University of Batna 1 جامعة باتنة
Faculty of Matter Sciences
Department of Chemistry

Laboratory of Materials Chemistry and the Living: Activity & Reactivity (LCMVAR)

Laboratory of Chemistry and Environmental Chemistry (LCCE)

The 3rd National Seminar on Chemistry and its Applications

(SNCA-3-2025)

الملتقى الوطني الثالث حول الكيمياء وتطبيقاتها

BOOK OF ABSTRACTS

Batna, 26-27 November, 2025

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Plenary conferences

From Molecular Engineering to Application: Tunable Nanomaterials for Advanced Technologies

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Abstract

Nanomaterials represent a versatile and rapidly evolving class of materials with significant potential across multiple strategic sectors, including environmental remediation, biomedicine, electronics, agriculture, and catalysis. The molecular engineering of these nanomaterials through appropriate functionalization provides them with new and adaptable multifunctional properties, enhances their interactions with surrounding environmental and biological targets, and improves their physicochemical and mechanical properties, as well as their stability and bioavailability. These advances open up new opportunities for the development of next-generation nanomaterial-based systems, providing more efficient, selective, and sustainable solutions for critical challenges spanning water treatment, health, and industrial processes.

This presentation will showcase representative examples of functionalized hybrid nanomaterials engineered to serve as adsorbents, catalytic systems, or sensing platforms for the selective detection, separation, and removal of environmental contaminants and pathogenic bacteria.

Le stress oxydant et le traitement alternatif par les plantes

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Résumé

Les espèces réactives de l'oxygène (ROS) constituent un groupe de substances de faible poids moléculaire formés comme sous-produits du métabolisme normal de l'oxygène et jouent un rôle important dans la signalisation cellulaire et l'homéostasie. Cependant, l'accumulation de ROS dans les cellules peut causer des dommages irréversibles aux molécules biologiques et aux membranes cellulaires, pouvant aboutir à la mort cellulaire, aboutissant au vieillissement et la genèse de plusieurs situations pathologiques, y compris l'athérosclérose, le cancer et les maladies pulmonaires et neuro-dégénératives.

Néanmoins, la production de ROS est équilibrée par l'action d'un système antioxydant endogène, constitué des enzymes superoxyde dismutase et catalase. Les composés phénoliques d'origine végétale, une partie essentielle de l'alimentation humaine, possèdent un cycle aromatique portant des groupes hydroxyles et leurs structures peuvent varier de phénols simples à des tannins complexes à haut poids moléculaire. Les plantes comptent plus de huit mille composés phénoliques différents, parmi lesquels les flavonoïdes représentent plus de la moitié.

Au cours de ces quelques dernières décennies, de nombreux rapports de recherche ont clairement plaidé pour un rôle décisif des composés phénoliques comme agents thérapeutiques dans le traitement de l'inflammation, du diabète, du cancer et des troubles neuro-dégénératifs. Par conséquent, cette étude a été conçue pour présenter un aperçu détaillé des ROS et des pathologies associées, ainsi que des études de cas sur les composés phénoliques de plantes médicinales, notamment la clématite, *Clematis flammula*, du frêne, *Fraxinus angustifolia*, du pistachier lentisque, *Pistacia lentiscus* et du peuplier noir, *Populus nigra*. Par conséquent, des preuves expérimentales sur le rôle des phénols végétaux en tant que nouveaux médicaments potentiels dans le traitement palliatif et alternatif de certaines maladies à caractère inflammatoire seront présentées et discutées.

Mots clés : *Clematis flammula*, *Fraxinus angustifolia, Pistacia lentiscus, Populus nigra* Composés phénoliques, Anti-inflammatoire

Thematic Conferences

TOPIC A: THEORETICAL CHEMISTRY AND MOLECULAR MODELING

TA1- In Silico Drug Discovery : Intégration du Docking et de la Dynamique Moléculaire dans la Prédiction Bioactive

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Résumé

La découverte de médicaments a profondément évolué avec l'avènement des méthodes *in silico*, qui permettent d'accélérer l'identification de molécules bioactives tout en réduisant les coûts expérimentaux. Parmi les outils les plus puissants de la modélisation moléculaire, le docking moléculaire et la dynamique moléculaire (MD) jouent un rôle essentiel dans la compréhension et la prédiction des interactions entre ligands et cibles biologiques. La conférence thématique « In Silico Drug Discovery : Intégration du Docking et de la Dynamique Moléculaire dans la Prédiction Bioactive » vise à explorer ces deux approches complémentaires et leur importance croissante dans la recherche pharmaceutique moderne.

Le docking moléculaire constitue une étape fondamentale dans le criblage virtuel. Il vise à prédire la position et l'orientation optimales d'un ligand lorsqu'il se lie à une protéine ou à tout autre macromolécule biologique. Grâce à des algorithmes efficaces, le docking génère différentes poses possibles du ligand et évalue leur affinité via des fonctions de scoring approximant l'énergie de liaison. Cette approche permet de filtrer rapidement des bibliothèques de millions de composés, identifiant ainsi les candidats présentant un potentiel thérapeutique élevé. Toutefois, malgré son efficacité, le docking repose sur une vision souvent statique des biomolécules, ce qui peut limiter la précision des prédictions, notamment lorsque la cible est flexible ou subit des changements conformationnels importants.

À ce stade, la dynamique moléculaire intervient comme un outil indispensable pour affiner et valider les résultats du docking. La MD simule le mouvement des atomes et des molécules dans le temps en prenant en compte les interactions physiques et l'environnement moléculaire (solvant, ions, température…). Cette approche permet d'étudier la stabilité du complexe ligand–protéine, d'observer l'évolution des interactions clés et d'identifier les transitions conformationnelles qui ne peuvent être détectées par les méthodes statiques. Les simulations offrent une vision dynamique et réaliste des phénomènes moléculaires, apportant des informations précieuses sur les mécanismes de liaison, l'adaptabilité du site actif et le comportement global du système.

L'intégration du docking et de la dynamique moléculaire dans un pipeline cohérent permet d'améliorer considérablement la fiabilité de la prédiction bioactive. Le docking sert de première

étape de sélection, tandis que la MD confirme et affine les résultats en évaluant la stabilité temporelle des complexes. Cette stratégie hybride est souvent complétée par des méthodes d'estimation d'énergie libre de liaison (telles que MM-PBSA ou MM-GBSA), qui offrent une meilleure évaluation thermodynamique de l'affinité ligand–cible. Cette combinaison d'outils permet d'obtenir des prédictions plus robustes tout en limitant les coûts computationnels et expérimentaux.

La conférence abordera également les avancées récentes qui renforcent le rôle des méthodes in silico dans la découverte de médicaments. L'essor de l'intelligence artificielle et du machine learning a profondément transformé le domaine en permettant d'améliorer les fonctions de scoring, de prédire l'affinité ligand-cible avec une précision accrue, et même de générer de nouvelles structures moléculaires optimisées. Les techniques de simulation avancées, telles que la métadynamique ou la dynamique moléculaire accélérée, augmentent l'échantillonnage conformationnel et permettent de capturer des événements moléculaires rares mais biologiquement pertinents.

Les défis demeurent néanmoins importants. Les simulations dépendent fortement de la qualité des structures tridimensionnelles et des champs de force utilisés. Certaines protéines complexes, notamment les récepteurs membranaires ou les protéines intrinsèquement désordonnées, restent difficiles à modéliser avec précision. De plus, malgré les progrès des infrastructures de calcul, la réalisation de simulations longues et l'analyse des trajectoires générées peuvent nécessiter des ressources importantes.

La conférence présentera des études de cas démontrant l'application réelle de ces outils dans des projets variés : identification d'inhibiteurs enzymatiques, modélisation d'interactions ligand–récepteur, recherche d'antagonistes pour des cibles thérapeutiques émergentes, ou encore repositionnement de médicaments existants. Ces exemples illustreront l'impact majeur des approches in silico dans les domaines de l'oncologie, des maladies infectieuses, des neurosciences et au-delà.

Cette conférence thématique met en avant l'importance stratégique de l'intégration du docking et de la dynamique moléculaire dans la découverte de médicaments. Ces méthodes, de plus en plus précises et accessibles, constituent aujourd'hui un pilier essentiel de la recherche biochimique et pharmaceutique. Elles offrent une opportunité unique d'accélérer l'identification de nouvelles molécules actives, tout en améliorant notre compréhension des mécanismes biomoléculaires fondamentaux.

Mots clés : Docking moléculaire, Affinité de liaison, Dynamique moléculaire, Modélisation in silico, Interaction ligand–protéine, Prédiction de l'activité biologique.

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TOPIC B: ANALYTICAL CHEMISTRY, ELECTROCHEMISTRY AND WATER CHEMISTRY

TB1- Les polluants émergents : L'apport du screening non ciblé pour une vision globale de la contamination »

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Résumé

Les eaux naturelles et potables contiennent de plus en plus de polluants émergents issus de l'activité humaine : résidus pharmaceutiques, cosmétiques, pesticides ou microplastiques. Ces substances, même à faibles doses, présentent des risques toxicologiques complexes et mal caractérisés, par exemple les microplastiques peuvent provoquer stress oxydatif, inflammation et déséquilibres microbiens [1]. Les approches analytiques ciblées actuelles sont insuffisantes pour détecter l'ensemble de ces composés et leurs produits de dégradation. Le screening non ciblé (NTS), fondé sur la spectrométrie de masse haute résolution, permet une cartographie complète de la contamination chimique, y compris la détection de métabolites et de composés non envisagés auparavant [2]. Son développement constitue un levier essentiel pour comprendre, surveiller et réduire la toxicité chimique globale des eaux.

Mots clés : Polluants émergents, Screening non ciblé (NTS)

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2. « Non-target screening in water analysis: recent trends of data evaluation, quality assurance, and their future perspectives. » Analytical & Bioanalytical Chemistry, 2024. Springer Link

TOPIC C: MATERIALS AND POLYMER CHEMISTRY, INORGANIC CHEMISTRY AND CATALYSIS

TC1- Valorization of 2-Chloro-3-Formylquinoline: Synthesis and Antimicrobial Evaluation of New Bioactive Derivatives

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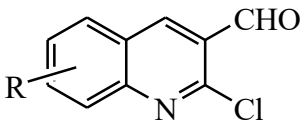
Abstract

Quinoline is an aromatic heterocycle consisting of a benzene ring fused to a pyridine ring. This fundamental structural motif is found in numerous natural alkaloids, such as quinine, as well as in various pharmaceutical molecules, including antimalarial, antibacterial, and anticancer agents. Owing to its aromatic stability and the presence of a basic nitrogen atom, quinoline exhibits a versatile chemical reactivity, making it an important platform for the design of new bioactive compounds.

Its derivative, 2-chloro-quinoline-3-carbaldehyde[1], is particularly reactive: the chlorine atom at position 2 facilitates nucleophilic substitution reactions, while the formyl group enables condensation reactions such as the Henry[2], Knoevenagel , and Baylis–Hillman [3] reactions.These properties make this compound a key intermediate for the synthesis of new bioactive heterocycles, such as tetrazolo[1,5-a]quinolones [4], pyranoquinolines [5] and epoxyquinolines [6].

Thus, quinoline and its derivatives represent a strategic class of compounds in medicinal and green chemistry, paving the way for the development of innovative molecules with high pharmacological potential.



2-Chloro-quinoline-3-carbaldehyde

Keywords: quinoline, 2-chloro-quinoline-3-carbaldehyde, heterocycle, bioactive compounds

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TOPIC D: CHEMISTRY OF NATURAL PRODUCTS, ORGANIC SYNTHESIS AND PHARMACEUTICAL CHEMISTRY

TD1- Insights into the Phytochemistry and Chimiotaxonomy Patterns of *Launaea* Cass. Genus (Asteracea) from Algerian Sahara

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Abstract

Medicinal plants in traditional pharmacopeia have been employed for the treatment and management of various ailments since the beginning of human civilization and continue to provide mankind with new remedies, such as, the oldest known medicinal systems of the world: Ayurveda, Arabian medicine, Chinese and Kempo medicine. The Materia Medica of Ibn Baytar (Andalusia, Spain, 1197–1248), is one of the oldest documents that describe the use of natural products for healing diseases in the mediterranean area. It listing about 1400 drugs, medicinal plants and foods, for treating human diseases. Actually, about 50,000 species of higher plants have been used for medicinal purposes and major pharmaceutical drugs have been either derived from or patterned after compounds from biological diversity.

Algeria with its large area and diversified climate has a varied flora, which is a source of rich and abundant medical matter and, in particular, Sahara part constitutes an important reservoir of many plants, which have not been investigated until today. Among this flora, some *Launaea* plants have been used in the Algerian traditional medicine as bitter stomachic, anti-tumour, insecticides and against skin diseases. Three of this species are used in Algerian Sahara ethnopharmacopea: *Launaea Nudicaulis, Launaea residifolia and Launaea arborescens*.

The aim of this conference is to present the recent trends on the nature of natural compounds constituents from the genus *Launaea Cass.*, especially those growing in Algerian Sahara and used as medicinal plants, together with their biological activities, and as chemotaxonomic markers for the botanical Asteraceae family.

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TD2- Bio-sourced Proteases: Green Catalysts for Sustainable Applications in Leather Processing and Agri-Food Industries

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Abstract

Microbial proteases have emerged as versatile bio-sourced catalysts with broad industrial applications, particularly in eco-friendly leather processing and sustainable agri-food production. In the leather industry, these enzymes offer an efficient alternative to traditional chemical treatments for dehairing and bating processes, significantly reducing pollution and improving product quality. In parallel, their use in the bioconversion of protein-rich agri-food by-products such as poultry feathers and shrimp shells, enables the generation of bioactive protein hydrolysates that can serve as natural feed additives for aquaculture, enhancing both nutritional and functional properties of fish diets.

In this study, two purified alkaline serine proteases produced by Anoxybacillus kamchatkensis and Aeribacillus pallidus were employed for the enzymatic hydrolysis of keratinous residues. The resulting hydrolysates were enriched in essential amino acids and bioactive peptides exhibiting antioxidant and enzyme inhibitory (ACE, DPP-IV) activities.

The findings highlight the dual industrial potential of these microbial proteases as green tools for cleaner leather processing and as bioactive sources for the agri-food sector. This bio-sourced

enzymatic approach contributes to the valorization of underutilized keratinous materials, aligning with the principles of green chemistry, circular bioeconomy, and sustainable industrial development.

Keywords: microbial proteases, leather processing, agri-food by-products, enzymatic valorization, circular bioeconomy, bioactive peptides

TD3- EXPLORING THE PHARMACOLOGICAL POTENTIAL OF SOME SELECTED AURES PLANTS: FROM ETHNOMEDICINAL KNOWLEDGE TO APPROVED CANDIDATES

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Abstract

Plant-derived molecules continue to play a pivotal role in modern drug design and discovery. In recent years, there has been a remarkable increase in the exploration, development, and advancement of herbal substances for pharmaceutical applications. Owing to their low toxicity, structural diversity, and multi-target mechanisms of action, bioactive compounds isolated from medicinal plants have demonstrated significant efficacy in preventing and treating oxidative, inflammatory, and microbial diseases, among others. The development of drugs from natural products typically involves several critical stages: the selection of plants based on their traditional use, extraction and purification of bioactive compounds, structural elucidation, and biological evaluation through *in vitro* and *in vivo* studies. Complementary computational approaches, such as molecular docking and ADMET prediction, further enhance the identification of therapeutic targets and the optimization of lead compounds. In this context, the present study explores the drug discovery potential of some selected medicinal plants from the flora of Aures region, Algeria. By integrating phytochemical, pharmacological, and computational approaches, we aim to bridge traditional knowledge with modern pharmacological research, thereby highlighting the promise of these plants as sources of novel therapeutic agents.

Keywords: Plant-derived molecules, biological activities, molecular docking and ADMET prediction.

Oral Conferences

Topic A Program

TOPIC A: THEORETICAL CHEMISTRY AND MOLECULAR MODELING		
N°	**Title**	**Autors**
O_{A1}	Intégration d'un e-pharmacophore et du docking moléculaire pour l'identification de nouveaux inhibiteurs de la protéase NS3/4A du virus de l'hépatite C (VHC)	Dr. Afaf Zekri **U-Biskra**
O_{A2}	Quantitative prediction of the octanol–organic carbon partition coefficient in organic compounds	Dr. Amel Bouakkadia **U-Khenchela**
O_{A3}	Molecular junctions with a perfect spin-filtering function based on half-metallic Zigzag Graphene Nanoribbons (ZGNRs)	Youcef Bensaidane **U-Laghouat**
O_{A4}	Basicity and Nucleophilicity Effect in charge transfer of AlH_3–base Adduct	Dr. Mohamed Aichi **U- Khenchela**
O_{A5}	Theoretical insights into the structure–antioxidant activity relationship of some flavonoids	Dr. Samiha Karoui **U-Batna 1**
O_{A6}	Molecular modeling study of pyrimidinone linked to thiazole derivatives	Dr. Hanane Tabbi **U-Batna 1**
O_{A7}	Étude des complexes binucléaires de Ruthénium à pont hydrure	Dr. Housny Maddi **U-Batna 1**

OA1- Intégration d'un e-pharmacophore et du docking moléculaire pour l'identification de nouveaux inhibiteurs de la protéase NS3/4A du virus de l'hépatite C (VHC)

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Résumé

La découverte rationnelle d'inhibiteurs antiviraux s'appuie largement sur le docking moléculaire. Nous avons mis en œuvre un criblage virtuel basé sur la structure (SBVS) intégrant un modèle e-pharmacophore dérivé du complexe Voxilaprévir–NS3/4A (PDB 6NZT), suivi d'un protocole de docking Glide (modes SP/XP) contre la protéase NS3/4A du VHC. Une bibliothèque de 65 220 composés issus de PubChem, sélectionnés pour 90 % de similarité avec des produits naturels actifs contre le VHC, a été filtrée ; 298 molécule s présentant les meilleurs scores de fitness ont ensuite été retenues pour le docking. L'efficacité de la méthode a été validée par une analyse d'enrichissement, démontrant une capacité de discrimination satisfaisante (ROC = 0,74 ; RIE = 4,7 ; AUC = 0,74). Cinq composés prioritaires, **CID 44326497**, **CID 142714408**, **CID 99999007**, **CID 129834837**, et **CID 129835078**, affichent des scores XP compris entre −9.316 et −7.220 kcal/mol, supérieurs à celui du ligand de référence Voxilaprévir (−4.886 kcal/mol), suggérant une affinité potentiellement accrue pour NS3/4A. Ensemble, ces résultats confirment la solidité de l'approche SBVS/docking et désignent plusieurs candidats prometteurs comme inhibiteurs de NS3/4A, justifiant des investigations expérimentales ultérieures.

Mots clé: VHC, NS3/4A, e-pharmacophore, docking moléculaire, validation par enrichissement.

OA2- Quantitative Prediction of the Octanol–Organic Carbon Partition Coefficient in Organic Compounds

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Abstract

Pesticides are a major environmental concern due to their persistence, bioaccumulation, and potential harmful effects on human health and ecosystems. Their physicochemical properties play a key role in determining their environmental distribution and fate. Chemometric methods can be used to analyze how these properties vary according to molecular structure, as represented by appropriate molecular descriptors. Quantitative Structure–Property Relationship (QSPR) models provide a comprehensive understanding of how molecular structure influences these properties. The octanol/carbon partition coefficient (Koc) is a critical parameter for predicting the mobility and bioavailability of pesticides in the environment. In this study, molecular descriptors were optimized and calculated using specialized molecular modeling software (HyperChem and Dragon). The QSPR model was then developed using The QSARINS [6] software was used for simple MLR analysis, employing ordinary least squares regression (OLS) and Genetic Algorithms for variable subset selection (GA-VSS) [7]. A dataset of 34 compounds was randomly divided into two subsets: a training set of 22 compounds for model development and a test set of 12 compounds for external validation. The values of the statistical parameters (coefficient of determination and prediction: R^2, Q^2EXT, standard deviation s, SDEPext, and SDEC) confirm the quality and relevance of the developed model. The model's applicability domain was assessed using Williams plots.

Keywords: QSPR methods; Pesticides, Octanol/Carbon Partition Coefficient (Koc); Multiple Linear Regression (MLR); Molecular Descriptors.

OA3- Molecular junctions with a perfect spin-filtering function based on half-metallic Zigzag Graphene Nanoribbons (ZGNRs)

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Abstract

One of the most researched types of graphene nanoribbon is the zigzag nanoribbon (ZGNR), which is essential to studies in molecular electronics and spintronics. The unique geometry of its edges sets it apart.We design spin filter devices based on (ZGNR), a carbon nanomaterial in which intrinsic magnetic moments combine with edge effects to produce a half-metallic property, using density functional theory in conjunction with the nonequilibrium Green's functions method. Such carbon-based devices can achieve over 100% spin filtering effect at low bias voltages, according to spin-resolved electrical transport investigations. Our research demonstrates that the magnetic and electronic characteristics of (ZGNR) nanoribbons, particularly the magnetic moments on the quasi-sp3 carbons, are responsible for the excellent SEF transport features. According to these intriguing findings, (ZGNR) nanomaterial has.

Keywords: NEGF, DFT, Molecular junctions. Biosensors.

OA4- Basicity and Nucleophilicity Effect in charge transfer of AlH_3–base Adduct

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Abstract

This study permits to explore the interactions involved in Lewis acid (AlH3) and Lewis bases: CO; H2O; NH3; PH3; PC13; H2S; CN-; OH-; O2-2; F-; N (CH3)3; N2; N2H4; N2H2; pyridine; aniline. By means of DFT theory calculations with B3LYP functional using 6-31G(d,p) basis set and in order to check the effects of both the donor and the acceptor in the establishment of the different adducts we focused mainly on the calculation of the energetic gap ΔEHOMO-LUMO, Gibbs energies ΔG, the angle (θ) in AlH3-Base and the interaction energy values Eint. The several parameters of the reactivity (electrophilicity index (ω) , nucleophilicity (N), chemical potential (μ), hardness (η) and polarizability (α) are also calculated to defined the weak interaction as well as to distinguish between the nucleophilicity and basicity of the different Lewis basis. Our results showed that the electronic charge transfer is estimated to be important in the systems where the interaction is established between Al and anionic bases, and the electron donor power is predictable for O-2, F-, OH- and CN-. The pseudo-tetrahedral adduct arrangements depend on the parameter geometries (bond length interaction and θ angle) and Gibbs energies ΔG characterizing the main stability.

Keywords: Lewis acid-base interaction, adduct, DFT, nucleophilicity, charge transfer.

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OA5- Theoretical Insights into the Structure–Antioxidant Activity Relationship of Some Flavonoids

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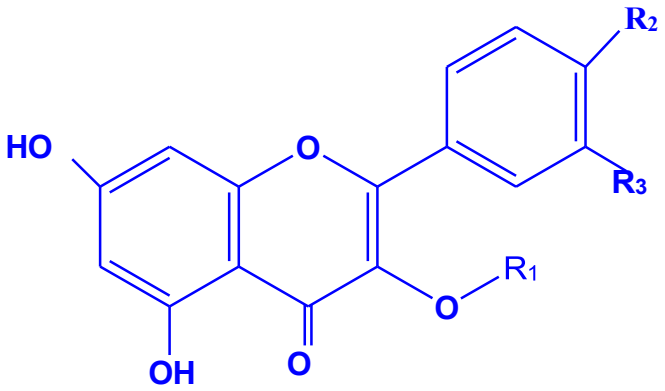
Abstract:

Flavonoids, which originate from plant secondary metabolites, enter the human body through daily dietary intake. These compounds attract considerable interest due to their strong antioxidant and radical-scavenging properties, suggesting a potential role in preventing various diseases and neutralizing free radicals, including those implicated in cancer.

In this study, we employed quantum chemistry methods to investigate the electronic, structural, and energetic properties of different activated forms.

Furthermore, to model interactions between proteins and flavonoid inhibitors, we used a range of molecular modeling techniques, including molecular mechanics, molecular docking, and molecular dynamics simulations.



Keywords: Flavonoid, Antioxidant, Antiradical, enzyme, Molecular docking.

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OA6- Molecular modeling study of pyrimidinone linked to thiazole derivatives

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Abstract

Nitrogen and sulfur heterocyclic compounds such as thiazoles have been consistently exploited over the years by industry and academia to provide drug candidates with interesting pharmacological properties, including antimicrobial [1], anticancer and anti- inflammatory [2] properties.
Furthermore, pyrimidinone derivatives also form a very remarkable class of heterocyclic compounds. They play an important role in the development of several broad -spectrum pharmaceuticals, such as antimicrobials, anti-HIV drugs, and antimalarials [3].
Density functional theory (DFT) has been widely used in the literature due to its efficiency and accuracy in evaluating a number of molecular properties [4]. Also, virtual screening obtained by molecular docking is a new method for calculating the affinity of a very large type of ligands for a known therapeutic purpose; it is faster and easier to use, and it is inexpensive compared to experimental screenings.

Therefore, this research work is placed in the context of a computational study of a series of thiazole derivatives linked to pyrimidinone in order to predict its chemical reactivity and to study the binding affinities of the drugs and the molecular interactions between compounds and the active site (protein-ligand) using Gaussian 09 software and molecular docking software which is MOE (Molecular Operating Environment) respectively.

Keywords: pyrimidinone; thiazole; DFT; docking; computational chemistry.

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OA7- Étude des complexes binucléaires de ruthénium à pont hydrure

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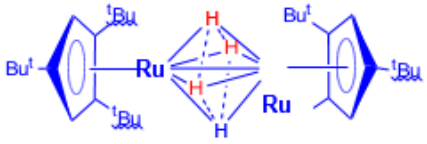
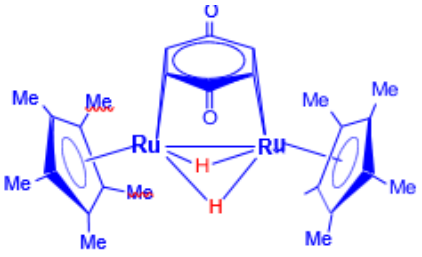
Résumé :

Cette étude propose une investigation zsystématique, menée par calculs DFT, de complexes binucléaires de ruthénium à base de Cp, en particulier Cp*Ru(μ-H)4RuCp* (A1) et CpRu(μ-H)2(μ- η^2-C6H4O2)RuCp (A2). Les calculs réalisés aux niveaux B3LYP et PBE0/def2-TZVP montrent un excellent accord entre les géométries optimisées et les données expérimentales, avec des écarts inférieurs à 0,1Å pour les distances Ru–Ru. L'analyse des orbitales frontières indique que A1 présente la plus grande stabilité électronique (écart HOMO-LUMO élevé), tandis que A2 se distingue par une réactivité plus marquée et des propriétés optiques renforcées. Enfin, MESP et l'analyse NBO mettent en évidence une forte délocalisation metal-ligand ainsi que la présence probable d'interactions agostiques dans A2.



A1



A2

Les calculs TD-DFT en solution d'acétonitrile montrent qu'A1 est un bon candidat pour la capture de lumière à haute énergie (transitions MLCT/ILCT intenses), alors qu'A2 est mieux adapté aux absorptions décalées vers le rouge. Enfin, les propriétés NLO mettent en évidence A3 comme le composé le plus prometteur pour les applications optoélectroniques. Ces résultats soulignent la corrélation entre la structure, la réactivité et les propriétés optiques de complexes à pont hydrure de ruthénium, offrant de nouvelles perspectives pour la conception de matériaux moléculaires multifonctionnels.

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TOPIC B: ANALYTICAL CHEMISTRY, ELECTROCHEMISTRY AND WATER CHEMISTRY

Topic B Program

N°	*Title*	Autors
OB1	Eco-friendly inhibition of biocorrosion using a lipopeptide biosurfactant: Structural characterization and MIC mitigation via SEM-EDX.	Soumia Hadjala **U-Blida 1**
OB2	Elimination de sulfur du bain de d'épilage des eaux usées de tannerie par une combinaison de précipitations et l'oxydation processus de lixiviation	Dr. Fatima Chemlal **U-Batna 1**

OB1- Eco-friendly inhibition of biocorrosion using a lipopeptide biosurfactant: Structural characterization and MIC mitigation via SEM-EDX

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Abstract:

Microbiologically influenced corrosion (MIC) is a major industrial and environmental issue, particularly in marine and aquatic systems where sulfate reducing bacteria (SRB) contribute to the rapid deterioration of metallic infrastructures. Conventional corrosion inhibitors are often toxic and non-biodegradable, prompting the need for sustainable alternatives. In this study, a lipopeptide biosurfactant, produced by a hydrocarbonoclastic bacterial strain isolated from marine sediment contaminated with hydrocarbons, was investigated for its anticorrosive properties against MIC under laboratory-controlled conditions.

The biosurfactant was produced under aerobic batch conditions at 30 °C using olive oil and ammonium nitrate as the sole carbon and nitrogen sources. Surface active performance was confirmed by a surface tension reduction to 28 $mN \cdot m^{-1}$, an oil displacement diameter of 70 mm, and an emulsification index (E24) of 75% after 48 hours. The compound was structurally identified as a lipopeptide using Fourier Transform Infrared Spectroscopy (FTIR) and UV- Visible spectrophotometry, confirming the presence of characteristic functional groups associated with peptide and lipid moieties.

To evaluate its performance against MIC, carbon steel coupons were exposed to SRB in the presence and absence of the biosurfactant. Scanning Electron Microscopy (SEM) revealed a significant reduction in bacterial adhesion and biofilm formation on treated surfaces. Energy Dispersive X-ray Spectroscopy (EDX) further confirmed a decrease in sulfur deposition, indicating inhibited sulfate reduction activity. After 30 days of exposure, the biosurfactant treatment achieved 81.3% efficiency in iron preservation and 91.2% reduction in sulfur accumulation, compared to untreated controls.

These findings highlight the potential of lipopeptide biosurfactants as efficient, ecofriendly corrosion inhibitors, capable of disrupting microbial colonization and electrochemical degradation processes. Their biodegradability, low toxicity, and structural stability make them promising candidates for sustainable corrosion mitigation in marine, water treatment, and industrial environments.

Keywords: Biosurfactants; Sulfate Reducing Bacteria (SRB); Microbiologically Influenced Corrosion (MIC); Biofilm Inhibition; SEM-ED

OB2- Elimination de sulfure du bain de d`épilage des eaux usées de tannerie par une combinaison de précipitations et l'oxydation processus de lixiviation.

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Résumé

Le traitement des eaux usées de dépilage provenant d'une tannerie algérienne (unité de Batna) a été réalisé à l'aide d'un procédé de lixiviation par précipitation chimique et oxydation. Tout d'abord, une extraction sélective du sulfure a été obtenue par précipitation chimique dans des conditions optimisées, entraînant une réduction de 95 % des ions sulfure. L'intégration du procédé de lixiviation par oxydation avec la précipitation chimique a renforcé l'élimination du sulfure, atteignant jusqu'à 98 %, tout en empêchant la production de boues.

De plus, la solution de $ZnSO_4$ peut être recyclée pour être utilisée dans un nouveau cycle de précipitation.

Cette étude examine l'efficacité d'une combinaison de précipitations et à l'oxydation processus de lixiviation dans la réduction de fortes concentrations de sulfures dans bain de d`epilage-pelannage de la tannerie de l'effluent à partir de l'un des principaux en cuir de tannage végétal de Batna, Algérie. D'abord, l'influence de divers paramètres de fonctionnement et les différents sels de zinc a été évaluée par rapport à la précipitation et le taux de dépôt de ZnS.

1. Le traitement des eaux usées de dépilage provenant d'une tannerie algérienne (unité de Batna) a été réalisé à l'aide d'un procédé de lixiviation par précipitation chimique et oxydation.
2. Tout d'abord, une extraction sélective du sulfure a été obtenue par précipitation chimique dans des conditions optimisées, entraînant une réduction de 95 % des ions sulfure. L'intégration du procédé de lixiviation par oxydation avec la précipitation chimique a renforcé l'élimination du sulfure, atteignant jusqu'à 98 %, tout en empêchant la production de boues.
3. De plus, la solution de $ZnSO_4$ peut être recyclée pour être utilisée dans un nouveau cycle de précipitation.

Mots-clés: Oxydation de lixiviation; Précipitations; Sulfure d'enlèvement des effluents de Tannerie; traitement de l'Eau.

TOPIC C: MATERIALS AND POLYMER CHEMISTRY, INORGANIC CHEMISTRY AND CATALYSIS

Topic C Program

N°	Title	Autors
O_{C1}	Enhanced Water Treatment Approaches: The Role of Cellulose Acetate / Natural Zeolite Membranes	Dr. Tahani-Achouak CHINAR **U-Batna 2**
O_{C2}	Etude de la cinétique de dégradation thermique des films d'emballage pcl/pvc/organo-argile nanoblends	Dr. Farida Yahiaoui **U-Batna 1**
O_{C3}	Valorization of Bentonite as Low-Cost Precursors for Ni-Based Catalysts for Hydrogen Production via the Dry Reforming of Methane	Dr. BOUDIAF Meriem **U- Bab-Ezzouar, Algeria.**
O_{C4}	Synthesis and characterization of quinoline derivatives using an optimized Henry reaction	Khelaf Rahima **U-Batna 1**
O_{C5}	Synthèse d'un Adsorbant Polymère Contenant le Motif 2-HydroxyBenzophénone : Application à l'Extraction des ions Plomb en Solution Aqueuse	Fairouz Aberkane **U-Batna 1**

OC1- Enhanced Water Treatment Approaches: The Role of Cellulose Acetate / Natural Zeolite Membranes

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Abstract:

The treatment of wastewater, whether originating from domestic or industrial sources, poses a significant challenge for environmental protection today. The reuse of this water is a solution that is already being implemented. Among the rapidly advancing techniques in this area, membrane filtration methods are particularly noteworthy.

In this study, we developed polymer membranes using cellulose acetate and zeolite obtained from a deposit in Bédjaia, Algeria, by adjusting their proportions. These membranes are designed to purify wastewater contaminated with dyes, especially from the textile and paper industries.

The morphology of these membranes was analyzed using Fourier transform infrared spectroscopy (FTIR) and scanning electron microscopy (SEM). The resulting filtrates were examined through UV spectroscopy to assess the membranes' effectiveness in removing methyl orange. The findings indicate that these membranes are effective in eliminating this organic dye, with their efficiency attributed to the adsorption capacity of natural zeolite, owing to its porous structure.

Keywords: *wastewater, protection, membranes, polymer, zeolite, porous.*

OC2- Étude de la cinétique de dégradation thermique des films d'emballage PCL/PVC/organo-argile nanoblends.

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Résumé :

Dans le cadre de cette étude, nous nous sommes intéressés à l'amélioration des propriétés thermiques du matériau PVC/PCL, par l'incorporation d'une faible quantité d'argile organiquement modifiée, au sein de leur matrice. Dans ce but, la cinétique de la dégradation thermique de mélange PVC/PCL et de leur nanoblends (PVC/PCL/OMMTs) sera étudiée de façon approfondie à l'aide de la méthode KAS et celle d'OFW.

Les résultats obtenus montrent que l'incorporation de 3% en poids d'argile modifié organiquement dans la matrice du PVC/PCL amélioré la stabilité thermique de ce dernier, par l'augmentation de sa température de début de dégradation (T_{onset}). De plus, l'étude cinétique de décomposition thermique a montré que les énergies d'activation apparentes de la première étape de dégradation Ea_1 des nanomatériaux PVC/PCL//OMMT1 et PVC/PCL/C30B est supérieure à celles du matériau PVC/PCL. Ces résultats confirment l'effet barrière de l'argile modifié organiquement sur la décomposition du matériau PVC/PCL. Tandis que celle du PVC/PCL/OMMT2 est inférieure à celle du PVC/PCL, ce qui confirme son effet catalytique.

Mots clés : *Poly (ε-caprolactone) ; Poly (chlorure de vinyle) ; Films d'emballage ; Montmorillonite ; la stabilité thermique, Cinétiques de dégradation ; nanoblends.*

OC3- Valorization of Bentonite as Low-Cost Precursors for Ni-Based Catalysts for Hydrogen Production via the Dry Reforming of Methane

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Abstract:

Since the Industrial Revolution, global energy demand has continued to rise in parallel with population growth, improved living standards, and globalization. Consequently, the atmospheric concentrations of the two major greenhouses gases—methane (CH_4) and carbon dioxide (CO_2)—have increased proportionally with energy consumption. Hydrogen production via the dry reforming of methane ($CH_4 + CO_2 \rightarrow 2H_2 + 2CO$) is gaining growing attention, as it simultaneously addresses two critical global challenges: the depletion of fossil resources and the mitigation of global warming through the utilization of CH_2 and CO_2 to produce synthesis gas ($H_2 + CO$).

Extensive efforts are being devoted to developing catalytic materials that are both cost-effective and highly active. Nickel-based catalysts have attracted significant interest due to their low cost, abundance, and catalytic activity comparable to that of noble metals. However, their rapid deactivation caused by coke deposition and particle sintering at high temperatures remains a major limitation. To enhance catalytic performance, suitable supports and promoters are often introduced. The cost of supports, however, represents a considerable barrier to large-scale applications.

In this communication, we explore the valorization of bentonite as low-cost, environmentally friendly, and thermally stable supports for the synthesis of Ni-based catalysts for the dry reforming of methane. Various preparation and treatment methods, along with physicochemical characterization results and catalytic performance evaluations, will be presented and discussed.

Keywords: *Dry reforming of methane, Nickel based catalysts, Bentonite, hydrogen generation.*

OC4- Synthesis and Characterization of Quinoline Derivatives Using an Optimized Henry Reaction

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Abstract

Quinoline derivatives, widely recognized for their broad spectrum of biological properties **[1,2]**, continue to attract significant interest in organic and medicinal chemistry. In the present work, we report the synthesis of a novel series of nitroaldol-based quinoline compounds **[3]** through an efficient Henry reaction protocol, affording the target molecules in high yields. Their structures were fully characterized using ^{1}H and ^{13}C NMR spectroscopy, FTIR analysis, and mass spectrometry. The synthesized derivatives demonstrated promising antimicrobial activity against several pathogenic microorganisms. Furthermore, Density Functional Theory (DFT) calculations provided theoretical support for the experimental findings, while in-silico pharmacokinetic evaluations revealed favorable oral absorption, membrane permeability, and overall bioavailability.

