Preamble

Heterocyclic chemistry has always known considerable growth thanks to the relevance of the heterocyclic compounds in practical applications, particularly in the fields of medicine, pharmacology, agrochemicals, electronics, polymers, organic conductive materials, corrosion inhibitors, pigments, dyes, and so on and so forth.

It is in this context that the 9th Trans Mediterranean Colloquium on Heterocyclic Chemistry is organized **Under the High Patronage of His Majesty King Mohammed VI**, by the presidency of Sidi Mohamed Ben Abdellah University, the Laboratory of Organic Chemistry of the Faculty of Science Dhar El Marhaz, in cooperation with the Scientific Committee of TRAMECH and with the sponsorship of the International Union of Pure and Applied Chemistry (IUPAC).

The main objectives of this conference are:

- Presentation of the latest research in the field of heterocyclic chemistry.
- Strengthening and development of the mobility of students and PhD students between the Mediterranean countries.
- Encouraging the exchange of new ideas and application experiences.
- Creating new partnerships with the industrial world to develop joint projects.
- Building networks for future research and partnership collaboration between international research / educational institutions.
- To highlight the contribution of chemistry for qualifying of human resources for the sustainable development of society
- Publication of the main results presented at this conference in the internationally indexed database Scopus.

This meeting is open to all national and international scientists from universities and industry interested in various aspects of heterocyclic chemistry, such as:

- New approaches to the synthesis of heterocyclic compounds.
- New heterocyclic compounds of pharmaceutical and agrochemical interest.
- Drug design.
- Applications to organic materials and nanomaterials.
- Study of different physical and chemical aspects of heterocyclic compounds.
- Sensitization of the world of industry on important chemical applications.
- Economic and environmental problems in connection with this chemistry.
- New chemistry for a sustainable development.
- Chemistry and knowledge economy.

As chairman of the 9th Transmediterranean Colloquium on Heterocyclic Chemistry (TRAMECH IX) and on behalf of the organizing committee, I have the great pleasure to warmly welcome you to Fez for this major event.

For its strong support for TRAMECH IX, I would like to thank the Presidency of Sidi Mohamed Ben Abdellah University. I also thank the Deanship of the Faculty of Science Dhar El Marhaz, the Deanship of the Faculty of Sciences and Technology and our partner's institutions:

- Faculty of Science and Technology
- Higher Normal School
- Thematic Pole of Research of SMBA University "Biotechnology"
- Thematic Pole of Research of SMBA University "Health, biomedical research, biomolecules and quality of Health",
- Thematic Pole of Research of SMBA University "Medicinal and Aromatic Plants"
- Thematic Pole of Research of SMBA University "Water and Environment"

and the TRAMECH IX sponsors.

TRAMECH IX will allow us to host **250** participants from **53** universities and research centers around the world, including **8** Moroccan universities, and to attend the opening conference given by **Professor Ei-Ichi Negishi (Winner of the 2010 Nobel Prize in Chemistry)**, **16** Plenary lectures, **12** Invited Lectures, **27** Short Talks, **190 Poster presentations**, and a round table on the development of scientific research in the field of heterocyclic chemistry. In addition, 2 short talks prizes and 2 posters prizes will be awarded.

We wish all TRAMECH IX participants a rewarding and memorable scientific meeting and a pleasant stay in the spiritual capital of Morocco.

TRAMECH IX Chairman

Professor Anouar Alami
Laboratory of Organic Chemistry-Faculty of Science Dhar El Mahraz
Sidi Mohamed Ben Abdellah University
Fez-Morocco

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Aziz Atmani	Former Director of the CURI, USMBA
Ahmed Iraqi	Honorary Dean

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Scientific Program with Short Biography of Plenary and Invited Speakers

Tuesday 21 November 2017	
Afternoon	
14:30 – 18:30	**Registration of participants** **Entrance hall of the Hotel Zalagh Park Palace**

Wednesday 22 November 2017	
Morning	
8:45 – 9:00	**Introductory presentation & start of the Scientific program of TRAMECH IX** **Florio Saverio & Alami Anouar** **Conference room "Thousand and One Nights"**
Session 1 – **Conference room "Thousand and One Nights"** **Moderators & Rapporteurs: Abdelali Kerbal & Branko Stanovik**	
9:00 – 9:30	**Plenary Lecture 1** **Lutz Friedjan Tietze** (**University of Göttingen – Germany**) Domino Reactions. The Green and Economical Art of Chemical Synthesis
9:40 – 10:10	**Plenary Lecture 2** **Abdelilah El Hallaoui** (**Sidi Mohamed Ben Abdellah University, Fez-Morocco**) Precursors and Derivatives of Heterocyclic Amines and Heterocyclic Amino acids. Synthesis – Study of Biological and Electrochemical Properties
Session 2 – **Conference room "Thousand and One Nights"** **Moderators & Rapporteurs: Belkheir Hammouti & Abdesslam Bentama**	
10:20 – 10:40	**Invited Lecture 1** **Stellios Arseniyadis** (**Queen Mary, University of London – United Kingdom**) New Developments in the Field of Pd-AAA
10:50 – 11:10	**Invited Lecture 2** **José Miguel Sansano Gil** (**University of Alicante – Spain**) Enantioselective Synthesis of Prolinates as Key Precursors of Bioactive Heterocycles
11:20 – 11:40	**Coffee break**
Session 3 – **Conference room "Thousand and One Nights"** **Moderators & Rapporteurs: Panayiotis Koutentis & Ahmed Iraqi**	
11:40 – 12:10	**Plenary Lecture 3** **Piotr Kaszyński** (**University of Vanderbilt – Poland**) Functional Materials Derived from π-Delocalized Radicals for Photovoltaics And Spintronic
12:20 – 12:50	**Plenary Lecture 4** **Metin Balci** (**Middle East Technical University, Ankara – Turkey**) Gold-Catalyzed and Base-Supported Cyclization Reactions of N-Propargylated Pyrrole, Indole and Benzene Derivatives: Synthesis of Heterocycles with New Scaffolds

Wednesday 22 November 2017	
Afternoon	
Session 4 _____ Conference room "Thousand and One Nights" **Moderators & Rapporteurs: Bahia Bennani & Ata Martin Lawson**	
15:15 – 15:45	**Plenary Lecture 5** **Dusan Berkes (University of Technology, Bratislava – Slovakia)** 3-Indolylglycines and γ-Oxo-α-Amino Acids as 1,3-Bifunctional Nucleophiles in the Synthesis of Heterocycles
15:55 – 16:-35	**Short Talks**
Session 5 _____ Conference room "Thousand and One Nights" **Moderators & Rapporteurs: Maria Emília da Silva Pereira de Sousa & Abderahim Lahrach**	
15:55 – 16:05	**Short Talk -1** **El Mostapha Rakib (Sultan Moulay Slimane University, Beni Mellal – Morocco)** Synthesis of new heterocyclic compounds based on N-N-cyclic azomethine imine scaffold
16:10 – 16:20	**Short Talk-2** **Mohamed Othman (University of Havre-Normandie – France)** New Development Around N-Acyliminium Ions Chemistry
16:25 – 16:35	**Short Talk-3** **Dahmane Tebbani (University of the Mentouri-Constantine Brothers, Algeria)** New Adamantyl Chalcones: Synthesis, Antimicrobial and Anticancer Activities

17:20–18:00	**Official Opening Ceremony** **Opening speech** **- Mr. Secretary of State in charge of Higher Education and Scientific Research** **- Mr. President of Sidi Mohamed Ben Abdellah University** **- Mr. Dean of the Faculty of Science Dhar El Mahraz** **- Mr. Dean of the Faculty of Sciences and Technology** **- Mr. President of Moroccan Group of Heterocyclic Chemistry** **- Mr. Chairman of the TRAMECH IX-Morocco**
Opening Scientific Session _____ Conference room "Thousand and One Nights" **Scientific Moderator: Saverio Florio**	
18:00 – 19:00	**Opening Conference** **Ei-Ichi Negishi (Purdue University, Indiana, USA "Winner of the Nobel Prize in Chemistry in 2010")** Magical Power of d-Block Transition Metals as Demonstrated by Catalytic Asymmetric C–C Bond Formation
19:00 – 19:30	**Coffee break**

Thursday 23 November 2017	
Morning	
Session 6_____**Conference room "Thousand and One Nights"** **Moderators & Rapporteurs: Lutz Friedjan Tietze & Mohamed El Yazidi**	
8:45 – 9:15	**Plenary Lecture 6** **Athina Geronikaki** (**University of Thessaloniki – Greece**) Synthesis and Biological Evaluation of Novel Substituted 2-[(5-Adamantane-1-yl) 1,3,4-Thiadiazol-2-yl) Imino]-5 Thiazolidinones
9:25 – 9:55	**Plenary Lecture 7** **François Couty** (**University of Versailles-St-Quentin-en-Yvelines – France**) From Azetidines to Orthogonal « Click » Reactions
Session 7_____Conference room "Thousand and One Nights" **Moderators & Rapporteurs: El Mokhtar Essassi & Abdelaziz Zerouale**	
10:05 – 10:25	**Invited Lecture 3** **Asuncion Barbero** (**University of Valladolid – Spain**) Access to Different Sized Heterocycles via Silyl-Prins Cyclization
10:35 – 10:55	**Invited Lecture 4** **Maria do Amparo Ferreira Faustino** (**University of Aveiro – Portugal**) Recent Development on Porphyrinic Chemistry and Applications
10:55 – 11:25	**Coffee break & Poster session 1 (PP01-PP37)**
Session 8_____Conference room "Thousand and One Nights" **Moderators & Rapporteurs: Mustapha Taleb & Mohamed Othman**	
11:25 – 11:55	**Plenary Lecture 8** **El Mokhtar Essassi** (**Mohamed V University – Morocco**) Recent Advances in Ring Transformations of Heterocyclic Compounds
12:05 – 12:35	**Plenary Lecture 9** **José Maria Lassaletta** (**Spanish National Research Council – Spain**) Atroposelective Synthesis of Axially Chiral Heterobiaryls

Thursday 23 November 2017	
Afternoon	
Session 9_____Conference room "Thousand and One Nights" **Moderators & Rapporteurs: Metin Balci & Adil Benjelloun Touimi**	
15:00 – 15:30	**Plenary Lecture 10** **Hamdullah Kilic** (**Atatürk University – Turkey**) Mechanistic Studies on the Epoxidation and Aziridination Reactions

15:40 – 16:10	**Plenary Lecture 11** **Adam Daïch** (**University of Havre – France**) Diversity in Aza-Heterocyclic Systems based on Tandem/Domino Reactions Involving Ionic Species
16:20 – 16:50	**Plenary Lecture 12** **Hussein El-Kashef** (**Assiut University – Egypt**) Synthetic Approaches for New Pyrazoles
17:00 – 17:20	**Invited Lecture 5** **Maria Emília da Silva Pereira de Sousa** (**University of Porto – Portugal**) Marine-Fungi Natural Products as Models for New Antibacterial Agents
17:25 – 17:50	**Coffee break & Poster session 2 (PP38-PP75)**
17:50 – 18:30	**Short Talks (Two sessions)**
Session 10_____Conference room "Thousand and One Nights" (Room A) **Moderators & Rapporteurs : Wafaa Abdou & Mouhcine Sfaira** **Session 11_____Conference room "Cabotine" (Room B)** **Moderators & Rapporteurs: Zakia Rais & Hamdullah Kilic**	
17:50 – 18:00	**Short Talk-4** **Asmae Mahfoud (Sidi Mohamed Ben Abdellah University, Faculty of Sciences Dhar El Mahraz, Fez-Morocco) –** (Room A) Synthesis of New Heterocyclic Compounds Based on (E)-2-Methyl-3-Arylidene Chroman-4-Ones
	Short Talk-5 **Mouad Filali (Sidi Mohamed Ben Abdellah University, Faculty of Science and Technology, Fez, Morocco) –** (Room B) Synthesis of Novel Heterocyclic Ligands Based of 3,6-Bis (Pyridin-2'-yl) Pyridazine and Evaluation of Their Antibacterial and Antioxidant Activities
18:05 – 18:15	**Short Talk-6** **Özdemir Dogan (Middle East Technical University, Ankara – Turkey) –** (Room A) Catalytic Asymmetric Synthesis of Pyrrolidine Derivatives
	Short Talk-7 **Meriem Fardioui (Moroccan Foundation Advanced Science, Innovation and Research, Rabat – Morocco) –** (Room B) Bio-active films based on styrylquinoxaline-grafted-Chitosan: Antibacterial and Fluorescent studies
18:20 – 18:30	**Short Talk-8** **Taoufik Akabli (Sidi Mohamed Ben Abdellah University, Polydisciplinary Faculty of Taza, Fez-Morocco) –** (Room A) 2D-QSAR and Pharmacophore Studies on N9-Substituted Harmine Derivatives as Potential Anticancer Agents
	Short Talk-9 **Jalal Isaad (Mohammed 1st University, Faculty of Science and Technologie, Al-Hoceima – Morocco)** (Room B) Green Synthesis of New Dyes Based on Pyrazolone Derivatives

Friday 24 November 2017	
Morning	
Session 12 Conference room "Thousand and One Nights" **Moderators & Rapporteurs: Carmen Najera & Fouad Ouazzani Chahdi**	
8:45 – 9:15	**Plenary Lecture 13** **Youssef Kandri Rodi** (Sidi Mohamed Ben Abdellah University, Fez, Morocco) Conception to the Biological and Anti-Corrosive Evaluation of New Organic and Heterocyclic Systems in the Laboratory " LCOA"
9:25 – 9:55	**Plenary Lecture 14** **Florio Saverio** (University of Bari Aldo Moro – Italy) Oxiranyllithiums: from Fleeting, Elusive Intermediates to Powerful Synthons
Session 13 Conference room "Thousand and One Nights" **Moderators & Rapporteurs: Lachkar Mohammed & Mehdi Chaouch**	
10:05 – 10:25	**Invited Lecture 6** **Damien Prim** (Lavoisier Institute of Versailles – France) A Unique Strategy-Several Topologies: Selected Examples of Helical, Twisted, Angular and Planar Architectures
10:35 – 10:55	**Invited Lecture 7** **Fawaz Aldabbagh** (Kingston University, London –United Kingdom) H_2O_2-HX in the Synthesis of Heterocyclic Quinones
11:05 – 11:30	**Coffee break & Poster session 3 (PP76-PP113)**
Session 14 Conference room "Thousand and One Nights" **Moderators & Rapporteurs: Artur Silva & Fatima Lamchouri**	
11:30 – 12:00	**Plenary Lecture 15** **Nativi Cristina** (University of Florence – Italy) The Cycloaddition Way to Saccharidic Anti-Pathogens

Friday 24 November 2017	
Afternoon	
Session 15 Conference room "Thousand and One Nights" **Moderators & Rapporteurs: El Mostapha Rakib & Mokhtar Fodili**	
15:30 – 16:00	**Plenary Lecture 16** **Victor de Freitas** (University of Porto, Porto – Portugal) Chemical and Physico-Chemical Properties of Flavylium Derivative Compounds: Putative Industrial Applications
16:10 – 16:30	**Invited Lecture 8** **Serge Thorimbert** (University Pierre and Marie Curie – France) Heterocycles : from Reactivity to Diversity

16:30 – 17:05	**Coffee break & Poster session 4 (PP114-PP150)**
17:05 – 18:00	**Short Talks (Two sessions)**
Session 16_____Conference room "Thousand and One Nights" (Room A) **Moderators & Rapporteurs : Hussein El-Kashef & Brahim Labriti** **Session 17**_____Conference room "Cabotine" (Room B) **Moderators & Rapporteurs: Nurllah Saracoglu & Mohamed Amari**	
17:05 – 17:15	**Short Talk-10** **Wafaa M. Abdou (National Research Centre, Cairo –Egypt)** – (Room A) Bisphosphonic Acids: New Therapeutic Players In Oncology
	Short Talk-11 **Seda Cinar (Hacettepe University, Ankara – Turkey)** – (Room B) A Novel Approach to the Synthesis of Alkyl-Substituted A3B Porphyrins
17:20 – 17:30	**Short Talk-12** **Hamid Elmouli (Cadi Ayyad University, Polydisciplinary Faculty of Safi – Morocco)** – (Room A) Polyethylenimines-Supported Catalysts for Copper(I)- Catalyzed Azide-Alkyne Cycloaddition Click Reactions in Aqueous Solvent
	Short Talk-13 **Mohammed Bakhouch (Sidi Mohamed Ben Abdellah University, Faculty of Sciences Dhar El Mahraz, Fez-Morocco)** – (Room B) Thioaurones as Synthons Towards Novel Heterocyclic Systems
17:35 – 17:45	**Short Talk-14** **Gönül Yapar (Istanbul Technical University, Istanbul - Turkey)** – (Room A) The Synthesis of New Bis(Morpholinophenoxy)Ethylene Glycol Podands and Investigation of Their Cation Recognition
	Short Talk-15 **Siham El Arrouji (Sidi Mohamed Ben Abdellah University, Faculty of Sciences Dhar El Mahraz, Fez-Morocco)** – (Room B) Evaluating Corrosion Inhibition Property of Some Pyrazole Derivatives for Mild Steel in 1M HCl: Insight from Electrochemical and Quantum Studies
17:50 –18:00	**Short Talk-16** **Yassir Filali Baba (Sidi Mohamed Ben Abdellah University, Faculty of Science and Technology, Fez, Morocco)** – (Room A) Synthesis, Biological Evaluation, and Characterization by NMR and X-Ray of Some Novel of 2-Oxo-1,2-Dihydroquinoline-4-Carboxylic Acid Derivatives
	Short Talk-17 **Morad Lamsayah (Mohammed 1st University, Faculty of Science, Oujda – Morocco)** – (Room B) Liquid–Liquid Extraction of Metal Ions by New Synthesized Pyrazole & Triazole N-Ligands, High Selectivity For Fe And Pb With TD-DFT Theorical Calculation
18:05 – 18:15	**Short Talk-18** **Mohammed Aarjane (Moulay Ismail University, Faculty of Science, Meknes, Morocco)** – (Room A) Synthesis and Antibacterial Study of Novel Acridone Derivatives Containing 1,2,3-Triazole
	Short Talk-19 **Cihangir Tanyeli (Middle East Technical University, Ankara–Turkey)**– (Room B) Organocatalytic Asymmetric Synthesis of Dihydronaphthofurans via Friedel-Crafts / Substitution Domino Type Reaction

Saturday 25 November 2017	
Morning	
Session 18_____Conference room "Thousand and One Nights" **Moderators & Rapporteurs : Cristina Nativi & Abdelhadi Lhassani**	
9:00 – 9:30	**Invited Lecture 9 (special topic)** **Mario Schiavoni** (Hemophilia and Rare Coagulopathies Centre – Italy) A New Era for Anticoagulant Agents: From Pharmaceutical Research to Clinical Setting
9:40 – 10:00	**Invited Lecture 10** **Islam Ullah Khan** (College University, Lahore – Pakistan) Bi-Aryl Pyrimidines: Potent Biologically Active Pharmacophores
Session 19_____Conference room "Thousand and One Nights" **Moderators & Rapporteurs : Mohamed Merzouki & José Maria Lassaletta**	
10:10 – 10:30	**Invited Lecture 11** **Ettaybi Mohamed** (Sidi Mohamed Ben Abdellah University, Fez-Morocco) Chemical genomics platforms for the discovery of bioactive compounds and understanding their mechanism of action
10:40 – 11:00	**Invited Lecture 12** **Arthur Silva** (University of Aveiro, Aveiro, Portugal) Chromones bearing unsaturated substituents at C-2 and C-3 as building blocks in cycloaddition and conjugate addition reactions
11:05 – 11:30	**Coffee break & Poster session 5 (PP151-PP188)**
11:30 – 12:10	**Short Talks (Two sessions)**
Session 20_____Conference room "Thousand and One Nights" (Room A) **Moderators & Rapporteurs : Ghali AlHouari & Dahmane Tebbani** **Session 21**_____Conference room "Cabotine" (Room B) **Moderators & Rapporteurs: Şirin Gülten & Hassane Faraj**	
11:30 – 11:40	**Short Talk-20** **Nurettin Menges (Yuzuncu Yil University, Van – Turkey) –** (Room A) Bicyclic Imidazole Skeletons via Alkyne Cyclization
	Short Talk-21 **Mohamed Adardour (Cadi Ayyad University, Semlalia Science Faculty, Marrakech – Morocco) –** (Room B) Synthesis of New Polyheterocyclic Systems by 1,3-Dipolar Cycloaddition Reactions
11:45 – 11:55	**Short Talk-22** **Rachid Azzallou (Laboratory of Biochemistry, Environment & Agri-food, Hassan II University, Mohammedia, Morocco) –** (Room A) Efficient and Green Synthesis of 2,3-Dihydroquinazolin-4(1*H*)-Ones Using Animal Bone Meal as a New Biocatalyst in Water
	Short Talk-23 **Naoual Habbati (Ibn Tofail Univrsity, Faculty of Science, Kenitra–Morocco) –** (Room B) Theoretical Study of Some Oxadiazoles Derivatives and their Iron Complexes in Corrosion Inhibition Process

12:00 – 12:10	**Short Talk-24** **Essam Hanashalshahaby (Hacettepe University, Ankara – Turkey) – (Room A)** Metal Free Alkylation Reaction of Heterocycles via Ketonic Mannich Bases
	Short Talk-25 **Hamza Tachallait (Mohamed V University, Faculty of Science, Rabat - Morocco) – (Room B)** Innovative synthesis of some modified C- and N-nucleosides analogous
12:15– 12:25	**Short Talk-26** **Nadia Bouzidi Kambouche (Ahmed Benbella University, Oran – Algeria) – (Room A)** Chemical Composition and Antioxidant Potential of *Pistacia* lentiscus L. Essential Oil from Oran (Algeria)
	Short Talk-27 **Salaheddine Boukhssas (Sidi Mohamed Ben Abdellah University, Faculty of Sciences Dhar El Mahraz, Fez-Morocco) – (Room B)** Synthesis and characterization of aminoalkyl and tetrazolic amino acid derivatives
12:30 – 13:15	**- Closing session of the symposium** **- Designation of the organizing country of the TRAMECH X in 2019** **Conference room "Thousand and One Nights"**

Ei-ichi Negishi
Winner of the Nobel Prize in Chemistry in 2010», Japan

H. C. Brown Laboratories of Chemistry,
Purdue University, West Lafayette, IN, USA

Ei-ichi Negishi, H. C. Brown Distinguished Professor of Chemistry, Purdue University, grew up in Japan and received his Bachelor's degree from the University of Tokyo in 1958. From 1958-1966, while working as a Research Chemist at Teijin, Ltd., Japan, Negishi spent 3 years (1960-1963) as a Fulbright-Smith-Mund Scholar at the University of Pennsylvania and obtained his Ph.D. in Chemistry.

In 1966, he joined Professor H. C. Brown's Laboratories at Purdue as a Postdoctoral Associate and was appointed Assistant to Professor Brown in 1968. Negishi went to Syracuse University as Assistant Professor in 1972 and began his life-long investigations of transition metal-catalyzed organometallic reactions for organic synthesis. Negishi was promoted to Associate Professor at Syracuse University in 1976 and invited back to Purdue University as Full Professor in 1979.

In 1999 he was appointed the inaugural H. C. Brown Distinguished Professor of Chemistry. He has received various awards, with the most representative being 1987 J.S. Guggenheim Fellowship, 1996 Chemical Society of Japan Award, 1998 ACS Award in Organometallic Chemistry, 1998–2001 Alexander von Humboldt Senior Researcher Award, Germany, 2000 Sir Edward Frankland Prize, Royal Society of Chemistry, UK, 2007 Yamada-Koga Prize, Japan, 2010 ACS Award for Creative Work in Synthetic Organic Chemistry, 2010 Japanese Order of Culture, 2010 Nobel Prize in Chemistry, 2010 UK Royal Society of Chemistry Honorary Fellowship Award, 2011 Fellow of the American Academy of Arts and Sciences, and 2014 elected into the National Academy of Sciences as a Foreign Associate.

Lutz Friedjan Tietze
Institute of Organic and Biomolecular Chemistry, Georg-August-University Göttingen
Germany

Lutz Friedjan Tietze studied chemistry at the universities of Freiburg and Kiel, Germany and obtained his doctorate under the supervision of Prof. B. Franck in 1968 in Kiel. He then worked as a research associate with Prof. G. Büchi at MIT, Cambridge, USA for two years and later with Prof. A. Battersby in Cambridge, UK. In 1975 he got his habilitation at the University of Münster and in 1977 he received a professorship at the University of Dortmund. Since 1978 he has been Professor and until 2012 also Director of the Institute of Organic and Biomolecular Chemistry at the Georg-August-University in Göttingen.

He was head of a Collaborative Research Centre (Sonderforschungsbereich), has served as a member of the DFG-Panel (Fachforum) for eight years and was dean and vice dean of the faculty of chemistry in Göttingen again for eight years. He is President of the German Steering Committee of the German Chemical Societies (DZfCh), member of the German Centre for Cardiovascular Research (DZHK) and in 2012 was honoured with the position of a Distinguished Research Professor.

Professor Tietze has received several prizes, including the award for his book on "Reactions and Syntheses" by the Fonds of the Chemical industry, the Grignard-Wittig Prize of the Société Française de Chimie, the Prix Charles Mentzer of the Société de Chimie Thérapeutique and the highly prestigious Emil Fischer Gold Medal of the German Chemical Society. He has received an honorary doctorate from the University of Szeged (Hungary), has been awarded with an honourable fellowship of the Indian Chemical Society (CRSI), has worked as a visiting professor at seven universities worldwide and is member of two academies of science in Germany as well as an honourable member of the Hungarian Academy of Science.

He has almost 480 scientific papers, 38 patents and six books to his name. His research focuses on the development of efficient and selective synthetic methods using domino reactions, which allow the preparation of complex molecules starting from simple substrates in an ecological and economical advantageous way. Moreover, he is working on the total synthesis of natural products as well as materials and on the development of new selective anticancer agents based on conjugates of tumor-selective monoclonal antibodies and enzymes as well as prodrugs of duocarmycin analogues.

El Hallaoui Abdelilah
Laboratory of organic chemistry
Faculty Of Sciences Dhar El Mahraz
Sidi Mohamed Ben Abdelah University, Fez, **Morocco**

Abdellah El Hallaoui obtained a state doctorate thesis in chemistry in 1984 at the university of Montpellier (France), “Synthesis of amino acides enantiomerically pure”. The same year, he was recruited as an organic chemistry teacher at Sidi Mohamed Ben Abdellah University, Fez, Morocco, where he teaches advanced organic chemistry, asymmetric synthesis and strategy of synthesis. In 1986, he was the founder member of Laboratory of Organic Chemistry (LCO) which he was responsible of amino acids team.

This laboratory LCO developed new methodologies of synthesis of heterocyclic amino acids and their precursors (heterocyclic amino-aldehydes and amino alcohols) as well as the studies of the biological, electrochemical and structural properties of the synthesized products. He has taken part by conferences and communications in national and international congresses and published the results of research (+120 publications and communications) in several international journals. He was the founder member of the first TRAMECH in 2000.

On the teaching and administrative level:

- Head of the Department of Chemistry at the Faculty of Science Dar El Mahraz, Fez, Morocco (1990-1992)
- Head of the Faculty of Science and Technology, Fez, Morocco (1992- 1999)
- Member of several scientific commissions.
- Member of several review and expertise boards.

Stellios Arseniyadis
School of Biological and Chemical Sciences
Queen Mary University of London
United Kingdom

Stellios Arseniyadis studied chemistry at Paris XI University and moved to Strasbourg to do his PhD under the guidance of Dr. Charles Mioskowski. In 2001, he joined Rhodia Chirex Inc. (Boston, USA) for an industrial placement where he worked on various palladium and copper-catalyzed aryl bond--- forming processes in collaboration with Professor Stephen L. Buchwald at MIT. After a postdoc with Professor Alan C. Spivey at Imperial College London (UK) working in the field of asymmetric organocatalysis,

Stellios Arseniyadis joined Professor K. C. Nicolaou's group at The Scripps Research Institute (USA) to work on the synthesis of new epothilone B analogues and on the total synthesis of vannusal A. In 2005, he joined the CNRS as a permanent researcher in the group of Professor Janine Cossy at ESPCI Paris where he was promoted to the rank of CNRS Director in 2015. The same year, Arseniyadis started his own group at Queen Mary University of London, which is principally interested in the development of new synthetic tools with an emphasis on structural and functional complexity. These methods span within the areas of organocatalysis, transition metal catalysis and, more recently, bio-hybrid catalysis.

52 Publications including 6 Angew. Chem. Int. Ed., 3 J. Am. Chem. Soc., 8 Org. Lett., 8 Chem. Commun., 1 ACS Catal., 1 Adv. Synth & Catal.
6 Book chapters
2 Books (Modern Tools for the Synthesis of Complex Bioactive Molecules. Eds. Janine Cossy, Stellios Arseniyadis, John Wiley & Sons, Inc., Hoboken, NJ, USA (2012), ISBN 13: 978---0470616185. Metathesis in Natural ProductSynthesis. Eds. Janine Cossy, Stellios Arseniyadis, Christophe Meyer, Wiley--- VCH, Weinheim, Germany (2010), ISBN---13: 978---3---527---32440---8.
>900 Citations, h---index 20
2015 CNRS Bronze medal – 2014 Thieme Chemistry Journal Award Editorial Board: Frontiers in Chemical Biology (Nature Publishing group)

José Miguel Sansano Gil
Departamento de Química Orgánica, Instituto de Síntesis Orgánica (ISO)
Centro de Innovación en Química Avanzada (ORFEO-CINQA).
University of Alicante, **Spain**

José Miguel Sansano Gil was born in Rojales (Alicante), studied chemistry at the University of Alicante, where he obtained his B.Sc. and Ph.D. degrees in 1988 and 1994, respectively. His thesis on sulfone chemistry was supervised by Prof. C. Nájera.

After spending a two-year postdoctoral stay at the University of Leeds (U.K.) with Prof. R. Grigg, he joined the University of Alicante in 1996, where he was appointed Associate Professor in 2001. In 2010 he was promoted to Full Professor at the same University. He was invited as a visiting Professor at Universidade Federal de Rio de Janeiro (Brazil) in 2010 and 2011 and at Chuo University (Tokyo, Japan) in 2014. He is co-author of more than 107 articles and he has supervised 11 PhD students. He is also co-founder of the spin-off company Medalchemy, S. L. at the University of Alicante. H index = 32, 30.76 citations/item.

Piotr Kaszynski
Centre of Molecular and Macromolecular Studies, Polish Academy of Sciences
Poland

Piotr Kaszynski is a Professor of Chemistry at the Centre of Molecular and Macromolecular Studies of Polish Academy of Sciences, Department of Chemistry University of Łódź, Poland, and Middle Tennessee State University, USA.

He received his M.Sc. degree from the Technical University of Warsaw, Poland in 1985, his Ph.D. degree in Organic Chemistry in 1991 (University of Texas at Austin), and habilitation in 2007 (University of Łódź).
He spent two years at Caltech as a postdoctoral fellow working in the area of organic magnetic materials, before joining Vanderbilt University in 1993. In 2015 he moved the bulk of his research programme to Polish Academy of Sciences and University of Łódź, while maintaining ties with Middle Tennessee State University.

His research is focused on the design, synthesis and characterization of organic materials for electrooptical, molecular electronics, photovoltaic and spintronic applications, and for studying of molecular magnetism in liquid crystalline media.

He is an author and co-author of nearly 170 peer-reviewed original publications, reviews and book chapters.

Metin Balcı
Department of Chemistry, Middle East Technical University, Ankara, **Turkey**

Metin Balcı was born in Erzurum, Turkey. He received his "Diplom Chemiker" degree in 1972 followed by a Ph.D. degree in 1976 from the University of Cologne, where he worked with Professor Emanuel Vogel. He did postdoctoral work at the University of Siegen (Germany), University of Puerto Rico and University of Florida.

In 1980 he joined the Department of Chemistry at the Atatürk University and he has been a full professor since 1987. He spent one year in 1986 at the University of Cologne and one year (1996-1997) at the Auburn University in USA as guest professor. In 1997 he moved to the Middle East Technical University in Ankara upon reputation. He retired in June 2015.

Metin Balcı has received many prizes: In 1983 "Junior Research Prize" from TUBITAK and "Scientific Prize" in 1989 from the same Institution.

Furthermore, in 1990 he was awarded the Scientific and Technology Foundation's "Scientific Prize" and the Chemistry Foundation's "Chemistry Prize", and in 1991 the Ministry of Public awarded him its "Scientific Prize". He is member of Turkish Academy of Sciences.

His main research interests include synthesis of cyclitols, endoperoxides, cyclic strained compounds, bromine chemistry and heterocyclic compounds and he has published 270 scientific papers.

Dusan Berkes
Slovak University of Technology, Bratislava, **Slovakia**

Dusan Berkes was born in 1957 and currently works as Associate Professor of Organic Chemistry at the Slovak University of Technology in Bratislava. He graduated summa cum laude in Chemistry and Pharmaceutical Technology at the Slovak Technical University in Bratislava in 1981.

In 1987 he obtained the Ph.D. in Organic Chemistry (supervisor Prof. J. Kovac) and was hired as Assistant Professor at the Faculty of Chemical and Food Technology of the Slovak University of Technology in Bratislava.

In 2002 he was appointed as Associate Professor of Organic Chemistry at the same University. From 2012 he is head of the independent university laboratory in Saneca Pharmaceuticals company. He was the post-doctoral fellow in the group of Professor Henry-Basch at the University Paris-Sud (France) and research fellow at the University of Le Havre (France). The main research interests are stereoselective nonproteinogenic amino acid synthesis, crystallization-induced asymmetric transformations, with the applications towards the synthesis of sphingolipid metabolism inhibitors.

2015 CNRS Bronze medal – 2014 Thieme Chemistry Journal Award Editorial Board: Frontiers in Chemical Biology (Nature Publishing group)

Athina Geronikaki
Aristotle University of Thessaloniki, School of Pharmacy, **Greece**

Athina Geronikaki graduated from Tashkent State University in 1971 specializing in organic chemist. In 1977 she defended her Ph.D thesis and received her Ph.D in Chemistry. In 1984 she graduated from School of Pharmacy of Aristotelian University of Thessaloniki. From 2006-2016 she is the Head of the Department of Pharmaceutical Chemistry. Since 2010 she is Full Professor of Medicinal Chemistry of School of Pharmacy of Aristotle University of Thessaloniki. In the period 2009-2011 she was Vice President of School of Pharmacy of Aristotle University of Thessaloniki.

In July 2013 Prof. Geronikaki was elected as a Full member of Mediterranean Academy of Science and Arts and in 2015 Member of European Academy of Science and Arts. Her scientific interests are chemistry of natural products isolation, determination of structure; chemistry of biologically active compounds and evaluation of their activity, using different computational methods.

She has organized three International conferences: Computational Methods in Toxicology and Pharmacology, Integrating Internet Resources (CMTPI) (2003) Thessaloniki; 4th Eurasian Meeting on heterocyclic Chemistry , 2006 , Thessaloniki, 8th CMTPI 2015 and the 23d Hellenic Symposium in Medicinal Chemistry, 2017.
She has published more than 130 papers and four book chapters. She has written four books for student. She has 23 Erasmus agreements and is University coordinator of Paul Ehrlich PhD Network in Medicinal Chemistry.

François Couty
University of Versailles-St-Quentin-en-Yvelines, **France**

François Couty earned his PhD at the University Paris VI in 1991 and his habilitation degree in 1999. Since 2001, he is full Professor of organic chemistry at the University of Versailles (France). He is currently the head of the "Institut Lavoisier de Versailles" a public laboratory administrated by the CNRS and the University of Versailles. He has published more than 135 scientific papers in the field of heterocyclic chemistry, total synthesis, and reactivity in organic chemistry.

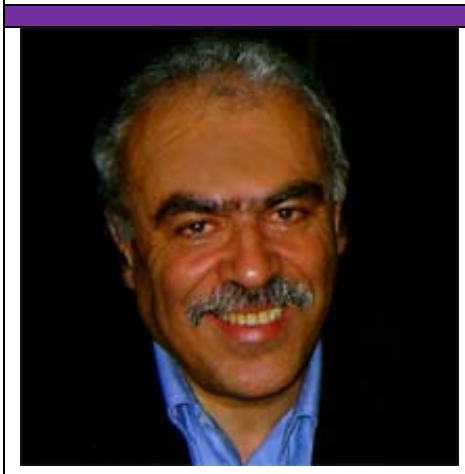
Asunción Barbero
Faculty of *Ciencias,Campus Miguel Delibes* University of Valladolid, **Spain**

Asunción Barbero was born in Burgos, Spain. She studied Chemistry at the University of Valladolid, and received her Ph.D degree at the same university working with Prof. Pulido. She then held Postdoctoral Marie Curie Fellowship at the University of Cambridge for two years working under the supervision of Prof. Ian Fleming in the study of stereocontrol in organic synthesis using silicon chemistry. She returned to Valladolid as Assistant Professor, was promoted to Associate Professor in 2001 and obtained the Spanish habilitation to full professor in 2012.

She has co-authored numerous international scientific publications and has delivered several invited and plenary lectures. Her current interests include the study of the silyl-cupration of multiple bonds and its application to the synthesis of natural and related products.

Maria do Amparo Ferreira Faustino
Department of Chemistry & QOPNA,
University of Aveiro, **Portugal**

Education
1992 - University of Aveiro, Portugal, "Licenciatura" (5 year BA degree) in Teaching of Physics and Chemistry
1999 - University of Aveiro, Portugal, PhD in Chemistry (Organic Chemistry). Thesis Title "Synthesis of new porphyrin derivatives and their potential application in PDT"
Work experience:
Organic chemistry
Organic synthesis; synthetic methodologies leading to tetrapyrrolic derivatives and their functionalization, Structural characterization mainly by, UV-Vis and fluorescence spectroscopy, NMR (mono and bi-dimensional), Mass spectrometry.
Scientific interests
Synthesis, reactivity and characterization of tetrapyrrolic macrocycles. Functionalization of porphyrin and related derivatives via cycloaddition reactions (Diels-Alder, 1,3 dipolar and 1,5-electrocyclizations) with structural features to be considered as dyes in solar cells (DSSC) and in medical and environmental applications (photodynamic therapy of neoplastic tissues, microorganisms photoinactivation, dermatologic formulations). Utilization of photochemical techniques to develop environmentally friendly approaches in the field of water treatment.
Supervision experience
27 MSc Thesis concluded and 1 MSc under development.
3 PhD Thesis concluded and 4 PhD under development
Scientific production: 120 publications, 2110 citations, H index: 26)
Research ID: J-5787-2012, Orcid: 0000-0003-4423-3802, Scopus Author ID: 6601979742



El Mokhtar ESSASSI
Laboratory of Heterocyclic Organic Chemistry Faculty of Science,
University Mohamed V – **Morocco**

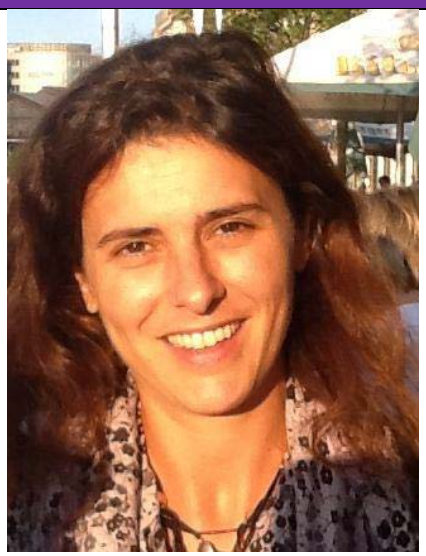
Professor El Mokhtar ESSASSI received his Ph.D in 1977 from the University of Sciences and Techniques of Languedoc (Montpellier, France) under the supervision of Professor Philippe VIALLEFONT. In 1977 he joined the Faculty of Science of Mohammed V University in Rabat as "Maître de Conférences" and was made full professor in 1981 at the same university.
In 1981 he founded the Heterocyclic Organic Chemistry Laboratory and the Moroccan Group of Heterocyclic Chemistry in 1999. He is a leading member of the organizing committee of the Moroccan National Meetings of Heterocyclic Chemistry (1993, 1996, 1998, 2000, 2002, 2007, 2009, 2011). He is the national coordinator for the pole of competence in Pharmacochemistry created in 2002.
Since 2010, he is the director of Composites Nanocomposites Center of Moroccan Foundation for Advanced Science, Innovation and Research (MASCIR).
He is currently a member of TRAMECH (Trans Mediterranean Colloquium on Heterocyclic Chemistry) scientific committee representing Morocco.
He was the chairman of TRAMECH III (Marrakech, 2004 and TRAMECH VII, (Rabat, 2013).
He is the editor in chief of Moroccan Journal of Heterocyclic Chemistry launched in 2002.
Professor ESSASSI was the co-director of NATO-ARW in 2009 (Detection of Biological Agents for the Prevention of Bioterrorism (Mass Spectrometry)) and co-director of NATO-ASI in 2013 and 2016 (Molecular Technologies for Detection of Chemical and Biological Agents). Professor ESSASSI is a resident member of HASSAN II Academy of Sciences and Techniques since 2006.

José María Lassaletta
Spanish National Research Council, **Spain**

José María Lassaletta received his B.Sc. and his Ph.D in 1990 under the supervision of Prof. Gómez-Guillén at the University of Seville. After postdoctoral work at the 'Instituto de la Grasa y sus Derivados' (CSIC) he joined the group of Professor Richard R. Schmidt (U. Konstanz, Germany).

In 1995 he moved to the Instituto de Investigaciones Químicas (CSIC, Seville), where he was promoted to Tenured Scientist in 1996, Research Scientist in 2005 and Research Professor in 2009. He has been recognized with the 'Felix Serratosa' Lecture (with Prof. Paul Wender, 2011) and the 'Ignacio Ribas' Medal from the Organic Chemistry Division of the Royal Society of Chemistry (2017).

He has been visiting professor at the Pierre y Marie Curie University (UPMC, Paris) in 2016. He is currently interested in the development of synthetic methodologies, cross-coupling & C–H activation strategies, ligand design, with emphasis in hydrazones & N-heterocyclic carbenes, and asymmetric organocatalysis.



Maria Emília da Silva Pereira de Sousa Laboratory of Organic and Pharmaceutical Chemistry, Faculty of Pharmacy, University of Porto, **Portugal**

Maria Emília da Silva Pereira de Sousa is a researcher at the Research Center CIIMAR and assistant professor of Organic and Medicinal Chemistry of the Faculty of Pharmacy of the University of Porto.

She obtained her degree in Pharmaceutical Sciences at the University of Porto in 1997 and her Ph.D in Pharmaceutical and Medicinal Chemistry from the same university in 2003, in the synthesis of chiral xanthones with antitumor activity. She held two post-doctoral internships in the project 083/02 Grices / Capes at the Federal University of São Carlos, SP, Brazil in August 2004 and February 2006.

Her area of scientific activity is centered on medicinal and pharmaceutical chemistry in particular, in the structure-based design and synthesis of potential drug candidates based on plant and marine natural product leads such as xanthones, flavonoids and other polyphenols, in studies of structure-activity relationships and preclinical/preformulation studies. Current research interests include: design and synthesis of P-glycoprotein modulators; design and synthesis of modulators of p53/negative regulators interaction; synthesis of anticancer drugs metabolites.

Other current activities include Member of the Scientific Board of the Master in Pharmaceutical Chemistry, FFUP; Member of International Doctoral Programme BiotechHealth Staff, UP (FCT PD-F 2012); Member of the editorial board Molecules (MDPI), Pharmaceuticals (MDPI), American Journal Pharmaceutical Sciences & Nanotechnology (Columbia International Publicating, USA); Reviewer of several Pharmaceutical Sciences scientific journals; Evaluation of international research projects.

Experience as scientific adviser: to date, she concluded the co/supervision of 2 posdoc, 4 PhD student, 8 Masters, 3 student ERASMUS, 9 research fellows. Currently, she is co/supervising, 3 PhD and 5 master students, and several undergraduate students.She is (co-)author of 1 international and 2 national patents, 1 book, 5 book chapters, 68 papers in international scientific periodicals with referees and 2 paper in national, 47 abstracts international circulation / national refereed scientific, 64 oral communications (18 invited) and 176 posters in conferences in the field of Medicinal Chemistry.

Hamdullah KILIC
Atatürk University, Department of Chemistry, Erzurum, **Turkey**

Hamdullah KILIC was born in Erzurum, Turkey, in 1966. He obtained a B.Sc. degree in 1992 from the Atatürk University and a Ph.D. degree in 1999 from the same University under the supervision of Prof. Dr. Metin BALCI. After carrying out postdoctoral work with Prof. Dr. Waldemar ADAM at the University of Würzburg through late 2000, he joined the faculty of Sciences at the Ataturk University as an assistant professor of chemistry and was promoted to associate professor of chemistry in 2005, and full professor in 2010. Since then, he has been full professor of Organic Chemistry at the Atatürk University.

His research programme focuses on the development of novel catalytic and stoichiometric reagents for the asymmetric construction of chiral building blocks, the use of hypervalent iodine reagents in organic synthesis. Other research interests include mechanistic investigations of epoxidation and aziridination reactions.mechanistic investigations of epoxidation and aziridination reactions.

Adam Daïch
Normandie University,
UNILEHAVRE
France

Adam Daïch was born in Aït Ouribel, Morocco, in 1961. After receiving his B.Sc. degree in chemistry in 1987 conjointly from the University Paris-VI and ENSCP High School at Paris, he completed his Ph.D in 1991 under the guidance of Professor B. Decroix at the University Le Havre Normandie (ULHN). Following two post-doctoral stints (1992–1993) as an associate with Dr. Ingenir F. Považanec at the Technical University of Slovakia of Bratislava and ATER at the ULHN, respectively, he joined Professor J. Morel's team in 1993 as an Assistant Professor. At the same University, he completed his 'habilitation' in 2000 and was promoted to the rank of full professor in 2004.

Professor Daïch is a team leader of one Eureca groups at URCOM-CNRS FR3038 of University Le Havre Normandie and his current research interests cover many topics including:

- Behaviour of cationic species towards the heterocyclization processes using N, O, S and Se heteroatoms as internal nucleophiles,
- Elaboration of cytotoxic and anticancer analogues of the natural products as topoisomerase-I/II poisons,
- Spiroindole and spirooxindoles-heterocyclic systems by domino/tandem and/or cascade protocols using versatile small reagents,
- Natural and unnatural aza-heterocyclic heterocyclic lactams with broad biological uses including FTase inhibition and anti-tubulin activity, and finally
- Asymmetric synthesis of hydroxylated pyrrolidines and indolizidines with glycosidases inhibitory potentials.

He has published more than 110 scientific papers, has one international patent, one chapter in a book and four articles in books.

Hussein El-Kashef
Chemistry Department, Faculty of Science, Assiut University,
Egypt

Dr. Hussein El-Kashef was born in El-Minia (Egypt) in 1945. He studied at Assiut University in Egypt and got all his degrees from the same university. He received his B.Sc. (special degree in Chemistry with distinction) in 1965, his M.Sc. in 1969 and Ph.D. in 1973.
He obtained a second doctorate degree (Docteur ès sciences Pharmaceutiques) from the University of Caen-France in 1994.
He was appointed as Assistant of Organic Chemistry at the Faculty of Science, Assiut University in 1965, and promoted to all his academic positions until Professor in 1982.
He has been Professor Emeritus from 2005 until the present day.
Dr. El-Kashef has been visiting professor at different universities and institutes in different countries:

In France: at the University of Caen, Marseille, Strasbourg, Nice – Sophia, Antipolis, Clermont–Ferrand I and Lille.
In Italy: at the University of Ferrara and Calabria.
In Germany: at the university Saarlandes; Saarbrücken, and Kaufmann institute of Lipids of Münster.
In Japan: at the university of Tohoku
In Yemen: at the University of Sana'a.

Prizes
Prize of Assiut University for Scientific Distinction (2001).
Chevalier dans l'ordre des palmes Académiques (from the French Governement , 2004).
Prize of Faculty of Science for the research of highest impact factor (2014)
Prize of Faculty of Science, Assiut University for the best research paper in Organic Chemistry (2016).

Kandri Rodi Youssef
Laboratory of Applied Organic Chemistry
Faculty of Sciences and technologies
Sidi Mohamed Ben Abdellah University

Professor of Organic Chemistry at Faculty of Sciences and technologies-Fez
Academic Record
2012: Professor Grade C. Université Sidi Mohamed Ben Abdellah – FST FES
2005: Professor Grade B. Université Sidi Mohamed Ben Abdellah – FST FES
1999: Professor Grade A. Université Sidi Mohamed Ben Abellah – FST FES
1995: Lecturer, Université Sidi Mohamed Ben Abdellah – FST FES
Participation in Academic and Scientific activities
- Head of the Research group of: Synthesis and Complexation of Compounds of Biological Relevance.
- Member of the Moroccan Group of Heterocyclic Chemistry.
- Referee for the Journal Marocain de Chimie Hétérocyclique.
- Referee for the Journal Materials & Environment Science.

Teaching Activities
- Organic Chemistry
- Bio-Organic Chemistry

Research Activities. Subjects
1/ Methodologies in Heterocyclic Chemistry
2/ Synthesis and functionalization of new heterocyclic systems
3/ Utilization of those heterocyclic substrates for the preparation of products of biological or therapeutic relevance (SCN, Cardiovascular system, anti-ache, diabetes, obesity, cancer etc..
Scientific Publications
170 publications in national and international journal
He has published more than 110 scientific papers, 1 international patent, 1 chapter in a book and 4 articles in a book.

Florio Saverio
Consortium CAMPUS
University of Bari Aldo Moro
Italy

Florio Saverio received his 'Laurea' in Chemistry at the University of Bari (Italy). Assistant Professor and Associate Professor of Organic Chemistry at the University of Bari till 1982, Full Professor of Organic Chemistry at the University of Lecce (1986–90) and University of Bari, chair of organic chemistry (1990–2012). Director of 'Consorzio Interuniversitario sulle Metodologie e Processi Innovativi di Sintesi' (CINMPIS) 1994-2014. President of the Division of Organic Chemistry of the Italian Chemical Society (1997–2001), vice President of the Italian Chemical Society (2007–10). He has been a member of the SAB and of NSC of the International Advanced School of Organic Chemistry of Ischia (IASOC School).

His research interests are concerned with mechanistic studies, stereochemistry, and asymmetric synthesis of small-ring heterocycles, chemistry and structural features of oxiranyl and aziridinyl anions applied to organic synthesis.

Prof. Florio Saverio published more than 200 papers. He received the following awards: the 'Ziegler-Natta Lecture' from the German Chemical Society (GDCh) in 2005, the 'Angelo Mangini Gold Medal' from the Division of Organic Chemistry of the Italian Chemical Society in 2007, Member Elected of the European Academy of Arts and Sciences, Salsburg in 2007, First Lecturer of the Slovenian-Italian Chemical Societies Lectureship for the year 2010, Silver Plate from Consortium CINMPIS in 2014.

Damien Prim
UMR CNRS 8180
Lavoisier Institute of Versailles,
France

Damien Prim is professor of organic chemistry at the University of Versailles St Quentin, France. He obtained his PhD in Organic Chemistry at the University Paul Verlaine in Metz under the supervision of Professor G. Kirsch (France, 1994). After a postdoctoral period in Professor L. Ghosez group at the University Catholique of Louvain, Belgium for his postdoctoral training, he came back to Metz as Assistant Professor and successively moved to the University of Pierre and Marie Curie as CNRS researcher (Paris, 1999), the University of Versailles St Quentin as Assistant Professor (Versailles, 2001) where he was promoted to professor of chemistry in 2004.

His current research interests include homogeneous catalysis and chemistry of planar, twisted and 3D-shaped molecular architectures.

Fawaz Aldabbagh
Kingston University, London
United Kingdom

Fawaz Aldabbagh obtained a PhD on organic radicals with Professor W. R. Bowman at Loughborough University, UK in 1997. Subsequently he completed 2 years postdoctoral work on nitroxide-mediated polymerizations with Professors W. K. Busfield and I. D. Jenkins at Griffith University, Brisbane, Australia. He gained his first independent academic position at the age of 28 at the National University of Ireland Galway in 2000. As a lecturer and then senior lecturer in chemistry, he supervised 22 PhDs to completion. He has published almost 80 peer-reviewed articles and reviews on heterocyclic chemistry, cancer research, and polymer chemistry. In June 2017, Fawaz accepted the offer of Professor of Medicinal and Pharmaceutical Chemistry at Kingston University, London, UK.

Cristina Nativi
Department of Chemistry "Ugo Schiff" University of Florence
Italy

Professor
Department of Chemistry
University of Florence

Current research interests

stereoselective glycosylation
sulfur-mediated reactions
design, synthesis and application of glycosides as immunostimulants or anti-pathogens
design and synthesis of matrix-metalloproteinases inhibitors
molecular recognition of carbohydrates

Publications and Patents

>140 papers and 5 patents

Education

1993-1994: Post Doc, University of Montréal (CDN) (Prof. S. Hanessian)
1989-1991: Fellowship, CNR, University of Florence
1987-1989: Grant (Swiss Government), Université de Lausanne (CH) (Prof. P. Vogel)
1980-1986: Chemistry Degree, University of Florence

Academic Career

2005-present: Full Professor, University of Florence
2000-2005: Associate Professor, University of Florence
1991-2000: Assistant Professor, University of Florence

Chair of the Italian Meeting-School of Carbohydrate Chemistry, Member of the Scientific committee of the Divisione Italiana of Carbohydrate Chemistry, of Giotto Biotech (start-up of the University of Florence), of the Leonardo da Vinci (LdV) BioBank and of FiorGen (Farmaco genomic Foundation).

Victor Freitas
Department of Chemistry and Biochemistry, Faculty of Sciences
Portugal

Victor Freitas graduated in Chemistry from the Faculty of Science of the University of Porto (FCUP) in 1984. In 1995, he obtained his PhD in Biological and Medical Sciences in the University of Bordeaux II (France).
After his PhD, he returned to the Department of Chemistry and Biochemistry (DQB) of FCUP where he has been developing his teaching and research activities. He is currently Full Professor in the University of Porto, member of the REQUIMTE-LAQV Research Centre and the leader of the Food Polyphenol Lab (http://www.foodphenolab.com) where he has been developing an independent research area involving polyphenol compounds focusing on a) the chemical transformations resulting from oxidation processes of polyphenolic pigments, including technological applications in the food industry; b) the interaction of different classes of polyphenols with proteins in the sensory and nutritional context; c) the antioxidant and biological properties of polyphenolic compounds.

Victor Freitas presents in his CV more than 240 original articles published in journals indexed in the Science Citation Index (SCI), several book chapters, numerous invited conferences, running multiple I&DT projects and several supervisions of Master and PhD students.

Serge Thorimbret
PIMC, University Pierre and Marie Curie, **France**

Education
1993: PhD of organic chemistry under the direction of Pr. J.P. Genêt
2003: Habilitation delivered by Université Pierre et Marie Curie

Professional experience
1993 - 94: Post-doctoral fellow. Max-Planck-Institut für Kohlenforschung. Pr. W.F. Maier.
1994 -95 : Assistant Professor. University P. et M. Curie. Pr. C. Agami.
1998 - 98: Academic Visitor. Imperial College. London. Pr. D. Craig.
1995- : Associate Professor Then Full Professor (2010) at the IPCM, UPMC.

Award
1989-93: French Ministry of Research and Technology fellowship
1993-94: Max Planck-Gesellschaft fellowship
1998 : Invited Prof., Florence University (July 1998) – Collaboration with prof G. Poli
1998-99 : NATO fellowship
1998-99 : Visiting Scientist. Imperial College. London
2009 : Valtva 2009. Financial support to visit Laboratories in Czech Republic
2014 : Visiting Prof., Nanyang Technological University. 10th-15th March 2014

Scientific Production
71 publications; 30 national and international conferences, 14 oral communications; h-index = 23
Review articles: 3; Book chapters: 2

Current research interests
- Organic Synthesis - Heterocyclic compounds - Reactivity
- Organometallic Chemistry – Catalysis – Artificial Metalloenzymes
- Hybrids Materials.

Mario Schiavoni
Hemophilia and Rare Coagulopathies Centre, Lecce, **Italy**

Desired employment / Occupational field
Medicine Doctor, specialist in Internal Medicine,
Hematology and Rare Haemostasis and Coagulation Diseases
Work experience
Clinical research in haemostasis and thrombosis fields
Occupation or position held
President of ONLUS ASSOCIATION AGAINST HEMORRAGIC AND THROMBOTIC DISEASES (A.L.M.E.T)-Italy
Main activities and responsibilities
- Past Director of Dep. of Internal Medicine-Hemophilia Centre_ Azienda Sanitaria Locale-Lecce (Italy)
- Education and training Scientific Director of post-graduate courses on Haemostasis and Thrombosis on the behalf and in collaboration with Italian Association of Hemophilia Centre (A.I.C.E.), Italian Association on Haemostasis and Thrombosis (S.I.S.E.T.)
- Personal competences 1990 - 1993 Professor of "Pathophysiology of Hemostasis" in the Faculty of Biological and Mathematical Sciences- University, Lecce (Italy)
- Since 1993 member of Italian Association of Hemophilia Centres (AICE)
- 2000-2001 professor of "Human Anatomy" – Institute of Pharmaceutical Chemistry – University of Bari (Italy)
- 2003-2013 member of European Hemophilia Therapy Standardisation Board (EHTSB)
- 2006 - 2008 Member of Executive Committee of Italian Society of Hemostasis and Thrombosis (S.I.S.E.T.)
-2008-2011 member of Executive Committee of Italian Association of Hemophilia Centres (AICE)

Mohamed ETTAYEBI
University SMBA, Fez, **Morocco**

EDUCATION : Ph. D., Molecular Genetics, State University of New York Buffalo, New York, USA
ACADEMIC POSITIONS: Professor of Molecular Genetics, and Coordinator of BBE consortium (Biodiversity, Bioenergy and Environment Research Group), School of Sciences, University SMBA in Fez
Visiting Professor:
- Institute for Infectious Disease Research, McMaster University, Canada
- Thermal Biology Institute, Montana State University in Bozeman, US
- International Center for Genetic Engineering & Biotechnology, Rome, Italy
ADMINISTRATIVE POSITIONS:
- Coordinator of Biodiversity, Bioenergy and Environment Research Consortium
- Coordinator of Environmental & Life Science Division. School of science and Engineering. Alakhawayn University in Ifrane, Morocco
- Head of the Department of Biological Sciences. University SMBA in Fez
- Coordinator of the Biotechnology/Biodiversity Research Unit Thermal Biology Institute in Montana State University, USA
- Founder and Director of Biotechnology Research Unit. University SMBA in
RESEARCH INTERESTS
- Drug discovery: This involves the utilization of chemical genomics in the search for new bioactive compounds from synthetic libraries and from natural resources with a special interest in anticancer drugs, antimicrobial synergism and combination therapy to combat drug resistance.
- Genetic Engineering applications in different fields: epidemiology (viruses, antibiotic resistance), ecology (Microbial biodiversity) and biotechnology (Industrial microbiology)
- Bioenergy: Biodiversity, Bioenergy & Environment Research Group (BBE) is a consortium composed of scientists involved in multidisciplinary research projects. BBE was founded and is coordinated by Prof Ettayebi and it includes different schools from the university of Fes, Rabat, And Tangier as well as international collaborating partners.

Islam Ullah Khan
Faculty of Science &Technology
GC University Lahore, **Pakistan**

Education
Ph.D in Chemistry from Kyushu University, Fukuoka, Japan, 1993

Administrative and Advisory Services
Dean, Faculty of Science and Technology (2nd tenure) since 30th December 2015.
Dean, Faculty of of Science and Technology (1st tenure) from 27th September, 2012 to 26th September, 2015.
Dean, (Acting) Arts & Social Sciences and Eingeeniring from 22nd October, 2012 to 26th September, 2015.
Look after charge of Vice Chancellor Office of GCU for 3 months (b/w 29.06.2013-30.07.2013, 20.06.2014-19.06.2014 and 13.06.2015-12.07.2015).
Chairman, Department of Chemistry from 25th March, 2010-17th June, 2014.

Areas of Research
- Synthesis of new organic molecules of pharmaceutical importance.
- Syntheses, applications and X-Ray crystallographic studies of new metal-organic frameworks.
- Development of novel HPLC and spectrometric methods for pharmaceutical and forensic analysis.
- Oxidative Stress studies using novel and contemporary analytical methods.
Supramolecular Chemistry – calixarenes: synthesis and inclusion properties.

He has published almost 281 peer-reviewed articles and reviews.

Artur Silva
University of Aveiro, **Portugal**

He obtained both the BSc (1987) and the PhD (1993) degrees at the University of Aveiro. He joined the Department of Chemistry of the same University in 1987 and was appointed to Auxiliary Professor in 1996, Associate Professor in 1999 and Full Professor in 2001. He published more than 553 SCI papers (h = 41), 1 e-book and 40 book chapters, 2 patents and delivery more than 51 lectures in scientific meetings. He supervised 25 PhD students and 35 MSc students; he participate / has participated in 21 financed Portuguese and European projects and in 8 bilateral financed projects with European Research Groups. He belongs to the editorial board of 6 scientific journals.

His research interests range over the chemistry of polyphenolic and nitrogen heterocyclic compounds, with special emphasis on the development of new synthetic routes, and also on the organocatalytic and metal-catalysed transformations. The second passion of his research is centred in the isolation and structural characterization of natural products from diverse terrestrial and marine sources. But all these scientific activities it is supported in his strong knowledge on NMR spectroscopy. The third axis of their research are focused on the synthesis of biologically active oxygen and nitrogen heterocyclic compounds, as well as on the evaluation of their antioxidant, anti-inflammatory, antitumor and antimicrobial activity in collaborations with other Portuguese and International research groups.

He is the director of the QOPNA research centre (150 researchers), president of the Portuguese Chemical Society, member of the Executive Board of EuCheMS and Fellow of the European Academy of Sciences.

Opening Plenary Conference

MAGICAL POWER OF d-BLOCK TRANSITION METALS AS DEMONSTRATED BY CATALYTIC ASYMMETRIC C–C BOND FORMATION

Ei-ichi Negishi*, Shiqing Xu

H. C. Brown Laboratories of Chemistry, Purdue University, West Lafayette, IN, USA

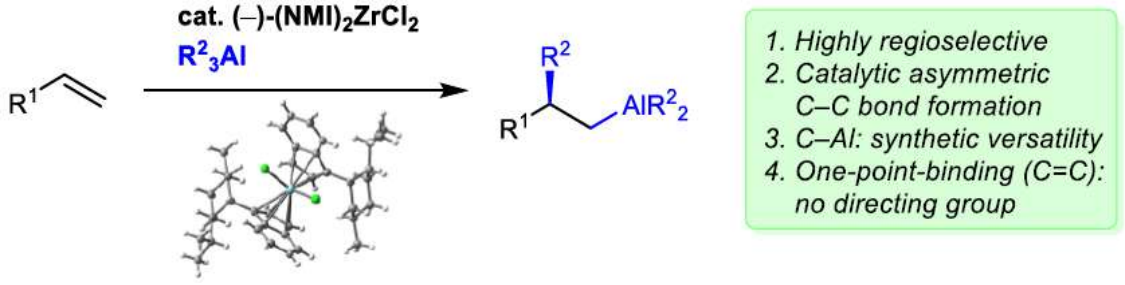
**For Correspondence: Email: negishi@purdue.edu*

Abstract

Over the past several decades, d-block transition metals have been increasingly recognized and used as catalysts for various chemical reactions. In most cases, their superb catalytic properties may be attributed to one or both of the following two: (1) ability to provide simultaneously one or more each of the valence-shell empty orbitals that serve as LUMOs and filled nonbonding orbitals that serve as HOMOs; (2) ability to undergo simultaneously both reduction and oxidation under one set of reaction conditions in one reaction vessel. A combination of these two properties can be exploited in devising a wide variety of useful catalytic reactions for formation and cleavage of C–C, C–H, C–O and other bonds.

For critically important C–C bond formation, i) reductive elimination, ii) carbometalation, and iii) migratory insertion may be exploited. The representative examples of reductive elimination and carbometalation are the Pd-catalyzed cross-coupling proceeding via reductive elimination and **Z**r-catalyzed **a**symmetric **c**arboalumination of **a**lkenes (ZACA reaction) proceeding via carbometalation.

In this lecture, recent advances of ZACA reaction will be discussed with emphasis on several methodological developments including: (i) ZACA–lipase-catalyzed acetylation–transition metal-catalyzed cross-coupling processes for preparing various enantiopure chiral alcohols; (ii) one-step homologation for the synthesis of deoxypropionates; (iii) the ZACA reaction of dienes to generate chiral cyclic compounds including those with all-carbon quaternary stereocenters.



Plenary Lectures

DOMINO REACTIONS. THE GREEN AND ECONOMICAL ART OF CHEMICAL SYNTHESIS

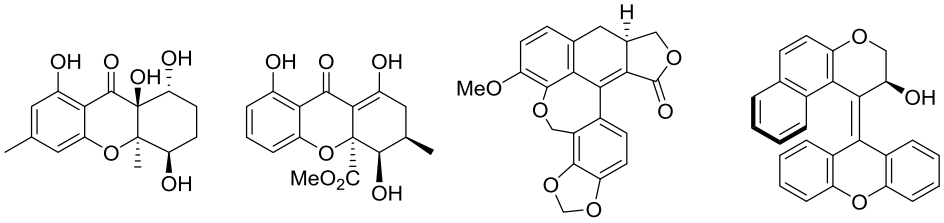
Lutz F. Tietze

Institute of Organic and Biomolecular Chemistry, Georg-August-University Göttingen, Tammannstr. 2, D-37077 Göttingen, Germany

Email: ltietze@gwdg.de

Abstract

The efficient synthesis of natural products, drugs, agrochemicals and materials is a very important aspect in academia and industry. To allow an ecologically and economically favourable approach in a green fashion the former stepwise procedures must be replaced by domino reactions which allow the preparation of complex molecules starting from simple substrates in a straight forward way. Domino reactions **[1]** allow the reduction of the amount of waste being formed and the preservation of our resources. Moreover, they are also favourable in an economical way since they consume less time and less material.



Diversonol (-)-Blenolid A Linoxepin Molecular Switches

The usefulness of the domino concept **[1]** is demonstrated with the syntheses of the fungal metabolites diversonol **[2]**, blennolide A **[3a]**, blennolide C **[3b]**, and gonytolide **[3b]**, as well as other natural products of the dimeric tetrahydroxanthenone type **[4]** using an enantioselective domino-Wacker/carbonylation/methoxylation reaction and of the natural aryldihydronaphthalene lignan linoxepine **[5]** employing a domino-carbopalladation/Heck reaction. The approach has also been applied for the synthesis of novel materials such as molecular switches **[6a-d]** and fluorescence dyes **[6e-f]**, using a domino-Sonogashira/carbopalladation/CH-activation reaction.

Keywords: Domino reactions; enantioselective synthesis; natural products; molecular switches; fluorescence dyes; Palladium; CH-activation.

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PRECURSORS AND DERIVATIVES OF HETEROCYCLIC AMINES AND HETEROCYCLIC AMINO ACIDS. SYNTHESIS, STUDY OF BIOLOGICAL AND ELECTROCHEMICAL PROPERTIES

Abdellah El Hallaoui

Laboratory of Organic Chemistry (LCO), Faculty of Sciences Dhar El Mahraz – University of Sidi Mohamed Ben Abdellah, Fez - Morocco

Email: elhallaoui.a@gmail.com

Abstract

Amines and heterocyclic amino acids **[1-3]** form a very wide and varied field of application, especially in the medical **[4]**, agrochemical **[5]** and surface processing **[6,7]**. The main objective of this conference is the synthesis and study of the biological and electrochemical properties concerning new series of precursors and derivatives of amines and heterocyclic amino acids.

The precursors of the described amino acids are obtained with excellent yields, following two strategies of the synthesis of the 4-methyl-4-O-Tosylmethyl-2-phenyloxazoline.

The preparation of heterocyclic carboxylic and phosphonic amino acid derivatives can have two different key steps: either the direct substitution reaction of the azid group of the α-azidoglycinate of methyl N-protected by a nucleophilic, or the dipolar cycloaddition reaction 1,3 over this azid group.

The tetrazolic derivatives referred to as TET, IND and IND-TET are obtained through the cycloaddition reaction (2+3) among the sodium azide and the related nitriles.

The structures of the synthesized products are elucidated, inter alia, on the basis of homo and hetero-nuclear 2D RMN analysis: ^{1}H-^{1}H, ^{1}H-^{13}C. In some cases, the ^{1}H-^{15}N, ^{13}C-^{15}N correlation was necessary **[8]**. The mono-crystals obtained are analyzed by X-ray diffraction.

Biological tests are performed on six amino acid derivatives against five strains of Gram+ and Gram- bacteria. The results obtained reveal a bactericidal activity of the compounds tested.

The electrochemical study of some heterocyclic amino acid precursors and derivatives shows that these compounds are potential corrosion inhibitors. The same applies to the amino tetrazole derivatives prepared.

Keywords: Phosphoric amino acids; Carboxylic amino acids; Aminotetrazoles; Oxazoline.

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FUNCTIONAL MATERIALS DERIVED FROM π-DELOCALIZED RADICALS FOR PHOTOVOLATICS AND SPINTRONIC

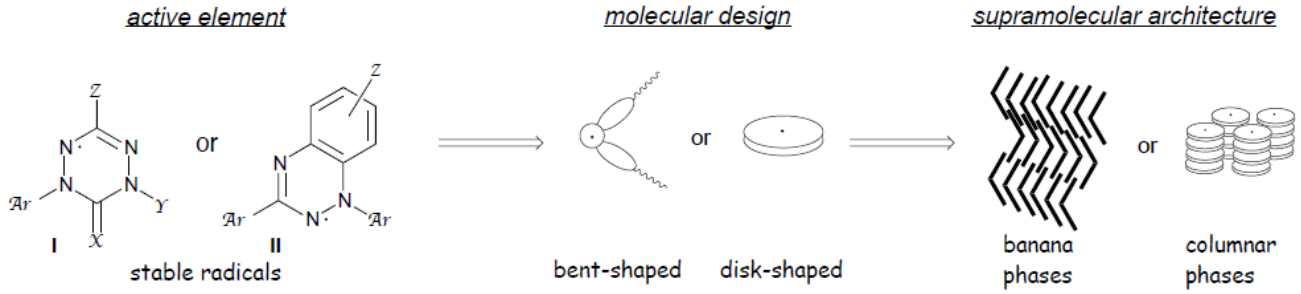
Piotr Kaszyński[1,2,3]

[1]*Centre of Molecular and Macromolecular Studies, Polish Academy of Sciences, 90-363 Łódź, Poland*
[2]*Faculty of Chemistry, University of Łódź, Tamka 12, 91403 Łódź, Poland.*
[3]*Department of Chemistry, Middle Tennessee State University, Murfreesboro, TN 37123, USA.*

Email: piotrk@cbmm.lodz.pl

Abstract

Open-shell organic systems are becoming increasingly important structural elements of advanced materials investigated for applications in molecular electronics, energy harvesting, memory and energy storage, and spintronics. In this context, we have been studying supramolecular assemblies of stable π-delocalized radicals, such as 6-oxoverdazyl derivatives (**I**) **[1]**. Recently, we have developed a new synthetic method **[2]**, which opened up a broader access to derivatives of benzo[*e*][1,2,4]triazinyl (**II**), an exceptionally stable radical. The new method has provided access to new types of molecular architectures **[3]** containing the benzo[e][1,2,4]triazinyl, and also to liquid crystalline derivatives exhibiting discotic (*Col*$_h$) and bent-core smectic (SmA) phases **[4]**. The latter were investigated for their thermal, magnetic and photovoltaic properties. SQUID measurements revealed that magnetic behavior of such materials depends on the structure/size of the Ar substituent at the N(1) position. Moreover, discotics containing the benzo[*e*][1,2,4]triazinyl (**II**) exhibit much stronger spin exchange interactions in both the fluid and crystalline phases, when compared to those of mesogenic 6-oxoverdazyl derivatives (**I**).



Acknowledgments: Financial support was provided by the National Science Center (2014/13/B/ST5/04525 and 2013/11/B/ST3/04193).

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GOLD-CATALYZED AND AND BASE-SUPPORTED CYCLIZATION REACTIONS OF *N*-PROPARGYLATED PYRROLE, INDOLE AND BENZENE DERIVATIVES: SYNTHESIS OF HETEROCYCLES WITH NEW SCAFFOLDS

Metin Balci

Department of Chemistry, Middle East Technical University, 06800 Ankara, Turkey

Email: mbalci@metu.edu.tr

Abstract

Compounds classified as heterocyclic probably constitute the largest and most varied family of organic compounds and they are well presented among pharmaceuticals. As part of our ongoing research program on the design and synthesis of heterocycles with new skeletons we developed new methodologies. The key feature of this methodology was the synthesis of N-propargyl pyrrole, indole, and benzene derivatives. Gold-catalyzed or NaH-supported cyclization of these compounds resulted in the formation of compounds given in Figure 1 **[1-9]**.

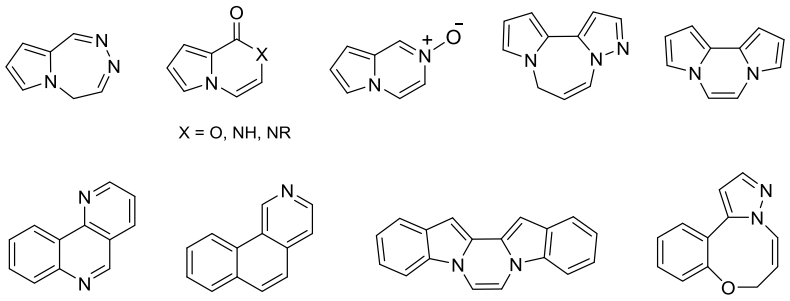

Figure 1. Structures of some synthesized compounds.

The gold-catalyzed reaction of pyrrole and indole oximes having N-propargyl group transferred the oxime functionality intramolecularly from one carbon atom to another carbon atom via 7-endo-dig cyclization process. This transformation is unprecedented in the literature and was named as oxime-oxime rearrangement **[6]**.

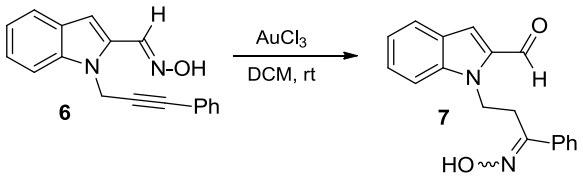

Figure 2. Oxime-Oxime Rearrangement

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3-INDOLYLGLYCINES AND γ-OXO-α-AMINO ACIDS AS 1,3-BIFUNCTIONAL NUCLEOPHILES IN THE SYNTHESIS OF HETEROCYCLES

J. Markus[1], B. Ferko[2], **D. Berkeš[2,*]**, A. Daïch[3]

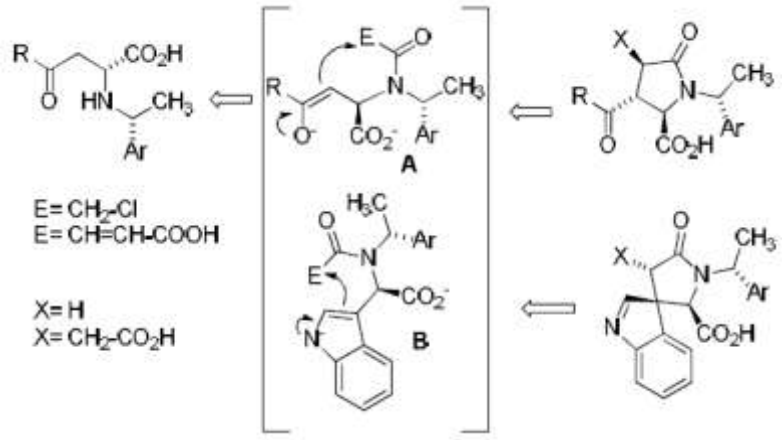
[1]*Saneca Pharmaceuticals a.s., Hlohovec, Slovakia*
[2]*Slovak University of Technology, Bratislava, Slovakia,*
[3]*Université du Havre, Le Havre, France*

**For correspondence: Email: dusan.berke@stuba.sk*

Abstract

During the last years, a significant effort has been focused on the design and preparation of novel nonproteinogenic amino acids and their synthetic applications. Enantiomerically pure *N*-substituted g-oxo-a-amino acids accessible *via* our CIAT applications in tandem with *aza*-Michael and Mannich reactions **[1]**. They represent suitable chiral synthons and have been used for the stereodivergent synthesis of ceramide metabolism inhibitors recently **[2]**.

