

University of M'sila



Faculty of Sciences, Department of Chemistry

Laboratory of **Organo-Therapeutic Substances**
and **Sustainable Processes (LOTSSPL)**



1st International Hybrid Seminar:

Green Chemistry and Artificial Intelligence: Towards Molecular Design
(GCAITMD'25)

October 21st–22nd, 2025, M'sila

Seminar Proceedings Book

GC AI TMD'25



1st International Hybrid Seminar on “Green Chemistry and Artificial Intelligence: Towards Molecular Design” (GCAITMD'25 M'sila - Algeria)

Preface

We are pleased to announce the organization of the First International Hybrid Seminar on “Green Chemistry and Artificial Intelligence: Towards Molecular Design” (GCAITMD'25), hosted by the Laboratory of Organo-Therapeutic Substances and Sustainable Processes (LOTSSP), Department of Chemistry, Faculty of Science, Mohamed Boudiaf University – M'sila, Algeria.

This international event provides an excellent platform for the scientific community to exchange ideas, share experiences, and strengthen collaboration between researchers, academics, and industrial partners at both the national and international levels. It also aims to guide doctoral students in their academic and research careers while encouraging the emergence of innovative scientific projects that address global sustainability challenges. The seminar covers a broad spectrum of topics in modern chemistry, including semi-synthetic materials, organic synthesis, environmental engineering, medicinal and pharmaceutical chemistry, natural bioactive compounds, and macromolecular systems (polymers/biopolymers). It seeks to disseminate recent advances and applied research outcomes that contribute to sustainable development and the improvement of human health.

A special emphasis is placed on the integration of artificial intelligence into chemical research and molecular design. AI now plays a pivotal role in predicting molecular properties, optimizing reaction pathways, and accelerating the discovery of new drugs and materials. By enabling data-driven innovation and reducing experimental costs, it contributes to the transformation of the chemical and pharmaceutical industries toward more efficient and sustainable practices.

Through the convergence of Green Chemistry and Artificial Intelligence, GCAITMD'25 aspires to inspire creativity, promote scientific excellence, and advance sustainable technological solutions for the benefit of both humanity and the environment.

Chair of GCAITMD'25

Webpage of the seminar : <https://www.univ-msila.dz/site/1st-international-conference-on-green-chemistry-and-artificial-intelligence-towards-molecular-design-gcaitmd25/>



Dr. BOULEGHLEM Hocine

1st International Hybrid Seminar on “Green Chemistry and Artificial Intelligence: Towards Molecular Design” (GCAITMD'25 M'sila - Algeria)

Objectives

This seminar aims to:

- ❖ Promote scientific research and exchange in the fields of green chemistry and artificial intelligence, and their applications in molecular design;
- ❖ Highlight the synergy between sustainable chemistry and intelligent technologies to achieve more efficient and targeted molecular design;
- ❖ Strengthen scientific collaboration among researchers, PhD students, and industrial professionals in related fields;
- ❖ Discuss recent trends and developments in green chemistry and the use of artificial intelligence for material and drug development;
- ❖ Foster a culture of sustainability in scientific and industrial research by reducing the environmental impact of chemical processes
- ❖ Encourage the exchange of experiences and innovations at both national and international levels.

Honorary Chairs

This supervision includes:

Professor Amar BOUDELLA, Rector of the University of M'Sila

Professor Rabah BOUNAR, who works at the Faculty of Sciences at the University of M'Sila

The Topics covered by the seminar

Topic 01: Green Chemistry, Organic Synthesis, and Molecular Modeling (organic/bio organic synthesis and phytochemistry)

Topic 02: Molecular Systems (polymer/biopolymer), Sustainable Development, Health, and the Role of Artificial Intelligence In Sustainability

Topic 03: Nanomaterials and Nanostructures for Energy and Environmental Applications

T4 / Topic 04: Valorization of Natural and Renewable Resources and Materials (bioprocesses and catalytic processes)

T5 / Topic 05: Applications of Artificial Intelligence In Molecular Design In Chemistry

Honorary chairs

Dr. Hocine BOULEGHLEM Director of GCAITMD'25

Co-chairs: Dr. Salima ZIDANE

Organizing committee

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Table of Contents	
Plenary	Page
Applications de l'énergie solaire thermique à la dépollution de l'eau et des sols <i>Prof. Mokhtar DJEHICHE</i>	02
Ecocatalysis and Asymmetric Organocatalysis, a New Vision of Green and Sustainable Chemistry <i>Prof. Nour-Eddine AOUF</i>	03
Chimie verte et intelligence artificielle pour les agrosystèmes durables : une synergie innovante pour optimiser l'association culturale blé-légumineuse <i>Prof. Wissem HAMDI</i>	04
Development of a prototype for hydrogen production and industrial and/or urban wastewater treatment using various electrochemical techniques based on solar energy <i>Prof. Nouredine HAMDI</i>	05
Synthesis of new green composite zeolite/activated carbon: adsorption of Non-Steroidal drug and volatile organic compounds <i>Prof. Nouredine HAMDI</i>	06
Supercondensateurs : la révolution énergétique au service des technologies de demain <i>Prof. Ahmed BAHLOUL</i>	07

Oral Communications	
Equilibrium, kinetic and thermodynamic studies of the biosorption of textile dye from aqueous solutions onto opuntia ficus indica Cords <i>LAIDANI Ykhlef</i>	09
Characterization and Electrochemical behavior of new synthesized zinc (II) tetradentate Schiff base complex <i>MAGHRAOUI Nadjah</i>	10
Antibacterial activity of hydroethanolic leaf extract of Ziziphuf spina christi against Gram positive and Gram negative bacteria <i>Dalila BENCHEIKH</i>	11
3D Printed Polymer Phononic crystal structures for the Detection and Characterization of Acetic Acid <i>Fahima ARAB</i>	12
Revealing the bioavailability and gastroprotective activity of polyphenols from Clematis flammula extract by in vitro digestion <i>ATMANI-KILANI Dina</i>	13
Antibacterial Activity of Green Synthesized NiO Nanoparticle and NiO-ZnO Nanocomposite using Limon Citrus Extract <i>Imane DJOUABI</i>	14
Electrodeposition and Characterization of Zn-Cu Alloy Thin Films <i>BENDEBANE Farida</i>	15
Sustainable Recovery of a Synthetic Polymer Waste Via a Bio-Based Polymer System <i>MOUFFOK Samir</i>	16
Coques de noyaux d'abricot comme biosorbant durable pour l'élimination efficace du colorant violet de cristal <i>TERCHI Smail</i>	17
Valorization of Algerian medicinal plants in medicine and cosmetology <i>ATMANI Djebbar</i>	18
Removal of nickel(II) in wastewater by nanochitosan <i>RAHALI Abdallaha</i>	19
Influence of Zinc Acetate Concentration on the Photoelectrochemical Performance of Chemically Deposited ZnO Films <i>BOUDERBALA Ibrahim Yaacoub</i>	20

1st International Hybrid Seminar on “Green Chemistry and Artificial Intelligence: Towards Molecular Design” (GCAITMD'25 M'sila - Algeria)

Plant-Driven Nanotechnology: CuO Nanoparticles and Their Light-Induced Degradation of Pollutants <i>KHENICHE Abdelhakim</i>	21
Valorisation nanoformulée des extraits d'Artemisia herba-alba pour la protection pré-récolte du blé contre les ravageurs <i>KABOUYA Imane</i>	22
Caractérisation physico-chimique et composition minérale d'une argile naturelle (Région de Soubella, M'Sila, Algérie) <i>LARKAT Karima</i>	23
Co-détection de l'eugénol et du butylhydroxytoluène par hydrodistillation verte et sélective d'héliotropium tenuiflorum (L.) utilisant de nouveaux solvants verts <i>BENDJELLOUL Sara</i>	24
The optimization of experimental conditions using Design Expert to enhance the oxidation of rhodamine B with persulfate in a sustainable solar system <i>BACHIRI Marwa</i>	25
Homogeneous Catalyzed Transesterification of Biodiesel: Application of the Box-Behnken Design <i>BENDEBANE Salima</i>	26
Electrosynthèse et analyse des propriétés electrocatalytiques d'électrodes modifiées par des films de polypyrrole fonctionnalisés contenant du nickel <i>NESSARK Faiza</i>	27
Enhancement of flow parameters and modeling of the rheological behavior of crude oil with and without additive <i>Mohamed Rafik BERINIE</i>	28
Analysis and Evaluation of the in vitro Antioxidant, Anti-enzymatic, Anti-mold and Cytotoxicity activities of Erodium trifolium (Cav.) <i>MESSAOUDI Noura</i>	29

Poster Communications

T1 PP 198	KAABI Ilhem	Molecular Docking Insights into the Dual Antioxidant and Enzyme-Inhibitory Potential of Azomethine SB	31
T1 PP 257	Chahrazed ESSEID	Etude phytochimique de l'extrait chloroforme d'une plante endémique saharienne du genre Pituranthos	32
T1 PP 305	Ahlem HACHELEF	Phytochemical analysis of Ranunculus arvensis L extracts	33
T1 PP 303	Hanane ZOUAOUI	Développement et caractérisation avancée de membranes composites à base de polyalcool vinylique modifié pour applications énergétiques et environnementales	34
T4 PP 90	FREIDJA Mohamed Lamine	In vitro Antioxidant and Antimicrobial Activity of Teucrium polium L. Extracts and Pistacia lentiscus L. Seeds' Oil	35
T1 PP 294	Faiza MERITATE	Phytochemical characterization of Eryngium pusillum Extracts	36
T5 PP 270	HARRAR Abdenassar	Integrating AI for Metabolite Identification from Mass Spectrometry Data: Challenges in Preprocessing and Neural Network Training	37
T5 PP 22	LATELLI Nadjia	Free Radical Scavenging Efficiency of Isatin Schiff Bases(O-H versus N-H). A DFT Study	38
T1 PP 60	FELLAHI Zineb	Synthesis, crystallographic study and molecular modeling of the compound edta chloride monohydrate	39
T3 PP 295	Soumia BENLECHHEB	Structural, optical and electronic properties of Cd _{0.25} Zn _{0.75} S semiconductor for energy and environmental applications	40
T1 PP 278	CHADI Sara	Activité antioxydante, anti-inflammatoire et antibactérienne d'Anthemis pedunculata	41
T2 PP 31	SAIDAT Fatma	Calorimétrie, résistance et microstructure d'un liant active à base de metakaolin	42
T1 PP 203	TAHARCHAOUCH E Djamel	Evaluation of the Hydrolytic Degradation of Triphenylmethane Dyes Using DFT and TD-DFT Methods	43
T1 PP 292	Faiza MERITATE	Assessment of Biological Activities of Medicinal Plant	44
T3 PP 50	HENINI Ghania	Evaluation of the biosorption kinetics and thermodynamics for the removal of textile dye from aqueous solutions using calcined opuntia ficus indica	45
T3 PP 181	SIASSI Abderrahim	Investigating the structural and optical properties of manganese oxide nanoparticles synthesized via the sol-gel method	46

1st International Hybrid Seminar on “Green Chemistry and Artificial Intelligence: Towards Molecular Design” (GCAITMD'25 M'sila - Algeria)

T3 PP 131	BEN KOUIDER Tayeb	Enhanced Methylene Blue Adsorption from Water Using Fe ₂ O ₃ -Decorated Kaolinite	47
T3 PP 2	OUADAH Mustapha	Amélioration de l'ultrafiltration des margines par couplage aux ultrasons « la sono-ultrafiltration	48
T3 PP 251	TEBERMACINE Ouarda	Physical and chemical properties of nanomaterial spinel oxide doped with magnesium.	49
T3 PP 230	MECHEHOUD Naima	Comparative Analysis of the Physicochemical and Morpho-Structural Characteristics of a Nanomaterial Synthesized by Sol-Gel, Precipitation, and Hydrothermal Methods	50
T3 PP 271	GHERBI Khouloud	A DFT study of the 2D nanomaterial -hydrogenated silicene	51
T3 PP 108	MAHI Ahmed	Etude de la Fixation Du Ni ²⁺ et Cr ³⁺ par la Resine Acide Para-Aminobenzoique-Formol	52
T3 PP 84	AMITOUCHE Dahbia	Iron-Vanadyl based Keggin Polyoxometallates for clean synthesis of Adipic Acid	53
T3 PP 273	BENDEBANE Hawa	Dégradation avancée du bleu de méthylène par un procédé Fenton-like modifié : Application du plan Box–Behnken	54
T5 PP171	MOKHTARI Djihad	First principle study on Half metallic properties of MnSb compound in the two structures hexagonal and zinc-blende, by employing Ab initio calculations	55
T3 P P 281	REFICE Lamouri	Investigation of structural, mechanical, electronic, optical, and dynamical properties of cubic MgLiF ₃ , MgLiH	56
T3 PP 21	HAMZA Laila	Magnesium Oxide Nanoparticles Synthesized Using Olive Leaf Extract for Environmental Remediation	57
T3 PP 297	Mustapha BOUBATRA	Enhanced Visible Eriochrome Black T Degradation using ZnS/TiO ₂ Heterojunction Nanocatalysts	58
T3 PP 142	ASSELI Rabah	Electrolytic synthesis and characterization of Ni-W alloys from a chloride bath and citrate as complexant.	59
T3 PP 137	Djaber SABAH	Removal of Dye Pollutants from Wastewater Using Activated Carbon Supported by Nano-oxides for the Adsorption Process	60
T4 PP 83	BENMAHAMMED Ahmed	Antibacterial,Antidiabetic,and Hepatoprotective Activites of the Polyphenol rich extract from pulicaria odora	61
T4 PP 72	GUETTOUCHI Ahlam	Molecular markers and their applications on the date palm (<i>Phoenix dactylifera L.</i>)	62
T4 PP 266	BRIKI Lyamine	Alkaline activation of a geopolymers based on industrial mineral waste	63
T4 PP 199	ZITOUNI Khalida	Enhancing Plant Fiber Properties via Chemical Modification: A Review	64
T4 PP 211	KEMEL Hadjer	Alkaloid Profiling of Peganum harmala Extract by LC-ESI-QTOF-MS/MS and Evaluation of Its Pharmacological Activity Against Cancer Cell Lines	65
T4 PP 25	DJELLAL Amel	Valorization of Olive Wood Ash for the Debittering Step in Green Table Olive Processing	66
T4 PP 239	BOUCHELKIA Imene	Hydrogen Production from Plastic Waste via Pyro-Gasification: Dynamic Simulation Using Aspen Plus	67
T4 PP 189	ASLOUM Abdelmadjid Yagoub	Toxic activity of the Chemical Components of <i>Coriaria myrtifolia</i> on the Survival of <i>Drosophila melanogaster</i> .	68
T1 PP 309	Abdelhalim SAADI	Health Risks of Consuming Spirulina Grown in Mineral-Enriched Media	69
T4 PP104	ZERROUKI Sara	Phytochemical investigation of an Algerian. Plant: a green approach for bioactive compounds discovery	70
T4 PP 33	CHEBIRI Fatima	Phytochemical Analysis and Evaluation of the Antioxidant Activity of Methanolic and Aqueous Extracts of <i>Cynoglossum creticum</i>	71
T4 PP 91	MEZHOUD Bilel	Punica Granatum derived compounds as green corrosion inhibitors for zinc in acidic environments	72
T5 PP 170	HENTABLI Mohamed	AI-Driven Modeling of Occupational Exposure Limits for Active Pharmaceutical Ingredients Using Cheminformatics and Machine Learning	73
T4 PP 302	Wassila REMACHE	Solar light-Induced Degradation of Cresol Red in the Presence of the Fe(III)-NTA Complex	74
T1 PP 14	Meriem HAMPLA	Formulation and Assessment of an Environmentally Friendly Dishwashing Detergent from Biosourced Surfactants	75

1st International Hybrid Seminar on “Green Chemistry and Artificial Intelligence: Towards Molecular Design” (GCAITMD'25 M'sila - Algeria)

T1 PP 99	BELHADDAD Oum El-Kheir	Qualitative and quantitative phytochemical analysis and biological activities of Fraxinus excelsior L extracts	76
T1 PP 9	AMAMRA Samra	Moringa Oleifera fruit extracts: Phytochemical Screening, Antioxidant and Antibacterial Activities	77
T1 PP 103	MOHAMADI Sabrina	Antimicrobial and antioxidant activities of aqueous extracts of Rhus tripartita species	78
T1 PP 215	CHENNA Malika	Valorization of biofloculants for the Textile dyes by coagulation Flocculation Green chemistry	79
T1 PP 303	Abdelouahab DIAFAT	Zinc tolerance and growth adaptation of malva sylvestris l. In Zinc contaminated soils	80
T1 PP 109	Abdeslem BOUZINA	Microwave-assisted synthesis of imino-acridine derivatives with antioxidant potential: combined in vitro and in silico investigations	81
T4 PP 95	Meftah ALLAL	Étude de la durabilité du béton contenant des granulats recyclés traités et de son amélioration face aux attaques chimiques	82
T4 PP 200	Aida KEMMOUNDJI	In vivo anti-inflammatory and antibacterial activities of n-Butanol Extract from an endemic Algerian Ficus	83
T1 PP 216	BOUDJELAL Amel	On Vivo wound healing and molecular docking studies support traditional use of Arisarum vulgare aqueous extract	84
T1 PP 03	SAGHIRI Khadijah	Structure-Based Design and Pharmacokinetic Studies of Novel GAC Inhibitors for Triple-Negative Breast Cancer	85
T1 PP 106	BENZEGGOUTA Naïrouz	Plantes Médicinales Anti-inflammatoires Citées dans la Médecine Prophétique	86
T1 PP 259	BOULEGHLEM Hocine	Eco-Responsible Extraction of Collagen from Food Waste: Towards a Green Approach	87
T1 PP 24	BENABILA Nabila	Theoretical Study of Excess Molar Volumes in Binary Mixtures of Alkoxyethanols and Selected Amines Using DFT	88
T1 PP 178	MAKOUF Naouel	Synthesis, Structure and Molecular Docking Studies of a Cobalt(II) Complex Derived from Phthalimide Ligands	89
T1 PP 220	BOUCHELOUCHE Kenza	Phytochemical screening, biological activity and corrosion inhibition of a medicinal plant	90
T1 PP 121	SAHKI Feriel Aouatef	Synthesis, Crystal Structures, Antioxidant Activity and Molecular Docking Studies of a Thiomethylbenzimidazole Ligand and Its Mononuclear Zn(II) Complex	91
T1 PP 163	SEBAI Ibtissam	Visible light induced hydrogen evolution from water on the hetero-system 10% NiO/ γ -Al ₂ O ₃	92
T1PP268	LACHACHE Sabira	Physicochemical study of Medicinal plants in the region,Algeria	93
T1 PP 78	HADJI Maroua	LC-MS/MS Characterization of Phenolics and Green Synthesis of Antibacterial Silver Nanoparticles from the Acetonic Extract of Algerian Daucus carota	94
T1 P P 260	ZIDANE Salima	Evaluation of a Binary Complex for Use in Cosmetics	95
T1 PP 245	BENADEL Zohra	Extraction And Treatment Of Cellulosic Fibers From Date Palm	96
T1 PP 300	CHABANE Sarra	Phytochemical Profile and Anticancer Potential of Pituranthos scoparius	97
T2 PP 75	CHETIOUI Souheyla	Cu(II) coordination polymer bearing diazenyl-benzoic ligand: Synthesis, physicochemical and XRD/HSA-interactions	98
T2 PP 193	KADI Souad	The role of Artificial Intelligence in sustainable smart food packaging: Recent advances	99
T2 PP 136	KALOUN Amina	: Optimized PVA-Based Cationic Membranes for Efficient Dual-Electrolyte Water Electrolysis.	100
T2 PP 13	GHERBAOUI Fatima	Contribution to the Study of the Physico-Chemical Quality of Water in the Hodna Basin	101
T2 PP 227	MOKRANE Amira	Thermal Stability of Sol-Gel Derived Hydroxyapatite for Ca/P Molar Ratio 1.67 and 1.5	102
T3 PP 64	MAALMI Mohamed	Experimental study of the effect of nitric acid on wollastonite synthesis via sol-gel method	103
T3 PP 147	GHARNOUT Zahia	PVA-Based Proton-Exchange Membranes for Energy-Efficient Dual-Electrolyte Water Electrolysis.	104
T3 PP 76	TURQUI Tarik	Eco-Friendly Synthesis of AgNPs Using Asteraceae Extract and Their Comparative Antioxidant Potential	105

1st International Hybrid Seminar on “Green Chemistry and Artificial Intelligence: Towards Molecular Design” (GCAITMD'25 M'sila - Algeria)

T3 PP 231	SAADI Taieb	Electronic structure, mechanical and optical properties of hydrogen storage alkaline amides XNH ₂ (X = Li, Na) compounds.	106
T3 PP 233	REDAOUI Samiha	The morphology ,electro chemical performance and characterization of nanostructured α -PbO prepared from spent lead acid battery negative plate	107
T3 PP 117	Oualid DILMI	Effect of potential on the electrochemical nucleation and growth of the nanostructured indium thin film	108
T3 PP150	LAKHAL Lynda	The effect of physical properties of nanostructural ZnSe quantum Dots	109
T3 PP 190	CHAHLAT Said	Computational Study of a Half-Heusler Alloy Using Ab Initio Methods	110
T3 PP 138	SADEDDINE Sarra	solvothermal syntesis ,characterization and antibacterial activity of undoped and Ag doped ZnO	111
T3 PP 212	MEZRAG Fadila	Band gap energies and optical properties in nanostructured semiconductor InAs: The Effect of Quantum Confinement	112
T3 PP 132	CHENAGUE Hanane	Spray Pyrolysis Deposition of Aluminum- Doped Zinc Oxide(AZO) Thin Films for Energy Applications	113
T3 P P133	TALHI Souaf	Removal of Methyl Orange dyes from water Utilizing Layered Double Hydroxide (NiFeCO ₃).	114
T3 PP 97	TIAIBA Wafa	Efficient Methylene Blue Adsorption: Experimental & DFT Analysis of H ₃ PO ₄ -Activated Date Palm Carbon	115
T3 PP 236	KHENICHE Abdelhakim	Optimisation des membranes protoniques à base de PVA sulfoné : effet des agents de réticulation sur les propriétés électrochimiques et thermomécaniques	116
T3 PP 192	DJELLALI Brahim Said	A Theoretical Framework for Modeling the Nonlocal Mechanical Behavior of Protein Networks in Biomolecular Resonant Sensors: Integrating Hydrogen Bonding and van der Waals Interactions	117
T3 PP 219	DILMI Souad	Electron-Phonon Coupling and Superconductivity in YC ₂ via first principle calculation	118
T3 PP 246	DJERIOUI Ammar	جسيمات اكسيد النحاس وتفككها الضوئي للملوثات بالاستعمال التقنيات الحديثة.	119
T3 PP 284	SALMI Somia	Investigation into the photocatalytic degradation of red congo dye using semiconductor	120
T4 PP 40	HERIZI Achwaq	Sustainable Valorization of Wastewater Sludge: Resource Recovery for Energy and Soil Applications	121
T4 PP 269	KOUIDRI Djamilia	Physicochemical Characterization of a Natural Fiber Extracted from Kochia indica	122
T4 P P 93	BOUCHAREB Samira	Bioprocessing and structural valorization of natural lignocellulosic fibers for sustainable material development	123
T4 PP 145	HADJ KOUIDER Boubakr	Analyse de la composition chimique du quinoa et perspectives de valorisation pour l'alimentation humaine	124
T4 PP 149	LALLOUCHE Bahia	Évaluation de la valeur nutritionnelle et de la composition chimique de plants de blé destinés à la fabrication de chlorophylle alimentaire	125
T4 PP 186	YOUSFI Samia	The effect of nitrate ions on the electrochemical behavior of brass.	126
T4 PP 58	ATTOUI Warda	Elaboration et caractérisation d'un matériau composite à base de caoutchouc naturel renforcé par des fibres de verres, fibres végétales et hybrides.	127
T4 PP 70	HADROUG Aldjia	Comparative GC/MS Analysis of Essential Oil Profiles in Origanum glandulosum Desf. from Algeria and Tunisia	128
T4 P P 283	BOUCHAREB Khaled	Climatic Impact on the Performance of a Parabolic Trough Solar Power Plant: Case of the Semi-Arid Northern Region of Algeria and Southern Spain	129
T1 PP 312	Yousra MIHOUNE	Synthesis and Antioxidant Evaluation of Nitrovanillin Derivatives	130
T4 PP 62	MEFTAH Lamya	Development of Activated Carbon from Almond Shells: Physico-Chemical Characterization and Application in Wastewater Treatment.	131
T4 PP 238	BELAMRI Kenza	Développement des batteries Zn/MnO ₂ pour le stockage des énergies renouvelables : une alternative écologique basée sur la valorisation des ressources minérales abondantes.	132
T4 P P188	NESSARK Faiza	Etude de la tenue a la corrosion d'un acier a304 modifie par un materiau composite : polypyrrole/TiO ₂	133
T4 PP 86	MERABET Sarra	Effect of Thermal Environmental fluctuations on the corrosion behaviour of low-carbon steel alloy in saline conditions	134

1st International Hybrid Seminar on “Green Chemistry and Artificial Intelligence: Towards Molecular Design” (GCAITMD'25 M'sila - Algeria)

T1 PP 307	Samir BOUACHA	Pharmacophore Generation, 3D QSAR model, Molecular Docking studies and in silico ADMET Screening of Benzimidazole Derivatives as HCV NS5B RNA-dependent RNA Polymerase Inhibitors	135
T4 PP 306	Malika MERZOUGUI	Effect of Deformation and Annealing on the Microstructure and Mechanical Behavior of a Magnesium Alloy	136
T1 PP 310	Sarra BEKRI	Preparation and application of biomass-derived activated carbon for wastewater remediation.	137
T5 PP 311	Hesna BENSEDDIK	Valorization of biological studies of medicinal plant « thapsia garganica »	138
T1 PP 302	Abdelouahab DIAFAT	In vivo and in vitro anti-inflammatory and anti-arthritis effect of Peganum harmala. L	139
T1 PP 304	DRIF Seif Eddine	Synthèse de ZnO nanoparticules dopés Charbon actif à base des grains d'olive pour le traitement des eaux usées par photocatalyse solaire	140
T3 PP 311	Samir HAMRIT	RF-Magnetron Sputtered Vanadium-Doped ZnO Thin Films Derived from Sol-Gel Nanopowder Targets on Flexible PEN Substrates.	141
T3 PP 182	Zoubida HAMMOU	Characterization and modification of an Algerian clay and its application as an adsorbent	142
T4 PP 288	Hamza MEGHERBI	The effect of phosphoric acid on the physicochemical properties of activated carbons made from biomass leaves: porosity characteristics, surface chemistry, and adsorption capacity	143
T4 PP 314	LAIFA Fakhreddine	Effect of Alkaline Treatment on the Crystallinity Index and Crystallite Size of Silybum Marianum Lignocellulosic Fibers	144
T4 PP 77	KOADRI Zainate	Valorization of Local Renewable Materials for Sustainable Construction: Mechanical Reinforcement of Clay Composites	145
T4 PP 248	ABCHICHE Hacina	Energy Recovery and Regeneration of Used Engine Oils: Comparison between Pyrolysis and Combined Treatment Methods	146
T3 PP 322	Walid MENASRI	FP-LAPW and Hybrid Functional Study of the Half-Metallic Behavior in CuMnInSe ₃	147
T4 PP 264	Maria BOUCHIBA	Manufacture and characterization of a tube made from sand and plastic waste	148
T1 PP 197	ADOUI Nabila	Etude phytochimique d'une plante utile en médecine traditionnelle <i>Hertia Cheirifolia</i>	149

Oral Communications “Online via Google Meet”

T1 OEL74	ARAB Houda	Theoretical study of the interaction between proteins; collagen, keratin and blue indigo dye by molecular docking approach	151
T1 OEL 157	CHERAFT-BAHLOUL Nassima	Effet protecteur de l'extrait brut de feuilles de <i>Clematis flammula</i> sur la cicatrisation des ulcères chez la souris.	152
T1 OEL 56	ALLAB Yacine	Redox Behavior and Antioxidant Activity of Tetrazole-Based Ni (II) Complexes: A Green Solid-State Synthesis and DFT Study	153
T1 OEL 128	YAHLA Sara	Essential Oil of <i>Teucrium aureo-candidum</i> as a Natural Antibacterial Agent against Resistant Pathogens: A Docking-Guided Approach	154
T1 OEL 148	MAYOUF Nozha	In vitro anti oxidant capacity , Phytochemical Evaluation and anti inflammatory activity by Bsa of hydro Methanolic Extract from fruit	155
T1 OEL 156	BENATTIA Mohamed	Optimisation de la production d'hydrogène vert par électrolyse PEM. Application de plan Box-Behnken	156
T1 OEL 107	MERDJA Khedidja	DFT and Molecular Docking Insights into New Thiohydantoin Derivatives with Potential Biological Activity	157
T2 OEL 226	ARIS Serine	Development of biocomposites based on palm fiber for sustainable applications	158
T1 OEL 125	CHERAITIA Amina	Mechano-enzymatic and deep eutectic solvent (DES) mediated sulfoxidation reactions	159
T1 OEL 256	CHEHROURI Manel	Palladium (II) complexes of amphiphilic azoles as recoverable catalysts in Suzuki-Miyaura cross-coupling reaction.	160
T1 OEL 209	HASNI Ferdaous	Investigation of New Inhibitors as Anti-Alzheimer Agents Through Molecular Modeling Methods	161
T1 OEL 242	ZETCHI Amel	Détermination d'une nouvelle voie d' accès aux β -aminocétone et leurs effets thérapeutiques	162

1st International Hybrid Seminar on “Green Chemistry and Artificial Intelligence: Towards Molecular Design” (GCAITMD'25 M'sila - Algeria)

T1 O EL 8	HANTOUR Razika	Dosage des composés phénoliques et évaluation de l'activité antioxydante d'une plante de la famille des Malvacées	163
T5 OEL 26	TOUATI Hana	Comparison of DFT and AI-Predicted IR and NMR Spectra of (R)- and (S)- 1-Fluoroethanol	164
T1 OEL 168	GHERZOULI Hiba	Phytochemical study and antioxidant activity evaluation of the methanolic extract of <i>Borago officinalis</i> L.	165
T1 OEL 225	MENNANA Imene	Nouvelle voie de synthèse de Naphtoxazinone par un nouveau catalyseur	166
T1 OEL 115	AZIZI Nassima	Contribution to the study of the biological effect of <i>Citrullus colocynthis</i> seeds	167
T1 OEL 115	CHAHBAOUI Narimene	Combined Pharmacophore Modeling, 3D-QSAR, Molecular Docking, and Molecular Dynamics Simulations for the Identification of Novel Curcumin Derivatives Against Pancreatic Cancer	168
T2 OEL 191	DIKES Loubna	Isolation and Characterization of Biocorrosive Bacteria from Industrial Systems: A Step Toward Sustainable Infrastructure Protection	169
T2 OEL 160	BAIRA Fayçal	Electronic Characteristics and Deformation of Nanotubes Under Influence of an Electric Field	170
T2 OEL 54	Rahla Miloud	Elaboration des matériaux composites renforcés par des fibres Naturelles	171
T3 OEL 279	BOUSEMAT Hadjer	Modélisation et investigation expérimentale du processus d'adsorption binaire sur un adsorbant nanostructuré	172
T3 OEL 39	BOUIGHI Habib	Simulation of heat dissipation by twisted surface fins	173
T3 OEL 258	ELHABCHI Yasmine	Microbial Nanoparticle Synthesis: a sustainable method for Biocorrosion Mitigation in Oil and Gas Pipelines	174
T5 OEL 55	BOUDAUD Asma	Evaluating AI Models for IR Spectral Analysis of Phenol: Accuracy and Limitations in Molecular Characterization	175
T4 OEL 66	DELHOUM Hadia	Valorization of natural resources: study of the antimicrobial activity of <i>Plectranthus amboinicus</i> (Cuban oregano) extract	176
T3 OEL 35	KHELOUFI Slimane	Influence of Zinc Acetate Concentration on the Photoelectrochemical Performance of Chemically Deposited ZnO Films	177
T4 OEL 41	BOUBLATA Nour El Imene	<i>Hyoscyamus albus</i> : Une Plante Médicinale et Agricole à Redécouvrir	178
T4 OEL 291	BOUBRIK Fairouz	Valorisation D'extrait Acétate D'éthyle De Thé Vert (<i>Camellia sinensis</i> L.) Comme Ressource Naturel Renouvelable	179
T4 OEL 180	TOUATI Fatima Zohra Batoul	Soil Valorization Strategies in Barley Cropping Systems in Arid Agroecosystems: The Case of Ziban	180
T4 OEL 243	BOUNOURI Yassine	Valorisation de matériaux naturels pour le traitement d'eaux colorées : cas de l'Orange II	181

Poster Communications “Online via Google Meet”

T4 PE 210	CHOUIKH Nesrine	Antioxidant properties and preventive effect of aqueous leaf extract of <i>Pistacia lentiscus</i> L. against Oxaliplatin-induced oxidative stress in isolated rat liver mitochondria	182
T4 PEL 80	MEBARKI Moubarek	Élimination des colorants bleu de méthylène et rouge Congo dans une solution aqueuse à l'aide de biomasse de fêrle.	183
T4 PEL 12	LAKAS Manal	Pharmacological insights into the anti-inflammatory and antioxidant activities of <i>Anvillea radiata</i>	184
T4 PEL 51	GUENANE Nesrine	De la plante au potentiel thérapeutique : propriétés antitumorales prédites de <i>Teucrium polium</i> L.	185
T4 PEL 69	SAIDI Asma	Pharmacotoxicological study of aqueous and hydro-methanolic extracts of <i>Pergularia tomentosa</i> L.	186
T4 PEL 265	Saliha TORCHE	Contribution to an ethnobotanical study on plants with antiseptic and healing properties in the Khenchela and Batna regions	187
T4 PEL 255	BADAOUI Fatima Zohra	Quantitative ethnobotanical survey on the cosmetic use of plants in Constantine-Algeria	188
T4 PEL 262	ATAOUAT Zana	L'effet de prétraitement chimique sur la production de biogaz à partir des boues de la station d'épuration	190

1st International Hybrid Seminar on “Green Chemistry and Artificial Intelligence: Towards Molecular Design” (GCAITMD'25 M'sila - Algeria)

T4 PEL 101	KOUROULOU Zoubida	Extraction and Characterization of a Biopolymer from Biomass Waste	191
T1 PEL 113	GUENANE Wissem	Caractérisation Chromatographique et Spectrophotométrique des Composés Phénoliques d'une Plante Médicinale	192
T4 PEL 144	BOUTARFA Soumia	Antimicrobial activity of fruit peels extracts cultivated in Algeria.	193
T4 PEL 29	HOUITI Kaouthar	Sustainable Biocatalysis Using Yeast-Derived Enzymes: A Green Approach to Molecular Design	194
T4 PEL 202	KHEMKHAM Aicha	Phenolic content, antioxidant activity of essential oils of <i>Teucrium polium</i> and <i>Artemisia herba alba</i> : combination effect	195
T4 P EL 140	SAAD Fatima	Valorization of Eggshell-Derived Biosorbent for Efficient Dye Removal from Wastewater	196
T4 P EL 285	SAOUDI Soulef	Determination of bioactive compounds, anti-inflammatory and antioxidant properties of hydroalcoholic extract of <i>Galium aparine</i> L	197
T4 P EL 73	BELAID Taous	Biosorption of Cu(II) using eggshell-alginate composite beads: kinetic and thermodynamic study	198
T4 P EL 286	HEDIA Nacera	Valorization of Faba Bean (<i>Vicia faba</i> L.) Residues through FTIR Characterization for Integration into Broiler Chicken Feed	199
T4 P EL 261	ADDA Messaouda	Characterization, phytochemical and biological activities of essential oils of few spontaneous plants in Tiaret region (Algeria).	200
T4 P EL 162	MELLAL Hanane	Enzymatic Bioprocesses from Thermal Bacterial Strains: Potential and Perspectives	201
T1 P EL 94	LAMOURI Abdelmouman	In silico exploring of phytochemistry components and in vitro bioactivity of essential oils: bioinformatics structure and biological prospects	202
T1 PEL19	ARAB Ouahiba	Phytochemical screening, therapeutic and medicinal virtues of a plant of the Ginkgoaceae family	203
T1 PEL 205	BOUNAB Souhila	Étude phytochimique et bioactivité des huiles essentielles d'une plante Asteraceae: <i>Artemisia herba-alba</i> provenance de Hassi Behbeh (wilaya de Djelfa, Algérie).	204
T1 PEL 222	FAR Hadjer	Organic Synthesis of New Proline-Based Metal Complexes: Spectroscopic Characterization and Antibacterial Potential	205
T1 PEL 45	BENAISSA Mohamed Rafik	Synthèse et Etude Théorique d'un Complexe de Cobalt(II) Incorporant un Triazole Substitué lié à la Phénanthroline	206
T2 PP02	BACHIR BEY Imene	Influence of Applied Voltage on the Fatigue Performance of Copper-Embedded Multifunctional Composites	207
T2 P EL 217	ABDELLAOUI Fatiha	Impact de l'antibiothérapie sur l'émergence de la résistance des Entérobactéries aux antibiotiques de la famille des bêta-lactamines	208
T2 P EL 207	FEKHAR Nassima	Resistance profile of <i>Staphylococcus aureus</i> (MRSA) isolates to antibiotics in infections in the hospital CHU in the West region of Algeria	209
T1 P EL 167	MAYOUF Nozha	Screening of Plant Extract for Antioxidant Activity and anti inflammatory effect by the method of egg albumin	210
T1 P EL 81	LAHRECHE Saadia	Removal of pollutant by adsorption process using an activated carbon adsorbents prepared from prickly pear fruit seeds	211
T3 P EL 224	MAKHLOUFI Mohamed Cherif	Green Chemistry for Environmental and Industrial Transformation	212
T5 P EL 37	GUENDOZ Djema	First principles calculations on structural, mechanical and optical properties of alkaline earth hydride CaH for hydrogen storage applications	213
T2 P EL 32	AMIRA Aicha	In vitro antibacterial activity of methanolic leaf extract of <i>Eucalyptus citriodora</i>	214
T5 P EL 11	REZAZI Sarah	Ai And Molecular Design: Harnessing Artificial Neural Networks For High-Fidelity Prediction Of Anti- Inflammatory Compounds	215
T3 P EL 104	BEKKAR Fadila	Highly Efficient Photocatalytic Degradation of Methylene Blue Dye Using Sodium Alginate/TiO ₂ Nanocomposites	216
T1 P EL 223	RADJA Djamaia Sabiha	Teneur en 5-hydroxyméthylfurfural (HMF) dans les miels de la région de Mostaganem	217
T1 P EL 213	GHECHAM Abdelmoudjib	In Silico Molecular Docking of LC-MS-Identified Phytocompounds as Potential α -Amylase Inhibitors	218
T3 P EL 277	BELAIDI Ouafa	Organometallic nanostructures for efficient dye removal: Towards greener water treatment technologies	219

1st International Hybrid Seminar on “Green Chemistry and Artificial Intelligence: Towards Molecular Design” (GCAITMD'25 M'sila - Algeria)

T3 P EL 263	ZITOUNI Imene	Functionalized Kaolin with Green-Synthesized TiO ₂ Nanoparticles for Dye Adsorption	220
T1 P EL 53	BOUNAB Bochra	A novel green synthesis of a nanomaterial using plant extract, optimization of operating parameters	221
T1 P EL 150	HEBBACHE Zahida Yasmina	Contribution of Pituranthos Scoparius to green chemistry : extraction and therapeutic valorization	222
T1 PEL 96	SADLI Houssam Eddine Mustapha	Polyphenolics Compounds and Antioxidant Activity Using DPPH Assay of Four Thymus Species from Western Algeria	223
T1 PEL87	BAKI Samira	Etude théorique de la réaction de cycloaddition dipolaire-1,3 du nitroso oxide avec le fluoroéthylène.	224
T1 PEL 208	KHELIFA Sonia	Box-Behnken experimental approach for the removal of cationic dyes via a green emulsified liquid membrane	225
T1 PEL 183	CHERAIET Zine Laabidine	Synthesis and biological activities α -amino phosphonate derivatives of thiadiazol	226
T1 PEL 100	LITIM Sarra	Antidiabetic Activity of Cold-Pressed Linseed and Chia Seed Oils	227
T1 PEL 01	BOUYA Sara	Développement de plateformes d'intelligence artificielle pour l'optimisation accélérée de catalyseurs en chimie verte : vers des procédés moléculaires plus innovants et performants	228
T1 PEL 154	SAOUDI Besma	Synthèse de dérivés polycycliques originaux comportant comme structure de base un noyau Pyrazole via une réaction d'arylation directe catalysée par le palladium	229
T1 PEL 214	BOUAFIA Waffa	In Silico Evaluation of Plant-Derived Flavonoids Identified by LC-MS as Potential Antibacterial Agents Against Gram-Positive and Gram-Negative Bacteria	230
T1 PEL 85	MEKKI Sofiane	Copper triazole complex supported on Fe ₃ O ₄ @SiO ₂ nanoparticles as eco-friendly nanocatalyst in solvent-free Biginelli reaction	231
T4 PEL 158	Karim TIGHILET	Impact of Extraction Methods on Phytochemicals and Bioactivity: A Green Chemistry Approach	232
T3 PEL 224	MAKHOULFI ALI	Multiscale Modeling Of Moisture Diffusion In Polymer/Clay Nanocomposites	233
T1 P EL 28	KARKOURI ILHAM	Computational Approaches to Screening Plant Phytochemicals: Molecular Docking, ADME Prediction, and Experimental Correlation: A Literature-Based Review	234
T4 P EL 122	SADOK Zeyneb	Valorisation of Alfalfa Sprouts as a Source of Antioxidant and Anti-Inflammatory Bioactive Compounds	235
T4 P EL 280	LAKHDARI Chafika	Green drying strategies and IA driven modeling for the valorization of capparid Spinoza buds as functional ingredients	236

Plenary



APPLICATIONS DE L'ENERGIE SOLAIRE THERMIQUE A LA DEPOLLUTION DE L'EAU ET DES SOLS

DJEHICHE Mokhtar



*Laboratoire des Matériaux Organiques, Université de M'sila, Pôle
Universitaire, Route Bourdj Bou Arreidj, M'sila 28000 Algérie*

E-mail address: mokhtar.djehiche@univ-msila.dz

Résumé : L'énergie solaire thermique constitue une composante essentielle des énergies renouvelables, au même titre que le photovoltaïque, l'éolien ou l'hydraulique. Contrairement au photovoltaïque, qui convertit directement le rayonnement solaire en électricité, le solaire thermique utilise cette énergie pour produire de la chaleur. Celle-ci est captée par des dispositifs spécifiques qui la transmettent à un fluide caloporteur (généralement de l'eau, de l'huile thermique ou un mélange eau-glycol). Le fluide chauffé peut ensuite être valorisé selon plusieurs usages : production d'eau chaude sanitaire, chauffage des bâtiments, approvisionnement des procédés industriels, ou encore production d'électricité dans des centrales solaires thermodynamiques. Dans cette présentation, nous mettons en lumière une application émergente et particulièrement prometteuse de cette technologie : l'élimination des polluants présents dans l'eau et dans les sols, grâce à des procédés thermiques et photo-thermiques favorisant la dégradation ou la désorption des contaminants.

Mots clés : Énergie solaire thermique ; Fluide caloporteur ; Dépollution ; Photo-dégradation ; Contaminants.

ECOCATALYSIS AND ASYMMETRIC ORGANOCATALYSIS, A NEW VISION OF GREEN AND SUSTAINABLE CHEMISTRY

Nour-Eddine AOUF, Professeur Emérite



L.C.O.A. Groupe de Chimie Bio-Organique, Faculté des Sciences, UBM Annaba.

E-mail address: aoufnoureddine18@gmail.com

Abstract: Every year, we discover with horror that we are depleting the planet's resources faster and faster. Earth Overshoot Day marks the date when humanity's demand for ecological resources and services in a given year exceeds what Earth can regenerate in that year. In 2025, Earth Overshoot Day lands on July 24, the earth is now living on credit. Green chemistry is the design of chemical products and processes that reduce or eliminate the use and generation of hazardous substances. Sustainable development as “development that meets the needs of the present without compromising the ability of future generations to meet their own needs”. 17 Sustainable Development Goals which are an urgent call for action by all countries it is a priority for the well-Being of the planet. Asymmetric organocatalysis has been a key part of pharmaceutical research and production. The methods pioneered by List and MacMillan have allowed synthesis of important molecules without the intensive use of environmentally damaging heavy metals. A new vision of green and sustainable chemistry based on a well-established concept named Ecocatalysis, this strategy is based on the capacity of plants to adapt to stresses caused by high concentrations of metal elements in their environment; In this contribution, we present some work from our group concerning the synthesis of α -aminophosphonates and hydroxyphosphonates, the chemistry of protective groups as well as the design of compounds for therapeutic purposes which use some principles of green chemistry.

Keywords: Sustainable development. Green chemistry. Ecocatalysis. Asymmetric organocatalysis. Eco-friendly synthesis.

CHIMIE VERTE ET INTELLIGENCE ARTIFICIELLE POUR LES AGROSYSTEMES DURABLES: UNE SYNERGIE INNOVANTE POUR OPTIMISER L'ASSOCIATION CULTURALE BLE–LEGUMINEUSE

Wissem HAMDİ¹, Amira SOUID¹, Amal ATTALAH¹



¹Université de Gabès, Institut Supérieur des Sciences et Techniques des Eaux, 6029 Gabès, Tunisie

*Corresponding author: Wissem Hamdi, Tel./Fax: +21697071986

E-mail address: wissemhamdi@yahoo.fr

Résumé : La chimie verte vise à réduire la dépendance aux intrants chimiques et à valoriser les processus biologiques pour améliorer la durabilité agricole. Dans ce cadre, l'association céréales–légumineuses constitue une approche agro–écologique prometteuse. Deux expérimentations ont été menées : en conditions semi-arides du Sud tunisien (2020–2022) et sur sols alluviaux pauvres en carbone, azote et phosphore, comparant le blé dur (*Triticum turgidum ssp. durum L.*) et le pois chiche (*Cicer arietinum L.*) en monoculture et en association. Les résultats révèlent une amélioration significative des paramètres agronomiques et biogéochimiques : augmentation de l'azote total du sol (+32 % et +29 %), du carbone total (+27 % et +24 %), de l'absorption d'azote par le blé (+26 % et +21 %) et du rendement (+23 % et +20 %). Concernant le phosphore, la disponibilité a progressé de +28,45 % en association, accompagnée d'une diminution du pH rhizosphérique (–0,44 et –0,11 unités) et d'une stimulation de la biomasse microbienne P. L'intégration de l'intelligence artificielle (IA) permet de renforcer ces résultats par la modélisation et la prédiction des dynamiques sol–plante–microbiote. Des approches de *deep learning* et de systèmes experts agricoles ont été appliquées à des jeux de données multi–sources combinant paramètres climatiques, propriétés physico–chimiques des sols, mesures issues de capteurs *IoT* (humidité, pH, température, nutriments) et données microbiologiques. Les modèles entraînés ont permis d'atteindre une précision prédictive de 85–90 % pour l'estimation des flux d'azote et de phosphore, et de 80–85 % pour la prévision des rendements en fonction de différents scénarios climatiques. Ces résultats démontrent la capacité de l'IA à optimiser en temps réel les densités des cultures associées, la gestion des nutriments et la réduction des apports d'engrais de synthèse. La synergie observée entre pratiques agricoles inspirées de la chimie verte et outils numériques intelligents confirme qu'il s'agit d'un levier stratégique pour la conception de systèmes agricoles plus durables, productifs, résilients et sobres en ressources.

Mots-clés : Association blé–légumineuse, Flux d'azote et de phosphore, Agrosystèmes durables, Chimie verte, Intelligence artificielle.

DEVELOPMENT OF A PROTOTYPE FOR HYDROGEN PRODUCTION AND INDUSTRIAL AND/OR URBAN WASTEWATER TREATMENT USING VARIOUS ELECTROCHEMICAL TECHNIQUES BASED ON SOLAR ENERGY

Boulbaba LOUHICHI, Wissem HAMDI, NOUREDDINE HAMDI.



*Higher Institute of the Sciences and Techniques of Waters of Gabes, Tunisia University of Gabes,
Department of Chemical Process Engineering, National Engineering School of Gabes,
Center of Research in Materials Sciences (CNRSM), B.P.73, 8020 Soliman, Tunisia*

E-mail address: boulbabaiaa@yahoo.fr

Abstract: This study addresses the dual challenges of sustainable energy production and wastewater treatment by developing and evaluating an integrated prototype. The research focuses on the treatment of industrial wastewater contaminated with recalcitrant organic compounds, such as tannic acid (TA), and the simultaneous production of green hydrogen. Advanced electrochemical processes, including electrocoagulation (EC) and the electro-Fenton reaction (E-Fenton), powered by solar energy, were investigated for their efficiency and environmental sustainability. Experimental results demonstrated the system's dual functionality. Electrocoagulation using aluminum electrodes significantly removed tannic acid, reducing a solution to 600 mg/L in 30 minutes, while simultaneously producing a hydrogen volume of $102.2 \times 10^{-6} \text{ m}^3$. The electro-Fenton process was found to be superior in pollutant degradation. The use of solar energy as the primary energy source highlighted the economic and environmental viability of the process by minimizing operating costs and carbon footprint.

Keywords: Electrocoagulation, Electro-Fenton, Tannic Acid, Green Hydrogen, Solar Energy, Wastewater Treatment, Advanced Oxidation Processes.

SYNTHESIS OF NEW GREEN COMPOSITE ZEOLITE/ACTIVATED CARBON: ADSORPTION OF NON-STEROIDAL DRUG AND VOLATILE ORGANIC COMPOUNDS

Noureddine Hamdi^{1,3}, Imen Amri¹, Aymen Amin Assadi²



¹ Higher Institute of Water Sciences and Techniques, University of Gabes, 6072 Zrig, Gabes, Tunisia

² College of Engineering, Imam Mohammad Ibn Saud Islamic, University, IMSIU, Riyadh 11432, Saudi Arabias

³ Composite Materials and Clay Minerals Laboratory, National Center for Research in Material Sciences, Technopole Borj Cedria, 8020 Soliman, Tunisia

*Corresponding author: Tel./Fax: +21697598648

E-mail address: nouryhamdi@gmail.com

Abstract : In this study, pure synthesised zeolite and synthetic activated carbon were investigated as adsorbents for Non-Steroidal drug (diclofenac) and volatile organic compounds (VOCs) such chloroform and dimethyl disulfide. Here, zeolites were synthesised from Illito-Kaolinitic clay of Tejra region (South-east of Tunisia), while a novel activated carbon was synthesised from wooden tongue depressor waste collected from hospitals during the first wave of covid-19 pandemic. The mineralogical properties of raw clay and the synthesized materials were determined using X-ray diffraction (XRD) and Attenuated Total Reflectance-Fourier Transform Infrared (ATR-FTIR) spectroscopy. Morphological characteristics were determined using scanning electron microscopy (SEM), which revealed a high degree of particle size uniformity in zeolite and a well-developed, clearly defined structure in activated carbon. The Na-P1 zeolite shows a high-cation exchange capacity, reaching 279 meq/100 g. BET (N₂ adsorption-desorption) analysis reveal a high specific surface area (1512 m²/g) and a mean pore volume equal to 0.621 cc/g. A fraction of the synthesised activated carbon has been added to zeolite which enhanced its mesopores characteristics, thus increasing its adsorption capacity. Additionally, Kinetic model data are well fitted to pseudo-second order. The Langmuir model provides the best fit for isothermal adsorption equilibrium data, and according to this model, the zeolite-activated carbon composite demonstrated a maximum adsorption capacity of 54.13 mg/g for chloroform and 28.16 mg/g for dimethyl disulfide.

Keywords: Natural clay, Covid-19 waste, Zeolites-activated carbon composite, Chloroform and DMDS gas adsorption, Adsorption modelling

SUPERCONDENSATEURS : LA REVOLUTION ENERGETIQUE AU SERVICE DES TECHNOLOGIES DE DEMAIN.



Ahmed BAHLOUL ^{1,2}

¹ Laboratoire des substances organo-thérapeutiques et des procédés durables, Faculté des sciences, Université Mohamed Boudiaf, M'sila, 28000

² Laboratoire d'électrochimie et d'environnement, Faculté des sciences et de latechnologie, Université Mohamed El Bachir El Ibrahimi, Bordj Bou Arréridj, 34000

E-mail address: ahmed.bahloul@univ-msila.dz

Résumé : Avec la transition énergétique et les avancées technologiques, il devient indispensable de repenser notre manière de stocker l'électricité. Dans ce contexte, les supercondensateurs jouent un rôle de plus en plus central. Bien plus qu'un simple complément aux batteries, ils offrent des performances impressionnantes et ouvrent de nouvelles perspectives. Contrairement aux batteries classiques, ils stockent l'énergie de façon physique plutôt que chimique, ce qui leur permet de délivrer une puissance exceptionnelle et de supporter des centaines de milliers de cycles sans se dégrader. Leur longévité quasi illimitée les rend particulièrement attractifs pour les applications où la fiabilité est cruciale. Les recherches récentes, notamment sur les supercondensateurs à base de graphène et d'autres matériaux nanostructurés, ont constamment repoussé les limites de la densité d'énergie. L'objectif est clair : combiner la puissance remarquable des supercondensateurs avec l'autonomie des batteries, pour imaginer des systèmes de stockage toujours plus performants et adaptés aux besoins de demain.

Mots-Clés : Supercondensateurs ; Graphène ; Transition énergétique ; Nanomatériaux ; Stockage d'énergie.

Oral Communications

EQUILIBRIUM, KINETIC AND THERMODYNAMIC STUDIES OF THE BIOSORPTION OF TEXTILE DYE FROM AQUEOUS SOLUTIONS ONTO OPUNTIA FICUS INDICA CORDS

L Aidani Ykhlef^{1,*}, HENINI Ghania², HENTABLI Mohamed³, BENDRISS Elhouari⁴

^{1,3}Laboratory Chemical Vegetal - Water – Energy, University of Chlef, Algeria

^{2,4}Laboratory Environment-Water, University of Chlef, Algeria

*Corresponding author: +213 7 98 61 11 48, l.ykhle@gmail.com

Abstract: This study explores the possibility of using opuntia ficus indica Cords to remove Bemacide Red from aqueous effluents. The removal of Bemacide Red was investigated in both batch and continuous processes. Batch mode adsorption studies were performed by varying parameters such as contact time, pH, initial Bemacide Red concentration and temperature. The different adsorption models Langmuir, Freundlich, Elivoch and Temkin were used for the mathematical description of the adsorption equilibrium, and it was found that the very well - equipped experimental data for the Langmuir model ($R^2=0.961$), the pseudo - first - order and pseudo - second - order kinetic models were applied to the experimental data. The experimental data fitted very well the pseudo-second-order kinetic model ($R^2= 0.965$) and also followed the model of intra particle diffusion for concentrations between 5 and 50 mg/L), whereas diffusion is not the only rate - control step. Finally the thermodynamic parameters for the adsorption of Bemacide Red onto cords were also determined. The negative sign of ΔS° shows the decreased randomness at the solid - solution interface during adsorption, and the negative sign of ΔH° indicates that the adsorption process is exothermic. The negative sign of ΔG° confirms the spontaneous nature of the adsorption process, physical reaction.

Keywords : Opuntia ficus indica cords, dye, Isotherm; Thermodynamics; Kinetics.

CHARACTERIZATION AND ELECTROCHEMICAL BEHAVIOR OF NEW SYNTHESIZED ZINC (II) TETRADENTATE SCHIFF BASE COMPLEX

MAGHRAOUI Nadjah^{1*}, MERZOUGUI Moufida¹ and OUARI Kamel²

¹ *Laboratory of Electrochemistry, Molecular Engineering and Redox Catalysis, Sétif-1 Farhat Abbas University, Algeria*

² *Laboratory of Electrochemistry and Environment, Faculty of Sciences and Technology, Mohammed El*

Bachir El Ibrahimi University, Bordj Bou Arreridj, Algeria

**Corresponding author: Tel./Fax: +213-0667-47-6607*

E-mail address: nadjah.magraoui@univ-bba.dz

Abstract: The first synthesis of imine function was performed by Hugo Schiff there is more than century. Most researchers have paid a particular attention to this class of compounds for its versatile structures inducing several applications in catalysis, electrocatalysis and in detection of biomolecules. This chemistry has been a considerable interest in coordination chemistry involving the transition metals as main reagents with Schiff bases as chelating agents. This is due to the fact that Schiff bases may stabilize many different metals in their various oxidation states In this work and regarding the influence of Schiff base structure on coordination of metal ions and the importance of zinc metal ion with their catalytic and electrocatalytic properties, we report herein the synthesis of a new Zinc (II) Schiff base complex through the reaction of a new Tétradentate ligand with a stoichiometric amount of zinc acetate in methanol. This zinc (II) complex was characterized by the different spectroscopic methods such as, UV visible, FT-IR. As well, the electrochemical Behavior of the complex in deoxygenated DMF solution containing LiCO₄ as a supporting electrolyte was explored using cyclic voltammetry.

Keywords: Synthesis, Schiff base complex, Spectroscopic characterization, Cyclic voltammetry.

ANTIBACTERIAL ACTIVITY OF HYDROETHANOLIC LEAF EXTRACT OF *ZIZIPHUS SPINA-CHRISTI* AGAINST GRAM-POSITIVE AND GRAM-NEGATIVE BACTERIA

Dalila BENCHEIKH ^{1,2*}, AICHOUCHE Abir ^{1,a}, BAKRI Chima ^{1,b}, SEDDIK Khennouf ^{2,a}, Saliha DAHAMNA ^{2,b}

^{1*}Department of Biochemistry and Microbiology, Faculty of Sciences, University of M'sila, University Pole, Road Bourdj Bou Arreidj, M'sila 28000, Algeria. <https://orcid.org/0000-0003-0992-2987>

²Laboratory of phytotherapy applied to chronic diseases. Department of Animal Biology and Physiology

^{1, a} Department of Biochemistry and Microbiology, Faculty of Sciences, University of M'sila, University Pole, Road Bourdj Bou Arreidj, M'sila 28000, Algeria.

^{1, b} Department of Biochemistry and Microbiology, Faculty of Sciences, University of M'sila, University Pole, Road Bourdj Bou Arreidj, M'sila 28000, Algeria.

^{2, a} Laboratory of phytotherapy applied to chronic diseases. Department of Animal Biology and Physiology,

^{2, b} Laboratory of phytotherapy applied to chronic diseases. Department of Animal Biology and Physiology,

* Correspondence: dalila.bencheikh@univ-msila.dz

Abstract: *Ziziphus spina-christi*, a member of the *Rhamnaceae* family, is a commonly used medicinal plant in Algeria. used historically to treat a variety of illnesses. The purpose of this study was to assess the hydroethanolic leaf extract of *Ziziphus spina-christi*'s antibacterial activity. The tests revealed a richness in bioactive compounds, notably polyphenols, with a content of 104.19 ± 0.07 mg GAE/g of extract. *Staphylococcus aureus*, *Bacillus subtilis*, *Salmonella*, et *Escherichia coli* were the four bacterial strains that were tested with three extract concentrations (200mg/ml, 400mg/ml, and 600mg/ml). The findings showed that as extract concentration rose, so did its antibacterial efficacy. *Salmonella* showed the least amount of activity, followed by Gram-positive bacteria (*S. aureus* and *B. subtilis*). At all tested concentrations, the extract did not cause any sensitivity in the Gram-negative bacterium *E. coli*. These results demonstrate *Ziziphus spina-christi*'s potential as a natural antibacterial agent that works especially well against Gram-positive bacteria.

Key words: Antibacterial activity, hydroethanolic extract, *Ziziphus spina-christi*, Gram-positive, Gram-negative

3D-PRINTED POLYMER PHONONIC STRUCTURES FOR THE DETECTION AND CHARACTERIZATION OF ACETIC ACID

Fahima ARAB*¹, Fares KANOUNI¹

¹*Research Unit in Optics and Photonics, Center for Development of Advanced Technologies, University of Setif 1, El- Bez, Setif, 19000 Algeria.*

*Corresponding author: Corresponding author: **Fahima Arab** (farab@cda.dz)

Abstract: The challenge today is to develop advanced detection techniques able to accurately and rapidly detect and characterize all types of liquids. An essential component of many industrial processes and environmental monitoring applications, acetic Acid. In this work, a simulation study carried out in COMSOL Multiphysics Software presented to investigate and evaluate the performance of 3D-printed phononic structures, specially designed for the highly sensitive detection of acetic acid range of 25–35% with a step size of 1%. The sensor uses transmission peaks to identify the fluids. These peaks result from the resonance mode generated by the cavity. In this way, the transmission coefficient is an essential measuring tool. Our results show the efficiency of these 3D-printed polymer acoustic structures in allowing real-time detection and characterization of acetic acid in a range of different concentrations, demonstrating superior sensitivity and selectivity. This study highlights the great potential of 3D acoustic printing technology in creating integrated, robust, and cost-effective sensor platforms, which paves the way for advances in sensing.

Keywords: 3D Phononic crystal, acetic acid, liquid sensors, FEM, Transmission spectre.

REVEALING THE BIOAVAILABILITY AND GASTROPROTECTIVE ACTIVITY OF POLYPHENOLS FROM *CLEMATIS FLAMMULA* EXTRACT BY *IN VITRO* DIGESTION

Dina ATMANI-KILANI^{1*}, Lydia KAROU¹, Djebbar ATMANI¹, Naima SAIDENE¹ and Lamia HANIFI¹

¹*Department of Physical Chemistry, University of Bejaia, Algeria*

*Corresponding author: Tel. +213-07-7324-2860 ; E-mail address: dina.kilani@univ-bejaia.dz

Abstract: *Clematis flammula* is a plant traditionally used to treat inflammatory conditions such as arthritis and peptic ulcer. This study aimed at evaluating the gastro-protective effect of *C. flammula* leaf extract through *in vitro* simulated digestion (INFOGEST method). The extract constituents' bioavailability and their antioxidant activities were evaluated by the quantification of polyphenols, flavonoids and sugars, and antioxidant activity (DPPH test) was assessed before and after the passage by the oral, gastric and intestinal stages of digestion. The results show an increase in the total polyphenols in the gastric phase (30.04mgEQ/g extract) compared to the oral one (19.7 mgEQ/g extract). Polyphenols were significantly high in the intestinal phase (33.5mgEQ/g extract) compared to the control (20.08 mgER/g extract). The tenure in flavonoids (31.67mgER/g extract) increased drastically in the test conditions (alpha amylase) of the oral phase, was equivocal in the control, normal (pH 3) and ulcer conditions (pH 2) of the gastric phase, and was upgraded in the intestinal phase in the test conditions (27.92 mgER/g extract) compared to control (7.13 mgER/g extract). The sugar levels followed the same trend as flavonoids in the oral phase, but increased in the gastric phase (22.83 mgEG/g extract) compared to control (14.25mg EG/g extract), favoured by both the high acidity and the presence of pepsin. While unchanged in the oral phase, antioxidant activity has increased in test conditions (pH 2) of the gastric (64.13%) and intestinal (49.17%) phases, suggesting a significant gastroprotective potential.

Clematis flammula may thus represent a promising natural alternative to conventional anti-ulcer therapies.

Keywords: *Clematis flammula*, INFOGEST, gastroprotective, DPPH.

ANTIBACTERIAL ACTIVITY OF GREEN SYNTHESIZED NiO NANOPARTICLE AND NiO-ZnO NANOCOMPOSITE USING LIMON CITRUS EXTRACT

Imane DJOUABI^{1*}, Mahdia TOUBANE^{2,3}, Nadia BOUKHERROUB^{2,3}, Samira TATA⁴, Djelal KHERIFI⁵, Ibtissem BELAID¹ and , Meriem Djanette BLIZAK⁶

¹N-body and Structure of Matter Laboratory (LNCSM), Cheikh Mohamed el Bachir El-Ibrahimi higher Normal School of kouba, Algiers,

²UR-MPE, M'hamed Bougara University, Boumerdes 35000, Algeria

³Department of Physics, Faculty of Sciences, University M'hamed Bougara of Boumerdes, 35000 Boumerdes, Algeria

⁴Laboratoire de Biologie des Systemes Microbiens (LBSM), Cheikh Mohamed el Bachir El-Ibrahimi higher Normal School of kouba, Algiers,

⁵Materials and Renewable Energy Laboratory, department of physics, university of M'sila, Algeria

⁶L-BMAB, M'hamed Bougara University, Boumerdes 35000, Algeria

*Corresponding author: Tel./Fax: +213-55324-38-87 ; E-mail address: imane.djouabi@g.ens-kouba.dz

Abstract

In this work, NiO nanoparticle and NiO-ZnO nanocomposite were fabricated via green synthesis method using limon citrus peel extract as an eco-friendly and cost effective approach. The structural characterization of as fabricated samples was carried out using X-ray diffraction (XRD). From XRD analysis we revealed that the NiO phase crystallizes in a cubic structure, with the presence of a characteristic peak of Ni phase observed at $2\theta = 44.56^\circ$, while the ZnO phase exhibits a hexagonal Wurtzite structure within the NiO-ZnO nanocomposite. For the pure NiO sample, the crystallite sizes were calculated to be 25.65 nm for the NiO phase and 32.9 nm for the residual metallic Ni. In the NiO-ZnO nanocomposite, the crystallite sizes were found to be 29.1 nm for the NiO phase and 30.2 nm for the ZnO phase. The antibacterial activity of the as-fabricated samples was found to be significant against *Micrococcus luteus* and *Bacillus subtilis* bacterial strains, with inhibition zone diameters of 22 mm and 15 mm, respectively. In contrast, the pure NiO nanoparticles exhibited no notable antibacterial effect, highlighting the crucial role of ZnO incorporation in enhancing the antimicrobial performance of the nanocomposite. The higher specific surface area of the NiO-ZnO nanocomposite allows for stronger interactions with the bacteria [3], thereby enhancing its antibacterial activity compared to pure NiO. This is likely due to the low reactivity of the pure NiO phase, combined with the presence of metallic Ni, which has a lower specific surface area.

