مؤتمر تونس الدولي الثاني والعشرون للكيمياء

TWENTY SECOND TUNISIA CHEMISTRY CONFERENCE

TCC 2024

Organized by the

Tunisian Chemical Society

15-18 December 2024

Laico Hotel
Yasmine Hammamet, Tunisia

Abstracts of Lectures and Communications
List of Participants

Tunisian Chemical Society - Short Program of TCC 2024

Sunday 15 December 2024	
14.00 - 17.00	**Welcoming participants, distribution of documents and check in**
17.00 - 17.15	**Opening Ceremony**
17.15 - 18.55	**Plenary Lecture 1 Michael KNORR** *UTINAM Institute, University of Franche-Comté, France*
19.00 - 19.30	**Registrations of participants (Resumption)**
19.30	***Dinner***
Monday 16 December 2024	
09.00 - 09.40	**Plenary Lecture 2 Nadine MILLOT** *Université de Bourgogne, Dijon, France*
09.45 - 10.25	**Plenary Lecture 3 Pascal MARCHAND** *Nantes Université, IICiMed, Nantes, France*
10.25-10.40	**Gathering for the group photo**
10.40 - 11.15	**Poster Session 1 (P 1 - P 42) Alphabetical Order**
11.30 – 13.00	**Oral Communications - Session 1 : OC 01 - OC 06**
13.00	***Lunch***
14.45 – 15.25	**Plenary Lecture 4 Julien BACHMANN** *Friedrich-Alexander University, Erlangen-Nürnberg, Germany*
15.30 – 16.30	**Oral Communications - Session 2 : OC 07 - OC 10**
16.30 – 17.15	**Coffee break + Poster Session 2 (P 43 - P 84) Alphabetical Order**
17.15 – 18.30	**Oral Communications - Session 3 : OC 11 - OC 15**
19.30	***Dinner***
Tuesday 17 December 2024	
09.00 – 09.40	**Plenary Lecture 5 Ismail ÖZDEMIR** *İnönü Üniversitesi, Malatya, Türkiye*
09.45 – 10.45	**Oral Communications - Session 4 : OC 16 - OC 19**
10.45 – 11.30	**Poster Session 3 (P 85 - P 126) Alphabetical Order**
11.30 – 12.15	**Oral Communications - Session 5 : OC 20 - OC 22**
13.00	***Lunch***
14.45 – 16.00	**Oral Communications - Session 6 : OC 23 - OC 27**
16.00 – 16.45	**Coffee break + Poster Session 4 (P 127 - P 175) Alphabetical Order**
17.00 – 19.00	**General Assembly of the Tunisian Chemical Society**
19.30	***Dinner***
21.00	**Election of the new National Bureau of the Tunisian Chemical Society**
Wednesday 18 December 2024 (morning)	
09.00 – 09.40	**Plenary Lecture 6 Tamer UĞUR** *Gazi University, Ankara, Türkiye*
09.45 – 11.30	**Oral Communications - Session 7 : OC 28 - OC 34**
11.45	**Closing Remarks and Poster Awards**
13.00	***Lunch, Check Out and Departure***

Foreword

Dear colleagues and participants,

It is with great pleasure that I welcome you all to this year's scientific event dedicated to the fascinating world of chemistry in the beautiful setting of Yasmine Hammamet, Tunisia. We are delighted that round 300 chemists from different fields have joined us to share the knowledge, insights and innovations that continue to shape our discipline.

I would like to express my sincere gratitude to our invited speakers, whose willingness to share their expertise and insights will undoubtedly enrich our discussions. Their contributions are invaluable, and we are delighted to have them with us.

Of course, my thanks also go to the various members of the Scientific and Organising Committees for their commendable and continuing efforts to ensure the success of this Conference.

And, of course, I must not forget my fellow chemists, professors, teachers and researchers from all the universities, colleges and institutes who have shown their strong support for TCC2024 either by exhibiting their work or by their presence. Some of our guests are from Algeria, Belgium, Democratic Republic of Congo, France, Germany, Libya, Nigeria, South Africa and Tükiye.

The Tunisian Chemistry Conference - TCC2024 - will feature 06 plenary lectures, 101 oral presentations and 173 poster presentations.

As we gather in this renowned tourist destination, I encourage each of you to take the opportunity to engage in meaningful conversations, share your ideas and network with fellow chemists. We have put together an exciting programme that I am sure will inspire and invigorate our community.

Let us make this conference an unforgettable experience of learning and collaboration.

Once again, welcome to TCC 2024 !

Pr. Mohamed Lotfi EFRIT
TCC 2024 Chairman
President of the Tunisian Chemical Society

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Imed LAAJIMI	*Tunisian Chemical Society*

TCC 2024 Program

	Sunday 15 December 2024
14.00 - 17.00	**Welcoming participants, distribution of documents and check in**
17.00 - 17.15	**Opening Ceremony**
17.15 - 18.55	**Lecture 1** **Michael KNORR** Chair : *Mohamed Lotfi Efrit* *UTINAM Institute, University of Franche-Comté, France* **Organometallic coordination chemistry of 2-azabutadienes: A versatile π-conjugated ligand system**
19.00 - 19.30	**Registrations of participants (Resumption)**
19.30	***Dinner***

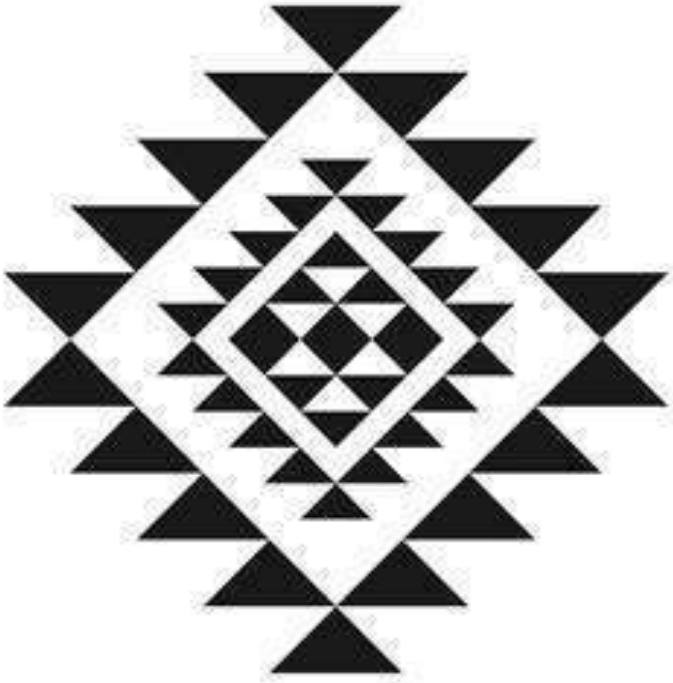
	Monday 16 December 2024 (Morning)					
09.00 - 09.40	**Lecture 2** **Nadine MILLOT** Chair : *Adel Megriche* *Université de Bourgogne, Dijon, France* **Engineered inorganic nanomaterials for biomedical applications**					
09.45 - 10.25	**Lecture 3** **Pascal MARCHAND** Chair : *Noureddine Allouche* *Nantes Université, IICiMed, Nantes, France* **Imidazo[1,2-a]pyrazine-based compounds targeting casein kinase 1 (CK1) for the development of novel anti-infective agents**					
10.25-10.40	**Gathering for the group photo**					
10.40 - 11.15	**Poster Session 1 (P 1 - P 42) Alphabetical Order** **Evaluators :** Taieb Ben Dhia, Fayrouz Djallouli, Djamel Berredjem & Abdelkader Bougarech					
	Oral Communications - Session 1					
	Room A - Chair: *Rym Abidi* ***Organic Chemistry***		***Room B -*** Chair: *Habib Boughzala* ***Inorganic Chemistry***		***Room C -*** Chair: *Mohamed Belhouchet* ***Nanotechnology & Materials Sciences***	
	Com.	*Communicating*	*Com.*	*Communicating*	*Com.*	*Communicating*
11.30 - 11.45	**OC-01A**	ARGOUBI Samar	**OC-01B**	ABASSI Khalil	**OC-01C**	AOULED ABDALLAH Marwa
11.45 - 12.00	**OC-02A**	AYACHI Abir	**OC-02B**	ADJIEUFACK Abel Idrice	**OC-02C**	BECHETNIA Mahran
12.00 - 12.15	**OC-03A**	AYOUNI Wissal	**OC-03B**	BAHLOUL Assala	**OC-03C**	BEN KACEM Imen
12.15 - 12.30	**OC-04A**	BEN MABROUK Nouha	**OC-04B**	CHELLEGUI Mohamed	**OC-04C**	BEN SALAH Manel
12.30 - 12.45	**OC-05A**	BOUSSANDEL Sirine	**OC-05B**	BEN SLIMEN Aya	**OC-05C**	ELLOUZE Nourchen
12.45 - 13.00	**OC-06A**	TALBI Imen	**OC-06B**	BELAROUI Lala Setti	**OC-06C**	GHARBI Chaima
13.00	***Lunch***					

	Monday 16 December 2024 (Afternoon)					
14.45 - 15.25	**Lecture 4** **Julien BACHMANN** Chair : *Latifa Bergaoui* *Friedrich-Alexander University, Erlangen-Nürnberg, Germany* **Atomic-layer approaches towards energy conversion and storage devices**					
	Oral Communications - Session 2					
	Room A - Chair: *Néjib Mekni* ***Organic Chemistry***		***Room B -*** Chair: Béchir Chaouachi ***Inorganic Chemistry***		***Room C -*** Chair: *Latifa Latrous* ***Nanotechnology & Materials Sciences***	
	Com.	*Communicating*	*Com.*	*Communicating*	*Com.*	*Communicating*
15.30 - 15.45	**OC-07A**	DEMS Lobna	**OC-07B**	BERRADJ Omar	**OC-07C**	REDOLFI Michaël
15.45 - 16.00	**OC-08A**	DHAOUADI Jihen	**OC-08B**	BOUHAJEB Oumayma	**OC-08C**	MHALLA Jalel
16.00 - 16.15	**OC-09A**	DRIDI Mohamed Ali	**OC-09B**	CHAKROUN CHERIF Yousra	**OC-09C**	MATTOUSSI Hedi
16.15 - 16.30	**OC-10A**	FADLI Khadidja	**OC-10B**	DHIFET Mondher		
16.30 - 17.15	**Coffee break + Poster Session 2 (P 43 - P 84) Alphabetical Order** **Evaluators:** Gaith Rigane, Haba Hamada, Yamina Berredjem & Boukhouite Amel					
	Oral Communications - Session 3					
	Room A - Chair: *Taïcir Ben Ayed* ***Organic Chemistry***		***Room B -*** Chair: Dalila *Hellali* ***Inorganic Chemistry***		***Room C -*** Chair: Kadri Younes ***Nanotechnology & Materials Sciences***	
	Com.	*Communicating*	*Com.*	*Communicating*	*Com.*	*Communicating*
17.15 - 17.30	**OC-11A**	GHANNOUCHI Ghada	**OC-11B**	GHORBALI Lokmen	**OC-11C**	RABAH Rawand
17.30 - 17.45	**OC-12A**	GHARBI Narjes	**OC-12B**	GHRAB Imen	**OC-12C**	SAIDANI Mohamed Ali
17.45 - 18.00	**OC-13A**	HAMDI Chayma	**OC-13B**	SAADAOUI Hadir	**OC-13C**	HAJJI Asma
18.00 - 18.15	**OC-14A**	FELKAOUI Nour El Houda	**OC-14B**	SALHI Sourour	**OC-14C**	BOUKLI-HACENE Leila
18.15 - 18.30	**OC-15A**	JEBRI Dorsaf	**OC-15B**	ABID Feriel	**OC-15C**	NGOY Bokolombe Pitchou
19.30	***Dinner***					

	Tuesday 17 December 2024 (Morning)					
09.00 - 09.40	**Lecture 5** **Ismail ÖZDEMIR** Chair : *Ridha Ben Salerm* *İnönü Üniversitesi, Malatya, Türkiye* **N-Heterocyclic carbene complexes and their catalytic activities**					
	Oral Communications - Session 4					
	Room A - Chair: *Rafaa Besbes* ***Organic Chemistry***		***Room B -*** Chair: *Mohamed Dammak* ***Catalyse and Polymer Science***		***Room C -*** Chair: *Zouhair Ksibi* ***Environment and Renewable Energy***	
	Com.	*Communicating*	*Com.*	*Communicating*	*Com.*	*Communicating*
09.45 - 10.00	**OC-16A**	KAOUACH Aicha	**OC-16B**	KHEDHIRI Lamia	**OC-16C**	BAFFOUN Arij
10.00 - 10.15	**OC-17A**	MASMOUDI Nihel	**OC-17B**	CHALLOUF Oumayma	**OC-17C**	BEN DLALA Sirine
10.15 - 10.30	**OC-18A**	MHASNI Olfa	**OC-18B**	GUERMASSI Youssef	**OC-18C**	BEN HAMOUDA Sofiane
10.30 - 10.45	**OC-19A**	MANCER Daya	**OC-19B**	FNENA Kamel	**OC-19C**	BOUABIDI Amen
10.45 - 11.30	**Poster Session 3 (P 85 - P 126) Alphabetical Order** **Evaluators :** Med Abderrahmane Sanhoury, Mohamed Hedi Attia, Abderrahmane Abdelli & Moufida Romdhani					
	Oral Communications - Session 5					
	Room A - Chair: *Souhaira Hbaieb* ***Organic Chemistry***		***Room B -*** Chair: Houcine Ammar ***Catalyse and Polymer Science***		***Room C -*** Chair: *Younes Moussaoui* ***Environment and Renewable Energy***	
	Com.	*Communicating*	*Com.*	*Communicating*	*Com.*	*Communicating*
11.30 - 11.45	**OC-20A**	AGOUILLAL Farid	**OC-20B**	RJILI Mohamed	**OC-20C**	HADDAD Larbi
11.45 - 12.00	**OC-21A**	AOUIDENE Mariem	**OC-21B**	MISSAOUI Kahla	**OC-21C**	MANNAI Faten
12.00 - 12.15	**OC-22A**	BENDAOUD Houcine	**OC-22B**	TOKOYI Vuyolwethu	**OC-22C**	WALENG Ngwako
13.00	***Lunch***					

	Tuesday 17 December 2024 (Afternoon)					
	Oral Communications - Session 6					
	Room A - Chair: Thouraya Barhoumi ***Organic Chemistry***		***Room B -*** Chair: *Sofiene Ben Hamouda* ***Water, Marine and Air Pollution***		***Room C -*** Chair: Hatem Majdoub ***Phytochemistry***	
	Com.	*Communicating*	*Com.*	*Communicating*	*Com.*	*Communicating*
14.45 - 15.00	**OC-23A**	OMRANI Assia	**OC-23B**	BEN ASSAKER Ibtissem	**OC-23C**	TOUBANE Amel
15.00 - 15.15	**OC-24A**	SALHI Sirine	**OC-24B**	BEN SALAH Sarra	**OC-24C**	KHITRI Walid
15.15 - 15.30	**OC-25A**	SAMB Issa	**OC-25B**	BOLTANE Khouloud	**OC-25C**	BOUCHNAK Houda
15.30 - 15.45	**OC-26A**	TRABELSI Yosra	**OC-26B**	DAGHFOUS Sinda	**OC-26C**	CHAKHARI Saida
15.45 - 16.00	**OC-27A**	TRIAA Nahla	**OC-27B**	TALEB Khadidja	**OC-27C**	KHEMIS Eya
16.00 - 16.45	**Coffee break + Poster Session 4 (P 127 - P 175) Alphabetical Order** **Evaluators :** Mongi *Ben Mosbah,* Salah Naghmouch, Slim Salhi & Omar Berradj					
17.00 - 19.00	**General Assembly of the Tunisian Chemical Society**					
19.30	***Dinner***					
21.00	***Election of the new National Bureau of the* Tunisian Chemical Society**					

	Wednesday 18 December 2024 (Morning)					
09.00 - 09.40	**Lecture 6** **Tamer UĞUR** Chair : *Nizar Bellakhal* *Gazi University, Ankara, Türkiye* **Rapid bacteria detection using functionalized nanoparticles: From microfluidic chip to paper strip**					
	Oral Communications - Session 7					
	Room A - Chair: *Saoussen Cherni* ***Environment and Renewable Energy***		***Room B -*** Chair: *Halim Hammi* ***Analytical Chemistry***		***Room C -*** Chair: *Malika Berredjem* ***Phytochemistry***	
	Com.	*Communicating*	*Com.*	*Communicating*	*Com.*	*Communicating*
09.45 - 10.00	**OC-28A**	MOUSSA Marwa	**OC-28B**	ASKRI Houyem	**OC-28C**	FAKHFAKH Jawhar
10.00 - 10.15	**OC-29A**	ZOUAGHI Mohamed Oussama	**OC-29B**	CHIBI Souaad	**OC-29C**	HABA Hamada
10.15 - 10.30	**OC-30A**	KETIR Wahiba	**OC-30B**	IBRI Aicha	**OC-30C**	IBN ELACHAOUIA Yosra
10.30 - 10.45	**OC-31A**	RABTI Amal	**OC-31B**	JEBALI Sami	**OC-31C**	EL HADI Djamel
10.45 - 11.00	**OC-32A**	SNOUSSI Aziza	**OC-32B**	KRAIEM Souhail	**OC-32C**	CHAHBANI Amna
11.00 - 11.15	**OC-33A**	NYABA Luthando	**OC-33B**	SMATI Houda	**OC-33C**	REGUIGUI Amira
11.15 - 11.30	**OC-34A**	MZOUGHI Zeineb	**OC-34B**	DHAOUADI Fatma	**OC-34C**	BOUAZIZI Ikram
11.45	**Closing Remarks and Best Posters Awards**					
13.00	***Lunch, Check Out and Departure***					



SPEAKERS' ABSTRACTS

Michael KNORR

Michael Knorr was born in 1959 in Würzburg, Germany. Graduate of the Julius-Maximilian University of Würzburg in 1985, his Master's degree was followed by a PhD (Dr. rer. nat.) in chemistry (1988) under the supervision of Prof. Ulrich Schubert on the synthesis and reactivity of organometallic silyl and stannyl complexes of iron and manganese. As post-doctoral fellow and associate researcher, he spent the next five years in France (with Pierre Braunstein, *Laboratoire de Chimie de Coordination*) at the Université Louis Pasteur (Strasbourg) and spent also some months in the research group of Prof. R. J. P. Corriu at the Université de Montpellier. In 1994, he joined the *Institute of Inorganic Chemistry* of Prof. Michael Veith at the University of the Saarland (Saarbrücken, Germany) to complete his habilitation thesis on the activation of unsaturated organic molecules by heterobimetallic transition metal complexes. After appointment to assistant professor (Privat-Dozent) in 1997, he moved back to Strasbourg to collaborate with P. Braunstein's laboratory and the *Institut Charles Sadron*. In 1999, he was appointed associate professor (PR 2) at the Université de Franche-Comté (Besançon, France) and was vice-director of the *Laboratoire de Chime et Électrochimie Moléculaire*. From 2000 - 2013 he led, first as associate professor (PR 2), then as full professor (PR 1), the research group *Matériaux et Surfaces Structurés* working on organic synthesis, coordination chemistry, molecular materials and the deposition of nano(micro) particles/thin films on surfaces/interfaces. From 2007-2011, he was also vice-director of the Institute *UTINAM - UMR CNRS 6213*. In 2014, he was promoted "Professeur Classe Exceptionnelle" (PR CE).

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Organometallic Coordination Chemistry of 2-Azabutadienes: A Versatile π-Conjugated Ligand System

Michael Knorr

Institut UTINAM - UMR CNRS 6213, Université de Franche-Comté, 25030 Besançon, France
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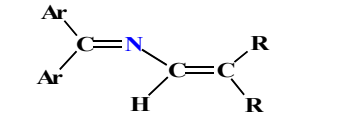
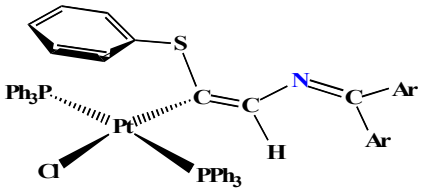
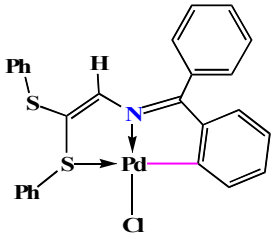
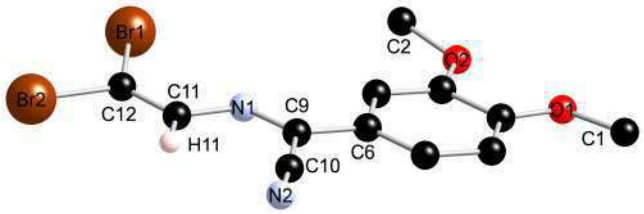
Due to the eminent role of Pd and Pt in organometallic synthesis and catalysis, formation of Pd- or Pt-carbon bonds with functional organic ligand systems is of great interest. We have synthesized a series of 1,1-diaryl-2-azabuta-1,3-dienes [Ar_2C=N-C(H) =CR_2] (R = Cl, SR, OR, NR_2) and related cyano-functionalized 2-azabutadienes [Ar(N≡C) C=N-C(H)=CX_2] (X = Cl, Br) and investigated their complexation onto various transition metal centres. Due to the presence of (*i*) two conjugated double bounds, (*ii*) an imine-type nitrogen atom and a thioether group as potential donors and (*iii*) reactive vinyl-halide bonds, these polydentate 2-azadienes constitute promising ligand systems for the construction of organometallic transition metal complexes (Mn, Re, Ru, Cu, Ag, Hg, Cd).



(Ar = Ph, C_6H_4Cl, C_6H_4Me, C_6H_4OMe)
(R = Cl, SR, OPh)







Depending on the reaction conditions, oxidative addition on [$Pd(PPh_3)_4$] affords s-alkenyl complexes or unusual bimetallic m-vinylidene complexes, possessing two different coordination spheres around Pd. The preparation and reactivity of a series of luminescent *C,N,S*-cyclometallated complexes ligated by [Ar_2C=N-C(H)=$C(SR)_2$] as pincer ligand has also been investigated. [1-6]

References

1) M. Knorr, G. Schmitt, M. M. Kubicki, E. Vigier, *Eur. J. Inorg. Chem.* **2003**, 514.
2) S. Jacquot, A. Kathyr, G. Schmitt, M. Knorr, M. M. Kubicki, O. Blacque, *Inorg. Chem. Commun.* **2006**, *8*, 610.
3) Jacquot-Rousseau, G. Schmitt, A. Khatyr, M. Knorr , M. M. Kubicki , E. Vigier, O. Blacque, *Eur. J. Org. Chem.* **2006**, 1555.
4) R. Kinghat, G. Schmitt, K. Ciamala, A. Khatyr, M. Knorr, S. Jacquot, Y. Rousselin, M. M. Kubicki, *Comptes Rendus Chimie* **2016**, *19*, 17516.
5) A. Schlachter, R. Kinghat, F. Guyon, P. D. Harvey, M. Knorr *et al.*, Dalton Trans. **2021**, *50,* 2945.
6) R. Kinghat, A. Khatyr, M. Knorr, C. Strohmann, M.M. Kubicki, *Chemistry* **2024**, *6*, 62-80.

Nadine MILLOT

Laboratoire Interdisciplinaire Carnot de Bourgogne, UMR 6303 CNRS/Université de Bourgogne, Nanosciences Department, Dijon, France

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Prof. Dr. Nadine Millot is Full Professor at the University of Bourgogne, France. After being deputy director of the ICB laboratory (about 380 members) and founder of the "Bio-Hybrid Nanoparticles & Nanostructures, BH2N" group, she is now vice-president of the University of Bourgogne, in charge of Research. She is member of the steering committee of the French national competency cluster in Nanoscience of CNRS, C'Nano France.

She has extensive expertise in the field of synthesis and characterization of nanoparticles and nanohybrids, particularly gold NPs for photothermal and biosensing applications, SPIONs as bimodal contrast agents, and titanate nanotubes developed for the nanovectorisation of active molecules.

She has published 86 papers, three book chapters and one patent. She has given more than 20 invited oral presentations in the last five years and has supervised 19 PhD students (three on going). She is author of a textbook on crystallography (Ed. Lavoisier, France) and she is an expert for several French and European agencies.

Engineered inorganic nanomaterials for biomedical applications

Julien Boudon and Nadine Millot

ICB laboratory, UMR 6303 CNRS/Université de Bourgogne, Dijon, France
E-mail: nadine.millot@u-bourgogne.fr

This communication addresses some new inputs in the field of theranostics by using engineered inorganic nanoparticles (NPs).

Multimodal imaging magnetite (Fe_3O_4) nanoparticles, used as contrast agent for MRI (Magnetic Resonance Imaging) / PET (Positron Emission Tomography) double imaging have been developed is our laboratory. In a first step and by means of a continuous hydrothermal process, surface-modified NPs were prepared. The second step consists in developing stable complexes with radionuclides on the surface-modified NPs with a chelating agent. *In vitro* and *in vivo* results were realized. These nanohybrids are promising contrast agents for MRI/ PET double imaging.[1]

We also demonstrated that titanate nanotubes (TiONts) elaborated by hydrothermal synthesis and developed as stable suspensions by surface chemistry engineering, are capable to increase the ionizing effect of radiation therapy in the case of glioblastoma and can also be used as novel transfection agents for cardiomyocytes. Furthermore, we have demonstrated that TiONts-docetaxel (DTX) nanohybrids are versatile nanocarriers to limit the systemic toxicity of taxanes and to improve the selectivity of radiotherapy (RT).[2] Our strategy is based on the intraprostatic injection of the TiONts-DTX nanohybrids in combination with RT. This is achieved by taking advantage of the TiONts morphology as well as their radiosensitization effect and by associating them with docetaxel molecules, also recognized for their potential to radiosensitization. We also grafted the surface of TiONts with AuNPs, for a resulting combined radiosensitizing effect.[3] Mice receiving nanohybrid-RT exhibited a significant tumor growth delay compared to mice receiving free DTX-RT.

Our last results concern hybrid gold nanorods (AuNRs). They were synthetized for immunotherapy, using biomolecules targeting death receptors of the tumor necrosis superfamily, coupled with hyperthermia. Heterobifunctional PEG were used for their functionalization. Different coupling strategies, including EDC/NHS, Schiff base formation after antibody oxidation and click chemistry, were then assessed to graft biomolecules to the AuNRs, and compare final immunotherapy efficiency.[4]

One of the strengths of our studies, is the exhaustive characterizations systematically realized to investigate: the aggregation state and colloidal stability of NPs (TEM, DLS, zeta potential measurements, UV-vis measurements as a function of time) and the surface chemistry modification (zeta potential measurements as a function of pH, XPS, IR and Raman spectroscopies).

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I - CAREER AND EDUCATION

Medicinal Chemistry department - Team UR 1155 IICiMed (Targets and Drugs for Infectious Diseases and Immunity) - School of Pharmacy - University of Nantes
January 2017: Deputy director of IICiMed research group and Head of Medicinal Chemistry department
September 2013: Professor of Organic Chemistry (1st class **September 2016** & exceptional class 1 **September 2022**)
June 2007: Habilitation in Medicinal Chemistry - Design, synthesis and biological evaluation of azaheterocyclic compounds
September 2001: Assistant Professor in Organic Chemistry
January 2000-August 2001: Lecturer in Organic Chemistry
November 1999: PhD Thesis in Medicinal Chemistry - Synthesis and biological evaluation of indole derivatives as immunosuppressive and anti-cancer agents **June 1996**: Master's degree in Pharmacochemistry

II - TEACHING - School of Pharmacy - Nantes

Organic Chemistry, Medicinal Chemistry, Spectroscopy (NMR, MS, IR) to Pharmacy students (Pharm. D.) from the first to the fifth year of the cursus and to Master students

III - ADMINISTRATIVE RESPONSIBILITIES

Prof Pascal Marchand held several administrative positions

IV - RESEARCH SUPERVISION

Research interests: Design, synthesis and biological evaluation of heterocyclic compounds for therapeutic purposes (mycology, parasitology, bacteriology and cancer). Inhibitors of kinase signaling pathways. ADMET properties of molecules of biological interest.

V - PUBLICATIONS, PATENTS and SCIENTIFIC PRODUCTION (see attached list)

- 71 international publications (h-index: 21).
- 4 international patents.
- 72 posters.
- 30 conferences as invited speaker & 23 oral communications.

VI - MISCELLANEOUS ACTIVITIES AND RESPONSIBILITIES

Some headlines of the activities and responsibilities:

1 - International research collaborations
- CAPES-COFECUB 2015/2018 & 2023/2026 Programme - Brazil
- Collaboration University of Toronto since 2021 - Canada
- Collaboration Ege University1, Izmir & Izmir Katip Celebi University2 since 2023 - Turkey
- Collaboration Assane Seck University of Ziguinchor 2021-2025 - Senegal
- Collaboration University of Sfax since 2021 - Tunisia

2 - National research networks
3- European research networks
4- Industrial research collaborations
5- Scientific societies
6- Expert reports
7- Organisation of congress

Web: https://pharmacie.univ-nantes.fr/pascal-marchand-1
https://orcid.org/0000-0001-7773-8642

Imidazo[1,2-a]pyrazine-based compounds targeting casein kinase 1 (CK1) for the development of novel anti-infective agents

Pascal MARCHAND

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According to a recent WHO report[1], leishmaniasis affects nearly 12 million people, with 350 million others at risk, and is responsible for nearly 40,000 deaths per year. In 2012, mainly due to global warming, visceral leishmaniasis (VL) was declared as a new emerging disease in Europe. Today, there is no effective vaccine, and the limited treatments are unfortunately too toxic and costly. In this context, there is a real emergency to develop new paradigms for antileishmanial therapy, which also limit the devastating impact of parasite resistance. While most of the current drugs as well as those in development target the parasite biology, we propose to target the exoproteome of *Leishmania*, and particularly excreted signalling kinases, to inhibit host-parasite interactions, which will restore the host cell ability to fight the parasite and limit the risk of resistance.
To this end, we selected and validated *Leishmania* casein Kinase I paralog 2 (L-CK1.2) as a drug target[2,3]. L-CK1.2 is essential for intracellular parasite survival and released in macrophages via extracellular vesicles[2]. Moreover, several evidence suggest that L-CK1.2 has been evolutionary selected to interact with and phosphorylate host proteins subverting the biological and immune functions of the macrophage[2]. Because of its dual role in the parasite and the host cell, targeting L-CK1.2 would kill the parasite while limiting the emergence of parasite resistance.
We previously reported the discovery of **CTN1122**[4,5], an imidazo[1,2-*a*]pyrazine derivative with promising antileishmanial properties that targets L-CK1.2 (Figure 1).

CTN1122

IC_{50} (amastigotes *L. major*) = 0.80 µM (CL)
IC_{50} (amastigotes *L. donovani*) = 2.74 µM (VL)
SI (RAW cells/amastigotes *L. major*) = 52.5
SI (RAW cells/amastigotes *L. donovani*) = 15.3
IC_{50} (*Lm*CK1) = 0.72 µM
SI_{CK1} = 1.3

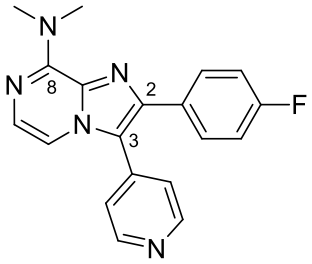

Figure 1. The hit compound **CTN1122**.

When tested *in vivo*, it reduces the parasite load in the liver and spleen of mice infected with *L. donovani*, as well as in the lesion of mice infected with *L. major* with a significant decrease in the size of the lesion.
Here, we present the TEXLEISH consortium, which, through a research program dedicated to this chemical series and its target, focuses on three main objectives (1) the optimization of this hit compound by generating new pharmacomodulations of **CTN1122,** (2) the identification of potential off-target effects to limit toxicity and side-effects by using state-of-the-art deconvolution methods and (3) the better understanding of the role of L-CK1.2 in host-pathogen interactions by using system-levels analyses. The TEXLEISH consortium will provide the first evidence that targeting the exoproteome of parasite for drug treatment is an innovative way to discover potent new drugs against leishmaniasis limiting the risk of selecting for drug resistant parasites.

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Academic Curriculum

since 1/2020	**ATLANT 3D Nanosystems** (Kongens Lyngby, Denmark) Co-founder and Director
since 7/2017	**University of Erlangen-Nürnberg** (Erlangen, D), Chemistry Department Full Professor (W3) and Chair, Chemistry of Thin Film Materials
2017-2/2022	**Saint Petersburg State University** (Saint Petersburg, RUS), Institute of Chemistry, Chair of Laser Chemistry and Laser Materials Science Secondary appointment: Full Professor
2012-2017	**University of Erlangen-Nürnberg** (Erlangen, D), Chemistry Department Associate Professor (W2) of Inorganic Chemistry
2009-2012	**University of Hamburg** (Hamburg, D), Physics Department Junior Professor (W1)
2007-2009	**University of Hamburg**, Physics Department Senior scientist with Prof. K. Nielsch
2006-2007	**Max Planck Institute of Microstructure Physics** (Halle, D) Alexander von Humboldt Research Fellow with Prof. U. Gösele
2001-2006	**Massachusetts Institute of Technology** (Cambridge, USA), Chemistry Dept. Ph. D. student with Prof. D. G. Nocera Doctor of Philosophy in Inorganic Chemistry, 2006
1997-2001	**University of Lausanne** (Lausanne, CH), Chemistry Department Undergraduate student — Diploma thesis with Prof. C. Floriani *Diplôme de chimiste*, 2001

Main Scientific Achievements and Awards

2004 - 2024	165 peer-reviewed articles (WoS h-index 34)
2008 - 2022	> 12 M€ of competitive third-party funding secured, including: • ERC Consolidator Grant (2015) and ERC Proof of Concept (2022) • coordination of one national and one EU consortium
2020	**Otto Mønsted Guest Professor**, Danish Technical University
2006	**Humboldt Research Fellowship**, Alexander von Humboldt Foundation
2001	**Presidential Fellowship**, MIT
2000	**Louis Pelet Prize**, University of Lausanne
1999	**Faculty Prize**, University of Lausanne

Atomic-layer approaches towards energy conversion and storage devices

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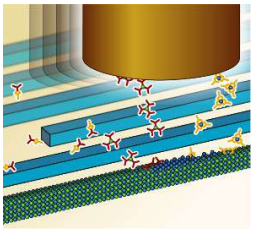
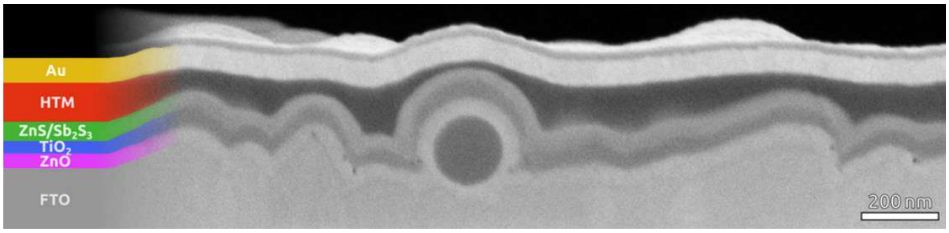
The conversion of energy between its light, electrical and chemical forms occurs at interfaces when charge carriers traverse from one phase to another. Therefore, in any energy conversion device the control of both the chemical identity of the interface and its geometry are paramount to optimizing the performance parameters. Atomic layer deposition (ALD) serves as an ideal tool for this, as it exploits molecular reactivity on surfaces to add individual layers of functional solids. In photovoltaics, it has enabled us to minimize the absorber layer thickness to 30 nm and design interface layers 1 nm thick only. One limitation of ALD is the range of materials accessible by it. We have circumvented it by depositing from dissolved precursors. If reagents do not need to be volatile, a broader variety of materials become possible in atomic-layer processing mode, including polymers, metal-organic frameworks and ionic semiconductors such as halide perovskites. Another limitation of ALD is related to its inherently slow nature and the large number of samples required for the prototyping of novel solar cell types. Atomic-layer additive manufacturing (ALAM) has been developed to enable rapid prototyping of microdevices by combining the principles of 3D printing and ALD. We have demonstrated that the self-limiting principles inherent to the surface chemistry of ALD result in high material quality, sharp line edges and extensive design flexibility in ALAM. This novel method delivers direct-patterning deposition, eliminates the need for lithographic processing and simplifies the process design for small-scale, decentralized prototyping and manufacturing of microdevices. Established ALD chemistry can be advantageously transferred to ALAM, whereas the user profits of lower material consumption, faster deposition and increased safety. Our first functional devices include sensors of temperature, corrosion and heavy metal pollutants as well as a simple solar cell.





İsmail ÖZDEMİR

Prof. Dr. İsmail Özdemir
Education: 1995 Inönü University, Ph.D.

Awards: 2005 TUBİTAK Young Scientist Award

Experiences:

1988-1997	Instructor at Inönü University, Faculty of Siences and Arts Department of Chemistry
1997	Lecturer at Inönü University, Malatya
1994	Visiting Researcer at University of Sussex, England for a period of five months.
1996	Collobarate research at University of Rennes, France for three months.
1999	Visiting researcher at University of Rennes, France for three months.
2000	Collobarate research at University of Rennes, France for three weeks.
2001	Visiting researcher at University of Rennes, France for one month.
2002-2015	Collobarate research at University of Rennes, France..
2008-2009	Director of Institute of Science and Techonology
2009-2016	Vice President of İnönü University
2013-2016	Dean of Faculty of Pharmacy
2007-2013	Turkish Scientific Research Council (TÜBİTAK), Member of BİDEB Committee
2017	Turkish Scientific Research Council (TÜBİTAK), Member of ARDEB Committee
2021	Director of Drug Apllication and Research Center

Scientific Interest

- Synthetic and spectroscopic studies in coordinating, metallo-organic and organometallic chemistry.
- Carbene complexes derived from electron-rich olefins.
- Catalytic properties of carbene complexes.
- Homogeneous Catalysis by Transition Metal Complexes
- Cross coupling reaction by Pd-NHC's
- C-H bond activation by N-heterocyclic carbene
- Catalysis in ionic liquids
- Transfer hydrogenation
- Biological activity of Metal-NHC complexes

Scientific activities :

- 360 publications, 3 book chapter;
- h-index: 46 (Google Scholar)

https://scholar.google.com/citations?user=M94IZpkAAAAJ&hl=tr&oi=ao

N-Heterocyclic Carbene Complexes and Their Catalytic Activities

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N-Heterocyclic carbenes, which are singlet carbenes integrated into a nitrogen-containing heterocycle, were initially studied by Wanzlick in the early 1960s [1]. Shortly thereafter, the first application of NHC as a ligand for metal complexes was independently described by Wanzlick [2] and Öfele [3] in 1968. Nevertheless, the field of N-heterocyclic carbenes as ligands in transition metal chemistry remained dormant until 1991 when a report on the extraordinary stability, isolation and storability of crystalline NHC by Arduengo et al. ignited a rapidly growing research field [4]. They have equivalent or superior donating characteristics, as well as generally stronger thermal stability and enhanced stabilizing effects than most commonly used phosphines [5].

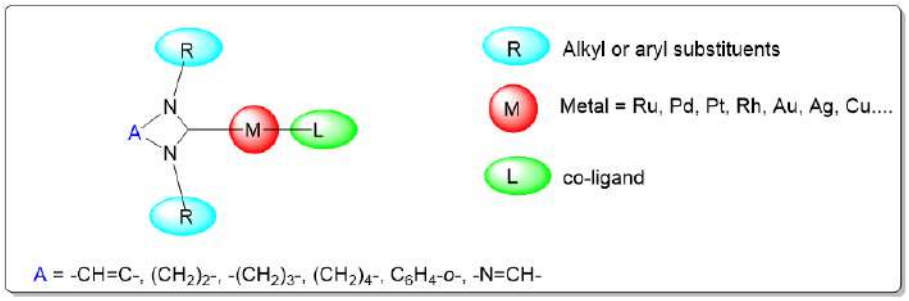

Figure 1. *N*-Heterocyclic carbene complexes.

N-Heterocyclic carbenes has been applied not only from a purely synthetic organometallic point of view but also to the use of NHC-transition metal complexes as catalyst, or catalyst precursor, for several transformations. NHC-modified organometallic systems in ruthenium-mediated olefin metathesis, C-H bond activation, furan formation, transfer hydrogenation, hydrogenation, or C-C coupling reactions using carbene complexes of palladium are now well recognized [6].

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Uğur Tamer is a Professor of Pharmacy Faculty at Gazi University in Turkey. He received Ph.D. degree in 2003 at Hacettepe University Department of Analytical chemistry. Under the mentorship of Professor Dr. Kadir Pekmez and Professor Dr. Attila Yıldız, his research focused on modified electrodes and conducting polymers. He was involved in Prof. Dr. Harry Mark's electroanalytical research group as a visiting scholar in the department of chemistry at Cincinnati University in 2002 and he had worked a post-doctoral researcher, working with Professor Curtis Shannon, in the Department of Chemistry and Biochemistry at Auburn University in 2005. He was involved in Raman research group as a visiting Professor, at University of Maine, Lemans, France. His research focuses on modified electrodes, electrochemical controlled micro-extraction, enantiomer separations, magnetic and anisotropic nanoparticles, surface modification, Raman spectroscopy and surface enhanced Raman scattering. His research group constructed a paper based microfluidic surface enhanced Raman spectroscopy (SERS) device that uses nanoparticle-embedded based microfluidic system. A microfluidic chip was also constructed using the surface micromachining technique for the determination of bacteria. He has published 160 peer-reviewed research papers and 6 book chapters.

Rapid bacteria detection using functionalized nanoparticles: From microfluidic chip to paper strip

Uğur Tamer

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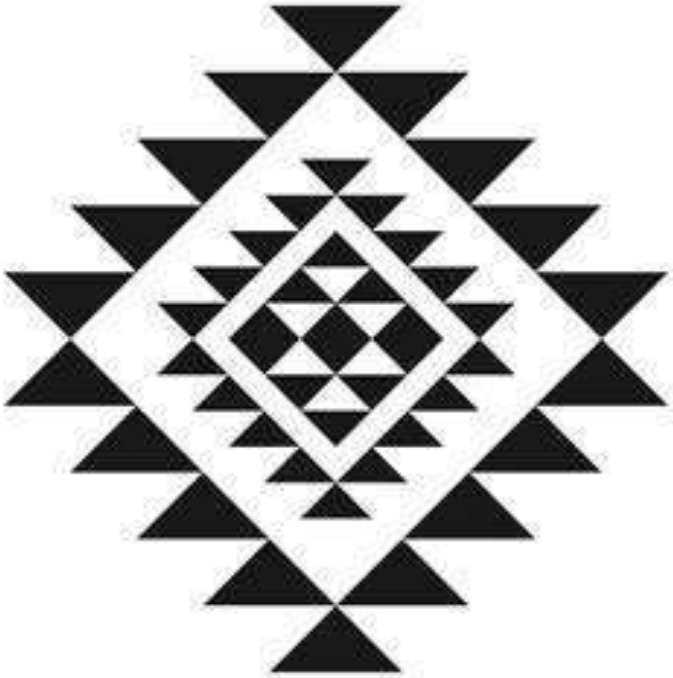
The rapid detection of bacteria has been one of the important issues due to serious and even fatal medical conditions result from bacterial infection or contamination. Golden standard method of indicating the presence of bacteria is culture assay, but the culture assay require at least a period of 24 hours or more. It is very difficult to detect these bacteria in a short time which makes this subject very important all over the world. For quantitative analysis, highly sensitive and accurate detection methods are needed to reach a lower limit of detection limits . PCR, ELISA or MALDI measurements have also been used for pathogen detection, however, the construction of sensitive and reproducible substrate is still a challenge. Especially, the paper microfluidics such as lateral flow immunoassay and microchip-based measurement are important approach and will be powerful alternatives to the expensive conventional techniques. The present study aims to find out the most proper bioactive chip preparation method to develop for the quantitative determination of bacteria. This presentation is mainly devoted to the tag based immunoassay technique and PCR analysis using microfluidic chip. In this work, we have synthesized magnetic nanoparticles which are suitable for immunomagnetic separation of microorganism. After immunomagnetic separation of bacteria from matrix, labeled nanoparticles were immobilized to the target bacteria on the surface of chip surface. Then, fluorescence or SERS measurement was performed. Magnetic nanoparticles were also used high-throughput DNA extraction method for pathogen detection in microfluidic chip. For this purpose, first time polymer brush coated monodisperse magnetic nanoparticles were prepared with interface-mediated RAFT polymerization to be used in DNA extraction process. After synthesizing magnetic nanoparticles, silica shell was coated on the magnetic nanoparticle core. Polymer brushes was immobilized on the amine functionalized silica layer using RAFT agent. The developed particle provided both the rapid extraction of DNA and high-yield DNA recovery without requiring extended incubation and elution time. The capture and lysis of bacteria in the blood sample were performed in the first part of the chip and this approach is quite new in this area. The design, preparation and surface modification of assay platform could be useable for the detection of target bacteria from complex matrices. The optimization strategies and the analytical performance of the chip -based assays will be presented.

Acknowledgements: Health Institutes of Türkiye (TUSEB) project number: 33033



LIST OF ORAL COMMUNICATIONS

Communicatings' Names	Ref
K. Abassi, A. Mezni, T. Ben Chaabane, A. Ben Ali And M. Bellardita *FSB - Bizerte* Enhanced photocatalytic performance of P25@ZnO composites for organic dye degradation under UV light	**OC01B**
F. Abid, P. S.S. Lacerda, A. J.D. Silvestre, A. F. Sousa *FSS - Sfax* Ring opening polymerization of biobased (macro)cyclic oligofuranoates for the development of greener polyesters	**OC15B**
A.I. Adjieufack, V. Liégeois, B. Champagne *University of Namur, Belgium* Deciphering the mechanism of the addition reaction between an intramolecular frustrated Lewis Pair and phenylisocyanate within bonding evolution theory (BET)	**OC02B**
F. Agouillal, D. Mancer, Y.I. Ait Hammou, W. Loudjani, N. Nasrallah *Houari Boumediene University, Algiers, Algeria* Antimicrobial activities of triterpenoids, ricinine and quercetin derivatives from methanolic extract of Ricinus communis and their molecular docking correlation	**OC20A**
M. Aouidene, H. Ben Jannet *FSM - Monastir* Vectorization of a sesquiterpene acid isolated from Inula viscosa leaves towards the semi-synthesis of new bioactive targets	**OC21A**
M. Aouled Abdallah, I. Abidli, O.M. Lemine, M. Bououdina, M. Zougagh, L. Latrous, A. Megriche *FST - Tunis* Green pomegranate peel and potato peel starch-derived magnetic nanocomposite as efficient sorbent of ascorbic acid extracted from fruit juices	**OC01C**
S. Argoubi, M.A.K. Sanhoury, E. Manoury, I. Chehidi *FST - Tunis* Solution behavior of tin(IV) chloride complexes with fluorinated phosphoramidates: A variable temperature NMR study	**OC01A**
H. Askri, B. Rzig, K. Djebeli, M. Maamar, N. Bellakhal *INSAT - Tunis* Modelling and optimization of chlorpheniramine treatment using anodic oxidation process on boron doped diamond electrode	**OC28B**
A. Ayachi, R. Besbes, M. Abarbri *FST - Tunis* Accès rapide et simple à de nouvelles 3-Alkyl-5-Alkylamino-7-Iodoisocoumarines et à leur fonctionnalisation via des réactions catalysées par le palladium.	**OC02A**
W. Ayouni, H. Riguene, A. Yahyaoui, M. Dhiabi, S. Dali, H. Ammar, S. Choura, M. Chamkha, R. Ben Salem, G. Rigane *FSS - Sfax* Microwave-assisted extraction of phenolic compounds from Hylocereus undatus fruit cultivated in Tunisia: Optimization RSM-CCD and HPLC-DAD identification.	**OC03A**
A. Baffoun, M. Ben Salah, N. Jaoued, T. Soltani, J. Thibonnet, S. Hbaieb *FST - Tunis* Synthesis and Characterization of Novel Calamitic Liquid Crystalline Compounds	**OC16C**

Communicatings' Names	Ref
A. Bahloul, M. Messaad, S. Salhi, C. Delaite, T. Dammak, M. Abdelhedi *FSS - Sfax* Crystal structure, DFT calculations, vibrational characterization, and Hirshfeld surface analysis of a novel zero-dimensional metal-halide hybrid $(C6H7ClN)_3 \cdot [SbCl_5] \cdot Cl$ exhibiting exceptional green emission	**OC03B**
M. Bechetnia, O. Hajlaoui, J. Boudon, C. Mirjolet, N. Millot, L. Bergaoui *INSAT - Tunis* Study of the effect of ultrasonication on the morphology and reactivity of MnO_2 layered structure	**OC02C**
L.S. Belaroui, L. Dali Youcef, A. Lopez Galindo *University of Oran, Algeria* Synthesis and characterization of zeolite LTA by hydrothermal transformation of a natural Algerian palygorskite	**OC06B**
I. Ben Assaker, S. Hamrouni, S. Aoun, M. Ridolfi *CRTEn - Borj Cédria* Atmosphere-controlled plasma-assisted surface engineering of $NiMoO_4$ for enhanced supercapacitor electrode performance	**OC23B**
S. Ben Dlala, M. Haj Romdhane, Z. Mzoughi, D. Le Cerf, H. Korri-Youssoufi, H. Majdoub *FSM - Monastir* Extraction and characterization of polysaccharides from Tunisian Broad Bean Pods: Physicochemical properties, rheological behavior and cytotoxicity	**OC17C**
S. Ben Hamouda, A. Msahel, N. Chaarana, Alberto Figoli *CRMN - Sousse* Study of azeotropic separation of MeOH/MTBE mixture by pervaporation by means of chitosan membranes elaborated by Deep Eutectic Solvents	**OC18C**
I. Ben Kacem, W. Mabrouk, K. Charradi, S. M.A.S. Keshk, N. Bellakhal *INSAT - Tunis* Improving proton exchange membrane performance: Incorporating layered double hydroxides in composite membranes of low-sulfonated polyether sulfone octyl sulfonamide	**OC03C**
N. Ben Mabrouk, C. Youssef, F. Saad, K. Hamden, H.Amed Ben Ammar *FSM - Monastir* Design and synthesis of a novel N-substituted pyrrole derivatives as alpha-glucosidase inhibitors: In vitro and in silico studies	**OC04A**
M. Ben Salah, T. Soltani, L. Saadaoui, N. Ben Hamadi, A. Guesmid, Z. Bouberka, A. Barrera, U. Maschke *FST - Tunis* Dielectric and electrical properties of liquid crystals doped with ferroelectric nanoparticles	**OC04C**
S. Ben Salah, M. Missaoui, A. Attia, G. Lesage, M. Heran, R. Ben Amar *FSS - Sfax* Treatment of real textile effluent containing indigo blue dye by hybrid system combining adsorption and membrane processes	**OC24B**
A. Ben Slimen, H. Najjar, A. Megriche *FST - Tunis* Effect of synthesis method on the physical and photocatalytic properties of Co_3O_4	**OC05B**

Communicatings' Names	Ref
H. Bendaoud, D. Salem, H. Saada, F. Mokdad, M. Romdhane *ENIG - Gabès* Study of extraction yield and corrosion inhibitory power of hydrolate from Euclyptus Diversifolia essential oil hydrodistillation : Optimization of experimental conditions using Surface Response Methodology	**OC22A**
O. Berradj, H. Bougherra *Mouloud Mammeri University, Tizi-Ouzou, Algeria* Synthesis, experimental characterization, and antioxidant evaluation of new ternary Cu(II) complexes of dimethylglyoxime and some amino-acids	**OC07B**
K. Boltane, A. Mnif *FST - Tunis* Removal of levofloxacin from aqueous solutions and economic assessment through electrocoagulation and bioadsorption	**OC25B**
A. Bouabidi, K. Ben Yahia, C. Ben Romdhane, S. Sghaeir, M. Romdhane, E. Saadaoui *FSG - Gabès* Nerium oleander L. in southern Tunisia: Genetic diversity, insecticidal and herbicidal activities of its aqueous extracts	**OC19C**
I. Bouazizi, H. Majdoub, E. Ben Salem *IPEIM - Monastir* Elaboration of an hybrid material based on doped hydroxyapatite and modified chitosan for medical application	**OC34C**
H. Bouchnak, A. Hamdi, J. Kraiem *Faculty of Pharmacy - Monastir* Synthesis of 3-aminohydantoin via condensation of hydrazines with isocyanates derived from α-aminoesters and preliminary study of their anti-inflammatory activity	**OC25C**
O. Bouhajeb, R. Hammami, B. Ünlü, M. Özacar, A. Megriche *FST - Tunis* Investigation of antibacterial activity of $MAPbCl_3$ synthesized with simple and modified ultrasound assisted process	**OC08B**
L. Boukli-Hacene, H. Mokri, M. Saidi *University of Tlemcen, Algeria* Synthesis and characterization of Zr based metal organic frameworks for enhancing the removal of typical organic dyes.	**OC14C**
S. Boussandel, W. Erb, F. Mongin, A. Samarat *FSB – Bizerte* Nouvelles mono- et diphosphines ferrocéniques chirales énantiopures	**OC05A**
A. Chahbani, N. Fakhfakh, H. Elhatmi, N. Zouari *ISBAM - Médenine, Gabès* Comparison between thermal treatment and microwave drying of garlic *(Allium sativum L.)* leaves: Kinetics modeling and changes in phenolic compounds profile	**OC32C**
S. Chakhari, F. Chabchoub, L. Ismaili *FSS - Sfax* New quinazoline hybrids as amyloid-β aggregation inhibitors with dual cholinesterase inhibition and antioxidant properties for Alzheimer's disease	**OC26C**
Y. Chakroun Cherif, W. Cherif, L. Ktari *FSS - Sfax* Temperature and pressure effects on phase transitions and structural stability in $CsPb_2Br_5$ and $CsPb_2Br_4I$ perovskite-derived halides	**OC09B**

Communicatings' Names	Ref
O. Challouf, S. Zaidi, A. Bougarech, T. Robert, M. Abid, H. Ammar, S. Abid *FSS - Sfax* Synthèse et propriétés de nouveaux polyesteramides furaniques à longue chaine aliphatique	**OC17B**
M. Chellegui, A. I. Adjieufack, M. Trabelsi, V. Liégeois, B. Champagne *FSS - Sfax* Revealing the driving forces of endo/exo stereoselectivity in Diels-Alder cycloadditions: Insights from reactivity and topological analysis	**OC04B**
S. Chibi, - *Saad Dahlab University, Blida, Algeria* Dielectric strength of methyl esters of vegetable oils from Ricinus communis and Jatropha curcas as a substitute for mineral oil in power transformers	**OC29B**
S. Daghfous, C. Gomri, E. Petit, E. Makhoul, M. Semsarilar, M. Cretin, C. Trellu, N. Bellakhal *INSAT - Tunis* A comparative study of the performance of two TiOx Magnéli Phase Anodes in the degradation of PFAS using advanced electrooxidation	**OC26B**
L. Dems, Z. Mzoughi, Pampat, H. Majdoub *FSM - Monastir* Characterization of Prickly Pear seed oils from various regions in Tunisia: Clinical and dermatological evaluations	**OC07A**
F. Dhaouadi *FSM - Monastir* Application of advanced analytical models to evaluate and analyze the adsorption mechanism of three emerging pharmaceutical pollutants on a phosphorus carbon adsorbent	**OC34B**
J. Dhaouadi, C. Hamdi, B. Ben Hassine, F. Aloui *FSM - Monastir* Synthesis and characterization of new functionalized bis-diarylethenes as precursors of helicenic structures	**OC08A**
M. Dhifet, H. Nasri *FSM - Monastir* Synthesis, spectroscopic properties and structural of the chlorido Fe(III) octaethylporphyrin complex	**OC10B**
M.A. Dridi, M. Hasyeoui, F. Lassagne, W. Erb, S. Touil, F. Mongin *FSB - Bizerte* Oxazolo[5,4-f]quinoxalines and related phosphorous compounds towards novel selective inhibitors of Glycogen Synthase Kinase 3α (GSK-3α): Development and effect on cancer cell therapy	**OC09A**
D. El Hadi, D. Boudjit *University of Blida, Algeria* Étude de l'influence de la taille des particules sur la qualité de l'huile essentielle de la poudre d'écorces de quelques variétés d'agrumes	**OC31C**
N. Ellouze, L. Marrodán Bretón, J.J. Serrano Olmedo, H. Maghraoui-Meherzi *FST - Tunis* Magnetic nanoparticles and hyperthermia: A synergy for tTargeted cancer treatment	**OC05C**

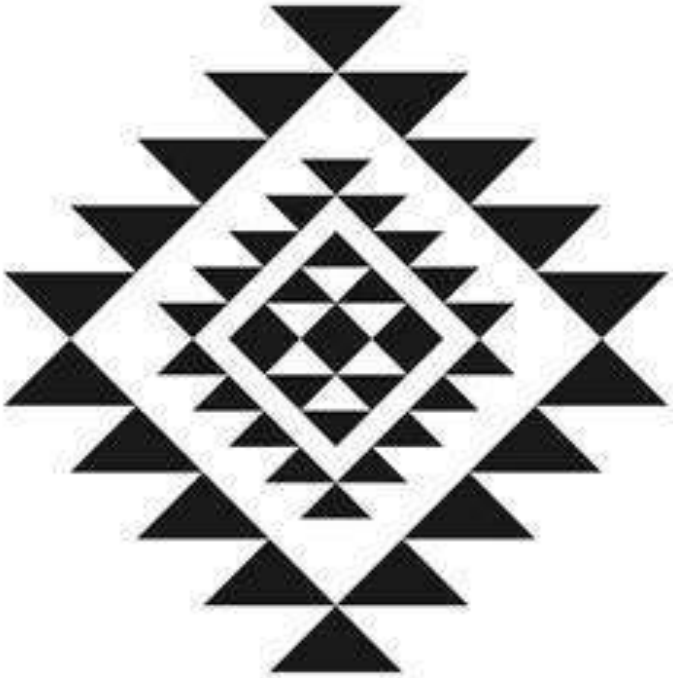
Communicatings' Names	Ref
K. Fadli, A. Bouchama, A. Tabbiche, N.E.H. Felkaoui, C. Chiter, M. Yahiaoui *Ferhat Abbas University, Sétif, Algeria* Hydrazine derivative as potent anticancer agent: Synthesis, crystal structure, in silico leukemia inhibition and computational studies	**OC10A**
J. Fakhfakh, K. Athmouni, H. Mallek-Fakhfakh, H. Ayedi, N. Allouche *FSS - Sfax* Structural features, antioxidant potential and protective effect of a polysaccharide from Lycium arabicum	**OC28C**
N.E.H. Felkaoui, A. Hellal, K. Fadli, Y. Miloudi *University of Constantine, Algeria* Synthesis, biological behavior analysis,and a theorical stady (docking and QSAR) of some aminophosphonates	**OC14A**
K. Fnena, A. Bellagi *FSG - Gafsa* Elaboration of a general Joule-Thomson effect inversion curve	**OC19B**
G. Ghannouchi, Z. Kibou, N. Choukchou-Braham, H. Ben Jannet, A. Romdhane *FSM - Monastir* Innovative synthesis of benzopyranic hydrazones: Comparative study of ultrasound-assisted and conventional methods with insights into drug design and α-amylase inhibition	**OC11A**
C. Gharbi, M. Mhadhbi, L. Khedhiri *INRAP - Sidi Thabet* Experimental investigation of nanomaterials MXenes for energy storage properties and conversion: Performances and progress	**OC06C**
N. Gharbi, S. Argoubi, E. Manoury, M.A. Sanhoury, R. Besbes *FST - Tunis* Synthesis and characterization of oxazaphospholidine-2-oxides bearing long alcoxy chains	**OC12A**
L. Ghorbali, M.F. Zid, H. Chebbi *FST - Tunis* Synthesis, crystal structure, vibrational study and optical properties of a new hybrid material $(C_5H_6BrN_2)_2[FeCl_4]Cl$	**OC11B**
I. Ghrab, H. Ben Attia, M.S. Abdelbaky, S. García-Granda, M. Dammak *FSS – Sfax* Synthesis, crystal structure, vibrational spectroscopy and thermal study of new chromium (III) based coordination complex	**OC12B**
Y. Guermassi, P. Rudolf, F. Raouafi *FSB – Bizerte* Reactions between carbon monoxide and hydrogen on the surface of interstellar dust grain analogs: Molecular dynamic simulation	**OC18B**
H. Haba, M. Belaid, A. Alabdul Magid, M.I. Badaoui, S. Mouffouk, C. Sayagh, S. Chabani, L. Voutquenne-Nazabadioko *University of Batna, Algeria* Phytochemistry of genus Centaurea grown in Algeria: Extraction, isolation, structural elucidation and chemotaxonomy	**OC29C**
L. Haddad, - *Echahid Hamma Lakhdar University, El Oued, Algeria* Adsorptive potential of Algerian mineral clay for organic pollutants: Experimental validation, RSM-based optimization, and AI-guided innovations	**OC20C**

Communicatings' Names	Ref
A. Hajji, E.D. Paul, S. Ahmed, L. Latifa, M.B. Inocencio, M. Adel *FST - Tunis* Core-shell carbon Dots@Silica-decorated heterostructured phosphate nanomaterials for ultrasensitive ratiometric temperature sensing	**OC13C**
C. Hamdi, J. Dhaouadi, B. Ben Hassine, F. Aloui *FSM - Monastir* Syntheses and characterizations of α,β-unsaturated nitriles: Insights into their photochemical evolution	**OC13A**
Y. Ibn Elachaouia, M. Affes, J. Fakhfakh, N. Allouche *FSS - Sfax* Etude chimique et valorisation biologique d'huiles essentielles issues de Ficus carica	**OC30C**
A. Ibri, N. Hosni, H. Maghraoui Meherzi *FST - Tunis* Synthesis, characterization, and applications of manganese oxide nanoparticles and nanocomposites	**OC30B**
S. Jebali, A. Labidi, H. Galai, L. Latrous *INRAP - Sidi Thabet* Sustainable and stability indicating liquid chromatography- mass spectrometry method for the quantitation of delafloxacin in pharmaceutical formulations	**OC31B**
D. Jebri, M. Znati, H. Ben Jannet *FSM - Monastir* Design and synthesis of new halogenated and nitrogen flavonoids	**OC15A**
A. Kaouach, Z. Kibou, N. Choukchou-Braham, H. Ben Jannet, A. Romdhane *FSM - Monastir* Synthesis and in silico study of new pyranopyrimidine derivatives	**OC16A**
W. Ketir, A. Bennada *Houari Boumediene University, Algiers, Algeria* Visible light induced (Zn^{2+}) reduction over (CuO/TiO_2) catalyst	**OC30A**
L. Khedhiri, C. Gharbi, C. Ben Nasr *INRAP - Sidi Thabet* Elaboration et caractérisation physico-chimique de nouveaux composés de coordination à base de thiocyanate	**OC16B**
E. Khemis, A. Zardi-Bergaoui, H. Ben Jannet *FSM - Monastir* Semi-synthesis of new structural analogs of harmine linked to 1,2,3-triazoles, anti α-amylase potential, Molecular Docking and ADMET Profiling	**OC27C**
W. Khitri, M. Chelghoum, D. Smati, A.C. Mitaine-Offer, T. Paululat, M.A. Lacaille-Dubois *Faculté de Médecine, Université of Oran, Algérie* Phenylethanoides : Isolement de molecules naturelles aux nombreuses activites biologiques	**OC24C**
S. Kraiem, S. Touil, A. Beotra, V. Mohamed-Ali, M. Almaadheed, S. Bouabdallah *FSB - Bizerte* Elimination profile of 20-hydroxyecdysone(20-OHE) in urine: Liquid-Liquid extraction and dilute and inject methodology using UHPLC/HRMS A comparative study	**OC32B**

Communicatings' Names	Ref
D. Mancer, F. Agouillal, K. Daoud *Houari Boumediene University, Algiers, Algeria* Infrared investigation of stearic acid interactions with tween 60 and soy lecithin for metformin solid lipid microparticles formulation	**OC19A**
F. Mannai, M. Ben Mosbah, M.N. Belgacem, Y. Moussaoui *FSG - Gafsa* Comparative study of conventional and combined ultrasound-assisted methods on the quality of mucilage extracted from Opuntia (Cactaceae) cladodes	**OC21C**
N. Masmoudi, M. Chtourou *FSS - Sfax* Synthèse multicomposants rapide et efficace de dérivés de 4H-pyrane assistée par ultrasons catalysée par LiOH.H2O en milieu aqueux	**OC17A**
H. Mattoussi, S. E. Donmez, S. Wang, U. Vorajee *Florida State University, USA* Investigating energy transfer interactions in perovskite quantum Dot-Dye assemblies	**OC09C**
J. Mhalla, Sana Saidi, Sondès Boughammoura *FSM - Monastir* Synergistic effect and formation of mixed SDS-TTAB micelles in aqueous media at 25°C	**OC08C**
O. Mhasni, F. Rezgui *INRAP - Sidi Thabet* An efficient one-step synthesis of a new series of mutifunctional olefins	**OC18A**
K. Missaoui, K. Ferchichi, N. Amdouni, J.L. Gómez Cámer, C. Pérez-Vicente, A. Bonilla, D. Cosano, Á. Caballero, G. F. Ortiz *FST - Tunis* Polyaniline coated $Na_3V_2(PO_4)_2F_3$ cathode enables fast sodium ion diffusion and structural stability in rechargeable batteries	**OC21B**
M. Moussa, A. Hamrouni ,H. Lachheb, M. Ferhi[d], I. Chérif, M. J.Sampaio, C. G. Silva, J. L. Faria *FSG - Gabès* Pt-doped g-C 3 N 4 photocatalyst for hydrogen production under visible light	**OC28A**
Z. Mzoughi, L. Dems, D. Le Cerf, H. Dhaouadi, H. Majdoub *FSM - Monastir* Effect of extraction methods on the physicochemical characteristics of polysaccharides from orange peels : Natural ingredients for cosmetic formulations	**OC34A**
B.P. Ngoy, Muthumuni Managa, Tebello Nyokong *University of Kinshasa, Dem. Rep. Congo* Laser flash photolysis of selected porphyrins	**OC15C**
L. Nyaba, Boitumelo P. Khunou, Philiswa N. Nomngongo *University of Johannesburg, South Africa* Application of nickel iron layered double hydroxides/activated carbon (NiFe-LDH@AC) composite for preconcentration and removal of Cr and As from water systems	**OC33A**
A. Omrani, H. Elleuch, F. Rezgui, M. Jridi, A. Ouerghui *ISB - Béja* A free catalytic α- regioselective N-allylic substitution of cycaromatic amines and their biological activities	**OC23A**

Communicatings' Names	Ref
R. Rabah, S. Ben Chaâbène, Z. Ksibi *FST - Tunis* TiO2 quantum dots on TiO_2 nanotubes: A novel approach to photocatalysis	**OC11C**
A. Rabti, F.K. Algethami, N. Raouafi *INRAP - Sidi Thabet* Ultrasensitive label-free detection using electrochemical capacitance spectroscopy for food safety, environmental, and medical applications	**OC31A**
M. Redolfi, S. Aoun, I. Ben Assaker *Université Sorbonne Paris Nord, , Villetaneuse, France* Growth and functionalization of metal oxide nanostructures by a MW plasma process for water treatment and green hydrogen production	**OC07C**
A. Reguigui, P.G. Ott, A. Darcsi, J. Bakonyi, M. Romdhane, Á.M. Móricz *ENIG - Gabès* Antibacterial and α-glucosidase inhibitors in the Salvia officinalis leaves	**OC33C**
M. Rjili, A. Aschi *FST - Tunis* Evaluation of properties and structural transitions of protein/polyanion complex coacervates	**OC20B**
H. Saadaoui, H. Ben Attia, M.S. Abdelbak, S. García-Granda, M. Dammak *FSS - Sfax* Synthesis, crystal structure, vibrational (FT-IR and Raman) and thermal behavior of new selenium hybrid material	**OC13B**
M.A. SAIDANI, A. Chmangui, L. S. Smiri, A. Fkiri *FSB - Bizerte* Hydrothermal Synthesis of Cu-Doped Au-ZnO Nanoparticles: Photocatalytic Activities	**OC12C**
S. Salhi, D. Kanzari-Mnallah, I. Jourdin, M. Knorr, J. Kirchhoff, H. M'rabet, M. L. Efrit, A. Ben Akacha *FST - Tunis* Synthesis and structural characterization of metal complexes coordinated by phosphonated thiosemicarbazones	**OC24A**
S. Salhi, A. Omri, R. Ben Salem, M. Benzina *FSS - Sfax* Oxidation of Congo red dye using modified natural hematite as heterogeneous catalyst	**OC14B**
I. Samb, M.L. Gaye, V. Michelet *Alioune Diop University, Bambey, Senegal* Réactions à économie d'atomes et respectueuses de l'environnement : Nouveaux catalyseurs supportés sur polymère recyclable	**OC25A**
H. Smati, Y. Ben Torkia, A. Ben Lamine *FSM - Monastir* Advanced analysis of the adsorption mechanism for odorants molecules on human olfactory receptor via statistical physics theory and molecular docking	**OC33B**
A. Snoussi, L. Latrous, A. Megriche *FST - Tunis* Synthesis of magnetic hydrochar from Hawthorn seeds for the determination of fluoroquinolones in chicken meat using magnetic solid-phase extraction, liquid chromatography and UV detection	**OC32A**

Communicatings' Names	Ref
I. Talbi, H. Abdelkafi *Novalix Tunisie* HTE kits: A strong optimization tool in organic synthesis Suzuki reaction as a model system	**OC06A**
K. Taleb, M. Bouras, I. Boufroukh, S. Saidi *Ahmed Ben Bella University, Oran, Algeria* Bioadsorbents for wastewater treatment	**OC27B**
V. Tokoyi, L. D. Mthembu, N. Deenadayalu *Durban University of Technology, Durban, South Africa* Acidity influence of 1-allyl-3-methylimidazolium-based ionic liquids on the conversion of glucose to levulinic acid (LA)	**OC22B**
A. Toubane, I. Bourega, S. Lahouazi, K. Daoud *Houari Boumediene University, Algiers, Algeria* Formulating an oral emulsion with an association of Carum carvi L. and Foeniculum vulgare Mill. using a planification experimental design	**OC23C**
Y. Trabelsi, M. Znati, H. Ben Jannet, J. Bouajila *FSM - Monastir* Semi-synthesis and biological screening of novel C28-modified triterpene acid derivatives from natural maslinic acid	**OC26A**
N. Triaa, M. Znati, H. Ben Jannet, J. Bouajila *FSM - Monastir* Hemi-synthesis of oleanolic acid derivatives: evaluation of their inhibition of acetylcholinesterase and α-glucosidase	**OC27A**
N. Waleng, T. S. Munonde, A. Mpupa, Y. Zhang, P. N. Nomngongo *University of Johannesburg, South Africa* Photoelectrochemical properties of magnetic amine based-MIL-101(Cr) hybrid material and its application in the degradation of acebutolol in water	**OC22C**
M.O. Zouaghi, D. Bensalah, S. Hassen, Y. Arfaoui, L. Mansour, N. Özdemir, H. Bülbül, N. Gurbuz, I. Özdemir, N. Hamdi *FST - Tunis* DFT study and anticancer evaluation of novel benzimidazole derivatives	**OC29A**
Y. Ammari, N. Baaalla, E.K. Hlil, S. Abid *FSB – Bizerte* Synthesis, structural, magnetic, optical and electronic studies of a novel Honeycomb Kagome polyoxometalate based copper(II) complex	**OC35**
G. Mbarki, C. Atzenhofer, H. Harmuth, R. Alouani, K. Nahdi *FSB – Bizerte* Synthesis and Characterization of Cordierite-Mullite Ceramic Phases from Tunisian Kaolin, Granite and Talc	**OC36**
F. Nouri, M. Trabelsi-Ayadi, R. Ternane *FSB – Bizerte* Synthesis, structural characterization and ionic conductivity of Apatite-type $Ca_{10-x}Na_x(PO_4)_{6-x}(SO_4)xF_2$ (x =0, 3, 6) materials	**OC37**



ABSTRACTS OF ORAL COMMUNICATIONS

Program of
Monday 16
December 2024

Solution behavior of tin(IV) chloride complexes with fluorinated phosphoramidates: A variable temperature NMR study

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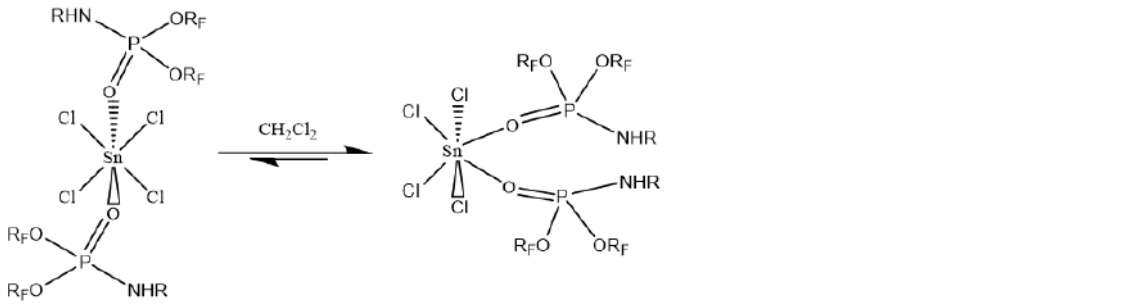
The chemistry of tin(IV) and organotin(IV) halides is increasingly attracting considerable interest due to their wide range of applications [1,2]. These compounds have recently emerged as potential candidates in the field of biomedical molecular imaging [3]. More recently, we have reported on the synthesis of new fluorinated phosphoramidates and their use as potential ligands towards tin tetrachloride [4-7]. It was shown that the stability of such complexes depends on the nature of substituents on the phosphorus atom. In the present work, we describe the solution behavior of new octahedral tin tetrachloride complexes with a novel series of fluorinated phosphoramidates with the general formula $[SnCl_4L_2]$ (L= $(R_FO)_2P(O)NHR$)) using variable temperature ^{31}P and ^{119}Sn NMR spectroscopy. The NMR data show that these complexes exist in solution at room temperature as mixtures of *cis* and *trans* isomers with predominance of the *cis* form. Importantly, the solution behavior of these complexes in the presence of excess ligand was studied with variable temperature ^{31}P NMR. The metal-ligand exchange barriers of the *cis* isomers were measured using the coalescence temperature method, giving values in the range 11.50-12.60 kcal/mol. The predominance of the *cis* isomer is consistent with a higher frequency shift (~10 ppm) of ^{119}Sn NMR signals for tin complexes as compared with those using analogous dialkyl amino ligands ($(R_FO)_2P(O)NR_2$). This suggests that the substitution of a dialkylamino by an alkylamino group does reduce the donor ability of such ligands, leading to the formation of higher proportions of the *cis* isomer.



