الملتقى السادس للباحثين الكيميائيين الشبان

SIXIÈME FORUM DESJEUNES CHERCHEURS CHIMISTES

FJCC 2025

Organisé par la

Section du Centre

de la

Société Chimique de Tunisie

09-11 Mai 20245

Palais des Sciences de Monastir
Monastir, Tunisie

Résumés des Conférences et des Communications
Liste des Participants

Société Chimique de Tunisie - Section du Centre
Programme Succint du FJCC 2025

	Vendredi 09 Mai 2025
08h00 - 09h00	**Inscription**
09h00 - 09h15	**Cérémonie d'Ouverture**
09h20 - 10h05	**Conférence Plénière 1 : Professeur Habib NASRI** | Présidente : Amira Bahy *FSM - Université de Monastir* **The Porphyrin : The Other Molecule of Life**
10h05 - 10h35	**Pause-café**
10h40- 11h25	**Conférence Plénière 2 : Professeur Hatem DHAOUADI** | Présidente : Zeineb Mzoughi *FSM - Université de Monastir* **Les Fluides Supercritiques : Une Révolution dans la Teinture Durable pour l'Industrie Textile**
11h30 - 12h30	**Communications Orales (15min) - Session 1 -** *Salle I* **- CO 1 - CO 4**
12h30 - 14h30	**Déjeuner libre**
14h30 - 15h30	**Communications Orales (15min) - Session 2 -** *Salle I et II* **- CO 5 - CO 12**
15h30 - 16h15	**Pause-café, Séance Posters (P 01 - P 22) Ordre alphabétique**
16h15 - 17h15	**Communications Orales (15min) - Session 3 -** *Salle I* **- CO 13 - CO 16**
	Samedi 10 Mai 2025
09h00 - 09h45	**Conférence Plénière 3 : Professeur Ayoub HAJ SAID** | Président : Mansour Znati *FSM - Université de Monastir* **Une Introduction aux Structures métallo-organiques (MOFs)**
09h45 - 10h25	**Pause-café**
10h25 - 11h10	**Conférence Plénière 4 : Professeur Mustapha MAJDOUB** | Président : Khaled Hriz *FSM - Université de Monastir* **Utilisation de la technologie micro-ondes en synthèse chimiques**
11h15 - 12h15	**Communications Orales (15min) - Session 4 -** *Salle I* **- CO 17 - CO 20**
12h15 - 14h30	**Déjeuner libre**
14h30 - 15h30	**Communications Orales (15min) - Session 5 -** *Salle I et II* **- CO 21 - CO 28 -**
15h30 - 16h15	**Pause-café, Séance Posters (P 23 - P 43) Ordre alphabétique**
16h15 - 17h15	**Communications Orales (15min) - Session 6 -** *Salle I* **- CO 29 - CO 32**
	Dimanche 11 Mai 2025
09h00 - 10h30	**Communications Orales (15min) - Session 7 -** *Salle I et II* **- CO 33 - CO 42**
10h30	**Clôture du FJCC 2025**

Avant-propos

Au nom des Comités Scientifiques et d'Organisation, c'est avec un immense plaisir que nous vous accueillons à Monastir, à l'occasion de ce Forum qui se tiendra du 09 au 11 mai 2025. Nous sommes ravis de votre présence et nous vous remercions pour votre participation. Nous espérons que ces journées seront riches en échanges, découvertes et pleines de collaborations fructueuses.

Le programme du FJCC 2025 comprendra 04 conférences plénières, 42 communications orales, 43 communications par affiche et 02 ateliers de formation portant sur le “Plan d’Expérience” et sur le “Docking Moléculaire”. Les langues officielles du congrès seront l'anglais et le français. Nous remercions vivement nos quatre conférenciers qui ont accepté de partager leurs expériences récentes dans leurs domaines respectifs lors de ce forum. Notre extrême reconnaissance va aussi à nos 02 formateurs pour les connaissances qu’ils vont partager avec les jeunes chercheurs afin de leur offrir une véritable opportunité d’apprentissage et de développement.

Le sixième Forum des Jeunes Chercheurs Chimistes (FJCC 2025) est une rencontre scientifique nationale qui offre une plateforme d'échange aux jeunes chercheurs en chimie. Cet événement leur permet de présenter leurs travaux originaux, de partager leurs projets novateurs et de discuter des expériences technologiques dans un cadre interactif.

Ce forum aspire à être un moteur d’innovation et un creuset d’idées nouvelles au service des avancées scientifiques et technologiques.

Nous espérons que cette rencontre apportera à nos jeunes chercheurs une expérience fructueuse d’apprentissage et de collaboration.

Une fois encore, bienvenue à Monastir et au 6ème Forum FJCC 2025 !

Pr. Hatem Majdoub

Président du FJCC 2025

Secrétaire Général de la Section du Centre de la Société Chimique de Tunisie

COMITÉ SCIENTIFIQUE

Hatem MAJDOUB (Président)	*FSM, Université de Monastir*
Latifa LATROUS	*IPEIEM, Université de Tunis El Manar*
Rym ABIDI	*FSB, Université de Carthage*
Ridha BEN SALEM	*FSS, Université de Sfax*
Houcine BARHOUMI	*FSM, Université de Monastir*
Faouzi ALOUI	*FSM, Université de Monastir*
Béchir CHAOUACHI	*ENIG, Université de Gabès*
Younes MOUSSAOUI	*FSG, Université de Gafsa*
Mansour ZNATI	*FSM, Universté de Monastir*
Moneim ZANNEN	*FSM, Universté de Monastir*
Sarra BOUDRIGUA	*FSM, Université de Monastir*
Kamel LANDOLSI	*FSM, Université de Monastir*
Ichraf NAGGAZI	*FSM, Université de Monastir*
Mejed CHEMLI	*FSM, Université de Monastir*

COMITÉ D'ORGANISATION

Khaled HRIZ	*FSM, Université de Monastir*
Amira BAHY	*FSM, Université de Monastir*
Zeineb MZOUGHI	*FSM, Université de Monastir*
Ahlem BEYAOUI	*FSM, Université de Monastir*
Chiraz YOUSSEF	*FSM, Université de Monastir*
Leila BAOUEB	*FSM, Université de Monastir*
Hannen JLIZI	*FSM, Université de Monastir*
Sondes BOURIGUA	*FSM, Université de Monastir*
Mariem ITAIMI	*FSM, Université de Monastir*
Souad OUANES	*FSM, Université de Monastir*
Anoura LAOUITI	*FSM, Université de Monastir*
Mehdi RAMMEH	*FSM, Université de Monastir*
AMIN MNIF	*FST, Université de Tunis El Manar*
Imed LAAJIMI	*Société Chimique de Tunisie, SCT*

Sixième Forum des Jeunes Chercheurs Chimistes - FJCC 2025

Programme des Ateliers de Formations

(Plan d'Expérience - Docking Moléculaire)

Mercredi 07 Mai 2025		
	Plan d'expérience Formateur : **Dr. Halim HAMMI**	**Docking** Formateur : **Dr. Mabrouk HORCHANI**
09h00 - 11h00	• Initiation aux notions des plans d'expériences : Facteurs (contrôlés et non contrôlés)	• Introduction sur l'amarrage moléculaire et son implication dans la conception de molécules thérapeutiques. • Installation des logiciels.
11h00 - 11h30	**Pause-café**	
11h30 - 12h30	• Initiation aux notions des plans d'expériences : Facteurs (quantitatifs et qualitatifs)	• Préparation des ligands.
12h30 - 13h30	**Déjeuner libre**	
13h30 - 15h00	• Initiation aux notions des plans d'expériences Niveaux (bas et haut) Réponses (variables dépendantes)	• Préparation des récepteurs (enzymes cibles)
15h00 - 15h30	**Pause-café**	
15h30 - 17h00	• Initiation aux notions des plans d'expériences Les types de plans - Formes géométriques	• Préparation du complexe : Récepteur-Ligand
Jeudi 08 Mai 2025		
09h00 - 11h00	• Interprétation des résultats Analyse statistique Applications : Exemples	• Application du Docking Moléculaire à des cibles thérapeutiques.
11h00 - 11h30	**Pause-café**	
11h30 - 12h30	• Interprétation des résultats Convertir des résultats statistiques en résultats concrets. Optimisation des conditions opératoires	• Application du Docking Moléculaire à des cibles thérapeutiques.
12h30 - 13h30	**Déjeuner libre**	
13h30 - 15h00	• Interprétation des résultats Applications : Exemples Méthodes indirectes (plans de deuxième degré, courbes isoréponses)	• Conception de résultats : figures, énergies de liaisons, etc.
15h00 - 15h30	**Pause-café**	
15h30 - 17h00	• Interprétation des résultats Applications sur le logiciel « NemrodW »	• Conception de résultats : figures, énergies de liaisons, etc.

Programme du Forum - FJCC 2025

Conférences Plénières, Communications Orales et par Affiches

Vendredi 09 Mai 2025				
08h00 - 09h00	**Inscription**			
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09h20 - 10h05	**Conférence Plénière 1 : Professeur Habib NASRI** | Présidente : Amira Bahy *FSM - Université de Monastir* **The Porphyrin : The Other Molecule of Life**			
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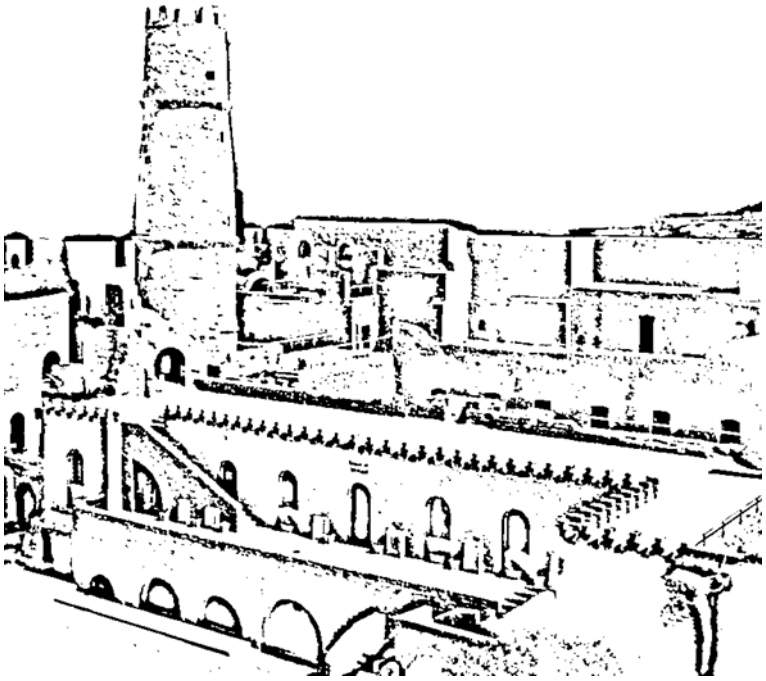
	Communications Orales (15min) - Session 1			
	Salle I - Président : Mejed Chemli			
11h30 - 11h45	CO-1	HORCHANI Mabrouk		
11h45 - 12h00	CO-2	ELHISS Sawsen		
12h00 - 12h15	CO-3	MACHERKI Ameni		
12h15 - 12h30	CO-4	KHEMIS Eya		
12h30 - 14h30	**Déjeuner libre**			
	Communications Orales (15min) - Session 2			
	Salle I - Présidente :Ichraf Nagazzi		**Salle II** - Présidente : Sarra Boudrigua	
14h30 - 14h45	CO-5	MAALEJ Emna	CO-9	BEN NEJMA Sadok Lamine
14h45 - 15h00	CO-6	BOLTANE Khouloud	CO-10	HAMROUNI Khaoula
15h00 - 15h15	CO-7	DJERIBI Malek	CO-11	JAAFAR Zouhour
15h15 - 15h30	CO-8	BEN DASSI Roua	CO-12	WALHA Sandra
15h30 - 16h15	**Pause-café, Séance Posters (P 01 - P 22) Ordre alphabétique** **Evaluateurs** : Mehdi Rammeh et Ichraf Nagazzi			
	Communications Orales (15min) - Session 3			
	Salle I - Présidente : Ahlem Beyaoui			
16h15 - 16h30	CO-13	BEN DLALA Sirine		
16h30 - 16h45	CO-14	CHOUAIBI Asma		
16h45 - 17h00	CO-15	FATNASSI Ameni		
17h00 - 17h15	CO-16	SGHAIER Zohra		

Samedi 10 Mai 2025				
09h00 - 09h45	**Conférence Plénière 3 : Professeur Ayoub HAJ SAID** | Président : Mansour Znati *FSM - Université de Monastir* **Une Introduction aux Structures métallo-organiques (MOFs)**			
09h45 - 10h25	**Pause-café**			
10h25 - 11h10	**Conférence Plénière 4 : Professeur Mustapha MAJDOUB** | Président : Khaled Hriz *FSM - Université de Monastir* **Utilisation de la technologie micro-ondes en synthèse chimiques**			
	Communications Orales (15min) - Session 4			
	Salle I - Présidente : Chiraz Youssef			
11h15 - 11h30	CO-17	REGUIGUI Amira		
11h30 - 11h45	CO-18	YAHIA Achwak		
11h45 - 12h00	CO-19	DEMS Lobna		
12h00 - 12h15	CO-20	MZOUGHI Zeineb		
12h15 - 14h30	**Déjeuner libre**			
	Communications Orales (15min) - Session 5			
	Salle I - Président : Houcine Barhoumi		**Salle II** - Président : Kamel Landoulsi	
14h30 - 14h45	CO-21	OUNIS DKHIL Yossra	CO-25	BEN AMOR Wala
14h45 - 15h00	CO-22	BOUHLEL Ines	CO-26	BOUMAIZA Fatma
15h00 - 15h15	CO-23	BERGAOUI Souad	CO-27	IBIDHI Salah
15h15 - 15h30	CO-24	ELABED Makram	CO-28	WANNASSI Jassem
15h30 - 16h15	**Pause-café, Séance Posters (P 23 - P 43) Ordre alphabétique** **Evaluateurs** : Semy Ben Chaabene et Mejed Chemli			
	Communications Orales (15min) - Session 6			
	Salle I - Président : Ibrahim Ayed			
16h15 - 16h30	CO-29	CHAABENE Marwa		
16h30 - 16h45	CO-30	DHIFET Mondher		
16h45 - 17h00	CO-31	ELGHARBI Safa		
17h00 - 17h15	CO-32	LASSOUED Ameni		

Dimanche 11 Mai 2025				
	Communications Orales (15min) - Session 7			
	Salle I - Président : Moneim Zannen		**Salle II** - Présidente : Imen Abdelhédi	
09h00 - 09h15	CO-33	TOUMIA Hiba	CO-38	MBAREK Awatef
09h15 - 09h30	CO-34	ZGUIR Imen	CO-39	KHALDI Rania
09h30 - 09h45	CO-35	HASNI Fatma	CO-40	MOUMEN Youssra
09h45 - 10h00	CO-36	BRAHIM Mariem	CO-41	BEN TIBA Ameni
10h00 - 10h15	CO-37	MABROUKI Nabil	CO-42	MISSAOUI Kahla
10h30	**Clôture du FJCC 2025**			



Résumés des Conférences

Habib NASRI

Professor Habib Nasri is a Professor Emeritus at the Faculty of Sciences of Monastir, University of Monastir, Tunisia, where he has had a distinguished academic career since 1990. He earned his PhD in 1987 from the University of Strasbourg 1 under the supervision of Professor R. Weiss. Following his doctoral work, Professor Nasri completed a postdoctoral research period between 1988 and 1990 with Professor W. R. Scheidt at the University of Notre Dame, Indiana, USA.In 1990, he joined the Faculty of Sciences of Monastir as an assistant professor, where he has steadily advanced in his academic career, achieving the rank of associate professor in 2001 and full professor in 2007. His research interests primarily revolve around porphyrins and porphyrin complexes. With more than 140 published articles and numerous contributions to the field, he has also supervised several Master's and PhD students. Between 2017 and 2024, Professor Nasri served as the Director of the Laboratory of Physical Chemistry of Materials, further strengthening his leadership in research. His work continues to contribute significantly to the development of material chemistry and the study of complex molecular structures.

The Porphyrin : The Other Molecule of Life

Habib NASRI

Laboratory of Physical Chemistry of Materials
Faculty of Science of Monastir, Environment Avenue, 5019 Monastir -TUNISIA
University of Monastir

Porphyrin macrocycles have been the subject of intense study in the last century and the last two decades because they are widely distributed in nature. As such, they serve as the prosthetic groups in a wide variety of primary metabolites, such as hemoglobin, myoglobin, cytochromes, catalases, peroxidases, chlorophylls, and bacteriochlorophylls. These species present a tetrapyrrolic ring known as porphyrin. The resulting aromaticity gives rise to the semiconducting properties that make these compounds of interest for a broad range of applications, including artificial photosynthesis, catalysis, molecular electronics, sensors, non-linear optics, solar cells and as photosynthesizers in the photodynamic therapy (PDT) of cancer.

Hatem DHAOUADI

Hatem Dhaouadi est un enseignant chercheur tunisien dans le domaine de la Chimie et du génie chimique. Titulaire d'un doctorat en Génie des Procédés de l'Institut National Polytechnique de Lorraine (INPL, France) en 1997, il a obtenu une Habilitation universitaire en Chimie en 2009 à l'université de Monastir et également une Habilitation à Diriger des Recherches (HDR) en Sciences et Technologies Industrielles en 2011 à l'Université Paul Cézanne d'Aix-Marseille. Depuis février 2017, il occupe le poste de Professeur de Génie Chimique à la Faculté des Sciences de Monastir (FSM), où il a précédemment été Maître de Conférences dans la même discipline et Assistant puis Maître-assistant de Chimie.

Hatem Dhaouadi est le fondateur et directeur du Laboratoire de Chimie de l'Environnement et des Procédés Propres (LR21ES04) depuis mai 2021. Il a également dirigé l'Unité de recherche Chimie Appliquée Environnement (UR13ES63) de 2015 à 2021. Ses travaux de recherche ont donné lieu à plus de 70 publications scientifiques et 30 communications internationales dans le domaine des sciences environnementales et des procédés propres.

Il est le fondateur et président de l'Association Tunisienne des Technologies Durables (ATuTeD) et a présidé plusieurs congrès internationaux, dont l'ICACE. Il a également encadré de nombreuses thèses et mastères.

Les Fluides Supercritiques : Une Révolution dans la Teinture Durable pour l'Industrie Textile

Hatem DHAOUADI

Laboratoire de Chimie de l'Environnement et des Procédés Propres (LR21ES04)
Faculté des Sciences de Monastir, Avenue de l'environnement 5019 Monastir -TUNISIE
Université de Monastir

L'industrie textile est l'une des plus polluantes au monde, notamment en raison de l'utilisation intensive d'eau, de produits chimiques toxiques et de procédés énergivores dans les processus de teinture. Face à ces défis environnementaux, les fluides supercritiques, en particulier le dioxyde de carbone supercritique (CO_2 supercritique), émergent comme une solution innovante et durable pour changer les pratiques de teinture. Cette conférence explore comment cette technologie peut transformer l'industrie textile en réduisant son empreinte écologique.

Les fluides supercritiques, qui se situent à un état intermédiaire entre le liquide et le gaz, possèdent des propriétés très intéressantes. Le CO_2 supercritique, par exemple, combine la densité d'un liquide avec la diffusivité d'un gaz, ce qui en fait un solvant idéal pour la teinture. Contrairement aux méthodes traditionnelles, la teinture par CO_2 supercritique ne nécessite pas d'eau, élimine l'utilisation de produits chimiques nocifs et réduit considérablement la consommation d'énergie. De plus, ce procédé permet une pénétration uniforme des colorants dans les fibres, offrant des résultats de teinture de haute qualité.

Dans cette conférence, nous aborderons les principes scientifiques sous-jacents aux fluides supercritiques et leur application dans la teinture textile. Nous examinerons les aspects chimiques des interactions fibre – colorant et les moyens de leurs améliorations. Nous examinerons également les avantages environnementaux de cette technologie, notamment la réduction de la consommation d'eau, l'élimination des rejets toxiques et la diminution des émissions de gaz à effet de serre.

Ayoub HAJ SAID

Dr Ayoub HAJ SAID est Professeur de chimie physique et Directeur Scientifique du Centre de Recherche en Microélectronique et Nanotechnologie (CRMN) de Sousse. Son expertise porte sur l'électrochimie appliquée et les sciences des matériaux. Ses intérêts de recherche incluent la synthèse de polymères conjugués et de différents nanomatériaux (nanofibres, matériaux nanoporeux, nanocomposites…) pour des applications optoélectroniques et le développement de capteurs. Pr Ayoub HAJ SAID est le coordinateur du « Projet de recherche et d'innovation sur la micro et la nanotechnologie pour les capteurs » (PRIMiNaS, Projet Horizon Europe - ref 101079485).

