respectueux du microbiote de la peau.

L'extrait d'amande douce a été obtenu à partir des fruits, puis analysé. Son potentiel antioxydant a été évalué à l'aide d'un test au peroxyde d'hydrogène (H_2O_2), tandis que la chromatographie liquide à haute performance (HPLC) a permis d'identifier plusieurs composés bioactifs majeurs, dont l'acide gallique (20,8 %), la quercétine (2,9 %), la rutine (0,2 %) et l'acide caféique (0,1 %).

Par ailleurs, l'extrait a démontré une activité antimicrobienne à large spectre, en particulier contre des bactéries Gram-positives (Staphylococcus aureus, Bacillus subtilis), Gram-négatives (Escherichia coli, Pseudomonas aeruginosa, Klebsiella pneumoniae), des levures (Candida albicans), ainsi que des champignons filamenteux (Aspergillus spp., Fusarium graminearum). Les concentrations minimales inhibitrices (CMI) se sont révélées faibles, notamment pour E. coli (1,6 mg/mL) et Fusarium graminearum (1,8 mg/mL).

L'ajout de glycérine dans certaines formulations a permis d'améliorer la texture du produit grâce à ses propriétés hygroscopiques et structurantes, tout en renforçant l'activité antimicrobienne, notamment vis-à-vis de souches résistantes comme P. aeruginosa.

L'étude rhéologique a révélé un comportement pseudoplastique pour l'ensemble des formulations, assurant une application agréable sur la peau. Un nouveau modèle de modélisation rhéologique a permis d'obtenir une meilleure corrélation (R^2) et des paramètres plus pertinents que ceux obtenus avec les modèles classiques, en particulier à faibles vitesses de cisaillement.

Enfin, des tests d'irritation cutanée réalisés in vivo sur dix volontaires sains n'ont mis en évidence aucune réaction indésirable, confirmant la bonne tolérance dermatologique de la crème.

Ces résultats mettent en avant le potentiel d'une formulation à base d'extrait d'amande douce et de glycérine comme cosmétique naturel aux propriétés antioxydantes, antimicrobiennes et hydratantes, soutenu par des données physico-chimiques et biologiques solides.

Keywords – amande douce, stress oxydatif, émulsions, rhéologie, glycérine

Phytochemical and in vitro antioxidant activity of the aqueous extract of Echium boraginaceae family

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Abstract –

Reactive oxygen species (ROS) and reactive nitrogen species (RNS) play an essential physiological role, but can cause oxidative stress when overproduced, leading to cellular alterations. Natural extracts from plants contain a variety of molecules that are biologically active in several biological activities, and natural antioxidants are receiving widespread attention due to their preventive effects. Echium sp. is a medicinal plant of the Boraginaceae family known for its bioactive substances. This study aimed to evaluate the phytochemical composition and antioxidant activity of the aqueous extract of Echium sp. This extract was obtained by decoction, and its total polyphenol content was measured using the Folin-Ciocalteu reagent method. The Lipid peroxidation method (thiocyanate technique) was used to estimate the antioxidant activity. The total polyphenol content was 90.78 ± 0.7 µg QE/mg E in dry weight expressed as gallic acid equivalents (GAE). aqueous extract showed moderate antioxidant activities with the lipid peroxidation method. Our results showed that the tested aqueous extract could be a promising natural antioxidant source.

Keywords – Echium sp.; polyphenol; aqueous extract; lipid peroxidation method.

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Influence of Deposition Time on the Electrochemical Growth of a Zinc Film on Graphite

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Abstract **–** Zinc is a metal widely used in electrochemistry, particularly for its anticorrosion properties, conductivity, and its role in energy storage devices. Its electrochemical deposition allows the preparation of thin metallic films, which are used in various technological fields. Chronoamperometry, a technique that monitors the evolution of current as a function of time after the application of a potential step, is particularly suitable for studying the growth of such films under controlled conditions. In this work, a metallic zinc film was prepared on a graphite electrode by potentiostatic deposition, starting from a potential chosen based on the cyclic voltammogram, where the reduction peak of Zn^{2+} ions appears at -1.58 V. The current decreases sharply in the first few seconds, indicating the rapid nucleation of zinc clusters on the graphite surface. After 25 seconds, the current stabilizes around -3.6 mA, suggesting that the diffusion of Zn^{2+} ions in the solution becomes the limiting step in film growth. To quantify the consumed charge, the deposited zinc mass, and the film thickness, deposits were made for 1, 2, 3, 4, and 5 minutes under identical conditions. The results show a proportionality between the film thickness and the treatment time, confirming a steady growth of the metallic film. This study highlights the effectiveness of potentiostatic control in the formation of thin zinc films.

Keywords – Zinc, Electrochemical deposition, Anticorrosion, Chronoamperometry, Metallic film.

Synthèse et caractérisation d'un bio-adsorbant et leur utilisation pour la rétention d'un polluant organique en lit fixe

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Résumé

Les éléments polluants qui sont introduits de manière importante dans l'environnement sont de nature organique tel que les colorants textiles et inorganique comme les métaux lourds. L'objectif de ce travail est d'éliminer un colorant cationique d'une solution synthétique en utilisant un bio-adsorbant à lit fixe. Ce matériau a été préalablement caractérisé au moyen de quelques techniques physico-chimiques et spectroscopiques tel que : la FTIR, MEB et le potentiel zêta. Ceci nous a permis d'établir une série de données avec les différentes propriétés de ce matériau. La cinétique en équilibre adsorbat/ adsorbant est une étape indispensable pour déterminer les isothermes d'adsorption. Une série des expériences a été étudiée en variant la hauteur du lit (0,5-1cm), le débit (2-4 ml. Min-1) et la concentration initiale du colorant (10-30 mg. L-1). Les résultats obtenus montrent que le temps de percé des courbes diminue avec l'augmentation du débit et de la concentration initiale, mais augmente avec l'augmentation de la hauteur du lit. Les modèles de Thomas et Yoon-Nelson ont permis une bonne prédiction des courbes de percée expérimentales.

Mots-clés : Bio-adsorbant ; Adsorption; Courbe de percé; Cinétique; Colorant.

Synthesis and characterization of ZnO doped regenerated activated carbon for water splitting applications

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Abstract – By incorporating regenerated activated carbon and Zinc oxide (ZnO) nanoparticles (Nps) to form a series of ZnO-RAC nanocomposites with a different weight ratio between ZnO nanoparticles and RAC particles. As part of the evaluation of the properties of the synthesized nanocomposites, FTIR, XRD, and SEM spectroscopy techniques were applied. In addition, the performance of the ZnO-RAC nanocomposite was evaluated in the water splitting (WS) process. As a result of the experiments, it was found that the ZnO-RAC nanocomposite was capable to split water into hydrogen and oxygen with excellent performance. The efficiency of the WS process over ZnO-RAC photocatalysts was greatly affected by the weight ratio between ZnO and regenerated activated carbon particles. In spite of the advantages offered by AC by increasing surface area, improving air quality, and charge separation, the maximum number of active sites are maintained while still maintaining sufficient ZnO content for effective photocatalytic activity. Therefore, ZnO and regenerated activated carbon have a synergistic effect that leads to the highest hydrogen production in water splitting. According to the results of this study, 3/5 was determined as the optimal ratio between ZnO and regenerated activated carbon.

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Keywords – regenerated activated carbon, ZnO-RAC nanocomposite, photcatalytic activity, weight ratio, hydrogen productivity

Evaluation of the in vitro toxicity of two different extracts from the bark of *Punica granatum* fruit: comparative study

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Abstract – *Punica granatum L.* belongs to the Lythraceae family and is commonly known as pomegranate and locally as Roman. Since ancient times, people have utilized pomegranate peel, seeds, fruit, and roots for their numerous medicinal benefits. They specifically aid in the treatment of severe intestinal and digestive conditions, parasite infections, and anemia prevention. Numerous studies have examined its phytochemical capabilities, demonstrating its anti-inflammatory, anti-diabetic, and antioxidant qualities. The aim of this study was to determine the flavonoid content of two different extracts (hydro-acetone and hydro-methanol) and to assess their toxicity in vitro. Therefore, the fruit peels of the plant were dried and ground to powder and brought into contact with aqueous acetone or aqueous methanol solvent and left to macerate for 24 hours. The flavonoid content was measured using the colorimetric technique and the toxicity of the extract was assessed using a haemolytic test on red blood cells, according to the method described by Shobana and Vidhya in 2016. As results, tests showed that the hydro-acetone and hydro-methanol extracts had low flavonoid concentrations. Toxicity analysis showed that haemolysis of human erythrocytes did not exceed 15% even after application of different concentrations of the two extracts. This research led us to determine that extracts of *Punica granatum L.* fruit bark have very low toxicity. Consequently, the in vitro and in vivo pharmacological potential of *Punica granatum* can be safely assessed.

Keywords – Punica granatum; Phytochemical properties; Total flavonoids; Haemolytic effect; Toxicity assay.

Prédiction de la pollution organique biodégradable dans les eaux usées à l'aide de modèles hybrides en intelligence artificielle

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Abstract **–** La Demande Biologique en Oxygène à 5 jours (DBO_5) constitue un indicateur essentiel de la pollution organique biodégradable dans les eaux usées, et joue un rôle clé dans la surveillance et la gestion des systèmes de traitement. Cette étude propose une approche de modélisation prédictive de la DBO_5 à partir de quatre variables environnementales couramment mesurées : la température, le pH, les matières en suspension, et le volume d'eau traité. Le modèle principal utilisé est le Extreme Learning Machine (ELM), un réseau de neurones à apprentissage rapide particulièrement adapté aux jeux de données environnementaux non linéaires. Pour améliorer la précision et la capacité de généralisation du modèle, deux versions hybrides ont été développées : ELM-DE, optimisé par l'algorithme d'évolution différentielle (Differential Evolution), et ELM-GA, optimisé par l'algorithme génétique (Genetic Algorithm). Les résultats expérimentaux ont montré que les versions hybrides surpassent le modèle ELM standard, avec une réduction significative des erreurs de prédiction (RMSE, MAE) et une amélioration des coefficients de performance (R^2, NSE). Parmi les deux approches hybrides, ELM-DE s'est révélé le plus performant, grâce à une exploration plus efficace de l'espace des hyperparamètres. Cette étude met en lumière l'intérêt des modèles hybrides en intelligence artificielle pour la chimie de l'environnement, en offrant des outils fiables, rapides et adaptatifs pour la prévision de la DBO_5 et la gestion optimale des procédés de traitement des eaux usées.

Mots-clés :DBO_5, ELM, Differential Evolution, Genetic Algorithm, Modélisation hybride, Chimie environnementale, Traitement des eaux usées

Biological Activities of Borgenaceae Plant Extracts from Oued Souf Region

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Abstract **–** The Boraginaceae family includes numerous plant species recognized for their pharmacological properties. This study focuses on evaluating the biological activities of plant extracts derived from Boraginaceae species naturally found in the arid environment of the Oued Souf region in Algeria.

Using a liquid-liquid extraction method, hydroalcoholic extracts and their fractions (n-hexane, ethyl acetate, butanol, and aqueous extracts) were prepared. The total phenolic content (TPC) was measured, while antioxidant and antibacterial activities were tested using the DPPH assay, TAC method, and agar diffusion technique. Furthermore, cytotoxicity was examined with a yeast cell model.

The results revealed that the plant is rich in phenolic compounds, with a total phenolic content of 21.26 mg GA/g extract. Among the fractions, the ethyl acetate extract displayed the strongest DPPH free radical scavenging activity, with an IC_{50} of 0.64 mg/mL. All extracts showed moderate to low inhibition of bacterial growth. Toxicity assessments demonstrated that the ethanolic extract is non-toxic to living cells at concentrations below 40 mg/mL.

Keywords – Biological Activities, Boraginaceae, Oued Souf Region.

Anti-oxidant activity of pomegranate peel extract

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Abstract – Pomegranate peels demonstrate anti-oxidant activity that can be used in the treatment of different pathologies and enhancement of the skin lightening and elasticity. The extract of pomegranate peel was tested for antioxidant activity using the DPPH radical scavenging assay. Determination of antioxidant activity by the DPPH radical was carried out according to the method described by Blois (1958), using ascorbic acid as a positive control. The results showed that the pomegranate peel extract presents an IC50 of 10.28µg/mL, which considered to be excellent compared with ascorbic acid (IC50=17.09µg/mL). It can be concluded that pomegranate peel extract has interesting anti-oxidant activity.

Keywords – Antioxidant, DPPH, pomegranate peel extract, skin

Biosynthèse des nanoparticules d'argent : une approche durable et antimicrobienne prometteuse

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Abstract – Le processus de biosynthèse des nanoparticules est reconnu pour sa durabilité, son respect de l'environnement, son absence de toxines et sa biocompatibilité. Ce processus repose sur l'utilisation de micro-organismes tels que les bactéries et les levures, qui agissent comme agents réducteurs et stabilisants. Dans cette étude, des bactéries pathogènes comme *Escherichia coli* ***ATCC25922*** et *Bacillus subtilis ATCC 6633* , ainsi que la levure *Saccharomyces cerevisiae* , ont été employées pour synthétiser des nanoparticules d'argent. Ces nanoparticules ont été caractérisées à l'aide de diverses techniques physico-chimiques, notamment la spectroscopie infrarouge à transformée de Fourier en mode ATR (ATR-FTIR), la spectroscopie UV-visible, et le microscope électronique à balayage (MEB). Leur activité antimicrobienne a également été évaluée in vitro par la méthode de diffusion en puits sur milieu solide.
Les résultats ont démontré que les nanoparticules d'argent synthétisées possèdent une efficacité bactéricide remarquable contre quatre souches bactériennes testées : *Escherichia coli ATCC25922* , *Salmonella enterica ATCC6017* , *Staphylococcus aureus ATTC43300* et *Pseudomonas aeruginosa ATCC9027*. Les données obtenues au cours de cette recherche mettent en évidence le potentiel significatif des nanoparticules d'argent dans les applications biologiques explorées. Par conséquent, les bactéries et levures se sont révélées être des agents efficaces pour la production de ces nanoparticules, avec une efficacité biologique qui ouvre la voie à leur incorporation dans des formulations destinées aux secteurs alimentaire, biomédical et pharmaceutique.

Keywords – Biosynthèse, Nanoparticules d'argent, Antimicrobien, Durabilité, Biocompatibilité.

Optimisation of extraction processes for essential oils from Algerian aromatic plants

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Abstract

Algeria has an extremely rich and varied flora of aromatic and medicinal plants, most of which exist in their natural state. For thousands of years, mankind has used various plants found in its environment to treat and cure all kinds of illnesses. These plants represent an immense source of potential bioactive compounds attributed to metabolites.

Currently, aromatic plants have a considerable advantage thanks to the gradual discovery of applications for their essential oils in healthcare, as well as their use in other areas of industrial interest, such as pharmaceuticals, cosmetics, and the food industry. Their many uses mean that they are increasingly in demand on world markets for their medicinal properties, to control their quality, and detect any specificity to add value.

Today, essential oils represent one of the most important active ingredients due to their therapeutic potential and constituents. Traditional extraction techniques such as hydrodistillation are widely used, but have their limitations in terms of efficiency and energy consumption.

In the context of optimising essential oil extraction processes, current research is focusing on improving conventional extraction processes to increase yields while preserving the quality of the oils obtained, and developing innovative methods such as microwave-assisted extraction, supercritical fluid extraction (in particular with CO_2), and ultrasound-assisted extraction.

Keywords: Aromatic plants, Essential oils, Hydrodistillation, Extraction, Clevenger, Volatile compounds.

Electrochemical Study of the Corrosion Behavior of Mild Steel and TA6V4 Alloy in Sodium Chloride Solution: Potential & Current Evolution

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Abstract **–** This study investigates the electrochemical corrosion behavior of two metallic materials, Mild steel and the TA6VA alloy, in a 35% sodium chloride (NaCl) solution at a controlled temperature of 37°C. Using electrochemical techniques, we traced the potential-time curves (E=f(T)) and current-potential curves (I=f(E)) to understand the corrosion dynamics of both materials. The corrosion process was studied through open-circuit potential (OCP) measurements and Tafel polarization curves. The results show that the corrosion potential of steel becomes increasingly negative, indicating intense corrosion and a lack of passivation, while the TA6V4 alloy exhibits an increase in corrosion potential, stabilizing over time due to the formation of a protective passive layer. The current of corrosion for steel was found to be higher than that of the TA6V4 alloy, indicating greater reactivity. These findings underline the importance of passivation in preventing corrosion, and the impact of chloride ions in disrupting passive layers. The study demonstrates that electrochemical techniques, including potentiometry and polarization measurements, are crucial in analyzing corrosion mechanisms and providing valuable insights for material selection in corrosive environments.

Keywords – Electrochemical corrosion, Mild Steel, TA6VA alloy,OCP, Tafel polarization, Corrosion current, Passivation, Potentiostat,Corrosion resistance.

Prédiction avancée de la DCO dans les eaux usées à l'aide des algorithmes CatBoost, Random Forest et AdaBoost

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Abstract – L'augmentation continue de la charge polluante dans les eaux usées représente un défi majeur pour les stations d'épuration, nécessitant des outils prédictifs efficaces pour anticiper les variations et optimiser les procédés de traitement. Cette étude vise à estimer la Demande Chimique en Oxygène (DCO), indicateur essentiel de la pollution organique, à partir de variables mesurées en continu telles que la température, le volume, le pH, la DBO_5 (Demande Biologique en Oxygène à 5 jours) et les matières en suspension.

Trois modèles d'apprentissage automatique supervisé ont été développés et comparés : CatBoost, Random Forest Regressor (RFR) et AdaBoost. Ces algorithmes ont été choisis pour leur aptitude à capturer des relations complexes et non linéaires entre les variables, ainsi que pour leur robustesse face aux données bruitées fréquemment rencontrées en environnement réel.

Les résultats expérimentaux montrent que le modèle CatBoost offre la meilleure précision prédictive, avec une réduction significative des erreurs (RMSE, MAE) et des coefficients de corrélation élevés (R, NSE). Le RFR obtient également de bons résultats, tandis qu'AdaBoost, bien qu'efficace, présente une légère instabilité sur certaines séries temporelles.

Cette recherche met en lumière l'apport des techniques d'intelligence artificielle dans le domaine de la chimie environnementale, en particulier pour la prévision de la DCO. Elle ouvre des perspectives prometteuses pour une gestion plus intelligente, proactive et durable des systèmes de traitement des eaux usées.

Keywords – Demande Chimique en Oxygène, Machine Learning, CatBoost, Random Forest, AdaBoost, Traitement des eaux usées, Chimie environnementale

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Pharmacokinetics-Based Molecular Docking Investigation of 3G75 Target Ligands

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Abstract – This work include several advanced molecular docking tools to study the interactions of our newly synthesized 1,3,4-thiadiazole derivatives in the active site of penicillin binding protein and DNA gyrase against Staphylococcus aureus, the enzymes targeted for antimicrobial agents. Results such as MolDock scores, binding energies, residue binding distances, etc. were identified and discussed in this present research. The molecules with best docking results were selected in order to calculate drug likenessand bioavailability using Molinspiration software. All the compounds obey Lipinski's rule and its extension and showed drug likeness. The pharmacokinetic parameters study was done using the AdmetSAR to display ADME and toxicity properties of these antimicrobial.

Keywords – 1, 3, 4-thiadiazol ; Antimicrobial ;Molecular docking ;Staphylococcus aureus

Swelling Behavior of Semi-Interpenetrating Sodium Alginate/Poly(acrylamide-co-acrylic acid) Hydrogels in Aqueous and Metal-Laden Environments

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Abstract : Water pollution by heavy metals poses serious threats to ecosystems and human health, driving demand for effective remediation materials. This study investigates sodium alginate/poly(acrylamide-co-acrylic acid) semi-interpenetrating hydrogels as potential solutions for water treatment. The hydrogels combine natural alginate's biocompatibility with synthetic polymers' robustness through a unique semi-IPN structure.

The materials exhibited pH-dependent swelling behavior, absorbing significantly more water at neutral pH than acidic conditions. Incorporation of alginate enhanced both swelling capacity and structural stability. When tested against common water contaminants (Pb^{2+} , Cd^{2+} , Cr^{3+}), the hydrogels demonstrated notable adsorption capabilities, particularly for chromium ions. study investigates the pH-responsive swelling behavior and heavy metal adsorption capacity of semi-interpenetrating network (semi-IPN) hydrogels composed of sodium alginate (Alg-Na) and poly(acrylamide-co-acrylic acid). The hydrogels were synthesized via free-radical polymerization, combining Alg-Na's linear chains with a crosslinked synthetic network to create a tunable, stimuli-responsive material.