Keywords: Phosphoramidate, tin complex, ligand exchange barrier, ^{31}P and ^{119}Sn NMR.

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Accès rapide et simple à de nouvelles 3-Alkyl-5-Alkylamino-7-Iodoisocoumarines et à leur fonctionnalisation via des réactions catalysées par le palladium.

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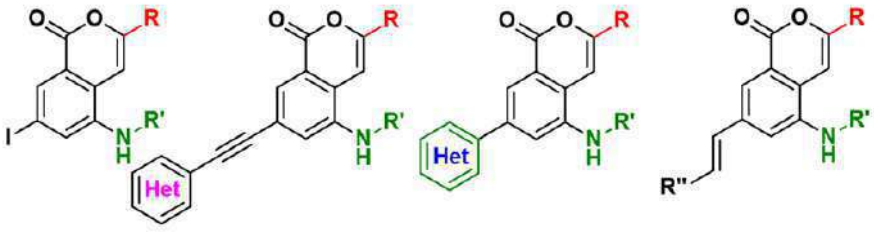
Le développement de méthodes efficaces pour la synthèse et la fonctionnalisation des isocoumarines présente une importance capitale en chimie médicinale et synthétique.[1] Cette étude propose une approche innovante et rapide pour la synthèse de nouvelles 3-alkyl-5-alkylamino-7-iodoisocoumarines et leur fonctionnalisation ultérieure.

La méthode de synthèse utilisé repose sur une procédure simple et à haut rendement, offrant un moyen efficace pour accéder à ces composés avec divers groupes fonctionnels.[2] Ensuite, des réactions catalysées par le palladium permettant d'introduire une variété de substituants sur le site iodé de ces molécules, augmentent efficacement la diversité des produits obtenus.

Les molécules synthétisées par cette méthode montrent un potentiel prometteur pour des applications futures par la découverte et le développement de nouveaux agents thérapeutiques.[2]



Key words: isocoumarine, catalysé par le palladium, agents thérapeutiques

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Microwave-Assisted Extraction of Phenolic Compounds from *Hylocereus undatus* Fruit Cultivated in Tunisia: Optimization RSM-CCD and HPLC-DAD Identification.

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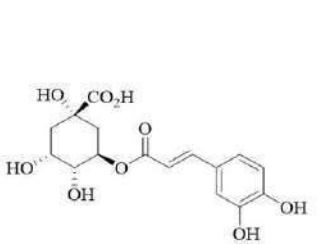
This study aimed to optimize the microwave-assisted extraction process for obtaining bioactive compounds from the peel and pulp of *Hylocereus undatus* fruit cultivated in Tunisia, utilizing response surface methodology. Total phenolic and flavonoid content, along with FRAP and DPPH activities, were optimized using a central composite design (CCD), considering three key variables: extraction time, temperature, and liquid-to-solid ratio. The optimal extraction conditions for peel and pulp were found to be 9.57 min, 42.20°C, 27.79 ml/g, and 10.08 min, 40.84°C, 31.52 ml/g, respectively. HPLC-DAD analysis identified chlorogenic and caffeic acids as well as rutin, quercetin, and luteolin-7-O-glucoside as major phenolic and flavonoid compounds. This Investigation highlights the promise of a sustainable and environmentally friendly extraction technique, supporting a circular economy model for the industrial-scale production of antioxidant-rich extracts from *Hylocereus undatus*.

Key words: antioxidant activity, total phenol, total flavonoid, DPPH, FRAP, RSM, HPLC-DAD, *Hylocere usndatus.*



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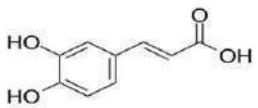

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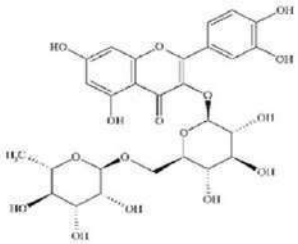
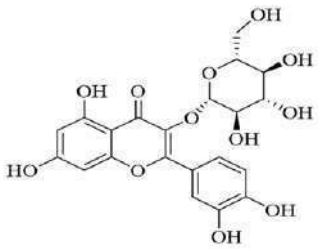
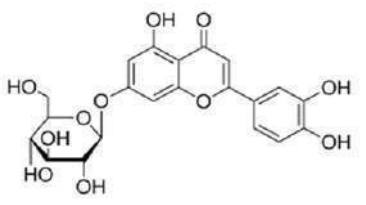


Rutin



Quercetin



Luteolin-7-o-glucoside

Design and synthesis of a novel N-substituted pyrrole derivatives as alpha-glucosidase inhibitors: In vitro and *In Silico* studies

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Diabetes mellitus (DM) still a chronic disease that have emerged as an immense crisis to public health in recent decades[1]. Among several enzymes, α-glucosidase participate in diabetes development by hydrolyzing the α-glucopyranosidic bond (α1-4) in complex carbohydrates subsequently releasing glucose.

In this work, a secure, straightforward, and manageable procedure have been emphasized to synthesized novel *N*-substituted pyrrole rings. Several synthetic steps were then constructed to create a sequence of pyrrole derivatives such as formylpyrroles, unsaturated compounds, halogenated derivatives and 3-pyrrolylpirimidines. This farmwork molecules were computationally investigated and docked into α-glucosidase active pocket. Satisfactory results were acquired which directed us to establish in vitro tests in terms of evaluating their anti-diabetic potential. The tested compounds have showed excellent IC_{50} values that make them promising α-glucosidase inhibitors for future drug development.

Key words: *N*-substituted pyrrole derivatives, antidiabetic activity, simulation *in silico*, α-glucosidase, in vitro.

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Nouvelles mono- et diphosphines ferrocéniques chirales énantiopures

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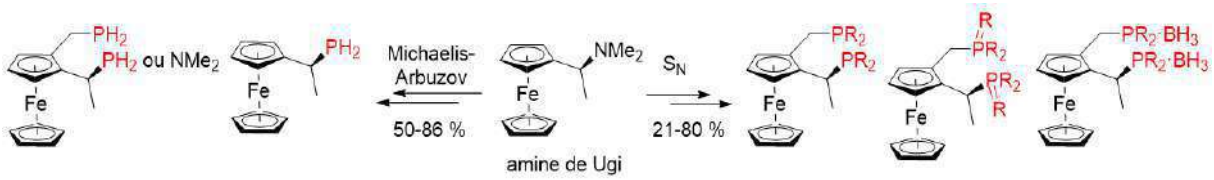
Depuis sa découverte en 1951,[1] le ferrocène et ses dérivés ont trouvé de nombreuses applications en chimie, notamment en catalyse, en tant que sondes et en chimie médicinale[2]. Les phosphines ferrocéniques, et en particulier les diphosphines, sont généralement considérées comme des ligands clés en catalyse organométallique[3]. Comparés aux ligands où la phosphine est directement liée au ferrocène, les (phosphinométhyl)ferrocènes ont fait l'objet de nettement moins d'études. Compte tenu de leur potentiel en synthèse asymétrique, et en nous inspirant de travaux réalisés sur une famille de diphosphines achirales similaires aux Josiphos[4], nous avons développé la synthèse d'une famille de diphosphines chirales énantiopures à partir de l'amine de Ugi. De plus, nous avons optimisé une variante de la réaction de Michaelis-Arbuzov permettant d'accéder à de nouvelles mono- et diphosphines primaires ferrocéniques chirales énantiopures stables, ouvrant la voie à leur fonctionnalisation future.



Mots-clés : phosphine énantiopure, réaction de Michaelis-Arbuzov, phosphine primaire, amine de Ugi.

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HTE kits: A strong optimization tool in organic synthesis Suzuki reaction as a model system

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High-Throughput Experimentation (HTE) has revolutionized organic synthesis by enabling the rapid screening and optimization of reaction conditions across diverse chemical transformations. This powerful approach accelerates the discovery and development of new compounds, allowing chemists to efficiently explore reaction parameters and pinpoint optimal conditions[1].

In the case of the Suzuki reaction, which facilitates the C-C bond formation between aryl halides and boronic acids to form biaryl compounds, HTE kits provide distinct advantages. They enable the simultaneous testing of various solvents, catalysts, and temperatures, allowing researchers to swiftly identify the best conditions for the reaction. This rapid, parallel testing speeds up the optimization process, leading to higher yields and greater reaction efficiency. With its user-friendly design, HTE kits allow laboratories to implement this technology without complex setups, making it accessible to researchers with varying levels of expertise[2].

Key words: HTE, Suzuki reaction, Parallel experimentation

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Characterization of Prickly Pear seed oils from various regions in Tunisia: Clinical and dermatological evaluations

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Vegetable oils are vital for our daily diet, offering energy and a wealth of essential nutrients. They are widely utilized in food and cosmetic products, including margarines, chocolates, cooking oils, soaps, and lotions [1]. A comprehensive examination was carried out to compare the chemical composition, encompassing fatty acids and total phenol content, of Prickly Pear seed oil sourced from six distinct regions in Tunisia (Monastir, Sbitla, Kairouan, Kef, Sidi bouzid, Kasserine). This study involved the systematic collection of oil samples from these diverse regions using the cold press method to ensure a thorough representation of geographical variations. Subsequently, a detailed chemical analysis of the samples was conducted to assess their fatty acid profiles, vitamin content, and levels of antioxidants. Preliminary findings unveiled significant variations, underscoring the need for further comprehensive investigations. Furthermore, clinical trials were conducted to evaluate the effects of these oils on human skin. Volunteer participants were engaged in trials aimed at assessing dermatological aspects such as hydration, skin texture enhancement, and reduction of skin imperfections. Results revealed that Prickly Pear seed oil sourced from the Monastir governorate, displayed noteworthy physicochemical characteristics and substantial sensory and dermatological benefits. Additionally, collaborative efforts with experienced dermatologists were initiated to delve into the impact of these oils on various skin conditions. Initial observations are encouraging, suggesting potential therapeutic advantages for specific dermatological concerns.

Key words: Prickly Pear seed oil, Chemical composition, Geographic variation, Physicochemical characteristics, Dermatological aspects.

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Synthesis and characterization of new functionalized bis-diarylethenes as precursors of helicenic structures

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Bisdiarylethenes are a class of organic compounds that have garnered significant interest as chromophores due to their unique optical properties and potential applications in materials science and photonics. These compounds exhibit remarkable photochromic behavior, allowing them to reversibly switch between different states upon exposure to light. This property is attributed to the structural features of bisdiarylethenes, which facilitate efficient light absorption and emission. The synthesis of bisdiarylethenes typically involves straightforward methods such as Diels-Alder reactions or Suzuki-Miyaura coupling, leading to high yields of functionalized derivatives. Characterization techniques, including NMR spectroscopy, UV-Vis spectroscopy, and fluorescence measurements, are employed to elucidate their structural and electronic properties. Recent studies have highlighted their applications in optoelectronic devices, molecular switches, and sensors, underscoring their versatility as chromophores in advanced materials. As research progresses, bisdiarylethenes continue to be a focal point for innovations in organic electronics and photonic technologies.

Keywords: Chromophores, Heck coupling, Absorption.

Oxazolo[5,4-*f*]quinoxalines and related phosphorous compounds towards novel selective inhibitors of Glycogen Synthase Kinase 3α (GSK-3α): Development and effect on cancer cell therapy

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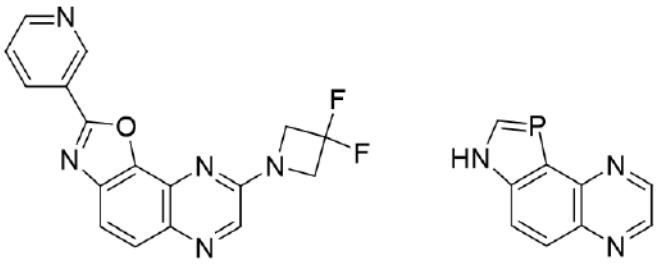
The serine/threonine kinases glycogen synthase kinase-3 (GSK-3) play an important role in numerous cellular processes. They are also implicated in human pathologies such as diabetes, bipolar disorder, schizophrenia, Alzheimer's, Parkinson's diseases and cancers.[1] However, the two isoforms, GSK-3α and GSK-3β, of this kinase do not play the same roles in these processes. Developing and modifying the oxazolo[5,4-*f*]quinoxaline in different positions was found as a promising way to obtain new α-selective inhibitors. As a result, the compound **MH-124** showed clear selectivity for the α isoform, with IC_{50} values of 17 nM and 239 nM on GSK-3α and GSK-3β, respectively. It was then evaluated against different types of cancer and found to significantly stop the growth of breast, skin and brain cancer cells.[2] Here, we report not only the development of **MH-124** analogues that have been evaluated for their activity on a panel of protein kinases, but also the synthesis of related original phosphorus-based tricyclic heterocycles.

Key words: Glycogen Synthase Kinase 3α, Cancer, Heterocycle, Organophosphorus



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Hydrazine derivative as potent Anticancer agent: Synthesis, crystal structure, In Silico Leukemia Inhibition and computational studies.

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The current and future most pressing challenges, such as access to affordable medications and healthcare, can be addressed through chemistry and chemical synthesis **[1-4]**. After exploring multiple bases in different treatments, new therapeutic agents based on Schiff bases (nitrogen-containing compounds) have attracted the attention of many medicinal chemists due to their promising potential **[5,6]**.
The Schiff bases we focused on in this study were derived from hydrazines; they represent an important class of iminic derivatives linked by N-N, exhibiting interesting physical, chemical, and biological properties **[7-9]**. In this study, a new nitrogen-containing compound will be synthesized through the reaction of hydrated hydrazine with an excess of the carbonyl derivative, and the product will be purified by column chromatography. The compound was characterized by spectroscopic techniques such as FT-IR, UV-VIS, 1H and 13C NMR, elemental analysis, and single-crystal X-ray diffraction at 100 K.
To evaluate the efficacy of our product as an anticancer drug accurately and precisely, we studied its interactions with 2B7F through molecular docking and MD simulation experiments. The results indicate that the isovanilline azine has the potential to effectively inhibit 2B7F, thus laying the foundation for the development of targeted treatments for HTLV-1-related disorders.

Key words: Azine Schiff Base, Crystal, DFT, Docking, HTLV-1, MD simulation.

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Innovative Synthesis of Benzopyranic Hydrazones: Comparative Study of Ultrasound-Assisted and Conventional Methods with Insights into Drug Design and α-Amylase Inhibition

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In the last two decades, N-acylhydrazone has emerged as a highly versatile and promising framework in drug design and medicinal chemistry [1,2]. In light of these developments, a series of twelve benzopyranic hydrazones (4a–l) were synthesized through the condensation reaction of benzopyran-hydrazide 3 (derived from the corresponding 2-amino-3-cyanopyrane 2) with various arylaldehydes, utilizing both conventional and ultrasound-assisted methods. The ultrasound approach demonstrated environmental advantages and superior efficiency compared to traditional heating methods, achieving comparable or higher yields in a shorter reaction time. The synthesized compounds were characterized using spectroscopic techniques (1H NMR, 13C NMR, HRMS), and their α-amylase inhibitory activities were predicted through molecular docking analysis. The simulations indicated that compounds 4h, 4j, and 4l exhibited high binding affinities for the α-amylase enzyme. Additionally, pharmacokinetic properties of the synthesized derivatives were predicted, suggesting that most compounds are likely to be orally active, as their physicochemical parameters fell within the desired range and complied with Lipinski's rule of five.

Key words: Benzopyrane, N-acylhydrazone, Green Chemistry, ultrasound irradiations, anti-α-Amylase, Molecular Docking, ADMET

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Synthesis and characterization of oxazaphospholidine-2-oxides bearing long alcoxy chains

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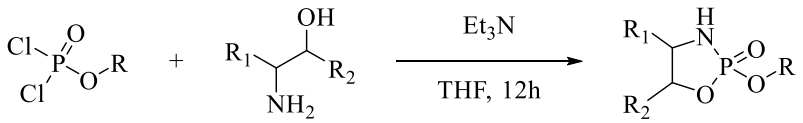
Organophosphorus compounds have played a pivotal role in biological processes, leading to extensive research into diverse functionalized phosphorus-containing heterocycles [1]. In particular oxazaphospholidines derived from amino alcohols and amino acids, have shown significant insecticidal, immunosuppressive and anti-inflammatory properties [2]. Various synthetic strategies have been developed for their production [3]. In continuation of our previous investigation on phosphoramidates and their derivatives [4,5], we report herein on the synthesis of new oxazaphospholidine-2-oxides (**1**-**8**). These compounds were produced using two methods; a one-pot synthesis and a tow-step method using phosphorodichloridates as intermediates (**1**-**8**). The results obtained using both methods were compared and showed that the latter method gives cleaner products in higher yields. All the products (**9**-**16)** were characterized using multinuclear (^{1}H, ^{13}C, ^{19}F and ^{31}P) NMR spectroscopy.



(**1**-**8**) (**9**-**16**)

65-75%

Key words : Amino alcohol, alkyl phosphorodichloridate, oxazaphospholidine, NMR spectroscopy.

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Syntheses and Characterizations of α,β-Unsaturated Nitriles: Insights into Their Photochemical Evolution

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A series of functionalized phenanthrene [1] derivatives was synthesized using a straightforward method, employing inexpensive reagents and mild conditions. The synthesis begins with the preparation of para-substituted benzyl bromide and chloride arylacetonitriles. These arylacetonitriles are subsequently used to synthesize α,β-unsaturated nitriles, whose photochemical evolution [2] is studied to form tri- and tetra-cyclic π-conjugated systems [3]. The resulting phenanthrenes were characterized by ^{1}H and ^{13}C NMR spectroscopy as well as FT-IR. UV-Vis absorption studies of these compounds in solution revealed significant behavior in the blue region of the visible spectrum, attributed to their π-conjugated electronic system.

Keywords: Phenanthrenes; Photolysis; Cyclization; Photooxidation.

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Synthesis, biological behavior analysis,and a theorical stady (docking and QSAR) of some aminophosphonates

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In search of new bioactive molecules, a series of new molecules of the phosphonate family have been synthesized via the Kabachnik-Fields reaction (phosphonate ester) and the Irani-Moedritzer reaction (phosphonic acids) [1] using microwave-assisted organic synthesis (SOAM) [2]. Their structures have been characterized by various spectroscopic methods including IR and UV-vis. The synthesized compounds were screened for their antimicrobial activity in vitro against Gram-positive bacteria (Staphylococcus aureus and Bacillus subtilis), Gram-negative bacteria (Escherichia coli and Salmonella typhimurium) and fungal strains (Candida albicans, Aspergillus niger et Penicillium notatum). Biological tests showed that all the compounds studied (Nb, No and Tc) exhibited high antibacterial and antifungal activities. In silico drug-likness using property prediction software (e.g. Molinspirtation[3], wissADME[4]), and molecular docking[5]. studies in the active site of the COVID 19 protein were performed to predict possible modes of interaction and binding energies of drug candidates at the molecular level. The results obtained are very encouraging and show that these molecules can be used in therapy.

Key words: aminophosphonic acid, aminophosphonate ester, drug-likness, COVID 19.

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Design and synthesis of new halogenated and nitrogen flavonoids

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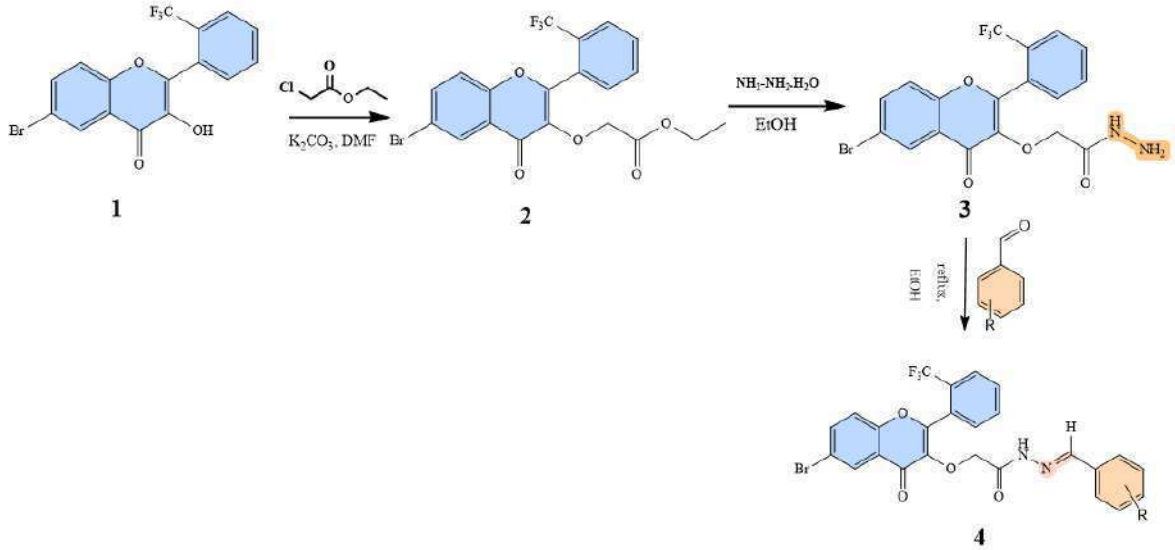
Flavonoids constitute a major group of polyphenolic compounds found in plants, fruits, vegetables, and nuts. Pharmacological research has consistently highlighted the diverse biological activities linked to the flavonoids rings system.[1] Due to their broad range of biological effects, this fragment has garnered notable attention in organic synthesis.

In this communication, we report an effective procedure of the synthesis of new flavonoid derivatives. This work began with the synthesis of an initial flavonol, from which we derived hydrazide **3**. Subsequently, hydrazide **3** was reacted with a range of aromatic aldehydes, resulting in the formation of new hydrazones of type **4**.



Key words: Flavonoids, synthesis, chemical functionalization

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Enhanced Photocatalytic Performance of P25@ZnO Composites for Organic Dye Degradation Under UV Light

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This study focuses on the synthesis and the study of the photocatalytic activity of ZnO and P25-based composites prepared using a simple ball-milling technique. The structural and optical properties of the materials were analyzed using comprehensive characterization techniques such as X-ray diffraction (XRD), Raman spectroscopy, diffuse reflectance spectroscopy (DRS), and scanning electron microscopy (SEM). The photocatalytic activity was evaluated by conducting the degradation of organic dyes under UV light. Commercial TiO2 (P25) was used as received, while ZnO was synthesized via a hydrothermal method using zinc acetate dihydrate, NaOH as precursors and PVP as surfactant. According to preliminary tests, P25 reduced 97% of Rhodamine B after 2 hours of irradiation, while the removal reached 85% with ZnO. By ball-milling, P25@ZnO composites containing various ZnO amounts (1, 3, and 5 wt%) were prepared to enhance the photocatalytic activity with respect the single photocatalysts. The composites exhibited high performance boosting up the degradation of rhodamine B to 99% after 2 hours. Bare ZnO was more active than P25 in the degradation of Rose Bengal and, also in this case, the coupled systems displayed better performance. After 30 minutes, P25@ZnO (5 wt%) degraded 71% of the dye, while by the composites containing 1 wt% and 3 wt% ZnO conversion increased up to 95%. Mechanistic studies using scavengers (t-BuOH, $Na_2C_2O_4$, benzoquinone, and $AgNO_3$) revealed that hydroxyl and superoxide species radicals played a critical role in the dyes degradation both by using P25 and ZnO photocatalysts. This study demonstrates the potential of P25@ZnO composites for effective photocatalytic applications in environmental remediation.

Key words: ZnO, TiO_2, Photocatalysis, Ball-milling composite synthesis, UV-light.

Deciphering the Mechanism of the Addition Reaction between an Intramolecular Frustrated Lewis Pair and Phenylisocyanate within Bonding Evolution Theory (BET).

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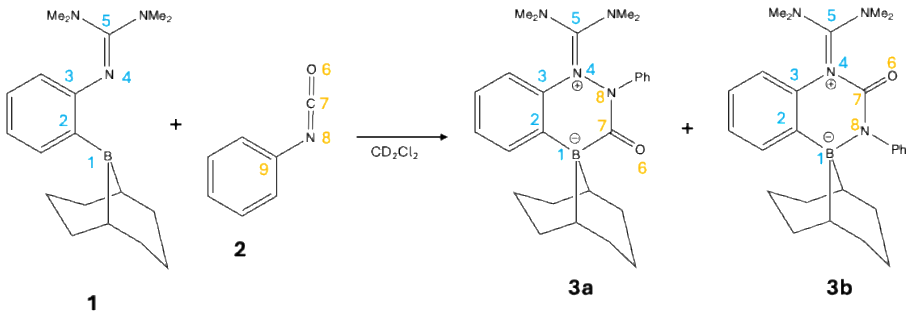
Frustrated Lewis Pairs (FLPs) are widely explored for the reduction of imines, carbonyl compounds, alkenes, and alkynes [1]. During their interaction with unsaturated compounds, they can easily undergo a 1,2-cycloaddition with C=X (O, N, and S) functional groups, leading to zwitterionic six-membered heterocycles [2]. Working in this perspective, Manankandayalage et al.[3] carried out the synthesis of **1** (a FLP) which has been added to the double bond of **2** (PhNCO) to form cyclic zwitterionic guanidinium borates containing new bonds (B–C[N] and N–N[C], Scheme 1).

The objective of this work concerns the understanding of the forming process of new bonds along this 1,2-cycloaddition reaction. Using the bonding evolution theory (BET) [4] based on DFT [M06-2X/6-311+G(d,p)] electronic structure calculations, the reaction mechanism leading to **3a** is described by three consecutive events : 1) the population of the initial C−N double bond is transferred to the C atom; 2) the B−C bond is formed, and 3) the N−N bond is created. Along the path leading to **3b**, the first step involves the formation of the B−N bond while the second one deals with that of the N−C bond.



Scheme 1. 1,2-cycloaddition reaction between **1** and **2**.

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Crystal structure, DFT calculations, vibrational characterization, and Hirshfeld surface analysis of a novel zero-dimensional metal-halide hybrid $(C_6H_7ClN)_3\cdot[SbCl_5]\cdot Cl$ exhibiting exceptional green emission

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This study presents a comprehensive investigation of a novel zero-dimensional metal-halide hybrid, $(C_6H_7ClN)_3\cdot[SbCl_5]\cdot Cl$, synthesized via the slow evaporation method. We focus on its crystal structure, vibrational properties, and optical characteristics.

The crystal structure was elucidated through single-crystal X-ray diffraction, revealing a unique framework and coordination environment. The structure comprises discrete $[SbCl_5]^{2-}$ anions surrounded by three organic cations and one loosely bound Cl^- anion, adopting the centrosymmetric space group $P\bar{1}$ in the triclinic system, with a unit cell containing Z = 2. Direct structural analysis techniques were employed, yielding refinement values of R1 = 0.02 and wR2 = 0.04, which confirm the intricate arrangement and stability of the framework. Additionally, Hirshfeld surface analysis was conducted to assess intermolecular interactions, with 2D fingerprint plots indicating that Cl···H interactions are the most dominant, accounting for 67.5% of all observed interactions. This significant contribution underscores the critical role of these interactions in stabilizing the molecular arrangement.

To further investigate the electronic structure and vibrational properties of the synthesized compound, Density Functional Theory (DFT) calculations were performed. The theoretical results exhibited strong correlation with experimental data, as validated by Fourier Transform Infrared (FTIR) and Raman spectroscopy, which identified distinct vibrational modes corresponding to both the organic and inorganic components of the hybrid material.

Comprehensive optical characterization demonstrated significant absorption in the visible spectrum, highlighting the compound's luminescent properties with an emission peak in the green region. The energy gap was determined through calculations supported by frontier orbital analysis and the density of states (DOS) spectrum, yielding a value closely aligned with the experimental results obtained using the indirect Tauc plot method.

Keywords: Antimony material; X-ray diffraction; DFT calculations; Luminescence; HOMO-LUMO energy gap; Molecular electrostatic potential.

Revealing the Driving Forces of Endo/Exo Stereoselectivity in Diels-Alder Cycloadditions: Insights from Reactivity and Topological Analysis

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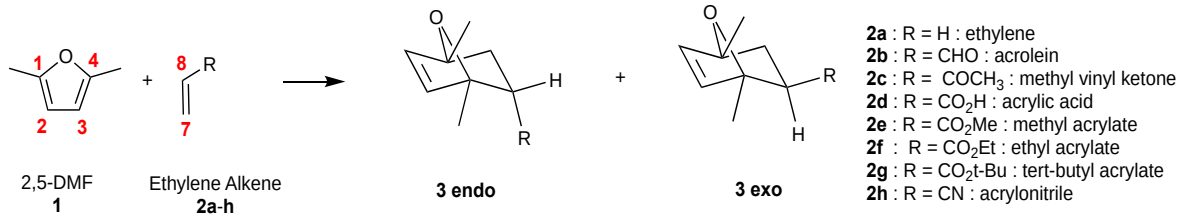
The [4+2] Diels-Alder (DA) reaction is crucial for synthesizing heterocycles and natural products. Understanding its reaction mechanisms has taken advantage of theoretical models, from the seminal frontier molecular orbital (FMO) theory to Density Functional Theory (DFT) and analysis schemes [1]. So, key tools such as Conceptual DFT (CDFT), Quantum Theory of Atoms-in-Molecules (QTAIM), and Bonding Evolution Theory (BET) reveal insights into th reaction polarity, the bonding evolution, and the (a)synchronicity [2]. On the other hand, the Distortion/Interaction-Activation Strain (DIAS) model further explains the stereoselectivity, including the relative endo/exo transition state energies [3].

In this work, DFT calculations at the IEFPCM(dichloromethane)/M06-2X/6-311+G(d,p) level have been enacted to study the DA cycloaddition between 2,5-DMF **1** and various ethylene derivatives **2a-h** (Scheme 1). The analysis reveals that ethylene derivatives act as electrophiles and 2,5-DMF as a nucleophile, with the activation of ethylene double bond increasing its electrophilicity and reaction polarity. The Gibbs free energy of activation decreases linearly with this increase in polarity. BET shows that an electron-withdrawing group on ethylene shifts the reaction mechanism from a synchronous to an asynchronous process. The DIAS model indicates that endo/exo selectivity is primarily influenced by differences in interaction energies.



Scheme 1. DA reactions between 2,5-DMF **1** and ethylene derivatives **2a-h**.

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Effect of synthesis method on the physical and photocatalytic properties of Co_3O_4

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This study examines the impact of two synthesis methods-solution combustion synthesis (SCS) [1] and ultrasound-assisted synthesis (sonochemistry)[2]- on the physical and photocatalytic properties of spinel cobalt oxide (Co_3O_4). The synthesized materials were characterized by Fourier-transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), and photoluminescence (PL) analysis to assess their structural properties. The photocatalytic efficiency of the Co_3O_4 samples was evaluated through the degradation of Congo red dye under visible light irradiation. The findings reveal that the synthesis method significantly affects the crystallinity, particle size, and surface defects of Co_3O_4.The Co_3O_4 synthesized via sonochemistry demonstrated superior photocatalytic performance, attributed to an increased surface area, higher defect density, and a reduced band gap from 1.9 to 1.82 eV, which enhanced charge separation and increased active sites. This work provides valuable insights into how different synthesis techniques can optimize Co_3O_4 performance for environmental applications, particularly in dye degradation.

Key words: cobalt oxide, ultrasound-assisted method, combustion synthesis, dye degradation.

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SYNTHESIS AND CHARACTERIZATION OF ZEOLITE LTA BY HYDROTHERMAL TRANSFORMATION OF A NATURAL ALGERIAN PALYGORSKITE

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In the present study, an Algerian palygorskite (Sif Pal, Figure 1a)[1,2] has been selected as Si source to synthesize zeolite LTA through a hydrothermal treatment by using sodium aluminate. Sif Pal is activated under reflux using hydrochloric acid solutions at different concentrations (4, 6 and 7 mol.L^{-1}) in a ratio of 50 g.L^{-1} and then analysed using XRD, SEM and XRF analysis. The selected product (PalH1) is mixed with NaOH solutions at different concentrations (1, 2, 3, 4 and 5 mol.L^{-1}), diverse $NaAl_2O_3$ quantities (1, 2, 3 and 5 g) and analyzed after several nucleation (1, 2, 3 and 5 h) and crystallization (6, 18 and 24 h) times to check the influence of these parameters on the synthesis of zeolite LTA. X-ray diffraction proved the presence of all characteristic peaks of zeolite LTA, and electron microscopy revealed the presence of the rhombohedra forms referring to zeolite LTA morphology (Figure 1b). To obtain almost pure (> 98%) zeolite LTA, the better experimental conditions are: 3 mol.L^{-1} of NaOH solutions, 3 g of sodium aluminate, 3 h for nucleation and 24 h for crystallization.

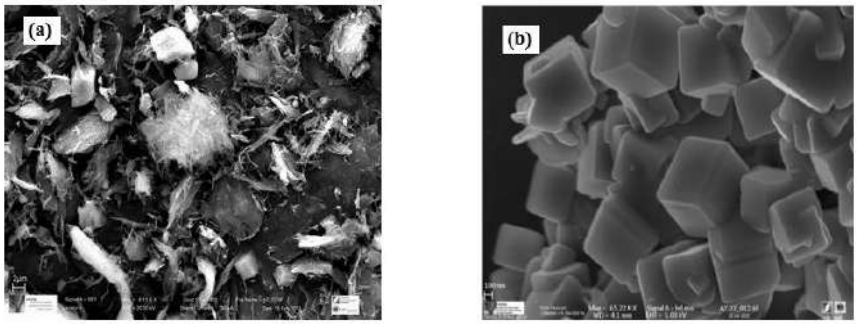

Fig. 1*. The SEM images of: (a) Algerian palygorskite (b) zeolite LTA.*

Key words: Algerian palygorskite, Hydrothermal synthesis, Zeolite LTA

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Synthesis, experimental characterization, and antioxidant evaluation of new ternary Cu(II) complexes of dimethylglyoxime and some amino-acids

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Four ternary copper (II) complexes of dimethylglyoxime (H_2dmg) as a primary ligand and tryptophan(Trp), proline(Pro), arginine(Arg) or lysin-monochlorhydrate(Lys-Cl) as a secondary ligand have been prepared and characterized by elemental analysis, conductivity, infrared spectra and electronic spectra. The IR study shows that dimethylglyoxime is coordinated to the metal ion in a bidentate manner with NN donor sites of the oxime function. The amino acid is coordinated by the carboxylate oxygen and the N atom of the amino acid. Spectroscopic studies have shown that the synthesized complexes have different geometries (square planar and octahedral). Some of these compounds were screened for their in-vitro antioxidant property using 2,2-diphenyl-1-picrylhydrazyl radical (DPPH$^{\cdot}$) free radical scavenging. The results obtained show that these complexes have a good antioxidant activity in comparison with ascorbic acid as positive control.

Keywords: Complexes, dimethylglyoxime, spectroscopic analysis, antioxidant property.

Investigation of antibacterial activity of $MAPbCl_3$ synthesized with simple and modified ultrasound assisted process

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The hybrid perovskite crystal structure, lead-based methylammonium chloride ($MAPbCl_3$), has been widely applied in optoelectronic devices and catalysis [1]. However, its antibacterial properties have been less investigated. In this study, $MAPbCl_3$ nanoparticles were synthesized using a simple, modified ultrasound-assisted process. The antibacterial activity of the synthesized nanoparticles was evaluated using the blood agar diffusion method [2], testing two pathogenic bacteria: Staphylococcus aureus (S. aureus), a Gram-positive bacterium, and Escherichia coli (E. coli), a Gram-negative bacterium. The synthesized nanoparticles were characterized using various techniques, including XRD, FTIR, UV-DRS, PL, impedance spectroscopy, and Mott-Schottky analysis. Only the $MAPbCl_3$ synthesized through simple ultrasound-assisted method using water as solvent showed antibacterial activity uniquely against the Gram-positive bacterium (S. aureus).

Key words: Hybrid perovskite**,** $MAPbCl_3$, ultrasound-assisted method, antibacterial activity

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Temperature and Pressure Effects on Phase Transitions and Structural Stability in $CsPb_2Br_5$ and $CsPb_2Br_4I$ Perovskite-Derived Halides

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All-inorganic lead halide perovskites, such as $CsPbBr_3$ or $CsPbI_3$, serve as excellent alternatives to the classical hybrid organic-inorganic perovskites, such as $CH_3NH_3PbI_3$. In contrast, all-inorganic perovskites exhibit outstanding light absorption properties in the visible range, making them suitable for solar energy applications. In this study, we focus on the synthesis of $CsPb_2(Br,I)_5$ using mechanochemical procedures. Our research includes synchrotron X-ray diffraction (SXRD) data, which are essential for determining the crystallographic evolution in the 295−753 K temperature range. Between room temperature and 573 K the crystal structure is refined in a 2D tetragonal framework, defined in the space-group $I4/mcm$, and consisting of layers of face sharing $[Pb(Br,I)_8]$ polyhedra. Above a transition temperature of T_t= 630 and 621 K, identified from DSC curves for $CsPb_2Br_5$ and $CsPb_2Br_4I$, respectively, a cubic 3D corner-sharing perovskite structure is identified, showing a substantial Cs and (Br,I) deficiency. Our diffuse reflectance UV-Vis-NIR spectroscopy measurements reveal optical gaps of approximately 2.93 and 2.50 eV, respectively, which agrees well with ab-initio calculations.

Key words: Mechano-chemical synthesis, synchrotron X-ray diffraction, phase transition, optoelectronic properties.

Synthesis, Spectroscopic Properties and Structural of the Chlorido Fe(III) Octaethylporphyrin Complex

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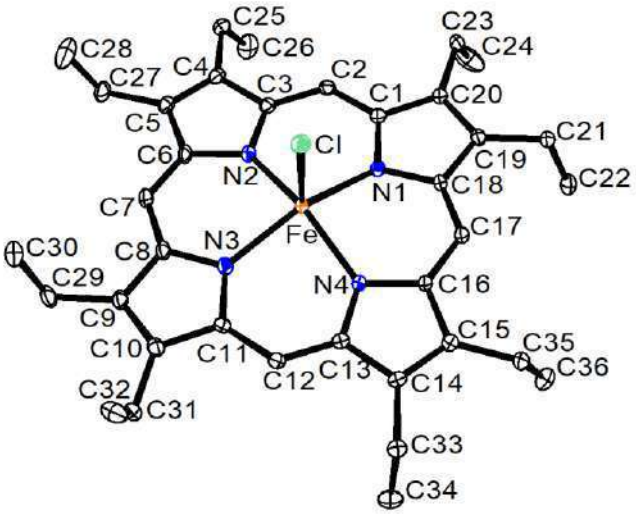
An Fe(III)-chlorido five-coordinate octaethylporphyrin complex with the formula [Fe^{III}(OEP)Cl] (**I**) (OEP = octaethylporphinato) has been prepared and described by electronic and IR spectroscopies. The synthesis of complex **I**, is used H_2OEP and $FeCl_2$ in the preparation procedure. The crystal structure of this chlorido Fe(III) octaethylporphyrin indicates that the mean equatorial distance between the iron ion and the four nitrogen atoms of the porphyrin (Fe-Np) is equal to 2.063(3) Å indicating that complex **I** is a ferric high-spin complex (S = 5/2) and has the $(d_{xy})^1(d_{xz})^1(d_{yz})^1(d_{z^2})^1(d_{x^2-y^2})^1$ ground state electronic configuration.



Keywords: Iron(III) octaethylporphyrin; Chlorido complex; DRX; UV-Visible.

Synthesis, crystal structure, vibrational study and optical properties of a new hybrid material $(C_5H_6BrN_2)_2[FeCl_4]Cl$

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In this work, we reported the synthesis and the structural study of a new hybrid material of formula $(C_5H_6BrN_2)_2[FeCl_4]Cl$. Various experimental techniques were used for the physico-chemical characterizations of the title compound : powder and single crystal X-ray diffraction, spectroscopic study (IR, solid UV-visible, diffuse reflectance and photoluminescence). Powder X-ray diffraction analysis confirmed the purity of the synthesised phase. Moreover, the different functional groups were identified using FT-IR spectroscopy. UV-visible absorption spectroscopy, diffuse reflectance and photoluminescence were used to measure the optical properties, showing that this compound has semiconducting properties. In addition, the single crystal X-ray diffraction study showed that the title compound $(C_5H_6BrN_2)_2[FeCl_4]Cl$ crystallizes in the monoclinic system with *C*2/c space group and the cell parameters are: a = 24,537(5) Å, b = 10,386(2) Å, c = 16,123(9) Å and β = 103,779(1)°. Hirshfeld surface analysis was used to explain the nature of intermolecular interactions, highlighting the importance of the H-bonds and the π–π interactions in the structure stabilization.

Key words: X-ray diffraction, Crystal structure, Hybrid material, Vibrational study, Optical properties, Hirshfeld surface

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Synthesis, crystal structure, vibrational spectroscopy and thermal study of new chromium (III) based coordination complex

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A new chromium (III) based coordination complex with the formula **[**$Cr(phen)(pydc)(H_2O)][Cr(pydc)_2]\cdot 2H_2O$ (H_2pydc= 2,6-Pyridinedicarboxylic acid and Phen= 1,10-Phenanthroline) has been synthesized using the hydrothermal method and characterized by single crystal X-ray diffraction (XRD), powder X-ray diffraction (PXRD), scanning electron microscope (SEM), vibrational measurements (IR and Raman) and differential scanning calorimetry (DSC).

The crystal structure analysis revealed the compound crystallizes in the monoclinic system with space group $P2_1/c$. The optimal parameters: a= 8.1993(3)Å, b= 27.3558(15)Å, c= 15.1233(7)Å, β= 101.898(4)°, V= 3319.3(3)$Å^3$ and Z= 4. The structure of the studied compound was stabilized by hydrogen bonds of type O−H···O and C−H···O and aromatic π···π interactions. Hirshfeld surface analysis, which converts the 3D d_{norm} surface into a 2D fingerprint plot, reveals that the intermolecular interactions O···H/H···O, H···H, and C···H/H···C are the dominant ones.

Scanning Electron Microscopy (SEM) and energy-dispersive X-ray spectroscopy (EDX) are used to study the uniformly prismatic morphology and the surface elemental composition.

Infrared absorption and Raman scattering spectroscopy were performed to establish the presence of the various complex chemical groups.

Thermal studies using differential scanning calorimetry (DSC) revealed that the investigated material seems to be stable up to 471 K.

Keywords: Chromium (III) complex, hydrothermal method, Hirshfeld surface analysis, IR, Raman, DSC.

Synthesis, crystal structure, vibrational (FT-IR and Raman) and thermal behavior of new selenium hybrid material

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A new hybrid material based on selenium with the formula $(C_{19}H_{43}N)SeBr_2$ was synthesized by the slow evaporation method at room temperature. This new material is characterized by single-crystal X-ray diffraction (XRD), powder X-ray diffraction (PXRD), scanning electron microscope (SEM) and differential scanning calorimetry (DSC).

The crystal structure was refined, revealing a monoclinic system $P2_1/m$. The optimal parameters are: a= 7.1667(5)Å, b= 7.4830(4)Å, c= 23.1779(16)Å, β= 96.826(6)°, V= 1234.18(14)Å^3 and Z =2. The asymmetric unit is built up from an isolated anionic entity $[SeBr_2]^-$ and a monoprotonated cationic entity $[C_{19}H_{43}N]^+$ which are developed in linear plans along the b-axis. Intermolecular hydrogen bonding, specifically of the C−H···Br type, plays a crucial role in stabilizing the crystal structure. Using Hirshfeld surface analysis, the intermolecular interactions are described and the 2D fingerprint plot is used to quantify them.

The Infrared and Raman spectroscopy studies lead to confirm the presence of bonds associated with the organic and inorganic entities. Scanning electron microscopy (SEM) and energy-dispersive X-ray spectroscopy (EDX) were employed to examine the surface prismatic morphology and elemental composition.

Finally, the thermal analysis reveals a reversible phase transition at 345/330 K upon heating/cooling respectively, giving rise to a thermal hysteresis phenomenon of ∼15 K.

Keywords: Selenium, Hybrid, Slow evaporation method, X-ray diffraction, PXRD, SEM, DSC.

Oxidation of Congo red dye using modified natural hematite as heterogeneous catalyst

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A heterogeneous catalyst, Cobalt doped Natural hematite (Co/Nat-Hem), was synthesized by impregnation method. Several techniques were used to characterize the prepared catalyst as BET, XRD, FT-IR, XRF and pHpzc. Solid characterization with XRD and BET showed that doped hematite particles were small in size, and large in surface area, as compared with the natural hematite. The catalytic performance of Co/Nat-Hem was tested by photo-Fenton oxidation of anionic Congo red (CR) as a model substrate. The efficiency of the process was investigated a function of the experimental parameters. Under the best experimental conditions: pH = 3; H_2O_2 concentration = 0.2 mol/L; and catalyst dose = 1 g/L, it was possible to remove about 97 % of the initial color in 30 min. A synergistic ratio of 28.5% was added to the oxidation rate using prepared catalyst. Leaching tests indicated a very low concentration of dissolved Cobalt ion and satisfactory stability of prepared catalyst.

Keywords: Hematite; Cobalt; Photo-Fenton; oxidation.

Ring opening polymerization of biobased (macro)cyclic oligofuranoates for the development of greener polyesters

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The increasing concerns regarding the massive use of polymers and the associated environmental pollution have stimulated considerable research efforts to deliver polymers from renewable resources as alternatives such as the furanic building blocks. However, in addition to the biobased origin of monomers, the development of greener strategies for polymers synthesis is absolutely fundamental. In this context, Ring Opening Polymerization (ROP) of cyclic esters can be considered as greener synthetic route due to atom-economy reasons and because it requires less severe reaction conditions than conventional bulk polyesterification [1]. Thus, in this work, we studied the combination of the advantageous of ROP as green pathway with the wide availability of the biobased furanic building-blocks. We focused, in one hand, on the synthesis of two furanic macrocycles, namely macrocyclic ethylene 2,5-furandicarboxylate (CEF) and macrocyclic hexamethylene 2,5-furandicarboxylate (CHF) via first cyclodepolymerization of the corresponding low molecular weight linear polyesters species under high dilution conditions and second pseudo high dilution condensation. In the other hand, the ROP of these two macrocycles was studied employing different reaction conditions in aim of producing high molecular weight polyesters. All the obtained species underwent thorough characterization using various analytical techniques: FTIR, ^{1}H and ^{13}C NMR, Intrinsic Viscosity, DSC and TGA.

Key words: Furanic polyesters, Ring Opening Polymerisation, Cyclic oligoesters, Green Chemistry.

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Green Pomegranate Peel and Potato Peel Starch-Derived Magnetic Nanocomposite as Efficient Sorbent of Ascorbic Acid Extracted from Fruit Juices

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This research focuses on developing a novel magnetic nanocomposite made from pomegranate peels, starch, and Fe_3O_4 nanoparticles, designed for two main purposes: the extraction of ascorbic acid from fruit juices via magnetic solid-phase extraction (MSPE) and its potential in hyperthermia applications. Physicochemical analyses (SEM, EDX-Map, IR, XRD, VSM) show that the nanocomposite possesses excellent properties for both sorbent and hyperthermia uses. Key MSPE parameters, such as elution solvent type, volume, time, sorbent amount, and extraction duration, were optimized. High-performance liquid chromatography demonstrated strong linearity ($R^2 \geq 0.9996$) across concentrations of 0.01 to 10 µg/L for ascorbic acid, with detection limits between 0.0014 and 0.012 µg/L. The method was successfully applied to real fruit juice samples, achieving recoveries between 92.48% and 103.76%, with RSDs ≤ 5.71%. In hyperthermia, the nanocomposite reached 42°C quickly (SAR of 35 W/g) under a magnetic field of 17 mT at 332 kHz. Density functional theory (DFT) calculations revealed key electrostatic interactions between the nanocomposite and ascorbic acid, primarily involving Fe^{2+} and -OH groups. This integrated experimental and computational approach offers valuable insights into designing adsorbents with high efficiency and fast kinetics.

Study of the Effect of Ultrasonication on the morphology and reactivity of MnO_2 layered structure

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In this study, MnO_2 triclinic birnessite crystalline structure was synthesized, and the effects of ultrasonication on their morphology, structure, colloidal stability and reactivity toward glutathione were investigated. Transmission electron microscopy analysis showed a progressive transformation of the oxide morphology with increased ultrasonication duration. This transformation induced the change from agglomerated nanosheets to exfoliated and separated forms, subsequently leading to the formation of nanofibres due to the fragmentation of the sheets. The colloidal stability was determined by recording absorbance spectra at one-hour intervals, with each spectrum measured as a function of wavelength. The maximum absorbance was then plotted as a function of time, providing insights into the evolution of nanoparticle stability in the studied medium These measurements showed that the ultrasonication significantly enhanced the colloidal stability of the nanosheets in water at pH 7.4. However, in simulated biological environments with high ionic strength, all samples exhibited low colloidal stability. As the duration of sonication increases, a reduction in hydrodynamic diameter, an improvement in pore size distribution and an increase in specific surface area were observed. Kinetic studies of the reaction between MnO_2 nanostructures and glutathione revealed that nanofibres exhibited a faster reaction rate compared to nanosheets. Additionally, the cytotoxicity of the two forms was assessed using the MTS assay on three tumor cell line. The results showed that both nanosheets and nanofibres of MnO_2 exhibited cytotoxic effects on all three cell lines.

Key words: MnO_2, nanosheets, nanofibers, ultrasonication, oncology, cytotoxicity, colloidal stability

Improving Proton Exchange Membrane Performance: Incorporating Layered Double Hydroxides in Composite Membranes of Low-Sulfonated Polyether Sulfone Octyl Sulfonamide

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A new method was used to create ion exchange membranes for fuel cell applications by blending Low Sulfonated PolyEther Sulfone Octyl Sulfonamide (LSPSO) with Layered Double Hydroxides (LDH) clay at varying ratios. The composite membranes were extensively characterized using different techniques to evaluate their structure and thermal properties. The results showed that the addition of LDH clay improved the thermal performance and proton conductivity of the membranes. This study suggests that LDH/LSPSO composite membranes have the potential to be used as efficient electrolyte membranes for fuel cells operating at high temperatures.

Keywords*:* Composite membrane, Layered double hydroxides Proton conductivity, LSPSO,

Dielectric and Electrical Properties of Liquid Crystals doped with Ferroelectric Nanoparticles

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The present work examines the impact of incorporating ferroelectric $Ba_{0.85}Sr_{0.15}TiO_3$ nanoparticles (NPs) on the thermodynamic, dielectric, electrical, ionic, and electro-optical properties of 4-cyano-4'-octylbiphenyl (8CB) as Liquid Crystal (LC). The introduction of ferroelectric NPs results in a notable elevation of the nematic-isotropic phase transition temperature, which is consistent with theoretical models. Impedance spectroscopy was employed to investigate bulk and interfacial phenomena, revealing a low-frequency relaxation mode attributed to space charge polarization. In comparison to the pure LC, the dielectric anisotropy and the DC conductivity were found to be increased in the doped samples. Furthermore, the reduction in the concentration of ions on the surface, their diffusion constant, and their mobility, coupled with a decrease in the threshold voltage, simultaneously indicate the trapping of ions by the ferroelectric NPs. The observed enhancement of conductivity and the screen effect make the dispersed ferroelectric NPs an optimal solution for addressing the issue of ionic contamination and eliminating its negative effects.

Keywords : Liquid crystals ; nanoparticles; dispersion; impedance spectroscopy; ion trapping

Magnetic Nanoparticles and Hyperthermia: A Synergy for Targeted Cancer Treatment

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Magnetic hyperthermia (MH) is a promising therapeutic strategy for targeted cancer treatment, based on the use of magnetic nanoparticles (NMPs) capable of generating localized heat under the effect of alternating magnetic fields. The main objective of this approach is to destroy cancer cells while minimizing damage to surrounding healthy tissues. In this perspective, we proceeded to the synthesis of zinc ferrite nanoparticles by the co-precipitation method. The nanoparticles thus obtained were stabilized by citric acid, a biocompatible stabilizing agent, to improve their dispersion in aqueous media and promote their interaction with biological cells. The structural and magnetic properties of nanoparticles have been thoroughly characterized by several analytical techniques, namely X-ray diffraction (XRD), infrared spectroscopy (IR), dynamic light scattering (DLS) and vibrating sample magnetometry (VSM). The cytotoxic activity of nanoparticles was evaluated by XTT, which allowed them to study their cell compatibility and tolerance. The results showed that these nanoparticles do not exhibit cellular toxicity and allowed for the determination of the maximum safe dose to be used for in vitro tests under magnetic field.

Keywords: Zinc Ferrite Nanoparticles, Cancer Treatment, Magnetic Hyperthermia, Nanomedicine.

Experimental investigation of nanomaterials MXenes for energy storage properties and conversion: Performances and progress

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The 2D nanomaterials field continues to grow and expand as more research in science engineering, such as energy storage [1], electronics [2], photocatalysis [3], sensing [4], medicine [5] and other fields. Among them, a new family of transition metal carbides $M_{n+1}X_nT_x$ has the great importance due to their huge physicochemical features including large surface area, good stability, excellent dispersion in various solvents, outstanding oxidation resistance, high electrical and thermal conductivity [6] that ensure as electrode for electrochemical energy storage. In this study, we provide in recent years a ready glance into the evolutionary development of the MXene family and great efforts are made globally in renewable energy technologies towards property improvement and electrochemical performance for energy storage and conversion devices such as metal-ion batteries and supercapacitors.

Keywords: MXene; Energy storage; Electrochemical performance.

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Growth and Functionalization of Metal Oxide Nanostructures by a MW Plasma Process for Water Treatment and Green Hydrogen Production

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Solar light and water are essential renewable energy resources. Their conversion into hydrogen through the photodecomposition of water is a promising solution to environmental problems associated with fossil fuel use. The photoelectrochemical decomposition of water offers low costs and high efficiency, facilitating the separation of H_2 and O_2 gases. Research has focused on metal oxide semiconductors such as TiO_2, ZnO, and Fe_2O_3, but their absorption limitations in the ultraviolet range and material degradation pose challenges for large-scale use. Recent studies have explored enhancing photocatalytic activity by coupling with other materials, aiming for broader solar spectrum absorption and effective charge separation. To produce green hydrogen, it is crucial to modify the structure of photocatalysts to reduce the recombination of electron-hole pairs. The main goal is to increase the conversion efficiency of these oxides for hydrogen production and pollutant degradation. In this work, the steps include designing supported nanostructures of TiO_2, WO_3, ZnO, and Fe_2O_3, created through anodization, followed by surface treatment utilizing microwave plasma for ion implantation. This work is conducted as part of a collaboration between two teams with expertise in the development of semiconductor materials [1] and plasma-surface interactions [2].

Key words: Green hydrogen, Photodecomposition, Nanostructures, Microwave plasma.

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Synergistic effect and formation of mixed SDS-TTAB micelles in aqueous media at 25°C

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The self-association in aqueous solutions of amphiphilic monomers dodecyl sulfate "SD^-" into "SDS" micelles $(C_{12}H_{25}SO_4Na) \equiv [(SD^-)_x, (Na^+)_a]^{Zap}$, beyond a critical concentration of micellization, c.m.c ≈ 8.3 10^{-3} mol.L^{-1} at 25°C, is governed by the intricate balance between "hydrophobic interactions" among the nonpolar side chains ($C_{12}H_{25}$), and the different "electrostatic-hydrophilic" interactions between the ionic head groups (SO_4^-), the counterions (Na^+), and water molecules.

The addition of tetradecyltrimethylammonium bromide "TTAB" ($C_{17}H_{38}N^+$, Br^-) gives rise to a new supplementary attraction between anionic and cationic monomers, respectively $C_{12}H_{25}SO_4^-$ and $C_{17}H_{38}N^+$ which could lead to a synergic effect lowering the c.m.c with a possible formation of a mixed micelle of type: $[(SD^-)_x, (Na^+)_a ; (TTA^+)_y, (Br^-)_b]^{Z'ap}$, with an apparent charge number: $Z'_{ap} = (-x + y + a - b)$.

This presentation concerns a conductemetric analysis of the mixed mixture (Water-SDS-TTAB) at 25°C and 1 atm, in order to prove the formation of mixed micelles. Theoretical interpretation of the results is based on a coherent thermodynamic approach taking into account micellisation and ionic condensation equilibria, according to a generalized Debye's model, and on the Onsager-Kim-MSA conductivity theory, which takes into account all the coupled friction effects that slow down the migration of micelles, of their monomers and counterions.

According to the reasonable approximations adopted: b = 0; x + y = 54, calculations show that mixtures (Water-SDS-TTAB) of SDS total concentrations between: 3.2110^{-3} and 3.42 10^{-3} mol.L^{-1}, and TTAB total concentrations between: 8.210^{-5} and 1.93 10^{-4} mol.L^{-1}, give rise to the formation of mixed micelles of structural composition (x, y, a), with: $49 \leq x \leq 54$; $0 \leq y \leq 5$; $21 \leq a \leq 32$; so that the apparent charge number Z'_{ap} varies relatively little from -22 to -23.

On the other hand, the limit equivalent conductivity $\lambda°_{micel}$ of the mixed micelle varies according to its structure (x, y, a) from 102 to 93 S.cm^2.$equiv^{-1}$. It is obtained by converging the theoretical conductivity of the mixture (χ^{theo}) with the experimental conductivity (χ^{exp}) at better than 3%. Therefore, within the limits of our approach and our calculations, we can conclude that the mixtures (Water-SDS-TTAB) studied, contain several types of spherical mixed micelles, each one is characterized by its structural composition (x, y, a).

Investigating Energy Transfer Interactions in Perovskite Quantum Dot-Dye Assemblies

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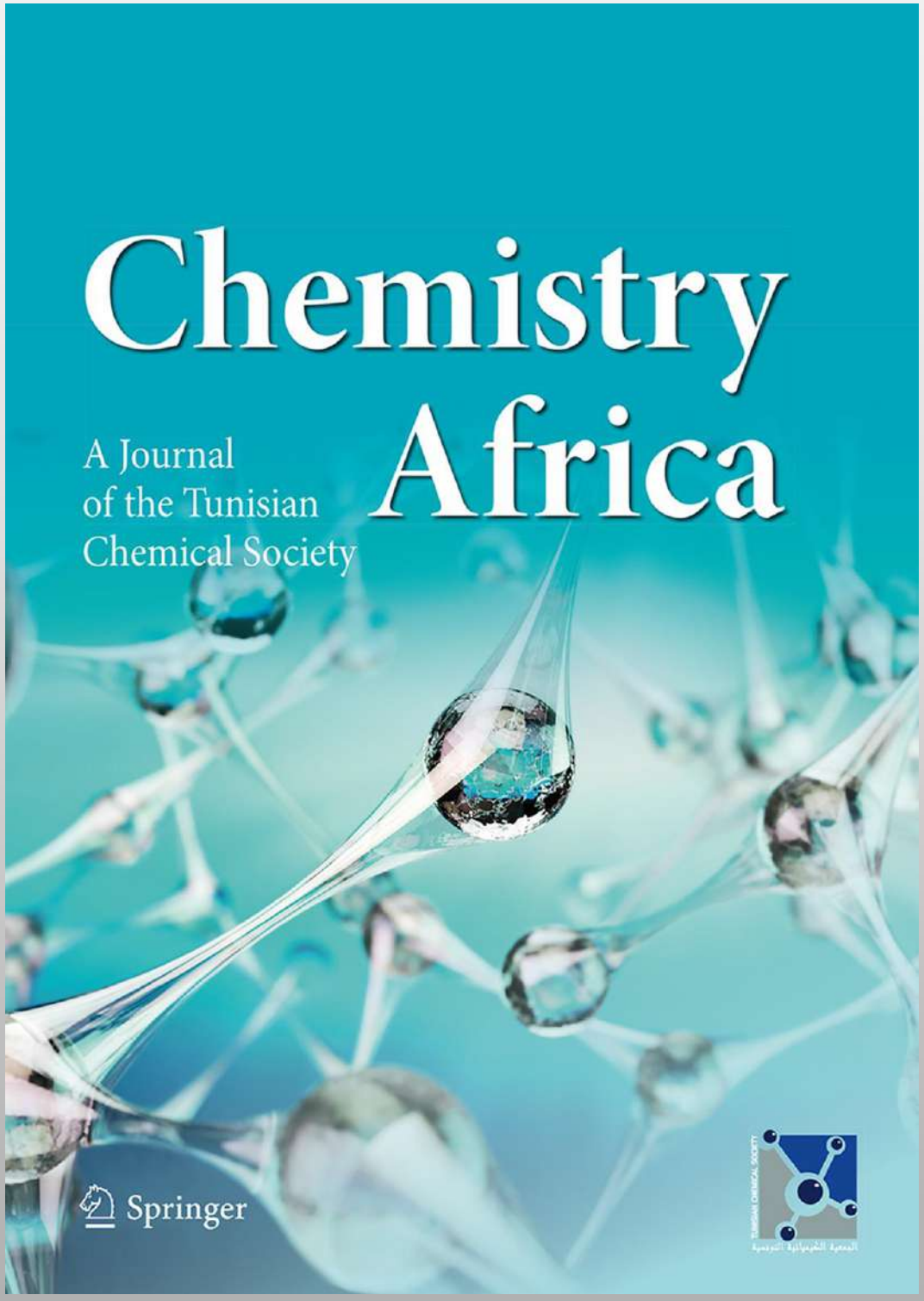
All inorganic colloidal perovskite quantum dots (PQDs) combine several tunable photophysical properties, large surface-to-volume ratios, high tolerance for structural defects and relatively easy to implement synthesis. These properties make them very attractive for use in processes relying on energy transfer (ET) interactions.