Now we present the convenient two-step synthesis of polysubstituted pyroglutamic acid derivatives. The key step of this sequence is a high diastereoselective intramolecular C-C bond formation *via* the enolates of the corresponding *N*-acylated g-oxo-a-amino acids. Additionally, the lecture will address the high structural analogy of over-mentioned enolates with enamine part of indolylglycines, and the straightforward synthesis of spiroindolyl derivatives will be presented too.



Several new stereoselective transformations of the prepared spiroindolenine derivatives targeting the polycyclic core of spiroindolyl alkaloids along with the new synthesis of indolylmaleimides from indolylglycines and the Povarov reaction will also be discussed **[3]**.

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SYNTHESIS AND BIOLOGICAL EVALUATION OF NOVEL SUBSTITUTED 2-[(5-ADAMANTANE-1-YL) 1,3,4-THIADIAZOL-2-YL) IMINO]-5 THIAZOLIDINONES

A. G eronikaki[a,*], M. Fesatidou[a], P. Zagaliotis[a], A. Ćirić[b],J. Glamočlija[b], M. Soković[b]

[a] *Aristotle University of Thessaloniki, School of Pharmacy, Thessaloniki 54124, Greece*
[b] *Mycological Laboratory, Department of Plant Physiology, Institute for Biological Research, Siniša Stanković, University of Belgrade, BulevarDespotaStefana 142, 11000, Belgrade, Serbia.*

**For correspondence: Email: geronik@pharm.auth.gr*

Abstract

Throughout the human history there has been a real struggle between human and various microorganisms which cause infections. Around the middle of the 20th century the progress of antimicrobial agents was great and the winner of that struggle proved to be the human. [1] The frequent and bad use of the antibacterial and antifungal drugs led to the wide phenomenon of the bacterial and antifungal resistance. [2] Usually, the infections are accompanied with inflammation, so, the researchers try to design and synthesize agents with dual action, both antimicrobial and antiinflammatory activity, in order to avoid burdening the patient with multiple medications.
The thiadiazole moiety has been connected -among others- to antimicrobial and antiinflammatory activity and the adamantane core has received considerable attention due to its wide range of pharmacological action.
So, this work presents the design, synthesis and biological evaluation of novel thiadiazole derivatives (Scheme 1). Following the prediction of several compounds' biological activity by the program PASS, seventeen novel compounds were selected and synthesized. The synthesis of the final compounds was carried out in 4 steps. In the final step, condensation between the intermediate thiazolidinones and different aromatic aldehydes took place, with high yield (39.1-74.7%). All the compounds are tested for their antibacterial, antifungal and antiinflammatory activity. Results will be presented.

Keywords: thiadiazole; antimicrobial; antifungal; adamantine.

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FROM AZETIDINES TO ORTHOGONAL « CLICK » REACTIONS

François Couty

Institut Lavoisier de Versailles, UMR CNRS 8180, Université de Versailles St-Quentin en Yvelines.45, av. des Etats-Unis, 78035 Versailles Cedex, France

Email: francois.couty@uvsq.fr

Abstract

Azetidines, eg. saturated four-membered ring nitrogen heterocycles, are much less studied thant their higher or lower homologues, pyrrolidines and aziridines. Besides, they combine specific reactivity owing to the strain present in the four-membered ring, and to the basicity of the amine. Few years ago, an original synthetic route towards these heterocycles was discovered in our group **[1]**, allowing an easy access to homochiral and functionnalized azetidines. This boosted studies directed to their reactivity, that selected pieces will be presented in this talk **[2]**. Azetidines display in some cases unexpected reactivity **[3]** that can be the driving force for the discovery of new reactions of broad value.
A recent example will be presented: it highlights the discovery process from an unexpected reaction in the field of azetines chemistry, to the development of a new process allowing to perform two consecutive orthogonal CuAAC click reaction on the same carbon atom, opening avenues for many applications **[4,5]**.

Keywords: thiadiazole; antimicrobial; antifungal; adamantine.

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RECENT ADVANCES IN RING TRANSFORMATIONS OF HETEROCYCLIC COMPOUNDS

El Mokhtar Essassi

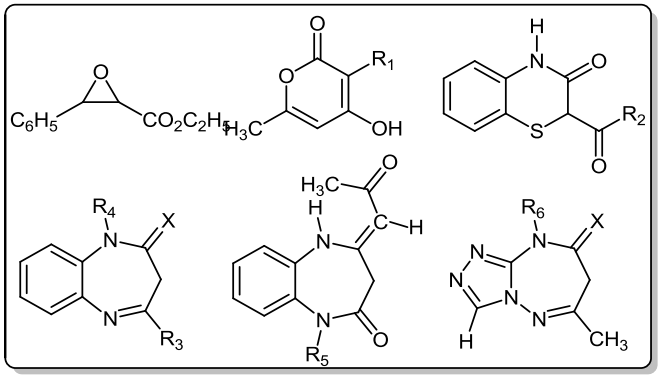
Laboratoire de Chimie Organique Hétérocyclique,URAC 21,
Centre de Recheches en Sciences des Médicaments
Pôle de Compétence Pharmacochimie
Centre Composites et Nanocomposites, MASCIR, Rabat, Morocco
Académie Hassan II des Sciences et Techniques

Email: emessassi@yahoo.fr

Abstract

Heterocyclic compounds play a vital role in biological systems and are of immense importance in the fields of pharmaceuticals, agrochemicals, and also in other industrial points of view. The development of new strategies and technologies for their synthesis have been studied. Thus ring transformations of heterocyclic systems constitute an useful tool in planning synthesis of target organic compounds. They are an interesting tool and beautiful class of organic reactions classified into four groups: classical ring transformation, degenerate ring transformation, ring contraction and ring enlargements and pseudo ring transformation or ring-chain transfer.

As starting materials we have used glycidic ester, triacetic acid lactone, dehydroacetic acid, 1,5-benzodiazepines, 1,4-benzothiazines, and triazolotriazepines. Reaction mechanisms of these ring transformations have been proposed and discussed.



Keywords: Domino reactions; enantioselective synthesis; natural products; molecular switches; fluorescence dyes; Palladium; CH-activation.

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ATROPOSELECTIVE SYNTESIS OF AXIALLY CHIRAL HETEROBIARYLS

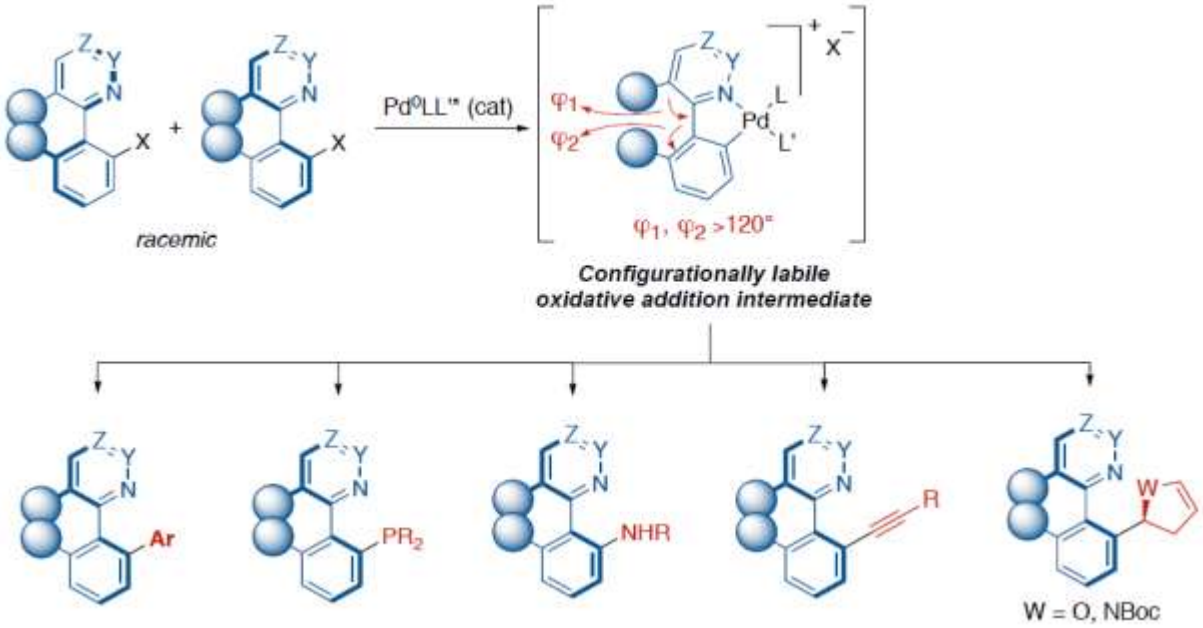
José M. Lassaletta

Instituto Investigaciones Químicas (CSIC-US), C/ Américo Vespucio, 49, 41092 Sevilla, Spain.

Email: jmlassa@iiq.csic.es

Abstract

The enantioselective synthesis of axially chiral heterobiaryls (e.g. 2-arylpyridines/isoquinolines) remains as one of the major synthetic challenges in the field of asymmetric cross-coupling reactions. In this lecture, a strategy based on Pd0-catalyzed dynamic kinetic asymmetric couplings of configurationally stable heterobiaryl electrophiles will be discussed. The strategy relies on the labilizacion of the stereogenic axis in the cationic oxidative addition intermediates and include Sukuki-Miyaura reactions **[1]**, C–P couplings **[2]**, Buchwald-Hartwig aminations **[3]**, copper–free Sonogashira couplings **[4]** and Heck reactions **[5]**.



Keywords: 1,3-dipolar cycloaddition; triazole; tetrazole; 2D NMR.

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MECHANISTIC STUDIES ON THE EPOXIDATION AND AZIRIDINATION REACTIONS

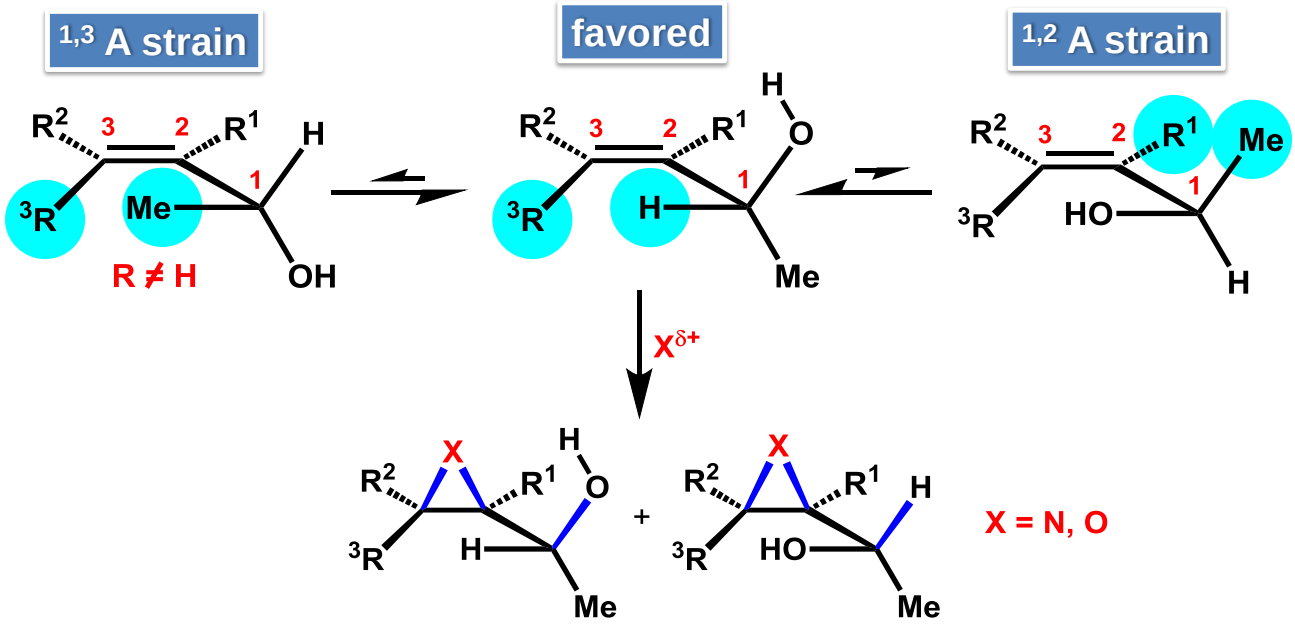
Hamdullah Kilic

Atatürk University, Department of Chemistry, Erzurum, Turkey

Email: hkilic@atauni.edu.tr

Abstract

Epoxidation and aziridination of double bonds are key reactions in synthetic chemistry, since they offer an access to preparation of synthetically useful products. A great deal of efforts has been devoted not only to development of novel methods but also mechanistic aspects of these reactions to elucidate the heteroatom-transfer processes. In this respect, conformationally fixed-chiral allylic alcohols have been used as mechanistic tools to rationalize heteroatom transfer mechanism.



The lecture will cover our recent mechanistic studies on the epoxidation and aziridination reactions of conformationally fixed-chiral allylic alcohols **[1-3]**.

Keywords: epoxidation; aziridination; allylic alcohol; diastereoselectivity.

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MECHANISTIC STUDIES ON THE EPOXIDATION AND AZIRIDINATION REACTIONS

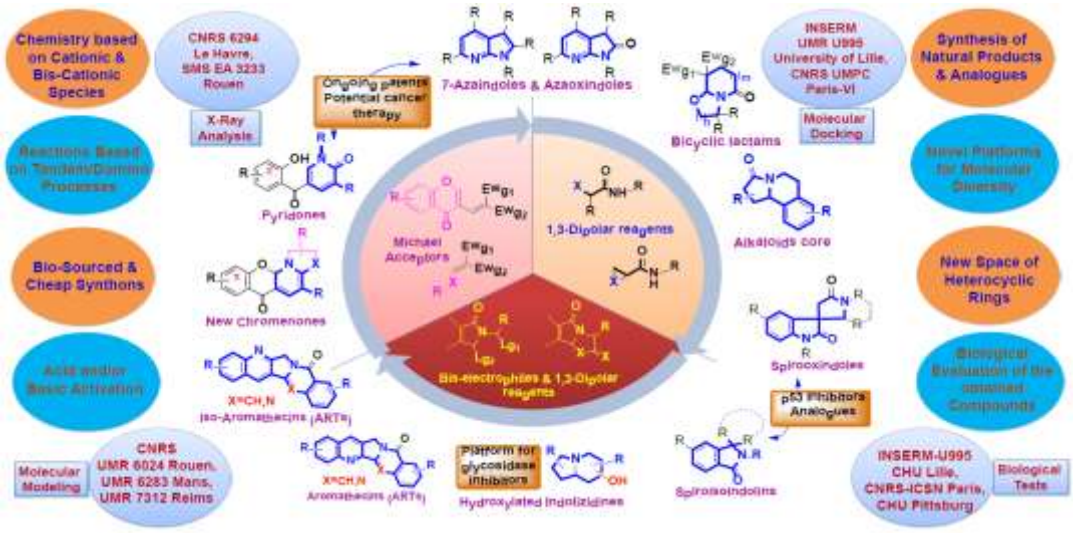
Adam Daïch

Normandie Univ, UNILEHAVRE, FR 3038 CNRS, URCOM-EA 3221, 76600 Le Havre, France.
Université Le Havre Normandie, UFR des Sciences et Techniques, 25 Rue Philippe Lebon, BP. 1123, F-76063 Le Havre Cedex, France.

Email: adam.daich@univ-lehavre.fr

Abstract

Our group at University of Le Havre-Normandy is interested since decades now in several research topics based in particular on the exploration of ionic chemistry. The synthetic methodologies we elaborate are generally simple and short and led to the construction of aza-heterocyclic platforms with promising biological activities. Among the targeted structures, below is given a non-exhaustive overview.



Besides the molecular hybrids derived of numerous alkaloids mentioned in this scheme (typically protoberberines, camptothecins, aromathecines, rutaecarpines, and luotonines known for their potent antitumor activities), it will be question in this presentation to discuss approaches developed to provide an array of highly functionalized compounds containing an aza-cyclic nuclei such as pyridone, indole, isoindole, oxindole and azaindole.
After determination and optimization of the best possible ways to these systems, certain compounds issued from these investigations showed inhibitive properties of the enzyme topoisomerase-I, tubulin polymerase and farnesyltransferase (FTase) inhibition activities including, more interestingly, tubulin and FTase dual activity explored for the first time.

Keywords: Ionic Chemistry; Aza-Heterocycles; Advanced Synthetic Intermediates; Tandem/Domino Process; Alkaloids; SAR Study; Bioactive Compounds; Health.

References

The references relative to these works and in particular those of these five last years can be found via the following link: https://urcom.univ-lehavre.fr/spip.php?article102.

SYNTHETIC APPROACHES FOR NEW PYRAZOLES

Hussein El-Kashef

Chemistry Department, Faculty of Science, Assiut University, 71516 Assiut Egypt

Email: elkashef@aun.edu.eg

Abstract

Pyrazole and its derivatives play an important role in medicinal and pesticide chemistry. They possess a wide range of bioactivities such as antimicrobial, anticancer, anti-inflammatory, antidepressant, anticonvulsant, antiparasitic, antipyretic, antiallergic, antihypertensive, antiviral activities **[1-12]** and as adenosine receptor antagonists **[13]**.

Zaleplon **[14]**, celebrex **[15]**, sildenafil **[16]**, allopurinol **[17]** and dipyrone **[18]** are some examples of pyrazole-based drugs which exist already in the market.
Many synthetic procedures exist for the synthesis of substituted pyrazoles. However, the development of simple, facile and efficient methodologies to get pyrazole derivatives and biologically active heterocycles containing the pyrazole moiety is always desired.
Several new pyrazole derivatives and pyrazole-containing heterocyclic systems have been synthesized using 1,3-disustituted-1*H*-pyrazol-5(4*H*)-one, or pyrazole aminonitrile and pyrazole aminoester derivatives as starting materials. Different synthetic strategies leading to different new pyrazole-based heterocyclic systems will be presented and discussed. The biological activities of some of the compounds prepared will be highlighted.

Keywords: Pyrazole; pyrazole derivatives; fused pyrazoles; five-membered ring; 1,2-diazole.

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CONCEPTION TO THE BIOLOGICAL AND ANTI-CORROSIVE EVALUATION OF NEW ORGANIC AND HETEROCYCLIC SYSTEMS IN THE LABORATORY ''LCOA''

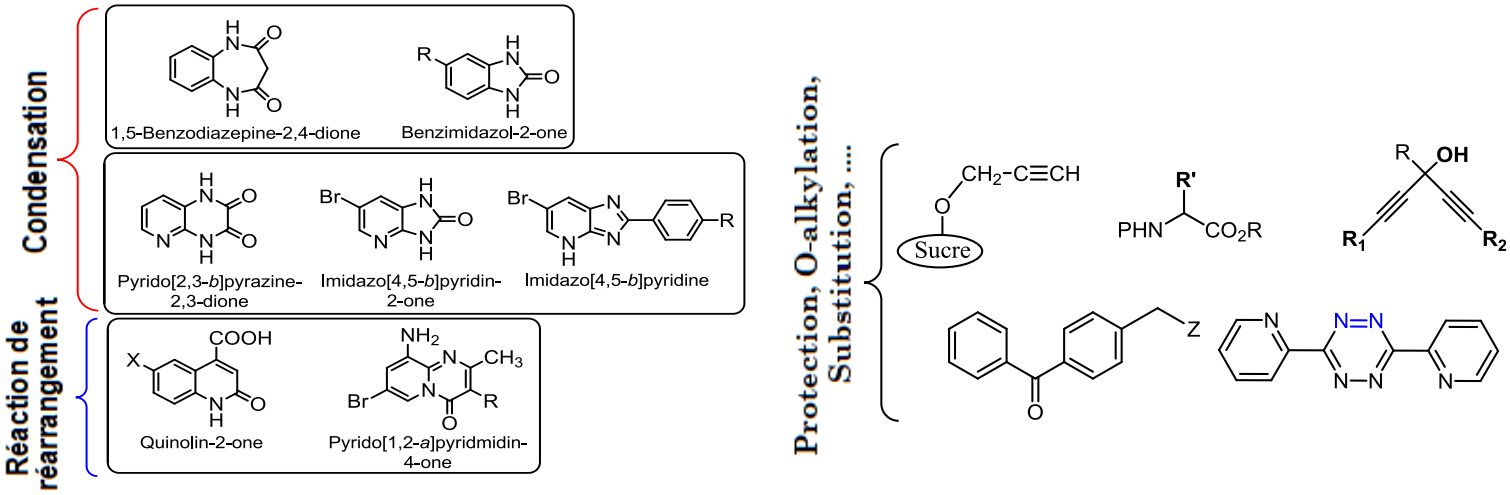
Y. Kandri Rodi*, A. Ben Tama, F. Ouazzani, E.M. El Hadrami

Laboratory of Applied Organic Chemistry, Faculty of Science and Techniques, Sidi Mohamed Ben Abdellah, University – Fez, Morocco.

Email: youssef_kandri_rodi@yahoo.fr, youssef.kandrirodi@usmba.ac.ma

Abstract

New approaches in heterocyclic synthesis have been used to discover new molecules that could be of potential therapeutic interest. During the last five years of research in the field of organic synthesis, we have synthesized new derivatives of great richness, characterized by a high molecular diversity (1,5-benzodiazepin-2,4-dione, imidazopyridine, benzimidazolone, quinoleines, sugars, aminoacids, dialcynylacrbinols, benzophenone, 3,6-bis(2-pyridyl) pyridazine …).



The synthesis methods adopted involve a limited number of substrate and reagent:

1- Compounds derived from *o*-phenylenediamine, 2,3-diaminopyridine, amino acid, sugar, benzophenone, etc. are engaged in cyclocondensation reactions under conventional conditions or under catalytic activation.

2- The heterocycles thus prepared have been used as raw materials to react with various reagents of choice making it possible to introduce various atoms or groups of atoms capable of rendering the compounds more soluble and capable of presenting potential activities in pharmacological, corrosive or materials for energy.

OXIRANYLLITHIUMS: FROM FLEETING, ELUSIVE INTERMEDIATES TO POWERFUL SYNTHONS

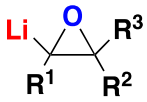
Saverio Florio

CINMPIS Consorzium, Università di Bari,
Via E. Orabona 4, 70125 Bari, Italy

Email: saverio.florio@uniba.it

Abstract

Strained cyclic compounds such as functionalized three-membered ring systems are of considerable contemporary interest due to their ability to impose conformational restrictions and to act as useful building blocks for the construction of relatively complex substances occurring frequently in natural products and biologically active molecules.
The chemistry of saturated small-ring heterocycles has been dominated till recently by ring opening reactions caused by nucleophilic reagents. The possibility that these rings could act as nucleophiles, in their anionic form, has been much less investigated at least till a few years ago. Once considered as fleeting, elusive intermediates, □-lithiated saturated small-ring heterocycles have risen to the state of useful synthons. Indeed, they can be generated by Li-H or Li-Sn, Li-Si, Li-halogen exchange from promptly available parent precursors. Their chemistry, structural properties including spectroscopic features, and synthetic applications are object of an ample literature **[1-5]**.



The present lecture will focus on heterosubstituted organolithiums such as lithiated aryloxiranes, their generation and synthetic applications. It will be shown that such reactive intermediates are good building blocks for the synthesis of functionalized epoxides, add to Fischer carbene complexes and nitrone ending up with the formation of highly functionalized, conformationally constrained cyclopropanes and oxazetidines, epoxylactones, alkenes, α-, β- and γ-aminoacids.
The configurational stability and the stereochemistry of their reactions will be discussed as well as the utility in asymmetric synthesis.

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THE CYCLOADDITION WAY TO SACCHARIDIC ANTI-PATHOGENS

Cristina Nativi

Department of Chemistry "Ugo Schiff" , University of Florence, via della Lastruccia,13 - 50019 Sesto Fiorentino (FI) Italy

Email: cristina.nativi@unifi.it

Abstract

Inverse electron-demand [4+2] cycloadditions involving glycals as electron rich dienophiles and alpha,alpha'-dioxothiones as electron poor dienes, are powerful reactions to afford *O*glycosides chemo-, regio- and stereoselectively. **[1]** Relying on these versatile reactions, diastereomerically pure *O*-glycosides have been prepared and used as starting material to obtain oligosaccharides, glycopeptides and glycoproteins. Among recent applications, the synthesis of a fucose mimetic and of two antigen mimetics (the mimetic of the melanoma antigen GM3 lactone and the mimetic of the mucin antigen Tn) will be discussed. **[2-3]** Thanks to their structure versatility, these three mimetics have been used to decorate multivalent constructs, including nanoparticles, **[4]** nano fibers, a cyclopeptidic (RAFT) **[5]** scaffold as well as proteins. Binding studies and biological assays run with the multivalent architectures will be presented.

Keywords: [4+2] cycloaddition; glycan mimetics; fucose-binding lectin; immunostimulants.

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CHEMICAL AND PHYSICO-CHEMICAL PROPERTIES OF FLAVYLIUM DERIVATIVE COMPOUNDS: PUTATIVE INDUSTRIAL APPLICATIONS

Victor de Freitas

REQUIMTE/LAQV, Departamento de Química e Bioquímica, Faculdade de Ciências, Universidade do Porto, Rua do Campo Alegre, 687, 4169-007 Porto, Portugal

Email: vfreitas@fc.up.pt

Abstract

Anthocyanins are natural flavylium pigments present in many flowers and fruits that are responsible for their appealing colors (from orange to blue). Despite their great interest, there are some drawbacks that have been limiting their technological applications such as their low chemical stability to pH change and their low solubility in lipophilic media **[1]**. In order to overcome these issues, natural-inspired chemistry reactions have been developed in order to synthesize new and more valuable pigments for different applications.

One of these classes of pigments are pyranoanthocyanins that were found for the first time in wines **[2]**. Their chemical formation pathway involves a cyclic addition onto carbon 4 and the hydroxyl group at the carbon 5 position of the anthocyanin, yielding a fourth ring that is responsible for the higher stability to hydration of these compounds when compared to the original anthocyanins. Over the years, several families of pyranoanthocyanins have been described in the literature including vitisins, methylpyranoanthocyanins, oxovitisins, acetylpyranoanthocyanins, pyranoanthocyaninphenolics, pyranoanthocyanin-flavanols, portisins, pyranoanthocyanin dimers **[2,3]**.

The diverse colors presented by pyranoanthocyanin pigments and their higher color stability at a wide pH range are important features indicating to have a great potential for different applications in foods, cosmetics, pharmaceuticals, dye-sensitizer solar cells among others.

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Invited Lectures

NEW DEVELOPMENTS IN THE FIELD OF Pd-AAA

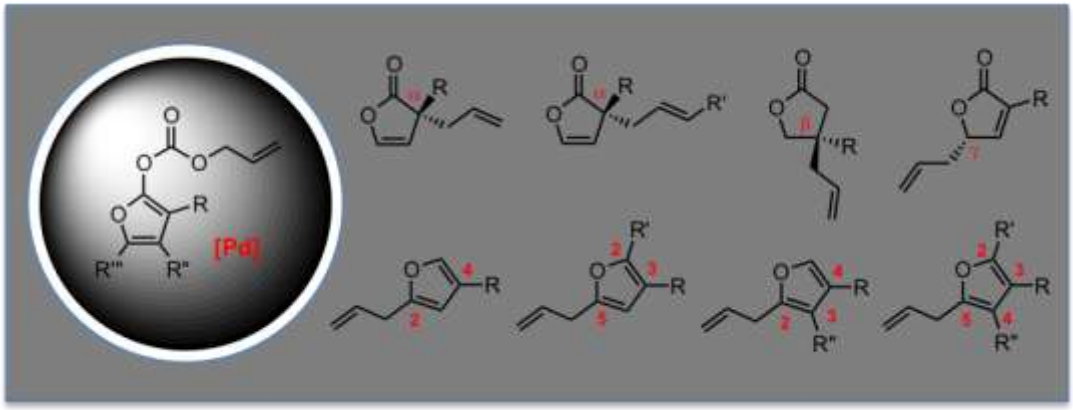
Stellios Arseniyadis

School of Biological and Chemical Sciences, Queen Mary University of London

Email: s.arseniyadis@qmul.ac.uk

Abstract

Since the pioneering work of Stoltz, Tunge and Trost about a decade ago, the palladium-catalysed asymmetric allylic alkylation reaction (Pd-AAA) has become a particularly attractive method for the enantioselective construction of C-C bonds. Our group has also contributed to this field of research by applying the Pd-AAA to cyclic dienol carbonates to afford diversely substituted heterocycles in a highly effective manner. This key reaction was also used in the total synthesis of various natural products, including (-)-nephrosteranic acid and (-)-roccelaric acid **[1-4]**.



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ENANTIOSELECTIVE SYNTHESIS OF PROLINATES AS KEY PRECURSORS OF BIOACTIVE HETEROCYCLES

José M. Sansano[a,b,*], Carmen Nájera[a], Miguel Yus[a]

[a]*Departamento de Química Orgánica, Instituto de Síntesis Orgánica (ISO), and Centro de Innovación en Química Avanzada (ORFEO-CINQA). Universidad de Alicante, Apdo. 99, E-03080-Alicante, Spain.*
[b] *Instituto de Síntesis Orgánica Universidad de Alicante, Apdo. 99, E-03080-Alicante, Spain.*

**For correspondence: Email: jmsansano@ua.es*

Abstract

Azomethine ylides are useful synthetic intermediates to access complex molecules, and in consequence, their precursors are valuable building blocks in the elaboration of structurally diverse biologically important heterocycles and natural products **[1]**. The main utility of these dipolar intermediates is as component of 1,3-dipolar cycloaddition (1,3-DC) together with electrophilic alkenes. Inter- and intramolecular versions of these types of 1,3-DCs provide a potentially flexible and versatile entry into the complex molecular framework with a pyrrolidine core. These cycloadditions reach a special dimension when the catalytic enantioselective process is successfully implemented. In this way, up to four contiguous stereogenic centers can be unambiguously generated in just one single step **[2]**.
Here, we demonstrate the utility of the enantioselectively generated prolinates as key building blocks for the generation of interesting molecules from the biological point of view. Thus, when acrylates are employed as dipolarophiles antiviral agents can be obtained. Nitroalkenes are useful to obtain nitroprolinates, which can be derived to analgesic, antituberculosis, inhibitors of farnesyl transferase, etc. Among this, they have been employed as organocatalysts in aldol reactions.

Keywords: 1,3-dipolar cycloaddition; prolinates; asymmetric catalysis.

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ACCESS TO DIFFERENT SIZED HETEROCYCLES VIA SILYL-PRINS CYCLIZATION

A. Barbero*, A. Diez-Varga, C. Díez-Poza

Departamento de Q Orgánica, Facultad de Ciencias,Campus Miguel Delibes, 47011 Valladolid, Spain.

**For correspondence: Email: asuncion.barbero@uva.es*

Abstract

Oxygen and nitrogen heterocycles are structures present in a large variety of biologically active compounds. Prins cyclization of acyclic precursors has emerged as one of the most efficient ways to prepare heterocycles **[1,2]**. The use of silylated alkenols as electron-rich alkene derivatives, in the so-called silyl-Prins cyclization, has shown to imply several advantages such as faster reactions or higher selectivity.

As part of our interest for the preparation of different sized heterocycles **[3,4]** using the chemistry of organosilanes, we here present an approach to the synthesis of different sized oxacycles and azacycles by means of a silyl-Prins reaction of silyl alkenols with an aldehydes. The factors controlling the process (such as substitution of the starting alcohol, nature of the Lewis acid, temperature, etc) will be discussed.

Keywords: Prins cyclization; organosilanes; stereoselective.

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RECENT DEVELOPMENT ON PORPHYRINIC CHEMISTRY AND APPLICATIONS

Nuno M. M. Moura[a], Ana T. P. C. Gomes[a,b], Kelly Castro[a,b], Mariana Q. Mesquita[a], M. Graça P. M. S. Neves[a], **M. Amparo F. Faustino[a,*]**

[a]*QPPNA and Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal*
[b]*Laboratory of Bioinorganic and Catalysis, Federal University of Paraná, Department of Chemistry, CP 19081, CEP 81531-990, Curitiba, Paraná, Brazil*

**For correspondence: Email: faustino@ua.pt*

Abstract

Porphyrins and analogues are a class of dyes that are being the object of intense research research for different applications in the last century due either to the important biological roles that they display or the interesting photophysical properties like strong light absorption, high emission, and an efficient ability to generate cytotoxic oxygen species when considered its use in medicine field. The use and efficacy of these macrocycles for a specific application is strongly dependent on their structural features that compounds can have, which explain the high number of studies related with the preparation and modification of natural and synthetic porphyrin derivatives. In particular, the use of synthetic macrocycles like porphyrins, corroles and phthalocyanines has been considered a good alternative to the use of natural porphyrins due to their less complex structures and easily synthetic accessibility. The usefulness of this type of derivatives can be improved through the adequate functionalization at β-pyrrolic positions or at meso positions.
In this communication, it will be discussed how simple transformations conducted in this type of templates can afford compounds with high PDT efficiency towards cancer cells and to photoinactivate microorganisms **[1-3]**.

Keywords: Porphyrins; Functionalization; Photodynamic Therapy.

Acknowledgements: Thanks are due to the University of Aveiro and FCT (Fundação para a Ciência e a Tecnologia) for the financial support to the QOPNA research project (FCT UID/QUI/00062/2013) through national funds and where applicable cofinanced by FEDER under the PT2020 Partnership Agreement, and also to the Portuguese NMR Network. ATPC Gomes, NMM Moura and MQMesquita thanks FCT for their postdoctoral and doctoral grants, SFRH/BPD/79521/2011, SFRH/BPD/84216/2012 and SFRH/BD/112517/2015 respectively. Kelly A. D. F. Castro also thanks CNPq for the post-doctoral scholarship (Process 201107/2014-7). The authors wish also to thank the financial support provided by the Project Transnational FCT-CNRST-Morocco 2017-2018.

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MARINE-FUNGI NATURAL PRODUCTS AS MODELS FOR NEW ANTIBACTERIAL AGENTS

Emília Sousa[1,2,*], Solida Long[1,2], Papichaya Boonpothong[1,2], Diana Resende[1,2], Artur M. S. Silva[3], Anake Kijjoa[1,4], Madalena Pinto*[1,2]

[1]*Laboratório de Química Orgânica e Farmacêutica, Departamento de Ciências Químicas, Faculdade de Farmácia, Universidade do Porto, Portugal*
[2]*CIIMAR – Centro Interdisciplinar de Investigação Marinha e Ambiental, Portugal*
[3]*QOPNA, Departamento de Química, Universidade de Aveiro, Portugal*
[4]*Instituto de Ciências Biomédicas Abel Salazar, Universidade do Porto, Portugal.*

**Email: madalena@ff.up.pt*

Abstract

The marine environment is an exceptional reservoir of bioactive natural products, many of which have unique structural features. Particularly fumiquinazolines, containing a pyrazino[2,1-b]quinazoline-3,6-dione core linked to an indole moiety have emerged in the last two decades have revealed very promising activities, especially in the field of chemotherapics **[1]**.
Nevertheless, some of them contain complex structures with unfavorable chemical stability and/or were isolated in small quantities as pure bioactive compounds.Herein, we highlight the emerging results within this class of natural products and our approach in the discovery of potential antibacterial agents through total synthesis of a marine product and their analogues. A highly efficient three-component one-pot methodology promoted by microwave irradiation was followed for the total syntheses of fumiquinazolines and several stereoisomers were obtained.

Keywords: Fumiquinazolines; antibacterial; total synthesis; fungi derived marine products.

Acknowledgements: This work was supported by the project INNOVMAR - Innovation and Sustainability in the Management and Exploitation of Marine Resources (reference NORTE-01-0145-FEDER-000035, within Research Line NOVELMAR), supported by North Portugal Regional Operational Programme (NORTE 2020), under the PORTUGAL 2020 Partnership Agreement, through the European Regional Development Fund (ERDF). To Dr Sara Cravo, for technical assistance.

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A UNIQUE STRATEGY - SEVERAL TOPOLOGIES: SELECTED EXAMPLES OF HELICAL, TWISTED, ANGULAR AND PLANAR ARCHITECTURES

Damien Prim

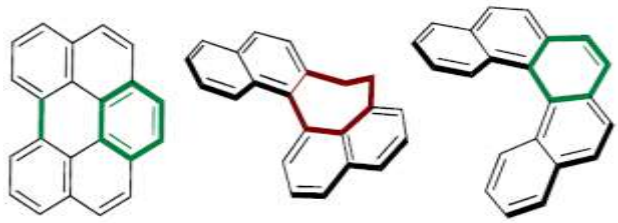
Institut Lavoisier de Versailles - UMR CNRS 8180
Université de Versailles St-Quentin-en-Yvelines 45 avenue des Etats-Unis 78035 Versailles

**For correspondence Email: damien.prim@uvsq.fr*

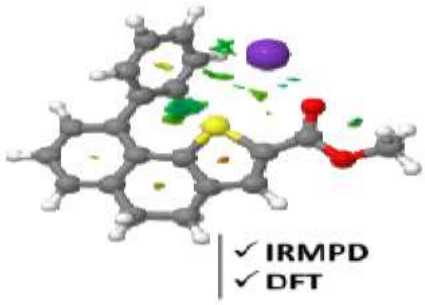
Abstract

The shape of molecular architectures is set by favourable interactions between atoms or functional groups but also often imposed by unfavourable connections as well as steric or electronic preclusions.

Within this context, the scientific community tends to mimic especially skillful biological processes in order control topology, complexity or diversity of well defined molecular architectures and reach accurate properties.
The access to helical, twisted, angular and planar architectures will be detailed from a unique molecular platform as shown hereby. Several aspects including synthesis, catalysis, characterization, theoretical calculations will be presented.



The impact of the presence, nature and position of heteroatoms embedded into such molecular architectures over their topology and properties will be also discussed. Finally, examples of topology / properties relationships will be given.



H_2O_2-HX IN THE SYNTHESIS OF HETEROCYCLIC QUINONES

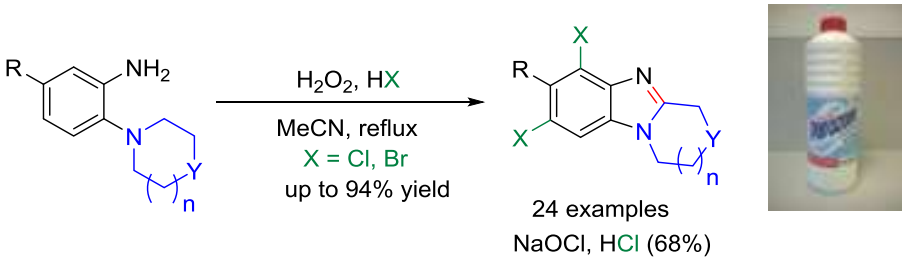
Fawaz Aldabbagh

Department of Pharmacy, School of Life Sciences, Pharmacy and Chemistry, Kingston University, Penrhyn Road, Kingston upon Thames, Surrey KT1 2EE, UK

Email: f.aldabbagh@kingston.ac.uk

Abstract

Our group is interested in the discovery of new heterocyclic quinone anti-cancer agents **[1-6]**. One-pot hydrogen peroxide and hydrohalic acid-induced ring closure of commercial *o*-cyclic amine substituted anilines gave new selectively dihalogenated benzimidazoles. Domestic bleach with HCl can be used for a one-pot ring-closure and chlorination **[7]**. There are many advantages to using H_2O_2 in synthesis; it is cheap and low in molecular weight with the by-product being water. This thought provoking presentation describes our use of H_2O_2-HX in the one-pot synthesis of new heterocyclic quinones from commercial anilines **[8,9]**.



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HETEROCYCLES: FROM REACTIVITY TO DIVERSITY

Serge Thorimbert

Sorbonne Universités, Université Pierre et Marie Curie, Institut Parisien de Chimie Moléculaire. F-75005 Paris, France.

Email: serge.thorimbert@upmc.fr

Abstract

Since 2010 our team works on the synthesis and the functionalization of original heterocycles. We prepared 2-substituted 4H-pyrido[e][1,3]oxazin-4-ones which have been identified in 2009 as a new potential source of original small molecules in a list of hundred virtually generated heteroaromatic rings **[1]**. These compounds have been the precursors for the preparation of original heterocycles (triazines, oxadiazoles, triazoles) including fluorescent one **[2]**. A second project is dealing with the reactivity of methyl coumalate **[3]** as a perfect substrate for the stereoselective preparation of various products such as dienoic acids, lactones, pyrans or even trifluoromethyl benzophenones.

We will present our results and discuss how they may enter into collaborative work.

Keywords: cycloaddition; heteroaromatic; fluorescence.

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A NEW ERA FOR ANTICOAGULANT AGENTS: FROM PHARMACEUTICAL RESEARCH TO CLINICAL SETTING

Mario Schiavoni*, Antonella Coluccia

Hemophilia and Rare Coagulopathies Centre P.O. "I.Veris delli Ponti", Scorrano
Azienda Sanitaria Locale-Lecce, Italy

**For correspondence: Email: marioschiavoni@gmail.com*

Abstract

Heparins, vitamin K antagonists (VKAs), and antiplatelet agents, mainly aspirin, have represented the most effective agents for prevention and treatment of thrombosis in clinical setting over the last 60 years. Nevertheless they have some limitations such as the risk of bleeding as well as the need of VKAs to be periodically monitored by laboratory controls, so that pharmaceutical research is committing itself to develop new drugs able to minimize disadvantages. Recently four novel oral anticoagulants are commercially available: dabigatran etexilate, rivaroxaban, apixaban, edoxaban. They, called "direct oral anticoagulants" (DOACs), may be given in fixed dose and do not require laboratory control **[1]**. Generally heparins and VKAs can inhibit different factors in the three phases of coagulation: initiation, propagation, and termination. DOACs target directly only one factor. Dabigatran inhibits thrombin while rivaroxaban, apixaban and edoxaban target F.Xa respectively **[2]**. More recently other new anticoagulants have been proposed such as inhibitors of FXI and FXII. The interest of these drugs derives from experimental data suggesting that they attenuate thrombosis without affecting hemostasis. FXI may be inhibited by FXI-antisense oligonucleotides, such as a 2′-O- (2-methoxyethyl) (2′-O-MOE) second-generation ASO, that specifically reduces human FXI messenger RNA expression in the liver and consequentely lowers hepatic synthesis of FXI. FXII may be considered a better potential anticoagulant than FXI, but data on FXII inhibition by ASO or specific antibodies are available only in experimental animal models **[3]**.

Keywords: heparins; vitamin K antagonists; direct oral anticoagulants (DOACs).

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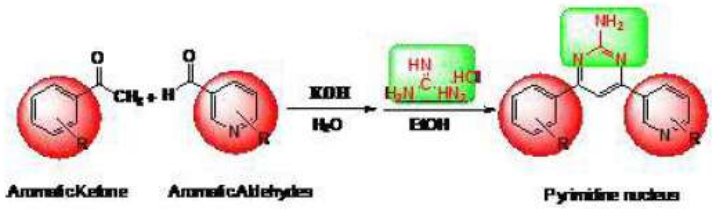
BI-ARYL PYRIMIDINES: POTENT BIOLOGICALLY ACTIVE PHARMACOPHORES

Islam Ullah Khan*,Tanzeel Ur Rehman, Sadaf Riaz

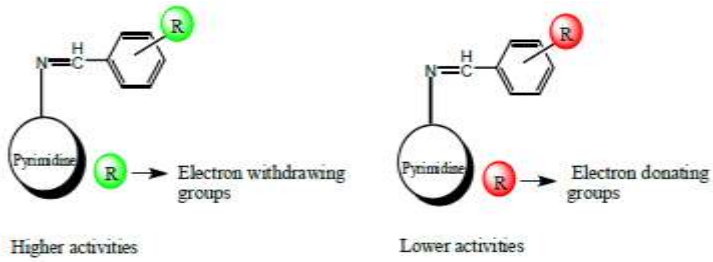
Department of Chemistry, GC University, Lahore 54000, Pakistan
**For correspondence: Email: iukhan@gcu.edu.pk*

Abstract

Chemistry of aza-heterocyclic compounds is an ever green field of organic synthesis and expanding area of research for chemists working not only in the area of natural products but also in the synthetic work.Pyridinecontainingcompounds are the most importantaza-heterocycles possessing wide range of biological activities. Their broad spectrum applications focus our research scheme to synthesize numerous novel compounds containing pyridine moiety and their preliminary screening would significantly develop bioactive compounds. Recently we devised an efficient procedure for the synthesis of novel substituted pyridine pyrimidinesand their significant derivatives as potent inhibitors (α, β-glucosidase,Lipoxygenase,) **[1,2]**.
Synthetic schemes are hereby illustrated



To further explore the contribution of different structural features exhibited by the compounds in relation bioactivities (% inhibition), we developed quantitative structure-activity relationship (QSAR) models. The knowledge furnished by such models unveils the structural trends present within set of compounds, and enable more rational future development.
Generally, it was noticed that pyrimidines containing para substituted phenyl ring exhibited higher activities than ortho and meta substituted phenyl ring as shown (Figure).



Keywords: 1,3-dipolar cycloaddition; prolinates; asymmetric catalysis.

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CHEMICAL GENOMICS PLATFORMS FOR THE DISCOVERY OF BIOACTIVE COMPOUNDS AND UNDERSTANDING THEIR MECHANISM OF ACTION

Mohamed Ettayebi

Sidi Mohamed Ben Abdellah University, Fez-Morocco

**For correspondence: Email: moettayebi@gmail.com*

Abstract

Chemical genomics combines chemistry with molecular genetics for exploring the function of unknown molecules and identifying biological pathways and processes via the use of small bioactive compounds. At the same time it, is being used to discover new bioactive chemicals using various cell-based screens. The most popular small model organisms used as screening platforms for the identification of small bioactive molecules and their molecular targets are the bacteria *Escherichia coli* and the yeast *Saccharomyces cerevisiae*. The efficiency and accuracy of genome-wide profiling was greatly enhanced with the use of barcoded gene deletion collections of such organisms.

Drug targets have traditionally been identified by the use of mutagenesis and conventional single nucleotide polymorphism (SNP)-mapping methodologies. However, the emergence of next generation sequencing (NGS) tools enabled a rapid nucleotide sequencing technologies that generate millions of sequence reads in short periods of time allowing precise genome wide comparisons.

Chemical-genomics profiling involves the screening of large chemical libraries against drug target families to rapidly identify and validate therapeutic targets. Indeed, hundreds of thousands of compounds can be screened with relative ease and large numbers of bioactive compounds can be assembled. The major challenge is in understanding the mechanism of action (MOA) and revealing mechanistic hypotheses for uncharacterized bioactive molecules.

We will present here new platforms for studying and identifying the biological target(s) of new bioactive compounds such as the use of reporter libraries, genome-wide deletion libraries, gene dosage, and deep sequencing to decipher the MOA of chemical compounds.

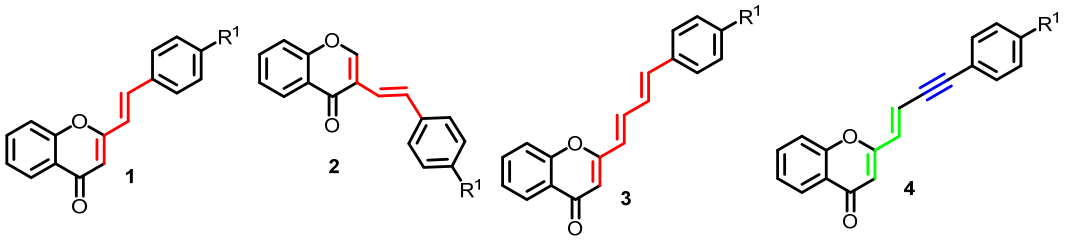
CHROMONES BEARING UNSATURATED SUBSTITUENTS AT C-2 AND C-3 AS BUILDING BLOCKS IN CYCLOADDITION AND CONJUGATE ADDITION REACTIONS

Artur M. S. Silva

Department of Chemistry & QOPNA, University of Aveiro, Campus de Santiago, 3810-193 Aveiro, Portugal
**For correspondence: Email: artur.silva@ua.pt*

Abstract

Chromones (or 4*H*-chromen-4-ones) are oxygen-containing heterocycles widely occurring in Nature foremost known for their biological and pharmacological properties **[1]**. It constitutes one of the most abundant group of naturally occurring compounds, although some of their classes are constituted by a small number of derivatives, such as the case of styrylchromones. This small class are constituted by nine natural derivatives and also by an huge number of synthetic analogues, which present important biological activities. Beyond that, they also have been involved in a series of chemical transformations very useful to create more complex and biological interesting new heterocycles **[2]**.
Taking into account our interest on the chemistry of chromones, namely on derivatives bearing unsaturated substituents at C-2 and C-3, we have established new synthetic routes for (*E*)-2- and 3-styrylchromones **1** and **2**, 2-[(1*E*,3*E*)-4-arylbuta-1,3-dien-1-yl]-4*H*-chromen-4-ones **3** and (*E*)-2-(4-arylbut-1-en-3-yn-1-yl)-4*H*-chromen-4-ones **4** and studied the reactivity of their unsaturated systems in cycloaddition and conjugate addition reactions **[2,3]**. In the present communication, it will be presented and discussed some results on the referred transformations.



Keywords: Chromones, Cycloaddition reactions, Conjugate Additions, MW-assisted organic transformations.

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Short Talks

SYNTHESIS OF NEW HETEROCYCLIC COMPOUNDS BASED ON N,N-CYCLIC AZOMETHINE IMINE SCAFFOLD

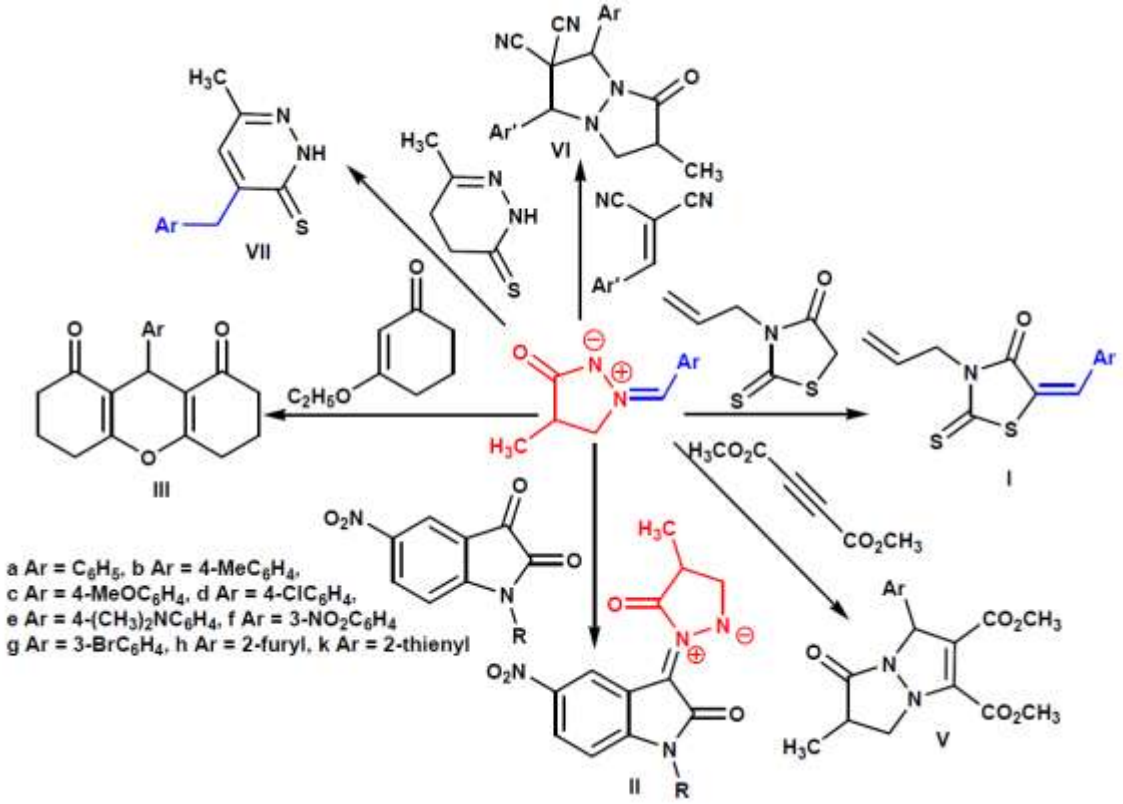
E. M. Rakib* R. El Ajlaoui, O. Amiri

Laboratoire de Chimie Organique et Analytique, Faculté des sciences et Techniques, Université Sultan Moulay Slimane, BP : 591, Beni-Mellal, Maroc.

**For correspondence: Email: elmostapha1@ymail.com*

Abstract

N,N′-Cyclic azomethine imines constitute a class of stable and easily accessible 1,3-dipoles and act as versatile and robust building blocks for the construction of structurally diverse N,N-bicyclic heterocycles with potential biological activities [**1**]. In this work, we investigated the reactivity of some heterocycles with various 4-methyl-3-oxo-1,2-pyrazolidinium ylides **2a-e**, in different conditions. These reaction conditions, lead unexpectedly to the formation of new heterocyclic compounds [**2,3**].



Keywords: 4-methyl-3-oxo-1,2-pyrazolidinium; heterocycles; cycloadducts.

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NEW DEVELOPMENT AROUND *N*-ACYLIMINIUM IONS CHEMISTRY

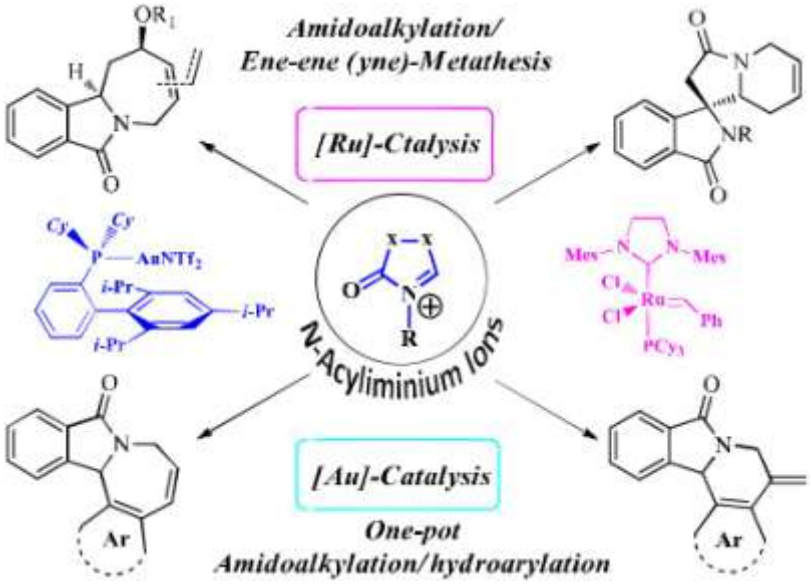
Mohamed Othman

Unité de Recherche en Chimie Organique et Macromoléculaire (URCOM, EA 3221, FR CNRS 3038), Université Le Havre-Normandie, 25 rue Philippe Lebon, BP 1123, 76063 Le Havre cédex, France

**For correspondence: Email: Mohamed.othman@univ-lehavre.fr*

Abstract

N-Acyliminium ions are important, reactive species in organic synthesis for the construction of carbon–carbon and carbon–heteroatom bonds **[1]**. The development of eco-friendly procedures for their implementation has recently became a subject of intensive investigations and Quite recently, our group has contributed to the development of improved conditions for *N*-acyliminium ion chemistry by documenting the use of **TIPSOTf, $HNTf_2$** and **$AuNTf_2$** as highly efficient catalysts for the α-amidoalkylation reaction.
These improved conditions triggered our curiosity to develop, in a first part, a novel approach combining our catalytic α-amidoalkylation reaction with a ring-closing metathesis, a strategy that allowed us to easily access to a new class of isoindolones (spirocyclic) compounds through the use of two catalytic processes **[2]**.



In a second part, we have used the dual hard/soft character exhibited by gold complexes to d v lopp d int mol cul "On -pot" F i d el-Crafts amidoalkylation/intramolecular hydroarylation sequence using $AuNTf_2$/$Ph_3PAuNTf_2$ as a model couple of gold catalysts **[3-4]**.

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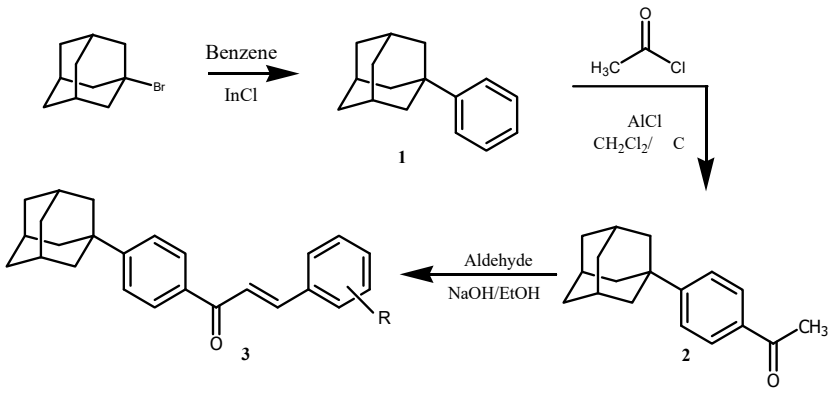
NEW ADAMANTYL CHALCONES : SYNTHESIS, ANTIMICROBIAL AND ANTICANCER ACTIVITIES

D.Tebbani[a]*, A. Tabbi[a], G. Turan-Zitouni[b], L. Rastrelli[c]

[a]Laboratoire des produits naturels et de synthèse, faculté des sciences, Université des frères Mentouri, Constantine, 25000 Algérie.
[b]Department of pharmaceutical chemistry, faculty of pharmacy, Anadolu University, Yunus Emre Campus 26470 Eskisehir, Turkey.
[c]Diparitmento di Farmacia, University of Salerno, Via Giovanni Paolo II 84084 Fisciano (SA), Italy.
***For correspondence : Email : dahmane.tebban@umc.edu.dz**

Abstract

Chalcones are very useful compounds due to their significant biological activity, which include anti-inflammatory, anti-oxidant, antiviral, antifungic, antitumor, antileishmanial, anti-HIV and others [1-3]. Chalcones are usually synthesized using the Claisen-Schmidt reaction, in basic medium in polar solvents, and purified by separation. Due to their abundance in plants and ease of synthesis, the chalcone class of compounds have attracted extensive studies. In recent years, the necessity of effective therapies has led to research in novel biologically active agents.
In the other hand, the incorporation of an adamantyl moeity into a variety of molecules results in compounds with relatively high lipophilicity, consequently they can modify the biological activity of these molecules.In almost all cases, an adamantyl-bearing compound will be more lipophilic than the corresponding without adamantyl analogue. We reported herein the synthesis, antimicrobial and anti-cancer activities of a new series adamantyl chalcones.



3a R=H, 3c R= Cl, 3d R= Br, 3f R= OMe, 3h R= SMe , 3l R=2-chloro-7 fluoro quinolyl, 3m R= 2-chloro-quinolyl.

Keywords : Adamantyl chalcones, Anticancer activity, MiaPaca2

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SYNTHESIS OF NEW HETEROCYCLIC COMPOUNDS BASED ON (E)-2-METHYL-3-ARYLIDENE CHROMAN-4-ONES

A. Mahfoud[a,*], M. Bakhouch[a], M. Chalkha[a], M. Akhazzane[b], A. Kerbal[a], M. El Yazidi[a], M. Daoudi[a] and G. Al Houari[a]

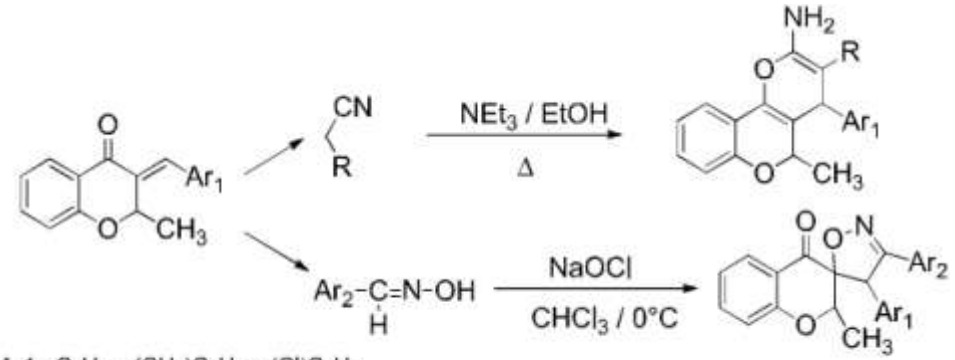
[a]*Laboratoire de Chimie Organique, Faculté des Sciences Dhar El Mahraz, Université Sidi Mohamed Ben Abdellah, BP: 1796, Fès, Morocco.*
[b]*Cité de l'innovation, Université Sidi Mohamed Ben Abdellah, Fès, Morocco.*

**For correspondence e-mail: asmae.mahfoud@hotmail.com*

Abstract

In our effort to synthesize new heterocyclic compounds with potential biological activity, we decided to study the behavior of (E)-2-methyl-3-arylidene chroman-4-ones with active methylene and nitrile oxide respectively, through cyclocondensation **[1]** and 1,3-dipolar cycloaddition.

In this work, we decided to describe in the first part the behavior of ethyl cyanoacetate and malononitrile with different (E)-2-methyl-3-arylidene chroman-4-ones in ethanol **[2]** in the presence of a base catalyst such as triethylamine **[3]**. And in the second part we studied the stereochemistry **[4,5]** of some new spiroisoxazolines obtained by the reaction of p-arylnitriloxide and (E)-2-methyl-3-arylidene chroman-4-ones.



Keywords: Michael 1,4-addition; Ethyl cyanoacetate; Malononitrile; dipolar-1,3 cycloaddition; *(E)*-2-methyl-3-arylidene chroman-4-ones.

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SYNTHESIS OF NOVEL HETEROCYCLIC LIGANDS BASED OF 3,6-BIS (PYRIDIN-2'-YL)PYRIDAZINE AND EVALUATION OF THEIR ANTIBACTERIAL AND ANTIOXIDANT ACTIVITIES

M. Filali, A. Ben-Tama*, E. M. EL Hadrami, S. Chakroune

Laboratoire de Chimie Organique Appliquée, Université Sidi Mohamed Ben Abdellah, Faculté des Sciences et Techniques, Route d'Immouzer, BP 2202 Fès, Maroc

**For correspondence: Email: bent_abslam@yahoo.fr / abdeslem.bentama@usmba.ac.ma*

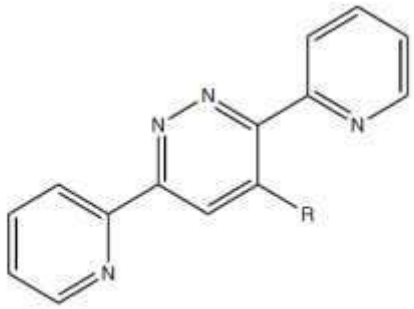
Abstract

A very large number of drugs and molecules which derived from natural substances, are heterocyclic compounds. These compounds are cyclic organic molecules having at least one different atom than carbon, such as nitrogen or oxygen. These kinds of molecules have considerable attention from researchers and industrialists because of their vast fields of application.

Heterocycles are very interesting chemical compounds in scientific research due to their potential for application in different fields, for which their synthesis has become a very important subject.

Indeed, the heterocycle constitutes the basic skeleton for a wide variety of compounds for chemical, biological, pharmacological and industrial interest.

In this point, we have been interested in the preparation of novel aromatic nitrogen heterocyclic ligands from dppn (3,6-bis (pyridin-2'-yl) pyridazine) (i.e. Scheme 1).



Scheme 1: Heterocycles based of dppn

After the synthesis and characterization of these molecules by different spectroscopic methods, a study of their antibacterial and antioxidant activity was carried out and showed a great activity related to the radical.

Keywords: heterocyles synthesis; (3,6-bis (pyridin-2'-yl) pyridazine); antibacterial; antioxydant.

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CTALYTIC ASYMMETRIC SYNTHESIS OF PYRROLIDINE DERIVATIVES

Özdemir Dogan

Middle East Technical University, Department of Chemistry, 06800 Ankara, Turkey

Email: dogano@metu.edu.tr

Abstract

Pyrrolidine derivatives are important building blocks of many natural compounds. Kainic acids and nicotine are two common examples. Literature has many methods for the synthesis of these compounds. Among these methods the most efficient one is the 1,3-dipolar cycloadditions of azomethine ylides with electron deficient olefins. By this method two "C-C" bonds and upto four stereogenic centers can be created. Recent studies related with this method mainly deals with the asymmetric construction of pyrrolidines using metal-catalysts and organocatalysts. Our group is also involved in developing a new chiral metal-catalysts and organocatalysts for the asymmetric synthesis of pyrrolidine derivatives via azomethine ylide chemistry. In this respect new amino alchol type chiral molecule complexed with zinc served as a good catalysts in the formation of pyrroldine structures in up to 84% ee which can be increased to >99% by crystallization **[1-4]**.

***Keywords*:** Asymmetric synthesis, pyrrolidines, azomethine ylides 1,3-dipolar cycloaddition

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BIO-ACTIVE FILMS BASED ON STYRYLQUINOXALINE-GRAFTED-CHITOSAN: ANTIBACTERIAL AND FLUORESCENT STUDIES

M. Fardioui[a,b,*], I. M. Kadmiri[c], A. Qaiss[a], R. Bouhfid[a]

[a]*Moroccan Foundation Advanced Science, Innovation and Research (MAScIR), Institute of Nanomaterials and Nanotechnology (INANOTECH). Rabat Design Center, Av Mohamed Jazzouli, Madinat El Irfane 10100, Rabat, Morocco*

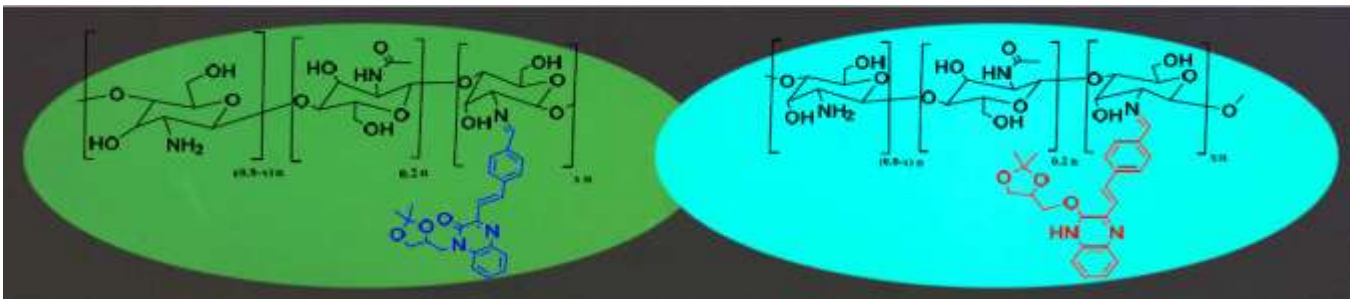
[b]*Laboratoire de Matériaux, électrochimie et environnement, Faculté des Sciences, Université Ibn Tofail, Kenitra,Morocco*

[c]*Moroccan Foundation Advanced Science, Innovation and Research (MAScIR), Biotechnologie verte. Rabat Design Center, Av Mohamed Jazzouli, Madinat El Irfane 10100, Rabat, Morocco*

**For correspondence: Email: fardimeriam@gmail.com*

Abstract

The quinoxalines derivatives constituted a large class of the heterocyclic compounds, due to their heterocyclic structure, quinoxalines derivatives are characterized by different biological activities, such as antibacterial activities **[1,2]**. In this work, two styryl-quinoxaline derivatives are synthetized in three steps; first 3-methylquinoxalin-2-one was prepared by condensation of o-phenylenediamine and ethyl pyruvate, then fused with 1,4-Phthalaldehyde to synthetize styryl-quinoxalin-2-one, followed by the alkylation of this latter by solketal tosylate. Structures of synthesized molecules were confirmed by FT-IR, ^{1}H, ^{13}C-NMR spectral data. The antibacterial test against Escherichia coli, Staphylococcus aureus, Bacillus subtilis and Pseudomonas Aeruginosa found a good activity of the two compounds against Pseudomonas Aeruginosa. These molecules are exploited to develop new active chitosan films by chemical grafting on the chitosan in solution followed by casting-evaporation process. Antibacterial test (against P. Aeruginosa) of the unmodified/modified chitosan films found all chitosan films are able to inhibit the growth of P.A by surface contact whose modified chitosan films were distinguished by their resistance to the antibacterial tests conditions, in contrary to unmodified chitosan, which are partially soluble in the same conditions.



Keywords: Styryl-quinoxaline; chitosan; solketal; antibacterial activity.

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2D-QSAR AND PHARMACOPHORE STUDIES ON N9-SUBSTITUTED HARMINE DERIVATIVES AS POTENTIAL ANTICANCER AGENTS

T. Akabli*, H. Toufik*, F. Z. Ahjyaje and F. Lamchouri

Laboratory of Materials, Natural Substances, Environment and Modeling (LMSNEM), Polydisciplinary Faculty of Taza, Sidi Mohamed Ben Abdellah University of Fez - Morocco.

*Corresponding authors: taoufik.akabli@usmba.ac.ma / hamid.toufik@usmba.ac.ma

Abstract

Heterocyclic compounds represent a wide range of natural products which play an important role in several areas due to their chemotherapeutic potential and their chemical novelty **[1]**. Thus, the β-carboline alkaloids, specially a planar heterocyclic with 2 N atoms at the first and 9th positions of the skeleton **[2]**, have attracted attention in medicinal chemistry due to their anti-cancer activity **[3]**.

A study of Quantitative Structure Activity Relationship (QSAR) was performed on a serie of 24 heterocyclic β-carbolines derivatives with cytotoxic activity divided into training and set test. The QSAR models were established using Principal Component Analysis (PCA), Partial Least Square (PLS) and Multiple Linear Regression (MLR) methods. The QSAR model was selected on the basis of various statistical parameters like: R^2 correlation coefficient, q^2 cross validation, R^2pred, standard error of estimation (SE) and fisher test (F). The best model was found having 5 descriptors with, R^2 = 0.73, q^2 = 0.50, fisher test = 7.63 and R^2pred = 0.88 and the 2D-QSAR analysis reveal that the cytotoxic activity of these compounds is governed by topological index, polar and steric descriptors. The pharmacophore model was built based on the six most active compounds. Results shown that the hydrophobic, hydrogen bond acceptor and the aromatic features are the important proprieties responsible of the activity of the β-carbolines derivatives studied in this work.

The 2D-QSAR and pharmacophore models developed will be used for the *in silico* screening of the new cytotoxic β-carbolines derivatives.

Keywords: Heterocyclic; β-carbolines derivatives; cytotoxicity; 2D-QSAR; pharmacophore.

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GREEN SYNTHESIS OF NEW DYES BASED ON PYRAZOLONE DERIVATIVES

J. Isaad[a,b,*], H. Bessbousse[c], A El Achari[d]

[a] *Faculté des Sciences & Techniques d'Al Hoceima, BP 34, 32003 Ajdir, Morocco* [b] *Université Mohamed, 1st. Bd Mohamed VI, BP: 717, 60000 Oujda, Morocco,*
[c]*Entité minéralurgie et procédé de traitement. OCP SA. Khouribga. Morocco*
[d]*Lille Nord de France University, Engineering and Textile Materials Laboratory, Lille, 2 Allée Louise et Victor Champier, 59100 Roubaix, France France*

** For correspondence: E-mail: j.isaad@ump.ac.ma*

Abstract

Heterocycles are an inescapable and integral feature of numerous diverse fields of chemistry. The organic dye chemistry is not an exception; heterocycles have been widely used in disperse dye chemistry. Recently, different eco-friendly synthetic methods were developed to prepare azoic dyes, and in this sense, an efficient and experimentally simple method to synthesis azoic dyes pyrazolone based **[1-3]** was developed in the presence of N-propyl-2-pyrrolidonium hydrogen sulfate ([H-NPP]HSO_4) supported on nano-sized silica-coated magnetite **[4]** as acid catalyst under solvent-free conditions in good to excellent yields.
The novel azoic dyes pyrazolone based were prepared with some advantages compared to the traditional synthesis methods such as a short reaction times, high yields and purity, easy work-up and reusability of catalyst.
The structure of these prepared azoic dyes was confirmed by UV-vis, NMR and mass spectroscopy, and the electronic properties of the new azo dyes were influenced by the substituent nature of the coupled pyrazolone moi ti s n d its compl m n t i ti s in th fo m d zoic compounds. Th sp ct oscopic d t ' s confi m th t th prepared azoic dyes existent in the hydrazone-keto and azo-enol tautomeric forms where the hydrogen bears by the *C–O–H* and *N-N– H* bonds are stabilized respectively by the nitrogen of the azo group and oxygen of both carbonyl groups present in the pyrazolone moiety.
In this presentation, a summary of the developed pyrazolone azoic dyes as well as their physic chemical properties will be presented.

Keywords: Pyrazolone; Azo dyes; nanoparticle; wate; reuse.

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BISPHOSPHONIC ACIDS: NEW THERAPEUTIC PLAYERS IN ONCOLOGY

Wafaa M. Abdou*, Azza A. Kamel

Chemical Industries Division, National Research Centre, Elbohouth St., Dokki, Cairo, Egypt

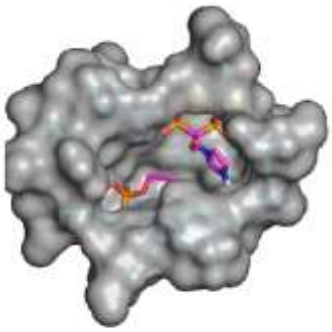
**For correspondence: Email: wabdou@link.net*

Abstract

In addition to inhibiting bone resorption, and chronic arthritis, bisphosphonates (BPs) and relevant BP-acids have also been shown to exhibit anti-tumor effects. *In vitro*, BPs inhibit proliferation and induce apoptosis in cultured human breast cancer cells. There is now a much greater appreciation of the benefits of introduction of BPs in oncology, which has dramatically changed the management of patients with cancer disease. Recently, BPs have been, however, proven to be the drugs of choice to:

i-Decrease in bone resorption in tumor disease.

ii- Decrease in hypocalcemia as a result of diminution of bone resorption that leads to a big decrease of new osteolytic lesions, and iii- Decease of fractures, which results in amelioration of pain and an improvement of the quality of life [1]. This antitumor potency of BPs, particularly *N*-BPs was attributed to the differences of their molecular mechanism of action. Thus, BPs can be grouped in two main different classes: first-generation is non-*N*-BPs and the second generation is *N*-BPs. First-generation of BPs, such as clodronate and etidronate, are metabolized intracellular to analogues of ATP by inhibiting ATP-dependent enzymes. In contrast, second- *N*-BPs, generation such as pamidronate and zoledronate, interfere with mevalonate biosynthetic pathway, by inhibiting farnesyl diphosphate (FPP) synthase [2]. Our recent, and present work considered an elaboration of a novel series of nitrogen- and/or sulfur heterocycles containing BP-acids. Several of these *N*-BP-acids reflected remarkable antitumor activity against breast, ovarian, and prostate carcinoma cell lines.



