BADJI MOKHTAR-ANNABA UNIVERSITY
FACULTY OF SCIENCES
Chemistry Department

# The first International Seminar on Medicinal Chemistry and Green Chemistry (1st IS MCGC)

November 13 to 14, 2024—Annaba, Algeria

# BOOK OF ABSTRACTS


AJET



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The first International Seminar on Medicinal Chemistry and Green Chemistry (1st IS MCGC)

November 13 to 14, 2024—Annaba, Algeria

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**Pr. BERREDJEM Malika:** Laboratory of Applied Organic Chemistry

**Seminar President**

**Pr. DJILANI Salah Eddine:** Laboratory of Synthesis and Organic Biocatalysis

**Editor**

Dr. Neghmouche Nacer Salah

**Editor-in-chief of journal**

Pr. Abdelkrim Rebiai

Published, January 2025.

# Acknowledgment

Dear Colleagues,

On behalf of the organizing committee, we would like to sincerely thank you for attending the First International Seminar on Medicinal Chemistry and Green Chemistry (1st IS MCGC), which was held at the University of Annaba, Algeria, on November 13-14, 2024.

The 1st IS MCGC aimed to bring together researchers, practitioners, and educators to exchange and share their experiences and research findings, as well as discuss practical challenges and solutions in the fields of Medicinal Chemistry and Green Chemistry. The seminar provided an excellent opportunity for scientific knowledge-sharing, fostering collaborations, and laying the groundwork for multidisciplinary and interdisciplinary research in these critical fields.

With the theme “Medicinal Chemistry and Green Chemistry,” the event featured two days of scientific sessions, keynote and invited lectures, oral and poster presentations, as well as valuable networking opportunities and a unique social program.

We deeply appreciate your participation and contributions, which played a crucial role in making the 1st IS MCGC a successful and enriching event. We look forward to future editions and continued collaboration in advancing research and innovation in Medicinal and Green Chemistry.

Yours sincerely,
Organizing Committee of 1st IS MCGC

# The first International Seminar on Medicinal Chemistry and Green Chemistry (1st IS MCGC)

**November 13 to 14, 2024 - Annaba, Algeria**

# Program


| | |
|---|---|
| 08h 00 – 09h 00 | **Reception of participants.** |
| 09h 00 – 09h 45 | **Official Opening** |

**SESSION CHAIRS : Pr. BERREDJEM Malika, Pr. DJILANI Salah Eddine**

**09h 45 – 10h 15** | **PLENARY CONFERENCE 1**

**Pr. HACINI Salih, University Oran 1**

**10h 15 – 10h 45** | **PLENARY CONFERENCE 2**

**Pr. KABOUCHE Zahia, University of Constantine 1**

**11h 00 – 11h 30 : Snack + POSTERS SESSION 1**

# ORAL SESSION 01

| | ROOM 1 | ROOM 2 | ROOM 3 |
|---|---|---|---|
| SESSION CHAIRS | Pr. LIACHA Messaoud<br>Pr. OUMEDDOUR Rabah | Pr. El-HATTAB Mohamed<br>Pr. HABA Hamada | Pr. ATTOUI YAHIA Ouassila<br>Pr. KADRI MEKKI |
| | Thematic conferences | | |
| 11h 30– 12h 00 | Pr.MARMINON Christelle | Pr. CHERITI Abdelkrim | Pr. DJOUAD Seif Eddine |
| 12h 00– 13h 30 | OR-001 ADJLANE Noureddine<br>OR-002 BACHA Maroua<br>OR-004 BENAOULA Sid Ahmed<br>OR-006 BOUSSAFI karima<br>OR-008 FEKIH Yasmine<br>OR-009 MAKHLOUF Mohammed Rabeh<br>OR-010 OUAMAR Fatma Lynda<br>OR-011 OUGHILAS.A | OR-27 BOUKRAÂ Djamila<br>OR-29 BOUGUERRA Nadia<br>OR-30 DALIA Farid<br>OR-32 MEKAOUI Radja<br>OR-33 MEZIANE KACI Zoubida<br>OR-34 BENAZZOUZ Kinza<br>OR-45 BELOUNIS Yousra | OR-57 BOUSKIA Soumaya<br>OR-58 ALEM Karima<br>OR-59 OTMANE RACHEDI Khadidja<br>OR-60 HIMRI Safia<br>OR-61 GHAMRI Mariem<br>OR-63 SOUKEHAL Souha Fatma Zohra<br>OR-64 HASNI Nour |

**13h 30 – 14h 30 Lunch**

# ORAL SESSION 02

| | ROOM 1 | ROOM 2 | ROOM 3 |
|---|---|---|---|
| SESSION CHAIRS | Pr. BOUCHAREB Fouzia<br>Pr. MERABET Mounia | Pr. KABOUCHE Zahia<br>Pr. CHERITI Abdelkrim | Pr. LANEZ Touhami<br>Pr. TRIKI Houria |
| 14h 30 – 16h 00 | OR-012 SANDELI Abd el-krim<br>OR-013 AMRI Yazid<br>OR-014 BADAOUI Kawther<br>OR-015 BANDOU Samira<br>OR-016 BOUATROUS Yamina<br>OR-005 BOUONE Yousra Ouafa | OR-037 TOUATI Naima<br>OR-038 KANTAOUI Aicha<br>OR-039 DJEKIDEL Alia<br>OR-041 BOUMAAZA Nour El-Houda<br>OR-042 CHELGHAM Abdelhakim<br>OR-043 AIT SI SAID Chahinez | OR-052 MOALLA REKIK Dorsaf<br>OR-057 BOUSKIA Soumaya<br>OR-036 MEHALAINE Souad<br>OR-051 BEDJOU Fatiha |

**16h 00 – 16h 30 : Coffee break + POSTERS SESSION 2**

# ORAL SESSION 03

| | ROOM 1 | ROOM 2 | ROOM 3 |
|---|---|---|---|
| SESSION CHAIRS | Pr. BERREDJEM Malika<br>Pr. MARMINON Christelle | Pr. AKKAL Saleh<br>Pr. TAIBI Faiza | Pr. DJILANI Salah Eddine<br>Pr. HAMEL Tarek |
| 09h 00 – 9h 30 | Thematic conferences | | |
| | Pr. KıRKıN GÖZÜKıRMıZı Celale | Pr. EL-HATTAB Mohamed | Dr. AIT KAKI Samira |
| 9h 30 – 10h 15 | OR-017 BOURAS Hadj Daoud<br>OR-018 HAMANA Haoua<br>OR-003 BAHADI Rania<br>OR-020 LAIB Ibtissam | OR-048 KECIS Hadjer<br>OR-049 BEN AMEUR Raoudha<br>OR-025 DEHMCHI Farouk<br>OR-065 ABDALLAH A. Mohamed | OR-046 ATIA Amina<br>OR-062 DADDA Noureddine<br>OR-053 DEMMAK Rym Gouta |

**10h 15 – 10h 45 Coffee break + POSTERS SESSION 3**

# ORAL SESSION 04

| | ROOM 1 | ROOM 2 | ROOM 3 |
|---|---|---|---|
| SESSION CHAIRS | Pr. BERREDJEM Malika<br>Pr. MARMINON Christelle | Pr. AKKAL Saleh<br>Pr. TAIBI Faiza | Pr. DJILANI Salah Eddine<br>Pr. HAMEL Tarek |
| 10h 45 – 13h 00 | OR-021 LANEZ Elhafnaoui<br>OR-022 MOUHEB Lynda<br>OR-023 SIRID Remache | OR-044 BEN MANSOUR Rim<br>OR-035 ALIBOUDHAR Hamza | OR-026 AMIRAT Sabrina<br>OR-028 TOUDERT Nadia<br>OR-055 BOUTEMEDJET Siham |

**13h 00– 13h 30 Closing Remarks, Awards Distribution**

**13h 30 Lunch**

# POSTER SESSIONS

**13/11/2024**

**SESSION 01: 11h00 – 11h30**

**SESSION 02: 16h00 – 16h30**

**14/11/2024**

**SESSION 03: 10h 15 – 10h 45**

## POSTERS SESSION 1

| JURY 01 | | JURY 02 | |
|---|---|---|---|
| Pr. BOUZEMI Nassima (Presidente) | | Dr. BOUASLA Radia (presidente) | |
| Dr. FEDDAOUI Dalila | | Dr. MELLOUK Karima | |
| Dr. REDJEMIA Rayenne | | Dr. GRINE Sara | |
| Dr. GHODBANE Racha | | phD. MANSOURI Achraf | |
| PhD. ALEM Aya | | PhD. BOUSSAKER Meriem | |
| P-002 | ACHOURI Rahma | P-151 | NADJI Ayoub |
| P-006 | BEKOUCHE Karima | P-152 | AZABI Warda |
| P-008 | BENREGGA Fatima Zohra | P-153 | BAATOUCHE Samia |
| P-012 | BOUBESSIL Mohamed | P-156 | BOUAFINA Khawla |
| P-013 | BOUGUESSA Sabrina | P-157 | BOUTAMDJA M. |
| P-014 | BOUKERCHE Khadidja | P-158 | DALIA Farid |
| P-022 | GHOUAFRIA Imane | P-160 | HAMDOUCHE Nadira |
| P-026 | HADJI Maroua | P-161 | LAROUM Rima |
| P-027 | HAIOUR Hasna | P-166 | ABRANE Rahma |
| P-031 | KRID Ferial | P-167 | REDJILI Selma |
| P-032 | KHELAF Rahima | P-168 | REZGOUN Sarra |
| P-033 | KHELFAOUI Malika | P-174 | ZOUCHOUNE Soria |
| P-038 | MANSAR Lina Nourhane | P-175 | ZOUIED  Daoiya |
| P-041 | MOUSSAOUI S | P-178 | RIAH Amel |
| P-043 | BOUASLA Nabila | P-179 | BOUKOUCHA Nada Hiba |
| P-044 | CHEMMAM Dounya Achwak | P-191 | RAHMANI Amina |
| P-045 | BENKHEDIR Abdelkarim | P-192 | HAMADA Hakim |
| P-046 | KEMMOUNDJI Aida | P-194 | DJILANI Imene |
| P-050 | FATMI Widad | P-195 | OTMANI Amar |
| P-053 | DJEGHADER Nour El-Houda | P-197 | BOUDEBAZ Khadidja |
| P-054 | AMIRA Khedidja | P-202 | CHOUIT Hanifa |
| P-061 | TENSAOUT Fatima | P-204 | MESSIKH Samia |
| P-062 | BOUNAAS Jihane | P-205 | BAIRA Kaouther |
| P-064 | SAKER Hichem | P-208 | ZINE Mounia |
| P-065 | ATTIA Amel | P-210 | KHAMMAR Rachida |
| P-066 | BOUFADENE Wassim | P-215 | LAFIFI Ismahan |
| P-067 | MEKDADE Loubna | P-217 | GHAMMIT Fehd |
| P-073 | BOUDEHANE Esma | P-219 | BENSAAD Mohamed Sabri |
| P-074 | BEKACHE Nour-elhouda | P-222 | LATRECHE Hanane |
| P-075 | MELLAHI Lamia | P-224 | REDJEMIA Rayenne |
| P-100 | ALLAOUA Zina | P-226 | AISSAOUI Mohamed |
| P-120 | BOUAFIA Zineb | P-227 | ALI RACHEDI Sofiane |
| P-123 | NASRI Meriem | P-228 | GHODBANE Racha |
| P-132 | GOUASMIA Raounak | P-233 | KADRI Rayene |
| P-135 | OUNISSI Ismahan | P-234 | RAZI Samra |
| P-136 | RAHAL Sarah | P-230 | DEKIR Ali |
| P-143 | TAFER Radia | P-236 | BOUDJOU-MECHOUCHE Souhila |
| P-146 | TORCHE Khouloud | P-149 | ALI AHMED Atef |
| P-148 | AOUACHRIA Chaima | P-242 | HAMMADI Maroua |

# POSTERS SESSION 2

| JURY 01 | | JURY 02 | |
|---|---|---|---|
| Pr. FERCHICHI Loubna (presidente) | | Dr. TOUDERT Nadia (Presidente) | |
| Dr. BENABBAS Rihab | | Dr. ZEKKAD Faridar | |
| Dr. SEDIK AMEL | | Dr. BAHADI Rania | |
| PhD. AMAMRA Roumaissa | | PhD. SAYED Rayene | |
| PhD. ZERRAD Chaima | | PhD. TLIBA Sourour | |
| P-005 | ALEM Aya | P-137 | BEN AMEUR Raoudha |
| P-010 | BOUASLA Radia | P-138 | RIZI Aicha |
| P-023 | GRIB Ismahene | P-139 | ACIDI Anissa |
| P-028 | HARROUS Imene | P-140 | SAYAD Rayene |
| P-030 | HESSAINIA Sihem | P-141 | SILINI Ilhem |
| P-040 | MOUSSAOUI Kamilia | P-142 | SIZIANI D. |
| P-048 | DJEDIOUI.A | P-144 | TARMOUL Houria |
| P-055 | BENABBAS Rihab | P-145 | TLIBA Sourour |
| P-058 | BARKAT Ramzi | P-147 | ZADEM Achwaq |
| P-059 | ZERROUK Roumeila | P-150 | AYAD Rabha |
| P-071 | ZERRAD Chaima | P-162 | MAHIEDDINE Cherifa |
| P-079 | AMAMRA Roumaissa Halima | P-163 | MELIANI Habib |
| P-080 | BAKHOUCHE Imene | P-164 | MOULAOUI Kenza |
| P-084 | DIAF Ilhem | P-235 | MANSOURI Achraf |
| P-085 | CHAFAA Nassiba | P-169 | TALBI Amina |
| P-087 | AHMIDA meryem | P-170 | ZANOUNE Kheira |
| P-088 | CHOHRA Djawhara | P-171 | ZAOUT Samiya |
| P-090 | SALHI Rim | P-172 | ZEFFOUNI Zakia |
| P-091 | SMAIL Safa | P-173 | ZOUAMBIA Yamina |
| P-092 | BAMBRA Moussa Abderrazak | P-176 | BOUGHELOUM Chafika |
| P-093 | CHELOUFI Hadjer | P-177 | BOUSSAKER meriem |
| P-094 | BECHEKER Abir | P-180 | BOUTERFAS Karim |
| P-095 | MEKIRCHA Fatiha | P-181 | BELHANI Billel |
| P-096 | GHORBAL Imene | P-183 | BOUCHEBCHEB Yasser |
| P-097 | MEBARKI Salsabil | P-184 | CHETTIBI Naouel |
| P-098 | AGABI Rania | P-185 | HAMOUD Fares |
| P-099 | HAMEL Imene | P-188 | BEZZINA Belgacem |
| P-101 | DJELLOUL Karima | P-189 | OURDJINI Zeyneb |
| P-102 | BOUTENNOUN Hanane | P-190 | LAYACHI Fayçal |
| P-110 | AOUDIA Hassiba | P-196 | RIBOUH Nazih |
| P-111 | BOUSSOUF Lilia | P-198 | KADRI Amira |
| P-112 | BOUASLA Ihcéne | P-199 | ATHMANI Sameh |
| P-114 | BENKACEM Rayenne | P-200 | BOUGHELOUM Khadidja |
| P-115 | BLIDA Rafika | P-203 | BELDJEZZIA Dounia |
| P-116 | DAAS Nesma Abir | P-209 | LOULOU Fatma |
| P-119 | LEMBOUB Chama | P-212 | SEDIK Amel |
| P-121 | ALEM Samia | P-213 | MEZIANI Ouafa |
| P-128 | ZAKKAD Farida | P-214 | AITKAKI Samira |
| P-133 | OUATMANI Toufik | P-216 | SAKHRAOUI Houssem Eddine El Yamine |
| P-134 | OUNACEUR Linda Sabrina | P-223 | TOUHAMI Imen |

# POSTERS SESSION 3

| JURY 01 | | JURY 02 | |
|---|---|---|---|
| Pr. BENAMIA Fatiha (presidente) | | Dr. BENZAID Chahrazad (presidente) | |
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| Dr. CHOHRA Djawhara | | Dr. ACIDI Anissa | |
| Dr. BENTOUMI Houria | | Dr. CHEMAM Yasmine | |
| PhD. MEZIANI Ouafa | | PhD. KADRI Amira | |
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| P-004 | AHMED LHADJ Sarah | P-103 | GUIBADJ Fatma Zohra |
| P-007 | BENAKACHA amira | P-104 | FEKHAR Mohamed |
| P-009 | BENSEMMANE Nachida | P-105 | SABOUR Smain |
| P-011 | BOUAZZAOUI Naima | P-106 | KHETTAR Filicia |
| P-015 | BOUKHELKHAL Mounira | P-107 | AIT-KACI Aourahoun |
| P-016 | BOUMEDINE Titem Liza | P-108 | ABDELLATIF Fahima |
| P-017 | CHELLALI Ferial | P-109 | ABBADENI Kawther |
| P-018 | CHIHANI Ouijdane Malak | P-113 | BENKHERARA Salah |
| P-019 | DELLALI Mohammed | P-117 | BEN SALAH Hichem |
| P-020 | DRIOUECHE Asma | P-118 | BENJEMAA Mariem |
| P-021 | DRAOUI Aïcha | P-122 | RADJA Lydia |
| P-024 | Amel GUERGAB | P-124 | BEN MIRI Yamina |
| P-025 | HACHACHE Naima | P-125 | BOUKADA Fadhela |
| P-029 | HELLEL Djamila | P-126 | TURQUI Tarik |
| P-034 | LAZELA Kahina | P-127 | MEJRI Nahla |
| P-035 | Imane LAZOUNI | P-129 | DJERIBIA Nahla |
| P-036 | LETTREUCH Hichem | P-130 | BENZID Amina |
| P-037 | MAHI Ahmed | P-131 | BERKOUD Moussa |
| P-039 | MERAD N. | P-154 | BENAISSA Mohamed Rafik |
| P-042 | BEN AMOR Mohammed Larbi | P-155 | BENCHIKH Imen |
| P-047 | AOUIFFAT Yacine | P-159 | DERKAOUI Samira |
| P-049 | KORTI Amira | P-182 | ZIDANE Mohammed |
| P-051 | RAHMANI Salah-Eddine | P-186 | ANEDE Nada |
| P-052 | SAYADAA Nardjis | P-187 | ZITOUNI-NOURINE Saida Hanane |
| P-056 | TAMMA Noureddine | P-193 | BOUSEKKINE Hicham |
| P-057 | ABADI Abderrezzak | P-201 | GHRIEB Hana |
| P-060 | BENALIA Halima | P-206 | GRINE Nahla |
| P-063 | MAHAMMEDI Hichem | P-207 | BOUAOUNE Ahmed |
| P-068 | LABRI Khadidja | P-211 | REBIZI Mohamed Nadjib |
| P-069 | KAIFES Chaima | P-218 | AMARNI Meriem |
| P-070 | BENSMAIL Souhila | P-220 | ZAOUT Samiya |
| P-072 | Mami I. R. | P-221 | M'ZYENE Fatima |
| P-076 | BENSABEUR Badra | P-225 | BELGHIT Mohamed Yazid |
| P-077 | BENSATAL Ahmed | P-229 | DERARDJA Imene |
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| P-081 | LAROUCI Rania | P-231 | BOUAKKADIA Amel |
| P-082 | ZAITRI Mohamed | P-232 | HADDAG Hamza |
| P-083 | KIRED Ibrahim | P-237 | DADDA Noureddine |
| P-086 | ZAAKANE Abla | P-001 | ABDI Yamina |
| P-240 | SBARTAI Hana | P-238 | HACHAMI Yasmine Rahma |
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# PLENARY CONFERENCES

The 1st International Seminar on
medicinal chemistry and green chemistry
(1st IS MCGC - Annaba 2024)

## Plenary conference 1

# La synthèse organique : de l'alchimie à la chimie verte

Pr. Salih HACINI

*Laboratoire de Chimie Fine LCF, Université Oran1 Ahmed Benbella*

**E-mail** : s_hacini@hotmail.com

**Resumé**

Avec ses perspectives infinies de création de molécules, la synthèse organique représente le domaine clé de la chimie organique. Son objectif majeur reste l'élaboration d'enchaînements fonctionnalisés, carbone-carbone et carbone-hétéroatome, avec une structure spatiale bien déterminée.

L'Alchimie « al-Kīmiyā » du Moyen-âge (environ du IV$^{ème}$ siècle, jusqu'au début du XVI$^{ème}$ siècle) peut être considérée comme l'ancêtre de la chimie moderne. Elle se propagea à l'Occident par les conquêtes arabes, et c'est à cette période que la distinction entre les deux termes commença à se généraliser.

C'est au cours du XX$^{ème}$ siècle, avec les avancées majeures de la chimie organique de synthèse et de la biochimie, que les grandes synthèses spectaculaires d'antibiotiques, de vitamines et autres médicaments essentiels, ont été mises au point. La découverte et le développement de nouvelles molécules bioactives a toujours représenté, un domaine de recherche essentiel pour la santé de l'homme et en particulier pour l'augmentation de son espérance de vie.

Ces recherches se sont poursuivies avec le développement de nouvelles méthodologies de synthèse l'utilisation de nouveaux catalyseurs plus efficaces, ainsi que par l'apport de nouveaux outils de recherche comme l'analyse rétro-synthétique et la modélisation moléculaire.

Une grande variété de molécules-cibles, de complexité structurale et stéréochimique croissante, a été ainsi synthétisée à ce jour par les chimistes qui continuent à relever régulièrement d'autres challenges.

Actuellement, la synthèse s'appuie de plus en plus sur les principes de chimie verte.

Durant ces vingt dernières années, la synthèse organique a considérablement amélioré l'éventail de ses outils (réactions et stratégies) ainsi que leur efficacité, dans une vision de développement durable.

C'est ainsi que les termes éco-synthèse ou bien synthèse éco-compatible (synthèse économique et écologique) sont de plus en plus utilisés.

La synthèse de molécules s'appuie de plus en plus sur les principes du développement durable, en exploitant au mieux le «réservoir» des produits naturels (source de carbone renouvelable), dont une grande partie reste encore peu explorée.

Les principales étapes du développement de ces recherches en synthèse organique seront abordées et illustrées au cours de cet exposé.

**Mots-clés**: Synthèse organique, alchimie, méthodologies de synthèse, chimie verte, développement durable.

## Plenary conference 2

# Bioactive secondary metabolites of Algerian medicinal plants

Zahia Kabouche

*Université frères Mentouri-Constantine 1, Laboratoire d'Obtention des Substances Thérapeutiques (LOST), Campus Chaabet-Ersas, 25000 Constantine, Algeria*

**E-mail** : zahiakabouche@umc.edu.dz

**Abstract**

Bioactive secondary metabolites (triterpenoid saponins, triterpenes, diterpenoids, polyphenols…) are found in Algerian medicinal plants belonging to various families (Lamiaceae, Astaraceae, Caprifoliaceae, Caryophyllaceae, Rosaceae, Linaceae..). The antioxidant, antimicrobial, anti-Alzheimer, antidiabetic, anti-inflammatory, analgesic and anticancer activities of several compounds, isolated from the studied plants, have been evaluated. A chemotaxonomic significance is also investigated.

**Keywords:** Antioxidant, antimicrobial, anti-Alzheimer, antidiabetic, anti-inflammatory, analgesic, and anticancer

# THEMATIC CONFERENCES

## Thematic conference

# Indeno[1,2-b]indol-10-one, a convenient and versatile scaffold in medicinal chemistry

Christelle Marminon

*University Claude Bernard Lyon 1, Cancer Research Center of Lyon,*
*UMR CNRS 5286, INSERM 1052, Lyon, France, 69373, christelle.marminon@univ-lyon1.fr*

**Abstract**

Indeno[1,2-b]indol-10-ones **1** are heterotetracyclic compounds (Figure 1). When partially saturated, these analogues have been found to be promising CK2 inhibitors[1,2], a human protein kinase involved in various human diseases among others cancer, neurodegenerative diseases, virus infection as SARS-CoV2…When completely aromatized, they become potent inhibitors of ABCG2, the breast cancer resistance protein, member of the ABC (ATP-binding cassette) transporters, involved in treatment resistance in a variety of human malignancies through active efflux of anticancer drugs[3].

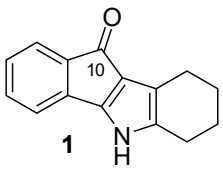


**Figure 1**: Structure of indeno[1,2-b]indol-10-ones **1**

In order to develop structure-activity relationship (SAR) studies, the original two step synthesis[4] was adapted. First, new eco-friendlier methods, using microwave irradiations or neat reactions for example, were developed to afford the desired key reagents i.e. substituted ninhydrins and enaminones. These analogues were then used to introduce substituents or functions on each of the positions, sometimes leading to regiochemistry concerns that will be discussed. Improvements were also made to afford the indeno[1,2-b]indol-10-ones.

Methods and optimizations to afford tailor made indeno[1,2-b]indol-10-ones will be presented, as well as their SAR on their two most important targets namely CK2 and ABCG2, two essential targets in the fight against cancer. But not only that, these compounds having shown others interesting activities...

**Keywords**: Indeno[1,2-b]indole-9,10-dione, CK2, ABCG2, microwave, SAR

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## Thematic conference

# Insights into the research of bioactive compounds and chimiotaxonomic patterns from the endemic warionia saharae

Abdelkrim CHERITI

*Phytochemistry and Organic Synthesis Laboratory*
*Faculty of Medicine, UTMB, Bechar, Algeria*

**E-mail**: karimcheriti@yahoo.com

**Abstract**

Medicinal plants in traditional pharmacopeia have been employed for the treatment and management of various ailments since the beginning of human civilization and continue to provide mankind with new remedies, such as, the Materia Medica of Ibn Baytar (Andalusia, Spain, 1197–1248), is one of the oldest documents that describe the use of natural products for healing diseases in the mediterranean area. Actually, about 50,000 species of higher plants have been used for medicinal purposes and major pharmaceutical drugs have been either derived from or patterned after compounds from biological diversity.

Algeria with its large area and diversified climate has a varied flora, which is a source of rich and abundant medical matter and, in particular, Sahara part constitutes an important reservoir of many plants, which have not been investigated until today. Among this flora, the medicinal specie Warionia saharae, an endemic to Algeria and Morocco growing in arid conditions has been used ethnobotanically for treatment of a variety of disorders.

The aim of this conference is to present the recent trends on the ethnopharmacological, phytochemical and biological activities of the endemic Warionia saharae. Sesquiterpene lactones, guaianolide-type sesquiterpene lactones, eudesmane type sesquiterpene, dimeric sesquiterpene lactones, dehydroleucodin, flavonoids as well as volatile compounds from essential oils, have shown to be the most common secondary metabolites, suggest that this endemic specie could be source of new bioactive compounds, and chemotaxonomic markers for the botanical Asteraceae family.

**Keywords:** Ethnopharmacopeae; Endemic; Asteraceae; Bioactivity; Sesquiterpene; Chimiotaxonomy; Sahara

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## Thematic conference

# Effects of nonthermal food processing technologies on the bioactive properties of spices and herbs

Celale Kırkın Gözükırmızı

*Department of Food Engineering, Faculty of Chemical and Metallurgical Engineering, Istanbul Technical University, Istanbul, Türkiye.*

**E-mail** : kirkin@itu.edu.tr

**Abstract**

Spices and herbs are basic ingredients of many food formulations. They are added to food in order to improve the flavor and color. Also, they have been known for their positive effects on human health, but they can be highly contaminated with microorganisms. Nonthermal technologies can be utilized for the decontamination of herbs and spices, as these methods do not lead to heat-related losses in the quality. For instance, gamma irradiation has been used for the sterilization of herbs and spices. In addition, other nonthermal methods, such as ultraviolet (UV) irradiation and cold plasma treatment, can be used for a similar purpose. Besides, the essential oils and extracts of herbs and spices can be effective in controlling the oxidation and microbial growth in foods. In addition, it is possible to employ nonthermal techniques, such as ultrasonication and pulsed electric field treatment, to enhance the extraction of bioactive compounds and the isolation of essential oils. However, these technologies can change the flavor, color, and bioactive composition of herbs and spices. Thus, the effects of nonthermal food processing technologies on the quality properties of herbs and spices, such as antioxidant activity, antimicrobial activity, and bioactive composition, need to be investigated. The changes depending on the process parameters including power, intensity, exposure time, etc. should also be explored. This study aimed to review the recent studies that evaluated the effects of nonthermal food processing techniques, such as gamma irradiation, UV irradiation, ultrasound, pulsed electric fields, and cold plasma, on the bioactive properties of herbs and spices.

**Keywords:** herbs, spices, food processing, bioactive, nonthermal

## Thematic conference

# Interaction of chemical, microbiological and ecological aspects in the brown alga Zonaria tournefortii

Sonia Hamiche, C. Ait Si Said, R. Larouci, Naima Bouzidi1 , Mohamed Reda Zahi, Yasmina Daghbouche, Abdelmalek Badis, Mohamed El Hattab

**Laboratory of Natural Products Chemistry and Biomolecules, Faculty of Sciences , University of Blida 1 Algeria*

**E-mail** : elhattab@univ-blida.dz

**Abstract**

Study was carried out on the brown alga Zonaria tourfortii harvested on the central coast of Algeria. The chemical study enabled the characterization of phenolic compounds, mainly acylphloroglucinol and chromones metabolites . The study isolated a significant quantity of allcis-5,8,11,14,17 eicosapentanoic acid (EPA). Based on a literature review, we have proposed a biosynthetic pathway leading from EPA to phenolic metabolites. Bacterial screening from the algal surface led to isolate 30 bacterial strains, including 26 Gram+ containing the Staphylococcus and Bacillus genus, and 4 Gram- containing the Acinetobacter and Enterobacteracea genus. In terms of activity profiles, strain S13 (identified as Bacillus amyloliquefaciens basing of 16S rRNA technic) proved highly interesting inhibitory activities against target germs, as well as its production of diffusible and volatile compounds. Bacterial cells from the B. amyloliquefaciens S13 strain were used to recover a volatile fraction. Analysis was carried out by gas chromatography-mass spectrometry. The main volatile compounds identified were: 13-epi-manoyl oxide (29.39%), manool (17.39%), 15,16-dinorlabd-8(20)-en13-one (13.17%), labda-8(17),13Z-dien-15-ol (9. 51%) and 3 -acetoxy-13 epimanoyl oxide (5.26%) belonging to the labdane class of diterpenes, the latter having never been described in the category of microbial volatile organic compounds. Ecological aspects were discussed.

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## Thematic conference

# Synthèse, evaluation de l'activité antitumorale de nouveaux sulfamidophosphonates analogues structuraux de la fotémustine, étude in silico

Seif-Eddine Djouad[1], Malika Berredjem[2], Fatima Zohra HADJADJ AOUL[3]

[1] *Laboratoire de chimie thérapeutique du Centre Hospitalo-Universitaire Benflis Touhami Batna, Algérie,*

[2] *Laboratoire de Chimie Organique Appliquée, Groupe Synthèse de Biomolécules et Modélisation Moléculaire, Faculté des Sciences, Département de Chimie, Université Badji Mokhtar-Annaba, Box 12, 23000 Annaba, Algérie,*

[3] *Laboratoire de Chimie thérapeutique Faculté de pharmacie d'Alger, Algérie*

**Résumé**

Le cancer représente un problème majeur de santé publique dont la prise en charge constitue un véritable défi aussi bien sur le plan thérapeutique que psychologique.
Actuellement, la recherche de nouvelles substances actives utilisées dans les thérapies ciblées orales est légitime et ouvre la possibilité d'un « virage ambulatoire » du traitement de ces pathologies.
Dans le but de concevoir des candidats médicaments antitumoraux ayant une biodisponibilité orale, nous avons préparés de molécules d'intérêt thérapeutique : α-sulfamidophosphonates en utilisant la synthèse chimique classique

L'évaluation de l'activité antitumorale in vitro d'une série des composés α-sulfamidophosphonates par le test MTT a révélé deux composés bioactives **1d, et 1g** qui ont présenté une activité moyenne sur les lignées cellulaires testées.
Une étude in silico a été effectuée pour tous les composés α-sulfamidophosphonates, Deux approches ont été exploitées : la modélisation moléculaire (la théorie fonctionnelle de la densité (DFT)) et la méthode QSAR (Quantitative Structure Activity Relationship). L'étude in silico a révélé des composés **1d, 1g** présentant une forte réactivité chimique et drogables, selon la règle de cinq de Lipinski.

Ainsi, l'étude d'amarrage de ces composés étudies a dévoilé de bonnes interactions ligand cible, les trois composés **1a, 1d** et **1g** ont montré une forte affinité vers la cible anticancéreuse GCPII : glutamate carboxypeptidase II (GCPII) cette inhibition est due principalement à la présence du groupement pharmacophore bioisotérique (O=S=O) qui donne la même liaison métallique avec l'ion $Zn^{+2}$ 1752 dans le site actif de la protéine GCPII.

À la fin, ces molécules **1d, 1g** pourvus de l'activité pharmacologique recherchée peuvent jouer le rôle des points de départ pour concevoir des médicaments idéals.

**Mots-clés :** α-sulfamidophosphonates, MTT, DFT, QSAR, GCPII.

## Thematic conference

# Recherche in silico de nouvelles molécules bioactives en oncologie : des méthodes CADD à l'immuno-informatique

Samira AITKAKI[1,2], Fayçal LAYACHI[1,2], Khair-Eddine KRAIM[1,3], Abdelhak NEGHRA[2] et Fouad FERKOUS[1]

[1.] *Laboratoire de recherche Chimie Organique Appliquée LCOA, UBMA*
[2.] *Laboratoire de Chimie Thérapeutique, département de Pharmacie, Faculté de Médecine, UBMA*
[3.] *Laboratoire Physicochimie et Biologie des matériaux, école supérieure normale de l'éducation technologique, Skikda, Algérie*

**E-mail:** kaki_samira@yahoo.fr

**Résumé**

Le processus de développement des médicaments devient de plus en plus rationnel et se base sur l'utilisation de moyens informatiques pour exploiter les avancés dans le domaine de la protéomique et de la génomique et les grandes bases de données.
Les méthodes de se basant sur la disponibilité de la structure de la protéine impliquée dans une pathologie donnée tel que le docking moléculaire, et / ou sur les méthodes de pharmacophores et équations 3D QSAR construits sur la base de la connaissance de ligands actifs sur une cible donnée, ont permis de mettre sur le marché un nombre important de médicaments. Nous citons comme exemples les anticancéreux inhibiteurs de plusieurs kinases à savoir l'imatinib, Sorafenib et dasatinib.

Des études in silico sont réalisées pour prédire les épitopes capables de déclencher des réponses immunitaires. L'immuno-informatique est la branche de la bioinformatique utilisée pour étudier la relation entre les réponses immunitaires et les épitopes prédits. Cette approche est un moyen innovant, rapide et précis.

Dans cette présente conférence, nous nous proposons de discuter deux protocoles de recherche de nouvelles molécules bioactives dans le traitement du cancer.

Dans le premier, l'objectif de l'étude est la recherche de nouveaux inhibiteurs de l'HDAC8 par un criblage virtuel basé sur le docking et la prediction des propriétés ADMET.

Dans le second, des molécules similaires aux composants naturels de l'huile de la graine de Pisticia lentiscus ont été amarrés dans la protéine PI3K. Cette cible a été prédite lors d'un criblage inverse par le serveur de prédiction Netinfer, comme cible potentielle de ces composants naturels constitués d'acides gras, des stérols, des polyphénols et d'antioxydants.

Enfin, nous donnerons un petit aperçu sur les méthodes in silico utilisées dans le processus de recherche des vaccins anti cancer basées sur épitopes.

**Keywords** : Docking, criblage virtuel, criblage inverse, vaccin, épitopes, ADMET

# ORAL COMMUNICATIONS

**Oral communication** **OR-002**

# Synthèse, caractérisation et étude de la capacité de détection de métaux lourds d'une base de Schiff dérivé de la pyridine

Maroua BACHA[1], Amel ZITOUNI[1], Brahim HARKATI[1] and Abdelkrim GOUASMIA[1].

[1] *Laboratory of Organic Materials and Heterochemistry, Department of Material Sciences, Faculty of Exact Sciences, Echahid Cheikh Larbi Tebessi University, Street of Constantine, 12002 Tebessa, Algeria.*

**E-mail:** maroua.bacha@univ-tebessa.com

**Résumé**

Les bases de Schiff et leurs complexes occupent une place prépondérante en chimie de coordination en raison de leur synthèse relativement facile et de la grande variété de leurs applications [1]. Leurs architectures adaptables favorisent une large gamme d'applications, allant de la catalyse à la reconnaissance moléculaire des ions [2]. D'autre part, la pyridine, en tant que ligand largement employé en chimie de coordination, forme des complexes métalliques qui trouvent des applications variées, notamment dans la catalyse organique et la fabrication de matériaux innovants.