Here, we probe the effectiveness of $CsPbBr_3$ perovskite quantum dots as energy transfer donors in hybrid PQD-dye assemblies. This is achieved by combining PQDs and various cyanine dye molecules that present zwitterionic moieties and/or salt groups, to promote stable binding, via electrostatic interactions, while allowing control over the spectral overlap properties in these donor-acceptor (D-A) pairs. This strategy enabled easy dispersion of the assemblies in ethanol, close separation distance, and control over D-A stoichiometry. Using steady-state and time-resolved fluorescence spectroscopy, we evaluated the impact of varying the dye structure, photophysical characteristics and dye-to-PQD ratio on the fluorescence properties of these conjugates. We have found that the fluorescence quenching efficiency measured for these pairs depends on key parameters including spectral overlap integral and number of dyes per assembly (i.e., valence). Our results confirm that a singlet ET mechanism takes place. Furthermore, a thorough analysis of the data has indicated that a combination of the Förster dipole-dipole coupling and Dexter charge transfer model is required to account for our findings in these donor-acceptor assemblies.

Keywords: Perovskite quantum dots, Donor-acceptor, Energy transfer interactions, Steady-state fluorescence, Time resolved fluorescence



TiO_2 QUANTUM DOTS ON TiO_2 NANOTUBES: A NOVEL APPROACH TO PHOTOCATALYSIS

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Among its many applications in the environmental and energy fields, TiO_2 photocatalysis is used for self-cleaning surfaces, air and water purification systems, sterilization, hydrogen evolution, and photoelectrochemical conversion [1]. Recently, nanotechnology has demonstrated that nano-sized titanium dioxide photocatalysts, are highly effective in photodegrading organic and inorganic contaminants in water [2]. In fact, several approaches have been employed to formulate structures and electronic properties of TiO_2 at the nanocrystal level, including the control of the band structure, doping and heterojunction interaction [4-6]. In this work, we present an alternative approach to constructing TiO_2 homojunctions by assembling TiO_2 quantum dots (QDs) onto titanium nanotubes (TNT). These homojunctions were thoroughly characterized using X-ray diffraction (DRX), Nitrogen physisorption, photoluminescence spectroscopy (PL), and UV-Visible spectroscopy. From the outcomes, a strong interfacial interaction between the TNT and TiO_2 QDs significantly reduces the recombination of photogenerated electron-hole pairs and enhances charge transport efficiency [7]. In terms of catalytic application, TiO_2 catalysts showed high photocatalytic activity for the degradation of methylene blue present in water (up to 70% in 140 min). Currently, efforts are being made to optimize and characterize other TiO_2-based catalysts, which exhibit promising performance and highlight alternative proposals and assumptions about QDs/support coupling. As a result of this work, a new vision of homojunction based on quantum dots is being created, and new paths are being opened for practical applications of photocatalysis in the field of water treatment.

Keywords: Heterogeneous photocatalysis, TiO_2, quantum dots, homojunction, semiconductor, water treatment.

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Hydrothermal Synthesis of Cu-Doped Au-ZnO Nanoparticles: Photocatalytic Activities

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This study reports a successful hydrothermal synthesis of Cu-doped Au-ZnO hybrid nanoparticles with controlled doping levels (Au-Zn1-xCuxO, where $0 < x < 1.5\%$) through a one-pot method using diethylene glycol (DEG) as the solvent. Systematic characterization was performed using X-ray diffraction, UV–Vis diffuse reflectance spectroscopy, and transmission electron microscopy. The results confirmed the successful incorporation of Cu into the Au-ZnO lattice, enhancing optical and structural properties. These hybrid materials are characterized by small Au nanoparticles that are well-dispersed and anchored onto a Cu-doped ZnO nanoparticle substrate. The photocatalytic capabilities of the synthesized nanoparticles were assessed in the degradation of Methylene Blue (MB) under solar light irradiation. The addition of 1% gold to ZnO nanoparticles increased the degradation rate from 45% for pure ZnO to 62% for Au-ZnO, attributed to the enhanced separation and transfer of photoinduced electron-hole pairs. Furthermore, the introduction of Cu into ZnO exhibited a characteristic volcano-like pattern in degradation efficiency, with the highest rate of 92% achieved for Au-Zn1-xCuxO ($x = 1\%$). These findings highlight the superior performance of Cu-doped Au-ZnO nanoparticles in degrading MB compared to undoped Au-ZnO and pure ZnO nanoparticles.

Key words: Copper-doped Au-ZnO, Hydrothermal method, Solar light, Methylene blue (MB)

Core-Shell Carbon Dots@Silica-Decorated Heterostructured Phosphate Nanomaterials for Ultrasensitive Ratiometric Temperature sensing

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KEYWORDS: Core-shell, Carbon Dots, Heterostructures, luminescence, optical thermometer, radiometric sensing.

High spatial resolution in temperature measurement is vital for biomedical applications, necessitating the creation of advanced nanoscale thermometers with exceptional performance and reliability. This study introduces core-shell carbon dots@silica (CDs@SiO2)-decorated manganese phosphate (Mn3(PO4)) nanomaterials as efficient ratiometric temperature sensors. These nanostructures display dual emission within the visible spectrum, making them ideal for biological temperature monitoring over a range of 293 to 343 K. The strong optical properties of the carbon dots enable precise temperature-dependent fluorescence behavior. The ratiometric response of the emission bands from the carbon dots and Mn3(PO4) shows a consistent decrease with rising temperature, achieving high relative sensitivity and minimal temperature error at room temperature. Furthermore, intralipid tests were conducted to confirm the sensors' efficacy under conditions mimicking biological tissue scattering. These findings highlight the advantages of core-shell nanomaterials and their promise for future biomedical sensing technologies.

Synthesis and Characterization of Zr based Metal Organic Frameworks for Enhancing the Removal of Typical Organic Dyes.

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Metal-organic frameworks (MOFs) are an attractive class of porous functional materials, generating significant interest across various academic and industrial fields, such as medicine, separation, catalysis, and adsorption, due to their extensive specific surface areas and tunability. In this study, we present the synthesis of a series of Zr-based metal-organic frameworks. The three synthesized Zr-MOFs exhibited numerous properties and advantages over other materials, including a simple synthesis procedure, good crystallinity, rigidity, and robust chemical stability. X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), scanning electron microscopy (SEM), and thermogravimetric analysis (TGA) were employed to analyze the as-synthesized Zr-MOFs.

The obtained MOFs were used to investigate and compare their performance in the adsorption kinetics of red telon dye (RTL) molecules. The effects of time, initial RTL concentration, adsorbent dose, pH, and temperature were examined. The pseudo-second-order kinetic model was found to be suitable for describing the adsorption kinetics of RTL dye onto the three Zr-based MOFs. The Langmuir isotherm model best fitted the adsorption data compared to the Freundlich and Temkin models for all three MOFs. Thermodynamic analysis demonstrated the spontaneous and exothermic nature of the dye removal processes.

The results will be discussed, indicating that the three Zr-based MOFs have potential applications for treating wastewater containing dyes.

Laser Flash photolysis study of selected Metal free, Zn and Ga 5,10,15,20- tetrakis(4-phenylderivatives) porphyrins

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The use of dyes such as porphyrins, phthalocyanines, naphthalocyanines, chlorins, bacteriochlorins and texaphyrins as photosensitizers for photodynamic therapy (PDT) and photodynamic antimicrobial chemotherapy (PACT) investigations has been reported by many researchers working for the improvement of cancer treatment or antimicrobial activity [1-2]. These dyes are good targets because of their excellent physicochemical properties including photostability. Zn 5,10,15,20-tetrakis[4-(benzyloxy) phenyl]porphyrins, Ga 5,10,15,20-tetrakis(4-bromophenyl)porphyrin, meso-tetrakis(4-nitrophenyl)gallium porphyrins, meso-tetra(4-carboxyphenyl)porphyrin tetramethyl ester which are among the abovementioned compounds have been recently synthesized and tested for the PDT application [3-6]. In extension of knowing the photophysicochemical properties of the four selected porphyrins, in this work we used laser flash photolysis to generate in organic solvents different reactive intermediates taking place during the photoreaction in excited states, their transient absorption spectra and their lifetimes. The overall mechanism including the reactive pathway has been proposed.

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Synthesis and *in silico* study of new pyranopyrimidine derivatives

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A novel series of anti-ischemic pyranopyrimidine derivatives **3a-o** was synthesized in three steps starting by α-aminocarbonitrile in one pot reaction and characterized by ^{1}H NMR, ^{13}C NMR experimental data. A molecular docking study was performed to investigate the possible inhibitory mechanism at the binding site of the target enzyme which reinforced the anti-ischemic activity of compounds **3b**, **3d**, **3k, 3l** and **3n**.

The analysis revealed the strength of intermolecular hydrogen bonding and hydrophobic interactions in the ligand-receptor complexes as significant descriptors to rationalize the inhibition results obtained.

Several physicochemical properties related to the pharmacokinetics of the synthesized derivatives were predicted. These properties were found to lie within the desired limit and we have noticed that all compounds are likely to be orally active as they obeyed Lipinski's rule of five.

Key words: α-aminocarbonitrile, pyranopyrimidine, anti-ischemic, molecular docking, ADMET

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Synthèse multicomposants rapide et efficace de dérivés de 4*H*-pyrane assistée par ultrasons catalysée par $LiOH.H_2O$ en milieu aqueux

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Les dérivés de 4*H*-pyrane occupent une place importante dans la chimie organique synthétique en raison de leurs nombreuses propriétés pharmacologiques et biologiques, telles que leur activité antitumorale [1], antimicrobienne et antibiotique [2]. Cette étude propose une méthode simple et efficace pour la synthèse de 4*H*-pyranes, utilisant une réaction de cyclocondensation multicomposants entre des aldéhydes aromatiques, du malononitrile et de l'acétoacétate d'éthyle. Ce procédé écologique repose sur l'utilisation des ultrasons et de l'eau comme milieu de réaction, permettant d'obtenir des 4*H*-pyranes avec de bons rendements à température ambiante. Le $LiOH{\cdot}H_2O$, un catalyseur commercial disponible, joue un rôle clé en activant à la fois la formation d'intermédiaires benzylidène et en agissant comme une base douce pour la production de 4*H*-pyranes. Grâce à la simplicité de la procédure, la rapidité des réactions, la propreté, le faible coût et la disponibilité immédiate du $LiOH{\cdot}H_2O$, cette méthode présente une grande efficacité et des rendements élevés, rendant cette approche particulièrement attrayante pour la synthèse de 4*H*-pyranes.

Key words: 4*H*-pyranes, Multicomposants, Cyclocondensation, Eau, $LiOH{\cdot}H_2O$, Ultrasons.

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An efficient *one-step* synthesis of a new series of mutifunctional olefins

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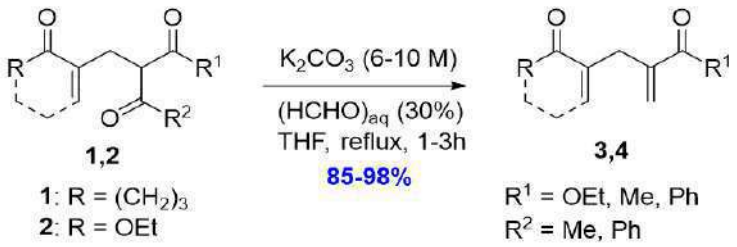
The *α,β*-unsaturated carbonyl derivatives have been found to be useful intermediates in organic chemistry [1] and for the synthesis of natural products as well as for various biologically active molecules [2]. The most famous synthetic methods for the preparation of these compounds are based on the Wittig reaction [3], the Horner–Wadsworth–Emmons reaction [4] and the decarboxylative Knoevenagel process [5]. Most of these procedures generally suffer from several major drawbacks including the requirement of metal catalysts, harsh reaction conditions and the use of expensive or complex starting materials.

We report herein an efficient, pratical and convenient protocol for the condensation of formaldehyde with a series of MBH reaction-derived β-dicarbonyl and β-phosphonoester compounds [6,7], using commercially available and inexpensive K_2CO_3 in a commonly available solvent such as THF. The *α,β*-unsaturated carbonyl compounds **3,4** were obtained in 95–98% yields, through a selective deacylation reaction (Scheme 1) [8].



Scheme 1. Synthesis of *α,β*-unsaturated carbonyl compounds from α-substituted 1,3-dicarbonyl compounds

Keywords: β-Dicarbonyl derivatives; Morita–Baylis–Hillman; Olefination; Wittig-Horner; Deacylation

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Infrared investigation of stearic acid interactions with tween 60 and soy lecithin for metformin solid lipid microparticles formulation

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Background: The formulation of solid lipid microparticles (SLM) as one of the lipid-based drug delivery systems has recently attracted tremendous interest as drug carriers for poorly water-soluble molecules [1].
SLM preparation using saturated fatty acid like stearic acid and surfactants like Tween 60 and soy lecithin leverages the unique properties and interactions of these components to achieve a stable and effective delivery system. Careful optimization of their ratios and processing conditions can enhance the performance of the final product. Hence, understanding the chemical interactions engaged between these excipients is crucial for enhancing the formulation stability as well as the releasing profiles [2]. Thus, Infrared spectroscopy is one of the valuable tools for studying these chemical interactions.
The present study aims to assess and optimize metformin SLM formulation using Fourier-transform infrared spectroscopy (FT-IR) namely for investigate the chemical interactions nature of the optimized microparticles [3].
Methods: Metformin-loaded SLMs were prepared using a double emulsion hot homogenization technique with a rotor-stator technique. The Fourier-transform infrared spectrometer FT-IR (Bruker's Alpha) equipped with an Attenuated Total Reflection (ATR) accessory in a diamond crystal was used to acquire the spectra of the components and so obtained SLMs. The acquisition was done from 4000 to 500 cm−1 range and controlled using Opus 6.5 software.
Results: The results showed an optimum encapsulation efficiency of 82% and a particle size of 2 µm. Tween 60 concentration had the most significant effect on particle size. The simple effects of the studied factors did not significantly affect encapsulation efficiency.
The FTIR spectrum of the physical mixture of all components exhibits characteristic peaks corresponding to the individual components.
According to the IR spectrum of the final obtained microparticles, characteristic metformin bands appeared. The N─H and C─H groups were ascribed to the absorption bands at 2929 cm-1 and 2853 cm-1, respectively. Also, the stearic acid FTIR spectrum shows a band at 3203 cm-1 corresponding to the elongation of the CH2 bond; two bands were found at 1699 cm-1 and 1550 cm-1, corresponding to the elongations of the C═O and COO- bonds, respectively. However, we note the disappearance of the FTIR bands of Tween 60 and soy lecithin in the final formulation, namely the region of 1100-1000 cm-1 corresponding to C─O─C stretching vibrations in the ether linkages of the polyoxyethylene chain of Tween 60 and the peaks in the region of 1200–1000 cm-1 correspond to the phosphate ester and phosphodiester groups of phospholipids in soy lecithin. This result shows the engagement of the disappeared groups in the system interactions.
Conclusion: Among the analyses of FTIR spectrum, both in the individual ingredients and in the final obtained formulation of Metformin-loaded SLMs, the characteristic hydrophobic interactions are observed between the long hydrocarbon chains of stearic acid and lecithin promoting hydrophobic interactions and helping to maintain the lipid matrix. Also, Tween 60 facilitates the emulsification of stearic acid, creating a stable lipid dispersion in the formulation. Lecithin and Tween 60 work synergistically to stabilize the formulation through emulsification and interaction with lipid components.
Shifts or changes in peak intensities relative to the individual component spectra indicate the formation of new chemical entities or changes in molecular conformation due to interactions between the components.

Keywords: Stearic acid, Tween 60, Soy lecithin, Metformin solid lipid microparticles Fourier-transform infrared spectroscopy (FT-IR).

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Antimicrobial activities of Triterpenoids, Ricinine and Quercetin derivatives from methanolic extract of *Ricinus communis* and their molecular docking correlation

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Background: Over the past two decades, numerous research projects worldwide have focused on developing new antibiotic leads [1]. Triterpenoids, which are bioactive phytochemicals composed of six isoprene units, exhibit various biological activities, including antimicrobial effects. Ricinine and its derivatives, as well as quercetin—a flavonoid known for its antioxidant and anti-inflammatory properties - also show enhanced antimicrobial activity.
Recent studies have shown that methanolic extracts from various parts of *Ricinus communis* contain several active compounds, including lupeol, amyrin, ricinine, and quercetin derivatives, which exhibit promising antibiotic activities [2]. However, the specific contributions of these bioactive compounds - whether individually or synergistically - remain less explored.
The present study aims to isolate and identify some constituents of *R. communis* leaves, their analytical characterization, on one side, and the correlation of their in-vitro with their in-silico bioactivities against selected bacteria and fungi to establish the contribution of the main active compounds from these mixtures [3].
Methods: Methanolic extract of *R. communis* leaves was obtained by the conventional maceration process, then, characterized by FTIR-NMR structural elucidation.
The obtained extract was *in-vitro* tested against five selected pathogens (*S.aureus, E.coli, P.aeruginosa, S.cerevesiae* and *A.niger*) using Inhibition Zone assessment in PCA, then the identified compounds were *in-silico* tested against ten protein receptors of the five selected pathogens using SwissDock, Chimera and Biovia Discovery Studio software kit to analyze the protein/ligand interactions.
Results: Our results showed that the maceration process allows a methanolic extract yield of 10.45%; the structural elucidation allows the identification of Ricinine, Lupeol, alpha-Amyrin, Quercetin, Quercetin-3-O- β- D-glucopyranoside and Quercetin-3-O- β-rutinoside in the obtained extract. *In-vitro* analysis shows that the lowest minimum inhibitory concentration (MIC) of the extract was found to be 7.5 ± 1.5 mg/mL against *Staphylococcus aureus*. Additionally, the minimum fungicidal concentration (MFC) of the extract was reported as 200 ± 10 mg/mL against *Saccharomyces cerevisiae*. The *In-vitro/In-silico* correlation shows that for *S.aureus*, ricinin is more active on the 4URM receptor (DS=-6.94), quercetin is more active on the 3FRA receptor (DS=-8.42) and finally Quercetin-3-O- β-D-glucopyranoside is more active on 3FRA (DS=-9.6). For *Saccharomyces cerevisiae*, lupeol is more active on the P47026 receptor (DS=-8.53), a-Amyrin and Quercetin-3-O-β-rutinoside are more active on the 4LXJ receptor with a DS=-8.77 and DS= -11.22 respectively.
Conclusion: Among the six studied compounds from the methanolic extract, ricinin is more active on the 4URM receptor of *Staphylococcus aureus* and lupeol is more active on the P47026 receptor of *Saccharomyces cerevisiae.*

Keywords: *Ricinus communis*, Molecular Docking, Antimicrobial activities, *In-vitro/In-silico* correlation.

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Vectorization of a sesquiterpene acid isolated from *Inula viscosa* leaves towards the semi-synthesis of new bioactive targets

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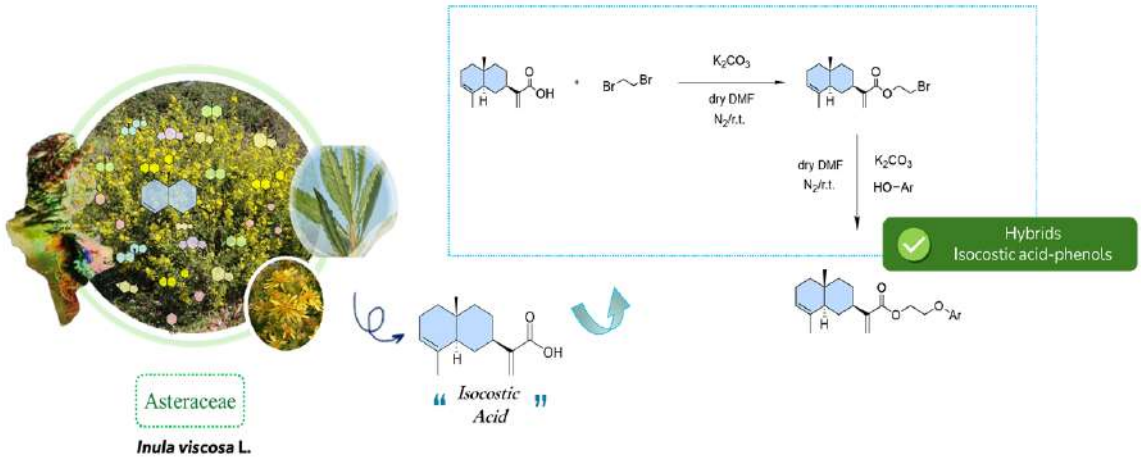
The remarkable abundance of sesquiterpene compounds in *Inula viscosa* has a significant biological interest.[2] This research led to the isolation of isocostic acid, a bioactive molecule which has several properties due to its predominance in the plant.[3] This secondary metabolite was used as a starting synthon to develop new bioactive targets with potential biological and pharmacological activities. In this study, we present an efficient method for the selective isolation of isocostic acid from the leaves of *I. viscosa*.

The biological and pharmacological relevance of isocostic acid which we isolated as well as the various biological interests of phenolic compounds,[2,4] prompted us to connect this natural acid to a series of phenolic derivatives, by exploring its reactivity, in ordrer to enhance its biological activities, and gain insight into its mode of action. The structures of the prepared derivatives from isocostic acid were characterized by ^{1}H and ^{13}C NMR spectral data.

Keywords : *Inula viscosa*, isolation, isocostic acid, semi-synthesis, sesquiterpene-phenolic derivaives.



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Study of extraction yield and corrosion inhibitory power of hydrolate from *Euclyptus Diversifolia* essential oil hydrodistillation *:* Optimization of experimental conditions using Surface Response Methodology

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Essential oils are one of the high value-added natural products. They are often extracted from aromatic and medicinal plants by steam. These substances have become increasingly in demand on the international market for their uses in various industrial formulations, particularly in pharmaceutical and cosmetic products. Hydrodistillation is the most popular standardized extraction technique (Afnor), especially for its better yield and relatively low cost compared to new techniques such as those using supercritical fluids or microwaves. Hydrodistillation processes generate liquid and solid residues (hydrolate and exhausted biomass) that are commonly rejected. The recovery of these by-products can be a fairly important subject of research. This work aims to find ways to recover the final hydrolate, from Eucalyptus essential oil extraction operation, as a bio-inhibitor of corrosion of ordinary steel in aerated acidic aqueous environments. The mass loss method was adopted to determine the corrosion inhibiting power of these products. This property is closely linked to the chemical composition of the residual hydrolate which, in turn, depends on the hydrodistillation conditions. A study based on a Box Behnken experimental design were conducted in the objective to evaluate the optimum operating parameters of hydrodistillation (extraction time, plant material/water ratio and heating power) allowing to obtain both maximum extraction yield and corrosion inhibiting power. Two mathematical models expressing the "Yield" and "Corrosion Inhibiting Power" responses as a function of the studied factors were obtained. Based on these models, the optimum conditions were determined using multi-criteria optimization method based on Desirability function.

Keywords : Corrosion, hydrodistillation, corrosion inhibitor, hydrolatel, response surface experimental design, Eucalyptus.

A free catalytic α-regioselective *N*-allylic substitution of cyclic Morita-Baylis-Hillman adducts with aromatic amines and their biological activities

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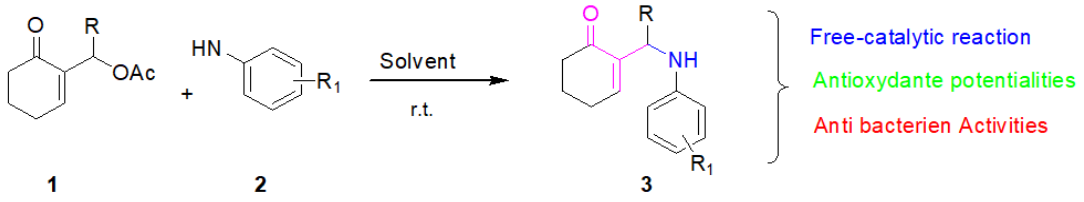
The carbon-nitrogen bond formation by N-nucleophilic substitution of allylic substrates play an important role for the diversity of synthetic compounds with biological activities[5]. The aza-Morita-Baylis-Hillman reactions has been investigated with a variety of catalyst system,[6] in particular the allylic substitution of MBH adduct with aromatic or aliphatic amines.

Herein, we wish to report our findings dealing with the direct allylation of various amines with MBH adducts, and their biological activities (**Scheme1**).



Scheme 1

The allylated aromatic amine **3** were afforded in good to excellent yields (50-92%) with highly α-regioselectivity, under free-catalytic conditions at room temperature.

Then, we evaluate the DPPH (2,2-diphenyl-1-picrylhydrazyl) scavenging activities of products **3**, the majority of them exhibit good to excellent antioxidant activity (IC_{50} µg/mL value 1,069 ±005; 276,57± 0,782) compared to that of BHT and caffeine (4.535 ± 0.04 and 4.725 ± 0.035, respectively).

Finelly, the results of antibacterial activity revealed that all chemical compounds **3** exhibited promising antibacterial activity against both Gram-negative and Gram-positive bacteria. and the MIC values varying from 62,5 to 500 µg/mL.

Key words: Morita-Baylis-Hillman, N-allylic substitution, biological activities.

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Synthesis and structural characterization of metal complexes coordinated by phosphonated thiosemicarbazones

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Thiosemicarbazones[1] and their metal complexes have received considerable attention in view of their variable binding modes, structural diversity and promising biological applications[2]. In this context, we synthesized a series of hitherto unknown thiosemicarbazones **2** using β-phosphonated hydrazones[3] **1** as precursors. Subsequently, these compounds featuring *N,S* donor sites were complexed with copper (I) and (II) salts to obtain phosphonated thiosemicarbazone complexes **3**. Both thiosemicarbazone **2** and the resulting five-membered chelate complexes **3** were characterized by spectroscopic analyses (IR, NMR, UV), and X-ray diffraction (XRD). The latter technique reveals the occurrence of extended hydrogen bonding. Their conformations were analyzed by Intrinsic Reaction Coordinate (IRC) calculations.

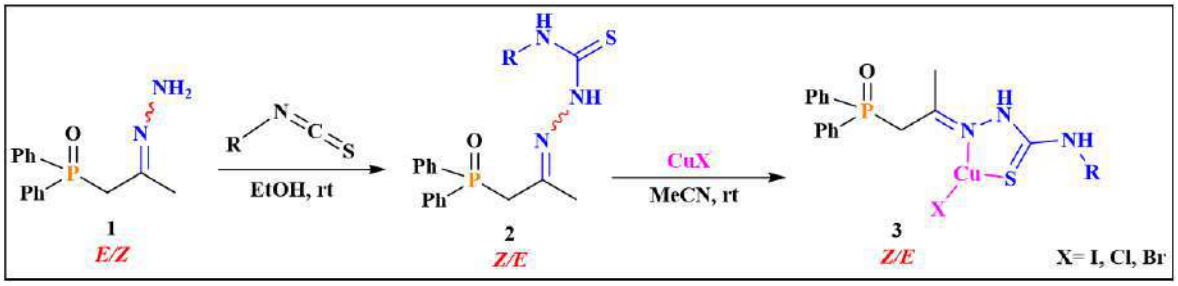

FIG. 1. Synthesis strategy leading to thiosemicarbazone complexes **3**

Key words: β-phosphonated thiosemicarbazone, chelate complexes, X-Ray Crystallography.

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Réactions à économie d'atomes et Respectueuses de l'Environnement : Nouveaux Catalyseurs Supportés sur Polymère Recyclable

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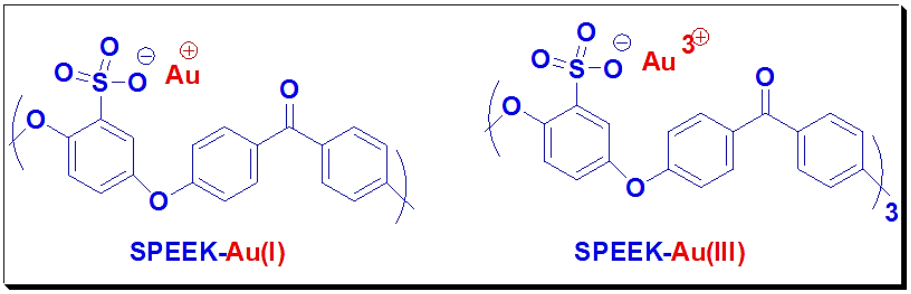
Le développement de la chimie organométallique a permis d'effectuer des réactions de cyclisations à des températures beaucoup plus basses en mettant en jeu des processus réactionnels beaucoup plus respectueuse pour l'environnement. Parmi celles-ci, la cycloisomérisation.

Le développement de nouveaux hétérocycles fonctionnalisés fait l'objet d'un intérêt croissant dans la littérature.[1] Ce concept répond à un double intérêt : d'une part, trouver des méthodes chimiques efficaces pour générer de tels composés constitue un challenge pour la communauté chimiste. D'autre part ces structures originales sont des candidats intéressants pour la recherche de composés d'intérêt biologique.[2]

Dans ces travaux nous sommes particulièrement intéressés au poly(éther éther cétone) ou PEEK, qui fait partie de la famille des poly(aryle éther cétone) (PAEK). Les dérives PAEK sont des thermoplastiques ayant des propriétés intéressantes et utilisées dans de nombreuses applications (transport, industrie, électroniques, médical, etc.…). Une fonctionnalisation du PEEK en passant par un intermédiaire chlorosulfoné suivie d'une hydrolyse nous a permis d'obtenir du SPEEK-OH. Et enfin le SPEEK-OH en solution dans l'eau à reflux avec du AuCl ou $AuCl_3$ permet d'obtenir nos catalyseurs recyclables supportés sur polymères.



Les premiers tests de nos catalyseurs sur les acides portant la propargyl et sur des diynes nous ont permis d'obtenir des lactones et cyclohex-2-enone. Ces travaux de cycloismérisations, nous ont aussi permis d'exploiter la réactivité de nos catalyseurs et de démontrer qu'ils sont recyclables.

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Semi-synthesis and biological screening 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 a variety of plants including olive pomace [1]. It has been reported to exhibit a range of biological activities, such as anti-inflammatory, anti-diabetic and analgesic effect [2]. In this study, maslinic acid has been isolated from olive pomace (*Olea europaea* L.) using an ultrasonic bath. A series of novel maslinic acid-arylidene derivatives was synthesized and the structures of the newly synthesized compounds were elucidated through ^{1}H NMR, ^{13}C NMR, and HRMS analyses. Subsequent *in vitro* assays were conducted to evaluate their inhibitory activities against 15-lipoxygenase and α-glucosidase enzymes. Several of the compounds demonstrated potent inhibitory effects on both enzyme activities. Notably, most derivatives exhibited good to moderate inhibition of 15-lipoxygenase, reaching an IC_{50} value of 50.94 µM. The evaluation of the antidiabetic potential against α-glucosidase revealed that some derviatives were found to be more active than the parent compound, maslinic acid. 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, Anti-inflammatory, Antidiabetic activities.

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Hemi-synthesis of oleanolic acid derivatives: evaluation of their inhibition of acetylcholinesterase and α-glucosidase

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Oleanolic acid, a natural triterpenic compound widely found in medicinal plants, is gaining increasing attention for its diverse biological properties [1,2]. In this study, we started by the extraction of this compound from olive pomace using an ultrasound-assisted extraction method, then used it as a starting material to hemi-synthesis a series of new derivatives bearing phenolic and coumarinic moieties. Their structures were characterized by ^{1}H NMR, ^{13}C NMR and HRMS analyses. The biological activities of these derivatives were evaluated with a particular focus on their inhibitory effects against α-glucosidase and acetylcholinesterase. These compounds showed no inhibition against acetylcholinesterase, but moderate inhibition of α-glucosidase. Some derivatives exhibited significant degrees of inhibition such as 61.56 and 54.32% against α-glucosidase. These results highlight the potential of oleanolic acid derivatives for new disease treatments, and underline the importance of natural compounds for therapeutic innovation.

Key words: Oleanolic acid, hemi-synthesis, α-glucosidase, acetylcholinesterase.

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Elaboration et caractérisation physico-chimique de nouveaux composés de coordination à base de thiocyanate

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La chimie de coordination des éléments de transition offre de grandes possibilités quant à la conception de nouveaux matériaux fonctionnels originaux qui en résultent de l'association des entités métalliques et de ligands organiques donnant lieu à des réseaux avec une grande flexibilité architecturale et ainsi une versatilité chimique qui leurs confèrent des propriétés exceptionnelles. Cette branche a connu un développement important pour un large éventail d'applications, dans des domaines en optique **[1]**, électronique **[2]**, mécanique **[3]**, stockage d'énergie **[4]**, environnement **[5]**, biologie **[6]** et médecine **[7]**. L'étude des matériaux de coordination qui évolue vers la complexité au niveau moléculaire nourrit la curiosité scientifique et les approches pluridisciplinaires ouvrent de nouveaux mondes fascinants. Le développement des composés de coordination biologiquement actifs apporte une richesse indéniable dans le domaine d'investigation de la chimie médicinale **[8, 9]**. Parallèlement, la reconnaissance du rôle des ions métalliques offre de nouvelles perspectives dans la conception des médicaments et attire l'attention sur les avantages d'étudier l'interaction des ions métalliques avec les molécules organiques. Bien évidemment, la recherche des médicaments puissants, sélectifs et offrant de large gamme d'activités thérapeutiques demeure de grande utilité aussi bien pour le monde académique qu'industriel. Plusieurs études récentes ont montré qu'il y avait un progrès significatif dans l'utilisation des complexes de métaux de transition comme médicaments visant à remédier plusieurs maladies humaines, comme le cancer, les infections, l'inflammation, le diabète et les désordres neurologiques.
En continuité avec l'étude et le développement des composés hybrides organiques-inorganiques, les résultats présentés dans ce travail sont consacrés à l'élaboration de nouveaux composés de coordination à base de thiocyanates à savoir: $(C_{11}H_{17}N_2O)_4[Co(NCS)_4]_2\cdot H_2O$, $(HPhPip)_2[Co(NCS)_4]$, $(C_6H_{17}N_3)_2[Co(NCS)_4]_2.4H_2O$, $(C_{10}H_{14}ClN_2)_2[Co(NCS)_4]$, à leurs caractérisations physico-chimiques et computationnelles au moyen de la méthode DFT et aussi à l'étude de leurs propriétés thermiques, électriques et biologiques que leurs structures laisseraient prévoir.

Mot clés : Thiocyanates, Structure, DFT, Propriétés thermiques, électriques et biologiques

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Synthèse et Propriétés de Nouveaux Polyesteramides Furaniques à Longue Chaine Aliphatique

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Compte tenu de l'impact environnemental que représentent les polymères provenant de la pétrochimie, la biomasse offre une solution durable en réduisant les émissions de gaz à effet de serre et la pollution. Les dérivés furaniques issus de la biomasse semblent jouer un rôle majeur dans la conception de polymères respectueux de l'environnement [1]. Dans cette étude, une série de poly (ester-amide) s, intégrant dans leur structure des noyaux mono- et bifuraniques [2] ont été synthétisé par la polycondensation en masse du dodécanediol et d'amido-diol (4-6) [3]. La structure de ces polymères a été vérifiée par des analyses de spectroscopie RMN^{1}H et infrarouge (IR-TF). Leur comportement thermique et leur dégradation hydrolytique ont également été examinés. En tenant compte de leurs caractères amorphes et cristallins, et de leur stabilité chimique, ces polyesteramides ont un potentiel considérable en termes d'applications dans différents secteurs.

Key words: Furane, Dodecandiol, Amidodiols, polyesteramides.

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REACTIONS BETWEEN CARBON MONOXIDE AND HYDROGEN ON THE SURFACE OF INTERSTELLAR DUST GRAIN ANALOGS: MOLECULAR DYNAMIC SIMULATION

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We live in a dusty Universe! Dust is not only found in our solar system among the planets, but it is present in a wide variety of objects throughout the Universe, mainly in those regions between stars called interstellar clouds. The interstellar medium particles -generally composed of an intimate mixture of silicate and carbon grains- and the interstellar gas are perpetually interacting. The aim of our study is to understand the dynamics of this interaction between the matter in the gas phase and the nanoparticles in new physical conditions and see how this influences the chemical complexity of space, particularly on the formation of planets. A coherent and interdisciplinary approach is required to quantify the active and catalytic role of dust in space [1].

First of all, we will produce in the laboratory dust particles analogous to the silicate dust observed in the interstellar medium. Then, we will perform experiments to study the reactions on the surface of the dust grains under astrophysical conditions and characterize the obtained products using the techniques: X-Ray Photoelectron Spectroscopy (XPS). Finally, we will exploit the results of our study to define relevant astrophysical environments using a molecular dynamic simulation and develop additional modules for these simulations that describe the new dust functionality.

Key words: Interstellar grains, interstellar gas, catalytic reactions, molecular dynamics simulation.

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Elaboration of a General Joule-Thomson effect inversion curve

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For practical engineering applications, the temperature variation resulting to a isenthalpic drop of pressure is extremely important for the super critical temperature gas study. The present work applies a statial method to generate a very precise Joule-Thomson effect inversion general curve with a relative deviation from the experimental and correlated data from the literature no more than 0.1%. The general curve was capable to predict the experimental inversion curve over a large interval of temperature even at a redued temperature up to 5.2.

Evaluation of properties and structural transitions of protein/polyanion complex coacervates

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In this work, we focus on the analysis of the Ovalbumin-PSSMA complex, which relies on the formation of coacervates using various methods, including UV-visible spectroscopy, Image-Based Dynamic Light Scattering (IDLS) and Small Angle Light Scattering (SALS). Turbidity has been precisely from spectroscopy employed to identify the critical pH values for complex formation (pH_C, $pH_{\varphi 1}$, $pH_{optimal}$, and $pH_{\varphi 2}$). Simultaneously, the IDLS technique has been used to thoroughly examine the $g_2(t)$ correlation and the size of the coacervate droplets, rich in proteins and poly electrolytes, within the liquid-liquid phase separation. Added to that, characterizing the Ovalbumin-PSSMA mixture through SALS allowed the plotting of scattered intensity I(q) to obtain the apparent radius of gyration R_G of rapidly diffusing particles. These analyses reveal that the growth of coacervate droplets is attributed to attractive electrostatic interactions within the complex.

Key words: Protein-polyelectrolyte complex, IDLS, SALS, Turbidity

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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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Acidity influence of 1-allyl-3-methylimidazolium-based ionic liquids on the conversion of glucose to levulinic acid (LA)

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Even though ILs have been revealed to operate as both solvents and catalysts in the catalytic transformation of cellulose into LA, their properties have also been shown to have an impact [1, 2]. Despite the high yields produced with these solvents, their acidity as potent catalysts for transformation reactions have sparked a lot of attention, particularly in biomass valoriation. [3, 4]. In this work 1-allyl-3-methylimidazolium based ILs were synthesized and characterized using the spectroscopic techniques, the obtained results showed a successful preparation of the ILs, with their overall thermal properties depicted to be impacted by different anions, and following this trend: [1-allyl-3-mim][HSO_4] > [1-allyl-3-mim][Form] > [1-allyl-3-mim][Dos] > [1-allyl-3-mim][Dos]. The estimated Brønsted acidic strength of ILs using the Hammett function was illustrated to follows this trend: [1-allyl-3-mim][Dos] > [1-allyl-3-mim][HSO_4] > [1-allyl-3-mim][Form] > [1-allyl-3-mim][Cl] (as per **Figure 1**). Using the Parr reactor and a Box–Behnken design, each IL was evaluated as a catalyst in the transformation reaction and the obtained results demonstrated clearly that the acidic strength, time, temperature, and catalyst loading parameters have an overall impact on the obtained LA yields.

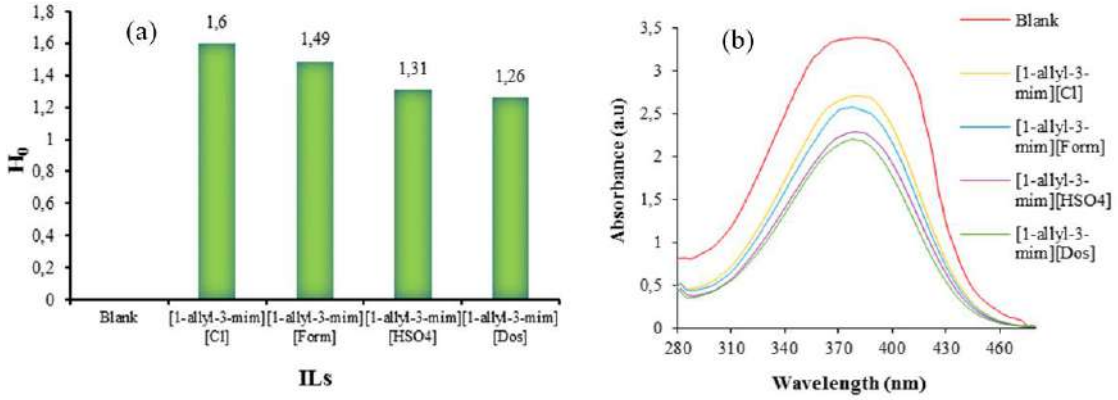

Figure 1: Estimated acidity strength values of the ILs (a) from the obtained UV-Vis absorbance spectra (b) using the Hammett function method.

Key words: Ionic liquids (ILs), lignocellulosic biomass, acidity, and levulic acid (LA)

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Atmosphere-Controlled Plasma-Assisted Surface Engineering of NiMoO4 for Enhanced Supercapacitor Electrode Performance

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The development of high-performance electrode materials is crucial for advancing energy storage systems, including supercapacitors and batteries, as they require both high energy density and power density. Transition metal oxides (TMOs), such as manganese oxide (MnO_2) [1], iron oxide (Fe_2O_3) [2], cobalt oxide [3,4], and $NiMoO_4$ [5], have shown promise in improving the electrochemical performance of pseudocapacitors due to their excellent catalytic properties, unique crystal structures, tunable surface morphologies, and multiple oxidation states that enable efficient redox charge transfer. Nanostructured electrode materials, in particular, are highly effective in facilitating mass transport, ion diffusion, and electron transfer, which significantly enhances electrochemical performance.

To improve the electrical conductivity of $NiMoO_4$-based electrodes, various nanostructured substrates have been explored as effective methods to boost the electrochemical behavior of semiconductors. Plasma treatment, a rapid and efficient process compared to conventional chemical synthesis, has emerged as a powerful tool for modifying electrocatalysts and inducing phase transformations. The reactive species generated during plasma treatment can interact with precursors to form new chemical bonds, altering the surface properties through etching, doping, and other mechanisms.

In this study, $NiMoO_4$ nanostructures were successfully synthesized onto nickel foam and stainless-steel mesh (SSM) substrates using a simple hydrothermal method. The surface of the synthesized materials was then functionalized through plasma treatment under various atmospheres (e.g., N2, H2, CH4). The resulting samples were characterized using X-ray diffraction (XRD), scanning electron microscopy (SEM), and energy-dispersive X-ray spectroscopy (EDX). Electrochemical performance was evaluated through cyclic voltammetry (CV), galvanostatic charge-discharge (GCD), and electrochemical impedance spectroscopy (EIS). The optimized $NiMoO_4$-CNT nanosheets exhibited exceptional energy storage capability with outstanding stability. This work demonstrates a viable plasma-assisted approach for enhancing the performance of supercapacitors based on transition of metal oxide electrode.

Key words: metal oxide, $NiMoO_4$, plasma treatment, supercapacitor performance.

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Treatment of real textile effluent containing indigo blue dye by hybrid system combining adsorption and membrane processes

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The rapid expansion of the textile industry in Tunisia has resulted in ever-increasing discharges of wastewater, making it necessary to set up treatment systems allowing i) its discharge into the environment or ii) to recycle the water in the textile plant. In this study, several unitary operations were tested in order to improve the treated water quality. Thus, the following unit operations were applied: adsorption using Natural Clay (NC) and Powdered Activated Carbon (PAC), ultrafiltration (UF) and nanofiltration (NF) individually or in synergy: UF, nanofiltration, PAC-UF, NC-UF, UF-NF et Adsorption-UF/NF. The experiments were carried out on real textile effluent containing Indigo blue dye. A threshold concentration was observed above which performance no longer increases. NF alone showed better reduction of COD (67%), color (78%), and turbidity (98%) than UF alone (26%, 48%, 95%, respectively). The coupling UF–NF showed a clear improvement in water quality in terms of color (99%) and COD (98%) with an improvement in the NF flux from 67.81 L/h.m2 to 90.62 L/h.m2. No fouling was observed for NF while it is significant during UF. The used of adsorption as pretreatment to filtration leads to an enhancement of the treatment performances with a removal of 99.9%, 99.5% and 79.5% respectively for turbidity, color and COD for NC-UF and a removal of 100%, 99.4% and 79.6% respectively for turbidity, color and COD for PAC-UF. Moreover, the addition of adsorbent controls the fouling and a constant and high flux is quickly attained and remains stable over time. The use of natural clay as adsorbent represents an economically profitable solution since it can be obtained locally and the clay used can be reused in the ceramic industry as an additive for road surfacing without the need for regeneration.

Keywords : Indigo blue, adsorption, natural clay, ultrafiltration, nanofiltration, hybrid process

Removal of levofloxacin from aqueous solutions and economic assessment through electrocoagulation and bioadsorption.

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The presence of organic micropollutants in aquatic environments represents an emerging form of pollution that disrupts ecosystems. This study adopts a systematic approach to evaluate two depollution processes for removing Levofloxacin (LVF): electrocoagulation using aluminum electrodes and adsorption utilizing nettle as a bioadsorbent. The objective is to optimize the operating parameters of each method to achieve energy efficiency, lower operating costs, and high removal performance. Electrocoagulation experiments were performed using a lab-scale EC cell, demonstrating that factors such as initial LVF concentration, inter-electrode distance, initial pH, current intensity, electrolysis time, electrode surface area, and NaCl dosage significantly influence removal efficiency. Meanwhile, the adsorption study revealed that nettle exhibits excellent removal capacity. The adsorption behavior of LVF on nettle was successfully modeled using the Langmuir and Freundlich isotherms, providing a detailed understanding of the removal process from water samples.

Keywords

Organic micropollutants, Levofloxacin (LVF), depollution processes, Electrocoagulation, Electrodes, Adsorption, bio-adsorbent, Nettle.

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A comparative study of the performance of two TiOx Magnéli Phase Anodes in the degradation of PFAS using advanced electrooxidation

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This study assessed the efficacy of two sub-stoichiometric titanium oxide anodes, designated TiO_{x1} and TiO_{x2}, in the electrochemical degradation of perfluorooctanoic acid (PFOA) and perfluorooctanesulfonic acid (PFOS).

The two anodes were employed in an electrolytic cell in conjunction with a carbon felt cathode for the purpose of evaluating the degradation of PFOA and PFOS through electro-oxidation and electro-oxidation coupled with electro-Fenton. Two concentrations, namely 2ppm and 0.2ppm were studied. At a concentration of 2ppm, electrolysis using the TiO_{x1} electrode resulted in the removal of 98% of PFOA (K= 0.0094 min^{-1}) and 99% of PFOS (K= 0.126 min^{-1}). In contrast, the TiO_{x2} electrode demonstrated a significantly lower degradation rate, with only 52% of PFOA (K= 0.0019 min^{-1}) and 82% of PFOS being degraded (K= 0.0075 min^{-1}).

The most effective degradation was achieved when electro-oxidation was coupled to electro-Fenton, using the TiO_{x1} electrode. This method resulted in the removal of 97% of PFOA (K= 0.014 min^{-1}) after only two hours of treatment and 100% of PFOS (K= 0.14 min^{-1}) after one and a half hours.

To further validate the performance of the TiO_{x1}, both anodes were characterised by RAMAN, scanning electron microscopy (SEM), X-ray diffraction (XRD) in surface and cross-section, and their compositions were compared with each other.

Additionally, the impact of organic matter on the degradation efficiency of PFOA at the 2ppm concentration level was examined to determine if it would impede the electrochemical decomposition process when using the TiO_{x1} anode or not.

Keywords: Degradation, Electro-oxidation (EOX), Electro-Fenton (EF), Perfluorooctanoic acid (PFOA), Perfluorooctanesulfonic acid (PFOS), Magnéli phase, Performance, Organic matter

BIOADSORBENTS FOR WASTEWATER TREATMENT

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With the gigantic development of modern industry, water pollution affects ecosystems and human health. It has become a major global concern [1,2]. Particularly, oily wastewater present important social and environmental issues. Various techniques have been proposed to address these issues; however, the efficacy and cost-effectiveness of these techniques for residual oil removal remain a great challenge. Adsorbent materials have been identified as a potentially valuable tool due to their usage in the final step for oil residues treatment. Therefore, new materials are urgently required that are biobased, environmentally friendly, biodegradable and sustainable.

Herein, we developed a feasible, efficient and cost-effective approach using bioadsorbents derived from agricultural waste for oily wastewater remediation. Adsorption data showed that the studied adsorbents exhibited a high efficiency for oil/water mixture separation and dyes removal. The findings are highly promising and suggest that the bioadsorbents used in this work could have significant potential for use in practical applications.

Key words: bioadsorbents, oil/water mixture, adsorption, porous structure.

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Synthesis and Characterization of Novel Calamitic Liquid Crystalline Compounds

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Four novel 4-(alkyloxycarbonyl)phenyl 3-fluoro-4-(tetradecyloxy)benzoate compounds with varying alkyl chain lengths were synthesized and characterized using Fourier Transform Infrared Spectroscopy (FT-IR) and Nuclear Magnetic Resonance (NMR) spectroscopy. The thermal and phase behaviors of these compounds were investigated through Polarized Optical Microscopy (POM) and Differential Scanning Calorimetry (DSC). The results revealed a diverse range of mesophases, including smectic and nematic phases, indicating their liquid crystalline properties. This study elucidates the relationship between molecular structure and liquid crystalline behavior, emphasizing the significant roles of terminal alkoxy groups and fluorine substituents in influencing thermal properties. Additionally, the dielectric properties of the compounds were assessed over a frequency range of 1 to 107 Hz, providing further insights into their potential applications in liquid crystal technologies.

Key words: Liquid Crystals, Mesophases, Thermal Properties, Dielectric Behaviour.

Extraction and Characterization of Polysaccharides from Tunisian Broad Bean Pods: Physicochemical Properties, Rheological Behavior and Cytotoxicity

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The expansion of fruit and vegetable processing industries has resulted in the production of considerable by-products, such as skins, peels, seeds, and pulp, which are rich in bioactive compounds like polyphenols, polysaccharides, and dietary fibers. This study focused on extracting polysaccharides from Tunisian broad bean pods using an acidified solution heated to 80 ºC for two hours. The structural characterization of the extracted polysaccharides (PBB) was performed using Fourier Transform Infrared Spectroscopy (FTIR), Gas Chromatography-Mass spectrometry (GC-MS. Size Exclusion Chromatography (SEC) analysis revealed that the polysaccharide had a weight-average molar mass of 1130 kDa. The flow behavior and viscoelastic properties of PBB solutions were assessed at concentrations of 10, 20, 30, and 40 g/L in water, as well as at 30 g/L in the presence of 1M $CaCl_2$ and NaCl. Importantly, cytotoxicity tests on Vero cells indicated that the PBB extracts were non-toxic at a concentration of 2500 µg/mL.

Key words: Vicia faba pods, Polysaccharide, Physical-chemical analysis, Flow behavior, Cytotoxicity

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Study of azeotropic separation of MeOH/MTBE mixture by pervaporation by means of chitosan membranes elaborated by Deep Eutectic Solvents

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The present study consists in studying azeotropic separation by pervaporation by means of chitosan membranes as well as those prepared by the Deep Eutectic Solvent PRO:SUF. First, we were interested in characterizing membranes developed for the understanding of compound separation mechanisms through SEM analysis, transmission infrared spectroscopy (FTIR-ATR), contact angle measurement, determination of mechanical properties as well as swelling rate. We then studied the influence of the operating temperature on the separation performance by pervaporation. Finally, a comparative study is made for membranes prepared by means of DES.

Key words: pervaporation, azeotropic separation, chitosan, contact angle

Nerium oleander L. in southern Tunisia: Genetic diversity, insecticidal and herbicidal activities of its aqueous extracts

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Seven *Nerium oleander* cultivars were identified and collected from the southern of Tunisia which are as follows: Villa Romaine (VR), Villa Romaine spontaneous (VRS), Roseum Plenum (RP), Mont Blanc (MB), Red (R), Petit Salmon (PS), Variegated (Var) and Alsace (Al). This seven *Nerium oleander* cultivars aqueous extracts were screened for their toxic effects against *Stator limbatus* (Horn, 1873). Wild Villa Romaine variety records the maximum percentage (53.33%) of adult emergence and the minimum value is recorded in both PS and MB varieties (20%). In the case of treatment with leaf extract, the highest viability was 70% recorded in MB variety while the lowest value of adult emergence was observed in Var variety (46.66%). Moreover, Phytotoxic activity of the 7 *Nerium oleander* cultivars extracts was investigated against the germination and seedling growth of *L. leucocephala*. Feeding by flowers extracts, the varieties MB et VRS were the most effective whose germination rate of *L. leucocephala* decreases to 11.66% compared with control (GR100%). While, the variety R was the least affective against this plant with a germination rate which exceeds 50% (55%). On the other hand, using leaf extracts, VRS remains the one who has the most phytotoxic effect against *L. leucocephala* which records a germination rate that does not over run 63,33%. However, the efficiency of MB extract as a phytotoxic substance retreats to become the least effective and the germination rate of *L. leucocephala* reached 91.66%. The overall results, suggest that in both insecticidal and herbicidal tests, *Nerium oleander* flower extracts were more effective than leaf extracts, suggesting their important biological activities. The chemical analysis of these extracts will enable us to identify their active compounds.

Key words: diversity, *Stator limbatus* (Horn, 1873), *Leucaena leucocephala*, *Nerium oleander* cultivars, phytotoxic, insecticidal activity.

Adsorptive Potential of Algerian Mineral Clay for Organic Pollutants: Experimental Validation, RSM-Based Optimization, and AI-Guided Innovations

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This study investigates the potential of Algerian mineral clay as an efficient adsorbent for removing organic dyes, namely methylene blue (MB), Congo red (CR), and methyl orange (MO), from water. Experimental results demonstrate significant adsorption capacities, with Langmuir isotherms showing high linearity (regression factors of 0.996, 1, and 1 for MB, CR, and MO, respectively) and Freundlich isotherms yielding regression factors of 0.990, 0.985, and 0.821, with MB displaying the highest adsorption affinity. Kinetic analysis indicates a pseudo-second-order model, with regression coefficients of 0.995, 0.874, and 0.952 for MB, CR, and MO, respectively. For precise optimization, response surface methodology (RSM) and artificial neural network (ANN) modeling were employed. These models considered variables such as initial dye concentration, clay mass, shaking speed, and pH, achieving close alignment between predicted and observed values. Optimal conditions recommended by the models included an initial dye concentration of 252 mg/L, clay mass of 10 mg, stirring speed of 350 rpm, and pH 10, achieving maximum dye removal efficiency. Furthermore, the comparative analysis of ANN and RSM showed the advantage of integrating AI-driven optimization, including a techno-economic evaluation, which enhanced both dye removal efficiency and cost-effectiveness. This comprehensive approach underscores the potential of combining mineral clay adsorption with AI techniques in sustainable wastewater treatment applications.

Key words: Adsorption, Mineral clay, Organic dye, RSM, ANN.

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Comparative study of conventional and combined ultrasound-assisted methods on the quality of mucilage extracted from *Opuntia* (Cactaceae) cladodes

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Opuntia (Cactaceae) mucilage is a renewable source of hydrocolloid carbohydrates with a high added value suitable for food and other industrial applications [1,2]. This study aims to evaluate the extraction efficiency of mucilage from *Opuntia* (Cactaceae) as a promising emulsifying agent using the conventional one-step method versus the combined conventional and ultrasound-assisted extractions. The obtained polysaccharide fractions were characterized by ATR-FTIR, XRD, and TGA. The results reveal that mucilages have a carbohydrate structure, an amourphous appearance, and good thermal stability in some temperature ranges. The emulsions stabilized with mucilage extracts were stable with a zeta potential between -22.1 ± 1.2 and -34.6 ± 1.7 mV [1]. The ultrasound-assisted extraction combined with the conventional method is considered a green technology for extracting polysaccharides.

Key words: mucilage, ultrasound, hydrocolloid, emulsifying agent.

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Photoelectrochemical properties of magnetic amine based-MIL-101(Cr) hybrid material and its application in the degradation of acebutolol in water

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Rapid advances in industries and agricultural practices have released various toxic pollutants into the aquatic environment over the past few decades [1]. Pharmaceuticals, among others, have been detected at concentrations that threaten human well-being and ecological balance [2][3]. This work successfully synthesised Fe_3O_4@NH_2-MIL-101(Cr) through a facile in-situ chemical co-precipitation method. The prepared materials were characterised using Fourier transform infrared spectroscopy (FTIR), energy dispersive X-ray spectroscopy (EDX), transmission electron microscopy (TEM) and Brunauer-Emmett-Teller (BET). The optoelectronic properties were determined using Photoluminescence (PL), Ultraviolet-visible spectroscopy, diffuse reflectance spectroscopy (UV-Vis DRS) and electrochemical impedance spectroscopy. The photocatalytic efficacy of the nanocomposite was assessed by the degradation of the acebutolol under visible light illumination. The results indicate that adsorption-desorption was attained after 60 min in the dark, and complete mineralisation was achieved after 180 min with the light on. According to scavenging experiments, superoxide radicals ($\cdot O_2^-$) were the main active species during photodegradation. The Nyquist plot obtained from electrochemical impedance spectroscopy (EIS) revealed that the Fe_3O_4@NH_2-MIL-101(Cr) nanocomposite had a reduced charge transfer resistance (R_{ct}), indicating separation and accelerated charge transfer at the interface. The obtained electron lifespan (τ_e) supported the results and it was found to be higher for the nanocomposite compared to the pristine materials. The photocatalytic mechanism revealed that the formed heterojunction followed the Z-scheme mechanism.

Keywords: Pharmaceuticals, advanced oxidation processes, photdegradation, photoelecrochemical properties.

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Formulating an oral emulsion with an association of Carum carvi L. and Foeniculum vulgare Mill. using a planification experimental design

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Essential oils are increasingly recognized for their therapeutic potential and their health benefits, but they are highly concentrated preparations and can cause symptoms of intoxication in case of overdose especially if ingested. The risk is greater when used pure, so it is best to introduce them into preparations or pharmaceutical forms such as emulsions.

The aim of this work is the formulation of an oral emulsion containing two EO: Foeniculum vulgare Mill. and Carum carvi L. using experimental design by evaluating formulas rheological and microscopical characteristics. For this purpose, a full factor screening experimental design was used by varying three main factors: mixing rate, emulsifying and thickening agents percentages on the formulas rheological properties.

The composition of the formulation and the process conditions were optimized to obtain the most stable emulsion, which was having the lowest viscosity, critical speed and consistency, with moderate process conditions.

Such a formulation seems promising as a drug for oral application.

Key words: Carum carvi L essential oil, Foeniculum vulgare Mill, oral emulsion, experimental design.

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PHENYLETHANOIDES : ISOLEMENT DE MOLECULES NATURELLES AUX NOMBREUSES ACTIVITES BIOLOGIQUES

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Les glycosides phényléthanoïdes (PhG) constituent une classe de composés hydrosolubles largement répandus dans les plantes. Ces composés se retrouvent dans les familles Scrophulariaceae, Oleaceae, Plantaginaceae, Lamiaceae et Orobanchaceae. Le genre *Phlomis* de la famille des Lamiaceae comprend 113 espèces. Quatre espèces poussent dans le nord de l'Algérie : *Phlomis herba-venti* L., *P.bovei* Noë, *P.caballeroi* Pau et *P.crinita* Cav **[1]**. En médecine traditionnelle algérienne, les espèces du genre *Phlomis* sont utilisées pour traiter les plaies et les ulcères.

L'objectif du présent travail est d'isoler des phenylethanoides glycosides à partir du *Phlomis bovei*, une plante peu étudiée sur le plan phytochimique

Cinq (5) phenylethanoides ont été isolé pour la premiére fois du *P.bovei*. Deux à partir des feuilles **(**verbascoside et angoroside C) et trois à partir des racines (leucosceptoside B, forsythoside B, et diacétyl martynoside)

Les composés ont été identifiés par analyse des données spectroscopiques 1D- (1H, 13C), 2D-RMN (1H–1H COSY, TOCSY, ROESY, HSQC, HMBC), spectrométrie de masse (ESI- et HR-ESI-MS) et par comparaison avec des données spectrales précédemment rapportées.

Mots-clés : phenyl ethanoides, isolement, *Phlomis bovei*, Algérie

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Synthesis of 3-aminohydantoin via condensation of hydrazines with isocyanates derived from α-aminoesters and preliminary study of their Anti-inflammatory activity

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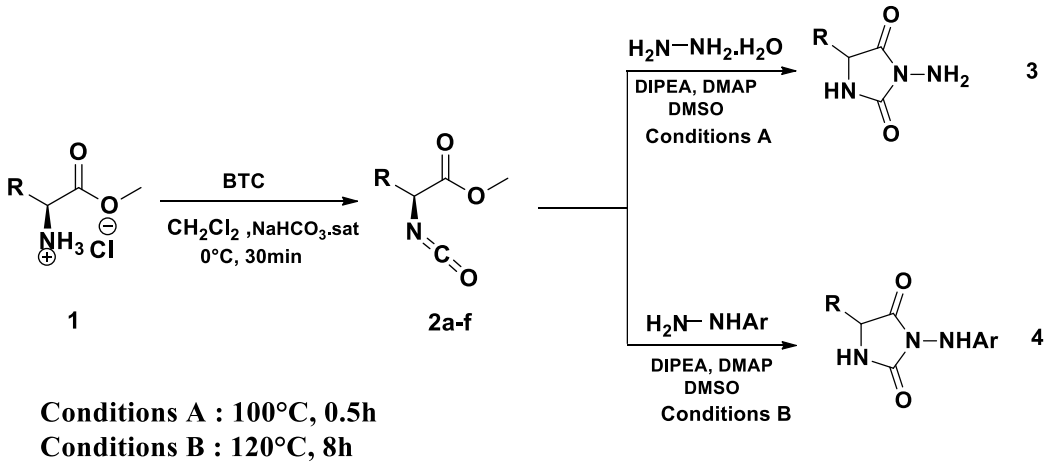
3-aminohydantoins, also known as 3-aminoimidazolidine-2,4-dione, are compounds with a relatively simple structure but of great significance of the field of medicinal chemistry due to their potential applications in therapeutic development. However, obtaining these compounds in their racemic form presents a challenge. Certain synthesis methods require highly advanced energy conditions[7],[8] and, in some cases, involves reagents that are not readily available or rely multiple-step reaction sequences, often spanning five or six stages[9].

In this work, we have developed a new two-step synthesis route starting from amino acid esters (scheme1). Thus, the compounds were characterised by ^{1}H NMR, ^{13}C NMR, TF-IR and HRMS). A biological study revealed that some of these compounds possess anti-inflammatory activities.



Scheme 1: Synthesis route of 3-aminohydantoins derivatives[10].

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New quinazoline hybrids as amyloid-β aggregation inhibitors with dual cholinesterase inhibition and antioxidant properties for Alzheimer's disease

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Alzheimer's disease (AD) is the leading cause of degenerative dementia in the elderly, marked by progressive cognitive decline and memory loss. Central to its pathology are extracellular amyloid-β (Aβ) plaques and intracellular neurofibrillary tangles formed by hyperphosphorylated tau proteins. Current research supports the amyloid cascade hypothesis, which links Aβ aggregation to neuronal degeneration in AD. Additionally, cholinergic dysfunction, characterized by reduced levels of acetylcholine (ACh), is a key feature, contributing to cognitive impairment.

In light of these dual pathological hallmarks, therapeutic strategies combining cholinesterase inhibition with modulation of Aβ aggregation are critical. Quinazoline derivatives have shown potential as multi-functional agents in AD, acting as cholinesterase inhibitors, Aβ aggregation modulators, and antioxidants.

This study proposes the development of new quinazoline-based molecules with multi-target activity. We synthesized functionalized quinazolines through a multi-step process, beginning with the reaction of 2-aminobenzonitrile derivatives with various orthoesters, followed by the introduction of substituted anilines. These novel compounds were evaluated for their ability to inhibit Aβ aggregation, cholinesterases, and oxidative stress. Preliminary biological tests revealed promising efficacy across these targets. Further biological assessments using the acidic quinazolines, obtained via a saponification reaction, indicate their potential as therapeutic agents for AD, offering both symptomatic relief and disease-modifying effects.

Keywords: Alzheimer's disease, Quinazoline, Cholinesterase, Amyloid-β, tau proteins, antioxidants

Semi-synthesis of new structural analogs of harmine linked to 1,2,3-triazoles, anti α-amylase potential, Molecular Docking and ADMET Profiling

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Harmine is a naturally occurring β-carboline alkaloid that was originally isolated from *Peganum harmala*. Various studies have revealed that it exhibits a broad spectrum of pharmacological properties, including anti-inflammatory, antibacterial, antiviral, anticancer, and anti-diabetic effects. [1,2] Thus, we aimed to isolate and modify this alkaloid from this plant to identify new antidiabetic candidates. Harmine (1) was quantitatively isolated from the chloroform extract of the *P. harmala* seeds. Subsequently, a series of novel harmines linked to 1,2,3-triazole derivatives (**4a-j**) was synthesized via 1,3-dipolar cycloaddition. Furthermore, Harmine and its structural analogs were characterized by ^{1}H, ^{13}C NMR, and HRMS. The synthesized compounds were assessed *in vitro* for their anti-α-amylase activity. Molecular docking was performed to investigate the behavior of our products with respect to the α-amylase enzyme. Predictive ADMET analysis of these compounds was realized to better understand their pharmacokinetic and drug-like properties. The obtained results showed that **4a**, **4b**, **4d**, **4f** and **4j** were actives and have potentially interesting antidiabetic effects.

Key words: Harmine, 1,3-dipolar cycloaddition, α-amylase, Molecular Docking, ADMET.

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Pt-doped g-C_3N_4 photocatalyst for hydrogen production under visible light

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Metal-free catalysis, particularly utilizing semiconducting $_g$-C_3N_4 (graphitic carbon nitride, CN), is currently a highly discussed subject due to its sustainability and promising performance in various crucial reactions. Despite its application as a photocatalyst, the efficacy of g-C_3N_4 under visible light remains constrained, primarily due to slow charge transfer, fast recombination of photogenerated electron/holes pairs (e-/h+), and limited surface area [1]. Consequently, numerous strategies have been explored to enhance its photocatalytic capabilities.