Mechanism of action of *N*-BPs

Keywords: *N*-heterocycles; terazoles; bisphosphonic acids (BP-acids); FPP- synthase docking.

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A NOVEL APPROACH TO THE SYNTHESIS OF ALKYL-SUBSTITUTED A3B PORPHYRINS

S. Cinar, P. Seyitdanlioglu, G. Altundal, C. Unaleroglu*

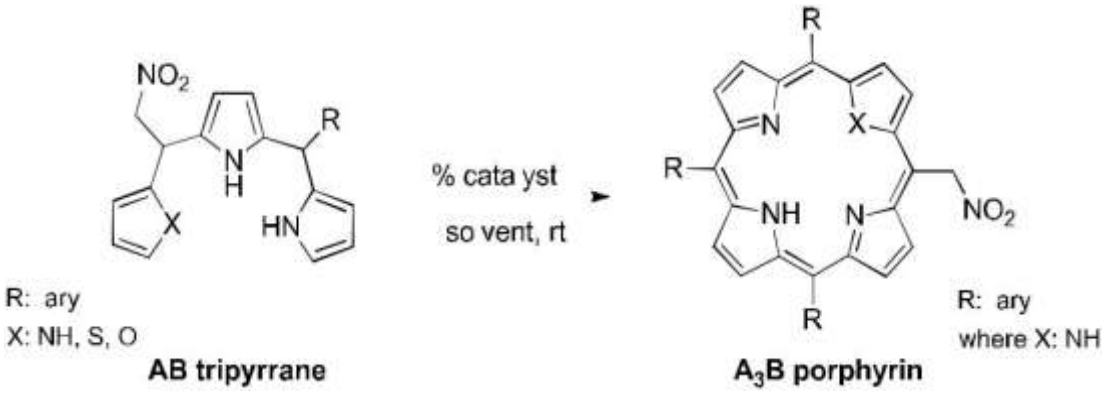
Hacettepe University, Chemistry Department, 06800 Beytepe, Ankara, Turkey

**For correspondence: canan@hacettepe.edu.tr*

Abstract

Porphyrin compounds are of great interest for their structural importance as they found use in biologic systems, material science or medical applications **[1,2]**. Synthesis of different functional groups bearing porphyrins at *meso*- positions have considerable attention due to their important physical properties and further applications. A number of methods have been developed for the synthesis of A2B2-, A3B- or ABCD type porphyrins. Reaction of aryl or alkyl aldehydes with pyrrole, dipyrromethane or bilane compounds were the synthetic routes to reach the desired porphyrins **[3]**.

In the presented work, we developed a new synthetic approach for the synthesis of A3B-porphyrins having nitroalkyl group. We first investigated the synthesis of AB-type tripyrrane compounds from the addition of dipyrromethanes to nitrovinyl arenes and then indicated their utilization to obtain the synthetically diffucult nitroalkyl substituted A3B-porphyrins.



Keywords: AB tripyrrane; A3B porphyrins; nitrovinyl arenes.

The authors thank to The Scientific and Technological Research Council of Turkey (no. 215Z042) for financial support.

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POLYETHYLENIMINES-SUPPORTED CATALYSTS FOR COPPER(I)-CATALYZED AZIDE-ALKYNE CYCLOADDITION CLICK REACTIONS IN AQUEOUS SOLVENT

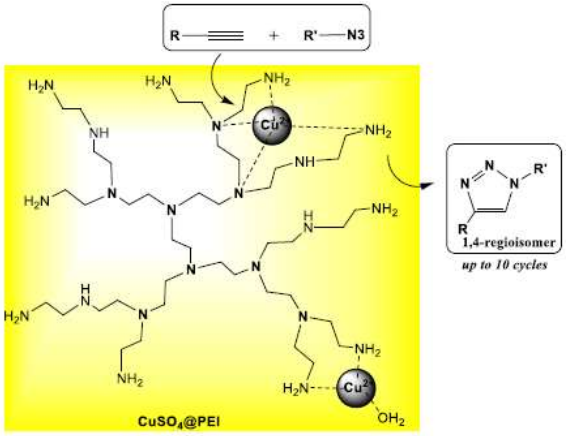
H. Elmouli[a], H. Ben El Ayouchia[a,*], H. Anane[a], M. R. Laamari[a], S.-E. Stiriba[a,b,*]

[a]*Laboratoire de Chimie Analytique et Moléculaire, LCAM, Faculté Polydisciplinaire de Safi, Université Cadi Ayyad, 46030 Safi, Morocco.*
[b]*Instituto de Ciencia Molecular / ICMol, Universidad de Valencia, C/. Catedrático José Beltrán Nº2, 46980 Paterna, Valencia, Spain.*

**For correspondence: Email: belayou@gmail.com*

Abstract

The Cu(I)-catalyzed azide-alkyne cycloaddition (CuAAC, known as the click reaction) is an established tool used for the construction of complex molecular architectures containing 1,4-triazolic moieties **[1,2]** While the use of copper as a catalyst is at the root of its immense success, the presence of copper metal traces is undesirable for most application and in particular biological complex systems. Generally, the moist applicable strategy in catalysis that prevents the presence of metals in the final products of the reaction rely on the immobilization of the pre-catalyst on a support , which can be readily removed from the final product, and ideally be reused for further reactions.



In this respect, polyethylenimine (PEI) a known hyperbranched polyamine was employed to immobilize the copper(II) sulfate pre-catalyst. The immobilized copper(II) complex, Cu@PEI was successfully employed in clicking a series of azide and alkynes in water at room temeparature in absence of any external reducing agent, affording regioselectively 1,4-disubstutued 1,2,3-triazoles in excellent yields (90-95%). The Cu@PEI was recovered by simple extraction and reused for up to ten cycles without loss of its activity **[3]**.

Keywords: Copper catalyst; Hyperbranched Polymer; azide-alkyne cycloaddition; CuAAC; 1,4-triazoles.

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THIOAURONES AS SYNTHONS TOWARDS NOVEL HETEROCYCLIC SYSTEMS

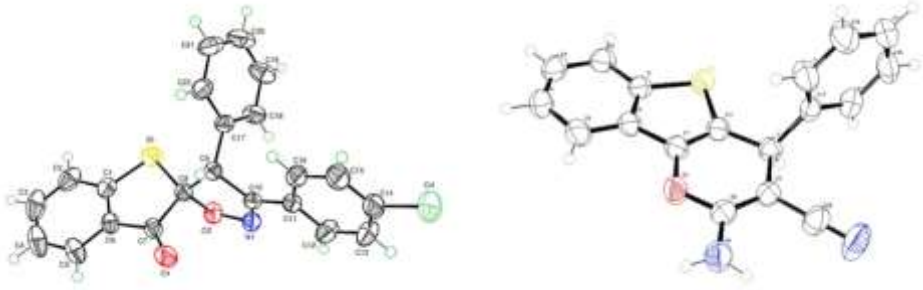
M. Bakhouch[a,*], M. Chalkha[a], A. Mahfoud[a], M. Akhazzane[b], G. Al Houari[a], M. Daoudi[a], M. El Yazidi[a]

[a]*Laboratoire de Chimie Organique, Université Sidi Mohamed Ben Abdellah, Faculté des sciences Dhar El Mahraz, BP: 1796, Fès, Maroc.*
[b]*Cité de l'innovation, Université Sidi Mohamed Ben Abdellah, Fès.*

**For correspondence: Email: mohamed.bakhouch@usmba.ac.ma*

Abstract

2-arylidenebenzo[b]thiophen-3(2H)-one and derivatives, known as thioaurones, are identified as synthetic thio analogues of the naturally-occurring aurones. These derivatives are attracting widespread interest due to the great interest they present **[1-4]**.
Allowing their use as potential starting materials for the synthesis of a wide range of heterocyclic compounds **[5].**
Meanwhile, the presence of an α,β-unsaturated ketone with an exocyclic double bond in the structure of thioaurones has pushed us to investigate their reactivity through 1,3-dipolar cycloaddition and cyclocondensation reactions, in an attempt to synthesise novel heterocyclic systems containing benzothiophene framework.[**6-10]**



***Keywords*:** 2-arylidenebenzo[b]thiophen-3(*2H*)-one; thioaurones; 1,3-dipolar cycloaddtion; cyclocondensation.

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THE SYNTHESIS OF NEW BIS(MORPHOLINOPHENOXY)ETHYLENE GLYCOL PODANDS AND INVESTIGATION OF THEIR CATION RECOGNITION

Gönül Yapar

Department of Chemistry, Faculty of Arts and Sciences, Istanbul Technical University, Maslak, 34469 Istanbul, Turkey

**For correspondence: Email: yaparg@itu.edu.tr*

Abstract

Ion binding macromolecules have an important role in functional organic chemistry because of their extraordinary strong physical and chemical properties, which are classified as supramolecules. The cation binding behaviors of such molecules are related their structure and stereochemistry, the donor atoms like oxygen, nitrogen, sulphur in the macrocyclic ring as well as the electropositivities of cations and atomic radii **[1]**. Macrocyclic compounds bearing ethyleneoxy units in their structure were called crown ether by Pedersen who reported the synthesis and strong complexing properties of those with metal cations in 1967 **[2]**. Crown ethers are mainly used in complex formation, cation binding with extraction, cation deactivation, anion activation: phase-transfer catalyst, sensors, ion-membran balancing agents and some other applications. Crown ethers containing different functional groups have been designed and synthesized and their tecnological applications have been extensively studied in chemistry, biology, pharmacy, medicine, and material science **[3-6]**.

In this work, polyether-type podands having different ring size were synthesized (n=0-4). The new compounds have morpholine units which are extremely versatile chemical with many important applications (Fig. 1). In the first part of the study, noncyclic crown ether derivatives, podans carrying morpholinophenol as end group, were synthesized in good yields. The structures of all compounds were identified by using FTIR, 1H NMR and mass spectroscopic methods. In the second part of the study, complex formations of the compounds with alkaline, alkaline earth and some transition metal ions have been investigated using steady state fluorescence spectroscopy in acetonitrile at 20°C **[7]**.

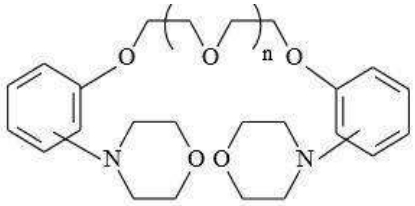

Figure 1: Bis(morpholinophenoxy)ethylene glycol podands

Keywords: Podand; non-cyclic crown ether; cation binding; complexation; macrocycle; fluorescence spectroscopy; morpholine.

Acknowledgements: This research study was partly supported by The Scientific and Technological Research Council of Turkey (TUBITAK)

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EVALUATING CORROSION INHIBITION PROPERTY OF SOME PYRAZOLE DERIVATIVES FOR MILD STEEL IN 1 M HCl: INSIGHT FROM ELECTROCHEMICAL AND QUANTUM STUDIES

S. El arrouji[a,*], K. Karrouchi[b], Z. Rais[a], M. Taleb[a], K. Ismaily alaoui[a], F. El hajjaji[a]

[a]*Laboratoire d'Ingénierie d'Electrochimie de Modélisation et d'Environnement (LIEME), FSDM Fès, Morocco*
[b]*Laboratoire National de Contrôle des Médicaments, DMP, Ministère de la Santé, Madinat Al Irnane, BP 6206, Rabat, Morocco*

**For correspondence: Email: elarroujisiham@gmail.com*

Abstract

The effect of synthesized Pyrazole derivatives, namely, 2-(3,5-dimethyl-1*H*-pyrazol-1-yl)-*N*'-[(*E*)-(4-methylphenyl)methylidene]acetohydrazide (DPM) and 2-(3,5-dimethyl-1*H*-pyrazol-1-yl)-*N*'-[(*E*)-(4-fluorophenyl)methylidene]acetohydrazide (DPF) on the corrosion of mild steel in 1M HCl solution was investigated by using weight loss and electrochemical methods. Both inhibitors act as mixed inhibitors and their adsorption on mild steel obeyed Langmuir's adsorption isotherm. The inhibition actions of these Pyrazole molecules are discussed in view of blocking the electrode surface. Scanning electron microscopy (SEM) studies of the metal surfaces confirmed the existence of an adsorbed film. Density functional theory (DFT) has been used to determine the relationship between molecular configuration and their inhibition efficiencies. The order of inhibition performance obtained from experimental results is successfully verified by DFT.

***Keywords*:** pyrazole; ptentiodynamic polarization; electrochemical impedance; SEM; DFT.

SYNTHESIS, BIOLOGICAL EVALUATION, AND CHARACTERIZATION BY NMR AND X-RAY OF SOME NOVEL OF 2-OXO-1,2-DIHYDROQUINOLINE-4-CARBOXYLIC ACID DERIVATIVES

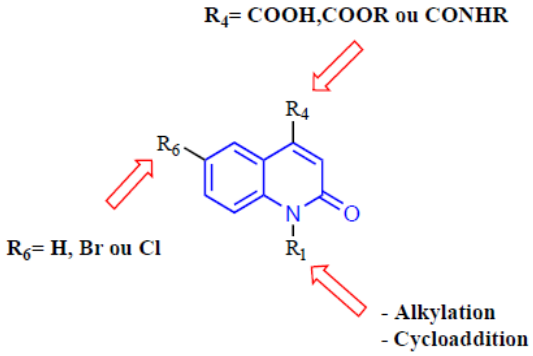
Y. Filali Baba[a,*], Y. Kandri Rodi[a], F. Ouazzani Chahdi[a], H. Misbahi[a], E.M. Essassi[b]

[a]*Laboratory of Applied Organic Chemistry, Faculty of Science and Technology, University Sidi Mohammed Ben Abdallah, Fez, Morocco.*
[b]*Laboratory of Organic Heterocyclic Chemistry, Faculty of Science, Ibn Battuta Avenue, Rabat, Morocco.*

**For correspondence: yassir.filali.baba@gmail.com*

Abstract

A heterocyclic quinolone with a large spectrum of activity **[1-5]**, has been synthesized and developed by a cyclo-condensation reaction from isatin and malonic acid. Firstly, 2-oxo-1,2-dihydroquinoline-4-carboxylic acid was obtained with an excellent yield. This compound was subject to different types of reactions following different steps to obtain a wide range of compounds. The structures of the prepared compounds have been determined by spectroscopic methods: IR, ^{1}H NMR, ^{13}C NMR and some of them were confirmed by single crystal X-Ray diffraction. The antioxidant activity of these compounds was evaluated using DPPH, FRAP and β-carotene bleaching techniques. Their antimicrobial activity was evaluated against *E. coli, S. aureus, B. subtilis*, *B. cereus* and *Salmonella typhi* using a microplate protocol.



Keywords: Quinolone; cyclo-condensation; esterification; alkylation; antioxidant and anti-bacterial.

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LIQUID–LIQUID EXTRACTION OF METAL IONS BY NEW SYNTHESIZED PYRAZOLE & TRIAZOLE N-LIGANDS, HIGH SELECTIVITY FOR Fe AND Pb WITH TD-DFT THEORICAL CALCULATION

M. Lamsayah[a,b,*], M. Khoutoul[a], A. Takfaoui[a], R. Touzani[a,b]

[a]*LCAE-URAC18, COSTE, Département de Chimie, Faculté des Sciences, Université Mohamed Premier, BP524, 60 000 Oujda, Maroc.*
[b]*Faculté Pluridisciplinaire de Nador, Université Mohamed Premier BP300, Selouane 62700, Nador, Maroc.*

**For correspondence: E-mail: moradsmc@hotmail.com*

Abstract

A sensitive and selective Liquid-Liquid extraction using four new ligands ***L1-L4*** as chelating agents for extraction of heavy metals from aqueous solution. Their capacities extraction of Fe^{2+}, Cu^{2+}, Cd^{2+}, Pb^{2+}, Co^{2+}, Zn^{2+} and Ni^{2+} were determined by atomic absorption measurement (AA). The ligands ***L2***, ***L3*** and ***L4*** show a high extractive affinity for Fe(II) (97.28%, 89.93% and 90.36% respectively) and Pb(II) (86.17%, 91.62% and 80.73% respectively) **[1]**. The effects of pH and ligand concentration upon extraction capability were investigated. The results revealed that the extraction of Fe(II) dependents on the pH with maximum extraction was obtained in the pH range of 6 to 7. A back-extraction of Fe(II) and Pb(II) lead us to recover them from aqueous solution (***L3*** gave 92.12% for Fe(II) and 85.66% for Pb(II) using H2SO4 and HNO3 aqueous acidic solution respectively). The theorical investigation using TD-DFT calculation has been reported as well.

Keywords: Liquid-Liquid extraction; heavy metals; atomic absorption; TD-DFT.

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SYNTHESIS AND ANTIBACTERIAL STUDY OF NOVEL ACRIDONE DERIVATIVES CONTAINING 1.2.3 TRIAZOLE

M.Aarjane*, Siham Slassi, Amina Amine*

Equipe de Recherche Chimie Moléculaire et Molécules Bioactives. Faculté des Sciences, Université Moulay Ismail – Meknès

** For correspondence: E-mail: aarjane.mohammed@gmail.com / amine_7a@yahoo.fr*

Abstract

Acridone compounds exist extensively in natural products. As a macrocyclic conjugated system with a rigid planar structure, acridone ring can be embedded in biological macromolecules such as DNA and possess potent antitumor, antiviral, antimalarial and antimicrobial bioactivity **[1]**. Owing to its strong fluorescence emission, it has also been applied to cell labeling and medical testing as a fluorescent pH indicator **[2]**.

1,2,3-Triazoles are important heterocycles in synthetic as well as medicinal chemistry due to its simple synthesis via click chemistry approach and a wide range of biological activities. 1,2,3-Triazoles with high dipole moment, considerable stability and capability for hydrogen bonding make it a favorable binder of biomolecular targets **[3]**.

The potential applications of these two classes of heterocycles led us to develop novel acridone derivatives containing 1.2.3 triazole, aiming to get potentially improved therapeutic agents. We reported in this work the synthesis via click chemistry approach of novel acridone derivatives containing 1.2.3 triazole, using Simple copper catalyzed 1,3-dipolar cycloadditions of ethyl 2-azidoacetate and acridone alkynes afford regioselective 1,4-disubstitued 1,2,3-triazoles with high yields. The synthesized compounds were characterized by FTIR, 1H NMR, 13C NMR, 2D NMR and evaluated for their antimicrobial activities. Interestingly, most of the compounds exhibit moderate to good activities against tested Gram-positive, Gram-negative bacterial strains.

***Keywords*:** Acridone; 1,3-dipolar cycloaddition; triazole; antimicrobial activities.

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ORGANOCATALYTIC ASYMMETRIC SYNTHESIS OF DIHYDRONAPHTHO- FURANS VIA FRIEDEL-CRAFTS / SUBSTITUTION DOMINO TYPE REACTION

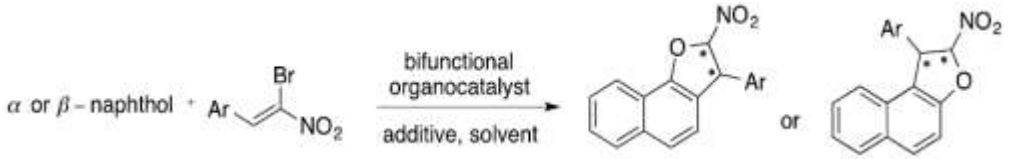
Cihangir Tanyeli

Middle East Technical University, Department of Chemistry

** For correspondence: E-mail: tanyeli@metu.edu.tr*

Abstract

Dihydronaphthofuran skeletons can be found in various pharmaceutical and natural products used in treatments **[1]**. Friedel-Crafts/substitution domino type reactions are practical for synthesizing these molecules. Applications of these reactions in domino type reactions are a trending topic in organocatalytic studies in the recent years **[2]**. In the present study, it was chosen as the key step in domino reaction to afford disubstituted dihydronaphthofuran derivatives possessing two chiral centers in enantiomerically enriched forms. For this purpose, (*Z*)-(2-bromo-2-nitrovinyl)benzene and or *β*–naphthol were used to perform model organocatalytic Friedel-Crafts/substitution domino type reaction (Scheme 1). Initial studies involve the screening of 2-aminoDMAP **[3]** based and quinine based bifunctional organocatalysts. After choosing the proper sterically bulked (tert-butyl **[4]**, 1-adamantyl, 2-adamantyl substituted) squaramide derived quinine based organocatalyst (Figure 1), the reaction conditions were optimized and getting the product in a very short duration (10-45 minutes) with 99% ee. The derivatization study was performed under the optimized condition.



Scheme 1. Organocatalytic Friedel-Crafts / substitution domino reaction

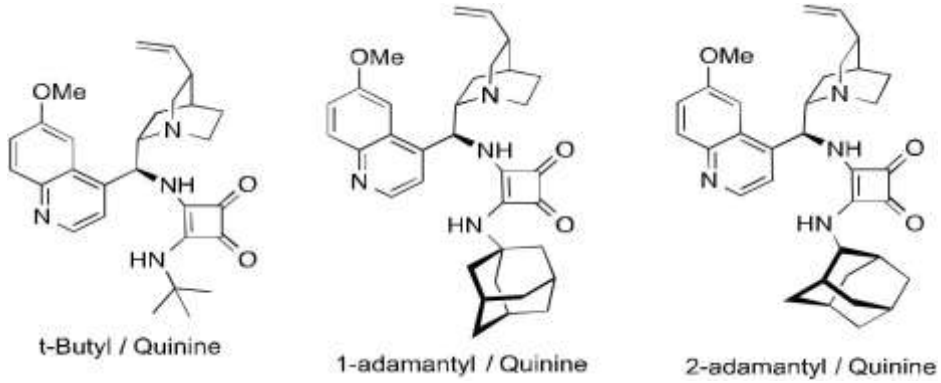


Figure 1. Sterically bulked squaramide derived quinine based organocatalysts

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BICYCLIC IMIDAZOLE SKELETONS VIA ALKYNE CYCLIZATION

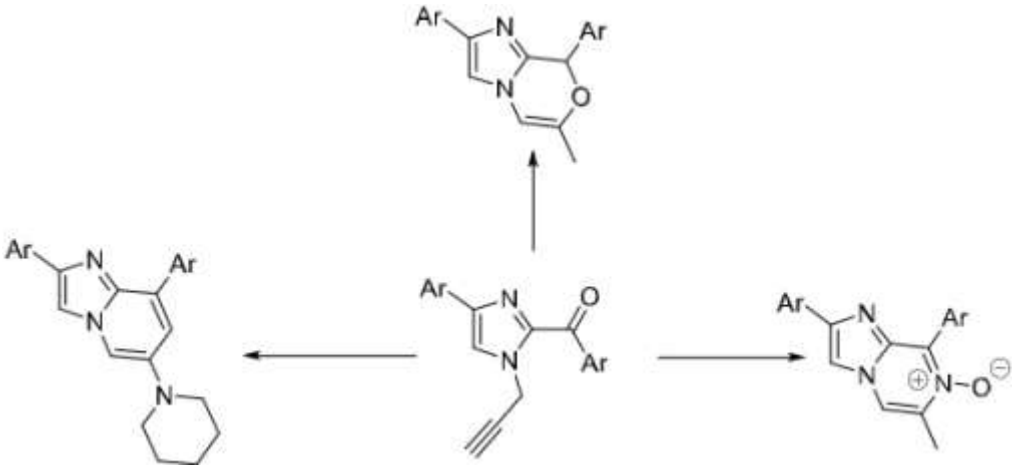
Burak Kuzu, Meltem Tan, **Nurettin Menges***

Faculty of Pharmacy, Yuzuncu Yil University, 65080, Van, Turkey

**For correspondence: nurettinmenges@gmail.com*

Abstract

Imidazole is an important ring and its derivatives gain more attention to be applied to many scientific fields such as drug industry, polymer science, and synthetic materials. To uncover unknown methodologies in order to synthesize new types of imidazole rings is big challenge and we have already studied on this skeletons. Alkyne cyclization opens a huge gate for many vital heterocyclic molecules. In this study, we have synthesized many unknown bicyclic imidazole skeletons and evaluated their toxicities with molecular mechanics models such as SAR, QSAR and/or Docking.



Scheme 1. Bicyclic imidazole skeletons

To synthisize bicyclic imidazole derivatives, N-propargyl-2,4-disubstituted-imidazole derivatives were consumed. Their cyclization reactions were done by means of either catalyst or base (Scheme 1).

This study is supported by Turkey Scientific and Technologic Research Agency TUBİTAK (115Z894).

SYNTHESIS OF NEW POLYHETEROCYCLIC SYSTEMS BY 1,3-DIPOLAR CYCLOADDITION REACTIONS

M. Adardour*, A. Baouid, A. El Qami, Y. Ben soumane

Laboratoire de Chimie Moléculaire, Département de Chimie, Faculté des Sciences Semlalia, BP 2390, Université Cadi Ayyad, 40001, Marrakech, Maroc.

**For correspondence: adardourmed@gmail.com*

Abstract

The study of five-membered heterocyclic systems has developed considerably in the demonstration of their biological activities. It is known that benzimidazole derivatives are among the heterocyclic compounds which have received the most attention because of their applications in such varied fields as medicine. Indeed, benzimidazole derivatives have been shown to have antimicrobial activity **[1-3]**, antiviral **[4,5]** and anticancer activity **[6,7]**.
The 1,3-dipolar cycloaddition reactions have opened very interesting synthetic routes and have led to the preparation of a wide variety of pentagonal heterocyclic. By developing our research focus, we are interested in the synthesis of new heterocyclic systems by clicking chemistry reactions.
The work we present in this paper deals with the dipolar condensation of diarylnitrilimines **[8]** and nitrile oxide **[9]** with 1-cyclohexenyl-3-(prop-2-ynyl)-1H-benzimidazol-2(3H)-one. The results obtained show that a single monocycloadduct is obtained in good yield whatever the amount of dipole used.
In summary, we have demonstrated that 1,3-dipolar cycloaddition of diarylnitrilimines and nitriles oxides on 1-cyclohexenyl-3-(prop-2-ynyl)-1H-benzimidazol-2(3H)-one was highly peri and regioselective.
The structures of these compounds were established by IR, ^{1}H NMR, ^{13}C NMR, mass spectral data. The structure of a compound was also confirmed by X-ray diffraction analysis.

Keywords: benzimidazolone; 1,3-dipolar cycloaddition; pyrazole; isoxazole.

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EFFICIENT AND GREEN SYNTHESIS OF 2,3-DIHYDROQUINAZOLIN-4(1*H*)-ONES USING ANIMAL BONE MEAL AS A NEW BIOCATALYST IN WATER

R. Azzallou[a,b,*], M. Ait Taleb[b], R. Mamouni[b], A. Benlhachemi[c], B. Bakiz[c], S. Villain[d], S. Lazar[a]

[a]*Laboratoire de Biochimie, Environnement & Agroalimentaire, URAC 36, Université Hassan II-Casablanca, BP 146, 20650 Mohammedia, Morocco.*
[b]*Equipe de Matériaux, Catalyse et Valorisation des Ressources Naturelles,*
[c]*Laboratoire Matériaux et Environnement, Université Ibn Zohr, BP 8108, 80000 Agadir, Morocco.* [d]*Institut Matériaux Microélectronique et Nanosciences de Provence, Aix Marseille Université, CNRS, Université de Toulon, IM2NP UMR 7334, 83957 La Garde, France*

**For correspondence: azzallourachid@gmail.com*

Abstract

Dihydroquinazolinones are of considerable interest as they exhibit biological properties, such as antitumor, antibiotic, antidefibrillatory, antipyretic, analgesic, antihypertonic, antihistamine, antidepressant and vasodilating behavior **[1-3]**.
In recent years, the direction of science and technology has been shifting more towards eco-friendly, natural product resources and reusable catalysts. Thus, natural biocatalysts are attractive candidates in the search for such solid support catalysts. The use of Animal Bone Meal (ABM) has recently received considerable attention as an inexpensive, nontoxic, also include high stability for various organic transformations to afford the corresponding products in excellent yields **[4-5]**.
In continuation of our research program concerning the application of our ABM catalyst, we wish report in this work a facile one-pot procedure for the synthesis of 2,3-dihydroquinazolin-4(1*H*)-ones by cyclocondensation of anthranilamide and aldehydes using ABM modified as catalyst.
We have achieved a facile and efficient method for the synthesis of a variety of 2,3-dihydroquinazolin-4(1*H*)-ones derivatives using ZnCl2/ABM as a reusable catalyst. Present methodology offers very attractive features such as reduced reaction times, higher yields and economic viability of the catalyst, when compared with conventional method as well as with other catalysts, which will have wide scope in organic synthesis. The simple procedure combined with easy of recovery and reuse of this catalyst make this method economic, begin and a waste-free chemical process for the synthesis of 2,3-dihydroquinazolin-4(1*H*)-ones. The catalyst can be prepared easily with readily available inexpensive reagents, which is heterogeneous and non-hazardous. We believe that this procedure is convenient, economic, and user-friendly process for the synthesis of 2,3-dihydroquinazolin-4(1*H*)-ones of biological and medicinal importance.

Keywords: Animal Bone Meal; 2,3-Dihydroquinazolin-4(1H)-ones; Anthranilamide; Aldehydes; Green chemistry protocols.

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THEORETICAL STUDY OF SOME OXADIAZOLES DERIVATIVES AND THEIR IRON COMPLEXES IN CORROSION INHIBITION PROCESS

N. Habbati[a,b,*], M. Benzakour[a], M. Mcharfi[a], M. Ebn. Touhami[b], Z. El Adnani[a], M. Sfaira[a], A. Touimi. Benjelloun[a]

[a]*Laboratoire d'Ingénierie des Matériaux, Modélisation et Environnement, Faculté des sciences Dhar EL Mahraz, Université Sidi Mohamed Ben Abdellah, BP : 1796, Fès, Maroc.*
[b]*Laboratoire d'ingénierie des Matériaux et d'Environnement: Modélisation et Application, Faculté des sciences, Université Ibn Toufail, BP 133 14000, Kenitra, Maroc*

**For correspondence: Email: nhabbati@yahoo.fr*

Abstract

Corrosion inhibitors are substances that preserve metals by prevening or reducing the corrosion rate process. The most effective organic inhibitors are π system and hetero cyclic organic compounds that contain atom such as O, N, P or S which facilitates its adsorption on the metal surface.
Several quantum chemical methods and molecular modeling techniques have been performed to correlate the inhibition efficiency of the inhibitors with their molecular properties. Using theoretical parameters helps to characterize the molecular structure of the inhibitors and to propose their interacting mechanism with surface.
The DFT/ B3LYP calculations were applied to investigate the relationship between electronic properties and corrosion inhibition efficiency of three oxadiazole derivatives: 2,5-bis (2-methyl phenyl)-1,3,4-oxadiazoles (2MPOX), 2,5-bis (3-methyl phenyl)-1,3,4-oxadiazoles (3MPOX) and 2,5-bis (4-methyl phenyl)-1,3,4-oxadiazoles (4MPOX) recently studied as a good inhibitor for mild steel .
The calculated quantum chemical parameters are E_{HOMO}, E_{LUMO}, ΔE, μ, χ and η. The interaction energies of the investigated inhibitors on the iron surface were studied to discuss the inhibition mechanism. Several modes of interactions between iron and oxadiazoles have been investigated: Fe-π, Fe-NN and Fe-NNO.

Keywords: DFT calculations; inhibitors; corrosion; surface.

METAL FREE ALKYLATION REACTION OF HETEROCYCLES VIA KETONIC MANNICH BASES

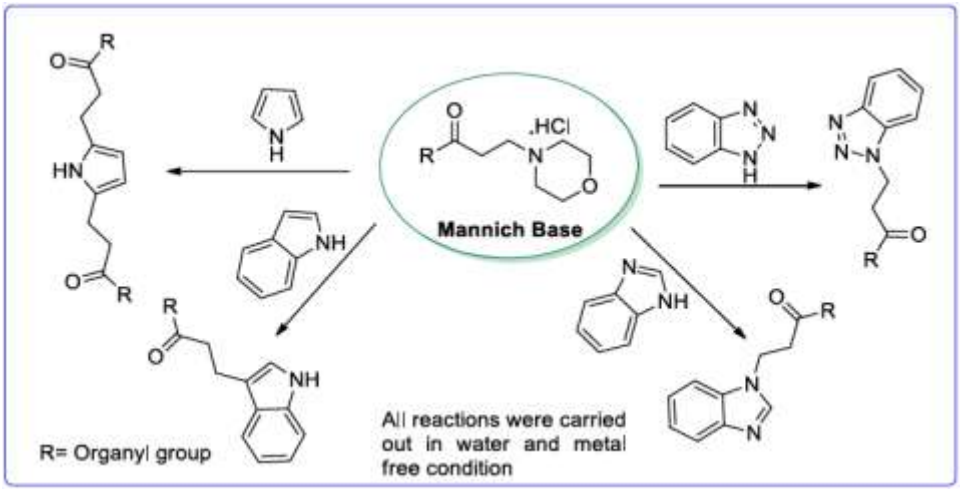
P. Seyitdanlioglu, D. Celik, **E. Hanashalshahaby**, C. Unaleroglu*

Department of Chemistry, Faculty of Science, Hacettepe University, PC: 06800, Ankara, Turkey

**For correspondence: Email: canan@hacettepe.edu.tr*

Abstract

Synthesis of alkyl substituted pyrrole, indole, benzimidazole and benzotriazole compounds are of special interest due to their biological activities **[1]**. The currently used methods in the synthesis of alkylation of these heterocycles are generally suffering from the use of metal catalysts, organic solvents and expensive unstable starting materials such as enones **[2]**. In this work, alkylation reactions of a variety of heterocycles such as 1*H*-indole, 1*H*-benzimidazole, 1*H*-benzotriazole and pyrrole were performed in environmentally friendly conditions via Michael addition of these heteroaromatics to the *in situ* generated vinyl ketones from ketonic Mannich bases.



Keywords: Ketonic Mannich bases; vinyl ketones; Michael addittion; pyrrole; 1*H*-indole; 1*H*-benzimidazole; 1*H*-benzotriazole.

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INNOVATIVE SYNTHESIS OF SOME MODIFIED *C*- AND *N*- NUCLEOSIDES ANALOGUES

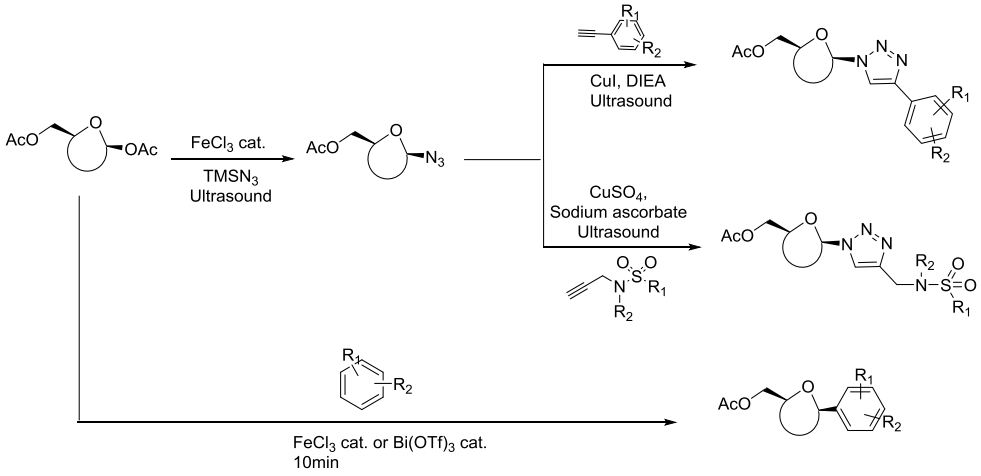
H. Tachallait[a,b], S. Alaoui[a,b], H. Marzag[a,b], M. Driowya[a,b], L. Demange[b,c], A. R. Martin[b], M. Dufies[d], G. Pagès[d], R. Benhida[b], K. Bougrin[a,*]

[a] *Laboratoire de Chimie des Plantes et de Synthèse Organique et Bioorganique, URAC23, Faculté des Sciences B.P. 1014, GEOPAC Research Center, Université Mohammed V Rabat, Maroc*
[b] *ICN, UMR CNRS 7272, Université de Nice Sophia-Antipolis-Université Côte d'Azur, Parc Valrose, Nice, France.*
[c] *Université Paris-Descartes, Sorbonne Paris Cité, UFR des Sciences Pharmaceutiques et UFR Biomédicale des Saints Pères, Paris, France.*
[d] *Institute for Research on Cancer and Aging ,UMR7884 CNRS and INSERM U1081 ,Université Côte d'Azur, Nice*

**For correspondence: Email: kbougrin@yahoo.fr*

Abstract

The *C*- and *N*-nucleosides are extensively used in medicinal chemistry due to their high value in pharmaceutical industry discovers, for example tiazofurin, ribavirin, AZT and cladribin have been approved as a drug for the treatment of certain types of viral and cancer diseases. Various approaches have been used for the synthesis of *C*- and *N*-nucleosides. We report here two routes, which have been developed by our research group. The first one, consists in the use of protected azidosugar as substrates for a subsequent functionalization through click chemistry **[1-2]**.The second route is based on the use of a Friedel-Craft mediated by an Lewis acid as catalysts, which leads to *C*-nucleosides in high yields and with an excellent stereoselectivity **[3]**. Among the series of *N*-nucleosides synthesized in the team, some products revealed an interesting cytotoxic activity against RCC4 and MDA-MB-231 cancer cells.



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CHEMICAL COMPOSITION AND ANTIOXIDANT POTENTIAL OF *PISTACIA* LENTISCUS L. ESSENTIAL OIL FROM ORAN (ALGERIA)

Nadia Bouzidi Kambouche*, Abdelkader Hamiani, Salima Bellahouel

Organic Synthesis Laboratory, Chemistry Department, Sciences Faculty, Oran1 Ahmed Benbella University, Oran, Algeria

**For correspondence: Email: kambouche@yahoo.fr*

Abstract

Essential oil from the leaves of *Pistacia lentiscus* L. growing in the Oran region in the west of Algeria was obtained by hydrodistillation with a 1.26 % yield on a dry weight basis. Spectrophotometric analyses were employed to highlight the scavenger capacity of this oil using the 2,2-diphenyl-1-picrylhydrazyl (DPPH) test. Twenty compounds were identified by GC and CG/MS analyses, and the main part of the compounds of the oil were terpinene-4-ol (41.24%) and α-terpineol (7.31%), α-pinene (9.48%), limonene (09.11%), β-myrcene (10.5 %), *p*-cymene (8.67 %) and α-phellandrene (2.20%), β-caryophyllene (12.62%) as major compounds.

The DPPH test shows that *Pistacia lentiscus* essential oil possesses antiradical activity. A linear correlation (correlation coefficient R^2 = 0.995, P <0.001) was found between the reduction of DPPH stable free radical and the concentration of *Pistacia lentiscus* essential oil.

Keywords: *Pistacia lentiscus;* terpinene-4-ol; *essential oil*; antioxidant activity.

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SYNTHESIS AND CHARACTERIZATION OF AMINOALKYL AND TETRAZOLIC AMINO ACID DERIVATIVES

S. Boukhssas, Y. Aouine, H. Faraj, A. Alami*, A. El Hallaoui, B. Labriti

Laboratoire de Chimie Organique, Faculté des Sciences Dhar El Mehraz, Université Sidi Mohamed Ben Abdellah, BP. 1796, Fès, Morocco

**For Correspondence: E-mail: alamianouar@yahoo.fr*

Abstract

Tetrazoles are an important class of nitrogen containing heterocycles with a wide range of medicinal and commercial applications **[1,2]**. Tetrazolyl analogs of amino acids exhibit versatile biologic activity, and some of them are known pharmaceuticals **[3]**. In addition, compounds of this type may be utilized in development of radiopharmaceuticals for positron emission tomography **[4]**.
In continuation of our investigations in the tetrazolic amino acids **[5]**, we described in this presentation the synthesis and characterization of some aminoalkyl and tetrazolic amino acid derivatives basing on different spectroscopic methods as NMR 2D.

Keywords: Tetrazole; aminoalkyl; α-amino acid; NMR 2D.

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Poster presentations

OPTIMIZATION OF ULTRASOUND-ASSISTED EXTRACTION OF YIELD AND PHENOLIC COMPOUNDS FROM *LAVANDULA STOECHAS* L. USING RESPONSE SURFACE METHODOLOGY

Y. Ez zoubi[a,*], M. Fadil[a], D. Bousta[b], B. Ihssane[a], M. Lachkar[c], A. Farah[a]

[a] *Laboratory of Applied Organic Chemistry, Faculty of Sciences and Technology, Sidi Mohamed Ben Abdellah University, B.P. 2202 – Route d'Imouzzer, Fez, Morocco*,

[b] *Faculty of Sciences Dhar El Mehraz, Sidi Mohamed Ben Abdellah University, Fez, Morocco*,

[c] *Engineering Laboratory of Organometallic and Molecular Materials (CNRST, URAC 19), Faculty of Sciences, University Sidi Mohamed Ben Abdellah, Po.Box 1796 (Atlas), 30000 Fez, Morocco.*

**For Correspondence: ezzoubiyassine@yahoo.fr*

Abstract

The effect of extraction conditions on yield and polyphenols contents by ultrasound-assisted extraction (UAE) was studied. Liquid/solid ratio (mL/g), ethanol concentration (%) and extraction time (min), were studied as variables using response surface methodology (RSM) for the extraction of polyphenols and yield from aerial parts of *Lavandula stoechas* L. of Morocco.

After the realization of experiments and data analysis, the optimum extraction yield (31.68%) was obtained by ensuring the following parameters: an ethanol concentration of 40%, a liquid/solid ratio of 30 mL/g and 32.62 min as time processing. The maximum extraction of total polyphenols (190.61 mg Gallic Acid Equivalents (GAE)/g dry matter) was obtained using a process time of 20 min, liquid/solid ratio of 29.08 mL/g and a concentration of ethanol of 40%. The optimization of two responses simultaneously has led to 24.2% as extraction yield and a total concentration polyphenols of 190.24 mg GAE/g, to get these responses, the following parameters must be adjusted: extraction time about 20.73 min, ratio of liquid/solid at 29.72 mL/g and ethanol proportion at 40.5% (v/v).

The experimental values under optimal conditions were in good consistent with the predicted values, which suggested UAE is validation model adopted in this study.

Keywords: *Lavandula stoechas*; Ultrasound assisted extraction; Phenolic Compounds; Response Surface Methodology; Morocco.

SYNTHESIS AND ELASTASE INHIBITION OF THIOPHENYL SUBSTITUTED HYDROXYIMIMO ESTERS

B. Hasdemir[1,*], Ö.Saçan[2], H. Yasa[1], H. Başpınar Küçük[1], A.S. Yusufoğlu[1], R. Yanardağ[2]

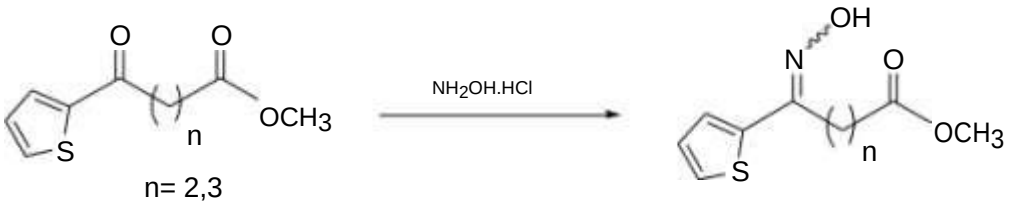
[1]*Division of Organic Chemistry, Department of Chemistry, Faculty of Engineering, Istanbul University, 34230-Avcilar, Istanbul, Turkey*
[2]*Division of Biochemistry, Department of Chemistry, Faculty of Engineering, Istanbul University, 34230-Avcilar, Istanbul, Turkey*

**For correspondence:* Email: karaefe@istanbul.edu.tr

Abstract

Oximes are very important compounds in organic synthesis and they can be successfully transformed to amide, amine, hydroxylamine and nitrile etc. Moreover, oxime compounds have gained great important in medicinal chemistry because of their potential biological activities such as antibacterial **[1]**, antitumor **[2]** and antiviral **[3]** etc.

In this study is aimed to synthesize and investigate the elastase inhibition activities of novel hetereoaryl substituted keto oxime esters. In the literature there is no data on the synthesis and the elastase inhibition of these compounds.



The obtained hydroxyimino esters were identified by spectroscopic (IR, ^{1}H-NMR, ^{13}C-NMR and Mass) analysis. All the test compounds exhibited antielastase activity. The enzyme inhibitory activities of these novel hydroxyimino esters were found to increase dose dependently.

Keywords: Hydroxyimino ester; elastase; inhibition

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INVESTIGATION OF GREEN INHIBIOR FOR ANTI-CORROSION ACTIVITY IN ACIDIC MEDIUM

A. Bouoidina[a,*], M. Chaouch[a], M. Taleb[b], A. Lahkimi[b], F. El-Hajjaji[b]

[a]*Laboratoire de génie des Matériaux et environnement, Faculté des sciences Dhar EL Mahraz, Université Sidi Mohamed Ben Abdellah, BP : 1796, Fès, Maroc.*
[b]*Laboratoire d'Ingénierie d'Electrochimie de Modélisation et Environnement, Université Sidi Mohamed Ben Abdellah, Fès, Maroc.*

**For correspondence: Email: asmae.bouoidina@gmail.com*

Abstract

The corrosion of metals, including mild steel is a serious problem in industries. Although serval options are availed for the protection of mild steel against corrosion, the use of green inhibitors is one of the best options. In most cases, the presence of heteroatom's as well as aromatic ring(s) facilitates the adsorption of the inhibitor on the metal surface. In this work, the corrosion inhibition of carbon steel was studied by using the essential oil of Polio in 1M HCl solution. This study was carried out by means of electrochemical impedance spectroscopy, potentiodynamic polarization and weight-loss measurements. It was found that Polio oil had high inhibition efficiency against corrosion of carbon steel in 1M HCl solution which reaches 90 % at 303 K for 1g/l. This efficiency strongly depended on inhibitor concentration, immersion time as well as temperature.

Polarization curves obtained clearly indicated that Polio oil acted as mixed-type inhibitor and adsorbed physically onto the mild steel surface. The EIS technique revealed that the charge transfer process was dominant in controlling the corrosion process, and using the scanning electron microscope we confirmed the adsorption of the inhibitor on the surface by the formation of a protective layer.

Keywords: steel; Corrosion; Inhibitor; EIS; Polarization; Gravimetric.

INVESTIGATION OF CORROSION INHIBITION EFFECT OF IMIDAZOPYRIDINE DERIVATIVES AS INHIBITORS ON C-STEEL IN HYDROCHLORIC ACID MEDIA

Elhachmia Ech-chihbi[1,2,*], R. Salim[1, 2], H. Oudda[1], F. El Hajjaji[2], M.Taleb[2]

[1]Laboratory of separation processes, Faculty of Science, University Ibn Tofail, Kenitra, Morocco [2]Laboratory of Engineering, Electrochemistry, Modeling and Environment (LIEME), Faculty of Science, University Sidi Mohamed Ben Abdellah, Fez, Morocco

**For correspondence: Email: chahbi.elhachmia@gmail.com*

Abstract

The corrosion inhibition of C- steel in 1M HCl was effectively studied by a newly synthesized imidazopyridine derivatives (IMD) using Electrochemical impedance spectroscopy (EIS), potentiodynamic polarization technique and gravimetric measurements. The results obtained showed that these compounds are a good inhibitors and inhibition efficiency reaches 94% at 10^{-3}M. The effect of the temperature of the aggressive medium was studied in the range 298-328K.

The imidazopyridine derivatives are physically and chemically adsorbed on the surface of the metal follows the Langmuir adsorption isotherm. The kinetic and thermodynamic parameters for C-steel corrosion and inhibitor adsorption, respectively, were determined and discussed.

Keywords: corrosion; inhibition; C-steel; imidazopyridine; HCl; EIS.

SYNTHESIS AND ANTIBACTERIAL ACTIVITY OF NEW 1,4-BENZOTHIAZIN-3-ONE DERIVATIVES

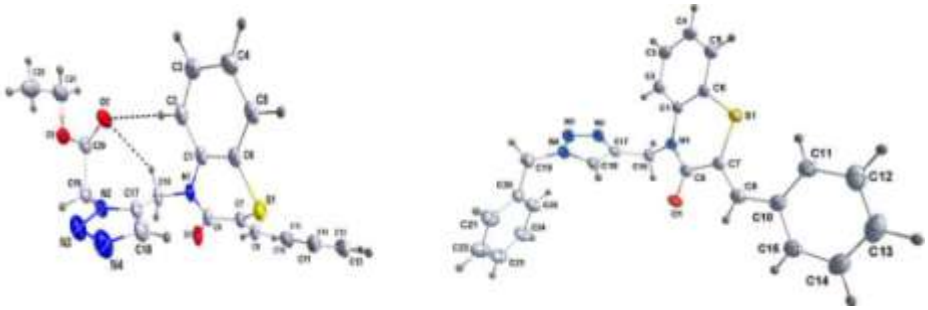
Mohamed Ellouz[1,*], Nada Kheira Sebbar[1], Zakaria Mennane[2], Reda Charof[2], El Mokhtar Essassi[1,3]

[1]*Laboratoire de Chimie Organique Hétérocyclique, Pharmacochimie, Av Ibn Battouta, BP 1014, Faculté des Sciences, Université Mohammed V, Rabat, Morocco.*
[2]*Département de bactériologie, Institut national d'hygiène, avenue Ibn Batouta, B.P. 769, Agdal, Rabat, 11000, Morocco.*
[3]*Moroccan Foundation for Advanced Science, Innovation and Research (MASCIR), Rabat, Morocco.*

**For correspondence: Email: Ellouz.chimie@gmail.com*

Abstract

In order to develop relatively small molecules as pharmacologically active molecules, novel 1,4-benzothiazine derivatives with triazole were synthesized. In this study, a series of 1,4-benzothiazin-3-one derivatives were developed by exploiting a click chemistry reaction using a Cu(I)-catalyzed and Huisgen [3 + 2] cycloaddition.
Starting from 2-(substituted)-3,4-dihydro-2H-1,4-benzothiazi-3-one, a number of 1,4-benzothiazine derivatives were also synthesized using different alkylating agents to give a 4-(substituted)-2-(substituted)-3,4-dihydro-2H-1,4-benzothiazi-3-one in good yields. All structures of the synthesized compounds were elucidated on the basis of spectral analyses (^{1}H, ^{13}C NMR, IR) and some of them were established by single-crystal X-ray diffraction.
The newly synthesized products were subjected to in vitro biological evaluation. The result indicated that the compounds show convincing antibacterial activities on different microorganisms.



***Keywords**:* 1,2,3-Triazole; 1,4-Benzothiazine; Antimicrobial activity; Cycloaddition; Spectroscopic methods.

SYNTHESIS, STRUCTURAL STUDY, ANTIBACTERIAL ACTIVITY AND THEORETICAL STUDY OF SOME ISOXAZOLINE CONTAINING 1,4-BENZOTHIAZIN-3-ONE NUCLEUS OBTAINED BY 1,3-DIPOLAR CYCLOADDITION REACTION

Nada Kheira Sebbar[a*], Zerzouf Abdelfettah[b], Mohamed Ellouz[a], Younes Ouzidan[c], H. Elmsellem[d], Fouzia Hlimi[a], Zakaria Mennane[e], Reda Charof[e], El Mokhtar Essassi[a,f]

[a]*Laboratoire de Chimie Organique Hétérocyclique, Centre de Recherche des Sciences des Médicaments, Pôle de Compétences Pharmacochimie, Mohammed V University in Rabat, Faculté des Sciences, Av. Ibn Battouta, BP 1014 Rabat, Morocco.*
[b]*Laboratoire de Chimie Organique et Etudes Physico-chimique, ENS Takaddoum, Université Mohammed V, Rabat, Morocco.*
[c]*Laboratoire de Chimie Organique Appliquée, Faculté des Sciences et Techniques, Université Sidi Mohamed Ben Abdallah, Fès, Morocco.*
[d]*Laboratoire de chimie analytique appliquée, matériaux et environnement (LC2AME), Faculté des Sciences, B.P. 717, 60000 Oujda, Morocco.*
[e]*Département de bactériologie, Institut national d'hygiène, avenue Ibn Batouta, B.P. 769, Agdal, Rabat, 11000, Morocco.*
[f]*Moroccan Foundation for Advanced Science, Innovation and Research (MASCIR), Rabat, Maroc.*

**For correspondence: Email: snounousebbar@gmail.com*

Abstract

1,4-Benzothiazine derivatives have constituted an important class of heterocycles, which, even when part of a complex molecule **[1]**, possess a wide spectrum of biological activities **[2]**, due to the presence of a fold along the nitrogen sulfur axis. The biological activity of some 1,4-benzothiazine derivatives is similar to that of phenothiazines, featuring the same structural specificity **[3]**. The role of 1,4-benzothiazine in medicinal chemistry was reviewed earlier **[4]**. Generally, 1,4-benzothiazine derivatives have found widespread applications as analgesic, antibacterial, anticancer, anthelmintic **[5-6]**. These properties indicate that 1,4-benzothiazine derivatives are a template that may be potentially useful in medicinal chemistry research and therapeutic applications. The 1,3-dipolar cycloaddition of arylnitrile oxides on the 4-allyl-2-(substituted)-3,4-dihydro-2*H*-1,4-benzothiazin-3-one led to polycyclic heterocyclic systems. The structure of the cycloadducts obtained was determined from 1H-NMR and 13C-NMR some structures and the proposed regiochemistry were confirmed by crystallographic studies. The synthesized products were subjected to *in vitro* biological evaluation. Several tested compounds showed significant antibacterial activities. A theoretical study was also performed. The results are in agreement with the experimental data.

Keywords: arylnitriloxides, 1,3-dipolar cycloaddition, 1,4-benzothiazin-3-one, Antimicrobial, crystallographic structural resolution.

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SYNTHESIS OF NEW HETEROCYLIC SYSTEMS DERIVATIVES OF 1,5-BENZODIAZEPINE

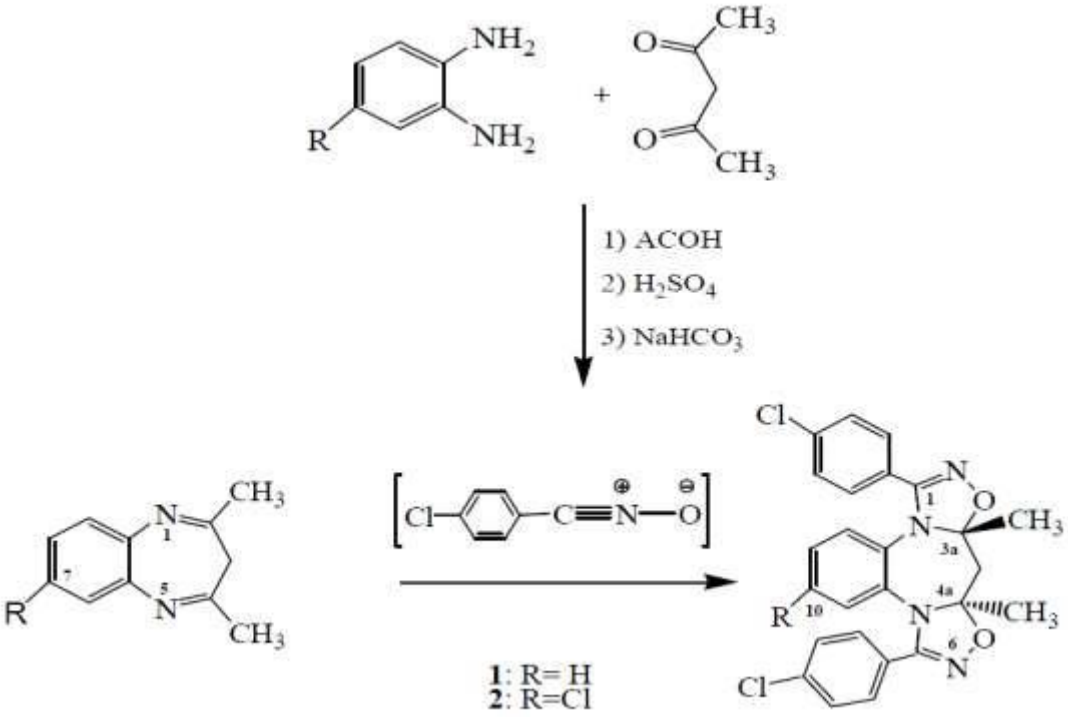
K. Nabih*, A. Baouid

Laboratoire Chimie Moléculaire, Faculté des Sciences -Semlalia, Université Cadi Ayyad, B.P.2390 Marrakech, Maroc.

**For correspondence: Email: khadija_nabih@yahoo.fr*

Abstract

Benzodiazepines are known by their remarkable activity on the central nervous system (CNS). They are widely used in medicine for the treatment of the anxiety (tranquillizers) and of insomnia (hypnotics/sedatives).
With the aim of contributing to developement of similar compounds to molecules having the interesting pharmacological properties, we synthesized of new benzodiazepines [1,2] **1** and **2**.



The structures of these molecules were established from spectral data (mass, ^{1}H NMR and ^{13}C NMR).

***Keywords**:* benzodiazepines, Heterocyclic, ^{1}H NMR, ^{13}C NMR

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ECO-FRIENDLY EXTRACTION OF CHITIN AND CHITOSAN BY MICROWAVE IRRADIATION; A GREEN APPROACH

H. El Knidri*, R. Belaabed, R. El Khalfaouy, A. Addaou, A. Laajeb, A. Lahsini

Laboratory of Science and Technology - Process Engineering, Higher School of Technology, Sidi Mohamed Ben Abdellah University, Fez MOROCCO

**For correspondence: Email: hakima.elknidri@usmba.ac.ma*

Abstract

This work concerns the valorization of waste products from fishing industry by eco-friendly extraction of chitin and chitosan.
Chitin is the second most common polymer after cellulose in earth, existing in the shells of crustaceans like crab, shrimp and lobster as well as in the cuticle of insects and the cell walls of fungicide. In this work the shrimp shells are used to extract chitin and chitosan.
Chitosan is a natural amino-polysaccharide derived from chitin, known as one of the most abundant organic materials in nature; it has been widely used in several applications due to its natural origin and exceptional properties such as biodegradability, biocompatibility, non-toxicity, and chelating of metal ions. Chitin and chitosan are characterized by degree of deacetylation, one of the most important chemical characteristics that can influence the performance of chitosan in many applications **[1-3]**.
Chitosan is usually prepared by a conventional heating method, which is time consuming (many hours up to days), that consumes a lot of energy and reagents.
In this study, a new ecological method, via microwave irradiation, was developed for the extraction of chitosan in a few minute, with decrease consumption of products and energy. The chitosan extracted was characterized by Fourier transform infrared spectroscopy (FTIR), Scanning electron microscopy (SEM) and X-ray diffraction (XRD), Nuclear magnetic resonance spectroscopy (NMR) and compared with the commercial chitosan.

Keywords: Chitin, chitosan, biodegradability, biomaterials, deacetylation, organic materials, microwave irradiation.

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SYNTHESIS, STRUCTURAL AND SPECTROSCOPIC STUDIES OF A NEW PHOSPHONIC ACID: (2-OXO-2-(THIOPHEN-2-YL)ETHYL) PHOSPHONIC ACID

H. Lamsaf [a,b,*], M. I. L. Soares[b] , S. M. V. Pinto[b] , M. S. C.Henriques[c], J. A.Paixao[c], A. Oulmekki[a],E. H. Elghadraoui[a], R. Fausto[b]

[a]*Chemistry Laboratory of Condensed Matter (LCMC), Faculty of Science and Technology Fez, University Sidi Mohammed Ben Abdellah, BP. 2202 Morocco*
[b]*CQC, Department of Chemistry, University of Coimbra, P-3004-535 Coimbra, Portugal* [c]*CFisUC, Department of Physics, University of Coimbra, P-3004-512, Portugal*

**For correspondence: Email: hafsae.lamsaf@usmba.ac.ma*

Abstract

This investigation deals with the synthesis, structural and spectroscopic characterization of a new phosphonic acid. Previous studies have revealed interesting properties of phosphonates for practical applications. For example, organometallic phosphonic acid derivatives have been shown to possess good properties for application in energy storage and catalysis. They have also been used in ion exchange and enantioselective intercalation reactions,as well as for the self-assembly of thin films possessing electroactive properties **[1]**.

In the present study, the novel (2-oxo-2-(thiophen-2-yl) ethyl) phosphonic acid has been synthesized from the corresponding thienyl β-ketophosphonate **[2]** *via* two-step route which involves first the reaction withtrimethylsilyl chloride, followed bythe trimethylsilyl phosphonate cleavage under methanolic conditions **[3]**.

Theobtained crystalline compound was investigated by X-ray diffraction, which revealed that the crystal is orthorhombic, $P2_12_12_1$ space group, with four molecules in the unit cell. The compound was also investigated by Raman spectroscopy, supported by electronic structure calculations undertaken at the DFT level of approximation. The computational studies allowed a detailed characterization of the potential energy surface of the compound and identification of the most stable conformers for the isolated molecule situation, and facilitated the interpretation of the vibrational spectroscopy data.

The new phosphonic acid derivative is now being used as a ligand in the synthesis of novel organometallic phosphonic acid complexes with different metal ions.

Keywords: synthesis; phosphonic acid; DFT calculations; Raman; X-ray diffraction.

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SYNTHESIS OF HETEROCYCLIC COMPOUNDS DERIVED FROM EUGENOL

F. El Aroussi*, A. Farah, E.M. El Hadrami*, A. Ben-Tama

Laboratoire de Chimie Organique Appliquée, Université Sidi Mohamed Ben Abdellah, Faculté des Sciences et Techniques, Route d'Immouzer, BP 2202 Fès, Maroc

**For correspondence: Email: fatima.elaroussi@usmba.ac.ma / elmestafa.elhadrami@usmba.ac.ma*

Abstract

This investigation deals with the synthesis, structural and spectroscopic characterization of a new phosphonic acid. Previous studies have revealed interesting properties of phosphonates for practical applications. For example, organometallic phosphonic acid derivatives have been shown to possess good properties for application in energy storage and catalysis. They have also been used in ion exchange and enantioselective intercalation reactions,as well as for the self-assembly of thin films possessing electroactive properties **[1].**
In the present study, the novel (2-oxo-2-(thiophen-2-yl) ethyl) phosphonic acid has been synthesized from the corresponding thienyl β-ketophosphonate **[2]** *via* a two-step route which involves first the reaction withtrimethylsilyl chloride, followed bythe trimethylsilyl phosphonate cleavage under methanolic conditions **[3]**.
Theobtained crystalline compound was investigated by X-ray diffraction, which revealed that the crystal is orthorhombic, $P2_12_12_1$ space group, with four molecules in the unit cell. The compound was also investigated by Raman spectroscopy, supported by electronic structure calculations undertaken at the DFT level of approximation. The computational studies allowed a detailed characterization of the potential energy surface of the compound and identification of the most stable conformers for the isolated molecule situation, and facilitated the interpretation of the vibrational spectroscopy data.
The new phosphonic acid derivative is now being used as a ligand in the synthesis of novel organometallic phosphonic acid complexes with different metal ions.

Keywords: synthesis; phosphonic acid; DFT calculations; Raman; X-ray diffraction.

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SYNTHESE ET PROPRIETES COMPLEXANTES DES COMPOSES DERIVES D'IMIDAZO [4,5-b] PYRIDINE

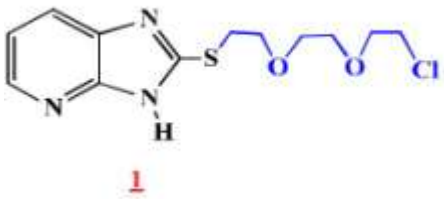
F. Lazrak[a,d], E.M. Essassi[a], Y. Kandri Rodi[b], J. Bellan[c] , M. Ansar[d] , J.Taoufik[d]

[a]*Laboratoire de Chimie Organique Hétérocyclique, Faculté des Sciences, Université Mohammed V, Rabat, Maroc*
[b]*Laboratoire de Chimie Organique Appliquée, Faculté des Sciences et Techniques, Université Sidi Mohamed Ben Abdallah, Fés, Maroc*
[c]*Laboratoire de Synthèse et Physicochimie de Molécules d'Intérêt Biologique, ESA CNRS 5068, Université Paul Sabatier, Toulouse, France*
[d]*Laboratoire de Chimie Thérapeutique, Faculté de Médecine et de Pharmacie, Université Mohammed V, Rabat, Maroc*

Abstract

Heterocyclic systems containing imidazo[4,5-b]pyridines aroused great interest by researchers because of their applications in pharmacology **[1,2]**, Moreover, the main feature of polyester and cyclic nitrogen or sulfur derivatives lies in their ability to form stable complexes with cations **[3]**, thus can be applied in various chemical and biochemical fields **[4]**.Thus it seemed interesting to prepare new derivatives of imidazo[4,5-b]pyridines by alkylation reactions in hetrogenous media using a phase transfer catalysis (CTP) **[5]**.

Compound **1** showed selectivity towards transition metals such as (Zn^{2+}, Cu^{2+}, Cd^{2+}). The sites of complexation are localized by vibrational spectroscopy, the formation constants of the different complexes are determined by UV spectrophotometry.



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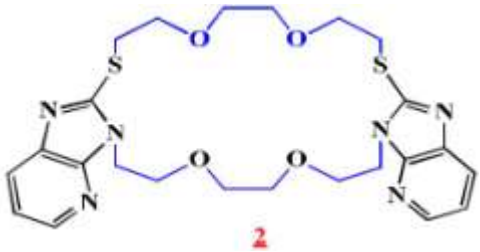

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Keywords: 2H-imidazo[4,5-b]pyridine-2-thione; bis chlorotriethyleneglycol; Phase Transfer Catalysis: complexation; UV spectrophotometry,

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SYNTHESIS OF THIOALKYL PYRAZOLONE DERIVATIVES

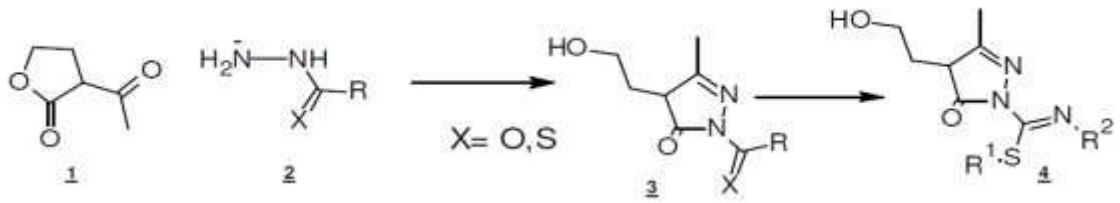
L. Hammal, S.Meksem, S. Baaziz, W. Frites

Organic Chemistry and Applied Laboratory, University of Sciences and Technology Houari Boumediene (USTHB), 16111 Algiers, Algeria.

**For correspondence: Email: lamou2007@yahoo.fr*

Abstract

Pyrazolone is a key structure in numerous compounds that occur in many drugs and synthetic products **[1,2]**. These compounds exhibit remarkable analgesic **[3]**, antitubercular **[4]**, antifungal, antibacterial **[5]**, anti-inflammatory **[6]**, antioxidant and antitumor activities **[7]**. Due to their easier preparation and rich biological activity, pyrazolone framework plays an essential role and represents an interesting template for combinatorial and medicinal chemistry. The synthesis of pyrazolone and its derivatives have engrossed substantial attention from organic and medicinal chemists for many years as they belong to a class of compounds with proven utility in medicinal chemistry.
4-(2-hydroxyethyl)-5-methyl-1,2-dihydro-3*H*-pyrazol-3-one 3 and its derivatives prepared using 3-acetyldihydrofuran-2(3*H*)-one, semicarbazide, thiosemicarbazide and its derivatives. 3-acetyldihydrofuran-2(3*H*)-one reacted with 1,2- diamino at reflux temperature in the presence of Ethanol as solvent following two different procedures: without catalyst or from an efficient and improved procedure using Keggin-type heteropolyacid (HPAs). In this case excellent yields and short reaction times were obtained. Alkylation of pyrazol-3-one derivatives 3 (X = S) in the presence of K_2CO_3 and alkyl halides gave derivatives of thio alkyl pyrazol-3-one 4.



Keywords: pyrazole; heteropolyacid (HPAs); furanone, semicarbazide.

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ULTRASOUND-ASSISTED GREEN AND ELEGANT SYNTHESIS OF NEW CLASS OF 1,2,3-TRIAZOLE AND ISOXAZOLE VIA TANDEM CATALYTIC 1,3-DIPOLAR CYCLOADDITION / RINGS CLEAVAGE REACTION

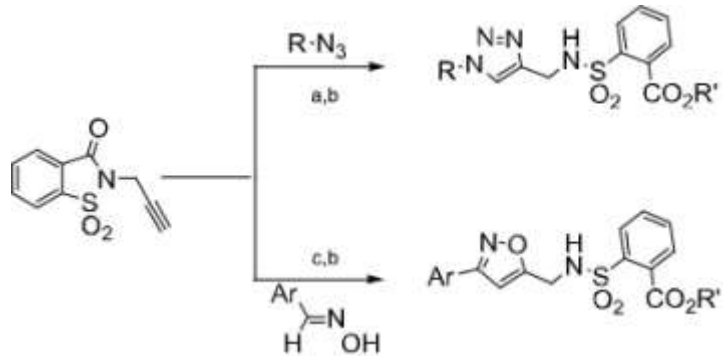
H. Tachallait, M. Driowya, A.Talha, A. Saber, K. Bougrin*

Laboratoire de Chimie des Plantes et de Synthèse Organique et Bioorganique, URAC23, Université Mohammed V, Faculté des Sciences B.P. 1014 Rabat, Maroc

**For correspondence: Email: kbougrin@yahoo.fr*

Abstract

1,3-Dipolar cycloaddition reaction is easy and efficient method for access to five-membered heterocyclic units **[1]**. One of the most important classes for 1,3-dipolar cycloaddition involves azide and nitrile oxide, which is a powerful method for the construction of biologically active aza-heterocycles especially substituted 1,2,3-triazole and isoxazole rings **[2]**.



Experimental conditions: (a,b) Cu(I)/tertiary amine, DCM; R'OH/Na
(c,b) Oxidant, DCM; R'OH/Na

To our knowledge, the synthesis of sulfonamide- triazoles and isoxazoles by a one-pot 1,3-dipolar cycloaddition/rings cleavage cascade carried out under ultrasound condition have not been reported.

Keywords: Sulfonamide; saccharin; triazole; isoxazole; click chemistry; catalysis; one pot.

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SYNTHESIS, CHARACTERIZATION AND ANTIOXIDANT ACTIVITY OF NEW 2,4-THIAZOLIDINEDIONES DERIVATIVES VIA 1,3-DIPOLAR CYCLOADDITION REACTION

F.Z. Thari[a], H. Tachallait[a], N. El Alaoui[a], K. Karrouchi[b,*], K. Bougrin[a,*]

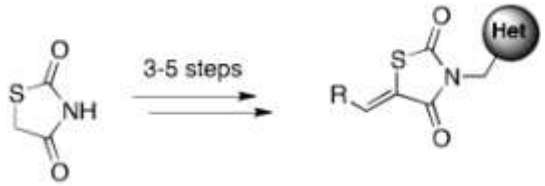
[a]*Laboratoire de Chimie des Plantes et de Synthèse Organique et Bioorganique, URAC23, Université Mohammed V, Faculté des Sciences B.P. 1014 Rabat, Maroc.*
[b]*Laboratoire National de Contrôle des Médicaments, Direction des Médicaments et de la Pharmacie, Ministère de la Santé, Rabat, Maroc.*

**For correspondence: Email: kbougrin@yahoo.fr / khalid.karrouchi@um5s.net.ma*

Abstract

Thiazolidinone is a heterocyclic ring system with multiple applications. In recent years, a large number of innovative drugs containing the thiazolidinone moiety have been developed, including hypoglycemic thiazolidinediones, aldose reductase inhibitors and new generation diuretics. It is an important scaffold known to be associated with several biological activities **[1-4]**.

In this communication, we report the synthesis and antioxidant activity of new 2,4-thiazolidinedione derivatives via 1,3-dipolar cycloaddition reaction. The structures of the newly synthesized compounds were confirmed by IR, NMR, mass spectral studies and structure analysis by single crystal X-Ray diffraction. All compounds were evaluated for their preliminary in vitro antioxidant activity.



Keywords: Synthesis; 1,3-dipolair cycloaddition; thiazolidinone; antioxidant activity.

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SYNTHESIS OF IMIDAZOPYRAZINE DERIVATIVES AND EVALUATION OF THEIR GENOTOXICITY AND CYTOTOXICITY VIA SAR-QSAR MODELS

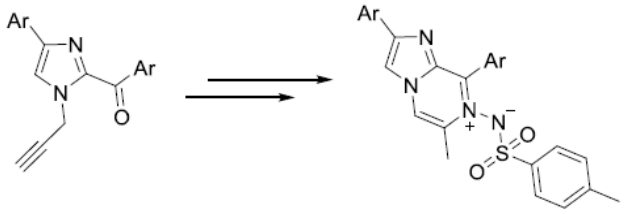
Burak Kuzu[a,*], Meltem Tan[a], Mehmet Taşpınar[b], Nurettin Mengeş[a]

[a]*Yuzuncu Yil University, Faculty of Pharmacy, Pharmaceutical Chemistry*
[b]*Yuzuncu Yil University, Faculty of Medicine, Medicinal Biology*

**For correspondence: E-mail: burak_30046@hotmail.com*

Abstract

Many compounds with imidazole ring are widely used in the treatment of many diseases in clinics. Since the imidazole ring was first reported in 1840, the synthesis of compounds with the imidazole ring has continued to attract interest at an increasing rate **[1]**. This is a consequence of the use of imidazole containing compounds in pharmaceutical industry, agricultural medicines, industrial, artificial receptors, complex ligands, biomimetic catalysts **[2]**. It is important that the imidazole ring be converted into its derivatives by various ringing reactions. For example imidazo[1,2-a]pyrazine rings are used for treatment very disease like Rheumatoid arthritis (RA) (autoimmune disease) **[3]**.
A new and effective method has been devised due to the limited imidazolopyrazine synthesis in the literature. According to this method, the condensation reaction with the imidazole-bonded carbonyl groups and Tos-hydrazine is carried out. After that obtained compound is characterized, subsequent intramolecular closure reaction is intended to give the pyrazine ring in the metal catalysed medium.



Scheme: The intended cyclization reaction

Once the characterization of the resulting cyclization product is made, genotoxic and cytotoxic studies will be carried out in vitro, bioactive potential will be investigated and theoretical QSAR and SAR modeling will be done depending on the result.

This study is supported by TUBİTAK (Grand no: 115Z894).

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SYNTHESIS OF NEW ISATIN DERIVATIVES CARRIED OUT BY 1,3-DIPOLAR CYCLOADDITION

I. Rayni*, Y. El Bakri, J. Sebhaoui, E.M. Essassi

Laboratoire de Chimie Organique Hétérocyclique URAC 21, Pôle de, Compétence Pharmacochimie, Av. Ibn Battouta, BP : 1014 Faculté des sciences, Université Mohammed V, Rabat, Maroc

**For correspondence: Email: irayni@yahoo.fr*

Abstract

This work consists of the synthesis of new heterocyclic systems containing isoxaline and indoline. The production of these compounds is carried out by reaction of 1,3dipolar cycloaddition of 1-allylindoline-2,3-dione with aryl nitrile oxides in chloroform for 4h. The structures of the products were established on the basis of the IR and NMR spectral data (^{1}H and ^{13}C) and confirmed by X-ray analyzes.
The products are likely to exhibit interesting pharmacological properties, since isatin and its derivatives are known for their sedative, anticonvulsant and anti-HIV effects.