Keywords

Nitroaldolquinoline, antimicrobial, DFT, *In silico* molecular docking, DNA-gyrase

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OC5- Synthèse d'un Adsorbant Polymère Contenant le Motif 2-HydroxyBenzophénone : Application à l'Extraction des ions Plomb en Solution Aqueuse

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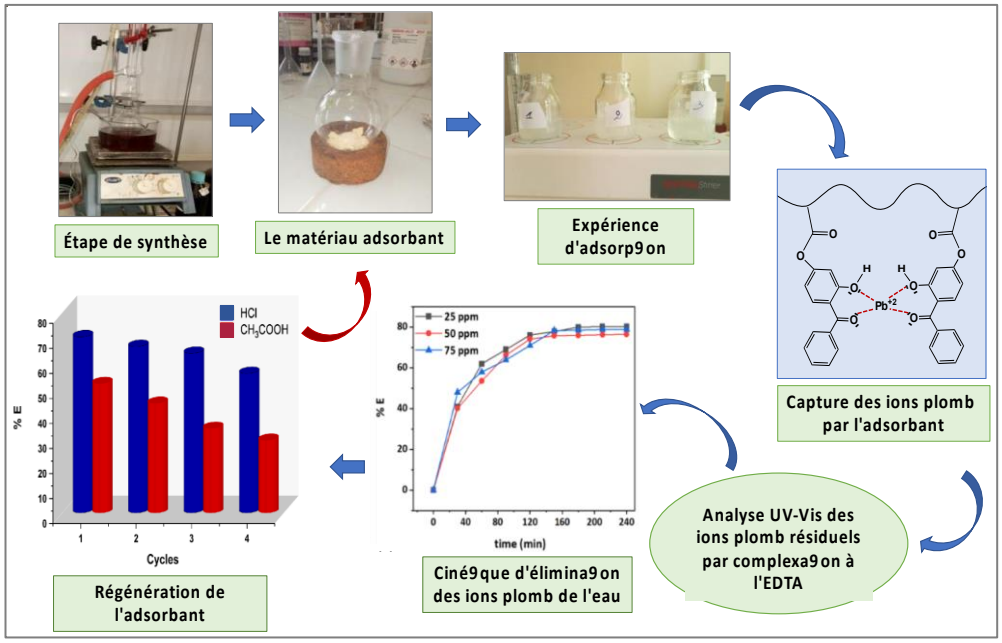
Résumé

La contamination de l'eau par les métaux lourds représente un risque sérieux pour les écosystèmes et la santé humaine en raison de leur toxicité, de leur persistance et de leur capacité à s'accumuler dans les organismes vivants. Dans cette étude, un nouveau matériau adsorbant, le poly(2-hydroxy-4-méthacryloyloxy benzophénone) (PHMB), a été synthétisé et utiliser pour l'extraction du plomb présent dans l'eau. Les structure du PHMB a été confirmées par les spectroscopies (FTIR, et la ^{1}H RMN et ^{13}C RMN). L'étude d'adsorption du plomb sur le PHMB a été déterminée par spectroscopie UV-visible. L'étude des isothermes d'adsorption a révélé que le modèle de Freundlich décrit le mieux le comportement du système, suggérant un adsorption multicouche favorable, avec une capacité maximale d'adsorption de 142,68 mg/g. L'étude cinétique a révélé que le processus d'adsorption était bien décrit par le modèle cinétique de pseudo-second ordre, indiquant que la chimisorption était le mécanisme d'adsorption dominant. De plus, le PHMB a conservé son efficacité après plusieurs cycles de régénération, attestant de sa bonne réutilisabilité et de sa forte affinité pour le Plomb.

Mots clés : Plomb ; Polymère adsorbant ; 2-hydroxy benzophénone ; Adsorption.



TOPIC D: CHEMISTRY OF NATURAL PRODUCTS, ORGANIC SYNTHESIS AND PHARMACEUTICAL CHEMISTRY

Topic D Program

N°	Title	Autors
O_{D1}	Approche novatrice pour le développement d'un gel anti-arthrose et l'identification des métabolites bioactifs du Trigonella foenum-graecum	Dr. MOKRANI Karima **U-Tarf**
O_{D2}	Etude phytochimique et biologique de l'extrait apolaire du frêne dimorphe d'Algérie.	Sabrine Bouhentala **U-Batna 1**
O_{D3}	Extraction, isolation and structural elucidation of some phytochemicals from a Halophytic plant.	Abdelbasset Tamersit **U-Batna 1**
O_{D4}	Promising preventive treatments for hypercholesterolemia and dyslipidemia from C. flammula and F. angustifolia extracts	Prof. Dina Atmani-Kilani **U-Bejaia**
O_{D5}	Essai de fabrication de chips de pommes	Hayet Benhamza **U- Eloued**
O_{D6}	Analyse LC-MS des composés phénoliques de Senecio glaucus et évaluation antioxydante	Dr. Meriem Belaid **U-Batna 1**
O_{D7}	Etude du profile de la plante Vicia onobrychioides par GC-MS et estimation de leur activitié antioxydante	Fatima Belahssini **U-Batna 1**
O_{D8}	Activités, antioxydants, anti-inflammatoire et antalgique des extraits de Thapsia garganica de la région de Bejaia	Prof. Fatiha Bedjou **U-Bejaia**
O_{D9}	Caractérisation physico-chimique d'une lipase partiellement purifiée chez Penicillium sp. isolée à partir des grignons d'olives	Benhassine Yousra **U-Annaba**
O_{D10}	Analyse phytochimique et évaluation des activités biologiques de l'extrait de Crataegus azarolus	Prof. Nassima Chaher **U-Bejaia**
O_{D11}	Un flavonol glycosylé isolé de l'espèce Malope malacoides L.	*Nour el-houda Bekache* ***U-Batna 1***

OD1- APPROCHE NOVATRICE POUR LE DEVELOPPEMENT D'UN GEL ANTI- ARTHROSE ET L'IDENTIFICATION DES METABOLITES BIOACTIFS DU TRIGONELLA FOENUM-GRAECUM

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Résumé

Trigonella foenum-graecum L.**,** communément appelé fenugrec, est une plante annuelle de la famille des Fabacées, reconnue pour ses propriétés médicinales et thérapeutiques. Originaire du bassin méditerranéen, elle est largement cultivée en Algérie et valorisée pour ses usages traditionnels, notamment dans le traitement des affections articulaires et inflammatoires.

Dans cette étude, un gel innovant à visée anti-arthrose a été développé à partir des graines de fenugrec, suivant une démarche intégrée combinant analyse phytochimique et évaluation biologique. Les métabolites secondaires ont été extraits et caractérisés, révélant une richesse significative en flavonoïdes (3 %), alcaloïdes (5 %), saponosides, huiles essentielles et quinones. Ces composés sont connus pour leur rôle dans les mécanismes anti-inflammatoires. L'activité anti-inflammatoire in vitro a été évaluée par l'inhibition de la dénaturation de l'albumine sérique bovine, un modèle largement utilisé pour prédire le potentiel thérapeutique des formulations topiques. Les résultats ont montré que le gel formulé exerce une inhibition significative, comparable à celle d'un anti-inflammatoire de référence (diclofénac), confirmant l'efficacité des composés bioactifs présents. Le mécanisme d'action supposé des flavonoïdes et saponosides repose sur plusieurs voies complémentaires. Les flavonoïdes inhibent les médiateurs pro-inflammatoires tels que les cytokines et les enzymes COX/LOX, réduisant la synthèse de prostaglandines et d'oxyde nitrique. Les saponosides contribuent à stabiliser les membranes cellulaires et à moduler la réponse immunitaire locale, renforçant ainsi l'effet anti-inflammatoire observé.

D'un point de vue technologique**,** la formulation du gel présente plusieurs innovations : elle repose sur une base hydrosoluble optimisée, favorisant la pénétration cutanée des composés bioactifs et assurant une libération prolongée. L'utilisation d'excipients biocompatibles et la stabilisation homogène du gel améliorent sa stabilité, sa conservation et son efficacité thérapeutique, offrant ainsi un produit sûr et performant. Cette étude illustre une approche novatrice en phytothérapie, combinant la valorisation des ressources végétales locales et le développement de solutions naturelles pour le soulagement des douleurs articulaires. La méthodologie employée pourrait servir de base pour d'autres formulations topiques à visée anti-inflammatoire et ouvre des perspectives pour la mise au point de produits phytothérapeutiques innovants.

Mots-clés : Trigonella foenum-graecum L., phytothérapie, formulation topique, gel anti- arthrose, métabolites bioactifs, activité anti-inflammatoire, innovation pharmaceutique.

OD2- Etude phytochimique et biologique de l'extrait apolaire du frêne dimorphe d'Algérie

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Résumé

Le frêne dimorphe (*Fraxinus dimorpha* Coss. et Dur.), appartenant à la famille des Oléacées [1], est une plante médicinale largement utilisée dans la pharmacopée traditionnelle pour le traitement de diverses maladies telles que la jaunisse, le paludisme, la pneumonie, les fractures osseuses et les plaies [2].

Afin de valoriser cette espèce et d'explorer son potentiel bioactif, une étude phytochimique et biologique a été effectuée. L'extrait *n*-hexane de *F. dimorpha* a été soumis à différentes techniques chromatographiques (VLC, CC, CCM …. etc.), ce qui a permis l'isolement de six composés purs. L'élucidation structurale de ces composés a été réalisée à l'aide des méthodes spectroscopiques RMN 1D (^{1}H et ^{13}C) et 2D (COSY, HSQC, HMBC, ROESY), ainsi que par spectrométrie de masse (HR-ESI-MS). Cette analyse a abouti à l'identification de six biomolécules appartenant à différentes classes chimiques à savoir un acide gras estérifié nouveau, un acide gras saturé, deux triterpènes pentacycliques et deux stérols.

L'activité antioxydante a été évaluée par les tests DPPH et ABTS. Les résultats ont montré que l'extrait *n*-hexane présente une capacité modérée de piégeage des radicaux libres, comparativement à l'acide ascorbique utilisé comme standard.

Mot clés: *Fraxinus dimorpha*, Chromatographie, RMN, HR-ESI-MS, Antioxydants.

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OD3- EXTRACTION, ISOLATION AND STRUCTURAL ELUCIDATION OF SOME PHYTOCHEMICALS FROM A HALOPHYTIC PLANT

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Abstract

Medicinal plants have been used as primary treatments in various cultures for thousands of years. They are a valuable resource for traditional medicine and have also become a significant source for many modern pharmaceuticals. These plants contain numerous classes of phytochemicals that exhibit interesting pharmacological activities. As a result, leveraging these plant-derived products for drug discovery presents a promising opportunity for developing novel therapeutic drugs. The present study involves the phytochemical screening, extraction, isolation, and structural elucidation of some phytochemicals from an Algerian halophytic plant. The results of the phytochemical screening revealed the presence of many classes of secondary metabolites known for their pharmacological properties, such as flavonoids, terpenoids, saponins, quinones, and coumarins. The phytochemical study of the petroleum ether and *n*-butanolic extracts led to the isolation of two phytosterols and two glycosylated flavonoids using various chromatographic methods. The chemical structures of the isolated compounds were identified using different spectroscopic analyses, including 1D NMR (^{1}H, ^{13}C), and 2D NMR (COSY, HSQC, and HMBC), and the comparison with literature data. These results highlight the importance of this Algerian halophyte plant as a natural reservoir of bioactive compounds that could contribute to future research in drug discovery.

Keywords: Halophytic plant, Extraction, phytosterols, Flavonoids, NMR Analyses.

OD4- Promising preventive treatments for hypercholesterolemia and dyslipidemia *from C. flammula* and *F. angustifolia* extracts

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Abstract:

Dyslipidemia, or metabolic syndrome, is associated with atherosclerosis and obesity, which are widespread due to bad nutritional habits. Researchers are looking for naturally derived remedies to supplement highly toxic statins. Clematis flammula and Fraxinus angustifolia are commonly used in Algeria for treating arthritis and inflammatory diseases. We attempted to test in vitro anti-lipase and anti-HMG-CoA reductase and in vivo, hypolipidemic and hypocholesterolemic effects. The results show that the administration of Triton X-100) as a hyperlipidemic agent increased significantly ($P < 0.0001$) the level of triglycerides (TG) by 34.41%, and serum total cholesterol (TC) by 196%. On the other hand, we observed a decline in TG levels reaching 12 and 55.56% in mice having received 100 and 200 mg/kg of F. angustifolia extracts, respectively, while they were reduced by 33.59 and 58.32% ($P < 0.0001$) by 100 and 200 mg/kgbw of C. flammula extracts, respectively. While C. flammula extracts had no significant effect on TC, F. angustifolia reduced it by 27.9 and 21.24%, following the administration of 100 and 200mg/kgbw, respectively, with, nevertheless, a weaker efficiency when compared to atorvastatin (40%). A significant inhibition on porcine pancreatic lipase type II was equally observed by F. angustifolia extract (97.15%; IC50: 3.55 µg / ml), higher than that exhibited by C. flammula extract 84.89% (IC50: 12.10 µg / ml), at the same concentration of 300µg/ml.

Moreover, the plant extracts had a negative impact on the activity of HMG CoA reductase, at the dose of 200 µg / ml, by suppressing its activity by more than 60%, (92.15%; IC50: 90.06 µg/ml) exhibited by F. angustifolia, comparable to that of C. flammula (61.87%; IC50: 96.57 µg / ml). Histological analysis of liver confirmed our results.

Our findings advocate both plants as natural sources of lead molecules against hypercholesterolemia and dyslipidemia.

Keywords: Hypercholesterelemia, Dislipidemia, Clematis flammula, F. angustifolia, Biological activity.

OD5- ESSAI DE FABRICATION DE CHIPS DE POMMES

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Résumé :

Le présent travail constitue une ébauche pour la réalisation d'un ensemble d'essais sur la fabrication des chips de pomme.
La caractérisation biochimique des chips de pomme obtenue à démontré qu'elle est riche en sucres comme elle constitue un important apport énergétique, pour cela ils sont consommés par tous les âges, particulièrement appréciés par les enfants.

Le test de dégustation ressort que les chips de pomme les plus appréciés sont ceux enrobés en sucre et cuit au four.

Mots clé : chips, pomme, caractéristique biochimique, four, test de dégustation.

OD6- Analyse LC-MS des composés phénoliques de *Senecio glaucus* et évaluation antioxydante

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Résumé :

Les espèces du genre *Senecio* sont historiquement employées en phytomédecine pour le traitement d'affections variées, incluant les infections, le rhumatisme, l'asthme, les processus inflammatoires et les douleurs musculaires. Parmi elles, *Senecio glaucus* (Asteraceae), herbacée annuelle originaire d'Afrique du Nord et d'Asie, suscite un intérêt croissant en raison de son usage empirique contre les états inflammatoires et certaines formes de cancer. Le genre se distingue par une remarquable richesse en métabolites secondaires, majoritairement des composés phénoliques, tels que flavonoïdes (myricétine, quercétine, lutéoline) et acides hydroxycinnamiques (caféique, férulique, sinapique), fréquemment rencontrés sous forme glycosylée ou méthoxylée. L'analyse chromatographique LC-MS des extraits acétate d'éthyle et *n*-butanol de S. glaucus a permis d'identifier plusieurs composés phénoliques et d'en évaluer

l'abondance relative. L'extrait acétate d'éthyle présente une forte teneur en myricétine et en son dérivé glycosylé, tandis que l'extrait *n*-butanol se caractérise par un profil plus diversifié dominé par la chrysine-6-*C*-glucoside et l'oroxyline A, suggérant un large potentiel pharmacologique.

OD7- ETUDE DU PROFILE DE LA PLANTE *vicia onobrychioides* PAR GC-MS ET ESTIMATION DE LEUR ACTIVITIES ANTIOXYDANTE

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Résumé :

La famille des Fabaceae est la troisième plus grande famille de plantes à fleurs après les *Orchidaceae* et les *Asteraceae* (environ 730 genres et plus de 19400 espèces selon le Royal Botanic Garden, Edinburgh 2010). Les plantes de cette famille sont connues pour leur utilisation en médecine traditionnelle. Notamment, les études phytochimique ont montré leur richesse en métabolites secondaire possédant des activités biologique intéressante en particule les isoflavonoïdes qui sont connu par leur pouvoir oxydant.

Le genre *vicia* est l'un des genres important de la famille de Fabaceaeses grains qui sont très riche en protéines ont été utilisés en cuisine, torréfiés, et comme aliment pour les voyageurs dans les déserts orientaux. Mais en Algérie ce genre est plus utilise comme fourrage pour les animaux. Il est représenté par 83 espaces dans la flore d'Algérie. Les études récentes sur les plantes de ce genre ont prouvé l'existence de plusieurs métabolites secondaires, en particules les flavonoïdes, les saponines. Ils ont aussi montres que ce genres possède une activité biologique antioxydants remarquable.

L'étude de l'extrait ether de pétrole de l'espèce *vicia onobrychioides* nous a conduit à identifier 39 produites qui appartiennes a 4 famille. Aussi la plante a montré une activité antioxydant remarquable.

Mots clés : Fabaceae, *vicia, vicia onobrychioides,* GC-MS, activité biologique, antioxydant.

OD8- Activités antioxydants, anti inflammatoire et antalgique des extraits de *Thapsia garganica* de la région de Bejaia

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Résumé :

L'objet de cette étude est la détermination de l'activité antioxydants, anti inflammatoire et antalgique des extraits de *Thapsia garganica*, plante poussant spontanément dans la région de Bejaia. Une étude de la toxicité a complété les résultats obtenus afin de déterminer soit la toxicité ou l'innocuité des extraits de cette plante.

A cet effet les différentes parties de la plante (racines, feuilles et fleurs) ont été cueillies, séchées et broyées. Les activités antioxydants ont été réalisées *in vitro*, cependant les activités anti inflammatoire et antalgique ont été réalisées *in vivo* sur des rats. Des tests de détermination des activités enzymatiques au niveau du foie et des reins ont permis de compléter ces évaluations.

Les résultats montrent un effet inhibiteur vis-à-vis du radical DPPH allant jusqu'à 89,83% et pouvoir réducteur important pour l'extrait des feuilles. Les tests de toxicité montrent peu d'effets sur les enzymes rénales et hépatiques, de plus la détermination de la DL50 montre que ces extraits ne sont pas toxiques.

L'activité anti inflammatoire a montré une inefficacité des extraits, cependant l'activité antalgique la plus importante (64,66%) a été obtenue avec l'extrait des fleurs.

OD9- Caractérisation physico-chimique d'une lipase partiellement purifiée chez *Penicillium* sp. isolée à partir des grignons d'olives

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Résumé :

Dans le cadre de la valorisation des déchets agroalimentaires, la recherche et la production d'enzymes lipolytiques chez les moisissures, une souche fongique *Penicillium* sp. a été isolée à partir des grignons d'olives (en dégradation) issus d'une huilerie de la région d'Annaba (Nord Est Algérien).

La production de lipase a été réalisée par fermentation sur milieu liquide à base de l'huile de soja (1%) (15°C, pH8, 5jours). Les cellules fongiques issues de la culture de la *Penicillium* sp. après incubation, sont éliminées par centrifugation à 10000×g pendant 20 minutes à 4 °C. Le surnageant récupéré, contenant les lipases, a été clarifié par filtration en utilisant des filtres seringue à porosité 0.45 µm. Les lipases obtenues ont été partiellement purifiés par sulfate d'ammonium 20%. Les effets de différentes températures (5, 15, 25, 35, 45) °C, de pH (3, 4, 5, 6, 7, 8, 9 10) et de quelques ions métalliques : Ca^{2+} ($CaCl_2$), Mn^{2+} ($MnSO_4$), Mg^{2+} ($MgSO_4$), Zn^{2+}

($ZnSO_4$), Cu^{2+} ($CuSO_4$), Fe^{2+} ($FeSO_4$) ; ont été testé sur l'activité lipolytique de la lipase partiellement purifiée.

Les résultats de la caractérisation physico-chimique ce cette lipase montrent son activité optimale est enregistrée à 15 °C, pH 6 et Fe^{2+} pourrait jouaient le rôle du meilleur cofacteur enzymatique. Cette étude a permis pour la première fois, la caractérisation physicochimique d'une lipase partiellement purifiée chez une souche fongique isolée à partir des grignons d'olives. Les caractéristiques physico-chimiques de cette lipase témoignent qu'elle est très prometteuse à l'échelle industrielle et d'intérêt économique important : notamment dans la synthèse d'intermédiaires chiraux et de composés thermosensibles, la détergence et la bio décontamination.

Keywords: Grignons d'olives; *Penicillium* sp.*; lipases*; temperature, pH, ions métalliques.

OD10- Analyse phytochimique et évaluation des activités biologiques de l'extrait de *Crataegus azarolus*

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Résumé

Cette étude visait à optimiser l'extraction des anthocyanes monomères totales à partir des fruits de *Crataegus azarolus* et à évaluer leurs activités biologiques. L'effet de plusieurs paramètres a été examiné, notamment le type et la concentration du solvant, la méthode d'extraction, l'amplitude de sonication, la durée d'extraction, la granulométrie et le rapport solide/solvant. Le méthanol à 80 % s'est révélé être le solvant le plus efficace, avec un rendement maximal de 205,69 ± 4,52 µg CRE/g. L'extraction assistée par ultrasons (100 % d'amplitude pendant 5 min) et une granulométrie inférieure à 63 µm ont permis d'obtenir la plus forte teneur en anthocyanes (225,76 ± 4,10 µg CRE/g). L'extrait obtenu a présenté une activité antioxydante élevée (CI_{50} DPPH = 193,53 ± 3,71 µg/mL) ainsi qu'un pouvoir réducteur et une capacité antioxydante totale significatifs. L'analyse phytochimique a confirmé la richesse en composés phénoliques. De plus, l' extrait a montré des activités anti- inflammatoires et antibactériennes notables. Ces résultats démontrent le potentiel de *C. azarolus* comme source naturelle d'antioxydants pour la formulation d'aliments fonctionnels et de compléments

nutritionnels.

Mot clés : *Crataegus azarolus*, anthocyanes, composés phénoliques, activité biologique.

OD11- Un flavonol glycosylé isolé de l'espèce *Malope malacoides* L.

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Résumé :

Malope malacoides L. est une espèce du genre *Malope,* appartenant à la famille des Malvaceae. Ce genre comprend trois espèces originaires d'Afrique du Nord, d'Europe et de la région Macaronésienne. Les études menées sur la famille des Malvaceae ont mis en évidence une grande diversité de métabolites secondaires, soulignant son importance dans les domaines de la phytochimie et de la pharmacologie. Parmi les principaux composés isolés figurent des alcaloïdes, des triterpènes, des flavonoïdes, des quinones et des coumarines, connus pour leurs propriétés biologiques variées.

De nombreuses recherches ont également rapporté que les plantes de cette famille présentent un large éventail d'activités pharmacologiques, incluant des effets analgésiques, anti-inflammatoires, antidiabétiques, anti-obésité, antioxydants, antimicrobiens, anxiolytiques, cardioprotecteurs, cytotoxiques, hépatoprotecteurs et néphroprotecteurs.

Le présent travail a pour objectif d'examiner le profil phytochimique de l'espèce *Malope malacoides* L. et d'identifier les composés présents dans cette espèce. L'analyse chimique de l'extrait d'acétate d'éthyle, effectuée à l'aide de méthodes chromatographiques, a permis l'isolement d'un composé pur. L'identification structurale, réalisée à partir des données spectroscopiques (RMN 1D et 2D), a permis de caractériser ce métabolite comme étant l'astragaline, un flavonoïde bien connu pour ses propriétés pharmacologiques multiples.

Mots-clés : Malvaceae, *Malope*, spectroscopie, Astragaline.

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PA28	A Computational approach of BEDT-TTF derivatives.	Dr. HANANE TABBI U-Batna 1
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PA1- Molecular interactions of bioactive antioxidants with cell adhesion proteins – a docking approach for potential biomaterial applications

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Abstract

Molecular docking is a valuable computational approach to investigate the potential interactions between antioxidants and target proteins. Although antioxidants are primarily known for their ability to scavenge free radicals rather than binding to specific receptors, docking studies allow researchers to explore unexpected or non-specific interactions with cell-adhesion proteins (Integrin αVβ3). In this study, four potent antioxidants (quercetin, gallic acid, ascorbic acid, curcumin, and resveratrol) were selected and docked against an integrin receptor as a model cell-adhesion protein. Their binding affinities were compared with a reference peptide (RGD), which naturally exhibits strong and specific adhesion to integrin. Preliminary docking results suggest that while the antioxidants show moderate to weak binding compared to RGD, some exhibit notable interactions that could guide the design of dual-function molecules with both antioxidant properties and receptor-binding capacity. These findings highlight the potential of docking as an exploratory tool for discovering new therapeutic or biomaterial applications of known antioxidant compounds.

Keywords: Molecular docking; Integrin αVβ3; Natural antioxidants; RGD peptide; Cell Adhesion; Biomaterials.

PA2- Modélisation thermodynamique de la spéciation du système Fe(II)–Fe(III)–H_2SO_4–H_2O en vue du traitement par électrodialyse

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Résumé:

Les métaux en solution aqueuse existent sous forme d'ions ou de complexes neutres et chargés. La détermination expérimentale de leur spéciation demeure difficile en raison du manque de techniques analytiques adaptées, d'où l'intérêt de la modélisation thermodynamique. Celle-ci permet d'élucider la distribution des espèces dissoutes, essentielle pour l'optimisation des procédés hydrométallurgiques. Dans cette étude, nous avons modélisé la spéciation d'une solution synthétique composée d'acide sulfurique (150 $g.L^{-1}$), Fe(II) (25,10 $g.L^{-1}$) et Fe(III) (1,10 $g.L^{-1}$), correspondant au système Fe(II)– Fe(III)–H_2SO_4–H_2O. Les coefficients d'activité ont été calculés selon la méthode étendue de Bromley, et les équations non linéaires résolues avec **FSOLVE** sous **MATLAB (2008)**. Les résultats révèlent la présence d'espèces anioniques, cationiques et neutres, dominées par HSO_4^-, H^+, Fe^{2+}, $FeHSO_4^+$, $FeSO_4^0$, SO_4^{2-} et $FeH(SO_4)_2^0$. Le modèle prédit une diminution des concentrations de H^+, SO_4^{2-}, Fe^{2+}, Fe^{3+} et des complexes associés avec l'élévation de température (25 –85 °C), attribuée à la formation d'espèces plus stables. Parallèlement, la force ionique décroît, tandis que les constantes d'équilibre augmentent avec la température, confirmant la validité du modèle proposé.

Mots clés : métaux ; spéciation ; modélisation ; thermodynamique ; Bromley.

PA3- PIGMENTS NATURELS ET SANTÉ : LES BIENFAITS DES ANTHOCYANES DE LA ROSELLE

SAIDJI NAWEL

PA4- Structure-Property Relationships in Dithienopyrrole D-π-A-π-D Compounds

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Abstract:

This study examines the electronic structure and nonlinear optical (NLO) properties of DTP-based D-π-A-π-D compounds using DFT and TDDFT methods. The effect of electron-withdrawing acceptors on intramolecular charge transfer was investigated. NLO responses were evaluated at 1064 and 1907 nm. Key parameters, including dipole moment, polarizability, and first hyperpolarizability, were analyzed. The hyperpolarizability density βxx(2) and total density of states (TDOS) were also examined.
Regional NLO contributions were quantified from volumetric electron density data. 2D and 3D visualizations were generated using Python-based KZ.py tools. These analyses highlight donor–acceptor interactions and resonance effects governing NLO performance.compare the theoretical results with experimental data.

Key words: NLO, Charge transfer, Hyperpolarizability, Electron-withdrawing, DFT

Références:
Kamal Ziadi, Abdellatif Aouragh, Abdelatif Messaoudi, "Structure-property analysis of dithienopyrrole-based D-π-A-π-D compounds: Electronic and nonlinear optical responses with advanced python-based visualizations ", Journal of Molecular Graphics and Modelling, Volume 140, 2025, 109113, ISSN 1093-3263, https://doi.org/10.1016/j.jmgm.2025.109113

PA5- NLO behaviour of fused-metallocene hydride complexes: Theorical predictions

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Abstract

Fused-metallocene hydride complexes are sophisticated organometallic systems in which transition metals coordinate with pentalene ligands (Pn^{*}, C_8Me_6) and bridging hydride atoms (μ_2-H, μ_3-H). These complexes possess remarkable chemical, structural, and electronic properties, rendering them highly effective in organometallic chemistry. Moreover, their unique attributes position them as strong candidates for Nonlinear Optics (NLO) and energy conversion technologies. Quantum chemical calculations have proved to be a valuable tool for understanding and predicting the non-linear optical responses of these materials.

This work focuses on predicting the behaviour and NLO responses of group 4 permethylpentalene lithium hydride complexes ($Pn^{*}M_2H_yLi.thf_x$, M= Ti, Zr and Hf) by analysing their first and second hyperpolarizability under varying external electromagnetic field intensities using DFT, TD-DFT, and SOS calculations. These calculations, performed at the ωB97XD/6-311+G(d)/SDD level in both static and dynamic regimes, revealed significant variations in NLO properties depending on the wavelength, the nature of the metal (Ti, Zr, Hf), and the number of Thf ligands. Our results indicate that Zr- or Hf-based systems with one Thf ligand exhibited interesting optical nonlinearity with a high hyperpolarizability response.
Correlating the structural properties of these complexes with their NLO performance (hyperpolarizability β, susceptibility γ) enables the prediction and identification of structure-activity relationships to guide the synthesis of optimized NLO materials.

Keywords: *Fused-metallocenes NLO, hyperpolarizability, DFT, TD-DFT*

PA6- Electronic Structure and Radical-Scavenging Pathways in Ferrocenyl Antioxidants

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Abstract

The antioxidant activity of two ferrocenyl derivatives, Fc-CA and Fc-FA, together with their parent ligands caffeic acid (CA) and ferulic acid (FA), was investigated using density functional theory (DFT) calculations. Three plausible mechanisms—hydrogen atom transfer (HAT), single-electron transfer–proton transfer (SET-PT), and sequential proton loss–electron transfer (SPLET)—were examined. Key physicochemical descriptors, including O–H bond dissociation enthalpy (BDE), proton dissociation enthalpy (PDE), ionization potential (IP), proton affinity (PA), electron transfer enthalpy (ETE), and HOMO/LUMO energies, were computed in the gas phase and in various solvents. The findings indicate that HAT is the most favorable mechanism in the gas phase and nonpolar (benzene) medium, whereas in polar solvents, the SPLET pathway predominates.

Keywords: Ferrocenyl derivatives; DFT; Antioxidant mechanism; HAT; SET-PT; SPLET; Solvent effect.

PA7- Theoretical Approach by DFT and TD-DFT to the Decolorization and Degradation of Synthetic Triphenylmethane Dyes

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Abstract

This study employs DFT and TD-DFT methodologies to investigate the reactivity descriptors, UV-Vis absorption spectra, and hydrolysis mechanisms of three cationic

triphenylmethane dyes: malachite green (MG^+), brilliant green (BG^+), and ethyl green (EG^{2+}). A range of exchange-correlation functionals, including GGA, hybrid, and range-separated types, were utilized to assess their influence on the theoretical properties. The calculated UV-Vis spectra indicate that the absorption maxima (λmax) decrease in the order of GGA > hybrid > range-separated functionals. Transition state theory calculations reveal that the hydrolysis activation barriers follow the sequence $BG^+ < MG^+ < EG^{2+}$ consistently in both gas phase and solution environments. Among the functionals tested, CAM-B3LYP yields the highest activation energies, while M06 predicts the lowest. These findings emphasize the significant impact of functional choice on accurately modeling the photophysical behavior and reaction kinetics, providing valuable insights into the degradation pathways of these cationic dyes.

Keywords : *Decolorization, Degradation , hydrolysis,Triphenylmethane dyes, DFT, TD-DFT,*

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PA8- Computational Exploration of the Anticancer Potential of Benzimidazole Derivatives

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Abstract

This study investigates the synthesis and biological evaluation of two benzimidazole-based compounds (2 and 3) for their anticancer potential against colon cancer cells (DLD-1) and normal human lung fibroblast cells (WI-38). Compound 3, featuring an anthracene moiety, exhibited superior antiproliferative activity with an IC_{50} value of 46.91 μM against DLD-1 cells, and demonstrated greater selectivity toward cancerous cells compared to compound 2. Computational approaches, including DFT calculations, molecular docking, and molecular dynamics simulations, further supported the experimental findings by revealing compound 3's enhanced reactivity and stable binding interactions with the

Caspase-9 protein (PDB ID: 2HQ6). Overall, these results highlight compound 3 as a promising and selective anticancer candidate.

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

PA9- Optical Properties of Materials: A Theoretical Approach

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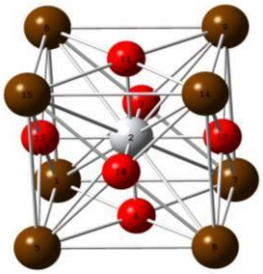
ABSTRACT

The spectroscopic and photophysical behavior of barium titanate ($BaTiO_3$) and polymer/$BaTiO_3$ composites have been highlighted by a large number of reports in last three decades, due to their luminescence properties. In an attempt to understand these properties, we undertook a theoretical study of polymer/$BaTiO_3$ composites using the density functional method (DFT) and time-dependent (TD-DFT) to determine their geometries and electronic structures DFT method, and also to study their first electronic excitations (energy, nature, transition probability). TD-DFT calculations with the use of hybrid functionals are shown to provide an excellent cost-effective computational approach for the treatment of the excited states of these composites. The present paper can provide the experimentalists with data to develop a working device using this system.



Barium titanate ($BaTiO_3$)

Keywords: Barium titanate; TD-DFT; Absorption spectrum; Charge transfer; electronic; excitations.

PA10- Inhibition of 5*α*-reductase by *Ficus carica* L: A DFT and Molecular Docking Approach to Stimulate Hair Regrowth

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Abstract

Androgenic alopecia (AGA) is a common condition linked to high levels of dihydrotestosterone (DHT), which is produced from testosterone by the enzyme 5α-reductase. Our research has shown that bioactive compounds from the leaves and fruit of Ficus carica L, particularly the triterpenoids constituents, which can inhibit the activity of 5α-reductase. We used density functional theory (DFT) calculations to identify the optimal molecular structures and the conceptual DFT to determine the active sites. Besides, the molecular docking study was used to analyze how these compounds block 5α-reductase and to predict their biological effects. We calculated several chemical properties, such as energy levels and reactivity, to understand how these compounds might interact with the 5α-reductase enzyme. The docking results indicate that these compounds can effectively bind to the 5α-reductase receptor, suggesting that Ficus carica L. could be a promising natural treatment for AGA.

Keywords: Fukui functions, molecular docking, Density functional theory, dipole moment

PA11- Computational Investigations of a Novel Schiff Base via DFT

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Abstract

Density functional theory has become a powerful computational tool for investigating the structural, electronic and reactivite properties of schiff base. In this study, DFT calculations were employed to optimize the molecular geometry and to evaluate various quantum chemical parametres of the compound. The theoretical study has been performed on the synthesized compound using DFT via B3LYP/6-31G(d,p) methods. The geometry optimization, molecular energy and molecular properties of **SBA** such as energy gap ,ionization potential (I), electron

affinity (A) ,global hardness (η) ,global softness (S) ,chem.ical potential (μ) , electophilicity (ω) and electronegativity (χ) were investigated using DFT. The obtained results demonstrate that DFT is an effective approach for elucidating the electronic structure and potential reactivity of **SBA**, supporting its application in coordination chemistry and biological systems.

Keywords: Schiff base, theorical studies, DFT, reactivity, optimization.

PA12- Theoretical Investigation into the Enhanced Non-Linear Optical Response of Yttrium-Boron Co-Doped Carbon Nanotubes

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Abstract

Single-walled carbon nanotubes (SWCNT) [1], is one-dimensional materials derived from rolled graphene sheets, possess highly tunable electronic and optical properties governed by their precise chirality. This intrinsic tunability makes them exceptionally promising for advanced technological applications. To fully exploit their potential, continuous research is focused on enhancing specific functionalities, such as the non-linear optical (NLO) response. Structural modifications, particularly through doping and co-doping [2], have been identified as a highly promising strategy to achieve superior NLO activity for novel device development. This computational study employs Density Functional Theory (DFT), utilizing the B3LYP functional with the 6-311G++(d,p) basis set, to investigate the influence of yttrium (Y) and boron (B) co-doping on the NLO properties of SWCNT. We specifically calculate and analyze key NLO features, including the dipole moment, polarizability, and first-order hyperpolarizability. Furthermore, we explore the co-doping mechanism by analyzing the structural and electronic properties (e.g. density of states) to ascertain how Y/B-doping modifies the electronic energy gap and introduces impurity levels, thereby influencing NLO activity. Comparative analysis between pristine and Y/B-doped SWCNT reveals a significant enhancement in the NLO performance of the studied structures, demonstrating their compelling potential for creating more efficient optoelectronic applications

Keywords: SWCNT, NLO, DFT, Co-doping, DOS.

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PA13- QSPR Study for enthalpies of combustion, ,formation and sublimation of monocarboxylic acids (C2 C20)

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Abstract

This study presents a quantitative structure–property relationship (QSPR) analysis for predicting the enthalpies of combustion, formation, and sublimation of monocarboxylic acids ranging from C2 to C20. A set of quantum chemical descriptors was calculated using density functional theory (DFT) at the B3LYP/6-31G(d,p) level to characterize molecular structure and reactivity. Multiple linear regression (MLR) models were developed and statistically validated using standard metrics, including R^2, and cross-validation coefficients and RMSE successively. R^2 =0.997597, Q^2_{loo}= 0.996138 RMSD = 9.85217.

The models demonstrated strong predictive capability and internal consistency, confirming the relevance of the selected descriptors. Furthermore, the influence of molecular size and branching on thermodynamic properties was systematically analyzed. The enthalpy values exhibited smooth trends along the homologous series, with minor deviations attributed to structural isomerism. This approach offers a reliable and cost-effective alternative to experimental measurements. The developed models can be employed in thermodynamic databases and molecular design.