Keywords: Semi-IPN hydrogels, pH-responsive materials, Sodium alginate, Heavy metals, Water pollution

Développement d'un nouveau biosorbant à base de biopolymère pour l'élimination des ions de Cu (II), Ni (II) et Zn (II)

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Abstract **–** Les écosystèmes peuvent être menacés par les effluents contenant des ions métalliques. Par conséquent, il est impératif de les éliminer des eaux de rejet avant qu'ils ne soient déversés dans la nature. La biosorption, processus simple et efficace, pourrait être une solution prometteuse pour le traitement de ces effluents. A cette fin, des essais de biosorption en batch ont été effectués afin d'éliminer les ions métalliques de Cu^{2+}, Ni^{2+} et Zn^{2+} grâce à un biosorbant à base de billes de chitosane réticulées avec de l'épichlorohydrine modifié par une réaction de carboxylation. Ce biosorbant a été caractérisé par IFTR, analyse élémentaire et DRX. Le pH isoélectrique de 9,3 du biosorbant a été également déterminé. Les réactions de réticulation et de carboxylation ont nettement amélioré les propriétés physico-chimiques du chitosane en lui conférant une grande capacité d'adsorption vis-à-vis des trois ions métalliques ; le biosorbant développé a démontré une capacité d'adsorption de 96, 56 et 57 mg/g de Cu^{2+} , Ni^{2+} et Zn^{2+} , respectivement. Dans un mélange composé par les trois ions métalliques, le biosorbant a présenté une sélectivité pour le Cu^{2+}. Les tests de désorption des trois ions métalliques dans une solution d'acide chlorhydrique 0,5 M ont montré que la désorption a été rapide et totale après quelques minutes d'immersion des biosorbant/Me^{2+} dans la solution d'acide.

Le chitosane et ses dérivés ont un potentiel important en tant que biosorbant pour le traitement des effluents industriels contenant des ions métallique.

Keywords – Chitosane, ions métalliques, épichlorohydrine, réaction de carboxylation, biosorption.

The efficient use of photocatalysis for the degradation of triphenylmethane dye

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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, due to their high oxidative potential and their non-selectivity, these radicals are very effective for the destruction of persistent organic pollutants.
Iron Phosphate (FePO4) was successfully synthesized via a simple method as a heterogeneous catalyst for photo degradation of textile dye in aqueous solution. The $FePO_4$ was identified by the X-ray diffraction, Fourier transform infrared spectroscopy analyses and the scanning electron microscopy image The analysis was completed by the pHPZC and the band gap energy. The photocatalytic performance of $FePO_4$ was investigated using reduction of methyl violet 2B as a model reaction. The results showed that $FePO_4$ had converted nearly 99% of methyl violet 2B under UV light with optimum operating conditions of 1 g L^{-1} of $FePO_4$, natural pH (pH 6.75), and 10 mg L^{-1} of methyl violet 2B, a kinetic study was also realized. The recyclable character of the catalyst under the optimum conditions for three cycles was successfully investigated without any structural modification of the $FePO_4$.

Keywords – waste water; Textile dye; Degradation; Catalyst; Photocatalysis.

Kinetic Study of Paracetamol Degradation by the UV/PDS Advanced Oxidation Process

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Abstract **–** The degradation kinetics of paracetamol (PCT) by the UV-activated peroxydisulfate (UV/PDS) advanced oxidation process were investigated under varying initial concentrations of PCT and peroxydisulfate (PDS) dosage. Two initial PCT concentrations (0.066 mM and 0.132 mM) were studied. Results showed that a higher PCT concentration led to a decrease in degradation efficiency, attributed to competitive inhibition for oxidizing radicals. In contrast, increasing the PDS dose up to 20 mM significantly enhanced degradation performance due to the greater generation of sulfate radicals. Kinetic modeling indicated that the degradation process follows a pseudo-second-order reaction model, demonstrating a strong dependency on the initial concentrations of both reactants. Under optimal experimental conditions (0.132 mM PCT, 20 mM PDS, pH 6, UV power of 30 W), a degradation efficiency of 92% was achieved within 240 minutes at 25 °C. These findings confirm that the UV/PDS process is highly effective for the treatment of emerging pharmaceutical contaminants such as paracetamol, provided that process parameters are carefully optimized. The study contributes to a better understanding of the reaction mechanisms and supports the application of advanced oxidation processes for water treatment purposes.

Keywords – Paracetamol, UV/PDS process, Degradation kinetics, Sulfate radicals, Pseudo-second-order reaction

Statistical Modeling and Optimization of the UV/PDS Process for Paracetamol Removal

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Abstract **–** This study presents a statistical modeling and optimization approach for the UV/PDS advanced oxidation process used in paracetamol (PCT) degradation. A central composite design (CCD) was employed to assess the influence of three key variables: initial PCT concentration, solution pH, and UV lamp power. The results indicated that increasing the initial PCT concentration negatively affects the degradation efficiency due to radical scavenging. The pH was found to be a critical parameter, with an optimal value of 6 promoting the efficient generation of reactive sulfate radicals. Additionally, increasing the UV lamp power significantly enhanced the degradation yield, regardless of the initial PCT concentration. Response surface methodology (RSM) allowed for the identification of optimal operational conditions: 0.132 mM PCT, pH 6, and UV power of 30 W. Under these conditions, a degradation efficiency of 92% was achieved within 240 minutes at 25 °C. The model developed in this study accurately predicts the system's behavior and highlights the synergistic effects of the studied parameters. These findings provide a valuable tool for the design and scaling-up of efficient treatment systems targeting pharmaceutical contaminants in aqueous environments.

Keywords – Paracetamol, Optimization, Response Surface Methodology (RSM), Sulfate radicals, Central Composite Design (CCD)

Synthesis, Characterization, and DFT Calculations of a New Schiff Base.

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Abstract – Schiff bases are considered as valuable compounds because of their versatility in the field of medicine and pharmaceuticals, a new Schiff base was synthesized by reacting an aldehyde with a primary amine in ethanolic solution. The ligand LV was characterized by a spectroscopic techniques such as FT-IR , In addition, a theoretical study has been performed on the synthesized compound using the density functional theory DFT via B3LYP/6-31G(d,p) methods. The geometry optimization, molecular energy and molecular properties of LV such as HOMO-LUMO band gaps, were investigated using DFT. At last, it appears that both the experimental and theoretical studies have confirmed the synthesis of our ligand, yielding a satisfactory result and demonstrating its reactivity.

Keywords – Schiff base, synthesis, characterization, DFT, optimization.

Electrochemical Insights into a Salicylaldehyde-Based Oxovanadium Schiff Base Complex

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Abstract

Schiff bases are widely used in coordination chemistry due to their ability to form stable complexes with transition metals. In this study, a tetradentate oxovanadium(IV) complex was synthesized via the reaction between salicylaldehyde and an aromatic amine, and its electrochemical properties were investigated in an organic medium.

The analysis was carried out using cyclic voltammetry (CV) on a glassy carbon electrode, with $LiClO_4$ as the supporting electrolyte, under a nitrogen atmosphere. The results showed that the electrochemical parameters (E_pc, E_pa, and ΔE_p) remained stable regardless of the scan rate. The anodic-to-cathodic peak current ratio approached unity, indicating a reversible electrochemical behavior of the complex.

Additionally, rotating disk electrode (RDE) experiments were conducted to determine diffusion coefficients, which were found to be in the order of 10^{-6} $cm^2 \cdot s^{-1}$, consistent with literature values. The resulting Levich plots exhibited linearity, confirming a diffusion-controlled regime for the electrochemical reactions at the electrode surface.

These findings highlight the redox stability of the oxovanadium complex and its potential relevance in advanced electrochemical applications.

Keywords – Aromatic amine; Cyclic voltammetry; Oxovanadium complex

Study of the Crystal Structure of Zwitterionic Imidazoles

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Abstract – In nature, catechol, also known as 1,2-dihydrobenzene, occurs naturally in small amounts in fruits and vegetables. It is additionally released into the environment during its production and use, primarily serving as an antiseptic, antifungal, and antioxidant in various industries such as chemical, rubber, photographic, pharmaceutical, and cosmetic.
From a toxicological perspective, catechol is considered a pollutant that can irritate the skin, eyes, and lungs. Prolonged exposure may lead to increased blood pressure and damage to kidney function and structure. It has been classified by the International Agency for Research on Cancer (IARC) as a Group 2B carcinogen, indicating it is possibly carcinogenic to humans.
This study focuses on the synthesis of 2-(1H-Imidazolin-2-yl)phenol and the characterization of its zwitterionic form, L_1, using spectroscopic methods and single-crystal X-ray diffraction. The research further investigates the catalytic properties of the in situ copper-imidazole complex (CuL_1) in the oxidation of 3,5-di-tert-butylcatechol (3,5-DTBC).
Imidazoles are highly significant chemically and have been extensively studied due to their role as complexing agents**.** Beyond their pharmaceutical relevance and biological activities , imidazole derivatives like imidazoline , featuring a phenyl hydroxyl group, have garnered interest for their various applications and their ability to form stable zwitterionic tautomeric forms through proton transfer from the ortho-hydroxy group to nitrogen. These interactions between oppositely charged entities enhance their stability.

Keywords – Catechol; Environmental impact; Imidazole derivatives; X-ray crystallography; Zwitterionic structure

Optimized Biotechnological Production of Hyaluronic Acid for Pharmaceutical Applications

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Abstract **–** Hyaluronic acid (HA) is a naturally occurring glycosaminoglycan with exceptional biocompatibility, hydration capacity, and regenerative properties, making it highly valuable in pharmaceutical and biomedical applications. This study focuses on the development and optimization of a bacterial fermentation process for HA production aimed at pharmaceutical use.

The process optimization involved adjusting key fermentation parameters—such as pH, temperature, nutrient composition, and incubation time, which led to a significant improvement in HA yield. The biopolymer was extracted, purified, and characterized using Fourier-transform infrared spectroscopy (FTIR) and high-performance liquid chromatography (HPLC), confirming its purity and structural integrity.

Pharmaceutical evaluation of the resulting HA demonstrated favourable properties in terms of viscosity, stability, and biocompatibility, validating its potential for use in injectable therapies, wound healing formulations, and ophthalmic products. This work supports the goal of local bioproduction of high-value molecules and aligns with the development strategy of the Algerian pharmaceutical industry, offering a promising alternative to imported materials.

Keywords – Hyaluronic acid, bacterial fermentation, pharmaceutical chemistry, biotechnology, local production, Algeria.

ULTRASOUND ASSISTED EXTRACTION OF PHENOLIC COMPOUNDS AND FLAVONOIDS FROM AQUEOUS EXTRACT OF PLANT FROM CRASSULACEAE FAMILY

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Abstract

Description du sujet: Ultrasound assisted extraction is a technique that uses sound waves to improve the extraction efficiency of bioactive compounds from plants, or other materials, this technique is a non-conventional process which gives a significant yield with a reduced solvent of extraction.

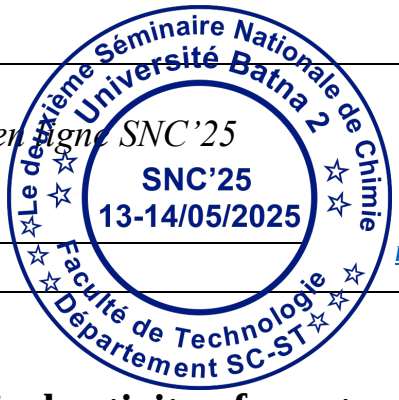
Objectifs: The objective of this work is to investigate the influence of extraction conditions assisted by ultrasound on the total polyphenols and the flavonoid contents.

Méthodes : Extraction of secondary metabolites is performed using ultrasound for 30 min at 40°c and 40 kH frequency. The total phenolic compounds were determined using Folin Ciocalteau's phenol reagent according to Singleton and Rossi (1965). And the total flavonoid contents using the aluminium chloride method Shahar B et al, 2023.

Résultats et Discussion: The results showed values were 31,02 % yield, 22,92 mg GAE/g for total phenolic acid and 45,49 mg QEq/ g for total flavonoids content.

Conclusion: The conditions defined above provide a fundamental for real applications in the extraction of bioactive compounds from the leaves of plant from the Crassulaceae family. However, additional research is needed to identify the molecules present in the optimized extract.

Keywords – Ultrasound, extraction, flavonoids, polyphenols, waves.



Theoretical study of the antiradical activity of carotenoid pigments using global reactivity indices

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Abstract – Carotenoids are the most widely distributed pigments in nature that gives their yellow, orange, and red colors to various fruits and vegetables. They are considered as efficient free radical scavengers because of their structural variety characterized by a long aliphatic polyene chain [1].
The present work aims to perform a computational analysis of the antiradical activity of three carotenoids, namely, phytoene (colorless), ζ-Carotene (pale yellow), lycopene (red) by considering the SET (single electron transfer) mechanism. The antiradical activity is expressed by the ability of carotenoid molecules to neutralize free radicals either by oxidation (giving electrons) or by reduction (accepting electrons). The antiradical activity of the studied systems is rationalized by the calculation of global reactivity indices, namely, the Parr's electrophilicity index ω and the global nucleophilic index (N) proposed by Domingo et al. [2], and the NEP (Nucleophilic-Electrophilic power) index proposed by us in the present work [3]. The calculations were carried out at the M06-2X/6-31+G(d,p) level of theory and the obtained results show clearly that red pigments, characterized by high values of NEP index, are better antiradical carotenoids compared with yellow or colorless pigments and the following sequence order was established: Phytoène < ζ-Carotène < lycopene in total agreement with experimental outcomes.

Keywords – Carotenoids, pigments, antiradical activity, reactivity indices, SET mechanism

Enhancing Performance: Cross-Linking Strategies for Improved Mechanical and Rheogical Properties in LDPE/iPP Polymer Blends

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Abstract **–** The creation of materials with precisely customized qualities is made possible by the fast-evolving field of polymer mix design.
To achieve the appropriate mechanical properties, it is crucial to comprehend the morphology that results from blends of immiscible polymers.
This study explores the complex interactions between structure and characteristics in both cross-linking-modified and unmodified LDPE and iPP blends.
Using both mechanical testing and rheological evaluations, our study provides important new informatio.
We discover that crosslinked materials have significantly higher viscosity, which suggests the creation of a three-dimensional network and improved stability.
Furthermore, after crosslinking, LDPE exhibits better behavior.Because more interchain links are formed after crosslinking, the melt flow index decreases, indicating increased resistance to flow and deformation.
Higher PP concentration in unmodified blends results in greater ductility and flexibility, whereas cross-linking causes rigidity. Cross-linking , on the other hand, improves flexibility by reducing rigidity in blends with less iPP.
Furthermore, the addition of crosslinking agents and iPP greatly increases mechanical strength, strengthen ing structural integrity.
Additionally, iPP inclusion and crosslinking improve impact resistance, making the materials appropriate for applications needing strong performance in demanding circumstances.
Keywords – LDPE/iPP, polymer, blends, resistance, performance.

Contribution To The Phytochemical Characterization Of *Ceratonia siliqua* L. Leaves

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Abstract – *Ceratonia siliqua* L. (FABACEAE) commonly known as Carob tree is a typical plant of the Mediterranean basin widely used in phytotherapy. In the aim to highlight some of the natural bioactive compounds that might be at the origin of its therapeutic properties, we were interested by a qualitative and quantitative phytochemical characterization of leaves of *Ceratonia siliqua* L. harvested from Tipaza region of the north of Algeria. Plant powder and an aqueous extract prepared by infusion from these latters have been subjected to a series of phytochemical screening tests in order to determine the main families of primary and secondary metabolites that constitute the carob leaves. Spectrophotometric assays to determine the total polyphenols and tannins content, were carried out on a methanolic extract of carob leaves prepared by maceration. The results of the phytochemical screening showed a significant presence of total polyphenols, flavonoids, gallic tannins, coumarins and mucilages. Leucoanthocyanins were moderately detected, whereas a faint presence of saponosides was demonstrated, however we noted the absence of alkaloids, glucosides, cathechic tannins and anthocyanins. The methanolic extract gave a yield of 38.07 %, and based on the spectrophotometric analysis it was found that the methanolic extract of the leaves contain a higher level of tannins estimated by (2892.16 µg TAE/mg DE) compared to total polyphenols content (396.05 µg GAE/mg DE). Given the results of the current study we may explain the significant medicinal value of *Ceratonia siliqua* L. by the diversity of its leaves in term of bioactive constituents such as phenolic compounds which in fact has already proven to be a great antioxidant, antimicrobial, antifungal…etc. agents

Keywords – *Ceratonia siliqua* L, Leaves, Phytochemical characterization, Total polyphenol, Tannins.

QSPR Applications on Heat of Combustion of Monocarboxylic Acids using the quantum molecular descriptors

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Abstract

Quantum chemical descriptors of 19 monocarboxylic acids (C_2–C_{20}) were computed using the DFT-B3LYP method with the 6-31G(d,p) basis set. These descriptors, in combination with experimental enthalpies of combustion (ΔH_{Comb}), were employed to develop a quantitative structure–property relationship (QSPR) model using multiple linear regression (MLR). The resulting three-descriptor model demonstrated excellent predictive accuracy, yielding a coefficient of determination R^2 = 0.999987, a leave-one-out cross-validated Q^2_{LOO} of 0.999982, and a root-mean-square deviation (RMSD) of 13.2584 . External validation further confirmed the model's robustness, with a predictive correlation coefficient Q^2_{ext} = 0.999986. These findings indicate that the QSPR model possesses both high estimation stability and strong predictive capability. Overall, the results highlight significant correlations between the molecular structure of monocarboxylic acids and their enthalpies of combustion (ΔH_{Comb}), as well as properties such as total energy, dipole moment, and lowest unoccupied molecular orbital energy.

Keywords: Quantum chemical descriptors, Multiple linear regression (MLR), Monocarboxylic acids, QSPR modeling, Density Functional Theory (DFT).

Digital Modeling of Heterocyclic Compounds Applied to Pharmaceutical Design

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Abstract **–** Imidazole, a heterocyclic compound found in natural products, biological systems, and pharmaceuticals, forms complexes with significant industrial applications. To explore structure-activity relationships (QSAR) of imidazole derivatives, this study investigates 31 compounds reported by Olson et al. as angiotensin II AT1 G-protein coupled receptor blockers. These derivatives include aminomethyl/acylmethylimidazoles (compounds 1–26, with biphenyl-tetrazole groups) and biphenyl-N-acylsulfonamide-imidazoles (compounds 27–31), which exhibit divergent biological effects attributed to structural variations. Geometrical, and electronic parameters were optimized using computational methods (AM1, PM3, B3LYP). QSAR analysis via multiple linear regression (MLR) identified key molecular descriptors correlating with receptor-blocking activity. Model validity was confirmed through leave-one-out (LOO) cross-validation, demonstrating strong agreement between experimental and predicted activity values. The results highlight the critical role of molecular structure in biological efficacy and validate the robustness of the QSAR models for designing targeted imidazole-based therapeutics.

Keywords – DFT, QSAR, Imidazole derivatives

Traitement des eaux usées par précipitation (eau usée d'une station de fabrication de détergents)

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Résumé : Ces dernières années la pollution des milieux aquatiques se fait de plus en plus importante et crée un déséquilibre écologique dans les écosystèmes aquatiques. Les rejets incontrôlés d'eaux usées dans les milieux naturels chargés en phosphore sont considérés comme une forme de pollution pour ces milieux. La lutte contre l'eutrophisation des cours d'eau consiste à réduire les apports phosphorés des eaux usées et une des techniques de déphosphatation de l'eau consiste à éliminer le phosphore au moyen de réactifs chimiques qui génèrent des précipités insolubles.

Dans ce contexte la présente étude se base sur l'élimination chimique du phosphore, sous forme de struvite, contenu dans une eau usée prélevée à partir de l'usine de fabrication de détergents Henkel.

L'approche expérimentale développée consiste à éliminer les phosphates présents dans l'eau usée à température constante et dans des conditions optimales de pH. Pour ce faire, l'eau usée a été analysée et les concentrations en phosphate/magnésium/ammonium ont été ajustées dans un rapport molaire de 1 /1 /1, respectivement, de façon à favoriser la précipitation maximale de struvite. Les caractéristiques des cristaux obtenus, dans la phase solide, ont été déterminées par des méthodes physiques d'analyse (MEB, IRTF, DRX, FRX). Les résultats obtenus nous ont permis de conclure que la méthodologie de déphosphatation par cristallisation contrôlée de struvite s'avère efficace et rentable (70.6%) dans l'élimination des phosphates à partir de l'eau usée utilisée.