Une Introduction aux Structures Métallo-Organiques (MOFs)

Ayoub HAJ SAID

[1.] *Centre de Recherche en Microélectronique et Nanotechnologie*
Technopôle de Sousse "Novation City", Sahloul Sousse 4054
[2.] *Faculté des Sciences de Monastir, Avenue de l'environnement 5019 Monastir -TUNISIE*
Université de Monastir

Depuis quelques années, la famille des Metal Organic Frameworks (MOFs) a attiré considérablement l'attention en raison de leurs structures hautement modulables permettant l'accès à une large gamme de matériaux nanoporeux et multifonctionnels. Ces matériaux hybrides nanostructurés peuvent être décrits comme des assemblages supramoléculaires de cations métalliques, ou des clusters oxo-métalliques, avec des ligands présentant plus qu'un centre de coordination. Ces matériaux possèdent une grande porosité et différentes fonctionnalités qui leur confèrent un grand potentiel pour des diverses applications. Dans cette intervention, un aperçu général sera présenté sur leurs méthodes de synthèse, leurs propriétés et leurs applications.

Mustapha MAJDOUB

DOCTEUR D'ETAT Es-SCIENCES PHYSIQUES
(Spécialité chimie des polymères)

mustapha.majdoub@fsm.rnu.tn , mustaphamajdoub@gmail.com
Tel: +(216) 73 501 787

Formation

- 1983: DEA de physicochimie macromoléculaire de l'UPMC, Université Paris 6
- 1985 : Thèse de doctorat en chimie des Polymères de l'UPMC, Université Paris 6
- 1998: Doctorat d'Etat Es-Sciences Physiques ***Spécialité chimie des polymères*** -Université de Tunis

Mobilité et fonctions occupées

- Depuis 2004: Professeur des Universités, à la Faculté des Sciences de Monastir
- 1998 - 2004 : Maître de Conférences à la Faculté des Sciences de Monastir
- 1992 - 1998 : Maître assistant à la Faculté des Sciences de Monastir.
- 1989 - 1992: Assistant à la Faculté des Sciences de Monastir.

Professeur invités :

- Université Paris 6, Paris Diderot (7 fois 1 mois)
- Université d'Évry val-d 'Essonne (1 mois)
- Université Pierre et Marie Curie, Paris 6 (1 mois)

Responsabilités administratives et Pédagogiques

- Membre élu du **conseil Scientifique** de la Faculté des Sciences de Monastir (1996-1999)
- ***Directeur du Laboratoire***, Polymères–Biopolymères-Matériaux Organique (2010 - 2014).
- ***Directeur du Laboratoire*** des Matériaux Avancés et Interfaces (LIMA) (2014-2024)
- ***Président de la commission des Doctorats*** et des Habilitations à la Faculté des Sciences de
- Monastir (Février 2014 à juillet 2024).

Activité de recherche et domaines de compétences

- *Synthèse et caractérisation des polymères semi-conducteurs dérivés de PPV (Application en opto-électronique et aux capteurs optiques).*
- *Synthèse de nouveaux polymères biosourcés, supramolécules fonctionnelles à base de cyclodextrines pour des applications aux capteurs.*
- *Microencapsulation pour applications en cosméto-textile.*

Domaines de compétences

- Synthèse et Modification chimique des polymères
- Activation par les microondes
- Synthèse organique

PRODUCTION SCIENTIFIQUE ET ENCADREMENT DE CHERCHEURS

- **23 thèses** soutenues dont 3 en cotutelle+ 3 thèses en cours
- **29 DEA et Mastères** (7 DEA + 22 Mastères de Recherche et 2 Mastères Appliqués).
  - https://scholar.google.com/citations?user=V-g1-EUAAAAJ&hl=fr
  - https://www.researchgate.net/profile/Mustapha-Majdoub
  - **ORCID iDhttps://orcid.org/0000-0003-0337-2937**

Utilisation de la technologie micro-ondes en synthèse chimiques

Mustapha MAJDOUB

Laboratoire des Matériaux Avancés et Interfaces (LIMA)
Faculté des Sciences de Monastir, Avenue de l'environnement 5019 Monastir -TUNISIE
Université de Monastir

L'activation des réactions chimiques par micro-ondes est un domaine de recherche qui a suscité un grand intérêt depuis les années 1990. Cette présentation concerne les nouveaux développements sur l'utilisation des technologies microondes en synthèse organique, inorganique et macromoléculaire.

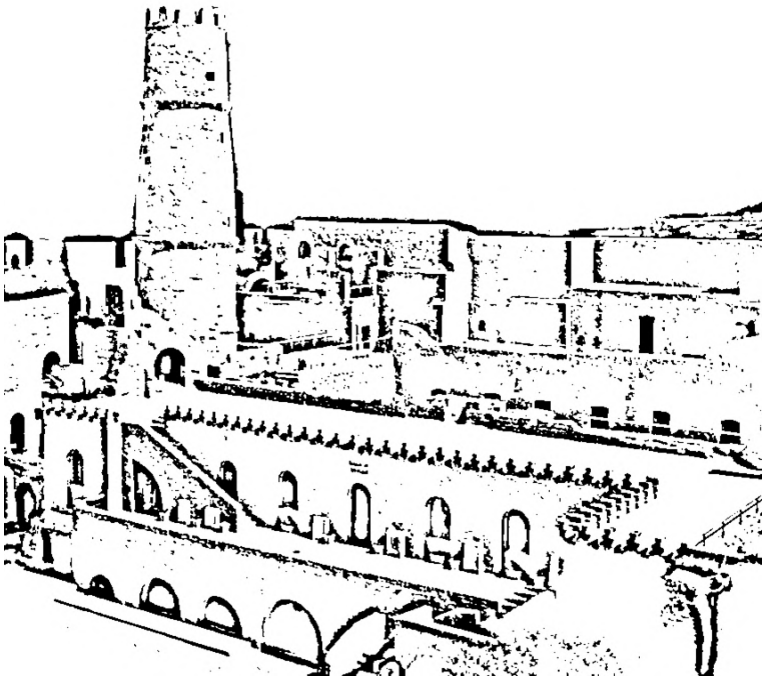
La première partie sera consacrée aux rappels du principe de fonctionnement des micro-ondes et leur utilisation en synthèse chimique et dans le domaine des matériaux.

La deuxième partie, concernera les réacteurs microondes adaptés et utilisés dans les laboratoires. Il s'agira du principe d'activation des réactions chimiques dans les fours microondes domestiques classiques et des réacteurs monomodes utilisés dans les laboratoires.

Dans la troisième partie nous développerons quelques exemples de synthèse des polymères et des synthèses organiques en solution et en milieu sec (sans solvant). Une étude comparative de l'activation par chauffage thermique et par les microondes sera développée à travers quelques exemples de synthèses.

Dans la dernière partie nous donnerons quelques exemples récents d'applications Industrielles de la Synthèse Chimique par Micro-ondes.

En conclusion, l'activation des réactions chimiques par micro-ondes offre un potentiel intéressant pour améliorer l'efficacité et la rapidité des processus chimiques, mais son application nécessite une compréhension précise des phénomènes physiques et chimiques impliqués pour éviter des effets indésirables.



Liste des Communications Orales

Noms des Communicants	Ref
BEN AMOR Wala, H. Ammar, R. Ben Salem, G. Rigane *FSS - Sfax* Microwave-assisted extraction of bioactive polyphenols from *Cucumis metuliferus*: Optimization and antioxidant evaluation	**CO 25**
BEN DASSI Roua, F. D'agostino, S. Ibidhi, H. Jemai, L. Giaramita, G. Tranchida, S. Sadok, A. Cherif, R. Driouich Chaouachi *ISBST - Sidi Thabet* Sustainable valorization of shrimp shell waste into chitosan nanofibers for efficient amoxicillin removal	**CO 8**
BEN DLALA Sirine, M. Haj Romdhane, S. Lakard, B. Lakard, D. Le Cerf, N. Jaffrezic-Renault, H. Ben Halima, H. Majdoub *FSM - Monastir* Valorization of *Vicia faba* wastes: Pectin extraction and its application as an eco-friendly corrosion inhibitor for mild steel	**CO 13**
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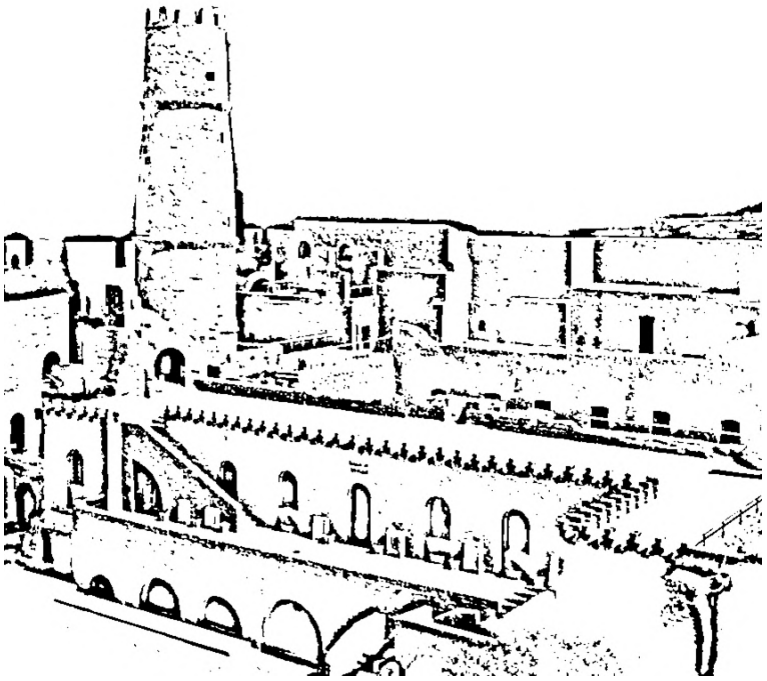

Résumés des Communications Orales

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Design, synthesis, ADMET profiling and *in silico* docking assessment towards M-Pro of novel pyrazolopyrimidinone derivatives as putative SARS-CoV-2 inhibitors.

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In addition to vaccines, antiviral drugs are fundamental to suppress COVID-19. Although, some inhibitor candidates have been determined to target the SARS-CoV-2 protein, there is still an urgent need to continue the search for new inhibitors of the SARS-CoV-2 main protease "Omicron P132H", as a recently discovered protein [1-2]. In this light, herein, in the search for therapeutic alternatives to treat COVID-19 in addition to its recent variants, we conducted a structure-based virtual screening using docking studies and ADMET predictions for a novel series of pyrazolo[3,4-d]pyrimidin-4(5H)-one of derivatives, which were synthesized *via* the condensation reaction of pyrazolopyrimidinone-hydrazide with a series of electrophiles. From the theoretical biological evaluation, interesting results were obtained based on the types of interactions formed and the binding energy values which were compared to the reference anti-SARS-CoV-2 redocked drug, 'Nirmatrelvir'.

Keywords: pyrazolopyrimidinone, SARS-CoV-2, docking, ADMET.

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Hyaluronic acid from poultry by-products: Isolation, characterization, and evaluation of biological activities

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The poultry industry is a rapidly expanding agricultural sector, highlighting the need for innovative strategies to valorize its by-products. Hyaluronic acid (HA), a key biopolymer found in high concentrations in rooster and chicken combs, was targeted in this study for extraction, purification, and characterization, alongside evaluation of its anti-inflammatory and gastroprotective properties.

HA samples, extracted from rooster and chicken combs (HAQ and HAP, respectively), were purified using anion exchange chromatography, yielding approximately 55.9 mg/g and 32 mg/g of defatted raw material. Structural characterization using FT-IR, 1D–^{1}H NMR and SEC/MALS/DRI/VD confirmed the identity of highly pure (>90%) hyaluronic acids with relatively low molecular weights: 180 kDa (HAQ) and 143.4 kDa (HAP).

Both HAQ and HAP exhibited significant, dose-dependent anti-inflammatory and gastroprotective effects. In the ethanol/HCl-induced ulcer model, pretreatment with either HAQ or HAP notably reduced gastric lesion severity. These effects were associated with modulation of gastric secretions (volume, pH, total acidity) and improved antioxidant status in gastric tissue, evidenced by increased CAT and SOD activity and reduced MDA levels. Therefore, these findings indicate that poultry by-products are a promising source of natural hyaluronic acid with therapeutic potential for gastrointestinal health.

Keywords: Poultry by-products, Hyaluronic acid, Physicochemical characterization, Biological properties.

Polysaccharides from Star Anise Pomace: Physico-chemical Characterization and Biological Evaluation

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In this study, a water-soluble polysaccharide was extracted from the seed pomace of *Illicium verum* (star anise) using hot water extraction followed by ethanol precipitation. The purified polysaccharide was structurally characterized by Fourier Transform Infrared Spectroscopy (FT-IR), Nuclear Magnetic Resonance (NMR), Size Exclusion Chromatography (SEC), and Gas Chromatography-Mass Spectrometry (GC-MS). GC-MS analysis of the acid-hydrolyzed polysaccharide revealed a complex mixture of monosaccharides, mainly arabinose (35.2%), rhamnose (18.7%), xylose (14.6%), mannose (10.3%), glucose (11.1%), and galactose (10.1%), indicating a heterogeneous polymer rich in arabinogalactans and rhamnogalacturonan-like regions [1,2]. The isolated polysaccharide was also evaluated for its biological activity. It demonstrated significant antioxidant capacity in DPPH and ABTS assays and moderate α-amylase inhibitory activity, suggesting potential use as a bioactive agent in functional food and pharmaceutical formulations [3,4].

Keywords: *Illicium verum*, polysaccharide, GC-MS, structural characterization, antioxidant activity, biological evaluation.

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Design, synthesis and *in silico* approach of anti-*Trypanosoma cruzi* activity of Harmine linked to 2-nitroimidazole derivatives

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Parasitic diseases have been a persistent threat to human health throughout history and various organisms cause a wide range of illnesses. Among these, Chagas disease, caused by the protoroan parasite *Trypanosoma cruzi*, stands out as a significant concern. Therefore, research on new therapeutic options is urgently required. Thus, a series of harmines linked to 2-nitroimidazole was synthesized *via* a mechanochemical reaction. Furthermore, molecular docking was conducted on two key molecular targets of *T. cruzi*, cruzipain (CRZ) and C14α-sterol demethylase (CYP51), to elucidate the potential molecular mechanisms of action of the synthesized derivatives. Several pharmacokinetic and toxicity parameters of these compounds were predicted *in silico*. Docking studies showed that the synthesized analogs can interact with the active sites of cruzain and CYP51 *via* hydrogen bonds and other covalent interaction. Moreover, pharmacokinetic prediction revealed that all best-scored compounds had drug-like characteristics for potential use as *Trypanosoma cruzi* inhibitors in Chagas disease. These results suggest that harmine linked to 2-nitroimidazole derivatives can be considered a potent, selective, and multi-target antitrypanosomal agents.

Key words: *Trypanosoma cruzi*, harmine, mechanochemistry, 2-nitroimidazole, *in silico*

Synthèse, étude *In Silico* et évaluation biologique des 4-Aminopyrimidine-5-carbonitriles

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De nos jours, le cancer est la maladie la plus grave qui menace la vie humaine. Plusieurs types de cancer tel que celui du colon et du poumon causent un nombre important de décès chaque année [1]. Par conséquent, le développement de nouveaux médicaments anticancéreux est un objectif et un défi majeur de la chimie médicinale moderne. D'un autre côté, les dérivés pyrimidiniques constituent une classe privilégiée de composés hétérocycliques présentant diverses applications biologiques et pharmaceutiques [2]. Dans ce contexte, nous avons développé une méthode simple et fiable de synthèse des 4-aminopyrimidine-5-carbonitriles par condensation des chlorhydrates d'amidine avec les éthers d'énols. L'évaluation des composés synthétisés pour leur activité antitumorale contre les lignées de cellules cancéreuses du côlon humain et les lignées de cellules cancéreuses du poumon humain a donné des résultats acceptables.

Mots clés : chlorhydrate d'amidine, pyrimidine, cancer

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The impact of inadequate plastic waste management and untreated wastewater discharge on the marine environment

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Plastics are water-insoluble polymers widely used across various industrial sectors due to their unique properties, such as flexibility, rigidity, heat resistance, and chemical stability [1]. However, these plastics–whether in the form of primary objects or smaller fragments called microplastics “MPs”, ranging from 1 µm to 5 mm–eventually reach the oceans, primarily via rivers, wastewater discharges, and terrestrial runoff. The distribution of these MPs is strongly influenced by local anthropogenic activities such as fishing and the discharge of domestic and industrial wastewater [2]. Inefficient waste management and the release of untreated wastewater into marine environments significantly contribute to plastic pollution [3] leading to the degradation of marine habitats, which are vital resources of food, energy, water, and biodiversity.

This research aims to assess the current state of plastic pollution in Tunisia, with a particular focus on the Gulf of Tunis. Microplastics concentrations in this area ranged from 0.626 to 22.32135 particles/m^3 across 3 out of the 9 sampling stations, with the highest concentrations recorded at stations located closest to the shore. High-density polyethylene (HDPE) particles were frequently detected. This pattern of particle distribution highlights the need to address the causes of pollution at the source in order to reduce discharges into the oceans, particularly from wastewater treatment plants, aquaculture farms, and the textile industry.

Key words: Plastic pollution, Marine ecosystems, Ecological degradation, Gulf of Tunis.

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New Hybrid Polyoxometalate-Based Material for Antitumor Drug Applications

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A novel hybrid material based on a Strandberg-type selenomolybdate cluster and 1,3-propanediaminium organic moieties, formulated as $(C_3H_{12}N_2)_2[Se_2Mo_5O_{21}]\cdot 4H_2O$, was successfully synthesized via a conventional solution-phase method. Single-crystal X-ray diffraction analysis confirmed that the compound crystallizes in the Orthorhombic system, with the $P2_12_12_1$ space group and with four crystallographically independent units per unit cell (Z = 4).

Comprehensive physicochemical characterizations, including scanning electron microscopy (SEM), X-ray diffraction analysis on powder (XRDP), Fourier-transform infrared (FT-IR) spectroscopy, ultraviolet-visible (UV-Vis) spectroscopy and thermogravimetric analysis (TGA), were conducted to elucidate the material's morphological, structural and thermal properties.

An intriguing cytotoxicity assay was performed on the material against Caco-2 colon cancer cells. The findings reveal that the compound effectively inhibits both the proliferation and migration of these cells within a specific concentration range, indicating its potential can be used as a therapeutic agent against colon tumours.

Keywords: hybrid material, Strandberg-type, solution-phase method, colon tumours.

Sustainable Valorization of Shrimp Shell Waste into Chitosan Nanofibers for Efficient Amoxicillin Removal

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The growing concern over environmental pollution–particularly the contamination of aquatic systems by pharmaceutical residues–has prompted the search for efficient, sustainable, and low-cost adsorbent [1]. Among such pollutants, antibiotics like amoxicillin (AMOX) are of particular concern due to their widespread use and potential to foster antibiotic resistance [2]. Conventional wastewater treatment methods often prove inefficient or costly, underscoring the need for greener alternatives. In this study, chitosan nanofibers were sustainably extracted from shrimp shell waste via a green protocol using a natural deep eutectic solvent (NaDES) assisted by ultrasound [3].

The resulting bio-adsorbent were thoroughly characterized: degree of deacetylation (81%), particle size distribution was assessed via laser diffraction and structural/morphological features were evaluated using Fourier Transform Infrared Spectroscopy and X-ray Diffraction, morphology and elemental composition using Transmission Electron Microscopy (TEM) coupled with Energy-Dispersive X-ray Spectroscopy (–EDX analyses., and surface charge behavior through the point of zero charge (pHpzc) analysis. The results, shows the extracted chitosan exhibited a high degree of deacetylation (81%) and a semi-crystalline structure. TEM images revealed nanofiber morphologies with diameters ranging from 9 to 70 nm. The point of zero charge (pH_pzc) was also determined to assess surface charge behavior.

The adsorption performance of the chitosan nanofibers was evaluated using AMOX as a model contaminant. The material exhibited a maximum AMOX removal efficiency of 91% at pH 7.5 confirming its high potential as a low-cost and eco-friendly solution for antibiotic removal from wastewater.

These results highlight the potential of sustainably extracted chitosan as an effective and low-cost adsorbent for antibiotic removal from water, contributing to environmentally friendly wastewater treatment solutions.

These findings demonstrate the effectiveness of valorizing marine biowaste into high-performance adsorbents, contributing to sustainable water treatment strategies.

Keywords: Chitosan, NaDES, Green extraction, Amoxicillin, Adsorption, Shrimp shell waste.