Keywords: Green synthesis; Limon Citrus; NiO; NiO-ZnO; Antibacterial activity

ELECTRODEPOSITION AND CHARACTERIZATION OF Zn–Cu ALLOY THIN FILMS

Farida BENDEBANE^{1*}, Salima BENDEBANE² and Hawa BENDEBANE²

1 Department of Chemistry, Faculty of Sciences, Badji Mokhtar Annaba-University, Algeria, Laboratory LOMOP,

2 Department of process engineering and energy, National Higher School of Technology and Engineering, Annaba-Algeria, Laboratory L3M,

3 Department of process engineering, Faculty of Technology, Badji Mokhtar Annaba-University, Algeria, LOMOP Laboratory.

**Corresponding author: Tel./Fax: +213-664-600-777 ; E-mail address: farida.bendebane@univ-annaba.dz*

Abstract: In order to develop and characterize thin films of a zinc-copper alloy a process of electroplating from a sulfate bath on a steel substrate was examined. Based on the experimental planning (Box-Behnken), the objective was to optimize the different factors influencing the coating quality in terms of micro-hardness. Zinc sulfate concentration, copper sulfate concentration, temperature and current density are the parameters tested. It was found that good coatings are obtained under the following optimal conditions: $I = 3 \text{ A/dm}^2$, $T = 50 \text{ }^\circ\text{C}$; $[\text{Zn}^{2+}] = 0,1 \text{ M}$; $[\text{Cu}^{2+}] = 0,3 \text{ M}$. For a theoretical response of 361.82 and experimental response of 358.78. In order to improve the quality of coating an addition of natural non-toxic additives was made. It was found that increasing the concentration of additives negatively affects the coating quality and it is the concentration 1 g/L that gives a fine, smooth, homogeneous surface and glossy coating. This result is confirmed by SEM-EDS analysis.

Keywords: Electrodeposition, Zn-Cu alloy, additive, optimization, RSM, characterizations.

SUSTAINABLE RECOVERY OF SYNTHETIC POLYMER WASTE VIA A BIO-BASED POLYMER SYSTEM

Samir MOUFFOK^{1*}, Mustapha KACI²

¹*Laboratoire de Valorisation et Recyclage de la Matière pour le Développement Durable (VRMDD),
Faculté de Génie Mécanique et Génie des Procédés, Université des Sciences et de la Technologie
Houari Boumediene 16111, Algeria*

²*Laboratoire des Matériaux Polymères Avancés (LMPA), Université de Bejaia 06000, Algeria*

*Corresponding author: E-mail address: samir.mouffok@usthb.edu.dz

Abstract: This study explores the sustainable recycling of synthetic polymer waste, specifically polymethyl methacrylate (PMMA), using a biopolymer. Chitosan (Cs), a bio-based biopolymer, was employed to enhance the environmental performance of the recycled material. PMMA waste was processed via extrusion to produce sheets for further analysis. Gel permeation chromatography (GPC) results showed a slight decrease in the average molecular weight of PMMA after extrusion processing due to thermal degradation. Fourier Transform Infrared Spectroscopy in Attenuated Total Reflectance mode (FTIR-ATR) revealed no significant changes in the chemical structure of recycled PMMA/Cs blends compared to their virgin counterparts. This suggests that chain scission is the primary degradation mechanism affecting PMMA during processing. Dynamic Mechanical Analysis (DMA) indicated a single glass transition temperature (T_g) for the blends, confirming the miscibility of PMMA and chitosan. The recycled PMMA/Cs blends exhibited slightly lower T_g values than those made with virgin PMMA, reflecting minor changes in thermal properties. While the incorporation of recycled PMMA led to a slight reduction in the thermal stability of the blends, it notably improved their water uptake capacity, demonstrating potential for enhanced biodegradability in environmentally sensitive applications.

Keywords: Sustainable materials ; polymer recycling ; Poly(methyl methacrylate) Waste ; Chitosan

**COQUES DE NOYAUX D'ABRICOT COMME BIOSORBANT DURABLE POUR
L'ÉLIMINATION EFFICACE DU COLORANT VIOLET DE CRISTAL**

TERCHI Smail

*Department of Chemistry, Faculty of Science, University of M'sila, University Pole, Road Bourdj Bou
Arreiridj, M'sila 28000 Algeria*

*Department of Chemistry, Faculty of Science, University of M'sila, University Pole, Road Bourdj Bou
Arreiridj, M'sila 28000 Algeria*

**Corresponding author: Tel./Fax: +213666589565 ; E-mail address: smail.terchi@univ-msila.dz*

Résumé : Cette étude examine le potentiel des coques de noyaux d'abricot (ASS) en tant que biosorbant économique et respectueux de l'environnement pour l'élimination du colorant violet de cristal (CV) à partir de solutions aqueuses. Le matériau ASS a été caractérisé par DRX, FTIR et TG-DTA révélant une composition riche en cellulose. Les expériences d'adsorption ont montré des performances optimales à pH 3 et à 40 °C, atteignant l'équilibre en 60 minutes. Les études cinétiques ont indiqué un mécanisme pseudo-second ordre, tandis que l'isotherme de Temkin décrivait le mieux le comportement d'adsorption, suggérant une chimisorption sur des sites hétérogènes. L'analyse thermodynamique a confirmé le caractère endothermique du processus, avec une variation de l'énergie libre de Gibbs (ΔG°) indiquant une spontanéité accrue à des températures plus élevées. Ces résultats positionnent l'ASS comme une alternative prometteuse et durable pour le traitement des eaux usées, valorisant ainsi un déchet agricole pour une élimination efficace des colorants.

Mots clés: Biomasses; traitement des eaux ;Valorisation des co-produits naturels.

VALORIZATION OF ALGERIAN MEDICINAL PLANTS IN MEDICINE AND
COSMETOLOGY

Djebbar ATMANI^{1*}, Dina KILANI¹, Souad KASMI Kenza, MOULAOUÏ and Tristan RICHARD²

¹ *Laboratory of Applied Biochemistry, Faculty of Life and Nature Sciences, University of Bejaia, 06000 Algeria.*

² *Université de Bordeaux, UR Œnologie, MIB, EA 4577, USC 1366 INRAE, Bordeaux INP, ISVV, F-33140, Villenave d'Ornon, France.*

*Corresponding author: Tel./Fax: +0-213-772-928314 ; E-mail address: djebbar.atmani.@univ-bejaia.dz

Abstract: Valorization of Algerian medicinal plants represents an interesting challenge since they provide local populations with medicines at no cost. This study aimed to examine various biological activities of *Fraxinus angustifolia* (Oleaceae) and *Pistacia lentiscus* (Anacardiaceae) for their potential use in human health. *Pistacia lentiscus* extracts showed a strong inhibition of lipid peroxidation induced by neurotoxic metals in mice brains, a dose-dependent cytoprotective effect on PC12 cells and a moderate inhibitory activity on acetylcholinesterase. Moreover, the extracts reversed behavioral, histological and biochemical alterations induced by Aluminum intoxication. On the other side, *Pistacia lentiscus* extracts exhibited a cytotoxic effect on human ovarian cancer cell lines A2780 and SKOV3 by inducing apoptosis and cell cycle arrest in phase G1. *Fraxinus angustifolia* extracts reduced edema in carrageenan-induced inflammation in mice, while inhibiting myeloperoxidase activity. Moreover, the extracts of *F. angustifolia*, significantly inhibited ear edema induced by tetraphorbol acetate and suppressed the cellular infiltration. *In vivo*, the vesicles loaded with the crude extract of *F. angustifolia* inhibited oxidative stress in human keratinocytes against H₂O₂ and attenuated edema and leukocyte infiltration by stimulating the repair of TPA-induced skin damage, thereby accelerating the wound healing process. Several experiments including Ames' and chromosomal aberration tests indicated that the used plant extracts are free of any genotoxicity, even showing antimutagenic action. Therefore, *Fraxinus angustifolia* can be used in superficial wound healing, while *Pistacia lentiscus* may be associated to chemotherapy in the treatment of cancer, as well as a palliative against deterioration of cognitive functions.

Keywords: *Pistacia lentiscus* ; *Fraxinus angustifolia* ; wound healing ; anticancer ; neuroprotection.

REMOVAL OF NICKEL(II) IN WASTEWATER BY NANOCHITOSAN

RAHALI Abdallaha , MOUSSAOUI Badredineb, NIHAL Bektasc.

Laboratory of Beneficial Microorganisms of Functional and Health Foods University of Mostaganem

Chemical Oxidation Laboratory Gebze University Türkiye.

abdallah.rahali@univ-msila.dz

Abstract: Nickel is one of the most toxic and dangerous heavy metals that pollutes the environment in general and water in particular. The objective of this work is to develop a simple method for treating urban wastewater by removing nickel. This method uses a natural adsorbent from shrimp waste (shells), nanochitosan prepared from chitin. The demonstration and reliability of the adsorption of nickel ions on nanochitosan were carried out by Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy coupled with energy dispersive spectroscopy (SEM-EDS) and zeta potential. The results obtained reveal that the optimal conditions for adsorption of nickel on nanochitosan are: pH = 9, initial concentration = 210.6 mg / L and time = 360 min. The maximum amount of nickel adsorbed equal to 85.7 mg/g of nanochitosan. The analysis of the experimental data at equilibrium indicates that the adsorption process is similar to the Freundlich model. Based on the kinetic study of adsorption, the pseudo-second-order kinetic model was found to be the best explanatory model of the adsorption process. Nanochitosan showed better regeneration performance for further use and therefore, it appears as a good, inexpensive biosorbent that can be used in the remediation of wastewater contaminated by heavy metals in general and nickel in particular.

Keywords: Adsorption, Chitin, Wastewater, Nanochitosan, Nickel.

INFLUENCE OF ZINC ACETATE CONCENTRATION ON THE PHOTOELECTROCHEMICAL PERFORMANCE OF CHEMICALLY DEPOSITED ZNO FILMS

Ibrahim Yaacoub BOUDERBALA^{1,2}, Abdelmadjid HERBADJI^{2,3} and Slimane KHELOUFI^{4*}

¹ *Laboratory of Physical Chemistry of Materials, Faculty of Sciences and Technology, Chadli Bendjedid University, 36000, El Tarf, Algeria*

² *Laboratory of Chemistry, Molecular Engineering and Nanostructures, University of Ferhat Abbas, 19000 Setif, Algeria*

³ *Applied Optics Laboratory, Institute of Optics and Precision Mechanics, University of Ferhat Abbas, 19000 Setif, Algeria*

⁴ *Laboratory: Growth and Characterization of New Semiconductors, University of Ferhat Abbas, 19000 Setif, Algeria*

*Corresponding author: KHELOUFI SLIMANE ; E-mail address: slimanekheloufi03@gmail.com

Abstract : This study explores the influence of zinc acetate (ZnAc) precursor concentration on the electrochemical and photocatalytic properties of zinc oxide (ZnO) thin films fabricated via the chemical solution deposition method. By systematically varying the ZnAc concentration from 0.25 M to 0.75 M, the study aims to establish the relationship between precursor concentration and film performance in both electrochemical and photocatalytic applications. Electrochemical impedance spectroscopy (EIS) and Mott-Schottky analysis were employed to assess the charge transport behavior and semiconductor properties of the films. Results demonstrated that higher ZnAc concentrations led to a notable improvement in charge transfer characteristics. Specifically, the film synthesized with 0.75 M ZnAc exhibited the lowest charge transfer resistance ($R_{ct} = 0.31 \text{ k}\Omega$) and the highest double-layer capacitance ($102.5 \text{ }\mu\text{F}$), indicative of enhanced charge carrier density and more efficient interfacial electron transfer. In parallel, the photocatalytic activity of the ZnO films was evaluated through the degradation of Rhodamine B (RhB) under UV irradiation. The ZnO film derived from 0.75 M ZnAc showed the most effective photocatalytic performance, as evidenced by a continuous and significant decrease in RhB absorbance over time. This activity is attributed to the generation of reactive oxygen species (ROS), particularly hydroxyl radicals ($\bullet\text{OH}$) and superoxide anions ($\bullet\text{O}_2^-$), formed by the UV-induced excitation of electron-hole pairs within the ZnO lattice. These species facilitate the oxidative breakdown of RhB into less harmful by-products. Overall, the findings underscore the pivotal role of precursor concentration in modulating ZnO thin film properties, with implications for their use in advanced photoelectrochemical and environmental remediation technologies.

Keywords: Zinc Oxide Thin Films ; Precursor Concentration ; Photocatalytic Degradation ; Electrochemical Performance

PLANT-DRIVEN NANOTECHNOLOGY: CuO NANOPARTICLES AND THEIR LIGHT-INDUCED DEGRADATION OF POLLUTANTS

Abdelhakim KHENICHE *, Imane Meriem KHALED² and Samiya RIZOUG³

¹*Department of Chemistry, Laboratory of Organo-Therapeutic Substances and Sustainable Processes, Faculty of Science, University of Mohamed Boudiaf-Msila, Algeria*

²*Department of Chemistry, Faculty of Science, University of Mohamed Boudiaf -Msila, Algeria*

³*Department of Chemistry, Laboratory of Inorganic Materials, Faculty of Science, University of Mohamed Boudiaf-Msila, Algeria*

*Corresponding author: Tel./Fax: (+213) 671 70 85 71; abdelhakim.kheniche@univ-msila.dz

Abstract : This study examines the environmentally sustainable synthesis of copper oxide (CuO) nanoparticles utilizing an aqueous extract of *Salvia barrelieri*, a medicinal plant indigenous to North Africa. The extract served as a natural reducing and stabilizing agent that substituted for toxic chemicals commonly used in traditional nanoparticle manufacturing. The resultant nanoparticles were analyzed using X-ray diffraction (XRD) and Fourier-transform infrared spectroscopy (FTIR), validating their crystalline structure and identifying essential functional groups originating from plant metabolites. The photocatalytic efficacy of the CuO–ZnO system was assessed by the degradation of Rhodamine B dye under natural sunlight and LED illumination. The impacts of dye concentration, catalyst dosage, and ZnO incorporation ratios were methodically analyzed. Optimal degradation was attained with 25 mg of CuO combined with 5% ZnO, demonstrating a synergistic action that improves photodegradation efficiency. The findings indicate the viability of *Salvia barrelieri* as a sustainable, local resource for sophisticated applications in environmental nanotechnology and wastewater treatment.

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

VALORISATION NANOFORMULEE DES EXTRAITS D'ARTEMISIA HERBA-ALBA POUR LA PROTECTION PRE-RECOLTE DU BLE CONTRE LES RAVAGEURS

Imane KABOUYA¹ et Khalil MESSADI²

¹ Université de Mohamed Boudiaf – M'sila, Département de sciences de la nature et de vie

² Université de sfax-Tunisie, Département de sciences de la nature et de vie

* E-mail address: kabouyaimane@gmail.com

Résumé : Éprouvant les conséquences néfastes des insecticides chimiques sur la santé environnementale et humaine la recherche actuelle s'oriente vers des solutions alternatives durables et respectueuses des écosystèmes. Les extraits végétaux, riches en métabolites secondaires bioactifs, représentent une source prometteuse de composés naturels à activité insecticide. Toutefois, leur efficacité peut être limitée par leur instabilité et leur faible biodisponibilité. L'objectif principal de cette étude est de formuler des extraits d'Artemisia herba-alba sous forme nanoencapsulée, en vue d'optimiser leur efficacité insecticide pré-récolte contre les principaux ravageurs du blé. L'extraction des composés actifs a été réalisée par hydrodistillation à l'aide d'un appareil de type Clevenger, avec un rendement de 1,2 %. Le traitement a été appliqué par pulvérisation foliaire, 10 à 15 jours avant la récolte. Les résultats ont révélé des taux de répulsion variant entre 68,33 % et 76,68 %. En parallèle, une réduction significative des infestations a été observée, notamment de 58,35 % pour *H. armigera* et *Z. tenebrioides*, et de 50,02 % pour *E. integriceps* hydro alcoolique. Les extraits ont ensuite été incorporés dans des nanoparticules polymériques biodégradables via la méthode d'émulsion-diffusion, en utilisant la lécithine et des biopolymères naturels. Les formulations obtenues ont été caractérisées physico-chimiquement (Taille moyenne des particules 135 ± 10 nm Potentiel zêta -32.5 mV Indice de polydispersité (PDI) 0.18 Efficacité d'encapsulation (EE%) 82.4%), puis testées in vitro et in vivo sur des insectes ravageurs courants du blé. Les résultats montrent une amélioration significative de l'efficacité insecticide des extraits nanoformulés, comparée aux extraits bruts, notamment en termes de mortalité, de persistance et de libération prolongée. Cette approche innovante, alliant phytochimie, nanotechnologie et protection intégrée des cultures, ouvre des perspectives prometteuses pour le développement de biopesticides de nouvelle génération, à la fois efficaces, écologiques et adaptés aux exigences de l'agriculture durable.

Mots-clés : Artemisia herba-alba, nanoformulation, extraits végétaux, insecticide naturel, ravageurs du blé, chimie verte, nanobiopesticide, agriculture.

CARACTERISATION PHYSICO-CHIMIQUE ET COMPOSITION MINERALE D'UNE ARGILE NATURELLE (REGION DE SOUBELLA, M'SILA, ALGERIE)

Karima LARKAT^{1*}, Azzedine BENYAHIA¹, Meftah ALLAL², Nadir DEGHEFEL² et Warda ATTOUI¹

¹Université de M'sila, Algeria, Faculté des sciences, laboratoire des matériaux inorganique

LMI

²Université de Biskra, Algeria, Faculté des sciences et technologie, laboratoire de Recherche en Génie Civil

*Département de chimie Université de M'sila.

Karima.larkat@univ-msila.dz

Résumé : Cette recherche contribue à une meilleure valorisation des ressources naturelles locales, en évaluant l'aptitude de l'argile pour des applications industrielles ou environnementales (traitement des eaux, stabilisation des sols, etc.). La faible hygroscopicité et la stabilité thermique observées suggèrent un potentiel pour des matériaux durables, réduisant ainsi l'impact écologique des procédés industriels. L'étude des propriétés physico-chimiques de l'argile jaune de la région de Soubella (M'Sila) révèle un pH légèrement alcalin (7,47), attribué à la présence de sels solubles basiques, tels que les bicarbonates et les silicates de métaux alcalins. Cette argile présente une faible hygroscopicité, comme en témoigne sa teneur en humidité réduite (1,38 %). Son indice de gonflement modéré (1,55 %) confirme une capacité limitée d'expansion en présence d'eau. La granulométrie des échantillons indique une répartition entre sable fin, moyen et grossier, ce qui influence leurs propriétés mécaniques et leur potentiel d'utilisation. La caractérisation par spectroscopie infrarouge à transformée de Fourier (FTIR) a permis de confirmer la présence de kaolinite et de quartz, en accord avec les résultats analytiques. L'analyse thermogravimétrique (ATG) a montré une perte de masse totale de 5,56 %, reflétant l'élimination de l'eau adsorbée et des impuretés organiques. Par ailleurs, la diffraction des rayons X (DRX) a été employée pour identifier les phases minérales dominantes et caractériser les minéraux argileux présents. Ces techniques combinées offrent une compréhension approfondie de la composition minéralogique et du comportement thermique de l'argile.

Mots-clés : Argile, propriétés physico-chimiques, composition minéralogique, DRX, ATG, FTIR.

Co-DETECTION DE L'EUGENOL ET DU BUTYLHYDROXYTOLUENE PAR HYDRODISTILLATION VERTE ET SELECTIVE D'*HELIOTROPIUM TENUIFLORUM* (L.) UTILISANT DE NOUVEAUX SOLVANTS VERTS

BENDJELLOUL Sara^{1*}, BENDEDDOUCHE Choukry Kamel¹

¹ Laboratoire de synthèse organique appliquée, Faculté des sciences exactes et appliquées, département de chimie, Université Ahmed Ben Bella Oran-1, Algeria

bendjelloulsara@gmail.com

Résumé : Actuellement, la demande en huiles essentielles est en forte croissance, notamment en raison de leur large utilisation dans les industries alimentaire, pharmaceutique et cosmétique. Parmi les différentes techniques d'extraction disponibles, l'hydrodistillation reste la méthode la plus couramment employée pour l'obtention des huiles essentielles. Cependant, cette méthode présente parfois des limitations, notamment en termes de rendement d'extraction, ce qui peut affecter son efficacité. Ce travail concerne une mise au point d'une nouvelle méthode d'extraction d'huiles essentielles en introduisant un liquide ionique comme additif dans l'hydrodistillation afin d'améliorer le rendement d'extraction. Grâce à leurs propriétés uniques, notamment leur non-volatilité, les liquides ioniques peuvent être utilisés comme agents d'extraction efficaces dans ce procédé. Cette approche représente une alternative prometteuse à l'hydrodistillation classique. L'objectif de ce travail est d'étudier la composition chimique de l'huile essentielle extraite de la partie aérienne d'*Heliotropium tenuiflorum* (L.) en utilisant l'analyse par chromatographie en phase gazeuse couplée à la spectrométrie de masse (GC-MS). Deux procédés d'extraction sont comparés : Extraction par hydrodistillation classique ; Extraction par hydrodistillation avec l'ajout d'un liquide ionique comme additif. Cette étude vise à évaluer l'influence de l'utilisation des liquides ioniques sur la composition chimique et le rendement de l'huile essentielle obtenue. Afin d'évaluer l'effet du liquide ionique sur l'extraction, la morphologie de la plante a été analysée à l'aide du microscope électronique à balayage (MEB). En conclusion, l'utilisation de la nouvelle méthode d'extraction a permis d'obtenir une augmentation significative du rendement. Une étude comparative, réalisée par GC-MS, des compositions quantitative et qualitative des huiles essentielles a révélé une meilleure sélectivité avec la méthode assistée par liquide ionique. De plus, une modification morphologique notable des structures végétales a été observée, confirmant l'efficacité du liquide ionique en tant qu'additif dans ce procédé d'extraction.

Mots-clés : Huile essentielle ; liquide ionique ; additif ; hydrodistillation ; *Heliotropium tenuiflorum* (L.).

THE OPTIMIZATION OF EXPERIMENTAL CONDITIONS USING DESIGN EXPERT TO ENHANCE THE OXIDATION OF RHODAMINE B WITH PERSULFATE IN A SUSTAINABLE SOLAR SYSTEM

Marwa BACHIRI¹, Mokhtar DJAHICHE¹, Nedjma LAHMAR¹

1. Laboratoire des matériaux inorganiques, Université Mohamed Boudiaf, M'sila, Algeria

Tel: 0666325328

E-Mail: marwa.bachiri@univ-msila.dz

Abstract : Rhodamine B dye poses a serious environmental threat due to its high toxicity, which is harmful to aquatic organisms and plants. The dye is also resistant to degradation, leading to its continuous accumulation in the ecosystem. In addition, it has been demonstrated that rhodamine B dye can block light penetration and disrupt the ecological balance, thereby degrading water quality. In order to address this challenge, the research relied on the chemical oxidation technique using potassium persulfate ($K_2S_2O_8$). The experimental design employed utilized the Box-Behnken method, a statistical technique for optimization, to assess the impact of critical variables on the efficacy of removal. These variables encompassed reaction time, temperature, oxidant concentration, and laboratory experiments. The objective of this multifaceted approach was to ascertain the optimal conditions for achieving maximum removal. However, reliance on conventional electrical heating for this process gave rise to a new challenge: high costs and carbon emissions. A pioneering solution was devised, entailing the conceptualization of a "Green House Cell" that employs solar radiation to produce the requisite thermal energy. The optimal conditions were meticulously applied through the utilization of this cell. The findings indicated a high removal efficiency that was comparable to laboratory performance, with significant environmental benefits, including the elimination of carbon emissions, and a low-cost solution for remote areas. The present work sets forth an integrated model that exemplifies the utilization of renewable resources (solar energy) to address significant pollutants and constitutes a sustainable strategy to address two challenges: Water contamination with resistant dyes and dependence on fossil fuels.

Keywords: Box-Behnken, Rhodamine B, Green House Cell, Oxidation

HOMOGENEOUS CATALYZED TRANSESTERIFICATION OF BIODIESEL: APPLICATION OF THE BOX-BEHNKEN DESIGN

Salima BENDEBANE¹, Hawa BENDEBANE², Farida BENDEBANE²

¹National Higher School of Technology and Engineering, Laboratory L3M, 23005, Annaba, Algeria,

²Laboratory LOMOP, Badji Mokhtar- Annaba University, BP 12, Annaba-Algeria

Abstract

This study focused on optimizing biodiesel production from waste cooking oil using homogeneous catalysis. The effects of four key parameters were investigated through a Box–Behnken experimental design: aqueous-to-organic phase ratio (A/O), NaOH concentration, temperature, and reaction time. Optimal conditions were determined as A/O ratio = 1:12, NaOH = 0.5 wt.%, temperature = 40 °C, and reaction time = 70 minutes. Under these conditions, the experimental yield reached 100%, while the predicted yield from the model was 107.71%, confirming the adequacy of the quadratic model ($R^2 > 0.99$). Potassium hydroxide (KOH) demonstrated the best catalytic performance among the tested bases and yielded biodiesel that met ASTM D6751 and EN 14214 standards (viscosity = 4.75 mm²/s, acid value = 0.28 mg KOH/g, density = 0.864 g/mL). FTIR spectroscopy confirmed effective ester formation, indicating successful transesterification. This optimized process demonstrates a sustainable route for valorizing waste cooking oil in Algeria, aligning with circular economy goals and environmental protection strategies .

Keywords: Biodiesel, Waste Cooking Oil, Homogeneous Catalysis, Transesterification, Box–Behnken Design, Process Optimization.

ÉLECTROSYNTHÈSE ET ANALYSE DES PROPRIÉTÉS ÉLECTROCATALYTIQUES
D'ÉLECTRODES MODIFIÉES PAR DES FILMS DE POLYPYRROLE FONCTIONNALISÉ
CONTENANT DU NICKEL

Faiza NESSARK^{1,2*}, Ali ALOUACHE³ and Mohamed EISSA⁴

¹Laboratoire d'Electrochimie et Matériaux (LEM), Université Ferhat Abbas Sétif 1, 19000, Algeria

²Département de Chimie, Faculté des Sciences, Université Mohamed Boudiaf M'Sila, 28000, Algeria

³Laboratoire N-Corps et Structure de la Matière, Ecole Normale Supérieure Kouba Alger,

16000, Algeria

⁴Polymers and Pigments Department, National Research Centre, Dokki, Giza 12622, Egypt

*Auteur correspondant : Tél. +213 775092906; E-mail : faiza.nessark@univ-msila.dz

Résumé : Les composites à base de polymères conducteurs révolutionnent l'électrocatalyse, grâce à leur conductivité soutenable, une activité redox et des effets synergétiques avec les nanomatériaux intégrés. Ils sont particulièrement utiles dans les applications de conversion d'énergie et de détection, notamment les piles à combustible, l'électrolyse de l'eau et la réduction du CO₂. Ce travail consiste en la préparation et en l'analyse des propriétés électrochimiques d'un matériau composite obtenu sur une électrode de carbone vitreux à partir d'un poly [acide 4-(pyrrol-1-yl méthyl) benzoïque], dans lequel est incorporé un métal de transition sous forme de microparticules (Ni²⁺), et ce, en vue de son utilisation comme matériau d'électrode en électrocatalyse. Le processus d'électrodéposition et la caractérisation du matériau d'électrode obtenu ont été examinés par voltampérométrie cyclique et par spectroscopie d'impédance. L'étude montre que ce nouveau matériau composite présente une activité électrocatalytique très importante. La modification de l'électrode par le film de polymère complexant permet de détecter les métaux par complexation de ces derniers. L'électrode ainsi obtenue peut être utilisée dans différentes applications, notamment, en électrocatalyse et protection des électrodes métallique et semi-conductrice contre la corrosion.

Mots clés : Matériau Composite ; Polypyrrole Fonctionnalisé ; Nickel ; Voltampérométrie Cyclique ; Spectroscopie d'Impédance.

ENHANCED OF FLOW PARAMETERS AND MODELING OF THE RHEOLOGICAL BEHAVIOR OF CRUDE OIL WITH AND WITHOUT ADDITIVE

Djamal Eddine DJEMIAT*^{1,2}, Mohamed Rafik BERINIE¹, Abdelbaki BENMOUNAH²

¹Laboratory of City, Hydraulic Environment and Sustainable Development, Hydraulic Department, University of M'sila, M'sila, Algeria.

²Research Unit, Materials, Processes and Environment (UR-MPE), Boumerdes University, Algeria.

*e-mail:djamaleddine.djemiat@univ-msila.dz

Abstract: The aim of this study is to determine how the aromatic compound tetrahydrofuran affects the rheological behavior of the oil and the percentage of energy consumption during the pumping process at 20, 30 and 50°C. The viscosity of the oil causes several problems for this process. Most of the time, researchers solve these problems by adding additives that make the oil less viscous. It is known the wax and asphaltene are responsible for oil viscosity, which is why there are many scientific studies that study the effect of additives on these two compounds. Machado et al , Li et al ,and Marenov et al examined the impact of polymers and co-polymers on oil viscosity by focusing on the wax contained in oil, and they found that the compounds do have an influence in lowering viscosity. The chemical additive was added at concentrations of 3000, 6000 and 9000 ppm. AR-2000 rheometer was used for rheological modeling, measurement of viscosity, yield point, and viscoelastic characteristics. The percent reduction in viscosity is dependent on the temperature and the concentration of the additive. With the addition of additives, the viscosity of crude oil decreased more than 34%, the power consumption of the pump by 26.90%. At a concentration of 9000 ppm, the yield stress is reduced more than 41%. The effect of the compound is significant at low shear rates, where the behavior is non-Newtonian, then decreases with increasing shear rates, where the behavior becomes Newtonian.

Keywords: crude oil; viscosity reduction; yield stress; consumption of a pump; viscoelastic behavior.

ANALYSIS AND EVALUATION OF THE *IN VITRO* ANTIOXIDANT, ANTI-ENZYMATIC, ANTI-MOLD AND CYTOTOXICITY ACTIVITIES OF *ERODIUM TRIFOLIUM* (CAV.)

Noura MESSAOUDI , Hamdi BENDIF , Khellaf REBBAS and Larbi DERBAK

Department of Natural and Life Sciences, Faculty of Sciences, University of M'sila, University Pole, Road BourdjBouArreidj, M'sila 28000, Algeria.

*e-mail: noura.messaoudi@univ-msila.dz

Abstract: Herbal medicine, one of the oldest therapeutic practices, continues to be an important alternative to synthetic pharmaceuticals due to its effectiveness and minimal side effects. Despite advancements in pharmaceutical chemistry, interest in plant-based treatments remains high, as many modern drugs originate from bioactive compounds found in medicinal plants. [1] The genus *Erodium*, belonging to the Geraniaceae family, derives its name from the Greek word *Erodium* (heron), a reference to the beak-like shape of its fruit [2]. Traditionally, *Erodium* species have been widely used in folk medicine across different cultures for treating a variety of ailments, including hemorrhages, digestive disorders, diabetes, urinary inflammation, and skin conditions [3]. *Erodium trifolium* (Cav.), an Algerian native species of the *Erodium* genus, has a history of traditional medicinal use but remain spoorly studied. Its phytochemical composition and potential biological activities have yet to be thoroughly explored. The study aims To evaluate the antioxidant, anti-enzymatic, anti-mold, and cytotoxic activities of *E. trifolium*, and to identify its bioactive compounds using Fourier Transform Infra red Spectroscopy. *E. trifolium* display spromising antifungal and antioxidant properties with low toxicity, supporting its potential use in natural preservative and therapeutic applications. Further studies are needed to isolate and characterize its active compounds and optimize extraction protocols.

Keys Words : *Erodium trifolium*; Antioxidant activity; Anti-mold activity

Poster Communications

MOLECULAR DOCKING INSIGHTS INTO THE DUAL ANTIOXIDANT AND ENZYME-INHIBITORY POTENTIAL OF AZOMETHINE SB

Ilhem KAABI^{1*}, Samra AMAMRA^{1,2} and Tahar DOUADI¹

¹Laboratory of Electrochemistry of Molecular Materials and Complexes (LEMMC), Department of Engineering Process, Faculty of Technology, Setif 1 University-Ferhat Abbas, 19000 Setif, Algeria

²Department of Matter Sciences, Faculty of Sciences and Technology, University Mohamed El Bachir El-Ibrahimi, Bordj Bou Arreridj, Algeria, 34000

*Corresponding author: Tel./Fax: +0-213-698-010778 ; E-mail address: kaabi_ilh@yahoo.fr

Abstract: Azomethines, for instance, 1-[(E)-(1H-1,2,4-Triazol-3-ylimino)methyl]-2-naphthol (SB), are of interest because they play a dual role in acting as corrosion inhibitors and antioxidants. Their π -electron-rich and heteroatom-rich molecular structure supports strong reactive oxygen species (ROS) and metal surface interactions, and therefore, they are found to be useful in industrial and biomedical applications. In this study, the SB multifunctional properties are explored in its corrosion inhibition of X48 carbon steel in 1 M HCl and as an antioxidant. Electrochemical tests (EIS, PDP) and gravimetric measurements identified SB's highest inhibition efficiency (94.24% at 5×10^{-4} M), which was due to chemisorption and physisorption mechanisms following Langmuir isotherm. Characterization of the surface (SEM, AFM, EDX) confirmed the formation of a protective Fe-SB complex. Computational studies, like DFT and QTAIM, highlighted SB's electron-donating character and non-covalent interaction with the steel surface. Molecular docking revealed SB's inhibitory activity as an inhibitor of xanthine oxidase, NADPH oxidase, and SARS-CoV-2 main protease, with binding energies of -98.21 to -109.59 kcal/mol, representing improved inhibitory activity against *Acidithiobacillus ferrooxidans* (1H10). The complementarity between theoretical and experimental approaches highlights SB's efficacy as a green corrosion inhibitor and antioxidant with material protective and biomedical applications. Docking results also validate its capacity to combat oxidative stress and microbial activity, positioning SB as a potential multi-purpose compound for green industrial and therapeutic applications.

Keywords: Azomethine; Antioxidant activity; QTAIM; Molecular docking.

Etude phytochimique de l'extrait chloroforme d'une plante endémique saharienne du genre *Pituranthos*

Chahrazed ESSEID ^{1,2*}, Zinelabidine CHINI ², Meriem AISSAOUI ^{1,2}, Eric MARCHIONI ³, Samir BENAYACHE ¹ et Fadila BENAYACHE ¹.

¹Unité de recherche Valorisation des Ressources Naturelles, Molécules Bioactives et Analyses Physicochimiques et Biologiques (VARENBIOMOL), Département de Chimie, Faculté des Sciences Exactes, Université Constantine 1, 25000 Constantine, Algérie.

²Département de chimie, Faculté des Sciences, Université Saad dahlab, Blida 1, 270 Route Soumâa - Blida-, Algérie

³Equipe de Chimie Analytique des Molécules Bioactives (IPHC-LC4, UMR 7178), Université de Strasbourg, Faculté de Pharmacie, 74 Route du Rhin, 67400 Illkirch, France.

*Corresponding author: Tel./Fax: +213-077-789-8818 ; E-mail address: esseidchahrazed@yahoo.fr

Résumé : Cette étude s'inscrit dans le cadre de la valorisation des ressources naturelles de l'Algérie. Nous avons soumis l'extrait au chloroforme des parties aériennes de cette plante à diverses techniques de chromatographie en phase liquide. Les structures des composés isolés ont été déterminées par une combinaison de méthodes spectroscopiques, notamment la spectrophotométrie UV-Visible, la résonance magnétique nucléaire monodimensionnelle (¹H, ¹³C et DEPT) et bidimensionnelle (HSQC, COSY, HMBC, NOESY), ainsi que la spectrométrie de masse haute résolution (HRESI-MS et HR-EI-MS). Ces travaux ont permis l'isolement et l'identification de 14 composés naturels, majoritairement de type coumarine, parmi lesquels 3 présentent des structures inédites, jamais décrites auparavant dans la littérature. Tous ces composés sont isolés pour la première fois à partir de cette plante. La découverte de trois structures nouvelles constitue un élément d'originalité remarquable, apportant une contribution significative à la chimiotaxonomie du genre *Pituranthos*, de la famille des *Apiaceae*, et à une meilleure connaissance de la flore algérienne.

Mots clés: *Pituranthos*; *Apiaceae* ; Coumarines.

PHYTOCHEMICAL ANALYSIS OF *RANUNCULUS ARVENSIS* L EXTRACTS

Ahlem HACHELAF, Ahmed TOUIL, Amar ZELLAGUI*, Salah RHOUATI

University Mentouri – Constantine Algeria, Faculty of science, laboratory of Natural Products and Organic Synthesis.

*Department of chemistry; Oum El Bouaghi, Algeria.

ahlem.hachelef@univ-msila.dz

Abstract: Medicinal Aromatic Plants play a valuable and important role in economic, social, cultural and ecological aspects of local communities the world over. They benefit virtually everyone on Earth through nutrition, toiletry, bodily care, incense and ritual healing. Algeria presents with the nature of their soils and its climate a great variety of vegetation. Phytochemical studies carried out on various *Ranunculus* species, which comprises 50 genera and 2000 species, revealed that they produce compounds belonging to different secondary metabolite groups, including triterpenesaponins, alkaloids, flavonoids, fatty acids and organic acids. Although several plants belonging to this genus have been shown to possess important biological properties such as antioxidant, antibacterial, antimicrobial. *Ranunculus arvensis* L. has long been used to treat a variety of medical conditions such as arthritis, asthma, hay fever, rheumatism, psoriasis, gut diseases and rheumatic pain. This study provides new scientific information about *R. arvensis* based on the phytochemical analysis and HPLC analysis. This work was carried out to investigate the quantitative determination of their crude phytochemicals in methanol, chloroform, ethyle acetate and butanol extracts the result reveal a significant value of flavonoids and phenolics observed via high performance liquid chromatography. Quantitative and qualitative analysis of various crude extracts indicated the presence of bioactive compounds as flavonoids and phenolics. Moreover, the above data indicate that, *R. arvensis* was also rich in rutin and caffeic acid. However, further studies are needed for the isolation of the natural products with fascinating biological and pharmacological properties.

Keywords: *Ranunculus arvensis*, Phenolic content, Flavonoid, HPLC

DEVELOPPEMENT ET CARACTERISATION AVANCEE DE MEMBRANES COMPOSITES A BASE DE POLYALCOOL VINYLIQUE MODIFIE POUR APPLICATIONS ENERGETIQUES ET ENVIRONNEMENTALES

Hanene ZOUAOUI¹ , Ahmed BAHLOUL^{1,2}, Hadjer LAIFAOU¹ et Imen DEBBACHE¹

¹ Laboratoire d'électrochimie et d'environnement, Faculté des sciences et de la technologie, Université Mohamed

El Bachir El Ibrahimi, Bordj Bou Arréridj, 34000

² Laboratoire des substances organo-thérapeutiques et des procédés durables, Faculté des sciences, Université Mohamed Boudiaf, M'sila, 28000

Résumé : Ce travail présente une étude approfondie sur le développement de membranes composites innovantes à base de poly(alcool vinylique) (PVA) modifié, destinées à des applications avancées dans le domaine énergétique et environnemental. La recherche a porté sur l'élaboration et l'optimisation de plusieurs formulations membranaires grâce à des protocoles de synthèse, incluant des méthodes de modification chimique contrôlée et des traitements post-synthèse spécifiques. L'approche méthodologique a permis d'obtenir des matériaux aux propriétés physico-chimiques et structurales remarquablement améliorées. Les caractérisations systématiques ont mis en évidence des performances exceptionnelles, avec une optimisation significative du comportement au gonflement et des propriétés d'hydratation, une augmentation notable de la capacité d'échange ionique, ainsi qu'une stabilité électrochimique démontrée par spectroscopie d'impédance sur plusieurs cycles. Les analyses structurales approfondies ont confirmé des modifications contrôlées des réseaux polymères, conduisant à une amélioration des propriétés stabilité thermique. Ces membranes composites présentent un potentiel prometteur pour diverses applications technologiques, particulièrement dans le domaine des énergies renouvelables (piles à combustible, systèmes d'électrolyse) et du traitement des eaux (procédés de séparation et de purification).

Keywords: Membrane composite, PVA modifiée, Propriétés électrochimiques, Matériaux polymères, Applications énergétiques.

IN VITRO ANTIOXIDANT AND ANTIMICROBIAL ACTIVITY OF TEUCRIUM POLIUM L. EXTRACTS AND PISTACIA LENTISCUS L. SEEDS' OIL

Mohamed Lamine FREIDJA^{1,2*}, Chorouk BELOUADAH¹, Feyrouz LASSAG¹, Zohra SALEM¹.

¹ Department of Microbiology and Biochemistry, Faculty of Sciences, University of M'sila , 28000 M'sila, Algeria

² Laboratory of Biomathematics, Biochemistry, Biophysics and Scientometry, Faculty of Natural and Life Sciences, University of Bejaia, 06000 Bejaia, Algeria

* Corresponding author: mohamedlamine.freidja@univ-msila.dz

Abstract: This study aims to evaluate the biological activities of *Teucrium polium* L. extracts, collected in the province of Boussâada (Sidi Ameer), , and *Pistacia lentiscus* L. Seeds' vegetal oil. Bioactive compounds were extracted from the aerial parts of *Teucrium polium* L. using two polar solvents: methanol and hydro-ethanol (20-80%), with extraction yields of 7.5% and 8.4%, respectively. Phytochemical screening revealed the presence of flavonoids and polyphenols as the dominant compounds. Antioxidant activity was assessed *in vitro* using DPPH• assay. The methanolic extract exhibited higher antioxidant activity ($IC_{50} = 31.6 \mu\text{g/mL}$) compared to the hydro-ethanolic extract ($IC_{50} = 34.00 \mu\text{g/mL}$), although both were less effective than the reference compound BHT ($IC_{50} = 21.7 \mu\text{g/mL}$). The antimicrobial activity of the methanolic extract was assessed using the agar-well diffusion method. It revealed inhibitory effects against *Escherichia coli*, *Staphylococcus aureus*, *Pseudomonas aeruginosa* and *Candida albicans*. In contrast, the hydroethanol extract had no significant effect. In addition, *Pistacia lentiscus* vegetable oil showed antibacterial activity only against *Staphylococcus aureus* and *Bacillus subtilus*. These results confirm the promising therapeutic potential of combining *Teucrium polium* L. extract with *Pistacia lentiscus* L. seeds' oil.

Keywords: *Teucrium polium* L., *Pistacia lentiscus* L., methanolic extract, hydro-ethanolic extract, vegetal oil, antioxidant activity, antibacterial activity.

PHYTOCHEMICAL CHARACTERIZATION OF *ERYNGIUM PUSILLUM* EXTRACTS

Faiza MERATATE^{1,2}, Aissa LALAOUI³, Khellaf REBBAS⁴, Salah AKKAL⁵, Ibrahim DEMIRTAS⁶, Karima BOUALI⁷, Khadija BEKHOUCHE⁷, Nesrine BENYERBAH¹, Athir GHATTOUCHE¹, Widad KHERFI¹.

¹*Departement of Chemistry, Faculty of Sciences, University of M'sila.*

²*Laboratoire des substances organo-thérapeutiques et Innovation d'énergie verte (SOLTIVER).*

³*University of M'sila, Algeria.*

⁴*Departement of Nature and Life Sciences, University of M'sila.*

⁵*Department of chemistry, University of Constantine, Algeria.*

⁶*Department of Chemistry, Türkiye.*

Abstract

Among the rare medicinal plant species that have not undergone in-depth biochemical studies, a plant from the genus *Eryngium* were selected, as these plants are known for their strong aromatic properties, with the aim of conducting a comprehensive phytochemical study. The methodology included the extraction of plant secondary metabolites using extraction techniques, employing solvents with varying polarities (water, ethanol) to ensure the widest possible range of active chemical compounds is extracted. The biological efficacy of the extracts was then evaluated through standardized tests, where they showed significant activity as antioxidants. Microbial activity against Gram-positive and négative bacterial strains, including its ability to inhibit free radicals in DPPH tests, which indicates its effectiveness as an antioxidant. The anti-inflammatory activity was also measured using in vitro laboratory bioassays, complemented by subsequent in vivo experiments. Regarding the in vivo anti-inflammatory activity study, we performed a paw edema test on laboratory mice using 1% formalin. The results showed that the ointment reduced the thickness of the edema, which seems to indicate a strong therapeutic potential in the treatment of inflammatory pain.

Keywords: Anti-inflammatory, *Eryngium*, Medicinal plants.

INTEGRATING AI FOR METABOLITE IDENTIFICATION FROM MASS SPECTROMETRY DATA: CHALLENGES IN PREPROCESSING AND NEURAL NETWORK TRAINING

Abdenassar HARRAR^{1,2*} and Hind Safa BENALI³

¹Department of Microbiology and Biochemistry, Faculty of Sciences, Laboratory of Biologie: Application en Santé et Environnement, University of M'sila, University Pole, Road Bordj Bou Arreridj, M'sila 28000, Algeria

²Laboratory of Organo-Therapeutic Substances and Sustainable Processes, University of M'sila

³Department of Microbiology and Biochemistry, Faculty of Sciences, University of M'sila,

*Corresponding author: Tel: +213 697 315 530 ; E-mail address: abdenassar.harrar@univ-msila.dz

Abstract: Developing AI models that can predict the identity of unknown metabolites in complex biological samples through analytical data analysis could revolutionize metabolomics research. Accurate identification of metabolites is essential for understanding biological processes, disease mechanisms, and the effects of drugs. Traditional methods often struggle with the complexity and volume of data, making efficient and accurate metabolite identification a challenging task. In this study, we developed and deployed an AI-based tool for metabolite identification using a multi-output neural network trained on processed MS/MS data. We trained a multi-output neural network model using TensorFlow, following a comprehensive process involving loading a processed dataset, encoding labels for Name and Formula columns, preprocessing and padding peaks to ensure uniform length, combining various features such as MW, ExactMass, and Num Peaks, scaling features using StandardScaler, splitting data into training (80%) and test (20%) sets, and defining and training the neural network model. For deployment, we developed a graphical user interface (GUI) using Tkinter. The neural network model successfully trained without system overload; however, it achieved very low accuracy, with all predictions being incorrect. We suspect the cause to be the method of preprocessing and converting the peaks to numerical format. The limitation of this study is the substantial amount of time required to identify the correct algorithm to preprocess and convert peaks accurately, train the model effectively, and integrate the findings into the GUI. Future research should focus on optimizing hyperparameters, improving data augmentation techniques, and integrating advanced visualization methods to enhance model performance and user experience.

Keywords: AI, Metabolite Identification, Neural Networks, Mass Spectrometry, Data Preprocessing

FREE RADICAL SCAVENGING EFFICIENCY OF ISATIN SCHIFF BASES(O-H VERSUS N-H). A DFT STUDY

Nadjia LATELLI ^a, Habiba BOUDIAF ^b

^aFaculty of Sciences , department of chemistry , University of M'sila, University Pole, Road Bourdj Bou Arreiridj, M'sila 28000. Algeria

^bFaculté des sciences de la matière, Département d'enseignement fondamental en SM , université El-Hadj Lakhdar Batna 1. Algeria

Corresponding authors: nadjia.latelli@univ-msila.dz

Abstract: This study explores the fundamental antioxidant mechanisms of a series of Schiff bases derived from isatin and its analogues. To achieve this, density functional theory (DFT) calculations were conducted using the hybrid M05-2X functional, the long-range corrected LC- ω PBE functional, and the 6-31+G(d,p) basis set. The molecular reactivity of these compounds was assessed using global and local reactivity descriptors in both the gas phase and various solvent environments. The results obtained from both computational models exhibit consistent trends in the gas phase and in non-polar media, highlighting hydrogen atom transfer (HAT) as the preferred pathway. However, increasing solvent polarity significantly alters the antioxidant behavior, with a greater contribution from the sequential proton loss electron transfer (SPLET) mechanism. Notably, the presence of the isatin moiety does not reduce the antioxidant potential of the disubstituted Schiff base derivatives, in agreement with previously reported experimental findings.

Key words: Schiff bases (isatin-thiocarbohydrazone), Antioxidant , M05-2X, LC- ω PBE

SYNTHESIS, CRYSTALLOGRAPHIC STUDY AND MOLECULAR MODELING OF THE COMPOUND EDTA CHLORIDE MONOHYDRATE

Zineb FELLAHI ^{1*}, Souheyla. CHETIOUI ² and Amel. DJEDOUANI³

¹Université Mohamed Chérif Messaadia Souk Ahras, Faculté des Sciences et de la Technologie, Laboratoire de sciences et technique de l'eau et environnement, Algeria

²Université Mohamed boudiaf, M'sila, Algeria

³Ecole Normale Supérieure de Constantine Assia Djebbar, Ville Universitaire Ali Mendjeli, 25000, Constantine, Algeria

* Corresponding author: zinou.fella12@univ-soukahras.dz

ABSTRACT: In recent years, the organic-inorganic hybrid materials have wide range of applications owing to their interesting chemical and physical properties. They are defined the composition of two parts at the molecular level, commonly, one of these parts is organic and the other is inorganic. These materials do not represent only a creative alternative to design new materials and compounds for academic research, but their improved or unusual features allow the development of innovative industrial applications. Nowadays, most of the hybrid materials that have already entered the market are synthesized and processed by using conventional soft chemistry based routes developed in the eighties . A new hybrid material ionic EDTA chloride monohydrate ($C_{10}H_{18}N_2O_8^{2+} \cdot Cl^- \cdot H_2O$) as a single crystal was synthesized by the simple reaction of Ethylene Diamine Tetra Acetic acid (EDTA) with hydrochloric acid in distilled water of an equimolar aqueous solution. The title crystal belongs to triclinic system with space group P_1 symmetry and $Z = 1$, $a = 5.3616(8) \text{ \AA}$, $b = 6.6477(9) \text{ \AA}$, $c = 10.4282(11) \text{ \AA}$ and $V = 343.94(8) \text{ \AA}^3$.

Keywords: EDTA , hybrid material, crystal structure, organic-inorganic.

**STRUCTURAL, OPTICAL AND ELECTRONIC PROPERTIES OF
Cd_{0.25}Zn_{0.75}S SEMICONDUCTOR FOR ENERGY AND
ENVIRONMENTAL APPLICATIONS**

BENLECHHEB Soumia

*Laboratory of Material Physics and its Applications, Faculty of Science, University of M'sila,
University Pole, Road Bordj Bou Arreridj, M'sila, 28000, Algeria*

Corresponding author: Tel./Fax: +213671655656 ; E-mail address: soumiaeva@gmail.com

Abstract: In this study, the structural, optical and electronic properties of the Cd_{0.25}Zn_{0.75}S semi-conductor compound were investigated. Structural characterization was performed to identify the crystalline phase, while optical behavior was examined through UV-Visible spectroscopy. The electronic properties were analyzed to estimate the band gap and evaluate the potential of this material for energy-related applications, The tunability of the band gap in Cd_{0.25}Zn_{0.75}S alloys, combined with their high absorption coefficients in the visible–UV range, reinforces the suitability of Cd_{0.25}Zn_{0.75}S for thin-film solar applications. The material shows efficient light–matter interaction due to its strong dielectric response and favorable refractive index, which can enhance charge carrier generation. Moreover, the partial substitution of Cd with Zn not only adjusts the optoelectronic behavior but also reduces the environmental impact, these characteristics make Cd_{0.25}Zn_{0.75}S a balanced choice for sustainable and high-performance energy devices.

Keywords: GGA, Semiconductor, optical properties, photovoltaic, UV-Visible spectroscopy.

**ACTIVITE ANTIOXYDANTE, ANTI-INFLAMMATOIRE ET ANTIBACTERIENNE
D'ANTHEMIS PEDUNCULATA**

Sara CHADI ^{1,3}, Sabah BOUMERFEG ^{2,3}, Thoraya GUEMMAZ ³, El yamine MESSOUAK ² and
Abderahmane BAGHIANI ³

¹ *Laboratoire de Caractérisation et de Valorisation des Ressources Naturelles, Faculté des Sciences de la Nature et de la Vie, Université Mohamed El Bachir El Ibrahimi, Bordj Bou-Arréridj, 34000, Algeria.*

² *Département de Biologie, Faculté des Sciences de la Nature et de la Vie, Université Mohamed El Bachir El Ibrahimi, Bordj Bou-Arréridj, 34000, Algeria.*

³ *Laboratoire de Biochimie Appliquée, Faculté des Sciences de la Nature et de la Vie, Université Ferhat Abbas Sétif 1, 19000, Algeria.*

*Corresponding author: Tel./Fax: +213-698-932-308 ; E-mail address: saradoc20172024@gmail.com

Abstract : L'introduction des antibiotiques dans la pratique médicale a révolutionné le traitement des maladies infectieuses, sauvant ainsi d'innombrables vies. Cependant, l'augmentation de la résistance aux antibiotiques est devenue une préoccupation majeure pour les cliniciens du monde entier. Cette résistance se traduit par une difficulté croissante à traiter efficacement diverses infections, ce qui conduit souvent à des impasses thérapeutiques. De plus, l'utilisation de composés antioxydants synthétiques est souvent associée à des effets secondaires indésirables. En conséquence, la recherche actuelle se concentre de plus en plus sur les molécules d'origine naturelle ayant des activités biologiques prouvées, dans le but de découvrir de nouveaux composés qui pourraient servir de base à de futurs agents thérapeutiques. Dans ce contexte, l'activité antioxydante, anti-inflammatoire et antibactérienne *in vitro* de l'extrait hydrométhanolique d'*Anthemis pedunculata* a été évaluée. L'extrait a présenté un rendement d'extraction de 24 %. Les dosages colorimétriques des polyphénols totaux et des flavonoïdes ont révélé que l'extrait brut d'*Anthemis pedunculata* est particulièrement riche en composés phénoliques et flavonoïdiques. L'activité antioxydante de cet extrait a été évaluée à l'aide de trois tests complémentaires : le piégeage du radical DPPH, le pouvoir réducteur (FRAP) et la chélation des ions ferreux. Les résultats ont mis en évidence un effet antioxydant significatif, avec une forte capacité de neutralisation des radicaux libres DPPH, un pouvoir réducteur élevé vis-à-vis des ions ferriques, ainsi qu'une bonne aptitude à la chélation du fer. Pour l'activité anti-inflammatoire, une importante inhibition de la dénaturation des protéines à différentes concentrations a été marquée. Le criblage antibactérien a révélé une forte activité contre les bactéries Gram positives et une inhibition modérée sur des souches Gram négatives. Selon ces résultats, l'extrait d'*Anthemis pedunculata* possède une activité antioxydante, anti-inflammatoire et antibactérienne significative *in vitro* et peut être utilisé dans le traitement du stress oxydatif et comme antibiotique alternatif en cas d'infections.

Mots clés: DPPH; antioxydant ; antibactérien ; anti-inflammatoire; *Anthemis pedunculata*

CALORIMÉTRIE, RÉSISTANCE ET MICROSTRUCTURE D'UN LIANT ACTIVÉ À BASE DE MÉTAKAOLIN

SAIDAT Fatma^A, BOUNAR Rabeh^B, MAKANI Abdelkadir^C, TAFRAOUI Ahmed^C

^A *Laboratoire de Génie Civil et Environnement (LGCE), Université de Mohamed Seddik Benyahya, Jijel (18000), Algérie*

^B *Université de M'sila C Laboratoire EMIA ex LFGM, université Tahri Mohamed, Bechar*

RESUMÉ : Au cours de ces dernières années l'utilisation de métakaolin comme addition pouzzolanique s'est développée en substitution partielle du ciment pour réduire la consommation de ciment et améliorer la durabilité du béton. En revanche, des manques de performances mécaniques des bétons incorporant du métakaolin apparaissent au jeune âge lorsqu'ils sont mûris à température ambiante. L'objectif de cette étude est de rechercher les moyens d'activer chimiquement le métakaolin dans les matrices cimentaires afin de faciliter sa dissolution et d'augmenter la vitesse de sa réaction pouzzolanique qui est lente pour recouvrer, aux jeunes âges, un niveau de performance équivalent à celui obtenu dans les bétons sans métakaolin. L'étude a été réalisée à l'échelle du mortier et traite de l'effet de l'activation du métakaolin par des sulfates alcalins sur différentes propriétés (temps de prise, résistance mécanique à la compression, chaleur d'hydratation...). L'activation avérée aux jeunes âges altère les résistances à plus long terme des mortiers (28 jours), quelle que soit la nature du sulfate alcalin, en contrecarrant l'action pouzzolanique propre du métakaolin. Les analyses physico-chimiques sur pâtes ont néanmoins confirmé l'activation à jeune âge du métakaolin dans la matrice, indépendamment de la nature du sulfate alcalin.

Mots Clés : métakaolin, liant activé, résistance mécanique, microstructure

EVALUATION OF THE HYDROLYTIC DEGRADATION OF TRIPHENYLMETHANE DYES USING DFT AND TD-DFT METHODS

D.TAHARCHAUCHE ^{1*}, N. MECHEHOUD ² and N, LATELLI ³

¹Department of Chemistry, Faculty of Sciences, University of Batna 1, 05000 Batna, Algeria

²Department of Technical Science, Institute of Hygiene and Safety, University of Batna 2, Fesdis, Algeria

³Department of Chemistry, Faculty of Sciences, University of Msila, Ichbilia, BP 166, 28000 M'sila, Algeria

*d.taharchaouche@univ-batna2.dz

Abstract: This study explores the DFT reactivity descriptors, UV-Vis spectra, and the hydrolysis mechanism of three cationic dyes (Malachite Green (MG), Brilliant Green (BG) and Ethyl Green (EG)) using various exchange-correlation functionals (global GGAs, hybrids, and range-separated functionals). The UV-Vis absorption spectra were obtained using time-dependent density functional theory (TD-DFT). The results indicate that the spectra follow a trend based on the type of functional used, with the GGA functionals giving the largest λ_{max} values, followed by the hybrid functionals and then the range-separated functionals. Regarding the hydrolysis mechanism, the energy barriers were calculated in both the gas and solution phases. The order of the barriers is $BG^+ < MG^+ < EG^{2+}$ in both phases. In comparison, the CAM-B3LYP functional gives the highest barriers for hydrolysis, while the M06 functional provides the lowest barriers in both phases.

Keywords : Triphenylmethane dyes, DFT, TD-DFT, Degradation , hydrolysis.

ASSESSMENT OF BIOLOGICAL ACTIVITIES OF MEDICINAL PLANT

Faiza MERATATE^{1,2}, Aissa LALAOUF³, Khellaf REBBAS⁴, Salah AKKAL⁵, Ibrahim DEMIRTAS⁶, Karima BOUALI⁷, khadija BEKHOUCHE⁷, Samiha LOBZI¹, Lamis KEBABI¹, Affaf GUERIBIS¹

¹*Departement of Chemistry, Faculty of Sciences, University of M'sila.*

²*Laboratoire des substances organo-thérapeutiques et Innovation d'énergie verte (SOLTIVER).*

³*University of M'sila, Algeria.*

⁴*Departement of Nature and Life Sciences, University of M'sila.*

⁵*Departement of Chemistry, University of Constantine*

⁶*Department of Chemistry, Türkiye.*

Abstract :Medicinal plants are a rich source of bioactive compounds with multiple health benefits. In this context, we carried out a phytochemical and biological study of medicinal plant belongs to the *Zygophyllaceae* family. The active compounds of this plant were extracted; the antimicrobial and antioxidant activities were studied, The Ethanolic extract of this plant possess a good antibacterial activity on *Pseudomonas aeruginosa* ATCC 27853 with a zone of inhibition of 15 mm while low activity was observed against *Staphylococcus aureus* ATCC 25923 and *Escherichia coli* ATCC 25922, with a zones of inhibition of 7 mm and 6 mm respectively. On the other hand the extract possess a good antioxidant activity. An ointment based on *Zygophyllum* extract was prepared, and its anti-inflammatory activity was evaluated in an experimental model of formaldehyde-induced inflammation in rats. The results showed a clear efficacy of the ointment, demonstrating its anti-inflammatory properties.

Keywords :: Medicinal Plants, Antimicrobial Activity, Antioxidant Activity, Ointment, anti-inflammatory.

EVALUATION OF THE BIOSORPTION KINETICS AND THERMODYNAMICS FOR THE REMOVAL OF TEXTILE DYE FROM AQUEOUS SOLUTIONS USING CALCINED OPUNTIA FICUS INDICA

HENINI Ghania^{1,*}, LAIDANI Ykhlef², HENTABLI Mohamed³, BENDRISS

Elhouari⁴

^{1,4}Laboratory Environment-Water, University of Chlef, Algeria

^{2,3}Laboratory Chemical Vegetal - Water – Energy, University of Chlef, Algeria

*Corresponding author: +213 7 79 55 60 65, g.henin@gmail.com

Abstract: In this study, the removal of Bemacide Red from synthetic wastewater was investigated using *Opuntia ficus indica* as adsorbent. The preparation method studied consists of chemical activation with H_3PO_4 , followed by pyrolysis at $600^\circ C$. The determinations of the concentrations of dye have been performed using an UV– visible spectrophotometer. The results obtained show $AC_{H_3PO_4}$ / Bemacide Red have an adsorption capacity ($q_m = 5.892$ mg/g). The adsorption process was rapid and reached equilibrium in 60 min of contact at $25^\circ C$ and $pH = 5.68$. The different adsorption models Langmuir, Freundlich, Temkin and Dubinin-Radushkevich were used for the mathematical description of the adsorption equilibrium, and it was found that the very well - equipped experimental data for the Langmuir model ($R^2 = 0.954$), the pseudo-first- and pseudo-second order kinetic models were applied to the experimental data. The experimental data fitted very well the pseudo-second-order kinetic model ($R^2 = 0.986$) and also followed the model of intra particle diffusion K_{dif} vary from 0.0445 to 0.107 $mg/(g \text{ min}^{1/2})$ for concentrations between 30 and 70 mg/L, whereas diffusion is not the only rate - control step. The thermodynamic parameters study show that, the negative value of ΔH° indicated that the adsorption of the dye on $AC_{H_3PO_4}$ was endothermic, the reaction was accompanied by a increase in ΔS° . The Gibbs free energy increased from -104.820 to -98.227 kJ/mol, respectively for Bemacide Red dye when the temperature was increased from 298 to 318 K. The studied system shows that the adsorption process is spontaneous.

Keywords : Adsorption, *Opuntia ficus indica* cords, Activated Carbon, Bemacide Red, Kinetics study, Thermodynamics

INVESTIGATING THE STRUCTURAL AND OPTICAL PROPERTIES OF MANGANESE OXIDE NANOPARTICLES SYNTHESIZED VIA THE SOL–GEL METHOD

Abderrahim SIASSI^{1,2,✉}, Rabie AMARI^{3,4}, Abdelhalim KAHOU^{1,2}, Bahri DEGHEFEL^{3,5},
Noudjoud LEBGAA^{2,6}, Salim DAOUDI^{1,2}

¹*Department of Matter Sciences, Faculty of Sciences and Technology, University of Mohamed El bachir El ibrahimi - Bordj Bou Arreridj. 34030, Algeria*

²*Laboratory of Materials Physics, Radiation and Nanostructures (LPMRN), University of Mohamed El bachir El ibrahimi - Bordj Bou Arreridj 34030, Algeria*

³*Laboratory of Materials and Renewable Energy, Faculty of Sciences, University of M'sila, Algeria.*

⁴*Department of Civil Engineering, Faculty of Technology, University of M'sila, Algeria.*

⁵*Department of Physics, Faculty of Sciences, University of M'sila, Algeria*

⁶*Department of Physics, Faculty of Sciences, University of Setif 1, Setif 19000, Algeria..*

✉*Corresponding Author Email: abderrahim.siassi@univ-bba.dz*

Abstract: Manganese oxide thin films were prepared using the sol–gel spin-coating method in this work. While numerous synthesis techniques are cited in the literature, this procedure utilized manganese acetate tetrahydrate ($(\text{CH}_3\text{COO})_2\text{Mn}\cdot 4\text{H}_2\text{O}$) with ethanol serving as the solvent. The synthesis began by dissolving a measured quantity of manganese acetate in ethanol, followed by the addition of MEA in a 1:1 molar ratio relative to manganese ions. The mixture was stirred continuously at 50 °C for 60 minutes to ensure homogeneity. The resulting sol was deposited onto glass substrates through spin coating at a speed of 2000 rpm for 30 seconds and subsequently annealed at 450 °C. Optical measurements showed that the fabricated films possess an indirect optical band gap of approximately 2.36 eV. Structural analysis by X-ray diffraction (XRD) confirmed the presence of a cubic Mn_2O_3 crystalline phase in the deposited layers.