Dans l'optique d'étudier le phénomène de la reconnaissance moléculaires des ions d'une base de Schiff, nous intéressons dans ce travail, à la synthèse d'une nouvelle molécule porte dans sa structure la pyridine et la fonction hydrazone. Ensuite, nous examinons leur capacité pour détecter les métaux lourds. Les différentes méthodes spectroscopiques (RMN$^{1}$H, $^{13}$C, IR et UV-Vis) ont été mises à profit pour établir les caractéristiques structurales du composé synthétisé. L'ajout des ions $Fe^{2+}$, $Zn^{2+}$, $Hg^{2+}$ et $Cd^{2+}$ aux solutions de ligand a entrainé un changement remarquable sur le spectre d'absorption du ligand libre. Le composé préparé montre une meilleure sélectivité pour les ions $Fe^{2+}$ et $Zn^{2+}$.

**Mots-clés** : Hydrazone, détection des ions, sélectivité, métaux lourds, polluants envirenmentals.

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**Oral communication** **OR-003**

# Synthesis of new copper (II) complexes derived from α-aminophosphonates

BAHADI Rania[1, 2], MANSOURI Achraf[1], GRIB Ismahene[1], BERREDJEM Malika[1]

[1]*Laboratoire de Chimie Organique Appliquée, Groupe Synthèse de Biomolécules et Modélisation Moléculaire, Département de Chimie, Faculté des Sciences, Université Badji-Mokhtar-Annaba, Boîte 12, 23000 Annaba, Algérie.*

[2]*Département Génie des Procédés, Faculté de Technologie, Université Chahid Mostfa Benboulaid - Batna 2-, 05000, Batna, Algérie.*

**E-mail:** rania.mriam@yahoo.fr

**Abstract**

Organophosphorus compounds are among the most prominent in modern organic chemistry due to their use in various fields, such as biology. The incorporation of metal ions into organic ligands can significantly alter their therapeutic effects and pharmacological properties. Due to the wide range of coordination geometries, metal complexes offer greater stereochemical variability in organic molecules and often introduce new elements of chirality **[1]**. The interaction between metal ions and α-aminophosphonate ligands, which contain donor groups, is limited in the context of our ongoing research into synthetic and biological applications. This has motivated us to explore the influence of metal ion interactions with these molecules and their biological activity **[2]**.

Our presented work focuses on the synthesis of new complexes derived from α-aminophosphonates. We employed a green synthesis method using microwave activation to drive the reaction, with the aim of synthesizing new anti-inflammatory agents. The reaction was conducted without catalysts.

Various spectroscopic methods, including **IR, UV-Vis**, and X-ray diffraction (**XRD**), were utilized to establish the structural characteristics of the complexes.

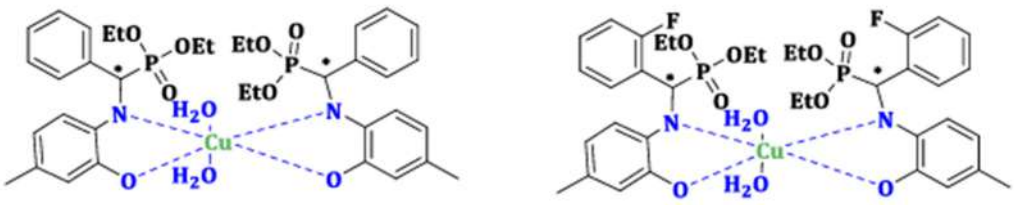


**Figure 01:** Structures of complexes

**Keywords**: Complexes, Anti-inflammatory activity, Microwave, α-aminophosphonates.

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**Oral communication** **OR-005**

# In vitro and in silico assessment of novel synthesized 4-hydroxyquinolone analogues as antioxidant agents.

Yousra Ouafa Bouone*, Abdeslem Bouzina, Rayene Sayad, Nour-Eddine Aouf

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

**E-mail:** bouoneyyo@gmail.com // yousra.ouafa-bouone@univ-annaba.dz

**Abstract**

The present work investigates the antioxidant activity of a set of 4-hydroxyquinolone analogues synthesized using an easy and rapid procedure involving both heterogeneous catalysis and microwave-assisted synthesis. Resulting 4-hydroxyquinolone derivatives were subjected to an in vitro assessment of their radical scavenging ability through several reliable assays including DPPH, ABTS, and FRAP assays. Results were found to be promising for many synthesized 4-hydroxyquinolone analogues especially two of them that exhibited encouraging $IC_{50}$ values compared to the employed standards. A complementary study consisting of an in silico investigation was completed including molecular docking that provided a better insight on how molecules act in the active site of the xanthine oxidase that is considered as a target for antioxidant activity, as well as a DFT study that helped to understand the structural composition of compounds, and to assess the most important and reactive regions of the molecules through mapping their electrostatic potential. Finally, an ADMET prediction was performed to apprehend pharmacokinetics properties necessary for the conception of novel drug-candidates.

**Keywords**: 4-hydroxyquinolone, Antioxidant activity, Molecular docking, DFT, ADMET

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**Oral communication** **OR-006**

# Grinding method: Green approach for the synthesis of flavonoïd isomers

Boussafi karima*[1,2], Didier Viallemin[2] and Boudebaz Khadidja[1]

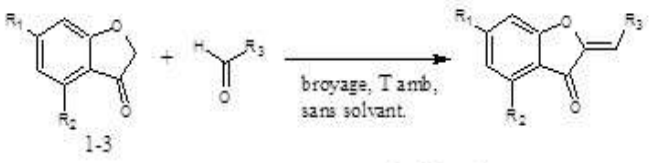
[1] *Laboratoire de Pharmacologie et Phytochimie. University of Jijel, Algeria*
[2] *ENSICAEN LCMT, UMR CNRS 6507, Normandie Université France, INC3M, FR 3038, Labex EMC3, Labex SynOrg, 14050 Caen, France.*

**E-mail:** boussafi.karima@yahoo.fr

**Abstract**

Reducing toxicity risks in organic chemistry is the primary goal of green chemistry. Our challenge was to prepare aurones (isomers of flavonoïds) under green conditions, using the technique of reactant grinding.

Grinding technique is a protocol compatible with the principles of green chemistry, applied to reactions processed through mechanical energy during the grinding of reactants using a mortar, allowing for energy transfer through friction. A series of aurones were synthesized by grinding method in a dry environment at room temperature, via condensation reaction of coumaranones with aryl aldehydes.




1: 6-hydroxybenzofuran-3(2*H*)-one
2: 4,6-dihydroxybenzofuran-3(2*H*)-one
3: naphtofuran-3(2*H*)-one

a: $R_3$= Ferrocène
b: $R_3$= 1,3-benzodioxole
d: $R_3$= 3,4,5-triméthoxybenzène

Fig: Condensation reaction

Adol condensation by grinding of the reactants is an effective approach. It leads to the selective formation of pure aurones, in a short time, with excellent yields.

In this study, we relied on molecular docking methods to evaluate the anti-inflammatory activity of synthesized aurones, which may exhibit the best affinities for the target of interest, inducible cyclooxygenase (COX-2) (PDB ID: 1pxx). Four aurones demonstrated greater inhibitory efficacy than the reference diclofenac with energies ranging from -9.2 to -8.7 kcal/mol.

**Keywords**: Green chemistry, solventless reaction, condensation reaction, aurones, grinding method.

**Oral communication** **OR-008**

# Synthèse des hétérocycles mixtes à partir de l'acide téréphtalique

Fekih Yasmine[1], Datoussaid Yazid[2], Choukchou-Braham Nourredine[3]

[1]*Laboratoire de Catalyse et synthèse en chimie organique, faculté des science, université de Tlemcen*

[2]*Laboratoire de Catalyse et synthèse en chimie organique, Ecole supérieur en science appliquées, Tlemcen*

[3] *Laboratoire de Catalyse et synthèse en chimie organique, faculté des science, université de Tlemcen*

**E-mail:** yasmine.fekih@univ-tlemcen.dz

**Abstract**

Les hétérocycles mixtes sont des composés chimiques très intéressants dans la recherche scientifique en raison de leur potentiel d'application dans différents domaines, pour cette raison leur synthèse est devenue un sujet très important.

Dans notre travail, nous avons opté pour la synthèse de dérivés du 1,2,4-triazole en raison de leur importance chimique et biologique.

Nous avons essayé de trouver une nouvelle voie de synthèse de ce composé à partir de l'acide téréphtalique, tout en modifiant certaines des conditions opératoires, telles que la base et l'acide, la température.

**Keywords**: Acide téréphtalique, hétérocycles, hétérocycles mixtes, 1,2,4-triazole.

**Oral communication** **OR-009**

# Eco-friendly synthesis of biosorbent based in chitosan-activated carbon/zinc oxide nanoparticles beads for efficiency reduction of cadmium ions in wastewater

Mohammed Rabeh Makhlouf [a, *], Malek Bendjaballah [a], Ferkous Hana [b], Ghouafria Imane [a], Benhamza Mohamed El Hocine [a]

[a] *Laboratoire d'Analyses Industrielles et Génie Des Matériaux, Université 8 Mai 1945 Guelma 24000, BP 401, Guelma, Algeria*

[b] *Département de Technologie, Université de Skikda, 21000, Skikda, Algeria*

**E-mail:** amindz24@gmail.com

**Abstract**

This study aims to synthesize a new bio-adsorbent through the dual valorization of agricultural and marine waste (date pits and shrimp shells) for the purification of cadmium-contaminated water. The bio-composite is synthesized by combining the properties of chitosan with activated carbon and zinc oxide nanoparticles (CS-AC/ZnO). The optimum ratio between AC/ZnO and CS is 1/2 (w/w) to achieve maximum removal. Successful synthesis was confirmed by the analysis of the composite using FTIR, XRD, SEM, BET, and EDX techniques. The specific surface area of the CS-AC/ZnO was 20.54 $m^2\ g^{-1}$, with a removal efficiency of 82%, which was higher than other adsorbents tested in this study.

Batch adsorption studies were carried out to investigate operational factors as well as the kinetics, isotherms, and thermodynamics of the adsorption mechanism. The adsorption of $Cd^{2+}$ was spontaneous and exothermic. Experiments demonstrate the preferential elimination of $Cd^{2+}$ in the presence of interfering ions such as $Na^+$, $K^+$ and $Mg^{2+}$. Non-linear modeling was used to analyze the adsorption isotherm and kinetics. The Freundlich and Redlich-Peterson isotherms, together with the pseudo-second-order kinetic model, were the best suited to the experimental data. The highest adsorption capacity determined by Langmuir was found to be 18.63 mg g-1. Remarkably, the adsorbent maintained high performance over 5 regeneration cycles, with a slight reduction in efficiency from 83.76% to 80.18%.

**Keywords**: Biosorption, Bio-composites, Chitosan-Activated Carbon/ZnO beads, Cadmium, ecofriendly and cost effectiveness.

**Oral communication** **OR-011**

# Antibacterial activity of hand disinfectant gel based on silver nanoparticles synthesized from aqueous extract of Satureja Calamintha ssp. Nepeta (L.) briq. from northwestern Algeria

OUGHILAS.A[1]*, BENAOULA.S[1] AMAR.A[1] CHAHED. A[1]TALEB.S[1]

[1] *Laboratory of Condensed Matter and Sustainable Development, University of Sidi Bel Abbes, LMCDD*

**E-mail** : oughilasargan@gmail.com
oughilasahmed@yahoo.fr.

## Abstract

**Context:** Staphylococcus aureus is a bacterium that causes bacteremia in patients with COVID-19 pneumonia. S. aureus is responsible for 80% of suppurative diseases, with the skin surface as its natural habitat. Therefore, it is crucial to maintain hand hygiene during a pandemic. Currently, people prefer to use convenient hand sanitizers. Most hand sanitizers contain alcohol, which has the potential to cause irritation. Thus, the active substance, which is biogenic silver nanoparticles from the extract of Calamintha ssp. Nepeta, is used as a substitute for alcohol.
**Objective:** Green synthesis of silver nanoparticles (AgNPs) with physicochemical characterization from the aqueous extract of the chosen plant. Development of the gel and the concentration of AgNPs that exhibited antibacterial effects against bacterial strains.
**Methods:** The AgNPs resulting from biochemical reduction, as well as the hand sanitizer gel, were tested for their antibacterial activities against the tested bacterial strains using the agar diffusion method.
**Results:** The results showed that the obtained AgNPs have a surface plasmon resonance (SPR) band at 415 nm and an ATR-FTIR spectrum displaying peaks corresponding to the functional groups of the biomolecules from the chosen plant extract, in addition to inhibition zones of 0 mm, 9.00 mm, and 14 mm observed for the plant extract, the corresponding AgNPs, and the gel with a concentration of 27% V/V, respectively, against the S. aureus strain.
**Conclusion:** The gel formulation of AgNPs was able to inhibit the growth of S. aureus with a moderate inhibition category. The hand sanitizer gel meets the requirements for organoleptic tests, pH, homogeneity, dispersibility, and adherence. However, the viscosity of the preparation did not meet the requirements.

**Keywords:** Extract of Satureja Calamintha ssp. Nepeta (L.) briq, Hand sanitizer gel, Silver nanoparticles, green synthesis, Antibacterial

**Oral communication** **OR-012**

# Advances in silver(I)-NHC complexes: Synthesis, molecular docking, and inhibition of cholinesterase: A step toward Alzheimer's therapy

Abd el-krim SANDELI[1,3]*, Ismahene BAZINE [1], Boutheina BOUALIA[2,3] , and İsmail ÖZDEMIR [3,4]

[1]*Pharmaceutical Sciences Research Center (CRSP), Constantine 25000, Algeria*
[2]*The molecular and structural environmental chemistry research unit, Faculty of Exact Sciences, Frères Mentouri - Constantine 1 - University, CONSTANTINE, ALGERIA*
[3]*İnönü University Drug Administration and Research Center, 44280-Malatya, TÜRKİYE*
[4] *Inönü University, Faculty of Arts and Sciences, Department of Chemistry, 44280-Malatya, TÜRKİYE*

**E-mail** : karim.sandeli.dz@gmail.com

**Abstract**

A series of novel silver(I)-N-heterocyclic carbene (NHC) complexes, along with their related benzimidazolium salt precursors, have been synthesized and thoroughly characterized through spectroscopic techniques and X-ray crystallography. The primary aim of this study was to explore the biological potential of these synthesized compounds, particularly as potent inhibitors with significant pharmacological properties. Comprehensive in vitro evaluations were conducted to determine their effectiveness in terms of anti- Alzheimer's properties. The inhibitory activities of these compounds on acetylcholinesterase (AChE) and butyrylcholinesterase (BChE) enzymes were screened in an in vitro complementary system. Among the tested compounds, silver(I)-NHC complexes (3a-f) demonstrated substantial inhibition of both AChE and BChE, surpassing the efficacy of standard reference drugs. Meanwhile, the benzimidazolium salts (2a-f) also showed considerable inhibitory effects against AChE and BChE. Molecular docking studies using AutoDock were performed to further investigate the binding interactions of the most active inhibitors within the active sites of AChE and BChE, aiding in the optimization of lead compounds. These results highlight the potential of silver(I)-NHC complexes for further development as therapeutic agents targeting Alzheimer's disease.

**Keywords**: Silver(I)-NHC complexes, Benzimidazolium salts, Acetylcholinesterase (AChE), Butyrylcholinesterase (BChE), α-Amylase inhibition, Molecular docking.

**Oral communication** **OR-013**

# Oxidation and corrosion inhibition study of some plant extracts from Saharan area arid and semi- arid

Yazid amri *[1], Mohammed abdelkader belalem[1] and Abdelkrim Gsassi[2]

[1] *Sciences and Environmental Research Laboratory, Department of Material Sciences, Faculty of sciences and technology, University of Tamanghasset, 11000 Tamanrasset (Algeria)*

[2] *University Amine El Okkal El Hadj Moussa Eg Akhamouk of Tamanghasset, 11000 Tamanrasset (Algeria)*

**E-mail:** amriyazid97@yahoo.com

**Abstract**

- Algeria has a diverse climate from north to south, which has made it possess a great diversity of plants, some of which have not yet been discovered.
- The Algerian desert contains medicinal plants that its residents use to treat their diseases in light of the arid climate.
- Balanite Aegyptiaca is a plant from arid area of Algeria (Tamanghasset)
- In this work we aimed to study the phytochemical properties and to evaluate the antioxidants and the corrosion inhibitory activity of some organic extract of the Balanite Aegyptiaca plant.
- The plant simple was collected and dried under suitable conditions and then ground.
- The oils were extracted by maceration method using many different solvents.
- Chemical detection revealed the presence of: saponins, terpenes, steroids, flavonoids, and coumarins. And the absence of proteins, phenols, tannins, alkaloids and saccharides.
- The antioxidant activity was studied using the DPPH test with hexane and $CH_2Cl_2$ extracts.
- According to $IC_{50}$, the results showed that the hexane extract had a higher inhibitory activity than $CH_2Cl_2$ extract compared to ascorbic acid.
- The inhibitory efficacy was studied by the mass loss method.
- The carbon steel CX70 was used in HCl (0.5M) in presence of hexane & $CH_2Cl_2$ plant extracts.
- The experimental results showed that by increasing the concentration of the two extracts, the inhibitory efficiency increased.
- We also obtained the maximum inhibitory effectiveness at a temperature of 80, with a slight difference for the two extracts.
- Scientists should focus on using green substances for a clean environment, which has become one of the biggest problems in the world.

**Keywords**: Organic extracts; Chemical detection; Balanite Aegyptiaca; DPPH; Carbon Steel CX70; corrosion.

**Oral communication** **OR-014**

# Antioxidant activity of new synthesized α-aminophosphonates

Kawther BADAOUI [1*] and Imene SEHOUT [1]

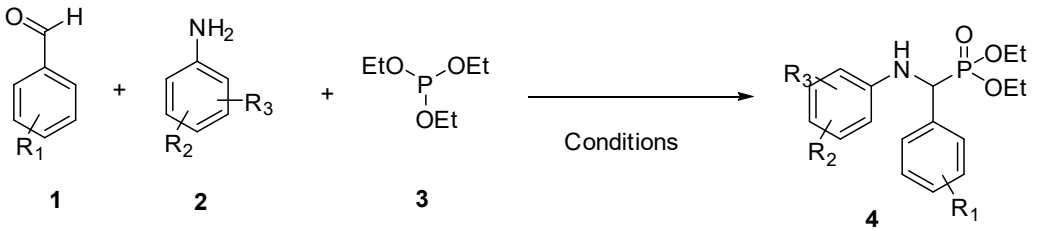
[1] *Laboratory of Synthesis of Bioactive Molecules, Department of Chemistry, Faculty of Exact Sciences, Freres Mentouri Constantine -1- University, Constantine, 25000, Algeria.*

**E-mail**: badaoui.kaouther7@gmail.com

**Abstract**

α-aminophosphonates represent an important part of organophosphorus compounds. α-aminophosphonates can be created by Kabachnik-Fields reaction with new and green methods [1]. α-aminophosphonates have a wide spectrum application in medicinal chemistry including antioxidant activity [2].

A series of new α-aminophosphonates was prepared by the condensation of an aromatic aldehyde, an aniline and a triethylphosphite in a ultrasonic bath under green conditions. Compounds were elucidated by 1H NMR, 13C NMR, 31P NMR and IR. This work is devoted for the in vitro antioxidant activity assessment of the target molecules. Tests were carried out in 96-well microplates and read in a spectrophotometer at the appropriate wavelength. Findings showed moderate to good results.




**Scheme**

**Keywords**: kabachnik-Fields reaction, α-aminophosphonates, antioxidant activity.

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**Oral communication** **OR-017**

# On-site production of iron nanoparticles using tamarix articulata for the removal of hexavalent chromium

Hadj Daoud Bouras [a,b,*], Aya Alterkaoui [c], Zelal Isik [c], Nadir Dizge [c]

[a] *Département d'Automatique et Électromécanique, Faculté des Sciences et de la Technologie, Université de Ghardaia, Ghardaia, Algeria*
[b] *Laboratoire de Valorisation et Conservation des Ecosystèmes Arides (LVCEA), Université de Ghardaia, Ghardaia, Algeria.*
[c] *Department of Environmental Engineering, Mersin University, Mersin, 33343, Turkey*

**E-mail:** hadjdaoud_bouras@yahoo.fr

**Abstract**

This research presents a novel and straightforward method for environmentally friendly in-situ synthesis of iron nanoparticles (TA-FeNPs) utilizing Tamarix articulata (TA) as both a reducing and stabilizing agent. To characterize TA and TA-coated FeNPs, UV-vis spectroscopy, X-ray diffraction, and scanning electron microscopy techniques were employed. Remarkably, the scanning electron microscopy images revealed micrometer-sized TA-FeNPs with irregular shapes and distinct sharp edges. The X-ray diffraction pattern lacked clear diffraction peaks, indicating the amorphous nature of the iron nanoparticles. The weight percentage of the Fe element was determined to be 2.16%. Interestingly, the removal efficiency of Cr (VI) displayed a significant decline, ranging from 99.06% to 35.85%, as the initial pH increased from 2 to 5. At a concentration of 25 mg/L, complete reduction of Cr (VI) was achieved. Moreover, the optimal conditions for complete reduction were observed at the original pH value of 5.2, with a dosage of 1 g/L, after a 60 min.

**Keywords**: Green chemistry, Tamarix articulata, Cr (VI) reduction, Fenton reaction, nanoparticles.

**Oral communication** **OR-018**

# Synthesis, structural characterization, and application of four rhodanine derivatives as dyes in solar cells

HAMANA Haoua, GOUASSMIA Abdelkrim, BOUMEDJOUT Meriem

*The Laboratory of Organic Materials and Heterochemistry*

**E-mail** : haouahamana@univ-tebessa.dz

**Abstract**

In this study, we synthesized four unique derivatives of rhodanine and elucidated their molecular structures through a range of meticulous physical and chemical analyses, including Nuclear Magnetic Resonance (NMR), Ultraviolet-Visible (UV-Vis) spectroscopy, and Infrared (IR) spectroscopy. Additionally, we investigated their potential utilization as potential dyes in solar cells. The synthetic procedures yielded high-purity compounds, facilitating subsequent analytical and applicative studies.

Furthermore, we evaluated the efficacy of these derivatives as dyes in solar cells, revealing promising results indicating their capability to enhance the performance of solar energy conversion devices.

In conclusion, the synthesized rhodanine derivatives exhibit significant promise as efficient dyes for integration into solar cells, supported by their meticulously elucidated molecular structures and demonstrated efficacy in photovoltaic applications. This study contributes to the advancement of sustainable energy technology and underscores the potential of organic dyes in increasing solar energy conversion efficiency.

**Keywords**: Rhodanine, Chemical analyses, Solar cells, Photovoltaic, Organic dyes, Conversion efficiency.

**Oral communication** **OR-019**

# Le petit chercheur scientifique et la transformation des plantes médicinales

Ali JARRAY

*Institut supérieur des sciences humaines Médenine Université de Gabes*

**E-mail** : Alijar2005@gmail.com

**Resumé**

Pour enrichir l'expérience des jeunes participants (6 à 12 ans) dans un club de protection de l'environnement au sein des établissements scolaires primaires de la région montagneuse du gouvernorat de Médenine, au sud de la Tunisie, nous avons mené une étude pratique de recherche qui se concentre sur une expérience éducative prometteuse pour le développement de l'esprit scientifique précoce chez les élèves du primaire. En effet, cette étude aborde l'efficacité des procédés de distillation qui influencent la qualité et les propriétés médicinales des essences ainsi que leur impact environnemental.

Cette étude met également en valeur l'importance des activités des clubs de l'environnement dans la conservation des plantes médicinales et la biodiversité. Elle promeut l'éducation sur les pratiques durables et responsables en matière de transformation des plantes médicinales selon des axes éducatifs et sociaux qui permettent de développer l'esprit scientifique précoce chez les élèves du primaire. De bons résultats ont été obtenus à savoir le développement de l'efficacité des procédés, l'étude de l'impact des activités du club sur la conservation des plantes médicinales et la biodiversité, et la promotion de l'éducation sur les pratiques durables et responsables en matière de transformation des plantes médicinales. Ceci met l'action que ce que nous avons appelé : le petit chercheur scientifique ».

Ces résultats permettent de mieux comprendre les enjeux et les bénéfices des activités du club en lien avec l'environnement et la santé, et préparent les enfants à la recherche scientifique dès un jeune âge. Ils favorisent la formulation d'hypothèses, la recherche de réponses adéquates et l'identification des types de plantes locales (comme le Thym et le Romarin à Beni-Kedach, Médenine en Tunisie) pour les transformer en produits médicaux directement exploitables dans leurs familles

**Keywords**: Keyword1, Keyword2, Keyword3, Keyword4, Keyword5, Keyword6.

**Oral communication** **OR-020**

# Therapeutic potential of silver nanoparticles from helianthemum lippii extract for mitigating cadmium-induced hepatotoxicity: Liver function parameters, oxidative stress, and histopathology in wistar rats

Ibtissam LAIB [1, 2, 3*], Boutlilis DJAHRA ALI[1,3], Ali Alsalme,[4] David Croun,[5] Mikhael Bechelany[5,6], Ahmed Barhoum[7]

[1] *Department of Cellular and Molecular Biology, Faculty of Natural and Life Sciences, El Oued University, El Oued 39000, El Oued, Algeria*

[2] *Higher School of Saharan Agriculture, El Oued, Algeria*

[3] *Laboratory of Biology, Environment and Health, Faculty of Natural and Life Sciences, El Oued University, El-Oued 39000, Algeria*

[4] *Department of Chemistry, College of Science, King Saud University, Riyadh, 11451, Saudi Arabia*

[5] *Institut Européen des Membranes, IEM, UMR-5635, Univ Montpellier, ENSCM, CNRS, Place Eugene Bataillon, 34095 Montpellier, France*

[6] *Gulf University for Science and Technology, GUST, Kuwait*

[7] *NanoStruc Research Group, Chemistry Department, Faculty of Science, Helwan University, Cairo, 11795, Egypt*

**E-mail** : ibtissambiochimie95@gmail.com

**Abstract**

This study explored the therapeutic potential of silver nanoparticles (Ag NPs) synthesized with a Helianthemum lippii extract for mitigating cadmium-induced hepatotoxicity in Wistar rats. The results of X-ray diffraction, UV-Vis spectrometry, and energy-dispersive X-ray spectroscopy with scanning electron microscopy confirmed the formation of Ag NPs with a cubic crystal structure and particle size from 4.81 to 12.84 nm. The Ag NP sub-acute toxicity study (2 mg/kg and 10 mg/kg) did not highlight any difference with untreated control rats (n=3 animals/group). Then, adult Wistar rats (n=5/group) were divided into one control (untreated/unexposed) and three experimental groups (Ag NPs alone, exposure to 50 mg/kg $CdCl_2$ in drinking water for 35 days, and exposure to $CdCl_2$ for 35 days followed by 0.1 mg/kg/day Ag NPs by intraperitoneal injection for 15 days). In the $CdCl_2$ exposed group, body weight was decreased, alanine and aspartate transaminase were significantly increased ($p < 0.05$ vs control), indicating hepatotoxicity, antioxidant defenses were decreased, and malondialdehyde levels increased. Liver architecture was altered (portal fibrosis, inflammation, necrosis, sinusoid and hepatic vein dilation, and cytoplasmic vacuolations). Treatment with Ag NPs after $CdCl_2$ exposure effectively attenuated some of the adverse effects of $CdCl_2$ exposure on liver function and architecture and increased body weight. This study contributes to the research on sustainable and eco-friendly approaches for NP synthesis, addressing toxicity concerns and offering potential applications for therapeutic strategies. It also supports the adoption of green synthesis methods, aligning with the growing emphasis on environmentally conscious practices in scientific research and healthcare.

**Keywords**: Silver Nanoparticles, Green Synthesis, Cadmium Toxicity, Hepatoprotective, Wistar Rats, Intraperitoneal Supplementation.

The 1st International Seminar on medicinal chemistry and green chemistry (1st IS MCGC - Annaba 2024)

**Oral communication** **OR-021**

# Synthesis, computational analysis, and bioevaluation of ferrocenylmethylnucleobase complexes: DFT calculations, ADMET profiling, molecular docking, and dynamics simulations

Elhafnaoui LANEZ[1,3,*], Mohammed larbi BEN AMOR[2,3], Touhami LANEZ[3]

[1]*University of El Oued, Faculty of Biology, Department of Cellular and Molecular Biology, 39000, El Oued, Algeria*

[2]*University of El Oued, Faculty of Technology, Department of Process Engineering and Petrochemical, P.O. Box 789, El Oued 39000, Algeria*

[3]*University of El Oued, Faculty of exact Sciences, Department of Chemistry, VTRS Laboratory, B.P.789, 39000, El Oued, Algeria*

**E-mail**: lanez-elhfanaoui@univ-eloued.dz

## Abstract

This study presents the synthesis, computational analysis, and bioevaluation of a new series of ferrocenylmethylnucleobase complexes (FcMeAd, FcMeCy, FcMeTh, and $(FcMe)_2Ad$) designed for potential antioxidant and antidiabetic applications. The synthesized complexes were characterized using a range of spectroscopic and electrochemical techniques, including Infrared (IR) spectroscopy, Proton Nuclear Magnetic Resonance ($^1$H NMR), Carbon-13 Nuclear Magnetic Resonance ($^{13}$C NMR), Cyclic Voltammetry (CV), and Ultraviolet-Visible (UV-Vis) spectroscopy, confirming their molecular structures. Density Functional Theory (DFT) calculations were performed to optimize molecular geometries, calculate frontier molecular orbitals, and assess electronic properties, revealing low energy gaps indicative of efficient intramolecular charge transfer. The pharmacokinetics and ADMET properties were evaluated in silico, demonstrating favorable drug-likeness profiles and non-toxic, non-carcinogenic characteristics. Molecular docking studies indicated strong binding affinities of the complexes with α-amylase and α-glucosidase enzymes, suggesting effective inhibition of these carbohydrate-hydrolyzing enzymes. Molecular dynamics simulations further confirmed the stability and persistence of these interactions. Complementary in vitro assays, including DPPH, ABTS, and FRAP, validated the antioxidant activity of the complexes, while enzyme inhibition assays targeting α-amylase and α-glucosidase corroborated their antidiabetic potential. Collectively, these findings highlight the combined efficacy of experimental and theoretical approaches in the design and evaluation of novel ferrocenyl-based therapeutics with promising antioxidant and antidiabetic properties.

**Keywords**: Ferrocenylmethylnucleobase, Antioxidant, antidiabetic, Molecular docking, Molecular dynamics simulations, Density Functional Theory, ADMET.

**Oral communication** **OR-022**

# A non-nitric acid method of dicarboxilic acids synthesis: organic solvent-free oxidation of ketone with hydrogen peroxide as oxidant.

Lynda MOUHEB[1], Leila DERMECHE[1,2], Nadine ESSAYEM[3] and Cherifa RABIA[2]

[1.] *Département de Chimie, Faculté des Sciences, Laboratoire de Chimie Appliquée et de Génie Chimique, (UMMTO), 15000 Tizi-Ouzou, Algérie.*

[2.] *Laboratoire de Chimie du Gaz Naturel, Faculté de Chimie, USTHB, BP32, El-Alia, 16111Bab-Ezzouar, Alger, Algérie.*

[3.] *Institut de Recherches sur la Catalyse et l'Environnement de Lyon, Université Lyon 1-UMR 5256 - CNRS- 2, avenue Albert Einstein, F-69626 Villeurbanne Cedex.*

**E-mail :** lynda.mouheb@ummto.dz

**Abstract**

In the current chemical industry framework, adipic acid, important precursor in the nylon production is obtained from oxidation of a mixture of cyclohexanone and cyclohexanol (KA oil) by nitric acid. However, the reduction of this latter leads to nitrogen oxides gases as by-products. Among them, $NO_2$ and NO are recycled and $N_2O_5$ and $N_2O$ are vented to the outside, thus contributing to global warming and ozone depletion.

The ecological synthesis of the adipic acid (AA) by catalytic way is of major interest. The purpose of our work joins in this context. Clean synthesis of adipic acid (AA) from oxidation of cyclohexanone was carried out at 90 °C, in the presence of hydrogen peroxide (30%) in free solvent, using Keggin-type polyoxometalates as catalysts. HPLC analysis of reaction mixture showed the formation of adipic, succinic and glutaric acids.

The salts were found to be effective for AA synthesis. $Sn_{1.25}PMo_{12}O_{40}$ led to the highest AA yield (56%) from cyclohexanone oxidation.

These results are very promising and emphasize our contribution to the development of a way of sustainable synthesis of the adipic acid, by targeting the substitution of the nitric acid, which presents numerous inconveniences: toxicity, effluent releases with strong impact on the environment, the corrosion of the installations.

**Keywords**: Keggin-type polyoxometalates, catalysts, green chemistry, adipic acid.

**Oral communication** **OR-023**

# A green corrosion inhibitor for carbon steel in acidic environments, electrochemical, AFM and SEM/EDS studies

Sirid Remache [1] [2], Adlene Benyamina [1] Ayache Boultif [3], Merzoug Benahmed [4]

[1] *Laboratory of Natural Resources and Management of Sensitive Environments, University of Oum El Bouaghi, 04000, Algeria.*

[2] *Centre for Scientific and Technical Research in Physico-Chemical Analysis BP 384, Z.I Bou-Ismail RP 42004, Tipaza, Algeria.*

[3] *Laboratory of Applied Chemistry and Materials Technology, University of Oum EL Bouaghi, 04000, Algeria.*

[4] *Laboratory of Organic Materials and Heterochemistry, University of Tébessa, 12002, Algeria.*

**E-mail** : sirid40@gmail.com

**Abstract**

The development of green inhibitors in corrosion control systems has been significant, as they provide effective corrosion protection and mitigate the negative consequences of metal degradation, while also contributing to sustainable applications. Safer industrial operations and infrastructure integrity can be achieved through the use of green inhibitors, which eliminate the need for traditional, often unsafe corrosion inhibitors.

This research is centered around the question of how the dichloromethane extract (DME) obtained from an Asteraceae plant (AP) can prevent carbon steel (CS) corrosion in a molar HCl solution.

The extract's anticorrosive activity was assessed using electrochemical impedance spectroscopy (EIS) and potentiodynamic polarization (PDP). We employed atomic force magnetic microscopy (AFM), scanning electron microscopy (SEM), and energy dispersive X-ray spectroscopy (EDS) to describe the surface roughness and morphology of (CS) samples with and without (DME) in acid media. The inhibition efficiency (IE) of DME was increased by increasing its concentration, reaching its maximum value of 76.49% at 500 ppm at 298K, but decreases with increasing temperature.

The (PDP) investigation indicates that the (DME) is a mixed-type inhibitor that has a predominant anodic effect. The (EIS) study validated the notion that increasing the level of (DME) raises the charge transfer resistance (Rct) while decreasing the double layer capacitance (Cdl) as a result of the development of a protective layer on the (CS) surface.

Furthermore, this research underscores the utility of dichloromethane extract (DME) obtained from an Asteraceae plant (AP) as a green corrosion inhibitor, which is crucial for developing ecologically acceptable methods of corrosion inhibition in acidic environments

**Keywords**: Green inhibitor, Plant extract, Asteraceae, corrosion, AFM, SEM/EDS.

**Oral communication** **OR-024**

# Synthesis, X-ray crystal structure and electrochemical properties of DAMN-based tetrathiafulvalene derivative

ZITOUNI Amel [1], BOUGUESSA Sabrina[1], BACHA Maroua[1] and GOUASMIA Abdelkrim [1].

[1] Laboratory of Organic Materials and Heterochemistry, Department of Material Sciences, Faculty of Exact Sciences, Echahid Cheikh Larbi Tebessi University, Street of Constantine, 12002 Tebessa, Algeria.

**E-mail:** amel.zitouni@univ-tebessa.dz

**Abstract**

Schiff bases enjoy the advantages of a rather straightforward synthesis and readily-modified structures. They are widely studied for their interesting biological and pharmacological activities. In addition, the presence of an imine linker contributes to their coordination with different metal ions, emphasizing their important position in coordination chemistry [1]. Synthesis of Schiff bases and its complexes derived from diaminomaleonitrile have gained recent interests as they have different applications in various areas [2], especially in the field of chemosensors for the detection of ionic and neutral species. On the other hand, tetrathiafulvalene (TTF) and its derivatives have played an important role in both the development of multifunctional organic materials, the construction of molecular devices and switchable supramolecular systems [3]. In this context, our research has been focused to the development of a new Schiff base combining the redox behavior of TTF unit and the coordination ability of the diaminomaleonitrile (DAMN). The prepared ligand was characterized by various spectroscopic techniques and X-ray diffraction. The electrochemical behavior of this compound indicates that it is promising for the construction of crystalline materials. As a preliminary study, the sensing ability of the new compound was studied with various cations by visual and UV visible techniques.

