Frontiers in Organic Synthesis and Polymer Science 2026

المؤتمر التاسع للكيمياء العضوية
والمؤتمر الخامس لعلوم وهندسة المواد البوليمرية

9TH ORGANIC CHEMISRY CONFERENCE
5TH SCIENCE AND ENGINEERING OF POLYMERIC MATERIALS

OCC SEPM

30 April-03 May 2026

Laico Hotel,
Yasmine Hammamet, Tunisia

Abstracts of Lectures and Communications
List of Participants

Foreword

We are pleased to welcome you to *Frontiers in Organic Synthesis & Polymer Science 2026*, organized by the Tunisian Chemical Society. This event brings together two established scientific meetings: - the 9th Organic Chemistry Conference (OCC) and the 5th Science and Engineering of Polymeric Materials (SEPM) - to foster rigorous scientific exchange and interdisciplinary collaboration.

The Organizing and Scientific Committees have prepared a rich program reflecting current advances and emerging directions in Organic Chemistry and Polymer Science. We are particularly grateful to the plenary speakers and invited researchers whose participation and expertise contribute significantly to the intellectual depth of the meeting.

The scientific program is structured to encourage active engagement through plenary lectures, oral presentations, and poster sessions. It provides a platform for the presentation of original research, critical discussion of recent developments, and the exploration of new perspectives across related disciplines.

With 12 plenary lectures, 54 oral communications, 100 posters presentations, and nearly 170 participants, the conference offers a substantial forum for discussion and discovery, with special attention to early-career researchers.

Beyond the scientific sessions, we are delighted to offer cultural activities, including a tour of Hammamet's landmarks, to enrich your experience and highlight Tunisia's heritage.

We trust this conference will provide a stimulating environment for scholarly interaction and collaboration, while your stay in Yasmine Hammamet will be both professionally rewarding and personally enjoyable. Finally, we warmly thank the conference chairs, whose commitment and availability have been essential in achieving our goals.

We also hope that your stay in Tunisia will be both professionally rewarding and personally enjoyable, enriched by the country's renowned hospitality and the setting of Yasmine Hammamet.

Sami LAKHDAR	**Ridha BEN SALEM**	**Younes MOUSSAOUI**	**Houcine AMMAR**	**Hatem MAJDOUB**
University of Toulouse, France *Co-chair of the OCC 2026*	University of Sfax *Co-chair of the OCC 2026*	University of Gafsa *Co-chair of the OCC 2026*	University of Sfax *Co-chair of the SEPM 2026*	University of Monastir *Co-chair of the SEPM 2026*

SCIENTIFIC COMMITTEE

Ridha BEN SALEM (Co-chair)
FSS - Sfax, University of Sfax, Tunisia

Semy LAKHDAR (Co-chair)
Univ. Paul Sabatier, Toulouse, France

Younes MOUSSAOUI (Co-chair)
FSG - Gafsa, University of Gafsa, Tunisia

Houcine AMMAR (Co-chair)
FSS - Sfax, University of Sfax, Tunisia

Hatem MAJDOUB (Co-chair)
FSM - Monastir, University of Monastir, Tunisia

Mohamed Lotfi EFRIT
FST - Tunis, University of Tunis El Manar, Tunisia

Amir HOVEYDA
Boston College, USA - University of Strasbourg, France

Krzysztof MATYJASZEWSKI
Carnegie Mellon University, Pittsburgh, USA

Mohamed Mehdi RAMMEH
FSM - Monastir, University of Monastir, Tunisia

Peter SCHREINER
University of Giessen, Germany

Cyrille BOYER
School of Chemical Engineering, Sydney, Australia

Jérôme Lacour
University of Geneva, Switzerland

Alessandro PEGORETTI
University of Trento, Italy

Laurence GRIMAUD
École Normale Supérieure, Paris, France

Sami BOUFI
University of Sfax, Tunisia

Anis TLILI
Claude Bernard University, Lyon, France

Frédéric GUITTARD
University of Nice, France

Christelle DELAITE
Université de Haute Alsace, Mulhouse, France

Stellios ARSENIYADIS
Queen Mary University, Londres, United Kingdom

Imen ABDELHEDI
FST - Tunis, University of Tunis El Manar, Tunisia

Thouraya BARHOUMI SLIMI
ISSTE - Borj Cédria, University of Carthage, Tunisia

ORGANIZING COMMITTEE

Latifa LATROUS
IPEIEM, University of Tunis El Manar, Tunisia

Adel MEGRICHE
FST - Tunis, University of Tunis El Manar, Tunisia

Béchir CHAOUACHI
ENIG, University of Gabès, Tunisia

Semy BEN CHAABENE
FST - Tunis, University of Tunis El Manar, Tunisia

Amine MNIF
FST - Tunis, University of Tunis El Manar, Tunisia

Mohamed Mehdi RAMMEH
FSM - Monastir, University of Monastir, Tunisia

Sami LAKHDAR
University of Toulouse, France

Imen ABDELHEDI
FST - Tunis, University of Tunis El Manar, Tunisia

Houcine AMMAR
FSS - Sfax, University of Sfax, Tunisia

Halim HAMMI
CNRSM - Borj Cédria, University of Carthage, Tunisia

Mohamed DAMMAK
FSS - Sfax, University of Sfax, Tunisia

Nizar BELLAKHAL
INSAT - Tunis, University of Carthage, Tunisia

Ridha BEN SALEM
FSS - Sfax, University of Sfax, Tunisia

Younes MOUSSAOUI
FSG - Gafsa, University of Gafsa, Tunisia

Rym ABIDI
FSB - Bizerte, University of Carthage, Tunisia

Hatem MAJDOUB
FSM - Monastir, University of Monastir, Tunisia

Mustapha HIDOURI
ISSAT - Gabès, University of Gabès, Tunisia

Mohamed Mouldi ABDELKAFI
FST - Tunis, University of Tunis El Manar, Tunisia

Imed LAAJIMI
Tunisian Chemical Society

Frontiers in Organic Synthesis & Polymer Science 2026

Program of the Conference

	Thursday 30 April 2026	
14.00 - 17.00	**Registration and check in**	
17.00 - 17.30	**Opening Ceremony**	
17.30 - 18.15		**Technical Talk** **Ali SAAD** **Chair:** Adel MEGRICHE *Publisher, Springer Nature* **Beyond Manuscripts: The AI Revolution in Scientific Publishing**
18.15 - 19.00		**Plenary Lecture 1** **Jérôme LACOUR** **Chair:** Stellios ARSENIYADIS *Department of Organic Chemistry, University of Geneva, Switzerland* **Stereoselective synthesis & catalysis with reactive metal carbenes**
19.00	***Dinner***	

	Friday 01 May 2026 (Morning)					
09.00 - 09.45		**Plenary Lecture 2** **Amir H. HOVEYDA** **Chair:** Sami LAKHDAR *Boston College, Chestnut Hill, Boston, United States* **Strategies in Deconstructive Synthesis**				
09.45 - 10.30		**Plenary Lecture 3** **Krzysztof MATYJASZEWSKI** **Chair:** Latifa LATROUS *Carnegie Mellon University, Pittsburgh, USA* **Advanced Materials with Precisely Controlled Macromolecular Architecture by Atom Transfer Radical Polymerization**				
10.30 - 10.45	**Technical Presentation** **Ghazy SHERIF** *Account Manager – Africa, KSA, UAE and Oman, ELSEVIER Life Sciences Solutions* **How Reaxys would support the ongoing chemistry research projects in Tunisia**					
10.45	**Group Photo Gathering**					
10.50- 11.45	**Poster Session 1 (P 1 - P 33) Alphabetical Order** | Evaluators: Amine GARCI & Semy BEN CHAABENE					
	Oral Communications - Session 1					
	Room A - Chair: Anis TLILI		**Room B - Chair**: Rafâa BESBES		**Room C - Chair**: Sami BOUFI	
	Com.	*Communicating | Topic A*	*Com.*	*Communicating | Topic C - E*	*Com.*	*Communicating | Topic F - J*
11.45- 12.00	**OC-01A**	ABDELLAOUI Mehdi	**OC-01B**	BEN HAJ MBAREK Asma	**OC-01C**	ABDELHEDI Imen
12.00 - 12.15	**OC-02A**	BEYAOUI Ahlem	**OC-02B**	JENDOUBI Ons	**OC-02C**	ALOULOU Hajer
12.15 - 12.30	**OC-03A**	DRIDI AMAL	**OC-03B**	LEJMI Maïssa	**OC-03C**	BHIRI Fatma
12.30 - 12.45	**OC-04A**	ALAMI Anouar	**OC-04B**	AMOR Amal	**OC-04C**	BEN HAMOUDA Sofiane
13.00	***Lunch***					

	Friday 01 May 2026 (Afternoon)					
14.00 - 14.45		**Plenary Lecture 4** **Frédéric GUITTARD** **Chair:** Alessandro PEGORETTI *University of Côte d'Azur, Nice, France* **Free Fluorine Surface Modification for Low Surface Energy Materials**				
14.45 - 15.30		**Plenary Lecture 5** **Anis TLILI** **Chair:** Ridha Ben SALEM *Claude Bernard University, Lyon, France* **Pentafluorosulfanylation Chemistry: New Frontiers and Beyond**				
	Oral Communications - Session 2					
	Room A - Chair: Noureddine ALLOUCHE		**Room B - Chair**: Anouar ALAMI		**Room C - Chair**: Abdelkader BOUGARECH	
	Com.	*Communicating | Topic A*	*Com.*	*Communicating | Topic B - C - D*	*Com.*	*Communicating | Topic F*
15.30- 15.45	**OC-05A**	ELMARY Pierre	**OC-05B**	SALHI Sourour	**OC-05C**	HLIMI Haythem
15.45 - 16.00	**OC-06A**	HAN Lulu	**OC-06B**	SAIDI Ilyes	**OC-06C**	MACHERKI Ameni
16.00- 16.15	**OC-07A**	HEDHLI Amel	**OC-07B**	YAKOUBI Chadia	**OC-07C**	RJILI Mohamed
16.15 - 16.30	**OC-08A**	YANG Yi	**OC-08B**	BEN NEJMA Sadok Lamine	**OC-08C**	SCHULLER Anne-Sophie
16.30 - 17.30	**Coffee break + Poster Session 2 (P 34 - P 66) Alphabetical Order** | Evaluators: Lassaad HEDHILI & Mustapha HIDOURI					
17.30 - 18.15		**Plenary Lecture 6** **Stellios ARSENIYADIS** **Chair:** Youness MOUSSAOUI *Queen Mary University, Londres, United Kingdom* **A journey into asymmetric allylic alkylation chemistry: From methodology development to natural product synthesis**				
18.15 - 19.00		**Plenary Lecture 7** **Christelle DELAITE** **Chair:** Frédéric GUITTARD *Université de Haute Alsace, Mulhouse, France* **Polymers for biomedicals applications**				
	Oral Communications - Session 3					
	***Room A* - Chair**: Hichem Ben SALAH		***Room B* - Chair**: Ali SAMARAT		***Room C* - Chair**: Slim SALHI	
	Com.	*Communicating | Topic A*	*Com.*	*Communicating | Topic D*	*Com.*	*Communicating | Topic F - G*
19.00- 19.15	**OC-09A**	JEBLI Nejib	**OC-09B**	HORCHANI Mabrouk	**OC-09C**	ZOUIDI Imen
19.15- 19.30	**OC-10A**	JMAI Momtez	**OC-10B**	TKA Najeh	**OC-10C**	GASMI Nesrine
19.30 - 19.45	**OC-11A**	KAOUACH Aicha	**OC-11B**	YAHYA Ahlem	**OC-11C**	GHAMMAGUI Fatma
19.45	***Dinner***					

	Saturday 02 May 2026 (Morning)					
09.00 - 09.45		**Plenary Lecture 8** **Peter R. SCHREINER** **Chair:** Jérôme LACOUR *Justus Liebig University, Giessen, Germany* **London Dispersion in Molecular Catalysis**				
09.45 - 10.30		**Plenary Lecture 9** **Sami BOUFI** **Chair:** Houcine AMMAR *University of Sfax, Faculty of Science, Sfax, Tunisia* **Biomass-Derived Nanomaterials: Processing, Functionalisation, and High-Value Applications**				
10.30 - 11.30	**Poster Session 3 (P 67 - P 98) Alphabetical Order |** Evaluators: Safa GAMOUDI & Halim HAMMI					
	Oral Communications - Session 4					
	Room A - Chair: Raoudha MEZGHANI JARRAYA		**Room B - Chair**: Aïcha ARFAOUI		**Room C - Chair**: Ane Sophie SCHULLER	
	Com.	*Communicating | Topic A - B - J*	*Com.*	*Communicating | Topic E*	*Com.*	*Communicating | Topic G - H - I*
11.30 - 11.45	**OC-12A**	KRISSAANE Nadia	**OC-12B**	BELTAIEF MEDDEB Imen	**OC-12C**	SELLAMI Dina
11.45 - 12.00	**OC-13A**	SAIDANI Dhia	**OC-13B**	BEN KHALIFA Maryem	**OC-13C**	ESSAFI Wafa
12.00 - 12.15	**OC-14A**	SLAMA Takwa	**OC-14B**	BOUHARB Narjess	**OC-14C**	MRABET Molka
12.15 - 12.30	**OC-15A**	TALBI Imen	**OC-15B**	ELNADI Hanan	**OC-15C**	BENBRAIEK Insaf
12.30 - 12.45	**OC-16A**	ELBIRGUI Kaouthar	**OC-16B**	HILELI Anwar	**OC-16C**	RAMANAVICIUS Arunas
13.00	***Lunch***					

	Saturday 02 May 2026 (Afternoon)
15.00	**Cultural Activities: Tour of Hammamet's Cultural Landmarks**
20.00	***Dinner***

	Sunday 03 May 2026 (Morning)			
09.00 - 09.45		**Plenary Lecture 10** **Pierre Henry DIXNEUF** **Chair:** Mohamed Lotfi EFRIT *University of Rennes, Rennes, France* **New Catalytic Reduction Processes for innovation in Heterocycle and Nitroarene Green Chemistry**		
09.45 - 10.30		**Plenary Lecture 11** **Alessandro PEGORETTI** **Chair:** Krzysztof MATYJASZEWSKI *University of Trento, Italy* **Functional interphases for structural composites**		
	Oral Communications - Session 5			
	Room A - Chair: Sami ZOUARI		**Room B - Chair**: Naceur HAMDI	
	Com.	*Communicating | Topic B*	*Com.*	*Communicating | Topic E*
10.30 - 10.45	**OC-17A**	BOUBAKRI Lamia	**OC-17B**	KHALDI Rania
10.45 - 11.00	**OC-18A**	HAMDI Rim	**OC-18B**	NGOM Ibrahima
11.00 - 11.15	**OC-19A**	MEZNI Dorsaf	**OC-19B**	ROMDHANE Ons
11.30	**Closing Ceremony** **Remarks and Best Posters Awards**			
13.00	***Lunch***			

TOPICS	ORGANIC CHEMISTRY		SCIENCE OF POLYMERS	
	A	**Innovations in Organic Synthesis** - New reagents, catalysts, strategies and concepts for organic synthesis - Stereoselective synthesis and asymmetric catalysis - Heterocyclic chemistry - Photoredox and organic electrochemistry	F	**Polymer Design & Engineering** - Polymer Synthesis & Macromolecular Engineering - Surface Modification & Interface Engineering of Polymers - Rheology, Physical Properties & Polymer Processing
	B	**Molecular Architectures: Metals & Beyond** - Organometallic chemistry - Supramolecular chemistry	G	**Sustainable & Advanced Materials** - Sustainable, Bio-based & Composite Polymer Materials - Self-Healing Polymers, Industrial Applications & Future Trends
	C	**Natural Products & Chemical Biology** - Total synthesis and biosynthesis of natural products - Bioorganic chemistry and chemical biology	H	**Nanostructured & Functional Polymers** - Polymer Colloids, Nanoparticles & Hybrid Nanomaterials - Hydrogels & Soft Nanocomposites - Advanced Membranes & Porous Polymer Materials
	D	**Medicinal Chemistry Horizons** - Drug discovery and medicinal chemistry	I	**Electronic & Smart Polymers** - Conductive, Thermoelectric & Electronic Polymers - Molecularly Imprinted Polymers (MIPs)
	E	**Green Chemistry & Smart Tools** - Sustainable chemistry - Physical and computational methods in organic chemistry	J	**Polymers for Life & Health** - Polymers for Life Science & Sensing Technologies

Speakers' Abstracts

Jérôme
LACOUR

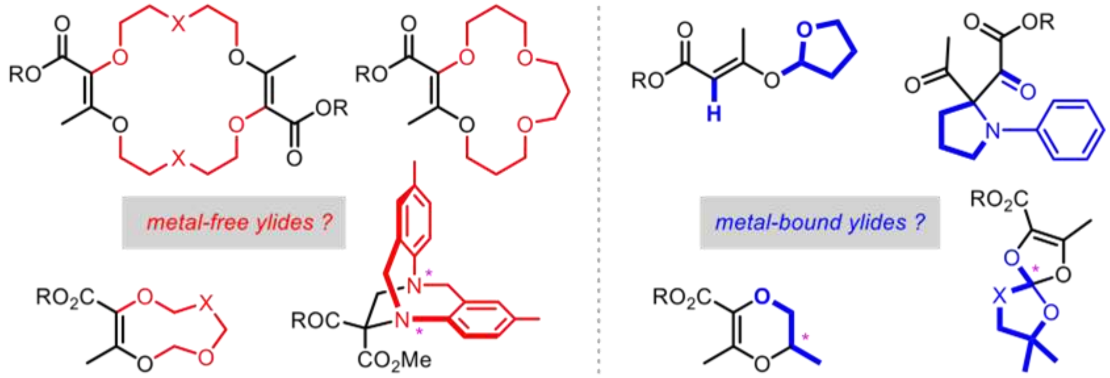
Jérôme Lacour was educated at the École Normale Supérieure (Ulm, Paris). He holds an Agrégation in Physical Sciences (major in Chemistry) and obtained in 1993 his Ph.D. in Chemistry at the University of Texas at Austin under the supervision of Prof. Philip D. Magnus. After post-doctoral studies in the laboratory of Prof. David A. Evans at Harvard University, he joined the Organic Chemistry Department of the University of Geneva in 1995. In 2001, he received the Sandoz Family Foundation professorship. Since 2004, he holds a full professor position in the department. Currently, his primary research interests are in asymmetric synthesis, catalysis and chiroptical spectroscopy using organic, physical organic, organometallic and coordination chemistry tools.

Stereoselective synthesis & catalysis with reactive metal carbenes

Jérôme Lacour

Department of Organic Chemistry, University of Geneva, Switzerland
E-mail: jerome.lacour@unige.ch

Recent progress on metal-catalyzed reactions will be presented - and those involving dirhodium,[1] CpRu [2], copper [3], iridium [4] and palladium [5] catalyzed decompositions of α-diazocarbonyls in particular. Attention will be given to routes affording ylide intermediates, metal-free or metal bound, and then functionally rich macrocyclic and heterocyclic derivatives. A large variety of stereoselective and enantiospecific transformations are available through these metal carbene reactions and subsequent ylide transformations.[1] Mechanistic investigations will be detailed during the lecture.



References

[1] a) K.-F. Zhang, N. Saleh, M. Swierczewski, A. Rosspeintner, F. Zinna, G. Pescitelli, C. Besnard, L. Guénée, T. Bürgi, J. Lacour, *Angew .Chem. Int. Ed.* **2023**, e202304075; b) A. Aster, F. Zinna, C. Rumble, J. Lacour, E. Vauthey, *J. Am. Chem. Soc.* **2021**, *143*, 2361-2371; c) A. Guarnieri-Ibáñez, A. de Aguirre, C. Besnard, A. I. Poblador-Bahamonde, J. Lacour, *Chem. Sci.* **2021**, *12*, 1479–1485; d) A. Homberg, J. Lacour, *Chem. Sci.* **2020**, *11*, 6362-6369; e) F. Zinna, S. Voci, L. Arrico, E. Brun, A. Homberg, L. Bouffier, T. Funaioli, J. Lacour, N. Sojic, L. Di Bari, *Angew. Chem. Int. Ed.* **2019**, *58*, 6952 –6956; f) A. Bosmani, A. Guarnieri-Ibáñez, S. Goudedranche, C. Besnard, J. Lacour, *Angew. Chem. Int. Ed.* **2018**, *57*, 7151-7155 .

[2] a) J. Viñas-Lóbez, N. Sellet, B. Fabri, G. Levitre, A. De Aguirre, A. I. Poblador-Bahamonde, C. Besnard, J. Lacour, *Org. Chem. Front.* **2026**, DOI: 10.1039/D1035QO01635E; b) O. Viudes, C. Besnard, A. F. Siegle, O. Trapp, T. Bürgi, G. Pescitelli, J. Lacour, *J. Am. Chem. Soc.* **2025**, *147*, 21121-21130; c) C. Montagnon, J. R. Bultel, C. Besnard, L. Guénée, J. Lacour, *Chem. Eur. J.* **2024**, e202401522; d) Y. Nikolova, B. Fabri, P. Moneva Lorente, A. GuarnieriIbáñez, A. de Aguirre, Y. Soda, G. Pescitelli, F. Zinna, C. Besnard, L. Guénée, D. Moreau, L. Di Bari, E. Bakker, A. I. Poblador-Bahamonde, J. Lacour, *Angew. Chem. Int. Ed.* **2022**, *61*, e202210798; e) J. Viñas-Lóbez, G. Levitre, A. De Aguirre, C. Besnard, A. I. Poblador-Bahamonde, J. Lacour, *ACS Org. Inorg. Au* **2021**, *1*, 11-17; f) T. Achard, L. Egger, C. Tortoreto, L. Guénée, J. Lacour, *Helv. Chim. Acta* **2020**, *103*, e2000190; g) T. Achard, C. Tortoreto, A. I. Poblador-Bahamonde, L. Guénée, T. Bürgi, J. Lacour, *Angew. Chem. Int. Ed.* **2014**, *53*, 6140–6144; h) C. Tortoreto, T. Achard, W. Zeghida, M. Austeri, L. Guénée, J. Lacour, *Angew. Chem. Int. Ed.* **2012**, *51*, 5847-5851 .

[3] a) C. Montagnon, R. Pertschi, C. Besnard, J. Lacour, *Adv. Synth. Catal.* **2024**, *366*, 1070-1077; b) S. Goudedranche, C. Besnard, L. Egger, J. Lacour, *Angew. Chem. Int. Ed.* **2016**, *55*, 13775-13779.

[4] Z. Zhong, C. Besnard, J. Lacour, *Org. Lett.* **2024**, *26*, 983-987.

[5] Z. Zhong, C. Besnard, J. Lacour, *Adv. Synth. Catal.* **2024**, *366*, 3029-3035.

Amir H. HOVEYDA

Amir H. Hoveyda is the Vanderslice Millennium Professor of Chemistry at Boston College, a position he has held since 1998. Since January 2019, he has also been the Director of Catalysis in Chemical Synthesis at the Institute for Supramolecular Science and Engineering at the University of Strasbourg. He was educated at Columbia University (B. A.), Yale University (Ph. D.; Schreiber) and Harvard University (postdoc; Evans). His honors include an NIH MERIT Award (2005), the Yamada-Koga Prize (2010), the American Chemical Society Award for Creative Work in Organic Synthesis (2014), the Eni Prize for Hydrocarbon Research (2014), and the American Chemical Society H. C. Brown Award for Creative Research in Synthetic Methods (2020). His research interests are in mechanism-based development of catalysts and methods for synthesis and deconstructive remodeling of complex bioactive molecules. Hoveyda is the co-founder of XiMo, AG.

Strategies in Deconstructive Synthesis

Amir H. Hoveyda

Boston College, Chestnut Hill, Boston, United States
Institute for Supramolecular Science and Engineering, University of Strasbourg, France

Skeletally remolded analogs of natural products enrich compound libraries, accelerating hit identification and drug discovery. In this Lecture, we will discuss streamlined, programmable and divergent deconstructive strategies for precise skeletal alteration of alkaloids and macrocycles. At the heart of these new strategies is a central diversification platform or hub, which can be systematically transformed to assorted expanded, contracted or distorted derivatives. The methods are practical, mild, efficient, and amenable to iteration; the requisite catalysts and reagents are inexpensive and readily accessible. The importance of the approach is highlighted by the results of in vitro screening studies against ten human cancer cell lines.

Krzysztof
MATYJASZEWSKI

Kris Matyjaszewski is J.C. Warner University Professor of Natural Sciences and director of the Center for Macromolecular Engineering at Carnegie Mellon University. In 1994, he discovered Cu-mediated atom transfer radical polymerization, which was commercialized in 2004 in the US, Japan, and Europe. He synthesized many advanced materials for biomedical, environmental, and energy-related applications. He has co-authored >1,380 peer-reviewed publications, (>216,000 citations, h-index 221) and 72 US patents. He is a member of the National Academy of Engineering, National Academy of Sciences, European, Australian, Polish, Hungarian, and Georgian Academies of Sciences. He received 2023 NAS Award in Chemical Sciences, 2021 Grand Prix de la Fondation de la Maison de la Chimie, France, 2017 Benjamin Franklin Medal in Chemistry, 2015 Dreyfus Prize in Chemical Sciences, 2011 Wolf Prize in Chemistry, 2009 Presidential Green Chemistry Challenge Award, 6 major Awards from the American Chemical Society, and fourteen doctorates honoris causa.

Advanced Materials with Precisely Controlled Macromolecular Architecture by Atom Transfer Radical Polymerization

Krzysztof Matyjaszewski

Carnegie Mellon University, Center for Macromolecular Engineering, Pittsburgh, PA, 15213, USA
matyjaszewski@cmu.edu

Various well-defined (co)polymers with precisely controlled macromolecular architecture were prepared under environmentally benign conditions, with ppm amounts of Cu-catalysts, in an aqueous environment, and in open-air with temporal control by light, electrical current, mechanical forces, or benign chemicals such as ascorbic acid. The dynamic exchange between active radicals and dormant species catalyzed by ppm amounts of copper catalyst in atom transfer radical polymerization (ATRP) enabled access to uniform star, comb, bottlebrush, or cyclic polymers with controlled chain composition, such as block, gradient, or periodic structures. Macromolecular engineering provided access to designed bioconjugates by covalently linking synthetic polymers with proteins or nucleic acids (DNA and RNA) and attaching polymers to inorganic surfaces such as nanoparticles or flat wafers. Such well-defined polymers and hybrid materials outperform conventional commercial products; they can self-assemble, self-repair, depolymerize back to monomers, and respond to external stimuli. They find applications in the areas of biomedicine, environment, and energy.

Frédéric
GUITTARD

Full Professor - *Bio-Inspired & Biobased Materials & Methods*

Dr. Frédéric Guittard received his PhD in Organic Chemistry in 1994 from University of Nice, (**France**), under Professor A. Cambon. He pursued postdoctoral research across Europe: at the University of Padova (**Italy**) with Professor Gambaretto on bisammoniums as biocide alternatives; at the University of Preston (**UK**) with Professor M. Holmes on lyotropic fluorinated surfactants; and at the Institute of Physics in Prague (**Czech Republic**) with Professor M. Glogarova on chiral liquid crystals. He later joined Theramex (**Monaco**), now Merck Inc. as head of industrial chemical development for hormonal substitutes.

In 1997, Dr. Guittard returned to the University of Nice as Associate Professor, becoming Full Professor in 2020 and Exceptional Class in 2014. In 2012, he transitioned from chemistry to physics, founding the “Surfaces & Interfaces” team on advanced materials. His research focuses on biomimetic and biobased approaches to active surfaces, structured around three axes: NanoTech, BioTech, and SmartTech. His group pioneered superhydrophobic and superoleophobic materials, ranking first in Europe and the USA, and second worldwide in 2017 for superoleophobic properties (*sources: web of science, scifinder*). He also develops hydrocarbon-based alternatives to fluorinated surfaces. In 2017, he established a new laboratory dedicated to Bioinspiration and Biobased Chemistry and Materials (www.unice.fr/nice-lab).

From 2004 to 2010, he directed the Chemistry Department at Nice University, creating apprenticeship-based Bachelor and Master programs (www.unice.fr/master-pro-mqm & www.unice.fr/bhpe) with 130 industrial partners. He has authored over 300 scientific articles, delivered 74 invited lectures, and is recognized internationally for his work on adhesion, anti-wetting, and surface properties.

Between 2010 and 2022, Dr. Guittard was visiting researcher at Bristol University (**UK**), the Institute of Physics (**Czech Republic**), Porto Alegre (**Brazil**), and the University of California, Riverside (**USA**). Since 2012, he has chaired the International Conference on Biobased and Biomimetic Materials & Chemistry (www.nice-conference.com), endorsed by MRS, EMRS, and IUPAC, and accredited in 2024 as a UNESCO Club.

He is also founder and director (2020–2024) of the CNRS national network “GDR-2088 Biomim,” uniting 98 laboratories and 700 researchers (www.gdr-biomim.com).

Contact: frederic.guittard@univ-cotedazur.fr - (+33)-06-6190-7404
Address: Univ. Cote d’Azur, Nice-lab, 9 rue J. Lauprêtre, 06200 Nice - France

Free Fluorine Surface Modification for Low Surface Energy Materials

Frédéric Guittard, Sonia Amigoni, Thierry Darmanin,

Université Côte d'Azur, N.I.C.E. Lab , 06200 Nice - France
frederic.guittard@univ-cotedazur.fr

Inspired by natural surfaces such as gecko feet and rose petals [1-2], controlling surface hydrophobicity and water adhesion is essential for applications like water-harvesting systems. Vertically aligned nanotubes are particularly appealing because of their high surface-area-to-volume ratio and adjustable porosity, which give rise to unique wetting behaviors [3]. Soft-template electropolymerization provides a simple and efficient approach for fabricating nanotubes with tunable characteristics. In aqueous media, hydrogen and oxygen bubbles generated during electropolymerization can create porosity within the material [4]. In organic solvents, we demonstrated that micelles form in the presence of water prior to electropolymerization, acting as soft templates that guide polymer growth [5]. The formation of nanotubular structures requires directing polymer growth along a single dimension (1D), which can be achieved using monomers capable of π-stacking interactions [6], provided that the polymerization rate remains sufficiently slow. Recently, we investigated triphenylamine-based molecules functionalized with thiophene or carbazole substituents at various positions. Their geometries and electronic structures were analyzed using DFT calculations at the B3LYP/6-31G(d) level. The optimized structures revealed non-planar conformations arising from steric interactions between conjugated units. Notably, carbazole substitution at the para position produced particularly promising results. We will also present a method for fabricating such surfaces without the use of templates. And finally, in aqueous media, the electrocrystallization of organic acids as in situ templates for pyrrole electropolymerization offers a promising route toward controlled surface structuring through the modulation of key electrochemical parameters.

Keywords: Bioinspired, Hydrophobicity, Water adhesion, Surface structures, Electrochemistry.

References

[1]. Darmanin, T.; Guittard, F. Superhydrophobic and superoleophobic properties in nature, Mater. Today, 2015, 18, 273–285.
[2].Guittard, F.; Amigoni, S.; Darmanin, T. Switchable and reversible wetting properties, Responsive Mat., 2026, 4:e70028.
[3]. Cheng, Z.; Gao, J.; Jiang, L. Tip geometry controls adhesive states of superhydrophobic surfaces, Langmuir, 2010, *26*, 8233–8238.
[4]. Fakhry, A.; Cachet, H.; Debiemme-Chouvy, C. Mechanism of formation of templateless electrogenerated polypyrrole nanostructures, Electrochim. Acta, 2015, 179, 297–303.
[5]. Fradin, C.; Orange, F.; Amigoni, S.; Szczepanski, C. R.; Guittard, F.; Darmanin, T. Micellar formation by soft template electropolymerization in organic solvents, J. Colloid Interface Sci., 2021, 590, 260–267.
[6]. Guittard F., Amigoni S., Darmanin T., Bioinspired and Biomimetic Wetting Properties, ACS Nano, 2025, 19, 36005-36026.

Anis TLILI

Anis Tlili is a CNRS Research Director. After studying chemistry at the Université de Bourgogne, he obtained a Master’s degree at the same university. He then completed his Ph.D. in late 2011 in the group of Dr. M. Taillefer (Montpellier, France). Subsequently, he joined the group of Prof. M. Beller (LIKAT, Rostock, Germany) for a postdoctoral stay, followed by a second collaborative postdoctoral position with the Cantat and Marinetti groups (CEA/ICSN, Paris). In 2014 he was appointed a CNRS Research Fellow in Lyon, and in 2024 he was promoted to Research Director. Since 2025 he has been the head of the Hydrazine and Polynitrogen Energetic Compounds Laboratory (LHCEP). His current research interests lie in the area of homogeneous and photoredox catalysis, with a particular focus on fluorine chemistry and the fundamental chemistry of N–N interactions. This includes the study of polynitrogen derivatives for space propulsion and applications in fine chemicals. In 2024 he was recently awarded the CNRS Bronze Medal.

Pentafluorosulfanylation Chemistry: New Frontiers and Beyond

Anis Tlili

CNRS research Director
Laboratoire LHCEP (UMR 5278), Université Claude Bernard Lyon 1
Mail : anis.tlili@univ-lyon1.fr

Despite the unique properties of the pentafluorosulfanyl (SF_5) group—such as high electronegativity, lipophilicity, and thermal stability—its broader application has been limited by the lack of practical, safe, and selective synthetic methods.[1] In this talk, we present two complementary strategies that address this long-standing challenge.

First, we demonstrate the direct activation of sulfur hexafluoride (SF_6), an inert and potent greenhouse gas, under metal-free and visible-light conditions. Using TDAE as a reductant, we achieved a two-electron reduction of SF_6 to generate a reactive SF_5-based fluorinating species. This reagent enabled key transformations, including deoxyfluorination of CO_2, desulfurization of CS_2, and the mild generation of $Cl–SF_5$ gas for chloro-pentafluorosulfanylation of unsaturated substrates.[2]

Second, we introduce the first family of air- and moisture-stable SF_5 reagents, including imine–SF_5,[3] which allows for selective formation of SF_5-containing four-membered rings via energy-transfer catalysis.[4] Together, these advances provide powerful new tools for incorporating the SF_5 motif under mild and scalable conditions, paving the way for broader use in synthetic, medicinal, and materials chemistry.

References

[1] *Chem. Rev.* **2025**, *125*, *17*, 8426–8476
[2] *Angew. Chem. Int. Ed.* **2022**, *61*, e202204623
[3] *Angew. Chem. Int. Ed.* **2025**, *64*, e202505146
[4] *J. Am. Chem. Soc.*, **2025**, *147*, 27905-27911.

Stellios
ARSENIYADIS

Queen Mary University of London, Department of Chemistry
Mile End Road, London E1 4NS, UK
s.arseniyadis@qmul.ac.uk

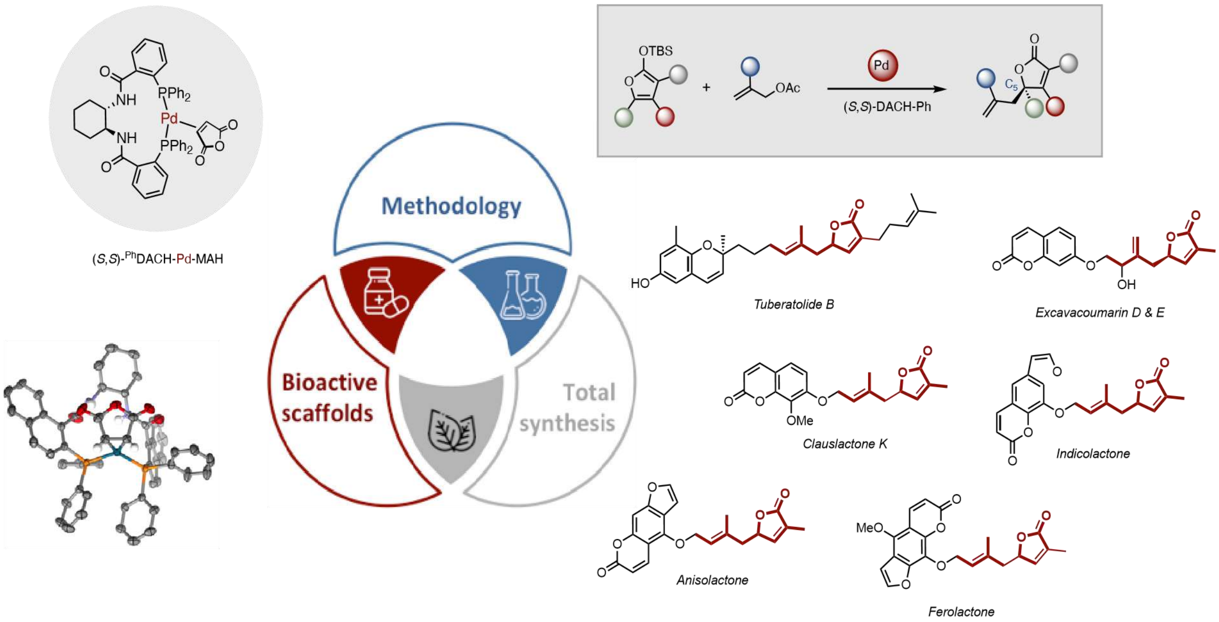
Stellios was born in Greece and raised in France. He received his PhD in 2002 from the University of Strasbourg under the guidance of Dr Charles Mioskowski. After various postdoctoral stints both in industry (at Rhodia Chirex in Boston in collaboration with Pr Stephen L. Buchwald, MIT) and in academia (with Pr Alan C. Spivey at Imperial College London and Pr. K. C. Nicolaou at The Scripps Research Institute), he started his academic career in France as a permanent CNRS Researcher in 2005 and was promoted to the rank of CNRS Director in 2015. The same year, he moved to the UK and joined Queen Mary University of London as a Reader in Organic Chemistry. His group is interested in the development of new synthetic tools with a special emphasis given to asymmetric catalysis and bio-hybrid catalysis with applications in natural product synthesis

A journey into asymmetric allylic alkylation chemistry: From methodology development to natural product synthesis

Stellios Arseniyadis

Queen Mary University of London, Mile End Road, E1 4NS, London, UK

For the past several years, the group has been interested in developing new synthetic tools with a special emphasis given to structural and functional diversity. These methods span within the areas of asymmetric transition metal catalysis, organocatalysis, photoredox catalysis and, more recently, bio-hybrid catalysis. In this context, we've been particularly interested in designing novel palladium-catalyzed asymmetric allylic alkylation reactions, ultimately applying them to the synthesis of natural products.[1] Notably, this has led to the development of bench stable, single component, chiral palladium pre-catalysts – developed in collaboration with the Leitch group (University of Victoria, Canada) and Servier (France) – which exhibit improved reactivity and selectivity across the field.[2] I'll present some of these results.



References

[1] For selected examples developed in the group, see: (a) P. Clark *et al. Chem. Commun*. **2025**, *61*, 19064-19067. (b) F. Richard *et al. Nat. Synth.* **2022**, *1*, 641-648. (c) T. Katsina *et al. Org. Lett*. **2019***, 21*, 9348-9352. (d) S. Aubert *et al*. *Org. Lett.* **2019**, *21*, 2231-2235. (d) T. Song *et al. Org. Lett*. **2019**, *21*, 603-607. (e) T. Song *et al. Chem. Eur. J.* **2018**, *24*, 8076-8080. (f) M. Nascimento de Oliveira *et al. Chem. Eur. J.* **2018**, *24*, 4810-4814. (g) M. Nascimento de Oliveira *et al. Org. Lett*. **2017**, *19*, 14-17. (h) S. Arseniyadis *et al. Synlett* **2013**, 2350-2364. (i) J. Fournier *et al. Angew. Chem. Int. Ed.* **2013**, *52*, 1257-1261. (j) J. Fournier *et al*. *Angew. Chem. Int. Ed.* **2012**, *51*, 7562-7566. For a recent review on the Pd-AAA of heterocyclic scaffolds, see: F. Richard *et al*. *Chem. Soc. Rev.* **2024**, *53*, 1936-1983.

[2] T. Keenan *et al. Nat. Commun.* ***2023****, 14, 8058.*

Christelle DELAITE

After graduating from the École Supérieure de Chimie Industrielle de Lyon and completing a PhD in polymerization catalysis, also in Lyon, Christelle Delaite was appointed professor in 2007 at the University of Haute-Alsace (Mulhouse). Specialising in macromolecular synthesis, Dr Delaite's research ranges from the synthesis of (co)polymers with complex architectures to the use of polymers in composites, functional coatings and in the biomedical field at the Laboratory of Photochemistry and Macromolecular Engineering, which she has headed since January 2023.

Polymers for biomedicals applications

Pr . Christelle Delaite

Laboratoire de Photochimie et d'Ingénierie Macromoléculaires
Université de Haute Alsace
3,b rue Alfred Werner
68093 Mulhouse cedex - France

This presentation will outline two approaches to the controlled and targeted administration of drugs.

The first approach involves the synthesis of amphiphilic graft copolymers comprising a hydrophobic poly(ε-caprolactone) backbone and hydrophilic poly(N-vinylpyrrolidone) or poly(N-vinylcaprolactam) grafts. The synthesis of these copolymers combines ring-opening cationic polymerization for the synthesis of the backbone and RAFT polymerization for the synthesis of the grafts, allowing for good control of molar masses. These copolymers are capable of micellisation in water and are therefore of interest for the delivery of drugs, particularly when the grafts have an LCST of around 37°C.

The second approach concerns the development of biocompatible magnetic nanocomposites comprising an iron oxide core and a poly(ethylene oxide) shell, developed for applications in cancer treatment via hyperthermia. We have decided to focus our attention on maghemite (ɤ-Fe_2O_3) and poly(ethylene glycol) in order to prepare materials combining the superparamagnetic properties of iron oxide (strong paramagnetic properties with very high susceptibility and no remanent magnetisation after the particles have been subjected to an external magnetic field), with the properties of the selected polymer, such as non-toxicity, bioresorbability and biocompatibility. To ensure strong adhesion between the macromolecules and the inorganic substrate, the polymer chains are covalently linked to the iron oxide nanoparticles.

Peter R. SCHREINER

Peter R. Schreiner is Liebig-Chair at Justus-Liebig-University Giessen, Germany. He was educated in Germany and the USA and became full professor in Giessen in 2002. Schreiner is a **member of Leopoldina – German National Academy of Sciences**, NRW-Academy of Sciences, Academy of Science (Mainz), and the Berlin-Brandenburg Academy of Sciences. He received the Dirac Medal (2003), the **Adolf-von-Baeyer-Award in 2017**, the RSC-Award in PhysOrgChem in 2019, the Academy Award of the Berlin-Brandenburg Academy in 2020, the **Arthur C. Cope Scholar Award 2021**, the **2024 Gottfried-Wilhelm-Leibniz Award** of the DFG, and the **2025 Schrödinger Medal**. His research interests include organocatalysis, reactive intermediates, quantum tunneling, and dispersion interactions.

London Dispersion in Molecular Catalysis[1]

Peter R. Schreiner

Institute of Organic Chemistry, Justus Liebig University, Heinrich-Buff-Ring 17,
35392 Giessen, Germany
e-mail: prs@uni-giessen.de; www.uni-giessen.de/schreiner

The *Gecko* can walk up a glass window because of the adhesion in hydrophobic setae on its toes that convey van der Waals (vdW) interactions with the surface. The attractive part of vdW-interactions is an electron correlation effect referred to as *London dispersion* (LD), which is directly related to polarizability. Only recently, LD has been appreciated in molecular chemistry as a key element of structural stability, chemical reactivity, and catalysis. Indeed, for increasingly larger struc-tures, the overall LD contribution grows rapidly and can amount to tens of kcal mol^{-1}. This presentation shows selected examples that emphasize the importance of inter- and intramolecular LD for molecules consisting mostly of first row atoms.[2] We note the synergy of experiment and theory that now has reached a stage where dispersion effects can be examined in fine detail. This forces us to re-consider our perception of steric hindrance and stereoelectronic effects, and even the transferability of chemical bond parame-ters from one molecule to another, both in structural chemistry[3] and, in particular, in reactivity[4] and catalysis.[4a, 5] We will also shed light on the possibilities to use machine learning approaches to improve catalytic reactions[6] and highlight the importance of optimizing for differences in activation free energies (vs. enantiomeric excess).[7]

This work was supported by the Deutsche Forschungsgemeinschaft and the European Research Council.

References

[1] a) J. P. Wagner, P. R. Schreiner, *Angew. Chem. Int. Ed.* **2015**, *54*, 12274-12296; b) L. Rummel, P. R. Schreiner, *Angew. Chem. Int. Ed* **2024**, *63*, e202316364; c) M. H. J. Domanski, M. Fuhrmann, P. R. Schreiner, *J. Am. Chem. Soc.* **2025**, *147*, 29611-29623.

[2] a) S. Rösel, C. Balestrieri, P. R. Schreiner, *Chem. Sci.* **2017**, *8*, 405-410; b) P. R. Schreiner, L. V. Chernish, P. A. Gunchenko, E. Y. Tikhonchuk, H. Hausmann, M. Serafin, S. Schlecht, J. E. P. Dahl, R. M. K. Carlson, A. A. Fokin, *Nature* **2011**, *477*, 308-311; c) S. Grimme, P. R. Schreiner, *Angew. Chem. Int. Ed.* **2011**, *50*, 12639-12642; d) A. A. Fokin, D. Gerbig, P. R. Schreiner, *J. Am. Chem. Soc.* **2011**, *133*, 20036-20039; e) S. Rösel, J. Becker, W. D. Allen, P. R. Schreiner, *J. Am. Chem. Soc.* **2018**, *140*, 14421-14432.

[3] a) J. M. Schümann, J. P. Wagner, A. K. Eckhardt, H. Quanz, P. R. Schreiner, *J. Am. Chem. Soc.* **2021**, *143*, 41-45; b) J. M. Schümann, L. Ochmann, J. Becker, A. Altun, I. Harden, G. Bistoni, P. R. Schreiner, *J. Am. Chem. Soc.* **2023**, *145*, 2093-2097.

[4] a) L. Rummel, M. H. J. Domanski, H. Hausmann, J. Becker, P. R. Schreiner, *Angew. Chem. Int. Ed.* **2022**, *61*, e202204393; b) M. H. J. Domanski, L. Rummel, S. N. Krug, H. Hausmann, E. Solel, P. R. Schreiner, *J. Org. Chem.* **2026**.

[5] C. Eschmann, L. Song, P. R. Schreiner, *Angew. Chem. Int. Ed.* **2021**, *60*, 4823–4832.

[6] O. Pereira, M. Ruth, D. Gerbig, R. C. Wende, P. R. Schreiner, *J. Am. Chem. Soc.* **2024**, *146*, 14576-14586.

[7] M. Ruth, T. Gensch, P. R. Schreiner, *Angew. Chem. Int. Ed.* **2024**, *63*, e202410308.

Sami BOUFI

Sami BOUFI, is a Professor at the Faculty of Sciences of Sfax, Tunisia. He obtained his PhD in Macromolecular Materials from the *Institut Polytechnique de Grenoble* and his Habilitation degree from the *University of Sfax* in 2001. His research focuses on the development and application of nanoscale particles derived from bio-based resources, including cellulose, starch, chitin, and lignin. His broader interests encompass polymers, composites and nanocomposites, as well as biomass valorisation. He is the author or co-author of more than 200 publications in peer-reviewed journals and book chapters, and serves on the editorial boards of several international scientific journals.

Biomass-Derived Nanomaterials: Processing, Functionalisation, and High-Value Applications

Sami BOUFI

Laboratoire LMSE (Sciences des Matériaux et Environnement)
Faculty of Science of Sfax-University of Sfax-Tunisia

This presentation highlights the main classes of nanoparticles derived from local biomass sources such as agricultural residues, starch, and crustacean shells. Focus is placed on nanocelluloses (NCs), chitin nanocrystals (ChNCs), starch nanocrystals (SNCs), and lignin-containing cellulose nanofibrils (LCNFs). Their production methods, morphology, and key properties will be briefly discussed, along with selected applications in advanced sustainable materials, including biodegradable plastics, nanocomposites, and smart systems.

The aim is to demonstrate that biomass, as an abundant and renewable resource, can serve as a versatile platform for producing a wide range of nanoparticles through simple, safe, and environmentally friendly processes. These materials offer significant advantages such as lack of toxicity, sustainability, cost-effectiveness, and ease of processing, making them promising candidates for sustainable and safe nanomaterials.

Pierre Henry DIXNEUF

Prof. Pierre H. Dixneuf
Emeritus Professor of Chemistry
University of Rennes, France

Research Focus

Founder of the Catalysis Group at Rennes (1985), Prof. Dixneuf has advanced organometallic and catalytic chemistry through:

- Selective alkyne transformations
- CO_2 incorporation into carbamates and carbonates
- Ruthenium-vinylidene and -allenylidene complexes in catalysis
- Enantioselective hydrogenation with chiral Ru catalysts
- Alkene metathesis for plant oil derivatives
- Catalytic C–H bond activation and functionalization (since 2007)

Recent work on soft hydrogenation catalysts and heterocycle/nitroarene transformations

Leadership Roles

- Deputy Director, CNRS Chemistry, Paris (1996–1999)
- Founder, Institut de Chimie de Rennes (2000)

Vice-President for Research, University of Rennes (2001–2004)

Publications

- Over **490 papers and reviews,** including 120 on green C–H bond modifications

Co-editor of **7 books**

Honors & Awards

Recipient of major **international prizes** from **Germany** (Humboldt, Wittig), **Italy** (Sacconi), **Spain** (Catalan), **Portugal** (Luso Prize), **China** (Chinese Chemical Society, 2014), **Taiwan**, **India** (Asima Chatterjee, B.D. Tylak), **Japan** (Yoshida), and **France** (Académie des Sciences IFP, Le Bel Prize).

Recognition

Foreign member of **four academies of sciences** in Europe and India.

New Catalytic Reduction Processes for innovation in Heterocycle and Nitroarene Green Chemistry

Pierre H. Dixneuf [1] and Min Zhang [2]

[1] *Institute of Chemical Sciences of Rennes, CNRS 6226, University of Rennes, Rennes, France*
[2] *South China University of Technology, Canton, China*
pierre.dixneuf@univ-rennes.fr ; minzhang@scut.edu.cn

The control of the reduction first step of substrates allows to trap the intermediates to create new reactions, avoiding full known reductions. The objective of the presentation is to show that new simple homogeneous and heterogeneous hydrogenation catalysts can interrupt their reduction of N-heteroarenes and of Nitroarenes to allow innovative combinations via green processes.

- Ruthenium(II) catalysts can be driven for partial reduction of N-Heteroarenes for diastereoselective Annulation of Azaarenes in methanol and formaldehydes[1].
- Iridium based catalyst allows partial hydrogenation with HCOOH of heterocycles leading to γ-AminoAcids in the presence of 1,2-Dicarbonyls.[2]
- Molecular Manganese catalysts in the presence of Fe(III) Lewis Acid allow the regioselective first step reduction of N-heterocycles into cyclic Imines to give access to Functional 2-Azabicyclo[2.1.1]Hexanes via Hydrodearomative [2π + 2σ] Cycloaddition of *Aza*-Arenes[3].

Simply made supported Cobalt catalysts allow selective first step hydrogenation, with HCO_2H, of abundant Nitroarenes, leading directly to 1,3-diaryl imidazolines, the NHC carbene precursors [4] By contrast, single atom Cobalt catalyst with HCO_2H allows the formation of hydroxylamine from Nitroarenes which can be trapped by aldehydes and alkynes to offer γ-lactams synthesis.[5] Supported Cobalt-DAPhen/C catalyst also allows the formation of hydroxylamine from nitroarenes but leading with formaldehyde and acrylates to functional g-amino acids.[6]

References

1. H Zhao, Y Wu, Z Tan, H Jiang, P. H. Dixneuf, Min Zhang, Nature Commun.2022,13,2393
2. H. Jia, Q. Liao, et al... P. H. Dixneuf, G. Vilé, and Min Zhang, J. Am. Chem. Soc. 2024, 146,31647.
3. Jian Yang, Bo-Xuan Yao, Huan-Feng Jiang, Shao-Fei Ni, Pierre H. Dixneuf, Min Zhang Angew. Chem. Int. Ed. 2025, e202505060
4. Jia-Lu Sun, C. Ci, H. Jiang, P. H. Dixneuf, Min Zhang, Angew. Chem. Int. Ed.2023, e202303007.
5. Jia-Lu Sun, H. Jiang, P. H. Dixneuf, Min Zhang, J. Am. Chem. Soc. 2024, 146, 11289.
6. H. Hua, C. Ci, P. H. Dixneuf, Min Zhang, J. Am. Chem. Soc. 2025, 147, 6572−6582

Alessandro PEGORETTI

Alessandro Pegoretti graduated in Materials Engineering at the University of Trento, Italy, in 1988. After a professional experience in industry, he has been Visiting Research Scientist at the Institute of Materials Science of the University of Connecticut (USA) between 1995 and 1997. From 1997 to 2001 he has been Aggregate Professor at the University of Modena (Italy) and then Associate Professor and Full Professor of Materials Science and Technology at the University of Trento (Italy) in 2002 and 2012, respectively. Since 2021 he is the Head of the Department of Industrial Engineering of the University of Trento.

From 2022 he is the Editor-in-Chief of Polymer Composites, the engineering and scientific journal of the Society of Plastics Engineers (SPE) serving the fields of reinforced plastics and polymer composites.

He has authored over 360 refereed publications, 2 books, 16 book chapters and 3 patents on various subjects in polymer and composites science and engineering. The main research interests are in the mechanics of polymer composites with a specific focus on the fiber-matrix interphase.

Functional interphases for structural composites

Alessandro Pegoretti

University of Trento, Italy

Safety of light engineering structures is of great importance since the structural integrity of a component may be compromised over time due to a variety of internal and external loads. The use of advanced materials, such as fiber-reinforced composites (FRCs), has become crucial in the manufacturing industry due to their superior properties. However, FRCs may suffer interfacial debonding, i.e. the nucleation and the propagation of cracks at the contact region between matrix and fibers. Robust interfacial adhesion and self-healing capability are crucial to reduce defects and extend the material service life. This seminar will present some of the most recent strategies investigated at the University of Trento to enhance the interfacial adhesion and concurrently add new functionalities such as strain monitoring or self-healing interfacial capabilities. These research areas involved the investigation of the interfacial region through the fabrication of single-fiber micro-composites in order to allow highly accurate estimations of the interfacial properties.