Mots clés - Pollution, Eutrophisation, Eau usée, Traitement, Cristallisation.

Electrochemical and DFT studies of Inhibition of copper corrosion in nitric acid in the presence of chemical compounds

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Abstract –

Understanding the corrosion process is key to discovering techniques that limit or prevent a metal's reactivity with its surroundings.

Copper is one of the most widely used metals in industry due to its important electrical and mechanical properties, and while the problem of corrosion is an obstacle [3], tests have been conducted to qualify amine-derived chemical compounds as corrosion inhibitors for copper in a 1M HNO_3 acidic medium at different concentrations. To this end, a theoretical study (Density Functional Theory) and an electrochemical study were proposed. The latter involves using electrochemical techniques such as polarization curves and electrochemical impedance spectroscopy.

According to preliminary experiments, the results obtained indicate that these compounds are good inhibitors at low concentrations.

Keywords – corrosion Inhibition, copper,DFT, polarisation, impédance.

ADSORPTION OF A NEW DERIVATE ESTER FROM ALGINIC ACID WITH METHYLENE BLUE DYE

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Abstract – In this work, the application of ester materials prepared by grafting different carbon chain lengths of diols in alginic acid (AA) by a simple, fast and efficient method for the adsorption of methylene blue (MB) is studied. The AA ester derivatives are characterized by Fourier transform infrared spectroscopy (FTIR), X-ray photoelectron spectroscopy (XPS), thermogravimetric analysis (TGA), derivative thermogravimetry (DTG), scanning electron microscopy (SEM), atomic force microscopy (AFM), and Zeta potential before and after MB adsorption. This study shows a significant improvement in the adsorption capacity of MB by AA after its esterification with a Qmax value up to 454.545 mg/g for the best adsorbent "Poly(AA-g-EG)". The experimental data are studied according to two isothermal models (Langmuir and Freundlich) and two kinetic models (pseudo-second order and intra-particle diffusion). The adsorption of MB is also evaluated thermodynamically. An adsorption mechanism of MB is established.

Keywords – Methylene blue, Adsorption, Alginic acid, Esterification, Chemical modification.

Computational insight into magnetoelectric trends and semi-metallic trends of double perovskite compounds K_2 $NaXBr_6$ (X = Ti, V) double perovskite compounds.

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Abstract **–** Double perovskites have gained importance in materials science. Our study explores the magneto electric characteristics of the K_2 $NaXBr_6$ series, where X is Ti or V. We used density functional theory (DFT) calculations to predict the magnetic properties. Our results revealed distinct electronic behaviors within this series. Which exhibited semi-metallic behavior indicating potential for spin-dependent electronic transport.

Keywords – double pérovskite sans plomb, optoélectronique, DFT et ferromagnétique.

Experimental Study of Salt Effects on the Liquid–Liquid Equilibrium of the Ternary System

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Abstract – This The study addresses liquid-liquid equilibria (LLE) for aqueous solutions containing electrolytes, specifically examining their impact on solvent extraction processes. Liquid-liquid extraction exploits differences in solubility to selectively transfer solutes from an aqueous to an organic phase. The presence of electrolytes such as potassium chloride (KCl) and calcium chloride ($CaCl_2$) significantly influences phase equilibria due to changes in intermolecular interactions, notably hydrogen bonding.

Experiments investigated the ternary system Water/Acetic Acid/1-Butanol without salts and compared it to systems containing varying concentrations of KCl and $CaCl_2$. Results demonstrated that increasing electrolyte concentrations enhanced the transfer of acetic acid from the aqueous phase to the organic phase. This phenomenon is attributed to hydration theory, suggesting ionic species reduce available water molecules around organic compounds, promoting their migration into the organic phase. Among the salts tested, $CaCl_2$ exhibited a more pronounced salting-out effect compared to KCl.

While the primary goal of salt addition is to enhance solvent selectivity and improve extraction efficiency, the potential environmental consequences of salt usage, such as increased salinity in effluents and ecological imbalance in receiving waters, must be carefully managed through sustainable practices. Elevated salt concentrations can lead to increased environmental concerns, including salt disposal issues, potential soil contamination, and negative effects on aquatic ecosystems due to high salinity levels. Studies highlight concerns about ecosystem disturbances and soil contamination from industrial and road salts, emphasizing the need for sustainable practices and effective waste management strategies to mitigate these impacts.

The reliability of the experimental data was validated using Othmer-Tobias and Hand correlations. Othmer-Tobias correlation effectively represented the system without salt and higher concentrations (10%, 15%) of $CaCl_2$, whereas Hand correlation provided superior accuracy for systems with KCl (5%, 10%, 15%) and the lowest concentration (5%) of $CaCl_2$.

Keywords – Liquid-Liquid Equilibrium, Salting-out Effect, Phase Equilibrium, Othmer-Tobias Correlation, Hand Correlation, Solubility, Environmental Impact.

Utilization of Pulsed Electromagnetic Fields for Water Treatment: A Novel Method for Improving Physicochemical Properties and Preventing Scale Formation

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Abstract **–** This study investigates a groundbreaking approach for water treatment using pulsed electromagnetic fields (PEMF), focusing on the enhancement of water's physicochemical characteristics and the prevention of scale deposition. By employing a custom-designed laboratory setup, two samples of municipal water were exposed to PEMF, resulting in notable alterations in essential water quality indicators. Key parameters such as electrical conductivity (EC), total dissolved solids (TDS), and hardness experienced considerable reductions, while dissolved oxygen (DO) levels were substantially increased. Specifically, EC showed a decrease of approximately 29%, TDS dropped by up to 44%, and DO saw an increase of over 22%. Additionally, the concentrations of calcium and magnesium ions—responsible for water hardness—were effectively reduced. These results suggest that the application of PEMF influences the behavior of dissolved ions and the formation of crystalline structures, presenting a promising, chemical-free alternative to conventional water treatment techniques. This method holds significant potential for improving water quality in diverse contexts, including industrial, agricultural, and environmental applications, where water softening and enhanced oxygenation are crucial.

Keywords – Pulsed Electromagnetic Fields, Water Quality Enhancement, Non-Chemical Treatment, Water Softening, Ionic Behavior Modification.

Synthesis, DFT calculations and molecular docking as antibacterial of *α*-aminophosphonates/ phosphates *α*-aminophosphonates

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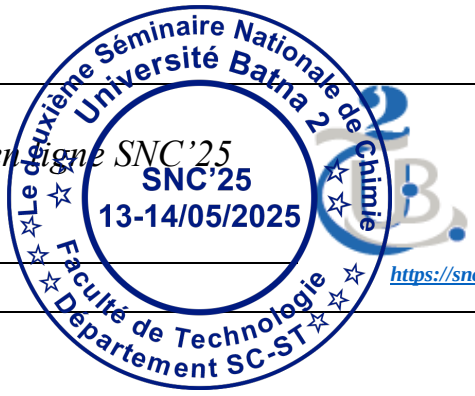
Abstract – The *α*-aminophosphonates are of great biochemical and pharmacological importance1,2 due to the association of phosphonate and amine. These molecules are phosphorus structural analogues of amino acid and are interesting for medicinal chemistry. *α*-Aminophosphonates derivatives have received much attention as enzyme inhibitors, pharmacogenic agents, haptens of catalytic antibodies, herbicidals, inhibitors of serine hydrolases. In this study, we have compared the stability and reactivity between the *α*-aminophosphonates/ phosphates α-aminophosphonates previously sunthesized as novel category. Theoretical DFT calculations of the synthesized compounds were carried out at CAM-B3LYP 6-31G (d,p) basis set to predict the molecular geometries and chemical reactivity descriptors. Frontier orbital energies (HOMO/LUMO) were described the charge transfer and used to predict structure-activity relationship study. Molecular docking studies confirmed strong interactions between the synthesized compounds and proteins. Notably, the phosphates α-aminophosphonates is more efficient than *α*-aminophosphonates. These results may indicate the importance of diethylphosphate inserted moiety to the diethyl hydroxyphenyl α-aminophosphonates and the possibility of the use of diethylphosphates diethyl *α*-aminophosphonates as potential antibacterial candidates.

Keywords –I α-Aminophosphonates, *Kabachnik–Fields* reaction, DFT calculations, molecular docking.



Removal of copper ions from aqueous solutions using Sodium hydroxide activated adsorbent derived from local low-cost agricultural wastes

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ABSTRACT

Heavy metals removal from aqueous solutions is very important research field especially while using natural adsorbents after physical or chemical modification, in present study a local agricultural waste of abundantly grass was used to prepare three adsorbents from raw material waste; first one Pyrolysed at 800 °C, second one Hydrothermal pyrolysed and the third one chemically activated with sodium hydroxide then pyrolysed at 800 °C, in order to select the best adsorption proprieties a preliminary tests were done on all these adsorbents in synthetic contaminated water with copper ions in different concentrations (10,20,40, 80 mg/l), the results showed best removal percentage was with NaOH activated adsorbent more than 90 % which was characterised by SEM/EDX, FTIR, and Point of Zero Charge (PZC), SEM images showed well defined tunnel shaped pores, PH effect was studied it was very important factor, PH between 5 to 6 was found the best for adsorption, Kinetic study showed best fit with pseudo second order model, FTIR characterisation showed its functional groups that may give the opportunity of ion exchange or coordination with heavy metals, the isotherm study is in progress to bring more information about its adsorption performance and for its optimization, additional analysis is programmed as well as XRD, BET and completed adsorption behaviour study in order to optimize this local grass to be within the best low-cost agricultural waste based adsorbents, more practical tests and analysis will be done to find out its capacity on industrial waste water to eliminate the toxic heavy metals.

Keywords: *Adsorption, Agricultural wastes, Copper, Heavy metals, Wastewater treatment.*

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Synthesis of New Rhodanine Derivatives and Evaluation of Their Antioxidant Activity Using Phenanthroline and SNP Methods

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Abstract

Rhodanine is a privileged heterocyclic scaffold known for its wide range of biological activities, especially its antioxidant potential. In this study, a series of novel rhodanine derivatives were synthesized through conventional organic synthesis techniques. The chemical structures of the synthesized compounds were confirmed using spectroscopic methods, including FT-IR and ^{1}H NMR spectroscopy.
The antioxidant activity of the compounds was evaluated using two well-established in vitro methods: Phenanthroline assay, which measures the ability of the compounds to chelate iron ions and prevent hydroxyl radical (•OH) formation,and the (SNP) assay, used to assess the inhibition of (NO•) production.
The results revealed that several synthesized compounds exhibited significant antioxidant activity, highlighting the influence of structural modifications on the biological performance of the rhodanine core. These findings suggest that the synthesized derivatives hold promise as potential candidates for the development of novel antioxidant agents.

Keywords – Rhodanine, Antioxidant activity, Phenanthroline, SNP, Organic synthesis, Biological evaluation.

Étude théorique des interactions entre le bisphénol A et le fluorure de polyvinylidène (PVDF): Mise en evidence de la liaison hydrogène.

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Abstract

Le bisphénol A (BPA) est un polluant organique largement répandu, reconnu pour ses effets endocriniens nocifs sur la santé humaine et l'environnement, ce qui justifie la recherche de méthodes efficaces pour son élimination. Cette étude théorique explore l'interaction entre le BPA et le polyfluorure de vinylidène (PVDF), un matériau économique réputé pour sa capacité d'adsorption du BPA. Afin de caractériser la nature de cette interaction, plusieurs outils de chimie théorique ont été utilisées : la densité d'états électroniques (TDOS), la théorie quantique des atomes dans les molécules (QTAIM) et l'analyse des interactions non covalentes (NCI).

L'énergie d'adsorption obtenue par la méthode ωB97X-D/6-311G(d,p), estimée à -97,74 kJ/mol, indique une forte affinité entre le BPA et le PVDF, typique d'un processus de physisorption. Les spectres TDOS révèlent l'émergence de nouveaux états électroniques dans le complexe BPA/PVDF, absents dans le PVDF isolé, traduisant une modification de sa structure électronique. Cette altération est attribuée à de puissantes interactions de type van der Waals, dominées par des liaisons hydrogène, comme le confirment les analyses QTAIM et NCI. Ces résultats démontrent que l'adsorption du BPA sur le PVDF repose essentiellement sur des interactions non covalentes, en particulier les liaisons hydrogène, soulignant ainsi le potentiel du PVDF comme matériau adsorbant pour la dépollution du bisphénol A.

Keywords : DFT, Bisphenol A, polyvinylidene fluoride, adsorption, QTAIM, NCI, TDOS

Evaluation de la qualité fertilisante des boues de la station d'épuration Ibn Ziad de la ville de Constantine

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Abstract **–** L'épandage agricole des boues résiduaires urbaines est une pratique courante régie par des normes et une réglementation. L'objectif du présent travail est l'évaluation de la disponibilité des éléments nutritifs dans les boues résiduaires de la station d'épuration des eaux de la ville de Constantine Ibn Ziad. Plusieurs schémas d'extraction ont été utilisés pour pouvoir évaluer la spéciation du carbone, du phosphore et de l'azote. Les résultats de l'analyse élémentaire (CHN) montrent la prédominance du carbone. Les résultats de la spéciation des trois éléments révèlent la prédominance de la forme organique. Parmi les espèces d'azote minéral, l'ammonium prédomine. La fraction apatite du phosphore est importante. Le phosphore Olsen disponible est de l'ordre de 700mg/kg. Le rapport C/N calculé indique la biodisponibilité de l'azote.

Keywords – Station d'épuration; Boues résiduaires; Carbone; Azote; Phosphore

Adsorption of Rhodamine B using low cost adsorbent obtained from orange peels: kinetics and equilibrium

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Abstract **–**Dyes are widely used for industrial, printing, food, cosmetic and clinical purposes as well as textile dyeing because of their chemical stability ease of synthesis, and versatility. Their stability causes pollution once the dyes are released into the environment in effluents. Adsorption with activated carbon is one of the most widely adopted techniques for removing these pollutants. However, due to its high cost and the difficulty of regeneration, low cost adsorbents derived from various natural wastes are used as effective adsorbents. The aim of this study is to illustrate the valorization of orange peels and their use for the processing of effluent charged in dyes. The retention of cationic dye Rhodamine B by chemical activated orange peels, in batch system, taking into account various physico-chemical parameters was studied. The results showed that retention of Rhodamine B is rapid, with equilibrium reached after 20 minutes. The kinetic was pseudo-second order, controlled by intraparticle diffusion. Maximum adsorption was recorded at pH=3, which was explained by the pHpzc of the material, orange peels, and by the molecular nature of the dye. The pHpzc was found to be around 2.03, indicating the acidic nature of the orange peels. The adsorption isotherm for Rhodamine B was studied; the given experimental data were well represented by the Langmuir and Freundlich model. Finally this study showed that oranges peel can be regarded as an interesting adsorbent for the removal of dyes from industrial wastewater effluents.

Keywords – Dyes; Orange peels; Rhodamine B; Adsorption; Kinetic and isotherm

Dédoublement cinétique par désacylation enzymatique du 1–phényléthyl acétate dans des milieux pauvres en eau : Effet d'addition de sels.

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Résumé **–** Les réactions de dédoublement cinétique enzymatique sont largement décrites comme des méthodes faciles à mettre en œuvre pour la préparation des molécules énantiomériquement enrichies ou pures. Parmi ces réactions, les dédoublements cinétiques par hydrolyse enzymatique conventionnelles sont modérément décrites, cela est due à plusieurs inconvénients, en l'occurrence la mauvaise solubilité des substrats dans le milieu aqueux, ce qui donne lieu à des sélectivités modérées avec de faibles rendements. Afin de remédier cette problématique, plusieurs paramètres ayant un impact crucial sur la sélectivité et la réactivité enzymatique peuvent être modulés, particulièrement en adoptant l'approche de l'introduction des additifs.

Dans le présent travail, nous avons étudié le comportement de quatre lipases, d'origines différentes, une immobilisée et trois libres: la ***CAL-B***, la ***PCL***, la ***CRL*** et la ***PPL***, lors de la réaction de dédoublement cinétique par désacylation lipasique, du 1-phényléthyl acétate, en présence de quatre sels : **Na_2CO_3, Na_2SO_4, Na_2HPO_4** et le **NaCl**, et ce dans le cadre de mieux comprendre leurs modes d'action dans des systèmes anhydre et micro-aqueux. Nous avons examiné l'effet de quelques paramètres pouvant intervenir d'une manière cruciale sur le déroulement de cette réaction tels que : l'hydrophobicité du milieu réactionnel et la nature de l'enzyme. Les résultats obtenus on montré un effet important de la nature des sels sur la réactivité et la sélectivité lipasiques dans les deux milieux examinés.

Keywords – Désacylation enzymatique ; Lipases ; Effet de sels ; Milieu anhydre ; Milieu micro-aqueux

Acylation énantiosélective de la 1-phényléthanamine et de la pentan-2-amine par catalyse enzymatique.

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Résumé – Les réactions de dédoublement cinétique par amidation enzymatique sont les plus sollicitées pour la séparation des énantiomères des substrats racémiques d'intérêt potentiel, en l'occurrence les amines. De ce fait, le développement de méthodes ou de paramètres susceptibles d'influer sur l'effet catalytique de ces enzymes est devenu pressant. Vu les impératifs et les obligations imposées par la Food and Drug Administration (FDA), qui exige une pureté énantiomérique ee > 99% sur toute molécule destinée aux marché des médicaments, nous avons focalisé notre intérêt sur la conception des amines et de leurs dérivés amides sous forme optiquement enrichie ou pure.

Au cours de ce travail, nous avons étudié la réaction de dédoublement cinétique par amidation enzymatique de deux amines primaires : la 1-phényléthanamie (1) et la pentan-2-amine (2). Nous avons examiné l'effet de quelques paramètres pouvant intervenir d'une manière cruciale sur le déroulement de cette réaction tels que : la nature de la lipase, la structure du nucléophile, l'hydrophobicité du solvant organique et la nature du donneur d'acyle.

Nous avons obtenus des résultats significatifs avec les deux amines dédoublées. L'énantiomère amide, le *(R)-N-*(1-phényléthyl) acétamide *(1a)* a été obtenu avec un ee =92% à une conversion de 46.5% et un facteur de sélectivité de 58, et l'énantiomère (*R)-N-(*pentan-2-yl) acétamide *(2a)* a été obtenu avec un ee > 93% à une conversion de 48%, en utilisant l'acétate d'éthyle comme donneurs d'acyle. Tandis que l'énantiomère *(R)-N-(*1-phényléthyl) dodecanamide a été récupéré avec un bon enrichissement énantiomérique de 96.4%, à une conversion de 48.6%, en utilisant l'acide laurique comme donneur d'acyle.

Keywords – Dédoublement cinétique; Lipases ; Amidation ; Amines primaires ; Amides énantiopurs.

Impact des polluants organiques persistants (pesticides) sur les milieux aquatiques et leur élimination par électro-oxydation : Cas de dégradation de l'herbicide fénuron

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Résumé –
La pollution hydrique par les rejets industriels et l'activité agro-industrielle particulièrement les produits chimiques organiques constituent une réelle menace pour l'environnement et la survie sur terre. Certains de ces produits sont très stables et difficiles à dégrader. Beaucoup de recherches ont porté sur une nouvelle classe de techniques d'oxydation : les procédés d'oxydation avancée (POA), il s'agit de technologies basées sur la génération d'espèces hautement oxydantes telles que les radicaux hydroxyles ($^{\bullet}OH$, E^{o} = 2.80 V/SHE) capables d'oxyder tout polluant organique jusqu'à la minéralisation. Dans ce contexte, cette étude porte sur l'application de la technique électro-oxydation pour le traitement des eaux chargées en polluant organique particulièrement un pesticide (fénuron) en utilisant une électrode (Ti/SnO_2-Sb_2O_3/PbO_2) que nous avons synthétisée dans notre laboratoire. L'objectif de ce travail est d'améliorer l'efficacité du procédé, dans ce but nous avons étudié l'influence de quelques paramètres sur l'élimination du fénuron tels que : la densité du courant, la nature de l'électrolyte support et le pH. Les résultats obtenus ont montré que l'augmentation de la densité de courant a un effet positif sur la cinétique de dégradation et de minéralisation. Par contre, l'effet de la variation du pH est faible. L'étude de l'effet de la nature de l'électrolyte support a fait ressortir que les meilleurs résultats sont obtenus avec de Na_2SO_4.