In this study, bulk CN was synthesized through the thermal treatment of a mixture of urea and melamine. Subsequently, to improve its crystallinity and photocatalytic performance, CN was loaded by Pt nanoparticles, resulting in the material denoted as Pt-CN. The materials were further characterized using XRD, FTIR, SEM, and N_2 adsorption at -196 ºC. Photocatalytic performance evaluation of the prepared materials was conducted under visible light, focusing on the hydrogen production using methanol and anisyl alcohol as sacrificial agents.

Key words: Photocatalysis, g-C_3N_4, .Pt, Hydrogen production

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DFT Study and Anticancer Evaluation of Novel Benzimidazole Derivatives

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This study reports the synthesis and detailed characterization of novel benzimidazole derivatives with strong potential as anticancer agents. Density functional theory (DFT) calculations were employed to optimize the geometric structures, showing excellent alignment with experimental results. The electronic properties of these compounds were examined, and their anticancer efficacy was tested across multiple cancer cell lines, including MDA-MB-231, MCF-7, and HT-29. Among them, compound 2a demonstrated particularly high cytotoxicity against the MDA-MB-231 breast cancer cell line, highlighting its promise as a therapeutic candidate. These results underscore the relevance of benzimidazole derivatives in the pursuit of next-generation anticancer drugs and offer valuable insights for advancing molecular design and drug development.

Key words: Benzimidazole derivatives, Density Functional Theory (DFT), Cytotoxicity, Anticancer agents, Molecular docking

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Visible light induced (Zn^{2+}) reduction over (CuO/TiO_2) catalyst

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Zinc (Zn^{2+}) has a high toxicity in water beyond a certain threshold concentration of (Zn^{2+}) in water is mainly due to incontrollable industrial discharges. This has a direct consequence on health and human beings. Several techniques are used to remedy these problems such as reverse osmosis, ion exchange resins and coagulation which require sophisticated equipment.

In this work, we have successfully tested the photo reduction of (Zn^{2+}) in the presence of (CuO/TiO_2) material under visible irradiation.

First, we synthesized TiO_2 by sol gel method. Then, ($10\%CuO/90\%TiO_2$) was prepared by co-precipitation method and characterized physically. The X-ray diffraction spectrum shows the existence of characteristic peak at (111) attributed to the CuO reflection. It exhibits a nano particle size (6 nm). The width band gap (2.36 eV) obtained from the Kubelka-Munk equation is well located to the sunlight.

As application, the (Zn^{2+}) photo reduction is sucesufully achieved in air-equilibrium suspension by ratio ($CuO\text{-}TiO_2/Zn^{2+}$) (1/1). The irradiation simples were analyzed by compexometric method, 96% of (Zn^{2+}) was reduced by photo catalytic process under optimal condition. In parallel, the photo production of hydrogen is carried out, 3.6 cm^3 of hydrogen gas was evolved.

Key words: nano particle, (CuO/TiO_2), visible light, (Zn^{2+}).

Ultrasensitive Label-Free Detection Using Electrochemical Capacitance Spectroscopy for Food Safety, Environmental, and Medical Applications

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Electrochemical capacitance-derived impedance spectroscopy (ECS) has emerged as a powerful tool for ultrasensitive and label-free biosensing, relying on changes in interfacial redox capacitance to detect specific analytes [1]. This method exploits surface-confined redox groups and mixed molecular films composed of recognition elements, such as protein or aptamers, to transduce the binding of analytes with high sensitivity.

For instance, we developed a capacitance-based biosensor for kanamycin detection at sub-femtomolar levels, incorporating melanin-like polymeric films and gold nanoparticles (AuNPs). This sensor achieved a detection limit of 0.3 fM and was successfully applied to detect kanamycin in milk samples, ensuring accurate monitoring of antibiotic residues in food products. Similarly, we applied ECS to detect nitrite ions in processed meats using a polydopamine/AuNP-modified electrode, with a detection limit of 1.98 μM, demonstrating its suitability for environmental monitoring. In addition, we engineered an aptasensor for acetamiprid detection in fortified tomato samples, utilizing magnetic beads and ferrocene to enhance redox properties, achieving a detection limit of 0.94 fM. We further demonstrated the versatility of ECS by detecting the breast cancer biomarker α-lactalbumin using a printed single-walled carbon nanotube (SWCNT)-based electrode modified with polycatechol. This sensor exhibited exceptional sensitivity and specificity, with a detection limit of 9.7 ng/mL.

These examples highlight the wide-ranging applicability of ECS for food safety, environmental monitoring, and medical diagnostics, offering an efficient, highly sensitive, and specific platform for real-world sample analysis.

Key words: capacitance, label-free detection, food safety, environmental monitoring

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Synthesis of Magnetic Hydrochar from Hawthorn Seeds for the Determination of Fluoroquinolones in Chicken Meat Using Magnetic Solid-Phase Extraction, Liquid Chromatography and UV detection

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Pharmaceuticals in biological matrix have been an environmental issue since the 1994s [1]. An important but often ignored aspect is the fate of antibiotic residues that reach the environment by different pathways. In this work, magnetic hydrochar from hawthorn seeds was successfully synthesized via the hydrothermal method and used as an adsorbent in magnetic solid-phase extraction (MSPE) for the separation of trace fluoroquinolone antibiotics (Ciprofloxacin and Delafloxacin) in chicken meat, followed by analysis using high-performance liquid chromatography (HPLC) with UV detection. The synthesized adsorbent was characterized using different techniques, including Fourier Transform Infrared (FTIR), scanning electron microscopy (SEM) and transmission electron microscopy (TEM). The separation of fluoroquinolone antibiotics was carried out on a C18 column using isocratic elution. The mobile phase consisted of acidified water (1% formic acid, pH 3) and acetonitrile in a 16:84 ratio. Various parameters influencing extraction efficiency were studied and optimized. Under the optimized conditions, the method provided excellent linearity, with the coefficient of determination (R^2) ranging from 0.9992 to 0.9995. Spiked recoveries were also high, ranging from 82.1% to 98.6%, with a relative standard deviation (RSD) of less than 4.5%.

Keywords: magnetic solid phase extraction (MSPE), carbon nanotubes, fluoroquinolones, chicken meat, HPLC-UV.

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APPLICATION OF NICKEL IRON LAYERED DOUBLE HYDROXIDES/ACTIVATED CARBON (NiFe-LDH@AC) COMPOSITE FOR PRECONCENTRATION AND REMOVAL OF Cr AND As FROM WATER SYSTEMS

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Text of the abstract A nickel-iron layered double hydroxides/activated carbon (NiFe-LDH@AC) composite was synthesised via hydrothermal assisted ultrasonic exfoliation and its structural properties and morphologies were characterised using various analytical characterization techniques. These include transmission electron microscopy (TEM), scanning electron microscopy coupled with energy dispersive spectroscopy (SEM-EDS), Fourier transform infrared (FT-IR) spectroscopy, Brunauer–Emmett–Teller (BET) and X-ray diffraction (XRD). The material was applied as an adsorbent for preconcentration and removal of As and Cr. The target analytes were quantified using inductively coupled plasma optical emission spectroscopy (ICP-OES). Under the optimal conditions, the preconcentration method was validated with respect to linearity, limits of detection (LOQ), accuracy, limits of quantification (LOQ) and precision. The linear ranges were 0.1-150 µg/L and 0.07-100 µg/L for As and Cr, respectively. The precision was investigated in terms of repeatability and reproducibility. The results were expressed in terms of relative standard deviation (%RSD) and the values were less than 5%. The LOD and LOQ ranged from 0.021-0.031 and 0.1-0.07 µg/L for As and Cr, respectively. Finally, the accuracy was validated by successfully analysing spiked samples and the recoveries ranged from 92.6-99.2%. The adsorbent was then explored for the removal of target analytes and adsorption capacities were 102 mg/g and 92.6 mg/g for As and Cr, respectively. The metal ions adsorption was evaluated using kinetics and isotherm models and the results followed pseudo second-order kinetics and Langmuir isotherms. Finally, the removal efficiency for spiked effluent wastewater samples ranged from 89.7-100%.

Key words: adsorption, Layered double hydroxide, wastewater

Effect of extraction methods on the physicochemical characteristics of polysaccharides from orange peels : Natural ingredients for cosmetic formulations

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The study evaluated and compared four extraction techniques—hot water extraction (HWE), supercritical fluid extraction (SFE), ultrasonic assisted extraction (UAE), and microwave assisted extraction (MAE)—to isolate polysaccharides from orange peels for cosmetic formulations. Although the extracted polysaccharides shared similar monosaccharide compositions, as confirmed by FT-IR and NMR spectroscopy, they exhibited differences in molecular weights, intrinsic viscosities, uronic acid content, and degrees of esterification, which influenced their solubility, viscosity, and gelling properties. These variations are crucial for their functional roles in cosmetics. Notably, the extracted polysaccharides showed strong antioxidant activity, making them promising natural antioxidants. When incorporated into cosmetic creams, the polysaccharides improved texture, adding cohesiveness and a refreshing sensation. Supercritical fluid extraction (SFE) proved to be the most efficient method, yielding high-quality polysaccharides while aligning with eco-friendly practices due to its use of non-toxic, non-flammable supercritical CO_2. The study emphasizes the potential of agro-food waste, such as orange peels, as a sustainable source of biopolymers for the cosmetic industry, supporting waste valorization and sustainability efforts.

Key words: Polysaccharides from orange peels, extraction techniques, supercritical fluid extraction (SFE), physicochemical properties, cosmetic formulations.

Treatment of chlorpheniramine by using an advanced oxidation process : Boron doped diamand electrode

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Due to the fact that medicines have been produced for years, their production has increased by orders of magnitude; as a result, they contribute to the pollution of water with pharmaceutical chemicals. These pollutants are adversely affecting the environment and all living organisms. Therefore, the elimination of these pollutants from aqueous effluents has emerged as a major problem. Apart from, electrochemical oxidation has also powerful ability to remove the target contaminants and anodic oxidation is considered as one of the environmental friendly process because it can conduct in aqueous solution and form active hydroxyl radicals (OH°) with high oxidation capability during the treatment. We hereby present a report on the anodic oxidation of chlorpheniramine-CLP, a pharmaceutical class antihistamine in an aqueous medium purposed to study its treatment by Boron-Doped Diamond BDDElectrode. The effectiveness of this process is governed by different operative parameters: the initial chlorpheniramine concentration, the electric current density (J), the treatment time and reaction medium temperature. This study aimed to determine the optimum conditions of chlorpheniramine treatments using anodic oxidation by Doehlert experimental design on a boron-doped diamond (BDD) electrode. The optimal conditions for the treating chlorpheniramine were 40.810-5 M concentration, electrical density of

The optimal current density for the formation of a biofilm was 87 mA cm-2 with a treatment time of 8 hours at 37 ºC and this resulted in 98% removal efficiency of chemical oxygen demand (COD) and a nitrate ions concentration of more than 95%. These results reflect the high efficiency of removing clofenamine from aqueous solutions via anodic oxidation on boron-doped diamond.

Keywords: Electrochemical treatment, Chlorpheniramine, BDD, COD determination.

Dielectric Strength of Methyl Esters of Vegetable Oils from *Ricinus communis* and *Jatropha curcas* as a Substitute for Mineral Oil in Power Transformers

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This study aims to compare the dielectric strength of methyl esters derived from vegetable oils, specifically those obtained from crude oils of *Jatropha curcas* and *Ricinus communis*, with that of mineral oil typically used in power transformers. Vegetable oils, known for their good thermal conductivity, are increasingly explored as alternatives to mineral oil due to their lower fire risk, biodegradability, and improved environmental footprint. The study investigates whether methyl esters derived from these natural sources can effectively replace mineral oil in power transformers. The methyl esters of *Jatropha curcas* (*JMEO*) and *Ricinus communis* (*RMEO*) are synthesized through transesterification, employing potassium hydroxide (KOH) as a homogeneous catalyst.

Key words: *Ricinus communis* oil, methyl ester of *Ricinus communis*, *Jatropha curcas* oil, methyl ester of *Jatropha curcas*.

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Synthesis, Characterization, and Applications of Manganese Oxide Nanoparticles and Nanocomposites

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Water pollution, particularly from industrial wastewater, is a major environmental issue due to the presence of harmful organic compounds like synthetic dyes, which are difficult to degrade using conventional methods [1]. Among the various solutions, photocatalysis has emerged as an eco-friendly approach, utilizing light to drive chemical reactions that effectively degrade harmful and toxic compounds [2], using specifically metal oxide nanoparticles show strong potential for enhancing photocatalytic activity, making them ideal for environmental remediation [3].

In this work, we synthesized manganese oxide nanoparticles Mn_3O_4, and nanocomposites with molybdenum dioxide (Mn_3O_4@MoO_2), that were developed using a simple chemical bath method. X-ray diffraction (XRD) reveals that Mn_3O_4 crystallized in a tetragonal phase, while Mn_3O_4@MoO_2 exhibit a monoclinic phase. Scanning electron microscopy (SEM) showed that Mn_3O_4 presented a nanosphere shape with an estimated size of 40 nm, while Mn_3O_4@MoO_2 exhibited two shapes: nanospheres with an estimated size of 55 nm and nanorods with an estimated length of 105 nm. Diffuse reflectance spectroscopy (DRS) revealed bandgap energies of 3.05 eV for Mn_3O_4 and 2.58 eV for Mn_3O_4@MoO_2. Photocatalytic tests for methylene blue (MB) degradation under sunlight showed that Mn_3O_4@MoO_2 nanocomposites exhibited a higher performance compared to Mn_3O_4 due to improved charge transfer that enhanced light absorption.

Key Words: Oxide nanoparticles, Nanocomposites, Mn3O4, MoO2, Heterogeneous photocatalysis, Methylene blue.

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Sustainable and stability indicating liquid chromatography-mass spectrometry method for the quantitation of delafloxacin in pharmaceutical formulations

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A sensitive, precise, accurate, and green analytical HPLC-ESI-MS method for the quantification of delafloxacin and its degradation products in pharmaceutical dosage forms has been optimized and validated. The best separation was achieved with isocratic elution, the mobile phase is composed of a mixture of 0.1% trifluoroacetic acid in water and acetonitrile 65:35 (v/v), the flow rate is 0.5 mL/min and the column used is Kinetex Core-shell C18 (250 × 4.6 mm, 5 µm). Forced degradation studies were performed to prove that the method is indicating of stability. The pharmaceutical substance is prone to oxidative (H_2O_2 3%), acidic (HCl 0.1 M) and basic (0.1 M) conditions. Delafloxacin proved to be susceptible to acidic (HCl 0.1 M), basic (0.1 M), and oxidative (H_2O_2 3%) conditions. The validation of the analytical method was carried out following the ICH guidelines [1]. The method was validated in terms of specificity, precision, linearity and accuracy. The limits of detection (LOD) and quantification (LOQ) of delafloxacin are respectively 0.005 and 0.017 µg mL^{-1}.

Key words: Delafloxacin, Pharmaceuticals, Liquid chromatography- mass spectrometry, Degradation products, Green chemistry.

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Elimination profile of 20-hydroxyecdysone(20-OHE) in urine: Liquid-Liquid extraction and dilute and inject methodology using UHPLC/HRMS : A comparative study

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Ecdysteroids are of interest as potenial sport performance enhancers, due to their anabolic effects. Several studies have been reported on the elimination profile of ecdysterone in urine and blood by applying different sample extraction and analysis techniques.

Since ecdysterone is introduced in the monitoring list of WADA in 2020, many of the antidoping laboratories introduced the monitoring of ecdysterone in their screening procedures, which can be liquid -liquid extraction, solid phase extraction or dilute and inject as per the extraction protocol followed by the respective laboratories.

The aim of the present study was to compare liquid liquid extraction and dilute and inject procedure using UHPLC high resolution mass spectrometry for the detection of supplement derived 20 OHE and its metabolite by administration to healthy volunteers.To carry out the same, two different supplement preparations were administered to two volunteers and their excretion profile was evaluated. It was aimed to match the scenario for the anti doping laboratories where the samples received would be from the athletes who may consume supplments containing ecdysterone.

An UHPLC-MS/MS method was developed for the detection of 20 hydroxy ecdysone (20 OHE) and its metabolite 14-deoxy 20OHE. The chromatographic separation was performed on Acquity UPLC®BEH C18 column (2.1 mm x 100, particle size 1.7 µm), the mass spectrometer was operated in positive mode ionisation (ESI+) with acquisition in full scan and MSMS mode simultaneously.

The results show the elimination profile with the peak concentration of 20 OHE at 4-5 hours and the mass accuracy was less than 2 ppm for the identification of 20 OHE (m/z 481.3160) and its metabolites 14-deoxy 20 OHE (m/z 465.3211) using either dilute and inject or liquid-liquid extraction.

Key words: 20-OHE, Excretion urine, LC-HRMS, Extraction, DS

Advanced analysis of the adsorption mechanism for odorants molecules on human olfactory receptor via statistical physics theory and molecular docking

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In the present paper, a double layer advanced model was used to investigate the adsorption process putatively involved in the olfactory perception of sotolone and abhexone molecules on the human olfactory receptor OR8D1. The number of adsorbed molecules or the fraction of adsorbed molecule per site, n, informed that the two odorants molecules are docked on OR8D1 binding sites with mixed parallel and nonparallel anchorages. Furthermore, the estimated molar adsorption energy ($-\Delta E1$ and $-\Delta E2$) were inferior to 40 kJ/mol for the two adsorption systems, which confirmed the physical nature and the exothermic character of the adsorption process. In addition, stereographic characterizations of the receptor sites surface were carried out through the determination of the receptor site size distribution (RSDs) via Kelvin equation, which spread out from 0.05 to 1.5 nm. The adsorption energy distributions (AEDs) via Polayni equation show an adsorption band spectrum localized between 17 kJ/mol and 22.5 kJ/mol for sotolone and abhexone molecules respectively. A molecular docking calculation was performed. The results indicate that the binding affinities are belonging to the spectrum of the energy band of the molecules sotolone and abhexone, with values 19.66 kJ/mol and 19.24 kJ/mol.

Keywords: Olfaction process; Statistical physics modeling; Sotolone; Abhexone; Molecular docking

Application of advanced analytical models to evaluate and analyze the adsorption mechanism of three emerging pharmaceutical pollutants on a phosphorus carbon adsorbent

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The double layer adsorption of sulfamethoxazole, ketoprofen and carbamazepine on a phosphorus carbon-based adsorbent was analyzed using statistical physics models. The objective of this research was to provide a physicochemical analysis of the adsorption mechanism of these organic compounds via the calculation of both steric and energetic parameters. Results showed that the adsorption mechanism of these pharmaceuticals was multimolecular where the presence of molecular aggregates (mainly dimers) could be expected in the aqueous solution. This adsorbent showed adsorption capacities at saturation from 15 to 36 mg/g for tested pharmaceutical molecules. The ketoprofen adsorption was exothermic, while the adsorption of sulfamethoxazole and carbamazepine was endothermic. The adsorption mechanism of these molecules involved physical interaction forces with interaction energies from 5.95 to 19.66 kJ/mol. These results contribute with insights on the adsorption mechanisms of pharmaceutical pollutants. The identification of molecular aggregates, the calculation of maximum adsorption capacities and the characterization of thermodynamic behavior provide crucial information for the understanding of these adsorption systems and to optimize their removal operating conditions. These findings have direct implications for wastewater treatment and environmental remediation associated with pharmaceutical pollution where advanced adsorption technologies are required.

Keywords: double layer adsorption, carbon-based adsorbent, pharmaceutical pollutants, statistical physics

Structural features, antioxidant potential and protective effect of a polysaccharide from *Lycium arabicum*

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A water-soluble polysaccharide called LAP was isolated from the fruits of *Lycium arabicum* and investigated. LAP contains carbohydrates (82.45 ± 1.23 %), protein (1.56 ± 0.21 %), and uronic acids (3.56 ± 0.34 %). The analysis of the monosaccharide composition revealed the presence of rhamnose, arabinose, galactose, glucose and mannose in a molar ratio of 4.7 : 1.5 : 1 : 8.7 : 16.4 : 5.6. The interpretation of its GC/MS, FT-IR and NMR data allowed to deduce that this polysaccharide is heterogeneous and highly branched. LAP displayed a strong antioxidant activity at low concentrations evaluated by the DPPH-radical scavenging, ferric reducing activity power FRAP, free radical scavenging ability, superoxide radical-scavenging and hydroxyl radical-scavenging abilities. Inhibition of erythrocyte hemolysis and lipid peroxidation was also assessed. In 5 h, LAP treatment allowed the protection of the damaged erythrocytes caused by AAPH and enabled to reduce the level of malondialdehyde (MDA) as well as to increase the reduced glutathione (GSH) level.

Keywords: *Lycium arabicum*, polysaccharide, antioxidant potential.

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Phytochemistry of genus *Centaurea* grown in Algeria: Extraction, Isolation, Structural elucidation and Chemotaxonomy

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The species *Centaurea omphalotricha, C. dissecta* and *C. granatensis* growing in Algeria, belong to *Centaurea* genus within the Cardueae tribe and subtribe Centaureinae of the Asteraceae family (Compositae) divided into 12 subfamilies and 35 tribes. Asteraceae is one of the largest and most important families in the plant order Asterales, containing more than 1620 genera and 23 600 species manifesting as either annual or perennial herbs, trees, and shrubs. They are widely distributed throughout the Mediterranean basin, Asia and America. Moroever, *Centaurea* species exhibit significant pharmacological interest as plants used in folk medicine for the treatment of skin cancer, rheumatism, insect bites, gastric ulcers, wounds, hemorrhoids, asthma and malaria. Previous reports on *Centaurea* plants indicated the occurrence sesquiterpene lactones, flavonoïds, triterpenoids, phytosterols, lignans, phenolic acids, coumarins, and alkaloids. However, flavonoïds and sesquiterpene lactones are the major components of this genus possessing many interesting biological activities such as antioxidant, anti-inflammatory, antimicrobial and anticancer properties. Phytochemical research of *Centaurea omphalotricha, C. dissecta* and *C. granatensis* led to the isolation of 60 secondary metabolites including sesquiterpene lactones, flavonoids, lignanes, polyphenols and triterpenoids. Their structures were elucidated by means of extensive 1D- and 2D-NMR, ESI-MS, hydrolysis acid and by comparison with reported data in the literature. Furthermore, the chemotaxonomic significance of all isolates was discussed.

Key words: *Centaurea*, Asteraceae, Sesquiterpenes, Flavonoids, Triterpenoids, NMR.

Etude chimique et valorisation biologique d'huiles essentielles issues de *Ficus carica*

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Depuis les nuits des temps, les plantes ont constitué la source majeure de médicaments puisqu'elles contiennent des principes actifs possédant plusieurs effets pharmacologiques. La flore Tunisienne constitue une réserve importante d'espèces végétales intéressantes. Les huiles essentielles et les principes actifs issus de ces plantes peuvent être employés dans divers secteurs tels que les industries agroalimentaire, cosmétique et pharmaceutique. Dans cette étude, on s'est intéressé à l'étude chimique et biologique de *Ficus carica.*

Nous avons entamé notre étude par l'extraction des huiles essentielles des écorces des tiges de *Ficus carica* récoltés pendant trois stades de maturation (été, automne et hiver) en utilisant la technique de l'hydrodistilation. Dans une deuxième étape, nous avons identifié les constituants de ces huiles moyennant la technique GC-MS. Dans une troisième étape, nous avons évalué leurs activités antioxydantes en utilisant deux méthodes (DPPH et CAT), leurs propriétés antibactériennes contre cinq bactéries et leurs effets antidiabétiques.

Les résultats montrent que les huiles essentielles sont douées de potentiels antioxydant et antidiabétique très intense. Cependant, des résultats modérés ont été rapportés contre les bactéries testées par rapport au contrôle positif Gentamicine.

Mots clés : *Ficus-carica*, huiles essentielles, GC-MS, activité antioxydante, activité antibactérienne, α- amylase.

Étude de l'influence de la taille des particules sur la qualité de l'huile essentielle de la poudre d'écorces de quelques variétés d'agrumes

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Le présent travail porte sur l'étude l'effet de la taille des particules sur la qualité de l'huile essentielle de la poudre d'écorces de cinq variétés d'agrumes. Les écorces ont été séchées, découpées, broyées et tamisées. L'extraction d'huile essentielle par hydrodistillation assistée par micro-ondes (HDMO) (dispositif type Clevenger monté sur micro-onde) a montré des avantages par rapport à l'hydrodistillation classique, notamment des temps d'extraction plus courts ainsi que des rendements supérieurs. Les résultats obtenus montrent que le diamètre moyen des particules de 350µm a donné le rendement le plus élevé en huile essentielle. Les rendements obtenus varient (en % mass) entre 2,2 et 7,66%. L'analyse par chromatographie en phase gazeuse (CPG) de trois échantillons de mandarine de la variété *Citrus reticulata Blanco* (180µm, 350µm et 500µm) a montrée des différences dans le nombre de pics et de composés identifiés pour chaque échantillon. De plus, la plus grande quantité de composés identifiés a été relevée dans l'échantillon de taille 350µm. D'autre part, la concentration du composé majeur (le limonène) la plus élevée a été observée dans l'échantillon de taille 500µm. Pour mieux interpréter les résultats obtenus, notre étude a été achevée par l'analyse de la poudre d'écorces de différentes tailles avant et après l'extraction d'huile essentielle, en utilisant le MEB (microscope électronique à balayage).

Mots clés: Extraction, micro-onde, agrume, huile essentielle, granulométrie, composition.

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Comparison between thermal treatment and microwave drying of garlic (*Allium sativum* L.) leaves: Kinetics modeling and changes in phenolic compounds profile

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The leaves of garlic (*Allium sativum* L.), known for their mild flavor and rich bioactive compounds. The present study investigated the influence of microwave drying (100–450 W) and oven temperature (40–70°C) on the color, phenolics profile and radical scavenging activity of garlic leaves. Effect of microwave power and oven temperature on drying kinetics modelling were also studied. Page's model was found to be the best for fitting the experimental drying kinetics. Specific energy consumption increased with increasing microwave power from 80 to 137 MJ/kg of water at 100 and 450 W, respectively, whereas the energy efficiency decreased.

Effective moisture diffusivity ranged from 0.211 to $0.718\times10-^{11}$ m^2/s, and the activation energy was determined as 34.66 kJ/mol using the modified Arrhenius equation. Drying at 450 W produced a very distinct product because the sample's ΔE value (24.87) was higher than those dried at lower microwave powers (ΔE = 14.66–16.86). Analysis by liquid chromatography coupled with mass spectrometry of garlic extracts resulted in identification of 5 phenolic acids and 11 flavonoids. Total identified phenolics in the fresh leaves was 1.28 mg/g extract, which increased for dried leaves at 100 W (5.6 mg/g extract), then gradually decreased to 2.7 mg/g extract at 450 W. Quercetin 3-O-rhamnoside was the main flavonoid extracted with 4 mg/g extract for the sample dried at 100 W Quercetin 3-O-rhamnoside emerged as the major compound (9.42 mg/g extract) in dried garlic leaves at 40°C. Furthermore, drying at 40°C increased phenolic content to ~12.5 mg/g extract, compared to fresh material (~1.28 mg/g extract). However, higher drying temperatures, such as 70°C, led to a significant decline, reducing the phenolic content to 7.33 mg/g extract. The leaves, when dried at 40°C, showed the greatest antioxidant potential, as assessed through DPPH• radical-scavenging activity.

Keywords: Garlic leaves; microwave drying; thermal treatment; drying modelling; phytochemical characteristics; anti-radical activity

Antibacterial and α-glucosidase inhibitors in the *Salvia officinalis* leaves

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Salvia officinalis is a plant which belongs to the Lamiaceae family and the genus *Salvia*. In traditional medicine, it has been used for the treatment of various kinds of diseases such as hyperglycemia and inflammations (mouth, bronchial asthma, angina, throat, and coughs). In this study, we discovered the compounds with antibacterial and anti-α-glucosidase activities from Tunisian *S. officinalis* extracts. For this reason, the leaves of this plant were collected from Gabes, Tunisia. Then, the extracts were prepared using ethyl acetate as a solvent. The combination of planar layer chromatography with *Aliivibrio fischeri*, *Bacillus subtilis*, and *Rhodococcus fascians* as well as α-glucosidase assays was used for the screening of bioactive compounds. For the identification of these compounds, electrospray ionization-mass spectrometry (ESI-MS) was utilized. Two isomer pairs of triterpenes were found as antibacterial and α-glucosidase inhibitors in the tested extracts. Our results demonstrated that leaves of *S. officinalis* may be useful as a therapeutic agent against hyperglycemia and pathogenic bacteria.

Keywords: *Salvia officinalis*, leaf part, extracts, planar layer chromatography, triterpenes.

Elaboration of an hybrid material based on doped hydroxyapatite and modified chitosan for medical application

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In this work, new hybrid materials were synthesized using freeze drying technique. Their chemical composition included a mineral component based on hydroxyapatite codoped with strontium and magnesium and an organic graft composed of modified chitosan. These composites could be used as scaffolds for bone tissue Engineering BTE. Indeed, chitosan was extract from shrimp shells. It is an ideal as a bone graft substituent [1]. This biopolymer is well known for its several properties including biocompatibility, low toxicity, biodegradability and antibacterial activity. However, its flexibility, its hydrophobic surface and its mechanical weakness disable this biopolymer for promoting the bone regeneration [1]. For that reason, a chemical modification was explored to enhance its hydrophility and its adhesion when is mixed with the major component hydroxyapatite. This mineral was synthesized by the co-precipitation method. Furthermore, hydroxyapatite doped with other minerals such as magnesium and strontium could approximately decrease the degradation of apatite in order to mimic the biomineralization process of apatite in bone tissue [2] and to fabricate the most efficient hybrid composite scaffold. The hybrid materials were characterized by XR diffraction, Infrared Spectroscopy and Thermal analysis.

Keywords : modified chitosan, doped hydroxyapatite, hybrid material, scaffold

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Synthesis, structural, magnetic, optical and electronic studies of a novel Honeycomb Kagome Polyoxometalate based copper(II) complex

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A novel hybrid copper complex, $C_{7.5}H_{36.3}Cu_2Mo_5N_3O_{31.4}P_2$, with a Honeycomb Kagome (HK) lattice, was prepared in aqueous solution. Single-crystal X-ray diffraction analysis revealed structural defects due to the non-stoichiometric occupancy of copper and water molecules, a characteristic commonly observed in advanced technologies such as solar cells and superconductors **[1]**. This compound contains two distinct copper(II) ions (one at Wyckoff position 4e and the second at 2d, with 60% occupancy), one and a half 2-methylpiperazinium cations, a unique Strandberg $[P_2Mo_5O_{23}]^{5-}$ anion, and coordinated as well as lattice water molecules. The negative Curie-Weiss temperature, from the Curie-Weiss fit of high temperature magnetic susceptibility data suggests antiferromagnetic interaction between Cu^{2+} moments. The power low behavior and magnetization data collapse indicate a random singlet state characteristic of quantum spin liquid. Electronic structure calculations reveal that the conduction band is dominated by Mo(3d) states, while the valence band features strong hybridization between N(2p), Cu(3d), and O(2p) states. Reflectance and fluorescence studies further elucidate the material's optical properties.

Key words: Magnetic Frustration, hybrid organic inorganic POMs-based materials

References

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Synthesis and Characterization of Cordierite-Mullite Ceramic Phases from Tunisian Kaolin, Granite and Talc

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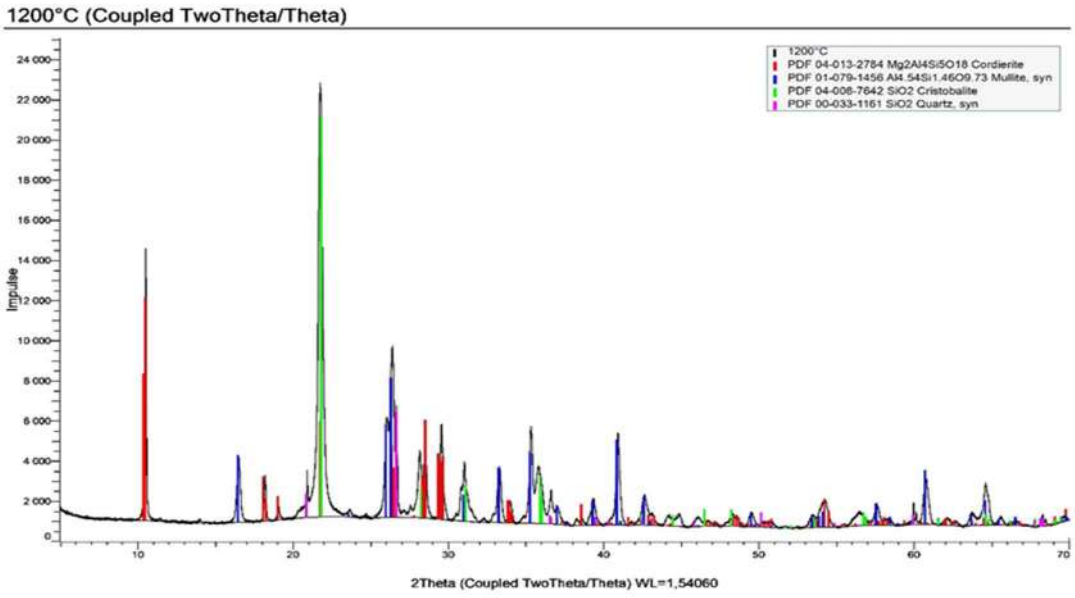
This study explores the synthesis of cordierite-mullite ceramic phases from natural raw materials such as Tunisian kaolin, granite and talc. The materials were characterized using X ray fluorescence (XRF), X-ray diffraction (XRD), scanning electron microscopy coupled with energy dispersive spectroscopy (SEM-EDX), infrared spectroscopy (IR) and differential thermal and thermogravimetric analysis (DTA-TG). The raw material mixture was thermally treated at temperatures ranging from 1000°C to 1200°C. Cordierite and mullite phases were observed at 1200°C
with an average porosity of 45.7% and a density of 1.51 g/cm³. The microstructure of the samples was also studied confirming the formation of stable ceramic phases. These results provide a better understanding of phase transitions in kaolin-granite talc systems and open the door to a potential application in refractory materials manufacturing.



Synthesis, structural characterization and ionic conductivity of Apatite-type $Ca_{10-x}Na_x(PO_4)_{6-x}(SO_4)_xF_2$ (x =0, 3, 6) materials

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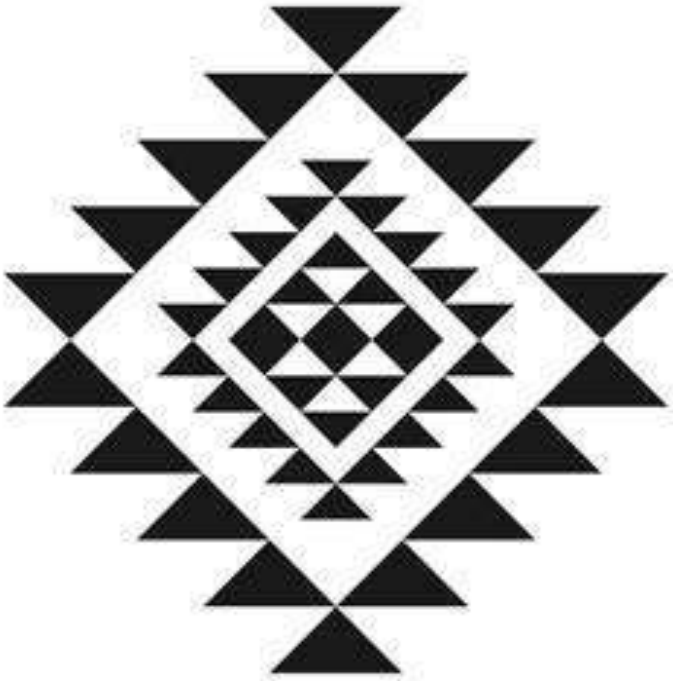
Phosphate-sulfate fluorapatites $Ca_{10-x}Na_x(PO_4)_{6-x}(SO_4)_xF_2$ (x =0, 3, 6) have been synthesized by the solid-state reaction at high temperature. The samples have been characterized by X-ray Diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), Raman scattering spectroscopy and Transmission Electron Microscopy (TEM) techniques. XRD study shows that these materials crystallize in the hexagonal system with P63/m as a space group. An impedance analysis has been used to analyze the electrical behavior of the samples at different temperatures. Evidence of temperature-dependent electrical relaxation phenomena is observed. The bulk resistance decreases with increasing temperature, showing a typical negative temperature coefficient of resistance (NTCR). Ac-conductivity measurements have been performed on a wide range of frequencies and temperatures. The ionic conductivity follows the Arrhenius and the Jonscher laws.



LIST OF POSTER COMMUNICATIONS

Communicatings' Names	**Ref**
K. Abaid, W. Erb, M. Blot, T. Roisnel, F. Mongin, T. Soufiane *FSB - Bizerte* Ferrocenephosphonates: copper-promoted synthesis and further functionalization	**PC 01**
S. Abdelli, O. Berradj, H. Bougherra *Mouloud Mammeri University, Tizi-Ouzou, Algeria* Synthesis and characterization of some metal complexes of curcumin with bipyridine and antioxidant application	**PC 02**
D. Abeira, B. Hamdi, B. Champagne *University of Namur, Belgium* Synthesis, characterizations, optical properties, and DFT investigation of a new organic-inorganic complex	**PC 03**
F. Abid, P. S.S. Lacerda, A. J.D. Silvestre, A. F. Sousa *FSS - Sfax* Advancement in the synthesis of poly(hexamethylene 2,5- furandicarboxylate) via ring opening polymerisation	**PC 04**
F. Agouillal, D. Mancer, N.E.H. Rayan Boudjema, M. Boutemine, T. Chaabane *Houari Boumediene University, Algiers, Algeria* Optimization of total oils, grease, and petroleum hydrocarbons recovery from oily petroleum sludges by freeze-thaw process	**PC 05**
N. Akwesi, Bokolombe P. Ngoy, John Mack, Tebello Nyokong *University of Kinshasa, Dem. Rep. Congo* Photophysical properties and photodynamic antimicrobial study of 2,6-dibromo-BODIPY substituted by 3-bromo 4-hydroxy styryl at 3,5 positions	**PC 06**
F. Alfirjany, S. Alshelmani, S. Salah, D. Jalaly, R. Alnajjar *Libyan International Medical University, Benghazi, Libya* Indole derivative as a possible treatment for breast cancer	**PC 07**
S. Alshelmani, F. Alfirjany, S. Salah, D. Jalaly, R. Alnajjar *Libyan International Medical University, Benghazi, Libya* Triazoles as HER2 inhibitors to overcome brest cancer resistance	**PC 08**
R.H. Amamra, R. Bouasla, M. Berredjem, L. Ferchichi, K. Mellouk *Badji Mokhtar University, Annaba, Algeria* Activité antioxydante de l'huile essentielle de Bubonium graveolens, Docking moléculaire, DFT et étude ADMET de trois dérivés.	**PC 09**
F. Amrouche, N. Bendjaballah-Lalaoui *Houari Boumediene University, Algiers, Algeria* Synthesis and characterization of hybrid materials based on graphene oxide and metal nanoparticles	**PC 10**
K. Ardhaoui *ISBAM - Médenine, Gabès* Détermination des enthalpies de dissolution dans l'eau d'apatites halogénées	**PC 11**
A. Arfaoui, M. Mendili, S. Aschi-Smiti *FST - Tunis* The effect of combined hypoxia and salinity stress on morphological, antioxidant activity and secondary metabolites of Ocimum basilicum L.	**PC 12**

Communicatings' Names	Ref
B. Assel, A.E. Maayoufi, F. Jomni, D. Hellali *FST - Tunis* Thermochemical and electric properties of lithium nitrate	**PC 13**
S. Assissila, S. Ben Ali, T. Triki, F. Guasmi *Institut des Régions Arides - Mednine* Physicochemical characterization of soils under two cultivation methods: Irrigated and non-irrigated	**PC 14**
F. Ayari, M. Mrabet, I. Kamoun, M. Oudni-M'rad, S. M'rad *Faculty of Pharmacy - Monastir* Activité protoscolicide des nanoparticules d'argent	**PC 15**
W. Ayouni, H. Riguene, W. Ben Amor, R. Ben Salem, G. Rigane *FSS - Sfax* Optimized ultrasound-assisted extraction of phenolic compounds from Hylocerus undatus cultivated in Tunisia and evaluation of antioxidant activity in vitro	**PC 16**
Z. Aziz, M.A. Boudjeltia, M.C. Terkhi, M.A. Bennani *Abdelhamid Ibn Badis University, Mostaganem, Algeria* Theoretical investigation of ternary semiconductors half-Heusler RhTaZ (Z = Si, Ge and Sn) for thermoelectric applications	**PC 17**
A. Bahloul, M. Messaad, M. Abdelhedi *FSS - Sfax* Crystal structure, DFT analysis, vibrational characterization, and Hirshfeld surface study of a novel zero-dimensional metal-halide hybrid with outstanding green emission	**PC 18**
L. Baklouti, D. Ben Salah, N. Hamdi *FSS - Sfax* Design of novel phthalocyanines as potential antimicrobial agents starting with synthesized phthalonitrile derivatives:Complexation, extraction	**PC 19**
N. Jegham, S. Gabsi, N.E.H. Ben Fatma, S. Bayoudh, F. Hfaeidh, M.L. Efrit, M.A. El Kaibi *Faculty of Pharmacy - Monastir* Castor oil and laxative activity: in silico exploration of the active components of castor oil	**PC 20**
L.S. Belaroui, Abderraouf Boudahri *University of Oran, Algeria* Enhancement of the antibacterial activity of modified Algerian palygorskite	**PC 21**
D. Belkheiri, S. Cheriet, A. Bouraiou *Ziane Achour University, Djelfa, Algeria* Photocatalytic degradation of methylene blue using ZnO thin layer	**PC 22**
N. Belkheiri, Z. Belkacem, M. Derdour, F. Mechrouh, R.M. Bachar, M. Fodili, M. Amari, P. Hoffmann *Université Ziane Achour, Djelfa, Algérie* Synthesis of New Derivatives of Benzimidazole-Cyclohexanones	**PC 23**
S. Bellatreche, M.A. Hasnaoui *Ahmed Ben Bella University, Oran, Algeria* Synthèse des silicoaluminophosphates nanoporeux à partir de plusieurs agents structurants	**PC 24**
C. Ben Aissa, B. Lepoittevin, J. Baudoux, S. Touil *FSB - Bizerte* Synthèse de nouveaux α-aminophosphonates thiophéniques d'intérêt	**PC 25**

Communicatings' Names	**Ref**
N. Ben Ameur, W. Sassi *CERTE - Borj Cédria* Ultra-rapid Rhodamine B removal by highly efficient recyclable blue crab crustacean	**PC 26**
J. Ben Attig, L. Latrous, I. Galvan, M. Zougagh, Á. Ríos *FST - Tunis* Rapid determination of malondialdehyde in serum samples using a porphyrin functionalized magnetic graphene oxide electrochemical sensor	**PC 27**
M. Ben Braiek, M. Chemeck, B. Ben Hassine *FSM - Monastir* Synthesis, characterization, and photophysical properties of functionalized six and seven-Membered-Ring carbohelicenes	**PC 28**
A. Ben Issa, N. Jaoued, S. Bejaoui, Y. Chevalier, C. Nardin, S. Hbaieb *FST - Tunis* Innovative valorization of Posidonia Lignin for biomedical and cosmetic applications	**PC 29**
A. Ben Khelifa, M. Dhifet, Ezzayani Khaireddine, A. N. Alanazi *FSM - Monastir* Bioactive porphyrin magnesium (II) complex. Synthesis, Molecular Structure and Spectroscopic characterization. Biological Activity and Molecular Docking studies.	**PC 30**
A. Ben Khelifa, M. Dhifet, Ezzayani Khaireddine, A.N. Alanazi, S. Moussa *FSM - Monastir* Synthesis, biological evaluation and molecular docking studies of a new magnesium (II) porphyrin complex	**PC 31**
N. Ben Mabrouk, C. Youssef, H. Ben Ammar *FSM - Monastir* Synthesis of a novel pyrrolyl-pyrimidine derivatives as antidiabetic agents: Molecular docking studies and ADMET prediction	**PC 32**
M. Ben Mosbah, Y. Moussaoui *FSG - Gafsa* Improved synthesis of 2,2′-arylmethylene bis(3-hydroxy-5,5 dimethyl-2-cyclohexene-1-one) derivatives catalyzed by KSF under microwave	**PC 33**
L. Benadda, A. Keniche, A. Aboura, C. Latati *University of Tlemcen, Algeria* Synthesis of new analogues of cinnamic acid : Bioactive compound in propolis	**PC 34**
A. Benayache, L. Lamoudi, K. Daoud *Houari Boumediene University, Algiers, Algeria* Coating uniformity: Influence of atomizing air pressure and spray rate	**PC 35**
A. Benayache, L. Lamoudi, K. Daoud *Houari Boumediene University, Algiers, Algeria* Optimisation de la formulation d'un comprimé orodispersible EBASTINE 10mg	**PC 36**
M.F. Benlamnouar, N. Bensaid, R. Badji *Research Center in Industrial Technologies, Algiers, Algeria* Electromechanical properties of dissimilar welds using different filler metal compositions	**PC 37**
S. Benmebarek, N. Djouambi, S. Bacha, I.E. Benmebarek, B.O. Boussaha, A.B. Mammeria *Université Alger 1, Algérie* Anti-inflammatory therapeutic treatment generated by the extract of "Capsaicin" Pepper	**PC 38**

Communicatings' Names	Ref
L. Benmekhbi, S. Mosbah, A.K. Baghdouch *Salah Boubnider University, Constantine, Algeria* Synthesis, characterization and biological evaluation of new polyphenol derivatives from3-benzyloxy-4-methoxybenzaldehyde	**PC 39**
N. Benosmane, A. Rebahi, K. Chaouche, Y. Moussaoui *M'hamed Bougara University, Boumerdes, Algeria* Enhancing solubility and molecular characterization of Ibuprofen-β-Cyclodextrin inclusion complexes through rapid microwave-promoted formation	**PC 40**
N. Benosmane, Y.M. Aksouh, K. Chaouche, Y. Moussaoui *M'hamed Bougara University, Boumerdes, Algeria* Assessment of heavy metal contamination in irrigation water, soil, and onion crops: A case study from the Isser and Zemmouri regions, Algeria	**PC 41**
S. Benrabeh, E. Zouaoui, K. Ben Yahia, M.L. Fauconnier, M. Romdhane, E. Saadaoui *FSG - Gabès* Variation in the Yield, chemical composition and antimicrobial activity of essential oils of four Eucalyptus species under different bioclimatic conditions	**PC 42**
Z. Benredjem, R. Delimi, I. Chaabna *Badji Mokhtar University, Annaba, Algeria* Cadmium removal from phosphate ore	**PC 43**
Z. Benredjem, T. Rouki, I. Chaabna, M.F. Ghorab *Badji Mokhtar University, Annaba, Algeria* Decontamination of water containing persistent dyes by heterogeneous photocatalysis under solar irradiation	**PC 44**
N. Bensaid, M.F. Benlamnouar, R. Badji *Research Center in Industrial Technologies, Algiers, Algeria* Influence of welding parameters and heat treatments on the electrochemical properties of TIG welds in AISI 430 steel	**PC 45**
D. Berdjane, A. Hafs, S. Achouri, A. Bendjama, B. Maalem *CRTI, Cheraga, Alger, Algérie* Electrochemical behavior of AISI1080 steel in marine environment applications	**PC 46**
S. Bergaoui, W. Zaaraoui, N. Braiek, A. Hadj Said *FSM - Monastir* Electrosynthesis and characterization oligomer deriving from m-propargylanisole	**PC 47**
S. Bergaoui, N. Braiek, W. Zaaraoui, A. Hadj Said *FSM - Monastir* Anodic synthesis of a new oligophenylene deriving from m-fluoroanisole	**PC 48**
O. Berradj, S. Abdelli *Mouloud Mammeri University, Tizi-Ouzou, Algeria* Synthesis, characterization and antioxidant application of some metal complexes of curcumin with bi-pyridine	**PC 49**
M. Berredjem, I. Grib, K. Otmane Rachedi, A. Dekir *Badji Mokhtar University, Annanba, Algeria* Efficient synthesis and characterization of new copper (II) complex with sulfonylphthalimide	**PC 50**
Y. Berredjem, S. Guerfi, N. Bensid, Y.Boutaleb, A.A. Ahmed, O. Belkadi, Y. Ait Ammar, N.E. Zenati *University of Annaba, Algeria* Application des nanoparticules à base de kaolin pour l'élimination des colorants en milieu aqueux	**PC 51**

Communicatings' Names	**Ref**
K. Boltane, S. Ben Ismail, H. Ben Boubaker, H. El Maleh, S. Dabboub, A. Mnif *FST - Tunis* Preliminary study of the abundance of microplastics on the surface waters of the Gulf of Tunis	**PC 52**
N. Bouabidi, H. Ben Jannet *FSM - Monastir* Semi-synthesis and in silico prediction of novel triterpenic acid derivatives	**PC 53**
M. Bouaoun, L. Benmekhbi *REMEDD Laboratory, University of Constantine 3, Algeria* Phytochemical Composition and Antibacterial Activity of Algerian medicinal plant (J.erratica Extracts)	**PC 54**
I. Bouazizi, H. Majdoub, D. Le Cerf, E. Ben Salem *IPEIM - Monastir* A Comparative Study between the organic grafts "Chitosan" and "Modified Chitosan" used in the fabrication of hybrid materials	**PC 55**
H. Boubertakh, Z. Kabouche, A. Khalfallah, A. Boudechicha, A. Kabouche *Frères Mentouri University, Constantine, Algeria* Profile HPLC analyses, antioxidant, antimicrobial activities of Achillea ligustica All.	**PC 56**
H. Bouchnak, A. Ben Hamda, R. Raddadi, A. Hamdi, M.A. Lassoued, J. Kraiem *Faculty of Pharmacy - Monastir* 3-aminohydantoins as a potential Anti-Diabetic Agents In vivo, in vitro and In silico studies	**PC 57**
A. Boudahri, N. Boceiri, A. Lazzaz, L. Belmahdi, L.S. Belaroui *Ahmed Ben Bella University, Oran, Algeria* Novel clay-Schiff base hybrid materials with promising antimicrobial properties	**PC 58**
M. Bouh, H. Najar *FST - Tunis* The study of the photocatalytic activity of a green synthesized material based on ZnO	**PC 59**
A. Bouhaouche, D. Mancer, A. Toubane, K. Daoud *Houari Boumediene University, Algiers, Algeria* 1-Etude de formulation d'une suspension buvable à usage pharmaceutque a base d'extrait de plantes encapsule.	**PC 60**
A. Bouhaouche, L. Chabou, Y. Seffari, K. Daoud *Houari Boumediene University, Algiers, Algeria* Study of melt granulation process applied to a pharmaceutical powder mixture	**PC 61**
M. Bouhjar, K. Zaghdoudi, N. Bellakhal *INSAT - Tunis* Enhancing Poultry Nutrition: Valorisation of Chicken Egg Shells for Calcium Supplementation - Describing the Shell Treatment Process, Physicochemical Characterization, and Microbiological Analysis.	**PC 62**
A. Boukhouiete, S. Boumendjel *Badji-Mokhtar University, Annaba, Algeria* Corrosion inhibition of carbon steel in acidic media using a natural compound	**PC 63**
L. Boukli-Hacene, H. Mokri *University of Tlemcen, Algeria* Effective adsorption of methylene blue with metal-organic framework UIO-66-NH2: Characterization and kinetic analysis	**PC 64**

Communicatings' Names	Ref
H. Boussehel, B. Guerira *University of Biskra, Algeria* Valorization of date palm fibers for biodegradable ldpe composites: effect of chemical treatment on material properties	**PC 65**
S. Chakhari, F. Chabchoub, L. Ismaili *FSS - Sfax* Synthesis and biological evaluation of new quinazolines for Alzheimer's disease treatment	**PC 66**
B. Champagne, F. Mairesse, T. Legat, S. Van Cleuvenbergen *University of Namur, Belgium* Second harmonic generation of l_β-cellulose nanocrystals in solution	**PC 67**
S. Cherni Namouchi, B. Essghaier *FST - Tunis* Synthesis, crystal structure, spectroscopic properties and potential biological activities of a binuclear copper(II) complex di(μ-hydroxo) di(μ-nitrato-O,O') bis(N,N,N',N'-tétraméthyléthylènediamine) cuivre(II) 7,5 hydrate $[Cu_2(OH)_2(NO_3)_2(C_6H_{16}N_2)_2].7,5\ H_2O$	**PC 68**
S. Cherni Namouchi, I. Jendoubi, M.F. Zid *FST - Tunis* Investigation of the physical properties of the new alluaudite-type molybdate $Ag_{0.30}Na_{3.70}Mn(MoO_4)_3$ for photocatalytic and the antimicrobial activity	**PC 69**
A. Chmangui, G. Mahfoudhi, W. Ben Ameur, M.R. Driss, S. Touil, S.Ondes Bouabdallah *FSB - Bizerte* Ultrasound-assisted extraction followed by liquid chromatography-FLD for isolation and assessment of polycyclic aromatic hydrocarbons in commonly consumed fish in Bizerte, Tunisia	**PC 70**
D. Dallali, C. Paris, K. Hamden, M. Varbanov, N. Allouche, J. Fakhfakh *FSS - Sfax* Fructooligosaccharides from Cynoglossum tubiflorus : Effect of the molecular size on their antidiabetic activity in high-fat diet and alloxan induced diabetic rats.	**PC 71**
H. Debbache, N. Khadhri, M.L. Belfar, R. Khiari, Y. Moussaoui, Y. Moussaoui, A. Omar Ayachi *Kasdi Merbah University, Ouargla, Algeria* Agrichar prepared from peanut shell by chemical activation: Functionalization with Fe and Ca and application for heavy metals	**PC 72**
J. Dhaouadi, C. Hamdi, B. Ben Hassine, F. Aloui *FSM - Monastir* Design and Characterization of π-Conjugated Architectures: Synthesis and Insights	**PC 73**
F. Djellouli, B. Chaib, H. Messaoudi, F. Miles, A. Dahmani *Houari Boumediene University, Algiers, Algeria* Phase diagram of sulfaméthoxazole + metronidazole system	**PC 74**
H. Djouama, R. Djouama *Mohamed Khider University, Biskra, Algeria* Electronic structure and optical properties of luminescent complexes: a computational investigation	**PC 75**
F. Dorbanne, W. Madaci, L. Mebrouki *M'hamed bougara University, Boumerdes, Algeria* Etude et formulation du fuel-oil IFO30 à partir des fuels lourds IFO80, 180, 380 et du gasoil	**PC 76**

Communicatings' Names	**Ref**
R. Dridi, B. Esghaier, M.F. Zid *FST - Tunis* Green synthesis of silver nanoparticles using Tunisian plant extract: Characterization and evaluation of biological activities	**PC 77**
M. Elakremi, L. Sillero, J. Labidi, R. Ben Salem, Y. Moussaoui *FSG - Gafsa* Microwave assisted extraction of compounds from the shell of Pistacia vera L. and characterization of the extracts	**PC 78**
H. Elhleli, F. Mannai, R. Khiari, M.N. Belgacem, Y. Moussaoui *FSG - Gafsa* Biosourced innovations from Opuntia ficus-indica: Environmental remediation and encapsulation applications	**PC 79**
A.E. Etsellah, H. Boughzala *FST - Tunis* synthesis and structural characterization of N, N-dimethyl-1, 3- propanediaminium penta bromobismuthate (III)	**PC 80**
R. Fakraoui, E. Dhahri, B. Champagne *FSS - Sfax* Experimental and theoretical studies of the structural, magnetic, and electronic properties of the La0.6Ca0.2Sr0.2MnO3 perovskite	**PC 81**
F. Ferkous, O. Meziani, S. Ait Kaki, K. Kraim, Y. Saihi *Badji Mokhtar University, Annaba, Algeria* Identification de nouveaux inhibiteurs de VEGFR2 comme agents anticancéreux à l'aide d'un criblage virtuel par docking moléculaire	**PC 82**
A. Fkiri, A. Mezni *FSB - Bizerte* Original strategy for facile synthesis of ZrO2 nanoparticles: Structural and optical properties.	**PC 83**
O. Fliss, N. Mekni *LNCM - Tunis* DFT calculations and mechanistic study of the 1,3-dipolar cycloaddition reaction between dichlorophosphoryl isocyanate and hydrocarbon azides	**PC 84**
O. Fliss, A. Labidi, L. Latrous *LNCM - Tunis* A DFT study of Favipiravir complexation through double iron (III) chelation	**PC 85**
O. Gatri, C. Fischmeister, M.L. Efrit *FST - Tunis* Synthèse de nouveaux dérivés de 1,2,4-triazole fonctionnalisés par des réactions de métathèse des oléfines.	**PC 86**
K. Ghanem, Nedjema Chérifi -Bennadji *Mohamed Khider University, Biskra, Algeria* The effect of welding currents on microstructure of steel	**PC 87**
G. Ghannouchi, H. Lazrag, Z. Kibou, N. Choukchou-braham, H. Ben Jannet, A. Romdhane *FSM - Monastir* Innovative green Synthesis of Novel Quinoline Hydrazones as Effective anti-α-amylase agents with in vitro and molecular docking insights	**PC 88**

Communicatings' Names	**Ref**
C. Gharbi, C. Ben Nasr, L. Khedhiri *INRAP - Sidi Thabet* Experimental study, crystallographic investigation, antimicrobial potency and molecular docking of Co (II) coordination complexes	**PC 89**
N. Gheraissa, B. Benamor, A.E. Chemsa, N. Cherrada *Higher School of Saharan Agriculture, El Oued, Algeria* Chemical analysis and antimicrobial activity of Salsola foetida extract against pathogenic bacteria	**PC 90**
L. Ghorbali, M.F. Zid, H. Chebbi *FST - Tunis* Structural and spectroscopic studies, Hirshfeld surface analysis and optical properties of copper (II) organic-inorganic hybrid material with 5-aminotetrazol ligand	**PC 91**
N. Guemras, L. Lamoudi, K. Daoud *Houari Boumediene University, Algiers, Algeria* Effect of volume on the crystallization of different paracetamol polymorphs	**PC 92**
N. Guemras, Daoud Kamel *Houari Boumediene University, Algiers, Algeria* Single-well technology for the determination of solubility and crystallization of drug	**PC 93**
S. Guerfi, Y. Berredjem, L. Boubakri, W. Koko, L. Mansour, N. Gürbüz I. Özdemir, N. Hamdi *University of Skikda, Algeria* Design of efficient benzimidazole-derived N-heterocyclic carbene Ag(I) catalysts for aldehyde-amine-alkyne coupling and their antioxidant and Enzyme inhibition	**PC 94**
N. Gürbüz, E. Evren, H. Karci, M. Dündar, I. Özdemir, A. Koç, I. Özdemir *İnönü Üniversitesi, Malatya, Türkiye* Synthesis and anticancer properties of benzimidazole selen derivatives	**PC 95**
N. Gürbüz, I. Slimani, H. Karci, M. Dündar, İ. Özdemir, A. Koç, İ. Özdemir *İnönü Üniversitesi, Malatya, Türkiye* In vitro anticancer activity against HCT116 and SH-SY5Y cell lines of new imidazolidine derivatives	**PC 96**
S. Hadjar, B. Harkati *Cheikh Larbi Tebessi University, Tebessa, Algeria* Phytochemical content and in silico molecular docking of P. albicans L plant	**PC 97**
A. Hajlaoui, G. Ghannouchi, Z. Kibou, N. Choukchou-Braham, H. Ben Jannet, A. Romdhane *FSM - Monastir* Synthesis of novel 1,2,3-triazole-linked chromene hybrids: In vitro anti-melanoma effects and in silico insights	**PC 98**
A. Hajlaoui, G. Ghannouchi, Z. Kibou, N. Choukchou-Braham, H. Ben Jannet, A. Romdhane *FSM - Monastir* Design and synthesis of novel benzopyran derivatives: An investigation by experimental and computational studies	**PC 99**
C. Hamdi, J. Dhaouadi, B. Ben Hassine, F. Aloui *FSM - Monastir* Bisdiarylethylenes: Towards New Horizons in Synthesis, Characterization and Applications	**PC 100**

Communicatings' Names	**Ref**
N. Hamdi, N. Touj, N. Gurbuz, I. Özdemir *ISSTE - Borj Cédria* Pd−PEPPSI-type expanded ring N-heterocyclic carbene complexes: Synthesis, characterization, and catalytic activity in Suzuki−Miyaura cross coupling	**PC 101**
M. Hamdouni, C. Hrizi, M. Knorr, C. Strohmann, S. Chaabouni *FSS - Sfax* Molecular self-assembly of 1D linear polyiodide in a 4-dimethylaminopyridinium salt: A Competition between halogen and hydrogen bond	**PC 102**
M. Hamdouni, C. Hrizi, M. Knorr, C. Strohmann, S. Chaabouni *FSS - Sfax* Molecular self-assembly of 2D T-shape polyiodide arrangement in triiodide of tetraethylammonium: Supramolecular structure and density functional theory-based optical properties	**PC 103**
L. Hammal, S. Baaziz *Houari Boumediene University, Algiers, Algeria* Synthesis of pyrrazole and pyrimidine structure	**PC 104**
Z. Hammami, A. Mezni *FSB - Bizerte* Effet du dopage au manganèse sur les propriétés électriques du ZnO	**PC 105**
B. Harkati, K. Aggoun, C. Belghit, T. Abbaz, H. Laouer, D. Villemin, A. Gouasmia *Larbi Tebessi University, Tebessa, Algeria* Electrochemical and theoretical of investigation of plan extract as a corrosion inhibitor for carbon steel in 1M HCl	**PC 106**
C. Hrizi, M. Hamdouni, M. Knorr, C. Strohmann, S. Chaabouni *FSG - Gabès* Reaction of Bi(NO3)3 with quinoxaline in the presence of HI: Synthesis of a graphite-like energetic compound by serendipity	**PC 107**
C. Hrizi, M. Essid, A. Khatyr, M. Knorr, C. Strohmann *FSG - Gabès* Unexpected formation of the Iodobismuthate Salt $(C_{14}H_{15}S_2N_2)_2(C_9H_{10}SN)_2[Bi_4I_{16}]$ upon reaction of the unsaturated ligand Z-PySCH$_2$CH=CHCH2SPy with BiI3	**PC 108**
S. Idoudi, B. Essghaier, M. Horchani, H. Ben Jannet, M.F. Zid, S. Namouchi Cherni *FST - Tunis* Biological activities and molecular doking of tris(8-quinolinolato-κ2N,O)cobalt(III) methanol solvate	**PC 109**
C. Jaffali, A. Khadhri, A. Synytsya, R. Bleha, P. Klouček, S. Aschi-Smiti *FST - Tunis* Extraction and characterization of cell wall polysaccharides from Tunisian (Pleurotus eryngii) fruiting bodies	**PC 110**
H. Jelizi, S. Boudriga, H. Ben Jannet, M. Knorr *FSM - Monastir* Asymmetric synthesis of enantiopure tetracyclic dispirooxindolopyrrolidine-piperidones via microwave-assisted multicomponent reaction: Crystallographic analysis, antimicrobial activity and in silico studies	**PC 111**
I. Jendoubi, B. Essghaier, S. N. Cherni, M.F. Zid *FST - Tunis* A novel green synthesis of CoFe2O4 Nanoparticles for photocatalytic and antimicrobial activity evaluation	**PC 112**

Communicatings' Names	Ref
G. Kabeya, - *University of Kinshasa, Dem. Rep. Congo* Photodynamic antimicrobial activity of selected metal free and tin based porphyrines	**PC 113**
N. Khadhri, Y. Moussaoui *FSG - Gafsa* Adsorption of indigo carmine dye onto activated carbon derived from Phoenix dactylifera petiole by fixed bed column	**PC 114**
N. Khebichat, B. Messaoudi, N. Benhadria *Higher School of Applied Sciences ASSA, Tlemcen, Algeria* On the adsorption of a dye by means of theory approach	**PC 115**
L. Khedhiri, C. Gharbi, M. Mhadhbi *INRAP - Sidi Thabet* A comparative study of MXenes' properties in previous researches for energy storage and conversion: Recent advances and perspectives	**PC 116**
O. Kheffache, S. Slyemi, H. Messaoudi *Ben Youssef Ben Khadda University, Algiers1, Algeria* Synthèse de 3,4-dihydropyrimidin-2-(1H) -one en présence de catalyseurs verts CoCuZnO et $CoCuZrO_2$ via la réaction de Biginelli	**PC 117**
E. Khemis, M. Ben Mustapha, I. Chaieb, R. Ascrizzi, G. Flamini, H. Ben Jannet, A. Zardi-Bergaoui *FSM - Monastir* Repellency and toxicity effect of volatile oils of Thapsia garganica L. growing in Tunisia against Red flour beetles	**PC 118**
W. Khitri, M. Chelghoum, D. Smati *Faculté de Médecine, Université of Oran, Algérie* Enquete ethnobotanique sur les plantes anticancereuses utilisees en medecine traditionnelle ALGERIENNE	**PC 119**
I. Khlifi, I. Gouti, S. García-Granda, H. Litaiem *FSS - Sfax* Structural behavior, thermal properties, electrical characterization and conduction mechanism study of the new potassium arsenate tellurate compound	**PC 120**
M. Kolli, S. Khelfi, I. Nouar *Ferhat Abbas University, Sétif, Algeria* Spinel synthesis from waste aluminium dross and dolomite ore	**PC 121**
A. Labidi, O. Fliss, T. Issa, M.F. Zid, R. Bensegueni, L. Latrous, A. Megriche *LNCM - Tunis* Synthesis, characterization, DFT and Molecular Docking study of the crystallized 6-methoxylated derivative of the antiviral drug favipiravir	**PC 122**
I. Laib, B. Djahra Ali, A. Alsalme, D. Cornu, M. Bechelany, A. Barhoum *University of El Oued, Algeria* Therapeutic potential of silver nanoparticles from Helianthemum lippii extract for mitigating cadmium-induced hepatotoxicity and nephrotoxicity in Wistar rats	**PC 123**
I. Lansari, K. Tizaoui, B. Benguella, A.F. Bendimerad, S.M. Bouchaour *University of Tlemcen, Algeria* The removal of a textile dye from aqueous solution using natural and modified chitosan	**PC 124**