List of Oral Communications

Communicatings' Names	**Ref**
I. Abdelhedi, E. Drockenmuller, H. Ben Romdhane *TCS / FST - Tunis* Oligo(ethylene glycol)-based Poly(1,2,3-triazolium) Ionenes obtained by *N*-Alkylation step growth polymerization	**OC 01C**
M. Abdellaoui, A. Tlili *Claude Bernard University, Lyon 1, France* First example of nitrogen-nitrogen bond formation through photocatalytic iminyl radical generation under visible light irradiation	**OC 01A**
A. Alami *Sidi Mohamed Ben Abdellah University, Fès, Morocco* Synthesis and characterization of new mono- and bi-heterocyclic α-aminophosphonate models via copper(I)-catalyzed "Click Chemistry" dipolar cycloaddition	**OC 04A**
H. Aloulou, R. Ben Amar *IPEIG - Gabès* Preparation and characterization of a novel polysulfone (PSF) ultrafiltration membrane modified with zinc oxide-graphene oxide (ZnO-GO) nanocomposites to improve permeability and antifouling properties	**OC 02C**
A. Amor, S. Bessalah, S. Jbahi, M. Hidouri *FSG - Gabès* Gelatin / Chitosan composite for wound healing applications	**OC 04B**
I. Beltaief Meddeb, Y. Arfaoui *IPEIN - Nabeul* DFT study of the Boulton-Katritzky base-catalysed rearrangement of some Z-arylhydrazones of 3-benzoyl-5-phenylisoxazoles into 2-aryl-4-acyl-2H-1,2,3-triazoles	**OC 12B**
A. Ben Haj Mbarek, M. Itaimi Dammak, C. Milanese, A. Laouani, D. Le Cerf, H. Majdoub, A. Papetti, H. Ben Jannet *FSM - Monastir* Selective NADES-mediated microwave extraction of Boswellia sacra polysaccharides: Balancing process yield with structural integrity	**OC 01B**
S. Ben Hamouda, N. Chaarana, A. Figoli *CRMN - Sousse* PEBAX membranes for water desalination by pervaporation process	**OC 04C**
M. Ben Khalifa, C. Hassouna, A.R. Allouche, M.H. V Baouab, R. Ben Chaabane, R. Mlika *FSM - Monastir* A computational study of glucose, galactose, and fructose interactions with an Fe(II) macrocyclic Schiff base complex	**OC 13B**
S.L. Ben Nejma, M. Othman, H. Ben Jannet, M. Znati *FSM - Monastir* Synthesis and in silico evaluation of Coladonin derivatives as potential carbonic anhydrase IX inhibitors	**OC 08B**
I. Benbraiek, V. Pifferi, S. Yatouji, L. Falciola, H. Barhoumi, N. Jaba *FSM - Monastir* Selective electrochemical detection of hexacosanoic acid (C26:0) in buffered medium using a MIP-modified SPCE	**OC 15C**
A. Beyaoui, I. Saidi, A. Romdhane, H. Ben Jannet *FSM - Monastir* Synthesis of new 1,2,4-oxadiazole derivatives of flavonol and in silico evaluation of their biological properties	**OC 02A**
F. Bhiri, M. Chemli, N. Sakly, M. Majdoub *FSM - Monastir* Carbon nanoparticle-carbazole polymer nanocomposites for resistive detection of volatile organic compounds	**OC 03C**

Communicatings' Names	**Ref**
L. Boubakri, I. Özdemir, H. Kelm, N. Hamdi *ISSTE - Borj Cédria* Cationic Tris-benzimidazole-silver(I) complexes: Synthesis, characterization, anticancer, and antimicrobial evaluation	**OC 17A**
N. Bouharb, L. Hedhili, M.H. Baouab *IPEIM - Monastir* Selective organic transformations of unsaturated fatty acids in olive pomace oils via heterogeneous catalysis	**OC 14B**
A. Dridi, M. Mastouri, R. Haudecoeur, S. Py, R. Besbes *FST - Tunis* Synthesis of novel 1,3,2-oxazaphospholidine-2-oxides via ring expansion of 2-hydroxymethylaziridines and evaluation as acetylcholinesterase inhibitors	**OC 03A**
K. Elbirgui, K. Benali, H. Charii, C. Merbouh, N. Iounes, S. Ibenmoussa *Hassan II University, Casablanca, Morocco* Differential acute toxicity of copper, lead, cadmium, and zinc to Artemia salina Nauplii and its modulation by natural biopolymers	**OC 16A**
P. Elmary, M. Abdellaoui, A. Tlili *Claude Bernard University, Lyon 1, France* Metal free photoinduced N-N radical coupling leading to difunctionalized triazones	**OC 05A**
H. Elnadi, M.O. Zouaghi, Y. Arfaoui *FST - Tunis* Turning NO_2 into high-value chemicals with CaO catalysts: A DFT study towards oxadiazolidinone synthesis	**OC 15B**
W. Essafi, M. Fehri, N. Jemili *INRAP - Sidi Thabet* Electrostatic complexation of oppositely charged polyelectrolytes in aqueous solution	**OC 13C**
N. Gasmi, L. Khalfa, G. Rossignolo, A. Lorenzetti, Y. Moussaoui *FSG - Gafsa* Designed from chemically recycled polyethylene furanoate packaging	**OC 10C**
F. Ghammagui, S. Ammar *FSG - Gabès* Sustainable biochar-based metal oxide composites for enhanced adsorption and photocatalytic degradation of organic dyes	**OC 11C**
R. Hamdi , J.F. Longevial, M. Sindt, C. Lefebvre, T. Boubaker *FSM - Monastir* Synthesis, quantification and reactivity of gold(I) N-heterocyclic carbenes complexes bearing a methacrylate moiety	**OC 18A**
L. Han, Yi Yang, A. Tlili *Claude Bernard University, Lyon1, France* Strain-release-driven synthesis of pentafluorosulfanylated four-membered rings under energy transfer photocatalysis	**OC 06A**
A. Hedhli, S. Ayachi, T. Boubaker *FSM - Monastir* Structure-reactivity relationships in para-X-substituted diethyl benzylidenemalonates: Insights from kinetics and DFT descriptors	**OC 07A**
A. Hileli, Z. Ghodbani, Y. Moussaoui, S. Gamoudi *FSG - Gafsa* Biomass-enhanced modified clay for industrial effluents treatment: performance and optimization	**OC 16B**
H. Hlimi, M. Mbarek *FSM - Monastir* Engineering donor–acceptor PPV–PFO copolymers for advanced organic optoelectronic devices	**OC 05C**

Communicatings' Names	**Ref**
M. Horchani, H. Ben Jannet, A. Romdhane *FST - Tunis* Design, synthesis, and in silico investigations of novel alkyl-phosphonate derivatives tethered to the antibiotic Ciprofloxacin	**OC 09B**
N. Jebli, S. Touil *ISSH - Jendouba* Direct access to 2,6-bis(diphenylphosphine oxide)-phenol derivatives	**OC 09A**
O. Jendoubi, S. Majdoub, H. B. Al-Hmadi, R. El Mokni, S. Angeloni, A.M. Mustafa, G. Caprioli, F. Maggi, S. Hammami *FSM - Monastir* HPLC-MS/MSPhenolic profile of *Salvia aegyptiaca* L growing in Tunisia	**OC 02B**
M. Jmai, H. Edziri, A. Dridi, M. Melliti, S. Py, R. Besbes, H. M'rabet *FST - Tunis* Isoxazolidine- and isoxazoline-linked thioether derivatives: Synthesis, antimicrobial activity, and in silico insights	**OC 10A**
A. Kaouach, L. Pagès, L. Jean, H. Ben Jannet, A. Romdhane *FSM - Monastir* Green synthesis, cytotoxic assessment, and computational study of novel spiroxindole–triazolyl–pyranopyrimidinone derivatives	**OC 11A**
R. Khaldi, A. Hedhli, T. Boubaker *FSM - Monastir* A predictive relationship between tautemeric equilibria and acidity of nitroalkanes in water	**OC 17B**
N. Krissaane, R. Hammami, N. Sadfi-Zouaoui, A. Arfaoui, M.L. Efrit *FST - Tunis* Biological evaluation and molecular docking studies of pyrrolidinones and pyrrolinones as potential antibacterial agents	**OC 12A**
M. Lejmi, B. Kouidhi , H. Rhim, M. Mastouri, A. Elaissi *Faculty of Pharmacy - Monastir* Chemical composition and biological activities of essential oils from five Eucalyptus species	**OC 03B**
A. Macherki, M. Itaimi Dammak, D. Le Cerf, M. Rey, H. Majdoub, A. Romdhane *FSM - Monastir* Extraction, structural analysis, and applications of Star Anise polysaccharide	**OC 06C**
D. Mezni, R. Kefi *FSB - Bizerte* Crystal structure study, spectroscopy, theoretical investigations, and biological evaluation of a hybrid material	**OC 19A**
M. Mrabet, I. Kamoun, M. Oudni-M'rad, S. M'rad, F. Ayari *FSM - Monastir* Synthesis and characterization of silver nanoparticles: The evaluation of their protoscolicidal activity against Echinococcus granulosus	**OC 14C**
I. Ngom, M.O. Zouaghi, I. Ferchichi, F. Guégan, I. Seck, Y. Arfaoui *FST - Tunis* Mechanistic DFT investigation of the cycloaddition reaction of nitrones with allene–propargyl equilibria toward isoxazoline and isoxazolidine derivatives	**OC 18B**
A. Ramanavicius, G. Zvirzdine, E. Mohsenzadeh, V. Liustrovaite, V. Ratautaite, E. Brazys, E. Nedzinskaite, G. Slaboseviciute, D. Plausinaitis, U. Prentice, G. Kaspute, A. Ramanaviciene *Centre for Physical Sciences and Technology (FTMC), Vilnius, Lithuania* The formation and application of molecularly imprinted conducting polymers	**OC 16C**

Communicatings' Names	**Ref**
M. Rjili, A. Aschi *FST - Tunis* A structural and dynamic comparison of gelatin- and ovalbumin-based coacervates	**OC 07C**
O. Romdhane, J. Kraiem *FSM - Monastir* Aerobic oxidation of aldehydes to carboxylic acids in aqueous solution of NaOH / NaCl	**OC 19B**
D. Saidani, R. Abderrahim *FSB - Bizerte* Efficient synthesis of quinazoline derivatives via cyclization of 2-aminobenzamide with ethyl chloroformate	**OC 13A**
I. Saidi, D. Mergby, A. Ben Arfa, M. Neffati, H. Najjaa, H. Ben Jannet *FSM - Monastir* Isolation, characterization, and evaluation of the herbicidal potential of phytochemical compounds derived from Inula viscosa L.	**OC 06B**
S. Salhi , A. Omri, R. Ben Salem, M. Benzina *FSS - Sfax* Optimization and modeling of photocatalytic degradation of anionic dye using Co-TiO2/hemathite catalyst	**OC 05B**
A.S. Schuller, X. Moreno, E. Lobry , C. Ley *University of Haute-Alsace, Mulhouse, France* Coupling UV irradiation and electrospinning for advanced polyurethane filtration membranes	**OC 08C**
D. Sellami, S. Zaidi, O. Challouf, T. Robert, M. Abid, S. Abid, A. Bougarech *FSS - Sfax* Bio-based furan-containing polyurethanes from bisfuranic polyesters and Desmodur® eco N: Synthesis, characterization, and application	**OC 12C**
T. Slama, S. Ayachi, T. Boubaker *FSM - Monastir* Synthesis and characterization of a push–pull dinitropyridine derivative for non-linear optics	**OC 14A**
I. Talbi, M. Jeanty *Novalix Tunisia* Strategic selection of building blocks for DNA encoded library design	**OC 15A**
N. Tka, P. Langer *FSM - Monastir* Synthesis and photophysical characterization of novel acridine-based hybrids	**OC 10B**
A. Yahya, A. Ayachi, F. Chtourou, Z. Benissa, N. Tene ; R. Jarraya, M. Treilhou, S. Zouari *FSG - Gafsa* Influence of hydrodistillation time intervals and drying period on the yield, chemical composition, and antioxidant activities of stems essential oils of Pituranthos chloranthus from the Er-hiba-Gafsa provenance (Southern Tunisia)	**OC 11B**
C. Yakoubi, C. Dehoux, M.L. Efrit, A. Arfaoui, Y. Genisson *FST - Tunis* Synthesis of pyrrolidines as enzyme modulators targeting glucocerebrosidase: Application to Gaucher disease	**OC 07B**
Y. Yang, L. Han, A. Tlili *Claude Bernard University, Lyon1, France* A shelf-stable reagent for photocatalytic radical pentafluorosulfanylation of styrene derivatives	**OC 08A**
I. Zouidi, A. Ben Slimane ; S. Gamoudi *FSG - Gafsa* Removal of methyl green dye by new biocomposite (activated carbon/polyaniline)	**OC 09C**

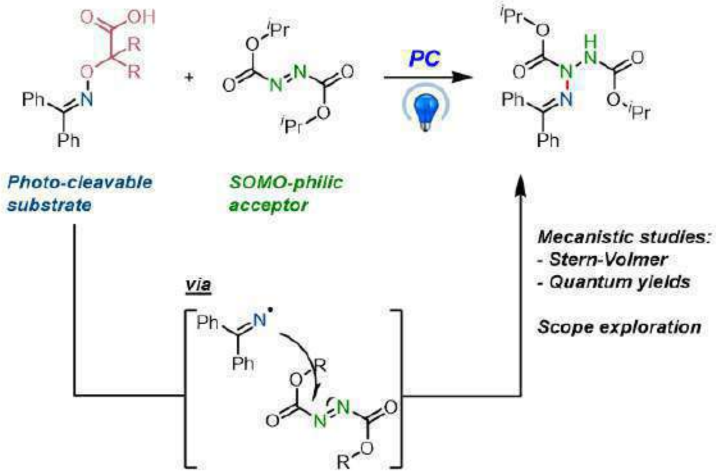
Abstracts of Oral Communications

Program of
Friday 01
May 2026

First example of nitrogen-nitrogen bond formation through photocatalytic iminyl radical generation under visible light irradiation

M. Abdellaoui, Dr. A. Tlili

Laboratoire Hydrazines et Composés Energétiques Polyazotés (LHCEP) UMR-CNRS 5278
2 Rue Victor Grignard, UCBL Campus de la Doua, 69622 Villeurbanne
e-mail: mehdi.abdellaoui@univ-lyon1.fr



Over the past two decades, nitrogen-centered radical rose a significant interest in the field of organic chemistry and taming their reactivity[1] progressively became a primary goal for different industries. Among these reactivities, nitrogen-nitrogen bond formation is of primary importance, notably for the design of novel High Energy Density Material (HEDM).[2] However, such couplings are sporadically described and the simple addition of a nitrogen radical on a nitrogen containing unsaturated compound has never been considered yet. The study herein describes the first example of a fully *aza* version of the Giese reaction between an iminyl radical and a diazene, considered here as a SOMOphilic acceptor.

Our approach leverages the photo-cleavable behavior of imin-oxy-alkyl carboxylic acids[3] to release a transient free iminyl radical by β-scission that readily performs the addition on the diazo-compound. The resulting polyfunctionalized triazone is endowed with one unprotected nitrogen fully compatible with various postfunctionalizations that are also explored in this study. *In-depth* experiments will be conducted by combining DFT and photochemical analyses to help rationalize the mechanism involved.

References

1. (a) Miller, D. C.; Choi, G. J.; Orbe, H. S., Knowles, R. R. *J. Am. Chem Soc.* **2015**, *137*, 13492. (b) Roos, C. B.; Demaerel, J.; Graff, D. E.; Knowles, R. R. *J. Am. Chem. Soc.* **2020**, *142*, 5974.
2. Selected publications from our group dealing with nitrogen containing HEDM: (a) Kalout, H.; Lansalot, M.; Bourgeat-Lami, E.; Morlet-Savary, F.; Lacôte, E.; Lavalée, J. *Adv. Funct. Mat.* **2024**, *34* , 2406299. (b) Bourgeois, L.; Hammoud, A.; Chalouni, L.; Baudoin, A.; Chefdeville, E. ; Lhoussain, K. ; Renault, A. ; Lesage de la Haye, J. ; Darwich, C. ; Lacôte, E. *Angew. Chem. Int. Ed.* **2025**, *64*, e202425279. (c) Eymann, J. ; Joucla, L. ; Jacob, G. ; Raynaud, J. ; Darwich, C. ; Lacôte, E. *Angew. Chem. Int. Ed.* **2020**, *60*, 1578-1582.
3. (a) Davies, J.; Sheikh, N. S.; Leonori, D. *Angew. Chem. Int. Ed.* **2017**, *56*, 13361-13365. (b) Morcillo, S. P.; Dauncey, E. M.; Kim, J. H.; Douglas, J. J.; Sheikh, N.; Leonori, D. *Angew. Chem. Int. Ed.* **2018**, *57*, 12945-12949.

Synthesis of new 1,2,4-oxadiazole derivatives of flavonol and in *silico* evaluation of their biological properties

Ahlem Beyaoui, Ilyes Saidi, Anis Romdhane and Hichem Ben Jannet

University of Monastir, Faculty of Science of Monastir, Laboratory of Heterocyclic Chemistry, Natural Products and Reactivity (LR11ES39), Team: Medicinal Chemistry and Natural Products,
Avenue of Environment, 5019 Monastir, Tunisia.

This work focuses on the synthesis of new 1,2,4-oxadiazole derivatives of flavonol through a four-step synthetic route. First, flavonol (3-hydroxy-2-phenyl-4*H*-chromen-4-one) was obtained *via* the condensation of 2-hydroxyacetophenone with benzaldehyde under basic conditions, followed by cyclization and oxidation, affording the product in a 79% yield. The synthesized flavonol was subsequently converted into a nitrile derivative and then into an amidoxime, a key precursor for the construction of the 1,2,4-oxadiazole ring. Cyclization of this intermediate with various acyl chlorides and orthoesters led to a series of new 3,5-disubstituted 1,2,4-oxadiazoles **(4a–h)**. The obtained compounds were isolated in good yields and characterized by ^{1}H NMR, ^{13}C NMR, and high-resolution mass spectrometry (HRMS)**.** Furthermore, an *in silico* molecular docking study was performed to evaluate the biological potential of these compounds, particularly their anti-α-amylase, anti-15-lipoxygenase, and cytotoxic activities.

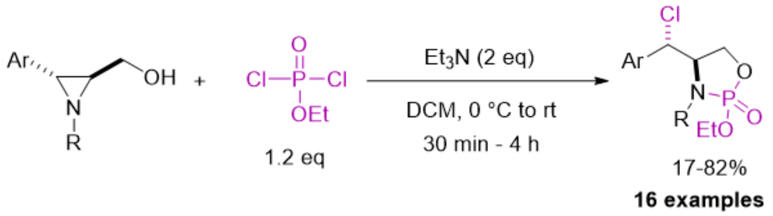
Keywords: flavonol; 1,2,4-oxadiazole; heterocyclic synthesis; molecular docking; anti-α-amylase; anti-15-lipoxygenase

Synthesis of novel 1,3,2-oxazaphospholidine-2-oxides *via* ring expansion of 2-hydroxymethylaziridines and evaluation as acetylcholinesterase inhibitors

Amal Dridi,[a,b] Mohamed Mastouri,[c] Romain Haudecoeur,[d] Sandrine Py [b] and Rafâa Besbes [a]

[a] *Laboratory of Analytical Chemistry and Electrochemistry, Organic Synthesis Team, LR99ES15-University of Tunis El Manar, Faculty of Sciences of Tunis, 2092 Tunis, Tunisia.*
[b] *Département de Chimie Moléculaire, UMR 5250 CNRS –Université Grenoble Alpes, 38058 Grenoble, France.*
[c] *School of Biomedical Engineering, Harbin Institute of Technology (Shenzhen), Shenzhen, Guangdong, China.*
[d] *Département de pharmacochimie Moléculaire, UMR 5063 CNRS-Université Grenoble Alpes, 38058 Grenoble, France.*
Email: amal.dridi@univ-grenoble-alpes.fr

2-Hydroxymethylaziridines represent valuable synthetic intermediates for the construction of diverse interesting heterocyclic systems.[1] In this communication, we report a simple and efficient approach for the synthesis of 1,3,2-oxazaphospholidine-2-oxides through the ring expansion of non-activated 2-hydroxymethylaziridines in the presence of ethyl dichlorophosphate, under mild conditions. Regio- and stereoselective aziridine ring opening yields α-chlorinated 5-membered ring heterocyclic compounds as the sole products of the reaction.



- **Molecular Docking**
Electrophorus electricus AChE
Insect AChE
Human AChE

- ***In vitro* assays**
Electrophorus electricus AChE

Some 1,3,2-oxazaphospholidine-2-oxides have been reported to exhibit anti-inflammatory,[2] antibacterial[3] or insecticidal[4] effects, however molecules containing such scaffold remain underinvestigated to date. Numerous organophosphorus compounds have been employed as insecticides due to their ability to inhibit acetylcholinesterase (AChE).[5] However, their use was subsequently prohibited because they also inhibit humans and animals AChE. More recently, AChE inhibition has emerged as an important therapeutic strategy for the treatment of Alzheimer disease.[6] Herein, we describe the preparation of 16 examples of 1,3,2-oxazaphospholidine-2-oxides along with the evaluation of these molecules as acetylcholinesterase (AChE) inhibitors using molecular docking and in vitro assays.

Key words: 2-hydroxymethylaziridine, 1,3,2-oxazaphospholidine-2-oxide, ring expansion, acetylcholinesterase inhibitors.

---

[1] Stanković, S.; D'hooghe, M.; Catak, S.; Eum, H.; Waroquier, M.; Van Speybroeck, V.; De Kimpe, N.; Ha, H.-J. Regioselectivity in the Ring Opening of Non-Activated Aziridines. *Chem. Soc. Rev.* **2012**, *41*, 643–665.

[2] Abdou, W. M.; Sabry, E.; Shaddy, A. A. Synthesis Approach and Biological Activity Evaluation of a Series of 1,3,2-Oxazaphosphole-2-Oxides against Inflammation and Nociception. *Monatsh. Chem.* **2019**, *150*, 283–294.

[3] Krishna, B. S.; Rao, A. J.; Naidu, K. R. M.; Rao, V. K.; Raju, C. N. Synthesis and Antibacterial Activity Studies of Novel 2-Substituted- 1,3,2-Oxazaphosphole-2-Oxide Derivatives of (*S*)-(+)-Prolinol. *Org. Commun.* **2010**, *3*, 98–105.

[4] Eto, M. Functions of Phosphorus Moiety in Agrochemical Molecules. *Biosci. Biotech. Biochem.* **1997**, *61*, 1-11.

[5] Sussman, J.; Harel M.; Frolow, F.; Oefner, C.; Goldman, A.; Toker, C .; Silman, I. Atomic Structure of Acetylcholinesterase from Torpedo Californica: A Prototypic Acetylcholine-Binding Protein. *Science*, **1991**, 253, 872-879.

[6] Schneider S., L. A Critical Review of Cholinesterase Inhibitors as a Treatment Modality in Alzheimer's Disease. *Dialogues Clin. Neurosci.* **2000**, 2, 111–128.

Synthesis and characterization of new mono- and bi-heterocyclic α-aminophosphonate models via copper(I)-catalyzed "Click Chemistry" dipolar cycloaddition

Anouar Alami

L3IA, Faculty of Sciences Dhar El Mahraz, Sidi Mohamed ben Abdellah University, Fez, Morocco

α-aminophosphonates constitute an essential class of bioactive molecules due to their structural analogy with α-amino acids. Their pharmacological properties are extensive, including anti-Alzheimer, antibacterial, anticancer, and antiviral activities. This work presents the design and synthesis of new heterocyclic α-aminophosphonate models incorporating triazole motifs.

The synthesis strategy is based on "Click Chemistry," specifically the 1,3-dipolar cycloaddition between a phosphonic azide dipole and various heterocyclic dipolarophiles, catalyzed by copper (I). This methodology was chosen for its total regioselectivity (exclusive formation of the 1,4-isomer), its mild operating conditions, and its high yields, reaching 90%.

Several new cycloadducts were synthesized, notably derivatives of carbazole, benzimidazole, and naphthalene. The structure of these new models was rigorously established through an in-depth spectroscopic study:

- 1D and 2D NMR (1H, 13C, 31P) confirmed the connectivity and regiochemistry.
- Infrared spectroscopy (IR) and High-Resolution Mass Spectrometry (HRMS) were employed.
- The structure of the naphthalene derivative was confirmed by X-ray diffraction (ORTEP view).

These new molecules are currently undergoing evaluation to determine their antiviral, antioxidant, and anticancer activities, opening promising perspectives in medicinal chemistry

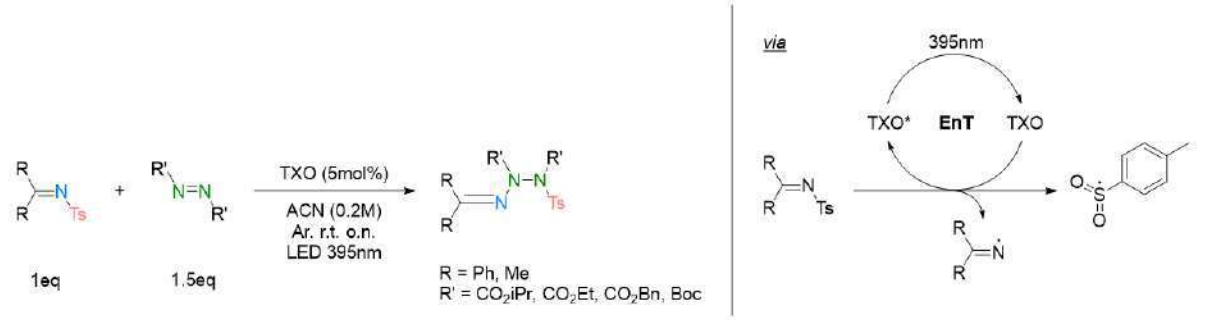
Keywords: α-aminophosphonates, Click Chemistry, CuAAC, Triazole, Heterocycles,
2D NMR, Bioactivity

Metal free photoinduced N-N radical coupling leading to difunctionalized triazones

Pierre Elmary, Mehdi Abdellaoui, Tlili Anis

LHCEP, UCBL Campus de la Doua
2 Rue Victor Grignard, Bâtiment Raulin
pierre.elmary@univ-lyon1.fr

Polynitrogen compounds always attracted attention, particularly in the pyrotechnic field since the cleavage of N-N bonds releases a significant amount of energy that can be exploited by the propellant industry[1]. Moreover, in the past few years, the N-N bonds are gaining interest in the pharmaceutical[2] field thanks to their metabolic properties[3]. However, the synthesis of these compounds represents a challenge due to the inherent instability of the N-N bonds in extended networks. In this work, we report a novel access to triazone compounds through a metal free photocatalysis by energy transfer (EnT)[4]. This reaction occurs through the homolytic cleavage of a tosylated imine[5] and leads to the difunctionalization of several diazenes. In this study, we aim both to adapt a flow version of our protocol for industrial purposes and help rationalize the reaction mechanism *via in-depth* photophysical analyses, kinetics and X-Ray study of key intermediates and products. Our experimental data will be strengthened by DFT calculations and PRE-experiments.



---

[1] O'Sullivan, O. T. & Zdilla, M. J. Properties and Promise of Catenated Nitrogen Systems As High-Energy-Density Materials. *Chem. Rev.* **120**,5682–5744(**2020**)

[2] https://cen.acs.org/people/nobel-prize/Click-bioorthogonal-chemistry-win-2022-Nobel-Prize-in-Chemistry/100/i36.

[3] Appel, K. E., Bauszus, M., Roots, I., Rühl, C. S. & Hildebrandt, A. G. Enzyme Catalysed Cleavage of the N-N Bond of N-Nitrosamines. in *Biological Reactive Intermediates III: Mechanisms of Action in Animal Models and Human Disease* (eds Kocsis, J. J., Jollow, D. J., Witmer, C. M., Nelson, J. O. & Snyder, R.) 959–970 (Springer US, Boston, MA, 1986). doi:10.1007/978-1-4684-5134-4_93.

[4] Jiang, Y.-S. *et al.* Photoinduced Difunctionalization of Diazenes Enabled by N–N Radical Coupling. *Org. Lett.* **25**, 6671–6676 (**2023**).

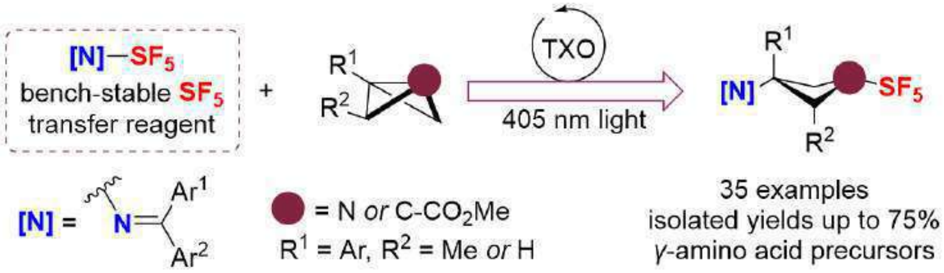
[5] Rodríguez, R. I. *et al.* Radical strain-release photocatalysis for the synthesis of azetidines. *Nat. Catal.* **7**, 1223–1231 (**2024**).

Strain-Release-Driven Synthesis of Pentafluorosulfanylated Four-Membered Rings under Energy Transfer Photocatalysis

Lulu Han, Yi Yang, and Anis Tlili *

CNRS, Université Claude Bernard Lyon 1, CNES, Ariane Group, LHCEP, Villeurbanne F-69622, France
Bâtiment Raulin, 2 Rue Victor Grignard 69622 VILLEURBANNE CEDEX, France.

Methods to prepare SF_5-containing molecules are of significant interest, as the pentafluorosulfanyl (SF_5) group imparts unique chemical and physical properties - such as high electronegativity, lipophilicity, and thermal stability - that are valuable in pharmaceuticals, agrochemicals, and materials science.[1] On the other hand, four-membered rings play a crucial role in molecular design. The three-dimensional shape of these rings is of particular importance, as their compact, rigid structure induces conformational constraints, enhancing their ability to interact more effectively and selectively with biological targets.[2] The use of our shelf-stable reagent,[3] imine-SF_5, enables selective access to four-membered ring SF_5-containing molecules under mild reaction conditions via a strain-release approach facilitated by energy-transfer catalysis. Mechanistic investigations provided insight into the reaction pathway. This approach advances pentafluorosulfanylation methodology, paving the way for future development (**Scheme 1**).[4]



References

[1] Sowaileh, M. F.; Hazlitt, R. A.; Colby, D. A. *ChemMedChem*. **2017**, *12* (18), 1481.
[2] Kraemer, Y.; Buldt, J. A.; Kong, W. Y.; Tantillo, D. J.; Pitts, C.R. et al. *Angew. Chem. Int. Ed.* **2024**, *63*, e202319930.
[3] YANG, Y.; HAN, L.; Taponard, A.; Khrouz, L.; Bucher, C.; Cyrille, M.; Médebielle, M.; Tlili, A. *Angew. Chem. Int. Ed.* **2025**, e202505146
[4] Yang, Y.; Han, L.; Canavero. L,; Brettnacher. L,; Khrouz. L,; Monnereau. C,; Médebielle. M,; Tlili. A. *J. Am. Chem. Soc.* **2025**, *147, 31, 27905.*
[5] Yang, Y.; Han, L.; Canavero. L,; Brettnacher. L,; Tlili. A. *Chem. Rev.* **2025**, *125,* 8426.

Structure-Reactivity Relationships in *para*-X-Substituted Diethyl Benzylidenemalonates: Insights from Kinetics and DFT Descriptors

Amel HEDHLI,[a] Sahbi AYACHI,[b] and Taoufik BOUBAKER[a]

[a] *Laboratoire de Chimie Hétérocyclique, Produits Naturels et Réactivité (LR11ES39), Faculté des Sciences, Université de Monastir, Avenue de l'Environnement, 5019 Monastir, Tunisie.*

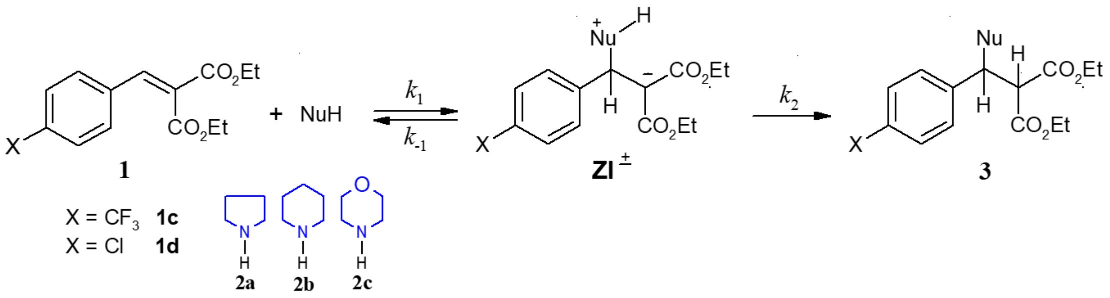
[b] *Laboratoire de Physico-chimie des Matériaux (LR01ES19), Faculté des Sciences, Université de Monastir, Avenue de l'Environnement, 5019 Monastir, Tunisie.*

Understanding and predicting electrophilic reactivity is essential for the rational design of functionalized organic molecules. In this study, we systematically investigated the reaction kinetics of para-X-substituted diethyl benzylidenemalonates **1c** (X = CF_3) and **1d** (X = Cl) with cyclic secondary amines **2a-c** in acetonitrile at 20 °C. The second-order rate constants (k) were measured and employed to evaluate the electrophilicity parameter (E) through the linear free energy relationship: $\log k\ (20\ °C) = s_N\ (E + N)$.

For derivatives **1h** (X = OH) and **1i** (X = NH_2), the E parameters were estimated from a well-established empirical correlation between E and the Hammett substituent constant (σ_p).

To rationalize the observed reactivity trends, density functional theory (DFT) calculations were performed on a series of ten para-X-substituted diethyl benzylidenemalonates **1a-j**. Correlations between E and several electronic and molecular descriptors were then examined, including the lowest unoccupied molecular orbital energy (ε_{LUMO}), the global electrophilicity index (ω), the dipole moment (μ), and molecular polarizability.

A nonlinear relationship was observed, highlighting the significant influence of geometric factors, particularly the dihedral angle between the phenyl ring and the C=C bond, on π-conjugation and, consequently, on the electrophilic reactivity of these systems.



References

[1] H. Mayr, M. Patz. Angew. *Chem. Int. Ed. Engl.*, **1994**, 33, 938-957.

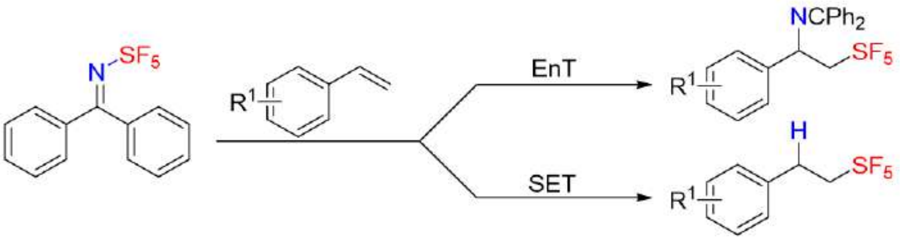
[2] A. Hedhli, A. Ghabi, H. Ayachi, S. Ayachi, T. Boubaker, *Chem. Eng. J.*, **2025**, 519, 1-15.

A Shelf-Stable Reagent for Photocatalytic Radical Pentafluorosulfanylation of Styrene Derivatives

Yi Yang, Lulu Han, and Anis Tlili *

CNRS, Université Claude Bernard Lyon 1, CNES, Ariane Group, LHCEP, Villeurbanne F-69622, France
Bâtiment Raulin, 2 Rue Victor Grignard 69622 VILLEURBANNE CEDEX, France.

We have developed the first family of air- and moisture-stable pentafluorosulfanylation (SF_5) reagents. Although the SF_5 group is a bioisostere of the trifluoromethyl group (CF_3)—exhibiting even greater electronegativity and lipophilicity, attributes that have earned it the nickname "super trifluoromethyl group"—the development of shelf-stable, non-toxic, and easy-to-handle SF_5 -incorporating reagents had remained elusive for over 70 years since its discovery. Our discovery enables the synthesis of per- and polyfluoroalkyl sub-stances (PFAS)-free fluorinated compounds, offering significant advantages over traditional CF_3 analogs. These new reagents exhibit promising reactivity under photochemical conditions, efficiently facilitating the formation of novel SF_5 -containing molecules. Moreover, our approach is compatible with the late-stage functionalization of complex molecules. Mechanistic studies have provided valuable insights into the underlying reaction pathways.



Scheme 1. Imino-pentafluorosulfanylated and hydropentafluorosulfanylation of styrene.

References

[1] Britton, R. et al. Nat. Rev. Methods Primers. **2021**, 1, 47.
[2] Y. Ogawa, E. Tokunaga, O. Kobayashi, K. Hirai, N. Shibata, iScience **2020**, 23.
[3] C. Zhang, K. Yan, C. Fu, H. Peng, C. J. Hawker, A. K. Whittaker, Chem. Rev. **2022**, 122, 167.
[4] N. D. Tyrrell, Org. Process. Res. Dev. **2023**, 27, 1422.
[5] P. R. Savoie, J. T. Welch, Chem. Rev. **2015**, 115, 1130.
[6] YANG, Y.; HAN, L.; Taponard, A.; Khrouz, L.; Bucher, C.; Cyrille, M.; Médebielle, M.; Tlili, A. Angew. Chem. Int. Ed. **2025**, e202505146.
[7] Yang, Y.; Han, L.; Canavero. L,; Brettnacher. L,; Tlili. A. Chem. Rev. **2025**, 125, 8426.

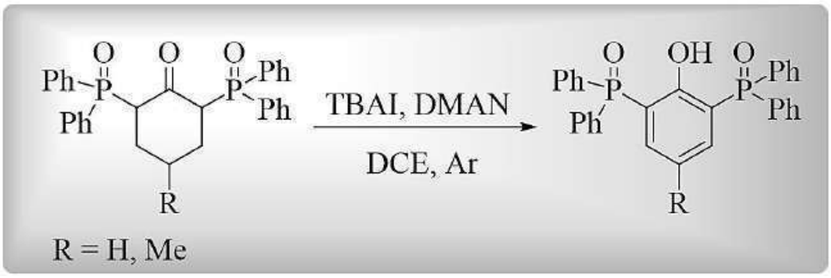
Direct access to 2,6-bis(diphenylphosphine oxide)-phenol derivatives

Nejib Jebli [a,b] & Soufiane Touil [a]

[a] University of Carthage, Faculty of Sciences of Bizerte, Laboratory of Hetero-Organic Compounds and Nanostructured Materials (LR18ES11), 7021 Jarzouna-Bizerte, Tunisia.
[b] University of Jendouba, Higher Institute of The Human Sciences of Jendouba,
Department of Sciences & Education, 8189 Jendouba, Tunisia.

π-Conjugated systems are a versatile class of functional materials due to their distinct electronic asymmetry and strong electron-withdrawing properties. By incorporating phosphine oxide units into extended π-frameworks, there is a notable impact on the frontier molecular orbitals, often resulting in lower LUMO energy levels while maintaining or slightly enhancing HOMO distributions. Furthermore, the presence of hydroxyl and phosphoryl groups encourages robust intermolecular interactions that influence solid-state arrangement and charge transfer. These characteristics enhance the appeal of these systems for optoelectronic and dielectric purposes. As part of this orientation, we report herein the direct dehydrogenative aromatization of α,α'-bis(diphenylphosphoryl)cycloalkanones in the presence of Tetra-n-butylammonium iodide (TBAI) and N,N,N',N'-tetramethylnaphthalene-1,8-diamine (DMAN), performed in dichloroethane (Scheme 1).

Keywords: α,α'-bis(diphenylphosphoryl)cycloalkanones, Dehydrogenation, bis(diphenylphosphoryl)phenols.



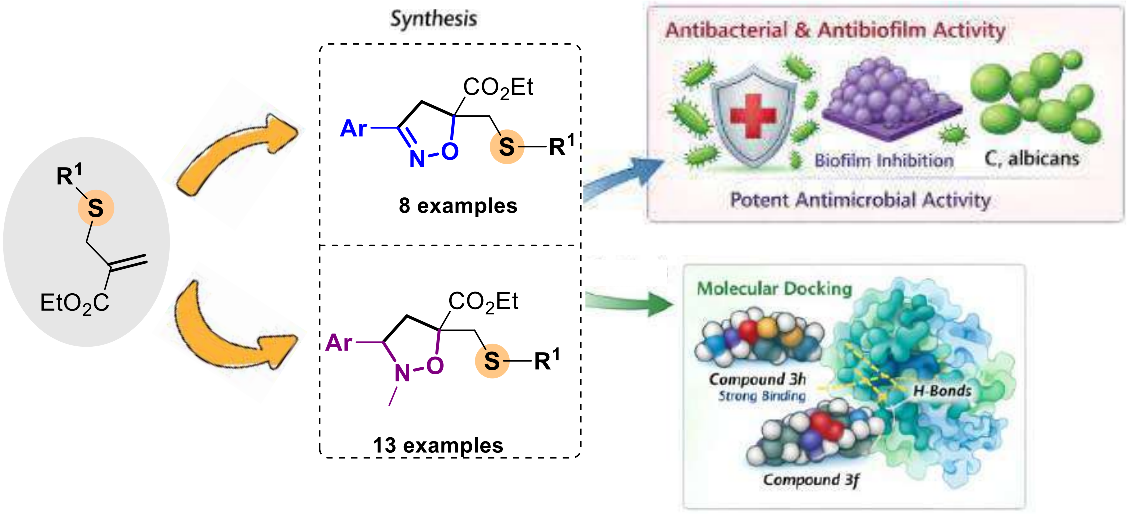
Scheme 1: dehydrogenation of α,α'-bis(diphenylphosphoryl)cycloalkanones

Isoxazolidine- and Isoxazoline-Linked Thioether Derivatives: Synthesis, Antimicrobial Activity, and *In Silico* Insights

Momtez Jmai [a,*], Hayet Edziri [b], Amal Dridi [c,d], Marwa Melliti [b], Sandrine Py [d],
Rafâa Besbes [c], Hedi M'Rabet [a]

a) Laboratory of Selective Organic and Heterocyclic Synthesis-Biological Activity Evaluation, SOHES, (LR17ES01), Faculty of Science of Tunis, University Tunis El Manar, Tunis 2092, Tunisia.
b) Laboratory of Transmissible Diseases and Biologically Active Substances, (LR99ES27), Faculty of Pharmacy, University of Monastir, 5000 Monastir, Tunisia.
c) Laboratory of Analytical Chemistry and Electrochemistry, LCAE, (LR99ES15), Faculty of Sciences of Tunis, University of Tunis El Manar, Tunis 2092, Tunisia.
d) Univ. Grenoble Alpes, CNRS, DCM, 38000 Grenoble, France.
E-mail **:** momtez.jmai@fst.utm.tn

A series of novel isoxazolidine and isoxazoline derivatives were synthesized and evaluated for their antimicrobial potential. Structure–activity relationship analysis revealed that the nature of the sulfur substituent and the electronic properties of the aryl group play a critical role in biological activity. Among the derivatives, compound **3h** demonstrated the most promising antibacterial activity, while compound **3f** showed remarkable antifungal efficacy. Molecular docking studies supported these experimental results, indicating strong binding interactions with key bacterial and fungal targets. The findings highlight these scaffolds as promising antimicrobial candidates and provide a foundation for further optimization and pharmacological exploration.



Scheme 1: Synthesis, Antimicrobial Activity, and Molecular Docking study of Isoxazolidine- and Isoxazoline- Linked Thioether

Key words: thioether, isoxazolidine, isoxazoline, antimicrobial, antibiofilm

Green Synthesis, Cytotoxic Assessment, and Computational Study of Novel Spiroxindole–Triazolyl–Pyranopyrimidinone Derivatives

Aicha Kaouach[a], Lucas Pagès[b], Ludovic Jean[b], Hichem Ben Jannet[a], Anis Romdhane[a]

a) *Laboratory of Heterocyclic Chemistry, Natural Products and Reactivity (LR11ES39), Team: Medicinal Chemistry and Natural Products, Faculty of Sciences of Monastir, University of Monastir, Avenue of Environment, 5019 Monastir, Tunisia.*

b) *Laboratory of Therapeutic Targets and Drug Design CiTCoM, (UMR 8038 – U1268), Faculty of Pharmacy, Paris Cité University, 4 Observatory Avenue, 75006 Paris, France.*

A series of novel spiroxindole–triazolyl–pyranopyrimidinone derivatives was synthesized from isatin using an eco-friendly and sustainable synthetic protocol. This methodology proved to be efficient, affording the target compounds in good to excellent yields. The molecular structures and purity of the synthesized derivatives were thoroughly confirmed through comprehensive spectroscopic techniques, including NMR and mass spectrometry analyses.

Furthermore, *in silico* studies were conducted to investigate the potential biological interactions of these compounds, which revealed promising cytotoxic activity. These computational findings highlight the potential of the synthesized spiroxindole–triazolyl–pyranopyrimidinone derivatives as valuable bioactive molecules for further exploration in drug discovery and development.

Keywords: Spiroxindole; Pyranopyrimidinone; Triazole; Green synthesis; Cytotoxic activity; *in silico*.

Selective NADES-Mediated Microwave Extraction of Boswellia sacra Polysaccharides: Balancing Process Yield with Structural Integrity

Asma BEN HAJ MBAREK [1,2], Mariem Itaimi Dammak [3], Chiara Milanese [4], Aicha Laouani [5], Didier Le Cerf [6], Hatem Majdoub [3], Adele Papetti [2], Hichem Ben Jannet [1]

[1]Laboratory of Chemistry of Natural Substances and Organic Synthesis, University of Monastir, Tunisia.
[2] Department of Drug Sciences, University of Pavia Viale Taramelli 12 27100, Pavia, (Italy)
[3] Laboratory of Interfaces and Advanced Materials (LR11ES55), University of Monastir, Tunisia.
[4] Department of Chemistry, Centre for Health Technologies (CHT), University of Pavia, Pavia, Italy
[5] Laboratory of Metabolic Biophysics and Applied Pharmacology, Faculty of Medicine, University of Sousse, Sousse 4002, Tunisia (c)
[6] Laboratory Polymers, Biopolymers & Surfaces, Normandy University, UNIROUEN, INSA Rouen, CNRS, PBS, France

The selection of natural deep eutectic solvents (NADES) for biopolymer recovery requires a nuanced understanding of the trade-off between extraction efficiency and macromolecular purity. This study explores the microwaves-assisted extraction (MAE) of polysaccharides from *Boswellia sacra*, focusing on the impact of NADES composition on structural characteristics. Initial screening of various NADES formulations revealed an inverse correlation between gravimetric yield and the intensity of characteristics vibrational band in FTIR spectra.

While certain NADES system provided higher crude yields, spectroscopic analysis identified that lower concentrations of key functional groups. Using a box-benkhen design (BBD), we optimized the extraction parameters: Time (min), Temperature (°C), and solid-to-liquid ratio (g/mL), specifically for the NADES system that prioritized structural quality. The resulting macromolecules were characterized via FTIR, SEC, DSC and TGA to evaluate their molecular weight and thermal stability. This work highlights the necessity of "Structure guided" solvent selection in green chemistry, providing that NADES can be tuned to isolate highly functionalized biopolymers for advanced applications in polymer science.

HPLC-MS/MSPhenolic Profile of Salvia aegyptiacaL. growing in Tunisia

Ons Jendoubi [a], Siwar Majdoub [a], Hekmat B. AL-Hmadi [b], Ridha El Mokni [c,d],
Simone Angeloni [e], Ahmed M. Mustafa [e], Giovanni Caprioli [e],
Filippo Maggi [e] and Saoussen Hammami [a]

[a] *Laboratory of Environmental Chemistry and Clean Processes(LR21ES04),*
Faculty of Sciences of Monastir, Monastir University, Monastir 5000, Tunisia
[b] *Department of Chemistry, College of Medicine, AL-Muthanna University, Samawah, Iraq.*
[c] *Department of Pharmaceutical Sciences "A", Laboratory of Botany, Cryptogamy and Plant Biology, Faculty of Pharmacy of Monastir, Avicenna street, Monastir University, Monastir 5000, Tunisia.*
[d] *Laboratory of Forest Ecology, National Research Institute of Rural Engineering, Water and Forests (INRGREF), IRESA, Carthage University, Ariana-2080, Tunisia.*
[e] *Chemistry Interdisciplinary Project (ChIP), School of Pharmacy, University of Camerino, via Madonna delle Carceris.n.c., I-62032, Camerino (MC), Italy.*

Among medicinal plants, species belonging to the genus *Salvia* are widely recognized for their rich content of phenolic compounds and their numerous biological activities. In particular, *Salvia aegyptiaca*, traditionally used in folk medicine, is considered as a potential source of natural bioactive molecules. Phenolic derivatives present in this plant are known for their antioxidant and pharmacological properties. This work aimed to characterize the phenolic compounds present in Tunisian *S.aegyptiaca* extracts obtained through maceration with solvents of varying polarity.HPLC-MS/MS analysis revealed a diverse range of phenolic acids and flavonoids. Their distribution varied depending on the extraction solvent. These findings confirm *S. aegyptiaca* as a promising source of natural phenolics.

Keywords: *Salvia aegyptiaca* L., Crude extracts, Phenolic derivatives, HPLC-MS/MS.

Chemical Composition and Biological Activities of Essential Oils from Five *Eucalyptus* Species.

Maissa Lejmi [a], Bochra Kouidhi [b], Hajer Rhim [c], Maha Mastouri [d], Ameur Elaissi [a]

[a] *Laboratory of Chemical, Galenic and Pharmacological Drug Development-(LR12ES09),*
Faculty of Pharmacy, University of Monastir, Avicenne street, 5000, Monastir, Tunisia.
[b] *Laboratory of Analysis, Treatment, and Valorization of Environmental Pollutants and Products,*
Faculty of Pharmacy, University of Monastir, Monastir, Tunisia
[c] *Microbiology Laboratory, CHU Fattouma Bourguiba, Monastir, Tunisia*
[d] *Laboratory of Transmissible Diseases and Biologically Active Substances (LR99ES27),*
Faculty of Pharmacy, University of Monastir, Monastir, Tunisia

The global escalation of antibiotic resistance in respiratory pathogens, including *Streptococcus pneumoniae*, *Staphylococcus aureus*, and *Klebsiella pneumoniae*, represents a critical public health challenge[1,2]. As conventional treatments for pneumonia and sinusitis decline in efficacy, exploring natural alternatives is imperative. Recognized by the European Pharmacopoeia for their potent antiseptic properties, *Eucalyptus* essential oils (EOs) represent a significant reservoir of bioactive compounds with proven efficacy against respiratory tract infections[3].

This study investigates the chemical composition and biological potential of EOs extracted from five *Eucalyptus* species: *E. loxophleba*, *E. torquata*, *E. salmonophloia*, *E. oleosa*, and *E. longicornis*.

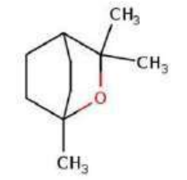
The EOs were extracted by hydrodistillation using a Clevenger-type apparatus. These oils were analyzed by GC/FID and GC/MS. Their antibacterial activities were tested against seven bacterial strains using two methods (disk diffusion and micro-dilution), and their antioxidant activities were evaluated against two free radicals, DPPH and ABTS. Data were interpreted through statistical analysis using SPSS 2023 software.

EO yields varied significantly among species ($p \leq 0,001$). Chemical analysis identified 115 compounds, representing between 95.40% and 98.10% of the total EOs. Their concentrations varied significantly depending on the species. Twenty-two major compounds (with a content > 2,0 % in at least one EO) were selected for statistical analysis. Four chemotypes were identified, such as the 1,8-cineole chemotype for *E. oleosa*.

Antibacterial activity varied significantly according to the EOs and the bacterial strains tested. The highest antibacterial activity was recorded for *E. longicornis* against all bacterial strains, even surpassing the effectiveness of amikacin. Structure-activity correlation shows that hydrocarbon monoterpenes (p-cymène, α-pinène) and terpenoids (trans-pinocarveol, globulol, thymol) are the most active against bacterial strains.

While antioxidant activity did not vary greatly between species and remained lower than that of Vitamin C, the *E. longicornis* EO rich in thymol, oxides, and terpenoids was the most active. These chemical families reduce free radicals through their antioxidant properties.

E. longicornis EO may serve as an alternative to antibiotics for treating certain respiratory infections of bacterial origin and for combating oxidative stress.



1,8 cineole

Keywords: *Eucalyptus* essential oils, Hydrodistillation, GS-analysis, Antibacterial activity, Antioxidant activity.

References

[1] Niederman MS, Torres A. Respiratory infections. Eur Respir Rev. 2022;31(166):1-2.

[2] Wang L, Qiao X liang, Ai L, Zhai J, Wang X xia. Isolation of antimicrobial resistant bacteria in upper respiratory tract infections of patients. 3 Biotech. 2016;6(2):166.

[3] European Directorate for the Quality of Medicines & HealthCare. **European Pharmacopoeia (Ph. Eur.)**. 11th ed. Strasbourg: Council of Europe; 2023.

Gelatin / Chitosan composite for wound healing applications

Amal Amor [1], Salma Bessalah [2], Samira Jbahi [1], Mustpha Hidouri [3]

[1] *Energy and Matter Research Laboratory, Centre National des Sciences et 3TechnologiesNucléaires (CNSTN),*
Pole technologique, 2020, Sidi Thabet-Tunisia
[2] *Livestock and Wildlife Laboratory, Arid Lands Institute (I.R.A), University of Gabès, Médenine, Tunisia*
[3] *Research laboratory: Energy, Water, Environment and processes, LREWEP (LR18ES35),*
National School of Engineers, University of Gabes, 6072 Gabes, Tunisia.

Gelatin (GEL) is a very attractive biomaterial for wound healing applications because they can retain cells and carry bioactive molecules such as growth factors. GEL has been classified as a biofriendly scaffold which interacts perfectly with cells, due to its similar structure to the extracellular matrix [1,2]. Gelatine (GEL)/ Chitosan (CH) wound dressing were prepared for wound healing applications. GEL-CH composite characterization and functional properties were determined with physico-chemical techniques such as Electron Paramagnetic Resonance (EPR), Fourier Transform Infrared spectroscopy (FTIR), X-ray diffraction (XRD) and impedance spectroscopy studies. Results revealed that EPR spectroscopy of un-irradiated GEL-CH showed 2 paramagnetic centers which correspond to g=2.077 and g= 2.079. After irradiation, no active centre was appeared. A dose-dependent decrease in the central signal intensity was detected then the ESR intensity almost disappears at 20 kGy. Gamma rays caused a slight increase in ion conductivity. FTIR measurements revealed decrease in peaks intensity and absorbance at C–H chains as well as C=O carboxyl groups at 20 kGy. XRD analysis does not show peak indicating crystallinity between a range of 2θ (15–30°). The current study, thus, reveals that GEL-CH composite could be effectively helpful in dressings for wound healing.

Keywords: Gelatin/Chitosan composite, Electron Paramagnetic Resonance, X-ray diffraction, Gamma Ray.

References

[1] Chaudhari AA, Vig K, Baganizi DR, Sahu R, Dixit S, Dennis V, Singh SR, Pillai SR. Future Prospects for Scaffolding Methods and Biomaterials in Skin Tissue Engineering: A Review. Int J Mol Sci. 2016 Nov 25;17(12):1974.

[2] Gurunathan S, Han JW, Eppakayala V, Jeyaraj M, Kim JH. Cytotoxicity of biologically synthesized silver nanoparticles in MDA-MB-231 human breast cancer cells. Biomed Res Int. 2013;2013:535796

Optimization and Modeling of Photocatalytic Degradation of anionic Dye Using Co-TiO_2/hemathite Catalyst

Sourour SALHI *[1, 2], Abdessalem OMRI [1], Ridha BEN SALEM [2], Mourad BENZINA [1]

[1] *Organic Chemistry Laboratory LR17ES08, Faculty of Sciences of Sfax, University of Sfax, Tunisia.*
[2] *Laboratory Eau Energie Environment (LR3E), Code: AD-10-02, Ecole Nationale d'Ingénieurs of Sfax, University of Sfax, Tunisia.*
Corresponding author E-mail: souroursalhi10@gmail.com

This study evaluates the catalytic effectiveness of the catalyst for the degradation of the azo dye Congo Red (CR) in an aqueous medium under heterogeneous photo-Fenton process. Using hydrogen peroxide, as an oxidant. The catalyst was prepared by a simple impregnation method from natural hematite. The hematite ferrous sample was characterized using several techniques such as : BET, SEM-EDX, XRD). Response surface methodology (RSM) was developed to reduce the number of experiments and reach optimal preparation conditions for the oxidation of CR dye. The parameters affecting the oxydation process, such as the mass of the catalyst, the concentration of the Congo Red dye and the pH of the solution, were studied. According to regression analysis, the experimental data and projected values showed an acceptable connection with an R^2 value of 0.9785. Based on the statistical data, the best conditions for the removal of the CR dye from aqueous solution by the prepared Co,TiO_2/Nat Hematite catalyst were: the mass of the catalyst 0.3 g, the concentration of the CR dye 50 mg/L and the pH of the solution 3. The maximum of oxidation, reached 91.06 %, using the previous conditions. The regeneration experiments proved that the resulting Co,TiO_2/Nat-Hematite catalyst still had a high removal capacity for Congo Red dye after three regeneration cycles. It has been demonstrated that natural hematite provides an appropriate support for the deposition of highly active and evenly distributed TiO_2 phases and cobalt.

Keywords: Dye removal ; Photo-Fenton Process; Natural hematite; Photochemical Oxidation

Isolation, characterization, and evaluation of the herbicidal potential of phytochemical compounds derived from *Inula viscosa* L.

Ilyes Saidi [1,2], Dhawya Mergby [3], Abdelkarim Ben Arfa [3], Mohamed Neffati [3],
Hanen Najjaa [3], Hichem Ben Jannet [1]

[1] Laboratory of Heterocyclic Chemistry, Natural Products and Reactivity (LR11ES39), Team: Medicinal Chemistry and Natural Products, Faculty of Science of Monastir, University of Monastir, Monastir, Tunisia.
[2] Higher School of Health Sciences and Techniques of Sfax (ESSTSS), University of Sfax, Sfax, Tunisia.
[3] Laboratory of Pastoral Ecosystems and Valorization of Spontaneous Plants and Microorganisms, Institute of Arid Regions Medenine, University of Gabes, Medenine, Tunisia.

Inula viscosa (syn. *Dittrichia viscosa*) is a perennial plant belonging to the Asteraceae family, widely distributed throughout the Mediterranean basin [1]. It is characterized by its viscous leaves rich in aromatic resins and by its late flowering period, from the end of summer until October, which promotes the presence of beneficial insects and serves as an important pollen source for bee overwintering. This plant has also been described as a source of fungicidal compounds against foliar diseases affecting several important crops, including cucumber, tomato, potato, wheat, and sunflower [2].

In order to further investigate the ecological and agronomic role of this plant, a phytochemical study was undertaken to explore its chemical composition and evaluate its allelopathic potential. This investigation led to the isolation of three sesquiterpenic acids (isocostic, viscic, and ilicic acids), as well as two sesquiterpene lactones (carabrone and inuviscolide). Their structures were determined using spectroscopic analyses (^{1}H and ^{13}C NMR) and by comparison with literature data. The isolated compounds were tested for their phytotoxic effects on the germination and growth of the weed *Setaria verticillata*. Among them, carabrone was identified as the allelochemical principle, exhibiting strong herbicidal potential, with complete inhibition observed at a concentration of 800 µM.

References

[1] Andolfi et al. (2013). Phytochemistry, 86, 112-120.
[2] Wang et al. (2004). Phytopathology, 94, 1042-1047.

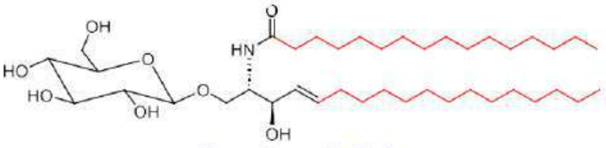
Synthesis of pyrrolidines as enzyme modulators targeting glucocerebrosidase: Application to Gaucher disease

Chadia YAKOUBI,[1,2] Cécile DEHOUX,[2] Mohamed Lotfi EFRIT,[1]
Aïcha ARFAOUI,[1] Yves GENISSON[2]

[1] *Laboratoire Synthèse organique sélective et hétérocyclique : Evaluation de l'activité biologique, Faculté de Sciences de Tunis, Université de Tunis El Manar, Tunisie.*
[2] *Laboratoire de Synthèse et Physico-Chimie de Molécules d'Intérêt Biologique (SPCMIB), UMR 5068, Université de Toulouse, France.*
Correspondance : chedia.yaakoubi@etudiant-fst.utm.tn

The pyrrolidine ring is one of the important and valuable heterocyclic compounds.[1] This five- membered ring containing nitrogen is also known as tetrahydropyrrole. This heterocyclic scaffold is present in medicinal and biological molecules as well as bioactive compounds and alkaloids due to the properties and characteristics of this ring.[2]

Various cyclization methods, such as the cycloaddition of amines and olefins, provide access to a wide variety of substituted pyrrolidine structures[3,4]. The study of the reactivity of these pyrrolidines, particularly in functionalization reactions, paves the way for the design of new immunosugar derivatives with improved pharmacological properties.[5] For example, in the case of Gaucher disease,[6] the most prevalent lysosomal storage disorder, the pathology is caused by mutations in the gene encoding the lysosomal enzyme glucocerebrosidase (GCase). The resulting decrease in GCase activity leads to the accumulation of glucosylceramide (GlcCer) within lysosomes, giving rise to a wide range of symptoms including hepatosplenomegaly, bone abnormalities, and neurological disorders.[7]



Glucosylceramide GlcCer

R_1 = H, alkyl, aryl
R_2 = H, OMe, OH, OC_6H_{13}, $-C_6H_{13}$

Pyrrolidines

In this context, we became interested in developing a new strategy for the synthesis of pyrrolidine derivatives from *α*-substituted dimethyl itaconate bearing *N*-, *O*- or *C*-alkyl chains, single or dialkyl, inspired by GlcCer and followed by evaluation of their activity on key enzymes, particularly GCase.

Key words: Pyrrolidines, Gaucher disease, lysosomal diseases, glucosylceramide, glucocerebrosidase.

References

[1] Nishida, A.; et al. Recent Advances in the Synthesis and Functionalization of Pyrrolidine Derivatives. *Chem. Rev*. **2020**, *120*, 3102.
[2] Vitaku, E.; Smith, D. T.; Njardarson, J. T. *Journal of Medicinal Chemistry*, **2014**, *57*, 10257.
[3] Compain, P.; Martin, O. R. *Actual. Chim*. **2007**, *307*, 25.
[4] Nájera, C.; Sansano, J. M. *Chem. Rev*. **2007**, *107*, 4584.
[5] Horne, G.; Wilson, F. X.; Tinsley, J.; Williams, D. H.; Storer, R. *Drug Discov. Today*. **2011**, *16*, 107.
[6] Kulkarni, A.; Chen, T.; Sidransky, E.; Han, T.-U. *Genes*, **2024**, *15*, 364.
[7] Parashuraman, S.; D'Angelo, G. *Chem. Phys. Lipids*. **2019**, *218*, 10.