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Synthesis of Potent Anticancer Agents From Parthenolides Extracted from *Anvillea Radiata*

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Anvillea radiata (commonly known as "nougd" or "chadjeret ed dhob") is a bushy sub-shrub from the Asteraceae family, native to the northern and central regions of the Algerian Sahara. This plant exhibits diverse biological activities, including antioxidant, anticholinesterase, anti-tyrosinase, anti-α-glucosidase, cytotoxic, antifungal, and antibacterial properties [1].

As part of our efforts to valorize natural bioactive compounds, we focused on extracting the two germacranolide epimers - 9*α*-hydroxyparthenolide and 9*β*-hydroxyparthenolide - the major constituents of *A. radiata*'s dichloromethane extract. These compounds are known for their significant biological activity, attributed to the presence of an *α*-methylene-*γ*-lactone moiety [2]. To enhance the pharmacokinetic profile and therapeutic potential of the natural product, we chemically modified 9*β*-hydroxyparthenolide through acetylation and aza-Michael addition. Density functional theory (DFT) calculations were employed to assess reactivity changes at each step of the semi-synthesis, providing deeper insights *into* the synthetic strategy. Additionally, *in silico* studies were conducted to evaluate key pharmacokinetic parameters, including ADME (Absorption, Distribution, Metabolism, Excretion) properties, Rule of Five (Ro5) compliance, and Fsp^3 values. Our modifications successfully improved the pharmacokinetic profile of the semi-synthetic derivatives compared to the natural compound.

Furthermore, molecular docking studies were performed to predict the ability of acetylparthenolide to inhibit the p53-MDM2 protein-protein interaction and block NF-κB nuclear translocation, suggesting potential anticancer activity for this molecule.

Keywords: *Anvillea radiata*, 9*α*, 9*β*-hydroxyparthenolide, Semisynthesis, DFT, *In silico*.

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Synthesis of Novel [6] Helicene Derivatives for OLED Applications: Experimental Photophysical and Chiroptical Properties

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Helicenes are polycyclic aromatic hydrocarbons composed of ortho-fused aromatic or heteroaromatic nuclei, presenting non-planar π-electron systems [1], which arise from steric hindrance between the terminal aromatic rings. These organic molecules exhibit exceptionally intense chiroptical properties, such as strong optical rotation and pronounced electronic circular dichroism (ECD). Their inherent chirality, high optical stability, and rigid helical structures have consistently attracted considerable interest across various interdisciplinary fields, including liquid crystals [2], sensors [3], chiral catalysts [4], ligands for asymmetric synthesis, and the synthesis of polymers and molecular motors, as well as biological applications.

A series of helically chiral hexacyclic helicenes bearing suitable functional groups have been synthesized in good overall yields through four-step sequences carried out under mild experimental conditions. The optical resolution of the racemic mixtures afforded the enantiomers P and M in high optical purity. Their chiroptical properties were thoroughly characterized. Furthermore, additional optical properties, including UV-vis absorption and photoluminescence, were investigated, revealing emissions in the visible region.

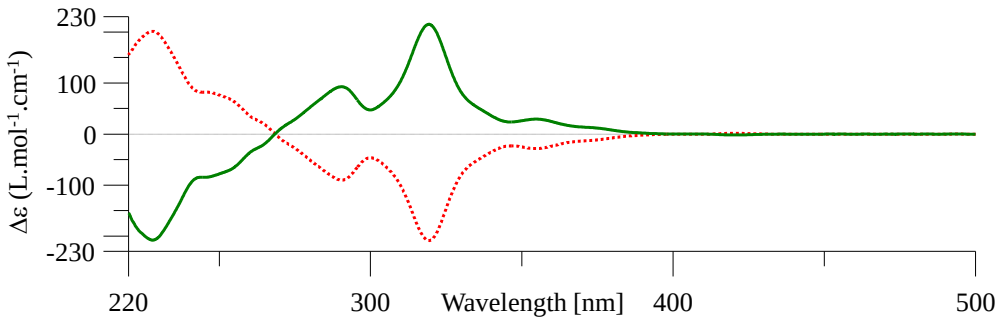

Figure: Electronic circular dichroism (ECD) spectra of (+)-**1** and (-)-**1** in CH_2Cl_2.

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Design, molecular docking and DFT study of chiral 1,2,3-triazolo-benzodiazepine as an allelopathy agent

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In the search for novel eco-friendly allelopathic agents, a series of chiral 1,2,3-triazolo-benzodiazepine derivatives were designed and investigated using an integrated computational approach. The molecular design was guided by the structural features of known benzodiazepine frameworks with potential for biological activity enhancement through triazole incorporation and chiral modulation. Density Functional Theory (DFT) calculations were employed to optimize the geometries, analyze electronic properties, and assess the reactivity of the designed molecules. Frontier molecular orbital (FMO) analysis and molecular electrostatic potential (MEP) maps provided insights into the active sites and electronic behavior [1]. Molecular docking studies were conducted against selected plant growth-related protein targets to evaluate the binding affinity and interaction profiles, revealing key binding interactions influenced by chirality and triazole substitution. The results suggest that these chiral 1,2,3-triazolo-benzodiazepine derivatives exhibit promising characteristics as allelopathic agents, with favorable binding energies and electronic properties conducive to biological activity. This study lays the groundwork for further in vitro and in vivo evaluation of these compounds as sustainable alternatives to synthetic herbicides [2].

Key words: Chiral 1,2,3-triazolo-benzodiazepine derivatives, Molecular docking, DFT, Allelopathic activity.

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Antimicrobial dynamics and DNA nicking within 1,3-propanediaminium dibromide and dichloride supramolecular frameworks: The critical role of strong hydrogen bonding and subtle molecular interactions

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Amine salt compounds are attracting increased attention due to their potential bioactive properties. This study explores the synthesis and detailed characterization of two novel amine salts, 1,3-propanediaminium dibromide (13DPBr) and 1,3-propanediaminium dichloride (13DPCl), through single-crystal X-ray diffraction, Hirshfeld surface analysis, and optical absorption spectroscopy. Structurally, 13DPBr crystallizes in the orthorhombic space group Pbcn, while 13DPCl crystallizes in the monoclinic space group P2/n. Supramolecular assemblies in both compounds are driven by strong N–H···X (X = Cl, Br) hydrogen bonds, alongside weaker C–H···X interactions. The optical absorption spectra indicated band gaps of 4.32 eV for 13DPBr and 4.56 eV for 13DPCl. The biological activities of these compounds were assessed through DNA nicking assays and antimicrobial tests. The antimicrobial properties were evaluated using agar diffusion assays against pathogenic bacterial strains, including *Salmonella enterica*, *Staphylococcus aureus*, *Escherichia coli*, and *Pseudomonas aeruginosa*. The Minimum Inhibitory Concentration (MIC) results demonstrated that both salts exhibited strong antibacterial activity, with 13DPBr showing higher efficacy against *Pseudomonas aeruginosa*. DNA nicking assays using pUC19 plasmid DNA revealed that both compounds offered significant protection against hydroxyl radical-induced DNA damage, preventing the degradation of plasmid DNA. These results highlight the potential of 13DPBr and 13DPCl as promising agents for antimicrobial and DNA protection applications.

Valorization of *Vicia faba* wastes: Pectin Extraction and its Application as an Eco-Friendly Corrosion Inhibitor for Mild Steel

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Polysaccharides derived from renewable resources are gaining increasing interest as sustainable and eco-friendly corrosion inhibitors [1]. This study focuses on the extraction of a polysaccharide from broad bean pods (Vicia faba), an agricultural by-product, and evaluates its potential in protecting mild steel from corrosion. The extracted polysaccharide (PBB) was characterized using Fourier-transform infrared spectroscopy (FTIR), gas chromatography-mass spectrometry (GC-MS), and size exclusion chromatography (SEC), revealing it to be a high molecular weight pectin. The anticorrosion efficiency of PBB was tested in a 0.1 M hydrochloric acid solution, where it achieved a maximum inhibition efficiency of 87.07% at a concentration of 0.7 g/L. Electrochemical techniques, including potentiodynamic polarization and electrochemical impedance spectroscopy (EIS), demonstrated that PBB effectively inhibited both anodic and cathodic corrosion processes. The adsorption of PBB on the steel surface followed the Langmuir adsorption isotherm, and FTIR and scanning electron microscopy (SEM) confirmed the formation of a protective film on the metal surface. This study emphasizes the potential of polysaccharides as effective, non-toxic, and environmentally friendly alternatives to traditional synthetic corrosion inhibitors.

Keywords: Broad bean polysaccharide, Structural characterization, Corrosion, Mild steel

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Optimization of ultrasound assisted extraction of polysaccharides from *Thymelaea hirsute L.* leaves

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Polysaccharides from Thymelaea hirsuta L. leaves were efficiently extracted using ultrasound-assisted extraction (UAE), a rapid and environmentally friendly technique. The extraction process was optimized using response surface methodology (RSM), specifically the Box-Behnken Design (BBD), to determine the optimal conditions for maximum yield. Under the optimized conditions—90 W ultrasonic power, 30 minutes of extraction time, and a water-to-powder ratio of 25.76 mL/g—a maximum yield of 21.60% was achieved. This yield is significantly higher than the 13.94% reported in a previous study employing conventional aqueous extraction, which required 3 hours.

Structural characterization by FT-IR spectroscopy confirmed the presence of characteristic polysaccharide functional groups, including hydroxyl and carboxyl groups.

These results demonstrate that UAE, when combined with statistical optimization through RSM-BBD, is a highly effective, time-efficient, and sustainable method for extracting bioactive polysaccharides from Thymelaea hirsuta L. leaves. This method holds great promise for applications in the pharmaceutical, cosmetic, and food industries.

Keywords: Polysaccharides; *Thymelaea hirsute*; UAE; ecofriendly extraction.

Lanthanides-strontium oxyapatites electrolyte for solid oxide fuel cells: Structure and ionic conductivity

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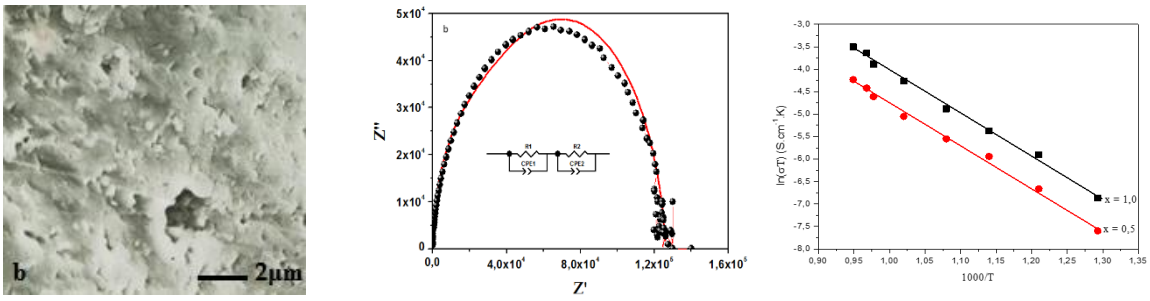
Graphical abstract

Densification $Sr_6Mg_1La_{2,5}(Nd,Gd)_{0,25}(PO_4)_2(SiO_4)_4O_{0.5}$ Ionic conductivity



Fuel cells (FCs) are among the most promising clean energy technologies,–due to their high efficiency and low environmental impact significant environmental benefits and exceptional efficiency in both electricity and energy production. They are increasingly recognized as a practical and effective solution for energy generation. Recently, Solid Oxide Fuel Cells (SOFCs), in particular, are attracting renewed interest for their ability to generate high power using ceramic electrolytes that conduct oxide ions (O^{2-}) have gained renewed interest, primarily for their capability to produce high-power energy by utilizing a ceramic electrolyte that conducts O^{2-} ions. Oxyapatite, known for its potential oxide ion conductivity, demonstrates promising ionic conduction properties, making it a candidate for use as a solid oxide electrolyte in SOFCs.

This study focuses on magnesium-doped rare earth-strontium silicated oxyapatites with the general formula $\mathbf{Sr_{7-x}Mg_xLa_{2.5}(Nd,Gd)_{0.25}(PO_4)_2(SiO_4)_4O_{0.5}}$ (x = 0.0–2.0), synthesized via mechanochemical milling. Characterization by XRD, FTIR, and ICP confirmed the formation of a hexagonal apatite phase (space group $P6_3/m$), with lattice parameters influenced by ion substitutionRietveld refinement showed that Mg^{2+} preferentially occupies metal(2) sites at low concentrations. After pressureless sintering at 1350 °C for 6 hours, dense ceramics (up to 90% relative density) were obtained. Impedance spectroscopy revealed improved ionic conductivity with increasing Mg content, peaking at x = 1.0. The conduction mechanism is interstitial, supported by excess oxide ions. These materials show strong potential as solid electrolytes for SOFC and battery applications.

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Structural and Mechanical Properties of Hydroxyapatite - zinc-Doped Tricalcium Phosphate Composites Bioceramics for Bone Tissue Engineering

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Autologous bone grafting remains the reference for orthopedic bone vacuum filling surgeries. However, its clinical application is limited due to factors such as limited availability, donor site complications, disease transmission risks, immune rejection, and high cost [1,2], for this reason, scientists are looking for an ideal synthetic material to replace bone transplantation. Calcium phosphate replacement is recently attracted attention and is considered a potential bone substitute [3,4].

In this study, we investigated the structural and mechanical properties of the composites (%HA-% (TCP-xZn)). The primary products of the composites, which are hydroxyapatite (HA) and zinc-doped and undoped tricalcium phosphate (TCP-xZn) (x=0; 0.1;0.3), were synthesized using the coprecipitation method. While the composites were carried out in solid-state suspension. The powders were characterized morphologically and structurally by X-ray diffraction, Fourier-transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), and specific surface area (SSA) analysis.

The relative density of the sintered samples reaches the highest value with x = 0.1 and reaches approximately 99% after sintering at 1200 °C for 3 hours for 0 and 10% HA. The prepared bioceramic materials were mechanically characterized using Young's modulus and Vickers hardness measurements. The overall trend of these parameters evolved similarly to the relative density, and the maximum values obtained of 134 GPa and 7.12 GPa respectively for the composite (20%HA-80%(TCP-0.1Zn)).

Keywords Hydroxyapatite, Tricalcium phosphate, Zinc, Mechanical properties

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Mai 2025

Optimization of Hydro-distillation Extraction of Essential oil from Tunisian *Lavandula* using Response Surface Methodology

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Hydro-distillation (HD) is a most used method for the isolation of essential oil from aromatic plants. Nevertheless, this technique has some drawbacks including low yield of essential oil and long extraction time. The ratio plant/water, steam flow rate, and extraction time are three important operating parameters that can influence the extraction yield. In this study, the response surface method linked with Box-Behnken Design was performed to optimize the parameters for HD. Then, the optimized HD conditions were determined. The ANOVA results revealed that HD time and steam flow rate had the greatest impact on the essential oil yield followed by ratio plant/water. Under the HD optimized conditions, the predicted yield of essential oil was very close to the experimental yield. For this reason, the leaves of Tunisian *Lavandula* were used in the present study. The extraction yield by HD was significantly higher than that of HD technique without optimization. Moreover, the HD time (few minutes) was reduced after optimization. Therefore, this study reveals that HD could be a good extraction method for extracting higher yields of Tunisian *Lavandula* essential oils after optimization of its operating parameters.

Keywords: *Lavandula*, Essential oil, Hydro-distillation, Optimization.

Traitement combiné des huiles essentielles de Thymus vulgaris L. et de Rosmarinus officinalis L : Optimisation des activités biologiques par la méthodologie de conception des mélanges

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Cette étude porte sur l'extraction combinée de plantes médicinales du sud de la Tunisie : les huiles essentielles (HE) de *Thymus vulgaris L.* (*T. vulgaris*) et de *Rosmarinus officinalis L.* (*R. officinalis*) ont été utilisées dans un traitement combiné, suivant une méthodologie de conception expérimentale (mix design**)** afin d'étudier leur effet synergique. La composition chimique des HE a été déterminée par chromatographie en phase gazeuse **(**GC**)** et GC couplée à la spectrométrie de masse (GC/MS), et plusieurs activités biologiques ont été évaluées. Les résultats de cette première étape ont révélé que le thymol et le bornéol étaient les principaux composés de l'HE de *T. vulgaris* et le 1,8-cinéole et l'α-pinène dominaient dans celle de *R. officinalis.* Par ailleurs, les tests biologiques ont mis en évidence une activité anti-inflammatoire marquée, ainsi qu'un effet anti-Alzheimer significatif pour les deux plantes. Enfin, l'analyse des combinaisons a montré que le mélange présentait une activité biologique supérieure à celle de chaque HE prise isolément, confirmant ainsi un effet synergique.

Mots clés : Huiles Essentielles, Synergique, Traitement Combiné, Activités Biologiques.

Potential of *Opuntia* cake oils for cosmetic formulations: Supercritical fluid extraction, stability, and chemical profile

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Oils extracted from prickly pear seed cake using various methods, particularly supercritical CO_2 and Soxhlet extraction, exhibited promising characteristics in terms of stability, chemical composition, and potential applications. Physicochemical, spectroscopic, and chromatographic analyses revealed rich profiles of unsaturated fatty acids, such as linoleic acid (59%) and oleic acid (30%), along with antioxidants like vitamin E (0.35 mg/g), which are essential for cosmetic and other applications. The oils also contained significant amounts of bioactive compounds, including tocopherols and flavonoids, which contribute to their antioxidant properties.

Stability tests, including thermal cycling (5 cycles between 4°C and 40°C) and mechanical stress testing (centrifugation at 3000 rpm for 15 min), demonstrated that these oils retain their integrity and key properties under stress. The oil extracted by supercritical CO_2 showed superior oxidative stability, with a low oxidation rate of 2.1 meq O_2/kg after 10 hours in the Rancimat test, making it ideal for long-term formulations. Emulsion tests further demonstrated that the oils are highly stable and do not separate under extreme conditions, confirming their suitability for cosmetic use.

In conclusion, oils extracted from prickly pear seed cake, particularly via supercritical CO_2, present high potential for cosmetic applications, offering both stability and efficacy. They represent a promising natural alternative for the formulation of skincare products, such as tanning oils and moisturizing creams, with the added benefit of enhanced oxidative stability and antioxidant properties.

Key words: Prickly pear seed oil, Supercritical fluid extraction, Chemical composition, Cosmetic formulations

Development and optimization of natural sunscreen formulations using prickly seed oil: Physicochemical and stability assessments

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This work focuses on the development and optimization of sunscreen formulations using prickly seed oil. Various concentrations of the oil and sun filters were tested, and the optimal sunscreen, containing 1% *Opuntia* seed oil and mineral filters, demonstrated excellent sun protection and remarkable stability. Stability was evaluated through centrifugation (3000 rpm for 30 min), thermal cycling (5 cycles between 4°C and 40°C), and oxidation tests (Rancimat test at 100°C for 10 hours), confirming its durability under different storage conditions.

Moreover, Sun Protection Factor (SPF) was measured using spectrophotometric methods (UV-Vis absorption) and physical measurements (reflectance and transmission). The results showed an SPF of 30, comparable to commercial sunscreens, providing effective protection against both UVA (320-400 nm) and UVB (280-320 nm) rays, while maintaining stability over time. UV reflection and transmission measurements confirmed an effective blocking range, with UV reflection at 320 nm at 85% and UV transmission at 290 nm below 10%.

Additionally, stability tests, including emulsion stability (centrifugation at 3000 rpm for 15 min) and accelerated aging tests (40°C for 4 weeks), revealed that the cream remained homogeneous and stable without phase separation or significant degradation. The Rancimat test indicated a low oxidation rate of 2.5 meq O_2/kg after 10 h, reinforcing the formulation's long-term viability. Overall, this study demonstrates that *Opuntia* seed oil, with its unsaturated fatty acid content (mainly oleic acid 48% and linoleic acid 27%) and antioxidant properties, is an excellent natural alternative for sunscreens, offering effective protection and environmental sustainability. Future work will focus on *in vivo* studies to validate sunscreen efficacy for sensitive skin and explore its application in moisturizers and anti-aging creams.

Keywords: *Opuntia ficus-indica*, Seed oil, Natural sunscreen, Stability and efficacy.