Keywords: Manganese oxide; DRX; sol gel; spin coating.

ENHANCED METHYLENE BLUE ADSORPTION FROM WATER USING Fe₂O₃-
DECORATED KAOLINITE

Tayeb BEN KOUIDER ^{1,*}, Lahcene SOULI ², Yazid DEROUICHE ¹

¹ Laboratoire Physico-Chimie des Matériaux et Environnement, Université ZIANE Achour, 17000 Djelfa, Algeria.

² Laboratory of Organic Chemistry and Natural Substances, Faculty of Exact Sciences and informatics, Ziane Achour University, 17000 Djelfa, Algeria.

*Corresponding author: Tel : +213779421387; E-mail address: * t.benkouider@univ-djelfa.dz

Abstract: The contamination of water bodies by synthetic dyes such as methylene blue (MB) represents a significant environmental concern due to their toxicity and persistence[1]. In this study, iron oxide (Fe₂O₃) nanoparticles were synthesized via a green route using natural extracts as reducing and stabilizing agents and subsequently incorporated into a kaolinite matrix to enhance their dye removal capability. The resulting Fe₂O₃/kaolinite nanocomposites were characterized using X-ray diffraction (XRD) and Fourier-transform infrared spectroscopy (FTIR), confirming successful nanoparticle formation and integration into the clay structure. Adsorption experiments conducted in aqueous media demonstrated the high efficiency of these nanocomposites in removing methylene blue, outperforming raw kaolinite. The enhanced adsorption capacity is attributed to the synergistic interaction between Fe₂O₃ and kaolinite, which increases the available surface area and active sites. These findings highlight the potential of Fe₂O₃/kaolinite nanocomposites as sustainable and effective adsorbents for the treatment of dye-contaminated water. This work contributes to the development of environmentally friendly water purification technologies targeting organic pollutants.

Keywords: Water pollution : Fe₂O₃ nanoparticles : kaolinite: methylene blue: XRD: FTIR

AMÉLIORATION DE L'ULTRAFILTRATION DES MARGINES PAR COUPLAGE AUX ULTRASONS « LA SONO-ULTRAFILTRATION »

Mustapha OUADAH ⁽¹⁾ ; Radia CHEMLAL ^(1,2) ; Nabil MAMERI ⁽¹⁾

1. Laboratoire de bioengineering et génie des procédés. Ecole National Polytechnique, Alger

2. Faculté des Sciences Biologiques, USTHB. Alger

Tel: 0671433931

E-Mail: ouadahmustapha@gmail.com

Résumé : Le bassin méditerranéen est touché par le problème de pollution engendrée par les rejets anarchiques des margines qui ayant une composition chimiques hétérogènes, leurs actions directe sur l'environnement à cause des éléments azotés et des composés phénoliques qui ont un effet néfaste. Dans la lutte contre ces éléments, différents procédés ont été développés. Dans ce travail le principe repose sur la comparaison entre deux procédés physiques : ultrason et ultrafiltration, essai par la suite, le couplage entre ces deux traitements pour voir l'impact sur la qualité de produit fini et l'effet sur le coût de traitement. La comparaison des résultats obtenus suite à ces différents traitements des margines montre qu'il est envisageable d'améliorer le taux d'élimination de la charge polluante de ces effluents par application de procédés intégrés (couplage des deux traitements) Le principe de ce procédé hybride repose sur l'amélioration des performances de l'ultrafiltration par combinaison aux ultrasons. Les résultats obtenus sont très prometteurs par rapport à l'ultrafiltration seule. En effet, on a enregistré des abattements aux alentours de 94% en DCO, 92% en COT, 74% en polyphénols, 76% en azote ammoniacal, disparition des acides gras et un effet stérilisant de 100%. Un autre constat très pertinent concerne la modification des propriétés dynamiques et rhéologique du fluide telle que la viscosité affecte directement les paramètres hydrodynamiques de l'UF, tel que débit du perméat. L'analyse de ces résultats nous encourage à conclure que le procédé avec l'ultrason améliore de manière très efficace les performances de l'ultrafiltration classique d'une part, augmentant le pouvoir dépolluant de système d'autre part.

Mots clés : Acide gras, Polyphénols, Margine, Ultrason, Ultrafiltration

PHYSICAL AND CHEMICAL PROPERTIES OF NANOMATERIAL SPINEL OXIDE DOPED WITH MAGNESIUM

TEBERMACINE Ouarda*

**University Mohamed Khider – Biskra Algeria, Faculty of Exact Sciences, Laboratory of Molecular Chemistry and Environment.*

**Department of Matter Sciences; Biskra, Algeria.*

ouarda.tebermacine@univ-biskra.dz

Abstract: Spinel ferrites, with the general formula AB_2O_4 , are a class of crystalline materials known for their remarkable chemical and thermal stability. These compounds have attracted extensive attention due to their wide range of applications in various technological and industrial fields. Spinel ferrites are commonly utilized in magnetic recording media, magnetic fluids, MRI enhancement, magnetically guided drug delivery, sensors, and pigments, among others. One of the notable members of the spinel family is calcium ferrite ($CaFe_2O_4$). It is considered particularly important due to its natural abundance, eco-friendly nature, and non-toxic behavior. Calcium ferrite nanoparticles (CFNPs) exhibit superparamagnetic properties and are known to function as efficient catalysts. Furthermore, CFNPs have been extensively studied for their adsorption performance in removing dyes from aqueous solutions, offering a more environmentally safe alternative compared to other ferrite materials. Spinel oxide ($0 \leq x \leq 0.5$) oxides synthesized by sol-gel method were investigated. X ray diffraction, fourier transform infrared spectroscopy, scanning electron microscopy, optical absorption measurements, were used to characterize the structure, morphological, optical properties of the samples. The studied compounds show a single spinel phase with a nanoparticles and the solubility of Magnesium in the spinel structure was limited to 50%. The optical band gap increases with increasing magnesium substitution from 2.88 to 3.00 eV.

Keywords: Spinel oxide, nanomaterials, sol-gel, X-ray diffraction, optical absorption

COMPARATIVE ANALYSIS OF THE PHYSICOCHEMICAL AND MORPHO-STRUCTURAL CHARACTERISTICS OF A NANOMATERIAL SYNTHESIZED BY SOL-GEL, PRECIPITATION, AND HYDROTHERMAL METHODS

N. MECHEHOUD ^{1*}, D.TAHARCHAOUCHE ² and N, LATELLI ³

¹*Department of Chemistry, Faculty of Sciences, University of Batna 1, 05000 Batna, Algeria*

²*Department of Technical Science, Institute of Hygiene and Safety, University of Batna 2, Fesdis, Algeria*

³*Department of Chemistry, Faculty of Sciences, University of Msila, Ichbilja, BP 166, 28000 M'sila, Algeria*

**naima.mechehoud@univ-batna.dz*

Abstract : In this work, we synthesized and characterized zinc oxide (ZnO) nanoparticles using three different methods: co-precipitation, sol-gel, and sonochemical synthesis. We aimed to determine the most effective synthesis method based on a small-scale application. The optical and morphological characteristics were analyzed using X-ray diffraction (XRD), which revealed the structural properties of our samples. The results showed that the ZnO powders, regardless of the synthesis method, crystallize in a hexagonal wurtzite structure, confirming the formation of ZnO. Grain size calculations indicated that the particles are in the nanometer range. The catalytic performance was evaluated by monitoring the degradation of methyl orange (MO), used as a model pollutant, under artificial UV irradiation. The results demonstrated that ZnO synthesized via the sonochemical method exhibited significant photocatalytic efficiency, achieving 96% degradation of methyl orange within 120 minutes. This result confirms the catalyst's ability to completely decolorize the solution. In contrast, the photocatalytic reaction using ZnO prepared by co-precipitation was the least efficient, likely due to the formation of new energy levels near the conduction band (CB), which increases the recombination rate and negatively affects photocatalytic performance.

Keywords: Zinc oxide, semiconductor, co-precipitation, sol-gel, sonochemistry, XRD, photocatalyst.

A DFT STUDY OF THE 2D NANOMATERIAL -HYDROGENATED SILICENE

Khouloud GHERBI^{*}, Hafid BELKHIR¹ and Mohamed Tahar KADRI¹

¹*Department of physics, Laboratory of studies of Surfaces and Interfaces of Solid Matter (LESIMS),
University of Badji Mokhtar Annaba, Algeria*

** Tel: +213-06-72-45-93-82; E-mail address: khouloud.gherbi@univ-annaba.dz*

Abstract: Two-dimensional (2D) nanomaterials such as graphene, silicene, germanene and borophene have received considerable attention in recent years due to their extraordinary physical and chemical properties, which make them promising candidates for the development of next generation nanoelectronics devices. Silicene is defined as a monolayer of silicon atoms arranged in a honeycomb structure. Density functional theory (DFT) was used to investigate the structural and electronic properties of a hydrogenated silicene sheet. We optimised the structure of a functionalised silicene sheet with H and the calculations showed that the lattice constant of the hydrogenated silicene sheet was $a = 3.89 \text{ \AA}$, the Si-Si bond length was 2.358 \AA , the Si-H bond length was 1.5 \AA and the buckling height was $\Delta z = 0.62 \text{ \AA}$. These values are larger than those obtained for a silicene sheet ($a = 3.86 \text{ \AA}$, Si-Si bond length = 2.284 \AA and $\Delta z = 0.45 \text{ \AA}$). In terms of electronic properties, our results show that functionalisation of hydrogenated silicene opens the band gap. We also found that the zero direct band gap at the K-point (semimetal) in silicene changes to a direct band gap at the Gamma-point (semiconductor, $E_g = 2.33 \text{ eV}$). Calculations of density and partial DOS were performed to evaluate the bonding characteristics of the structures. These calculations showed sp^3 hybridisation, and charge density calculations showed the types of bond lengths (Si-Si and Si-H). To verify the stability of hydrogenated silicene, we calculated the phonon dispersion along the high symmetry points in the Brillouin zone.

Keywords: DFT; Hydrogenated silicene; bond length; buckling; semiconductor

ETUDE DE LA FIXATION DU Ni²⁺ ET Cr³⁺ PAR LA RESINE ACIDE PARA-AMINOBENZOIQUE-FORMOL

MAHI Ahmed^{1*}, DAHO Bouabdellah² et CHADLI El hadj³

^{1*}Polymers Chemistry Laboratory (LCP) BP 1524, Ahmed Ben Bella, Oran1 31000, Algeria.

²Engineering Physics Laboratory, University of Ibn Khaldoun Tiaret 14000, Algeria.

³Department of chemistry, Faculty of Material Science; University of Ibn Khaldoun BP 78 Zaaroura;Tiaret 14000, Algeria

*Corresponding author: Tel./Fax: +21396127735 ; E-mail address: ahmedmahi761@gmail.com

Abstract: This work touches the problem of hydrous pollution resulting from heavy metals such as chromium and nickel. Many studies were undertaken to eliminate these pollutants among them the use of the derivatives phenolic resins. The analysis of the results enabled us to evaluate the aptitude of the phenolic resins and their derivative to complex this pollutant from their elimination. In conclusion, the resin seems to have a much better affinity for Cr³⁺ than for Ni²⁺. In Algeria, water pollution approached dangerous levels in the 1970s as a result of large volumes of untreated sewage being dumped into rivers, lakes and coastal areas by expanding industry and urban centres. In northern Algeria, where heavy industries are concentrated, most of the treatment plants do not work well enough, and moreover the most serious problem remains the contamination of groundwater, which results not only from the fact that the factories evacuate untreated water and pile up their waste without any particular precautions, but also from the abuse of chemicals used in agriculture. Groundwater is generally considered to be the best source of drinking water, and contamination often threatens the water supply. Potability is the essential characteristic of urban tap water, which requires raw water from all which can constitute a risk to the health of the consumer. It is necessary to carry out a double elimination, first the suspended solids and then the pathogens (bacteria, parasites, viruses). Another pollution, more dangerous and less visible than that caused by suspended solids, is due to heavy metals; it is micropollution that has as its main origin the discharge of industrial effluents contaminated by these micropollutants such as (Hg, Pb, As, Ni, etc.) into the natural environment. The objective of this work is to synthesize a resin on a laboratory scale capable of fixing micropollutants, in particular nickel and chromium. In this study, we developed resin-based adsorbent carriers. (PARA-FORMOL). This elaboration is made from inexpensive precursors, but requiring original techniques using fairly developed concepts, mainly those related to purification. The phenomenon of adsorption of these metals on the supports thus constituted is studied in order to take advantage of this type of adsorbent. The results obtained state that these adsorbents are effective in their ability to bind the heavy metals nickel and chromium with variable adsorption rates depending on the metal considered. By contributing these results, this study can thus contribute to a certain extent to solving the problem of contamination of resources intended for human consumption.

Keywords: Phenolic resins, polycondensation, heavy metals, chemical adsorption.

IRON-VANADYL BASED KEGGIN POLYOXOMETALLATES FOR CLEAN SYNTHESIS OF ADIPIC ACID

Dahbia AMITOUCHE^{1*}, Ibtissam SEBAI², Sihem MOUANNI², Tassadit MAZARI¹, Mohamed HAOUAS³, Catherine ROCH MARCHAL³ and Cherifa RABIA²

¹*Chemical Engineering and Applied Chemistry Laboratory (LCGA). UMMTO, Tizi Ouzou 15000, Algeria*

²*Natural Gas Chemistry Laboratory, Faculty of Chemistry, USTHB, BP32, El-Alia, 16111 Bab-Ezzouar, Algeria*

³*ILV-UMR 8180 CNRS, Lavoisier Building, University of Versailles-St Quentin-en-Yvelines 78035 Versailles Cedex, France*

*Corresponding author: Tel: +213 5 49 76 70 73 ; E-mail address: dahbia.amitouche@ummto.dz

Abstract: Polyoxometallates could be used as catalysts for oxidation of various organic substrates with hydrogen peroxide or oxygen. The presence of counter-ions significantly influences the structure of Keggin-type POMs by modulating their stability, crystal arrangement, and solubility. These counter-ions also affect the acidic, redox, and catalytic properties of POMs by altering the electronic distribution around the metal cluster and facilitating or inhibiting interactions with substrates. In this work, a new series of Keggin-type polyoxometalates (POMs) was synthesized via cationic substitution by combining vanadyl (VO^{2+}) and iron (Fe^{3+}) ions. The resulting compounds were evaluated as catalysts (1%) for the oxidation of cyclohexanone (30mmol) to adipic acid, using hydrogen peroxide (H_2O_2 / 30 %) as green oxidant at 90 ° C over a period of 20 hours. The structural and physicochemical characterization of the catalysts $\text{HVO}_x\text{Fe}_y\text{PMo}_{12}\text{O}_{40}$ was performed using infrared spectroscopy (IR), X-ray diffraction (XRD), thermal analysis (TGA/DSC), UV - Vis spectroscopy, and cyclic voltammetry. Among the tested catalysts, the vanadyl-containing system ($\text{HVOPMo}_{12}\text{O}_{40}$) exhibited the highest catalytic performance, yielding a high conversion to adipic acid. The final product was identified and characterized through melting point determination, IR spectroscopy and high-performance liquid chromatography (HPLC).

Keywords : Heteropolysalts ; Catalytic oxidation ; Hydrogen peroxide ; Adipic acid ; Polyoxometallates.

DEGRADATION AVANCEE DU BLEU DE METHYLENE PAR UN PROCEDE FENTON-LIKE MODIFIE : APPLICATION DU PLAN BOX- BEHNKEN

Hawa BENDEBANE¹, Salima BENDEBANE², Farida BENDEBANE¹

¹ *Laboratory LOMOP, Badji Mokhtar- Annaba University, BP 12, Annaba-Algeria*

² *National Higher School of Technology and Engineering, Laboratory L3M, 23005, Annaba, Algeria,
bendebanehawa@yahoo.fr*

Résumé : Le présent travail vise à développer et à optimiser les paramètres influençant la dégradation du bleu de méthylène (BM) à l'aide d'un procédé Fenton-like modifié, reconnu pour son efficacité dans l'élimination des colorants organiques persistants présents dans les effluents industriels. À cette fin, un plan d'expériences de type Box-Behnken (RSM) a été appliqué, en faisant varier trois facteurs clés : la concentration du catalyseur ($[Fe^{2+}]$), la concentration de l'oxydant ($[K_2S_2O_8]$) et la concentration initiale du colorant. L'étude a permis de déterminer des conditions optimales de fonctionnement : $[Fe^{2+}] = 2,88$ ppm, $[K_2S_2O_8] = 10$ ppm et concentration initiale de BM = 14,39 ppm. Ces paramètres ont conduit à un rendement de dégradation théorique de 99,15 %, confirmé expérimentalement par un taux de 99,17 %. L'efficacité du procédé a ensuite été testée sur différentes matrices aqueuses réelles, révélant l'ordre suivant : Eau distillée (99,17 %) > Eau industrielle (98,93 %) > Eau de mer (98,91 %) > Eau minérale (98,88 %) > Eau de source (98,68 %). Ces résultats mettent en évidence la robustesse du procédé dans des environnements diversifiés.

Mots-clés : Photo-oxydation assistée (POA), Fenton-like modifié, bleu de méthylène (BM), optimisation, plan de surface de réponse (RSM).

FIRST PRINCIPLE STUDY ON HALF METALLIC PROPERTIES OF MNSB COMPOUND IN THE TWO STRUCTURES HEXAGONAL AND ZINC-BLENDE, BY EMPLOYING AB INITIO CALCULATIONS

Djihad MOKHTARI^{1,2}, Zoulikha CHARIFI^{2,3} and Hakim BAAZIZ^{2,3}

¹ Department of Physics, Higher Normal School of Bousaâda - M'sila (Algeria)

² Laboratory of Physics and Chemistry of Materials, University of M'sila, Algeria

³ Physics Department, Faculty of Science, University of M'sila (Algeria)

Corresponding author: Tel: +213698515244 ; mokhtari.djihad@ens-bousaada.dz

Abstract: An ab initio study was performed using the full potential linearized augmented plane wave (FP-LAPW) method within the framework of density functional theory (DFT). The realization of this study requires the use of the code (WIEN2k), to study the structural, electronic and magnetic properties of the binary compound MnSb in the two structures hexagonal and zinc-blende, several approximations were used, namely the generalised gradient approximation (GGA), local density approximation (LDA), EV-GGA (Engel-Vosko) and mBJ (modified Becke-Johnson). The calculation showed that the stable case of the MnSb compound is the spin-polarized (magnetic) case regardless of the approximation applied (LDA or GGA) in the hexagonal and zinc-blende structures. The MnSb compound is a metal in the hexagonal phases, but in the zinc-blende phase it is a Half-metallic. The decrease in the energy gap in the same phase (zinc-blende) is observed in both EV-GGA and mBJ approximations. While in the LDA approximation the gap increases. In the case of GGA, it is noted that the latter remains almost the same. in the zinc-blende structure the total magnetic moment for the MnSb compound (4 μ B).

Keywords: DFT, Half metallic, Magnetic properties, mBJ, zinc-blende structures.

INVESTIGATION OF STRUCTURAL, MECHANICAL, ELECTRONIC, OPTICAL, AND DYNAMICAL PROPERTIES OF CUBIC MgLiF₃, MgLiH₃

L. REFICE^{1*}, A. BENAMER¹

¹*Department of physical science, Higher Normal School of Boussaâda, 28001 Boussaâda, Algeria.*

* *refice.lamouri@ens-bousaada.dz*

Abstract: Ab initio calculations were performed for the cubic antiperovskites Borides and carbides MgLiF₃, MgLiH₃. to study the structural, elastic and electronic properties from the ternary MgLiF₃, MgLiH₃. We have employed the local density approximation (LDA) and the generalized gradient approximation (GGA) for the exchange and correlation potential. The equilibrium lattice constants and the bulk modulus and its pressure derivative are calculated and compared with available experiment and theoretical results. we have also predicted the elastic constants, Young's modulus (E), Poisson ratio (ν), shear modulus (G). The contribution of the different bands was analysed from total and partial density of states curves.

Keywords: Intermetallic compounds, Ab initio calculations, Elastic properties.

MAGNESIUM OXIDE NANOPARTICLES SYNTHESIZED USING OLIVE LEAF EXTRACT FOR ENVIRONMENTAL REMEDIATION

Laila HAMZA^{1*}, Souhaila MENACEUR², Ahlem KEROUR¹ and Salah Eddine LAOUINI²

¹ *University of Science and Technology Houari Boumediene, USTHB, Faculty of Physics, Laboratory of Semiconductor Materials and Metal Oxides (LMSOM), Algiers, Algeria.*

² *University of El Oued, Faculty of Technology, Laboratory of Biotechnology Biomaterial and Condensed Matter, Eloued, Algeria.*

**Corresponding-author email: laila.hamza.2009@gmail.com*

Abstract/ Magnesium oxide nanoparticles (MgONPs) were synthesized via a simple, eco-friendly method employing olive leaf extract as a natural reducing and stabilizing agent. This green synthesis approach not only adheres to the principles of sustainable and environmentally benign chemistry but also leverages the phytochemical constituents of olive leaves such as polyphenols, flavonoids, and organic acids to mediate the formation and stabilization of the nanoparticles. The use of plant-based extracts eliminates the need for toxic chemical reagents and high-energy input, offering a safe, cost-effective, and scalable alternative for nanoparticle production. UV–Visible spectroscopy revealed a characteristic absorption peak at 278 nm confirming MgO nanoparticle formation, while X-ray diffraction (XRD) analysis demonstrated the crystalline nature of the particles with an estimated average size of approximately 20 nm. The photocatalytic activity of the biosynthesized MgO NPs was investigated under natural sunlight irradiation, targeting the degradation of organic pollutants. The nanoparticles exhibited remarkable photocatalytic efficiency, achieving degradation rates of 95% for Rose Bengal and 90% for Methyl Orange dyes within 120 minutes. These results underscore their potential application in wastewater treatment. Additionally, the MgO NPs demonstrated a high removal efficiency of approximately 90% against a selected insecticide, further highlighting their broad-spectrum environmental remediation capability.

Keywords: Photocatalysis, Nanoparticles, magnesium -oxides, Greensynthesis, Synthetic dyes.

ENHANCED VISIBLE ERIOCHROME BLACK T DEGRADATION USING ZNS/TIO₂ HETEROJUNCTION NANOCATALYSTS

Mustapha BOUBATRA ^{*1,2,4} Meriem HAMLA ^{2,4} Samra AMAMRA ^{3,4}

¹Laboratory of Electrochemistry and Environment (LEE), Mohamed El Bachir El-Ibrahimi University - Bordj Bou Arreridj- 34030, Algeria.

²Laboratory of Energetics and Solid-State Electrochemistry (LEES), Ferhat Abass University of SETIF, 19000, Algeria

³Laboratory of Electrochemistry of Molecular and Complex Materials (LEMMC), Faculty of Technology, Department of Process Engineering, University Ferhat Abbas Setif-1, DZ-19000, Setif, Algeria

⁴Department of Matter of Sciences, Faculty of Science and Technology, Mohamed El Bachir El-Ibrahimi University, Bordj Bou Arreridj, Algeria

*Corresponding author: Tel./Fax: +213 662 698 530 ; E-mail address: m.boubatra@univ-bba.dz

Abstract/ Constructing stable and efficient heterostructure photocatalysts is pivotal for solar energy conversion and for applications like environmental purification. In this study, we synthesized multiple ZnS/TiO₂ heterojunction nanocatalysts using a hydrothermal technique. As detailed in the X-ray Diffraction (XRD) results, the nanostructure included a few-layer ZnS nanosheet on which multiple anatase TiO₂ nanocrystals were anchored. The diffuse reflectance spectroscopy (DRS) results showed that the composite's (2.81 eV for the optimal sample) bandgap was lower than that of pure TiO₂ (3.2 eV) which also improved visible light absorption. The optimized 25 wt% ZnS/TiO₂ composite had remarkable photocatalytic activity (12 times greater than pure TiO₂) and surpassed the production rate of a 1 wt% Pt/TiO₂ catalyst under visible irradiation of 150 mW.cm⁻². In the photocatalytic degradation of Eriochrome Black T (EBT), the same catalyst produced 96% degradation in 25 minutes, with a rate constant 7 times greater than that of pure TiO₂, demonstrating outstanding performance

Keywords : Photocatalysis, Heterojunction, Zinc sulfide (ZnS), Titanium dioxide (TiO₂), Pollutant degradation.

ELECTROLYTIC SYNTHESIS AND CHARACTERIZATION OF NI-W ALLOYS FROM A CHLORIDE BATH AND CITRATE AS COMPLEXANT.

Rabah ASSELI*¹

¹*Energetic and Solid-State Electrochemistry Lab., Department of Processes Engineering, Ferhat
Abbas-Setif1 University, Setif, 19000, Algeria.*

**Corresponding author: Tel./Fax: +213-658-041-683 ; E-mail address:
mohamedrabah7070@gmail.com*

Résumé : L'objectif de ce travail était d'étudier les conditions de électrodéposition de Ni et l'alliage Ni-W. Ainsi un bain de watts classique de nickelage a été modifié à cet effet. L'introduction de l'ammoniaque à côté du citrate a changé radicalement le comportement des deux systèmes Ni/Ni²⁺ et W /WO₄²⁻. Ainsi, le mécanisme de déposition du Nickel et de son alliage Ni-W a été élucidé. La déposition du Ni-W est de type anormal. La vitesse de déposition des deux métaux est améliorée par l'augmentation à la fois de la température et du pH de la solution. Le mode de nucléation de ces alliages à pH neutre et à température ambiante suit un modèle de nucléation instantanée et de croissance en trois dimensions. À l'exception du cas des faibles surtensions pour les premiers instants où elle suit le mode progressif. L'analyse morphologique et compositionnelle effectuée par MEB et EDX ont été exploitées. La synthèse des dépôts de Nickel allié au tungstène a été rendue possible grâce à la modification du bain de watts. D'après les résultats de la microanalyse, la composition de l'alliage est étroitement liée aux conditions de déposition, particulièrement au potentiel imposé. Ainsi, plus le potentiel appliqué est cathodique, moins sera la teneur en tungstène dans le dépôt. Des surfaces relativement lisses et des fissures très fréquentes pour tous les films ont été observées. D'après les résultats de l'EIS obtenus, une haute stabilité en milieu corrosif (NaCl 3.5%) est celle de l'alliage Ni-W déposé à -1.10 V /ECS le moins cathodique, ainsi l'élément W qui est un facteur primordial améliorant la résistance à la corrosion.

Mots clés: Electrodeposition; alliages Ni-W; nucléation; bain de watts

REMOVAL OF DYE POLLUTANTS FROM WASTEWATER USING ACTIVATED CARBON SUPPORTED BY NANO-OXIDES FOR THE ADSORPTION PROCESS

Djaber SABAH^{1*}, Merabet SARRA¹ and Hamida KHADIDJA², Selmane TAHAR³

¹*Inorganic Materials Laboratory, Department of Chemistry, Faculty of Sciences, University Mohamed Boudiaf-M'sila, 28000, Algeria.*

²*Department of chemical industrial, college of science and technology, University Biskra, 07000, Algeria*

³*Department hydraulic and civil engineering, Faculty of technology, University of Ghardaïa*

**Corresponding author: Tel./Fax: +213.675.25.37.45; E-mail address: sabah.djaber@univ-msila.dz*

Abstract: The presence of organic dyes in wastewater is a significant environmental concern due to the associated severe health risks and negative impacts on aquatic ecosystems. This study aims to generate highly efficient activated carbon from palm petioles, offering a cost-effective solution. The primary focus of the research was on investigating the properties of this specific type of carbon. Various analytical techniques, including FTIR, XRD, iodine number, methylene blue number and pH_{PZC} analysis, were employed to characterize the activated carbon. The study also examined the carbon's ability to adsorb synthetic dyes, particularly methyl orange (OM), in a batch system. The findings revealed that the activated carbon (AC) material exhibited a specific surface area ($\text{SBET}=792.8\text{m}^2/\text{g}$) and pore volume ($\text{V}_{\text{Total}}=7\text{cm}^3/\text{g}$). It was observed that the OM dye displayed rapid absorption kinetics within the initial minutes and reached equilibrium swiftly. The kinetic data for the system's components were effectively described by pseudo-second-order kinetic models and intraparticle diffusion. Moreover, the Langmuir model provided the best fit, indicating maximum adsorption capacities (q_{max}) of 73.76 mg/g for the OM dye. These results highlight the potential of utilizing carbon derived from low-cost palm petioles as a valuable adsorbent for the removal of pollutants, especially synthetic dyes.

Keywords: Methyl orange, adsorption, pollution, palm

ANTIBACTERIAL, ANTIDIABETIC, AND HEPATOPROTECTIVE ACTIVITIES OF THE POLYPHENOL-RICH EXTRACT FROM *PULICARIA ODORA*

Ahmed BENMAHAMMED¹, BEDREDDINE Meriem², Abdelkader BASLI¹

1. *Laboratory of Interaction Research, Biodiversity, Ecosystems and Biotechnology. Faculty of Sciences, University of Skikda, Skikda, Algeria.*
2. *Department of Science of Matter, Faculty of Science and Technology, Mohamed El-Bachir El-Ibrahim University of Bordj Bou Arreridj, City Bordj Bou Arreridj, 34000, Algeria.*

*Corresponding author: Tel./Fax: +213-540-55-2283 ; E-mail address: ah.benmahammed@gmail.com

Abstract: *Pulicaria odora*, a medicinal plant belonging to the Asteraceae family, is widely used in traditional medicine for its therapeutic benefits. This study aimed to characterize the polyphenolic compounds present in the hydro-methanolic (70%) leaf extract of *P. odora* and to evaluate its main biological activities, including antioxidant, cytotoxic, antimicrobial, antidiabetic, anti-inflammatory, larvicidal, and protective effects. Bioactive compounds were identified using HPLC-MS/MS analysis. Various standardized in vitro assays were employed: DPPH and FRAP tests for antioxidant capacity, *Artemia salina* lethality assay for cytotoxicity, agar diffusion and solid medium dilution for antimicrobial activity, and the crystal violet microplate method for antibiofilm assessment. Antidiabetic activity was evaluated via yeast cell glucose uptake and α -amylase inhibition. Anti-inflammatory activity was assessed through anti-hemolytic effect and inhibition of protein denaturation. Larvicidal activity was tested on *Culex pipiens* larvae, and an in vivo study on Wistar rats was conducted to evaluate the protective effects of the extract against metribuzin-induced toxicity. The hydromethanolic extract showed a yield of 17.1% in phenolic compounds and was rich in bioactive flavonoids and phenolic acids. It exhibited notable antioxidant activity ($IC_{50} = 192.24 \mu\text{g/mL}$ for DPPH), although less potent than ascorbic acid. The extract was non-cytotoxic ($LC_{50} > 100 \mu\text{g/mL}$) and showed moderate antimicrobial activity against *Staphylococcus aureus*, *Escherichia coli*, *Pseudomonas aeruginosa*, and several fungal strains, with inhibition zones ranging from 11 to 23 mm and MIC values as low as 1.25 mg/mL. Strong antibiofilm activity was observed, with inhibition rates ranging from 38% to 93%. The extract enhanced glucose uptake at low concentrations and inhibited α -amylase activity comparably to acarbose, indicating a dual antidiabetic mechanism. The in vitro anti-inflammatory activity was moderate, with limited protection against oxidative hemolysis and weak inhibition of protein denaturation at low doses. Larvicidal activity was dose-dependent, reaching 66.66% mortality at 1 mg/mL after 72 hours. The in vivo study confirmed significant hepatoprotective and antioxidant effects against metribuzin-induced toxicity. These findings highlight *Pulicaria odora* as a promising source of bioactive compounds with antioxidant, antimicrobial, insecticidal, and protective properties. Further investigations are warranted to elucidate its mechanisms of action and fully explore its therapeutic potential in biomedical, agricultural, and food applications.

Keywords: *Pulicaria odora*, polyphenols, LC/ESI-MS/MS, antioxidants, antimicrobial activity, larvicidal effect, metribuzin, protective effect, antidiabetic, anti-inflammatory.

MOLECULAR MARKERS AND THEIR APPLICATIONS ON THE DATE PALM (*PHOENIX DACTYLIFERA* L.)

A. GUETTOUCHI

¹Department of sciences of nature and life, Faculty of the sciences, University Mohamed Boudiaf, M'sila 28000, Algeria

Abstract : Molecular markers are a good way to study genetic diversity, and to introduce them into plant improvement programs according to the importance of each plant. Molecular markers have been used in many studies of many plants (wheat, barley, maize....). For date palms, many molecular markers (RAPD, ISSR, SSR ...) have been used for several purposes, The most important of which is the molecular identification of date palm varieties and the study of the genetic convergence between the varieties and the use of them to identify the types of resistance to diseases, for example the varieties resistant to the disease of Bayoud, and also to verify the genetic compatibility of the vitro-plants obtained from tissue culture and if there are mutations, Through molecular markers. Can molecular markers be used to identify more about date palm inheritance? Can molecular markers help treat endangered palm diseases?

Key words: Date palm, molecular markers, molecular identification, resistance, tissue culture.

ALKALINE ACTIVATION OF A GEOPOLYMER BASED ON INDUSTRIAL MINERAL WASTE

Lyamine BRIKI^{1*}, Mohammed Rissel KHELIFA², Belkacem BENZEROUAL³ and Kamel ZIDANI⁴

¹*Department of Civil Engineering, University of Batna2, Algeria*

²*Department of Civil Engineering, University of Sherbrooke, Canada*

³*Department of Geography and Territorial Planning, University of Batna2, Algeria*

⁴*Department of Mechanical Engineering, University of Batna2, Algeria*

*Corresponding author: Tel.: +213-(0)661-667-653 ; E-mail address: l.briki@univ-batna2.dz

Abstract: This article aims to highlight the alkaline activation of a new ecological geopolymer-type material, which is attracting growing interest in the construction industry, by promoting raw materials with low environmental impact, consequently reducing CO₂ emissions resulting from the decomposition of carbonate during firing, and thus preserving natural resources intended for the manufacture of Portland cement. We used glass powder and metakaolin as an activator of the chemical reaction to transform it into a hard and very compact material. Three formulations were studied, with different mass contents of glass powder and metakaolin, namely: 95% glass powder + 5% metakaolin, 85% glass powder + 15% metakaolin and 70% glass powder + 30% metakaolin. This new material was synthesized using physicochemical and mechanical analysis processes; the results obtained are very promising, especially with the mass combination of 70% glass powder and 30% metakaolin.

Keywords: Geopolymer ; glass powder ; metakaolin ; materials ; environment.

ENHANCING PLANT FIBER PROPERTIES VIA CHEMICAL MODIFICATION: A REVIEW

Khalida ZITOUNI^{1,2*}, Azzedine BENYAHIA³ and Mourad FERHAT²

¹Department of chemistry, University of Bouira, Algeria

²Department of chemistry, University of M'sila, Algeria

*Corresponding author: Tel: 0658957507; E-mail address: k.zitouni2025@gmail.com

Abstract: Plant fibers, mainly composed of cellulose, hemicellulose, and lignin, are promising renewable materials but face challenges such as high moisture absorption, poor adhesion to polymer matrices, and low thermal stability. This study is a review about the chemical modification of plant fibers, focusing on various treatment methods, their effects on fiber properties, characterization techniques, and potential applications in composites and other industries. Chemical modification techniques such as alkalization, acetylation, silanization, and graft copolymerization are widely employed to enhance fiber properties by improving surface chemistry, mechanical strength, and compatibility with composites. Characterization methods like FTIR, SEM, DSC, and XRD help analyze these modifications and their effects on fiber morphology, crystallinity, and thermal behavior. Chemically treated fibers exhibit better interfacial bonding, reduced moisture uptake, and improved dimensional stability, making them more suitable for diverse applications in composites, textiles, and construction materials. Additionally, recent research emphasizes eco-friendly and sustainable modification methods to minimize environmental impact while maintaining or enhancing fiber performance, highlighting future trends toward green and bio-based treatments.

Keywords: Plant fibers ; Chemical modification ; Industrial applications

ALKALOID PROFILING OF *PEGANUM HARMALA* EXTRACT BY LC-ESI-QTOF-MS/MS AND EVALUATION OF ITS PHARMACOLOGICAL ACTIVITY AGAINST CANCER CELL LINES

Hadjer KEMEL^{1*}, Lamia BENGUEDOUAR¹ and Nesrine CHOUIKH¹ and Mohamed SIFOUR¹

¹Laboratory of Molecular Toxicology, Faculty of Nature and Life Sciences, University of Jijel, Algeria

*Corresponding author: Tel./Fax: +213-558-884-106 ; E-mail address: hadjerkemel@gmail.com

Abstract: The medicinal plant *Peganum harmala*, widely used in Algerian traditional medicine, has attracted interest for its potential anticancer properties. This study explores the cytotoxic and antimigratory effects of the n-butanol (*n*-BuOH) extract obtained from *P. harmala* seeds. The inhibitory effect on cancer cell migration was assessed using the scratch wound assay, while cytotoxic activity was evaluated against the human pancreatic cancer cell line PANC1[3]. Chemical analysis of the extract via LC-ESI-QTOF-MS/MS led to the identification of 37 distinct metabolites, primarily comprising β -carboline alkaloids (harmaline and harmine), quinazoline derivatives (including peganol and peganine), and glycosylated flavonoids. The extract exhibited notable cytotoxicity with an IC₅₀ value of 51.71 ± 5.28 μ g/mL and significantly reduced cell migration at 24, 48, and 72 hours. These findings suggest that the biological activity of the extract may result from synergistic interactions among its various bioactive polyphenolic compounds.

Keywords: Peganum harmala, Alkaloids, harmaline, Anticancer.

VALORIZATION OF OLIVE WOOD ASH FOR THE DEBITTERING STEP IN GREEN TABLE OLIVE PROCESSING

DJELLAL Amel¹, METTOUCHI Soraya¹, TAMENDJARI Abderezak¹ and Sylia AMRANE¹

1 Laboratoire de Biochimie Appliquée, Faculté des Sciences de la Nature et de la Vie, Université de Bejaia, 06000, Algeria

E-mail : amel.djellal@univ-bejaia.dz

Abstract: The olive industry produces various by-products, including olive wood ash generated from pruning and combustion. Traditionally regarded as agricultural waste, this ash is in fact rich in valuable minerals such as potassium, calcium, and magnesium, offering untapped potential in sustainable food processing. One of the major challenges in table olive production is the fruit's intense natural bitterness, which necessitates debittering treatments prior to consumption. The conventional method, particularly the Spanish style, relies heavily on sodium hydroxide (NaOH), raising both environmental and health concerns due to its chemical nature. In response to the growing demand for cleaner and more eco-friendly alternatives, this study investigates the potential reuse of olive wood ash as a natural alkaline agent in the processing of green table olives. We examined and compared the effects of olive wood ash and NaOH on two green olive varieties: Gordal and Sevilla. The study assessed key biochemical markers at the end of spontaneous fermentation, including total polyphenols, ortho-diphenols, flavonoids, and carotenoids. The findings revealed that olives treated with ash retained higher carotenoid levels and lower flavonoid content than those treated with NaOH in both varieties. As for polyphenols and ortho-diphenols, the Gordal variety debittered with ash exhibited higher concentrations compared to the NaOH treatment, while the Sevilla variety showed the opposite trend. These results suggest that olive wood ash can be successfully integrated into the olive processing chain, not only reducing the reliance on synthetic chemicals but also modulating the bioactive compound profile of the final product. This innovative approach aligns with circular economy principles and opens new pathways for sustainable, clean-label production in the table olive industry.

Mots clés: Table olives, Spanish style, ashes, polyphenols, orthodiphenols, carotenoids, debittered

HYDROGEN PRODUCTION FROM PLASTIC WASTE VIA PYRO-GASIFICATION: DYNAMIC SIMULATION USING ASPEN PLUS

Imene BOUCHELKIA^{1*}, Hacina ABCHICHE¹, MARIR Aymen¹, Souhila KADEM¹, Mounir MELLAL¹

¹ *Laboratory of Matter's Valorization and Recycling for Sustainable Development (VRMDD) USTHB University of Sciences and Technology Houari Boumediene, El Alia BP32, 16111, Bab Ezzouar, Algiers, Algeria*

*Corresponding author: Tel./Fax: +213-540-257-937 ; E-mail address: ibouchelkia@usthb.dz,

Abstract: Energy recovery from plastic waste via pyro-gasification offers a scalable pathway to mitigate environmental burdens while supplying high-value energy carriers. This study presents a comprehensive Aspen Plus model developed to optimize sustainable hydrogen production from the pyrolysis of representative plastic wastes (HDPE, PET, and waste tires). The simulation framework couples RYield blocks to describe initial thermal degradation of polymer matrices with RGibbs blocks to capture subsequent thermodynamic re-equilibration of gaseous intermediates, enabling an integrated representation of the transition between pyrolysis and partial gasification under near-equilibrium assumptions. A systematic sensitivity analysis was conducted on key operational variables—temperature, pressure, and air (oxidant) input—to quantify their influence on syngas composition (H₂, CO, CH₄, CO₂), hydrogen selectivity, and suppression of undesired byproducts such as tar and CO₂. Results reveal that elevated temperatures significantly enhance hydrogen and carbon monoxide formation, with hydrogen yield from HDPE peaking near 800 °C, while finely tuned air addition and moderate pressures control the trade-off between partial oxidation and reduced-species generation. The model's predictive capability was validated by comparing its outputs for waste tire gasification against published data from Mitta et al., demonstrating consistent trends in syngas composition and hydrogen/CO yields under comparable operating conditions. The calibrated model identifies optimal operating windows and highlights inherent process trade-offs, providing a robust decision-support tool for the design and scale-up of plastic-to-hydrogen reactors. Prospective work includes experimental validation of broader feedstock mixtures, coupling with detailed energy and exergy analyses, and embedding life-cycle-based environmental assessment to position pyro-gasification within circular economy strategies for green hydrogen production.

Keywords: Pyrolysis, gasification ; plastic waste ; hydrogen ; Aspen Plus ; modeling

TOXIC ACTIVITY OF THE CHEMICAL COMPONENTS OF CORIARIA MYRTIFOLIA ON THE SURVIVAL OF DROSOPHILA MELANOGASTER

ASLOUM Abdelmadjid Yagoub ¹, BENHISSEN Saliha ^{1,2}, HEDJOULI Zakaria ¹, BOUNADJI Siham¹, HABBACHI Wafa ², REBBAS Khellaf ^{2,3}.

¹Department of Natural and Life Sciences, Faculty of Sciences, University of M'sila, University Pole, Road Bourdj Bou Arreiridj, M'sila 28000, Algeria

²Laboratoire de Neuro-Endocrinologie Appliquée. Département de Biologie, Faculté des Sciences, Université

Badji – Mokhtar, BP 12, 23 000 - Annaba, Algeria.

³Laboratoire d'Agro-Biotechnologie et de nutrition en zones arides et semi arides/ Equipe de recherche de

gestion des ressources naturelles et environnement, Université Ibn Khaldoun, Tiaret, Algeria.

*Corresponding author: Tel./Fax: +21376522325 ; E-mail address: abdelmadjid-yagoub.asloum@univ-msila.dz

Abstract: The increasing resistance of mosquitoes to synthetic insecticides necessitates the exploration of plant-derived alternatives. In this study, larvicidal activity of alcoholic extracts of *Nicotiana glauca* (Solanaceae) and *Ruta chalepensis* (Rutaceae) is tested against fourth-instar larvae of *Culiseta longiareolata* (Culicidae), avian malaria vector. The plants were chosen because of their known bioactive properties. The experimental design involved exposing fourth-instar larvae to varying concentrations of plant extracts under controlled laboratory conditions. The measured mortality levels, with *R. chalepensis* exhibiting particularly strong insecticidal potential. Analysis indicated that this species attained 50% mortality at concentrations several orders of magnitude below required for *N. glauca* to exhibit similar effects. *R. chalepensis* was indicated by the results as a most promising mosquito control due to its rapidity of action and low LC values. The delayed action of *N. glauca* could be attributed to its neurotoxic mode of action. Both extracts present eco-friendly alternatives to synthetic larvicides but with field trials and evaluation on non-target organisms needed. Synergistic mixtures of these plant compounds and their efficacy against other vector species should be the area of research in the future.

Keywords: *Nicotiana glauca* , *Ruta chalepensis* *Culiseta longiareolata* larvicidal activity.

HEALTH RISKS OF CONSUMING SPIRULINA GROWN IN MINERAL- ENRICHED MEDIA

Abdelhalim SAADI^{1,2}, Hocine BOULEGHLEM², Sadok BOUKHCHINA¹, Abdelhamid GUELIL³ and Salima ZIDANE¹

¹Lipid Biochemistry Laboratory, Department of Biology, Faculty of Sciences of Tunis, 2092 ELmanar, Tunisia

² Laboratory of Therapeutic Organic Substances and Sustainable Processes (LTOSSP), Mohamed Boudiaf University of M'Sila

³Applied Chemistry Laboratory, University Mohamed Khider-Biskra, Algeria

* Corresponding author Email: msilamedical@gmail.com

Abstract: The present study investigates the potential health risks associated with the consumption of *Arthrospira platensis* (spirulina) cultivated in media enriched with various mineral salts and trace elements. The biochemical composition, metal bioaccumulation, and possible toxicological impacts were assessed using spectroscopic and chromatographic analyses. Results revealed that enrichment with certain minerals, while enhancing protein and pigment content, led to significant accumulation of heavy metals such as iron, zinc, and, in some cases, trace amounts of cadmium and lead. These findings highlight the importance of strict monitoring of cultivation conditions to ensure the safety of spirulina-based dietary supplements.

Keywords : *Arthrospira platensis*; Spiruline; Enrichissement minéral; Oligoéléments; Métaux lourds; Toxicité

PHYTOCHEMICAL INVESTIGATION OF ALGERIAN MEDICINAL PLANTS: A GREEN APPROACH FOR BIOACTIVE COMPOUND DISCOVERY

Sara ZERROUKI¹, Ratiba MEKKIOU²

¹Laboratory of Organo-Therapeutic Substances and Sustainable Processes (OTSSPL), Department of Chemistry, Mohamed Boudiaf University of M'sila, Algeria

²Unité de recherche: Valorisation des Ressources Naturelles, Molécules Bioactives et Analyses Physico-chimiques et Biologiques (VARENBIOMOL), Université des Frères Mentouri Constantine 1, Constantine, Algeria.

**E-mail: sara.zerrouki@univ-msila.dz*

Abstract: In the framework of green chemistry, phytochemical studies represent a sustainable and environmentally friendly approach to drug discovery. This research focuses on the extraction, identification, and characterization of bioactive compounds from selected Algerian medicinal plants using green solvents and eco-compatible techniques. Preliminary results reveal the presence of diverse secondary metabolites, including flavonoids, and phenolic compounds, known for their antimicrobial and antioxidant activities. Furthermore, the integration of chemometric analysis and artificial intelligence tools enhances the efficiency of compound screening and prediction of biological activities. This study highlights the potential of phytochemistry as a key pillar of green molecular design, aligned with the principles of sustainability and innovation in pharmaceutical research.

Keywords: Phytochemistry, Green Chemistry, Medicinal Plants, Bioactive Compounds, Artificial Intelligence, Algeria

**PHYTOCHEMICAL ANALYSIS AND EVALUATION OF THE
ANTIOXIDANT ACTIVITY OF METHANOLIC AND AQUEOUS
EXTRACTS OF *CYNOGLOSSUM CRETICUM***

Fatima CHEBIRI¹, Hassina GUERGOUR¹, Sabah BOUMERFEG², Asma MEZITI², Yuva BELLIK²,
Hiba GHERZOULI¹, Mohamedredha AIDEL¹ and Nasreddine MEKHOUKH³

¹*Health and Environment Laboratory (SANENV), Faculty of Natural and Life Sciences and Earth and Universe Sciences, Mohamed El Bachir El Ibrahimi University, Bordj Bou Arréridj, Algeria*

²*Department of Biology, Faculty of Natural and Life Sciences, Mohamed El Bachir El Ibrahimi University, Bordj Bou Arréridj, Algeria*

³*Department of Physico-Chemical Biology, Faculty of Natural and Life Sciences, University of Bejaia, 06000 Bejaia, Algeria*

*Corresponding author: Tel./Fax: +213-654-200-029; E-mail address: fatima.chebiri@univ-bba.dz

Abstract: In the context of valorizing Aromatic and Medicinal Plants (AMPs), *Cynoglossum creticum*, a species belonging to the Boraginaceae family, is attracting increasing scientific interest due to its traditional uses. However, it remains poorly studied in terms of phytochemical composition and biological properties. This work aims to characterize the bioactive compounds of this plant and evaluate its antioxidant potential. Aerial parts were subjected to maceration extraction using 75% methanol and distilled water. Total polyphenol content was determined using the Folin-Ciocalteu method, and flavonoid content by the aluminum chloride method. Antioxidant activity was assessed using the DPPH radical scavenging assay [4]. The methanolic extract showed higher concentrations of polyphenols (84.73 ± 6.95 mg GAE/g extract) and flavonoids (29.96 ± 0.24 mg QE/g extract), along with a stronger antioxidant capacity ($IC_{50} = 0.89 \pm 0.12$ mg/mL), compared to the aqueous extract ($IC_{50} = 4.15 \pm 0.3$ mg/mL). These findings highlight the richness of *C. creticum* in antioxidant compounds and suggest its potential as a valuable natural source for the development of pharmacological formulations or nutraceuticals. Further studies may support its application in the design of innovative bioproducts derived from medicinal plants.

Keywords: *Cynoglossum creticum*; methanolic and aqueous extracts; polyphenols; flavonoids; antioxidant activity.

PUNICA GRANATUM DERIVED COMPOUNDS AS GREEN CORROSION INHIBITORS FOR ZINC IN ACIDIC ENVIRONMENTS

Bilel MEZHOUD^{*1,2}, Mina BOULKROUNE²

¹ *Department of Chemistry, Faculty of Exact Sciences and Computer Science, Mohamed Sedik Ben Yahia University, B.P 98 Ouled Aissa, 18000, Jijel, Algeria*

² *Unit for Environmental Chemistry and Molecular Structural Research, CHEMS, University of Frères Mentouri Constantine 1, Constantine, Algeria*

E-mail : bilelmezhoud@univ-jijel.dz

Abstract: Traditional corrosion inhibitors are mostly composed of organic and inorganic substances that are often toxic, expensive, and harmful to both the environment and human health. Consequently, recent research has increasingly focused on the development of 'natural corrosion inhibitors'. Plants, in particular, offer a renewable and eco-friendly source of corrosion inhibitors with high efficiency, affordability, and broad availability. The corrosion inhibition performance of *Punica granatum* extract as a natural inhibitor for zinc in 0.5 M HCl solution was evaluated using weight loss and electrochemical polarization methods. The findings demonstrated that the extract exhibits a mixed-type inhibition mechanism. A maximum inhibition efficiency of 81.9% was achieved at a concentration of 600 ppm. The corrosion rate decreased with increasing inhibitor concentration and rose with increasing temperature. The adsorption of the extract on the zinc surface followed the Langmuir adsorption isotherm.

Keywords: Corrosion, Natural Inhibitors, Zinc, Acidic Solutions, Polarization Techniques.

AI-DRIVEN MODELING OF OCCUPATIONAL EXPOSURE LIMITS FOR ACTIVE PHARMACEUTICAL INGREDIENTS USING CHEMINFORMATICS AND MACHINE LEARNING

Mohamed HENTABLI^{1,2*}, Ykhlef LAIDANI^{3,*}, Ghania HENINI⁴, Yamina MORSLI²

Laboratory of Biomaterials and Transfer Phenomena, Theoretical and Computational Chemistry in Process Engineering Team, Faculty of Technology, University Yahia Fares of Medea 26000, Medea, Algeria.

² Process Engineering Department, Faculty of Technology, Hassiba Ben Bouali University of Chlef, Hay Essalem, P.O. Box 151, Chlef 02000, Algeria.

³ Laboratory of Vegetal Chemistry-Water-Energy, Hassiba Ben Bouali University of Chlef, Hay Essalem, P.O. Box 151, Chlef 02000, Algeria.

⁴Laboratory Environment-Water, University of Chlef, Algeria

*Corresponding author: Tel./Fax: +213663810937 ; E-mail address: hentabli.mohamed92@gmail.com

Abstract: This study introduces an artificial intelligence (AI) framework to predict Time-Weighted Average Occupational Exposure Limits (OEL-TWAs) for 54 active pharmaceutical ingredients (APIs), leveraging cheminformatics and Support Vector Machine (SVM) algorithms. By translating molecular structures into descriptors (e.g., lipophilicity, molecular weight, hydrogen-bonding capacity), the model achieved robust predictive accuracy ($R^2 = 0.82$, RMSE = 0.45 log units), outperforming traditional toxicology-dependent methods. Key advantages include accelerated OEL-TWA derivation, reduced reliance on costly animal studies, and scalability to novel pharmaceuticals. Feature importance analysis aligned predictions with toxicokinetic principles, validating the model's scientific relevance. Cross-validation and external testing confirmed its reliability, offering a cost-effective tool for regulatory compliance and workplace safety. This AI-driven approach not only streamlines risk assessment but also supports dynamic updates to safety guidelines in fast-evolving pharmaceutical industries. Future work will expand the dataset and integrate deep learning to enhance precision, underscoring AI's transformative role in modern occupational health strategies.

Keywords: Artificial Intelligence, Occupational Exposure Limits, Cheminformatics, Machine Learning, Pharmaceutical Safety, Predictive Modeling.

SOLAR LIGHT-INDUCED DEGRADATION OF CRESOL RED IN THE PRESENCE OF THE Fe(III)-NTA COMPLEX

Wassila REMACHE*¹, Oualid DILMI ³, Nassira SERAGHNI ², Nafissa BOUBAZINE ¹, Sihem BELAIDI ², Hasna BOUCHARREB ⁴ and Tahar SEHILI ²

¹ Department of Chemistry, Faculty of Exact Sciences and Computer Science, University of Jijel, 18000 Jijel, Algeria

² Laboratory of Environmental Science and Technology, Frères Mentouri University, Constantine 1, Constantine, 25000, Algeria

³ Department of S.M, faculty of Science and Technology, Mohamed El Bachir El Ibrahimi University Bordj Bou Arreridj, 34000, Algeria

⁴ Department of Chemistry, Faculty of Sciences, University of Algiers 1, Benyoucef BENKHEDDA, Algeria

*Corresponding author: tel: +213774609553

Email adress: remache.wassila@univ-jijel.dz

Abstract: In this work, the iron(III)–nitrilotriacetate complex (Fe(III)–NTA) was synthesized via a stoichiometric approach to activate peroxymonosulfate (PMS) for the generation of sulfate radicals, powerful oxidizing agents produced through the cleavage of PMS's peroxy bond upon activation. This system was applied for the degradation of cresol red (CR) under solar irradiation. Upon exposure to sunlight, Fe(III)–NTA undergoes ligand-to-metal charge transfer (LMCT), leading to the in-situ formation of Fe²⁺, which continuously activates PMS and sustains CR degradation. The Fe(III)–NTA/PMS system achieved complete degradation of CR within 15 minutes under the following conditions: initial CR concentration of 0.05 mM, [Fe(III)–NTA] = 0.9 mM, PMS = 4 mM, and pH = 2.3. Quenching experiments suggested that SO₄^{•-} radicals play a significant role in the degradation process. However, since the inhibition was not complete, this indicates that other radicals, such as the superoxide anion (O₂^{•-}), which is also generated during the photolysis of the Fe(III)-NTA complex under solar irradiation, also contribute to CR oxidation.

Keywords: Red cresol; radicaux sulfates; iron(III)–nitrilotriacetate complex; Peroxymonosulfate.

FORMULATION AND ASSESSMENT OF AN ENVIRONMENTALLY FRIENDLY DISHWASHING DETERGENT FROM BIOSOURCED SURFACTANTS

Meriem HAMLAM^{1,2*}, Rafik AY¹ and Samra AMAMRA¹

¹*Department of Sciences of Matter at the Faculty of Science and Technology, Mohamed El Bachir El Ibrahimi University, Bordj Bou Arréridj, 34030 El Anceur, Algeria.*

²*Energetics and Solid-State Electrochemistry Laboratory (ESEL) at the Department of Processes Engineering - Faculty of Technology - Ferhat Abbas University, 19000 Sétif, Algeria.*

*Corresponding author : meriem.hamla@univ-bba.dz

Abstract: This work emphasizes the importance of developing and synthesizing a liquid dishwashing detergent for household use. By employing a rigorous scientific approach, we aimed to create an innovative formulation that meets stringent quality and safety requirements. This also provides a solid foundation for future developments, integrating crucial criteria such as sustainability, biodegradability, and respect for human health and the environment. The results obtained align perfectly with physicochemical and microbiological standards. The resulting formulation exhibits optimal characteristics: a neutral pH of 7.02, a viscosity of 65.86 Pa·s, good foaming and cleaning power, and satisfactory long-term stability. Microbiological analyses confirmed the absence of pathogens, ensuring the product's safety. A comparison with several commercial products demonstrated the competitiveness of the synthesized formulation in terms of both efficacy and quality.

Keywords: Dishwashing detergent ; Eco-friendly ; Microbiological analysis ; Physicochemical properties ; Biosourced surfactants.

QUALITATIVE AND QUANTITATIVE PHYTOCHEMICAL ANALYSIS AND BIOLOGICAL ACTIVITIES OF *FRAXINUS EXCELSIOR L* EXTRACTS

Oumelkheir BELHADDAD*¹, Salima ZIDANE¹, Hocine BOULEGHLEM^{1,2}, Sabrina MOHAMADI¹, KENZA BOUCHELOUCHE¹, Wafa ZAIBET³ and Leila BOUZIDI⁴

¹ Laboratory of Therapeutic Organic Substances and Sustainable Processes (LTOSSP), Department of Chemistry, Faculty of Sciences, University of M'Sila, University Pole, Road Bourdj Bou Arreiridj, M'sila 28000, Algeria

² Laboratory of Process Engineering, Department of Process Engineering, University Ferhat Abbas-Setif 1 DZ-19000 Setif, Algeria

³ Applied Organic Chemistry Laboratory (LCOA), University Badji Mokhtar of Annaba, Annaba, Algeria

⁴ Laboratoire des Matériaux Polymériques Multiphasiques (LMPMP), Département de Génie des Procédés. Faculté de Technologie, Université Ferhat Abbas, Sétif-1, Algérie

*Corresponding author: E-mail address: oumelkheir.belhaddad@univ-msila.dz

Abstract: The aim of this study was to determine the phytochemical screening and an evaluation of the antioxidant and antibacterial activity of leaves of *Fraxinus excelsior L.* In this study, the crude plant extracts obtained by three different methods of extraction (ethanol, methanol, and water) were collected and tested for the presence of phytochemicals. The tests revealed the presence of flavonoids, tannins, sterols, and triterpenes in all extracts. The qualitative analysis using TLC showed the presence of flavonoids in different extracts. This result was confirmed by a quantitative analysis based on the dosage of phenolic compounds. The results proved that alcoholic extracts represent a significant source of phenolic compounds. The DPPH free radical scavenging method was used for antioxidant activity analysis. All the extracts exhibited good antioxidant activity; the methanol extract exhibited the highest radical scavenging activity ($IC_{50}=35,39 \pm 0,99 \mu\text{g/ml}$ from maceration extraction). The extracts were also checked in the lab for their ability to fight bacteria against two types (*Escherichia coli* and *Staphylococcus aureus*) using the disc diffusion method. The results showed that all extracts exhibited moderate antibacterial activity against both bacteria.

Keywords: *Fraxinus excelsior*, Polyphenols, Flavonoids, Antioxidant, Antibacterial activity.

MORINGA OLEIFERA FRUIT EXTRACTS: PHYTOCHEMICAL SCREENING, ANTIOXIDANT AND ANTIBACTERIAL ACTIVITIES

Samra AMAMRA^{*1,2}, Ilhem KAABI²

¹Department of Matter Sciences, Faculty of Sciences and Technology, University Mohamed El Bachir El-Ibrahimi, Bordj Bou Arreridj, Algeria, 34000.

²Laboratory of Electrochemistry of Molecular Materials and Complexes (LEMMC). Department of Engineering Process, Faculty of Technology, University Ferhat Abbas Setif-1, Setif, Algeria, 19000.

*Corresponding author: E-mail address: samra.amamra@univ-bba.dz

Abstract: The natural antioxidants, more recently, have attracted considerable attention of users and researchers largely on account of adverse toxicological reports on some synthetic antioxidants. In this context, medicinal plants are being viewed as easily available and potent source of antioxidants as they contain a mixture of different chemical compounds that may act individually or in synergy to cure disease and improve health. In fact, Medicinal plants are still the mainstay of about 70–80 % of the world population, largely in developing countries, for primary health care needs because of better cultural acceptability, better compatibility with the human body and lesser side effects. For this reason, in this study, We carried out an extraction of two types of substances, namely polyphenolic extract and vegetable oil from the fruit of a tree called *Moringa oleifera*, which we then subjected to antioxidant and antibacterial tests, After carrying out the phytochemical screening test, to identify the main compounds such as flavonoids, tannins.... The results of the experiments revealed that the *Moringa* plant contains flavonoids and tanins. Furthermore, the evaluation of the antioxidant activity of the extracts by the DPPH test showed a positive result for the methanolic extract. And moderate antibacterial activity for both extracts. As a result, the Moringa tree is an effective source of compounds with nutritional and health value.

Keywords: Antioxidant; DPPH; Antibacterial Activity; Moringa ; Flavonoids.

ANTIMICROBIAL AND ANTIOXIDANT ACTIVITIES OF AQUEOUS EXTRACTS OF *RHUS TRIPARTITA* SPECIES

Sabrina MOHAMADI^{1*}, KENZA BOUCHELOUCHE¹ et OUM Elkheir BELHADDAD¹

¹Département de Chimie, Faculté des Sciences, Université de M'Sila, Pôle Universitaire, Route Bourdj Bou Arreidj, M'sila 28000, Algérie

*Corresponding author: Tel./Fax: +213-698-56-9114 ; E-mail address: *sabrina.mohamadi @univ-msila.dz*

Abstract: The importance of natural plants such as *Rhus tripartita* lies in their natural bioactive substances like polyphenols and flavonoids. These plants are used for therapeutic purposes against diseases. In this study, we investigated the phytochemical, antioxidant, and antibacterial activity of the aqueous extracts of *Rhus tripartita* from M'sila region of Algeria. The aqueous extracts were obtained using decoction and infusion methods. Phytochemical screening revealed the presence of various groups of secondary metabolites, such as flavonoids, tannins, saponosides, alkaloids, terpenoids, steroids and mucilages, etc. The total polyphenol and flavonoid content in the aqueous extracts was determined using the Folin-Ciocalteu method [1] and the AlCl₃ method [2], respectively. The results show that the extract obtained by decoction was the richest in polyphenols (210.677±3.411µgEAG /mg of extract) and flavonoids (23.642±0.642 µg EQ/mg of extract). The results of the antioxidant activity studied by the DPPH test [3] determined that this extract is the most active by its IC₅₀ value (16.531µg/ml). The extracts were also tested for their antibacterial activity in vitro against four bacterial strains (*Escherichia coli*, *Bacillus subtilis*, *Pseudomonas aeruginosa* and *Staphylococcus aureus*) using the disk diffusion method[4]. The antibacterial results showed that the highest activity was attributed to the decoction extract against *Bacillus subtilis*, with a maximum zone of inhibition of 13 mm.

Keywords : *Rhus tripartita*, secondary metabolites, antibacterial activity, flavonoïds, antioxidant activity, DPPH.

VALORIZATION OF BIOFLOCCULANTS FOR THE TEXTILE DYES BY COAGULATION FLOCCULATION GREEN CHEMISTRY

Malika CHENNA^{1*}, Samir BOUACHA², Nadia LARDJANE³, Hakim LOUNICI⁴ et Ali CHENNA⁵

^{1*}*Université de M'sila, Algeria.*

²*Laboratoire des biotechnologies Environnementales et génie des procédés BIOGEP, Ecole Nationale Polytechnique, B.P. 182-16200, El Harrach, Algiers, Algeria.*

³*Faculté des Sciences Biologiques et des Sciences Agronomiques, Université Mouloud Mammeri de Tiziouzou, Algiers, Algeria*

⁴*Laboratoire des Sciences et Techniques de l'Environnement, Ecole Nationale Polytechnique, BP 182 El-Harrach, Algiers, Algeria*

⁵*Faculté des Sciences et Sciences Appliquées, Department of chemistry, Université de Bouira, Bouira, Algeria*

*Corresponding author: Tel. /Fax: +213 792 79 26 41 ; E-mail address: *malika.chenna@univ-msila.dz*

Abstract : This study aims to exploit *Moringa oleifera* seeds and use them for industrial wastewater treatment. The seeds were used as a liquid (extracts) as biocoagulants. The objective of to optimize the factors influencing the removal of textile dyes by a physicochemical treatment, coagulation- flocculation, using an experimental design. By carrying out the tests and analysing the data, the screening of the factors made it possible to identify the optimum conditions necessary to obtain better elimination. These operating conditions are pH, coagulant dose, the concentration of initial solutions, and stirring speed. Our study demonstrated the importance of applying the design of experiments methodology, particularly the response surface methodology (RSM). A full factorial design allowed the optimization of operational parameters affecting flocculation coagulation. Green chemistry offers a sustainable and responsible approach to dye coagulation-flocculation, contributing to a more environmentally friendly future while meeting industrial needs. Integrating green chemistry into dye coagulation-flocculation offers a sustainable advantage that meets today's environmental challenges while optimizing industrial processes.