PA14- DFT-Based Study of the Structural and Electronic Characteristics of Isoquercetin

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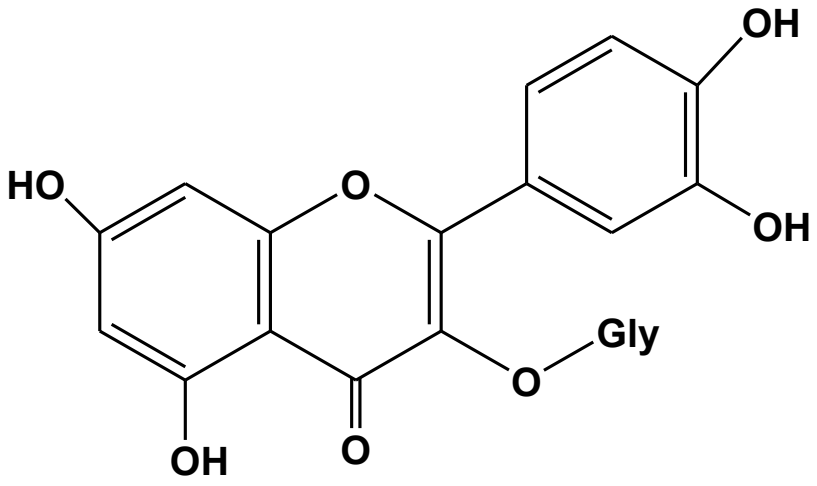
Abstract:

Flavonoids are widely distributed in a broad range of fruits and vegetables and are well known for their remarkable biological activities, including anti-inflammatory, antioxidant, and antiradical properties. These bioactive compounds play a crucial role in protecting biological systems against oxidative stress and are therefore of considerable interest in medicinal and pharmaceutical research. Among them, isoquercetin has attracted increasing attention owing to its potent biological activity and therapeutic potential.

In the present study, quantum chemistry methods were employed to gain deeper insight into the molecular behavior of isoquercetin at the atomic level. Density Functional Theory (DFT) calculations were performed using the B3LYP functional in combination with the 6-311++G(2d,2p) basis set. This computational approach enabled a comprehensive investigation of the electronic structure, optimized geometry, and energetic properties of various activated forms of isoquercetin. The obtained results provide valuable information on the reactivity and stability of isoquercetin, thereby contributing to a better understanding of its physicochemical properties and potential biological activity.



Keywords: Flavonoid, Antioxidant, Antiradical, enzyme, Molecular docking.

PA15- The Hidden Order: Quantum Perspectives on Hybrid Crystalline Matter

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Abstract:

The design of selenium-based hybrid crystalline materials represents a promising route toward multifunctional compounds with tunable structural, electronic, and optical properties. Theoretical chemistry and molecular modeling provide valuable tools to elucidate the relationship between crystal structure and physicochemical behavior at the atomic scale.

In this study, Density Functional Theory (DFT) was employed to investigate the optimized geometries, frontier molecular orbitals (HOMO–LUMO), and charge density distributions of a newly synthesized selenium-containing hybrid complex. Calculations were performed using the B3LYP/6-31G(d,p) level of theory. The optimized geometry displayed a stable configuration characterized by tetrahedral coordination around the selenium center. The HOMO was primarily localized over the donor atoms (N, O), while the LUMO was distributed on the selenium moiety, indicating efficient intramolecular charge transfer.

Molecular Electrostatic Potential (MEP) analysis revealed electron-rich regions surrounding selenium atoms, suggesting their role as reactive centers in intermolecular interactions. Density of States (DOS) and natural bond orbital (NBO) analyses further confirmed the delocalization of electron density and hybrid orbital participation in Se–C and Se–O bonds. The theoretical optical gap (≈3.20 eV) implies semiconducting behavior consistent with hybrid crystal characteristics.

The integration of theoretical and crystallographic approaches enables a deeper understanding of the bonding nature and stability of selenium-based materials. Such insights open perspectives for the rational design of hybrid systems with potential applications in optoelectronics, catalysis, and energy materials.

Keywords: Selenium-based materials; Hybrid crystals; Density Functional Theory; Molecular modeling; Structure–property relationship.

PA16- Theoretical study of biological molecules

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Abstract:

Toxic gases are very harmful for both the environment and human health. They can cause air pollution, damage plants and animals, and even lead to serious diseases in humans. Because of these problems, scientists are working hard to develop sensors that can detect toxic gases quickly and accurately [1]. In recent years, biosensors have become an exciting field of research. These devices use biological materials to recognize specific substances in the environment [2]. Among them, DNA and other nucleic acids have shown great potential because they can form stable and selective complexes with metals or other molecules. By using these unique properties, researchers hope to create new, sensitive, and eco-friendly sensors that can help protect both people and nature [3]. The aim of our work is to study a potential biosensor for detecting toxic gases (H_2S, SO_2, NH_3, CO, CO_2, NO, and NO_2)., which is based on thymine base pair linked with Cobalt [thymine-Co-thymine] and copper [thymine-Cu-thymine]. All structures are optimized at **DFT/M062X/6-311G+(d,p)** level of theory implemented in **Gaussian16** code. LanL2DZ basis set was used for cobalt and copper.

Keywords: DNA, biosensors, DFT.

PA17- Theoretical study, Prediction by DFT calculations of new bis malonamides derivatives

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Abstract

In recent years, considerable attention has been devoted to the structures of malonamide-based compounds in order to assess their therapeutic potential against various disease targets. Notably, some derivatives have been synthesized as γ-secretase inhibitors, which are considered promising candidates for Alzheimer's disease treatment due to their ability to influence amyloid-β production **[1]**. Furthermore **DFT** plays a crucial role in organic chemistry by providing detailed insights into molecular structure, electronic properties, and reaction mechanisms. It allows researchers to predict chemical reactivity, stability, and spectroscopic behavior with high accuracy and relatively low computational cost. **DFT** helps visualize electron density distribution, optimize molecular geometries, and explore transition states in reactions.

In our study, we focused on the molecular properties associated with the Frontier Molecular Orbitals (FMOs) of the synthesized molecules, such as ionization potential, electron affinity, global hardness, chemical potential, electrophilicity index, and hardness values. The energy gap between the **HOMO** and **LUMO** orbitals was also analyzed, as it provides valuable insight into the kinetic stability and chemical reactivity of the prepared compounds.

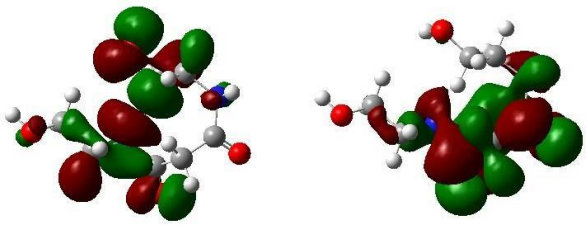

Figure: Homo and lumo figure of the molecule **3a**

Keywords: DFT- Theoretical study- malonamide

PA18- Atomistic Mechanism of Adenine Chemisorption on Silica Nanoclusters: A DFT Investigation of Electronic Structure and Interfacial Bonding

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Abstract

This detailed Density Functional Theory (DFT) study offers a thorough quantum-mechanical description of the interfacial electronic characteristics and adsorption mechanism controlling the interaction between a modeled nano-silica cluster (SiO_{10}) and adenine, a basic purine nucleobase. The study determines that chemisorption via the $–N_2$ site is the most kinetically advantageous and thermodynamically stable pathway by methodically evaluating five different adsorption configurations. Strong interfacial bonding is indicated quantitatively by a significant adsorption energy (E_{ad} = -4.19 eV), a characteristically short interfacial Si–N bond distance (1.81 Å), and a highly spontaneous Gibbs free energy change (ΔG = -79.3 kcal/mol). Electronic structure analysis revealed a remarkable 35% reduction in the HOMO-LUMO band gap, signifying enhanced electronic conductivity attributable to significant charge transfer from the adenine's highest occupied molecular orbital to the silica cluster's lowest unoccupied molecular orbital. This charge-transfer complex formation was further corroborated by Electron Localization Function and Non-Covalent Interaction analyses, which provided

explicit evidence of electron density delocalization at the interface and characterized the specific hydrogen bonding interactions responsible for structural stabilization. The elucidation of these fundamental physico-chemical principles underlying nucleobase adsorption on silica surfaces provides critical insights for the rational design and development of advanced silica-based biosensing platforms, targeted drug delivery systems, and next-generation functional nanomaterials with tailored interfacial properties.

Keywords: Adsorption, Nucleobase, Silica cluster, DFT theory, Biosensing.

PA19- TD-DFT computational study of some complexes with Ruthenium(II) based TTF terpyridine ligands

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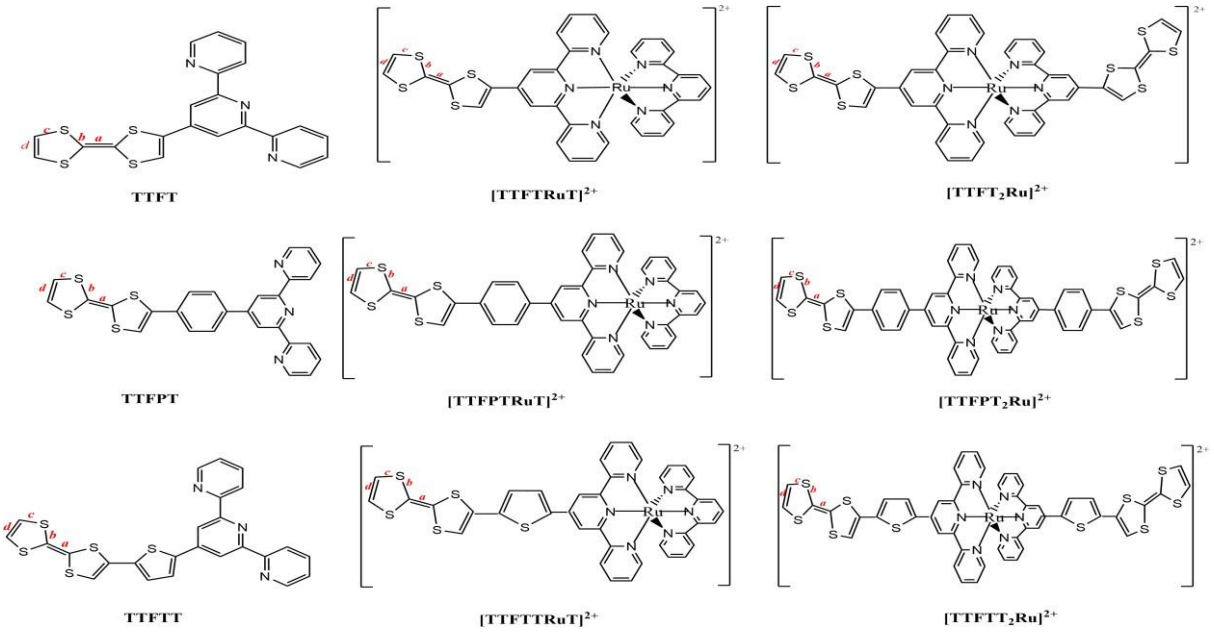
Abstract:

Theoretical calculations were performed with the Gaussian16 package [1]. The DFT method was employed with the B3LYP functional (Becke's three parameter nonlocal exchange functional with the Lee-Yang-Parr correlation function) [2, 3] and the LANL2DZ basis set for the ruthenium atom and the 6-31G(d,p) basis set for the other atoms. The geometry optimizations were carried out in the gas-phase and the minima, confirmed by frequency calculations. UV absorption energies were calculated using the TD-DFT method and frontier molecular orbital energies were also calculated at the same level of DFT theory.



Mots clés: TD-DFT, UV-visible, TTF-terpyridines - ruthenium(II) complexes

Références

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(2019): 118-124

PA20- THERMODYNAMIC ASSESSMENT OF THE Ga-Ho SYSTEM BY CALPHAD APPROACH

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Abstract

A theoretical investigation of the binary Ga-Ho (Gallium-Holmium) phase diagram has been performed using thermodynamic modeling of the liquid phase based on the Redlich- Kister polynomial formalism. The formation enthalpies of the liquid solution were described as a function of composition and temperature by introducing interaction parameters between gallium and holmium atoms. These parameters were optimized to reproduce available experimental

thermodynamic and phase equilibrium data. The Ga-Ho binary includes several intermetallic compounds reported in experimental work, commonly listed as Ga_6Ho, Ga_3Ho ($L1_2$/$AuCu_3$-type), Ga_2Ho.

The resulting model provides a consistent description of the liquid phase behavior and enables the calculation of key thermodynamic quantities such as the Gibbs free energy, activity coefficients, and mixing enthalpies. The calculated phase diagram exhibits good agreement with experimental observations, confirming the reliability of the Redlich–Kister approach for representing the excess thermodynamic properties of the Ga–Ho system. This theoretical study contributes to a better understanding of the thermodynamic interactions in rare-earth– gallium alloys and provides a useful basis for future CALPHAD assessments and alloy design.

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Thermodynamic assessment / CALPHAD of Ho-Ga (critical assessment; provides a CALPHAD parameter set or discussion). (thermodynamic assessment of the Ho- Ga system).

PA21- Analyse de la structure électronique des complexes dioxo à l'aide des calculs quantiques basés sur la DFT

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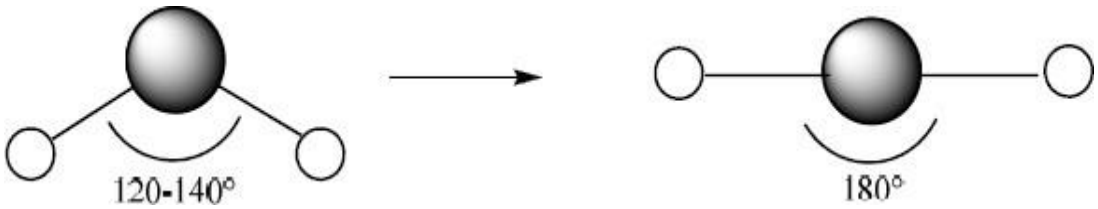
Abstract:

Ce travail comprend une étude sur les entités isoélectroniques MO_2^{+n} (M =U, Th, W, Mo). L'objectif est d'étudier l'importance des effets relativistes sur le choix de la géométrie (linéaire, coudée) qui peuvent être adoptés par ces composés et de mieux comprendre le rôle clé des orbitales 5f des actinides par rapport aux orbitales d des éléments de transition. Tous les calculs ont été effectués à l'aide de la méthode DFT/ZORA/TZP/BP86.



Mots clés: Actinides, métaux de transition, isoélectronique, DFT, ZORA.

PA22- Etude du docking moléculaire de l'alginate de sodium complexé aux ions calcium : valorisation biomédicale potentielle.

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Résumé– L'alginate de sodium est un biopolymère naturel couramment utilisé dans le domaine biomédical en raison sa biocompatibilité, sa biodégradabilité et sa capacité à former des gels en présence d'ions calcium (Ca^{2+}). Quand l'alginate de sodium est mis en présence des ions calcium, il génère une structure tridimensionnelle, connue sous le nom de « egg-box
», ce qui optimise ses caractéristiques mécaniques et biologiques. Ces gels résultants constituent des matériaux excellents pour l'encapsulation et la libération contrôlée de molécules bioactives. Notre recherche utilisant le docking moléculaire nous aide à simuler les interactions entre les chaînes d'alginate et les ions calcium, avec l'objectif de comprendre plus précisément les mécanismes de liaison et d'améliorer la conception de ces hydrogels. Les résultats montrent que ces hydrogels en présence de Ca^{2+} peuvent accroître la bioactivité de la molécule et servir de plateformes efficaces pour des applications pharmaceutiques.

PA23- Theoretical study of the structural parameters and the descriptors of the reactivity of herbicide terbutryn

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ABSTRACT

A structural theoretical study by molecular modeling of terbutryn in order to discuss the reliability of the chemical model used as well energy study on local and global descriptors to know their reactivity. The calculations were performed on using density functional theory (DFT) with the hybrid functional B3LYP at base 6-311++G(d,p) in isolated and solvated phase , using the Gaussian 16 package. The effect of the solvent is introduced using the theoretical model CPCM.

Key words : CPCM, terbutryn, DFT, local and global descriptors.

PA24- Molecular Docking and Pharmacokinetic Assessment of Alkaloid Compounds

PA25- Évaluation in-silico de l'activité anti bactérienne d'un dérivé ferrocènique (FcMA)

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Résumé : Les composés de ferrocene sont des composés organométalliques qui ont montré une activité biologique très importante contre de nombreuses maladies, car notre étude vise à comprendre l'effet de certains de ces dérivés sur l'inhibition antibiotique potentiel. Cependant, pour valider son utilisation, il est nécessaire de suivre ses effets secondaires et sa cytotoxicité. Le but de notre étude est d'évaluer l'activité antibactérienne de la N-Férocénylméthylaniline in silico. Les résultats ont montré in silico en évaluant les propriétés physico-chimiques et la pharmacocinétique du dérivé du ferrocène via le serveur web swiss ADME qui montre une réponse

à la base de Lipniski et Veber en raison de la solubilité et de la facilité d'absorption du dérivé. Le Docking moléculaire a montré une interaction entre le dérivé et de la protéine membranaire d'Escherichia coli pas des liaisons électrostatiques entre les acides aminés de la protéine et les ligands étudiés.

Mot clés : ferrocène, activité antibactérienne, docking moléculaire , in-silico , swiss ADME.

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PA26- DFT Investigation of Carmustine Adsorption on Si-Doped Fullerene for Targeted Drug Delivery

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Abstract:

Due to its excellent biocompatibility and outstanding bioavailability, fullerene has emerged as a highly promising candidate for use as a nanocarrier in advanced drug delivery systems [1]. Carmustine, a well-established anticancer agent recognized for its effectiveness in suppressing tumor growth and improving patient survival, remains one of the most potent chemotherapeutic drugs in current cancer therapy [2,3]. In this study, DFT calculations using B3LYP functional and 6-31G++(d,p) basis set under aqueous-phase conditions were performed to evaluate the potential of Si-doped fullerene as a carrier for Carmustine drug. Key parameters, including adsorption energy, frontier molecular orbitals (FMO) analysis, and density of states (DOS), were analyzed to elucidate the adsorption mechanism and electronic characteristics of the Carm–SiC_{19} complex. The results reveal strong and stable adsorption of Carmustine on Si-doped fullerene surface, accompanied by notable changes in electronic properties, suggesting its potential for targeted and controlled drug release, thereby reducing systemic accumulation and minimizing adverse effects. Overall, these findings underscore the promising capability of Si-doped fullerene as an efficient and site-specific nanocarrier for anticancer drug delivery.

Keywords: Density functional theory (DFT) -SiC_{19}-Carmustine- Cancer –Adsorption-Drug delivery

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PA27- Synthesis and In Silico Study of a new α- aminophosphonate derivative as Potential α-Glucosidase Inhibitor

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Abstract:

This study aims to evaluate the potential of a new α-aminophosphonate derivative as inhibitor of the α-glucosidase enzyme using an in silico approach. FT-IR, UV–Vis approaches were used to confirm the structure of the new α-aminophosphonic acid. The study employed molecular docking methods. The structure of the α-glucosidase enzyme was obtained from the Protein Data Bank (PDB ID : *5ZCB*), while the 3D structure of α-aminophosphonic acid was generated and optimized using Gaussian 09. Docking simulations were conducted using iGMDOCK version 2.1, and interaction results were analyzed using Discovery Studio. The analyzed parameters included binding affinity values and the interactions between ligands and active site residues of the enzyme. The results showed that α-aminoposphonic acid, exhibited strong binding affinity value : -88.10 kcal/mol. Based on molecular docking analysis, the investigated α-aminophosphonic acid indicate great potential for further development as antidiabetic agents.

Keywords: α-Aminophosphonic acid, molecular docking, α-glucosidase enzyme, antidiabetic.

PA28- Computational approach of BEDT-TTF derivatives

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Abstract

Organic semiconductors are generally pi-conjugated materials, in which the transport mechanisms are quite different from those conventionally described in solid -state physics with inorganic semiconductors [1]. The Bis(ethylenedithio)tetrathiafulvalene (BEDT-TTF) compound is of major importance in scientific and applied fields due to its remarkable electronic properties [2]. In the field of conductive and insulating materials, it constitutes the basis of numerous organic salts with conductive capacities capabilities [3]. Some of these salts even exhibit superconducting properties at temperatures up to 11.6 K [4].

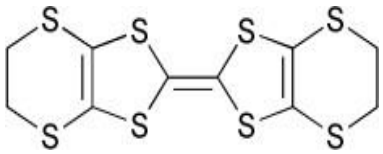

Figure 1. Molecular structure of BEDT-TTF.

Keywords: BEDT-TTF, DFT, chemical reactivity, nonlinear optics, natural bonding orbitals.

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PA29- Étude théorique de la réaction atmosphérique du 4-hydroxy-2- pentanone (4H2P) avec le radical OH

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Résumé:

La cinétique et le mécanisme de la réaction du 4-hydroxy-2-pentanone (4H2P) avec l'oxydant atmosphérique OH ont été réalisés en utilisant des calculs théoriques quantiques. La théorie fonctionnelle de la densité DFT B3LYP / 6-311 $^{++}$ G (2d, pd), les méthodes CBS-QB3 et G3B3 sont utilisé pour explorer les voies de réaction. est utilisée pour obtenir les constantes de vitesse de la réaction sur une gamme de température de 278-400 K et à la pression atmosphérique. Cette étude délivre la première détermination théorique et cinétique de la constante de vitesse pour les réactions du 4H2P avec OH. La constante de vitesse obtenue au niveau CBS- QB3 // B3LYP (6-311G ++ (2d, pd)) à 289 k est de 4.97×10^{-11} cm^3 $molécule^{-1}$ s^{-1}.

La différence entre les résultats obtenus et les valeurs trouvées dans la théorie peut s'expliquer par le fait que 4H2P est un hydroxycétone d'une chaîne carbonée linéaire plus grande.

Mots-clés: Hydroxycétone, Cinétique, CBS-QB3, G3B3, atome de OH, constante de Vitesse, 4H2P.

PA30- Theoretical study of New Inhibitors as Anti-cancer Agents Through Molecular Modeling Methods

PA31- Investigation of free radical scavenging activities of some Isatin Schiff bases (O-H versus N-H). A DFT Study

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Abstract:

In the present study we analyze various mechanisms of primary antioxidant action of a series of Schiff bases of isatin and its derivatives. For the purpose, theoretical calculations have been performed by means of density functional theory (DFT), using the hybrid functional M05-2X, range-separated functional LC-ωPBE and 6-31+G (d, p) basis set. The reactivity of these Schiff bases has been investigated and interpreted using chemical reactivity descriptors in gas and solvents phase. The two computational approaches used provide identical mechanisms trends in gas and non -polar phase and they are shown that the hydrogen atom transfer (HAT) mechanism is more favored. In contrast, the polarity of the solvent plays a crucial role in the antioxidant activity mechanism, as a higher solvent polarity enhances the contribution of the sequential proton loss electron transfer (SPLET) mechanism. It is found that the isatin group did not suppress the antioxidant effect of the disubstituted Schiff bases products as suggested by the experimental results.

PA32- Antileishmanial activity of dihydrosyrindine and syringine: molecular modelling, bioactivity, molecular docking, and dynamic simulations

Oussama Khaoua

PA33- QUANTUM CHEMICAL INVESTIGATION OF SILYL CATION–LEWIS BASE COMPLEXES: STRUCTURAL FEATURES AND STABILITY VIA DFT AND NBO ANALYSIS

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Abstract

This work delves into how steric and electronic influences govern the structural and energetic properties of Si–P bonds within silicon-based cationic systems coordinated to phosphine ligands. Through comprehensive computational analysis, it is shown that $(CH_3)_3Si^+$ forms the most compact Si–P linkages (2.01–2.03 Å), a result of low spatial hindrance and effective orbital overlap. Slightly elongated bond lengths (2.03–2.05 Å) occur with $(C_2H_5)_3Si^+$, while the most extended distances (2.08–2.10 Å) are associated with Ar_3Si^+, where both steric congestion and electron-withdrawing aromatic rings impede close approach. The angular parameters reflect similar trends; bulky phosphines such as $(C_2H_5)_3P$ induce broader Si–P–R bond angles (e.g., up to 121° with Ar_3Si^+) relative to less hindered analogs like $(CH_3)_3P$.

Energetically, the $(CH_3)_3Si^+\cdots(CH_3)_3P$ pair exhibits the strongest interaction (~–28 kcal/mol), a result of well-balanced spatial arrangement and electrostatic compatibility. In contrast, electron donation trends derived from charge transfer calculations reveal that $(C_2H_5)_3P$ is more effective in transferring electron density than $(CH_3)_3P$, aligning with predictions based on steric and electronic parameters. Natural Bond Orbital (NBO) evaluations further demonstrate that increased σ-donation correlates with greater interaction strength, as evidenced by more negative interaction energies. Conversely, Ar_3Si^+ consistently engages in weaker associations, hindered by the electron-withdrawing character of its aromatic substituents.

Altogether, this study emphasizes the nuanced interdependence between geometry and electronic structure in modulating Si–P bonding, offering design principles for future silicon-phosphine architectures relevant to catalysis and materials development.

Keywords: Sillyl cations, Lewis bases, Density Functional Theory, Natural Bond Orbital analysis.

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PA34- Exploration du mécanisme antioxydant des méthoxyphénols par approche DFT

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Résumé

Les antioxydants sont des composés capables, grâce au don d'électrons, de réagir de manière sûre avec les radicaux libres, stoppant leurs réactions et les transformant en molécules inoffensives. Dans cette étude, nous avons utilisé la théorie de la fonctionnelle de la densité (DFT) afin d'élucider les mécanismes des méthoxyphols. Les calculs ont été réalisés au niveau LC-ωPBE

L'analyse s'est centrée sur le groupe phénolique OH, en évaluant les enthalpies des réactions associées aux mécanismes antioxydants primaires : transfert d'atome d'hydrogène (HAT), transfert d'électron suivi d'un transfert de proton (SET-PT) et perte de proton suivie d'un transfert d'électron (SPLET). Le modèle de solvatation CPCM a été utilisé pour les calculs en solution, dans des milieux polaires et non polaires.

Les enthalpies associées à ces processus ont été calculées en phase gazeuse et en solution pour déterminer la voie la plus favorable selon le milieu. Les résultats montrent que le HAT prédomine en phase gazeuse, tandis que le SPLET devient plus favorable en solvants polaires. Cette différence met en évidence l'importance de l'environnement chimique dans le contrôle du mécanisme antioxydant

Mots clés : Antioxydants, DFT, mécanismes, méthoxyphénols.

PA35- DFT-Based Quantum Chemical Analysis and Molecular Modeling of Heterocyclic Compounds for Predicting Reactivity and Biological Activity

Adjoul Dounia

TOPIC B: ANALYTICAL CHEMISTRY, ELECTROCHEMISTRY AND WATER CHEMISTRY

Topic B Program

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P_{B2}	Artificial neural network modeling of adsorptive removal of Malachite Green from aqueous solution.	**Dr. Houria Rezala U-Khemis-Miliana**
P_{B3}	Performance evaluation of 2-mercaptobenzothiazole for corrosion protection of aluminum	**Dr. Abdeldjabbar Messaoudi U-Ouargla**
P_{B4}	Green Synthesis of Copper Oxide Nanoparticles Using Peel Extracts of Cucurbita pepo.	**Bouzidi Ali U-Ouargla**
P_{B5}	Electrochemical Fabrication and Characterization of Ni–Al_2O_3 Composite Coatings on Steel	**Dr. Rekaik Mouna U-Médéa**
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P_{B11}	Evaluation of the Inhibitory Properties of Glycine Against Copper Corrosion in 1M HNO_3	**Dr. ABDERRAHIM Karima U-Annaba**
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P_{B18}	Elabration of thin films by electrodeposition of copper II complex	**Dr. Nawal BOUNAB U-Batna 1**
P_{A19}	Current-Dependent Lithium-Ion Concentration Profiles Across the Electrolyte and Their Evolution at Electrode Interfaces in Lithium-Ion Batteries	**Dr. Afaf Djaraoui U-Batna1**
P_{B20}	Removal of Cephalexin from aqueous solutions by adsorption onto activated carbon: kinetics, isotherms and regeneration study	**Dr. Roumaissa Boumaraf U-Batna 1**
P_{B21}	Recovery of Na_2SO_4/Fe_2O_3 Nanocomposite Material from the Chemical spent pickling bath and Its Application in Electrochemical Sensors for Heavy Metal Ion Detection in Aqueous Medium	**Dr. Afaf Lalmi U-Batna 1**

PB22	Élimination de l'amoxicilline des eaux par adsorption sur charbon actif	**Houda Djouza** **U-Skikda**

PB1- Détermination par absorption atomiques les éléments métallique dans les eaux potables

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Abstract:

La qualité naturelle des eaux souterraines et de surfaces peut être altérée par l'activité humaine. La détérioration de la qualité de l'eau est appréciée par mesures des paramètres physico-chimique et bactériologique. Dans le d'une détérioration jugée importante, l'eau ne sera plus considérée comme potable pour la consommation humaine.

Notre travail consiste à étudier les concentrations de certains métaux présents dans les eaux potables destinées à la consommation des populations. Nous avons dosé des éléments métalliques tels que le sodium (Na), le calcium (Ca), magnésium et plomb (Pb) dans les eaux potable par absorption atomique. Cette technique rapide qui commence être a se généralisé est un outil indispensable permettant de mesurer des concentrations en éléments de l'ordre ug. Toute fois les méthodes physico-chimique restent les plus répandues dans un grand nombre de laboratoire d'analyses.

Keywords: eaux potable**,** absorption atomique SAA**,** polluants toxiques métallique, Na, Mg, Ca, Pb.

PB2- Artificial neural network modeling of adsorptive removal of Malachite Green from aqueous solution

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Abstract

In this study, the adsorptive removal of malachite green (MG) from aqueous solutions onto clays has been studied. Corresponding results were simulated using an artificial neural network. Materials were characterized by X-ray fluorescence spectrometry, Fourier transform infrared spectroscopy, X-ray diffraction and nitrogen adsorption at 77K. Sorption experiments were carried out in the discontinuous mode, examining the influences of contact time, adsorbent dose, suspension pH, initial MG concentration and temperature. The neural network topology was 4–10- 1 and exhibits the optimal architecture with the strongest correlation coefficients (R = 0.9158 and 0.9998) and the smallest mean square errors (MSE = 0.0025 and $4.6797e^{-05}$) for commercial and Algerian bentonite, respectively. The results predicted by this model show a good agreement with experimental data. Maximum MG adsorption of 166.33 and 81.91 mg/g were obtained by commercial bentonite and local Algerian bentonite, respectively at following conditions: 5 min, pH medium, 25 ± 1 °C, 100 mg/L and adsorbent dose of 0.6 and 1.2 g/L for commercial bentonite and local Algerian bentonite, respectively. The thermodynamic parameters such as the changes in Gibbs free energy, enthalpy, and entropy are determined. The MG adsorption is physical, spontaneous and exothermic.

Keywords: Artificial Neural Network, Malachite Green, Adsorption, Bentonite.

PB3- Performance evaluation of 2-mercaptobenzothiazole for corrosion protection of aluminum

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Abstract

The corrosion of metals, particularly aluminum, constitutes a major industrial concern due to substantial economic losses and detrimental effects on equipment and manufacturing processes. Consequently, the pursuit of efficient and eco-friendly organic inhibitors has garnered heightened interest in recent years, as they provide alternatives to conventional, hazardous inhibitors.

This study seeks to assess the efficacy of the novel organic chemical, 2-mercaptobenzothiazole, in mitigating aluminum corrosion in an acidic environment (1M HCl). A multi-method approach was employed, incorporating gravimetric measurements to ascertain mass loss rates, static electrochemical analysis (Tafel curves), and electrochemical impedance spectroscopy (EIS) to elucidate the inhibitory mechanism and adsorption characteristics.

The electrochemical experiments indicated that 2-mercaptobenzothiazole demonstrates significant

corrosion inhibition efficacy. At 20 ppm, the corrosion current decreased from 7.62 to 0.24 mA/cm², while the polarization resistance increased from 1.89 to 46.12 Ω.cm², resulting in an inhibitory efficiency of 96.87%. Conversely, EIS spectra revealed that the peak transfer resistance (Rt) value was seen at 10 ppm (393 Ω.cm²) with an efficiency of 99.8%, signifying the establishment of a robust and efficient barrier layer. Adsorption modeling investigations indicated that the adsorption behavior aligned more closely with the Frumkin (R^2 = 0.818) and Temkin (0.791) models, suggesting multi-site adsorption with lateral interactions among the adsorbed molecules.

Keywords: corrosion, aluminum, 2-mercaptobenzothiazole, efficiency, adsorption.

PB4- Green Synthesis of Copper Oxide Nanoparticles Using Peel Extracts of Cucurbita pepo.

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Abstract

This study aims to investigate the efficiency of green synthesis in the preparation of copper oxide nanoparticles (CuONPs) using pumpkin peel extract. The prepared samples were characterized using a set of analytical and physicochemical techniques, including Fourier Transform Infrared Spectroscopy (FTIR), Ultraviolet–Visible Spectroscopy (UV-Vis), X-ray Diffraction (XRD), Scanning Electron Microscopy (SEM), and Energy-Dispersive X-ray Spectroscopy (EDX). The results revealed the formation of pure and crystalline nanoparticles within the monoclinic phase.

These findings highlight the potential of plant extracts as eco-friendly and sustainable mediators for the synthesis of multifunctional nanoparticles, emphasizing the importance of tailoring plant extract constituents to achieve optimal surface properties suitable for targeted applications, particularly in photocatalysis and antimicrobial activity.

Keywords: green synthesis, nanoparticles, copper oxide nanoparticles, pumpkin.

PB5- Electrochemical Fabrication and Characterization of Ni-Al_2O_3Composite Coatings on Steel

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Abstract

The growing demand for advanced coatings with enhanced properties has motivated the development of composite electrolytic deposits, achieved by incorporating solid particles into a nickel matrix. This study focuses on producing a nickel–alumina (Al_2O_3) composite coating characterized by high hardness and chemical stability. The coatings were electrodeposited from a chloride-based electrolyte containing nickel ions and fine alumina particles. Structural and morphological analyses were performed using X-ray diffraction (XRD) and scanning electron microscopy (SEM). Corrosion resistance was evaluated in
0.5 M NaCl and 0.5 M K_2SO_4 solutions by polarization measurements. The results demonstrate that the composite coatings exhibit significantly improved corrosion resistance compared to pure nickel deposits.

Keywords: Corrosion, Nickel, Electroplating, Alumina, Composite Deposition, Steel.

PB6- Impact Environnemental des Techniques Photocatalytiques sur les Contaminants Aquatiques

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Résumé:

La photolyse du lindane en solution aqueuse représente une méthode prometteuse pour la

dégradation de ce pesticide toxique, largement utilisé mais désormais interdit dans de nombreux pays en raison de son impact environnemental négatif. L'utilisation de la lumière proche-visible et UV, en particulier à des longueurs d'onde inférieures à 320 nm, permet d'initier des réactions photochimiques complexes. En présence du polyoxométallate $PW_{12}O_{403}^{-}$, des études ont montré que le lindane se décompose efficacement en dioxyde de carbone (CO) et en acide chlorhydrique (HCl). Ce processus de dégradation commence rapidement, souvent en quelques minutes, ce qui souligne l'efficacité potentielle de la photocatalyse dans la purification des eaux contaminées.

Un des résultats les plus intéressants est la capacité de minéralisation en l'absence de dioxygène, indiquant que les radicaux hydroxyles (OH) jouent un rôle clé en tant qu'oxydants primaires. Cela ouvre des perspectives pour l'application de cette technologie dans des conditions où l'oxygène est limité, comme dans les milieux aquatiques profonds ou pollués. La compréhension des mécanismes sous-jacents de cette dégradation photocatalytique pourrait également conduire à de nouvelles approches pour traiter d'autres contaminants organiques dans les systèmes aquatiques, contribuant ainsi à la protection de l'environnement et à la qualité de l'eau.

Mots-clés : lindane, polyoxométallates, dégradation photocatalytique, minéralisation.

PB7- Removal of Methylene Blue by Adsorption onto sulfuric acid (H2SO4) Activated carbon derived biomass

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Abstract:

The purification of wastewater is a vital concern for the preservation of the environment and public health. Removing methylene blue, a commonly used dye in the industry, poses a significant challenge. An effective method to achieve this is through the use of activated carbon. Activated carbon is a porous material with the ability to selectively adsorb organic compounds present in wastewater, including methylene blue.

In this study, three activated carbons prepared from Ziziphus seeds by sulfuric acid activation were examined using Fourier transform infrared (FTIR) and scanning electron microscopy (SEM). They were used as adsorbents for the removal of methylene blue. The effects of various experimental parameters, such as the adsorbent dosage and particle mass, initial dye concentration, and contact time, were investigated. The maximum adsorption capacities of methylene blue by the activated carbon under optimized conditions reached 57.43%. The results suggest that Ziziphus seed activated carbon could be used as an economical and commercially viable adsorbent material in wastewater treatment for the removal of basic dyes.

Keywords: biomass, pollution, chemical activation, adsorption

PB8- Comparative Adsorptive Removal of Anionic Dyes on Granular Activated Carbon: Isotherm and Kinetic Modeling

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Abstract

This study investigated and compared the adsorption performance of granular activated carbon (GAC) toward two anionic dyes, Acid Black 210 (NA210) and Acid Green 20 (VA20). The experimental results showed that the maximum dye removal occurred under strongly acidic conditions (pH = 2), achieving efficiencies of 98.78% for NA210 and 96.33% for VA20 at an initial concentration of 150 mg/L. Adsorption efficiency decreased with increasing temperature, indicating that the process was exothermic in nature. At an initial dye concentration of 100 mg/L, the adsorption capacity for VA20 (18 mg/g) exceeded that for NA210 (10 mg/g), which may be attributed to the stronger affinity of VA20 molecules toward the GAC surface. Isotherm modeling revealed that the adsorption of NA210 was best described by the Langmuir type II model, suggesting monolayer adsorption on a homogeneous surface. In contrast, the adsorption of VA20 followed the Dubinin–Radushkevich (D–R) model, indicating a predominantly physical adsorption mechanism governed by mesoporous diffusion. Kinetic analysis demonstrated that the pseudo-second-order (PSO) model provided the best fit for both dyes, implying that the overall process is controlled mainly by chemisorption involving electrostatic interactions between the dye molecules and the active sites of GAC.