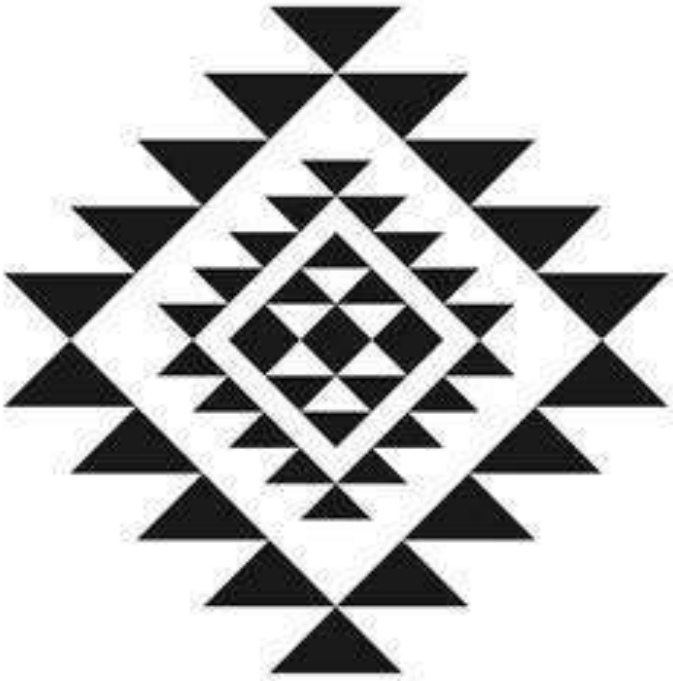
Communicatings' Names	**Ref**
R. Laroum, A. Benouatas, N. Hamdouni, W. Zemamouche, A. Boudjada, A. Debache *Larbi Ben M'Hidi University, Oum El Bouaghi, Algeria* Crystal structure and Hirshfeld surface analysis of (Z)-3-methyl-4-(thiophen-2-ylmethylidene)isoxazol-5(4H)-one	**PC 125**
B. Maalem, S. Abderrahmane, S. Athmani, B. Bezzina, A. Youbi, H. Khelfi, K. Moussaoui, D. Berdjane *Badji Mokhtar University, Annaba, Algeria* Valorization of black cumin cake as an eco-friendly inhibitor of corrosion on Stainless Steel 316L in 1M HCl through chromatography analysis, experimental and theoretical studies	**PC 126**
S. Majdoub, M. Ben Salah, T. Soltani, U. Maschke, S. Hbaieb *FST - Tunis* Azo Dyes for Enhancing Optical Properties and Developing Multifunctional Liquid Crystal Materials	**PC 127**
F. Mannai, M.N. Belgacem, Y. Moussaoui *FSG - Gafsa* In vitro digestion of vegetable oils encapsulated with Opuntia (Cactaceae) polysaccharides	**PC 128**
A. Manseri, S. Caillol, R. Auvergne, G. Boutevin, B. Boutevin, M. Grimaldi, P. Balaguer *CNRS Occitanie EST* Understanding glycidylation reaction for the formation of pure mono, diglycidyl and dual monomers as glycidyl methacrylate of vanillyl alcohol	**PC 129**
B. Mansouri, Z. Ksibi *FST - Tunis* Catalytic treatment of ONAS wastewater	**PC 130**
M. Medjani, W. Zemamouche, O. Brihi, A. Boudjada *Frères Mentouri University, Constantine, Algeria* Hirshfeld surface analysis, molecular conformation and docking investigation of 4,6-dichloro-2-methylpyrimidine	**PC 131**
A. Mejri, P. Soriano-Molina, S. Miralles-Cuevas, J.A. Sánchez Pérez *ISSTE - Borj Cédria* Fe3+-NTA as iron source for solar photo-Fenton at neutral pH in raceway pond reactors	**PC 132**
G. Mejri, B. Essghaier, M.F. Zid, S. Namouchi Cherni *FST - Tunis* Structural, physicochemical characterization and antimicrobial activities of a catena-poly[[aqua(nitrato-κ²O,O')(1,10-phénanthroline)cadmium(II)]-μ-nitrato-κ²O:O'] [$Cd(NO_3)_2(C_{12}H_8N_2)(H_2O)$]n	**PC 133**
M. Mendili, I. Degano, S. Aschi-Smiti, A. Khadhri *FST - Tunis* The parietin, a key pigment in Xanthoria parietina: characterization and application in textile dyeing	**PC 134**
O. Mhasni, F. Rezgui *INRAP - Sidi Thabet* Straightforward hydroxymethylation of α-substituted β-keto esters with formaldehyde	**PC 135**
Y. Miloudi, A. Kedjadja, S. Ikhlef, Z. Kabouche *University of Skikda, Algeria* An efficient (NHC) copper (I)-catalyst for the synthesis of 1,2,3-trisubstituted triazoles	**PC 136**

Communicatings' Names	Ref
K. Missaoui, K. Ferchichi, N. Amdouni, D. Cosano, R. Liu, S. Pan, H. Zhanning, Y. Su, M. Luo, Y. Yang, G. F. Ortiz *FST - Tunis* Effects on the structure and electrochemical reactivity of surface modified magnesium cobalt oxide	**PC 137**
A. Mnasri, N. Hamdi *ISSTE - Borj Cédria* Molecular docking studies of dicoumarols and their corresponding epoxycoumarins	**PC 138**
N. Mnasri, E. Elaloui *IPEIG - Gafsa* Mesoporous silica-based systems containing silver nanoparticles for trapping and immobilizing iodine from the gas phase	**PC 139**
C. Mouffouk, S. Mouffouk, H. Medghoul, M. Mehdaoui, H. Hamada *Mustapha Benboulaid University, Batna 2, Algeria* The assessment of *in vitro* cytotoxic, anti-inflammatory, antimicrobial, antioxidant, and hemolytic effects of the species *Eryngium triquetrum* Vahl	**PC 140**
C. Mouffouk, S. Mouffouk, S. Mouffouk, H. Hamada *Mustapha Benboulaid University, Batna 2, Algeria* The evaluation of pharmacological effects of the species *Suaeda monodiana*	**PC 141**
M. Moussa, A. S. Mestre, A. Hamrouni, H. Lachheb, A. Houas, O. C. Monteiro *FSG - Gabès* Treated graphitic carbon nitride for enhanced photodegradation of caffeine under visible light	**PC 142**
R. Msaadi, W. Sassi, S. Ammar, M.M. Chehimi *FSG - Gabès* An optimized comparative process for the adsorption of methyl green by biomass and its biochar	**PC 143**
Z. Mzoughi, K. Khwaldia, D. Le Cerf, H. Majdoub *FSM - Monastir* Enhancing food preservation with bio-films: Incorporating polysaccharides from pepper wastes for sustainable packaging solutions	**PC 144**
R. Nasri, M.F. Zid *FST - Tunis* Physical properties and photocatalytic activities of NaLi1.07Co2.94(MoO4)5 nanoparticles	**PC 145**
S. Neghmouche Nacer, A. Abadi, P. De Frémont, S. Dagorne, F. Louafi *University of Eloued, Algeria* Synthesis and Electrochemical Characterization of a Novel Imidazolium-Based Salt for Catalytic and Energy Applications	**PC 146**
M. Nouadji, S. Marmi, L. Abdelli, H. Marmi, Z. Hamida *University of Biskra, Algeria* Inhibition of steel corrosion in the middle of hydrochloric acid by aqueous extract for olive leaves	**PC 147**
A. Omrani, M. Hraoui, F. Rezgui, M. Jridi, A. Ouerghui *ISB - Béja* One-pot synthesis of 1,2,3-triazoles acetamide and vanillin derivatives via nucleophilic substitution in α-position of cyclic Morita-Baylis-Hillman adducts and 1,3-dipolar cycloaddition and evaluation of their biological activities	**PC 148**
S-E. Rahmani, N. Rebizi, T. Benderrah *University of Djelfa, Algeria* Antioxidant status of methanolic extract of Algerian steppic Onopordum acanthium L.	**PC 149**

Communicatings' Names	**Ref**
M.N. Rebizi, N. Belkheiri, S.E. Rahmani *University of Djelfa, Algeria* Synthesis, biological activity and enantioseparation of iminonaringenine	**PC 150**
A. Reguigui, H. Bendaoud, M. Romdhane *ENIG - Gabès* Yield optimization of essential oil from Tunisian *Lavandula* leaves	**PC 151**
S. Rennane, N. Bendjaballah-Lalaoui *Houari Boumediene University, Algiers, Algeria* Batch adsorption experiments of methylene blue using different sand-bentonite mixtures	**PC 152**
M. Rjili, A. Aschi *FST - Tunis* Effect of a globular protein on the dynamical behavior of long-chain polyanion in dilute regime	**PC 153**
S. Saad, F. Mannai, I. Dávila-Rodríguez, J. Labidi, Y. Moussaoui *FSG - Gafsa* Zizyphus lotus cellulose for methyl orange elimination	**PC 154**
S. Sakouhi, S. Ben Younes, J. Bouajila, A. Mhamdi *FST - Tunis* In vitro and in silico approach for evaluating the antioxidant, anti-inflammatory and anti-hemolytic potential of 5-hydroxyferulic acid	**PC 155**
S. Salhi, D. Kanzari-Mnallah, I. Jourdin, M. Knorr, J. Kirchhoff, H. Mrabet, M. L. Efrit, A. Ben Akacha *FST - Tunis* Synthesis and structural characterization of β-phosphonated thiosemicarbazones: Investigation of their Z/E interconversion by NMR and DFT computing	**PC 156**
S. Salhi, A. Omri, R. Ben Salem, M. Benzina *FSS - Sfax* Parametric and kinetic study of the methylene blue degradation by homogeneous photochemical processes	**PC 157**
W. Sassi, J.Y. Hihn *ISSAT - Gabès* The TiO2/Ti3C2 MXenes structure in toxic metal removal using combined batch/electrochemical processes: ADOX and OAP	**PC 158**
W. Sassi, J.Y. Hihn *ISSAT - Gabès* MB and CR selective adsorption onto amorphous perlite: CCD optimization and mechanisms	**PC 159**
H. Slaouti Messaoudi, H. Kabir, I. Belkhettab, S. Boutamine *Houari Boumediene University, Algiers, Algeria* Study on The reactivty of some amino acids with molybdenum.	**PC 160**
A. Souamti, A. Jraba, A. Megriche *FST - Tunis* Investigations on p-n heterojunction MoO3/M-oxide nanocomposites for catalytic and energy storage applications	**PC 161**
F. Taleb, M. Ben Mosbah, Y. Moussaoui *FSG - Gafsa* Transforming waste to wealth: Biolignin production from spent coffee grounds	**PC 162**

Communicatings' Names	Ref
R. Testas, Z. Benredjem, I. Chaabna, R. Delimi, M.F. Ghorab, H. Belbel *Badji Mokhtar University, Annaba, Algeria* Synthesis of ZnO/AC Activity Composite and Photocatalytic Degradation of Methylene Blue under UV irradiation	**PC 163**
K. Tizaoui, Z. Guebli, I. Lansari, K. Chaibet, L. Bouaoud, L. Meddour Boukhobza, N. Marouf *Houari Boumediene University, Algiers, Algeria* Application de procédé photocatalytique à la dégradation d'un polluant pharmaceutique (Prednisone)	**PC 164**
N. Touahri, A. Benadda, J.P.Holgado *Houari Boumediene University, Algiers, Algeria* Catalytic properties of modified Hexaaluminate catalysts by nickel and iron in OCM.	**PC 165**
S. Wahabi, S. Selmi, A. Ayari, K. Gharbi, H. Sebai *ISB - Béja* Phytochemical properties of Arbutus unedo L. fruits decoction extract and evaluation of its protective activity against acetic acid-induced ulcerative colitis in rat	**PC 166**
A. Yacoub, Z. Ksibi *FST - Tunis* Catalytic treatment of wastewater	**PC 167**
S. Yebdri, O. Nehar, R. Mahboub, T. Roisnel, L. Boukli-Hacene, S. Louhibi *Abou Bakr Belkaid University, Tlemcen, Algeria* Synthesis and characterization of a zwitterionic imidazolyl-phenol derivative: Catalytic properties in the oxidation of 3,5-Di-tert-butylcatechol	**PC 168**
C. Zidani, D. Kherbouche, L. Benhabib *University of Tlemcen, Algeria* Design and investigation of a conical solar furnace powered by optical fibers	**PC 169**
C. Zidani, A. Ghomri, D. Kherbouche, F. Lassouani *University of Tlemcen, Algeria* Development of a predictive model for the photovoltaic cells performance evaluation	**PC 170**
S.H. Zitouni-Nourine, N. El Yebdri, N. Belyagoubi-Benhammou, F. El-Houaria Zitouni-Haouar, F. Atik Bekkara, N. Kambouche, A. Gismondi, H. Toumi *Ahmed Ben Bella University, Oran, Algeria* Etude phytochimique et évaluation des activités antioxydantes et anti hémolytiques des bourgeons de Ficus carica, Olea europaea et Prunus avium de la région de Tlemcen (Algérie)	**PC 171**
S.H. Zitouni-Nourine, N. Belyagoubi-Benhammou, N. El Yebdri, F. El-Houaria Zitouni-Haouar, I. Gasmi, Y. Kerzabi, H. Toumi *Ahmed Ben Bella University, Oran, Algeria* Etude phytochimique et évaluation des activités biologiques de l'extrait méthanolique de la racine d'Echinops spinosissimus subsp. bovei	**PC 172**
Y. Ammari, N. Baaalla, S. Abid *FSB - Bizerte* Ab-initio studies of electronic, thermoelectric and superconducting properties of vanadium nitride material	**PC 173**
M.R. Belmecheri, H. Touati *Université M'hamed Bougara, Boumerdes, Algérie* Etude par des méthodes théoriques des interactions du 1-fluoroethanol en phase liquide	**PC 174**

Communicatings' Names	**Ref**
L. Hamdaoui, R. Amri, H. Oudadesse, T. Rebaia, H. Keskes *Faculty of Medicine, Sfax* Exploration of in vivo toxicity and tolerance of bioactive glass 46S6 associated with chitosan after implantation applications in *Wistar* rats	**PC 175**
S. Hazourli, M. Bendai, M. Cherifi, W. Atba, B. Mansouri *Badji Mokhtar University, Annaba, Algeria* Adsorption de colorants alimentaires sur du charbon actif à base de noyaux de datte greffés	**PC 176**
B. Mansouri, S. Hazourli *Université Badji Mokhtar, Annaba, Algérie* Phénomènes de transport et décontamination électrocinétique de l'aluminium et des sulfates d'une boue de laiterie	**PC 177**
F. Nouri, G. Panczer, Y. Guyot, M. Trabelsi-Ayadi, R. Ternane *FSB - Bizerte* Synthesis and luminescent properties of Eu^{3+}-doped phosphate-sulfate fluorapatites $Ca_{10-x}Na_x(PO_4)_{6-x}(SO_4)_xF_2$	**PC 178**
K. Ouaad, C. Allach, S. Rahmi *Université Houari Boumediene, Alger, Algérie* Elaboration par voie solution et caractérisation des mélanges à base d'un polymère synthétique, d'un biopolymère et de nanocharge. Etude des propriétés	**PC 179**
S. Salhi, A. Omri, R. Ben Salem, M. Benzina *FSS - Sfax* Study of the adsorption of an anionic dye on a mineral siderite	**PC 180**
A. Wahbi, M.A. Dridi, I. Dridi, H. Alimi, S. Touil *FSB - Bizerte* Convenient synthesis, antibacterial activity and in silico studies of novel 6-phenoxy-4,5-dihydro-1,2,6-oxazaphosphinine 6-oxides	**PC 181**



ABSTRACTS OF POSTER COMMUNICATIONS

Ferrocenephosphonates: Copper-promoted synthesis and further functionalization

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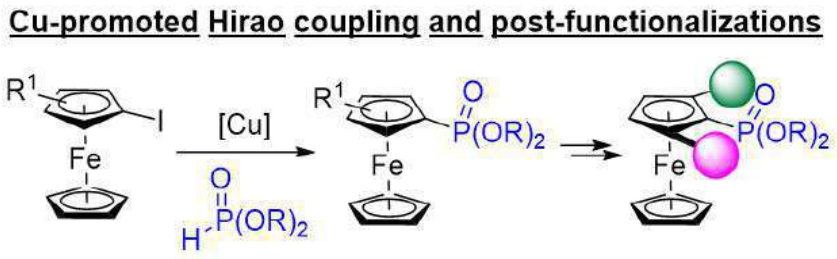
Ferrocenephosphonate make up an important class of organometallic derivatives with a wide range of useful applications in organic synthesis and coordination chemistry. Here, an approach based on a copper-promoted Hirao coupling is reported. Further functionalization based on regioselective deprotolithiation and both Negishi and Suzuki-Miyaura cross-coupling reactions is also described to reach original derivatives.



Key words: Ferrocene, Phosphonate, Copper, Cross-coupling, Deprotolithiation.

Synthesis and characterization of some metal complexes of curcumin with bipyridine and Antioxidant application

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In this contribution, some transition metal complexes of general formula [M(Cur)(Bpy)X], M = Co, Ni, Cu or Mn, Cur = curcumin, Bpy = bipyridine and X= halogen have been synthesized by the reaction of metal with curcumin as primary ligand and bipyridine as secondary ligand in ethanol solution. The composition of the complexes has been characterized by conductivity measurement, IR and UV-visible spectroscopy. The stability and solubility of the prepared complexes were determined.

The evaluation of the antioxidant power of the complexes was carried out using the DPPH$^{\cdot}$ The results showed that the complexes have antioxidant activity compared to a control antioxidant.

Key words: Curcumin; bipyridine; antioxidant; DPPH.

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Synthesis, characterizations, optical properties, and DFT investigation of a new organic-inorganic complex

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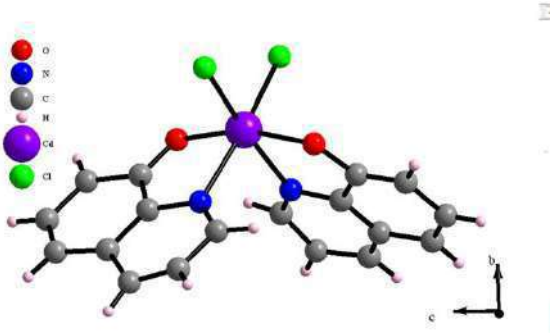
This poster reports on the synthesis and characterization of a new hybrid organic-inorganic crystals presenting interesting optical properties. The compound has been prepared using the solvothermal method [1] by mixing 8-hydroxyquinoline [2] with $CdCl_2$. Crystals have been grown and have been characterized by single-crystal X-ray diffraction to unravel the structural properties and the nature of the intermolecular interactions. Each unit cell is composed of two 8-hydroxyquinoline molecules coordinating a $CdCl_2$, which adopts an octaedral structure. The organic molecules play the role of bidentate ligands coordinating the Cd(II) cations by their nitrogen and oxygen atoms. In the crystal, these clusters form chains, connected via π-π interactions and H bonds. These have been further characterized by analyzing the Hirshfeld surfaces and their 2D fingerprint diagrams. Then, systematic vibrational, thermal, and optical characterizations have been performed. The material displays fluorescence after being irradiated at 285nm. To support these experimental characterizations, quantum chemistry calculations, enacted using density functional theory, have been carried out to determine the structural and electronic properties of this crystal using the Crystal23 code.



Unit formula of $CdCl_2(C_9H_6NO)_2$

Key words: organic-inorganic salts, bidentate ligands, structural and optical properties, Hirshfeld surfaces, DFT calculations.

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ADVANCEMENT IN THE SYNTHESIS OF POLY(HEXAMETHYLENE 2,5- FURANDICARBOXYLATE) via RING OPENING POLYMERISATION

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Synthetic polymers are a versatile family of materials in which polyesters are among the most used today due to a wide range of high-performance properties. However, most commercial polyesters are still derived from fossil feedstocks and their synthesis is typically carried out via bulk step-growth polymerization, while effective, often involves harsh conditions. Several initiatives such as the United Nations 2030 Agenda for Sustainable Development are driving research towards the use of renewable resources and of eco-friendlier polymer synthesis following the Green Chemistry principles. In this vein, biomass components such as cellulose, hemicelluloses, lignin, and vegetable oils are promising raw materials for the synthesis of building-block monomers and of biobased polyesters thereof. Importantly, ring-opening polymerization (ROP) of macrocyclic esters is a greener alternative, offering atom economy efficiency since no by-product is produced, besides the fact that typically mild reaction conditions, and high polymerization rates are involved [1]. In this work, we studied in first the synthesis of macrocyclic hexamethylene 2,5-furandicarboxylate (CHF) via cyclodepolymerization of the corresponding low molecular weight linear polyesters species under high dilution conditions. Secondly, the ROP of these macrocyclic oligoesters was accomplished using various metal catalysts under different time and temperature conditions. The obtained macrocyclic and their related polymers were characterized using various analytical techniques.

Key words: macrocyclic hexamethylene 2,5-furandicarboxylate, ring-opening polymerization, greener synthesis.

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Optimization of total oils, grease, and petroleum hydrocarbons recovery from oily petroleum sludges by freeze-thaw process

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Background: Petroleum hydrocarbon wastes are a significant global issue resulting from fossil fuel extraction and refining. Improper disposal poses serious risks, particularly to contaminated soils regarding their effects on soil microbiology, human health, and ecosystem degradation [1].
Over the past two decades, various methodologies have been explored for the treatment and valorization of oily petroleum sludges, specifically aimed at recovering oil and safely disposing of hazardous residues [2]. The focus has been on the most straightforward and environmentally friendly "Green processes", among them, the solvent extraction technique is a straightforward process that involves mixing oily waste with a solvent to enhance oil miscibility while allowing most water and solids to be removed as impurities through gravitational settling or centrifugation. Also, freeze/thaw treatment has emerged as a cost-effective dewatering technique, utilizing the expansion of water droplets when frozen to promote the coalescence of emulsified water and alter interfacial tension, which aids in dewatering [3].
The objective of this study is to investigate and optimize the most important parameters affecting the performance of total oils, grease, and petroleum hydrocarbons (T-O-G-PH) recovery from high-moisture petroleum sludge by using a combination of solvent extraction and freeze/thaw treatment.
Methods: Solvent extraction and freeze/thaw treatment combination consist of one first step of solvent/petroleum sludge mixture and shaking, followed by a second step of freezing at -20°C/12 h. After that, the frozen mixture was then thawed. The optimized parameters using the Response Surface Methodology were: Solvent/Sludge Ratio, Shaking duration (min), and thawing temperature.
Results: The optimized conditions for the T-O-G-PH recovery process show that the combination of solvent ratios of 60% and 70% with a shaking time of 15 minutes and a thawing temperature of 35 °C seem very adequate for further recovery ranging from 15 to 98%. The significant binary interactions are solvent ratios-thawing temperature and solvent ratios- shaking duration.
Conclusion: Optimized solvent extraction - freeze/thaw combination process is suitable for the T-O-G-PH recovery from Oily petroleum sludges at 98% using acceptable solvent amounts of 65% and processing in short duration at natural ambient temperature.

Keywords: Oily petroleum sludges, Total Oils – Grease - Petroleum Hydrocarbons recovery, Solvent extraction - Freeze/thaw combination, Green processes, Response Surface Methodology.

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Photophysical properties and photodynamic antimicrobial study of 2,6-dibromo - BODIPY substituted by 3-bromo 4-hydroxy styryl at 3,5 positions

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Boron dipyromethene known as BODIPY dyes has attracted many researchers because of their different applications in bioimaging, photodynamic therapy, solar cell sensitization and photodynamic antimicrobial chemotherapy. In this work, 3-bromo 4-hydroxy styryl bodipy, and 2,6 - dibromo - BODIPY were synthesized and used Photodynamic antimicrobial chemotherapy activity against Staphylococcus aureus and E. Coli. In the best of my knowledge, 2,6-Dibromo-3,5-distyryl BODIPY dye used in this work is novel. The results found in this study are promising for both negative and positive gram bacteria used.

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Indole Derivative as a Possible Treatment for Breast Cancer

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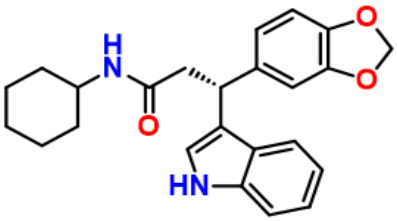
EGFR and HER-2 are epidermal growth factor receptors that are members of the ErbB family of receptor tyrosine kinases; their overexpression affects the development and progression of breast cancer. The current drugs are subject to resistance, and new drugs with novel mechanisms of action are required. Indole compounds are well-known to have promising biological activity along with good anticancer activity. Herein, we attempt to screen a database of 9,753 indole derivatives against epidermal growth factor receptors EGFR and HER2. High throughput virtual screening followed by standard precision and extra precision docking identified 20 compounds as possible inhibitors for EGFR proteins. These 20 compounds were docked against the active site of the five mutations of HER2, including D769Y, L755S, T798I, V777L, and Del755-759, along with the wild type. The preliminary results showed that compound 5886 has a promising activity, with a docking score of -6.904 kcal/mol against EGFR and -9.65, -9.51, -9.79, -9.69, -10.05, -9.77 against wild, D769Y, L755S, V777L, T798I, and Del755-759, respectively. Further molecular dynamics simulation for 500 ns revealed that compound 5886 was stable inside EGFR and HRE2^{T798I}, indicating the promising activity of this compound against BC. Further, in vitro testing and ADME profiling for this compound are considered.



5886

Keywords: Docking, molecular dynamics, Cance, Drug design, HTVS

Triazoles as HER2 Inhibitors to Overcome Brest Cancer Resistance

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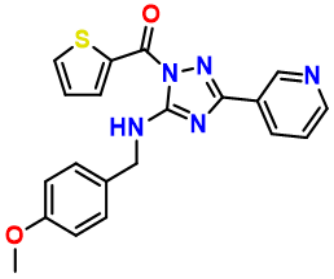
Cancer, a major global health issue, is a broad set of horrifying diseases characterized by unchecked cell growth. Activating the epidermal growth factor receptor (EGFR) promotes tumor development, invasion, and metastasis, making it a crucial component in epithelial malignancies. HER2 is a protein expressed at increased levels in 15% to 20% of breast cancers, and these tumors are referred to as HER2-positive breast malignancies. Triazoles are a significant category of heterocyclic compounds with interesting pharmacological properties. In this research, we attempt to find new drug candidates against breast cancer using in silico techniques. A database of 4000 triazole derivatives was screened against EGFR using HTVS, and the best compounds were further investigated for their potential as inhibitors for HER2 wild type along with the most common mutations that include D769Y, L755S, T798I, V777L, and Del755-759. The docking result showed that compound D116-0314 has a good docking score throughout all mutation and wild types with a docking score of -7.968 kcal/mol against $HER2^{T798I}$ compared to -6.321 kcal/mol of lapatinib. Molecular dynamic simulations revealed the stability of D116-0314 inside the active site of HER2T798I, suggesting promising activity toward breast cancer. *In vitro* testing and ADME profiling of the compound is under investigation.



D116-0314

Keywords: Docking, molecular dynamics, Cance, Drug design, HTVS

Activité antioxydante de l'huile essentielle de Bubonium graveolens, Docking moléculaire, DFT et étude ADMET de trois dérivés.

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Pour valoriser les plantes aromatiques et médicinales algériennes, cette étude s'est concentrée à la fois sur l'évaluation de l'activité antioxydante de l'huile essentielle de la plante bubonium graveolens qui appartient à la famille des astéracées, et sur l'étude in silico de ses fraction, l'extraction a été faite par hydrodistillation.
L'activité antioxydante, mesurée à l'aide du test de piégeage des radicaux libres DPPH, a montré des résultats antioxydants significatifs par rapport aux références de BHT et d'acide ascorbique, indiquant la présence de composés bioactifs responsables de l'activités antioxydante.
Trois molécules majeures ont été sélectionnées pour réaliser l'étude in silico. La stabilité et la réactivité moléculaire de ces molécules ont été calculées à l'aide des énergies HOMO-LUMO, de l'écart d'énergie, du potentiel chimique (μ), de l'électronégativité (χ), de la dureté (η) et de la mollesse (S). Une analyse in silico par le biais de docking moléculaire et d'évaluation pharmacocinétique a été utilisée pour évaluer son activité biologique et ses propriétés de similitude avec des médicaments. Les études in silico DFT, ADMET, de docking moléculaire et de dynamique moléculaire confirment que les résultats présentent une plus grande affinité avec les tests in vitro réalisés pour la sélection de nouveaux produits d'origine naturelle.

Mots clés: Bubonium graveolens, huile essentielle, activité antioxydante, DFT, docking moléculaire, ADME/Toxicité

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Synthesis and characterization of hybrid materials based on graphene oxide and metal nanoparticles

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The development of carbon nanomaterials in nanosciences has opened an important new field of research for all carbon allotropes. The present work focuses on the synthesis of graphene oxide (GO) using the modified Hummers method based on oxidative chemical exfoliation [1]. We also synthesized hybrid materials: (i) GO/Cobalt oxide in spinel form and (ii) GO/Cobalt nanoparticles via a simple one-pot reaction in an aqueous medium containing a high concentration of cobalt (II) nitrate hexahydrate [2].

The GO and the two prepared composites were characterized using various techniques such as XRD, SEM, Raman Spectroscopy, and FTIR-ATR.

The obtained results confirmed the structure and morphology of graphene oxide (GO) by the presence of the different chemical bonds detected.

The results revealed that cobalt oxide is predominant in the GO/Co_3O_4 composite, probably due to the 1:2 ratio between graphene oxide and cobalt oxide. Furthermore, the characterization results of the material based on OG and [Co $(NO_3)_2.6H_2O$] showed that a high concentration of metal ions in solution leads to deoxygenation of the functional groups of this composite. In addition, metal ions bind to the oxygen sites of GO, facilitating the anchoring of cobalt oxide nanoparticles on the surface of OG.

Key words: Graphene oxide, Hybrid materials, Cobalt oxide, Cobalt nitrate hexahydrat

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Détermination des enthalpies de dissolution dans l'eau d'apatites halogénées

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Les apatites calciques de formule $Ca_{10}(PO_4)_6X_2$ (avec X un halogène), sont impliquées dans de nombreux domaines comptant les sciences médicales, les biomatériaux (génie des tissus osseux, nanomédecine) [1], la géologie [2], ou encore les sciences de l'environnement (immobilisation des phosphates et des composés métalliques, sciences nucléaires) [3,4], et en particulier connues pour leur utilisation comme matrice de stockage pour les éléments radioactifs, où la manipulation de ces matériaux nécessite la connaissance de leur stabilité et autres propriétés de dissolution dans l'eau. En effet ces dernières se dissolvent totalement dans les acides forts mais elles sont très peu solubles dans l'eau.

Dans des recherches précédentes [5,6], des mesures de l'enthalpie de dissolution des apatites calciques fluorées et hydroxylés dans l'acide nitrique à différentes concentrations nous ont permis de proposer et de confirmer différents mécanismes de dissolution des apatites calciques, selon les domaines du pH des solutions de solvant. A partir de ces résultats, les enthalpies de dissolution des apatites calcique fluorées et hydroxylées dans l'eau ont été déduites. Dans le présent travail, moyennant ce modèle de calcul nous avons déterminé les enthalpies de dissolution dans l'eau, d'apatites variablement halogénées, $M_{10}(PO_4)_6Cl_2$, $Pb_{10}(PO_4)_6Br_2$ avec (M = Ca, Sr, Ba) qui sont des matériaux candidats pour stocker des halogènes radioactifs [7]. Ces enthalpies sont négatives, et conformément à la loi de Van't Hoff, ces apatites auront une dissolution dans l'eau rétrograde avec la température, et donc très limitées si jamais ces matériaux sont stockés dans des décharges géologiques profondes connues pour leur haute température et risque d'infiltration et ruissellement d'eau.

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The effect of combined hypoxia and salinity stress on morphological, antioxidant activity and secondary metabolites of *Ocimum basilicum* L.

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In the literature, the effects of root hypoxia and salinity on many plants have been extensively studied. However, data on the combined effects of these two stresses on the growth of the species of basil are scarce. In this work, the effects of combined waterlogging and salinity stresses are studied on the changes of the enzymatic antioxidant system and the morphological alterations of the species of basil, *Ocimum basilicum* L. Thus, the question that arises is to determine if, during a combined salinity-hypoxia stress, the effect of one would be corrected by the effect of the other. During 7 days of treatment, it seems that basil tolerates hypoxia well in terms of weight growth and is sensitive to salinity or combined stress. It seems, also, that basil tolerates hypoxia well in terms of the content of secondary metabolites and antioxidant activity; plants under this stress show a higher content of secondary metabolites (total polyphenols, total flavonoids, and proanthocyanidins) compared to control plants or plants under saline stress, especially in aerial organs. Similarly, antioxidant activity is very important in hypoxia plants. Considering these results, basil seems to adopt a mechanism of synthesis of secondary metabolites mainly in aerial organs. It also seems that hypoxia has reduced the negative effect of salinity on weight growth, antioxidant activity, and bioactive compounds. Thus, hypoxia improves the tolerance of basil to salinity when we impose on basil a combined hypoxia-salinity constraint for a short duration (7 days) and under moderate salinity (50 mM NaCl).

Keywords: Basil, *Ocimum basilicum* L, hypoxia, salinity, combined-stress, weight growth, secondary metabolites, antioxidant activity.

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Thermochemical and electric properties of Lithium Nitrate

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Considerable interest has been generated in lithium nitrate due to its potential applications in various fields particularly in lithium batteries and thermal storage and transfer systems.

Our current interest revolves around thermochemical and electric properties of this nitrate.

Lithium nitrate is characterized by only one solid state between room temperature and its melting point. Melting temperature and the corresponding enthalpy were measured by STA/DTA and DSC techniques.

While, electrical conductivity, dielectric permittivity, and impedance were measured across a range of frequencies and temperatures by using the impedance spectroscopy technique.

The variation of AC conductivity (σ_{ac}) with frequency shows a distinct behavior: at low frequencies, the conductivity is practically constant which corresponds to the dc bulk conductivity (σ_{dc}). However in the high-frequency region, the σ_{ac} shows significant variation with frequency. Therefore the ac conductivity can be investigated by Jonscher's power law.

In terms of dielectric properties, both the dielectric constant (ε') and dielectric loss (ε") decrease with increasing frequency and stabilize at higher values. At low frequencies, the dielectric constant presents a dispersion phenomenon, which can be attributed to charge carrier accumulation at the interface between the electrodes and the $LiNO_3$ material.

Regarding the impedance analysis, the real part of the impedance (Z′) decreases as temperature increases in the low-frequency region, indicating thermally activated conductivity [1]. At higher frequencies, Z′ continues to decrease as temperature rises, but remains constant beyond 100 Hz [2]. In contrast, the imaginary part of the impedance (Z″) initially increases with frequency, reaching a maximum value ($Z''max = 1.20 \times 10^{11}$) at 0.1 Hz (fmax) before decreasing at frequencies beyond 1 Hz. This variation in Z″ is likely due to the presence of immobile species or electrons at lower temperatures and defects or vacancies at higher temperatures [3].

Key words: electrical conductivity, dielectric permittivity, impedance spectroscopy

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Physicochemical characterization of soils under two cultivation methods: Irrigated and non-irrigated

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Arid and semi-arid regions, defined by irregular and minimal rainfall, experience significant physical and chemical soil degradation due to water scarcity, compaction, and reduced fertility. This study aims to characterize the physico-chemical properties (including texture, pH, electrical conductivity, total lime, and organic matter) and assess mineral element concentrations (such as sodium, potassium, calcium, nitrogen, and magnesium) in soils from irrigated and non-irrigated fields across four regions in southern Tunisia (Djerba, Zarzis, Gabes, Benikhdach). Given the essential role of soil conditions in crop growth and productivity, this comparative study reveals important distinctions: non-irrigated soils tend to exhibit unique granulometric profiles (with higher sand and clay content), likely due to the lack of consistent water input, while irrigated soils show increased levels of minerals, organic matter, and electrical conductivity, likely influenced by regular irrigation and soil treatments.

Key words: soil, physico-chemical characteristics, irrigated and non-irrigated

Activité protoscolicide des nanoparticules d'argent

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L'échinococcose hydatique (kyste hydatique) est une anthropozoonose due au développement du stade larvaire du cestode *Echinococcus granulosus sensu lato* chez l'homme. La chirurgie, qui est le traitement de choix, nécessite l'utilisation d'un produit protoscolicide afin d'éviter le développement de nouveaux kystes dans l'organisme en cas d'essaimage de protoscolex vivants. L'efficacité et la rapidité d'action de la solution utilisée constitue donc un facteur essentiel afin de réduire le risque d'échinococcose secondaire. L'utilisation de nanoparticules d'argent (NP-Ag) comme produit protoscolicide pourrait être une nouvelle alternative à explorer.

Dans la présente étude, quelques préparations faisant intervenir des agents réducteurs d'origine naturelle ont conduit à la formation de nanoparticules d'argent dotées d'une activité anti-parasitaire intéressante. En effet, une mortalité de 70 % a déjà été observée après seulement 1 minute de mise en contact, pour atteindre 94 % de mortalité au bout de 5 minutes. Dans une étude faite par Rahimi et *al.* [1], une mortalité de 90 % a été notée au bout de 120 minutes d'exposition.

Les NP-Ag préparées ont été caractérisées par diffusion dynamique de la lumière, spectrophotométrie UV/Vis et par la mesure du potentiel zêta. L'échantillon le plus actif montre une bande située à 400 nm qui est attribuée aux NP-Ag. D'autre part, la distribution de la taille des agglomérats est bimodale avec des tailles allant de 10 à 30 nm et de 100 à 200 nm. Quant à la faible valeur du potentiel zêta (- 44 mV), elle indique une bonne stabilité des agglomérats en solution.

Dans cette étude, il a été aussi révélé que les clusters d'argent (Ag_n), Ag_2O ainsi que les nanoparticules de palladium sont inefficaces.

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Optimized Ultrasound-Assisted Extraction of Phenolic Compounds from *Hylocerus Undatus* Cultivated in Tunisia and Evaluation of Antioxidant Activity in Vitro.

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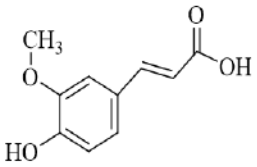
Hylocereus undatus has garnered considerable interest for its notable health benefits, attributed to its rich content of bioactive compounds. This study aimed to optimize the ultrasound-assisted extraction of phenolic compounds from the peel and pulp of *Hylocereus undatus* cultivated in Tunisia. Central composite design (CCD) combined with response surface methodology (RSM) was employed to assess the effects of extraction time (6.96 - 17.04 min), temperature (33.18 - 66.81°C), and solvent-to-material ratio (13.18 - 46.81 ml/g) on extraction efficiency. Optimal conditions for extracting bioactive compounds were established as 11.84 min, 52.20°C, and 30 ml/g for peel, and 13.07 min, 48.13°C, and 31.18 ml/g for pulp. These results provide a foundation for the development of an industrially viable, eco-friendly extraction process to obtain valuable bioactive metabolites from *Hylocereus undatus* peel and pulp.

Key words: antioxidant activity, total phenol, total flavonoid, DPPH, FRAP, RSM, *Hylocereus undatus.*



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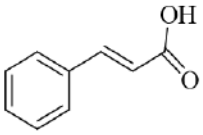

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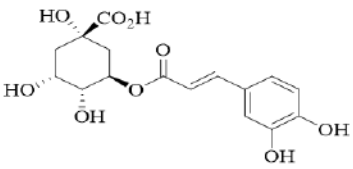

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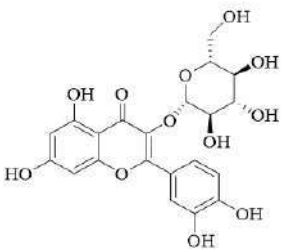

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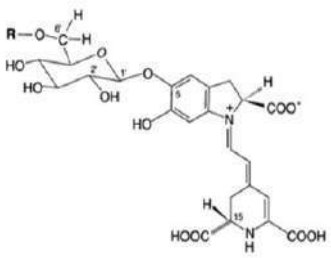

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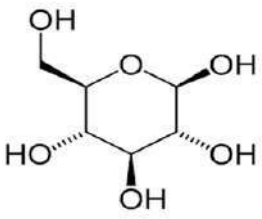

Glucose

Theoretical investigation of ternary semiconductors half-Heusler RhTaZ (Z = Si, Ge and Sn) for thermoelectric applications

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The structural, electronic, elastic, thermodynamic and thermoelectric properties of RhTaZ (Z = Si, Ge and Sn) half-Heusler materials have been studied using density functional theory. We have found that the compounds studied can be experimentally synthesized. Also, RhTaZ (Z = Si, Ge and Sn) alloys exhibit a semiconductor behavior following the Slater-Pauling rule. The elastic properties calculated confirm that our compounds are mechanically stable. Using Debye's quasi-harmonic model, the thermodynamic properties of these half-Heusler alloys were investigated. For the study of thermoelectric properties, the semi-classical Boltzmann theory, as implemented in the BoltzTraP code, has been used. The high values obtained from the figure of merit for RhTaZ (Z = Si, Ge and Sn) compounds suggest that they are promising candidates for thermoelectric applications at low and high temperatures.

Keywords: Half-Heusler; density functional theory (DFT); semiconductor behavior; thermodynamic and thermoelectric properties.

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Crystal Structure, DFT Analysis, Vibrational Characterization, and Hirshfeld Surface Study of a Novel Zero-Dimensional Metal-Halide Hybrid with Outstanding Green Emission

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This study provides an in-depth exploration of a novel zero-dimensional metal-halide hybrid, $(C_6H_7NCl)_3 \cdot [SbCl_5] \cdot Cl$, synthesized via slow evaporation. Emphasis is placed on its crystal structure, vibrational characteristics, and optical properties.

Single-crystal X-ray diffraction reveals a unique structural framework featuring discrete $[SbCl_5]^{2-}$ anions coordinated by three organic cations and one loosely bound Cl^- anion. The structure adopts the centrosymmetric triclinic space group $P\bar{1}$ with Z = 2 in the unit cell. Refinement values (R1 = 0.02, wR2 = 0.04) confirm the intricate stability and arrangement of this framework. Hirshfeld surface analysis, supplemented with 2D fingerprint plots, identifies Cl···H interactions as the dominant intermolecular forces, contributing 67.5% of the interactions and underscoring their role in structural stability.

Density Functional Theory (DFT) calculations were conducted to explore electronic structure and vibrational behaviour, showing strong agreement with experimental FTIR and Raman spectroscopy data. These analyses revealed distinct vibrational modes associated with both organic and inorganic components of the hybrid material.

Detailed optical studies indicate strong absorption within the visible range, with a significant green luminescent emission peak. The energy gap, derived from frontier orbital and DOS spectrum analyses, aligns closely with experimental values obtained from the indirect Tauc plot method, confirming the compound's luminescent properties.

Keywords: Antimony material; X-ray diffraction; DFT calculations; Luminescence; HOMO-LUMO energy gap; Molecular electrostatic potential.

Design of Novel Phthalocyanines as Potential Antimicrobial Agents Starting With Synthesized Phthalonitrile Derivatives: Complexation, Extraction

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New phthalonitrile derivatives **1-4** were considered as the key intermediates for the synthesis of new phthalocyanines. Their capacity to bind various transition metal and heavy metal cations was studied in methanol. The absorbance and conductivity were measured using UV spectrophotometry. Spectral and elemental investigations revealed the structures of the newly synthesized phthalocyanines. The complexes formed were analyzed, and their stability constants were determined through digital data processing. The ability of water to extract these compounds in dichloromethane was also examined. It was discovered that compound **1** had a lower affinity for metal picrates compared to compound **2-4**, especially Fe(III). The stoichiometry of the complex was confirmed by conducting conductivity studies. The antimicrobial properties of the novel compounds were investigated, and it has been established that have compounds **9**, **12** and **13** potent inhibitory activities against both Gram-positive and Gram-negative bacteria and fungi.

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Castor oil and laxative activity: In silico exploration of the active components of castor oil

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Introduction: Castor oil has long been recognized for its laxative activity, used in traditional and conventional medicines for the treatment of constipation The objective of this study was to investigate the mechanism of action of castor oil as a laxative through computational modeling.

Materials and methods: We used an in silico approach, leveraging computational tools, to explore the laxative mechanism of castor oil. we performed molecular docking for the major constituents of the castor oil with the molecular target 6AK3, using AutoDock Vina.

Results and discussion: Molecular docking showed that ricinoleic acid has a strong affinity for the chosen molecular target, reflecting its pivotal role in mediating the laxative effect of castor oil. Additionally, These studies confirmed that the laxative effect of castor oil is mainly mediated by the activation of EP3 receptors located on smooth muscle cells of the digestive tract.

Ricinoleic acid, to which laxative activity is attributed, demonstrated significant affinity with a binding energy score of -7.3 kcal.mol^{-1}, thus strengthening the hypothesis of its involvement in laxative activity.

Interestingly, other components of the castor oil showed even stronger affinities than ricinoleic acid.The best docking scores were attributed to β-tocotrienol, δ- tocopherol and γ-tocopherol with scores of -9.5, -9.1 and -9.0 kcal/mol, respectively.

The significant affinity observed during molecular docking suggests potential synergistic effects with ricinoleic acid on intestinal motility. This highlights the need for further exploration through in vitro and in vivo experiments.

Conclusion: In conclusion, our study delved into the molecular mechanisms underlying the laxative activity of castor oil, focusing on ricinoleic acid as the primary active constituent.

we have to conducted a virtual screening of other molecules related to ricinoleic acid using the Python Dockstring package than undertook an in silico prediction of their physicochemical, pharmacokinetic, and toxicological parameters using SwissADME and PkCSM websites.

Key words : castor-oil, in silico, laxative

ENHANCEMENT OF THE ANTIBACTERIAL ACTIVITY OF MODIFIED ALGERIAN PALYGORSKITE

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The present work aims at the synthesis, characterization and evaluation of the antibacterial activity of samples with and without clay. The clay chosen is Algerian palygorskite (Sif-Pal)[1, 2], the first is functionalized with an N-salicylidene aniline named HSA-Pal described with Boceiri et al. 2023[3]. In addition, the second is prepared with zinc oxide by the sol-gel process followed by calcination (ZnO-Pal). The antibacterial activity of each sample was evaluate using the minimum inhibitory concentration (MIC) method.

The MIC results of ZnO-Pal without calcination, showed significant inhibition against *Staphylococcus aureus* and *Staphylococcus aureus (MRSA)* starting from 4 $mg.mL^{-1}$, *Escherichia coli* from 8 $mg.mL^{-1}$ and *Pseudomonas aeruginosa* from 16 $mg.mL^{-1}$, with a predominant sensitivity towards Gram-positive bacteria. In contrast, ZnO-Pal with calcination demonstrated a specific antimicrobial activity against *Staphylococcus aureus* and *Staphylococcus aureus (MRSA)* at concentrations of 0.5 $mg.mL^{-1}$ and 1 $mg.mL^{-1}$, respectively, without notable impact on *Pseudomonas aeruginosa* and *Escherichia coli*. Furthermore, raw palygorskite (Sif Pal) showed no antibacterial effect, with a minimum inhibitory concentration (MIC) of 16 $mg.mL^{-1}$ for all tested bacterial strains. Conversely, the HSA sample (salicylideneaniline Schiff base) exhibited significant antibacterial activity against both Gram-positive and Gram-negative bacteria, with an MIC of 0.5 $mg.mL^{-1}$ for each type of bacteria. Notably, *Pseudomonas aeruginosa* showed higher sensitivity to the HSA-Sif Pal compound compared to enterobacteria and Gram-positive bacteria, with an MIC of 2 $mg.mL^{-1}$, suggesting promising potential for the development of effective antimicrobial agents.

Key words: Palygorskite; Schiff base; MIC method; *Staphylococcus aureu*; Escherichia *coli*; *Pseudomonas aeruginosa*.

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Photocatalytic degradation of methylene blue using ZnO thin layer

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Methylene blue (MB) is environmentally persistent, toxic, carcinogenic and mutagenic [1]. It is often considered as a model pollutant in water remediation. Many technologies have been developed for the removal of MB from its waste effluent before its release into the environment.

Photocatalysis permits its degradation/mineralization [2]. Among the most used semiconductors, ZnO stands out as a photocatalyst due to its unique properties such as stability, high optical sensitivity, low-cost and non-toxic nature [3] and, also, because of its large excitation binding energy (60 meV) and wide band gap (3.0 - 3.3 eV) [4].

Most of the ZnO based photocatalysts were in the form of suspended particles. However, suspended nanoparticles have several drawbacks, including difficulty in separation or filtration of the photocatalysts and blocking of UV light by suspended particles. Thus, the challenge in photocatalysis is the recovery of the photocatalyst on suitable substrates after wastewater treatment.

The objective of this work was to evaluate the photocatalytic activity of zinc oxide (ZnO) thin layer for methylene blue (MB) degradation.

ZnO thin film was grown on indium tin oxide (ITO) coated glass substrate by electrodeposition process. The electrolyte bath used for the films elaboration consisted on 0.1M of $ZnSO_4.7H_2O$. The deposition was carried out at 65°C for 45 min with an applied potential of -7.2 V. After deposition, the samples was rinsed by deionized water and dried under the air. The elaborated sample was annealed at 500°C during 60 min and under a fixed heating rate of 10°C min^{-1}.

The degradation of MB was calculated using UV-Vis absorption from the samples before and after the photocatalytic process. The maximum percentage of degradation (72 %) was obtained during 7 h, with the operational parameters which are the following: C_0: 25 mg L^{-1}; solution volume: 50 mL; ZnO film surface: 2 cm^2; radiation: 0.67 W/m^2 and λ 334 nm.

Key words: ZnO, Thin layer, Methylene blue, Photocatalytic degradation.

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Synthesis of New Derivatives of Benzimidazole-Cyclohexanones.

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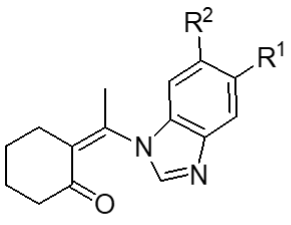
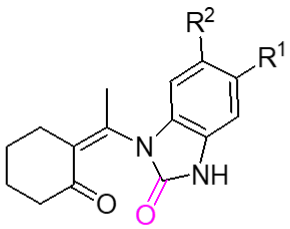
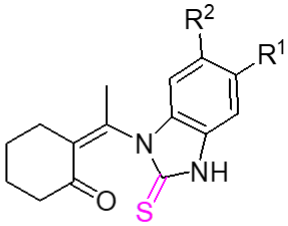
Heterocyclic compounds are significant in organic chemistry due to their diverse biological activities. Recently, the design and synthesis of new molecules for crop health and human welfare have gained importance. Benzimidazoles, in particular, have proven vital in medicinal chemistry, serving as proton pump inhibitors and antiviral agents, and exhibiting properties such as antimicrobial, anticonvulsant, analgesic, anti-inflammatory, anti-diabetic, antiprotozoal, antipsychotic, antioxidant, and antitumoral effects [1]. Some, like thiabendazole and albendazole, are commonly used as antihelmintic drugs [2]. The structures of benzimidazolone and benzimidazolothione feature interesting biological properties and include a constrained ring system with two nitrogen atoms linked by an ethylene bridge [3, 4]. This work reports the synthesis and characterization of new benzimidazole-cyclohexanone derivatives **3a-d**, **4a-d** and **5a-d** under different reaction conditions (**Scheme 1**).



3a-d



4a-d



5a-d

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Synthèse des silicoaluminophosphates nanoporeux à partir de plusieurs agents structurants

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Dans le début des années 1980, Les aluminophosphates (AlPO4-n) sont des tamis moléculaires, ils ont été découverts par des recherches à Union Carbide Corp [1]. A. Tuel et al. ont initié une activité intense dans la synthèse des matériaux inorganiques ayant des compositions et une architecture particulières de la charpente aluminophosphate [2].
Dans cette étude, plusieurs échantillons ont été synthétisés dans des conditions hydrothermales en utilisant premièrement la Morpholine comme agent de direction de structure. Ensuite, un mélange de deux agents structurant (TEAOH+Morpholine) a été utilisé. L'effet de l'agent structurant organique, la nature des sources de silicium et leur teneur sur la phase cristalline du matériau ont été étudiées et les résultats ont été comparés à ceux qui ont obtenus à partir d'autres études rapportées dans ce domaine. Les cristaux ont été caractérisés par diffraction de rayon X (DRX) et infrarouge(IR). D'une part, différentes phases ont été obtenues en utilisant le Morpholine comme agent structurant dans certaines conditions de synthèse. D'autre part, les résultats montrent que la combinaison de TEAOH et Morpholine aboutit à une structure AFI (SAPO-5) tant dit que le morpholine est l'agent approprié pour la synthèse de la SAPO-34, selon les résultats de notre étude.

Mots clés: l'aluminophosphate ; synthèse ; agent structurant ; SAPO-34 ; SAPO-5

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Synthèse de nouveaux α-aminophosphonates thiophéniques d'intérêt

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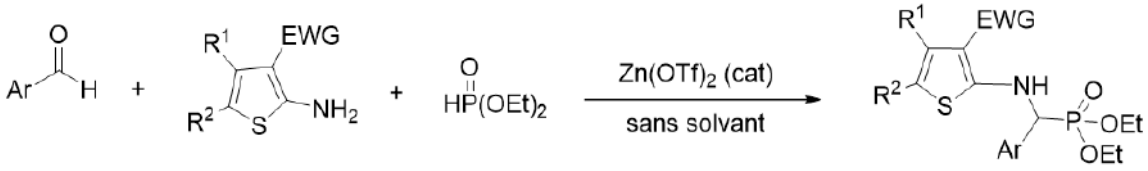
Les α-aminophosphonates sont des analogues structuraux des α-aminoacides et peuvent mimer l'état de transition dans l'hydrolyse des peptides. Ils sont notamment connus comme inhibiteurs d'enzymes HIV protéase, anticancéreux et agents antithrombotiques [1]. D'autre part, les 2-aminothiophènes sont des motifs intéressants dans la conception de molécules biologiquement actives en raison de leur affinité avec diverses cibles biologiques. L'incorporation de tels pharmacophores dans les α-aminophosphonates pourrait donc améliorer leur activité biologique dans le traitement de nombreuses maladies. [2]

Dans le cadre de cette orientation, cette présentation décrit la synthèse d'une nouvelle famille d'α-aminophosphonates thiophéniques, *via* une condensation *one-pot* à trois composants de type Kabachnik-Fields d'aldéhydes, de 2-aminothiophènes fonctionnalisés et de dialkylphosphites, catalysée par le triflate de zinc. Cette méthode qui propose des conditions douces et sans solvant présente également l'avantage d'être flexible et de conduire à des rendements bons à excellents. De plus, cette séquence propose l'utilisation d'un catalyseur Zn(OTf)2 reconnu pour sa faible toxicité et son faible impact écologique, ce qui rend cette méthode particulièrement intéressante pour la synthèse d'une large gamme de produits pour les tests biologiques.



Mots clés : α-aminophosphonates, 2-aminothiophènes, réaction de Kabachnik-Fields.

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Ultra-rapid Rhodamine B removal by highly efficient recyclable blue crab crustacean

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This research investigates the removal of Rhodamine B dye (RB) from both synthetic and real wastewater using locally sourced crustacean waste biomass. The granulometric analysis showed an even distribution of the biomass microparticles. The investigation into surface charge revealed an acidic pH of zero charge. By optimizing the adsorption process using Central Composite Design (CCD) modeling, the study identified optimal conditions for RB concentration, reactor temperature, and contact time, resulting in a maximum yield and a maximum adsorption capacity (Qmax). Kinetic and isothermal studies had occurred. Namely, pseudo-first, pseudo-second orders, intra-diffusion and Elovich models.

SEM micrographs displayed biomass particle swelling post-RB adsorption, while FTIR analysis indicated an increase in the crystalline order of crustacean waste chitosan chains. Furthermore, applying these optimal conditions to real industrial wastewater were also studied.

This work stands out for its transition from laboratory-scale reactors (in mL) to real industrial-scale wastewater applications (in L) and for assessing the biomass's affinity for Rhodamine B in a mixture containing similar dyes, showcasing its selective/simultaneous adsorption abilities.

Rapid determination of malondialdehyde in serum samples using a porphyrin-functionalized magnetic graphene oxide electrochemical sensor

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An electrochemical sensor based on a screen-printed carbon electrode (SPCE) modified with porphyrin-functionalized magnetic graphene oxide (TCPP-MGO) was developed for the sensitive and selective determination of malondialdehyde (MDA), an impor tant biomarker of oxidative damage, in serum samples. The coupling of TCPP with MGO allows the exploitation of the magnetic properties of the material for separation, preconcentration, and manipulation of analyte, which is selectively captured onto the TCPP MGO surface. The electron-transfer capability in the SPCE was improved through derivatization of MDA with diaminonaphthalene (DAN) (MDA-DAN). TCPP-MGO-SPCEs have been employed to monitor the differential pulse voltammetry (DVP) levels of the whole material, which is related to the amount of the captured analyte. Under optimum conditions, the nanocomposite-based sens ing system has proved to be suitable for the monitoring of MDA, presenting a wide linear range (0.01-100 µM) with a correlation coefficient of 0.9996. The practical limit of quantification (P-LOQ) of the analyte was 0.010 µM, and the relative standard deviation (RSD) was 6.87% for 30 µM MDA concentration. Finally, the developed electrochemical sensor has demonstrated to be adequate for bioanalytical applications, presenting an excellent analytical performance for the routine monitoring of MDA in serum samples.

Key words: Porphyrin-functionalized magnetic graphene oxide, Screen-printed carbon electrode, Electrochemical sensor, Malondialdehyde, Serum samples.

Synthesis, characterization, and photophysical properties of functionalized six and seven-Membered-Ring carbohelicenes

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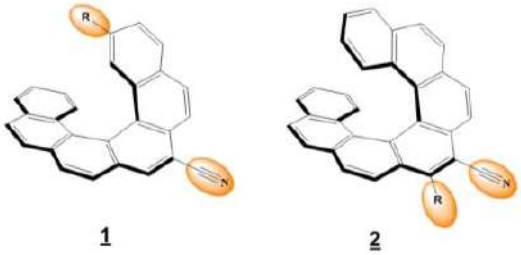
Helicenes are unique helical chromophores possessing advanced and well-controlled spectral and chemical properties owing to their diverse functionalization and defined structures.

Functionalization, of a helicene, may have either the purpose of modifying the electronic properties of the parent helicene, c.g., by adding electron-withdrawing groups, or the scope of providing the helicene with a "handle", which can be reacted to bind the molecule to a metal surface, or again to allow for complexation of the helicene with metal ions.

In this context, the purpose of this study is to screen our continuing efforts on the synthesis of new functionalized helical scaffolds. The synthetic approach followed in this work is founded on the use of 4-Bromophenylacetonitrile as a convenient building block to provide the appropriate 1,2-diarylethene via Knoevenagel condensation. Helicenes precursors were then properly transformed into the functionalized helicene under UV irradiation. Upon success of this this goal, it was interesting to investigate experimental chiroptical, photophysical and electrochemical behaviors of such derivatives. Moreover, the cyano group grafted on the polyaromatic structure serves for increasing the solubility of the helicene in organic solvents, may improve its photophysical properties and may convert the helix skeleton into variously substituted large derivatives through different couplings.



Key words: Helicene, Polyaromatic, Photooxydation, Photophysical properties

Valorization of Posidonia Oceanica Lignin: Sustainable Extraction and Characterization for Innovative Pharmaceutical and Cosmetic Applications

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Lignin, a natural polymer abundant in Posidonia oceanica fibers, shows promising potential for pharmaceutical and cosmetic applications due to its inherent antioxidant, antimicrobial and anti-inflammatory properties. Its versatility is further enhanced by the ease with which it can be transformed into micro- and nanoparticles or thin active layers, making it ideal for innovative uses in health and beauty products. This research emphasizes the sustainable valorization of Mediterranean marine resources, contributing to the development of high-quality, environmentally friendly materials.

In this study, we focused on the preparation and characterization of Posidonia oceanica fibers and the chemical extraction of lignin. The fibers underwent a series of cleaning and processing steps before being analyzed by spectroscopic and chromatographic techniques to assess their structural and chemical properties. Solvent-based methods were then used to extract the lignin, which was characterized to determine its chemical composition and molecular structure.

In this study, advanced analytical techniques, in particular quadrupole time-of-flight mass spectrometry (QTOF-MS), were used to provide a detailed characterization of the molecular structure of lignin extracted from Posidonia. The results reveal a complex and diverse composition, highlighting the potential of this lignin for industrial applications. This research thus paves the way for the exploration of new sustainable material solutions incorporating Posidonia lignin, with promising prospects for innovation in this field.

Key words: Posidonia, lignin extraction, characterization, biotechnological processes.

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Bioactive porphyrin magnesium (II) complex. Synthesis, Molecular Structure and Spectroscopic characterization. Biological Activity and Molecular Docking studies.

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We have synthesized and characterized porphyrin structures by UV-visible, IR and fluorescence spectroscopy studies and single crystal XRD analysis; H_2(TPP) (**I**) (meso-tetraphenylporphyrin), [Mg(TPP)(DMF)] (**II**); (DMF: dimethylformamide) and [Mg(TPP)(H_2O)].2(4-CNpy) (**III**); (4-CNpy: 4-Cyanopyridine). The crystal packing of the porphyrin structures is stabilized by intermolecular hydrogen bonds and by intermolecular C–H···Cg π interactions where Cg is the centroid of the phenyl and pyrrole rings. UV-Vis spectroscopic data confirmed the creation of *Mg*-meso-porphyrin complexes by the red-shifted Soret bands for our derivatives compared to the free-base porphyrin. The optical gap energy values of (I), (II) and (III) are 1.92, 2.07 and 2.00 eV. Gram-positive and Gram-negative bacteria were tested against free porphyrin (I), metallated porphyrin (II) and complex (III). The results show that the magnesium porphyrin derivative is highly effective compared to H_2TPP free-base porphyrins and metallated porphyrin [Mg(TPP)] and has higher inhibition character against the tested bacteria. The molecular docking of the complex (III), in the active sites of bacterial proteins was carried out to detect the degree of antibacterial activity of recognition.

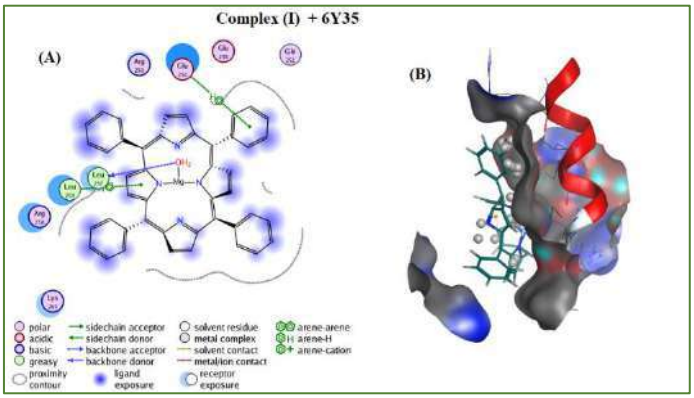

Figure : Molecular Docking Interaction diagram for the porphyrin compound with protein active site (6Y35); (A) best docking interaction, (B) surfaces maps.

Synthesis, biological evaluation and molecular docking studies of a new magnesium (II) porphyrin complex

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A new bioactive material of magnesium porphyrin complex [Mg(TPP)](H2O)2].2/3(2.2.2).1/3(Bz) (I), (TPP = meso--tetraphenylporphyrinato and (2.2.2) = cryptand, and Bz is benzene (C6H6)) has been synthesized and characterized by Single-crystal X-ray diffraction (SCXRD). The title compound crystallizes in trigonal crystal system in space group P-3. The magnesium ion is coordinated to four nitrogen atoms of the porphyrin core and two oxygen atoms of the axial ligands. The crystal packing is stabilized by inter-and intramolecular hydrogen bonds, and by weak C–H…Cg π interactions leading to a bi-dimensional network. In order to confirm the crystal structure, the photophysical properties have been evaluated by infrared (IR), proton nuclear magnetic resonance 1H NMR and UV-Vis spectroscopy. UV-Visible absorption spectrum of complex (I) displayed a red shifted Soret (429 nm) and Q (567 and 609 nm) bands due to the extended conjugation. The IR, and 1H NMR confirm the crystal structure. Finally, bioactivity investigations revealed that free porphyrin H2TPP, [Mg(TPP)] and complex (I) could be used as potential novel significant antibacterial agents. The docking of the free base porphyrins, metallated and the complex (I), in the active sites of bacterial proteins *EEscherichia coli* (1ECL) and *Aspergillus Niger* (3K4P) was carried out to detect the degree of antibacterial activity of recognition.

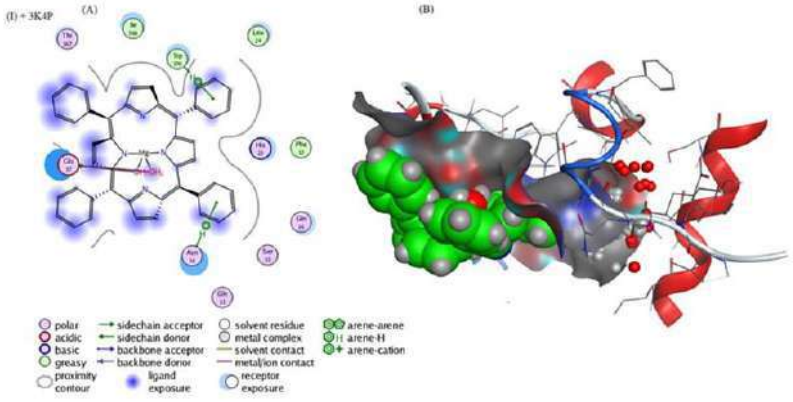

Figure : Molecular Docking Interaction diagram for the compound (I) with the protein active site (3K4P); (A) best docking interaction, (B) surfaces maps.

Synthesis of a novel pyrrolyl-pyrimidine derivatives as antidiabetic agents: Molecular Docking studies and ADMET prediction

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Diabetes mellitus is a significant global health concern, with a high prevalence of type 2 diabetes, necessitating effective treatments to manage the condition[1].Additionally, various drugs have been used to treat diabetes and improve insulin sensitivity[2]. Among several enzymes, α-amylase have been explored as potential antidiabetic agent [3].

In this present work, a novel serie of 3-pyrrolylpyrimidines was synthesized from several formylpyrroles, guanidine and dibenzoylmethane. These synthesized analogues were evaluated in terms of their α-amylase inhibitory potential using *in silico* studies. The majority of these compounds exhibited different hydrogen bonds with the active site of the Human pancreatic Alpha-amylase (PDB: 3baj) and showed promising potential for future development as α-amylase inhibitors. In another term, and with the intention of optimizing and streamlining the process of drug development, the ADMET profiling of the synthesized compounds was predicted theoretically through chemoinformatic tools in order to determine their pharmacokinetic proprieties and to ensure their efficacy and safety profiles for clinical use.

Key words: Pyrrolylpyrimidine, antidiabetic activity, α-amylase, docking, ADMET.

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Improved synthesis of 2,2′-arylmethylene bis(3-hydroxy-5,5 dimethyl-2-cyclohexene-1-one) derivatives catalyzed by KSF under microwave

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Because of the good control of the particle size, morphology, uniformity thus large specific surface area of mesoporous silica nanoparticles provides for large adsorption capacities interesting for biotechnology, also biomedicine.

In this work, MCM-41 mesopourous silica was obtained from tetraethoxysilane using C_{18}TAB as pore template. 2,2'arylmethylene bis (3-hydroxy-5,5-dimethyl-2-cyclohexene-1-ones) were synthesized in a one-step using a new method taking into account the principles of green chemistry; such as atom saving, handling with inexpensive reagents, saving time and simplicity of procedures while respecting the environment. Functionalized mesostrutured silica were obtained by coupling the MCM-41 with 2,2'arylmethylene bis (3-hydroxy-5,5-dimethyl-2-cyclohexene-1-ones) using 3-(triethoxysilyl) propyl isocyanate as coupling agent.

We have succeeded in obtaining Functionalized MCM-41 silica nanoparticles. UV-Vis spectroscopy shows the modification of the organic structure while passing from one step to another. From the thermogravimetric analysis, it can be said that functionalization is not completed.

Key words: MCM-41, Nanoparticles, Functionalization, Green chemistry.