Mots clés – Traitement des eaux, procédés d'oxydation avancée, électro-oxydation, électrode Ti/SnO_2-Sb_2O_3/PbO_2 et pesticide

Détermination des paramètres influençant le rendement de cristallisation de l'acide salicylique

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Résumé **–** Cette étude vise à optimiser le rendement du procédé de cristallisation par antisolvant d'un composé d'intérêt pharmaceutique. Le plan d'expériences Box-Behnken a été utilisé pour évaluer l'influence de trois paramètres opératoires critiques : le rapport volumique (antisolvant/solvant), le débit d'antisolvant et la concentration initiale, sur le rendement de cristallisation de l'acide salicylique. Les résultats ont confirmé que le rapport volumique avait un impact significatif sur l'efficacité de la cristallisation, permettant d'identifier des conditions optimales pour maximiser le rendement. Le rendement prédit optimal atteint 98 % pour un rapport volumique (antisolvant/solvant) de 2, une concentration initiale de 4 g/20 mL et un débit d'antisolvant de 15 mL/min. Les tests de validation du modèle mathématique ont montré une forte corrélation entre les valeurs prédites et les valeurs expérimentales. Ces résultats offrent des perspectives pertinentes pour l'optimisation des procédés de cristallisation, avec des applications potentielles dans l'industrie pharmaceutique, notamment pour améliorer la pureté et la reproductibilité des produits.

Mots-clés *– Acide salicylique, Cristallisation par antisolvant, Optimisation, Méthodologie de surface de réponse, Plan Box-Behnken.*

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Evaluation comparative de la capacité antioxydante des extraits de feuilles et d'écorces de tiges de *Zizyphus spina-christi* L. de la région du Souf

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Résumé **–** L'intérêt croissant pour l'utilisation d'antioxydantes naturels comme alternatives aux antioxydantes synthétique, conduit à rechercher de nouvelles sources locales d'antioxydants naturels pouvant être utilisées dans la biotechnologie industrielle. Dans la présente étude, nous avons examiné et comparer la capacité antioxydante de certains extraits de la plante médicinale *Zizyphus spina-christi* du Souf afin de sélectionner les extraits les plus prometteuses comme des antioxydants naturels efficaces, pour cette raison nous avons déterminé l'activité antioxydante à l'aide d'essais de *β*-carotene/acide linolique (méthode spectrophotométrique) pour les extraits d'hexane, dichloromethane, méthanol et aqueux des feuilles et d'écorce de tige de cette plante.

Nos résultats ont montré que les valeurs de l'activité antioxydante (AA %) de ces échantillons à 24 h et celles à 48 h étaient différentes de manière très significative (P< 0.001: ***). L'extrait de dichloromethane des feuilles a montré une activité antioxydante élevée de 88.75% après 24h et 77.64% après 48h. Les extraits de méthanol et aqueux d'écorce de tige présentent une activité antioxydante similaire et supérieure aux extraits d'hexane et de dichloromethane, avec des valeurs de AA% = 78.59% et 77.35% successivement après 24h, elle diminue légèrement à 73.48% et 72.71% après 48h.

Sur la base de nos résultats, nous pensons que l'extrait de dichloromethane de feuilles et les extraits de methanol et aqueux d'écorce de tige de *Ziziphus spina-christi* de la région de Souf ont été considérés comme des sources les plus prometteuses en tant qu'antioxydants pouvant être introduits dans les industries pharmaceutiques.

Mots-clés – Antioxydantes naturels – Biotechnologie industrielle – Essais de β-carotene/ acide linolique - Région de Souf - Ziziphus spina-christi

From Structure to Function: Characterizing Alginate Semi-IPN Hydrogels for Single/Binary Heavy Metal Removal

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Abstract : Semi-interpenetrating polymer network (semi-IPN) hydrogels composed of sodium alginate and poly(acrylamide-co-acrylic acid) were characterised for the removal of heavy metals from contaminated water. Structural analysis confirmed a porous, pH-responsive network with interconnected channels that facilitate ion diffusion. FTIR spectroscopy and SEM imaging verified the successful incorporation of polymers and the presence of functional groups capable of binding metal ions. These hydrogels exhibited excellent swelling capacity and high adsorption efficiency for Pb^{2+} , Cd^{2+} , and Cr^{3+} ions.In single-metal systems, the hydrogels demonstrated varying adsorption capacities, with cadmium and lead showing the highest uptake. In binary-metal systems, competitive adsorption was observed, driven by the metals' ionic radius, charge, and coordination affinity. The alginate content had a significant influence on both the structural features and the metal-binding selectivity of the hydrogels, affecting their overall adsorption performance and swelling behaviour.This study provides important insights into the relationship between composition, structure, and performance of semi-IPN hydrogels. The results highlight their potential to be tailored for efficient and selective removal of heavy metals, particularly in complex contamination scenarios involving multiple ions. These materials show great promise as eco-friendly adsorbents for environmental remediation and offer a sustainable approach to water purification in real-world applications.

Keywords: Hydrogel characterization, Binary metal systems, Semi-interpenetrating polymer network , Sodium alginate, Environmental remediation

Understanding Nitrobenzene Adsorption on Apricot Stone-Based Activated Carbon Using Statistical Physics Analysis

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Abstract **–** Nitrobenzene (NB), a chemical widely used in the manufacture of explosives, organic compounds, and plastics, is frequently released into the environment, posing significant ecological and health hazards even at trace concentrations. Classified as a hazardous, mutagenic, and carcinogenic substance, NB exhibits strong resistance to biodegradation, resulting in its long-term persistence and accumulation in various environmental compartments.

In the present study, the removal of NB from aqueous solutions was investigated using activated carbon derived from apricot stones (APS). The adsorbent was synthesized via chemical activation with phosphoric acid, resulting in a carbon material with a high specific surface area (1762 $m^2\ g^{-1}$), a large micropore volume (0.98 $cm^3\ g^{-1}$), and a relatively low mesopore volume (0.11 $cm^3\ g^{-1}$). The surface of APS exhibited a low acidic character, with a point of zero charge (pH_{PZC}) of 4.3. The material achieved a maximum NB adsorption capacity of 295.63 mg g^{-1} at 298 K.

To elucidate the adsorption mechanism, three statistical physics models were employed to fit the NB adsorption isotherms: (1) a monolayer model with a single adsorption energy, (2) a monolayer model with two distinct adsorption energies, and (3) a double-layer model with two adsorption energies. Based on the statistical physics analysis, the double-layer model provided the best fit, enabling the estimation of steric and energetic parameters. The findings revealed that two to three adsorption sites are involved in the fixation of NB molecules on the APS surface, with adsorption governed predominantly by physical interactions.

Keywords – Water pollution, Activated carbon, Nitrobenzene, Double layer model

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Photocatalytic Enhancement of AgCl-Based Materials for Visible Light Applications

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Abstract

To increase the photocatalytic activity of AgCl for environmental applications, a simple precipitation–deposition technique was established for the synthesis of the $CoFe_2O_4$/AgCl complex. For that, the phase of the nanoparticles was identified by X-ray diffraction (XRD), and the morphology was investigated by scanning electron micrograph (SEM), The gap energies of $CoFe_2O_4$(CFO) and AgCl, evaluated from the UV-VIS diffusion reflectance, were found to be 1.46 eV and 3.20 eV, respectively. For the photodegradation of the acid orange dye, some operating parameters such as the mass ratio of $CoFe_2O_4$/ AgCl, the catalyst, the pH of the solution and initial AO61 concentration were optimized. 25%/75% mass ratio of CFO/ AgCl, catalyst dose of 1.25 g/L, pH ~ 6 and 50 mg/L initial concentration were found as optimal conditions for the degradation performance under visible light with an efficiency of 93% within only 240 min. Moreover, this hetero-system demonstrated effective oxidation by facilitating photo-electron transport with the deference potential.

Keywords : $CoFe_2O_4$/ AgCl ; Catalyst ; Photodegradation ; Dye ; Environment.

Energy Decomposition Analysis of Ethylène Diamine TétraAcétique (EDTA)

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Abstract

The determination of the physicochemical properties of molecular systems crucially relies on intermolecular interactions. The energies associated with these interactions are usually calculated using theoretical methods such as Hartree-Fock (HF), MP2, and CCSD(T). Energy Decomposition Analysis (EDA), initially developed by Morokuma and refined by Ziegler and Rauk [1], is a method that involves performing DFT calculations on each fragment in isolation. This allows for the decomposition of intermolecular interactions into different energetic components:

$\Delta E_{int} = \Delta E_{orb} + \Delta E_{elect} + \Delta E_{pauli}$ (1)

Within the framework of the mono-electronic approximation, the orbital interaction energy (ΔE_{orb}) represents the stabilizing interactions that are established between two electrons and their respective orbitals.

The electrostatic energy (ΔE_{elect}) quantifies the interaction between the fragments, based on the distribution of their electron density.

The Pauli repulsion energy (ΔE_{pauli}) arises from the fact that two electrons with the same spin cannot occupy the same spatial region, which generates a destabilizing effect.

This quantitative analysis aims to evaluate the relative importance of ionic and covalent interactions in the coordination bonds of M-EDTA complexe (where M = Ni, Zn, Fe). The energy decomposition is performed according to equation (1), following the original method by Morokuma, as it was improved by Ziegler and Rauk [2].

Keywords
EDA, DFT, EDTA

Caractérisation physico-chimique du charbon actif dérivés des résidus agricoles locaux et leur efficacité dans l'élimination des polluants

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Abstract **–** This study aims to characterize an activated carbon used for the removal of pollutants from aqueous solutions using a combination of Scanning Electron Microscopy (SEM), Energy Dispersive X-ray Spectroscopy (EDX), and X-ray Diffraction (XRD). The SEM analysis revealed a porous surface structure of the activated carbon, with well-distributed pores that are favorable for adsorption processes. EDX analysis provided detailed information on the elemental composition of the activated carbon surface, highlighting the presence of carbon, oxygen, and trace amounts of metals. XRD analysis showed that the activated carbon has a predominantly amorphous structure with minimal crystalline phases, which suggests a high surface area ideal for pollutant adsorption. Adsorption tests demonstrated that the activated carbon is particularly effective in removing heavy metals and organic pollutants such as dyes and pharmaceutical residues from water. The combined use of SEM, EDX, and XRD offered valuable insights into the relationship between the structural and chemical properties of the activated carbon and its adsorption performance. This study underscores the importance of understanding the surface morphology and crystallinity of activated carbon to enhance its effectiveness in water treatment applications.

Keywords – adsorption, characterization, xrd,sem,edx

Étude comparative de l'extraction et de la composition phénoliques de deux plantes médicinales: Tisane et thé

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Résumé – *Aloysia citriodora* et *Camellia sinensis* sont des plantes médicinales qui sont largement utilisées en médecine traditionnelle en Algérie. L'objectif de cette étude est d'étudier la composition phénolique et flavonoïde obtenus par macération, Les rendements sont 7.95 % et 15.15% pour la Tisane et le Thé respectivement. La teneur des polyphénols totaux a été déterminée en utilisant le réactif Folin-Ciocalteu, elles sont de l'ordre de 168,125mgEAG/g Ps et 120,65mgEAG/g Ps pour la Tisane et le Thé respectivement, et les flavonoïdes ont été évalués par la méthode des chlorures d'aluminium $AlCl_3$, la teneur est estimée à 34,275 mgEQ/ g Ps et 6,475 mgEQ/ g Ps pour la Tisane et le Thé respectivement. La teneur en cendre a été déterminée par la méthode de calcination, les valeurs obtenues par cette méthode nous ont permis de conclure que l'extrait de thé présente la plus grande teneur en cendres avec un taux de 46.95%. En fin, on peut dire que les deux plantes ne sont pas seulement médicinale et agroalimentaire ils sont aussi des sources de matériaux naturels qui ont un impact significatif sur le plan biologique.

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Keywords – Plantes médicinales, verveine, *Aloysia citriodora*, thé, *Camellia sinensis*, polyphénols, activité antioxydante.

Un polymère à empreinte moléculaire (PEDOT:PSS-Ppy-rGO) intégré dans une électrode flexible hybride 3D ultra-sensible pour la détection picomolaire de dopamine

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Résumé

Ce travail décrit le développement d'un nouveau capteur électrochimique pour la détection sélective et sensible de la dopamine (DA) construit à partir du nanocomposite polymérique PEDOT:PSS-Ppy-rGO. La plateforme de détection est obtenue par electro dépôt et réduction électrochimiques en une seule étape de PEDOT:PSS, Ppy et rGO sur la surface de l'électrode flexible sérigraphie (SPCE) pour améliorer l'efficacité du transfert d'électrons. La structure et la morphologie du capteur (MIP)SPCE/PEDOT:PSS-Ppy-rGO ont été caractérisées par la technique physicochimique : microscopie électronique à balayage (MEB). Les propriétés électrochimiques du capteur ont été étudiées par voltamétrie cyclique, spectroscopie d'impédance électrochimique et la voltametrie différentielle à impulsions. Le capteur électrochimique présente une large plage linéaire de détection allant de 0,1 nM à 12 nM. La limite de détection et la sensibilité obtenues sont de 8,47 picomolaires (pM) et 2,70 µA/nM, respectivement. L'analyse d'échantillons réels de dopamine a été réalisée avec un extrait d'échantillons de cerveau bovin dilués dans du PBS sous des conditions contrôlées. Enfin, le nanocomposite MIP 3D a démontré des attributs impressionnants en termes de sélectivité, de reproductibilité et de stabilité. De plus, l'efficacité de récupération observée lors des tests sur des échantillons réels confirme collectivement l'adéquation du capteur de dopamine développé pour diverses applications analytiques pratiques.

Mots clé – Polymère à empreinte moléculaire ; Dopamine ; Détection électrochimique ; PEDOT ; Ppy .

Fabrication and Characterization of TiO_2 Thin Films via Spin-Coated Sol-Gel Route

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Abstract –

Titanium Oxide TiO_2 has an interesting properties (high chemical stability, high refractive index and transparency in the visible...) that allow to use it in several applications. The Sol-Gel process is based on the conversion of a liquid into a solid phase by a series of chemical reactions of the hydrolysis and condensation type of the molecular solution of extreme purity. In all samples, the starting solution contains Titanium Tetraisopropoxide used as dissolved with different solvent ethanol, methoxy, methanol, and propanol then we deposited on glass substrates by sol-gel method. The films were analyzed by the UV-Visible spectroscopy, and the SEM.

The results obtained by the UV-Visible spectrum indicated that the transmission of the films in the visible is about 90%. The preferential orientation is (101). The surface morphology was studied by using the Scanning Electron Microscope.

Keywords – Thin films, Titanium Dioxide, Sol-Gel (spin-coating), solvents.

Caractérisation et performance du charbon actif dérivé de cheveux humains pour l'adsorption d'un colorant textile

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Abstract

L'industrie textile est largement identifiée comme l'une des principales sources de pollution à l'échelle mondiale, engendrant des rejets annuels qui dépassent les cent millions de mètres cubes. Face aux défis environnementaux critiques posés par les polluants issus de ce secteur, la nécessité d'identifier et de mettre en œuvre des solutions efficaces est devenue une évidence pressante.

La présente étude explore l'utilisation de charbon actif préparé à partir de cheveux humains pour l'élimination d'un de ces colorants textiles en solution aqueuse par adsorption. L'adsorbant a été caractérisé par diverses analyses physicochimiques, notamment la spectroscopie infrarouge à transformée de Fourier (FTIR), la diffraction des rayons X (DRX) et la détermination du point de charge zéro (pHpzc).

De plus, des tests tels que la mesure de la teneur en humidité, les indices de tétrachlorure de carbone, de benzène et d'iode, ainsi que l'adsorption de bleu de méthylène, ont été réalisés pour évaluer les qualités et les performances du charbon actif.

L'influence du temps de contact, du pH et de la température sur le processus d'adsorption a été étudiée. Les résultats ont montré que l'équilibre est atteint après 60 minutes, et que la cinétique d'adsorption est bien décrite par un modèle de pseudo-second ordre. L'étude démontre l'efficacité du charbon actif issu de cheveux humains pour l'adsorption du Vert Acide 4G, avec un taux d'élimination atteignant 98,50 %.

Keywords – Colorant; charbon actif; cheveux humain; cinétique;Adsorption

Optimisation du dosage direct des ions Cr(VI) par Spectrophotométrie UV-Visible – Application à la spéciation du chrome dans l'eau

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Résumé **–** L'objectif de la présente étude et de proposer une méthode simple et accessible pour la détermination des concentrations des espèces du chrome dans l'eau. Le dosage direct des ions Cr(VI) par spectrophotométrie UV-visible est optimisé puis utilisé pour le dosage des ions Cr(III) et le dosage du chrome total. Les effets du pH et de la présence des ions étrangers sont évalués.

Les résultats obtenus, montrent que le dosage direct des ions Cr(VI) peut être réalisé à pH ≤6 à 350nm avec une droite d'étalonnage qui s'étale jusqu'à 100mg/L, et à pH ≥8 à 372nm avec une droite d'étalonnage qui s'étale jusqu'à 25mg/L. Dans les deux cas, la limite de détection est de 0,02mg/L. Dans les eaux chargées en ions métalliques autres que ceux du fer, le dosage doit être réalisé à pH très acide (pH: 2). La présence des anions oxalate, citrate, acétate, tartrate n'a aucun effet. Le dosage direct des ions Cr(VI) ne peut pas être réalisé dans le domaine de pH 6,5<pH<8 et en présence des ions Fe(II) et Fe(III).

En milieu alcalin, le dosage direct des ions Cr(VI) peut être bien appliqué au dosage des ions Cr(III) après oxydation par H2O2 en absence des ions Ni(II), Cd(II), Zn(II), Fe(II), Fe(III), et Mg(II). La présence des ions Co(II), Cu(II), Mn(II), oxalate, citrate, acétate et tartrate n'a aucun effet. Dans les mêmes conditions, la méthode de dosage proposée permet le dosage du chrome total.

Mots clés: *analyse des eaux, spectrophotométrie UV-visible, Cr(VI), Cr(III), métaux de transition*

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Utilisation des charbons à base de noyaux de dattes pour l'adsorption du produit organique

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Abstract – Cette étude souligne l'importance de l'innovation et de la chimie écologique pour élaborer des solutions durables face aux enjeux environnementaux contemporains. Le recours à des matériaux biosourcés pour la purification de l'eau représente un progrès notable vers des méthodes industrielles plus durables et responsables, contribuant ainsi à la préservation de notre environnement et de nos ressources naturelles.

Ce travail porte sur l'analyse du processus d'adsorption de la matière polluante bémacide bleu (BB) sur des matériaux dérivés de végétaux robustes tels que les noyaux de dattes. Dans un premier temps, nous avons procédé à la synthèse de charbons de diverses tailles de particules (d1 et d2) à partir des noyaux de datte par calcination.

Nous avons opté pour une étude de l'élimination du BB par les charbons ayant les plus hauts taux de rétention, 98,65 % pour le charbon (C-d1) et 87,73 % pour le charbon (C-d2). D'après nos tests, il s'agit des charbons calcinés à 700°C.

Des tests d'adsorption ont été réalisés pour déterminer l'affinité des charbons synthétiques envers le BB afin d'améliorer son élimination. L'analyse cinétique indique que l'équilibre est atteint après dix minutes pour C-d1 et deux minutes pour C-d2, et que le modèle du pseudo-second-ordre est celui qui représente le processus d'adsorption.

Les données thermodynamiques suggèrent que l'adsorption du BB sur C-d1 est un processus endothermique, tandis que la fixation du BB par C-d2 est exothermique.

Keywords – noyaux de dattes ; matériaux ; fixation du BB ; processus d'adsorption ; données thermodynamiques.

Valorisation de *Carlina hispanica* : Extraction et caractérisation de l'oxyde de carline et exploration de ses propriétés bioactives

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L'Algérie, caractérisée par sa diversité bioclimatique, possède une flore riche en métabolites naturels bioactifs. Dans ce contexte, cette étude s'intéresse à *Carlina hispanica*, une plante médicinale réputée pour sa richesse en composés acétyléniques, dans le but de valoriser son huile essentielle à travers une double approche chimique et biologique.

L'huile essentielle a été extraite des parties aériennes par hydrodistillation. L'analyse chimique a été réalisée par chromatographie en phase gazeuse (CPG) et CPG couplée à la spectrométrie de masse (CPG/SM). Le composé majoritaire, l'oxyde de carline, a été isolé par chromatographie sur colonne puis identifié par des techniques spectroscopiques, notamment la RMN.