Keywords: Synthesis; indoline; 1,3-dipolar cycloaddition; isoxazoline.

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THE ONE-POT SYNTHESIS OF 1,2/3-TRIOLS FROM CORRESPONDING ALLYLIC HYDROPEROXIDES

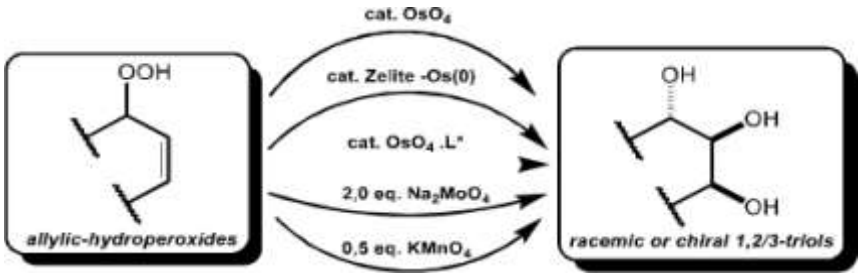
Mehmet Serdar Gültekin[a,*], Haydar Göksu[b], Önder Metin[a]

[a]*Department of Chemistry, Faculty of Sciences, Atatürk University, 25240-Erzurum, Turkey*
[b] *Kaynaşlı Vocational College, Düzce University, 81900-Kaynaşlı, Düzce, Turkey*

**For Correspondence: Email: gultekin@atauni.edu.tr*

Abstract

The triols syntheses were archived with both racemic and chiral reaction condition in high yields without using any co-oxidant (H2O2, t-BuOOH, NMO, etc.) in water/acetone at room temperature.
Polyhydroxylated organic compounds including inositols, quercitols, conduritols, glucose, and cyclic triols are an important class of compounds found in plants and some cyclitols, such as glycerol, ethylene glycol, are often used in the production of industrial materials. Additionally, most cyclitols possess a wide range of important biological activities such as glycosidase inhibitory effect and antibiotic effect. Recently, the enantioselective synthesis of polyhydroxylated organic compounds has received considerable attention due to their useful biological activity and synthetic utility **[1].**



In this method, allylic hydroperoxide group was used as both a co-oxidant and a source of hydroxyl groups. Cyclic or linear allylic hydroperoxides were prepared by photooxygenation of the corresponding alkenes according to reported procedure in literature **[2-4].** The triols syntheses were archived with both racemic and chiral reaction condition in high yields without using any co-oxidant (H_2O_2, t-BuOOH, NMO, etc.) in water/acetone at room temperature. In our study, facile, efficient and practically methods for the one-pot synthesis of 1,2/3-triols from the allylic hydroperoxides were developed by using 0.5 eq. KMnO4, 2.0 eq. Na_2MoO_4, cat. OsO_4, cat. zeolite-confined osmium (0) nano-clusters or cat. OsO_4-chiral cinchona alkaloids complex.

Keywords: Intramolecular atom transfer; allylic hydroperoxides; Oxidation.

Acknowledgment: *This study was supported partially by the Scientific and Technological Research Council of Turkey (TUBITAK) (Project No: 109T815) and Ataturk University Scientific Research Project Council (Projects No: 2010/32; 2011/93 and FAD-2017/6107).*

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SYNTHESIS OF NOVEL DERIVATIVES OF 6-METHYL-QUINOXALINE-2,3-DIONE AND 6-METHYL-QUINOXALINE-2,3-DITHIONE

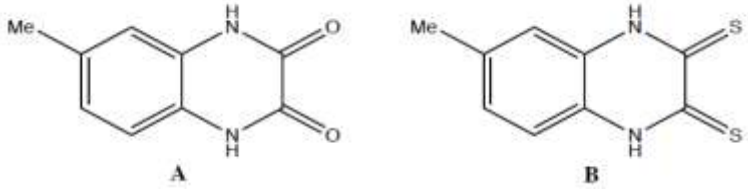
A. Zouitini[a,*], Y. Kandri Rodi[a,*], K. Misbahi[a], F. Ouazzani Chahdi[a], E.M.Essassi[b]

[a]*Laboratory of Applied Organic Chemistry, Faculty of Science and Technology, Sidi Mohammed Ben Abdallah University, Fez, Morocco.*
[b]*Laboratoire de Chimie Organique Hétérocyclique, URAC 21, Pôle de Compétences Pharmacochimie, Mohammed V University, Faculté des Sciences, Av. Ibn Battouta, BP 1014 Rabat, Morocco*

**For correspondence: Email: ayman.zouitini@gmail.com / youssef_kandri_rodi@yahoo.fr*

Abstract

The synthesis of quinoxalines has been intensively studied in the past, especially because of the diverse biological activities ascribed to many representatives of this class of compounds.
The quinoxaline moiety is present in a large variety of physiologically active compounds, with applications varying from medicinal to agricultural. Various quinoxalines exhibit biological activities including antibacterial **[1]**, anti-inflammatory **[2]**, anticancer **[3]**, kinase inhibitors **[4]**, antitumor **[5]**, and antidiabetic **[6]**.
The 6-methyl-1,4-dihydroquinoxaline-2,3-dione **(A)** was synthesized by the condensation of 4-methyl-o-phenylenediamine with oxalic acid under reflux in hydrochloric acid solution. Then the compound **(A)** was reacted with phosphorus pentasulfide P_2S_5 in presence of pyridin affording to 6-methyl-1,4-dihydroquinoxaline-2,3-dithione **(B)**.
In order to prepare other quinoxaline-2,3-diones and quinoxaline-2,3-dithiones disubstituted Compounds **(A)** and **(B)** were exposed to alkylation reactions under the conditions of phase transfer catalysis using monohalogenated agents.



Keywords: quinoxaline-2,3-dione; Alkylation; *o*-phenylenediamine.

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NANO DIPHOSPHATE AS NEW CATALYST FOR SYNTHESIS OF PYRANOPYRAZOLES

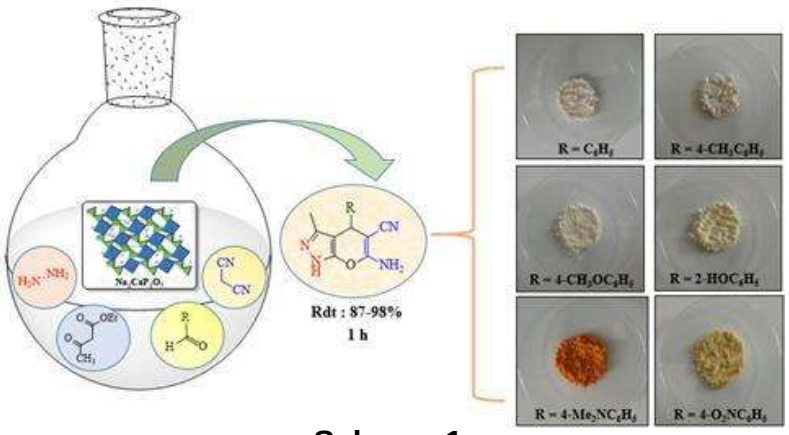
R. Jouhari[a], **A. Elmakssoudi**[a,]*, M. Dakir[a], M. Elabbassi[a], M. Zahouily[b]

[a]*Laboratoire de Synthèse Organique, Extraction et Valorisation (LSOEV), Université Hassan II de Casablanca, Faculté des Sciences Ain Chock, Casablanca.*
[b]*Laboratoire de Matériaux, Catalyse & Valorisation des Ressources Naturelles (LMaCaVa) Université Hassan II de Casablanca, FST Mohammedia*

**For correspondence: Email: h.elmakssoudi@gmail.com*

Abstract

Pyranopyrazoles represent an important class of heterocyclic compounds. They find applications as pharmaceutical ingredients and biodegradable agrochemicals **[1]**. The most straightforward synthesis of this heterocyclic system involves a four-component coupling of aromatic aldehyde, malononitrile, ethyl acetoacetate, and hydrazine hydrate. A number of methods have been reported for the synthesis of pyranopyrazoles employing different catalysts. In continuation of our investigation on the use of nano-$Na_2CaP_2O_7$ as catalyst **[2]** and our interest in synthesis of heterocycles containing a pyran ring systems **[3]**, we report an efficient and facile synthesis of a series of pyranopyrazoles using nano-structured diphosphate ($Na_2CaP_2O_7$) as catalyst (Scheme 1).



Scheme 1

The method offers several advantagesincluding high yields, short reaction times, a simple work-up procedure and catalyst reusability for several runs.

Keywords: nano-structured diphosphate; pyranopyrazoles; four-component reaction.

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ELECTROCHEMICAL REDUCTIVE AMINATION OF BENZALDEHYDE

A. Haouat,[a,b,*], F. Louafi[a], A. Chibani[a]

[a]*Unité de Recherche CHEMS, Université des Frères Mentouri,Constantine, 25000, Algérie*
[b]*Université d'El oued, El Oued, Algérie*

**For Correspondence: anays.org@gmail.com*

Abstract

In biological and chemical systems, the reductive amination of aldehydes and ketones is an important transformation, which allows the direct conversion of carbonyl compounds into amines using simple operations **[1]**.
A variety of reducing agents, such as sodium cyanoborohydride ($NaBH_3CN$), [$NaBH(OAc)_3$], pyridine-borane (pyr-BH_3) have been developed for this conversion. The reductive aminations with $NaBH_3CN$ are successfully carried out using a five-fold excess of amine at pH 6–8. However, the use of expensive and highly toxic $NaBH_3CN$ that carries the risk of having residual cyanide in the product as well as in the work-up stream makes this procedure less attractive. Clearly, the use of $NaBH_3CN$ is not acceptable in the context of green synthesis, especially in industry **[2]**. Our approach is electrochemical reduction of benzaldehyde in presence of primary amines (scheme.1). Several medium were tested. All conversion of benzaldehyde to secondary amines in good yields has been carried out in CH_3COOLi at potential-controlled. This is a highly efficient and mild procedure that is applicable for a wide variety of substrates.

Keywords: reductive amination; amines; aldehydes, elctroreduction.

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THEORETICAL STUDY OF COPPER ACETONITRILE EFFECTS ON FUKUI INDICES AND REGIOSELECTIVITY USING DENSITY FUNCTIONAL THEORY (DFT)

A.Ghaleb[a,*], A. Aouidate[a], T. Lakhlifi[a], M.Bouachrine[b], H. Maghat[c], A. Sbai[a]

[a]*Molecular Chemistry and Natural Substances Laboratory, school of Science Moulay Ismail University, Meknes, Morocco.*
[b]*Laboratory of chemistry and biology applied to the environment, school of Science Moulay Ismail University, Meknes, Morocco.*
[c]*EST, Moulay Ismail University, Meknes, Morocco.*

**For Correspondence: E-mail: adib.ghaleb@gmail.com*

Abstract

Copper-catalyzed azide–alkyne cycloaddition (CuAAC) is a straightforward way for making covalent connections between building blocks containing various functional groups. It has been used widely in organic synthesis, medicinal chemistry, polymer chemistry, and bioconjugation applications. Using copper acetonitrile as catalyst for click reaction (CuAAC) lead to a non-concerted reaction, and affect fukui indices to determine the polar sites, therefor predict the favorable regioisomer (1,4-regioisomer) and explain the contradiction obtained to the experimental results. The huge difference of activation barriers between catalyzed and uncatalyzed reaction indicate that is a selective reaction.

Keywords: Click reaction; 1,3-dipolar cycloaddition; 1,2,3-triazole; regioselectivity; fukui indices.

ANTIOXYDANT ACTIVITY OF DIFFERENT EXTRACTS OF *ZIZYPHUS LOTUS* FROM NORTH OF MOROCCO

K. Ammor[a,*], D. Boucetta[b], S. Jennane[a], A. Chaqroune[a] , F. Mahjoubi[a]

[a]*Laboratory of Process Engineering and Environmene, Faculty of Sciences Dhar Mahraz, University Sidi Mohamed Ben Abdellah, BP : 1796, Fez, Morocco.*
[b]*Laboratory of Neuroendocrinology and Nutritional Environment and Climate, University of Sidi Mohamed Ben Abdellah, BP : 1796, Fez, Morocco*

**For correspondence: Email: kenza.ammor1@gmail.com*

Abstract

Zizyphus lotus, also known as Jujube, is a medicinal plant largely found in the Mediterranean region including Algeria **[1]**. The fruit of this plant is consumed by local population for the treatment of several pathologies such as digestive disorders, obesity, urinary troubles and skin infections **[2,3]**.
The objective of this work is to study the antioxidant activity of hydro-ethanolic and aqueous extracts of *Zyziphus lotus* by using three methods, DPPH, FRAP and total antioxidant activity.
The results of the antioxidant activity showed that the aqueous extract of *Zyziphus lotus* have a higher antioxidant activity than the aqueous extract by using the three methods.

Keywords: Extracts, *Zyziphus lotus*, antioxidant activity

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NEW IN-SITU PREPARED CATALYSTS FOR CATECHOLASE MOLDING

R. El Ati*, Y. Kaddouri, A. Mouadili, A.Takfaoui, M.El Kodadi, R.Touzani

Laboratory of Applied Chemistry and Environment, COSTE, Faculty of Science, Mohammed Premier University, Oujda-Morocco

**For Correspondence: Email: rafika.elati@gmailcom*

Abstract

Catalysis solves many problems in the course of chemistry reactions, especially for green, economical and less polluting chemistry.
In this work, we will investigate new catalysts to reproduce the catalytic activity of the enzyme catechol oxidase (CO) in order to demonstrate the structural parameters essential to the reactivity of the enzyme and to understand the mechanism of action **[1]**. We compared the potentialities of the complexes formed in situ as well as the synthesized complex, as catalysts of the oxidation reaction of catechol to o-quinone **[2]**.

Keywords: Catechol; *In situ;* complexes; oxidation.

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ANTIBACTERIAL, ANTIOXIDANT ACTIVITIES AND MUTAGENICITY OF 1,2-BIS(2-(2-MORPHOLINOPHENOXY)ETHOXY)ETHANE

Gönül Yapar

Department of Chemistry, Faculty of Arts and Sciences, Istanbul Technical University, Maslak, 34469 Istanbul, Turkey

For Correspondence: E-mail: yaparg@itu.edu.tr

Abstract

Ion binding macromolecules are important and rapid growing group of organic chemistry. These compounds are classified as supramolecules due to their physical, chemical and biological activities. Macrocyclic compounds bearing oxyethylene units called coronand and open chain form of those called podands **[1]**. Morpholine is an amino ether; which is an important molecule, due to its functionality and importance in chemical and biological applications. Despite, the ether function of the molecule is typically inert; most of the reactions occurs over seconder amine group. A number of morpholine derivatives are used as analgesics and local anesthetics, moreover as respiratory and vasomotor stimulants. Furthermore; morpholine is used in pharmaceutical applications such as choleretics, antispasmodics, analeptics and as antimalarials. Molecules having morpholine in their structures are used as bactericides, fungucides and herbicides due to their antimicrobial behaviours **[2-4].**

In this study, morpholine units as substituents were attached to the aromatic part of opened-chain macrocyclic ether. 1,2-Bis(2-(2-morpholinophenoxy)ethoxy)ethane molecule was tested against C. albicans, A. niger, Penicillium sp., E. coli and S. aureus by using serial 96-well microbroth dilution method **[5]**. Ampicillin was used as reference antibiotic in the study. The CUPRAC (Cupric Reducing Antioxidant Capacity) method was used for antioxidant measurements **[6]**. Trolox was used as referance antioxidant in CUPRAC method. For detecting mutagenicity of 1,2-bis(2-(2-morpholinophenoxy)ethoxy)ethane molecule (Fig. 1) Ames test was used on S. Typhimurium TA 100 strain **[7]**.

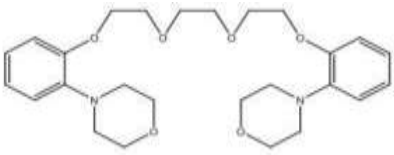

Figure 1: 1,2-Bis(2-(2-morpholinophenoxy)ethoxy)ethane

Acknowledgements: *This research study was partly supported by The Scientific and Technological Research Council of Turkey (TUBITAK)*

Keywords: Podand; morpholine; antimicrobial; antibacterial; antioxid ant

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SYNTHESIS OF NOVEL BISINDOLYLMETHANE DERIVATIVES AS AIE MATERIAL

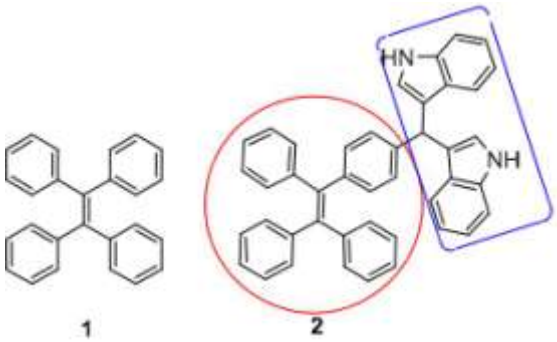
Farrokh Lafzi[a], Berrak Ertugrul[a], Haydar Kilic[b,c], **Nurullah Saracoglu[a,*]**

[a]*Department of Chemistry, Faculty of Sciences, Atatürk University, 25240 Erzurum, Turkey*
[b]*East Anatolia High Technology Application and Research Center, Atatürk University 25240, Erzurum, Turkey*
[c]*Oltu Vocational School, Atatürk University, 25400, Erzurum, Turkey*

**For correspondence: Email: nsarac@atauni.edu.tr*

Abstract

Luminescent molecules with aggregation-induced emission (AIE) that are not fluorescent in solution but are highly emissive in the aggregate or solid state **[1]**. The design and synthesis of AIE luminophores have attracted much interest due to high-tech applications of these materials in various optoelectronic and biological devices, such as organic lighting-emitting diodes (OLEDs), chemosensors, and bioprobes **[2-4]**. In this communication, we prepared bisindolemethane substituted tetraphenylethylenes as a new AIE system. Furthermore, their photophysical properties are currently underway.



Acknowledgment: This study is supported by the coordination of scientific research projects of Atatürk University (Project number: **2016/162** and **FAD-2017/6107**). We would like to thank Atatürk University for its support.

Keywords: Indole; tetraphenylethylene; aggregation-induced emission.

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A NEW APPROACH TO PREPARE DERIVATIVES OF 1, 3- DITHIOLE-2-THIONE

D. Jeroundi*, S. Chakroune, E.M. El Hadrami, A. Ben-Tama

Laboratory Of Applied Organic Chemistry, Sidi Mohamed Ben Abdellah University, Faculty Of Science And Technology, Road Immouzer, BP 2202 Fez, Morocco

**For correspondence: Email: douniajeroundi@gmail.com*

Abstract

The 1,3- ditiole-2- thione ring system is recognized to be widely used as donor components in the preparation of molecular conductors and superconductors **[1–6]** and that's because of their electron-donating ability and their attractive reversible redox properties. On the other hand, the study of five-chain heterocyclic systems (triazoles, oxazoles) has been considerably developed due to the demonstration of their biological activities **[7-9]**.
However, the discovery of new compounds containing the thiolone remains a challenging area of research. Herein we report different methods (alkylation, condensation and click- chemistry) for the synthesis of new polysubstitued thiolone derivatives able to present potential pharmacological activities.

Keywords: 1,3- dithiole-2- thione ring; click chemistry; biological potential.

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SYNTHESIS, STRUCTURAL STUDY, ANTIBACTERIAL ACTIVITY AND THEORETICAL STUDY OF SOME ISOXAZOLINE CONTAINING 1,4-BENZOTHIAZIN-3-ONE NUCLEUS OBTAINED BY 1,3-DIPOLAR CYCLOADDITION REACTION

Nada Kheira Sebbar[a,*], Zerzouf Abdelfettah[b], Mohamed Ellouz[a], Younes Ouzidan[c], H. Elmsellem[d], Zakaria Mennane[e], Reda Charof[e], El Mokhtar Essassi[a,f]

[a]*Laboratoire de Chimie Organique Hétérocyclique, Pharmacochimie, Av Ibn Battouta, BP 1014, Faculté des Sciences, Université Mohammed V, Rabat, Morocco.*
[b]*Laboratoire de Chimie Organique et Etudes Physico-chimique, ENS Takaddoum, Université Mohammed V, Rabat, Morocco.*
[c]*Laboratoire de Chimie Organique Appliquée, Faculté des Sciences et Techniques, Université Sidi Mohamed Ben Abdallah, Fès, Morocco.*
[d]*Laboratoire de chimie analytique appliquée, matériaux et environnement (LC2AME), Faculté des Sciences, B.P. 717, 60000 Oujda, Morocco.*
[e]*Département de bactériologie, Institut national d'hygiène, avenue Ibn Batouta, B.P. 769, Agdal, Rabat, 11000, Morocco.*
[f]*Moroccan Foundation for Advanced Science, Innovation and Research (MASCIR), Rabat, Maroc.*

**For correspondence: Email: snounousebbar@gmail.com*

Abstract

The chemistry of 1,4-benzothiazine derivatives have constituted an important class of heterocycles, which, even when part of a complex molecule **[1]**, possess a wide spectrum of biological activities **[2]**, due to the presence of a fold along the nitrogen sulfur axis. The biological activity of some 1,4-benzothiazine derivatives is similar to that of phenothiazines, featuring the same structural specificity **[3]**. The role of 1,4-benzothiazine in medicinal chemistry was reviewed earlier **[4]**. Generally, 1,4-benzothiazine derivatives have found widespread application as analgesic, antibacterial, anticancer, anthelmintic **[5-6]**. These properties indicate that 1,4-benzothiazine derivatives are a template that may be potentially useful in medicinal chemistry research and therapeutic applications. The 1, 3-dipolar cycloaddition of arylnitrile oxides on the 4-allyl-2-(substituted)-three, 4-dihydro-2*H*-1,4-benzothiazin-3-one led to polycyclic heterocyclic. The structure of the obtained cycloadducts was determined from ^{1}H-NMR and ^{13}C-NMR, and for some structures confirmed the proposed regiochemistry by crystallographic studies. The synthesized products were subjected to *in vitro* biological evaluation. Several tested compounds showed significant antibacterial activities. A theoretical study was also performed. The results are in agreement with the experimental data.

Keywords: arylnitriloxides, 1,3-dipolar cycloaddition, 1,4-benzothiazin-3-one, Antimicrobial, crystallographic structural resolution.

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A SIMPLE SYNTHESIS FOR N^2-SUBSTITUTED SPIRO PYRAZOLO[4',3':5,6]PYRANO[2,3-*D*]PYRIMIDINE AS A NEW SCAFFOLDS FOR ANTIVIRAL AGENTS

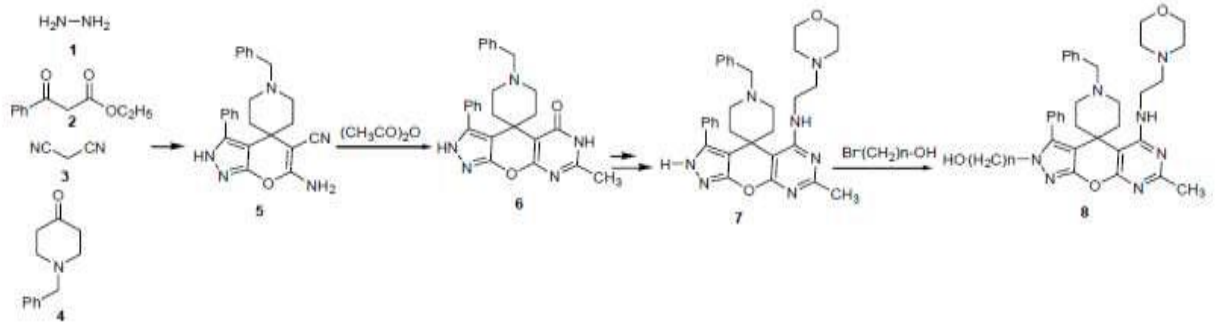
Sami A. Al-Hussain[a], **Magdi E. A. Zaki[a,b,*]**

[a]*Faculty of Science, Department of Chemistry, Al-Imam Muhammad Bin Saud Islamic University, Riyadh 11632, Kingdom of Saudi Arabia*
[b]*Photochemistry Department, National Research Centre, Cairo 12622, Egypt.*

**For correspondence: Email: mezaki@imamu.edu.sa*

Abstract

A recent knowledge of Multi-component reactions chemistry (MCR) suggests that the necessary material of life, in particular, pre-biotic organic molecules, might be formed by MCR in water as an efficient and eco-friendly method for the synthesis of pyranopyrazole **[1]**. N^2-substituted fused pyranopyrazole considered to be an active promising class of fused pyrazoles **[2]** possessing a diverse spectrum of biological activity. Among antibacterial, antifungal, antimicrobial, anti-inflammatory, and analgesic.



The present work describes the synthesis of pyranopyrazole using 4 component reactions protocol, hydrazine **1**, phenyl acetoacetate **2**, malononitrile **3** and 1-(2-phenylethyl)piperidin-4-one **4**, led to the formation of compound **5**.Treatment of compound **5** with acetic anhydride afforded compound **6** which transformed to 6-substituted pyrazolopyranopyrimidines **7**. Alkylation of N-^{2} of compound **7** led to the formation of N^2- substituted spiro fused pyrazoles. The structure of all obtained compounds was proved by NMR- and IR-spectroscopy, the all new compounds has been submitted for biological activity studies and virtual screening.

Keywords: Multi-component reactions chemistry; pyranopyrazole; N^2- substituted spiro fused pyrazolo.

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AN EFFICIENT SYNTHESIS OF NEW HYBRID MOLECULES CONTAINING OXADIAZAPHOSPHOLE-5-CARBOXYLATE AND 2-PYRONE MOIETIES

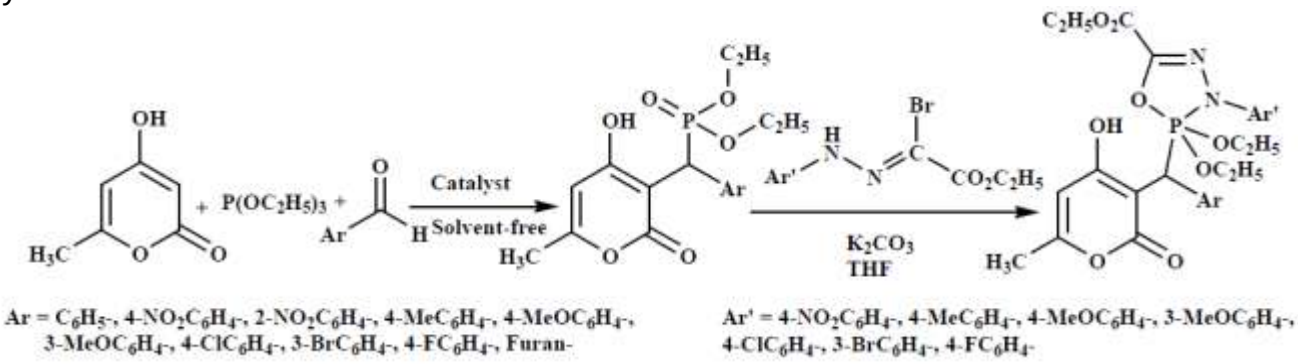
A. Ihammi*, L. Bouissane, M. Chigr, E. M. Rakib*

Laboratoire de Chimie Organique et Analytique, Faculté des sciences et Techniques, Université Sultan Moulay Slimane, BP : 591, Beni-Mellal, Maroc.

**For correspondence: Email: elmostapha1@ymail.com / azizihammi@gmail.com*

Abstract

The synthesis of 2-pyrones and their derivatives has attracted much attention in the context of the biological activities of these compounds induced by the hetero-cyclic moiety [**1-4**]. These compounds display a wide range of biological activities such as cytotoxic, antibiotic and antifungal activity. Phosphonate derivatives have considerably attracted the attention of organic chemists due to their wide range of applications in agriculture and bio-chemistry. For example, phosphonate derivatives are used as insecticides, herbicides, fungicides and plant-growth regulators in the area of agricultural chemistry **[5]**. Extensive efforts have been made to introduce convenient and efficient methods for the synthesis of phosphonates [**6,7**]. In view of the aforementioned success, we planned to explore the possibility of introducing a oxadiazaphosphole group into a pyrone ring through multicomponent reaction and 1,3-dipolar cycladditions.



Keywords: 2-pyrone; oxadiazaphosphole; cycloadducts.

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SYNTHESIS OF NOVEL 1,3,4-THIADIAZOLES USING A MONOTERPENE ISOLATED FROM ESSENTIAL OIL OF *CEDRUS ATLANTICA*

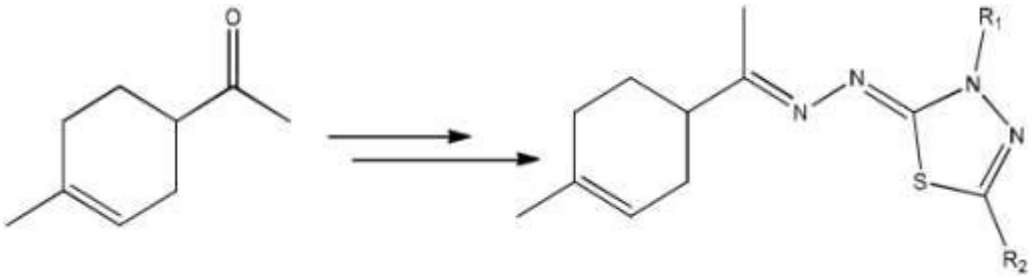
M. Fawzi[a,*], A. Auhmani[a], My.Y. Ait Itto[a], A. Oubella[a], A. Auhmani[a] A. Riahi[b], S. Chevreux[b] and E.M. Ketatni[c]

[a]*Laboratory of Organic Synthesis and Physico-Molecular Chemistry, Department of Chemistry, Faculty, of Sciences Semlalia, B.P. 2390, Marrakech 40001, Morocco,*
[b]*Institute of Molecular Chemistry of Reims, CNRS UMR 7312 Bat.Europol'Agro, Moulin Of the Housse UFR Sciences, B.P.1039-51687 Reims Cedex 2, France, and*
[c]*Laboratory of Applied Spectro-Chemistry and Environment, University Sultan, Moulay Slimane, Faculty of Science and Technology, PO Box 523, Beni-Mellal, Morocco.*

**For Correspondence: Email*: fawzi.mourad93@gmail.com

Abstract

Five membered heterocyclic compounds have been reported to exhibit a wide range pharmacological effects amongst them 1,3,4-thiadiazoles. In pharmaceutical and agrochemical domain, 1,3,4-thiadiazoles display a broad spectrum of biological activities including antibacterial **[1]**, antimicrobial **[2]**, anticancer **[3]** anti-inflammatory **[4]**, antileishmanial **[5]**, antidepressants **[6]**, antituberculosis **[7]**, antioxidant **[8]**. In addition, 1,3,4-thiadiazoles are widely applied in optics and electrochemistry. Prompted by the aforementioned findings, we used an monoterpene isolated from of the essential oil of *Cedrus atlantica* to prepare a new series of 1,3,4-thiadiazole derivatives as shown below.



Keywords : synthesis; monoterpene; thiadiazole.

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ANTIOXIDANT ACTIVITIES AND TOTAL PHENOLIC AND FLAVONOIDS CONTENT VARIATIONS OF LEAVES EXTRACTS OF *LAURUS NOBILIS* FROM MOROCCO

A. Tarog*, F.El kamari, Y.El Atki, I.Aouam, B. Lyoussi, A. Abdellaoui

Laboratory of Physiology Pharmacology and Environmental Health, Department of Biology, Faculty of Sciences Dhar Mehraz, University Sidi Mohamed Ben Abdellah, B.P. 1796, Atlas, Fez, Morocco.

**For correspondence: Email*: tarog.amal@gmail.com

Abstract

Reactive oxygen species (ROS) are produced by cellular metabolism and by exogenous agents in the cells. These ROS may induce oxidative damage to various biomolecules in cells such as DNA, carbohydrates, proteins which in turn leads to cardiovascular and neurodegenerative diseases, *Laurus nobilis* is an evergreen shrub belongs to the Lauraceae family and is native to the Mediterranean region it's used in tradional Moroccan medicine and as condiments. The present study was undertaken to determine antioxidant activity, total phenolic and flavonoid content of ethanol, methanol, ethyl acetate and aqueous extracts of leaves of *Laurus nobilis.* Antioxidants properties were measured using three tests: free radical scavenging activities against 2, 2-diphenyl-1-picrylhydrazyl, reduction of molybdate and reducing (Fe^{3+}_Fe^{2+}) power. Total phenolic content was measured by Folin Ciocalteu reagent. The results ethanol and water extracts showed antioxidant activities unlike ethyl acetate. Aqueous extract exhibited a higher DPPH radical scavenging (IC50=0,07mg/ml) and reducing of molybdate 545,83±5,89 Equivalent to ascorbic acid(mg)/g dry extract. The strong antioxidant activity of water extract wich was probably due to its high content of phenols 494, 86 ±3, 62 mg gallic acid equivalent/g dry extract. Ethanol and water extracts showed the high total falvonoid content with values: 153,33±3,59 and 127, 25±2,60 mg Equivalent rutin/g dry extract respectively.

Our results suggested a potent and excellent antioxidant activity of *Laurus nobilis* extracts, and could be considered as a potential source of a biomolecules for pharmaceutical industry.

Keywords: *Laurus nobilis;* antioxidant activity; DPPH; phenols; total flavonoid.

NEW ASSAY METHOD OF THE ATRACTYLOSIDE AND CARBOXYATRACTYLOSIDE

S. Errai[a,*], Y. Khabbal[b], M. Faid[c], A. Maataoui[d], M. Benbella[d], A. Abdellaoui[a]

[a]*Laboratory of Physiology, Pharmacology Health and Environment Unit of Bioremediation and Environment, Department of Biology. Faculty of Sciences Dhar EL Mahraz, Université Sidi Mohamed*
[b]*Laboratory of pharmacologie. Faculty of Medicine and Pharmacy, University of Fez BP. 1893; Km 2.200, Sidi Hrazem Road, Fez 30000, Morocco*
[c]*Institue agronomic and vétairinaire Hassan II, Rabat, Morocco*
[d]*National School of Agriculture, Meknes, Morocco*

**For correspondence: Email: siham.errai1@usmba.ac.ma*

Abstract

Atractylis gummifera L. or thistle glue, is a plant of the Asteraceae family, known in Arabic as Addad or choûk el-eulk. It is a plant of the Mediterranean region, found in North Africa and southern Europe **[1]**. In Morocco, the plant is frequently found in nature in the wild form, and is characterized by the production of a highly toxic glycoside called atractyloside (ATR) **[2,3]**. The objective of this study is the development of a new method of determining the plasma levels of atractyloside in the roots of thistle glue. Method: Root samples were collected in the region of Fés boulmane, and extracts were analyzed by the system of ultra-violet spectrometery (JASCO-530). Results: The validation of our method is based on the recommendations of ICH guidelines for the adaptation of new analytical techniques. The coefficient of determination is 0.99, the limit of detection and quantification are respectively 93 µg / ml, 310 µg / ml. While the sensitivity is 0.2927, which reduces the risk of interference in the dosage of the active ingredient of the thistle glue plant. Discussion: Many methods for the determination of atractyloside and carboxyatractyloside are published, often based on the use of liquid chromatography, gas or techniques cumbersome, complex and lacking in sensitivity and specificity.Conclusion: The results of our study show that this new method is practical, simple and applicable to all types of laboratories.

Keywords: Atractylis gummifera; Atractyloside; Carboxyatractyloside; Assay; Plasmatique determination.

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SYNTHESIS AND ANTIBACTERIAL ACTIVITY OF 2-BENZAMIDO-2-((2-METHOXY-2-OXOETHYL)AMINO)ACETATE

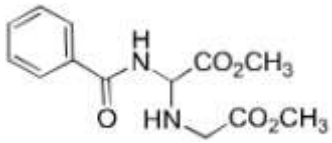
O. Karai, Y. Aouine, H. Faraj, A. Alami*, A. El Hallaoui, B. Labriti

Laboratoire de Chimie Organique, Faculté des sciences Dhar EL Mahraz, Université Sidi Mohamed Ben Abdellah, BP : 1796, Fès, Maroc.

**For Correspondence: Email: alamianouar@yahoo.fr*

Abstract

Heterocyclic amino acids play a predominant role in the synthesis of peptides and proteins, since they increase the resistance of peptides to enzymatic degradation **[1]**. In addition, these building blocks and their derivatives are present in a number of potentially active against various fungal strains and many of them got wide acceptance clinical trials **[2,3]**.
We described in this communication the preparation of 2-benzamido-2-((2-methoxy-2-oxoethyl)amino)acetate. This preparation approach is based on *N*-alkylation method (Figure).



Figure

The obtained product was characterized on the basis of 1D and 2D NMR spectroscopy (^{1}H, ^{13}C) in addition to MS data and it was also tested *in vitro* for its antibacterial activity against Gram-positive and Gram-negative bacteria.

Keywords: *N*-alkylation; antibacterial activity; Heterocyclic α-amino acid.

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SYNTHESIS AND STRUCTURAL CHARACTERIZATION OF (2-PHENYL-4,5-DIHYDROOXAZOLE-4,4-DIYL)DIMETHANOL

H. El Madani El Alami, S. Boukhssas, Y. Aouine, H. Faraj, A. Alami*, A. El Hallaoui, B. Labriti

Laboratoire de Chimie Organique, Faculté des sciences Dhar El Mahraz, Université Sidi Mohamed Ben Abdellah, BP : 1796, Fès, Maroc.

**For Correspondence: Email: alamianouar@yahoo.fr*

Abstract

The oxazoline ring is important constituent of bioactive natural products **[1]** and pharmaceuticals **[2]**. Oxazolines are five-membered heterocyclic compounds having one double bond and present an interesting structure on which to build a wide variety of compounds having properties which make them of interest in many fields of application.
Continuing our investigations in the use of oxazoline derivatives **[3]** in heterocyclic synthesis of α-amino acids, we described in this communication the preparation of (2-phenyl-4,5-dihydrooxazole-4,4-diyl)dimethanol (Figure).

Figure

The structure of the synthesized compound was established on the basis of NMR spectroscopy (^{1}H, ^{13}C), X-ray crystallography and MS data.

Keywords: Oxazoline derivatives; Heterocyclic α-amino acid.

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MICROWAVE-ASSISTED SYNTHESIS OF CHROMENO[3,4-*b*]XANTHONES AND (BENZO[*c*]CROMENYL)CHROMONES

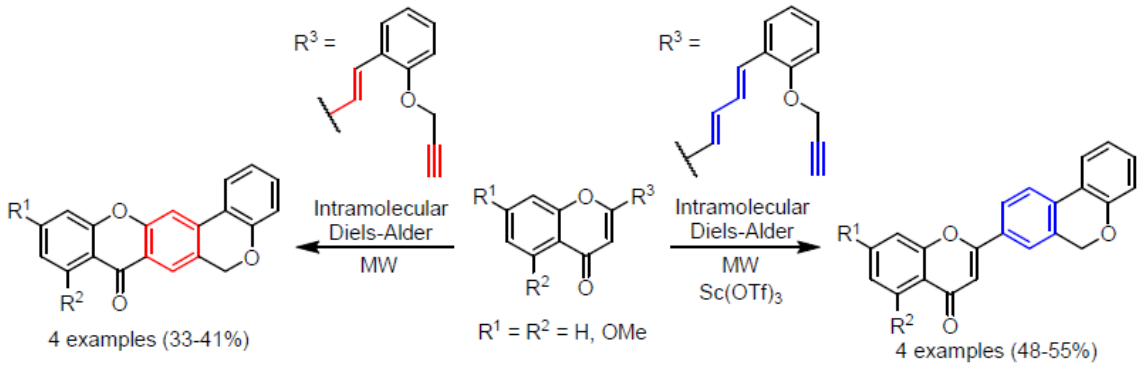
Hélio M. T. Albuquerque[a,*], Clementina M. M. Santos[a,b], José A. S. Cavaleiro[a], Artur M. S. Silva[a],

[a]*Department of Chemistry & QOPNA, University of Aveiro, Campus de Santiago, 3810-193 Aveiro, Portugal.*
[b]*School of Agriculture, Polytechnic Institute of Bragança, Campus de Santa Apolónia, 5300-253 Bragança, Portugal.*

**For correspondence: Email: helio.albuquerque@ua.pt*

Abstract

Following previous reports dealing with the reactivity of chromone derivatives in Diels-Alder reactions, series of novel (*E*)-2-[2-(prop-2-yn-1-yloxy)styryl]chromones and of 2-{(1*E*,3*E*)-4-[2-(prop-2-yn-1-yloxy)phenyl]buta-1,3-dien-1-yl}chromones were designed and synthesized through aldol condensation of 2-methylchromones with 2-propargyloxy(benzaldehyde and cinnamaldehyde), respectively. Both chromone derivatives were used as substrates in microwave-assisted intramolecular Diels-Alder reactions, affording chromeno[3,4-*b*]xanthones and (benzo[*c*]chromenyl)chromones. This is the first report involving chromone derivatives in intramolecular Diels-Alder reactions for the synthesis of new oxygen heterocycles, namely xanthones and flavones **[1-2]**.



Keywords: propargyloxychromones, intramolecular Diels-Alder, flavones, xanthones, MW - assisted organic transformations.

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ANALYTICAL APPLICATION OF XANTHONE DERIVATIVES AS CHIRAL SELECTORS FOR LIQUID CHROMATOGRAPHY

Ye Zaw Phyo[a], Carla Fernandes[b,c,*], M. Elizabeth Tiritan[b,c,d], Sara Cravo[b,c], Artur M.S. Silva[e], Anake Kijjoa[a], Madalena M.M. Pinto[b,c],

[a]*Instituto de Ciências Biomédicas Abel Salazar, Universidade do Porto, Portugal*
[b]*Laboratório de Química Orgânica e Farmacêutica, Departamento de Ciências Químicas, Faculdade de Farmácia, Universidade do Porto, Portugal*
[c]*Centro Interdisciplinar de Investigação Marinha e Ambiental (CIIMAR/CIMAR), Universidade do Porto, Portugal*
[d]*CESPU, Instituto de Investigação e Formação Avançada em Ciências e Tecnologias da Saúde, Gandra, Portugal*
[e]*Departamento de Química & QOPNA, Universidade de Aveiro, Aveiro, Portugal*

**For correspondence: Email: cfernandes@ff.up.pt*

Abstract

Xanthones are oxygenated heterocyclic compounds with a dibenzo-γ-pyrone scaffold, well known in Medicinal Chemistry **[1]**. In addition to the interesting biological/pharmacological activities **[2,3]**, these small molecules were exploited for analytic proposals as selectors for liquid chromatography (LC) in enantioseparation methods **[4]**.
Herein, we describe the development of three new chiral stationary phases (CSPs) based on chiral derivatives of xanthones. These chiral selectors, obtained by multi-step synthetic pathways, were covalently bonded to silica and then packed into LC stainless-steel columns.
The LC enantioresolution capability of the CSPs was evaluated, under normal phase elution conditions, using different standard racemates as well as a library of enantiomeric mixtures of xanthones prepared "in-house". The new chiral stationary phases revealed good enantioselectivity mainly for the enantiomeric mixtures of xanthone derivatives.

Keywords: chiral derivatives of xanthone; chiral selectors; liquid chromatography.

This work was supported through national funds from Foundation for Science and Technology (FCT) and European Regional Development Fund (ERDF) and COMPETE under the projects PEst-C/MAR/LA0015/2013, PTDC/MAR- BIO/4694/2014 (POCI-01-0145-FEDER-016790), QOPNA (FCT UID/QUI/00062/2013), and INNOVMAR (Innovation and Sustainability in the Management and Exploitation of Marine Resources) - NORTE-01-0145- FEDER-000035, Research Line NOVELMAR, Chiral–Drugs -CESPU -2017 and the Portuguese NMR Network. Y.Z. Phyo thanks the Erasmus Mundus Action 2 (Lotus Plus project) for a PhD's scholarship, and also the IUPAC grant destined to facilitate the participation at the TRAMECH-IX.

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ANALYSE COMPARATIVE DES HUILES ESSENTIELLES DU *Rosmarinus officinalis* DE DIFFÉRENTES RÉGIONS MAROCAINES

M. El Yemni[a,d,*], N. Eloutassi[a,b], M. Taleb[c], M. Chaouch[a], A. Bouia[d]

[a]*Laboratoire de Génie des Matériaux et Environnement, Faculté des Sciences Dhar El Mahraz, Université sidi Mohammed ben Abdellah, Fès, Maroc.*
[b]*Laboratoire des Sciences de la Vie, Centre Régional des Métiers de l'Education et de la Formation, Fès, Maroc.*
[c]*Laboratoire d'ingénierie, d'électrochimie, de modélisation et d'environnement, Faculté des Sciences Dhar El Mahraz, Université Sidi Mohammed Ben Abdellah, Fès, Maroc*
[d]*Laboratoire de Biotechnologie, Faculté des Sciences Dhar El Mahraz, Université Sidi Mohammed Ben Abdellah, Fès, Maroc*

**For Correspondence: Email: yemni.majda@usmba.ac.ma*

Abstract

Ce travail s'intéresse à la comparaison du rendement et de la composition chimique des huiles essentielles extraites à partir de variétés de *Rosmarinus officinalis* spontanées et cultivées. La technique d'extraction des huiles essentielles utilisée est l'hydro-distillation et les deux paramètres physiques qui ont été déterminés sont l'indice de réfraction et la densité. La composition chimique a été réalisée par la chromatographie en phase gazeuse couplée à la spectrométrie de masse (CPG-SM). Le rendement du romarin sauvage en huiles essentielles selon les régions étudiées (Boulmane, Berkane, Bouiblane et Errachidia) varie entre 0.52 et 0.96 % et pour le romarin cultivé à la région de Fès, il est de 0.80 %. L'analyse par CPG-SM, a permis d'identifier 42 composés. La composition chimique de l'huile essentielle de différents échantillons (spontané et cultivé) est similaire qualitativement, mais il existe des différences quantitative entre certains composés.

Keywords: *Rosmarinus officinalis*, huile essentielle, indice de réfraction, densité, CPG-SM.

SYNTHESIS, STUDY AND CHARACTERIZATION OF BISBENZIMIDAZOLE DERIVATIVES

A. Ouaket*, S. Hamdouch, F. Moughaoui, Z. Anbaoui, M. Berrada, A. Bennamara, N. Knouzi

Biomolecules and Organic Synthesis Laboratory, Faculty of science Ben M'sik, University Hassan II of Casablanca, Morocco.

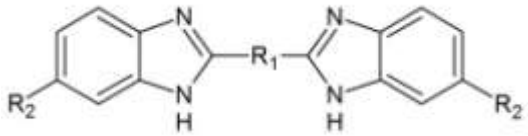
**For correspondence: Email: amine.ouaket@gmail.com*

Abstract

An heterocyclic ring is a cyclic organic compound in which we will find one or several types of atoms. The heterocyclic molecule can count several heteroatoms of the same nature or different **[1]**.

The role of heterocyclic compounds has become more and more important in recent years particularly in the design of new classes of compounds with demonstrated activities (corrosion inhibitors, dyes and stabilizers…), as well in the medicinal field (vitamins, hormones, antibiotics and anti-tumor…) **[2]**.

Among these heterocyclic compounds are the benzimidazoles, the series of benzimidazole is one of the most versatile in therapeutic chemistry.



R_1	-$(CH_2)_n$-	-$(CHOH)_n$-	-C_6H_4-
R_2	-H-NO_2	-CH_3-Cl	-Br

In the framework of our research on the development of new routes for the synthesis of benzimidazole compounds, we report in this work a study of heterocyclic systems of bis-benzimidazole type that known have therapeutic activities.

These molecules and their derivatives display a wide range of pharmacological activity, and their inhibitory properties as regards the replication of polio viruses, adenosine deaminase, and casein kinase have been fully demonstrated. For instance it is known that 1,2-bis(2-benzimidazyl)-1,2-ethanediol shows antifungal and anti-polio viruses character, and that ligand such as 1,4-bis(2-benzimidazyl)-1,2,3,4-butanetetraol have a negative effect on intracellular viruses **[3,4]**.

To achieve these syntheses, we studied different parameters for the reactions in order to determine the conditions for obtaining the best results.

Keywords: Benzimidazole, bisbenzimidazole, heterocyclic, synthesis, therapeutic activities, pharmacological activity.

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PROPERTIES OF TWO ISOMERIC BIS-TRIPODS BASED ON PYRAZOLE

I. Bouabdallah[a,b,*], I. Zidane[c], R. Touzani[d], D. Eddike[e], S. Radi[f], A. Haidoux[g], L. Ait M'Barek[h], A. Zyad[h], A. Melhaoui[a], B. Hacht[i], A. Ramdani[a]

[a]*Laboratoire de Chimie Organique, Macromoléculaire et Produit Naturels, URAC 25, Faculté des Sciences, Université Mohammed Ier, BP 524, 60 000 Oujda, Maroc.* [b]*Équipe de Recherche en Chimie et Didactique, CRMEF - Région d'Orientale,Maroc.* [c]*Faculté des Sciences, Université Ibn Tofail – Kénitra.* [d]*Faculté Pluridisciplinaire, Université Mohammed Ier, 62700 Selouane, Nador, Maroc.*
[e]*Laboratoire de Chimie Inorganique d'Etat solide, Faculté des Sciences, Université Mohamed Ier,Oujda, Maroc.*
[f]*Laboratoire de Chimie Appliquée et Environnement,Université Mohammed Ier, Oujda, Maroc.*
[g]*Laboratoire de Physico-chimie de la Matière Condensée, Université de Montpellier II, Place Eugène Bataillon, 34095 Montpellier, France.*
[h]*Laboratoire d'Immunologie, Biochimie et biologie Moléculaire, Faculté des Sciences et Technique, Béni-Mellal.*
[i]*Département de Chimie, Faculté des Sciences, Université Mohammed Ier, Oujda, Maroc.*

**For correspondence: Email: bouabib2002@yahoo.fr*

Abstract

Two bis-tripod compounds **1** **[1]** and **2** **[2]** were prepared respectively by the reaction of 1-(hydroxymethyl)-3,5-dimethylpyrazole and 3-chloromethyl-1,5-dimethylpyrazole with para-phenylenediamine (**Figure 1**). These products were characterized by IR, ^{1}H-NMR, ^{13}C-NMR, mass spectrometry and elemental analysis. The X-ray structures **[2]**, cytotoxic activities **[3],** liquid-liquid extraction **[4]** and catalytic properties **[5]** of these isomers were reported.

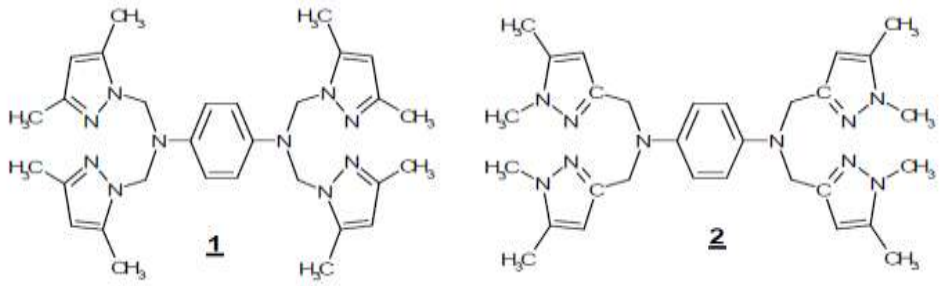

Figure 1. Structures of bis-tripods **1** and **2**

***Keywords*:** bis-tripod; pyrazol; isomer properties.

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CHEMICAL AND ELECTROCHEMICAL EVALUATION OF NEW PYRIDAZINE DERIVATIVE AS A CORROSION INHIBITOR FOR CARBON STEEL IN MOLAR HYDROCHLORIC ACID

R. Salim[a,b,*], E. Ech-chihbi[a,b], H. Oudda[a], F. El Hajjaji[b], M.Taleb[b]

[a]*Laboratory of separation processes, Faculty of Sciences, University Ibn Tofail, Kenitra, Morocco*
[b]*Laboratory of Engineering, Electrochemistry, Modeling and Environment (LIEME), Faculty of Sciences, University Sidi Mohamed Ben Abdellah, Fez, Morocco*

**For correspondence: Email: salimrajae@gmail.com*

Abstract

The inhibition of pyridazine derivatives on carbon steel in molar hydrochloric acid has been evaluated using electrochemical impedance spectroscopy (EIS), potentiodynamic polarization and weight loss measurement. The experimental results show that these compounds acted as an efficiency inhibitor against the carbon steel corrosion in HCl 1M and this efficiency increased with inhibitor concentration. The polarization curves indicated that the studied compounds acted as mixed type inhibitors. The EIS technique revealed that the charge transfer process as dominant in controlling the corrosion of carbon steel. The parameters thermodynamic of activation and adsorption were calculated.

Keywords: pyridazine; carbon steel; inhibition; adsorption.

SYNTHESIS OF NEW 2-[(5-METHYL-ISOXAZOL-3-YL)-METHYL]-BENZIMIDAZOLE DERIVATIVES FROM CYCLOADDUCTS OF A 1,5-BENZODIAZEPINE

Jihad Sebhaoui, Youness El Bakri, El Mokhtar Essassi*

Laboratoire de Chimie Organique Hétérocyclique, Centre de Recherche des Sciences des Médicaments, Pôle de Compétences Pharmacochimie, URAC 21, Faculté des Sciences, Mohammed V University Rabat, Avenue Ibn Battouta, BP 1014, Rabat, Morocco.

**For correspondence: Email: emessassi@yahoo.fr*

Abstract

The value of the benzimidazole derivatives based mainly on their pharmacological activities and complexing properties. We are interested in the synthesis of such compounds from 1,5-benzodiazepin-2-one derivatives which are also an important class of bioactive products and a raw material useful for the preparation of various heterocyclic ring systems. The purpose of our work is synthesis of substituted benzimidazoles with triazol ring to increase the activity of the synthetized compounds. Furthermore, these compounds can be used as ligands to complex different metals.

We will discuss the synthesis, alkylation and copper-catalysed 1,3-cycloadditon of 4-(2-oxo-propylidene)-1,5-benzodiazepin-2-one wich leads to the isoxazolylméthylbenzimidazole derivatives by the action of hydroxylamine in ethanol. Then we will discuss results of the complexation study of benzimidazol derivatives with copper.

Keywords: Copper-catalysed 1,3-cycloadditon; 1,5- benzodiazepine-2-ones; benzimidazole, alkylation; complexation.

PYRAZOLE COMPOUNDS: NEW POTENTIAL APPLICATIONS WITH DFT-IR CALCULATION STUDIES

Y. Kaddouri[a,*], R. El Ati[a], F. Abrigach[a], M. El Kodadi[b] and R. Touzani[a,c]

[a]*LCAE, University of Mohammed First, Oujda, Morocco*
[b]*CRMEF Oriental, Oujda, Morocco*
[c]*Multidisciplinary Faculty, Nador, Morocco*

**For correspondence: Email: Yassine.kaddouri92@gmail.com*

Abstract

We report herein, our project concerning the development of an efficient method to prepare monopyrazle (a), bispyrazole (b) and tetrapyrazole (c) functional compounds, with the opportunity to change easily structure, substituents, and armed for getting huge and divers library compounds.
These methods take advantage of the vast number of commercially available starting materials containing functional and aliphatic or aromatic amines. The structural and the electronic diversity of pyrazolic compounds open many and potential applications such as inhibitor of corrosion **[1]**, many biological properties **[2]**, efficient extractants of heavy metals **[3]**, DFT-IR calculations **[4]**, and catalysis **[5]**, these applications will be highlight too.

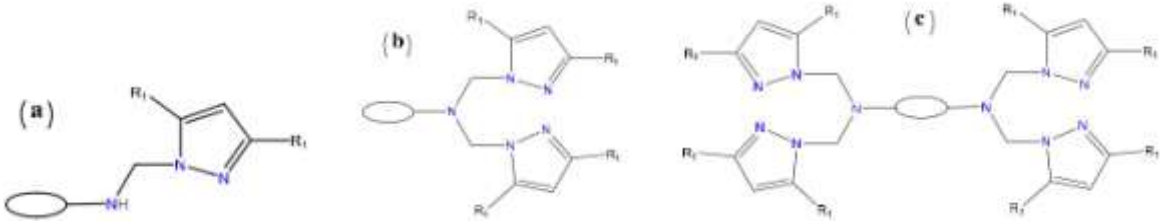

Figure 1 Structure of our classes of products

Keywords: Pyrazole; N-donor electron rich; corrosion; bioactivity and catalysis; DFT-IR calculations.

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HEMISYNTHES OF NEW HETEROCYCLIC SYSTEMS: 1,3-DIPOLAR CYCLOADDITION OF NITRILIMINES ON TRANS ANETHOLE

Y.Ben Soumane[a,b,*], L. Haimmad[a], M. Adardour[a], E.M. El Hadrami[b], A. Baouid[a] And A. Ben-Tama[b]

[a]*Laboratoire de Chimie Moléculaire, Département de Chimie, Faculté des Sciences Semlalia, BP 2390, Université Cadi Ayyad, 40001, Marrakech, Maroc.*
[b]*Laboratoire de Chimie Organique Appliquée, Université Sidi Mohamed Ben Abdellah, Faculté des Sciences et Techniques, BP 2202 Fès, Maroc.*

**For correspondence: Email: Yahya.bensoumane@usmba.ac.ma*

Abstract

In recent years, pyrazole derivatives are an important class of heterocyclic compounds. They have attracted a lot of attention through their important biological activity, such as fungicides **[1]**, insecticides **[2]**, acaroids **[3]**, herbicides **[4]**, antibacterial **[5]** and anti-cancer activity **[6]**. The use of 1,3-dipolar cycloaddition reaction on a natural product such as Trans anethole gives pyrazole derivatives. The Trans anethole is the major component in essential oil of several plants such as anise **[7]**, star-anise **[8]** and fennels **[9]**.
In this work, we focused our efforts on the preparation of new heterocyclic systems pentagonal by the condensation of 1,3-dipolar cycloaddition reaction from Trans anethole with nitrilimines. We obtained three heterocyclic products, two are cycloadduits regioisomerics and the third comes by eliminating of the molecule H2 from the majority cycloadduit.
The structures of synthesized regioisomers were established on the basis of spectroscopic data (IR, ^{1}H NMR, 13C NMR spectroscopy, mass spectroscopic data) and the X-ray crystallography. This 1,3-dipolar cycloaddition is higly regioselective.

Keywords: pyrazole, 1,3-dipolar cycloaddition, Trans anéthole, nitrilimines, regioisomers.

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SYNTHESES OF HETEROCYCLIC PYRIDINE LIGANDS BINDING AND COMPLEXATION WITH TRANSITION METALS OF SPIN

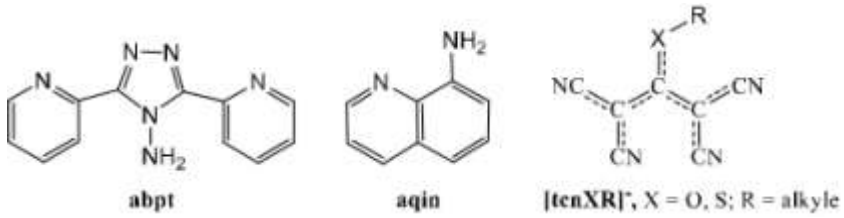
R. Motei[a,b,*], A. Ben-Tama[b], E.M. El Hadrami[b], S.Triki[a]

[a]UMR CNRS 6521- Université de Bretagne Occidentale, 6, Avenue Le Gorgeu, 29238 Brest [b]Laboratoire de Chimie Organique Appliquée, Université Sidi Mohammed Ben Abdellah, Faculté des Sciences et Techniques, BP 2202, Fès, Maroc

**For correspondence: Email: rachid_cmb@yahoo.fr*

Abstract

The Nitrogen heterocyclic products are very useful in various fields: materials, pharmacy, agriculture, medicine, etc. **[1,2]**. In this communication we present the synthesis of novel magnetic molecular materials based on polyazotated heterocyclic ligands and polynitrile anion, as well as the study of the influence of their structural characteristics on magnetic properties **[3,4]** (Schema).



Schema: Some examples of synthesized pyridine ligands

Keywords: Heterocyclic; polynitrile anion; materials.

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VALORIZATION OF ETHANOLIC EXTRACT OF A.visnaga AS ANTIOXIDANT AND INHIBITOR OF CORROSION

S. Aourabi[a], M. Sfaira[a,*], F. Mahjoubi[b]

[a]*Laboratoire Génie des Matériaux et environnement, Faculté des Sciences Dhar El Mahraz, Université Sidi Mohamed Ben Abdellah, Fès, Maroc*
[b]*Laboratoire des Matériaux, Electrochimie et Environnement, Faculté des Sciences, Université Ibn Tofaîl, BP. 133 – 14000, Kénitra, Maroc*

**For correspondence: Email: msfaira@yahoo.com*

Abstract

In this work we were interested in the valuation of the ethanolic extract of the aerial part of A.visnaga recently extracted by ultrasound as antioxidant and corrosion inhibitor of mild steel in a 1M HCl medium.
The study of the antioxidant activity of the extract object of study is carried out by two methods namely the DPPH and the total antioxidant activity (TAC).
Concerning the study of the anti-corrosion activity of the extract object of study is carried out by different methods namely electrochemical impedance spectroscopy, potentiodynamic polarization and weight loss measurement.
The results show that this extract exhibits an important antioxidant activity. For the latter the inhibition obtained by the DPPH method is 75% and TAC is 824.63 (mg BHT / g of extract). Concerning the anticorrosive power of steel, the tests show that the efficiency increases with the concentration of the inhibitor. The effect of temperature on the inhibition efficiency of this steel was studied at a temperature range of 25 to 65 + 1°C. The polarization curves indicate that the extract studied acts as a mixed type inhibitor. The thermodynamic parameters of adsorption are calculated and show that the process is spontaneous. The combined effects of concentration temperature and kinetic parameters of the steel dissolution process have all suggested that the ethanolic extract of A.visnaga acts by adsorption on steel through physical and chemical interactions.

Keywords: Extract; antioxidant activity; anti-corrosion activity; adsorption.

SYNTHESIS OF NEW 2-SUBSTITUBED INDOLE DERIVATIVES

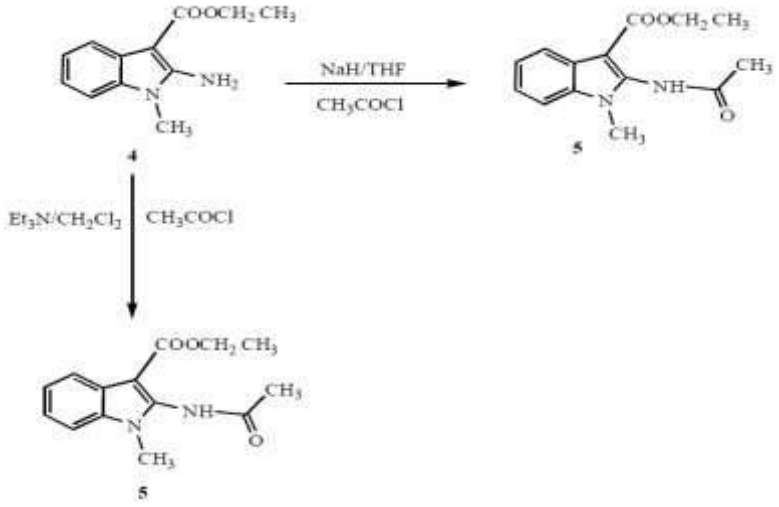
K. Nabih[a,*], J-Y. Mérour[b], A. Baouid[a]

[a]*Laboratoire Chimie Moléculaire, Faculté des Sciences-Semlalia, Université Cadi Ayyad, B.P.2390 Marrakech, Maroc.*
[b]*Institut de Chimie Organique et Analytique, CNRS-Université d'Orléans, France*

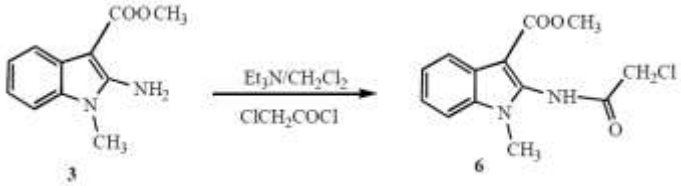
**For correspondence: Email: khadija_nabih@yahoo.fr*

Abstract

Indole moiety is very small but is fascinated by scientists because of the diverse biological activities **[1,2]** by not only indole but its various substituted derivatives as well.
Acylation of ethyl-2-amino-1-methyl-1H-indol-3-carboxylate was established according to two methods. These two methods of synthesis gave a satisfactory yield.



The results obtained above have encouraged us to carry out the acylation of methyl-2-amino-1-methyl-1H-indol-3-carboxylate.



The structures of these molecules were established from spectral data (mass, ^{1}H NMR and ^{13}C NMR).

Keywords: Indole; Acylation; ^{1}H NMR; ^{13}C NMR.

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THEORETICAL INVESTIGATION OF NEW TRIPHENYLAMINE-BASED ORGANIC SENSITIZERS FOR DYE-SENSITIZED SOLAR CELLS

A. Slimi[a,*], A. Touimi Benjelloun[a], M. Benzakour[a], M. Mcharfi[a], M. Hamidi[b], M. Bouachrine[c]

[a]*ECIM/LIMME, Faculty of sciences Dhar El Mahraz, University Sidi Mohamed Ben Abdallah, Fez, Morocco*
[b]*Moulay Ismail University, Faculty of Sciences and Technology, Errachidia, Morocco*
[c]*ESTM, Moulay Ismail University MEM, High School of Technology, Meknes, Morocco*

**For correspondence: Email: sli.ahmed@yahoo.com*

Abstract

Organic Dye-Sensitized Solar Cells (DSSCs) are a low-cost alternative of our renewable energy sources in the past decades because they have potential to get high power conversion efficiency (PCE) and their devices are easy to fabricate **[1]**. Numerous efforts have been applied to acquire novel organic dyes with higher efficiency. Although experimental molecular modification is a powerful and straightforward route to get new dyes, the synthesis process is not only expensive but time consuming. On the other hand, theoretical analysis of the electronic structure of conjugated systems can establish the relationships between molecular structure and electronic properties.

In this study, we present the theoretical analysis on the geometries and electronic properties of six new conjugated compound based on triphenylamine synthesized by Yu et al. **[2]**. The theoretical ground-state geometry and electronic structure of the studied molecules were investigated by the DFT method at B3LYP level with 6-31 G (d, p) basis set. Also, the UV-vis spectra was simulated with the TD-DFT method using CAM-B3LYP functional and 6-31 G (d, p) basis set in THF solvent **[3,4]**. The calculated frontier orbital energies HOMO and LUMO and energy gaps showed that the energy gaps of the studied molecules differ slightly about 2.7 eV depending on the different structures, and the Voc is in the range 1,57–1,62 eV. Our results suggest that the studied molecules are expected to be promising candidates for dyes sensitized solar cells (DSSCs).

Keywords: *Energy, Triphenylamine,* DSSCs, *TD-DFT, THF, UV-visible, electronic properties.*

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SYNTHESIS AND PHARMACOLOGICAL STUDY OF PYRIDO [2,3-b] PYRAZINE DERIVATIVES

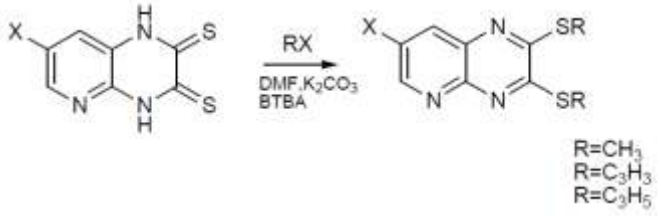
M. Sikine[a], Y. Kandri Rodi[a,*], M. Chraibi[b], A. Kandri Rodi[a], F. Ouazzani Chahdi[a], K. Fikri Benbrahim[b] and E.M.Essassi[c]

[a]*Laboratoire de Chimie Organique Appliquée, Université Sidi Mohamed Ben Abdellah, Faculté des Sciences et Techniques, Route d'Immouzzer, BP 2202, Fès, Morocco.*
[b]*Laboratoire de biotechnologie microbienne, Université Sidi Mohammed Ben Abdallah, Faculté des Sciences et Techniques, Route Immouzer, BP 2202 Fès, Morocco*
[c]*Laboratoire de Chimie Organique Hétérocyclique URAC 21, Faculté des Sciences, Université Mohammed V,Avenue Ibn-Batouta, Rabat, Maroc.*

**For correspondence: Email: youssef_kandri_rodi@yahoo.fr*

Abstract

The pyrido[2,3-b]pyrazine derivatives are interest the chemical application and biological activities. Moreover, the novel heterocyclic pyridopyrazine have diffrents activities, presents VIH-1 integrase inhibitors, anticancer, anti-inflammatory, and anti-bacterial.
New series of pyrido[2,3-b]pyrazine were synthesized by alkylation with various substituted aryl, and has good yield. The all compounds exhibited antibacterial activities against different strains *Staphylococcus aureus*, and *Escherichia coli*. These latter's were characterized by their ^{1}H, ^{13}C RMN and X-ray diffraction.



Keyswords: pyrido[2,3-b]pyrazine; alkylation; CTP; antibacterial activity.

EFFICIENT AND SAFE SYNTHESIS OF NOVEL SULFONAMIDE-ISOXAZOLINE SCAFFOLDS THROUGH 1,3-DIPOLAR CYCLOADDITION REACTION IN AQUEOUS MEDIA

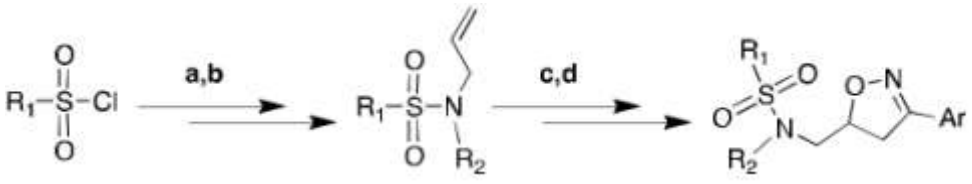
A.Talha, H.Tachallait, K. Bougrin*

Laboratory of Plant Chemistry and Organic and Bioorganic Synthesis, URAC23, University of Mohammed V, Faculty of Sciences, Avenue Ibn Battouta, BP:1014, 10000 Rabat, Morocco.

**For correspondence: Email: kbougrin@yahoo.fr*

Abstract

Sulfonamides have received significant relevance in modern organic chemistry and are very privileged class of compounds in synthetic and medicinal chemistry. Sulfonamides and isoxazoline are omnipresent motifs seen in many of natural products and pharmaceutically active compounds **[1,2]**. In this work, we have synthesized a series of isoxazoline linked to sulfonamides moiety exploiting the click chemistry approach in aqueous media. Also, the same isoxazoline derivatives **3** can be evolved biologically as antibacterial, antifungal and antioxidant.



1 **2** **3**

Experimental conditions:

a: Base, primary amine, aprotic solvent. **b**: allyl bromide, base, secondary sulfonamide.
c: arylaldehyde, Base, NH_2OH,HCl, aprotic solvent. **d**: **2**, aldoxime, oxidant, water

Keywords: Tertiary sulfonamides, Isoxazolines, Click chemistry.

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A NEW AND EASY METHOD FOR SYNTHESIS OF 1,5-DISUBSTITUED 1,2,3-TRIAZOLE BY METAL-FREE REGIOSELECTIVE 1,3-DIPOLAR CYCLOADDITION REACTION

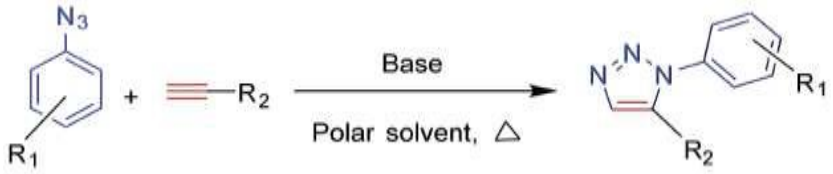
Y. Halabi, H.Tachallait, A. Saber, A.Talha, K. Bougrin*

Laboratory of Plant Chemistry and Organic and Bioorganic Synthesis, URAC23, University of Mohammed V, Faculty of Sciences, Avenue Ibn Battouta, BP:1014, 10000 Rabat, Morocco.

**For correspondence: Email: kbougrin@yahoo.fr*

Abstract

The synthesis of 1,4-disubstitued 1,2,3-triazole have an easy access by the copper (I)-catalysed regioselective cycloaddition CuAAC of azides with terminal alkynes **[1,2]**. These heterocylces have shown a widespread applications in medicinal chemistry, chemical biology, and materials science. Therefore the usefulness of 1,4- disubstitued generates interest in regioisomeric 1,5-disubstituted 1,2,3-triazoles. Generally, the regioisomer 1,5-disubstituted was synthesized via ruthenium- catalyzed cycloaddition or by using aggressive reagents of lithium or magnesium **[3]**. We envisioned a new transition metal free procedure for the synthesis of 1,5-disubstituted 1,2,3- triazoles in polar solvent under reflux in a basic medium, with an experimentally easy and simple reaction, affording 1,5-disubstituted 1*H*-1,2,3-triazoles in good to excellent yields.



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REGIOSELECTIVE SYNTHESIS OF NEW ISOXAZOLINES DERIVATIVES OF RHODANINE NUCLEUS *VIA* 1,3-DIPOLAR CYCLOADDITION USING CATALYTIC KI IN AQUEOUS MEDIA

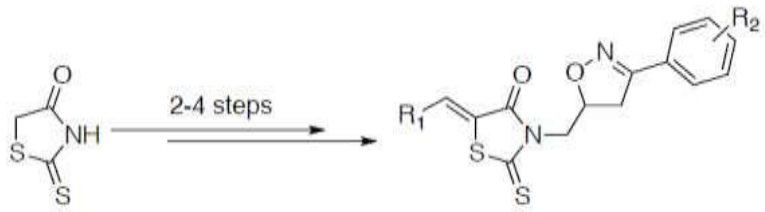
W. Belhaj, A. Talha**,** H. Tachallait, K. Bougrin*

a Laboratory of Plant Chemistry and Organic and Bioorganic Synthesis, URAC23, University of Mohammed V, Faculty of Sciences, Avenue Ibn Battouta, BP:1014, 10000 Rabat, Morocco.

**For correspondence: Email: kbougrin@yahoo.fr*

Abstract

Aza-heterocyclic compounds, such as rhodanine and isoxazoline analogues have shown numerous biological activities **[1]**. They represent a highly important class of compounds, which are widely used in materials science, agrochemistry, and medicinal chemistry **[2]**. Therefore, there is continuing interest in the development of convenient, efficient, and green synthetic methods for their construction **[3]**. Recently, hypervalent iodine reagents have been introduced in many different transformations owing to their mild reaction conditions and environmentally friendly nature **[4]**.



Expérimental conditions : a) aldehyde, base b) allylation c) préparation of nitrile oxide d) 1,3-dipolar cycloaddition

In this communication, we described an efficient synthesis of new rhodanine-isoxazoline analogues *via* a 1,3-dipolar cycloaddition. This reaction involves hypoiodite mediated catalytic oxidative cyclization of aldoximes and *N*-allylrhodanine derivatives as dipolarophile. In all cases, only one regioisomer was obtained, the products were characterized by comparing IR, NMR and MS data.

Keywords: Isoxazolines, Rhodanine, 1,3-dipolar cycloaddition, hypervalent iodine, catalytic oxidations.