Synthesis of new analogues of cinnamic acid : Bioactive compound in propolis

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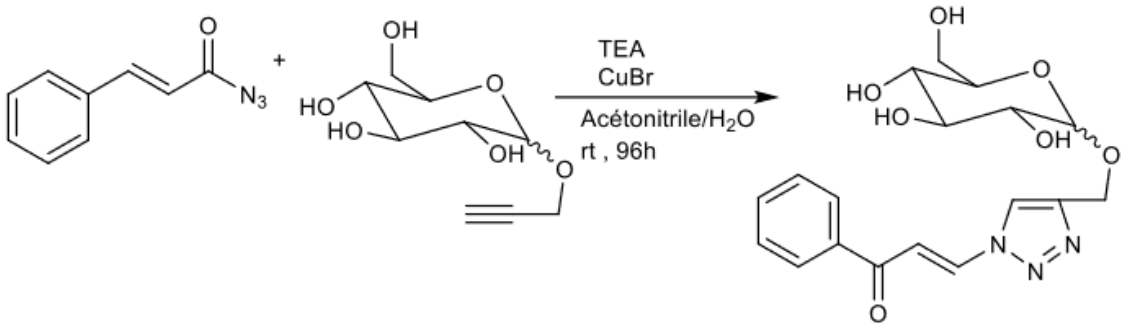
Propolis, also known as bee glue, is a sticky, resinous substance produced by bees to protect their hive and perform other functions such as mummifying intruders to prevent decomposition, filling cavities in the hive and restricting entry to the hive during the winter Numerous studies have shown that propolis has a wide range of therapeutically significant activities, including antioxidant, antimicrobial, anticancer, antiulcer, antidiabetes and immunomodulatory properties. Cinnamic acid is studied not only for it biological[1] activity in propolis but also because of its very specific structure, it has various possibilities of substitution on the cinnamic skeleton as well at the level of the carboxylic group, even on the double bond and the aromatic nucleus this leads to a wide choice of analogue to modulate a biological activity. for this we chose to synthesize a series of analogue, characterized by NMR and IR.



Key words: Synthesis, propolis, cinnamic acid, analogues.

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Coating Uniformity: Influence of Atomizing Air Pressure and spray rate

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Polymer films are applied to pharmaceutical solids for cosmetic, protective, or functional purposes [1] [2]. The application process is quite complex, with multiple variables related to the substrate characteristics, coating formulation, processing equipment, and processing conditions [3][4].

The purpose of this study was to investigate the effect of atomizing air pressure, spray rate on coating uniformity, and film coat quality. Parameters characterizing coating uniformity were the mass variance of the film-coated tablets and the variance of the film thickness inside a tablet. For this analysis, we took into account the film coat's thickness as well as the proportion of weight growth.

A Labe scale drum coater was used for the trials, with three distinct spray rates ranging from 1 to 2 ml/min and atomizing air pressures ranging from 1 to 3 bars. Throughout the coating process, all other parameters remained unchanged. The quality and homogeneity of a film coat can be demonstrated to be significantly influenced by the atomizing air pressure.

We noticed an increase in the weight gain of the tablets with the increase in atomizing air pressure. The film coating was thicker when sprayed at 2 and 3 bars than when sprayed at 1 bar. The smooth tablets and a small film thickness variance will produce at an atomizing air pressure of 2.0 bars. The weight gain and coating film thickness were directly proportional to the spray rate. An increased flow rate increased the amount of the coating solution deposited on the tablet surface, thereby increasing weight gain and coating thickness. The smooth tablets with a lower surface roughness and a small film thickness variance will produce at a spray rate of 1 ml/min.

Keywords: Coating uniformity; Atomizing air pressure; Spray rate, Weight gain; Film thickness, roughness surface.

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Optimisation de la formulation d'un comprimé orodispersible EBASTINE 10mg

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Un médicament générique est une copie d'un médicament original (princeps) conçue pour le remplacer à moindre coût une fois que le brevet ou le certificat complémentaire de protection de ce dernier a expiré. L'utilisation des génériques reste le seul moyen de rendre les médicaments accessibles à une large part de la population des pays du tiers monde [1].
Les comprimés orodispersibles sont des comprimés non enrobés conçus pour se dissoudre rapidement dans la bouche avant d'être avalés. Ils contiennent des superdésintégrants qui accélèrent la dissolution ou la dispersion du principe actif en provoquant la désintégration du comprimé en contact avec de l'eau ou de la salive [2].
L'objectif de notre recherche est d'optimiser la composition du générique EBASTINE 10 mg afin d'obtenir une formulation qui offre une libération optimale du principe actif et une désintégration plus rapide proche de celle du princeps KESTIN. Pour atteindre cet objectif nous adopterons la méthode de modification des facteurs (diluants, désintégrants) et mettrons en œuvre deux méthodes de formulations : la compression directe et granulation humide.
Différents modèles mathématiques ont été utilisés pour modéliser la cinétique de dissolution du générique et du princeps KESTIN. Une étude comparative des profils de dissolution du princeps et du générique a été effectué en utilisant la méthode du « Fit factor ».
Les résultats obtenus ont montré que la formulation la plus efficace est la formule F5, qui est obtenue par granulation humide. En outre, la comparaison des profils de dissolution du générique et du princeps a confirmé leur similitude.

Mot clés : EBASTINE, médicament générique, médicaments princeps, dissolution, orodispersible, superdésintegrant

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Electromechanical Properties of Dissimilar Welds Using Different Filler Metal Compositions

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In this study, dissimilar welding of ferritic stainless steel with copper was carried out using the TIG (tungsten inert gas) welding technique. The quality of the weld is influenced by the chemical composition of the filler wire, which varies based on the different materials used. Thus, the welding was performed using four types of filler metals with different chemical compositions: duplex-stainless alloy, copper alloy, and nickel alloy. The corrosion behavior of the welds was then studied to identify the filler metal that offers the best resistance to corrosion. To achieve this, corrosion tests were conducted using parameters such as the most aggressive corrosion medium, NaCl, along with varying corrosion time and corrosion rate. In the results, the Tafel curve provided the corrosion potential and electromechanical properties of dissimilar welds. Additionally, the samples were characterized both before and after corrosion to observe the initiation of corrosion, identify corrosion-sensitive phases, and analyze the corrosion layer formation using optical microscopy and scanning electron microscopy, also it was concluded that nickel alloy filler has the best electromecanical behavior for these types of dissimilar welds.

Key words: Filler metal, Electromechanical properties, A1Cu, AISI 430, TIG Welding, Dissimilar weld

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Anti-inflammatory therapeutic treatment generated by the extract of “Capsaicin” Pepper

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Phytotherapy, practiced for thousands of years, is based on the use of medicinal plants in various forms, such as herbalism, aromatherapy and homeopathy. The chili pepper, a species widely cultivated worldwide, is recognized not only as a staple food in many ethnic cuisines, but also as a medicinal plant. The antimicrobial, antioxidant, antimutagenic, hypocholesterolemic and immunosuppressive properties of its secondary metabolites make it a valuable ingredient in various medical treatments and a versatile resource. Capsaicin, the main active component of chili pepper, is known for its analgesic and anti-inflammatory properties, which explains its widespread use in traditional and folk medicines worldwide.

The formulated cream has a semi-solid consistency, a light orange color and a slightly refreshing minty odor, has good homogeneity and a pH close to the skin. The latter has undergone various quality control tests such as homogeneity and stability. Tests were carried out using the Folin-Ciocalteu assay method to qualify total polyphenols and the DPPH method to measure antioxidant activity. Using these methods, we were able to determine the chemical composition of the peppers and evaluate their biological properties.

Key words : Capsaicin, chili pepper, essential oil, anti-inflammatory, ointment, CG-MS.

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Synthesis, Characterization and biological evaluation of new polyphenol Derivatives From3- benzyloxy-4-methoxybenzaldehyde

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Chalcones are products of condensation of simple or substituted aromatic with simple or substituted acetophenones in presence of alkali. Chalcone constitute an impartment group of natural products and some of them possess a wide range of biological activities such as anticancer[1] antitubercular, antiviral, also they are used as anti-malarial, anti protozoal, anti-inflammatory, immunomodulatory[2], nitric oxid inhibition, tyronase inhibition, cytotoxic, antimicrobial. A natural medicine genus Angelica is known to contain large number of naturally occurring chalcones. Chalcone derivatives are recognized for NLO properties and have good crystallization ability, these molecules are also used as starting materials in the synthesis of UV absorption filters in polymers, photorefractive polymers, photosensitizers in bicolor films, sweeteners in food technology, and in holographic recording technology.

A series of chalcone derivatives (2a–i) were prepared via the reaction of 3-benzyloxy-4-methoxybenzaldehyde with the appropriately acetophenon derivatives. The structures of all the new chalcone derivatives (2a–i) synthesized in this study were established on the basis of ^{1}H NMR and ^{13}C NMR spectral data, and elemental analyses The antibacterial activity of the synthesized compounds (**2a- i**) was carried out by well diffusion and MIC method.

Key words: Chalcones, antibacterial activity, 3-benzyloxy-4-methoxybenzaldehyde,

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Enhancing Solubility and Molecular Characterization of Ibuprofen-β-Cyclodextrin Inclusion Complexes through Rapid Microwave-Promoted Formation

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This study investigates the formation of inclusion complexes between Ibuprofen (IB) and β-cyclodextrin (β-CD) under microwave irradiation, focusing on enhancing solubility and understanding molecular interactions [1]. The solubility of IB increased linearly with β-CD concentration, as depicted by the phase solubility diagram, revealing a 1:1 stoichiometry and an estimated stability constant (Ks) of 74.42 M-1. Various methods for preparing IB/β-CD complexes were explored, resulting in solubility enhancements ranging from 1.550 ± 0.006 to 4.421 ± 0.003 mg/ml compared to free IB solubility of 1.391 ± 0.004 mg/ml. FT-IR analysis indicated characteristic shifts in absorption bands, confirming the formation of inclusion complexes, which was further supported by 1H NMR spectra revealing upfield chemical shifts for β-CD and IB protons [2].

Distinct differences in proton shifts observed between complexes prepared via Heating Reflux (HR) and Microwave Reflux (MR) suggest unique interactions or conformations within the β-CD cavity under different heating conditions. Overall, this study provides comprehensive insights into the formation and characterization of IB/β-CD inclusion complexes, offering significant implications for their potential pharmaceutical applications

Key words: Inclusion complex, β-cyclodextrin, Supramolecular interaction, Ibuprofen, Phase solubility study, Microwaves irradiation, ^{1}H NMR.

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Assessment of Heavy Metal Contamination in Irrigation Water, Soil, and Onion Crops: A Case Study from the Isser and Zemmouri Regions, Algeria

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This study thoroughly assesses heavy metal contamination in onions cultivated in Boumerdes, Algeria's Isser and Zemmouri regions, focusing on potential health risks from consumption. Analysis of irrigation water, soil, and onion samples revealed concentrations of essential and toxic heavy metals including iron (Fe), copper (Cu), zinc (Zn), cadmium (Cd), chromium (Cr), lead (Pb), and nickel (Ni). Atomic Absorption Spectroscopy (AAS) was utilized for accurate quantification, with results compared against FAO/WHO 2001 standards [1].

In Isser:
- Irrigation water showed elevated copper (Cu) at 0.72 mg/L and zinc (Zn) at 0.19 mg/L.
- Soil analysis at Site 01 indicated high levels of copper (Cu) at 68.41 mg/kg, zinc (Zn) at 62.12 mg/kg, and lead (Pb) at 71.63 mg/kg.
- Onion samples from Site 01 exceeded permissible limits for chromium (Cr) at 3.1 mg/kg and lead (Pb) at 0.31 mg/kg in bulbs.

In Zemmouri:
- Irrigation water showed elevated nickel (Ni) at 0.18 mg/L, chromium (Cr) at 0.09 mg/L, and copper (Cu) at 0.14 mg/L.
- Soil analysis indicated elevated lead (Pb) at 64.32 mg/kg and nickel (Ni) at 11.21 mg/kg.
- Onion samples from Zemmouri (Site 02) had high zinc (Zn) at 49.40 mg/kg and iron (Fe) at 541.31 mg/kg in leaves, with iron exceeding limits (437.65 mg/kg) in leaf analysis.

These findings underscore significant health risks associated with consuming these vegetables due to their elevated concentrations of heavy metals [2].

Key words: Heavy Metals, Soil contamination, Vegetables, Health risk, irrigation waters.

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Variation in the Yield, chemical composition and antimicrobial activity of essential oils of four *Eucalyptus* species under different bioclimatic conditions

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The present work investigates the quantitative and qualitative variations of essential oils from the leaves of five *Eucalyptus* species; *E. salmonophloia, E. torquata, E. lesouefii*and *E. astringens,* in different locations in Tunisia and highlights their antimicrobial activities. A trial was carried out during winter season of 2021 and samples collected from arboreta from different parts of Tunisia characterized by two climates; semi-arid and arid. The obtained results refer to presence of high significant differences between species and locations. The hydrodistilled oils obtained from arid regions (0.39-4.63%) recorded higher yield compared to semi-arid regions (0.27-3.74%) for all species studied. GC/MS analysis indicated a significant variation in oil composition among and within species. A total of 99 compounds were identified. However, there are main and common compounds such as 1,8-cineole, α-pinene, transpinocarveol, β-eudesmol, torquatone, spathulenol and globulol. Studied EOs showed significant inhibitory activity against all microbial strains tested. However, a microbicidal effect against gram negative bacteria *E. coli* and *S. marcescens* and against the fungus *C. tropicalis* was observed, with the oils extracted from **E. lesouefii** cultivated in the El Hanya arboretum in semi-arid climate being the most active.

Key words: *Eucalyptus* essential oil; chemical composition; antimicrobial activity; environmental effect

Cadmium removal from phosphate ore

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Phosphate rock is a valuable material that is used for the production of large phosphorus chemicals. However, this natural material usually contains some toxic elements such as cadmium(Cd). Cd is a non-nutritive metal regarded as harmful to both humans and the environment. Themain toxic effects of Cd on human health are the kidney and renal cortex diseases. Other effectswere observed on pulmonary, cardiovascular, and musculoskeletal systems, in addition to including Cd as a human carcinogen. In order to reduce the cadmium content in the phosphate ore, an original method was studied and consists of coupling both leaching and electrodialysis. The effects of process parameters, such as reaction time, nature, and concentration of the extracting agent, liquid/phosphate ore ratio, pH, temperature, and current density, were investigated. The obtained results show that the cadmium extraction from phosphate ore using simple batch leaching does not reduce the cadmium content to the required level. However, the application of leaching- electrodialysis coupled method at optimum current density of 10 mA cm−2 increases the cadmium extraction efficiency up to 84.3%. This synergetic process could be applied to thetreatment of phosphate ore containing cadmium.

Key words: Phosphate ore, cadmium, leaching, electrodialysis, coupled process

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Decontamination of water containing persistent dyes by heterogeneous photocatalysis under solar irradiation

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For several years, water pollution has become one of the most interesting current concerns, especially after the great general industrial development that threatens the health and environmental system; this is what led to insist on the development of research for the purification and reuse of water. Among several water treatment techniques, photocatalysis seems an efficient and clean process, in addition to its use in water treatment, photocatalysis has found several applications in the field of the environment, namely in the purification of indoor and outdoor air. This present study focused on the degradation of water containing two types of recalcitrant dyes "Congo Red and Crystal Violet" by heterogeneous photocatalysis based on virgin TiO2 and TiO2 doped with nitrogen in the presence of solar irradiation. The results obtained show that photocatalysis based on TiO2 doped with nitrogen under solar irradiation is more effective. The improvement in the degradation efficiency of crystal violet using TiO2-N compared to virgin TiO2 ranges from 53.4% to 97.56% after doping. However, the improvement in the degradation of Congo Red from 83.7% by virgin TiO2 to 92.8% by TiO2-N. Given these encouraging results, this technique can be used in the treatment of water contaminated by recalcitrant dyes.

Key words: Phosphate ore, cadmium, leaching, electrodialysis, coupled process

Influence of Welding Parameters and Heat Treatments on the Electrochemical Properties of TIG Welds in AISI 430 Steel

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This study investigates the influence of welding parameters, alloying elements (Al and Ti), and heat treatments on the mechanical and electrochemical properties of TIG welds in AISI 430 ferritic stainless steel. Electrochemical tests, including polarization measurements and impedance spectroscopy, were performed to assess corrosion resistance. The results show that pulsed current, particularly at low frequencies, enhances both mechanical performance and corrosion resistance by reducing the formation of intergranular martensite. The addition of Ti and Al promotes an equiaxed microstructure and improves intergranular corrosion resistance. The post-weld heat treatment at 800°C restored corrosion resistance, demonstrating the effectiveness of this approach. These findings provide guidance for optimizing welding processes for ferritic stainless steels in corrosive environments.

Key words: TIG welding, AISI 430 ferritic stainless steel, heat treatments, electrochemical tests, mechanical properties.

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ELECTROCHEMICAL BEHAVIOR OF AISI1080 STEEL IN MARINE ENVIRONMENT APPLICATIONS

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Threaded rods are used in mechanical and metal structures for industrial applications. They are generally designed in steel to be subsequently heat treated to improve their performance when commissioning in the agro-exploitation structures. These rolled rods, have problems related to their low resistance to the various loads to which they are subjected during their commissioning corrosion [1, 2, 3]. Thus, the goal of this work is to study the effect of the surrounding environment on intrinsic and electrochemical properties by seeking to optimize various treatments in order to improve the performance of these rods made of steel [4]. The results of the mechanical, microstructural and electrochemical investigations performed on the treated steel gave lower corrosion rates than those of the standard steel, thus indicating a higher resistance to corrosion since their use is in a corrosive environment that would facilitate the fall of their mechanical characteristics and to protect the natural resources [5].

Key Words: Rods Steel, agriculture structures, Corrosion, Microstructure.

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Electrosynthesis and characterization oligomer deriving from m-propargylanisole

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The anodic oxidation of m-propargylanisole is studied in acetonitrile on a platinum electrode. Preparative electrolysis at constant current leads to the formation of two types of oligomers. The first is soluble but the second is insoluble in all common solvents. The latter develops in the form of a film that deposited on the anode during scanning potential by cyclic voltammetry. The study of the surface morphology by scanning electron microscope showed that this deposit becomes very thick after 60 cycles and cracks deeply.

The physico-chemical characterizations of the obtained products show that they are oligomers derived from m-propargylanisole, which are thermally stable and semiconductor.

Keywords: Conjuguted polymers; m-propargylanisole; Electron transfer; Oligophenylenes

Anodic synthesis of a new oligophenylene deriving from m-fluoroanisole

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The electrochemical study of m-fluoroanisole (m-FA) is realized by cyclic voltammetry and preparative electrolysis in acetonitrile on a platinum electrode. The voltammetric analysis shows the formation of a compact and homogeneous film on the anode during successive scans of the potential.

The preparative electrolysis at high concentration leads to the formation of two oligomers. The first is soluble; the second is a deposit, insoluble in most usual solvents. Their chemical structures are characterized by FTIR, NMR and UV.

The physico-chemical study of these new oligophenylenes showed that they are thermally stable and semi-conductor.

Keywords: m-Fluoroanisole, Conjuguted polymers, Electrosynthesis, Semi-conductor

Synthesis, characterization and Antioxidant application of some metal complexes of curcumin with bi-pyridine

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In this contribution, some transition metal complexes of general formula [M(Cur)(Bpy)X], M = Co, Ni, Cu or Mn, Cur = curcumin, Bpy = bipyridine and X= halogen have been synthesized by the reaction of metal with curcumin as primary ligand and bipyridine as secondary ligand in ethanol solution. The composition of the complexes has been characterized by conductivity measurement, IR and UV-visible spectroscopy. The stability and solubility of the prepared complexes were determined. The evaluation of the antioxidant power of the complexes was carried out using the $DPPH^{\cdot}$ The results showed that the complexes have antioxidant activity compared to a control antioxidant.

Keywords: Curcumin; bipyridine; antioxidant; DPPH.

Efficient synthesis and characterization of new copper (II) complex with sulfonylphthalimide

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Sulfonamides and their derivatives are a well-known class of physiologically active compounds with a wide range of medical uses. These compounds have been widely used in many different fields including antibacterial, antifungal, antimalarial, and anticancer agents.

In recent years, there has been a significant focus on the investigation of transition metal complexes due to their extensive usage in diverse areas of chemical, biological, and environmental significance. sulfonamide compounds are a significant class of ligands in the domain of transition metal coordination chemistry. Copper complexes of sulfonamides offer a dual mechanism of action, combining the antimicrobial activity of the sulfonamide ligand with the inherent antimicrobial properties of copper ions. This synergistic effect enhances their effectiveness in combating infections and promoting wound healing in burn patients.

Sulfonylphtalimide have two strong coordination sites, making them excellent ligands for complexation with metal ions. The desired complexes were synthesized in a single step using two equivalents of sulfonylphthalimide and one equivalent of $CuCl_2 \cdot 2H_2O$. The reaction was carried out under reflux in ethanol for 3 hours. The formation of the complex was confirmed by a color change, with the mixture turning dark green, indicating significant progress in the reaction. After precipitation and filtration, a green powder was collected with a good yield. The structure of the complex was identified by IR, UV-visible, and XRD analyses.

APPLICATION DES NANOPARTICULES A BASE DE KAOLIN POUR L'ELIMINATION DES COLORANTS EN MILIEU AQUEUX

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Notre présent travail a pour objectif principal : l'étude de l'adsorption d'un colorant cationique à savoir le Cristal Violet (CV) en milieux aqueux, en utilisant des nanoparticules à base de kaolin bio synthétisés par hydro extraction continu afin de récupérer les agents réducteur d'une plante naturel. Nos matériaux ont été caractérisé par différentes méthodes d'analyse à savoir la Diffraction de Rayon X et FTIR afin d'évaluer leurs propriétés. L'élimination de cette substance a été suivie par spectrophotométrie UV/Visible. Dans notre étude nous avons utilisé une approche dans le but d'étudier l'optimisation par conception des cinq paramètres à savoir (la masse, le pH et la température du milieu, la concentration du contaminant, et le temps de contacte), et d'étudier le mécanisme réactionnaire respectivement. Les résultats obtenus ont révélés que l'élimination du cristal violet par adsorption avec le kaolin bio synthétise sont des approches prometteuses avec un rendement allant jusqu'à 100%.

Mots Clés : Nano particules, Colorant cationique, Photo dégradation, Adsorption, Plan d'expériences (plan factoriel fractionnaire), Traitement des eaux.

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Preliminary study of the abundance of microplastics on the surface waters of the Gulf of Tunis

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This study focuses on the assessment of microplastic abundance in the Gulf of Tunis, located on the northeastern coast of Tunisia, which has been subjected to significant urban and industrial expansion; rivers also constitute a direct pathway through which plastics enter the oceans. This study reflects the results of a sampling campaign conducted in October 2024. A total of 3 stations (S_1, S_2 and S_3) were sampled along a T_1 radial with a spatial resolution of 1.5 to 6 miles. Floating microplastics were collected with a manta net and each sample is characterized by geographical parameters and hydrographic parameters (conductivity, temperature, depth and pH). The results showed that the size of detected microplastic particles (MPs) ranged from 10 µm to 1300 µm. Both stations S_1 and S_2 indicated that the most dominant particle shape was fragments while the most abundant form for station S_3 were film. The microplastic concentrations ranged from 0.3 to 1.568 particles m^{-3}. Besides, the highest concentrations were recorded at station S_1. The polymer type of each particle was identified by Fourier Transform Infrared Spectroscopy-Attenuated Total Reflectance (FTIR-ATR) technique, where the most abundant polymer was high-density polyethylene (HDPE) at all stations analyzed with 72% particles with transparent color.

Key words: Microplastics, Marine Pollution, Polymer, Surface Waters, FTIR-ATR.

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Semi-synthesis and in *silico* prediction of novel triterpenic acid derivatives

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Triterpenoids, secondary metabolites naturally present in many plants, possess hepatoprotective, antimicrobial, antioxidant, anti-inflammatory, and anticancer properties[1]. The olive tree (**Olea europaea** L.) exhibits promising phytochemical properties due to the presence of triterpenoids such as oleanolic acid. Given the biological significance of this hydroxy acid, our aim was to isolate it from olive pomace and use it as a starting material for the synthesis of a new series of amino hybrid molecules. All synthesized compounds were characterized using spectroscopic (NMR) and spectrometric (ESI-HRMS) techniques. The inhibitory activity of all the synthesized products against inducible nitric oxide synthase (iNOS) was predicted through molecular docking, as proposed by the Way2Drug server. The results showed that all derivatives exhibited strong inhibitory potential.

Key words: *Olea europaea* L., Oleanolic acid, Anti-inflammatory, molecular docking.

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Phytochemical Composition and Antibacterial Activity of Algerian medicinal plant (J.erratica Extracts)

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The Asteraceae plant species J.erratica, was the subject of this pharmaceutical chemistry study investigating the phytochemical composition and antibacterial activity of its extracts.
In our study on J.erratica, the qualitative phytochemical analysis revealed varied presence of bioactive compounds between chloroform and methanolic extracts. The methanol extract showed a richer profile, with positive results for polyphenols, flavonoids, tannins, glycosides, cardiac glycosides, coumarins, and terpenoids, indicating a high potential for antioxidant and bioactive properties. In contrast, the chloroform extract demonstrated the presence of steroids, free quinones, and terpenoids, suggesting a different bioactivity profile focused on non-polar constituents. The extract of J.erratica exhibited significant antibacterial activity against selected bacterial pathogens, demonstrating strong effectiveness, particularly against Escherichia coli, with an inhibition zone of 28 mm. The antimicrobial activity was confirmed using a disk diffusion technique on two bacterial strains: Staphylococcus aureus (Gram-positive) and Escherichia coli (Gram-negative). This antibacterial potency is likely attributed to the presence of bioactive compounds such as steroids, quinones, and terpenoids, highlighting J. erratica as a promising natural source of antibacterial agents with potential applications in pharmaceutical research.

Key words: Flavonoids, Tannins, Terpenoids, Antibacterial activity

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A Comparative Study between the organic grafts “Chitosan” and “Modified Chitosan” used in the fabrication of hybrid materials

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The aim of this work is to study the main differences between the native chitosan extracted from shrimp shells [1] and the obtained one after doing a chemical modification. The Infrared Spectroscopy, Size Exclusion Chromatography and Nuclear Magnetic Resonance were explored to evaluate the size and the number of monomers before and after treatment.
Furthermore, two hybrid materials were produced by Freeze- Drying technique. The first was composed of pure hydroxyapatite and the native chitosan as an organic graft while the second composite was synthesized with the same mineral component, using similar manner and the unique changement was in the use of modified chitosan. Characterization by Infrared Spectroscopy and XR Diffraction were realized to evaluate the effect of the organic graft on the performance of composite.

Keywords : native chitosan, modified chitosan , composite, comparative study

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Profile HPLC analyses, antioxidant, antimicrobial activities of *Achillea ligustica* All.

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Achillea species belonging to the family Asteraceae is a widely distributed medicinal plant throughout the world and has been used since ancient time. Due to its biologically active substances, we aimed to investigate the total phenolic content and to evaluate the antioxidant properties of Ethyl acetate extract from *Achillea ligustica* All., total phenolic was evaluated using gallic acid as standard, and the phenolic profile was characterized using HPLC. The antioxidant activity was determined by two methods: free radical-scavenging activity ($DPPH^{\cdot}$) methods and radical scavenging ($ABTS^{\cdot+}$) assay. The antimicrobial activity was performed 5 microbial strains. A total of twenty-five phenolic compounds belonging to phenolic acids and flavonoids were detected. Furthermore, the extract showed strong antioxidant activity and antimicrobial activity due to their richness in phenolic compounds.

Key words: *Achillea ligustica* All., Phenolic profile, HPLC, DPPH, ABTS, Antioxidant, antimicrobial

3-aminohydantoins as a potential Anti-Diabetic Agents *In vivo, in vitro* and *In silico* studies

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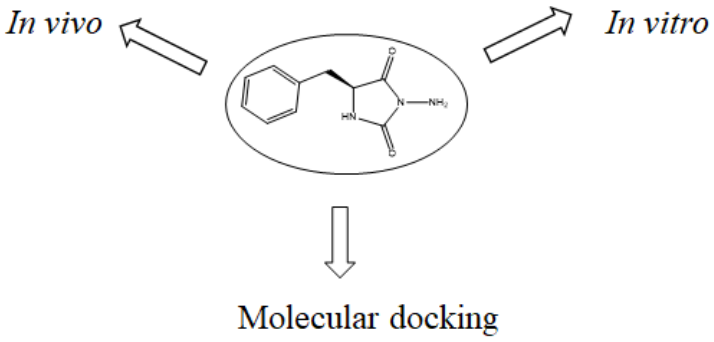
The treatment for Diabetes represents a therapeutic challenge due to the absence of a definitive cure for the disease. In this work, we studied the effect of a 3-aminohydantoin derivative on Diabetes, synthesized from L-phenyl alanine. The molecule was characterized by various spectral techniques (NMR, IR-TF and HRMS). Additionally, we employed solid dispersion as the galenic form to enhance the biodisponibility. The effect of this molecule on Diabetes was investigated through *in vivo, in vitro* studies, as well as molecular docking. The results obtained was promising.



Novel clay-Schiff base hybrid materials with promising antimicrobial properties

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This study focuses on the synthesis, characterization, and evaluation of the antibacterial properties of two novel clay-Schiff base composites. Two types of clay minerals Montmorillonite (Lalithe) [1] and Palygorskite (Sif Pal) [2] were functionalized with the N-salicylideneaniline Schiff base to form modified materials named HSA-Lalithe and HSA-Sif Pal, respectively. The newly synthesized materials were characterized using X-ray diffraction (XRD) and Fourier transform infrared spectroscopy (FT-IR). Their antibacterial activity was tested against Gram-positive bacteria (*Staphylococcus aureus and MRSA+*) and Gram-negative bacteria (*Escherichia coli and Pseudomonas aeruginosa*) using the agar dilution method on Mueller-Hinton agar (MHA). The minimum inhibitory concentration (MIC) results revealed moderate antibacterial activity across all four bacterial strains. Notably, HSA-Lalithe exhibited superior activity against *Staphylococcus* aureus and *Pseudomonas aeruginosa* compared to HSA-Sif Pal, likely due to the swelling nature of Lalithe and the presence of the Schiff base within its interlayer structure.

Key words: Montmorillonite, Palygorskite, N-salicylideneaniline, Antibacterial, Multi-resistant bacteria

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The study of the photocatalytic activity of a green synthesized material based on ZnO

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The textile industry releases a significant amount of dyes into wastewater, which poses environmental hazards and threatens living organisms. The degradation of these dyes using photocatalysts has garnered attention from various research groups. In this study, we focused on the photocatalytic activity of a synthesized material based on zinc oxide. We studied the influence of different parameters for the degradation of the methyl orange such as the pH, the darkness time, the catalyst's masse. Results indicate that the zinc oxide synthesized via an environmentally friendly method can be utilized for various environmental and industrial applications.

Keywords: photodegradation, photocatalysis, dye, sunlight

ETUDE DE FORMULATION D'UNE SUSPENSION BUVABLE A USAGE PHARMACEUTQUE A BASE D'EXTRAIT DE PLANTES ENCAPSULE

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Les suspensions pharmaceutiques sont des dispersions hétérogènes d'un solide dispersé dans un milieu liquide sous forme de particules insolubles. La formulation d'une suspension est une activité consistant à fabriquer des produits stables et possédant des propriétés spécifiques, en mélangeant différentes matières premières.

L'objectif de cette étude est de formuler une suspension pharmaceutique buvable à usage pharmaceutique à base d'extrait d'un mélange de trois plantes à intérêt pharmaceutique, cet extrait est encapsulé afin d'obtenir des micro particules qui seront la suite mise en suspension. Cet extrait est utilisé comme étant une cure hépato protectrice à l'égard de la maladie du psoriasis qui peut être une résultante de la mauvaise élimination des toxines de la peau, et donc lié aux intestins ou au foie. La première partie de ce travail consiste en une étude de pré formulation dans laquelle nous avons étudié l'effet des paramètres de formulation de la phase dispersante à savoir la concentration des agents de suspension à savoir la concentration de la gomme guar ainsi que le glycérol sur son comportement rhéologique afin d'aboutir à une suspension la plus stable possible sur la base de la méthodologie des plans d'expériences en utilisant le logiciel JMP® ou nous avons étudié l'effet de chaque facteur étudié et interaction sur les réponses sélectionnées. La deuxième partie concerne l'étude de formulation de la suspension finale. Les résultats obtenus au cours de la première partie ont démontré qu'après l'ajustement des courbes d'écoulement et de viscosité par le modèle de sisko et le modèle de carreau respectivement, nous avons constaté que l'ensemble des préparations ont un comportement d'un fluide rhéofluidifiant (pseudo plastique). Au cours de cette étude, le domaine de variation des paramètres de formulation, dans lequel les suspensions présentent un comportement rhéologique et une vitesse de sédimentation et une stabilité d'intérêt ont été identifiés.

Mots-clés : Suspension, pharmaceutique, stabilité.

Study of melt granulation process applied to a pharmaceutical powder mixture

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In this work we present a study of a melt granulation process for capsule filling, applied to a pharmaceutical powder mixture using ibuprofen as the active ingredient and polyethylene glycol (PEG) as the melt binder. The study of melt granulation first required the design and implementation of an experimental apparatus equipped with the necessary measuring instruments, simulating a high shear granulator. Once the installation was completed, we explored two methods of binder incorporation: the in situ method and the melt-in method. The tests were conducted under different operating conditions. Additionally, the study focused on evaluating the characteristics of the obtained granules and analyzing the effects of the operating conditions on these characteristics. The evaluated properties included particle size distribution, porosity, flowability, and the dissolution of the active ingredient. In conclusion, this study provides information on optimizing the conditions for melt granulation for the production of pharmaceutical granules intended for capsule filling.

Keywords : Melt granulation, ibuprofen, polyethylene glycol, high shear granulator, pharmaceutical formulation.

Enhancing Poultry Nutrition: Valorisation of Chicken Egg Shells for Calcium Supplementation - Describing the Shell Treatment Process, Physicochemical Characterization, and Microbiological Analysis.

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In order to enhance the quality of eggshells for consumption, this study aims to valorize eggshells as a calcium supplement in the diet of laying hens. Beyond the beneficial properties of the product, our solution provides an alternative to calcium carbonate sourced from limestone quarries, which incurs certain costs. Additionally, the inherent properties of our eggshells are more advantageous.

Exploring an alternative source of calcium to effectively supplement the calcium requirements of hens would be advantageous for both the hens themselves and their breeders.

When dietary sources of calcium are insufficient, calcium is withdrawn from the medullary bone of the laying hen. Calcium deficiency can result in the production of eggs with poor shell quality, leading to lower-grade products and financial losses for breeders. Globally, the poultry industry plays a critical role in meeting the demand for animal calcium.

From an environmental perspective, our project gives a second life to waste material that holds significant potential for valorization, while also contributing to a circular and local economy. Furthermore, the physicochemical and microbiological analyses of both the raw material and the final incorporated feed meet the standards, with a calcium content of approximately 7.58%, far exceeding the values obtained with rocky calcium bicarbonate, which does not exceed 3.5% with the same percentage in the formulation, while respecting the appropriate granulometry. The microbiological analyses conducted on the shells are satisfactory and allow for safe incorporation into the formula. However, we still need to optimize the calcium-enriched formulas to meet the needs of the industry.

Keywords: consumed eggshell, valorization, calcium Enrichment, decontamination process, Poultry Nutrition, Circular Economy.

Corrosion inhibition of carbon steel in acidic media using a natural compound

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Corrosion is a complex process that has engaged the attention of academics in the fields of chemistry and materials science for decades. It has a negative impact on the environment and the economy. The use of hazardous chemicals as inhibitors has been restricted due to their adverse environmental consequences. Plant-derived natural inhibitors offer several benefits, including potent inhibitory effects, lack of toxicity, biodegradability, and environmentally sustainable origins. The objective of this work was to study the inhibitive power of a natural organic compound (the essential oil of clove) on API 5L X60 pipeline steel in an acidic medium (HCl) using gravimetric and electrochemical methods. The results revealed that adding clove essential oil to the corrosive medium considerably slows down the corrosion process and that the maximum inhibitory efficiency of 86.97% is obtained for a concentration of 400 ppm in inhibitor.

Key words: Corrosion, inhibitor, API 5L X60 steel, Eessential oil of clove.

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Effective Adsorption of Methylene Blue with Metal-Organic Framework UIO-66-NH2: Characterization and Kinetic Analysis.

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In recent years, new and highly promising porous materials known as Metal-Organic Frameworks (MOFs) or coordination polymers have been discovered and used for dye adsorption. These MOFs possess unique characteristics such as high porosity, large specific surface area, and significant pore volume and size. In our study, we focused on evaluating the MOF UIO-66-NH2 for the adsorption of methylene blue. The adsorption capacity increases with the amount of MOF, achieving a maximum yield of 76% with 15 mg of adsorbent. The optimal conditions for methylene blue adsorption with UIO-66-NH2 were found to be at an initial dye concentration of 10 mg/L and a pH of 11. Kinetic modeling indicates that the adsorption process follows a pseudo-second-order kinetic model. Langmuir, Freundlich, and Temkin adsorption isotherms were applied to the equilibrium experimental data, and the Langmuir model was determined to be the most appropriate. The thermodynamic analysis showed that the adsorption process is exothermic and spontaneous, with a negative $\Delta G°$ at various temperatures. These results demonstrate that UIO-66-NH2 exhibits excellent efficiency in the adsorption of methylene blue.

Valorization of date palm fibers for biodegradable ldpe composites: Effect of chemical treatment on material properties

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The widespread use of composite materials necessitates sustainable end-of-life solutions due to extensive waste generation. Biodegradable alternatives offer a promising path, which can be achieved by replacing the matrix with biodegradable polymers or incorporating biodegradable fibres into existing materials. However, the latter often requires chemical modification of both fibres and matrix to optimise interfacial adhesion. This study explores the valorization of date palm crop residues as biodegradable fibres (DPF) for reinforcing low-density polyethylene (LDPE) with rates of 10, 20, and 30 wt%, investigating the impact of alkali treatment on composite properties. Results demonstrate a significant influence of treatment on interfacial adhesion, mechanical performance, and biodegradability. Fourier-transform infrared spectroscopy confirmed that the structure of the palm fibre had changed after treatment. The absence of the C=O peak at 1722 cm^{-1} suggests partial hemicellulose hydrolysis in the alkaline environment, as evidenced by the broken C-O-C bonds. This aligns with the disappearance of the lignin C=O peak at 1218 cm^{-1}. Moreover, a diminished C=C peak at 1512 cm^{-1} indicates both lignin and hemicellulose degradation due to the alkaline treatment. Mechanical testing revealed decreasing tensile strength and elongation at break with increasing fibre loading. The decrease in tensile strength is evaluated at 13, 12.3 and 11.2 MPa for the formulations with 10%, 20% and 30% reinforcement, respectively, but treatment significantly improved these metrics. The Young modulus and Shore D hardness exhibited opposite trends, increasing with fibre content and improving with treatment, explained by the rigid nature of the date palm fibre compared to the thermoplastic matrix. Water absorption measurements indicated a reduced uptake for treated composites compared to their untreated counterparts, suggesting improved durability. This behaviour is clearly due to the decrease in hydroxyl groups after treatment. This makes the filler much less water-repellent and improves the interface between the filler and matrix in the PE-BD/FPD composites. Thus, after treatment, the external topology of the fibre changes and the fibre becomes more hydrophobic, leading to good fibre/matrix interaction. Thermal ageing at 120°C resulted in colour and mass loss, highlighting the need for further investigation into enhancing heat resistance.

These findings showcase the potential of date palm fibre-reinforced LDPE composites as a sustainable and tunable alternative to traditional materials. While treatment significantly improves several vital properties, optimization of the process and long-term durability assessments are crucial for successful implementation.

Key words: Polyethylene, Date palm, Alkali treatment, Water absorption.

Synthesis and biological evaluation of new Quinazolines for Alzheimer's disease treatment

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Alzheimer's disease (AD) is the most common form of degenerative dementia in the elderly, characterised by a progressive decline in cholinergic function[1,2]. AD is characterised by the presence of extracellular plaques consisting of the accumulation of amyloid beta peptide (Aβ) and intracellular deposits in the form of neurofibrillary tangles of hyperphosphorylated tau protein. Recent research has emphasised the amyloid hypothesis, suggesting that amyloid β (Aβ) plays a critical role in AD, with a strong correlation between neuronal death and Aβ aggregates in the brains of AD patients.

Cholinergic neurons are the most damaged in AD, resulting in low levels of acetylcholine (ACh), which can be alleviated by the administration of acetylcholinesterase (AChE) inhibitors. A literature review revealed that quinazoline derivatives have diverse therapeutic potential for AD as modulators/inhibitors of Aβ, AChE, BuChE and as protective agents (antioxidants).

In this work, we propose to develop new multi-targeted molecules with simultaneous activity as antioxidants, cholinesterase inhibitors for symptomatic relief, and more specific properties to impede disease progression, mainly targeting the amyloid aggregation cascade by inhibiting Aβ aggregates (see Figure 1). To achieve this goal, we carried out a multi-step reaction starting with the reaction of 2-aminobenzonitrile derivatives with different orthoesters, followed by the addition of different substituted anilines to produce functionalised quinazolines. Preliminary biological tests showed promising activity in inhibiting amyloid-β aggregation and cholinesterases, as well as antioxidant properties. We then carried out biological evaluations for the treatment of Alzheimer's disease using the corresponding acidic quinazolines obtained by a saponification reaction.

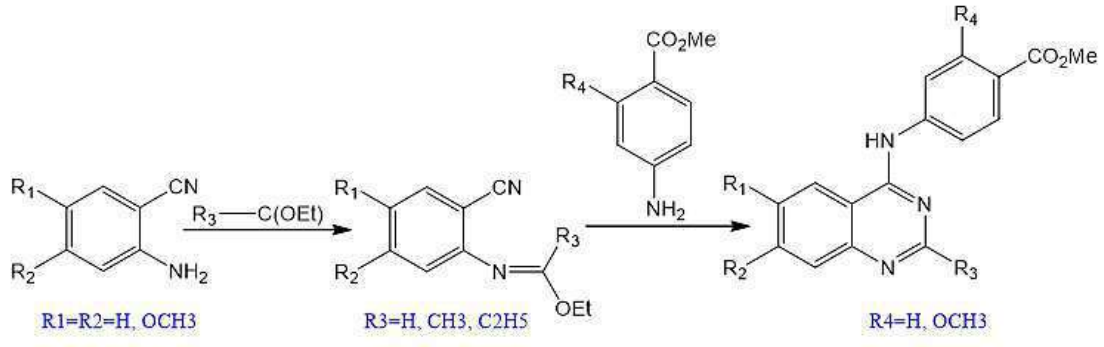

Figure: Access routes to the desired compounds.

Keywords: Maladie d'Alzheimer, Cholinesterase, Amyloid-β, Quinazoline/ Alzheimer's disease, Cholinesterase, Amyloïde-β, Quinazoline.

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Second Harmonic Generation of I_β-Cellulose nanocrystals in solution

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Nonlinear optics is the field of study of light-matter interactions, and it encompasses a wide variety of phenomena of interest for the development of photonics materials capable of signal treatment, light frequency tuning, etc… Among them Second Harmonic Generation (SHG) is a one-step phenomenon involving the conversion of pairs of photons of frequency ω into photons of frequency 2ω. At the molecular scale, SHG is governed by the first hyperpolarizability tensor β while by the second-order nonlinear optical (NLO) susceptibility $\chi^{(2)}$ at the macroscopic scale. A key factor for materials to perform SHG is the absence of centrosymmetry.

Good candidates for potential applications are cellulose nanocrystals, which whom the bulk itself is non-centrosymmetric, but which also tend to self-align into chiral nematic phases over a critical concentration.[1] I_β cellulose is the most abundant allomorph and has been selected for the present study. A collaborative work involving on one side experimental hyper-Rayleigh scattering and depolarization ratio measurements, and on the other side theoretical prediction of the crystalline bulk NLO susceptibility $\chi^{(2)}$ tensor at the quantum level, has been carried out to unravel the origin of the NLO properties of I_β cellulose nanocrystals in aqueous solution.

The quantum chemistry (QC) computations were performed at the Kohn-Sham DFT level of approximation with Periodic Boundary Conditions (PBC), employing gaussian functions basis sets. Some of the present authors recently benchmarked this approach considering reference NLO crystals[2] in order to establish the requirements (basis set, exchange-correlation functional, lattice summation thresholds, Brillouin zone sampling) to obtain $\chi^{(2)}$ tensors close to the experimental values. In this poster, the experimental data of I_β cellulose nanocrystals are analyzed at the light of the QC results to get insights about the various contributions to the first hyperpolarizability, being from the bulk or related to the surface state of these nanocrystals.

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Synthesis, Crystal Structure, Spectroscopic Properties and Potential Biological Activities of a binuclear copper(II) complex Di(µ-hydroxo) Di(µ-nitrato-O,O') Bis(N,N,N',N'-tétraméthyléthylènediamine) cuivre(II) 7,5 hydrate $[Cu_2(OH)_2(NO_3)_2(C_6H_{16}N_2)_2].7{,}5\ H_2O$

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Binuclear copper complexes hold considerable promise across various fields, from catalysis and bioinorganic chemistry to material science and medicine. Their flexible coordination environment and redox activity make them versatile in a wide range of applications, particularly in mimicking natural enzymatic functions, designing new materials, and developing therapeutic agents.

The synthesized complex crystallizes in the monoclinic system with space group *C*2/*m*. This complex has a binuclear structure, with the unit represented in Fig.1. The two copper atoms are connected by two hydroxyl bridges and two nitrate groups. Each Cu^{2+} ion is surrounded by six atoms, forming an octahedron elongated along the z-axis due to the Jahn-Teller effect, which is often observed in hexacoordinated complexes containing divalent copper.

The structure can be described as a succession of layers parallel to the (001) plane, formed by $[Cu_2(OH)_2(NO_3)_2(C_6H_{16}N_2)_2]\cdot 7.5\ H_2O$ complexes, separated by a sheets of water molecules. The cohesion of the structure is ensured by hydrogen bonds and Van der Waals interactions, leading to a three-dimensional framework.

The crystalline phase was analyzed for crystallographically independent cations using Hirshfeld surface analysis. The copper complex, characterized by IR and UV-visible spectroscopy and thermogravimetric analysis, demonstrated significant microbial inhibition and biofilm disruption, suggesting potential for anti-virulence therapies.

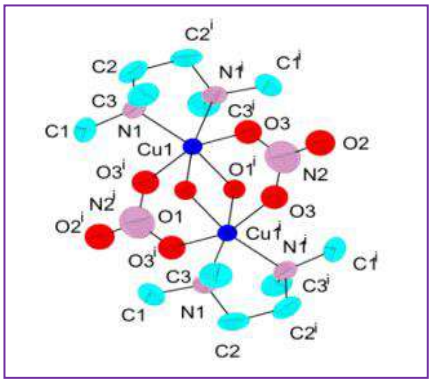

Fig.1: Representation of the binuclear copper complex $[Cu_2(OH)_2(NO_3)_2(C_6H_{16}N_2)_2]\cdot 7.5\ H_2O$

Key words: XRD, Dinuclear, Hirshfeld Surface analysis, Antimicrobial, Anti-virulence.

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Investigation of the physical properties of the new alluaudite-type molybdate $Ag_{0.30}Na_{3.70}Mn(MoO_4)_3$ for photocatalytic and the antimicrobial activity

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Molybdate-type alluaudite is a structural variant of the alluaudite mineral, where molybdate ions (MoO_4^{2-}) replace phosphate groups (PO_4^{3-}). Its open framework enables fast ion transport, making it a candidate for energy storage in sodium-ion and lithium-ion batteries. These materials also exhibit tunable electrochemical, catalytic, and magnetic properties, depending on the cations present, offering potential for applications in batteries and catalysis **[1]**.

A yellow single crystal of the new alluaudite-type molybdate $Ag_{0.30}Na_{3.70}Mn(MoO_4)_3$ (Fig.1) was synthesized via solid-state reaction. Single-crystal X-ray diffraction confirmed that it crystallizes in the monoclinic system, space group C2/c, with a three-dimensional framework characterized by $Mn_2Mo_3O_{14}$ layers parallel to the (100) plane linked by MoO_4 tetrahedra, forming two types of hexagonal channels where cations reside. FTIR analysis confirmed the presence of $(MoO_4)^{2-}$ groups, while UV-visible spectroscopy determined its optical band gap.

The compound exhibits antiferromagnetic behavior and thermally activated electrical conduction, as indicated by impedance spectroscopy. Photocatalytic tests demonstrated efficient degradation of methylene blue, and antibacterial studies revealed strong activity against both gram-positive and gram-negative bacteria.

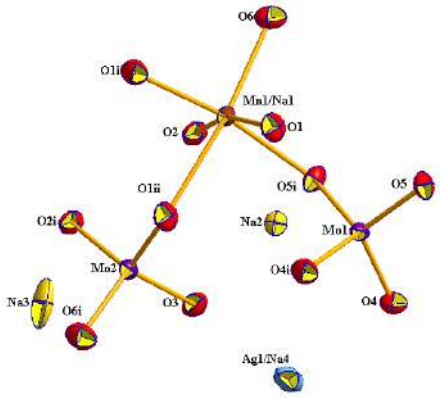

Fig.1: ORTEP diagram of $Ag_{0.30}Na_{3.70}Mn(MoO_4)_3$ with displacement ellipsoids drawn at 50% probability.

Key words: Molybdate-type alluaudite, X-ray diffraction, Optical band gap, Impedance spectroscopy, Antimicrobial studies.

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Ultrasound-assisted extraction followed by liquid chromatography-FLD for isolation and assessment of polycyclic aromatic hydrocarbons in commonly consumed fish in Bizerte, Tunisia

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Marine fish are consumed in large quantities as a nutritious food by humans. However, ingestion of fish contaminated by chemicals such as polycyclic aromatic hydrocarbons (PAHs) can pose a serious threat to human health [1]. PAHs are a class of highly carcinogenic and mutagenic compounds; sixteen of them have been considered priority pollutants by the regulation authorities. In this work, a simple and sensitive automated method, consisting of ultrasound assisted extraction UAE coupled with high-performance liquid chromatography-fluorescence detection (HPLC-FLD), was developed for the determination of PAHs in fish samples. Fifteen PAHs standards were separated within 70 min by HPLC-FLD using a Supelcosil PAH column with an acetonitrile/water gradient elution program as the mobile phase. Under optimal conditions, the proposed method has been validated and the results showed good linearity (R^2> 0.995) for all the studied PAHs obtained in the concentration range of 40-400 ng mL^{-1}. The limit of detection and limit of quantification were in the range of 0.01-0.41 ng/g ww and 0.033-1.37 ng/g ww respectively. PAHs in fish samples were extracted by ultra-sonication in hexane/acetone, and the cleanup of the extracts was performed by glass columns containing silica gel with alumina, and successfully analyzed by HPLC-FLD, with good recovery rates above 60% in spiked fish samples for all analytes. The proposed method showed high reproducibility having intra-day and inter-day precision less than 10%.

Key words: polycyclic aromatic hydrocarbons, ultrasound-assisted extraction, Fish, contamination, liquid chromatography-fluorescence detection.

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Fructooligosaccharides from *Cynoglossum tubiflorus* : Effect of the molecular size on their antidiabetic activity in high-fat diet and alloxan induced diabetic rats.

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The use of acetylation followed by silica gel column purification allowed the isolation of eight fructooligosaccharides (FOS) from the ethanolic extract of *Cynoglossum tubiflorus* roots. Each FOS was identified by analyzing its FT-IR, HRMS/MS and NMR data, including ^{1}H, ^{13}C and 2D NMR, H-H COSY, HMBC and NOESY. In diabetic rats treated with a series of FOS from Glc-(Fru)$_3$ to Glc-(Fru)$_7$, a significant inhibition of intestinal α-amylase was observed. This activity increases proportionally with the FOS molecular size. It was found that they delay the absorption of total cholesterol (TC), LDL-cholesterol (LDL-C) and increase HDL-cholesterol (HDL-C) in a molecular size-dependent manner. This inhibitory effect on the activity of the digestive enzyme causes a significant ($p < 0.05$) reduction in the level of glucose in the blood as an anti-diabetic action. The ethanolic extract exerts a significant effect against α-amylase as well as antihyperglycemic and antihyperlipidemic activities, while its acetylation suppresses these effects. Therefore, this study demonstrates for the first time that pure FOS act as efficient agents in preventing hyperglycemia and hyperlipidemia and that this action evolves in the same manner with their molecular size.

Keywords: *Cynoglossum tubiflorus*, fructooligosaccharides, hyperglycemia, hyperlipidemia, antidiabetic.

Agrichar prepared from peanut shell by chemical activation: Functionalization with Fe and Ca and application for removal of

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In this study, peanut shell-derived activated carbon, produced by orthophosphoric acid activation, was used as a material to adsorb methylene blue (MB). An optimization process was conducted to determine the optimal values for the adsorption parameters, including adsorbent dosage, temperature, pH, and contact duration. The outcomes of experiments were analyzed using four adsorption isotherms, while the pseudo-first and second-order models were deployed for assessing the kinetics. The adsorption of MB achieved equilibrium after 120 minutes, following the pseudo-second-order kinetic model. The Langmuir model accurately represented the adsorption process and achieved a maximum amount adsorbed of 219.7 mg/g at 25 °C. The thermodynamic variables (ΔH^0, ΔG^0, and ΔS^0) were calculated by investigating the impact of temperature, revealing that the adsorption was both exothermic and spontaneous. Carbon functionalization with Fe^{3+} or Ca^{2+} ions enhances the adsorption capacity and expedites the adsorption process, with equilibrium being achieved in 70 minutes and 50 minutes, respectively.

Keywords: Peanut shell, Chemical activation, Activated carbon, Functionalization, Methylene blue, Adsorption.

Design and Characterization of π-Conjugated Architectures: Synthesis and Insights

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Polycyclic aromatic hydrocarbons (PAHs) represent a vital class of compounds characterized by the presence of two or more fused benzene rings. Their unique chemical properties, structural diversity, and photoelectric characteristics have attracted considerable attention, making them essential materials for electronic device development and promising candidates as semiconductors. This study focuses on the synthesis of a series of functional bis-diarylethene derivatives, achieved with high yields under mild reaction conditions. These derivatives were synthesized *via* Heck coupling of brominated 1,2-diarylethenes that feature reactive functional groups. The absorption properties of the target compounds were thoroughly investigated in solution, revealing a significant absorption in the UV region.

Keywords: Aromatic compounds, Chromophores, Heck coupling, Absorption.

Phase Diagram of Sulfaméthoxazole + Metronidazole System

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Keywords: drug; Solid - liquid equilibrium; DSC,

Drug formulation often implies the preparation of multicomponent systems based both on drug-drug and drug- excipient combinations. It is well-known that drug-excipient interactions can deeply influence the technological and biopharmaceutical properties of solid dosage forms. Thermal analysis is often employed to evidence such interactions.
Metronidazole is an antibacterial drug and commonly used in combination with other antibiotics[1].Sulfamethoxazole is a broad-spectrum antimicrobial agent[2].These drugs are used due to their low cost relatively and ability to act against common bacterial diseases efficiently.The purpose of this study was to describe and characterize co-crystal formation of sulfamethoxazole and Metronidazole [3].
Using Differential scanning calorimetry, we have determined the solid-liquid phase diagram for Sulfaméthoxazole (1) + Metronidazole (2) mixture.
A typical DSC curves obtained are shown in figure 1a. The systems are eutectic because the first peak appeared at the constant temperature. For each system, this composition is estimated by the intersection of the two curves of solubility by extrapolation and then localized with more precision by the determination of eutectic heat versus molar fractions for each system. The eutectic composition is found at the fraction of maximum. Figure 1b show the plots of the experimental SLE for the binary mixture.

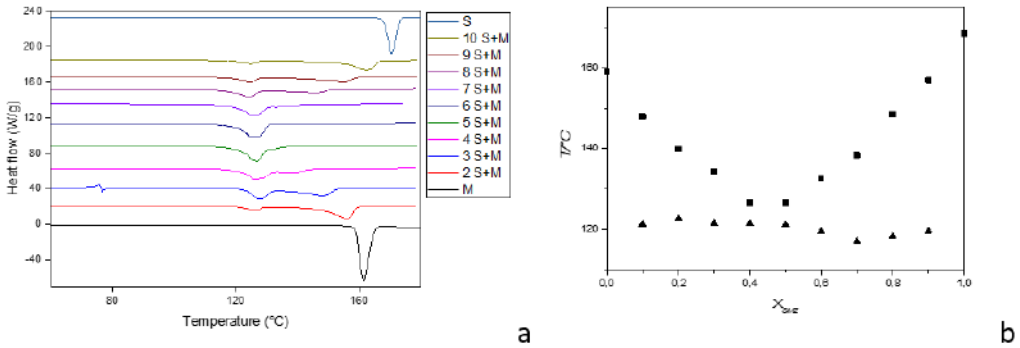

Figure 1. Experimental and predicted SLE phase diagrams of Sulfaméthoxazole (1) Métronidazole (2) mixture.

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Electronic structure and optical properties of luminescent complexes: A computational investigation

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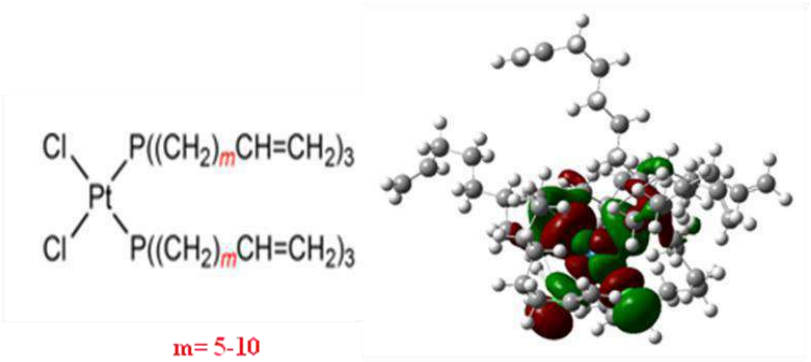
Molecular materials based on the assemblage of organometallic fragments and Phosphine-olefin ligands ligands are among the most studied compounds in coordination chemistry. This is due to their relatively good stability combined with their excited-state and redox properties which confer them interesting physical properties in several domains (magnetism, optics, electrochemistry…).

The work to be presented has focused on the study of a series of molecules with $P(CH_2)_mCH=CH_2$ moieties synthesized in the laboratory of John A. Gladysz. [1-2]



TD-DFT calculations are shown to provide an excellent cost-effective computational approach for the treatment of the excited states of these complexes.

Key words: TD-DFT, Phosphine-olefin, Molecular materials, excited states.

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Etude et formulation du fuel-oil IFO30 à partir des fuels lourds IFO80, 180, 380 et du gasoil

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Le fuel est un combustible dérivé du pétrole, utilisé comme carburant pour les engins agricoles, les bateaux de pêche et les engins de travaux publiques, l'objectif principales est de formuler du fuel-oil 30cst à partir des fuels lourds en diminuant leurs viscosités par l'addition du gasoil.

Tout d'abord on passe par l'étude des caractéristiques physico-chimiques de ces produits afin d'assurer leur conformité. Au cours de ce travail nous avons effectué l'étude de compatibilité de ces mélanges à différentes proportions pour assurer l'homogénéité et la stabilité, ensuite on a montré que l'ajout du gasoil diminue la viscosité, ce qui nous a permis de poursuivre les autres tests.

Enfin ces résultats indiquent que les produits formulés sont conformes et rentables, prêt à être commercialisé et utilisé pour les moteurs diesel.

Mots clés : Fuel-oil, gasoil, point d'écoulement, viscosité.

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Green Synthesis of Silver Nanoparticles Using Tunisian Plant Extracts: Characterization and Evaluation of Biological Activities

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The green synthesis of nanoparticles using plant extracts has emerged as a highly promising field due to its extensive range of biomedical applications [1, 2]. In this study, we report for the first time the successful biosynthesis of silver nanoparticles (AgNPs) using Anagallis monelli extract. The synthesized nanoparticles were characterized using UV-Vis spectroscopy, transmission electron microscopy (TEM), X-ray diffraction (XRD), and Fourier-transform infrared spectroscopy (FTIR). The structural analysis revealed that the AgNPs possess a face-centered cubic (fcc) structure, with an average crystallite size of 22 nm. The biosynthesized AgNPs demonstrated exceptional antioxidant and antimicrobial activities, indicating their potential for various biomedical applications. Antioxidant capacity was assessed through DPPH, total antioxidant activity (TAA), and ferric reducing antioxidant power (FRAP) assays. The AgNPs exhibited strong antibacterial effects, particularly against Gram-positive species Staphylococcus aureus and Micrococcus luteus, with inhibition zones of 15 mm and 16 mm, respectively, as determined by the agar well diffusion method. In contrast, Gram-negative bacteria, including Escherichia coli, Serratia marcescens, and Klebsiella pneumoniae, displayed smaller inhibition zones (11-12 mm). Additionally, the AgNPs demonstrated significant lysozyme activity and the ability to inhibit and eradicate biofilms. Remarkably, the synthesized nanoparticles were also highly effective against Candida albicans, exhibiting superior antifungal activity compared to Fluconazole (25 µg), with notable morphological alterations observed in Candida cells. These findings highlight the potential of Anagallis monelli-derived silver nanoparticles for future applications in antimicrobial and antifungal treatments.

Key words: Silver nanoparticles (AgNPs), Green synthesis, Plant extracts, Antimicrobial activity

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Microwave assisted extraction of compounds from the shell of Pistacia vera L. and characterization of the extracts

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Plants are already recommended as a safer alternative to chemical products since they have less negative effects. The use of goods derived from medicinal plants has significantly increased in recent years. Due to their medicinal properties, plants are used as a primary health care aid in the form of plant extracts or their active components.

The purposes of this investigatory study were to determine the chemical composition of the extracts of Pistacia vera L. shell from the region of Gafsa (Tunisia) obtained by microwave assisted extraction (MAE), as well as the evaluation of their biological effects. The determination of the chemical composition of extract was performed by Gas chromatography-mass spectrometry (GC-MS). The antioxidant activities of extract were performed using free radical scavenging ability (DPPH), The ferric reducing antioxidant power assay (FRAP), and ABTS radical scavenging assay. Antimicrobial activity was assessed in vitro using the disk-diffusion assay.

Finally, the shell of Pistacia vera could be considered as a cheap source of bio-compounds with antiradical potential and antimicrobial effect.

Key words: *Pistacia vera* L shell., MAE, antioxidant properties, antimicrobial capacities.

Biosourced innovations from *Opuntia ficus-indica:* Environmental remediation and encapsulation applications

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This study focused on the valorization of plant biomass "*Opuntia ficus-indica*" for the development of innovative biosourced materials. Here are two important uses of the work that was done: (i) making activated carbon to soak up waste water; and (ii) using mucilage from cactus as a coating for making microcapsules. First, we prepared activated carbon from the trunk shavings of *Opuntia ficus-indica* and we tested its adsorbent power with respect to p-nitrophenol retention. We found that the adsorption of p-nitrophenol follows the pseudosecond-order model, reaching equilibrium in 120 minutes, based on all the kinetic parameters. From the isotherm modeling results, the Langmuir model was found to be the most credible model to describe the adsorption of p-nitrophenol on the activated carbon from *Opuntia ficus-indica* with a maximum adsorption capacity of 16.83 mg/g. In the second part, we created a process for making sunflower oil microcapsules using different mucilaginous parts that were taken from *Opuntia ficus-indica* rackets and precipitated at various pH levels. The microencapsulation of sunflower oil was carried out by the coacervation process with different crosslinking systems: cactus mucilage / carboxymethylcellulose and cactus mucilage / chitosan. We characterized the different cactus extracts and the resulting microcapsules. Fourier transform infrared spectroscopy analysis of the mucilages revealed the presence of key polysaccharides, such as galactose and pectin, within the mucilage. Scanning electron microscopy showed that for the mucilages precipitated at pH=4 and pH=12, most of the particles adhered together and caused the formation of compact and linked agglomerates. However, incomplete crosslinking was observed in the microstructure of the mucilage obtained at pH=2. The mucilaginous extracts made the encapsulation process easier. This led to microcapsules with a narrow size range of 4 to 12 μm in diameter and encapsulation rates between 83% and 87%. These results confirmed that coacervate droplets were deposited around the oil droplets. They also showed that the formation and subsequent deposition of coacervate particles happened in steps, including through complex coacervation. In conclusion, both approaches yielded materials with promising properties, offering viable solutions for the sustainable valuation of abundant industrial waste from a renewable source. These results suggest potential applications in environmental remediation and materials science, highlighting the importance of developing environmentally friendly processes for resource recovery.

Synthesis and structural characterization of N, N-dimethyl-1, 3- propanediaminium penta bromobismuthate (III)

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Hybrid organic-inorganic materials have garnered significant attention due to their unique properties and potential applications in various fields such as optoelectronics and photovoltaic. In this study, we report the synthesis and the structural characterization of N, N-dimethyl-1, 3-propanediaminium penta bromobismuthate (III), obtained by slow evaporation of 3-diméthylaminopropylamine with $BiBr_3$.

The crystal structure consists of $(C_5H_{16}N_2)^{2+}$ cations and $(BiBr_5)^{2-}$ anions. The crystallographic data reveal that the compound crystallizes in the $P2_1/n$ monoclinic space group, with unit cell parameters: a = 8.0436 (6) Å, b= 15.3624 (10) Å, c= 12.680 (1) Å, β = 93.208 (4) °, Z=4 and V= 1564.4 (2) $Å^3$.

A detailed analysis of the crystal structure shows that the $(BiBr_5)^{2-}$ anions in the inorganic part are connected through corner-sharing, forming a chain-like arrangement represented in Figure 1. The organic moiety spread in the empty space around the 1D inorganic chains. The structureis stabilized by N—H…Br and C—H…Br hydrogen interaction, linking the organic and inorganic parts and ensuring the hybrid structure cohesion.

Key words: Organic-inorganic, hybrid, bromobismuthate.

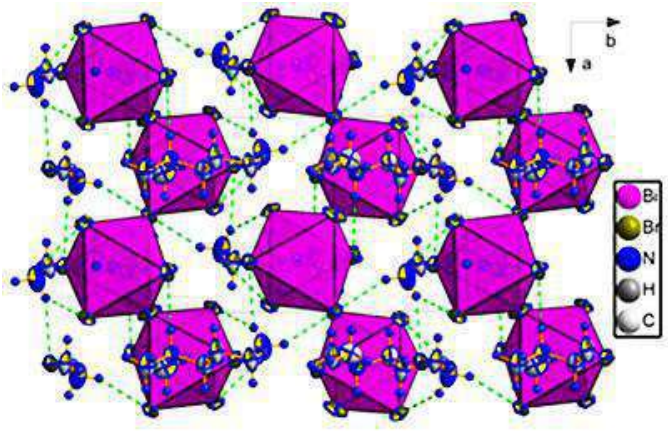

Figure 1: The crystal structure of $(C_5H_{16}N_2)$ [$BiBr_5$] showing the alternate organic-inorganic packing view.

Experimental and theoretical studies of the structural, magnetic, and electronic properties of the $La_{0.6}Ca_{0.2}Sr_{0.2}MnO_3$ perovskite

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In this study, we examined the structural, magnetic, and magnetocaloric properties of a $La_{0.6}Ca_{0.2}Sr_{0.2}MnO_3$ composite. This composite was created by blending two citric-gel manganite-based oxides: $La_{0.6}Ca_{0.4}MnO_3$ and $La_{0.6}Sr_{0.4}MnO_3$, in mole fractions of 60% and 40%, respectively. X-ray diffraction analysis, using Rietveld refinement, revealed that the sample crystallize in an orthorhombic structure with the Pbnm space group. The SEM techniques confirmed the formation of single-phase materials with excellent mapping distribution, with mean size of 37.8723 ± 0.5536nm. The M-T curve demonstrates second-order magnetic phase transitions at the Curie temperature (Tc = 340.01 K), shifting from a ferromagnetic (FM) to a paramagnetic (PM) state. Our results reveal significant magnetic entropy changes, indicating a substantial magnetocaloric effect. Notably, the magnetic entropy change reaches a peak value of 5.763 J/kg.K, along with a considerable relative cooling capacity of 335.3512 J/kg, observed under a magnetic field change of 5 T. To support these experimental characterizations, quantum chemistry calculations, enacted using density functional theory, have been carried out to determine the structural, electronic and magnetic properties of this compound using the Crystal23 code.