Les propriétés biologiques de l'huile ont été évaluées par des tests antioxydants (DPPH, β-carotène, $FeCl_2$), antimicrobiens (diffusion sur disque, microplaque) et anti-inflammatoires (inhibition de la dénaturation protéique). Des substances standards (BHT, EDTA, gentamicine, amphotéricine B, diclofénac) ont été utilisées comme références.

L'huile essentielle s'est révélée riche en oxyde de carline (81,1 %), lequel a montré une activité antioxydante, antifongique et anti-inflammatoire significative. Ces résultats suggèrent le potentiel thérapeutique de cette molécule naturelle.

En conclusion, *Carlina hispanica* apparaît comme une source prometteuse de composés bioactifs, et l'oxyde de carline se positionne comme un candidat intéressant pour le développement de produits naturels à visée thérapeutique ou cosmétique.

Keywords : Carlina *hispanica*, oxyde de carline, activité biologique, spectroscopie RMN, CPG/SM.

Clay-polymer biocomposites: valorization of raw materials and adsorbents of the future for water treatment

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Abstract – Biocomposites can be defined as materials that consist of two or more chemically and physically different phases separated by a distinct interface. Alginate obtained from cell walls of brown sea-weed is the most widely used biopolymer for preparing hydrogel beads for wastewater treatment due to their biocompatibility, biodegradability, large scale availability, lower cost and nontoxicity. Clays supported on calcium alginate beads have been reported to improve the mechanical and thermal stabilities of the beads and to simplify the separation procedures compared to the use of natural clay.

The purpose of this study is to prepare bio-adsorbent beads based on citrus peel waste, Algerian bentonite, activated carbon and calcium alginate for the removal of two organics polluants from industry wastewater in discontinuous modes. The identification of adsorbent was carried out by various analyzes: elemental analysis, FTIR spectroscopy, X-rays diffraction (DRX), BET, and SEM. The adsorption of bisphenol A and trichlorophenol by the bio-adsorbent was carried out according to various parameters which influence the process such as, the initial concentration of the adsorbate, the pH of the adsorbate solution and temperature. Isotherms and adsorption kinetics have also been studied and treated with different mathematical models. The results showed that the kinetics followed the pseudo-second-order model and the isotherms are well described by the Langmuir model

Keywords – Marterial, morphology, polymer, Adsorption, biocomposite, alginate.

Antimicrobial activity of Peganum.harmala essential oil against several bacteria and fungi

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Abstract **–** Infectious diseases have always been the number one enemy threatening health and well-being. With increasing numbers of infectious diseases, growing resistance of pathogens, and declining roles of antibiotics in the treatment of infectious diseases, it is becoming increasingly difficult to treat new infectious diseases, and there is an urgent need to develop new antibiotics to change the situation. Natural products tend to exhibit many special biological properties. The genus *Peganum* (Zygophyllaceae) has garnered significant attention for it is rich in bioactive compounds, that exhibit potent antibacterial, antifungal, antiviral, and antiparasitic activities. This Research highlights the plant's ability to inhibit a variety of pathogenic microorganisms by assessing the antibacterial activity of the essential oil against several bacteria and fungi using disc diffusion method on MH medium. The results showed that the fungal strains are very sensitive with a significant effect on LCP, LCK, L23, L43, *LRM* with diameters ranging from 22.5 mm, 61 mm, 42.5 mm and 57.5 mm, 19mm respectively. As for tested bacteria, the results show a very strong inhibitory activity against *P.aeuroginosa* and a slight inhibitory activity was observed on the *Staphylococcus aureus* strain with a diameter of 18 mm. While the bacterial strains *Bacillus subtilis*, *Micrococcus luteus* marked no inhibitory zone. In the present work, the agar diffusion test showed that the EO of *P. harmala* have high antimicrobial property and have the potential to inhibit multi drug resistance strains.

Keywords – Antimicrobial activity ; Peganum harmala ; essential oil ; microorganisms ; pathogens.

Séparation de bleu de méthylène de l'eau par adsorption sur les nanoparticules de maghémite modifiées et imprégnées dans des capsules d'alginates

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Résumé **–** Dans ce travail, nous présentons la méthode de préparation de nanoparticules magnétiques de maghémite (γ-Fe_2O_3) ainsi que leur encapsulation dans des billes d'alginate afin d'obtenir des billes magnétiques (A/γ-Fe_2O_3). Ces matériaux ont été caractérisés par différentes techniques analytiques en vue de leur utilisation comme adsorbants pour la séparation du bleu de méthylène de l'eau.

Pour prédire les quantités maximales de bleu de méthylène adsorbées par nos matériaux, des isothermes d'adsorption ont été étudiées. Les résultats ont montré que la quantité adsorbée augmente progressivement jusqu'à atteindre un plateau correspondant à la capacité maximale d'adsorption. Les modèles de Langmuir et de Freundlich ont été appliqués à nos données expérimentales. Les coefficients de corrélation (R^2), obtenus par régression non linéaire, indiquent que le modèle de Langmuir s'ajuste mieux aux données. Cela suggère que l'adsorption se fait sur des sites énergétiquement identiques, impliquant que les sites actifs de la maghémite et de l'alginate interagissent de manière similaire avec le bleu de méthylène, conduisant à une adsorption en monocouche.

Les capacités d'adsorption maximales théoriques de γ-Fe_2O_3 et A/γ-Fe_2O_3 (155,25 et 438,6 $mg \cdot g^{-1}$, respectivement) sont proches des valeurs expérimentales obtenues (141,3 et 418,7 $mg \cdot g^{-1}$, respectivement), ce qui est confirmé par la superposition des isothermes théoriques de Langmuir. Ces résultats confirment l'efficacité de ces matériaux comme adsorbants prometteurs pour l'élimination du bleu de méthylène, tout en soulignant leur caractère magnétique, qui facilite leur séparation rapide et efficace après le traitement des eaux. d.

Mots clés – eau; adsorption; bleu de méthylène; maghémite; alginate.

Extracts of wormwood as green inhibitors of corrosion of XC55 steels in acidic media

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Abstract – The protection of the environment and especially of materials is a priority for scientists and industrialists. In this context, to combat corrosion often encountered in industry, is used to test and evaluate extracts or oils of the Sagebrush plant as corrosion inhibitors against acidic media such as 1N hydrochloric acid from API X55 carbon steel. Three extracts were prepared using solvents, then the study of the inhibitory effect of these extracts on API X55 steel in a hydrochloric acid medium is started. The results obtained from weight loss measurements indicate that the first extract has good corrosion resistance with an efficiency of 81,62% at 25°C, the second with an efficiency of 75.32% and the third 77.39%. The thermodynamic adsorption coefficients indicated the presence of spontaneous adsorption on the surface of the XC55 steel according to the Langmuir isotherm of the extract of the three solvents. These results indicate that these extracts can be used as green corrosion inhibitors.

Keywords – Corrosion, green inhibitor, steel API XC55

Study of Corrosion Inhibition of Mild Steel in H_2SO_4 by a Green Plant Extract: Effects of Temperature and KI

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Abstract **–** This study focuses on evaluating the corrosion inhibition efficiency of *Agave americana* extract (EAA) for mild steel in a 0.5 M H_2SO_4 solution, at concentrations of 500, 1000, 1500, and 2000 ppm. The synergistic effect of potassium iodide (KI) at 10^{-3} M, as well as the influence of temperature, were investigated using Electrochemical Impedance Spectroscopy (EIS). Surface analyses were also carried out using Scanning Electron Microscopy (SEM) and Atomic Force Microscopy (AFM). The impedance spectra obtained in the presence of EAA exhibited a single capacitive loop, indicating a charge transfer-controlled mechanism. The maximum inhibition efficiency reached 76.58% at 2000 ppm. The addition of 10^{-3} M KI significantly enhanced the inhibition performance, increasing the efficiency to 81.87% at the same EAA concentration. The temperature effect was studied at 298, 308, 318, and 328 K. A maximum efficiency of 94.78% was observed at 328 K in the presence of the synergistic system (2000 ppm EAA + 10^{-3} M KI). The observed decrease in activation energy in this case suggests a chemisorption mechanism. AFM observations revealed a notable decrease in the average surface roughness after treatment with 2000 ppm of EAA, confirming the formation of a protective adsorbed film on the mild steel surface.

Keywords – Corrosion; green inhibitor; electrochemistry; characterization; medium.

Potential of ionic liquids (ILs) in organic synthesis: a literature approach

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Abstract – In the current context of sustainable chemistry, the search for more environmentally friendly reaction media has become a priority. Ionic liquids (ILs) have thus emerged in recent years as versatile tools in organic synthesis, capable of acting simultaneously as solvents, catalysts, or supports. Their modular structure allows their physicochemical properties to be precisely adjusted to the specific requirements of the reactions, which contributes to improving their efficiency, selectivity, and sustainability. This multifunctionality paves the way for greener and more efficient catalytic processes. In addition, ILs have demonstrated their effectiveness in a wide range of transformations, whether single-step or multi-step reactions, in homogeneous or two-phase media. Thanks to these characteristics, they now appear as essential levers for the optimization of modern organic processes and the transition to more sustainable chemistry.

Keywords – ionic liquids (ILs); organic synthesis; catalysis.

Valorisation des feuilles d'une plante de la famille des Astéracées : extraction par ultrason et potentiel antioxydant

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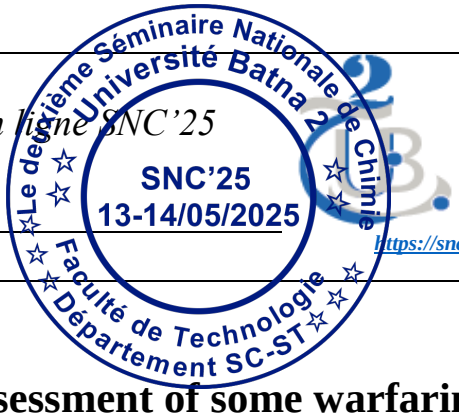
Résumé **–** L'extraction des composés phénoliques à partir des feuilles d'une plante de la famille des Astéracées a été réalisée à l'aide de la technique d'extraction assistée par ultrasons. Cette méthode, considérée comme respectueuse de l'environnement, présente de nombreux avantages, notamment un gain de temps, une réduction de la consommation de solvant et une meilleure préservation des composés bioactifs. L'objectif de cette étude était d'obtenir un extrait riche en polyphénols totaux (TPC), des métabolites secondaires dotés de propriétés antioxydantes, anti-inflammatoires et protectrices vis-à-vis du stress oxydatif. L'extraction a été conduite à l'aide d'une solution hydroalcoolique à 55 % d'éthanol, à une température modérée de 35 °C, pendant 10 minutes. Sous ces conditions, le rendement en TPC a atteint 222,46 mg EAG/g d'extrait sec, ce qui met en évidence l'efficacité du procédé utilisé. Par ailleurs, l'évaluation de l'activité antioxydante de l'extrait par le test DPPH a révélé un taux d'inhibition radicalaire élevé, à hauteur de 91,46 %, confirmant la richesse de l'extrait en composés actifs. Ces résultats suggèrent un fort potentiel de valorisation de cette plante dans des domaines tels que la cosmétique et l'agroalimentaire.

Mots clés– Astéracées, extraction, polyphénols, activité antioxydante, DPPH.



DFT calculation and toxicity assessment of some warfarin derivatives

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Abstract **–** Warfarin is one of the potent vitamin K antagonists. Its derivatives have shown higher anticoagulant activity compared to warfarin itself. Therefore, we decided herein to investigate chemical, structural, electrical properties and the toxicity of some novel warfarin derivatives.

Density functional theory (DFT/B3LYP) with 6-311G++ (d,p) as a basis set was used to have insight into warfarin derivatives reactivity. Hence, their electronic properties of the studied compounds have been calculated using Maestro. It is worth pointing that all the derivatives had lower energy gap than warfarin which indicates their higher reactivity. Overall, all the derivatives had a positive values of chemical softness (S) chemical hardness (η) that allow assuming the derivatives ability to participate in molecular interactions.

Toxicity assessement of the studied derivatives was performed in order to ensure their safety. ProTox-II web tool results clearly indicated that the studeied compounds are non- mutagenic, non-cytotoxic, non-carcinogenic, non-cardiogenic, non nephrogenic and have no nutritional toxicity.

Based on these results it can be assumed that these new warfarin derivatives will potentially be promising for anticoagulant therapy.

Keywords –DFT; toxicity; warfarin; derivatives.

Enhanced Optical and Electrical Properties of Electrodeposited ZnO Thin Films for High-Frequency Optical Sensing Applications

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Abstract **–** In this work, zinc oxide (ZnO) thin films were prepared on ITO substrates using electrodeposition technique at different applied voltages of 7 V, 8 V, and 9 V. The structural, optical, and electrical properties of the films were studied using X-ray diffraction (XRD), UV–Vis, and Hall effect measurements. The results revealed that the prepared films exhibit a hexagonal wurtzite structure with a preferred growth direction along the (002) plane, along with an improved grain size. The optical properties showed high transparency in the visible light region and strong absorption in the UV region. The electrical measurements indicated an increase in the charge carrier concentration and mobility (both electrons and holes), a decrease in the resistance, and an enhancement in the conductivity with increasing applied voltage. Based on these results, high-frequency optical sensors were simulated using the prepared ZnO thin films. The results showed promising optical and electrical properties, including energy conversion efficiencies. The results demonstrate promising energy conversion efficiencies of 20.64, 20.72 and 20.78% for ZnO thin films deposited at − 7, − 8, and − 9 V/SCE respectively, This confirms the suitability of the prepared ZnO thin films for high-frequency optical sensing applications.

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Keywords – High-frequency optical; ZnO thin films; Electrical proprieties.

Adsorption Study of Textile Dye basic blue Sandocryl onto pods of wild carob

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Abstract – Large quantities of dye have been discharged into the aquatic environment without appropriate treatment. Industrial wastewater has caused serious environmental and health problems. This work is dedicated to studying the process of removing a basic dye, blue Sandocryl BS, using an adsorbent derived from natural waste, specifically the pods of wild carob (GC). The results of this removal show that: an adsorbent dose of 0.5 g/L, a contact time of 60 minutes, and the natural pH of the BS solution for a concentration of 20 mg/L are the optimal conditions. Under these conditions, the BS removal rate is 92.85%, with a capacity of 36.91 mg/g. The kinetics of BS removal by the GC adsorbent align better with the pseudo-second-order model, showing an excellent correlation coefficient (R^2). The study of the influence of temperature allows to assess the thermodynamic values. These values show that the adsorption is exothermic and spontaneous.

Keywords – Bleu sandocryl, Adsorption, Valorization, Environnement

Effect of a new green catalyst on methyl salicylate synthesis

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Abstract **–** Currently, acid catalysts are widely used in various organic synthesis processes to enhance reaction efficiency, reduce reaction times, and improve product yields. However, the use of these acid catalysts can also present significant drawbacks.

This project explores an innovative and sustainable alternative: **banana peel ash**, a natural catalyst, for the synthesis of **methyl salicylate**—an ester of great interest due to its valuable biological properties.

The study also investigates the influence of several key parameters on the reaction's yield and kinetics, such as catalyst amount, temperature, and catalyst regeneration

Based on the results obtained, banana peel ash has proven to be a highly efficient natural catalyst for the synthesis of methyl salicylate. This finding opens promising perspectives for its application in the synthesis of various organic compounds, representing a significant advancement in green chemistry through the valorization of agricultural waste.

Noteworthy aspects of this protocol include high yields, short reaction times, catalyst recyclability, and simple product isolation.

Keywords- Esterification; Banana peel; Heterogeneous catalyst; Methyl Salycilate

Computational analysis of corrosion inhibition by an organic compound

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Abstract **–** Computational methods have become invaluable tools in the study of corrosion and corrosion inhibition, offering a cost-effective and efficient way to evaluate the properties of inhibitor molecules and their interactions with metallic surfaces. Various computational techniques have been employed for this purpose, including molecular dynamics (MD) simulations, Monte Carlo (MC) simulations, and density functional theory (DFT). The objective of this study is to perform a quantum calculation based on DFT. The DFT-based quantum chemical calculation was achieved by means of the Dmol3 module to obtain the complete geometrical optimized structure of organic molecule type of quaternary ammonium. The GGA exchange-correlation function and a double numerical basis set with polarization (DNP) were chosen. The quantum chemistry in order to calculate the electronic proprieties such us: highest occupied molecular orbital energy (E_{HOMO}), lowest unoccupied molecular orbital energy (E_{LUMO}), LUMO-HOMO energy gaps(ΔE), dipole moments(μ), ionization potential (I), hardness (η), and softness (σ). The MC simulations were utilized to investigate the adsorption orientation and interaction of the corrosion inhibitor on mild steel with Fe (110).

Keywords –Corrosion inhibitor, computational methods, DFT, MC simulation, organic compound.

Traitement des eaux riches en polluants organiques par une matrice à base d'hydroxyapatite

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Abstract **–** Le secteur textile est l'un des plus grands utilisateurs de colorants, et ses opérations de teinture nécessitent des quantités significatives d'eau, d'énergie et de substances chimiques. Cette activité engendre ainsi des effluents abondants, fréquemment contaminés par des polluants tels que les métaux lourds, les composés organiques résistants à la dégradation et divers sels. Ces rejets représentent un risque majeur pour les milieux aquatiques et peuvent également avoir des effets néfastes sur la santé humaine.

La présente recherche porte sur le développement de granulés poreux à base d'hydroxyapatite et de métakaolin (HAP-MK-GP). Elle vise principalement à examiner leur potentiel en tant que matériaux adsorbants pour la dépollution de solutions aqueuses contenant différents types de colorant. L'étude met en lumière les capacités d'adsorption du matériau conçu, tout en explorant de manière approfondie les mécanismes physico-chimiques régissant l'interaction entre les sites actifs des granulés et les molécules de colorant.

Keywords: colorants organique, hydroxyapatite, géopolymère, adsorption

Theoretical Study Transition metal Complexes OF N, S- Derivatives Ligands

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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

Phytochemical Constituents and Antioxidant Activity of Peels of Two Citrus Varieties

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Abstract

Citrus fruits, celebrated for their nutritional and sensory attributes, generate peels that constitute 50-60% of the fruit's mass. These peels, often discarded, are rich in bioactive compounds, making them valuable for sustainable food innovation and functional beverage development. This study compares the phytochemical composition and antioxidant activity of Citrus aurantium (bitter orange) and Citrus limetta (sweet lemon) peels. Peels were processed into powders and analyzed for physicochemical properties and phytochemicals. At 25% incorporation, C. aurantium peels showed higher polyphenol (data not specified), flavonoid (16.25±0.056 mg/100g), flavonol (25.71±0.042 mg/100g), and tannin (1734.01±0.113 mg/100g) content, while C. limetta peels had elevated carotenoids (1047.3±0.056 mg/100g). Antioxidant activity, assessed via DPPH (49.35±0.282% inhibition for C. aurantium vs. lower for C. limetta) and ABTS (87.81±0.226% inhibition for C. aurantium vs. lower for C. limetta) assays, was stronger in C. aurantium, reflecting its richer phytochemical profile. Both varieties enhanced beverage nutritional value, with increasing powder incorporation boosting phytochemical content and antioxidant capacity. These results highlight citrus peels as potent natural antioxidant sources, with C. aurantium and C. limetta offering distinct profiles for tailored functional beverages, promoting health and by-product valorization.

Keywords – Citrus peels, bioactive compounds, phytochemicals, antioxidants, antioxidant activities, functional beverage.

Proteomic analysis of sweet kernel of an Algerian apricot variety (*Prunus armeniaca L.*) by combinatorial peptide ligand libraries and LC-MS/MS

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Abstract – *Prunus armeniaca* L., commonly known as the apricot, is a widely cultivated fruit-bearing plant, particularly prevalent in the Mediterranean region and Algeria is currently the 5th world producer with 239,700 tonnes (FAO, 2010). The plant is renowned for its nutritional richness, containing sugars, mono- and polysaccharides, polyphenols, fatty acids, sterol derivatives, carotenoids, glucosides, and volatile compounds. From time immemorial, *P. armeniaca L.* has been used in folk medicine as a remedy for various diseases, and only recently has it been investigated for its biological activities, such as antimicrobial, antioxidant, hepatoprotective, and anti-inflammatory effects. The beneficial effects on health are primarily due to the presence of unsaturated fatty acids. However, the importance of proteomic investigation to further understand its nutritional function has not been thoroughly evaluated. We here propose a proteomic evaluation of apricot kernel in order to update the *armeniaca* data bank including the minor protein components. The proteomic approach based on Combinatorial peptide ligand library technology, coupled to mass spectrometry, has been applied to extensively map the proteome of apricot seed identifying 178 proteins. Bioinformatics analysis using Gene Ontology (GO) classification of their biological functions was also performed. A preliminary investigation using an *in silico* web-available BIOPEP tool suggested that the two most abundant expressed proteins, Prunin1 and Prunin2 appear to contain tetra- and tripeptides with potential angiotensin-converting enzyme I (ACE) inhibitory and antioxidant activities, as well as the ability to stimulate the release of vasoactive substances.