**Keywords :** Tetrathiafulvalene, Sensing ability, DAMN, Schiff base, Metallic cations

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**Oral communication** **OR-026**

# Caractérisation des composés phénoliques de capparis spinosa L(Kabbar) algérien et évaluation de leur pouvoir biopesticide

AMIRAT Sabrina [1*], SADOU Nina [1], MAKNI Samar [2], SERIDI Ratiba[1], TOUNSI Slim [2]

[1] Laboratory of Plant Biology and Environment (LBVE) «Medicinal Plants» Axis, Faculty of Sciences, Department of Biology, Badji Mokhtar University, Annaba, Algeria.

[2] Laboratory of Biopesticides (LB Pest), Center of Biotechnology of Sfax, University of Sfax, P.O. Box 1177, 3018 Sfax, Tunisia.

**E-mail :** sabrinaamirat@univ-annaba.org

**Abstract**

Capparis spinosa L « Câprier » de la famille des Capparidaceae est un arbuste spontané xérophyte et héliophile, très répondu dans le bassin méditerranéen.
L'utilisation des pesticides chimiques a provoqué une détérioration de notre environnement.

Le recours aux molécules bioactives d'origine végétale demeure une excellente alternative. Dans cette optique Les parties de la plante ayant subi une extraction assistée par ultrason avec un système de solvant hydro-éthanol 80%.

Une analyse par HPLC-DAD confirmant la richesse de notre plante en métabolites secondaires, tel que : Acide gallique ; Hydroxycortisol ; Acide caféique ; Catéchols, Acide Ellagique ; Acide Coumarique ; Acide férulique ; Vanilline.

Nos extraits ont accusé des teneurs en PPT de (131.821 ± 0.37 mg EAG/g ES) pour les feuilles et (152.261 ± 0.20 mg EAG/g ES) pour les fruits avec des taux en Flavonoïdes totaux et Tanins totaux respectivement de (21.340 ± 1.12 mg EQ/g ES) (15.67 ± 0.30 mg EC/g ES) pour les feuilles et (21.000 ± 2.38 mg EQ/g ES) (12.03 ± 0.55 mg EC/g ES) pour les fruits.

Dans la perspective de l'exploration d'un éventuel pouvoir biopesticide, nous avons testé les extraits des différentes parties de C. spinosa sur les souches phytopathologiques suivantes : Fusarium oxysporum CTM 10402 ; Botrytis cinerea LPAP 630 ; Aspergillus niger CTM 10099 **;** Agrobacterium tumefaciens B6 ; Agrobacterium tumefacien**s** C58.

Les résultats enregistrés montrent une activité antifongique et antibactérienne absolue où nous avons enregistré des rapports CMF/CMI = 1 et CMB/CMB = 1. Sauf pour : Fusarium oxysporum CTM 10402 avec un rapport CMF/CMI > 4.

**Keywords**: Capparis spinosa ; HPLC-DAD ; souches phytopathogènes ; Biopesticide

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**Oral communication** **OR-028**

# Contribution à l'étude phytochimique de ampelodesma mauritanica: impact du solvant sur la capacité antioxydante, caractérisation et quantification de quelques composés phénoliques par HPLC.

TOUDERT Nadia[1], ZEKKAD Farida[2] ZERRAD Chaima[2], BOUTEMEDJET Siham[2], DJILANI Salah Eddine[2]

[1]*Laboratory of Physical Chemistry of Materials, El Chadli Ben Djedid University, El Tarf, Algeria*

[2]*Laboratory of Synthesis and Organic Biocatalysis, Badji Mokhtar University, Annaba, Algeria*

**E-mail :** n.toudert@univ-eltarf.dz

**Abstract**

Dans ce travail, la capacité antioxydante des extraits de racines et de feuilles d'Ampelodesma mauritanica a été évaluée en utilisant des tests in-vitro (ABTS, DPPH et PPM). Une étude a également été menée sur l'impact des variations du solvant d'extraction (rapport méthanol-eau) sur cette activité. Les résultats montrent que le solvant méthanol-eau avec un rapport de 70:30 a été le plus actif, en termes d'activité antioxydante, que ce soit pour les extraits de feuilles ou de racines. Par ailleurs, dans ces conditions, les extraits de feuilles ont démontré leur capacité antioxydante la plus élevée.

En outre, l'HPLC a permis d'identifier certains composés phénoliques présents dans les divers extraits d'Ampelodesma mauritanica. Les résultats indiquent que les composés les plus représentatifs sont l'acide gallique, l'acide protocatéchique, l'acide hydrate de catéchine et l'acide caféique. De plus, et en raison de sa forte polarité, l'acide gallique est le produit le plus extrait par les solvants alcooliques (comme le méthanol ou le butanol) que les autres acides identifiés.

**Keywords** : Extraction ; HPLC ; Composés polyphénoliques ; Activité antioxydante ; ABTS ; DPPH.

**Oral communication** **OR-030**

# Etude chimique, caracterisation physique et evaluation du potentiel antioxydant d'huiles essentielles de quatre plantes medicinales aromatiques de la flore algerienne

DALIA Farid [(1)], BENSOUICI. Ch [(2)], LALAOUNA. A [(1)], BELKHIRI. A [(1)]

[(1)] *Laboratoire d'Innovation et de Développement d'Actifs Pharmaceutiques (IDAP), Université de Constantine 3, Algérie*

[(2)] *Centre de recherche en Biotechnologie -CRBT- de Constantine, Algérie*

**E-mail** : FARIDDALIA.21@GMAIL.COM

**Resumé**

Depuis la plus haute antiquité, les plantes ont servi de pharmaco thèque naturelle à l'homme pour se soigner, et celles à essence sont particulièrement ciblées.

Dans sa phase initiale, le présent travail entrepris à travers une série d'enquêtes ethnopharmacologiques dans le Nord-est Algérien, nous a permis de confirmer l'engouement toujours présent de la part de la population des régions enquêtées envers la phytothérapie traditionnelle en général, avec une réputation de bon profil, de tolérance et d'innocuité. Ces plantes médicinales aromatiques ont été identifiées formellement sur le plan botanique, et parmis lesquelles figurent : l'Origanum vulgare, Thymus capitatus, Aloysia triphylla et Eucalyptus globulus.

Les profils chromatographiques des huiles essentielles (HEs) établis par CPG-MS. Celui d'A.triphylla étudiée a révélé une composition chimique caractéristique de l'espèce, à savoir une prédominance du D-Limonène et E- et Z-Citrals. Cependant, l'échantillon analysé a montré une relative forte teneur en Spathulénol et alpha-Terpinéol. Les HEs de T.capitatus et d'O.vulgare ont montré des compositions typiques des espèces Nord-Africaines, avec une prédominance des phénols. Des fortes proportions de thymol et carvacrol (57,57 et 10,53%, respectivement) trouvées dans l'HE de T.capitatus, Alors que l'HE d'O.vulgare contenait des fortes proportions de thymol / γ-Terpinène / p-Cymène (38,96 / 25,45 / 18,31%, respectivement. La composition de l'HE d'E.globulus est dominée par le 1,8-cinéole, caractère partagé par de nombreuses huiles récoltées dans différentes régions d'Algérie.

Les résultats des tests antioxydants des HEs étudiées selon les méthodes ABTS, DPPH, GOR et CUPRAC ; ont montré que parmis les quatre HEs testées, celles d'O.vulgare et de T.capitatus ont révélé une importante activité antioxydante, comme le montrent les valeurs des concentrations ($CI_{50}$ et $A_{0,50}$) obtenues par les deux méthodes (ABTS+, CUPRAC). Ces résultats suggèrent que les HEs d'O.vulgare et de T.capitatus pourraient être une source potentielle d'antioxydants naturels.

**Mots-clés :** Plantes médicinales aromatiques ; Phytothérapie ; CPG-MS ; Activité antioxydante ; Origanum vulgare ; Thymus capitatus.

**Oral communication** **OR-034**

# Physicochemical, phytochemical, and biological characterization of Moringa oleifera

Kinza Benazzouz

*Mouloud Mammeri University of Tizi-Ouzou, Faculty of Biological and Agricultural Sciences, Department of Biochemistry and Microbiology, Laboratory of Protection and Valorization of Agrobiological Resources*

**E-mail**: kinzabenazzouz@gmail.com

**Abstract**

Moringa oleifera is a tree belonging to the Moringaceae family, native to India. It is a plant of nutritional and medicinal interest. The present work focuses on the physicochemical and phytochemical study, as well as the evaluation of the biological activities of Moringa oleifera seed extracts. Phytochemical screening revealed the presence of active secondary compounds such as steroids, anthocyanins, glucosides, and saponins. The results of the total polyphenol content assay using the Folin-Ciocalteu reagent method showed that the aqueous extract has a content of 43.21 ± 0.5 mg GAE/g DW. Two strains were tested for their ability to form biofilms on Congo Red (CR) medium, namely Staphylococcus aureus ATCC 25923 and Escherichia coli ATCC 25922. It was found that only S. aureus forms biofilms. The anti-biofilm activity of the aqueous extracts (pure extract, ½ diluted extract) of Moringa oleifera seeds showed a significant effect with inhibition zone diameters of 23 mm and 19 mm, respectively. Similarly, the antibacterial activity of the aqueous extracts (pure and ½ diluted) exhibited a strong inhibitory effect on the growth of Staphylococcus aureus ATCC 25923 and a moderate effect against Escherichia coli ATCC 25922, with inhibition zone diameters of 20 mm and 14 mm, and 9 mm and 8 mm, respectively.

**Keywords:** Moringa oleifera, total polyphenols, aqueous extract, anti-biofilm activity, antibacterial activity.

**Oral communication** **OR-035**

# Chemical composition of essential oils, optimization of phenolic compounds extraction and evaluation of antioxidant and anti-inflammatory properties of Anagyris foetida

Hamza Aliboudhar[1*], Zineb Lakache[2] and Fayçal Boukhari[1]

[1] Laboratory of Functional Organic Analysis, Faculty of Chemistry, University of Sciences and Technology Houari Boumediene (USTHB), El-Alia, Bab-Ezzouar, Algiers, Algeria

[2] Laboratory of Ethnobotany and Natural Substances, Department of Natural Sciences, Ecole Normale Superieure (ENS), Kouba, Algiers, Algeria

**E-mail**: haliboudhar@yahoo.fr

**Abstract**

Anagyris foetida has been utilized in traditional medicine for a long time to address various ailments such as digestive, respiratory, and skin conditions. Despite this, scientific research on its secondary metabolites is still limited. This study seeks to fill this gap by investigating the extraction and optimization of essential oils and phenolic compounds from different parts of Anagyris foetida using various extraction techniques. We aimed to validate and highlight some of the plant's traditional uses by evaluating the antioxidant and anti-inflammatory properties of the extracts. Essential oils were extracted from the leaves and aerial parts using hydrodistillation and microwave-assisted hydrodistillation, with the chemical profiles analyzed via gas chromatography-mass spectrometry (GC-MS). The analysis revealed distinct chemical profiles with significant variations in the composition and concentration of 33 identified compounds, depending on the extraction method. Phenolic compounds were optimized through experimentation with different solvents and conditions, achieving the highest phenolic and flavonoid contents using reflux heating in ethyl acetate at 60°C for 4 hours. Antioxidant activity was assessed using the 2,2-diphenyl-1-picrylhydrazyl (DPPH) assay, revealing moderate potential compared to the standard BHT, with IC50 values of 346.56 ± 33.67 µg/mL for the leaves and 287.14 ± 30.31 µg/mL for the stems. Anti-inflammatory activity was evaluated, in vivo, using the carrageenan-induced mouse paw edema inhibition method, demonstrating that the leaves had a stronger inhibitory effect compared to the stems, with maximum inhibition of 38.92% for the leaves and 20.53% for the stems at a concentration of 300 mg/mL, relative to the positive control (aspirin). This study highlights the pharmacological potential of Anagyris foetida as a valuable source of bioactive compounds, supporting its traditional uses and paving the way for new medicinal applications.

**Keyword:** Anagyris foetida, essential oil, phenolic compounds, antioxidant activity, anti-inflammatory activity.

**Oral communication** **OR-041**

# A comprehensive review of phytochemical characterization in cherry cultivars: Key bioactive compounds, medicinal potential and therapeutic applications

Nour El-Houda BOUMAAZA [1, 2*], Abdelkader DJOUAMAA [1], Hana BOUZAHOUANE [1,3], Moundji TOUARFIA [1], Kaouther LAIBI [1,2], Rayene DJABOURABI [1,2], Azzedine CHEFROUR [1, 4]

[1] *Faculty of Natural and Life Sciences, Mohamed Cherif Messaadia University – Souk Ahras*
[2] *Organic and Interdisciplinary Chemistry Laboratory E0841400.*
[3] *Laboratory of Environmental Biosurveillance, Department of Biology, Faculty of Sciences, Badji Mokhtar University, BP 12, El Hadjar, Annaba 23000, Algeria*
[4] *Development and control of hospital pharmaceutical preparations, Faculty of Medicine, Badji Mokhtar university-Annaba.*

**E-mail** : n.boumaza@univ-soukahras.dz

**Abstract**

Cherry tree (Prunus spp.) is known not only for its delicious fruits but also for its medicinal properties, especially the fruits and peduncles, but these benefits are often marginalized in modern medical practice. This comprehensive review focuses on the phytochemical characterization of the fruits and peduncles of the world's most widely cultivated cherry cultivars, comparing their bioactive compounds and therapeutic potential. This review includes a meta-analysis of phytochemical studies conducted on major cherry cultivars such as “Bing” (Prunus avium), “Montmorency” (Prunus cerasus), “Rainier” (Prunus avium) and “Stella” (Prunus avium). Data were collected from studies published between 2012 and 2024. The analysis specifically compares the phenolic, anthocyanin and flavonoid content and antioxidant capacity of the fruits and peduncles of these cultivars. The review reveals significant differences in phytochemical content between cultivars. For example, the sweet cherry cultivar “Bing” shows the highest anthocyanin content (120–160 mg/100 g), contributing to its strong antioxidant properties, while the sour cultivar “Montmorency”, despite its lower anthocyanin content (90–110 mg/100 g), shows a higher concentration of flavonoids and phenolic acids, especially in the cherry peduncles. “Reinier” cherries, known for their light colour, have lower anthocyanin levels (60–80 mg/100 g) but have a higher vitamin C content, enhancing their overall antioxidant capacity. The peduncles of all cultivars were found to be rich in polyphenols and flavonoids, which exhibit strong anti-inflammatory properties. In particular, the peduncles of the “Stella” cultivar had the highest flavonoid content, with potential applications in anti-inflammatory therapies. The phytochemical diversity in both the fruit and peduncle of cherry cultivars offers great medicinal potential, with each cultivar offering unique, often neglected advantages as a valuable source of bioactive compounds with therapeutic potential, particularly for anti-inflammatory and antioxidant applications.

**Keywords**: Cherry cultivars, phytochemicals, anthocyanins, flavonoids, antioxidant properties, therapeutic applications.

**Oral communication** **OR-042**

# Human cancer cell Lines inhibition by extracts from phlomis crinita

Abdelhakim Chelgham[1,2,*], Abdelkader Saadi [2], Ricardo Calhelha[3]

[1] *Laboratory of Natural Bio-Resources, Hassiba Benbouali University of Chlef, Algeria.*
[2] *Faculty of Life and Natural Sciences, Hassiba Benbouali University of Chlef, Algeria.*
*3 Centro de Investigação de Montanha (CIMO), Bragança, Portugal*

**E-mail**: a.chelgham@univ-chlef.dz

**Abstract**

Phlomis crinita Cav., a traditional Algerian medicinal plant, is used to treat lesions and burns. This study aimed to investigate the potential antiproliferative properties of its leaves, flowers, and rhizomes hydromethanolic extracts against five human tumor cell lines: AGS (gastric adenocarcinoma), CaCo2 (colorectal adenocarcinoma), HeLa (cervical carcinoma), MCF-7 (breast adenocarcinoma), and NCI-H460 (non-small cell lung carcinoma). And a non-tumor cell line, Vero (African green monkey kidney) was aslo used. Total phenolic compounds (TPC) and flavonoid content (FC) were quantified using spectrophotometric methods. TPC was determined using the Folin-Ciocalteu reagent, and FC was measured using the aluminum chloride colorimetric assay. Antiproliferative activity was evaluated using the sulforhodamine B (SRB) assay. Results revealed significant variations in TPC and FC among the extracts. The rhizome extract displayed the highest levels of both TPC (128.15 µg EAG/mg DW) and FC (46.91 µg QE/mg DW), followed by the leaf and flower extracts. All extracts exhibited antiproliferative activity against tumor cell lines, with the rhizome extract demonstrating the most potent effects. The AGS cell line was the most sensitive to the extracts, while the HeLa cell line was resistant. Importantly, none of the extracts displayed toxicity against the Vero (non tumor cell line), demonstrating a favorable safety profile. The rhizome extract exhibited the lowest $GI_{50}$ values against the tumor cell lines, indicating its superior antiproliferative potential. The $GI_{50}$ values for the rhizome extract against AGS, CaCo2, MCF-7, and NCI-H460 were 178.11 µg/mL, 212.33 µg/mL, 234.56 µg/mL, and 259.93 µg/mL, respectively. These findings suggest that Phlomis crinita extracts, particularly the rhizome extract, could be promising sources of natural anti-cancer agents. Further studies are warranted to elucidate the underlying mechanisms of action and to explore their potential therapeutic applications

**Keywords**: Phlomis crinita, Antiproliferative activity, Herbal medicine, phenolic compounds, flavonoids, cancer cell lines

**Oral communication** **OR-043**

# Cosmetic potential of olive mill wastewater fractions

Chahinez Ait Si Said, O. Touafek, Mohamed El Hattab

*Laboratory of Natural Products Chemistry and Biomolecules, Faculty of Sciences, Saad Dahlab University of Blida, 1- POB 270, Soumaa Road, Blida, Algeria.*

**E-mail:** aitsisaid.18@gmail.com

**Abstract**

Antioxidants are highly important gradients used to preserve cosmetic products and reduce the effect of oxidative stress on the skin. The present work explores the possibility of using seven different fractions separated from olive mill wastewater (OMW) extract as effective ingredients which can be used in cosmetic formulations deemed mainly by their photoprotective effects. In this purpose, the sample was collected from an oil mill in the Blida region (Algeria). A crude ethyl acetate extract was prepared from OMW according to a well-established protocol; the yield of the extract obtained was 4%. From the extract, different fractions were prepared by fractionating the total extract on an open column chromatography. All the fractions obtained show great antioxidant activity and photoprotective effects in smaller concentrations. Combinations of fractions were excellent choice for cosmetic use.

Phytochemical study of the different fractions was assessed by evaluating the total phenolic and flavonoid compounds for all fractions studied as the main compounds found in OMW are phenols like hydroxytyrosol, tyrosol, phenolic acids like caffeic, quinic and ferulic acids which show great therapeutic activities.

**Keywords**: Olive mill wastewater, fractionation, phenolic compounds, photoprotective activity, sun protection factor.

**Oral communication** **OR-044**

# Cardioprotective effects of protocatechuic acid on hydrogen peroxide and -cobalt chloride-induced cardiomyocyte injuries

Rim Ben Mansour[1], Hélène Talarmin [2], Riadh Ksouri[1], and Wided Megdiche-Ksouri[1]

[1] *Laboratory of Aromatic and Medicinal Plants, Centre of Biotechnology of Borj-Cedria, BP 901, 2050 Hammam-Lif, Tunisia*

[2] *Université de Bretagne Occidentale, Faculté de Médecine et des Sciences de la Santé, EA 4324 Laboratoire de Physiologie ORPHY, 29200 Brest, France*

**E-mail**: rim.bmansour@gmail.com;

**Abstract**

Oxidative stress disrupts the normal redox state within the human body, potentially leading to numerous chronic diseases, including cardiac and hypoxia-related injuries… Antioxidant properties of some bioactive components have been proposed to be capable of controlling such disordersThis study aims to assess the potential protective effect of Protocatechuic acid (3,4-dihydroxybenzoic acid, PCA) on $CoCl_2$ and $H_2O_2$-challenged $H_9C_2$ cardiomyoblast cells. In vitro antioxidant capacities and the potential protective effect of PCA on $CoCl_2$ and $H_2O_2$-challenged $H_9C_2$ cardiomyoblast cells were assessed. Biochemical markers of enzymatic antioxidant defense system by assessment of SOD and CAT activities and glutathione peroxidase (GPx) and MDA levels were evaluated. Exposure of cultured $H_9C_2$ cells to $CoCl_2$-simulated hypoxia or $H_2O_2$-oxidative stress induced over-activity of superoxide dismutase and Catalase and decrease in GPx and excess in MDA level. Pretreatment with PCA, attenuated significantly $CoCl_2$ and $H_2O_2$ challenged cardiomyoblasts injury by restoring cell viability (≈ 100%), oxidative balance and MDA level. These results indicate that PCA may become in the future efficacious and safe substances that reduce the side effects of the oxidative stress and can be therapeutically effective candidate in cardiac disorders.

**Keywords**: Cytoprotection; $CoCl_2$-induced hypoxia; $H_2O_2$-induced oxidative stress, $H_9C_2$ cells; Protocatechuic acid.

**Oral communication** **OR-045**

# Etude in vitro et in silico de l'activité antibactérienne de l'extrait aqueux de racines de Carthamus caeruleus L.

Yousra Belounis [1], Idir Moualek [1], Ali Dekir [2], Hillal Sebbane [1], Karim Houali[1]

[1] Laboratory of Analytical Biochemistry & Biotechnology Research, Faculty of Biological Sciences and Agricultural Sciences, University Mouloud Mammeri, Tizi-Ouzou 15000, Algeria

[2] Laboratory of Applied Organic Chemistry, Synthesis of Biomolecules and Molecular Modelling Group, Sciences Faculty, Chemistry Department, Badji-Mokhtar Annaba University, Box 12, Annaba 23000, Algeria

**E-mail:** belounisyousraw@gmail.com

**Resumé**

Dans le but de valorisation des ressources naturelles et de l'utilisation traditionnelle de plantes médicales en Algérie, cette étude exploite l'effet antibactérien de Carthamus caeruleus L. Comme il existe peu d'études sur cette plante malgré son potentiel thérapeutique important, ce travail vise à caractériser les biomolécules présentes dans l'extrait aqueux de racines de C. caeruleus L. et à évaluer son activité antibactérienne à travers une étude in vitro et in silico. Les dosages spectrophotométriques ainsi que les résultats de l'HPLC ont révélé la richesse de l'extrait en biomolécules avec 22 composants. Le potentiel antibactérien est étudié en utilisant la méthode de diffusion sur gélose et de microdilution contre neuf souches bactériennes de référence. Les résultats montrent que les racines possèdent la meilleure activité avec des zones d'inhibition comprise entre 10,5 ± 0,7 et 16,5 ± 0,12 mm et des MIC entre 2,34 ± 0,02 et 150 ± 0,052 mg/ml sur les souches testées. L'extrait était également capable d'inhiber la croissance de Staphylococcus aureus ATCC 25923 et d'Escherichia coli ATCC 25922. En outre, en étudiant son effet sur la membrane bactérienne comme un mécanisme antibactérien probable, aucune fuite des acides nucléiques et aucun dommage membranaire n'a été détecté. Cependant, les résultats du docking moléculaire réalisé sur les biomolécules révélées par HPLC ont montré une affinité et une stabilité importante pour l'ADN gyrase. On peut donc conclure que la présente étude rapporte une activité antibactérienne et une efficacité importante de Carthamus caeruleus L.

**Mots-clés** : Carthamus caeruleus L, racines, HPLC, activité antibactérienne, docking moléculaire.

**Oral communication** **OR-049**

# The physicochemical and phytochemical characteristics of Tunisian Pistacia lentiscus fruit oil

Raoudha Ben Ameur[1], Mohamed Ayadi[2] and Noureddine Allouche[1]

[1] *Natural Substances Team (LR17ES08), Faculty of Sciences of Sfax, Laboratory of Organic Chemistry, University of Sfax, Sfax, Tunisia*

[2] *Olive Tree Institute, UR: Cultivated Plant Protection and Environment, Sfax, Tunisia*

**E-mail :** mehdiraoudha@yahoo.fr

**Abstract**

This study aims to comprehensively examine the chemical composition, physicochemical characterization, as well as antioxidant of Pistacia lentiscus fruit oil (PLFO). PLFO containing high amounts of phenolic and flavonoid compounds exhibits a powerful antioxidant capacity. In this context, the potential of PFLO was evaluated using DPPH radical scavenging and reducing power methods. However, tocopherols were quantified at a content of 1249.16 mg $g^{-1}$ of oil. In PLFO, β-carotene was identified as a major carotenoid with a content of 7.22 ± 0.05 mg $kg^{-1}$ of oil. Our results showed that the prominent class of fatty acids was represented by monounsaturated fatty acids (42.73%), followed by saturated fatty acids (33.99%) and polyunsaturated fatty acids (23.13%). The different ratios of fatty acids were determined (PUFA/MUFA = 0.54, PUFA/SAFA = 0.68 and MUFA/SAFA = 1.25). The obtained results related to saturated and polysaturated fatty acids ratios were in line with the recommendations of the World Health Organization (WHO). The principal fatty acid (FA) consisted in oleic acid (41.32%), followed by linoleic acid (23.08%). A comparison was made with Moroccan and Algerian PLFO showing that Tunisian PLFO is the richest in linoleic acid. On the other hand, a study was carried out on the DSC thermogram of PLFO which illustrates the variation of enthalpy values with increasing heating temperature. PLFO presented a simple thermogram with two distinct peaks.

**Keywords**: Pistacia lentiscus, physicochemical characterization, antioxidant effect, essential fatty acids, tocopherols.

**Oral communication** **OR-052**

# Incorporation of Allium Cepa L. on transformed refrigerated meat

Dorsaf Moalla Rekik[1], Imen Kallel[2], Ahmed Bayoudh[3]

[1:] Department of Biology, Faculty of Sciences, University of Sfax

[2:] Research Laboratory of Toxicology, Microbiology Environmental, and Health (LR17ES06), Faculty of Sciences of Sfax, Po Box 1171, 3000 Sfax, University of Sfax, Tunisia

[3:] Laboratory of Enzyme Engineering and Microbiology, Engineering National School of Sfax (ENIS), University of Sfax, Tunisia

**E-mail:** rmdorsaf@gmail.com

**Abstract**

The impact of onion extract on refrigerated meat was investigated by adding dried green onion waste to salami and storing it at 4°C for 90 days. During this storage period, the microbiological quality was closely monitored, and a variety of assessments—including physico-chemical, microbiological, and sensory evaluations—were conducted.

Adding dried green onion waste to salami and storing it at 4°C for 90 days effectively suppressed the growth of several microorganisms, including total coliforms, FMAT, yeasts, molds, and Salmonella. This antimicrobial action is attributed to the natural compounds present in onions, which have been shown to reduce microbial contamination effectively due to antioxidant components.

By substituting 0.6% of nitrate and nitrite with 0.1% onion extract in the salami formulation, the shelf life at 4°C was extended by 10 days compared to commercial products. This demonstrates the potential of using onion extract as a natural preservative to extend the storage life of refrigerated meat preparations.

The addition of onion extract while maintaining the organoleptic, microbiological, and color qualities preferred by consumers. Sensory evaluations confirmed that the meat treated with onion extract retained desirable characteristics, making it a viable natural preservative alternative.

The study highlights the potential of substituting traditional preservatives like nitrate and nitrite with onion extract. This approach not only enhances the safety of the meat product but also aligns with consumer preferences for natural ingredients.

The findings support the safe and effective use of natural preservatives like onion extract in refrigerated meat products. The incorporation of onion extract can extend shelf life, inhibit microbial growth, and maintain the quality attributes preferred by consumers, making it a promising alternative to synthetic preservatives.

**Keywords**: Allium Cepa, refrigerated meat, salami, physico-chemical, microbiological, sensory evaluations.

**Oral communication** **OR-053**

# Activité antibactérienne d'un nouveau sesquiterpène isolé d'une plante endémique : Myrtus nivellei

DEMMAK Rym Gouta[1*], TENIOU Soumia[2], MOKRANI El Hassen[2], BENSEGUENI Abderrahmane[2]

[1] *Département de médecine, Université Salah Boubnider-Constantine 3; 25000 Constantine, Algerie*

[2] *Laboratoire de Biochimie Appliquée, Département des Sciences de la Nature et de la Vie, Université Frères Mentouri-Constantine 1; 25000 Constantine, Algerie*

**E-mail**: rym.demmak@univ-constantine3.dz

**Abstract**

Myrtus nivellei Batt. & Trab est une plante médicinale utilisée par la population locale en Algérie (les Touaregs) pour traiter plusieurs troubles telle que les diarrhées et la fièvre. Très peu d'informations sont disponibles sur la phytochimie et les activités biologiques de cette plante. L'objectif de cette étude est d'examiner l'activité antimicrobienne de la partie aérienne de Myrtus nivellei par fractionnement bio-guidé, afin de séparer et d'identifier les composés les plus actifs.

Les parties aériennes réduites en poudre (500 g) ont été extraites par macération en utilisant trois solvants successifs (dichlorométhane, méthanol et éthanol-eau, 1:1 v/v, 3 × 1 L chacun). Les solvants ont ensuite été évaporés de manière exhaustive pour obtenir 75,0 g d'extrait dichlorométhane (DCM), 80,2 g d'extrait méthanol et 63,0 g d'extrait hydro-alcoolique. Un premier criblage antimicrobien a été réalisé pour les trois extraits sur une large gamme de concentrations allant de 1,20 mg/mL à 0,03 mg/mL contre 36 souches microbiennes, dont 35 bactéries et une levure.

Les résultats ont montré que sur les trente-six souches microbiennes étudiées, chaque extrait de M. nivellei inhibait en moyenne une quinzaine de micro-organismes. Neuf d'entre eux étaient simultanément sensibles aux trois extraits, mais avec des CMI différentes, allant de 0,07 à 0,60 mg/mL. L'extrait de dichlorométhane (19 g) a été fractionné par chromatographie centrifuge partitionnée, en utilisant le système Arizona W (n-heptane/AcOEt/MeOH/eau 6:1:6:1; v/v), ce qui nous a permis d'obtenir 54 mg du composé 1. Ce dernier a été identifié par SM et RMN 1D et 2D comme un sesquiterpène jamais rapporté dans la littérature scientifique. Le composé 1 a ensuite été testé en microplaque contre 4 bactéries pathogènes et la CMI était de 9,7 µg/mL.

En conclusion, ces résultats suggèrent que le composé 1 pourrait être un candidat potentiel pour surmonter la résistance aux antibiotiques.

**Keywords** : activité antibactérienne, fractionnement bio-guidé, Myrtus nivellei, sesquiterpène.

**Oral communication** **OR-055**

# Étude phytochimique et évaluation du pouvoir antioxydant d'une étude phytochimique et évaluation du pouvoir antioxydant d'une plante Saharienne par deux méthodes d'extraction différentes

BOUTEMEDJET Siham[1], TOUDERT Nadia[2]

[1] *Laboratory of Synthesis and Organic Biocatalysis, Badji Mokhtar University, Annaba, Algeria*
[2] *Laboratory of Physical Chemistry of Materials, El Chadli Ben Djedid University, El Tarf, Algeria*

**E-mail** : sihemziad@yahoo.fr

**Résumé**

Ce travail a pour but l'étude phytochimique et l'évaluation du pouvoir antioxydant d'une plante médicinale de l'est Algérien par deux méthodes d'extraction.
La première partie a été réservée au screening phytochimique et à la quantification des polyphénols et des flavonoïdes quant à la deuxième concerne l'étude de l'activité antioxydante des extraits préparés dans différents solvants par deux méthodes d'extraction différentes : conventionnelle et assistée par ultrasons.

Les résultats montrent que la plante est assez riche en composés phénoliques et les meilleures teneurs ont été observées pour l'extrait aqueux. L'étude de l'activité antioxydante par la technique du radical DPPH a montré que les meilleurs résultats sont donnés par l'extraction sous ultrasons.

**Mots-clés :** Plante médicinale, Extraction, Ultrasons, Activité antioxydante.

**Oral communication** **OR-057**

# Synthesis, molecular docking, and DFT study of novel sulfonamide derivatives bearing amino ester and benzamide moieties

Soumaya BOUSKIA, Chafika BOUGHELOUM

*Laboratory of Advanced Systems and Materials, Sciences Faculty, Badji Mokhtar-Annaba University, P.o.Box 12, Annaba. 23000, Algeria.*

**E-mail** : soumaya.bouskia@univ-annaba.org

**Abstract**

Sulfonamides, a class of organic compounds characterized by the group ($-SO_2NH_2$), are known for their varied pharmacological properties, including antibacterial, anti-inflammatory, anti-diabetic and anticancer effects [1-3]. Our current research aims to synthesize novel sulfonamide derivatives that incorporate aminoester and benzamide groups. Benzamides, are prevalent in various biologically active natural compounds and pharmaceuticals, provide a structural framework that allows them to interact with diverse biological targets, leading to a wide range of pharmacological activities. These compounds were synthesized through a one-step reaction involving sulfonamides and benzioc acid, using a solid coupling agent.

To explore the interactions between the synthesized molecules and human carbonic anhydrase II (PDB IDs: 2AW1, 3SH4), we conducted molecular docking studies and performed a DFT analysis using the B3LYP/6-31G(d,p) method.

**Keywords**: Sulfonamides, Benzamides, Molecular docking, DFT.

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**Oral communication** **OR-058**

# Etude comparative de l'effet inhibiteur de la curcumine et de l'acide rosmarinique sur la cyclooxygénase 2 par docking moléculaire

ALEM Karima [1*], ALEM Samia [2], ATHMANI Walid , DJOUDER Chaouki [1], BOUMENDJEL Amel[1] et MESSARAH Mahfoud [1].

[1] *Laboratoire de Biochimie et Toxicologie Environnementale, Département de Biochimie, Faculté des Sciences, Université de Badji Mokhtar, Annaba, 23000, Annaba, Algérie*

[2] *Laboratoire de recherche "Ecologie des Systèmes Terrestres et Aquatiques. Département de Biologie, Faculté des Sciences, Université de Badji Mokhtar, Annaba, 23000, Algérie*

**E-mail:** karima.alem@univ-annaba.dz

**Résumé**

La cyclooxygénase 2 (COX-2) est une enzyme clé principalement responsable de l'activité inflammatoire, étant surexprimée et induite par de nombreux facteurs pro-inflammatoires. Ainsi, son inhibition constitue une alternative efficace pour contrôler l'inflammation. Dans ce contexte, les produits naturels à base de plantes offrent une voie thérapeutique prometteuse. L'objectif de notre travail est d'évaluer l'effet inhibiteur de deux composés naturels, la curcumine et l'acide rosmarinique sur la COX-2 humaine par docking moléculaire en utilisant les logiciels AutoDockTools et Discovery Studio 2021 Client. Les résultats obtenus ont indiqué que l'énergie de liaison de la curcumine avec la COX-2 montre une affinité plus élevée (ΔG = - 8,8 kcal/mol) par rapport à l'acide rosmarinique (ΔG = - 7.9 kcal/mol) avec des interactions plus stables de type hydrophobes et hydrogènes. De plus, les propriétés physicochimiques et pharmacocinétiques de la curcumine analysées par le serveur SwissADME sont meilleures que celles de l'acide rosmarinique. Ces résultats suggèrent que la curcumine, un composé naturel aux propriétés remarquables, est un inhibiteur plus efficace de la COX-2 que l'acide rosmarinique.

**Mots-clés:** Inflammation, Cyclooxygénase, Curcumine, Acide rosmarinique, Docking moléculaire.

**Oral communication** **OR-059**

# In Silico study DFT and molecular docking of Saussurea Lappa's major bioactive compounds

Khadidja Otmane Rachedi[1], Aicha Rizi[1], Anissa Acidi[1], Chelbi lilya[2], Radia Bouasla[1], Malika Berredjem[1]

[1] *Laboratory of Applied Organic Chemistry LCOA, Synthesis of biomolecules and molecular modelling Group, Badji -Mokhtar - Annaba University, Bo x 12, Annaba 23000, Algeria*

[2] *Laboratory of Applied Neuroendocrinology,, Department of Biology, Faculty of Science, Badji - Mokhtar - Annaba University, Bo x 12, Annaba 23000, Algeria*

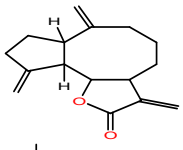
**E-mail** :k.otmanerachedi@yahoo.com

**Abstract**

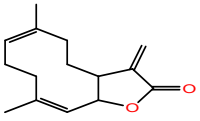
A theoretical study (DFT, ADMET, POM and molecular docking) of the Indian Costus plant (Saussurea Lappa) has been carried out. This plant is rich in secondary metabolites and belongs to the Asteraceae family. An alcoholic extract's treatment of this plant with Hexane allowed us to obtain a yield of 14.28%. The two major bioactive compounds of the roots Costus plant are Dehydrocostus lactone (DHC) and Costunolide. Given the biological and pharmacological importance of these two compounds, we have been carried out a DFT study of these two active compounds in order to predict their chemical reactivity using the Gaussian09 software [1]. Maestro version 16.8 software [2] has been also used for a molecular docking study of these two compounds. In order to estimate the pharmacokinetics of these molecules, as well as their similarity to drugs, an ADME study [3] has been carried out. The findigs of this study show that (DHC) and Costunolide have interactions with the target protein, they also have a good pharmacokinetic properties with good bioavailability. The DFT study indicates that Costunolide is more reactive than (DHC).