Keywords: Adsorption; Granular Activated Carbon (GAC); Acid Black 210 (NA210); Acid Green 20 (VA20)

PB9- Electrochemical Traitement of Phenol Using PbO_2 Chemical-Based Composite Anodes

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PB10- Visible-Light Photocatalytic Elimination of Gallic Acid over Modified Perovskite Oxides

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Abstract:

Gallic acid, a common aromatic compound originating from industrial and agricultural effluents, has become a serious environmental concern due to its toxicity and limited biodegradability. Developing efficient photocatalytic systems capable of degrading such pollutants under visible light is therefore essential for sustainable water purification. In this study, advanced modified perovskite oxides were designed and evaluated as visible-light-driven photocatalysts for the effective degradation of gallic acid. The aim was to clarify how compositional tuning and surface modifications influence charge carrier dynamics, reactive species generation, and overall photocatalytic efficiency. The materials were synthesized via controlled methods and characterized by X-ray diffraction (XRD), UV–Vis diffuse reflectance spectroscopy (DRS), Fourier-transform infrared spectroscopy (FTIR), and electron microscopy (SEM/TEM), Brunauer–Emmett–Teller (BET) surface area analysis, and X-ray photoelectron spectroscopy (XPS). These techniques were used to establish correlations between structure, morphology, and optical properties. Photocatalytic degradation experiments under visible-light illumination revealed rapid and efficient removal of gallic acid, with reaction rates strongly dependent on surface and structural features. Mechanistic studies using selective radical scavengers confirmed that hydroxyl radicals and photogenerated holes are the main reactive species responsible for the degradation process. This work provides new insights into the structure–activity relationship of modified perovskite oxides and demonstrates their potential as efficient and sustainable photocatalysts for the elimination of persistent organic contaminants in water.

Keywords: modified perovskite oxides, photocatalysis, gallic acid, visible light, water treatment.

PB11- Evaluation of the Inhibitory Properties of Glycine against Copper Corrosion in 1M HNO_3

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Abstract:

This work was dedicated to studying the inhibitory effect of glycine (GLY) on copper corrosion in nitric acid medium (1M HNO_3) using various techniques: open-circuit potential monitoring, polarization curves, electrochemical impedance spectroscopy (EIS), gravimetry, density functional theory (DFT) calculations, optical microscopy (OM), and SEM-EDS analysis. The results obtained from these methods indicate that the studied glycine acts as an anodic inhibitor, with a maximum efficiency of 92.24% at a concentration of 10^{-4} M. Observations by OM and SEM-EDS reveal the formation of a stable and insoluble protective layer that limits electrolyte access to the metal surface.

Keywords: Corrosion, Copper, inhibitors of corrosion , glycine.

B12- Cyclic Voltammetric Detection of Chlorantraniliprole Residues in Tomato Aqueous Extracts: Integration of Electrochemical and Water Chemistry Approaches

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Abstract:

Electrochemistry provides a powerful and sensitive approach for detecting and quantifying pesticide residues in agricultural and environmental samples. In this study, the insecticide Chlorantraniliprole—widely applied for lepidopteran pest control—was investigated using cyclic voltammetry (CV) while integrating a water chemistry perspective to assess its persistence and electrochemical behavior in aqueous tomato extracts. Measurements were carried out with a modified glassy carbon electrode (GCE) within a potential range of –1.0 to +2.0 V, at a scan rate of 25 mV s^{-1} and a pH of 6.5.

The proposed electrochemical method exhibited excellent sensitivity, achieving a detection

limit of 0.01 µg mL^{-1} and recovery rates ranging from 85% to 98%. From a water chemistry standpoint, the results provided insights into the stability and degradation pathways of Chlorantraniliprole in aqueous environments. Overall, this combined electrochemistry–water chemistry approach highlights the capability of electrochemical techniques not only for rapid monitoring of pesticide residues but also for understanding their environmental behavior, thus contributing to risk assessment and sustainable management of phytosanitary products.

Keywords:

Electrochemistry; Water chemistry; Chlorantraniliprole; Pesticide residues; Cyclic voltammetry; Tomato extracts.

PB13- Amélioration des propriétés physico-chimiques des conducteurs organiques synthétisés chimiquement : Application dans le domaine de traitement des eaux usées.

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Résumé

Dans ce travail, nous avons synthétisé un polymère conducteur, la polyaniline, par voie chimique, suivi par une caractérisation à l'aide de différentes techniques. La polyaniline obtenue a été analysée par spectroscopie FT-IR afin d'identifier et de confirmer la présence des groupements fonctionnels souhaités, par diffraction des rayons X (DRX) pour étudier sa morphologie et déterminer la taille des cristallites, ainsi que par analyse thermique (ATG) pour évaluer ses propriétés thermiques. Enfin, ses performances ont été testées dans le cadre de l'élimination des colorants de l'eau à travers plusieurs méthodes : adsorption, photocatalyse, voltamétrie cyclique et électrolyse. Les résultats ont montré que la polyaniline présente une efficacité élevée en voltamétrie cyclique et en électrolyse, tandis que ses performances en adsorption et en photocatalyse restent faibles.

Mots clés : Polyaniline, dopage, synthèse chimique, polymère conducteur, électrolyse.

PB14-Treatment of Industrial Wastewater from the Berkawi Basin, Ouargla, by Electrocoagulation

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Abstract:

The sustainable management of industrial wastewater represents a major environmental challenge due to the presence of persistent organic and inorganic pollutants that are difficult to remove using conventional treatment methods.
Electrocoagulation is an innovative electrochemical process based on the *in situ* generation of coagulant ions from sacrificial aluminum electrodes. These ions react with contaminants to form stable aggregates that can be easily separated by sedimentation or filtration.

This study aims to evaluate the efficiency of electrocoagulation in treating wastewater produced by petroleum industries in the Berkawi Basin, Ouargla. The obtained results pH = 6.5, COD removal = 90%, TSS removal = 93%, total petroleum hydrocarbons (TPH) = 95%, Pb = 97%, Zn = 90%, and Cu = 96% demonstrate that electrocoagulation is an effective, economical, and environmentally friendly alternative to conventional physicochemical treatment methods. Moreover, integrating this process within a combined treatment approach (electroflocculation and photocatalytic flocculation) can further improve the quality of reusable water, thereby contributing to the achievement of sustainable development goals and advancing green chemistry practices.

Keywords: petroleum industry wastewater, electrochemical treatment, pollutants, sustainable development.

PB15- Study of the effectiveness of some new corrosion inhibitors against steel

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Abstract:

Steel is composed of at least two elements, primarily iron and then carbon. It is essentially the carbon content that gives the alloy the properties of the metal we call "steel". Due to the durability of steel, its high production and installation costs, most industries have adopted several measures aimed at extending the lifespan of this valuable material [1].To counteract this undesirable phenomenon, organic inhibitors, whose mode of action generally results from their adsorption onto the metal surface, are the most frequently used. Their inhibitory action is linked to the formation of a more or less continuous barrier, but of finite thickness, which

prevents the solution from reaching the metal [2]. Inhibitors are unique in that they are the only means of intervention from the aggressive environment, making them an easy and inexpensive method of corrosion control, provided that the product(s) used are moderately priced [3]. Furthermore, it is important to understand the mode of action of inhibitory molecules, their cost, their application limitations, and their toxicity in order to use them with a sufficient safety margin [4]. A corrosion inhibitor is a chemical compound that, when added in low concentrations to a corrosive environment, slows down or stops the corrosion process of a metal placed in contact with that environment [5, 6]. In this work, we were interested in the evaluation of the effectiveness of salts in the prevention of corrosion of steel in a solution of H2SO4 0.5M by mass loss and electrochemical methods. Different conditions were chosen (different temperatures and inhibitor concentrations). The high-resolution scanning electron microscope was used to examine the steel surface morphology. According to the different experiments, the bis-phosphonium salts studied are mixed-type inhibitors. The adsorption of the inhibitors on the metal surface follows the Langmuir adsorption isotherm. The order of the EI determined from experimental measurements correlates perfectly with the surface analysis.

Keywords: bis-phosphonium salts; Steel; Inhibitor; Electrochemical method; Mass loss; Corrosion. Weight loss; DFT

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PB16- Groundwater Quality and Agricultural Suitability in the Continental Intercalaire Aquifer of Southern Algeria: Insights from Hydrochemical and GIS Analyses

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Abstract

The Ouled Djellal region, located in southern Algeria, is characterized by an arid to semi-arid climate where groundwater from the Continental Intercalaire (CI) aquifer represents the primary source of water for both irrigation and domestic use. In the absence of perennial surface water, groundwater plays a crucial role in sustaining agricultural productivity and socio-economic activities. This study aims to evaluate the hydrogeochemical characteristics and agricultural suitability of groundwater by integrating water quality indices with Geographic Information System (GIS) techniques. Sixteen groundwater samples were collected and analyzed for major cations and anions, electrical conductivity (EC), pH, temperature (T°), and total dissolved solids (TDS). Hydrochemical classification identified two dominant water types: Ca– Mg–SO_4 and Na–SO_4, reflecting the influence of evaporation, ion exchange, and water– rock interactions. The saturation index (SI) results indicate that most samples are oversaturated with respect to calcite, dolomite, and gypsum, whereas halite remains undersaturated. Irrigation water quality indices—including EC, sodium adsorption ratio (SAR), and sodium percentage (%Na)—suggest that while most samples are suitable for irrigation, certain zones exhibit elevated salinity and sodium hazards. Spatial distribution maps generated using GIS reveal increasing groundwater mineralization toward the downstream and eastern parts of the study area. Effective management strategies are therefore essential to ensure the sustainable use of groundwater resources in this arid environment.

Keywords: Groundwater, Hydrochemical facies, Water–rock interaction, Irrigation suitability, Ouled Djellal.

PB17- Influence of the thermodynamic properties of Zn2+, Cu2+, and Mg2+ on the inhibition of calcium carbonate precipitation, by Controlled Chemical Degassing Method (LCGE)

PB18- Elabration of thin films by electrodeposition of copper II complex

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Abstract

The objective of this research work is to study the electrochemical propreties of copper II complex by cyclic voltammerty methode, the process of elaboration of thin films by electrodeposition of copper II complex on the FTO and ITO surfaces was carried out. The atomic force microscope (AFM) analysis showed the thin films morphology.

Keywords: electrochemical propreties, cyclic voltammetry, thin films, AFM

PB19- Current-Dependent Lithium-Ion Concentration Profiles Across the Electrolyte and Their Evolution at Electrode Interfaces in Lithium-Ion Batteries

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Abstract –

This work investigates how the applied current influences lithium-ion concentration profiles along the electrolyte and at the electrode–electrolyte interfaces in lithium-ion batteries. A one-dimensional Nernst– Planck model under electroneutrality conditions was solved using a finite difference scheme to simulate ionic transport during galvanostatic charge–discharge cycles. The results show that the concentration distribution is nearly uniform at low current, while higher current values generate steep concentration gradients, particularly at the anode/electrolyte and cathode/electrolyte interfaces. During discharge, lithium-ion depletion occurs near the anode interface and accumulation near the cathode, whereas the opposite trend appears during charging. These interface-driven gradients intensify with increasing current, reflecting stronger polarization and reduced transport efficiency. The study highlights the critical role of current load in governing ion distribution across the electrolyte and provides insight into the limitations imposed by interfacial transport phenomena in lithium-ion batteries.

Keywords: Lithium-ion concentration profile, electrode–electrolyte interface, current density, ionic transport, Nernst–Planck model.

PB20- Removal of Cephalexin from aqueous solutions by adsorption onto activated carbon: kinetics, isotherms and regeneration study

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Abstract:

Wastewater from urban and hospital sources is a significant pathway for the release of pharmaceutical residues, including β-lactam antibiotics, into aquatic environments. Cephalexin, a first-generation cephalosporin widely prescribed in human medicine, has been repeatedly detected at low concentrations in treated effluents, raising concerns about ecological impacts and the development of antimicrobial resistance. In this work, adsorption onto activated carbon is investigated as an advanced treatment option to reduce cephalexin levels in synthetic solutions and pre-treated real waters. The effect of key operating and solution parameters is examined, including activated carbon dose, contact time, initial cephalexin concentration, pH, ionic strength and the presence of natural organic matter. The results highlight a high affinity of cephalexin for activated carbon under optimized conditions, which can be attributed to the combined contribution of the large specific surface area and the surface chemistry of the adsorbent. The adsorption mechanism involves π–π interactions between aromatic moieties, hydrogen bonding and electrostatic interactions, all of which are strongly influenced by the acid–base speciation of cephalexin and the surface charge of the carbon. The kinetic data are satisfactorily described by a pseudo-second-order model. Equilibrium data are in accordance with the Langmuir isotherm model. Regeneration tests show that the activated carbon can be reused for several adsorption cycles with only a moderate loss in removal efficiency. Thus, the study demonstrates that adsorption onto activated carbon is a robust and flexible approach for the tertiary treatment or polishing of effluents containing cephalexin, and can be effectively combined with other processes such as membrane filtration or advanced oxidation.

Keywords:

Water treatment; Cephalexin; Antibiotics; Activated carbon; Adsorption; Isotherms; Kinetics.

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PB21- Recovery of Na_2SO_4/Fe_2O_3 Nanocomposite Material from the Chemical spent pickling bath and Its Application in Electrochemical Sensors for Heavy Metal Ion Detection in Aqueous Medium

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Abstract

The presence of heavy metal ions in the environment represents a major ecological issue due to their toxic impact on ecosystems and the health of living organisms. These contaminants can lead to various harmful effects, disrupting the natural balance. To address this, the scientific community has focused its efforts on developing effective methods to identify and quantify these pollutants in water bodies. Among the available techniques, electrochemical sensors offer significant advantages, including high accuracy, rapid detection, and a particularly efficient analytical mechanism, often surpassing traditional methods.

In this research, the Na_2SO_4/Fe_2O_3 nanocomposite was synthesized from a metal stripping bath using the co-precipitation method. The final material was then subjected to various characterization techniques such as Scanning Electron Microscopy (SEM), X-ray Diffraction (XRD), Fourier Transform Infrared Spectroscopy (FTIR), and Raman Spectroscopy. The study of the electrochemical behavior of Na_2SO_4/Fe_2O_3 as a metal ion detector was conducted in an aqueous medium in the presence of Cu and Pb ions at different concentrations, using two electrochemical techniques: Cyclic Voltammetry (CV) and Square Wave Voltammetry (SWV).

During this investigation, specific concentrations of Cu ions (0.1, 0.2, 1, and 5 mg/L) and Pb ions (0.03, 0.05, 0.1, 0.15, and 0.2 mg/L) were meticulously studied to evaluate the response of the nanocomposite. The results obtained demonstrate an excellent electrochemical detection capability of Na_2SO_4/Fe_2O_3 concerning heavy metal ions, even during simultaneous detections. These results offer promising prospects for the recovery of nanomaterials from stripping baths, as a replacement for traditional costly synthesis methods.

Keywords: electrochemical, detection, sensors, spent pickling bath, nanocomposites

PB22- Approche synergique de la dialyse de Donnan et de l'oxydation de Fenton pour l'élimination améliorée de l'ammonium et de la demande chimique en oxygène (DCO) dans les effluents de délavage de tannerie

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Résumé

Cette étude examine l'application séquentielle de la dialyse de Donnan (DD) et de l'oxydation de Fenton pour éliminer efficacement les ions ammonium (NH_4^+) et la demande chimique en oxygène (DCO) dans les eaux usées réelles de délavage. Les effluents de délavage contiennent des niveaux élevés d'azote, principalement en raison du sulfate d'ammonium, et des valeurs de DCO pouvant atteindre 3000 mg/L. Dans la première étape, la DD avec une membrane échangeuse de cations monovalents (CMX) a été utilisée pour éliminer sélectivement les ions NH_4^+. Les effets du ratio NH_4^+/Na^+, de la plage de pH et de la concentration initiale en ammonium sur l'efficacité et la sélectivité de la DD ont été soigneusement évalués. Dans des conditions optimales, la DD a réduit la concentration de NH_4^+ de 94 %, passant de 980 mg/L à 54 mg/L. Ensuite, l'oxydation de Fenton a été appliquée pour réduire la DCO, avec une réduction de 97 % (de 2880 mg/L à 66,24 mg/L) dans des conditions optimales : pH 3,0, 2 g/L de H_2O_2, 0,03 g/L de Fe^{2+} et un temps de réaction de 90 minutes. Ces résultats confirment l'efficacité du processus combiné DD-Fenton comme une solution durable et pratique pour le contrôle de la pollution et la récupération des ressources dans le traitement des eaux usées de délavage de tannerie.

Mots-clés

Récupération de l'ammonium ; Membrane cationique monovalente ; Effluent de délavage de tannerie ; Dialyse de Donnan ; Processus de Fenton.

TOPIC C: MATERIALS AND POLYMER CHEMISTRY, INORGANIC CHEMISTRY AND CATALYSIS

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PC3	Green Synthesis of Hematite (α-Fe2O3) Nanoparticles Using Biological Precursors and Stabilizing Agents	**Dr. Youcef BAHLOUL U-BATNA 1**
PC4	Enhanced photocatalytic degradation using inorganic materials	**Dr. ATOUT Hicham U-Setif 1**
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PC15	Processing and Purification of Natural Precursors for the Phase Formation of Magnesium Aluminate Spinel	**NOUAR Ilhem U-Setif 1**
PC16	Structural study of a new polymorph based on barbituric acid	**Dr. Wahiba Falek1 U-Khenchela**

P_{C17}	Synthesis, characterization, and magnetic properties of a heterometallic ligand	**Dr. Falek Wahiba U-Khenchela**
P_{C18}	Structural, Microstructural and Magnetic properties of The Ball Milled FeCoP Powder Mixtures	**Dr. Hanane Berkani U- Khenchela**
P_{C19}	Characterisation by gel permeation chromatography of HALS-stabilised LDPE films aged under severe climatic conditions (Sub-Saharan region)	**Dr. ABDELHAFIDI ASMA ENS-Laghouat**
P_{C20}	Study of the different physical and mechanical properties of composite materials made of polyethylene and fibers	**NOUIOUA Nour Elhouda U-Biskra**
P_{C21}	THE EFFECT OF AG DOPED MAGNESIUM OXIDE NANOPARTICLES ON THE ANTIBACTERIAL ACTIVITY	**Dr. Nouhad ROUABAH U-Batna 1**
P_{C22}	Crystal structure and Hirshfeld surface analysis of Isoxazolones derivative.	**Dr. Rima Gheribi U-Oum El bouaghi**
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P_{C24}	Photoluminescence Characterization of Graphene Oxide Reduced and Decorated by Different Acetates	**Dr. Touafek Naima ENSB-Constantine**
P_{C25}	Synthesis of a biopolymer reinforced with plant fiber (ALFA)	**Dr. Amel Samia CHABIRA U-Batna 2**
P_{C26}	Morphological and physico-chemical properties of HALS-stabilized LDPE films photo-oxidated	**Dr. ABDELHAFIDI ASMA HSP Laghouat**
P_{C27}	Procédé d'extraction et de purification de l'hydroxyapatite à partir de phosphate naturel pour applications biomédicales	**Yasmine Nasri U-Sétif 1**
P_{C28}	POAs appliqués à la dégradation du méthyle orange sur l'oxyde de fer Fe_2O_3	**Asma meriche U-Jijel**
P_{C29}	Metal-organic framework based on imidazole derivatives and anhydrous zinc (II) chloride metal: crystallographic analysis, Hirshfeld surface, and Theoretical study.	**Kerkatou Redouane U-Constantin 1**
P_{C30}	Effect of Alkali Treatment on the Mechanical Strength of Alfa Fiber/Polyester Composites	**Addour Yakout U-M'sila**
P_{C31}	Synthèse, caractérisation et étude électrochimique des propriétés électrocatalytiques d'un complexe de manganèse à base de Schiff pentadentée	**Dr. Naoual ZOBEIDI U-Ouargla**
P_{C32}	Synthesis, crystal structure and Hirshfeld surface analysis of (2-Methyl-imidazol-1yl)-acetic acid ethyl ester	**Kerkatou Mounia ENS-Constantine**
P_{C33}	Synthèse et caractérisation d'un nouveau composé PVC 4000 M – 1,12-Diaminododécane pour l'extraction des métaux lourds des eaux polluées	**Dr. Ahmed TABCHOUCHE U-Ouargla**
P_{C34}	Metal-organic framework based on imidazole derivatives and anhydrous zinc (II) chloride metal: crystallographic analysis, Hirshfeld surface, and Theoretical study.	**Kerkatou Redouane U-Constantine 1**
P_{C35}	Clay-Catalyzed Polymerization of Styrene: The Effect of Clay Type and Their Processing Mode on Polystyrene Performance	**TABET HABIBA U-SKIKDA**
P_{C36}	Nanofiltration of Cephalexin from Aqueous Solutions: Rejection Mechanisms, Operating Conditions and Fouling Behavior	**Dr. Sami khettaf U-Batna 1**

P_{C37}	Effect of Alkali Treatment on the Mechanical Strength of Alfa Fiber/Polyester Composites	**Addour Yakout U-M'sila**
P_{C38}	Préparation et caractérisation des matériaux hybrides à base de poly (aniline-ci-2aminophenyle disulfide) aves différentes quantités de SiC	**Dr. Sarah benyakhou U-Mascara**
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P_{C42}	EFFECT OF Fe2O3, ZnO AND Sb2O3 ON DIELECTRIC PROPERTIES OF 0.02Pb[(Fe1/5, Zn1/5, Sb3/5)O3 - xPbZrO3 - (0,98-x)PbTiO3] LEAD PIEZOCERAMICS	**Dr. Khiouani Adel U-Batna 1**
P_{C43}	Élimination du Plomb en Solution Aqueuses Par Adsorption Sur Un Polymère Fonctionnel : Études des isothermes d'adsorption	**Dr. Fairouz Aberkane U-Batna 1**
P_{C44}	Unraveling Metal–Support Interactions in Ni/TiO_2-Modified Bentonite Catalysts for DRM: Insights from In Situ XPS	**Boudiaf Meriem U-USTHB**
P_{C45}	Adsorption of Crystal Violet Dye Dissolved in Aqueous Solutions on Activated Carbon Prepared from Peanut Shells	**Dr. Abdelhek MEKLID U-Biskra**
P_{C46}	Nanofiltration of Cephalexin from Aqueous Solutions: Rejection Mechanisms, Operating Conditions and Fouling Behavior	**Dr. Sami khettaf U-Batna 1**
P_{C47}	Evaluation of the Inhibitory Properties of Glycine Against Copper Corrosion in 1M HNO_3	**Karima ABDERRAHIM U-Annaba**

PC1- Enhanced Structural, Thermal, and Thermoelectric Properties of Neodymium-Substituted Sodium Cobaltate Nanocomposites

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Abstract

Sodium cobaltate-based materials have emerged as promising candidates for thermoelectric applications due to their layered structure, favorable charge transport properties, and intrinsic thermal stability. In this study, $Na_{0.74}CoO_2$ nanocomposites were modified through partial substitution of sodium by neodymium, yielding a series of $Na_{0.74-x}Nd_xCoO_2$ (x = 0–0.2) compositions prepared via the sol–gel method. X-ray diffraction confirmed that the parent material maintained its hexagonal phase, while secondary $NdCoO_3$ reflections appeared at higher Nd concentrations. Scanning electron microscopy revealed a noticeable decrease in porosity with increasing dopant content. Optical analysis using UV–Vis absorption and Tauc plots indicated a slight band gap widening, from 2.87 to 2.94 eV. Thermal expansion studies exhibited non-linear behavior, with the $Na_{0.64}Nd_{0.1}CoO_2$ composition showing the lowest thermal expansion coefficient, highlighting its enhanced structural stability. Regarding thermoelectric response, all samples exhibited positive Seebeck coefficients (61.6–140 μV/K). Among them, $Na_{0.64}Nd_{0.1}CoO_2$ demonstrated the lowest electrical resistivity (34.26 μΩ·m at 830 K) and the highest power factor (0.4425 W/K^2 at 1070.5 K). These findings underline the potential of $Na_{0.64}Nd_{0.1}CoO_2$ as a promising thermoelectric material for practical energy conversion applications.

Keywords:

Sodium cobaltate, Nanocomposites, XRD, SEM, Band gap, Thermal expansion, Seebeck coefficient, Electrical resistivity, Power factor.

PC2- Study and characterization of a semi-conductive material based on polypyrrole and ZnO nanoparticles.

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Abstract:

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 study, polypyrrole (PPy) was synthesized via oxidative polymerization using ammonium persulfate (APS) in the presence of various dopants: hydrochloric acid (HCl), dodecylbenzene sulfonic acid (DBSA), and sodium dodecyl sulfate (SDS). PPy/ZnO Nanocomposites were subsequently prepared by in situ polymerization with varying ZnO contents (5–20%) in the presence of DBSA and SDS. Fourier transform infrared spectroscopy (FTIR) analysis confirmed the incorporation of surfactants into the PPy matrix and revealed interactions between the N–H groups of PPy and ZnO Nanoparticles. Thermogravimetric analysis (TGA) indicated a significant enhancement in the thermal stability of PPy when doped with SDS or DBSA, with further improvement upon the addition of ZnO. Scanning electron microscopy (SEM) showed that both the particle morphology and size were influenced by the choice of dopant and the presence of ZnO. UV– Visible spectroscopy revealed changes in the PPy band gap upon the addition of SDS, DBSA, and ZnO. Finally, electrical conductivity, measured by the four-point probe method, was highest for SDS- doped PPy (0.11 $S \cdot cm^{-1}$) and further increased with the incorporation of ZnO, reaching a percolation threshold at 5% ZnO.

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

PC3- Green Synthesis of Hematite (α-Fe_2O_3) Nanoparticles Using Biological Precursors and Stabilizing Agents

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Abstract

The development of environmentally friendly synthesis methods has become a central objective in green chemistry. In this work, hematite **(α-Fe_2O_3)** nanoparticles were prepared using bio-based approaches that rely on natural extracts and biological residues as precursors, stabilizing agents, and **pH** regulators.

Different green routes were explored, including the use of eucalyptus leaf and orange peel extracts, which acted simultaneously as natural reducing and stabilizing agents, enabling control over the size and morphology of the nanoparticles. The obtained nanoparticles were characterized by X-ray diffraction **(XRD),** Fourier-transform infrared spectroscopy **(FTIR),** and **UV–Visible** spectroscopy. The results confirmed the successful formation of crystalline hematite phases, with an optical band gap of about **2.1 eV.** This study highlights the feasibility of replacing conventional chemical precursors with low - cost, locally available biological resources, thereby reducing the environmental footprint of synthesis processes. Beyond the ecological benefits, the bio-

synthesized hematite nanoparticles open new opportunities for applications in photocatalysis, energy conversion, and biological fields.

Keywords: Hematite nanoparticles, Green synthesis, XRD, FTIR, UV–Vis spectroscopy.

PC4- Enhanced photocatalytic degradation using inorganic materials

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Abstract:

The aim of this study is to achieve a higher photocatalytic degradation through two process at the same time : heterogeneous photocatalysis and heterogeneous photo- Fenton like under UV, Visible and Sun light. The as-prepared catalysts based on Fe, TiO2 and graphene oxide were synthesized by different method for methylene blue (MB) degradation. Graphene oxide was prepared from graphite via Hummer's method, and the reduction of graphene oxide along $FeTiO_2$ nanoparticles was obtained through a hydrothermal process. The resulting catalysts were characterized different methods .
The photocatalytic degradation of MB was evaluated under UV, visible and Sun light irradiation, revealing that the catalyst $FeTiO_2$/rGO exhibited significantly higher photocatalytic activity than TiO_2, TiO_2/rGO and $FeTiO_2$. Notably, the highest
photocatalytic activity was observed for the $FeTiO_2$/rGO and achieve 100% of degradation yield.

Key words: Fenton like, Photocatalysis, Methylene blue, Graphene oxide.

PC5- Reinvestigation of cesium hydrogen oxalate crystal structure, Hirshfeld surface analysis, enrichment ratio and voids analysis

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Abstract:

As part of our research regarding the elaboration of novel coordination polymers (CPs) with oxalate ligand, involving the combination of trivalent transition metals and alkali metals [1-3], attempts to prepare a bimetallic compound with Cr and Cs atoms led to colorless single crystals which have been isolated and identified as $CsHC_2O_4$ [4]. Due to the lack of some structural data, the structure has been reinvestigated with new and more accurate crystallographic data [5], allowing the redefinition of a new formula $Cs_2(C_2O_4)(H_2C_2O_4)$ (I), instead of the one proposed earlier [4]. The asymmetric unit contains one Cs atom, a half oxalate ligand and a half oxalic acid molecule. The structure of (I) is made up of zigzag files of CsO_{11} polyhedra, linked by opposite faces via the $C_2O_4^{2-}$ ions, forming double layers that are separated by $H_2C_2O_4$ ligand layers in the [001] direction. A moderate H bond is established along [101] direction between the two organic ligands, while a weak intramolecular H bond is formed within the $H_2C_2O_4$ molecule, playing a role in the structural polymerization. Hirshfeld surface analysis and its corresponding 2D fingerprint plots revealed that Cs···O contacts are the main contributors to the crystal packing, followed by O···C, O···O, and O···H contacts. Enrichment ratio calculations showed that O···C, Cs···O and O···H contacts have the highest values, indicating strong preferential interactions and suggesting that these are the major forces driving the crystal packing. Void analysis revealed a very densely packed structure with no significant cavities, suggesting good mechanical properties.

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PC6- Novel Water Treatment Technology Utilizing Membranes: Polyethylene/Natural Zeolite

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ABSTRACT:

The treatment of wastewater, whether from domestic or industrial sources, represents a crucial challenge for environmental protection today. The reuse of this water is a solution that is already being implemented. Among the rapidly developing techniques in this field, membrane filtration methods stand out particularly.

In this research, we have designed polymer membranes from polyethylene and zeolite sourced from a deposit located in Bédjaia, Algeria, by adjusting the proportions. These membranes aim to purify wastewater contaminated by dyes, particularly in the textile and paper industries.

The morphology of these membranes was studied using Fourier transform infrared spectroscopy (FTIR) and scanning electron microscopy (SEM). The obtained filtrates were analyzed by UV spectroscopy to determine the effectiveness of these membranes in eliminating methyl orange. The results reveal that these membranes are effective in removing this organic dye, and this effectiveness is attributed to the adsorption capacity of natural zeolite, due to its porous structure.

Keywords: wastewater, membrane, polymer, zeolite.

PC7- Élaboration de céramiques hautes performances dopées par des nanomatériaux pour des applications technologiques avancées

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Abstract

Les travaux menés au cours de cette mémoire s'inscrivent dans l'étude de Céramique e de type BZT et structure de pérovskite ABO_3. Cette étude est effectuée en variant X et en effectuant des substitutions au site A de la structure de la pérovskite par un Mélange des dopants ($CaCO_3$; MgO) Cette étude porte donc sur deux parties principales :

La première partie concerne la synthèse BZT à partir d'un mélange des oxydes et dopants.

La deuxième partie est engagée dans l'étude de caractérisation et propriété diélectrique d'un nouveau matériau céramique de type BZT et de la structure du système de formule général : $Ba_x(Ca_{0.7}Zn_{0.3})_{1-x}Ti_{0.8}Zr_{0.2}O_3$ abrégé (BCMTZ) avec : $0{,}96 \leq X \leq 0.99$

Pour atteindre notre objectif, l'étape d'élaboration suivie pour la synthèse de notre céramique est la méthode par voie solide.

Afin d'homogénéiser la solution solide et de stabiliser la structure cristalline, ces échantillons ont été traités thermiquement à différentes températures de frittage de 1050, 1100, 1150, 1175 et 1190

C°.
Plusieurs analyses peuvent être utilisées pour l'identification morphologique et structurelle, telles que analyse infrarouge (IR). Sont conduit aux conclusions suivantes :
Afin d'atteindre la température de frittage optimale, l'influence de la température de frittage sur la densité et la porosité a été étudiée. Cette température (1190 C°) correspond à la densité maximale, donc la porosité minimale correspond également à des produits de meilleure qualité.

Mots clés : Céramique, pérovskite, PZT, frittage

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PC8- Sr/Co-Doped Pr_2NiO_4 Cathodes for Alkaline Fuel Cells

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Abstract:

Layered nickelate materials are being investigated as potential cathodes for alkaline fuel cells due to their mixed conductivity and structural stability. This work reports the synthesis of Pr2NiO4 and Pr1.95Sr0.05Ni0.95Co0.05O4 by the citrate method, followed by characterization using X-ray diffraction (XRD) and scanning electron microscopy (SEM). Sr and Co doping was found to enhance both electrical conductivity and electrochemical reactivity. The results demonstrate that the doped compound exhibits superior performance compared to the pristine material, confirming its potential as a promising cathode for alkaline fuel cells.

Keywords: Nickelates; Pr_2NiO_4; Sr/Co-doping; Citrate method; Electrochemical properties; Alkaline fuel cells.

PC9- Structural reinvestigation, thermal analysis and correction to the formula of Ba(II) Cu(II) phthalate coordination polymer

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Abstract:

The self-assembly of fascinating coordination polymers (CPs) remains a topical research subject. Materials of interest in terms of applications in several fields, environment, storage, gas separation, catalysis, optoelectronics, etc [1]. They result from multifunctional organic ligands combined with metals by coordination bonds, sometimes associated to supramolecular interactions.

The title heterobimetallic complex has been synthesized from aqueous solution of a mixture of H_2BDC acid, barium and copper salts. Biagini Cingi *et al* have previously reported a basic description of the structure [2]. In this previous study, they speak of a complex with four water molecules of different nature. Our study allowed a new refinement with significant better precision with all H atoms positions. The asymmetric unit consists of one Ba(II) cation, one Cu(II) cation, two o-phthalate dianions and four water molecules In fact. The new formula $[BaCu(OOC\text{-}C_6H_4\text{-}COO)_2(H_2O)_4]$ highlights the four coordination water molecules, major difference noted. This result is confirmed by TGA/DTA. The dehydration occurs from 105°C to 180 °C with the departure of the four coordination water molecules; the experimental value of 11.44 % is in agreement with the theoretical percentage of 11.97 % [3].

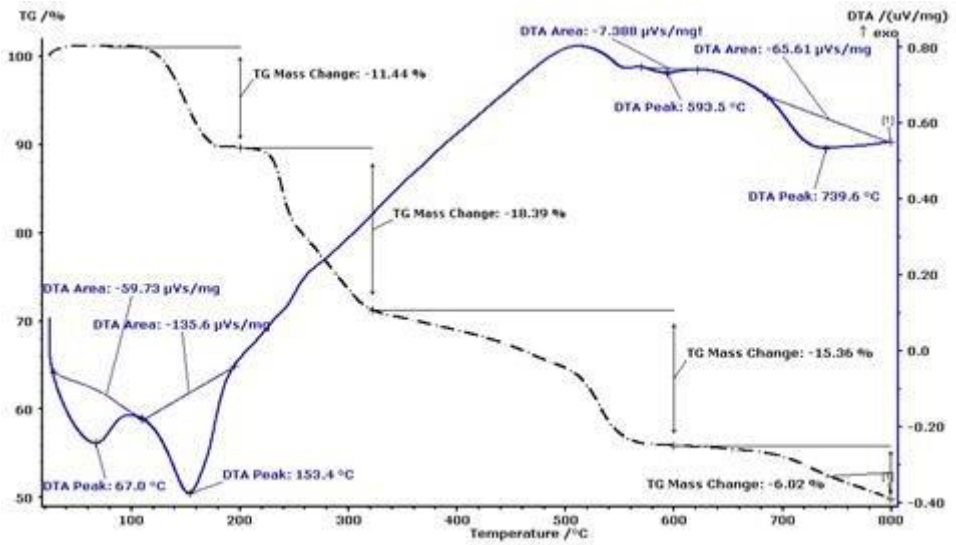

Figure 1. TGA/TDA curves of $[BaCu(OOC\text{-}C_6H_4\text{-}COO)_2(H_2O)_4]$

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PC10- The Crystal Structure, Hirshfeld Surface interactions, optical/Nonlinear Optical properties and evaluation of the antioxidant activity of 8-(3-chloropropanamido)quinolin-1-ium chloride: Experimental and theoretical studies

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Abstract

The title compound, 8-(3-chloropropanamido)quinolin-1-ium chloride, (C 12 H 11 ClN 2 O)$^{+}\cdot$Cl^{-} (**Q1**), was synthesized via the reaction of quinolin-8-amine with 3-chloropropanoyl chloride. It was characterized by single-crystal X-ray diffraction analysis, and by infrared, and ^{1}H and ^{13}C NMR spectroscopies. Hirshfeld surface analysis and two-dimensional fingerprint plots were used to quantify the interatomic interactions present in the crystal. The antioxidant activity of the synthesized compound was evaluated by the 2,2-diphenyl-1-picrylhydrazyl hydrate (DPPH) radical scavenging, cupric reducing capacity (CUPRAC) and ABTS radical scavenging activity, showed an average inhibition. The molecular structure of Q1 is determined by DFT calculations at wb97xd/6- 311g(d) levels. Local and global reactivity descriptors were computed to predict the reactivity of the title compound. Furthermore, TD-DFT calculation is also used to determine the optical properties of the Q1 in the gas and solvents. We found excellent agreement between the calculated results and the experimental data. Moreover, the quantum calculations showed that the title compound is a potential candidate for second- and third-order NLO applications.

Keywords: Crystal structure, Quinoline, HS, Antioxidant activity, DFT and TD-DFT calculations.

PC11- Influence of the Crystalline Structure and morphology on the Electrocatalytic Properties of NiFe Alloys for the Hydrogen Evolution Reaction

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Abstract:

The present work is part of a research project aiming at the fabrication of a quaternary Graphene-Metal composite material and its characterization as an electrocatalyst for the hydrogen evolution reaction (HER) in alkaline water electrolysis. This study focuses on a NiFe alloy synthesized from a bath with different molar ratios. To precisely determine the elemental composition and the molar ratios of the deposited alloy, the crystallographic structure and the phase identification of the synthesized NiFe alloy were investigated using X- ray Diffraction (XRD). The structural characterization confirmed the formation of the NiFe alloy and provided insight into the preferred crystallographic orientation. The synthesized NiFe alloy was found to have good corrosion resistance in aggressive media, with improved electro-catalytic properties towards the HER in alkaline solution [2]. Specifically, the alloy with an optimal molar ratio exhibited better catalytic properties for hydrogen evolution in alkaline media than electrodes based on Ni or Fe separately, demonstrating the critical role of composition and structure, as verified by XRF and XRD, in enhancing electrocatalytic performance.