Salvia Hispanica (Chia) Seed Extract Mediated Green Synthesis of ZnO Nanoparticles for Photocatalytic Degradation of Diclofenac and *p*-Nitrophenol

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Zinc oxide nanoparticles (ZnO NPs) were successfully synthesized using a simple and ecofriendly precipitation method route, employing a capping agent derived from chia seeds (*Salvia hispanica*). X-ray diffraction (XRD) analysis confirmed the formation of ZnO with a hexagonal wurtzite crystal structure and revealed an average crystallite size of less than below 30 nm. Scanning electron microscopy (SEM) showed distinct quasi-spherical and nanorod morphologies, while energy-dispersive X-ray spectroscopy (EDX) verified the elemental composition presence of zinc and oxygen. Diffuse reflectance spectroscopy (DRS) indicated substantial UV light absorption, with the ZnO NPs exhibiting a band gap of 3.25 eV significant activity in the UV region, with the nanoparticles exhibiting a band gap of 3.25 eV. The photocatalytic performance efficiency of the synthesized ZnO NPs was evaluated by their ability to degrade diclofenac sodium (DCF) and para-nitrophenol (4-nitrophenol, PNP) under UV-LED irradiation, achieving pollutant removal efficiencies exceeding 98% achieving pollutant removal rates exceeding 98%. The degradation mechanism pathway was further elucidated through detailed characterization of the reaction intermediates. These findings highlight the potential of ZnO NPs synthesized from chia seed extract for effective environmental remediation of pharmaceutical and organic pollutants.

Keywords: ZnO; Green Synthesis; *Salvia hispanica*; Chia Seeds; Photocatalytic Degradation; Pharmaceuticals; Diclofenac; *p*-Nitrophenol.

Smartphone-Based Fluorimetric Detection of Hg^{2+} Using a Carbazole-Modified Chitosan Bio-Nanocomposite Probe

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The U.S. Agency for Toxic Substances and Disease Registry (ATSDR) classifies mercury as one of the most toxic heavy metals.**[1]** Research has shown that even at very low concentrations (a few parts per million), mercury ions (Hg^{2+}), released into the soil by chemical industries, can cause severe damage to the brain, as well as to the immune, renal, and endocrine systems.**[2]** Therefore, strict monitoring of drinking water quality is essential to protect public health.

Although elemental analysis techniques such as atomic absorption spectroscopy (AAS), selective atomic fluorescence spectroscopy (SAFS), and specific methods (EPA 1631 and 7471) provide high sensitivity, reliability, and accuracy, they are expensive and lack portability, limiting their application in field conditions. In this study, we present a simple and innovative method for fabricating a fluorimetric sensor using carbazole-functionalized chitosan for the detection of mercury ions (Hg^{2+}) in aqueous solutions. The chitosan is extracted from the shells of the Tunisian shrimp *Parapenaeus longirostris*, with a high degree of deacetylation (95%).

Functionalizing chitosan with carbazole units is an effective strategy to improve its chemical properties and broaden its applications. Specifically, this modification enhances its ability to complex with heavy metals, particularly mercury.

To address field detection needs, we propose a portable, cost-effective, and environmentally friendly method based on a fluorescence assay, using a smartphone as the analytical tool. The developed probe is a bio-nanocomposite combining carbazole-modified chitosan (Cs-Car) with silver nanoparticles (Ag NPs). This system provides a rapid and sensitive response, with a limit of detection (LoD) in the range of hundreds of nanomoles/L.

Keywords: Chitosan, carbazole, Ag NPs, bio-nanocomposite probe, Hg^{2+} detection.

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Electropolymerization of a new semiconducting material emitting in the green spectrum

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A new thermally stable material was prepared by electrochemical oxidation of m-FA. The preparative study gives rise to two oligomers, one soluble in chloroform and another insoluble in most common solvents. IR and ^{1}H and ^{13}C NMR spectroscopic analyses showed that the structure is of polyphenylene type. The forbidden band gap width of the synthesized material, determined both electrochemically and optically, is practically the same (3.4 - 3.56 eV). In addition, the chloroform-soluble oligomer is photoluminescent and emits light in the green region of the spectrum. These characteristics suggest that this material could be a candidate promoter for OLED devices.

Keywords*:* Conjuguted polymers, Electropolymerisation, Semi-conductring, Photoluminescence

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Valorisation Chimique du PET : Une Route Vers des Nouveaux Copolyesteramides Ecologiques

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L'utilisation des polyesteramides issus de monomère naturel pouvant combiner les propriétés des polyesters (dégradabilité, facilité de mise en œuvre) avec celle des polyamides (bonne résistance mécanique, température de fusion élevée) apparait donc à priori intéressante.

Dans le cadre de la valorisation des déchets plastiques, ce travail porte sur l'élaboration de nouveaux polyesteramides semi-aromatiques à partir du poly(téréphtalate d'éthylène) (PET)-déchet. Par une approche innovante de polycondensation à l'état fondu, le bis(hydroxyéthyl)téréphtalate (BHET), obtenu par glycolyse du PET, a été combiné à la ß-alanine, un acide aminé naturel.

Une série de polyesteramides (PEAs) a été synthétisée par polycondensation en masse de BHET et de la β-alanine, en modifiant les ratios massiques des deux comonomères BHET/ß-alanine variant de 90/10 à 10/90.

Ces matériaux ont été caractérisés par des techniques spectroscopiques telles que la FTIR et le RMN ^{1}H, permettant de confirmer leur structure chimique. Les propriétés thermiques ont été étudiées par calorimétrie différentielle à balayage (DSC) et analyse thermogravimétrique (ATG), et les masses molaires ont été déterminées par chromatographie d'exclusion stérique (SEC).

Les résultats obtenus révèlent des propriétés thermiques et structurales prometteuses, positionnant ces nouveaux matériaux comme des candidats intéressants pour des applications dans les textiles techniques et l'ingénierie tissulaire.

Mots clés: Polyesteramides, β-Alanine, BHET, Glycolyse, PET-déchet, Valorisation.

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Microwave-Assisted Extraction of Bioactive Polyphenols from Cucumis metuliferus: Optimization and Antioxidant Evaluation

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This study focused on optimizing the microwave-assisted extraction of polyphenols and their antioxidant activity from *Cucumis metuliferus* peel and pulp. A central composite design (CCD), integrated with response surface methodology (RSM), was employed to optimize three key variables: extraction duration (6.29–20 minutes), temperature (33.18–66.81°C), and liquid-to-solid ratio (13.18–46.81 ml/g). For the peel, optimal extraction was achieved at 11.27 minutes, 40°C, and a 30 ml/g ratio, leading to maximum yields of total phenolics (198.52 mg GAE/g DW), flavonoids (116.26 mg QE/g DW), and antioxidant capacities measured by DPPH (41.72 µg/ml) and FRAP (201.84 µM BHT/g DW). Similarly, the pulp exhibited the highest bioactive compound content under conditions of 15.76 minutes, 50.50°C, and a 30.54 ml/g ratio, with corresponding TP, TF, DPPH, and FRAP values of 236.71 mg GAE/g DW, 161.11 mg QE/g DW, 39.86 µg/ml, and 234.83 µM BHT/g DW, respectively. These optimized parameters highlight a green and effective method for extracting antioxidant-rich polyphenols, with promising implications for applications in food, pharmaceutical, and cosmetic industries.

Key words: antioxidant activity, total phenol, total flavonoid, DPPH, FRAP, RSM, *Cucumis metuliferus.*

Simultaneous Biosorption of Cationic Dyes onto Activated Orange Peels Using Doehlert Design

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Two cationic dyes were removed using a low-cost adsorbent prepared from activated orange peels (AOP). The AOP was characterized and evaluated as an effective adsorbent for the removal of methyl violet (MV) and methylene blue (MB) from both single and binary systems. The effect of adsorbent dose, initial dye concentration, pH and temperature were investigated. Initially, a preliminary study was conducted to define the experimental domain. Then a full factor design was employed to determine the influence of the main parameters and their interactions on the adsorption process. Based on the results obtained, response surface methodology (RSM) using the Doelhert design was applied to identify the optimum operating conditions and to predict response values at any point within the experimental domain.

Keywords: Adsorption, Cationic Dyes, Activated orange peels, Competitive removal, Optimization, Doehlert design

Optimization of Green Resveratrol Extraction Using Ultrasound-Assisted DES Solvent: Box–Behnken Design and Antioxidant Activity Evaluation

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Resveratrol is a natural polyphenol with antioxidant activity and numerous health benefits [1]. Deep eutectic solvents (DESs), a new class of eco-friendly solvents, have been combined with the ultrasonic-assisted extraction (UAE) technique [1]. This study aimed to develop an ultrasonic-assisted extraction (UAE) method using DESs for the extraction of resveratrol from red grapes. The optimization was performed through Response Surface Methodology (RSM) operated with a Box-Behnken design (BBD). The ultrasound-assisted extraction was accomplished by varying three key parameters: ultrasonication temperature (30 - 70°C), extraction time (10 - 60 min), and biomass-solvent ratio (10 - 40 mL). The extracted resveratrol recovery was measured using High-Performance Liquid Chromatography with UV detection (HPLC-UV), while antioxidant activity was assessed through DPPH free radical scavenging and FRAP assays. The Box-Behnken design predicted the maximum yield of resveratrol utilizing the following optimal conditions: 60 min extraction time, 70°C temperature, and 21.21 mL solvent volume. The maximal resveratrol yield was evaluated to 0.16 mg/g of biomass and the measured parameters matched the predicted results. The retention time for resveratrol was approximately 5 minutes, demonstrating the high precision of the developed HPLC method. Moreover, a comparative study confirmed that the optimized DES-based UAE resulted in higher resveratrol extraction yields and antioxidant activity compared to other extraction methods. Hence, DESs are considered promising green solvents with selective and efficient properties for extracting bioactive compounds from medicinal plants.

Keywords: Antioxidant activity, green extraction, Box Benkhen Design, Resveratrol

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A Novel Fe_2O_3@DCTA-Ag Nanocomposite Sensor for Lead Detection: Box-Behnken Design Optimization and Real-World Applications

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A novel Fe_2O_3@DCTA-Ag composite was synthesized for the first time and used to develop a highly reliable electrochemical sensor for Pb^{2+} detection. Differential pulse voltammetry, optimized via a Box-Behnken design (BBD) and response surface methodology (RSM), evaluated key parameters (pH, contact time, drop volume, drying time). The sensor exhibited linear detection from 0.2 nM to 10 µM, with a low detection limit of 0.2 nM and excellent selectivity against interfering ions. Tested in food (rice, corn, milk, honey, tea) and environmental samples (pond water), it demonstrated high sensitivity, stability, and reproducibility, confirming its potential for food safety applications.

Keywords: Fe_2O_3 nanoparticles, Box-Behnken design (BBD), response surface methodology (RSM), Portable electrochemical sensor, Lead ions, Differential pulse voltammetry.

Use of Tetraphenyl(hydroxyl)imidazole for Colorimetric Detection of Iodide: Optical Properties, Computational Characterizations, NBO, QTAIM, and NCI-RDG Analyses

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The Optical, structural, electronic, and energetic properties of tetraphenyl (hydroxyl) imidazole were carried out using the B3LYP-D3/6-311G (d, p) level theory. Complexation of imidazole compound with Br^-, Cl^-, CN^-, SCN^-, NO_3^-, CH_3COO^-, SO_4^- and I^- anions have been analyzed using experimental UV spectroscopy (The UV-Vis spectroscopy was employed to examine the interaction of the imidazole compound with various anions including Br^-, Cl^-, CN^-, SCN^-, NO_3^-, CH_3COO^-, SO_4^- and I^- . Data indicated that the addition of various anion ions in imidazole solutions exhibited negligible change in the absorption spectrum. However, the intensity of the absorbance was well improved in the presence of I^- (While most anions induced negligible changes in the absorption spectra, the presence of iodide led to a significant enhancement of absorbance and a visible reddish-orange color.). A reddish orange color was observed with the appearance of new peak at 368 nm (experimental spectra) and 337 nm (theoretical spectra) (this was accompanied by the appearance of new absorption bond at 368nm (experimental) and 337nm (theoretical), demonstrating high selectivity towards I-). This proved that the studied imidazole has a high selectivity towards iodide over other competitive anions.
Imidazole compound detected I^- in the range 0-30 µM, showing good linear relationships between concentration and absorption change (R^2 = 0.93), with a detection limit of 0.73 µM (The sensor showed a linear response in the iodide concentration range of 0–30 µM (R^2 = 0.93), with a low detection limit of 0.73 µM.).
The interaction (between the imidazole and iodide) of iodide with the colorimetric chemo sensor was discussed (was further analyzed) using Natural Bond Orbital (NBO) [1], and Quantum Theory of Atoms in Molecules (QTAIM) analyses based on Reduced Density Gradient (RDG), employing the 6-311G(d,p)/LANL2DZ(I) level [2]. Taking into consideration the Reduced Density Gradient (RDG) theory using 6-311G (d, p)/lanl2dz(I) method [3]. Adsorption energy (E_{ad}), vibrational spectra and Frontier molecular orbitals (FMOs) were used to detect the presence of I^-. The adsorption energy, vibrational spectra, and frontier molecular orbitals (FMOs) were also evaluated to characterize the sensing mechanism.
Overall, the present finding exhibited that Imidazole displayed suitable properties to design good I^- sensors.

Keywords: Tetraphenyl(hydroxyl)imidazole, Iodide detection, Chemo Colorimetric sensor, Natural Bond Orbital NBO, QTAIM Quantum Theory of Atoms in Molecules, RDG analysis. Reduced Density Gradient.

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Crystal Structure and Spectroscopic Investigations (FT-IR, UV/Vis) of a Novel (η^1-hydrogencarbonato) five-coordinate High-spin Iron(II) Picket Fence Porphyrin Complex

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In this work we have prepared the novel (η^1-hydrogencarbonato) iron(II) picket fence porphyrin with the formula [K(2,2,2-crypt)][Fe^{II}(TpivPP)(η^1-HCO_3)] (**I**) (where TpivPP is (α,α,α,α-terakis(*o*-pivalamidophenyl)(porphinato) anion and (2,2,2-crypt) is cryptand-2,2,2). The complex **I** was characterized by UV/Vis and IR spectroscopy and single crystal X-ray diffraction molecular structure. These techniques show that the HCO_3^- axial ligand is coordinated to the Fe^{2+} metal ion in a monodentate mode. This compound crystallizes in the *$P2_1/n$* space group with one ion complex [Fe^{II}(TpivPP)(HCO_3)]$^-$ and one counterion [K(2,2,2-crypt)]$^+$. Compound (**I**) exhibits a non-planar conformation with major *doomed* and *saddle* distortions. The average equatorial iron-pyrrole nitrogens [Fe—N_p= 2.107 (2) Å] bond length and the distance between the iron and the 24-atom core of the porphyrin ring [Fe—P_C = 0.5744 (6) Å] are longer than those of all other similar five-coordinate iron(II) high-spin (S = 2) porphyrinates. This is probably due to the electronic repulsion of the d_{x2-y2} and d_{xy} orbitals by the negative charge of the pyrrole nitrogens. This structure, which is the first one reported on an hydrogencarbonato-iron(II) porphyrin species, confirms the high-spin-state of the hydrogencarbonato derivative and shows that the coordination sphere of the iron atom is strongly affected by the monodentate axial ligand from the pocket side of the TpivPP porphyrin.

Keywords: porphyrin, axial ligand, iron, X-ray.

New cobalt (II) bidentate complexes with N_2O_2 Schiff base ligands: Synthesis, characterization, optimized yield, and antibacterial evaluation

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This study reports the synthesis and characterization of novel bidentate cobalt (II) complexes derived from two N_2O_2-donor Schiff base ligands: 1,2-di(furan-2-ylmethylene)hydrazine and 1,2-di(1-(furan-2-yl)ethylidene)hydrazine. The synthesized compounds were characterized using NMR, FT-IR, and UV-visible spectroscopy. To enhance the efficiency of the synthetic procedure, a Taguchi method-based optimization, leveraging artificial intelligence principles, was implemented. This optimization significantly improved the reaction yields by systematically controlling key parameters. Furthermore, the antibacterial activity of the synthesized complexes was evaluated against Escherichia coli, Staphylococcus aureus, Salmonella typhimurium, and Pseudomonas aeruginosa, revealing potential for further investigation in the field of antimicrobial agents.

Synthesis and Physicochemical Characterization of a Novel Gold(III) Porphyrin Complexes

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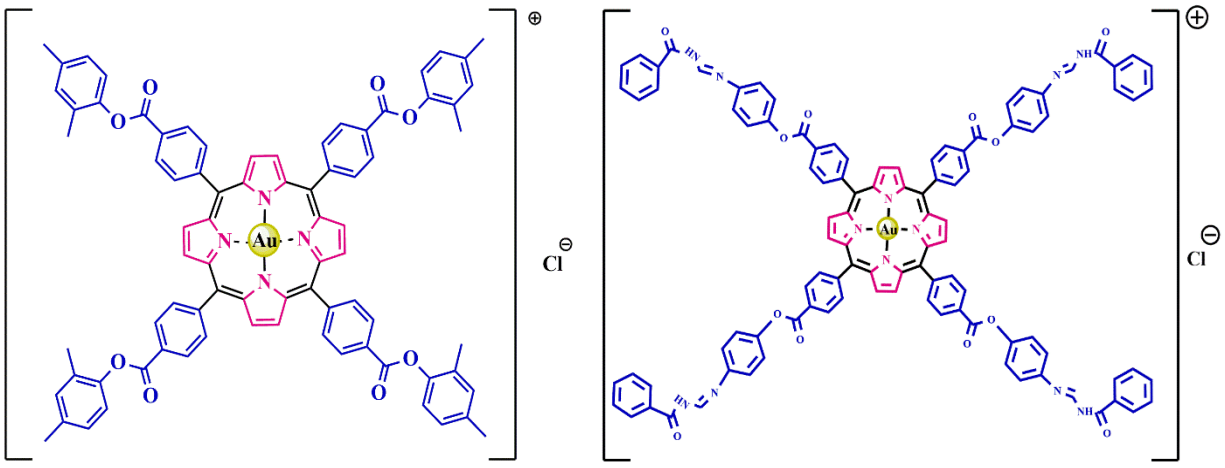
As cancer research continues to grow, many compounds are being explored for their potential to treat different types of cancer **[1] [2]**. Among these, gold-based metalloporphyrin compounds are gaining interest because they often show strong anticancer activity and are less toxic than platinum-based drugs. In this work, we describe the preparation and basic characterization of a new gold metalloporphyrin complexes. The study includes analysis using UV-visible, (IR), and proton nuclear magnetic resonance (^{1}H NMR) spectroscopy. The complexes studied are {*meso*-tetra(*p*-[4((benzamidomethylene)amino)phenyl benzoate])porphyrin} gold(III) [Au^{III}(TBAPP)]Cl and the {*meso*-tetra(*p*-(2,4-dimethylphenylbenzoate))porphyrin} gold(III) [Au^{III}(TDPP)]Cl coordination complexes.

Keywords: Gold(III) porphyrin complexes; UV-visible; NMR; IR.



Structures of the [Au^{III}(TDPP)]Cl and [Au^{III}(TBAPP)]Cl complexes.

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Programme du Dimanche 11 Mai 2025

Advancing Microsupercapacitor Technology: Laser-Fabricated MOF Electrodes for Enhanced Performance

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Laser-induced graphene (LIG) functionalized with copper-based metal-organic frameworks (Cu-MOFs) presents a promising approach for developing advanced flexible electronics [1]. In this work, we introduce a facile one-step synthesis strategy combining laser photothermal processing with drop-casting deposition to achieve uniform Cu-MOF integration on LIG substrates [2]. Structural and chemical characterization confirms the successful formation of well-dispersed Cu-MOF crystals on the conductive LIG framework.

Electrochemical evaluation reveals that the Cu-MOF-LIG hybrid electrodes exhibit superior performance in supercapacitor applications compared to pristine LIG. Notably, the modified electrodes demonstrate a substantial enhancement in specific capacitance, energy density, and long-term cycling stability. These findings highlight the potential of Cu-MOF-LIG composites as high-performance, flexible electrode materials for next-generation energy storage devices.

Keywords: Laser-induce graphene LIG , energy storage , copper-MOF .

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Synthesis and Spectroscopic Characterization of a New Cobalt(II) Meso-aryl Porphyrin Complex

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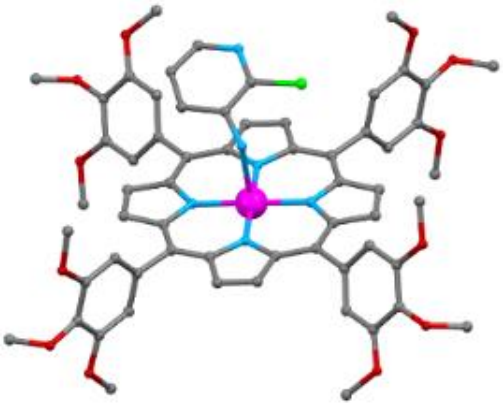
The biological relevance of cobalt metalloporphyrin complexes stems from their structural similarities to cobalamins **[1]**, which feature a porphyrin-like architecture. They are recognized as excellent compounds to explore in the development of new catalysts **[2]**, sensor **[3]**. In this study, we concentrate on the synthesis, crystal structure, and spectroscopic characterization (UV-visible, IR, NMR). of the 3-amino-2-chloropyridine{*meso*-tetrakis(3,4,5-trimethoxyphenyl)porphyrin}cobalt(II) complex with their formula [Co^{II}(TTMPP)(3-A-2Clpy)]•$2H_2O$. This new metalloporphyrin crystallizes in the triclinic crystal system (*P-1* space group) with the cell parameters: a = 7.8240(8) Å, b = 12.7807(12) Å, c = 14.3179(6) Å, α = 85.664(6) °, β = 76.444(5) °, γ = 89.517(8)°. The final R values are: R_1 = 0.0554 and Rw_2 = 0.1303 and the Goodnee of fit is S = 1.204.