Keywords: Magnetic entropy, magnetocaloric effect, electronic properties, exchange interaction, DFT.

Identification de nouveaux inhibiteurs de VEGFR2 comme agents anticancéreux à l'aide d'un criblage virtuel par docking moléculaire

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Les thérapies ciblées ont été développées pour traiter le cancer dans le but de réduire les effets secondaires associés à la chimiothérapie. Parmi les cibles prometteuses, on trouve les inhibiteurs des récepteurs à tyrosine kinase, notamment l'enzyme VEGFR2, qui constitue le principal transducteur de l'angiogenèse tumorale[1].Dans cette étude, un criblage virtuel par docking moléculaire a été effectué sur une chimiothèque de produits naturels « Selleckchem » dans le but de découvrir de nouveaux inhibiteurs anticancéreux du VEGFR2, plus efficaces et moins toxiques.

Après validation du protocole de docking par redocking de la protéine 6GQO (RMSD = 0,82) et sélection du SORAFENIB comme ligand de référence, l'outil « Glide Virtual Screening Workflow » de Schrödinger a été utilisé pour cribler la chimiothèque. Seules les meilleures poses, présentant un score supérieur à celui du médicament SORAFENIB et établissant des interactions avec les résidus clés, ont été retenues. Par la suite, une seconde filtration de ces poses a été effectuée en fonction des propriétés ADME-Tox à l'aide des serveurs ADMETlab 2.0, PreADMET et PkCSM.

Deux hits ont été sélectionnés, présentant des caractéristiques prometteuses en tant que nouveaux inhibiteurs potentiels du VEGFR2. Ces molécules seront soumises à un criblage virtuel par pharmacophore/QSAR, suivi de tests *in vitro* pour valider les résultats obtenus.

Keywords: Cancer, Virtual screening, Docking, Sorafenib, VEGFR2.

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Original Strategy for Facile Synthesis of ZrO_2 nanoparticles: Structural and Optical properties.

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A new synthesis method of ZrO_2 nanoparticles is presented in this work, and this novel approach allows one to produce zirconium dioxide owing to a modified polyol process that makes use of 1.3-propanediol as a solvent. The structure and morphology of the nanoparticles were characterized by high-resolution transmission electron microscopy, transmission electron microscopy, X-ray diffraction and and UV-Vis diffuse reflectance spectroscopy. The results showed that quasi-spherical ZrO_2 nanoparticles with sizes in the range 5-15 nm was formed. Their morphology, size and colloidal stability are driven by the Polyol solvent. Under UV excitation, a strong visible photoluminescence emission, due to the radiative recombinations of the electron-hole pairs photo-generated in the ZrO_2 nanoparticles, was observed. This optical property, together with the easy synthesis process, makes the ZrO_2 CNCs a promising candidate for applications

Key words: ZrO_2 nanoparticles, polyol medium, 1.3 propandiol, Optical properties.

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DFT Calculations and Mechanistic Study of the 1,3-Dipolar Cycloaddition Reaction between Dichlorophosphoryl Isocyanate and Hydrocarbon Azides

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Tetrazole heterocyclic compounds have broad applications in various fields, particularly tetrazolin-5-one derivatives, which are noted for their potential use as herbicides [1] and as drugs for treating obesity [2]. Phosphorylated compounds are also well known for their roles as herbicides, drugs, and polymeric building blocks [3].

The 1,3-dipolar cycloaddition reaction between the highly reactive dichlorophosphoryl isocyanate (Cl_2PONCO) and hydrocarbon azides R-N_3, (R = decyl, benzyl and phenyl) has been investigated using theoretical approaches.

A Density Functional Theory (DFT) study clarified the geometrical characteristics, thermodynamic and kinetic parameters, as well as the atomic charge distribution of the substrates and transition state. Analysis of the reaction pathway, obtained through the Intrinsic Reaction Coordinate (IRC) method, [4] indicates that the formation of the thermodynamic reaction products follows a concerted mechanism.

Key words: DFT, theoretical calculations, isocyanate, azide, 1,3-dipolar cycloaddition.

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A DFT study of Favipiravir complexation through double iron (III) chelation

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This study was performed to examine an idea about full chelation of Iron (Fe) by well-known Favipiravir as a possible mechanism of action for medication of COVID-19 patients. To this aim, formations of Fe- mediated dimers of Favipiravire were investigated by performing density functional theory (DFT) computations of electronic and structural features for singular and dimer models.

Keywords: Favipiravir, COVID-19, iron chelation, DFT,

Synthèse de nouveaux dérivés de 1,2,4-triazole fonctionnalisés par des réactions de métathèse des oléfines.

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Au cours des dernières années, les dérivés plateforme de triazoles se sont imposés comme des composés de premier plan dans le domaine pharmaceutique, suscitant un vif intérêt chez les chercheurs pour l'étude de leurs propriétés.[1] Dans ce travail, nous avons développé une nouvelle méthode one-pot répondant aux critères de la chimie verte pour la synthèse de dérivés 1,2,4-triazole à partir d'imidates simples. Cette méthode présente de nombreux avantages, comme un schéma de synthèse plus court, des rendements plus élevés ou encore l'utilisation de réactifs moins toxiques. Par ailleurs, nous avons modifié ces triazole plateformes par métathèse des oléfines en utilisant le catalyseur Hoveyda de 2ème génération, afin de diversifier en une seule étape les structures de ces dérivés pour ensuite étudier leurs activités biologiques

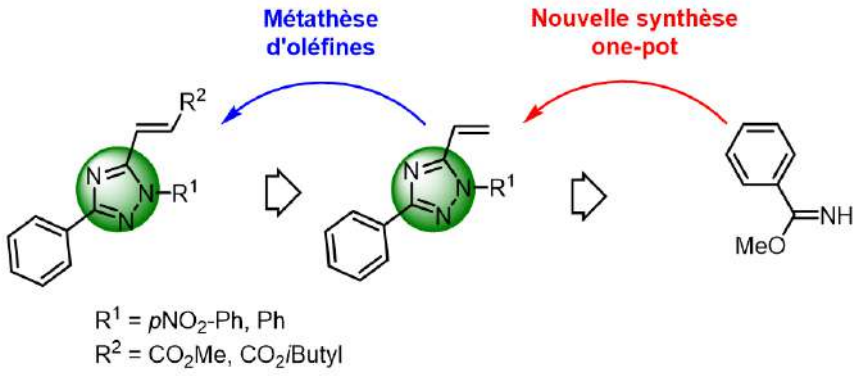

Schéma 1 : Schéma retro-synthétique de nouveaux dérivés de 1,2,4-triazoles fonctionnalisés.

Mot clé : triazole, imidate, métathèse

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The Effect of Welding Currents on Microstructure of steel

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Changes in microstructure affect weld formation and need to be controlled since weld failure is related to the microstructure of the heat affected zone. This research focuses on studying the variation of electric arc welding (SMAW) current on the microstructures of the heat affected metal weld zone of X60 steel. To achieve the research goal, X-ray diffraction (XRD) was used in the heat-affected zones and welding areas. As is evident from the analysis of the experimental results of welded joints, welding parameters have an effect on the grain types and structural phase characteristics of the welded structure.

Keywords: Microstructure, SMAW, Steel, XRD.

Innovative Green Synthesis of Novel Quinoline Hydrazones as Effective Anti-α-Amylase Agents with In Vitro and Molecular Docking Insights

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The N-acylhydrazone scaffold has been recognized as a prominent pharmacophore in various bioactive compounds, interacting with multiple molecular targets [1,2]. A series of 14 quinoline hydrazones (3a-n) was synthesized using both ultrasonic vibrations and conventional methods through the condensation reaction of quinoline hydrazide 2 with different arylaldehydes in an aqueous medium. Compared to conventional techniques, the ultrasonic method achieved significantly higher yields and faster reaction times. The synthesized compounds were characterized using mass spectrometry, ^{1}H-NMR, ^{13}C-NMR, and other spectral analyses. Their α-amylase inhibitory activity was evaluated in vitro, with acarbose serving as a standard reference. Four analogs showed significant activity with **IC50** values ranging from **34.50 ±12 to 0.44 ± 21** μM, compared to the standard acarbose **IC50 = 9.83 ±23** μM, and they exhibited a non-competitive and uncompetitive modes of inhibition as confirmed by kinetic studies. Additionally, molecular docking studies were conducted to elucidate the binding affinity with the target enzyme, while ADMET properties were simulated to evaluate their drug-like characteristics, indicating that the noteworthy compounds displayed favorable in silico ADMET profiles.

Key words: quinoline, N-acylhydrazone, green chemistry, ultrasound-assisted, alpha-amylase inhibitors, molecular docking, ADMET

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Experimental study, crystallographic investigation, antimicrobial potency and molecular docking of Co (II) coordination complexes

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Two complexes $[Co(NCS)_4]_2$ $(C_6H_{17}N_3)_2$. $4H_2O$ (I) and $(C_{10}H_{14}N_2Cl)_2$ $[Co(NCS)_4]$ (II) were synthesized and characterized by physicochemical evidences. According to compound (I), the molecular structure consists of anionic hybrid layer, while $(C_6H_{17}N_3)^{2+}$ cations, are mainly trapped onto successive between these latter, forming corrugated organic layers. However, the atomic arrangement of compound (II) is composed of NH_2^+ groups and inorganic anions, which are linked via N–H…S hydrogen bonds to form anionic layer's parallel to (a, b) plane. The organic cations are inserted between anionic layers to form a three-dimensional network structure. The inter-contacts in the crystal packing were envisioned quantitatively using Hirshfeld surface analysis by 2D fingerprint plots in order to elucidate short contacts resulting from the structural data. The vibrational properties were discussed experimentally by means of IR spectroscopy. Electronic and computational features are examined by quantum chemical studies. The antimicrobial effects were surveyed in vitro against clinical bacterial strains with lysozyme and anti-biofilm activities. Molecular docking investigation divulged significant interactions and binding affinities into active sites.

Keywords: Synthesis; Structural analysis; Molecular docking; antimicrobial potency.

Chemical analysis and antimicrobial activity of *Salsola foetida* extract against pathogenic bacteria

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The present study investigates the biological efficacy of *Salsola foetida* (Chenopodiaceae vent), a wild plant found in the Algerian desert, focusing on its potential antibacterial properties. The objectives involved testing the MeOH extract (70%) of *S. foetida* aerial parts for antibacterial activity against six bacterial strains, quantitative determination of phenolic content, HPLC, and FT-IR analysis. The MeOH extract exhibited significant antibacterial activity against *L. innocua*, *S. aureus*, *E. coli*, and *P. aeruginosa*, while showing weak effects against *B. subtilis* and *S. typhimurium*. The study concludes that *S. foetida* holds promise as a source of bioactive compounds for applications in the food, pharmaceutical, and cosmetic industries, emphasizing its potential significance in these sectors.

Key words: MeOH extract, *Salsola foetida*, Antibacterial activity.

Structural and spectroscopic studies, Hirshfeld surface analysis and optical properties of copper (II) organic-inorganic hybrid material with 5-aminotetrazol ligand

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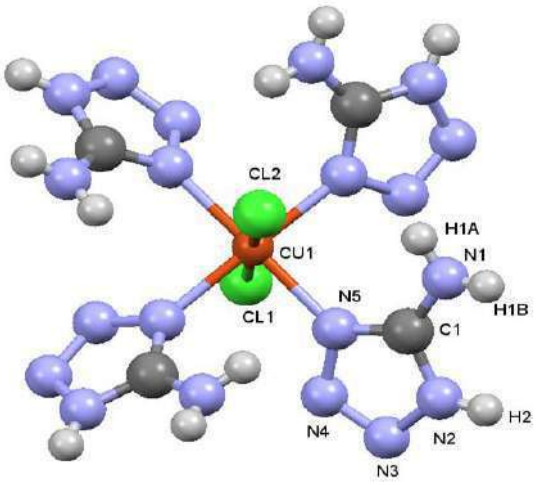
A novel organic-inorganic hybrid material with 5-aminotetrazol ligand of formula $[CuCl_2(CH_3N_5)_4]$ was successfully synthesized at ambient temperature by slow evaporation. The title compound was characterized by experimental physicochemical methods. We have investigated the crystal structure, FTIR, reflectance diffuse and optical properties. Indeed, single crystal X-ray diffraction analysis indicated that the compound crystallizes in the tetragonal space group *P*4nc with the cell parameters a = 9,471(3) Å, c = 8,822(1) Å.



The molecular structure of title compound showing only the atom number labeling of the asymmetric unit.

Investigation of the optical properties of the compound confirmed its semiconducting properties. Photoluminescence proprieties were also reported. The structural determination showed that π–π interactions and hydrogen bonds are implicated in the crystal packing, as investigated by the Hirshfeld surface.

Key words: X-ray diffraction, Crystal structure, Hybrid material, Vibrational study, Optical properties, Hirshfeld surface.

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Effect of volume on the crystallization of different paracetamol polymorphs

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Crystallization is an important operation during the manufacture of pharmaceutical active ingredients because it allows to modify the physicochemical characteristics of a molecule with therapeutic activity thus generating polymorphic forms such as its stability and bioavailability. Polymorphism represents more than 80% of molecules of pharmaceutical interest.

This work is based on the study of the crystallization by cooling of a molecule of pharmaceutical interest in this case paracetamol.

The behavior of this molecule in pure solvents allows to elucidate different crystalline forms in a stagnant medium represented by the single-well system. The influence of supersaturation, the polarity of the solvent have shown a significant influence on the nature of the crystals obtained as well as the crystal size distribution.

Key words: crystallization by cooling, polymorphism, solubility, solvents, nucleation, volume.

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Single-well technology for the determination of solubility and crystallization of drug

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This work is based on the study of crystallization by cooling of drug in a single-well system in a few milliliters of solvent developed within the laboratory.

This system made it possible to follow the appearance of the first crystal as well as the growth in a few milliliters. Hence the determination of the solubility, the nucleation temperature as well as the size of the crystals.

Different parameters were studied, namely supersaturation, polarity of solvents.

The crystals obtained analysis with X-ray diffraction and scanning electron microscopy showed different polymorphic forms with different crystal sizes.

Single-well technology is useful for the determination of solubility and crystallization parameters

Key words: drug, crystal, single well technology, XRD, SEM**.**

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Design of efficient benzimidazole-derived *N*-heterocyclic carbene Ag(I) catalysts for aldehyde-amine-alkyne coupling and their antioxidant and Enzyme inhibition

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This article describes the synthesis of a series of New unsymmetrical *N*,*N*-disubstituted benzimidazolium salts **2a-f** and their Ag(I) N-heterocyclic carbene (NHC) complexes **3a-f**. All compounds were characterized by ^{1} H and ^{13}C Nuclear Magnetic Resonance (NMR), Fourier Transform Infrared Spectroscopy (FTIR), and elemental analysis. Furthemore the antioxidant activity of these compounds was evaluated by using ABTS and DPPH radical scavenging assays as well as their ability to inhibit the acetylcholine esterase (AChE) enzyme. The antioxidant activity showed that the compounds, particularly compound **2** displayed effective antioxidant activities.In addition preliminary catalytic studies using all the silver complexes **3a-f** were performed on three-component coupling reaction of a series of aldehydes with alkynes and amines was demonstrated. Most of these reactions led to formation of the expected propargylamines in good conversions using low amounts catalyst. Silver-based A^3 -coupling was achieved for secondary amines using a diverse set of alkynes to afford propargyl amines with good conversion of up to 90 %. The present approach is environmentally benign and water is generated as the sole byproduct.

Key words: New unsymmetrical *N*,*N*-disubstituted benzimidazolium, complexes, Enzyme inhibition, **antioxidant**

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Synthesis and Anticancer Properties of Benzimidazole Selen Derivatives

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N-Heteocyclic carbenes (NHC) are cyclic carbenes carrying at least one α-amino substituent and are widely used ligands in organometallic and catalytic chemistry. NHCs are strong Lewis bases and generally form stronger and more stable bonds with metals than similar phosphines [1]. Organochalcone compounds find application in organic synthesis, biochemistry, organic superconductors and the synthesis of semiconductor materials [2]. Selenium-containing heterocyclic compounds have an important place among organoselenium compounds [3]. Selenium is an important micronutrient in human nutrition. Selenium deficiency is seen to cause diabetes, cancer and immune system disorders [4]. Organo-selenium compounds for the prevention of cancer were first identified in the 1980s. Later, clinical trials of organo-selenium showed excellent results as anticancer agents. Selenium increases immunity by preventing chromosome damage. In recent years, it is also known that elemental selenium has been used as a reactant in the synthesis of Se-NHCs [5].

In this study, Se derivatives containing benzimidazole nucleus were prepared and their anticancer activities were investigated. The current research study aims to provide alternatives to some selenium derivatives. The structures of all compounds were characterized by ^{1}H NMR, ^{13}C NMR and HR-AM spectroscopy techniques.

Key words: Benzimidazole, Selenium, Anticancer activity

Note : This work was financially supported by the Technological and Scientific Research Council of Turkey TÜBİTAK-CNRST-122Z261.

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In vitro Anticancer Activity against HCT116 and SH-SY5Y cell lines of New Imidazolidine Derivatives

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Imidazole has become an important synthon in the development of new drugs. Its derivatives show different biological activities such as antibacterial, anticancer, antiviral, anti-inflammatory and antifungal activities which have been widely reported in the literature [1,2]. Creating safe and effective anticancer pharmaceuticals with an imidazolidine heterocyclic ring was the goal of this project. Starting with 1-(2-hydroxypropyl)imidazoline and N,N-dimethylformamidedimethyl acetal, substituted-imidazolidine derivatives (3a-h) have been generated. The anti-tumor potential of the imidazolidine derivatives (3a-h) was further investigated using the human colon cancer cell line HCT116 and the human neuroblastoma cell line SH-SY5Y. All of the synthesized compounds, with the exception of one salt, were active against the tow cells line. According to the results of biological tests, the inhibitory concentration (IC50) values ranged from 45.44 µM to 663.73 µM.

Key words: imidazolidine, anticancer activity, HCT116, SH-SY5Y.

Note: This work was supported by the Technological and Scientific Research Council of Turkey (TÜBİTAK) for Post-Doc Research Fellowship Programme (2216B-TWAS)

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Phytochemical content and in silico molecular docking of P. albicans L plant

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P. albicans L (plantaginaceae) is used in traditional therapy and is one of several medicinal plants known in Algeria and Tunisia due to their variety of therapeutic properties. Jaceosidin is a flavonoid extracted from this plant experimentally by a phytochemical process and identified using spectroscopic analysis (UV-VIS, IR, RMN 1H, RMN 13C). In current literature, it has been reported that jaceosidin has anti-inflammatory and antioxidant activities, as well as antibacterial and anti-cancer activities. In this case, the experimental part was fed back by theoretical investigation to demonstrate jaceosidin bioactivity. In fact, we studied the pharmacokinetic properties of the molecule through simulation, such as ADME, bioavailability, and anti-oxidant potency. In addition, the interaction between jaceosidin and MM9 enzyme were determined *in silico* by molecular docking.

Keywords : Flavonoid, Extraction, In silico, Molecular docking, ADME.

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Synthesis of Novel 1,2,3-Triazole-Linked Chromene Hybrids: In Vitro Anti-Melanoma Effects and In Silico Insights

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Hybrid structures derived from entities with established biological properties offer a promising strategy for enhancing molecular diversity, making them valuable tools in the development of potential therapeutic agents [1]. Among these, five-membered heterocycles, especially 1,2,3-triazole compounds, have attracted considerable interest over the past decade and are widely utilized in organic chemistry [2]. Our work fits into this optical and focuses on the synthesis of novel hybrid 1,4-disubstituted triazole derivatives using a copper(I) catalyst. The structures of the synthesized products were confirmed through spectroscopic analyses (HRMS, NMR). In vitro assessments revealed that some derivatives exhibited activity against murine (B16F10) and human (IGR-39) melanoma cell lines. Molecular docking studies indicated that these compounds bind to several potential target proteins, including B-Raf Kinase^{V600E}, EGFR, and Human MEK1 kinase. Additionally, the physicochemical, pharmacokinetic, and toxicological properties of the synthesized analogs were found to be within desirable limits, demonstrating a promising ADMET profile.

Key words: Chromene-based triazoles, Melanoma, Molecular docking

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Design and Synthesis of novel benzopyran derivatives: An Investigation by Experimental and Computational Studies

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Elevated blood glucose levels are a critical factor in diabetes mellitus (DM), with approximately 90% of diabetic patients affected by type 2 diabetes mellitus (T2DM) [1]. An effective strategy for managing T2DM involves reducing postprandial hyperglycemia by retarding carbohydrate digestion and absorption, primarily through the inhibition of carbohydrate-hydrolyzing enzymes such as α-amylase [2]. Therefore, there is a great demand to develop new and safe therapeutic agents for T2DM with minimal side effects.

In the light of these findings, we report herein the synthesis of a new series of heterocyclic compounds *via* molecular hybridization, combining the benzopyran moiety with various pharmacophores, including pyrazole, pyrrole, and pyrrolidinedione. The synthesized compounds were characterized using spectroscopic methods (^{1}H NMR, ^{13}C NMR, and HRMS) and evaluated for their ability to inhibit the α-amylase enzyme. The results demonstrated that these derivatives displayed significant α-amylase inhibitory activity. Structure-activity relationship (SAR) analyses, supported by *in silico* and kinetic studies, provided insights into the interactions of these compounds with the target protein α-amylase.

Key words: Benzopyran, molecular hybridization, α-amylase, Molecular docking, ADMET

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Bisdiarylethylenes: Towards New Horizons in Synthesis, Characterization and Applications

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A comprehensive methodology for creating new bisdiarylethylene derivatives begins with the preparation of a diarylethylene from para-substituted benzyl bromide. This arylacetonitrile was then used to synthesize an α,β-unsaturated nitrile via the Knoevenagel reaction, followed by Heck coupling [1] with various styrénes to produce functionalized bisdiarylethylenes exhibiting intriguing structural and electronic properties. The final products were characterized by NMR, IR, and UV-Vis spectroscopy, which revealed distinctive spectroscopic features and promising optical properties. These bisdiarylethylenes are identified as potential precursors to helicenes [2] and semiconductor materials, opening new avenues in organic electronics [3] and advanced materials chemistry.

Keywords: Helicenes; bisdiarylethylenes; diarylethylene; Heck coupling.

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Pd-PEPPSI-Type Expanded Ring N-Heterocyclic Carbene Complexes: Synthesis, Characterization, and Catalytic Activity in Suzuki-Miyaura Cross Coupling

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In this work, we have synthesized a series of six unsymmetrical benzimidazolium salts **2**, featuring an isobutyl on one of their nitrogen atoms and a various alkyl groups on the other one and their pyridine enhanced precatalyst preparation stabilization and initiation (PEPPSI) themed palladium *N*-heterocyclic carbene complexes [$PdCl_2$(NHC)(Py)]. All the products were isolated in satisfactory yields (75-85%). The synthesis of these novel palladium PEPPSI complexes involved reacting NHC precursors with $PdCl_2$ in pyridine at 60 °C in the presence of excess K_2CO_3. The structures of all compounds have been characterized by ^{1}H NMR, ^{13}C NMR, HRMS and IR spectroscopy, as well as elemental analysis techniques, which support the proposed structures. The catalytic activity of the six complexes was assessed in the Suzuki-Miyaura cross-coupling of phenylboronic acid and aryl halides. The reactions required only a low catalyst loading (0.1 mol%) and were carried out under mild aerobic conditions in a green, water-based solvent mixture. High yields of biphenyl derivatives were achieved with all the aryl bromides tested, irrespective of the presence of electron-donating or withdrawing substituents on their aromatic ring. When 1-Chloro-4-methyl-benzene, a representative served as substrate, complex 3a became mostly inactive, whereas with the 1-Chloro-4-nitro-benzene catalyst 3a maintained a high activity

Keywords: palladium *N*-heterocyclic carben complex; benzimidazole; Suzuki-Miyaura cross coupling; C-C bond formation; water.

Molecular self-assembly of 1D linear polyiodide in a 4-dimethylaminopyridinium salt: A Competition between Halogen and Hydrogen Bond

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A new 1D linear polyiodide, $C_7H_{11}N_2^+ \cdot I_3^- \cdot 0.5H_2O$, was synthesized by slow diffusion method in solution. It consists of an arrangement of tri-iodide ions, organized in one-dimensional linear chain, stabilized by the 4-dimethylaminopyridinium ligand. An asymmetry of the tri-iodide anions is observed and is associated to the I···I halogen and hydrogen bonding interactions. The generation of the resulting supramolecular network for this compound was found to be driven by hydrogen-bond assisted self-assembly. The crystal structure of the compound was found to be supported essentially by H···I interactions between organic molecules and tri-iodide anions. An additionally stabilization by O···H/H···O interactions due to the presence of water molecules occurs. The dominant intermolecular interactions and their directionality have been examined by Hirshfeld surfaces and fingerprint analysis. The $C_7H_{11}N_2 \cdot I_3 \cdot 0.5H_2O$ compound was characterized further by FT-IR and Raman spectroscopies, TGA/DTG and UV-visible absorption by means of thin films method **[1]**.

Key words: Triiodide, Molecular structure, Supramolecular assembly, Raman spectroscopy, TD-DFT theory.

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Molecular self-assembly of 2D T-shape polyiodide arrangement in triiodide of tetraethylammonium: Supramolecular structure and density functional theory-based optical properties

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The preparation of the tri-iodide salt, $(C_2H_5)_4N^+ \cdot I_3^-$, synthesized by the slow diffusion method in solution, is reported. It consists of an arrangement of triiodide ions, organized into two-dimensional T-shaped sheets, stabilized by the tetraethylammonium ligands. An asymmetry of the tri-iodide anions is observed in the structure, and is associated to the I···I halogen and hydrogen bonding interactions. The generation of the resulting supramolecular network for this compound was found to be driven by hydrogen-bond assisted self-assembly. The compound was characterized further by FT-IR and Raman spectroscopies, TGA/DTG and UV-visible absorption by means of thin films method. The target compound was also studied computationally using Density Functional Theory (DFT) and time-dependent DFT (TD-DFT) approaches to explore its potential performances and to rationalize the experimental results. An electronic transition from $3\sigma_g$ to $3\sigma_u^*$ has been proven to dominate intramolecular charge transfer occurring for $(C_2H_5)_4N \cdot I_3$. This electronic communication leads to an HOMO-LUMO energy gap of 4.255 eV **[1]**.

Key words: Triiodide, Molecular structure, Supramolecular assembly, Raman spectroscopy, optoelectronic properties, TD-DFT theory, HOMO-LUMO gap.

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SYNTHESIS OF PYRRAZOLE AND PYRIMIDINE STRUCTURE

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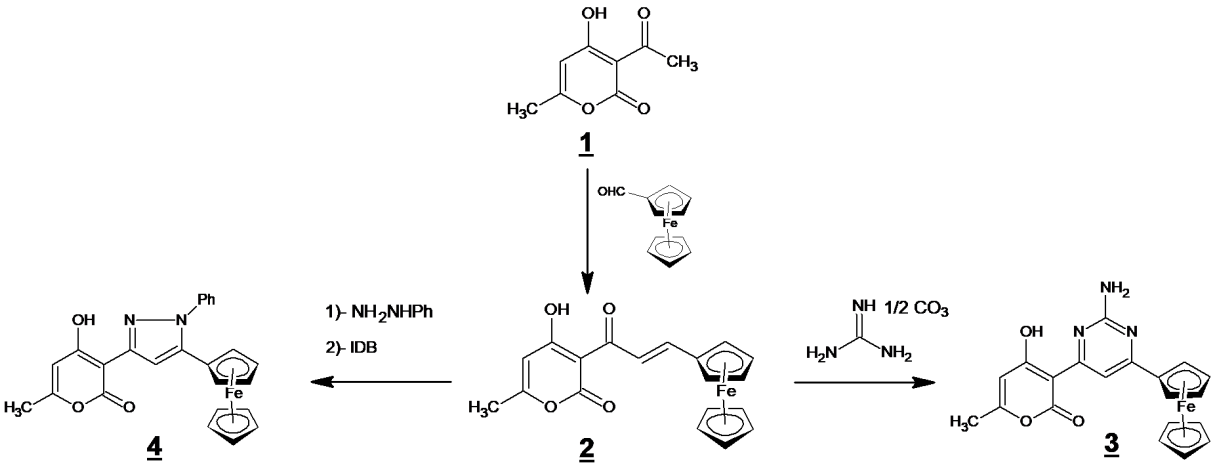
keywords : Pyrrazole ; Pyrimidine ; Dehydroacetic acid

Pyrazoles and pyrimidines represent an important class of nitrogen heterocycle in organic chemistry, given their large biological potential. [1,2,3]

We present in this work the synthesis of a pyrimidine derivative **3** and a pyrazole derivative **4** from the intermediate **2** (obtained by condensation of ferrocene carboxaldehyde and dehydroacetic acid **1**).

Compound **3** is obtained by the action of guanidine carbonate on chalcone **2**. Compound **4**was obtained by the action of phenyl hydrazine on compound **2**, the intermediate obtained is oxidized with iodobenzene acetate.



Scheme 1: Synthesis of derivatives **3** and **4**

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Effet du dopage au manganèse sur les propriétés électriques du ZnO

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Le présent travail est consacré pour la synthèse et la caractérisation des nanoparticules (NPs) ZnO dopé au manganèse (Mn/ZnO), par la suite nous envisageons d'étudier ses propriétés électriques. Nous avons utilisé la méthode hydrothermale pour la synthétisé des nanocristaux ZnO dopés à 3% au Manganèse. L'analyse des propriétés électriques a été réalisée à l'aide de mesures de photocourant et d'impédance à différentes températures. Les résultats montrent que les Nps ZnO pur présentent une densité de photocourant supérieure à celle du ZnO dopé à 3 % au manganèse, indiquant une séparation de charge plus efficace. De plus, l'impédance a révélé que la résistance des échantillons diminue avec l'augmentation de la température, et la conductivité électrique du $Zn_{0.97}Mn_{0.03}O$ s'est avérée inférieure à celle du ZnO. Nous avons également observé que la structure des produits et les mécanismes de conduction sont influencés par le dopage au Mn, mettant en évidence son impact sur les performances électriques et photocatalytiques. Ces résultats fournissent des informations précieuses pour l'optimisation des applications photocatalytiques basées ~~sur~~ des NPs ZnO dopé au Mn.

Mots-clés : ZnO, dopage au Mn, photocourant, conductivité électrique.

Electrochemical and Theoretical Investigation of Plant Extract as a Corrosion Inhibitor for Carbon Steel in 1M HCl

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Carbon steel is one of the commonly used materials in the industry. The cleaning process of these materials often involves the use of acidic solutions, which can result in significant financial losses. Currently, solutions based on synthetic chemical products are used, but they have major drawbacks such as high cost and toxic environmental impact. Therefore, researchers are turning to the development of more affordable, eco-friendly, and biodegradable inhibitors. In this study, we evaluated the potential of an extract from species belonging to the Apiaceae family grows in northeastern Algeria. We used advanced electrochemical techniques, including Electrochemical Impedance Spectroscopy and Potentiodynamic Polarization Curves, as well as surface analysis using MEB equipped with an EDS analysis system. The extract characterization was done as well as the identification of major compounds of the extract, subjected to a theoretical study using the DFT method, to obtain an idea of the major compound that adsorbs on the steel surface. MEB-EDS analysis confirmed the experimental results, thus validating the effectiveness of plant extract as a corrosion inhibitor.

Key words: Extract, Corrosion, DFT, MEB-EDS.

Reaction of $Bi(NO_3)_3$ with quinoxaline in the presence of HI: Synthesis of a Graphite-Like Energetic Compound by serendipity

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Treatment of an acetone solution of $Bi(NO_3)_3$ with quinoxaline (Qx) in the presence of hydroiodic acid produces in moderate yield the crystallographically characterized 1D-polymeric salt-like iodobismutate $[(Qx\text{-}H)BiI_4]_n$ (**1**), whose negative charge is balanced by mono-protonated quinoxalinium counterions. The main product is an unusual tetra(nitrated) quinoxaline derivative, namely 5,6,7,8-tetranitro-1,2,3,4-tetrahydroquinoxaline-2,3-diol (**2**), which was formed accidently under mild reaction conditions. The molecular structure of this organic compound **2** was determined by single-crystal X-ray diffraction and its strong intermolecular interactions giving rise to a supramolecular three-dimensional network were assessed by a Hirshfeld surface analysis. Structural analysis reveals that the crystal structure is supported essentially by O–H···O and N–H···O intermolecular hydrogen bonds and additionally stabilized by N–O···π interactions. The ground-state molecular structure of this novel organic heterocycle has been optimized by DFT calculation. High density, positive heat of formation and very good thermal stability according to thermal analysis by TGA, DTA and DSC characterize tetranitro compound **2** as energetic material **[1]**.

Key words: Quinoxaline, Bismuth iodide, Crystal structure, DFT, Energetic compound, Graphite-Like structure.

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Unexpected Formation of the Iodobismuthate Salt $(C_{14}H_{15}S_2N_2)_2(C_9H_{10}SN)_2[Bi_4I_{16}]$ upon Reaction of the Unsaturated Ligand Z-PySCH$_2$CH=CHCH$_2$SPy with BiI_3

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The olefinic dithioether (*Z*)-1,4-bis(pyridin-2-ylthio)but-2-ene *Z*-PyS(CH$_2$CH=CHCH$_2$)SPy (L) was prepared by the treatment of *cis*-ClCH$_2$CH=CHCH$_2$Cl with in situ generated potassium pyridine-2-thiolate Py-SK and analyzed by IR and NMR spectroscopy. To investigate the chemistry of polynuclear iodobismuthate complexes, two equivalents of BiI_3 were reacted with L in the MeOH solution to afford the anionic tetranuclear title compound $(C_{14}H_{15}S_2N_2)_2$ $(C_9H_{10}SN)_2[Bi_4I_{16}]$ with a *N*-protonated (*Z*)-1,4-bis(pyridin-2-ylthio)but-2-ene as a counterion. Compound **1** was characterized by IR and UV spectroscopy; the formation of a tetranuclear framework was ascertained by a single-crystal X-ray diffraction study performed at 100 K. Furthermore, an unusual Bi(III)-meditated cyclization of one Z-PyS(CH$_2$CH=CHCH$_2$)SPy ligand occurred, affording the bicyclic pyridinium salt 3-vinyl-2,3-dihydrothiazolo[3,2-a]pyridinium bearing a terminal vinyl group, compensating the second negative charge of the $Bi_4I_{16}^{4-}$ cluster anion. The SCXRD characterization was completed by a Hirshfeld surface analysis, revealing some secondary interactions occurring in the crystal **[1]**.

Key words: Bismuth triiodide, olefinic dithioether, crystal structure, Hirshfeld analysis, supramolecular structure.

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Biological activities and molecular doking of tris(8-quinolinolato-κ^2*N*,*O*)cobalt(III) methanol solvate

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Cobalt complexes with 8-hydroxyquinoline hold a privileged status in medicinal chemistry, highlighting the significant importance of this class of compounds [1]. The crystal structure of the compound was identified as belonging to the monoclinic system, with space group *P*21/*n*. The unit cell, illustrated in Fig.1, contains three deprotonated 8-HQ ligands, which adopt a distorted octahedral geometry. Notably, the complex also crystallizes with a methanol molecule, although this molecule is not part of the cobalt coordination sphere. The compound displayed remarkable antibacterial activity and enhanced antifungal effects against Candida compared to the positive control. This efficacy can be attributed to its anti-biofilm and anti-virulence properties. Additionally, it exhibited a specific inhibitory effect on the lipopolysaccharides of Klebsiella pneumoniae. Moreover, molecular docking demonstrated that 8-HQ shows promising results through its interactions with the target CYP51 from the pathogen Candida albicans (PDB: 5v5z). The interactions include an H-bond with Tyr505, a Pi-alkyl interaction with Pro230, and a Pi-Pi stacking interaction with Tyr64.

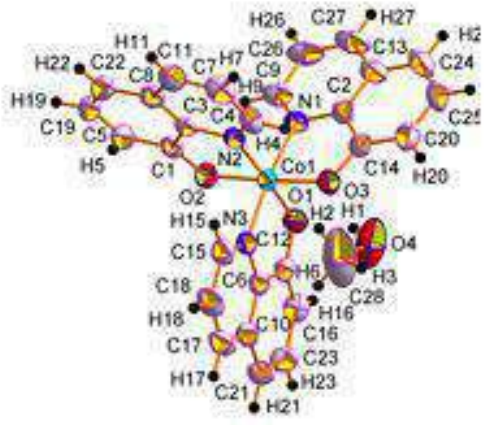

Fig.1 Asymmetric unit of compound $[Co(C_9H_6NO)_3].(CH_3OH)$

Key words: XRD, Antibacterial and antifungal activities, molecular docking.

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Extraction and characterization of cell wall polysaccharides from Tunisian (*Pleurotus eryngii*) fruiting bodies

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This study investigates the composition of polysaccharides isolated from the fruiting bodies of two *Pleurotus eryngii* varieties, *P. eryngii* var. *elaeoselini* and *P. eryngii* var. *ferulae*. The total polysaccharides, β-glucan, and α-glucan content were quantified. Polysaccharide fractions were extracted using microwave-assisted methods with hot water, with 1 mol L^{-1} aqueous sodium hydroxide, and followed by dimethyl sulfoxide DMSO. Purification of polysaccharidic fraction soluble in hot water was performed using proteolytic enzymes. Monosaccharide composition, FTIR, and NMR analyses were conducted to elucidate the structures of the polysaccharide fractions. Results indicate that the β-glucan content of *P. eryngii* var. *elaeoselini* is twice that of *P. eryngiums* var. *ferulae*. Glucose was the predominant neutral sugar in all fractions across the strains. The neutral sugar content was relatively high in the extracts (58-79%) but lower in the insoluble parts (28-49%) due to the presence of chitin. FTIR and NMR spectra revealed that the purified hot water extracts are mixtures of (1→4)-α-D-glucan, (1→6)-β-D-glucan, and branched mannogalactan. The dominant polysaccharide in the alkali-soluble fractions is branched (1→3)(1→6)-β-D-glucan, with unbranched (1→3)-α-D-glucan being a minor constituent.

Key words: King oyster mushroom, Polysaccharide, structure, β-d-glucan

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Asymmetric synthesis of enantiopure tetracyclic dispirooxindolopyrrolidine-piperidones via microwave-assisted multicomponent reaction: Crystallographic analysis, antimicrobial activity and in silico studies

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In an attempt towards the development of new antimicrobials, we synthesized by microwave-assisted multicomponent reaction (MCR) of enantiopure (E,E)-3,5-bisarylidene-N-[(S)-(-)-methylbenzyl]-4-piperidones, isatin and α-amino esters a series of optically active tetracyclic dispirooxindolopyrrolidine-piperidones. The beneficial and promising features of this protocol such as simple operational procedure, short reaction time (10 min), and high product yields (up to 97%) make it an efficient eco-friendly approach offering a powerful mean to expand the structural diversity of spirooxindoles.

This approach appears hugely advantageous for high-throughput screening processes in drug discovery research. In addition, crystallographic parameters and inter- and intramolecular interactions occurring in spiropyrrolidine-fused piperidone derivative 4g were examined through single-crystal XRD analysis allowing to determine the absolute configuration of the enantiopure compound. The resulting optically active heterocycles were screened for their in vitro antimicrobial potency against a variety of pathogenic organisms. The preliminary biological assessment indicated that most of the screened products display higher antimicrobial activity than the standard reference drugs Ampicillin and Griseofulvin, while the remaining compounds exhibited good to moderate activity against bacteria and fungi. In addition, in silico molecular docking and predictive ADMET studies for the more active spirocompounds were carried out.

Molecular docking methods confirmed the binding efficacy of candidates 4c and 4l through low score energy values and the establishment of diverse bonds with active site residues active of selected targets. Finally, the ADMET profiling of the most active spiroheterocycles proved their remarkable drug-like and pharmacokinetic properties.

A novel green synthesis of $CoFe_2O_4$ Nanoparticles for photocatalytic and antimicrobial activity evaluation

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Green synthesis of nanoparticles is an eco-friendly method that uses natural biological agents such as plant extracts, bacteria, or fungi to reduce and stabilize metal ions. This process avoids toxic chemicals, making it more sustainable and energy-efficient compared to conventional methods. This green method provides a safer and more cost-effective approach to nanoparticle production. $CoFe_2O_4$ nanoparticles, valued for their magnetic and catalytic properties, are applied in drug delivery, environmental cleanup, and magnetic devices.

This paper reports a novel green fabrication of cobalt ferrite ($CoFe_2O_4$) nanoparticles (NPs) from Artemisia plant extract. The NPs were characterized by different spectroscopic techniques. The Fourier transform infrared (FTIR) spectrum exhibited intrinsic stretching at the tetrahedral position of Fe–O at 591 cm^{-1} and the octahedral stretching of Co–O at 402 cm^{-1} respectively. The fine diffraction pattern in the X-Ray diffraction analysis (XRD) showed the formation of well-crystalline NPs. The mean crystallite size of the NPs was calculated to be 20 nm. The High-resolution Transmission Electron Microscopic (TEM) analysis showed roughly spherical shape and irregular morphology of the NPs. Optical properties were analyzed by UV-Vis diffuse reflectance spectroscopy. The optical absorbance was measured to determine the optical band gap using Kubelka-Munk function. The photocatalytic activity of the $CoFe_2O_4$ NPs was examined against the methylene blue (MB) dye, showing 82% degradation under UV-Visible light. The reusability experiment showed that the catalytic activity was not much decreased even till the 4^{th} cycle. The antibacterial activity of the synthesized $CoFe_2O_4$ NPs was tested against Bacillus subtilis, Staphylococcus aureus, Bacilus pumilis, Escherichia coli, Pseudo monas aeruginosa, and Salmonella abony through the Agar well diffusion method. The $CoFe_2O_4$ NPs gave strong antibacterial potential against gram positive and negative bacteria, it was able to affect growth and virulence factor of bacterial and fungal species.

Key words: $CoFe_2O_4$ NPs, Green synthesis, photocatalytic, antioxidant; antimicrobial

Photodynamic antimicrobial activity of selected metal-free and tin porphyrins

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Photosensitization is considered nowadays as one of the alternatives for antimicrobial and photodynamic therapy treatment by researchers. Different dyes such as bodipy, phthalocyanines and porphyrins are used for this purpose. In this study selected metal-free porphyrins and tin 5 10 15 20 -tetrakis (4-bromophenyl) porphyrin and meso-tetra (4-carboxyphenyl) tetramethyl ester porphyrins were synthesized and used for the inhibition of staphylococcus aureus and Salmonella including E.Coli. Irradiation was performed using 530 nm and 650 nm LED lamps. Dyes used in this work showed good results for metalated compared to free base.

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Adsorption of Indigo Carmine dye onto activated carbon derived from *Phoenix dactylifera petiole* by fixed bed column

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Activated carbon obtained from date palm petiole (AC-PT) by chemical activation was used as an efficient adsorbent for the removal of indigo carmine dye (IC) from aqueous solutions. The Thomas, Yoon-Nelson and Yan models were applied to adapt the experimental data of the continuous adsorption of IC. The experimental breakthrough data, including the saturation adsorption capacities, breakthrough times, for the studied pollutant were evaluated by varying the flow rate. The Bohart-Adams model fit perfectly to the initial part of the breakthrough curve ($C_t/C_0<0.5$), and the hole curve was well fit by the Yoon-Nelson and Thomas model.

Key words: Activated carbon, date palm petiole, indigo carmine, Continuous adsorption.

On the adsorption of a dye by means of theory approach

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The treatment of wastewaters becomes a matter of great interest and it is necessary to develop efficient and cost-effective methods to solve this environmental problem. Advanced oxidation processes (AOPs) emerge as an attractive way for the treatment of wastewater containing organic substances. In fact, most AOPs are based on the generation of powerful hydroxyl radicals, which are highly reactive and non-selective. The oxidation potential of these radicals is 2.8 V. Therefore, the AOPs are able to oxidize a great number of organic compounds like aliphatic and aromatic organic molecules. Besides their many uses as coloring matters, dyes with triphenylmethane structure, have found extensive use in industry of textiles, drugs, printing inks, laboratory indicator cosmetic industries and as biological stains.

Bormophenol blue (BPB) is a prominent acid dye, accomplished of making direct links with basic groups in tissue-constituents, used as a color mark to monitor the process of agarose gel electrophoresis and polyacrylamide gel electrophoresis, coloring proteins in paper electrophoresis.

Bromophenol blue is also a pH indicator at neutral pH and it is an anionic dye and a member of triphenylmethane dyes family. It is usually used in many industrial areas for various purposes, e.g. textile, biological stain, dermatological agent, veterinary medicine. Due to various harmful effects of these dyes, the degradation of them was subjected of various works.

In this study, Density functional theory (DFT) was used to strengthen the critical role of the adsorption of the solid surface in determining the oxidation rate of pollutants in iron oxide/H_2O_2 systems.

A comparative study of MXenes' properties in previous researches for energy storage and conversion: Recent advances and perspectives

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MXenes with the general formula of $M_{n+1}X_nT_X$ are yielded through exfoliation of the ternary class of carbides materials MAX phases, where M is a transition metal (Ti, Zr, Hf, V, Nb, Ta, Cr, Sc), X usually represents a non-metal (C or N) and T_X denotes the surface termination groups related to the etchant solvents (-OH, =O and F). MXenes have emerged as promising nano-materials in many applications. Recently, they are used as electrodes for developing efficient energy storage and conversion systems in virtue of the metallic conductivity, high Li storage capacity, high theoretical capacitance, low diffusion barrier and hydrophilic surfaces. According to previous researches, MXenes have various properties depending on the composition, structure, and processing conditions **[1, 2]**. For instance, the 2D MXenes with binairy metals offer even better flexibility in tuning of properties than single metal carbides [3, 4]. In the present study, we provide evidence of the effects of transition metal on the MXenes' electronic properties and electrochemical performance for energy sectors.

Keywords: MXene; electronic properties; binary metals transition.

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Synthèse de 3,4-Dihydropyrimidin-2-(1H) -one en présence de Catalyseurs verts CoCuZnO et $CoCuZrO_2$ via la réaction de Biginelli

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La réaction de Biginelli est l'une des réactions multicomposants les plus étudiées. Elle permet la synthèse d'un produit complexe unique présentant des propriétés biologiques, thérapeutiques et pharmaceutiques, telles que des activités antivirales, antibactériennes, anti-inflammatoires et antitumorales [1-3]. Ces réactions sont particulièrement intéressantes pour leurs avantages économiques et écologiques, connus sous le terme de "chimie verte". En conditions homogènes, cette réaction peut être limitée par plusieurs facteurs tels que l'utilisation de solvants toxiques ou inflammables, ce qui peut être jugé inapproprié selon les principes de la chimie verte. Par conséquent, l'utilisation de catalyseurs en phase hétérogène a été proposée comme une approche alternative. Dans ce contexte, nous avons choisi d'étudier la réaction de Biginelli pour la synthèse de 3,4-Dihydropyrimidin-2-(1H)-one (DHPM) en milieu hétérogène en utilisant des catalyseurs $CoCuZrO_2$ et CoCuZnO préparés par la méthode sol-gel. L'utilisation de ces derniers dans les conditions douces s'affiche comme des outils précieux pour le développement d'une chimie plus durable et plus respectueuse de l'environnement**.** Les r**é**sultats de l'activité catalytique ont montré que le système $CoCuZrO_2$ est plus efficace avec un rendement en DHPM de 85% en utilisant 0,01g de catalyseurs à 100°C pendant 3h sans solvant.

Mots-clés : chimie verte, phase hétérogène, catalyseurs, Biginelli

Repellency and toxicity effect of volatile oils of *Thapsia garganica* L. growing in Tunisia against Red flour beetles

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Recent studies have highlighted the promising role of aromatic plant-derived volatile oils in the management of insect pests. [1] Red flour beetles are well-known insects that primarily target stored food products and cause significant damage. Thus, this study pioneered the exploration of the chemical composition, repellency, and toxicity properties of the volatile oils of *Thapsia garganica* seeds against these insects. Oil composition was analyzed using gas chromatography coupled with mass spectrometry (GC/MS) and flame ionization detection (GC/FID). The major compound detected was 1,4-diméthylazulene, comprising 51.3% of the total oil composition. This study revealed remarkable results regarding the efficacy of the oil against insects. It has potent repellent properties and high toxicity effect causing of 93% of mortality after 24 hours of exposure. These findings suggest that volatile oils from *T. garganica* could serve as an effective natural alternative to conventional insecticides.

Key words: *Thapsia garganica*, volatile oils, pest management, red flour beetles.

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ENQUETE ETHNOBOTANIQUE SUR LES PLANTES ANTICANCEREUSES UTILISEES EN MEDECINE TRADITIONNELLE ALGERIENNE

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Le cancer est un problème majeur de santé publique. Actuellement, une personne sur cinq dans le monde développe un cancer au cours de sa vie. Il est à l'origine de près de 10 millions de décès par an et représente l'une des principales causes de mortalité dans le monde **[1].** L'Algérie a enregistré plus de 50 000 nouveaux cas de cancer en 2020.
Suite aux données de l'OMS, 80 % de la population mondiale a recours aux plantes pour prévenir ou traiter diverses pathologies notamment le cancer
L'intérêt populaire pour la phytothérapie n'a jamais cessé d'évoluer. Les chercheurs y ont découvert environ 60.000 espèces dont 3.000 plantes ayant des propriétés anticancéreuses.
L'objectif de la présente étude est de faire le point sur l'utilisation des plantes médicinales par les patients atteints de cancer.
Une enquête descriptive transversale a été menée auprès de 300 patients cancéreux suivies au niveau du service d'oncologie d'Oran, Algérie.
Nos résultats montrent que 48% soit 144 patients ont recours à la phytothérapie en association avec le traitement conventionnel. Lors de cette étude, nous avons recensé 21 espèces présumées anticancéreuses appartenant à 19 familles. La plus utilisée est le *Berberis vugalis* L. à 35.2% suivie par *Prunus persica* L. et *Aristolochia longa* L. avec un pourcentage respectif de 16.55 % et 11.03 %.

Key words: Médecine traditionnelle, plante, cancer, Algérie

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Structural behavior, thermal properties, electrical characterization and conduction mechanism study of the new potassium arsenate tellurate compound

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The new compound $K_3(HAsO_4)(H_2AsO_4).Te(OH)_6$(KAsTe) has been synthesized in order to determine the structural behavior , the temperature transitions and to specify the electrical properties as well as the conduction mechanism. It is obtained by hydrothermal preparation method and proves to crystallize in the monoclinic system with centrosymmetric space group *C*2/*c*. In this atomic arrangement, two types of polyhedra (TeO_6 and $HAsO_4$) were observed in the presence of K^+ cations. The stability and the cohesion of the crystal structure were ensured via O–H···O hydrogen bonds. Thermal analysis (DSC, DTA and TG) revealed the presence of the phase transitions and the temperature of the decomposition. Additionally, in this current work, electrical properties based on the impedance measurements were determined. Before and after the decomposition of the studied material, the complex impedance diagrams at different temperatures were fitted into two equivalent circuit types, each circuit built up by a series combination of grains and grains boundary elements. The thermal evolution of the conductivity σ_{dc} displayed an Arrhenius type behavior and suggested that this material is an ionic protonic conductor at high temperature whereas the σ_{ac} conductivity is accounted for in terms of two processes that can be assigned to a hopping transport mechanism. These processes are the correlated barrier hopping (CBH) model in the first region (before the decomposition), as well as the non-overlapping small polaron tunneling (NSPT) model in the second region (after the decomposition).

Key words: Crystal structure, Hydrothermal method, Phase transitions temperatures, DSC, Conductivity, equivalent circuits.

Spinel synthesis from waste aluminum dross and dolomite ore

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Aluminum melting industries generate large quantities of aluminum dross that are mainly composed of alumina (Al_2O_3). They can also contain other chemical compounds such as: $MgAl_2O_4$, AlN, $NaAlCl_4$, $Al(OH)_3$, Al_2S_3, NaCl, KCl, $FeSO_3$... Some chemicals such as: AlN, Al_4C_3, Al_2S are very dangerous and harmful to the environment and humans because they can react with the surrounding humidity and generate dangerous and toxic gases (H_2, CH_4, NH_3, H_2S…). Over the last few decades, several research studies have been conducted on the recovery of aluminum dross. It was demonstrated the possibility of their use to synthesize high purity γ-alumina, aluminum sulfate, calcium aluminates, and to manufacture refractory materials and active catalyst. Aluminum dross are also used to make spinel composites, and little research works were devoted to the synthesis of spinel.

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

In this work, we were interested in the study of powders synthesized from aluminum dross and dolomite by dissolution-precipitation-calcination process. Local aluminum dross from the company AMR (El-Eulma, Setif (Algeria) was used as alumina (Al_2O_3) source and dolomite from Teioualt djebel as MgO source to promote the formation of spinel.

In first stage, the starting materials were characterized. According to the chemical analysis, a mixture (Al dross/dolomite) which theoretically gives an equimolarAl_2O_3/MgO final composition was optimised. The starting materials were subjected to the adopted synthesizing protocol comprising: dissolution of each material independently, precipitation and calcination. The obtained powder was characterized by several physicochemical methods (XRD, FTIR, SEM, EDX, laser granulometry). It was found that obtained powder was composed of spinel ($Mg_{0.4}A_{2.4}O_4$) as a major phase associated to alumina (Al_2O_3) with traces of some impurities (CaO, $SiO_{2...}$). The particles of the obtained grain powder are in agglomerated state and have a micronic size (5.6 μm- 8.71 μm).

Key words: Aluminum dross, alumina, dissolution, precipitation, spinel

Synthesis, characterization, DFT and Molecular Docking study of the crystallized 6-methoxylated derivative of the antiviral drug favipiravir

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In response to the COVID-19 pandemic which has led to millions of victims worldwide, Favipiravir (FAV) has attracted significant interest as a promising antiviral treatment for this disease. This study focuses on the synthesis of a Favipiravir derivative, 3-hydroxy-6-methoxypyrazine-2-carboxamide, using iron (III) as a catalyst. The compound was thoroughly characterized through various analytical techniques, including single-crystal X-ray diffraction, infrared (IR) spectroscopy, UV-visible spectroscopy, and $^{1}H/^{13}C$ NMR spectroscopy. The crystallographic analysis revealed that the enol form predominates in the solid state, while UV and NMR studies demonstrated a tautomeric equilibrium in solution. Furthermore, density functional theory (DFT) calculations were performed to evaluate the chemical parameters, electronic affinity, and molecular electrostatic potential of the compound. Investigations into Mulliken atomic charges and chemical reactivity descriptors were also conducted. Finally, docking simulations of the two tautomeric forms were performed against the SARS-CoV-2 main protease (PDB: 6LU7) and the spike receptor-binding domain (PDB: 7BZ5) to assess their binding affinity. The results exhibited strong binding affinities for key amino acid residues within the receptors, particularly with the enol form. These findings suggest that the synthesized derivative may hold potential as a therapeutic agent for COVID-19 and related diseases.

Keywords: Favipiravir derivative, COVID-19, single XRay, Lewis acid, Molecular docking

Therapeutic Potential of Silver Nanoparticles from *Helianthemum lippii* Extract for Mitigating Cadmium-Induced Hepatotoxicity and Nephrotoxicity in Wistar Rats

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This groundbreaking study delves into the remarkable therapeutic potential of silver nanoparticles (Ag NPs) synthesized from *Helianthemum lippii* extract to counteract cadmium-induced hepatotoxicity and nephrotoxicity in Wistar rats. Through meticulous characterization using X-ray diffraction, UV-Vis spectrometry, and energy-dispersive X-ray spectroscopy, we confirmed the successful synthesis of Ag NPs with a distinct cubic crystal structure and particle sizes ranging from 4.81 to 12.84 nm. Our sub-acute toxicity assessments at doses of 2 mg/kg and 10 mg/kg revealed no significant adverse effects compared to untreated controls. The experimental protocol involved exposing Wistar rats to 50 mg/kg $CdCl_2$ for 35 days, leading to significant liver and kidney damage, characterized by reduced body weight, elevated liver enzymes, impaired renal function, oxidative stress, and severe tissue alterations. Remarkably, the subsequent administration of Ag NPs (0.1 mg/kg/day) led to substantial recovery, ameliorating hepatic and renal dysfunction, restoring body weight, and significantly reducing oxidative stress. This study not only highlights the profound therapeutic efficacy of Ag NPs but also champions the eco-friendly synthesis of nanoparticles, aligning with sustainable practices in medical research and therapeutic development. The findings underscore a novel, green approach to mitigating heavy metal toxicity, offering promising avenues for future research and therapeutic applications.

Key words: Silver Nanoparticles, Green Synthesis, Cadmium Toxicity, Hepatoprotective, Nephroprotective, Oxidative Stress, Wistar Rats.

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THE REMOVAL OF A TEXTILE DYE FROM AQUEOUS SOLUTION USING NATURAL AND MODIFIED CHITOSAN

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The textile industry is widely recognized as one of the main sources of global pollution, generating discharges exceeding one hundred million cubic meters per year. Given the environmental issues posed by pollutants from the textile industry, the need to find adequate solutions quickly became evident.

In this context, the present work focused on the use of natural materials such as commercial and modified chitosan in the sorption of a textile dye (Acid Green 4G). Several physicochemical analyses were conducted to characterize our materials.

Batch adsorption revealed the influence of several parameters (contact time, initial concentration, temperature) on the sorption capacity. Different isotherm models were applied (Langmuir and Freundlich) to assess the capacity of the materials used for dye retention. The results obtained demonstrated the practical and economic relevance of using chitosan in the depollution of contaminated water.

Keywords: Depollution, sorption, chitosan, textile dye, Acid Green 4G.

Crystal structure and Hirshfeld surface analysis of (Z)-3-methyl-4-(thiophen-2-ylmethylidene)isoxazol-5(4H)-one

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Isoxazolones show some interesting biological properties. They are inhibitors of the factorization of tumor necrosis alpha (TNF-α) [1] and antimicrobial [2].They are used for the treatment of cerebrovascular disorders and as muscle relaxants. They are also herbicides and fungicides [3]. On the other hand, isoxazolone derivatives constitute excellent intermediates for the synthesis of various heterocycles such as pyridopyrimidines, quinolines and undergo various chemical transformations [4]. For these reasons, these compounds have been the subject of several investigations.

The present method for their synthesis is a three-component polycondensation between an aromatic aldehyde, ethyl acetoacetate and hydroxylamine hydrochloride under different conditions and for our part we propose here the use of a food additive, tolerated in organic agriculture, very inexpensive, highly available and a safe catalyst, in an aqueous medium. In the present study, we report on the synthesis, molecular and crystal structure together with a Hirshfeld surface analysis of (Z)-3-methyl-4-(thiophen-2-ylmethylidene)isoxazol-5(4H)-one.

Key words: crystal structure, π–π interactions, isoxazolone, hirshfeld surface.

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Valorization of black cumin cake as an eco-friendly inhibitor of corrosion on Stainless Steel 316L in 1M HCl through chromatography analysis, experimental and theoretical studies

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In this work, austenitic stainless steel (316L SS) in 1M HCl was treated with Black Cumin Cake Extract (BCCE), which was made using hydrochloric acid maceration during 24 hrs as a solvant. The inhibitory behavior was investigated using weight loss technique (WL), potentiodynamic polarization (PDP) and electrochemical impedance spectroscopy (EIS). UV-visible, FTIR, and gas chromatography mass spectrometry (GC-MS) were the methods used to characterize BCCE. The identification of the principal compounds included in BCCE was made possible using GC-MS. Inhibition effciency increases with increase in concentration of the inhibitor. In addition, computational calculations were carried out using the B3LYP functional and density functional theory (DFT), using adsorption locator modules on basis set 6-311G+ (d, p), Monte Carlo (MC) simulation was carried out to corroborate the experimental results; scanning electron microscopy, and spectrometric dispersive energy (SEM-EDX) with and without an inhibitor, the obtained micrographs of 316L SS confirm the existence of a protective film, the BCCE of an effective corrosion inhibitor. We can conclude that the BCCE has two benefits: it effectively inhibits corrosion for 316L in 1M HCl and, by recovering this waste, acts as a good environmental protection agent. The surface condition of 316L SS was investigated using profilometry, the maximum inhibitory efficacy is 87.54 % at 2.10^{-2} v/v BCCE by EIS technique; induction and charge transfer phenomena led to the latter's adsorption. BCCE exhibits inhibitory efficience behavior. The presence of the inhibitor film is confirmed by profilometry and SEM micrographs.

Keywords: Black Cumin Cake; Green inhibitor; HCl; 316L; EIS; DFT; Gas Chromatography-Mass Spectrometry.

Azo Dyes for Enhancing Optical Properties and Developing Multifunctional Liquid Crystal Materials

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Liquid crystals are unique materials that exhibit properties between those of conventional liquids and solid crystals. They possess a degree of molecular order that allows them to flow like a liquid while retaining some structural properties typical of solids. Liquid crystals have been extensively used in various applications such as optoelectronic devices, biomedical applications, sensors and biosensors, and packaging. In this study, we focused on the doping of liquid crystals with azo dyes. By incorporating azo dyes into liquid crystal systems, researchers can manipulate optical properties such as birefringence and absorption, leading to improved performance in various applications. Microscopic observation of nematic liquid crystals doped with azo dyes reveals intriguing interactions and enhancements in their properties. Azo dyes, especially those that can undergo photoisomerization, significantly affect the alignment and behavior of nematic liquid crystals under light exposure.

In addition, the ability of azo dyes to modify birefringence and absorption in liquid crystals opens new avenues for applications. Fluorescence spectroscopy has been used to visualize the localization of low-molecular-weight azo dye molecules at topological defects in the nematic liquid crystal matrix, highlighting how these defects can trap and interact with dye molecules, enhancing their optical properties.

Key words: liquid crystals, azo dyes, birefringence, absorbance, various applications.

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In vitro digestion of vegetable oils encapsulated with *Opuntia* (Cactaceae) polysaccharides

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Microencapsulation is an effective and economical method for protecting sensitive compounds [1]. In this work, vegetable oils were microencapsulated through coacervation technique using *Opuntia* (Cactaceae) polysaccharides and chitosan as core-shell materials. Polysaccharides were extracted from *Opuntia* cladodes using the combined conventional and ultrasound-assisted method [2]. The encapsulation efficiency (EE) was found to be around 97%. Morphological studies have shown successful oil entrapment within core shells with fine particle sizes. Thermogravimetric analysis has revealed improved core protection with high thermal stability. The in vitro digestion of the produced microcapsules was examined. The results indicated that the microcapsules remain intact under oral conditions, exhibiting a gradual release of oil during stomach digestion and a rapid release in the small intestine. Microcapsules could serve as efficient carriers for encapsulating sensitive components and functional oils.

Key words: *Opuntia*, polysaccharides, encapsulation, coacervation

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Understanding glycidylation reaction for the formation of pure mono, diglycidyl and dual monomers as glycidyl methacrylate of vanillyl alcohol

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The glycidylation reaction of vanillyl alcohol was studied taking into account the difference in reactivity between phenol and the aromatic methylol of vanillyl alcohol [1]. The analysis of reaction of epichlorohydrin on phenol and methylol alcohols allowed to demonstrate that the phase transfer catalysts (TBAC) activate phenol and not the methylol at room temperature, whereas Soda activates both phenol and methylol alcohols. Additionally, the elimination of the epichlorohydrin excess must be carried out before closing the chlorohydrin in the presence of NaOH to obtain pure mono glycidyl derivatives. Finally, the amount of reagents (epichlorohydrin and NaOH) has a minor role on the selectivity but not on the oligomerization. Thus, we obtained pure mono and diglycidyl monomers without purification by column chromatography. Hence, the present study demonstrated that mono-glycidyl, diglycidyl and dual monomers from vanillyl alcohol can be produced at industrial-scale following this routes, which is an important result allowing industrialization. This work on the optimization of the synthesis thus completes the work of Stanzione [2, 3] and ours, which had already demonstrated thermo-mechanical properties equivalent to those of the DGEBA. Thus by providing for the first time the demonstration of the absence of endocrine effect, we offer real substitutes for DGEBA and MAGLY.

Mots Clés: polymères biosourcés, époxy, glycidylation, éther glycidylique, vanilline, alcool vanillique

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Catalytic treatment of ONAS wastewater

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The objective of this work was to investigate the photocatalytic oxidation reaction in the presence of H_2O_2 using cobalt-based metal catalysts supported on TiO_2, SiO_2, and TiO_2/SiO_2 for the degradation of an azo dye, methyl orange. The sol-gel method was employed to synthesize aerogel supports, which were subsequently used to prepare various catalysts containing a fixed proportion of cobalt via dry impregnation. All supports and catalysts were calcined under an air flow at temperatures ranging from 450 °C to 550 °C.

The textural and structural properties of the solids were characterized by measuring the specific surface area using the BET method. Nitrogen adsorption-desorption analysis revealed similar isotherms with varying hysteresis loops, indicating differences in texture and pore distribution. X-ray diffraction (XRD) analysis showed the presence of the anatase phase in TiO_2-based supports and catalysts, while SiO_2-based supports exhibited an amorphous phase.

Catalytic tests demonstrated significant activity in methyl orange degradation for Co-TiO_2, Co-TiO_2/SiO_2, and TiO_2/SiO_2 supports, particularly with prolonged reaction times. This catalytic behavior appears to be related to the increase in average pore diameter and pore volume, enhancing cobalt-support interaction and optimal dispersion of the metallic phase on the support surface.

Additionally, the use of these catalysts, along with an industrial byproduct (coal fly ash), in the catalytic treatment of wastewater from the ONAS (National Sanitation Utility of Tunisia) showed variable effectiveness depending on the case. Future work will focus on further exploring the potential of fly ash, with the aim of optimizing its properties and pursuing a patent that would promote its use as a catalyst in wastewater treatment, encouraging industries to adopt this sustainable approach.

Key words: catalysts, photocatalytic oxidation, wastewater treatment, degradation of methyl orange

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HIRSHFELD SURFACE ANALYSIS, MOLECULAR CONFORMATION AND DOCKING INVESTIGATION OF 4,6-DICHLORO-2-METHYLPYRIMIDINE

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In order to understand the behavior of the methyl radical (CH3), a systematic study is carried out on benzene or cyclic products derived from highly symmetrical molecules substituted by methyl and halogen. In our overall work, we determined on the one hand the crystal structure of 4,6-dichloro-2-methylpyrimidine (DMP2) which is resolved from X-ray diffraction from a single crystal at room temperature.

Using the Crystal Explorer program, we analyzed the Hirshfeld surface, understand the crystal stacking and identified the intermolecular interactions that ensure cohesion in the crystal. In parallel with the experimental study, we undertook theoretical calculations of the conformation of the isolated molecule of DMP2 using the methods of DFT (Density Functionnal Theory) [1]. Optimization calculations of the molecular conformation of DMP2 using the program chain GAUSSIAN09 [2] and the functional MPW1PW91 and the base Lanl2DZ gave a C1 conformation with results very close to the experiment for lengths and for angles.

The Raman and infrared spectroscopy calculations undertaken from the optimization results using the same functional MPW1PW91 and the Lanl2DZ set of bases led to frequency values very close to the experimental results. The conformation closest to the experimental results undergoes an additional Docking study to study the therapeutic capacities of DMP2 against anti-oxidant activity and Alzheimer's disease.

Mots-clés : Diffraction, DFT, Surface de Hirshfled, Conformation, Spectroscopie, Docking.