PC12- Comparison between different type of zeolite

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Abstract

Zeolites, as a class of inorganic microporous crystalline materials, are widely used in catalysis, adsorption–separation, and ionexchange. In general, zeolite materials are synthesized under hydrothermal–solvothermal conditions, and the reaction gel medium contains the framework atoms, solvents, templates or structure- directing agents (SDAs), and mineralizers. Systematization and understanding of zeolite synthesis have been tremendous, but the detailed molecular mechanism of zeolite nucleation is still unknown.

At this study, we reported tow deferent synthesis zeolite A and T zeolite. A and T-type zeolite were synthesized using sodium aluminate as the starting material. The synthesis was carried out by activating the reactive source, followed by hydrothermal treatment of the activated concretes for 72 hours at a temperature of 100°C. As temperature increases to 100 °C, zeolite presented itself as a major phase in the system at time of crystallization. The synthesized samples were characterized by X-ray diffraction (XRD) on an X-ray diffractometer (CuKa radiation, BRUKER, D8 ADVANCE). The infrared (IR) spectra were recorded as thin KBr wafers

containing about 2 wt% sample on a FT-IR spectrometer (NICOLET, NEXUS 670). The crystalline size and morphology were determined by scanning electron microscopy (SEM) (FEI, QUANTA 200). XRD, FTIR and SEM instruments were used to monitor the behavior of zeolite crystals with respect of temperature and time.

Keywords: zeolite, material, synthetic, characterization.

PC13- Characterisation by gel permeation chromatography of HALS-stabilised LDPE films aged under severe climatic conditions (Sub-Saharan region)

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Abstract

The characterization of LDPE films stabilized by hindered amine light stabilizers (HALS) and exposed to natural weathering was performed using Gel Permeation Chromatography (GPC). The films were prepared as polymer solutions by dissolving them in analytical-grade xylene at 50°C. This procedure allowed for precise evaluation of molecular weight distribution and the degree of macromolecular chain degradation. Results indicate that the weight-average molecular weight (Mw) initially increases during exposure. This is attributed to predominant intermolecular crosslinking reactions, as evidenced by the polydispersity index (PDI) rising to 1.364. Subsequently, both the number-average molecular weight (Mn) and (Mw) gradually decrease during prolonged weathering, due to the prevalence of main-chain scission processes. GPC analysis demonstrated that HALS addition significantly restricted the reduction in molecular weight and mitigated the increase in polydispersity. This suggests that nitroxyl radicals effectively quench polymer peroxyl radicals and suppress Norrish type I and II photo-oxidation pathways. These findings confirm that HALS impart robust, long-term stabilization to LDPE films, maintaining their mechanical integrity and prolonging their functional lifespan under extreme environmental stress.

Keywords: HALS , GPC, Mw, PDI, Peroxyl

PC14- Effect of Calcination Temperature on the Formation of Spinel Phase

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Abstract:

Spinel is of a good interest for several structural applications. The aluminum dross contains significant amounts of alumina, can be used as alumina source for spinel preparation. However, Dolomite $CaMg(CO_3)_2$ can be also used for the spinel preparation as an MgO source. In this work, we studied the synthesis of Mg-Al by using these materials. The adopted synthesizing process involves three significant stages: leaching, precipitation and calcination. The preparation was carried out by grinding The two materials. After that, we washed the aluminum dross with distilled water, to eliminate the contained salts and release the toxic gases. The two materials were submitted to several characterization tests such as XRF, XRD, laser granulometry and FTIR. The leaching process for aluminum dross and dolomite in sulfuric acid encompasses various parameters (T, t, C and S/L ratio), the solution was characterized using Atomic Absorption Spectroscopy and Inductively Coupled Plasma Mass Spectrometry.

X-ray fluorescence results revealed that used dolomite was mainly composed Of CaO (~31.37% wt.) and MgO (~22.22% wt.), with the presence of minor amounts of other oxides. The major crystalline phases identified in dolomite ore were dolomite mineral associated to a few quantities of calcite. The analysis by laser granulometry showed that ground dolomite exhibits the mean particle size d 50 =291.5µm. The FTIR spectrum of natural dolomite showed a strong band at around 730 cm -1 attributed to mineral dolomite, while the band observed at 873 cm -1 corresponds to the vibration of carbonates (C-O bond). For the used aluminum dross, alumina is the major component (~ 59.80% in wt.). Several other components are present at lower quantities, such as MgO (~12.75% wt.), CaO (~6.26% wt.), and SiO 2 (~5.46% wt.). After washing by water, the aluminum dross and the dried resulted residues were submitted to characterization. XRF showed the improvement of the alumina percentage (~72%) in the washed dross du to the remove of salts (NaCl and KCl) as was suggested by the XRD tests conducted on the washing residue. This result demonstrated the importance of washing aluminum dross as a prior step to be adopted in all our spinel synthesis experiments. For aluminum dross, the major crystalline phases identified were aluminum oxide (Al 2 O 3), spinel (MgAl 2 O 4). The mean particle size was found d 50 = 255.8µm. The transmittance curves recorded by Fourier Transform Infrared spectroscopy carried out on aluminum dross showed absorption bands at 418 cm -1 due to Ca-O stretching, and band at 473cm -1 corresponding to the Mg-O bending. The peak observed in the 450 cm -1 is due to Al-O bending vibrations and the Al - O stretching modes are also found between 500 and 600 cm -1. The optimal extraction conditions for aluminum and magnesium from their major sources have been determined using (AAS) and (ICP). The highest concentration of aluminum (597 mg/L) in the aluminum dross leaching solution was achieved after leaching during 120 minutes at T= 70°C. The highest concentration of magnesium (296.7 mg/L) in the dolomite leaching solution was obtained at a temperature of 65°C during 15 minutes. During the precipitation stage, NH_4OH was used as the base at different temperatures. XRD analysis revealed that the most intense spinel peak was obtained at 40 °C. Pour les précipités du mélange M1 et M2 calcinés à 1100°C sont présents : l'alumine (Al_2O_3), la magnésie (MgO) et peu de spinelle. L'augmentation de la température de calcination à 1300 °C pour le mélange M1 a renforcé la présence du spinelle, par réaction fort probable de l'alumine libre avec la magnésie libre.Pour les précipités du mélange M3 calcinés à 1100°C, le spinelle est la phase majoritairement formée suivie de l'alumine et de la magnésie. Il

ressort que la préparation du spinelle à partir du mélange M3, par précipitation à 40°C et calcination des précipités à 1100°C est la voie la plus pertinente, puisque cette température de calcination est relativement faible à ce qu'on peut trouver dans la littérature.

Keywords: spinel, synthesis, dolomite, aluminum dross, Alumina, MgO.

PC15- Processing and Purification of Natural Precursors for the Phase Formation of Magnesium Aluminate Spinel

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Abstract:

Spinel ($MgAl_2O_4$) or magnesium aluminate is a very interesting ceramic due to its important physical, chemical, and mechanical properties, making it a material of choice in various applications in advanced technology. The classical method for synthesizing spinel consists of the solid phase reaction, using magnesium oxide (MgO) and alumina (Al_2O_3) as starting materials. Unfortunately, the involved costs are high due to the price of the raw materials and the very high temperature required for the achievement of the reaction.

This work aims to study the synthesis of Mg-Al spinel or $MgAl_2O_4$ from natural and local raw materials, highly abundant and available with low costs: kaolin of Tamazert (Jijel) as an alumina source (Al_2O_3) and dolomite of Djebel Teioualt (Oum El Bouaghi) as MgO source. The new adopted technique offers the possibility to make the synthesis possible at low temperatures while ensuring good control of the particle size and morphology with a simple and economical experimental procedure (dissolution-purification-precipitation and calcination). We conducted leaching of calcinated kaolin and dolomite by modifying leaching parametres such as acid concentration, temperature, and duration…

The most effective parameters for extracting magnesium from their respective sources were determined through Atomic Absorption Spectroscopy (AAS) and Inductively Coupled Plasma Mass Spectrometry (ICP).

Keywords: Kaolin, dolomite, spinel, synthesis, Alumina, MgO

PC16- Structural study of a new polymorph based on barbituric acid

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ABSTRACT:

The new tetragonal polymorph of dichlorobarbituric acid, $C_4H_2Cl_2N_2O_3$, forms a ribbon structure linked by N—H…O hydrogen bonds along the [001] axis. Two ribbons, linked by a second-order rotation axis, are associated by Cl…O contacts, and four pairs of such chains are arranged around a fourth-order roto-inversion axis.

In the new crystal structure of (**a**), a ribbon consists of two parallel strands. Neighboring molecules forming the same strand are linked to each other by N—H•••O═C bonds via their C6 carbonyl groups. Two strands of the same ribbon are linked by a second set of N— H•••O═C interactions involving the C2 carbonyl group. These interactions form two independent $R_3^3(12)$ rings. The molecules of the same strand are linked together by a translation along the [001] axis. In addition, the ribbon has a sliding plane oriented perpendicular to its mean plane.

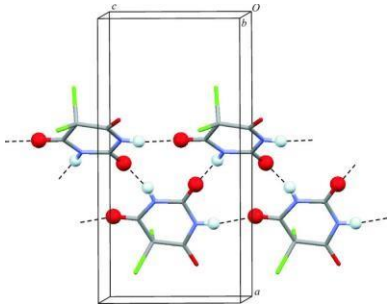

Fig.1. A view along the *b* axis of the H-bonded C-3 tape structure of (**a**).

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PC17- Synthesis, characterization, and magnetic properties of a heterometallic ligand

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ABSTRACT:

Following the structural synthesis of the new pyridylmethyliminomethyl ligands, their magnetic properties were investigated using direct and alternating current magnetic susceptibility measurements. The paramagnetic metal ions present in theseaggregates exhibit weak antiferromagnetic coupling, characterized by a slow relaxation of their magnetization. This is the first report describing the use of this versatile ligand to target 3d–4f coordination clusters.

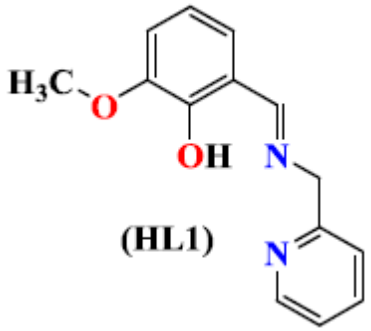

Fig. 1. Structure and coordination modes of the ligand (L1)(**a**).

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PC18- Structural, Microstructural and Magnetic properties of The Ball Milled FeCoP Powder Mixtures

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Abstract Ball milling technique was used to obtaine FeCoP powder mixtures in a high-energy planetary ball mill. Phases formation, microstructural, structural and magnetic properties of the milled powders are studied as a function of milling time by X-ray diffraction (XRD) using the MAUD program which is based on the Rietveld method and vibrating sample magnetometry (VSM). A nanocrystallines α-Fe(P) solide solution in addition to $Co_{75}Fe_{25}$ binary phase with the same *bcc* structure and Im-3m space group were detected after 1h of milling. Further milling time (up to 2h) gives rise to the proportion of the $Co_{75}Fe_{25}$ binary phase. The crystallite size of the α-Fe(P) solid solution remarkably decreased but was nearly stable for the $Co_{75}Fe_{25}$ phase. The mechanical results reveal that the bulk modulus of elasticity for the α-Fe(P) solid solution is less than that of the $Co_{75}Fe_{25}$ phase. Higher powders milling time (3 h) exhibit higher, coercive field, H_c and remanence-to-saturation ratio than those obtained at lower milling times. The highest value of the saturation magnetization, M_s, is observed after one hour of the milling time.

Keywords: Ball milling, FeCoP powders, XRD, Rietveld refinement, magnetic properties.

PC19- Characterisation by gel permeation chromatography of HALS-stabilised LDPE films aged under severe climatic conditions (Sub-Saharan region)

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Abstract

The characterization of LDPE films stabilized by hindered amine light stabilizers (HALS) and exposed to natural weathering was performed using Gel Permeation Chromatography (GPC). The films were prepared as polymer solutions by dissolving them in analytical-grade xylene at 50°C. This procedure allowed for precise evaluation of molecular weight distribution and the degree of macromolecular chain degradation. Results indicate that the weight-average molecular

weight (Mw) initially increases during exposure. This is attributed to predominant intermolecular crosslinking reactions, as evidenced by the polydispersity index (PDI) rising to 1.364. Subsequently, both the number-average molecular weight (Mn) and (Mw) gradually decrease during prolonged weathering, due to the prevalence of main-chain scission processes. GPC analysis demonstrated that HALS addition significantly restricted the reduction in molecular weight and mitigated the increase in polydispersity. This suggests that nitroxyl radicals effectively quench polymer peroxyl radicals and suppress Norrish type I and II photo-oxidation pathways. These findings confirm that HALS impart robust, long-term stabilization to LDPE films, maintaining their mechanical integrity and prolonging their functional lifespan under extreme environmental stress.

Keywords: HALS , GPC, Mw, PDI, Peroxyl.

PC20- Study of the different physical and mechanical properties of composite materials made of polyethylene and fibers.

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Abstract

In recent efforts to enhance the mechanical properties of synthetic polymers, alternative reinforcing fillers like lignocellulosic materials are gaining traction. These materials, derived from eco-friendly agricultural waste, hold significant promise in tackling pressing environmental issues. Their biodegradability and ease of collection from agricultural residues make them an environmentally responsible choice.This study aims to investigate the influence of silane coupling agents and alkali treatments on palm fibers on the mechanical, thermal, and water absorption properties of polyethylene (PE) composites. Infrared spectroscopy will be employed to analyze the impact of these fiber treatments. We anticipate that treated fibers will lead to improved mechanical properties compared to untreated composites. Additionally, scanning electron microscopy (SEM) images are expected to reveal strong interfacial adhesion between the PE composite surfaces and treated fibers, potentially improving both heat stability and water resistance.

Keywords: coupling agent, adhesion, polyethylene, fibre, and alkali treatment.

PC21- THE EFFECT OF AG DOPED MAGNESIUM OXIDE NANOPARTICLES ON THE ANTIBACTERIAL ACTIVITY

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Abstract:

Currently, the search for efficient, cheap, and green treatment processes for wastewater is a challenge around the world. Also, Bacteria resistance to antibiotics is one of the biggest challenges facing human health today. In this work, an attempt has been made to synthesized Ag doped MgO nanoparticles and investigate their antibacterial effects . we report the structural, optical, and morphological properties of Ag :MgOnanoparticles .

In this investigation, Ag doped MgO NPs were successfully synthesized by sol gel methods. Analysis via scanning electron microscopy (SEM) confrmed their agglomerated quasi- spherical shape with a size range of 20-50 nm. The X-ray difraction (XRD) pattern exhibited prominent peaks at planes (200) and (220), indicating the high crystallinity of MgO and Ag doped MgO NPs. Fourier transform infrared spectroscopy (FT-IR) of Ag doped MgO showed slight shift to higher wave number which might be due to the introduction of Ag as a dopant.

However, the Ag-doped MgO samples exhibit better antibacterial activities compared to pure MgO.Surprisingly, 3% Ag- MgO shows the best antibacterial activity.It is assumed that the more formed Ag nanoparticles will occupy the defect sites on the surface of MgO particles and thus hinder preventing the adsorption of oxygen to produce ROS. Thus the adsorption of oxygen to generate ROS. The results of this present study indicated that this material have very effective antibacterial properties and there is a direct relationship between the concentration of nanoparticles and the rate of elimination of bacteria, and the antibacterial effect is a bactericidal effect .Where the smaller nanoparticle ,the grater the effect of antibacterial.

Keywords: Magnesium oxide nanoparticles, Antibacterial activity ,sol- gel , E. coli and P. aureus

PC22- Crystal Structure and Hirshfeld Surface Analysis of Isoxazolones Derivative

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Abstract

Isoxazolones possess notable biological activities, including inhibition of tumor necrosis factor alpha (TNF-α) [1] and antimicrobial [2] effects. They are also applied in the treatment of cerebrovascular conditions and as muscle relaxants, in addition to serving as herbicides and fungicides [3]. Moreover, derivatives of isoxazolone are valuable intermediates in the synthesis of diverse heterocyclic compounds such as pyridopyrimidines and quinolines, and they participate in various chemical reactions. Due to these versatile properties, they have attracted considerable research interest.

The current synthesis method involves a three-component polycondensation reaction using an aromatic aldehyde, ethyl acetoacetate, and hydroxylamine hydrochloride under varying conditions. In this study, we propose a green approach using a food -grade additive, which is approved for use in organic farming, cost-effective, widely available, and environmentally safe, as a catalyst in water. We present the synthesis, molecular and crystal structure, and a Hirshfeld surface analysis of a derivative of isoxazolone.

Keywords: Crystal structure, π–π interactions, Isoxazolone, Hirshfeld surface.

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PC23- Etude Structurel du Compose Hybride à Base de Sulfate

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Résumé

La structure cristalline du composé ***hydrogènphosphite de 4-méthyle anilinium*** **(*Bis-p-MEANPx)*** cristallise dans le groupe d'espace ***P-1*** du le système triclinique, est construite à la base d'une unité asymétrique constituée de deux cations 4- méthyle anilinium (**CH_3-C_6H_4-NH_3^+*)* et deux anions hydrogènphosphite (**$H_2PO_3^-$**) **(Figure 1).** La structure du composé ***Bis-p-MEANPx*** est formée de feuillets constitués par les cations organiques (***CH_3-C_6H_4-NH_3^+)*** entre lesquels se situent les anions minéraux ***H_2PO_3.*** Ces ions sont liés entre eux par des liaisons hydrogène fortes et forment d'une part des chaînes infinies ***$[(H_4P_2O_6)]^{2-}$*** **(Figure 2)** le long de l'axe b. La cohésion intermoléculaire entre les anions et les cations est assurée par un réseau de liaisons hydrogène de type N-H…O et O-H…O.

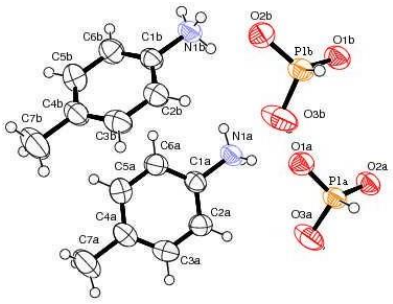

Figure 1 : L'unité asymétrique du composé Bis-p-MEANPx

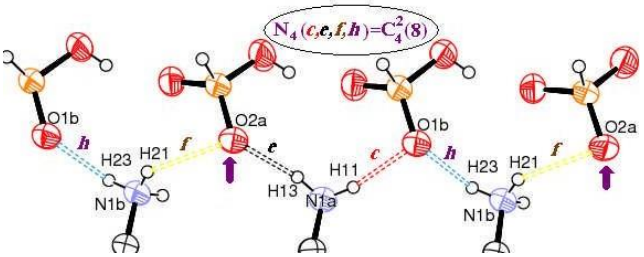

Figure 2 : Chaine infinie

Dans la structure les groupements anioniques $H_2PO_3^-$ forment des chaînes en zigzag qui se développent suivant la direction de l'axe b en alternance avec les couches des groupements organiques $CH_3\text{-}C_6H_4\text{-}NH_3^+$.

Une étude détaillée des différentes liaisons hydrogène, assurant la cohésion dans l'édifice cristallin, nous a permis de déterminer leurs graphes binaires, formés principalement par des cycles et des chaînes infinies, ainsi que les graphes d'ordre supérieurs entre plusieurs types de liaisons.

Keywords: Synthèse, Composé hybride, Crystal, RX, Liaison hydrogène et l'édifice cristallin.

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PC24- Photoluminescence Characterization of Graphene Oxide Reduced and Decorated by Different Acetates

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Abstract

This study investigates the synthesis and photoluminescence (PL) behavior of graphene oxide (GO) and reduced graphene oxide (rGO) prepared by the modified Hummers method and chemically reduced using sodium, nickel, and lead acetates. Graphene, a two-dimensional carbon material, exhibits outstanding electrical and mechanical properties, but its lack of a bandgap limits optical applications. Oxidizing graphene introduces oxygen-containing functional groups that open a bandgap and enable photoluminescence. GO was synthesized by oxidizing graphite to graphite oxide, and then exfoliated into graphene oxide sheets. Reduction was carried out by a reflux method in dimethylformamide using different acetates. Photoluminescence spectroscopy was employed to analyze the optical response of pure and reduced GO under excitation wavelengths ranging from 350 to 450 nm. Pure GO exhibited a broad PL emission between 420 and 720 nm with a main peak at 570 nm, corresponding to radiative recombination of electron–hole pairs in

sp^2 clusters. The PL intensity increased nearly threefold when the excitation wavelength decreased from 450 to 350 nm, showing strong excitation dependence. After chemical reduction using sodium, nickel, and lead acetates, the PL emission bands exhibited a red shift, with characteristic peaks at 550 nm, 580 nm, and 640 nm, respectively, for excitation wavelengths of 350 nm, 380 nm, and 410 nm. These variations reveal that the reducing agent strongly influences the degree of deoxygenation and the restoration of sp^2 carbon networks. Sodium acetate produced the most efficient reduction, enhancing the optical emission, while nickel and lead acetates showed weaker effects. These results highlight that the type of acetate used plays a key role in tuning the optical properties of graphene oxide. This work opens new perspectives for the controlled design of GO-based materials for optoelectronic and photonic applications.

PC25- Synthesis of a biopolymer reinforced with plant fiber (ALFA)

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Abstract

The objective of this work is to synthesize a starch-based biopolymer reinforced with plant fiber (Alfa). Three types of composites were produced: one containing only the biopolymer, the second formulated with plant fiber without chemical treatment, and the last made with chemically treated fiber. A natural aging protocol was carried out on the composites. Various analyses and tests were performed on material samples taken at regular intervals, such as FTIR spectroscopy, X-ray diffraction (XRD), and mechanical tensile testing. The results obtained show that the presence of an organic filler in the matrix of this biopolymer improves its resistance to degradation and increases its mechanical properties.

Keywords: biodegradable, biopolymer, plant filler (ALFA), XRD, FTIR, mechanical testing.

PC26- Morphological and physico-chemical properties of HALS-stabilized LDPE films photo-oxidated

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Abstract

The addition of hindered amine light stabilizers (HALS) significantly enhances the long-term stability of low-density polyethylene (LDPE) greenhouse films exposed under severe sub-

Saharan weathering conditions. Over a 24- month exposure period, HALS slows down significantly the carbonyl (I-C = 6) and vinyl groups'(I-V=0,8) formation during exposure. indicating effective peroxyl radical deactivation by nitroxide, thus inhibiting Norrish photo-oxidation reactions , as demosterated by FTIR.However DSC analysis of HALS stabilised films exposed revealed a modest increase in crystallinity around 5%, indicating limited structural changes. Additionally, the stabilizer effectively inhibited crosslinking reactions, as supported by the unchanged concentration of vinylidene groups during aging. These results indicat the crucial role of HALS in preserving the structural of LDPE films under harsh environmental conditions, thereby extending the service life and performance of agricultural plastics.

Keywords: HALS, Photo-oxidation , FTIR, , DSC, Crystallinity Index, I-C

PC27- Procédé d'extraction et de purification de l'hydroxyapatite à partir de phosphate naturel pour applications biomédicales

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Abstract :

L'hydroxyapatite (HA) est un biomatériau d'intérêt majeur dans le domaine des substituts osseux, grâce à sa biocompatibilité, sa bioactivité et sa similitude chimique avec la phase minérale de l'os humain. Dans ce travail, une hydroxyapatite a été élaborée à partir d'un phosphate naturel local, dans une démarche de valorisation des ressources disponibles et de production à faible coût destinée aux applications biomédicales.

Les poudres obtenues ont été caractérisées par **fluorescence X (FRX)** pour la composition chimique, **diffraction des rayons X (DRX)** pour l'analyse de la phase cristalline, **spectroscopie infrarouge à transformée de Fourier (FTIR)** pour l'identification des groupes fonctionnels, **analyse thermique (ATG/ATD)** pour l'étude de la stabilité thermique, et **microscopie électronique à balayage couplée à l'analyse EDX (MEB/EDX)** pour la morphologie et la distribution élémentaire. Les résultats confirment la formation d'une hydroxyapatite pure, bien cristallisée et homogène, présentant un rapport Ca/P proche de la valeur théorique

Les essais **in vitro** réalisés dans un fluide physiologique simulé (SBF) ont révélé la formation d'une couche apatite en surface, indiquant une excellente bioactivité. Ces performances démontrent le potentiel de cette hydroxyapatite issue du phosphate naturel pour la fabrication de substituts osseux et d'échafaudages bioactifs. Des études **in vivo** sont actuellement envisagées afin d'évaluer la réponse biologique, la biocompatibilité tissulaire et la capacité d'intégration osseuse, ouvrant ainsi la voie au développement d'implants personnalisés à base de biocéramique locale.

Mots-clés : hydroxyapatite, phosphate naturel, biomatériaux, substitut osseux.

PC28- POAs appliqués à la dégradation du méthyle orange sur l'oxyde de fer Fe_2O_3

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Résumé

Ce travail vise à étudier l'adsorption du méthyle orange, un colorant anionique, en milieu neutre et acide, ainsi que sa dégradation en utilisant du Fe_2O_3 synthétisé par la méthode sol- gel combustion.

Les principaux résultats MEB-EDAX ont confirmé la composition chimique du Fe_2O_3, montrant un pourcentage atomique d'oxygène (13,03 %) et de fer (86,48 %). Le spectre DRX a confirmé la présence de la phase Fe_2O_3 dans l'échantillon, tandis que le spectre FTIR-ATR a révélé les bandes caractéristiques de ce composé, notamment à 518 cm^{-1} (correspondant à Fe– O) et à 431, 385 et 240 cm^{-1} (correspondant à O–Fe–O).

Les études cinétiques et d'équilibre de l'adsorption du méthyle orange (MO) ont été réalisées en mode batch (pH libre et acide, R = 1 g/L, [MO] = 50 mg/L). L'analyse cinétique a montré que la réaction de surface suit un modèle de pseudo-second ordre. L'efficacité d'adsorption est de 8,67 % en milieu neutre et de 64,10 % en milieu acide.

Les résultats et conditions expérimentales de l'élimination du MO par les POAs sur Fe_2O_3 sont résumés comme suit :

Les conditions optimales en milieu hétérogène pour la dégradation du MO par le procédé Fenton en présence de Fe_2O_3 sont : $[MO]_0$ = 30 mg/L, masse de catalyseur Fe_2O_3 = 1 g/L, $[H_2O_2]$ = 150 mM et pH = 3.

- **Sans lumière :** Rendement = **65 %**
- **Avec lumière :** Rendement = **96 %**

En milieu homogène, les conditions optimales pour la dégradation du MO par le procédé Fenton sont : $[MO]_0$ =50 mg/L, $[Fe^{2+}]$ = 0,1 mM, $[H_2O_2]$ = 5 mM, pH = 3, le Rendement : 96 %**.**

Mots clés : Pollution de l'eau, MO, oxyde de fer, POAs.

PC-29 Metal-organic framework based on imidazole derivatives and anhydrous zinc (II) chloride metal: crystallographic analysis, Hirshfeld surface, and Theoretical study.

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Abstract:

This paper presents a combined experimental and computational study of two new mononuclear Zinc(II) coordination compounds. The (I) and (II) complexes have been synthesized and characterized by NMR, UV, FTIR and single crystal X-ray diffraction techniques. The single crystal X-ray analyses reveal that the centrosymmetric ZnII cation in both complexes (I) and (II) is tetrahedrally coordinated by two chelating imidazole oxime ligands and by two chlorine atoms in a distorted tetrahedral geometry. The intremolecular interactions were found to play an important role in determining the most favorable structure of the free ligands, therefore controlling the final coordination mode. The cohesion of the structure and stability are ensured by intermolecular O–H···O, O–H···N, O–H···Cl and C–H···O hydrogen bonds. Hirshfeld surface analysis was performed to study the nature of intermolecular interactions within the crystal structure via 3D and 2D fingerprint surfaces and to demonstrate H-bonding with close contacts in crystal via dnorm surface. The stability of the prepared ZnII complexes has been evaluated through the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO), and energy gap. The molecular geometries and electronic transitions of the two complexes and their ligands in the ground state have been calculated using the mPW1PW91 basis at the TZVP level of theory.

Keywords : crystal X-ray ,NMR, UV, FTIR, H-bonding, Zn(MICO)2Cl2 , Zn(MIPMO)2Cl2, Hirshfeld surface ,LUMO , HOMO , mPW1PW91, TZVP

PC30- Effect of Alkali Treatment on the Mechanical Strength of Alfa Fiber/Polyester Composites

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Abstract

Researchers are showing increasing interest in plant fiber reinforced composites due to their eco-friendliness, low density, low cost and amazing mechanical properties. However, some challenges remain for researchers in this field, most notably poor adhesion between the polymer matrix and the plant fibers, which reduces the mechanical properties of composites reinforced with these fibers. This study aims to improve the adhesion between the matrix and the reinforcement

by chemically treating Alfa fibers (Stipa tenacissima) with a 3 wt% NaOH solution at different times (1, 3, 5 and 24 h). FTIR, DRX, GTA and tensile tests were conducted. XRD tests showed that the crystallinity index of 3% alkali treated Alfa fibers for 5 h increased by 36.26%, compared to that of untreated fibers. The results also revealed that the mechanical properties of composites reinforced with treated fibers outperformed those reinforced with untreated fibers. These findings can contribute to the development of high mechanical performance composites, which can be competitive with those prepared with synthetic fibers.

Keywords: composite, Stipa tenacissima, adhesion, tensile strength, alkaline treatment

PC31- Synthèse, caractérisation et étude électrochimique des propriétés électrocatalytiques d'un complexe de manganèse à base de Schiff pentadentée

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Résumé :

Ce travail s'inscrit dans le cadre du développement de nouveaux complexes de métaux de transition à visée électrocatalytique. Il porte sur la synthèse, la caractérisation structurale et l'étude électrochimique d'un complexe de manganèse(II) dérivé d'une base de Schiff pentadentée, obtenue à partir du ligand 5,5'-dibromo-N,N'-bis(salicylidène)bis(3- aminopropylamine).

L'objectif principal est d'examiner la réactivité électrochimique de ce complexe, ainsi que son activité catalytique dans la réaction d'époxydation du cyclooctène, réaction modèle de l'oxydation sélective des alcènes. Cette étude vise à mieux comprendre le rôle du centre métallique de manganèse dans les processus d'activation de l'oxygène moléculaire et à évaluer l'influence du groupe fonctionnel NH de la base de Schiff, susceptible d'agir comme base axiale favorisant la coordination et l'activation de l'oxygène au niveau du site métallique.

Les expériences électrochimiques ont été réalisées à l'aide de la voltamétrie cyclique, technique permettant de suivre les processus rédox impliqués et de déterminer les conditions optimales de catalyse homogène. L'étude du complexe [Mn(II)-Cl-L] a été conduite sous atmosphères d'azote et d'oxygène, sur une électrode de carbone vitreux (CV), et dans divers solvants organiques — diméthylsulfoxyde (DMSO), diméthylformamide (DMF) et acétonitrile (AN) — afin d'évaluer l'influence du milieu réactionnel sur les propriétés électrochimiques.

Les résultats obtenus suggèrent la formation d'espèces métal-oxo du type Mn(V)=O, jouant un rôle clé dans les mécanismes d'oxydation. Ces observations confirment l'intérêt de ce type de complexes de manganèse à base de Schiff pentadentée en tant que catalyseurs potentiels pour les réactions d'oxydation sélective et les applications électrocatalytiques avancées.

Mots-clés : Complexes à base de Schiff, manganèse(II), métaux de transition, électrocatalyse, voltamétrie cyclique, époxydation, polymétallation, oxydation sélective.

PC32- Synthesis, crystal structure and Hirshfeld surface analysis of (2-Methyl-imidazol-1yl)-acetic acid ethyl ester

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Abstract

In the framework of our research work, we synthesized 2-(methyl-imidazol-1-yl)-acetic acid ethyl ester, an imidazole-based organic compound of structural and supramolecular interest. This molecule consists of a methyl-substituted imidazole ring linked through a methylene bridge to an ethyl acetate group, forming a stable heterocyclic system (Fig. 1). The coexistence of donor and acceptor sites in the molecular structure promotes the formation of intra- and intermolecular hydrogen bonds, which play an important role in the stabilization of the crystal packing.

The synthesized compound was characterized by infrared (IR) and UV–visible spectroscopy, confirming the presence of the main functional groups and the electronic transitions within the molecule. The single-crystal X-ray diffraction study revealed that the structure crystallizes in the triclinic system with space group P-1, showing well-defined hydrogen bonding interactions that contribute to the supramolecular arrangement. In order to gain a deeper understanding of the intermolecular contacts and surface interactions, a Hirshfeld surface analysis was also performed.

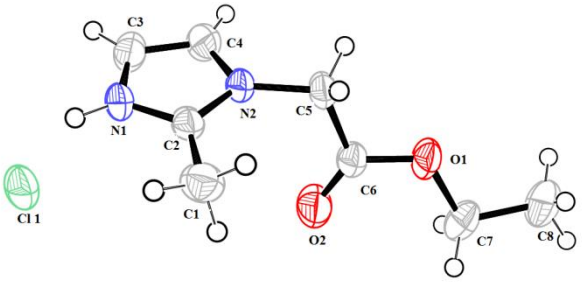

Figure 1 : Ortep of 2-methyl-imidazol-1yl)-acetic acid etyle ester

PC33- Synthèse et caractérisation d'un nouveau composé PVC 4000 M – 1,12- Diaminododécane pour l'extraction des métaux lourds des eaux polluées

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Résumé :

Le polychlorure de vinyle (PVC) constitue aujourd'hui l'un des polymères les plus utilisés dans les domaines industriels, domestique et environnemental. Sa popularité repose sur ses excellentes propriétés mécaniques, chimiques et thermiques, ainsi que sur la possibilité de le modifier chimiquement afin d'obtenir des matériaux aux fonctionnalités spécifiques.
Dans le cadre de ce travail, nous avons entrepris la modification chimique de la matrice du PVC 4000 M par réaction avec l'amine aliphatique primaire 1,12-diaminododécane. Cette fonctionnalisation vise à introduire des groupes amines actifs susceptibles de complexer et d'adsorber les ions métalliques lourds présents dans les eaux contaminées. Le produit obtenu, un nouveau polymère composite PVC–1,12-diaminododécane, a été synthétisé, caractérisé et évalué pour son efficacité dans le traitement et la dépollution des eaux usées.

La caractérisation structurale du polymère modifié a été réalisée à l'aide de techniques spectroscopiques telles que la spectroscopie UV-Visible, la spectroscopie infrarouge (IR), ainsi que la mesure de conductivité électrique, permettant de confirmer la réussite de la modification et d'évaluer la capacité d'adsorption des métaux lourds.
Cette approche s'inscrit dans une perspective de développement de matériaux polymériques éco compatibles capables de contribuer efficacement à la protection de l'environnement et à la gestion durable des ressources en eau.

Mots-clés : Polychlorure de vinyle (PVC 4000 M), 1,12-diaminododécane, métaux lourds, adsorption, traitement des eaux, polymère fonctionnalis.

PC34- Metal-organic framework based on imidazole derivatives and anhydrous zinc (II) chloride metal: crystallographic analysis, Hirshfeld surface, and Theoretical study.

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Abstract:

This paper presents a combined experimental and computational study of two new mononuclear Zinc(II) coordination compounds. The (I) and (II) complexes have been synthesized and characterized by NMR, UV, FTIR and single crystal X-ray diffraction techniques. The single crystal X-ray analyses reveal that the centrosymmetric ZnII cation in both complexes (I) and (II) is tetrahedrally coordinated by two chelating imidazole oxime ligands and by two chlorine atoms in a distorted tetrahedral geometry. The intremolecular interactions were found to play an important role in determining the most favorable structure of the free ligands, therefore controlling the final coordination mode. The cohesion of the structure and stability are ensured by intermolecular O–H···O, O–H···N, O–H···Cl and C–H···O hydrogen bonds. Hirshfeld surface analysis was performed to study the nature of intermolecular interactions within the crystal structure via 3D and 2D fingerprint surfaces and to demonstrate H-bonding with close contacts in crystal via dnorm surface. The stability of the prepared ZnII complexes has been evaluated through the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO), and energy gap. The molecular geometries and electronic transitions of the two complexes and their ligands in the ground state have been calculated using the mPW1PW91 basis at the TZVP level of theory.

Keywords : crystal X-ray ,NMR, UV, FTIR, H-bonding, Zn(MICO)2Cl2 , Zn(MIPMO)2Cl2, Hirshfeld surface ,LUMO , HOMO , mPW1PW91, TZVP

PC35- Clay-Catalyzed Polymerization of Styrene: The Effect of Clay Type and Their Processing Mode on Polystyrene Performance

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Abstract: The purpose of this work is to synthesize composites based on clay used as a synthesis medium. Cation exchange and modifications are performed to improve the dispersion of the clay to generate leaflets that promote the attraction forces and consequently the adhesion of the polymer chains which will act in their turn in a positive manner if not synergistic.
This method of synthesis is carried out in solution; The composites prepared are characterized according to a protocol that makes it possible to understand and detect the phenomenon according to the method of preparation and the structural changes. For this purpose, Fourier Transform Infrared Spectroscopy characterizations were used to better understand the mechanism of function of our system, as well as the following techniques: DSC; ATG, hardness and density. The results of the composites studied, proven that clay is an ideal support for the anionic polymerization of styrene at the same time is a good catalyst for biodegradation.

Key words: styrene / sodium clay / organophilic / in situ polymerization / DSC.