Keywords: Cobalt (II) porphyrin complex; X-ray molecular structure; UV-visible; NMR, IR.



Molecular Structure of the [Co^{II}(TTMPP)(3-A-2Clpy)] complex.

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Synthesis, characterization of new hybrid compounds Based on Hydroxyapatite for Biomedical Applications

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Hydroxyapatite (CaHAp) is a synthetic biomaterial and has been found to promote new bone formation when implanted in a bone defect site. However, its use is often limited due to its slow osteointegration rate and low antibacterial activity, particularly where HA has to be used for long term biomedical applications. This work describes the synthesis and characterization of modified hydroxyapatite by two biopolymers: Agar agar and Gellan Gum. The obtained materials were characterized using various techniques by studying the properties of the powder and comparing them with those of unmodified hydroxyapatite. The X-ray diffraction (XRD) studies revealed the phase and the effects of the modification on the CaHAp surface. The chemical composition of the samples was evaluated by energy dispersive X-ray analysis (EDX). Furthermore, the antimicrobial properties of the modified hydroxyapatite were evaluated against ***Escherichia coli*** ATCC 35218 and ***Pseudomonas aeruginosa*** (ATCC 27853). The results of the biological assays suggested that the samples show great potential for being used in the development of novel materials for biomedical applications.

Keywords: Hydroxyapatite, Gellan Gum, antibacterial activity.

Synthesis and Characterization of Modified Hydroxyapatite with Biopolymers for Biomedical Application

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Hydroxyapatite is a substance of great importance in many applications, particularly in the medical field. In the context of this study, we focused on the synthesis of hydroxyapatite and the functionalization of this material by combining it with polymers. A sample was prepared by grafting two polymers each time onto the surface of the hydroxyapatite material (CaHAp-CS-CMC). The obtained product was characterized by X-ray diffraction, IR absorption spectroscopy, scanning electron microscopy (SEM), and thermal analysis (TGA-DTA). After surface modification (CaHAp), X-ray diffraction shows that the crystallinity was slightly affected by the presence of chitosan and carboxymethylcellulose. Infrared spectroscopy reveals the presence of new absorption bands attributed to the organic group. The results obtained confirm that the polymers have been well grafted onto the surface of the CaHAp. The thermograms (ATD-TGA) show the thermal stability of the materials; moreover, they show mass losses attributed to the decomposition of organic molecules. Observations using scanning electron microscopy for the material show that the morphology of the apatite material was altered due to surface functionalization by the different polymers. The result of these studies indicated that CaHAp-CS-CMC with optimal properties can be used in various biomedical applications.

Keywords: hydroxypatite, chitosan, carboxymethyl cellulose, Biomedical Application

Xanthan bio-polymer modified hydroxyapatite-powders: Synthesis, characterization, and adsorption efficiency toward Methylene blue

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Dye removal from wastewater is of prominence due to its hostile effects on human health and the environment. Adsorption is found to be a promising technique to eliminate dye wastes due to its high removal capacity at low concentration. The precipitation technique was used to prepare calcium Hydroxyapatite-Xanthan (CaHAp-Xan) hybrid materials. Chemical analysis, X-ray powder diffraction, infrared spectroscopy, specific surface area, thermogravimetry, and scanning electron microscopy were used to analyze the materials and the organic-inorganic interfaces. XRD and SEM investigations demonstrated that the presence of biopolymer had an impact on both the structural and morphological properties as well as the crystallinity. The PO_4^{3-} vibration modes are visible in the IR spectra, and new vibration modes mostly associated with Xan are observed at 1594, 2878, and 3246 cm^{-1}. Additionally, following surface modification by biopolymers, the specific surface area was reduced. The ability of the two materials CaHAp and CaHAp-Xan to sorb methylene blue (MB) from aqueous solutions was assessed. The adsorption kinetics results best fitted the pseudo-second- order model. The isotherm data agreed well with the Freundlich model. The adsorption capacities values of porous composites CaHAp-Xan 5% and CaHAp achieved 277 mg/g and 144 mg/g, respectively. The non-spontaneous and exothermic nature of the adsorption was demonstrated by the thermodynamic parameters (ΔG°, ΔH°, and ΔS°). The obtained results indicated that CaHAp-Xan is a potential adsorbent that can effectively remove MB and other contaminants from aquatic media.

Keywords: Hydroxyapatite, Xanthan Gum, Methylene blue, Adsorption.

SYNTHESIS, SPECTROSCOPIC AND STRUCTURAL CHARACTERIZATION OF A NEW Cobalt (II) PORPHYRIN COMPLEX

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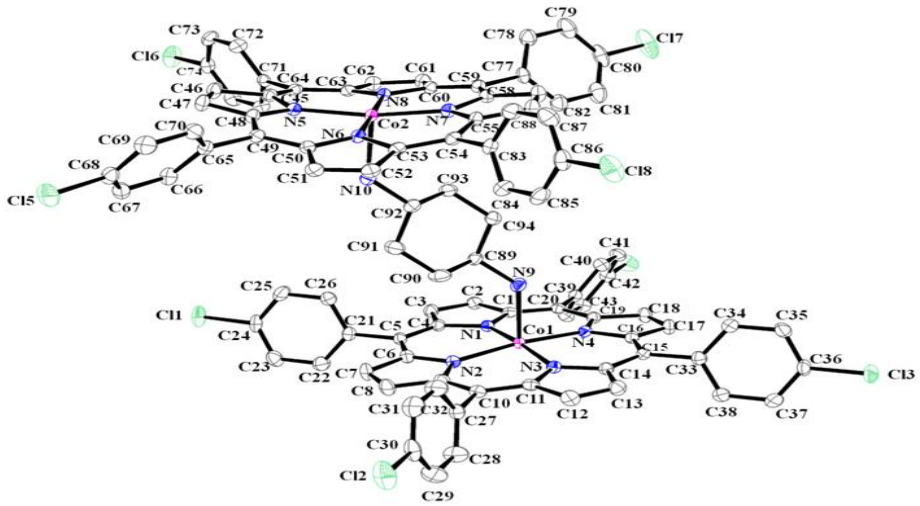
The aim of this work is the synthesis of a new cobalt(II) Metalloporphyrin with formula **[{Co^{II}(TClPP)}$_2$(μ2-dace)]•C_6H_{14}•$CHCl_3$ (I)** where TClPP is the *meso*-tetra(*para*-chlorophenyl)porphyrin . Compound **(I)** was prepared by the reaction of the [Co(TClPP)] staring material with an excess of dace in chloroforme. This complex was characterized by UV–visible, IR and proton NMR spectroscopy. We also characterized this species by single crystal X-ray Molecular structure. The data collection was made at low temperature (150 K) and complex **(I)** crystalizes in the triclinic crystal system with the *P-1* space group. The cell parameters are: ***a*** = 16.6467(17) Å, ***b*** = 16.7361(17) Å, ***c*** = 19.716(2) Å and ***α*** = 84.111(4)°, ***β*** = 66.856(4)° , ***γ*** = 60.209(3)°. **V** = 4353.7(8) Å^3, ***Z*** = 2. The reability factors are R_1 = 0.0418 and ***wR2*** = 0.0978. The cobalt (II) cation Co1 is coordinated by four N atoms of the four pyrrole groups of porphyrin (TClPP) and an N5 atom of the axial ligand trans-1,4-diaminocyclohexane (dace) and Co2 is coordinated by four pyrrole N atoms and an N10 atom of the axial.



Molecular structure of [{Co^{II}(TClPP)}$_2$(μ2-dace)]•C_6H_{14}•$CHCl_3$.

Keywords: Metalloporphyrin, complex, cobalt, X-ray.

Electrophilic Reactivity of Benzochalcogenadiazoles toward Cyclic Secondary Amines : A Mayr Scale Approach

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In this study, the electrophilicity parameter E of benzochalcogenadiazole was determined at 20 °C using Mayr's linear free-energy relationship. This was based on kinetic investigations of electrophilic addition reactions with a series of cyclic secondary amines in DMSO.

$$\log k\ (20\ °C) = S_N\ (E + N) \qquad (1)$$

Additionally, the kinetic study of the reactions between 2,1,3-benzothiadiazole and the same set of amines revealed that the second-order rate constant k follows equation (1). As a result, the electrophilicity parameter E of this compound was successfully determined and incorporated into Mayr's universal electrophilicity scale.

Furthermore, a significant correlation was observed between the $\log k_1$ values and the pK_a values of the amines (measured in DMSO), highlighting the relevance of this approach for a comprehensive characterization of electrophilic reactivity in solution.

Keywords: Kinetics, Mayr approach, Nucleophilic addition, Structure–reactivity correlation

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Synthesis and Characterization of Zeolitic Imidazolate Framework-8 Zif-8 combined with ruthenium nanoparticules

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A green and eco-friendly synthesis route was adopted to prepare zeolitic imidazolate framework-8 (ZIF-8), a highly porous and stable Metal-Organic Framework (MOF). To enhance its functional potential for advanced applications, particularly in sensing, ZIF-8 was doped with ruthenium (Ru) nanoparticles, resulting in the formation of a hybrid nanocomposite, Ru@ZIF-8. The synthesis was conducted under mild conditions, without the use of toxic solvents or harsh reagents, highlighting its sustainability. The structural integrity and morphology of both ZIF-8 and Ru@ZIF-8 were systematically characterized using X-ray diffraction (XRD), scanning electron microscopy (SEM), Brunauer–Emmett–Teller (BET) surface area analysis, and Fourier-transform infrared (FTIR) spectroscopy. Cyclic voltammetry (CV), differential pulse voltammetry (DPV), and electrochemical impedance spectroscopy (EIS) were utilized to evaluate the electrochemical activity.

Key Words : Green synthesis , Ruthenium nanoparticles ,Zeolitic imidazolate framework-8 (ZIF-8) , Nanocomposites , electrochemical activity.

Trace level Electrochemical Detection of HMF in Honey based on electrochemical deposition of Hkust-1

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In this work, we report the electrochemical synthesis of HKUST-1 [1] (Cu-BTC) metal-organic framework onto a conductive substrate for the development of an electrochemical sensor targeting the detection of 5-hydroxymethylfurfural (HMF) in honey[2]. The synthesis was carried out under controlled conditions to ensure uniform growth and stability of the MOF layer. The electrochemical behavior of the modified electrode was characterized using cyclic voltammetry (CV), while square wave voltammetry (SWV) was employed for the quantitative detection of HMF. The HKUST-1-modified sensor demonstrated excellent performance, including high sensitivity and a remarkably low limit of detection (LOD), making it a promising platform for food quality monitoring[3].

Keywords: Electrochemical sensors, Metal–organic framework, Electrochemical deposition, 5-Hydroxymethylfurfural, Honey quality analysis

Acknowledgment: *This work was supported by the PRIMINAS project ref (101079485) funded by the EU whose financial contribution is gratefully acknowledged.*

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Polyaniline coated $Na_3V_2(PO_4)_2F_3$ cathode enables fast sodium ion diffusion and structural stability in rechargeable batteries

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$Na_3V_2(PO_4)_2F_3$ (NVPF), a typical sodium super ion conductor (NASICON) type structure, has attracted much interest as a potential positive sodium ion battery [i]. However, the inherently poor electronic conductivity of phosphates compromises the electrochemical properties of this material [ii, iii]. Here, we develop a general strategy to improve the electrochemical performance by preparing a new composite material «polyaniline (PANI)@NVPF» using a Pickering emulsion method. The XRD and Raman results indicated a successful PANI coating without affecting the NASICON-type structure of NVPF, and enhanced the interfacial bonding between the two components. Also, the TGA and SEM analyses revealed that the PANI content influenced the thermal stability and morphology of the nanocomposites. As result, the sodium test cells exhibited multi-electron reactions and a better rate performance for PANI@NVPF nanocomposites as compared to NVPF. Specifically, 2%PANI@NVPF maintained 70% of its initial capacity at 5C. Ex situ EPR revealed the existence of mixed valence states of vanadium (V^{4+}/V^{3+}) in both discharge and charge processes. Consequently, the successful PANI coating into the sodium superionic conductor framework improved the sodium diffusion channels with a measurable increase of diffusion coefficients with cycling (ca. 3.25 10^{-11} $cm^2\ s^{-1}$). Therefore, PANI@NVPF nanocomposites are promising cathode candidates for high rate sodium-ion battery applications.

Keywords: PANI; $Na_3V_2(PO_4)_2F_3$ (NVPF); Conducting Polymer; composite materials; sodium-ion battery

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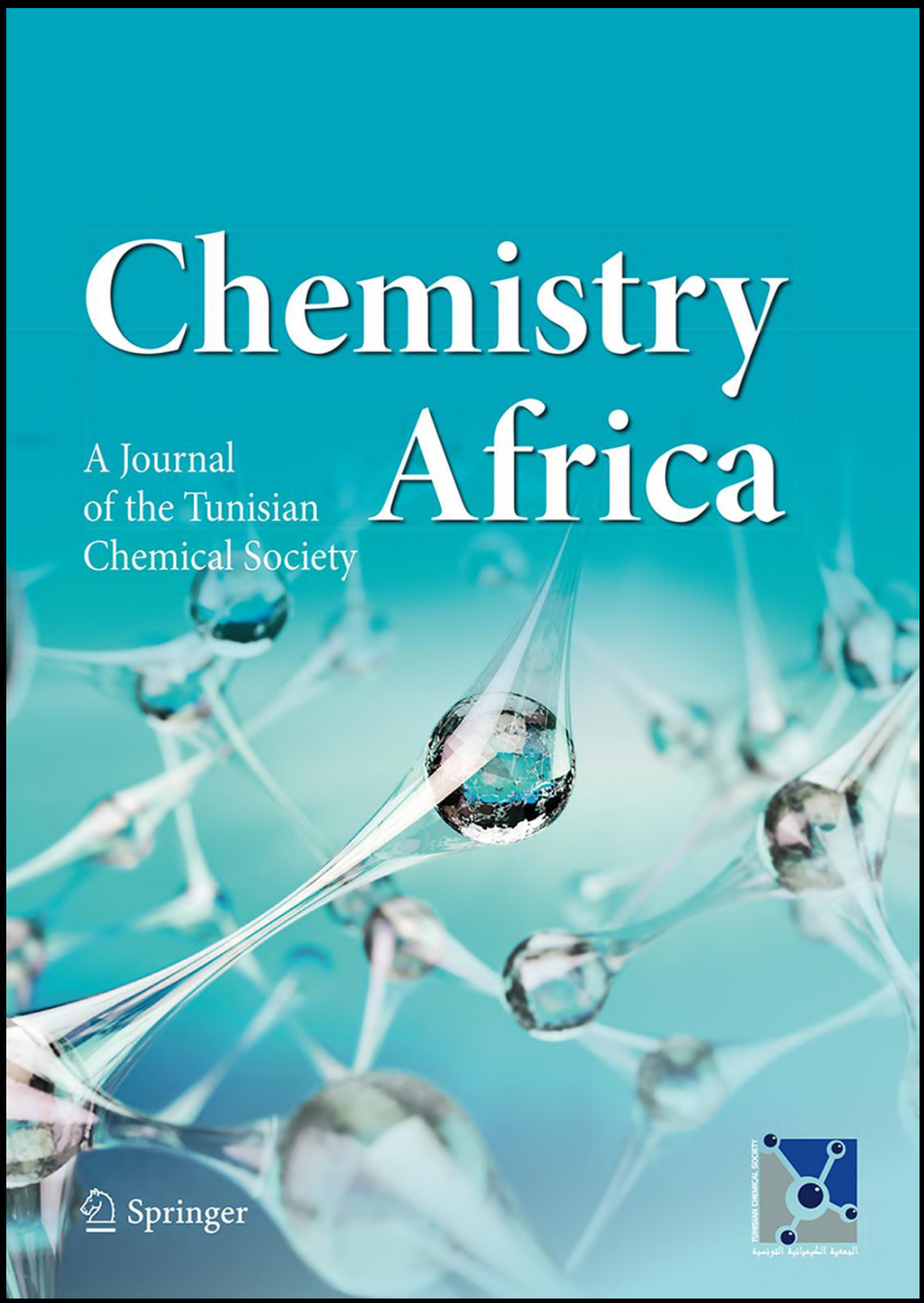

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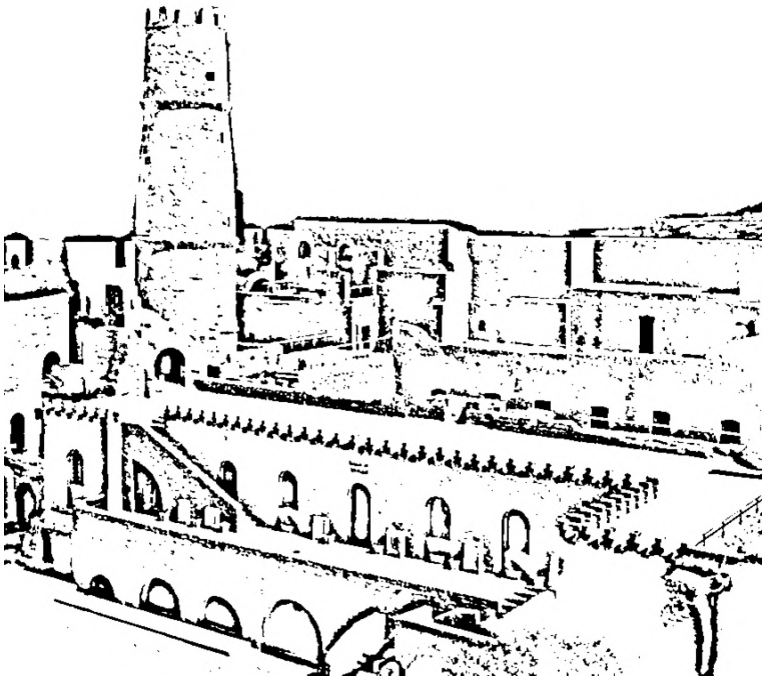

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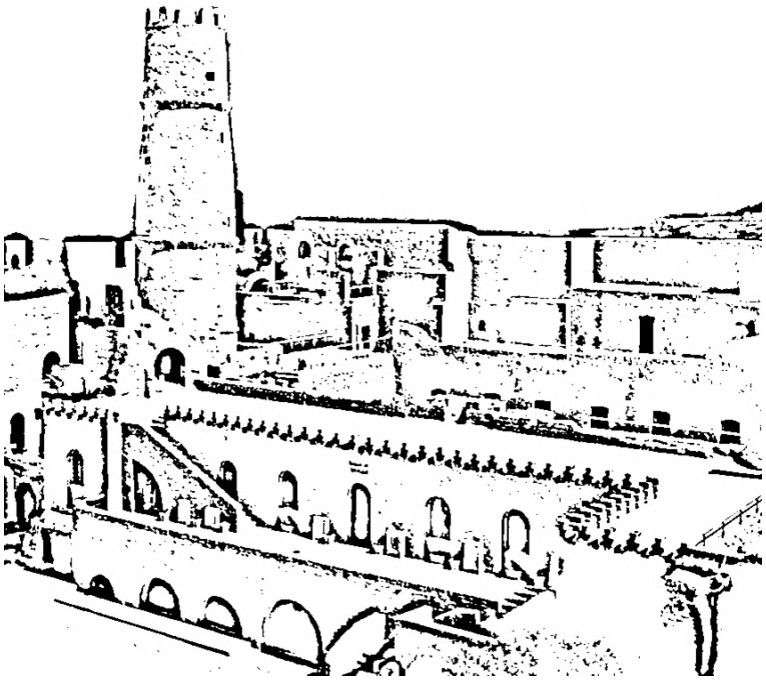

Résumés des Communications Posters

Sustainable Thin-Film Materials Based on Bio-Based Polymers Doped with Nanoparticles: Structural and Optical Property Analysis

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The growth of hybrid nanocomposites, an interdisciplinary field, is finding expanding applications in piezoelectric sensors, LEDs, solar cells, and various domains such as optoelectronics, energy, catalysis, and biomedicine.

This study focuses on the synthesis of chitosan-based membranes and investigates the effects of incorporating $BiFeO_3$ (BFO) nanoparticles using structural and optical characterization techniques.