**Keywords**: Indian Costus, bioactive compound, DFT, ADME, docking.

**DHC**



**Costunolide**



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**Oral communication** **OR-060**

# Molecular modeling of inclusion complexes as drug delivery systems

Safia Himri [*1,2], Belgacem Bezzina[3] and Hemza kouarta[4]

[1] *Laboratory of Reaction Engineering, Department of Process Engineering, Faculty of Mechanical Engineering and Process Engineering, BP32 El Alia USTHB, BEZ, Algiers, Algeria.*
[2] *University of 8 May 1945- Guelma.*
[3] *Research Center in Industrial Technologies (CRTI), P.O.Box 64, Cheraga, 16014.Algiers, Algeria.*
[4] *LEAM, Department of Physic, Faculty of Sciences, University of Badji Mokhtar Annba, Algeria.*

**E-mail**: himri.safia@gmail.com // himri.safia@univ-guelma.dz

**Abstract**

Molecular recognition is of profound importance in biology and therapeutics. The cyclodextrins (CDs) are of particular interest in this regard. Among various approaches CDs have contributed a lot to this aspect of drug delivery, because of having fairly rigid and well-defined hydrophobic cavities and hydrophilic outer surfaces, they can act as molecular receptors (hosts) for a wide variety of organic and inorganic, as well as biological and pharmaceutical guest molecules, forming host–guest complexes or supramolecular assemblies. The cavity size of β-cyclodextrin (β-CD) is more appropriate than other CDs to encapsulate a great variety of molecules. The drugs, to be pharmacologically active, must possess some degree of aqueous solubility, as well as they should be lipophilic to permeate the biological membranes via passive diffusion. If a drug is hydrophilic, the dissolved drug molecule will not penetrate from the aqueous exterior into a lipophilic biomembrane. The use of β-CD on drug solubility, bioavailability, safety, stability and as a carrier in drug formulation may be achieved by formation of inclusion complexes with drug molecules.

Norepinephrine, NP, is a member of the catecholamine family of compounds known to possess pharmacological activities as neurotransmitters and hormones. It is used to treat cases of low blood pressure because as a stimulant of the sympathetic nervous system it increases the heart rate and blood pressure.

**Keywords**: β-cyclodextrin, Norepinephrine, Inclusion complex, PM3 and DFT.

**Oral communication** **OR-062**

# Hirshfeld's 3D surface and charge density of 2-methylanilinium dihydrogen phosphite obtained using theoretical model (DFT)

Noureddine DADDA[1], Amel MESSAI[2], Malika MEDJALDI[3] and Karima DADDA[4]

[1] *Laboratory of Synthesis and Organic Biocatalysis, Department of Chemistry, Badji-Mokhtar-Annaba University, Algeria*

[2] *ISMA laboratory, Faculty of Sciences and Technology, Abbes Laghrour University Khenchela, 40000, Algeria.*

[3] *Laboratory of SATIT, University Abbes Laghrour Khenchela, Algeria.*

[4] *Laboratoire des Matériaux Semi-conducteurs et Oxydes Métalliques (LMSOM), Départements des Matériaux et Composants, Faculté de Physique, Université des Sciences et de la Technologie Houari Boumediene (USTHB), Alger, Algérie.;*

**E-mail** :naouridadda2@gmail.com

**Abstract**

The 2-methylanilinium dihydrogen structure was determined at 100 K using a multipolar atom model. Theoretical structure factors were calculated from the periodic functional density theory, used to refine a theoretical multipolar charge density model (Theo-Mult). The 3D Hirshfeld surfaces calculations were computed for intermolecular interactions. The Fourier residual electron density maps analysed in the aromatic and the carboxylic plane for IAM model and multipolar model taken at 100 K showed that the multipolar model is the clearest, considering the deformation's electron density. The electron density distribution associated to multipolar (Mult) and Theo-Mult models was studied.

**Keywords:** 2-methylanilinium dihydrogen phosphite; Crystal structure; Hirshfeld surface; Electronic density; DFT.

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**Oral communication** **OR-063**

# Computational modeling of intermolecular interactions in β-cyclodextrin inclusion complex

[1] Souha. Fatma. Zohra. Soukehal, [1]Djamel. Bouchouk, [1]Tahar. Abbaz

*[1] Laboratory of Organic Chemistry and interdisciplinary, Mohamed Cherif Messaadia University., Souk Ahras, 41000, Algeria.*

**E-mail:** f.soukehal@univ-soukahras.dz

**Abstract**

Many promising pharmaceutical compounds are hindered by excessive volatility or low solubility, which can compromise their biological activity and make them difficult to handle. Cyclodextrins offer a solution to these challenges by forming inclusion complexes with these molecules.

A theoretical study was conducted to investigate the inclusion mechanism between a bioactive molecule and the macromolecule cyclodextrin. The study involved simulating the inclusion of the guest molecule within the host molecule and optimizing the resulting structure using DFT calculation methods. The goal was to determine geometric and energetic parameters, as well as perform NBO, NMR and NCI analyses, to predict and validate the formation of the complex and the various intermolecular interactions contributing to its stability.

**Keywords**: β−cyclodextrin, Inclusion complex, DFT, NBO, NMR, NCI.

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**Oral communication** **OR-064**

# In-Silico profiling of Schiff Base derivatives against MCF-7 cell lines: Docking study and ADMET analysis

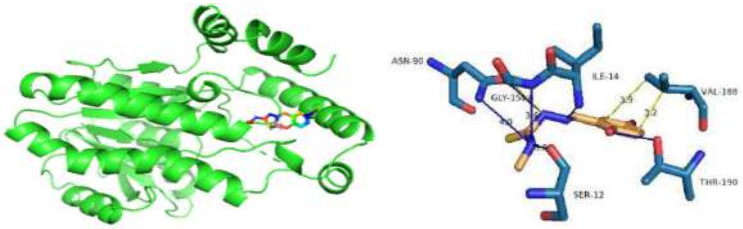
Nour HASNI[a,*] , Rayene KADRI[a*] , Mekki KADRI[a*]

[a] *Laboratoire de Chimie Physique , Université 8 Mai 1945,24000 Guelma , Algérie*

**E-mail:** nourhsn234@gmail.com

**Abstract**

N, S-donor ligands, which contain both nitrogen and sulfur atoms, play a crucial role in coordination chemistry due to their versatile coordination abilities and significant biological relevance. Among these, thiosemicarbazone ligands, characterized by the general formula $R_1NH–C(=S)–NH–N=CH–R_2$, demonstrate exceptional donor properties that enhance their bioactivity in medicinal chemistry. These ligands are notable for their flexibility and reactivity, as well as their unique tautomeric characteristics, which facilitate diverse bonding modes with metal ions. The complexation of thiosemicarbazone ligands with transition metals such as Co(II), Ni(II), Cu(II), and Zn(II) has been extensively studied [2]. These metal complexes are recognized as promising candidates in drug development, offering therapeutic applications that include antioxidant, anticancer, anti-inflammatory, antimalarial, antimicrobial, and anti-tuberculosis effects [3]. The ability of these complexes to interact with biological targets underlines their potential for treating various diseases, especially cancer. To explore their anticancer potential, we conducted a molecular docking study against MCF-7 cell line proteins (PDB IDs: 1FDW, 2WTT, 5GWT). The docking calculations revealed that both the ligands and their corresponding metal complexes exhibited significant affinities for the cancer targets, indicating their potential as effective anticancer agents. This finding is crucial as it paves the way for further experimental validation and development of these compounds as therapeutic options for breast cancer.




In addition to the docking studies, comprehensive computational analyses were performed to tackle challenges in drug discovery. These molecular docking analyses elucidate the interactions and binding energies of the compounds with amino acids [5], providing insights into their mechanisms of action. Furthermore, a thorough evaluation of ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) properties is essential to assess the therapeutic potential of these metal complexes. This assessment ensures that the compounds possess favorable bioavailability, which is vital for efficient absorption and distribution within biological systems.

Moreover, understanding metabolic pathways is crucial for predicting potential toxicity, thereby enabling the design of safer and more effective therapeutic agents. By integrating these evaluations, we can better establish the safety and efficacy of thiosemicarbazone complexes, positioning them as viable candidates for clinical applications in cancer treatment and beyond.

**Keywords**: N-Methyl Thiosemicarbazide, Schiff base, molecular docking, ADMET, MCF-7, anticancer breast.

**Oral communication** **OR-065**

# Phytochemical, antioxidant, antibacterial activity and chemical composition for Opuntia strepthacanta, thorn-less Opuntia ficus indica and thorn Opuntia ficus indica in Libya.

[1,2]Abdalla A. Mohamed, [2]Taher Abdalhameed, [3]Khaled Aburass, [4]Ftaim Taher Gammoudi, [4] Salah M. Azwai, [4]Ibrahim M. Eldaghayes, [4]Aboubakar M. Garbaj, [5]Lazhar Zourgui and [1]Bassem Khemakhem

[1]*Laboratory of Plant Biotechnology, Sfax. Faculty of Sciences, PB 1171, University of Sfax, 3038 Sfax, Tunisia.*

[2]*Department of Medical Nutrition, Biomedical Research Team, Faculty of Medical Technology, University of Zawia. Libya*

[3]*National Medical Research Center, Zawia Libya.*

[4]*Department of Microbiology and Parasitology, Faculty of Veterinary Medicine, University of Tripoli. Libya*

[5]*University of Gabes, Research lab. BMA 'Biodiversities, Molecules, Applications" Department of Biological Engineering, Higher Institute of Applied Biology of Medenine(ISBAM), Tunisia*

**E-mail** : a.alrmah@zu.edu.ly

**Abstract**

**Background:** Opuntia, commonly called prickly pear, is a member of the Cactaceae family that originated in Central America but is now grown in Europe, the Middle East, and northern Africa. Many Opuntia species were grown in Libya, including Opuntia strepthacanta, thorn-less Opuntia ficus indica, and thorn Opuntia ficus indica. Prickly pear fruits and cladodes contain beneficial components including phenolic acids, flavonoids, and colors. Studies have discovered a substantial link between phenol concentration in Opuntia spp: extracts and antibacterial and antioxidant activities.
**The objective of work** to assess the in vitro antioxidant and antibacterial properties and the phytochemical components of Opuntia cladode extracts from three species of Opuntia cladodes in Libya.
**Methodology**: in this work, three cladode extracts for Opuntia species in Libya were examined for differences in their chemical composition, antioxidant and antibacterial properties, total phenolic content (TPC), and total flavonoid content (TFC). Results: Opuntia strepthacanta had the highest TPC for ethanolic and aqueous extracts, respectively (112.23 ± 0.96 mg GAE/g and 94.61 ± 0.81 mg GAE/g), while the thorn Opuntia ficus indica had the highest TFC and tannin contents for ethanolic and aqueous extracts, respectively (75.70 ± 0.75, 63.82 ± 0.64 mg CAT/g and 0.620 ± 0.030, 0.523 ± 0.025 mg CAT/g). The thorn-less Opuntia ficus indica have great antibacterial against all bacteria strain in the study.
**Conclusion:** The findings revealed that Opuntia species in Libya are a great source of biomolecules with high antiradical and antibacterial properties that might be exploited in functional food.

**Keywords:** phytochemical, antioxidant, Opuntia ficus indica, antibacterial, Opuntia strepthacanta

# POSTER COMMUNICATIONS

The 1st International Seminar on medicinal chemistry and green chemistry (1st IS MCGC - Annaba 2024)

**Poster communication** **P-001**

# Multi-component synthesis of 2-[Aryl(arylamino)methyl]furo[3,2-c]pyran-3,4-diones and of 3-[3-Aryl-3-aryl amino) acryloyl]-4-hydroxypyran-2-ones

Y. Abdi[a,b], D. Siziani[a,b], M. Kelbouz[a], I. Tennci[a], Z. Attou[b], N. Bensouilah[b]

[a)] *Applied sciences laboratory LSA, Ecole Nationale Supérieure des Technologies Avancées, Cité Diplomatique, ex. Centre biomédical, Dergana, Bordj El Kiffan, Algiers, Algeria*

[b)] *Laboratory of Applied Organic Chemistry, Faculty of Chemistry (LAOC), University of Sciences and Technology Houari Boumediene, USTHB, PB 32, El-Alia, Bab-Ezzouar, 16111 Algiers, Algeria*

**E-mail:** yamina.abdi@ensta.edu.dz

## Abstract

In cascade transformations[1] and multicomponent reactions[2] as tools in the synthesis of complex biologically important compounds.[3]An earlier report has shown that a one-pot, four-component reaction of 2-bromoacetophenones with aldehydes, primary amines, and ammonium acetate under solvent-free conditions has provided highly functionalized imidazole scaffolds.[4]
Herein, we investigate the chemical behaviour of α-Br-DHA (1) under similar multicomponent reaction conditions, 4 aiming to build up novel structural dyads of pyran-2-ones.

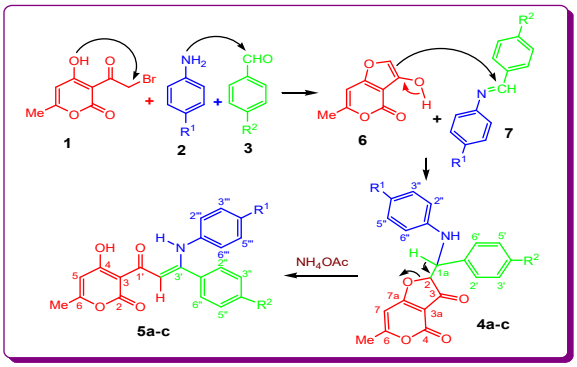
At first, we discovered that the three-component reaction of equimolar quantities of α-Br-DHA (**1**) with anilines **2** and benzaldehydes **3** in refluxing ethanol unexpectedly afforded 2-[aryl(arylamino)methyl]-6-methyl-4H-furo[3,2-c]pyran-3,4(2H)-diones **4a–c** in excellent yields (87–96%) and short reaction time (30 min, Scheme 1).

A similar protocol in the presence of 1.5 equivalents of ammonium acetate in refluxing ethanol surprisingly gave 3-[3-aryl-3-(arylamino)acryloyl]-4-hydroxy-6-methyl-2H-pyran-2-ones **5a–c** in 88–96% yields within 120 minutes.

The structures of the resulting furo[3,2-c]pyran-3,4-diones **4a–c** were established from their extensive 2D NMR analyses (HSQC, HMBC, and NOESY) and mass spectrometric data.

In conclusion, we have described a one-pot, three component reaction of α-bromodehydroacetic acid with anilines and benzaldehydes resulting in a high-yielding preparation of novel 2-[aryl(arylamino)methyl]-6-methyl-4H-furo[3,2-c]pyran-3,4(2H)-diones **4a–c** and demonstrated their diastereoselective tautomerism under basic conditions to (Z)-3-[3-(aryl)-3-(aryl amino) acryloyl]-4-hydroxy-6-methyl-2H-pyran-2-ones **5a–c**.

We have also obtained these latter compounds through a one-pot, three-component reaction of α-Br-DHA, anilines, benzaldehydes catalyzed by ammonium acetate.




**Scheme 1 .** Possible mechanistic pathway for the formation of furopyran-3,4-diones 4a-c and tautomerism via 1,3-proton shift to 3-enaminone-pyran-2-one 5a-c.

**Keywords**: DHA, DHA-Br, MCR, green chemistry, organic synthesis, Heterocyclic ligands.

**Poster communication** **P-002**

# Microwave utilization in esterification reaction as a green energy

ACHOURI Rahma[1,2], MELAIS Nedjma[1,3], YAHIA Wassila[1,4].

[1]*Department of Chemistry, Faculty of Sciences ,University of 20 August 1955 – Skikda - B.P. 26 street El-Hadaiek 21000 Skikda - Algeria.*

[2]*Physical chemistry laboratory of surfaces and interfaces -LRPCSI ,University of 20 August 1955 – Skikda - B.P. 26 street El-Hadaiek 21000 Skikda - Algeria.*

[3]*Eco-compatible asymmetric catalysis laboratory, university Badji Mokhtar-Annaba, Algeria.*

[4]*Organic Synthesis and Biocatalysis Laboratory,Department of Chemistry, Faculty of Sciences ,University Badji Mokhtar Annaba, BP 12 23000 Annaba, Algeria.*

**E-mail:** achourirahma95@gmail.com

**Abstract**

Microwave use in esterification accelerates the reaction, reducing it from hours to minutes. This method, applying direct microwave heating, enhances selectivity and yields, minimizing by-products. It's a green energy option, significantly cutting energy usage and reducing solvent quantities. This approach aligns with sustainable, eco-friendly chemical synthesis, showing promise for more environmentally conscious reactions. Herein, we present studies on the resolution of (R/S) - 4-chromanol used for the preparation of enantiomerically pure building blocks in a green fashion [1]. The microwave irradiation is widely used in organic chemistry [2].

We have reported a convenient procedure for the lipase-catalyzed acylation with succinic anhydride as acylating agent [3] under unconventional activation.

**Keywords**: microwave, biocatalysis, eco-friendly, acylation, resolution.

**Poster communication** **P-003**

# A catalytic approach for N−S bond formation from Iminyl radicals under flow conditions and batch

Adnane HALIMA SALEM*[1,2,3], Abdellah MILOUDI[1,3] and José ALEMAN[4,5]

[1]*Laboratoire de Chimie Fine, Département de Chimie, Faculté des Sciences Exactes et Appliquées, Université Oran-1, BP1524, El Mnaouer, 31100, Oran, Algeria.*

[2]*Département de Chimie, Faculté des sciences Exactes, Université de Mascara, Av. Cheikh El Khaldi, Mascara 29000, Algérie*

[3]*Département des Classes Préparatoires en Sciences et Technologies, Ecole Nationale Polytechnique d'Oran Maurice-Audin, BP1523, ElMnaouer, 31100, Oran, Algeria.*

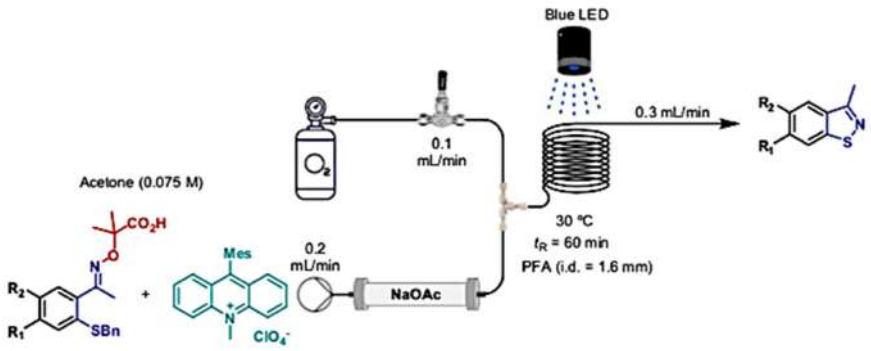
[4]*Organic Chemistry Department, Módulo 1, Universidad Autónoma de Madrid, 28049 Madrid, Spain.*

[5]*Institute forAdvanced Research in Chemical Sciences (IAdChem), Universidad Autónoma de Madrid, 28049 Madrid, Spain.*

**E-mail:** adnane.halima-salem@enp-oran.dz

**Abstract**

Isothiazoles, which contain two electronegative heteroatoms (nitrogen and sulfur) in a 1,2-relationship, are important scaffolds in medicinal chemistry and agriculture industry. A sustainable synthesis of isothiazoles has been developed using an α-amino-oxy acid auxiliary and applying photoredox catalysis (Scheme 1). This simple strategy features mild conditions, broad scope and wide functional group tolerance representing a new environmentally friendly option to prepare these highly valuable heterocycles. Furthermore, the synthetic value of the method is highlighted by the preparation of a natural product derivative and the implementation of the reaction in a continuous flow setup.




**Scheme 1:** Synthesis of Isothiazoles.

**Keywords**: Isothiazoles, Photocatalysis, Metal Free, α-amino-oxy acid.

**Poster communication** **P-005**

# Synthesis, characterization & conductivity study of hexamethylenetetramine - metal (ii) complexes

Aya Alem[1]*, Yasser Bouchebcheb[1], Dalila Fedaoui[1], Zerrad Chaima[1]

[1]*Laboratory of Synthesis and Organic Biocatalysis (LSBO), Organic Synthesis and Medicinal Chemistry Group, Department Of Chemistry, Faculty of science, BADJI Mokhtar-Annaba University, P.O. Box 12, Annaba 23000, Algeria*

**E-mail**: ayaalem2608@gmail.com

**Abstract**

The heterocyclic tetradentate donor ligand hexamethylenetetramine (HMTA, $C_6H_{12}N_4$) has been employed in medicine as an antibacterial remedy for infections of the urinary tract [1]. There have been reports on the synthesis of some metal hexamethylenetetramine complexes among the multi-dentate nitrogen donor ligands, as well as their antibacterial properties [2].

For this reason, investigations into HMTA coordination compounds with various metal salts has garnered a lot of interest.

Herein we present synthesis of HMTA-Ni (II), and Cu (II) complexes. The nickel complex has two molecules of hexamethylenetetramine, whereas the copper (II) complexes only include one. Infrared and UV-visible spectroscopy and conductivity, have all been used to characterize these compounds. The findings point to octahedral coordination, where HMTA and aqua ligands are linked to the center metal ion. Infrared and UV-visible spectroscopy methods have also been used to create and characterize complexes containing hexamethylenetetramine and thiocyanate ion as coligands [3].

**Keywords**: Hexamethylenetetramine, Complexes, UV-Visible, Nickel complexes, cooper complexes.

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**Poster communication** **P-006**

# Ecofriendly green synthesis of copper oxide nanoparticles using the UM plant extract and their application for the cristal violet dye degradation

Karima Bekouche[1], Daoiya Zouied[2], Malika Khelfaoui[2]

[1]*Department of Process Engineering University Aout 20, 1955-Skikda.*
[2]*Laboratory of Chemical Engineering and Environment of Skikda (LGCES), University-20 Aout-1955-Skikda, Algeria.*

**E-mail**: krmbekouche21@yahoo.com

**Abstract**

The green synthesis method, which employs natural plant extracts, has recently gained considerable interest within the scientific community. This is due to the significant advantages it offers in comparison to other physical and chemical methods, which are generally disfavored due to their high costs, toxic and unsafe nature. The green synthesis approach plays a vital role in the field of nanotechnology, where scientists are directing their attention towards the identification of novel plant extracts that are rich in carboxyl and phenol groups. These extracts have the potential to serve as effective reducing and capping agents in the synthesis of nan scale particles with size ranging 1-100 nm, including metal, oxide, and polymer nanoparticles. In this study, a novel plant extract derived from U.M (collected from the north of Algeria in February) was used in the bio-synthesis of copper oxide nanoparticles by reducing the copper oxide ions present in copper nitrate. The as-synthesized copper oxide nanoparticles were characterized with a variety of techniques, including X-ray diffraction (XRD), ultraviolet-visible (UV-Vis) spectroscopy, and energy dispersive X-ray spectroscopy (EDX). The photoreduction activity of U.M-mediated copper oxide nanoparticles was investigated in the photodegradation of crystal violet dye. Copper oxide nanoparticles with a monoclinic structure were successfully biosynthesized, exhibiting a removal capacity of crystal violet exceeding 90% within 70 minutes. Moreover, the study indicates that doping copper oxide NPs with noble metals has been demonstrated to enhance the degradation of dyes to a value exceeding 98%.

**Keywords**: U.M plant extract, green synthesis, copper oxide, nanoparticles, crystal violet dye

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**Poster communication** **P-008**

# Valorization of Azerole biomass and elimination of BM

[a]Benregga Fatima.Zohra, [b] Maghchiche. Abdelhak, [c] Yousfi.Chaima

*[a] Faculty of Exact Sciences and Sciences of Nature and Life, Department of Material Sciences, Larbi Tebessi University, Tebessa, Algeria*

*[b] Department of Pharmacy, Faculty of Medicine, Batna2 University, Batna Algeria*

*[c] National Higher School of Biotechnology University of Constantine3, Constantine, Algeria*

*[a,b] Laboratory of Organic Materials and Heterochemistry (LMOH) Larbi Tebessi University, Tebessa Algeria*

**E-mail**: fatima .benregga @univ-tebessa.dz

**Abstract**

Activated carbon has long been known as an adsorbent. It is characterized by its large specific surface area, porous structure, and thermostability, among other properties. It can be prepared from any solid material containing a high proportion of carbon, often through carbonization followed by physical or chemical activation.

Our work has a dual aspect, the valorisation of waste biomass. And on the other hand, the study of the absorbing efficiency of activated carbon.The goal of the present study is the valorisation of farm food industry wastes , whereas hundred thousand's tonnes are produced every year.

The Azerole (Zoorour) is a medicinal plant with several therapeutic properties. These fruits are also rich in polysaccharides (cellulose and pectin) and aromatic amino acids; hence, they are rich in carbon, making them suitable for conversion into charcoal.

To valorize natural materials and reduce pollution, azerole waste has been used as a raw material in the production of charcoal through chemical activation with phosphoric acid, followed by a carbonization step. We studied pH, ash content, moisture content, and iodine index for characterization. A comparative study with commercial charcoal C Merck regarding removing the BM dye was conducted using a UV-visible technique. The different results showed that the prepared charcoal is comparable to industrial charcoal and could be used in water treatment.

**Keywords**: Coal, Azerole, Carbonization, Activation, Adsorption.

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**Poster communication** **P-009**

# Synthesis and enhanced photocatalytic performance of $CoAl_2O_4$ nano-sheets: Structural characterization and degradation of organic pollutant under visible light

BENSEMMANE Nachida [1,*], MEDJADJI Hamza [1], BOULAHOUACHE Ali [1,2], IMELHAINE Adel [3], SALHI Nassima [1,2]

[1,*] *Laboratoire LCPMM, Faculté des Sciences, Université BLIDA1, B.P 270, Route de Soumaa, BLIDA, Algérie.*

[2] *Laboratoire de Chimie du Gaz Naturel, Faculté de Chimie, USTHB, BP32, El-Alia, 16111 Bab Ezzouar, Alger, Algérie.*

[3] *Département de chimie, Faculté des Sciences, Université BLIDA1, B.P 270, Route de Soumaa, BLIDA, Algérie.*

**E-mail:** bensemmane_nachida@univ-blida.dz

## Abstract

In this study, $CoAl_2O_4$ nano-sheets were synthesized via the sol-gel method, using propionic acid as a chelating agent. The material's structure, chemical bonding, morphology, composition, and optical properties were evaluated using various techniques as: X-ray diffraction (XRD), FT-IR spectroscopy, UV-visible diffuse reflectance spectroscopy (DRS), and scanning electron microscopy coupled with energy-dispersive X-ray spectroscopy (SEM-EDX). XRD analysis of the calcined powder confirmed the formation of a pure spinel phase, with an average particles size of 35 nm. SEM analysis revealed a sheet-like morphology with lower porosity, while EDX confirmed the expected presence of cobalt (Co), aluminum (Al), and oxygen (O). X-ray photoelectron spectroscopy (XPS) provided the surface electronic states of the elements.

The photocatalytic activity of the $CoAl_2O_4$ spinel was performed through the degradation of methylene blue, an organic pollutant model, under visible light irradiation. Various parameters, including solution pH and the presence of electron acceptors, were examined. At pH ~7, a degradation rate of 15.73% was observed within 90 minutes, whereas near-complete degradation (~100%) was achieved at pH ~3 after 90 minutes in the presence of the electron acceptor $K_2S_2O_8$.

**Keywords**: $CoAl_2O_4$, Sol-gel, Spinel, Photocatalytic-degradation, Methylene blue.

**Poster communication** **P-010**

# Synthesis of novel sulfonamide-aziridine hybrid molecules, theoretical study DFT and molecular docking.

BOUASLA Radia[1,2], BOUSSAKER Meriem[1], OTMANE RACHEDI Khadidja[1,3], DEKIR Ali[1], BERREDJEM Malika[1]

[1]*Laboratory of Applied Organic Chemistry, Synthesis of Biomolecules and Molecular Modelling Group, Department of Chemistry, Sciences Faculty, Badji-Mokhtar-Annaba University, Box 12, 23000 Annaba, Algeria.*

[2]*National Higher School of Technology and Engineering, Preparatory Classes Department, 23005, Annaba, Algeria.*

[3]*Chadli Bendjedid University, Natural, and Life Sciences faculty, El-Tarf, 36000, Algeria*

**E-mail :** r.bouasla@ensti-annaba.dz

**Abstract**

Bibliographic studies show that heterocyclic compounds containing nitrogen, sulfur and / or oxygen, has shown remarkable pharmacological activity. Among the different classes of heterocyclic compounds, mainly nitrogenous structures are present in many natural compounds of plant, animal or synthetic origin. These structures are sometimes associated with each other but in most cases, they are linked to very diverse structural patterns.

Aziridines are an important class of heterocyclic compounds; basically, they are a fully saturated three-member ring containing one nitrogen and two carbon atoms. This moiety is present in certain natural and synthetic products having a known beneficial biological activity.

On the other hand, the sulfonamide moiety is frequently found in antimicrobial drugs, acting by inhibiting the activity of bacterial enzymes. It can also be found in compounds exhibiting anti-inflammatory properties, they are often used in medicinal chemistry.

The combination of sulfonamide and aziridine can create a molecule with both antibacterial properties associated with sulfonamides and reactive properties characteristic of aziridines.

In this study, the new sulfonamide-aziridines derivatives were designed and successfully synthesized starting from chlorosulfonyl isocyanate, diverse amines and dibromoethane. The compounds were obtained in good yield, and their chemical structures have been determined by 1H NMR and HRMS spectra.

A theoretical study of synthesized compounds by DFT and molecular docking were performed to identify their chemical reactivity and to confirm their stability in the cavity of the biological target.

**Keywords**: sulfonamide, aziridine, molecular docking, DFT study.

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**Poster communication** **P-011**

# Use of supercritical $CO_2$ "Green chemistry" for the extraction of melon seed oil and identification of its fatty acid composition

[1]* Naima Bouazzaoui, [2] Jalloul Bouajila, [2] Severine Camy, [2] Jean-Stephane Condoret

[1] *University of Science and Technology Mohamed Boudiaf, Chemical Engineering Department, El Mnaouar, BP 1505, Bir El Djir 31000, Oran, Algeria,*

[1] *Laboratory of Organic Chemistry, Natural substances and Analysis (COSNA), Tlemcen University, Algeria*

[2] *Laboratory of Chemical Engineering, Toulouse University, INP, UPS, UMR, CNRS 5503, Toulouse, France*

**E-mail** : naima.bouazzaoui@univ-usto.dz

**Abstract**

The demand for natural products with high purity is rapidly expanding. Indeed, the high cost of organic solvents, increasing stringent environmental regulations and new requirements of the medical and food industries for ultra-pure and high value-added products have increased the need for new and clean technologies for the processing of foods. Thus, the aim of this work was to investigate the SC-$CO_2$ extraction of oil from melon (Cucumis melo L. Inodorus) seeds.

The oil was extracted by soxhlet using hexane and by supercritical $CO_2$ technology operating under a set of pressures and temperatures. Fatty acids composition was analyzed by gas chromatography and gas chromatography mass spectrometry.

The results showed that the melon seeds were rich in lipids. The yield of oil with SC-$CO_2$ extraction increased with increasing pressure. The highest extraction yield was 34% and was obtained at 70 MPa and 57°C. The major fatty acids extracted by soxhlet were palmitic, stearic, oleic and linoleic with the respective percentages of 5,95%, 2,87%, 21,95% and 69,24%. Extraction by supercritical $CO_2$ technology gave same results as compared to Soxhlet as regards oils.

Moreover, the SC-$CO_2$ technology afforded a safe mean of obtaining edible oils without using any contaminant organic solvent with yields that compared with soxhlet extraction.

**Keywords:** Cucumis melo, seed oil, supercritical fluid extraction, green chemistry, fatty acids.

**Poster communication** **P-012**

# Synthesis of silver, zinc and silver-doped zinc nanoparticles based on AG plant extract and evaluation of their crystal violet degradation efficiency

Mohamed boubessil[1,2,3*]; Daoiya Zouied[4]; Malika Khelfaoui[4] Nasrine Ammouchi[1,5] Youghourta Belhoucine[1]

[1] *Department of Process Engineering, Faculty of Technology, 20 August 1955 University of Skikda, P.O. Box 26, El Hadaik Road, 21000, Skikda, Algeria.*

[2] *Laboratory of Physico-Chemical research of Surfaces and Interfaces, 20 August 1955 University of Skikda, Algeria.*

[3] *Laboratory of Catalysis, Bio-Process and Environment, Department of Process Engineering, University of 20 August 1955, Skikda, Algeria*

[4]*Laboratory of Chemical Engineering and Environment of Skikda (LGCES), University-20 Aout-1955-Skikda, Algeria.*

[5] *Department of Technology, Faculty of Technology, 20 August 1955 University of Skikda, Algeria.*

**E-mail**: m.boubessil@univ-skikda.dz

**Abstract**

The search for a cost-effective and environmentally friendly method for wastewater treatment is a global challenge. Therefore, this study investigated the removal of pollutants from wastewater using zinc oxide, silver and silver-doped zinc nanoparticles synthesized using the extracts of the plant AG. Green synthesis of nanoparticles is a simple, rapid, cost-effective and environmentally friendly method that has successfully removed organic dyes from wastewater. The crystal violet degradation results for the different synthesized nanoparticles show that: silver-doped ZnO exhibits higher photodegradation efficiency than undoped ZnO for the different syntheses where the efficiency reaches 98.42% after a time of 100min in the presence of the plant Atractylis gummifera.

**Keywords**: green synthesis of nanoparticles; ZnO; Ag; Ag/ZnO ; crystal violet degradation.

**Poster communication** **P-013**

# Synthesis and characterization of macromolecules precursors of materials for applications in optoelectronics.

Bouguessa Sabrina[1,*], Amel zitouni[1], Saigaa Narimane [1], Ayoub Nadji[1], Gouasmia Abdelkrim[1].

[1] *Laboratoire de matériaux organique et héterochimie / Université de Tébessa, Tébessa, Algerie.*

**E-mail:** sabrina.bouguessa@univ-tebessa.dz // sbouguessa@hotmail.com

**Abstract**

One of the most attractive current objectives is to create semiconductor polymers with remarkable optoelectronic properties.
In this context, we are interested in the synthesis and characterization of a new series of potential precursors of such polymers.

On the basis of a retrosynthetic study of the targeted polymers, two types of key molecules of the olefination reaction of Horner-wadsworth-Emmons were retained.
Compound of type I: concerns dialdehyde with extensive π-conjugated system.
Compound of type II: involves aryl units disubstituted by two phosphonate functions.

During this synthsis, several types of reactions were used, among which the palladium-catalyzed Sonogashira coupling.

In order to confirm the structure of new molécules obtained, we used the usual analysis techniques suchas UV-Visible, Infrared and 1H NMR.

**Keywords**: Organic semiconductor materials, coupling of Sonogashira, optoelectronics.

**Poster communication** **P-016**

# Extraction et optimisation éco-responsable de la nanocellulose à partir d'un déchet forestier innovant

BOUMEDINE Titem Liza[1,2], KEDDAR Mohamed Nadir[2] .

[1] *Laboratoire de Protection des Ecosystèmes en Zones Arides et Semi-arides*
[2] *Laboratoire Dynamique, interaction et réactivité des systèmes*

**E-mail** :boumedine.titemliza@univ-ouargla.dz

**Résumé**

La santé humaine est de plus en plus liée aux innovations en chimie verte, qui vise à réduire l'impact environnemental des procédés chimiques. La valorisation des déchets forestiers, riches en cellulose, offre une solution durable pour extraire la nanocellulose, un biomatériau clé pour les bioplastiques. Qui sont bénéfiques pour la santé humaine car ils minimisent l'exposition aux produits chimiques toxiques. L'extraction de la nanocellulose utilise des méthodes écologiques telles que la délignification à la soude, le blanchiment au peroxyde d'hydrogène et l'hydrolyse acide à l'acide acétique, produisant un matériau léger, résistant, biodégradable, et possédant d'excellentes propriétés mécaniques et antimicrobiennes. Les bioplastiques à base de nanocellulose se décomposent plus rapidement que les plastiques conventionnels, réduisant ainsi la pollution par les microplastiques et les risques de contamination alimentaire et les perturbation endocriniennes, tout en contribuant à une meilleure qualité de l'air, de l'eau et des sols, ce qui est bénéfique pour la santé des générations futures. Dans ce travail, la nanocellulose a été extraite à partir de la valorisation d'un déchet forestier non exploité. L'extraction a été effectuée en combinant un traitement alcalin à l'aide de NaOH, suivi d'un blanchiment au H2O2 et enfin une hydrolyse acide avec de l'acide acétique. En premier , une optimisation du traitement alcalin a été réalisée en faisant varier la concentration du NaOH (C1 ;C2 ;C3 ;C4) , la température (T°1 ;T°2 ;T°3 ), la durée de la réaction(60 ;90 ;120 ;180 min). L'efficacité du traitement a été déterminée par le calcul du rendement de la quantité de matière délignifiée. Un rendement maximal de 92,88% a été obtenu avec les paramètres (C2/T°1/60min), pour prouver l'efficacité de ce traitement un dosage de lignine a été fait selon la norme D1106-96. Puis on passera à l'optimisation du blanchiment puis à l'hydrolyse acide, et enfin l'élaboration et caractérisation du bioplastique.