PC37- Effect of Alkali Treatment on the Mechanical Strength of Alfa Fiber/Polyester Composites

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Abstract

Researchers are showing increasing interest in plant fiber reinforced composites due to their eco-friendliness, low density, low cost and amazing mechanical properties. However, some challenges remain for researchers in this field, most notably poor adhesion between the polymer matrix and the plant fibers, which reduces the mechanical properties of composites reinforced with these fibers. This study aims to improve the adhesion between the matrix and the reinforcement by chemically treating Alfa fibers (Stipa tenacissima) with a 3 wt% NaOH solution at different times (1, 3, 5 and 24 h). FTIR, DRX, GTA and tensile tests were conducted. XRD tests showed that the crystallinity index of 3% alkali treated Alfa fibers for 5 h increased by 36.26%, compared to that of untreated fibers. The results also revealed that the mechanical properties of composites reinforced with treated fibers outperformed those reinforced with untreated fibers. These findings can contribute to the development of high mechanical performance composites, which can be competitive with those prepared with synthetic fibers.

Keywords: composite, Stipa tenacissima, adhesion, tensile strength, alkaline treatment

PC38- Préparation et caractérisation des matériaux hybrides à base de poly (Aniline-Co2Aminophenyldisulfide) avec différents masses de SiC

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Abstract

Dans ce travail, des nanocomposites à matrice (aniline –Co- 2Aminophenyldisulfide) ont été synthétisés par polymérisation chimique, en utilisant le persulfate d'ammonium comme oxydant et l'acide chloridrique comme dopant, avec différents masses du carbure de silicium (SiC). L'hybride organique-inorganique a été caractérisé par diffraction des rayons X (DRX), spectroscopie infrarouge à transformée de Fourier (FTIR), la spectroscopie ultraviolette (UV). Les résultats confirment la formation réussie des composites. Les résultats montrent la formation de copolymére sur la surface De renfort. les échantillons résultants gardent toujours des conductivités

élevées. Les propriétés électrochimiques du composite ont été caractérisées par la voltammétrie cyclique. La comparaison entre les différents échantillons montre que l'activité électrochimique dépend significativement de la quantité de renfort ajoutée.

Keywords: nanocomposites, copolymères, aniline, 2aminophenyldisulfide, carbure de silicium.

PC39- Dielectric and magnetic properties at room temperature of a doped NBT- type ceramic material

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Abstract:

During these last twenty years, a very important research activity was dedicated to the study of Lead- free piezoelectric ceramic compounds, which can replace PZT ceramics. The main objective of this work is based on the study of the doping effect on structural, electrical and magnetic properties of NBT type material.

Replacing lead with other environmentally friendly elements has opened up many avenues of research. This is why we focused on stud ying compounds with the formula $Na_{0.5}Bi_{0.5}TiO_3$. XRD spectra confirmed the purity of the phases at calcination temperature of 900°C. Density measurements suggest these samples have good properties. We also studied the electrical and magnetic properties of this material.

Key words: DRX, magnetic properties, NBT, perovskite.

PC40- Plant-Based Nanotechnology: CuO Nanoparticles for Light-Induced Pollutant Degradation

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Abstract

This study explores an eco-friendly method for synthesizing copper oxide (CuO)

nanoparticles using an aqueous extract of *Salvia barrelieri*, a medicinal plant native to North Africa. The plant extract functioned as a natural reducing and stabilizing agent, replacing the hazardous chemicals typically used in conventional nanoparticle production. The resulting CuO nanoparticles were characterized by X-ray diffraction (XRD) and Fourier-transform infrared spectroscopy (FTIR), confirming their crystalline structure and identifying functional groups derived from plant metabolites. Photocatalytic performance was evaluated through the degradation of Rhodamine B dye under natural sunlight and LED light, examining the effects of dye concentration, catalyst dose, and ZnO loading. The best degradation efficiency was achieved with 25 mg of CuO supplemented with 5% ZnO, highlighting a synergistic enhancement in photocatalytic activity. Overall, the results demonstrate that *Salvia barrelieri* provides a sustainable, locally available resource for advanced applications in environmental nanotechnology and wastewater treatment

Keywords: Salvia barrelieri extract, Photocatalysis, Rhodamine B, CuO

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PC41- $CH_3NH_3SnI_3$: Matériau Pérovskite Sans Plomb pour Dispositifs Photovoltaïques et Optoélectroniques

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Abstract :

Les pérovskites hybrides organiques–inorganiques à base d'halogénures métalliques ont émergé comme des matériaux prometteurs pour la prochaine génération de dispositifs optoélectroniques, grâce à leurs excellentes propriétés de transport de charge et à la possibilité d'ajuster finement leur structure électronique. Parmi elles, la pérovskite sans plomb $CH_3NH_3SnI_3$

($MASnI_3$) suscite un intérêt croissant en tant qu'alternative respectueuse de l'environnement aux matériaux contenant du plomb, tout en conservant des performances électroniques comparables. Dans ce travail, nous étudions les propriétés structurales, optiques et électroniques de $MASnI_3$ en combinant des caractérisations expérimentales et des calculs ab initio basés sur la théorie de la fonctionnelle de la densité (DFT). Le matériau cristallise dans une structure pérovskite déformée, présente une forte absorption de la lumière dans le domaine visible et possède un gap direct adapté aux applications photovoltaïques et aux photodétecteurs. Nos analyses montrent que l'incorporation de Sn^{+2} introduit des caractéristiques électroniques particulières tout en maintenant une grande mobilité des porteurs, bien que l'oxydation partielle de Sn^{+2} constitue un défi majeur affectant la stabilité à long terme. Nous discutons également des stratégies visant à améliorer sa stabilité environnementale et thermique, notamment par l'ingénierie de composition et la passivation de surface. Cette étude met en évidence le potentiel de $MASnI_3$ comme pérovskite sans plomb pour des technologies optoélectroniques durables et fournit des pistes pour optimiser ses performances dans les dispositifs futurs.

Key words: DFTcalculation;Optical Properties; Perovskites.

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PC42- EFFECT OF Fe_2O_3, ZnO AND Sb_2O_3 ON DIELECTRIC PROPERTIES OF 0.02Pb[(Fe1/5, Zn1/5, Sb3/5)O3 - xPbZrO3 - (0,98-x)PbTiO3] LEAD PIEZOCERAMICS

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Université de Batna 1

PC43- Élimination du Plomb en Solution Aqueuses Par Adsorption Sur Un Polymère Fonctionnel : Études des isothermes d'adsorption

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Résumé

Le plomb (Pb^{2+}) est un polluant hautement toxique qui menace la santé humaine, il peut causer des dommages graves et permanents à de nombreux organes, notamment le système nerveux. Cette étude évalue l'efficacité d'un nouveau matériau, le poly(2-hydroxy-4-méthacryloyloxy benzophénone) (PHMB), pour l'élimination du Pb^{2+} de l'eau. Le monomère 2-hydroxy-4-méthacryloyloxy benzophénone (HMB) a été synthétisé et polymérisé pour obtenir l'adsorbant PHMB. Le PHMB et le HMB ont été caractérisés par des techniques spectroscopiques (FTIR, RMN ^{1}H et ^{13}C). L'efficacité d'élimination du Pb^{2+} dans les échantillons d'eau a été examinée par spectroscopie UV-visible en utilisant l'EDTA comme agent complexant. Les résultats ont montré qu'une élimination optimale du Pb^{2+} est obtenue à pH 6 avec une concentration de PHMB de 0,75 g/L. L'analyse des isothermes d'adsorptions a montré que le modèle de Freundlich était le plus approprié, indiquant une adsorption multicouche et favorable du Pb^{2+}, avec une capacité d'adsorption maximale de 142,68 mg/g. Par ailleurs, le PHMB a conservé environ 80 % de son efficacité après plusieurs cycles de régénération ; sa réutilisabilité et sa forte affinité pour le Pb^{2+} en font un candidat prometteur pour une purification de l'eau durable et pratique.

Mots clés : Ions plomb ; monomère ; Polymérisation radicalaire ; Poly(2-hydroxy-4-méthacryloyloxy benzophénone) ; Adsorption.

PC44- Unraveling Metal–Support Interactions in Ni/TiO_2-Modified Bentonite Catalysts for DRM: Insights from In Situ XPS

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Abstract:

Understanding metal–support interactions at the atomic level is crucial for designing stable nickel catalysts for dry methane reforming (DRM). In this work, in situ X-ray photoelectron spectroscopy (XPS) was employed as the primary tool to elucidate the surface and electronic transformations occurring in Ni catalysts supported on natural (Na-Bent) and TiO_2-modified bentonite (TiO_2-Bent) under calcination, reduction, and DRM reaction conditions. Catalysts (15 wt% Ni) were characterized using XRF, XRD, BET, SEM, TPR-H_2, Raman, and in situ XPS. While conventional characterizations revealed expected structural and textural modifications upon TiO_2 incorporation, XPS provided unique insights into the evolution of oxygen species (O 1s), framework elements (Si 2p, Al 2p), titanium (Ti 2p), and nickel (Ni 2p). After reduction, Ti^{4+} partially transforms into Ti^{3+}, generating TiO_{2-x} species with oxygen vacancies. These species migrate toward Ni nanoparticles, forming a thin overlayer that strengthens metal–support interactions and prevents nickel reoxidation during DRM. In contrast, Ni on Na-Bent undergoes significant reoxidation and structural instability, as reflected by pronounced changes in Ni 2p and O 1s spectra after reaction. These surface phenomena directly correlate with catalytic performance: TiO_2-modified catalysts maintain activity and resist coking under concentrated DRM conditions, whereas Na-Bent catalysts deactivate rapidly. This study demonstrates the central role of in situ XPS in revealing dynamic interfacial processes that govern catalyst stability and performance, highlighting TiO_2-modified clays as cost-effective, structurally robust supports for DRM.

Keywords: Dry reforming of methane, Nickel based catalysts, TiO_2- modified Bentonite, In-situ XPS.

PC45- 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, peanutsshells,water.

PC46- Evaluation of the Inhibitory Properties of Glycine Against Copper Corrosion in 1M HNO_3

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TOPIC D: CHEMISTRY OF NATURAL PRODUCTS, ORGANIC SYNTHESIS AND PHARMACEUTICAL CHEMISTRY

Topic D Program

N°	Title	Autors
P_{D1}	Essential Oils of Two Medicinal Plants as Antidiabetic Agents: Phytochemical Characterization and Multiscale Evaluation Through In Vivo, In Vitro, and In Silico Approaches	**Dr. Mohmmed Larbi BENAMOR U-Eloued**
P_{D2}	PIGMENTS NATURELS ET SANTÉ : LES BIENFAITS DES ANTHOCYANES DE LA ROSELLE	**SAIDJI NAWEL ENS KOUBA**
P_{D3}	Perturbations de surface des croûtes biologiques du sol	**BENHAMZA Hayet U-Eloued**

PD4	Nouvelles entités moléculaires issues de la vanilline et de 1,3-dithioles : études structurales, électroniques et biologiques	**Chaima Aouachria U-Tébessa**
PD5	Évaluation in vitro de l'activité d'inhibition de l'α-amylase, de l'α-glucosidase des polysaccharides extraits des fruits de Balanites aegyptiaca Del. récoltés au Sahara algérien	**Dr. Malika SEDDIKI U-Ghardaïa**
PD6	Contribution à l'étude de l'activité antibactérienne du miel naturel d'origine Algérien	**Dr. Ouartsi Nouha U-Annaba**
PD7	Toxicity assessment of phenolic-rich extracts from hawthorn (Crataegus laciniata)	**Naima SAIDENE U-Bejaia**
PD8	Microwave-Assisted Extraction of Bioactive Compounds from Carthamus caeruleus L. Roots: Comparative Efficiency and Antibacterial Activity	**Dr. ISSAADI Halima Meriem U-USTHB**
PD9	Nouveau Dérivé Soufré De La Vanilline : Synthèse, Caractérisation Et Evaluation In Silico De Son Potentiel Antibactérien	**Takoua Belghit U-Tebessa**
PD10	PHYTOCHEMICAL STUDY AND PHARMACOLOGICAL VALORIZATION OF THE GENUS LIMONIUM	**Dr. Badra Bouzghaia U-Batna 2**
PD11	Développement d'une nouvelle formule naturelle pour la cicatrisation des brûlures	**Dr. Faiza SALHI U-Khenchela**
PD12	Phenolic and Lipid Composition of Oilseeds from Southeastern Algeria Nutritional and Biological Insights	**Lahmadi Bechira U-Ourgla**
PD13	Ethnobotanical Study Of medicinal plant Ziziphus spina-christi (jujube)	**Dr. Guediri Imane U-Eloued**
PD14	Eco-Friendly Method of Synthesizing Cinnamic acid by Catalyzed Oxidation Natural Cinnamic aldehyde, Theoretical Study (Docking and DFT)	**Dr. Radia Bouasla HNSTE-Annaba,**
PD15	Efficient Production of Glycerol Monostearate by Biocatalysis using a Lipase from Autochthon Microorganisms	**BOUAZIZ OUALID U-Annaba**
PD16	ISOLATION AND STRUCTURE ELUCIDATION OF ISOFLAVONOÏDS FROM ONONIS MITISSIMA L. AND BIOLOGICAL ACTIVITIES	**Dr. Saliha Besbas U-Batna-1**
PD17	Extraction-guided isolation and preliminary chemical profiling of antimicrobial and antibiofilm metabolites from Streptomyces albidoflavus S19.	**Dr. Samiha SOUAGUI U-Béjaia**
PD18	Evaluation des Activités biologiques d'une plante médicinale	**Bouabdallah Rania Chaima U-setif-1-**
PD19	Phenolic and volatile profiling using HPLC-DAD and GC-MS analyses of an Algerian Auresian Thymus vulgaris with its antioxidant and antimicrobial evaluation	**Nourelhouda Benelmufti U-Constantine 1**
PD20	Chemistry Characterization and In Vitro Evaluation of the Antioxidant and Cytotoxicity Potential of Cyclocybe cylindracea Strain TMES42 (Agaricomycetes) from Algeria	**Dr. TOUMI Mohammed Esseddik U-Constantine 1**
PD21	Synthesis and characterization of organic molecule with antibacterial activity	**Dr. Hanane Berkani U-Khenchela**

PD22	Chemical composition, Epidemiology and Ethnomedicinal Treatment of Urolithiasis in South Western Algeria	**Dr. Sekkoum karima Hopital 240- Bechar**
PD23	PHARMACOLOGICAL EVALUATION OF THE METHANOLIC EXTRACT OF SUAEDA MONODIANA MAIRE: IN VITRO ANTI-INFLAMMATORY, ANTIMICROBIAL, ANTIOXIDANT, AND PHOTOPROTECTIVE PROPERTIES	**Dr. Soumia Mouffouk U-Batna 1**
PD24	EVALUATION OF TOTAL BIOACTIVE CONTENT AND ANTIOXIDANT POTENTIAL OF AN ALGERIAN MEDICINAL PLANT	**Abdelbasset TAMERSIT U-Batna 1**
PD25	COMPLEMENT ALIMENTAIRE A BASE D'UNE PLANTE MEDICINALE	**Dr. Ghanem Hasna U-Batna1**
PD26	Phytochemical study of Phlomis herba-venti L (lamiaceae)	**Dr. Bouzergoune Fouzia U-Batna 1**
PD27	Antioxidant activity and total phenolic and flavonoid contents of Coronilla juncea	**Dr. Kherkhache Hayat U-Djelfa**
PD28	Synthesis and physico-chemical characterization of Schiff bases	**BOUZID Imene U-Setif 1**
PD29	ANTIMICROBIAL AND ANTIOXIDANT EFFECTS OF SPECIES HEDYSARUM PALLIDUM	**Kenza Hazine U-Batna1**
PD30	VALORISATION PHYTOCHIMIQUE ET ANTIOXYDANTE DE CLEMATIS FLAMMULA UTILISEE EN MEDECINE TRADITIONNELLE ALGERIENNE	**LYDIA KAROU U-Bejaia**
PD31	Acetylcholinesterase Inhibitory and Antioxidant Activities of Cold-Pressed Sesame Oil	**Litim Sarra Abdelhafid U-Mila**
PD32	PURIFICATION AND ISOLATION OF A TRITERPENOID FROM A MEDICINAL SPECIES BELONGING TO THE BORAGINACEAE FAMILY	**Djouhaina Makhlouf U-Batna-1**
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PD52	ETUDE DU PROFILE DE LA PLANTE vicia onobrychioides PAR GC-MS ET ESTIMATION DE LEUR ACTIVITIES ANTIOXYDANTE.	**Fatima Belahssini U-Batna1**
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PD54	Profil phytochimique et potentiel biologique de Convolvulus cantabrica L. (Convolvulaceae)	**Dr. Zina ALLAOUA U-BATNA 1**
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PD56	Green Synthesis, In-vitro Antifungal Activities, and Molecular Docking Studies of Pyranopyrazoles Derivatives	**Dr. Boukezzoula Faiza U-Batna 1**
PD57	Etude phytochimique de trois plantes médicinales récoltées dans le Nord Est Algérien (région de Séraidi)	**Prof. Djelloul Radia U-Tarf**

P_{D58}	Biological Evaluation of Novel Nitroaldol-Based Quinoline Compounds as Antimicrobial Agents	**Khelaf Rahima U-Batna 1**
P_{D59}	LCMS-MS ET L'EVALUATION DE L'ACTIVITE ANTIOXYDANTE IN VITRO DE L'EXTRAIT HYDROALCOHOLIC DE LA PLANTE VICIA ONOBRYCHIOIDES	**Fatima BELAHSSINI U-Batna1**
P_{D60}	Isolation of some pentacyclic saponins from scabiosa stellata with in vivo and in silico antifebrile and anti-inflammatory insights	**Dr. Chaima Mouffouk U-Batna 1**
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P_{D62}	Zeolite Based Drug Delivery Systems: Controlled Release of Ibuprofen for Enhanced Therapeutic Efficacy	**BENBEKAI Rima U-Setif 1**
P_{D63}	Pistacia lentiscus Seed Oil as a Natural Anti-Inflammatory Agent: Evidence from In Vitro Assays	**Dr. Kenza Moulaoui U-Bejaia**
P_{D64}	Optimized ultrasonic-assisted deep eutectic solvents extraction of Populus nigra buds, phytochemical screening, biological activities, and MPO inhibition.	**Debbache Benaida Nadjet U-Bejaia**
P_{D65}	Biotechnological potential of marine bacteria from contaminated sites: A case study from the fishing port of Khemisti, Tipaza, Algeria	**Soumia HADJALA U-Blida**
P_{D66}		**Ben Ali Mustapha U-Ouargla**

PD1- Essential Oils of Two Medicinal Plants as Antidiabetic Agents: Phytochemical Characterization and Multiscale Evaluation Through In Vivo, In Vitro, and In Silico Approaches

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Abstract

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

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

PD2- PIGMENTS NATURELS ET SANTÉ : LES BIENFAITS DES ANTHOCYANES DE LA ROSELLE

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Résumé :

Les anthocyanes extraites de la Roselle (*Hibiscus sabdariffa*) sont des pigments naturels appartenant à la famille des flavonoïdes, reconnus pour leurs puissantes propriétés antioxydantes. Elles jouent un rôle essentiel dans la neutralisation des radicaux libres, contribuant ainsi à la prévention du stress oxydatif et des maladies chroniques telles que les maladies cardiovasculaires, le diabète de type 2 et certains types de cancer.

En plus de leurs effets antioxydants, les anthocyanes de la Roselle possèdent des propriétés anti-inflammatoires, antihypertensives et hépatoprotectrices. Elles favorisent également la santé vasculaire et pourraient améliorer la mémoire et les fonctions cognitives.

Grâce à leur stabilité à pH acide, elles sont aussi utilisées comme colorants naturels dans les aliments et les boissons, offrant une alternative saine aux colorants synthétiques.

Ce travail vise extraire des anthocyanes à partir de la Roselle, à évaluer leur éfficacité, et à étudier les conditions influençant leur stabilité.

L'objectif de notre travail était d'améliorer la stabilité de l'extrait d'anthocyanines de fleurs de Roselle en étudiant l'effet des conditions de stockage, de la température et du pH.

Mots clés : Anthocyanes, Roselle, Extraction.

PD3- Perturbations de surface des croûtes biologiques du sol

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Résumé :
Élément important de nombreux écosystèmes arides à l'échelle mondiale est la croûte biologique du sol, une croûte composée de lichens, de cyanobactéries, de mousses et d'algues. Les croûtes sont extrêmement sensibles aux perturbations de surface et aux incendies, et la perturbation des croûtes peut diminuer la fertilité et la stabilité du sol, ce qui entraîne une moindre disponibilité des nutriments pour les plantes vasculaires et une perte de sol importante de l'écosystème. Les taux de récupération naturelle se sont avérés très lents. Toutes les surfaces encroûtées étaient plus stables que le sable nu. De plus, les croûtes de sol précédemment perturbées se sont révélées moins résistantes aux nouvelles perturbations que les croûtes de sol précédemment non perturbées. Ces croûtes organiques sont présentes toute l'année. Pour ces raisons, la gestion des régions arides et semi-arides devraient refléter le rôle important que ces croûtes jouent dans la stabilité de la surface du sol et devraient réduire autant que possible les perturbations de ces croûtes biologiques.

Mots clé : croûtes de sol ; perturbations ; récupération ; surface ; stabilité.

PD4- Nouvelles entités moléculaires issues de la vanilline et de 1,3-dithioles : études structurales, électroniques et biologiques

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Résumé
Dans le présent travail, nous décrivons pour la première fois la réticulation de la vanilline avec divers dérivés 1,3-dithiol-2-thione portant une large gamme de substituants. Cette nouvelle classe originale de molécules 1,3-dithiole dérivées de la vanilline a été obtenue par une méthode de substitution en une seule étape, réalisée en milieu phosphite. Le processus réactionnel implique la désulfuration du 1,3-dithiol-2-thione ainsi qu'un transfert d'hydrogène de la position C5 du 4-hydroxy-3-méthoxybenzaldéhyde vers la position C2' de l'anneau dithiole.

L'identification des nouveaux composés a été assurée par différentes techniques spectroscopiques, incluant l'IR, l'UV-Visible, RMN ^{1}H, RMN ^{13}C ainsi que RMN bidimensionnelle (^{1}H-^{13}C HSQC et HMBC), complétées par la spectrométrie de masse à haute

résolution (HRMS). Leur comportement électrochimique a également été étudié par voltammétrie cyclique. De plus, les structures cristallines ont été confirmées par diffraction des rayons X. L'analyse de la densité électronique totale a permis de localiser les régions électrophiles et nucléophiles.

Ces nouveaux dérivés de la vanilline présentent une activité neuroprotectrice intéressante dans le cadre de la prise en charge de la maladie d'Alzheimer, et révèlent en outre un potentiel antidiabétique notable.

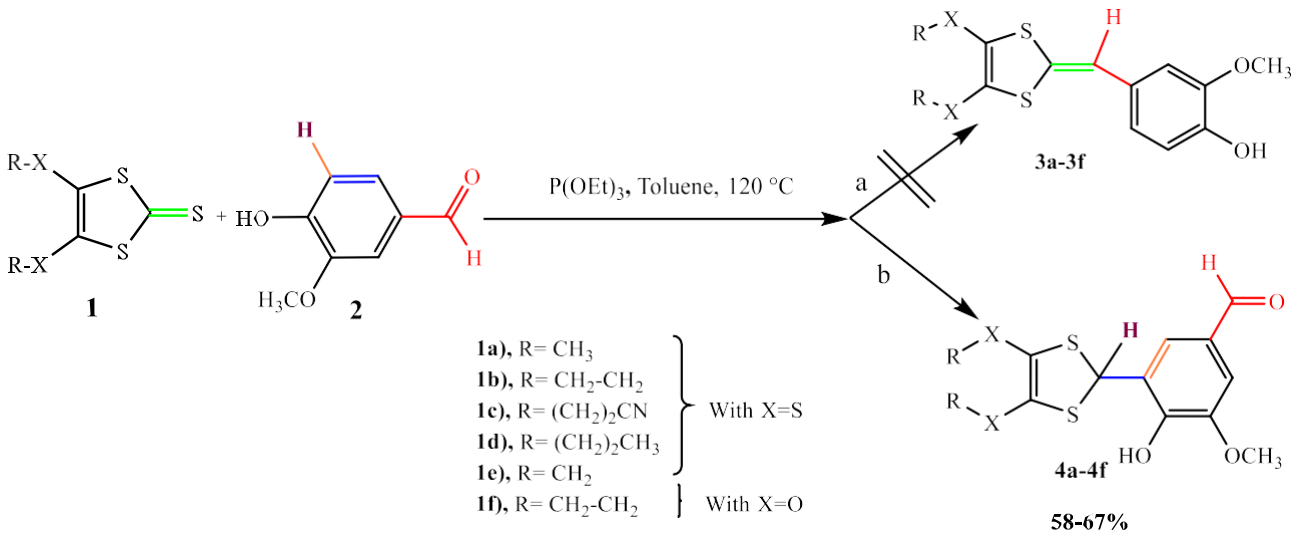

Schéma 1 : Synthèse des molécules cibles. Voie a : composés envisagés 3a-3f ; Voie b : composés obtenus 4a-4f.

PD5- Évaluation in vitro de l'activité d'inhibition de l'α-amylase, de l'α-glucosidase des polysaccharides extraits des fruits de *Balanites aegyptiaca* Del. récoltés au Sahara algérien

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Résumé

La présente étude vise à évaluer *in vitro* l'activité hypoglycémique des polysaccharides hydrosolubles des fruits de *Balanites aegyptiaca* Del. (BA) récoltés dans la wilaya de Tamanrasset.

La caractérisation préliminaire de l'extrait est déterminée par les dosages colorimétriques, FT-IR et GC/SM-EI. Le rendement d'extraction par macération dans l'eau distillée à 60°C est de 2,09 ± 0,12 %. BA présente un taux élevé en oses totaux (85,77 ± 0,21 %) et des teneurs faibles en protéines (7,39 ± 0,06 %) et polyphénols (1,34 ± 0,02 %). Son spectre FT-IR présente les bandes caractéristiques des polysaccharides. L'analyse de GC/SM-EI montre que BA est constitué de 34,06% d'acide galacturonique, 27,82% d'arabinose, 15,63% de galactose, 9,71% de glucose, 7,04% de xylose et de 5,74% de rhamnose. L'évaluation de l'activité hypoglycémique de BA a révélé une inhibition modérée de l'α-glucosidase, atteignant 23,75 % à 10 mg/mL, avec une IC_{50} de 27,117 ± 0,737 mg/mL. Cette activité reste nettement inférieure à celle de l'acarbose (IC_{50} = 1,108 ± 0,006 mg/mL). De même, l'extrait a montré une activité inhibitrice vis-à-vis de l'α-amylase (IC_{50} = 44,132 ± 0,926 mg/mL), bien que significativement plus faible que celle de l'acarbose (IC_{50} = 0,051 ± 0,001 mg/mL).

Mots clés : polysaccharides, *Balanites aegyptiaca,* α-glucosidase, α-amylase, GC/SM-EI.

PD6- Contribution à l'étude de l'activité antibactérienne du miel naturel d'origine Algérien

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Résumé :

Le miel est l'un des produits naturels est très connu pour ses caractéristiques nutritionnelles et thérapeutiques en raison de la grande variété de ses composants et de leur contribution à plusieurs activités biologiques telles que les antioxydants, les antimicrobiens. Le présent travail rapporte sur l'évaluation de l'effet antibactérien de quatre échantillons de miel naturel (miel d'Arbousier, d'Eucalyptus, de Jujubier et de Montagne) aux concentrations de 100, 75, 50 et 25%, récoltés de trois sites du territoire de Skikda. Il s'agit de Filfila, Azzaba et Oum Toub. L'activité antibactérienne des différents échantillons de miel naturel a été testée sur trois bactéries pathogènes, résistantes aux antibiotiques, isolées des infections urinaires et cutanées, à savoir *Escherichia coli, Pseudomonas aeruginosa* et *Staphylococcus aureus.* L'activité antibactérienne a été déterminée par la méthode de diffusion en milieu gélosé.

Les résultats obtenus ont montré que les miels exercent une activité inhibitrice intéressante vis- à-vis des bactéries testées. Cet effet inhibiteur a été constaté pour les quatre échantillons de miel, avec des différences d'un échantillon à un autre et d'une souche bactérienne à une autre. La majorité des miels testés, à une concentration de 50%, ont montré un pourcentage d'inhibition allant de 65 à 75% pour *Escherichia coli*. *Staphylococcus aureus* est le microorganisme le plus sensible aux différents miels testés avec un pourcentage d'inhibition estimé à 98% pour des concentrations de 100% et 75%. Une vaste étude est nécessaire pour prendre en considération les types de miel qui inhibent les souches microbiennes et leur concentration optimale afin de l'utilisé comme antibiotique naturel.

Mots clés: activité antibactérienne, miel naturel, Escherichia coli, Pseudomonas aeruginosa

PD7- Toxicity assessment of phenolic-rich extracts from hawthorn (*Crataegus laciniata*)

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Abstract:

Introduction: Hawthorn (Crataegus spp.) is traditionally used in cardiovascular and metabolic disorders, largely due to its high phenolic content. Despite its therapeutic potential, establishing a safety profile remains essential for pharmaceutical applications. This study aimed to evaluate the acute toxicity of phenolic-rich extracts from Crataegus laciniata leaves.
Materials and Methods: The extract was obtained using ultrasound-assisted extraction. Acute toxicity was assessed by administering a single oral dose of 2000 mg/kg to experimental animals, which were monitored daily for 14 days for mortality and clinical or behavioral signs of toxicity. Blood samples were collected in heparinized tubes, centrifuged, and analyzed for liver function (ALT, AST, ALP, total/direct/indirect bilirubin) and kidney function (urea, creatinine). Histopathological examinations of liver and kidney tissues were also performed.
Results: No mortality or abnormal behavioral signs were observed in treated groups. Biochemical analyses showed no significant alterations in hepatic or renal function markers compared with controls. Histopathological evaluations of liver and kidney confirmed normal architecture, with no evidence of structural damage.
Conclusion: The absence of mortality, behavioral changes, biochemical alterations, and histopathological lesions indicates that Crataegus laciniata leaf extracts are safe at the tested dose. These findings support their potential use as safe natural products in health-promoting and pharmaceutical formulations, while further studies are recommended to assess chronic toxicity and long-term safety.

Keywords: *C.laciniata*, phenolic compounds, Acute toxicity, Histopathology.

PD8- Microwave-Assisted Extraction of Bioactive Compounds from *Carthamus caeruleus* L. Roots: Comparative Efficiency and Antibacterial Activity

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Abstract

The study aimed to develop an eco-friendly extraction method to recover bioactive compounds from traditionally used *Carthamus caeruleus* L. roots by comparing conventional and modern techniques using ethanol as extractive solvent.

Three extraction methods were applied: Microwave-Assisted Extraction (MAE; 3 min at 450 W), Soxhlet extraction (4 h at 60 to 80°C), and cold maceration (72 h at ambient temperature). Extraction efficiency was assessed by extractive yield (%), total phenolic content (TPC), and total flavonoid content (TFC). The optimal extract was then evaluated for its antibacterial activity against gram-negative and gram-positive bacteria via disk method.

The results revealed distinct differences in extraction efficiency and bioactive compound recovery among the methods. MAE achieved a yield of 6.61% in just 3 minutes, slightly lower than Soxhlet (7.10%) and maceration (7.25%), which required significantly longer durations. However, MAE delivered a significantly higher TPC (30.78 ± 0.37 mg GAE/g) than Soxhlet (25.14 ± 0.41 mg GAE/g) and nearly six times that of maceration (5.42 ± 0.51 mg GAE/g). Similarly, MAE-extracted TFC (23.38 ± 0.09 mg QE/g) surpassed Soxhlet (22.39 ± 0.34 mg QE/g) and was more than double that of maceration (9.96 ± 0.04 mg QE/g). The MAE extract demonstrated mild antibacterial activity, showing the largest inhibition zone (24 mm) against *Escherichia coli* ATCC 25922 and the smallest (9 mm) against *Candida albicans* ATCC 10231.

Overall, this study indicated that MAE is a rapid and efficient extraction technique that enhances phenolic and flavonoid compounds recovery by minimizing thermal degradation due to reduced exposure time compared with conventional techniques. Further optimization of MAE parameters is necessary to enhance antibacterial potency and maximize the therapeutic potential of *Carthamus caeruleus* L. root phytoconstituents.

PD9- Nouveau Dérivé Soufré De La Vanilline : Synthèse, Caractérisation Et Evaluation In Silico De Son Potentiel Antibactérien

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Résumé

La vanilline, un composé aromatique oxygéné bioactif, constitue une structure de référence dans la synthèse de dérivés biologiquement actifs [1–3]. Les composés hétérocycliques et notamment leurs dérivés soufrés présentent une importance particulière en raison de leur activité

significative dans les systèmes naturels et synthétiques [4] .
Dans ce travail, un nouveau dérivé de la vanilline, portant un groupement 5,6-dihydro-4H-cyclopentaddithiole-2-yl, a été obtenu par réaction de condensation entre la vanilline et une sélénone en milieu trialkylphosphite, sous irradiation ultrasonore. La structure du composé a été confirmée par spectroscopies IR, RMN ^{1}H et RMN ^{13}C.
En outre, les propriétés ADMET in silico ainsi que les affinités de liaison par docking moléculaire ont été évaluées vis-à-vis de trois protéines cibles essentielles (gyrase B de *S. aureus*, MurE de *E. coli* et bromodomaine BD2 de *C. albicans*). Les résultats, comparés aux ligands de référence B48, SZN et 8HZ, suggèrent que ce nouveau dérivé soufré de la vanilline pourrait présenter un intérêt biologique notable.

Mots clés : Vanillin, 1.3-dithiol-2-selenone, Fonctionnalisation, propriétés ADMET

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PD10- PHYTOCHEMICAL STUDY AND PHARMACOLOGICAL VALORIZATION OF THE GENUS *LIMONIUM*

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Abstract
As part of our research aiming to conduct a literature review on the genus *Limonium*, the bibliographical analysis reveals that *Limonium* is the most dominant genus within the family Plumbaginaceae, with about 600 species, and a high diversity observed in the Mediterranean region.
In Algeria, the genus *Limonium* includes 23 species recorded in the Northeast of the country, of which eight are endemic: *L. gougetianum, L. duriaei, L. gummiferum, L. minutiflorum, L. delicatulum, L. cymuliferum, L. ramosissimum,* and *L. tunetanum*.
Phytochemical studies carried out on *Limonium* have highlighted a very diverse reservoir of secondary metabolites; the main compounds isolated from this genus are phenolic compounds,

notably flavonoids of the myricetin and quercetin types, as well as their glycoside derivatives, and phenolic acids such as gallic acid. These molecules are considered chemotaxonomic markers of the genus *Limonium*.
The richness in secondary metabolites of *Limonium* species is manifested by a diversity of pharmacological activities, notably antioxidant activity attributed to phenolic compounds, as well as antimicrobial, enzymatic, anticancer, and other activities. This pharmacological valorization helps to explain the use of these plants in traditional medicine.

Keywords : Limonium, Plumbaginaceae, flavonoids , antioxidant activity, antimicrobial activity.

PD11- Développement d'une nouvelle formule naturelle pour la cicatrisation des brûlures

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Résumé

Les plantes médicinales et les traitements naturels utilisés dans le soin des plaies ont démontré leur efficacité et constituent de véritables alternatives aux produits pharmaceutiques de synthèse, souvent associés à des effets secondaires indésirables. Les composés bioactifs présents dans les plantes médicinales favorisent la cicatrisation des plaies et la régénération tissulaire grâce à des mécanismes d'action spécifiques.
Cette étude, fruit d'une innovation développée par les chercheurs du laboratoire **ISMA**, vise à élaborer une pommade originale composée à 100 % d'ingrédients naturels. Chacun des constituants de cette préparation a montré une activité significative dans le traitement des plaies et la réduction des cicatrices cutanées.
L'hydrodistillation a été employée pour l'extraction des huiles essentielles. Divers tests physico-chimiques ont ensuite été réalisés sur les huiles extraites, notamment la détermination du rendement, des caractéristiques organoleptiques, l'analyse en CCM, la mesure du pH, de la densité, de l'indice de réfraction, ainsi qu'une analyse spectroscopique FTIR.
La partie aérienne de la plante médicinale a été utilisée pour les analyses phytochimiques. Les tests réalisés sur la poudre végétale ont confirmé la présence de plusieurs familles de métabolites secondaires, dont des huiles essentielles, tanins, stérols insaturés, terpènes, cardénolides, saponines, alcaloïdes et flavonoïdes.
Le principe actif a été isolé par macération à froid pendant 96 heures. L'évaporation sous vide de la solution obtenue a permis d'extraire une substance huileuse (rendement : 4,72 %), constituant l'ingrédient actif principal de la pommade.
Enfin, la pommade a été formulée par fusion en utilisant plusieurs substances naturelles, afin d'obtenir une texture homogène et stable.

Mots-clés : Pommade innovante, *plant médicinal*, huile de *Pistacia lentiscus*, cicatrisation des plaies, réduction des cicatrices.

PD12- Ethnobotanical Study Of medicinal plant Ziziphus spina-christi (jujube)

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Abstract:

Our study aims to document local knowledge related to the use of medicinal plants in the treatment of skin inflammations and allergies in the El Oued region, in light of the lack of sufficient scientific studies on the effectiveness of these plants and their methods of use.

The study sought to identify the most commonly used plant species, the parts of the plants employed, and the common methods of preparation and application among the local population.

From this study, we identified a wide range of medicinal plants used by people in the region to treat skin allergies and inflammations. We selected most frequently cited plants:

- Ziziphus spina-christi (jujube)

Based on this, we developed a questionnaire on the use of these plants and distributed 100 copies across various population groups. The study spanned two months, during which the results revealed a rich body of traditional knowledge that has been orally transmitted across generations, along with a strong reliance on certain plants known for their traditional effectiveness.

Keywords: Medicinal plants, skin allergies and inflammations, herbs, El Oued, jujube (Ziziphus spina-christi).

PD13- Eco-Friendly Method of Synthesizing Cinnamic acid by Catalyzed Oxidation Natural Cinnamic aldehyde, Theoretical Study (Docking and DFT)

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Abstract

Cinnamaldehyde is a naturally occurring organic compound responsible for the

characteristic flavor and aroma of cinnamon. It is the primary constituent of cinnamon bark oil, particularly from species such as *Cinnamomum verum* and *Cinnamomum cassia*. Chemically, it belongs to the class of aromatic aldehydes. Cinnamaldehyde is widely utilized in the food, fragrance, and cosmetic industries. Beyond its sensory properties, it also demonstrates various biological activities including antimicrobial, antifungal, and antioxidant effects making it a compound of significant interest in both traditional medicine and modern scientific research.
In our study, *Cinnamomum zeylanicum* essential oil (EO) was extracted using hydrodistillation, a widely adopted and environmentally friendly technique. The separation and purification of the active constituent of *C. zeylanicum* were initially performed using silica gel column chromatography.