***Keywords*:** Apricot; combinatorial peptide ligand libraries (CPLL); GO analysis; LC-MS/MS; proteomics.

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

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Abstract

Industrial wastes contain significant amounts of heavy metals that can harm human health and threaten the ecosystem. The development of innovative technologies that respect the environment has become essential to protect them. To this end, new approaches minimizing the risks of hazardous chemicals, and in particular green chemical engineering for the extraction of heavy metals from industrial wastes must be widely developed.The aminopolycarboxylate (APC) acids have been widely used as ligands to capture heavy metals. Therefore, the APC structures are also known for their good possibilities for heavy atom recovery.[1]

Conceptual density functional theory (DFT) is widely applied in various fields to understand chemical reactions using the isolated properties of reactants.[2]

Due to the low biodegradability and toxicity of traditional APCs such as EDTA and NTA, it has become highly desirable to substitute them with biodegradable and environmentally friendly chelating agents such us EDDM and EDDG.

Currently, several industrial research groups are investigating whether new agents such as $EDDS^{4-}$, $EDDM^{4-}$, $EDDG^{4-}$, …., can replace the previous generation of chelating agents like $EDTA^{4-}$ and NTA^{3-}. Additionally, they are examining whether the reaction conditions used in various industries that utilize $EDTA^{4-}$ need to be modified to achieve maximum efficiency with easily biodegradable replacement ligands. The answers lie in the predominant chemical speciation in industrial processes and the reaction kinetics between these chelants and metal ions.

Keywords –APC, DFT, EDTA, EDDM and EDDG

Synergistic Effect of Cefalexin and Zn-Fe Alloy Coatings for Corrosion Protection of SAE 1008 Steel in Acidic Media

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Abstract – This study investigates the potential of cefalexin, a β-lactam antibiotic, as a corrosion inhibitor for SAE 1008 steel in a 1 M HCl solution, in combination with Zn-Fe alloy coatings. Electrochemical measurements, gravimetric analysis, and microstructural characterization techniques (SEM-EDS) were employed to evaluate the corrosion resistance of the coated samples. The results demonstrate that Zn-Fe coatings significantly mitigate steel corrosion, and the incorporation of cefalexin further enhances the protective effect, particularly at higher concentrations. Morphological analyses reveal notable alterations in the coating's structure and composition depending on the inhibitor concentration, highlighting the potential of this combined approach for industrial applications requiring robust corrosion protection in aggressive environments.

Keywords – Corrosion, Zn-Fe alloy, Corrosion inhibitor, SAE 1008 steel, SEM-EDS

Application d'une nouvelle génération d'agents complexants pour l'élimination des ions métalliques lourds dans divers déchets.

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Résumé :

Les agents complexants sont largement utilisés dans de nombreux secteurs industriels, car ils permettent de contrôler efficacement les ions métalliques traces dans des domaines tels que le nettoyage, le textile, la production de pâtes et papiers, le traitement des eaux, l'agriculture et l'industrie agroalimentaire. Cependant, la faible biodégradabilité de ces ligands et leur accumulation dans l'environnement suscitent de plus en plus de préoccupations. Il est donc souhaitable de remplacer l'acide éthylènediaminetétraacétique (EDTA) et l'acide diéthylènetriaminepentaacétique (DTPA) par des agents chélatants plus respectueux de l'environnement. Jusqu'à présent, ces acides et leurs sels ont été utilisés comme composants dans des produits chimiques ménagers, des cosmétiques, des engrais modernes à base de microéléments et des produits agrochimiques.

L'objectif de ce travail est d'étudier la complexation des métaux de transition avec des ligands de nouvelle génération en utilisant des méthodes de fonctionnelle de densité. Des optimisations géométriques et un modèle de solvatation du continuum (COSMO) ont été réalisés. Les énergies de solvatation des métaux Mn^{2+}, Co^{2+}, Ni^{2+}, Cu^{2+} et Zn^{2+}, ainsi que leurs énergies de complexation avec des ligands de nouvelle génération (de charge totale -2), ont été calculées. Nous avons démontré que la réaction de complexation des métaux de transition avec ces ligands de nouvelle génération est favorable, conduisant à la formation du complexe métal-ligand le plus stable.

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Keywords – Aminopolycarboxylate, DFT, GLDA. ISA

Analyse chimique des panneaux solaires dégradés dans les zones désertiques par les techniques EDS et XRD

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Résumé :

Cette étude porte sur l'analyse chimique approfondie des panneaux solaires ayant subi une dégradation dans les environnements désertiques, en utilisant les techniques complémentaires de spectroscopie à dispersion d'énergie (EDS) et de diffraction des rayons X (XRD). Dans les régions désertiques, les panneaux photovoltaïques sont exposés à des conditions environnementales extrêmes, notamment des températures élevées, des variations thermiques importantes, une forte irradiation UV et des particules abrasives transportées par le vent, qui accélèrent leur détérioration.

Notre recherche a examiné trois échantillons de panneaux solaires (S1, S2 et S3) ayant respectivement 17, 13 et 7 ans d'exploitation dans des conditions désertiques. L'analyse EDS a révélé la présence progressive d'éléments contaminants comme l'aluminium, le calcium et le silicium provenant des dépôts de poussière, ainsi qu'une oxydation croissante des contacts métalliques. La quantification des éléments a démontré une corrélation directe entre la durée d'exposition et le niveau de contamination superficielle.

Les analyses XRD, complétées par un affinement de Rietveld, ont permis d'identifier les phases cristallines présentes et leur évolution temporelle. Un pic caractéristique à 2θ=28,1° correspondant à la phase de quartz a été observé dans tous les échantillons, avec une intensité variable suggérant des modifications structurelles progressives. L'échantillon le plus ancien (S1) présente des pics additionnels à 2θ=13°, 21°, 26° et 29,1°, absents dans les échantillons plus récents, indiquant la formation de nouvelles phases cristallines résultant probablement de la dégradation à long terme.

Les résultats obtenus contribuent à une meilleure compréhension des mécanismes de dégradation des panneaux solaires en milieu désertique et pourraient guider le développement de revêtements protecteurs plus efficaces et de protocoles de maintenance adaptés pour prolonger la durée de vie des installations photovoltaïques dans ces environnements hostiles.

Mots-clés:
Énergie photovoltaïque, dégradation des panneaux solaires, environnement désertique, spectroscopie EDS, diffraction XRD, affinement de Rietveld, contamination de surface, phases cristallines, vieillissement des matériaux, énergies renouvelables.

Caractérisation de la résistance à la corrosion des revêtements en alliage Zn-Ni électrodéposés

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Abstract **–** La corrosion constitue un défi majeur dans de nombreux secteurs industriels, entraînant d'importantes pertes économiques. Cette étude porte sur l'électrodéposition de revêtements en alliage Zn-Ni sur de l'acier doux (à faible teneur en carbone) et évalue leur résistance à la corrosion. Différents bains électrolytiques ont été préparés, avec et sans l'incorporation d'additifs organiques tels que la saccharine et le 2-butyne-1,4-diol.

Les résultats montrent que l'utilisation de ces additifs améliore significativement les propriétés des revêtements, notamment une microdureté accrue, une rugosité de surface réduite et une meilleure résistance à la corrosion. Les analyses EDS et DRX ont révélé une teneur plus élevée en nickel dans les revêtements contenant des additifs, ce qui est corrélé à un déplacement du potentiel de corrosion vers des valeurs plus anodiques et à une résistance à la polarisation accrue.

Le revêtement formulé avec à la fois de la saccharine et du 2-butyne-1,4-diol a montré les meilleures performances, présentant la microdureté la plus élevée, le taux de corrosion le plus faible et la plus grande résistance au transfert de charge. Ces résultats mettent en évidence le potentiel des revêtements Zn-Ni enrichis en nickel, en particulier ceux élaborés avec des additifs organiques appropriés, comme candidats prometteurs pour prolonger la durée de vie des composants en acier dans des environnements corrosifs agressifs.

Keywords –Résistance à la corrosion – Électrodéposition – Additifs organiques – Protection – Revêtements en alliage Zn-Ni

Mechanistic Studies of Phenolic Antioxidant in Reaction with Hydroxyl and Superoxide Radicals

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Free radicals are chemical compounds with unpaired electrons. The most frequently encountered free radicals include superoxide anion radical ($O_2^{\cdot -}$), hydroxyl radical ($HO^{\cdot}$), alkyl radical ($R^{\cdot}$), alkoxy radical ($RO^{\cdot}$), peroxy radical ($ROO^{\cdot}$) and nitric oxide radical ($NO^{\cdot}$). Owing to the great potential of free radicals to react with various compounds by electron transfer, proton transfer, H-atom abstraction or addition reaction, they are considered responsible for a series of undesired processes, such as aging, material degradation, food deterioration and many diseases. Therefore, much interest has been focused on finding antioxidants to prevent the radical induced impairments in chemical, food and pharmaceutical industries.
Hydroxytyrosol and Tyrosol are phenolic antioxidants that exist in a variety of natural sources. The main source in human diet is olive oil. These two molecules are particularly interesting, and they are widely been used in the pharmaceutical field (e.g. the cardiovascular treatment and treatment against aging) because they are good scavengers of Reactive Oxygen Species (ROS) like hydroxyl ($HO^{\cdot}$) and superoxide ($O_2^{\cdot -}$) radicals.

This work is a theoretical study using quantum chemistry methods for studding of the hydroxytyrosol and the tyrosol with the radicalizing reactive species of oxygen ($HO^{\cdot}$ and $O_2^{\cdot -}$) by considering approaches of the radical towards potentially interesting sites of attacks.

Keywords- hydroxytyrosol, tyrosol, activity antioxidant, $O_2^{\cdot -}$, $HO^{\cdot}$, DFT.

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

Effective removal of methyl orange dye from water media using ZnAl-LDH@Biochar composite

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Abstract – Large quantities of dyes are produced and consumed daily across various industrial sectors, such as paper, cosmetics, pharmaceuticals, and especially the textile industry. Textile effluents typically contain a wide variety of dyes, among which azo dyes constitute a major class of synthetic organic compounds. Due to their toxicity, low biodegradability, and potential carcinogenicity, these dyes represent a significant source of water pollution, posing serious risks to aquatic ecosystems and human health. Therefore, their removal is essential for reducing pollution and protecting the environment.

In this study, ZnAl-LDH integrated with biochar were synthesized via a co-precipitation method subsequently calcination at 500 °C for 4 hours to develop a novel composite adsorbent for the elimination of methyl orange (MO) from aqueous solutions. The synthesized composite was characterized using XRD, FT-IR, SEM, and BET) analysis to determine its crystalline phases, functional groups, surface morphology, and specific surface area. Batch adsorption experiments were conducted to evaluate the removal performance of MO, focusing on adsorption kinetic, isotherm studies and the effect of initial solution pH. The kinetic data were best fitted by the pseudo-second-order (R^2 = 0.997) and Avrami (R^2 = 0.987) models compared the pseudo-first-order model (R^2 = 0.923) indicating that equilibrium was achieved after 3 hours of contact. Isotherm modeling of the adsorption data using Langmuir, Freundlich, and Redlich-Peterson equations revealed that the Langmuir model provided the best fit, with a calculated monolayer adsorption capacity of 768.01 mg/g. The point of zero charge (pH_{PZC}) of the composite was 10.73, with optimal MO removal observed at pH 7. Overall, this study highlights the hight potential of ZnAl@Biochar composite as efficient and cost-effective adsorbent for the removal of MO from wastewater.

Keywords – layered double hydroxides; biochar; composite; methyl orange; adsorption.

Removal of Organic Dyes (Methylene Blue and Brilliant Green) Using Dowex 50W x8 Resin: An Experimental Approach in Environmental Chemistry.

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Abstract **–** Water pollution caused by organic dyes such as Methylene Blue (MB) and Brilliant Green (BG) is a major environmental concern due to their toxicity and persistence. This experimental study evaluates the effectiveness of Dowex 50W x8 ion-exchange resin for the removal of these dyes from aqueous solutions. The results demonstrate that this material exhibits excellent adsorption capacity, achieving removal efficiencies exceeding 81% after just 50 minutes of contact. Analysis of operational parameters reveals that the process is strongly influenced by pH, with optimal adsorption occurring in acidic conditions for MB (pH 4-6) and in neutral to slightly basic conditions for BG (pH 6-7). Adsorption isotherm studies show that the system perfectly follows the Langmuir model, suggesting monolayer adsorption on the resin surface. Kinetic analysis indicates that the mechanism follows pseudo-second-order kinetics. Thermodynamic parameters confirm that the process is spontaneous and exothermic. These results position Dowex 50W x8 resin as an efficient, cost-effective, and environmentally friendly adsorbent for treating water contaminated with cationic organic dyes. The simplicity of implementation and demonstrated effectiveness open promising prospects for industrial applications in textile effluent treatment.

Keywords -- Adsorption, ion-exchange resin, Methylene Blue, Brilliant Green, kinetic modeling.

Synthesis, Characterization, crystal structure and Hirshfeld surface analysis of a binuclear Cu(II)-salen complex

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Abstract **–** The discovery of new transition metal complexes with salicylaldehyde Schiff base played a significant role in the growth and development of coordination chemistry for their applications, properties, interesting structures and wide range of physicochemical characteristics.

Salen ligands containing aromatic ring p-conjugated systems have also enabled metal complexes to exhibit fascinating electrical conducting properties. Salen ligand's simplistic synthesis route makes the development of metal complexes time-efficient and less expensive.

This research study presents a sound report on the synthesis, crystal structure, x-ray diffraction, FT-IR and Electrical characterization of a Cu (II)-Salen complex. $[Cu_2(C_{16}H_{14}N_2O_2)_2]$ was synthesized, and its structure was determined in triclinique space group P -1 with the following parameters: a=6.9171(10), b=13.729(2) , c=14.527(2) Å , α=97.390(12) , β = 87.390(12), γ=104.617(12) , and Z = 4. The crystal structure was stabilized by an extensive network of C-H....O hydrogen bonds, as well as π–π stacking interactions. Hirshfeld surface analysis indicates that the most significant contacts in the crystal packing are H···H (49.6%), C···H (14.1%).

Keywords – Schiff base complex, Single-crystal X-ray diffraction, Hirshfeld surface analysis,FT-IR.

Investigation of the antioxidant of the methanolic extract of aerial part of *Globularia alypum*

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Abstract – Medicinal plants are a very important source of therapeutic drugs for medical use because they contain a variety of secondary metabolites and bioactive chemicals that give them multiple therapeutic potentials. The goal of this research is to investigate some biological activities of the methanolic extract of the material part of Gloubular alypum. All preliminary tests have confirmed the presence of various metabolites like flavonoids, polyphenols, flavanols and other metabolites.
Additionally, various antioxidant activity will be assessed using two technics, DPPH and FRAP, and the inflammatory effect will be tested in vivo. According to the results, the extract exhibited strong anti-inflammatory activity and an important antioxidant activity with these concentrations 0,153, 0,116, and 0,110 (µg/ml). According to current research findings and comparisons with earlier studies, Gloubularia alypum exhibits therapeutic activity. This explains why it is used in alternative medicine and motivates us to conduct further research.

Keywords – Antioxidant activity, DPPH technic, Globularia alypum , preliminary screening.

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Activité antioxydante des extraits d'*Artemisia absinthium*

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Résumé_ La présente étude était consacrée à l'évaluation de l'activité antioxydante d'***Artemisia absinthium***. La plante a été extraite de trois manières : infusion, décoction et macération, et le rendement de l'extraction a été estimé à **8,39 %**, **16,235 %** et **0,7 %**, respectivement. La méthode de décoction a donné le meilleur rendement par rapport aux autres méthodes. Le criblage phytochimique a également révélé la présence des tannins, des saponosides, des mucilages et des alcaloïdes. Les polyphénols ont été déterminés selon la méthode au réactif de Folin-Ciocalteu. Les résultats ont été les suivants : **9,997 ± 0,0217**, **12,17 ± 0,0321** et **76,2051 ± 0,2114 mg d'équivalent acide gallique/g d'extrait** pour les extraits obtenus par infusion, décoction et macération, respectivement. Les flavonoïdes ont été estimés à l'aide de la méthode $AlCl_3$, et leur concentration était la suivante : **0,064 ± 0,198**, **0,088 ± 0,009** et **1,842 ± 0,0007 mg d'équivalent quercétine/g d'extrait** pour les extraits obtenus à partir des méthodes d'extraction mentionnées (infusion, décoction et macération), respectivement. En comparant l'activité antioxydante des trois extraits en utilisant le radical libre DPPH à celle du standard BHT, estimée à **3,601 µg/ml**, les résultats ont montré que les extraits présentaient une activité faible en comparaison avec celle du standard.

.

Keywords – **:** *Artemisia absinthium, polyphénols, flavonoïdes, activité antioxydante, DPPH, BHT.*

Determination of asphaltene and Subfractions aromatic structure from 1H NMR and 13C NMR

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Abstract –

Asphaltenes, defined as petroleum organic compounds, impede oil operations due to their propensity to form floccules and their tendency to accumulate on pipes utilized for production and transportation. Mullins and colleagues have proposed a modified Yen model, which focuses on asphaltene molecules. Spectroscopic techniques, particularly nuclear magnetic resonance (NMR) spectroscopy, have proven to be effective methods for the study of complex compounds, with particular applications in the analysis of the chemical nature of suspended molecules and their fragments. This study utilized 1H NMR and 13C NMR to ascertain the structural parameters of Algerian asphaltenes and subfractions. NMR spectra are indicative of the asphaltene's rich and complex nature. In order to extract useful information, a systematic approach is required to accurately identify and quantify the molecular nature of 1H NMR spectra. In this study, it was observed that subfraction one (AS1) contains more aromatic structures when the aromatic peaks are well resolved (6.5–9.5 ppm). In contrast, the other fractions are composed of aliphatic structures. The aliphatic peaks are further divided into three types of protons according to their position relative to the aromatic core.

Keywords – Asphaltene ,subfraction, aromatic , 1H NMR ,13C NMR

Synthesis and characterization of date stones biochar for nitrate removal from aqueous solutions

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Abstract **–** Nitrate ions present in agricultural and agri-food effluents are the major cause of water pollution leading to eutrophication and health risks due to methemoglobinemia.

The treatment of these effluents before discharge is then imperative. Many biological and physicochemical processes have been implemented for the treatment.

However, adsorption is a promising alternative due to its simplicity and speed. In this context, the main objective of the work presented is to study the nitrate removal on biochar prepared by date stones (DSB). Biochars were prepared at different pyrolysis temperatures (700, 800, 900 and 1000 ^{0}C) in order to select the best biochar with the highest nitrate removal efficiency and determine the main its characteristics, was characterized by FTIR, MEB, DRX, pH_{pzc}.

The adsorption results highlighted that nitrate was effectively removed (76 %) when using DSB-1000 ^{0}C. Our contribution paves the way for future investigations for the recovery of plant waste, namely date stones or other by operators in the field of water treatment by the adsorption process.

Keywords – Adsorption; Biochar; Date stone; Nitrate.

Treatment of water synthetically polluted with hexavalent chromium using an innovative waste product, sunflower seed shells, in dynamic mode.

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Abstract

The valorization of non-hazardous natural and industrial/agriculture wastes has got a lot of attention from the scientific and industrial communities as clean and alternative low-cost materials for environmental remediation. The present work aims to evaluate the sorption ability of valorized sunflower seed shells (SSS) for the recovery of toxic Cr(VI) in bed column systems. Waters contaminated with Cr(VI) can lead to many human health diseases and environmental perturbations. The tolerance limit for chromium Cr(VI) in drinking water is set at 0.05 mg/L according to the World Health Organization.