**Mots-clés :** nanocellulose, bioplastique, valorisation, déchet forestier, optimisation, santé

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**Poster communication** **P-017**

# Synthèse innovante de composés hétérocycliques copmlexes par la réaction de Vilsmeier-Haack

Ferial Chellali [1;*], Yazid Datoussaid [1,2], Attar Tarik [2,]

[1] *Laboratoire de catalyse et synthese en chimie organique , Facultée de sciences, Université de Tlemcen, BP119, Tlemcen 13000,Algerie.*

[2] *Ecole superieure des sciences appliqués de Tlemcen (ESSAT), BP 165, Bel Horizon,Tlemcen 13000, Algerie.*

[3] *Laboratoire de toxicomed, Unoversité de Tlemcen, BP 119, Tlemcen 13000, Algerie.*

**E-mail** :ferialchelali@gmail.com

**Résumé**

Depuis sa découverte, la réaction de Vilsmeier-Haack a trouvé de nombreuses applications en synthèse organique, devenant un outil polyvalent pour la formation de divers composés hétérocycliques d'intérêt à la fois medical,industriel et pharmacetique. De plus, le réactif de Vilsmeier-Haack est largement utilisé pour la chloroformylation de la β-chloroacroléine et la cyclisation aromatique de la β-formylchromone, permettant la formation de structures hétéroaromatiques complexes par réaction de condensation ou d'un couplage. Ces composés, en raison de la présence de la fonction aldéhyde, agissent comme des intermédiaires clé dans la préparation de nouvelles molécules bioactives. L'intérêt croissant pour cette réaction découle de sa capacité à générer des échafaudages hétérocycliques variés et fonctionnalisés, jouant un rôle crucial dans la conception de médicaments et de matériaux spécialisés. Notre laboratoire s'intéresse à l'offre une voie facile, directe et prometteuse vers une large gamme de systèmes aromatiques biologiquement actifs tels que les dérivés de thiophènes et de chromones. Au cours de nos recherches, nous avons synthétisé avec succès différents dérivés de β-aryl-β-chloroacroléine et de β-formylchromone à partir de dérivés d'acétophénones, avec des rendements satisfaisants. Ces composés ont ensuite été utilisés comme précurseurs pour la création de nouveaux hétérocycles soufré et oxygéné a partir des reaction simple et en deux étapes, offrant ainsi une opportunité pour la découverte de nouveaux agents thérapeutiques potentiels.

Dans cette communication, nous présentons les résultats de nos recherches récentes, qui mettent en avant les dernières applications du réactif de Vilsmeier-Haack dans la synthèse de composés hétérocycliques aux propriétés biologiques varies comme des activité antioxydant, antibacterial anticorrosive et antinflamatoire.

**Mots-clés**: réactif de Vilsmeier-Haack, β-aryl-β-chloroacroléine, β-formylchromone, chloroformylation, hétérocyles complexes, aldéhyde

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**Poster communication** **P-018**

# Study of the effect of biosynthesis zinc nanoparticles for experimental anemia in rats

Ouijdane Malak Chihani [1], Aya Omane [1], Samir Derouiche [1,2]

[1] *Department of Cellular and Molecular Biology, Faculty of Natural and Life Sciences, El Oued University, El Oued 39000, Algeria;*

[2] *Laboratory of Biodiversity and application of biotechnology in the agricultural field, Faculty of natural and life sciences, El Oued University, El-Oued 39000, Algeria.*

**E-mail** :melekchihani@gmail.com

**Abstract**

This study aims to examine the preparation of zinc nanoparticles (ZnNPs) and evaluates their efficacy against experimental anemia in rats. An in vitro study characterized zinc oxide nanoparticles using standard analytical methods and protocols. For the in vivo study, fifteen male albino Wistar rats were randomly assigned to three groups (n = 5): healthy rats (Control group), exp anemic rats (exp group) and exp anemia rats treated with zinc nanoparticles (ZnNPs) group. Experimental Anemia was induced using phenylhydrazine. Treatments were given to the rats for three weeks (20 days). Various parameters, including hematological, biochemical, oxidative stress markers, and histopathological studies of spleen and kidney tissues, were assessed. The characterization results of ZnNPs confirmed the robust of proteins with oval and multifaceted shapes, sizes (220 nm), and immobilization yields of 80.68% for ZnNPs. Furthermore, the in-vivo study results showed significant improvements in hematological and biochemical parameters in treated group compared to the exp group. There was also a notable reduction in oxidative stress markers, indicating the therapeutic effects of ZnNPs. Histopathological examinations revealed a complete recovery in the kidney and spleen tissues of rats treated with ZnNPs. In conclusion, this study confirms that the zinc oxide nanocomposites is highly effective in treating anemia.

**Keywords**: ZnNPs, camel milk, casein, anemia, phenylhydrazine, rats.

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**Poster communication** **P-021**

# Study synergetic effects on anti-inflammatory and analgesic activity of essential oils of Artemisia campestris, Citrus limon and Citrus aurantium

Aïcha Draoui*, Mohamed Ouinten, Nadhir Gourine, Chafia Tigrine, Mohamed Yousfi

*Laboratories des Sciences Fundamentals (LSF), University of Amar Telidji, Laghouat, BP. 37G, (03000), Laghouat, Algeria*

**E-mail**: draoui.aichaa@gmail.com

**Abstract**

The aim of the present work was the determination of the chemical composition and The investigation possible presence of synergetic effects by mixtures of OEs [C.a/ A.c] ("v/v"): in order to reduce the effective applied dose and reach synergistic combinations that enhance the therapeutic efficacy to be used instead of chemical anti-inflammatory drugs that have gastro-intestinal side effects.
The chemical composition of major constituents of Artemisia campestris : (β- pinene : 27.40%) ,(Limonene : 14.33%),(γ-Terpinene : 8.33%) ,(α-pinene: 8.30%), (β-myrcene 5.94%), and (α-Curcumene : 5.22%). Only one major compound "limonene" was identified for Lemon and Naranj, with respective concentrations of 91.69% and 43.86% respectively.

First of all, the results of the test on acute inflammation activity, by reducing the thickness of 1% of edema, and for treatments with doses of 200 mg/kg, showed that the inhibitory effects (after 4h) were equal to: 49,59 %; 34.19 % and 24.58%, for Dgouft, Lemon and Naranj oils, respectively. Alternatively, and regarding to their mixtures (Dgouft/Naranj: 20/80 "v/v"), (Lemon / Naranj: 50/50) and (Dgouft/Lemon/Naranj: 20/40/40), the inhibition values were equal to: 49.59% ; 23.14% and 46.90%, respectively. That combinations of multiple (AC) with the essential oils of peel citrus promote synergistic anti-inflammatory effect.

Secondly, the effect of essential oils on the Analgesic activity (by reducing the number of convulsions caused by the stimulation of visceral chemical receptors with acetic acid 1%), gave inhibition levels at (200 mg/kg): 23.43%; 17.83%; 30.55%; 20.98% and 37.83%, for the Dgouft, Lemon, Naranj, the mixture of (Dgouft/Naranj) and (Dgouft/Lemon/Naranj), respectively.
(in vivo), quantitative determination of synergy between EO (C.a/ A.c) . (Analgesic activity 3h) (CI < 1) (CI = 0.34, 0.21 and 0.28 for 100, 200 and 400 mg / kg, respectively). For $ED_{50}$ of EO (C.a/ A.c). The dose reduction index showed that the (C.a) dose can be reduced 4.94 -folds, and (A.c) dose can be reduced 7.15-folds in the combination when compared with the EDs50 of each essential oil, The favorable DRI (>1) allows dose reduction that leads to toxicity reduction.

Our results point to a possible synergism between the active compounds at the Essential oil mixtures, probably acting in different pharmacological receptors.

**Keywords**: Artemisia campestris, Citrus limon , Citrus aurantium , Synergic effect , Anti-inflammatory , Analgesic activity

**Poster communication** **P-022**

# A comprehensive study on the enhanced corrosion inhibition of copper in HCl solution using 3,4-dimethoxy phenylthiosemicarbazone (DMPTS): Experimental, characterization, and theoretical insights.

Imane GHOUAFRIA [1] Hana FERKOUS [2], Mohamed Rabah MAKHLOUF[1], Delimi Amel[2], Aïda Rebaïa Nadji[1]

[1]*Laboratory of Industrial Analysis and Materials Engineering, Department of Process Engineering ,Faculty of Science and Technology, University 8 May 1945, Guelma, Algeria*
[2]*Laboratoire de Génie mécanique et Matériaux, Faculté de Technologie, Université de Skikda, 21000, Algeria*

**E-mail:** imaneghouafria24@gmail.com

**Abstract**

This study investigates the effectiveness of 34-dimethoxy phenyl thiosemicarbazone (DMPTS) as a corrosion inhibitor for copper in a 1M HCl environment. A combination of experimental methods, including gravimetric analysis, electrochemical impedance spectroscopy, and surface characterization techniques (SEM, AFM, and EDX), was employed to analyze the inhibitory performance of DMPTS. Theoretical studies, such as Density Functional Theory (DFT), were also used to explore the molecular structure and inhibition mechanism of DMPTS. Results show that DMPTS effectively reduces the corrosion rate of copper, with inhibition efficiency increasing with DMPTS concentration. At 400 ppm, the inhibitor exhibited an efficiency of 89%. The study highlights the chemisorption process, supported by theoretical simulations, and suggests DMPTS as a promising, eco-friendly alternative for corrosion prevention in acidic environments.

**Keywords**: Schiff Base, Copper, Corrosion, DMPTS, electrochemistry, AFM, SEM, DFT Calculations.

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**Poster communication** **P-023**

# Hémisynthèse de 1,4-dihydropyridines via la réaction de Hantzsch dans des conditions vertes

GRIB Ismahene[1]*, BAHADI Mohamed Réda[1], AMOUCHI Houssem[1], BAHADI Rania[1, 2], BERREDJEM Malika[1]

[1]*Laboratoire de Chimie Organique Appliquée, Groupe Synthèse de Biomolécules et Modélisation Moléculaire, Département de Chimie, Faculté des Sciences, Université Badji-Mokhtar-Annaba, Boîte 12, 23000 Annaba, Algérie.*

[2]*Département Génie des Procédés, Faculté de Technologie, Université Chahid Mostfa Benboulaid - Batna 2-, 05000, Batna, Algérie.*

**E-mail:** ismahanegrib@yahoo.fr

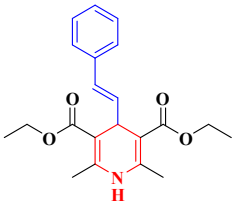
**Abstract**

Les composés hétérocycliques azotés jouent un rôle important en chimie médicinale. Vue leur rôle dans le processus biochimique, ils ont été largement utilisés comme unité constructive dans le développement des médicaments. Les 1,4-dihydropyridines (1,4-DHPs) et leurs dérivés forment une classe importante de molécules actives dans le domaine pharmaceutique. L'hétérocycle DHP est un motif commun dans plusieurs composés préconisés comme l'hypertension, anti-tuberculose, Anticancéreux, antibacterial, Antiepileptique, …etc. Les DHPs commerciales tel l'amlodipine, l'isradipine, la nifedipine… sont utilisées dans le traitement des maladies cardiovasculaires y compris l'hypertension.

D'autre part Le cinnamaldéhyde possède des propriétés antimicrobiennes, anti-inflammatoires, et pourrait même jouer un rôle dans la gestion du diabète de type 2.

L'objectif de notre travail est la modification structurale du composé naturel qui permis l'obtention du produit de l'hemisynthèse « Diethyl (E)-2,6-dimethyl-4-styryl-1,4-dihydropyridine-3,5-dicarboxylate » 92%.

La synthèse des dérivés de 1,4-dihydropyridine a été réalisée par la condensation de trois composants via la réaction de Hantzsch en utilisant l'acétoacétate d'éthyle, la cinnamaldéhyde et l'ammoniaque. La réaction a été effectuée sous irradiations ultrasoniques comme source d'activation verte et en absence des solvants organiques et des réactifs toxiques. Les molécules synthétisées sont obtenues avec de bons rendements.




**Mots-clés** : Hémisynthèse, 1,4-dihydropyridine, la réaction de Hantzsch, irradiations ultrasoniques

**Poster communication** **P-024**

# α-amylase inhibitory and antioxidant activity of the phenolic compounds of Pistacia atlantica oil

Amel GUERGAB[1]. Chahrazed HAMIA[1] . Mohamed YOUSFI[1]

[1]*Laboratoire des Sciences Fondamentales (LSF). Université Amar Télidji. Laghouat. BP 37G. 03000 Laghouat. Algeria*

**E-mail** : amelguergab@gmail.com

**Abstract**

One of the objectives of food industry is to seek new resources that preferably presents nutritional values. For human health. The search for effective. Natural compounds with antioxidant activity and α-Amylase inhibitory effects has been intensified in recent years to replace the synthetic products.

The aims of this study are to evaluate α-Amylase inhibitory effects and the antioxidant activity using in vitro assays by an organic extract of Pistacia atlantica fruit from southern Algeria.

The Phenolic compounds were obtained with from the Pistacia atlantica fruit oil. respectively. Then. we studied their inhibitory effects on α-amylase enzymes. The antioxidant potential was determined in vitro with DPPH tests.

The total phenolic contents in phenolic Compounds of total lipid between 16. 14 and 39. 38 mg GAE/100 g. The total flavonoid contents determined by the AlCl3reagent ranged from 3.14 to 20.41 mg QE/100 g. The condensed tannin contents showed little variations between Pistacia atlantica cultivars.

The antioxidant activity measured by the DPPH radical scavenging assay of different standards used in this study showed an important activity. with IC50 values ranging from 0.26 to 0.53 mg/ml while.

Almost sample inhibited the a-amylase. and the inhibitory activities IC50 ranged from 3.98 ± 0.21 to 11.24 ± 0.32.

This study is the first report on potential inhibition of phenolic compounds of these fruits oil extracts on the digestive enzyme. α-amylase.

**Keywords**: Enzyme inhibition. Pistacia atlantica. phenolic compounds. DPPH. α amylase

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**Poster communication** **P-025**

# Evaluation des propriétés physicochimiques des dérivés de xanthane obtenues par fonctionnalisation chimique

Naima Hachache[1*], Yamina Zouambia[1], Maachou Hamida[2], Randa Arous[3], Saloua Slama[3]

[1]*Faculté de Technologie, Laboratoire Matériaux et Environnement (LME) Université Yahia Fares de Médéa, Algérie*
[2]*Faculté des sciences, Laboratoire Matériaux et Environnement (LME), Université Yahia Fares de Médéa, Algérie*
[3]*Faculté des sciences Université Yahia Fares de Médéa, Algérie*

**E-mail:** hachache.naima@univ-medea.dz

**Résumé**

Ce travail est consacré à la modification chimique de la gomme xanthane par amidation en utilisant deux amines qui sont le triéthylamine et l'octylamine. L'amidation a été réalisée sous l'influence de différents paramètres : rapport massique xanthane /amine (1/2, 1/5 et 1/10) et le temps de contact (24h, 48h et 72h). Les dérivés de xanthane ainsi obtenus ont été soumis aux différents tests physicochimiques (FTIR, test de solubilité, pouvoir émulsifiant……). Les résultats obtenus ont montré que tous les dérivés de xanthane obtenus sont solubles dans l'eau. Les mesures de la tension de surface ont montré que les dérivés de xanthane amidés sont dotés de propriétés tensioactives avec une valeur minimale de la tension de surface de l'ordre 49.9 dyn/cm. De plus, l'utilisation des dérivés de xanthane amidés dans la formulation des émulsions de type huile dans eau a permis d'améliorer l'activité émulsifiante de 66.66% pour le xanthane natif à 96.72% pour le xanthane amidé.

**Mots-clés**: Xanthane, amidation, tension de surface, propriétés émulsifiantes

**Poster communication** **P-026**

# Green synthesis of silver nanoparticles using methanolic extract of Foeniculum vulgare and evaluating the antibacterial properties

HADJI Maroua[1], BENDIF Hamdi[1], DJEDIOUI Abdallah[2], HADJI Toka[3], SMAILI Tahar[1]

[1] Department of Natural and Life Sciences, Faculty of Sciences, University of M'sila, Algeria.
[2] Department of Biochemistry, Faculty of Sciences, Badji Mokhtar University, Annaba, Algeria.
[3] Department of Biology and Plant Ecology, University of Mentouri Brothers Constantine, Algeria.

**E-mail**: mar.hajjii88@gmail.com

**Abstract**

Green chemistry is increasingly focused on developing eco-friendly approaches to synthesize bioactive compounds for medicinal purposes. In this context, silver nanoparticles (AgNPs) have emerged as a promising area of study due to their wide-ranging antibacterial properties. This research presents a green synthesis of AgNPs using Foeniculum vulgare methanolic extract, highlighting its potential as antibacterial agent. The process involves extracting phenolic compounds using maceration method, followed by the biological synthesis of silver nanoparticles by mixing 10 mL of the methanolic extract with 90 mL of a 1 mM $AgNO_3$ solution. The pH of the mixture was adjusted to 8, and the reaction was allowed to proceed at room temperature in the absence of light. The formation of nanoparticles was visually confirmed by a color shift from yellowish-green to dark brown. The resulting AgNPs were separated through centrifugation at 10,000 rpm for 10 minutes, thoroughly washed with deionized water, and then dried at 50°C. Furthermore, the characterization of AgNPs was done by measuring the absorbance in the wavelength range of 200–800 nm using a UV-VIS spectrophotometer. Moreover, the antibacterial efficacy of the biosynthesized AgNPs was tested against common pathogenic bacteria, including Escherichia coli, Staphylococcus aureus, Pseudomonas aeruginosa, and Bacillus subtilis, using the agar diffusion method. The study also determined the minimum inhibitory concentration (MIC) and minimum bactericidal concentration (MBC) through liquid culture assays. The AgNPs exhibited significant antibacterial activity, with inhibition zones ranging from 12 to 18 mm, and MIC values between 40 and 12.5 µg/mL. Additionally, a synergistic effect was observed when AgNPs were combined with conventional antibiotics, enhancing their antibacterial potency. These results demonstrate the potential of methanolic extract-mediated AgNPs as an effective, eco-friendly antibacterial agent.

**Keywords**: Silver, Nanoparticles, Foeniculum vulgare, Antibacterial activity.

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**Poster communication** **P-027**

# Preparation des pyranotacrines (quinolein-3-yl)-tacrine) à activite biologique potentielle

Haiour Hasna [a], Bouraiou Abdelmalek [b], Belfaitah Ali [a]

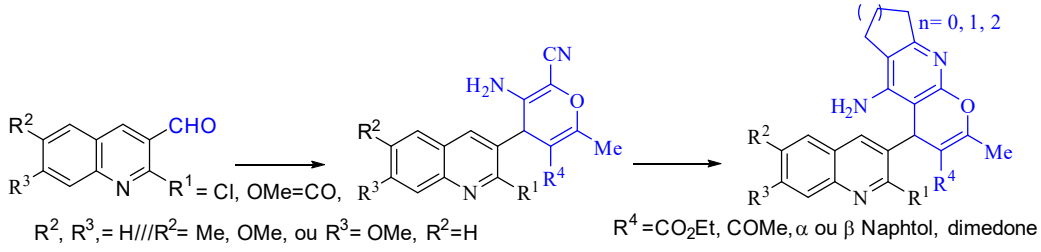
[a] *Equipe de recherche «Synthèse de Molécules à Objectif Thérapeutique ». Laboratoire des Produits naturels d'Origine végétale et de la Synthèse Organique.*

[b] *Unité de recherche de chimie et de l'environnement, et moléculaire structurale, Université Frère Mentouri Constantine 1. Route Ain El bey. Constantine 25000. Algérie*

**E-mail** : hasna.haiour@umc.edu.dz // freehasna2011@gmail.com

**Résumé**

La Tacrine, est la première molécule à avoir été proposée pour ses propriétés cholinergiques dans les essais thérapeutiques de la maladie d'Alzheimer (MA), a permis d'envisager un traitement symptomatique des démences de type Alzheimer. Elle agit principalement en inhibant l'activité enzymatique de l'acétylcholinestérase et en freinant la dégradation de l'acétylcholine dans l'espace synaptique du système cholinergique. L'effet indésirable majeur de la tacrine est son hépatotoxicité qui se traduit par l'élévation réversible des transaminases hépatiques sanguines, en particulier, l'alanine aminotransférase (ALAT). Le travail réalisé dans notre laboratoire repose sur la préparation, de quelques dérivés hétérocycliques originaux hautement et diversement fonctionnalisés analogues structuraux de la Tacrine, à partir des dérivés hybrides (quinoléin-3-yl)-4H-pyrane. Les pyranotacrines (quinoléin-3-yl)-tacrine) ont été préparés dans les conditions standards de la réaction de Friedländer. L'évaluation biologique in vitro (tests anti-Alzheimer) de quelques pyranotacrines (PTs) tel que la mesure de l'hépatotoxicité, la détermination du pouvoir inhibiteur envers l'Acétylcholinestérase et la Butyrylcholinestérase, l'agrégation induite de □-amyloïdes Aβ, la neuroprotection et la neurotoxicité, ont montré que ces pyranotacrines (PTs) sont des agents multi-puissants, non-hépatotoxiques, inhibiteurs non compétitif de l'acétylcholinestérase et de l'agrégation induite de □-amyloïdes, neuro-protecteurs et non neurotoxiques pour le traitement de la maladie d'Alzheimer.




**Mots-clés**: Quinoléine, hétérocycle, Maladie d'Alzheimer, Tacrine, activité biologique.

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**Poster communication** **P-028**

# Évaluation du potentiel allélopathique de l'extrait aqueux d'une plante appartenant à la famille de Zingiberaceae Curcuma longa L

HARROUS Imene[1], AÏT HAMLET Smina[2], AMIAR Abir[1], BOUMENDJEL Amel[1], MESSARAH Mahfoud[1]

[1]*Laboratoire de Biochimie et de Toxicologie Environnementale, Faculté des Sciences, Université Badji-Mokhtar, Annaba, B.P.12, 23000, Algérie*

[2]*Laboratoire de Toxicologie Cellulaire, Faculté des Sciences, Université Badji-Mokhtar, Annaba, B.P.12, 23000, Algérie*

**E-mail** : rahmaimmunologie@gmail.com

**Abstract**

**Introduction:** l'allélopathie est un phénomène biologique, qui consiste en tout effet direct ou indirect, positif ou négatif, d'une plante sur une autre à travers la production de molécules chimiques libérées dans l'environnement. Les molécules mis en jeu dans ce phénomène sont principalement des métabolites secondaires (molécules aromatiques, terpènes, alcaloïdes ...), impliqués dans des interactions allélopathiques. Ces composés ont d'abord été caractérisés par leur rôle protecteur contre les bioagresseurs (insectes, bactéries, champignons ...), mais ils peuvent également affecter la croissance d'autres plantes.
**Objectifs:** l'évaluation de l'activité allélopathique potentielle de Curcuma longa L. sur les carottes.
**Méthodologie :** après avoir obtenu des feuilles bien dressées, les carottes ont été inondées par les extraits aqueux de C. longa (décoctés, infusés et macérés) à une concentration de 50 mg/ml. Leur aspect a été suivi pendant environ 5 semaines maximum pour voir les modifications apparentes sur les feuilles et les tiges. L'incubation est faite à température ambiante. L'exploration de l'activité allélopathique des différents extraits aqueux sur la croissance des feuillages est réalisée par un test de mise en évidence de l'existence d'effets inhibiteurs ou stimulants.
**Résultats:** l'examen allélopathie a montré que le décocté de C. longa a présenté un effet allélopathique immédiat. Les plantes meurent après trois jours, et même après régénération avec l'eau ordinaire, cela prouve que les molécules hydrophiles de cet extrait aqueux jouent un rôle similaire à celui d'un bio-herbicide.
**Conclusion:** les mélanges des extraits aqueux étudiés peuvent être utilisés comme herbicides, à condition de vérifier profondément leur efficacité et leur toxicité sur d'autres plantes cibles, et d'élucider la nature chimique des molécules responsables de cette allélopathie.

**Keywords**: Zingiberaceae, Curcuma longa L, extrait aqueux, activité allélopathique, carottes.

**Poster communication** **P-030**

# Synthesis, DFT calculations and molecular docking as antimicrobial activity of 3-(benzothiazol-2-yl)-2-(4-nitrophenyl)-3,4-dihydro-2h-benzo[1,3] oxazine as novel compound.

Sihem HESSAINIA[a], Samia GUEZANE-LAKOUD[a] and Zinelaabidine CHERAIET[b]

[a] *Ecocompatible Asymmetric Catalysis Laboratory (LCAE) Badji Mokhtar Annaba-University, B.P 12, 23000 Annaba, Algeria*

[b] *Organic Synthesis Laboratory Modeling and Optimization of Chemical Processes (LOMOP) Badji-Mokhtar Annaba University, Annaba BP12. Annaba, Algeria.*

**E-mail:** Shessainia@gmail.com

**Abstract**

Benzoxazines are a well-known class of natural compounds recognized for their wide range of biological activities, such as antimicrobial, antifungal, anti-inflammatory, antiparasitic, and plant pathogen-fighting properties [1-2]. Benzoxazines derivatives have been also studied as important heterocyclic system for building natural and designed reflecting synthetic compounds. Benzoxazine is a fused heterocycles compound and also serves as core part of various pharmaceutically active compounds [3]. Recently, a significant progress in the synthesis of 1,4-benzoxazine were developped [4]. In this context, we have synthesized the 3-(benzothiazol-2-yl)-2-(4-nitrophenyl)-3,4-dihydro-2h-benzo[1,3] oxazine as novel compound in three steps, the first one concerns the condensation of 2-amino-benzothiazole with salicylaldehyde in ethanol at reflux to form the 2-((benzothiazol-2-ylimino) methyl) phenol, followed by reduction using sodium borohydride ($NaBH_4$), giving the 2-((benzothiazol-2-ylamino) methyl) phenol as second step. The third step translates to the intermolecular cyclization of this last in the presence of nitrobenzaldehyde in acetonitrile at reflux for 4 hours, the desired product was obtained with 60°C chemical yield. This novel compound was characterized by spectroscopic analyses. Theoretical DFT calculations of this compound was carried out using B3LYP 6-31G (d,p) basis set to predict the molecular geometries and chemical reactivity descriptors. Molecular docking study are implemented to analyze the binding energy with protein to be considered as antimicrobial candidate.

**Keywords:** Benzoxazines, DFT, Molecular docking, antimicrobial activity.

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**Poster communication** **P-031**

# Extracts of peel of P.granatum grenade as green inhibitors for cupronickel in NaCl 3%

Ferial Krid[1*]; Mohamed boubessil[1,2,3]; Nasrine Ammouchi[1,4]; Youghourta Belhoucine[1]

**Laboratoire de recherche en génie chimique et environnement de Skikda LGCES , Faculté de Technologie, Université du 20 Août 1955-Skikda, Algérie.*

*[1] Department of Process Engineering, Faculty of Technology, 20 August 1955 University of Skikda, P.O. Box 26, El Hadaik Road, 21000, Skikda, Algeria.*

*[2] Laboratory of Physico-Chemical research of Surfaces and Interfaces, 20 August 1955 University of Skikda, Algeria.*

*[3] Laboratory of Catalysis, Bio-Process and Environment, Department of Process Engineering, University of 20 August 1955, Skikda, Algeria*

*[4] Department of Technology, Faculty of Technology, 20 August 1955 University of Skikda, Algeria.*

**E-mail**: f.krid@univ-skikda.dz

**Abstract**

The inhibition performance of extract of P.granatum in controlling corrosion of Cu–Ni (90/10) alloy in synthetic seawater and synthetic seawater containing different concentrations of $NaCl_3$% has been investigated. Electrochemical impedance, potentiodynamic polarization, were employed to evaluate the inhibitor performance. The results of impedance studies show that both charge transfer resistance and film resistance increase with an increase in extract concentration and at a concentration of 1g/l, extract P.granatum functions as an excellent inhibitor with an inhibition efficiency of 99.72%. The phase angle Bode plots are more broadened and showed a phase maximum of 81 in the presence of APT. The APT film is highl y protective evenat a temperature of 60°C. Potentiodynamic polarization studies inferred that extract P.granatum functions as a cathodic inhibitor.

**Keywords**: P.granatum ; inhibiteur ; extrait de plante ; cupronickel ; corrosion.

**Poster communication** **P-032**

# Synthesis of epoxyquinolines derivatives

Rahima Khelaf [a], Noura Benbellat [a], Fatiha Guenfoud [b], Mohammed Laabassi [c], Paul Mosset [d]

[a] *Département de Chimie, Faculté des Sciences de la Matière, Université Batna 1, 5000, Batna, Algérie.*
*Laboratoire de Chimie des Matériaux et des Vivants : Activité-Réactivité (LCMVAR).*
[b] *Département de Pharmacie, Faculté de Sciences médical, Université Batna 2, 5000, Batna, Algérie.*
*Laboratoire de Chimie des Matériaux et des Vivants : Activité-Réactivité (LCMVAR).*
[c] *Département des Sciences et Technologies, Faculté de technologie, Université Batna 2, 5000, Batna, Algérie.*
[d] *CNRS, ISCR (Institut des Sciences Chimiques de Rennes), Université de Rennes, UMR 6226, F-35000 Rennes, France*

**E-mail** : rahima.khelaf@univ-batna.dz

**Abstract**

Quinoline derivatives, renowned for their diverse biological activities, have been a focal point in medicinal chemistry research. This study presents a novel synthetic approach for the preparation of multifunctionalized epoxyquinoline derivatives. Our strategy involves a series of carefully orchestrated reactions, including protection, substitution, deprotection, epoxidation, and oxidation steps. These transformations enable the introduction of various functional groups onto the quinoline scaffold, enhancing its structural diversity and potential biological properties.

The synthesized compounds were characterized using state-of-the-art analytical techniques, including NMR spectroscopy, mass spectrometry, and elemental analysis. Structural elucidation confirmed the successful incorporation of the desired functional groups and the formation of the target epoxyquinoline derivatives.

These multifunctionalized epoxyquinolines represent promising candidates for further exploration in drug discovery. Their unique structural features and potential biological activities make them attractive targets for the development of novel therapeutic agents. Future studies will focus on evaluating the biological properties of these compounds in various disease models.

**Keywords**: quinoline, synthesis, epoxyquinoline, multifunctionalized, drug discovery.

**Poster communication** **P-033**

# Degradation of an organic dye in aqueous phase by green synthesis of nanoparticles using an Algerian medicinal plant

Malika Khelfaoui [1, 2] Daoiya Zouied [1, 2]

[1] *Laboratoire LGCES, Faculté de Technologie, Université du 20 Août 1955, Skikda, Algérie*
[2] *Département de Génie des Procédés, Université du 20 Août 1955, Skikda Algérie*

**E-mail** : m.khelfaoui@univ-skikda.dz // khel.mal80@yahoo.fr.

**Abstract**

Water is the most important raw material on our planet for humans, animals, plants, and microorganisms. Water pollution is one of the major challenges facing humanity today, and dyes from the textile industry are a major contributor to this pollution that causes degradation and loss of wildlife and flora. Methylene blue is the dye most commonly used in the dyeing of cotton, wood and silk. It can cause eye burns responsible for permanent injury to the eyes of humans and animals. Its inhalation can give rise to breathing difficulties and its ingestion by the mouth produces a burning sensation, causes nausea, vomiting, perspiration and profuse cold sweats. Bleaching rejects from the textile industry is often difficult because organic dyes are not degraded by conventional treatments, such as biological treatments. Several treatments have been proposed including precipitation/coagulation, oxidation, reverse osmosis, membrane processes. These treatments have proven to be effective, but in most cases very expensive. In order to contribute to the fight against this danger, our study is focused on the degradation of an organic dye in the aqueous phase, by a green process using an Algerian medicinal plant and metal oxides, under the influence of certain parameters such as; the pH, the initial concentration and the mass. The results show a better degradation of the dye at acidic pH with a yield of 90%.

**Keywords:** dye, degradation, plant, pollution, water.

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**Poster communication** **P-038**

# LC-MS analysis and antioxidant activity of plant.

MANSAR Lina Nourhane[1], AMEDDAH Souad[1], MENAD Ahmed[1], HABA Hamada[2], BELAID Meriem[2]

[1]*Laboratory of Biology and Environment University of Mentouri Bothers Constantine1*
[2]*Laboratory of Chemistry and Environmental Chemistry LCCE, Batna 1 University.*

**E-mail:** mansarlina2@gmail.com
linanourhene.mansar@doc.umc.edu.dz

**Abstract**

Acute pancreatitis (AP) is a common inflammatory disease characterized by damage and inflammation of the pancreas. It is a serious condition of the digestive system that remains a clinical challenge in the last decade. This study investigated the potential protective role of Anabasis sp (AEAO), an algerian medicinal plant, against l-arginine-induced AP in mice. The severity of AP was evaluated by measuring biochemical and oxidative stress markers in blood samples and pancreatic tissue. Our results showed that Anabasis sp suppressed the development of l-arginine-induced AP by significantly reducing serum amylase and lipase levels. It also reduced levels of MDA (a marker of oxidative stress) and increased levels of the antioxidant glutathione (GSH) and superoxide dismutase enzyme (SOD). Additionally, to enrich the knowledge of the variation of the chemical composition of AEAO, LC-MS/MS analyses were carried out. These findings suggest that AEAO may have an antioxidant effect in mice with acute pancreatitis and could potentially be used as a novel treatment for AP. This protective effect may be due to its bioactive constituent.

**Keywords**: Anabasis sp; acute pancreatitis; GSH related enzyme; Oxidative stress, LC-MS/MS.

**Poster communication** **P-042**

# Investigation of essential oil extraction, GC/MS evaluation, and assessment of antioxidant properties in two medicinal plant species indigenous to southern Algeria

Mohammed larbi BEN AMOR[1,3,*], Elhafnaoui LANEZ[2,3,*] , Touhami LANEZ[3]

[1]*University of El Oued, Faculty of Technology, Department of Process Engineering and Petrochemical, P.O. Box 789, El Oued 39000, Algeria*

[2]*University of El Oued, Faculty of Biology, Department of Cellular and Molecular Biology, 39000, El Oued, Algeria*

[3]*University of El Oued, Faculty of exact Sciences, Department of Chemistry, VTRS Laboratory, B.P.789, 39000, El Oued, Algeria*

**E-mail:** benamor-mohmmedlarbi@univ-eloued.dz

**Abstract**

The utilization of medicinal plants for therapeutic purposes has been deeply rooted in traditional medicine practices. In this study, we focus on the extraction, Gas Chromatography-Mass Spectrometry (GC/MS) analysis, and evaluation of Antioxidant activity of essential oils derived from two indigenous medicinal plants native to the southern region of Algeria. The extraction process employs hydro-distillation technique to ensure optimal yield and preservation of bioactive compounds. Subsequently, GC/MS analysis is conducted to identify and quantify the chemical constituents present in the essential oils, providing insights into their phytochemical composition.

Furthermore, the Antioxidant potential of these essential oils is investigated through in vitro assays utilizing UV-Vis spectroscopy. The assay methodology is designed to assess the ability of the essential oils to modulate key parameters associated with free radicals. Complementing these experimental analyses, computational studies are performed using induced fit docking and Molecular Dynamics Simulation (MDS) techniques, spanning a simulation period of 100 nanoseconds. Through in silico simulations, we aim to elucidate the molecular interactions between bioactive components of the essential oils and target proteins implicated in stress oxidative.

The integration of experimental and computational approaches provides a comprehensive understanding of the therapeutic potential of these medicinal plants in managing stress oxidative. This multidisciplinary investigation contributes to the advancement of natural product-based drug discovery and underscores the significance of traditional knowledge in modern scientific research.