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SYNTHESIS OF NEW CYCLOPROPANIC THIOSEMICARBAZONES FROM (R)-CARVONE

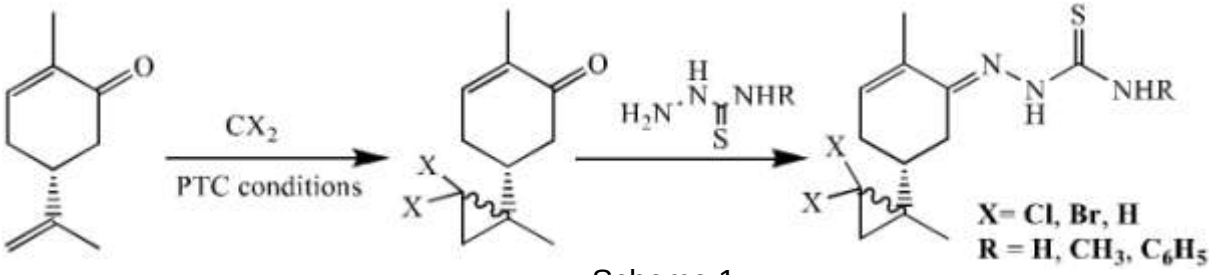
A.Oubella[a,*], M. Y. Ait itto[a], A. Bimoussa[a], A. Auhmani[a], M. Fawzi[a], A. Riahi[b], A. Auhmani[a]

[a]*Laboratoire de Physico-Chimie Moléculaire et de Synthèse Organique Département de Chimie Faculté des Sciences Semlalia, Marrakech.*
[b]*Université de Reims Champagne-Ardenne ICMR UMR CNRS 6229 Bât. Europol'Agro - Moulin de la Housse BP. 1039 - 51687 Reims Cedex 2 France.*

**For correspondence: Email: oubellaali1@gmail.com*

Abstract

Thiosemicarbazones are useful compounds which have been studied for extended periods because of their biological activities such as anti-malarial **[1]**, anti-cancer **[2]** and anti-HIV **[3]**. They also could be valuable intermediates for the preparation of hexagonal or pentagonal heterocyclic systems by heterocyclisation reactions. Because of the presence of nitrogen and sulfur atoms, they are usually used as donor ligands in the preparation of biological active complexes **[4-6]**.
This work is the continuity of a research program developed in our laboratory on the valorization of natural substances. It aims at the preparation of new cyclopropanic thiosemicarbzones with terpenic skeleton which could have biological properties.



Scheme 1

Our synthesic strategy begins with cyclopropanation reaction of naturally occurring (R)-Carvone followed by condensation reaction of the resulting product with thiosemicarbazides (Scheme 1). The structure of all the newly prepared compounds are confirmed by ^{1}H and ^{13}C NMR spectroscopy.

Keywords: 1,3-dipolar cycloaddition.

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A NOVEL ROUTE TO 1,4-DIHYDROQUINOXALINE FOR BIOLOGICAL PROPERTIES

A. El Janati[a,*], Y. Kandri Rodi[a], F. Ouazzani Chahdi[a], Y. Ouzidan[a], E. M. Essassi[b]

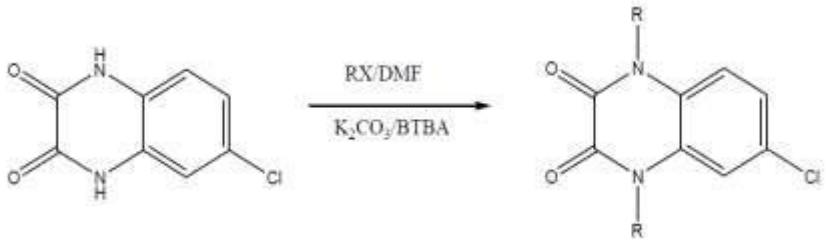
[a]*Laboratory of Applied Organic Chemistry, Faculty of Science and Technology, University Sidi Mohammed Ben Abdallah, Fez, Morocco.*
[b]*Laboratoire de Chimie Organique Hétérocyclique, URAC 21, Pôle de Compétences Pharmacochimie, Université Mohammed V, Faculté des Sciences, Av. Ibn Battouta, BP 1014 Rabat, Morocco.*

**For correspondence: Email: alieljanati@gmail.com*

Abstract

The development of new chemically synthesized molecules represents a major strategy for the discovery and preparation of new substances of biological interest. The quinoxaline heterocyclic is among the classic divisions of organic chemistry, which develop fastest.In fact, studies have shown that this type of compound has several biological activities such as anti-tumors **[1]**, anticancer **[2]**, antioxidant **[3]**, anticoagulant **[4]**, antinomic **[5]**, Antibacterial and anti-inflammatory **[7]**, anti-plasmodial **[8]**. They are also used as neuroprotective agents **[9]**.

To a solution of 6-chloro-1,4-dihydroquinoxaline-2,3-dione 0,3g (1,53 mmol) in DMF (20 ml), we have added 0.52g (3,84 mmol) of potassium carbonate and 0,1 mmol of tetra-n-butyl ammonium (BTBA), after 10 min of stirring 3,85 mmol of the halogenated reagent were added, then the mixture was allowed to stir at room temperature for 36 hours. After filtration of salts, the DMF was evaporated under reduced pressure and the residue obtained is dissolved in dichloromethane, the organic phase was dried over Na2SO4 and then concentrated. The mixture obtained was chromatographed on Silica gel column (eluent : hexane/ethyl acetate (3/1)).



Structures of the obtained compounds were confirmed by ^{1}H and ^{13}C NMR spectroscopy.

Keywords: quinoxaline-2,3-dione; Alkylation, biological properties.

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EFFECIENT SYNTHESIS OF 4-SUBSTITUTED PYRAZOLIDIN-3-ONES

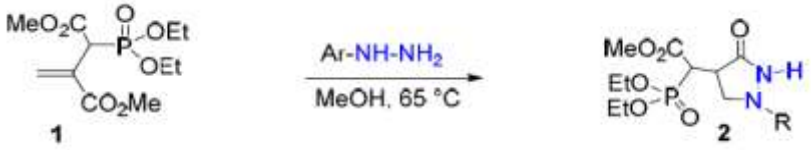
A. Arfaoui[a,b,*], F. Saâdi[a], H.Chebbi[c], G. Barozzino-Consiglio[b], K. Renault[d], J. Legros[b], H. Amri[a], J. Maddaluno[b]

[a]*Université de Tunis El Manar, Faculté des Sciences de Tunis, Laboratoire SOHES, 2092 Tunis, Tunisie.*
[b]*Normandie Université, INSA Rouen, CNRS, COBRA Laboratory (UMR 6014 & FR3038), 76000 Rouen, France.*
[c]*Université de Tunis El Manar, Faculté des Sciences de Tunis, Laboratoire de Matériaux, Cristallochimie et Thermodynamique Appliquée, 2092 Tunis, Tunisie.*
[d]*Université de Normandie, CNRS, COBRA (UMR 6014), 76000 Rouen, France.*

**For correspondence: Email: acha.arfaoui@gmail.com*

Abstract

Pyrazolidin-3-ones derivatives represent an interesting class of heterocyclic compounds, which possess a wide range of biological and pharmacological activities **[1]**. In this context and considering the importance of these attractive target products, we present in this communication an efficient method for the synthesis of 4-substituted pyrazolidin-3-ones **2 [2]** from a convenient coupling reaction of two equivalents of aryl hydrazines with allyl phosphonate **1**, involving a two-step sequence: conjugate addition of the hydrazine to the terminal ethylenic carbon of the phosphonocarboxylate **1** leading to an γ-aminoester, which undergoes a spontaneous 5-*endotrig* cyclization to provide functionalized pyrazolidin-3-ones **2** in good yields.



Keywords: Allyl phosphonate; methanol; aryl hydrazines; pyrazolidin-3-ones.

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SYNTHESIS OF POLYAZOTES HETEROCYCLIC LIGANDS FOR THE DESIGN OF NEW SPIN TRANSITION IRON (II) COMPLEXES

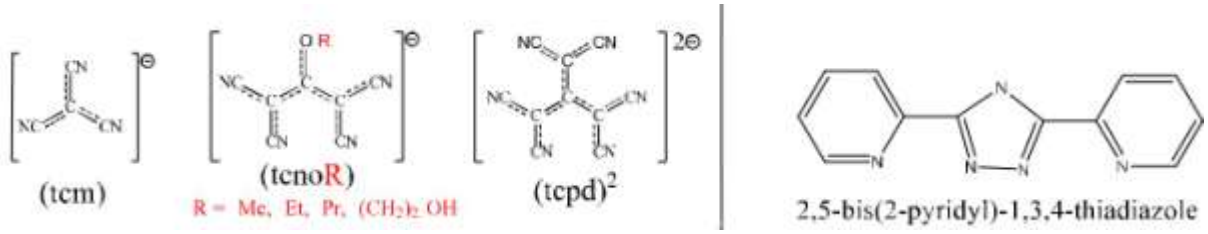
R. Motei[a,b,*], S. Triki[a], A. Ben-Tama[b], E.M. El Hadrami[b]

[a]*UMR CNRS 6521- Université de Bretagne Occidentale, 6, Avenue Le Gorgeu, 29238 Brest*
[b]*Laboratoire de Chimie Organique Appliquée,Faculté des Sciences, BP 2202, Fès, Maroc*

**For Correspondence: Email: rachid_cmb@yahoo.fr*

Abstract

For many years, our group has been interested in the synthesis of new heterocyclic ligands and polynitriles anions with original magnetic properties such as spin cross-over.



Scheme 1. Examples of ligands and anions used

In this context, we have considered the use of the 2,5-bis (2-pyridyl)-1,3,4-thiadiazole heterocyclic co-ligand due to its rigidity and its potential bridging ligand character. Associated with Fe (II) salts and several polynitriles anions, it leads to a new series of original derivatives characterized by a broad structural variety (Figure 1). We present here the synthesis and structural characterizations of the first polynuclear complexes.

Keywords: heterocyclic ligands; polynitriles anions; spin cross-over.

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ETUDE DE LA REACTIVITE D'ENAMINES CYCLIQUES SUR DES AZIDES ORGANIQUES

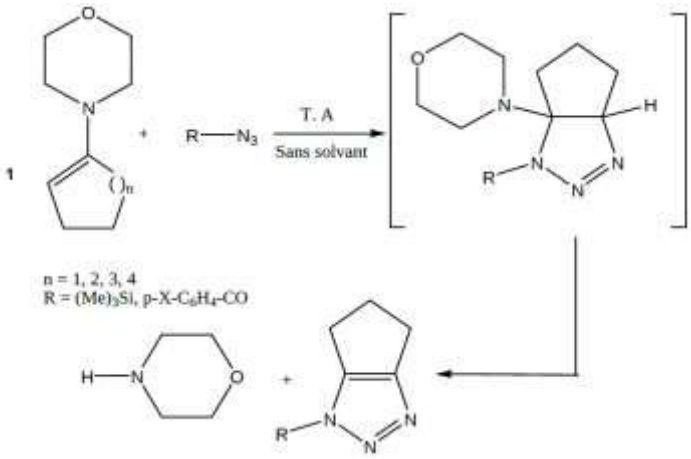
A. Chenni[a,b,*], M. Hamadouche[a], D. El Abed[a]

[a]*Laboratoire de Chimie Fine (LCF), Faculté des Sciences Exactes et Appliquées, Université d'Oran 1 Ahmed Ben Bella, Oran, Algérie*
[b]*Centre Universitaire Nour Bachir El-Bayadh BP 900, 32000,*

**For Correspondence: Email: ch.sarah336@yahoo.fr*

Abstract

La recherche sur la synthèse des hétérocycles est très répandue dans le domaine de la chimie organique, autant parce qu'elle requiert une planification synthétique particulière que parce que les hétérocycles sont souvent des pièces maîtresses de cibles synthétiques d'intérêt biologique **[1]**. Parmi ces hétérocycles, on retrouve les (1,2,3)-triazoles, composés obtenus par réaction de cycloaddition [3+2] **[2]**.
Dans ce travail nous allons étudier la réactivité d'énamines cycliques (dipolarophiles) sur des aryl et acylazides (dipôle-1,3). (Schéma).



L'addition des *azides* organiques aux *ènamines* cycliques à température ambiante et sans solvant, conduit à des triazolines instables qui se dégradent en triazoles bicycliques avec des rendements appréciables.
Les produits obtenus ont été caractérisés par les techniques spectroscopiques usuelles : IR, RMN ^{1}H et du ^{13}C.

Keywords: Azide organique, ènamine, cycloaddition [3+2], triazolines, triazoles

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SYNTHESIS, CHARACTERIZATION AND BIOLOGICAL EVALUATION OF NEW THIABENDAZOLE DERIVATIVES VIA 1,3-DIPOLAR CYCLOADDITION

K. El Bourakadi[a,b], **M. E. M. Mekhzoum[a,*]**, E.M. Essassi[a,b], A. Qaiss[a], R. Bouhfid[a]

[a]*Moroccan Foundation Advanced Science, Innovation and Research (MAScIR), NANOTECH, Rue Mohamed Al Jazouli Madinat Al Irfane Rabat, Morocco*
[b]*Laboratoire de Chimie Organique Hétérocyclique, URAC 21, Pôle de Compétence Pharmacochimie, Av Ibn Battouta, BP 1014, Faculté des Sciences, Mohammed V University, Rabat, Morocco*.

**For correspondence: Email: m.mekhzoum@mascir.com*

Abstract

The importance of thiabendazole derivatives in various fields, has attracted much attention in recent years because of their biological and pharmacological activities such as antimicrobial **[1]**, anthelmintic **[2]**], anticancer **[3]**. Because of its structural similarity to the chelating agents, thiabendazole often used as ligands in coordination chemistry. In addition to these properties, some thiabendazole compounds are widely used in other fields, including medicine, food chemistry **[4]**, This compound has also been used in agricultural as fungicide **[2]**. In the purpose of evaluating and developing new compounds with potential biological activity, we have substituted thiabendazole by the triazole moiety using 1,3-dipolar cycloaddition reaction between an alkyne and an azide. Triazole and many of its derivatives exhibit a variety of biological actions, and wide applications in organic synthesis. For that matter an interesting series of thiabendazole-based cycloadduit were synthesized in good yields and their chemical structures were determined through elemental analyses and spectroscopic studies namely ^{1}H, ^{13}C NMR, FT-IR, and MS, all the synthesized compounds were tested over a range of concentrations to investigate their anti-bacterial activity.

Keywords: thiabendazole; triazole; 1,3-dipolar cycloaddition; biological activity.

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FIRST SYNTHESIS OF NATURAL BROMOPHENOLS INCLUDING SULPHONE UNIT

Abdullah Menzek*, Çetin Bayrak

Department of Chemistry, Faculty of Science, Atatürk University, Erzurum-25240, Turkey

**For Correspondence: E-mail: amenzek@atauni.edu.tr*

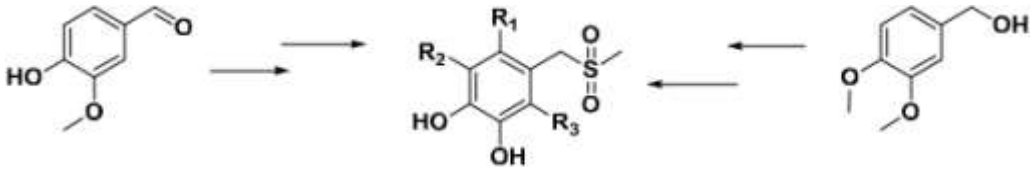
Abstract: Natural bromophenols 3,4-dibromo-5-((methylsulfonyl)methyl)benzene-1,2-diol (**1**) and 3,4,6-tribromo-5-((methylsulfonyl)methyl)benzene-1,2-diol (**2**) were synthesized.

Introduction:

Natural bromophenols are frequently isolated from marine red algae of the family Rhodomelaceae and have important biological activities such as antimicrobial, carbonic anhydrase and antioxidant activities **[1,2]**. Natural bromophenols including sulphone unit **1** and **2** were isolated from marine red alga *Rhodomela confervoides* and marine red alga *Symphyocladia latiuscula*. They exhibit antioxidant activity **[2]**.

Result and and Discussion

To synthesis natural bromophenols **1** and **2**, vanillin (**3**) and (3,4-dimethoxyphenyl)methanol (**4**) were used as starting material. The bromophenols **1** and **2** were obtained from the reactions such as bromination, substitution, demethylation, acetilation, oxidation and hydrolysis of **3** and **4**.



3 — 1) $R_1 = R_2 = Br, R_3 = H$; 2) $R_1 = R_2 = R_3 = Br$ — 4

Keywords: Bromination; demethylation; natural product; sulphone.

Authors thank TUBITAK (113Z702) and Ataturk university (FAD-2017-6107).

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PREPARATION AND CHARACTERIZATION OF IMMUNOGENS FOR ANTIBODY PRODUCTION AGAINST PROGESTERONE

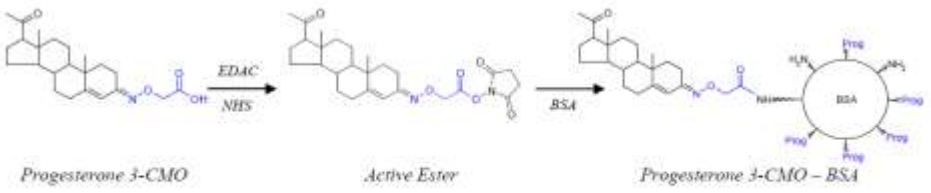
A. Moutaouakkil[a,*], A. Moussaif[a], M. Chentouf[b], N. El Abbad[a]

[a]*Unité de Biotechnologie et d'Ingénierie des Biomolécules, Division des Sciences du Vivant, Centre National de l'Energie, des Sciences et des Techniques Nucléaires, BP. 1382 RP. Rabat 10001*
[b]*Unité de Recherche sur les Production Animales, Centre Régional de la Recherche Agronomique de Tanger, INRA, 78 Bd Sidi Mohamed Ben Abdellah 90000, Tanger*

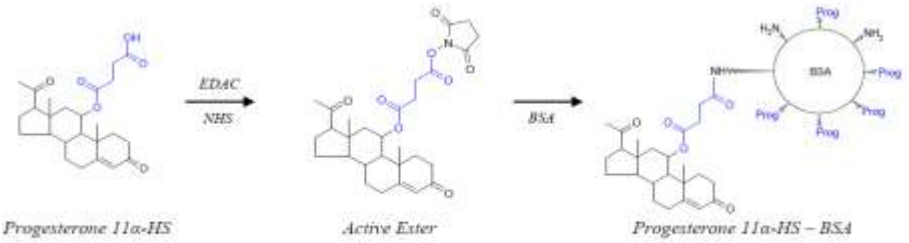
**For Correspondence: E-mail: moutaouakkil@cnesten.org.ma*

Abstract

Small molecules such as steroids are usually non-immunogenic and hence do not elicit an immune response unless coupled with some macromolecules such as proteins. To generate antibodies against steroids for immunoassay applications, they are first modified to link with the protein carrier **[1]**. The functional group of the steroid (hapten) governs the selection of the conjugation method to be employed. Common procedures of conjugation use amine and carboxylic acid groups on the steroid and the protein carrier **[2]**. The most frequently used carrier protein for conjugation is bovine serum albumin (BSA).
In this study, we report the preparation of progesterone-BSA conjugates using activated ester method **[3]** which we modified according to our conditions (Schemes 1 and 2). The obtained immunogens were then characterized by spectrophotometeric analysis and gel electrophoresis to determine the extent of conjugation (hapten density on carrier protein).



Scheme 1



Scheme 2

Keywords: Progesterone; Hapten; Antibodies; Immunoassay applications.

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AN EFFICIENT REUSABLE PYRIDINIUM SALTS AS A CATALYST FOR A MULTICOMPONENT REACTION

M. A. Redouane[a,*], R. Laroum[a], N. Khiri[a], A. Debeche[a]

[a]*Laboratoire de synthèse des molécules d'intérêts biologiques, Faculté des sciences exactes, Université des Frères Mentouri Cons tantine 1, BP : 25017, Constantine, Algérie.*

**For correspondence: Email: redouaneabdenour3@gmail.com*

Abstract

Many advances in benzopyran chemistry have been made in view of their important biological activities **[1-4]**, such as anti-cancer **[5]** and anti-bacterial **[6]**.
In addition, pyridinium salts are a very important class of catalysts in view of the ease of their preparation and low toxicity, In this work, we have evaluate the catalytic efficiency of various pyridinium salts in the synthesis of 4H-pyran by a multicomponent reaction, using an aromatic aldehyde, an enolizable carbonyl and malononitrile, in aqueous EtOH. The most efficient of these catalysts was used to elaborate a series of benzopyrane derivatives from various aromatic
aldehydes after the optimization of reaction conditions. The promising points for this methodology is the high efficiencies, short reaction times, mild reaction conditions, and simplicity which makes it a desirable and useful method for the synthesis of 4Hbenzo[b]pyrans as biologically interesting compounds.

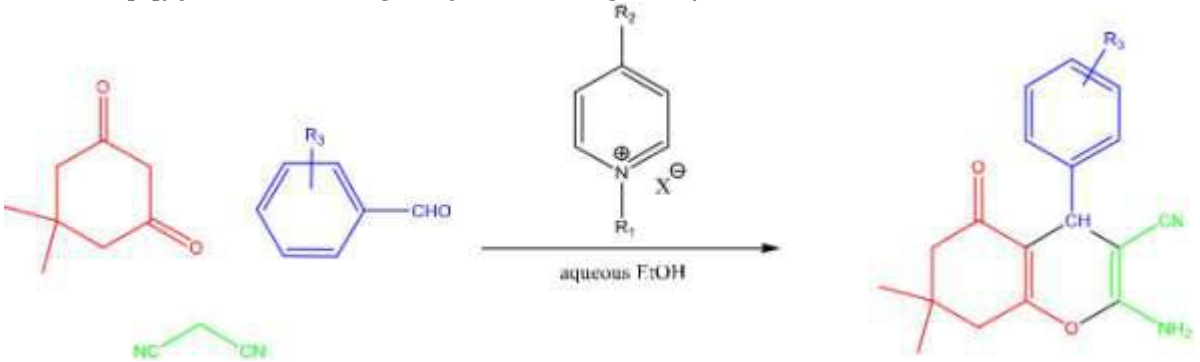

Figure 1: benzopyrane derivatives synthesis catalyzed by pyridinium salts

Keywords: pyridinium salts; tetrahydr o[b]benzopyr ane; multicomponent reaction; ionic liquid.

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SYNTHESIS OF SPIROISOXAZOLINES AND ITS TRANSFORMATION TO TRISUBSTITUTES ISOXAZOLES BY TREATEMENT WITH TRIETHYLAMINE

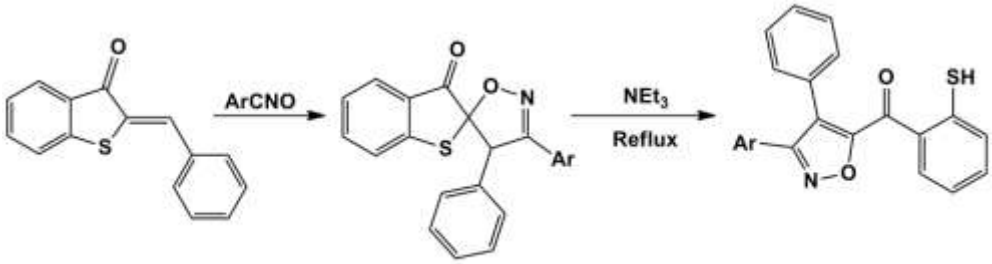
M. Bakhouch[a,*], M. Chalkha[a], A. Mahfoud[a], M. Akhazzane[b], G. Al Houari[a], M. Daoudi[a], M. El Yazidi[a]

[a]*Laboratoire de Chimie Organique, Université Sidi Mohamed Ben Abdellah, Faculté des sciences Dhar EL Mahraz, BP: 1796, Fès, Maroc.*
[b]*Cité de l'innovation, Université Sidi Mohamed Ben Abdellah, Fès.*

**For Correspondence: E-mail: mohamed.bakhouch@usmba.ac.ma*

Abstract

2-Isoxazolines are attractiong widespread interest due to their use as building blocks for the synthesis of medicinally relevant compounds and novel heterocycles **[1,2]**. They constitute a class of heterocycles that are most commonly assembled by 1,3-dipolar cycloaddition reaction of nitrile oxides and alkenes **[3]**. That found promissing application in organic chemistry due to its versatility as a synthetic intermediate to obtain new types of functionalized compounds **[4]**. In order to ensure continuation of our ongoing research, and inspired by the behaviour of thioaurones with nitrilimines **[5]**. We aimed, in this work to study and describe the action of triethylamine on spiroisoxazolines previously synthesised (scheme) **[6,7]**.
The structure of the synthesized products was corroborated by spectroscopic analysis: IR, ^{1}H-NMR and ^{13}C-NMR.



Ar = C_6H_5 , p(Me)C_6H_4, p(MeO)C_6H_4 , p(Cl)C_6H_4 , C_4H_4S

Keywords: 2-isoxazoline; isoxazole; 1,3-dipolar cycloaddition; nitrile oxides; ring cleavage.

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A COMPARATIVE STUDY OF CHITIN EXTRACTION USING CONVENTIONAL METHOD AND MICROWAVE TECHNOLOGY

H. El Knidri*, R. Belaabed, R. El Khalfaouy, A. Addaou, A. Laajeb, A. Lahsini

Catalysis, Materials and Environment Laboratory, Sidi Mohamed Ben Abdellah University, Fez, Morocco
Address:Higher School of Technology BP 2427 Road Imouzzer 30000 - Fez

**For correspondence: Email: hakima.elknidri@usmba.ac.ma*

Abstract

This work concerns the valorization of waste products from fishing industry by eco-friendly extraction of chitin and its derivatives.
Chitin is the second most common polymer after cellulose in earth, existing in the shells of crustaceans like crab, shrimp and lobster as well as in the cuticle of insects and the cell walls of fungicide. In this work the shrimp shells are used to extract the chitin.
Chitosan, main derivative of chitin, is a natural amino-polysaccharide known as one of the most abundant organic materials in nature, it has been widely used in several applications due to its natural origin and exceptional properties such as biodegradability, biocompatibility, non-toxicity, and chelating of metal ions. Chitin and chitosan are characterized by degree of deacetylation, one of the most important chemical characteristics that can influence the performance of chitosan in many applications **[1–3]**.
Chitin is usually prepared by a conventional heating method, which is time consuming (many hours up to days), that consumes a lot of energy and reagents.
In this study, a new ecological method, via microwave irradiation, was developed for the extraction of this natural polymer in a few minute, and a comparative study of chitin extraction by conventional method and microwave technology was made.
The chitin extracted was characterized by Fourier transform infrared spectroscopy (FTIR), Scanning electron microscopy (SEM) and X-ray diffraction (XRD).

Keywords: Chitin, biomaterials, deacetylation, organic materials, microwave irradiation.

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SYNTHESIS OF ONE INDOLE-MODIFIED TETRAPHENYLETHYLENE AS A POTENTIAL AIE-LUMINOGEN

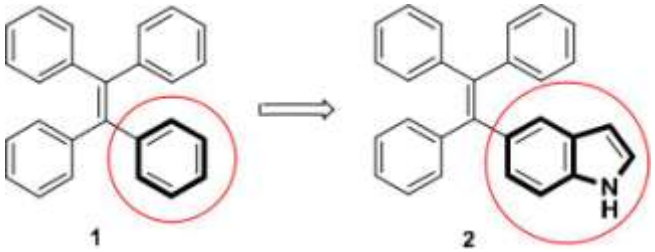
Farrokh Lafzi[a], Berrak Ertugrul[a], Haydar Kilic[b,c], **Nurullah Saracoglu[a,*]**

[a]*Department of Chemistry, Faculty of Sciences, Atatürk University, 25240 Erzurum, Turkey*
[b]*East Anatolia High Technology Application and Research Center, Atatürk University 25240, Erzurum, Turkey*
[c]*Oltu Vocational School, Atatürk University, 25400, Erzurum, Turkey*

**For correspondence: Email: nsarac@atauni.edu.tr*

Abstract

Aggregation-induced emission (AIE) has attracted much interest in a design of new fluorescent-based optoelectronic and biological devices such as chemical sensors and bio-imaging agents **[1]**. Especially, tetraphenylethylenes (TPEs) have been widely employed as strong AIE-luminogenic materials **[2]**. The indole moiety is a very important component of natural products and bioactive compounds and plays an important role in biochemistry and medicine **[3]**. Therefore, we aimed synthesis of novel TPE-analogue replacing one of the phenyl rings in TPE with indole in this communication.



1 2

Acknowledgment: This study was supported by the Scientific and Technological Research Council of Turkey (TUBİTAK, Project number: **116Z175**). We would like to thank TÜBİTAK for its support.

Keywords: Tetraphenylethylene; indole; Knoevenagel condensation; McMurry reaction; Suzuki coupling.

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INVESTIGATION OF ANTIFUNGAL AND ANTICANDIDAL ACTIVITIES OF 1,2-BIS (2-(2-MORPHOLINOPHENOXY)ETHOXY)ETHANE

Gönül Yapar

Department of Chemistry, Faculty of Arts and Sciences, Istanbul Technical University, Maslak, 34469 Istanbul, Turkey

For Correspondence: E-mail: yaparg@itu.edu.tr

Abstract

Macrocyclic polyether compounds have growing interest and importance in chemistry, biochemistry and material science because of a variety of applications. The most important property of these molecules is that they are not only able to bind the cations, they also capable to selective discriminate and bind strongly a cation among the others. Because of selective binding characteristic of macrocyclic compounds, they can be used as sensors to detect some metal ions that have importance in environmental chemistry and biological systems **[1,2]**. In resent years, numerous studies have been conducted on biomedical potentials of crown ethers such as ion transporter channels, antimicrobial and antitumor activity **[3]**. It is well known that morpholine and molecules bearing morpholine moiety in their structure exhibit a wide spectrum of pharmacological and biological activities such as analgesic, anti-inflammatory **[4]**, antihyperlipidemic **[5]**, antimicrobial and antioxidant activity **[6]**.

In this study, morpholine is a substituent on aromatic part of open-chain macrocyclic ether (Fig.1). Antifungal and anticandidal activities of 1,2-bis(2-(2-morpholinophenoxy)ethoxy)ethane molecule were tested by using serial 96-well microbroth dilution method **[7-8]**. Fluconazole was used as standard antifungal drug.

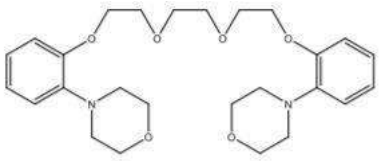

Figure 1: 1,2-Bis(2-(2-morpholinophenoxy)ethoxy)ethane

Acknowledgements: This research study was partly supported by The Scientific and Technological Research Council of Turkey (TUBITAK)

Keywords: Podand; morpholine; antimicrobial; antifungal; anticandidal.

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REACTIONS OF MAJOR ENDOPEROXIDES OBTAINED FROM 5- AND 6-CHLOROCYCLOHEPTADIENES WITH TETRAZINE

Y. Çetinkaya[a,b]*, A. Menzek[a] , M. E. Şengül[a]

[a]*Department of Chemistry, Faculty of Science, Atatürk University, 25240 Erzurum,Turkey.*
[b]*Department of Food Technology, Oltu Vocational School, Atatürk University, 25400 Oltu-Erzurum, Turkey.*

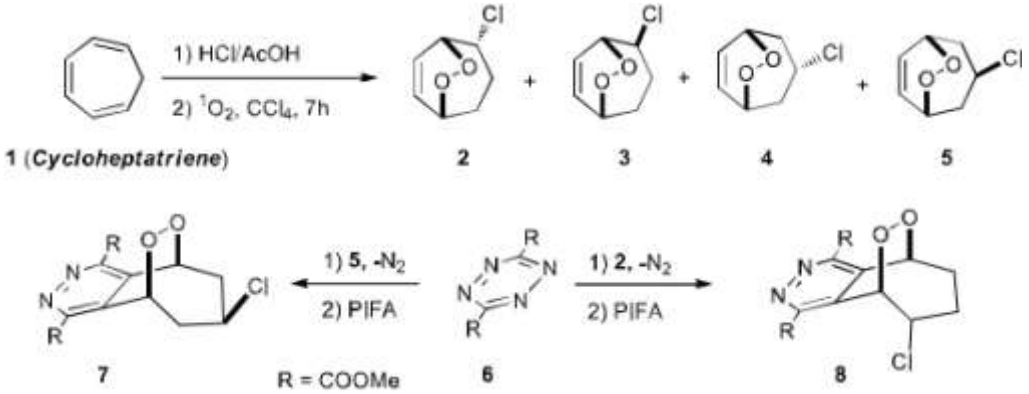
**For correspondence: Email: yasincetinkaya1@gmail.com / yasin.cetinkaya@atauni.edu.tr*

Abstract

Photooxygenations of 5-and 6-chlorocycloheptadiens obtained by addition of HCl to cycloheptatriene gave four endoperoxides whose two are major products (**2** and **5**) for each of the corresponding dienes. Pyridazine derivatives **7** and **8** including O–O bonds were obtained from the reactions of **2** and **5** with dimethyl 1,2,4,5-tetrazine-3,6-dicarboxylate (**6**).

Introduction

Tetrazine **6** is an important diene for inverse Diels-Alder reactions because it easily reacts with electron-rich olefins. The reactions of unsaturated endoperoxides with tetrazine (**8**) are known **[1,2]**.



Result and Discussion

As seen above, four chloroendoperoxides **2-5** whose **2** and **5** are major products for each of the corresponding dienes were obtained from reactions of cycloheptatriene with HCl and ^{1}O2, respectively **[3,4]**. Pyridazine derivatives **7** and **8** were synthesized from the reactions of **6** with **2** and **5**.

Keywords: Endoperoxide; tetrazine; inverse Diels-Alder reaction; pyridazine.

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DFT INVESTIGATION OF FOUR QUINOXALINE DERIVATIVES AS STEEL CORROSION INHIBITORS

Z. El Adnani*, M. Mcharfi, M. Sfaira, M. Benzakour, A.T. Benjelloun

Laboratoire d'Ingénierie des Matériaux, de Modélisation et d'Environnement, LIMME, Faculté des Sciences Dhar El Mahraz, Université Sidi Mohammed Ben Abdellah, USMBA, BP 1796, 30000 Atlas, Fès, Morocco

**For correspondence: Email: zinebeladnani@gmail.com*

Abstract

B3LYP/6-31G(d,p) calculations were conducted on four quinoxaline derivatives, three of which (Q=O, Q=S, Q=2O) were previously reported as good mild steel corrosion inhibitors in acidic media, to establish a correlation between their structural electronic properties and corrosion inhibition efficiencies. The global reactivity descriptors, such as the Energy of the Highest Occupied Molecular Orbital (E_{HOMO}), the Energy of the Lowest Unoccupied Molecular Orbital (E_{LUMO}), the gap energy ($\Delta E=E_{LUMO}-E_{HOMO}$), the dipole moment ($\mu$), the Ionization Potential (I), the Electron Affinity (A), the electronegativity (χ), the global hardness (η), the global softness (σ) and the fraction of electron transferred (ΔN), were in good agreement with the available experimental results. Besides, a high inhibition efficiency for Q=2S, experimentally unstudied, could be expected. Fukui functions calculations were performed to gain some insights into the local reactivity centres. Based on their results an investigation of the possible Fe complexes, by the studied compounds, was conducted to bring about their possible adsorption mechanisms onto the steel surface. Given the intricate and particular nature of the iron atom, three spin multiplicities (singlet, triplet and quintet) were first considered. The complexation study showed that the quintet Fe-quinoxaline complexes were the most stable. Full geometry optimization process led to ten final iron complexes; Fe-Ph and Fe-2O/2S for Q=2O/2S and Fe-Ph, Fe-O/S, and Fe-N for Q=O/S. The results proved the higher stability of the complex Fe-2S when compared to the others, while Fe-Ph appeared to be the least stable complex.

Keywords: DFT; Corrosion inhibition; Quinoxaline; Fukui functions; Complexes ; Spin multiplicities.

NEW EXTRACTION METHOD OF ATRACTYLOSIDE AND CARBOXYATRACTYLOSIDE

S. Errai[a,*], Y. Khabbal[b], M. Faid[c], A. Maataoui[d], M. Benbella[d], A. Abdellaoui[a]

[a]*Laboratory of Physiology, Pharmacology Health and Environment Unit of Bioremediation and Environment Department of Biology. Faculty of Sciences Dhar EL Mahraz, Université Sidi Mohamed Ben Abdellah, BP : 1796, Fès, Maroc.*
[b]*Laboratory of pharmacologie. Faculty of Medicine and Pharmacy, University of Fez BP. 1893; Km 2.200, Sidi Hrazem Road, Fez 30000, Morocco*
[c]*Institue agronomic and vétairinaire Hassan II, Rabat, Morocco*
[d]*National School of Agriculture, Meknes, Morocco*

**For correspondence: Email: siham.errai1@usmba.ac.ma*

Abstract

Evaluation of lethal doses (LD) of Atractylis gummifera's toxic principles namely, atractyloside, and carboxyatractyloside **[1-2]**. has already been the subject of sporadic studies. However, most of these studies are old and based on the use of products resulting from improper extraction technique. Thus, we found useful to initiate a work to enrich and update data on Atractylis gummifera's DL50.This work includes assessment of the plant's toxic power and validation of a new extraction method to obtain the highest yield of active principle from the plant. Roots of Atractylis gummifera used for this study were collected in August 2014 in Morocco. They were first dried under shade then, reduced to powder to undergo the new extraction method. The resulting extract was administered to wistar rats by gavage. The results presented here, indicate that the extraction method is more effective than others techniques already published and the DL50 value of Atractylis gummifera found in this study is 0.48 g / Kg.

Keywords: *Atractylis gummifera,* Atractyloside, Carboxyatractyloside*,* extraction method, DL_{50}

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SYNTHESIS AND *IN VITRO* ANTIOXIDANT ACTIVITY OF SOME NEW HETEROCYCLIC CARBOXYLIC A,A-DIAMINOESTERS

O. Karai, H. Faraj, A. Alami*, A. El Hallaoui, B. Labriti, S. El Hajji, Y. Aouine

Laboratoire de Chimie Organique, Faculté des Sciences Dhar El Mehraz, Université Sidi Mohamed Ben Abdellah, BP : 1796,Fés, Morocco

**For Correspondence: E-mail: alamianouar@yahoo.fr*

Abstract

The synthesis of new α-carboxylic aminoesters containing heterocyclic systems occupies an important place in the realm of synthetic organic chemistry **[1-3]**, Heterocyclic α-Amino acids are the fundamental units of life because of their wide utility of such compounds as components of proteins, peptides and as starting materials for the synthesis of naturally occurring biologically active compounds **[4-6]**.
In our previous work, Heterocyclic α-Amino acids show biological properties including antioxidant activity **[7]**.
In view of these observations and in continuation of our previous work in heterocyclic chemistry, the prepared compounds were synthesized and screened for their *in vitro* antioxidant activity.
The structures of obtained compounds were confirmed by ^{1}H, ^{13}C NMR, IR, Mass spectrometry, Elemental analysis and X-ray analysis.

Keywords: Amino ester; Heterocyclic compound; Amine; antioxidant activity,

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SYNTHESIS AND CHARACTERIZATION OF AN OXAZOLINIC DERIVATIVE, PRECURSOR OF α-METHYL-4-(5-PHENYL-2*H*-TETRAZOL-2-YL)ALANINE

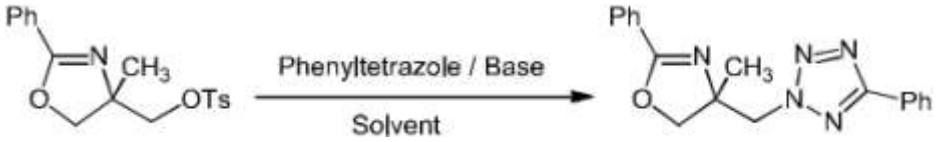
S. Boukhssas, Y. Aouine, H. Faraj, A. Alami*, A. El Hallaoui, B. Labriti

Laboratoire de Chimie Organique, Faculté des Sciences Dhar El Mehraz, Université Sidi Mohamed Ben Abdellah, BP : 1796,Fés, Morocco

**For Correspondence: E-mail: alamianouar@yahoo.fr*

Abstract

Tetrazoles are important heterocycles with a wide range of applications in specialty explosives, information recording systems, photography, new materials, coordination chemistry and pharmaceuticals **[1]**. In the latter application; they are carboxylic acid bioisosteres **[2]**.
Continuing our investigations in the use of oxazoline derivatives **[3]** in heterocyclic synthesis of α-amino acids, we described in this communication the preparation of an oxazolinic precursor of α-methyl-4-(5-phenyl-2*H*-tetrazol-2-yl)alanine (Scheme). This preparation approach is based on the nucleophilic substitution of an oxazolinic derivative.



The desired product was obtained after purification by column chromatography on silica gel, as white solid, with a satisfying yield and its structure was characterized on the basis of NMR spectroscopy in addition to the elemental analysis and MS data.

Keywords: Tetrazole, *N*-alkylation; Oxazoline derivatives; Heterocyclic α-amino acid.

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SYNTHESIS, CHARACTERIZATION AND ANTIBACTERIAL ACTIVITIES OF SOME NEW COMPOUNDS DERIVED FROM *N*-ALKYLATION OF PROTECTED AZIDO GLYCINE

O. Karai, Y. Aouine, H. Faraj, A. Alami*, A. El Hallaoui, B. Labriti

Laboratoire de Chimie Organique, Faculté des Sciences Dhar El Mehraz, Université Sidi Mohamed Ben Abdellah BP : 1796, Fés, Morocco

**For Correspondence: E-mail: alamianouar@yahoo.fr*

Abstract

Heterocyclic amino acids play a predominant role in the synthesis of peptides and proteins, since they increase the resistance of peptides to enzymatic degradation **[1]**, or as precursors to β-lactams and that family of antibiotics **[2]**.In addition, these building blocks and their derivatives are present in a number of potentially biologically useful natural products **[3]**.
We described in this work the preparation of two new compounds derived from glycine. This preparation approach is based on N-alkylation methods **[4,5]**.
The structures of the synthesized compounds were determinate by $_{1}$H, $_{13}$C NMR, MS data in addition to elemental analysis. These biomolecules have diverse biological and pharmacological actions, as antimicrobial and antioxidant **[6,7]**.

Keywords: Amino ester; Heterocyclic compound; Amine; antioxidant activity,

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ORIGINAL DOMINO AZA-MICHAEL-*ih*DIELS-ALDER REACTION TO VARIOUS 3-VINYL-1,2,4-TRIAZINES TO ACCESS POLYSUBSTITUTED TETRAHYDRO-1,6-NAPHTYRIDINES

J. Jouha[a,b,*], F. Buttard[a], M. Lorion[a], C. Berthonneau[c], M. khouili[b], M-A. Hiebel,[a] G. Guillaumet[a],J-F. Brière[c], F. Suzenet[a]

[a]*Université d'Orléans, CNRS, ICOA (UMR 7311), 45067 Orléans, France.*
[b]*Université Sultan My Slimane - Faculté des Sciences et Techniques, BP 523, 23000 Beni-Mellal, Maroc.*
[c]*Normandie Univ, INSA Rouen, UNIROUEN, CNRS, COBRA*, 76000 Rouen, France.

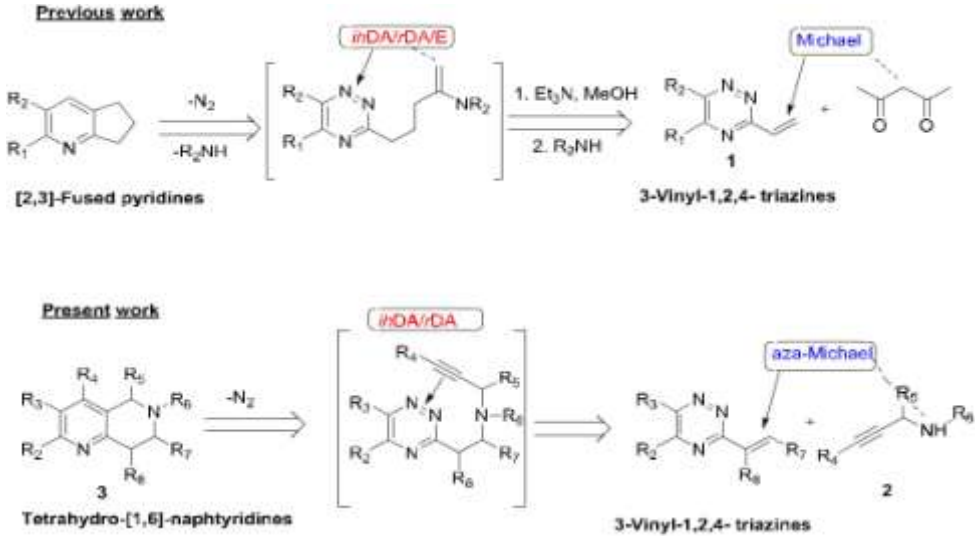
**For correspondence: Email: jabranejouha@gmail.com*

Abstract

Nitrogen containing heteroaromatic compounds, such as di-, tri- and tetrazines are well known to undergo inverse-electron-demand hetero-Diels-Alder (*ih*DA)/ retro-Diels-Alder (*r*DA) reactions as π-electron-deficient *aza*-diene with a wide range of electron-rich dienophile partners **[1]**.

In this context, previous studies in our group validated the possible use of 3-vinyl-1,2,4-triazines **1** as original Michael acceptors in a sequential process involving a conjugated addition followed by an enamine promoted *ihDA*/ *rDA*/ elimination sequence **[2,3]**.

We are now focusing on the evaluation of the potential of these new electrophilic platforms with nitrogen nucleophiles such as propargylamine derivatives **2** bearing a triple bond as dienophile. The aim of this methodology is to open a new route to highly substituted tetrahydro-[1,6]-naphtyridines scaffolds **3** which are poorly described in literature **[4]**.



Keywords: 3-vinyl-1,2,4-triazine; aza-Michael reaction; domino sequence; tetrahydro-1,6-naphtyridines.

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PROCESS INTENSIFICATION FOR THE AZIRIDINES SYNTHESIS USING CONTINUOUS-FLOW REACTORS

F. Siopa*, J.P.M. Antonio, C.A.M. Afonso

The Research Institute for Medicines (iMed.ULisboa), Faculty of Pharmacy,University of Lisbon, Av. Prof. Gama Pinto, 1649-003, Lisboa, Portugal

**For Correspondence: Email: filipasiopa@ff.ulisboa.pt*

Abstract

The discovery of potent biological properties of aminocyclopentitols and the promise that such effects might be exploited as an advantage in medicine have encouraged their synthesis.[1] An attractive approach for the synthesis of these compounds is the photochemical transformation of pyridinium salts to bicyclic-aziridines followed by aziridine ring-opening to afford aminocyclopentene derivatives. However, the reported productivity under batch conditions is low $2.7E^{-3}$ - 1.33 g/L/h and 0.01- 0.36 g/L/h, using respectively water and methanol as nucleophile/solvent.[2] An increasingly popular solution to solve the aforementioned problem is the development of continuous-flow reactors.[3] We hereby present the development and comparison of home-made continuous-flow reactors, consisting of a fluorinated ethylene propylene tube (FEP) reactor and two parallel quartz reactors containing two different internal diameters and their application on the photochemical transformation of 1-*n*-butyl and 1-allyl pyridinium bromide salts to the correspondent α-hydroxycyclopenteno-aziridines (6-azabicyclo[3.1.0]hex-3-en-2-ols).

Keywords: Photoreaction, aziridine, flow reactions, aminocyclopentitols

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THEORETICAL INVESTIGATION OF NEW ORGANIC MATERIALS BASED ON 8-ALKYL-8H-THIENO[2,3-b]INDOLE FOR DSSCS

M. Hachi[a,*], A. Touimi Benjelloun[a], S. Elkhattabi[a,b], A. Fitri[a], M. Benzakour[a], M. Mcharfi[a], M. Hamidi[c], M. Bouachrine[d]

[a]*LIMME, Faculty of Sciences Dhar El Mahraz, University Sidi Mohamed BenAbdallah, Fez - Morocco.*
[b]*ENSA, University Sidi Mohammed Ben Abdellah, Fez - Morocco.*
[c]*URMM/UCTA, FST Errachidia, University Moulay Ismaïl, Errachidia - Morocco.*
[d]*ESTM, (LASMAR), University Moulay Ismaïl, Meknes - Morocco.*

**For correspondence: E-mail: hachimohamed1990@gmail.com*

Abstract

In this work, a theoretical investigation by DFT and TD-DFT methods has been performed to determine the electronic, photovoltaic and spectroscopic properties of new heterocyclic dyes based on 8-alkyl-8H-thieno [2,3-b] indole synthesized recently **[1]**.Different bridge groups were introduced to investigate their effects on the electronic structure. Moreover, several physical parameters (EHOMO, ELUMO, Egap, λ_{emis}, λ_{abs}, Voc, ΔGinject,...) were determined from the fully optimized structures using B3LYP/6-31G (d, p) level. The absorption and emission spectra were also obtained with TD-DFT method using PBE0 functional and 6-31(d,p) basis set in chloroform (CHCl3) solvent which have proved their effectiveness in the study of analogous systems **[2-4]**. All calculations were performed with Gaussian 09 program supported by Gauss View 5.0 interface. Our results suggest that the studied molecules are expected to be promising candidates for dyes sensitized solar cells (DSSCs).

Keywords: Thieno[2,3-b]indole; heterocyclic dyes; DFT; TD-DFT; electronic, photovoltaic and spectroscopic properties.

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PARALLEL SYNTHESIS OF NOVEL DERIVATIVES OF PYRROLOBENZODIAZEPINE LIBRARY

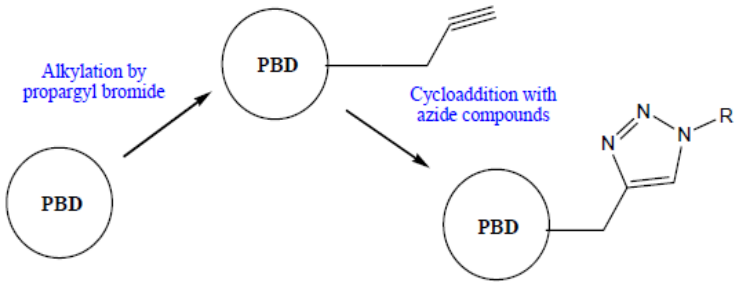
D. Jeroundi[a,*], S. Chakroune[a], E.M. El Hadrami[a], A. Ben-Tama[a], Y. Kandri Rodi[a], E.M. Essassi[b]

[a]*Laboratory Of Applied Organic Chemistry, Sidi Mohamed Ben Abdellah University, Faculty Of Science And Technology, Road Immouzer, BP 2202 Fez, Morocco*
[b]*Laboratory of Heterocyclic Organic Chemistry, Competence Center Pharmacochemistry, Mohammed V-Agdal University, BP 1014 Avenue Ibn Batouta, Rabat Morocco.*

**For correspondence: E-mail: douniajeroundi@gmail.com*

Abstract

The pyrrolobenzodiazepines (PBDs), of which the natural products abbeymycin, DC-81 and fuligocandin B are typical examples, are a class of molecule that has attracted significant interest due the antitumour and antibiotic activity of several members **[1–5]**. PBDs with additional fused rings such as the circumdatin **[6]**, bretazenil **[7]** and the 1, 2, 3-triazolo-fused system **[8]** are attractive as potential antitumour compounds, neurological agents, and protease inhibitors, respectively. As a result of this interest, the fusion of the PBD ring with other rings (oxazole, triazole …) has attracted attention.
In the present communication, we report the synthesis of new derivatives of PBD by action of alkyl halides on pyrrolo [2,1-c] [1,4] benzodiazepine 1 under the conditions of the CTP. The reaction led to the formation of compound 2, after this we have implemented the reaction of 1,3-dipolar cycloaddition using derivatives of PBD as dipolarophiles and alkyl azides as dipoles.



The structures of these products were determined using ^{1}H NMR, ^{13}C NMR. The study of their biological activities will be realized to evaluate their importance.

Keywords: 1,3-dipolar cycloaddition, Triazole, Pyrrolobenzodiazepine, Biological evaluation.

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SYNTHESIS OF SOME THIOXANTHENES BY INTRAMOLECULAR FRIEDEL-CRAFT ALKYLATION

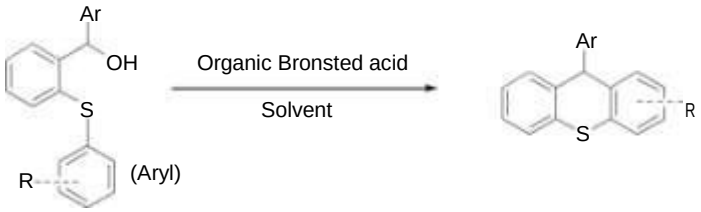
T.Yıldız*, H.Yaşa, B. Hasdemir, H.B. Küçük

Istanbul University, Faculty of Engineering, Department of Chemistry, Organic Division, 34320 Avcilar-Istanbul – Turkey

**For Correspondence: E-mail: tulayyil@istanbul.edu.tr*

Abstract

Compounds of thioxanthene have some typical biological activities such as enzyme inhibition, antiviral and anti-bacterial activities. Besides these properties, they are used in the construction of neuroleptic and antidepressive drugs. Since it is a group of antipsychotic drugs which are used in the treatment of schizophrenia and other psychotic disorders, there are many uses such as drug chemistry **[1,3]**.
In this work, thioxanthenes were synthesized by intramolecular Friedel-Craft alkylation of the appropriate thioether alcohols by an organocatalytic protocol. In the intramolecular Friedel-Crafts alkylation reaction, various organic Bronsted acids were tested for the first time and the best organocatalyst was identified. The original 9H-thioxanthenes were synthesized and purified by chromatographic methods and the structures were determined by ^{1}H-NMR, ^{13}C-NMR, IR, GC-MS and elemental analyzes. Subsequently, the drug activities of these valuable thioxanthenes will be also examined.



Keywords: thioxanthenes; intramolecular cyclization; Friedel-Crafts alkylation; Bronsted acids

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ANTICORROSION POTENTIAL OF POLIO ESSENTIAL OIL ON MILD STEEL IN HYDROCHLORIC ACID SOLUTION: GRAVIMETRIC, ELECTROCHEMICAL, THERMODYNAMIC AND THEORETICAL INVESTIGATIONS

A. Bouoidina[a,*], M. Chaouch[a], M. Taleb[b], A. Lahkimi[b], F. El-Hajjaji[b]

[a]*Laboratoire de génie des Matériaux et environnement, Faculté des sciences Dhar EL Mahraz, Université Sidi Mohamed Ben Abdellah, BP : 1796, Fès, Maroc.* [b]*Laboratoire d'Ingénierie d'Electrochimie de Modélisation et Environnement, Université Sidi Mohamed Ben Abdellah, Fès, Maroc.*

**For correspondence: Email: asmae.bouoidina@gmail.com*

Abstract

Every year, industry pays a massive and rising cost for its corrosion problems. Research and development into new materials, processes and initiatives to combat this loss is increasing, and new findings are constantly coming to light which can help to beat corrosion problems throughout industry. This work is inscribed in the frame of valorization of the essential oil of Polio as an efficacies corrosion inhibitor.

The study of the extract of Polio at different concentrations of inhibitor in acid medium HCl 1M is evaluated by the electrochemical and gravimetric methods. Our results of electrochemical impedance spectroscopy (EIS) indicate that the value of inhibition efficiency increased with increasing concentration of inhibitor and finally reached 90 % for the optimal concentration of 1 g/l. Moreover, the polarization measurements shown that the Polio acts essentially as a mixed-type inhibitor and from the gravimetric results, the thermodynamic parameters of activation of corrosion process also calculated and discussed.

In the second part, the quantum mechanics calculations have been applied within the framework of the density functional theory (DFT) to the major molecules of Polio oil in order to determine the structural and electronic parameters of the molecule responsible for imparting on the extract its high inhibition efficiency as corrosion inhibitor.

Keywords: steel; Corrosion; Inhibitor; EIS; Polarization; Gravimetric

PHYTOCHEMICAL PROFILE, ANTIOXIDANT ACTIVITY AND TOTAL PHENOLIC CONTENT OF EXTRACTS OF CAROB SEED PEELS OF MOROCCO

I. Lakkab*, H. El Hajaji, B. El Bali and M. Lachkar

Engineering Laboratory of Organometallic and Molecular Materials "LIMOM", (CNRST-URAC 19), Faculty of Sciences, Sidi Mohamed Ben Abdellah University in Fez-Morocco.

**For correspondence: Email: lakkab.imane@gmail.com*

Abstract

The Carob tree (*Ceratonia siliqua L.)* belongs to the Caesalpinaceae sub family of the family Leguminoseae. It's widely cultivated in the Mediterranean area and Middle East. The world production of carob pods is estimated about 315.000 tons per year in which Morocco occupied the forth position after Spain, Italy and Portugal (FAO, 2014). This rate is depending on the cultivar, region, and farming practices.

Constituents of seeds are: peel (30-33%), endosperm (42-46%) and embryo or germ (23-25%). The endosperm is composed by natural polysaccharide named galactomannan that is used to produce a natural food additive E410 or commonly known as locust bean gum LBG exhausted in various domains, especially in food industry as flavoring, emulsifier and gelling agent **[1]**. The germ flour contains a high level of proteins which are suitable for human and animal nutrition **[2]**.

The seeds are dehusked with dilute sulfuric acid or thermal mechanical treatment. After that, the endosperm is separated from the embryo and seed peel. In the majority of time peels are eliminated **[3]**.

In this work, we sought to recuperate carob seed peel and establish its phytochemical profile. Apart of that we evaluated its antioxidant activity by using three in-vitro antioxidant models including 1,1-diphenyl-2-picrylhydrazyl (DPPH) scavenging assay, reducing power and total antioxidant capacity of the extracts of carob seed peel produced in Morocco.

Carob seed peel extracts contain high amounts of polyphenols with strong antiradical, antioxidant capacity and reducing properties which might constitute an important source of natural antioxidants which can be used in food and/or pharmaceutical industry.

Keywords: Ceratonia siliqua; peel; phytochemical screening; Dpph; Frap; phosphomolybdenum assay.

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THIABENDAZOLUIM SURFACTANT FOR CLAY MODIFICATION AND THEIR APPLICATION IN NANOCOMPOSITES

K. EL Bourakadi[a,b,*], M. M. Mekhzoum[a], E. M. Essassi[a,b], A. Qaiss[a], R. Bouhfid[a]

[a]*Moroccan Foundation Advanced Science, Innovation and Research (MAScIR), Institute of Nanomaterials and Nanotechnology (INANOTECH). Rabat Design Center, Av Mohamed Jazzouli, Madinat El Irfane 10100, Rabat, Morocco*

[b]*Laboratoire de Chimie Organique Hétérocyclique, URAC 21, Pôle de Compétence Pharmacochimie, Av Ibn Battouta, BP 1014, Faculté des Sciences, Mohammed V University, Rabat, Morocco.*

**For correspondence: Email: khadijaelbourakadi16@gmail.com*

Abstract

The physical and chemical interactions of expandable clays with organic molecules have been studied extensively since the introduction of organically modified clays **[1]**. As a result of these studies, a substantial industry has been established to utilize organoclays. Currently organoclays have been used in different field in industrial scale such as, adsorbents of organic pollutants in soil, paints, cosmetics, personal care products and wastewater treatment **[2,3]**. Recently, considerable attention has been given to the application of organoclays materials in the field of polymer-clay nanocomposite. Interesting characteristic that render organoclay suitable for this purpose is its organophilic character. In this respect, various organic molecules have been used as organic modification for the montmorillonite clay **[4]**. Herein, a series of *N*-alkyl thiabenzaolium surfactant were synthesized and structurally characterized by using different analyses including NMR, MS, Single-crystal X-ray diffraction. These organic compounds were used as clay modification reagents to produce effectively intercalated and thermally stable organophilic clays via cationic exchange process. The detailed characterizations of organoclays produced were performed by X-ray diffraction (XRD), Fourier transform infrared spectrometer (FTIR) and thermogravimetric (TGA) analyses. A computational method of DFT/B3LYP was used to speculate the impact of the alkyl chain length and the effet of concentration (CEC) of surfactant on the interlayer distance of the organically intercalated. These results help to understand the microstructure of thiabendazolium-modified MMT and guide their relevant engineering applications.

Keywords: thiabendazolium, quaternization; alkyl halide; *surfactant, DFT calculation*.

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3D-QSAR STUDY AND MOLECULAR DOCKING OF 4-ANILINOQUINOLINE TRIAZINES AS POTENTIAL ANTIMALARIALS

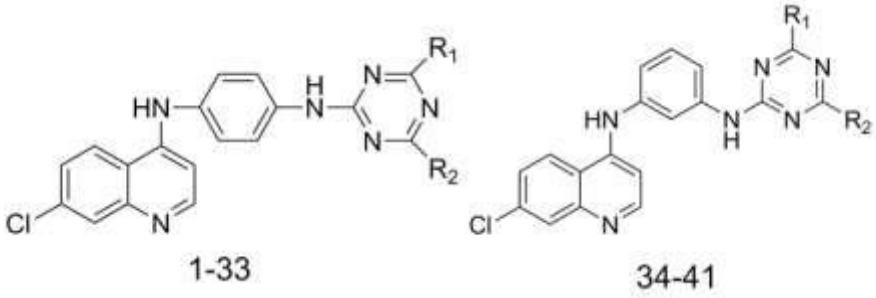
H. Hadni*, M. El Hallaoui

Engineering Materials, Modeling and Environmental Laboratory, Faculty of Science Dhar Mehraz, Sidi Mohammed Ben Abdellah University, B.P. 1796, Atlas, Fes, Morocco.

**For correspondence: Email: hadni.hanine@yahoo.fr*

Abstract

QSAR investigations of 41 hybrids of 4-Anilinoquinolinetriazines **[1]**, known for their potential antimalarial activity, were carried out using descendant multiple regression analyses (MLR), and artificial neural networks (ANN). Quantum chemical descriptors were calculated with the use of the DFT-B3LYP method, with the basis set 6-31G. The correlation coefficients calculated by MLR and ANN values are 0.87 and 0.92 respectively. The ANN model test indicates that this model is statistically significant and shows a very good stability towards data variation in leave-one-out (LOO) cross validation. The observed activity was further substantiated by molecular docking study of compounds 11 and 38 on both wild and quadruple mutant type of pf-DHFR-TS to highlight the structural features of hybrid molecules **[2,3]**. The purpose of the present work is to better understand the predicted binding modes and key protein-ligand interactions in order to develop criteria for selecting compounds. This methodology could be used in future studies to design new antimalarial drugs.



The general structure of the 4-Anilinoquinoline triazine hybrids.

Keywords: antimalarial activity; (QSAR); multiple linear regression (MLR); artificial neural networks (ANN), cross-validation (CV); Molecular docking.

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THEORETICAL CONFORMATIONAL ANALYSIS OF OPIATE PEPTIDES LEU-ENKEPHALIN (H-TYR-GLY-GLY-PHE-LEU-OH) AND ITS TWO THIOAMIDE ANALOGS (H-TYR-GLYΨ[CSNH]GLY-PHE-LEU-OH) AND (H-TYR-GLY-GLYΨ[CSNH]PHE-LEU-OH)

C. Ameziane Hassani[a], **M. Houssat**[a,*], J.E. Hazm[b]

[a]*Laboratory of Applied Chemistry, Faculty of Science and Technology, Sidi Mohamed Ben Abdellah University. BP 2202, Fez, Morocco.*
[b]*Laboratory of Mechanical Engineering, Faculty of Science and Technology, Sidi Mohamed Ben Abdellah University. BP 2202, Fez, Morocco.*

**For correspondence: Email: mourad.houssat@usmba.ac.ma*

Abstract

In order to find information on the native structure of the Leu-Enkephalin opiate peptide, the parent peptide and its two thioamide analogs (Thio-Gly2)Leu-Enkephalin and (Thio-Gly3)Leu-Enkephalin were studied by the theoretical method PEPSEA **[1]**. This comparative conformational analysis showed that the active conformation is a β turn structure centered on Gly3 and Phe4. Moreover, this study showed also that the more active analog (Thio-Gly2)Leu-Enk **[2]** has a lower tendency to adopt this structure. Consequently, its high activity can only be explained by its long lifetime due to its resistance to enzymatic hydrolysis, following the substitution of the amide linkage by the thioamide one. The weakly active analog (Thio-Gly3)Leu-Enk **[2]** does not adopt this structure and prefers instead a β turn structure centered on Gly2 and Gly3. This study also confirmed the importance of the distances between the Tyr and Phe residues at positions 1 and 4 **[3]**, and that of the terminal Tyrosine N-H group which must be free of any intramolecular hydrogen bond in order to be available in the molecular recognition process **[4]**.

Keywords: Opiate peptide; Thioamide-peptide; Conformational analysis; Molecular recognition; Enzymatic hydrolysis.

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SYNTHESIS AND CHARACTERIZATION OF NOVEL OXAZOLINIC DERIVATIVES, PRECURSORS OF α-METHYL-3-(1*H*-PYRAZOL-1-YL)ALANINE

S. Hajib, A. El Hallaoui, A. Alami*, S. El Hajji, H. Faraj, B. Labriti, K. Boujdi and Y. Aouine

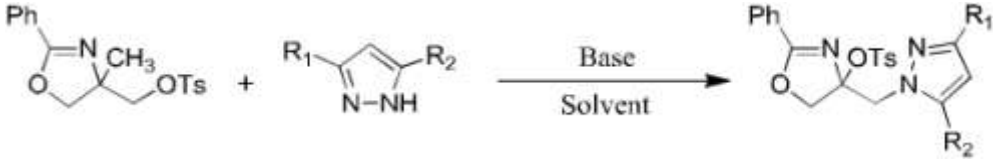
Laboratoire de Chimie Organique, Faculté des sciences Dhar EL Mahraz, Université Sidi Mohamed Ben Abdellah, BP : 1796, Fès, Maroc.

**For correspondence: Email: alamianouar@yahoo.fr*

Abstract

Pyrazole and its derivatives attract the attention of the chemical community mainly on account of the wide spectrum of their pharmacological activities, including antibacterial, antidepressant, anti-inflammatory, antitumor **[1]**. They are widely used as agrochemicals **[2]**.

Continuing our investigations in the use of oxazoline derivatives **[3]** in heterocyclic synthesis of α-amino acids, we described in this communication the preparation of two oxazolinic precursors of α-methyl-3-(1*H*-pyrazol-1-yl)alanine (Scheme). This preparation approach is based on the nucleophilic substitution of an oxazolinic derivative. The desired products were obtained, with a satisfying yield and their structures were characterized on the basis of MS and ^{1}H, ^{13}C NMR spectra.



Keywords: Pyrazole, *N*-alkylation, Oxazoline derivatives, Heterocyclic α-amino acid.

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STUDY OF CRISTALLINITY BEHAVIOR OF CELLULOSE HARD-WOOD COMPONENT USING FT- IR SPECTROSCOPY AND X-RAY DIFFRACTION

S. Fellak*, A. Boukir*

Department of Chemistry, Faculty of Sciences and Techniques of Fez, Sidi Mohamed Ben Abdellah University, B.P. 2202 -Imouzzer road -Fez-Morocco

**For Correspondence Email: aboukir@gmail.com ; soumaya.fellak@gmai.com*

Abstract

Cellulose wood component constitute one of the most abundant and renewable biopolymer in nature biosynthesized largely in the cell wall. It is a linear 1,4-β-glucan polymer, where the monomer units are able to form highly ordered structures, which is due to the result of extensive interaction through intra- and intermolecular hydrogen bonding of the three hydroxyl groups present in each cellulose unit **[1]**. Furthermore, the feature of crystallinity in cellulose is one of the most important characteristics contributing to its physical, chemical and mechanical properties and that remains a field of active study today.

In our work, study of crystallinity behaviors executed on four hardwood samples pertaining to 17^{th}, 18^{th}, 20^{th} and 21^{st} centuries and originated from Agadir region (south of Morocco) during exposure time to the natural degradation process using FT-IR spectroscopy and X-ray diffraction.

In the spectra of FT-IR patterns it has been shown that the band at 1318 (δ CH2 in crystallized cellulose I), 1163 (CH2 in crystallized I cellulose) and 898 cm^{-1} (νC1-O-C of β-(1-4)-glycosidic linkage between glucose) shift towards a lower intensities upon degradation level. This decline can be justified by decreasing cellulose crystallinity accompanied by an increase of disordered structure (amorphous form) identified by the absorptions located at 1337 and 1156 cm^{-1}.

XRD results revealed a decrease in peak intensity at 22.6° 2θ for the (200) crystallographic plan assigned to cristalline cellulose fraction passing from un-degraded sample to degraded one, as well as in the crystallinity index (CrI %), exception made for the sample dating to 20^{th} century when the increase of CrI% (from 43% to 48%) be explained by that the partially degraded cellulose was capable to form a new and larger cristals. While, no significant changes was observed on cristallite seize (D200) suggesting that the microcristalline structure was not significantly affected and broken during exposure time to the natural degradation.

Whatever, the present data developed a detailed understanding of changes that occur at the cellulose microcrystalline structure and may be applicable to other types of cellulose polymorphs.

Keywords: Hard-wood, cellulose, crystallinity, degradation, FT-IR spectroscopy, X-ray diffraction.

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SYNTHESIS, CHARACTERIZATION AND ANTIMICROBIAL ACTIVITY OF THIOQUINOXALINONE AND α-NAPHTOL FUSED EXO-BICYCLIC 1,2,3-TRIAZOLO-1,4-OXAZINES

M. Missioui[a,b], M. El fal[a,c], M. Ouhssine[b] and Y. Ramli[a,*]

[a]*Laboratory of agro-physiology, biotechnology, environnement and quality, Département of biology, Ibn-Tofail University, BP, 133, 14000, Kenitra, Morocco.*
[b]*Medicinal Chemistry Laboratory, Faculty of Medicine and Pharmacy, Mohammed V University, 10170, Rabat, Morocco.*
[c]*Laboratory of Organic Heterocyclic Chemistry URAC 21, Faculty of Sciences, Mohammed V University, 10170, Rabat, Morocco*

**For Correspondence: E mail: mohcinemissioui@gmail.com and yramli76@yahoo.fr*

Abstract

thioquinoxalinone and α-naphtol compounds were reacted with epichlodrine by a nucleophilic reaction, to give a terminal oxirane compounds, the result products were reacted with an excess of azide ion, the following step consists in a propargilation reaction followed by a quick and spontaneous 1,3 dipolar intramolaicular cycloaddition reaction **[1]**. All the synthesized compounds structures were established on the basis of spectral analysis and were evaluated for their entimicrobial activity.

***Keywords*:** 1,3-dipolar cycloaddition; triazole; oxazine; antimicrobial activity.

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HEMISYNTHESIS OF NEW TRIAZOLYL DERIVATIVES USING SESQUITERPENIC HYDROCARBON

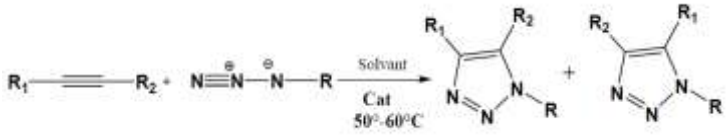
A. Bimoussa*, A. Auhmani, A. Oubella, My.Y. Ait Itto, A. Auhmani

Laboratoire de synthèse organique et physico-chimie Moléculaire, Université Cadi Ayyad, Faculté des Sciences Semlalia, Département de chimie, B P 2390, Marrakech, Maroc.

**For Correspondence: Email: bimoussa_@hotmail.com*

Abstract

The 1, 2, 3-triazoles and their derivatives are known by their important biological activities, such as antiseptic, antifungal **[1]**, anti-inflammatory **[2]** and antimicrobial **[3]**. To prepare new triazolyl derivatives, we used a sesquiterpenic hydrocarbon extracted from Atlas cedar essential oil. Thus, The 1,3-dipolar cycloaddition reaction between sesquiterpenic azide and the terminal alkynes gives a series of new 1,2,3-triazole derivatives. There structures were identified by ^{1}H and ^{13}C NMR and IR spectral analyses.



***Keywords*:** 1, 2,3-triazoles; sesquiterpenic; 1,3-dipolar cycloaddition

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ELECTROCHEMICAL AND THERMODYNAMIC STUDIES ON CORROSION INHIBITION OF PSB IN MOLAR HYDROCHLORIC ACID

M. Driouch[a,*], N. Achinie[a], E. Elassiri[a], M. Beniken[a], M. Sfaira[a], M. Benzakour[a], M. Ebn Touhami[b]

[a]*Laboratoire d'Ingénierie des Matériaux, de Modélisation et d'Environnement (LIMME), Faculté des Sciences, Université Sidi Mohammed Ben Abdellah, B.P. 1796–30000, Fès, Morocco.*
[b]*Laboratoire d'Ingénierie des Matériaux et Environnement : Modélisation et Application (LIMEMA), Faculté des Sciences, Université Ibn Tofaïl, B.P. 133–14000, Kénitra, Morocco.*

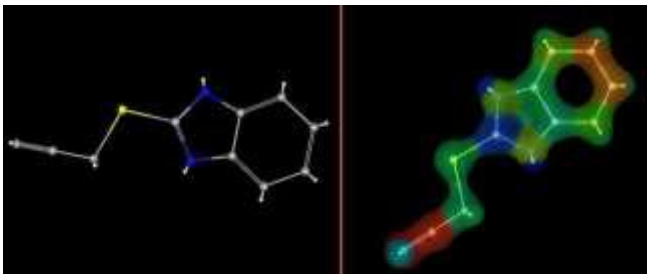
**For Correspondence: Email: majid.driouch.fsdm@gmail.com / msfaira@yahoo.com*

Abstract

The ***2-(prop-2-yn-1-ylsulfanyl)-1H-1,3-benzodiazole PSB*** has been investigated as corrosion inhibitor for mild steel in 1M HCl by means of potentiodynamic polarization PP fitted with Tafel, Stern, Stern & Geary methods **[1]** as well as EIS measurements. The EIS data were analyzed to model the inhibition process by an appropriate equivalent circuit model, in order to understand the mechanism of the process that takes place at the electrode / solution interface and to differentiate the different elementary steps which the global process referring to their relaxation time.

The obtained results showed that PSB revealed a good corrosion inhibition which increased with the inhibitor concentration reaching circa 95 % at 10^{-4} M of PSB. Potentiodynamic polarisation revealed the mixed type character of this organic compound. The Nyquist and Bode diagrams indicated that the diagrams corresponding to the high concentrations highlighted two time constants; the first capacitive semicircle observed at high frequency could be attributed to a charge transfer process and the neighbouring second semicircle to the inhibitor's adsorption onto the metal surface.

The adsorption data fitted well to Langmuir, El-Awady, Frumkin and Temkin. The thermodynamic parameters and the intrinsic properties of PSB (protonation: (pKa, isoelectric point), Charge, polarizability…) and of the metal (PZN) converged to a double character of the adsorption process though predominantly chemical. The scanning electron microscopy testified the formation of a protective film over the surface.



Keywords: Benzodiazol; Carbon steel; Acid corrosion; Corrosion Inhibition; Stern & Geary.

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KINETIC-THERMODYNAMIC PROPERTIES OF A POLYACRYLAMIDE AS CORROSION INHIBITOR OF CARBON STEEL IN 1.0M HCl

M. Beniken[a,*], M. Driouch[a], M. Sfaira[a,*], B. Hammouti[b], M. Ebn Touhami[c], M.A. Mohsin[d]

[a]*Laboratoire d'Ingénierie des Matériaux, de Modélisation et d'Environnement (LIMME), Faculté des Sciences, Université Sidi Mohammed Ben Abdellah, B.P. 1796–30000, Atlas – Fès, Morocco.*
[b]*LCAE-URAC18, Faculté des Sciences, Université Mohammed Premier, BP 717 – 60000, Oujda, Morocco*
[c]*Laboratoire d'Ingénierie des Matériaux et Environnement : Modélisation et Application (LIMEMA), Faculté des Sciences, Université Ibn Tofaïl, B.P. 133–14000, Kénitra, Morocco.*
[d]*Department of Chemistry, University of Sharjah, Sharjah, P.O. Box 27272, United Arab Emirates.*

**For Correspondence: Email: mustapha.beniken@yahoo.fr / msfaira@yahoo.com*

Abstract

The efficiency of a polyacrylamide (PA), recently synthesized by inverse emulsion polymerization, was evaluated for corrosion inhibition of C38 in 1.0 M HCl solution, by means of electrochemical impedance spectroscopy, potentiodynamic polarization and weight-loss measurements. The effects of temperature and immersion time as well as kinetic parameters values of steel dissolution process were determined and discussed. The adsorption of PA on C38 obeyed Langmuir followed by El-Awady, Flory-Huggins, Temkin and Frumkin adsorption isotherms. A discussion of the treatment results of each model was given. Combined effects suggested that PA acted as mixed-type inhibitor, by adsorption on C38 via both physical and chemical interactions of nonprotonated and protonated molecules.