Several parameters influencing adsorption were studied, such as flow rate, bed height and Cr(VI) concentration. Overall, the highest efficiency was found at 66.10% under the following conditions: flow rate 2 mL min^{-1}, Cr(VI) concentration 10 ppm, bed height 30 mm.

Keywords – Adsorption, hexavalent chromium, Sunflower seed shells, wastwater, dynamic mode.

Antioxidant Potential of Two Rutaceae Plants: A Comparative Approach Using ABTS and Phenantroline Assays

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Abstract – *Ruta montana* and *Ruta chalepensis*, two species from the Rutaceae family, are well known for their medicinal properties and richness in bioactive compounds. This study aimed to assess their antioxidant potential through polyphenol, flavonoid, and tannin contents, along with antioxidant activity evaluated using ABTS and phenantroline assays. The aerial parts of both plants were collected, dried, and extracted using a hydroethanolic solution. Total polyphenols were determined by the Folin-Ciocalteu method, flavonoids by the aluminum chloride colorimetric assay, and tannins using the vanillin method. Antioxidant activities were evaluated by two methods: ABTS, which measures radical scavenging ability, and phenantroline, which assesses ferric reducing power. *Ruta montana* showed higher polyphenol (57.8 µg GAE/mg extract) and tannin (6.99 µg CATE/mg extract) contents, whereas *Ruta chalepensis* had higher flavonoid levels (18.23 µg QE/mg extract). Both species exhibited promising antioxidant activities in both assays, reflecting the strong reducing and radical scavenging capacity of their extracts.
In conclusion, the findings highlight the antioxidant potential of *Ruta montana* and *Ruta chalepensis*, linked to their phenolic composition. These plants may serve as valuable sources of natural antioxidants for pharmaceutical or nutraceutical applications. Future studies should focus on isolating individual compounds and investigating additional biological activities such as antimicrobial or anti-inflammatory effects.

Keywords – Rutaceae Plants; polyphenol; flavonoid; tannin; ABTS; phenantroline

The effect of sulphur-containing organic compound as corrosion inhibitor of copper in NaCl medium, experimental and theoretical studies

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Abstract – Herein, the efficiency of sulphur-containing organic compound as corrosion inhibitor in NaCl solusion was studied via electrochemical impedance spectroscopy (EIS), and potentiodynamic polarization (PDP) methods. The obtained results indicated that the tested inhibitor act as an excellent mixed type corrosion inhibitor for copper in NaCl solution reached a maximum efficiency of 99.98% at 10−3 M, and their adsorption obeys Langmuir adsorption isotherm. The formation of a protective film of inhibitor on the copper surface, was investigated via various techniques such as scanning electron microscopy (SEM) and atomic force microscopy. Quantum chemical calculations, DFT, and Fukui indices were also applied to describe the adsorption mechanism. MD simulations were also performed to describe the ability of the tested inhibitor molecule to adsorb on the Cu (111).

Keywords – Corrosion inhibitor; Copper; EIS; DFT

Eco-Friendly Synthesis of $Bi_{1\ 2}ZnO_{2\ 0}$ /Bi_2O_3 Composite Using Prickly Pear Peel: A Sustainable Photocatalyst for Beibrich Scarlet Dye Degradation

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Abstract –

This study focuses on the green synthesis of a $Bi_{1\ 2}ZnO_{2\ 0}$ -type sillenite material using prickly pear peel extract as a natural reducing and stabilizing agent, and explores its photocatalytic potential for the degradation of organic dyes. The structural, morphological, and optical properties of the synthesized material were thoroughly characterized by X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), and optical band gap analysis. Preliminary photocatalytic experiments revealed promising activity in the UV-driven degradation of Beibrich Scarlet (BS) dye, highlighting the material's potential for environmental applications. To further enhance photocatalytic performance, different proportions of Bi_2O_3 were incorporated into the $Bi_{1\ 2}ZnO_{2\ 0}$ matrix using the same eco-friendly synthesis method. The resulting $Bi_{1\ 2}ZnO_{2\ 0}$ /Bi_2O_3 composites exhibited a marked improvement in photocatalytic efficiency, with complete degradation of BS achieved within 80 minutes under UV irradiation. This enhancement is attributed to the formation of a Type II heterojunction, which promotes more efficient charge separation and reduces recombination rates. Overall, the findings demonstrate that green-synthesized $Bi_{1\ 2}ZnO_{2\ 0}$ -based materials, particularly when modified with Bi_2O_3 , offer significant promise as efficient, stable, and sustainable photocatalysts for the treatment of wastewater contaminated with persistent organic pollutants.

Keywords – $Bi_{1\ 2}ZnO_{2\ 0}$ -type selenite, Bismuth oxide, Beibrich scarlet, photocatalysis, UV light

Electrochemical and mechanical properties of nickel coatings elaborated on copper from a chloride bath

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Abstract – This study investigates the electrochemical and mechanical properties of nickel coatings electrodeposited on copper substrates from a chloride bath using cyclic voltammetry at various temperatures (25°C to 55°C). The morphological characterization of the coatings was conducted via optical microscopy and white light interferometry, while microhardness was assessed using the Vickers method. Electrochemical performance was evaluated in 0.5 M NaCl solution through electrochemical impedance spectroscopy (EIS) and DC polarization measurements. The results show a clear correlation between deposition temperature and coating properties. As the temperature increased, the coatings exhibited improved mechanical strength and smoother surface morphology. At 25°C, the average microhardness was 85.7 HV, which progressively increased to 99.3 HV at 55°C. The surface of the 55°C coating was significantly smoother with fewer pits, indicating improved deposition quality and reduced susceptibility to chloride-induced defects. Furthermore, the electrochemical analysis revealed that the coating deposited at 55°C demonstrated superior corrosion resistance, with the highest charge transfer resistance (Rc=13,670 Ω·cm²), suggesting enhanced barrier properties. This behavior is likely due to the dense and low-porosity nature of the nickel layer formed at elevated temperatures. Overall, the findings highlight that electrodeposition at 55°C optimizes both the mechanical and corrosion-resistant performance of nickel coatings, making it a promising condition for protective metal finishing applications.

Keywords – Corrosion resistance ; Nickel coatings ; Electrodeposition ; EIS; Microhardness ; CV; Surface characterization

Green Synthesis and Bioactive Potential of Thiophene Derivatives

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Abstract – Thiophenes represent a major class of heterocyclic compounds that have garnered significant attention due to their structural diversity and wide-ranging applications in medicinal chemistry, materials science, and agrochemicals. Among the various thiophene derivatives, 3-aminothiophenes are of particular interest because of their high chemical reactivity and their ability to serve as versatile building blocks in the synthesis of complex bioactive molecules. The presence of an amino group on the thiophene ring facilitates further functionalization, making these compounds valuable intermediates in the design of heterocyclic frameworks with potential biological activity.In the context of our ongoing research on heterocyclic compound synthesis, we have developed a novel, rapid, and environmentally friendly synthetic protocol for producing a new class of mixed heterocycles containing both sulfur and nitrogen atoms. Our methodology begins with the chloroformylation of commercially available ketones, followed by a two-step cyclization process that yields 3-aminothiophenes in moderate but reproducible yields. These key intermediates were then employed in the synthesis of a variety of novel derivatives, several of which exhibit promising therapeutic properties.This innovative approach contributes not only to the field of green chemistry but also opens new perspectives for the discovery and development of biologically active molecules with potential pharmaceutical applications.

Keywords – 3-Aminothiophene; Chloroformylation; Cyclization; Mixed heterocycles; Biological activity.

Synthèse étude structurale et évaluation de l'activité antifongique d'un complexe de Nickel dérivé du DHA

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Abstract:

Durant de longues années, le nickel était considéré comme un élément toxique et aucun intérêt biologique n'a été établi pour cet élément. Il est le plus allergisant de tous les métaux. Plus de 12% de la population y est allergique [1, 2]. Ce n'est qu'en 1975 qu'il a été montré que le nickel était présent dans l'uréase qui est une enzyme contenue dans certaines plantes [98]. Depuis, un intérêt considérable a été apporté au rôle biologique du nickel, et les études ne cessent de montrer son importance dans la formation de sites actifs dans différentes métalloprotéines telles que : hydrogénase, carbone monoxide déhydrogenase, méthyl-S-coenzyme-M méthyl réductase et uréase [1, 3, 4].

Dans ces enzymes, le nickel est souvent entouré d'atomes d'azote et d'oxygène. Les complexes avec des ligands ayant pour atomes donneurs l'oxygène et l'azote constituent de bons modèles pour étudier ces systèmes. Dans le present travaille nous avons synthètise et caracteriser par les methodes spectroscopioques et RX plus l'évaluation de l'activité antifongique d'un complexe de Nickel dérivé du l'acide dehydroqcetique (DHA).

mots clef : DHA, étude cristallographique et spectroscopique, activité antifongique

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Étude inhibitrice de l'extrait de plante médicinale sur l'acier XC48 dans une solution de chlorure d'hydrogène 1M

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Résumé – En raison de l'énorme croissance des problèmes environnementaux causés par l'application de certains inhibiteurs de corrosion toxiques, la recherche d'inhibiteurs respectueux de l'environnement, également appelés inhibiteurs verts, a été incitée, en raison de leurs biodégradabilités, de leurs non-toxicités. En plus d'être respectueux de l'environnement et écologiquement acceptables, les produits végétaux sont peu coûteux et facilement disponibles et renouvelables.

Le but de ce travail est de vérifier l'efficacité inhibitrice de l'extrait d'un *PLANTE MEDICINALE*, sur la corrosion de l'acier XC48 dans une solution de chlorure d'hydrogène 1 M, en utilisant les différentes techniques telles que la polarisation potentiodynamique, et la spectroscopie d'impédance électrochimique. Les résultats obtenus ont montré que l'extrait inhibe de manière satisfaisante la corrosion de l'acier dans la solution acide.

Keywords – l'efficacité inhibitrice, Plantes médicinales, polarisation potentiodynamique, spectroscopie d'impédance ,

Waste Valorization for the Design of an Efficient Photocatalyst under Real Solar Conditions

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Abstract – This study explores photocatalysis as an environmentally friendly and effective solution for the degradation of organic pollutants, focusing on the development of a novel, low-cost, and sustainable photocatalyst derived from waste materials. Three materials were synthesized by calcination at 900 °C for one hour: PHO1 (from one type of waste), PHO2 (from another), and PHOM (a mixture of both). The photocatalysts were characterized using X-ray diffraction (XRD), X-ray fluorescence (XRF), UV-Visible spectroscopy, scanning electron microscopy (SEM), and energy-dispersive X-ray spectroscopy (EDS). The results show that PHOM exhibits enhanced crystallinity, good structural stability, and the lowest band gap (2.86 eV), compared to 3.46 eV for PHO2 and 5.86 eV for PHO1, allowing for more efficient absorption of solar light. Photocatalytic performance was evaluated using methylene blue under solar irradiation. PHOM achieved 95% degradation within 5 minutes at an initial concentration of 10 mg/L, with a kinetic rate constant of 0.042 min^{-1} (R^2 = 0.993). At higher concentrations, the rate constants remained significant: 0.0386 min^{-1} (R^2 = 0.988) at 20 mg/L and 0.0350 min^{-1} (R^2 = 0.967) at 30 mg/L. In contrast, PHO1 and PHO2 showed much lower efficiencies across all conditions. These findings highlight the effectiveness of the synergy between the selected waste materials in designing an innovative photocatalytic material. PHOM emerges as a promising, sustainable, and economical solution for water depollution under natural sunlight.

Keywords – Photocatalysis; Waste valorization; Solar irradiation;

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Synthèse étude structurale et évaluation de l'activité antifongique d'un complexe de Nickel dérivé du DHA

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Abstract:

Durant de longues années, le nickel était considéré comme un élément toxique et aucun intérêt biologique n'a été établi pour cet élément. Il est le plus allergisant de tous les métaux. Plus de 12% de la population y est allergique [1, 2]. Ce n'est qu'en 1975 qu'il a été montré que le nickel était présent dans l'uréase qui est une enzyme contenue dans certaines plantes [98]. Depuis, un intérêt considérable a été apporté au rôle biologique du nickel, et les études ne cessent de montrer son importance dans la formation de sites actifs dans différentes métalloprotéines telles que : hydrogénase, carbone monoxide déhydrogenase, méthyl-S-coenzyme-M méthyl réductase et uréase [1, 3, 4].

Dans ces enzymes, le nickel est souvent entouré d'atomes d'azote et d'oxygène. Les complexes avec des ligands ayant pour atomes donneurs l'oxygène et l'azote constituent de bons modèles pour étudier ces systèmes. Dans le present travaille nous avons synthètise et caracteriser par les methodes spectroscopioques et RX plus l'évaluation de l'activité antifongique d'un complexe de Nickel dérivé du l'acide dehydroqcetique (DHA).

mots clef : DHA, étude cristallographique et spectroscopique, activité antifongique

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Prediction of Polymer Refractivity: QSPR Approach

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Abstract **–** Understanding the molecular basis of polymers is essential for advancing applications in materials science, particularly in optics and photonics. In this study, we developed a quantitative structure-property relationship (QSPR) model to predict the refractive index of a series of polymers, using theoretical descriptors derived from their molecular structure. The geometries were optimized using the semi-empirical PM3 method, and the descriptors calculated using Dragon software (version 5.5). Genetic algorithms (GA) were used to select the relevant variables, and multiple linear regression (MLR) was used to build the model. The model was validated in accordance with OECD guidelines, with an assessment of the area of application using the Williams diagram to identify the influential compounds. The internal and external validations confirmed the robustness and predictive performance of the model, which achieved an R^2 coefficient of determination of 97.2% and a Q^2_LOO prediction coefficient of over 96%.

Keywords – QSPR; Optical properties; Molecular descriptors; Multiple linear regression; polymers.

Analyse phytochimique d'Ecballium elaterium (L.) A. Rich.

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Abstract

Le concombre d'âne (Ecballium elaterium) est une espèce indigène du sud de l'Europe, du bassin méditerranéen et de l'Afrique, parfois cultivée pour ses usages en tant que plante médicinale. Cette étude a comparé la teneur en composés phénoliques (polyphénols, flavonoïdes et tanins) des feuilles d'Ecballium elaterium en utilisant deux méthodes d'extraction différentes.

Les résultats ont montré que les feuilles présentaient des teneurs totales en polyphénols variables, avec des valeurs de 38,50 et 31 mg d'équivalents d'acide gallique par gramme de matière sèche. Les teneurs en tanins variaient entre 20,01 et 17,52 mg/g, tandis que des teneurs intéressantes en flavonoïdes ont été observées, allant de 86,14 à 119,04 mg/g.

Ces résultats suggèrent que les extraits de feuilles d'Ecballium elaterium pourraient constituer une source prometteuse en phytochimie et en phytothérapie, avec un potentiel d'application dans le domaine pharmaceutique.

Keywords – Ecballium elaterium;polyphénols;flavonoides;tanins;phytochimie

Analysis and Study of a Magneto-Hydrodynamic micromixer

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Abstract – Microfluidic devices have become increasingly common in various sectors recently, including chemistry, environmental technology, biotechnology, and biomedicine. Fluids must frequently be pumped from one area of the device to another in these applications. In the meantime, adequate fluid mixing is also necessary. The characteristic length of the microchannel is frequently relatively short, and the mixing time with low diffusivity needs to be increased. Consequently, in order in order to accelerate the mixing procedure, a more beneficial microdevice needs to be developed. One feasible method of pumping and mixing is magnetohydrodynamics (MHD). This work proposes a novel magnetohydrodynamic micro-mixer that numerically analyses the mixing properties of two distinct electrolyte solutions. The Comsol multiphysics code is used to analyze in detail flow characteristics such as fluid velocity, current density, pressure and fluid mass fraction. The effect of the magnetohydrodynamic phenomenon on the characteristics of the pumping and mixing functions across the different voltages applied to the electrodes will be discussed.

Keywords – Flow rate, Lorentz force;;, Magneto-hydrodynamic (MHD); Micromixer; Mixing performance.

Molecular Modeling of Antioxidant and Antifungal Compounds from Cymbopogon schoenanthus Interacting with 1URM and 2KCN Proteins

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Abstract **–** Molecular Modeling of Antioxidant and Antifungal Compounds from Cymbopogon schoenanthus Interacting with 1URM and 2KCN Proteins El hassasna Souhir1 , Hadjar Sameh1* Boumedjout Meriam1* , Houmana Haoua 1* , Harkati Brahim 1* 1 Laboratory of Organic Materials and Heterochemistry, Echahid Cheikh Larbi Tebessi University, Constantine Road, Tebessa 12002, Algeria *souhir.elhassasna@univ-tebessa.dz ABSTRACT This work is part of a molecular modeling study that was conducted by performing molecular docking using the MOE software. The study focused on specific molecules with antioxidant properties binding to the 1URM protein, and other molecules exhibiting antifungal properties binding to the 2KCN protein. These molecules are present in the leaf and root extracts of the Cymbopogon schoenanthus plant. Our findings revealed noteworthy results, indicating that the molecules bind tightly to their respective target proteins, forming significant interactions within specific binding sites. This suggests a potential impact on the enzyme's activity. Keywords: Antioxidant, Antifungal, Cymbopogon schoenanthus, molecular docking, MOE, 1URM and 2KCN protein.

Keywords – Antioxidant, Antifungal, Cymbopogon schoenanthus, molecular docking, MOE, 1URM and 2KCN protein.

RECUPERATION ET SEPARATION DE LA MATIERE ORGANIQUE DANS LES EAUX USEES : APPLICATION DE LA CHROMATOGRAPHIE IONIQUE POUR UNE VALORISATION DURABLE

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Abstract – Les acides aminés, composants essentiels des protéines, jouent un rôle crucial dans une multitude de processus biologiques et biochimiques. Leur séparation et leur identification sont donc des tâches fondamentales dans les domaines de la biochimie, de la biotechnologie, de la médecine, et des sciences alimentaires. Parmi les nombreuses techniques disponibles pour la séparation des acides aminés telles que la chromatographie, l'électrophorèse, et la spectrométrie de masse. Parmi ces méthodes, la chromatographie échangeuse d'ions(CEI)) est l'une des plus couramment utilisées en raison de sa précision, de sa reproductibilité, et de sa capacité à séparer les acides aminés en fonction de leurs charges ioniques.

Cette recherche s'inscrit dans le cadre de l'application des technologies propres visant l'économie et le recyclage de l'eau, ainsi que la valorisation des polluants (matières organiques). Elle porte sur la séparation des acides aminés libres contenus dans l'eau de lavage du blé par chromatographie d'échange d'ions.

On s'intéressera tout particulièrement à :

- ✓ la séparation du mélange d'acides aminés à travers une résine échangeuse d'ions.
- ✓ Les acides aminés élus dans la colonne en fonction de leur acidité
- ✓ La détection et la quantification de ces acides aminés.

Keywords – Acides aminées, échanges d'ions, chromatographie,

Computational Evaluation of the Antioxidant Properties of Several Schiff Base Derivatives in the Presence of Diverse Free Radicals: A DFT Study

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Abstract **–** A series of Schiff bases, including 5-chloroisatin-thiocarbohydrazone, underwent a computational investigation using Density Functional Theory (DFT) at the M05-2X/6- 31+(d,p) and LC-ωPBE/6-31+(d,p) levels of theory. These calculations were performed in both the gas phase and in solution, employing solvent models. Global reactivity descriptors were computed to elucidate the antioxidant reactivity of these compounds under both conditions. Furthermore, reaction enthalpies associated with key primary antioxidant mechanisms—Hydrogen Atom Transfer (HAT), Single Electron Transfer–Proton Transfer (SET–PT), and Sequential Proton-Loss Electron-Transfer (SPLET)—were explored. The influence of solvent polarity on the predicted antioxidant activity was also examined.

Keywords – Schiff bases, DFT; reactivity antioxidant, solvent effect

Adsorption And Corrosion Inhibitive Properties Of Amino Acid Leucine On Mild Steel In Hydrochloric Acid Media

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Abstract **–**this study, adsorption of amino acid Leucine on mild steel (MS) surface in 0.5M HCl solution and its corrosion inhibition effect was studied in both short and long immersion times (over 120h). For this purpose, a series of techniques, such as potentiodynamic polarization, electrochemical impedance spectroscopy (EIS), linear polarization resistance (LPR), gravimetric, surface photographs, hydrogen evolution (V_{H2}–t) and change of open circuit potential with immersion time (Eocp–t) were utilized. The values of activation energy for MS corrosion and the thermodynamic parameters, such as adsorption equilibrium constant (K_{ads}), free energy of adsorption (G_{ads}), adsorption heat (Hads) and adsorption entropy (Sads) values were calculated and discussed. The potential of zero charge (Epzc) of MS in inhibited solution was studied both after short and long immersion times by EIS method, and a mechanism of adsorption process was proposed. Results showed that leucine performed excellent inhibiting effect for the corrosion of MS in 0.5 HCl solution and inhibition efficiency is higher than 99% after 120h at 10^{-2} M.Inhibition efficiency was discussed in terms of strongly adsorption of inhibitor molecules on the metal surface and forming a protective film. Surface photographs showed a good surface coverage on the metal surface.