**Keywords**: Medicinal Plants, Essential Oil Extraction, GC/MS Analysis, Antioxidant Activity.

**Poster communication** **P-043**

# Phytochemical screening of flax seeds

BOUASLA Nabila[1,2*], GUENADIL Fawzi [1], YOUBI Asma[2], ABDERRAHMANE Sihem[2], ZITOUNI Achouak[1]

[1]*Université Chadli Bendjedid-El Tarf, B.P 73, El Taref 36000, Algeria*
[2]*Surface Engineering Laboratory (L.I.S), Faculty of Sciences, Badji Mokhtar -Annaba University, P.o.Box 12, Annaba 23000, Algeria*

**E-mail :** n.bouasla@univ-eltarf.dz

**Abstract**

For thousands of years, mankind has used flax seed, which offers a range of interesting nutrients. Their composition varies according to variety and environmental conditions. In general, flax seed is rich in oil (30-45%), protein (10-30%) and dietary fibre (25-32%). The seed coats contain mainly polyphenols and carbohydrate compounds. Flax is recognised as a functional food or source of functional ingredients due to its content of alpha-linolenic acid, lignans and non-starch polysaccharides, all of which have beneficial effects on disease prevention. Despite the scientific evidence encouraging the consumption of flaxs eed, many people remain uninformed about the benefits of this product and its potential uses in food production. This study focused on the phytochemical analysis of flax seed, highlighting the presence of various compounds such as alkaloids, anthocyanins, volatile oils, tannins, phenols and sterols.

**Keywords:** flax seed, phytochemical analysis, lignans, food production

**Poster communication** **P-046**

# Bioactivity and antioxidant properties of n-Butanol extract from indigenous Algerian ficus

Aida KEMMOUNDJI[1], Mouna SAOUDI[2], Thamere CHEREIT[1, 3], Ramdane SEGHIRI[1]

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

[2] *Laboratory of molecular and cellular biology, University of brothers Mentouri, Route Ain el Bey,Constantine 25017, Algeria*

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

**E-mail:** aydakemmoundji@gmail.com

**Abstract**

Exploring natural products for their potential health benefits has increased interest in the phytochemical properties of various species extracts. This study investigates the antibacterial and antioxidant activities of the n-butanol extract from an endemic Algerian ficus, prepared from the dried ficus plant and subjected to various in vitro assays to evaluate its biological activities. The antibacterial activity they assessed using the well-diffusion method in DMSO, against a panel of gram-positive and three gram-negative bacteria, including *Staphylococcus aureus*, *Escherichia coli*, *Morganelle morganii*, and *Pseudomonas aeruginosa*. The extract demonstrated significant antibacterial activity, particularly against Pseudomonas aeruginosa and Escherichia coli. Antioxidant activity was evaluated using a DPPH (2,2-diphenyl-1-picrylhydrazyl) radical scavenging assay. The n-butanol extract exhibited strong DPPH radical scavenging activity with 84.13% at 0.5 mg/ml with an IC50 value of 0.218 mg/ml, indicating its potential as a natural antioxidant. The results suggest that the n-butanol extract from ficus species possesses potent antibacterial and antioxidant properties, making it a promising candidate for further development in pharmaceutical and nutraceutical applications.

**Keywords**: ficus, Moraceae, antioxidant activity, DPPH assay, bioactivity.

**Poster communication** **P-048**

# Etude des activités biologiques de l'huile essentielle et l'extrait d'une plante aromatique et médicinale « Thymus algériensis »

DJEDIOUI Abdallah, BOUASLA Ihcene, BOUBIDI Fatima, KOUCH Mina, DERBALI Karim, HAMROUNE Aicha.

*Département de Biochimie - Faculté des Sciences- Université Badji Mokhtar-Annaba-Algérie.*

**E-mail:** djediouiabdallah@yahoo.fr

**Résumé**

Ce travail a pour but la valorisation de la végétation algérienne et ses ressources naturelles. Par l'étude morphologique d'une plante médicinale et aromatique provenant de la wilaya de Guelma et appartenant à la famille des Lamiacées « Le thymus Algériensis ».

Après extraction de l'huile essentielle par hydrodistillation et récupération d'extrait aqueux de la plante on a procédé à une étude phytochimique pour mettre en évidence la présence des Tannins, Leuco-anthocyanes, Saponines et les flavonoides. Suivi par un dosage de la teneur en polyphénols, montre que la quantité des polyphénols est maximale égale à 0.96 mg /ml d'acide gallique.

Le rendement d'HE est d'une valeur de 2.40%. Cette HE a été soumis à plusieurs tests in vitro a fin d'évaluer sa capacité antioxydante par le test DPPH avec un pourcentage d'inhibition = 1.59 %. Nos résultats montrent que l'HE présente un rendement plus ou moins élevé mais une activité antioxydante relativement faible.

Finalement, le T. Algériensis représente une source naturelle très diversifié riche en molécules bioactifs qui peuvent être très intéressant et bénéfiques pour les futures études en pharmacologie, biotechnologie, cosmétologie.

**Mots-clés :** Thymus algériensis, huile essentielle, composé bioactives, polyphénols, activité antioxydante

**Poster communication** **P-049**

# Determination of total phenolic, flavonoid content, and antioxidant activity of *Leucaena leucocephala* extract

KORTI Amira [1*], Djilani Ghemam Amara[2], Chemsa Ahmed El khalifa[2]

[1]*Faculty of Natural and Life Sciences - Laboratory of Biology, Environment, and Health - University of ECHAHID HAMMA LAKHDAR EL-OUED"*

[2] *Faculty of Natural and Life Sciences - Laboratory of Biology, Environment, and Health - University of ECHAHID HAMMA LAKHDAR EL-OUED"*

**E-mail**: amira-korti@univ-eloued.dz

**Abstract**

This study aimed to evaluate the antioxidant and antibacterial properties, along with the total flavonoid and phenolic content, of leaves and flowers of *L. leucocephala* using five different nonpolar and polar solvents, including hexane, chloroform, ethanol, and n-butanol. The free radical scavenging activity was assessed using the 2,2-Diphenyl-1-Picrylhydrazyl (DPPH) assay, while the reducing power was measured by the Ferric Reducing Ability of Plasma (FRAP) assay. Total flavonoid content was determined using the aluminum chloride method, and total phenolic content was measured by the Folin-Ciocalteu method. Antibacterial activity was evaluated through a disc diffusion assay. The n-butanol and ethanol flower extracts demonstrated superior antioxidant and antibacterial potential compared to the leaf extracts in the same solvents. Additionally, the leaf and flower extracts exhibited higher flavonoid and phenolic content. Therefore, it can be concluded that due to the presence of secondary metabolites such as phenols and flavonoids in both the leaf and flower extracts, they hold promise as natural sources of antioxidant and antibacterial agents.

**Keywords**: *Leucaena leucocephala*, Anti-bacterial, Anti-oxidant, Flavonoid, Phenolic, DPPH.

**Poster communication** **P-050**

# Phytochemical screening and evaluation of the antienzymatic activity of Hydro-methanolic extract of *corchorus olitorius L.* leaves.

Widad FATMI, HARICHE Abla, Bouderbala Ismahene

*Laboratory of Health and Environment, Faculty of Nature and Life Sciences and Earth and Universe Sciences, University El-Bachir El-Ibrahimi, Bordj Bou Arreridj, 34000, Algeria.*

**E-mail** : w.fatmi@univ-bba.dz

**Abstract**

In the context of valorizing medicinal plants from the Algerian and Mediterranean flora, this study aimed to conduct phytochemical analysis and assess the antioxidant and anti-enzymatic activities of the hydromethanolic extract of *Corchorus olitorius L.* leaves, known as Moulokhia in Algeria. A crude extract of the plant's leaves was obtained through maceration in 70% methanol. Phytochemical analysis unveiled the abundance of secondary metabolites in the species, notably polyphenols (193.84 mg GAE/g DE), flavonoids (14.26 ± 0.039 mg QE/g DE), and condensed tannins (94.074 ± 0.0091 mg CE/g DE). The antioxidant potential of the methanolic extract was gauged using three tests - total antioxidant capacity (TAC), DPPH radical scavenging, and ferric reducing power (FRAP), all demonstrating significant activity. Furthermore, the hydromethanolic extract of Corchorus olitorius leaves displayed notable anti-enzymatic activity by inhibiting alpha-amylase with an IC50 value of 4.62 ± 0.98 mg/ml. In essence, this research underscores the substantial biological activities of Corchorus olitorius, hinting at its promising potential for pharmacological applications.

**Keywords**: Corchorus olitorius L., polyphenols, flavonoids, antioxidant activity, anti-enzymatic activity.

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**Poster communication** **P-051**

# Antioxidant status of ethanolic extract of steppic *Malva sylvestris L.*

Salah-Eddine RAHMANI[1*], Nadjib REBIZI[1], Noureddine GHERRAF[2]

[1]*Department of Matter Sciences, Faculty of Exact Sciences, Ziane Achour University of Djelfa, Algeria.*

[2]*Laboratory of Natural Resources and Management of Sensitive Environments, University of Oum El Bouaghi, Algeria*

**E-mail:** rahmanidz@yahoo.fr

**Abstract**

The natural resources of antioxidants have garnered considerable attention in contemporary research aimed at the prevention and scavenging of free radicals. The primary objective of our investigation is to assess the antioxidant activity, total phenolic content, and total flavonoid content of the ethanolic extract derived from *Malva sylvestris L.* (commonly referred to as "Khubbayz") in the Djelfa district of the Algerian steppe. The quantification of total phenols and flavonoids was conducted utilizing the Folin-Ciocalteu reagent method and the aluminium chloride method, respectively. The evaluation of antioxidant activity was performed employing the 1,1-diphenyl-2-picrylhydrazyl (DPPH) assay. The total phenolic and flavonoid contents of the ethanolic extract from the aerial portions of Malva sylvestris L. were quantified as 36.18±0.46 mg GAE/g (DW) and 18.32 ±0 .14 mg QE/g (DW), respectively. The antioxidant efficacy of the ethanolic extract of Malva sylvestris L., as determined by the DPPH assay, exhibited a concentration-dependent response, yielding an IC50 value of 264.32µg/ml, with a maximum percentage of 56% observed at 400 µg/ml, which was lower than that of ascorbic acid, which reached 78% at 300 µg/ml. The findings indicate a significant antioxidant capacity for the ethanolic extract obtained from the local Malva sylvestris L.; however, this potential requires validation through other methods.

**Keywords**: *Malva sylvestris L.*; Ethanolic extract; Antioxidant; DPPH

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**Poster communication** **P-053**

# Study of principal metabolites in the aqueous extract of *Arbutus unedo* leaves

Djeghader Nour El-Houda[1,2*], Amira Khedidja [2,3] and Delhoum Hadia[4]

[1] *Department of Biology, Faculty of Life and Natural Sciences, University of Badji Mokhtar, Annaba-Algeria*

[2]*Laboratory of Physical, Chemistry and Biology of Materials, Skikda-Algeria*

[3] *Department of Natural Sciences, Higher Normal School of Technological Education of Skikda-Algeria.*

[4] *Department of Biology, Faculty of Life and Natural Sciences, University of Djilali Bounaama-Khemis Meliana*

**E-mail** : djeghader_nour@yahoo.fr

**Abstract**

Arbutus unedo, commonly known as the strawberry tree, is a plant that remains relatively unknown in terms of its nutritional and industrial value among the Algerian population, and its consumption is seasonal. Despite this lack of awareness, the strawberry tree has significant medicinal value; various studies have shown that its consumption is associated with a reduced risk of developing certain diseases such as hypertension and diabetes, due to its biological properties. The aim of this study was to evaluate the composition of secondary metabolites in the leaves of *Arbutus unedo*. The leaves were collected from the municipality of Treat, Annaba Province, dried, and then ground using a mechanical grinder to obtain a powdered form. The preparation of the aqueous extract of the strawberry tree was carried out by infusion. After filtration, the resulting extract was subjected to a phytochemical screening to detect the presence of various secondary metabolites. The results revealed that the screening tests were positive for all the tested metabolites, including tannins, alkaloids, flavonoids, saponins, and terpenes. These results suggest that *Arbutus unedo* leaves contain a diversity of potentially beneficial bioactive compounds.

**Keywords**: Arbutus unedo, secondary metabolites, aqueous extract, phytochemical screening.

**Poster communication** **P-054**

# Phytochemical study of the aqueous extract of *Pistacia lentiscus* leaves

Amira Khedidja[1,2*], Zaoui Khouloud[3], Maar Ramzi[3], Semouma Dounia[3], Djeghader Nour El-Houda[2,4]

[1]*Department of Natural Sciences, Higher Normal School of Technological Education of Skikda, Algeria.*

[2]*Laboratory of Physical, Chemistry and Biology of Materials, Skikda*

[3]*Department of Biology, Faculty of Life and Natural Sciences, 20 August 1955 University, Skikda, Algeria*

[4]*Department of Biology, Faculty of Life and Natural Sciences, Badji Mokhtar University, Annaba, Algeria*

**E-mail**: amira_khedidja@yahoo.com

**Abstract**

Mastic tree, scientifically known as Pistacia lentiscus, is one of the aromatic medicinal plants with significant therapeutic properties. It is widely spread in the regions of the Mediterranean basin and is utilized in various other aspects of life due to its distinctive properties. The objective of this study is to unveil some active chemical substances present in the aqueous extract of *Pistacia lentiscus* leaves collected from Treat- Annaba. The results obtained confirmed the presence of saponins, tannins, and flavonoids, and the absence of terpenes and alkaloids in the aqueous extract of this plant, confirmed by color changes and the appearance of foam after the addition of certain chemical reagents and distilled water. These substances have numerous medicinal benefits, including antioxidant, antibacterial, antiviral, and anti-inflammatory activities, among other characteristics.

**Keywords**: Pistacia lentiscus, aqueous extract, chemical reagents, active chemical substances, antioxidant activity.

**Poster communication** **P-055**

# Contribution à l'étude d'une plante médicinale algérienne à huile essentielle

BENABBAS Rihab[1], CHOHRA Djawhara[1], SAIDI Ouided[2], BENTOUMI Houria[1], AOUF Noureddine[1].

[1] *Laboratoire de chimie organique appliquée, équipe de chimie bio-organique, Département de Chimie, Faculté de sciences, Université de Badji-Mokhtar, Box 12, 23000, Annaba, Algérie*

[2] *Laboratoire de pharmacognosie, Département de pharmacie, Faculté de médecine, Université Badji-Mokhtar, Annaba, Algérie.*

**E-mail :** benabbas.rihab@outlook.com

**Résumé**

La Lavande stéchade ou *« **Lavandula stoechas L**.* » est une espèce appartenant à la famille des Lamiaceae. Ses effets spectaculaires justifient sa large utilisation en phytothérapie et en médecine classique. Elle est riche en huiles essentielles douées d'efficacité curative et préventive. L'objectif visé par cette étude, est de contribuer à la recherche d'un traitement d'appoint aux traitements chimiques et de minimiser les phénomènes de résistance aux antibiotiques. En effet, l'intérêt de la lavande réside dans son huile essentielle qui a été extraite à partir des feuilles et des sommités fleuries séchées de cette plante par le procédé d'Hydrodistillation, ce mode d'extraction a fourni un rendement modéré de 0.70% à 1.2%. L'analyse qualitative par chromatographie sur couche mince (CCM) d'huile essentielle de lavande nous a permis d'identifier certains de ses composants odoriférants majoritaires tels que le linalol et le 1,8-cineol. Ensuite, une évaluation de l'activité antimicrobienne de cette huile essentielle, a été testée sur dix souches bactériennes et une souche de levure, par la méthode de diffusion sur disques stériles, elle a permis de dévoiler la sensibilité de quelques souches avec un diamètre d'inhibition plus au moins important : Une sensibilité très remarquée des souches bactériennes : Escherichia coli ATCC 25922, E.coli BLSE, Serratia marcescens, Acinetobacter baumannii, Staphylococcus aureus ATCC00, et de la souche de levure : Candida albicans. Une sensibilité moyenne de : E.coli ciprofloxacine Resistante, Klebsiella pneumonia Carbapenemase +, Klebsiella pneumonia Carbapenemase -, Staphylococcus aureus Atcc 29213. Contrairement à Pseudomonas aeruginosa qui est très résistant à cette essence. Enfin, ce travail n'est qu'une tentative de participation à des travaux de recherches scientifiques dont l'objectif principal était la valorisation de la flore Algérienne et la collaboration dans la mise au point de nouveaux principes bioactives naturels plus efficace et moins nocifs.

**Mots-clés :** Lavandula stoechas L. ; Hydrodistillation ; CCM ; Activité antimicrobienne.

**Poster communication** **P-056**

# Study of phenolic and mineral components of potato tuber (*Solanum tuberosum L.*) grown in Oued Souf region.

TAMMA Noureddine

*Laboratory of Applied Chemistry and Environment , Department of Chemistry, Faculty of Exact Sciences, University of El Oued, Algeria*

**E-mail:** noureddine.tamma@gmail.com

**Abstract**

To discover the extent of the therapeutic value of the active products contained in the potato (*Solanum tuberosum L.*) plant of the regions of Al-Trifawi and Ouarmes and to continue previous research, we conducted an applied study on phenolic extracts. We studied their chemical and biological effectiveness through antioxidant activity and analysis of minerals present in the plant's tubers.

- The chemical detection of secondary metabolites showed that the studied extracts contained phenols and flavonoids.
- The phenolic extract that recorded the highest yield of the potato peel extract of the Al-Trifawi region was 3.072%.
- By estimating the total content of phenols using the Folin-Ciocalteu method and estimating the total content of flavonoids using $AlCl_3$ and by UV and visible spectroscopy, it was found that the potato extract from the Ouarmes region contains the largest amount of polyphenols estimated at 72.86 mg EAG/g and also contains the largest amount of flavonoids estimated at 4.095 mg EQ/g, compared to these results with the international standards, which estimated polyphenols between: (123-441 mg EAG/100g).
- The study of the antioxidant activity of the extracts using the DPPH test showed that the $IC_{50}$ values obtained were the highest activity for inhibiting DPPH in the Phenolic extract of potato peels from the Ouarmes region.
- The minerals were quantitatively estimated by volumetric calibration and multiscale visible spectroscopy.The results showed that the highest value was reached for magnesium in the Ouarmes area, which was estimated at (81.15 mg/100g) for the pulp and peels of potato tuber, which is a better value than that recorded in the international standards.
- In conclusion of what we have presented in this research, we can say that potato tubers grown in the Ouarmes area are better than the Trifawi area, and this is due to the difference in the quality of fertilizer.

Finally, given the encouraging results obtained from potato tuber extracts, they can be valued and qualified to be among the most used plants in nutrition.

**Keywords**: Solanum tuberosum L., phenolic and mineral components, antioxidant activity (DPPH).

**Poster communication** **P-057**

# Phytochemical composition, antioxidant potential, and antibacterial/antifungal activities of *Azadirachta indica* (Neem) leaf extracts from arid environments: A case study in the El Oued region

Abadi Abderrezzak[1], Wassima Lakhdari[2,3], Neghmouche Nacer Salah[1],Abderrahmene Dehliz[2]

[1] *University of El Oued, Faculty of Exact Sciences, Chemistry Department, P.O. Box 789, El Oued 39000, Algeria.*

[2] *National Institute of Agronomic Research of Algeria, Sation of Sidi Mehdi, Touggourt, 30200, Algeria.*

[3] *Biology Department, Faculty of Life and Nature Sciences, Valcore Laboratory, University of Boumerdes, Algeria.*

**E-mail:** abadi-abderrezzak@univ-eloued.dz

**Abstract**

The chemical composition and biological properties of *Azadirachta indica* (Neem) leaf extract from arid environments were investigated. LC-MS analysis identified several bioactive compounds, including quercetin, oleanolic acid, salicin, and catechin. The extract exhibited notable antioxidant activity, with DPPH scavenging activity at a concentration of 25.01 ± 0.71 µg/mL and an IC50 value higher than that of the β-carotene bleaching assay (22.29 ± 0.66 µg/mL) and the ABTS assay (45.09 ± 1.23 µg/mL). Antibacterial tests revealed that Escherichia coli, Pseudomonas aeruginosa, Staphylococcus aureus, and Bacillus subtilis were susceptible to the extract, with minimum inhibitory concentrations (MICs) ranging from VHC to 30 mg/mL. Additionally, antifungal activity was observed against *Alternaria* sp., *Fusarium solani*, and *Thielaviopsis paradoxa*. These findings suggest that neem leaf extract from arid regions holds significant biological activities, supporting its traditional use in medicine and agriculture.

**Keywords**: *Azadirachta indica*, neem, phytochemical composition, antioxidant activity, antimicrobial activity.

**Poster communication** **P-058**

# Screening chimique et evaluation de l'activité antioxydante d'une plante médicinale : *Anthemis maritima l.* de la région du Cap de Garde, Annaba.

BARKAT Ramzi[1] , SADOU Nina[1], SERIDI Ratiba[1], MECHENTEL Lina[1], TOUAHRIA Nadia Gghofrane[1].

[1]*Laboratoire de Biologie végétale et environnement (LBVE), Université Badji Mokhtar Annaba, ALGERIE.*

**E-mail:** ramzi.barkat@univ-annaba.org

**Resumé**

Les plantes médicinales sont des matières premières utilisées pour des fins thérapeutiques, aromatiques, culinaires, et dans la fabrication de cosmétiques, médicaments, aliments naturels, et autres produits de santé. Elles sont une source riche en métabolites secondaires aux structures chimiques variées et possédant une large gamme d'activités biologiques. Parmi ces plantes, nous avons choisi *Anthemis maritima L*, cette dernière est une plante médicinale endémique à l'Algérie, récoltée au Cap de Garde de Annaba. Le choix de cette espèce endémique est guidé par son intérêt thérapeutique.

En premier nous nous sommes intéressés au criblage phytochimique pour étudier la composition chimique de la drogue végétale (feuilles) de Anthemis maritima, cette étude a mis en évidence la présence de 4 principes actifs : Alcaloïdes, Flavonoïdes, Tanins, Saponosides. Ces derniers sont considérés comme étant des substances naturelles bioactives qui présentent un intérêt d'une part dans la phytothérapie et d'autre part dans l'industrie cosmétique et agroalimentaire.

La deuxième partie a été consacrée à l'évaluation de l'activité antioxydante sur l'extrait éthanolique obtenu par macération à partir de la partie aérienne (Feuilles) de notre espèce, par la méthode de réduction du radical DPPH , le résultats obtenu révèle une valeur d'IC50 de l'extrait éthnolique de 47.54 ± 0.310 mg/ml contre une valeur de 0.93 ± 0.002 mg/ml pour le BHT (antioxydant de référence) .Cet extrait présent une capacité antioxydante moyenne contre le radical DPPH, modérée par rapport au standard BHT. Les raison peuvent être liées à une faible présence des polyphénols dans cet extrait.

**Mots-clés :** Plantes Médicinales. Anthemis maritima L. Antioxydant. Screening.

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**Poster communication** **P-062**

# Chemical characterization, phenolic and flavonoid contents and evaluation of antioxidant and anti-Alzheimer potential of chloroform extract from *Myrtus*

BOUNAAS Jihane[1], BASLI Abdelkader[1], OUNISSI Ismahan[1]

[1]*Laboratory of Interaction Research, Biodiversity, Ecosystems and Biotechnology, Faculty of Sciences, University of Skikda, Skikda, Algeria.*

**E-mail:** bounaas.jihane@gmail.com

## Abstract

The use of medicinal plants has retained an undisputed place in practice, due to their effectiveness in various therapeutic procedures. This work focused on the plant of the *genus Myrtus*, a medicinal plant belonging to the family Myrtaceae which is known for their antidiabetic, antidiarrheal, antirheumatic and anti-inflammatory effect. Therefore, this study aimed to evaluate the antioxidant and anticholinesterase potential of chloroform extract from the plant *Myrtus* as well as its phenolic and flavonoid contents and explore its chemical compounds using LC-ESI-MS/MS analysis. The quantification of total phenols and flavonoids showed that the extract has a significant source of these bioactive compounds, measuring 67.23 ± 1.01 mg EAG/g DW and 41.94 ± 1.17 mg EQ/g DW, respectively. The antioxidant activity was carried out using DPPH radicals scavenging and FRAP assay. The evaluation of antioxidant activity showed that the chloroform extract had an interesting ability to reduce iron and trap the free radical DPPH. The FRAP method given an optical density equal to 16.55 ± 0.55 µg/ml, while the $IC_{50}$ obtained from the DPPH assay was 13.70 ± 0.32 µg/ml. The chloroform extract exhibited the most promising anticholinesterase activity, with $IC_{50}$ values of 170.35 ± 0.21 µg/mL against acetylcholinesterase (AChE) and 34.61 ± 2.00 µg/mL against butyrylcholinesterase (BChE), which were comparable to galantamine in BChE and lower in AChE. A total of 42 standards were employed in the LC-MS/MS analysis, and the phytochemical profiling revealed the presence of 18 distinct phenolic compounds within the extract, including 7 phenolic acids, 8 flavonoids, 1 benzaldehyde, 1 Coumarin, and 1 carotenoid, and 4 other phytochemical compounds (BHT, 2 vitamins and 1 dicarboxylic acid). This genus possesses antioxidant properties that may be attributed to the presence of phytocomponents, thereby representing a viable source of natural compounds for potential therapeutic applications in the treatment of Alzheimer's disease.

**Keywords**: Myrtus, LC-ESI-MS/MS, anticholinesterase, antioxidant, polyphenol, flavonoid.

**Poster communication** **P-065**

# Phenolic compound profile of an eastern Algerian spice : Characterization by LC/ESI/MS

ATTIA Amel [1]*, OUKIL Naima[1] , Gali Lynda[2]

[1] *Department of Microbiology/Laboratory of Plant Biology and Ethnobotany/University of Béjaia*
[2]*Centre de rcherche en Biotechnologie / Constantine*

**E-mail*:** amel.attia@univ-bejaia.dz

**Abstract**

Numerous studies show that antioxidants play an essential role in maintaining human health, preventing and treating diseases, due to their ability to reduce oxidative stress. In recent years, there is great interest for identifying alternative natural and safe sources of food antioxidants, and the search for natural antioxidants, especially of plant origin. The majority of natural antioxidants are phenolic compounds, and the most important groups of natural antioxidants are the tocopherols, flavonoids and phenolic acids. In order to investigate the polyphenolic profile of the *Laurus nobilis L*. leaf extracts obtained by ultrasounds assisted extraction, LC/ESI/MS analysis was carried out. A total of 12 phenolic compounds, consisting of phenolic acids, flavonols, flavan-3-ols, flavones and were identified. The phenolic content of the bay laurel plant was found by comparing it with standards. The most abundant compound was determined to be vanillic acid (459 ng/ml). Vanillic acid was followed by quercitin (326.09ng/ml). Therefore, these two compounds can be defined as the main compounds found in the structure of the LN. Luteolin (1.67 ng/ml) and o-coumaric acide acid (0.625 ng/ml) compounds were determined as the least common minor compounds in the structure of the LN. The LC-MS/MS method is an effective method for identifying and quantifying these components. Thanks to this method, quality control of herbal products and supplements obtained from the bay plant can be made.

**Key words:** phenolic compounds, antioxydants, LC/ESI/MS

**Poster communication** **P-067**

# Dosage des éléments nutritifs des feuilles de Stevia cultivée au sud algérien

MEKDADE Loubna [1*], MADI Nassim [2], SAHRAOUI Hossem [1], HADJADJ Nasreddine[1]

[1]*Centre de Recherche en Biotechnologie (C.R.Bt)- Constantine, Algérie.*

[2] *Centre de Recherche en Technologies Agro-Alimentaires (CRTAA)- Béjaia, Algérie*

**E-mail**:l.mekdade@crbt.dz

**Resumé**

*Stevia rebaudiana* est une plante sucrée produisent des glycosides hypocaloriques appelés glycosides de stéviol qui possèdent un pouvoir sucrant jusqu'à 450 fois supérieur à celui du saccharose. Eu égard à l'intérêt croissant pour les aliments naturels faibles en calories, les glycosides de stéviol suscitent de plus en plus d'intérêt. Notre étude se fixe ainsi comme objet de déterminer la valeur nutritionnelle de feuilles de *Stevia* cultivée en Algérie afin d'envisager son introduction progressive dans l'alimentation du consommateur algérien. Pour ce faire, nous avons cultivé *Stevia* rebaudiana sous serre au niveau de la région de Ghardaia. Les feuilles de Stevia séchées et broyées ont fait l'objet d'une évaluation de la qualité nutritionnelle par un dosage des lipides, protéines, carbohydrates, fibres, humidité, cendres, et valeur énergétique. La composition minérale des feuilles de *stevia* a été étudiée par spectrométrie de fluorescence des rayons X. Par ailleurs, nous avons testé quatre méthodes pour l'extraction de glycosides de stéviol à savoir ; l'extraction par infusion, décoction, ultrasons, et micro-ondes.

Nos résultats révèlent que la composition proximale des feuilles de Stevia était comme suit : lipides 3.22 ± 0.05 %, protéines 9.19 ± 1.002%, carbohydrates 56.78 ± 17.20%, fibres brutes 0.33 ± 0.005 %, humidité 7.70 ± 0.03%, cendres 22.75 ± 17.33%, et valeur énergétique 252.165 ± 61,42 Kcal/g. L'étude de la composition minérale révèle que les feuilles de *Stevia* sont très riches en calcium (38.68 %) et en potassium (36.14 %). Les techniques d'extraction des glycosides ont présenté des rendements jusqu'à 37,35 ± 0,71%, cependant l'analyse statistique ANOVA n'a révélé aucune différence significative ($p < 0.05$). On en conclue que la méthode d'extraction n'a pas d'effet sur le rendement. Nos résultats confirment que la *Stevia* est une plante riche en éléments nutritifs essentiels pour l'organisme, sa culture et sa production à grande échelle en Algérie contribuerait à la consolidation de la sécurité alimentaire et nutritionnelle.

**Keywords**: Stevia, glycosides de stéviol, édulcorants hypocaloriques.

**Poster communication** **P-069**

# Quantification of sugars in pollen grains of four pistacia atlantica (anacardiaceae).

Chaima Kaifes[1], Mohamed Yousfi[2], Hamid Guenane[3].

[1] *Material sciences University Amar Télidji of Laghouat, Laboratory of Fundamental Sciences*
[2] *Material sciences University Amar Télidji of Laghouat, Laboratory of Fundamental Sciences*
[3] *biology, University Amar Télidji of Laghouat, Laboratory of Fundamental Sciences.*

**E-mail:** c.kaifes@lagh-univ.dz

**Abstract**

Pollen grains are a rich source of essential minerals, amino acids, lipids, polyphenols sugars and they are often considered as a complete food for human beings. Sugars are essential biomolecules that play a variety of structural and functional roles in living organisms and source of energy, in our work we focused on the quantification of sugars of four pollen aqueous extracts from Pistacia atlantica flowers.

Pollen grains were collected from four flowers of pistacia atlantica trees in different regions, these grins were macerated in mixture of methanol/water, after isolation of phenolic compounds with ethyl-acetate, the aqueous fraction was used for the quantification of sugars The spectrophotometric determination of sugars revealed that the content of this phytocompound were found in all the aqueous samples using (debois et al, 1956) method, which ranged between (6 -16 GluE mg/g DM).

We can say now that pollen grains collected from trees flowers are a good source of energy substances and can be proposed as a supplement.

**Keywords**: Pistacia atlantica; Pollen; Extraction; Sugars

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**Poster communication** **P-071**

# Etude de l'effet des solvants sur l'extraction des polyphénols par Soxhlet

Zerrad Chaima[1], Toudert Nadia[2], Djilani Salah Eddine[1], Amamra Roumaissa[1], Alam Aya[1], Zekkad Farida[1]

[1]*Laboratoire de Synthèse et Biocatalyse Organique, Université Badji Mokhtar, Annaba, Algérie*

[2]*Laboratoire de physico-chimie des Matériaux, Université Chadli Bendjedid, El Tarf, Algérie*

**E-mail:** Chaimazerrad141@gmail.com

**Resumé**

Cette étude a pour objectif d'évaluer l'impact du choix du solvant sur l'efficacité de l'extraction des polyphénols en utilisant la méthode Soxhlet, qui permet une extraction optimale grâce à la circulation continue du solvant à travers le matériau végétal. Trois solvants ont été utilisés à savoir l'éthanol, l'acétate d'éthyle et l'hexane, et ils ont été comparés afin de déterminer leur capacité à extraire les polyphénols totaux à partir d'une plante donnée.

Les résultats montrent que la polarité du solvant joue un rôle déterminant dans l'efficacité de l'extraction. Parmi les solvants testés, l'éthanol a permis d'obtenir l'extraction la plus efficace des polyphénols, en raison de sa grande affinité avec les groupes hydroxyles des composés phénoliques. L'acétate d'éthyle, bien que moins performant, a néanmoins réussi à extraire certains polyphénols spécifiques. En revanche, l'hexane, un solvant non polaire, s'est avéré beaucoup moins efficace pour extraire ces composés.

L'analyse des extraits par spectrophotométrie UV-Vis et chromatographie liquide haute performance (HPLC) a permis de quantifier les polyphénols totaux et d'identifier certains composés phénoliques particuliers. Les rendements d'extraction dépendent non seulement du type de solvant, mais également de la durée de l'extraction, de la température, et de la nature de la matrice végétale.

En conclusion, cette étude souligne l'importance cruciale du choix du solvant pour l'extraction des polyphénols, et offre des recommandations sur les solvants les plus adaptés pour des applications spécifiques dans les domaines de la phytothérapie et des produits naturels.

**Mots-clés** : Polyphénols , Soxhlet, spectrophotométrie UV-Vis, HPLC.

**Poster communication** **P-074**

# Isolation and identification of β-sitosterol.

Nour-elhouda Bekache[1], Sonia Chabani[1,2], Hamada Haba[1]

[1] *Laboratory of Chemistry and Environmental Chemistry (LCCE), Department of Chemistry, Faculty of Matter Sciences, University of Batna 1, Algeria*

[2] *Higher National School of Renewable Energies, Environment and Sustainable Development, Batna, Algeria*

**E-mail**: nourelhouda.bekache@univ-batna.dz.

**Abstract**

Malope, a genus within the Malvaceae family, comprises three distinct species native to North Africa, Europe, and the Macaronesia region. Research on the Malvaceae family has uncovered a diverse array of secondary metabolites, underscoring its significance in pharmacology and phytochemistry. These metabolites encompass saponins, triterpenes, tannins, flavonoids, quinones, and coumarins. Additionally, members of the Malvaceae family have demonstrated a broad spectrum of biological activities, including analgesic, anti-inflammatory, antidiabetic, anti-obesity, antioxidant, antimicrobial, anxiolytic, cardioprotective, cytotoxic, hepatoprotective, and nephroprotective effects.

The present work consists examining the phytochemical profile of the species. and identifying the compounds present in this plant. Chemical analysis of the ethyl acetate extract, using chromatographic methods, facilitated the isolation of compounds. Spectroscopic techniques were subsequently employed to identify β-sitosterol.

**Mots-clés** : Malvaceae, Malope, spectroscopy, β-sitosterol.

**Poster communication** **P-075**

# Preventive effect of Atriplex halimus L. on cadmium provoked hepatic injury in rats

Lamia MELLAHI [1], Samia BENZAZIA [2], Safia NADJI [2], Abdelkader BASLI [1], Fouzi BOULKENAFET [2]

[1] *Laboratory of Research Interactions, Biodiversity, Ecosystems and Biotechnology, Department of Natural and Life Sciences, Faculty of Sciences, University 20 August 1955 Skikda, Algeria*

[2] *Department of Natural and Life Sciences, Faculty of Sciences, University 20 August 1955 Skikda, Algeria*

**E- mail :** lamiamellahidz@gmail.com // l.mellahi@univ-skikda.dz

**Abstract**

The present study was designed to estimate the preventive effect of Atriplex halimus L. aerial parts against cadmium intoxication in liver rats. 42 male albino rats were divided into 6 groups of 7 rats each: Control (G1), Atriplex halimus (G2 : 400 mg/ kg/ d et G3 : 600 mg/ kg/ d), cadmium (G4 : 8.8 mg/ kg/ d), cadmium (G4 : 8.8 mg/ kg/ d) + Atriplex halimus (G5 : 400 mg/ kg/ d et G6 : 600 mg/ kg/ d) for 40 days. Aqueous extract of aerial parts of Atriplex halimu was was given by gavage. At the end the experiment, body weight gain and relative liver weight were estimated and liver enzyme markers (AST, ALT, ALP) and GSH were analysed by spectrophotometry. Histopathological studies on hepatic tissue were also performed by the method of Hematoxylin and Eosin staining. Cadmium administrated to rats caused an alteration in physiological parameters (body and organs weigh) and hepatic enzymes markers (AST, ALT, ALP) and GSH. In addition, Histopathological studies showed a massive degeneration in liver tissue in cadmium exposed rats. However, treatment by Atriplex halimus especially preventive effect ameliorated most of the adverse effects induced by cadmium. Atriplex halimus restored the altered of physiological, biochemical and histopathological changes. The present study suggests that Atriplex halimus could be a substantially promising hepatoprotective agent against cadmium toxic effects and may be against other hepatotoxic chemical or drugs.