***Keywords*:** Polyacrylamide; Acid corrosion; Corrosion inhibition; Adsorption isotherms.

CYCLOCONDENSATION AND CHARACTERIZATION OF NOVEL 5-CHLORO-1*H*-INDOLE-2,3-DIONE DERIVATIVES

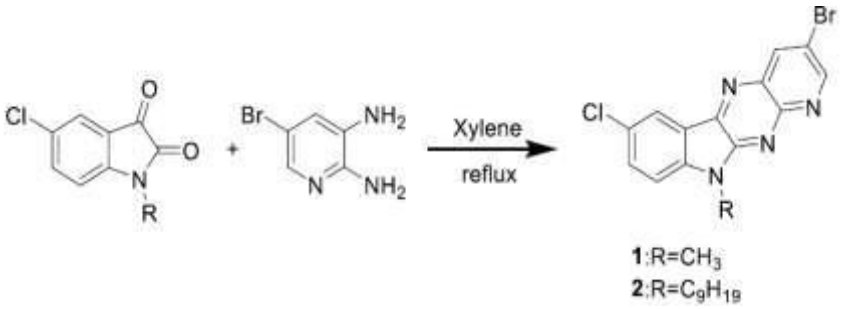
Z. Tribak[a,*], M.K. Skalli[a], O. Senhaji[b], Y. Kandri Rodi[c], A. Haoudi[a], M. Filali Baba[d], E.M. Essassi[e]

[a]*Laboratory of Applied Chemistry, Sidi Mohamed Ben Abdellah University, Faculty of Science and Technology of Fes, Morocco.*
[b]*Laboratory of Applied Physical Chemistry, Moulay Ismaïl University, Faculty of Sciences and*
[c]*Laboratory of Applied Organic Chemistry, Sidi Mohamed Ben Abdellah University, Faculty of Science and Technology of Fes, Morocco.*
[d]*Laboratory of Engineering, Electrochemistry, Modeling and Environment, Faculty of Sciences Dhar Mehraz, Sidi Mohamed Ben Abdellah University, B.P: 1796, Fez, Morocco*
[e]*Laboratoire de Chimie Organique Hétérocyclique, Pô le de Compétences Pharmacochimie, Mohammed V University in Rabat, BP 1014, Avenue Ibn Batouta, Rabat, Morocco*

**For Correspondence: E-mail: tribak.zineb@gmail.com*

Abstract

Isatin, possessing an indole nucleus having both the keto and lactam moiety has aroused tremen-dous curiosity due to its diverse biological and pharmacological studies. From literature survey it is well known that isatin heterocycles exhibit manifold importance in the field of medicinal chemistry as a potent chemotherapeutic agent **[1,2]**.
In order to multiply the family heterocyclic compound from 5-Chloro-1*H*-indole-2,3-dione, we report here the synthesis of new compounds shown in the scheme-1 via the cyclocondensation between 5-chloroisatin derivatives and Diamino-5-Bromopyridin **[3]**.
The synthesized compounds were characterized by spectral analysis of, ^{1}H-NMR and ^{13}C-NMR **[4]**.



Scheme 1

Keywords: Isatin, 5-Chloroisatin, heterocyclic, Cyclocondensation, NMR.

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NEW METHOD OF REGIOSELECTIVE SYNTHESIS OF 1,2,3-TRIAZOLYL NUCLEOSIDES *VIA* CLICK CHEMISTRY CATALYSED WITH COPPER NANOPARTICULES SUPPORTED ON SILICA AND UNDER ULTRASONIC ACTIVATION

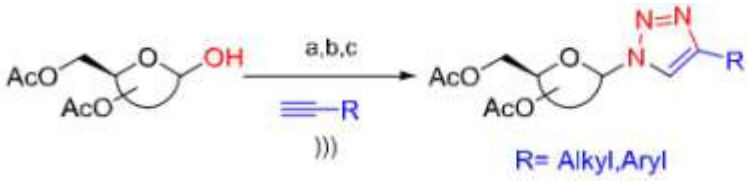
A. Talha[a], A. Mourhly[b], M. Driowya[a], H. Tachallait[a], M. Halim[b], S. Arsalane[b], K. Bougrin[a,*]

[a]*Laboratory of Plant Chemistry and Organic and Bioorganic Synthesis, URAC23, University of Mohammed V, Faculty of Sciences, Ibn Battuta Avenue, PO Box 1014, 10000 Rabat, Morocco.*
[b]*Center for Materials Science, Laboratory of Materials, Nanotechnologies and Environment, Mohammed V University, Faculty of Sciences, Ibn Battuta Avenue, PO Box 1014, 10000 Rabat, Morocco.*

**For correspondence: Email: kbougrin@yahoo.fr*

Abstract

The triazole ring is often found in various drugs, probably because of its ability to form hydrogen bonds with the active site. The making of triazoles in drugs was usually prepared by the Copper-catalyzed azide−alkyne cycloaddition (CuAAC) **[1]**. The major limitations of existing CuAAC protocols have been in terms of catalyst homogeneity, thus creating the problem of catalyst / product separation and the required addition of reducing agents limits their use in industrial processes **[2]**. Recently, copper nanoparticles (CuNPs) are used as an alternative catalyst to conventional systems **[3].**



***Experimental Conditions*: (a) : Ac_2O, LA; (b) : $TMSN_3$, LA, DCM; (c) : CuNPs ,Reducing agent, Aprotic solvant**

The aim of our work is to keep abreast of scientific advances in the application of nanoparticles in heterogeneous catalysis, for that we have realized the 1.3-dipolar cycloaddition azide-alkyne "click chemistry" with a new nanocatalyst system CuNPs supported on amorphous mesoporous silica, under ultrasound irradiation for obtaining derivatives of type 1'- (1,2,3-triazolyl) -nucleosides 4-substituted which can have significant biological activities.

Keywords:Nanoparticles, 1,3-Dipolar cycloaddition, Click chemistry, 1,2,3-Triazoles, Nucleosides.

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SYNTHESIS OF HAPTENS OF CHLORPYRIFOS-ETHYL AND ITS METABOLITES

I. Maftouh[a,b,*], A. Moussaif[a,*], A. Iddar[a], N. El Abbadi[a], A. Mesfioui[b]

[a]*Biotechnology and Biomolecular Engineering Unit, National Centre for Nuclear Energy, Sciences*
[b]*Genetics - Neuroendocrinology and Biotechnology Laborartory, IbnTofaïl University, Faculty of Sciences, Kenitra, Morocco.*

**For correspondence: Email: i_maftouh@yahoo.fr a.moussaif@cnesten.org.ma*

Abstract

The O,O'-Diethyl-3,5,6-trichloropyridin-2-yl phosphorothioate, commonly named as Chlorpyrifos-ethyl, is an organophosphorus insecticide which is widely used in agriculture worldwide. During its penetration into the soil and / or into the crop, it undergoes degradation by physical, chemical and biological means to give rise to several metabolites **[1-2]**.
In this work, we propose to study this insecticide as well as two of its metabolites, namely: the O,O'-diethylhydroxyphosphorothioate and the 3,5,6-trichloro-2-pyridinol which is the primary degradation product. The global objective is to conceive an immunoassay tool to evaluate this pesticide's residue level in agricultural products. This tool will allow detecting both the Chlorpyrifos-ethyl and the products of its degradation, whereas other classical analytical methods permit only the detection of the mother molecule **[1]**.
The main phase of an immunoassay consists of producing antibodies. For small molecules such as Chlorpyrifos-ethyl, it is suitable to synthetize haptens which will be conjugated to carrier proteins so that the analytical structure becomes immunogenic **[3]**. Indeed, the presented method involves the hapten synthesis, for the three above products, with different spacer arms which the structures have been identified by nuclear magnetic resonance and have been verified using infrared spectrometry. Then, each obtained hapten has been used for the generation of polyclonal antibodies in rabbit using the hapten-protein (bovine serum albumin) conjugate carrier through N-hydroxysuccinimide active esters to make immunogens **[1]**.

Keywords: Antibodies; Chlorpyrifos-ethyl; Hapten; Hydroxide pyridine; Organophosphorus.

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SYNTHESIS AND REACTIVITY STUDY OF THIAZOLIDINONES

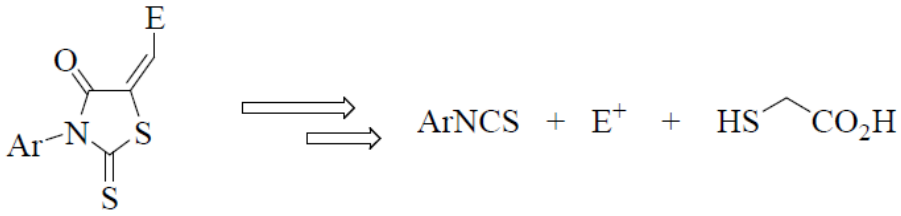
Mohammed Benabdallah[a,*], Zahira Kibou[b], Noureddine Choukchou-Braham[a]

[a]*Laboratoire de Catalyse en Chimie Organique, Faculté des Sciences, Université Abou-Beker Belkaid, B.P. 119, 13000 Tlemcen, Algeria*
[b]*Centre Universitaire Belhadj Bouchaib d'Ain Témouchent, BP 284, 46000 Ain Témouchent, Algeria*

**For correspondence: Email: m.benabdallah1977@gmail.com*

Abstract

Compounds such as the oxygenates, nitrogen and the sulphur ones have attracted the scientific researchers' attention. Among these heterocyclic compounds, the thiazolidinones **[1]** which play an appealing role as a basic skeleton for the synthesis of several extensively applied products in the pharmaceutical **[1]** and therapeutic industry **[1]** as antiviral, anticonvulsants, antibacterial and anti-inflammatory and so on. Moreover, they are also a potential candidate as an anti-cancer drug **[1]**.
However, we used a domino effect to synthesise a new series of heterocyclic with five functioned links, especially thiazolidinones series (schema 1), using a key synthon thioglycolic acid under mild conditions respecting the few criteria of green chemistry.



Schema 1: Synthesis of 3-aryl-2-thioxothizolidin-4-ones

Keywords: thioglycolic acid; 2-thioxothizolidin-4-one; Condensation of knoevenagel; Domino reaction; green chemistry.

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SYNTHESIS OF NEW MOLECULES OF BENZIMIDAZOLOTHIONE STRUCTURE

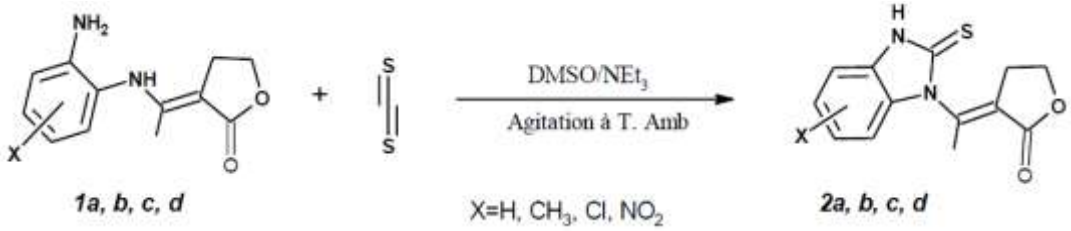
Mohamed Amari[a,b,*] and Mokhtar Fodili[b]

[a]*Faculty of Chemistry, USTHB, BP 32 ElAlia Bab Ezzouar, Algiers, Algeria*
[b] *Laboratoire COSNa, UZA, Route de Laghouat, Djelfa, Algeria*

**For correspondence: Email: amarimod@hotmail.fr*

Abstract

The recent literature reveals an interest growing for benzimidazolothiones, because of their use in diverse domains **[1]**, such as antimicrobial agents and in the industrial domain. They are used as anticorrosive agents **[2]** and adsorbants of the heavy metals **[3]**. We have obtained the Enaminones **1** by condensation of 1,2-
phenylenediamines on the acetylbutyrolactone and we have elucidated by stereochemical study **[4]**. Subseqently, compounds 1 react with the disulfure of carbon in the DMSO in presence of basic catalysis of the triethylamine under magnetic agitation and at room temperature to isolate the structure **2**. Products **2** are obtained with yields between 40 and 85%.



1a, b, c, d *2a, b, c, d*

Compounds **2** were determined by NMR ^{1}H and ^{13}C, spectrometry of mass and RX analysis.

Keywords: benzimidazole; acetylbutyrolactone; NMR ^{1}H, ^{13}C.

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ANTIMICROBIAL ACTIVITY OF A NEW CLASS OF PYRROLOBENZODIAZEPINE

D. Jeroundi[a,*], S. Chakroune[a], E.M. El Hadrami[a], A. Ben-Tama[a], Y. Kandri Rodi[a], E.M. Essassi[b]

[a]*Laboratory Of Applied Organic Chemistry, Sidi Mohamed Ben Abdellah University, Faculty Of Science And Technology, Road Immouzer, BP 2202 Fez, Morocco*
[b]*Laboratory of Heterocyclic Organic Chemistry, Competence Center Pharmacochemistry, Mohammed V-Agdal University, BP 1014 Avenue Ibn Batouta, Rabat Morocco.*

**For Correspondence: E-mail: douniajeroundi@gmail.com*

Abstract

In recent years, the field of heterocyclic chemistry has become increasingly important. Indeed, heterocyclic structures, whether of synthetic or natural origin, appear as a particularly interesting support in very varied fields (pharmacy, medicine, industry ...). Pyrrolo [2,1-c] [1,4]benzodiazepines are among the heterocyclics which have attracted considerable interest because of their important activities, including antibiotic, anti-tumor **[1,2]**, antiviral activity and anxiolytic properties. The remarkable broad spectrum of activities of the naturally produced PBDs **[3]** encouraged the synthesis of several PBDs. In present work, novel PBDs derivatives of the benzodiazepine by alkylation of pyrrolo [2,1c] [1,4] benzodiazepines are studied for their antimicrobial activity.
For that, we alkylated the PBDs with different alkyl halides under the phase transfer conditions. Then, an attempt has been made to highlight the biological activity of alkylPBDs by testing their antimicrobial action against several types of bacteria.
The structures of these products were determined using ^{1}H NMR, ^{13}C NMR.

***Keywords*:** Pyrrolobenzodiazepine, antimicrobial evaluation, CTP.

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CYCLOADDITION AND CYCLOCONDENSATION OF (E)-2-(4-ARYLBENZYLIDENE)-3-PHENYL INDANONES

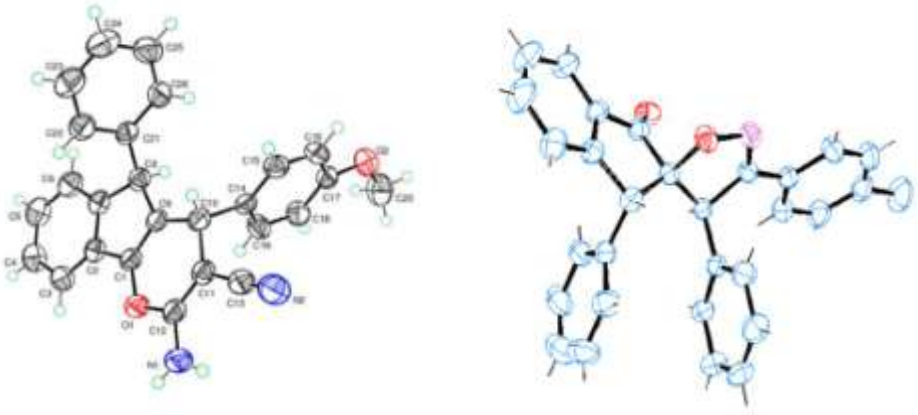
A. Mahfoud[a,*], M. Bakhouch[a], M. Chalkha[a], M. Akhazzane[b], A.Kerbal[a], M.El Yazidi[a], M. Daoudi[a] and G. Al Houari[a]

[a]*Laboratoire de Chimie Organique, Faculté des Sciences Dhar El Mahraz, Université Sidi Mohamed Ben Abdellah, BP: 1796, Fès, Morocco.*
[b]*Cité de l'innovation, Université Sidi Mohamed Ben Abdellah, Fès, Morocco.*

**For correspondence e-mail: asmae.mahfoud@hotmail.com*

Abstract

In this work, we used the cyclocondensation and the dipolar-1,3 cycloaddition reactions to synthesize new amino-indeno-pyran-3-carbonitriles and spiroisoxazolines. These molecules are known for their biological properties such as herbicidal, anti-tumoral **[1]**, anti-HIV **[2]** and antiproliferative **[3]**.
We obtained these amino-indeno-pyran-3-carbonitriles and spiroisoxazolines by the action of (E)-2-(4-arylbenzylidene)-3-phenyl indanones with malononitrile **[4]** and nitrile oxide **[5]** respectively.
The Orteps of the obtained molecules are given below.



Keywords: Malononitrile; dipolar-1,3 cycloaddition; nitrile oxide; E)-2-(4-arylbenzylidene)-3-phenyl indanones.

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SYNTHESIS OF NEW COPPER-AMINOPYRIDINESCOMPLEXES

F. Nouali[a,*], Z. Kibou[a,b], M. Benabdallah[a], N. Choukchou-Braham[a]

[a]*Laboratoire de Catalyse et Synthèse en Chimie Organique, Université de Tlemcen, B.P.119, 13000 Tlemcen, Algeria*
[b]Centre Universitaire de Ain Témouchent, Institue des Sciences, BP 284, 46000 Ain Témouchent, Algeria

**For correspondance:* E-mail: *noualifatiha46@yahoo.fr*

Heterocyclic compounds are the preferred source of various study subjects in our laboratory **[1-2]**. They have received much attention because of their applications in biology **[3]** and coordination chemistry **[4].**
2-Aminopyridines constitute an important class of heterocyclecompounds with different group of electron donor or proton acceptor, they have received much attention due to their antifungal, anti-inflammatory, analgesic, antipyretic and antimicrobial activities **[5].**
In this work, we present a new method for the preparation of 2-Aminopyridines and their uses as ligands complexing to copper. The synthesis and characterization of the copper(II) complexes of a series of aminopyridineligands is described.

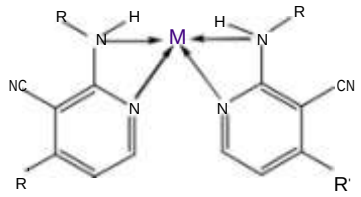

Figure 1: Complexe structure

Keywords*:* Heterocyclic compound; 2-Aminopyridines; copper; complexes.

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APPROACH TO THE TOTAL SYNTHESIS OF A NEW ANALOGUE OF HALICLAMINE A.

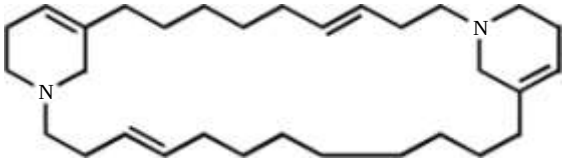
I. Khettar*, G. Ferouani, A. Selka, C. Ziani-Cherif

Laboratoire de catalyse et synthèse en chimie organique, Faculté des sciences, Université de Tlemcen.

**For Correspondence: Email: jokerch2014@gmail.com*

Abstract

Haliclamine A **[1]** is a bis-tetrahydropyridine alkaloid having one unsaturated carbon chain which was isolated for the first time from the sponge Chimney HaliclonaGenus by Fusetani and Coll in 1989.
Biological tests have shown that Haliclamine A has very interesting biological activities such as: cytotoxicity, antifungicity and antimicrobial against Gram-Escherichia Coli, or Gram + Staphylococcus Aureus **[2,3]**.
In this work we have been interested in the total synthesis of an analogue of haliclamine A by simple and effective reactions which are already done in our laboratory.



Haliclamine A

Keywords: Haliclamine A;Total synthesis; bis-tetrahydropyridine; antimicrobial.

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SYNTHESIS AND PHOTOPHYSICAL STUDIES OF NOVEL N-ACYLHYDRAZONE BASED ON ACRIDONE

Mohammed Aarjane*, Siham Slassi, Amina Amine*

Equipe de Recherche Chimie Moléculaire et Molécules Bioactives. Faculté des Sciences, Université Moulay Ismail - Meknès

**For correspondence: Email: aarjane.mohammed@gmail.com / amine_7a@yahoo.fr*

Abstract:

Fluorescent heterocyclic compounds are of particular interest, because they exhibit unique electrical and optical properties such as emitters for electroluminescence devices, molecular probes for biochemical research, in traditional textile and polymer fields, fluorescent whitening agents and photo conducting materials **[1]**.
Acridone derivatives, as an important kind of tricycle nitrogen heterocycle, have been used for the production of dyes and some valuable drugs. Particularly, some of them are found to be efficient fluorescent chemosensors for recognition of transition metal ions such as Hg^{2+} **[2]** and emitters for luminescence studies **[3]**. Also, acridine orange (3,6-dimethylaminoacridine) is a nucleic acid selective metachromatic stain valuable for cell cycle determination.
In this work, we present the synthesis of novel N-acylhydrazone acridone by the condensation of 9-oxo-9,10-dihydroacridine-4-carboxylic acid hydrazide with various aldehydes. Physical spectral and analytical data have confirmed the structures of the synthesized dyes. The optical and solvatochromic properties of these compounds were investigated and the results showed that they show very interesting photophysical properties. Furthermore, density functional theory (DFT) calculations of fluorescent dyes were performed to provide the optimized geometries and relevant frontier orbitals.

***Keywords*:** Acridone; fluorescence; photophysical study.

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SYNTHESIS OF CYCLIC PEPTIDES USING BIS(2-SULFANYLETHYL)AMIDO PEPTIDE AS LATENT THIOESTER SURROGATE

E. Boll[a], J-P. Ebran[a], H. Drobecq[a], **O. El-Mahdi[b,*]**, L. Raibaut[a], N. Ollivier[a], O. Melnyk[a]

[a]*Institut Pasteur de Lille, UMR 8161 - M3T – Mechanisms of Tumorigenesis and Target Therapies, F-59000 Lille, France.*
[b]*Laboratoire Ressources Naturelles et Environnement, Faculté Polydisciplinaire de Taza, BP 1223, Taza gare, Maroc.*

**For correspondence: ouafaaelmahdi@yahoo.fr*

Abstract

Cyclic peptides are valuable tools in chemical biology and pharmaceutical science. In contrast to linear peptides, these ring-shaped variants have shown a higher selectivity for binding, an improved proteolytic stability and a defined conformation, which enable them to be used as privileged scaffolds in drug design but also for mimicking protein epitopes and disrupting protein-protein interactions **[1]**.
Various synthetic strategies for producing backbone-cyclized peptides or proteins have been explored and known continuously improvements particularly with the emergence of native chemical ligation which consists in the chemoselective reaction of a *C*-terminal peptide thioester with an *N*-terminal cysteinyl peptide **[2]**. However, significant synthetic challenges in producing cyclic peptides especially larger ones (up to 50 amino acids residues) have precluded a prolific use in biomedical research. In most cases, the cyclic product ring size is restricted to length of peptides that can be accessed from solid phase peptide synthesis and the efficiency of the cyclization reactions. Herein, we will present an attractive approach based on *N*-acylperhydro-1,2,5-dithiazepine incorporated as a *C*-terminal amido moiety of a target peptide by solid-phase Fmoc chemistry **[3]**. This key functional moiety is an amide-based thioester surrogate with particularly appealing properties that have enabled the design of controlled chemoselective amide bond ligation which can be integrated in effective sequential chemical ligation process giving access to desired backbone cyclized peptides **[4]**.

Keywords: Native chemical ligation; thioester; bis(2-sulfanylethyl)amide; Fmoc-SPPS; cyclative ligation.

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MICROWAVE AND ULTRASOUND ASSISTED SYNTHESIS AND REACTIVITY OF PYRIDAZINONES

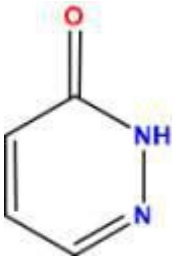
Y. Zaoui[a,*], Y. Boukharsa[a], J. Taoufik[a], M. Ansar[a]

Laboratory of Therapeutic Chemistry, Faculty of Medicine and Pharmacy of Rabat, Mohammed V University of Rabat, BP 6203 10000 Av Mohammed Belarbi Alaoui, Rabat

For Correspondence: Email: younes.zaoui@um5s.net.ma

Abstract

Heterocyclic chemistry, have shown, in the last decades an interesting and various chemical core like tetrahydroquinolines, benzotriazole, diazepine, pyridazine, thiazole, pyrazole. Different studies integrated several way to synthetize those class of molecule.
Pyridazin-3(2H)-ones constitute an important core in heterocyclic chemistry. Interesting biological and pharmaceutical studies showed the importance of this class of molecule, also agrochemistry activities have been highlighting. Differents synthesis of this heterocylic class of molecules have been reported in the literature. It include novel ways of synthesis by microwave and ultrasound. Those novel ways showed facil methods and interesting results than conventional synthesis.



Keywords : Pyridazin-3(2H)-one, microwave, ultrasound, biological activities.

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SYNTHESIS OF HETEROCYCLIC COMPOUNDS DERIVATIVES OF γ-PYRONE

Salima Tabti[a,*], Amel Djedouani[b]

[a]*Laboratoire Matériaux et systèmes électroniques, Universite Mohamed el Bachir El Ibrahimi, El Anasser, 34000, Bordj Bou Arreridj, Algeria*
[b]*Laboratoire de Physicochimie Analytique et Cristallochimie des Materiaux Organometalliques et Biomoleculaires, Universite Constantine 1, 25000, Constantine, Algeria*

**For correspondence: Email: thabti_sa@yahoo.fr*

Abstract

The synthesis of α,β-unsaturated carbonyl compounds by the condensation of dehydroacetic acid DHA with carboxaldehyde RCHO derivatives [pyrrole-2; and -4-(dimethylamino) phenyl] afforded four chalcone ligands (L1-L2), These compounds when carbonyl group is conjugated with an alkene, from which they derive special properties. There are characterized by IR, UV-Vis, NMR proton elemental analysis and mass spectroscopy.
L1 and L2 were characterized by X-ray crystallography. Molecules crystallize with four and two molecules in the asymmetric unit, respectively and adopt an E conformation about the C=C bond. Both structures are stabilized by an extended network O-H … O. Furthermore, N-H … O and C-H … O hydrogen bonds are observed in L1 and L2 structures, respectively.

***Keywords**:* chalcone, DHA, heterocyclic compound, γ-pyrone

SYNTHESIS AND THEORETICAL STUDY OF SOME 1,4-BENZOXAZINE DERIVATIVES OBTAINED BY 1,3-DIPOLAR CYCLOADDITION REACTION

Fouzia Hlimi[a]*, Nada Kheira Sebbar[a], Younes Ouzidan[b], M. Salah[c], Hamza El Hadki[c], Said Kitane[d], Oum Kalthoum Kabbaj[c], El Mokhtar Essassi[e]

[a]*Laboratoire de Chimie Organique Hétérocyclique, Centre de Recherche des Sciences des Médicaments, Pôle de Compétences Pharmacochimie, Mohammed V University in Rabat, Faculté des Sciences, Av. Ibn Battouta, BP 1014 Rabat, Morocco.*
[b]*Laboratoire de Chimie Organique Appliquée, Université Sidi Mohamed Ben Abdallah, Faculté des Sciences et Techniques, Route d'Immouzzer, BP 2202 Fès, Morocco.*
[c]*Laboratoire de Spectroscopie Modélisation Moléculaire Matériaux et Environnement (LS3ME), Université Mohammed V - Faculté Des Sciences, Rabat, Maroc.*
[d]*Laboratoire de Chimie Appliquée, Ecole Nationale de l'Industrie Minérale, Agdal, Rabat, Morocco*
[e]*Moroccan Foundation for Advanced Science, Innovation and Research (MASCIR), Rabat, Morocco.*

**For correspondence: Email: fouziahlimifsr@gmail.com*

Abstract

The 1,4-benzoxazine structure has attracted considerable interest due to its wide range of biological and therapeutic properties. 1,4-Benzoxazine nucleus is present in a large number of pharmacologically active molecules described as anti-inflammatory **[1]**, antiulcer **[2]**, antipyretic **[3]**, antifungal **[4]**, and others agents **[5]**. The 1,3-dipolar cycloaddition of diarylnitrilimines on the 1,4-benzoxazine derivative led to polycyclic heterocyclic systems. The structure of the obtained cycloadducts was determined from ^{1}H-NMR and ^{13}C-NMR. Geometries optimization of all molecules considered in this study were fully optimized by using gradient corrected DFT with Becke's three-par ameter hybrid exchange functional and the *Lee-Yang-Parr* correlation functional (B3LYP) and with the 6-31G basis. A theoretical study of the synthesized products was also performed. The results are in agreement with the experimental data. The directly calculated energy of highest occupied molecular orbital EHOMO, the lowest unoccupied molecular orbital ELUMO, energy gap (ΔE) dipole moment (μ), and total electronic energy of the three isomers, are all in good agreement with the available experimental data.

Keywords: 1,3-dipolar cycloaddition, 1,4-benzoxazine, Density functional theory (DFT), Fukui function, Softness indices, Electrophilicity index.

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NOVEL AMINO ACID MODELS DERIVED FROM 1,5-BENZODIAZEPINE: SYNTHESIS OF 4-METHYL-1,3-DIHYDRO-2H-1,5-BENZOZEPIN-2-ONE

K. Dioukhane, A. Alami*, L. Gaye, H. Faraj, A. El. Hellaoui, I. Labriti, O. Karai, S. Boukhssas, S. Hajib, Y. Aouine

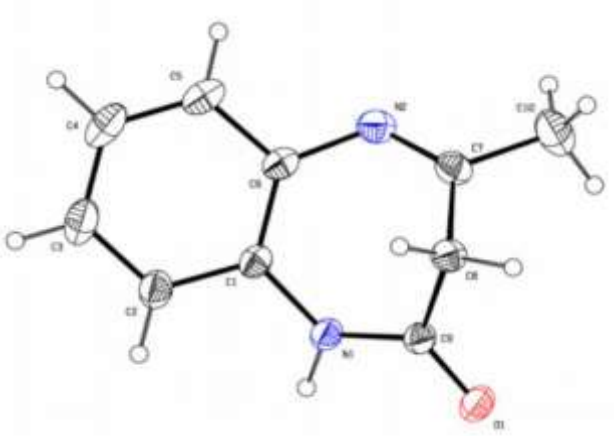
Laboratoire de Chimie Organique (LCO), Faculté des Sciences Dhar El Mahhraz, Université Sidi Mohammed Ben Abdellah ; Fès BP 1796 – Atlas, Fès, Maroc

**For correspondence: Email: alamianouar@yahoo.fr*

Abstract

Benzodiazepines have a great success due to their simplicity for synthesis, their numerous reactive sites, their efficacy, their low lethal risk in case of abuse, etc. We have especially developed an original method for synthesizing 4-methyl-1,3-dihydro-2H-1,5-benzozepin-2-one.

Benzodiazepines are among the most widely used drugs in the world **[1]** because they possess anti-convulsant, anxiolytic or hypnotic and muscle relaxant properties **[2,3]**. We have especially developed an original method for synthesizing 4-methyl-1,3-dihydro-2H-1,5-benzozepin-2-one.



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TOTAL PHENOLIC CONTENT, FLAVONOID CONCENTRATION AND ANTIOXIDANT ACTIVITIES OF LEAVES EXTRACTS OF *Vitex agnus castus L.* GROWING WILD IN MOROCCO

F. Elkamari*, A.Taroq, Y. EL Atki, I. Aouam, B. Lyoussi, A. Abdellaoui

Laboratory of Physiology Pharmacology and Environmental Health, Department of Biology, Faculty of Sciences Dhar EL Mehraz, University Sidi Mohamed Ben Abdellah, B.P. 1796, Atlas, Fez, Morocco.

*For correspondence: Email: kamarisapiens@gmail.com

Abstract

Vitex agnus-castus L. (verbanacee) commonly known as Chaste tree, is a shrub widely distributed in the Middle East and Southern Europe. Traditionally used for the treatment of several health problems and symptoms, such as premenstrual ones and spasmodic dysmenorrhea, certain menopausal conditions, insufficient lactation and acne. Several reports have been indicate that *Vitex agnus castus* contained flavonoids, diterpenoids, and essential oils. To our knowledge, no data are available on the antioxidant activities of moroccan vitex agnus castus. The aim of this work was to evaluate the antioxidant activity of four extracts from leaves of vitex agnus castus growing wild in Morocco. *In vitro* antioxidant activity, total phenolic content and total flavonoid content of different extracts (ethanol, methanol, ethyl acetate and water), were determined using spectrophotometric methods. The total phenolic content ranged from 10 ± 0.2 to 53.33± 1.38 mg Eq GAE/gDW, The total flavonoid concentrations varied from 13.66 ± 0.33 to 95.33 mg RE/gDW. Ethanolic exstract of *vitex agnus castus leaves* showed the highest phenolic and flavonoid concentration and strong antioxidant activity. Therefore, Moroccan vitex agnus castus can be regarded as promising candidates for natural plant sources of antioxidants with high value.

Keywords: Antioxidant activity; flavonoids; *vitex agnus castus L.*; phenols

SESAMUM INDICUM: EFFECT OF MINERAL STRESS ON MORPHO- PHYSIOLOGICAL PARAMETERS

S. Errai[a,*], A. Maataoui[b], H. Bezaidi[b], M. Elmidaoui[b], M. Benbella[b]

[a]*Laboratory of Physiology, Pharmacology Health and Environment Unit of Bioremediation and Environment Department of Biology, Faculty of Sciences Dhar El Mahraz, Fez – Morocco.*
[b]*National School of Agriculture, Meknes, Morocco.*

**For correspondence: Email: siham.errai1@usmba.ac.ma*

Abstract

Morocco is characterized by an aromatic and medicinal flora rich and little known. The objective of this work is to study the response of sesame (Sesamum indicum) to mineral stress. To meet this objective, a test was conducted hydroponically in a growth chamber in the Department of Agronomy in the National School of Agriculture. Seedlings were transplanted into nutrient solution with two plants per pot with a capacity of 600ml. Nutrient solutions tested corresponded to 10% (T1), 20% (T2) and 40% (T3) of the solution of Hoagland. Parameters of growth and development if the species were measured. The results showed that almost all parameters of growth and development were affected by mineral stress. The height of sesame for T1 and T2 treatments was lower than that of T3, a reduction of 81% to 70 DAS. The rate reductions in leaf area compared to the control, T1 and T2 treatments were respectively 85.05% and 69.37% (T3> T2> T1). Meanwhile, the most significant reductions of the dry matter, compared to the control 70DAS, ranged from 43.77% to 69.29% in T2 to T1. Similarly, reductions in the total solids compared to the control were 44.58% for T2 and T1 at 67.52%. for A 50DAS, allocation of dry matter to the aerial part was similar ranging from 63% for T3 to 61% for T1. Similar results were obtained by **[1,2]**. Allocated to the roots dried material was larger than that allocated to the rod.

Keywords: *Sesamum indicum*; mineral stress; hydroponics; growth; development.

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SYNTHESIS AND ANTIBACTERIAL ACTIVITY OF METHYL 1-(1-BENZAMIDO-2-METHOXY-2-OXOETHYL)PYRROLIDINE-2-CARBOXYLATE

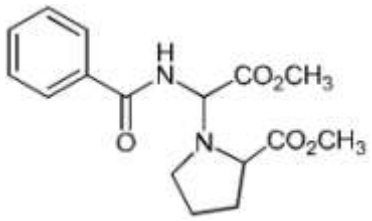
O. Karai, Y. Aouine, H. Faraj, A. Alami*, A. El Hallaoui, B. Labriti

Laboratoire de Chimie Organique, Faculté des sciences Dhar EL Mahraz, Université Sidi Mohamed Ben Abdellah, BP : 1796, Fès, Maroc.

**For correspondence: Email: alamianouar@yahoo.fr*

Abstract

Heterocyclic amino acids play a predominant role in the synthesis of peptides and proteins, since they increase the resistance of peptides to enzymatic degradation **[1]** .In addition, these building blocks and their derivatives are present in a number of potentially active against various fungal strains and many of them got wide acceptance clinical trials **[2,3]**.
We described in this communication the preparation of methyl 1-(1-benzamido-2-methoxy-2-oxoethyl)pyrrolidine-2-carboxylate. This preparation approach is based on *N*-alkylation method (Figure).



Figure

The obtained product was characterized on the basis of 1D and 2D NMR spectroscopy (^{1}H, ^{13}C) in addition to MS data and it was also tested *in vitro* for its antibacterial activity against Gram-positive and Gram-negative bacteria.

Keywords: *N*-alkylation; antibacterial activity; Heterocyclic □-amino acid.

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ARYLATION OF 5-AMINOINDOLE VIA Pd(II)-CATALYZED C-H ACTIVATION

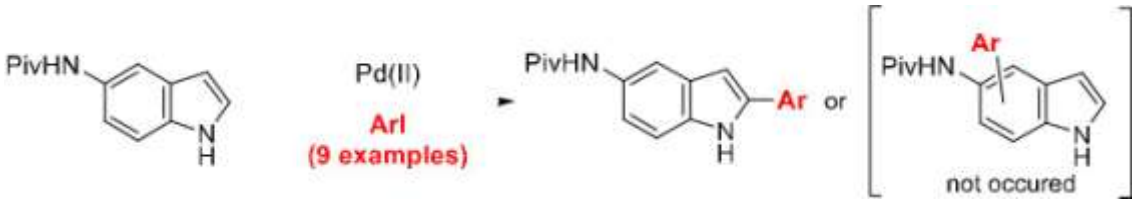
Yunus Taskesenligil[a], Haydar Kilic[b,c], Farrokh Lafzi[a], **Nurullah Saracoglu[a,*]**

[a]*Department of Chemistry, Faculty of Sciences, Atatürk University, 25240 Erzurum, Turkey*
[b]*East Anatolia High Technology Application and Research Center, Atatürk University 25240, Erzurum, Turkey*
[c]*Oltu Vocational School, Atatürk University, 25400, Erzurum, Turkey*

**For correspondence: Email: nsarac@atauni.edu.tr*

Abstract

Due to its biological significance, the indole is often considered a privileged scaffold in the drug chemistry **[1]**. Since the indole framework is a key structural feature commonly found in natural products and bioactive molecules, the indole functionalization has therefore been one of the major goals of synthetic organic chemists seeking to develop new chemical transformations **[2]**. Furthermore, indole-based ligands can easily complex into metal centers and their functions as highly efficient catalytic systems have also been reported **[3]**. In this work, an arylation of 5-aminoindole via Pd(II)-catalyzed C-H activation was investigated using iodobenzenes as aryl sources. Despite the presence of the directing group at amine, the reaction displayed the direct C2-arylation of indole in good yields and with high regioselectivity.



***Keywords*:** C-H activation; arylation; indole; Palladium; directing group.

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EFFICIENT HEAVY METAL IONS DETECTION BY PORPHYRINIC BASED CHEMOSENSORS

Nuno M.M. Moura[a,b], M. Amparo F. Faustino[a], Carlos Lodeiro[b], **M. Graça P.M.S. Neves[a,*]**

[a]*Department of Chemistry and QOPNA, University of Aveiro, Campus de Santiago, 3810-193 Aveiro, Portugal.* [b]*CentrBIOSCOPE Research Team, UCIBIO, REQUIMTE, Departamento de Química, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, 2829-516 Caparica, Portugal.*

**For correspondence: Email: gneves@ua.pt*

Abstract

Due to the high pollution levels affecting several parts of the globe, particularly those highly industrialized, monitoring efficiently the presence of metals *in situ* and on real time has become a major issue. Research on the applications of colorimetric and fluorescent sensors to be used in the recognition and sensing of a wide range of analytes has emerged as an area of considerable relevance **[1]**. These type of probes exhibit unique advantages when compared with other techniques, namely cost-effective, high stability, enable rapid, facile and real-time detection, and application in environmental, medical, and biochemical fields as well as in industry **[2]**.
The chemical and physical properties displayed by tetrapyrrolic macrocycles render them particularly attractive to be used in a wide range of fields like supramolecular chemistry, catalysis, electronic materials, sensors and medicine **[3]**. In the particular case of molecular recognition, tetrapyrrolic macrocycles have characteristics that make them unique: i) light stability and chemical reactions; ii) high absorption coefficients in the visible; iii) fluorescence emission; iv) high Stokes deviations; v) specific fingerprints that facilitate the analysis of receptor-analyte interactions, namely by UV-vis spectroscopy or fluorescence **[4]**. In this communication we will describe the synthesis of beta substituted porphyrins with different moieties through simple and efficient synthetic approaches and their sensing ability towards metal ions in solution, gas-phase and when supported in solid polymers **[5]**.

Keywords: Porphyrin, Chemosensor, Heavy metal ions, Binding studies.

Acknowledgements: Thanks are due to FCT/MEC for the financial support to the QOPNA research Unit (FCT UID/QUI/00062/2013), through national founds and when applicable co-financed by the FEDER, within the PT2020 Partnership Agreement, and also to the Portuguese NMR Network. Thanks are also due to FCT-CNRST 2017-2018 Portugal Morocco bilateral agreement and Nuno MM Moura thanks FCT for their Post-Doc scholarship SFRH/BPD/84216/2012.

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EXPERIMENTAL AND THEORETICAL TOOLS FOR CORROSION INHIBITION STUDY FOR MILD STEEL IN HYDROCHLORIC ACID MEDIUM BY NEW INDANONES DERIVATIVES

A. Saady[1,*], M.Taleb[1], K. Ismaily Alaoui[1], A. El Biache[1], A. Mahfoud[1], Ghali Alhouari[1], S. Echihi[2], B. Hammouti[3]

[1]*Laboratoire d'Ingénierie d'Electrochimie, Modélisation et d'Environnement (LIEME), Faculté des sciences/Université Sidi Mohammed Ben Abdellah, Fès, Maroc*
[2]*Laboratoire des matériaux, nanotechnologie et environnement. Faculté des Sciences, Université Mohammed V, Rabat, Ibn Battouta, BP 1014 Rabat, Maroc*
[3]*Laboratoire de chimie analytique appliquée, matériaux et environnement (LC2AME), Faculté des Sciences,*
B.P.717, 60000 Oujda, Morocco

**For correspondence: Email: Saady.asmae2014@gmail.com*

Abstract

The corrosion inhibition for mild steel in hydrochloric acid Medium by some Indanones derivatives namely 2-(4-methylbenzylidene)-3-oxo-2,3-dihydro-1Hf-indene-1-carboxylic acid (**A1**), 2-(hydroxymethylene)-3,3-dimethyl-3-oxo-2,3-dihydro-1H-indene-1-one (**A2**) and 2-
benzylidene-3-oxo-2,3-dihydro-1H-indene-1-carboxylic acid (**A3**) are evaluated experimentally using weight loss measurements, Tafel polarization and electrochemical impedance spectroscopy (EIS) techniques and theatrically using the density functional theory (DFT).
For each species we found that, the corrosion inhibitors for mild steel in HCl 1M solution are excellent: in the presence of 10^{-3} M at 303 K the efficiency of inhibition of **A1**, **A2** and **A3** are respectively in the order of 91,76% ; 87,41% and 89,93% , the Adsorption on the steel surface obeys the Langmuir isotherm and the potentiodynamic polarization studies revealed that the investigated compounds behaves as a mixed-type inhibitor. Impedance data were analyzed by equivalent electric circuit and revealed a frequency distribution of the capacitance, simulated as constant phase element. The DFT calculation (B3LYP in combination of the 6-31G (d, p) basis set) are also applied for the determination of structural parameters of A1,A2 and A3, the results of weight loss are in and were in reasonable agreement with electrochemical studies.

Keywords: corrosion inhibitor; indanones derivatives; Mild steel; hydrochloric acid; polarization; impedance; Electrochemical; DFT.

APPLICATION OF SLUDGE COMPOST IN THE FIELD FOR SUSTAINABLE DEVELOPMENT

K. Lahlou[a,*], M. Ben Abbou[b], Z. Majbar[a], M. El Haji[b], M. Taleb[a], Z. Rais[a]

[a]*Laboratory of Electrochemistry's Engineering, Modeling and Environment (LIEME), Faculty of Sciences, Université Sidi Mohamed Ben Abdellah, BP : 1796, Fès, Maroc*
[b]*Laboratory Industrial, Energy and Technology of Plastics and Composites, ENSEM- Casablanca*

**For correspondence: Email: knizaalahlou@gmail.com*

Abstract

The preservation of water resources and soil in Morocco against uncontrolled sludge storage, thus promoting the protection of public health and the environment are part of the major environmental problems that preoccupied the researchers and Moroccan authorities. In this context, we have upgraded waste water treatment plant's sludge of Fez city in the composting process by mixing them with others organic wastes conforming to the standard NFU44-095 and acting as a soil fertilizer **[1]**.
The purpose of this study is to apply sludge's compost in the field farmer's conditions for the cultivation of the potato in order to improve its nutritional quality, vegetative growth and production as well as the quality of the soil. The results were compared with the planting of the same crop in the bare soil, corrected by manure or modified by compost without sludge.
The results showed a significant increase in the parameters of vegetative growth and production compared to bare soil and manure. Nutritional quality is the same for all crops tested. Potatoes have a total carbohydrate content of 18.5 g/100 g of cooked potato, 3.4% protein and 81% starch.

Keywords: Sludge, co-compost, vegetative growth, production, food quality.

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IMPACT OF THE INDUSTRIAL EFFLUENTS OF THE DOKKARAT AREA ON UPSTREAM OF OUED FEZ AND ON THE NEARBY POPULATION

Y. Metarfi[a,*], Z. Rais[a], M. Taleb[a], K. EL Rhazi[b] A. Kherbeche[c], S. Lairini[d], F. El Madani[a]

[a]*Laboratoire d'Ingénierie d'Electrochimie, de Modélisation et d'Environnement (LIEME), Faculté des sciences, Université Sidi Mohammed Ben Abdellah, Fès, Maroc.*
[b]*Laboratoire d'Épidémiologie, Recherche Clinique et Sante Communautaire, faculté de Médecine et de Pharmacie Fès.*
Université Sidi Mohammed Ben Abdellah, Fès, Maroc.
[c]*Laboratoire de Catalyse, Matériaux et Environnement (LCME), Ecole Supérieur de Technologie-Fès, Université Sidi Mohammed Ben Abdellah, Fès, Maroc.*
[d]*Laboratoire de Bio-industrie et Technologie Agroalimentaire (LBTA), Ecole Supérieur de Technologie-Fès,*
Université Sidi Mohammed Ben Abdellah, Fès, Maroc.

**For correspondence: Email: Yousra.metarfi@yahoo.fr*

Abstract

The demographic growth of our planet is accompanied by an impressive social and economic development. Related to a large uncontrolled use of chemicals and irrational exploitation of natural resources, particularly water that is used by the majority of industries and rejected out without any treatment. This point represents a major cause of environmental degradation, and affects human health.
In this study we focused on:

T. To evaluate the quality of Oued Fez water, which crosses the Dokkarat industrial area, in order to determine concentrations of pollutants from the liquids discharged of various industries in the area of study. The majority of the industries reject out their liquids effluents in the oued without any prior treatment
U. Conduct a cross-sectional epidemiological study among the adjacent population of the area of study that uses the water of the oued in its daily activities. The data collected from the survey were processed by the SPSS software.

The results of the study reveal human, material and organizational constraints that all responsible authorities must be involved in to propose recommendations and solutions to further improve the industrial sector and protect health and environment.

Keywords: industries, toxic chemicals, water pollution, environment, human health.

SYNTHESIS AND CHARACTERIZATION OF CONDUCTING POLYMERIC NANOCOMPOSITES EMBEDED WITH NANOCLAY

Kamal .I. Aly*, Muhamed Gamal and Marwa M. Sayed

Polymer Laboratory 122, Chemistry Department, Faculty of Science, Assiut University, Assiut, 71516, Egypt

**For Correspondence: E-mail: kamalaly@aun.edu.eg*

Abstract:

A new series of polymeric nanocomposite and conducting polyarylidenecycloalkanones based on cyclalkanones moieties in the main chain were synthesized by insitu polymerization technique. Two model compounds were prepared from the reaction of each cycloalkanone monomer with benzaldehyde and their structures were determined by using single crystal x-ray diffraction. The structure of the monomers and copolymers was confirmed by elemental and spectral analyses. The resulting nanocomposites polymers were characterized by elemental and spectral analyses, beside solubility and viscometry measurements. X– ray analysis showed these polymers having high degree of crystallinity in the region $2\theta = 5 – 60°$. In addition, the morphological properties of selected examples were tested by SEM of these nanocomposites polymers were measured.

Keywords: polymeric nanocomposite; Thermal properties; nanoclay; Cycloalkanones.

*Chairman of Chemistry Department, Faculty of Sciences, Assiut University, Assiut, 71516, EGYPT.

SYNTHESIS, CHARACTERIZATION AND ANTIBACTERIAL ACTIVITY OF COMPLEXES OF ZINC (II) WITH A SERIES OF BIDENTATES HETEROCYCLIC LIGANDS: SYNTHESIZED IN ONE STEP BY PALLADIUM CATALYSIS

Amal Benzai[a,*], Fazia Derridj[a,b] , Fatiha Abdemalek[a], Rachid Touzani[c] , Henri Doucet[b]

[a]*Laboratory of Physics and Materials Chemistry (LPCM), Faculty of Sciences, UMMTO, BP 17, 15000 Tizi Ouzou, Algeria*
[b]*Laboratory of Catalysis and Organometallics, Institute of Chemical Sciences of Rennes, UMR 6226 CNRS,Campus of Beaulieu, 35042 Rennes, France.*
[c]*Laboratory of Applied Chemistry and Environment, COSTE, Faculty of Science, Mohammed Premier University,Oujda-Morocco*

**For Correspondence: Email: benz_amel@yahoo.fr*

Abstract

Compounds containing heterocycles are extremely useful in pharmacy. Indeed, more than half of the drugs currently used contain a heterocycle. Their preparation by inexpensive methods while respecting the environment (limited and non-toxic releases during synthesis) Is therefore one of the major challenges of chemistry research in the coming decades. Furthermore, the synthesis of these biaryl compounds possessing biological or physical properties is of considerable interest for the industry **[1]**.
Our work falls within this perspective. So, we have synthesized bidentate heterocyclic ligands derived from benzoxazole, in a single step by arylation of heteroarenes via activation / functionalization of C-H bonds with heteroaryl halides and palladium catalysts such as PdCl(DPPB)(C_3H_5) **[2]**. In addition, we have synthesized zinc complexes with these heterocyclic ligands derived from benzoxazole.Indeed, zinc complexes have considerable interest in the coordination chemistry due to their multiple applications in biology and catalysis. These complexes of formula, [Zn (L^{1-3})Cl_2] with the heterocyclic ligands were characterized by elemental analysis and spectral methods : (Infrared spectroscopy, proton nuclear magnetic resonance as well as carbon and electron absorption spectrography). On the basis of the data, structural models have been proposed for all synthesized complexes. Finally, the antibacterial activity of the ligands as well as that of the complexes was evaluated in vitro against different pathogenic bacteria by the diffusion method on agar. *The ligands and their zinc complexes have shown remarkable growth inhibition of bacteria especially on Escherichia coli and Staphylococcus aureus.*

Keywords: heterocycle; arylation; C-H bonds; palladium; catalysts.

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SYNTHESIS OF NEW FUSED HETEROCYCLIC RING SYSTEMS USING ISOXAZOLONES AS PRECURSOR

Rima Laroum*, Abdenour M. Redouane, Abdelmadjid Debache

Laboratoire de Synthèse de Molécules d'Intérêts Biologiques, Département de Chimie, Faculté des Sciences Exactes, Université Frères Mentouri Constantine, 25000 Constantine, Algérie

**For Correspondence: Email: laroum.rima@gmail.com*

Abstract

Multicomponent reactions (MCRs) have drawn great interest in modern organic synthesis and medicinal chemistry because they are one-pot processes bringing together three or more components and show high atom economy, high selectivity and higher yield as well **[1]**. In addition, the MCRs are easy to perform, economic, inexpensive, quick, and involve simple experimental procedures **[2]**.
The MCRs generally provide access to highly functionalized heterocyclic compounds; these compounds can be used as a basis for the design of new active molecules or the creation of a library of compounds **[3]**.
Among the wide variety of heterocycles compounds that have been explored for developing pharmaceutically important molecules, isoxazolones derivatives have played an important role **[4]**.
Therefore, in the context of multicomponent reactions we developed a new process for the synthesis of isoxazolones. The synthesized isoxazolone derivatives were then used as key intermediate for the synthesis of some new heterocycles, namely pyrazoloisoxazoles.

Keywords: Multicomponent reactions, isoxazolones, pyrazoloisoxazoles.

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THEORETICAL STUDIES ON TAUTOMERISM OF 5,5'-DIISOPROPYL-3,3'-BIPYRAZOLE

I. Bouabdallah[a,b,*], M. Rahal[c,d], T. Harit[a], A. El Hajbi[d], F. Malek[a], D. Eddike[e], M. Tillard[f]

[a]*Laboratoire de Chimie Organique, Macromoléculaire et Produit Naturels, URAC 25, Faculté des Sciences, Université Mohammed I[er], BP 524, 60 000 Oujda, Maroc.*
[b]*Équipe de Recherche en Chimie et Didactique, CRMEF - Région d'Orientale,Maroc.*
[c]*Laboratoire de Chimie Physique, Faculté des Sciences, Université Chouaib Doukkali,El Jadida, Maroc.*
[d]*CRMEF - Région Laayoune Boujdour Saguia El Hamra, Maroc.*
[e]*Laboratory of Inorganic Solid State Chemistry, University Mohammed the first, Oujda, Morocco.*
[f]*Agrégats, Interfaces, Matériaux pour l'Energie, Institut Charles Gerhardt,UMR 5253,CNRS-UM2,CC1502, Université de Montpellier 2, Sciences et Techniques du Languedoc,2 Place Eugène Bataillon, 34095 Montpellier Cedex, France.*
**For Correspondence: E-mail: bouabib2002@yahoo.fr*

Abstract

To gain a better understanding of the tautomerism of 5,5'-diisopropyl-3,3'-bipyrazole (**Figure 1**), theoretical studies were performed using the ab initio HF and DFT methods **[1]**. Several structural and molecular properties, total molecular energies, relative energetic stabilities, tautomeric equilibrium constants, kinetic parameters, Mulliken net charges and pKa values for three tautomers were calculated. Tautomer **I** presenting a large junction distance between the pyrazolic rings is the most stable. Forms **II** and **III** have respectively higher dipole moment and more acidic character.

Figure 1. Tautomeric forms for 5,5'-diisopropyl-3,3'-bipyrazole

Keywords: C,C-linked; bipyrazole; Ab initio; DFT; tautomer.

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SYNTHESIS AND STRUCTURAL DETERMINATION O NEW BENZIMIDAZOLES

M. Loughzail*, M. Adardour, A. Baouid

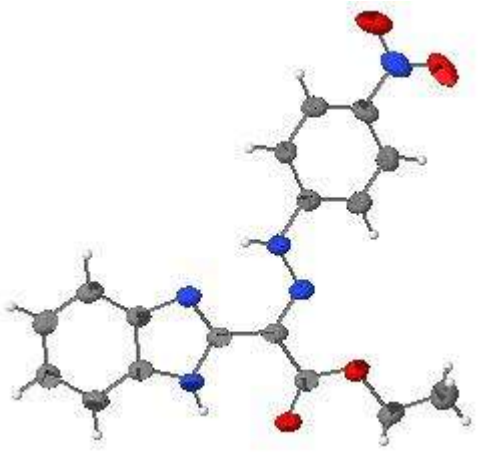
Laboratoire de Chimie Moléculaire, Equipe de Chimie des Hétérocycles et Valorisation des Extraits des Plantes, Département de Chimie, Faculté des Sciences-Semlalia, B.P 2390 40001 Marrakech, Maroc.

**For correspondence:Email: loughzail@gmail.com*

Abstract

Benzimidazole-based drugs exhibit a wide range of different biological activities as a result of changing the groups on the core structure. These biological activities include anti-cancer **[1]**, bactericidal **[2]**, fungicidal **[3]**, analgesic **[4]** and anti-viral properties **[5]**. Some have cardiovascular applications **[6]** while some derivatives have been synthesized and evaluated for inhibition of HIV-1 infectivity **[7]**.
Since the synthesis of the first benzimidazole prepared by Hoebrecker **[8]**, a number of methods have been reported for the synthesis of benzimidazole and its derivatives. These methods include the coupling of o-phenylenediamines and carboxylic acids, anhydrides, esters, amides, acid chlorides, lactones, nitriles, aldehydes… **[9]**.
In view of our interest in the development of new heterocyclic, we are pleased to report a general and simple procedure for the preparation of a series of new benzimidazoles **[10]**. Initially, we synthesize several keto-esters which are reactive with o-phenylenediamine to give ethyl 2-(1H-benzimidazol-2-yl)-2-[2-(4-nitrophenyl)hydrazinylidene]acetate and its derivatives. The structure elucidation of the benzimidazoles was determined on the basis of mass, NMR spectral data (^{1}H and ^{13}C) and confirmed by X-ray diffraction.

Keywords: Arylhydrazone, Cetones, Benzimidazole, crystal structure.



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SYNTHESIS AND EVALUATION OF NEW DERIVATIVES OF QUINOXALINE-2,3-DIONE

A. Zouitini[a,*], Y. Kandri Rodi[a,*], K. Misbahi[a], F. Ouazzani Chahdi[a], E.M.Essassi[b]

[a]*Laboratory of Applied Organic Chemistry, Faculty of Science and Technology, Sidi Mohammed Ben Abdallah University, Fez, Morocco.*
[b]*Laboratoire de Chimie Organique Hétérocyclique, URAC 21, Pôle de Compétence, Pharmacochimie, Av IbnBattouta, BP 10014, Faculté des Sciences, Université Mohammed V, Rabat, Maroc*

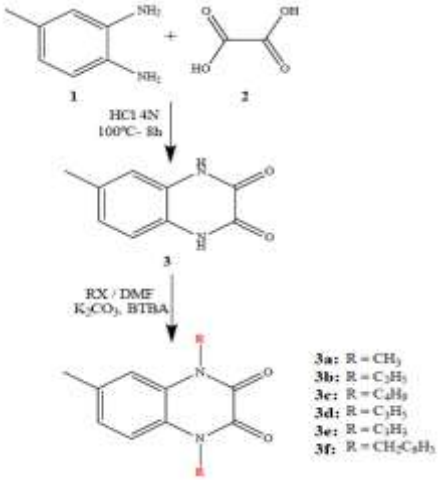
**For Correspondence: Email: ayman.zouitini@gmail.com / youssef_kandri_rodi@yahoo.fr*

Abstract

Quinoxalines are a versatile class of nitrogen containing heterocyclic compounds and they constitute useful intermediates in organic synthesis and medicinal chemistry. Quinoxaline derivatives possess a broad spectrum of biological activities including anti-bacterial **[1]**, anti-inflammatory **[2]**, anticancer **[3]**, kinase inhibitors **[4]**, antitumor **[5]**, and antidiabetic **[6]**.

The 6-methyl-1,4-dihydroquinoxaline-2,3-dione **3** was synthesized by the condensation of 4-methyl-*o*-phenylenediamine **1** with oxalic acid **2** under reflux in hydrochloric acid solution.

In order to prepare other quinoxaline-2,3-diones disubstituted Compound **3** was exposed to alkylation reactions under the conditions of phase transfer catalysis using monohalogenated agents leading to alkylated products **3a-3f**.



Keywords: quinoxaline-2,3-dione; Alkylation; *o*-phenylenediamine.

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SYNTHESIS AND CHARACTERIZATION OF NOVEL 1*H*-INDOLE-2,3-DIONE DERIVATIVES: ALKYLATION AND 1,3-DIPOLAR CYCLOADDITION

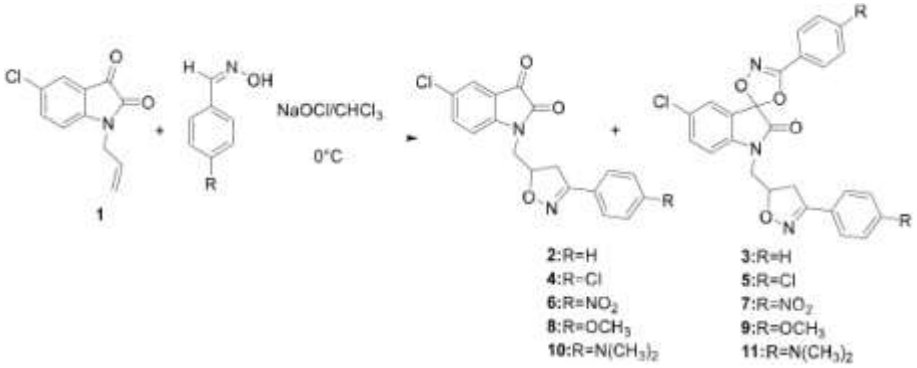
Z. Tribak[a,*], M.K. Skalli[a], O. Senhaji[b], Y. Kandri Rodi[c], A. Haoudi[a], M. Filali Baba[d], El Mokhtar Essassi[e]

[a]*Laboratory of Applied Chemistry, Sidi Mohamed Ben Abdellah University, Faculty of Science and Technology of Fes, Morocco.*
[b]*Laboratory of Applied Physical Chemistry, Moulay Ismaïl University, Faculty of Sciences and Technology of Errachidia, Morocco.*
[c]*Laboratory of Applied Organic Chemistry, Sidi Mohamed Ben Abdellah University, Faculty of Science and Technology of Fes, Morocco.*
[d]*Laboratory of Engineering, Electrochemistry, Modeling and Environment, Faculty of Sciences Dhar Mehraz, Sidi Mohamed Ben Abdellah University, B.P: 1796, Fez, Morocco*
[e]*Laboratoire de Chimie Organique Hétérocyclique, Pôle de Compétences Pharmacochimie, Mohammed V University in Rabat, BP 1014, Avenue Ibn Batouta, Rabat, Morocco*

**For Correspondence: E-mail: tribak.zineb@gmail.com*

Abstract

Isatin derivatives are endogenous natural compounds under intense development in medicinal chemistry. A wide variety of these compounds have valuable pharmacological activities. The novel 5-Chloroisatin and 5-Bromoistin derivatives were synthesized by the alkylation reaction on the nitrogen atom N, using a brominated alkylating agent in DMF under phase transfer catalysis conditions (PTC).
In order to multiply the family heterocyclic compound from 5-Chloro-1*H*-indole-2,3-dione containing isoxaline, dioxazoline and indoline via 1,3- dipolar cycloaddition reaction which is a very useful in organic synthesis and using 1-allyl-5-chloro-indole-2,3-dione as dipolarophile and aryl nitrile oxides as 1,3-dipoles. The reaction leads to the expected products with good yields and structures of various compounds are determined by the analytical techniques NMR ^{1}H, ^{13}C and X-ray crystallographic study.



Keywords: 5-Chloroisatin Alkylation; PTC; 1,3-dipolar cycloaddition; X-ray.

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DFT STUDY OF ORGANIC MOLECULES OF TYPE D-π-A BASED ON TRIPHENYLAMINE USED IN DSSC

A, Chiki[a,*], A. Touimi Benjelloun[a], S. Elkhattabi[a,b], A. Fitri, M. Bourass[a], M. Benzakour[a], M. Mcharfi[a], M. Hamidi[c], M. Bouachrine[d]

[a]*LIMME, Faculty of Sciences Dhar El Mahraz, University Sidi Mohamed BenAbdallah, Fez - Morocco.*
[b]*ENSA, University Sidi Mohammed Ben Abdellah, Fez - Morocco.*
[c]*URMM/UCTA, FST Errachidia, University Moulay Ismaïl, Errachidia - Morocco.*
[d]*ESTM, (LASMAR), University Moulay Ismaïl, Meknes - Morocco.*

**For correspondence: hamidchiki23@gmail.com*

Abstract

Recently, a lot of works has been applied in the field of dye-sensitized solar cells (DSSC).Their advent came at a time when the quest for alternative energy was high. Triphenylamine based organic dyes with D–π–A structure as sensitizer for DSSCs attain considerable attention due to their high molar absorption coefficient.
In this work, we designed eight molecules they possess the same donor group which is triphenylamine, the same acceptor group which is cyanoacrylic acid and eight different bridges. All the calculations are performed by the program Gaussian 09, using the DFT method and the TD-DFT approach. The B3LYP/6-31G (d,p) was used to calculate the energies of frontiers moleculars orbital's (EHOMO, ELUMO), and enery of gap (Egap = ELUMO-EHOMO).The CAM-B3LYP/6-31G (d,p) level was used to calculate the excitation energy (Eabs.) and the maxima of absorption wavelengths (**λ**max) in solvent. The predicted **λ**max for the eight molecules give values close to those obtained experimentally which allows us to say that these can be used as dyes in the photovoltaic cells because of their very good characters.

Keywords: Triphenylamine Derivatives, Dyes; DSSC; DFT; TD-DFT; Photovoltaic properties.

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UNDERSTANDING THE MECHANISM AND REGIOSELECTIVITY IN THE SYNTHESIS OF 1,2,3-TRIAZOLES *VIA* CuAAC REACTIONS: A DFT STUDY

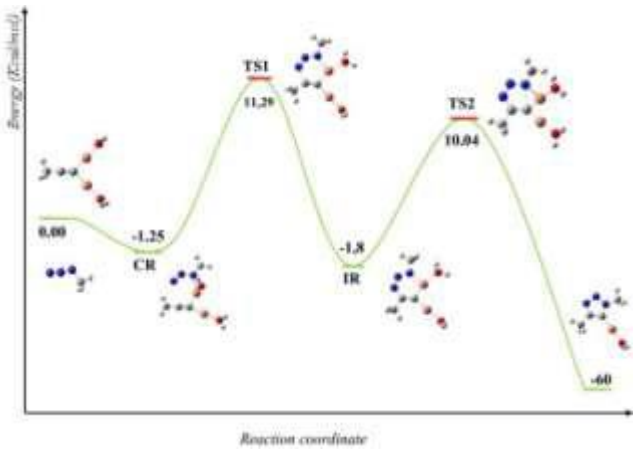
H. Ben El Ayouchia[a,*], H. Anane[a], L.R. Domingo[b], S.-E. Stiriba[a,c]

[a]*Laboratoire de Chimie Analytique et Moléculaire, Faculté Polydisciplinaire de Safi, Université Cadi Ayyad, 46030 Safi, Morocco.*
[b]*Departamento de Química Orgánica, Universidad de Valencia, C/. Dr. Moliner Nº50, 46100 Burjassot, Valencia, Spain.*
[c]*Instituto de Ciencia Molecular / ICMol, Universidad de Valencia, C/. Catedrático José Beltrán Nº2, 46980 Paterna, Valencia, Spain.*

**For correspondence: Email: belayou@gmail.com*

Abstract

In this contribution, the mechanistic pathway of the copper(I)-catalyzed azide-alkyne cycloaddition reactions has been studied by using DFT calculations in light of the latest thermodynamic and structural foundlings **[1]**. In fact, coordination of copper to the alkyne carbon atom produces a drastic change in the mechanism along the more favorable 1,4-disubstitued triazol isomer. The process is characterized by a strong nucleophile/electrophile interaction. The subsequent C2—N3 bond formation constitutes the rate-determining step in affording the triazol moiety. The analysis of the global and local electrophilicity/nucleophilicity derived from *Parr Function* allows to explain correctly the reactivity and regioselectivity of the Copper catalyzed cycloaddition **[2]**. Both catalyzed and uncatalyzed [3+2] cycloaddition reactions of azide-alkyne are going to be compared and discussed from the mechanistic and regioslectivity points of view.



***Keywords*:** Azide-alkyne cycloaddition; CuAAC; 1,4-triazoles; mechanism; regioselectivity; Parr Function, DFT.

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THEORETICAL STUDY: NEW LOW BAND-GAP CONJUGATED ORGANIC MATERIALS BASED ON INDOLINE FOR PHOTOVOLTAIC APPLICATIONS

R. Elmouhi[a,*], S. El khattabi[b], A. Touimi Benjelloun[a], M. Benzakou[a], M. Mcharfi[a], M. Hamidi[c], M. Bouachrine[d]

[a]*(ECIM), LIMME, Faculty of Sciences Dhar El Mahraz, University Sidi Mohamed Ben Abdallah, Fez Morocco*
[b]*ENSAF, University Sidi Mohamed Ben Abdallah, Fez.*
[c]*URMM/UCTA, FST Errachidia, University Moulay Ismaïl, Errachidia - Morocco*
[d]*ESTM, University Moulay Ismail, Meknes Morocco*

For Correspondence: Email: Rahma.elmouhi@usmba.ac.ma

Abstract:

Novel designed organic compounds donor-acceptor-π-acceptor (D-A-π-A) used for Bulk Heterojunction organic solar cells (BHJ) based on the heterocycles indoline compounds as a donor, were studied by density functional theory (DFT) and time-dependent DFT (TD-DFT) approaches, to shed light on how the π-conjugation order influence the performance of the solar cells. This study includes the predicting of the energy of HOMO and LUMO levels, the gap energy, the Voc (open circuit voltage) and λmax of absorption and other quantum parameters. The results show that these materials as good candidates for use in photovoltaic applications.

Keywords: Indoline; organic solar cells; TD-DFT; UV; optoelectronic properties; Voc (open circuit).

THEORETICAL INVESTIGATION OF EFFECTS OF HETEROCYCLES AS π-BRIDGES ON THE PERFORMANCES OF ALKYLAMINE-BASED ORGANIC DYES

S. El Khattabi[a,b,*], A.T. Benjelloun[a], M. Benzakour[a], M. Mcharfi[a]

[a]*Laboratoire Ingénierie des Matériaux, de Modélisation et d'Environnement, Faculté des sciences Dhar EL Mahraz, Université Sidi Mohamed Ben Abdellah, BP : 1796, Fès, Maroc.*
[b]*Laboratoire d'Ingénierie, Systèmes et Applications, Ecole Nationale des Sciences Appliquées, Université Sidi Mohamed Ben Abdellah, BP : 72, Fès, Maroc.*

**For Correspondence: E-mail: souad.elkhattabi@usmba.ac.ma*

Abstract

In this work, we were carried out theoretical study using DFT and TD-DFT calculations of a series of novel organic D-π-A dyes comprising dialkylamine as electron donor and cyanoacrylic acid group as an electron acceptor and anchoring group. The π-conjugated bridge in the designed D-π-A dyes is constituted by the heterocycles groups, such as, 3,4-ethylenedioxythiophene (EDOT) or diketopyrrolopyrrole (DPP) linked to the thiophene or to the phenyl. The HOMO, LUMO, Gap energy, λmax, and ΔGinject of these compounds have been calculated and analyzed. Specific attention has been paid at the relationship between the performances of the DSSCs and the conjugate bridge. Thus, the geometries, electronic structures and absorption properties of the photovoltaic organic dyes have been investigated in detail.

***Key words**:* Photovoltaic organic dyes, D-π-A, Dialkylamine, EDOT, DPP.

SYNTHESIS OF NOVEL IMIDAZOLE LIGANDS AND THEIR COMPLEXES AND EVALUATION OF THEIR ANTIBACTERIAL ACTIVITY

S. Slassi[a,*], M. Aarjane[a], A. El-Ghayoury[b], A. Amine[a,*]

[a]*Equipe de recherche Chimie Moléculaire et Molécules Bioactives, Faculté des Sciences – Meknès, Université Moulay Ismail, Meknès, Maroc*
[b]*Laboratoire MOLTECH Anjou, Université d'Angers, UMR 6200, CNRS, 2 Bd. Lavoisier, 49045 Angers Cedex, France*

**For Correspondence: Email: siham.slassi@gmail.com / amine_7a@yahoo.fr*

Abstract:

Coordination chemistry of Schiff bases has attracting considerable attentions of researchers in the field of chemical science as well as in medical science for their immense biological activities and bears a curious history.
Since imidazoles have been shown to exhibit interesting biological activities, this heterocyclic ring became a major source of interest for chemists to develop new imidazole derivatives and to explore their various pharmacological potentials. In another hand, Schiff bases and their metal transition complexes show a growing interest themselves due to their important role in many biological systems. It has been observed that metal ions have considerable effect on the antimicrobial activity of antibiotics. Similarly metal ions are known for their antitumor activity.
We report herein the synthesis and characterization of new Schiff bases based on imidazole moiety by condensation of salicylaldehyde and imidazole derivatives. Zn(II) and Cu(II) complexes of these ligands were also prepared and identified by crystallography. All the derivatives have been screened for their antibacterial activities against gram-positive and gram-negative multi resistant bacterial strains.

Keywords: Imidazole; Schiff base; Coordination compounds; Antibacterial activity

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CLICK CHEMISTRY FOR A FACILE SYNTHESIS OF NOVEL TRIAZOLYL DERIVATIVES OF TOTAROL

Y. Laamari[a,*], E. ID Abdelmalek[a], A. Auhmani[a], My Y. Ait Itto[a], Ab. Auhmani[a], S. Stiriba[b,c], M. Khouili[d]

[a]*Laboratoire de Synthèse Organique et Physico-Chimie Moléculaire, Département de Chimie, Faculté des Sciences, Semlalia, Université Cadi-Ayyad, B.P 2390, Marrakech 40001, Maroc,*
[b]*Equipe de Chimie Moléculaire, Matériaux et Modélisation, Faculté Poly-disciplinaire, Université Cadi Ayyad, BP 4162, 46000 Safi, Morocco*
[c]*Instituto de CienciaMolecular/ICMol, Universidad de Valencia, C/. Catedrático José Beltrán, 2, 46980 Paterna, Valencia, Spain*
[d]*Laboratoire de Chimie Organique et Analytique, Faculté des Sciences et Techniques Béni-Mellal, Université Sultan Moulay Slimane, B.P. 523, 23000 Béni-Mellal Maroc.*

**For correspondence: Email: yassine.laamari@edu.uca.ac.ma*

Abstract

Click chemistry of natural products has acquired a great reputation in recent years for the development of bioactive natural product analogs. Some of the molecules studied include alkaloids **[1]**, coumarins **[2]**, saponins **[3]**, steroids **[4]** and triterpenes **[5]**. Triazoles and their derivatives have a great importance in medicinal chemistry and can be used for the synthesis of numerous heterocyclic compounds with different biological activities such as antiviral, antibacterial, antifungal, anti-tuberculosis, anticonvulsant, antidepressant, anti-inflammatory,antineoplastic and anticancer **[6,7]**. Thus, the design and synthesis of novel triazole derivatives is the prospective direction for the development of novel anticancer agents with better curative effect, lower toxicity as well as higher selectivity.
Based on the above cited findings and inspiration from the potential anticancer activities of triazoles, we approached this work to synthesize novel triazolyl derivatives by using Totarolas starting material. All the structures ofnewly synthesized compounds were confirmed by ^{1}H and ^{13}C NMR.