Keywords: Optimization · Response Surface Methodology · Textile Dye · Coagulation-Flocculation, Green Chemistry.

**ZINC TOLERANCE AND GROWTH ADAPTATION OF MALVA SYLVESTRIS L.
IN ZINC CONTAMINATED SOILS**

Abdelouahab DIAFAT^a , Ahmed BAHLOUL^{bc}, Abdelmalek MERIBAI^a , Farid BOUAZIZ^a
, Hammoudi MEKHALFI^a ,

a: Laboratory of Characterization and Valorization of Natural Products, Faculty of Nature and Life Sciences,

University Mohamed El-Bachir El-Ibrahimi, of Bordj Bou Arreridj, 34000, Algeria.

b: Laboratory of Electrochemistry and Environment, Faculty Sciences and Technology, University Mohamed El-

Bachir El-Ibrahimi, of Bordj Bou Arreridj, 34000, Algeria.

c: Department of chemistry, Faculty of Sciences, University of Mohamed Boudiaf, M'sila, 28000, Algeria.

Abstract: Contamination of soils with various pollutants, including heavy metals, poses significant challenges for plant growth and ecosystem sustainability. Understanding the tolerance mechanisms and growth adaptations of plants in contaminated soils is crucial for developing effective strategies for phytoremediation and ecological restoration. Phytoremediation is an emerging, cost-effective remediation technology that uses plants to remove or degrade organic and inorganic contaminants from soil and water. *Malva sylvestris* plants were growing in pots containing soil artificially contaminated with Zn at concentrations of 100, 200 and 300 mg/kg. Parameters such as regular monitoring of the plants, growth rate, and dry matter are measured to evaluate the effect of zinc on plant growth. The obtained results indicate that the control plants continued to grow until the end of the study. After treatment with different concentrations of zinc; 100, 200 and 300 mg/kg, the plants showed slowed growth, and a decrease in stem size. The values of the ash content in the aerial part are 1.306 % in the control, and 1.52 %, 1.484 %, 1.426 % for the concentration of 100, 200 and 300 mg/kg, respectively. In the root part, the values of the ash content are 0.158 % in the control group, and 0.3 %, 0.276 % and 0.224 % for 100, 200 and 300 mg/kg respectively. Analysis using atomic absorption spectrometry revealed that this plant accumulates only small quantities of zinc. Therefore, it can be concluded that the *Malva sylvestris* plant tolerates soils contaminated with zinc but it is not considered as a zinc hyper-accumulator plant.

Keywords: Zn-contaminated soils, *Malva Sylvestris*, phytoremediation, phyto-extraction.

MICROWAVE-ASSISTED SYNTHESIS OF IMINO-ACRIDINE DERIVATIVES WITH ANTIOXIDANT POTENTIAL: COMBINED *IN VITRO* AND *IN SILICO* INVESTIGATIONS

Abdeslem BOUZINA^{1*}, Rachida MANSOURI², Zineb AOUF¹, Houria BENTOUMI¹,
Yousra Ouafa BOUONE¹, and Nour Eddine AOUF¹

¹Laboratory of Applied Organic Chemistry, Bioorganic Chemistry Group, Department of Chemistry, Sciences Faculty, Badji-Mokhtar - Annaba University, Box 12, 23000 Annaba, Algeria.

²Environmental Research Center, Alzon, 23000 Annaba, Algeria.²Department, Institution, Country

*Corresponding author: Tel: 0654776845; E-mail address: abdeslem.bouzina@univ-annaba.dz.

Abstract: In the drive toward safer and more sustainable chemistry, researchers continue to face major challenges particularly in reducing toxic waste from outdated synthetic methods and achieving efficient reactions without relying on hazardous organic solvents and reagents. Today, developing environmentally friendly and safe laboratory practices, without sacrificing the performance of traditional chemical approaches, is essential. This objective is fully aligned with the core principles of green chemistry established by its pioneers. Microwave-assisted has emerged as a powerful and eco-friendly method for the rapid production of diverse molecules. It offers high yields, improved selectivity, and better reaction efficiency. This technique has found wide application in heterocycle synthesis and has shown particular effectiveness in the preparation of acridine derivatives. In this study, a series of imino-acridine derivatives was synthesized via the condensation of various enaminones with aromatic aldehydes under microwave irradiation, without the use of a catalyst. This method offers several advantages, including short reaction times, good yields, and adherence to green chemistry standards achieved by avoiding harmful reagents and employing simple, environmentally benign conditions. To assess the antioxidant potential of the synthesized compounds, *in vitro* assays using the DPPH radical scavenging method were conducted. The results revealed significant antioxidant activity among the compounds. In addition, molecular docking and molecular dynamics simulations were performed to explore the binding interactions of the compounds with the active site of xanthine oxidase, a key enzyme involved in oxidative stress. These computational results supported the experimental findings.

Keywords: Imino-acridines; microwave synthesis, antioxidant test, *in silico* studies.

ÉTUDE DE LA DURABILITE DU BETON CONTENANT DES GRANULATS RECYCLES TRAITES ET DE SON AMELIORATION FACE AUX ATTAQUES CHIMIQUES

Meftah ALLAL^{12*}, Leila ZEGHICHI², Karima LARKAT³

¹Laboratoire de Recherche en Génie Civil, Université de Biskra, 07000 Biskra, Algeria.

²Laboratoire des Éco-matériaux, Procédés Chimiques et Développement Durable, Université de Biskra, 07000 Biskra, Algeria.

³Laboratory of Inorganic Materials LMI, University of M'sila, 28000, Algeria.

*Corresponding-author-only@gmail.com (meftah.allal@univ-biskra.dz)

Résumé : Le béton recyclé traité développé dans cette étude présente des performances mécaniques et chimiques élevées, adaptées aux exigences du génie civil et hydraulique. Sa résistance accrue et sa durabilité en font un matériau fiable, même en conditions environnementales extrêmes telles que les cycles thermiques intenses et l'humidité élevée. Sa tenue face à l'eau, notamment en matière d'hydratation et de résistance aux agressions chimiques, le rend particulièrement adapté aux infrastructures hydrauliques comme les barrages, canaux et stations de traitement des eaux. La durabilité a été évaluée à travers plusieurs indicateurs : absorption capillaire, résistance à la compression, et résistance aux attaques chimiques (sulfates et acides). Les tests ont été réalisés conformément aux normes ASTM C 1012-89 (sulfates) et ASTM C 267-97 (acides), avec immersion des échantillons dans des solutions à 5 % de HCl et H₂SO₄ durant 700 jours. Enfin, une analyse microstructurale par MEB-EDX a permis de suivre l'évolution de la portlandite (Ca(OH)₂), indicateur clé de la stabilité chimique du béton. Ces résultats confirment la capacité du béton recyclé traité à maintenir ses propriétés dans des milieux agressifs sur le long terme.

Mots-clés : béton recycle, caractérisations physico-chimique, durabilité, Résistance aux attaques chimiques, encapsulation.

IN VIVO ANTI-INFLAMMATORY AND ANTIBACTERIAL ACTIVITIES OF N-BUTANOL EXTRACT FROM AN ENDEMIC ALGERIAN FICUS

Aida KEMMOUNDJI¹, Abdallah Kherbache^{2,3}, Thamere CHEREIT^{1,4}, Ramdane SEGHIRI¹

¹ *Unité de Valorisation des Ressources Naturelles, Molécules Bioactives et Analyse Physicochimiques et Biologiques (VARENBIOMOL), Université des Frères Mentouri, 25000 Constantine, Algeria*

² *Department of Microbiology and Biochemistry, Faculty of Sciences, University of M'sila, M'sila, Algeria*

³ *Laboratory of Applied Biochemistry, Faculty of Natural and Life Sciences, University Ferhat Abbas, Setif, Algeria*

⁴ *Département de science de la matière, faculté des sciences exactes et sciences de la nature et de la vie, université Larbi Ben M'hidi, Oum el Bouaghi, Algeria.*

*Corresponding author: Tel : 05.41.93.03.33; E-mail address: ayda.kemmoundji@student.umc.edu.dz

Abstract: Exploring natural products for their potential health benefits has increased interest in the phytochemical properties of various species extracts. This study investigates the antibacterial and anti-inflammatory activities of the *n*-butanol extract from an endemic Algerian *ficus*, prepared from the dried ficus plant and subjected to various in vitro assays to evaluate its biological activities. The antibacterial activity they assessed using the well-diffusion method in DMSO, against a panel of gram-positive and three gram-negative bacteria, including *Staphylococcus aureus*, *Escherichia coli*, *Morganella morganii*, and *Pseudomonas aeruginosa*. The extract demonstrated significant antibacterial activity, particularly against *Pseudomonas aeruginosa* and *Escherichia coli*. The anti-inflammatory activity of *n*-butanol extract was evaluated by using xylene-induced, and the results showed a higher inhibition 74±1.4% comparison with indomethacin 70±1.7%. The results suggest that the *n*-butanol extract from *ficus* species possesses potent anti-inflammatory and antibacterial properties, making it a promising candidate for further development in pharmaceutical and nutraceutical applications.

Keywords: Ficus, Moraceae , anti-inflammatory, antibacterial

IN VIVO WOUND-HEALING AND MOLECULAR DOCKING STUDIES SUPPORT THE TRADITIONAL USE OF ARISARUM VULGARE AQUEOUS EXTRACT

Zineb BOUAFIA ^{1,2}, Amel BOUDJELAL ^{1,2*}, Souhila BOUAZIZ-TERRACHET ^{3,4}, Antonella SMERIGLIO ⁵, Mustapha Mounir BOUHENNA ⁶, Ilyas YILDIZ ⁷, Ibrahim DEMIRTAS ^{8,9} and Domenico TROMBETTA ⁵

¹Department of Microbiology and Biochemistry, Faculty of Sciences, University of M'sila, Algeria;

²Laboratory of Biology: Applications in Health and Environment, University of M'sila, Algeria;

³Laboratory of Applied Chemistry and Materials, University of Boumerdes, Algeria;

⁴Laboratory of Theoretical Physico-Chemistry and Computer Chemistry, Faculty of Chemistry, USTHB, Algeria;

⁵Department of Chemical, Biological, Pharmaceutical and Environmental Sciences, University of Messina, Italy;

⁶Centre de Recherche Scientifique et Technique en Analyses Physico-Chimiques (CRAPC), Bou-Ismaïl, Algeria;

⁷Foundation of the Faculty of Health Sciences, Nutrition and Dietetics Department, Iğdir University, Turkey;

⁸Department of Biochemistry, Faculty of Science and Art, Iğdir University, Iğdir, Turkey;

⁹Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Ondokuz Mayıs University, Samsun, Turkey.

*Amel BOUDJELAL; e-mail: amel.boudjelal@univ-msila.dz

Abstract: In Algerian traditional medicine, *Arisarum vulgare* O. Targ. Tozz. (Araceae), locally known as “Elbgouga”, is widely used to treat eczema, wounds and burns. Investigate, using *in vivo* and *in silico* molecular docking techniques, the possible effects of *A. vulgare* ultrasound-assisted aqueous extract (AVAE) on wound healing for the first time. The phytochemical profile was elucidated by LC-ESI-MS/MS analysis. Wistar albino rats were used *in vivo* tests to evaluate the AVAE ointment's acute cutaneous toxicity and wound-healing potential (1, 2, and 5% AVAEO). Through *in silico* investigations, TNF- α , IL-1 β , MMP-9, TGF- β , VEGF, and EGFR were examined as possible therapeutic targets [3]. Twenty-seven phytochemicals, belonging mainly to the flavonoids and phenolic acids' class were identify and semi-quantify. The 5% AVAEO-treated group showed a significantly greater ($p < 0.001$) wound contraction (8–20 days) with respect to untreated and petroleum jelly groups, whereas no statistically significant difference was observed with respect to the Madecassol[®]-treated group. On the contrary, the two lower dosages (1 and 2% AVAEO) showed no statistically significant effects. Docking studies showed that *A. vulgare* bioactive compounds may have therapeutic effects on wound healing by targeting with high affinity TNF α , IL-1 β , MMP-9, TGF- β R1, VEGF and EGFR, counteracting inflammation, angiogenesis and oxidative unbalance, and promoting wound repair. This study demonstrated as that AVAE possess *in vivo* wound healing properties and no dermal toxicity, shading light also on the potential therapeutic targets involved.

Keywords: *Arisarum vulgare* O. Targ.Tozz.; traditional medicine; LC-ESI-MS/MS analysis; *in vivo* wound healing activity; *in silico* molecular docking studies.

STRUCTURE-BASED DESIGN AND PHARMACOKINETIC STUDIES OF NOVEL GAC INHIBITORS FOR TRIPLE-NEGATIVE BREAST CANCER

Khadijah SAGHIRI⁽¹⁾, BEN ADEL Zohra⁽¹⁾, Ismail DAOUD^(2,3), Nadjib MELKEMI⁽¹⁾.

1. *Laboratory of Molecular Chemistry and Environment (LMCE), Department of Chemistry, University Mohamed Khider, Biskra, Algeria*
2. *University Mohamed Khider, Department of Matter Sciences, BP 145 RP; (07000) Biskra, Algeria*
3. *Laboratory of Natural Substances and Bioactive (LASNABIO), University of Abou- BakrBelkaid, 13000, Tlemcen, Algeria*
Tel: +213782915558
E-Mail: khadijah.saghiri@univ-biskra.dz

Abstract : Triple-negative breast cancer (TNBC) is an aggressive subtype of breast cancer lacking targeted therapies. In this study, we explored the inhibitory potential of novel Withangulatin A (WA) derivatives targeting the allosteric site of glutaminase C (GAC), a promising therapeutic target in TNBC. A structure-based drug design approach was employed using molecular docking, molecular dynamics (MD) simulations, molecular electrostatic potential (MEP) analysis, and pharmacokinetic profiling. Docking studies revealed that four WA derivatives—W5, W8, W13, and W18—exhibited strong binding affinity to the allosteric site of GAC, occupying the same pocket as known inhibitors BPTES and CB-839. These top-ranked compounds were further validated via 600 ns MD simulations, confirming the stability of the ligand–protein complexes (3UO9-W5, 3UO9-W8, 3UO9-W13, and 3UO9-W18). Key stabilising interactions involved residues PHE322 (A) and LEU323 (A), as well as ARG317 (B), indicating a conserved binding mode. MEP analysis highlighted that the carbonyl oxygen atoms represent the most electrophilic regions, suggesting potential reactive hotspots. These findings were consistent with the observed hydrogen bonding patterns within the allosteric pocket. ADMET predictions showed that compounds W8 and W13 have favorable pharmacokinetic properties, closely resembling the reference compound CB-839, with good oral bioavailability and low toxicity risks. Collectively, these results suggest that W8 and W13 are promising lead candidates for further development as a novel class of allosteric GAC inhibitors for the treatment of TNBC.

Keywords: Withangulatin A derivatives – Molecular Docking/Dynamic simulations – Glutaminase C–Pharmacokinetics – MEP analysis

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PLANTES MEDICINALES ANTI-INFLAMMATOIRES CITEES DANS LA MEDECINE PROPHETIQUE

Nairouz BENZEGGOUTA

Département de Chimie, Faculté des Sciences, Université de M'sila, Algérie

nairouz.benzagouta@univ-msila.dz

Résumé: La Médecine Prophétique est une mine d'or d'informations sur plusieurs plantes médicinales ou alimentaires ayant des vertus thérapeutiques. Parmi ces plantes il y a l'aloë, la nigelle, le gingembre et l'olivier, qui possèdent des effets anti-inflammatoires en plus d'autres effets. L'effet anti-inflammatoire est dû à la présence de plusieurs molécules actives comme : les polysaccharides, thymoquinone, gingerols, oleuropéine. Ces plantes sont essentielles dans notre quotidien pour traiter ou prévenir l'inflammation ainsi que d'autres maladies, à condition de bien connaître les doses thérapeutiques.

Mots clés : Médecine Prophétique – Effet anti-inflammatoire – Aloë – Nigelle – Gingembre – Olivier.

ECO-RESPONSIBLE EXTRACTION OF COLLAGEN FROM FOOD

WASTE: TOWARDS A GREEN APPROACH

Hocine BOULEGHLEM^{*1,2}, Salima ZIDANE^{1,2}, Hadjer BOUKHALFA¹ and Norhane ABDELKBIR¹

¹Department of Chemistry, Faculty of Sciences, Mohamed Boudiaf University of M'Sila

Address: University Campus, Bordj Bou Arreridj Road, 28000 M'Sila, Algeria.

² Laboratory of Therapeutic Organic Substances and Sustainable Processes (LTOSSP), Mohamed Boudiaf University of M'Sila

³Applied Chemistry Laboratory, University Mohamed Khider-Biskra, Algeria

* Corresponding author Email: hocine.boulegblem@gmail.com

Abstract: The eco-responsible extraction of collagen and gelatin from animal-derived food waste including bovine hides, bones, and fish by-products offers a sustainable alternative to conventional biopolymer sources. This approach valorizes underutilized agro-industrial residues, thereby reducing the environmental burden associated with their disposal and illustrating the principles of circular economy and bioeconomy. The extraction process involves several key steps: pretreatment and cleaning of the biomass, demineralization with acidic or alkaline solutions, and subsequent recovery of native collagen. Collagen can then be partially hydrolyzed by thermal or enzymatic methods to yield gelatin. The resulting biopolymers display properties compliant with industrial standards for safety, quality, and functional performance in pharmaceutical, cosmetic, and food sectors. This valorization pathway provides several advantages, including the abundance and low cost of raw materials, a marked reduction of environmental pollution, and opportunities to design high-yield, eco-friendly processes. Nonetheless, technological optimization is still required to preserve collagen's structural integrity, improve extraction selectivity, and enhance the purity of the final product. Thus, the exploitation of animal food waste as an alternative source of collagen and gelatin represents not only a promising direction for scientific and industrial innovation, but also a strategic response to contemporary challenges of sustainability, waste management, and competitiveness within health and wellness industries.

Keywords: Collagen; Gelatin; Animal waste; Valorization; Enzymatic hydrolysis; Green extraction; Sustainable development; Bioeconomy.

THEORETICAL STUDY OF EXCESS MOLAR VOLUMES IN BINARY MIXTURES OF ALKOXYETHANOLS AND SELECTED AMINES USING DFT

Nabila BENABILA^{1*}, Hamza Serrar^{2,3}, Souheyla Chetioui^{4,5}

¹ *Laboratory of Therapeutic Organic Substances and Sustainable Processes (LTOCSP) Mohamed Boudiaf University of M'Sila, 28000 M'sila, Algeria,*

² *The National Higher School of Biotechnology - Taoufik Khaznadar, constantine, Algeria.*

³ *Laboratory of Mathematical Physics and Subatomic Physics (LPMPs), Mentouri Brothers University - Constantine 1*

⁴ *VEHDD Laboratory, University of M'sila, 28000 M'sila, Algeria,*

⁵ *Research Unit for Chemistry of the Environment and Molecular Structural, University of Constantine 1, Constantine 25000, Algeria.*

*Corresponding author: Tel: 0697550559 ; E-mail address: nabila.bennabila@univ-msila.dz

Abstract:

This study investigates the volumetric properties and molecular interactions of binary mixtures composed of alkoxyethanols and selected amines through theoretical calculations based on Density Functional Theory (DFT) employing the B3LYP/6-31G++(d,p) basis set. The chosen solvents are recognized for their green chemistry applications due to their environmentally friendly nature. Geometry optimizations of individual components and their binary mixtures were performed to compute energies, molecular volumes, and vibrational spectra, aiming to elucidate the nature of intermolecular interactions, particularly hydrogen bonding. Theoretical excess molar volumes were analyzed and correlated with available experimental data to gain deeper insights into the influence of molecular interactions on the physical properties of the mixtures. The results reveal significant volumetric behavior changes driven by interactions between alkoxyethanols and amines, supporting the use of these solvents in designing more sustainable and eco-friendly chemical processes. This work provides an integrated theoretical framework that complements experimental studies within the scope of green chemistry.

Keywords : Density Functional Theory (DFT), Excess Molar Volume, Binary Mixtures, Alkoxyethanols, Amines.

SYNTHESIS, STRUCTURE AND MOLECULAR DOCKING STUDIES OF A COBALT(II) COMPLEX DERIVED FROM PHTHALIMIDE LIGANDS

Naouel MAKOUF^{1*} and Ismail BOUKRINA²

^{1*} *Laboratoire des substances organo-thérapeutiques et procédés durables, Département de chimie, Faculté des sciences, Université Mohamed Boudiaf - M'sila – Algérie.*

² *Department of chemistry, Faculty of science, University Mohamed Boudiaf of M'sila, Algeria.*

*Corresponding author: Tel. +213 699 17 16 94; E-mail address: naouel.makouf@univ-msila.dz

Abstract : In this work, we report the synthesis and structural characterization of a cobalt(II) complex formulated as $[\text{Co}(\text{C}_{10}\text{H}_6\text{NO}_4)_2(\text{C}_7\text{H}_{10}\text{N}_2)(\text{H}_2\text{O})_2]$, obtained through a sustainable solution-phase reaction involving N-phthaloylglycine and 4-(dimethylamino)pyridine (DMAP) as organic ligands. Single-crystal X-ray diffraction analysis reveals a mononuclear cobalt center in a distorted octahedral geometry (CoN_2O_4), coordinated by DMAP through nitrogen atoms in the axial positions, and by N-phthaloylglycine through carboxylate oxygen atoms in the equatorial plane, along with two water molecules. The supramolecular architecture is stabilized by intermolecular hydrogen bonding and π - π stacking interactions. Considering the known bioactivity of phthalimide and DMAP derivatives, molecular docking studies were conducted to assess the interaction of the complex with biological targets, supporting its potential as a metal-based therapeutic agent. This work highlights the integration of green synthetic methods, crystallography, and computational modelling in the design of novel bioinorganic frameworks.

Keywords: Cobalt(II) complex, Phthalimide, Green synthesis, Crystal structure, Molecular docking.

PHYTOCHEMICAL SCREENING, BIOLOGICAL ACTIVITY AND CORROSION INHIBITION OF A MEDICINAL PLANT

Kenza BOUCHELOUCHE^{1,2*}, Oum Elkheir BELHADDAD^{1,2} and Sabrina MOHAMADI^{1,2}

¹University of M'Sila, Faculty of Sciences, Department of Chemistry, PO Box 166 Ichebilia, 28000 M'Sila, Algeria;

²Laboratory of Therapeutic Organic Substances and Sustainable Processes (LTOSSP).
kenza.bouchelouche@univ-msila.dz (*corresponding author)

Abstract: *Pulicaria odora*, a member of the Asteraceae family, is a medicinal plant commonly used in traditional and pharmaceutical practices for its healing properties in Algeria. The aim of this work is to study the phytochemical screening, Determination of total polyphenols of and total flavonoids content in plant extracts. The study also evaluated the antioxidant, antibacterial, and anti-corrosive activity of extracts from this plant, obtained through maceration using solvents of varying polarity as well as through aquatic extraction via decoction and infusion. The results of phytochemical screening show the presence of gallique tannins, mucilage, total flavonoids, catechic tannins, alkaloids, bones, reducing compounds, and small quantities of saponins. The total polyphenol content analysis showed that the ethanolic extract had the highest concentration of polyphenol and flavonoid. The results of the DPPH test showed that the ethanol extract had the highest antioxidant activity. Additionally, the ethanol, decoction, and infusion extracts all exhibited significant activity against *Pseudomonas aeruginosa* and *Bacillus cereus* bacteria. Furthermore, the corrosion inhibition experiment yielded positive results within 48 hours.

Keywords: *Pulicaria odora*, antioxidant activity, antibacterial activity, corrosion inhibition.

SYNTHESIS, CRYSTAL STRUCTURES, ANTIOXIDANT ACTIVITY AND MOLECULAR DOCKING STUDIES OF A THIOMETHYLBENZIMIDAZOLE LIGAND AND ITS MONONUCLEAR Zn(II) COMPLEX

Feriel Aouatef SAHKI^{1,2*}, Mehdi BOUCHOUIT¹, Ouided BENSLAMA³, Rafika BOUCHENE^{4,5}, Sofiane BOUACIDA^{1,5} and Abdelmalek BOURAIOU¹

¹Research Unit of Environmental and Structural Molecular Chemistry (CHEMS), University of Frères Mentouri Constantine 1, 25000, Algeria

²Laboratory of Organo-Therapeutic Substances and Sustainable Processes, Department of Chemistry, Faculty of Sciences, Mohamed Boudiaf University - M'sila, Algeria.

³Laboratory of Natural Substances, Biomolecules and Biotechnological Applications, Department of Natural and Life Sciences, Faculty of Exact Sciences and Natural and Life Sciences, University of Oum El Bouaghi, Oum El Bouaghi 04000,

⁴Laboratory of Analytical Sciences, Materials and Environment, University of Oum El Bouaghi, Oum El Bouaghi 04000,

⁵Department of Material Sciences, Faculty of Exact Sciences and Natural and Life Sciences, University of Oum El Bouaghi, Oum El Bouaghi 04000, Algeria. *Corresponding author: Tel./Fax: +213793518312 ; E-mail address: feriel-aouatef.sahki@univ-msila.dz

Abstract: In this study, a novel thiomethylbenzimidazole ligand (MIMTMB) and its mononuclear Zn(II) complex were synthesized and characterized through FTIR, NMR, and single crystal X-ray diffraction techniques. Crystallographic data revealed a distorted tetrahedral geometry for the Zn(II) complex, stabilized by hydrogen bonding interactions and π - π stacking [3]. Intermolecular interactions within both structures were further examined using Hirshfeld surface analysis, which highlighted the dominant role of H \cdots H and Cl \cdots H interactions in structural cohesion [4–5]. The antioxidant activity was evaluated using the DPPH radical scavenging assay, where MIMTMB exhibited superior activity (44.80%) compared to its Zn complex (14.84%) [6]. Molecular docking studies targeting cytochrome c peroxidase (PDB: 2x08) confirmed MIMTMB's stronger binding affinity (-5.7 kcal/mol) relative to the Zn complex (-2.4 kcal/mol), with key hydrogen bonds and hydrophobic interactions contributing to its high reactivity [7, 8]. Furthermore, in silico drug-likeness and ADMET profiling of MIMTMB, based on Lipinski and Veber rules, indicated favorable pharmacokinetics, oral bioavailability, and BBB penetration, though potential hepatotoxicity and respiratory risks were also noted [9,10]. These findings position MIMTMB as a promising candidate for the development of antioxidant agents with biomedical applications.

Keywords: Benzimidazole; Zinc complex; Single crystal; Antioxidant activity; Docking molecular.

VISIBLE LIGHT INDUCED HYDROGEN EVOLUTION FROM WATER ON THE HETERO-SYSTEM 10% NiO/ γ -Al₂O₃

Ibtissam SEBAI^{1,2*}, Radia BAGTACHE³, Dahbia AMITOUICHE⁴, and Mohamed TRARIF⁵

¹ *Department of Physical Science, Higher Normal School of Bousaada, Bousaada, Algeria*

² *Laboratory of Natural Gas Chemistry, Faculty of Chemistry University of Science and Technology Houari Boumediene, Algiers, Algeria*

³ *Laboratory of Electrochemistry-Corrosion, Metallurgy and Inorganic Chemistry, Faculty of Chemistry University Of Science And Technology Houari Boumediene, Algiers, Algeria*

⁴ *Department of Chemistry, Faculty of Sciences, Mouloud Mammeri University, Tizi Ouzou, Algeria*

⁵ *Laboratory of Storage and Valorization of Renewable Energies, Faculty of Chemistry, University Of Science And Technology Houari Boumediene, Algiers, Algeria*

*Corresponding author: E-mail address: sebai.ibtissam@ens-bousaada.dz

Abstract: Hydrogen is known as a clean and ecological energy source due to its potential to significantly reduce reliance on fossil fuels and mitigate climate change. The photocatalytic reduction of water appears to be a promising long-term energy solution. Therefore, the aim of this work is to develop novel photocatalyst for the photocatalytic hydrogen evolution. The NiO/ γ -Al₂O₃ hetero-system has been successfully synthesized via a wet impregnation. Where, the XRD pattern confirmed the presence of characteristic peaks corresponding only to γ -Al₂O₃ and NiO phases. The optical gap was found to be narrow at 1.51 eV and the transition is directly permitted. The capacitance measurement indicates *n*-type semiconductor and the potential of conduction band ($-0.35 V_{SCE}$), is more cathodic than the H₂O/H₂ level ($\sim -0.3 V_{SCE}$) at pH \sim 13 leading to a thermodynamically favorable H₂ evolution under visible light irradiation. The photocatalytic procedure was carried out using Na₂SO₄ solution (10^{-3} M) at 50 °C. Supporting NiO on alumina γ -Al₂O₃ lead to in a significant increase in photoactivity by 42% compared to unsupported NiO, attributed to improved surface characteristics, better dispersion, and more efficient electron transfer. The energy bands of NiO are pH insensitive while the level H₂O/H₂ changes by $-0.6 V pH^{-1}$, The best photoactivity was obtained at pH \sim 12. This property was judiciously exploited to have an optimal band bending and an enhancement of 25% was obtained. A quantum yield of 0.67% was achieved under optimal conditions.

Keywords: Nickel oxide, Hydrogen, Visible light, Alumina, Photocatalytic reduction of water.

PHYSICOCHEMICAL STUDY OF MEDICINAL PLANTS IN THE MSILA REGION, ALGERIA

Sabira LACHACHE^{1*}, Ghania BENAICHE² and Rebbas KHELLAF²

¹*Department of chemistry, Mohamed Boudiaf University of Msila, Algeria*

²*Department of Natural Sciences and Life, Mohamed Boudiaf University of Msila, Algeria*

**Sabira LACHACHE : Tel./Fax: +213697268000; E-mail address: sabira.lachache@univ-msila.dz*

Abstract: Algeria's flora, and in particular the El-Hodna region, is characterized by its richness and diversity, harboring numerous endemic and medicinal species. Thanks to a favorable Mediterranean climate, this region is home to botanical families such as the Fabaceae and many others, which play a crucial role both for the local ecosystem and for the populations who use them for medicinal and culinary purposes [1]. In this context, this work deals with a study of phytochemical polyphenols and flavonoids in flowers and leaves of this plant. The preliminary screening based on specific tests confirmed the presence of substances having great therapeutic values such as: flavonoids, tannins and coumarins [2]. The quantitative estimation of total polyphenols by the Folin-Ciocalteu method, and total flavonoids by the method of Aluminum chloride $AlCl_3$ [3] showed that the flowers and leaves are very rich in these compounds.

Keywords: Genista, secondary metabolites, El-Hodna.

LC-MS/MS CHARACTERIZATION OF PHENOLICS AND GREEN SYNTHESIS OF ANTIBACTERIAL SILVER NANOPARTICLES FROM THE ACETONIC EXTRACT OF ALGERIAN DAUCUS CAROTA

Maroua HADJI^{1*}, Soundouss HADJI², Khadidja DEHIMI³, Toka HADJI³, Tahar SMAILI¹

¹ Department of Natural and Life Sciences, Faculty of Sciences, University of M'sila, PO Box 166 Ichebilia, 28000, Algeria.

² Department of Physics, Faculty of Sciences, University of M'sila, PO Box 166 Ichebilia, 28000, Algeria.

³ Department of Microbiology and Biochemistry, Faculty of Sciences, University of M'sila, PO Box 166 Ichebilia, 28000, Algeria.

⁴ Department of Biology and Plant Ecology, University of Mentouri Brothers Constantine 1, P.O. Box, 325 Ain El Bey Way, Constantine, 25017, Algeria

*Corresponding author: E-mail address: maroua.hadji@univ-msila.dz

Abstract: In the search for safe and sustainable antimicrobial agents, green chemistry offers a valuable alternative to conventional chemical synthesis by using plant extracts for nanoparticle production. This study aimed to analyze the phenolic composition of *Daucus carota* subsp. *maximus* acetonetic extract, to synthesize silver nanoparticles (AgNPs) using the extract via a green method, and to evaluate their antibacterial activity following the approach of combining phytochemical profiling, green synthesis, and antibacterial testing. The phenolic profile of the extract was determined by LC-ESI-MS/MS, which revealed 16 phenolic compounds known for the ions reducing power with a total concentration of 8.809 mg/g. AgNPs were synthesized by adding the extract to an aqueous solution of AgNO₃. A color change from yellow to dark brown and an absorbance peak at 420 nm in UV-visible spectroscopy confirmed nanoparticle formation. The antibacterial activity of the biosynthesized AgNPs was tested against four bacterial strains (*Escherichia coli*, *Staphylococcus aureus*, *Pseudomonas aeruginosa*, and *Bacillus subtilis*) using the agar diffusion method and minimum inhibitory concentration (MIC) testing. The inhibition zones ranged from 12 to 22 mm, while MIC values varied between 50 and 25 µg/mL. These results demonstrate the effectiveness of *Daucus carota* extract in reducing silver ions and producing stable nanoparticles with significant antibacterial activity. The study underlines the potential of Algerian wild plants in green nanotechnology and supports their use in developing new antimicrobial materials for future biomedical applications.

Keywords: Green synthesis; Silver nanoparticles; *Daucus carota* subsp. *maximus*; Phenolic compounds.

EVALUATION OF A BINARY COMPLEX FOR USE IN COSMETICS

Salima ZIDANE^{1,2*} Hocine BOULEGHLEM^{1,2}, BENMANSOUR Khawla¹ and BEN LATRECHE Nassira¹

¹Department of Chemistry, Faculty of Sciences, Mohamed Boudiaf University of M'Sila
Address: University Campus, Bordj Bou Arreridj Road, 28000 M'Sila, Algeria.

² Laboratory of Therapeutic Organic Substances and Sustainable Processes (LTOSSP), Mohamed Boudiaf University of M'Sila

³Applied Chemistry Laboratory, University Mohamed Khider-Biskra, Algeria

* Corresponding author Email: salima.zidane@univ-msila.dz

Abstract: The integration of binary or ternary complexes of natural bioactives represents an innovative approach in cosmetics, aiming to enhance the stability, bioavailability, and efficacy of formulations. This study investigates the synergistic effect of microphytes (*Spirulina*, *Chlorella*) combined with natural additives (carob pod, chitosan) to develop nutraceutical supplements and cosmetic applications. *Spirulina* and *Chlorella*, rich in proteins, amino acids, vitamins, minerals, and bioactive pigments such as phycocyanin and chlorophyll, are well-recognized for their strong antioxidant, anti-inflammatory, and antibacterial activities. Experimental assays comparing different formulations revealed that (*Spirulina*–carob) exhibited significant antioxidant activity (71%), marked anti-inflammatory potential (82%), and good antibacterial effects. Meanwhile, (*Spirulina*–*Chlorella*–chitosan) demonstrated excellent anti-inflammatory activity (84%) along with substantial antibacterial efficacy. Based on these findings, cosmetic prototypes (cream, ointment, gel, soap) were formulated using *Spirulina* as the core ingredient, and confirmed their biological effectiveness, particularly against skin inflammation and microbial growth. These results highlight that combining natural bioactives allows the design of multifunctional cosmetic products that combine efficacy, safety, and sustainability. This approach not only enhances the valorization of *Spirulina* and plant biomass but also aligns with the growing demand for natural and innovative formulations in the global cosmetic industry.

Keywords: *Spirulina*, *Chlorella*, binary complexes, carob, chitosan, cosmetics

EXTRACTION AND TREATMENT OF CELLULOSIC FIBERS FROM DATE PALM

BENADEL Zohra⁽¹⁾, Khadijah SAGHIRI⁽²⁾, BENYAHIA Azzeddine⁽³⁾,

¹. University Mohamed boudiaf Department of Matter Sciences M'sila ,Algeria

². Laboratory of Molecular Chemistry and Environment (LMCE), Department of Chemistry, University Mohamed Khider

Tel: +213779600370. E-Mail: zohrabenadel23@gmail.com

Abstract : The date palm (*Phoenix dactylifera*) is a major agricultural crop cultivated extensively in North Africa, the Arabian Gulf—particularly Saudi Arabia—Pakistan, and India . Various techniques have been reported in the literature for extracting fibers from different parts of the date palm, each with distinct advantages and limitations. Mechanical extraction, as well as chemical and biological treatments, have been employed to isolate cellulose fibers from non-cellulosic constituents such as lignin and hemicellulose. The choice of extraction technique is critical for producing high-performance fibers. An effective process should yield pure, long, and fine fibers with minimal structural damage. Among the methods most frequently cited in the literature are mechanical extraction and alkaline treatment with sodium hydroxide (NaOH). In the present study, Palm leaves were collected from a local farm in Algeria M'sila . The material was washed, dried, and cut into small pieces before dispersion in distilled water to form a paste. This was followed by alkaline treatment with an NaOH–water solution to solubilize the fibers. Delignification was subsequently carried out using sodium chlorite (NaClO₂). Additional bleaching steps and treatment with potassium hydroxide (KOH) solution were applied prior to a dilute acid treatment with sulfuric acid (H₂SO₄). The resulting insoluble fraction was thoroughly washed and neutralized. Fiber characterization was conducted in Algeria using infrared (IR) spectrometry and other analytical techniques.

Keywords: Date palm (*Phoenix dactylifera*) – cellulosic fibers – fiber extraction – alkaline treatment (NaOH) – acid treatment (H₂SO₄) –IR spectrometry

PHYTOCHEMICAL PROFILE AND ANTICANCER POTENTIAL OF *PITURANTHOS SCOPARIUS*

Sarra CHABANE^{1,2}, Amel BOUDJELAL^{2,3}, Aslı YILDIRIM KOCAMAN⁴, Ibrahim DEMIRTAS^{5,6}

¹Department of Veterinary, Faculty of Sciences, University of M'sila, Algeria.

²Laboratory of Biology: Applications in Health and Environment, University of M'sila, Algeria.

³Department of Microbiology and Biochemistry, Faculty of Sciences, University of M'sila, Algeria.

⁴Research Laboratory Practice and Research Center, Iğdir University, 7600, Iğdir, Türkiye .

⁵Ondokuz Mayıs University, Faculty of Science and Art, Department of Chemistry, Samsun, Turkey

⁶Department of Biochemistry, Faculty of Science and Art, Iğdir University, Iğdir, Turkey

*Corresponding author: Tel: +2136660655387 ; E-mail address: sarra.chabane@univ-msila.dz

Abstract: Medicinal plants have always been used as traditional medicines to treat human ailments, *Pituranthos scoparius* (*Apiaceae*), holds significant traditional importance in Algeria for the treatment of asthma and rheumatism, diabetes, urinary infections. The objective of this study was to investigate for the first time the phytochemical composition of *Pituranthos scoparius* methanolic extract and essential oil, as well as to evaluate their anticancer potential. The chemical composition of the extract and essential oil was carried out using LCMS and GCMS techniques to identify their major bioactive compounds. The anticancer effects were evaluated against the colorectal cancer (HT29) and liver cancer (HEPG2) cell lines using MTT assay. Two major compound were identified by LC-MS/MS analysis, chlororganic acid and trans-ferulic acid. The composition of essential oil was investigated by GC-MS/MS analysis. The major component is: α pinene (37,11%). The methanolic extract possesses notable antiproliferative effects on HEPG2 cells, which intensify over time and with increasing concentration, then the essential oil has a strong antiproliferative effect on HEPG2 cells, with its potency increasing over time and at higher concentrations. This study aims to identify the phytochemical composition of *Pituranthos scoparius* extract and essential oil and assess their anticancer potential. The findings of this research could contribute to the development of new plant-based therapeutic agents for cancer treatment.

Keywords: *Pituranthos scoparius*; traditional uses; LC-MS/MS analysis; GC-MS/MS analysis; anticancer potential.

CU(II) COORDINATION POLYMER BEARING DIAZENYL-BENZOIC LIGAND: SYNTHESIS, PHYSICO-CHEMICAL AND XRD/HSA-INTERACTIONS

Souheyla CHETIOUI^{1,2*}, Ilhem BENSEHIL^{1,4}, Sihem MENASSEL¹, Nabila BENABILA³

1 Faculty of Technology, University of M'sila, 28000 M'sila, Algeria.

2 Research Unit for Chemistry of the Environment and Molecular Structural, University of Constantine 1, Constantine 25000, Algeria.

3 Faculty of Science, Department of Chemistry, University of Msila, 28000 M'sila, Algeria

4 Laboratory of Surfaces and Interfaces Studies of Solid Materials, University of Setif 1, Algeria.

**Corresponding author: souheyla.chetioui@univ-msila.dz*

Abstract : Azo ligands are very important in the field of pigments, dyes and advanced material. These compounds demonstrate one of the most broadly applied organic materials that are appealing to scientists due their different applications. They can coordinate to transition metal in a wide coordination mode and employ the N as a ligating donor. New binuclear copper(II) complex $[Cu_2L_2]$ zig-zag coordination polymer (CCP) have been synthesized via one-pot copper(II) acetate/(E)-2-((2-hydroxynaphthalen-1-yl)diazenyl)benzoic dye through an in situ aqua doubly deprotonated ligand substitution reaction. The coordination polymer complex was characterized by spectroscopic and CHN-elemental analysis. The crystal structure has been specified by the XRD-method exhibiting that the Cu(II) center geometry is with five-coordinated distorted tetragonal pyramidal. The desired CCP structure chains are connected into a 2D-Supramolecular assembly via one C-H...O H-bond and enhanced by a π - π stacking interactions. These interconnections strengthened the lattice of CCP that originated the formation of super thermal CCP complexes. The fundamental vibrational wavenumbers and electron transfer in the free ligand are combined with the complex before and after coordination to demonstrate the spectral behavior of L -2 in the desired zig-zag CCP. The 2D-fingerprint (2D-FP) and Hirshfeld surface analysis (HSA) computations were served to prove the 2D-network packed crystal lattice interactions.

THE ROLE OF ARTIFICIAL INTELLIGENCE IN SUSTAINABLE SMART FOOD PACKAGING: RECENT ADVANCES

Souad KADI^{1,2*}

¹*Department of natural and life sciences, Laboratory of Organo-Therapeutic Substances and Sustainable Processes, University of M'sila, University Pole, Road Bordj Bou Arreidj, M'sila 28000, Algeria*

²*University of Sciences and Technology Houari Boumediene, Laboratory of Polymeric Materials, Faculty of chemistry, BP 32, El Alia, Algiers 16111, Algeria*

**Corresponding author: Tel./Fax: +0-065-763-2746 ; E-mail address: souad.kadi@univ-msila.dz*

Abstract: Artificial intelligence (AI) is a multidisciplinary field of computer science that focuses on developing algorithms, models, and systems capable of mimicking human-like cognitive functions such as learning, reasoning, problem-solving, and decision-making. Food safety and packaging materials are the two main areas of attention for modern packaging technologies. In addition to protecting from outside contaminants, food packaging guarantees freshness, preservation, and an extended shelf life. Modern technology combined with conventional preservation techniques has improved food quality and safety. Additionally, waste or by-products from the fruit and vegetable industry are widely used to create biodegradable packaging options, offering a more sustainable approach. Artificial Intelligence plays a pivotal role in revolutionizing the food packaging. It optimizes various aspects of the packaging process, enhancing efficiency, safety, and sustainability. AI enables smart packaging solutions, incorporating sensors and data analytics to monitor and control factors such as freshness, temperature, and shelf life. This ensures that food products remain in optimal condition throughout the supply chain. AI is transforming the food packaging industry in numerous innovative ways: intelligent labels, shelf-life optimization, robotic packing, enhanced sustainability and food safety, inventory management, food safety and traceability, personalized packaging and marketing, resources conservation and energy reduction [7]. This contribution provides recent developments in smart food packaging materials, with some examples for the application of AI in food packaging.

Keywords: Artificial intelligence, smart food packaging, sustainability.

OPTIMIZED PVA-BASED CATIONIC MEMBRANES FOR EFFICIENT DUAL-ELECTROLYTE WATER ELECTROLYSIS.

Amina KALOUN ^{1*}, Zahia GHARNOUT ¹, Abdallah MERROUCHE¹

¹Laboratory of Inorganic Materials, University of M'Sila, Faculty of Sciences, Department of Chemistry, PO Box 166 Ichebilia, 28000 M'Sila, Algeria

*Corresponding author: Tel./Fax: +213-552-62-5054; E-mail address: amina.kaloun@univ-msila.dz

Abstract: In this study, cationic polymer membranes based on polyvinyl alcohol (PVA) and chemically modified by the incorporation of sodium silicate (Na_2SiO_3) were developed for energy-related applications, particularly in dual-electrolyte water electrolysis systems. Two membranes containing different weight percentages of Na_2SiO_3 (5% and 10%) were prepared, and the membrane with 10 wt% was selected due to its superior electrochemical performance. Subsequently, the selected membrane underwent a freeze–thaw treatment ($-20\text{ }^\circ\text{C}$ for 16 hours) to enhance its structural properties and ionic transport behavior. The results showed that freezing reduced the swelling degree from (320%) to (280%), indicating a significant improvement in mechanical stability. In parallel, the ionic conductivity increased from 1.26 to 3.97 mS/cm, and the cationic permselectivity improved to reach 95%, reflecting high ion transport efficiency. The ion exchange capacity (IEC) was also evaluated, with the treated membrane showing a value of 21 meq/100g compared to 50 meq/100g for the untreated sample. Structural analysis using FTIR and XRD confirmed the incorporation of silicate and the morphological changes induced by the thermal treatment. When tested in a dual-electrolyte electrolysis cell (2M NaOH / 2M H_2SO_4), the treated membrane enabled a reduction in operating voltage from 2.8 V to 1.73 V, which led to an energy efficiency increase to approximately 54%, outperforming several results reported in previous studies. These findings suggest the potential for significant energy savings and enhanced performance in sustainable hydrogen production. This study demonstrates that combining Na_2SiO_3 incorporation with freeze–thaw processing offers a simple, cost-effective, and efficient strategy to enhance polymer membrane performance without requiring complex chemical modifications, making it a promising candidate for clean energy applications.

Keywords: Cationic membrane, PVA, sodium silicate (Na_2SiO_3), freeze–thaw treatment, dual-electrolyte electrolysis, ionic conductivity, permselectivity, ion exchange capacity (IEC), sustainable energy, FTIR, XRD.

CONTRIBUTION TO THE STUDY OF THE PHYSICO-CHEMICAL QUALITY OF WATER IN THE HODNA BASIN

Fatima GHERBAOUI ^{1,2}, Ammar SASSOUI ³ and Ettayib BENSACI ³

¹*Département des Sciences Agronomiques, Université Mohamed El Bachir El Ibrahimi, Bordj Bou Arreridj, ALGERIE.*

²*Laboratoire de Santé et environnement, Département Sciences Biologiques, Université Mohamed El Bachir El Ibrahimi, Bordj Bou Arreridj, ALGERIE.*

³*Département des Sciences de la nature et de la vie, Université de M'sila, M'sila, ALGERIE.*

**Corresponding author: Tel./Fax: 0661440128; E-mail address: fatima.gherbaoui@univ-bba.dz*

Abstract: This study contributes to the physico-chemical characterization of water quality in the Hodna Basin, located in a semi-arid region of Algeria. These water resources are of critical importance for both hydrological balance and agricultural productivity, particularly in areas where water availability is limited. As such, monitoring their pollution status is essential to ensure their sustainability. In the studied region, industrial development and agricultural intensification have been increasing over the years, leading to significant pollutant discharges into aquatic systems. Water sampling campaigns were conducted during April and May 2017 at 24 sampling stations distributed along five wadis forming part of a sub-watershed. Various physical parameters were measured in situ using a multiparameter probe, including pH, temperature, salinity, and electrical conductivity. Additionally, chemical analyses were carried out to evaluate pollution and mineralization indicators, such as nitrite and orthophosphate concentrations, total dissolved solids (TDS), salinity, and dissolved oxygen levels. The findings revealed that most of the measured parameters exceeded the permissible limits established by Algerian standards, as well as international guidelines set by the WHO and FAO for irrigation water, except for pH values which remained within normal ranges. The high concentrations of pollutants are mainly attributed to agricultural runoff and domestic wastewater. This environmental degradation poses serious threats to ecosystem health and public safety.

Keywords: Water quality; physico-chemical; aquatic pollution; Hodna Basin; semi-arid region.

THERMAL STABILITY OF SOL-GEL DERIVED HYDROXYAPATITE FOR CA/P MOLAR RATIO 1.67 AND 1.5

Amira MOKRANE^{1*}, Menad HERAIZ¹ and Fatima-Zohra MEZAH¹

¹Physics and Chemistry of Materials Laboratory, Department of Physics, Mohamed Boudiaf University, 28000, M'sila, Algeria.

*Corresponding author: Tel./Fax: +213552376251 ; E-mail address: amira.mokrane@univ-msila.dz

Abstract: Hydroxyapatite (HA: $\text{Ca}_{10}(\text{PO}_4)_3(\text{OH})_2$) is a crucial mineral component of bones and teeth. It is widely used in biomedical applications due to its excellent biocompatibility. Their physical, chemical, and biological properties are significantly influenced by the synthesis parameters, including the initial (Ca/P) ratio and the calcination temperature. So, this study investigates the impact of heat treatment on stability of HA, synthesized via the sol-gel method. Two different (Ca/P) molar ratios (1.67 and 1.5) were chosen. HA was synthesized using triethyl phosphate and calcium nitrate tetrahydrate. A mixture of ethanol and distilled water was employed as the solvent. The aging, gelling, and drying process occurred at 90°C for one day. The dried gels were calcined at 700°C for one hour. The samples were then heat-treated at 1100°C, 1200°C, and 1300°C. The structural evolution of the synthesized phases was analyzed using X-ray diffraction (XRD) and Fourier-transform infrared spectroscopy (FT-IR). XRD patterns indicated HA formation in all samples, along with CaO. Additionally, β -tricalcium phosphate (β -TCP) was observed as a secondary phase in the sample with (Ca/P) ratio of 1.5. At 1100°C, an increase in the intensity of HA peak was remarked, along with a decrease in the intensities of CaO and β -TCP. At 1200°C and 1300°C, β -TCP completely disappeared, and α -TCP emerged, indicating a phase transition from β -TCP to α -TCP. FT-IR spectra confirmed the XRD findings. The formation of biphasic calcium phosphate composites (HA and TCP) enhance the biological activity of these composites and ensure their mechanical stability [4].

Keywords: Hydroxyapatite ; Sol-gel ; Thermal stability.

EXPERIMENTAL STUDY OF THE EFFECT OF NITRIC ACID ON WOLLASTONITE SYNTHESIS VIA SOL-GEL METHOD

Mohamed MAALMI^{1*}, Fatima Zohra MEZAH¹ and Menad HERAIZ¹

¹ *Department of Physics, Physics and Chemistry of Materials Laboratory University of M'sila Msila, Algeria*

**Corresponding author: Tel./Fax: 06 98 00 63 06; E-mail address: mohamed.maalmi@univ-msila.dz*

Abstract: This study is devoted to examine the effect of nitric acid on the synthesis of wollastonite (CaSiO₃) via sol-gel method. This technology allows low-temperature production of powders at nanometer scale and has some benefits compared to conventional techniques. Wollastonite has been used in several biomedical applications such as artificial dental roots and bone filling biomaterial because it is biocompatible and bioactive. Artificial implants based on wollastonite have found wide usage in the field of orthopedics to treat bone deficiencies. The bioactivity of wollastonite originates because of the presence of silicon, which facilitates the metabolism of new bone formation. In this study, calcium nitrate (Ca(NO₃)₂) and tetraethyl orthosilicate (C₈H₂₀O₄Si: TEOS) were used as the source of calcium and silicon, respectively. Nitric acid was used as solvent with different concentrations (2, 1.5, 1, and 0.5 M). To analyze the structural evolution of formed phases, different techniques were used: X-ray diffraction (XRD), spectrometer FTIR-ATR, and Raman spectroscopy. Dielectric measurements were also conducted. The obtained results indicated the formation of larnite at 800°C for all products. When the products were heat treated at 1000°C, β-wollastonite was formed. But as the concentration of nitric acid decreased, the proportion of larnite declined, β-wollastonite increased, and a new phase, α-wollastonite, also resulted with an appreciable percentage at 0.5 N concentration of nitric acid. The obtained results showed that the concentration of nitric acid has a major impact on the nature and proportions of the phases formed.

Keywords: Sol gel ; Wollastonite ; XRD

PVA-BASED PROTON-EXCHANGE MEMBRANES FOR ENERGY-EFFICIENT DUAL-ELECTROLYTE WATER ELECTROLYSIS.

Zahia GHARNOUT^{1*}, Amina KALOUN¹, Aicha Belhadj¹, Abdallah MERROUCHE¹ and Laid TELLI¹

1 Department of Chemistry, Faculty of Science, University of M'sila, M'sila 2800, Algeria.

**Corresponding author: Tel./Fax: +213-672-49-0667 ; E-mail address: zahia.gharnout@univ-msila.dz*

Abstract: Membranes based on polyvinyl alcohol (PVA) and phosphoric acid (H₃PO₄) have been prepared and characterized using various experimental techniques, including X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), electrochemical impedance spectroscopy (EIS), ion exchange capacity (IEC), Water uptake (W_U) and permselectivity. When used between two NaCl solutions, these membranes have exhibited relatively high ionic conductivity. In particular, the PVA-H(20 wt.%) membrane has demonstrated a maximum ionic conductivity of $1.2 \cdot 10^{-3} \text{ S cm}^{-1}$ with sufficient ion exchange capacity of 0.52 meq.g^{-1} . These properties make this proton exchange membrane a promising candidate for electrochemical applications. This membrane has been employed in a dual-electrolyte water electrolyzer in order to reduce the energy consumed during electrolysis. The results have shown that the voltage of dual-electrolyte electrolysis has been on average 0.9 V lower than that of conventional alkaline electrolysis, under the same conditions. Furthermore, in both dynamic and static operation, an energy saving of around 38% has been achieved for the same amount of electricity consumed, compared to traditional electrolysis. These findings **may demonstrate** the utility of dual-electrolyte electrolysis and highlight the potential of PVA-H membranes for sustainable energy applications.

Keywords: Dual-electrolyte system, Membrane, PVA, Proton conductivity, proton-exchange membranes, Low-energy water electrolysis.

ECO-FRIENDLY SYNTHESIS OF AGNPS USING ASTERACEAE EXTRACT AND THEIR COMPARATIVE ANTIOXIDANT POTENTIAL

Tarik TURQUI ^{1*}, Ghania BENAICHE ² and Imen BENKOUIDER³

^{1*}*Department chimistry, Inorganic Materials Laboratory, Faculty of Science, University of M'sila, University Pole, Road Bordj Bou Arreridj, M'sila 28000 Algeria Country*

²*Laboratory of Therapeutic Organic Substances and Sustainable Processes (LTOCSP), common truck department of Nature and Life sciences, Faculty of Science, University of M'sila, University Pole, Road Bordj Bou Arreridj, M'sila 28000 Algeria.*

³*Laboratory of Physics and Quantum Chemistry, Mouloud Maameri University of Tizi-Ouzou, Department of Chemistry, Faculty of Science, University of M'Hamed Bouguara, Boumerdès, Route de la Gare Ferroviaire, Boumerdès 35000, Algeria*

*Corresponding author: Tel: +213671922812; E-mail address: tarik.turqui@univ-msila.dz

Abstract: The Asteraceae family is widely recognized for its rich phytochemical profile and therapeutic potential. In this study, the aerial parts of *A.C spices* were collected, shade-dried, and extracted using a methanol-water mixture (30:70 v/v) at 25°C through successive maceration cycles. In parallel, silver nanoparticles (AgNPs) were synthesized using an aqueous extract of the same plant specie *A.C* following an environmentally friendly approach in line with green chemistry principles. A silver nitrate (AgNO₃) solution was gradually added to the plant extract, resulting in a visible color change from yellow to brown, suggesting the formation of AgNPs. This was further supported by FTIR analysis performed on both the methanolic extract and the synthesized nanomaterial (*AC-AgNPs*), which enabled the identification of functional groups involved in reduction and stabilization processes. The antioxidant activity of both the plant extract and the nanostructure was assessed using the DPPH• radical scavenging assay[4]. The results revealed notable differences in radical scavenging capacity, indicating that the (*AC-AgNPs*) significantly enhanced the biological performance. These preliminary findings highlight the promising therapeutic potential of *A.C* extract and its (*AC-AgNPs*), particularly in improving antioxidant effectiveness. Moreover, the study underscores the relevance of this approach in the context of green chemistry, offering a pathway for the development of eco-friendly, bioactive nanomaterials with prospective applications in pharmaceutical and environmental fields.

Keywords: Asteraceae ; aqueous ; nanostructure

ELECTRONIC STRUCTURE, MECHANICAL AND OPTICAL PROPERTIES OF HYDROGEN STORAGE ALKALINE AMIDES XNH_2 (X = LI, NA) COMPOUNDS

T.SAADI^{a, b, *}, Z. CHARIFI^{a, b, *}, H. BAAZIZ^{a, b}, T. GHELLAB^{a, b}

^a Department of Physics, Faculty of Science, University of M'sila, 28000 M'sila, Algeria

^b Laboratory of Physics and Chemistry of Materials, University of M'sila, Algeria

* Corresponding author: E-mail address: taieb.saadi@univ-msila.dz

zoulikha.charifi@univ-msila.dz, Phone: +21335556453, Fax: +21335556453

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Abstract: Using first-principles calculations based on density functional theory (DFT), the structural and electronic properties of XNH_2 (X = Li, Na) hydrides were investigated. The exchange–correlation energy was treated using both the generalized gradient approximation (GGA) and the local density approximation (LDA). Under ambient conditions, XNH_2 (X = Li, Na) is stable in a tetragonal structure. At elevated pressures, these complex hydrides undergo a structural phase transition from the orthorhombic $PbCl_2$ -type phase to the tetragonal phase, and the corresponding transition pressures were determined. The electronic density of states analysis indicates that these hydrides are semiconductors with a direct Γ – Γ band gap when using both GGA and LDA approximations. The calculated results show good agreement with available experimental and theoretical data. As newly studied materials, XNH_2 (X = Li, Na) hydrides could be effectively utilized in the design of promising prototype devices for hydrogen storage applications.

Keywords: DFT, complex hydrides, hydrogen material, electronic structure, Energy gap.

THE MORPHOLOGY ,ELECTRO CHEMICAL PERFORMANCE AND CHARACTERIZATION OF NANOSTRUCTURED α -PbO PREPARED FROM SPENT LEAD ACID BATTERY NEGATIVE PLATE

REDAOUI SAMIHA^{1*}, DAKHOUCHE ACHOUR¹

¹ *Laboratory of inorganic materials, Departement of chemistry, Faculty of science, University of M'sila, University pole, Road Bourdj Bou Arreiridj, Msila 28000-Algeria*
Affiliation 1

* **Corresponding author:** Samiha Redaoui, samiha.redaoui@univ-msila.dz

Abstract: Early, millions of lead acid batterie/s (LABs) are thrown after their failure. They constitute a source of contamination of the environment and a great attaint for the human health. Many processes, either pyrometallurgical or hydrometallurgical, have been developed to produce metallic lead from the spent LABs. However, pyrometallurgical routes require high temperature (around 1000 °C), which not only consume huge amounts of energy but also easily produce SO₂ and lead dust if the desulfation is not fully completed, bringing secondary contamination to the environment. The aim of this work was the synthesis and characterization of nanostructured PbO obtained from spent lead acid batteries negative plate. The negative plates of used battery are made up of large amounts of PbSO₄ and smaller amounts of Pb. The PbSO₄ was desulfated with (NH₄)₂CO₃ to obtain PbCO₃ which is then calcined in air at different temperatures. In this work we are interested in studying the effect of temperature on the nature and the morphology of the products of the calcination process. The results shows that at a 450°C we obtain α -PbO, at 500°C β -PbO, after these temperature we get a mixture of lead oxides α -PbO, β -PbO, and minium Pb₃O₄. α -PbO granules have sizes around 26 nm with a mesoporous materials and BET surface area was equal to about 4 m²/g

Keywords: Lead, nanostructured pbo, lead acid battery, lead oxides, waste recycling.

EFFECT OF POTENTIAL ON THE ELECTROCHEMICAL NUCLEATION AND GROWTH OF THE NANOSTRUCTURED INDIUM THIN FILM

Oualid DILMI*^{1,2}, Hadjira BENHEDID³, Wassila REMACHE⁴, Tahir HABILA⁵ and Rabah ASSELI⁶

¹Department of S.M, Faculty of Science and Technology, Mohamed el Bachir el Ibrahimi University, Bordj Bou Arreridj, 34000, Algeria.

²Laboratory of Physics of Materials and its Applications, Mohamed Boudiaf University, M'sila, 28000, Algeria.

³Department of Biological Sciences, Faculty of Natural Sciences, Life and Earth Sciences, University of Ghardaia, Ghardaia, 47000, Algeria.

⁴Department of Chemistry, Faculty of Exact Science and Computer sciences, Mohamed Seddik Benyahia University, Jijel, 18000, Algeria.

⁵Department of physics, Higher Normal School of BouSaada, Boussaada, 28201, Algeria.

⁶Energetic and Solid-State Electrochemsistry Laboratory, Ferhat Abbas-Setif1 University, Setif, 19000, Algeria.

*Corresponding author: Tel./Fax: +213-777-271-263; E-mail address: oualid.dilmi@univ-bba.dz

Abstract: The indium is a shiny gray metal similar to gallium and thallium whose tetragonal crystal structure . In recent years; indium and its alloys attract more attention owing to its good propriety. It can be used in several domains in our life among them the use in solar cells in photoactive thin films such as CuInGaSe₂ (CIGS) CuInSe₂ (CIS) In₂Se₃. In this work, cyclic voltammetry and chronoamperometry were used to study the influence of potential on the electrocrystallization kinetics of electrodeposited indium on platinum and ITO (Indium Tin Oxide) substrates from acid medium (PH=4.2) containing indium trichloride InCl₃ and sodium citrate at ambient temperature. The potentiostatic current transients were analyzed according to Scharifker-Hills model. The morphological characterization of the deposits was carried out by Scanning Electron Microscopy (SEM), whereas the Atomic Force Microscopy (AFM) was used to investigate its roughness. The obtained results showed that the nucleation mechanism of (In) on the two substrates is instantaneous with a three-dimensional growth of the hemispherical nuclei. The nucleation density (N₀) and the max of time (t_m) evolves exponentially with the applied potential, whereas the max of current density (i_m) is linearly evolved with the applied potential, the grains of the obtained deposits at -1.2 and -1.3 V vs. SCE have spherical forms with nanometric sizes and possesses less rough surface.

Keywords: electrodeposition; indium; nanostructure, kinetics; nucleation; growth

THE EFFECT OF PHYSICAL PROPERTIES OF NANOSTRUCTURAL ZNSE QUANTUM DOTS

Lynda LAKHAL¹, Fadila MEZRAG², N.BOUARISSA³

¹ *Laboratory of Materials Physics and Its Applications, University of M'sila, 28000 M'sila*

E-mail des auteur correspondant : lakhal.lynda@univ-msila.dz

Abstract: The current investigation attempts to explore the effects of physical properties of nanostructural ZnSe on spherical quantum dots. Hence, this research uses the pseudopotential approach, based on the data collected and analyzed, it has been shown that spherical quantum dots change significantly the physical properties of nanostructural ZnSe relatively to the bulk [2]. In other words, the direct energy gap has been incredibly changed in accordance to the bulk values which are obtained. As a result of this finding, the possibility of gaining other new physical properties was significantly decreased the bulk.

Keywords: : Quantum dots, nanostructural ZnSe, physical properties, spherical quantum dots

COMPUTATIONAL STUDY OF A HALF-HEUSLER ALLOY USING AB INITIO METHODS

Said CHAHLAT ¹✉, Lahcene NASRI ², Sabrina BOUNAB ¹, Abdelouheb BENTABET ² and Lakhdar CHELALI ³

¹ M'sila University, Laboratory of physics and chemistry of materials, M'sila, Algeria

² Bordj Bou-Arredj University, Laboratoire de Caractérisation et Valorisation des Ressources Naturelles (LCVRN), Algeria

³ M'sila University, Laboratory of materials physics and its applications, M'sila, Algeria

*Corresponding author: Tel: +213773701239 ; E-mail address said.chahlat@univ-msila.dz

Abstract: We used the WIEN2k software's full-potential linearised augmented plane wave (FP-LAPW) method to study the mechanical behaviour of a Half-Heusler compound. We used the Murnaghan equation of state to improve the crystal structure of the compound and find the equilibrium lattice parameter. We found that the elastic constants satisfied the Born criteria for cubic crystals after doing some math. This proved that the substance we looked at was stable in terms of mechanics. We used the Voigt-Reuss-Hill approximation to figure out the Poisson's ratio, Young's modulus, shear modulus, and bulk modulus. The Pugh ratio showed that the compound is flexible. The analysis of the elastic anisotropy index also demonstrated that the elastic properties change slightly depending on the direction. These data suggest that this chemical is strong and flexible in general. In other words, it can be employed when robust structures and good mechanical performance are needed. This theoretical study is the first step in making and testing Half-Heusler materials for use in thermoelectric devices and other mechanical uses.