Synthesis and *In Silico* Evaluation of Coladonin Derivatives as Potential Carbonic Anhydrase IX Inhibitors

Sadok Lamine BEN NEJMA [a], Mohamed OTHMAN [b],
Hichem BEN JANNET [a], Mansour ZNATI [a]

[a)] *Laboratory of Heterocyclic Chemistry, Natural Products and Reactivity (LR11ES39), Team: Medicinal Chemistry and Natural Products, Faculty of Sciences of Monastir, University of Monastir, Avenue of Environment, 5019 Monastir, Tunisia.*
[b)] *Normandie University, URCOM, UNILEHAVRE, FR3021, UR 3221, 25 Rue Philippe Lebon, BP 540, F-76058 Le Havre, France.*

Human carbonic anhydrases are vital pH-regulating enzymes, with isoforms IX and XII serving as key cancer targets reachable through various inhibitors. Among these, coumarins act uniquely by blocking the entrance to the active site rather than binding directly to the zinc ion[1]. Coladonin is a natural sesquiterpene coumarin isolated from the Tunisian endemic plant, *Ferula tunetana,* was known to have interesting cytotoxic activity[2]. Also, this natural molecule showed a selective inhibition of carbonic anhydrase XI and XII, which are expressed in hypoxic tumors[3].

As part of our ongoing interest in the valorization of natural bioactive compounds, we extracted coladonin from *F. tunetana* seeds then and performed chemical modifications (alkylation and [3+2] cycloaddition) to synthesize novel derivatives with promising anticancer potential. Subsequently, *in silico* studies were conducted to predict ADME (Absorption, Distribution, Metabolism, and Excretion), toxicity, and binding affinity of these molecules toward carbonic anhydrase IX and anticancer efficacy.

Key words: *F. tunetana,* Coladonin, [3+2] cycloaddition, Carbonic anhydrase IX, *In silico.*

---

[1] Supuran, C. T. (2020). “Coumarin carbonic anhydrase inhibitors from natural sources”. J. Enzyme Inhib. Med. Chem. **35** (1), 1462−1470.

[2] Jabrane, A., et al. (2010). "Two New Sesquiterpene Derivatives from the Tunisian Endemic Ferula tunetana Pom." Chemistry & Biodiversity **7**(2): 392-399.

[3] Mustafa, M., et al. (2025). "Selective Inhibition of Carbonic Anhydrase IX and XII by Natural Coumarin Coladonin and Its Derivatives: Promising Antimelanoma and Antiglioblastoma Agents." ACS Medicinal Chemistry Letters **16**(6): 1190-1196.

Design, synthesis, and *in silico* investigations of novel alkyl-phosphonate derivatives tethered to the antibiotic Ciprofloxacin

Mabrouk HORCHANI, Hichem BEN JANNET, Anis ROMDHANE

Laboratory of Heterocyclic Chemistry, Natural Products and Reactivity (LR11ES39), Team: Medicinal Chemistry and Natural Products, Faculty of Science of Monastir, University of Monastir, Avenue of Environment, Monastir 5019, Tunisia

Ciprofloxacin was patented in 1983 by Bayer A.G. and approved in 1987 by the United States Food and Drug Administration (USFDA) [1] Ciprofloxacin is an antibiotic agent in the fluoroquinolone class used to treat bacterial infections such as urinary tract infections and pneumonia [2].

Encouraged by the aforementioned findings, we designed and synthesized a series of novel hybrid derivatives of Ciprofloxacin using the Arbuzov reaction as the key synthetic strategy. This approach involved the reaction of appropriate intermediates with a range of trialkyl phosphites, enabling the introduction of phosphonate-based functionalities and the generation of structurally diverse ciprofloxacin–phosphonate hybrids. Additionally, theoretical studies were conducted to investigate the predicted biological potential of the synthesized compounds. In particular, molecular docking analyses were performed to evaluate their possible inhibitory mechanisms against target Enzymes. The findings showed significant intermolecular interactions with key amino acid residues within the active site, suggesting promising inhibitory activities. These interactions suggest that the synthesized derivatives may exhibit promising inhibitory activity and could serve as potential candidates for further biological evaluation.

References

[1] Zhang HL, Tan M, Qiu AM, Tao Z, Wang CH. Antibiotics for treatment of acute exacerbation of chronic obstructive pulmonary disease: a network meta-analysis. BMC Pulm Med. 2017 Dec 12;17(1):196.

[2] Sharma PC, Jain A, Jain S, Pahwa R, Yar MS. Ciprofloxacin: review on developments in synthetic, analytical, and medicinal aspects. J Enzyme Inhib Med Chem. 2010 Aug;25(4):577-89.

Synthesis and Photophysical Characterization of Novel Acridine-Based Hybrids

Najeh TKA and Peter Langer

Laboratory of Asymmetric Synthesis and Molecular Engineering for Organic Electronic Materials (LR18ES19),
Monastir University, Faculty of Sciences of Monastir
Universität Rostock, Institut für Chemie, Albert-Einstein-Str.3a, 18059 Rostock, Germany
najeh_tka@yahoo.fr

The acridine scaffold consists of rigid nitrogen containing tricyclic aromatic system that forms an extended π-conjugated planar structure favoring efficient electronic delocalization. The incorporation of additional electronically active fragments into the acridine core can further enhance π–π stacking interactions and modulate the electronic distribution within the molecule. Such structural modifications play a key role in tuning the photophysical behavior of acridine-based hybrids, leading to characteristic optical properties. Our recent research work[1,2] focuses on the design and synthesis of new 2,4-diaryl and 2,4-bis(arylethynyl)-9-chloro-5,6,7,8-tetrahydroacridine via one-pot double Sonogashira and Suzuki–Miyaura cross-coupling. The resulting compounds were subjected to optical and electrochemical investigations, including evaluation of UV-visible absorption and fluorescence properties, and were further analyzed using density functional theory (DFT) calculations to explore their electronic structures and frontier molecular orbital profiles. These studies afford insights into the electronic and photophysical behavior of tetrahydroacridine scaffolds, which are important prerequisites for the rational design of acridine derivatives with potential applications in medicinal chemistry and materials science

Keywords: novel acridine derivatives, cross-coupling reactions, optical and electrochemical investigations, materials science.

References

1. Tka, N.; Hadj Ayed, M.A.; Ben Braiek, M.; Jabli, M.; Langer, P. *Beilstein J. Org. Chem.,* **2021**, 17, 2450-2461.

2. Tka, N.; Hadj Ayed, M.A.; Ben Braiek, M.; Jabli, M.; Chaaben, N.; Alimi, K. ; Jopp, S. ; Langer, P. *Beilstein J. Org. Chem.*, **2021**, 17, 1629–1640.

Influence of Hydrodistillation Time Intervals and Drying Period on the Yield, Chemical Composition, and Antioxidant activities of stems essential oils of *Pituranthos chloranthus* from the Er-hiba-Gafsa Provenance (Southern Tunisia)

Ahlem Yahya[ab], Amani Ayachi[c], Fatma Chtourou[d], Zina Benissa[a], Nathan TENE[e]; Raoudha Jarraya[c], Michel Treilhou[e], Sami Zouari[a,f]

a) Laboratory of Medicinal and Environmental Chemistry, High Institute of Biotechnology of Sfax, University of Sfax, Tunisia
b) Faculty of Sciences of Gafsa, University of Gafsa
c) Laboratory of Organic Chemistry LR17ES08, Natural Substances Team, Faculty of Sciences of Sfax, University of Sfax, P.B 1171, Sfax 3000, Tunisia
d) Laboratory of Electrochemistry and Environment, National School of Engineers of Sfax, University of Sfax, Sfax, Tunisia
e) Equipe BTSB-EA 7417, Institut National Universitaire Jean-François Champollion, Université de Toulouse, Place de Verdun, 81012 Albi, France
f) Engineering National School of Sfax, University of Sfax, Sfax, Tunisia

The main objective of this study was to investigate the influence of hydrodistillation time intervals (0–60, 60–120, 120–180, and 180–240 min) and drying duration (one month (OM) and one year (OY)) on the yield, chemical composition, and antioxidant activities of stems essential oils (EOs) of *P. chloranthus* collected from the Er-hiba-Gafsa provenance. EOs yields were highest during the early interval (0–60 min), with OM samples producing a higher yield (0.53%) compared to OY samples (0.45%). The major constituents were α-pinene and *α*-phellandrene (monoterpene hydrocarbons), *L*-terpinen-4-ol (oxygenated monoterpene), *cis*-asarone and allyltetramethoxybenzene (phenylpropanoids), which allowed the identification of four new chemotypes. Regardless of hydrodistillation time, *cis*-asarone was occurred at relatively higher rates in the dried stems EOs for OM compared to OY. Antioxidant activities were evaluated using DPPH and FRAP assays. Stem EOs dried for one year and hydrodistilled at 0–60 min and 120–180 min exhibited the strongest antioxidant activities, with IC_{50} values of 0.72 and 0.74 mg/mL, respectively, and the same value of EC_{50} (1.55 mg/mL) for both hydrodistillation times. Overall, these results demonstrate that drying duration and hydrodistillation time were the key determinants of Er-hiba-Gafsa stems EOs yields, their chemical compositions, and their antioxidant activities.

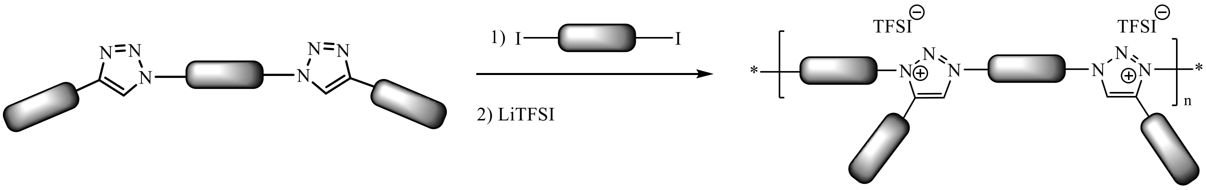
Key words: *Pituranthos chloranthus*; essential oil hydrodistillation time; drying duration; antioxidant activities; chemotype.

Oligo(ethylene glycol)-based Poly(1,2,3-triazolium) Ionenes obtained by *N*-Alkylation Step Growth Polymerization

Imen Abdelhedi-Miladi,[a] Eric Drockenmuller,[b] and Hatem Ben Romdhane [a]

[a] Université de Tunis El Manar, Faculté des Sciences de Tunis, Laboratoire de Chimie (Bio)Organique Structurale et de Polymères (LR99ES14), Tunis, El Manar, 2092, Tunisia
[b] Université Claude Bernard Lyon 1, CNRS, Ingénierie des Matériaux Polymères, UMR 5223, Lyon, 69622, France

Poly(ionic liquid)s (PILs) and ionenes are promising polyelectrolytes for energy storage and separation.[1,2] PILs are generally prepared from ionic liquid monomers or by post-polymerization modification, whereas ionenes are obtained by Menshutkin step-growth polymerization (poly(*N*-alkylation)). CuAAC polyaddition enables access to poly(1,2,3-triazolium)s PILs via post-polymerization *N*-alkylation of neutral poly(1,2,3-triazole)s,[3] but their direct synthesis via poly(*N*-alkylation) has not yet been reported. Herein, we report the first synthesis of poly(1,2,3-triazolium) ionenes (PTIs) via AA+BB step-growth polymerization of oligo(ethylene glycol)-based bis(1,2,3-triazole)s, prepared by CuAAC, with α,ω-diiodotetraethylene glycol, followed by anion metathesis with LiTFSI (Scheme 1).



Scheme 1: Synthesis of poly (1,2,3-triazolium)s ionenes

The resulting materials were characterized by NMR, ESI-HRMS, TGA, and DSC. PTIs showed ionic conductivity up to 4.5×10^{-5} S cm^{-1} at 30 °C under anhydrous conditions, as determined by broadband dielectric spectroscopy. This work introduces a straightforward and unprecedented route to 1,2,3-triazolium-based ionenes, thereby broadening the scope of main-chain polyelectrolytes for electrochemical applications.

Key words: 1,2,3-triazolium, CuAAC, Ionenes, Ionic conductivity.

References

[1] Yuan, J., Mecerreyes, D., Antonietti, M. Prog. Polym. Sci. 2013, 38 (7), 1009–1036.
[2] Lee, J. S., Hocken, A., Green, M. D. Mol. Syst. Des. Eng. 2021, 6 (5), 334–354.
[3] Dimitrov-Raytchev, P., Beghdadi, S., Serghei, A., Drockenmuller, E. J. Polym. Sci. Part Polym. Chem. 2013, 51 (1), 34–38.

Preparation and characterization of a novel polysulfone (PSF) ultrafiltration membrane modified with zinc oxide-graphene oxide (ZnO-GO) nanocomposites to improve permeability and antifouling properties

Hajer Aloulou [1,2*], Raja Ben Amar [1]

[1] *Research Unit 'Advanced Technologies for Environment and Smart Cities',*
Faculty of Sciences of Sfax, University of Sfax, Tunisia
[2] *Department of Chemical, Preparatory Institute for Engineering Studies of Gabes,*
University of Gabes, Gabes 6029, Tunisia
* Corresponding author. Email: hajer.aloulou89@yahoo.fr

Effluents from pharmaceutical industry pose significant environmental threats due to their complex and recalcitrant nature, including low biodegradability, high organic load, and the presence of emerging contaminants such as pharmaceutical residues. In this study, polysulfone (PSF) ultrafiltration membranes were modified with zinc oxide-graphene oxide (ZnO-GO) nanocomposites at varying loadings (0.6 and 1.2 wt.%) via the phase inversion method to enhance their separation efficiency and photocatalytic performance. Physicochemical characterization was performed using scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDXS), Fourier transform infrared spectroscopy (FTIR), contact angle analysis, and mechanical strength testing. The photocatalytic performance of the membranes was evaluated through the degradation of diclofenac (DCF), a model pharmaceutical contaminant, under UV irradiation (24 W) at an operating pressure of 3 bar. The membrane incorporating 0.6 wt% ZnO-GO exhibited the best overall performance, achieving a high-water flux of 19.12 L m^{-2} h^{-1} bar^{-1} and an 80% DCF removal efficiency. Furthermore, antifouling evaluation using bovine serum albumin (BSA) demonstrated a rejection rate of 91% and a flux recovery ratio (FRR) exceeding 86%, indicating strong resistance to fouling. These results demonstrate the potential of PSF/ZnO-GO nanocomposite membranes as high-performance, multifunctional systems for the advanced treatment of pharmaceutical wastewater, combining efficient filtration with photocatalytic degradation capabilities.

Keywords: PSF; ZnO-GO; Mixed Matrix Membrane; Diclofenac; Photodegradation, Antifouling properties

Carbon Nanoparticle-Carbazole Polymer Nanocomposites for Resistive Detection of Volatile Organic Compounds

Fatma BHIRI, Mejed CHEMLI, Naoufel SAKLY, Mustapha MAJDOUB

Interfaces and Advanced Materials Laboratory (LIMA), Faculty of sciences of Monastir, TUNISIA.

In this work, a carbazole-based semiconducting polymer synthesized via Wittig polycondensation was employed for the development of nanocomposite materials dedicated to the resistive detection of volatile organic compounds (VOCs). Thin sensing layers were prepared by dispersing spherical carbon nanoparticles (~40 nm) into a solution of the conjugated polymer, followed by deposition onto interdigitated resistive transducers using a drop-casting technique.

The electrical properties of the nanocomposites were investigated as a function of the carbon nanoparticle content. A typical percolation behavior was observed, with the electrical resistance decreasing significantly as the nanoparticle loading increased. The percolation threshold was determined at approximately 20.8 wt% of carbon nanoparticles, corresponding to the formation of a three-dimensional conductive network within the polymer matrix.

The sensing performance of the nanocomposite layers was evaluated toward several volatile organic compounds including methanol, ethanol, isopropanol, chloroform, dichloromethane, acetone, toluene, dimethylformamide and acetic acid. While most vapors produced negligible responses, significant resistive variations were observed for chloroform, dichloromethane and acetone, with the strongest response obtained for chloroform.

The optimized nanocomposite containing 20 wt% carbon nanoparticles exhibited reversible sensing behavior and a quasi-linear response toward chloroform concentrations in the ppm range, with a detection limit of 94.65 ppm. The sensing mechanism is attributed to the combined effects of electrical percolation and polymer swelling induced by solvent–polymer interactions. These results highlight the potential of carbazole-based semiconducting polymer/carbon nanoparticle nanocomposites as promising materials for VOC sensing applications.

Keywords: Carbazole-based semiconducting polymer, Nanocomposites, Resistive gas sensors, Percolation threshold, Chloroform detection

PEBAX membranes for water desalination by pervaporation process

Sofiane Ben Hamouda [a], Nadia Chaarana [a], and Alberto Figoli [b]

[a)] *CRMN, Centre for Research on Microelectronics and Nanotechnology of Sousse, NANOMISENE Lab, LR16CRMN01,4054,Technopark of Sousse, Tunisia*

[b)] *Institute on Membrane Technology, ITM-CNR, Via P. Bucci 17/c, 87036 Arcavacata di Rende (CS), Italy*

Hydrophobic dense membrane PEBAX were prepared, and their suitability for a water pervaporation process was studied. The effects of the following parameters on the water flux were determined as operating conditions [brine inlet temperature (28–54°C) and NaCl concentration in the feed brine (0–3.5 mol L^{-1})]. A water flux of 1.3–7 g m^{-2} h^{-1} was obtained using this type of membranes. It was found that, for our application, the optimal specifications for our membrane is a thickness of 100 mm and an operating temperature of 50°C that allow us to have a water flux of 7 g m^{-2} h^{-1} in the permeate side. These data are required for the manufacturing of a novel desalination system based on this type of dense membranes.

Keywords: PEBAX membrane ; pervaporation ; permeate flux ; activation energy

Engineering Donor–Acceptor PPV–PFO Copolymers for Advanced Organic Optoelectronic Devices

Hlimi Haythem,[1] Mohamed Mbarek*

* hlimihaythem1@gmail.com
mohamedmbarek99@yahoo.fr

[a] *LR: Synthèse asymétrique et ingénierie moléculaires des matériaux nouveaux pour l'électroniques Organiques (LR18ES19) Faculté des Sciences de Monastir, Université de Monastir-Tunisie.*

[b] *Faculty of Sciences Gabes, University of Gabes*

A novel donor–acceptor PPV–PFO diblock copolymer was successfully designed and synthesized through an oxidative polymerization strategy. The material was thoroughly characterized using infrared spectroscopy (IR), Raman spectroscopy, thermogravimetric analysis (TGA), UV–visible absorption, photoluminescence (PL), and time-resolved photoluminescence (TRPL) to investigate its structural, thermal, and photophysical properties. The copolymer displays excellent thermal stability and broad absorption across the visible spectrum, accompanied by a reduced band gap relative to the individual homopolymers. In addition, efficient Förster resonance energy transfer between the PPV and PFO segments significantly enhances the exciton lifetime. These results highlight the promising potential of the synthesized copolymer for advanced organic optoelectronic applications.

Key words: Donor-acceptor architecture; Photophysical properties; Organic optoelectronics; conjugated polymers

Extraction, Structural Analysis, and Applications of Star Anise Polysaccharide

Ameni Macherki (a), Mariem Itaimi Dammak (b), Didier Le Cerf (c), Marcel Rey (d),
Hatem Majdoub(b), Anis Romdhane(a)

(a) Monastir University, Laboratory of Heterocyclic Chemistry, Natural Products and Reactivity, Faculty of Sciences of Monastir, Monastir 5000, Tunisia (a)
(b) Monastir University, Laboratory of Interfaces and Advanced Materials, Faculty of Sciences of Monastir, Monastir 5000, Tunisia (b)
(c) Normandie University, UNIROUEN, INSA Rouen, CNRS, PBS, 76000 Rouen, France (b)
(d) Münster University, Institute of Physical Chemistry, Corrensstr. 28/30, 48149 Münster, Germany(d)

Illicium verum (star anise) is an aromatic plant rich in bioactive compounds. In this study, a water-soluble polysaccharide was extracted from its seeds and characterized using FTIR, UV-Vis, and SEC analyses to evaluate its chemical, physicochemical, and structural properties. The results revealed the presence of typical carbohydrate functional groups and a homogeneous molecular weight distribution, indicating good structural stability. This polysaccharide is mainly composed of neutral sugars and exhibits good water solubility. Its rheological properties and gel-forming ability were evaluated, showing interesting viscoelastic behavior. Moreover, it demonstrated potential applications as a thickening, stabilizing, and emulsifying agent in food, cosmetic, and pharmaceutical systems. The effect of polysaccharide concentration on the viscosity and stability of emulsions was systematically investigated, revealing a positive correlation between concentration and emulsion stability. Its biodegradability and non-toxicity further highlight its potential as a sustainable alternative to synthetic polymers. These findings provide insights into the structure–function relationship of the star anise polysaccharide and emphasize its applicability in designing environmentally friendly formulations with enhanced functional performance.

Keywords: *Illicium verum*, polysaccharide, emulsions, sustainability

A Structural and Dynamic Comparison of Gelatin- and Ovalbumin-Based Coacervates

Mohamed Rjili *, Adel Aschi

Laboratory of Physics of Soft Matter and Physics of Fluids, LR99ES16,
Faculty of Sciences of Tunis, University of Tunis El Manar, 2092 Tunis, Tunisia
* Presenting author. Tel: (+216) 40979359; E-mail: mohamed.rjili@fst.utm.tn

The complexation between proteins and polyelectrolytes is a fundamental process with extensive applications, from food science to drug delivery. This study provides a comprehensive comparative analysis of the structure and dynamics of complexes formed between a single strong polyanion, poly(4-styrenesulfonic acid-co-maleic acid) sodium salt (PSSMA), and two distinct protein partners: Gelatin and Ovalbumin (OVA). We selected these proteins to represent two extremes of protein structure and flexibility—Gelatin being a large, flexible, and amphoteric protein, and Ovalbumine being a small, rigid, globular one. Our research began by systematically mapping the phase behavior of both systems as a function of solution pH using turbidimetry. This allowed us to precisely identify the critical pH values and the optimal coacervation points where aggregation is at its peak. To further characterize the internal structure of the aggregates, we utilized ultra-small angle light scattering (USALS) across the entire pH range. This powerful technique revealed key structural differences between the PSSMA-Gelatin and PSSMA-OVA aggregates, providing detailed insights into their internal architecture. To specifically probe the slow dynamics of the dense phase, we employed image dynamic light scattering (IDLS) at the point of optimal coacervation. Our findings reveal that the choice of protein partner significantly impacts every aspect of the complexation process. We observed substantial differences in the critical pH values required for complex formation, the internal structures of the resulting aggregates, and the slow dynamics of the coacervate phase. These results offer critical insights into how the intrinsic properties of a protein—such as its flexibility, charge distribution, and size—fundamentally dictate the final properties of the resulting polyelectrolyte-protein materials. Ultimately, this work highlights the crucial role of protein choice in the rational design and engineering of functional materials.

Keywords: Complex Coacervation, Protein, Polyelectrolyte, Ultra-Small Angle Light Scattering (USALS), Fractal Structure, Image Dynamic Light Scattering (IDLS)

Coupling UV Irradiation and Electrospinning for Advanced Polyurethane Filtration Membranes

Anne-Sophie Schuller [1*], Xenia Moreno [1, 2], Emeline Lobry [2], Christian Ley [1]

[1] *Laboratoire de Photochimie et d'Ingénierie Macromoléculaire, Mulhouse, France*
[2] *Institut de Chimie des Procédés pour l'Énergie, l'Environnement et la Santé, Strasbourg, France*
[*]e-Mail: anne-sophie.schuller@uha.fr

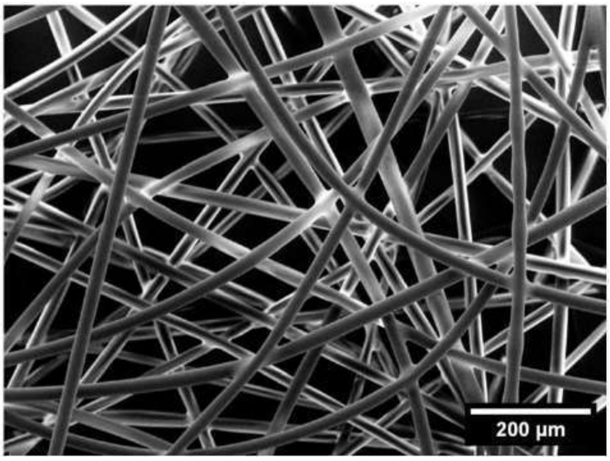


Figure 1. SEM image of fibers obtained by electrospinning under UV irradiation at 200 mW/cm^2

Electrospinning is a technique enabling the production of nonwoven fibrous mats through the emission of a polymer solution jet subjected to an electric field.[1] This process results in fibers with diameters typically ranging from a few hundred nanometers to several micrometers.[2] Electrospinning is characterized by a residence time between the needle and the collector of less than one second, associated with a jet velocity on the order of 0.5 m·s^{-1}.[3] Similarly, jet elongation strongly depends on the viscoelastic properties of the solution, making their control-together with a sufficiently fast polymerization kinetics-one of the major challenges in coupling electrospinning with UV-induced polymerization. The aim of this work is to demonstrate the feasibility of in-flight, in situ photopolymerization coupled with electrospinning, using solvent-free formulations, for the development of fibrous membranes. Accordingly, the kinetics and photo-rheological properties of polyurethane acrylate (PUA) oligomer formulations were investigated, despite their sensitivity to oxygen. To limit oxygen inhibition, a thiol was introduced as a hydrogen donor, enabling the regeneration of active radicals capable of sustaining the polymerization.[4] The formulations were processed using a coupled electrospinning/UV setup at irradiances ranging from 150 to 200 mW·cm^{-2}. Fibrous mats with an average fiber diameter of 22 ± 3.7 µm (Figure 1) were obtained, demonstrating the feasibility of the approach and opening new pathways for the preparation of electrospun membranes.

References

1. Xue, J., Wu, T., Dai, Y., Xia, Y. *Chem. Rev.*, 2019, **119**, 5298–5415.
2. Greiner, A., Wendorff, J. H. *Angew. Chem. Int. Ed.*, 2007, **46**, 5670–5703.
3. Bellan, L. M., Craighead, H. G., Hinestroza, J. P. *J. Appl. Phys.*, 2007, **102**, 094308.
4. Courtecuisse, F., Cerezo, J., Croutxé-Barghorn, C., Dietlin, C., Allonas, X. *J. Polym. Sci. Part Polym. Chem.*, 2013, **51**, 635–643.

Removal of Methyl Green dye by new biocomposite (activated carbon/polyaniline)

Imen Zouidi [a,b]; Amel Ben Slimane [c]; Safa Gamoudi [a]

[a] *Laboratory of Composite Materials and Clay Minerals, National Center for Research in Materials Science, Technopole Borj Cedria, B.P. 73, 8027, Soliman, Tunisia*
[b] *University of Gafsa, Faculty of Sciences of Gafsa, Gafsa 2112, Tunisia.*
[c] *University of Gafsa, Faculty of Sciences of Gafsa, Laboratory for the Application of Materials to the Environment, Water and Energy (LR21ES15), Gafsa 2112, Tunisia.*
Email: hajerzwidi@gmail.com

The development of industrial activity causes the emission of various toxics effluents in the environment which pose a threat to the ecosystem. Therefore, their elimination has become a priority and constitutes currently a major preoccupation for scientists. In this context, we have focused our research to synthesize the new composite based on conductive polymer and activated carbon locally available source such as Thymelaea hirsuta wood THW. We initially started our work by the pretreatment and carbonization of the THW, and then we prepared a conductive composite THW/PANI by the In-situ chemical polymerization method. Subsequently, the composite was applied for the removal of Methyl Green dye (MG) from aqueous solutions. Experimental parameters such as temperature, contact time, initial dye concentration, and adsorbent mass were studied. The equilibrium isotherms were analyzed using the Freundlich and Langmuir models. BET analysis confirmed the presence of a mesoporous structure and found a specific surface area of 10.20 m^2/g and a pore diameter of 187.14 Å. Adsorption equilibrium was achieved within 70 minutes, as determined by kinetic analysis. Pseudo-second-order kinetics described MG adsorption. Freundlich modeling showed maximum adsorption capacities of 10.10 mg/g at 70mg/L of MG. The adsorption was spontaneous and exothermic, consistent with thermodynamic parameters. Isosteric heat of adsorption indicated physisorption with weak intermolecular interactions between the dyes and the composite surface.

Keywords: carbon, PANI, composite, adsorption, methyl green.

Designed from Chemically Recycled Polyethylene Furanoate Packaging

Nesrine Gasmi [1,2], Leila Khalfa [3,4], Gabriele Rossignolo [5],
Alessandra Lorenzetti [5], Younes Moussaoui [1,6]

[1] *University of Gafsa, Faculty of Sciences of Gafsa, Gafsa 2112, Tunisia*
[2] *University of Gafsa, Faculty of Sciences of Gafsa, Laboratory of Application of Materials to Environment, Water and Energy (LR21ES15), Gafsa 2112, Tunisia*
[3] *Applied Thermodynamics Unit Research, ENIGabes, Zrig Gabes, Tunisia*
[4] *National School of Engineers of Gafsa (eniga), University of gafsa, 2112, Gafsa, Tunisie*
[5] *Università di Padova, Dept. of Industrial Engineering, Via F. Marzolo 9, 35131 Padova, Italy*
[6] *University of Sfax, Faculty of Sciences of Sfax, Organic Chemistry Laboratory (LR17ES08), Sfax 3000, Tunisia*
Email address: nesrinegasmi.g@gmail.com ; y.moussaoui2@gmail.com

Chemical recycling by depolymerization has become a very important future end-of-life option for turning plastics highly resistant to biodegradation into a portfolio of useful chemicals. One bottleneck for chemical recycling, is however, the high energy demand and often long reaction times required. Aminolysis has been suggested as a relatively cost-effective and easy-to-implement feedstock recycling pathway. Microwave irradiation, a well-established technique in organic synthesis, has also been successfully employed in the chemical recycling of plastics. In the present work, an efficient and fast end-of-life management option for non-degradable polyethylene furanoate (PEF) thermoplastic, a promising fully biobased alternative to PET, was established. This chemical recycling approach involves transforming PEF polyester, through catalyst- and solvent-free microwave-assisted aminolysis, into two new value-added furanoate diamines featuring high melting points (T_m>140°C). To prove their suitability in polymerization, the imine polycondensation of prepared monomers with an aromatic dialdehyde was successfully carried out under mild conditions, yielding two novel aromatic-aliphatic polyimines. The latter are semi-crystalline materials exhibiting good thermal performance, high T_m values in the range of 160-295 °C, and an excellent resistance to heat up to 365°C. Such attractive thermal properties are highly demanded in a wide range of practical applications, including aerospace, automotive, and electronics. Transforming sustainable furanoate-based packaging materials into a library of new diamine-type building blocks and high-performance polyimines, rather than sending them to landfill or incineration, is an important strategy to add value to waste and help reduce plastic pollution.

Keywords: Polyethylene Furanoate; Chemical recycling; Aminolysis; Schiff-base; Polyimine; Polyester

Sustainable Biochar-Based Metal Oxide Composites for Enhanced Adsorption and Photocatalytic Degradation of Organic Dyes

Fatma Ghammagui, Salah Ammar

Research laboratory; Chemistry, Electrochemistry, and Materials for Environment.
Faculty of Sciences of Gabes; University of Gabes, 6072 Gabes, Tunisia
Email: ghammaguifatima339@gmail.com ; Mobile Number: +216 95 12 19 26

The discharge of dye-containing effluents from industrial activities represents a significant environmental concern due to their toxicity, persistence, and resistance to conventional treatment methods. Developing sustainable, low-cost, and efficient materials for wastewater remediation remains a critical challenge.

In this study, biomass valorization was employed to produce biochar via pyrolysis under oxygen-limited conditions. Several biomass sources were initially screened based on their adsorption capacity toward model organic dyes, and the most efficient precursor was selected for further composite fabrication.

Biochar-based metal oxide composites were subsequently synthesized to enhance both adsorption and photocatalytic degradation performance. The materials were evaluated through UV–Visible spectrophotometry, monitoring the decrease in dye absorbance over time under irradiation.

The composite systems exhibited significantly improved removal efficiency compared to individual components, demonstrating a clear synergistic effect. The enhanced performance is attributed to improved surface adsorption properties and more efficient separation of photogenerated charge carriers, leading to increased reactive species formation.

These findings highlight the potential of biochar-based hybrid materials as sustainable and effective candidates for advanced wastewater treatment applications.

Keywords: Biochar; Biomass; Metal oxides; Photocatalysis; Adsorption; Wastewater treatment.

Program of
Saturday 02
May 2026

Biological Evaluation and Molecular Docking Studies of Pyrrolidinones and Pyrrolinones as Potential Antibacterial Agents

Nadia KRISSAANE,[1] Rania Hammami,[2] Najla Sadfi-Zouaoui,[2]
Aïcha Arfaoui,[1] Mohamed Lotfi Efrit[1]

[1] Selective and Heterocyclic Organic Synthesis Laboratory: Evaluation of Biological Activity LR17ES01, Faculty of Sciences of Tunis, University of Tunis El Manar, 2092 Tunis, Tunisia.
[2] Laboratory of Mycology, Pathologies and Biomarkers LR16ES05, Faculty of Sciences of Tunis, University of Tunis El Manar, 2092 Tunis, Tunisia.
Correspondance : krissaane.nadia@etudiant-fst.utm.tn

Functionalized γ-butyrolactams are important scaffolds in organic and medicinal chemistry.[1],[2] In this study, efficient conjugate addition-cyclization strategies enabled the synthesis of saturated and unsaturated γ-lactams and assess their antibacterial activity. Pyrrolidin-2-ones were obtained from dimethyl itaconate and primary amines under mild conditions,[3] while pyrrolin-2-ones were synthesized from dimethyl α-bromomethylfumarate via Michael addition followed by cyclization.[4] Evaluation against Escherichia coli, Staphylococcus aureus, Pseudomonas aeruginosa, and Enterococcus faecalis showed that antibacterial activity was influenced by both ring system and substitution pattern. Molecular docking[5] with the LasR protein of *P. aeruginosa* indicated favorable binding interactions, supporting the biological results. These findings support the potential of this class of compounds for further antibacterial development.

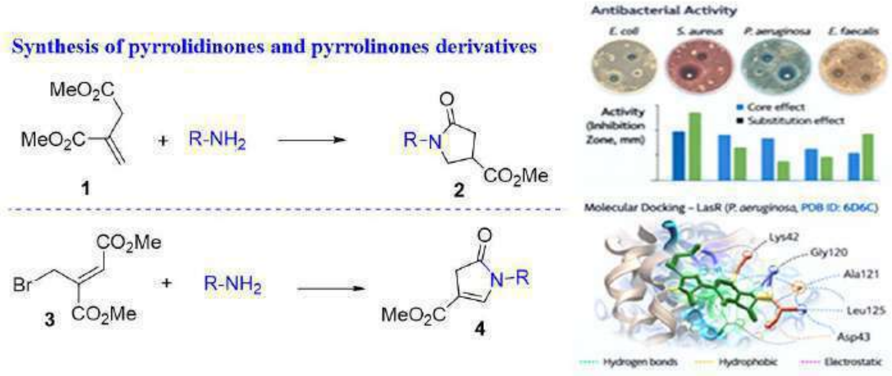


Figure 1: LasR docking and key active-site interactions.

Keys words: Pyrrolidinones, pyrrolinones, itaconic diester, primary amines, antibacterial activity.

References:
[1] Anusevičius, K.; Slaninaitė, E.; Jonuškienė, I.; Sapijanskaitė, B.; Vaickelionienė, R.; Mickevičius, V. *Chem. Technol.* **2014**, *65*, 1.
[2] Asif, M.; Alghamdi, S. *Russ. J. Org. Chem.* **2021**, *57*, 1700.
[3] Mansour, T. S.; Jin, H. *Bioorg. Med. Chem. Lett.* **1991**, *1*, 757.
[4] Beshes, R.; Villiéras, M.; Amri, H. *Indian J. Chem., Sect. B* **1997**, 5.
[5] D. Duhovny, R. Nussinov, H.J. Wolfson, *Lect. Notes Comput. Sci.* **2002**, *2452*, 185.

Efficient Synthesis of Quinazoline Derivatives via Cyclization of 2-Aminobenzamide with Ethyl Chloroformate

D. Saidani and R. Abderrahim

University of Carthage, Faculty of Sciences of Bizerte, Laboratory of Ressources Matériaux, Valorisation et Écosystème (RME code LR19ES20), Zarzouna 7021, Bizerte, Tunisia

Quinazolines represent an important class of nitrogen-containing heterocycles with wide applications in medicinal and organic chemistry. In this work, we report an efficient approach for the synthesis of quinazoline derivatives through the cyclization of 2-aminobenzamide with ethyl chloroformate ($ClCO_2Et$) as the cyclizing reagent.

The reaction proceeds under mild conditions and affords the quinazoline framework in good to excellent yields. This protocol provides a straightforward pathway with limited formation of side products and avoids the use of harsh reaction conditions. The structures of the synthesized compounds were confirmed by IR, ^1H NMR, and ^{13}C NMR spectroscopy, supporting the successful formation of the targeted heterocyclic system.

This method represents a practical and reliable strategy for the preparation of quinazoline derivatives and may serve as a useful platform for the development of biologically relevant heterocyclic molecules.

Synthesis and characterization of a push–pull dinitropyridine derivative for non-linear optics

Takwa SLAMA,[a] Sahbi AYACHI,[b] and Taoufik BOUBAKER[a]

[a] *Laboratory of Heterocyclic Chemistry, Natural Products and Reactivity (LR11SE39), Faculty of Sciences of Monastir, University of Monastir, Avenue de l'Environnement, 5019 Monastir, Tunisia.*

[b] *Laboratory of Physico-Chemistry of Materials (LR01ES19), Faculty of Sciences, University of Monastir, Avenue of the Environment, 5019 Monastir, Tunisia*

This study presents a multi-faceted characterization of 2-(pyrrolidin-1-yl)-3,5-dinitropyridine (DNP-Pyr), a compound synthesized via nucleophilic aromatic substitution (S_NAr), to evaluate the impact of the pyrrolidine donor group on the dinitropyridine core. The molecular structure was confirmed by NMR (^{1}H and ^{13}C) and FT-IR spectroscopies, showing excellent agreement with theoretical results based on Density Functional Theory (DFT/B3LYP).

Hirshfeld surface analysis and QTAIM theory reveal that the crystal stability is primarily governed by π–π interactions and hydrogen bonding. The electronic properties, investigated by cyclic voltammetry and UV-visible spectroscopy, indicate a pronounced intramolecular charge transfer (ICT), confirmed by a reduction in the HOMO-LUMO gap (3.838 eV) compared to its precursor. Furthermore, molecular dynamics simulations, combined with the study of non-linear optical (NLO) properties, highlight high hyperpolarizability values, suggesting that DNP-Pyr is a promising candidate for advanced applications in optoelectronics and organic photonics.

References:

1) T. Slama, Z. Mazouz, B. Abdelaziz, S. Bouazizi, I. Cherif, A. Ghabi, B. Gassoumi, H. Kaur, S. Patané, T. Boubaker, S. Ayachi. J. Mol. Liq., **2025**, 418, 126722-126744.
2) A. Hedhli, A. Ghabi, H. Ayachi, S. Ayachi, T. Boubaker. Chem. Eng. J., **2025**, 519, 164656- 164668.

Strategic Selection of Building Blocks for DNA Encoded Library Design

Imen TALBI [a], Matthieu JEANTY [b]

a) Novalix Tunisia
b) Novalix France

DNA-Encoded Libraries (DELs) have become a powerful technology for the rapid identification of bioactive small molecules by enabling the screening of extremely large chemical spaces in a single experiment. The success of DELs critically depends on the availability of small molecule building blocks that are not only structurally diverse but also synthetically robust under DNA-compatible conditions. From a synthetic chemistry perspective, the challenges are clear: reactions must proceed in aqueous or mixed media at moderate temperature and controlled pH, while maintaining DNA integrity. These constraints impose strict requirements on functional group tolerance, chemoselectivity, and reagent stability, making the design and preparation of suitable building blocks the limiting factor for DEL chemical space.

In this work, we present strategies for the organic synthesis of DEL-compatible building blocks, focusing on multi-step transformations that maximize structural complexity while preserving DNA-tolerant functionality. We explore reactions, stability considerations, and chemoselectivity challenges, highlighting how these factors dictate which chemical motifs can be reliably incorporated into libraries. By addressing the synthetic bottlenecks at the building block stage, we demonstrate a practical roadmap to expand DEL-accessible chemical space and enable more ambitious library designs.

Key words: DEL, Building block synthesis, Drug discovery

References

[1] *Chem. Rev*. **2021**, 121, 12, 7155–7177.
[2] *RSC Adv.*, **2021**, 11, 2359-2376.

Differential Acute Toxicity of Copper, Lead, Cadmium, and Zinc to *Artemia salina* Nauplii and Its Modulation by Natural Biopolymers

Kaouthar ELBIRGUI [1,2]*, Kamal BENALI [3], Hassan CHARII [4], Chaimaa MERBOUH [2],
Nadia IOUNES [2], Samir IBENMOUSSA [1]

1 Laboratory of Chemistry and Biochemistry, Nutrition, Environment and Health - Faculty of medicine and pharmacy of Casablanca, Rue Tarik Ibnou Ziad, 20250, Casablanca, Morocco.
[2] Laboratory of Ecology and Environment, Faculty of Sciences Ben M'Sick, Hassan II University. Avenue Cdt Driss El Harti, B.P.7955 Sidi Othmane. Casablanca. Morocco.
[3] Laboratory of chemical and biochemical sciences, Green process Engineering (CBS), Mohammed VI Polythecninc University, Ben Guerir, Morrocco.
[4] Chemical Process and Applied Materials Laboratory, Poly disciplinary Faculty, Sultan Moulay Slimane University, BP 592 Beni-Mellal, Morrocco.
*E-mail address: kaouthar.elbirgui-etu@etu.univh2c.ma

Acute toxicity bioassays are widely used to assess the ecotoxicological risks posed by chemical pollutants in aquatic ecosystems. The present study evaluated the acute toxicity of four heavy metal sulfates copper, lead, cadmium, and zinc, toward *Artemia salina* nauplii and investigated the potential of natural biopolymers to mitigate their toxic effects. *Artemia* cysts were hatched under controlled laboratory conditions, and stage II nauplii were exposed for 24 hours to increasing concentrations of each metal, following standardized bioassay procedures, with potassium dichromate employed as a reference toxicant. Mortality data were used to determine median and total lethal concentration values. The results demonstrated pronounced differences in metal toxicity, with copper showing the highest toxicity, followed by lead, cadmium, and zinc. In parallel assays, the addition of chitin, phosphorylated chitin, micro-fibrillated cellulose, and phosphorylated micro-fibrillated cellulose significantly reduced naupliar mortality, indicating a decrease in metal bioavailability. Phosphorylated biopolymers exhibited the strongest protective effects, highlighting the importance of functional group modification in enhancing metal-binding capacity. Overall, this study confirms the sensitivity of *Artemia salina* as a model for acute toxicity assessment and demonstrates the potential of chitin- and cellulose-based biopolymers as eco-friendly agents for mitigating heavy metal toxicity in aquatic environments.

Keywords : *Artemia salina*; heavy metals; acute toxicity; biopolymers.

DFT study of the Boulton-Katritzky Base-catalysed Rearrangement of some Z-arylhydrazones of 3-benzoyl-5-phenylisoxazoles into 2-aryl-4-acyl-2H-1,2,3-triazoles

Imen Beltaief Meddeb and Youssef Arfaoui

Laboratory of Applications, Characterizations, and Modelling of Materials (LR18ES08),
Faculty of Sciences of Tunis, University of Tunis El Manar, 2092, Tunisia.

A theoretical investigation based on density functional theory (DFT) was carried out to clarify the mechanism of the base-catalyzed monocyclic Boulton–Katritzky rearrangement [1,2] of Z-arylhydrazones derived from 3-benzoyl-5-phenylisoxazoles into 2-aryl-4-phenylacyl-2H-1,2,3-triazoles. These heterocyclic compounds [3,4] hold considerable importance in chemical and pharmaceutical fields due to their diverse applications. Intrinsic reaction coordinate calculations were performed at the B3LYP /6-31G (d, p) level. The results indicate that the rearrangement proceeds through a concerted one-step pathway. Solvent polarity was found to exert only a minor influence on both activation and reaction free energies. In contrast, the nature of the base significantly affects the reaction kinetics, with tert-butoxide providing the lowest activation barrier. Substituent effects on the aromatic ring, which encompass a range of different electronic effects, were shown to have a limited impact on the reaction energetics.

References

1. Liu J, Chen C, Kotagiri R, Yang W, Cai Q (2019) A Simple Transformation of 1-(Isoxazol-3-yl) ureas to 5-(2-oxoalkyl)-2,4-dihydro-3H-1,2,4-triazol-3-ones through Base-Promoted Boulton-Katritzky Rearrangement. Advanced Synthesis & Catalysis 361(3): 481-484. https://doi.org/10.1002/adsc.201801357

2. Romade S, Lsdeme M (2019) Strategies Towards the Synthesis of N^2-Substituted 1,2,3-Triazoles. An Acad Bras Ciênc 91(1). https://doi.org/10.1590/0001-3765201820180751

3. Pozharskii AF, Katritzky AR, Soldatenkov AT (2011) Heterocycles in Life and Society: An Introduction to Heterocyclic Chemistry. Biochemistry and Applications; John Wiley & Sons: New York. books.google.com.

4. Eicher T, Hauptmann S, Speicher A (2013) books.google.com. The Chemistry of Heterocycles (Structure, Reactions, Syntheses, and Applications); WileyVCH: Weinheim, books. google. com.

A Computational Study of Glucose, Galactose, and Fructose Interactions with an Fe(II) Macrocyclic Schiff Base Complex

Maryem Ben Khalifa [1,3] *, Chaima Hassouna [2], Abdul-Rahman Allouche [3],
Mohamed Hassen V Baouab [2], Rafik Ben Chaabane [1], Rym Mlika [1]

[1] Laboratory of Advanced Materials and Interfaces (LIMA), Faculty of Sciences of Monastir, University of Monastir, Avenue of Environment, 5000 Monastir, Tunisia
[2] Physico-Chemistry Laboratory of Innovative Materials, LR (24ES16), Preparatory Institute for Engineering Studies of Monastir, University of Monastir, Avenue of the Environment, 5000 Monastir, Tunisia
[3] Institute of Light and Matter, UMR5306, University of Lyon 1-CNRS, 69622 Villeurbanne Cedex, Lyon, France

The structural flexibility of monosaccharides and the electronic complexity of transition metal complexes make the description of their interactions challenging, thus requiring a quantum chemical approach to better understand their structural and energetic properties. In this work, the interactions between three monosaccharides (glucose, galactose, and fructose) and the $[Fe(II)(C_{40}H_{24}N_4)]^{2+}\cdot 2Cl^-$ complex were studied. Molecular dynamics simulations with the semi-empirical PM7 level were used to generate structures, from which 500 geometries of each sugar/$[Fe(II)(C_{40}H_{24}N_4)]^{2+}\cdot 2Cl^-$ complex were selected. After PM7 optimization and removal of duplicates, 60 structures were selected for further optimization using DFT with the B3LYP functional. Two-step DFT optimizations were performed: first with the 6-31G* basis set, then with a larger basis set (6-311+G(d) for H, C, N, O, and Cl; LANL2DZ for Fe). The results indicate that the sugars interact with the $[Fe(II)(C_{40}H_{24}N_4)]^{2+}\cdot 2Cl^-$ complex through a hydrogen bond between a hydroxyl group of the monosaccharide and a chloride counterion. The stability of the complexes follows the order: Fructose > Galactose > Glucose.

Keywords: Interaction, Glucose, Galactose, Fructose, $[Fe(II)(C_{40}H_{24}N_4)]^{2+}\cdot 2Cl^-$, Molecular dynamics, PM7, DFT.

Selective Organic Transformations of Unsaturated Fatty Acids in Olive Pomace Oils via Heterogeneous Catalysis

Narjess Bouharb, Lassaad Hedhili*, Med Hassen Baouab

Université de Monastir, Institut Préparatoire aux Études d'Ingénieurs de Monastir (IPEIM),
Laboratoire de Physico-Chimie des Matériaux Innovants LR24ES16, Monastir, Tunisia
lassaad.hedhili@ipeim.u-monastir.tn

Olive pomace oils contain a high proportion of **long-chain fatty acids** characterized by well-defined **organic molecular signatures**. The lipid fraction is dominated by **oleic acid** (*cis-9-octadecenoic acid*, $\mathbf{C_{18}H_{34}O_2}$, C18:1, $\Delta 9$), accompanied by **linoleic acid** (*cis,cis-9,12-octadecadienoic acid*, $\mathbf{C_{18}H_{32}O_2}$, C18:2) and saturated fatty acids such as **stearic acid** (*octadecanoic acid*, $\mathbf{C_{18}H_{36}O_2}$, C18:0). These molecules share a common **carboxylic acid function (–COOH)** and differ mainly by their **degree of unsaturation**, which governs their reactivity and physicochemical properties.

This work investigates the **selective organic reduction of C=C double bonds** in unsaturated fatty acids through heterogeneous catalysis. After a simplified pretreatment and purification of the oil, catalytic reactions were conducted using **palladium on activated carbon (Pd/C)** and **magnetic iron oxide ($\mathbf{Fe_3O_4}$)** catalysts. The study focuses on molecular-level transformations involving π-bond adsorption, hydrogen transfer, and saturation of unsaturated carbon chains.

Gas chromatography (GC-FID) analyses show a progressive conversion of **oleic acid (C18:1)** into **stearic acid (C18:0)**, corresponding to the selective hydrogenation of the carbon–carbon double bond while preserving the carboxylic function. Pd/C exhibits high activity due to Pd^0 surface sites promoting π-complexation with unsaturated chains, whereas Fe_3O_4 induces milder and partially selective transformations.

These molecular modifications directly affect key **structure–property relationships**, including **degree of saturation, oxidative stability, melting behavior, and molecular rigidity**. The results provide a clear **organic chemistry interpretation** of lipid reactivity and demonstrate how heterogeneous catalysis enables the **controlled transformation of naturally occurring organic molecules**, in line with sustainable and selective organic synthesis.

Turning NO_2 into High-Value Chemicals with CaO Catalysts: A DFT Study towards Oxadiazolidinone Synthesis

Hanan Enadi,[a] Mohamed Oussama Zouaghi,[a] Youssef Arfaoui [a] *

[a] *Laboratoire Applications, Caractérisations et Modélisation de Matériaux (LR18ES08), Faculté des Sciences de Tunis, Université de Tunis El Manar, Tunis, 2092, Tunisia. (a)*

Nitrogen dioxide (NO_2) [1] is both a major atmospheric pollutant and a reactive species of considerable interest in catalysis. Here, we use density functional theory (DFT) [2] to examine its adsorption on a $(CaO)_{16}$ cluster model of the CaO(001) surface and its subsequent reaction with 1,2-dimethylaziridine to yield oxadiazolidinone derivatives. Two adsorption modes were identified: a chelating and a non-chelating geometry. According to energy decomposition analysis, the chelating mode binds more strongly (-30.36 kcal·mol^{-1}), largely through electrostatic, polarization, and donor–acceptor effects, while the non-chelating mode (-22.24 kcal·mol^{-1}) is stabilized mainly by dispersion. These results highlight the ability of CaO surfaces [3,4] to strongly capture NO_2, providing the initial step for its activation and subsequent transformation. Natural Bond Orbital analysis further points to a rich network of charge-transfer interactions in the chelating complex, consistent with its enhanced stability. Reaction pathway calculations suggest that adsorbed NO_2 promotes ring opening of the aziridine via C–H activation, with a moderate barrier of 31.74 kcal·mol^{-1} and an overall exergonic profile ($\Delta rE = -9.30$ kcal·mol^{-1}). When solvent effects are considered (CPCM), the barrier decreases in polar media, which may facilitate the transformation. Taken together, these findings suggest that CaO surfaces not only capture NO_2 efficiently but may also provide a sustainable route for its conversion into heterocycles of potential value.

Keywords: NO_2, Catalysis, DFT computation, Heterogenous catalysis, CaO, Solvent effects.

References

[1] J.H. Seinfeld, Atmospheric Chemistry and Physics: From Air Pollution to Climate Change, 1st ed, John Wiley & Sons, Incorporated, Newark, 2016.
[2] [S. Grimme, J. Antony, S. Ehrlich and H. Krieg, J. Chem. Phys., 2010, 132, 154104.
[3] M. Sharifi, S. Tangestaninejad, M. Moghadam, A. Marandi, V. Mirkhani, I. Mohammadpoor-Baltork, S. Aghayani, Metal-organic frameworks-derived CaO/ZnO composites as stable catalysts for biodiesel production from soybean oil at room temperature, Sci Rep 15 (2025) 3610.
[4] C. Di Valentin, A. Figini, G. Pacchioni, Adsorption of NO and NO2 on terrace and step sites and on oxygen vacancies of the CaO(100) surface, Surface Science 556 (2004) 145–158.

Biomass-Enhanced Modified Clay for Industrial Effluents Treatment: Performance and Optimization

Anwar Hileli [1,2*], Zahwa Ghodbani [3], Younes Moussaoui [2,4], Safa Gamoudi [1]

[1] Laboratory of Composite Materials and Clay Minerals, National Center for Research in Materials Science, Technopole Borj Cedria, B.P. 73, 8027, Soliman, Tunisia.
[2] University of Gafsa, Faculty of Sciences of Gafsa, Gafsa 2112, Tunisia.
[3] University of Gafsa, National Engineering School of Gafsa, Sidi Ahmed Zarroug - 2112, Gafsa, Tunisia.
[4] University of Sfax, Faculty of Sciences of Sfax, Organic Chemistry Laboratory (LR17ES08), Sfax 3029, Tunisia
e-mail: anwarhl173@gmail.com (A. Hileli)

The development of sustainable materials for wastewater treatment has become an important environmental priority. In this study, a novel bioflocculant, BioC3, was synthesized from *Opuntia ficus-indica* cactus juice and smectite-rich raw clay from El Fahs (Tunisia). The material was characterized using physicochemical analyses, FTIR, and XRD to investigate its structural stability and functional composition.

The flocculation performance of BioC3 was evaluated using textile and hydraulic industrial effluents and compared with five reference materials: synthetic cationic polyacrylamide (Syn-F), crude cactus juice, raw clay, purified clay, and organophilic modified clay. Key parameters such as pH, conductivity, and turbidity were monitored.

A comparative study with the synthetic flocculant under varying conditions (dose, stirring speed, stirring time, and pH) showed that BioC3 consistently achieved higher turbidity removal and improved water clarification. These results highlight BioC3 as a promising eco-friendly alternative to conventional synthetic flocculants for industrial wastewater treatment.

Keywords: industrial effluent, clay, cactus juice, bioflocculant, turbidity, conductivity.

Bio-Based Furan-Containing Polyurethanes from Bisfuranic Polyesters and Desmodur® eco N: Synthesis, Characterization, and Application

Dina Sellami [a], Sami Zaidi [a], Oumayma Challouf [a], Tobias Robert [b], Majdi Abid [c],
Souhir Abid [a,c] and Abdelkader Bougarech [a]

[a] *Faculté des Sciences, Laboratoire de Chimie Appliquée HCGP, Université de Sfax, Sfax 3038, Tunisia*
[b] *Fraunhofer Institute for Wood Research–Wilhelm-Klauditz-Institut WKI, Riedenkamp 3,*
38108 Braunschweig, Germany
[c] *Department of Chemistry, College of Science, Jouf University, P.O. Box 2014, Sakaka,*
Aljouf, Kingdom of Saudi Arabia

Over the last decades, furan-based monomers, particularly 2,5-furandicarboxylic acid (FDCA) and 5,5'-isopropylidene bis(ethyl 2-furoate) (DEF), have attracted considerable attention for polymer synthesis owing to their rigid, aromatic-like ring structure, which has been shown to significantly enhance the physicochemical properties of the resulting materials [1,2]. While FDCA has already been explored as a building block in the development of bio-based polyurethanes [3], DEF has, to the best of our knowledge, not yet been used in this field, representing a notable gap in the literature.

In this work, novel furan-based polyurethanes were prepared through polyaddition of hydroxyl-terminated polyesters derived from DEF *via* polycondensation with succinic acid and 1,6-hexanediol, with the bio-based isocyanate Desmodur® eco N 3700. A comprehensive evaluation of the physicochemical properties of the resulting polyurethanes was subsequently conducted, alongside preliminary application tests on glass and wood substrates, in order to assess their practical suitability as bio-based coating or adhesive materials.

References

[1] Wei, S., Liu, L., Duan, Y., Chen, X., Tian, B., Yuan, P., Lv, S., Zhang, Y. (2025). *European Polymer Journal*, 241, 114364.
[2] Challouf, O., Zaidi, S., Bougarech, A., Abid, M., Robert, T., Ammar, H., Abid, S. (2024). *Polymer*, 312, 127577.
[3] Bruckbauer, A., Hays, S. S., Guan, Z., Frisch, T., O'Shea, K., Mayfield, S. P., Bae, J., Pokorski, J. K., Burkart, M. D. (2025). *ACS Applied Polymer Materials*, 7, 13226–13235.

Electrostatic complexation of oppositely charged polyelectrolytes in aqueous solution

Mariem Fehri [a,b], Nouha Jemili [a,b] and Wafa Essafi [a,b]

[a] *Laboratoire Matériaux, Traitement et Analyse, Institut National de Recherche et d'Analyse Physico-Chimique, Pôle Technologique de Sidi Thabet, 2020 Sidi Thabet, Tunisia.*
[b] *Université de Tunis El Manar, Faculté des Sciences de Tunis-Département de Chimie, 2092 Tunis, Tunisia.*

In this work, the electrostatic complexation of strong hydrophilic polyelectrolytes (PEs) in aqueous solution was studied as a function of different parameters, such as the chemical charge density of the polyanion, the chain length of both polyelectrolytes and the polymer concentration. The hydrophilic polyanion is a copolymer of acrylamide and sodium acrylamido methyl propane sulfonate, prepared by radical polymerization and then well characterized chemically, while the polycation is a commercial Polydiallyldimethylammonium chloride. Polyelectrolyte complexes 'PEC' were investigated and characterized by a set of complementary experimental techniques, namely Dynamic Light Scattering, zetametry, Isothermal Titration Calorimetry, viscosimetry, optical microscopy and Small Angle X ray Scattering.

For this PAMAMPS–PDADMAC based system, the formation of colloidal complexes of size between 100 and 150 nm was detected either before charge stoichiometry ($Z[+]/[-] < 1$) or at the same time as coacervation. On the other hand, the complexation reaction is only endothermic in agreement with one step mechanism of complexation. This behaviour shows that ***coacervation*** takes place, indicating that despite the strong interaction between the cationic and the anionic charges, the system is weakly interacting.

Keywords: polyelectrolyte complexes; hydrophilic polyelectrolytes, polyanion, polycation, colloids ; coacervates.