In this work, our synthesis strategy is based by hemisynthetic reaction conducted under environmentally friendly conditions. The oxidation of cinnamaldehyde was carried out in the presence of ethanol with concentrated sulfuric acid as catalysts assisted by ultrasonic waves. The structure of the compound was characterized using X-ray diffraction and NMR spectroscopy.

Keywords: Cinnamon, Cinnamaldehyde, Cinnamic Acid, Essential oil, Ultrasonic Irradiations, Oxidation

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PD14- Efficient Production of Glycerol Monostearate by Biocatalysis using a Lipase from Autochthon Microorganisms

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ABSTRACT

Enzymes are highly efficient biological catalysts of protein nature, endowed with great functional specificity. They are essential components of many industrial processes, such as the production of detergents and pharmaceuticals[1]. Among enzymes, lipases were considered as a great biotechnological and industrial catalyst after carbohydrases and proteases[2]. Due to their selectivity and specificity lipases as biocatalyst offer a useful way of synthesizing highly purified single fatty acid containing monoglycerides (MGs)[3]. In order to improve the selectivity of glycerol monoesterification, synthesis by enzyme catalysis was attempted as an alternative synthesis method[4]. The present study reports an enzymatic synthesis of GMS using lipase from a thermophilic Actinomycete strain Cpt29 isolated from chicken compost collected from a local farm in northeast of Algeria. For maximum GMS production several reaction parameters (substrate molar ratio, solvent effect, reaction time and enzyme load) were studied. The autochthon extracellular lipase resulted in significant production of GMS in organic medium where upper than 90% conversion of stearic acid was achieved. A 2.2-fold increase in GMS production was recorded under the optimal reaction parameters compared to the literature.

Keywords: Lipase, Monoglycerides, Actinomycetes, Esterification.

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PD16- Isolation and structure elucidation of isoflavonoïds from *Ononis mitissima* L. And biological activities

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Abstract

The genus *Onions* L. is one of the most important genera of the family Fabaceae, with about of 75 species distributed mainly in Mediterranean region, Canary Islands, Europe and Central Asia. The species *O. mitissima* is an annual plant, erect or ascending, glabrescent, not spiny. It is very common in the Mediterranean region of Europe, Asia and Africa. The present work describes the isolation and structure elucidation of two isoflavonoïds namely: formononetin (1) ononin (2) and a new one named formononetin -7-O-[*S*-3-hydroxy-3-methylglutaryl-(1→6)]-β-D-glucopyranoside (3) (Figure 1). The separation process for these compounds was based on chromatographic methods (VLC, TLC and CC) and structural elucidation by modern methods of spectroscopic analysis (NMR, high resolution mass spectrometry HR-ESI-MS, measurement of the optical rotation $[\alpha]_D^{20}$) and by comparison with data from the literature. In the biological part of this work, we have evaluated the antioxidant activity of the crude extracts (PE, EtOAc and *n*-BuOH) by three different methods including scavenging of the free radical DPPH, ferric reducing antioxidant power and total antioxidant capacity and the anti-inflammatory activity was studied by the egg albumin denaturation method. The results of antioxidant activity by DPPH showed that the EtOAc extract exhibited a greater antioxidant capacity than those of PE and *n*-BuOH extracts with an IC50 27.3 ± 0.015 µg/mL, compared to the BHT as a reference (22.32 ± 0.02). In addition, the EtOAc extract displayed the highest antioxidant activity, in ferric reducing antioxidant power and total antioxidant capacity with values of 122.23 ± 0.014 and 16.44 ± 0.0012 µg EAA/mg ex compared to the results of *n*-BuOH and PE extracts. All the tested extracts had moderate anti-inflammatory activity with the percentages of inhibition at 21.96, 33.41 and 11.48 % respectively, compared to diclofenac (86,72 %).

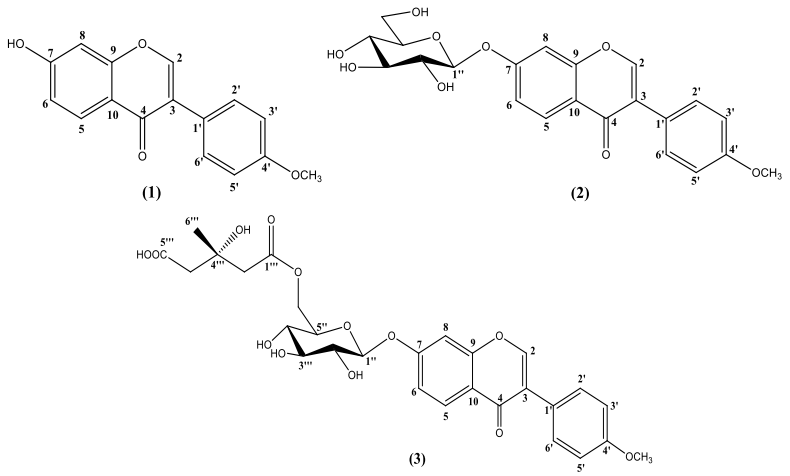

Figure 1: Structures of isolated compounds.

Keywords: *Ononis mititssima* L., Isoflavonoïds, Antioxidant activity, anti-inflammatory activity.

PD17- Extraction-guided isolation and preliminary chemical profiling of antimicrobial and antibiofilm metabolites from *Streptomyces albidoflavus* S19.

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Abstract:

Extraction-guided fractionation of *S. albidoflavus* S19 revealed multiple bioactive metabolites across bacteria and fungi, with UV–Vis excluding polyene signatures and HPLC-DAD indicating at least ten chromatographic entities under reversed-phase elution. SPE-enriched fractions (notably 50% acetonitrile) retained activity against *E. coli, V. cholerae,* MRSA, and *Candida albicans*, facilitating LC–MS annotation of ions at m/z 559, 1025, 1086, and 1085 that tentatively align with known *Streptomyces* metabolites in databases but remain unassigned pending further purification and structure elucidation by NMR and high-resolution MS workflows typical of modern dereplication. The extract demonstrated antibiofilm efficacy against *Staphylococcus aureus* strains LGA 251, FRI 56, and ATCC 29213 with biofilm reductions of 64%, 56%, and 47% at 9 mg/L, and against *P. aeruginosa strains* P.a 893 and P.a 258 with 66% and 40% reductions at 18.5 mg/L, respectively, complementing planktonic inhibition data. Total phenolics were 12.22 ± 0.04 mg GAE/g extract and flavonoids 1.45 ± 0.062 mg/g, with antioxidant capacities of ABTS IC*50 of* 6.68 *mg/ml and DPPH IC*50 of 25.16 mg/ml, supporting multiparametric chemical and pharmacological characterization.

Keywords: Natural products chemistry**;** Dereplication and LC–MS**;** Antibiofilm metabolites; non-polyenic antifungals; Phenolics and flavonoids

PD18- Evaluation des Activités biologiques d'une plante médicinale

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Résumé :

Évaluation du potentiel biologique de l'extrait hydrosoluble des parties aériennes de la plante appartient à la famille Myrtaceae à conduits des résultats intéressante notamment activité antibactérienne par méthode de diffusion sur gélose donne des résultats significatifs avec une concentration de 250µg/mL . De même, l'activité antifongique a été testée sur différentes souches fongiques donne des zones d'inhibition importantes de (11-28mm). L'ensemble des tests réalisés met en évidence une efficacité significative d'extrait contre les micro-organismes bactériens et fongiques, suggérant une action antimicrobienne polyvalente et prometteuse pour des applications biomédicales.

Mots clé : Myrtaceae, antibactérien, antifongique, gélose, applications biomédicales

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PD19- Algerian Auresian Thymus vulgaris with its antioxidant and antimicrobial evaluation

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Abstract

The current study aimed to analyze the chemical profile of Thymus vulgaris gathered from the Aurès zone using HPLC-DAD and GC-MS methods, as well as to assess its antioxidant and antimicrobial properties. The essential oil (TVEO) and methanol extract (TVME) yielded 0.5% and 6.7%, respectively. The GC-MS analysis determined 76 volatile chemicals, with eucalyptol

(11.14%), α-terpinyl acetate (9.62%), (+)-2-bornanone (8.96%), 1R-α-pinene (8.74%), ledol (6.43%), and α-gurjunene (5.92%) being the main components. The HPLC-DAD profile revealed the presence of 18 compounds, with epicatechin (75.22 mg/g), caffeic acid (4.31 mg/g), luteoline-7- glucoside (2.11 mg/g), apeginin-7-glucoside (1.84 mg/g), naringenin (1.26 mg/g), and tyrosol (1.03 mg/g) being the main ingredients. TVME contained polyphenols and flavonoids (77.6 ± 0.9 µg GAE/mg and 107.36 ± 27.56 µg QE/mg, respectively) with moderate antioxidant (2.94 ± 0.04 mg/ml and 34.03 ± 0.13%) and antimicrobial capabilities (9.08 ± 1.66 mm). In fact, (+)-2-bornanone, α-gurjunene, ledol, luteoline-7-glucoside and tyrosol were determined for the first time in T. vulgaris with high levels.

Keywords: HPLC-DAD, GC-MS, antioxidant activity, antimicrobial activity.

PD20- Chemistry Characterization and In Vitro Evaluation of the Antioxidant and Cytotoxicity Potential of *Cyclocybe cylindracea* Strain TMES42 (Agaricomycetes) from Algeria

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ABSTRACT: Edible and medicinal mushrooms are a rich source of nutrients and chemical substances with several interesting therapeutic activities such as anti-diabetic, antimicrobial, anti-obesity, immunomodulation, and anti-cancer activities. In the present study, we examined the medicinal and chemical properties of an Algerian mushroom *Cyclocybe cylindracea* strain TMES42. Different extracts were obtained from sequential liquid-liquid extraction using three solvents of increasing polarity (chloroform, ethyl acetate and butanol). Antioxidant potential was

evaluated using different methods (DPPH, ABTS, FRAP, and phenanthroline assays). The phenolic composition of acetate-ethyl-extract (AcEt-Ext) was characterized under LC-ESI-MS-MS analysis, and the antiproliferative effect was determined against the breast-maligned cell line MCF-7. Results demonstrated that the studied mushroom has a promising cytotoxic activity. Its AcEt-Ext fraction showed significant antioxidant activities as well as high phenolic acid and total phenolic content compared with other fractions. This fraction induced breast malignant cell cytotoxicity, exhibiting an IC_{50} value of 59.84 ± 4.06 µg/ml, and demonstrated a significant selectivity index; these findings suggest that *C. cylindracea* could be regarded as a promising natural therapeutic agent.

KEY WORDS: *Cyclocybe cylindracea* strain MEST42, medicinal mushrooms, bioactive compounds, antioxidant, LCESI-MS/MS, cytotoxic activity.

PD21- Synthesis and characterization of organic molecule with antibacterıal activity

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Abstract:

The preparation of the Schiff base was finished from condensation reaction between acetophenone and sulfamerazine. The mixture was left under reflux for 2 hours. After cooling in at room temperature; the mixture was cooled in an ice bath for a few minutes. After a few days; crystals shaped needles have been obtained.The FTIRspectrophotometer Perkin Elmer recorded the spectra within the range of 4000 to 400 $cm^{-1}$was used to confirm the structure of the obtained compound. The FTIR spectra typically showed a characteristic peak in 1636 cm^{-1} which is indicative of the C=N group. The antibacterial efficacy of this compound was also tested on two different types of bacteria *Escherichia coli* and *Saccharomyces cerevisiae* using disc diffusion method. The Schiff base derivative showed a good efficiency for all types of tested bacteria strains. The obtained compound could be used as a good antibacterial agent.

Keywords: Schiff base, infrared spectroscopy, biological effect, bacterium, structural stud

PD22- Chemical composition, Epidemiology and Ethnomedicinal Treatment of Urolithiasis in South Western Algeria

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***Abstract*:**
Urolithiasis is painful urological disorder due to the formation of stones in the urinary system and influenced by several factors such as: epidemiological, biochemical and genetic. In Algeria, is one of the most common diseases and constitute a public health and is largely influenced by the quality of drinking water, diet and climatic conditions.
The aim of the present study is to analyze the epidemiological data (age and sex) on urinary stones, the medicinal plants used in the management of urolithiasis in two regions of south western Algeria (El Bayadh and Bechar) and to evaluate the percentage of the stone type according to chemical composition obtained by morph-constitutional analysis by IRTF of urinary stones collected from patients of these regions.
The results of the epidemiological investigation showed a large predominance in male gender and then most calculus were located in the upper urinary tract. Calcium oxalate stones represent the main form of urolithiasis, affecting males more than females. Our ethnomedicinal analysis revealed that the local population use of various medicinal plants, either as mixtures or as single plant extracts, particularly to the management of pain caused by urolithiasis.

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PD23- PHARMACOLOGICAL EVALUATION OF THE METHANOLIC EXTRACT OF SUAEDA MONODIANA MAIRE: *IN VITRO* ANTI-INFLAMMATORY, ANTIMICROBIAL, ANTIOXIDANT, AND PHOTOPROTECTIVE PROPERTIES

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Abstract

Plants are valuable sources of bioactive metabolites with promising therapeutic potential. These natural compounds are of great interest due to their strong antibacterial, anti-inflammatory, antioxidant, and wound-healing properties, even at low concentrations, without causing toxicity or adverse effects. Their multiple pharmacological properties can also improve therapeutic outcomes and promote faster healing. This study examines the biological activities of the methanolic extract obtained from *Suaeda monodiana*. The antioxidant activity was evaluated using five different assays, and the sun protection factor (SPF) was determined. Hemostatic activity was assessed by measuring plasma recalcification time, while the anti-inflammatory effect was investigated through heat-induced hemolysis and albumin denaturation tests. Furthermore, antimicrobial activity was tested using the agar disc diffusion method against seven microbial strains. As a result, the tested extract has a rich chemical composition and possesses interesting photoprotective (SPF at 46.49±0.05) and antioxidant activities. The crude extract significantly shortens the clotting time and inhibits the growth of all the tested strains with minimum inhibitory concentrations ranging between 31.25 to 250 µg/mL. Moreover, this extract showed the ability to inhibit protein denaturation (IC_{50} at 1.22±0.8 mg/mL) and to protect the erythrocyte membrane (IC_{50} at 2.39±0.3 mg/mL). Furthermore, the species *S. monodiana* could be used in pharmaceutical formulations for the treatment of several diseases due to its interesting biological properties.

Keywords: *Suaeda monodiana*, antibacterial, anti-inflammatory, antioxidant, and wound healing.

PD24- EVALUATION OF TOTAL BIOACTIVE CONTENT AND ANTIOXIDANT POTENTIAL OF AN ALGERIAN MEDICINAL PLANT

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Abstract

The present study focuses on quantifying total bioactive content and evaluating antioxidant activity in crude extracts from an Algerian medicinal plant. The levels of terpenoids, flavonoids and phenolic compounds in the crude extracts were determined using standardized spectrophotometric assays, whereas antioxidant activity was assessed through various *in vitro* methods, including ferric reducing antioxidant power (FRAP), total antioxidant capacity (TAC), iron chelation, and CUPRAC assays. The results showed that the *n*-butanolic extract had the highest total phenolic content (422.6 µg GAE/mg) and total flavonoid content (103.82 ± 0.23 µg QE/mg), followed by the ethyl acetate extract. In contrast, only the petroleum ether extract contained detectable levels of terpenoids (26.16 µg EUA/mg). Additionally, all tested crude extracts displayed significant antioxidant activities across all assays. The *n*-butanol extract demonstrated the strongest reducing

power ($A_{0.5}$ = 3.75 ± 0.20 µg/mL), exceeding the activities of all reference standards (BHA, BHT, and ascorbic acid). Overall, these findings emphasize the promising antioxidant activity of this Algerian medicinal plant, especially in its polar fractions, and support its potential as a valuable natural source of bioactive compounds.

Keywords: Medicinal plant, Total bioactive content, Antioxidant activity.

PD25- COMPLEMENT ALIMENTAIRE A BASE D'UNE PLANTE MEDICINALE

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Résumé

Depuis de nombreuses années, les plantes médicinales jouent un rôle très important dans la médecine et la pharmacologie. Aujourd'hui, on estime qu'environ 80% de la population mondiale repose sur des préparations botaniques comme médicaments pour répondre à leurs besoins de santé.

L'etude présentée dans ce travail a porté sur une éspèce de la famille Cupressaceae ainsi que l'étude de ces utilisations traditionnelles et la préparation des gélules en poudre à partir de cette plante et ces bienfaits pour le système digestif. Cette espèce est trés répondus en Afrique du Nord (Algérie, Maroc et Tunisie). En effet, les éspèces de ce genre sont très utilisées en médecine traditionnelle Algérienne pour traiter diverses maladies tels que les maladies de peau et d'estomas.

Mot clé : Pharmacologie; Cupressaceae; plante médicinale.

PD26- Phytochemical study of *Phlomis herba-venti L* (lamiaceae)

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Abstract

Phlomis herba-venti L, belonging to the Lamiaceae family, is a medicinal plant traditionally used for its anti-inflammatory, antioxidant, and antimicrobial properties. In this

study, a phytochemical investigation was carried out on the aerial parts of *Phlomis herba-venti* to identify and isolate its major constituents. Successive extraction with solvents of increasing polarity followed by chromatographic purification of the diethyl ether extract led to the isolation of two compounds: a sterol, **stigmasterol**, and an iridoid, **lamiide**. Their chemical structures were elucidated using spectroscopic methods, including 1D NMR of proton (1H) and carbon (13C), as 2D NMR experiments such as COSY (proton-proton correlations), HSQC, and HMBC. Their structures were also confirmed by mass spectrometry (ESI-MS).

Preliminary phytochemical screening also revealed the presence of flavonoids, phenolic compounds, and terpenoids. The isolation of stigmasterol and lamiide confirms the chemical richness of *phlomis herba-venti* and supports its traditional medicinal uses. These findings contribute to the valorization of this species as a potential source of bioactive natural products with pharmacological interest.

Keywords: *phlomis herba*-venti, phytochemical study, stigmasterol, lamiide, natural compounds, Lamiaceae.

PD27- Antioxidant activity and total phenolic and flavonoid contents of *Coronilla juncea*

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Abstract

The aim of this work is the investigation of the antioxidant activity, total phenolic and flavonoid contents of different parts of *Coronilla juncea* L. extracts (seeds, flowers, stems and roots). In The antioxidant activity was evaluated using three different assays. In 2,2- diphenyl-1-picrylhydrazyl (DPPH) radical and phosphomolybdate assays, flowers exhibited a remarkable inhibitory effect (EtOAc extract half maximal inhibitory concentration (IC50) = 62.25 ± 0.35 and *n*-BuOH extract 80.23 ± 3.73 µg/mL) followed by stems extracts (*n*-BuOH extract IC50 = 71.03 ± 4.20 µg/mL) in DPPH assay and by seeds (*n*-BuOH extract IC50 = 88.03 ± 3.70 µg/mL) in phosphomolybdate assay. Compared with other parts of *C. juncea*, seeds extracts showed also the best generation of superoxide anion (EtOAc extract IC50 = 100.25 ± 1.55 µg/mL) followed by flowers (*n*-BuOH extract IC50 = 113.73 ± 3.89 µg/mL).To the best of our knowledge, this

investigation reported for the first time the quantification of phenolic and flavonoid contents and assessed the antioxidant activity of four different parts of *Coronilla juncea*, indicating its potential application in therapeutic purposes.

PD28- Synthesis and physico-chemical characterization of Schiff bases

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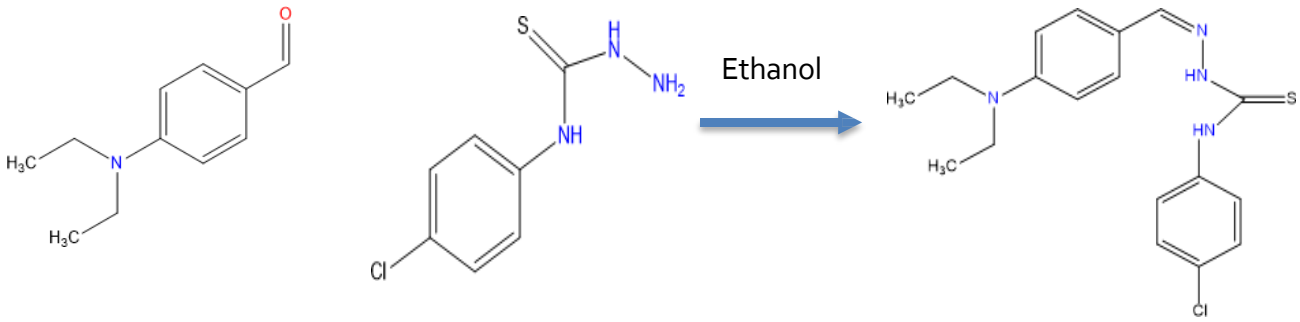
Abstract

Schiff bases are synthesized through a condensation reaction between substituted primary amines and substituted aromatic aldehydes or ketones. They constitute an important class of organic compounds with significant medicinal and pharmaceutical relevance. Many synthetic organic analogues contain imine groups, which are notable for their wide range of applications in organic, biological, medicine, and analytical chemistry [1–3]. Schiff bases and their analogues, particularly those containing a sulfur atom, exhibit diverse biological and pharmacological activities, including antimicrobial, anti-inflammatory, anticancer, antioxidant, and antidiabetic properties [4]. In this perspective, we synthesized the compounds following the sequence according to the sequence below.



Keywords: Synthesis, Schiff bases.

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PD29- ANTIMICROBIAL AND ANTIOXIDANT EFFECTS OF SPECIES *HEDYSARUM PALLIDUM*

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Abstract

Bioactive molecules and plant-derived extracts have gained growing interest in the pharmaceutical industries owing to their protective roles against microbial and oxidative stress-mediated pathologies. In this context, the present study evaluates the antioxidant and antimicrobial effects of the species *Hedysarum pallidum*, belonging to the Fabaceae family, which is widely employed in traditional medicine to treat several viral, inflammatory, and infectious disorders. The quantification of the total terpenoids, flavonoids, and phenolic contents was carried out using several colorimetric methods. The antimicrobial activity was evaluated by the agar disk diffusion assay against seven microbial strains, and the antioxidant activity was assessed using two different techniques, including the DPPH radical scavenging effect and reducing power assay. The results revealed the richness of this species in many classes of secondary metabolites, such as flavonoids, saponins, tannins, and coumarins, which contribute to its pharmacological activities. The butanolic extract demonstrated a significant DPPH radical scavenging effect and ferric-reducing power, indicating its potential antioxidant capabilities. And possesses moderate antimicrobial effects against the clinical strains *Enterobacter sp, Streptococcus D and E.coli.* Furthermore, it can be concluded that the species *H.pallidum* may represent a promising source of antimicrobial and antioxidant molecules.

Keywords: *H.pallidum*, antimicrobial, antioxidant, flavonoids.

PD30- Valorisation phytochimique et antioxydante de *clematis flammula* utilisée en medecine traditionnelle algerienne

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ABSTRACT

Clematis flammula (C. flammula), plante de la famille des Ranunculaceae, est largement utilisée en médecine traditionnelle en Algérie pour ses propriétés thérapeutiques. Cette étude vise à analyser son extrait hydro-alcoolique à travers une caractérisation phytochimique (UPLC-ESI-MS/MS), minérale (XRF) et une évaluation de l'activité antioxydante [1 ;2] (DPPH et ABTS). L'analyse a permis d'identifier plusieurs composés phénoliques, dont des flavonoïdes (quercétine, lutéoline, rutine, myricétine…), des acides phénoliques (caféique, férulique, salicylique…) ainsi qu'un stilbène (resvératrol). L'extrait s'est également révélé riche en minéraux essentiels comme le calcium, le magnésium et le fer. Par ailleurs, une forte activité antioxydante a été observée, avec des valeurs de CI_{50} de 0,100 ± 0,003 mg/mL (DPPH•) et 0,089 ± 0,004 mg/mL (ABTS•+). Ces résultats mettent en évidence la richesse de *C. flammula* en composés bioactifs, soulignant son potentiel en tant qu'agent antioxydant à usage nutritionnel ou thérapeutique.

Keywords: *Clematis flammula,* Caractérisation, UPLC-ESI-MS/MS, XRF, Activité antioxydante.

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PD31- Acetylcholinesterase Inhibitory and Antioxidant Activities of Cold-Pressed Sesame Oil

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Abstract :

Cold-pressed vegetable oils are increasingly recognized for their nutritional and therapeutic potential due to their retention of natural bioactive compounds such as tocopherols, phytosterols, and lignans. The present study aimed to evaluate both the acetylcholinesterase (AChE) inhibitory activity and antioxidant potential of cold-pressed sesame oil, comparing its performance with the standard inhibitor galantamine and synthetic antioxidants including BHA, BHT, and α-tocopherol. The AChE inhibitory activity of cold-pressed sesame oil was assessed at concentrations ranging from 3.125 to 200 µg/mL. The oil demonstrated a moderate inhibitory effect, with values increasing from 20.86 ± 0.34% to 50.72 ± 0.31%, and an IC_{50} of 186.29 ± 2.36 µg/mL. In contrast, galantamine, used as a positive control, exhibited significantly higher inhibition levels, reaching 94.77 ± 0.34% at 200 µg/mL with an IC_{50} of 6.27 ± 1.15 µg/mL. These results suggest that cold-

pressed sesame oil possesses mild acetylcholinesterase inhibitory activity, potentially attributed to its bioactive components such as sesamin, sesamolin, and tocopherols, which may interact with the enzyme's active site.

To further assess the bioactivity of the oil, its antioxidant capacity was measured using ABTS and DPPH radical scavenging assays. The oil showed a concentration-dependent increase in activity, with ABTS inhibition ranging from 7.45% at 12.5 µg/mL to 19.95% at 800 µg/mL, and DPPH inhibition from 3.68% to 16.01% over the same range. However, the oil did not achieve 50% inhibition in either assay, resulting in IC_{50} values above 800 µg/mL. By comparison, synthetic antioxidants demonstrated significantly stronger activity, with IC_{50} values of 6.14 µg/mL (BHA), 12.99 µg/mL (BHT), and 13.02 µg/mL (α-tocopherol).

The relatively low radical scavenging ability of sesame oil is likely related to the limited solubility of its lipophilic constituents in aqueous systems used for these assays. Despite this limitation, cold-pressed sesame oil retains compounds known to exert antioxidant effects in vivo through mechanisms such as lipid peroxidation inhibition and reactive oxygen species modulation.

Overall, the findings demonstrate that cold-pressed sesame oil exhibits moderate AChE inhibitory and weak in vitro antioxidant activities, suggesting that its bioactive potential may be more pronounced in biological systems rather than in chemical radical assays. Future studies should employ lipid-phase antioxidant models, investigate in vivo neuroprotective mechanisms, and explore synergistic combinations with other natural extracts to enhance its functional efficacy.

Keywords:

Cold-pressed sesame oil, acetylcholinesterase inhibition, galantamine, antioxidant activity, ABTS, DPPH, neuroprotection, IC_{50}.

PD32- PURIFICATION AND ISOLATION OF A TRITERPENOID FROM A MEDICINAL SPECIES BELONGING TO THE BORAGINACEAE FAMILY

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Abstract

Boraginaceae family, commonly known as borage family comprises approximately more than 140 genera and 2000 species widely distributed in temperate regions. The species of this family possess a wide range of secondary metabolites, mainly flavonoids, phenolic acids, triterpenoids, and alkaloids, which contribute to their diverse biological activities such as antioxidant and

antimicrobial. In the aim of this study, we are interested in the phytochemical investigation of the plante *Moltkia ciliata*. The species was collected and dried, then macerated in the solvent mixture (Ethanol-H_2O/70:30) for 72 h at room temperature. After filtration, a liquid/liquid extraction was realized by organic solvents with increasing polarity namely petroleum ether (PE), ethyl acetate (EtOAc) and *n*-BuOH and concentrated to dryness to get three extracts. Furthermore, a phytochemical screening was realized by different protocols and reagents where the results indicated the presence of several bioactive compounds. The purification of the Oleanolic (triterpenoid) was achieved by using different chromatographic techniques such as column chromatography (SiO_2), thin layer chromatography and the structure was elucidated by spectroscopic analysis, including 1D NMR and 2D NMR. Moreover, the isolation and identification of this triterpenoid are reported from *Moltkia ciliata* for the first time.

Keywords: Boraginaceae, Phytochemical screening, Triterpenoid, Chromatography, NMR

PD33- Synthesis and Theoretical Evaluation of a New *α*-aminophosphonate Derivative

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Abstract

The development of novel bioactive compounds remains a major focus in modern organic and pharmaceutical chemistry. In this study, a new α-aminophosphonate derivative was synthesized through a Kabachnik-Fields reaction. Density functional theory DFT was employed to investigate their molecular geometry and electronic features, providing insight into their reactivity and stability. Molecular docking studies using Autodock Vina were then performed to predict their possible interactions with a pharmacologically relevant protein and to estimate binding affinities. In addition, in silico ADME analyses were carried out to evaluate the pharmacokinetic and drug-likeness properties. The obtained results indicate that the synthesized compound possesses promising biological potential and could be considered as a candidate for further investigation.

Keywords: Synthesis, α-aminophosphonic acid, DFT calculations, molecular docking.

PD34- CARACTERISTIQUES GEOTECHNIQUES ET GEOCHIMIQUE D'UN GISEMENT PLOMBO-BARYTE : MINE SOUTERRAINNE D'ICHEMOUL_WILAYA DE BATNA

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Résumé

Ce travail porte sur l'étude géotechnique et géochimique d'un site minier souterrain de plombo-barytine situé à Ichmoul, dans la wilaya de Batna. L'objectif est de caractériser la nature des formations encaissantes, les propriétés géotechniques des roches, ainsi que leur composition chimique afin de fournir une évaluation complète du potentiel de ce gisement.

L'approche adoptée repose sur des observations de terrain (relevés géologiques, échantillonnage), des analyses en laboratoire (pétrographie, essais géotechniques) et une analyse chimique par fluorescence X (XRF).

Les investigations géologiques ont révélé la complexité de la structure du gisement, avec une minéralisation concentrée dans les calcaires dolomitisés d'âge Albo-Aptien, et une forte fracturation due à la genèse du pli anticlinal.

Les analyses minéralogiques ont confirmé la présence de barytine associée à la dolomite et à la galène, avec des textures variées et des signes d'altération, soulignant l'hétérogénéité de l'environnement géologique.

Les analyses chimiques, notamment par XRF, ont attesté de la haute pureté de la barytine d'Ichemoul, bien que légèrement inférieure aux normes API pour une utilisation directe dans le forage sans traitement préalable. La présence de minéraux accessoires et d'éléments traces témoigne de la complexité géologique du gisement et nécessite une approche de traitement adaptée.
Les études géotechniques ont mis en évidence une hétérogénéité significative des matériaux, avec des variations importantes des caractéristiques mécaniques. La bonne compacité et résistance des formations calcaires et marneuses assurent une stabilité générale des excavations souterraines, mais la présence de zones de fragilité et de sols compressibles nécessite un suivi rigoureux et des mesures de soutènement appropriées.
L'évaluation des méthodes d'exploitation a confirmé l'efficacité des techniques de chambre et pilier et d'exploitation par tranchée pour l'extraction du minerai.

Mots-clés : barytine, galène, mine souterraine, géotechnique, Ichmoul , XRF.

PD35- The quantification of some secondary metabolites and in vitro anti-inflammatory effect of a plant belonging to the genus Centaurea

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ABSTRACT

The genus *Centaurea* of the family Asteraceae is common throughout the globe. It has more than 600 species, among which 42 species grow spontaneously in Algeria. Species belonging to this genus are used in folk medicine to treat various diseases, such as diarrhea, diabetes, rheumatism, malaria, hypertension, and tonics. Most of the therapeutic and pharmaceutical properties of medicinal plants are associated with their richness in several classes of secondary metabolites, notably the presence of flavonoids, terpenoids, and phenolic compounds. The present study aims to estimate the total bioactive contents and to evaluate the anti-inflammatory effect of crude extracts prepared from a *Centaurea* plant. The results indicated that the various extracts of *Centaurea* had moderate to low tannins and terpenoid contents and contained high amounts of phenolic and flavonoid compounds. On the other hand, these extracts inhibit thermally-induced protein denaturation in a dose-dependent manner. Their efficacy was significant and comparable to that of the standard anti-inflammatory drug. It could be concluded that the studied species could constitute a rich source of secondary metabolites with anti-inflammatory effects.

Keywords: *Centaurea*, anti-inflammatory, terpenoids, secondary metabolites.

PD36- Isolement et identification des acides phénoliques à partir de l'espèce *Centaurea dissecta*

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Résumé

La recherche des principes actifs extraits des plantes aromatiques et médicinales est d'une importance capitale car elle permet la mise au point de médicaments pour entretenir la santé de l'être humain. C'est pour cette raison qu'on s'est intéressé à ce genre d'investigation dans notre laboratoire de recherche. La présente étude se focalise principalement sur l'espèce *Centaurea dessicta* de la famille Asteraceae. La famille Asteraceae se caractérise par sa richesse en métabolites secondaires d'intérêt biologique tels que les triterpènes, les composés phénoliques, et les sesquiterpènes. Les plantes du genre *Centaurea* sont réputées en médecine traditionnelle pour soigner de nombreuses maladies.

Le but principal de notre travail consiste à isoler et identifier des métabolites secondaires qui peuvent avoir une activité biologique à partir des différents extraits organiques de l'espèce *Centaurea D*.

L'extraction hydro-alcoolique : éthanol/eau, la séparation et la purification chromatographique : VLC, CC et CCM des extraits éther de pétrole et acétate d'éthyle obtenus à partir de la plante entière *Centaurea D*., nous ont permis d'isoler et identifier 13 acides phenoliques.

Keywords:

Centaurea dessicta, Asteraceae, étude phytochimique, Acides phenoliques.

PD37- Synthesis, Structural Characterization, and Antioxidant Evaluation of Salicylaldehyde-Derived Schiff Bases and Their Reduced Analogues

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Abstract:

A series of Schiff bases and their corresponding secondary amines were synthesized through the condensation of salicylaldehyde derivatives with two aminophenol derivatives, followed by $NaBH_4$

reduction. The structures of the synthesized compounds were confirmed by FT-IR and NMR spectroscopy, and their melting points were determined experimentally. The antioxidant potential was investigated using five complementary assays (ABTS, DPPH, FRAP, phenanthroline, and CUPRAC). Statistical analysis (ANOVA, $p < 0.001$) revealed significant differences among the tested compounds. According to Duncan's multiple range test, two coumpounds exhibited the highest antioxidant activities, outperforming the standard antioxidants BHA, BHT, and ascorbic acid. The results highlight the impact of structural variations, particularly hydroxyl group positioning, on the antioxidant potential of salicylaldehyde-derived Schiff bases. These findings suggest that such compounds represent promising scaffolds for designing efficient antioxidant agents with pharmaceutical relevance.

Keywords:
Schiff bases, secondary amines, antioxidant activity, structure–activity relationship, green synthesis.

PD37- Assessment of the Antibacterial Effects of Artemisia herba-alba, a Medicinal Plant

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Abstract

Medicinal plants represent an inexhaustible source of traditional and effective remedies thanks to the various active compounds they contain, highlighting the importance of directing research toward new molecules. The present study focuses on the evaluation of the antibacterial activity of the medicinal plant *Artemisia herba-alba* (traditionally used in Algeria) against 20 multidrug-resistant pathogenic strains, in order to identify the most promising plant. *Artemisia herba-alba* yielded a high essential oil content of about 2.63%. Evaluation of the antibacterial activity of the crude essential oil showed that Gram-positive strains were more sensitive than Gram-negative strains, with significant MIC and MBC values. It can be concluded that *A. herba-alba* represents a recent source of bioactive molecules, mainly essential oils, which may serve as potential alternatives to conventional antimicrobial agents.

Keywords: *Artemisia herba-alba*, essential oil, MIC, MBC.

PD38- Assessment of the Antibacterial Effects of *Artemisia herba-alba*, a Medicinal Plant

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Abstract

Medicinal plants represent an inexhaustible source of traditional and effective remedies thanks to the various active compounds they contain, highlighting the importance of directing research toward new molecules. The present study focuses on the evaluation of the antibacterial activity of the medicinal plant *Artemisia herba-alba* (traditionally used in Algeria) against 20 multidrug-resistant pathogenic strains, in order to identify the most promising plant. *Artemisia herba-alba* yielded a high essential oil content of about 2.63%. Evaluation of the antibacterial activity of the crude essential oil showed that Gram-positive strains were more sensitive than Gram-negative strains, with significant MIC and MBC values. It can be concluded that *A. herba-alba* represents a recent source of bioactive molecules, mainly essential oils, which may serve as potential alternatives to conventional antimicrobial agents.

Keywords: *Artemisia herba-alba*, essential oil, MIC, MBC.

PD39- Antifungal activity of *Origanum majorana* L. essential oil against several *Candida* species

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Abstract

In light of the alarming rise in resistance of pathogenic yeasts to conventional antifungal agents, the search for natural alternatives has become a priority. This study aims to evaluate the antifungal activity of the essential oil of *Origanum majorana* L. against six clinical strains of *Candida*, namely: *C. albicans*, *C. tropicalis*, *C. glabrata*, *C. dubliniensis*, *C. famata*, and *C. parapsilosis*.

The oil was extracted by hydrodistillation from the aerial parts of the plant and tested *in vitro* using the disc diffusion method and microdilution in liquid medium.

The results revealed inhibition zones ranging from 19 to 32 mm, with MICs and MFCs varying between 0.19 and 1.56 mg/mL, and 0.19 to 6.25 mg/mL, respectively. These findings highlight the promising therapeutic potential of *O. majorana* essential oil as a natural alternative for the treatment of candidiasis.