Keywords: Half-Heusler compounds ; Elastic properties ; WIEN2k ; DFT ; Mechanical stability

SOLVO-THERMAL SYNTHESIS, CHARACTERIZATION AND ANTIBACTERIAL ACTIVITY OF UNDOPED AND Ag DOPED ZnO

Sara SADEDDINE ^{1*}, Samir HAMRIT ¹, Abdelhafid MAHROUG ¹ and Hanane CHENAGUE¹

¹ *Laboratory of Materials Physics and Its Applications, Physic Department, Faculty of science, Mohamed Boudiaf university, M'sila, Algeria*

Tel: +213-783-120-265; E-mail address: sara.sadeddine@univ-msila.dz

Abstract: Zinc oxide (ZnO) is a multifunctional semiconductor material widely investigated due to its outstanding physicochemical properties. These include environmental abundance, biocompatibility, non-toxicity, chemical and thermal stability high optical transparency in the visible region, and a wide direct band gap (~3.3 eV) with a large exciton binding energy(60 meV).Undoped and Ag-doped ZnO nanoparticles were successfully synthesized via a solvo-thermal method at 130°C. The resulting nano-powder underwent comprehensive characterization using various techniques including X-ray diffraction, scanning electron microscopy (SEM), and energy-dispersive X-ray spectroscopy (EDX). The analyses confirmed the high purity of the undoped ZnO and Ag-doped ZnO particles. Structural properties were thoroughly investigated using X-ray diffraction, revealing a hexagonal würtzite structure and face-centred cubic silver). SEM imaging of the nanoparticles displayed the particles as spherical in shape. The analysis using energy dispersive X-ray spectroscopy (EDS) provided details regarding the composition and concentration of elements within the synthesized nano-powder. The EDS spectrum displayed multiple distinct peaks, confirming the presence of Zn, O and Ag elements in the ZnO nano-powder. Notably, no peaks associated with other elements were detected, underscoring the high purity of the produced nano-powder. Results showed that ZnO: Ag nano-composites exhibited enhanced antimicrobial efficacy compared to pure ZnO. The inhibition zone increased with silver content, highlighting the potential of ZnO: Ag as a promising candidate for antimicrobial applications.

Keywords: Nanoparticles; Ag-doped ZnO; Solvo-thermal method. Anti-bacterial activity.

BAND GAP ENERGIES AND OPTICAL PROPERTIES IN NANOSTRUCTURED SEMICONDUCTOR INAS: THE EFFECT OF QUANTUM CONFINEMENT

Fadila MEZRAG^{1,2*}, Nadir BOUARISSA^{1,2}

¹Laboratory of Materials Physics and Its Applications, University of M'sila, 28000 M'sila, Algeria

²Physics Department, Faculty of Science, University of M'sila, 28000 M'sila, Algeria

*Corresponding author: Tel. +213664209226; E-mail address: fadila.mezrag@univ-msila.dz

Abstract: In the zinc-blende phase, the impact of quantum confinement on the band gap energies and refractive index of spherical semiconductor nanostructured InAs has been examined. Utilizing a pseudopotential approach, this study emphasizes the connection between the electronic and optical properties and the size of quantum dots. The results indicate that quantum confinement results in a significantly larger fundamental energy gap, whereas the refractive index decreases notably. This study underscores the influence of quantum confinement on the electronic properties of semiconductor quantum dots and their potential for various technological applications.

Keywords: Band gap energy; Optical properties; InAs semiconductors; Quantum dots.

SPRAY PYROLYSIS DEPOSITION OF ALUMINUM-DOPED ZINC OXIDE (AZO) THIN FILMS FOR ENERGY APPLICATIONS

Hanane CHENAGUE^{1*}, Samir HAMRIT¹, Abdelhafid MAHROUG¹ and Sara SADEDDINE¹

¹ *Laboratory of Materials Physics and Its Applications, Physic Department, Faculty of science, Mohamed Boudiaf university, M'sila, Algeria*

*Tel: +213-696-303-565; Email address: *hanane.chenague@univ-msila.dz*

Abstract: Recently, aluminium-doped zinc oxide (AZO) thin films have gained significant attention as promising transparent conductive oxide (TCO) materials for applications in solar cells, light-emitting diodes (LEDs), sensors, and photo-catalysis. This interest is due to their excellent optical transparency, high electrical conductivity, and lower cost compared to traditional indium-based TCOs. This study investigated how varying aluminium doping concentrations affects the physical properties of zinc oxide thin films. All AZO thin films were successfully deposited on glass substrates at a temperature of 475 ± 5 °C using spray pyrolysis technique. At optimal doping levels (~2-3 at% Al), AZO demonstrates an impressive combination of low resistivity (around $10^{-2} \Omega \cdot \text{cm}$) and high transmittance in the visible range ($\approx 90\%$). These characteristics make AZO ideal for use as transparent electrodes in solar cells, organic LEDs (OLEDs), and touch panels. The tunable band gap of AZO and its plasmonic behaviour in heavily doped forms open up new possibilities for applications in near-infrared optoelectronics and smart windows. Additionally, X-ray diffraction (XRD) results confirmed a wurtzite structure with a distinct orientation primarily along the (002) direction, while scanning electron microscopy (SEM) indicated that all samples were continuous and homogeneous over large areas.

Keywords: AZO thin films; Spray pyrolysis; Transparent electrodes; Opto-electronics.

REMOVAL OF METHYL ORANGE DYES FROM WATER UTILIZING LAYERED DOUBLE HYDROXIDE (NiFeCO₃)

Souad TALHI¹ and Achour DAKHOUCHE¹.

Inorganic Materials Laboratory, Chemistry Department, Faculty of Science, Mohammed Boudiaf University - Msila, Algeria.

souad.talhi@univ-msila.dz

Abstract: Water has faced significant threats over the past few decades due to rapid development. To meet the growing demand for products, industrial and agricultural activities have accelerated, resulting in the introduction of numerous pollutants into water sources. This situation can lead to the contamination of water with various chemicals, including dyes, pharmaceuticals, metals, fertilizers, refining materials, and pathogenic bacteria. Among these, dyes are particularly prevalent, as various colored materials are widely used as pigments in the textile, food, and pharmaceutical industries. In recent decades, a class of anionic clays known as layered double hydroxides (LDHs) or hydrotalcite-like compounds (HTlc) has garnered significant interest from both industry and academia. Although LDHs occur naturally as minerals, they can also be synthesized relatively easily and cost-effectively. The structure of LDHs consists of positively charged brucite-like sheets, with the positive charges balanced by the intercalation of anions in the hydrated interlayer regions. LDHs exhibit relatively weak interlayer bonding, resulting in an exceptional capacity to capture both organic and inorganic anions. LDHs have been studied for their potential applications in a wide range of important fields, including catalysis, magnetization, polymerization, electrochemistry, polymerization, photochemistry, and environmental applications. In this study, a NiFeCO₃ layered double hydroxide was synthesized via co-precipitation and characterized for its application as a photocatalyst in the removal of persistent organic compounds from water. All the results indicate that NiFeCO₃ layered double hydroxides (LDHs) are among the most widely used adsorbents for treating hazardous and toxic pollutants in aqueous solutions. Their structural properties, appropriate interlayer spacing, exceptional ion exchange capacity, and high removal efficiency contribute to this status. In the past decade, the use of LDHs for the effective adsorption of various environmental pollutants, including dyes, heavy metals, and pharmaceutical compounds, has garnered increasing attention.

Keywords: Hydrotalcite, Layered double hydroxides (LDHs), photocatalytic, dyes, adsorption.

EFFICIENT METHYLENE BLUE ADSORPTION: EXPERIMENTAL & DFT ANALYSIS OF H₃PO₄-ACTIVATED DATE PALM CARBON

TIAIBA Wafa^{1*}, Abdelbaki ²

¹ Department of Chemistry, Faculty of Science, Univer-sity of Mohamed Boudiaf, M'sila 28000, Algeria.

*Corresponding author: Tel./Fax: +213669551456 ; E-mail address: wafa.tiaiba@uviv-msila.dz

Abstract: This study addresses the challenge of treating industrial wastewater containing complex, hazardous chemical compositions by developing a sustainable method using cost-effective activated carbon (AC) derived from date palm fibers. Chemical activation with phosphoric acid (H₃PO₄) at a 150% impregnation ratio yielded the optimal adsorbent (AC150) for methylene blue (MB) removal. Characterization via SEM, FTIR, and BET analysis revealed a high specific surface area of 771.115 m²·g⁻¹. Experimental data demonstrated exceptional MB adsorption capacity (772.857 mg·g⁻¹), following the Langmuir isotherm model. Theoretical DFT studies strongly supported experimental results, confirming the adsorption mechanism is driven by HOMO-LUMO interactions at nitrogen, sulfur, and phenyl sites, with a high binding energy of 34.36 kJ·mol⁻¹. This work establishes H₃PO₄-activated date palm carbon as an efficient adsorbent for organic pollutant removal in wastewater treatment.

Keywords: Date Palm fiber. Activated carbon. Characterization. MB dye elimination. Optimization

OPTIMISATION DES MEMBRANES PROTONIQUES A BASE DE PVA SULFONE : EFFET DES AGENTS DE RETICULATION SUR LES PROPRIETES ELECTROCHIMIQUES ET THERMOMECHANIQUES

Abdelhakim KHENICHE ¹*, Samiya RIZOUG ², and Amira TALLAI ²

¹*Department of Chemistry, Laboratory of Organo-Therapeutic Substances and Sustainable Processes, Faculty of Science, University of Mohamed Boudiaf-Msila, Algeria*

²*Department of Chemistry, Faculty of Science, University of Mohamed Boudiaf -Msila, Algeria*

*Corresponding author: Tel./Fax: (+213) 671 70 85 71

abdelhakim.kheniche@univ-msila.dz

Abstract : Ce travail vise à améliorer les performances des membrane échangeuse de protons (PEMFC), en se basant sur l'amélioration des propriétés électriques et la stabilité thermomécanique. Des séries des membranes poreuses de PVA ont été élaborées par sulfonation à l'aide de l'acide 5-sulfosalicylique (SSCA) et réticulées avec l'acide glutamique (AG) et l'acide α -cétoglutarique (Keto) afin d'optimiser leurs performances. Les spectres FTIR-ATR ont confirmé le processus de sulfonation et de réticulation, révélant la présence de groupes ester (O–C–O) et sulfonique (O–S=O). L'hydrophilicité du PVA pur s'est traduite par un taux de gonflement élevé (450 %), tandis que la membrane PVA/SSCA/AG a présenté le taux de gonflement le plus faible (39,02 %), associé à une meilleure intégrité structurale. Les essais mécaniques ont montré que la sulfonation augmente la flexibilité, tandis que la résistance à la traction diminue ; un compromis optimal entre flexibilité et résistance a été obtenu avec la réticulation à l'AG. Les mesures thermogravimétriques ont révélé une stabilité thermique considérable, la membrane PVA/Keto ne commençant à se dégrader qu'au-delà de 500 °C. Les tests électrochimiques ont indiqué que les membranes non réticulées présentaient la capacité d'échange ionique la plus élevée (0,89 meq/g) et la meilleure conductivité protonique ($4,7 \times 10^{-3}$ S/cm) pour PVA/SSCA, attribuées à la présence de groupes sulfonique libres. En revanche, les membranes réticulées ont vu leur conductivité diminuer à ($2,3 \times 10^{-3}$ S/cm) pour PVA/Keto et $1,74 \times 10^{-3}$ S/cm pour PVA/AG, tout en bénéficiant d'une meilleure stabilité structurale. En conclusion, la membrane PVA/SSCA/AG présente des performances équilibrées, alliant bonne conductivité, faible gonflement et stabilité mécanique.

Keywords: Membranes protoniques, PVA, Sulfonation, stabilité thermique, conductivité.

A THEORETICAL FRAMEWORK FOR MODELING THE NONLOCAL MECHANICAL BEHAVIOR OF PROTEIN NETWORKS IN BIOMOLECULAR RESONANT SENSORS: INTEGRATING HYDROGEN BONDING AND VAN DER WAALS INTERACTIONS

DJELLALI Brahim Said¹, BOUROUINA Hicham¹, KHOUNI Soumia¹, LAMARI Abir¹, MAIZA Yahia¹, MEKTOUT Mohamed¹, ELAIHAR Lamine¹

¹ *Laboratory of Physics of Materials and its Applications*

¹ *Department of Physical Sciences Higher Normal School of Bou-Saada, Bou-Saada, 28200 M'sila, Algeria*

* *Corresponding author: djellali.brahimsaid@ens-bousaada.dz*

Abstract: This study investigates the modulation of resonant frequencies in nanoscale resonator systems induced by molecular adsorption, with a particular focus on the effects of shear deformation, spatially non-uniform adatom distribution, and atomic-scale interactions, all within the framework of nonlocal elasticity theory. The adsorption phenomenon is modeled as a spatially distributed energy exchange between the microbeam biosensor and the spike protein, providing a rigorous framework for quantifying biologically induced mechanical perturbations. The dynamic response of the system is formulated using a dual-level approach that integrates functional microbeam mechanics with a localized representation of biomolecular adsorption. Intermolecular van der Waals interactions are incorporated through the Lennard-Jones (6–12) potential, ensuring a physically accurate modeling of adsorption dynamics. The moment of inertia and shear forces are computed within the nonlocal Timoshenko beam theory, with residual stresses modeled as internal axial loads. Numerical simulations demonstrate that the observed shifts in resonant frequency are highly sensitive to the mechanical characteristics of the adsorbed species, surface interaction parameters, and the biosensor-protein configuration. These results highlight the critical influence of nanoscale binding interactions in enhancing the mechanical compliance of the biosensor, thereby modulating its vibrational characteristics. The proposed model not only encapsulates the essential physics of biomolecular interactions but also offers a predictive framework for detecting variations in mass and density associated with spike proteins and viral particles, explicitly accounting for the nature of molecular bonding at the interface.

Keywords: Nonlocal behavior, van der waals interaction, resonance frequency, adsorbed adatoms, statistical distribution, interatomic potential.

ELECTRON-PHONON COUPLING AND SUPERCONDUCTIVITY IN YC₂ VIA FIRST PRINCIPLE CALCULATION

Souad DILMI^{1*}, Salima SAIB² and Nadir BOUARISSA³

¹*Department physique, Université of M'sila, Algérie*

**Corresponding author: Tel./Fax: +213698471219*

E-mail address: souad.dilmi@univ-msila.dz

Abstract: In this work, we have studied the Structural, electronic and superconducting properties of the intermetallic compound YC₂. All calculations were performed by the first-principles calculations using the plane wave pseudo potential (PP-PW) based on the density functional theory DFT and PDFT implemented in the QUANTUM ESPRESSO code, For the exchange correlation function we used the generalized gradient approximation GGA of Perdew–Burke–Ernzerhof (PBE). Our results are in agreement with the available experimental and theoretical data .The obtained low value of electron phonon coupling parameter confirmed that YC₂ is a weak coupling Bardeen-Copper-Schrieffer (BCS) superconductor.

Keywords: PP-PW ; DFT ; QUANTUM ESPRESSO; electron-phonon coupling ; coupling Bardeen-Copper-Schrieffer (BCS)

جسيمات اكسيد النحاس (CuO) وتفككها الضوئي للملوثات بالاستعمال التقنيات الحديثة

جريوي عمار, مسقم احلام, جريوي بشرى

قسم الكيمياء، مخبر الكيمياء المواد، كلية العلوم، جامعة محمد بوضياف بالمسيلة
قسم الكيمياء، كلية العلوم، جامعة محمد بوضياف، مسيلة الجزائر

هاتف / فاكس: +213 (0660915551)

البريد الإلكتروني

ammardjerioui@univ.msila.dz

المخلص: يركز هذا البحث على التخليق الأخضر لجسيمات أكسيد النحاس النانوية (CuO) باستخدام المستخلص المائي لنبات *Salvia barrelieri*، وهو نبات طبي موطنه شمال إفريقيا. عمل مستخلص *Salvia barrelieri* كمادة مختزلة ومثبتة طبيعية، مما أتاح الاستغناء عن المواد الكيميائية السامة المستخدمة عادة في عملية التخليق. أكد حيود الأشعة السينية (XRD) والتحليل الطيفي بالأشعة تحت الحمراء بتحويل فورييه (FTIR) البنية البلورية وأظهر المجموعات الوظيفية الهامة للجسيمات النانوية المشتقة من نواتج الأيض النباتية. تم تقييم النشاط التحفيزي الضوئي لنظام CuO-ZnO من خلال دراسة تحلل صبغة الرودامين B تحت ضوء الشمس الطبيعي وضوء LED. وأجريت دراسة منهجية لتركيز الصبغة، وجرعة الحفاز، ونسبة إضافة ZnO. تم تحقيق أعلى نسبة تحلل عند استخدام 25 ملغ من CuO و5% من ZnO، حيث أظهر هذا المزيج تأثيراً تآزرياً عزز من عملية التحلل الضوئي. *barrelieri* يمكن اعتباره بديلاً محلياً وصديقاً للبيئة للطرق التقليدية المعقدة في تكنولوجيا النانو البيئية ومعالجة مياه الصرف.

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

INVESTIGATION INTO THE PHOTOCATALYTIC DEGRADATION OF RED CONGO DYE USING SEMI-CONDUCTOR

Somia SALMI^{1*}, achour DAKHOUCHE²

¹ *Department of Chemistry, University of Mohamed Boudiaf-M'Sila, Algeria.*

² *Department of Chemistry, University of Mohamed Boudiaf-M'Sila, Algeria.*

somia.salmil@univ-msila.dz.

Abstract: Organic dyes have become a major source of environmental contamination, such as surface and groundwater contamination. Due to their persistent character (chemical stability), they are difficult to degrade. which is why several processes, including absorption, chemical oxidation, ion exchange, reverse osmosis, precipitation, biological treatments, and photocatalysis, have been developed to treat water contaminated with organic dyes. Among these, semiconductor-based photocatalysis is the most important method for degrading organic dyes in wastewater. Therefore, this study will focus on the manufacturing of titanium dioxide and its application in the photodegradation of organic pollutants. Initially, titanium dioxide with a nanotubular morphology was developed through electrochemical anodization of a metallic titanium plate and characterized by different methods DRX ,MEB .In the second part, we applied our semiconductor for the photodegradation of Red congo, considering the variations in the various factors that influence the photoactivity of TiO₂.

Keywords: Titanium dioxide, photodegradation, electrochemical anodization, wastewater.

SUSTAINABLE VALORIZATION OF WASTEWATER SLUDGE: RESOURCE RECOVERY FOR ENERGY AND SOIL APPLICATIONS

Achwaq HERIZI^{1,3*}, Chouki FARSI², Azzedine BENYAHIA^{3,1}, Lamy MEFTAH¹ and Abdel Hamid GUELIL⁴

¹*Department of Chemistry, Faculty of Science, Mohamed Boudiaf University, M'sila, Algeria.*

²*Department of Mechanical Engineering, Faculty of Technology, Mohamed Boudiaf University, M'sila, Algeria.*

³*Laboratory of City, Environment, Hydraulics and Sustainable Development, Mohamed Boudiaf University, M'sila, Algeria.*

⁴*Department of Material Science, Mohamed Khider University, Biskra, Algeria.*

E-mail address: Achwaq.herizi@univ-msila.dz

Abstract: The increasing environmental pressures linked to the expansion of wastewater treatment infrastructure in Algeria have intensified the need for effective and sustainable management of residual urban sludge. This study aims to evaluate the valorization potential of sludge produced by the Sidi Aïssa wastewater treatment plant, focusing on its possible recovery as a renewable resource. A comprehensive physico-chemical and mineralogical characterization of sludge samples was performed following standard analytical protocols reported in the literature, enabling a detailed understanding of their composition, mineral phases, and properties. The analysis revealed a high content of organic matter and nutrient-rich components, supporting two valorization pathways: its application as an agricultural soil amendment and its conversion into biogas for renewable energy generation. These results were assessed in terms of their environmental, economic, and operational relevance, highlighting the potential of integrating sludge valorization into sustainable waste management strategies. The findings underline not only the feasibility of reducing environmental burdens associated with sludge disposal but also the opportunity to recover valuable resources, contributing to circular economy models and local energy autonomy. This work provides a practical contribution to the ongoing efforts in resource recovery and environmental protection, with perspectives for further application in similar urban contexts and potential industrial partnerships in the field of renewable energy and natural resource valorization.

Keywords: Urban sludge; valorization; renewable energy; biogas; resource recovery.

PHYSICOCHEMICAL CHARACTERIZATION OF A NATURAL FIBER EXTRACTED FROM KOCHIA INDICA

Djamila KOUIDRI ^{1,*}, Mansour ROKBI ¹, Zineelabidine RAHMOUNI ², Younes KHERBICHE ¹ and Samira BOUCHAREB ^{1,3}

¹ *Department of mechanical Engineering, Faculty of technology, University of M'sila, M'sila, Algeria.*

² *Department of Civil Engineering, Faculty of technology, University of M'sila, M'sila, Algeria.*

³ *Laboratoire de Matériaux et Mécanique des Structures (LMMS). Université de M'sila. Algeria.*

**Corresponding author: Tel. +213668023345; E-mail address: djamila.kouidri@univ-msila.dz*

Abstract: In this study, innovative cellulose fibers were successfully extracted from the kochia Indica (*Bassia indica*) plant with the aim of using them as potential reinforcement in composite materials. The morphological structure of the fibers was examined through Scanning Electron Microscopy (SEM), which provided detailed surface observations. The structural properties, including crystallinity and functional groups, were analyzed using X-ray Diffraction (XRD). Thermogravimetric Analysis (TGA) was conducted to evaluate the thermal stability of the fibers. Anatomical analysis confirmed the significant presence of fibroblasts within the fiber structure. Furthermore, ATR-FTIR analysis verified the lignocellulosic composition of the fibers, highlighting the presence of lignin, cellulose, and hemicellulose. Physical characterization revealed that the fibers exhibited a density of 1.065 ± 0.025 g/cm³ and an average diameter of 145.58 ± 7.89 μm. The crystallite size was measured at 2.23 nm, while the crystallinity index reached 40.12%. The activation energy required for the degradation process was determined to be 32.74 kJ/mol. The thermal analysis indicated that the fibers maintain stability up to 260.24 °C, with the maximum degradation occurring at approximately 321.23 °C. The obtained results were compared to existing literature to validate their relevance. Overall, *Bassia Indica* fibers demonstrate promising characteristics and can be considered a suitable candidate for reinforcing lightweight bio-composites in sustainable material applications.

Keywords: *Bassia Indica*; Natural Cellulose Fiber; Morphological Characterization; Thermal Stability; Bio-composites.

BIOPROCESSING AND STRUCTURAL VALORIZATION OF NATURAL LIGNOCELLULOSIC FIBERS FOR SUSTAINABLE MATERIAL DEVELOPMENT

Samira BOUCHAREB ^{1*}, Mansour ROKBI ² and Mohamed BENHAMIDA ³

¹ Department of mechanical engineering, university Mohamed Boudiaf of M'sila (28000), Algeria

² Department of mechanical engineering, university Mohamed Boudiaf of M'sila (28000), Algeria

³ Department of physic, university Mohamed Boudiaf of M'sila (28000), ALGERIA

samira.bouchareb@univ-msila.dz

Abstract

the valorization of natural lignocellulosic fibers. Among the most promising approaches, enzymatic bioprocessing stands out as a green, selective, and efficient method to enhance fiber properties without relying on harsh chemical treatments. This study explores the application of specific enzymes, including cellulases, hemicellulose, pectinases, and lignin-degrading oxidoreductases, in the treatment of plant-based fibers. The enzymatic action leads to the partial removal of non-cellulosic components, surface cleaning, and improved fiber separation, thereby enhancing fiber-matrix adhesion and mechanical performance in composite applications. The impact of enzymatic processing on the biochemical composition, morphology (as observed via SEM), and thermal behavior (TGA) of the treated fibers was assessed. Results indicate that enzymatic treatments significantly increase fiber crystallinity and surface roughness, while preserving structural integrity, making them suitable for sustainable bio-based material development. The study also discusses how fiber response varies with environmental factors and source location, underlining the importance of adapting bioprocessing strategies to the intrinsic variability of natural resources.

Keywords: Enzymatic treatment, lignocellulosic fibers, fiber valorization, green bioprocessing, sustainable materials

ANALYSE DE LA COMPOSITION CHIMIQUE DU QUINOA ET PERSPECTIVES DE VALORISATION POUR L'ALIMENTATION HUMAINE

Boubakr HADJ KOUIDER^{1*}, Bahia LALLOUCHE¹, ACHOUCHE Maroua¹ and HADJ
HAFSI Soumia¹

¹Department of Agricultural Sciences, Faculty of Sciences, Mohamed Boudiaf University, Laboratory of Biodiversity and Biotechnological Techniques of Plant Resource Development, Algeria

*Corresponding author: Tel./Fax: +213-556-259-9497 ; E-mail address: boubakr.hadjkouider@univ-msila.dz

Résumé : Le quinoa, considéré comme une pseudo-céréale, appartient à la famille des Chenopodiaceae, originaire, des Andes, suscite un intérêt croissant en tant qu'aliment fonctionnel. Grâce à sa richesse en protéines complètes, en acides aminés essentiels et en micronutriments, et surtout à son absence naturelle de gluten, il représente une alternative nutritionnelle précieuse pour les personnes atteintes de la maladie cœliaque. Intégré dans des produits comme les barres nutritionnelles ou sous forme de compléments alimentaires, le quinoa peut répondre aux besoins spécifiques de cette population vulnérable (Bazile et al., 2015 ; Chenine et Sahli, 2020). Le quinoa, riche en protéines de haute qualité représentant environ 17 % de sa composition, contient principalement des globulines 11S et des albumines 2S. Sa digestibilité et ses propriétés fonctionnelles peuvent être optimisées par des méthodes de modification, élargissant ainsi son utilisation dans les produits végétaux (Cui et al., 2023). Cette étude s'inscrit dans l'objectif de la valorisation du quinoa dans l'alimentation humaine nous avons procédé à l'analyse de sa composition chimique. Les résultats obtenus montrent que le quinoa est riche en Potassium (0,32 %), Fer (0,29 %), Phosphore (0,20 %), Magnésium (0,10 %), Soufre (0,12 %) et le Zinc avec un pourcentage 0,00296 %. Par contre, aucune trace de Gluten n'a été détectée dans la farine des échantillons analysés.

Mots clés: Quinoa; composition chimique; proteïns; alimentation humaine.

EVALUATION DE LA VALEUR NUTRITIONNELLE ET DE LA COMPOSITION CHIMIQUE DE PLANTS DE BLE DESTINE A LA FABRICATION DE CHLOROPHYLLE ALIMENTAIRE

Bahia LALLOUCHE^{1*}, Boubakr HADJ KOUIDER¹, Ines F. Zohra BENAÏSSA¹ and RAHMOUNI Ritadj¹

¹*Department of Agricultural Sciences, Faculty of Sciences, Mohamed Boudiaf University, Laboratory of Biodiversity and Biotechnological Techniques of Plant Resource Development, Algeria.*

*Corresponding author: Tel./Fax: +000-000-000-000 ; E-mail address: bahia.lallouche@univ-msila.dz

Résumé : La chlorophylle est un pigment naturel essentiel dans le processus de photosynthèse, et elle a suscité un intérêt croissant en tant que complément alimentaire grâce à ses propriétés antioxydants, purifiantes et stimulantes. Avec cette demande croissante, la culture de plantes riches en chlorophylle est devenue un domaine prometteur, notamment dans le cadre de la nutrition saine [1]. Dans ce contexte, ce travail se concentre sur la production de plants de Blé et la valorisation de leurs composés bioactifs, tels que la chlorophylle, dans le domaine des compléments. Il aborde également les conditions agricoles optimales, les techniques de culture, et les méthodes d'extraction et de valorisation de la chlorophylle à des fins alimentaires. Cette étude vise également à évaluer le potentiel de ces cultures en tant que ressource locale et durable pour le développement d'un complément alimentaire naturel à haute valeur ajoutée. Les résultats ont révélé que le blé présente des teneurs globalement plus élevées en chlorophylle a (29,851 µg/g MF), b (45.395 µg/g MF) et totale (75.24 µg/g MF), ce qui en fait une source privilégiée pour l'extraction de chlorophylle à usage nutritionnel. Cette richesse en pigments photosynthétiques est accompagnée d'une forte concentration en minéraux essentiels, notamment le Potassium (1,26 %), le Phosphore (0,31 %), le calcium (1,26 %), le Sodium (0,25 %), le Manganèse (0.00251%) et le soufre (0,22 %), ainsi que des traces de nickel, de ruthénium et de rubidium. Ces éléments renforcent la valeur biologique et fonctionnelle des feuilles de blé dans un contexte de complémentation alimentaire.

Mots clés: Chlorophylle; Blé; valeur nutritionnelle; composition chimique.

THE EFFECT OF NITRATE IONS ON THE ELECTROCHEMICAL BEHAVIOR OF BRASS

Samia YOUSFI^{1*}, Khadija BERARMA² and Cheikh MOKRANI³

¹Department of Chemistry, Laboratory of inorganic materials, University of Msila-Mohamed Boudiaf, 28000 M'sila, Algeria

* Tel. /Fax: +0213-07-70-88-46-44; E-mail address: samia.yousfi@univ-msila.dz

Laboratoire des matériaux inorganiques /Département de Chimie, Faculté des Sciences, Université de Msila-Mohamed Boudiaf-28000 M'Sila, Algeria

Abstract: Brasses are copper alloys whose main addition element is zinc (5 to 45%). Currently they have taken a predominant place in our daily lives, and they are in widespread use in many industries, such as pipes, valves, and faucets thanks to their excellent physico-chemical, mechanical and thermal properties. Copper alloys (brass) are eminently suited in systems that transport water due to their corrosion resistance, high thermal and electric conductivity, excellent workability, as well as exceptional anti-bacterial properties. However, these alloys are subject to corrosion problems, an electrochemical process, in which corrosion species present in the surrounding environment, as well as engines corrosion engines consume the substrate through oxidation. The chemical composition of water, including the presence of anions such as nitrates (NO_3^-), can affect their durability. Even in traces amounts, they can produce enormous damage to installations and brass parts. We focused our attention on the study of the effect of nitrate ions on the electrochemical behaviour of brass. Several electrochemical techniques (cyclic voltammetry and impedance spectroscopy) were used for the characterization of the working electrode which allowed us to conclude that: The abandoned potential (E_{ab}), for brass, shifts from the beginning of immersion towards positive values to stabilize after 2 hours of immersion around a value close to that of copper; The concentration of 50 mM (nitrate ions) has the maximum effect on the electrochemical behaviour of the electrodes; Electrochemical impedance spectroscopy analysis shows that the reaction processes are very complicated involving processes of metal dissolution and formation of precipitates on the surface of the metal substrate

Keywords: Brass, corrosion, polarization curve, impedance spectroscopy

ELABORATION ET CARACTERISATION D'UN MATERIAU COMPOSITE A BASE DE CAOUTCHOUC NATUREL RENFORCEE PAR DES FIBRES DE VERRES, FIBRES VEGETALES ET HYBRIDES

Warda ATTOUI, Elhadi DEBIH, azzedine MELOUKI, Azzedine BENYAHIA

Chemistry Department, Sciences Faculty M'sila University, laboratory, City, inorganic materials 28000, M'sila Tel:0778222659, Email: warda.attoui@univ-msila.

Abstract les composites à matrice élastomère renforcés par des fibres de verre et des fibres végétales représentent une classe émergente de matériaux hybrides, combinant des performances mécaniques et thermiques satisfaisantes à une empreinte environnementale réduite. L'intégration de fibres naturelles biodégradables dans une matrice polymère, souvent à base de caoutchouc, permet d'améliorer la légèreté, la flexibilité et la durabilité des composites, tout en réduisant les coûts de production et l'impact écologique. Le renforcement par des fibres de verre confère au matériau une rigidité et une résistance accrues, tandis que les fibres végétales (telles que le lin, le jute ou le sisal) apportent un caractère renouvelable et durable au système composite. Le choix des fibres, leur nature, leur orientation ainsi que leur compatibilité avec la matrice jouent un rôle déterminant dans les propriétés finales du matériau. Ces composites trouvent de nombreuses applications dans des secteurs variés tels que l'automobile, l'aéronautique, la construction et l'industrie du pneumatique, où la recherche de matériaux alliant performance et responsabilité environnementale devient prioritaire. Ainsi, le développement de ces matériaux multifonctionnels s'inscrit pleinement dans une démarche d'innovation durable, répondant aux exigences croissantes de l'industrie en matière de performances techniques, de légèreté et de respect de l'environnement.

Keywords: Composite, luffa, Adhesion, Tensile strength, Alkaline treatment

**COMPARATIVE GC/MS ANALYSIS OF ESSENTIAL OIL PROFILES IN
ORIGANUM GLANDULOSUM DESF. FROM ALGERIA AND TUNISIA**

Aldjia HADROUG^{1*}, Rachid BELHATTAB² and Khellaf REBBAS³

¹ Department of Chemistry, University pole, Bordj Bou Arreridj road, M'Sila 28000 Algeria

² Laboratory of Applied Microbiology, Ferhat Abbas Setif I University, Setif 19000, Algeria

³ Department of Life and Natural Sciences, University pole, Bordj Bou Arreridj road, M'Sila 28000
Algeria

*Corresponding author: Tel.: 0660-34-3599 ; E-mail address: aldjia.hadrougue@univ-msila.dz

Abstract: The essential oils (EOs) of *Origanum glandulosum* Desf., an endemic subspecies of Algeria, were analyzed to determine their chemical composition using Gas Chromatography-Mass Spectrometry (GC-MS). A total of 82 constituents were identified, accounting for 84% of the EO content. The profile was primarily dominated by monoterpenes (59.9%), followed by sesquiterpenes (15.5%) and other compounds (7.8%). Thymol (32.77%) was the predominant compound, with other notable components including anisole (4.27%), p-cymene (3.83%), β -linalool (3.6%), and β -pinene (3.23%), positioning the oil as a thymol-dominant chemotype. These findings are consistent with previous studies on similar Algerian species. The sesquiterpene profile was particularly characterized by β -sesquiphellandrene (4.78%) and caryophyllene (2.48%). A comparative analysis with data from *Origanum glandulosum* specimens collected in Tunisia and other Algerian regions revealed regional variations in EO composition, with certain compounds showing varying levels of dominance across different geographical areas. This research provides a comprehensive understanding of the chemical diversity of *Origanum glandulosum* in North Africa, offering insights with potential applications in fields such as green chemistry and natural product development. These findings also open avenues for further exploration of EO variability and its implications for industrial contexts.

Keywords: *Origanum glandulosum*, essential oils, GC-MS, thymol, regional variation.

CLIMATIC IMPACT ON THE PERFORMANCE OF A PARABOLIC TROUGH SOLAR POWER PLANT: CASE OF THE SEMI-ARID NORTHERN REGION OF ALGERIA AND SOUTHERN SPAIN

Khaled BOUCHAREB^{1,2,*}, Khellaf BELKHIRI^{1,2} and Nabila IHADDADENE¹

¹Department of Mechanical Engineering, Med Boudiaf University, BP 166, M'sila 28000, Algeria.

²Laboratory of Materials and Mechanics of Structure L.M.M.S, University of M'sila, M'sila 28000, Algeria.

*Corresponding author: Tel: 0661-83-96-22 ; E-mail address: khaled.bouchareb@univ-msila.dz

Abstract: Among the various sustainable electricity generation technologies, concentrated solar power stands out as one of the most efficient and practical solutions for generating electricity in an environmentally sustainable manner. In this study, we assessed the feasibility of constructing a concentrated solar power plant using parabolic trough collector technology similar to the Andasol-1 power plant located in southern Spain in the M'Sila region of northern Algeria. The aim was to determine the climatic impact of the northern semi-arid region of Algeria on the performance of this power plant compared to its original location. The analysis was conducted using the System Advisor Model software. The reference plant has a capacity of 50 MW and is equipped with a thermal energy storage system. The results indicate that when the Andasol-1 power plant is hypothetically installed in M'Sila, it is capable of generating electricity continuously throughout the year from 11:00 a.m. to 7:00 p.m., with an average power output ranging between 15 MW and 50 MW. Simulation outcomes demonstrate that the M'Sila site offers superior performance compared to southern Spain. If the Andasol-1 plant were relocated from its current location in southern Spain to M'Sila in northern Algeria, its annual electricity production would increase by approximately 14%. The study demonstrated that the semi-arid climatic conditions and strong solar energy potential of the M'Sila region are suitable for the deployment of such power plants. These projects ease the load on conventional thermal power plants during peak periods and contribute to reliable, long-term clean energy generation.

Keywords: Concentrated solar power plants, Parabolic trough collector, Thermal energy storage system, System Advisor Model (SAM).

SYNTHESIS AND ANTIOXIDANT EVALUATION OF NITROVANILLIN DERIVATIVES

Yousra MIHOUNE ¹, Souad DJELLALI ², Nouara ZIANI ³, Yasmin ABDELOUAHED ⁴

¹ Department of Chemistry, Faculty of Sciences, University Ferhat Abbas Setif 1, 19000, Setif, Algeria

² Laboratory of Physical Chemistry of High Polymers, University Ferhat Abbas Setif 1, 19000, Setif, Algeria

Corresponding-author email: youssramihoune@gmail.com.

Abstract: Vanillin is a well-known aromatic compound primarily used as a flavoring agent, but it also possesses remarkable antimicrobial and preservative properties. Numerous derivatives of vanillin have shown diverse biological activities, including anticancer, antioxidant, antibacterial, antitubercular, antimalarial, antiviral, anti-inflammatory, anti-Alzheimer, and anti-diabetic effects, confirming their pharmacological significance. In the present work, nitrovanillin was synthesized through the nitration of vanillin using nitric acid as a source of nitro groups and dichloromethane (DCM) as the solvent, under low-temperature conditions (below 5°C), resulting in a good yield. The obtained compound was characterized using UV-Vis and FTIR spectroscopy, thin-layer chromatography (TLC), and melting point determination, confirming the successful introduction of the nitro group. The UV-Vis spectrum of nitrovanillin exhibited characteristic absorption peaks at 217, 252, and 275 nm, corresponding to $n \rightarrow \sigma^*$ transitions, while FTIR analysis revealed a strong band near 1552 cm^{-1} , attributed to the N–O stretching vibration. The antioxidant activity of the compound was evaluated at an initial concentration of 800 mg/mL using several assays, including DPPH, ABTS, FRAP, phenanthroline, and silver nanoparticles (SNP) methods. The results demonstrated that vanillin showed moderate antioxidant capacity, while nitrovanillin exhibited enhanced activity, particularly in the phenanthroline and SNP tests. These findings highlight the potential of nitrovanillin as a promising antioxidant agent, emphasizing the importance of structural modification in improving the biological and functional properties of natural compounds such as vanillin, with possible applications in food preservation, pharmaceuticals, and materials science.

Keywords : vanillin, nitrovanillin, antioxidant activity

DEVELOPMENT OF ACTIVATED CARBON FROM ALMOND SHELLS: PHYSICO-CHEMICAL CHARACTERIZATION AND APPLICATION IN WASTEWATER TREATMENT

MEFTAH lamya^{1,2}, TERCHI Smail^{1,2}, DEGHFEL Bahri^{1,3}, Achwaq HERIZI², Abdelhamid Guelil⁴

¹ *Laboratory of Materials and Renewable Energies. Mohamed Boudiaf University of M'Sila, Faculty of Sciences, M'Sila, Algeria*

² *Department of Chemistry, Faculty of Sciences, Mohamed Boudiaf University of M'Sila, M'Sila, Algeria*

³ *Department of Physics, Faculty of Science, University of M'Sila, Algeria, Mohamed Boudiaf University of M'Sila, Algeria.*

⁴ *Département de Chimie de la matière, Faculté des Sciences, Université Mohamed khider, Biskra
Lamya.meftah@univ-msila.dz*

Abstract: human well-being worldwide. Among the emerging solutions, adsorption using bio-based adsorbents offers a sustainable and cost-effective approach for removing various contaminants from wastewater. This study explores the valorization of almond shells an underutilized agro-industrial residue by converting them into activated carbon. The physicochemical properties of the produced activated carbon were characterized through point of zero charge (pH_{pzc}) determination and Fourier Transform Infrared Spectroscopy (FTIR). A series of batch adsorption experiments was conducted to assess the influence of operational parameters such as contact time, pH, adsorbent dose, and temperature on adsorption performance and kinetics. Furthermore, the potential integration of nanomaterials is discussed as a means to enhance the adsorption efficiency and expand the functional scope of these bio-adsorbents. Promoting such renewable, low-cost, and accessible materials contributes to the development of innovative strategies in sustainable wastewater treatment.

Keywords: Almond Shells; Activated Carbon; Adsorption; Bio-adsorbents; Wastewater Treatment; Agro-waste; Nanomaterials

DEVELOPPEMENT DE BATTERIES Zn/MnO₂ POUR LE STOCKAGE DES ENERGIES RENOUVELABLES : UNE ALTERNATIVE ECOLOGIQUE BASEE SUR LA VALORISATION DES RESSOURCES MINERALES ABONDANTES

Kenza BELAMRI^{1*}, Laid TELLI¹ and Larbi ZERROUAL¹

¹Department de chimie, University de M'sila, Algeria

*Corresponding author: Tel 0657086312; E-mail address: *kenza.belamri@univ-msila.dz*

Résumé : Face à l'augmentation des défis environnementaux et de la demande en sources d'énergie, le stockage des énergies renouvelables est devenu l'un des axes clés pour réaliser une transition énergétique durable. En ce sens, les batteries zinc/dioxyde de manganèse (Zn/MnO₂) se présentent comme une solution prometteuse et une alternative environnementale aux systèmes traditionnels à base de lithium. Les batteries alcalines au (MnO₂/Zn) sont des systèmes de stockage d'énergie électrique prometteurs en raison de leurs nombreux avantages tels que : leur haute sécurité, l'abondance des matériaux utilisés (Mn ...), un faible coût et leur non-inflammabilité, en plus de la conductivité ionique élevée de leur électrolyte. Cependant, ces batteries souffrent de plusieurs problèmes en milieu alcalin, - parmi lesquels on cite : la faible tension (1.5 V) ce qui sa densité d'énergie et la formation de substances irréversibles au niveau des électrodes entraînant une dégradation significative de la capacité. Afin de contribuer à l'amélioration des caractéristiques de telles batteries, nous avons réalisé une cellule MnO₂/Zn à double électrolyte de pH différent : un catholyte acide (H₂SO₄) et un anolyte alcalin (KOH) séparés par une membrane échangeuse d'ion. Les performances de cette cellule ont été évaluées par : voltampérométrie cyclique et chronopotentiométrie. En effet, la cellule MnO₂/Zn à double électrolyte présente une tension à vide de 2.6 V contre 1.5 V pour une cellule MnO₂/Zn usuelle. Ainsi, l'étude cinétique a montré une meilleure réversibilité des électrodes avec des courants de fonctionnement, en décharge et en charge, trois fois supérieures. Ainsi, les performances de la cellule étudiée sont nettement meilleures que celles d'une cellule classique.

Keywords: Les batteries zinc/dioxyde de manganèse; double électrolyte ;les énergies renouvelables.

ÉTUDE DE LA TENUE A LA CORROSION D'UN ACIER A304 MODIFIE PAR UN MATERIAU COMPOSITE : POLYPYRROLE/TiO₂

Faiza NESSARK^{1,2*}, Mohamed EISSA³ and Ali ALOUACHE⁴

¹Laboratoire d'Electrochimie et Matériaux (LEM), Université Ferhat Abbas Sétif 1, 19000, Algérie

²Département de Chimie, Faculté des Sciences, Université Mohamed Bouafia M'Sila, 28000, Algérie

³Polymers and Pigments Department, National Research Centre, Dokki, Giza 12622, Egypt

⁴Laboratoire N-Corps et Structure de la Matière, Ecole Normale Supérieure Kouba, Alger,
16000, Algérie

*Auteur correspondant : Tél. +213 775092906; E-mail : faiza.nessark@univ-msila.dz

Résumé : La corrosion de l'acier est un défi persistant, notamment dans les environnements difficiles tels que les environnements marins, industriels et pétroliers. Les matériaux composites, en particulier ceux à base de polymères et de nanomatériaux, offrent des solutions innovantes combinant protection barrière, inhibition active et mécanismes d'auto-réparation intelligents. Ce travail consiste en la préparation et en l'analyse des propriétés électrochimiques d'un matériau composite obtenu sur l'acier A304 à partir d'un polypyrrole et de nanoparticules de TiO₂. Le processus d'électrodéposition et la caractérisation du matériau d'électrode obtenu, ont été examinés par voltampérométrie cyclique et par spectroscopie d'impédance. Une disparition totale des pics d'oxydations et de réductions d'aciers dans les milieux corrosifs ont été observés, lors de l'analyse de ces électrodes une fois modifiés par un matériau composite (PPy + TiO₂), obtenus pour différents teneurs en TiO₂, dans une solution de NaCl. Ceci atteste bien qu'une amélioration de la tenue à la corrosion a été obtenue après l'électrodéposition de film de polypyrrole (PPy) et de matériau composite (PPy + TiO₂). En milieu NaCl, les voltampérogrammes montrent lors du balayage négatif un retour inversé, caractérisé par un pic d'oxydation très intense due à la piquration de la couche passive d'oxyde formé sur la surface de l'acier par les ions chlorures lors du balayage de potentiel positif.

Mots-clés : Polypyrrole ; Nanoparticules de TiO₂ ; Acier A304 ; Voltampérométrie Cyclique ; Spectroscopie d'Impédance.

EFFECT OF THERMAL ENVIRONMENTAL FLUCTUATIONS ON THE CORROSION BEHAVIOUR OF LOW-CARBON STEEL ALLOY IN SALINE CONDITIONS

Sarra MERABET^{1,2*}, Laid TELLI¹ and Cheikh MOKRAN²

Chemical Department, faculty of sciences, University of Mohamed Boudiaf, 28000, Algeria.

**Corresponding author: Tel./Fax: +213-657104684 ; E-mail address: sarra.merabet@univ-msila.dz*

Abstract: Corrosion gradually compromises the integrity of metal structures through deterioration caused by exposure to aggressive environmental conditions. Research on corrosion focuses on three main aspects: safety, cost, and preservation. This degradation occurs via electrochemical processes influenced by factors such as oxygen, moisture, and contaminants. Most metals and alloys, particularly iron and steel, corrode spontaneously due to thermodynamic instability in air and water. This study based on the variation of temperature of the 3.5% NaCl solution, we chose to control the corrosion of low-carbon steel alloy. The methods employed in this work were weight-loss (WL), Tafel polarization curves and electrochemical impedance spectroscopy (EIS). The surface morphology of this alloy was investigated using scanning electron microscopy and optical microscopy. The results reveal that the open circuit potential (OCP) shifted negatively with increasing temperature, suggesting the start of corrosion processes. The corrosion potential degenerates more quickly at higher temperatures, which is associated with a faster corrosion rate. The EIS indicated that the corrosion resistance of low-carbon steel alloy decreased at high temperatures. According to the results of polarization curves, the corrosion current density increased in high temperatures. The surface of our material was covered by a huge number of the accumulated corrosion products as the temperature climbed, the roughness of metal increased, and the volume and size of corrosion products dramatically increased. Nyquist and Bode plots show that the corrosion processes of our alloy are complex and depend on the temperature of the corrosive medium. The weight-loss shows a similar tendency.

Keywords: Corrosion, low-carbon steel alloy, EIS, chloride solution, Tafel polarization.

**PHARMACOPHORE GENERATION, 3D QSAR MODEL,
MOLECULAR DOCKING STUDIES AND IN SILICO ADMET
SCREENING OF BENZIMIDAZOLE DERIVATIVES AS HCV NS5B
RNA-DEPENDENT RNA POLYMERASE INHIBITORS**

Samir BOUACHA^{*1}, Malika CHENNA¹

*Faculty of Technology, Department of common base, University Pole, Road Bordj Bou Arreridj,
M'sila, 28000 (Algeria)*

**Corresponding author: Tel: +213775191391 ; E-mail address: samir.bouacha@univ-msila.dz*

Abstract: The current examination has been centered on 3D features and configurations responsible for biological activity of benzimidazole derivatives as HCV- NS5B polymerase inhibitors. The best pharmacophore model generated consisted of six features AHNRRR-1: one acceptor (A), one hydrophobic (H), one negatively ionizable, (N) and three aromatic rings (R). The developed pharmacophore features were used to derive a predictive atom-based 3D QSAR model. The developed models were statistically acceptable (pred $R^2 = 0.85$; $Q_2 = 0.436$). Structure-based docking studies were carried out to investigate the intermolecular interaction between the benzimidazole derivatives and the 2HAI receptor. Active ligands 11, 24 and 22 have the highest activity and the best docking scores. The insilico ADMET screening of these compounds also performed and the values of all the properties are within the recommended values. The information obtained from pharmacophore, 3D QSAR model, molecular docking and ADMET screening can be used for the design of benzimidazole derivatives as potent inhibitors of hepatitis C virus NS5B RNA-dependent RNA polymerase.

Keywords: Pharmacophore, 3D QSAR model, Docking, Benzimidazole derivatives, HCV NS5B polymerase, ADMET properties.

EFFECT OF DEFORMATION AND ANNEALING ON THE MICROSTRUCTURE AND MECHANICAL BEHAVIOR OF A MAGNESIUM ALLOY

Malika MERZOUGUI^{1,2}, Ismail BENCHERIFA³, Hiba AZZEDDINE¹, Denis SOLAS⁴, François BRISSET⁴, Thierry BAUDIN⁴

¹ *Laboratory of Materials and Renewable Energy, Faculty of Sciences, University of M'sila, University Pole, Road Bourdj Bou Arreiridj, M'sila 28000, Algeria.*

² *Department of TCSNV, Faculty of Sciences, University of M'sila, University Pole, Road Bourdj Bou Arreiridj, M'sila 28000, Algeria.*

³ *Department of Mechanical Engineering, University of Biskra, B.P.145, 07000 Biskra, Algeria*

⁴ *Université Paris-Saclay, CNRS, Institut de chimie moléculaire et des matériaux d'Orsay, 91405, Orsay, France.*

merzougui.malika@univ-msila.dz

Abstract: In this study, the effect of hot-rolling and annealing treatment on the microstructure and mechanical properties of the Mg–0.6Gd (wt.%) alloy was explored using Electron backscatter diffraction (EBSD) analysis and Vickers microhardness measurement. The EBSD results revealed that hot-rolling at 450 °C for 20% of thickness reduction led to the fragmentation of initial grains and the creation of a high number of twins. Increasing the thickness reduction to 80% led to the formation of a refined equiaxed microstructure due to the dynamic recrystallization process. Annealing treatment at 450 °C for 1 h causes the disappearance of twins and notable grain growth. Microhardness value increased with increasing thickness reduction due to the production of lattice defects such as dislocations. In contrast, the microhardness decreased after annealing treatment due to static recrystallization and grain growth.

Keywords: Deformation, Magnesium alloys, microstructure, recrystallization dynamics.

PREPARATION AND APPLICATION OF BIOMASS-DERIVED ACTIVATED CARBON FOR WASTEWATER REMEDIATION

Sarra BEKRI ^{*1}, Firouz CHERDOUD ², Brahim ABDELKEBIR ³, Nadjah MAGHRAOUI ¹, Hayette FAID ¹.

¹Department of Environmental Engineering, Mohamed El Bachir El Ibrahimi University, Bordj Bou Arréridj, P.O. Box 34000, Algeria.

²Department of Chemistry, Mohamed Boudiaf University, Pole, Road to Bordj Bou Arréridj, M'sila 28000, Algeria.

³Department of Hydraulic and Civil Engineering, Ghardaïa University, Zone Scientifique, BP 455, Ghardaïa 47000, Algeria

*Corresponding author: E-mail: sarra.bekri@univ-bba.dz

Abstract: The valorization of biomass waste and the purification of aqueous effluents have become major environmental challenges. In this study, eggshells were used as an alternative resource for the production of activated carbon through thermal activation, with the aim of applying it to wastewater treatment. The resulting material exhibited remarkable textural and chemical properties: an iodine number of 262.6 mg/g indicating moderate microporosity, and a high methylene blue index (732.7 mg/g) revealing well-developed mesoporosity suitable for the adsorption of large organic molecules such as dyes and surfactants. Boehm titration revealed a balanced distribution of acidic (6.67 mmol/g) and basic (6.00 mmol/g) surface groups, enhancing the functional diversity of the surface. Moreover, the pH_{pzc} value of 10.2 confirmed the ability of the activated carbon to interact effectively with anionic or cationic species depending on the solution pH. Application tests on industrial effluents demonstrated a significant reduction in organic load and turbidity, particularly with a decrease in COD (362 → 8 mg/L), BOD₅ (340 → 50 mg/L), and turbidity (up to 56.8 NTU) under slightly basic conditions and an optimal contact time of 120 minutes. However, the removal of nitrates and nitrites remained limited, suggesting the need to combine this process with complementary treatment methods. These findings highlight the great potential of eggshells as a sustainable, low-cost, and locally available raw material for the production of activated carbon, offering an innovative and eco-friendly solution for aqueous effluent remediation.

Keywords: Activated carbon, Eggshells, Adsorption, Aqueous effluents.

**VALORIZATION OF BIOLOGICAL STUDIES OF MEDICINAL PLANT
« THAPSIA GARGANICA »**

Hesna BENSEDDIK¹, Faiza MERATATE^{1,2}, Aissa LALAOUI³, Salah AKKAL⁴,
Khellaf REBBAS²

¹*Département de chimie, Université de M'sila, Algérie.*

²*Laboratoire des Substances Organiques Thérapeutiques et des Procédés Durables (LTOSSP),
Département de Chimie, Faculté des Sciences, Université de M'Sila, Pôle Universitaire, Route Bourdj
Bou Arreiridj, M'sila 28000, Algérie*

³*Département des Sciences Naturelles et de la Vie, Université de M'sila, Algérie.*

⁴*Département de chimie, Université de Constantine, Algérie.*

**Corresponding author E-mail : benseddikhasna@gmail.com*

Abstract : *Thapsia garganica* is a widespread species in Algeria, best known for the use of its roots in cooking and traditional medicine. This medicinal plant has been known since ancient times for its curative and preventive efficacy, it belongs to the apiaceae family. In our study we aimed to assess the evaluation of biological activities of this plant. We started this work with the methanolic extraction of all the components contained in the plant in order to obtain a crude extract, which we separated with different polar solvents “petroleum ether, chloroform, and ethyl acetate and n-butanol” The flavonoids were evaluated by the method of aluminum chlorides AlCl₃, the content is estimated at 5.6009 mg EQ / g dry matter in the crude extract. The DPPH test has attracted a lot of attention due to its speed, sensitivity and reproducibility. The IC₅₀ of the different extracts are compared with the BHT standard. The IC₅₀s in the order of antioxidant power were: petroleum ether (42,2938144 mg/ml) l'acetate ethyl (0,67893784mg /ml; BHT (0.0059 mg / ml). Depending on the results we have obtained, we can predict that flavonoids are first class antioxidant agents.

Keywords: *Thapsia garganica*, flavonoids content, DPPH.

IN VIVO AND IN VITRO ANTI-INFLAMMATORY AND ANTI-ARTHRITIC EFFECT OF PEGANUM HARMALA. L

Abdelouahab DIAFAT^a , Mounira DEHIRI^a , Ahmed BAHLOUL^a , Abdelmalek MERIBAI^a , Widad FATMI^b , Farid BOUAZIZ^a , Lekhmici ARRAR^c .

^a *Laboratory of Characterization and Valorization of Natural Products, Faculty of Nature and Life Sciences, University El-Bachir El-Ibrahimi, Bordj Bou Arreridj, 34000, Algeria.*

^b *Laboratory of Health and Environment, Faculty of Nature and Life Sciences, University El-Bachir El-Ibrahimi, Bordj Bou Arreridj, 34000, Algeria.*

^c *Laboratory of Applied Biochemistry, Faculty of Nature and Life Science, Ferhat Abbas University, Setif 1, Algeria*

*Corresponding Author: abdelouahab.diafat@univ-bba.dz

Abstract: Medicinal plants are potential sources of natural products that play an important role in preventing different human diseases; the aim of the present study is to evaluate the anti-inflammatory and the anti-arthritic effect of *Peganum harmala* L. The anti-inflammatory effects were evaluated in vitro by bovine serum albumin (BSA) denaturation inhibition test and in vivo using xylène-induced ear edema model. Arthritis was induced in rats by intradermal immunization with type II collagen emulsified in Freund's Adjuvant, then arthritic rats were treated with *P. harmala* hydromethanolic extract (PhHm) for 21 days and for 40 days for preventive and curative study, respectively, using two doses (50 and 100 mg/kg/Day). Results showed that PhHm extract significantly inhibited the BSA denaturation. It had also a good anti-inflammatory effect in xylene-induced ear edema model. *P. harmala* extract significantly inhibited arthritic development. Treatment with the plant extract also nearly normalized counts of platelets and total leukocytes. In conclusion, the current study demonstrated that the hydromethanolic extract of *P. harmala* plays an effective role in the anti-inflammatory effect and in both prevention and curative treatment of collagen-induced arthritis.

Keywords: Rheumatoid arthritis, type II collagen, *Peganum harmala* L., anti-inflammatory, anti-arthritic.

SYNTHESE DE ZnO NANOPARTICULES DOPES CHARBON ACTIF A BASE DES GRAINS D'OLIVE POUR LE TRAITEMENT DES EAUX USEES PAR PHOTOCATALYSE SOLAIRE

DRIF Seif Eddine*¹, TERCHI Smail ¹

*¹Laboratoire des matériaux et Energie Renouvelable (LMER), Faculté des sciences, université
Mohammed Boudiaf de M'sila, Route BBA 28000*

**Corresponding author: Tel./Fax: +213659399304; E-mail address: seifeddine.drif@univ-msila.dz*

Abstract

Les nanoparticules de ZnO dopés par Charbon Actif (préparé au sein de notre laboratoire à base des grains d'olive) sont caractérisés par DRX, MEB, EDS, UV-Visible et Infrarouge. Le charbon actif poreux (OSAC) a été synthétisé à partir de noyaux d'olives locaux en utilisant l'activation à l'acide phosphorique, obtenant une surface spécifique élevée de 823,07 m²/g. Les résultats de caractérisation des ZnO nanoparticules dopé par le charbon actif des grains d'olive montrent que les NPs synthétisées ont des caractéristiques très importantes (taille des particules, surface spécifique, énergie de GAP ...) Ces matériaux ont été utilisés au traitement des eaux usées de la sortie d'une station d'épuration pour améliorer la qualité des eaux usées urbaines en vue d'une éventuelle réutilisation agricole.

Keywords: ZnO nanoparticules, Charbon actif, Photocatalyse solaire, traitement des eaux usées.

**RF-MAGNETRON SPUTTERED VANADIUM-DOPED ZNO THIN FILMS
DERIVED FROM SOL-GEL NANOPOWDER TARGETS ON FLEXIBLE PEN
SUBSTRATES**

Samir HAMRIT ^{1*}, Abdelhafid MAHROUG ¹, Hanane CHENAGUE ¹, Sara SADEDDINE¹

¹ *Laboratory of Materials Physics and Its Applications, University of M'sila 28000, Algeria*

Email: Samir.hamrit@univ-msila.fr

Abstract

This study demonstrates the successful deposition of nanostructured vanadium-doped zinc oxide (VZO) thin films onto flexible PEN substrates using RF-magnetron sputtering at room temperature. The sputtering target was a compacted nano powder, synthesized via a sol-gel method with supercritical drying. Analysis confirmed the VZO nanoparticles and the resulting thin films possessed a pure hexagonal wurtzite structure, with nanoparticle sizes between 25 and 40 nm. The films exhibited a dense, columnar nanostructure. By varying the vanadium content in the target, an optimal doping level of 2 at.% was identified, yielding films with a low resistivity of approximately $6.0 \times 10^{-4} \Omega \cdot \text{cm}$, a Hall mobility of $19 \text{ cm}^2 \cdot \text{V}^{-1} \cdot \text{s}^{-1}$, and an average visible-light transmittance exceeding 75%. These properties make the films promising candidates for flexible transparent conductive oxide applications.

Keywords: V-doped ZnO, Thin films, PEN substrate, RF magnetron sputtering, TCO

CHARACTERIZATION AND MODIFICATION OF AN ALGERIAN CLAY AND ITS APPLICATION AS AN ADSORBENT

HAMMOU Zoubida ^{1*}, Aissaoui RAGADIA² and Makhloufi SOFIANE³

¹*Faculty of Exact Sciences and Computer Science University of Djelfa BP3117 Djelfa – Algeria*

²*Faculty of Exact Sciences and Computer Science University of Djelfa BP3117 Djelfa - Algeria.*

³*Faculty of Engineering Sciences University of Djelfa BP -3117 Djelfa - Algeria.*

* *Tel./Fax: 0779374989 ; E-mail address: zoubida.hammou@univ-djelfa.dz*

Abstract: In recent years, clays have played a significant role in a wide range of environmental problems, and their applications are constantly increasing. The increasing importance attached today to the protection of natural environments and the improvement of water quality. In response to these problems, we sought a simple and less expensive method to preserve the environment in order to removal and decomposition of inorganic pollutants in water. This work aims to study three types of Algerian clay, modify them after purification, and then use them as adsorbents to reduce nitrate levels in drinking water. After modification, we obtained four samples of each clay type: acid-activated clay, sodium clay, and organic clay, in addition to the purified raw clay of each type. The physical and chemical properties of these types before and after modifications revealed significant changes in their structures. Adsorption experiments also demonstrated the effectiveness of the modified clay used in reducing nitrate levels in aquatic media. The pollutant removal rate ranged between 60% and 90%, and the highest percentage was for the organic clay of each type. The raw clay also reached a removal rate of 60% but in an acidic medium (PH=2).

Keywords: Clay, adsorption, nitrate, water, pollutant inorganic. Organophiles

THE EFFECT OF PHOSPHORIC ACID ON THE PHYSIOCHEMICAL PROPERTIES OF ACTIVATED CARBONS MADE FROM BIOMASS LEAVES: POROSITY CHARACTERISTICS, SURFACE CHEMISTRY, AND ADSORPTION CAPACITY

Hamza MEGHERBI^{1*}, Abdelbaki REFFAS¹

¹Department of chemistry, Laboratory of Inorganic Materials, Algeria

*Corresponding author: Tel: +213799455078; E-mail address: Hamza.megherbi@univ-msila.dz

Abstract: Dye pollution poses a serious ecological threat to aquatic environments, emphasizing the need for advanced and sustainable water treatment solutions. Activated carbon-derived materials have gained recognition as efficient sorbents for the removal of such contaminants. In this study, we present a novel biomass-derived activated carbons (MC-ACs), produced through thermal treatment at 450 °C under ambient atmospheric conditions. The effects of H₃PO₄ were evaluated through various techniques, including BET surface area analysis, FESEM-EDS imaging, XPS, FT-IR-ATR, Raman spectroscopy. The specific surface area (SSA) increased from 642m²/g to 1237m²/g, total pore volume increased from 0.29cm³/g to 0.97cm³/g, and the mean pore diameter increased from 1.9 nm to 3.2 nm by increasing the impregnation ratio from 30 wt.% to 150 wt.%. The pH_{pzc} of MC-ACs exhibited an acidic character, owing to the presence of oxygen-containing functional groups such as hydroxyl, carboxyl, metaphosphate (-PO₃⁻), phosphates, and pyrophosphate groups, as indicated by XPS and FT-IR analysis. At a room temperature of 22 °C, the Methylene blue (MB) adsorption was lowest with MC-AC30% (42.28 mg/g) and highest with MC-AC150% (290.68 mg/g), showing increased adsorption capacity as the H₃PO₄ impregnation ratio rose from 30 to 150 wt.%.

Keywords: Activated carbons; Adsorption; Methylene blue; Specific surface area; Phosphoric acid

EFFECT OF ALKALINE TREATMENT ON THE CRYSTALLINITY INDEX AND CRYSTALLITE SIZE OF *SILYBUM MARIANUM* LIGNOCELLULOSIC FIBERS

LAIFA Fakhreddine ^{1,2*}, ROKBI MANSOUR ¹, ZAOUI MOUSSA ^{1,2}, Amroune SALAH ¹ and Yousfi SAMIA ³

¹ Department of mechanical Engineering, Faculty of technology, University of M'sila, 28000, Algeria

² Laboratoire de Matériaux et Mécanique des Structures (LMMS). Université de M'sila. Algeria

³ Department of Chemistry, Laboratory of inorganic materials, University of M'sila-Mohamed Boudiaf, 28000 M'sila, Algeria

*Tel. +0213-0770-270-225 ; E-mail address: fakhreddine.laifa@univ-msila.dz

Abstract: This study investigates the effect of alkaline treatment on the crystalline structure of natural Silybum Marianum (milk thistle) fibers using X-ray diffraction (XRD) analysis. The fibers were treated with sodium hydroxide (NaOH) solutions at concentrations of 1% and 3% for 1 h and 3 h, respectively, followed by neutralization with sulfuric acid (H₂SO₄) and drying at 68 °C. The XRD patterns revealed three major characteristic peaks at approximately $2\theta = 21^\circ$, 36° , and 72° , corresponding to the (002), (040)/(200), and (004) crystallographic planes of cellulose and amorphous regions of cellulose, respectively. The crystallinity index (CI) significantly increased notably from 64% to 68% after alkaline treatment, indicating a transition from a predominantly amorphous structure in the raw sample (SM NT) to a more ordered structure in the treated samples (SM T0101H and SM T0303H). The crystallite size (CS), calculated using the Scherrer equation, decreased slightly from 3.17 nm (untreated) to about 2.6–2.7 nm (treated), suggesting minor local disorganization accompanied by improved ordering within the crystalline domains. This structural evolution is attributed to the partial removal of amorphous constituents such as lignin, pectin, and hemicellulose, which promotes better alignment of cellulose chains. Overall, the alkaline treatment enhances the crystallinity, rigidity, and potential performance of Silybum Marianum fibers, thereby improving their suitability as reinforcement materials in bio-based composite applications.