Synthesis and characterization of silver nanoparticles: The evaluation of their protoscolicidal activity against *Echinococcus granulosus*

Molka Mrabet [a], Inès Kamoun [b], Myriam Oudni-M'rad [b], Selim M'rad [b], Faouzi Ayari [a]

[a] University of Monastir, Faculty of Pharmacy of Monastir, Laboratory of Chemical, Galenic & Pharmacological Development of Drugs-LR12ES09, University of Monastir, Avicenna Street, 5000 Monastir, Tunisia
[b] University of Monastir, Faculty of Pharmacy of Monastir, Laboratory of Medical and Molecular Parasitology-Mycology (LP3M)- LR12ES08, University of Monastir, Avicenna Street, 5000 Monastir, Tunisia

Cystic echinococcosis (CE) is a zoonotic infection caused by the larval stage of *Echinococcus granulosus sensu lato* in humans, and remains a significant global public health and economic concern. Although surgical removal of the cyst remains the treatment of choice, it requires strict precautions to prevent parasitic dissemination resulting from cyst rupture. In this context, the use of silver nanoparticles (Ag NPs) has emerged as a promising therapeutic strategy due to their nanoscale dimensions and their high biological efficacy at low concentrations. In the present study, Ag NPs were synthesized through a simple and environmentally friendly green chemistry approach, using naturally derived reducing agents. The synthesis conditions were optimized to obtain NPs with enhanced antiparasitic activity. Remarkably, exposure of protoscoleces to these Ag NPs resulted in a rapid protoscolicidal effect with 70% mortality observed after only 1 minute of exposure, increasing to 94% within 5 minutes. The most active sample exhibited a characteristic UV/VIS band, centered at 400 nm, confirming the formation of Ag NPs. Dynamic Light Scattering (DLS) analysis revealed a bimodal size distribution, with particle populations ranging from 10 to 30 nm and from 100 to 200 nm, indicating the presence of primary nanoparticles along with larger aggregates. In addition, the measured zeta potential value of - 44 mV suggests a high colloidal stability of the nanoparticle dispersion in solution. The X-ray diffraction analysis further confirmed the formation and crystalline nature of the silver nanoparticles. The study also revealed that silver clusters (Ag_n) and silver oxide (Ag_2O) exhibited no significant antiparasitic activity under the investigated conditions, highlighting that the observed protoscolicidal effect is specifically associated with the density of Ag NPs.

Keywords: Silver nanoparticles, green synthesis, physicochemical characterization methods, protoscolicidal activity

Selective Electrochemical Detection of Hexacosanoic Acid (C_{26}:0) in Buffered Medium Using a MIP-Modified SPCE

Insaf Ben Braiek [1,2,4], Valentina Pifferi [2], Sonia Yatouji [3], Luigi Falciola [2],
Houcine Barhoumi [4], Nejeh Jaba [1]

[1] University of Monastir, Preparatory Institute for Engineering Studies of Monastir, Laboratory of Physical Chemistry of Innovative Materials (LR24ES16), 5019, Monastir, Tunisia.
[2]Dipartimento di Chimica, Università degli Studi di Milano, Via Golgi 19, 20133 Milan, Italy
[3]University of Monastir, Faculty of Medicine of Monastir, Laboratory of Nutrition, Functional Foods and Vascular Health (LR11ES55),5000, Monastir, Tunisia.
[4] University of Monastir, Faculty of Sciences of Monastir, Interfaces and Advanced Materials Laboratory (LR12ES05), 5019, Monastir, Tunisia.

Hexacosanoic acid (C_{26}:0), a very-long-chain saturated fatty acid (VLCFA), has recently emerged as a novel lipid biomarker of Alzheimer's disease (AD), offering new opportunities for electrochemical sensing and strong potential for early diagnosis. Traditionally, this biomarker is quantified using chromatographic techniques, which are expensive, time-consuming, and require complex instrumentation.

To provide a simpler alternative, a molecularly imprinted polymer (MIP) sensor was fabricated via the electropolymerization of pyrrole (Py) in the presence of C_{26}:0 as the template molecule on a screen-printed carbon electrode (SPCE). Electrochemical over-oxidation enabled template removal and the formation of selective recognition cavities. Cyclic voltammetry (CV) and differential pulse voltammetry (DPV) were used to evaluate the sensor's performance.

The developed MIP–SPCE platform demonstrated rapid response, good stability, and high selectivity, offering promising perspectives for the early detection of Alzheimer's disease.

Keywords: Alzheimer's disease; Lipid biomarker; Molecularly imprinted polymer (MIPs); Electrochemical sensor; Polypyrrol.

The Formation and Application of Molecularly Imprinted Conducting Polymers

A. Ramanavicius [1]*, G. Zvirzdine [1], E. Mohsenzadeh [1], V. Liustrovaite [2], V. Ratautaite [1],
E. Brazys [2], E. Nedzinskaite [1], G. Slaboseviciute [1], D. Plausinaitis [2],
U. Prentice [1], G. Kaspute [1], A. Ramanaviciene [2]

1. State Research Institute Center for Physical and Technological Sciences (FTMC), Department of Nanotechnology, LT-10257, Vilnius, Lithuania.
2. Vilnius University, Institute of Chemistry, Faculty of Chemistry and Geosciences, NanoTechnas - Center of Nanotechnology and Materials Science, LT-03225 Vilnius, Lithuania.
*arunas.ramanavicius@chf.vu.lt

The development of molecularly imprinted polymers (MIPs) is very promising research and technology direction, because MIPs can be exploited in the design of sensors, drug delivery systems and in other technological applications [1]. Some research shows that MIPs imprinted by relatively small [2] and relatively large [3] targets can be designed and exploited as recognition elements of sensors. The major challenges during the formation/application of MIPs are related to the selection of polymer suitable for the formation of cavities, which are complementary to targeted analyte. To facilitate advances during the selection of the most suitable polymer we are using computational methods including DFT calculations. The next important challenge is the adaptation of polymerization protocol, during our MIP-related research we mostly are using electrochemical methods for the formation of conducting polymer layers. The advantage of electrochemical methods is that they enable precise control of polymerization reaction, what is important for the adjustment of proper morphology and thickness of formed MIP layer. The other challenging issue is the removal of template from polymeric matrix, which is also important for selectivity and sensitivity of formed MIP layer towards imprinted target. To remove entrapped template various solvents and combined physico/chemical methods are applied. Then the detection of analyte is performed, which could be based on any sensitive analytical method. In here reported research we have used electrochemical methods, which enable us to estimate analyte concentration by several different ways.

Acknowledgement: This research was supported by Central Project Management Agency (CPVA) Project No 10-038-T-0330.

References

[1] M. Drobysh, V. Ratautaite, E. Brazys, A. Ramanaviciene, A. Ramanavicius. Molecularly imprinted composite-based biosensor for the determination of SARS-CoV-2 nucleocapsid protein. Biosensors and Bioelectronics, 2024, 251, 116043. https://doi.org/10.1016/j.bios.2024.116043

[2] G. Zvirzdine, S. Zukauskas, A. Rucinskiene, E. Mohsenzadeh, R. Boguzaite, A. Ramanaviciene, M. Pogorielov, V. Ratautaite, A. Ramanavicius. Electrochemical salicylic acid sensor based on molecularly imprinted polypyrrole. ACS Applied Materials and Interfaces, 2025, 17, 57475−57485. https://doi.org/10.1021/acsami.5c11951

[3] V. Liustrovaite, V. Ratautaite, A. Ramanaviciene, A. Ramanavicius. Detection of the SARS-CoV-2 Nucleoprotein by Electrochemical Biosensor based on Self-Assembled Monolayer Supported Molecularly Imprinted Polypyrrole Formed on Gold Nanoparticle Modified Screen-Printed Electrode. Biosensors and Bioelectronics, 2025, 272, 17092. https://doi.org/10.1016/j.bios.2024.117092

Program of
Sunday 03
May 2026

Cationic Tris-benzimidazole-silver(I) complexes: Synthesis, characterization, anticancer, and antimicrobial evaluation

Lamia BOUBAKRI [a], İsmail ÖZDEMIR [b,c], Harald Kelm [d], Naceur HAMDI [a]

[a)] Research Laboratory of Environmental Sciences and Technologies (LR16ES09), Higher Institute of Environmental Sciences and Technology, University of Carthage, Hammam-Lif, Tunisia.
[b)] Department of Chemistry, Catalysis, Research, and Application Center, İnönü University, Malatya, Turkey
[c)] Drug Administration and Research Center, İnönü University, 44280-Malatya, Turkey
[d)] Department of Chemistry, RPTU Kaiserslautern-Landau, Erwin-Schrödinger-Str. Geb. 54, 67663 Kaiserslautern, Germany
Email: boubakri_lamia@yahoo.co.uk

Heterocyclic compounds are cyclic organic structures containing one or more heteroatoms within the ring. Nitrogen-containing heterocycles, in particular, are fundamental components of many natural and synthetic drugs.[1] Benzimidazole, a prominent member of this family found in various natural compounds, is highly valued for its versatile biological properties, including antimicrobial, antitumor, and antiviral activities.[2] While pharmaceutical research has extensively investigated metal-N-heterocyclic carbene (NHC) complexes in recent years, there is growing interest in the coordination chemistry of silver(I) azole complexes. Silver is biologically inactive in its pure metallic form but easily ionizes into silver cations (Ag^+), which offer low toxicity, enhanced stability, and significant therapeutic potential.[3] In this study, N-alkyl benzimidazole derivative ligands and their new Ag(I) complexes were synthesized and characterized. The anticancer and antimicrobial activities of these compounds were evaluated against Gram-negative bacteria, Gram-positive bacteria, and fungal strains.

Keywords: N-alkylbenzimidazole, silver complex, anticancer, antimicrobial activity.

---

[1] Vitaku, E.; Smith, D. T.; Njardarson, J. T., J. Med. Chem., 2014, 57 (24), 10257–10274.

[2] (a) Barker, H. A.; Smyth, R. D.; Weissbach, H., J. Biol. Chem., 1960, 235 (2), 480–488. (b) Al-Blewi, F. F.; Almehmadi, M. A.; Aouad, M. R., Chem. Cent. J., 2018, 12, 110.

[3] (a) Hanif, M. ; Noor, Muhammad, A. ; M. ; Ullah, F. ; Tahir, M.N. ; Khan, G.S. ; Khan, E., Inorganics., 2023, 11 (4), 152. (b) Sindelar, Z. ; Kopel, P., Inorganics., 2023, 11 (3), 113.

Synthesis, Quantification and Reactivity of Gold(I) N-Heterocyclic Carbenes Complexes Bearing a Methacrylate Moiety

Rim HAMDI [a,b], Jean-François LONGEVIAL[b], Michéle SINDT[b],
Corentin LEFEBVRE[c] and Taoufik BOUBAKER[a]

a) Laboratoire de Chimie Hétérocyclique, Produits Naturels et réactivité (LR11ES39), Faculté des Sciences de Monastir, Université de Monastir, Avenue de l'environnement, Monastir-Tunisie 5019, Tunisia
b) Laboratoire de Chimie Physique – Approche Multi-échelles des Milieux Complexes (LCP-A2MC), Université de Lorraine, ICPM, 1 Boulevard Arago, 57000 Metz Cedex 03, France
c) Laboratoire de Glycochimie et des Agroressources d'Amiens (LG2A), Université de Picardie Jules Verne 10, rue Baudelocque, Amiens 80000, France

This study investigates a series of gold(I) N-heterocyclic carbene (NHC) complexes bearing a methacrylate fragment. The objective is to synthesize eight complexes, including four mono-gold(I) and four bis-gold(I) NHC derivatives, obtained in yields ranging from 63% to 98%. Following their synthesis, these complexes were quantitatively characterized according to the Mayr reactivity approach to determine their electrophilicity parameters and gain insight into their intrinsic reactivity.

Two representative complexes from this series were examined toward sulfur-based nucleophiles to evaluate the feasibility of a Michael-type addition onto the methacrylate moiety, with the perspective of future bioconjugation applications. Density functional theory (DFT) calculations corroborate these observations, predicting an activation energy at least 4 kcal/mol lower for nucleophilic attack at the gold(I) center compared to the methacrylate group.

Overall, these results suggest that gold(I) NHC complexes may inherently behave as "clickable" platforms, questioning the necessity of introducing additional clickable functionalities in bioconjugation in bioconjugation strategies.

Keywords : N-heterocyclic carbenes, gold(I) complexes, methacrylate, Mayr reactivity approach.

References

[1] R. Hamdi, I. Staccioni, J. Gerber, S. Rup-Jacques, J. Hertzog, V. Carré, M. Sindt, C.Lefebvre, T. Boubaker, J. F. Longevial. Journal of Organometallic Chem., **2025.**
[2] N. G. J. Clayden, S. Warren, P. Wothers. Journal of Organic Chemistry., **2001**.
[3] J. F. Longevial, C. Rose, L. Poyac, S. Clément, S. Richeter. Eur. J. Inorg. Chem. **2021**.

Crystal Structure Study, Spectroscopy, Theoretical Investigations, and Biological Evaluation of a Hybrid Material

Dorsaf Mezni & Riadh Kefi

Laboratory of Materials Chemistry, Faculty of Sciences of Bizerte, 7021 Zarzouna, Tunisia.

In this study, the synthesis and structural characterization of a new complex, $Ni(C_6H_9N_2)_2(H_2O)_{42}\cdot 4H_2O$ (abbreviated as Ni-3AMP), were carried out. Single-crystal X-ray diffraction confirmed a triclinic crystal system with an octahedral coordination environment around the Ni^{2+} ion. Spectroscopic investigations, including FT-IR, UV–Vis, and photoluminescence analyses, verified the presence of key functional groups such as –OH, $–NH_2$, and –C=C–. These analyses revealed a strong blue emission, while theoretical calculations (DFT/CAM-B3LYP/LanL2DZ) corroborated the observed structural and electronic properties. Hirshfeld surface analysis of Ni-3AMP showed that approximately 45% of all contacts are dominated by H···O interactions, corresponding to hydrogen-bond interactions of the C–H···O, N–H···O, and O–H···O types. Molecular docking simulations using two P. aeruginosa targets (7PTF and 7PTG), representing the ATPase domain of the DNA gyrase subunit B, demonstrated a higher binding affinity of Ni-3AMP compared to ciprofloxacin (CIP), a standard antibacterial drug, with binding affinities of −139.60 kJ/mol (7PTF@Ni-3AMP), −108.90 kJ/mol (7PTF@CIP), −130.27 kJ/mol (7PTG@Ni-3AMP), and −110.84 kJ/mol (7PTG@CIP), and the formation of 11, 10, 5, and 5 hydrogen bonds, respectively. In vitro antimicrobial tests further revealed strong antibacterial activity, particularly against P. aeruginosa and E. coli, surpassing that of ciprofloxacin. These results suggest that Ni-3AMP is a promising multifunctional agent with potential applications in biomedical therapeutics and optoelectronics.

A Predictive Relationship between Tautemeric Equilibria and Acidity of Nitroalkanes in Water

Rania KHALDI, Amel HEDHLI and Taoufik BOUBAKER

Laboratoire de Chimie Hétérocyclique, Produits Naturels et Réactivité, Université de Monastir,
Faculté des Sciences, Avenue de l'Environnement, 5019 Monastir, Tunisia

The proton transfer reactions of the nitronate anion derived from 1-hydroxy-2,2-dinitroethane with HCl and carboxylic acid buffers were investigated in aqueous solution at 25 °C through combined kinetic and thermodynamic analyses. Mechanistic investigation enabled the determination of the acidity constants associated with O-protonation ($pK_a^{NO2H} = 1.67$) and C-protonation ($pK_a^{CH} = 3.78$), which are among the weakest reported for nitroalkanes in water. The intrinsic rate constant ($\log k_0 = 1.60$), determined using the Marcus formalism, is significantly lower than that typically observed for nitrile protonation, reflecting the strong resonance stabilization of the conjugate base by the electron-withdrawing NO_2 groups.

By combining literature data with the results obtained in this work, a predictive relationship between the tautomeric equilibrium constant ($pK_N = pK_a^{CH} - pK_a^{NO2H}$) and the acidity constant (pK_a^{CH}) of nitroalkanes in water was established. This previously unreported linear correlation enables estimation of the acidity constants of nitronic acids for four nitroalkanes that were previously experimentally inaccessible, providing new insights into structure–reactivity relationships governing protonation at carbon and oxygen sites.[11]

Keywords : Nitroalkanes; Nitronate anions; Proton transfer kinetics; Acidity constants; Tautomeric equilibria; Marcus theory ; Aqueous solutions.

---

[1] : R. Khaldi, A. Hedhli, T. Boubaker., ChemPhysChem **2025**, 26.

Mechanistic DFT Investigation of the Cycloaddition Reaction of Nitrones with Allene–Propargyl Equilibria toward Isoxazoline and Isoxazolidine Derivatives

Ibrahima Ngom [1,3], Mohamed Oussama Zouaghi [1], Imen Ferchichi [1],
Frédéric Guégan [2], Insa Seck [3] and Youssef Arfaoui [1]

[1] Laboratoire de Caractérisations, Applications et Modélisation de Matériaux (LR18ES08), Faculté des Sciences de Tunis, Université de Tunis El Manar, Tunisie
[2] IC2MP (Institut de Chimie des Milieux et des Matériaux de Poitiers), Université de Poitiers, France
[3] Laboratoire de Chimie de Coordination Organique, Département de Chimie, Faculté des Sciences et Techniques, Université Cheikh Anta Diop de Dakar (UCAD), BP 5005, Dakar-Fann, Sénégal

The [3+2] cycloaddition (32CA) reaction is a key transformation for the synthesis of biologically relevant five-membered heterocycles such as isoxazolidines. In this study, a detailed density functional theory (DFT) investigation is carried out to analyze the cycloaddition between a nitrone dipole and four competing dipolarophiles, including two allenes (A1, A2) and two propargyl derivatives (P1, P2) coexisting in equilibrium. Calculations were performed at the PBEPBE/6-311+G(d,p) level, with solvent effects taken into account using the CPCM model.

Frontier molecular orbital (FMO) analysis and global reactivity descriptors indicate that the reaction proceeds via a normal electron-demand mechanism, where the nitrone behaves as a nucleophile and the dipolarophiles act as electrophiles. Regioselectivity is rationalized using Houk's rule, revealing preferential interactions between the nitrone oxygen and the most electrophilic carbon centers. Transition-state analyses show highly asynchronous and polar pathways, with early O–C bond formation dominating the reaction mechanism. Natural Energy Decomposition Analysis (NEDA) highlights the crucial role of charge-transfer and reorganization energies, as well as the impact of nitrone substitution on activation barriers and kinetic selectivity.

Overall, this work provides valuable insights into the electronic factors controlling reactivity and selectivity in nitrone-based cycloadditions involving allenic and propargylic systems.

Keywords: Nitrone; [3+2] cycloaddition; DFT; Regioselectivity; Allenes; Propargyl derivatives; NEDA

References

[1] Huisgen R., 1968, 1,3-Dipolar cycloaddition reactions, Journal of Organic Chemistry, 33, 2291–2300.
[2] Piotrowska D.G., Głowacka I.E., Schols D., Snoeck R., Andrei G. et al., 2019, Novel isoxazolidine and γ-lactam analogs of homonucleosides, Molecules, 24(22), 1–23.
[3] Parr R.G., Yang W., 1989, Density functional theory of atoms and molecules, Oxford University Press, New York.
[4] Perdew J.P., Burke K., Ernzerhof M., 1996, Generalized gradient approximation made simple, Physical Review Letters, 77, 3865–3868.
[5] Fukui K., 1964, Role of frontier orbitals in chemical reactions, Molecular Orbitals in Chemistry, Physics, and Biology, Academic Press, New York.

Aerobic oxidation of aldehydes to carboxylic acids in aqueous solution of NaOH / NaCl

Ons Romdhane, Jamil Kraiem

Laboratory of Chemical, Galenic and Pharmacological Drug Development-(LR12ES09), Faculty of Pharmacy, University of Monastir, Avicenne street, 5000, Monastir, Tunisia.

Carboxylic acid-containing compounds are widely used in the food, cosmetic, and pharmaceutical industries. Although carboxylic acids are easily obtained at the laboratory scale, highly efficient and environmentally friendly transformations remain rare [1,2]. Most oxidation methods often rely on hazardous reagents, expensive catalysts, and often conducted in harmful solvents. In the framework of the research activities of our team which is interested in green chemistry [3,4], we have established a new green synthesis route of carboxylic acids. Our approach presents the advantages of being efficient, simple, economic, and more respectful of the principles of green chemistry. We report here an efficient, catalyst-free method for the aerobic oxidation of aldehydes to carboxylic acids in aqueous solution of NaOH/ NaCl under mild conditions. Molecular oxygen (1atm) was employed as the sole oxidant and water as green solvent. This protocol is applicable to a broad scope of aldehydes, providing the corresponding carboxylic acids in excellent yields without the need of complex purification steps. Notably, the process is easily operated and characterized by high selectivity, with no detectable side-product formation.

Keywords: Oxidation, Aldehydes, Green chemistry, Carboxylic acids, water

---

References

[1] Liu, M., Wang, H., Zeng, H., Li, C.-J., *Sci. Adv*, 2015, 1, e1500020, 1-9.
[2] Liu, M., Li, C.-J., *Angew. Chem. Int. Ed.*, 2016, 55, 10806–10810.
[3] Kraiem, J., Ghedira, D., Ollevier, T., *Green. Chem*, 2016, 18, 4859.
[4] Kraiem, J., Ollevier, T., *Green. Chem*, 2017, 19, 1263.

List of Poster Communications

Communicatings' Names	Ref
H. Abdellaoui, H. Habli *FSM - Monastir* Ionic character and nonadiabatic effects in AgLi: An Ab Initio perspective	**PC 01**
S. Abdellaoui , A. Taissir, S. Mlayah-Bellalouna, N. Srairi-Abid, M.F. Zid, R. Ksiksi *FST - Tunis* Synthesis, structure, characterization and antitumor activity of $(NH_4)_6[V_{10}O_{28}]$ 5H_2O	**PC 02**
S. Abdellaoui , A. Taissir, S. Mlayah-Bellalouna, N. Srairi-Abid, M.F. Zid, R. Ksiksi *FST - Tunis* Synthesis, structure, characterization and antitumor activity of $(NH_4)_4[H_2V_{10}O_{28}]$ 8H_2O	**PC 03**
A. Achour Khedhiri, K. Hriz, M. Zannen *FSM - Monastir* Synthesis and characterization of novel functionalized chitosan-based materials	**PC 04**
T. Aissa, D. Aissaoui-Zid, N. Srairi-Abid, M.F. Zid, R. Ksiksi *FST - Tunis* Design and therapeutic evaluation of a novel decavanadate-based hybrid material as a potent therapeutic agent for aggressive tumors	**PC 05**
S. Akretche, L. Lamoudi, D. Chergui, L. Kerbouche, N. Bousbia, A. Touri, I. Drici *Houari Boumediene University, Algiers, Algeria* Study of the extraction of molecules of interest from local sources	**PC 06**
M.H.V Baouab, K. Abbassi *IPEIM - Monastir* Investigating the impact of substitution and metal type on the structural, morphological, thermal, and optical properties of newly substituted Schiff base g-C3N4 derivatives	**PC 07**
H. Barhoumi, A. Elloumi, J. Wannassi, F. Echouchene *FSM - Monastir* Hybrid nanocomposite-based sensing materials for urea detection in human blood serum matrices	**PC 08**
I. Beltaief Meddeb, Y. Arfaoui *IPEIN - Nabeul* DFT study of the Boulton-Katritzky base-catalysed rearrangement of some Z-arylhydrazones of 3-benzoyl-5-substituted isoxazoles into 1,2,3-triazoles	**PC 09**
C. Ben Aissa, S. Touil *FSB - Bizerte* Design and synthesis of new thiophenyl α-aminophosphonates with potential biological interest	**PC 10**
C. Ben Aissa, J. Rouden, J. Baudoux, S. Touil *FSB - Bizerte* Synthesis of novel thiophene-derived *N*-bisphosphonates	**PC 11**
R. Ben Ameur, S. Soltani, N. Hamdaoui, M. Treilhou, N. Allouche *FSS - Sfax* Exploring the bioactivity of R. tripartitum leaf ethyl acetate extract: A cheminformatics-driven study of its antioxidant, anti-inflammatory, anti-α-amylase, and anti-acetylcholinesterase properties	**PC 12**
N.E.H. Ben Ammar, A.H. Hamzaoui *CNRSM - Borj Cédria* Extraction and optimization of cellulose from Alfa fiber (Stipa tenacissima) via alkaline treatment for incorporation into a polypropylene matrix	**PC 13**

Communicatings' Names	Ref
A. Ben Haj Mbarek, M. Itaimi Dammak, C. Milanese, A. Laouani, D. Le Cerf, H. Majdoub, A. Papetti, H. Ben Jannet *FSM - Monastir* A sustainable biorefinery approach: Selective isolation of Hawthorn polysaccharides via microwave-assisted extraction using Natural Deep Eutectic Systems	**PC 14**
A. Ben Romdhane, N.E.H. Ben Fatma, F. Hfaeidh, M. Laribi *Faculty of Pharmacy - Monastir* In silico evaluation of hexahydrocannabinol as a potential analgesic agent targeting opioid receptors	**PC 15**
A. Ben Romdhane, N.E.H. Ben Fatma, F. Hfaeidh, M. Laribi *Faculty of Pharmacy - Monastir* Computational discovery of novel cannabinoid-derived ligands targeting opioid receptors	**PC 16**
A. Benayache, L. Lamoudi, K. Daoud *Houari Boumediene University, Algiers, Algeria* Coating uniformity: influence of atomizing air pressure and spray rate	**PC 17**
A. Beyaoui, M. Kaplan, S. Jlizi, A. Ceyhan Goren, H. Ben Jannet *FSM - Monastir* Phytochemical profiling and biological activities of the trunk bark of Acacia cyclops trunk bark: in vitro combined with in silico approach	**PC 18**
K. Boltane, R. Ben Sghaier, S. Ben Ismail, P. Mira Mourão, A. Mnif *FST - Tunis* Synthesis of magnetic nanoparticles for the removal of polymeric pollutants from water	**PC 19**
L. Boubakri, N. Gürbüz, I. Özdemir, H. Kelm, N. Hamdi *ISSTE - Borj Cédria* Design of novel N-alkylbenzimidazole-silver(I) catalysts for aldehyde–amine–alkyne coupling	**PC 20**
S. Boubakri, R. Lafi, N. Saidi, W. Mabrouk *CERTE - Borj Cédria* Efficient removal of anionic dyes from aqueous media using a zeolite/chitosan/laser-induced graphene hybrid material	**PC 21**
D. Bouchouk, F.Z. S. Soukehal *Mohamed Cherif Messaadia University, Souk Ahras, Algeria* Synthesis and characterization of new peptide analogues obtained by sulfahydantoin opening reactions	**PC 22**
S. Boussandel, W. Erb, F. Mongin, A. Samarat *FSB - Bizerte* From ferrocene-fused xanthones to functionalized cyclic ferrocene derivatives	**PC 23**
N. Bouzayani, F. Bonnaterre, A. Joncour, P. Ciapetti, B. Vivet, H. Prevet, M.A. Pena Pinon, D. Triki, R. Cedeno, Y. Fischer, P. Schambel, J. Nomme, L. Wick, C. Ronin, N. Membre, M. Poirot, N. Huss-Braun, A. Bonhoure, E. Laigre, E. Klein, I. Talbi, M. Jeanty, N. Weidner, S. Gratzer, J. Guillemont *FSM - Monastir* Efficient synthesis and structure–activity relationships of a novel class of PI4Kβ inhibitors identified from a Novalix DEL library	**PC 24**
S. Briki, I. Souii, H. M'rabet *FST - Tunis* Bis(allyl-α-aminophosphonates) and bis(propargyl-α-aminophosphonates) derivatives: New synthesis from bis(α-aminophosphonates)	**PC 25**
I. Chaari, B. Rabeh, A.H. Hamzaoui *CNRSM - Borj Cédria* Magnetic Tunisian clay nanocomposite: A sustainable and separable adsorbent for rapid cationic dye removal from aqueous solutions	**PC 26**

Communicatings' Names	**Ref**
K. Charradi, R. Lafi, J. Chékir, N. Saidi, W. Mabrouk *CERTE - Borj Cédria* Fabrication of laser-induced graphene on polyethersulfone membranes and its application to rhodamine B adsorption	**PC 27**
W. Cheikhrouhou, H. Ben Jouira, S. Boufi *Centre of Biotechnology - Borj Cédria* Eco-friendly phosphorylation of chitin nanocrystals for enhanced mechanical and flame-retardant performance in bio-based nanocomposites films	**PC 28**
S. Chelli Lakhdar, S. Lakhdar *Paul Sabatier University, Toulouse, France* Laser Flash Photolysis: A Key Technique for Unraveling Polar and Radical Mechanisms	**PC 29**
Y. Dgachi, J. Marco-Contelles, L. Ismaili, F. Chabchoub *FSS - Sfax* Rapid synthesis and molecular modeling of new kojotacrines derivatives against Alzheimer's disease	**PC 30**
S. EL Ghali, I. Alvarez-Serrano, B. Sotillo, A. Badri, F. Aloui *FSM - Monastir* Facile Sol-Gel combustion synthesis of Fe_3O_4–$LiNiVO_4$ nanocomposite for energy storage and photocatalytic applications	**PC 31**
N. El Guesmi, F. Maurel *CRMN - Sousse* Theoretical investigation of the photochromic mechanism of tetrahydroindolizine (THI) derivatives	**PC 32**
A. Elaissi, H. Haj Salem, R. Chaâbane-Banaoues, H. Babba *Faculty of Pharmacy - Monastir* Chemical composition and antifungal activity of the essential oil of Origanum majorana L.	**PC 33**
A. Elaissi, H. Haj Salem, R. Chaâbane-Banaoues, H. Babba *Faculty of Pharmacy - Monastir* Chemical composition and antifungal activity of Geranium graveolens essential oil	**PC 34**
M. Elakremi, Y. Moussaoui, R. Ben Salem *FSG - Gafsa* Eco-friendly valorization of medicinal plant essential oils: Phytochemical and biofunctional assessment	**PC 35**
H. Elnadi, M.O. Zouaghi, Y. Arfaoui *FST - Tunis* Insights on the mechanism of the reaction between NO and aziridines with and without CaO catalyst	**PC 36**
K. Essid, M. Derbel, I. Trabelsi *FSS - Sfax* Esterification of tertiary alcohols with mixed aromatic-fatty anhydrides using Lewis acid as heterogeneous catalyst	**PC 37**
K. Essid, M. Gharsalli, W. Jahouach-Rabai *FSS - Sfax* Reactivity of mixed lipid anhydrides in the acylation of certain phenolic compounds extracted from olive pomace oil	**PC 38**
A. Fatnassi, M. Hidouri *ENIG - Gabès* Structural and electrical properties of Nd_{7-x} Li_x Sr_3 $(SiO_4)_6O_{1,5-x}$ $(0 \le x \le 1)$ oxyapatite ceramics	**PC 39**
A. Fatnassi, M. Hidouri *ENIG - Gabès* Optical Characterization of Nd_{7-x} Li_x Sr_3 $(SiO_4)_6O_{1,5-x}$ $(0 \le x \le 1)$ ceramics	**PC 40**

Communicatings' Names	**Ref**
M. Ferjani, A. Achour Khedhiri, M. Zannen, A. Lahmar, H. Barhoumi *FSM - Monastir* Engineering oxygen vacancies in $Na_{0.5}Bi_{0.5}TiO_3$-based perovskites for improved photocatalytic performance	**PC 41**
K. Fnena, A. Bellagi *FSG - Gafsa* Compute of the second coefficient of Viriel and elevation of the Boyle temperature	**PC 42**
N. Gasmi, L. Khalfa, G. Rossignolo, A. Lorenzetti, Y. Moussaoui *FSG - Gafsa* Microwave-assisted chemical recycling of bio-based poly(ethylene furanoate) by aminolysis	**PC 43**
A. Ghabi, J.C. Guillemin, T. Boubaker *FSM - Monastir* Access to primary α-phosphino- and α-arseno-nitriles: Synthesis, characterization, and comparison with α-aminonitriles	**PC 44**
F. Ghammagui, S. Ammar *FSG - Gabès* Sustainable biochar-based composites for enhanced dye removal from wastewater	**PC 45**
R. Ghorbali, H. Ghalla, L. Sellaoui *FSM - Monastir* Theoretical insights into the adsorption of Eriochrome Black T on apatite silicates: Steric and energetic analysis	**PC 46**
A. Haloui, K. Essalah, M.A.K. Sanhoury, N. Amdouni *FST - Tunis* A computational study of one-bond ^{31}P-^{19}F spin-spin coupling constants in some nerve agent related organophosphorus-fluorine derivatives	**PC 47**
N. Hamdi, S. Guerfi, L. Boubakri, Y. Berredjem *ISSTE - Borj Cédria* Design of efficient benzimidazole-derived N-heterocyclic carbene Ag(I) catalysts for aldehyde-amine-alkyne coupling and their antioxidant and enzyme inhibition	**PC 48**
N. Hamdi, N. Gurbuz, I. Özdemir, L. Mansour *ISSTE - Borj Cédria* Pd−PEPPSI-type expanded ring N-heterocyclic carbene complexes: Synthesis, characterization, and catalytic activity in Suzuki−Miyaura cross coupling	**PC 49**
N. Hammami, F. Chabchoub, E. Maalej *FSS - Sfax* Regioselective synthesis of functionalized pyrimidine derivatives via cyclocondensation reactions	**PC 50**
A. Hileli, Z. Ghodbani, Y. Moussaoui, S. Gamoudi *FSG - Gafsa* Bio-based clay composite for industrial effluent treatment: Performance and process optimization	**PC 51**
H. Hlimi, M. Mbarek *FSM - Monastir* Nanoscale engineering of PPV and PFO conjugated polymer nanowires via template wetting	**PC 52**
M. Horchani, H. Ben Jannet, A. Romdhane *FST - Tunis* Design and efficient synthesis of novel antibiotic derivatives (ciprofloxacin) with in silico assessment supporting their predicted biological efficacy	**PC 53**
K. Hriz, M. Essid, H. Zrida, K. Hassine *FSM - Monastir* Water-soluble chitosan-based fluorescent probe for Al^{3+} detection: Synthesis and sensing performance	**PC 54**

Communicatings' Names	**Ref**
B. Jedidi Yaich, H.M. Sbihi *FST - Tunis* Geoclimatic influence on the composition and quality of Tecoma stans seed oils from Tunisia and Saudi Arabia	**PC 55**
B. Jedidi Yaich, H.M. Sbihi *FST - Tunis* Comparison of fatty acid composition and bioactive properties of Marrubium vulgare seed oil and canola oil	**PC 56**
W.E.Q. Jemmali, M. Bouzid, A. Ben Lamine *FSM - Monastir* Mechanistic and predictive study of MB adsorption on biochar derived from Lantana camara	**PC 57**
W.E.Q. Jemmali, M. Bouzid, A. Ben Lamine *FSM - Monastir* ANN-based prediction of dye adsorption efficiency on Fe_3O_4-modified activated carbon	**PC 58**
O. Jendoubi, S. Majdoub, H. B. Al-Hmadi, R. El Mokni, G. Zengin, S. Hammami *FSM - Monastir* Antioxidant and enzyme inhibitory activities of Tunisian Salvia aegyptiacaL extracts	**PC 59**
M. Jmai, I. Soui, H. Edziri, H. M'rabet *FST - Tunis* Isoxazolidinyl-based nitrogen heterocycles: Efficient synthesis, antibacterial, antibiofilm activity, and in silico evaluation against EGFR and microbial targets	**PC 60**
Y. Kacem, S. Mehrez *FSM - Monastir* Synthesis of new chiral hydantoins starting from α-amino acids	**PC 61**
N. Kadri, A. Bougarech, S. Abid, M. Baltas, H. Ammar *FSS - Sfax* Synthetic approach to functionalized endoperoxide derivatives based on syncarpic acid for antimalarial drug discovery	**PC 62**
A. Kaouach, L. Pagès, L. Jean, H. Ben Jannet, A. Romdhane *FSM - Monastir* Synthesis, molecular docking, DFT Studies, and pharmacokinetic evaluation of spiroxindole pyranopyrimidinones as α-amylase inhibitors	**PC 63**
J. Kraiem *Faculty of Pharmacy - Monastir* Eco-friendly acylation and benzylation of Friedel-Crafts catalyzed with low-loaded ferric chloride under green conditions	**PC 64**
R. Ksiksi, M.F. Zid *FST - Tunis* Polyoxometalates: From synthesis to industrial and medical applications	**PC 65**
Y. Lahmer, H. Hammi *INSAT - Tunis* Valorization of deinking sludge in polymer composites	**PC 66**
L. Lamoudi, S. Akretche, N. Guemras, N. Bousbia, K. Daoud *Houari Boumediene University, Algiers, Algeria* Impact of freeze-drying on the chemical stability and biological activity of bioactive compounds in *Spirulina platensis*	**PC 67**
M. Lejmi, B. Kouidhi, H. Rhim, M. Mastouri, A. Elaissi *Faculty of Pharmacy - Monastir* Antibacterial and antioxidant potential of five Eucalyptus species against respiratory pathogens.	**PC 68**

Communicatings' Names	**Ref**
F. Mannai, A. Feriani, H. Al Busaidi, M.N. Belgacem, Y. Moussaoui *FSG - Gafsa* *Opuntia* (Cactaceae) mucilage mixed with polyvinyl alcohol for biodegradable packaging composite film formulation	**PC 69**
H. Meliani, A. Benguerdi, A. Harir, N. Menadi , N. Menadi, M.A. Bouzidi, A. Kerfouf *Djillali Liabes University; Sidi Bel Abbes; Algeria* Quality of water surface and analyzes in the Tessala Mountain water table, Wilaya of Sidi Bel-Abbes, Algeria	**PC 70**
D. Mezni, R. Kefi *FSB - Bizerte* A new 0D tin(IV) hybrid with dual functionality: Yellow–green photoluminescence and molecular docking evaluation of $(C_6H_{16}N_2)[SnCl_6]\cdot 4H_2O$	**PC 71**
T. Missaoui, R. Besbes *FST - Tunis* Synthesis of new imidazolidine-2-thiones from α,β-diaminoesters	**PC 72**
A. Najahi, Q. Tarrés, M. Delgado-Aguilar, J.L. Putaux, S. Boufi *FSS - Sfax* Eco-friendly conversion of biomass into functional lignocellulosic nanofibrils via maleic acid-assisted hydrothermal treatment	**PC 73**
T.Y. Namoussa *Shahid Hama Lakhdar University, El Oued, Algeria* Synthesis of green hybrid nanomaterials to enhance solar distillation efficiency and water production	**PC 74**
K. Nasri, L. Sellaoui, M. Mbarek *FSM - Monastir* Adsorption of heavy metal ions on activated carbon: Modelling and interpretation	**PC 75**
I. Ngom, F. Guégan, I. Seck, Y. Arfaoui *FST - Tunis* DFT mechanistic investigation of electrooxidative allene dioxygenation mediated by TEMPO	**PC 76**
M.H. Oueslati, A. Guetat, J. Bouajila *IPEIB - Bizerte* Phytochemical characterization of isolated compounds from Deverra tortuosa (Desf.) seeds: Evaluation of cytotoxic, α-glucosidase and antibacterial activities	**PC 77**
M.H. Oueslati, A.H. Harrath *IPEIB - Bizerte* Chemical composition and in vitro cytotoxic activities of the essential oil of Lavandula atriplicifolia Benth	**PC 78**
F. Rais, K. Oueslati, A. Naifar, N. Adhoum *IPEIK - Kairouan* Computer-assisted statistical physics study of Rotenone adsorption onto chemically engineered activated carbons	**PC 79**
A. Ramanaviciene, N. German, A. Ramanavicius, A. Popov, A. Kausaite-Minkstimiene *Vilnius University, Lithuania* The impact of gold nanostructures and enzymatically synthesized polymer layers in glucose biosensor design	**PC 80**
S. Ramanavicius , A. Raveendran, G. Paulikaite, S. Ali, O. Gogotsi, A. Ramanaviciute, V. Korniienko, M. Pogorielov, A. Ramanavicius *MB Sensografa, Vilnius, Lithuania* Functionalization of MXenes for the sensing and removal of pharmaceutical organic compounds	**PC 81**

Communicatings' Names	**Ref**
A. Ramanaviciute, E. Mohsenzadeh, V. Korniienko, M. Pogorielov, G. Zvirzdine, U. Prentice, G. Kaspute, S. Ramanavicius, A. Ramanavicius *MB Sensografa, Vilnius, Lithuania* In silico design of molecularly imprinted polymers	**PC 82**
M. Riahi, N. Amdouni, J. Nemchi *FST - Tunis* Thermal, mechanical and rheological behavior of PVC filled with ATH and MDH electrical cable applications	**PC 83**
O. Romdhane, J. Kraiem *FSM - Monastir* Efficient solvent-free synthesis of thymol/thymoquinone mixtures via catalyzed oxidation and evaluation of their antibacterial activity	**PC 84**
D. Saidani, M. Smadhi, R. Abderrahim *FSB - Bizerte* Efficient synthesis and spectroscopic characterization of a novel benzo-1,3-Diazine-2-thione derivative from 2-aminobenzonitrile	**PC 85**
O. Salah, N. Raouafi, W. Mabrouk *FST - Tunis* Aminated PES/Carbon black membranes for laser-induced graphene electrodes	**PC 86**
S. Salhi, A. Omri, R. Ben Salem, M. Benzina *FSS - Sfax* Enhanced photocatalytic degradation of Congo Red using Co-TiO_2/hematite catalyst: Modeling and optimization approach	**PC 87**
D. Sellami, S. Zaidi, O. Challouf, T. Robert, M. Abid, S. Abid, A. Bougarech *FSS - Sfax* Bio-based 5,5'-isopropylidene bis(ethyl 2-furoate) as a renewable building block for water-borne polyurethane dispersions	**PC 88**
D. Siziani, Y. Abdi, F.Z. Rihel, M. Kelbouz, K. Ferhah, R. Cheggou, Z. Attou, N. Bensouilah *National School of Advanced Technologies, Algiers, Algeria* One-pot synthesis of fused chromene-furanopyran under microwave Investigation on the solvatochromism. Determination of dipole moments	**PC 89**
F. Smail, M. Amara *National Higher School of Advanced Technologies, Algiers, Algeria* Synthesis and development of polymer-based nanoparticle mixed matrix membranes	**PC 90**
H. Smati, M. Bouzid, Y. Ben Torkia, A. Ben Lamine *FSM - Monastir* Advanced investigation of the adsorption process of coumarin compounds on mouse olfactory receptors: Statistical physics modeling and molecular docking	**PC 91**
E.W. Thiam, A.H. Barry, N. Claiser, M. Souhassou *University of Nouakchott, Mauritania* Synthesis and structural characterization of a novel hybrid organic-inorganic polyoxovanadate framework	**PC 92**
N. Tka *FSM - Monastir* The design of acridine-based hybrids as potential anticancer agents	**PC 93**
N. Touj, L. Delaude *ISSTE - Borj Cédria* Fluorinated rhodium complexes: Synthesis, characterization, and investigation of fluorine–metal interactions in transfer hydrogenation	**PC 94**

Communicatings' Names	**Ref**
A. Wahbi, W. Tahri, K. Kaabi, A. Chatti, C. Ben Nasr, J.F. Cavalier, S. Touil *FSB - Bizerte* Green synthesis, antibacterial activity and molecular docking study of γ-phosphonyloxime derivatives	**PC 95**
A. Yahya, A. Ayachi, F. Chtourou, Z. Benissa, N. Tene, R. Jarraya, M. Treilhou, S. Zouari *FSG - Gafsa* Influence of hydrodistillation time intervals and drying period on the yield, chemical composition, and antioxidant activities of Pituranthos chloranthus stems essential oils from the Sbiba-Kasserine provenance (Southern Tunisia)	**PC 96**
I. Zouidi, C. Arfaoui, S. Gamoudi *FSG - Gafsa* Fabrication and characterization of a new ceramic membrane from Tunisian clay: Application to industred wastewater treatment	**PC 97**
H. Zrida, K. Hassine, K. Hriz *FSM - Monastir* New fluorescent material based on anthracene and triazole for blue organic light emitting diode	**PC 98**
N. Akremi, M. Idia, I. Ayed, A. Rayes *FSG - Gabès* A chloro-ligated Lindqvist hexatungstate stabilized by a neutral chloroalkylamine: Synthesis, structural elucidation, and supramolecular topology of $Na_3(C_5H_{13}NCl)[ClW_6O_{19}]$	**PC 99**
N. Akremi, I. Ayed, A. Rayes *FSG - Gabès* Dibromoarylammonium-stabilized Lindqvist hexatungstate dihydrate: Synthesis, crystal architecture, and supramolecular water networks in $(C_7H_8NBr)_2[W_6O_{19}]\cdot 2H_2O$	**PC 100**

Abstracts of Poster Communications

Ionic Character and Nonadiabatic Effects in AgLi: An Ab Initio Perspective

Hadir Abdellaoui, Héla Habli

Université de Monastir, Faculté des Sciences de Monastir, Laboratoire de Physique Quantique et Statistique,
Avenue de l'Environnement 5019, Monastir, Tunisie
Emails : hadirabed7@gmail.com ; hablihela@gmail.com

Over the past decades, cold and ultracold diatomic molecules have become a major focus in molecular physics. Heteronuclear metal dimers are of particular interest due to their roles in astrophysics, laser cooling, and microelectronics. In this work, we present a detailed ab initio investigation of the AgLi molecule. We use non-empirical pseudopotentials for the Ag^+ and Li^+ cores, combined with Core Polarization Potentials to include core–valence correlation. The two valence electrons are treated using a Full Configuration Interaction approach.

We compute adiabatic potential energy curves and spectroscopic constants for low-lying electronic states of Σ^+ and Π symmetries, in both singlet and triplet multiplicities, below the Li^+Ag^- ionic limit. Several excited states show strong ionic character. This is confirmed by permanent dipole moments that follow a -1/R asymptotic behavior at large internuclear distances. This ionic contribution leads to multiple avoided crossings in the adiabatic representation and complicates the description of nuclear dynamics.

To overcome this limitation, we develop diabatic representations for the $^{1,3}\Sigma^+$ and $^{1,3}\Pi$ electronic states. We apply the Variational Effective Hamiltonian method with an effective metric to obtain a unitary transformation that yields smooth diabatic states. This representation captures nonadiabatic couplings and provides a clearer description near ionic-neutral crossing regions. These results offer a reliable theoretical framework for guiding experimental efforts aimed at forming cold AgLi molecules.

Keywords: Avoided crossings, Dipole moments, Nonadiabatic couplings, Ionic character, Diabatization.

Synthesis, structure, characterization and antitumor activity of $(NH_4)_6[V_{10}O_{28}]\cdot 5H_2O$

ABDELLAOUI SOUROUR[1*], AISSA TAISSIR[1], MLAYAH-BELLALOUNA SAOUSSEN [2],
NAJET SRAIRI-ABID[2], MOHAMED FAOUZI ZID[1] & KSIKSI REGAYA[1,3*]
* abdellaouisourour24@gmail.com

[1] *University of Tunis El Manar, Faculty of Sciences of Tunis, Laboratory of Materials, Crystal Chemistry and Applied Thermodynamics, 2092 El Manar II, Tunis, Tunisia.*
[2] *University of Tunis El Manar, Laboratory of Venoms and Therapeutic Molecules, Pasteur Institute of Tunis, Tunis 1002, Tunisia*
[3] *University of Carthage, High Institute of Preparatory Studies in Biology and Geology (ISEP-BG) of Soukra, Tunisia*

A new decavanadate compound, $(NH_4)_6[V_{10}O_{28}]\cdot 5H_2O$, was synthesized and characterized by single crystal X-ray diffraction. The decavanadate compound crystallizes in the monoclinic system with space group C2/c and the following unit cell parameters: a = 11.631(2) Å, b = 17.210(1) Å, c = 16.911(2) Å and β = 108.50(2)°. The formula unit of $(NH_4)_6[V_{10}O_{28}]\cdot 5H_2O$ compound is formed by decavanadate cluster $[V_{10}O_{28}]^{6-}$, six ammonium cations and five water molecules (**Figure 1**). The compound was characterized by: infrared absorption spectroscopy, powder X-ray diffraction, and UV-visible spectroscopy. The compound has been tested against brain cancer.

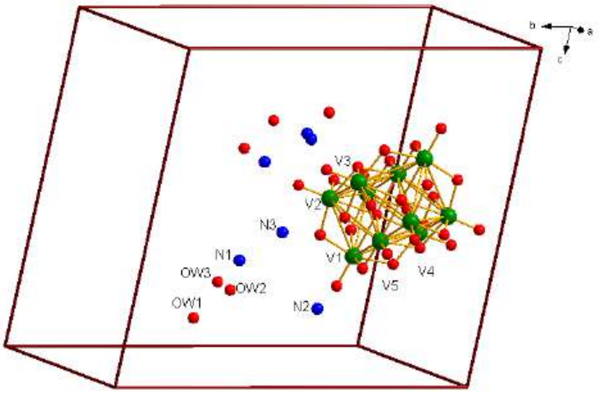


Figure 1. Unit cell of $(NH_4)_6[V_{10}O_{28}]\cdot 5H_2O$

Keywords: Decavanadate, Synthesis, X-Ray diffraction, Structure, Brain cancer

Acknowledgments: We would like to thank the Tunisian Ministry of Higher Education and Scientific Research for the financial support of this work in a project to evaluate research results under the code **VRR 25/26**.

Synthesis, structure, characterization and antitumor activity of $(NH_4)_4[H_2V_{10}O_{28}]\cdot 8H_2O$

ABDELLAOUI SOUROUR[1*], AISSA TAISSIR[1], MLAYAH-BELLALOUNA SAOUSSEN [2],
NAJET SRAIRI-ABID[2], MOHAMED FAOUZI ZID[1] & KSIKSI REGAYA[1,3*]
* abdellaouisourour24@gmail.com

[1] *University of Tunis El Manar, Faculty of Sciences of Tunis, Laboratory of Materials, Crystal Chemistry and Applied Thermodynamics, 2092 El Manar II, Tunis, Tunisia.*
[2] *University of Tunis El Manar, Laboratory of Venoms and Therapeutic Molecules, Pasteur Institute of Tunis, Tunis 1002, Tunisia*
[3] *University of Carthage, High Institute of Preparatory Studies in Biology and Geology (ISEP-BG) of Soukra, Tunisia*

A new acid decavanadate compound, $(NH_4)_4[H_2V_{10}O_{28}]\cdot 8H_2O$, was synthesis by slow evaporation at room temperature. The compound was identified by single-crystal X-ray diffraction and characterized using infrared absorption spectroscopy, powder X-ray diffraction and UV-visible spectroscopy. Single-crystal X-ray diffraction analysis revealed that: $(NH_4)_4[H_2V_{10}O_{28}]\cdot 8H_2O$ crystallizes in the triclinic system with space group P-1 and the following unit cell parameters: a = 10.171(2) Å, b = 10.297(7) Å, c = 16.742(5) Å, α = 83.53(4) °, β = 108.50(5) °, and γ = 70.96(8) °. The unit cell is formed by one $[H_2V_{10}O_{28}]^{4-}$ group, four ammonium cations and eight water molecules (**Figure 1**). The cohesion the structure is ensured by O–H…O and N–H…O hydrogen bonds and van der Waals interactions. The prepared compound was tested against brain cancer, in collaboration with a team from the Pasteur Institute of Tunis, and showed a very promising effect against the U89 cell line.

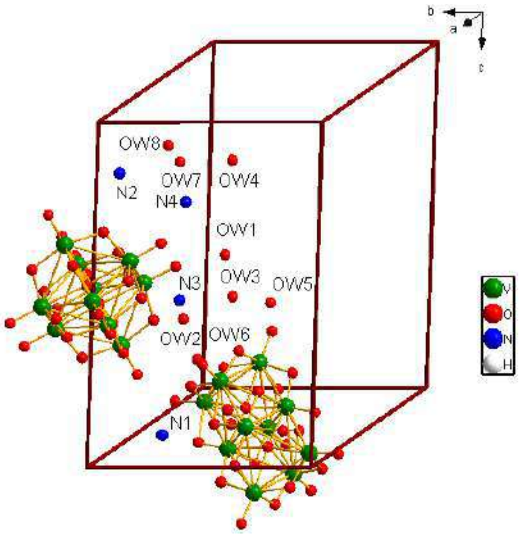


Figure 1. Unit cell of $(NH_4)_4[H_2V_{10}O_{28}]\cdot 8H_2O$

Keywords: Decavanadates, Synthesis, X-Ray diffraction, Structure, Brain cancer

Acknowledgments: We would like to thank the Tunisian Ministry of Higher Education and Scientific Research for the financial support of this work in a project to evaluate research results under the code **VRR 25/26**.

Synthesis and Characterization of Novel Functionalized Chitosan-Based Materials

Arwa Achour Khedhiri, Khaled HRIZ, Moneim ZANNEN

Laboratory of Interfaces and Advanced Materials, Faculty of Sciences of Monastir, University of Monastir, Bd. of the Environment, 5019 Monastir, Tunisia.

Chitosan is a biopolymer derived from the deacetylation of chitin, which is obtained from crustacean shells. It is well known for its rich chemistry, which originates from the functional groups along its polymer backbone, particularly hydroxyl and amino groups in its macromolecular structure. Furthermore, the chemical modification of chitosan generally leads to the development of new materials with enhanced properties, enabling a wide range of applications in pharmacy, food and medicine, water treatment, and environmental remediation [1]. Moreover, the introduction of different substituents can endow chitosan with additional functionalities. For example, grafting long alkyl chains can improve its hydrophobic character, enhance its solubility in organic solvents, and significantly tailor its physicochemical properties.

The synthesized material was characterized using XPS, UV–Vis spectroscopy, XRD, and SEM. Morphological analysis was performed using scanning electron microscopy in order to investigate the influence of chemical modifications on the surface of chitosan. It is clearly observed that their morphology differs from that of pure chitosan.

In addition, XPS characterization further confirms the incorporation of functional groups and enables the determination of the degree of chitosan modification. The obtained results confirmed the successful incorporation of the targeted functional groups into the chitosan side chains.

Keywords: Chemical modification, Chitosan, Alkylation, polymer.

References

[1] Mansour H, El-Sigeny S, Shoman S, Abu-Serie MM, Tamer TM. Preparation, Characterization, and Bio Evaluation of Fatty N- Hexadecanyl Chitosan Derivatives for Biomedical Applications. Polymers. 2022; 14(19):4011. https://doi.org/10.3390/polym14194011.

Design and Therapeutic Evaluation of a Novel Decavanadate-Based Hybrid Material as a Potent Therapeutic Agent for Aggressive Tumors

Taissir AISSA [1], Dorra Aissaoui-ZID [2], Najet Srairi-ABID [2],
Mohamed Faouzi ZID [1] & Regaya KSIKSI [1,3]

[1] *University of Tunis El Manar, Faculty of Sciences of Tunis, Laboratory of Materials, Crystal Chemistry and Applied Thermodynamics, 2092 El Manar II, Tunis, Tunisia.*
[2] *University of Tunis El Manar, Laboratory of Biomolecules, Venoms and Theranostic Applications (LR20IPT01), Pasteur Institute of Tunis, Tunis 1002, Tunisia*
[3] *University of Carthage, High Institute of Preparatory Studies in Biology and Geology (ISEP-BG) of Soukra, Tunisia*

Researching novel treatments to combat aggressive cancers is a major challenge in oncology. Polyoxometalates (POMs), specifically decavanadate $[V_{10}O_{28}]^{6-}$, have emerged as promising bioactive materials due to their structural versatility, redox activity, and ability to inhibit the proliferation of cancer cell lines. In this context, new potential drugs based on decavanadates are being developed as possible treatments for skin and breast tumors [1-2]. This study explores the synthesis, structure-function relationship, and antiproliferative effects of a novel decavanadate compound: hexa-[methylimidazolium] decavanadate(V) dihydrate, characterized using single-crystal X-ray diffraction, FT-IR, UV-Vis, and ^{51}V-NMR spectroscopies. The compound crystallizes in the monoclinic system space group $P2_1/n$. The Hirshfeld surface (HS) and their relative two-dimensional fingerprint plots (2D-FP) reveal that the structure is dominated by O…H/H…O and H…H contacts. Interestingly, this decavanadate compound $(C_4H_7N_2)_6V_{10}O_{28}\cdot 2H_2O$ inhibit the viability of IGR39 and MDA-MB-231 cells with IC_{50} values of 0.96 µM and 0.83 µM, respectively, after 72 h of treatment. The cytotoxicity assays of this compound in human cancer cell lines underscore its potential as a candidate for developing novel organometallic drugs with antitumoral properties.

Keywords: Advanced Materials; Decavanadate; XRD; Anticancer; Targeted Therapy.

Funding: Ministry of Higher Education and Scientific Research of Tunisia (VRR code of this project: **VRR 25/26)**

References

[1] J.B. Heistein, U. Acharya, S.K.R. Mukkamalla. Malignant Melanoma. StatPearls Treasure Island (FL) (2023). PMID: 29262210

[2] S.M. Mousavi, and al., 2022, Inorg. Chem. Commun. 146 110074

Study of the extraction of molecules of interest from local sources

AKRETCHE Soraya [1], LAMOUDI Lynda [2], CHERGUI Dallal [1], KERBOUCHE Lamia [1], BOUSBIA Nabil [1], TOURI Amira [3], DRICI Imene [3]

[1] *Laboratory of Industrial Process Engineering Sciences (LSGPI). Faculty of Mechanical Engineering and Process Engineering, University of Science and Technology Houari Boumediene (U.S.T.H.B.), P.O. Box 32 El Alia, 16111 Bab Ezzouar, Algeria.*

[2] *Transfer Phenomena Laboratory. Faculty of Mechanical Engineering and Process Engineering, University of Science and Technology Houari Boumediene (U.S.T.H.B.), P.O. Box 32 El Alia, 16111 Bab Ezzouar, Algeria.*

[3] *Faculty of Mechanical Engineering and Process Engineering, University of Science and Technology Houari Boumediene (U.S.T.H.B.), P.O. Box 32 El Alia, 16111 Bab Ezzouar, Algeria*

In this study, we extracted curcumin from *Curcuma longa* L., which is characterized by interesting properties. Soxhlet extraction produced a yellow-orange ethanolic extract with a yield of 7.183%, containing three curcuminoids identified by thin-layer chromatography (TLC) and nine volatile and semi-volatile substances identified by gas chromatography-mass spectrometry (GC-MS). The ethanolic extract showed antioxidant activity superior to that of ascorbic acid, with an IC50 of 1.477 mg/L.

Regarding antibacterial activity, the extract inhibited the activity of Staphylococcus aureus at a concentration of 0.1 mg/mL, suggesting potential efficacy against other pathogenic bacteria at higher concentrations. These results indicate that curcumin extracted from Curcuma longa L. has significant potential for food and pharmacological applications.