The films were fabricated using a solution-casting technique, with BFO particles incorporated into the chitosan matrix at concentrations of 4%, 8%, 10%, 25%, and 30%. Characterizations were performed using structural techniques such as X-ray diffraction (XRD) and scanning electron microscopy (SEM), as well as optical techniques including UV-visible spectroscopy.

X-ray diffraction analysis confirms that the films retain the crystalline structure of the $BiFeO_3$ nanoparticles, with no formation of secondary phases. SEM observations reveal a uniform distribution of nanoparticles within the chitosan matrix, with no signs of agglomeration in the CS/BFO films. To investigate the influence of $BiFeO_3$ on the optical properties of the polymer, the transmittance and reflectance spectra of the CS/$BiFeO_3$ composites were analyzed. A significant change in optical behavior is observed at 6% BFO, marked by the appearance of characteristic nanoparticle absorption bands in the visible range.

Keywords : Chitosan, nanoparticle, composite, membranes.

Electrochemical Sensor Based on MOF/@BCN for Simultaneous Detection of cadmium and lead

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Heavy metal pollution, particularly from cadmium (Cd^{2+}) and lead (Pb^{2+}), poses serious risks to both human health and the environment. Exposure to these toxic metals can lead to severe health issues, including kidney damage, bone demineralization, and even cancer **[1]**.

In this study, a MOF@BCN composite was synthesized and employed as a novel electrochemical sensor for the simultaneous detection of Cd^{2} and Pb^{2}. The electrochemical properties and sensing performance of the sensor were evaluated using differential pulse voltammetry (DPV). The sensor demonstrated a low detection limit and high sensitivity, making it a promising candidate for heavy metal monitoring.

Keywords: MOF, electrochemical sensor, heavy metals, differential pulse voltammetry.

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Poly (diallyldimethylammonium chloride) Functionalized Calcium Hydroxyapatite: Synthesis, and Application in Adsorption of Eriochrome Black T Dye

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In this work, Hydroxyapatite- poly (diallyldimethylammonium chloride) (CaHAp-PolyDADMAC) composites were successfully synthesized using a co-precipitation technique. The prepared hybrid materials were analyzed using X-ray diffraction (XRD), Fourier Transform Infrared Spectroscopy (FT-IR), Scanning Electron Microscopy (SEM), Energy Disperse X-Ray analysis (EDX) and Thermogravimetric Analysis (TGA/DTA). The crystalline phase of CaHAp was not affected by the modification with PolyDADMAC. The functionalized CaHAp particles displayed different sizes and poorly defined shapes. The EDX analysis of modified CaHAp showed the presence of nitrogen element of PolyDADMAC, and calcium, phosphorus, oxygen, and carbon characteristics of unmodified CaHAp. The hybrid materials were further used for the adsorption of Eriochrome Black T (EBT) under varying operational conditions such as pH, contact time, initial concentration, and temperature. At optimum conditions (T = 20°C, pH = 5, time = 40 min) the maximum adsorption capacities were equal to 98.8 mg/g and 236 mg/g for CaHAp and CaHAp- PolyDADMAC 3%, respectively. The kinetics of adsorption complied well with the pseudo-second-order model, suggesting a chemisorption process. The adsorption mechanism was exothermic, and non-spontaneous. Overall, the obtained high adsorption capacities confirmed that the synthesized hybrid materials could be used as efficient adsorbents of hazardous anionic dyes.

Keywords: Hydroxyapatite, Poly (diallyldimethylammonium chloride), Eriochrome Black T, Adsorption.

An innovative magnetic L-lysine-dialdehyde nanocellulose for sono-chemical heterogeneous catalysis in the green synthesis of ultrapure tri-substituted imidazoles

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In this study, we report the first ultrasound-assisted synthesis of magnetically modified L-lysine dialdehyde nanocellulose and its application in an efficient and eco-friendly catalytic process. The nanomaterial denoted as [Lys-g-DANC) @Fe_3O_4] was successfully characterized using various structural, morphological, thermal, optical and magnetic techniques.

Subsequently, it was utilized as a heterogeneous nanocatalyst in a one-pot multicomponent synthesis of tri-substituted imidazoles under green conditions. The catalytic process conducted under ultrasound irradiation using only 0.03 g of [Lys-g-DANC)@Fe_3O_4] in 10 mL of ethanol at 45 °C, resulted in excellent product yields ranging from 83.45% to 97.13% within a short reaction time (1.5–3 h). The structures of obtained imidazole derivatives were confirmed by FTIR and NMR spectroscopic techniques.

This work highlights the superior catalytic performance of magnetic L-lysine nanocellulose compared to conventional thermal methods, demonstrating advantages such as enhanced yields, reduced reaction times, facile catalyst recovery, and efficient recyclability [1].

Keywords: Magnetic L-lysine nano-catalyst; Heterogeneous catalyst; Tri-Substituted imidazole derivatives.

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Design and Evaluation of Isoxazole-Modified Chitosan: A Novel Biopolymer with Enhanced Anti-Ulcer Properties

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Isoxazoles are five-membered heterocyclic compounds containing nitrogen and oxygen, known for their wide range of biological activities, including antibacterial, antifungal, anticancer, anti-inflammatory, and anti-ulcer properties.[1] Their ease of synthesis and pharmacological efficiency, particularly as selective COX-2 inhibitors, have sparked strong interest in the medical field.

Chitosan is a natural polymer derived from chitin, widely recognized for its biocompatibility, biodegradability, and non-toxicity. These characteristics, combined with its numerous biological properties (antibacterial, antifungal, wound-healing, etc.), make it a highly promising material. Owing to these attributes, chitosan is used in various fields such as pharmaceuticals, biotechnology, cosmetics, food processing, textiles, and agriculture.[2] In recent years, interest in this biopolymer has continued to grow, particularly in the pharmaceutical sector, where research is increasingly focused on its chemical modification to enhance its performance and expand its applications.

In this context, this study aims to valorize shrimp waste by extracting chitosan and chemically modifying it through the grafting of isoxazole groups via O-alkylation. This approach seeks to combine the pharmacological benefits of both compounds to create an innovative biopolymer with enhanced anti-inflammatory and anti-ulcer properties. Molecular docking studies were conducted to evaluate the interactions between the modified chitosan and biological targets, in order to compare its effectiveness with that of unmodified one. This work opens up promising perspectives for the development of therapeutic materials aimed at treating gastrointestinal ulcers.

Key words: chitosan, isoxazole, modification, anti-ulcer, molecular docking

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Reaction of 4(-2-Aminoethyl)morpholin with the (Chloro) Meso-Tetra(para-fluorophenyl)porphyrinato Cobalt(III) Complex. Spectroscopic, and Structural Characterizations

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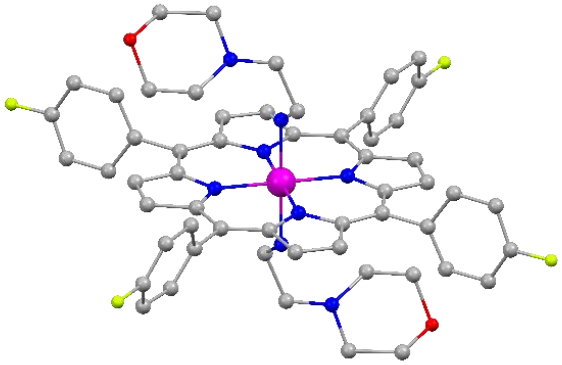
Cobalt(III) porphyrin complexes have a range of applications, particularly in the field of catalysis and bioinorganic chemistry. For example, cobalt(III) porphyrin complexes have been investigated for their electrochemical properties, including their use as electrocatalysts for fuel cells and other electrochemical processes **[1]**. These complexes can facilitate electron transfer reactions and have potential applications in energy conversion and storage **[2]**.
In this work, we have focused on the synthesis of a new cobalt(II) metalloporphyrin with formula **$[Co^{III}(TFPP)(C_6H_{12}N_2O)_2]Cl$ (I)** where TFPP is the *meso*-tetra(*para*-fluorophenyl)porphyrin. Compound **(I)** was prepared by the reaction of the [Co(TFPP)] staring material with an excess of 4(-2-Aminoethyl)morpholin in dichloromethane. This complex was characterized by UV–visible, IR and proton NMR spectroscopy. We also characterized this species by single crystal X-ray Molecular structure. The data collection was made at low temperature (200 K) and complex **(I)** crystalizes in the monoclinic crystal system with the C2/c space group. The cell parameters are: ***a*** = 28.128(6) Å, ***b*** = 12.778(3) Å, ***c*** = 18.353(4) Å, ***β*** =128,18(3)° and Z = 4.



Molecular structure of $[Co^{III}(TFPP)(C_6H_{12}N_2O)_2]Cl$.

Key words: Cobalt(III) porphyrin; X-ray molecular structure.

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Investigation of the aggregation behaviour of the anionic surfactant sodium dodecyl sulfate in ionic liquids in 1-allyl-3 -methylimidazolium bromide and N-allyl-N, N-dimethylethylammonium bromide

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The dynamics and aggregation behavior of sodium dodecyl sulfate (SDS) in 1-allyl-3 -methylimidazolium bromide [Amim]Br and N-allyl-N, N-dimethylethylammonium bromide (N112A-Br) are characterized by conductivity, density and TurbiScan measurements. The critical micellization concentration (CMC) was determined from the conductivity measurements and increased with adding 1-allyl-3-methylimidazolium bromide and decreased with the addition of [Amim] Br compared to solutions containing pure SDS. The decrease in CMC of SDS with increased concentration of [Amim]Br penetrates. We observe a positive change in apparent molar volume V in these systems containing SDS and both ions. We also observe clear evidence that the IL ions affect micelle size compared to pure SDS in water. To better understand these observations, we focus on DFT computer simulation to study the structure of SDS micelles in aqueous IL solutions. The plausible physicochemical interactions in the mixed system of sodium dodecyl sulfate (SDS) and 1-allyl-3-methylimidazolium bromide ([Amim]Br), along with N-allyl-N, N-dimethyl ethyl ammonium bromide (N112A-Br), were further explored through a computational simulation study. This study utilized density functional theory (DFT) with the B3LYP method, using Gauss View 5.0.9 and a 3-21G basis set.

Keywords: Ionic liquids, surfactant aggregation, computational simulations, co-surfactant, counterion dissociation.

Development and Electrochemical Evaluation of ZIF-8 and Its Derived Porous Carbon for Aqueous Supercapacitor Applications

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In this study, we investigated the electrochemical performance of Zeolitic Imidazolate Framework-8 (ZIF-8) and its derived porous carbon (PC) as electrode materials for energy storage applications, specifically targeting electric double-layer capacitors (EDLCs). Both materials were mixed with 5 wt% polyvinylidene fluoride (PVDF) as a binder. To evaluate their intrinsic electrochemical behavior, we first employed a well-known reversible redox system-ferri/ferrocyanide (5 mM) in 0.1 M $LiNO_3$-as the electrolyte. Cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS) revealed that the porous carbon exhibited superior electrochemical characteristics, including higher redox peak currents, lower charge transfer resistance, and a larger electroactive surface area, reflecting efficient electron transfer and ion diffusion. The study then focused on testing the materials in a neutral aqueous electrolyte (5 M $LiNO_3$) to assess their capacitive performance. The porous carbon electrode showed significantly higher specific capacitance compared to ZIF-8 in CV measurements. Furthermore, galvanostatic charge-discharge (GCD) analysis confirmed the ideal EDLC behavior of the porous carbon, with linear and symmetric charge/discharge profiles. It also demonstrated outstanding cycling stability, retaining 91.48% of its initial capacitance after 2000 cycles.

Keywords: Zeolitic Imidazolate Framework-8; porous carbon; cyclic voltammetry; electrochemical impedance spectroscopy; supercapacitor applications.

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Polysaccharide from Fennel Leaves: Extraction, Physicochemical Characterization, and Application as a Corrosion Inhibitor for Mild Steel

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Traditional chemical products used as corrosion inhibitors have significant environmental impacts [1], while polysaccharides extracted from renewable natural resources provide an eco-friendly and sustainable alternative [2]. This study focuses on the extraction and characterization of polysaccharides from *Foeniculum vulgare* (fennel) leaves, a renewable and cost-effective resource, and evaluates their effectiveness as corrosion inhibitors for mild steel in a 1 M hydrochloric acid solution.

The inhibition efficiency was assessed using mass loss measurements, potentiodynamic polarization, and electrochemical impedance spectroscopy (EIS). The results revealed a maximum efficiency at an optimal concentration of 2 g/L. The polysaccharides acted as mixed-type inhibitors, effectively reducing both anodic and cathodic reactions. Surface morphology analysis using scanning electron microscopy (SEM), along with infrared spectroscopy (FTIR), confirmed the formation of a protective film that limits metal dissolution. These results highlight the potential of fennel polysaccharides as green, effective, and non-toxic alternatives to conventional synthetic corrosion inhibitors.

Keywords: Corrosion, Mild steel, Green inhibitors, *Foeniculum vulgare* polysaccharide

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Qualitative Phytochemical Screening and pharmacological activities of extracts and oil of Algerian *Petroselinum crispum, Apiaceae*

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Medicinal plants are rich in bioactive components that are utilized to treat various human ailments. They are crucial to healing as well. Phytochemical constituents are responsible for the medicinal activity of plants. Phytochemical screening is an important step in identifying bioactive compounds present in particular medicinal herbs. Obesity, and multidrug resistance to pathogenic microorganisms and olso oxidative stress are major challenges in the health care systems and pharmaceutical industries. This study aimed to screen phytoconstituents, and estimate total phenols, flavonoids contents, antioxidant, and antimicrobial activities of *Petroselinum crispum* extracts and essential oil. The antioxidant capacity of buthanol, dichloromethane extracts and essential oil was evaluated by employing DPPH radical scavenging. All samples were also tested against Gram-positive (*Staphylococcus aureus*...) and Gram-negative (*Escherichia coli*…) bacterial species using the disk diffusion method.
The presence of the identified phytochemical components makes the leaves pharmacologically active. In the proximate analysis the leaf nutrients in the plants that are useful for many pharmacological activity, *Petroselinum crispum* showed the highest phenol content in the ethyl acetate extract and and flavonoid content in the n-BuOH and AE extracts who contain the highest flavonoid concentration at (144.44±0.07 mg/g) and (100.97±0.04 mg/g), respectively. Results using the DPPH method showed strong free radical scaringing activity for three extracts, this activity decreased with increasing concentration in the following order n-BuOH>AE>DCM.

Key words; Phytoconstituents, antioxidant capacity, bacterial species.

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A New (4,4'-Bipyridine) Zinc(II) Metalloporphyrin Structure for the Electrochemical Sensing of Dopamine

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This work continues our series of investigations into the electronic and structural properties of divalent metal porphyrin complexes [1-2], with a particular focus on zinc(II) metalloporphyrins. In this context, we have synthesized the coordination compound [Zn(TMPP)(4,4'-bpy)]•$CHCl_3$ (I), where TMPP denotes meso-tetra(para-methoxyphenyl)porphyrinate and 4,4'-bpy refers to 4,4'-bipyridine. The compound was thoroughly characterized using UV-Vis, fluorescence, IR, and ^1H NMR spectroscopy, ESI-HRMS mass spectrometry, and single-crystal X-ray diffraction analysis. this compound was successfully employed as an electrochemical sensor for the detection of dopamine (DA) using the square wave voltammetry (SWV).

Mots clés: Zinc(II) metalloporphyrin, X-ray molecular structure, UV-Vis, Dopamine

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Spectroscopic characterization and Binding interaction of heavy metal onto the Surface Receptor of the Azobenzene: DFT and experimental approach

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The azobenzene derivative 1-arylazo-2-naphthol was synthesized and characterized by elemental analysis, IR, UV–Vis, and ^{1}H NMR spectroscopy. DFT calculations at the B3LYP-D3/IEF-PCM level were performed to explore electronic properties (MEP, NPA, FMOs) and solvent effects [1,2]. Theoretical results indicated increased molecular reactivity in polar solvents, especially acetonitrile. No significant azo–hydrazone tautomerism was observed. Red and blue shifts in absorption spectra reflected π-conjugation and possible tautomeric forms, enhancing photostability.

The compound was investigated as a sensor for Cu^{2+}, Mg^{2+}, Ni^{2+}, and Zn^{2+} ions. Binding studies revealed the strongest interactions with Ni^{2+}, followed by Cu^{2+} and Zn^{2+}, while Mg^{2+} showed the weakest affinity. After cations chemisorption on azoic molecule a bathochromic shift in UV–Vis spectra, particularly for the Ni^{2+} complex, confirmed successful coordination. The azobenzene system demonstrates promising properties for use as a selective optical sensor for heavy metal ions.

Keywords: Azobenzene, MEP, NPA, FMOs, solvent effects and adsorption energy.

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Sustainable extraction of high-quality polysaccharides from *opuntia* cake using Supercritical CO_2 for cosmetic applications

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This study investigates the extraction of polysaccharides from prickly pear seed cake using two distinct methods: classical extraction and supercritical CO_2 extraction. The physicochemical and functional properties of the extracted polysaccharides were evaluated, revealing that, while both methods yield similar base compositions, significant differences in structure and properties were observed due to the extraction technique employed.

Fourier-transform infrared spectroscopy (FTIR), nuclear magnetic resonance (NMR), and gas chromatography-mass spectrometry (GC-MS) analyses showed that the polysaccharides extracted via supercritical CO_2 (PGF-CO_2) exhibit enhanced structural integrity and purity. These improvements translated into better interactions with other ingredients in hydrating cream formulations. Specifically, FTIR spectra confirmed the presence of characteristic polysaccharide bands with stronger peaks in the PGF-CO_2 sample, suggesting higher purity. NMR analysis identified the typical sugar backbone structure, while GC-MS confirmed the absence of solvent residues and other impurities.

Moreover, stability tests, including centrifugation at 3000 rpm for 10 min, thermal cycling (5 cycles between 4°C and 40°C), and emulsion stability, demonstrated superior performance of creams containing polysaccharides extracted by supercritical CO_2. These creams exhibited better oxidative stability, with a reduced oxidation rate of 1.8 meq O_2/kg after 12 hours in the Rancimat test, compared to creams made with polysaccharides from classical extraction.

In conclusion, Supercritical CO_2 extraction efficiently produces stable, high-quality polysaccharides from prickly pear seed cake, offering a sustainable solution for cosmetic formulations.

Key words: Prickly pear seed cake, Polysaccharides, Supercritical CO_2 extraction, Eco-friendly cosmetics.

Green extraction of polysaccharide from pomegranate peel using natural deep eutectic solvent extraction: Comparison and biological activity

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The pomegranate (*Punica granatum* L.), belongs to the *Punicaceae* family, is considered a "super tree" due to its high nutritional value and potential medicinal properties [1]. These benefits are attributed especially for their rich content of bioactive compounds, including polysaccharides, proteins, fatty acids and polyphenols [2]. In this study, we extracted PPC and PPN, two pectic polysaccharides extracted from pomegranate peels, using conventional and natural deep eutectic solvents (NADES), respectively. Subsequently, the polysaccharides were characterized using various analytical methods, such as FT-IR, UV, DSC, SEC/MALS/VD/DRI, NMR (1D and 2D), and GC/MS analyses. The antioxidant potential of the extracted polysaccharides was evaluated by DPPH, FRAP, and ABTS radical scavenging assays, in addition to α-amylase inhibitory activity. The results showed that PPN had significantly higher antioxidant and anti-diabetic potential than PPC, indicating its potential for therapeutic applications.

Key words: Pomegranate, polysaccharide, Natural deep eutectic solvent, physico-chemical characterization, α-amylase inhibitory

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Advanced Statistical and Deep Learning Approaches for the Optimization of Schiff Base Synthesis and Bioactivity

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A series of novel Schiff base compounds were synthesized via the condensation of hydrazine with various carbonyl derivatives. The resulting compounds were thoroughly characterized using FT-IR spectroscopy, UV-visible spectroscopy, and both ^{1}H and ^{13}C nuclear magnetic resonance. The synthetic process was optimized using Central Composite Design, an effective technique for experimental design and statistical analysis. The study focused on identifying the optimal reaction conditions to maximize both yield and product purity.

Computational modeling approaches, including Response Surface Methodology and Artificial Neural Networks, were employed to predict and enhance synthesis outcomes. Antibacterial activity assessments revealed minimum inhibitory concentration values ranging from 0.070 to 1.250 mg mL^{-1}, with significant activity observed against Gram-negative bacterial strains.