Keywords: Silybum Marianum, alkaline treatment, X-ray diffraction (XRD), crystallinity index, crystallite size, bio-based composites.

VALORIZATION OF LOCAL RENEWABLE MATERIALS FOR SUSTAINABLE CONSTRUCTION: MECHANICAL REINFORCEMENT OF CLAY COMPOSITES.

Koadri ZAINATE^{1,a}

¹*Ecole Normale Supérieure de Bousaada, Algeria.*

^a *Corresponding author :Tel:+213796820937 ; E-mail address: Koadri.zaiante@ens-bousaada.dz.*

Abstract : This study explores the valorization of abundant and largely Local Renewable Materials namely palm fibers and red clay from southern Algeria, aiming to enhance their application in sustainable construction. These natural, eco-friendly and renewable materials exhibit notable mechanical properties, making them viable candidates for environmentally responsible building solutions. The objective of this experimental investigation was to evaluate the effect of alkali treatment duration on the mechanical performance specifically, the compressive and flexural strength of red clay-based composites reinforced with palm fibers. The broader aim is to promote maximum utilization of locally available materials while minimizing environmental impact, thereby encouraging the use of these biocomposites in rural and low-cost construction settings. In the initial phase, red clay was combined with varying proportions of cement and lime to identify the optimal binder ratio for composite formulation. In the subsequent phase, palm fibers were treated with a 4% (w/w) sodium hydroxide (NaOH) solution for different durations: 3, 7, 24 and 48 hours. Mechanical testing revealed a clear enhancement in both flexural and compressive strength in the composites reinforced with treated fibers, with the most significant improvement observed at 7 hours of alkali treatment, with strength increases of about 57% (flexural) and 60% (compressive) compared to untreated composites. These improvements highlight the effect of fiber surface modification in strengthening the bond between fiber and matrix and improving overall structural behavior. The results underline the potential of using environmentally friendly, cost-free materials like treated palm fibers as sustainable and efficient reinforcements in clay-based construction. Furthermore, their use aligns with global goals for reducing the ecological footprint of building materials by offering positive outcomes for both the environment and surrounding ecosystems.

Keywords: Renewable Materials, Palm fibers, red clay, sustainability, mechanical properties, alkali treatment, rural construction, natural composites, eco-friendly materials, environmental impact.

ENERGY RECOVERY AND REGENERATION OF USED ENGINE OILS: COMPARISON BETWEEN PYROLYSIS AND COMBINED TREATMENT METHODS

Hacina ABCHICHE^{1*}, Imane BOUTALEB², Imene Bouchelkia¹, Bilal ZANOUN¹, Wissal GUALOUZE¹

¹*Laboratory of Matter's Valorisation and Recycling of Materials for Sustainable Development (VRMDD), University of Sciences and Technology Houari Boumediene, El Alia BP32, 16111, Bab Ezzouar, Alger, Algeria*

²*Naftal Central Laboratory, Fuel Branch, P.O. Box 70, Dar El Beida, Algiers, ALGERIA*

**Corresponding author; E-mail address: habchiche2@gmail.com*

Abstract: The transport sector generates a large amount of waste, particularly used engine oils, which contain harmful contaminants for both the environment and human health. The recovery of these oils is a significant challenge for sustainable development and environmental preservation. The central laboratory of Naftal addressed the issue of managing used engine oils. Energy recovery of these oils was explored through an approach focused on hazardous waste valorization. Two treatment strategies were compared: thermal pyrolysis and regeneration by liquid-liquid extraction and flocculation, followed by an adsorption process. The results showed that the regeneration method using flocculation produced the best products, very close to conventional fuels, followed by pyrolysis and regeneration by extraction. Among the adsorbents tested, activated carbon proved to be the most effective for the final treatment of regenerated oils, as it efficiently absorbs heavy metals and organic matter, producing results close to the desired standards.

Keywords: Used Engine Oils, Thermal pyrolysis, Liquid-liquid extraction, Adsorption, Energy Recovery

FP-LAPW AND HYBRID FUNCTIONAL STUDY OF THE HALF-METALLIC BEHAVIOR IN CuMnInSe₃

Walid MENASRI^{1,*}, Sabah FETAH¹, Saadia DIDAOU¹

¹*Laboratory of materials and renewable energy, Faculty of science, University of M'sila, 28000 M'sila, Algeria.*

*Corresponding author; E-mail address: *walid.menasri@niv-msila.dz*

Abstract : Density Functional Theory (DFT) within the framework of the Full-Potential Linearized Augmented Plane Wave (FP-LAPW) method was employed to investigate the structural properties of the quaternary chalcogenide CuMnInSe₃ crystal. The calculations were carried out within the Generalized Gradient Approximation (GGA), using the Perdew et al. (2008) GGA-PBEsol functional. Spin-polarized DFT calculations were performed, and the obtained equilibrium structural parameters show good agreement with the available experimental data. For the electronic and magnetic properties, the Tran–Blaha modified Becke–Johnson (TB-mBJ) and Heyd–Scuseria–Ernzerhof (HSE) hybrid functionals were used to improve the accuracy of the calculated band gap for this magnetic and semiconductor material. Based on the analysis of the spin-polarized band structures and density of states, the CuMnInSe₃ compound is predicted to exhibit half-metallic character, with a total magnetic moment of 6 μ B per unit cell. Furthermore, the electronic structure is found to be better described by an indirect band gap of the X– Γ type.

Keywords: Density Functional Theory (DFT); CuMnInSe₃; Half-metallic semiconductor; Magnetic properties; Band structure; FP-LAPW method.

MANUFACTURE AND CHARACTERIZATION OF A TUBE MADE FROM SAND AND PLASTIC WASTE

BOUCHIBA Maria¹*, ROKBI Mansour¹, SAIB Cherif¹

¹*Department/Mechanical engineering, University of M'sila, Algeria*

*Corresponding author; E-mail address: *maria.bouchiba@univ-msila.dz*

Abstract : In a global context where the sustainability, performance, and cost-effectiveness of materials have become priorities, composite materials are emerging as cutting-edge solutions, capable of meeting the growing demands of users while taking environmental issues into account. Thanks to their superior properties compared to traditional materials—particularly in terms of strength, lightness, and longevity—these composites open the way to numerous applications in construction, infrastructure, transportation, and resource management. With this in mind, our research aims to design a new composite material based on natural sand and polypropylene (PP), a lightweight, recyclable, and strong thermoplastic polymer. This combination leverages the mechanical qualities of sand and the flexibility of PP to develop an innovative tube that is economical, efficient, and environmentally friendly. By integrating locally available and potentially recycled materials, our approach is fully in line with a circular economy approach, while providing concrete solutions to the challenges of ecological transition and technical performance optimization. The results obtained demonstrate that these tubes can withstand hydrostatic pressures exceeding 8 bar, with an estimated circumferential Young's modulus of 11 GPa and a very low water absorption rate. These performance characteristics suggest their suitability for integration into a broad spectrum of applications, particularly in environments requiring high mechanical strength and minimal moisture sensitivity.

Keywords: Materials innovation; composite materials; composite tube; eco-materials; plastic recycling.

**ETUDE PHYTOCHIMIQUE D'UNE PLANTE UTILE EN MEDICINE
TRADITIONNELLE *HERTIA CHEIRIFOLIA***

Nabila ADOUI, Hamdi BENDIF

Département des sciences de la nature et de la vie, Faculté des sciences. Laboratoire de biodiversité et techniques biotechnologiques pour la valorisation des ressources végétales. Université de M'sila 28000.Algérie.

*Corresponding author; E-mail address: *nabila.adoui@univ-msila.dz.*

Résumé : L'objectif de la présente recherche est l'étude de composition chimique et les propriétés biologiques de la plante *Hertia cheirifolia* (L.) de la famille des Astéracées, qui est réputée par ses vertus thérapeutiques à travers l'évaluation de leurs effets anti-oxydant, insecticide et antibactérienne afin de mieux comprendre leurs potentiels thérapeutiques. La méthodologie implique l'extraction des composants de la plante par macération, donnant des extraits concentrés méthnolique et hénanique. Les polyphénols ont été dosés à l'aide de la méthode de Folin-Ciocalteu et l'activité antioxydante a été évaluée à l'aide du test DPPH. Les tests d'activité insecticide del'huile essentielle et des extraits méthanolique et hénanique ont inclus des évaluations par contact et répulsion sur des adultes de *Tribolium confusum* , avec des applications directes pour mesurer la mortalité des insectes. Tandis que l'activité antibactérienne a été étudiée par la technique de diffusion sur disque pour une évaluation quantitative. Les résultats ont montré un rendement d'extraction élevé de 41.38%,8.30 % pour l'extrait méthanolique et hénanique respectivement et un rendement moyen pour le l'huile essentielle (2.1g). Les extraits de *Hertia cheirifolia* se sont avérés riches en composés phénoliques avec un taux égale à 299.6176 GAE/mg. En ce qui concerne l'activité antioxydante, les extraits méthanolique et hénanique ont présentés des valeurs d'IC50 de 42.70mg/ml et 292.59 mg/ml respectivement soulignant un potentiel antioxydant considérable. Pour l'activité insecticide, les tests ont montré une faible mortalité chez les insectes exposés aux extraits et une moyenne mortalité au l'huile essentielle, démontrant ainsi une légère efficacité dans la lutte contre les insectes nuisibles. De plus une activité antibactérienne non significative a été observée sur toutes les souches bactériennes testées.

Mots clés : *Hertia cheirifolia*, Polyphénols, Antioxydante, Insecticide, Antibactérienne, *Tribolium confusum*

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THEORETICAL STUDY OF THE INTERACTION BETWEEN PROTEINS; COLLAGEN, KERATIN AND BLUE INDIGO DYE BY MOLECULAR DOCKING APPROACH

Houda ARAB^{1*}, Rida MASMOUDI¹, Sami KHETTAF¹, Saad BOUCHEKIOUA² and Ammar DIBI¹

¹Laboratory of Chemistry and Environmental Chemistry (LCCE), Department of Chemistry,
Faculty of Material Sciences, University of Batna-1, Batna, Algeria.

²Pharmaceutical Sciences Research Center (CRSP), Constantine, Algeria.

*Corresponding author: Tel./Fax: +213 674742807 ; E-mail address: houda.arab@univ-batna.dz

Abstract: It is important to highlight the significance of Industrial dyes interactions in biological applications. These dyes, such as blue indigo, are widely used in the textile manufacturing process, specifically in denim production. However, some studies have indicated their potential toxicity due to interactions with structural proteins in the human body, such as keratin and collagen. These proteins play a key role in maintaining the cohesion and elasticity of skin tissues, while keratin provides strength to hair, nails, and skin, cells while collagen contributes to the strength and elasticity of skin tissues. Prolonged exposure of human skin to these pigments may lead to structural damage to these proteins, most likely due to oxidative mechanisms resulting from chemical reactions with the pigment compounds. Accordingly, a simulation study was proposed to investigate the interactions between blue indigo and (collagen, keratin proteins). Using molecular docking technique to better understand how this dye affects the structural integrity and biological function of these essential proteins. The docking calculation was performed by AutoDock vina, 3D dimensional crystal structure collagen and keratin proteins (collagen (PDB: 7CWK) and (keratin (PDB: 6JFV)). was obtained from the protein database <http://www.rcsb.org./pdb>. The calculations of indigo were performed on using density functional theory (DFT) with the hybrid functional B3LYP at base 6-311++G(d,p) in isolated phase, using the Gaussian 16 package.

Keywords: Blue indigo, Collagen and keratin proteins, DFT, Molecular docking, PDB

EFFET PROTECTEUR DE L'EXTRAIT BRUT DE FEUILLES DE *CLEMATIS FLAMMULA* SUR LA CICATRISATION DES ULCERES CHEZ LA SOURIS

Nassima CHERAFT-BAHLOUL¹, Dina ATMANI¹, Meriem BERBOUCHA-RAHMANI¹, Marie-Hélène ANTOINE², Cécile HUSSON², Caroline STEVIGNY³, Joëlle NORTIER² et Djebbar ATMANI¹

1.Laboratoire de Biochimie Appliquée, Faculté des Sciences de la Nature et de la Vie, Université de Bejaia, Bejaia 06000, Algeria ;

2.Laboratoire de néphrologie expérimentale, Université libre de Bruxelles - Campus Erasme, Anderlecht, Belgique ;

3.Laboratoire plantnut, Université libre de Bruxelles - Campus Plaine, Bruxelles, Belgique

**Auteur correspondant Tél.00213556693235*

e-mail : nassima.cheraft@univ-bejaia.dz

Résumé : L'ulcère gastro-duodéal est une affection qui se manifeste par des lésions de la muqueuse gastrique résultant d'un déséquilibre entre les facteurs agressifs et les mécanismes de défense. Bien que les thérapies antiulcéreuses chimiques soient efficaces, elles peuvent entraîner des effets indésirables . A cet effet, comme une alternative prometteuse, la thérapie à base des plantes médicinales propose des solutions efficaces pour le traitement de cette pathologie. Dans ce contexte, nous avons entrepris une évaluation de l'effet de cicatrisation de l'extrait brut de feuilles de *Clematis flammula* (EFCF), sur les ulcérations induites par un agent ulcérogène (éthanol 96%), ainsi que l'activité inhibitrice de la peroxydation lipidique, après avoir déterminé ses teneurs en composés phénoliques. Les résultats de l'analyse quantitative ont montré que l'extrait EFCF est riche en phénols totaux, en flavonols glycosylés, en anthocyanes et en tannins. Par ailleurs, cet extrait a exhibé une forte activité d'inhibition de la peroxydation lipidique (>90% à 100 µg/ml), comparativement à l'acide ascorbique. D'autre part, l'analyse macroscopique des lésions internes visibles dans les estomacs des souris testées a révélé que l'extrait EFCF, à différentes doses (50, 100 et 150 mg/kg), a induit une réduction significative des lésions gastriques induites par l'agent ulcérogène. Cette réduction a été dose-dépendante, avec des taux d'inhibition des ulcérations très significatifs ($P < 0,01$), comparativement au groupe traité avec l'oméprazole (20 mg/kg). Ces résultats suggèrent que cette plante constitue une source prometteuse d'agents antioxydants, capables de contribuer à la prévention et la cicatrisation des ulcères.

Mots clés : *Clematis flammula*, peroxydation lipidique, ulcère, souris.

REDOX BEHAVIOR AND ANTIOXIDANT ACTIVITY OF TETRAZOLE-BASED NI (II) COMPLEXES: A GREEN SOLID-STATE SYNTHESIS AND DFT STUDY

Yacine ALLAB^{1, 2*}, Sabah CHIKHI^{1, 3}, Safia DJEBBAR¹, Sihem Zaater⁴, Selma AKCHA¹ and Afaf BOUCHOUCHA¹

1 Laboratoire d'Hydrométallurgie et Chimie Inorganique Moléculaire, Faculty of Chemistry, Houari Boumediene Sciences and Technology University, BP 32, El Alia, Bab Ezzouar, Alger, Algeria

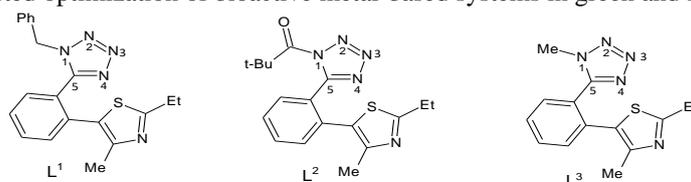
2 Département des Classes Préparatoire, Ecole Supérieure d'Agriculture Saharienne d'Adrar, 01000 Adrar, Algeria.

3 UMR 6226 CNRS-Université de Rennes 1 “Organométallique, Matériaux et Catalyse”, Campus de Beaulieu, 35042 Rennes, France.

4 Laboratoire de Physico-Chimie Théorique et de Chimie Informatique, Faculté de Chimie, Houari Boumediene Sciences et Technologie, Université, BP 32 El Alia, 16111 Alger, Algeria.

*Corresponding author: E-mail address: yacinecm34@gmail.com

Abstract :Research in the development of new metal complexes with biologically relevant ligands possessing donor sites such as nitrogen, oxygen, and sulfur has attracted considerable interest, as the biological properties of these ligands often improve upon coordination with metal ions. In this context, the rational design of metal complexes with biologically active ligands represents a key strategy in green chemistry for developing functional materials with enhanced redox and antioxidant properties. In the present study, we report the synthesis of novel nickel (II) complexes via an environmentally friendly solid-state method, employing a series of tetrazole-based ligands (L1–L3) previously developed by our group (Scheme 1). These ligands coordinate through the N3 nitrogen atom of the tetrazole ring, forming octahedral Ni(II) complexes with the general formula $[\text{Ni}(\text{L})_2\text{Cl}_2(\text{H}_2\text{O})_2] \cdot 2\text{H}_2\text{O}$, as confirmed by analytical, spectroscopic, and thermogravimetric analysis. Electrochemical characterization via cyclic voltammetry revealed that electron-donating substituents cause cathodic shifts in reduction potentials, while electron-withdrawing groups induce anodic shifts and enhance antioxidant activity. The antioxidant potential was quantitatively assessed using the DPPH radical scavenging method, showing superior performance compared to standard references. Electron withdrawing effect of the substituents on the ligands enhanced the antioxidant activity of the ligands and their Ni (II) complexes. To elucidate structure–activity relationships, density functional theory (DFT) calculations were carried out on both the ligands and their Ni (II) complexes. The computational results confirmed the coordination mode and geometric stability, and provided insight into the electronic factors influencing redox and antioxidant behavior. This work highlights how integrating green synthetic approaches with computational chemistry enables the molecular design of transition metal complexes with improved biological functionalities. The study offers a foundation for further development of AI-assisted optimization of bioactive metal-based systems in green and sustainable chemistry.



Scheme 1. Structure of the different ligands.

Keywords: Nickel (II) complex, TGA, Tetrazole derivatives, DFT, cyclic voltammetry and Antioxidant activity.

ESSENTIAL OIL OF *TEUCRIUM AUREO-CANDIDUM* AS A NATURAL ANTIBACTERIAL AGENT AGAINST RESISTANT PATHOGENS: A DOCKING-GUIDED APPROACH

Sara YAHLA *¹, Belkacem GORDO ¹, Kamel MSAADA², Omar MESSAOUDI ^{3,4,5}, Mohammed GHERIB ¹ et Abdel Ilah AMROUCHE ¹

¹ *Laboratory Sustainable Management of Natural Resources in Arid and Semi-Arid Zones, Department of SNV, Institute of Science, University Center Naama*

² *Laboratory of Medicinal and Aromatic Plants, Biotechnology Center in Borj Cedria Technopole, Tunisia*

³ *Department of Biology, Faculty of Science, University of Amar Telidji, Laghouat, Algeria*

⁴ *Laboratory of Applied Microbiology in Food, Biomedical and Environment, Abou Bekr Belkaïd University, 13000, Tlemcen, Algeria*

⁵ *Research Unit of Medicinal Plant (RUMP) Attached to Center of Biotechnology (CRBt, 3000, Constantine), Laghouat 03000, Algeria*

*Corresponding author: (213) 0662007011; E-mail: yahla@cuniv-naama.dz

Abstract : This study aimed to evaluate the antimicrobial potential of *Teucrium aureo-candidum*, an endemic aromatic plant from the Naâma region of Algeria. The main objective was to determine the chemical composition of its essential oil, extracted by hydrodistillation from aerial parts collected in Moghrrar and Djeniène Bourezg, and to assess its antibacterial activity. Gas chromatography analyses (GC-FID and GC-MS) identified 45 compounds accounting for 87.73% of the oil, with a predominance of sesquiterpenes hydrocarbons (29.53%) and oxygenated sesquiterpenes (30.06%). Major constituents included τ -muurolol (11.35%), γ -cadinene (5.24%), δ -cadinene (4.24%), α -muurolene (4.04%), and α -cadinol (3.30%), while monoterpenes were present in lower amounts. Antibacterial activity was tested against selected Gram-positive and Gram-negative strains using disc diffusion and microdilution methods, showing notable effectiveness, particularly against Gram-positive bacteria. In parallel, an in silico molecular docking study was conducted to investigate the interaction between major oil components and the FabI enzyme (enoyl-acyl carrier protein reductase), a critical target in bacterial fatty acid synthesis, using triclosan as a reference inhibitor. The results highlighted α -cadinol, spathulenol, caryophyllene, and α -muurolene as promising FabI inhibitors, with better bioavailability and lower toxicity profiles compared to triclosan. These findings position *T. aureo-candidum* essential oil as a valuable natural resource for the development of novel antibacterial agents, offering potential applications in the ongoing fight against antibiotic-resistant pathogens.

Keywords: Essential oil, *Teucrium aureo-candidum*, GC-MS, Antibacterial activity, Molecular docking.

IN VITRO ANTI OXIDANT CAPACITY , PHYTOCHEMICAL EVALUATION AND ANTI INFLAMMATORY ACTIVITY BY BSA OF HYDRO METHANOLIC EXTRACT FROM FRUIT

Nozha MAYOUF¹, Soumia BOUTARFA¹, Soulef SAOUDI², Khaoula AROUA⁴ , Nassima LEULMI⁴, Hanane MELLAL¹

¹Laboratory of Biotechnology, Water, Environment and Health Faculty of Nature and Life Sciences, University Abbes laghrour khenchela , Algeria.

² Laboratory of Phytotherapy Applied to Chronic Diseases², Department of Biology and Animal Physiology, Univ Setif 1, 19000, Algeria.

³Laboratory of Mycology , biotechnology and microbial activity³, Constantine 1. Department of Molecular and Cellular Biology Faculty of Natural and life Sciences, University of Abbes Laghrour, 40004, Khenchela, Algeria

⁴Plant protection laboratory in agricultural and natural environments against crop pests⁴. Department of Agronomic Sciences, Faculty of Natural and life Sciences, University of Abbes Laghrour, 40004, Khenchela, Algeria
Correspondance : nozhabiole91@gmail.com/ nozha.mayouf@univ-khenchela.dz

Abstract: Natural antioxidants are becoming increasingly popular because of their importance in preventing and treating many diseases , especially those sourced from fruits and vegetables, have garnered attention due to their potential health benefits and safety profiles compared to synthetic alternatives. This study investigates the antioxidant properties ,chemical composition and anti inflammatory effect of hydro methanolic extract derived from the fruit of *Cydonia oblonga Mill* collected in Khechela, Algeria. Maceration was used for hydro methanolic extraction, followed by both quantitative and qualitative chemical analyses. The antioxidant capacity of the extract was evaluated using Total anti oxidant capacity and evaluation of in vitro anti inflammatory power by colorimetric methods relating to the denaturation of bovine serum albumin (BSA).In this study the result obtained suggest that this fruit extract have high level of total sugars with a value of 27.73 ± 0.81 mg D-glucose/ g and low amount of proteine 1.58 ± 0.075 mg/g.Furthermore, the extract exhibited significant antioxidant activity, with EC₅₀ values of 0.43 ± 0.22 mg/mL for the TAC assay . The extract of *Cydonia oblonga Mill* was rich in proteines and sucres Concerning the anti-denaturation activity, the methanolic extract showed a high percentage of BSA inhibition of 84.98%, at the concentration of 18mg/mL.Coclusion : These findings highlight the potential of *Cydonia oblonga Mill* fruit as a valuable source of natural antioxidants, contributing to the prevention of oxidative stress-related diseases. Given their notable biological activity.

Key words : Anti oxidant, Inflammatory , BSA, *Cydonia oblonga* .

OPTIMISATION DE LA PRODUCTION D'HYDROGENE VERT PAR ELECTROLYSE PEM. APPLICATION DE PLAN BOX-BEHNKEN

Mohamed BENATTIA^{1*} and Salima BENDEBANE¹

¹National Higher School of Technology and Engineering, Laboratory L3M, 23005, Annaba, Algeria,

*Corresponding author: m.benattia@ensti-annaba.dz

Résumé : Dans une optique de transition énergétique durable, cette étude s'inscrit dans le cadre de la chimie verte en explorant la production d'hydrogène vert par électrolyse PEM. Une méthode statistique basée sur le plan Box-Behnken a permis d'optimiser trois variables : la tension appliquée (P), le débit d'eau (Q) et la qualité de l'eau, pour une durée d'électrolyse fixée à 60 minutes. Les conditions optimales déterminées sont : une tension de 3,5 V, un débit de 100 mL/min d'eau osmosée, conduisant à une production maximale d'hydrogène de 101,00 mL, avec un rendement faradique de 71,82 %. L'analyse de la variance révèle que la tension appliquée, son interaction avec la qualité de l'eau, ainsi que le terme quadratique de cette dernière, exercent une influence significative sur la quantité d'hydrogène produite. Ces résultats offrent une meilleure compréhension des paramètres clés à maîtriser pour améliorer l'efficacité du procédé.

Mots-clés : Hydrogène vert, électrolyse PEM, Box-Behnken, optimisation, chimie verte.

DFT AND MOLECULAR DOCKING INSIGHTS INTO NEW THIOHYDANTOIN DERIVATIVES WITH POTENTIAL BIOLOGICAL ACTIVITY

Khedidja MERDJA¹, Mansour DEBDAB¹

¹Laboratory of Synthesis and Catalysis (LSCT), Faculty of Materials Sciences, University Ibn Khaldoun-Tiaret, Tiaret 14000, Algeria.

*Corresponding author: Tel./Fax: +213793855096 ; E-mail address: merdja.khadidja@gmail.com

Abstract

The focus of this work is on synthesising novel thiohydantoin derivatives **2(a-c)**, akin to leucettamine B analogs, via microwave-assisted transamination reactions. This reaction was carried out between 3-alkyl-5-dimethylamino-2-thioxo-imidazolidin-4-one **1(a-c)** and aniline. Confirmation of the structural integrity of the synthesized compounds was given using NMR and MS spectroscopy, and their configurations were validated through DFT calculations. Analyses encompassed molecular electrostatic potential, frontier molecular orbitals, HOMO-LUMO energies, energy band gap, and global chemical reactivity descriptors, providing comprehensive insights into their characteristics. The investigation extended to the biological domain, employing substance activity spectra prediction (PASS) and molecular docking with Autodock Vina4 program. Notably, this holistic assessment aimed to gauge the potential regulatory effect of the compounds on cholesterol. The integration of this approach leads to a better understanding of compound design and potential applications, covering drug design and broader biomedical contexts.

Keywords: DFT calculations; thiohydantoin derivatives ; HOMO-LUMO energies; microwave irradiation; molecular docking

MECHANO-ENZYMATIC AND DEEP EUTECTIC SOLVENT (DES) MEDIATED SULFOXIDATION REACTIONS

Amina CHERAITIA^{1,2*}, Chuhan LI¹, Michele CROTTI¹, Naima MERABET² and Daniele CASTAGNOLO¹

¹*Department of Chemistry, University College London, Marshgate Building, Manufacturing Futures Lab, 7 Sidings Street, E20 2AE, London, United Kingdom.*

²*Laboratoire de Pharmacologie et de phytochimie, Faculté des Sciences Exactes et Informatique, Université de Jijel, 18000 Jijel, Algeria.*

*Corresponding author: Tel./Fax: +213555509805 ; E-mail address: cheraitiaa22@gmail.com

Abstract: The oxidation of sulfide substrates into sulfoxides is a common reaction in organic chemistry and it finds broad application in the pharmaceutical, chemical and agrochemical industries. Drugs such as omeprazole, armodafinil or sulindac, contain a sulfoxide moiety which is crucial for their pharmaceutical activity. The sulfoxide motif can also be found in natural products such as the garlic components allicin, ajoene and garlicnins B-2 and L-1 as well as in chiral ligands used in asymmetric organic syntheses, such as the Skarzewsky's ligand. Many sulfoxidation catalytic methods, including photo-, organo- and biocatalytic methods, have been developed to date with the aim to make such transformation more sustainable and in line with principle of Green Chemistry. This work describes the development and green assessment of three sulfoxidation methodologies, which combine biocatalysis with mechanochemistry, and the use of deep eutectic solvents (DESs). A new mechano-enzymatic method where sulfoxides are prepared under mechanochemical conditions with CALB biocatalyst, UHP and AcOEt, was first developed, followed by a mechanochemical method requiring only lactic acid (LacOH) and UHP. Finally, a DES-mediated method where sulfoxides are generated by the reaction of UHP with a LacOH based DES media was developed. All the three methodologies afforded sulfoxide products selectively with high yields.

Keywords: Sulfoxide; Mechanochemistry; Biocatalysis; Deep Eutectic Solvent; Mechano-enzymatic

PALLADIUM (II) COMPLEXES OF AMPHIPHILIC AZOLES AS RECOVERABLE CATALYSTS IN SUZUKI-MIYAUURA CROSS-COUPPLING REACTION

Manel CHEHROURI^{1,2*}, Ali Othman ADIL³ and José Miguel SANSANO⁴

¹*Département des Sciences Physiques, Ecole Normale Supérieure de Mostaganem ENS, Mostaganem, Algeria.*

²*Laboratoire de Synthèse Organique, Physico-Chimie, Biomolécules et Environnement LSPBE, Département de Chimie Physique, Faculté de Chimie, Université des Sciences et de la Technologie d'Oran Mohamed Boudiaf –USTO-MB, Oran, Algeria.*

³*Laboratoire de Synthèse Organique Bioactive, Département de Chimie Physique, Faculté de Chimie, Université des Sciences et de la Technologie d'Oran, Mohamed Boudiaf-USTO-MB, Oran, Algeria.*

⁴*Departamento de Química Organica, Instituto de Síntesis Organica and Centro de Innovacion en Química Avanzada (ORFEO-CINQA), Universidad de Alicante, Alicante, Spain.*

*Tel: +213-069-777-8473; E-mail adress: chehrouri.manel@gmail.com.

Abstract: The Suzuki-Miyaura cross-coupling reaction is one of the most useful and versatile ways to achieve different series of compounds (preferentially biaryls) where a new Csp²-Csp² bond is formed. The resulting molecules derived from this transformation have different applications in many areas: in the preparation of natural products, nucleoside surrogates, drugs, liquid crystals and pharmaceutically interesting compounds. The Suzuki-Miyaura coupling reactions in environmentally friendly solvents such as water or alcohols have a particular importance. In this sense, the importance of the nature of the ligands of the palladium complex determine the availability to run couplings to perform a later recovery or reuse of them in this media. The employment of ligands with surfactant nature, coordinated to the palladium atom, is crucial to recycle the catalytic system and is not very frequent in organic chemistry. So, in this work, initially two complexes of palladium (II) were prepared using 4-amino-5-pentadecyl-3,4-dihydro-2H-(1,2,4)triazole-3-thiol and 5-pentadecyl-3H-(1,3,4)-oxadiazole-2-thione as ligands and Pd(OAc)₂ and K₂PdCl₄ as palladium sources respectively in chloroform. Their structures was characterized by: IR, RMN, mass spectra (ESI) and microanalysis. After the ability of these complexes to operate in Suzuki-Miyaura cross coupling between iodo anisol and p-tolylboronic acid was studied. In order to optimize the conditions of this reaction, several parameters have been changed, such as: solvent, base, temperature and the quantity of the catalyst. The use of the combination of water/ ethanol as solvent in equal proportions in a bath at 100 °C using KOH as a base and palladium complexe (2 mol%) afforded an excellent conversion and very clean reaction product (99 % and 96% yields respectively). The recovery of the catalytic species has been surveyed, the nature of the employed solvent water/EtOH and also nature of the catalyst that was a brown sticky dense oil. These characters were permit to recover the catalyst and reuse it up to the fifth recycled experiment arising very high yield with total efficiency and they have ability to run a new process with the same efficiency (more than 5 cycles).

Keywords: Palladium complexes; Catalyst; Recycling; Suzuki-Miyaura.

DEVELOPMENT OF BIOCOMPOSITES BASED ON PALM FIBER FOR SUSTAINABLE APPLICATIONS

Serine ARIS^{1*}, Azzedine BENYAHIA¹ and Nadir DEGHEFEL²

¹*City, Environment, Society and Sustainable Development Laboratory, Department of chemistry, University of M'sila, Algeria*

²*Chemistry of Inorganic Materials Laboratory, Department of chemistry, University of M'sila, Algeria*

**Corresponding author: Tel./Fax: +213660998217 ; E-mail address: serine.aris@univ-msila.dz*

Abstract : This study investigates the development of a composite material using unsaturated polyester resin as the matrix and palm fiber, treated with varying concentrations of NaOH, as reinforcement. The palm fibers underwent chemical treatment with NaOH at different concentrations to enhance interfacial bonding by removing impurities and improving surface roughness. The composites were fabricated via hand lay-up or compression molding. Fourier Transform Infrared Spectroscopy (FTIR) was employed to analyze the chemical changes in the fiber surface post-treatment, confirming the removal of lignin and hemicellulose. Mechanical properties were assessed through tensile testing, revealing improved tensile strength with optimal NaOH concentration due to enhanced fiber-matrix adhesion. X-ray Diffraction (DRX) analysis provided insights into the crystallinity changes in the treated fibers, correlating with mechanical performance. The results demonstrate that NaOH-treated palm fiber composites exhibit superior mechanical properties and thermal stability, making them suitable for sustainable applications in industries such as construction and automotive.

Keywords: Unsaturated polyester ; Tensile strength ; Chemical treatment ; Composite material ; Mechanical properties.

INVESTIGATION OF NEW INHIBITORS AS ANTI-ALZHEIMER AGENTS THROUGH MOLECULAR MODELING METHODS

Ferdaous HASNI¹, Ismail DAOUD^{2,3} and Nadjib MELKEMI¹

1. *Group of Computational and Medicinal Chemistry LMCE. Laboratory, University of Mohamed Khider Biskra, Biskra 07000, Algeria*

2. *Department of Matter Sciences, University Mohamed Khider, BP 145 RP, Biskra 07000, Algeria*

3. *Laboratory of Natural Substances and Bioactive (LASNABIO), University of Abou-BakrBelkaid, Tlemcen 13000, Algeria*

**Corresponding author: Tel./Fax: 0698922968 ; E-mail address: ferdaous.hasni@univ-biskra.dz*

Abstract: Neurodegenerative diseases damage the nervous system and lead to a variety of complex progressive chronic issues. Alzheimer's disease (AD) is one such case. The most common form of dementia is a degenerative disorder of the brain that leads to memory loss, confusion, and behavioral changes. The main drug classes currently used to treat AD are acetylcholinesterase (AChE) and butyrylcholinesterase (BChE) inhibitors. In this study, we investigated the inhibitory effects of a series of newly synthesized compounds of 2-hydroxy-N-phenylbenzamide derivatives on AchE and BchE, using molecular modeling approaches such as molecular docking and dynamics simulation. Molecular docking was performed to analyze the complex score and different types of interactions present between certain amino acids of the protein studied and that of ligands. On the other hand, The best docking complexes, L18 and L6', were used as simulation inputs to evaluate the stability of the complex (protein–ligand). These results were verified using molecular dynamics simulations, demonstrating the strength of both complexes. All these methods allow us to identify new inhibitors that have potential against this disease and can be suggested as new drugs against Alzheimer's disease.

Keywords: Alzheimer's disease; Inhibition; AChE/BuChE; Molecular docking; Molecular Dynamics.

DÉTERMINATION D'UNE NOUVELLE VOIE D'ACCÈS AUX B-AMINOCETONES ET LEUR EFFETS THERAPEUTIQUES MISE AU POINT D'UNE NOUVELLE VOIE D'ACCES AUX B-AMINOCETONES ET ETUDE DE LEURS EFFETS THERAPEUTIQUES

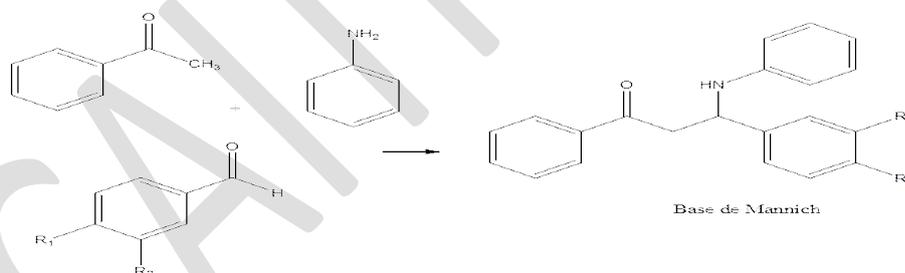
A.ZETCHI^{a, b *}, I.MENNANA^{a, b}, S.NEMOUCHI^{a, b}, I.SEHOUT^{a, b}

^a Département de chimie, Faculté des sciences exactes,, campus de Chaabat Erssas, Université Mentouri de Constantine1, Algeria

^b Laboratoire de synthèse des molécules bioactives SYMBIO.

E-mail address: melitazetchi@gmail.com Phone: +213540261328

Résumé : La chimie organique moderne se focalise sur les problématiques d'économie (étapes, atomes, énergie). Les réactions à composants multiples (RCMs), visant à synthétiser des produits hautement fonctionnalisés en une unique opération chimique, s'inscrivent précisément dans ce contexte. Par conséquent, ces réactions connaissent aujourd'hui un intérêt considérable tant dans le secteur industriel que académique. L'utilité des β -aminocétones dans notre quotidien a fait de leur méthode de préparation, nommée la réaction de Mannich [1], une des réactions à composants multiples les plus importantes ; de part les produits synthétisés comme la *Nisoxetine* antidépresseur et le *tolmetin* qui représentent la structure de *Mannich*[2].



L'efficacité d'une synthèse organique dépend essentiellement du catalyseur qui focalise le plus de chercheurs, car de là en dépendent l'économie en temps et en énergie, cela nous a exhortés à mener une étude de la réaction de Mannich et ce facteur. Le criblage catalytique nous a orientés sur la détermination de nouveaux catalyseurs dont les essais préliminaires se sont vus très concluants. La généralisation de la voie, après optimisation avec les trois bibliothèques des réactifs, a généré une chimiothèque de *bases de Mannich* avec de très bons rendements.

Mots clés : DFT, RCMs, réaction de Mannich, β -aminocétones, criblage.

DOSAGE DES COMPOSES PHENOLIQUES ET EVALUATION DE L'ACTIVITE ANTIOXYDANTE D'UNE PLANTE DE LA FAMILLE DES MALVACEES

Hantour RAZIKA^{1*}, Benabdesslem YASMINA¹ et Ghomari SAMIA¹

¹Laboratoire de Nutrition, Pathologie, Agro-Biotechnologie, et Santé (LAB-NUPABS); équipe : Agro-Biotechnologie et Développement Durable (ABDD),SNV Faculty, UDL-SBA.

*Corresponding author: Tel.0655245960 ; E-mail address:hantourrazika27@gmail.com

Résumé : Depuis l'Antiquité, les plantes médicinales sont considérées comme des remèdes essentiels dans le traitement de nombreuses maladies, en raison de leur richesse en composés bioactifs. Parmi elles, la mauve, membre de la famille des Malvaceae, se distingue par son importance. *Malva sylvestris*, l'une des espèces les plus répandues dans le bassin méditerranéen, est largement utilisée en médecine traditionnelle ainsi qu'en alimentation. Elle est particulièrement prisée pour sa forte concentration en composés phénoliques, mucilages, flavonoïdes et antioxydants, qui lui confèrent de précieuses propriétés bénéfiques pour la santé. L'objectif de ce travail est, dans un premier temps, de rechercher et de quantifier les composés phénoliques présents, notamment les polyphénols totaux, les flavonoïdes et les tanins. Le second objectif consiste à évaluer l'activité antioxydante des extraits, à l'aide des tests DPPH, FRAP et de l'évaluation de l'activité antioxydante totale. L'extraction des feuilles de *Malva* a été réalisée par deux méthodes : la macération et l'extraction assistée par ultrasons. Les résultats montrent que les deux extraits sont riches en composés polyphénoliques, en particulier en flavonoïdes, et présentent un fort pouvoir antioxydant. En conclusion, *Malva sylvestris* se révèle être une plante médicinale prometteuse grâce à sa richesse en composés phénoliques, notamment les flavonoïdes, et à son activité antioxydante marquée. Ces résultats confirment son potentiel d'utilisation dans les domaines pharmaceutique et nutritionnel, en tant que source naturelle de molécules bioactives.

Mots clés: Malva sylvestris ,Dpph ,Frap ,bioactives.

COMPARISON OF DFT AND AI-PREDICTED IR AND NMR SPECTRA OF (R)- AND (S)-1-FLUOROETHANOL

Hana TOUATI^{1*}, Hafida AMMAR-AOUCHICHE¹ and Mohamed Réda BELMECHERI¹

¹Department of Chemistry, University of M'hamed Bougara of Boumerdes, Algeria

*Corresponding author: Tel./Fax: +213553528869 ; E-mail address: hanatouati661@gmail.com

Abstract :Advancements in artificial intelligence (AI) have enabled the prediction and visualization of molecular behavior with increasing accuracy. In this study, a comparative spectroscopic characterization of the enantiomers (R)- and (S)-1-fluoroethanol was conducted using both quantum chemical calculations and AI-assisted tools. Infrared (IR) spectra were simulated using the B3LYP functional combined with two basis sets: 6-31+G** and 6-31++G**. Theoretical ¹H and ¹³C NMR chemical shifts were computed using the GIAO method with the same basis sets. All calculations were performed in both gas and solvent phases using Gaussian 09, and visualized with GaussView. In parallel, the NMR spectra were predicted using the online platform nmrd.org, based on symbolic machine learning algorithms. A detailed comparison was made between AI-based predictions and the DFT-calculated spectra. Results showed strong consistency for NMR in the gas phase, while some solvent-dependent deviations were observed. IR spectra also revealed minor differences between the two enantiomers, mainly in the fingerprint region. Data analysis and graphical representation were conducted using Google Colab and Python libraries including Pandas and NumPy. This multi-method approach highlights the strengths and limitations of AI in comparison to quantum methods for stereoisomeric spectral differentiation.

Keywords: Artificial Intelligence (AI) ; IR Spectroscopy ; NMR Spectroscopy.

**PHYTOCHEMICAL STUDY AND ANTIOXIDANT ACTIVITY
EVALUATION OF THE METHANOLIC EXTRACT OF *BORAGO
OFFICINALIS* L.**

Hiba GHERZOULI^{1*}, Sabah BOUMERFEG², Asma MEZITI³, Hassina GUERGOUR⁴, Yuva BELLIK⁵, Fatima CHEBIRI⁶, Mohamedredha AIDEL⁷, Chawki BENSOUICI⁸ and Nasreddine MEKHOUKH⁹

¹ *Laboratory of Health and Environment, Mohamed El Bachir El Ibrahimi University, Bordj Bou Arreridj, 3400, Algeria*

² *Faculty of Life and Nature Sciences, Mohamed El Bachir El Ibrahimi University, Bordj Bou Arreridj, 34000, Algeria*

³ *Research Center of Biotechnology, Ali Mendjli Nouvelle ville UV 03, BP E73 Constantine, Algeria*

*Corresponding author: Tel./Fax: +213 557 92 09 48; E-mail address: hiba.gherzouli@univ-bba.dz

Abstract; This study focuses on the phytochemical analysis and antioxidant activity evaluation of the methanolic extract of the aerial parts of *Borago officinalis* L., a medicinal plant known for its therapeutic potential. The methanolic extraction yielded 20.87%. Quantitative analysis revealed a high total phenolic content ($132.97 \pm 0.95 \mu\text{g GAE/mg}$), followed by hydrolysable tannins ($80.08 \pm 1.49 \mu\text{g TAE/mg}$), flavonoids ($53.71 \pm 2.96 \mu\text{g QE/mg}$), and flavonols ($45.37 \pm 1.81 \mu\text{g RE/mg}$). Antioxidant activity was assessed using several in vitro assays. The DPPH test showed moderate activity with an IC_{50} value of $580.53 \pm 2.63 \mu\text{g/mL}$, while the ABTS assay demonstrated a stronger effect ($\text{IC}_{50} = 183.26 \pm 1.20 \mu\text{g/mL}$). Reducing power was evaluated through FRAP and o-phenanthroline assays, with $\text{A}_{0.5}$ values exceeding $200 \mu\text{g/mL}$, indicating low reducing potential. The silver nanoparticle (SNP) assay revealed limited reducing ability for silver ion reduction, with an $\text{A}_{0.5}$ value greater than $400 \mu\text{g/mL}$. These findings highlight the richness of *Borago officinalis* L. in secondary metabolites, particularly phenolic compounds, and confirm its antioxidant potential through different mechanisms.

Keywords: *Borago officinalis* L.; methanolic extract; phytochemical characterization; antioxidant activity.

NOUVELLE VOIE DE SYNTHÈSE DE NAPHTOXAZINONE PAR UN NOUVEAU CATALYSEUR

Imene MENNANA ^{1*}, Amel ZETCHI¹, Houria BERRHAIL BOUDOUDA ², and Taous BOUMOUD¹

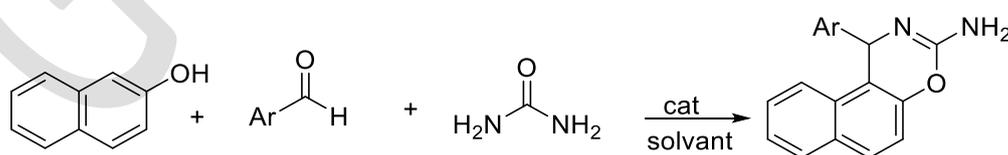
¹Department de chimie, Université des frères Mentouri Constantine 1, Algeria

²Department de science de la matière, Université d'Oum el Bouaghi, Algeria

*Corresponding author: Tel.: +213 794026054; E-mail address:

mennana.imene@umc.edu.dz

Résumé : Les oxazinones ont reçu une attention considérable en raison de leurs propriétés biologiques étendues et de leurs activités pharmacologiques. Il a été prouvé que la présence d'un autre fragment hétérocyclique améliore les caractéristiques biologiques de plusieurs composés. Par conséquent, il a été conçu pour synthétiser des dérivés d'oxazinones contenant des noyaux biologiquement actifs. De nouveaux dérivés d'oxazinones ont été synthétisés en tant que médicaments anti-inflammatoires, antimicrobiens et anti-VIH et diverses autres activités chimiques et pharmacologiques. La naphtoxazinone est un type très important d'échafaudages hétérocycliques dans le domaine de la chimie organique naturelle et synthétique en raison de leurs incroyables effets biologiques et pharmacologiques spéciaux. Par exemple, les dérivés de la naphtoxazinone présentent des propriétés antibactériennes. Ces composés sont également utilisés comme précurseurs pour la synthèse de ligands chiraux d'aminophosphine catalysés asymétriquement. Nous présentons un protocole efficace et respectueux de l'environnement pour la synthèse de dérivés des naphtoxazinones qui sont obtenues par une réaction multicomposante en utilisant un aldéhyde, β naphtolet urée, en utilisant un nouveau catalyseur.



Keywords: réaction multicomposant ; synthèse one-pot ; naphtoxazinone

CONTRIBUTION TO THE STUDY OF THE BIOLOGICAL EFFECT OF
CITRULLUS COLOCYNTHIS SEEDS

AZIZI Nassima^{1*}, SEGHIER Hanane ² and BOUABIDA Hayette²

¹Applied Biology Department, Echahid Echeikh Larbi Tebessi University, Tebessa. Algeria

²Living Beings Department, Echahid Echeikh Larbi Tebessi University, Tebessa. Algeria

*Corresponding author: Tel./Fax: +213. 0667754299 ; nassima.azizi@univ-tebessa.dz

Abstract: This study was carried out to evaluate the antibacterial, antioxidant, and antidiabetic activity of the ethanolic extract of *Citrullus colocynthis* seeds. The extract was obtained by maceration using ethanol. The yield of the maceration was estimated at 2.25%. Phytochemical screening revealed the presence of : flavonoids, catechin tannins, steroids, saponins, alkaloids, gallic tannins, quinones, and terpenes. Antibacterial activity was determined using the diffusion method on Muller-Hinton agar. The antibacterial activity study showed that the extract has a strong effect on Gram positive and Gram-negative strains and a more effective activity on *Candida* strains. The determination of the Minimum Inhibitory Concentration (MIC) was done by the microdilution method, tested on *Staphylococcus aureus*, *Klebsiella pneumoniae*, *E. coli*, *Enterococcus*, and *Candida albicans*. MIC values ranged between 0.31 mg/mL and 0.25 mg/mL. The calculation of the MBC/MIC ratio showed that the ethanolic extract has a bactericidal effect on the bacterial strains tested and the *Candida* strains. The antioxidant activity study by the DPPH method revealed that *Citrullus colocynthis* has a stronger activity at a concentration of 500 µL/mL with an inhibition percentage of 98.50% and 90% respectively. The study of the antidiabetic activity revealed a stronger activity ranging from 60 to 65%, whereas metformin shows a weaker inhibitory effect, limited to 40%. *Citrullus colocynthis* can be used as an alternative to antibiotics in the treatment of infectious bacterial diseases.

Keywords: *Citrullus colocynthis*; phytochemical screening; antibacterial activity; DPPH test; antidiabetic activity.

COMBINED PHARMACOPHORE MODELING, 3D-QSAR, MOLECULAR DOCKING, AND MOLECULAR DYNAMICS SIMULATIONS FOR THE IDENTIFICATION OF NOVEL CURCUMIN DERIVATIVES AGAINST PANCREATIC CANCER

Narimene CHAHBAOUI^{1*}

*1 Group of Computational and Pharmaceutical Chemistry, LMCE Laboratory, University of Biskra, BP 145 Biskra, 07000, Algeria *Corresponding author: Tel./Fax: +213-792082509 ;*

E-mail address: narimene.chahbaoui@univ-biskra.dz

Abstract : Pancreatic cancer, often referred to as the “silent killer,” remains among the most aggressive and intractable malignancies. The PI3K α signaling pathway has emerged as a critical target in pancreatic tumor progression, making it a focal point for therapeutic development. Curcumin derivatives, known for their structural diversity and bioactivity, have shown potential as PI3K α inhibitors. In this study, we employed an integrated computational pipeline involving pharmacophore modeling, atom-based 3D-QSAR analysis, molecular docking, and molecular dynamics simulations to identify promising curcumin-derived PI3K α inhibitors. The pharmacophore model (AAHRR_1) was constructed from biologically active curcumin derivatives with cytotoxic effects against the Panc-1 cell line. It served as the basis for a statistically robust 3D-QSAR model with strong internal and external validation ($R^2 = 0.990$, $Q^2 = 0.971$). The model's reliability was confirmed via Y-randomization and Tropsha's criteria, and its performance was supported by enrichment analysis. Subsequently, the validated pharmacophore was used to screen a curated dataset of curcumin-related compounds from PubChem. From this screening, two candidates (CID156189304 and CID154728220) were prioritized based on favorable docking scores and predicted pharmacokinetic profiles, both outperforming the reference compound Alpelisib. Subsequent molecular dynamics simulations confirmed their stability within the PI3K α binding pocket. These results support the potential of curcumin-based scaffolds as selective PI3K α inhibitors and demonstrate the effectiveness of integrated in silico methodologies in early-stage anticancer drug discovery.

Keywords: Panc-1; Curcumin derivatives; Pharmacophore modeling; 3D-QSAR; Molecular docking; MD simulations

ISOLATION AND CHARACTERIZATION OF BIOCORROSIVE BACTERIA FROM INDUSTRIAL SYSTEMS: A STEP TOWARD SUSTAINABLE INFRASTRUCTURE PROTECTION

DIKES Loubnaa*, DRICHE El-hadja, FARES Chahinezb, EL HABCHI Yasminea SEBAIHIA
Mohameda

a Laboratory of Molecular biology , Genomic and Bio-Informatic (LBMGB)), Sciences of Nature and Life (SNV), HassibaBenbouali University of Chlef, Hay Salem, 02000 Chlef, Algeria

bDepartment of technology, HassibaBenboualiUniversity Chlef, Algeria

Email: l.dikes@univ-chlef.dz

phone : 0541168572

Abstract : Biocorrosion, caused by microbial activity, accounts for up to 25% of material degradation in industrial systems, leading to significant economic losses and safety hazards. This study isolates and characterizes biocorrosive bacteria from industrial environments, including cooling towers, wastewater treatment plants, and pipelines. Key bacteria identified include *Desulfovibrio vulgaris*, *Pseudomonas aeruginosa*, and *Acidithiobacillus ferrooxidans*, which are major contributors to microbial-induced corrosion (MIC). Specifically, *D. vulgaris* was responsible for 42% of the observed corrosion, while *P. aeruginosa* and *A. ferrooxidans* contributed 30% and 18%, respectively. Using 16S rRNA sequencing and biochemical assays, the study confirmed the identity of these microbes and examined their corrosion mechanisms. Findings show that these bacteria accelerate corrosion through biofilm formation, production of sulfuric acid, and generation of hydrogen sulfide (H₂S), which significantly degrade metal surfaces. This research highlights the need for effective management of biocorrosion in industrial systems and demonstrates the potential of biopolymer solutions in enhancing infrastructure protection. By offering sustainable alternatives to conventional corrosion inhibitors, biopolymers contribute to long-term infrastructure resilience and sustainable development.

Keywords: Biocorrosion ,Microbial-Induced Corrosion, Industrial Systems and Sustainable Infrastructure.

ELECTRONIC CHARACTERISTICS AND DEFORMATION OF NANOTUBES UNDER INFLUENCE OF AN ELECTRIC FIELD

Fayçal BAIRA^{1,*}, Sara ZIDANI², Kaouther BAIRA¹

¹*Department of Sciences and technology, Faculty of technology, University ofBatna 2, Alleys 53, Constantine Avenue. Fesdis, Batna 05078, Algeria*

²*Department of Food Technology, Laboratory of Food Science (LSA), Institute of Veterinary and Agricultural Sciences, University of Batna 1 Had) Lakhdar, Alleys May 19 Biskra Avenue, Batna, 05000, Algeria*

*: *Tel./Fax: +213666665839 ; E-mail address:f.baira@univ-batna2.dz*

Abstract : The recent progress achieved in the synthesis and characterization of nanostructures has been spurred by the necessity to develop growth strategies to adapt the properties of these materials for specific applications. Studies related to morphology and dimensionality control have drawn particular interest in recent years because of their increasing roles in the domains of electronic and thermal transport, along with the enhancement of different properties at the nanometer scale. This is especially important in the case of one-dimensional (1D) structures. Among 1D nanostructures, semiconductors with nanotube-like morphology have garnered a lot of interest because of their interesting properties. Nanotubes have an ideal morphology for studying electrical transport mechanisms in 1D systems, which makes them fitting for utilization in many applications such as the manufacture of nano-lasers, field-effect transistors, nano-resonators, actuators and field emitters, Several semiconductor materials have been synthesized in the form of nanotubes such as silicon (Si). indium phosphide (InP), titanium dioxide (TiO₂) oxide zinc (ZnO). The oxide semiconductor activity is focused on ZnO and its alloys. It has received considerable attention in recent years in various fields . Interest in ZnO nanotubes formed the focus of our study which was conducted specifically on the structural and electronic properties of diverse zinc oxide nanotubes using density function theory (DFT).

Keywords: Titanium dioxide (TiO₂); Oxide zinc (ZnO); Density Function Theory (DFT)

ELABORATION DES MATERIAUX COMPOSITES RENFORCES PAR DES FIBRES NATURELLES

Miloud RAHLA^{1*}, Nadir DEGHEFEL^{2*}, Azzedine BENYAHIA^{3*}

¹ *Laboratory City, Society, Environment and Sustainable Development, University of M'sila,*

² *Inorganics Materials Laboratory, University M'sila Algeria*

**Corresponding e-mail: miloud.rahla@univ-msila.dz*

Abstract : Les préoccupations environnementales croissantes liées aux plastiques ont stimulé la recherche active d'alternatives aux matériaux dérivés du pétrole. Une des solutions prometteuses repose sur l'innovation utilisant des ressources naturelles et renouvelables. Dans ce contexte, les biocomposites émergent comme une option durable, substituant les matrices et fibres synthétiques par des biomatériaux, notamment des fibres naturelles. Bien que ces matériaux présentent des avantages économiques et écologiques significatifs, leur développement se heurte à des défis techniques, en particulier la compatibilité fibre-matrice, nécessitant des traitements physico-chimiques pour optimiser leurs performances. Face aux limites des méthodes conventionnelles de caractérisation mécanique, les techniques de contrôle non destructif (CND) gagnent en importance grâce à leur précision et leur capacité à évaluer les propriétés des matériaux sans altération. Nos travaux de recherche portent sur le développement d'un composite renforcé par des déchets naturels. Pour garantir une adhésion optimale entre la matrice thermoplastique et les fibres végétales, ces dernières ont été traitées par des méthodes physiques et chimiques, utilisant différentes concentrations d'hydroxyde de sodium (NaOH) et de permanganate de potassium (KMnO₄), à des températures variables. Les essais réalisés incluent des analyses avancées telles que la spectroscopie infrarouge à transformée de Fourier (FTIR) et la diffraction des rayons X (DRX), ainsi que des études de cinétique de sorption d'eau. Les propriétés mécaniques ont été évaluées à travers des tests de traction, flexion trois points, compression et dureté, assurant une caractérisation complète du matériau.

Keywords: Adhésion, fibre Natural , traitement chimique

MODELISATION ET INVESTIGATION EXPERIMENTALE DU PROCESSUS D'ADSORPTION BINAIRE SUR UN ADSORBANT NANOSTRUCTURE

Hadjer BOUSEMAT ^{1,2*}, Samira ZIANE-HEZIL ^{1,a}, Saadiya BENATMANE ^{1,b}, Naima HAMMOUDI ^{2,a}, Halima DELLALI ^{2,b}

*Laboratoire des Structures, Élaboration et Applications des Matériaux Moléculaires (SEA2M)
Département de Génie des Procédés, Faculté des Sciences et de la Technologie
Université Abdelhamid Ibn Badis, Mostaganem, Algeria
Auteur correspondant : hadjer.bousemat.etu@univ-mosta.dz*

Résumé : Cette étude examine l'adsorption binaire de polluants anioniques sur une argile naturelle à structure 2:1 (Be) et sur sa forme nanostructurée (B-8N) obtenue par activation acide. Une caractérisation complète a été réalisée à l'aide de l'analyse thermogravimétrique et thermique différentielle (ATG/ATD), de la diffraction des rayons X (DRX), de la microscopie électronique à balayage (MEB), de l'analyse de la surface spécifique par la méthode BET et de la spectroscopie infrarouge à transformée de Fourier (FTIR). Ces analyses ont confirmé la modification structurale, l'augmentation de la surface spécifique et le développement de caractéristiques nanostructurées après traitement acide. Des expériences d'adsorption en discontinu ont été menées à pH constant (6,4) en conditions binaires. Les données d'équilibre ont été modélisées à l'aide des isothermes de Langmuir et de Langmuir étendu, tandis que l'analyse cinétique a montré que le modèle du pseudo-second ordre décrivait le mieux le processus, indiquant que la chimisorption est le mécanisme prédominant. Les paramètres thermodynamiques (ΔG° , ΔH° , ΔS°) ont confirmé le caractère spontané de l'adsorption. La programmation sous MATLAB a été utilisée pour l'ajustement des modèles, la génération de surfaces isothermes en 3D et la validation des modèles théoriques. Par ailleurs, les expériences de désorption et de régénération ont montré que l'adsorbant nanostructuré (B-8N) conserve une efficacité élevée d'adsorption au cours de cycles successifs, confirmant sa stabilité et sa réutilisabilité. Dans l'ensemble, l'activation acide a transformé l'argile brute 2:1 en un adsorbant nanostructuré présentant une capacité d'adsorption supérieure, une robustesse structurelle et un fort potentiel de régénération, en faisant un matériau prometteur et durable pour le traitement des eaux usées.

Mots clés: Argile ; Adsorption binaire ; Équilibre ; Eaux usées ; Régénération.

SIMULATION OF HEAT DISSIPATION BY TWISTED SURFACE FINS

Nardjes BENGHERBIA¹, Habib BOUIGHI² and Hocine BOUKORTT³

¹*Department, Of Mechanics, Laboratory of Energetic Process and Nanotechnologies (LPEN) University of Blida 1, P.O. Box 270 Blida 09000 Algeria.*

²*Department, Of Mechanics, Laboratory of Environmental Technology Research. LTE, ENP MA-Oran, BP 1523 ElMnaouer, 31000, Oran, Algeria.*

³*Department, Of Mechanics, Laboratory of Renewable Energy and Materials LERM Faculty of Technology Univ of Yahia Fares Medea.*

**Corresponding author: Tel./Fax: +213661387384 ; E-mail address: habibtmt99@gmail.com*

Abstract: High-performance cooling is an essential requirement for modern microprocessors that generate large amounts of non-uniform heat distribution. Heat sinks have traditionally been used for thermal management. In this study, the effects of certain design parameters on the performance of the flat plate heat sink were analyzed. Heat transfer simulations were performed using COMSOL finite element analysis software to understand the variation in heat flux and temperature of the heat sink. Three parameters were varied: the number of fins, the heat flux and the material of the heat sink, and a comparison of the heat flux distribution and temperature between the Twist fin heat sink with a difference in the number of fins [4].

Keywords: Heat sink, convection, fins, cooling.

MICROBIAL NANOPARTICLE SYNTHESIS: A SUSTAINABLE METHOD FOR BIOCORROSION MITIGATION IN OIL AND GAS PIPELINES

Yasmine ELHABCHI^{1*}, El-Hadj DRICHE¹, Loubna DIKES¹ and Chahinez FARES²

¹*Laboratory of Molecular Biology, Genomic and Bioinformatic (LBMGB), Faculty of Nature and life sciences, Hassiba Benbouali University of Chlef, Hay Salem, 02000 Chlef, Algeria*

²*Faculty of Technology, Hassiba Benbouali University of Chlef, Chlef, Algeria*

*Corresponding author: Tel./Fax: +213665206145; E-mail address: y.elhabchi@univ-chlef.dz

Abstract : Microbial synthesis of nanoparticles offers a compelling solution to energy and environmental challenges, particularly in the context of mitigating biocorrosion in oil and gas pipelines. Currently, there are various chemical processes used to produce nanoparticles, but they have a negative effect on the environment. Leveraging the natural metabolic pathways of microorganisms, nanoparticles can be produced through eco-friendly, bottom-up biosynthetic processes. The aim of our study is to investigate the microbial synthesis of nanoparticles as a sustainable and multifunctional approach for mitigating biocorrosion in oil and gas pipelines as well as enhancing energy efficiency and contributing to environmental protection. Nanoparticles produced microorganisms exhibit strong antimicrobial activity against corrosive microbial communities that accelerate pipeline degradation, particularly sulphate reducing bacteria (SRB). Their deployment in pipeline systems, either as part of protective coatings or through targeted injection and by their properties including small size, high surface area, and bioactive properties they can inhibit microbial colonization, disrupt biofilm formation, reduce corrosion rates, and enhance the longevity of infrastructure. Compared to conventional chemical biocides, microbially synthesized nanoparticles are environmentally friendly, cost-effective, and adaptable to extreme operational conditions. By aligning microbial synthesis of nanoparticles with green nanotechnology principles, this approach supports sustainable energy infrastructure, reduces environmental toxicity, and promotes green nanotechnology.

Keywords: biocorrosion; biocorrosion mitigation; nanoparticles; microorganisms.

**EVALUATING AI MODELS FOR IR SPECTRAL ANALYSIS OF PHENOL:
ACCURACY AND LIMITATIONS IN MOLECULAR CHARACTERIZATION**

Asma BOUDAUD^{1*}, Mebrouk DJEDID², Mokhtar BENALIA², and Mounira GUERMIT¹

¹*Department of The Common Trunk Sciences and Technology, Laboratory of Process Engineering, Materials and Environmental, Faculty of Technology, Amar Telidji University of Laghouat, Laghouat, Algeria*

²*Department of Process Engineering, Laboratory of Process Engineering, Materials and Environmental, Faculty of Technology, Amar Telidji University of Laghouat, Laghouat, Algeria*

**Corresponding author: Tel./Fax: +213675562047; E-mail address: a.boudaoud@lagh-univ.dz*

Abstract: This study evaluated the performance of four publicly available artificial intelligence (AI) models in interpreting and analyzing the infrared (IR) spectrum of phenol. All models accurately calculated the degree of unsaturation as 4 and successfully identified key functional groups and bond types, including C=O, C=C, O-H, and C-H stretches. However, notable differences were observed in the completeness of bond identification, the recognition of substitution patterns, and the accuracy of structural representations. ChatGPT and Gemini delivered concise and largely accurate analyses, with Gemini demonstrating superior performance in identifying monosubstitution patterns on the benzene ring. In contrast, while DeepSeek and Grok correctly recognized functional groups, both exhibited limitations in structural accuracy, with Grok showing the most pronounced errors. These findings underscore the current strengths and limitations of AI models in IR spectroscopy, highlighting the need for advancements in structural visualization and comprehensive bond mapping to improve molecular interpretation accuracy.

Keywords: Artificial Intelligence (AI); Infrared (IR) Spectroscopy; Phenol; Molecular Characterization.