Keywords: curcuma, extraction, curcumin, analysis, activities.

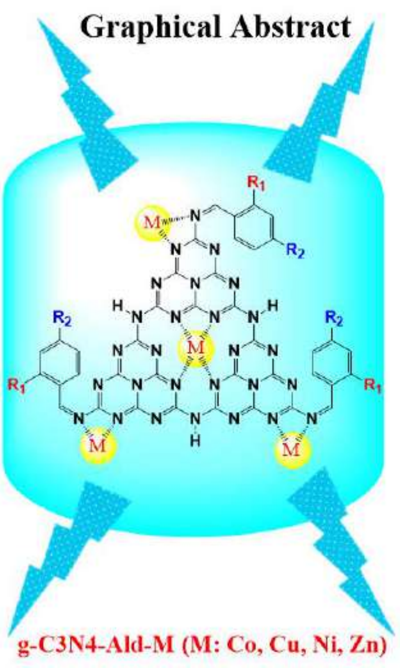
Investigating the impact of substitution and metal type on the structural, morphological, thermal, and optical properties of newly substituted Schiff base g-C_3N_4 derivatives

Mohamed Hassen V Baouab, Kaouther Abbassi

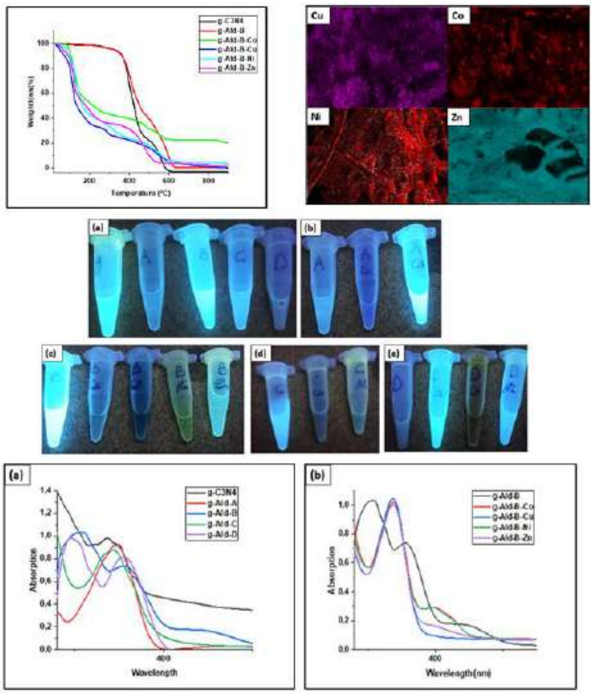
Laboratoire Physico-Chimie des Matériaux Innovants LR24ES16,
IPEIM, Monastir, Université de Monastir, Tunisie
E-mail address: hbaouab@yahoo.fr / hassen.baouab@ipeim.rnu.tn

This work designs functional g-C_3N_4 hybrids through substituted Schiff base modification (-OH, -Br, –OCH_3, -N $(CH_3)_2$) and metal complexation (Co, Cu, Ni, Zn). SEM reveals substituent-driven morphologies: bromo/hydroxy creates microtubes, while -$N(CH_3)_2$ yields smooth nanopores. FTIR confirms successful modification via new O–H (3050–3200 cm^{-1}) and C =N (1612 cm^{-1}) vibrations while preserving the heptazine core (1270-1750 cm^{-1}), with metal coordination evidenced by distinct M-O/N bond (Ni-O at 600 cm^{-1}, Co-O at 619 cm^{-1}). XRD confirms crystallinity enhancement (28–30◦ peaks) for electron-donating groups, with metal integration preserving matrix integrity. UV–Vis shows substituent-dependent absorption shifts ($\Delta\lambda$=30–50 nm) and fluorescence emission modulation via metal coordination. Nickel/cobalt complexes exhibit greater thermal stability than pristine g-C_3N_4, while copper/zinc produce ultrasmooth surfaces ideal for interfacial applications. Elemental mapping validates uniform metal distribution, revealing metal-substituent-morphology correlations that guide the design of functional surfaces. These hybrids demonstrate how molecular engineering can tailor carbon nitride architectures for specific optoelectronic and catalytic performance.

Keywords: g-C_3N_4, new synthesis procedure, characterization, Optical Properties


Graphical Abstract

g-C3N4-Ald-M (M: Co, Cu, Ni, Zn)



Hybrid Nanocomposite-Based Sensing Materials for urea detection in human blood serum matrices

Abir Elloumi [1], Jassem Wannassi[1], Fraj Echouchene [2] and Houcine Barhoumi [1]

(1) Laboratory of Interfaces and Advanced Materials, Faculty of Sciences,
University of Monastir, 5019 Monastir, Tunisia.
(2) Laboratory of Electronics and Microelectronics LR99ES30, Faculty of Sciences,
University of Monastir, Tunisia.

A molecularly imprinted polymer (MIP) of Urea (Ur) followed by ZIF-7 layer was investigated by using the electropolymerization of pyrrole (Py) on glassy carbon electrode (GCE). The preparation of ZIF-7/MIP matrix and quantitative measurements were performed by cyclic voltammetry (CV) and differential pulse voltammetry (DPV), respectively. Various physiochemical parameters monitoring the analytical performances of the developed MIP structure such as Py and Ur concentration in prepolymerization mixture, number of cyclic voltammetric scans, pH of electrolyte solution and accumulation time. The optimization of parameters was achieved using Plackett–Burman Design and Central Composite Design. The calibration curve demonstrated linearity over urea concentration range from 1×10^{-7} M to 1×10^{-5} M with a correlation coefficient of 0.98. The detection limit of urea was about 7×10^{-8} M. The developed MIP sensor has been successfully applied to detect urea in human blood serum matrices with good recovery between 109% and 123%.

Keywords: Molecularly Imprinted Polymer; Urea sensor; CV and DPV measurements; CCD and PBD design.

DFT study of the Boulton-Katritzky Base-catalysed Rearrangement of some Z-arylhydrazones of 3-benzoyl-5-substituted isoxazoles into 1,2,3-triazoles

Imen Beltaief Meddeb and Youssef Arfaoui

Laboratory of Applications, Characterizations, and Modelling of Materials (LR18ES08),
Faculty of Sciences of Tunis, University of Tunis El Manar, 2092, Tunisia.

A density functional theory (DFT) study was performed to elucidate the base-catalyzed monocyclic Boulton–Katritzky rearrangement [1,2] of Z-arylhydrazones derived from 3-benzoyl-5-phenylisoxazoles into triazoles [3,4]. Calculations at the B3LYP/6-31G (d, p) level indicate that the reaction proceeds via a concerted one-step mechanism. Substituent effects on the aromatic ring are modest, while isoxazoles containing different substituents exhibiting diverse electronic properties at C-5 significantly enhance reactivity. In this case, both electron-donating and electron-withdrawing groups lead to a noticeable reduction of the activation barrier.

References

1. Milyutin CV, Komogortsev AN, Lichitsky BV (2024) Synthèse de 1,2,3-triazoles contenant un motif allomaltol à partir de pyrano [2,3-*d*] isoxazolones substituées via un réarrangement de Boulton-Katritzky catalysé par une base. Beilstein J Org Chem 20 : 1334–1340. https://doi.org/10.3762/bjoc.20.117

2. Jianghao L, Haowen M, Jiehao Z, Wei Z, Qian C (2023) Synthesis of Pyrrolo [3,2] pyrimidin-4-ones via Cascade Alkyne−isocyanide [3＋2] Cycloaddition/Boulton-Katritzky Rearrangement/Ring Expansion Process. Acta Chimica Sinica 81. DOI :10.6023/A23040164 https://doi.org/10.1021/acs.jpca.9b08675

3. Buscemi S, Pace A, Pibiri I, Vivona N, Lanza CZ, Spinelli D (2004) Fluorinated Heterocyclic Compounds − The First Example of an Irreversible Ring-Degenerate Rearrangement on Five-Membered Heterocycles by Attack of an External Bidentate Nucleophile. Eur J Org Chem (5): 974-980. https://doi.org/10.1002/ejoc.200300737

4. Boulton AJ (1973) Lectures in Heterocyclic Chemistry; Academic Press: London, UK Vols 1 and 2

Design and synthesis of new thiophenyl α-aminophosphonates with potential biological interest

Chérifa Ben Aissa et Soufiane TOUIL [a]

[a] *Laboratory of Hetero-Organic Compounds and Nanostructured Materials (LR18ES11),*
Faculty of Sciences of Bizerte, University of Carthage, Jarzouna 7021, Tunisia;
soufiane.touil@fsb.rnu.tn

This study describes a rapid and flexible access to α-aminophosphonates bearing thiophenic moiety. These structural analogs of α-amino acids have received significant attention due to their broad-spectrum biological activities, including anticancer, antiviral, and enzyme inhibitory properties. Independently, recent work has also demonstrated very interesting biological properties for various thiophene derivatives [1]. Considering the role of these two components in this field, we first undertook the synthesis of substituted thiophenes bearing a primary amine in close proximity to the sulfur atom. Next, these functionalized compounds were evaluated in the Kabachnik–Fields reaction and the Aza-Pudovik reaction [2]. Thus, we report the highly efficient synthesis of thiophenic α-aminophosphonates via a one-pot three-component condensation of aldehydes, dialkyl phosphites and 2-aminothiophenes catalyzed by zinc triflate. Our objective is now to evaluate the antiviral activity of these novel thiophene aminophosphonates [3]. Currently, we are targeting enantiopure derivatives using asymmetric organocatalysis through the nucleophilic addition to carbonyl and related compounds using modified cinchona alkaloids and proline derivatives.

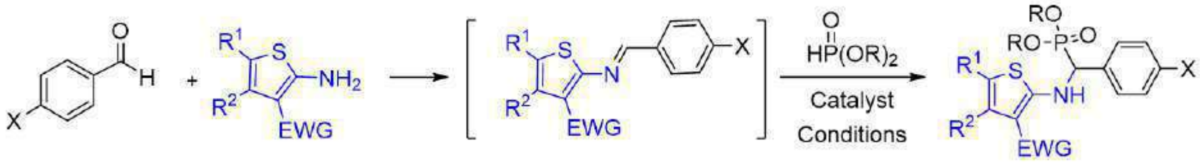


Figure 1

Keywords: Aminophosphonates; Kabachnik-Fields reaction; Aza-Pudovik reaction; Organocatalyst

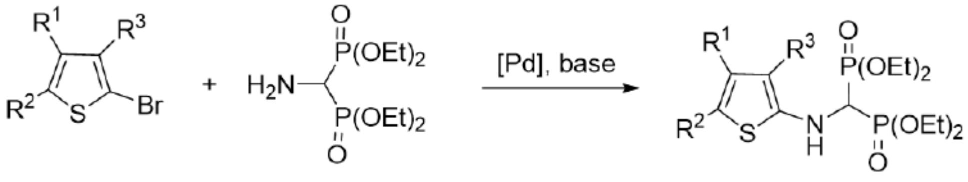
Synthesis of novel thiophene-derived *N*-bisphosphonates

Chérifa Ben Aissa,[a] Jacques Rouden,[b] Jérôme Baudoux,[b] Soufiane Touil [a]

[a] *University of Carthage, Faculty of Sciences of Bizerte, Laboratory of Hetero-Organic Compounds and Nanostructured Materials (LR18ES11), 7021 Jarzouna, Tunisia.* E-mail: soufiane.touil@fsb.rnu.tn
[b] *Normandie Univ, ENSICAEN, UNICAEN, CNRS, Laboratoire de Chimie Moléculaire et Thio-organique (LCMT) UMR 6507, 6 Bd du Maréchal Juin, 14000 Caen, France.* E-mail: jerome.baudoux@ensicaen.fr

Over the years, research interest in aminobisphosphonates has surged rapidly, owing to their interesting biological effects as highly effective inhibitors of bone resorption that exert their action *via* inhibition of human farnesyl pyrophosphate synthase, a mevalonate pathway enzyme in osteoclasts. Several examples of aminobisphosphonates have been already commercialized as drugs of choice for the treatment of osteoporosis, skeletal complications of malignancies, Paget's disease, multiple myeloma, hypercalcemia, fibrous dysplasia and many bone metastases of cancers [1]. On the other hand, the thiophene scaffold is considered to be privileged in drug design due to its favorable biological profile and differential binding affinity to diverse microbiological targets [2], and the incorporation of such a pharmacophore into bisphosphonates could improve their biological activity, in conformity with the active substructure combination principle.

With this in mind, and in the frame of our research program on the synthesis of novel phosphorus-containing compounds with possible biological properties, we now report a simple and straightforward approach to unprecedented thiophene-derived *N*-bisphosphonates, through the palladium-catalyzed cross-coupling of 2-bromothiophene derivatives with aminomethylenebisphosphonate (Scheme 1).



Scheme 1

Keywords: Aminobisphosphonates; thiophenes; palladium catalysis.

References

[1] J. E. Grove, R. J. Brown. D. J. Watts, *J. Bone Miner. Res.* **2000**, *15*, 971.
[2] V. Duvauchelle, P. Meffre, Z. Benfodda, *Eur. J. Med. Chem.* **2022**, *238*, 114502.

Exploring the Bioactivity of *R. tripartitum* Leaf Ethyl Acetate Extract: A Cheminformatics-Driven Study of Its Antioxidant, Anti-Inflammatory, Anti-α-Amylase, and Anti-Acetylcholinesterase Properties.

Raoudha Ben Ameur [1], Siwar Soltani [1], Nourhène Hamdaoui [2],
Michel Treilhou [3], Noureddine Allouche [1]

[1] *Laboratory of Organic Chemistry LR17ES08, Natural Substances Team, Faculty of Sciences of Sfax, University of Sfax, P.B. 1171, Sfax 3000, Tunisia*
[2] *Laboratory of Biomathematics LR22ES01, Faculty of Sciences of Sfax, University of Sfax, Tunisia*
[3] *Equipe BTSB-EA 7417, Institut National Universitaire Jean-François Champollion, Université de Toulouse, Place de Verdun, 81012 Albi, France*

The purpose of this study is to evaluate the biological properties of *R. tripartitum* leaves and identify the biomolecules that show promise. Ethyl acetate extracts from *R. tripartitum* leaves were tested in vitro for their phytochemical composition and anti-inflammatory, anti-acetylcholinesterase, antioxidant, and α-amylase properties. Regarding the ethyl acetate extract, it demonstrated the greatest in vitro enzyme inhibitory activity against acetylcholinesterase (IC_{50} = 0.186 mg/mL), α-amylase (0.100 mg/mL) and anti-inflammatory (0.151 mg/mL), respectively. LC-HESI-MS/MS analysis identified 28 compounds, including phenolic acids, flavonoids, and fatty acids. The major compounds were quercetin and kaempferol, as well as their derivatives: quercetin-*O*-glucoside, quercetin-*O*-xyloside, kaempferol-*O*-glucoside, and kaempferol-*O*-pentoside. The molecular docking study showed kaempferol-*O*-pentoside as a potent inhibitor of α-amylase and acetylcholinesterase, with binding affinities of -9.3 and -10.9 kcal/mol. Pharmacokinetic and toxicology analyses confirmed its drug-like properties. This study highlights the potential of *R. tripartitum* leaf ethyl acetate extract for use in food processing and disease treatment.

Extraction and Optimization of Cellulose from Alfa Fiber (Stipa tenacissima) via Alkaline Treatment for Incorporation into a Polypropylene Matrix

Nour Elhouda Ben AMMAR, Ahmed Hichem Hamzaoui

LVMU, National Research Center in Materials Science, Borj Cedria Technopark

Natural fiber-based composite materials are attracting growing interest as a sustainable alternative to conventional synthetic reinforcements (carbon, glass), whose manufacturing is energy-intensive and recycling is complex. In this context, Alfa fiber (*Stipa tenacissima*), a xerophilous plant abundant in North Africa and particularly in Tunisia, represents a promising plant resource due to its high cellulose content (≈ 39.5%).

This work focuses on the extraction of cellulose from Alfa stems by alkaline treatment with sodium hydroxide (NaOH), and on the optimization of operating conditions using response surface methodology via the NemrodW software. A second-degree composite experimental design with three factors - temperature (X_1), NaOH concentration (X_2), and treatment duration (X_3) - was implemented, generating 19 experiments.

The established mathematical model ($R^2 = 0.933$) was statistically validated by Fisher tests for regression ($F = 13.90 > F_{tab} = 3.18$) and validity ($F = 4.92 < F_{tab} = 6.26$). The optimal conditions identified — T = 85°C, [NaOH] = 4 M, duration = 6.5 h — allow achieving a cellulose content of approximately **77%**, with fibers exhibiting a smooth topography, a characteristic yellow coloration, and near-total disintegration of non-cellulosic compounds.

These results confirm the potential of Alfa fiber as a bio-based reinforcement for polypropylene matrix composites, whose manufacturing by twin-screw extrusion will constitute the next step of this project.

Keywords: Alfa, cellulose, alkaline extraction, experimental design, NemrodW, PP/natural fiber composites, XRF.

A Sustainable Biorefinery Approach: Selective Isolation of Hawthorn Polysaccharides via Microwave-Assisted Extraction using Natural Deep Eutectic Systems

Asma BEN HAJ MBAREK [1,2], Mariem Itaimi Dammak [3], Chiara Milanese [4], Aicha Laouani [5], Didier Le Cerf [6], Hatem Majdoub [3], Adele Papetti [2], Hichem Ben Jannet [1]

[1] Laboratory of Chemistry of Natural Substances and Organic Synthesis, University of Monastir, Tunisia.
[2] Department of Drug Sciences, University of Pavia Viale Taramelli 12 27100, Pavia, (Italy)
[3] Laboratory of Interfaces and Advanced Materials (LR11ES55), University of Monastir, Tunisia.
[4] Department of Chemistry, Centre for Health Technologies (CHT), University of Pavia, Pavia, Italy
[5] Laboratory of Metabolic Biophysics and Applied Pharmacology, Faculty of Medicine, University of Sousse, Sousse 4002, Tunisia (c)
[6] Laboratory Polymers, Biopolymers & Surfaces, Normandy University, UNIROUEN, INSA Rouen, CNRS, PBS, France

The Transition toward sustainable phytopharmaceutical production requires the replacement of volatile organic solvents with ecofriendly alternatives. *Crataegus azarolus* (Howthorn) is a ptofilic source of bioactive polysaccharides, yet traditional extraction methods are often hindered by low efficiency and high environmental costs. In this study, a “green” extraction platform was developed by pairing Microwave-Assisted Extraction (MAE) with Natural Deep eutectic solvents (NADES). Seven choline chloride-based NADES were synthesized and screened for extraction selectivity. Structural integrity and purity were monitored via FTIR spectroscopy. To maximize recovery, a three-level Box-Behnken Design (BBD) was employed to optimize temperature (X1), Time (X2), and solid-to-solvent ratio (X3). The Lactic Acid cleavage (LA:ChCl) system demonstrated superior selectivity, facilitated by the acidic cleavage of the plant cell wall matrix. Statistical analysis (ANOVA) confirmed a highly significant quadratic model ($p<0.0001$). The optimal conditions were identified as a temperature of 90°C, an extraction time of 18.3 min, and solid-to-solvent ratio of 45 mL. under these parameters, a maximum yield of 29.77% was predicted, which was experimentally validated (29.45 ±0.32%). The MAE-NADES approach significantly reduced extraction time compared to conventional methods while maintaining high structural purity. This study provides a robust, scalable, and green framework for the selective recovery of high-value biopolymers from botanical sources, aligning with the core principles of circular economy and green engineering.

In silico evaluation of hexahydrocannabinol as a potential analgesic agent targeting opioid receptors

Asma Ben Romdhane [1], Nour El Houda Ben Fatma [2], Firas Hfaeidh [3], Meriem Laribi [4]

[1] *Faculty of Pharmacy of Monastir, Monastir, Tunisia*
[2] *Pharmacy department, Charles Nicole Hospital, Tunis, Tunisia*
[3] *National Agency for Medicines and Health Products*
[4] *Pharmacy department, Mohamed Kassab Institute of Orthopedics, Tunis, Tunisia*

Introduction: Hexahydrocannabinol (HHC), a semi-synthetic cannabinoid derivative, has recently appeared on the international market as a novel psychoactive substance. While its recreational use is growing, its pharmacological profile remains poorly understood. This study aimed to explore the potential analgesic effects of HHC by examining its interactions with the three primary opioid receptors: mu (μ), delta (δ), and kappa (κ), using computational methods.

Materials and methods: Molecular docking simulations were conducted to assess HHC's binding affinity for μ, δ, and κ opioid receptors using PyRx v0.8, followed by redocking with Smina vOct 15 2019 to refine the results. Ligand–receptor interactions were analyzed using 2D and 3D visualizations in PyMol 3.1.5.1 and Discovery Studio v25.1.0.24284 to identify key binding residues. Additionally, physicochemical, pharmacokinetic, and toxicological properties were predicted via ADMETLab 3.0.

Results: HHC showed consistent binding affinity toward μ, δ, and κ opioid receptors, forming energetically favorable ligand–receptor complexes. HHC adopted a stable conformation within each receptor's hydrophobic cavity. Notable interactions with conserved residues such as Asp149 in the μ receptor and Asp128 in the δ receptor were observed. Physicochemical predictions indicated that HHC complies with Lipinski's rule of five, supporting its drug-like properties. However, it exhibited high lipophilicity, which could enhance membrane permeability and brain access while potentially limiting solubility. Pharmacokinetic predictions suggested good intestinal absorption and blood–brain barrier penetration.

Toxicological assessments did not identify major concerns for acute toxicity or mutagenicity, indicating a preliminary acceptable safety profile.

Conclusion: This computational study suggests HHC could interact effectively with μ, δ, and κ opioid receptors. Further experimental research is needed to confirm its pharmacological effects and therapeutic potential.

Computational discovery of novel cannabinoid-derived ligands targeting opioid receptors

Asma Ben Romdhane [1], Nour El Houda Ben Fatma [2], Firas Hfaeidh [3], Meriem Laribi [4]

[1] *Faculty of Pharmacy of Monastir, Monastir, Tunisia*
[2] *Pharmacy department, Charles Nicole Hospital, Tunis, Tunisia*
[3] *National Agency for Medicines and Health Products*
[4] *Pharmacy department, Mohamed Kassab Institute of Orthopedics, Tunis, Tunisia*

Introduction: Developing safer, more effective pain relievers remains challenging due to the limitations of traditional opioids. In this context, cannabinoid-based compounds are increasingly recognized for their role in modulating pain pathways. Among these, hexahydrocannabinol (HHC), along with related compounds, may serve as a promising source of new bioactive molecules. This study aimed to identify the most promising HHC-related analogue based on predicted opioid receptor affinity and a favorable pharmacological profile.

Materials and Methods: HHC-related compounds were obtained from the PubChem database, and the crystallographic structures of μ (mu), δ (delta), and κ (kappa) opioid receptors were sourced from the Protein Data Bank. Molecular docking was carried out using PyRx v0.8 and refined using Smina vOct 15 2019 followed by analysis of ligand-receptor interactions. Selected molecules were evaluated for physicochemical, pharmacokinetic, and toxicity parameters using ADMETLab 3.0. The final candidate was chosen based on a combination of opioid receptor affinity and a favorable predicted pharmacological profile.

Results: A library of 973 HHC analogues was screened through structure-based virtual docking against μ-, κ-, and δ-opioid receptors. Primary docking identified 660, 782, and 473 candidates for δ, κ, and μ receptors, respectively. Refinement reduced these to 514, 710, and 431 ligands. Cross-receptor affinity analysis revealed 275 analogues with strong predicted binding across all three targets. Further analysis narrowed the set to 108 compounds based on binding mode evaluation, and ADMET filtering identified nine analogues with favorable in silico pharmacological profiles. Among these, one lead analogue - (6aR,10aR)-6,6,9-trimethyl-3-(5,5,5-trifluoropentyl)-6a,7,10,10a-tetrahydro-6H-benzo[c]chromen-1-ol - demonstrated consistent high predicted affinity for μ-, κ-, and δ-opioid receptors, stable orthosteric binding, and favorable pharmacological properties, making it the most promising candidate.

Conclusion: This in silico study underscores the pharmacological potential of HHC-related analogues as opioid receptor ligands. These findings lay the groundwork for further preclinical research to assess their potential as novel therapeutics candidate.

Coating Uniformity: Influence of Atomizing Air Pressure and spray rate

BENAYACHE ASSIA, LAMOUDI Lynda, DAOUD Kamel

Laboratory of transfer phenomena. Faculty of Mechanical Engineering and Process Engineering.
USTHB. Algeria

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 considered 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 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.

References

[1] Porter SC, Felton LA. Techniques to assess film coatings and evaluate film-coated products. Drug Dev Ind Pharm. 2010;36(2):128–42.

[2] Bruce HF, Sheskey PJ, Garcia-Todd PFelton LA. Novel lowmolecular-weight hypromellose polymeric films for aqueous film coating applications. Drug Dev Ind Pharm. 2011;37:1439–45.

[3] Felton LA. Film coating of oral solid dosage forms. In: Swarbrick J, editor. Encyclopedia of pharmaceutical technology. 3rd ed. New York: Informa Healthcare; 2006. p. 1729– 47. 8. [4]Porter SC, Verseput RP, Cunningham CR. Process optimization using design of experiments. Pharmaceut Technol (USA). 1997;21(Oct):60–70.

Phytochemical profiling and biological activities of the trunk bark of *Acacia cyclops* trunk bark: *in vitro* combined with *in silico* approach

Ahlem Beyaoui [a], Muammer Kaplan [b], Salma Jlizi [a],
Ahmet Ceyhan Goren [c], Hichem Ben Jannet [a]

[a] *University of Monastir, Faculty of Science of Monastir, Laboratory of Heterocyclic Chemistry, Natural Products and Reactivity (LR11ES39), Team: Medicinal Chemistry and Natural Products, Avenue of Environment, 5019 Monastir, Tunisia.*
[b] *TUBITAK Marmara Research Centre, Institute of Chemical Technology, 41470, Gebze, Kocaeli, Turkiye*
[c] *Gebze Technical University, Faculty of Basic Sciences, Department of Chemistry, Gebze, Kocaeli, Turkiye*

Acacia cyclops, mainly introduced in Tunisia for the purpose of restoring natural rangelands, is recognized as a reservoir of phenolic compounds with pharmacological activity.[1,2] The aim of this study was to analyze the phytochemical profile of *Acacia cyclops* trunk bark ethyl acetate extract using LC–tandem mass spectrometry for the first time, along with evaluating its antioxidant and anti-tyrosinase properties. Consequently, we determined the total phenolic and flavonoid contents of the extract under investigation and identified and quantified 19 compounds, including phenolic acids and flavonoids. In addition to assessing their antioxidant potential against DPPH and ABTS assays, in vitro and *in silico* studies were conducted to evaluate the tyrosinase inhibitory properties of the *A. cyclops* extract. The ethyl acetate trunk bark extract exhibited a substantial total phenolic content and demonstrated significant antioxidant activity in terms of free radical scavenging, as well as notable tyrosinase inhibitory action. The substantial anti-tyrosinase activity of the examined extract was revealed through molecular docking analysis and druglikeness prediction of the main selected compounds. These findings suggest that *A. cyclops* extract holds promise as a potential treatment for skin hyperpigmentation disorders.

Keywords: *Acacia cyclops*; phenolic compounds; LC–MS/MS; antioxidant activity; tyrosinase inhibition; molecular docking.

---

[1] Jelassi A., Cheraief I., Hamza M. A., Jannet H. B., Journal of Food Composition and Analysis, 2014, 33: 49–54. https://doi.org/10.1016/j.jfca.2013.11.001

[2] Plants 2023, 12(19), 3486*;* https://doi.org/10.3390/plants12193486

Synthesis of magnetic nanoparticles for the removal of polymeric pollutants from water

Khouloud BOLTANE [a,c], Rafika BEN SGHAIER [b], Sana BEN ISMAIL [c],
Paulo MIRA MOURÃO [d,e], Amine MNIF [a]

[a)] University of Tunis El Manar, Faculty of Sciences of Tunis, Mineral Chemistry Laboratory
[b)] CNRSM-Composite Materials and Clay Minerals Laboratory, Technopole of Borj Cedria, Tunisia
[c)] National Institute of Marine Sciences and Technologies, Marine Environment Laboratory
[d)] Department of Chemistry and Biochemistry, University of Évora, Portugal
[e)] Mediterranean Institute for Agriculture, Environment and Development & CHANGE, Évora, Portugal

Magnetic nanoparticles have proven to be promising materials for water treatment due to their large specific surface area, strong adsorption capacity, and ease of separation from aqueous media by an external magnetic field. These properties make them particularly effective for the removal of persistent contaminants from aquatic systems. In this study, magnetite (Fe_3O_4) nanoparticles were synthesized using a simple and cost-effective co-precipitation method and then evaluated for the removal of a synthetic polymer commonly found in aquatic environments. The synthesized nanoparticles were characterized using various analytical techniques to investigate their morphology, structure, and chemical composition. Batch experiments were conducted to assess the polymer removal efficiency under different experimental conditions. The results demonstrated that the Fe_3O_4 nanoparticles exhibit a strong affinity for the targeted contaminating polymer, enabling its efficient removal at a rate of 98%. The magnetic properties of the material also enabled rapid recovery of the nanoparticles after treatment with an external magnetic field, facilitating their reuse and achieving a yield of 80%. Our results highlight the potential of magnetite nanoparticles synthesized by co-precipitation as an efficient and practical approach for treating water contaminated by synthetic polymers.

References

[1] Ba-abbad, M. M., Benamour, A., Ewis, D., Mohammad, A. W. (2022). Synthesis of Fe_3O_4 Nanoparticles with Different Shapes Through a Co-Precipitation Method and Their Application. JOM. https://doi.org/10.1007/s11837-022-05380-3

[2] Hu, L., Zhou, J., Kitazawa, D. (2025). Electrostatic Interactions Override Surface Area Effects in Size Dependent Adsorptive Removal of Microplastics by Fe_3O_4 Nanoparticles. Sustainability, 17,8878, 1–20. https://doi.org/https://doi.org/10.3390/su17198878

Design of Novel N-Alkylbenzimidazole-silver(I) catalysts for aldehyde-amine-alkyne coupling

Lamia BOUBAKRI [a], Nevin Gürbüz [b,c], İsmail ÖZDEMIR [b,c], Harald Kelm [d], Naceur HAMDI [a]

[a) Research Laboratory of Environmental Sciences and Technologies (LR16ES09), Higher Institute of Environmental Sciences and Technology, University of Carthage, Hammam-Lif, Tunisia.
[b) Department of Chemistry, Catalysis, Research, and Application Center, İnönü University, Malatya, Turkey
[c) Drug Administration and Research Center, İnönü University, 44280-Malatya, Turkey
[d) Department of Chemistry, RPTU Kaiserslautern-Landau, Erwin-Schrödinger-Str. Geb. 54, 67663 Kaiserslautern, Germany
Email: boubakri_lamia@yahoo.co.uk

The multicomponent reaction (MCR), specifically the A3-coupling (aldehyde–alkyne–amine), represents a highly efficient strategy for the synthesis of propargylamines.[1] From a sustainability standpoint, MCRs are particularly advantageous as they enable the construction of complex molecular frameworks while significantly reducing reaction time, solvent waste, and energy consumption.[2] While various catalytic systems have been explored, silver(I) complexes, particularly those featuring highly electron-donating N-heterocyclic carbene (NHC) ligands have recently emerged as superior candidates due to their ability to facilitate A3-coupling under exceptionally mild conditions.[3] Motivated by these considerations, we have synthesized a series of novel N-coordinated silver complexes. Following their characterization through spectroscopic methods, we evaluated their catalytic performance in A3-coupling reactions to elucidate the specific impact of ligand architecture on catalytic efficiency.

Keywords: N-alkylbenzimidazole, N-coordinated silver complex, A3-coupling.

---

[1] (a) V.A. Peshkov, O.P. Pereshivko, E.V. Van der Eycken, *Chem. Soc. Rev.*, 41 (2012) 3790. (b) S. Sakaguchi, T. Kubo, Y.A. Ishii, *Angew. Chem. Int. Ed.*, 40 (2001)

[2] B. Ganem, *Acc. Chem. Res.*, 42 (2009) 463.

[3] (a) A. D'Amato, M. Sirignano, S. Russo, R. Troiano, A. Mariconda, P. Longo, *Catalysts*., 13 (2023) 811. (b) M.N. Rao, R. Manne, J.M. Tanski, R. Butcher, P. Ghosh, Mol. Catal., 529 (2022) 112515. (c) Y. Li, X. Chen, Y. Song, L. Fang, G. Zou, Dalton Trans., 40 (2011) 2046.

Efficient Removal of Anionic Dyes from Aqueous Media Using a Zeolite/Chitosan/Laser-Induced Graphene Hybrid Material

Saber Boubakri*, Ridha lafi, Naila Saidi, Walid Mabrouk

CERTE, Laboratory Water, Membrane and Environmental Biotechnology,
BP 273, Borj Cedria, Soliman 8020, Tunisia.
* E-mail address: boubakrisaber772@gmail.com

Industrial wastewater containing anionic dyes such as Methyl Orange (MO) and Congo Red (CR) is a major environmental challenge due to their stability, persistence, and toxicity, requiring efficient and sustainable treatment solutions. In this study, a zeolite–chitosan–laser-induced graphene (LIG) composite was synthesized and evaluated as an effective adsorbent for removing these dyes from aqueous solutions. The physicochemical properties of the composite were comprehensively characterized using Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), scanning electron microscopy (SEM), and Brunauer–Emmett–Teller (BET) surface area analysis. Batch adsorption experiments were carried out to evaluate the influence of key operational parameters, including solution pH, contact time, initial dye concentration, and temperature, on adsorption performance. The adsorption kinetics were well described by the pseudo-second-order model, indicating that chemisorption plays a dominant role in the adsorption process. Equilibrium data were best fitted by the Freundlich isotherm model, suggesting heterogeneous surface characteristics and a multilayer adsorption mechanism. The enhanced adsorption capacity of the composite can be attributed to the synergistic effects of its constituents: the high surface area and ion-exchange properties of zeolite, the abundance of functional groups and electrostatic interactions provided by chitosan, and the strong π–π interactions and abundant adsorption sites offered by laser-induced graphene. These combined features significantly improve dye uptake efficiency compared to the individual components. Overall, the results show that the zeolite–chitosan–LIG composite is an efficient, eco-friendly adsorbent for removing anionic dyes from wastewater.

Keywords: Anionic dyes; Zeolite–chitosan– laser-induced graphene (LIG); Adsorption; Eco-friendly adsorbent.

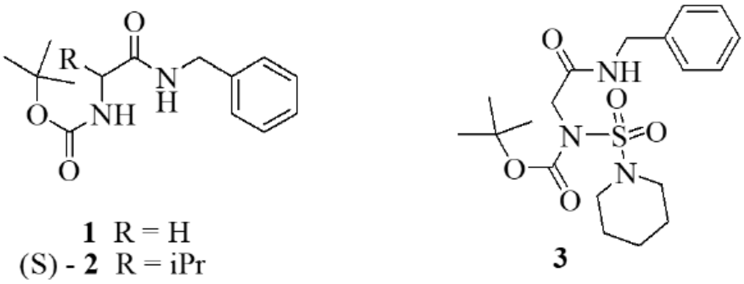
SYNTHESIS AND CHARACTERIZATION OF NEW PEPTIDE ANALOGUES OBTAINED BY SULFAHYDANTOIN OPENING REACTIONS

Djamel Bouchouk, Fatma Zohra Souha Soukehal

Laboratoire de Chimie Organique et Interdisciplinarité, Université Mohamed Cherif Messaadia,
Souk Ahras, 41000, Algérie
E-Mail: d.bouchouk@univ-soukahras.dz

Sulfhydantoin from glycine or *L*-valine is used as a precursor via heterocyclic opening reactions. The operating conditions used during electrophilicity tests influence the reactivity of heterocycles, the best control of the electrophilicity of our molecules and consider as well as their use as enzyme inhibitors. The regioselectivity of the reactions carried out in various nucleophilic media leads to three new linear products derived from acetamide and butanamide and which are analogous to the peptide structures, Fig1.

The synthetic methodology adopted and the realization of a process for opening sulfhydantoins which are derived from glycine and *L*-valine, which are used as generators for new derivatives which have mimetic structures at peptides under different nucleophilic conditions, these heterocycles have also been investigated in peptide chemistry. The objective of these syntheses was to use them as generators of functionalized peptide analogues for potential enzyme inhibition. The structures of the synthesized products **1**-**3** have been elucidated and confirmed by the usual spectroscopic methods.



1 R = H
(S) - **2** R = iPr

3

Fig.1.

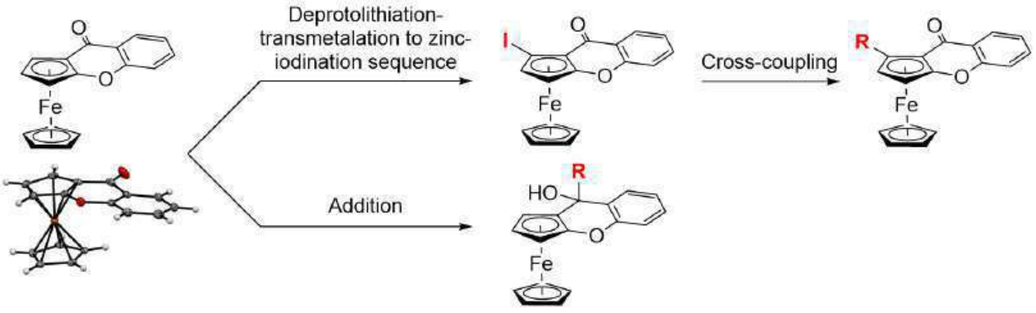
Keywords: Opening reactions; Sulfahydantoin; Electrophilicity; Peptide; Enzyme inhibitors

From Ferrocene-Fused Xanthones to Functionalized Cyclic Ferrocene Derivatives

Sirine Boussandel [1,2], William Erb [1], Florence Mongin [1], Ali Samarat [2]

[1] *Univ Rennes, CNRS, ISCR (Institut des Sciences Chimiques de Rennes) - UMR 6226, F-35000 Rennes, France*
[2] *University of Carthage, Faculty of Sciences of Bizerte, LR18ES11, Laboratory of Hetero-Organic Compounds and Nanostructured Materials, 7021 Bizerte, Tunisia*
sirine.boussandel@etudiant.univ-rennes.fr

Planar chiral ferrocene derivatives have attracted considerable interest among synthetic chemists due to their numerous applications in asymmetric catalysis, medicinal chemistry, and materials science.[1] Recent studies have highlighted effective cyclization strategies for the synthesis of planar chiral heterocyclic ferrocene derivatives via palladium-catalyzed intramolecular C–H arylation. These approaches provide powerful tools for the construction of original ferrocene scaffolds with high enantioselectivity and structural diversity.[2] Inspired by these methodologies, we sought to develop a complementary approach towards related cyclic ferrocene ketones. The key ferrocene-fused xanthone was prepared in racemic or enantiomerically pure form and then subjected topost-functionalization. A part from addition reaction onto the ketone, a directed deprotolithiation under Barbier conditions, using a ZnCl chelate as an electrophilic trap, followed by iodolysis, was optimized.[3]The resulting iodinated derivative was then subjected to various cross-coupling reactions with the aim of generating a diverse series of functionalized cyclic ferrocene ketones.



References

[1] (a) Hayashi, T.; Togni, A., Eds. *Ferrocenes*; VCH: Weinheim, Germany, **1995**. (b) Togni, A.; Halterman, R. L., Eds. *Metallocenes*; VCH: Weinheim, Germany, **1998**. (c) Štěpnička, P., Ed. *Ferrocenes*; Wiley: Chichester, U.K., **2008**. (d) Dai, L.-X.; Hou, X.-L., Eds. *Chiral Ferrocenes in Asymmetric Catalysis*; Wiley: Chichester, U.K., **2010**. [2] (a) Liu, C-X.; Gu, Q.; You, S-L. *Trends Chem.* **2020**, *2*, 8. (b) Gao, D-W.; Zheng, C.; Gu, Q.; You, S-L. *Organometallics*.**2015**, *34*, 4618. (c) Xu, B-B.; Ye, J.; Yuan, Y.; Duan. W-L. *ACS Catal*. **2018**, *8*, 11735. [3] (a) Dayaker, G.; Sreeshailam, A.; Chevallier, F.; Roisnel, T.; Krishna, P. R.; Mongin, F. *Chem. Commun*. **2010**, *46*, 2862. (b) Tazi, M.; Erb, W.; Halauko, Y. S.; Ivashkevich, O. A.; Matulis, V. E.; Roisnel, T.; Dorcet, V.; Mongin, F. *Organometallics*. **2017**, *36*, 4770. (c) Dayaker, G.; Erb, W.; Blot, M.; Gros, P. C.; Hedidi, M.; Chevallier, F.; Hilmersson, G.; Roisnel, T.; Dorcet, V.; Bentabed-Ababsab, G.; Mongin, F. *New J. Chem*. **2021**, *45*, 22579.

Efficient Synthesis and Structure-Activity Relationships of a Novel Class of PI4Kβ Inhibitors Identified from a Novalix DEL Library

Nadia BOUZAYANI [a], Florence BONNATERRE [b], Agnès JONCOUR [b], Paola CIAPETTI [c], Bertrand VIVET [c], Hugues PREVET [d], Miguel Angel PENA PINON [c], Dhoha TRIKI [d], Ruel CEDENO [c], Yaëlle FISCHER [c], Philippe SCHAMBEL [c], Julian NOMME [c], Lea WICK [c], Céline RONIN [c], Nathalie MEMBRE [c], Matthieu POIROT [c], Nathalie HUSS-BRAUN [c], Anna BONHOURE [c], Eugenie LAIGRE [c], Emmanuel KLEIN [c], Imen TALBI [a], Matthieu JEANTY [d], Nathalie WEIDNER [c], Sabine GRATZER [c] and Jérôme GUILLEMONT [d]

a) Novalix, Pépinière d'entreprises, Technopole Sidi Thabet, 2020-Ariana - TUNISIA
b) Novalix, 102 avenue Gaston Roussel, Bâtiment Galien, 93230 Romainville, France
c) Novalix, 16 rue d'Ankara, 67000 Strasbourg, France
d) Novalix, Campus de Maigremont, BP615 27106, Val-de-Reuil CEDEX, France

Human rhinovirus (HRV) belongs to the Picornaviridae family and is responsible for several pathologies, including acute upper and lower respiratory tract infections, pneumonia, and bronchiolitis. Phosphatidylinositol 4-kinase IIIα (PI4KA) and IIIβ (PI4KB) phosphorylate phosphatidylinositol to generate phosphatidylinositol 4-phosphate (PI4P), a lipid that plays a key role in membrane dynamics and lipid homeostasis. Pathogenic viruses hijack PI4Ks to manipulate PI4P levels and thereby promote their replication. Consequently, viruses of the Picornaviridae family are sensitive to direct inhibition of PI4KB, which disrupts viral replication. Targeting host kinases has therefore emerged as a promising antiviral strategy against viruses such as HRV.

Novalix has developed a DNA-encoded library (DEL) platform comprising over 400 million compounds and leveraged this technology to expand the chemical diversity of PI4KB inhibitor scaffolds. In this work, we report the synthesis of a series of benzimidazole-based compounds, prepared through efficient synthetic routes, that demonstrated inhibitory activity against PI4KB.

Key words: HRV, Picornaviridae, PI4K, DEL

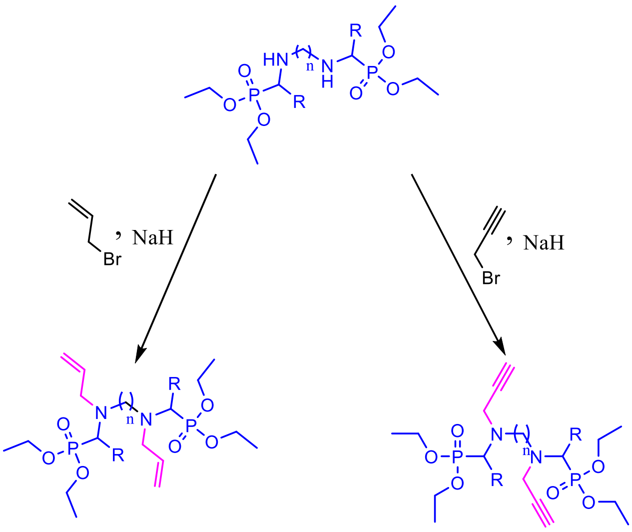
Bis(allyl-α-aminophosphonates) and bis(propargyl-α-aminophosphonates) derivatives: new synthesis from bis(α-aminophosphonates)

Sirine Briki, Ichrak Souii, Hédi M'rabet

Selective Organic & Heterocyclic Synthesis Biological Activity Evaluation Laboratory (LR17ES01), Department of Chemistry, Faculty of Sciences of Tunis, University of Tunis El Manar, 2092 Tunis-Tunisia.

Email: briki.sirin@etudiant-fst.utm.tn

Bis(α-aminophosphonates),[1,2] are notable for their strong ability to suppress bone resorption and their application as corrosion inhibitors owing to their potent metal-chelating properties[3]. In the present work, we performed a straightforward synthesis of two new bis(allyl-α-aminophosphonates) and bis(propargyl-α-aminophosphonates) derivatives. This approach involves the selective functionalization of bis(α-aminophosphonates) with allyl and propargyl groups.



Keywords: bis(α-aminophosphonates), bis(allyl-α-aminophosphonates), bis(propargyl-α-aminophosphonates).

References*:*

[1] Souii, I.; Sanhoury, M.A.; Vicario, J.; Jiménez-Aberásturi, X.; Efrit, M.L.; M'rabet, H.; de los Santos, J.M. Synthesis and Characterization of a New Series of Bis(allylic-_-aminophosphonates) under Mild Reaction Conditions. Molecules **2023**, 4678. https://doi.org/10.3390/molecules28124678.

[2] Souii, I.; Jmaî, M; M'rabet, H. Synthesis, In Silico molecular docking, and ADMET analysis of 1,4-terephthalic bis(α-aminomethanephosphonate) derivatives. Journal of Molecular Structure **2026**, 146040. https://doi.org/10.1016/j.molstruc.2026.146040.

[3] Deyab, M.A.; Abdeen, M.M.; Hussien, M.; E. El-Sayed, I.; Galhoum, A.; El-Shamy, O.A.A.; Abd Elfattah, M. Novel Corrosion Inhibitor for Carbon Steel in Acidic Solutions Based on α-Aminophosphonate (Chemical, Electrochemical, and Quantum Studies). Molecules **2023**, 4962. https://doi.org/10.3390/molecules28134962.

Magnetic Tunisian clay nanocomposite : A sustainable and separable adsorbent for rapid cationic dye removal from aqueous solutions

Islèm CHAÂRI, Bochra RABEH, Ahmad Hichem HAMZAOUI

[1] *National Center for Research in Materials Sciences, Tunis, Tunisia*
[2] *Faculty of Science, Tunis, Tunisia*
*Presenting author e-mail: islem.chaari@cnrsm.rnrt.tn
Tel: (+216) 56800680; Fax: (+216) 216 79 325 314;

The treatment of dye-contaminated aqueous solutions, representative of textile effluents, remains a critical environmental challenge. This study presents a novel, sustainable, and easily separable adsorbent: a nanocomposite of Tunisian natural clay coated with magnetite (Fe_3O_4) nanoparticles. The successful synthesis of the hybrid material was confirmed by XRD and FTIR analyses.

The adsorption performance was evaluated using Crystal violet (CV) as a model cationic pollutant. The Clay@ Fe_3O_4 nanocomposite demonstrated exceptionally fast and efficient removal, with adsorption equilibrium reached within 20 minutes. The process followed pseudo-second-order kinetics and the Langmuir isotherm model, revealing a high maximum adsorption capacity of 61 mg/g a significant improvement over raw clay.

The key innovation lies in the material's magnetic property, allowing for complete and rapid separation from water using a simple magnet after treatment, which addresses a major practical drawback of powder adsorbents.

Keywords : Magnetic adsorbent, clay nanocomposite, dye removal, sustainable material.

Fabrication of Laser-Induced Graphene on Polyethersulfone Membranes and Its Application to Rhodamine B Adsorption

Ridha Lafi [a], Jalila Chékir [a], Khaled Charradi [b,*], Neila Saidi [a], Walid Mabrouk [a]

[a] CERTE, Laboratory Water, Membrane and Environmental Biotechnology,
BP 273, Borj Cedria, Soliman 8020, Tunisia.
[b] CRTEn, Nanomaterials and Systems for Renewable Energy Laboratory, Research and Technology Center of Energy, Technoparc Borje Cedria, BP 095, Hammam Lif, Tunisia.
Corresponding author email: charradikaled2010@gmail.com

This study presents an investigation of Rhodamine B (Rh B) adsorption using Laser-Induced Graphene (LIG) synthesized from a sulfonated polyether sulfone sulfonamide precursor. Physicochemical characterization confirmed the porous morphology and surface charge favorable for dye adsorption, with a maximum adsorption capacity of 277.77 mg/g. Thermodynamic analysis revealed an exothermic adsorption process, suggesting spontaneous dye–adsorbent interactions governed by surface heterogeneity. Rh B, representative of toxic aromatic dyes commonly used in the textile and printing industries, was employed as a model pollutant. Statistical physics modeling indicated a multimolecular adsorption geometry primarily driven by π–π stacking and hydrophobic interactions. Furthermore, an artificial neural network (ANN) model exhibited excellent predictive performance ($R^2 = 0.9992$), highlighting its potential for adsorption process optimization. These findings demonstrate that LIG is a promising, scalable, and AI-enhanced adsorbent for industrial wastewater treatment and sustainable environmental technologies.

Keywords: Laser-Induced Graphene. Adsorption. Rhodamine B. Water Treatment.

Eco-Friendly Phosphorylation of Chitin Nanocrystals for Enhanced Mechanical and Flame-Retardant Performance in Bio-Based Nanocomposites Films

Wafa Cheikhrouhou[1], Hatem Ben Jouira[1], Sami Boufi[2]

[1] *Laboratory of Extremophile Plants, Centre of Biotechnology of Borj Cedria,*
B.P. 901, Hammam-Lif 2050, Tunisia
[2] *University of Sfax, Faculty of Science, LSME, BP1171-3018 Sfax, Tunisia*
E-mail: cheikhrouhouw@gmail.com

Chitin, a renewable and environmentally friendly biomass resource, has gained significant attention due to its abundance and unique properties. Chitin nanocrystals are particularly promising as reinforcing agents in bio-based composites, offering lightweight and high-strength characteristics. However, their intrinsic flammability remains a major limitation for applications requiring improved thermal stability and flame resistance. In this study, phosphorylated chitin nanocrystals (P-ChNCs) were successfully synthesized from crab shell waste through a simple H_3PO_4/urea pretreatment followed by high-pressure homogenization. Compared to conventional acid hydrolysis, this approach offers notable advantages, including lower acid concentration, higher yield, and milder operating conditions. The reinforcing potential of P-ChNCs was evaluated by preparing nanocomposite films with filler contents of up to 15 wt%, and the results were compared against those of acid-hydrolyzed ChNCs. The flame retardancy introduced by phosphorylation was also characterized, addressing one of the key drawbacks of conventional chitin nanocrystals. Additionally, the biodegradability of P-ChNCs in aquatic media was assessed using biological oxygen demand measurements and compared to that of neat chitin. Overall, this work demonstrates the potential of phosphorylated chitin nanocrystals as a multifunctional nanofiller combining reinforcing and flame-retardant properties for sustainable packaging applications.

Laser Flash Photolysis: A Key Technique for Unraveling Polar and Radical Mechanisms

Saloua Chelli-Lakhdar, Sami Lakhdar

CNRS/Université Toulouse III-Paul Sabatier, Laboratoire Hétérochimie Fondamentale et Appliquée, LHFA
UMR 5069, 31062 Toulouse Cedex 09, France
saloua.chelli-lakhdar@utoulouse.fr

Laser flash photolysis (LFP) is a powerful technique for elucidating fast reaction mechanisms through direct detection of transient intermediates and evaluation of their reactivity. Excited-state dynamics are characterized by monitoring ground-state recovery and lifetimes of photoinduced absorptions over nanosecond to millisecond timescales in the visible and near-infrared regions, with ~7 ns time resolution.[1]

We apply LFP to investigate three mechanistic scenarios.

- ✓ First, the nucleophilicity of structurally constrained phosphorus compounds is quantified via reactions with phosphonium reference electrophiles within the Mayr framework under pseudo-first-order conditions.
- ✓ Second, the mechanism of tandem olefin cross-metathesis and *E–Z* isomerization is elucidated by tracking the transient absorption of the photocatalyst radical anion. [2]
- ✓ Third, a distinct reactivity mode enabled by quantum mechanical tunneling (QMT) is demonstrated, where a cyclohexadiene derivative (terpinene) serves as a hydrogen atom donor under mild photochemical conditions, enabling activation of alkyl and aryl halides. Although thermodynamically and kinetically unfavorable classically, this pathway becomes accessible via tunneling, bypassing the conventional activation barrier.[3]

---

[1] a) J. C. Scaiano, *Acc. Chem.Res*. **1982**, *15*, 252; b) D. Duonghong, J. Ramsdenand, M.Gratzel, *J. Am. Chem.* Soc., **1982**, *104*, 2917; c) D. Bahnemann, A. Henglein, J. Lilie, L. Spanhel, *J. Phys. Chem*., **1984**, *88*, 709, d) D. Bahnemann, A. Henglein, L. Spanhel, *Faraday Discuss. Chem. Soc*., **1984**, *78*, 151; e) G. Rothenberger, J. Moser, M. Grätzel, N. Serpone, D. K. Sharma, *J. Am. Chem. Soc*., **1985**, *107*, 8054; f) D. W. Bahnemann, M. Hilgendorff and R. Memming, *J. Phys. Chem. B*, **1997**, 101, 4265.

[2] S. E. Cherif, A. Ghosh, S. Chelli, I. M. Dixon, J. Kraiem, S. Lakhdar, *Chem. Sci.,* **2022**, *13*, 12065.

[3] T. Constantin, B. Górski, M. J. Tilby, S. Chelli, F. Juliá,J. Llaveria, K. J. Gillen, H. Zipse, S. Lakhdar, D. Leonori *Science* **2022**, *377*, 1323.

RAPID SYNTHESIS AND MOLECULAR MODELING OF NEW KOJOTACRINES DERIVATIVES AGAINST ALZHEIMER'S DISEASE

YOUSSEF DGACHI [a], JOSE MARCO-CONTELLES [c],
LHASSANE ISMAILI [b] and FAKHER CHABCHOUB [a]

[a] *Laboratory of Applied Chemistry: Heterocycles, Lipids and Polymers, Faculty of Sciences of Sfax, University of Sfax. B. P 802. 3000 Sfax-Tunisia*
[b] *Laboratoire de Chimie Organique et Thérapeutique, UFR SMP, 19 rue Ambroise Paré, Université de Franche-Comté Université Bourgogne Franche-Comté, CHRU Besançon, F-25000 Besançon, France*
[c] *Laboratory of Medicinal Chemistry (IQOG, CSIC) C/ Juan de la Cierva 3, 28006-Madrid, Spain.*
email: youssefdgachi@gmail.com

In this report we describe the synthesis and molecular modeling of new kojotacrines derivatives. In the field of molecular modeling, docking is a method which predicts the preferred orientation of one molecule to a second when bound to each other to form a stable complex. The QSAR study, molecular docking and molecular dynamics simulations were performed to explore the influence of the structural features and investigate the molecular mechanism of ligands interactions with the human cholinesterases (hAChE).

Since compound KT2d has a chiral centre at the pyran ring, the reported biological data refer to the racemic mixture, and the observed whole result is a combination of the effects of both enantiomers. Nevertheless, to obtain more information about the binding properties, docking studies were performed on both (R)- and (S)-enantiomers of compound KT2d. The docking procedure was applied to the whole protein target, without imposing the binding site ("blind docking"). Flexible docking experiments have been performed for (R)- and (S)-enantiomers of KT2d. To address receptor flexibility in hAChE, the rearrangement of the side chains of eight residues, Trp286, Tyr124, Tyr337, Tyr72, Asp74, Thr75, Trp86, and Tyr341 was allowed. The movement of these residues may increase the size of the gorge and thus facilitate the access of bulky ligands to the catalytic site. Both (R)- and (S)-enantiomers of compound KT2d were studied in docking simulations. The binding energy of (S)-enantiomer (-10.4 Kcal/mol) was lower than that of the (R)-enantiomer (-9.6 Kcal/mol).

Keywords: Alzheimer's disease; molecular modeling; kojotacrines.

References

[1] Martins C, Carreiras MC, Le_on R, et al. Synthesis and biological assessment of diversely substituted furo[2,3-b]quinolin-4- amine and pyrrolo[2,3-b]quinolin-4-amine derivatives, as novel tacrine analogues. Eur J Med Chem 2011;46:6119–30.

[2] Dgachi Y, Ismaili L, Knez D, et al. Synthesis and biological assessment of racemic benzochromenopyrimidinimines as antioxidant, cholinesterase, and A$\beta_{1\text{-}42}$ aggregation inhibitors for Alzheimer's disease therapy. ChemMedChem 2016; 11:1318–27.

Facile Sol–Gel Combustion Synthesis of Fe_3O_4–$LiNiVO_4$ Nanocomposite for Energy Storage and Photocatalytic Applications

Siwar El Ghali [a], Inmaculada Álvarez-Serrano [b], Belén Sotillo[c],
Abdessalem Badri [d,e], Faouzi Aloui [a]

a) Laboratory of Asymmetric Synthesis and Molecular Engineering of Organic Materials for Organic Electronics (LR18ES19), Faculty of Sciences, University of Monastir, 5019 Monastir, Tunisia.
b) Dep. Inorganic Chemistry, Chemistry Faculty, University Complutense of Madrid, 28040 Madrid, Spain.
c) Dep. Materials Physics, Physics Faculty, University Complutense of Madrid, 28040 Madrid, Spain.
d) Laboratory of Interfacial and Advanced Materials, Faculty of Sciences (FSM), University of Monastir, 5019 Monastir, Tunisia.
e) Faculty of Sciences and Technics, University of Kairouan, 9100 Sidi Bouzid, Tunisia.

A Fe_3O_4–$LiNiVO_4$ nanocomposite was synthesized via a sol–gel combustion method followed by calcination. X-ray diffraction confirmed the coexistence of magnetite and $LiNiVO_4$ phases, while FTIR spectroscopy verified the presence of characteristic Fe–O, V–O and Ni–O bonds. Electron microscopy showed aggregated porous particles with homogeneous elemental distribution, indicating effective integration between both components. Magnetic measurements revealed superparamagnetic behavior at room temperature, with saturation magnetization decreasing from 74.8 emu g^{-1} for Fe_3O_4 to 35.64 emu g^{-1} for the composite due to the incorporation of the weakly magnetic $LiNiVO_4$ phase. Electrochemical evaluation as lithium-ion battery anodes demonstrated improved coulombic efficiency, rate capability, and cycling stability compared with pure magnetite. The composite delivered discharge capacities of 455 mAh g^{-1} at 1000 mA g^{-1} and retained ~250 mAh g^{-1} after 100 cycles at 300 mA g^{-1}. In addition, the material exhibited combined adsorption–photocatalytic activity toward methylene blue removal with a total efficiency of 88.64%. The enhanced performance is attributed to synergistic interactions between Fe_3O_4 nanoparticles and the $LiNiVO_4$ matrix, which improve structural stability, electron transport, and active surface area. These results demonstrate that the Fe_3O_4– $LiNiVO_4$ nanocomposite is a promising multifunctional material for energy storage and environmental remediation applications.