**Keywords:** Atriplex halimus, cadmium, hepatotoxicity, Rats, liver, Histopathological.

**Poster communication** **P-077**

# Evaluation of saponins of cucurbita moschata duch for antiurolithiatic activity

BENSATAL. Ahmed [1], BENALIA Nadjat[2]

[1] *Laboratory of physical chemistry of Materials and Environment, University Ziane Achour , Djelfa,BP 3117 ,17000, Algeria*

[2]*Department of Chemistry, University Ziane Achour , Djelfa,BP 3117 ,17000, Algeria*

**E-mail** : a.bensatal@univ-djelfa.dz

**Abstract**

The species of Cucurbita is a very common shrub in Algeria. Saponins are one of the most important products of secondary metabolites, and their many biological activities are been proven. Leaf, pulp, and seeds of Cucurbita plants are a very rich source of phytochemicals compounds; one of the most common members of this family is Cucurbita moschata.Duch.

The objective of this study is to evaluate in vitro the activity antilithiasic of saponins of the seeds of this shrub, by the model of turbidimetry. In the purpose of studying the Anti-lithiasis activity this work was divided into three minor studies which are: nucleation assay, growth assay, and aggregation assay. In this assay, changes in absorbance representing the inhibition percentage for nucleation, growth, and aggregation crystals that were in vitro prepared, were calculated with and without inhibitor by spectrophotometer UV.

The results indicate a very important biological activity of saponins against kidney stone formation that goes up to a limit of 75,43% in the nucleation stage, 83,11% in the growth stage, and 98,31% in the aggregation stage.

The concentration of saponins extraction is a very significant factor in the Anti-lithiasis activity so the higher the concentration is the bio-activity goes higher. In conclusion, saponin compounds shown a very strong Anti-lithiasis activity even in comparison with citrate inhibitor

**Keywords**: Cucurbita moschata, Saponins, Antiurolithiatic, Turbidimetry.

**Poster communication** **P-079**

# Extraction des polyphenols et l'activité biologique de la plante Napaulius graveolens

Amamra Roumaissa Halima , Mellouk Karima, Ferchichi Loubna , Bouasla Radia, Zerrad Chaima, Benzayed Chahra

*Laboratoire de synthèse organique et biocatalyse. Faculté des sciences. Université Badji-Mokhtar. Annaba*

**E-mail** : amamraroumaissa22@gmail.com

**Resumé**

Les plantes occupent une place fondamentale dans notre monde, elles assurent la production primaire, construisent des couverts végétaux ainsi elles participent fortement à la régulation du climat et au cycle de l'eau, des nombreuses substances actives qu'elles recèlent, utilisées notamment en médecine. En effet, Nauplius graveolens est une des plantes médicinales utilisée traditionnellement dans le cas de diabéte, la migraine et l'infection microbienne.

L'objectif de ce travail est l'extraction des polyphenols ainsi que l'activité antioxydante, antimicrobienne et anti-inflammatoire de différents extraits obtenant de cette plante appartenant à la famille des astéracées.

L'extraction a été faite par Soxhlet en utilisant des solvants de différentes polarités

L'évaluation de l'activité antimicrobienne des molécules par la méthode de diffusion sur puits a montré une activité très significative contre certaines souches bactériennes et fongiques. L'évaluation de l'activité antioxydante des molécules par le test de piégeage du radical libre DPPH a donné des résultats antioxydants significatifs par rapport à les références BHT et l'acide ascorbique, ces résultats révèlent la présence des composés bioactifs qui sont responsables des activités antioxydantes et antimicrobiennes. L'évaluation de l'activité anti-inflammatoire des extraits par le test de dénaturation de la protéine de l'albumine de sérum bovin (BSA) montre que cette plante possède un pouvoir pharmacologique.

**Mots-clés** : Astéracées, nauplius graveolens, Activité biologique, Extraction, Sohxlet, plante médicinale.

**Poster communication** **P-081**

# Nanoencapsulation of tetraaclinis articulate essential oil and evaluation of its antibacterial activity

Rania Larouci, Mohamed Reda Zahi, Chahinez Ait Si Said, Smain Sabour, Ouassila Touafek, Mohamed El Hattab

*University of Saad Dahleb Blida1, Faculty of science, Department of chemistry, Laboratory of Natural Products Chemistry and Biomolecules.*

**E-mail:** laroucirania79@gmail.com

**Abstract**

Essential oils are naturally derived aroma compounds, with wide-spectrum biological activities [1]. However, essential oils have been described as strong natural antimicrobial agents [2]. The crescent interest in the use of essential oils as natural antimicrobials and preservatives in different fields has been driven in the last years by the growing consumers' demand for natural products with improved microbial safety [1]. Nevertheless, the strong reactivity and hydrophobicity of essential oils provide a significant obstacle to their direct integration into multiple preparations. Nanotechnology is a tool used to improve the essential oils properties, which can be incorporated as nano-sized delivery systems in order to overcome their limitations [3]. Tetraclinis articulata (Cupressaceae), locally called "Al Araar" is an endemic, medicinal and aromatic species of northwestern Africa (Morocco, Algeria and Tunisia) [4]. Various parts of this tree are used in folk medicine for its multiple therapeutic effects, it is mainly used against childhood respiratory, intestinal infections, gastric pains, diabetes and hypertension [5]. Many studies have reported that the essential oil of Tetraclinis articulata has a high antibacterial potential [6]. The main object of this study is to determine the antibacterial activity of the essential oil of Algerian Tetraclinis articulata extracted from its dried leaves and its nanoemulsion. The essential oil obtained showed high antibacterial activity against the majority of the strains tested, with CMI values ranging between 2.5 and 5 µl/ml. The prepared formulation was transparent with tiny droplets, about 23.9 nm in diameter of the smallest ones, and had good stability under normal storage conditions. Also, the formulation exhibited moderate to good antibacterial activity against all the tested strains, with values of CMI ranging from 46.66 to 66.66 µl/ml.

**Keywords:** Essential oil, Tetraclinis articulata, nanoemulsion, Antibacterial activity.

**Poster communication** **P-082**

# Détermenation de l'activite antioxydante des extraits composés phénoliques défferentes de sorgho (sorghumbicolor l .moench)

Zaitri Mohamed, Belhadi Badreddine, Mohamed Benalia, Mohamed Yousfi; Ould-Kior Reda, Djabali Djaafar, Boubekeur Nedjmie.

*Université de Laghouat*
*Université Amar Telidji De Laghouat Département De Sciences De La Matière Faculté De Sciences Laboratoire Des Sciences Fundamentals (LSF)*

**E-mail** : medzaitri@gmail.com

**Résumé**

Le sorgho fait partie du groupe des plantes les plus anciennement cultivées dans le monde. Il est cultivé partout dans les zones arides d'Afrique, d'Asie, des Amériques, d'Europe et d'Australie. Le but de cette étude est d'évaluer les produits alimentaires naturels et leur rôle en tant qu'antibiotiques alternatifs en testant l'efficacité biologique des composés phénoliques de différents extraits sous l'influence de quatre systèmes pour les variétés de plantes de sorgho.

Les résultats ont montré que la teneur en phénols totaux lors de l'extraction avec le Système (Acétone/Eau) variait de 0,00 à 3,73 (mg TAE/g) dans la farine de sorgho. Cette teneur est beaucoup plus élevée que sa teneur lors de l'extraction avec les systèmes (Méthanol) , (Méthanol/Eau) d'un rapport de (8/2 : v/v) et (Acétone), tandis que les tanins variaient de 0,32 à 18,42 (mg EC/g) avec le système (Acétone/Eau) d'un rapport de (7/3 : v/v). Les résultats ont également montré que la teneur en phénols totaux des feuilles était deux fois plus élevée que son contenu dans la panicule et la tige. Alors que dans les tanins, elle était élevée dans la tige par rapport aux feuilles et à la panicule.

Les résultats de l'étude de l'activité anti oxydante de divers extraits phénoliques de la farine de sorgho ont montré une grande capacité anti radicalaire, ainsi qu'une capacité réductrice des ions fer III, notamment dans la variété S4B1.

**Mots-clé** : Sorgho, composés phénoliques, tanins, activité, antioxydant DPPH, FRAP.

**Poster communication** **P-083**

# Dosage et evaluation de l'activite antioxydante d'extraits lipidiques de cupressus sempervirens

Kired Ibrahim, Benalia Mohamed, Boulenouar Noureddine, Yousfi Mohamed

*École Normale Supérieure de Laghouatensl (ensl)*

**E-mail:** i.kired@ens-lagh.dz

**Résumé**

Historiquement, dans toutes les civilisations et sur tous les continents, l'Homme a utilisé les plantes aromatiques, d'abord dans l'alimentation, puis à des fins médicinales. Cupressus sempervirens appartient à la famille des Cupressaceae est un arbre vivace, l'une des plantes appréciées pour ses propriétés antioxydantes, antibactériennes et anti-inflammatoires, largement utilisées en médecine traditionnelle. Dans ce travail, deux échantillons (extrait lipidique) provenant de deux zones différentes (Djelfa et Laghouat) ont été prises pour le dosage de l'α tocophérol et l'évaluation de leurs l'activité antioxydante. Les teneurs en α tocophérol varient considérablement de 3,03 ±0,03 mg/g matière végétale à 2,55±0,05 mg/g matière végétale D'autre part, l'activité antioxydante par le test DPPH des deux extraits lipidiques indiquent que ces extraits inhibent le radical stable DPPH avec des pourcentages d'inhibition 82.20% de l'échantillon provenant de Djelfa et 63.39% de l'échantillon de Laghouat. Ces résultats prouvent que la région de collecte des échantillons influe sur le contenu en tocophérols ainsi qu'à l'activité antioxydante.

**Mots-clés :** Cupressus sempervirens, α -tocophérol, lipides, DPPH.

**Poster communication** **P-084**

# Le plantain une mauvaise herbe aux multiples vertus : screening phytochimiques et études de la composition chimique du plantain lancéolé.

DIAF Ilhem[1*], CHELOUFI Hadjher[1], HALKOUM Roufia[1]

[1] *Université Chadli Ben Djedid El Tarf, BP :73, El Tarf 36000, Algérie.*

**E-mail**: ilhemdiaf@rocketmail.com

**Abstract**

Depuis les temps les plus reculés, les plantes constituaient une réponse de choix pour fournir, de façon naturelle, à l'organisme les substances nécessaires pour maintenir son équilibre vital. A travers les siècles et les continents, les hommes ont su acquérir la connaissance des plantes et de leurs propriétés thérapeutiques. La recherche dans le domaine des substances végétales constitue actuellement un composant important dans la chimie verte. Les plantes médicinales constituent une matière première alternative dans l'industrie pharmaceutique et cosmétique, et ceci grâce leurs propriétés biologiques.

Dans ce travail nous souhaitons contribuer à la valorisation d'une plante appartenant à la famille des plantaginacéés, a savoir le plantain lancéolé comme plante médicinale. Une meilleure connaissance de la composition chimique de cette plante ainsi que ses propriétés biologiques pourra aider à valoriser cette plante dont les vertus sont peu connues.

**Keywords**: plante médicinale, plantaginacéés, plantain lancéolé.

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**Poster communication** **P-086**

# Phytochemical study and anti-inflammatory activity in vivo of Malva sylvestris L. flowers.

Zaakane Abla[a,b] , Missoun Fatiha[b], Zaouani Mohamed[c], Amari Ouda Nesrine[a]

[a]*Laboratoire de Structure, Elaboration et Application des Materiaux Moleculaires (SEA2M), Faculte des Sciences Exactes et de l'Informatique (FSEI), University of Abdelhamid Benbadis, Mostaganem, Algeria.*

[b]*Laboratory of Sciences and Techniques of Animal Production,Faculty of Nature and Life Sciences, Abdelhamid Ibn BadisUniversity, Mostaganem, Algeria.*

[c] *Laboratory of Food Hygiene and Quality Insurance System of Higher Veterinary School Algeries, Algeria.*

**E-mail** : Abla.planta@gmail.com

**Abstract**

Malva sylvestris L is a medicinal plant usually known as khobiza in Algeria, native to Asia and Europe. The flowers of this plant are used by the populations in traditional medicine in the treatment of respiratory and digestive inflammations and are well known also for its emollient effects. The aqueous extraction of dried flowers from the Malva sylvestris L. plant allowed to optain a yield of 20%. The phytochemical screening showed that the extract is very rich in mucilage, as well as flavonoids and phenols. Carrageenan was used to induce inflammation in mice, the percentage inhibition of edema (% INH), the percentage increase in paw edema volume (% AUG) and histological study were used to evaluate the anti-inflammatory activity of M sylvestris flowers in vivo on wistar rats. The results show that the treatment with extract of M sylvestris presents a significant anti-inflammatory activity at dose 200 mg / kg compared to control group during the whole period of experimentation. These results were confirmed by the histological study in the paws of mice. The data obtained in this study on Malva sylvestris L suggests its potential as a safe anti-inflammatory agent for use in the treatment of various inflammatory diseases.

**Keywords**: Malva sylvestris L, flowers, extraction, phytochemical screening, anti-inflammatory activity, Carrageenan**.**

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**Poster communication** **P-087**

# Analyse des activités biologiques de l'huile de cade : Vers de nouvelles stratégies en thérapie naturelle

Ahmida meryem[1], Zaddam Mustapha Hichem [1], Silini Ilhem[1], Djaber Nesrine[1], Bensouici Chawki[2], Boumendjel Amel[1], Messarah Mahfoud[1] & Boumendjel Mahieddine[1]

[1]*Laboratoire de Biochimie et de Toxicologie Environnementale, Faculté des Sciences, Université de Badji Mokhtar, Annaba, Algérie*

[2]*Centre de Recherche en Biotechnologie Ali Mendjli Nouvelle Ville, Constantine, Algérie*

**E-mail** : meryem.ahmida@univ-annaba.dz

**Résumé**

Le Juniperus oxycedrus, ou genévrier cade, est une espèce méditerranéenne utilisée pour produire l'huile de cade, reconnue pour ses propriétés antiseptiques et dermatologiques. Des études récentes ont révélé ses potentiels antioxydants, antidiabétiques et inhibiteurs de l'acétylcholinestérase (AChE), indiquant des applications thérapeutiques prometteuses. Dans cette recherche les analyses spectrométriques ont montré que cette huile est riche en polyphénols (275,21 ± 3,14 µg EAG/mg), bien que sa teneur en flavonoïdes soit relativement faible (28,23 ± 1,91 µg QE/mg). Divers tests ont été effectués pour évaluer son activité antioxydante. L'huile de cade a démontré une activité antioxydante modérée avec une $IC_{50}$ de 19,40 ± 0,45 µg/mL dans le test de réduction du fer, par rapport à l'acide ascorbique ($A_{0.5}$ de 6,73 ± 1,15 µg/mL). Par la méthode de la phénanthroline, elle a montré une activité notable ($IC_{50}$ de 11,52 ± 0,48 µg/mL), bien que moins efficace que le standard BHT ($IC_{50}$ de 2,12 ± 0,04 µg/mL). Dans le test GOR, l'huile de cade a également affiché une activité modérée ($IC_{50}$ de 21,93 ± 0,47 µg/mL), comparée au BHA ($IC_{50}$ de 5,38 ± 0,06 µg/mL), montrant une capacité limitée dans le piégeage des radicaux libres. Cependant, l'huile de cade a démontré une activité antidiabétique remarquable, avec une capacité d'inhibition de l'α-amylase ($IC_{50}$ de 95,19 ± 2,37 µg/mL) supérieure à celle de l'acarbose ($IC_{50}$ de 365,93 ± 1,70 µg/mL). Elle a aussi montré une inhibition modérée de l'AChE ($IC_{50}$ de 61,08 ± 1,19 µg/mL), inférieure à celle de la galantamine ($IC_{50}$ de 6,27 ± 1,15 µg/mL), mais efficace à des concentrations élevées. En conclusion, bien que l'huile de cade présente une activité antioxydante inférieure aux standards de référence, elle présente un potentiel intéressant pour la gestion du diabète de type 2 et pourrait constituer un adjuvant potentiel dans le traitement des maladies neurodégénératives.

**Mots-clés** : Huile de cade, polyphénols, flavonoïdes, propriétés antioxydantes, propriétés antidiabétiques, anticholinestérases.

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**Poster communication** **P-088**

# Identification par HPLC-DAD de polyphénols d'une plante médicinale Algérienne (Amaranthaceae)

CHOHRA Djawhara, BENABBAS Rihab, BENTOUMI Houria, AOUF Noureddine

*Laboratoire de Chimie Organique Appliquée, Equipe de Chimie Bio-organique, Département de Chimie, Université Badji Mokhtar-Annaba, 2300.*

**E-mail**: djawharachohra123@yahoo.com

**Résumé**

Algérie, par la diversité de son climat et de ses sols, offre une flore particulièrement riche en plantes médicinales et aromatiques. Ces ressources végétales constituent un réservoir inépuisable de substances bioactives, susceptibles d'être utilisées à des fins pharmaceutiques, agroalimentaires et cosmétiques.

Les composés phénoliques sont des produits largement distribués dans le règne végétal constituent un groupe de plus de 8000 molécules. Plusieurs recherches récentes ont été menées sur les composés phénoliques en général et sur les flavonoïdes en particulier, en raison de leurs diverses propriétés physiologiques qui sont attribuées principalement à leur effet antioxydant.

Le présent travail est une contribution à la valorisation d'une plante algérienne à caractère médicinal de la famille des Amaranthaceae. L'extrait méthanolique des parties aériennes de cette plante a été mené à une analyse spectrophotométrique, pour déterminer sa teneur en polyphénols totaux et en flavonoïdes totaux. Une identification des composés phénoliques contenant dans cet extrait a été effectuée par une HPLC/DAD.

La teneur en polyphénols a été déterminée par spectrophotométre selon la méthode Folin-Ciocalteu (45.18 ± 0.80 mg EAG/g ES), tandis que la teneur en flavonoïdes a été déterminée selon la méthode de chlorure (99.53 ± 1.88 µg EC/g ES). Ces résultats montrent que la plante est très riche en polyphénols et en flavonoïdes ce qui ce qui traduit leurs utilisation en médecine traditionnelle algérienne comme un antioxydant.

L'analyse HPLC/DAD a été effectuée avec 11 standards phénoliques Les résultats montrent que la plante est très riche en polyphénols avec des grandes concentrations en acide benzoïque, acide chlorogénique et en épicatéchine.

La richesse de cette plante en polyphénols traduit ses utilisations en médecine traditionnelle. Cette étude n'est qu'une étude préliminaire à un travail plus approfondi sur la composition de cette plante.

**Mots-clés**: Flavnoides, polyphenols, HPLC, Amaranthaceae

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**Poster communication** **P-090**

# Phytochemical analysis, anti-antioxidant and anti-inflammatory potential of myrtle berries Myrtus communis L.

Rim SALHI[1,*], Nadia AMESSIS-OUCHEMOUKH[1], Roukia BOUIZAR[1], Rania AGABI et Abel ZENATI[1].

[1] *Faculté des Sciences de la Nature et de la Vie, Laboratoire de Biomathématiques Biophysique Biochimie et Scientométrie, Université A. MIRA de Bejaia,06000 Bejaia, Algérie*

**E-mail:** rim.salhi@univ-bejaia.dz

**Abstract**

Common myrtle belonging to the Myrtaceae family is a widespread species in the Mediterranean basin and several parts of which (leaves or fruits) are used for therapeutic, cosmetic or food purposes. The fruits are consumed naturally or in infusion, as well as to make jams, jellies or liqueurs. The objective of this study was to estimate the content of bioactive compounds (total phenols, flavonoids and anthocyanins) as well as to evaluate the biological activities (antioxidant, anti-inflammatory) of extracts of freeze-dried powders of wild myrtle berries harvested in the Bejaïa region. The antioxidant activity of extracts of mature fruits of Myrtus communis was evaluated by different methods (DPPH, ABTS, ferrozine) in order to obtain a complete vision of the antioxidant capacity of this fruit. The anti-inflammatory activity was evaluated using two in-vitro methods: the inhibition of protein denaturation and the inhibition p of proteases. The Folin ciocalteu method showed a considerable amount of total polyphenols. The determination of total flavonoids with AlCl3 showed a good concentration of flavonoids. The extract showed excellent antioxidant activity using various methods, as well as good anti-inflammatory potential. This high activity is probably due to the high content of bioactive compounds such as flavonoids, polyphenols and anthocyanins.

**Key words:** Myrtus communis L., Polyphenols, anti-inflammatory activity, DPPH, ABTS, ferrozine.

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**Poster communication** **P-093**

# Phytochemical study of Noble laurel medicinal plant

Hadjer Cheloufi [a, b], Ilhem DIAF [b], Ismahene GRIB [a, b], Malika Berredjem[a]

[a] *Laboratory of Applied Organic Chemistry, Synthesis of Biomolecules and Molecular Modelling Group, Badji-Mokhtar. Annaba University, Box 12, 23000 Annaba, Algeria*

[b] *El-Tarf University, BP N ° 73, 36000, El-Tarf, Algeria*

**E-mail:** h.cheloufi@univ-eltarf.dz

**Abstract**

Noble laurel is a medicinal aromatic plant belonging to the lauracea family; this plant is rich in secondary metabolites. It is widely used in Algeria in traditional or alternative medicine, due to their multiple therapeutic effects[1]. Our work focuses on a phytochemical study of Noble laurel extract. The secondary metabolites screening revealed the presence of tannins, sterols, alkaloids, essential oil, coumarins, cardinolides, saponins and flavonoids. As flavonoids are known by their antioxidant [2] and anti-inflammatory activities[3], on the other hand they play a crucial role in the cardiovascular and euro-degenerative diseases treatment[3]. For this reason, a dosage of flavonoids has been carried out, in order to determine the flavonoids content in Noble laurel of our region.

**Keywords**: Noble laurel, Secondary metabolites, Photochemical screening, Flavonoids.

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**Poster communication** **P-094**

# Contribution to the study of the phytochemical composition and antioxidant activity of Salicornia Arabica

BECHEKER Abir, BOUCHAHDENE Souheila, LEMBOUB Chama, ZAALANI Achwak, ZENDI Roumaissa, REGHIS hayette, BOUMENDJEL Mahieddine

*Laboratory of Biochemistry and Environmental Toxicology, Faculty of Sciences, Badji Mokhtar Annaba University Algeria*

**E-mail** : bechekerabir@hotmail.com

**Abstract**

To promote the utilization of medicinal plants from the Algerian flora, we investigated Salicornia arabica, an original and rich medicinal plant known for its ability to thrive in salt-rich soils. This endemic species possesses notable nutritional, medicinal, and pharmacological properties. The evaluation of its antioxidant, anti-inflammatory, antimicrobial, anti-diabetic, and antidepressant activities is of significant interest for human health. Salicornia arabica has been used in the treatment and prevention of several cardiovascular diseases and cancers. This study aims to analyze the chemical composition and assess the antioxidant activity of Salicornia arabica. Samples were collected from the "Salines" region in the department of Annaba (North-East of Algeria). Phytochemical screening revealed the presence of various secondary metabolites, including quinones, tannins, and flavonoids. The results demonstrated the presence of polyphenols and flavonoids, with respective concentrations of 24.83 ± 0.024 µg EAG/mg DW and 42.23 ± 0.019 µg EQ/mg DW. The antioxidant activity, assessed using the DPPH assay, showed an $IC_{50}$ value of 243.72 ± 0.0018 µg/mL for the methanolic extract. This work provides a preliminary contribution that may support further research on a broader range of medicinal plants.

**Keywords:** Salicornia arabica, antioxidant activity, phenols, flavonoids.

**Poster communication** **P-098**

# Comparative analysis of morphological, phytochemical content, and antioxidant activity of Algerian bee pollen

AGABI Rania[1] , KADRI Nabil[1,2] , BOUNCER_MERZOUK Hafida[1] , SALHI Rim[1] , BOUIZAR Roukia1 , ZENATI Abel[1] , BUJOR Oana-Crina[3] , BADULESCU Liliana[3]

[1] *Laboratory of Biomathematics, Biophysics, Biochemistry, and Scientometrics, Department of Food Sciences, Abderrahmane Mira University, Targa Ouzemmour, Bejaia, Algeria.*

[2] *Department of Biological Sciences, Faculty of Natural and Life Sciences and Earth Sciences, University of Bouira, Drissi Yahia Street, Bouira, Algeria.*

[3] *Research Center for Studies of Food Quality and Agricultural Products, University of Agronomic Sciences and Veterinary Medicine of Bucharest, Marasti Blvd. 59, Bucharest, Romania*

**E-mail** : rania.agabi@univ-bejaia.dz ,

**Abstract**

Bee pollen, a widely used dietary supplement known for its curative properties, was investigated in this study through a comparative analysis of its morphological characteristics, phytochemical content, and antioxidant activity. Dehydrated bee pollen samples were collected from Algerian beekeepers and analyzed to explore the variability in color, which facilitated the separation and examination of pollen grains using Scanning Electron Microscopy (SEM). The SEM analysis highlighted distinct morphological differences among pollen grains from various samples, reflecting the diversity of floral sources in different regions. The study measured the total phenolic content, which ranged from 17.34 ± 0.26 mg EAG/g to 24.72 ± 0.08 mg EAG/g, and the total flavonoid content, which varied from 5.95 ± 0.69 mg EQ/g to 12.71 ± 0.93 mg EQ/g. These bioactive compounds are known for their antioxidant properties, which contribute to the health benefits of bee pollen. The antioxidant activity of the samples was assessed through IC50 values, ranging between 0.2015 mg/ml and 0.38 mg/ml, indicating varying degrees of antioxidant potential among the different samples. These findings emphasize the significant potential of bee pollen as a functional food resource, providing essential bioactive compounds for both bee health and human nutrition. Additionally, the results suggest that Algerian bee pollen could serve as a valuable source of natural antioxidants for the nutraceutical and pharmaceutical industries. This comparative analysis contributes to a better understanding of the regional differences in bee pollen composition and highlights its diverse applications in promoting health and wellness. The 1st International Seminar on medicinal chemistry and green chemistry (1st IS MCGC - Annaba 2024)

**Keywords**: Bee pollen, SEM, phenolic compounds, antioxidant activity, phytochemicals, Morphology

The 1st International Seminar on
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**Poster communication** **P-099**

# Isolation and cultivation of Spirulina from cyanobacterial bloom from Lake Oubeira: Optimisation of growth conditions and nutritional potential

Hamel Imene Nesrine[1*], Nasri Hicham[1] , Djemli Samir[2,]

[1]*Department of Marine Sciences, Biodiversity and Ecosystem Pollution Laboratory, Chadli Bendjedid University, El Tarf, Algeria*

[2]*Department of Biology, Applied Neuroendocrinology Laboratory, Badji Mokhtar University, Annaba, Algeria.*

**E-mail:** i.hamel@univ-eltarf.dz*

**Abstract**

As part of my research project, I undertook the isolation and cultivation of Spirulina, a cyanobacterium recognised for its many applications, particularly in the health and food sectors. The species was isolated from cyanobacterial bloom samples taken from Lake Oubeira, a freshwater lake in eastern Algeria, renowned for its biodiversity and classified as a Ramsar site for its ecological importance. The lake is part of the El Kala national park, a protected nature reserve.

The samples were processed to isolate Spirulina, which was then grown in the laboratory under controlled conditions. The culture was carried out at an optimised temperature of 35°C, in a culture medium enriched with nutrients and chemicals specific to the diet of this cyanobacterium. This approach makes it possible to recreate conditions conducive to the rapid, healthy growth of Spirulina.

This study focuses on the environmental conditions that influence the growth of Spirulina and seeks to optimise the culture parameters to maximise its production in the laboratory. The culture medium used, rich in mineral salts, trace elements and organic compounds, has been carefully selected to provide this cyanobacterium with the nutrients it needs for its development.

Spirulina is widely recognised for its health benefits, particularly as a superfood. It is extremely rich in protein, containing all the essential amino acids, as well as vitamins (B12, K, etc.), minerals and powerful antioxidants, such as phycocyanine, a pigment with beneficial effects. Because of its high nutritional value, Spirulina is used in various food products and as a nutritional supplement.

My research aims to gain a better understanding of the optimal conditions for growing Spirulina in a controlled environment, while exploring its potential applications in the fields of biotechnology and functional food. The results of this study could also be used to develop large-scale production methods, with a view to exploiting the benefits of Spirulina in the fight against malnutrition and the promotion of human health, while contributing to the conservation of local biodiversity.

**Keywords**: Spirulina, Cyanobacteria, Bloom, Lake Oubeira, Functional feeding.

**Poster communication** **P-100**

# Phytochemical study and evaluation in vitro of antioxidant activity of the endemic plant vicia onobrychioides (FABACEAE).

Zina ALLAOUA[1], Fatima BELAHSSINI[1], khaled ben elwalid MAHDADI[1], Imane BENABDELAZIZ[1], Haba HAMADA[1].

[1]*Laboratoire de Chimie et Chimie de l'Environnement (L.C.C.E), Département de Chimie, Faculté des Sciences, Université de Batna 1, Algérie*

**E-mail :** zina.allaoua@univ-batna.dz

**Abstract**

The genus Vicia is one of the important genera of the Fabaceae family, the third largest family of flowering plants after Orchidaceae and Asteraceae. In Algeria, the genus Vicia is represented by 83 spaces, and it is commonly used as fodder for animals. Grains of this type are very rich in protein and widely used in cooking. Phytochemical studies have shown the richness of genera of this plant in secondary metabolites with interesting biological activities such as polyphenols, flavonoids and saponins. Moreover, that it has remarkable antioxidant biological activity.

The present work focuses on the phytochemical study and evaluation of the antioxidant activity of hydro-alcoholic extract from the aerial parts of Vicia onobrychioides.

Phytochemical screening of the extract using different qualitative tests; led us to find that this plant is very rich in secondary metabolites, especially flavonoids and polyphenols. The determination of total polyphenols and flavonoids in the same extract using spectrophotometric determination methods; proved that the plant is very rich in compounds.

In addition, we tried to estimate the in vitro antioxidant potential on the hydro-alcoholic extract. This estimate was made by two methods: trapping of the free radical DPPH and reduction of ferric iron by FRAP test, the plant shows remarkable and interesting antioxidant activity.

In conclusion, these remarkable results encourage us to complete the phytochemical and biological study by purifying and knowing the chemical composition of these compounds and testing their biological importance.

**Key Words**: Fabaceae, Vicia, polyphenols, biological activity, antioxidant activity, Vicia onobrychioides.

**Poster communication** **P-101**

# Étude de la qualité d'un sérum cosmétique à base de réglisse : Evaluation de ses caractéristiques physico-chimiques et de ses activités biologiques en vue d'une approbation pour ses effets anti-âge et éclaircissant.

Karima DJELLOUL, MOKRANI, Radia DJELLOUL, HAOULI Khaoula, Mohamed Lotfi SOUICI,
Hamza HADDAG, Imen TOUHAMI, ZERNIZ Nawel

*Laboratoire Ecologie Fonctionnelle et Evolutive, Université Chadli Bendjedid El Tarf (Algérie)*

**E-mail:** djelloul-karima@univ-eltarf.dz

**Résumé**

Ce travail consiste en la préparation d'un sérum anti tache, à base de la racine de Glycyrrhiza glabra L

Cette préparation nous a conduits à l'étude de caractérisation organoleptique, physicochimiques, suivi d'une activité biologique « activité antioxydante et le suivi biologique de l'activité anti inflammatoire »

Le dosage colorimétrique de Folin-Ciocalteu nous a permis d'avoir une idée sur les variations qualitatives des composés phénoliques précisément les polyphénols totaux élevées, avec une teneur 85.78 ± 1.02 mg EAG /mg.

L'étude de l'activité anti-oxydante a montré que l'extrait méthanolique de la poudre de réglisse est riche en antioxydant lui donnant une efficacité contre le radical DPPH. à laquelle l'inhibition de l'activité anti-oxydante est de 50%.

Par ailleurs, l'extrait méthanolique obtenu à partir de la poudre de réglisse présente une activité anti-inflammatoire légèrement supérieure à celle du diclofénac. Par exemple, à une concentration de 200µg/ml, l'activité anti-inflammatoire de l'extrait méthalonique est de 96,35 ± 0,84, tandis que celle du diclofénac est de 94,17 ± 0,42.

Ces résultats sont encourageants afin d'approfondir l'étude de la qualité du sérum dans le but de pouvoir la commercialiser.

**Mots-clés :** Sérum anti tache, glycyrrhiza glabra ; Romarin, propriétés physico-chimiques, activité antioxydante, activité inflammatoire.

**Poster communication** **P-102**

# GC-MS analysis of bio-active compounds in hydro-methanolic extract of Ceratonia Siliqua fruits and their antioxidant potential

Hanane Boutennoun [1,2], Ghania Bourzama[3], Lilia Boussouf[2,4], NassimaBalli[1,5], LilaBoulekbache-Makhlouf[2,], Khodir Madani[2,6]

[1] *Department of Molecular and Cell Biology, Faculty of Nature and Life Sciences, University of Jijel, 18000 Jijel, Algeria*

[2] *Laboratory of Biomathematics, Biophysics, Biochemistry and Scientometry (L3BS), Faculty of Natural and Life Sciences, University of Bejaia, 06000 Bejaia, Algeria*

[3]*Badji Mokhtar University, Annaba, Faculty of Sciences, Department of Biochemistry, Laboratory of Biochemistry and Environmental Toxicology, 23000, Annaba, Algeria*

[4] *Department of Applied Microbiology and Food Sciences, Faculty of Nature and Life Sciences, University of Jijel, 18000 Jijel, Algeria*

[5]*Laboratory of Biotechnology, Environment and Health, Faculty of Nature and Life Sciences, University of Jijel, 18000 Jijel, Algeria*

[6] *Agri-Food Technologies Research Center, Targua Ouzemmour Road, 06000 Bejaia, Algeria*

**E-mail** : biologiehanane@yahoo.fr

**Abstract**

The bioactive components of Ceratonia Siliqua fruits have been evaluated using GC/MS. The chemical compositions of C. Siliqua fruits and fruits were investigated using Gas Chromatography–Mass Spectrometry, while the mass spectra of the compounds found in the extract was matched by the National Institute of Standards and Technology (NIST) library. GC/MS analysis of ethanolic extract of C. Siliqua fruits revealed the existence of oleic acid as major constituent. The qualitative analysis of ethanolic extract of C. Siliqua fruits showed that tannin, saponin, flavonoids, terpenoids, carbohydrate and phenols present in the extract. The quantitative determination of C. Siliqua fruits showed that extract is rich in polyphenols and flavonoid (45.597±2.203 mg EAG/gEB and 12.46±2.235mg EQ/g EB respectively). This study demonstrated that extract exhibited high free radical scavenging activity as showed by the low IC50 values for DPPH and for H2O2 scavenging assays. The results of this study offer a platform of using C. Siliqua fruits an herbal alternative for various diseases.

**Keywords**: Ceratonia Siliqua, bioactive compounds, GC MS, antioxidant effect.

**Poster communication** **P-103**

# Optimisation de l'extraction des composés phénoliques de Rosmarinus officinalis par l'utilisation de la méthode des surfaces de réponse.

Guibadj Fatma Zohra., Boukhalkhal Sarah., Benguechoua Imene Mebarka., Yousfi Mohamed.

*Université Ammar Telidji Laghouat*
*Laboratoire de Sciences Fondamentales (LSF), Université Ammar Telidji Laghouat- Algérie*

**E-mail** : fz.guibadj@lagh-univ.dz

**Résumé**

Les plantes aromatiques constituent une alternative thérapeutique très importante, par ce qu'elles sont capables de produire de nombreuses molécules bioactives appartenant à différentes familles chimiques largement exploitées en médecine.

Le romarin. Rosmarinus Officinalis, est une plante aromatique très répondue dans notre pays et largement utilisée en médicine traditionnelle. Beaucoup d'études ont été consacrées sur les composés des métabolites secondaires de cette plante notamment les huiles essentielles.

Dans cette étude, nous nous sommes intéressés à déterminer les conditions optimales de l'extraction des composés phénoliques en utilisant la méthode des surfaces de réponse par le plan d'expérience de Box-Behenken. L'optimisation est faite par la détermination des trois paramètres (temps, température et le rapport masse de la matière végétale/volume du solvant) afin d'obtenir la meilleure teneur en composés phénoliques totaux. Les résultats indiquent que les valeurs optimales de ces paramètres sont: t =30 min, T = 45° C et V = 50 ml, et que la valeur de la teneur en composés phénoliques est égale à 54,17 mg EAG/g MS.

Ces résultats montrent que le romarin est riche en composés phénoliques connus par leur activité antioxydante, ce qui encourage à l'exploiter en industrie agro-alimentaire.

**Mots-clés :** Rosmarinus Officinalis, composés phénoliques, surface de réponse, Box-Behenken.

**Poster communication** **P-104**

# Valorisation du mucilage de Malva sylvestris L. : extraction, propriétés et applications potentielles

Mohamed Fekhar, Meriem Kamilia Gasmi, Yasmina Daghbouche *, Naima Bouzidi,

Mohamed El Hattab

*Laboratoire de Chimie des Substances Naturelles et de BioMolécules (LCSN-BioM)*

**E-mail:** ydaghbouche@yahoo.fr

**Resumé**

Cette étude a exploré le potentiel du mucilage extrait des feuilles de Malva sylvestris L. comme alternative naturelle et durable aux agents chimiques synthétiques couramment utilisés dans les formulations alimentaires, cosmétiques et pharmaceutiques. Trois méthodes d'extraction (conventionnelle, par ultrasons et par micro-ondes) ont été comparées afin d'optimiser le rendement et la qualité du mucilage.