Development of a novel non-enzymatic electrochemical sensor for creatinine quantification in real samples

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Creatinine, a metabolic byproduct of creatine phosphate from muscle and protein metabolism, is released at a constant rate by the body and serves as a critical biomarker for renal function [1]. Abnormal creatinine levels in biological fluids are strongly linked to severe health conditions, including kidney failure [2], muscular disorders [3], and cardiovascular diseases [4]. Accurate and sensitive quantification of creatinine is therefore vital for early diagnosis and effective management of these diseases. In this work, a novel CuNPs@MIL-88B composite was synthesized and employed to develop a highly sensitive electrochemical sensor for creatinine detection. The electrochemical behavior and sensing performance were evaluated using differential pulse voltammetry. The sensor exhibited a broad linear detection range from 0.002 µM to 5 µM, an outstanding detection limit of 1.5 nM, and excellent selectivity against interfering biomolecules. The applicability of the sensor was successfully validated in human serum samples, exhibiting high recovery rates and confirming its potential for clinical diagnostics.

Keywords: Copper nanoparticles, Creatinine, electrochemical sensor, MIL-88B, Differential pulse voltammetry.

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Calendula aegyptiaca Polar Extract: Phyto-constituents, Antioxidant activity and *In-vivo* Toxicity.

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Plants are appreciated as an infinite source of active compounds. Multiple investigations have revealed that the genus *Calendula* (Asteraceae) is rich in active chemicals, particularly phenolic compounds, which supported the growing interest in scientific research on this genus' species.

Calendula aegyptiaca is a poorly studied plant in terms of chemistry and biology. The aerial part polar extract was tested for chemical composition and biological activities. Our plant's principal phyto-constituents were flavonoids, phenolic acids, and saponins detected using high-performance liquid chromatography combined with negative electrospray ionization mass spectrometry (HPLC-HESI-MS). Antioxidant activity test performed on this extract showed significant values compared to extracts with lower polarities. Subacute toxicity test on Wistar female rats by oral administration with dosages greater than 100x those employed for anti-inflammatory[1] and anti- diabetic activities[2] did not cause ruins to the rats, and the results demonstrated unexpected anti-hyperuricemic power at relevant doses.

According to our findings, *Calendula aegyptiaca* total aerial part polar extract can be considered as a potential new source with significant biological effects.

Keywords: *Calendula aegyptiaca*, HPLC-HESI-MS, phenolic acids, flavonoids, saponins, antioxidant activity, subacute toxicity, anti-hyperuricemic activity.

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Investigation de la variation de la composition du bio-verre 45S5 sur les propriétés mécaniques

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Les biomatériaux sont au croisement de plusieurs disciplines comme la médecine, la biologie, la chimie, l'ingénierie tissulaire et la science des matériaux. Ils jouent un rôle essentiel dans le domaine médical et représentent un enjeu majeur, aussi bien sur le plan social qu'économique. Ces matériaux regroupent une large gamme de produits, ils peuvent être d'origine naturelle ou synthétisés à l'aide de diverses approches chimiques, impliquant l'usage de métaux, de polymères, de céramiques ou encore de matériaux composites. Leur diversité et leur évolution sont directement liées à la complexité des tissus et organes du corps humain. L'étude de l'efficacité de ces matériaux doit considérer non seulement les aspects de biocompatibilité mais aussi les aspects d'ostéo-induction et d'ostéo-formation. De plus, ces matériaux doivent présenter des propriétés physico-chimiques leur permettant de résister aux contraintes de dégradation liées au milieu biologique dans lesquels se trouvent. Ainsi, l'évaluation des biomatériaux nécessite une caractérisation physico-chimique, mécanique statique et dynamique (composition, structure chimique, densité, morphologie, propriétés mécaniques, électriques, etc.). Dans ce travail, nous nous sommes intéressés à l'optimisation des propriétés mécaniques des biomatériaux afin de trouver le matériau idéal qui résiste aux diverses sollicitations. Nous avons étudié la variation de la composition des bio-verres, nous avons trouvé que l'augmentation de la concentration massique de CuO dans le bio-verre 45S5 donne une augmentation aussi bien de la densité et du module de Young que celle des vitesses longitudinale et transversale. Alors, une adaptation de la composition chimique des matériaux est nécessaire pour répondre aux contraintes biomécaniques, mais également répondre aux réactions cellulaires au contact.

Mots clés: Biomatériaux, propriétés physico-chimiques, optimisation, module de Young, biocompatibilité.

Synthesis and Characterization of Gold(I) N-Heterocyclic Carbenes Complexes Baring Methacrylate Moiety

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The study focuses on gold(I) N-heterocyclic carbene (NHC) complexes. The research aims to synthesize a family of four mono- and four bis-gold(I) N-heterocyclic carbene complexes, each bearing a methacrylate motif, with yields ranging from 63% to 98%. Two model complexes from this series were tested toward sulfur-based nucleophilic attack to assess the possibility of a Michael addition to the acrylate motif, with a view to future bioconjugation. Experimental results reveal that thiolate addition occurs exclusively at the gold(I) center, regardless of whether the N-heterocyclic carbene is a mono- or a bis-carbene, leaving the acrylate motif untouched. This outcome is supported by theoretical calculations, which predict an activation energy of at least 4 kcal/mol favoring nucleophilic attack at the gold(I) center. These findings suggest that gold(I) NHC complexes could serve as effective "clickable" motifs in themselves, challenging the necessity of further functionalizing them with additional clickable groups for bioconjugation applications.

Mots clés: *N*-heterocyclic carbenes, gold, methacrylate

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Antidiabetic activity of a novel chitosan derivative containing triazole/carbazole moieties

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Diabetes is a chronic metabolic disorder. Other than medication, adaptation of the diet is also considered one of the most effective methods of controlling blood sugar levels. Today's available therapies for diabetes, including insulin and a variety of oral hypoglycemic agents, are associated with serious side effects. Consequently, many promising studies have been reported for the development of several natural substances, in particular polysaccharide derivatives, which are suitable for both treatment and prevention of diabetes and any other associated health issues. Polysaccharides bearing heterocyclic groups are receiving considerable attention, especially triazole derivatives, owing to their wide range of biological activities. Chitosan is the second most abundant and renewable polysaccharide on earth after cellulose. Chitosan and its derivatives have been proved to show a variety of biological activities. The current work focuses on the synthesis and characterization of a new chitosan derivative created by click chemistry, for biological benefits involving anti-diabetic activity. This compound is soluble in common organic solvents. The structure was confirmed by XPS and IR-FT. The thermal characterization was carried out by differential scanning calorimetry (DSC).

Key words : Chitosan , clickc chemistry, anti-diabetic activity

Discovery of novel barbituric acid derivatives as antimicrobial agents, molecular structure, in vitro investigation by molecular docking and DFT study

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Barbituric acid and its derivatives continue to attract interest due to their broad spectrum of biological activities [1]. In this study, a series of novel barbituric acid derivatives were designed, synthesized, and evaluated for their antimicrobial potential. The molecular structures of the synthesized compounds were characterized using spectroscopic techniques. Their antimicrobial activity was assessed in vitro against a panel of Gram-positive and Gram-negative bacteria, as well as fungal strains[2]. To gain insights into the mechanism of action at the molecular level, docking studies were carried out targeting key microbial enzymes, revealing favorable binding affinities and interactions within active sites. Additionally, Density Functional Theory (DFT) calculations were performed to optimize the geometry and investigate electronic properties such as frontier molecular orbitals (HOMO–LUMO), energy gaps, and molecular electrostatic potential (MEP) surfaces. The DFT results supported the reactivity and stability profiles inferred from docking analysis. Collectively, these findings highlight the promising antimicrobial potential of the synthesized barbituric acid derivatives and provide a rational basis for further structural optimization and development.

Keywords: Barbituric acid, antimicrobial activity, molecular docking, DFT.

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Selective Extraction of Pure Polysaccharides from Olive Leaves via Three-Phase Partitioning (TPP): A Novel One-Step Method for Enhanced Antioxidant Profiling

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Olive leaves (*Olea europaea L.*), a widely available agro-industrial by-product, are known for their rich content of bioactive polysaccharides. However, most conventional extraction techniques lead to the co-extraction of polyphenols and proteins, forming complex polysaccharide–polyphenol–protein matrices that complicate functional evaluation. In this study, we propose a **novel, one-step extraction approach using the Three-Phase Partitioning (TPP) method**, aimed at isolating **high-purity polysaccharides** while eliminating interfering phenolic and protein compounds. This method offers a selective separation under mild conditions without the need of organic solvents or multi-step purification. The extracted polysaccharides were characterized by colorimetric analysis, FT-IR spectroscopy, and SEC, and their antioxidant activity was evaluated using ABTS and ORAC assays. Results demonstrated a high yield of structurally intact, phenol-free polysaccharides with significant antioxidant potential. This innovative TPP-based method offers a cleaner, simpler, and more efficient alternative for obtaining functional polysaccharides from olive leaves, making it especially promising for applications in food, pharmaceutical, and biomaterial development where purity is essential.

Keywords: Olive leaves (*Olea europaea L.)*, polysaccharide, Three-Phase Partitioning (TPP), antioxidant activity.

Synthesis and characterization of Activated carbons from agro-waste of palm trunk fiber : Application for azo dye removal

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In this work, the activated carbon of palm trunk fiber was prepared by the thermochemical activation method [1, 2] for the adsorptive removal of azo dyes known for their toxicity [3], including methylene blue (MB) and methyl orange (MO) from aqueous solution. This preparation was realized with activated factor phosphoric acid H_3PO_4 at 450 °C in different impregnation ratios, which varied within the following range : 30, 60, 100, and 150 wt %. Investigated adsorbents were characterized using several methods such as X-ray diffraction, N_2 sorption, energy-dispersive X-ray spectroscopy, and scanning electron microscopy techniques. The effect of adsorbent dosage was evaluated and discussed. The results show that the adsorption capacity increases with increasing the mesoporous of the activated carbons. At 150 wt % H_3PO_4 ratios were found to be appropriate for efficient adsorption of the (MO) dye (~862 $mg \cdot g^{-1}$) and (MB) dye (~508 $mg \cdot g^{-1}$). Isotherm data were investigated according to Langmuir and Freundlich equations. The obtained results revealed that the Langmuir model provides the best fit for the cationic MB dye while the Langmuir and Freundlich models offer the best fit for anionic MO dye.

Mots clés: Activated carbons; Characterized; Adsorptive removal; Palm trunk fiber, Azo dyes

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Photocatalytic degradation of Acridine orange dye and real textile wastewater via ZnO nanoparticle supported natural Tunisian clay

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In this study, sol gel synthesis route was used to prepare ZnO nanoparticles and ZnO modified natural and abundant bentonitic clay [1, 2]. ZnO and ZnO-clay nanocomposites were characterized by X-ray diffraction, N_2 adsorption-desorption, transmission electron microscopy techniques and tested for Acridine orange dye photodegradation using artificial UV irradiation. Experimental data indicates that ZnO-clay was an efficient photocatalyst under UV irradiation and in the presence of H_2O_2 oxidant (around 97.8 % of Acridine orange removal and 82.7 % mineralization were achieved after 90 min). Photocatalytic degradation data of Acridine orange followed the first-order removal rate with three materials : pure clay, ZnO and ZnO-clay and the apparent rate constant increased with photocatalyst performance. Synthetic photocatalyst ZnO-clay was reused three times without an apparent decrease in its degradation efficiency even after 3 runs (94.7 % of AO removal), proving the high stability and reutilisability. As well, ZnO-clay was tested in the treatment of a real textile effluent and obtained results (80.6 % of effluent mineralization) confirm its great performance in the environmental decontamination.

Mots clés: Photocatalyse; ZnO-clay; Acridine orange; Mineralization; UV irradiation

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Phytochemical profile, antibacterial potential and *in silico* studies of flowers, berries and roots extracts of *Solanum elaeagnifolium* growing in Tunisia

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Solanum elaeagnifolium, commonly known as silverleaf nightshade, is a perennial weed belonging to the Solanaceae family, native to the Americas. However, it is now recognized as one of the most invasive plant species globally. Despite its toxicity and invasive nature, *S. elaeagnifolium* offers several beneficial uses in the medical field, owing to its diverse phytochemical composition. Plant extracts have been shown to exhibit significant antioxidant and antimicrobial activities. The aim of this work was to assess the phytochemical profile of *Solanum elaeagnifolium* flowers, berries and roots extracts using HPLC-MS/MS, as well as to evaluate their antibacterial activity *in vitro* combined with an *in silico* approach. The total phenolic and flavonoid contents of the studied extracts were determined, and 16 compounds, including phenolic acids and flavonoids, were identified and quantified. Antibacterial activity showed promising results against a multitude of microbes. Furthermore, molecular docking analysis and drug-likeness prediction of the primary compounds confirmed the notable antibacterial effects of the extracts. These findings suggest that *S. elaeagnifolium* could be a promising candidate for treating drug-resistant pathogens.

Keywords: *S. elaeagnifolium*, HPLC-MS/MS, Polyphenols, Molecular Docking, Antibacterial.

Combined Computational Approaches For Developing New Anti-Hepatitis B Drug Candidates: 3D-QSAR, Molecular Docking

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Hepatitis B is a life-threatening viral infection caused by the Hepatitis B virus (HBV), representing a significant global public health challenge, necessitating the discovery of new molecules with potential anti-hepatitis activity. In this work, sulfamoyl-benzamide derivatives as potent anti-hepatitis agents were collected from the literature to generate a 3D-QSAR model and conduct molecular docking. The 3D-QSAR model was successfully generated with a high regression coefficient R^2 = 0.94 and an excellent cross-validated determination coefficient Q^2_{cv} = 0.53 for the training set. Furthermore, the model developed showed good predictive ability, with a high predictive value Q^2 = 0.70 for the test set. Then, the results were used to discover novel molecules with a potential anti-hepatitis activity using the structure-based virtual screening. Based on successful results obtained by virtual screening, ten compounds were selected as potential inhibitors with highly predicted activities, binding interactions, and acceptable ADME properties.

Keyword: ADME, Docking, 3D-QSAR, hepatitis, sulfamoyl-benzamide.

Discovery of New Inhibitors of Tubulin via Structure-Based Virtual Screening

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In this study, we aimed to develop a three-dimensional quantitative structure activity relationship (3D-QSAR) for a set including 62 cytotoxic quinolines as anticancer agents with tubulin inhibitory activity. The model was built and shown to be statistically significant, with a high correlation coefficient (R2 = 0, 87), cross-validation coefficient (Q2 = 0, 72), and F value (72.3). The generated 3D contour maps were used to reveal the structure activity relationship of the compounds. The model was then used to virtually screen the ZINC database with the aim of identifying novel chemical scaffolds as potential tubulin inhibitors and predicting their potential activity. Further, in silico predicted ADME properties were investigated for the most promising molecules. Based on the results of the above studies, 5 new molecules were proposed as tubulin inhibitors with high binding affinity, activity prediction, and favorable ADME properties.

Keywords: Tubulin, 3D-QSAR, anticancer, Virtual screening, ADME, ZINC.

Preparation, Spectroscopic Characterization, And Molecular Structure Of A Tin(IV) Porphyrin Complex

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Porphyrins are a class of macrocyclic compounds known for their versatile coordination chemistry and remarkable electronic properties. Among them, tin porphyrins have attracted increasing attention due to their unique structural characteristics and promising applications in various fields, including catalysis [1]…. We have prepared a new coordination compound; the tin (IV) porphyrin complex $[Sn^{IV}(TTP)(C_9H_9O_3)_2]$. This species was characterized by UV-Visible, IR, NMR, and X-ray crystallography.

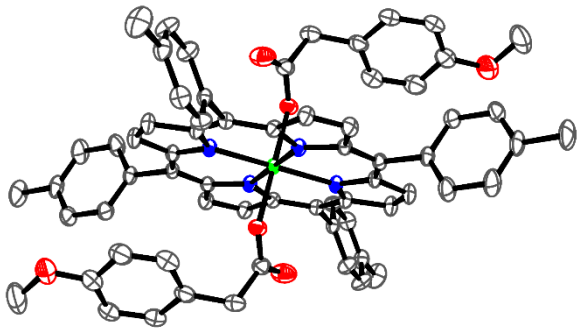

Figure 1 : Tin (IV) porphyrin complex $[Sn^{IV}(TTP)(C_9H_9O_3)_2]$

Key words: Tin (IV), porphyrin complex,

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Physicochemical and Fatty Acid Profile of *Moringa* Seed Oil Extracted

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In this study, the oil was extracted from *Moringa oleifera* seed cake by cold pressing, a gentle method that helps preserve thermosensitive compounds. The extraction yield was evaluated, and physicochemical analyses were performed, including acid value, peroxide value, iodine value, and saponification value, in accordance with AFNOR and ISO standards. The fatty acid profile was determined by gas chromatography coupled with a flame ionization detector (GC-FID) after methylation. The oil was found to be rich in oleic acid (C18:1, 72.6%), followed by palmitic acid (C16:0, 9.4%) and stearic acid (C18:0, 7.1%), with a low content of polyunsaturated fatty acids. These results indicate that *Moringa* seed cake oil exhibits excellent oxidative stability, significant nutritional quality, and can be utilized in the food, cosmetic, and pharmaceutical industries.

Keywords: *Moringa oleifera*, seed cake oil, cold pressing, GC-FID, fatty acids, quality indices.

Synthesis And Physicochemical Characterization Of A New Cobalt(II) Porphyrin Complex

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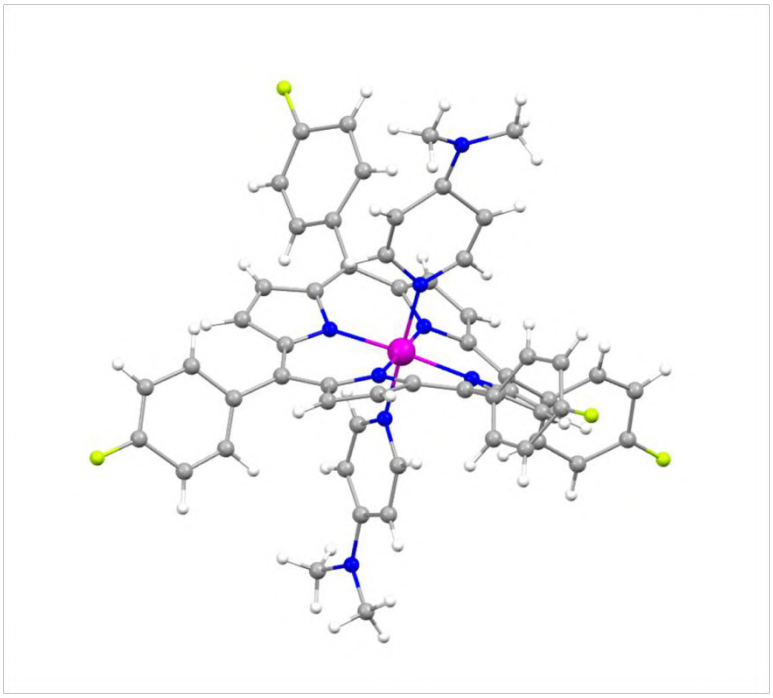
Cobalt porphyrins are an exceptional class of metalloporphyrins, renowned for their versatile chemical and catalytic properties, which have made them a focal point of research across various scientific fields.

This work aims at synthesizing a novel metalloporphyrin of cobalt(II). with the formula **[Co^{II}(TFPP)$(DMAP)_2$] (I)**, where TFPP is the meso-tetra(para-fluorophenyl)porphyrin and DMAP is 4-dimethylaminopyridin .Compound (I) was prepared by the reaction of the [**Co^{II}(TFPP)]** with an excess of 4-dimethylaminopyridin in chloroform. This complex was characterized by UV-visible, IR, mass spectrum, proton NMR spectroscopy and cyclic voltammetry.



Molecular structure of [Co^{II}(TFPP)$(DMAP)_2$].

Synthèse verte de nouveaux dérivés d'urée fluorés et évaluation de leur activité anti-inflammatoire

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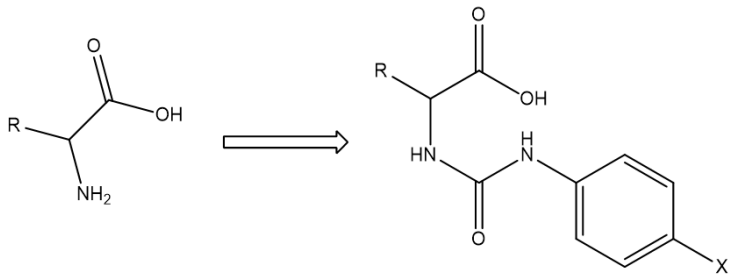
Une série de nouveaux dérivés d'urée fluorés a été développée par une méthode verte, respectueuse de l'environnement, à partir d'acides aminés en milieu aqueux alcalin. Les composés obtenus ont été caractérisés structurellement à l'aide de données spectroscopiques (RMN ^{1}H, ^{13}C et HRMS).