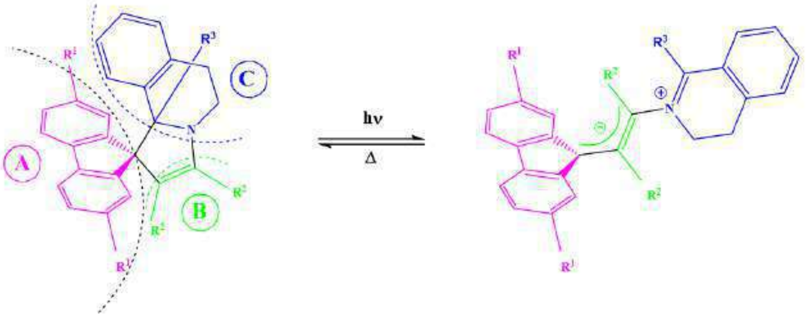
Key words: nanocomposite, multifunctional, energy storage, environmental remediation

Theoretical Investigation of the Photochromic Mechanism of Tetrahydroindolizine (THI) Derivatives

Nizar El Guesmi [a,b] and François Maurel [c]

a) *Département de chimie, Faculté des Sciences, Avenue de l'Environnement, 5019 Monastir, Tunisie.*
b) *CRMN, Centre for Research on Microelectronics and Nanotechnology of Sousse, NANOMISENE Lab, LR16CRMN01,4054,Technopark of Sousse, Tunisia.*
c) *Université de Paris, ITODYS, CNRS, F-75006 Paris, France*

Photochromic compounds are an important class of functional materials that exhibit reversible changes in molecular structure and optical properties upon light irradiation. This unique behavior provides significant potential for applications in optoelectronic devices, sensors, and molecular switches. In the present work, DFT calculations were performed to gain insight into the ring-opening and ring-closure mechanisms as well as the electronic transitions responsible for the observed photochromic behavior of tetrahydroindolizine (THI) derivatives. Geometry optimizations of both the closed spiro and open forms were performed to evaluate the relative stability of the molecular species involved in the photochromic process. The analysis of the frontier molecular orbitals indicates that UV irradiation promotes an electronic transition facilitating the ring-opening process and leading to the formation of a highly conjugated betaine species responsible for absorption in the visible region. Furthermore, exploration of the potential energy surface reveals that the thermal back-reaction proceeds through a two-step pathway involving a rotational isomerization (*transoid* → *cisoid*) followed by a 1,5-electrocyclization, regenerating the initial spiro form. The theoretical results indicate that both the nature and position of substituents play a crucial role in modulating intermediate stability and activation energy barriers, providing useful insights for the rational design of advanced photoresponsive materials.



THI-form (colorless) **Betaine-form (colored)**

Keywords: Photochromism ; Tetrahydroindolizine (THI) ; Reaction pathway ; DFT calculations

Chemical composition and antifungal activity of the essential oil of *Origanum majorana* L.

Hounaida Haj Salem [a], Raja Chaâbane-Banaoues [b], Hammouda Babba [b], Ameur Elaissi [a]

a) Laboratory of Chemical, Galenical and Pharmacological Development of Drugs (LR12ES09),
Faculty of Pharmacy of Monastir, University of Monastir, Monastir, Tunisia
b) Research Laboratory in Medical and Molecular Parasitology-Mycology (LR12ES08),
Faculty of Pharmacy of Monastir, University of Monastir, Monastir, Tunisia

The essential oil of *Origanum majorana* L. is recognized for its anti-infectious, anti-inflammatory, and antioxidant properties. Several chemotypes exist, including those with carvacrol, thymol/carvacrol, or linalyl acetate/linalool. Currently, no quality control standards govern its commercialization in Tunisia, and studies on its effectiveness against cutaneous microorganisms remain limited.

The essential oil marketed in Tunisia was analyzed by GC/MS and GC/FID, then tested against five fungal strains using disc diffusion and microdilution methods. Eighty-four compounds, distributed across thirteen chemical classes, were identified, representing 91% of the oil. The predominant class was monoterpene esters, with *trans*-sabinene hydrate as the major compound (31.64%), followed by hydrocarbon monoterpenes (31.64%) dominated by *p*-cymene (12.35%), sabinene (7.23%), and γ-terpinene (5.76%).

Antifungal activity varied significantly depending on the strain ($p < 0.05$). The highest activity was observed against *Trichophyton rubrum* and *Trichophyton mentagrophytes*, with inhibition zones greater than 90 mm and MICs of 0.156 mg/ml and 0.625 mg/ml, respectively, surpassing that of voriconazole. The disc diffusion and microdilution methods showed concordant results.

The essential oil of *Origanum majorana* L. represents a promising alternative against certain fungal strains responsible for skin conditions.

Keywords: Essential oils, *Origanum majorana* L., GC, antifungal activity, *trans*-sabinene hydrate.

Chemical Composition and Antifungal Activity of *Geranium graveolens* Essential Oil

Hounaida Haj Salem [a], Raja Chaâbane-Banaoues [b], Hammouda Babba [b], Ameur Elaissi [a]*

a) Laboratoire de Développement Chimique, Galénique et Pharmacologique des Médicaments (LR12ES09),
Faculté de Pharmacie de Monastir, Université de Monastir, Monastir, Tunisie
b) Laboratoire de Recherche en Parasitologie-Mycologie Médicale et Moléculaire (LR12ES08)
de la Faculté de Pharmacie de Monastir, Tunisie

Geranium graveolens L'Hér., belonging to the Geraniaceae family, is a perennial aromatic plant cultivated in Tunisia. Essential oil (EO) extracted from this plant is commercially available in Tunisia for therapeutic purposes. However, the absence of specific quality control standards governing its commercialization is currently a concern. Furthermore, research on its effectiveness against fungi responsible for skin conditions remains limited. This study aimed to analyze the chemical composition and evaluate the antifungal activity of *Geranium graveolens* essential oil against five fungal strains responsible for skin infections.

After analysis by GC/MS and GC/FID, the EO was tested against five fungal strains using the disk diffusion and broth microdilution methods. A total of 83 compounds, distributed among twelve different chemical classes, were identified, representing 86.22% of the total essential oil composition. The predominant chemical class consisted mainly of monoterpene alcohols (46.14%), with citronellol (30.43%) and geraniol (11.12%) as the dominant compounds. Monoterpene esters ranked second (10.67%), with citronellyl formate as the major compound (6.59%). Sesquiterpene alcohols ranked third (8.40%) and were primarily dominated by γ-eudesmol (4.30%).

The results of the essential oil growth inhibition tests on fungal strains did not vary significantly among the strains, except for *Candida albicans* ($p < 0.05$). The most pronounced activity was observed against *Trichophyton rubrum*, with an inhibition zone diameter > 90 mm and a minimum inhibitory concentration (MIC) of 0.156 mg/mL. This essential oil exhibited higher activity than the antifungal drug Voriconazole (inhibition zone diameter ranging from 40 to 60 mm). Comparative analysis of the results showed consistency between the two methods. In conclusion, *Geranium graveolens* essential oil could be utilized as an alternative to conventional antifungal agents against certain fungal strains responsible for skin infections.

Keywords: Essential oil, GC/FID, GC/MS, antifungal activity.

Eco-Friendly Valorization of Medicinal Plant Essential Oils: Phytochemical and Biofunctional Assessment

Manel Elakremi [a,b], Younes Moussaoui [a,b] & Ridha Ben Salem [a]

[a)] *University of Sfax, Faculty of Sciences of Sfax, Organic Chemistry Laboratory (LR17ES08), Sfax, Tunisia.*
[b)] *University of Gafsa, Faculty of Sciences of Gafsa, Tunisia.*
Email of communicant: manel.elakremi@yahoo.com

This study investigates the bioactive properties of a combined essential oil extracted from *Thymus vulgaris* L., *Syzygium aromaticum* L., and *Origan marjolaine* L., with a particular focus on its antioxidant and antimicrobial performance. The essential oils were obtained by hydrodistillation, and the total phenolic content (TPC) was quantified using the Folin–Ciocalteu assay, reaching 165.2 ± 4.5mg GAE/g.

The antioxidant activity was evaluated using DPPH, ABTS, and ferric reducing antioxidant power (FRAP) assays. The mixture exhibited high antioxidant capacity, with values of 420 ± 12 mg TE/g, 450 ± 15 mg TE/g, and 400 ± 10 mg TE/g, reflecting strong free radical scavenging ability and significant reducing power.

Antimicrobial effectiveness was assessed through the disc diffusion technique, revealing pronounced inhibitory effects against both Gram-positive and Gram-negative bacterial strains. The findings indicate that the phenolic constituents of thyme, clove, and marjoram oils may act synergistically, thereby strengthening both antioxidant and antimicrobial activities.

The essential oil blend is a natural source of active compounds that can be used in food preservation, medicine, and health products. Its use offers an environmentally friendly approach to reducing oxidative damage and controlling microbial growth, which can enhance the shelf life of food products and improve the efficacy of pharmaceutical formulations.

Keywords: *Thymus vulgaris* L.; *Syzygium aromaticum* L.; *Origan marjolaine* L., essential oil; antioxidant activity; antimicrobial activity.

Insights on the mechanism of the reaction between NO and aziridines with and without CaO catalyst

Hanan Enadi, Mohamed Oussama Zouaghi, Youssef Arfaoui [*]

Laboratoire Applications, Caractérisations et Modélisation de Matériaux (LR18ES08),
Faculté des Sciences de Tunis, Université de Tunis El Manar, Tunis, 2092, Tunisia. (a)

The reactions between nitric oxide (NO) [1] and an aziridine on gas phase and on calcium oxide (CaO) surfaces are investigated using Density Functional Theory to explore the formation of valuable nitrogen-containing heterocycles. Gas-phase analyses identify CH-side ring opening of aziridine as the most favorable pathway for radical attack by NO, leading to stable intermediates and products such as oxadiazolidines and diazetidines. [2] Solvent effects are found to further enhance the reactivity, with water notably reducing activation barriers. [3] Also, we show that electron-withdrawing groups significantly lower activation energies and improve reaction spontaneity. Besides, the CH cleavage mechanism is confirmed to be energetically preferred while the reaction occurs at the CaO(100) surface or CaO cluster, facilitated by surface basicity and favorable transition state stabilizations. Natural Bond Orbital (NBO) analysis shows the radical character development and charge redistribution during key steps. Further, periodic computations reveal that the oxadiazolidine production over the CaO(100) slab is kinetically favored compared to the diazetidine synthesis, whereas in gas phase this is due to thermodynamical considerations. These results provide insights into the reactivity of NO on oxide surfaces and should help guiding the design of efficient NO capture and transformation strategies for synthetic and environmental applications.

Keywords: NO, Catalysis, DFT computation, Heterogenous catalysis, CaO, Solvent effects.

References

[1] D.-H. Nguyen, C. Lin, C.-T. Vu, N.K. Cheruiyot, M.K. Nguyen, T.H. Le, W. Lukkhasorn, T.-D.-H. Vo, X.-T. Bui, Tropospheric ozone and NO x : A review of worldwide variation and meteorological influences, Environmental Technology & Innovation 28 (2022) 102809

[2] W.S. Epling, L.E. Campbell, A. Yezerets, N.W. Currier, J.E. Parks, Overview of the Fundamental Reactions and Degradation Mechanisms of NOx Storage/Reduction Catalysts, Catalysis Reviews 46 (2004) 163–245.

[3] M. Cossi, N. Rega, G. Scalmani, V. Barone, Energies, structures, and electronic properties of molecules in solution with the C-PCM solvation model, J Comput Chem 24 (2003) 669–681.

Esterification of tertiary alcohols with mixed aromatic-fatty anhydrides using Lewis acid as heterogeneous catalyst

Marwa Derbel, Iteb Trabelsi, Kamel Essid *

Laboratory of Organic Chemistry (LR17/ES08): Department of Chemistry, Faculty of Sciences in Sfax, Tunisia
* Corresponding author: kamelessid.issat@yahoo.fr
https://orcid.org/0000-0002-5949-1508

The fatty acid esters constitute an important class of useful chemical intermediates in the synthesis of several products such as amides, sulfonates and fatty alcohols [1]. These compounds are essential chemicals that are widely used in food, pharmaceutical, cosmetic, detergent, plasticizer, lubricant, cosmetic, textile, and other industrial applications [2].

We describe a novel and efficient method for the synthesis of fatty esters by the esterification reaction of tertiary alcohol with mixed carboxylic- fatty anhydrides using Lewis acid as heterogeneous acid catalyst. Influence of various reaction parameters such as molar ratio (anhydride/alcohol), catalyst amount, and type of mixed anhydride were studied to optimize the conditions for maximum yield.

In the present work, we have investigated the reactivity of some mixed anhydrides of fatty acid in the esterification reaction of tertiary alcohol and in the presence of Lewis acid as a heterogeneous catalyst. We have optimized the conditions for maximum yields of esterification by varying different reaction parameters.

Keywords : Tertiary alcohol, Lewis acid, heterogeneous catalyst, fatty acid ester.

References :

1. De Paiva E J.M, Corazza ML, Sierakowski MR, Wärnå J, Murzin DY, Wypych F, Salmi T (2015) Influence of two different alcohols in the esterification of fatty acids over layered zinc stearate/palmitate. Bioresour Technol193: 337-344
2. Martínez M, Oliveros R, Aracil J (2011) Synthesis of Biosurfactants: Enzymatic Esterification of Diglycerol and Oleic Acid. 1. Kinetic Modeling. Ind Eng Chem Res 50: 6609-6614

Reactivity of mixed lipid anhydrides in the acylation of certain phenolic compounds extracted from olive pomace oil

Maissa Gharsalli [a], Wafa Jahouach-Rabai [b], Kamel Essid [a*]

[a)] Laboratory of Organic Chemistry LR17ES08: Faculty of Sciences in Sfax,
Route de Soukra Km 3,5 – BP 1171-3000, Sfax, Tunisia
[b)] Laboratory of Energy and Materials for Nuclear Sciences Development,
National Centre of Nuclear Sciences and Technologies, Ariana, Tunisia;
[*] Corresponding author: kamelessid.issat@yahoo.fr
https://orcid.org/0000-0002-5949-1508

The anhydrides were prepared in the presence of triethylamine in the organic solvent by a reaction between fatty acid and acid chloride. Mixed aromatic palmitic were more reactive and selective than the aliphatic anhydrides. The palmitic group was the most involved in acylation. Good yields of fatty esters were obtained with total conversion of mixed anhydrides. Lipid esters are prepared from mixed fatty anhydrides by esterification. These esters are high-value-added intermediates used in industrial applications. We describe the synthesis and characterization of the obtained esters.

The esterification reaction was realized, first with some primary and secondary alcohols in the presence of resin Amberlyst-15. Then, in order to study the reactivity of lipid anhydrides as reaction intermediates with certain molecules among phenolic compounds, the qualitative and quantitative study of phenolic compounds, extracted by SPE (solid-phase extraction), was carried out by liquid chromatography coupled to mass spectroscopy (LC-MS). Phenolic compounds extracted with this recent method on a solid phase, often referred to as "polyphenols," are responsible for the good oxidation stability of oils.

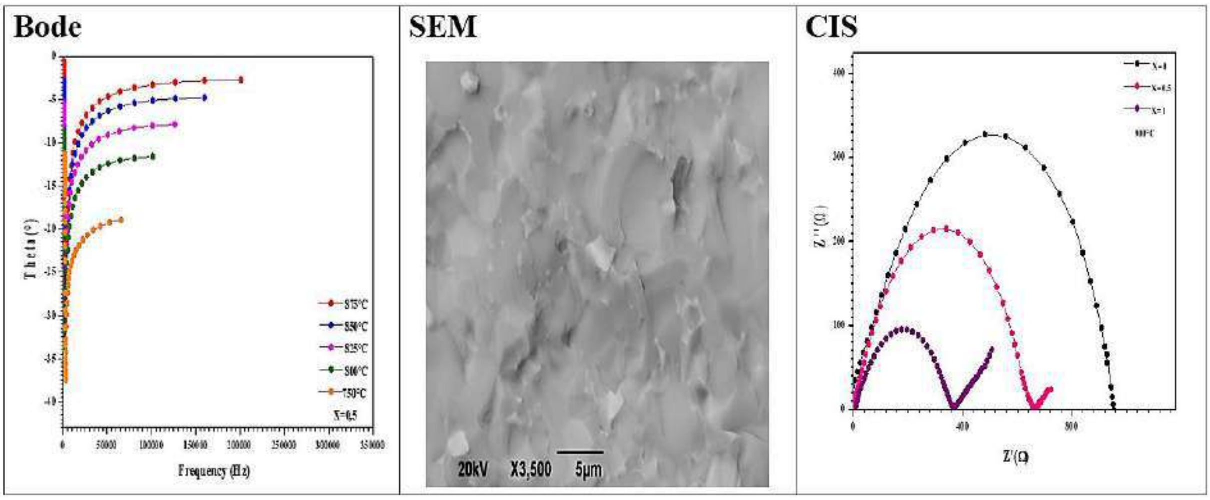
Keywords : Lipid anhydride; phenolic compounds; esterification; oxidation stability, olive pomace oil.

Structural and Electrical properties of Nd_{7-x} Li_x Sr_3 $(SiO_4)_6O_{1,5-x}$ $(0 \leq x \leq 1)$ Oxyapatite Ceramics

Ameni Fatnassi, Mustapha Hidouri

Research laboratory: Energy, Water, Environment and processes, LREWEP (LR18ES35),
National School of Engineers, University of Gabes, 6072 Gabes, Tunisia

Graphical abstract: Nd_{7-x} Li_x Sr_3 $(SiO_4)_6$ $O_{1,5-x}$



This study explores the electrical properties of Nd_{7-x} Li_x Sr_3 $(SiO_4)_6O_{1,5-x}$ $(0 \leq x \leq 1)$ ceramics as potential electrolytes for Solid Oxide Fuel cells (SOFCs) applications. Lithium substitution at the Nd site was explored to enhance ionic conductivity. The ceramics were synthesized via a mechanochemical route followed by optimized sintering. Comprehensive characterization including X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), inductivel coupled plasma (ICP), and impedance spectroscopy was performed. Structural analysis confirms the formation of a single-phase hexagonal apatite structure ($P6_3/m$). The results demonstrate a pronounced enhancement in ionic conductivity with increasing Li content, reaching a maximum of $1,85.10^{-4}S.Cm^{-1}$ at 875°C for x=1, attributed to improved oxygen-ion transport within the apatite lattice.

Keywords: Oxyapatite, solid state synthesis, Structural Refinements, Ionic conductivity.

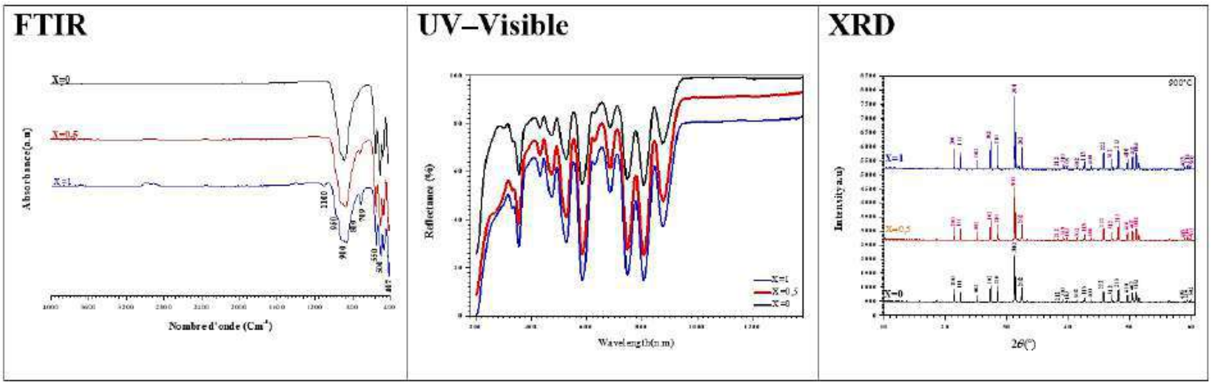
- *Full Name*: Ameni FATNASSI (PHD student in Chemistry)
- *Email*: amenifatnassi1996@gmail.com | • *Mobile Number*: +216 24 81 41 36

Optical Characterization of Nd_{7-x} Li_x Sr_3 $(SiO_4)_6O_{1,5-x}$ $(0 \leq x \leq 1)$ Ceramics

Ameni Fatnassi, Mustapha Hidouri

Research laboratory: Energy, Water, Environment and processes, LREWEP (LR18ES35),
National School of Engineers, University of Gabes, 6072 Gabes, Tunisia

Graphical abstract: Nd_{7-x} Li_x Sr_3 $(SiO_4)_6$ $O_{1,5-x}$



This study explores the optical properties of $Nd_{7-x}Li_xSr_3(SiO_4)_6O_{1,5-x}$ $(0 \leq x \leq 1)$ ceramics, focusing on their potential as a specialized laser and phosphor host material. While previous research has demonstrated the effectiveness of single-ion doping in oxyapatites, the impact of co-doping specifically the substitution of Nd with Li remains underexplored. The introduction of Li aims to enhance optical properties, inspired by the beneficial effects observed with other dopants such as lanthanides.

The ceramics were synthesized using a cost-effective mechano-chemical method, followed by optimized densification to achieve high relative density. Structural analyses (XRD, FTIR, ICP, SEM) confirm the formation of a pure apatite phase with a hexagonal structure (space group P63/m). Rietveld refinement indicates that Li and Nd ions preferentially occupy specific crystallographic sites. Nd^{3+} typically exhibits strong absorption bands in the near-infrared (NIR) region, most notably around 800–810 nm, which corresponds to the $^4I_{9/2} \rightarrow {}^4F_{5/2}, {}^2H_{9/2}$ transition. This makes these materials excellent candidates for laser diode pumping. The silicate matrix (as opposed to a phosphate matrix) often provides a slightly different crystal field splitting, which can broaden these absorption bands, potentially increasing the tolerance for pump wavelength fluctuations. The main laser emission occurs in the NIR region, typically centered around 1060–1070 nm (corresponding to the $^4F_{3/2} \rightarrow {}^4I_{11/2}$ transition.

- *Full Name*: Ameni FATNASSI (PHD student in Chemistry)
- *Email*: amenifatnassi1996@gmail.com | • *Mobile Number*: +216 24 81 41 36

Engineering Oxygen Vacancies in $Na_{0.5}Bi_{0.5}TiO_3$-Based Perovskites for Improved Photocatalytic Performance

Ferjani Mohamed [a], Arwa Achour Khedhiri [a], Moneim Zannen [a],
Abdelilah Lahmar né [b], Houcine Barhoumi [a]

[a] *Laboratory of Interfaces and Advanced Materials, Faculty of Sciences of Monastir,*
University of Monastir, Bd. of the Environment, 5019 Monastir, Tunisia.
[b] *Laboratoire de Physique de la Matière Condensée (LPMC), Université de Picardie Jules Verne,*
Pôle Scientifique, 33 rue Saint-Leu, 80039 Amiens Cedex 1, France.

Lead-free perovskites based on $Na_{0.5}Bi_{0.5}TiO_3$ have attracted considerable attention as promising functional materials for sustainable environmental applications, particularly in water remediation. Among the various optimization strategies, defect engineering has emerged as an effective approach to tailor electronic properties and enhance photocatalytic performance [1,2].

In this work, modified $Na_{0.5}Bi_{0.5}TiO_3$-based perovskites were investigated to elucidate the role of structural defects in photocatalytic activity. X-ray diffraction analysis confirmed the formation of a single-phase perovskite structure, while Raman spectroscopy provided valuable insights into lattice distortions and local structural disorder. Furthermore, X-ray photoelectron spectroscopy (XPS) revealed the presence of oxygen vacancies and mixed valence states, highlighting defect-induced electronic modifications [3,4,5].

The photocatalytic activity was evaluated through the degradation of organic dyes under irradiation, demonstrating an enhanced performance compared to the pristine material. This improvement is attributed to defect-induced oxygen vacancies, which facilitate charge carrier separation and promote the generation of reactive species.

Key words: Lead-free perovskites, NBT, defect engineering, photocatalysis, water remediation, oxygen vacancies

---

References

[1] Zannen, M.; Khemakhem, H.; Kabadou, A.; Es-Souni, M. *Structural, Raman and electrical studies of 2 at.% Dy-doped NBT.* Journal of Alloys and Compounds, 2013, 555, 56–61.

[2] Wang, P.; Yu, F.; Chi, Y.; Wu, X.; Lin, M.; Lin, C.; *et al. Enhanced piezo-photocatalysis in* $Bi_{0.5}Na_{0.5}TiO_3$*@Ag composite for efficient degradation of multiple organic pollutants.* Journal of Environmental Management, 2022, 323, 116186.

[3] Han, W.-H.; Koh, J.-H. *Shrinkage mechanism and enhanced piezoelectric properties of Ta-doped* $0.94Bi_{0.5}Na_{0.5}TiO_3–0.06BaTiO_3$ *lead-free ceramics.* Ceramics International, 2018, 44(5), 5352–5358.

[4] Ayadh, S.; Touili, S.; Amjoud, M.; Mezzane, D.; Gouné, M.; Ghanbaja, J.; Benyoussef, M.; Uršič, H.; Suban, N.; Raihane, M.; Kutnjak, Z.; El Marssi, M. *Improvement of piezocatalytic performance of* $Na_{0.5}Bi_{0.5}TiO_3$ *perovskite using K doping for efficient Rhodamine B degradation.* Journal of Water Process Engineering, 2025, 79.

[5] Quach, V.-D.; Harsan, A.; Spadaro, M. C.; *et al. Formation of oxygen vacancies at the metal–*TiO_2 *interface for enhanced photocatalytic hydrogen production.* Advanced Science, 2025, 12(32), e01835.

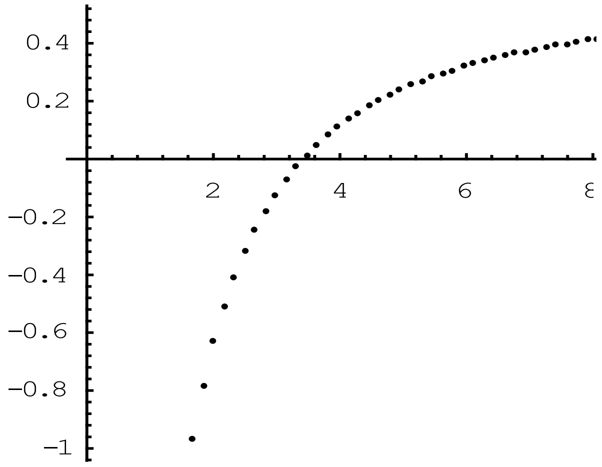
Compute of the second coefficient of Viriel and evaluation of the Boyle temperature

Fnena Kamel[a, b, c], Bellagi Ahmed

Laboratory of Thermal and Thermodynamics of Industrials Processes, TThIP
a) *Faculty of Sciences of Bizerte, University of Carthage*
b) *National School of Engineers, University of Monastir*
c) *Faculty of Sciences of Gafsa, University of Gafsa*

Accurate knowledge of the thermophysical properties such as the Boyle temperature is desirable for many applications in Cryogenics. In this work we use the Lennard-Jones[1] potential to calculate the second coefficient of Viriel [2] for Argon. A simple equation was proposed which correlates the second coefficient and temperature (plotted in the proposed figure). Very accurate prediction of the experimental value was observed.

Key words: Second coefficient of Viriel, Lennard-Jones Potential, Boyle temperature.



References

[1] A. Michels, T. Wassermann, W. Van Seenter, Appl. Sci. Res., A4, 52, (1953).
[2] K. Fnena, Inversion de l'effet de Joule Thomson, étude des courbes différentielles et intégrales et modélisation à l'aide d'équation d'état, Thèse de Doctorat FSB-ENIM (2004).

Microwave-Assisted Chemical Recycling of Bio-Based Poly(ethylene Furanoate) by Aminolysis

Nesrine Gasmi[1,2], Leila Khalfa[3,4], Gabriele Rossignolo[5],
Alessandra Lorenzetti[5], Younes Moussaoui[1,6]

[1] *University of Gafsa, Faculty of Sciences of Gafsa, Gafsa 2112, Tunisia*
[2] *University of Gafsa, Faculty of Sciences of Gafsa, Laboratory of Application of Materials to Environment, Water and Energy (LR21ES15), Gafsa 2112, Tunisia*
[3] *Applied Thermodynamics Unit Research, ENIGabes, Zrig Gabes, Tunisia*
[4] *National School of Engineers of Gafsa (eniga), University of gafsa, 2112, Gafsa, Tunisie*
[5] *Università di Padova, Dept. of Industrial Engineering, Via F. Marzolo 9, 35131 Padova, Italy*
[6] *University of Sfax, Faculty of Sciences of Sfax, Organic Chemistry Laboratory (LR17ES08), Sfax 3000, Tunisia*
Email address: nesrinegasmi.g@gmail.com ; y.moussaoui2@gmail.com

The increasing demand for sustainable materials has stimulated interest in the recycling and valorization of bio-based polymers such as polyethylene furanoate (PEF). In this work, the depolymerization of PEF was investigated through an aminolysis process assisted by microwave irradiation under controlled temperature and reaction time conditions. This approach aims to promote the chemical recycling of fully bio-based furanic polyesters and to recover valuable monomers. The process led to the formation of a new series of furanic diamine monomers, including both aliphatic and aromatic derivatives. The obtained products were characterized using thermogravimetric analysis, differential scanning calorimetry, Fourier-transform infrared spectroscopy, and nuclear magnetic resonance spectroscopy to confirm the formation of the target monomers. The results demonstrate that the polyester can be efficiently depolymerized under microwave-assisted aminolysis conditions. Furthermore, new polymers were synthesized from the recovered monomers under mild conditions. Preliminary results indicate an enhancement of thermal stability after polymerization, indicating the potential of this strategy for the valorization and recycling of bio-based furanic polyesters.

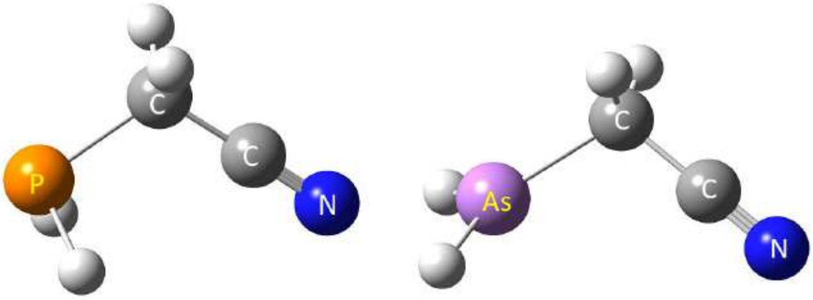
Keywords: Furanic diamine monomers; Aminolysis; Furanic polyesters

Access to Primary α-Phosphino- and α-Arseno-Nitriles: Synthesis, Characterization, and Comparison with α-Aminonitriles

Amira GHABI [a,b], Jean-Claude GUILLEMIN [b] and Taoufik BOUBAKER [a]

a) Laboratoire de Chimie Hétérocyclique, Produits Naturels et réactivité (LR11ES39), Faculté des Sciences de Monastir, Université de Monastir, Avenue de l'environnement, Monastir-Tunisie 5019, Tunisia
b) Université de Rennes, Ecole Nationale Supérieure de Chimie de Rennes, CNRS, ISCR − UMR6226, F-35000 Rennes, France

Through a chemoselective reduction of dichlorophosphines and dichloroarsines, we successfully synthesized and characterized simple primary α-phosphino- and α-arseno-nitriles. These compounds were characterized by NMR and IR spectroscopy. In general, their kinetic stability decreases from phosphorus to the corresponding arsenic derivatives, which is consistent with trends commonly observed for related compounds. Furthermore, in the ^1H NMR spectra, these chiral phosphines and arsines exhibit diastereotopic protons in the PH_2 and AsH_2 groups, a feature that has not been reported for the NH_2 group in α-aminonitriles. Finally, these newly synthesized analogues of well-known α-aminonitriles open new perspectives for further investigations of their spectroscopic behavior and chemical properties.



Keywords : Chemoselective reduction process, primary α-phosphino- and α-arseno-nitriles, diastereotopic protons.

References

[1] Amira Ghabi, Takwa Slama, Amel Hedhli, Taoufik Boubaker, Jean-Claude Guillemin. Inorg. Chem. **2024**, 63, 24, 11311–11316.
[2] Holger SP Müller, Jes K Jørgensen, Jean-Claude Guillemin, Frank Lewen, Stephan Schlemmer. Mol. Spectroscopy. **2023**, 111777, 394.

Sustainable Biochar-Based Composites for Enhanced Dye Removal from Wastewater

Fatma Ghammagui, Salah Ammar

Research laboratory; Chemistry, Electrochemistry, and Materials for Environment.
Faculty of Sciences of Gabes; University of Gabes, 6072 Gabes, Tunisia
Email: ghammaguifatima339@gmail.com ; Mobile Number: +216 95 12 19 26

The increasing discharge of industrial dyes into water bodies poses serious environmental and health risks. Developing sustainable and efficient treatment materials has therefore become a major research priority.

In this work, biomass was valorized to produce biochar through pyrolysis under oxygen-limited conditions. Several biomass sources were initially evaluated based on their adsorption capacity toward model dyes, and the most efficient one was selected for composite preparation.

Biochar was then combined with metal oxides to develop hybrid composites aimed at enhancing both adsorption and photocatalytic degradation processes. The photocatalytic performance was assessed using UV–Visible spectrophotometry, which showed a continuous decrease in dye absorbance over time.

The composite systems demonstrated improved pollutant removal efficiency compared to individual components, highlighting a synergistic interaction between biochar and metal oxides. The enhanced performance is attributed to improved adsorption properties and better separation of photogenerated charge carriers.

These results confirm the potential of biochar-based composites as promising, low-cost, and environmentally friendly materials for wastewater treatment applications.

Keywords: Biochar-based composites; Biomass valorization; Dye removal; Photocatalysis; Sustainable materials.

Theoretical Insights into the Adsorption of Eriochrome Black T on Apatite Silicates: Steric and Energetic Analysis

Rihab Ghorbali*, Houcine Ghalla, Lotfi Sellaoui

University of Monastir, Faculty of Sciences of Monastir, Laboratory of Quantum and Statistical Physics,
LR18ES18, Environment Street 5019 Monastir, Tunisia
* gorbalirihab2020@gmail.com

This study investigates the adsorption behavior of Eriochrome Black T (EBT) onto four apatite silicate materials, namely SrMil, CaMil, SrCal, and CaCal. The adsorption mechanism was analyzed using theoretical parameters derived from equilibrium isotherms, interpreted through a statistical physics model assuming multilayer adsorption. The steric parameter (n) provides insight into the molecular orientation and aggregation of EBT on the adsorbent surfaces. The obtained values suggest a multimolecular adsorption mechanism, where dye molecules are arranged in a non-parallel configuration.

The results indicate that EBT adsorption proceeds via the formation of two to three successive layers, depending on the nature of the adsorbent. The maximum adsorption capacities vary between 290 and 420 mg/g, with SrMil showing the highest performance. Furthermore, the calculated adsorption energies ($\Delta E < 40$ kJ/mol) reveal that the process is governed by physisorption, mainly driven by Van der Waals interactions and hydrogen bonding.

Overall, the reversible adsorption behavior and high adsorption capacity highlight the effectiveness of apatite silicates, particularly SrMil, as promising materials for the removal of organic dyes from aqueous environments.

A computational study of one-bond ^{31}P-^{19}F spin-spin coupling constants in some nerve agent related organophosphorus-fluorine derivatives

Abir Haloui [a], K. Essalah [b,c], M.A.K. Sanhoury [d,e], N. Amdouni [a]

[a] *Laboratory of Characterization, Applications and Modeling of Materials, Department of Chemistry. Faculty of Sciences of Tunis, University of Tunis El Manar 2092, Tunis, Tunisia*
[b] *Laboratory of Selective Organic and Heterocyclic Synthesis-Biological Activity Evaluation, SOHES, (LR17ES01), University of Tunis El Manar, Faculty of Sciences of Tunis, Department of Chemistry Tunis, El Manar 2092, Tunisia*
[c] *Preparatory Institute for Engineering Studies (IPEIEM), University of Tunis El Manar, B.P 244, Tunis 2092.*
[d] *Laboratory of Structural Organic Chemistry: Synthesis and Physico-chemical Studies, Department of Chemistry. Faculty of Sciences of Tunis, University of Tunis El Manar 2092, Tunis, Tunisia*
[e] *Materials Chemistry Research Unit, Department of Chemistry. Faculty of Sciences and Techniques, UN, Nouakchott, Mauritania*

Organophosphorus–fluorine compounds (OPFCs) bearing P–F bond have attracted considerable interest due to their chemical reactivity that allows them to be used as either mechanistic probes or potent inhibitors of enzymatic reactions. OPFC insecticides and nerve agents act primarily by inhibiting acetylcholinesterase enzyme (AChE) [1–5]. They all have fluoride as leaving group for reaction with AChE upon P-F cleavage. This suggests the importance of studying such a bond for more insights in mechanistic and enzymatic reactions. In this presentation, we report on DFT calculations of one-bond phosphorus-fluorine spin-spin coupling constants, ${}^{1}J_{P\text{-}F}$, in three phosphoryl fluoride derivatives (POF_3, $Me_2NP(O)F_2$ and $(Me_2N)_2P(O)F$) as well as a parent nerve agent (Sarin) using B3LYP, BHandH, PBE0, M06, M06L and M062X functionals combined with pcJ-1, pcJ-2, 6-31+g(d,p), TZVP and aug-cc-pVTZ basis sets. The prediction of ${}^{1}J_{P\text{-}F}$ values was preceded by a geometry optimization for each compound at M062X/aug-cc-pVTZ level of theory. Both geometry and magnetic parameter calculations were performed in solution by taking into consideration the SCRF solvent effect formalism with IEF-PCM model. Among the functionals used, M06, M06L and BHandH were found to be the most suitable in predicting ${}^{1}J_{PF}$ values to accurately reproduce the experimental data. This study could contribute significantly to the well known correlations between biological activity and structure of such compounds for the development of antidotes to related nerve agent intoxications.

References

[1] P.A. Bartlett, L.A. Lamdem, Bioorg. Chem. 14 (1986) 356–377.
[2] R. Engel, Chem. Rev. 77 (1977) 349–367.
[3] J.J. De Frank, in: J.W. Kelly, T.O Baldwin (Eds.), Applications of Enzyme Biotechnology, Plenum Press, New York, 1991, pp. 165 180;
[4] T.H. Kim, K.A. Oh, N.J. Park, N.S. Park, Y.J. Kim, E.K. Yum, Y.S. Jung, J. Appl. Biomed. 4 (2006) 67–72.
[5] K. Essalah, M.A. Sanhoury, M.T. Ben Dhia, M. Abderrabba, M.R. Khaddar, Tin tetrachloride adducts with phosphoryl ligands: A DFT study, *J. Mol. Struct. THEOCHEM*, 942, 2010, 110-114.

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

Guerfi Samiaa, [1, 2*], Lamia Boubakri [3], Berredjem Yamina [1,2,4] and Naceur Hamdi [3]

1 Faculté de technologie, Département de génie des procédés et de pétrochimie, université 20 août 1955Skikda.
2 Laboratoire des sciences et technologies de l'eau et de l'environnement, Faculté des sciences et technologies, Département des sciences des matières, Université Mohammed Cherif Messaadia, Souk_Aharas 41000. Algérie.
3 Research Laboratory of Environmental Sciences and Technologies (LR16ES09), Higher Institute of Environmental Sciences and Technology, University of Carthage, Hammam-Lif, Tunisia
4 Laboratoire de Traitement des Eaux et de Valorisation des Déchets Industriels, Faculté des Sciences, Département de Chimie, Université Badji-Mokhtar, B.P.12, Annaba 23000, Algérie.

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 % [1-2]. The present approach is environmentally benign and water is generated as the sole byproduct.

References

[1] S. Al-Nasser, N. Touj, S. Alomar, L. Mansour, M. Sauthier, N. Gurbuz, I. Ozdemir, N. Hamdi.. *Green Chem. Lett. Rev.* **2024**, *17*, 2370268.
[2] S. Al-Nasser, M. H. Abdulla, N. Alhassan, M. -A. Vaali-Mohammed, S. Al-Omar, N. Hamdi, Y. Elnakady, S. Matou-Nasri, L. Mansour. A. *Medicina* **2024**, *60*, 1379.

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

Nevin Gurbuz [1] Ismail Özdemir[1], Lamjed Mansour[2] and Naceur Hamdi*[3]

[1] *İnönü University, Catalysis Research and Application Center, Malatya, 44280, Turkey,*
[2] *Zoology Department, College of Science, King Saud University, Saudi Arabia,*
P.O. Box 2455, Riyadh 11451, Saudi Arabia
[3] *Research Laboratory of Environmental Sciences and Technologies (LR16ES09), Higher Institute of Environmental Sciences and Technology, University of Carthage, Hammam-Lif, Tunisia*
Corresponding author: *E-Mail: hamdi.naceur@isste.ucar.tn, Tel: +2198503980

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.

References:

[1] N. Touj, N. Gürbüz, N. Hamdi, S. Yas¸ar, ˙ I. Ozdemir, Inorg. Chim. Acta 478 (2018) 187–194, https://doi.org/10.1016/j.ica.2018.04.018. [2] I. Slimani, L. Boubakri, N. Özdemir, L. Mansour, I. Özdemir, N. Gürbüz, S. YAŞAR, M. Sauthier and N. Hamdi, Inorganica Chimica Acta.,2022,532,120747

Regioselective Synthesis of Functionalized Pyrimidine Derivatives via Cyclocondensation Reactions

Nozha HAMMAMI [a], Fakher CHABCHOUB [a], Emna MAALEJ [a,b]

[a] *Laboratory of Applied Chemistry: Heterocycles, Lipids and Polymers, Faculty of Sciences of Sfax,*
University of Sfax, BP 802, Sfax 3000, Tunisia
[b] *Laboratory of Molecular and Cellular Screening Processes, Centre of Biotechnology of Sfax,*
P.O. Box 1177, Sfax 3018, Tunisia

In this work, we report a direct and effective method to synthesize two distinct series of regioisomeric pyrimidines: 6-oxo-5-cyanopyrimidines and ethyl 4-aminopyrimidine-5-carboxylates.

By reacting amidinium salts with α, β-unsaturated Michael acceptors under specific conditions, we successfully steered the reaction toward specific constitutional isomers. We first optimized thepreparation of the starting materials amidine hydrochlorides and ethoxyalkylidene cyanoacetates achieving high yields.

We then focused on the condensation step, demonstrating how subtle changes in the reaction environment allow for the preferential formation of either the cyanopyrimidinone or the ethyl 4-aminopyrimidine-5-carboxylates scaffold. The structures of all new compounds were confirmed using 1D/2D NMR, IR, and melting point analysis. These polyfunctionalized products serve as versatile "building blocks" for medicinal chemistry, offering a reliable route to diverse bioactive molecules.

Bio-Based Clay Composite for Industrial Effluent Treatment: Performance and Process Optimization

Anwar Hileli [1,2*], Zahwa Ghodbani [3], Younes Moussaoui [2,4], Safa Gamoudi [1]

[1] Laboratory of Composite Materials and Clay Minerals, National Center for Research in Materials Science, Technopole BorjCedria, B.P. 73, 8027, Soliman, Tunisia.
[2] University of Gafsa, Faculty of Sciences of Gafsa, Gafsa 2112, Tunisia.
[3] University of Gafsa, National Engineering School of Gafsa, Sidi Ahmed Zarroug - 2112, Gafsa, Tunisia.
[4] University of Sfax, Faculty of Sciences of Sfax, Organic Chemistry Laboratory (LR17ES08), Sfax 3029, Tunisia.
e-mail: anwarhl173@gmail.com (A. Hileli)

Addressing the need for greener wastewater treatment solutions, this work explores a bio-based flocculant derived from natural resources. A composite material (BioC3) was prepared by integrating *Opuntia ficus-indica* cactus extract with smectite-rich clay collected from El Fahs, Tunisia. Its structural and chemical features were examined through physicochemical characterization, FTIR, and XRD analyses.

The efficiency of the developed material was tested on textile and hydraulic industrial effluents and benchmarked against several reference systems, including a conventional synthetic polyacrylamide. Performance evaluation was based on changes in turbidity, pH, and conductivity.

Experimental results under different operating conditions (flocculant dosage, mixing intensity, contact time, and pH) revealed that BioC3 provides enhanced clarification efficiency, achieving greater turbidity reduction than the synthetic counterpart. These findings demonstrate the potential of this clay-biomass composite as a sustainable and effective alternative for industrial effluent treatment.

Keywords: industriel effluent; clay ; cactus ; juice ; bioflocculant ; turbidity ; conductivity.

Nanoscale Engineering of PPV and PFO Conjugated Polymer Nanowires via Template Wetting

Hlimi Haythem,[1] Mohamed Mbarek*

[a] *LR: Synthèse asymétrique et ingénierie moléculaires des matériaux nouveaux pour l'électroniques Organiques (LR18ES19) Faculté des Sciences de Monastir, Université de Monastir-Tunisie.*
[b] *Faculty of Sciences Gabes, University of Gabes*
* mohamedmbarek99@yahoo.fr

Nanostructured conjugated polymers exhibit unique physicochemical properties as a result of their synthesis within confined templates. In this work, polymeric nanowires were successfully fabricated using a template-assisted impregnation method (template wetting). Specifically, nanoscale synthesis of poly(para-phenylenevinylene) (PPV) and poly(fluorene) (PFO) nanowires was achieved. The resulting nanostructures were thoroughly characterized to elucidate their morphological, structural, and optical properties at the nanoscale. Structural analysis and optical investigations revealed distinct features associated with nanoscale confinement. Notably, evidence of reabsorption phenomena (trivial energy transfer) as well as charge transfer processes was observed in coaxial nanostructures. Furthermore, an enhancement of PPV emission was achieved through the incorporation of the PFO luminophore, attributed to efficient energy transfer mechanisms. The significant overlap between the absorption and emission spectra of PPV and PFO supports the occurrence of both energy and charge transfer processes within these nanostructures.

Key words: Donor-acceptor architecture; Photophysical properties; photonics; conjugated polymers

Design and efficient synthesis of novel antibiotic derivatives (ciprofloxacin) with *in silico* assessment supporting their predicted biological efficacy

Mabrouk HORCHANI, Hichem BEN JANNET, Anis ROMDHANE

Laboratory of Heterocyclic Chemistry, Natural Products and Reactivity (LR11ES39),
Team: Medicinal Chemistry and Natural Products, Faculty of Science of Monastir, University of Monastir,
Avenue of Environment, Monastir 5019, Tunisia

Ciprofloxacin is an antibiotic agent in the fluoroquinolone class used to treat bacterial infections such as urinary tract infections, sexually transmitted infections (gonorrhea and chancroid, skin and soft tissue infection, bone, joint infections, prostatitis, pneumonia, typhoid fever, gastrointestinal infections, lower respiratory tract infections, inhalation anthrax (post-exposure prophylaxis), plague, and salmonellosis, acute bacterial exacerbation of chronic bronchitis [1-2].

Encouraged by the above informations, a series of novel ciprofloxacin derivatives have been synthesized *via* the combination of the hydrazide-ciprofloxacin with a series of cyclic anhydrides in refluxing 1,4-dioxane and in the presence of a catalytic amount of acetic acid. In addition, we carried out theoretical studies to explore the predicted biological potential of the synthesized compounds. Specifically, we focused on molecular docking to predict their inhibitory mechanisms against target bacteria. The results revealed notable intermolecular interactions with key amino acids in the active site, indicating promising inhibitory potentials.

References

[1] Apangu T, Griffith K, Abaru J, Candini G, Apio H, Okoth F, Okello R, Kaggwa J, Acayo S, Ezama G, Yockey B, Sexton C, Schriefer M, Mbidde EK, Mead P. Successful Treatment of Human Plague with Oral Ciprofloxacin. Emerg Infect Dis. 2017 Mar;23(3):553-5

[2] Unemo M, Lahra MM, Cole M, Galarza P, Ndowa F, Martin I, Dillon JR, Ramon-Pardo P, Bolan G, Wi T. World Health Organization Global Gonococcal Antimicrobial Surveillance Program (WHO GASP): review of new data and evidence to inform international collaborative actions and research efforts. Sex Health. 2019 Sep;16(5):412-42

Water-Soluble Chitosan-Based Fluorescent Probe for Al^{3+} Detection: Synthesis and Sensing Performance

Khaled Hriz, Mariam Essid, Habiba Zrida, Khaoula Hassine

University of Monastir, Faculty of Sciences of Monastir, Laboratory of Interfaces and Advanced Materials (LIMA), Bd. of the Environment, 5019 Monastir, Tunisia

Valorizing marine biowaste, this study reports the design of a novel water-soluble fluorescent chitosan derivative for Al^{3+} sensing. High-purity chitosan (97% DDA) extracted from shrimp shells was sequentially functionalized via a click chemistry and a Wittig reaction, introducing triazole and styrylanthracene fluorophore units to yield the ***Cs-Tri-An*** probe. A structural characterization (FT-IR, NMR) confirmed the successful synthesis and quantitative functionalization by Wittig reaction. **Cs-Tri-An** exhibits pronounced blue emission and organic semiconductor properties in aqueous solution. Its fluorescence sensing performance revealed a "turn-on" response toward Al^{3+}, with a 57 % enhancement. The probe forms a stable complex with Al^{3+} (binding constant $K = 6.9 \times 10^4\ M^{-1}$) and achieves a nanomolar detection limit (LOD = 49.11 nM). These results demonstrate the successful modification of chitosan into a high-performance sensing material, highlighting its significant potential for monitoring Al^{3+} cations in environmental and biological systems.

Keywords: Chitosan; Click chemistry; Water-soluble polymer; Optical properties; fluorescent probe; Aluminum ion detection.

Geoclimatic Influence on the Composition and Quality of *Tecoma stans* Seed Oils from Tunisia and Saudi Arabia

Belsem Jedidi, Hassen Mohamed Sbihi

Faculty of sciences of Tunis, Department of chemistry, laboratory of (BIO) organic, structural and Polymer chemistry, 2092 University of Tunis El Manar, Tunisia

Recently, interest in high-value seed oils has increased due to their nutritional, functional, and economic potential. This study aimed to investigate the influence of geoclimatic conditions on the composition and quality of *Tecoma stans* seed oils, through a comparative approach between samples originating from Tunisia and Saudi Arabia.

The oils were extracted and characterized in terms of their fatty acid profiles, minor compounds (tocopherols and tocotrienols), as well as their physicochemical properties and oxidative stability. The results revealed significant variations in lipid composition and quality parameters depending on geographic origin.

Moreover, the contents of natural antioxidant compounds and the oxidative stability index showed notable differences between oils from the two regions, suggesting a strong influence of climatic and environmental conditions on the final oil quality.

Overall, these findings highlight the critical role of geoclimatic factors in the variability of *Tecoma stans* seed oil composition and quality, and emphasize the potential of this plant resource for valorization according to its origin.

Comparison of Fatty Acid Composition and Bioactive Properties of *Marrubium vulgare* Seed Oil and *Canola* Oil

Belsem Jedidi, Hassen Mohamed Sbihi

Faculty of sciences of Tunis, Department of chemistry, laboratory of (BIO) organic, structural and Polymer chemistry, 2092 University of Tunis El Manar, Tunisia

This study aims to compare the seed oil of *Marrubium vulgare* (MVSO) with canola oil, in order to evaluate their differences in fatty acid composition and bioactive properties. Both oils were analyzed for their fatty acid profiles, tocopherol and sterol contents, as well as their physicochemical properties and oxidative stability.

Results show that MVSO differs from canola oil by its higher content of essential polyunsaturated fatty acids, particularly linolenic (omega-3) and linoleic (omega-6) acids, and by a sterol profile enriched in β-sitosterol. Its tocopherol content, predominantly γ-tocopherol, provides good oxidative stability and notable functional potential.

In comparison, canola oil exhibits a more conventional lipid profile with a slightly less balanced omega-6/omega-3 ratio. These differences indicate that MVSO could serve as an interesting alternative to conventional oils, offering benefits for nutritional, cosmetic, and industrial applications, while contributing to the diversification of high-value plant oil sources.

Mechanistic and Predictive Study of MB Adsorption on Biochar Derived from *Lantana camara*

Wihed ElQods Jemmali [a]*, Mohamed Bouzid [b], Abdelmottaleb Ben Lamine [a]

[a] *Laboratory of Quantum and Statistical Physics, University of Monastir, Faculty of Sciences of Monastir,*
Monastir, 5019, Tunisia
[b] *Centre for Research on Microelectronics and Technology CRMN, Technopark of Sousse,*
B.P.334, 4054, Sahloul, Sousse, Tunisia

This study investigates the potential of biochar derived from Lantana camara L. to adsorb methylene blue (MB). Using a statistical physics-based double-layer model, the adsorption behavior on two biochars, BC_L600 and BC_S600, was examined, revealing that each active site can capture single or multiple MB molecules indicating multimolecular, non-parallel adsorption. Temperature-dependent experiments showed that BC_L600 achieved the highest adsorption capacity (~55 mg g^{-1}). Adsorption energy calculations confirmed that the process is thermodynamically favorable and primarily driven by physical interactions, with Gibbs free and internal energy analyses providing further mechanistic insight. Complementing this, an artificial neural network (ANN) model accurately predicted adsorption capacities closely matching experimental results. This combined approach demonstrates how integrating statistical physics and machine learning can deepen understanding of adsorption mechanisms and enable reliable predictions of biochar performance under varied conditions.

Keywords: Adsorption, Statistical physics, Methylene blue dye, Lantana camara L., Artificial Neural Network

***Corresponding Author:** E-mail address: wihedjemmali@gmail.com (Wihed ElQods Jemmali).

ANN-Based Prediction of Dye Adsorption Efficiency on Fe_3O_4-Modified Activated Carbon

Wihed ElQods Jemmali [a]*, Mohamed Bouzid [b], Abdelmottaleb Ben Lamine [a]

[a] *Laboratory of Quantum and Statistical Physics, University of Monastir, Faculty of Sciences of Monastir,*
Monastir, 5019, Tunisia
[b] *Centre for Research on Microelectronics and Technology CRMN, Technopark of Sousse,*
B.P.334, 4054, Sahloul, Sousse, Tunisia

This study explores the adsorption behavior of Methyl Orange (MO) and Rhodamine B (RhB) from aqueous solutions using activated carbon functionalized with Fe_3O_4 magnetic nanoparticles (Fe_3O_4/AC). Statistical physics-based adsorption models, including isotherm analysis, were employed to elucidate the adsorption mechanisms at the molecular scale. Among the tested models, the monolayer Hill model provided the best fit for describing the adsorption of both dyes onto the Fe_3O_4/AC adsorbent.

The obtained results reveal that MO adsorption follows a multimolecular interaction mechanism, whereas RhB adsorption proceeds via a mixed parallel process. The maximum adsorption capacity of RhB (178 mg/g) was found to be significantly higher than that of MO (145 mg/g) at 298 K, indicating a stronger affinity of RhB toward the adsorbent surface. Furthermore, the calculated adsorption energies suggest that the interactions between dye molecules and the Fe_3O_4/AC surface are predominantly governed by physical forces.

In addition, an Artificial Neural Network (ANN) model was developed to predict and optimize adsorption performance under varying operational conditions. The ANN predictions showed excellent agreement with experimental data, demonstrating high accuracy and reliability. Overall, the combined use of statistical physics modeling and ANN analysis provides deeper insight into the adsorption mechanisms and highlights the effectiveness of Fe_3O_4/AC as a recyclable and efficient adsorbent for dye removal from wastewater.

Keywords: Adsorption; Statistical physics; Methyl Orange Fe_3O_4 ; Artificial Neural Network

***Corresponding Author:** E-mail address: wihedjemmali@gmail.com (Wihed ElQods Jemmali).

Antioxidant and Enzyme Inhibitory Activities of Tunisian Salvia aegyptiacaL. Extracts

Ons Jendoubi [a], Siwar Majdoub [a], Hekmat B. AL-Hmadi [b], Ridha El Mokni [c,d],
Gokhan Zengin [e] and Saoussen Hammami [a*]

[a] Laboratory of Environmental Chemistry and Clean Processes(LR21ES04), Faculty of Sciences of Monastir, Monastir University, Monastir 5000, Tunisia.
[b] Department of Chemistry, College of Medicine, AL-Muthanna University, Samawah, Iraq.
[c] Department of Pharmaceutical Sciences "A", Laboratory of Botany, Cryptogamy and Plant Biology, Faculty of Pharmacy of Monastir, Avicenna street, Monastir University, Monastir 5000, Tunisia.
[d] Laboratory of Forest Ecology, National Research Institute of Rural Engineering, Water and Forests (INRGREF), IRESA, Carthage University, Ariana-2080, Tunisia.
[e] Department of Biology, Science Faculty, Selcuk University, Konya, Turkey

The genus *Salvia* is considered as a rich natural resource due to its various properties and application in diverse sectors, mainly in pharmaceuticals, cosmetics, and food industry. The present study investigated the antioxidant and enzyme inhibitory activities of Tunisian *S. aegyptiaca* extracts obtained using solvents of different polarities. The antioxidant effects were assessed using DPPH, ABTS, FRAP, CUPRAC, and phosphomolybdenum assays. Enzyme inhibition activity was evaluated against α-amylase, α-glucosidase, acetylcholinesterase, butyrylcholinesterase and tyrosinase. The methanolic extract exhibited the strongest antioxidant activity and significant inhibitory effects against α-amylase and α-glucosidase, highlighting its potential as a natural source of bioactive phenolic compounds with promising antioxidant and enzyme inhibitory properties.

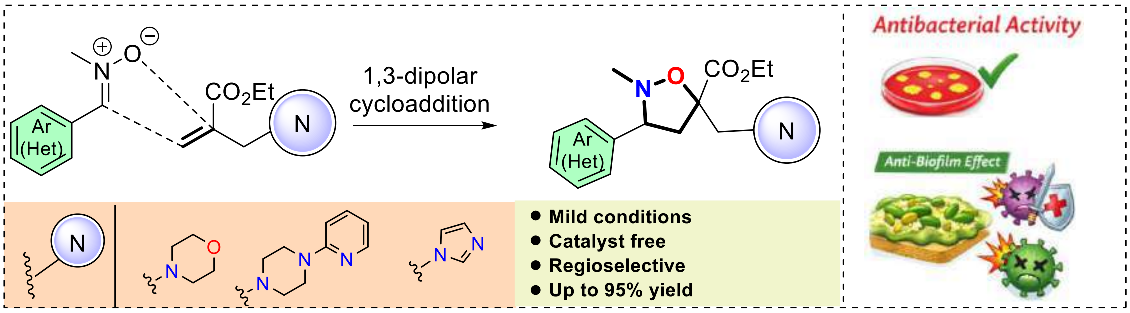
Keywords: *Salvia aegyptiaca*, Crude extracts, Antioxidant activity, Enzyme inhibition.