Keywords – Corrosion inhibitors; Inhibition mechanism; Electrochemical impedance spectroscopy (EIS); gravimetric ; Potential of zero charge (PZC).

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Greenly synthesized zeolite (ZSM-5) as sustainable materials for corrosion protection : Design, technology and application

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Abstract **–**The advancement and application of efficient and cost-effective anticorrosive materials are a critical priority due to significant safety and financial risks associated with corrosion.
Advances in corrosion prevention have led to significant cost savings, ranging from $375 to $875 billion annually. Numerous reports highlight the well-examined and validated application of zeolites in protective coatings.Zeolite coatings self-heal by forming passivating oxide films, which shield damaged zones from corrosion.The self-repair mechanism in zeolite coatings stems from their capacity to generate anticorrosive oxide layers (passivation) at defect sites.These coatings autonomously heal via passivation—the creation of protective oxide films that inhibit corrosion in compromised areas.
The synthesis of zeolites from the traditional hydrothermal method is associated with several drawbacks including their high cost and discharge of harmful gases such as oxides of nitrogen (NO_x) and greenhouse gases (CO_2 and CO).
Eco-friendly zeolite synthesis methods have been developed, including solvent-free and organotemplate-free processes, safer organic templates, green solvents, and energy-efficient heating . One-step reactions (OSRs) have also been employed. Recent studies have characterized the self-healing capabilities and corrosion inhibition mechanisms of these sustainably produced zeolites.

Keywords –Zeolite (ZSM-5), corrosion protection, Organotemplate-free synthesis, Green synthesis and Fly ash.

Extraction a deux phases aqueuses du colorant Orange G par micelles mixtes (non ionique – cationique)

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Abstract **–** L'objectif de ce travail est l'extraction par coacervat de l'Orange G., Pour l'extraire de sa solution aqueuse, nous avons choisi de travailler avec un tensioactif non ionique (Oxo-$C_{10}E_3$) aisément, rapidement biodégradable et un tensioactif cationique hexadecyltrimethylammonium bromide (CTAB).
Les résultats expérimentaux d'extraction de l'Orange G en solution aqueuse, en fonction du pourcentage massique du tensioactif non ionique, X_t (Oxo-$C_{10}E_3$) et la température, T, sont exprimés par les trois grandeurs suivants : pourcentage du colorant extrait (E), concentration résiduelle en colorant dans la phase diluée ($X_{s,w}$) et fraction volumique du coacervat(Φ_c) à l'équilibre. La méthode de lissage empirique a été utilisée, ou les résultats obtenus pour chaque paramètre ont été représentés sur des diagrammes tridimensionnels
Les valeurs ainsi calculées sont cohérentes avec les mesures. Le rendement d'extraction avec le tensioactif non ionique Oxo-$C_{15}E_7$ est de 55 % est atteint dans des conditions optimales. La réduction de la concentration en soluté dans la phase diluée a été réduite à environ 400 fois et passe à 98% lorsqu'une petite quantité (0,025% massique) du CTAB a été combiné avec Oxo-$C_{10}E_3$ dans un système de micelles mixtes.

Keywords – point de trouble, micelles mixtes, extraction par point de trouble, colorant Orange G.

Extraction a deux phases aqueuses du colorant Orange G par micelles mixtes (non ionique – cationique)

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Keywords –point de trouble, micelles mixtes, extraction par point de trouble, colorant Orange G.

Etude du comportement thermodynamique des fluides frigorigènes à base de CO_2

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Abstract – L'impact négatif des fluides synthétiques sur l'environnement a incité les chercheurs à utiliser des réfrigérants naturels. Bien que ces liquides ne soient pas nocifs pour l'environnement, certains d'entre eux peuvent présenter un danger du fait de leurs Inflammabilités et toxicités. C'est pourquoi le dioxyde de carbone est si loin devant les autres fluides naturels. Les propriétés thermodynamiques du dioxyde de carbone dictent un cycle transcritique.

Notre travail consiste à étudier le comportement thermodynamique des mélanges binaires à base de CO_2 qui sont considérés comme des fluides de travail alternatifs prometteurs dans les cycles frigorifiques et énergétiques en raison de leurs excellentes performances et de leur respect de l'environnement. L'équilibre liquide-vapeur des mélanges binaires à base de CO_2 constitue la base pour le calcul de l'enthalpie de mélange et de la capacité calorifique, éléments essentiels pour l'analyse thermodynamique.

Keywords –Equilibre vapeur-liquide, Melanges binaires `a base de CO2 ,Lignes critiques

Effet de la Centrifugation sur la Cinétique de Déshydratation Osmotique et les Propriétés Physico-chimiques de la Pomme

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Abstract **–** La présente étude vise à évaluer l'effet d'un prétraitement par centrifugation sur la déshydratation osmotique (DO) de cubes de pomme (Malus domestica). Deux procédures expérimentales ont été comparées : une DO classique et une DO précédée d'une centrifugation à 2800 tr/min à 30°C pendant 10, 20 et 30 minutes. Les paramètres physico-chimiques évalués comprenaient le pH, le degré Brix (°Brix) et la couleur, ainsi que les indicateurs cinétiques de perte en eau (WL%), de gain en solutés (SG%) et de perte en poids (WR%). Les résultats montrent que la centrifugation a significativement augmenté la perte en eau (WL%), le gain en solutés (SG%) et la perte en poids (WR%) par rapport à la DO simple. En particulier, une centrifugation de 30 minutes a permis d'atteindre une perte en eau de 53,35%. Le degré Brix des échantillons prétraités était également plus élevé, indiquant un gain accru en solides solubles. Le pH a diminué au cours du processus pour les deux conditions, avec une diminution plus marquée dans les échantillons prétraités, traduisant une plus grande perméabilité cellulaire.

Le prétraitement par centrifugation améliore la cinétique de déshydratation osmotique en favorisant les transferts de masse et en influençant positivement les paramètres physico-chimiques de la pomme. Cette technique pourrait être exploitée pour optimiser les procédés de préservation et de transformation des fruits.

Mots-clés: Centrifugation, Déshydratation osmotique, pomme, degré Brix. pH, transferts de masse.

Effet de la Variation d'Amplitude sur le Coefficient de Frottement de l'Eau Distillée dans une Forme Ondulée

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Résumé –

L'écoulement des fluides dans les conduites courbées revêt une importance particulière dans plusieurs applications en ingénierie, telles que les coudes de tuyaux, les serpentins de refroidissement et de chauffage, les passages de pales de turbomachines et les prises d'air des avions.

Cette étude expérimentale a été réalisée pour voir l'effet de la variation d'amplitude sur le facteur de perte de pression de l'eau distillée, dans des tubes périodiquement ondulés. Des tubes en aciers inoxydables 316L ont été testées, trois formes périodiques en C cycliquement ondulées avec des différents rayons de courbures R= 80,120, 160mm, avec une longueur totale de 6m pour chaque tube. Les résultats montrent que le facteur de frottement a varié selon le nombre d'ondulation au premier ordre. Le taux de variation a atteint 2,9% d'augmentation du coefficient de frottement dans la région turbulente pour le rayon 80mm lorsque le nombre de Dean est compris entre 352,06 et 5398,38.

Mots-clés – acier inoxydable316L, eau distillée, région turbulente, facteur de perte de pression, forme périodique.

Investigating FSW Tool Degradation: Insights from Gleeble-Based Thermo-Mechanical Simulation.

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Abstract **–** Friction Stir Welding (FSW) is a solid-state joining technique that has transformed welding practices in aerospace, nuclear, and transportation industries. By avoiding material melting, FSW minimizes common fusion-welding defects, including porosity, solidification cracking, and distortion. Although the method has traditionally been applied to aluminum alloys, its use has expanded to materials such as steel, titanium, copper, and nickel-based superalloys. A persistent challenge in FSW is the accelerated degradation and wear of welding tools, particularly as material thickness increases and welding speeds rise.

This study forms part of an extensive investigation into the mechanisms behind FSW tool wear, integrating experimental evaluations and advanced simulations. Specifically, we present a physical model that examines the thermal and mechanical cycles experienced by the tool material. By comparing the effects of repeated heating and cooling cycles against prolonged steady-state conditions, we isolate the factors that influence tool degradation. Metallographic and fractographic analyses provide valuable insights into how these cycles alter tool steel properties, shedding light on failure mechanisms. These findings pave the way for targeted strategies to enhance tool longevity and reliability in high-demand FSW applications.

Keywords –Friction Stir Welding, thermal and mechanical cycles, longevity and reliability

Characterization of FSW Tool Degradation and Failure

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Abstract Friction Stir Welding (FSW) is a solid-state joining technique widely used across industries such as aerospace, nuclear, and transportation for its ability to avoid melting materials and thereby eliminate fusion-welding defects like porosity, solidification cracking, and distortion. Initially developed for aluminum alloys, FSW has since been successfully applied to materials such as steel, titanium, copper, and nickel-based superalloys. Despite these advantages, a significant challenge is the accelerated degradation and wear of FSW tools—particularly H13 steel and cobalt-based MP159—when welding thicker base metals at higher speeds. In this study, a detailed analysis was conducted to characterize tool wear and failure mechanisms through both non-destructive and destructive evaluations, complemented by analytical and physical simulations. Scanning Electron Microscopy (SEM) revealed that the tool's surface degradation is strongly linked to microstructural factors, with the presence of three distinct hardness regions contributing to fractures and wear. These insights provide a foundation for improving tool performance and extending tool life in demanding FSW applications.

Keywords: *FSW,* *Degradation,* *Failure,* *SEM,* *Tool.*

Studies of physical properties of new ceramic

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Abstract – 0.05 $Pb[Fe_{1/2}Nb_{1/2}]O_3$-0.05 $Pb[Ni_{1/3}Nb_{2/3}]O_3$-0.90 $Pb[Zr_xTi_{(1-x)}]O_3$ (abbreviated PFN-PNN-PZT) piezoelectric ceramics with varying Zr/Ti ratio, which locate in the vicinity of the morphotropic phase boundary (MPB), were prepared by a conventional mixed-oxide route. The dielectric constant (ε) reach the maximum values at x = 0.51. The electric properties of the system were investigated and indicate that the MPB of the tetragonal and rhombohedral phase lies in the range $0.49 < x < 0.53$.This reflects the transition from tetragonal phase to rhombohedral phase, which makes this material a good candidate for high-power multilayer piezoelectric transformer applications.

Keywords – PZT, Morphotropic phase boundary, Piezoelectric properties, Electric properties.

Formulation d'un gel anti-inflammatoire à base d'une plante médicinale

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Le retour aux produits naturels suscite un intérêt croissant pour la formulation de produits cosmétiques et thérapeutiques à base d'ingrédients biodégradables, adaptés aux peaux sensibles et capables de répondre à divers besoins. Dans cette optique, l'objectif de ce travail est de développer un hydrogel topique à base d'extrait hexanique de *Centaurea acaulis* (partie racinaire) à visée anti-inflammatoire.

L'analyse chimique de cet extrait a été réalisée par chromatographie en phase gazeuse (CPG) et CPG couplée à la spectrométrie de masse (CPG/SM), ce qui a permis l'identification de 9 constituants représentant 92,6% de la composition totale de l'extrait.

Cette étude préliminaire propose une formulation simple, composée d'un agent gélifiant (CARBOPOL), d'un co-solvant (éthanol) et de l'extrait actif de *C. acaulis*. Le gel obtenu présente une texture homogène, une couleur jaunâtre et une viscosité satisfaisante.

Les tests anti-inflammatoires, réalisés par inhibition de la dénaturation des protéines, ont montré que les hydrogels à 1%, 0,5% et 0,1% d'extrait actif présentaient des taux d'inhibition supérieurs à ceux du contrôle, le gel de diclofénac de sodium.

Au regard des résultats prometteurs, nous proposons de développer un gel naturel à 1% de principe actif, visant à obtenir une efficacité équivalente, voire supérieure, à celle du gel commercial de diclofénac de sodium à 1%.

Keywords *: Hydrogel, Centaurea acaulis, Anti-inflammatoire, Extrait hexanique, CPG/SM.*

Numerical simulation of thermal stress during CdTe vertical Bridgman crystal growth

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Abstract – This study numerically examines the impact of varying crucible size on the shape of the crystal/melt interface and the distribution of thermal stresses during the growth of CdTe single crystals via the vertical Bridgman process. A two-dimensional model for fluid flow and heat transfer, incorporating solidification, was developed. The Navier-Stokes equations for the melt and the heat conduction equation for the crystal was solved using a control volume-based finite difference approach. Thermal elastic stress fields was derived from the temperature field by employing a plane strain model within the axi-symmetric geometry of a cylindrical crystal. The results indicate that the shape of the melt/crystal interface become increasingly concave, the maximum value of thermal stress in the crystal reduces as the crystal grows. Our numerical simulations demonstrate a strong correlation with existing literature findings.

Keywords –vertical Bridgman, CdTe, thermal stresses.

Étude des composés bioactifs et propriétés antioxydante de l'extrait phénolique *Corchorus olitorius*

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Abstract –

Corchorus olitorius est une plante utilisée en médecine traditionnelle et connue pour sa richesse en composés bioactifs tels que les polyphénols et les flavonoïdes. Ces molécules suscitent un intérêt croissant en raison de leurs effets potentiels sur la santé. Dans le cadre de cette étude, une analyse phytochimique de l'extrait phénolique de *Corchorus olitorius* a été réalisée, ainsi que l'activité antioxydante en vue du développement de nouveaux agents bioactifs. L'estimation quantitative des polyphénols totaux a été déterminer selon la méthode de Folin-Ciocalteu et des flavonoïdes par la méthode au trichlorure d'aluminium. Par ailleurs, l'évaluation de l'effet antioxydant de l'extrait phénolique été réaliser selon la méthode de FRAP et le test du DPPH. Les résultats ont montré que l'extrait phénolique des feuilles de *Corchorus olitorius* est riche en polyphénol ainsi qu'en flavonoïdes, de plus, la plante dispose d'un pouvoir réducteur du fer comparable à celui de l'acide ascorbique, et une forte capacité à neutraliser les radicaux libres, représentés par le radical DPPH comparé à l'acide gallique, ce qui est prometteur pour d'éventuelles applications biomédicales.

Keywords – Composés bioactifs, *Corchorus olitorius*, Activité antioxydante, Application biomédicales.

ETUDE THEORIQUE DES PROPRIETES STRUCTURALES ET SPECTROSCOPIQUES DE LA 3,4',5,7-TETRAMETHOXYFLAVONE

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Abstract **–** Les recherches phytochimiques de l'extraction des huiles essentielles de feuilles de Kaempferia parviflora [1], plante thaïlandaise d'intérêt médicinale, ont abouti à l'isolement de quatre composés. Le 3,5,7-Trimethoxy-2-(4-methoxyphenyl)-4H-1-benzopyran-4-one ou 3,4',5,7-tetramethoxyflavone est un métabolite secondaire isolé à partir de cette source végétale. L'analyse Rx sur monocristal a été utilisée pour l'authentification de la structure de ce composé isolé [2] et sa structure a été élucidée par l'analyse élémentaire, FT-IR, UV, RMN 1H, RMN 13C [3].

Dans notre travail, nous nous intéressons à l'étude théorique par la méthode DFT (Density Functional Theory) [4] des propriétés structurales, moléculaires, électroniques, et spectroscopiques de la 3,4',5,7-tetramethoxyflavone (Figure 1).Une comparaison des résultats théoriques avec les valeurs expérimentales a été effectuée et des conclusions ont été tirées .

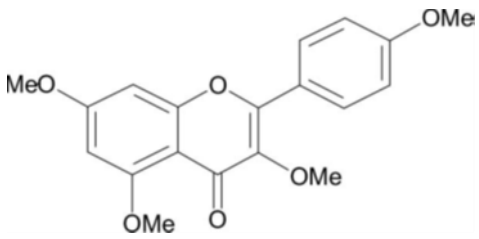

Figure 1: Structure chimique du composé étudié la 3,4',5,7-tetramethoxyflavone

Keywords *: Hétérocycle , Structure moléculaire, DFT, spectroscopie, propriétés biologiques.*

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Influence of Milling Time on the Structural and Magnetic Behavior of Nanostructured $Ni_{50}Ti_{50}$ Alloys Synthesized by High-Energy Ball Milling

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Abstract **–** This research investigates how milling duration impacts the morphological, structural, and magnetic properties of nanostructured $Ni_{50}Ti_{50}$ powders synthesized through high-energy mechanical alloying using a Fritsch Pulverisette 7 planetary ball mill. Scanning electron microscopy (SEM) combined with energy-dispersive X-ray spectroscopy (EDS) revealed a distinctive particle folding mechanism, diverging from the traditional fragmentation and cold-welding behavior typically seen during mechanical milling. As milling time increased, the powders exhibited a decrease in particle size and the development of a more homogeneous spherical equiaxed morphology. X-ray diffraction (XRD) patterns indicated the presence of multiple structural phases, including amorphous content, NiTi-martensite (Ms), NiTi-austenite (As), and a solid solution (SS) phase. Rietveld refinement and magnetic analysis emphasized the significant influence of the amorphous phase on both the martensitic start (Ms) and remanent magnetization (Mr) values. After 72 hours of milling, the coercivity (Hc) reached 285.8 Oe, and the martensitic phase content increased to 21.58%, underscoring the role of prolonged milling in tailoring functional properties.

Keywords – NiTi alloy, mechanical alloying, milling time, amorphous phase, martensitic transformation, coercivity, nanostructured powders, Rietveld refinement, magnetic properties, particle morphology

Structural and Optical Investigation of Cu/AZO Bilayers Prepared by RF Magnetron Sputtering for Transparent Electrode Applications

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Abstract **–** Aluminum-doped zinc oxide (AZO) thin films, known for their wide band gap and advantageous properties, have emerged as promising candidates for various nano- and micro-scale technological applications. The integration of elemental metals with AZO layers has opened innovative pathways in device engineering and circuit integration. This study aims to both fabricate and evaluate optimized thin film structures. A multi-step approach was adopted: (i) a multi-target RF magnetron sputtering configuration was employed, (ii) deposition parameters were optimized, (iii) copper/AZO bilayers were synthesized, and (iv) the resulting samples underwent detailed structural analysis. The Cu/AZO bilayers exhibited a wurtzite hexagonal crystal structure with a strong (002) c-axis orientation. Copper monolayers were confirmed to be uniform and continuous. Notably, the incorporation of copper enhanced the optical performance of the films, making them particularly suitable for applications in photovoltaics and as transparent conductive electrodes in solar energy devices.

Keywords – Al-doped ZnO, AZO thin films, RF magnetron sputtering, Cu/AZO bilayers, transparent electrodes, photovoltaics, optical properties, wurtzite structure

Young's and shear moduli determination of electroluminescent porous silicon

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Abstract – The discovery of visible electroluminescence in porous silicon, even at room temperature (RT), has attracted considerable interest. With an energy gap 0.5 eV higher than that of its crystalline counterpart; this semiconducting material has opened up new application areas such as optoelectronics, microelectronics, and Nano electronics. However, this electroluminescence phenomenon can only be observed when its porosity reaches a high level of around 80%. Furthermore, this high porosity makes it very fragile and its characterization more challenging. Hence, we investigate its very delicate elastic properties by acoustic nondestructive technique. Thus, we first determine the acoustic signatures of the material at different operating frequencies and film thicknesses. It is found that the determined acoustic signatures are dominated by the substrate response, i.e. completely attenuated for larger thicknesses. Thus, to overcome such a difficulty we apply the one-parameter law to determine the longitudinal wave velocity (V_L) of these layers. Finally, using different acceptable approximations, we derive specific formula for the elastic constants as a function of only V_L. The application of such formula led to the first evaluation both elastic moduli of this highly porous silicon: Young's modulus, E = 1.30 GPa and the shear modulus, G = 0.60 GPa. This result is very important in the design of surface acoustic wave devices.

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Keywords – Porous silicon, Acoustic signatures, Young's modulus, Shear modulus