Keywords: *Origanum majorana* L., *Candida* spp., essential oil, antifungal activity,

PD40- Flower plant from the *Asparagaceae* family as natural drug resources to treat Alzheimer's disease and inflammation

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Abstract

Inflammation is a complex biological response of vascular tissues to harmful stimuli. The main cause of a cognitive decline in patients with AD is the loss of cholinergic neurons in the brain, leading to impairment of cholinergic transmission. Developing new drugs from natural resources is always of interest to limit these processes in the human body.

Our study highlights the ability of the hydraulic and hydroalcoholic extracts of Flower plant from *the Asparagaceae* family to effectively inhibit inflammation by preventing protein denaturation, as well as their ability to inhibit acetylcholinesterase, which is known as the key enzyme in the breakdown of ACh, remains a promising approach for the treatment of AD. The importance of the results of the flower extracts encouraged the separation of three compounds from the butanolic extract, which could be responsible for these enzymatic activities, using chromatographic methods, while identifying them using spectrometric methods.

Keywords: Inflammation, acetylcholinesterase, extract, separation, chromatography.

PD41- Anti-inflammatory Activity of the Ethyl Acetate Extract of *Convolvulus Cantabrica*

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Abstract

The genus Convolvulus (family Convolvulaceae) comprises over 250 species of annual and perennial herbaceous plants, with about 50 distributed across North Africa and the Sahara Desert [1]. Several members of this genus have been traditionally employed as food sources, flavoring agents, medicinal herbs, and ornamental plants [2]. Phytochemical investigations have revealed that Convolvulus species contain a diverse range of bioactive constituents, including tropane alkaloids, calystegins, coumarins, phenolic compounds, and phytosterols. These compounds have been associated with various pharmacological properties, including diuretic, hypoglycemic, antioxidant, antitumor, antibacterial, and antifungal activities [3,4].

Convolvulus cantabrica L. (Convolvulaceae) is a medicinal plant widely distributed across North Africa and traditionally valued for its nutritional and therapeutic uses. This study aimed to investigate the phytochemical composition and anti-inflammatory potential of the ethyl acetate extract obtained from its aerial parts. Phytochemical screening revealed a high content of polyphenolic compounds, while biological evaluation demonstrated marked anti-inflammatory activity. These results indicate that C. Cantabrica possesses significant pharmacological potential and may serve as a promising natural source of bioactive compounds for pharmaceutical and nutraceutical development.

Keywords: Convolvulaceae, *Convolvulus cantabrica*, antioxidant, anti-inflammatory , polyphenolic

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PD42- Optimization of the extraction of anthocyanins from hawthorn fruits using methodology of the response surface and evaluation of their anti- inflammatory activity

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Abstract

The exploration of hawthorn fruits, traditionally valued for their nutritional properties and culinary applications, reveals their immense potential as a source of bioactive compounds with significant medical relevance. This study focused on optimizing the extraction of anthocyanins (ATC), natural pigments renowned for their therapeutic benefits, using ultrasound-assisted extraction techniques guided by response surface methodology (RSM). The extraction process was fine-tuned by varying methanol concentration (40–100%), extraction duration (0.5–6 minutes), and ultrasonic amplitude (20–100%) to maximize the yield of these medically important compounds.
The study also evaluated the in vitro anti-inflammatory properties of the extracted anthocyanins, emphasizing their inhibition of cyclooxygenase (COX) enzymes and nitric oxide (NO•) radicals—both critical targets in inflammation-related disorders. Optimal extraction conditions were established as 80% methanol, a 5-minute extraction time, and 80% ultrasonic amplitude, with methanol concentration identified as the key influencing factor ($R^2 = 0.97$). The extracted anthocyanins exhibited notable biological activities, including a 53% inhibition of COX (IC_{50} = 88 mg/ml) and a 77% reduction of NO• radicals (IC_{50} = 1.802 mg/ml).
These findings underscore the pioneering role of chemical techniques in enhancing the medicinal value of natural resources such as hawthorn. The optimized extraction process not only contributes to the understanding of bioactive compound isolation but also paves the way
for the development of innovative pharmaceutical solutions to address inflammatory conditions.

Keywords: Hawthorn, Anthocyanin, Ultrasound-assisted extraction, Anti-inflammatory activity, Medical chemistry, Pharmaceutical applications

PD43- Etude phytochimique de la plante *Rhamnus alaternus*

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Résumé

Ce travail porte sur l'investigation phytochimique des parties aériennes de la plante *Rhamnus alaternus* L., une espèce appartenant à la famille des Rhamnaceae appartenant à la famille Rhamnaceae, comprend 45-55 genres et environ 900 espèces. C'est une famille cosmopolite, distribuée dans les régions tropicales et parfois tempérées. Les plantes *Rhamnus* largement utilisées en médecine traditionnelle contre purgative, digestif, diurétique, laxatif, hypotensif et pour traitement de divers symptômes hépatiques et les maladies du foie et du pancréas, possèdent des activités biologiques intéressantes telles que antibactérienne, anticancéreuse et antioxydante,…ect, ceci s'explique dans une certaine mesure par la richesse de cette famille en composés triterpéniques, phénoliques sous forme de flavonoïdes, quinones et les anthraquinones.

L'investigation phytochimique de l'extrait acétate d'éthyle de l'espèce *R. alaternus* a abouti à l'isolement de cinq composés : lupéol **(1)**, acide oléalonique (**2**)**,** acide acétoxyoléan-12-èn-28- oique **(3),** *β*-sitostérol (**4**) and daucostérol (**5**). Leurs structures moléculaires ont été établies grâce à la combinaison des différentes méthodes spectroscopiques RMN 1D (^{1}H, ^{13}C *J*-modulé et DEPT) et 2D (COSY, HSQC et HMBC), la spectrométrie de masse ESI-MS et la comparaison avec les données de la littérature.

Mots clés : Rhamnaceae, *Rhamnus alaternus*, triterpènes, RMN 1D et 2D.

PD44- Crystal structure, Hirshfeld surface analysis and energy frameworks of salen-type Schiff base complex

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Abstract

A condensation of primary amine and aldehyde or ketone in a specific solvent can easily produce a compound named a Schiff base. Structurally, the carbonyl group (C=O) of the aldehyde or ketone is replaced by an imine or azomethine group. To form metal complexes, the Schiff base ligand is added to a metal precursor in an appropriate ratio, along with suitable experimental conditions. Commonly, the multidentate Schiff bases coordinate to metals through the imine nitrogen and another nitrogen or oxygen atom from a proper functional group from its neighborhood.

Schiff-base complex of Cu(II) has been synthesized and characterized by single-crystal X-ray crystallography which revealed the crystallization of LCu(II) as Orthorhombic with space group Pbca. A Hirshfeld surface analysis was undertaken to investigate and quantify the intermolecular interactions. In addition, energy frameworks were used to examine the cooperative effect of these intermolecular interactions across the crystal, showing dispersion energy to be the most influential factor in the crystal organization of the compound.

Keywords

Synthesis - DRX - Hirshfeld surface analysis .

PD45- ETUDE DES EFFETS DE QUELQUES GROUPEMENTS DIRECTEURS DANS LE COUPLAGE PALLADO-CATALYSE DU PYRAZOLE

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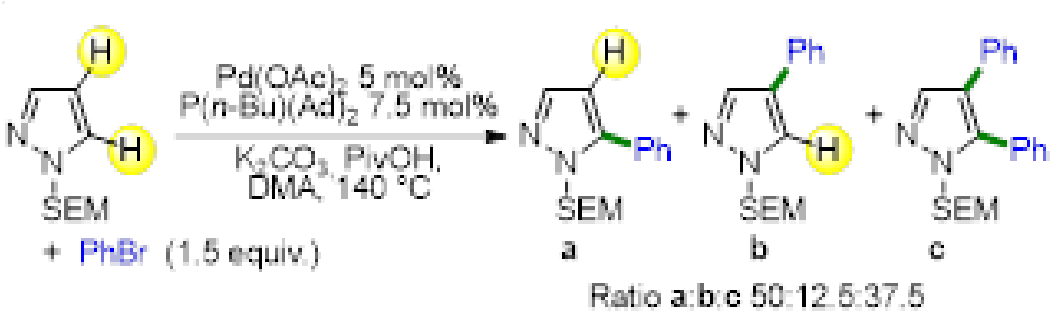
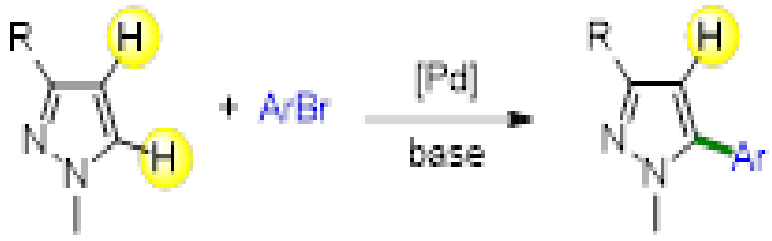
Abstract :

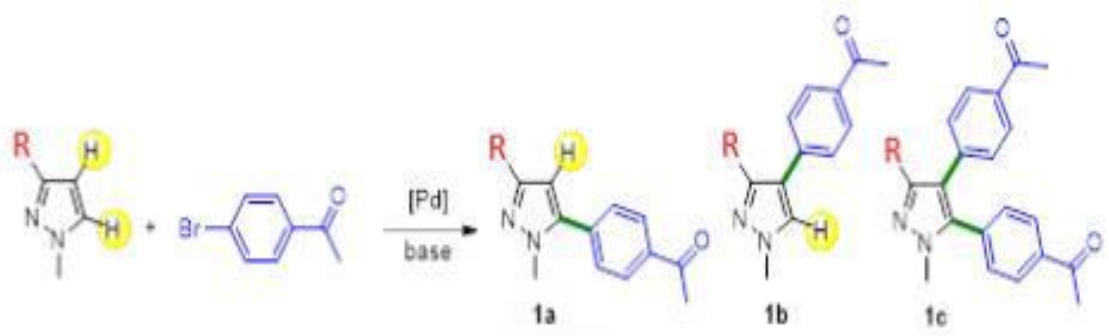
Depuis la découverte du couplage catalysé par le palladium d'halogénures d'aryle avec des dérivés hétéroaryliques, des résultats très intéressants ont été rapportés par plusieurs groupes. En revanche, à notre connaissance, le couplage direct de pyrazoles avec des halogénures d'aryle via une activation/fonctionnalisation de la liaison C-H a attiré beaucoup moins d'attention. Sames et ses collaborateurs1 ont établi la régiosélectivité de l'arylation C-H catalytique des pyrazoles.



Notre équipe de recherche a récemment développé un nouvel axe de recherche réservé à la synthèse et à l'évaluation de la sélectivité du couplage direct de pyrazole avec des halogénures d'aryle via une activation / fonctionnarisation de la liaison C-H.



L'objectif de notre travail est de déterminer la sélectivité de la réaction de C-H activation sur les pyrazoles substitués sur la position C32.



L'objectif poursuivi à travers ce travail s'intègre vers l'étude de l'influence des substituants en position C3 du pyrazole (R=CF3, CHO, Br, CN, CO2Me) sur le couplage direct avec des halogénures d'aryle via une réaction de C-H activation en utilisant l'acétate de palladium [Pd(OAc)2)] comme catalyseur en présence d'acétate de potassium. Cette étude nous a permis l'obtention des produits désirés avec de bons rendements. Tous les produits synthétisés ont été identifiés par les méthodes spectroscopiques usuelles.

Keywords: *Couplage direct, C-H activation, Palladium, Pyrazole*

Référence :

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PD46- CHEMICAL CHARACTERIZATION AND EVALUATION OF THE BIOLOGICAL ACTIVITIES OF A NOVEL PLANT-DERIVED RENNET

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ABSTRACT

One of the most significant sectors with intriguing economic revenue is the manufacture of cheese and other dairy products.
in fact, rennet from various animal and microbiological sources must be used to coagulate mil k in the first stage of the cheese-producing cycle. there has been a global scarcity of calf rennet for several decades. numerous rennet alternatives, including bovine and porcine pepsins, were used by industries; nevertheless, their widespread proteolytic nature and other social restrictions (the product is n ot halal) have led to their commercial failure. researchers developed several microbial coagulants as a result of this failure; these were very effective and readily available, but the dairy industry was hesitant to adopt them because of th eir low quality and decreased productivity. several tests were carried out to verify the product's effectiveness. the results show that this formula has a lot of secondary metabolites (polyphenol, flavonoid, anthocyanin, tannins), as well as high coagulant properties and a number of antioxidant and antibacterial properties. this rennet is a natural, organic, and halal vegetable rennet intended for cheese industries and people interested in dairy products production. it is a novel product made by combining a number of algerian native herbs and plants with coagulant, medicinal, and nutritional qualities.

Keywords: Chemical Characterization, Biological Activities, Dairy Products, And Plant-Based Rennet.

PD47- Synthesis, Crystal Structure, and Multimodal Antioxidant Assessment of 1,3,5-Tris(cyclohexyl)-1,3,5-triazinane

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Abstract:
Triaza heterocycles are versatile small-molecule frameworks with growing relevance in redox chemistry and bioactive materials. We report the synthesis, structure elucidation, and antioxidant evaluation of a new member of this family, 1,3,5-tris(cyclohexyl)-1,3,5- triazinane. The target compound was prepared by condensing cyclohexylamine with formaldehyde under mild conditions,

followed by purification to afford a crystalline solid suitable for X-ray analysis. Comprehensive characterization ($^{1}H/^{13}C$ NMR, FT-IR) confirmed the expected composition and purity. Single-crystal X-ray diffraction established the triazinane core, revealed the N-cyclohexyl substitution pattern, and defined key conformational features relevant to molecular recognition and redox behavior. Antioxidant activity was assessed using complementary, mechanism-informative assays. Radical scavenging was examined by ABTS•+ decolorization; reducing capacity was evaluated with the FRAP method; nitric-oxide quenching was monitored in the sodium nitroprusside (SNP) system; and iron-chelating ability was probed via the 1,10-phenanthroline test. Appropriate blanks and reference standards were included to control for assay interference and to support qualitative comparisons across methods. Across this panel, the compound displayed measurable activity consistent with a multimodal antioxidant profile encompassing radical scavenging, reducing power, modulation of NO•, and Fe2+ binding. These findings highlight a structurally simple, readily accessible triaza scaffold that integrates crystallographically verified architecture with broad antioxidant behavior. The results motivate further structure– activity exploration of triazinanes as tunable redox modulators and potential leads for applications in oxidative-stress mitigation and materials stabilization.

Keywords: hexahydro-1,3,5-triazine; triazinane; cyclohexylamine; crystal structure; ABTS; FRAP; sodium nitroprusside; phenanthroline; antioxidant.

PD48- A Combined In Vitro and In Silico Assessment of the Biological Activities of Ferrocene Derivative

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Abstract

Ferrocene derivatives have attracted considerable scientific interest due to their unique organometallic structure, redox properties, and versatile pharmacological potential. These compounds have shown promise in various biological applications, including anti- inflammatory, anti-diabetic, and anticancer activities. In this study, a combined in vitro and silico evaluation was performed to investigate the biological activities of a selected ferrocene- based compound FM.
The in vitro assays focused on anti-diabetic and anti-inflammatory potentials, using acarbose and diclofenac as reference drugs, respectively. FM exhibited superior inhibitory activity compared to the reference drugs, with IC50 values of 0.175 (µg/ml) for anti- inflammatory activity versus 3.25 (µg/ml) for diclofenac, and 0.015 (µg/ml) for anti-diabetic activity versus 0.189 (µg/ml) for acarbose, indicating enhanced efficacy. Molecular docking studies provided further insight into the binding

modes of FM, revealing strong and stable interactions with the active sites of alpha-amylase and BSA. In addition, ADMET predictions suggested favorable pharmacokinetic properties, acceptable drug-likeness, and low toxicity, supporting its potential as a safe and effective therapeutic candidate.

The consistency between the in vitro and in silico results highlights the reliability of the integrated approach and confirms FM as a promising lead compound for the development of potential anti-inflammatory and anti-diabetic therapeutics.

Keywords: Ferrocene Derivatives, BSA, α-amylase, anti-inflammatory activity, Anti- Diabetic.

PD49- Chemical Composition of the Essential Oil from *Centaurea* sp. Collected in Algeria

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Abstract

The genus *Centaurea* (Asteraceae) comprises a wide range of aromatic and medicinal species traditionally used in folk medicine. In this study, the essential oil was extracted from the aerial parts of Centaurea sp., collected in Algeria, using hydrodistillation. The oil was then analyzed by gas chromatography coupled with mass spectrometry (GC-MS) to determine its chemical profile.

The analysis revealed a complex mixture of 45 volatile compounds, representing 98.01% of the total oil content. Limonene (25.02%), methyl-cyclohexane (23.73%), and o-cymene (13.20%) were identified as the major constituents. These compounds are frequently found in essential oils with known therapeutic, antioxidant, and aromatic properties. The results provide the first insight into the volatile composition of *Centaurea* sp. from this region and contribute to the chemotaxonomic characterization of the genus. This preliminary work highlights the potential of *Centaurea* essential oil as a source of valuable natural compounds and sets the foundation for future studies on its biological properties, such as antimicrobial, antioxidant, and anti-inflammatory activities.

Keywords: *Centaurea* sp., essential oil, GC-MS, volatile compounds, limonene, Asteraceae, Algeria.

PD50- Les NaDES : nouveaux milieux verts pour la synthèse d'α-aminophosphonates

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Résumé :

Traditionnellement, les synthèses organiques sont réalisées avec des procédés énergivores et dans des solvants parfois dangereux, toxiques, persistants dans l'environnement et difficiles à éliminer. Ces effets méphitiques ont conduit à une prise de conscience croissante au sein de la communauté scientifique et industrielle, quant à la nécessité de réduire l'empreinte écologique de ces processus. Pour répondre à ces enjeux, la communauté scientifique et industrielle se tourne de plus en plus vers l'utilisation de solvants naturels et biosourcés dans les synthèses organiques[1] qui sont issus de ressources renouvelables comme les algues, les plantes ou encore les huiles essentielles.

La chimie verte cherche à réduire l'impact environnemental des procédés chimiques. Dans ce cadre, la synthèse des α-aminophosphonates dans des solvants eutectiques profonds naturels (NaDES) constitue une avancée importante. Cette approche durable et efficace permet de produire ces composés bioactifs, utiles en pharmacie et en agrochimie, tout en respectant mieux l'environnement.

Afin d'étendre l'utilisation des solvants eutectiques naturels profonds (NaDES), nous avons étudié leur efficacité et leurs limites sur la synthèse de dérivés d'α-aminophosphonate via la réaction multicomposants de Kabachnik-Fields. Nous avons obtenu ces dérivés avec de bons rendements. Les structures chimiques de ces nouvelles molécules ont été confirmées par les différentes méthodes spectroscopiques : RMN ^{1}H, ^{13}C et ^{31}P. Ces molécules ont montré une bonne activité antibactérienne et antifongique.

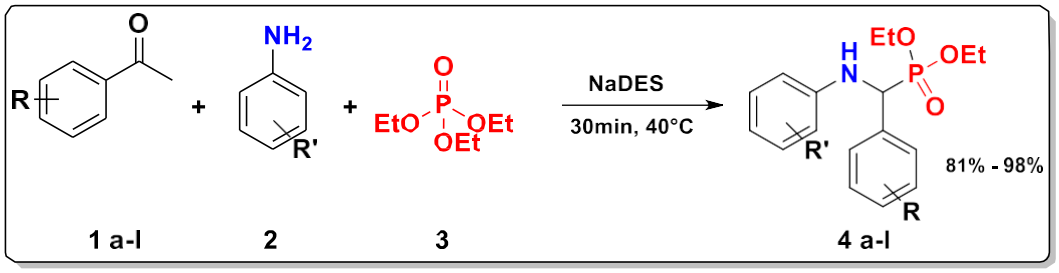

Schéma 1 : Synthèse de nouveaux composés dérivés d'α-aminophosphonatesc dans les NaDES

Mots clés : α-aminophosphonates ; NaDES, chimie verte, Kabachnik

[1] (a) Y. L. Gu Green Chem., 2012, 14 , 2091 —2128 RSC . (b) M. C. Bubalo , S. Vidović , I. R. Redovniković and S. Jokić , J. Chem. Technol. Biotechnol., 2015, 90(9), 1631-1639.

PD51- Etude de la catalyse du polyethylene glycol via La réaction à composant multiple 'Mannich'

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Résumé :

Les RCMs visent la synthèse des produits hautement fonctionnalisés en une unique opération chimique vu que la chimie organique moderne se focalise sur les problématiques d'économie (étapes, atomes, énergie). Par conséquent, ces réactions connaissent aujourd'hui un intérêt considérable tant dans le secteur industriel qu'académique. L'utilité des *β-aminocétones* dans notre quotidien a fait de leur méthode de préparation, nommée la réaction de Mannich, une des réactions à composants multiples les plus importantes tels que Moban neuroleptique ainsi que Osenervan antiparkinson. Dans ce travail, nous proposons une nouvelle procédure simple, efficace, générale et respectueuse de l'environnement pour la synthèse des β-aminocétone en faisant réagir, avec de bons rendements, trois composants, qui sont un aldehyde aromatique, une amine et une cetone.

Un criblage catalytique nous a orientés sur la détermination d'un nouveau catalyseur dont les essais préliminaires se sont vus très concluants. La généralisation de la voie, après optimisation avec les trois librairies des réactifs, a généré une chimiothèque de bases de Mannich avec de très bons rendements.

Mots clés : Réactions à composants multiples, réaction de Mannich, Bases de Mannich, , β-aminocétones, criblage.

PD52- ETUDE DU PROFILE DE LA PLANTE *vicia onobrychioides* PAR GC-MS ET ESTIMATION DE LEUR ACTIVITIES ANTIOXYDANTE

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Résumé :

La famille des Fabaceae est la troisième plus grande famille de plantes à fleurs après les *Orchidaceae* et les *Asteraceae* (environ 730 genres et plus de 19400 espèces selon le Royal Botanic Garden, Edinburgh 2010). Les plantes de cette famille sont connues pour leur utilisation en médecine traditionnelle.

Notamment, les études phytochimique ont montré leur richesse en métabolites secondaire possédant des activités biologique intéressante en particule les isoflavonoïdes qui sont connu par leur pouvoir oxydant. Le genre *vicia* est l'un des genres important de la famille de Fabaceae ses grains qui sont très riche en protéines ont été utilisés en cuisine, torréfiés, et comme aliment pour les voyageurs dans les déserts orientaux. Mais en Algérie ce genre est plus utilise comme fourrage pour les animaux. Il est représenté par 83 espaces dans la flore d'Algérie. Les études récentes sur les plantes de ce genre ont prouvé l'existence de plusieurs métabolites secondaires, en particules les flavonoïdes, les saponines. Ils ont aussi montres que ce genres possède une activité biologique antioxydants remarquable.

L'étude de l'extrait ether de pétrole de l'espèce *vicia onobrychioides* nous a conduit à identifier 39 produites qui appartiennes a 4 famille. Aussi la plante a montré une activité antioxydant remarquable.

Mots clés : Fabaceae, *vicia, vicia onobrychioides,* GC-MS, activité biologique, antioxydant.

PD53- L'isolement d'un nouveau flavonoïde glycosylé à partir de l'espèce *Diplotaxis erucoides*

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Résumé

L'étude de la chimie des plantes est toujours d'une brûlante actualité malgré son ancienneté. Cela tient principalement au fait que le règne végétal représente une source importante d'une immense variété de molécules bioactives. De ce fait, nous avons choisi d'étudier la plante *Diplotaxis erucoides* appartenant à une large famille de plantes d'une importance scientifique et économique majeure, qui est la famille Brassicaceae. Les plantes de cette famille ont été employées comme antidiabétiques, antibactériennes, antifongiques, anticancéreuses et antirhumatismales. L'étude phytochimique de l'extrait butanolique obtenus à partir de la partie aérienne de cette plante a abouti à l'isolement d'un nouveau flavonoïde glycosylé: Kaempférol-3-*O*-[α-L-rhamnopyranosyl-(1-2)-*β*-D-xylopyranosyl]-7-*O*-α-L- rhamnopyranoside appelé Diploerucoides A. Sa structure moléculaire ont été établies grâce à la combinaison des différentes méthodes spectroscopiques RMN 1D (^{1}H, ^{13}C) et 2D (COSY, HSQC et HMBC), la spectrométrie de masse ESI-MS et la comparaison avec les données de la littérature.

Mots clés : *Diplotaxis erucoides,* flavonoïde glycosylé , RMN 1D, RMN 2D, spectrométrie de masse

PD54- Profil phytochimique et potentiel biologique de *Convolvulus cantabrica* L. (Convolvulaceae)

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Résumé

Le présent travail propose une étude approfondie de *Convolvulus cantabrica* L., une plante appartenant à la famille des Convolvulaceae et au genre *Convolvulus.* L'investigation a porté à la fois sur les aspects chimiques et biologiques.

L'analyse par chromatographie en phase gazeuse couplée à la spectrométrie de masse (GC-MS) a révélé la présence d'un ensemble de métabolites secondaires, notamment des esters d'acides gras, des acides gras, des alcools sesquiterpéniques, des alcènes et des alcools gras.

Les extraits testés, notamment ceux à l'acétate d'éthyle et au butanol, ont montré une forte activité antioxydante lors des essais DPPH, ABTS et FRAP, comparativement aux extraits d'autres espèces du même genre. De plus, l'extrait au pétrole éther a révélé une activité anti- inflammatoire intéressante. Concernant l'activité antibactérienne, les extraits à l'acétate d'éthyle, hydroalcoolique et au pétrole éther ont inhibé la croissance de *Bacillus cereus*.

Dans l'ensemble, ces résultats indiquent que *Convolvulus cantabrica* L. est riche en métabolites secondaires, notamment en polyphénols, et présente des activités biologiques significatives, en particulier des propriétés antioxydantes.

Mots-clés : *Convolvulus cantabrica* L., GC-MS, antioxydante, anti-inflammatoire, antibactérienne.

PD55- Investigation phytochimique et propriétés pharmacologiques d'une plante Aurésienne du genre *Silene*

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Résumé:

De nos jours, la valeur des plantes médicinales est largement reconnue, principalement en raison de leur capacité à fournir des composés bioactifs utilisés comme sources potentielles pour le développement de nouveaux médicaments. Lorsqu'elles sont associées aux outils de la bio-informatique, ces plantes offrent une alternative naturelle, mieux tolérée par l'organisme et présentant relativement peu d'effets secondaires dans le traitement de diverses maladies chroniques.

Dans ce cadre, la présente étude vise à fournir une description complète du profil phytochimique d'une espèce du genre *Silene* poussant dans les Aurès, à l'aide de l'analyse (GC- MS), ainsi qu'à évaluer son potentiel pharmacologique à travers différentes approches *in vitro*.

L'analyse phytochimique par GC-MS a révélé la présence de 57 composés, appartenant principalement aux familles des acides gras et esters, des sucres, ainsi que des terpènes et stéroïdes. Sur le plan pharmacologique, l'extrait chloroformique a montré la meilleure activité antiradicalaire, accompagnée d'un facteur de protection solaire (SPF) élevé et comparable à celui de l'extrait éther de pétrole.

Ce travail met en évidence, une fois de plus, le potentiel pharmacologique prometteur des espèces végétales algériennes. Des études *in vivo* supplémentaires demeurent nécessaires pour confirmer et approfondir ces résultats préliminaires.

Mots-clés : *Silene*, SPF, Aurès, GC-MS, antioxydant, flore algérienne.

PD56- Green Synthesis, In-vitro Antifungal Activities, and Molecular Docking Studies of Pyranopyrazoles Derivatives

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Abstract:

This study explores the multicomponent synthesis of Pyranopyrazoles derivatives. These compounds are particularly valuable in medicinal chemistry due to their therapeutic potential [1, 2].

The findings contribute to sustainable practices in the development of novel therapeutic agents, highlighting the importance of eco-friendly catalysis in pharmaceutical research. Furthermore, the resulting Pyranopyrazoles were tested for antifungal activity, demonstrating effectiveness against various fungal strains, which may open new avenues for treating fungal infections. Additionally, theoretical studies (docking) were conducted to reinforce the findings. Overall, this research aims to streamline synthesis processes in medicinal chemistry while promoting ecological sustainability.

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PD57- Etude phytochimique de trois plantes médicinales récoltées dans le Nord Est Algérien (région de Séraidi)

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RESUME

Le présent travail de recherche porte sur la caractérisation phytochimique de trois espèces sélectionnées et récoltées dans la région de Séraidi, Wilaya d'Annaba.

Les tests du screening phytochimiques révèlent l'existence de différents métabolites secondaires: polyphénols, flavonoïdes, tanins, anthocyanes, stérols et triterpènes, quinones, cardénolides et les saponosides avec absence des alcaloïdes dans l'*Urtica dioica*. L'extraction des principes actifs a été effectuée sur les feuilles séchées des 3 plantes choisies, par macération dans une solution hydro-éthanolique à 80%. L'étude quantitative des extraits polyphénoliques a été réalisée au moyen des dosages spectrophotométriques, nous a permis la détermination de la teneur totale des polyphénols et des flavonoïdes avec des valeurs consécutives de 24.32µg EAG/mg et 3.267µg EQ/mg d'extrait de *Cytisus triflorus* ; 20.088µg EAG/mg et 4.396µg EQ/mg d'extrait de *Ziziphus lotus* ; 16.36µg EAG/mg

et 5.945µg EQ/mg d'extrait *d'Urtica dioica*.

Les analyses spectrales par GC/MS nous ont fait ressortir les composés contenus dans les extraits phénoliques étudiés. Les spectre ont recensé 09 composés pour ***Cytisus triflorus*** avec une molécule majoritaire Acide 4-hydroxy-3-méthoxybenzoïque; 17 composés pour *Urtica dioica*, avec la prédominance de l'Acide gallique et 11 composés pour *Zizyphus lotus* dont Hexahydroxydiphenoyl-glucose est majoritaire.

L'évaluation *in vitro* de l'activité antioxydante des extraits polyphénoliques de trois plantes a été réalisée par la méthode de piégeage du radical DPPH. Ces extraits présentent des valeurs intéressantes d'IC50 avec 155.163µg/ml pour *Urtica dioica*, 70.684µg/ml pour *Cytisus triflorus* et 104.829µg/ml pour *Ziziphus lotus*.

Mots clés : *Ziziphus lotus, Cytisus triflorus, Urtica dioica*, screening phytochimique, GC/MS, Région de Seraidi.

PD58- Biological Evaluation of Novel Nitroaldol-Based Quinoline Compounds as Antimicrobial Agents

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Abstract

Quinoline derivatives have attracted considerable attention due to their broad and potent biological properties, particularly their antimicrobial effects against a wide range of pathogenic microorganisms **[1,2]**. Motivated by these activities, we synthesized a new series of nitroaldol quinoline derivatives **[3]** using an efficient Henry reaction that provided the compounds in high yields. Structural characterization was confirmed through ^{1}H and ^{13}C NMR, FTIR, and mass spectrometry analyses.

Biological evaluation demonstrated that several of the synthesized derivatives exhibited noteworthy antimicrobial activity, indicating that the introduction of the nitroaldol moiety contributes positively to the biological potential of the quinoline scaffold. These results suggest that the new derivatives could serve as promising candidates for further development as antimicrobial agents.

To support the experimental findings, Density Functional Theory (DFT) studies were performed, offering insights into the electronic features and stability of the molecules. In addition, in-silico ADME predictions revealed favorable pharmacokinetic properties, including good oral absorption, membrane permeability, and bioavailability. Collectively, these results highlight the relevance of the newly synthesized nitroaldol quinoline derivatives as potential lead structures in the search for effective antimicrobial compounds.

Keywords
Nitroaldolquinoline, antimicrobial, DFT, *In silico* molecular docking, DNA-gyrase

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PD59- LCMS-MS ET L'EVALUATION DE L'ACTIVITE ANTIOXYDANTE IN VITRO DE L'EXTRAIT HYDROALCOHOLIC DE LA PLANTE VICIA ONOBRYCHIOIDES.

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Résumé

La famille des Fabacées (ou légumineuses) est une famille de plantes cosmopolites, troisième en nombre d'espèces et deuxième en importance économique. Elles sont reconnaissables à leurs fleurs papilionacées, leurs feuilles composées et leurs fruits en gousses. Elles se caractérisent par une relation symbiotique avec des bactéries (Rhizobium) dans leurs racines qui fixent l'azote atmosphérique, permettant de ne pas nécessiter d'engrais azotés. La famille Fabaceae est connue par la présence des polyphénols dans ces espèces, elle est la troisième plus grande famille de plantes à fleurs après les *Orchidaceae* et les *Asteraceae*. Les études phytochimique ont montré la richesse des plantes de cette famille en métabolites secondaire possédant des activités biologique intéressante en particule les polyphénols qui sont connu par leur pouvoir oxydant.

Le genre *Vicia* est l'un des genres important de la famille de Fabaceae. Ses grains sont très riche en protéines et très utilisés en cuisine. En Algérie, le genre *Vicia* est représenté par 83 espaces, et il est couramment utilisés comme fourrage pour les animaux. D'après les dernières études en phytochimie les plantes de ce genre sont riches en plusieurs métabolites secondaires comme les polyphénols, les flavonoïdes et les saponines. Ils ont aussi montres que ce genres possède une activité biologique antioxydants remarquable.

L'étude de l'extrait hydro-alcoolique des parties aériennes de l'espèce *Vicia onobrychioides* par LCMS-MS nous a conduit a déterminer 20 produits qui sont principalement des flavonoides. Aussi, nous avons essayé d'estimer le potentiel antioxydant in vitro sur l'extrait hydro-alcoolique. Cette estimation a été faite par deux méthodes : piégeage du radical libre DPPH et réduction du fer ferrique par test FRAP, la plante montre une activité antioxydant remarquable et intéressantes.

Mots clés : Fabaceae, *Vicia*, LCMS-MS, flavonoïdes, activité antioxydante.

PD61- Isolation and Identification of components of the aerial partextracts From an Algerian *Cistus ruficomus* Viv

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Abstract

The genus *Cistus* belonging to the Cistaceae family contains approximately 110 species of evergreen and semi-evergreen shrubs, distributed in America, Europe and North Africa. However, the Mediterranean region is considered its center of diversity. Some *Cistus* species possess a number of interesting biological activities as antibacterial, and antioxidant free radical-scavenging.

The chemical investigation of the AcOEt and n-BuOH extracts of the species *Cistus. ruficomus* Viv (aerial parts) led to the isolation of 11 natural compounds including a neolignan glucoside, six flavonoids, two benzoic acid derivatives and two quinic acid derivatives. These compounds were obtained by the alternating use of different chromatographic methods such us CC, VLC, TLC and HPLC.

The structures of all the isolated compounds 1-11 were elucidated using different spectroscopic methods including 1D NMR (^{1}H and ^{13}C NMR) and 2D NMR (COSY H-H, TOCSY HSQC, DEPTQ and HMBC), Mass spectrometry, measurement of the optical rotation $[\alpha]^{D}_{20}$ and by comparison with literature data.

Keywords: Cistus ruficomus Viv, Cistaceae, NMR 1D and 2D.

PD64- Optimized ultrasonic-assisted deep eutectic solvents extraction of Populus nigra buds, phytochemical screening, biological activities, and MPO inhibition.

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Abstract:

Algeria, thanks to its geographical location and diverse climate, is rich in natural resources. Combining knowledge of traditional plant uses and scientific research on active constituents. This study focuses on the phytochemical compounds with anti-inflammatory potential from *P. nigra* buds. Box–Behnken response surface design was used to optimize ultrasound-assisted extraction parameters for phenolic compounds, followed by an evaluation of myeloperoxidase activity in vitro, as well as molecular docking to further elucidate macromolecular–ligand interactions. Optimization results for ultrasound-assisted extraction revealed a total phenolic content of 42.87 ± 0.33 mg GAE/g dw, obtained with 66.54% lactic acid at 35 °C for 20 minutes.

In addition, the in vitro evaluation of the extract's enzymatic activity revealed strong inhibitory activity, with an IC50 of 0.084%. Furthermore, molecular docking of the most abundant phytochemical compounds in the extract interacting with the myeloperoxidase active site showed the formation of hydrogen bonds, Pi–alkyl, and Pi–sigma interactions, with high binding affinities of −9.0 and −10.1 kcal/mol attributed to esculoside and M-rhamnosyl-hexosyl-acyl-quercetin, respectively.

Our results demonstrate the efficiency of phenolic compound extraction using ultrasound as an energy source and lactic acid as an alternative solvent. In addition, the selected compounds exhibit strong anti-inflammatory activity and may serve as core structures for the design of more potent inhibitors.

Keywords: *Populus nigra* buds; myeloperoxidase; optimization; Box–Behnken.

PD65- Biotechnological potential of marine bacteria from contaminated sites: A case study from the fishing port of Khemisti, Tipaza, Algeria

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Abstract:

The marine environment affected by hydrocarbon contamination represents a complex ecosystem hosting highly specialized microbial communities. Among these, biosurfactant-producing bacteria play a key role due to their ability to alter surface interactions, disperse hydrocarbons, and facilitate their natural degradation. These microorganisms are therefore essential contributors to the self-purification processes occurring in polluted marine areas.

In this context, the fishing port of Khemisti (Tipaza, Algeria) provides a particularly relevant site of investigation, as its marine environment is regularly exposed to port activities that can lead to hydrocarbon inputs. Physicochemical analyses confirmed a significant level of contamination, characterized by elevated concentrations of petroleum compounds. Such chronic pollution creates a selective pressure that promotes the establishment of resistant and metabolically adapted microorganisms. From the collected samples, sixteen distinct bacterial isolates were obtained. Several demonstrated the ability to produce biosurfactants, while one isolate showed particularly strong activity in qualitative assays. Morphological characterization combined with 16S rRNA gene sequencing identified this strain as belonging to the genus *Bacillus*, a group well-known for its biotechnological potential and resilience in hydrocarbon-polluted marine environments.

Overall, this study highlights the fishing port of Khemisti as a natural reservoir of microorganisms with promising bioremediation potential. It also emphasizes the microbial diversity of the Algerian marine environment and the ecological significance of biosurfactant-producing *Bacillus* species in coastal areas impacted by hydrocarbons.

Keywords: Microbial biodiversity – Marine bacteria – Biosurfactants – Hydrocarbon contamination – Algeria.