Isoxazolidinyl-Based Nitrogen Heterocycles: Efficient Synthesis, Antibacterial, Antibiofilm Activity, and *In Silico* Evaluation Against EGFR and Microbial Targets

Momtez JMAÏ [a], Ichrak Soui [a], Edziri Hayet [b], and Hedi M’RABET [a].

a) Laboratory of Selective Organic and Heterocyclic Synthesis-Biological Activity Evaluation, SOHES, (LR17ES01), Faculty of Science of Tunis, University Tunis El Manar, Tunis 2092, Tunisia
b) Laboratory of Transmissible Diseases and Biologically Active Substances, (LR99ES27), Faculty of Pharmacy, University of Monastir, 5000 Monastir, Tunisia
E-mail : momtez.jmai@fst.utm.tn

Developing new molecular structures targeting biological systems is crucial for drug design.[1] This study introduces the efficient synthesis of isoxazolidinyl-based nitrogen heterocycles via regioselective, catalyst-free 1,3-dipolar cycloaddition between allylic amine-substituted acrylates and aryl nitrones. This method produces various isoxazolidinyl-linked compounds with morpholine, piperazine, and imidazole groups. Most of the synthesized compounds exhibited good antibacterial activity against Gram-positive and Gram-negative bacteria, along with notable antibiofilm potential. Furthermore, *in silico* molecular docking studies against *S. aureus* (PDB ID: 2XCT), *E. coli* (PDB ID: 3G7E), *C. glabrata* (PDB ID: 5JLC), and EGFR tyrosine kinase (PDB IDs: 1M17 and 4HJO) revealed moderate to high binding affinities. Notably, compounds **3k** and **3m** exhibited superior binding affinities compared reference drug. In addition, ADMET predictions indicated favorable pharmacokinetic and drug-like properties, highlighting the potential of these compounds as promising scaffolds for medicinal chemistry applications.[2]



Scheme 1: Design and in silico study of isoxazolidinyl-based nitrogen heterocycles

Key words: Isoxazolidine, Antibacterial activity, Molecular docking, ADMET prediction.

---

[1] Taruneshwar Jha, K.; Shome, A.; Chahat; Chawla, P. A. *Bioorganic Chemistry* **2023**, *138*, 106680.
[2] Jmai, M.; Soui, I.; M’rabet, H. *Chemistry Africa*, **2025**, *8*, 3365.

Synthesis of new chiral hydantoins starting from α-amino acids

Yakdhane Kacem and Syrine Mehrez

Laboratory of Chemical, Galenic, and Pharmacological Development of Drugs (LR 12ES09),
University of Monastir, Faculty of Pharmacy

In the first part of this communication, we present a new green and efficient synthesis method for obtaining fluorinated and non-fluorinated urea derivatives from natural amino acids. *In silico* studies on toxicity and physicochemical properties showed that the non-fluorinated candidate compounds exhibited favorable characteristics as well as acceptable similarity with existing drugs. Moreover, the *in vivo* results revealed that some of these compounds possess promising anti-inflammatory activity.

In the second part, we describe a new simple, efficient, and one-step protocol for the synthesis of hydantoins from the urea derivatives obtained in the first part. We also develop studies aimed at evaluating the therapeutic potential of the synthesized molecules. These studies have particularly focused on the *in vitro* and *in silico* evaluation of their antibacterial properties, revealing promising results.

Synthetic Approach to Functionalized Endoperoxide Derivatives Based on Syncarpic Acid for Antimalarial Drug Discovery

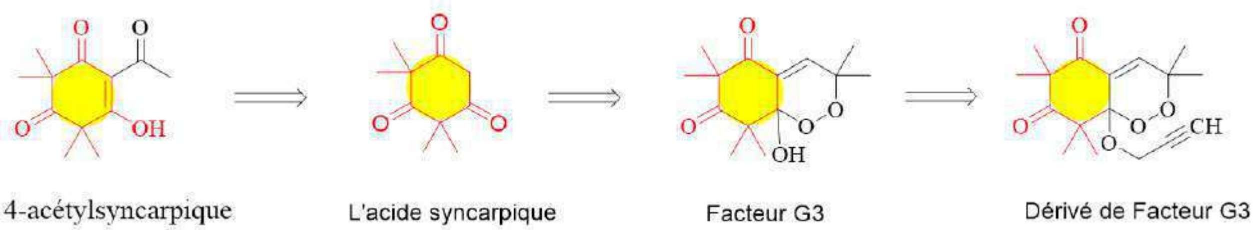
Naka Kadri [a], Abdelkader Bougarech [a], Souhir Abid [a,b], Michel Baltas [c], Houcine Ammar [a]

[a] Laboratory of Applied Chemistry: Heterocycles, Lipids and Polymers, Faculty of Sciences of Sfax,
University of Sfax, BP 802, Sfax 3000, Tunisia
[b] Department of Chemistry, College of Science, Jouf University, P.O. Box 2014, Sakaka, Aljouf, 21
Kingdom of Saudi Arabia
[c] Laboratoire de Chimie de Coordination du CNRS UPR8241, Inserm ERL 1289 Team « Nouvelles molécules
antiplasmodiques et approches pharmacologiques », 205 route de Narbonne,
BP 44099, Toulouse Cedex 31077, France

Malaria is a vector-borne disease predominantly found in Sub-Saharan Africa, Asia, and Latin America[1]. The increasing resistance to existing drugs highlights the urgent need for new, affordable antimalarial therapies[2]. Based on a literature review, we identified the crucial role of the peroxyketal function in enhancing antimalarial activity within the series of Factor G compounds, as demonstrated by both in vitro and in vivo studies.

The objective of this work is to synthesize derivatives of Factor G3 by introducing alkyl groups into its structure, in order to better understand and improve their antiplasmodial activities. Factor G3, a heterocyclic compound, is synthesized from syncarpic acid and an appropriate aldehyde, initially forming a Mannich base, followed by the release of a ketonic dienol and subsequent.

auto-oxidation leading to the formation of FG3. This compound can also be naturally found in the leaves of Eucalyptus grandis (native to Australia), where it plays a defensive role in the plant. This multifaceted approach aims to contribute to the global fight against malaria through the development of innovative antimalarial agents.



Scheme: Synthesis of G3 Factor Derivative (propargyl)

Keywords: Malaria, Endoperoxides, Factor G3.

References

[1] Hotez, P. J., Aksoy, S., Brindley, P. J. & Kamhawi, S. World neglected tropical diseases day. PLoS Negl. Trop. Dis. 14, 1–4 (2020).

[2] Benoit-Vical, F., Paloque, L. & Augereau, J. M. Plasmodium falciparum resistance to artemisinin-based combination therapies (ACTs): Fears of widespread drug resistance. Bull. Acad. Natl. Med. 200, 477–490 (2016).

Synthesis, Molecular Docking, DFT Studies, and Pharmacokinetic Evaluation of Spiroxindole Pyranopyrimidinones as α-Amylase Inhibitors

Aicha Kaouach [a], Lucas Pagès [b], Ludovic Jean [b], Hichem Ben Jannet [a], Anis Romdhane [a]

a) *Laboratory of Heterocyclic Chemistry, Natural Products and Reactivity (LR11ES39), Team: Medicinal Chemistry and Natural Products, Faculty of Sciences of Monastir, University of Monastir, Avenue of Environment, 5019 Monastir, Tunisia.*

b) *Laboratory of Therapeutic Targets and Drug Design CiTCoM, (UMR 8038 – U1268), Faculty of Pharmacy, Paris Cité University, 4 Observatory Avenue, 75006 Paris, France.*

A novel series of anti-α-amylase spiroxindole pyranopyrimidinone derivatives (3a–i) was efficiently synthesized through a three-step synthetic pathway starting from 4H-pyran α-aminocarbonitrile via a one-pot reaction protocol. The structures of the synthesized compounds were unambiguously confirmed by ^{1}H NMR and ^{13}C NMR spectroscopic analyses. Molecular docking studies were carried out to investigate the binding interactions and potential inhibitory mechanism of the synthesized derivatives within the active site of the target enzyme. The docking results identified compounds **3h**, **3i**, and **3g** as the most promising α-amylase inhibitors.

Furthermore, key physicochemical and pharmacokinetic properties were predicted *in silico* to evaluate the drug-likeness of the synthesized molecules. All derivatives exhibited favorable pharmacokinetic profiles and satisfied Lipinski's rule of five, suggesting their potential as orally bioavailable anti-α-amylase agents.

Keywords: Spiroxindole derivatives; Pyranopyrimidinone; α-amylase inhibitors; molecular docking; ADME prediction

Eco-Friendly Acylation and benzylation of Friedel-Crafts Catalyzed with Low-loaded Ferric Chloride Under Green Conditions

Jamil Kraiem

Laboratoire de développement chimique, galénique et pharmacologique des médicaments (LR12ES09), Faculté de Pharmacie de Monastir, Université de Monastir, Tunisie

The Friedel–Crafts reactions are fundamental Processes extensively employed in both academic research and industrial applications. The major drawbacks of these reactions are the use of toxic solvents, the need of high energy conditions, and sometimes the use of stoichiometric quantities of metal catalysts, resulting in the generation of large quantities of waste. We have developed new methods that have improved the ecological aspect of some Friedel-Crafts reactions, such as, the acylation and the benzylation of arenes. [1, 2, 3] These methods use green solvents, such as propylene carbonate, quatalytic quantities of iron^{-III} chloride as the catalyst, and are carried out under relatively mild conditions. These methods overcome the major limitations of traditional Friedel–Crafts réactions and represent a significant advancement in green chemistry.

References :

[1] S. E. Cherif, M. Chehaibi, R. Raddadi, M. Fustier-Boutignon, S. Lakhdar and J. Kraïem, ***RSC Adv.***, 2025,**15**, 31088-31094.
[2] H. Slimi, S. E. Cherif, I. Jemaa and J. Kraiem, ***Chemistry Africa*** 2025, **8**, 4161–4168.
[3] H. Slimi, Z. Litim, T. Ollevier and J. Kraïem, ***ACS Omega*** 2023, **8,** 44558–44570.

Polyoxometalates: From Synthesis to Industrial and Medical Applications

KSIKSI Regaya [1,2] & Mohamed Faouzi ZID [1]

[1] *University of Tunis El Manar, Faculty of Sciences of Tunis, Laboratory of Materials, Crystal Chemistry and Applied Thermodynamics, 2092 El Manar II, Tunis, Tunisia.*

[2] *University of Carthage, High Institute of Preparatory Studies in Biology and Geology (ISEP-BG) of Soukra, Tunisia.*

Polyoxometalates (POMs) are compounds of oxygen and transition metals (e.g., V, Nb, Ta, Mo, W) in their highest oxidation states. They can also contain a variety of heteroatoms (e.g., P, As, Si, Ge) **[1]**.

Polyoxometalates (POMs) have potential applications in various fields of science and technology (catalytic, magnetic, and electrochemical) due to their properties such as thermal stability, redox activity, and solubility in both polar and nonpolar solvents POMs have been extensively studied in hydrogen production by photocatalysis as cocatalysts with excellent multi-electron transfer capabilities. More recently, POMs have emerged as a new class of photosensitizers for the photocatalytic evolution of H_2 **[2-4]**.

POMs also have potential applications in biomedicine. Indeed, numerous studies have demonstrated potent antitumor, antiviral, and antibacterial activities of POMs **[5-6]**.

Acknowledgments: We would like to thank the Tunisian Ministry of Higher Education and Scientific Research for the financial support of this work in a project to evaluate research results under the code **VRR 25/26**.

References

1. K. Y. Monakhov, W. Bensch and P. Kögerler, The Royal Society of Chemistry, Chemical Society Reviews, **2015**, 44, 8443.
2. M. Louati, R. Ksiksi, L. Jouffret, M. F. Zid, Crystal Structure Theory and Applications, **2019**, 8, 1.
3. Q. Shen, J. Carlos. G. García, W. Sun, X. Lai, H. Pang and H. Ma, Green Chemistry, **2021**, 23, 3104.
4. B. C. Mirjana, M. Lacković, J. Lalatović, S. Ali. Mougharbel, U. Kortz and Z. K. Danijela, Current Medicinal Chemistry, **2020**, 27, 3365.
5. J. C. Chermann, M. Raynaud, C. Jasmin and G. Mathé, Nature, **1970**, 227, 173.
6. Y. Tajima, A review of the biological and biochemical effects of tungsten compounds, **2001**, 4, 129.

Valorization of Deinking Sludge in Polymer Composites

Yoldez LAHMER*, Halim HAMMI

Laboratory for Valorization of Useful Materials, CNRSM, Technopole Borj Cedria,
Soliman, Tunisia

Deinking sludge generated from the paper recycling industry represents significant industrial waste, posing major environmental challenges. Its valorization in polymer composites offers a sustainable solution by reducing environmental impact while enabling the development of new materials. This study aims to evaluate the incorporation of deinking sludge as a filler in a polypropylene matrix and to analyze its effect on the mechanical properties of the resulting composites. The sludge was first dried and ground before being incorporated at different loadings (5% and 10% by weight) into a polypropylene matrix. The composites were prepared by melt mixing followed by shaping, and mechanical tests were conducted to evaluate tensile strength, stiffness, and elongation at break. The results show that a 5% loading provides the best balance between stiffness, strength, and deformation capacity, with improved ductility and satisfactory mechanical performance attributed to a relatively homogeneous dispersion of particles within the matrix. At 10% loading, although stiffness increases, a significant reduction in strength and elongation at break is observed, indicating material embrittlement due to particle agglomeration and restricted mobility of polymer chains. Overall, the mechanical performance is optimal at 5% sludge content. The incorporation of deinking sludge into polymer composites therefore represents a promising route for industrial waste valorization. Future work will focus on optimizing the incorporation range (3–7%), exploring higher loadings (up to 15%), improving interfacial adhesion using compatibilizers such as maleic anhydride grafted polypropylene (PP-g-MA), and conducting advanced morphological and thermal analyses (SEM, XRD, FTIR, TGA/DSC) as well as evaluating durability and environmental impact.

Impact of Freeze-Drying on the Chemical Stability and Biological Activity of Bioactive Compounds in *Spirulina platensis*

Lynda Lamoudi [1], Soraya Akretche [2], Nadjet Guemras [1], Nabil Bousbia [2] and Kamel Daoud [1]

[1] Laboratory of Transfer Phenomena. Faculty of Mechanical Engineering and Process Engineering, University of Science and Technology Houari Boumediene (U.S.T.H.B.), P.O. Box 32 El Alia, 16111 Bab Ezzouar, Algeria.
[2] Laboratory of Industrial Process Engineering Sciences. Faculty of Mechanical Engineering and Process Engineering, University of Science and Technology Houari Boumediene (U.S.T.H.B.),
P.O. Box 32 El Alia, 16111 Bab Ezzouar, Algeria.

The microalga *Spirulina platensis* represents an important source of biomolecules of interest, particularly proteins, polyphenols, and pigments such as phycocyanin, which are recognized for their biological properties. Preserving these bioactive compounds is a major challenge due to their sensitivity to processing and storage conditions. Among preservation techniques, freeze-drying (lyophilization) appears to be a gentle method capable of limiting chemical degradation.

This study aims to evaluate the impact of freeze-drying on the chemical stability and biological activity of bioactive compounds in spirulina, through a comparison between fresh biomass and freeze-dried biomass. Samples were obtained from an experimental culture and then subjected to a vacuum freeze-drying process. Analyses focused on the quantification of proteins, total polyphenols, and mineral elements, as well as the evaluation of antimicrobial activity.

The results highlight a partial decrease in phenolic compounds after freeze-drying, indicating a certain sensitivity of these metabolites to drying conditions. A modification of antimicrobial activity was also observed, suggesting an influence of the process on overall bioactivity. In contrast, major nutritional constituents, particularly proteins, were generally preserved, confirming the relevance of freeze-drying as a stabilization technique.

These findings underline the importance of controlling freeze-drying parameters in order to optimize the preservation of the chemical and biological properties of biomolecules. This approach falls within the field of bioorganic chemistry, highlighting the relationships between chemical structure, stability, and biological activity. It also opens perspectives for the use of spirulina as a source of functional compounds in nutraceutical, pharmaceutical, and cosmetic applications.

Keywords: *Spirulina platensis*; Freeze-drying; Bioactive compounds; Chemical stability; Biological activity

---

Bibliographical references:

1. Papalia T., Sidari R., Panuccio M.R. *Impact of Different Storage Methods on Bioactive Compounds in Arthrospira platensis Biomass*. *Molecules*. 2019 ;24(15) :2810.
2. Navikaitė-Šnipaitienė V., Liudvinavičiūtė D., Rutkaitė R., Syrpas M. *Antioxidant Capacity and Thermal Stability of Arthrospira platensis Extract Encapsulated in Starch Sodium Octenyl Succinate with Freeze-, Spray-, and Nanospray-Drying*. *Molecules*. 2025 ;30(6) :1303.
3. Ramadan M.F., Asker M.M.S., Ibrahim Z.K. Functional bioactive compounds and biological activities of Spirulina platensis lipids. *Czech Journal of Food Sciences*. 2008;26:211–222.

Antibacterial and Antioxidant Potential of Five *Eucalyptus* Species Against Respiratory Pathogens.

Maissa Lejmi [a], Bochra Kouidhi [b], Hajer Rhim [c], Maha Mastouri [d], Ameur Elaissi [a]

[a] Laboratory of Chemical, Galenic and Pharmacological Drug Development-(LR12ES09),
Faculty of Pharmacy, University of Monastir, Avicenne street, 5000, Monastir, Tunisia.
[b] Laboratory of Analysis, Treatment, and Valorization of Environmental Pollutants and Products,
Faculty of Pharmacy, University of Monastir, Monastir, Tunisia
[c] Microbiology Laboratory, CHU Fattouma Bourguiba, Monastir, Tunisia
[d] Laboratory of Transmissible Diseases and Biologically Active Substances (LR99ES27),
Faculty of Pharmacy, University of Monastir, Monastir, Tunisia

In recent decades, while antibiotics have revolutionized the treatment of bacterial infections, their excessive and inappropriate use has led to the emergence of widespread antimicrobial resistance a critical global health crisis [1]. According to the World Health Organization (WHO), bacterial pathogens were associated with approximately 55.4 million deaths in 2019, representing 55% of global mortality. Specifically, respiratory infections caused by resistant strains are ranked among the top ten global health threats, accounting for an estimated 1.5 million deaths annually [2]. As conventional treatments for pneumonia and sinusitis lose efficacy against pathogens such as *S. pneumoniae*, *S. aureus*, and *K. pneumoniae*, exploring natural bioactive alternatives is imperative.

Recognized by the 11th edition of the European Pharmacopoeia for their antiseptic properties, *Eucalyptus* essential oils (EOs) offer a promising reservoir of compounds against respiratory infections [3]. This study evaluates the chemical profile and biological potential of EOs from five species (*E. loxophleba, E. torquata, E. salmonophloia, E. oleosa, and E. longicornis*) to identify potent natural alternatives for managing bacterial respiratory diseases and oxidative stress.

Essential oils (EOs) were extracted from leaves via hydrodistillation and characterized using GC/FID and GC/MS. Antibacterial susceptibility was evaluated against seven respiratory pathogens using disk diffusion and broth micro-dilution methods. Antioxidant capacity was assessed via DPPH and ABTS assays. Statistical significance was determined using SPSS 12.0.

Chemical profiling revealed significant variations in EO composition across species. The antibacterial activity was influenced by the EO type, the bacterial strain, and the testing method, with Gram-positive bacteria exhibiting higher sensitivity than Gram-negative strains. *E. longicornis* EO, characterized by its richness in β-cymene, 1,8-cineole, α-pinene, trans-pinocarveol, and thymol, emerged as the most potent extract, showing inhibition zones > 20 mm and occasionally surpassing commercial antibiotics. In contrast, *E. torquata* EO (rich in torquatone) was the least active (< 10 mm). Notably, the lowest Minimum Inhibitory Concentration (MIC) and Minimum Bactericidal Concentration (MBC) values (1.56 µl/ml) were recorded for *E. torquata* and *E. salmonophloia* against *Staphylococcus aureus* ATCC 29213. Regarding antioxidant potential, although all EOs remained less effective than Vitamin C, *E. longicornis* showed the highest radical scavenging activity. This performance is attributed to the synergistic interactions of its phenolic compounds (thymol), oxides, and terpenoids.

These findings highlight *E. longicornis* EO as a robust natural candidate for developing antimicrobial and antioxidant agents to manage respiratory infections and oxidative stress.

Keywords: *Eucalyptus* essential oils, Antibacterial activity, disk diffusion, micro-dilution, Antioxidant activity, DPPH, ABTS.

References

[1] Zhang Q. Global situation and WHO strategy on traditional medicine. Tradit Med Mod Med. 2018;01(01):11-3.
[2] World Health Organization. **WHO highlights huge scale of death from tobacco-related lung disease**. Geneva: World Health Organization; 2019.
[3] European Directorate for the Quality of Medicines & HealthCare. **European Pharmacopoeia (Ph. Eur.)**. 11th ed. Strasbourg: Council of Europe; 2023.

Opuntia (Cactaceae) mucilage mixed with polyvinyl alcohol for biodegradable packaging composite film formulation

Faten Mannai [a,b], Anouer Feriani [c], Harith Al Busaidi [d],
Mohamed Naceur Belgacem [e], Younes Moussaoui [b,f]

[a] University of Gafsa, Faculty of Sciences of Gafsa, Laboratory for the Application of Materials to the Environment, Water and Energy (LR21ES15), Gafsa 2112, Tunisia
[b] University of Gafsa, Faculty of Sciences of Gafsa, Gafsa 2112, Tunisia
[c] University of Gafsa, Faculty of Sciences of Gafsa, Laboratory of Biotechnology and Biomonitoring of the Environment and Oasis Ecosystems, Gafsa 2112, Tunisia
[d] University of Technology and Applied Sciences, Alrustaq, Oman
[e] University of Grenoble Alpes, CNRS, Grenoble INP, LGP2, Grenoble F-38000, France
[f] University of Sfax, Faculty of Sciences of Sfax, Organic Chemistry Laboratory (LR17ES08), Sfax 3000, Tunisia

Mucilage extracted from *Opuntia* using an ultrasound-assisted method [1] was incorporated at varying concentrations into glycerol-plasticized polyvinyl alcohol (PVOH) films. The films were characterized in terms of their structural, physicochemical, mechanical, barrier, and thermal properties, as well as their solubility and biodegradability. The PVOH–mucilage films exhibited uniform structures, indicating strong intermolecular interactions. The incorporation of 3% mucilage improved transparency, mechanical performance, barrier properties, wettability, and thermal stability. Despite their high solubility in freshwater within 48 hours, the films demonstrated rapid biodegradation in soil, achieving complete degradation within 21 days [2]. Additionally, the films exhibited antibacterial activity against *Staphylococcus aureus* and *Pseudomonas aeruginosa*, highlighting their potential as eco-friendly materials for sustainable packaging applications.

References

[1] Mannai, F., Elhleli, H., Mosbah, M. B., Khiari, R., Nacer, S. N., Belgacem, M. N., & Moussaoui, Y. (2024). Comparative study of conventional and combined ultrasound-assisted methods on the quality of mucilage extracted from Opuntia ficus-indica cladodes. *Industrial Crops and Products*, *214*, 118566.

[2] Mannai, F., Elhleli, H., Feriani, A., Al Busaidi, H., Belgacem, M. N., & Moussaoui, Y. (2025). Opuntia (Cactaceae) mucilage mixed with polyvinyl alcohol for biodegradable packaging composite film formulation. *Food Packaging and Shelf Life*, *51*, 101583.

QUALITY OF WATER SURFACE AND ANALYZES IN THE TESSALA MOUNTAIN WATER TABLE WILAYA OF SIDI BEL-ABBES, ALGERIA

MELIANI Habib (1+2), BENGUERDI Abdelkadir (2), HARIR Abdallah(2), MENADI Noreddine (3), MENADI Norredine(4), BOUZIDI Mohamed Ali (1+2), KERFOUF Ahmed(1+2)

[1+2] Laboratory of Spaces Eco-Development, ITMA, Department of Environmental Sciences, Faculty of Nature and Life Sciences, Djillali Liabes University of Sidi Bel-Abbès, Algeria

E-mail: habib.meliani@univ-sba.dz ou melianihbib@yahoo.fr ou melianihabib@gmail.com

[2] Department of Environmental Sciences, Faculty of Nature and Life Sciences, Djillali Liabes University of Sidi Bel-Abbès, Algeria

[3] Laboratory of Spaces Eco-Development, ITMA, Department of Environmental Sciences, Faculty of Nature and Life Sciences, Djillali Liabes University of Sidi Bel-Abbès, Algeria

[4] Laboratory of Biotoxicology, ITMA, Department of Biology, Faculty of Nature and Life Sciences, Djillali Liabes University of Sidi Bel-Abbès, Algeria

Water is today threatened by pollution as a result of such degradation of water resources. Knowledge of water quality is an essential condition for establishing a management system that will help to secure water supply in the future.

Our research consists first of all to determine the water quality of Mount Tessala, based on physicochemical and bacteriological analyzes of the water from three surface sources, (Attouche, Tafaksite and Merice). We have studied the effect of some physicochemical parameters which are mainly: temperature, pH, electrical conductivity, TDS, salinity and turbidity; as well as the bacteriological parameters, which are based on the detection and enumeration of total germs (total coliforms, E-coli, and fecal streptococci).

Keywords: water, pollution, physico-chemical, bacteriological, source, Tessala

A New 0D Tin(IV) Hybrid with Dual Functionality: Yellow-Green Photoluminescence and Molecular Docking Evaluation of $(C_6H_{16}N_2)[SnCl_6]\cdot4H_2O$

Dorsaf Mezni & Riadh Kefi

Laboratory of Materials Chemistry, Faculty of Sciences of Bizerte, 7021 Zarzouna, Tunisia.

In this study, the synthesis and characterization of a new organic–inorganic hybrid material, trans-2,5-dimethylpiperazin-1,4-diium hexachlorostannate(IV) tetrahydrate, $(C_6H_{16}N_2)[SnCl_6]\cdot4H_2O$, were carried out. Single-crystal X-ray diffraction revealed that the compound crystallizes in an orthorhombic system (space group Pccn), consisting of isolated $[SnCl_6]^{2-}$ octahedra, organic dications $[C_6H_{16}N_2]^{2+}$, and water molecules interconnected through an extensive three-dimensional hydrogen-bonding network involving N–H···Cl and O–H···Cl interactions.

Spectroscopic investigations, including FT-IR, UV–Vis, and photoluminescence analyses, confirmed the vibrational and electronic properties of the material, in good agreement with density functional theory (DFT) calculations. Hirshfeld surface analysis highlighted the dominant role of intermolecular interactions in stabilizing the crystal structure. Optical absorption measurements revealed a direct band gap of 3.75 eV, indicating the semiconducting nature of the material.

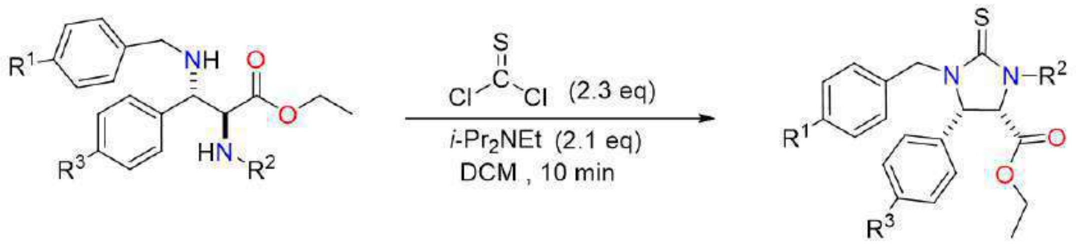
Molecular docking simulations with the target proteins 1JIN and 9KW2 demonstrated significant binding affinity, suggesting that this hybrid complex could act as a potential inhibitor. Taken together, these results combining structural stability, optical properties, and biological activity indicate that this material is a promising candidate for applications in optoelectronics and pharmacology.

Synthesis of new imidazolidine-2-thiones from α,β-diaminoesters

Takwa MISSAOUI, Rafâa BESBES

Laboratoire de Chimie Analytique et Electrochimie, Equipe de Synthèse Organique, LR99ES15, Université de Tunis El Manar, Faculté des Sciences de Tunis, Campus Universitaire, 2092 Tunis, Tunisie.

α,β-Diaminoesters [1] constitute versatile substrates for the development of new synthetic methodologies leading to functionalized sulfur and nitrogen heterocycles. In this work, we studied the condensation reaction of α,β-diaminoesters with thiophosgene in the presence of diisopropylethylamine as a base. This transformation leads to the formation of imidazolidine-2-thiones [2], structural motifs found in many natural molecules and biologically active compounds [3].



R^1 = *i*-Pr, c-C_3H_5, c-C_5H_9, c-C_6H_{11}, c-C_7H_{13}, c-C_8H_{15}
R^2 = H, F, Cl, OMe
R^3 = Cl

Keywords: aziridines, heterocycles, α,β-diaminoesters, imidazolidine-2-thiones.

References :

[1] Qaroush, A. K.; Eftaiha, A. F.; Smadi, A. H.; Assaf, K. I.; Al-Qaisi, F. M.; Alsoubani, F. *ACS Omega* **2022**, *7* (26), 22511-22521.
[2] Błaszczyk, R.; Gajda, A.; Zawadzki, S.; Czubacka, E.; Gajda, T. *Tetrahedron* **2010**, *66* (52), 9840-9848.
[3] Scarsil, A. ; Ponassi, M. ; Brullo, C. ; Rosano, C. ; Spallarossa, A. *Molecular diversity*, **2023**, 27, 1285-1295.
[4] Slama, S.; Elemine, B. O.; Besbes, R. *Synthetic Communications* **2013**, *43* (17), 2286-2293.

Eco-Friendly Conversion of Biomass into Functional Lignocellulosic Nanofibrils via Maleic Acid-Assisted Hydrothermal Treatment

Amira Najahi [1], Quim Tarrés [2], Marc Delgado-Aguilar [2], Jean-Luc Putaux [3], Sami Boufi [1]

[1] *University of Sfax, Faculty of Science, LSME, BP1171-3018 Sfax, Tunisia*
[2] *LEPAMAP-PRODIS Research Group, University of Girona*
[3] *Univ. Grenoble Alpes, CNRS, CERMAV, F-38000 Grenoble, France*
E-mail: najahiamira1@gmail.com

Lignin-containing cellulose nanofibrils (LCNF) have emerged as promising bio-based nanomaterials due to their intrinsic hydrophobicity, ultraviolet (UV) shielding capability, and reduced water sensitivity compared to lignin-free counterparts. In this study, LCNF with lignin contents up to 21 wt% were successfully produced from untreated date palm residues via a sustainable and scalable process. The method combines hydrothermal treatment (120-150 °C) in the presence of 20-30 wt% maleic acid, followed by high-pressure homogenization, yielding over 70 wt% nanofibrils. Comprehensive characterization was conducted to evaluate chemical composition, degree of polymerization, morphology, and colloidal and rheological behavior, providing insight into the impact of maleic acid-assisted hydrothermal treatment on fibrillation efficiency. The resulting LCNF exhibited effective nanoscale disintegration while preserving significant lignin content. Nanopapers fabricated from LCNF suspensions showed reduced mechanical strength compared to lignin-free cellulose nanofibril films, but demonstrated improved hydrophobicity. A mechanistic pathway is proposed to explain the role of hydrothermal treatment in facilitating biomass deconstruction and nanofibril formation. Overall, this work presents an efficient route for converting agricultural waste into value-added nanomaterials, eliminating the need for energy- and chemical-intensive delignification steps, and advancing the development of sustainable lignocellulosic nanomaterials for functional applications.

Synthesis of Green Hybrid Nanomaterials to Enhance Solar Distillation Efficiency and Water Production

Namoussa Tedjani Yahia

laboratory of Biodiversity and Application of Biotechnology in Agriculture.
University of El Oued, Algeria
namoussa-tedjaniyahya@univ-eloued.dz

Despite the increasing climate pressures contributing to global water scarcity, achieving the targets of Sustainable Development Goal 6 – clean water and sanitation – remains critical.
The nanocomposite Fe_2O_3–Dy_2O_3 (FD) was created utilizing a green technique based on an ethanolic extract of palm leaves rich in plant phenolic chemicals. Analytical methods such as FTIR, XRD, XPS, and EDS proved the accurate development of the nanostructure.
When heated to 700 °C, FD changes into its magnetic variant known as c-Fe_2O_3–Dy_2O_3 (c-FD
The enhanced solar distiller, featuring sealed glass tubes filled with Fe_2O_3–Dy_2O_3 nanofluids, was examined for performance. These nanofluids increased the absorption of solar energy and heat retention by improving thermal conductivity. As a result, the system ran at higher temperatures, which boosted evaporation rates and increased freshwater output. The sealed design also prevented nanoparticle leakage, ensuring water purity and promoting long-term operational reliability.

Keywords: Green nanocomposite; Fe_2O_3–Dy_2O_3 nanoparticles; Hybrid nanomaterials; Solar still enhancement; Sustainable water production

Adsorption of heavy metal ions on activated carbon: Modelling and interpretation

Khawla Nasri [1,3], Lotfi Sellaoui [2], Mohamed Mbarek [1*]

1 University of Monastir, Laboratory of Asymmetric Synthesis and Molecular Engineering of Materials for Organic Electronic (LR18ES19), Faculty of Sciences of Monastir, 5019, Monastir, Tunisia
2 CRMN, Centre for Research on Microelectronics and Nanotechnology of Sousse, NANOMISENE, LR16CRMN01, 4054 Sousse, Tunisia
Faculty of Sciences Gabes, University of Gabes
*Corresponding Author: mohamedmbarek99@yahoo.fr

This study reports an analysis of Pb^{2+} and Cu^{2+} removal using activated carbon (AC) obtained from durian skin. Pb^{2+} and Cu^{2+} adsorption tests were carried out at 30 – 50 °C and pH 5.5 to interpret the heavy metal – durian skin AC systems. A monolayer model was applied to simulate experimental isotherms, and the results indicated that the removal of these target pollutants was a multi-ionic process. The saturation adsorption capacities of this AC improved with increasing aqueous solution temperature, ranging from 81 to 139 mg/g for Pb^{2+} and from 95 to 180 mg/g for Cu^{2+} under the tested operating conditions. The calculated interaction energies indicated a physisorption mechanism. Durian skin AC offers competitive performance in purifying wastewater and industrial streams polluted by heavy metals. The results of this study can be useful in improving water cleaning via AC in various industrial sectors.

Keywords: Enhanced adsorption modeling, Environmental depollution, Carbonaceous-based materials

DFT Mechanistic Investigation of Electrooxidative Allene Dioxygenation Mediated by TEMPO

Ibrahima Ngom [1,3], Frédéric Guégan [2], Insa Seck [3] and Youssef Arfaoui [1]

[1] Laboratoire de Caractérisations, Applications et Modélisation de Matériaux (LR18ES08), Faculté des Sciences de Tunis, Université de Tunis El Manar, Tunisie
[2] IC2MP (Institut de Chimie des Milieux et des Matériaux de Poitiers), Université de Poitiers, France
[3] Laboratoire de Chimie de Coordination Organique, Département de Chimie, Faculté des Sciences et Techniques, Université Cheikh Anta Diop de Dakar (UCAD), BP 5005, Dakar-Fann, Sénégal

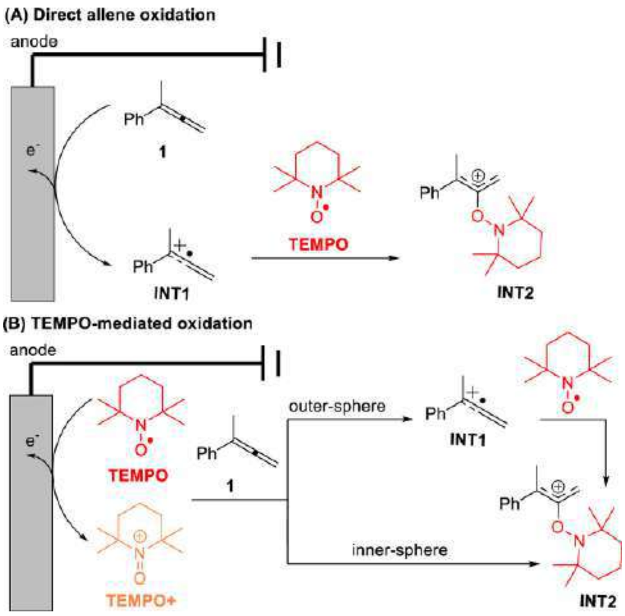
Allenes exhibit a distinctive cumulated π-system that enables unique radical reactivity; however, their electrochemical functionalization remains insufficiently explored. Herein, we present a comprehensive mechanistic investigation of an electro oxidative dioxygenation of allenes mediated by TEMPO (2,2,6,6-tetramethylpiperidine-1-oxyl), leading to the formation of a synthetically valuable vinyl-TEMPO intermediate.

A density functional theory (DFT) calculation was employed to elucidate the reaction mechanism. Electrochemical studies indicate an initial outer-sphere oxidation of TEMPO to $TEMPO^+$, followed by single-electron transfer (SET) to the allene substrate to generate a radical cation intermediate. Subsequent regioselective trapping and oxygen incorporation furnish the dioxygenated product. Substituent effects strongly influence the stability of radical and carbocationic intermediates, thereby governing both reactivity and selectivity.

Les calculs théoriques indiquent que la transformation est cinétiquement accessible, avec des barrières d'activation modérées (~4 $Kcal.mol^{-1}$), et conduit à un produit thermodynamiquement stabilisé.

L'étude met également en évidence un effet marqué des substituants sur la réactivité, ceux-ci modulant à la fois la hauteur des barrières énergétiques et la stabilité des intermédiaires réactionnels, probablement via des effets électroniques ou stériques.

Par ailleurs, le choix de l'acétonitrile comme solvant apparaît particulièrement pertinent : sa polarité et sa capacité à stabiliser les espèces ioniques ou radicalaires formées au cours du processus électro-oxydatif sont en accord avec les observations expérimentales [1], confirmant ainsi sa compatibilité avec le mécanisme proposé.



Keywords: Electrochemistry; Allenes; TEMPO; Radical Chemistry; DFT Mechanistic Study

---

References:

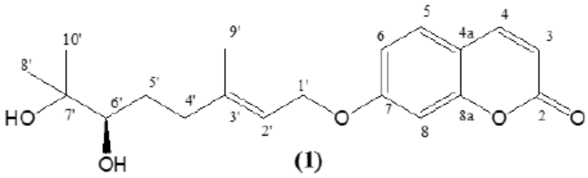
[1] Elucidating the Mechanism of Electrooxidative Allene Dioxygenation: Dual Role of Tetramethylpiperidine N-Oxyl (TEMPO)" (DOI: 10.1021/jacs.4c10431) published in the **Journal of the American Chemical Society** by Ken S. Lee, Federico Barbieri, Emanuele Casali, Elijah T. Marris, Giuseppe Zanoni, and Jennifer M. Schomaker.

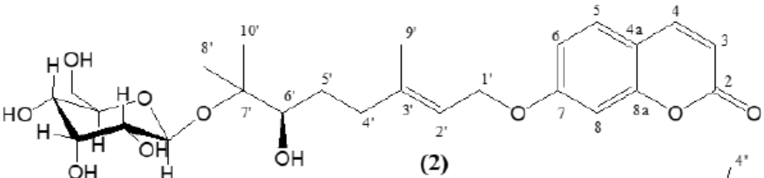
Phytochemical characterization of isolated compounds from *Deverra tortuosa* (Desf.) seeds: Evaluation of cytotoxic, α-glucosidase and antibacterial activities

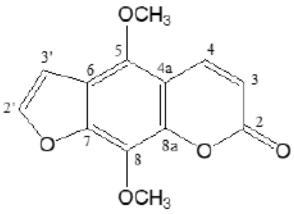
Mohamed Habib Oueslati [1], Arbi Guetat [2], Jalloul Bouajila [3]

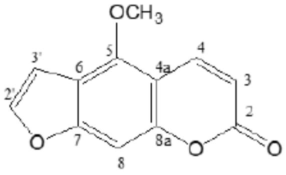
[1] University of Carthage, Faculty of Science Bizerte, Laboratory of Hetero-Organic Compounds and Nanostructured Materials, Zarzouna, Tunisia
[2] Northern Border University, College of Science of Arar, P.O. Box 1231, Arar 91431, Kingdom of Saudi Arabia.
[3] Laboratoire de Génie Chimique, UMR 5503, Université de Toulouse, CNRS, INPT, UPS, Toulouse, France

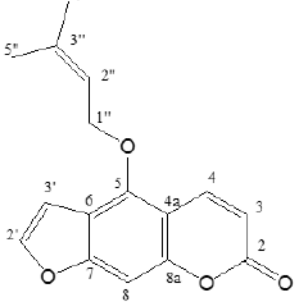
Deverra tortuosa (Desf.) DC (Syn. Pituranthos tortusus (Desf.) Benth. & Hook.f.) is a species belonging to the Apiaceae family that is common in the Northern Region of Saudi Arabia. The plant is well known in traditional medicine along the Arabian ecoregion. In the framework of the present study, the crude extract of n-hexane and ethyl acetate of the seeds were fractionated to purify major bioactive secondary metabolites. Five compounds were identified for the first time from the seeds of D. tortuosa: Marmin 1, Pituranthoside 2, Isoimperatorin 3, Bergapten 4 and Isopimpinellin 5. Their structures were elucidated using 1D and 2D NMR, (ESI)-MS and IR spectroscopic analyses. The cytotoxic, α-glucosidase and antibacterial activities of the pure phytochemicals were also evaluated.


(1)


(2)


(5)


(4)


(3)

Chemical composition and in vitro cytotoxic activities of the essential oil of *Lavandula atriplicifolia* Benth

Mohamed Habib Oueslati [a], Abdel Halim Harrath [b]

[a] *University of Carthage, Faculty of Science Bizerte, Laboratory of Hetero-Organic Compounds and Nanostructured Materials, Zarzouna, Tunisia*

[b] *King Saud University, College of Science, Department of Zoology, P.O. Box 2455, 1145 Riyadh, Saudi Arabia*

Plants of the Lavandula genus have been widely used in folk and traditional medicine. The aim of this study was to evaluate the qualitative and quantitative chemical composition of the essential oil of the aerial parts of Lavandula atriplicifolia (EOAPLA) grown in Saudi Arabia and its potential cytotoxicity to cancer cell lines. The essential oil was characterized and quantified by GC–MS and GC-FID. The potential cytotoxicity of the essential oil was evaluated against colorectal (LoVo) and hepatocellular (HepG2) car cinoma cell lines by using the MTT and lactate dehydrogenase (LDH) cytotoxicity assays. A total of 36 compounds were identified that constituted 92.3% of the total oil. The chemotype of the species was dominated by C-10 massoia lactone (46.65%) as the major compound followed by oxygenated monoter penes (28.43%). This is the first report to describe the presence of the rare compound massoia lactone in the essential oils from Lavandula species. The data revealed that EOAPLA inhibited the growth of LoVo and HepG2 cells in a dose-dependent manner. Treatment with 10 lg/mL EOAPLA for 2 days resulted in sig nificant damage to LoVo cells in comparison with the control. In contrast to the control cells, the LoVo cells showed morphological alterations such as cytoplasmic condensation, shrinkage, and the formation of debris. Moreover, EOAPLA treatment induced apoptosis in LoVo cells since it increased the expression of caspase 3/7. The cytotoxic and anti-proliferative properties of EOAPLA make it a good candidate for treatment of various cancers.

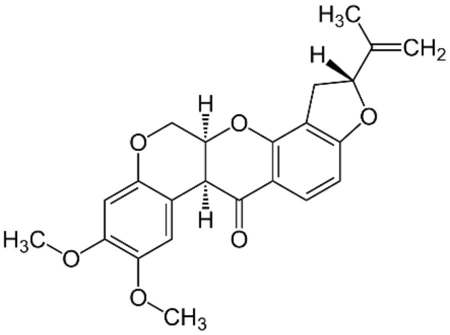
Computer-Assisted Statistical Physics Study of Rotenone Adsorption onto Chemically Engineered Activated Carbons

Rais Fayçal; Oueslati Kods; NaifarAmin ; Adhoum Nafaa

Laboratoire de Chimie, Matériaux et Modélisation (LCMM) à l'Institut Préparatoire aux Etudes d'Ingénieurs de Kairouan, Université de Kairouan

email : faicelrais@yahoo.fr

To address the environmental toxicity of rotenone insecticide with the following chemical structure: we employed statistical physics within the grand canonical ensemble to investigate the adsorption behavior of rotenone on three adsorbents (AC, AC-A, and AC-P) across 288–313 K. Three statistical models were numerically developed to fit the experimental isotherms, each incorporating parameters that describe probable molecular adsorption scenarios. Analysis revealed that adsorption on AC (rot/AC) is best described by the dual-layer dual-energy framework (DDEF), on AC-A (rot/AC-A) by the monolayer single-energy framework (MSEF), and on AC-P (rot/AC-P) by the monolayer dual-energy framework (MDEF). Steric evaluation indicated δ values between 0.98 and 1.08, reflecting predominantly non-parallel molecular orientations and the possibility of multiple species occupying single cavities, enabling aggregation. Energetic interactions with AC-A remained below 35 kJ/mol, suggesting van der Waals forces dominate adsorption. Pore size distribution (PSD) revealed primarily macroporous adsorbents (peak ~ 4 × 10^{-7} m), indicating surface accumulation rather than confinement governs adsorption. At higher temperatures, the adsorption energy distribution (AED) broadened with an increased population of high-energy sites (~ 1.5–2.0 × 10^{4} J/mol), consistent with moderated adsorption activity under thermal agitation.



Keywords : Rotenone, Activated Carbon, PSD, AED, Statistical Physics and adhesion isotherms.

The Impact of Gold Nanostructures and Enzymatically Synthesized Polymer Layers in Glucose Biosensor Design

Almira Ramanaviciene [1,2]*, Natalija German [2], Arunas Ramanavicius [1],
Anton Popov [1,2], Asta Kausaite-Minkstimiene [1,2]

[1] *NanoTechnas – Center of Nanotechnology and Nanomaterials, Faculty of Chemistry and Geosciences, Vilnius University, Vilnius, Lithuania;*
[2] *Department of Immunology and Bioelectrochemistry, Scientific Research Institute Centre for Innovative Medicine, Vilnius, Lithuania.*
* almira.ramanaviciene@chf.vu.lt

Glucose biosensors play a crucial role in clinical diagnostics, particularly in diabetes management and continuous glucose monitoring. The performance of electrochemical biosensors largely depends on the materials used for biosensor design. Some challenging bioanalytical problems, such as sensitivity, low limit of detection, specificity, reproducibility, and analysis duration, can be addressed by using various gold nanostructures on the electrode surface [1,2], while the operational stability of biosensors and linear range of analyte detection can be improved by using enzymatically synthesized π-π conjugated polymers, such as polyaniline (PANI) and polypyrrole (Ppy) [3,4]. Additionally, the combination of gold nanostructures and polymers offers advantages for biosensor performance in real samples, particularly by enhancing the analytical signal and improving resistance to interfering species.

The aim of this study was to evaluate the efficiency of PANI and Ppy layers formed by enzymatic polymerization on the surface of a graphite rod electrode, initially pre-modified with electrochemically synthesized dendritic gold nanostructures and glucose oxidase. The analytical characteristics of biosensors after the enzymatically initiated formation of PANI and Ppy layers were evaluated and compared. The applicability of glucose biosensors based on the Ppy layer was assessed in real samples.

References:

1. A. Ramanaviciene, N. German, A. Kausaite-Minkstimiene, A. Ramanavicius. *Chemosensors* 2021, 9, 188.
2. N. German, N., A. Ramanavicius, J. Voronovic, A. Ramanaviciene. *Microchimica Acta* 2010*,* 168, 221-229.
3. A. Ramanavicius, A. Kausaite, A. Ramanaviciene, A. *Analyst* 2008, 133, 1083-1089.
4. N. German, A. Ramanaviciene, A. Ramanavicius. *Polymers* 2021, 13, 2173.

Functionalization of MXenes for the Sensing and Removal of Pharmaceutical Organic Compounds

S. Ramanavicius [1,2]*, A. Raveendran [2], G. Paulikaite [2], S. Ali [2], O. Gogotsi [3],
A. Ramanaviciute [1,4], V. Korniienko [5,6], M. Pogorielov [5,6], A. Ramanavicius [1,4]

1. MB Sensografa, D. Riešė, LT-14262, Vilniaus rajonas, Lithuania;
2. State Research Institute Center for Physical and Technological Sciences (FTMC), Department of Nanotechnology, LT-10257, Vilnius, Lithuania;
3. Y-Carbon LLC (Carbon-Ukraine), Kyiv 04116, Ukraine;
4. Vilnius University, Institute of Chemistry, Faculty of Chemistry and Geosciences, NanoTechnas - Center of Nanotechnology and Materials Science, LT-03225 Vilnius, Lithuania;
5. Institute of Atomic Physics and Spectroscopy, University of Latvia, LV-1004 Riga, Latvia;
6. Biomedical Research Centre, Sumy State University, 40007 Sumy, Ukraine.
simonas.ramanavicius@ftmc.lt

Functionalized MXenes have emerged as promising materials for sensing and removing pharmaceutical organic compounds from aquatic environments due to their high surface area, tunable surface chemistry, hydrophilicity, and excellent optical and electronic properties. In particular, Mxene-based platforms are increasingly being explored for environmental monitoring due to their low cost, rapid response, and high sensitivity and selectivity [1]. By introducing suitable functional groups or decorating the Mxene surface with nanostructures, the interaction between Mxenes and pharmaceutical contaminants can be significantly enhanced, enabling both efficient detection and effective removal [2].

In sensing applications, Mxene-based colorimetric systems operate by inducing visible color changes upon interaction of target pharmaceutical molecules, enabling simple, real-time, and direct detection [3]. Surface modification of Mxenes with plasmonic nanoparticles, metal nanoclusters, polymers, or specific binding ligands can improve analyte recognition and amplify optical responses. These changes are often associated with variations in localized surface plasmon resonance, charge transfer, or catalytic activity, which can be monitored by absorption spectroscopy. For removal applications, Mxene functionalization plays a key role in improving adsorption capacity and selectivity toward pharmaceutical organic compounds. The presence of surface functional groups and hybrid components can promote electrostatic attraction, hydrogen bonding, π–π interactions, and other interfacial mechanisms that facilitate the capture of pollutant molecules in water [4]. In this study, functionalized Mxenes were investigated as both sensors and adsorbents for the removal of organic pharmaceutical compounds from simulated wastewater samples.

Acknowledgement: This research was funded by HORIZON-MSCA-2021-SE-01-01 “Towards development of new antibacterial strategy for dentistry” 101086441 ARGO.

References

[1] S. Zukauskas et al., “Electrochemical real-time sensor for the detection of Pb(II) ions based on $Ti_3C_2T_x$ MXene,” Science of The Total Environment 2024, 950, 175190; https://doi.org/10.1016/j.scitotenv.2024.175190
[2] F. Q. Yang et al., “Colorimetric Sensors: Methods and Applications,” Sensors 2023, 23, 9887; https://doi.org/10.3390/s23249887
[3] I. Navitski et al., MXene-Based Chemo-Sensors and Other Sensing Devices, Nanomaterials 2024, 14(5), 447; https://doi.org/10.3390/nano14050447
[4] S. Adomavičiūtė-Grabusovė et al., “Selective Enhancement of SERS Spectral Bands of Salicylic Acid Adsorbate on 2D $Ti_3C_2T_x$-Based MXene Film,” Chemosensors 2021, 9, 223; https://doi.org/10.3390/chemosensors9080223

In Silico Design of Molecularly Imprinted Polymers

A. Ramanaviciute [1,2]*, E. Mohsenzadeh [3], V. Korniienko [4,5], M. Pogorielov [4,5], G. Zvirzdine [1],
U. Prentice [1], G. Kaspute [1], S. Ramanavicius, A. Ramanavicius

1. MB Sensografa, D. Riešė, LT-14262, Vilniaus rajonas, Lithuania;
2. Vilnius University, Institute of Chemistry, Faculty of Chemistry and Geosciences, NanoTechnas - Center of Nanotechnology and Materials Science, LT-03225 Vilnius, Lithuania;
3. State Research Institute Center for Physical and Technological Sciences (FTMC), Department of Nanotechnology, LT-10257, Vilnius, Lithuania;
4. Institute of Atomic Physics and Spectroscopy, University of Latvia, LV-1004 Riga, Latvia;
5. Biomedical Research Centre, Sumy State University, 40007 Sumy, Ukraine.
agneramanaviciute@gmail.com

Molecularly imprinted polymer (MIP)-based structures are highly promising for the detection and extraction of various analytes. In this research, density functional theory (DFT) is applied for the in-silico design of MIPs. During the simulated formation of MIPs, we assess the most suitable monomers, characterise the formed oligomers, and evaluate the formation of binding sites and the rebinding energies of imprinted templates [1,2]. The most promising oligomers are evaluated to identify those optimally suited for the imprinting of selected target molecules. Binding energies, formation of hydrogen bonds, electrostatic potential maps, and electrochemical properties are considered. Conformation analysis is also applied for the more efficient prediction and characterization of molecularly imprinted cavities. Furthermore, the influence of the solvents (water, dimethyl sulfoxide, etc.) on the formation of hydrogen bonds and analyte binding energies is assessed [3]. The modelling of binding sites enables us to achieve improved sensitivity and higher specificity in the designed MIPs compared to non-imprinted polymers (NIPs). Therefore, NIPs are also modelled as reference systems to assess the efficiency of the MIPs. The integration of nanomaterials, which can enhance the performance of MIPs and induce additional properties such as antibacterial activity, can also be predicted and modelled. This research guides the development of MIP-based sensors and systems dedicated to the selective extraction of specific organic compounds.

Acknowledgement: This research was funded by HORIZON-MSCA-2021-SE-01-01 “Towards development of new antibacterial strategy for dentistry” 101086441 ARGO.

References

[1] E. Mohsenzadeh, V. Ratautaite, E. Brazys, S. Ramanavicius, S. Zukauskas, D. Plausinaitis, A. Ramanavicius. Design of Molecularly Imprinted Polymers (MIP) using Computational Methods: a Review of Strategies and Approaches. WILEY Interdisciplinary Reviews Computational Molecular Science 2024. 2024;14:e1713 https://doi.org/10.1002/wcms.1713

[2] E. Mohsenzadeh, V. Ratautaite, E. Brazys, S. Ramanavicius, S. Zukauskas, D. Plausinaitis, A. Ramanavicius. Application of computational methods in the design of molecularly imprinted polymers (review). Trends in Analytical Chemistry, 2024, 171, 117480. https://doi.org/10.1016/j.trac.2023.117480

[3] E. Brazys, V. Ratautaite, E. Mohsenzadeh, R. Boguzaite, A. Ramanaviciute, A. Ramanavicius, Formation of molecularly imprinted polymers: strategies applied for the removal of protein template (Review). Advances in Colloid and Interface Science, 2025, 337, 103386. https://doi.org/10.1016/j.cis.2024.103386

Thermal, Mechanical and Rheological Behavior of PVC Filled with ATH and MDH Electrical Cable Applications.

Mouna Riahi [1], Noureddine Amdouni [1], et Jawher Nemchi [2]

[1] *Laboratoire : Caractérisation applications et modélisation des matériaux,*
Faculté des Sciences de Tunis. Code labo :LR18ES08
[2] *Société Tunisienne des Câbles Électriques, Z.I. GROMBALIA – 8030 TUNISIA*

Polyvinyl chloride (PVC) is extensively used in the cable industry due to its cost-effectiveness and ease of processing. However, its intrinsic thermal and mechanical limitations can restrict its performance under demanding service conditions, particularly in terms of thermal stability and fire resistance.

In this study, PVC-based formulations were developed by incorporating mineral fillers, namely aluminum hydroxide (ATH) and magnesium hydroxide (MDH), in the presence of calcium carbonate ($CaCO_3$**)**. The main objective is to investigate the influence of these additives on the physical properties and processing behavior of the material.

Thermal properties were evaluated using thermogravimetric analysis (ATG), revealing enhanced thermal stability in the modified compositions. In addition, Fourrier-transform infrared spectroscopy (FTIR) was employed to assess the interactions between the polymer matrix and the incorporated fillers. Mechanical testing indicated an increase in material stiffness while maintaining an acceptable level of flexibility.

Overall, the results demonstrate that the incorporation of ATH and MDH significantly alters the physico-mechanical behavior of PVC, leading to improved processability and enhanced performance for advanced industrial applications.

Efficient solvent-free synthesis of thymol/thymoquinone mixtures via catalyzed oxidation and evaluation of their antibacterial activity

Ons Romdhane, Jamil Kraiem

Laboratory of Chemical, Galenic and Pharmacological Drug Development-(LR12ES09), Faculty of Pharmacy, University of Monastir, Avicenne street, 5000, Monastir, Tunisia.

Thymoquinone is a high-value natural phenolic compound with documented hypoglycemic [1], antioxidant [2], and anti-inflammatory [3] activities. While traditionally isolated from *Nigella sativa*, it can be synthesized via thymol oxidation, however, conventional methods often rely on hazardous oxidants and expensive catalysts. Within our green chemistry research framework [4,5], we developed an efficient, solvent-free catalytic route to produce thymol/thymoquinone mixtures. This approach is simple, cost-effective, and aligns with green chemistry principles. The results demonstrate a synergistic potential of the mixture, offering a promising eco-friendly alternative to conventional antibiotics for treating bacterial infections, notably against E. coli and S. epidermidis. The antibacterial activity was evaluated by determining the Minimum Inhibitory Concentration (MIC) using the microdilution method and the Minimum Bactericidal Concentration (MBC) via inoculation on Mueller-Hinton agar. General methods NMR spectra were acquired using $CDCl_3$ as solvent, running at 300 MHz for ^1H, and at 75 MHz for ^{13}C, while product distribution was analyzed via GC-MS. Reactions were carried out in a pressure tube with a stirrer bar at 50ºC.

Keywords: thymol, thymoquinone, oxidation, catalyst, MIC, MBC.