L'analyse par docking moléculaire a mis en évidence de fortes interactions, notamment par liaisons hydrogène, entre ces composés et les enzymes COX-1 et COX-2. Sur cette base, une sélection de composés a été soumise à une évaluation in vivo de leur activité anti-inflammatoire. Les résultats expérimentaux obtenus corroborent les prédictions issues des études in silico, confirmant que les affinités de liaison observées par modélisation moléculaire sont représentatives des effets anti-inflammatoires mesurés in vivo.



X= F, CF_3

Effects on the structure and electrochemical reactivity of surface modified magnesium cobalt oxide

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Polyaniline coated magnesium cobalt oxide nanocomposites (PANI@$MgCoO_2$) are synthesized by a cost-effective method. The structural, chemical, morphological, thermal and surface characterizations (X-ray diffraction, electron microscopy, thermogravimetry, Raman and X-ray photoelectron spectroscopies) confirm the presence of a thin layer of conducting polymer (~ 40 nm) in which the benzenoid and quinoid (C_6H_4) rings are surrounded by imine (=N-) and amine (-NH-) nitrogen on the particles of the cubic oxide. Their electrochemical reactions are studied in magnesium cells using the dual combination of sodium and magnesium ions in the electrolyte. A strong interaction at the interface of PANI and $MgCoO_2$ improved the electrochemical properties and revealed a single-phase insertion/extraction reaction mechanism into/from the cubic structure. These PANI@$MgCoO_2$ nanocomposites exhibited enhanced reversible capacity (103.4 – 153 mA h g^{-1}) at ~ 1 V vs. Mg^{2+}/Mg, Warburg (26.5 Ω $s^{-1/2}$) and diffusion ($6.92 \cdot 10^{-14}$ cm^2 s^{-1}) coefficients as compared to pristine material. These results show that the proposed coating can be used for electrodes in the field of rechargeable magnesium hybrid batteries (MHRBs).

Keywords: $MgCoO^2$; Conductive Polymer; Pickering emulsion composite materials; hybrid battery

Cold-pressed oil from Tunisian *Pistacia lentiscus* fruits: Physicochemical characterization and cosmetic valorization potential

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This study investigates the extraction and physicochemical characterization of *Pistacia lentiscus* oil obtained by cold pressing of ripe fruits collected in the Zaghouan region of Tunisia. The cold press method preserved the integrity of thermolabile compounds, yielding an oil extraction efficiency of 9.4 ± 0.3% (w/w). The physicochemical properties of the extracted oil were determined according to standard protocols. The acid value was 4.2 ± 0.1 mg KOH/g oil, indicating moderate free fatty acid content. The peroxide value was 5.6 ± 0.2 meq O_2/kg, reflecting good oxidative stability. The iodine value was 84.5 ± 1.0 g I_2/100 g, and the saponification value was 186.8 ± 2.5 mg KOH/g, both suggesting a predominance of unsaturated and medium-chain fatty acids. The refractive index at 20°C was measured at 1.467, and the relative density was 0.910 g/cm³. Gas chromatography analysis revealed a fatty acid profile dominated by oleic acid (C18:1, 46.8%), palmitic acid (C16:0, 26.5%), and linoleic acid (C18:2, 20.54%), with minor components including stearic acid and arachidic acid. Additionally, spectroscopic analyses confirmed the typical triglyceride structure of the oil, with FTIR, ^{1}H, and ^{13}C NMR revealing characteristic signals of ester bonds, unsaturated fatty acids, and the glycerol backbone.

These results highlight the suitability of *Pistacia lentiscus* fruit oil as a promising natural ingredient for cosmetic formulations, especially for skin repair, anti-aging, and emollient applications. Its richness in essential fatty acids, antioxidants, and its physicochemical stability positions it as a valuable candidate for sustainable cosmetic valorization.

Key words: *Pistacia lentiscus*, cold-pressed oil, physicochemical characterization, cosmetic valorization

Highly efficient $K_3NaCo_4(MoO_4)_6$/ H_2O_2 system for photocatalytic degradation of azo dyes

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$K_3NaCo_4(MoO_4)_6$ catalyst has been prepared using a solid-state reaction method. First, its crystal structure is determined from single-crystal X-ray diffraction data. This material crystallizes in trigonal system, space group $R3^-$ (No.148) with cell parameters a = 14.434(3) Å and c = 19.811(6) Å. The crystal structure of the title compound can be described by the junction of ribbons and MoO_4 tetrahedra by sharing vertices to give a three-dimensional framework in which Na^+ and K^+ cations are resided. Second, the as prepared sample has been characterized by X-ray diffraction (XRD), Fourier transform infrared (FTIR), Raman spectroscopy, UV–visible spectroscopy, scanning electron microscope (SEM) and EDX analysis. The SEM analysis demonstrates the presence of agglomerates with uniform nanoparticles having different crystallite sizes. FTIR and Raman spectra confirm the presence of characteristic MoO4 tetrahedra. Moreover, the optical band gap was found to be 3.5 eV. Finally, the photocatalytic removal of Acid Yellow (AY) organic azo dye was investigated under solar light in the presence of photocatalyst and H_2O_2. A good photocatalytic activity for the degradation of AY dye has been noted with a removal rate reaching 90 % when adding H_2O_2 at optimum reaction. The elimination of AY increased with the addition of 5 mM H_2O_2 concentration.

Imino and Amino orthopyridine-Appended Calix[4]arene and Thiacalix[4]arene Derivatives in *1,3*-Alternate Conformation: Rational Formation of Binuclear and Tetranuclear Complexes

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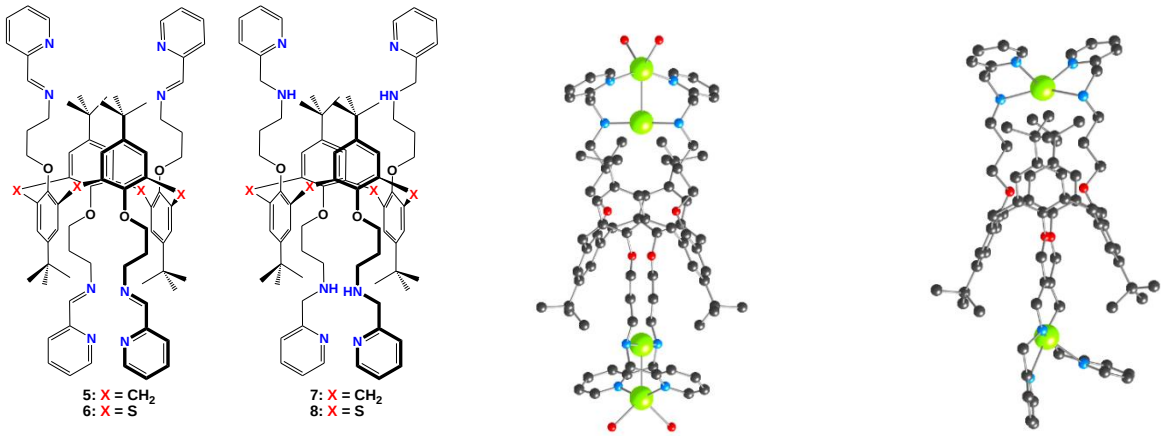
Four new multivalent ligands **5**–**8** derived from calix[4]arene and thiacalix[4]arene backbones in 1,3-alternate conformation bearing *ortho*-imino- and *ortho*-amino-methylpyridine chelating sites have been designed, prepared and characterized.



Owing to the imposed 1,3-alternate conformation of the backbone, ligands **5**–**8** offer two coordinating pockets composed of two sets of chelates located above and below the mean plane of the macrocyclic framework. Ligands **6**–**8**, independent of the nature of the anion associated with the Ag^+ cation (AgX; X = BF_4^-, PF_6^-, SbF_6^-, AsF_6^-, NO_3^-), form dinuclear silver complexes in solution and in the solid state. Ligand **7**, in the presence of an excess of Ag^+, also forms tetranuclear silver complexes **7**-$(AgBF_4)_4$ and **7**-$(AgNO_3)_4$ in the presence of two different auxiliary ligands (H_2O or NO_3^-) that have been characterized in the solid state. Due to a rather short Ag–Ag distance of about 2.89 Å, the tetranuclear complex **7**-$(AgBF_4)_4$ is emissive in the solid state, at 298 K (λ_{exc} = 295 nm, λ_{em} = 425 nm), which results from argentophilic interactions between the closely positioned silver cations.

Advancements in the Valorization of Ethyl Cyanoacetate: Exploring Novel Applications in Heterocyclic Chemistry

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The synthesis of novel triazole and succinimide derivatives from ethyl cyanoacetate represents a promising approach for developing compounds with potential applications in both pharmaceutical and industrial fields [1]. Ethyl cyanoacetate is a highly versatile precursor, owing to its reactive cyano and ester functional groups, enabling the construction of heterocyclic frameworks via targeted transformations [2].

This study focuses on the strategic functionalization of ethyl cyanoacetate through cyclization, condensation, and alkylation reactions to afford 1,2,4-triazole and succinimide derivatives. The synthetic methodologies include intramolecular condensation, and CuAAC (copper-catalyzed azide-alkyne cycloaddition) click chemistry for triazole formation. The resulting compounds were characterized by spectroscopic techniques to confirm their structures. These derivatives are anticipated to exhibit potential applications in pharmaceuticals and materials science due to their unique structural features and reactivity profiles.

Key words : Click Chemistry, Ethyl cyanoacetate, Heterocycles

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Synthesis, Spectroscopic Analysis, X-ray Crystallography, and Study of a Novel Iron(III) Meso-Tetra-3,5-Dimethoxyphenyl Porphyrin Complex

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Ferric porphyrins have long been, and continue to be, a central subject of extensive study due to their electronic, magnetic, and stereochemical properties, which closely resemble those of ferric heme proteins [1]. Most ferric porphyrins can be synthesized relatively easily and crystallized in a stable and pure form. In this work, we focused on the synthesis of meso-tetra(3,5-dimethoxyphenyl) porphyrin (H_2TDMPP) and the preparation of new iron porphyrin complexes with the dimethylaminopyridine (DMAP) axial ligand. Specifically, we investigated the synthesis, crystal structure, as well as the UV-visible, IR, ^{1}H NMR, cyclic voltammetry, and mass spectrometry data of the Fe^{3+}(T3,5-OMePP)$(DMAP)_2$ complex. This complex, with the formula [Fe^{3+}(T3,5-OMePP)$(DMAP)_2$], crystallizes in the monoclinic crystal system (space group $P2_1/n$) with the following cell parameters: a = 13.019(3) Å, b = 24.314(5) Å, c = 20.076(4) Å, β = 96.13(3)°, V = 6318(2) Å^3, Z = 4, R_1 = 0.0437, wR_2 = 0.0988, and S = 1.093.

Keywords: Fer(III) porphyrin complex; X-ray molecular structure; UV-visible, Cyclic voltammetry; Mass spectrometry; 1H NMR

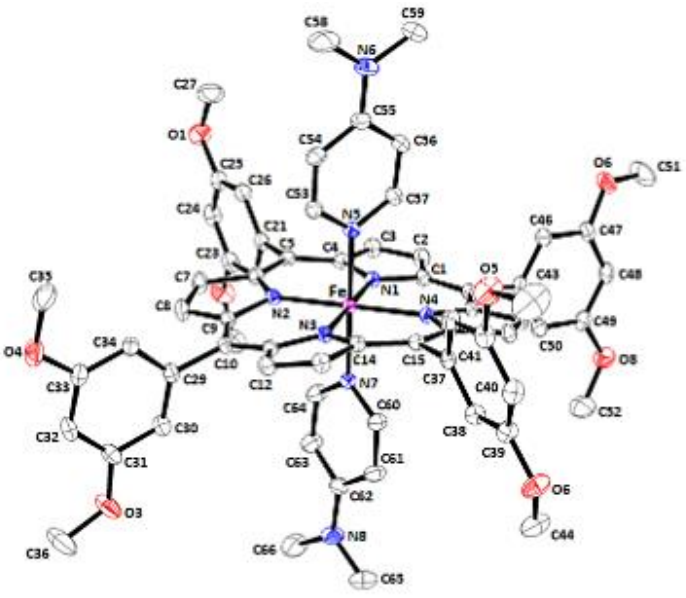

Figure 2: Ortep diagram of the [Fe^{III} (T3,5-OMePP)$(DMAP)_2$]

Structural and Mechanical Properties of zinc-doped tricalcium phosphate Bioceramics for Bone Tissue Engineering

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Autologous bone transplantation remains the reference for almost all orthopedic bone vacuum filling surgeries. However, it has limited sources, complications in the donor area, a risk of disease transmission, immune rejection and high prices, which have limited clinical applications [1,2], for this reason, scientists are looking for an ideal synthetic material to replace bone transplantation. Calcium phosphate replacement is recently attracted attention and is considered a potential bone substitute [3,4]. In this study, we investigated the structural and mechanical properties of the composites (%HA-%(TCP-xZn)). The primary products of the composites, which are hydroxyapatite (HA) and zinc-doped and undoped tricalcium phosphate (TCP-xZn) (x=0; 0.1; 0.3), were synthesized using the coprecipitation method. While the composites were carried out in solid-state suspension. The different synthesized powders were characterized morphologically and structurally by diffraction (XRD), spectrometry (FTIR), analysis (SEM), and specific surface area (SSA). The relative density of the sintered samples reaches the highest value with x = 0.1 and reaches approximately 99% after sintering at 1200 °C for 3 hours for 0 and 10% HA. The prepared bioceramic materials were mechanically characterized using Young's modulus and Vickers hardness measurements. The overall trend of these parameters evolved similarly to the relative density, and the maximum values obtained of 134 and 7.12 GPa respectively for the composite (20%HA-80%(TCP-0.1Zn)).

Keywords Tricalcium phosphate, Zinc, mechanical properties

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A Novel Trinuclear Copper MOF for High-Performance Micro-Supercapacitors: Synthesis and Characterization

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Metal-organic frameworks (MOFs) represent an emerging class of porous materials with significant potential for energy storage applications. In this study, we report the solvothermal synthesis of a novel trinuclear copper-based MOF, constructed from copper nitrate and dimethylpyrazol-naphthalene diimide (H_2NDI-H) [1], exhibiting high porosity and an exceptionally large specific surface area. Structural and morphological characterization was performed via powder X-ray diffraction (PXRD) and scanning electron microscopy (SEM), while thermogravimetric analysis (TGA) and low-temperature N_2 adsorption measurements were employed to assess thermal stability, surface area, and pore size distribution.

As a proof of concept, the MOF was integrated into micro-supercapacitor electrodes using laser-assisted printing [2]. Electrochemical evaluation revealed outstanding performance, including high specific capacitance, excellent rate capability, and remarkable cycling stability. These results demonstrate the viability of laser-printed MOF-based electrodes for next-generation miniaturized energy storage devices.

Keywords: MOF, Trinuclear ,naphtalene, microsupercapacitor , Laser-assisted printing , energy storage

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Semi-synthesis and *in silico* prediction of novel C28-modified triterpene acid derivatives from natural maslinic acid

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Maslinic acid is a pentacyclic triterpene acid widely found in various plants, particularly in olive pomace (*Olea europaea* L.) [1]. It has been reported to exhibit a range of biological activities, including anti-inflammatory, anti-diabetic and analgesic effects [2]. In this study, maslinic acid was isolated from olive pomace using an ultrasonic bath. A series of novel maslinic acid-arylidene derivatives was synthesized their structures were confirmed by ^{1}H NMR, ^{13}C NMR, and HRMS analyses. Molecular docking simulations were conducted to investigate the binding interactions between the synthesized compounds and the EGFR target protein, revealing consistently strong binding affinities across all derivatives. These findings suggest that these derivatives hold significant promise as lead candidates for further pharmacological development.

Key words: Olive pomace, Maslinic acid derivatives, Semi-synthesis, *in silico*, Molecular Docking

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Semi-synthesis of novel oleanolic acid derivatives: Evaluation of their anticancer activity and molecular docking studies

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Oleanolic acid (OA), a natural triterpenic compound widely found in medicinal plants [1], is gaining increasing attention for its diverse biological effects [2]. In this study, we synthesized a novel series of OA derivatives incorporating phenolic and coumarin moieties. Their structures were characterized by ^{1}H NMR, ^{13}C NMR and HRMS analyses. The biological activities of these derivatives were assessed, with a particular focus on their 15-lipoxygenase inhibitory effects and anticancer properties against tumor cell lines (HCT-116 and LS-174T), as well as the non-tumor cell line HEK-293. Most derivatives showed enhanced cytotoxic activity compared to OA. This cytotoxic potential was further supported by molecular docking studies. These results highlight the critical role of natural compounds in driving innovation in treatment strategies and the potential of oleanolic acid derivatives as novel therapeutic options.

Key words: Oleanolic acid, hemi-synthesis, anticancer activity, docking studies.

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Box-Behnken Optimized Fe_2O_3@DCTA-Ag Nanocomposite Sensor for Lead Detection in Real Samples

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A novel Fe_2O_3@DCTA-Ag composite was synthesized for the first time and employed in the development of a highly sensitive and reliable electrochemical sensor for Pb^{2+} detection. The sensor's performance was systematically optimized using differential pulse voltammetry (DPV), combined with a Box-Behnken design (BBD) and response surface methodology (RSM), to assess the influence of key experimental parameters, including pH, contact time, drop volume, and drying time. The optimized sensor exhibited a wide linear detection range from 0.2 nM to 10 µM, with an impressively low detection limit of 0.2 nM. Notably, it demonstrated exceptional selectivity, effectively distinguishing Pb^{2+} from potential interfering ions, ensuring accurate and interference-free detection even in complex sample matrices.

Keywords: Box-Behnken design (BBD), response surface methodology (RSM), Portable electrochemical sensor, Lead ions.

Novel aryl Benzothiazole Derivatives: Potential Neuroprotective Agents Against Alzheimer's Disease, In Silico Study and ADMET Profiling

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Alzheimer's disease (AD) is a neurological illness characterized by increasing cognitive decline and memory loss. Therapeutic endeavors are still trying to identify novel agents in the etiology of AD. In this context, benzothiazoles and benzoxazoles rings have shown promising outcomes as neuroprotective agents in AD models [1,2].

In this present work, various heteroarenes bearing benzothiazole moieties were synthesized from 2-mercaptophenol and heteroaromatic aldehydes. Several modifications were applied on these synthesized compounds to give formylated derivatives, aryl-benzothiazole bromides, and arylbenzothiazole alkene. Then, a molecular docking study was performed on acetylcholinesterase [1] (AChE) and amyloid-beta [2] ($A\beta_{1\text{-}42}$), two key enzymes associated directly to AD progression. All the synthesized compounds were tested and docked into the two protein's active sites in term of evaluating their anti-Alzheimer potential. The results have shown that the AD inhibitory potential increase in which the formylated and the halogenated derivatives presented the excellent energy scores along with hydrogen interactions with the active site of the protein target. After that, the ADMET profile of the selected compounds was simulated through chemoinformatic tools in order to determine their physio-chemical, pharmacokinetic proprieties and toxicity to ensure their efficacy and safety profiles for clinical use.

Key words: Arylbenzothiazole, Alzheimer's disease, docking, ADMET.

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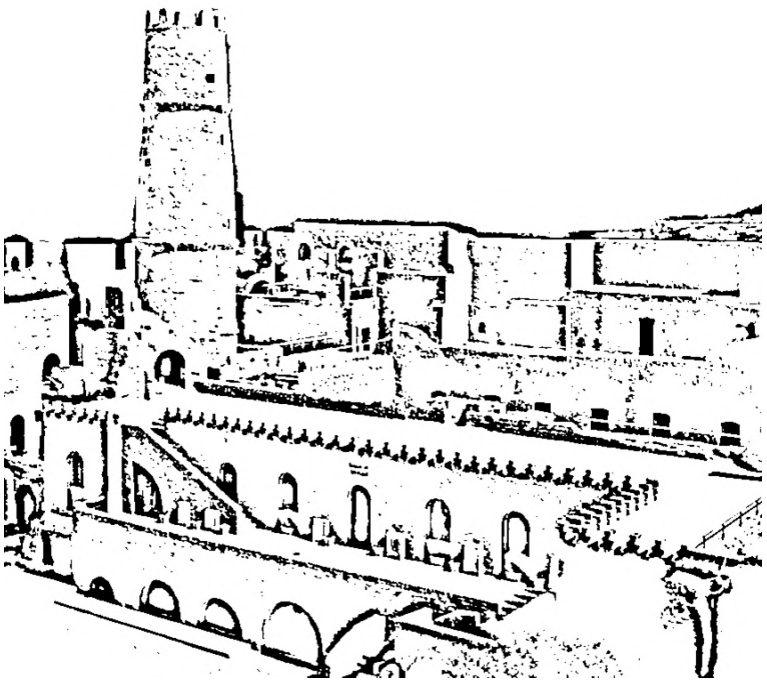

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