**VALORIZATION OF NATURAL RESOURCES: STUDY OF THE
ANTIMICROBIAL ACTIVITY OF *PLECTRANTHUS AMBOINICUS* (CUBAN
OREGANO) EXTRACT**

Hadia DELHOUM^{1*}, Khadidja AMIRA^{2,3} et Nour elhouda DJEGHADER^{3,4}

¹*Department of Natural and Life Sciences, Djilali Bounaama University, Khemis Meliana, Algeria*

²*Higher Normal School of Technological Education of Skikda, Algeria*

³*Laboratory of Physics, Chemistry, and Biology of Materials, Skikda, Algeria*

⁴*Department of Natural and Life Sciences, Badji Mokhtar University, Annaba, Algeria*

*Corresponding author: Tel: +213670000117; E-mail address: hadia.delhoum@univ-dbkm.dz

Abstract: *Plectranthus amboinicus*, commonly known as Cuban oregano, is a succulent aromatic plant belonging to the Lamiaceae family, found in many tropical and Mediterranean regions Ślusarczyk et al., 2021. Recognized for its distinctive flavor and medicinal properties Akinbo et al., 2018, this herb is traditionally used to treat various respiratory conditions, thanks to its anti-inflammatory and antiseptic properties, while also being appreciated in culinary applications Dos Santos Silva et al., 2020. In this study, we evaluated the antimicrobial activity of the ethanolic extract obtained from the leaves of *Plectranthus amboinicus*. The disk diffusion method was used to test the effectiveness of the extract against three pathogenic bacteria: *Escherichia coli*, *Pseudomonas aeruginosa*, and *Staphylococcus aureus*. The extraction yield was 19.23%. The antibiogram revealed the sensitivity or resistance of these bacteria to certain antibiotics, notably oxacillin and fusidic acid. The results showed that the ethanolic extract exhibited significant antimicrobial activity against all bacterial strains, with particularly strong efficacy against *Staphylococcus aureus*, which displayed inhibition zones up to 17.8 mm. These findings suggest that *Plectranthus amboinicus* could be a promising natural resource for developing new antimicrobial agents, highlighting its properties within the framework of sustainable bioprocesses.

Keywords: Antimicrobial activity; ethanolic extract; *Plectranthus amboinicus*.

INFLUENCE OF ZINC ACETATE CONCENTRATION ON THE PHOTOELECTROCHEMICAL PERFORMANCE OF CHEMICALLY DEPOSITED ZnO FILMS

Ibrahim Yaacoub BOUDERBALA^{1,2}, Abdelmadjid HERBADJI^{2,3} and Slimane KHELOUFI^{4*}

¹ *Laboratory of Physical Chemistry of Materials, Faculty of Sciences and Technology, Chadli Bendjedid University, 36000, El Tarf, Algeria*

² *Laboratory of Chemistry, Molecular Engineering and Nanostructures, University of Ferhat Abbas, 19000 Setif, Algeria*

³ *Applied Optics Laboratory, Institute of Optics and Precision Mechanics, University of Ferhat Abbas, 19000 Setif, Algeria*

⁴ *Laboratory: Growth and Characterization of New Semiconductors, University of Ferhat Abbas, 19000 Setif, Algeria*

*Corresponding author: KHELOUFI SLIMANE ; E-mail address: slimanekheloufi03@gmail.com

Abstract: This study explores the influence of zinc acetate (ZnAc) precursor concentration on the electrochemical and photocatalytic properties of zinc oxide (ZnO) thin films fabricated via the chemical solution deposition method. By systematically varying the ZnAc concentration from 0.25 M to 0.75 M, the study aims to establish the relationship between precursor concentration and film performance in both electrochemical and photocatalytic applications. Electrochemical impedance spectroscopy (EIS) and Mott-Schottky analysis were employed to assess the charge transport behavior and semiconductor properties of the films. Results demonstrated that higher ZnAc concentrations led to a notable improvement in charge transfer characteristics. Specifically, the film synthesized with 0.75 M ZnAc exhibited the lowest charge transfer resistance ($R_{ct} = 0.31 \text{ k}\Omega$) and the highest double-layer capacitance ($102.5 \text{ }\mu\text{F}$), indicative of enhanced charge carrier density and more efficient interfacial electron transfer. In parallel, the photocatalytic activity of the ZnO films was evaluated through the degradation of Rhodamine B (RhB) under UV irradiation. The ZnO film derived from 0.75 M ZnAc showed the most effective photocatalytic performance, as evidenced by a continuous and significant decrease in RhB absorbance over time. This activity is attributed to the generation of reactive oxygen species (ROS), particularly hydroxyl radicals ($\bullet\text{OH}$) and superoxide anions ($\bullet\text{O}_2^-$), formed by the UV-induced excitation of electron-hole pairs within the ZnO lattice. These species facilitate the oxidative breakdown of RhB into less harmful by-products. Overall, the findings underscore the pivotal role of precursor concentration in modulating ZnO thin film properties, with implications for their use in advanced photoelectrochemical and environmental remediation technologies.

Keywords: Zinc Oxide Thin Films ; Precursor Concentration ; Photocatalytic Degradation ; Electrochemical Performance.

***HYOSCYAMUS ALBUS* : UNE PLANTE MEDICINALE ET AGRICOLE A REDECOUVRIR**

Nour El Imène BOUBLATA¹ ; Sarra HABBACHI¹; Amira HABBECHÉ^{1,4} ; Wafa HABBACHI¹ ; Saliha BENHISSEN^{1,3} ; Khellaf REBBAS^{2,3} et Abdelkrim TAHRAOUI¹

¹Laboratoire de Neuroendocrinologie Appliquée. Département de Biologie, Faculté des Sciences, Université Badji Mokhtar Annaba 23000, Algeria.

²Laboratoire d'Agro-biotechnologie et de Nutrition dans les zones arides et semi-arides, Université Ibn Khaldoun, Tiaret, Algeria.

³Département de Biologie, Faculté des Sciences-Université Med Boudiaf, M'Sila 28000.

⁴Département d'Ecologie et Environnement. Faculté des Sciences. Université 20 Aout 1955 Skikda
Tel : 00213540909101 / email : imeneboublata@gmail.com

Abstract: L'intérêt croissant pour les biopesticides d'origine végétale résulte de leur impact réduit sur la santé humaine et l'environnement. *Hyoscyamus albus*, une plante saharienne appartenant à la famille des Solanacées, est connue pour sa richesse en composés bioactifs, notamment les alcaloïdes tropaniques, qui lui confèrent des propriétés biologiques intéressantes. Toutefois, ses effets sur les organismes vivants, en particulier sur le métabolisme, demeurent peu explorés. La présente étude vise à évaluer les effets d'un extrait aqueux de *H. albus* sur certains paramètres biochimiques chez le rat Wistar, après un traitement de 7 jours. Les analyses ont porté sur les concentrations sériques de créatinine, de triglycérides, de cholestérol total et de glucose, afin d'appréhender l'impact métabolique de l'extrait. Les résultats montrent des modifications significatives des taux de créatinine, de triglycérides et de cholestérol chez les animaux traités. Chez les femelles, une hypoglycémie notable a été observée, suggérant une influence hormonale ou sexuelle différenciée. Ces résultats témoignent de l'activité métabolique potentielle de l'extrait, probablement liée à la présence de composés à effets antioxydants, anti-inflammatoires, antidiabétiques et hypolipidémiques. Ainsi, *H. albus* se révèle être une plante d'intérêt pour une double valorisation : d'une part comme biopesticide naturel dans un contexte agroécologique, et d'autre part comme source potentielle de molécules bioactives à usage thérapeutique. Néanmoins, des investigations supplémentaires, notamment toxicologiques et mécanistiques, s'imposent pour confirmer ces observations et garantir la sécurité d'utilisation de cette plante dans les domaines médicaux ou agroalimentaires.

Keywords : Biopesticide végétal ; *Hyoscyamus albus* ; Paramètres biochimiques ; Lutte biologique ; Valorisation thérapeutique.

**VALORISATION D'EXTRAIT ACETATE D'ETHYLE DE THE VERT
(CAMELLIA SINENSIS L.) COMME RESSOURCE NATUREL
RENOUVELABLE**

Fairouz BOUBRIK*¹, Tahar BOUBELLOUTA ¹

¹Laboratory of Characterization and Valorization of Natural Resources (L.C.V.N.R), faculty of life and natural sciences and of earth and universe sciences, Mohamed El Bachir El Ibrahimi University, 34000, Bordj Bou Arreridj, Algeria.

*corresponding author: Tel./Fax: +213666080329 ; e-mail address: fairouz.boubrik@univ-bba.dz

Abstract : Les extraits des plantes représentent des et ressources naturels renouvelables et sûres prometteuses à la pasteurisation et à la conservation synthétique. Cette étude visait à valoriser les molécules bioactives d'extrait acétate d'éthyle de thé vert (*Camellia sinensis* L.) afin de les utiliser comme conservateurs alimentaires naturels et ressources naturels renouvelables dans le jus d'orange naturel non pasteurisé. Nous avons examiné les qualités physicochimiques, microbiologiques et sensorielles du jus traité avec l'extrait acétate d'éthyle de thé vert pendant 28 jours de stockage à 4 °C, avec des mesures effectuées tous les 7 jours. Les résultats ont montré que l'extrait acétate d'éthyle de thé vert a significativement amélioré les indicateurs de qualité en réduisant les réactions de brunissement et en inhibant l'activité de la pectine méthylestérase ($p < 0,05$). Cependant, le pH et l'acidité titrable sont restés inchangés ($p > 0,05$). L'extrait acétate d'éthyle de thé vert a significativement ($p < 0,05$) amélioré les propriétés microbiologiques et sensorielles du jus d'orange en réduisant la charge microbienne et en rehaussant le goût, la couleur, la saveur et l'acceptabilité globale. Au regard de ces résultats très prometteurs, les molécules bioactives provenant de *Camellia sinensis* L. pourraient être utilisées comme conservateurs alimentaires naturels et ressources naturels renouvelables, constituant ainsi une alternative aux conservateurs chimiques de synthèse.

Keywords: Valorisation, Extrait acétate d'éthyle, *Camellia sinensis* L., Ressource naturel renouvelable.

SOIL VALORIZATION STRATEGIES IN BARLEY CROPPING SYSTEMS IN ARID AGROECOSYSTEMS: THE CASE OF ZIBAN

Fatima Zohra Batoul TOUATI¹ and Abdelbaset BOUMADDA²

^{1,2} *Department of Agronomic Sciences, Kasdi Merbah University of Ouargla, Algeria*

**Corresponding author E-mail address: touati.fatimazohrabatoul@univ-ouargla.dz*

Abstract: The study assesses soil valorization techniques under barley cropping systems in the arid agroecosystem of Ziban, Algeria. A structured survey of 45 farmers in three sectors of the Ouled Djellal commune was conducted to identify farmer typologies regarding soil management practices. Results indicated that 52.2% of farmers received agricultural training, 47.8% used chemical fertilizers exclusively, and only 21.7% engaged in green or green-organic fertilization methods; deep tillage was practiced by 34.8% of respondents, and 43.5% of them adopted no tillage. Organic manure was applied by 47.8% of farmers. Furthermore, 82.6% did not receive government subsidies, while 86.9% sold their barley on local or mixed markets. Multiple Correspondence Analysis (MCA) explained 64.46% of total variance on two dimensions, revealing four typical farmer profiles: traditional organic valorizers (26.1%) working under ecologically sustainable low-input approaches; modern organic valorizers (17.4%) working on integration of organic inputs, training, and market access; synthetically intensive farmers (34.8%) relying on chemical inputs and deficient institutional supports; transitioning mixed-profile farmers (21.7%) applying both types of inputs without any structured guidance. This study indicates that agronomic practices and socio-economic factors collectively affect soil valorization; thus, improved access to technical advisory services regarding organic inputs for farmers' associations should be established to promote sustainable soil use in the arid regions of Algeria.

Keywords: Soil valorization; Arid agroecosystem; Agricultural practices; Sustainable agriculture.

VALORISATION DE MATERIAUX NATURELS POUR LE TRAITEMENT D'EAUX
COLOREES : CAS DE L'ORANGE II

Yassine BOUNOURI^{1*}, Dyna SADOUNE ²

¹Laboratoire de Physico-chimie des Matériaux et Catalyse, Faculté des Sciences Exactes,
Université de Bejaia, Targa ouzemmour 06000, Algeria.

²Département de chimie, Faculté des Sciences Exactes, Université de Bejaia, Targa ouzemmour
06000, Algeria.

*Corresponding author: Tel./Fax: +213-774-92-6459 ; E-mail address: yassine.bounouri@univ-bejaia.dz

Abstract : De nos jours, l'homme utilise d'importantes quantités d'eau douce pour ses besoins domestiques et industriels, ce qui entraîne sa contamination par divers éléments toxiques ou indésirables (particules solides, agents pathogènes, composés organiques et minéraux, etc.). Une fois souillées, ces eaux sont souvent rejetées dans le milieu naturel sans traitement préalable, ce qui peut avoir des conséquences néfastes sur les écosystèmes aquatiques (faune et flore) ainsi que sur la santé humaine. Les colorants organiques figurent parmi les principaux polluants présents dans les eaux usées. Plusieurs classes de ces colorants se caractérisent par une grande stabilité, une forte résistance à la dégradation et un potentiel cancérigène ou mutagène pour l'être humain. Dans le cadre de la valorisation de deux matériaux adsorbants, à savoir le charbon actif et l'argile, cette étude a pour objectif l'élimination d'un polluant organique (l'Orange II) à partir de solutions aqueuses. Les résultats obtenus ont montré que les masses optimales des adsorbants sont respectivement de 0,3 g pour le charbon actif et de 0,4 g pour l'argile. L'efficacité d'adsorption augmente avec la concentration initiale du colorant, et le processus est favorisé en milieu acide. Les vitesses d'agitation optimales ont été déterminées à 600 tr/min pour le charbon actif et 800 tr/min pour l'argile. La température exerce un effet positif sur l'adsorption, avec une efficacité maximale observée à 40 °C pour les deux adsorbants. La modélisation cinétique a révélé que le processus suit le modèle de pseudo-second ordre pour les deux matériaux. Par ailleurs, le modèle de Langmuir s'est avéré le plus adapté pour décrire l'isotherme d'adsorption d'Orange II. Les valeurs du facteur de séparation R_L indiquent que l'adsorption est favorable dans tous les cas étudiés. L'étude thermodynamique a montré que l'adsorption est de nature physique et endothermique, et qu'elle n'est pas spontanée à 25 °C.

Mots clés : Adsorption, Orange II, charbon actif, argile, cinétique d'adsorption.

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ANTIOXIDANT PROPERTIES AND PREVENTIVE EFFECT OF AQUEOUS LEAF EXTRACT OF *PISTACIA LENTISCUS* L. AGAINST OXALIPLATIN-INDUCED OXIDATIVE STRESS IN ISOLATED RAT LIVER MITOCHONDRIA

Nesrine CHOUIKH^{1*}, Lamia BENGUEDOUAR¹, Hadjer KEMEL¹ and Mohamed SIFOUR¹

¹Laboratory of Molecular Toxicology, Faculty of Nature and Life Sciences, University of Jijel, 18000 Jijel, Algeria.

*Corresponding author: Tel./Fax: +213698916951; E-mail address: chouikh.nesrine@univ-jjel.dz

Abstract : Oxaliplatin (OXA) is a chemotherapeutic agent primarily used in the treatment of colorectal cancer. Despite its efficacy, it can cause several adverse effects, notably oxidative stress. This study evaluates the antioxidant effects of the aqueous leaf extract of *Pistacia lentiscus* L. (ALEPL) and its potential to counteract OXA-induced mitochondrial oxidative stress in rat livers. The phenolic and flavonoid contents were quantified using the Folin-Ciocalteu and trichloroaluminum methods, respectively. In vitro antioxidant activity was assessed based on hydroxyl radical (OH[•]) and superoxide anion radical scavenging capacities. *In vitro* experiments were also conducted using mitochondria isolated from Wistar rat livers, treated with ALEPL in a dose-dependent manner and OXA. Our findings demonstrated that ALEPL contains a high concentration of phenolic compounds and exhibits notable antioxidant activity, with IC₅₀ values of 32.62 ± 5.32 µg/mL for hydroxyl radical scavenging and 205.08 ± 5.77 µg/mL for superoxide anion radical scavenging. ALEPL pretreatment effectively restored mitochondrial antioxidant enzyme activities, increased glutathione (GSH) levels, and reduced lipid peroxidation induced by OXA. These results suggest that ALEPL has the potential to serve as a natural antioxidant, supporting cancer treatment by mitigating chemotherapy-induced oxidative stress. Future studies should investigate its application as an adjuvant in clinical settings to enhance chemotherapy efficacy while reducing its side effects.

Keywords: *Pistacia lentiscus*; oxidative stress; oxaliplatin; mitochondria; antioxidant.

ÉLIMINATION DES COLORANTS BLEU DE METHYLENE ET ROUGE CONGO DANS UNE SOLUTION AQUEUSE A L'AIDE DE BIOMASSE DE FERULE

Moubarek MEBARKI^{1*}, Yasmine BENABDESLAM ¹ and Kadda HACHEM ^{1,2}

1 Département of Agronomie And Nutrition Sciences, Faculté of nature and life Sciences, University Dr.

Moulay Tahar of Saida, BP 138 cité ENNASR, 20000 Saida, Algeria

2 Laboratoire des Productions, Valorisations Végétales et Microbiennes, LP2VM, Faculté des Sciences, Université des Sciences et de la Technologie d'Oran Mohamed Boudiaf, BP 1505, El M'Naouar, 31000 Oran, Algeria

**Corresponding author: Tel./Fax: +213-774-83-1842 ; E-mail address: mebarek.mebarki@univ-saida.dz*

Abstract : La production industrielle de colorants génère des effluents hautement colorés et souvent non biodégradables, posant des risques pour l'environnement et la santé en raison de leur toxicité. Cette étude évalue l'utilisation des tiges de fêrulle (*Ferula communis L.*) de la région de Saida comme biosorbant pour traiter des eaux contaminées par deux colorants : le Rouge Congo (RC) et le Bleu de Méthylène (BM). Les résultats montrent des pH optimaux de 6 pour le BM et de 8 pour le RC, avec une adsorption rapide atteignant l'équilibre après 120 minutes. Le BM présente une capacité d'absorption supérieure, atteignant 33,83 mg/g contre 21,0 mg/g pour le RC. Le modèle de Langmuir décrit bien les données d'adsorption, avec des coefficients de corrélation R² supérieurs à 0,95. Cette étude souligne le potentiel de la biomasse de fêrulle pour traiter les eaux colorées, offrant une alternative efficace aux méthodes traditionnelles.

Keywords: Biosorption, Bleu de méthylène, Rouge Congo, Fêrulle.

PHARMACOLOGICAL INSIGHT INTO THE ANTI-INFLAMMATORY AND ANTIOXIDANT ACTIVITIES OF ANVILLEA RADIATA

Manal LAKAS^{1*}, Ibrahim SIFI², Imed eddine KADI³

1 Laboratory of Biological and Agronomic Sciences, Amar Thelidji University of Laghouat, Algeria

2 Laboratory of Fundamental Sciences, Amar Telidji University of Laghouat, Algeria

3 Research unit in medicinal plants of Laghouat, affiliated to the research center in biotechnology of Constantine, Algeria

**Corresponding author: Tel/Fax: +213699303021; E-mail address: m.lakas@lagh-univ.dz*

Abstract *Anvillea radiata* is a traditional Algerian medicinal plant with reported anti-inflammatory and antioxidant properties. This study aimed to evaluate its inhibitory effect on 15-lipoxygenase (15-LOX) and its antioxidant potential using both *in vitro* and *in silico* approaches. The anti-inflammatory activity was assessed using the FOX (Ferrous Oxidation–Xylenol Orange) assay, which measures lipid hydroperoxides produced by LOX activity. The antioxidant capacity was evaluated through DPPH, FRAP, and ABTS assays. Additionally, molecular docking simulations were performed using AutoDock Vina to investigate the interaction of key phytochemicals from *A. radiata* with the LOX active site. Results showed a significant inhibition of LOX activity by the plant extract and notable antioxidant effects across all three assays. Docking results revealed strong binding affinities between the plant's bioactive compounds and the LOX active site, supporting the *in vitro* findings. This study highlights the potential of *A. radiata* as a dual-function natural agent, with both lipoxygenase inhibitory and antioxidant activities, and supports its traditional use in managing inflammation and oxidative stress.

Keywords: *Anvillea radiata*, Anti-inflammatory activity, LOX inhibition, Molecular docking.

**DE LA PLANTE AU POTENTIEL THERAPEUTIQUE : PROPRIETES
ANTITUMORALES PREDITES DE *TEUCRIUM POLIUM* L.**

Nesrine GUENANE^{1,2}, Boulanouar BAKCHICHE ^{1,2}, Farouk BENACEUR ^{1,2} Fathi BERRABA^H et
Wissam GUENANE ^{1,2}

¹ *Laboratoire de sciences biologiques et agronomiques (LSBA), Université Amar Thelidji, Laghouat
03000, Algeria*

² *Unité de Recherche sur les Plantes Médicinales (RUMP), Centre de Recherche en Biotechnologie
(CRBt), Laghouat 03000, Algeria*

*Auteur de la correspondance : Tel./Fax: +213673449591 ; E-mail address: n.guenane.gpr@lagh-
univ.dz

Abstract : *Teucrium polium* L., une plante médicinale du bassin méditerranéen, a été étudiée pour ses propriétés antioxydantes, anti-inflammatoires et antitumorales. Dans ce travail, nous avons évalué l'activité biologique de l'huile essentielle (HE) et de l'extrait phénolique (EP) des parties aériennes de la plante récoltée dans la région du Sahara Algerian *Teucrium Polium*. L'extrait phénolique a révélé une teneur élevée en composés phénoliques totaux (110,59 mg GAE/g) et a montré une forte activité antioxydante avec une valeur IC₅₀ de 8,74 µg/mL contre le radical DPPH. L'analyse GC-MS de l'huile essentielle a permis d'identifier 33 composés, dont les principaux sont la fenchone (31,25 %), le 3-carène (15,77 %) et l'oxyde de limonène (9,77 %). Des études *in silico* ont été menées pour prédire les interactions moléculaires entre les principaux composés de l'HE et la protéine NF-kappa B, impliquée dans les processus inflammatoires et cancéreux. Trois molécules myrtenal, myrtenol et verbénol ont montré une forte affinité de liaison, avec le myrtenal présentant la meilleure stabilité et la plus faible énergie libre de liaison selon les simulations de dynamique moléculaire.

Mots clés : *Teucrium polium* L. ; Huile essentielle ; NF-kappa B ; DPPH.

PHARMACOTOXICOLOGICAL STUDY OF AQUEOUS AND HYDRO-METHANOLIC EXTRACTS OF *PERGULARIA TOMENTOSA* L.

Asma SAIDI^{1,2*}, Nadjiba TOUALBIA ¹ and Leila HAMBABA²

¹Department of natural and life sciences, faculty of natural and life sciences and earth and universe sciences , University of Mohamed Khider, Biskra 07000, Algeria

²Laboratory of Biotechnology of Bioactive Molecules and Cellular Physiopathology (LBMBPC), Department of Microbiology and Biochemistry, Faculty of Natural and Life Sciences, University Batna , 05078, Algeria *Corresponding author: Tel./Fax: +213-552-62-5054 ; E-mail address: asma.saidi@univ-biskra.dz

Abstract: In the search of new drugs to treat several diseases and to face various epidemic and pandemic situations, plants may be a good candidate resource due to their therapeutic characters. Unfortunately, the toxicology profile of many species of them has not been validated yet, including the Saharan species *Pergularia tomentosa* L. (Asclepiadaceae). The present work submitted to investigate the oral acute toxicity of aqueous (PAE) and MeOH80% (PME) extracts of *P. tomentosa* aerial-parts. The toxicological study was performed on *Swiss albino* male mice. Compared to control group (n=5), a single dose of 2000 or 5000mg/kg of each tested extracts was sequentially administrated (10ml/kg) to animals (groups 2-5). The mortality, variation of bodyweight and behavior changes were daily observed during a period of 14 days. The Hematological and biochemical parameters of blood samples were also analyzed at the end of the experiment. The obtained results showed that some clinical signs were observed only during the first 3 days on animals of group 2 and 3 given PAE (2000 and 5000mg/kg). However, no mortality and no significant bodyweight changes were seen, compared to control group. Moreover, a significant ($p \leq 0.05$) increase in liver parameters was noted in group 2 and 3. In addition, WBCs values have been increased significantly in all treated groups (2-5). Based on OECD guidelines N°425, *P. tomentosa* is classified as nontoxic drugs from category 5, with oral LD₅₀ >2000 mg/kg(b.w). That allow their use in complete safety at selected therapeutic doses in further studies.

Keywords: *Pergularia tomentosa*, Toxicological study, Hematological analysis, Biochemical analysis, Behavior changes.

CONTRIBUTION TO AN ETHNOBOTANICAL STUDY ON PLANTS WITH ANTISEPTIC AND HEALING PROPERTIES IN THE KHENCHELA AND BATNA REGIONS

Saliha TORCHE ^{1*}, Selma BENHIZIA², Hibat Allah NEFISSI³ and Khadidja SAHRAOUI⁴

¹Laboratory of Toxicology and Pharmacology, Institute of Veterinary Sciences, University Frères Mentouri, Constantine1, 25000, Constantine, Algeria

²Animal Pathology Research Laboratory PADESCA, Institute of Veterinary Sciences, University Frères Mentouri, Constantine1, 25000, Constantine, Algeria

³Veterinary Doctor, Batna, Algeria

⁴Veterinary Doctor, Khenchela, Algeria

*E-mail: s.torche17@gmail.com; saliha.torche@umc.edu.dz, Tel.: +213775842948

ABSTRACT : This study aims to document the medicinal plants with antiseptic and healing properties, in order to preserve and disseminate traditional medicinal knowledge that would otherwise be lost. Thirty herbalists were interviewed in semi-structured interviews to gather ethnobotanical data in the states of Batna and Khenchela. Ethnobotanical information collected focused on medicinal plants, including the specific parts of plants used, methods of preparation, modes of use, and the types of ailments treated. The frequency of citations (FC) was calculated in order to evaluate the plant species that were utilized by the regions. Through our investigation, we were able to identify 20 plant species that are used for their antiseptic and healing properties. Among them, *Juniperus phoenicie*, *Artemisia herba alba*, and *Teucrium polium* which have higher citation frequencies (FC) of 14.77%, 11.36% and 11, 36% respectively. These species belong to 16 different botanical families were *Lamiaceae* (31.25%) is the most mentioned. Leaves (26.32%) were the most utilized plant part, and the preparation of a decoction (47.37%) was the most preferred method of processing and application. A large portion of the plants was consumed as herbal tisane (63.16%) by oral administration for the treatment of internal infections (57.89%). Furthermore, 47.37% were used topically as powder or essential oil. The results obtained are a very valuable source of information for the regions studied and for the national medicinal flora. They can be regarded as a source of data for scientific investigations into new natural chemicals in the fields of phytochemistry and pharmacology.

Keywords: Medicinal plants; Ethnobotanical survey; Antiseptic; Healing

QUANTITATIVE ETHNOBOTANICAL SURVEY ON THE COSMETIC USE OF
PLANTS IN CONSTANTINE-ALGERIA

Fatima Zohra BADAOU^{1,2*}

¹*Department of Pharmaceutical Engineering, Faculty of Processes Engineering, Salah Bounider University-Constantine 3, Constantine 25000, Algeria*

²*Process Engineering Laboratory for Sustainable Development and Health Products, Constantine*

**Corresponding author: Tel: 06-62-36-33-37 ; E-mail address: fatimazohra.badaoui@univ-constantine3.dz*

Abstract: An ethnobotanical survey on the use of plants for cosmetic purpose was carried out in the wilaya of Constantine-Algeria. The main objective of this study is to identify the plants used in cosmetics and their relative importance within the population. The study was set up over a six-weeks period running from April 2024 to the end of May 2024 to conduct a survey on plants used in cosmetics. The ethnobotanical study was carried out following a series of surveys using a pre-established questionnaire in French and Arabic, in order to gather the identity characteristics of 106 informants and their knowledge of the cosmetic use of plants. Ethnobotanical indices (relative frequency of citation, use value, informant consensus factor and fidelity level) were determined. The majority of the participating population are young students who use essential oils purchased from herbalists for skin care. Most participants find herbal cosmetics natural, healthy, available and affordable. The highest relative citation frequency and use value (RFC = 0.34, UV = 0.58) were attributed to Aloe vera L. the high value of informant consensus factor was recorded for the skin care category (ICF = 0.79). The survey carried out in the wilaya of Constantine has given an idea on the cosmetic use of plants, and can serve as a basis for orienting the algerian market towards natural products.

Keywords: Constantine, cosmetics, ethnobotanical indices, plants.

L'EFFET DE PRETRAITEMENT CHIMIQUE SUR LA PRODUCTION DE BIOGAZ A PARTIR DES BOUES DE LA STATION D'EPURATION

Zana ATAOUAT^{1*}, Abdelmadjid HABCHI¹, Mohamed El Amine DAHOU²

¹ *laboratoire Energie, Environnement et Système d'information (LEES), Université d'Adrar*

² *Laboratoire des Matériaux Catalytique et Procédés Industriels, Université d'Adrar*

*Corresponding author: Tel./Fax: 0558190369; E-mail address: ataouat.zana@univ-adrar.edu.dz

Résumé : Cette étude porte sur l'évaluation expérimentale de l'influence d'un prétraitement chimique alcalin, utilisant deux solutions à 10 % (m/m) — l'hydroxyde de sodium (NaOH) et l'hydroxyde de potassium (KOH) — sur la digestion anaérobie des boues d'une station d'épuration située à Timimoun, dans le sud-ouest de l'Algérie. La digestion a été réalisée en mode batch, sous conditions mésophiles (35 ± 2 °C). Plusieurs paramètres de stabilité du processus ont été suivis, notamment le pH, les acides gras volatils (AGV), l'alcalinité et le volume de biogaz produit. En parallèle, des indicateurs de performance du traitement, tels que la demande chimique en oxygène (DCO) et la teneur en matière organique, ont été analysés. Les résultats obtenus après 15 jours de digestion montrent un impact positif du prétraitement alcalin, avec une augmentation du volume de biogaz de 61 % pour le KOH et de 40 % pour le NaOH, par rapport au témoin. Cette amélioration est attribuée à la capacité des agents alcalins à rompre les liaisons complexes, facilitant ainsi la dégradation de la matière organique par les micro-organismes anaérobies. Cette recherche confirme l'efficacité du prétraitement alcalin dans l'optimisation de la production de méthane à partir des boues, et souligne son potentiel pour le développement de technologies de bioénergie durables et économiquement viables, notamment dans les régions fortement productrices de déchets.

Keywords: Digestion anaérobie; Prétraitement chimique; Biogaz.

EXTRACTION AND CHARACTERIZATION OF A BIOPOLYMER FROM BIOMASS WASTE

Zoubida KOUROULOU^{1,2*}, Mahmoud BELALIA^{1,2}, Fouad MEKHALEF BENHAFSA³, Fatima Zohra BELKACEM^{1,2}, Halima DELALI^{1,2} and Asmae BENABBOU^{1,2}

¹*Department of Chemistry, University of Mostaganem, Mostaganem, 2700, Algeria.*

²*Laboratory of Structure, Elaboration and Application of Molecular Materials (SEA2M), University of Mostaganem, Mostaganem, 2700, Algeria.*

³*Center for Scientific and Technical Research in Physico-Chemical Analyzes, CRAPC, BP384, Bou-Ismaïl, 42004, Tipaza, - Algeria.*

**Corresponding author: Tel./Fax: +213557605119; E-mail address: zoubida.kouroulou.etu@univ-mosta.dz*

Abstract: In the context of renewable resource valorization, this study focuses on the extraction and characterization of cellulose from locally available lignocellulosic biomass. The extraction process was developed using a mild, environmentally friendly chemical treatment, allowing for the selective removal of lignin and hemicelluloses. The extracted cellulose was analyzed by Fourier Transform Infrared Spectroscopy (FTIR), confirming the presence of typical cellulose functional groups and indicating good purity. Thermogravimetric Analysis (TGA) was also conducted to assess the thermal stability of the obtained biopolymer. Results show a thermal behavior consistent with pure cellulose, highlighting its potential for bio-based material development. This work contributes to the sustainable transformation of biomass into valuable materials, aligned with the principles of green chemistry and circular economy.

Keywords: Biopolymer, Biomass valorization, Green chemistry, FTIR analysis, Thermogravimetric analysis

**CARACTERISATION CHROMATOGRAPHIQUE ET
SPECTROPHOTOMETRIQUE DES COMPOSES PHENOLIQUES D'UNE PLANTE
MEDICINALE**

Wissam GUENANE², Omar MECHRAOUI^{1,2}, Aissa TOUNSSI^{1,2} Fathi BERRABA^H et Nesrine
GUENANE ^{1,2}

¹ *Laboratoire de sciences biologiques et agronomiques (LSBA), Université Amar Thelidji, Laghouat
03000, Algeria*

² *Unité de Recherche sur les Plantes Médicinales (RUMP), Centre de Recherche en Biotechnologie
(CRBt), Laghouat 03000, Algeria*

**Auteur de la correspondance : Tel./Fax: +213696909876 ; E-mail address: w.guenane.gpr@lagh-
univ.dz*

Abstract : Les plantes médicinales constituent une source importante de composés bioactifs, notamment les polyphénols et les flavonoïdes, qui jouent un rôle essentiel dans leurs propriétés antioxydantes et thérapeutiques. Cette étude a pour objectif d'identifier, de caractériser et de quantifier ces composés dans un extrait d'une plante médicinale à l'aide de techniques chromatographiques et spectrophotométriques. L'extraction des métabolites secondaires a été réalisée à l'aide d'un solvant hydro-méthanolique. L'analyse qualitative et quantitative des composés phénoliques a été effectuée par chromatographie liquide à haute performance (HPLC). Le dosage des polyphénols totaux a été réalisé selon la méthode de Folin-Ciocalteu, tandis que les flavonoïdes ont été quantifiés par complexation au chlorure d'aluminium, selon une méthode colorimétrique. Les résultats ont révélé une teneur élevée en composés phénoliques, avec une présence marquée d'acide caféique, d'acide chlorogénique et d'acide gallique. Ces données confirment le potentiel bioactif de la plante étudiée et ouvrent des perspectives prometteuses pour des applications pharmacologiques futures.

Mots clés : Plante médicinale – Composés phénoliques – Polyphénols – Flavonoïdes – HPLC – Spectrophotométrie – Folin-Ciocalteu – Chlorure d'aluminium – Activité bioactive – Extraction hydro-méthanolique.

ANTIMICROBIAL ACTIVITY OF FRUIT PEELS EXTRACTS CULTIVATED IN ALGERIA.

BOUTARFA Soumia^{1,2,*}, MAYOUF Nozha^{1,2}, BRAHIMI Aya Malek¹ and OUANADA Nora¹

1 Faculty of natural and life Sciences, University Abbès Laghrour, Khenchela, Algérie

2 Laboratoire de biotechnologie, eau, environnement et santé, Faculté de sciences naturelles et de vie, Université de Khenchela, Algérie

**Corresponding author: Tel./Fax: +213664667046 ; E-mail address: soumia.boutarfa@univ-khenchela.dz*

Abstract: Medicinal plants, particularly fruit peels, have been recognized for their bioactive substances, which can treat various health issues. Research shows that fruit and vegetable peels contain phenolics, flavonoids, tannins, and terpenoids with antibacterial and antioxidant properties, making them potential solutions for addressing antimicrobial resistance. Orange and pomegranate peels, particularly *Citrus sinensis* and *Punica granatum*, are particularly valuable in Algerian agriculture. This study investigated the antimicrobial activities and phytochemical content of hydro-methanolic and hydro-ethanolic peel extracts from *Punica granatum* (pomegranate) and *Citrus sinensis* (orange). The various extracts were evaluated against five pathogenic bacterial strains: *Bacillus cereus*, *Staphylococcus aureus*, *Escherichia coli*, *Klebsiella pneumoniae*, *Pseudomonas aeruginosa*, and four clinical strains of *E. coli*, at different concentrations, utilizing disc diffusion assays. The findings indicated that both fruit peel extracts were effective against the examined strains. Moreover, ethanolic and methanolic extracts of pomegranate exhibited significantly enhanced inhibitory activities, particularly against *Staphylococcus aureus*, *Escherichia coli*, and *Pseudomonas aeruginosa*. Conversely, orange peel extracts demonstrated intermediate efficacy, with methanolic extracts surpassing their ethanolic counterparts. Moreover, the minimum inhibitory concentration tests validated the enhanced antibacterial efficacy of pomegranate peel extracts, which demonstrated effectiveness at far lower concentrations than orange extracts. Additionally, the plant extracts underwent phytochemical screening, revealing the presence of flavonoids, polyphenols, saponins, tannins, quinones, and terpenoids. Quantitative analysis indicated a significant abundance of flavonoids, with values between 24 ± 0.050 and 60 ± 0.80 mgCE/g. These findings confirm the antibacterial efficacy of these fruit byproducts and suggest their potential application as medicinal agents.

Keywords: Antimicrobial activity; citrus peels, phytochemical analysis, pomegranate

SUSTAINABLE BIOCATALYSIS USING YEAST-DERIVED ENZYMES: A GREEN APPROACH TO MOLECULAR DESIGN

Kaouthar HOUITI^{1*}, Smail MEHDA² and Pietro PUZZINI³

¹*Department of Cellular and Molecular Biology, Faculty of natural sciences and life, Laboratory of Biology, Environment, and Health, University of El-Oued, El-Oued 39000, Algeria.*

²*Department of Agronomy, Faculty of Natural and Life Sciences, University of El-Oued, El-Oued 39000, Algeria.*

³*Department of Agricultural, Food, and Environmental Sciences, University of Perugia Perugia,,Italy*

*Corresponding author: Tel./Fax: +213669342032 ; E-mail address: houiti-kaouthar@univ-eloued.dz

Abstract: Yeast-derived enzymes are increasingly recognized for their exceptional catalytic potential and ecological compatibility in green chemistry . This review synthesizes recent advances (2021–2025) in the application of enzymes from unconventional yeasts, particularly extremophilic species, as highly adaptable biocatalysts in sustainable molecular design. This work compiles and compares biochemical characterizations, catalytic applications, and process optimizations from current literature, with a focus on their potential integration into circular bioprocesses and green industrial platforms. Key findings reveal that these enzymes exhibit unique properties such as broad substrate tolerance, high stereoselectivity, and operational stability under harsh industrial conditions, making them highly attractive for low-impact synthesis. Moreover, their natural resistance to temperature, salinity, and pH shifts enables efficient biotransformations in non-conventional environments. In addition, their eukaryotic origin supports post-translational modifications, enhancing their versatility in pharmaceutical and agrochemical pathways. The enzymes' capacity to operate in solvent-minimized or solvent-free conditions, and their compatibility with biodegradable systems, underline their significance in future-oriented catalysis. Furthermore, recent insights suggest that combining biocatalyst selection with computational tools may open new frontiers in enzyme performance modeling . Ultimately, this review highlights the strategic importance of yeast-derived enzymes as sustainable tools, not only for their inherent biochemical strength, but also for their alignment with the evolving goals of green chemistry and environmentally responsible innovation .

Keywords: Yeast-derived enzymes; Biocatalysis; Green chemistry; Sustainable synthesis; Enzyme valorization.

PHENOLIC CONTENT, ANTIOXIDANT ACTIVITY OF ESSENTIAL OILS OF *TEUCRIUM POLIUM* AND *ARTEMISIA HERBA ALBA*: COMBINATION EFFECT

Aicha KHEMKHAM^{1*}, Salim IMRAZEN¹ and Larbi FEITAS¹

¹*Faculty of sciences of nature and life, Ziane Achour University of Djelfa, Algeria*

**Corresponding author: Tel : +0-069-612-7023 ; E-mail address: aicha.khemkham@univ-djelfa.dz*

Abstract: The pharmaceutical industry utilizes medicinal plants due to the presence of active chemical compounds that serve as agents for drug synthesis. Plant essential oils are widely regarded as safe and effective natural antioxidants and antibacterial agents, and they are also considered promising candidates for cancer treatment. Many studies have reported the potential synergistic effects of essential oils as an effective strategy to enhance their bioactivity. However, the combined effects of essential oils derived from plants cultivated in the steppic region of Djelfa have been rarely investigated. This study proposes, for the first time, an examination of the synergistic antioxidant activity of essential oils extracted from two aromatic and medicinal plants. *Teucrium polium* and *Artemisia herba-alba*, from the Djelfa region. *Teucrium polium* belongs to the family of Lamiaceae and *Artemisia herba-alba* belongs to the family of Asteraceae. The essential oils were extracted by hydrodistillation of the aerial parts of the plants. The total phenolic content was assessed by Folin ciocalteu reagent. The antioxidant properties were evaluated using α -diphenyl- β -picrylhydrazyl (DPPH) radical scavenging activity [4]. The essential oil from *Artemisia herba alba* gave a yield of 1.46% and from *Teucrium polium* 0.57%. Total polyphenol content: the essential oil of *Artemisia herba alba* contained 20.97 mg EAG/g HE, while the extract of *Teucrium polium* contained 15.73 mg EAG/g HE. In the DPPH test, the two EOs of *Teucrium polium*, *Artemisia herba alba* and their mixture had an IC₅₀ of 81.52 μ g/ml, 32.70 μ g/ml and 55.52 μ g/ml, respectively. Antioxidant activity varies from one species to another. These medicinal plants in general remain of great economic and health interest. Application of mixture of essential oils is promising for food additives in order to prevent or delay the oxidative degradation of foods.

Keywords: *Artemisia herba-alba*, *Teucrium polium*, Essential oil, Combination effect, Antioxidant activity

VALORIZATION OF EGGHELL-DERIVED BIOSORBENT FOR EFFICIENT DYE REMOVAL FROM WASTEWATER

Fatima SAAD^{1*}, Boumediene BOUNACEUR¹

¹*Department of Chemistry, University of Oran 1, Algeria*

*Corresponding author: E-mail address: fatimasaad9@yahoo.com

Abstract: This study demonstrates the transformation of eggshell waste into an efficient, eco-friendly biosorbent for dye removal from contaminated water. Through chemical treatment and high-temperature calcination (900°C), the modified eggshells achieved a 94.5% removal efficiency for synthetic dyes, including trisacrylamide blue, methylene blue, and methyl orange. The biosorbent exhibited robust performance across a wide pH range (4–9) and maintained 85% of its initial adsorption capacity after multiple regeneration cycles. Structural analysis via FTIR and XRD confirmed the formation of active surface sites and enhanced porosity, which improved dye capture. UV-Vis spectroscopy verified near-complete decolorization, with absorbance values reduced to baseline levels. Compared to untreated eggshells and commercial adsorbents, the modified material showed superior performance and cost-effectiveness. This work presents a dual environmental benefit: (1) valorization of agricultural waste into a functional material and (2) an affordable solution for textile wastewater treatment. The simplicity, scalability, and sustainability of this approach highlight its potential for industrial applications, aligning with circular economy principles. By addressing both waste management and water pollution challenges, this study offers a practical strategy for eco-friendly water purification.

Keywords: Eggshell waste, Biosorbent, Dye removal, Wastewater treatment, Sustainable materials.

DETERMINATION OF BIOACTIVE COMPOUNDS, ANTI-INFLAMMATORY AND ANTIOXIDANT PROPERTIES OF HYDROALCOLIC EXTRACT OF *GALUIM APARINE L*

Soulef SAOUDI, Wafa TADRENT, Nihed BARGHOUT, Dounia Zad BEN LATRECHE, Nozha MAYOUF, BETTIHI Sara, Assia BENTAHAR, Saliha DJIDEL, Amel BOUAZIZ, Saliha DEHAMNA, Seddik KHENNOUF

Laboratory of Phytotherapy Applied to Chronic Diseases, Department of Biology and Animal Physiology, Univ Setif 1, 19000, Algeria.

Laboratory of Biotechnology, water, Environement and Health, Faculty of Nature and Life Sciences. University Abbeès Laghrour, Khenchela. Algeria.

**Corresponding author: Tel. 0667234849; Email: Soulef2016bio@gmail.com*

Abstract: Oxidative stress is the cause of a number of diseases and is driving the search for new antioxidant remedies. *Galium aparine L* is a widespread plant in temperate zones, commonly known as bedstraw, belonging to the Rubiaceae family and traditionally used for its medicinal applications. The aim of the present study was to investigate the antioxidant and anti-inflammatory activities following quantification of bioactive compounds, in particular polyphenols, flavonoids and tannins from hydroethanolic extracts of *Galium aparine L* leaves and stems harvested in the Beni Ourthilan region, wilaya of Sétif. *In vitro* antioxidant activity was estimated using four different tests: DPPH, ferrous iron chelation, reducing power and β -carotene. Quantitative estimation of total phenolic compounds using the spectrophotometric method showed that the extract is rich in polyphenols, flavonoids and tannins. This study showed that the extract has excellent antioxidant power. These results may be attributed to the quality of the phenolic compounds and flavonoids in this extract. The *in vitro* anti-inflammatory activity was assessed using the thermal denaturation method for BSA and ovalbumin. This study showed that the extract had an important capacity to protect BSA against thermal denaturation (71.78% at 10 mg/ml). Similarly, analysis of the protection of ovalbumin against denaturation with value of $62.00 \pm 2.26\%$ at 20 mg/ml. In conclusion, the results of this work have enabled us to confirm that the plant has very good antioxidant, coagulant and anti-inflammatory properties, which merit greater interest from the pharmaceutical and parapharmaceutical sectors.

Key words: *Galium aparine L*, antioxidant, anti-inflammatory, polyphenols.

BIOSORPTION OF Cu(II) USING EGGSHELL-ALGINATE COMPOSITE BEADS: KINETIC AND THERMODYNAMIC STUDY

T. BELAID^{1*}, S. OUKHEMAMOU¹, Z. CHEMACHE¹, S. BEY¹, M. BENAMOR¹

¹ *Laboratory of Membranes Processes, and Techniques of separation and recovery (LPMTSR),*

Faculty of Technology, University of Bejaia, Algeria

Tel./Fax: +213-774-09- 6634 ; E-mail : taous.belaid@univ-bejaia.dz

Abstract: Heavy metal pollution, particularly from copper ions (Cu^{2+}), poses serious environmental and health risks due to their persistence and toxicity. This study investigates the use of eggshell powder, a low-cost and sustainable biosorbent, encapsulated in sodium alginate beads to enhance handling and adsorption efficiency. The composite beads were prepared by extrusion and ionotropic gelation in a calcium chloride solution. Batch adsorption experiments demonstrated that optimal copper removal occurs at $\text{pH} > 4$, with $m \geq 4$ g of eggshell powder, 80 minutes of contact, 200 rpm stirring, and room temperature. The adsorption behavior followed the Langmuir isotherm, indicating monolayer adsorption on a homogeneous surface. The maximum adsorption capacity reached 50 mg/g. Thermodynamic analysis showed that the process is spontaneous and endothermic, with a low enthalpy change ($\Delta H^\circ = 2.694$ kJ/mol), suggesting physisorption as the dominant mechanism. These results highlight the potential of alginate–eggshell composite beads as efficient and eco-friendly biosorbents for Cu^{2+} removal in wastewater treatment.

Keywords: Eggshell powder, Alginate beads, Copper removal, Adsorption isotherm.

VALORIZATION OF FABA BEAN (VICIA FABA L.) RESIDUES THROUGH FTIR CHARACTERIZATION FOR INTEGRATION INTO BROILER CHICKEN FEED

HEDIA Nacera¹, MEZIANE Ahmed Malika¹, BRADA Marwa Ilham¹, ROUAM Djawad², SADOK Zeyneb¹, NEHARI Assia¹

¹*LBRN Laboratoray, Department of Food Sciences, University of Chlef Algeria*

²*Geo-Environment and Spatial Development Laboratory, University of Muspapha Stambouli,*

**Corresponding author: Tel./Fax: +213797165660 ; E-mail address: hedianacera27000@gmail.com*

Abstract: The valorization of agro-industrial residues as renewable resources represents a promising strategy within the framework of sustainable food systems and circular economy. In this study, faba bean (*Vicia faba* L.) residues were investigated with the aim of integrating them into broiler chicken feed as a sustainable and functional ingredient. Samples were collected, dried, finely ground, and subjected to proximate analysis and Fourier Transform Infrared Spectroscopy (FTIR) in order to determine their biochemical composition. Results showed a crude protein content of 14.62% (± 0.29), confirming the nutritional value of faba bean residues for poultry diets. The FTIR spectra revealed characteristic absorption bands in the region 1200–1000 cm^{-1} , corresponding to C–O and C–C stretching vibrations of polysaccharides, particularly starch and hemicelluloses. Additional bands around 1650–1540 cm^{-1} were associated with amide I and II vibrations, indicating the presence of proteins, while a broad band near 3300 cm^{-1} reflected O–H stretching linked to polysaccharides and structural water. These signals confirmed the coexistence of carbohydrates, proteins, and functional groups. These findings demonstrate that faba bean residues have a dual nutritional potential (protein and energy) and can be effectively integrated into broiler chicken diets. This research supports the valorization of natural and renewable resources while contributing to sustainable poultry production in line with the principles of circular economy and bioprocessing.

Keywords: Faba bean residues, FTIR, renewable resources, circular economy.

**CHARACTERIZATION, PHYTOCHEMICAL AND BIOLOGICAL ACTIVITIES OF
ESSENTIAL OILS OF FEW SPONTANEOUS PLANTS IN TIARET REGION
(ALGERIA)**

Adda MESSAOUDA^{1*}, Omar YAMINA¹ and Doukani KOULA²

Laboratory of Agro-Biotechnology and Nutrition in the Semi-arid Zone , faculty of nature and life sciences, university of Tiaret ,Algeria.

University of Ibn Khaldoun Tiaret- Algeria.

**Corresponding author: Tel./Fax: +2137 95 93 79 27 ; E-mail address:
addamessaouda2013@gmail.com*

Abstract: Researchers are looking for novel ways to treat infections since germs are becoming more resistant to traditional medicines at an alarming rate. Among these, essential oils (HE) appear as promising natural agents thanks to their antimicrobial properties. Rich in compounds such as phenols, terpenes and aldehydes, essential oils have demonstrated an ability to inhibit the growth of many bacterial strains, including those resistant to antibiotics. Plants with therapeutic value are valued. The identification of the chemical components of essential oils from some aromatic and therapeutic plants that are widely utilized by Mediterranean Basin residents. One can access hydro distillation in the University of Tiaret laboratory after collecting species, washing, drying, and allowing light and air to enter in compliance with a clearly established methodology. Chromatography in phase gazeuze coupled to mass spectrometry was used to examine these hydro-distilled essential oils. With an extraction yield of 1.13%, the essential oil yield from *Mentha spicata* produced using the hydro distillation process is indeed high. Nineteen (19) chemicals are found by CPG/MS chromatographic analysis, with pulegone accounting for 42.32% of the total. Monoterpenes and sesquiterpenes make up the rest. Enhancing medicinal plants contributes to the preservation of ancient medical methods and traditional knowledge. In an attempt to strengthen Algeria's economy and increase the value of its bioresources, it also promotes the cultivation and commercialization of these plants, which helps the economies of areas with high biodiversity.

Key words: Essential oil, *Mentha spicata*, hydro distillation, and antibacterial activity, Tiaret

ENZYMATIC BIOPROCESSES FROM THERMAL BACTERIAL STRAINS: POTENTIAL AND PERSPECTIVES

Hanane MELLAL ^{1,2*}, Khaoula AROUA ³, Oumaima NAILI ^{1,2}, Saida HANOUN ², Nozha MAYOUF ^{1,2} and OUANAS Miyada^{2,4}

¹ *Laboratory of Biotechnology, Water, Environment and Health, Faculty of Natural and Life Sciences, University of Abbès Laghrour-Khenchela, Algeria*

² *Department of Molecular and Cellular Biology, Faculty of Sciences, University of Abbès Laghrour-Khenchela, Algeria*

³ *Department of Agronomy, Faculty of Sciences, University of Abbès Laghrour-Khenchela, Algeria*

⁴ *Department of Ecology, Faculty of Sciences, University of Abbès Laghrour-Khenchela, Algeria*

*Corresponding author: E-mail address: hanane.mellal@univ-khenchela.dz

Abstract: Extreme environments, such as thermal springs, represent invaluable reservoirs of microorganisms endowed with unique metabolic capabilities. In this context, the present study aims to explore the enzymatic potential of thermophilic bacteria isolated from the Hammam Tamersite thermal spring (Khenchela, Algeria), with a view to their valorization in sustainable industrial bioprocesses. Ten thermophilic bacterial strains were isolated and subjected to phenotypic and enzymatic characterization. Several strains exhibited diverse enzymatic profiles, with significant activities in amylase, protease (caseinase, gelatinase), and oxidase. In particular, strains E3, E4, and E12 demonstrated a broad spectrum of hydrolytic activities, suggesting strong potential for applications in biomass degradation, agro-food processing, and industrial wastewater treatment. The strains also showed good tolerance to extreme conditions (temperature, salinity, pH), which are desirable traits for robust biocatalytic processes. Preliminary identification revealed genera known for their biotechnological relevance, such as *Geobacillus*, *Thermus*, and *Anoxybacillus*. This study highlights the potential of these thermal bacteria as sources of thermostable enzymes and opens promising avenues for the development of eco-efficient bioprocesses. Future work will focus on molecular identification, purification, and detailed characterization of the target enzymes, as well as the evaluation of their performance under industrial conditions.

Keywords: *Thermophilic bacteria; Thermostable enzymes; Bioprocesses; Biotechnological valorization; Thermal springs*

***IN SILICO* EXPLORING OF PHYTOCHEMISTRY COMPONENTS AND *IN VITRO*
BIOACTIVITY OF ESSENTIAL OILS: BIOINFORMATICS STRUCTURE AND
BIOLOGICAL PROSPECTS**

Abdelmouman LAMOURI^{1*}, Miryam OUIS² and Fethi BENBELAÏD³

¹*Microbiology, Laboratory of Environment and Sustainable Development, Department of Biology, Faculty of Natural and Life Sciences, University of Relizane, Algeria*

²*Plant physiology, Laboratory of Environment and Sustainable Development, Department of Biology, Faculty of Natural and Life Sciences, University of Relizane, Algeria*

³*Microbiology, Department of Biology, Faculty of Sciences and Technology, University of Temouchent, Algeria*

*Corresponding author: Tel: +213-772-73-9794 ; E-mail address: abdelmouman.lamouri@univ-relizane.dz

Abstract : With growing interest in phytobiotics as natural sources of essential oils compounds, the need to decode their phytochemical profiles and understand their bioactivity is increasing. Modern *in silico* tools combined with *in vitro* bioassays open new avenues for therapeutic and preventive applications of essential oils. This study aims to integrate *in silico* bioinformatics and *in vitro* testing to gain a deeper understanding of their mechanisms and therapeutic importance against human and veterinary microbial diseases, exceeding traditional methods of random drug selection. The active components of selected essential oils were identified through phytochemical analysis. Molecular docking simulations were used to predict interactions with key microbial protein targets. Complementary antimicrobial assays were performed *in vitro*, supported by structural-functional analysis using bioinformatics tools. *In silico* analysis demonstrated strong binding affinity for aldehydes and monoterpenes, as well as key compounds such as carvacrol, thymol, and linalool, which exerted potent inhibitory effects against microbial target receptors and enzymes. Structural analysis revealed the importance of molecular conformation in enhancing binding affinity. These results confirmed the effectiveness of these compounds, with antimicrobial efficacy exceeding 85% in some oil samples against bacterial and viral strains. The combination of *in silico* and *in vitro* analysis approaches has proven efficient in identifying and validating active compounds, reducing the need for extensive experimental testing. Bioinformatics enhances the predictive power of research and drives the discovery of pharmacologically relevant phytochemicals. We propose expanding the use of databases and exploiting their results to develop effective and eco-friendly treatment solutions.

Keywords: Phytobiotics; Phytochemicals; Diseases; Molecular docking; Bioassays.

**PHYTOCHEMICAL SCREENING, THERAPEUTIC AND MEDICINAL VIRTUES
OF A PLANT OF THE GINKGOACEAE FAMILY**

Ouahiba ARAB^{1*}, Fatiha SEBIH^{1,2}, Salima BELLAHOUEL¹, Nadia KAMBOUCHE¹

¹ : *Laboratoire de synthèse organique et appliquée (LSOA), Département chimie, Faculté sciences exactes et appliquées, Université Oran 1 Ahmed BEN BELLA, BP 1524 El M'naouer, 31000 Oran, Algeria.*

² : *Laboratoire de synthèse organique et appliquée, Département génie chimique, Faculté de chimie, Université des Sciences et de la Technologie d'Oran Mohamed-Boudiaf USTOMB, BP 1505 El M'naouer, 31000 Oran, Algeria.*

*Corresponding author: Tel./Fax: +213675268469 ; E-mail address: arab.ouahiba39@gmail.com

Abstract: Phytotherapy is an alternative medicine that promises to heal naturally with plants. This therapy uses all the elements of a plant, and was publicly recognized by the French Ministry of Health as a medicine in its own right in the 1980s. Phytotherapy medications are titrated in active ingredients. In other words, they contain a more or less significant, but always known, concentration of active substances. For the past hundred years, synthesis has been squelching plant-derived medications, aside from antibiotics and anti-tumor drugs. However, thanks to the development of molecular-level testing, natural products are opening up new research avenues. Algeria is a country with a significant reservoir of medicinal and phytotherapeutic plants that must be exploited for various uses, particularly in the manufacture of medicines. In Algeria, more than 500 medicinal plants have been identified, as well as rare medicinal plants growing only in Saharan regions and others endemic to North African countries. Our plant is considered a living fossil. Its green leaves, often composed of two lobes (bilobed), are full of important therapeutic and medicinal properties. Whether for its vasodilatory effect on blood circulation or its antioxidant effect, this plant is used as a dietary supplement for memory, and has proven effective in treating disorders related to cerebral vascular insufficiency: memory loss, decreased concentration, dizziness, headaches, hearing loss, ringing in the ears, tinnitus, senile dementia, and early Alzheimer's disease. This study aims to determine the bioactive molecules present in this plant through phytochemical screening, using color/precipitation reactions and thin-layer chromatography techniques. This work therefore makes it possible to determine the richness of this species in secondary metabolites, in order to enhance and exploit it in various fields, particularly medicinal and cosmetic.

Keywords: medical plant, phytotherapy, secondary metabolites, phytochemical screening, bioactive molecules

**ÉTUDE PHYTOCHIMIQUE ET BIOACTIVITE DES HUILES ESSENTIELLES
D'UNE PLANTE ASTERACEAE: ARTEMISIA HERBA-ALBA PROVENANCE DE
HASSI BEHBEH (WILAYA DE DJELFA, ALGERIE)**

BOUNAB Souhila, MEDJEBER Mohammed, BERKANE Zakia Imane, MAHDJOUB Dalal, DIF Imane et MAAZOUZ Seif –Eddine

Centre de recherche en Agropastoralisme (CRAPast) Djelfa, Algeria.

*Corresponding author: Tel: +213 0-778-76-66 58 ; E-mail address: *bounabsouhila@gmail.com*

Résumé : Les plantes médicinales sahariennes représentent une richesse phytothérapeutique encore peu exploitée. Cette étude porte sur l'analyse phytochimique et l'évaluation des propriétés biologiques des huiles essentielles d'*Artemisia herba-alba*, une plante médicinale endémique du Sahara Algerian, traditionnellement utilisée dans la médecine populaire pour ses effets antiseptiques, antispasmodiques et digestifs. L'extraction des huiles essentielles a été réalisée par hydrodistillation, suivie d'une analyse par chromatographie en phase gazeuse couplée à la spectrométrie de masse (CPG-SM). Les résultats ont mis en évidence une richesse en composés bioactifs Monoterpéniques oxygénés tels que le camphre (25 %), le 1,8-cinéole (18 %) et Cétones tels que la thuyone (15 %) et le borneol (8 %). Les Sesquiterpènes et les Esters se présentent en faible quantité tels que le Caryophyllène, germacrène et l'Acétate de bornyle Les tests d'activités biologiques ont révélé un fort pouvoir antimicrobien vis-à-vis de souches bactériennes pathogènes (*E. coli*, *S. aureus* et *Enterrococcus feacalis*) et une activité antifongique modérée. Par ailleurs, les tests antioxydants (DPPH) ont montré une bonne capacité de piégeage des radicaux libres. Ces résultats confirment le potentiel thérapeutique d'*Artemisia herba-alba* et soutiennent son intégration dans les applications pharmaceutiques et cosmétiques. La valorisation de cette ressource saharienne pourrait contribuer au développement de produits naturels innovants tout en préservant le patrimoine médicinal local.

Mots-clés : Phytochimie, Huiles essentielles, *Artemisia herba-alba*, Activités biologiques, Djelfa.

**ORGANIC SYNTHESIS OF NEW PROLINE-BASED METAL COMPLEXES:
SPECTROSCOPIC CHARACTERIZATION AND ANTIBACTERIAL POTENTIAL**

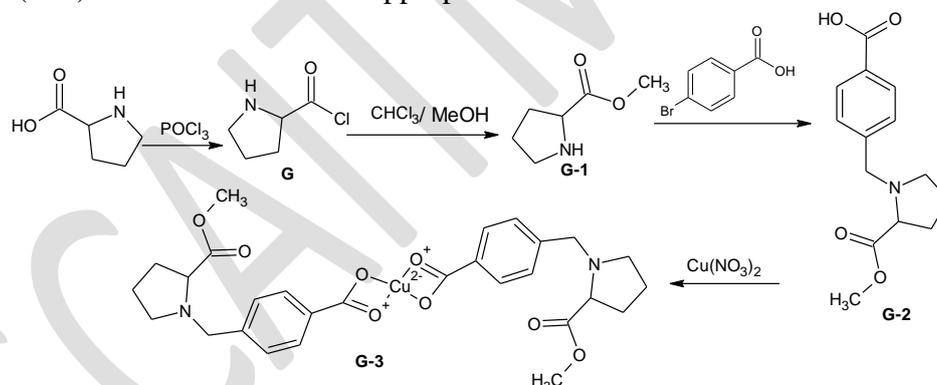
Hadjer Far¹, Tahar BENAÏSSA¹, Sofiane DAOUDI¹ and DjallalEddine ADLI²

¹ Department of Chemistry, Physical Chemistry Studies Laboratory, University of Dr. Moulay Tahar, Saïda 20000, Algeria

² Department of Biology, Faculty of Science, University of Dr. Moulay Tahar, Saïda 20000, Algeria

* Tel: 0669421027 ; E-mail address: Hadjer.far@gmail.com

Abstract: Recent studies have highlighted the chemistry of amino acids and azole derivatives, emphasizing their biological significance and potential applications in pharmaceuticals and biology. Their metal complexes are of particular interest, prompting the development of synthesis methods for these compounds. Metal complexes offer a versatile platform for designing novel therapeutic agents and play essential roles in the pharmaceutical industry and agriculture. The target compounds (G-3) were synthesized through a multi-step process, beginning with the esterification of pyrrolidine-2-carbonyl chloride with methanol. The resulting ester was then reacted with 4-bromobenzoic acid in a mixture of 60% acetone and 40% water to produce compound (G-2). Finally, the products (G-3) were obtained by refluxing compound (G-2) in methanol with the appropriate metal.



The obtained products were characterized by various spectroscopic methods, including IR, UV and NMR (¹H, ¹³C). The chemical substances were synthesized in our laboratory; they were then tested for the purpose of enhancing its antibacterial capacities against gram negative bacteria (*Klebsiella pneumoniae* ATCC700603, *Citrobacter freundii* ATCC8090, *Salmonella typhi* ATCC13311, *Enterobacter cloacae* ATCC13047) and gram positive bacteria (*Staphylococcus aureus* ATCC25923).

Keywords: Proline; Complex; Schiff base; Bactericidal activity; Inhibitor.

**SYNTHESE ET ETUDE THEORIQUE D'UN COMPLEXE DE COBALT (II)
INCORPORANT UN TRIAZOLE SUBSTITUE LIE A LA PHENANTHROLINE**

Mohamed Rafik BENAÏSSA^{1*}, Mohammed HAMADOUCHE¹, Imane Temer², Asmaa MOSTEFAI² and Sofiane DAOUDI³

¹ *Département de Chimie, Laboratoire de chimie fine, Faculté des sciences exactes et appliqués, Université d'Oran1 Ahmed Ben Bella, Oran, Algeria.*

² *Département de Chimie, Laboratoire de modélisation et méthodes de calculs. Faculté des Sciences et de la Technologie. Université de Saida Dr Moulay Tahar, Saida, Algeria.*

³ *Département de génie des procédés, Laboratoire d'études physico-chimiques, Faculté de technologie, Université de Saïda Dr Moulay Tahar, Saida, Algeria.*

Tel./Fax: +213-541-936-320 ; E-mail address: rafikbenaissa1994@gmail.com

Résumé : Une étude conjointe expérimentale et théorique au niveau DFT a été réalisée afin de déterminer les propriétés spectroscopiques et les paramètres géométriques d'un complexe organométallique dérivé d'une base de Schiff. Le ligand objet de complexation a été obtenu par fonctionnalisation de la phenanthroline et incorporation du noyau triazole via un pont méthylène, par une synthèse multi-étape des réactions de substitution, d'addition, de cyclisation. Le site de l'imine obtenu par condensation avec une amine et du groupement triazole, ont été mis à profit comme sites de coordination avec le cation Co^{+2} , donnant ainsi des complexes métalliques hybrides douées d'applications biologiques et catalytiques. Le choix du 1,2,4 triazole a été motivé par le fait que ce dernier constitue un fragment connu pour être incorporé dans une grande variété de nombreux composés thérapeutiquement actifs et reconnu dans la littérature par sa stabilité chimique, sa capacité de coordination avec des ions métalliques universels et son importance dans l'industrie et le système biologique et leur application dans divers domaines. Ces complexes métalliques, possèdent des propriétés magnétiques très intéressantes, en particulier lorsqu'il s'agit de la géométrie tétraédrique ou distordue la plus stable, facilitant leur étude des interactions ligand métal, par IR, UV-visible, Raman. Les résultats obtenus montrent une grande cohérence entre les grandeurs spectroscopiques. Par ailleurs l'analyse NBO, les énergies et les formes des orbitales frontières (HOMO et LUMO) permettent également de mettre en évidence les mécanismes de donation et d'acceptation d'électrons, crucial pour comprendre la structure et la réactivité de ces complexes.