Keywords: Click Chemistry; Totarolas; Triazoles

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INHIBITIVE EFFECT OF 5-CHLORO-10-THIA1,8-DIAZATRICYCLO [7.5.0.0$^{2.7}$] TETRADECA-2, 4, 6, 8-TETRAENE ON CORROSION OF CARBON STEEL IN 0.5 M H_2SO_4 AT 35°C

M. Driouch[a,*], N. Achnine[a], E. Elassiri[a], M. Beniken[a], M. Sfaira[a], M. Benzakour[a], M. Ebn Touhami[b]

[a]*Laboratoire d'Ingénierie des Matériaux, de Modélisation et d'Environnement (LIMME), Faculté des Sciences, Université Sidi Mohammed Ben Abdellah, USMBA, B.P. 1796–30000, Atlas – Fès, Morocco.*
[b]*Laboratoire d'Ingénierie des Matériaux et Environnement : Modélisation et Application (LIMEMA), Faculté des Sciences, Université Ibn Tofaïl, B.P. 133–14000, Kénitra, Morocco.*

**For Correspondence: E-mail: majid.driouch.fsdm@gmail.com*

Abstract

The inhibiting action of mercaptobenzimidazole derivative namely [***5-chloro-10-thia1,8-diazatricyclo [7.5.0.0$^{2.7}$] tetradeca-2, 4, 6, 8-tetraene***] (DMBI) carbon steel in 0.5M Sulfuric acid solution at 35°C, has been studied by a series of known techniques such potentiodynamic polarization (Tafel, Stern & Geary) and electrochemical impedance spectroscopy (EIS). The results obtained from different techniques were in good agreement. This result showed that this organic compound revealed a good corrosion inhibition and that the inhibition efficiency is increased with the inhibitor concentration reaching circa 90 % at 10^{-3} mol $L^{-1}$of (DMBI) . Potentiodynamic polarization suggested that it is a mixed type of inhibitor. Two time constants determined by the charge-transfer and the adsorption of the inhibitor, respectively, can be readily outlined. The adsorption of DMBI on the carbon steel surface, in 0.5M H_2SO_4 solution, obeyed to the Langmuir isotherm with a very high negative value of the standard Gibbs free energy of adsorption $\Delta G°ads$ (chemisorption).

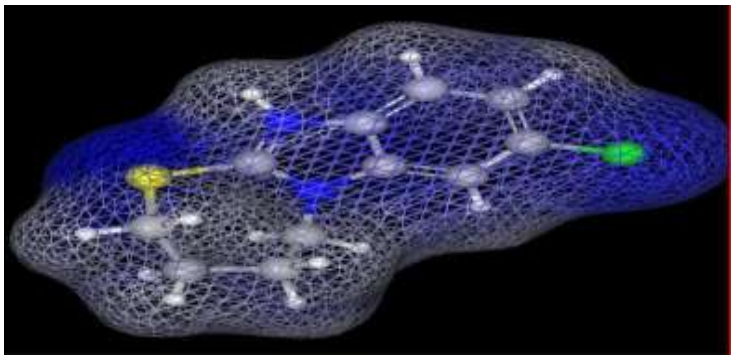

Figure : Structure of The 5-chloro-10-thia1,8-diazatricyclo [7.5.0.0$^{2.7}$] tetradeca-2, 4, 6, 8-tetraene

Keywords: Benzimidazole; Carbon steel; Acid corrosion; Corrosion Inhibition; Stern & Geary.

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EXTRACTION, CHARACTERIZATION AND INVESTIGATION OF ESSENTIAL OIL FROM ORANGE ZEST AS ECO-FRIENDLY CORROSION INHIBITOR FOR MILD STEEL IN ACIDIC SOLUTION

Z. Bensouda[a,*], M. Sfaira[a], A. Farah[b], M. Ebn Touhami[c]

[a]Laboratory of Engineering Materials, Modeling and Environment, University of Sidi Mohamed Ben Abdellah USMBA – Fez, Faculty of Sciences, B.P 1796, Fez, Atlas, Morocco.
[b]Laboratory of Applied Organic Chemistry, University of Sidi Mohamed Ben Abdellah USMBA – Fez, Faculty of Sciences and Technology. Route Immouzer Fez, Morocco.
[c]Laboratory of Electrochemistry, Corrosion and Environment, Ibn Tofail University, Faculty of Sciences - Kenitra, BP 133,14000, Morocco.

**For correspondence: Email: bensouda@yahoo.com*

Abstract

Current research efforts now focus on the development of the novel, cheaper, nontoxic, highly efficient and eco-friendly corrosion inhibitors as alternatives to different inorganic and organic compounds. In this context, Orange Zest Essential Oil denoted hereafter (OZEO) was investigated as an eco-friendly corrosion inhibitor for mild steel in 1M HCl medium utilizing different techniques such as Gas Chromatography-Mass Spectrometry (GC-MS), weight loss, electrochemical and Scanning Electron Microscope (SEM) associated with energy dispersive X-ray spectroscopy (EDX). The obtained results indicated that this essential oil acts as an eco-friendly efficient corrosion inhibitor for mild steel in 1 M HCl and the inhibition efficiency reach up to 75% at 2.5 g $L^{-1}$of OZEO. The electrochemical techniques revealed that OZEO acted as mixed inhibitor with a predominantly anodic action, facilitating the formation of an adsorbed film over the mild steel surface. The adsorption obeyed to Langmuir adsorption isotherm indicating monolayer adsorption and involved physisorption character. SEM examination and EDX analysis of the mild steel surface confirmed the existence of a protective adsorbed film.

***Keywords*:** Eco-friendly corrosion inhibitor; Essential oil; GC-MS; SEM; EDX, Adsorption.

NEW GREEN SYNTHESIS OF 1.8-DIOXODECAHYDROACRIDINE DERIVATIVES AND POLYHYDROQUINOLINES, VIA TWO NATURAL CATALYSTS IN A SOLVENT-FREE MEDIUM

I. Sehout*, A. Debache

Laboratory synthesis of molecules of biological interest, Department of Chemistry; Faculty of exact science; University of Constantine 1, Constantine, Algeria, 25000

**For correspondence: Email: sehoutimene@yahoo.fr*

Abstract

Requirements of modern chemistry, including the development of new synthesis with new secure, economic and environmentally protocols guide us to the field of green chemistry **[1]**. The development of solvent-free organic synthetic methods has become an important research area, aiming to save energy and to prevent hazardous solvent waste and toxicity in chemical processes. On the other hand, the catalyst is the most important factor in organic synthesis for its important role in a reaction by its presence or by its intervention. Green chemistry has allowed the emergence of new horizons in the field of catalysis; it is now the ninth principle of green chemistry. Several green methods were applied as microwave, ultrasound, ionic liquids **[2]**, nanoparticles. On our part we have contributed to this effect by the development of two new natural catalysts, inexpensive, non-toxic and very available, which are ascorbic acid and acetyl salicylic acid.

We applied our two new natural catalysts in the Hantzsch reaction, which is a multicomponent reaction; it is considered as a green reaction, by the fact they generate in record time and with good yields molecular structures with great complexity. The achieved results are remarkable, we could synthesize a range of 1.8-dioxodecahydroacridine derivatives (6), and polyhydroquinolines (7) with yields ranging between (47-99) % in the time range from (1.5-6) hours, we also enriched the bibliography molecules by synthesis of authentic molecules.

Keywords: Hantzsch reaction; green synthesis; solvent free medium; ascorbic acid and acetyl salicylic acid.

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PALLADIUM-CATALYZED REGIOSELECTIVE DIRECT C-H ARYLATION OF PYRAZOLO [3,4-D]PYRIMIDINES

Mohamed El Hafi[a,b,*], Mohammed Naas[a,b], Mohammed Loubidi[b], Jabrane Jouha[b], Youssef Ramli[c], Joel T Mague[d], El Mokhtar Essassi[a], and Gérald Guillaumet[b]

[a]*Laboratoire de Chimie Organique Hétérocyclique URAC 21, Pôle de Compétences Pharmacochimie, Mohammed. V University in Rabat BP 1014, Avenue Ibn Batouta, Rabat, Morocco*
[b]*Institut de Chimie Organique et Analytique, Université d'Orléans, UMR CNRS 7311, BP 6759, 45067 Orléans Cedex 2, France*
[c]*Laboratoire de Chimie Thérapeutique, Faculté de Médecine et de Pharmacie, Mohammed V University in Rabat BP 6203, Avenue Mohamed Belarbi El Alaoui, Rabat, Morocco.*
[d]*Departement of Chemistry, Tulane University, New Orleans, LA 70118, USA*

**For Correspondence: E-mail address: elhafi.mohamed1@gmail.com*

Abstract

Nitrogenous bicycles are an apparently endless field of organic and biological research. In this study we disclose an efficient pathway to the synthesis of the pyrazolo [3,4-*d*] pyrimidine scaffold in three steps from allopurinol. This key intermediate was engaged in the first example of regioselective C-H arylation catalyzed by palladium to access a library of 3-substituted-1-methyl-4-phenyl-1*H*-pyrazolo[3,4-*d*]pyrimidines.

Keywords: Nitrogenous bicycles; 1*H*-pyrazolo [3,4-*d*] pyrimidines; C–H arylation; regioselectivity; 1,10-Phenanthroline; Palladium.

1,4-DIHYDROPYRIDINE SYNTHESIS UNDER THE GREEN REACTION CONDITIONS

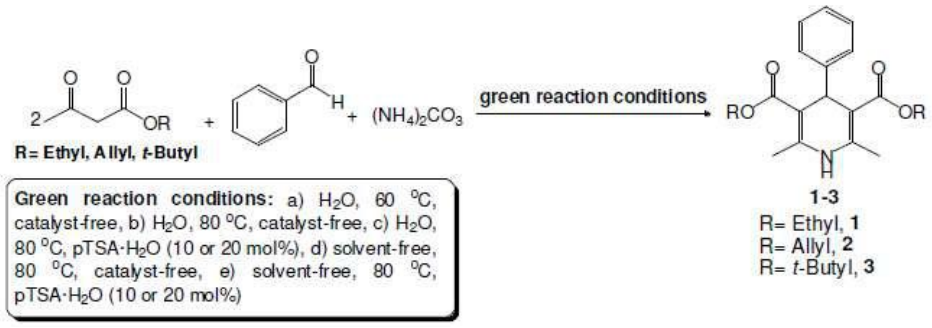
Ş. Gülten*, Ö. Ergin

Çanakkale Onsekiz Mart University, Faculty of Arts and Sciences, Department of Chemistry 17020 Çanakkale, Turkey

**For Correspondence: Email: sgulten@comu.edu.tr / siringulten@hotmail.com*

Abstract

1,4-Dihydropyridines (1,4-DHPs) are class of *N*-containing heterocycles having a six membered ring generated via multicomponent Hantzsch reaction in 1882. 1,4-DHP derivatives exhibit a wide range of biological activities such as antihypertensive, anti-inflammatory, antianxiety, vasodilation, analgesic, neuprotectant, bronchodilation, anticonvulsant, antidepresant and antitumor. 4-Aryl-1,4-DHPs are used in the treatment of hypertansion and cardiovascular diseases as a calcium channel blockers **[1-3]**.
In the our work, green chemistry conditions such as water/catalyst-free, water/pTSA·H_2O catalyst, water-free/catalyst-free and water-free/pTSA·H_2O catalyst were applied to synthesis of one-pot four-component Hantzsch reaction. Three 1,4-DHP derivatives from benzaldehyde, β-keto ester (ethyl acetoacetate, allyl acetoacetate and *t*-butyl acetoacetate) and ammonium carbonate were prepared efficiently under the green reaction conditions. Our procedures are simple and environmentally friendly, pTSA·H_2O is commercially available and inexpensive **[1-3]**. The synthesized compounds were confirmed by IR, ^{1}H-NMR and ^{13}C-NMR analyses.



Keywords: 1,4-Dihydropyridine; 1,4-DHP; Hantzsch Synthesis; Green reaction; pTSA.

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SYNTHESIS OF NEW [1,6]-NAPHTHYRIDINONES HETERCOCYCLIC SCARFFOLDS VIA MULTICOMPONENT REACTION

N. Mehiaoui*, Z. Kibou, M. Benabdallah, N. Choukchou-Braham

Laboratoire de Catalyse et Synthèse en Chimie Organique, Université de Tlemcen, B.P.119, 13000 Tlemcen, Algérie

For correspondence: Email: mehiaoui.nawel@gmail.com

Abstract

The nitrogenous compounds including the [1,6]-naphthyridinones are an important structural unit found in many natural compounds with biological and pharmaceutical activity **[1].** There are many literature sources describe numerous synthetic approaches lead to this compounds **[2].**
The present work report an efficient one-pot multicomponent synthesis of new substituted[1,6]-Naphthyridinones (Fig.1) under solvent-free conditions, in good yields.

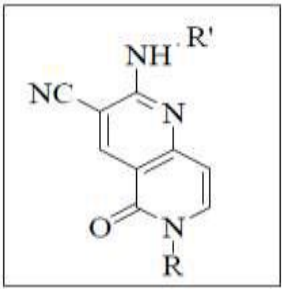

Figure 1: Structure of [1,6]-Naphthyridinones

Keywords: [1,6]-naphthyridinones; 2-pyridones; 2-aminopyridines; one-pot reaction; solvent-free reaction.

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SYNTHESIS OF XANTHONE DERIVATIVES BASED ON MARINE NATURAL MODELS WITH PROMISING BIOLOGICAL ACTIVITIES

Diana I. S. P. Resende[a,b], Emília Sousa[a,b], Madalena M. M. Pinto[a,b,*]

[a]*Laboratory of Organic and Pharmaceutical Chemistry, Faculty of Pharmaceutical Sciences, University of Porto, Porto, Portugal.*
[b]*Interdisciplinary Centre of Marine and Environmental Research (CIIMAR), Matosinhos, Portugal.*

**For correspondence: Email: madalena@ff.up.pt*

Abstract

Nature has been an important source of medicinal products for millennia, with many useful drugs developed from terrestrial and marine sources. Due to the development of new techniques and methodologies (sampling techniques, established culture methods, genome mining, etc.) marine organisms have been heavily sampled in the last two decades, and have become an important source of secondary active metabolites working as raw materials or models for interesting pharmacologically active compounds **[1]**.

Herein, we present a new methodology towards the synthesis of halogenated xanthone derivatives based on marine natural models. Our approach involves the synthesis of the xanthone scaffold via benzophenone intermediate **[2]**, followed by halogenation. The synthesized compounds had been screened for antibacterial activity with very encouraging results. Synthetic details as well as structure characterization (by 1D and 2D NMR studies) of the new synthesized compounds will be presented and discussed.

Keywords: xanthone; marine; halogenation.

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AN UNUSUAL REARRANGEMENT OF 5,5-FUSED RING SYSTEM INTO 5,6-BICYCLE

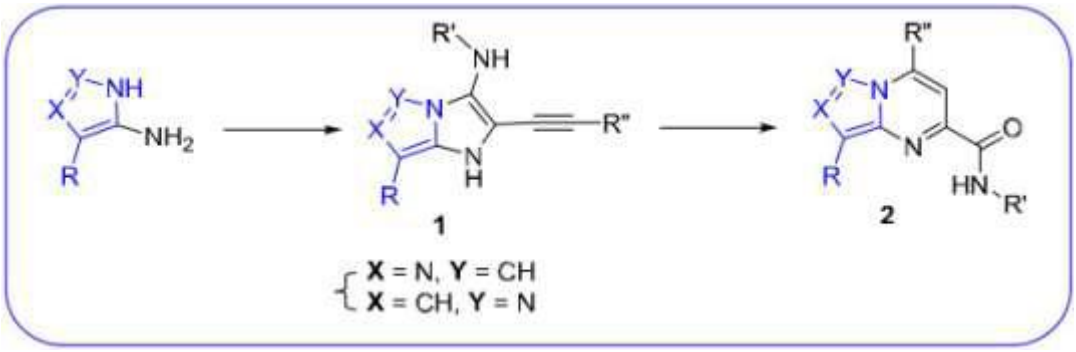
K. Gambouz[a,b,c,*], M. Loubidi[a,c] , Z. Tber[c], M. Driowya[c], S. El Kazzouli[b], M. Akssira[a], G. Guillaumet[c]

[a]*Laboratoire de Chimie Physique et Chimie Bioorganique URAC 22 FSTM Université Hassan II – Casablanca – Maroc.*
[b]*Faculté Euromed de Génie, Université Euro-Méditerranéenne de Fès –route de Meknès, Fès – Maroc*
[c]*Institut de Chimie Organique et Analytique, Université d'Orléans, UMR cnrs 7311, Orléans – France.*

For Correspondence: Email: gambouzkhadija@gmail.com

Abstract

Imidazo[1,5-a]pyrimidines or pyrazolo[1,5-a]pyrimidines are potent medicinal scaffolds that exhibit a large spectrum of biological activities concerning mainly the treatment of many widespread diseases such as leukemia **[1]**, Parkinson's disease, Gaucher's disease, schizophrenia **[2]** to name a few.



The multicomponent reaction of aldehydes, imidazoles or pyrazoles and isocyanides led us to a low-cost library of compounds **1**. These latter are engaged in a rearrangement in presence of iodine and tetrahydrofuran at room temperature to give derivatives 2 with different propargyl aldehydes on the one hand and with 1H-imidazo[1,2-b]pyrazole on the other.

In this poster communication we will describe the synthesis of this molecular rearrangement of **1** to afford **2**.

Keywords: imidazole, pyrazole, rearrangement, multicomponent reaction.

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ENANTIOSELECTIVE SYNTHESIS OF 4-PIPERIDONE

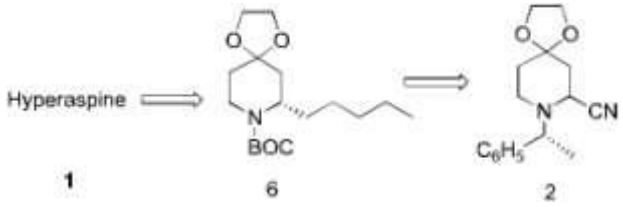
Fadila Louafi[a,*], Van Ha Vu[b], Jean Pierre Hurvois[b], Nicolas Girard[c], Ronan Marion[b]

[a]*Frères Mentouri Constantine University, Route Ain el bey, Constantine, Algeria*
[b]*Sciences Chimiques de Rennes, UMR 6226, CNRS−Université de Rennes 1,2 Avenue Leon Bernard, 35043 Rennes Cedex, France*
[c]*Faculté de Pharmacie, Université de Strasbourg UMR 7200 CNRS/UDS, 74 Route du Rhin, 67401 Illkirch Graffenstaden, France*

**For Correspondence: E-mail:* falouafi@umc.edu.dz

Abstract

Piperidine derivatives are part of a large group of substances that are found in Nature and in pharmaceuticals **[1]**. As a result of their various biological properties, these compounds and their structural analogues have been the subject of numerous synthetic approaches devoted to the construction of their heterocyclic core **[2]**.



Scheme 1

Our interest in the development of new methodology for the stereoselective synthesis of hyperaspine **1 [3]**. Our approach was based on the elaboration of α-amino nitrile 2, which was prepared by electrochemical means. The final stereochemical approach was to use Beak's lithiation-alkylation sequence of 4-piperidone (−)-6 to control the trans or the cis relationship between the α and the α′-substituents **[4]**. The main results of this synthesis will be presented.

Keywords: piperidine; alkylation; 4-piperidone; stereoselective synthesis.

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REACTIONS OF SPIRO-INDOLENINES WITH NUCLEOPHILES

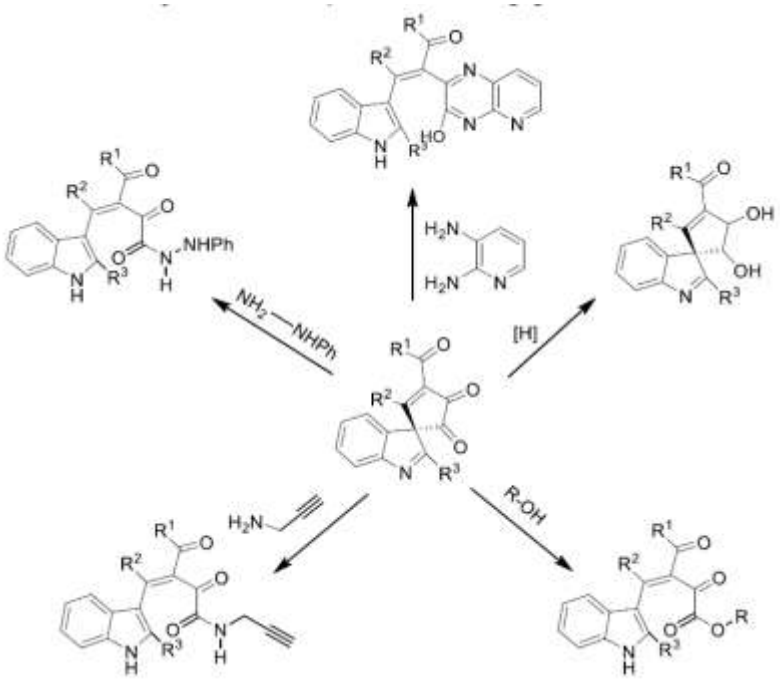
M. Tan*, N. Mengeş, B. Kuzu

Yuzuncu Yil University, Faculty of Pharmacy, 65080, Van, Turkey

**For Correspondence: Email: meltemtan@yyu.edu.tr*

Abstract

Alkaloids are natural products that are essential for the life of living organisms and defined as an important group of compounds with biological, pharmacological, psychological and chemical activity. Also spirocyclic alkaloids are important heterocyclic molecules found in nature. Spirocyclic alkaloids are composed of many different heterocyclic rings and also spirocyclic alkaloids containing indole are quite common **[1]**.



Scheme 1. Reactions of spiro-structured molecules with nucleophiles.

This work has developed a method for the synthesis of novel spiro indolenine compounds. The reaction of spiro-structured molecules with important nucleophiles has been investigated **[2]**.

Keywords: Alkaloid; spirocyclic alkaloid; spiroindolenine.

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SYNTHESIS AND CHARACTERIZATION OF IONIC LIQUIDS BASED ON ALKYL-SUBSTITUTED THIABENDAZOLIUM

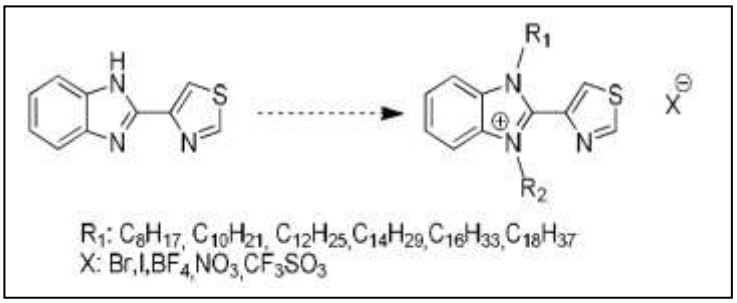
K. EL Bourakadi[a,b,*], M.E.M. Mekhzoum[a], E.M. Essassi[a,b], A. Qaiss[a], R. Bouhfid[a]

[a]*Moroccan Foundation Advanced Science, Innovation and Research (MAScIR), NANOTECH, Rue Mohamed Al Jazouli Madinat Al Irfane Rabat, Morocco.*
[b]*Laboratoire de Chimie Organique Hétérocyclique, URAC 21, Pôle de Compétence Pharmacochimie, Av Ibn Battouta, BP 1014, Faculté des Sciences, Mohammed V University, Rabat, Morocco*.

**For correspondence: Email: khadijaelbourakadi16@gmail.com*

Abstract

Ionic liquids are defined as organic salts, mostly consisting of organic cations and inorganic anions having a melting point of less than 100° C. In recent years, the research on ionic liquids continues to be dominated in different areas due to their unusual reactivity in synthetic and their various applications **[1]**. They have been used as solvents **[2]** and heat transfer media **[3]**. In addition, thiabendazolium have also been used as fungicides in agriculture **[4]**. In this work, we have been interested in synthesizing new ionic liquids using thiabendazole moiety as precursor molecule in order to evaluate their thermal and biological activities. The synthesis of the compounds is shown in the scheme below.



Keywords: thiabendazolium; ionic liquid; anion metathesis; melting point.

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STUDY OF THE COMPLEMENTATION OF THE GLICLAZIDE MOLECULE WITH THE TRANSITION METALS

M.Loukili[1,2,*], A. Moussaif[1,*], Y.Ramli[3], N.Bentaleb[1] and EM. Essassi[2]

[1]National Center of Energy, Sciences and Nuclear Techniques, Rabat, Morocco
[2]Laboratory of Heterocyclic Organic Chemistry, Mohammed V University, Rabat, Morocco
[3]Medicinal Chemistry Laboratory, Faculty of Medicine and Pharmacy, Mohammed V University, Rabat, Morocco

For correspondence: Email: loukili@cnesten.org.ma / a.moussaif@cnesten.org.ma

Abstract

Gliclazide is a molecule that belongs to the family of sulfonylureas, also known as hypoglycemic sulfonamides. These are antidiabetics used in the treatment of type 2 diabetes. Their mechanism of action is based on stimulation of the pancreas in order to increase the release of insulin. Like any drug, Gliclazide is likely to cause some undesirable effects, among them a possible iron deficiency anemia considered the most common form of anemia. It is characterized by a decrease in the level of hemoglobin in the blood following a lack or a bad fixation of the iron in the organism.
The purpose of our study is to determine whether Gliclazide complexes the iron molecule, thus preventing its fixation by the organism or if it's complex other elements such as Magnesium, Calcium or Potassium thus indirectly influencing the fixation of iron. We are also called to establish an approach to remedy this complementation while preserving the therapeutic specificities of the molecule.

Keywords: Gliclazide, complexation, transition metals, coordination chemistry

NOVEL 2-MERCAPTOBENZIMIDAZOLE DERIVATIVES: SYNTHESIS AND EVALUATION OF ITS ANTIBACTERIAL AND ANTIOXIDANT ACTIVITIES

Latifa El Ouasif[1], Abdelhakim Bouyahya[2], Rachid Zniber[1], Mostafa El Ghoul[1], Redouane Achour[1], Hind Chakchak[3], Ahmed Talbaoui[2], Houria El Boury[2], Nadia Dakka[2] and Youssef Bakri[2]

[1]*Laboratory of Organic Heterocyclic Chemistry, (URAC 21) Pole of Competence Pharmacochemistry, Mohamme d V University, Faculty of Science, Ibn Battuta Avenue BP 1014 RP, Rabat, Morocco*
[2]*Biochemistry-Immunology Laboratory, Mohamed V University, Faculty of Science, Ibn Battuta Avenue BP 1014 RP, Rabat, Morocco*
[3]*National Centre for Scientific and Technical Research, Rabat, Morocco*

Abstract

In the present study, a series of novel 2-mercaptobenzimidazolium were synthesized. These compounds can be prepared by condensation of 2-mercaptobenzimidazole with the various alkylating agents under the conditions of phase transfer catalysis, followed by a quaternization. The newly synthesized compounds were subjected to in vitro biological evaluation. The antibacterial activity was evaluated with diffusion assay and optical density method. The antioxidant activity was carried out using DPPH free radical scavenging assay. The result indicated that some compounds show convincing antibacterial activities against two microorganisms: *Escherichia coli* and *Staphylococcus aureus.* While these molecules have not shown any interesting antioxidant effects.

Keywords: 2-mercaptobenzimidazole; 2-mercaptobenzimidazolium; Antibacterial activity; Antioxidant activity.

MICHAEL ADDITION OF NITROGEN-HETEROCYCLES ON CHALCONES TOWARDS B-HETEROARYLATED (C–N BOND)

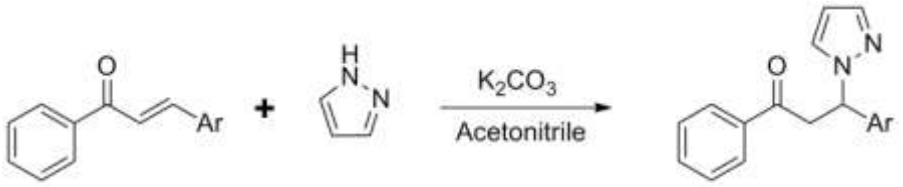
M. Chalkha[a], M. Bakhouch[a], A. Mahfoud[a], M. Akhazzane[b], G. Al Houari[a], M. Daoudi[a], M. El Yazidi[a,*]

[a]*Laboratoire de Chimie Organique, Université Sidi Mohamed Ben Abdellah, Faculté des sciences Dhar EL Mahraz, BP: 1796, Fès, Maroc.*
[b]*Cité de l'innovation, Université Sidi Mohamed Ben Abdellah, Fès.*

**For correspondence: E-mail: elyazidimohamed@hotmail.fr*

Abstract

Nitrogen-containing heteroarenes are often found in various natural products, materials and biologically active compounds of pharmaceutical interest **[1]**. Obviously, development of simple and efficient processes to N-heteroarenes has always attracted considerable attention **[2,3]**.
The most preferred and atom-efficient strategy is the conjugate addition of NH-bearing nucleophiles to activated α,β-unsaturated ketones **[4,5]**.
this study was dealed to the exploration of this strategy to N-bearing heterocycles involving intramolecular conjugate addition of the heteroatom to α,β-unsaturated carbonyls.
The structures of the prepared compounds were determinate by spectroscopic methods: ^{1}H-NMR, ^{13}C-NMR, FT-IR.



Ar = C_6H_5 , p(Me)C_6H_4 , p(MeO)C_6H_4 , p(Cl)C_6H_4

***Keywords**:* heteroarenes; chalcones; Michael addition; NMR.

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FINE-TUNING OF THE MEDICINAL PROPERTIES OF GINGEROL BY INCLUSION INTO GAMMA-CYCLODEXTRIN

S. S Braga*, J. M. Pais, B. F. Pereira, S. M. Cardoso

QOPNA research unit, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal.

**For correspondence: Email: sbraga@ua.pt*

Abstract

Gingerols comprise a series of bioactive compounds isolated from ginger rhizomes. The most abundant are 6-gingerol, 8-gingerol and 10-gingerol. In the present work, these compounds were extracted from fresh ginger by maceration with acetone and purified using chromatographic methods. The gingerols were subsequently encapsulated into gamma-cyclodextrin to afford a microcrystalline product. Solid-state characterization of the encapsulated gingerols was carried out by microanalysis, FT-IR, powder X-ray diffraction and thermogravimetry, showing the formation of a stable complex with channel-packing, a typical structural feature for gamma-cyclodextrin inclusion complexes in the solid state **[1]**. The anti-oxidant activity of gingerols, measured by the ABTS assay, was slightly superior to that of the reference (trolox), remaining practically unchanged after encapsulation; in turn, the No scavenging ability of gingerols was found to be low compared to the reference, ascorbic acid, having a slight increase with encapsulation. The most relevant action of gingerols, both free and encapsulated, was the inhibition of the inflammatory enzyme 5-lipooxygenase, with an activity 2-3 times higher than that of ascorbic acid.

Keywords: Ginger extract, gingerols, gamma-cyclodextrin, inclusion complexation, *in vitro* biological evaluation.

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EFFECT OF TEMPERATURE AND TIME ON THE ANTICORROSIVE POWER OF A NEW SCHIFF BASE MOLECULE ON MILD STEEL IN ACIDIC MEDIUM

Imene Benmahammed[1,*], Tahar Douadi[2], Saifi Issaadi[3]

[1,2]*Laboratoire d'Electrochimie des Matériaux Moléculaires et Complexes LEMMC, Département de Génie des Procédés, Faculté de Technologie, Université Ferhat Abbas Sétif-1, Algérie.*
[3]*Faculté des sciences, département de Chimie, Université Ferhat Abbas Sétif-1, Algérie.*

**For Correspondence: Email: imene.benmahammed@yahoo.fr*

Abstract

Corrosion of a material is its degradation; it can have mechanical causes such as friction or chemical causes. To remedy to this problem, we use inhibitors as a mean to combat corrosion. Heterocyclic compounds with various substituents are considered to be the effective corrosion inhibitors for metals in acid media **[1–6]**.
The first step in the mechanism of action of an inhibitor in acid solutions is the adsorption of organic molecule on metal. Adsorption depends mainly on the nature and external load of metal, the chemical structure of the molecule, the type of aggressive electrolyte and the temperature of the corrosion reaction.
In this context, we are interested in the study of electrochemical inhibition of corrosion of mild steel which is the metal most used commonly in industrial applications due to its excellent mechanical properties and low cost in hydrochloric acid HCl 1 M, by addition of various concentrations of a new schiff base molecule an interval of temperature ranging from 25 to 55°C after 30 minutes of immersion time in order to evaluate the influence of this factor on inhibitory power of the schiff base compound. From the results of the polarization curves, the increase in temperature causes an increase in the values of the corrosion current density (i_{corr}) in the entire field of temperature (25-35-45-55°C), even in the corrosive medium alone (HCl 1 M) confirming a growing metal dissolution.This increase in the presence of inhibitors is lower than in the control. These results confirm that the studied compound inhibits corrosion in the temperature range studied.
Using the method of weight reduction, we have studied the evolution of the corrosion rate and the inhibitory efficacy at different immersion time (16 h, 24 h, 48 h and 72 h) at 25°C in the aggressive environment HCl 1 M in absence and in presence of inhibitor, which allowed us to have important notions about the stability of the film thus formed during the phenomenon of inhibition. The rate of corrosion of mild steel XC48 and inhibitory efficiency of the compound studied vary slightly with the immersion time. This behavior may be linked to the strong adsorption and the formation of a film on the metal surface.

Keywords: Corrosion, immersion time, inhibitor, mild steel, schiff base, temperature.

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IMPROVEMENT OF CELLULASES ENZYMES ACTIVITY PRODUCED BY YEAST THE GENUS TRICHOSPORON

H. Toujer[1,3,*], N. Benchemsi[2], M. Ettayebi[3], A. Janati Idrissi[3], H. Bekkari[1,3]

[1]Sidi Mohamed Ben Abdellah University, Faculty of Sciences Dhar El Mahraz, Laboratory of Biotechnology, PO Box 1796, 30003 Fez-Atlas, Morocco.
[2]Sidi Mohamed Ben Abdellah University, Faculty of Sciences & Techniques Saiss, Laboratory of Ecology and environment, PO Box 1796, 30000 Fez, Morocco.
[3]Sidi Mohamed Ben Abdellah University, Faculty of Sciences Dhar El Mahraz, Biodiversity, Bioenergy and Environment Research Group (BBE), PO Box 1796, 30003 Fez-Atlas, Morocco.

**For correspondence: Email: hananetou@gmail.com*

Abstract

The lignocellulose saccharification into fermentable sugars for the production of bioethanol requires successive reactions catalyzed by cellulase enzymes. However, the high cost and low production efficiency of these enzymes are the main obstacles to their industrial application in the production of ethanol. Indeed, the search for novel yeast strains producing cellulases is of a great value to the bio-industry **[1-2]**.
In this study we conducted a characterization of cellulases enzymes; Carboxymethylcellulase (CMCase) and Filter paper activity (FPase) produced by yeast isolate of the genus Trichosporon. The variation in CMCase and FPase activity as a function of pH and temperature showed that these enzymes are more active at 60°C. with an optimum pH of 4 to 6 for FPase and 5 for CMCase.
The maximum activity was detected after 10 min of incubation (0.235 IU / ml), for CMCase and 15 min of incubation (0.144 IU / ml) for FPase.
The CMCase enzyme has a Km of 0.7mg / ml and a Vmax of 10 IU / ml. The study of the effect of the monovalent and divalent metal ions shows that the CMCase and FPase activities are higher in the presence of ions; K^+, Na^+ Hg^{2+}, Ca^{2+}, $(NH4)^{2+}$, Cu^{2+}, Zn^{2+}, Mn^{2+}, Fe^{2+}, Co^{2+}, Mg^{2+}. We expect that other enzymes are produced by this yeast isolate in order to catalyze the hydrolysis of several substrates, namely powdered cellulose, starch, inulin, and pectin.
The yeast strain described here could be used for the degradation of lignocellulosic biomass in the context of industrial production of bioethanol.

***Keywords*:** Yeast; Cellulases; Carboxymethylcellulase; Filter paper activity; bioethanol.

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ANTIOXIDANT ACTIVITIES AND TOTAL PHENOL CONTENT OF EXTRACTS OF *TEUCRIUM POLIUM* GROWING WILD IN MOROCCO

Y. El Atki*, I. Aouam, F. El kamari, A. Taroq, B. Lyoussi, A. Abdellaoui

Laboratory of Physiology Pharmacology and Environmental Health, Department of Biology, Faculty of Sciences Dhar Mehraz, University Sidi Mohamed Ben Abdellah, B.P. 1796, Atlas, Fez, Morocco

**For correspondence: Email: yassinelbs@gmail.com*

Abstract

The objective of the present study was to determine, for the first time, antioxidant activities, total polyphenols and total flavonoids contents of methanol, ethanol, water and ethyl acetate extracts of Moroccan germander (*Teucrium polium)***.** Total polyphenols and flavonoids contents were determined spectrophotometrically using gallic acid and rutin as standards. Antioxidant activities was evaluated in vitro by three assays namely Free radical scavenging activity against 1,1-diphenyl-2-picrylhydrzyl (DPPH), reducing antioxidant activity (FRAP) and total antioxidant capacity. The total polyphenols contents were higher in the methanol extract. The flavonoid content of water was significantly higher ($P<0.05$) than all the other extracts. The methanolic extract showed the highest antioxidant activity as measured by DPPH and FRAP assays with IC50 values of 0.37±0.02 mg/ml and 0.32 ± 0.01 mg/ml respectively. The total antioxidant capacity assay showed that the water extract had a significant activity with value 215.1 ± 9.03 mg equivalent to ascorbic acid/g dry weight. The ethyl acetate extract had a weak antioxidant activity in the three tests. These results showed that Moroccan Germander, is a rich source of phenols and natural antioxidant compounds, which can be used as a natural food preservative.

Keywords: Germander; polyphenols; flavonoids contents; antioxidant activity; Folk medicine.

EFFECT OF MINERAL STRESS ON MORPHO- PHYSIOLOGICAL PARAMETERS OF NIGELLA SATIVA

S. Errai[a,*], A. Maataoui[b], H. Bezaidi[b], M. Elmidaoui[b], M. Benbella[b]

[a]*Laboratory of Physiology, Pharmacology Health and Environment Unit of Bioremediation and Environment Department of Biology. Faculty of Sciences Dhar EL Mahraz, Université Sidi Mohamed Ben Abdellah, Fès, Morocco*
[b]*National School of Agriculture, Meknes, Morocco*

**For correspondence: Email: siham.errai1@usmba.ac.ma*

Abstract

Nigella Sativa is a very known plant in the Arab world for its nutritional use and therapeutic purpose. The objective of this work is to study the response of this plant (Nigella Sativa) to mineral stress condition. To meet this objective, a test was conducted hydroponically in a growth chamber at the Department of Agronomy exactly in the National School of Agriculture in Meknes, Morocco. Seedlings were transplanted into nutrient solution with two plants per pot with a capacity of 600ml. Nutrient solution test corresponded to 10 % (T1), 20 % (T2) and 40 % (T3) Hoagland solution. Parameters of growth and development of the species were measured. The results showed that almost all parameters of growth and development were affected by mineral stress. At the end of the experiment, plant height of T1 was significantly reduced compared to T3. The stress treatment (T1) has developed a number of branches by much higher than in T3 treatment plant. A leaf area was reduced compared to the control. The total solids accumulated by T3 were higher compared with those accumulated by T1 and T2. Reducing the number of pods in T1 compared to T3, was significant. Similarly, the number of seeds per pod and 1000 seed weight were affected by the mineral stress. After 60 days of growth allocated to aerial parts, dry matter was important. Similar results were obtained by **[1,2]**.

Keywords: *Nigella Sativa*; mineral stress; hydroponics; growth; development.

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SYNTHESIS AND *IN VITRO* ANTIOXIDANT ACTIVITY OF NEW POLYHYDROXYLATED FLAVON-3-OLS AND 3-HYDROXY-2-STYRYLCHROMONES

J.L.C. Sousa[a,*], C. Proença[b], M. Freitas[b], E. Fernandes[b], A. M. S. Silva[a]

[a]*QOPNA, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal*
[b]*UCIBIO, REQUIMTE, Laboratory of Applied Chemistry, Department of Chemical Sciences, Faculty of Pharmacy, University of Porto, Rua de Jorge Viterbo Ferreira, 228, 4050-313 Porto, Portugal*

**For correspondence: Email: joanasousa@ua.pt*

Abstract

Flavon-3-ols and 2-styrylchromones (2-SCs) are two well-known classes of natural and synthetic compounds, which display important biological activities **[1,2]**. Particularly, the antioxidant activity of these derivatives has attracted much attention, because some of them possess essential structural features for scavenging reactive oxygen (ROS) and nitrogen species (RNS), such as the presence of (i) a catechol moiety in the B ring, (ii) the C2=C3 double bond in conjugation with the carbonyl group at C-4 and (iii) free hydroxyl groups at C-3 and other positions of their skeletons **[3]**.
In the present work, efficient methodologies were designed to synthesize flavon-3-ol and 3-hydroxy-2-SC derivatives with specific substitution patterns. Therefore, *o*-dihydroxylated derivatives **1a,b** and **2a,b** were prepared, presenting a catechol moiety in the A or B rings (Figure 1). Moreover, polyhydroxylated ones **1c** and **2c** were also obtained, containing a catechol group in both rings (A and B) (Figure 1). The scavenging activity of the synthesized compounds was addressed against the most common ROS [superoxide radical ($O2^{\bullet-}$), hydrogen peroxide (H2O2), hypochlorous acid (HOCl), singlet oxygen ($^1O2$) and peroxyl radical ($ROO^{\bullet}$)] and RNS [nitric oxide ($^{\bullet}NO$) and peroxynitrite anion ($ONOO^-$)] **[4]**. All the synthetic details as well as the new stablished structure/antioxidant activity relationships will be presented and discussed.

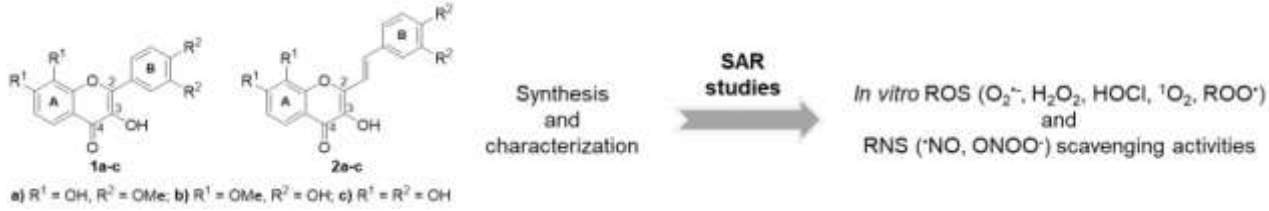

Figure 1

Keywords: flavon-3-ols; 3-hydroxy-2-styrylchromones; ROS; RNS; antioxidant activity.

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THE EFFECT OF HETEROCYCLIC COMPOUNDS FROM AROMATIC AND MEDICINAL PLANTS ON THE HYDROPHOBICITY OF CEDAR WOOD

F. Bennouna[a,*], M. Lachkar[b], Soumya El Abed[a,c], Saad Ibnsouda Koraichi[a,c]

[a]*Laboratory of Microbial Biotechnology, University Sidi Mohamed Ben Abdellah, Faculty of Science and Technology, Po. Box 2202, 30007, Fez, Morocco*
[b]*Engineering Laboratory of Organometallic and Molecular Materials, University Sidi Mohamed Ben Abdellah, Faculty of Sciences, Po. Box 1796, 30000, Fez, Morocco*
[c]*Regional University Centre of Interface, University Sidi Mohamed Ben Abdellah, Po. Box 2626, 30000, Fez, Morocco*

**For correspondence: Email: fadoua.bennouna@usmba.ac.ma*

Abstract

Cedar wood is sensitive to different agent of degradation such as fungi and bacteria which adhere to the wood surface and form biofilms **[1]**. The microbial adhesion step is considered as critical point in the biofilm formation process. It depends on hydrophobicity, surface tension, and electron donor–electron acceptor properties of both material and microbial surface **[2–4]**.
Thus, the development of non-biocidal solutions for wood protection with good environmental profile has become an overriding concern for these last years. So, the aim of this study is to evaluate the effect of heterocyclic compounds from aromatic and medicinal plants on the hydrophobicity and the electron donor–electron acceptor character of cedar wood.
The results show a hold of the hydrophobicity of cedar wood qualitatively and quantitatively after 1h of treatment ($\Delta Giwi$ = -11.62 mJ/m^2). Indeed, the treatment with the essential oil has increased the electron donor character with value of γ^- = 25.46 ± 0.41 mJ/m^2.

Keywords: Cedar wood; hydrophobicity; heterocyclic compounds.

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CONSEQUENCES MECANIQUES DE L'ATTAQUE SULFATIQUE EXTERNE SUR LES BETONS CONFECTIONNEES PAR LES EAUX USEES EPUREES DE LA VILLE D'ER-RACHIDIA

F.Z. Bouaich*, S. Naamane, N.H. Mtarfi, Z. Rais, M. Taleb, A. Lahkimi, N. Bouslamti,H. Chaouki

Laboratoire d'Ingénierie d'Electrochimie, de Modélisation et d'Environnement, Faculté des sciences Dhar El Mehraz, B.P. 1796, 30000 Atlas Fès, Maroc

**For correspondence: Email: bouaich.isbtp@gmail.com*

Abstract

Les bétons utilisés comme réacteurs chimiques supportant des solutions très agressives, dans des constructions dans la mer, dépôt de déchets chimiques industriels ou dans la construction sur des sols gypseux,...exigent une qualité spécifique.
Ce travail a un double objectifs. Le premier est de valoriser les eaux usées épurées (EUE) de la station d'Er-Rachidia afin de réduire la surexploitation des eaux souterraines et le coût d'utilisation de l'eau potable dans le béton. Le deuxième est d'élaborer un béton résistant aux attaques sulfatiques. Pour cela, trois types de bétons ont été confectionnés selon la norme NF P 18-404 et dans des éprouvettes cylindriques normalisées 16x32 cm avec des agrégats concassées. Après leur conservation pendant 24h, ils ont été démoulés et trempés dans trois types d'environnements différents:

- immersion dans l'eau du robinet,
- immersion dans l'eau de mer et
- immersion dans une solution à 5% de l'acide sulfurique (H_2SO_4) pure pendant trois mois.

Le suivi de la qualité des bétons élaborés a été réalisé en fonction du temps par mesure des paramètres physiques et mécaniques. Celui de la durabilité, a eu lieu par mesure de la perte de masse, du pH de chaque solution d'attaque ainsi que la dimension des éprouvettes.
Les résultats obtenus montrent que le béton élaboré avec les eaux usées épurées présente une résistance mécanique comparable au béton élaboré avec l'eau potable, et une durabilité satisfaisante dans les milieux agressifs.

Keywords: Béton, environnement, solutions agressives, acide sulfurique, eaux usées épurées, durabilité.

ELECTROCHEMICAL AND QUANTUM CHEMICAL INVESTIGATION OF SOME PYRAZOLE-THIAZOLE COMPOUNDS AS MILD STEEL CORROSION INHIBITORS IN MOLAR HYDROCHLORIC ACID

K. Ismaily Alaoui[1], M. Taleb[1], S. El Arrouji[1], Z. Rais[1], F. Abrigach[2], M. Khoutoul[2], A. Aouinti[2], B.Hammouti[2], R. Touzani[3]

[1]*Laboratoire d'Ingénierie d'Electrochimie de Modélisation et Environnement, Faculté des Sciences Dhar El Mahraz, Université Allal Ben Abdellah, BP 1796, 30000 Atlas, Fès, Morocco*

[2]*Laboratoire de Chimie Appliquée et Environment (LCAE-URAC18), Faculté des Sciences, Université Mohammed Premier, B.P. 717, M-60000 Oujda, Morocco*

Abstract

One of the primary approaches to controlling acidic corrosion is the employment of organic corrosion inhibitors, which is often proposed to be the most economical solution. The inhibitive effect of organic compounds depends on this its ability to adsorb on metallic surface.

Inhibition of mild steel corrosion by two combined pyrazole-thiazole compounds (N-[(3,5-dimethyl-1H-pyrazol-1-yl)methyl]-1,3-thiazol-2-amine, P-Th and bis(N,N-bis[(3,5-dimethyl-1H-pyrazol-1-yl)methyl]-1,3-thiazol-2-amine) 2P-Th in 1M HCl was studied by weight loss, potentiodynamic polarization and electrochemical impedance spectroscopy. Results obtained reveal that these compounds reduce significantly the corrosion rate of mild steel, their inhibition efficiency increased with inhibitor concentration. Potentiodynamic polarization study show that these compounds are mixed-type inhibitors with cathodic predominance in 1M HCl. Impedance experimental data revealed a frequency distribution of the capacitance, simulated as constant phase element. The inhibition efficiencies obtained from cathodic Tafel plots gravimetric and EIS methods were in good agreement.

The various thermodynamic parameters of dissolution and adsorption processes were evaluated in order to elaborate adsorption mechanism. Adsorption of studied inhibitors obeyed Langmuir adsorption isotherm model.

B3LYP/6-31G (d, p) quantum chemical calculations are performed to optimize geometries and obtain properties depending on the electron density for Pyrazole-Thiazole derivatives studied in order to ascertain any correlation between the inhibitive effect and the structures of inhibitors.

Keywords: Mild steel; HCl, Inhibition; Corrosion; Pyrazole-Thiazole derivatives; Adsorption; Langmuir isotherm; DFT calculation.

PHYSICOCHEMICAL AND BACTERIOLOGICAL QUALITY OF OUED FEZ AND SEBOU RIVER DOWNSTREAM OF FEZ AFTER THE LAUNCH OF THE WASTEWATER TREATMENT PLANT: ASSESSMENT SPATIO-TEMPORAL MAPS, MOROCCO

N. Idrissi[1,*], F. Z. Elmadani[1], K. El Rhazi [2], C. Nejjari [2], Z. Rais[1], M. Taleb[1]

[1]*Laboratory of Engineering, Electrochemistry, Modeling and Environment, Faculty of Science Agdal, Sidi Mohammed Ben Abdellah University, Fez, Morocco.*
[2]*Laboratory of Epidemiology and Public Health, Faculty of Medicine and Pharmacy, Sidi Mohammed Ben Abdellah University, Fez, Morocco.*

**For correspondence: Email: nisrine.idrissi@hotmail.fr*

Abstract

This study aims to present a assessment the quality of surface waters in Oued Fez and Sebou River downstream the city of Fez, who receive different industrial effluents . The study of the space-time monitoring of physical-chemical parameters and bacteriological of the different sites, compared to Moroccan standard of rejection. Reveals than a since Oued Fez surface water prior to wastewater treatment plant (WWTP) and Sebou River downstream from the confluence are chemically and bacteriologically contaminated. They are characterized by high turbidity, high content in suspended substances, namely nitrites and orthophosphates, and high microbial contamination by fecal coliforms FC, Escherichia coli EC and Intestinal Enterococci IE.
This study revealed the need for constant monitoring in places where environmental degradation is caused by sewage discharges coming from the city of Fez, that can haves adverse effects on the wastewater treatment plant (WWTP) of Fez city, also on the health of the population and the aquatic life of Oued Sebou. The developed GIS based environmental database will serve as a reference study for study the Decision Support System which will assist decision makers in assessing and monitoring the water pollution.

Keywords: Water quality; waterborne diseases; WWTP; Sebou River.

WATER COMPATIBLE SYNTHESIS OF *TRANS-4,5*-DIAMINO-CYCLOPENT-2-ENONES FROM FURFURAL

R.F.A. Gomes*, N. Esteves, C.A. Afonso

Research Institute for Medicines (iMed.ULisboa) Faculty of Pharmacy, Universidade de Lisboa, Av. Prof. Gama Pinto, 1649-003, Lisboa, Portugal

**For correspondence: Email: rafaelgomes92@live.com.pt*

Abstract

The ever increasing population growth, aligned with the concomitant industrial development leads to an enlarged demand for chemicals and energy. The fact that oil reservoirs are being depleted is a concern and the increased demand will hasten this depletion. New sustainable sources for fuels and bulk chemicals are of the highest interest, and biomass is the most attractive alternative for oil based products. Furan aldehydes such as furfural and 5-hydroxymethylfurfural (HMF), easily obtained from xylose or fructose respectively, are included in the U.S. Department of Energy top 10+4 list of biobased materials **[1]**. The transformation of the five member heterocycle furfural to important *trans*-4,5-diamino-cyclopent-2-enones (CP) was first described by Batey and coworkers promoted by Dysprosium in dry acetonitrile **[2]**. This work focus on the development of methodologies to prepare CP in water both as an environmentally friendly procedure with potential catalyst recycling and the possibility of using the cyclopentenone formation reaction as a platform to insert non-natural functionality on biomolecules (enone) **[3]**.

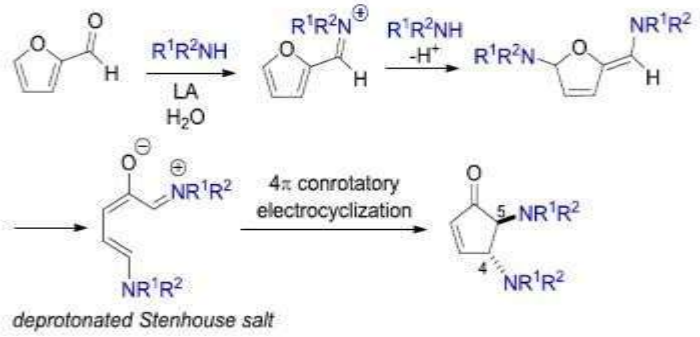

Figure 1 Mechanism for the Lewis acid promoted formation of 4,5-diamino-cyclopent-2-enone from furfural

Keywords: furfural; 1,2-diamino-cyclopent-2-enone; catalyst recycling.

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SYNTHESIS AND CHARACTERIZATION OF NEW HETEROCYCLIC COMPOUNDS α-AMINOPHOSPHONIC ESTERS VIA NUCLEOPHILIC SUBSTITUTION REACTIONS AND 1,3-DIPOLAR CYCLOADDITION

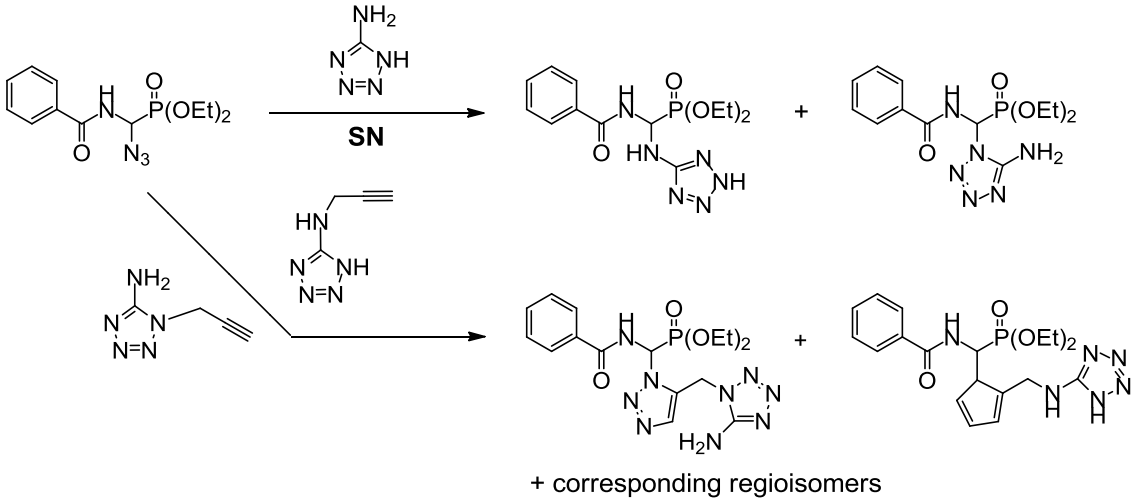
K. Fall*, H. Faraj, A. Alami, A. El Hellaoui, B. Labriti, S. El Hajji, Y. Aouine

Laboratory of Organic Chemistry, Faculty of Science Dhar El Mahraz, Sidi Mohamed Ben Abdellah University, Fez, BP. 1796 – Morocco

**For correspondence: Email: serigneabdoukhadirfall@gmail.com*

Abstract

The heterocyclic α-aminophosphonic acids interest increasingly both the researchers and industrialists because of their wide spectrum of activity they present. The interest granted to heterocyclic amino acids is due mainly to their important pharmacological and electrochemical industrial utility **[1,2]**.
Following the work on the synthesis of α-aminophosphonic and carboxylic esters **[3]**, we present the synthesis of new α,α-diaminophosphonic esters, glycine derivatives. These compounds are obtained by nucleophilic substitution reactions and 1,3-dipolar cycloaddition of α-azido aminosters *N*-protected by different aminotetrazole.



The compounds whose structures are confirmed by IR spectroscopy, ^{1}H-NMR, ^{13}C-NMR and spectrochemical studies, will be subjected to screening studies of pharmacological and biological activities.

Keywords: Aminophosphonic esters; heterocyclic compounds; Nucleophilic substitution; N-protected aminoester; 1,3-dipolar cycloaddition.

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SYNTHESIS AND CHARACTERIZATION OF NEW PRECURSORS OF 1,2,3-TRIAZOLIC AMINO ALDEHYDES VIA CLICK CHEMISTRY

S. Hajib, A. El Hallaoui, A. Alami*, S. El Hajji, H. Faraj, B. Labriti, K. Boujdi and Y. Aouine

Laboratoire de Chimie Organique, Faculté des sciences Dhar EL Mahraz, Université Sidi Mohamed Ben Abdellah, BP. 96, Fès, Maroc.

**For correspondence: Email: alamianouar@yahoo.fr*

Abstract

1,2,3-Triazoles are present in a number of compounds with assorted biological activities such as anticancer, antibacterial, antifungal, anti-tubercular, and anti-HIV properties **[1,2]**. The copper(I)-catalyzed azide-alkyne cycloaddition (CuAAC) is the most widely used method for the synthesis of 1,4-disubstituted 1,2,3-triazoles from a wide range of organic azides and terminal alkynes **[3–7]**.
We described in this communication the preparation of new oxazolinic precursors of 1,2,3-triazolic - amino aldehydes. This preparation approach is based on the Cu(I)-catalyzed azide-alkyne cycloaddition (Scheme).

R = $CH_3\ (CH_2)_2\ CH_2$; $HO\ CH_2\ CH_2$; $CH_3\ CH_2(OH)$

The obtained products were characterized on the basis of NMR spectroscopy (^1H, ^{13}C, ^{15}N and 2D ^1H-^{15}N HMBC) in addition to the elemental analysis and MS data.

Keywords: 1,3-dipolar cycloaddition; triazole; click chemistry.

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SYNTHESIS OF 2-(FLUORINATED ARYL)PYRIDINE DERIVATIVES VIA PALLADIUM-CATALYZED C-H BOND ARYLATION OF FLUOROBENZENES USING 2-HALOPYRIDINES AS ARYL SOURCES

R. Boyaala[a,b,*], R. Touzani[b,c,] , V. Guerchais[a], J.-F.Soulé[a], H. Doucet[a]

[a]*Institut des Sciences Chimiques de Rennes, UMR 6226 CNRS-Universite de Rennes, UMR 6226 CNRS-Universite de Rennes, "organometalliques: Materiaux et Catalyse", Campus de Beaulieu, 35042 Rennes, France.*
[b]*Laboratoire de Chimie Appliquée et Environnement (LCAE), Faculté des Sciences, Université Mohamed Premier, Oujda, Morocco*
[C]*Faculté Pluridisciplinaire de Nador, Université Mohammed Premier, BP : 300, Selouane 62700, Nador, Morocco*

**For correspondence: rababboyaala@outlook.fr*

Abstract

In the past decade, palladium-catalyzed C-H activation/C-C bond-forming reactions have emerged as promising new catalytic transformations; however, development in this field is still at an early stage compared to the state of the art in cross-coupling reactions using aryl and alkyl halides.
We report herein on palladium-catalyzed direct arylation of (poly)fluorobenzene derivatives in the presence of 2-halopyridines for the one-step synthesis of 2-[(poly)fluorinated aryl] pyridine derivatives. The reactivity of 2-bromopyridines is strongly dependent on its substituents at the C6 position.

Keywords: 2-arylpyridine; C-H activation; catalysis; Fluorinated molecules; Palladium.

THEORETICAL AND EXPERIMENTAL STUDY OF THE INHIBITORY EFFECT OF A PYRIDINE-BASED ORGANIC COMPOUND AGAINST THE CORROSION OF MILD STEEL IN 1M HCl MEDIUM

A. Saady*, M. Taleb, K. Ismaily Alaoui, A. El Biache

Laboratory of Engineering, Electrochemistry, Modeling and Environment (LIEME), Faculty of Sciences, University Sidi Mohamed Ben Abdellah, Fez, Morocco

**For correspondence: E-mail: Saady.asmae2014@gmail.com*

Abstract

Several methods are available to prevent or delay the corrosion of metallic materials by ensuring their protection when they are in contact with very aggressive media such as the hydrochloric acid medium, heterocyclic compounds are widely used as corrosion inhibitors of metals and alloys in the acid etching process and industrial cleaning.
In this work, we are interested in the protection of mild steel against corrosion in 1M HCl, using an organic pyridine-based compound (DPA) as a corrosion inhibitor. This study was carried out by stationary and transient electrochemical methods as well as theoretical methods. The results obtained show that the inhibitory efficiency increases with the increase in the concentration of DPA but decreases with the increase of the temperature. The potentiodynamic polarization measurements showed that the inhibitor is of the mixed type, so the thermodynamic parameters of adsorption and activation were discussed. On the other hand, the adsorption of the inhibitor on the surface of the mild steel obeys the Langmuir isotherm. The results obtained from electrochemical and weight loss studies were in reasonable agreement.
Quantum chemical approach using DFT at B3LYP/6-31G (d, p) level of theory, was used to calculate some structural and electronic properties of pyridine studied to ascertain the correlation between their experimental inhibitive efficiencies and some of the computed parameters.

Keywords: Pyridine, corrosion, C38 steel, adsorption, DFT.

NEW IMIDAZOTHIAZOLE-CHALCONE DERIVATIVES: SYNTHESIS AND EVALUATION OF THEIR ANTIFUNGAL AND ANTIBACTERIAL ACTIVITIES

M. Koudad [1,2,*], C. Elhammouti[2], A. Elaatiaoui[1,2], A. Oussaid[1], M. Allali[3], N. Benchat[2]

[1]*LACPRENE Department of Chemistry, Polydisciplinary Faculty of Nador, UMP*
[2]*Laboratory of Applied Chemistry and Environments (LCAE), Faculty of Sciences, University Mohammed Premier, Oujda*
[3]*Institut Supérieur des professions infirmières et techniques de santé, ISPITS-Fès, site El Ghassani, 30000 Fes Morocco.*

**For correspondence: E-mail: koudad.mohammed@yahoo.com)*

Abstract

Fused heterobicyclic systems have gained much importance in the field of medicinal chemistry because of their broad spectrum of physiological activities. Among the heterocyclic rings containing bridgehead nitrogen atom, imidazothiazoles derivatives are especially attractive because of their different biological activities.such as antifungal ,antimicrobial, anticancer, anti-inflammatory, antioxidant, antiviral and antitumor activities.

A large number of synthetic routes have been reported for the synthesis of chalcones, the most classical and general being the Claisen--Schmidt condensation. Chalcones and their derivatives have a huge importance in medicinal chemistry, displaying a wide range of important pharmacological activities.

Imidazothiadiazole chalcon occupy a prominent place in medicinal chemistry because of their significant properties as therapeutics.

This has generated much interest in the synthesis of new classes of heterocyclic systems, thereby to explore their biological properties.

Recently much interest has been focused on the synthetic routes of Imidazo [2,1-b]thiazole derivatives and their biological activity. Since the imidazo[2,1-b]thiazole derivatives have been reported in the literature as antibacterial, antifungal, antihelmintic and antitumour agents.

A series of imidazothiazole chalcon derivatives were synthesized by the condensation of 6-phenylimidazo[2,1-b]thiazole-5-carbaldehyde with deferent ketones.Their chemical structures have been confirmed by means of IR, H-NMR data and by elemental analysis. Investigation of antimicrobial and antifungal activity of compounds was done by dilution method against 3 pathogenic bacteria,2 pathogenic fungi .

SYNTHESIS AND ANTICORROSIVE ACTIVITY OF A POLYACRYLAMIDE ON C-STEEL IN ACIDIC MEDIA

M. Beniken[1,*], M. Driouch[1], M. Sfaira[1]*, B. Hammouti[2], M. Ebn Touhami[3], M.A. Mohsin[4]

[1]Laboratoire d'Ingénierie des Matériaux, de Modélisation et d'Environnement (LIMME), Faculté des Sciences, Université Sidi Mohammed Ben Abdellah, USMBA, B.P. 1796–30000, Atlas – Fès, Morocco.
[2]LCAE-URAC18, Faculté des Sciences, Université Mohammed Premier, BP 717 – 60000, Oujda, Morocco
[3]Laboratoire d'Ingénierie des Matériaux et Environnement : Modélisation et Application (LIMEMA), Faculté des Sciences, Université Ibn Tofaïl, B.P. 133–14000, Kénitra, Morocco.
[4]Department of Chemistry, University of Sharjah, Sharjah, P.O. Box 27272, United Arab Emirates.

**For Correspondence: Email: mustapha.beniken@yahoo.fr*

Abstract

The efficiency of a polyacrylamide (PA), recently synthesized by inverse emulsion polymerization, was evaluated, on the basis of concentration, for corrosion inhibition of C38 in 1.0 M HCl solution, by means of electrochemical impedance spectroscopy (EIS), potentiodynamic polarization and weight-loss measurements. A comparison of the PA inhibitor behaviour in both acidic media 1.0 M HCl and 0.5 M H_2SO_4, was investigated at 3×10^{-6} mol L^{-1}. The chemical structure of PA was confirmed by FTIR and ^1H NMR and the experimental conditions were designed to produce high molecular weight. The molecular weight was determined by the Gel Permeation Chromatography and the viscosity average molecular weight method. The effects of concentration on inhibition efficiency were determined and discussed. The inhibitor was of mixed-type, influencing predominantly the anodic process. The charge transfer process was dominant in controlling the corrosion of C-steel. The electrochemical impedance was satisfactorily simulated by an interface model having one or two time constants.

Keywords: Polyacrylamide, Acid corrosion, Acid inhibition. Adsorption.

SYNTHESE ET ETUDE DU POUVOIR ALLELOPATHIQUE DE NOUVEAUX SYSTEMES HETEROCYCLIQUES A SQUELETTE TERPENIQUE

A. N'ait Ousidi*, My. Y. Ait Itto, Az. Auahmani, H. Bouamama, A. Riahi, A. Auahmani

Laboratoire de synthèse organique et physico-chimie Moléculaire, Faculté des Sciences, Université Cadi Ayyad, Marrakech - Maroc

**For Correspondence: Email: docabdellah@gmail.com*

Abstract

Les composés hétérocycliques occupent une place importante en chimie thérapeutique et par conséquent dans la synthèse organique. La diversité structurale confère a ces composés des propriétés biologique diverses.
Les résultats bibliographiques les plus récentes révèlent un intérêt croissant pour les systèmes hétérocycliques en raison de leurs applications dans de nombreux domaines différents tels que la biologie la pharmacologie ou la chimie industrielle. En effet de nombreux hétérocycles pentagonaux contenant du soufre et de l'azote , tels que les thiazolidinones sont connus pour présenter un large spectre d'activités biologiques tels que des anticonvulsivants **[1]** contre le VIH **[2-4]** antimicrobienne **[5-7]** anti-inflammatoire et anti- cancer **[8,9]**.
Compte tenu des propriétés intéressantes mentionnées ci-dessus et en tant que continuation des travaux réaliser au sien de notre laboratoire **[10,11]** pour préparer de nouveaux systèmes hétérocycliques avec d'éventuelles activités biologiques améliorées, nous rapportons ici la synthèse de nouveaux hétérocyles en utilisant des réactions d'hétérocyclisation et de cycloaddition 1,3-dipolaire, à partir de (1R)-camphre et (R)-Carvone thiosemicarbazones, ainsi que l'évaluation de leur du pouvoir allelopathique. Les structures des cycloadduits nouvellement synthétisés ont été établies sur la base de leurs données spectroscopiques : IR, RMN ^{1}H, ^{13}C et Masse.

Keywords: hétérocyles, cycloaddition 1,3-dipolaire, heterocyclisation, pouvoir allelopathique.

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COPPER ON CELLULOSE: A HETEROGENEOUS CATALYST FOR CLICK SYNTHESIS IN WATER

L. Bahsis[a,*], H. Ben El Ayouchia[a], A. Ben-Tama[b], E.M. El Hadrami[b], H.Anane[a], S.-E. Stiriba[a,c,*]

[a]*Laboratoire de chimie analytique et moléculaire, Faculté Polydisciplinaire de Safi, Université Cadi Ayad, Safi, Morocco.*
[b]*Laboratoire de Chimie Organique Appliquée (LCOA), Faculté des Sciences et Techniques, BP 2202, Fès, Morocco.*
[c]*Instituto de Ciencia Molecular (ICMol), Universidad de Valencia, C/ Catedrático José Beltran, 46980, Valencia, Spain.*

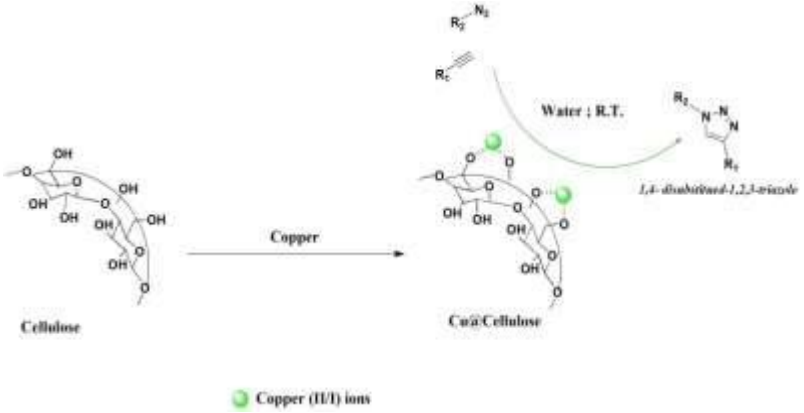
**For correspondance: E-mail: bahsis.lahoucine@gmail.com / stiriba@uv.es*

Abstract

Since its development by Sharpless and Meldal **[1]**, the Cu(I)-catalyzed [3+2] cycloaddition reaction between terminal acetylenes and azides (CuAAC) has emerged as a clickable strategy for the rapid and efficient assembly of molecules with diverse functionality. The major limitations of existing CuAAC protocols is their realization in terms of homogeneous nature of catalysts, thus leading to separation problems of catalyst/product(s), together with the requirement of adding reducing agents and stabilizing ligands to the catalyst. Therefore, the development of stable and recyclable heterogeneous copper catalysts with improved catalytic activity in absence of any oxidizing/reducing agents is highly desirable.

We now report a new greener catalytic system based on bio-polymer by using cellulose copper-supported the active catalytic copper (I/II). The catalytic activity of Cu@Cellulose was assessed in the regioselective synthesis of 1,4-disubstituted-1,2,3-triazoles by clicking a variety of organic azides and terminal alkynes in water as solvent. This bio-heterogeneous catalysis protocol offers several advantages in term of inexpensive and biocompatible catalyst that can be easily recovered and reused up to five times in high yields, without significant decrease in activity or selectivity.

Keywords: Click chemistry; azides; alkynes; copper (I); cellulose; triazole; cycloaddition.



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SYNTHESIS AND OPTIMIZATION OF NEW MOLECULES DERIVATIVES OF PYRIDO[2 ,3-b]PYRAZINE

M. Sikine[a], Y. Kandri Rodi[a,*], A. Kandri Rodi[a], K. Misbahi[a], S. Sabir[a], A. Bentama[a], F. Ouazzani Chahdi[a] et E.M. Essassi[b]

[a]*Laboratoire de Chimie Organique Appliquée, Faculté des Sciences et Techniques Université Sidi Mohamed Ben Abdallah, Fès, Maroc.*
[b]*Laboratoire de Chimie Organique Hétérocyclique URAC 21, Faculté des Sciences, Université Mohammed V, Avenue Ibn-Batouta, Rabat, Maroc.*

**For Correspondence: Email: youssef_kandri_rodi@yahoo.fr*

Abstract

The chemistry of heterocyclic compounds is very extensive and predominant place in industry and pharmaceuticals. . the novel heterocyclic pyrido[2,3-b]pyrazine have a potential as antitumor agent have pharmacological activities including anticancer activities, anti-inflammatory, anti-malariale, anti-bacterial and exhibit good inhibitory action in the corrosion of metals. On the other hand, the modification of the pyrido[2,3-b]pyrazine base structure is capable of exalting their activity, it is for this reason that we have envisaged synthesed new products possessing the motif of pyrido[2,3-b]pyrazine. The latter have been used as raw materials for the preparation of compounds capable of presenting potential biological activities. We were able to carry out the thionation of novel heterocyclic derivatives possessing a pyrido [2,3-b] pyrazine motif, there after, the alkylation reaction was carried out under the conditions of phase transfer catalysis. The structures were identified by the usual spectroscopic analyzes: NMR (1H, 13C), IR, mass spectrometry and x-ray diffraction.

Keywords: Heterocyclic; pyridopyrazine; alkylation; CTP; thionation.

GREEN AND ELEGANT SYNTHESIS OF SOME MODIFIED ARYL AND HETERO-ARYL *C*-AND *N*- NUCLEOSIDES ANALOGUES

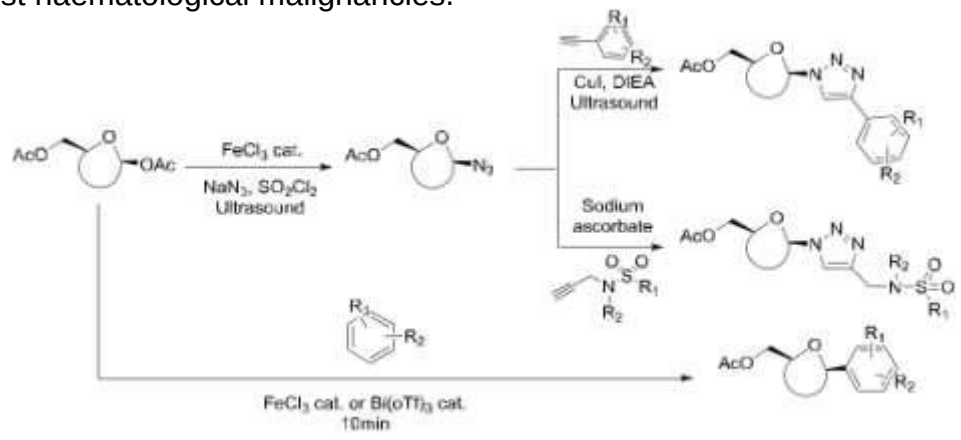
H. Tachallait[a,b], S. Alaoui[a,b], H. Marzag[a,b], A. Saber[a,b], L. Demange[b,c], A. R. Martin[b], M. Dufies[d], G. Pagès[d], R. Benhida[b,*], K. Bougrin[a,*]

[a]*Laboratoire de Chimie des Plantes et de Synthèse Organique et Bioorganique, URAC23, Université Mohammed V, Faculté des Sciences B.P. 1014 Rabat, Maroc*
[b]*CN, UMR CNRS 7272, Université de Nice Sophia-Antipolis-Université Côte d'Azur , Parc Valrose, Nice, France.*
[c]*Université Paris-Descartes, Sorbonne Paris Cité, UFR des Sciences Pharmaceutiques et UFR Biomédicale des*
[d]*Institute for Research on Cancer and Aging ,UMR7884 CNRS and INSERM U1081 ,Université Côte d'Azur, Nice*

**For correspondence: Email: kbougrin@yahoo.fr*

Abstract

The *C*-nucleosides are widely used in medicinal chemistry due to their high value as therapeutic agents and biochemical probes. For example, tiazofurin has been approved as an orphan drug for the treatment of certain type of haematological malignancies. Various approaches have been used for the synthesis of *C*-nucleosides. We report here two routes which have been developed by our research group.The first one, consists in the use of a Friedel-Craft mediated by an Lewis acid as catalysts, which leads to aromatic ribosides and glucosides in high yields and with an excellent stereoselectivity **[1]**.The second route is based on the use of azaglycosides as substrates for a subsequent functionalization through click chemistry **[2-3]**. Among the series of *C*-nucleosides synthesized in the team, some products revealed an interesting cytotoxic activity against haematological malignancies.