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Fe^{3+}-NTA as iron source for solar photo-Fenton at neutral pH in raceway pond reactors

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This work presents, for the first time, a kinetic study of the solar photo-Fenton process at neutral pH mediated by the Fe^{3+}-NTA complex (molar ratio 1: 1) applied to remove contaminants of emerging concern (CECs). To this end, wastewater treatment plant (WWTP) secondary effluents were treated in a raceway pond reactor (RPR) at pilot plant scale with 0.1 mM Fe^{3+}-NTA and 0.88 mM H_2O_2 under average solar UVA irradiance of 35 W/m^2. Sulfamethoxazole and imidacloprid, at 50 μg/L of initial concentration each, were selected as model CECs. Up to 40% of the sum of both model CECs was removed from simulated WWTP effluent by the Fe^{3+}-NTA Fenton-like process, and >80% was removed by solar photo-Fenton. The effect of liquid depth in the reactor was evaluated, showing an increase of the treatment capacity from 12 mg CEC/m^2·h to 18 mg CEC/m^2·h when liquid depth increased from 5 to 15 cm. Afterwards, these results were validated with real WWTP effluents and compared with the results obtained with the Fe^{3+}-EDDS complex under the same operating conditions. The same CEC removal rates were obtained with Fe^{3+}-NTA and Fe^{3+}-EDDS at 5 cm of liquid depth (kinetic constants of 0.110 min^{-1} and 0.046 min^{-1} for sulfamethoxazole and imidacloprid, respectively). Conversely, at 15 cm of liquid depth, the degradation rates were lower with Fe^{3+}-NTA (kinetic constants of 0.034 min^{-1} for sulfamethoxazole and 0.017 min^{-1} for imidacloprid), whereas with Fe^{3+}-EDDS the values were 0.076 min^{-1} and 0.047 min^{-1} for sulfamethoxazole and imidacloprid, respectively.

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Structural, physicochemical characterization and antimicrobial activities of a *catena*-poly[[aqua(nitrato-κ^2O,O')(1,10-phénanthroline)cadmium(II)]-μ-nitrato-$\kappa^2O:O'$] [Cd $(NO_3)_2(C_{12}H_8N_2)(H_2O)]_n$

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Cadmium complexes with 1,10-phenanthroline ligands are a significant area of study in coordination chemistry due to their unique structural, photophysical, and biological properties. Cadmium-phenanthroline complexes have been explored for various applications, including as luminescent materials, catalysts, and in studies of DNA interactions due to their binding affinity to biomolecules. However, cadmium is a toxic heavy metal, so the biological and environmental implications of these complexes also raise interest in understanding their reactivity and impact. Their photoluminescent properties make them useful in sensor technologies, while their structural versatility is key in material science and supramolecular chemistry [1].

This compound crystallizes in the monoclinic $P2_1/c$ space group. Each Cd^{II} ion is surrounded by two N atoms from a 1,10-phenanthroline ligand, and five O atoms from a water molecule and three nitrate anions, with two in bridging mode and one in chelating mode, forming a seven-coordinate CdO5N2 environment. Each cadmium(II) center is bridged to two others by two nitrate anions to produce a zigzag chain structure along the [010] direction. O—H···O hydrogen bonding interactions link adjacent chains into a two-dimensional network parallel to (001).

The cadmium complex was characterized using various techniques, including IR spectroscopy and thermogravimetric analysis. It exhibited notable antifungal activity against Candida species, specifically **Candida albicans** and **Candida tropicalis**, with inhibition zones ranging from 42 to 45 mm at higher concentrations (50 mg/ml) and from 32 to 35 mm at 1/16 dilutions.

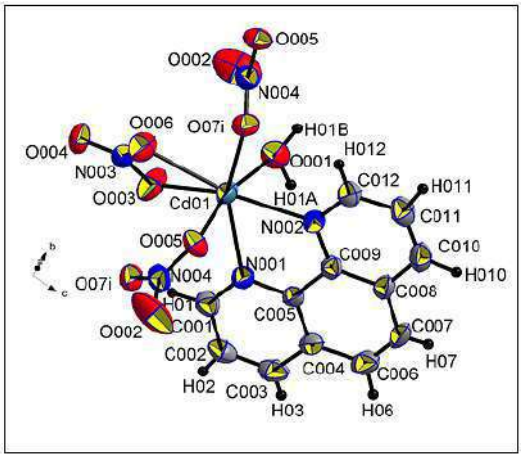

Figure 1: Asymmetric unit of $[Cd(NO_3)_2(C_{12}H_8N_2)(H_2O)]_n$

Key words: Cadmium complex, structural study, TG analysis, biological activity.

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The parietin, a key pigment in *Xanthoria parietina*: characterization and application in textile dyeing

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In a world where sustainability and ecology are given priority, the search for natural coloring agents is becoming increasingly attractive as a promising substitute for synthetic coloring agents, which are frequently linked to environmental and health issues. *Xanthoria parietina* stands out among these natural dyes for its ability to produce vivid, long-lasting colors. The objective is to evaluate the coloring properties of isolated parietin versus those of *X. parietina* extract to ascertain if parietin is the principal pigment.

The extract of *X. parietina* was obtained by extraction with boiling water and fermentation with ammonia (10%). These extracts were used to dye wool and canvas samples, with and without mordants. Dyeing properties were assessed by resistance to ammonia fermentation and boiling water. Analytical techniques such as high-performance liquid chromatography (HPLC-DAD) and mass spectrometry (LC-MS) were used to carry out chemical characterization of the dyes. Pure parietin was isolated for comparative dye tests on textile samples mordanted with alum.

The methanolic extract of *X. parietina* allowed us to identify several compounds. 16 compounds were identified, including parietin. HPLC-DAD data showed that the dominant compound in *X. parietina* is parietin. The *X. parietina* compounds formed a complex with the mordants and tissues. However, this makes it impossible to identify them. Samples dyed with separated parietin and *X. parietina* extract share identical colorimetric values, indicating that parietin is the primary lichen chemical responsible for the dyeing properties of this lichen. Parietin is therefore the molecule responsible for the coloring obtained by *X. parietina*.

This study establishes parietin as a promising alternative to synthetic dyes offering an eco-friendly solution for the textile industry while helping to preserve lichen biodiversity. These results pave the way for new applications of lichen metabolites in sustainable natural dyes.

Key words: LC-MS, natural dyes, parietin, textile dyeing, *Xanthoria parietina*

Straightforward hydroxymethylation of α-substituted β-keto esters with formaldehyde

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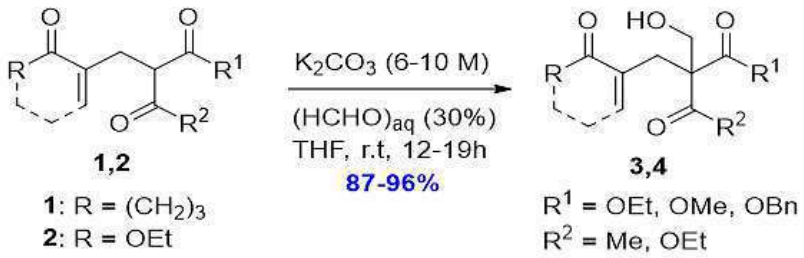
Hydroxymethylation using aqueous formaldehyde is one of the most efficient methods for the introduction of a C1 moiety [1] and although several reports of hydroxymethylation by this route are known, they typically make use of paraformaldehyde, stabilized formaldehyde or in situ generation from [2].

In general, the previous methods for the hydroxymethylation of 1,3-dicarbonyl compounds with formaldehyde needed catalysts or catalytic system such as $Fe(NO_3)_3.9H_2O$ and sodium dodecylbenzenesulfate [3], Pd(II), Pt(II)-(R)-BINAP complexes [4], dinuclear Ni_2-Schiff base complex [5] or iron-containing ionic liquid [6].

Herein, we describe a highly efficient hydroxymethylation of α-substituted β-dicarbonyl compounds [7,8] with formaldehyde using commercially available and inexpensive K_2CO_3 in THF at room temperature, affording the corresponding products in high yields (Scheme 1) [9].



Scheme 1. Hydroxymethylation of acetylated β-keto esters and β-diester compounds

Keywords : Hydroxymethylation; β-Dicarbonyl derivatives; Morita-Baylis-Hillman; Formaldehyde; Tetrasubstituted carbon

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An efficient (NHC) Copper (I)-catalyst for the synthesis of 1,2,3-trisubstituted triazoles

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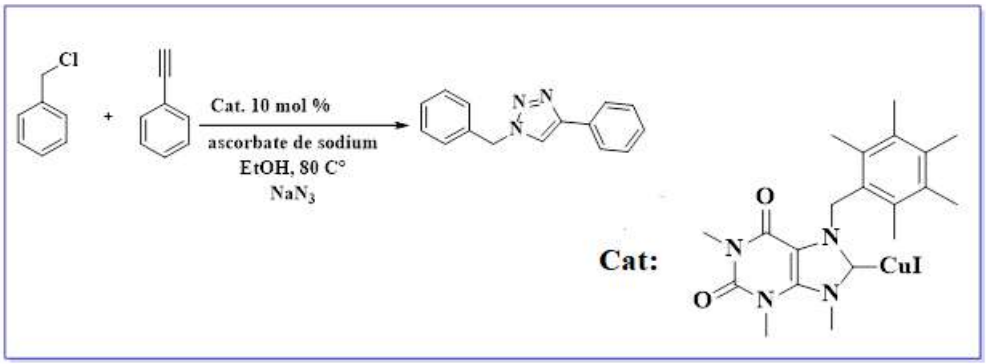
1,2,3-Triazoles are attractive molecules and widely used in organic synthesis, materials sciences, drug development, and bioconjugation chemistry [1]. Thus, the privileged 1,2,3 triazole motif has not only been extensively utilized by synthetic organic chemists, but also by chemists working in fields as diverse as bio-conjugation [2] and anion/cation recognition [3], The Cu(I)-catalyzed Huisgen 1,3-dipolar cycloaddition reaction between alkynes and azides (CuAAC) for constructing triazole cycles, which was independently reported by Sharpless et al. Recently, N-heterocyclic carbenes (NHC) is firmly occupied an important place in the ancillary ligand for homogeneous catalysis partially for substitution of the phosphine ligands. Herein, we investigate the catalytic activity of the synthesized complexes (NHC-Cu) for the Huisgen cycloaddition reaction of in situ generated azides and terminal alkynes to synthesize triazoles.



Key words: NHC, Huisgen cycloaddition, triazoles, Cu(I)-catalyzed.

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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

Molecular docking studies of dicoumarols and their corresponding epoxycoumarins

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Warfarin and dicoumarol [1,2] were just a few examples of biological and pharmacological products that contained coumarin derivatives. Dicoumarol has been thoroughly explored as a natural anticoagulant medication [3,4] due to its use in pharmaceutical study. series of 3,3-arylidene bis (4-hydroxycoumarins) 2 were synthesized by the reaction of aromatic aldehydes with 4-hydroxycoumarin using dodecylbenzenesulfonic acid as Brønsted acid-surfactant catalyst in aqueous media and under microwave irradiation. The present method is operationally simple and the use of water as the reaction medium makes the process environmentally benign. The epoxydicoumarins 5 were then obtained with a good yield by heating 3,3′-arylidenebis-4-hydroxycoumarins in acetic anhydride. Techniques such as elemental analysis, ^{1}H, ^{13}C NMR, and infrared spectroscopy were employed to characterize these compounds. The synthesized compounds displayed good antibacterial potential against different bacterial strains. Furthemore, a molecular docking simulation has been performed to evaluate the antibacterial activities and the probable binding modes of the studied compounds 2a-f and 5a-g toward the active sites of a series of well-known antibacterial targets.

Key words: dicoumarols, N-heterocyclic carbenes, biological activities, molecular docking.

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Mesoporous silica-based systems containing silver nanoparticles for trapping and immobilizing iodine from the gas phase

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Submicron-in-size silica particles with controllable morphology, particle size and mesoporosity, have been prepared under basic conditions making use of cationic alkyltrimethylammonium surfactants as porogens. Gaseous nitrogen adsorption, XRD and TEM experiments revealed quasi-spherical homodispersed objects possessing regular mesopores of the MCM-41 type; lengthening of the hydrophobic tail of the template resulted in smaller particles with greater intraparticle pores. The aggregation and sintering of individual silica particles during the calcination step led to the formation of particle clusters comprising interparticle voids, as evidenced by the ^{129}Xe NMR and TEM studies. The calcined particles were subsequently loaded with metallic silver. The measurements of iodine adsorption onto Ag-functionalized materials from the gas phase were supplemented by XRD, SEM/EDX, and TGA/DTA studies. It was demonstrated that the functionalized silica retained much gaseous iodine in an irreversible manner, mainly as an 'interfacial' AgI. The best compromise between the textural parameters and the post-synthesis functionalization was obtained for the large-pore silica templated with C_{18}TAB. Indications about the presence of silver metal nanoparticles, displaying certain heterogeneity in size and shape, within the pores of this sample were given based on the analysis of ^{129}Xe NMR spectra supplemented by UV-Visible absorption spectra and powder XRD patterns in the wide-angle region. The material can be recommended for the entrapment and immobilization of radioactive iodine in the nuclear industry since it guarantees that the adsorbed pollutant is primarily localized within the material pores and is thermally stable up to 800 K in air.

Key words: Mesoporous silica, gaseous iodine entrapment, Ag nanoparticles, ^{129}Xe NMR characterization.

The assessment of *in vitro* cytotoxic, anti-inflammatory, antimicrobial, antioxidant, and hemolytic effects of the species *Eryngium triquetrum* Vahl.

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Bioactive molecules had a growing interest in pharmaceutical industries owing to their protective roles against inflammatory, microbial, and oxidative stress-mediated pathological processes. For this reason, research on new molecules from natural sources constitutes an interesting topic for scientific research [1-2]. The present study aims to evaluate the biological effects of the methanolic extract prepared from the medicinal species *Eryngium triquetrum*. The quantification of the total bioactive contents was carried out using several colorimetric methods. The anti-inflammatory effect was tested using the denaturation of BSA method. In addition, the antioxidant activity was evaluated by six different assays including DPPH and hydroxyl radical scavenging effects, ferric-reducing antioxidant activity, copper-reducing antioxidant capacity, Total antioxidant capacity, and ferric iron chelation tests. The cytotoxicity was performed according to the brine shrimp lethality test and the hemolytic effect was evaluated using the erythrocyte model. Furthermore, the antimicrobial effect was assessed using disc agar diffusion assay against six microbial strains. According to the results, *E. triquetrum* extract is rich in several bioactive compounds with many pharmacological activities such as tannins, glycosides, flavonoids, and saponins. Moderate concentrations of polyphenols, flavonoids, and triterpenoids were estimated (29.94 ±0.12 ug eq GA/mg, 5.61± 0.41µg EQ/mg, 54.18± 2.71 µg EUA/mg respectively). The crude extract showed moderate antioxidant effects in all tested methods and a strong anti-inflammatory activity with a percentage of 89.82% at 5 mg/ml. However, a low hemolytic activity was detected (30% at 2.5 µg/mL). While a significant cytotoxic effect was estimated with LD50 at 5.49 µg/ml. However, moderate to low antimicrobial proprieties were found against *S. pneumoniae*, *Enterocoques* sp, *C. albicans* strains.
In conclusion, *E. triquetrum* could be an important source of bioactive compounds with potential therapeutic, pharmaceutical and nutritional applications.

Key words: *Eryngium triquetrum*, antioxidant, anti-inflammatory, and cytotoxic effects.

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The evaluation of pharmacological effects of the species *Suaeda monodiana*

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The efficient cutaneous wound healing process constitutes a critical challenge for clinical and fundamental research. Indeed, agents that prevent bacterial infections, the excessive production of free radicals, and inflammation may enhance wound healing. In this context, the biological activities of the methanolic extract prepared from the species *Suaeda monodiana* Maire were assessed. The antioxidant activity was tested by five different methods, and the sun protection factor was measured. The hemostatic activity was evaluated by determining plasma re-calcification time, and the anti-inflammatory effect was carried out by heat-inducing hemolysis and albumin denaturation tests. The antimicrobial activity was evaluated by the agar disk diffusion assay against seven strains. As a result, the tested extract has a rich chemical composition and possesses interesting photoprotective (SPF at 46.49±0.05) and antioxidant activities. This extract showed the ability to inhibit protein denaturation (IC50 at 1.22±0.8 mg/mL) and to protect the erythrocytes membrane (IC_{50} at 2.39±0.3 mg/mL). Moreover, the Methanol extract significantly shortens the clotting time and inhibits the growth of all the tested strains with minimum inhibitory concentrations ranging between 31.25 to 250 µg/mL. Furthermore, due to its pharmacological properties, *S. monodiana* species could be used in pharmaceutical formulations for the treatment of skin diseases

Key words: Anti-inflammatory, Antimicrobial, Hemostatic, Photoprotective, *S. monodian*

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Treated graphitic carbon nitride for enhanced photodegradation of caffeine under visible light

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In this study, bulk GCN (BGCN) was synthesized through the thermal treatment of a mixture of urea and melamine. Subsequently, to improve its crystallinity and photocatalytic performance, BGCN underwent further processing at 500 ºC, resulting in the material denoted as TGCN500. A comparative analysis was conducted with another sample obtained through an alternative treatment in ethylene glycol (EG) at 150 ºC, designated as BGCN/EG. EG was chosen due to its high boiling temperature and its active role as a solvent during semiconductor preparation, contributing to the enhancement of optical, structural, and catalytic properties of BGCN [1]. The materials were further characterized using XRD, FTIR, DRS, and N_2 adsorption at -196 ºC. Photocatalytic performance evaluation of the prepared materials was conducted under visible light, focusing on the degradation of caffeine as a microcontaminant model.

XRD data confirmed the successful synthesis of GCN, with TGCN500/EG exhibiting the highest BET area value (25 m^2/g) and the most promising optical response under visible light. Photocatalytic assays under visible radiation revealed the superior performance of the treated materials.

Key words: photocatalysis, caffeine, GCN,TGCN500

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An optimized comparative process for the adsorption of methyl green by biomass and its biochar

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This study aims to evaluate the efficiency of raw biomass from palm bark (RPB) and its derived biochar (PBC) for treating wastewater containing dyes through adsorption. Structural and morphological analyses of RPB and PBC were performed using Fourier-transform infrared spectroscopy and scanning electron microscopy. The adsorption performance of RPB and PBC for removing methyl green (MG) was further examined in batch mode. The CCD model generated optimal conditions for both materials, with a contact time of 80 and 39 minutes, an MG concentration of 137 and 150 mg/L, and a medium temperature of 306 K for biomass and biochar, respectively. Kinetic studies showed that the adsorption of MG was well described by the pseudo-second-order model. A thermodynamic study indicated that the adsorption process is exothermic and that adsorption is not spontaneous under standard conditions.

Key words: biochar, Biosorption, removal dye, optimization

Enhancing food preservation with bio-films: Incorporating polysaccharides from pepper wastes for sustainable packaging solutions

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The study investigated the development of bio-films incorporating polysaccharides derived from pepper waste to assess their potential for food preservation. By varying the concentrations of polysaccharides, the researchers examined their effects on the films' antimicrobial, physicochemical, mechanical, optical, and structural properties. Results showed that polysaccharide inclusion significantly enhanced the films' antioxidant capacity, particularly against the DPPH radical, suggesting the potential to extend food shelf life by reducing oxidative damage. The bio-films also exhibited strong antimicrobial activity, effectively inhibiting pathogens such as *Escherichia coli* and *Staphylococcus aureus*. Physicochemical analysis revealed a reduction in water vapor permeability, moisture content, and solubility, while the films became mechanically stronger with increased tensile strength, improving their durability as packaging. Optical changes included a slight darkening (reduced luminosity) and a shift toward yellow (increased b* value), which may impact packaging aesthetics. Scanning electron microscopy (SEM) showed a smooth and uniform polysaccharide distribution, and FTIR spectroscopy indicated interactions between film components, influencing their overall properties. X-ray diffraction (XRD) confirmed the films' structural stability despite the addition of polysaccharides. In conclusion, the study demonstrated that bio-films made from natural polysaccharides derived from chili waste could improve food packaging by enhancing food quality and safety, while also promoting the sustainable use of agricultural by-products.

Key words: Pepper wastes, bio-films based polysaccharides, antimicrobial properties, physico-chemical characterizations, sustainable packaging.

Physical properties and photocatalytic activities of $NaLi_{1.07}Co_{2.94}(MoO_4)_5$ nanoparticles

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In this work, we report the photocatalytic degradation of Acid Brown dye (AB) found in leather industry wastewater under sunlight and in presence of new prepared nanoparticles. The new photocatalyst has been synthesized by a solid state reaction method and from the mixture of Na_2CO_3, $LiNO_3$, $Co(NO_3)_2.6H_2O$ and $(NH_4)_6Mo_7O_{24}$. First, the reactants were dissolved in distilled water. Then the resulting mixture was dry evaporated at 80°C for 12 h. Then, the obtained residue was manually ground and heated at 400°C for 12 h. Thereafter, this powder is again reground and heated at 500°C. Finally, it was slowly cooled to room temperature. The synthesized photocatalyst was characterized using X-ray Powder Diffraction (XRPD), Raman, FTIR, Scanning Electron Microscopy (SEM), UV-vis-NIR spectrophotometry. The title compound was crystallized in the triclinic system, space group P-1. The structure can be described by the succession of different types of layers connected by sharing vertices and edges to lead a three-dimensional framework with tunnels in which the Na þ cations reside. Raman and IR studies confirm the existence of MoO_4^{2-} functional groups. The title compound is a wide-band-gap semiconductor with a value around 3.3 eV. SEM image and qualitative EDX analysis show that the nanoparticles (NPs) are distributed in a homogeneous way with large agglomeration and uniform porous structure. The EDAX spectrum revealed the presence only the elements: Na, Mo, Co and O with no impurities detected. The photocatalytic decomposition of Acid Brown organic dye load in tannery wastewater was studied. A maximum of 56% removal dyes was attained after 5 h. With the addition of hydrogen peroxide as an oxidant, the degradation efficiency increased to 90%. The photodegradation kinetics followed the pseudo first order with a constant rate k equal to 2.9 10^{-1} h^{-1} and 1.5 10^{-1}, respectively with and without adding H_2O_2. An important reduction in the chemical oxygen demand (COD) were observed. In fact, maximum removal of COD (80%) was observed with the addition of H_2O_2.This environment friendly and economical photocatalyst can be efficiently applied to the treatment of real leather industry wastewater with a notable reduced.

Keywords: synthesis; Leather wastewater treatment; Crystal structure; Acid Brown dye removal; Solar photocatalytic.

Synthesis and Electrochemical Characterization of a Novel Imidazolium-Based Salt for Catalytic and Energy Applications

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The unique ionic and tunable properties of imidazolium salts make them valuable candidates for applications in catalysis and energy storage systems. In this study, we report the synthesis of a novel imidazolium-based salt, designed to optimize stability and electrochemical activity. The synthesis process was optimized to achieve high yield and purity, confirmed through spectroscopic and analytical techniques. The electrochemical behavior of the compound was thoroughly characterized using cyclic voltammetry and electrochemical impedance spectroscopy to assess redox stability, conductivity, and electron transfer capabilities. Results indicate that the new imidazolium salt exhibits a stable redox profile with favorable conductivity, positioning it as a potential material for applications in catalytic systems and ionic conductors. Comparative analysis with related imidazolium salts highlights improvements in stability and electrochemical performance, underscoring the structural features responsible for enhanced activity. This research contributes valuable insights into the electrochemical properties of imidazolium salts, supporting their expanded use in sustainable and energy-efficient technologies.

Keywords: Imidazolium salt, Electrochemical characterization, Cyclic voltammetry, Redox stability, Ionic conductivity, Catalysis, Energy storage.

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Inhibition of steel corrosion in the middle of hydrochloric acid by aqueous extract for olive leaves

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The aim of this work is to study the inhibition of corrosion of C45 steel by a green water extract inhibitor of olive leaves in the acid medium of 1M HCl as a corrosion medium, where this study was conducted in the way of mass loss as well as analysis of the steel surface by electronic microscopy (MEB) and X-ray diffraction (XRD).

In the mass loss method, the effect of concentration, temperature and immersion time of steel on the corrosion rate and inhibition efficiency in the absence and presence of inhibitor, where our results reflect the inhibition efficiency increases by increasing the concentration up to 90.93766658% in 5 (g/l). And it increases with the temperature increase at 323 (k) to 97.14665702, and on the other hand, the inhibitory efficiency increases in the concentration of 5 (g/l). To register 97.94604587% in 24 hours and then decrease at the time of submersion 168 hours. Thermodynamic transaction values for adsorption of olive leaf extract inhibitor on the surface of the metal proved that this adsorption is a physical adsorption and follows the Langmuir isotherm. Results obtained through electronic microscopy (MEB) and X-ray diffusion (XRD) confirm a protective layer formed on the steel surface of the inhibitor's C45 in the middle of 1M HCl.

Key words: corrosion, carbon steel, green inhibitor, adsorption, water extract for olive leaves

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One-pot synthesis of 1,2,3-triazoles acetamide and vanillin derivative via nucleophilic substitution in α-position of cyclic Morita-Baylis-Hillman adducts and 1,3-dipolar cycloaddition and evaluation of their biological activities

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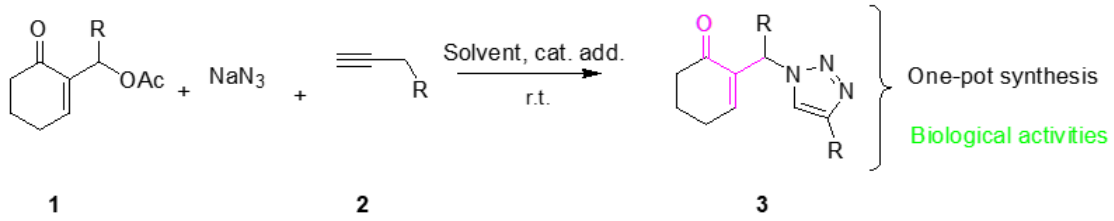
1,2,3-triazole-fused heterocycles are known to exhibit a wide range of biological activities such as antimicrobial activity against Gram positive bacteria[1], selective β_3 adrenergic receptor agonism[2], and antianxiety activity[3]. So, it is important to develop new and more efficient synthetic methods to a diverse array of 1,2,3-triazole pharmacophores.

Herein, an efficient method is described for the regioselective synthesis of α-substituted 1,2,3-triazoles acetamide and vanillin, in high yields from a variety of Morita-Baylis-Hillman acetates[4] and terminal alkynes with sodium azide using CuI as a catalyst, in DMF at room temperature. (**Scheme1**).



Scheme 1

The 1,2,3-triazoles **3** were afforded in good to excellent yields (51-91%) with exclusive α-regioselectivity and at room temperature. Furthermore, we described the different DPPH (2,2-diphenyl-1-picrylhydrazyl) scavenging activities of MBH triazole acetamide and vanillin **3** as well as their antibacterial activity.

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Antioxidant status of methanolic extract of Algerian steppic *Onopordum acanthium* L.

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Onopordum acanthium L. of the Asteraceae family, native of Europe and Asia. It has been used for many pharmacological properties. These properties are due its rich phytochemical composition. The aim of our work is to evaluate the antioxidant activity, total phenolic content, and total flavonoid content of the methanolic extract of this species in Djelfa district of the Algerian steppe. The quantification of total phenols and flavonoids was conducted utilizing the Folin-Ciocalteu reagent method and the aluminium chloride method, respectively. The evaluation of antioxidant activity was performed employing the 1,1-diphenyl-2-picrylhydrazyl (DPPH) assay. The total phenolic and flavonoid contents of the methanolic extract of *Onopordum acanthium* L. were quantified as 38.16±0.42 mg GAE/g (DW) and 19.62±0.12 mg QE/g (DW), respectively. The antioxidant efficacy of the methanolic extract of *O. acanthium* L., as determined by the DPPH assay, exhibited a concentration-dependent response, yielding an IC_{50} value of 62.84µg/ml, with a maximum percentage of 62% observed at 300 µg/ml, which was lower than that of ascorbic acid with 76% at 300 µg/ml. The findings indicate a significant antioxidant capacity for the methanolic extract obtained from the local *Onopordum acanthium* L.; however, this potential requires validation through other methods.

Key words: *Onopordum acanthium* L., methanolic extract, antioxidant, dpph.

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Synthesis, Biological Activity and Enantioseparation of Iminonaringenine

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In this work it was interested in the synthesis, biological activity and the chiral separation of enantiomers and diastereomers of Iminonaringenine. The various syntheses are performed based on condensation reactions of primary amines and diamines the structures of these compounds have been proved by spectroscopic methods IR, UV, NMR^{1}H and NMR^{13}C. These products have undergone varied biological activities, such as antibacterial activities, antioxidant and antifungal. As regards the antibacterial effect, we used five bacterial strains: Staphylococcus aureus, Bacillus subtilis, Listeria monocytogenes Escherichia coli, Pseudomonas aeroginosa. The results allowed us to say that the majority of the synthesized products have an inhibitory power all the tested micro-organisms. The antifungal tests against Fusarium oxysporum f.sp. albedinis were negative. The results of antioxidant activity the DPPH and β-carotene have been shown that these derivatives presented a very important activity on free radicals. The HPLC enantiomeric separation of fourteen Iminonaringenine was accomplished in the normal phase and organic polar mode, using six polysaccharides derived chiral stationary phases (Chiralcel OD-H, Chiralcel OD, Chiralcel OJ, Chiralpak AD, Chiralpak IA and Chiralpak IB) and various n-alkane/alcohol mobile phases. The enantioseparation of these new prepared shows that the chiral recognition mechanism of each stationary phase has been suggested, and based on the chemical nature and conformation of the chiral selector.

Key words: Iminonaringenine, HPLC, Biological activities, Enantioseparation, DPPH.

Yield optimization of essential oil from Tunisian *Lavandula* leaves

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Lavandula is a plant which belongs to the Lamiaceae family. In traditional medicine, the essential oils of this plant have been used as antioxidant, antimicrobial, anti-inflammatory, anti-depressive, and insecticidal agents. In this research work, we studied the optimization of the yield extraction of Tunisian *Lavandula* essential oil. For this reason, the leaves of this plant were collected from Gabes, Tunisia. Then, they were dried and used for the extraction of essential oil using hydrodistillation. For the optimization of the yield extraction, the effects of three different parameters including extraction time, heating power, and ratio plant/water on the yield were studied. Different extraction yields were obtained depending on the studied parameter. Our results demonstrated that extraction yield of *Lavandula* essential oil can be varied not only by the extraction time but also by other parameters like heating power and ratio plant/water.

Keywords: *Lavandula*, leaf part, essential oil, hydrodistillation, optimization.

Batch adsorption experiments of methylene blue using different sand-bentonite mixtures

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The purpose of this study was to advance the understanding of the adsorption of methylene blue on sand-bentonite mixtures in the context of their use in the lining of waste storage facilities. Discontinuous adsorption studies were carried out to study the adsorption of methylene blue, at different initial concentrations (5-200mg/L), on different sand-bentonite mixtures.

To do this, different sand-bentonite mixtures (0% to 8% bentonite) were tested to estimate their adsorption capacity for methylene blue and to study the adsorption kinetics of this dye. The results obtained showed that the 6% bentonite mixture adsorbs the greatest amount of methylene blue over the entire range of initial concentrations studied with an average adsorption percentage equal to 83%. Experimental data on the adsorption of methylene blue on sand/bentonite mixtures were examined using four kinetic models: pseudo-first order, pseudo-second order, Elovich model and intraparticle diffusion model. The results obtained showed that the adsorption kinetics of methylene blue on different sand/bentonite mixtures is well described by the pseudo-second order model. The intraparticle diffusion model has an important role, but it cannot be considered as the only limiting step during the adsorption process of methylene blue on the different sand-bentonite mixtures.

According to these results, it was found that sand-bentonite mixtures are promising adsorbents for the retention of methylene blue, resulting from industrial discharges. Therefore, they reduce the migration of this dye to groundwater.

Keywords: Adsorption, Methylene blue, Sand-bentonite mixtures

Effect of a globular protein on the dynamical behavior of long-chain polyanion in dilute regime

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The aim of this study is to determine the hydrodynamic radius of four characteristic pH values (pHφ1, pHc, pHφ2, pHopt) to determine the autocorrelation function. The analysis of these results provides us with information on the different states of complex formation of a strong polytectrolyte and a globular protein on the structure, dynamics and stability of the mixture variation in the amount of protein influences the shrinkage process of the NaPSS chain adsorption of the protein onto the NaPSS backbone by binding called patches is affected by the presence of repulsive electrostatic interactions of neighboring proteins.

Key words: DLS, polyelectrolyte, NaPSS, protein, ovalbumin, hydrodynamic radius.

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Zizyphus lotus cellulose for methyl orange elimination

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This study highlights the importance of alkaline delignification as a crucial pretreatment for extracting cellulose fiber from the trunk of *Zizyphus lotus*. The resulting cellulose is examined for its potential usage in methyl orange adsorption. The adsorption process is being investigated in batch mode, and numerous parameters such as pH, adsorbent dose, duration, initial concentration, and temperature were evaluated. There were 85-96% recoveries of the adsorbed methyl orange from the generated adsorbent after three sorption-desorption cycles. This demonstrated the remarkable effectiveness of cellulose derived from *Zizyphus lotus* for methyl orange adsorption, as well as its enormous capacity for organic dye removal from aqueous solutions.

Keywords: *Zizyphus lotus*, Cellulose, alkaline delignification, adsorption, Methyl orange

In vitro and In silico Approach for Evaluating the Antioxidant, Anti-Inflammatory and anti-hemolytic Potential of 5-Hydroxyferulic acid

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Text of the abstract: In our pursuit of novel drug candidates with antioxidant and anti-inflammatory properties, we focused on 5-hydroxyferulic acid (5-OHFA), a derivative of ferulic acid (FA) that has been demonstrated to confer health benefits. This study assesses the biological activity of 5-OHFA through the utilization of in vitro experimentation and in silico analyses. The antioxidant activity of the compound was evaluated using a series of in vitro assays, including the DPPH, ABTS, FRAP, and Fe(II)-chelating assays. 5-OHFA exhibited considerable radical scavenging activity, with IC50 values of [10,7 µM] for DPPH, [3,03 µM] for ABTS, [76,12 µM] for ferrous ion chelation, and [3,56 µM] for ferric reducing power. Furthermore, 5-OHFA demonstrated the ability to inhibit the denaturation of egg albumin and bovine serum albumin (BSA), which serve as models for inflammation. Furthermore, after incubation, it showed a slight toxic effect on erythrocytes with IC50 value of [29,53 µM]. In silico studies were conducted using the SwissADME and Protox III tools, which included molecular docking and ADME/toxicity predictions. The results of these analyses indicate that 5-OHFA exhibits favorable oral bioavailability, high gastrointestinal absorption, and low blood-brain barrier permeability, with no significant toxicity. The docking study demonstrated favorable binding interactions between 5-OHFA and various target proteins, including NADPH oxidase (PDB ID: 2CDU), xanthine oxidase (PDB ID: 1FIQ), and lipoxygenase (Furthermore, 15-LOX (PDB ID: 3V99), cyclooxygenase (COX-2, PDB ID: 3LN1) and Myeloperoxidase (MPO, PDB ID: 1DNU) demonstrated generally lower binding energies than FA, indicating stronger interactions. The collective findings from the in vitro and in silico investigations substantiate the potential of 5-OHFA as an antioxidant and anti-inflammatory agent, there by establishing it as a promising candidate for further investigation in the development of therapeutic agents.

Key words: 5-hydroxyferulic acid; phytochemicals; antioxidant activity; inflammation; hemolytic activity; antioxidant activity; molecular docking

Synthesis and structural characterization of β-phosphonated thiosemicarbazones: Investigation of their Z/E interconversion by NMR and DFT computing

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Thiosemicarbazone compounds[1] and their metal complexes exhibit noteworthy antiviral, antituberculous, antibacterial and antitumor properties[2]. Consequently, the synthesis of novel thiosemicarbazone ligands holds both theoretical and practical importance. In this context, phosphonated thiosemicarbazone ligands **2** were synthesized by combining β-phosphonated hydrazones **1** with isothiocyanate derivatives. All the synthesized products were characterized by multinuclear NMR, FT-IR spectroscopy and X-ray crystallography. To study the interconversion equilibrium of Z/E isomers, variable temperature experiments were realized. In order to determine the more stable isomer in solution a DFT calculations study were performed at B3LYP/6-311+G (d, p).

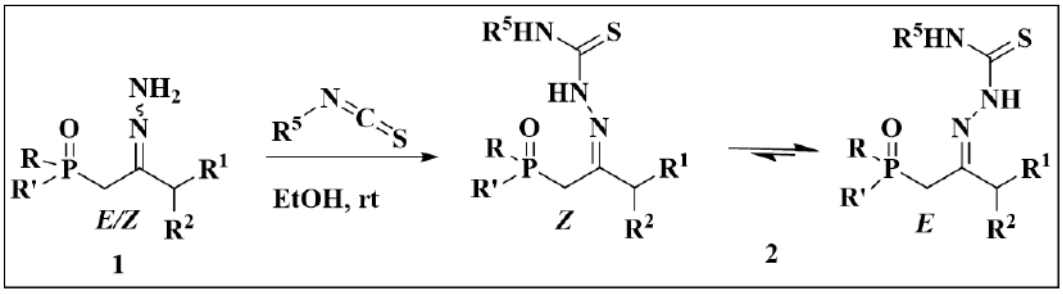

FIG. 1. Synthesis strategy of phosphonated thiosemicarbazones 2

Key words: β-phosphonated thiosemicarbazone, IRC, X-Ray Cristallography.

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Parametric and kinetic study of the methylene blue degradation by homogeneous photochemical processes

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This work studies the removal of methylene blue by the following advanced oxidation processes: UV, UV/H_2O_2, UV/$S_2O_8^{2-}$, Fenton and photo-Fenton. The UV/H_2O_2 system appears more reproducible than that of UV/$S_2O_8^{2-}$. The elimination was maximal after 60 min of reaction for a H_2O_2 concentration equal to 0.2 mol/L. The photooxidation of MB by the UV/H_2O_2 process was described by the pseudo first order kinetic. The appreciable difference between the treatment systems is due to the quantity of $HO^{\bullet}$ radicals formed by each process. The results obtained showed that the photo-Fenton process was the most efficient for the oxidation of MB.

Keywords: Methylene blue, oxidation, photo-Fenton, hydroxyl radical.

The TiO_2/Ti_3C_2 MXenes structure in Toxic Metal Removal using Combined Batch/Electrochemical Processes: ADOX and OAP

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This work addresses a significant research gap by presenting the latest advancements in MXenes materials, including adsorbents and photo-catalysts, for selective separations in water treatment, specifically targeting the removal of heavy metals. Some hypotheses have been made using the TiO_2-Ti_3C_2 as MXene and the Cr and Cu as the toxic metal. These pollutants pose a grave environmental concern as they adversely impact the quality of water bodies, thereby affecting various living organisms. The work demonstrates the superior separation capabilities of MXenes materials in eliminating such toxic compounds. Additionally, MXene-based composites have garnered considerable interest as photo-catalysts for contaminant degradation due to their exceptional thermal and optical properties, hydrophilicity, substantial surface area, customizable chemical characteristics, high chemical stability, regular planar configurations, high metallic conductivity, and numerous derivative products. Literature highlights numerous MXene-based materials exhibiting fascinating separation performance when compared to other available two-dimensional (2D) materials. The potential of MXene-based composites in toxic metals removal is noteworthy; however, several challenges need to be addressed to enable their practical applications in real water environments.

MB and CR selective adsorption onto amorphous perlite: CCD optimization and mechanisms

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Herein, the selectivity/simultaneously adsorption associated with Congo Red (CR) and Methylene Blue (MB) has been efficiently undertaken via amorphous perlite. Under optimum conditions of 38 min, 96 mg/L and 312°K for the contact time, the dye concentration, and the temperature, respectively, the optimization study using central composite design (CCD) matrix gave rise to high adsorption yields of 82.22 and 96.65 % for CR and MB, respectively. Importantly, kinetic and isotherm studies attested that the batch adsorption occurs as intra-diffusional mass transport onto porous material. The obtained thermodynamic parameters are indicative of an endothermic/spontaneous physisorption process. In addition, the FTIR analysis suggests that the adsorption process disrupted the short-range compounds order of perlite samples, revealing the marked crystallinity decrease of the adsorbent after adsorption. Finally, application of these optimum conditions tests on real industrial wastewater show that the adsorption was simultaneous at neutral pH and at 312°K, whereas CR and MB can be selectively adsorbed at pH 4 and 9, respectively.

Study on The Reactivty of Some Amino acids with Molybdenum

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The amino acids have a wide range of applications in biology and exhibit remarkable activity. Metal-coordinated complexes of ligands containing nitrogen and oxygen atoms, on the other hand, are more important than those free ligands.

In our research we have synthesized two complexes of amino acids-molybdenum using glycine and cysteine to investigate their antioxidant and antibacterial activities, which we then compared to the ligands.

In this work a direct reaction between amino-acids (glycine and cysteine) and Molybdenum were put together to synthesis two different complexes, the contained powders was characterized by examination of their elemental analysis and spectral studies (Infra-red, NMR, UV-Vis and thermal (TGA)).

The complexes have been tested with DPPH essays and antimicrobial by disk diffusion, in order to assess its antioxidant and antibacterial activities respectively the studies appear promising results.

Keywords: Amino acids, complex of Molybdenum.

Investigations on p-n heterojunction MoO_3/M-oxide nanocomposites for catalytic and energy storage applications

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Solvothermal technique is successfully led to develop the p-n heterojunction nanomaterials based on a MoO_3 oxide known as MoO_3/MO_x (M=Ti, Cu, Zn). The resulting nanoparticles were characterized by X-ray diffraction (XRD), FTIR spectroscopy, DRS spectroscopy, and Transmission Electron Microscopy (TEM). Results confirm the high purity of the prepared composites. The synthesized materials exhibit high degradation yields of methyl blue under UV irradiation, with a maximum of 99% in about a 120 min of time irradiation. This behavior can be explicated by the higher specific surface area of nanometric particles and their wide gap energies. The MB degradation rate decrease as a function of the added oxide nature.

With their wide gape energies, the MoO_3-based nanocomposites behave as semiconductors and exhibit high electrical conduction at moderate temperatures. Activation energy values vary between 0.39 and 1.12 eV in the [100-250 °C] temperature range.

The resulting properties suggest that prepared nanocomposites are suitable for catalytic and electrochemical applications.

Key words: Molybdates, Nanomaterials, Catalytic properties, energy storage

Transforming Waste to Wealth: Biolignin Production from Spent Coffee Grounds

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Text of the abstract: Coffee ranks as the second most traded commodity after petroleum. According to the International Coffee Organization (ICO, 2024), yearly coffee consumption was estimated to be ~ 9.98 million kg during 2020-2021 [1]. The production, processing, and consumption stages produce vast amounts of waste, creating challenges in managing coffee by-products. Spent coffee grounds, especially from instant coffee production and brewing, are garnering more interest due to their abundant availability (6 million tons per year) [2]. Over the past years, there has been growing interest in SCG due to its potential applications in various sectors. This study focuses on identifying and examining biolignin extracted from spent coffee grounds (SCG). Various techniques like Fourier-transform infrared spectroscopy (FTIR), elemental analysis, solid-state 13C cross-polarization magic angle spinning (13C CP/MAS) NMR, and thermogravimetric analysis (TGA/DTA) were performed to analyze the chemical structure and thermal stability of the isolated biomaterial. The surface morphology was observed using Field Emission Scanning Electron Microscopy (FESEM).

Key words: Spent coffee grounds, biolignin, biomass, extraction, chemical structure

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Synthesis of ZnO/AC Activity Composite and Photocatalytic Degradation of Methylene Blue under UV irradiation

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Advanced oxidation processes (AOPs) have become increasingly essential in recent decades due to their ability to degrade a wide range of organic and inorganic contaminants. Among these processes, heterogeneous photocatalysis stands out as a particularly promising method for the treatment of contaminated waters. Its effectiveness based on radical oxidation, triggered by the interaction with highly reactive free radicals generated in the environment.
This study presents the preparation and evaluation of the photocatalytic activity of a ZnO composite supported on derived activated carbon (ZnO/AC) for the degradation of methylene blue (MB) under UV irradiation. The ZnO/AC composite was synthesized using the sol-gel method and characterized with different analysis tehnics. Various physicochemical parameters were studied. The results demonstrated that the synthesized ZnO/AC composite exhibited excellent photocatalytic activity for the degradation of methylene blue under UV irradiation.

Keywords: Heterogeneous photocatalysis, ZnO/Activated carbon, Photocatalytic degradation, Persistant organic polluant.

Application de procédé photocatalytique à la dégradation d'un polluant pharmaceutique (Prednisone)

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La prednisone est largement utilisée comme produit pharmaceutique. Il a une action anti-inflammatoire, destiné principalement aux humains. Cette substance organique pénètre dans l'environnement par les eaux usées et les rejets pharmaceutiques, ce qui entraîne des problèmes menaçant les écosystèmes et la santé publique [1]. Le présent travail consiste à étudier la dégradation photocatalytique de la prednisone en utilisant l'oxyde de zinc comme précurseur. Pour optimiser les meilleures conditions de dégradation du la prednisone, nous avons procédé aux variations des paramètres : concentration en catalyseur ZnO (5000; 1000 et 2000mg/L) ; concentration initiale en prednisone (10 ; 15 et 20mg/L). La dégradation de ce polluant a été suivie par spectrophotométrie UV/Vis. La synthèse de photocatalyseur ZnO caractérisé par L'ATG, DRX, MEB, IR, la BET a permis l'obtention d'un rendement de dégradation de 60% au bout de 300 min d'irradiations UV 365nm [2].

Mots clés : Prednisone, ZnO, Photocatalyse et dégradation.

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Catalytic Properties of modified Hexaaluminate Catalysts by Nickel and Iron in OCM.

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Solid-state reaction synthesis methods based on calcination and grinding have been used to produce hexaaluminates. However, these techniques lead to low specific surface areas (≤1m2/g) due to high temperatures (>1400°C) and low catalytic activity. New methods have been developed to overcome this problem. Depending on the preparation method used, it is possible to obtain catalysts with different morphologies, phases of varying compositions, systems with greater or lesser metal-support interactions and consequently different catalytic activity and stability.

A series of Ni, Fe,-modified hexaaluminates $BaM_xAl_{12-x}O_{19-\alpha}$ (M=Fe, Ni; x=0.15) were prepared by the citrate method. Once the catalysts are obtained, they are subjected to calcination in air at different temperatures, in order to study the effect of temperature and dispersed metals. The solids are calcined at T=1000°C; 1200°C and investigated for OCM.

The oxidative coupling reaction of methane (OCM) is generally a heterogeneous catalytic process with the aim of obtaining ethane and ethylene by transforming methane into more valuable products from a chemical and energetic point of view.

The physico-chemical properties of the solids were investigated using XRD, BET, TPR, ATG/DSC, SEM and XPS.

Key words: OCM, Nickel, Fer, Hexaaluminates, High Surface Area.

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Phytochemical properties of *Arbutus unedo L.* fruits decoction extract and evaluation of its protective activity against acetic acid-induced ulcerative colitis in rat

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We aimed in the present research to evaluate the ameliorative effect of *Arbutus unedo* fruits decoction extract (AUFDE) against ulcerative colitis (UC) induced by acetic acid intoxication in rat as well as the mechanisms implicated in such protection. Adult male Wistar rats were separated into six groups: Control (H_2O), acetic acid (AA), AA + various doses of AUFDE (75, 150, and 300 mg/kg, b.w.,p.o.), and AA+ sulfasalazine (100 mg/kg, b.w.,p.o.) during 10 days. All rats were kept fasting overnight and ulcerative colitis was induced by rectal infusion of AA (300 mg kg^{-1}, b.w.) (3%, v/v, 5 mL kg^{-1}, b.w), for 30 s. The colon was excised and macroscopically examined to measure ulcerated surfaces and the ulcer index. The LC-MS analysis revealed the presence of 11 phenolic compounds with rutin being the main major component. Results of the *in vivo* assay showed that AUFDE pre-treatment significantly reduced acetic acid (AA)-induced colonic mucosa lesion sand attenuates histopathological alterations. Also, AUFDE limited the oxidative status induced by AA in the colonic mucosa, as assessed by MDA and H_2O_2 increased levels and the depletion of both enzymatic activities and non-enzymatic levels. Furthermore, AA intoxication increased iron and calcium levels in plasma, while AUFDE pretreatment regulated all intracellular mediators deregulation and significantly reduced inflammatory markers such as CRP and ALP levels. Our data suggest that the AUFDE exerted a potential protective effect against AA-induced colitis in rat.

Key words: Ulcerative colitis, Arbutus *unedo, Oxidative* stress, Inflammation, Rat.

Catalytic treatment of wastewater

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The objective of this work was to study the wet oxidation reaction catalyzed with metal catalysts based on iron supported on Zirconia oxide and bimetallic catalysts based on cobalt andiron deposited on ZrO2, in order to degrade one of the endocrine disruptors: Triclosan. In this study, we used the sol-gel route for the development of aerogel supports. These supports are subsequently used to prepare a series of catalysts based on iron alone or iron and cobalt with fixed percentages by dry impregnation. All these catalysts are reduced under a flow of hydrogen at 300°C. The study of the textural and structural properties of the solids was carried out by measuring the specific surface area by the BET method and by TPR. The N2 adsorption-desorption analysis of the different solids shows similar isotherms with the ZrO2 support, with varied hysteresis loops which reflects different textures and porous distributions. The TPR-H2 profiles show the non-reducibility of ZrO2. TPR analysis of the catalysts shows peaks characteristic of the reduction of iron and cobalt. The results of the catalytic tests show that the monometallic iron-based catalyst supported on ZrO2, the bimetallic catalyst impregnated simultaneously on theZrO2 support and the product X present significant catalytic activity in the degradation of Triclosan. This seems to be due to an increase in the average diameter of the pores and the pore volume which results in better iron-support interaction and therefore good dispersion of the metallic phase on the ZrO2 surface. The use of these catalysts and a product X for the catalytic treatment of ONAS wastewater showed their effectiveness to different degrees.

As perspectives: This study will be supplemented by other work on product X which should be further analyzed with a view to obtaining a patent which highlights it and encourages manufacturers to use it as a catalyst in the treatment Wastewater.

Synthesis and Characterization of a Zwitterionic Imidazolyl-Phenol Derivative: Catalytic Properties in the Oxidation of 3,5-Di-tert-butylcatechol

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In nature, catechol, also known as 1,2-dihydrobenzene, occurs naturally in small amounts in fruits and vegetables. It is additionally released into the environment during its production and use, primarily serving as an antiseptic, antifungal, and antioxidant in various industries such as chemical, rubber, photographic, pharmaceutical, and cosmetic.
From a toxicological perspective, catechol is considered a pollutant that can irritate the skin, eyes, and lungs. Prolonged exposure may lead to increased blood pressure and damage to kidney function and structure. It has been classified by the International Agency for Research on Cancer (IARC) as a Group 2B carcinogen, indicating it is possibly carcinogenic to humans.
This study focuses on the synthesis of 2-(1H-Imidazolin-2-yl)phenol and the characterization of its zwitterionic form, L_1, using spectroscopic methods and single-crystal X-ray diffraction. The research further investigates the catalytic properties of the in situ copper-imidazole complex (CuL_1) in the oxidation of 3,5-di-tert-butylcatechol (3,5-DTBC).
Imidazoles are highly significant chemically and have been extensively studied due to their role as complexing agents **[1,2].** Beyond their pharmaceutical**[3,4]** relevance and biological activities **[5]**, imidazole derivatives like imidazoline, featuring a phenyl hydroxyl group, have garnered interest for their various applications **[6,7]** and their ability to form stable zwitterionic tautomeric forms through proton transfer from the ortho-hydroxy group to nitrogen. These interactions between oppositely charged entities enhance their stability **[8]**.

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

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Design and investigation of a conical solar furnace powered by optical fibers

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A theoretical study of the heat transfer process that takes place in a special solar furnace is presented. Taking into account the possibility of transport of concentrated solar energy using optical fibres, we predict what may be expected in solar furnaces making use of such fibres.
The aims of this study are to optimize the coupling of a paraboloidal dish, which concentrates direct solar irradiance with dual axes tracking component, and the optical fibre, which transmits concentrated solar energy.
We present the daily power obtained at the output of the optical fibre, the power supply is estimated to be 20W at the end. Then we show that the energy transported is diffused until the enclosure then disperse inside it, the receiver absorbs this energy. Temperatures higher than 1600°K may be reached while maintaining very good efficiency. Such furnaces have the extra advantage of having temperature gradients, which may be perfectly determined.

Key words: concentrated solar energy, optical fibre, solar lighting, solar furnace.

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Development of a predictive model for the photovoltaic cells performance evaluation

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In this wok, we focus on photovoltaic solar energy as part of renewable energies. The latter is particularly interesting as it is infinite, the most abundant, fairly distributed, and mainly, for the fact that Algeria has about 3200 hours of sunshine per year, benefiting from a climatic situation favorable to the application of solar techniques. However, Cell efficiency and performance stability remains a primary concern. The main objective of this study is to investigate the impact of environmental conditions on the performance of photovoltaic cells of modules installed in the desert region in south of Algeria. The work developed in this thesis concerns the study of photovoltaic (PV) modules in real conditions of use (outdoors). Our work will be carried out by simulation on the software Origin and comparing its results to others obtained on excel, it embodies the prediction of maximum power of cells contained in the photovoltaic modal ISOFOTON 100. We will take into account several parameters such as lighting, temperature...The correlation between these variables and PV power is calculated then we will evaluate the output from the PV system based on known environmental input data. In this research, all available weather data are used to predict the PV power. Meteorological and power data are analyzed using a statistical approach to identify the order of significance of the input variables. TWO predictive models are suggested as a function of irradiance and number of cells shaded. Based on the system studied the modal predict that the value of the maximum power if the number of cells shaded was in fact zero is 70.459 W, if the number of cells shaded increases by one, the maximum power will decrease by -10.982W and that if the amount of solar radiation increases by 1W/m², the maximum power will increase by 0.0476.

Key words: Photovoltaic; Solar cells; Renewable energy; Regression; Correlation.

Etude phytochimique et évaluation des activités antioxydantes et anti hémolytiques des bourgeons de *Ficus carica, Olea europaea* et *Prunus avium* de la région de Tlemcen (Algérie)

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Le présent travail étudie les propriétés pharmacologiques des macérations de bourgeons de trois plantes : le figuier *(Ficus carica)*, l'olivier (*Olea europaea*) et le cerisier *(Prunus avium)*. Les bourgeons ont été macérés dans un mélange de solvants appropriés pour en extraire les principes actifs. L'objectif principal est de quantifier les composés bioactifs tels que les polyphénols totaux, les flavonoïdes et les tanins présents dans les macérats. Les méthodes analytiques employées incluent des dosages spécifiques pour chaque groupe de composés. En plus de la caractérisation phytochimique, des tests biologiques ont été effectués pour évaluer les propriétés antioxydantes et anti-hémolytiques des extraits. Les résultats obtenus montrent des différences significatives dans les teneurs en polyphénols totaux, flavonoïdes, et tanins entre les trois types de bourgeons étudiés. De plus, les résultats obtenus ont révélé que les extraits possèdent des activités antioxydantes et anti-hémolytiques notables, avec des variations en fonction de l'espèce végétale. En conclusion, ce travail démontre le potentiel thérapeutique des macérats de bourgeons de figuier, d'olivier et de cerisier, soutenant l'utilisation de la gemmothérapie comme approche naturelle dans la prévention et le traitement de diverses affections.

Mots-clés : Gemmothérapie - Bourgeons - Macération -polyphénols- Propriétés antioxydantes, hémolytiques._

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Etude phytochimique et évaluation des activités biologiques de l'extrait méthanolique de la racine *d'Echinops spinosissimus* subsp. bovei

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Echinops spinosissimus Turra subsp. bovei (Asteraceae) est une plante médicinale Algérienne dont les racines et les inflorescences sont utilisées traditionnellement, comme agents hypertensifs et dans le traitement des hémorroïdes. La présente étude porte sur la composition phytochimique, les propriétés antioxydantes, antimicrobiennes et cicatrisantes de l'extrait méthanolique de la racine *d'E. spinosissimus* subsp. bovei. La teneur en polyphénols totaux, en flavonoïdes et en tanins condensés a été également déterminée. En outre, le profil phénolique a été établi par HPLC/MS. Les résultats montrent que L'extrait méthanolique étudié est principalement composé d'apigénine, de kaempférol et de leurs dérivés. Il a montré une activité antioxydante vis-à-vis du radical DPPH, avec une IC50 de 7,99 ± 0,28mg/mL et une TAC de 30,30±0,54mg AAE/g DW, ainsi qu'un effet antibactérien, en particulier contre *P. aeruginosa*. Les pourcentages de contraction des plaies de l'essai in vivo ne témoignent pas d'une propriété significative de cicatrisation même si les observations histopathologiques confirment une meilleure qualité de cicatrisation. *E. spinosissimus* pourrait représenter une source de substances phytochimiques ayant des effets bénéfiques potentiels pour la santé humaine en tant qu'agents antioxydants et antibiotiques, cette espèce mérite également de faire l'objet d'autres études afin de mettre en evidence d'autres substances phytochimiques à diverses propriétés pharmacologiques.

Mots clés: *Echinops spinosissimus* Turra, polyphénols, HPLC/MS, activité antioxydante, antibactérienne, cicatrisante.

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Ab-initio studies of electronic, thermoelectric and superconducting properties of vanadium nitride material

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Transition metal nitrides (TMNs), such as vanadium and titanium nitrides, exhibit remarkable hardness, corrosion resistance, and thermal stability. These properties make them valuable in coatings, catalysis, and electronics. Additionally, their superconducting properties further enhance their technological significance **[1-2]**. In this paper ab initio method is used to report, the comprehensive investigation of the electronic structure of vanadium nitride (VN) based on first principal calculation. The band structure, density of states, and Fermi surfaces were obtained and discussed deeply. The V(d) states cross the Fermi level which confirm the metallic behavior of the system. The electron phonon coupling (EPC) strength and the spectral function are computed. The superconducting critical temperature was investigated using the McMillan Allen-Dens formalism. The results show strong agreement with experimental data, confirming that the superconductivity of VN nitride follows the conventional phonon-mediated mechanism. Additionally, thermoelectric computations reveal that the compound has good electrical conductivity

Key words: vanadium nitride (VN), Fermi surfaces, Density of states, superconductivity

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Etude par des méthodes théoriques des interactions du 1-fluoroethanol en phase liquide

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La chimie computationnelle a révolutionné le domaine de la chimie, en particulier la chimie organique, en fournissant une boîte à outils puissante pour simuler et comprendre les interactions complexes des molécules [1]. Elle permet aux expérimentateurs chimistes de visualiser les structures moléculaires, de prédire les résultats des réactions et d'explorer des domaines de la chimie difficiles ou impossibles à étudier expérimentalement [2]. Avec l'avènement de méthodes informatiques avancées, telles que la mécanique quantique et la dynamique moléculaire, les chimistes peuvent désormais étudier le comportement des molécules au niveau atomique avec une précision remarquable [3].

Ce qui rend la chimie computationnelle si importante est qu'elle étend et améliore le travail des expérimentateurs et elle permet d'économiser du temps et des ressources du laboratoire en permettant aux chercheurs de tester des hypothèses et d'évaluer les résultats expérimentaux [4].

Nous avons, dans ce travail, étudié les deux isomères optiques du 1-fluoroéthnol. Dans un premier temps nous avons procédé au choix de la méthode et de la base à utiliser, puis au calcul des énergies des interactions entre le 1-fluoroéthanol et le solvant en comparaison avec la phase gazeuse. Nous avons par ce travail pu déterminer une zone ou un domaine dans lequel nous pouvons procéder à une séparation entre ces deux isomères optiques.

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Exploration of in vivo toxicity and tolerance of bioactive glass 46S6 associated with chitosan after implantation applications in *Wistar* rats

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Bioactive glass particle used in the repair of bone defects. This material undergoes a series of surface in vivo reactions, which leads to osteointegration. In this study, we evaluated the effect of the bioactive glass synthesis, associated with 16% of chitosan on in vivo bioactivity with biochemical parameters, liver-kidney histological structure. These composites were testified and implanted in ovariectomized *wistar* rat. The serum and organs (liver and kidney) of all groups, control and treated rats, were collected to investigate the side effects of our composite, in comparison with control and ovariectomized rats. Also, the implants, before and after implantation, were prepared for analysis using physicochemical techniques such as Fourier transform infrared spectroscopy and X-ray diffraction. Our results have shown the stability of natremia, kaliemia, calcemia and phosphoremia. The histological structures of liver and kidney in implanted rats are intact compared to control and ovariectomized rats. The obtained biological studies have shown that the composite is biocompatible in vivo and it cause neither biochemical nor histological perturbation. The results highly recommend the implementation of the prepared composite in the evolution of biomaterials for bone tissue regeneration.

Keywords: In vivo, Biocompatibility, Bioactive Glass, Chitosan, Liver, Kidney

Adsorption de colorants alimentaires sur du charbon actif à base de noyaux de datte greffés

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Dans cette étude, il a été choisi d'éliminer d'une solution aqueuse, de colorants alimentaires reconnus toxiques à savoir l'azorubine et l'amarhante codés E122 et E123 successivement. Le procédé d'adsorption sur du charbon actif à base de noyaux de dattes (CND) brutes et greffées avec Al_3^+/Fe_3^+, a été choisi comme alternative de traitement en raison de sa rapidité, son efficacité et son faible cout. La capacité d'adsorption maximale est d'environ 6 mg/g pour E122 et 8 mg/g pour E123 correspondant à pH 2, 1g/L de matériau et 30 min de temps d'agitation ou d'équilibre adsorbant/adsorbat. D'autre part, l'influence du rapport massique ND_{Brute}/(Fe/Al) sur l'adsorption, a montré que globalement, 100 mg de Fe/Al suffisent à obtenir le maximum d'adsorption que ce soit pour le colorant E122 ou E 123.

Key words: Colorant, Anionique., Adsorption., Noyaux de dates

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PHENOMENES DE TRANSPORT ET DECONTAMINATION ELECTROCINETIQUE DE L'ALUMINIUM ET DES SULFATES D'UNE BOUE DE LAITERIE

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La décontamination électrocinétique des boues et des sols est une technique innovante et efficace qui permet l'extraction de métaux et/ou composés organiques toxiques des sols ou des boues pollués. Son intérêt vient du fait qu'elle utilise un faible courant électrique qui circule entre deux électrodes inattaquables. Différents phénomènes physiques peuvent être générés par ces systèmes électrodes/sol ou boue, on peut citer l'électro-osmose, l'électrophorèse, l'électromigration et les phénomènes chimiques liés aux réactions électrochimiques prés des électrodes, telle que l'électrolyse de l'eau. L'objectif de cette étude est orienté vers la justification des phénomènes régissant l'application de cette technique électrocinétique pour la décontamination de la boue de laiterie de son aluminium et de ses sulfates résultant de la clarification des eaux résiduaires par coagulation-floculation au sulfate d'aluminium. Si la boue est stockée sans traitement, ces constituants constitueraient alors une nuisance pour l'environnement. Les résultats de l'application de ce procédé sont satisfaisants; les décontaminations obtenues sont de l'ordre de 72 % pour l'aluminium et 90 % pour les sulfates. Les phénomènes d'électromigration et d'électro-osmose sont majoritaires pour le transport de ces éléments vers les électrodes correspondantes.

Key words: Phénomènes, électrocinétique, aluminium, sulfates boue laiterie.

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Synthesis and luminescent properties of Eu^{3+}-doped phosphate-sulfate fluorapatites $Ca10{-}xNax(PO4)6{-}x(SO4)xF_2$

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A series of phosphate-sulfate fluorapatites $Ca_{10-x}Na_x(PO_4)_{6-x}(SO_4)_xF_2$:$Eu^{3+}$(2%) (x = 0, 3, 6) has been synthesized by the solid-state reaction at high temperature. The samples were characterized by X-ray diffraction, Infrared spectroscopy and Raman scattering spectroscopy. Eu^{3+} luminescence properties were investigated at 77 K using site selective and time-resolved spectroscopy. Lifetimes and the color points were calculated. The emission spectra and luminescence decays of Eu^{3+} ions indicate that there is an energy transfer between different sites occupied by Eu^{3+}.

ELABORATION PAR VOIE SOLUTION ET CARACTERISATION DES MELANGES A BASE D'UN POLYMERE SYNTHETIQUE, D'UN BIOPOLYMERE ET DE NANOCHARGE. ETUDE DES PROPRIETES.

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Des mélanges binaires et ternaires à base de bentonite organiquement modifiée, originaires de Maghnia Algeria (OBT) [1, 2], poly (éthylène-co-acide acrylique) (PEAA) contenant 20% en moles d'acide acrylique et d'acétate de butyrate de cellulose (CAB) on été élaboré par la méthode d'intercalation en solution dans du tétrahydrofurane (THF) comme solvant. Ces mélanges binaires et ternaires ont été étudiés par diffraction des rayons X (DRX), microscopie électronique à balayage (MEB), spectroscopie FTIR/ATR, calorimétrie différentielle à balayage (DSC) et analyse thermogravimétrique (ATG).

L'analyse FTIR/ATR a révélé l'incorporation de la nanocharge au sein de la matrice polymère confirmée par l'apparition des bandes caractéristiques des nanocharges attribuées aux différents groupements de l'argile. L'effet de l'argile organique et de sa dispersion au sein de la matrice de mélange sur la morphologie et le comportement thermique des mélanges PEAA / CAB de différents rapports et de leurs mélanges d'hybrides ternaires correspondants est discuté. ATG a mis en évidence une diminution significative de la stabilité thermique

Mots-clés : Mélanges binaires et ternaires, poly (éthylène-co-acide acrylique), Acétate de butyrate de cellulose, Bentonite

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Study of the adsorption of an anionic dye on a mineral siderite

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The main objective of this work is the valorization of a natural material "siderite" collected from the Djebel Djerissa region for its use in the adsorption of Congo red dye in aqueous solution. Physicochemical analyses of natural siderite confirmed that this ore was characterized by an iron oxide content of 57 %, a specific surface area of 35.72 m^2/g and a porosity of 28 %. The results of the adsorption of CR on siderite showed that the adsorption percentage depends on the initial concentration of the dye, the contact time, the pH, the mass of the adsorbent and the temperature. An adsorbed quantity of CR equal to 37.72 mg/g was obtained after 90 min of reaction, at a pH = 3 and a temperature of 40 °C for an initial concentration of the dye equal to 50 mg/l. The thermodynamic study of the adsorption of this dye shows that the adsorption process is spontaneous, favorable and endothermic.

Keywords: Siderite, adsorption, Congo red, Thermodynamic study.

Convenient synthesis, antibacterial activity and in silico studies of novel 6-phenoxy-4,5-dihydro-1,2,6-oxazaphosphinine 6-oxides

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Herein we report a convenient three-step synthesis of a new class of oxazaphosphorines, namely 6-phenoxy-4,5-dihydro-1,2,6-oxazaphosphinine 6-oxides, through the microwave-assisted conjugative addition of diphenyl phosphite to α,β-unsaturated ketones, followed by oximation and intramolecular cyclization. The newly synthesized oxazaphosphorines were screened for their *in vitro* antibacterial activity against Gram-positive (*Staphylococcus aureus*) and Gram-negative (*Escherichia coli*, *Salmonella typhimurium* and *Pseudomonas aeruginosa*) bacteria. The obtained results were also correlated with the *in silico* molecular docking studies in DNA gyrase enzyme active site. Indeed, O,N,P-heterocycles also known as oxazaphosphorines, have attracted great interest due to their valuable pharmacological effects as anticancer [1], antibacterial [2], and anticholinesterase [3] agents.

Key words: O,N,P-heterocycles, 1,2,6-oxazaphosphinines, γ-ketophosphonates, γ-oximophosphonates, antibacterial activity, molecular docking.

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