Mot Clés : Base de Schiff, triazole, cation métallique, DFT, NBO.

INFLUENCE OF APPLIED VOLTAGE ON THE FATIGUE PERFORMANCE OF COPPER-EMBEDDED MULTIFUNCTIONAL COMPOSITES

I. BACHIR BEY ^{a*}, F. SI AHMED ^b and S. MANSOUR ^c

^a *Laboratory of Materials Science and Engineering (LSGM), University of Science and Technology Houari Boumediene (USTHB), Algiers, Algeria.*

^b *Laboratory of Materials and Chemical Process Sciences (LSMPC), University of Science and Technology Houari Boumediene (USTHB), Algiers, Algeria.*

^c *Materials Technology Laboratory, University of Science and Technology Houari Boumediene (USTHB), Algiers, Algeria)*

**Corresponding Author E-mail: ibachirbey@usthb.dz*

Abstract : The behavior of a multifunctional composite material with an embedded 0.05 mm copper foil strip under cyclic loading was investigated. Materials able to bear load while conducting electricity are crucial in various applications in high-tech industries. The effects of applied stress and voltage levels on the material response were analyzed. The composite was subjected to tensile and fatigue tests. The results revealed that the introduction of the 0.05 mm copper foil had an impact on the Maximum Tensile Resistance (MTR). The examination of fatigue-damaged specimens provided important insights into the evolution of the copper/composite interface debonding area under different loading conditions. Fatigue test results allowed the plotting of fatigue curves and the establishment of fatigue equations specific to each voltage level ($U = 5, 9, \text{ and } 12 \pm 0.3 \text{ V}$). These results also highlighted the influence of electrical voltage, showing that higher voltage levels improved fatigue resistance. Epoxy resin was chemically dissolved to restore the damaged copper. Naked-eye inspection, along with scanning electron microscope (SEM) observations, revealed important aspects of the metallic insert behavior, including the coexistence of ductile and brittle rupture features and the influence of voltage on the fractured surface.

Keywords: Multifunctional composite material; fatigue; electrical tension; metallic insert; debonding

IMPACT DE L'ANTIBIOTHERAPIE SUR L'EMERGENCE DE LA RESISTANCE DES ENTEROBACTERIES AUX ANTIBIOTIQUES DE LA FAMILLE DES BETA-LACTAMINES

Fatiha ABDELLAOUI^{1,2}, Ahmed MARROKI^{1,3}, Leila BOUSMAHA-MARROKI^{1,2}, Nassima FEKHAR^{1,2,4}, Khaoula Nihed ADLA^{1,2}, and Bénali BEGHADLI²

¹*Department of Biology, Faculty of Natural and Life Sciences (SNV), University Djillali Liabès of Sidi Bel Abbès, Algeria.*

²*Environment and Health Research Laboratory (LRES), Faculty of Medicine, University Djillali Liabès of Sidi Bel Abbès, Algeria.*

³*Laboratory of Microbial Genetic, Faculty of Natural and Life Sciences, University Oran1, Oran 31100, Algeria.*

⁴: *Université Tahri Mohamed of Béchar, Algeria*

Corresponding author: Tel./Fax: +213551931024 ; E-mail address: fatiha.microbiologiste@gmail.com, fatiha.abdellaoui@univ-sba.dz*

Abstract : L'émergence de la résistance des Entérobactéries aux antibiotiques de la famille des bêta-lactamines constitue une menace croissante pour la santé publique. Cette résistance est souvent favorisée par l'usage excessif ou inapproprié des antibiotiques en milieu hospitalier et communautaire. Ces bactéries représentent l'un des groupes les plus redoutables et les plus fréquemment isolés, notamment en milieu hospitalier. Ainsi, l'émergence de souches résistantes dans ce contexte est devenue une préoccupation majeure, rendant indispensable l'utilisation de méthodes diagnostiques fiables pour contrôler cette résistance. Une étude a été réalisée au sein du service de pneumologie du CHU de Tlemcen pour la sélection de souches entérobactériennes résistantes, isolées chez des patients présentant une infection respiratoire et atteints BPCO, l'asthme et la dilatation des bronches (DDB). Les données cliniques ont montré que 43,75 % des patients étaient BPCO, 37,5 % d'asthme et 18,75 % de DDB, avec un âge moyen de 59 ans. Sur le plan thérapeutique, le céfotaxime était l'antibiotique le plus prescrit (68,75 %), suivi de l'Augmentin (18,75 %). L'analyse microbiologique a révélé que 63,63 % des souches isolées étaient des entérobactéries, majoritairement du genre *Klebsiella* et *Enterobacter*, dont 92,85 % présentaient une résistance élevée aux bêta-lactamines, malgré leur sensibilité naturelle à cette classe. Ces résultats soulignent l'urgence d'une gestion rationnelle de l'antibiothérapie et d'une surveillance continue des résistances.

Keywords: Antibiothérapie, Résistance bactérienne, Entérobactéries, Bêta-lactamines, infections respiratoires .

RESISTANCE PROFILE OF STAPHYLOCOCCUS AUREUS (MRSA) ISOLATES TO ANTIBIOTICS IN INFECTIONS IN HOSPITAL CHU IN THE WEST REGION OF ALGERIA

FEKHAR Nassima^{*1,2,3}, BOUSMAHA Leila^{1,2}, MARROUKI Ahmed^{1,2,4}, BELAGUID Soumia³, BENMOULOUD Khadra³, ABDALAOUI Fatiha^{1,2} (1), ADLA Khawla Nihad^{1,2} BEGHADLI Bénali²

1Department of Biology, Faculty of Natural and Life Sciences, Djilali Liabès University of Sidi-Bel-Abbès, Sidi Bel Abbès, Algeria

2Laboratory of Environmental and Health Research, Faculty of Medicine, Djilali Liabès University of Sidi-Bel-Abbès, Sidi Bel Abbès, Algeria

3Department of Biology, Faculty of Natural and Life Sciences, Tahri Mohamed Bechar University, Algeria.

4 Laboratory of Microbial Genetics, Faculty of Natural and Life Sciences, University Oran 1, Oran Algeria

**E-mail: nassima.fekhar27@gmail.com, Tel : 0666168184*

Abstract : Methicillin-resistant *Staphylococcus aureus* (MRSA) has spread throughout the world and has become a threat to public health. and has become highly endemic in many geographical areas. This pathogen causes morbidity and mortality in hospitals. The aim of this study was to determine the prevalence of MRSA at and to determine its antibiotic resistance profile. A questionnaire was completed by the patients concerned, indicating age, sex, type of operation, department of stay, and occurrence of post-operative infection. 41 *Staphylococcus aureus* isolates from routine microbiological samples were collected from four hospitals in the West region of Algeria between January and March 2024. The disk diffusion method, according to CA-SFM standards, 14 antibiotics (3 beta-lactams, 2 aminosides, 2 glycopeptides, 3 macrolides, 2 glycopeptides, colistin, and fusidic acid) were used to determine the susceptibility of MRSA. The results showed that all 41 strains were MRSA; 96% were resistant to cefotaxim, augmentin, oxacillin, fosfomycin, and fusidic acid; 54.4% were resistant to erythromycin; 45.5% were resistant to tetracycline; and 36.6% were resistant to gentamycin. The results of this study highlight the need for ongoing surveillance of MRSA and antibiotic resistance in general. It is important to extend this work in order to draw up strong recommendations.

Key words: Emerging resistance, *Staphylococcus aureus* MRSA,

SCREENING OF PLANT EXTRACT FOR ANTIOXIDANT ACTIVITY AND ANTI INFLAMMATORY EFFECT BY THE METHOD OF EGG ALBUMIN

Nozha MAYOUF¹, Soumia BOUTARFA¹, Soulef SAOUDI², Khaoula AROUA⁴, Nassima LEULMI⁴, Hanane MELLAL¹

¹Laboratory of Biotechnology, Water, Environment and Health Faculty of Nature and Life Sciences, University Abbes lghrouk khenchela, Algeria.

²Laboratory of Phytotherapy Applied to Chronic Diseases², Department of Biology and Animal Physiology, Univ Setif 1, 19000, Algeria.

³Laboratory of Mycology, biotechnology and microbial activity³, Constantine 1. Department of Molecular and Cellular Biology Faculty of Natural and life Sciences, University of Abbes Laghrour, 40004, Khenchela, Algeria

Plant protection laboratory in agricultural and natural environments against crop pests⁴. Department of Agronomic Sciences, Faculty of Natural and life Sciences, University of Abbes Laghrour, 40004, Khenchela, Algeria

Correspondance : nozhabiole91@gmail.com/ nozha.mayouf@univ-khenchela.dz

Abstract : Since the ancient times, a great variety of plants have been used for therapeutic purposes. Most parts of plants have been used as extracts and may possess anti-inflammatory and antioxidant properties related to diseases such as diabetes, atherosclerosis, neurodegenerative, or cancer. In addition, plant extracts, as anti-inflammatory agents, can regulate the composition of the gut microbiota. . The aim of this study was to assess the anti oxidant and anti-inflammatory activity of aqueous extract from the medicinal plant *Eucalyptus globules*. Material and methods : This study of *Eucalyptus globules* focused on phytochemical screening, Determination of flavonol, protein and sugar compounds content by the colorimetric methods and evaluation of in vitro anti inflammatory capacity by the method of egg albumin. Results: The estimation of sucres, flavonol and protein showed that the aqueous extract contains a high amount of sugar, flavonol and protein respectively : 535.58 ± 0.052 mg D-glucose/g ; 3 ± 0.02 mg / g extract ; $2.025.3 \pm 0.003$ mg /g extr respectively. The quantitative evaluation of the scavenging power on SOD showed that the extract is active with IC₅₀ values of 7.72mg/mL. Concerning the anti-denaturation activity, the extract showed a high percentage of egg albumin inhibition 91.51% at the highest concentration. Thus, our results indicated that the extract had a significantly good anti-denaturation activity, compared to diclofenac. Conclusion. Our study show clearly that the aqueous Extract of *Eucalyptus globules* has a significant anti-denaturing property.

Keywords: Denaturation, Aqueous, flavonol, *Eucalyptus globules*.

**REMOVAL OF POLUTANT BY ADSORPTION PROCESS USING AN
ACTIVATED CARBON ADSORBENTS PREPARED FROM PRICKLY P
EAR FRUIT SEEDS**

LAHRECHE Saadia^{1,2}, KAID M'hamed ², BENYOUCEF Abdelghani ¹

¹ *Water Science and Technology Laboratory, University of Mustapha Stambouli Mascara, Mascara 29000, Algeria.*

² *Laboratory of Physico-Chemical Studies, University of Saïda, BP 138, Saïda 20000, Algeria.
Lahrechmg2010@gmail.com*

Abstract: Cadmium is a more toxic heavy metal. It enters the environment as metallic, inorganic, and organic mercury compounds through various industries such as the paper industry, gold and silver mining, the electrical industry, fungicides, and pharmaceuticals. It is widely dispersed in the environment in excessive concentrations and beyond a certain limit, it can cause more serious risks, deadly and carcinogenic diseases to human beings and thus it can cause environmental problems. This is the reason why the retention of this pollutant in wastewater is a big topic of research these. As a remedy, adsorption has been considered a preventive method that has the advantage of being able to be applied to the treatment of various effluents and thus provided for the protection of the environment where several adsorbents are used for the treatment of aqueous effluents. The reuse of agricultural waste is one of the objectives of the associated environmental property, which has become an important choice that has several advantages for waste treatment, such as free availability, a simple technique, a low cost, and a simple regeneration. In this study, we were interested in preparing an activated carbon product from the prickly pear fruit seeds, by several steps under different chemical and thermal treatments and were characterized by different spectrometric methods. Then it was tested as a biosorbent for the removal of Cd (II) from wastewater to broaden the scope of its application, and it gives good results with the various works carried out previously. The parametric study reveals encouraging results.

Keywords: *Pollutant, Cd (II), Adsorption, Activated Carbon, Prickly Pear Fruit Seeds.*

**GREEN CHEMISTRY FOR ENVIRONMENTAL AND INDUSTRIAL
TRANSFORMATION**

MAKHLOUFI Mohamed Cherif ^{1*}, Billel ZAHAF²

¹*Unité de recherche revêtements, matériaux et environnement, Département Génie des Procédés, Faculté de Technologie, Université M'hamedBougara, Avenue de l'indépendance, 35000, Boumerdes, Algerie*

²*Laboratoire de Synthèse Pétrochimique, Département Génie des Procédés Chimiques et Pharmaceutiques, Faculté des Hydrocarbures et de la Chimie, Université M'hamedBougara, Avenue de l'indépendance, 35000, Boumerdes, Algerie*

**Corresponding author: Tel./Fax: +213-558-926-398 ; E-mail address: makhloufi.mohamed.cherif@gmail.com*

Abstract: Green Chemistry represents a forward-thinking paradigm in chemical science, emphasizing the design, synthesis, and application of chemical products and processes that minimize harm to human health and the environment. Over the past decades, significant advancements have been made in developing innovative, efficient, and cleaner chemical methodologies. These include novel synthetic routes, safer reaction conditions, and the integration of sustainable feedstocks and catalysts. Moreover, Green Chemistry extends beyond research labs into education, equipping the next generation of chemists with the principles and practices necessary for conducting environmentally responsible science. This shift is not only fostering a culture of sustainability within the chemical community but also yielding tangible benefits for industry, public health, and ecological systems. As such, Green Chemistry continues to shape a more sustainable and conscientious future for both the scientific world and society at large.

Keywords: Green Chemistry ; Cleaner chemical ; environment ; sustainability

FIRST PRINCIPLES CALCULATIONS ON STRUCTURAL, MECHANICAL AND OPTICAL PROPERTIES OF ALKALINE EARTH HYDRIDE CaH₂ FOR HYDROGEN STORAGE APPLICATIONS

Djemaa GUENDOZ^{1,2}, Zoulikha CHARIFI^{2,3} and Hakim BAAZIZ^{2,3}

¹Physics Department, High Normal School of Bousaada (Algeria)

²Laboratory of physics and chemistry of materials, University of M'sila (Algeria)

³Department of Physics, Faculty of Science, University of M'sila, 28000 M'sila, Algeria

*Corresponding author: Tel./Fax:0662573881; E-mail address: djemaa.guendouz@ens-bousaada.dz

Abstract: Self-consistent ab initio calculations of the structural, electronic, optical and mechanical properties of CaH₂ earth hydride within the framework of Density Functional Theory (DFT) is performed. Generalized gradient approximation (GGA) and local density approximation (LDA) are employed to treat exchange-correlation potential. Modified Becke-Johnson (mBJ) exchange potential with a proper choice of basic parameters is used to calculate the electronic band-structure, density of states and optical properties. Strikingly, an excellent agreement between calculations and experiment is obtained. Under ambient conditions, the conventional form stable at room temperature and atmospheric pressure of CaH₂ is the orthorhombic structure complicated PbCl₂-type with *Pnma* as space group. In this phase, each unit cell contains four CaH₂ molecules. The primitive cell contains four atoms of Ca and two inequivalent H (labeled as H1 and H2 atoms at 4c sites. The Ca atom is surrounded by nine H ions. At high pressure, the structure is hexagonal (Ni₂In-type) with P6₃/mmc space group. The unit cell contains two molecules per formula unit, where two hydrogen H atoms are located at 2d (H1) and 2a (H2) sites, whereas the metal atoms X(X= Ca, Sr and Ba) occupy the 2c sites. Under ambient conditions, CaH₂ is found to be structurally stable in the orthorhombic (PbCl₂-type) structure. Total energy minimization indicates that examined alkaline hydride undertake a structural phase transition from the orthorhombic (PbCl₂-type) to hexagonal (Ni₂In-type) phase. Investigation of electronic density of states reveals that the hydrides is insulator. Furthermore, optical parameters such as, dielectric function, reflectivity and absorption coefficients as functions of wave length of incident light are computed and analyzed. Remarkably, CaH₂ are found to exhibit strong optical anisotropy. In addition, elastic constants of the single-crystal and polycrystalline forms of the investigated hydrides are numerically estimated and interpreted. The Voigt-Reuss-Hill (VRH) approximation is used to estimate the elastic constants of a surfaced polycrystalline hydride in terms of its crystallographic texture and the elastic constants of the constituting single crystals under high pressure. The calculated optical and mechanical properties are in good agreement with previous theoretical and experimental studies.

Keywords: Alkaline earth hydride; Hydrogen storage; DFT; Electronic structure.

IN VITRO ANTIBACTERIAL ACTIVITY OF METHANOLIC LEAF EXTRACT OF *EUCALYPTUS CITRIODORA*

Aicha AMIRA¹, Nadia KADJOUJ¹, Azzedine BOUNAMOUS², Houyem ABDEDAIM¹ and Faiza BENARIFA¹

¹Department of Biological and Agricultural Sciences, Institute of Natural Sciences, University Center Abdelhafid Boussouf of Mila, Mila, Algeria.

²Laboratory of Natural Sciences and Materials, Institute of Natural Sciences, University Center Abdelhafid Boussouf of Mila, Mila, Algeria.

*Corresponding author: ai.amira@centre-univ-mila.dz

Abstract: Multidrug-resistant bacteria have prompted intensified research into alternative antimicrobials, with medicinal plants identified as valuable natural sources. *Eucalyptus* leaf extracts have been widely recognized for their therapeutic properties, including notable antibacterial activity. The aim of this study is to evaluate the antibacterial activity of the methanolic leaf extract of *Eucalyptus citriodora*. We evaluated the antibacterial activity of the methanolic extract of *Eucalyptus citriodora* leaves using the disk diffusion method on Mueller-Hinton agar medium. The results showed significant activity of the methanolic extracts against *Pseudomonas aeruginosa* with inhibition zones varying between 23.41 and 11.01 mm followed by *Bacillus subtilis* and *Staphylococcus aureus* with inhibition zones ranging from 22.07 to 12.66 mm, and 11.28 to 9.55 mm, respectively. On the other hand, *Escherichia coli* was resistant to the extract. These results suggest that the methanolic extract of *Eucalyptus citriodora* may serve as an alternative antimicrobial agent, especially in the face of rising multidrug-resistant bacterial infections.

Keywords : Multidrug-resistant bacteria, methanolic extract, antibacterial activity, *Eucalyptus citriodora*.

AI AND MOLECULAR DESIGN: HARNESSING ARTIFICIAL NEURAL NETWORKS FOR HIGH-FIDELITY PREDICTION OF ANTI-INFLAMMATORY COMPOUNDS

Sarah REZAZI¹

*¹Department of Processes Engineering, Institute of Sciences, Tipaza University Center, Oued merzoug, Tipaza 42000, Algeria . *Corresponding author: E-mail: rezazi.sarah@gmail.com*

Abstract: The integration of AI into molecular design is revolutionizing drug discovery by enabling accurate prediction of biological activity from chemical structure. This work explores the use of artificial neural networks (ANNs) to model anti-inflammatory activity across 532 structurally diverse compounds, described by 165 molecular descriptors. Feature optimization was performed using stepwise elimination, resulting in a refined input space for enhanced model performance. A data-driven strategy was applied to optimize ANN topology, guided by error function minimization and maximized generalization. The best-performing model yielded a correlation coefficient of 96.04% and a mean absolute relative error below 1%. These findings validate deep learning as a powerful predictive tool and highlight its utility in streamlining lead identification and virtual screening processes.

Keywords: Artificial Intelligence, Molecular design, Drug discovery, Molecular descriptors.

HIGHLY EFFICIENT PHOTOCATALYTIC DEGRADATION OF METHYLENE BLUE DYE USING SODIUM ALGINATE/TiO₂ NANOCOMPOSITES

Fadila BEKKAR^{1*}, Hadjer BELHAOUA¹, Faiza BETTEHER¹ and Rachid MEGHABER

¹ *Département de chimie, Faculté de sciences exacta et appliqué, Université Oran 1 Ahmed Ben Bella*

**Corresponding author: Tel.(+213)790233742; E-mail address: fadilabekkar0@gmail.com*

Abstract: In this study, nanocomposites membranes based on sodium alginate (SA) and titanium dioxide (TiO₂) nanoparticles were successfully developed using an ultrasound-assisted synthesis method. This green and efficient technique promotes the homogeneous dispersion of TiO₂ nanoparticles within the biopolymer matrix, resulting in improved interfacial compatibility and enhanced mechanical and functional properties of the membranes. The synthesized nanocomposites membranes were characterized using infrared and diffuse reflectance spectroscopies, whereas the morphology was analyzed using X-ray diffraction (XRD) and transmission electron microscopy (TEM) techniques. The photocatalytic efficiency of the sodium alginate/TiO₂ nano hybrids was evaluated through the degradation of methylene blue (MB), a common cationic dye used to evaluate water treatment performance. The results revealed that these nanocomposite membranes show strong photocatalytic activity when exposed to light, which can be attributed to the effective interaction between the alginate matrix and the TiO₂ nanoparticles. In addition to their performance, the membranes demonstrated good stability and could be reused multiple times, making them attractive for sustainable environmental applications. Combining a biodegradable polymer with a well-known photocatalyst offers a promising path toward the development of environmentally friendly and efficient solutions for wastewater treatment.

Keywords: Sodium alginate; TiO₂ nanoparticles; Nanocomposite membranes; Photocatalytic; Water treatment

TENEUR EN 5-HYDROXYMETHYLFURFURAL (HMF) DANS LES MIELS DE LA REGION DE MOSTAGANEM

RADJA Djamaia Sabiha *, Mounia HOMRANI, Abelkader DAHOU et Abd Elkader HOMRANI

Département d'agronomie, Laboratoire des sciences et techniques de production animales, Faculté SNV, Algeria

**Corresponding author: salih191@gmail.com*

Abstract : Le HMF est le résultat de dégradation du fructose et du glucose dans un milieu acide, potentiellement toxique pour l'homme, dans les miels frais, le HMF n'est présent qu'à l'état de traces et sa teneur augmente avec la température, la durée de stockage. L'objectif de cette étude était de déterminer la teneur en 5-hydroxyméthylfurfural dans les miels de la région de Mostaganem Soixante quinze (75) échantillons de miels ont été récoltés durant la période qui s'étend du mois de Mai à Octobre 2023. Le taux d'HMF des échantillons des miels a été mesuré par méthode de spectrophotométrie le principe de cette méthode est basé sur la détermination de l'absorbance UV d'HMF à deux longueurs d'onde 284 nm et 336 nm. Les valeurs de la teneur en HMF des échantillons des miels oscillent de $5,19 \pm 0,26$ à $45,54 \pm 0,93$ mg/kg avec une moyenne de $16,14 \pm 9,61$ mg/kg. Les résultats obtenus s'accordent avec les normes recommandées par le Codex Alimentarius, exception faite pour quatre échantillons présentant des teneurs supérieures à 40mg/kg (E62, E63, E66, E70). Cette augmentation de la concentration en HMF peut se justifier par un chauffage lors de l'extraction pour faciliter l'écoulement du miel. Sur 75 échantillons de miels 45 présentent une teneur en HMF inférieure à 15mg/kg, ces miels sont considérés comme des miels de qualité, ont trouvé des teneurs entre 0,17 à 571,9mg/kg dans les miels du centre et l'Est Algerian. La détermination de la teneur en HMF est une excellente méthode pour l'appréciation du vieillissement et du chauffage des miels.

Keywords: Miel ; HMF ; Mostaganem.

**IN SILICO MOLECULAR DOCKING OF LC-MS-IDENTIFIED
PHYTOCOMPOUNDS AS POTENTIAL α -AMYLASE INHIBITORS**

Abdelmoudjib GHECHAM¹ and Waffa BOUAFIA²

¹*Department of Organismal Biology, Faculty of natural and life sciences, Biotechnology Laboratory of the Bioactive Molecules and Cellular Physiopathology, Mustapha Ben Boulaid, Batna 2 University, Batna, Algeria.*

²*Common Core Department, Faculty of natural and life sciences, Mustapha Ben Boulaid, Batna 2 University, Batna, Algeria.*

**Corresponding author: Tel./Fax: +2130665232692; E-mail address: a.ghecham@univ-batna2.dz*

Abstract: α -Amylase plays a crucial role in starch digestion, and its inhibition is a key strategy for managing blood sugar levels in diabetes. While synthetic inhibitors like acarbose are effective, their side effects have prompted the search for safer, natural alternatives. This study aims to evaluate the binding potential of ten compounds previously identified by LC-MS in a medicinal plant extract, using molecular docking to complement experimental α -amylase inhibitory data. The crystal structure of α -amylase (PDB ID: 1HX0) was retrieved from the RCSB Protein Data Bank. The docking grid was defined by a box of $40 \times 40 \times 40 \text{ \AA}^3$ centered at coordinates $x=34.5$, $y=33.2$, $z=36.8$. Ten ligands; Coumaric acid, Ferulic acid, Isoorientin, Gallic acid, Protocatechuic acid, Quercitrin, Vitexin, Vicenin II, p-hydroxybenzoic acid, and p-hydroxybenzaldehyde were geometry-optimized using Chem3D to achieve stable, low-energy conformations. The protein was prepared with Discovery Studio by removing water molecules and heteroatoms and adding polar hydrogens. Molecular docking simulations were performed using AutoDock Vina. Docking results indicated that Vicenin II (-9.7 kcal/mol), Isoorientin (-8.9 kcal/mol), Quercitrin (-8.8 kcal/mol), and Vitexin (-8.7 kcal/mol) exhibited the strongest binding affinities toward α -amylase, comparable or superior to acarbose (-8.7 kcal/mol). However, Isoorientin and Quercitrin violated Lipinski's Rule of Five, displayed poor predicted intestinal absorption, and were not expected to cross the blood-brain barrier. The molecular docking study reinforces in vitro findings, highlighting Vicenin II, Isoorientin, Quercitrin, and Vitexin as promising α -amylase inhibitors, with Vicenin II showing the highest binding affinity and favorable drug-like properties.

Keywords: Molecular Docking, α -Amylase Inhibition, LC-MS, Phytochemicals, Diabetes Management.

ORGANOMETALLIC NANOSTRUCTURES FOR EFFICIENT DYE REMOVAL: TOWARDS GREENER WATER TREATMENT TECHNOLOGIES

Ouafa BELAIDI¹, Samia SAAIDIA¹, Hamida BEKAKRIA¹ and Zahia BENREDJEM²

¹Chemistry Department, Chadli Bendjedid University - El-Tarf, Algeria

² Chemistry Department, Badji Mokhtar University, Annaba, Algeria

ou.belaidi@univ-eltarf.dz

Abstract: This work focuses on the design and application of a nanostructured coordination complex for the photocatalytic degradation of a model organic dye under UV and simulated solar irradiation. The synthesized material, based on transition metal centers coordinated with nitrogen-rich ligands, was characterized by its high surface reactivity and photostability. A systematic investigation of key operational parameters—including catalyst dose, initial dye concentration, and pH—revealed that optimal degradation occurs under mildly acidic conditions and at low catalyst loading. Under these conditions, the photocatalyst achieved up to 98 % dye removal within 120 minutes of light exposure. The study highlights the potential of metal-organic nanostructures as effective and sustainable materials for environmental remediation. These findings support their integration into advanced oxidation processes (AOPs) for dye-contaminated wastewater treatment, combining structural tunability, light responsiveness, and green chemistry principles.

Keywords: Coordination nanomaterial; Dye degradation; Advanced oxidation; Water treatment.

FUNCTIONALIZED KAOLIN WITH GREEN-SYNTHEZED TiO₂ NANOPARTICLES FOR DYE ADSORPTION

Imene ZITOUNI¹, Nassira ZABAT² and BOUNAB Bochra¹

¹Laboratory of Organic Synthesis-Modeling and Optimization of Chemical Processes

²Department of Process Engineering, Faculty of Engineering, Badji Mokhtar-Annaba University, P.O. Box 12 Annaba 23000, Algeria..

Tel./Fax: 213541462632 ; E-mail address: imene.zitouni@univ-annaba.dz

Abstract: The science behind the nanotechnology is to create or synthesized nano-sized materials, which are very useful across the entire field. The green synthesis is a fruitful emerging process that is environment friendly and low-cost as well. During the last decade, a plenty of work on green synthesis of TiO₂ nanoparticles had been practiced. Water is an essential resource for life, but the growing world population, accelerated urbanization, climate change and industrialization are critically affecting water quality and freshwater availability. The textile industry, which through its textile dyeing wastes significantly increases water pollution. Many techniques have been designed to address this environmental crisis, including adsorption by various materials, both natural and synthetic. Both TiO₂ and clay have gained immense popularity in this field, for obtaining nanomaterials effective in wastewater remediation. For this purpose, we synthesized a modified clay/TiO₂ nanocomposite based on a green synthesis method. First of all, modified TiO₂ nanoparticles were synthesized using a plant extract (*Salvia rosmarinus*). Then, these nanoparticles were incorporated into clay (Algerian kaolin) under certain conditions. The optimization of the main parameters such as temperature, stirring time, clay mass, extract concentration and TiO₂ mass were studied by testing the obtained nanocomposite on a model pollutant methylene blue likely to be found in textile waste. Satisfactory results were obtained, and confirmed by SEM/EDS characterization.

Keywords: Green synthesis, Titanium dioxide, nanoparticle, textile water, leaf extracts, EDS.

A NOVEL GREEN SYNTHESIS OF A NANOMATERIAL USING PLANT EXTRACT, OPTIMIZATION OF OPERATING PARAMETERS

Bouchra BOUNAB^{*1}, Nacéra ZABAT¹, Imen ZITOUNI¹ and Imen HARBI¹

*Laboratory of Organic Synthesis-Modeling and Optimization of Chemical Processes,
Department of Process Engineering, Faculty of Engineering, Badji Mokhtar-Annaba University, P.O.
Box 12 Annaba 23000, Algeria*

**Corresponding author: Tel: +213-668-855-291; E-mail address: bouchra.gp.chimique@gmail.com*

Abstract: Industrial waste, which contains toxic and dangerous substances, is the main source of wastewater pollution. This is particularly true of the dyes used in the textile industry. These products cause unprecedented damage to the ecosystem. To solve these problems, various treatment methods have been employed. Adsorption processes have the greatest potential. Green synthesis is a method used to synthesis nanomaterials from plant extracts. The importance of nanomaterials lies in the fact that, at this scale, they have emerging characteristics that could have a significant impact in many fields. In this study, we optimized the operating parameters for the synthesis of a tungsten oxide nanomaterial (WO₃), which is synthesized by green synthesis using a Pistacia lentiscus leaf extract. The synthesized nanomaterial was characterized by scanning electron microscopy (SEM) and energy dispersive spectroscopy (EDS). The study focused on optimizing the operating parameters for the tungsten oxide nanomaterial, including variations in: the concentration of the plant extract, the concentration of the precursor used and the concentration of a precipitating agent. Optimization was carried out using adsorption tests with an organic dye (methylene blue).

Keywords: Adsorption; organic dyes; nanomaterial; green synthesis.

**CONTRIBUTION OF *PITURANTHOS SCOPARIUS* TO GREEN CHEMISTRY :
EXTRACTION AND THERAPEUTIC VALORIZATION**

Zahida Yasmina HEBBACHE^{1*}, Yazid FOUJIL-CHERIF² and Mokhtar FODILI¹

¹Laboratory of Organic Chemistry and Natural Substances, University Ziane, Djelfa, Algeria

²Laboratory of Functional Organic Analysis, Department of Organic Chemistry, Faculty of Chemistry, University of Sciences and Technology Houari Boumediene (USTHB), Algeria

*Zahida Yasmina HEBBACHE : Tel. +213542169197 ;

E-mail address: hebbachezahidayasmina@gmail.com

Abstract : *Pituranthos scoparius* (Apiaceae), an endemic Saharan plant commonly found in the arid regions of Algeria, has long been used in traditional medicine to relieve pain, inflammation, and digestive disorders. This study focuses on evaluating its therapeutic potential through the analysis of essential oils extracted using various techniques, particularly microwave-assisted extraction, a more sustainable and efficient alternative to conventional methods. The chemical composition of the essential oils was identified and characterized using Gas Chromatography–Mass Spectrometry (GC-MS), revealing a predominance of Dillapiol (16.38-37.21%), α -Pinene (0.48-10.84%) and Myristicin (4.21-9.37%), all recognized for their anti-inflammatory and antioxidant properties. The biological activities of the extracts varied depending on the extraction method, showing the impact of technical parameters on pharmacological performance. The essential oil exhibited significant anti-inflammatory and analgesic effects, as confirmed by in vivo tests. Its antibacterial activity, while moderate, was still notable. These findings validate the traditional uses of the plant in Saharan communities and suggest its potential integration into the development of herbal medicines. Moreover, the low observed toxicity enhances the safety profile of the extracts, which is essential for therapeutic application. Considering its abundance in bioactive compounds and the underutilized diversity of Algerian flora, *Pituranthos scoparius* stands out as a promising natural source for developing new anti-inflammatory and analgesic agents.

Keywords: *Pituranthos Scoparius* ; Anti-inflammatory activity ; Analgesic activity.

POLYPHENOLICS COMPOUNDS AND ANTIOXIDANT ACTIVITY USING DPPH ASSAY OF FOUR THYMUS SPECIES FROM WESTERN ALGERIA

Houssam Eddine Mustapha SADLI^{1*} and Zoubir BELMOKHTHAR²

¹ Département de biotechnologie, Mohammed Boudief -Oran- Universty , Laboratory of Plant and Microbial Valorization and production (LP2VM), Algeria

² Département de environnementale sciences, Djilali Liabes de Sidi Bel-Abbé University s, Laboratory of Plant and Microbial Valorization and production (LP2VM), Algeria

*Corresponding author: Tel./: +213-696-1222-75 ; E-mail address: houssam.sadli@univ-usto.dz

Abstract: The genus *Thymus* is one of the most abundant genera in the Lamiaceae family, with 315 species worldwide. Thyme species exhibit optimal growth in the Western Mediterranean and Western Asia regions, and can also be grown in a different area of the world. The objective of this investigation was to evaluate the polyphenolic compounds and their correlation with antioxidant activities using DPPH assay for polar extract (hydroethanolic (70%) and aqueous extracts) . This study focused on four thyme populations from western Algeria: *Thymus pallescens* de Noé from both Sidi Bel Abbès and Ain Témouchent regions, *Thymus vulgaris* from Ain Témouchent region, and *Thymus capitatus* from Sidi Bel Abbès region.

The quantification of total phenolic compounds (TPC) revealed that both aqueous and hydroethanolic extracts of *T. pallescens* de Noé from Ain Témouchent exhibited the highest TPC concentrations among all tested samples. The evaluation of antioxidant properties through DPPH assay demonstrated that all extracts from the three investigated species possessed significant antioxidant activities at varying levels, with a remarkable free radical scavenging potential observed in *T. pallescens* extracts compared to *T. vulgaris* and *T. capitatus* extracts. These results suggest a promising therapeutic potential for these *Thymus* species native to western Algeria, supporting further research into their bioactive compounds and potential pharmaceutical applications.

Keywords: *Thymus* genus; Phenolics compounds; DPPH.

ETUDE THEORIQUE DE LA REACTION DE CYCLOADDITION DIPOLAIRE-1,3 DU NITROSO OXIDE AVEC LE FLUOROETHYLENE

Samira BAKI ^{1*}

¹ *Laboratoire de Chimie Physique Macromoléculaire, Département de Chimie, Faculté des Sciences Exactes et Appliquées, Université Oran 1 Ahmed Ben Bella, B.P 1524 El M'naouar, Oran 31005, Algeria.*

* s.baki@yahoo.fr

Résumé : L'objectif de ce travail est de faire une étude théorique de la réaction de cycloaddition dipolaire-1,3 du nitroso oxide **1** avec le fluoroéthylène **2**, en utilisant la méthode semi-empirique AM1. Dans cette réaction, deux produits régioisomères sont possibles (Figure). Il faut également tenir compte de l'isométrie endo et exo.

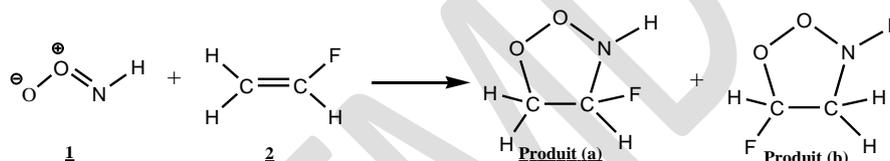


Figure. Réaction de cycloaddition dipolaire-1,3 du nitroso oxide **1** avec le fluoroéthylène **2**.

Ce travail consiste à faire une étude électronique et géométrique des réactifs mis en jeu puis une application de la théorie des orbitales frontières à la réaction étudiée. Ensuite, une étude détaillée des mécanismes réactionnels possibles, par détermination des états de transition et des produits correspondants, ce qui permet des discussions et des comparaisons des résultats théoriques obtenus.

Mots clés : Cycloaddition, Nitroso oxide, Fluoroéthylène, AM1, Etat de transition, Produit, Orbitale, Régiosélectivité.

BOX-BEHNKEN EXPERIMENTAL APPROACH FOR THE REMOVAL OF CATIONIC DYES VIA A GREEN EMULSIFIED LIQUID MEMBRANE

KHELIFA Sonia^{1*}, **BENDEBANE Salima**², **BENDEBANE Farida**³, **BENDEBANE Hawa**¹, and **ISMAIL Fadhel**⁴

¹*Department of Chemistry, Faculty of Sciences, Badji Mokhtar Annaba-University, Algeria, Laboratory LOMOP,*

²*Associate Professor, Department of process engineering and energy, National Higher School of Technology and Engineering, Annaba-Algeria, Laboratory L3M,*

¹*Professor, Department of Chemistry, Faculty of Sciences, Badji Mokhtar Annaba-University, Algeria, Laboratory LOMOP,*

⁴*Professor, Department of process engineering, Faculty of Technology, Badji Mokhtar Annaba-University, Algeria, LOMOP Laboratory.*

**sonia.khelifa@univ-annaba.dz*

Abstract : This work is part of an effort to reduce the environmental impact of petroleum-based organic solvents, which are frequently used in emulsified liquid membrane (ELM) processes. To this end, a green emulsion liquid membrane (GELM) process was developed using soybean oil, a non-toxic and economical solvent, as a diluent. A mixture of Malachite Green (MG) and Rhodamine B (Rh-B) dyes was selected as the model pollutant dissolved in the aqueous phase. The membrane was made up of Span 80 as a surfactant, sulfuric acid as the internal phase, and soybean oil as a diluent. The extraction conditions were optimized using Box-Behnken, considering the concentration of Span 80=6%, the concentration of sulfuric acid (0.05M), and the external phase/emulsion volume ratio ($V_{ext}/V_{em} = 5$) as optimal conditions. Under these optimal conditions, an extraction efficiency of 98.58% of the dye mixture was achieved.

Keywords: Green emulsion liquid membrane (GELM), soybean oil, pollution control, malachite green, rhodamine B, Box-Behnken design.

SYNTHESIS AND BIOLOGICAL ACTIVITIES α -AMINO PHOSPHONATE DERIVATIVES OF THIADIAZOL

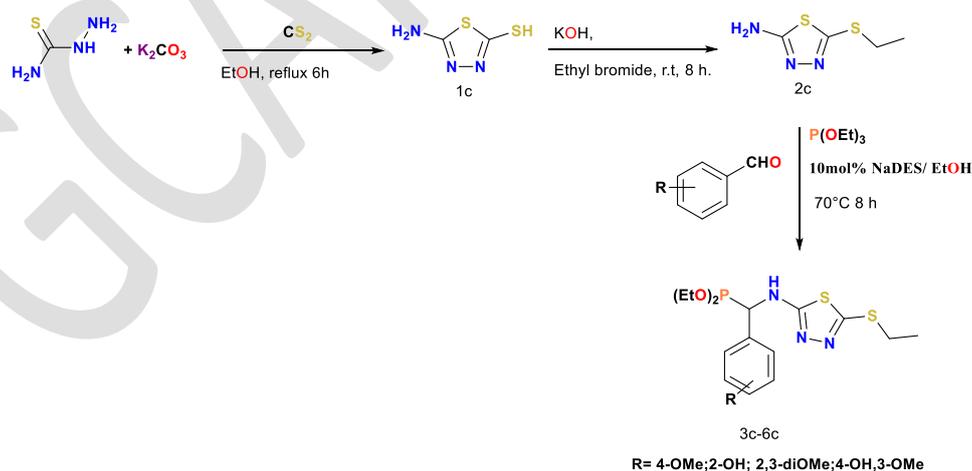
Zinelaabidine CHERAIET¹, Zineb SMAALI¹

¹Laboratoire des Matériaux Organiques et Hétérochimie (LMOH), Département des sciences de la matière, Université Echahid-Larbi Tébessi, Tébessa. Route de Constantine 12002, Tébessa (Algeria).

*Corresponding author: Tel. +213 673834821 ;

E-mail address: zinelaabidine.cheraiet@univ-tebessa.dz

Abstract: Organophosphorus compounds have attracted considerable attention due to their wide-ranging biological significance and versatile applications. Among them, α -aminophosphonates are particularly important yet challenging to synthesize, underscoring the demand for innovative and environmentally friendly approaches. In this study, we describe a simple *one-pot* synthesis of novel α -aminophosphonates *via* the Kabachnik-Fields reaction bearing 5-(ethylthio)-1,3,4-thiadiazol-2-yl) derivatives using deep eutectic solvents as catalyst. The synthesized molecules were rationally designed and synthesized according to the principle of synergic bioactive substructures. The synthesized compounds were obtained with a moderate yield without chromatographic work-up and were characterized by the usual spectroscopic methods: ¹H NMR, ¹³C NMR, HSQC, and HMBC. Some compounds were evaluated for *in vitro* antioxidant (DPPH and SPF) and anti-inflammatory activity in order to demonstrate the potential spectrum of the obtained α -aminophosphonates.



Keywords: 1, 3, 4-thiadiazol, α -aminophosphonates, Kabachnik-Fields reaction, antioxidant and anti-inflammatory.

ANTIDIABETIC ACTIVITY OF COLD-PRESSED LINSEED AND CHIA SEED OILS

Sarra LITIM^{1*}, Sabah BOUKERIA¹ and Radhia DERIOUCH¹

¹*Plant biotechnologie, Natural and Life Sciences, Algeria .*

Abdelhafid Boussouf-Mila University Center .

**Corresponding author: Tel./Fax: +0-054-051-4735 ; s.litim@centre-univ-mila.dz*

Abstract: This study investigates the in vitro antidiabetic potential of cold-pressed linseed (*Linum usitatissimum*) and chia (*Salvia hispanica*) seed oils through their inhibitory activity on the α -glucosidase enzyme, a validated target in the management of postprandial hyperglycemia [1]. Using established spectrophotometric enzyme inhibition assays, the oils were tested across concentrations ranging from 62.5 to 4000 $\mu\text{g/mL}$. Linseed oil exhibited greater efficacy ($\text{IC}_{50} = 21.79 \pm 0.33 \mu\text{g/mL}$) than chia oil ($\text{IC}_{50} = 30.69 \pm 0.27 \mu\text{g/mL}$), while the synthetic drug acarbose showed much lower potency ($\text{IC}_{50} = 3650.93 \pm 10.70 \mu\text{g/mL}$). These results demonstrate a dose-dependent inhibitory effect and highlight the potential of natural oils as functional alternatives for managing type 2 diabetes. The high inhibitory activity of linseed and chia oils is likely linked to their bioactive compound profiles, including unsaturated fatty acids and phenolics, which are known for their metabolic benefits. Their superior performance relative to acarbose suggests applications in green nutraceutical development and dietary-based glycemic control strategies. These findings align with recent trends in plant-based therapies and underscore the relevance of sustainable bioresources in addressing chronic diseases. Overall, the study contributes to expanding the scientific basis for the use of cold-pressed oils as effective antidiabetic agents, offering implications for industrial innovation, preventive healthcare, and the advancement of functional foods.

Keywords: Antidiabetic activity, chia oil, linseed oil, cold-pressed oils, natural bioactives.

**DEVELOPPEMENT DE PLATEFORMES D'INTELLIGENCE ARTIFICIELLE
POUR L'OPTIMISATION ACCELEREE DE CATALYSEURS EN CHIMIE VERTE :
VERS DES PROCEDES MOLECULAIRES PLUS INNOVANTS ET PERFORMANTS**

BOUYA Sara¹ & EL KADIRI Kenza¹

¹Université Ibn Tofail

¹Laboratoire des Sciences Economiques et Politiques Publiques (LSEPP), Maroc

**Corresponding author: sarra.bouya@uit.ma*

Résumé : L'intégration de l'intelligence artificielle (IA) dans le domaine de la chimie verte ouvre de nouvelles perspectives pour la conception rationnelle et l'optimisation accélérée des procédés catalytiques. Cette étude présente le développement d'une plateforme basée sur l'IA visant à améliorer l'efficacité et la durabilité des catalyseurs hétérogènes et homogènes. Grâce à des algorithmes d'apprentissage automatique entraînés sur des ensembles de données expérimentales et computationnelles, nous avons élaboré des modèles prédictifs capables de cribler rapidement des candidats catalytiques à partir de leurs descripteurs structuraux et électroniques. La méthodologie repose sur la curation de données, l'ingénierie de descripteurs, l'entraînement de modèles et la validation croisée à l'aide de bases de réactions chimiques diversifiées. Les résultats montrent une réduction significative du temps de découverte, une amélioration de la sélectivité des réactions et une meilleure précision dans la prédiction des rendements. La plateforme a permis d'identifier de nouvelles structures catalytiques prometteuses, notamment pour la conversion du CO₂ et la valorisation de la biomasse. L'utilisation d'outils d'IA interprétables a également permis d'extraire des connaissances chimiques utiles à la formulation de nouvelles hypothèses pour la conception de catalyseurs. Cette approche constitue un cadre évolutif pour intégrer l'IA dans la recherche en chimie verte, en facilitant la transition vers des procédés moléculaires plus performants, durables et innovants. Les résultats obtenus illustrent le potentiel des technologies fondées sur les données pour accélérer la découverte et enrichir la compréhension en catalyse et en ingénierie chimique durable.

Mots-clés : Intelligence artificielle ; Chimie verte ; Optimisation des catalyseurs ; Apprentissage automatique ; Conception moléculaire

**SYNTHESE DE DERIVES POLYCYCLIQUES ORIGINAUX COMPORTANT
COMME STRUCTURE DE BASE UN NOYAU PYRAZOLE VIA UNE REACTION
D'ARYLATION DIRECTE CATALYSEE PAR LE PALLADIUM**

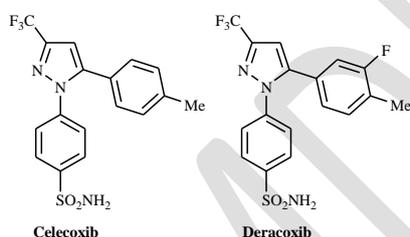
Besma SAOUDI¹, Norman LE FLOCH² and Henri DOUCET³

¹University of Constantine 1 - Frere Mentouri, Constantine, Algeria

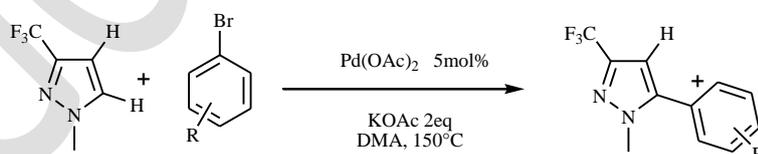
^{2,3}Univ Rennes, CNRS, ISCR-UMR 6226, 35000, Rennes, France

Tel: +213 796 00 92 50 ; E-mail: besma.saoudi@umc.edu.dz

Abstract : Les dérivés hétéroaryles, y compris les arylpyrazoles, sont des briques moléculaires importantes de la synthèse organique en raison de leurs propriétés biologiques.



Dans le cadre du développement de la chimie des hétérocycles, et particulièrement celui de la chimie verte, notre équipe de recherche a récemment développé un nouvel axe de recherche réservé exclusivement 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 3 (le 1-méthyl-3-trifluorométhyl)pyrazole avec des dérivés du bromobenzène en utilisant 5 mol% d'acétate de palladium [Pd(OAc)₂] comme catalyseur en présence d'acétate de potassium (KCH₃CO₂) au reflux du DMA.



Nous avons pu développer une approche simple, respectueuses de l'environnement et très efficaces pour la synthèse d'une large gamme de dérivés arylpyrazoles (16 nouveaux produits) avec des rendements élevés. Tous les produits synthétisés ont été identifiés par les méthodes spectroscopiques usuelles.

Keywords: Dérivés polycycliques ; Couplage direct ; Arylpyrazoles.

IN SILICO EVALUATION OF PLANT-DERIVED FLAVONOIDS IDENTIFIED BY LC-MS AS POTENTIAL ANTIBACTERIAL AGENTS AGAINST GRAM-POSITIVE AND GRAM-NEGATIVE BACTERIA

Waffa BOUAFIA¹ and Abdelmoudjib GHECHAM²

¹*Common Core Department, Faculty of natural and life sciences, Mustapha Ben Boulaid, Batna 2 University, Batna, Algeria.*

²*Department of Organismal Biology, Faculty of natural and life sciences, Biotechnology Laboratory of the Bioactive Molecules and Cellular Physiopathology, Mustapha Ben Boulaid, Batna 2 University, Batna, Algeria.*

*Corresponding author: Tel./Fax: 066963741 ; E-mail address: w.bouafia@univ-batna2.dz

Abstract: The rise of antibiotic-resistant bacteria has intensified the search for new antimicrobial agents, particularly from natural sources such as medicinal plants. This study investigates the antibacterial potential of five flavonoid compounds, previously identified through LC-MS, by evaluating their interactions with key bacterial targets using molecular docking. The aim is to support and complement in vitro antibacterial activity findings. Molecular docking was performed using AutoDock Vina on two bacterial target proteins. For *Staphylococcus aureus* (Gram-positive), the UDG/UGI complex (PDB ID: 3WDG) was used, and for *Pseudomonas aeruginosa* (Gram-negative), the PBP3 complex (PDB ID: 4WEK) was selected. The docking grid was set with dimensions $20 \times 20 \times 20 \text{ \AA}^3$ and centered at coordinates $x=34.5$, $y=33.2$, $z=36.8$. Ligands (Isoorientin, Quercitrin, Vitexin, and Vicenin II) and two reference drugs (Oxacillin and Ceftazidime) were geometry-optimized using Chem3D. Protein receptors were prepared in Discovery Studio by removing water molecules and heteroatoms, and adding polar hydrogens. Oxacillin displayed a binding affinity of -5.9 kcal/mol with *S. aureus*, closely followed by Quercitrin (-5.8 kcal/mol) and Isoorientin (-5.6 kcal/mol). Vitexin and Vicenin II showed slightly lower affinities (-5.3 kcal/mol). Against *P. aeruginosa*, Ciprofloxacin showed -2.7 kcal/mol , whereas all tested flavonoids demonstrated comparable or improved affinities, with Quercitrin again being the strongest binder (-3.1 kcal/mol). The docking results highlight Quercitrin and related flavonoids as promising candidates for antibacterial development, with binding affinities comparable to or better than standard antibiotics. These findings underscore their potential as lead compounds in the fight against bacterial resistance.

Keywords: Molecular Docking, LC-MS, Flavonoids, Antibacterial Activity, *Staphylococcus aureus*, *Pseudomonas aeruginosa*.

COPPER TRIAZOLE COMPLEX SUPPORTED ON Fe₃O₄@SiO₂ NANOPARTICLES AS ECO-FRIENDLY NANOCATALYST IN SOLVENT-FREE BIGINELLI REACTION

Sofiane MEKKI^{1,2*} and Salima SAIDI BESBES¹

¹Laboratoire de Synthèse Organique Appliquée (LSOA), Université Oran 1, Département de Chimie,
Bp 1524 El M'Naouer, Oran 31000, Algeria.

²Ecole Supérieure en Génie Electrique et Energétique d'Oran, BP 64 CH2 Achaba Hanifi-USTO-
Oran 31000, Algeria.

*Corresponding author: Tel./Fax: +213-794-026-169 ; E-mail address: mekkisoufiane16@yahoo.fr

Abstract: Magnetic nanoparticles (MNPs) have attracted increased attention during the last decades in a wide range of applications including nanomedicine, drug delivery, bioimaging, environment, and particularly in catalysis. In this field, the unique properties of MNPs such as small particle size, high surface-area-to-volume ratio and chemical stability allow the enhancement of their reactivity performance compared to conventional bulk catalysts. In addition, due to their superparamagnetic properties, these particles can be easily controlled and separated from the reaction medium by an external magnetic field without any chemical degradation of the active sites. The use of time and energy consuming separation procedures as centrifugation and filtration is thus avoided and the recycling process is simplified for successive nanocatalyst reuse in batch reactions. Magnetic nanocatalysts can be used in heterogeneous catalysis either for their intrinsic magnetic properties such as Fe, Ni, and Co, or as solid supports for the immobilization of others active catalysts including metal catalysts, organocatalysts or biocatalysts. In the present work, a novel hybrid heterogeneous catalyst based on 1,2,3-triazole complex of copper supported on core-shell Fe₃O₄@SiO₂ nanoparticles was designed and characterized by using various techniques such as infrared spectroscopy (FTIR), X-ray diffraction (XRD), thermogravimetry analysis (TGA), scanning electron microscopy (SEM) and energy-dispersive X-ray spectroscopy (EDX). The magnetic nanocatalyst was successfully employed for the synthesis of different functionalized 3,4-dihydropyrimidin-2(1H)-ones by a one-pot multicomponent condensation reaction under solvent-free conditions. The developed ecofriendly catalytic protocol showed several advantages including high yields, short reaction time and easy workup and purification conditions.

Keywords: Magnetic nanoparticles, Biginelli reaction, dihydropyrimidinones, solvent-free, heterogeneous catalysts, green chemistry, one-pot condensation.

IMPACT OF EXTRACTION METHODS ON PHYTOCHEMICALS AND BIOACTIVITY: A GREEN CHEMISTRY APPROACH

Karim TIGHILET^{1,2*} and Sihem AIT ATMANE²

¹ Department of Biology, Faculty of Natural Sciences and Life and Earth Sciences, University of Bouira 10000, Bouira, Algeria

² Laboratory of Plant Biotechnology and Ethnobotany, Faculty of Natural and Life Sciences, University of Bejaia, 06000, Bejaia, Algeria

*Corresponding author: Tel./Fax: +213-540-015-468; E-mail address: k.tighilet@univ-bouira.dz

Abstract : In line with the sustainable valorization of local plant resources and green chemistry principles, this study investigates the effect of two extraction methods, maceration and ultrasound-assisted extraction, on the yield, phytochemical composition, and biological activities of *Myrtus communis*, *Pistacia lentiscus*, and *Rhamnus alaternus*, three medicinal plants widely used in traditional Algerian phytotherapy. Extraction yields varied depending on the method, with ultrasound showing superior performance: 17.4% for *P. lentiscus* compared to 12.6% via maceration. Ultrasound extracts also exhibited higher total phenolic content, reaching 289.17 mg GAE/g for *M. communis*, and flavonoid content up to 114.64 mg QE/g for the same species. Antioxidant activity, assessed using DPPH and ABTS^{•+} assays, showed strong radical scavenging power, notably in *M. communis*, with a DPPH IC₅₀ of 19.04 µg/mL. Antibacterial tests revealed a maximum inhibition zone of 21 mm against *Staphylococcus aureus* using *R. alaternus* extract. Moreover, *P. lentiscus* exhibited significant anti-inflammatory activity, inhibiting protein denaturation by 86.45% at 100 µg/mL. These findings confirm the critical impact of extraction technique on extract efficacy and highlight the relevance of green approaches, especially ultrasound-assisted extraction, for enhancing bioactive compound recovery. This work contributes to the rational valorization of Algerian flora in a context of sustainable development and natural healthcare.

Keywords: Green chemistry, ultrasound extraction, phenolic compounds, antioxidant activity, medicinal plants.

MULTISCALE MODELING OF MOISTURE DIFFUSION IN POLYMER/CLAY NANOCOMPOSITES

Makhloufi ALI^{*}, Gueribiz DJELLOUL¹, Jacquemin FREDERIQUE² et Freour SYLVAIN²

¹*Faculté de Technologie, Laboratoire de Génie Des Procédés, Université Amar Télidji, Laghouat, Algeria*

²*Institut de Recherche en Génie Civil et Mécanique (UMR CNRS 6183), Nantes Université, Saint-Nazaire, France*

Email: makh.ali1988@gmail.com

Abstract: In this work, a multiscale modeling approach was used to analyze the moisture absorption behavior in polymer/clay nanocomposites, with the development of a new method for determining the representative elementary volume (REV), thereby improving the accuracy of the modeling and the representation of the actual structure of these materials. Two structural configurations were examined: exfoliated and intercalated. The results showed that moisture diffusion follows Fickian behavior, with a significant decrease in the diffusion coefficient as the nanoclay content increases, due to the barrier effect of the clay platelets within the polymer matrix. The exfoliated structures proved to be more effective than the intercalated ones in limiting moisture absorption.

Keywords: Moisture diffusion; multiscale modeling; nanocomposite; polymer; clay.

COMPUTATIONAL APPROACHES TO SCREENING PLANT PHYTOCHEMICALS: MOLECULAR DOCKING, ADME PREDICTION, AND EXPERIMENTAL CORRELATION: A LITERATURE-BASED REVIEW

Ilham KARKOURI^{1,2*}, Mohammed Laid TLILI^{1,3} and Nour Elhouda MEKHADEMI^{1,4}

¹*Department of Cellular and Molecular Biology, Faculty of Natural Sciences and Life, University of El-Oued, El-Oued, Algeria.*

²*Laboratory of Biology, Environment, and Health, University of El-Oued, El-Oued, Algeria.*

³*Biogeochemistry of Desert Environments Laboratory of Ouargla University, Algeria.*

⁴*Laboratory of the Development and Technology of Saharan Resources (VTRS), University of El-Oued, El-Oued, Algeria.*

*Corresponding author: Tel./Fax: +213797077454 ;

E-mail address: karkouri-ilham@univ-eloued.dz

Abstract: Traditionally, identifying the activities of plant bioactive compounds has required extensive laboratory work. Nowadays, computational modeling tools are widely used to screen phytochemicals for their pharmacological properties. This review highlights recent progress in the application of molecular docking and in silico ADME (Absorption, Distribution, Metabolism, and Excretion) prediction for evaluating the biological and pharmacokinetic potential of secondary metabolites. Literature published between 2021 and 2025 was examined to identify studies using tools such as AutoDock Vina, SwissADME, and pkCSM. Notably, compounds like thymol and carvacrol from *Thymus vulgaris* and *Origanum vulgare* exhibited strong antimicrobial effects. When combined with antibiotics, thymol and carvacrol reduced the minimum inhibitory concentration (MIC) for bacterial strains, demonstrating synergistic effects. Docking and experimental studies on *Centaurea lycaonica* revealed that apigenin and myristoleic acid showed notable binding affinities against α -amylase and α -glucosidase. Extracts from this plant also exhibited strong antioxidant activity and significant FRAP activity. In silico ADME predictions further revealed favorable drug-likeness and absorption profiles for several candidates. Integrating molecular docking with AI-based computational techniques—such as molecular dynamics simulations and QSAR modeling—offers a rapid and cost-effective way to screen a wide range of phytochemicals, which helps accelerate drug discovery. However, experimental studies remain essential.

Keywords: Phytochemicals; Molecular Docking; Artificial Intelligence; Drug Discovery; Antioxidant.

VALORISATION OF ALFALFA SPROUTS AS A SOURCE OF ANTIOXIDANT AND ANTI-INFLAMMATORY BIOACTIVE COMPOUNDS

SADOK Zeyneb^{1*}, NEHARI Assia¹ and KOICHE Malika¹

¹Laboratory of Natural and Local Bio-Resources, Faculty of Natural and Life Sciences, Department of Food Science and Human Nutrition, Hassiba Ben Bouali University, Chlef, Algeria

*Corresponding author: Tel: 06.98.33.11.80 ; E-mail address: z.sadok@univ-chlef.dz

Abstract: The search for plant-based bioactive compounds with antioxidant and anti-inflammatory properties continues to attract significant scientific interest. In this context, the present study investigates the methanolic extract of Alfalfa (*Medicago sativa*) sprouts for its antioxidant and anti-inflammatory potential. Extraction was performed by maceration using 80% methanol, which is known to efficiently solubilize phenolic compounds. The total polyphenol content was measured using the Folin–Ciocalteu method, yielding 649.36 mg gallic acid equivalents (GAE) per 100 g of dry weight. Total flavonoid content, determined via the aluminum chloride colorimetric assay, was 96.94 mg GAE/100 g dry matter. Antioxidant activity assessed through the DPPH radical scavenging method revealed a significant free radical inhibition capacity, confirming the extract's strong antioxidant profile. Furthermore, *in vivo* anti-inflammatory activity was evaluated in a formalin-induced paw edema model in Wistar rats. The extract showed dose-dependent inhibition of inflammation, achieving 50.10% and 70% inhibition at 100 mg/kg and 200 mg/kg, respectively. Notably, the higher dose outperformed Diclofenac (60.50% inhibition at 50 mg/kg), the reference anti-inflammatory drug. These results highlight the rich composition and dual bioactivity of Alfalfa sprouts, supporting their potential application in natural product chemistry, functional food formulation, and the development of nutraceuticals .

Keywords: Alfalfa sprouts , Anti-inflammatory activity, Antioxidant activity , Bioactive compounds.

GREEN DRYING STRATEGIES AND AI-DRIVEN MODELING FOR THE VALORIZATION OF *CAPPARIS SPINOSA* BUDS AS FUNCTIONAL INGREDIENTS

LAKHDARI Chafika^{1,2*}, DJELLAL Samia^{1,2}, ADOUANE Meriem^{1,2}, REMINI Hocine², DAHMOUNE Farid², KADRI Nabil²

¹Laboratoire de Gestion et Valorisation des Ressources Naturelles et Assurance Qualité (LGVRNAQ), Faculté des Sciences de la Nature et de la Vie et des Sciences de la Terre, Université de Bouira, 10000 Bouira, Algeria

²Département de Biologie, Faculté des Sciences de la Nature et de la Vie et des Sciences de la Terre, Université de Bouira, 10000 Bouira, Algeria

Abstract: *Caper buds (Capparis spinosa)*, an abundant and underutilized Mediterranean resource, are rich in bioactive compounds such as polyphenols and flavonoids, with promising applications in functional foods and nutraceuticals. This study explores eco-efficient drying strategies for the valorization of *C. spinosa* buds, focusing on the preservation of their active ingredients and functional properties through green processing. Three low-impact drying technologies—convective drying, vacuum drying, and microwave drying—were applied under varied conditions. Their influence on moisture kinetics, color retention (HunterLab), total phenolic content (TPC), total flavonoid content (TFC), and antioxidant activity (DPPH, ABTS, FRAP) was assessed. Among the tested methods, vacuum drying at 80 °C best preserved the functional quality of the buds (TPC = 30.18 mg GAE/g DW, TFC = 10.27 mg QE/g DW, DPPH = 0.249 mg/mL, ABTS = 4.448 mg/mL), while minimizing degradation and ensuring color stability ($\Delta E = 7.47$). To enhance process understanding, a meta-heuristic Dragonfly Algorithm was used to model the drying kinetics and support data-driven decision-making for sustainable process design. The integration of artificial intelligence enabled accurate prediction of drying behavior, contributing to energy-efficient and quality-preserving treatment protocols. This work demonstrates the potential of combining green chemistry principles with AI-based modeling for the valorization of plant-derived bioresources. It supports the development of sustainable bioprocesses to transform caper buds into high-value functional ingredients, reinforcing circular bioeconomy objectives and clean-label food innovation.

Keywords: *Capparis spinosa*, drying optimization, Dragonfly Algorithm, bioactive compounds, functional foods.

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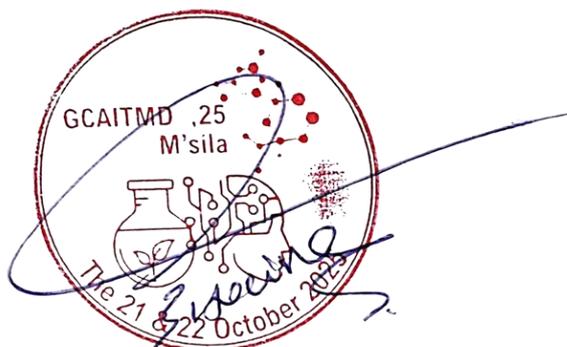


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