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CONTRIBUTION TO THE SYNTHESIS OF NEW BIOACTIVE MOLECULES FROM QUINOXALINE

A. Nadeem[a,*], Y.ramli[b], EL.Essassi[a]

[a]*Laboratoire Laboratoire de Chimie Organique Hétérocyclique, pharmacochimie Faculté des sciences, Université Mohammed V, Av Ibn Battouta: BP 10140, Rabat, Maroc*
[b]*CN, Laboratoire Thérapeutique chimie ,Faculty of Medicine and pharmacy Université Mohammed V,10140 Rabat.*

**For correspondence: Email: nadeemabad2017@gmail.com*

Abstract

In the framework of the research carried out in our laboratory, in order to prepare new molecules with interesting pharmacological power, namely analgesics **[1]**, anti-inflammatories **[1]**, antifungals **[2]**, antibacterial drugs **[3]**, anticancer **[4]**. We have developed the synthesis of novel quinoxaline derivatives via sulfurization **[5]**, and alkylation reactions under the conditions of liquid-solid phase transfer catalysis with various alkylating agents. The various products obtained were characterized by ^{1}H, ^{13}C, IR and mass.

Keywords: quinoxqline; sulphidation; CTP alkylations; Biological activity.

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ONE-POT THREE-COMPONENT SYNTHESIS OF THP-5-CARBOXAMIDE DERIVATIVES

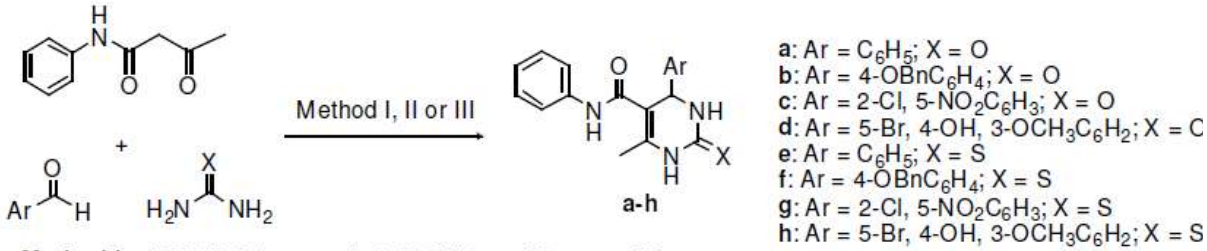
Ş. Gülten*, U. Gezer, E. A. Gündoğan

Çanakkale Onsekiz Mart University, Faculty of Arts and Sciences, Department of Chemistry 17020 Çanakkale, Turkey

**For Correspondence: Email:* sgulten@comu.edu.tr , siringulten@hotmail.com

Abstract

The synthesis of various new tetrahydropyrimidine (THP) derivatives bearing a phenylcarbamoyl group at C (5) position by one-pot three-component reaction was described in good yields. The reaction of acetoacetanilide as the 1,3-dicarbonyl component with various aromatic aldehydes (benzaldehyde, 4-benzyloxybenzaldehyde, 5-bromovanilin and 2-chloro-5-nitrobenzaldehyde) and urea/thiourea in the presence of either a catalytic amount of *p*-toulenesulfonic acid monohydrate (pTSA·H_2O) or concentrated HCl as an efficient catalyst leads to Biginelli compounds **[1,2]**. The synthesized compounds were confirmed by IR, ^{1}H-NMR, ^{13}C-NMR, mass and elemental analyses.



Method I: pTSA·H_2O (10 mmol%), EtOH (15 mL), 80-90 °C
Method II: conc. HCl (10 mmol%), solvent-free, 80-90 °C
Method III (Classical Biginelli conditions): conc. HCl (10 mmol%), EtOH (1 mL), 80-90 °C

This work was supported in part by Çanakkale Onsekiz Mart University (BAP 2008/28).

Keywords: Biginelli reaction; tetrahydropyrimidine; urea; thiourea.

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A NEW STRATEGY FOR THE SYNTHESIS OF NOVEL AMINOPYRIDO [2,3-*d*]PYRIMIDINES

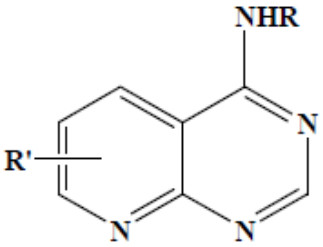
F. Belhadj[a,*], Z. Kibou[a,c], M. Benabdallah[a], N. Choukchou-Braham[a], D. Villemin[b]

[a]*Laboratoire de Catalyse et Synthèse en Chimie Organique, Université de Tlemcen, B.P.119, 13000 Tlemcen, Algérie*
[b]*LCMT, ENSICAEN, UMR CNRS 6507, 6 Bd du Maréchal Juin, 14050 Caen, France*
[c]Centre Universitaire de Ain Témouchent, Institue des Sciences, BP 284, 46000 Ain Témouchent, Algeria

**For correspondance: Email: fbelhadj88@yahoo.fr*

Abstract

The nitrogen heterocycles are a class of heterocyclic compounds with different applications in various fields, whether pharmacology, agricultural chemistry or chemical industry where various patents were fielded. Thus, several new synthetic methods have been described in literature where synthesis, reactivity and biological properties of pyrimidines moieties are given. Pyrido[2,3-*d*]pyrimidines derivatives are reported to possess antitumor, antibacterial and anti-inflammatory activities **[1-4]**.
In this communication, we present a new approach for the synthesis of substituted aminopyrido[2,3-d] pyrimidine **(**Scheme1**)** under solvent-free conditions.



Scheme1: Structure of aminopyrido[2,3-d] pyrimidines

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IN SITU SYNTHESIS UNI, BI OR THREE-DIMENSIONAL NETWORKS WITH VERY VARIED TOPOLOGIES CONTAINING IMIDAZOLE OR TETRAZOLE AS HETEROCYCLIC COMPOUNDS

Mohamed Abdellatif bensegueni[a,*], Aouatef Cherouana[a], Slimane Dahaoui[b]

[a]*Unité de Recherche de Chimie de l'Environnement et Moléculaire Structurale. Université frères Mentouri-Constantine25000. Algérie*
[b]*CRM2, UMR CNRS 7036, Faculté des Sciences et Technologies, Université de Lorraine, Institut Jean Barriol,*
BP 70239, 54506 Vandoeuvre-lès-Nancy Cedex, France

**For correspondence: Email: bensegueni.abdellatif@gmail.com*

Abstract

Numerous examples have illustrated the ability of the ligands containing the nitrile function to link metal centers forming complexes, and also have the ability to be converted into tetrazole functions insitu by [2+3] Cycloaddition reaction **[1-3]**, thus promoting the formation of complexes based on this type of ligands and the construction of new uni, bi or three-dimensional networks with very varied topologies.
Herein we examine and the report the crystal structure of complexes, coordination polymers and hybrid compounds and we study their hydrogen bonding network and topologies.

Keywords: In-Situ synthesis; Topology; hydrogen bonds; X-Ray diffraction.

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SYNTHESIS OF NEW BIOACTIVE MOLECULES FROM (4Z)-(2-OXOPROPYLIDENE)-1,2,4,5-TETRAHYDRO-2H-1,5-BENZODIAZ EPINE-2-ONE

Jihad Sebhaoui, Youness El Bakri, El Mokhtar Essassi*

Laboratoire de Chimie Organique Hétérocyclique, Centre de Recherche des Sciences des Médicaments, Pôle de Compétences Pharmacochimie, URAC 21, Faculté des Sciences, Mohammed V University Rabat, Avenue Ibn Battouta, BP 1014, Rabat, Morocco.

**For Correspondence: E-mail: emessassi@yahoo.fr*

Abstract

Benzodiazepines have recently received great importance because of their wide range of therapeutic and pharmacological properties. Many members of diazepine family are nowadays widely used as anticonvulsant, antianxiety, analgesic, sedative, antidepressive, and hypnotic agents.
Our work consists of the synthesis of new 1,5-benzodiazepine derivatives starting from (4Z)-(2-oxopropylidene)-1,2,4,5-tetrahydro-2H-1,5-benzodiazepine-2-one using alkylating agents, potassium carbonate and Tetra-n-butylammonium bromide as a Phase-transfer catalyst (PTC) in dimethylformamide and evaluating their biological activity.
Structures of the synthesized compounds were identified by x-ray data, (^{1}H,^{13}C) NMR and IR spectroscopy.

***Keywords**:* synthesis; 1,5-benzodiazepine; PTC; crystal structure.

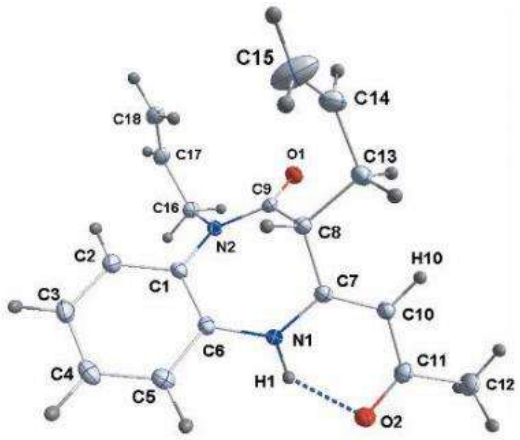

Figure: (4Z)-4-(2-Oxopropylidene)-1,3-bis(prop-2-en-1-yl)-2,3,4,5-tetrahydro-1H-1,5-benzodiazepin-2-one.

ANALYSIS OF CARBAMATE PESTICIDES: IMMUNOLOGICAL TECHNIQUES

N. Bellemjid[a,b,*], A. Moussaif[a,*],A. Iddar[a], N. El Abbadi[a] A. Mesfioui[b]

[a]*National Centre for Nuclear Energy, Sciences and Technologies, Rabat, Morocco.*
[b]*Faculty of Sciences University IbnTofaïl, Kenitra, Morocco.*

**For correspondence: Email: najwabellemjid@gmail.com / a.moussaif@cnesten.org.ma*

Abstract

Carbamates are a family of organic compounds carrying an R-HN- (C = O) O-R' function.
They are, in fact, substituted esters of carbamic acid or a substituted amide.
Carbamates, used as insecticides since the 1950s, are intensively used in Moroccan agriculture: in the loukkus and in the al -gharb region. The use of carbamates is the most important (28%) followed by nitrogenous heterocycles (22 %) **[1]**.
In order to control the fate of chemical contaminants and residues of pesticides used massively on crops in Morocco and to reduce their impact on public health, we aimed to develop an immunoanalytical assay for some carbamates such as Carbendazim (or benzimidazol-2-ylcarbamate), which is an active substance belonging to the benzimidazole family.
For the development of the carbendazim immunoassay system, production of polyclonal antibodies is required, but carbendazim are molecules of low molecular weight and are non-immunogenic (hapten). It is necessary to couple them to large molecules, usually protein (BSA, KLH). This coupling requires a chemical feasibility study to determine the synthesis pathway and chemical reactions (Anchoring of a "carbon chain arm" or of a peptide nature) necessary to obtain the hapten (s) without changing either the structure or the physicochemical properties of the carbamates in question.
After coupling the synthesized haptens and their injections to the rabbits, according to a pre-defined immunization protocol **[2]**; the antisera collected will be used for the realization of the immunoassay systems and the quantification of the carbendazim in the different matrices.

Keywords: Pesticides; Carbamates; Carbendazim; immunoassay; polyclonals antibodies.

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MODIFICATION, PHYSICOCHEMICAL CHARACTERIZATION AND POTENTIAL USE OF PINE CONE SAWDUST IN WASTEWATER TREATMENT

R. Ouafi[a,*], H. El Knidri[b], Z. Rais[a], M. Taleb[a], A. Laajeb[b], A. Lahsini[b]

[a]*Laboratory of Electrochemistry Engineering, Modeling and Environment. Faculty of Science, Dhar El Mahraz, Sidi Mohamed Ben Abdellah University, Fez, Morocco.*
[b]*Catalysis, Materials and Environment Laboratory, Higher School of Technology, Sidi Mohamed Ben Abdellah University, Fez, Morocco.*

**For correspondence: redouane.ouafi@usmba.ac.ma*

Abstract

Heavy metals pollution is becoming one of the major environmental problems requiring intensive efforts to be solved. New technologies, easy to implement deserve special attention. Indeed, adsorption using untreated and pretreated sawdust to remove heavy metals from wastewater has shown its proofs as a promising alternative to traditional physicochemical methods. These available and cheap materials can be involved in an efficient and economically appealing process of depollution **[1-3]**.
This study investigates the physicochemical characterization, the pretreatment and the potential use of pine cone sawdust. The sawdust samples were chemically modified using acid and basic treatment. A composite of pine cone sawdust and chitosan was prepared as well.
The characterization was realized in order to determine the physical and chemical properties of the modified sawdust and obtain information on the active sites involved in the pollutants adsorption. Physicochemical characterization includes Scanning Electron Microscope (SEM), Fourier Transform Infrared spectroscopy (FTIR), etc.

Keywords: Sawdust; chitosan; physicochemical characterization; modification.

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SYNTHESIS AND CHARACTERIZATION OF BENZIMIDAZOLE-2-THIONE DERIVATIVES FOR HEAVY METAL EXTRACTOR APPLICATIONS

A. Moussaif[1,*], Y. Abidi[1,*], Y. Ramli[3], F. Hlimi[2], A. El Yahyaoui[1], H. El Bari[4], E.M. Essassi[2]

[1]*National Center of Energy, Sciences and Nuclear Techniques, Rabat, Morocco*
[2]*Laboratory of Heterocyclic Organic Chemistry, Mohammed V University, Rabat, Morocco*
[3]*Medicinal Chemistry Laboratory, Faculty of Medicine and Pharmacy, Mohammed V University, Rabat, Morocco*
[4]*Laboratory of Biotechnology, Environment and Quality Ibn Tofail University - Kenitra – Morocco*

**For correspondence: Email: a.moussaif@cnesten.org.ma*

Abstract

For more than a century, human activities related to metal production have had a significant impact on natural environments, leading to an accumulation of metals in soils, sediments and waters. Heavy metals are present in all compartments of the environment, but in general in very small quantities.
In the context of the removal of toxic metals from liquid media (drinking water), we develop new molecules derived from benzimidazole-2-thione. These chemical modifications, with respect to the starting molecule, affect the structure of the molecule at depth and make it possible to obtain a hydrophilic cavity capable of binding the metals. In addition to their fundamental interest, these ligands exhibit, depending on the partial or total chemical substitution of the residual amine and mercaptan functions, a selectivity with respect to the heavy metal ions, with respect to the physiological cations such as Ca^{2+}, K^{+}, etc. ...
The complexation of 1,2-bis (2-mercaptobenzimidazolyl) ethane by polluting metals Hg (II), Pb (II) and Cd (II) raised the problem of how metal-benzimidazole interactions are described. We have shown that the latter are different depending on the metal used. This result in the type of complex obtained for each metal.

Keywords: Complexation; heavy metals; benzimidazole; organic sensor; ligand.

REGIO- AND STEREOSPECIFIC SYNTHESIS OF A NOVEL DIMETHOXYDIBROMO INOSITOL

Latif Kelebekli*, Kadir Aksu

Department of Chemistry, Ordu University, 52200 Ordu, Turkey

**For Correspondence: Email: lkelebekli@odu.edu.tr*

Abstract

Inositols and their derivatives are important class of biologically active natural products **[1]**. Interestingly one or more methyl ethers of these inositols have been isolated from plants and these methyl inositols are presumed to have important functions in plant biology. *Chiro*-inositol is one of naturally occurring inositol isomers, in which d -chiro-inositol has been effectively employed in management of polycysic ovary syndrome **[2]**. In addition to this, *myo*-Inositol and D-*chiro*-inositol, which are inositol izomers, have been showed to possess insulin-mimetic properties, found acting as second messengers in the insulin intracellular pathway **[3]**. Recently, their methyl-inositols or methoxy inositols have been synthesized from some natural compounds **[4]**. In connection with the inositols, halo-substituted inositols (such as dimethoxydicloro compound, methoxydibromo, dimethoxyfloro compound) have also gained importance over the last decade **[5]**.

Dimethoxydibromo inositol was synthesized starting from p-benzoquinone. Bromination of p-benzoquinone was followed by the reduction of the carbonyl groups with $NaBH_4$ to give a dioldibromo compound. Dimethoxy conduritol-B was synthesized from the reaction of the dioldibromo compound with CH_3ONa in methanol followed by controlled bromination to obtain a novel inositol derivative. The structures of all synthesized compounds were characterized by spectroscopic methods.

Keywords: Inositol, methoxy conduritol-B, halogene inositol.

*This study is supported by a grant (Project Number: **AR-1324**) from Scientific Research Projects Committee of Ordu University.

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QUANTUMCHEMISTRYINVESTIGATIONOFSOLVENTEFFECTONTHEIONIZATION POTENTIALOFTWOANTI-INFLAMMATORYMOLECULES:ASPIRINAND ACETAMINOPHEN

H. Amzal

Laboratoire de Biochimie-Immunologie, Faculté des Sciences, 4 Avenue Ibn Battouta B.P.: 1014 RP, Rabat - Morocco

For correspondence: Email: amzalhassane@gmail.com

Abstract

Antioxidant activity is tightly related to molecular electronic structure and to solvent. In this theoretical investigation, i have used Ab-initio method and accurate solvation model to explore the molecular electronic structure and to compare the electron -mediated antioxidant activity of two anti-inflammatory drugs (aspirin and acetaminophen) in gas and in the polar solvents (water and ethanol). Quantum calculation had been done at the DFT level theory including solvation model (SM8) for sightseeing electronic structures and prediction of an antioxidant indicator: ionization energy. DFT calculations at BP86 level theory and at the 6-31+G(d) basis set show that: Where an electron transfer is the processes underlying antioxidant activity, acetaminophen is more powerful antioxidant than aspirin in a gas phase, water and ethanol. A decrease of IP is observed from gas to polar solvent for acetaminophen and aspirin. The electron transfer is more facilitated in the polar solvents(waterandethanol)thaningas.

Keywords: Antioxidant; Aspirin; Acetaminophen; Ionization Potential; DFT; Solvation Model, SM8.

SYNTHESIS AND CHARACTERIZATION OF NEW ISOXAZOLES PREPARED VIA 1,3-DIPOLAR CYCLOADDITION

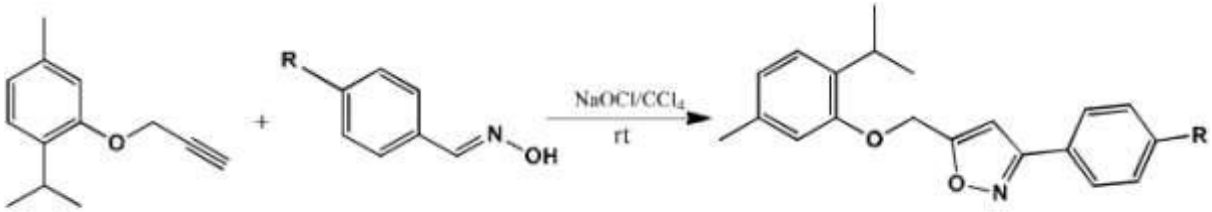
Azzeddine Sahbi, El Mestafa El Hadrami*, Abdeslem Ben-Tama

Laboratoire de Chimie Organique Appliquée, Université Sidi Mohamed Ben Abdellah, Faculté des Sciences et Techniques, Route d'Immouzer, BP 2202 Fès, Maroc

**For Correspondence: Email: elmestafa.elhadrami@usmba.ac.ma*

Abstract

1,2-Isoxazoles are oxygen–nitrogen (O,N) heterocycles that are important building blocks for the construction of a variety of compounds with medicinal applications **[1]** exhibiting antitumor **[2]**, anti-HIV **[3]**, antifungal **[4]**, antibacterial **[5]** and anti-inflammatory [6] functionalities. In addition to their potential applications, they can be conveniently modified, allowing thus the transformation of molecules with simple structures into functional complex systems **[7,8]**. This makes them very attractive intermediates with synthetic utility **[9]**.
we report herein the preparation of a series of isoxazoles heterocycles containing thymol fragment. Indeed, the 1,3-dipolar Cycloaddition of thymol with various aryl nitrile oxide moieties has afforded a new set of thymol-1,2-isoxazole compounds with promising biological activities.



Keywords: isoxazoles; 1,3-dipolar Cycloaddition; thymol.

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SYNTHESIS AND CHARACTERIZATION OF AMINO BI-1,2,3-TRIAZOLES

S. Hajib, A. El Hallaoui, A. Alami*, S. El Hajji, H. Faraj, B. Labriti, and N.Bergadi

Laboratoire de Chimie Organique, Université Sidi Mohamed Ben Abdellah, Faculté des sciences Dhar EL Mahraz, BP: 1796, Fès, Maroc.

**For correspondence E-mail: alamianouar@yahoo.fr*

Abstract

Lately, heterocyclic compounds containing in their structure 1,2,3-triazole framework have attracted considerable attention owing to their applications in pharmaceutical and agrochemical domains **[1,2]**. They are most commonly assembled by 1,3-dipolar cycloaddition reaction of azides and alkynes. In fact, the cycloaddition between an organic azides and alkynes lead to 1,2,3-triazole unite **[3]**. As an alternative approach Click chemistry represent a useful pathway to synthesis these kind of heterocyclic compounds with high regioselectivity **[4]**.
In continuation of our ongoing research **[5,6]**, we describe herein the synthesis of bicyclic compound contain two rings of 1,2,3-triazol framework, from 2-amino-2-ethylpropane-1,3-diol as starting material in three steps.
Products obtained in the various stages of syntheses are characterized by the spectroscopic methods of analyses.
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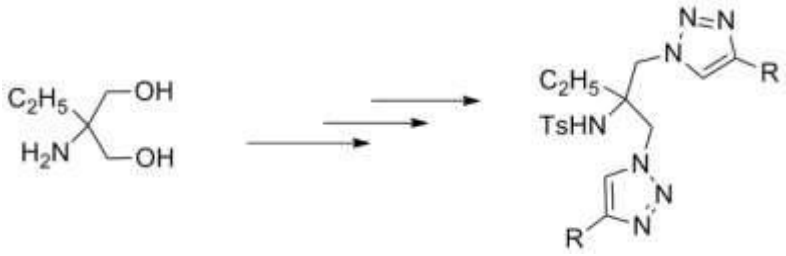

Keywords: 1,2,3-triazole; azide; 1,3-dipolar cycloaddition; Click chemistry.

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SYNTHESIS AND CARBONIC ANHYDRASE INHIBITORY PROPERTIES OF NOVEL CYCLOHEXANONYL BROMOPHENOL DERIVATIVES [1]

Abdullah Menzek[a,*], Halis T. Balaydin[a,c], Murat Şentürk[d]

[a]*Department of Chemistry, Faculty of Sciences, Atatürk University, Erzurum-25240, Turkey.* [b]*Artvin Çoruh University, Education Faculty, Artvin-08000, Turkey*
[c]*Recep Tayyip Erdoğan University, Education Faculty, Rize-53100, Turkey.*
[d]*Agri Ibrahim Cecen University, Department of Chemistry, Agri-04100, Turkey.*

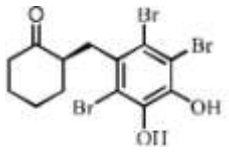
**For Correspondence: E-mail: amenzek@atauni.edu.tr*

Abstract

Natural product cyclohexanonyl bromophenol 2(R)-2-(2,3,6-tribromo-4,5-dihydroxybenzyl)-cyclohexanone (**1**) was synthesized as a racemic. In addition to this, its derivatives with Br, OMe, CO, and OH were also obtained. Carbonic anhydrase activities of synthesized the compounds were investigated.

Introduction

The naturally occurring cyclohexanonyl bromophenol **1** was isolated bromophenol from the red alga *Symphyocladia latiuscula and* and its antioxidant property was reported **[2]**.



Cyclohexanonyl bromophenol 1

Result and Discussion

Reaction of starting material 1,2,4-tribromo-3-(bromomethyl)-5,6-dimethoxybenzene with enamine derivatives of cyclohexanone gave derivatives with OMe of natural compound **1** as racemate. But, demethylation of this compound did not give natural compound **1** as racemate. This natural bromophenol **1** was obtained by derivatives with OAc of starting material. Other derivaties of **1** were also obtained. Inhibition of four human carbonic anhydrase (hCA, EC 4.2.1.1) isozymes I, II, IV, and VI, with synthesized compounds was investigated.

Keywords: Carbonic anhydrase; bromination; bromophenols; cyclohexanone with benzyl; enamine.

Authors thank DPT (2010K120440), Artvin Çoruh university (2011-F30.02.21 and the other universities.

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SYNTHESIS, X-RAY CRYSTAL STRUCTURE AND CATECHOLASE ACTIVITY INVESTIGATION OF NEW LIGANDS DERIVED FROM DHA

A. Djedouani[a,b,*], H. Boulemche[a], S. Tabti[a], Y. Benrabah[a], H. Mousser[a,b], R. Touzani[c,d]

[a]*Laboratoire de Physicochimie Analytique et Cristallochimie des Matériaux Organométalliques et Biomoléculaires, université Constantine 1, route Ain el bay 25000 , Algérie.*
[b]*Ecole normale superieure de constantine, ville universitaire Constantine 3, 25000, Algérie.*
[c]*Laboratoire de Chimie Appliquée et Environnement, LCAE-URAC18, COSTE,Faculté des Sciences, Université Mohamed Premier, BP524, 60000 Oujda, Morocco.*
[d]*Faculté Pluridisciplinaire Nador BP 300, Selouane, 62702 Nador, Maroc.*

**For correspondence: Email: djedouani_amel@yahoo.fr*

Abstract

Schiff bases are important precursors in various organic syntheses. The Schiff base ligands are immense coordinating compounds. It forms stable complexes with different transition metal ions. The mixed ligand complexes formation was an important aspect in inorganic and analytical chemistry. The uses of mixed ligand complexes in various fields diverted us to develop novel methodologies with increased atom economy, they are also used as catalyst.
In this study we tested the ability of copper complexes with Schiff bases ligands, prepared in situ as catalysts in the oxidation reaction of catechol O-quinone in the presence of air oxygen **[1-3]**.
We found that the catalytic activity of the complexes studied is influenced by different parameters:

- The nature of the ligands,
- The nature of the anions which bind with the metal,
- The nature of the solvent,
- The substrate concentration.

Keywords: Catecholase; Copper; Oxidation reaction; Schiff base.

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ANTI-CORROSIVE PROPERTIES OF 1,4-BENZOTHIAZINE DERIVATIVES ON MILD STEEL CORROSION IN 1M HCl SOLUTION: EXPERIMENTAL AND THEORETICAL STUDIES

K. Abdu[a,c,d,*], N. Kheira Sebbar[a*], H. Elmsellem[b], M. Ellouz[a], F. Hlimi[a], N. Abad[a], I. Ben Maïmoun[c], A. Dahdouh[d], E.M. Essassi[a,e]

[a]*Laboratoire de Chimie Organique Hétérocyclique, Centre de Recherche des Sciences des Médicaments, Pôle de Compétences Pharmacochimie, Faculté des Sciences, Rabat, Morocco.*
[b]*Laboratoire de chimie analytique appliquée, matériaux et environnement (LC2AME), Faculté des Sciences, BP. 717, 60000 Oujda, Morocco.*
[c]*Laboratoire de Physico-Chimie des Matériaux, Université Abdelmalek Essaâdi, Faculté des Sciences, BP 2121, 93000 Tétouan, Morocco.*
[d]*Laboratoire de Chimie Organique Appliquée Université Abdelmalek Essaâdi, Faculté des Sciences, BP 2121 Tétouan, Morocco.*
[e]*Moroccan Foundation for Advanced Science, Innovation and Research (MASCIR), Rabat Design Center, Rue Mohamed Al Jazouli, Madinat El Irfane, Rabat, Morocco.*

**For correspondence: Email: khaledabdufsr@gmail.com*

Abstract

1,4-Benzothiazin-3-one derivatives possess various pharmacological properties and play vital role in neurodegenerative diseases, such as Parkinson's disease and Alzheimer disease **[1]**, vasodilators **[2]**, anti-cataract agents **[3]**, dopamine D4, Na^+/H^+ exchange inhibitors **[4]**, matrix metalloproteinase inhibitors **[5]**. The corrosion inhibitory effect of two benzothiazine derivatives, namely 2-(3-oxo-2,3-dihydro[1,4]-benzothiazin-4-yl)acetic acid (P1) and 2-(2-benzylidene-3-oxo-2,3-dihydro[1,4]-benzothiazin-4-yl)acetic acid (P2) for mild steel in 1M HCl has been studied using electrochemical impedance spectroscopy (EIS), Tafel polarization curves and weight loss measurements. It was found that the inhibition efficiency of the two investigated inhibitors increases with increase in concentration of inhibitors. P1 and P2 show corrosion inhibition efficiency of 92 and 90%, respectively at 10^{-3}M and 308 K. Impedance experimental data revealed a frequency distribution of the capacitance, simulated as constant phase element. Potentiostatic polarization study showed that P1 and P2 are mixed-type inhibitors in 1M HCl. The results obtained from electrochemical and weight loss studies were in reasonable agreement. The adsorption of P1 and P2 on steel surface obeys Langmuir's adsorption isotherm. The correlation between inhibition efficiency and molecular structure of the inhibitors is investigated by determination of chemical indexes, which were performed using density functional theory (DFT) at (B3LYP/6-31G) (d,p) level.

Keywords: 1,4-Benzothiazine; Mild steel; Polarization; Electrochemical impedance spectroscopy; Quantum chemical calculations (DFT).

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SYNTHESIS OF BENZIMIDAZOLONE, BENZIMIDAZOLOTHIONE AND BENZIMIDAZOLE DERIVATIVES FROM 2-ACETYLCYCLOHEXANONE

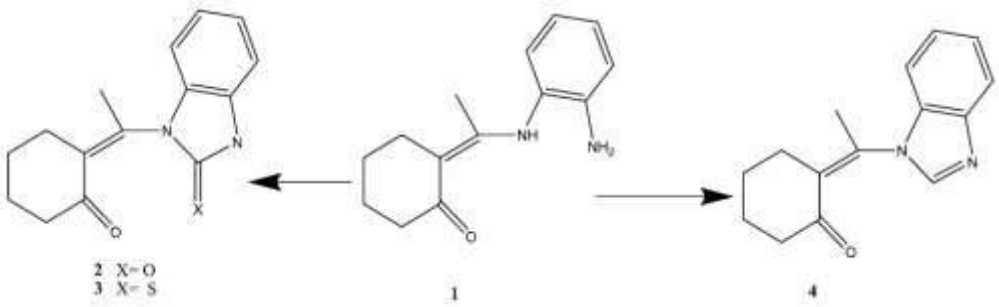
R. M. Bachar[a], M. Derdour[a], N. Belkheiri[a], M. Amari[a], **M. Fodili[a,*]**, P. Hoffmann[b]

[a]*Université Ziane Achour, Laboratoire de Chimie Organique & Substances Naturelles, Djelfa, Algeria*
[b]*Université de Toulouse, UPS, LSPCMIB (Laboratoire de Synthèse et Physico-Chimie de Molécules d'Intérêt Biologique)*

**For correspondence: Email: fodilimokhtar@hotmail.com*

Abstract

The benzimidazolone and benzimidazolothione ring structures possess a number of interesting biologically properties and constitute a constrained ring system with two nitrogen atoms linked by an ethylene bridge, as diazoles ring system **[1,2]**. As part of our effort to study the reactivity of diamine derivatives in Mannich type reactions, we previously report the synthesis of a series of benzimidazoles, benzimidazolones and benzodiazepines starting from o-phenylenediamines **[3]**. Here the study is extended to the condensation of a series of ophenylenediamines (O-PDA), triphosgene, thiosulfide and DMA-DMF with 2-Acetylcyclohexanone leading to new benzimidazolones **2**, benzimidazolothiones **3** and benzimidazoles derivatives, respectively, passing by intermediate **1** (Scheme).



Keywords: 2-Acetylcyclohexanone; benzimidazolone; benzimidazolothione; Benzimidazole.

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VICARIOUS NUCLEOPHILIC SUBSTITUTION IN NITRO DERIVATIVES OF INDAZOLES

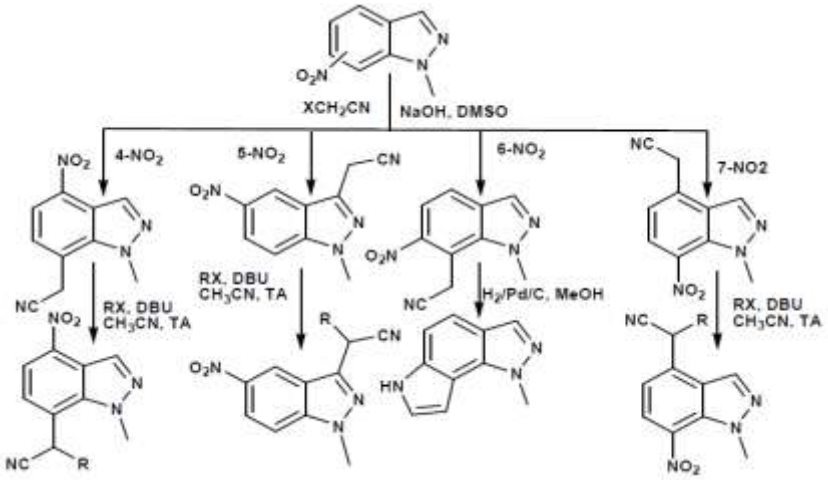
M. Eddahmi*, L. Bouissane, E. M. Rakib*

Laboratoire de Chimie Organique et Analytique, Faculté des sciences et Techniques, Université Sultan Moulay Slimane, BP : 591, Beni-Mellal, Maroc.

**For correspondence: Email: elmostapha1@ymail.com / eddahmi.med@gmail.com*

Abstract

Vicarious nucleophilic substitution (VNS) of hydrogen provides a convenient method for the introduction of functional groups into aromatic and heterocyclic rings [**1-4**]. This two-step reaction proceeds via addition of carbanions containing leaving groups X at the carbanionic center to the nitroaromatic ring followed by the base-induced β-elimination of HX from intermediate σ-adducts. The products of VNS reactions are key intermediates in the synthesis of useful and new heterocyclic compounds. In this communication, we investigated the VNS reaction of nitroindazole derivatives with 4-chlorophenoxyacetonitrile to obtain new substituted indazole derivatives as precursors for the synthesis of polyheterocyclic compounds of pharmacological importance. Indazole derivatives have been used widely in medicinal chemistry and drug discovery [**5-9**].



Keywords: nitroindazoles; VNS, substituted indazole.

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EFFECT OF MINERAL STRESS ON MORPHO-PHYSIOLOGICAL PARAMETERS OF *TRIGONELLAE FOENUGRAECI*

S. Errai[a,*], A. Maataoui[b], H. Bezaidi[b], M. Elmidaoui[b], M. Benbella[b]

[a]*Laboratory of Physiology, Pharmacology Health and Environment Unit of Bioremediation and Environment Department of Biology. Faculty of Sciences Dhar EL Mahraz, Université Sidi Mohamed*
[b]*National School of Agriculture, Meknes, Morocco*

**For correspondence: Email: siham.errai1@usmba.ac.ma*

Abstract

Trigonellae Foenugraeci is an extremely important medicinal plant for health, its use and very common in Morocco. The objective of this work is to study the response of fenugreek (Trigonellae Foenugraeci) on mineral stress. To meet this objective, a test was conducted hydroponically in a growth chamber at the Department of Agronomy in the National School of Agriculture. Seedlings were transplanted into nutrient solution with two plants per pot with a capacity of 600ml. Nutrient solutions tested corresponded to 10 % (T1), 20 % (T2) and 40 % (T3) Hoagland solution. Parameters of growth and development in both species were measured. The results showed that almost all parameters of growth and development were affected by mineral stress. At the end of the experiment, plant height of T1 was significantly reduced by 41% compared to T3. The stress treatment (T1) has developed a number of branches per plant much higher (3.5) than in the T3 treatment (2.16). The rate reductions in leaf area at T1 were 73.58 % compared to the control. The total solids accumulated in T3 were greater than 34% compared to 70DAS accumulated in T1. Reducing the number of pods in T1 compared to T3, was of the order of 67 %. Similarly, the number of seeds per pod and 1000 seed weight were affected by mineral stress, respectively 1 and 7 against 13.3 and 3.4 g. Similar results were obtained by **[1,2,3]**.

Keywords: *Trigonellae Foenugraeci*; mineral stress; hydroponics; growth; development.

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SYNTHESIS, CHARACTERIZATION AND ANTIMICROBIAL ACTIVITY OF NEW HETEROCYCLIC CARBOXYLIC α,α-DIAMINOESTERS

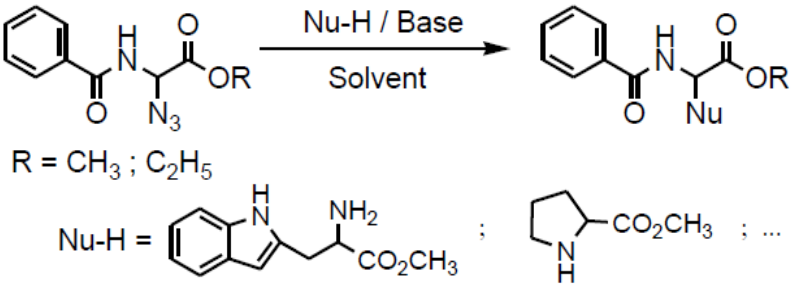
O.Karai, H. Faraj, A. Alami*, A. El Hallaoui, B.Labriti, S.El Hajji, Y.Aouine

Laboratoire de Chimie Organique, Faculté des Sciences Dhar El Mehraz, Université Sidi Mohamed Ben Abdellah, BP : 1796,Fés, Morocco

**For Correspondence: E-mail: alamianouar@yahoo.fr*

Abstract

Due to their important biological activities, the synthetic heterocyclic α-amino acids are widely studied and they have found interest and applications in many fields of chemistry, biochemistry and pharmacy **[1]**.
Continuing our research concerning heterocyclic α-amino acids which present interesting biological activity **[2]**, we present here the synthesis of new carboxylic α,α-diaminoesters derivatives .
Our strategy is based on the nucleophilic substitution of methyl α-azidoglycinate N-benzoyl-ated with different functionalized amines (scheme).



The prepared compounds were tested in vitro for their antibacterial activity against Gram-positive bacteria (Basillus subtilis and staphylococcus aureus), than Gram-negative bacteria (Escherichia coli and salmonelle).
The structures of obtained compounds were confirmed by ^{1}H, ^{13}C NMR, IR, Mass spectrometry, Elemental analysis and X-ray analysis.

Keywords: Amino acid; Heterocyclic compound, Amine; Nucleophilic substitution; Methyl α-azidoglycinate.

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SYNTHESIS OF NEW 2(3H)-BENZOXAZOLONE,6-[1-OXO-3-(2- FURANYL)-2-PROPENYL] AND SPECTRAL INVESTIGATION WITH ADVANCED NMR TECHNIQUES AND THE NMR SHIFT REAGENT [Eu(fod)3]

Cavit Kazaz[a,*], Sinan Bilginer[b], Feyza Sena Engin[b], Halise İnci Gül[b]

[a]*Department of Chemistry, Faculty of Science, Atatürk University, 25240,Erzurum Turkey*
[b]*Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Ataturk University, 25240, Erzurum*
**For Correspondence: Email:* ckazaz@atauni.edu.tr

Abstract

NMR shift reagents have experienced increasing popularity particularly in the area of spectral clarification. Chemical shift reagents are organic complexes of paramagnetic rare earth metals from lanthanide series. One of the commonly used complexes in the determintaion of structures of organic compounds is tris-(7,7-dimethyl-1,1,2,2,2,3,3-heptafluoroocta-7,7-dimethyl-4,6-dionato)-europium-III **Fig.1**, frequently abbreviated as Eu(fod)3.

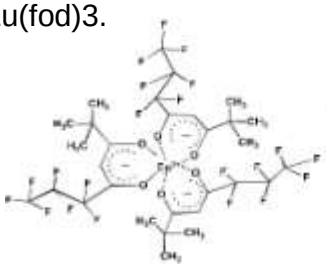

Fig.1

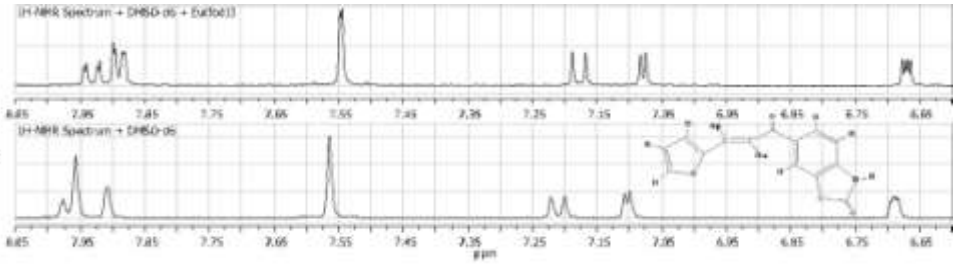

Fig.2

Keywords: NMR Shift Reagent; the Multiplicity of the Signal; 2D NMR.

Introduction

Lanthanide complexes produce spectral simplification in the NMR spectrum of any compound with relatively basic pair of electron (an unshared pair) which can coordinate with Eu^{+3}. Typically, aldehydes, ketones, alcohols, thiols, ethers and amines all interact **[1]**. The amount of chemical shift of protons depend on the distance separating the metal (Eu^{+3}). Because chemical shifts of several groups of protons are all very similar, which shows their proton resonances in the same area of the spectrum and often peak overlap so extensively that individual peaks and splitting can not be extracted. In this case, this method is very useful for structural assignments.

Result and and Discussion

In this work, the structural assignments of 2(3H)-Benzoxazolone,6-[1-Oxo-3-(2-Furanyl)-2-Propenyl] compound **[2]** was elucidated by NMR shift reagent [Eu(fod)3] and advanced NMR techniques **[3]**. Gül and her group synthesized of 2(3H)-Benzoxazolone,6-[1-Oxo-3-(2-Furanyl)-2-Propenyl] compound seen in the ^{1}H-NMR spectrum **Fig.2**. However, it was observed in the ^{1}H-NMR spectrum that the proton signals do not overlap with the structure of the compound. Especially, the signals of α-β protons resonances were in the same area of the spectrum. 10 mg of Eu(fod)3 was added to the sample to determine the multiplicity of the signal. Thus, the multiplication of the signals in the ^{1}H-NMR spectrum of the compound recorded as a result of coordination of Eu^{+3} with the nucleophilic centers was clearly observed**.**

We are grateful to Atatürk University for supporting this work.

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RISKS ASSOCIATED WITH TOXIC CHEMICAL ELEMENTS RESPONSIBLE FOR ENDOCRINE DISEASES IN THE DOKKARAT_VILLE AREA OF FEZ

Fatimazahra Elmadani[a,b,*], N. Idrissi[a,b], N.H. Mtarfi[a,b], Y. Metarfi[a,b], A. Omor[a,b], K. El Rhazi[c], M. Merzouki[a,d], M. Taleb[a,b], Z. Rais[a,b]

[a]*Faculty of Science Dhar El Mahraz, Sidi Mohamed Ben Abdallah University, Department of Chemistry*
[b]*Laboratory of Electrochemistry, Modeling and Environment Engineering (LIEME), Faculty of Sciences Dhar El Mahraz, Sidi Mohamed Ben Abdallah University*
[c]*Laboratory of Epidemiology, Clinical Research and Community Health. Faculty of Medicine and Pharmacy of Fez, Sidi Mohamed Ben Abdallah University*
[d]*Laboratory of Biotechnology (LB), Faculty of Medicine and Pharmacy of Fez, Sidi Mohamed Ben Abdallah University*

*****For correspondence: Email: elmadani.fatimazahra@gmail.com*

Abstract

In Morocco, the revolution in industrial and agricultural activities is contributing to the increase in water pollution, which causes the appearance of serious diseases of endocrine origin. The industrial sector is experiencing widespread use of toxic chemicals that threaten the environment and humans in a disturbing and alarming way, some of which is transported by water in the neighboring oued or infiltrated by soil into the aquifers groundwater.

The objective of this study is to know the main causes of toxic chemicals responsible for endocrine disrupters in the population adjacent to the estimated polluting industries of the zone Dokkarat - city of Fez.

The study consisted first of all of a cross-sectional epidemiological survey of 380 people from the study population and, secondly, an assessment of the polluting load of oued waters near the area studied.

The analysis of the survey data shows a strong correlation between the excessive use of chemicals and the appearance of endocrine pathological signs and the evaluation of the pollutant load of oued Fez waters, which are analyzed by measurement of physico-chemical and biological parameters, the majority of the results of which do not comply with the standards for surface water quality.

***Keywords*:** Endocrine disruptors; pollutants; epidemiological study; contamination.

ENVIRONMENTAL BEHAVIOR OF CEMENT MORTARS ENCLOSING SEWAGE SLUDGE ASH

S. Naamane*, N.H. Mtarfi, F.Z. Bouaich, Z. Rais, M. Taleb

Laboratory of electrochemical engineering, modeling and environment, Faculty of Sciences Dhar El Mehraz, BP 1796, 30000 Atlas, Fez, Morocco

**For correspondence: Email: saranaamane@hotmail.com*

Abstract

Certainly the reuse of wastes and by-products as cementitious additions brings technical, economical and environmental benefits to cement. However, this reuse should not disregard the hazardous nature of these wastes. Consequently, it is essential to study the environmental behavior and the leachability of cement mixtures enclosing wastes.

This paper investigates the leachability of cement based mortars containing various percentages of the waste material obtained from the incineration of sewage sludge, i.e. sewage sludge ash (SSA). The SSA were characterized by inductivity coupled plasma-atomic emission spectrometer, X-ray diffraction, scanning electron microscopy, and fourier transform infrared analysis, plus NF EN 12457 and XP CEN/TS 14429 leaching tests. Additionally, the influences of SSA on mortar physical and mechanical properties were also examined. The leaching behavior of heavy metals in crashed and monolithic mortars were assessed using NF EN 12457, XP CEN/TS and 14429 NF PX31-211 leaching tests. Results illustrate that the use of SSA in cement based materials is environmentally feasible and proves to be a suitable way of a safe reuse of SSA.

Keywords: Sewage sludge ashes; Cement; Physico-chemical and mechanical characterization; leaching behavior; Environmental evaluation.

VALORIZATION OF EUCALYPTUS WOOD SAWDUST IN THE PRODUCTION OF ACTIVATED CARBON AND ITS APPLICATION IN THE TREATMENT OF PRETREATED OLIVE MILL WASTEWATER

Z. Majbar[a], I. Adadi[a], K. Lahlou[a], M. Ben Abbou[b], M. Nawdali[c], H. Bouka[b], M. Taleb[a], M. El Haji[d], Z. Rais[a,*]

[a]*Laboratory of Engineering, Electrochemistry and Modeling Environment (LEEME), Faculty of Sciences Fez,Morocco.*
[b]*Laboratory of Natural Resources and Environment, University Sidi Mohammed Ben Abdallah Faculty Polydisciplinary, Taza, Moccoro .*
[c]*Laboratory of Chemistry of Condensed Matter (LCCM), University Sidi Mohammed Ben Abdallah, Faculty of Sciences and Technology, Fez, Morocco.*
[d]*Laboratory Engineering research - OSIL team Optimization of Industrial and logistics Systems, University Hassan II, Superior National School of Electricity and Mechanic (ENSEM), Casablanca, Morocco.*

**For correspondence: Email: zakia.rais@usmba.ac.ma*

Abstract

Activated carbons are materials which are characterized by a good adsorption capacity of several kinds of pollutants. However, they are very expensive despite their effectiveness. Our study contributes on the one hand to the production of an activated carbon from the eucalyptus wood processing residues, and on the other hand to its use as an adsorbent material for the treatment of olive mill wastewater (OMW) pretreated by electrocoagulation because of their high charge of non-biodegradable organic matter.
Activation of the wood sawdust was carried out by phosphoric acid and modified by hydrochloric acid (CA-HCl).
The adsorption of pollutants on wood sawdust activeted charbon was evaluated by the measurement of chemical oxygen demand (COD), phenolic compounds and color intensity. Influence of contact time, adsorbent mass, initial pH and initial concentration of OMW to phenolic compounds and COD on the effectiveness of the treatment was determineted. The results of the adsorption were modeled by Langmuir and Frendlich isotherms.
The characterization of the pretreated OMW shows that they are slightly acidic, carry a non-biodegradable organic charge of 48 g of $O_2.L^{-1}$, and a phenolic charge of 1.81 $g.L^{-1}$.
The adsorption kinetics record that the optimal time of adsorption of these pollutants is 4 h 30 min and is described by a pseudo second order kinetics. The adsorption isotherms of the various adsorbent / adsorbate couples studied are satisfactorily described by the Freundlich model.

Keywords: adsorption; olive mill wastewater; kinetic; isotherms.

CATALYTIC SYNTHESIS OF AMINOALCOHOLS IN ONE STEP FROM OLEFINS VIA α-BROMOALCOHOLS

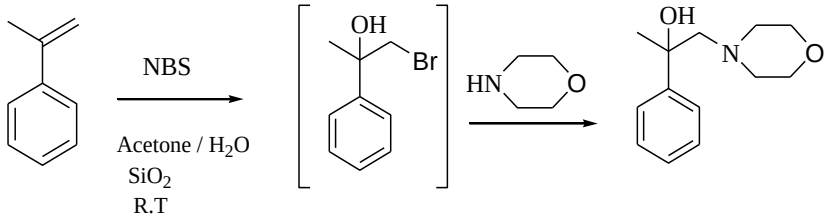
S. Oubaassine*[a, b], B. Boualy[c], L. El Firdoussi[a]

[a]*Equipe de Chimie de Coordination et Catalyse, Département de Chimie, Université Cadi Ayyad, Faculté des Sciences Semlalia, BP 2390, 40001 Marrakech, Morocco.*
[b]*Leibniz-Institut für Katalyse e. V. (LIKAT Rostock) Albert-Einstein-Str. 29 a 18059 Rostock, Germany*
[c]*Laboratoire de Chimie et Modélisation Mathématique, Université Hassan 1er, Faculté Polydisciplinaire de Khouribga, B.P 145, 25000 Khouribga, Morocco*

For Correspondence: Email: oubaassine.89@gmail.com

Abstract

Aminoalcohols are structural units present in many synthetic and natural products possessing potent biological activity **[1]**. Indeed, the 1,2-aminoalcohol's function is present in the widely consumed drug propanolol, a β–blocking agent and in the structure of serine protease inhibitors **[2-4]**. They have attracted more the attention of chemists with a number of different strategies being devised for their construction **[5-7]**
Herein, we report an efficient novel methodology for the regioselective synthesis of 1,2-aminoalcohols from vicinal bromoalcohols prepared in-situ from alkenes. The optimization of these reactions was studied with methylstyrene, chosen as model substrate, in the presence of catalytic amount of SiO_2.



Commercially available silica (SiO_2) was found to be highly effective catalyst for one-pot synthesis of vic- aminoalcohols from olefins via α–bromoalcohols using morpholine as nitrogen fragment donor. The conversion of various olefins has been successfully carried out under mild conditions. This novel methodology led to the corresponding aminoalcohols in a good to excellent yields and shows a high degree of regioselectivity.

Keywords: aminoalcohols; α–bromoalcohols; olefins; amines.

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DEVELOPMENT OF NEW ANTIBACTRIAL AGENTS

Assia Keniche [1,2] , Samia Bellifa , Hafida Hassaine and oseph Kajima Muengi

[1]*Laboratoire de Chimie Organique, Substances Naturelles et Analyses (COSNA). University of Tlemen, Algeria.*
[2]*Centre Universitaire de Maghnia, Tlemcen, Algeria.*
[3]*Laboratoire de microbiologie appliquée à l'agroalimentaire au biomédical et a l'environnement (LAMAABE), University of Tlemen, Algeria.*

Corresponding author: keniche assia yahoo.fr

Abstract

By using the peptide coupling protocol, a simple straightforward synthesis of functionalized aziridines has been developed. By means of this synthetic strategy from readily available N-phtaloyl acide and 2- methylbenzosulfonate aziridine using DCC as coupling agent, new tosylates aziridines could be obtained. The coupling reactions occurred without ring opening of the three membered ring. This work describes new results of our ongoing research targeting new derivatives of biological interest. All the compounds were screened for their antibacterial activity, they all showed comparable moderate to good growth inhibitory activity with reference to Tetracyclin and Gentamicin.

Keywords: Aziridines, phtaloyl acide, strained heterocycles, Antibiotics.

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SYNTHESIS AND ANTIDEPRESSANT ACTIVITY OF 5-(BENZO[B]FURAN-2-YLMETHYL)-6-METHYLPYRIDAZIN-*3(2H)*-ONE DERIVATIVES

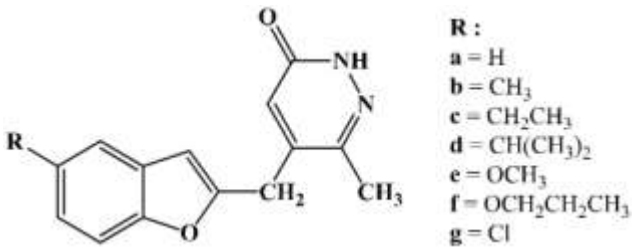
Y. Boukharsa[1,*], B. Meddah[2], R. Yvette Tiendrebeogo[2], A. Ibrahimi[4], J. Taoufik[1], Y. Cherrah[2], A.Benomar[3], My E.A. Faouzi[2], M. Ansar[1]

Laboratory of Therapeutic Chemistry, Faculty of Medicine and Pharmacy, BP 6203, Rabat Institutes, Mohammed V University, Rabat, Morocco
Laboratory of Pharmacology and Toxicology, Pharmacokinetic Research Team, Faculty of Medicine and Pharmacy, Rabat Institutes, Mohammed V University, Rabat, Morocco
Faculty of Medicine and Pharmacy, Research Center for Clinical Epidemiology and Therapeutic Trials, Mohammed V University, Rabat Institutes, Rabat, Morocco
Biotechnology Laboratory, Faculty of Medicine and Pharmacy, Rabat Institutes, Mohammed V University, Rabat, Morocco

**For Correspondence: Email: boukharsay@yahoo.fr*

Abstract

A new series of pyridazin-3-one derivatives were designed, synthesized and evaluated for their pre-clinical antidepressant effect on Swiss mice. Among the series, compounds **6c**, **6d** and **6f** exhibited significant activity profile in forced swimming test. Compounds **6c** and **6d** were most efficacious, which at dose of 50 $mg.kg^{-1}$ reduced the time of immobility by 42.85 and 38.09 %, respectively, as compared to the standard drug fluoxetine which reduced the immobility time by 45.23 % at the dose of 32 $mg.kg^{-1}$. All the test and standard compounds were administered orally 60 min before the test. Interestingly, all active compounds did not cause any significant alteration of locomotor activity in mice as compared to control, indicating that the hybrids did not produce any motor impairment effects. The results indicate that pyridazin-*3(2H)*-one derivatives may have potential therapeutic value for the management of mental depression.



Keywords: Pyridazin-*3(2H)*-one derivatives; Antidepressant activity; Forced swimming test (FST); Locomotor activity.

Various Posters

ELABORATION AND CHARACTERIZATION OF SOLAR CELLS BASED ON PEROVSKITE MATERIALS

Choukrallah Karim[a,b,*], Lmai Fatima[a] and Derkaoui Souad[b]

[a]*Laboratory of Renewable Energy and Dynamics of Systems (LREDS) Faculty of Sciences Ain chock University Hassan II of Casablanca*
[b]*Laboratory of Physics of Materials, Microelectronics, Automatic and Thermal Transfer (LPMMATT) Faculty of Sciences Ain chock University Hassan II of Casablanca.*

**For correspondence: Email: karimchoukrallah@gmail.com*

Abstract

Solar energy is one of the most important resources in our modern life. Photovoltaic is the most im-portant technology to render the solar energy usable since photovoltaic solar cells harvest light coming from sun and convert sunlight into electrical energy. Recently, an amazing light perovskite absorber was introduced into the so-called solid-state dye sensitized solar cells (ssDSSC) system to replace the dye, opening the new field of research. Perovskite solar cells (PSCs) open a new era in photovoltaic. Applications based on hybrid (organic-inorganic) perovskites have flourished in recent years, Since the boom of the latter as a low-cost material for cells Photovoltaics. Hybrid perovskite has become "black gold" for cells Photovoltaics. Since 2009, the date of first introduction of a hybrid perovskite in A photovoltaic cell, the efficiency of these cells has quadrupled, and has just reached Record yields equal to those of silicon-based cells. The predicted yield for Perovskite-based cells is of the order of 30%, thus exceeding that of the cells silicon.
Hybrid perovskites are semiconductor molecular crystals containing a portion Organic and an inorganic part, obtained by self-assembly during spin-coating on a substrate.
The subfamily of perovskites of type AMX3, called perovskites 3D, has very good conduction proper-ties and an optical gap for collecting. The wavelengths of the solar spectrum, it is therefore very well suited to applications Photovoltaics.
The components in the perovskite solar cell include: the compact metal oxide blocking layer, the elec-tron transport layer, the lead halide perovskite layer, the hole transport layer and the back contact, we focused on the preparation and improving the properties of the electron transport layer and the perov-skite layer.

Keywords: Solar energy; photovoltaic, perovskite; hybrid; 3D.

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EXTRACTION OF POLYPHENOLS (WASTEWATER, OLIVE LEAF) BY MICROWAVE, CLASSIC AND COLD HEATING

N. Sylla*, H. Elhajji, K. El Kacem

Laboratoire de chimie Analytique et d'électrochimie, Faculté des sciences Université Mohamed V, BP : 10000, Rabat, Maroc.

For Correspondence: Email: nabinty62@yahoo.fr

Abstract

The present work is a comparison between microwave-assisted extraction, extraction by conventional heating and cold extraction of the polyphenols contained in the mixture (Wastewater, olive leaf). The olive leaves are added to the wastewater to enrich it with polyphenols. Microwave-assisted extraction has the advantage of reducing the extraction time and the extract obtained is richer in polyphenols. This has been shown by qualitative and quantitative analysis of the various extracts obtained by the three different extraction techniques, carried out by spectrophotometry at different wave lengths 280, 330 and 350 nm, by HPLC, Antioxidant activity and the level of total polyphenols and flavonoids.

***Keywords*:** Wastewater; Olive leaves; Polyphenols; Extraction; Microwave.

REACTIVE POWER COMPENSATION BASED ON CAPACITOR BANK IN PRESENCE OF RENEWABLE ENERGY

M. Dib*, A. Nejmi

Laboratoire d'Automatique, de Conversion d'Energie et de Microélectronique, Faculté des Sciences et Techniques, Université Sultan Moulay Slimane, BP : 523, Béni Mellal, Maroc.

**For correspondence: Email: dib2017.mohamed@gmail.com*

Abstract

If solar panels are installed and connected to an industrial electrical installation, the active power absorbed by the power grid decreases due to the power supplied by the photovoltaic system and consumed by the installation. Thus, the ratio between the reactive and the active power absorbed by the network changes.

Particular attention must therefore be paid to compensation to avoid paying penalties because of a low cos phi which could seriously reduce the economical benefits of a renewable energy facility.

The compensation equipment must be reviewed, both for the installed capacity and for the type of construction.

Metalized and impregnated paper capacitors are the most robust solution for industrial compensation. The resistance of these capacitors is obtained thanks to the excellent mechanical characteristics of the paper, to which are added the properties of the oil impregnation.

Metalized paper capacitors are particularly suitable for electrical installations with high harmonic currents and / or very high operating temperatures. They are used in making filters on "troubled" installations.

Indeed, thanks to the stability of their capacity over time, these capacitors make it possible to maintain the adjustment of the filter's frequency, even in the presence of very high operating temperatures

Keywords: Reactive power; active power; capacitor bank; renewable energy.

PALLADIUM NANOPARTICLES SUPPORTED NATURAL PHOSPHATE: A HIGH EFFICIENT AND RECYCLABE CATALYST FOR DEHYDROGENATION

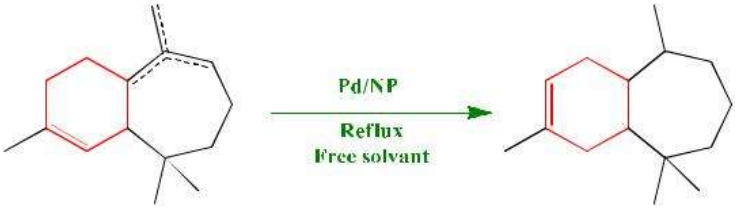
Mekkaoui Ayoub Abdelkader[a,b,*], Jennane Sanae[a], El Houssame Soufiane[a], Boualy Brahim[a], El Firdoussi Larbi[b]

[a]*Laboratoire de Chimie et Modélisation Mathématique, Université Hassan 1er, Faculté Polydisciplinaire de Khouribga, B.P : 145- 25000 Khouribga Morocco.*
[b]*Equipe de Chimie de Coordination et Catalyse, Département de Chimie, Université Cadi Ayyad, Faculté des Sciences Semlalia, BP 2390, 40001 Marrakech, Morocco.*

**For Correspondence: Email: mekk.ayoub@gmail.com*

Abstract

Heterogeneous catalysis is a catalytic process with two types of catalysts: bulk and supported. The supported catalyst plays a crucial role according to their high surface area, their controllable porosity and well defined structure.
As part of our studies directed toward the development of a new supported catalyst, we have focused our attention on the preparation and characterization of palladium supported catalysts due to their high performance.
Herein, we report the preparation of different catalysts supported on natural phosphate (Pd/NP) by incipient wetness impregnation method. Firstly, Palladium nanoparticles (Pd°) was prepared and supported on natural phosphate by incipient wetness impregnation method followed by calcination at 600°C for 3h. Furthermore the follow-up of reduction and preparation of palladium nanoparticles was carried out by UV-vis spectra. Moreover the prepared catalyst was characterized by IR, XRD, SEM, EDX and BET analysis.



As a catalytic application of the prepared Pd/NP catalyst, aryl himachalene was successfully prepared in a higher yield from naturally occurring himachalenes. In order to improve the feasibility of our system, the catalytic aromatization reaction of different terpenes has been carried out.

Keywords: Supported catalyst; natural phosphate; palladium nanoparticles; dehydrogenation; terpenes.

EFFECT OF HEAT TREATMENT ON THE SURFACE PROPERTIES OF SELECTED BITUMINOUS SHALE FOR CATIONIC DYE SORPTION

Asmae Gouza*, Kenza Fanidi, Sanaa Saoiabi, Abdelaziz Laghzizil, Ahmed Saoiabi

Laboratoire de Chimie Physique Générale, Faculté des Sciences, Université Mohammed V, Av. Ibn batouta BP.1014 Agdal Rabat, Morocco,

**For correspondence: Email: Asmae_gouza@yahoo.fr*

Abstract

Due to increasing contamination of water and soils by industrial production, there is a crucial need for new natural sorbents that are cost-effective, environmental friendly for pollutant removal. In this context, Moroccan oil shale from Tangier Region (OST) was characterized and evaluated for methylene blue (MB) remediation as model for cationic dye **[1-5]**. The maximal sorption capacity of the dried OST100 (>100 mg g^{-1}) is higher than that of calcined OST550 (80 mg g^{-1}) and OST950 (60 mg g^{-1}) samples. The pseudo-second-order kinetic model and Freundlich equation were found the most adequate to reproduce the experimental data. The effect of the thermal treatment of this oil shale on its sorption capacity was investigated, demonstrating that the active sites from shale play an important role for MB removal. As a result, this natural, widely available and low-cost resource can be a good adsorbent used for many removal applications of specific pollutants.

Keywords: Oil shale; Thermal treatment; Valorization; Surface properties; Dye adsorption

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HEMISYNTHESIS OF NEW 1,2,3-TRIAZOLE SYSTEMS DERIVED FROM A MAJOR ACTIVE INGREDIENT OF CLOVE ESSENTIAL OIL

A.Taia, M. Essaber, A. Aatif, M. Adardour, A. Kaouni and Y. Dizrofo

Laboratory of Molecular Chemistry, Department of Chemistry, Faculty of Sciences Semlalia, BP 2390, Cadi Ayyad University, 40001, Marrakech, Morocco.
E-mail : tatamajid@gmail.com

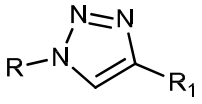
Abstract

Studies on essential oils have shown that they have a broad spectrum of activity as antioxidants, anti-inflammatory, antibacterial, antiviral ... [1].

In order to contribute to the valuation of the essential oil of cloves, we have studied the reactivity of its main active ingredient and the hemisynthesis of these new analogues by fusion of a heterocyclic five-membered 1,2,3-triazoles.

The importance of 1,2,3-triazole systems lies in their antibacterial, antiviral, antiepileptic, antiallergic [3,5], anti-cancer [6] and antimorphic biological activities [7]. Their synthesis was reported for the first time by Pechmann in 1888 [2].

The new 1,2,3-triazole systems are obtained in a good yield and regioselectively by reacting the true alkyne with different types of azides.



1,2,3- Trlazollc compound

Keywords: Essential oil, main active ingredient, 1,2,3-triazole, 1,3-dipolar cycloaddition, pharmaceutical, biological activity.

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RHENIUM(I) AND TECHNETIUM(I) COMPLEXES OF A NOVEL TRIAZOLE-BASED ON LIGAND CONTAINING AN ARYLPIPERAZINE PHARMACOPHORE

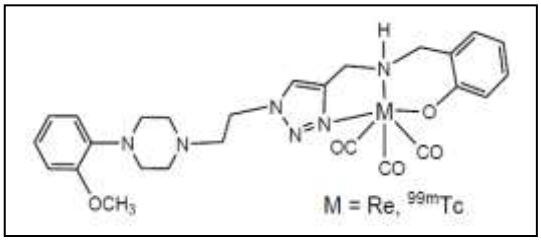
Achour SERIDI[a,b,*], Yassine AIMENE[b], mekki KADRI[b], Eric BENOIST[a]

[a]*Laboratoire de synthèse et de physicochimie de molécules d'intérêt biologique (SPCMIB) - UMR 5068 - CNRS-Université Paul Sabatier 118, route de Narbonne - 31062 Toulouse cedex 09 .France*
[b]*Laboratoire de Chimie Physique, Université de Guelma, BP401, 24000 Guelma, Algérie.*

**For correspondence: Email: seridi_a@yahoo.fr*

Abstract

The design, synthesis, and preliminary radiolabeling evaluation of new N,N,O-type triazol – amino - phenol ligand for the $[M(CO)_3]^+$ core, where M= ^{99m}Tc or Re, are described. The capability of the ligand to bind this technetium core is initially demonstrated by using the cold substitute $[Re(CO)_3]^+$. We opted for the click chemistry as a synthetic strategy (schem1) to prepare these new ligand. The interest of this reaction between an azide and an acetylene derivative regiospecifically leads to 1,2,3-triazoles 1,4-disubstituted mild operating conditions allow the use of azides and / or acetylenic compounds variously functionalized and the triazole ring can participate in the complexation of various metal ions ("Click chelate concept" developed by R. Schibli) [4]. Spectral data, of the rhenium (I) complex as well as the ^{99m}Tc-labelling are reported. Both complexes were neutral and iso-structural. Moreover, the ^{99m}Tc-complex presented a suitable lipophilic character for its use as a CNS imaging agent. These new tridentate, ligand is able to chelate the $[^{99m}Tc(CO)_3]^+$ core because radiolabeling yields ranged from 85-90% and the resulting complexes were stable as long as 24 h.



Scheme 1. Studied metallic complexes

Keywords: Triazol; Click chemistry; rhenium; technetium.

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NOVEL COMPOSITE CATALYST FROM PALLADIUM AND NANOCELLULOSE AEROGEL FOR CROSS-COUPLING CATALYTIC PROCESSES: PREPARATION AND APPLICATIONS FOR ACCESS TO NEW BIOACTIVE HETEROCYCLIC MOLECULES

Ouafa Moujahid[a,*], M.L. Belachemi[a,*], H. Kaddami[a], Y. Madich[a,b]

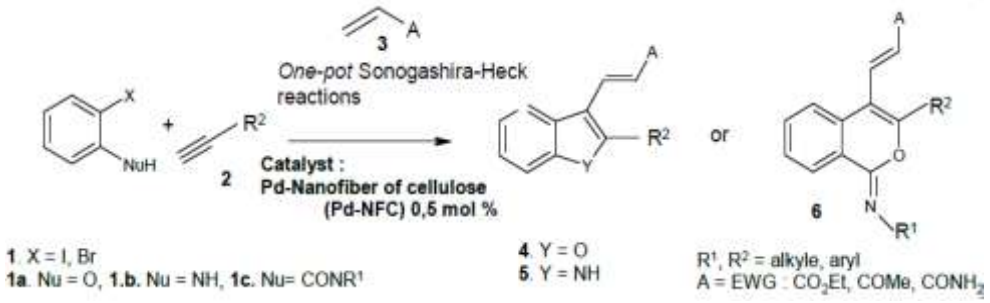
[a]*Laboratory of organometallic and Macromolecular chemistry – Composites materials, department of chemical sciences – Faculty of Sciences and Technology of Marrakech - University Cadi Ayyad*
[b]*Universidad del Pais Vasco UPV/EHU, Departamento de Quimica Organica II, Facultad de Ciencia y tecnologia, Apartado 644, Bilbao, 48080, Spain.*

**For correspondence: E-mail: Ouafa.moujahid@gmail.com; belachemi@yahoo.fr*

Abstract

These last years, a considerable number of homogeneous palladium catalysts have been used to obtain high yields of desired product. However, separation of catalyst and ligands from the final product is the problem to be solved. In this regard, studies on heterogeneous catalysts have drawn much attention because they can be easily separated and recovered **[1,2]** despite the fact that their catalytic activity is lower than that of homogeneous catalysts. Nowadays, green chemistry has attracted considerable attention particularly in organic synthesis due to its economic and environmental aspects **[3,4].** An increasing number of studies have focused on variety of supports for the immobilization or incarceration of palladium (0) nanoparticles with aim of showing biodegradability, water –miscibility and the metal ion uptake ability for palladium catalyzed cross-coupling reactions.

In this paper, the palladium catalysts supported on a matrix of cellulose nanofibers aerogel (NFC) were prepared and characterized. These Pd-catalysts have been used in heterogeneous catalysis to perform cross-coupling reactions to lead to new heterocyclic derivatives. We have already described the preparation of products **4-6** in preparatively useful yields starting from Sonogashira adducts derived from functionalized haloarenes **1** and alkynes **2**, and then using palladium- catalyzed *one-pot* Sonogashira/heterocylization/Heck-type-coupling cascades with an alkene **3** under oxidative conditions reactions and under homogeneous catalysis **[5]**.



Keywords: cellulose nanofiber; palladium; catalysts; Heck and Sonogashira reactions.

References

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SYNTHESIS AND ELASTASE INHIBITION OF THIOPHENYL SUBSTITUTED HYDROXYIMINO ESTERS

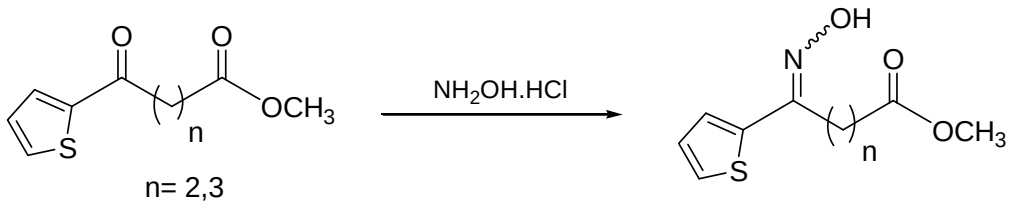
B. Hasdemir[1*], Ö.Saçan[2], H. Yasa[1], H. Başpınar Küçük[1], A.S. Yusufoğlu[1], R. Yanardağ[2]

[1]Division of Organic Chemistry, Department of Chemistry, Faculty of Engineering, Istanbul University, 34230-Avcilar, Istanbul, Turkey
[2]Division of Biochemistry, Department of Chemistry, Faculty of Engineering, Istanbul University, 34230-Avcilar, Istanbul, Turkey

**For correspondence: Email: karaefe@istanbul.edu.tr*

Abstract

Oximes are very important compounds in organic synthesis and they can be successfully transformed to amide, amine, hydroxylamine and nitrile etc. Moreover, oxime compounds have gained great important in medicinal chemistry because of their potential biological activities such as antibacterial [1], antitumor [2] and antiviral [3] etc.
In this study is aimed to synthesize and investigate the elastase inhibition activities of novel hetereoaryl substituted keto oxime esters. In the literature there is no data on the synthesis and the elastase inhibition of these compounds.



The obtained hydroxyimino esters were identified by spectroscopic (IR, ^{1}H-NMR, ^{13}C-NMR and Mass) analysis. All the test compounds exhibited antielastase activity. The enzyme inhibitory activities of these novel hydroxyimino esters were found to increase dose dependently.

Keywords: Hydroxyimino ester; elastase; inhibition

References

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SYNTHESIS AND CHARACTERIZATION OF SOME NEW HETEREOARYL SUBSTITUTED δ-KETIMINE ESTERS

B.Hasdemir*, H.Yaşa, T.Yıldız, H.B. Küçük

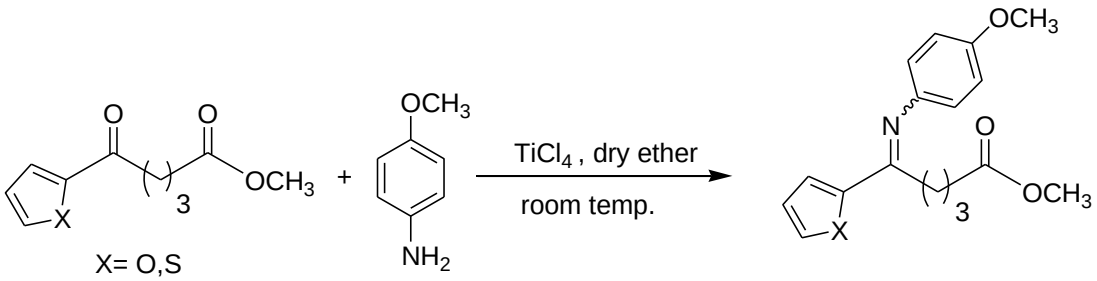
Istanbul University, Faculty of Engineering, Department of Chemistry, Organic Division, 34320 Avcilar-Istanbul/Turkey

E-mail: karaefe@istanbul.edu.tr

Abstract

Imines are compounds containing an azomethine group and are known as Schiff bases. These compounds are biologically important due to the presence of >C=N moiety, therefore, they are a class of important compounds in medicinal and pharmaceutical field. In recent years, several studies have been reported that imine compounds show biological activities including antibacterial [1], antifungal [2] and anticancer activities [3] [.

In this study, new hetereoaryl substituted δ-ketimine esters were synthesized by condensation of p-anisidine with keto esters in presence of lewis acid.



The obtained ketimine esters were identified by spectroscopic (IR, ^{1}H-NMR, ^{13}C-NMR and Mass) analysis. The isomerization (*E*/*Z* ratio) of these compounds was determined by ^{1}H-NMR spectrum.

Keywords: keto ester; ketimine ester; lewis acid.

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