References

[1] Bamosa, A.O., Ali, B.A., Sowayan, S.A., Saudi Pharmaceutical Journal, 1997, 5, 126-129.
[2] Lutterodt, H., Luther, M., Slavin, M., Yin, J.J., Parry, J., Gao, J.M., Yu, L.L., LWT-Food Sci. Technol, 2010, **43**(9), 1409–1413.
[3] Al-Ghamdi, M.S., Journal of Ethnopharmacology, 2001, 76, 45-48.
[4] Kraiem, J., Ghedira, D., Ollevier, T., Green. Chem, 2016, 18, 4859.
[5] Kraiem, J.; Ollevier, T., Green. Chem, 2017, 19, 1263.

Efficient Synthesis and Spectroscopic Characterization of a Novel Benzo-1,3-Diazine-2-thione Derivative from 2-Aminobenzonitrile

D. Saidani, M. Smadhi and R. Abderrahim

University of Carthage, Faculty of Sciences of Bizerte, Laboratory of Ressources Matériaux,
Valorisation et Écosystème (RME code LR19ES20), Zarzouna 7021, Bizerte, Tunisia

The development of efficient synthetic approaches for nitrogen- and sulfur heterocyclic containing compounds remains an important objective in organic synthesis due to their potential applications in various areas of chemistry.

In this work, a simple and efficient synthetic strategy for the preparation of a novel benzo-1,3-diazine-2-thione derivative starting from 2-aminobenzonitrile is described. The synthetic route involves the formation of an amidrazone intermediate through reaction with hydrazine, followed by treatment with carbon disulfide, which promotes cyclization leading to the target compound.

The structure of the synthesized compound was confirmed by IR, ^{1}H NMR, and ^{13}C NMR spectroscopy. The obtained spectroscopic data are consistent with the proposed molecular structure.

This straightforward method provides a practical approach for the synthesis of new nitrogen- and sulfur heterocyclic compounds and may offer useful perspectives for further studies in synthetic and medicinal chemistry.

Aminated PES/Carbon Black Membranes for Laser-Induced Graphene Electrodes

Ons SALAH [a], Nourddine RAOUAFI[a]* and Walid MABROUK [b]

[a] *Laboratory of Sensors and Biosensors, Department of Chemistry, Faculty of Science, University of Tunis, Tunis, Tunisia*
[b] *Center for Research and Water Technologies, Water Research and Technologies Centre, Borj Cedria technopark, Tunisia*
*E-mail: ons.salah@etudiant-fst.utm.tn

Aminated polyethersulfone (NH_2-PES)/carbon black composite membranes were developed as precursors for laser-induced graphene (LIG) electrodes. Carbon black enhances the electrical conductivity and improves laser–material interaction during CO_2 laser irradiation, enabling the formation of a porous and conductive carbon-based electrode after laser processing.

The materials were characterized by optical profilometry, FTIR, and TGA, while electrochemical performance was evaluated using cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS).

The LIG electrodes obtained from membranes containing carbon black showed improved electrochemical performance compared to pristine membranes.

Their application was demonstrated for electrochemical sensing of ascorbic acid (AA) showing promising analytical performance.

Keywords

NH2-PES membrane, Carbon Black, composite membrane, Laser Induced Graphene

---

References

N. Kurra, Q. Jiang, P. Nayak, et H. N. Alshareef, « Laser-derived graphene: A three-dimensional printed graphene electrode and its emerging applications », *Nano Today*, vol. 24, p. 81-102, févr. 2019, doi: 10.1016/j.nantod.2018.12.003.

S. Baachaoui, W. Mabrouk, A. Rabti, O. Ghodbane, et N. Raouafi, « Laser-induced graphene electrodes scribed onto novel carbon blackdoped polyethersulfone membranes for flexible high-performance microsupercapacitors », *J. Colloid Interface Sci.*, vol. 646, p. 1-10, sept. 2023, doi: 10.1016/j.jcis.2023.05.024.

S. Baachaoui *et al.*, « Laser-induced porous graphene electrodes from polyketimine membranes for paracetamol sensing », *R. Soc. Open Sci.*, vol. 10, n° 8, p. 230294, août 2023, doi: 10.1098/rsos.230294.

Enhanced Photocatalytic Degradation of Congo Red Using Co-TiO_2/Hematite Catalyst: Modeling and Optimization Approach

Sourour SALHI *[1, 2], Abdessalem OMRI [1], Ridha BEN SALEM [2], Mourad BENZINA [1]

[1] *Organic Chemistry Laboratory LR17ES08, Faculty of Sciences of Sfax,*
University of Sfax, Tunisia.
[2] *Laboratory Eau Energie Environment (LR3E), Code: AD-10-02,*
Ecole Nationale d'Ingénieurs of Sfax, University of Sfax, Tunisia.
Corresponding author E-mail: souroursalhi10@gmail.com

This study investigates the catalytic performance of a catalyst for the degradation of Congo Red (CR) dye in aqueous solution through a heterogeneous photo-Fenton process using hydrogen peroxide as in oxidant. The catalyst was synthesized by a simple impregnation method using natural hematite. The prepared ferrous hematite sample was characterized by several analytical techniques, including BET surface analysis, SEM-EDX, and XRD. Response Surface Methodology (RSM) was applied to minimize the number of experiments while determining the optimal conditions for CR oxidation. Several factors influencing the oxidation process were examined, such as catalyst dosage, Congo Red concentration, and the pH of the solution. Regression analysis revealed a good agreement between experimental and predicted results, with a coefficient of determination (R^2) of 0.9785. Statistical analysis indicated that the optimal conditions for removing CR from aqueous solutions using the prepared Co/TiO_2 supported on natural hematite catalyst were a catalyst mass of 0.3 g, a CR concentration of 50 mg/L, and a solution pH of 3. The maximum of oxidation efficiency of 91.06% was achieved. These results confirm that natural hematite serves as an effective support for the uniform dispersion and high activity of TiO_2 and cobalt phases.

Keywords: Congo Red ; Photo-Fenton Process; Natural hematite; Photochemical Oxidation

Bio-Based 5,5'-Isopropylidene Bis(ethyl 2-furoate) as a Renewable Building Block for Water-Borne Polyurethane Dispersions

Dina Sellami [a], Sami Zaidi [a], Oumayma Challouf [a], Tobias Robert [b], Majdi Abid [c],
Souhir Abid [a,c] and Abdelkader Bougarech [a]

[a] *Faculté des Sciences, Laboratoire de Chimie Appliquée HCGP, Université de Sfax, Sfax 3038, Tunisia*
[b] *Fraunhofer Institute for Wood Research–Wilhelm-Klauditz-Institut WKI, Riedenkamp 3,*
38108 Braunschweig, Germany
[c] *Department of Chemistry, College of Science, Jouf University, P.O. Box 2014, Sakaka,*
Aljouf, Kingdom of Saudi Arabia

Polyurethanes are versatile polymers widely used in foams, coatings, adhesives, and elastomers because of their adjustable mechanical and thermal properties [1]. However, their dependence on petrochemical resources has increased interest in sustainable, biobased alternatives. Furan-based polyurethanes are a promising option. In particular, 2,5-furandicarboxylic acid (FDCA) has shown performance comparable or superior to fossil-based materials in water-borne polyurethane dispersions, especially regarding pendulum hardness, tensile strength, and glass transition temperature [2]. In this work, 5,5'-isopropylidene bis(ethyl 2-furoate) (DEF), a related bisfuranic monomer, is studied for the first time as a renewable building block for polyurethane synthesis. Two series of water-borne polyurethane (WPU) dispersions were prepared and compared. In the first series, DEF-based oligoesters were synthesized by polycondensation of DEF with succinic acid and 1,6-hexanediol to obtain hydroxyl-terminated polyols with controlled molecular weights. In the second series, a petrochemical polyester based on dimethyl terephthalate (DMT) was prepared as a reference, following comparable experimental conditions. All oligoesters were then reacted with a bio-based oligomeric isocyanate in the presence of DMPA as an internal emulsifier to produce stable aqueous WPU dispersions. The obtained films were characterized to evaluate their potential as coating materials. This study highlights the influence of the bisfuranic structure on WPU properties and its potential as a sustainable alternative to conventional aromatic petrochemical building blocks.

References

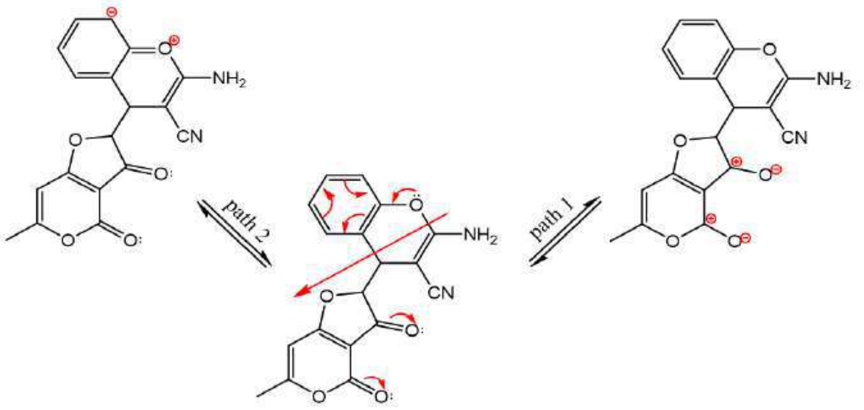
[1] Wu, S., Ma, S., Zhang, Q., Yang, C. (2025. *Polymer*, 327, 128361.
[2] Papadopoulos, L., Malitowski, N. M., Zamboulis, A., Friebel, S., Bikiaris, D., Robert, T. (2023). *Reactive and Functional Polymers*, 190, 105622.

One-pot synthesis of fused chromene-furanopyran under microwave Investigation on the solvatochromism, Determination of dipole moments

D. Siziani [1,2], Y. Abdi [1,2], F.Z. RIHEL [1], M. Kelbouz [1], K. Ferhah [3], R. Cheggou [3],
Z. Attou [2], N. Bensouilah [2]

[1] Applied sciences laboratory LSA, Ecole Nationale Supérieure des Technologies Avancées, Cité Diplomatique, ex. Centre biomédical, Dergana, Bordj El Kiffan, Algiers, Algeria
[2] Laboratory of Applied Organic Chemistry, Faculty of Chemistry (LAOC), University of Sciences and Technology Houari Boumediene, USTHB, PB 32, El-Alia, Bab-Ezzouar, 16111 Algiers, Algeria
[3] Laboratoire des Technologies Innovantes (LTI), Ecole Nationale Supérieure de Technologie avancées, Algiers, Algeria

The current study involves the synthesis of new serie of chromene-furanopyran -3-carbonitriles, using a quick chemical process of a multi-component type reaction under microwave irradiation [1]. Recently, the 2-amino- 4 H -chromenes have been used in technological areas, for instance, as laser dyes, optical brighteners, fluorescence markers, pigments, cosmetics and biodegradable agrochemicals [2].
The steady-state optical absorption and fluorescence spectra of three amino aryl-4H-furo[3,2-c]pyran -4H-chromene-3-carbonitrile derivatives. The ground state (µg) and excited state (µe) dipole moments were determined by the solvatochromic shift method using Kawski-Bilot and Ravi et. al. equations. The study of dipole moments, in the ground and the excited states of the molecules, provides crucial information about the electronic and geometric structure of the molecule in its short-lived state. Moreover, knowledge of the excited-state dipole moment is very important for designing new compounds with the desired optical properties. The excited-state dipole moment of fluorescent dye molecules such as those studied in this report is also able to determine the range of tenability of their emission energy as a function of the medium polarity [3].



References
[1] D. Siziani, B.E.C. Ziani, Y. Abdi, N. Bensouilah, B. Boutemeur-Kheddis, C. Ziani, L. Boukkena, M. Hamdi, O. Talhi, K. Bachari, A.M.S. Silva, J. Mol. Struct. 1264 (2022) 133236.
[2] W. Kemnitzer, J. Drewe, S. Jiang, H. Zhang, Y. Wang, J. Zhao, C. Crogan-Grundy, L. Xu, S. Lamothe, H. Gourdeau, R. Denis, B. Tseng, S. Kasibhatla, S.X. Cai, J. Med. Chem. 50 (2007) 2858–2864.
[3] D. Siziani, Y. Abdi, B. Bezzina, Z. Attou, N. Bensouilah, B. Boutemeur, J. Mol. Struct. 1319 (2025) 139473.

Email address: * Dhaouya SIZIANI dhaouya.siziani@ensta.du.dz

Synthesis and Development of Polymer-Based Nanoparticle Mixed Matrix Membranes

Fatima SMAIL, Mourad AMARA

Laboratory for Hydrometallurgy and Molecular Inorganic Chemistry, Faculty of Chemistry
USTHB, BP32 EL Alia, Bab Ezzouar,16011 ALGER
National Higher School Of Advanced Technologies Algeria,
Lycée Emir Abdelkader Bab El Oued Alger DZ‹ 16001
Email sma-fatima@hotmail.fr / fatima.smail@ensta.edu.dz

The current trend in membrane technology focuses on the development of new materials and membrane structures to reduce fouling effects while improving biocompatibility and introducing specific functionalities. However, hydrophilic membranes tend to swell in water, which leads to a loss of mechanical strength and a reduction in solute retention.

In this work, polyethersulfone (PES) membranes were fabricated by varying the composition of a collodion solution containing ZnO nanoparticles and metal–organic frameworks (MOFs). The physicochemical characteristics of the fabricated membranes were investigated, and permeability and retention tests were performed.

The membranes were characterized using Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), and thermogravimetric and differential thermal analyses (TGA/DTA) to determine their functional groups, morphology, and thermal properties.

To evaluate the selectivity of the prepared membranes, they were placed in a two-compartment diffusion cell into which a mixed solution of copper, nickel, and zinc metal ions was introduced.

Keywords: Membranes, polymer, polyelectrolyte, nanoparticle and metals

Advanced investigation of the adsorption process of coumarin compounds on mouse olfactory receptors: Statistical physics modeling and molecular docking

Houda Smati (a*), Mohamed Bouzid (b), Yosra Ben Torkia (a), Abdelmottaleb Ben Lamine (a)

(a) Laboratory of Quantum and Statistical Physics LR 18 ES 18, Faculty of sciences of Monastir,
University of Monastir, Environnement Street, 5019 Monastir, Tunisia
(b) CRMN, Centre for Research on Microelectronics and Nanotechnology of Sousse, NANOMISENE,
LR16CRMN01, Code Postal 4054, Sousse, Tunisia

A statistical physics framework was employed to elucidate the olfaction mechanism through a putative adsorption process involving coumarin compounds on mouse olfactory receptors Olfr924, Olfr285, and Olfr1016. Both monolayer and double-layer adsorption models were utilized to describe the interactions between the odorant molecules and the receptor sites. Experimental data were analyzed in terms of steric and energetic parameters characterizing the adsorption mechanism. Steric analysis indicated that the two odorant molecules exhibit both parallel and non-parallel orientations to the receptor binding sites, suggesting a mixed anchoring behavior. The estimated adsorption energies values, ranging from 13.563 to 33.872 kJ/mol, suggest that the coumarin compounds are physically adsorbed onto the receptors. Moreover, the application of statistical physics modeling enabled a detailed steric characterization of the receptor surface through binding site size distributions (BSDs), as well as an energetic characterization via adsorption energy distributions (AEDs). To complement the microscopic analysis, a macroscopic thermodynamic study was also performed, providing further insight into the adsorption behavior of coumarin compounds on the olfactory receptors. Subsequently, molecular docking analysis highlights the specific interaction patterns formed between the three mouse olfactory receptors and the coumarin ligands.

Keywords: Statistical physics; Coumarin; Olfr924; Olfr285; Olfr1016; adsorption entropy; molecular docking.

Synthesis and Structural Characterization of a Novel Hybrid Organic-Inorganic Polyoxovanadate Framework

El Waleda Moustapha Thiam [a], Aliou Hamady Barry [a],
Nicolas Claiser [b], Mohamed Souhassou [b]

[a] *Materials Chemistry Research Unit, Department of Chemistry, Faculty of Science and Technology, University of Nouakchott, Mauritania.*
[b] *CRM2 Laboratory, UMR CNRS 7036, Faculty of Science and Technology, University of Lorraine, France.*

The chemistry of Polyoxovanadates (POVs) is attracting growing interest due to their vast structural diversity and remarkable properties in catalysis, magnetism, and materials science. This study reports the synthesis by slow evaporation and the structural elucidation of a new hybrid organic-inorganic compound. The core of the structure consists of a decavanadate anionic cluster, stabilized by a complex network of non-covalent interactions. Single-crystal X-ray diffraction analysis reveals that the inorganic unit is surrounded by organic cations derived from 2-amino-4-methylpyridine. These organic entities play a crucial "template" role, ensuring crystal cohesion through a dense system of N-H...O hydrogen bonds. The structural arrangement highlights a strong synergy between the high-symmetry vanadium cluster and the organic cations. These directional interactions directly influence the thermal stability and electronic properties of the material. This new complex enriches the family of vanadate-based hybrid materials and opens perspectives for the development of new tunable catalytic systems.

Keyword: Polyoxovanadate (POVs), Decavanadate, Hybrid materials, Slow evaporation, Crystal structure, 2-amino-4-methylpyridine, Hydrogen bonding

The Design of Acridine-Based Hybrids as Potential Anticancer Agents

Najeh TKA

Laboratory of Asymmetric Synthesis and Molecular Engineering for Organic Electronic Materials (LR18ES19), Monastir University, Faculty of Sciences of Monastir.

najeh_tka@yahoo.fr

Cancer is one of the leading causes of mortality worldwide and continues to pose a significant global health burden. Although numerous chemotherapeutic agents have been developed, many of them suffer from limitations such as toxicity, poor selectivity toward tumor cells, and the emergence of multidrug resistance. The development of new anticancer agents remains a major priority in pharmaceutical research. Acridine-based compounds[1,2] have attracted significant attention because of their ability to interact with DNA and disrupt cell proliferation. A notable example is Amsacrine, an acridine derivative used clinically in the treatment of leukemia. Its mechanism of action involves inhibition of the enzyme Topoisomerase II, which is essential for DNA replication and repair. A recent strategy in medicinal chemistry involves the design of acridine-based molecular hybrids[3,4], in which the acridine scaffold is combined with other bioactive pharmacophores to enhance anticancer efficacy and reduce side effects. In The present work, we discuss the design principles of new acridine-based hybrids and their potential as anticancer agents.

Keywords: Heterocyclic compounds, acridine derivatives, anticancer activity.

References

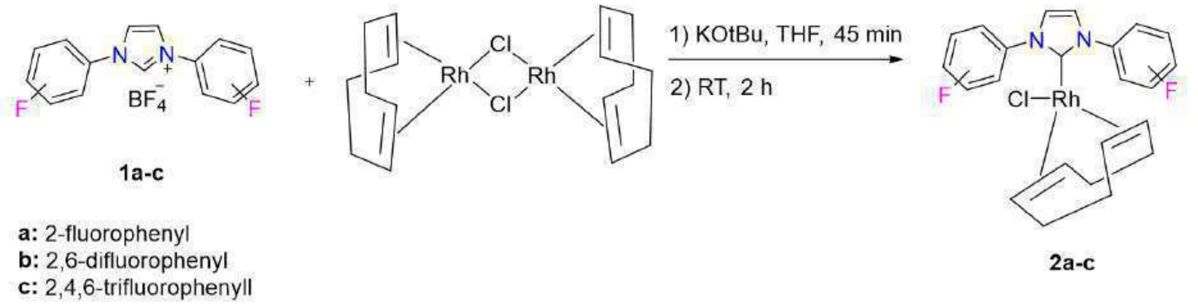
1. Denny, W. A. (2002). Acridine derivatives as chemotherapeutic agents. *Current Medicinal Chemistry*.
2. Belmont, P., Bosson, J., Godet, T., & Tiano, M. (2007). Acridine and acridone derivatives as antitumor agents. *Anti-Cancer Agents in Medicinal Chemistry*.
3. Gellerman, G., et al. (2015). Design and synthesis of novel acridine-based anticancer agents. *Bioorganic & Medicinal Chemistry*.
4. Cholewiński, G., Dzierzbicka, K., & Kołodziejczyk, A. (2011). Natural and synthetic acridines as anticancer agents. *Pharmacological Reports*.

Fluorinated Rhodium Complexes: Synthesis, Characterization, and Investigation of Fluorine–Metal Interactions in Transfer Hydrogenation

Nedra Touj [a,b] and Lionel Delaude [a]

[a] *Laboratory of Organometallic Chemistry and Homogeneous Catalysis,*
University of Liege, Allée du six août 13, 4000 Liege, Belgium.
[b] *Research Laboratory of Environmental Sciences and Technologies (LR16ES09), Higher*
Institute of Environmental Sciences and Technology, University of Carthage, Hammam-Lif, TUNISIA.
Email : toujnedra@gmail.com

The properties of metal complexes are strongly influenced by the electronic and steric characteristics of the ligands bound to the metal center. Understanding and quantifying these effects are essential for predicting catalytic behavior. n this context, three different Rh complexes with the generic formula [(NHC)RhCl(COD)] (2a–c) were synthesized from $[RhCl(COD)]_2$ using fluorinated imidazolium salts (scheme 1) and fully characterized by NMR spectroscopy (^1H, ^{13}C, ^{19}F), IR and HR-MS. [1] The presence of fluorine is expected to influence both the electronic distribution and the spatial environment around the rhodium center. This investigation aims to assess how fluorine–metal interactions may influence the catalytic behavior of rhodium NHC complexes in the reaction of transfer hydrogenation. [2]



Scheme 1. Synthesis of [(NHC)RhCl(COD)] complexes **2a–c**.

Key words: Rhodium complexes, N-hetrocyclic carbene, Fluorine–metal interactions, Catalytic behavior, Electronic proprieties.

References

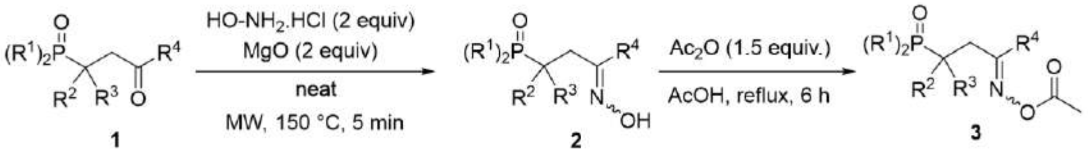
[1] N. Touj, F. Mazars, G. Zaragoza, L. Delaude. *Beilstein J. Org. Chem.* **2023**, *19,* 1947–1956.
[2] M. S. S. Jamil, S. Alkaabi, A. K. Brisdon. *Dalton Trans*. **2019**, *48*, 9317-9327.

Green Synthesis, Antibacterial Activity and Molecular Docking Study of Γ-Phosphonyloxime Derivatives

Aymen Wahbi [a]*, Wiem Tahri [b], Kamel Kaabi [c], Abdelwaheb Chatti [b], Cherif Ben Nasr [c], Jean-François Cavalier [d] and Soufiane Touil [a]

[a] *Laboratory of Hetero-Organic Compounds and Nanostructured Materials (LR18ES11), University of Carthage, Faculty of Sciences of Bizerte, 7021 Jarzouna, Tunisia.*
[b] *Laboratory of Biochemistry and Molecular Biology, Risks Related to Environmental Stress, Struggle and Prevention (UR17ES20), University of Carthage, Faculty of Sciences of Bizerte, 7021 Jarzouna, Tunisia.*
[c] *Laboratoire de Chimie des Matériaux, Faculté des Sciences de Bizerte, Université de Carthage, Carthage 1054, Tunisia.*
[d] *Aix-Marseille Univ., CNRS, LISM UMR 7255, IMM FR3479, Marseille, France.*
E-mail: aymen.wahbi@fsb.ucar.tn; aichamhamdi1987@gmail.com; tahri.wiem@yahoo.fr; dridiimentun@gmail.com; dridimedali20@hotmail.com; kamel_kaabi@yahoo.fr; chattiabdel@yahoo.fr; cherifbennasr48@gmail.com; jfcavalier@imm.cnrs.fr; soufiane.touil@fsb.rnu.tn

Herein we report an efficient, fast and green approach to γ-phosphonyloximes in 5 min, through the microwave-assisted oximation of γ-phosphonylketones under solvent-free conditions. These oximes can be converted into the corresponding *O*-acetylated derivatives, by reaction with acetic anhydride. Study of the molecular structure characteristics of the synthesized compounds, in order to gain more insight into the molecular geometry, intermolecular interactions and electronic properties, was performed by various spectroscopic tools including FT-IR, NMR (^{1}H, ^{31}P, ^{13}C) spectroscopy, mass spectrometry and single crystal X-ray diffraction analysis, and by theoretical calculations using the DFT/B3LYP/6-311+G* basis set. Intermolecular interactions within the crystal structure were further investigated by Hirshfeld surface analysis. The title compounds were screened for their *in vitro* antibacterial activity against Gram-positive bacterium (*Staphylococcus aureus* NCTC 6571) and three Gram-negative bacteria (*Escherichia coli* JW 1772, *Pseudomonas aeruginosa* SH 38, and *Salmonella typhimurium* ATCC 14028). The biological assays showed that the *O*-acetylated derivatives exhibited appreciable antibacterial activities. *In silico* molecular docking studies in *E. coli* FabH enzyme active site were performed in order to corroborate these results and to predict at the molecular level the possible interaction modes and binding energies for both the *O*-acetylated γ-oximophosphonate **3** and its free γ-oximophosphonate **2** analogue, as compared with those of a reference FabH inhibitor. Indeed, oximes are also known for their antibacterial, antiviral, and anticancer properties [1-3]. Oxime derivatives also have applications as peptide modifiers [4-6] and herbicide agents [7].



Scheme 1. Synthesis of γ-oximophosphonates and phosphine oxides (**2**) and *O*-acetyl-γ-oximophosphonates (**3**).

Keywords: γ-phosphonyloximes; microwave irradiation; green synthesis; X-ray diffraction; antibacterial activity; molecular docking.

References

[1] Bednarczyk-Cwynar, B., Zaprutko, L., Recent Advances in Synthesis and Biological Activity of Triterpenic Acylated Oximes, Phytochem. Rev., vol. 14, (2015), pp. 203-231.
[2] Fylaktakidou, K.C., Hadjipavlou-Litina, D.J., Litinas, K.E., Varella, E.A., Nicolaides, D.N., Recent Developments in the Chemistry and in the Biological Applications of Amidoximes, Curr. Pharm. Des. Vol. 14, (2008), pp. 1001-1047.
[3] Nikitjuka, A., Jirgensons, A., Synthesis, Chemical and Biological Properties of Aziridine-1-carbaldehyde Oximes (Minireview), Chem. Heterocycl. Compd. Vol. 49, (2014), pp. 1544-1559.
[4] Agten, S.M., Dawson, P.E., Hackeng, T.M., Oxime Conjugation in Protein Chemistry: from Carbonyl Incorporation to Nucleophilic Catalysis, J. Pept. Sci. vol. 22, (2016), pp. 271-279.
[5] Ulrich, S., Boturyn, D., Marra, A., Renaudet, O., Dumy, P., Oxime Ligation: a Chemoselective Click-Type Reaction for Accessing Multifunctional Biomolecular Constructs, Chem. Eur. J. vol. 20, (2014), pp. 34-41.
[6] Li, X.-G., Haaparanta, M., Solin, O., Oxime Formation for Fluorine-18 Labeling of Peptides and Proteins for Positron Emission Tomography (PET) Imaging: A Review, J. Fluorine Chem. Vol. 143, (2012), pp. 49-56.
[7] Sevilla-Morán, B., López-Goti, C., Alonso-Prados, J.L., Sandín-España, P., Degradation of Cyclohexanedione Oxime Herbicides, Herbicides: Advances in Research, (2013), pp. 101-130.

Influence of Hydrodistillation Time Intervals and Drying Period on the Yield, Chemical Composition, and Antioxidant activities of *Pituranthos chloranthus* stems essential oils from the Sbiba-Kasserine Provenance (Southern Tunisia)

Ahlem Yahya [ab], Amani Ayachi [c], Fatma Chtourou [d], Zina Benissa [a], Nathan TENE [e]; Raoudha Jarraya [c], Michel Treilhou [e], Sami Zouari [a,f]

a) Laboratory of Medicinal and Environmental Chemistry, High Institute of Biotechnology of Sfax, University of Sfax, Tunisia
b) Faculty of Sciences of Gafsa, University of Gafsa
c) Laboratory of Organic Chemistry LR17ES08, Natural Substances Team, Faculty of Sciences of Sfax, University of Sfax, P.B 1171, Sfax 3000, Tunisia
d) Laboratory of Electrochemistry and Environment, National School of Engineers of Sfax, University of Sfax, Sfax, Tunisia
e) Equipe BTSB-EA 7417, Institut National Universitaire Jean-François Champollion, Université de Toulouse, Place de Verdun, 81012 Albi, France
f) Engineering National School of Sfax, University of Sfax, Sfax, Tunisia

This study evaluates the combined effects of drying duration and hydrodistillation time on the yield, chemical composition, and antioxidant activities of *Pithuranthos chloranthus* stems essential oils (EOs) from the Sbiba-Kasserine provenance. EOs were recovered at successive time intervals (0–60, 60–120, 120–180, 180–240 min) from plant material dried for one month (OM) and one year (OY). The highest yields (0.45%) of EOs were occurred during the first interval (0–60 min) for both drying duration. GC–MS analysis revealed a notable chemical variability as influenced by both factor, particularly in the abundance of monoterpene hydrocarbons family (α-pinene, α-phellandrene, 3-carene, β-cymene, α-terpinene). Across all hydrodistillation time, the evolution of the rates of oxygenated monoterpenes recorded for EOs stems dried during OM and OY was mostly linked to the percentage of L-terpinen-4-ol considered as the main compound in this group. Antioxidant activities, measured via DPPH and FRAP assays, was modulated by both factors (drying duration and hydrodistillation time). In fact, stems EOs dried of OM showed the strongest DPPH scavenging (IC_{50} = 0.80 mg/mL) across all hydrodistillation time, whereas EOs stem dried for OY recovered at 60-120 min exhibited the highest FRAP activity (EC_{50} = 1.70 mg/mL). These finding demonstrate that drying duration and hydrodistillation time were the key factors determining the variation of the yields, the chemical compositions, and the antioxidant activities of Sbiba-Kasserine stems EOs.

Key words: *Pituranthos chloranthus*; essential oil hydrodistillation time; drying duration; antioxidant activities;chemotype.

Fabrication and characterization of a new ceramic membrane from Tunisian clay: Application to industred wastewater treatment

Imen ZOUIDI [a,b]; Chaima ARFAOUI [c]; Safa GAMOUDI [a]

[a] Laboratory of Composite Materials and Clay Minerals, National Center for Research in Materials Science, Technopole Borj Cedria, B.P. 73, 8027, Soliman, Tunisia
[b] University of Gafsa, Faculty of Sciences of Gafsa, Gafsa 2112, Tunisia.
[c] University of Gafsa, National Engineering School of Gafsa, Sidi Ahmed Zarroug - 2112, Gafsa, Tunisia
Email :hajerzwidi@gmail.com

In wastewater treatment, the application of ceramic membranes has gained significant attention due to their potential for highly effective filtration. These membranes are typically produced using methods such as spin coating, dip-coating, and spray coating. This research demonstrates the effective treatment of wastewater using cost-effective porous ceramic membranes, The corresponding support was prepared by a Pressing method using Tunisian clay alone followed by the addiction of a magnesium carbonate additive to improve certain parameters crucial to filtration sintering from 950 to 1100 °C. The selection of this foundational material is justified by its very low cost and its abundant availably within the region. Various analytical techniques, including XRD and MEB were employed to investigate the properties of these ceramic membranes. Furthermore, the influence of sintering temperature and $MgCO_3$ concentration on support properties, such as porosity and mechanical strength, was rigorously examined. Our findings significantly indicates that the $MgCO_3$ additive significantly enhances open porosity, achieving a maximum of 52.6%. The average pore size was determined to be approximately 0,7 µm, making this membranes selected for microfiltration of domestic wastewater.

Keywords: Clay, Ceramic membrane, Pressing method, microfiltration, Wastewater

New fluorescent material based on anthracene and triazole for blue organic light emitting diode

Habiba Zrida, Khaoula Hassine, Khaled Hriz

Advanced Materials and Interfaces Laboratory University of Monastir, Faculty of Sciences of Monastir,
Boulevard de l'Environnement, 5019 Monastir, Tunisia

Over recent decades the whole world has undergone rapid technological advancement driving energy revolution. Extensive research on these themes has been developed, including mainly organic electronics that field at the interface of molecular chemistry, materials science, and device engineering. One of its most remarkable successes is the organic light-emitting diode (OLED), which has changed the display world. Among the three primary colors (red, green, and blue) required for creating full-color displays. Small organic molecules are preferred candidates for emissive layers due to their well-defined structure, ease of purification, and ability to be vacuum-deposited to form high-quality thin films. Significant progress has been achieved through subtle but strategic chemical modifications.

Our contribution occurs within the framework of molecular architecture through the development of a new blue fluorescent material containing anthracene and triazole groups. Indeed, anthracene derivatives have demonstrated promising characteristics as blue-emitting materials for OLEDs. However, the presence of only the anthracene group in the structure presents certain problems, such as instability in the presence of light and oxygen and poor solubility, which limits the possibilities of using it as an active layer in electronic devices. Consequently, the insertion of heterocycles into organic devices is necessary. The triazole group is known for its optical application in nonlinear systems and is also considered an electron-transporting group in OLED fabrication. The prepared compound by Wittig reaction exhibits good solubility in common organic solvents. Its structure was confirmed by ^{1}H NMR and FT-IR spectroscopy. The optical properties were determined by UV-vis spectroscopy, and the energy levels were obtained by cyclic voltammetry. The various properties were further evaluated using a computational DFT study.

Key words: Organic material; Triazole; optoelectronics properties; DFT study.

Addendum Poster 99

A Chloro-Ligated Lindqvist Hexatungstate Stabilized by a Neutral Chloroalkylamine: Synthesis, Structural Elucidation, and Supramolecular Topology of $Na_3(C_5H_{13}NCl)[ClW_6O_{19}]$

Narmine Akremi (1), Msaadi Idia (1), Ibrahim Ayed (2) and Ali Rayes (1)

(1) Laboratory of Catalysis and Materials for the Environment and Processes LRCMEP (LR19ES08),
Faculty of Sciences of Gabes, University of Gabes, 6072, Tunisia
(2) Laboratory of Physical Chemistry of Materials (LR01ES19), Faculty of Sciences in Monastir,
Avenue de l'Environnement, Monastir, 5019, Tunisia

The functionalization of Lindqvist-type polyoxometalates through direct halide ligation to the metal–oxide core provides an effective route to tune their electronic structure, redox behavior, and supramolecular properties. Monosubstituted Lindqvist anions, $[XW_6O_{19}]^{n-}$, form a distinct subclass in which substitution of a terminal oxo ligand disrupts centrosymmetry, leading to anisotropic physicochemical characteristics. The use of neutral organic amines as structure-directing agents further expands crystal engineering possibilities without requiring protonation.

In this work, we report the reflux-assisted synthesis and comprehensive characterization of a new chloro-functionalized Lindqvist hexatungstate, $Na_3(C_5H_{13}NCl)[ClW_6O_{19}]$, incorporating a neutral chloroalkylamine molecule. Single-crystal X-ray diffraction confirms a monosubstituted $[ClW_6O_{19}]^{3-}$ core, where one W=O bond is replaced by W–Cl, inducing symmetry lowering while maintaining typical W–O bond distances. Charge neutrality is ensured by Na^+ cations, and the organic molecule contributes to crystal packing through hydrogen bonding and Cl-based interactions.

Hirshfeld surface analysis reveals dominant O···H contacts, followed by $Na^+\cdots O$ and Cl-related interactions. UV–Vis spectroscopy shows a red-shift of ligand-to-metal charge transfer bands relative to the parent cluster, attributed to W–Cl bonding and reduced symmetry, while high-energy bands confirm the W(VI) oxidation state.

These results demonstrate the accessibility of chloro-ligated Lindqvist clusters under mild conditions and highlight the role of neutral co-formers in stabilizing hybrid architectures. This approach offers new opportunities for designing asymmetrically functionalized polyoxometalates with potential applications in catalysis and molecular recognition.

Keywords: Chloro-substituted Lindqvist hexatungstate; functionalized polyoxometalate; neutral co-former; crystal engineering; halide ligation; supramolecular interactions; Hirshfeld analysis; UV–Vis spectroscopy.

Dibromoarylammonium-Stabilized Lindqvist Hexatungstate Dihydrate: Synthesis, Crystal Architecture, and Supramolecular Water Networks in $(C_7H_8NBr)_2[W_6O_{19}]\cdot 2H_2O$

Narmine Akremi (1), Ibrahim Ayed (2) and Ali Rayes (1)

(1) Laboratory of Catalysis and Materials for the Environment and Processes LRCMEP (LR19ES08),
Faculty of Sciences of Gabes, University of Gabes, 6072, Tunisia
(2) Laboratory of Physical Chemistry of Materials (LR01ES19), Faculty of Sciences in Monastir,
Avenue de l'Environnement, Monastir, 5019, Tunisia

The Lindqvist-type hexatungstate $[W_6O_{19}]^{2-}$ is a key isopolyoxometalate cluster composed of six edge-sharing WO_6 octahedra. In this work, we report the synthesis and structural characterization of a new hydrated hybrid compound, $(C_7H_8NBr)_2[W_6O_{19}]\cdot 2H_2O$, incorporating brominated methylanilinium cations. The compound was obtained via reflux of sodium tungstate dihydrate with a brominated 4-methylaniline derivative, followed by slow evaporation to yield single crystals.

Single-crystal X-ray diffraction confirms the integrity of the Lindqvist core with typical W–O distances. The structure consists of two protonated organic cations and two lattice water molecules per anion. Strong N–H···O hydrogen bonds connect the cations to terminal oxo ligands, while lattice water molecules generate extended O–H···O networks linking neighboring units into supramolecular chains. Additional stabilization arises from Br···O and Br···Br interactions. Hirshfeld surface analysis reveals dominant O···H contacts (≈ 42%), followed by Br···H and Br···O interactions. UV–Vis spectroscopy shows intense O→W LMCT transitions below 330 nm, consistent with a W(VI) framework.

These results highlight the cooperative role of hydrogen bonding, halogen interactions, and lattice water in directing supramolecular assembly in hydrated POM-based materials.

Keywords: Lindqvist hexatungstate; isopolyoxometalate; crystal engineering; hydrogen bonding; halogen interactions; Hirshfeld analysis.

List of Participants

Nr.	Last Name	First Name	Institution	Email	Ref.
1	ABDELHEDI	Imen	TCS / FST - Tunis	imen.abdelhedi@fst.utm.tn	**OC 01C**
2	ABDELKAFI	Mohamed Mouldi	TCS / FST - Tunis	mouldiabdelkafi@gmail.com	**-**
3	ABDELLAOUI	Hadir	FSM - Monastir	hadirabed7@gmail.com	**PC 1**
4	ABDELLAOUI	Mehdi	Claude Bernard University, Lyon 1, France	mehdi.abdellaoui@univ-lyon1.fr	**OC 01A**
5	ABDELLAOUI	Sourour	FST - Tunis	abdellaouisourour24@gmail.com	**PC 2 - 3**
6	ABIDI	Rym	TCS / FSB - Bizerte	abidi_rym@yahoo.fr	**-**
7	ACHOUR KHEDHIRI	Arwa	FSM - Monastir	achourkhedhiriarwa@gmail.com	**PC 4**
8	AFOUCHAL	Maouia	Mohammed 5 University, Rabat, Morocco	maouia_afouchal@um5.ac.ma	**-**
9	AISSA	Taissir	FST - Tunis	taissir.aiissa@gmail.com	**PC 5**
10	AKRETCHE	Soraya	Houari Boumediene University, Algiers, Algeria	kelfat.soraya@gmail.com	**PC 6**
11	ALAMI	Anouar	Sidi Mohamed Ben Abdellah University, Fès, Morocco	anouar.alami@usmba.ac.ma	**OC 04A**
12	ALLOUCHE	Noureddine	FSS - Sfax	noureddineallouche@yahoo.fr	**-**
13	ALOULOU	Hajer	IPEIG - Gabès	hajer.aloulou89@yahoo.fr	**OC 02C**
14	AMARA	Zacharias	Conservatoire National des Arts et Métiers, Paris, France	zacharias.amara@lecnam.net	**-**
15	AMMAR	Houcine	TCS / FSS - Sfax	houcine_fss@yahoo.fr	**-**
16	AMOR	Amal	FSG - Gabès	amalamor466@gmail.com	**OC 04B**
17	ARFAOUI	Aïcha	FST - Tunis	acha.arfaoui@gmail.com	**-**
18	ARSENIYADIS	Stellios	Queen Mary University, London, United Kingdom	s.arseniyadis@qmul.ac.uk	**Conf 6**
19	BAOUAB	Mohamed Hassen V	IPEIM - Monastir	hbaouab@yahoo.fr	**PC 7**
20	BARHOUMI	HOUCINE	FSM - Monastir	houcine.barhoumih@yahoo.com	**PC 8**
21	BARHOUMI SLIMI	Thouraya	TCS / ISSTE	thouraya.barhoumi@isste.ucar.tn	**-**
22	BELLAKHAL	Nizar	TCS / INSAT - Tunis	nizar_bellakhal@yahoo.fr	**-**
23	BELTAIEF MEDDEB	Imen	IPEIN - Nabeul	imen.beltaiefmeddeb@ipein.ucar.tn	**OC 12B - PC 9**
24	BEN AISSA	Cherifa	FSB - Bizerte	cherifabenaissa22@gmail.com	**PC 10 - 11**
25	BEN AMEUR	Raoudha	FSS - Sfax	raoudha.benameur@fss.usf.tn	**PC 12**
26	BEN AMMAR	Nour El Houda	CNRSM - Borj Cédria	nourelhouda.benammar@gmail.com	**PC 13**
27	BEN CHAABENE	Semy	TCS / FST - Tunis	semy.benchaabene@fst.utm.tn	**-**
28	BEN HAJ MBAREK	Asma	FSM - Monastir	asmabenhajmbarek@gmail.com	**OC 01B - PC 14**
29	BEN HAMOUDA	Sofiane	CRMN - Sousse	sofianebenhamouda819@gmail.com	**OC 04C**
30	BEN KHALIFA	Maryem	FSM - Monastir	maryembenkhalifa99@gmail.com	**OC 13B**
31	BEN NEJMA	Sadok Lamine	FSM - Monastir	sadekaminebennejma@gmail.com	**OC 08B**
32	BEN ROMDHANE	Asma	Faculty of Pharmacy - Monastir	asmaabenromdhane@gmail.com	**PC 15 - 16**

Nr.	Last Name	First Name	Institution	Email	Ref.
33	BEN SALAH	Hichem	FSS - Sfax	hichembensalah9@gmail.com	-
34	BEN SALEM	Ridha	TCS / FSS - Sfax	ridhabensalem@yahoo.fr	-
35	BEN SGHAIER	Rafika	CNRSM - Borj Cédria	rafika.bensghaier@gmail.com	-
36	BENAYACHE	Assia	Houari Boumediene University, Algiers, Algeria	assiaben90@gmail.com	**PC 17**
37	BENBRAIEK	Insaf	FSM - Monastir	insafbenbrik@gmail.com	**OC 15C**
38	BESBES	Rafâa	FST - Tunis	rafaa.besbes@fst.utm.tn	-
39	BESSAYADIA	Salem	FSM - Monastir	bessayadiasalem@gmail.com	-
40	BEYAOUI	Ahlem	FSM - Monastir	ahlemm.beyaoui@gmail.com	**OC 02A - PC 18**
41	BHIRI	Fatma	FSM - Monastir	fatmabhiri4@gmail.com	**OC 03C**
42	BOLTANE	Khouloud	FST - Tunis	khouloud.boltane@fst.utm.tn	**PC 19**
43	BOUBAKRI	Lamia	ISSTE - Borj Cédria	boubakri_lamia@yahoo.co.uk	**OC 17A - PC 20**
44	BOUBAKRI	Saber	CERTE - Borj Cédria	boubakrisaber772@gmail.com	**PC 21**
45	BOUCHOUK	Djamel	Mohamed Cherif Messaadia University, Souk Ahras, Algeria	d.bouchouk@univ-soukahras.dz	**PC 22**
46	BOUFI	Sami	University of Sfax, Tunisia	sami.boufi@fss.rnu.tn	**Conf 9**
47	BOUGARECH	Abdelkader	FSS - Sfax	abdelkader.bougarech@fss.usf.tn	-
48	BOUHARB	Narjess	IPEIM - Monastir	narjessbouharb57@gmail.com	**OC 14B**
49	BOUSSANDEL	Sirine	FSB - Bizerte	sirine.boussandel@etudiant.univ-rennes.fr	**PC 23**
50	BOUZAYANI	Nadia	FSM - Monastir	nbouzayani@novalix.com	**PC 24**
51	BRIKI	Sirine	FST - Tunis	brikisirine0@gmail.com	**PC 25**
52	CHAARI	Islem	CNRSM - Borj Cédria	islem.chaari@cnrsm.rnrt.tn	**PC 26**
53	CHAOUACHI	Bechir	TCS / ENIG - Gabès	bechir.chaouachi@enig.rnu.tn	-
54	CHARRADI	Khaled	CERTE - Borj Cédria	charradikaled2010@gmail.com	**PC 27**
55	CHEIKHROUHOU	Wafa	Centre of Biotechnology - Borj Cédria	cheikhrouhouw@gmail.com	**PC 28**
56	CHELLI LAKHDAR	Saloua	Paul Sabatier University, Toulouse, France	saloua.chelli-lakhdar @utoulouse.fr	**PC 29**
57	DAMMAK	Mohamed	FSS - Sfax	meddammak@yahoo.fr	-
58	DELAITE	Christelle	Haute Alsace University, Mulhouse, France	christelle.delaite@uha.fr	**Conf 7**
59	DGACHI	Youssef	FSS - Sfax	youssefdgachi@gmail.com	**PC 30**
60	DIXNEUF	Pierre Henry	University of Rennes, Rennes, France	pierre.dixneuf@univ-rennes.fr	**Conf 10**
61	DRIDI	Amal	FST - Tunis	amal.dridi@etudiant-fst.utm.tn	**OC 03A**
62	EFRIT	Mohamed Lotfi	TCS / FST - Tunis	medlotfi.efrit@fst.utm.tn	-
63	EL GHALI	Siwar	FSM - Monastir	siwarelghali98@gmail.com	**PC 31**
64	EL GUESMI	Nizar	CRMN - Sousse	nizar.elguesmi@fsm.rnu.tn	**PC 32**
65	ELAISSI	Ameur	Faculty of Pharmacy - Monastir	aelaissi@yahoo.fr	**PC 33 - 34**
66	ELAKREMI	Manel	FSG - Gafsa	manel.elakremi@yahoo.com	**PC 35**

Nr.	Last Name	First Name	Institution	Email	Ref.
67	ELBIRGUI	Kaouthar	Hassan II University, Casablanca, Morocco	kaouthar.elbirgui@gmail.com	**OC 16A**
68	ELMARY	Pierre	Claude Bernard University, Lyon 1, France	pierre.elmary@univ-lyon1.fr	**OC 05A**
69	ELNADI	Hanan	FST - Tunis	hananalnadi6@gmail.com	**OC 15B - PC 36**
70	ESSAFI	Wafa	INRAP - Sidi Thabet	essafi.wafa@inrap.rnrt.tn	**OC 13C**
71	ESSID	Kamel	FSS - Sfax	kamelessid.issat@yahoo.fr	**PC 37 - 38**
72	FATNASSI	Ameni	ENIG - Gabès	amenifatnassi1996@gmail.com	**PC 39 - 40**
73	FERJANI	Mohamed	FSM - Monastir	ferjeeni.mouhamed.fm@gmail.com	**PC 41**
74	FNENA	Kamel	FSG - Gafsa	chimiphy@yahoo.fr	**PC 42**
75	GAMOUDI	Safa	IPEIM - Monastir	safagamoudi@gmail.com	**-**
76	GARCI	AMINE	INRAP - Sidi Thabet	garci1amine@gmail.com	**-**
77	GASMI	Nesrine	FSG - Gafsa	nesrinegasmi.g@gmail.com	**OC 10C - PC 43**
78	GHABI	Amira	FSM - Monastir	ghabiamira12@gmail.com	**PC 44**
79	GHAMMAGUI	Fatma	FSG - Gabès	ghammaguifatima339@gmail.com	**OC 11C - PC 45**
80	GHORBALI	Rihab	FSM - Monastir	gorbalirihab2020@gmail.com	**PC 46**
81	GUITTARD	Frédéric	University of Nice, France	frederic.guittard@univ-cotedazur.fr	**Conf 4**
82	HALOUI	Abir	FST - Tunis	abir.haloui@fst.utm.tn	**PC 47**
83	HAMDI	Naceur	ISSTE - Borj Cédria	hamdi.naceur@isste.ucar.tn	**PC 48 - 49**
84	HAMDI	Rim	FSM - Monastir	rimhamdi1997@gmail.com	**OC 18A**
85	HAMMAMI	Nozha	FSS - Sfax	nozhahammami85@gmail.com	**PC 50**
86	HAMMI	Halim	TCS / CNRSM - Borj Cédria	halimhammi2015@gmail.com	**-**
87	HAN	Lulu	Claude Bernard University, Lyon1, France	hll121525@163.com	**OC 06A**
88	HEDHILI	Lassaad	IPEIM - Monastir	lassaad.hedhili@ipeim.u-monastir.tn	**-**
89	HEDHLI	Amel	FSM - Monastir	hedhli.amel.fsm@gmail.com	**OC 07A**
90	HIDOURI	Mustapha	TCS / ISSAT - Gabès	mustapha.hidouri@laposte.net	**-**
91	HILELI	Anwar	FSG - Gafsa	anwarhl173@gmail.com	**OC 16B - PC 51**
92	HLIMI	Haythem	FSM - Monastir	hlimihaythem1@gmail.com	**OC 05C - PC 52**
93	HORCHANI	Mabrouk	FST - Tunis	horchani.mabrouk@gmail.com	**OC 09B - PC 53**
94	HOVEYDA	Amir H.	Boston College, United States	amir.hoveyda@bc.edu	**Conf 2**
95	HRIZ	Khaled	FSM - Monastir	khaledhriz@gmail.com	**PC 54**
96	JEBLI	Nejib	ISSH - Jendouba	nejib.jebli@yahoo.com	**OC 09A**
97	JEDIDI YAICH	Belsem	FST - Tunis	j.belsem@yahoo.fr	**PC 55 - 56**
98	JEMMALI	Wihed ElQods	FSM - Monastir	wihedjemmali@gmail.com	**PC 57 - 58**
99	JENDOUBI	Ons	FSM - Monastir	jendoubions.hs@gmail.com	**OC 02B - PC 59**
100	JMAI	Momtez	FST - Tunis	momtez.jmai@fst.utm.tn	**OC 10A - PC 60**

Nr.	Last Name	First Name	Institution	Email	Ref.
101	KACEM	Yakdhane	FSM - Monastir	kacemyakdhane@gmail.com	**PC 61**
102	KADRI	Naka	FSS - Sfax	nakakadri98@gmail.com	**PC 62**
103	KAOUACH	Aicha	FSM - Monastir	kaouach893@gmail.com	**OC 11A - PC 63**
104	KHALDI	Rania	FSM - Monastir	raniakhaldi24@gmail.com	**OC 17B**
105	KRAIEM	Jamil	Faculty of Pharmacy - Monastir	jamilkraiem@gmail.com	**PC 64**
106	KRISSAANE	Nadia	FST - Tunis	krissaane.nadia@etudiant-fst.utm.tn	**OC 12A**
107	KSIKSI	Regaya	FST - Tunis	rksiksi@gmail.com	**PC 65**
108	LAAJIMI	Imed	Tunisian Chemical Society	imed.laajimi@fst.utm.tn	**-**
109	LACOUR	Jérôme	University of Geneva, Switzerland	Jerome.Lacour@unige.ch	**Conf 1**
110	LAHMER	Yoldez	INSAT - Tunis	yoldezlahmer2@gmail.com	**PC 66**
111	LAKHDAR	Sami	University of Toulouse, France	sami.lakhdar@univ-tlse3.fr	**-**
112	LAMOUDI	Lynda	Houari Boumediene University, Algiers, Algeria	lamoudilynda@gmail.com	**PC 67**
113	LATROUS	Latifa	TCS / IPEIEM - El Manar	latifa.latrous@ipeiem.utm.tn	**-**
114	LEJMI	Maïssa	Faculty of Pharmacy - Monastir	maissa.lejmi0098@gmail.com	**OC 03B - PC 68**
115	MACHERKI	Ameni	FSM - Monastir	amenimacherki@gmail.com	**OC 06C**
116	MANNAI	Faten	FSG - Gafsa	mannai_faten@yahoo.com	**PC 69**
117	MATYJASZEWSKI	Krzysztof	Carnegie Mellon University, Pittsburgh, USA	km3b@andrew.cmu.edu	**Conf 3**
118	MEGRICHE	Adel	TCS / FST - Tunis	adel.megriche@fst.utm.tn	**-**
119	MELIANI	Habib	Djillali Liabes University; Sidi Bel Abbes; Algeria	melianihabib@gmail.com	**PC 70**
120	MEZGHANI JARRAYA	Raoudha	FSS - Sfax	raoudha.jarraya@fss.usf.tn	**-**
121	MEZNI	Dorsaf	FSB - Bizerte	meznidorsaf2@gmail.com	**OC 19A - PC 71**
122	MISSAOUI	Takwa	FST - Tunis	missaouitakwa5@gmail.com	**PC 72**
123	MNIF	Amine	TCS / FST - Tunis	amine.mnif@fst.utm.tn	**-**
124	MOUSSAOUI	Younes	TCS / FSG - Gafsa	y.moussaoui2@gmail.com	**-**
125	MRABET	Molka	FSM - Monastir	molka17.mrabet@gmail.com	**OC 14C**
126	NAJAHI	Amira	FSS - Sfax	najahiamira1@gmail.com	**PC 73**
127	NAMOUSSA	Tedjani Yahia	Shahid Hama Lakhdar University, El Oued, Algeria	namoussa-tedjaniyahya@univ-eloued.dz	**PC 74**
128	NASRI	Khawla	FSM - Monastir	mohamedmbarek99@yahoo.fr	**PC 75**
129	NGOM	Ibrahima	FST - Tunis	ibrahima.ngom@etudiant-fst.utm.tn	**OC 18B - PC 76**
130	OUESLATI	Mohamed Habib	IPEIB - Bizerte	ouesmed74@gmail.com	**PC 77 - 78**
131	PEGORETTI	Alessandro	University of Trento, Italy	alessandro.pegoretti@unitn.it	**Conf 11**
132	RAIS	Fayçal	IPEIK - Kairouan	faicelrais@yahoo.fr	**PC 79**
133	RAMANAVICIENE	Almira	Vilnius University, Lithuania	almira.ramanaviciene@chf.vu.lt	**PC 80**
134	RAMANAVICIUS	Arunas	Centre for Physical Sciences & Technology (FTMC), Vilnius, Lithuania	arunas.ramanavicius@chf.vu.lt	**OC 16C**

Nr.	Last Name	First Name	Institution	Email	Ref.
135	RAMANAVICIUS	Simonas	MB Sensografa, Vilnius, Lithuania	simonas.ramanavicius@gmail.com	**PC 81**
136	RAMANAVICIUTE	Agne	MB Sensografa, Vilnius, Lithuania	agneramanaviciute@gmail.com	**PC 82**
137	RAMMEH	Mohamed Mehdi	TCS / FSM - Monastir	mehdiram@yahoo.fr	**-**
138	RIAHI	Mouna	FST - Tunis	mounariahichammem@gmail.com	**PC 83**
139	RJILI	Mohamed	FST - Tunis	mohamed.rjili@fst.utm.tn	**OC 07C**
140	ROMDHANE	Ons	FSM - Monastir	onsromdhane99@gmail.com	**OC 19B - PC 84**
141	SAAD	Ali	Publisher, Springer Nature	ali.saad@springernature.com	**Tech. Talk**
142	SAIDANI	Dhia	FSB - Bizerte	saidanidhia71@gmail.com	**OC 13A - PC 85**
143	SAIDI	Ilyes	FSM - Monastir	sisoelyesaidi@live.fr	**OC 06B**
144	SALAH	Ons	FST - Tunis	ons.salah@etudiant-fst.utm.tn	**PC 86**
145	SALHI	Slim	FSS - Sfax	slim.salhi@fss.usf.tn	**-**
146	SALHI	Sourour	FSS - Sfax	souroursalhi10@gmail.com	**OC 05B - PC 87**
147	SAMARAT	Ali	FSB - Bizerte	ali.samarat@gmail.com	**-**
148	SCHREINER	Peter R.	University of Giessen, Germany	prs@uni-giessen.de	**Conf 8**
149	SCHULLER	Anne-Sophie	University of Haute-Alsace, Mulhouse, France	anne-sophie.schuller@uha.fr	**OC 08C**
150	SELLAMI	Dina	FSS - Sfax	dina.sellami.etud@fss.usf.tn	**OC 12C - PC 88**
151	SIZIANI	Dhaouya	National School of Advanced Technologies, Algiers, Algeria	dhaouya.siziani@ensta.edu.dz	**PC 89**
152	SLAMA	Takwa	FSM - Monastir	takwaslama200@gmail.com	**OC 14A**
153	SMAIL	Fatima	National Higher School of Advanced Technologies, Algiers, Algeria	fatima.smail@ensta.edu.dz	**PC 90**
154	SMATI	Houda	FSM - Monastir	smatihouda2495@gmail.com	**PC 91**
155	TALBI	Imen	Novalix Tunisia	italbi@novalix.com	**OC 15A**
156	THIAM	El Waleda	University of Nouakchott, Mauritania	el-waleda.thiam@univ-lorraine.fr	**PC 92**
157	TKA	Najeh	FSM - Monastir	najeh_tka@yahoo.fr	**OC 10B - PC 93**
158	TLILI	Anis	Claude Bernard University, Lyon 1, France	anis.tlili@univ-lyon1.fr	**Conf 5**
159	TOUJ	Nedra	ISSTE - Borj Cédria	toujnedra@gmail.com	**PC 94**
160	WAHBI	Aymen	FSB - Bizerte	wahbi.aymen@gmail.com	**PC 95**
161	YAHYA	Ahlem	FSG - Gafsa	ahlemyahyaa@gmail.com	**OC 11B - PC 96**
162	YAKOUBI	Chadia	FST - Tunis	chedia.yaakoubi@etudiant-fst.utm.tn	**OC 07B**
163	YANG	Yi	Claude Bernard University, Lyon1, France	18321122152@163.com	**OC 08A**
164	ZNATI	Mansour	FSM - Monastir	znatimansour@yahoo.fr	**-**
165	ZOUARI	Sami	ENIS - Sfax	sami.zouari@enis.tn	**-**
166	ZOUIDI	Imen	FSG - Gafsa	hajerzwidi@gmail.com	**OC 09C - PC 97**
167	ZRIDA	Habiba	FSM - Monastir	zridahabiba@gmail.com	**PC 98**
168	AKREMI	Narmine	FSG - Gabès	rayesali1969@gmail.com	**PC 99 - 100**