L'analyse spectroscopique IR-TF a permis d'identifier les principaux groupements fonctionnels du mucilage et de mettre en évidence l'influence des différentes méthodes d'extraction sur sa composition chimique, tout en permettant de prédire la teneur en mucilage dans la plante sans traitement préalable des échantillons. La présence de polysaccharides, notamment le galactose, l'arabinose et le rhamnose, a été confirmée par chromatographie sur couche mince.

Une analyse approfondie des propriétés physico-chimiques, biologiques et fonctionnelles du mucilage ont été évaluées. Les propriétés fonctionnelles, comme la capacité et la stabilité d'émulsion et de mousse, se sont révélées croissantes avec l'augmentation de la concentration en mucilage.

Malgré une activité antioxydante modérée ($CI_{50}$ de 1,45 mg/mL), aucune activité antibactérienne n'a été détectée. Toutefois, les tests microbiologiques ont confirmé l'absence de micro-organismes pathogènes.

Enfin, l'utilisation du mucilage comme émulsifiant dans la formulation d'une crème hydratante a montré des résultats satisfaisants en termes de stabilité du produit final, offrant ainsi de nouvelles perspectives pour le développement de produits cosmétiques naturels et performants.

**Mots-clés**: Malva sylvestris L, mucilage, extraction, spectroscopie IR-TF, propriétés fonctionnelles, crème hydratante.

**Poster communication** **P-105**

# Etude comparative de l'activité antioxydante de l'huile essentielle de Cinnamomum Zeylanicum avant et après son immobilisation par adsorption sur un matériau naturel (argile)

Smain SABOUR[1,2*], Mohamed Reda ZAHI [1], Nadia NEDJARI, Wissam AISSANI, Mohamed EL HATTAB [1]

[1] *Département de chimie, Laboratoire de chimie des produits naturels et biomolécules, Université Blida-1, Algérie*

[2] *Département de Technologie, Laboratoire Chimie Physique des Interfaces des Matériaux Appliqués à l'Environnement, Université Blida-1, Algérie*

**E-mail** : sabour.smain@gmail.com

**Resumé**

L'étude des huiles essentielles et de leurs composés bioactifs, a suscité un intérêt croissant auprès des secteurs pharmaceutiques et agroalimentaires. En effet l'utilisation de ces additifs naturels (très connus par leurs activités biologiques) a pour objectifs d'assurer la sécurité, de maintenir et/ou d'améliore les propriétés sensorielles des produits de consommation. Toutefois leur faible stabilité au stockage, leur grande sensibilité à l'oxydation, et leur forte volatilité, présentent de vrais obstacles pour leur développement industriel

Pour surmonter ces problèmes, notre travail consiste premièrement à l'extraction de l'huile essentielle de Cinnamomum Zeylanicum par entrainement à la vapeur d'eau. Après la caractérisation physico-chimique de l'huile et l'étude de son activité antioxydante vis-à-vis le radical libre DPPH°, notre étude s'est portée sur l'immobilisation (adsorption) de l'huile essentielle de Cinnamomum Zeylanicum, sur un matériau naturel très abondant dans la nature (argile), dans le but d'une part de la protéger contre la dégradation physico-chimique (oxydation), induite par son exposition à l'oxygène, à la lumière, à l'humidité et la température, et d'autre part de contrôler sa libération dans un environnement approprié. Les résultats trouvés indiquent :

1- Une capacité puissante de l'huile à neutraliser les radicaux libres DPPH ($IC_{50}$ = 1.4mg/ml).
2- l'huile de Cinnamomum Zylanicuma a été adsorbée sur l'argile avec un rendement égale à 23% (adsorption compétitive avec l'éthanol)
3- La cinétique de désorption de l'huile, montre sa libération facile dans le milieu réactionnel (t = 24 heures).

**Mots-clés**: huile essentielle, Cinnamomum Zylanicuma, argile, adsorption et relargage, activité antioxydante.

**Poster communication** **P-106**

# Des édulcorants naturels pour un avenir durable : Eco-extraction et purification des glycosides de stéviol à partir de Stevia rebaudiana.

KHETTAR Filicia[1], ASMANI Katia Louiza[1], RADJA Lydia[1], BERKOUD Moussa[1], ACHAT Yasmine[2], LEFSIH Khalef[1,2].

[1] *Laboratoire d'écologie, Biotechnologie et Santé, Université Mouloud Mammeri de Tizi-ouzou.*
[2] *Laboratoire de Biomathématiques, Biophysique, Biochimie et Scientométrie, Université de Bejaia.*

**E-mail** : filicia.khettar@ummto.dz

**Resumé**

À l'ère de la recherche de solutions naturelles pour améliorer notre alimentation, les glycosides de stéviol se distinguent comme une alternative remarquable aux édulcorants synthétiques. Ces composés, extraits de la plante Stevia rebaudiana (Bertoni), offrent un pouvoir sucrant exceptionnel 200 à 300 fois supérieur au saccharose, tout en étant exempts de calories, ce qui augmente leur intérêt dans l'industrie agroalimentaire et les secteurs liés à la santé. En plus de leur capacité à remplacer le sucre, les glycosides de stéviol possèdent des propriétés bénéfiques pour la santé, notamment des effets antioxydants, anti-inflammatoires, et antidiabétiques, ce qui en fait des candidats prometteurs pour des applications thérapeutiques. Dans ce contexte, cette étude porte sur l'extraction écologique de ces glycosides à partir des feuilles de Stevia rebaudiana cultivée en Algérie. Pour ce faire, un protocole d'extraction verte optimisé, considéré comme une approche plus respectueuse de l'environnement, a été réalisé, suivi d'une purification par recristallisation par un antisolvant. En outre, l'efficacité du procédé a été évaluée par une caractérisation des composés extraits à l'aide de la spectroscopie infrarouge à transformée de Fourier (FTIR), afin de confirmer la présence des groupements fonctionnels caractéristiques des glycosides de stéviol. Les résultats préliminaires ont révélé la présence de plusieurs groupes fonctionnels, notamment les groupes hydroxyle (-OH), carbonyle (C=O), méthyle ($-CH_3$), ainsi que des liaisons éther (C-O-C) et des liaisons carbone-carbone insaturées (C=C). Ces résultats confirment l'efficacité de cette approche pour isoler les composés d'intérêt. Des travaux supplémentaires sont prévus pour évaluer les activités biologiques de cet extrait dans le cadre d'une application médicale ou para-pharmaceutique. Ces recherches s'inscrivent dans une démarche de valorisation des ressources locales pour répondre à des besoins globaux de santé et de nutrition.

**Mots-clés**: Stevia rebaudiana, Glycosides de stéviol, Extraction verte, Recristallisation, FTIR.

**Poster communication** **P-107**

# GC-MS profiling of volatile fractions of aqueous extracts from aerial parts of Cytisus villosus Pourr.

Ait-kaci Aourahoun K.[1,2*] et Fazouane F.[2]

[1]*Research Laboratory on Biodiversity, Biotechnology, Environment and Sustainable Development, Faculty of Sciences, M'Hamed Bougara University, Boumerdes, Algeria.*
[2]*Food Technology Laboratory, Faculty of Technology, M'Hamed Bougara University, Boumerdes, Algeria.*

**E-mail**: k.aitkaci@univ-boumerdes.dz

**Abstract**

The volatile fraction of aqueous extracts of plants is of great importance because of its wide applications in aromatherapy, pharmaceuticals, perfumes and chemical ecology. In this work, the possible presence of valuable volatile components in the aqueous extracts of the medicinal leguminous shrub Cytisus villosus, was evaluated by GC-MS analysis. The presence of 26 compounds were revealed in leave volatile fraction obtained with ethyl acetate-hexane solvent, with palmitic acid (7,54 %) and 9,12,15-Octadecatrien-1-ol, (Z,Z,Z)- (5,85 %), as major compounds. Among the 12 components identified in the flower diethylether-hexane fraction, linoleic (26,2%) and palmitic (22,15%) fatty acids were predominant ones. Both volatile fractions showed the presence of some interesting compounds such as antioxydants Tyrosol and BHT in addition to dihydroactiniodiolide with acetylcholinesterase inhibitory activity. Hence, the presence of such phytochemicals could justify the phytotherapeutic use of C. villosus.

**Keywords**: Cytisus villosus, aqueous extract, volatiles, GC-MS.

**Poster communication** **P-108**

# High liquide chromatography analysis, antimicrobial and antioxidant properties of Melissa officinalis L extracts

Fahima ABDELLATIF[1], Dahmane DAHMANE[1], Kawther ABBADENI[1]

[1]*Laboratoire de Recherche sur les Produits Bioactifs et la Valorisation de la Biomasse, Ecole Normale Supérieure Kouba, Alger, Algérie. B.P. 92, Kouba Alger, Algérie*

**E-mail** : Fahima.abdellatif@g.ens–kouba.dz

**Abstract**

In order to enhance natural products value, Melissa officinalis (lemon balm) aerial part (leaves) has been studied in this work. Hence, the objective of this study is to determine the chemical composition of the studied plant polyphenols extracts using. HPLC/DAD, as well as evaluate their flavonoid extracts' antioxidant and antimicrobial activities using DPPH• and disk diffusion methods, respectively. The results of phenols chemical composition showed the existence of two phenolic acids, five flavonic aglycones and six heterosides, while the biologic results of the plant flavonoid extracts exhibited the existence of a good antioxidant and antimicrobial activities.

**Keywords**: Melissa officinalis, Flavonoids, HPLC/DAD, Solvent extraction, Antioxidant, Antimicrobial activities, DPPH test.

**Poster communication** **P-109**

# Composition chimique et activité antioxidante de l'huile essentielle de Mentha spicata

Kawther ABBADENI[1], Fahima ABDELLATIF[1], Mohammed ABDELHADI[1], Dahmane DAHMANE[1]

*Laboratoire de Recherche sur les Produits Bioactifs et la Valorisation de la Biomasse, Ecole Normale Supérieure Kouba, Alger, Algérie. B.P. 92, Kouba Alger, Algér*

**E-mail** : kawthar.abadni19@g.ens-kouba.dz

**Résumé**

Depuis des milliers d'années, les plantes médicinales ont joué un rôle crucial dans la recherche pharmaceutique et le développement de médicaments. Afin de mettre en avant les plantes médicinales Algériennes, nous avons travaillé sur la Menthe (Mentha spicata). La menthe est utilisée pour réduire les douleurs, les nausées et la diarrhée. Des échantillons de la partie aérienne de M. spicata algérienne ont été récoltés en printemps 2021. Huile essentielle de M. spicata a été extraite par hydrodistillation en mode Clevenger pendant 4 heures. Pour identifier divers composants, nous avons analysé l'huile essentielle par la chromatographie en phase gazeuse, ainsi que la chromatographie en phase gazeuse couplée à la spectrométrie de masse. La $IC_{50}$ de l'huile essentielle de M. spicata a été évaluée en utilisant un test de DPPH pour évaluer son activité antioxidante. Nous avons obtenue un rendement de l'huile essentielle 0,66% (v/m). Les résultats d'analyse chromatographique obtenus est plus de 10 composés chimiques. Le composé principale était le Carvone (61,88 %), les autres composants présents en teneurs appréciables tels que: le limonène (10,37 %), le 1,8-cineole (08,77 %), le β-caryophyllene (02,23%) et le myrcène (01,42%). L'huile essentielle de M. spicata a une activité anti oxidante moyenne. Carvone est le compose majoritaire dans l'huile essentielle de M. spicata. La Carvone est une monocyclique, La molécule de carvone appartient à la famille des terpènes et possède un carbone asymétrique. Elle est utilisée comme arôme, en parfumerie et en aromathérapie.

**Mots-clés:** Mentha spicata, GC-MS, Huile essentielle, Carvone, Activité Antioxidante.

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**Poster communication** **P-111**

# Chemical composition and antibacterial activity of essential oils from Achillea odorata, Satureja vulgare and Origanum vulgare

Lilia Boussouf [1,2], Ghania Bourzama[3], Hanane Boutennoun [2,4], Nassima Balli [4], Lila Boulekbache-Makhlouf [2]

[1]*Mohammed SeddikBenyahia University, Faculty of Nature and Life Sciences, Department of Applied Microbiology and Food Sciences, 1800 Jijel, Algeria*

[2]*University of Abderrahman Mira, Faculty of Nature and Life Sciences, Laboratory of Biomathematics, Biophysics, Biochemistry and Scientometry, 06000 Bejaia, Algeria*

[3]*Badji Mokhtar University, Annaba, Faculty of Sciences, Department of Biochemistry, Laboratory of Biochemistry and Environmental Toxicology, 23000, Annaba, Algeria*

[4]*Mohammed SeddikBenyahia University, Faculty of Nature and Life Sciences, Department of Molecular and cell biology, 1800 Jijel, Algeria*

**E-mail** : boussouflilia@yahoo.fr

**Abstract**

In recent years, the rapid growth in antimicrobial resistance (AMR) has become a global concern. Essential oils derived from plants that include bioactive components with proven antioxidative and antibacterial activities could be a potential solution to arrest this problem. In the present work, the antibacterial activity and the phytochemical composition of Achillea odorata, Satureja vulgare and Origanum vulgare essential oils were investigated. The essential oils obtained by hydrodistillation from leaves were analyzed by GC–MS. The antibacterial activity of these oils has been evaluated against bacterial strains isolated from pathological samples of hospitalized patients using the agar well diffusion method. The GC-MS study revealed the presence of D-menthone (60.14%), Chrysanthenone (15% ) and □-terpinene (36,76 %) as the major compounds for Satureja vulgare, Achillea odorata and Origanum vulgare respectively. The tested essential oils showed variable degrees of antibacterial activity. The leaves essential oil from the three plants has a potential to be used as a natural antibacterial agent.

**Keywords**: Essential oils, Chemical composition, Antibacterial activity.

**Poster communication** **P-112**

# Contribution à l'évaluation de l'activité antioxydante des extraits issus de : Mentha spicata L. et Lavandula stoechas L.

Bouasla Ihcéne[1,2,*] ; Boussaid Aya ; Mokhnache Nour El Houda ; Bouasla Asma[1,3].

[1]*Laboratoire Chimie Organique et Interdisciplinaire (LCOI), Université Mohamed Chérif Messaâdia Souk Ahras.*

[2]*Département de Biochimie, Faculté des Sciences, Université Badji Mokhtar- Annaba.*

[3] *Département de Biologie, Faculté des Sciences de la Nature et de la Vie, Université Mohamed Chérif Messaâdia Souk Ahras.*

**E-mail**: Bouasla.ihcene@gmail.com

**Résumé**

La présente étude a été établie dans le cadre de la contribution à l'évaluation du pouvoir antioxydant des deux espèces qui appartiennent à la famille des Lamiaceae.

Durant la partie expérimentale de notre étude, deux extraits végétaux « extrait pure de la menthe : Mentha spicata L. et l'huile essentielle de la lavande : Lavandula stoechas L. » ont été soumis à des tests in vitro qui visent à évaluer leurs propriétés antioxydante vis-à-vis le radical libre diphényl-1-picry-hydrazyl «test DPPH », la réduction du fer ferrique $Fe^{3+}$ en fer ferreux $Fe^{2+}$ « test FRAP » ainsi que le complexe oxydant phosphomolybdène « test PPM ».

L'évaluation de l'activité antioxydante a mis en valeur le pouvoir anti radicalaire des extraits testés avec des $IC_{50}$ qui varient entre [0,178 « Lavandula stoechas L. » et 1,872 « Mentha spicata L. »].

En conclusion, il s'avère clairement que les deux espèces étudiées peuvent constituer une source naturelle pour les futures études qui s'intéressent à la recherche des nouveaux médicaments pour traiter les maladies liées au stress oxydant

**Mots-clés :** Lavandula stoechas L. ; Mentha spicata L. ; Activité antioxydante ; test DPPH, test FRAP ; test PPM.

**Poster communication** **P-115**

# Phytochemical study of ethanoic extracts from Inula viscosa.L

Rafika BLIDA

*Université Badji- Mokhtar- Annaba, Faculté des sciences, Département de Chimie*
*Laboratoire de synthèse Organique, Modélisation, Optimisation et Procédé chimique*

**E-mail** : blidarafika@yahoo.fr

**Abstract**

Inula viscosa.L is a species belonging to the Asteraceae family. It is native to the Mediterranean basin [1]. This plant is well distributed along the coasts of southern Europe, the Middle East and North Africa , and is very common in northern Algeria [2].

The aim of this study is to qualitatively assess the medicinal plants abandoned in Algeria, and more specifically in the Annaba region.

Inula viscosa.L essential oil, extracted by microwave-assisted hydrodistillation from fresh and dry leaves at two sites, Sidi Amar and Seraidi in Annaba, using water as solvent, is obtained with distinct yields.

The yield of oils obtained from fresh and dry leaves was better with dry leaves (4% and 3.35%), and a comparison of the results from the two sites showed that the Sidi Amar site was richer in essential oil (4% and 3.35%) than the Seraidi site (0.19%-0.01%) and (00%-0.04%).

Phytochemical screening based on specific tests enabled us to characterize the following groups: flavonoids, tannins, coumarins, alkaloids, saponins and glycosides. The presence of these compounds in viscous Inula and the use of extraction solvents of different polarity: water, acetone, ethanol and hexane gave highly variable and very distinct results, according to their content and presence.

**Keywords**: Inula Viscosa. L, essential oil, microwave-assisted hydrodistillation.

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**Poster communication** **P-116**

# Biochemical characterization of an essential oil Laurus nobilis, used as an alternative to chemical pesticides on the larvivorous fish Gambusia affinis

Daas Nesma Abir [1], Chouahda Salima[1]

[1]*University of Badji-Mokhtar, Annaba, Algeria*

**E-mail**: daasnesma@yahoo.com

**Abstract**

The efficacy of essential oils against mosquito larvae has been highlighted, being used as an alternative to chemical insecticides in a vector control program. However, few works demonstrate the side effects of these substances on non-target organisms. This study focuses on the potential side effects of an essential oil of Laurus nobilis, on a culiciphagous fish and reference biological control agent, Gambusia affinis. First, we analyzed the biochemical composition of the essential oil using the gas chromatography technique coupled with mass spectrometry. Then, preliminary acute toxicity tests were carried out (96 hours), with the application of different concentrations of the essential oil (1, 5, 10, 50 mg/L), added to the fish-rearing water of both adult and fry individuals of G. affinis, which were collected within a site considered as relatively healthy: El-Karma (Annaba). Gas chromatography demonstrated the different biochemical compounds of the essential oil, with 1,8-cineole as the main compound. In addition, we recorded no mortality after 96 hours, with no side effects on both fry and female adults, for all the concentrations provided. Our results indicate that this essential oil does not present any danger, and can therefore be used in eradicating mosquitoes with no eventual risk to Gambusia affinis.

**Keywords**: Gambusia affinis, Essential Oil, Laurus nobilis, GC/MS, Chemical composition.

**Poster communication** **P-117**

# Phenolic profile assessment by LC-MS/MS and biological activities of Tunisian Simmondsia chinensis leaves: in vitro and in silico studies

Siwar Soltani[a], Noura Baccouch[a], Thomas Michel[c], Noureddine Allouche[a]

and Hichem Ben Salah[a,*]

[a] *Organic Chemistry Laboratory LR17-ES08 (Natural Substances Team), Faculty of Sciences of Sfax, PB 1171, 3000 Sfax, University of Sfax, Tunisia.*

[b] *Université Côte d'Azur, CNRS, Institut de Chimie de Nice UMR 7272, 06108 Nice, France.*

**E-mail :** hichembensalah9@gmail.com

**Abstract**

The aim of this study was to evaluate the biological activities of Simmondsia chinensis from Tunisia and characterise its bioactive compounds. The methanolic extract showed the highest antioxidant activity and total phenolic content (976.03 GAE/g extract). It also showed significant anti-acetylcholinesterase and antibacterial activity. Ethyl acetate and methanolic extracts showed potent anti-diabetic effects with $IC_{50}$ values of 42 and 40 µg/mL, respectively. HPLC-ESI-MS/MS analyses identified flavonoids and lignans as the major phenolic compounds in the methanolic extract. Molecular docking showed the potential interactions of these major compounds with the target enzymes. Consequently, these findings indicate that S. chinensis is a highly valuable natural resource with potential industrial applications.

**Keywords:** Simmondsia chinensis; HPLC ESI-MS/MS; chemical composition; biological activities; molecular docking study

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**Poster communication** **P-118**

# Extraction optimisée des polysaccharides du marc de café : Une approche phytochimique au service de l'économie circulaire

BenJemaa Mariem[1], BenHadid Feriel[1], Bachkouel Sarra[1], Mejri Nahla[1], Falleh Hanen[1], Hammemi Mejdi[1], Abdennebi-Najar Latifa[2], Ksouri Riadh[1]

[1]*Laboratory of Aromatic and Medicinal Plants, Biotechnology Center of Borj Cedria, BP 901, Hammam-Lif 2050, Tunisia.*

[2]*Centre de Recherche Saint-Antoine (CRSA), Sorbonne University, INSERM UMR_S_938, 75020 Paris, France.*

**E-mail:** mariem.benjemaa@cbbc.rnrt.tn

**Résumé**

Cette étude visait l'optimisation de l'extraction des polysaccharides à partir du marc de café en vue de sa valorisation. Ainsi, deux méthodes d'extraction ont été essayées, à savoir l'extraction par pression et l'extraction par ultrasons. Les polysaccharides obtenus ont fait l'objet d'une comparaison du rendement d'extraction, des caractéristiques physiques et des activités biologiques. Les résultats ont souligné que la méthode d'extraction présente un effet significatif sur le rendu quantitatif, qualitatif et fonctionnel des polysaccharides extraits à partir du marc de café. En effet, l'extraction des polysaccharides par pression a donné un rendement 4 fois plus important que celui obtenu par la méthode par ultrasons. Concernant la composition en monosaccharides, les résultats de l'analyse par CLHP ont montré que les polysaccharides obtenus par les deux méthodes d'extraction ont été composés principalement par les mêmes 3 sucres, mais à différents pourcentages : le pourcentage du glucose a été similaire (6,5%) pour les 2 méthodes, alors que le polysaccharide obtenu par sonication a été plus riche en xylose (12,347%) que celui obtenu par pression (9,437%). La caractérisation physique des polysaccharides étudiés a souligné que la méthode d'extraction des polysaccharides n'a pas d'effets significatifs uniquement sur le pH et la conductivité, alors que la couleur et le potentiel Zeta des polysaccharides ont été influencés. L'étude de la viabilité des macrophages (RAW 264.7) traités par les polysaccharides étudiés a montré une absence de cytotoxicité même à la concentration 400mg/ml. L'évaluation de la capacité des deux polysaccharides à neutraliser le radical DPPH a exhibé une meilleure efficacité du polysaccharide obtenu par pression (91,5%). En conclusion, cette étude met en évidence le potentiel des polysaccharides extraits du marc de café et ouvre la voie à de nouvelles perspectives dans leur utilisation pour leur utilisation dans la promotion de la santé et le développement de produits fonctionnels.

**Mots-clés :** Marc de café, Extraction, Polysaccharides, Caractérisation physique, Activités biologiques.

*Ce travail a été élaboré dans le cadre du projet PRIMA MEDGOAT-2023

**Poster communication** **P-119**

# Contribution to the study of the phytochemical composition, antioxidant and antibacterial activities of Nasturtium officinale

LEMBOUB Chama, BOUCHAHDENE Souheila, BECHEKER Abir, BRAHMIA Safa, MEDJAHED Chaima, MEGUIMI Rim, MERABET Halima, BOUMENDJEL Mahieddine

*Laboratory of Biochemistry and Environmental Toxicology, Faculty of Sciences, Badji Mokhtar Annaba University Algeria*

**E-mail:** chama.88@hotmail.fr

**Abstract**

Nasturtium officinale, commonly known as watercress, is a perennial plant from the Brassicaceae family traditionally used to treat a variety of ailments, including hyperglycemia, hypertension, asthma, cough, inflammation, and cancer. This plant is particularly rich in vitamins C, A, K, E, B6, B2, B9, and B5, alongside essential minerals such as lutein, zeaxanthin, iron, calcium, iodine, folic acid, manganese, magnesium, zinc, copper, phosphorus, and potassium. Composed of 95% water, it also contains proteins, fats, and fibers. This study investigated the chemical composition, antioxidant activity, and antibacterial properties of Nasturtium officinale collected during spring from the Seraïdi region in Annaba department (North-East of Algeria). The results revealed the presence of polyphenols and flavonoids, with concentrations of 43.54 ± 0.031 µg EAG/mg DW and 18.23 ± 0.019 µg EQ/mg DW, respectively. The antioxidant activity, assessed using the DPPH method, showed an $IC_{50}$ value of 347.42 µg/mL for the methanolic extract, with an antiradical activity of 0.0028. Regarding antibacterial activity, the methanolic extract exhibited inhibitory effects against Staphylococcus aureus, with inhibition zones of 4 mm and 5 mm at concentrations of 100 mg/mL and 200 mg/mL, respectively. Against Enterococcus faecalis, inhibition zones were measured at 5 mm for 100 mg/mL and 10 mm for 200 mg/mL. These preliminary findings underscore the significant therapeutic potential of Nasturtium officinale, warranting further research to fully elucidate its health benefits and applications.

**Keywords**: **Nasturtium officinale**, phenols, flavonoids, antioxidant activity, antibacterial activity

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**Poster communication** **P-120**

# Exploring therapeutic potential of Arisarum vulgare via in-Vitro, in-Vivo, and in-Silico biological activities

Zineb Bouafia[1,2], Amel Boudjelal[1,2], Souhila Bouaziz-Terrachet[3,4], Souheila Bouchahdane[5], Mustapha Mounir Bouhenna[6], Ibrahim Demirtas[7]

[1]*Department of Microbiology and Biochemistry, Faculty of Sciences, University of M'sila, Algeria*
[2]*Laboratory of Biology: Applications in Health and Environment, University of M'sila, Algeria*
[3]*Laboratory of Applied Chemistry and Materials, University of Boumerdes, Algeria*
[4]*Laboratoire de Physico-Chimie Théorique et de Chimie Informatique, USTHB, Algeria*
[5]*Department of Biochemistry, Faculty of Sciences, University of Annaba, Algeria*
[6]*Centre de Recherche Scientifique et Technique en Analyses Physico-Chimiques Bou-Ismail, Algeria*
[7]*Department of Biochemistry, Faculty of Science and Art, Igdir University, Igdir, Turkey*

**E-mail:** zineb.bouafia@univ-msila.dz

**Abstract**

Arisarum vulgare O. Targ.Tozz. (Araceae), locally known as "Elbgouga", holds significant traditional importance in Algeria for the treatment of various human ailments, including pain, infections, inflammation, digestive disorders, cancer, skin problems, eczema, wounds, and burns. The aim of this study was to explore for the first time the phytochemical profile, antioxidant, antibacterial, inhibitory effects on acetylcholinesterase (AChE) and butyrylcholinesterase (BChE) enzymes, DNA protection, and capacity to promote wound healing.Preliminary phytochemical experiments were conducted to evaluate the major classes of bioactive compounds, in addition to the total phenol and flavonoid amount in AVEE. An LC-MS/MS analysis was conducted to clarify the phytochemical composition of this particular botanical species. The antioxidant capacity was assessed using DPPH and ABTS radical scavenging tests. The agar diffusion approach was used to ascertain the antibacterial efficacy against four bacteria. Cholinesterase enzyme inhibition was evaluated using a colorimetric method that relies on Ellman's reaction. The protective effects of AVEE on pBR322 plasmid DNA damaged by $H_2O_2$ and UV treatment were assessed by their DNA-breaking forms. The in vivo acute dermal toxicity and wound healing potential of the AVEE ointment (1-5% AVEO) were also investigated, and histological analyses were carried out on biological samples. Five protein targets were the subject of an in silico molecular docking investigation (TNFα, TGFBR1, IL-1ß, GSK-3ß, and NOS) .The screening of phytochemicals revealed a significant concentration of phenolic compounds mainly flavonoids. Three major compounds were identified by LC-MS/MS analysis, belonging mainly to the class of flavonoids, with Rutin as the most abundant compound , followed by Hesperidin . A conspicuous presence of isoquercitrin was also found. Small amounts of flavonoids and phenolic acids were also detected . DPPH assay showed higher antioxidant capacity compared to the ABTS assay. AVEE was effective against all selected bacterial strains; however, the highest zone of inhibition was noted against Enterococcus feacium. The extract of the plant significantly inhibited both AChE and BChE . The ethanolic extract of A. vulgare and Quercetin exhibited more significant DNA protection action in form I, compared to form II. The AVEO formulation may be safely administered by topical application. A statistically significant wound contraction was discovered in the group treated with 5% AVEO compared to the groups that were not treated or treated with petroleum jelly. Furthermore, there was no notable disparity detected between the group treated with 5% AVEO and the group treated with the reference drug. Moreover, the topical application of the formulation improved histological parameters. In silico study showed that rutin, hesperidin, and isoquercetrin had a high affinity to the five main targets that might contribute to the wound healing potential of A. vulgare ethanolic extract. The impressive biological capabilities of A. vulgare indicate that the plant has the ability to be a valuable origin of bioactive chemicals with various medical applications.

**Keywords**:Arisarum vulgare; LC-MS/MS analysis; antioxidant activity; antibacterial potential; DNA protection; acute dermal toxicity; wound-healing properties; in silico.

**Poster communication** **P-121**

# Effet répulsif des huiles essentielles du Pelargonium graveolens contre les moustiques

Samia Alem[1*], Karima Alem[2], Nazih Ribouh[3], Youssouf Driouche[4], and Zihad Bouslama[1,4]

[1]*Laboratory of Aquatic and Terrestrial Ecology, Department of Biology, Faculty of Sciences, Badji Mokhtar University, BP. 12, Annaba, Algeria*

[2]*Laboratory of Biochemistry and Environmental Toxicology, Department of Biochemistry, Faculty of Sciences, Badji Mokhtar University, BP.12 , Annaba, Algeria.*

[3]*Laboratary Nanomaterials for corrosion and surface treatment, Department of Chemistry, Faculty of Sciences, Badji Mokhtar University, BP. 12, Annaba, Algeria*

[4]*Environmental Research Center, Alzon, BP.72 A, Menadia, Annaba, Algeria*

**E-mail** : samia.alem@univ-annaba.dz

**Resumé**

Environ 17% des maladies infectieuses au niveau mondial sont provoquées par différents vecteurs comme les moustiques, les tiques et d'autres.

L'usage massif des insecticides chimiques contre ces insects a provoqué d'énormes perturbations de l'environnement notamment la toxicité sur la santé humaine et les autres organismes non cible ; ce qui nécessite de développer de nouvelles stratégies de contrôle plus efficaces.

Le recours à des ressources naturelles d'origine végétale à activité répulsive à base d'huiles essentielles représente une alternative respectueuse de l'environnement.

L'objectif de ce travail est l'évaluation de l'effet répulsif de faible concentrations des HEs afin de déterminer la concentration optimale à utiliser pour la synthèse d'un répulsif contre les moustiques.

Les HEs des feuilles du Pelargonium graveolens ont été extraites par hydrodistillation puis ont été analysées par la CPG-SM afin de les tester contre les moustiques.

37 composés ont été déterminé dont les majoritaires sont citronellol (43.27 %), Geraniol (16.3%), α-pinene (4.58%)

Les résultats des essais suggèrent que les concentrations de 1 %, 1,25 % et 1,50 % ont permis d'obtenir un effet répulsif optimal pendant les 15 premières minutes suite à l'application des HEs et que le temps de protection augmente avec l'augmentation de la concentration de l'HE.

**Mots-clés** : Huiles essentielles, plante aromatique, effet répulsif, CPG-SM, moustique

**Poster communication** **P-122**

# Green extraction of Aloe brevifolia polysaccharides: A biotechnological solution for sustainable applications.

RADJA Lydia[1], LEFSIH Khalef[1,2], BERKOUD Moussa[1], KHETTAR Filicia[1], ZERROUKI Taous[1], LAZRI Aziza[1]; ACHAT Yasmine[2]

[1]*Laboratory of Ecology, Biotechnology and Health, Mouloud Mammeri University of Tizi ouzou*
[2]*Laboratory Biomathematics Biophysics Biochemistry and Scientometry, university of Bejaia*

**E-mail**: lydia.radja@ummto.dz.

**Abstract**

Aloe brevifolia, a succulent plant widely used in traditional medicine, is known for its therapeutic properties, including antioxidant, anti-inflammatory, and anticancer effects. This study focuses on the green extraction, purification, and characterization of polysaccharides from this plant, as well as the evaluation of their antioxidant activity. The extraction of polysaccharides was carried out using a solid-liquid method, followed by purification through the eco-friendly three-phase partitioning (TPP) technique, which minimizes the use of harmful solvents. The obtained polysaccharides were characterized by Fourier Transform Infrared (FTIR) spectroscopy, which revealed the presence of esterified pectins. The TPP method proved particularly effective in enhancing the purity of the polysaccharides by significantly reducing protein content. The monosaccharide composition of the polysaccharides was further confirmed using Thin Layer Chromatography (TLC), demonstrating the presence of rhamnose and galacturonic acid**.** The antioxidant activity of the purified polysaccharides was measured using the DPPH assay, a commonly used method to evaluate the free radical scavenging capacity. The results showed that the polysaccharides from Aloe brevifolia exhibit significant antioxidant activity, with a free radical reduction percentage of 30.47%, compared to 9.20% for ascorbic acid, used as a positive control. This marked antioxidant activity is attributed to the presence of acemannan, an acetylated polysaccharide abundant in Aloe brevifolia, known for its potent antioxidant effects. These findings support the idea that Aloe brevifolia could be a valuable source of natural bioactive compounds, suitable for use in the pharmaceutical and cosmetic industries. The high sugar content and low protein content further highlight the potential of this plant in the development of innovative therapeutic and cosmetic products.

**Keywords**: Aloe brevifolia, polysaccharides, green extraction, FTIR, antioxidant activity.

**Poster communication** **P-123**

# Medicinal interest of Algerian Pinus halepensis resin

Meriem NASRI, Imene BAKHOUCHE , Hanane ABED

*Laboratory of Health and Environment, Faculty SNV-TU, University Bordj Bou Arreridj 34000, Algeria.*

**E-mail** : meriem.nasri@univ-bba.dz

**Abstract**

Pinus halepensis resin known under the vernacular name "Elk el Snober" is one of the plant substances that has many biological properties, widely used in traditional Algerian medicine as a treatment for various diseases. The present study aims to estimate the content of polyphenols and flavonoids and the evaluation of the antioxidant and anti-inflammatory activity of the aqueous extract of Aleppo pine resin. The content of total polyphenols is 103.457 ± 0.765 µg EAG/mg of dry extract. The flavonoid content is 23.524 ± 0.143 µg EQ/mg dry extract. The antioxidant effect of the aqueous extract of Aleppo pine resin tested in vitro using the DPPH test, shows that this extract has a strong DPPH radical scavenger activity. The extract showed antioxidant activity with $IC_{50}$ of 0.347 ± 0.156mg/ml. The anti-inflammatory activity was evaluated by the protein denaturation inhibition test of ovalbumin, which revealed a significant inhibition of protein denaturation. In conclusion, Aleppo pine resin could be a potential source of the compounds bioactives with antioxidant and anti-inflammatory potential.

**Keywords**: Resin, Pinus halepensis, Polyphenols, Flavonoids, Antioxidant, DPPH, Anti-inflammatory activity.

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**Poster communication** **P-124**

# Chemical profiling, antioxidant activity, and fungitoxic potential of essential oils against food-contaminating fungi

Yamina Ben Miri [1] and Amina Benabdallah [2]

[1]*Department of Biochemistry and Microbiology, Faculty of Sciences, Mohamed Boudiaf University, BP 166 M'sila, 28000, M'sila, Algeria.*

[2] *Laboratory on Biodiversity and Ecosystem Pollution, Faculty of Life and Nature Sciences. University Chadli Bendjedid, El-Tarf, 36000, Algeria .*

**E-mail :** yamina.benmiri@univ-msila.dz

**Abstract**

This study examines the chemical composition and bioactive properties of essential oils (EOs) extracted from Mentha pulegium, Myrtus communis, and Mentha piperita, focusing on their antioxidant and antifungal activities. Gas chromatography-mass spectrometry (GC-MS) analysis identified the major volatile constituents of each EO. M. pulegium EO was characterized by high levels of pulegone (60.82%) and 5-methyl-2-(-1-methylethyl)-cycloxanone (14.27%). M. communis EO was predominantly composed of α-pinene (46.7%) and 1,8-cineole (22.0%), which together constituted 98.3% of the oil. M. piperita EO contained menthol (40.0%), 1,8-cineole (26.0%), and menthone (25.0%), accounting for 97.0% of its composition. The antioxidant activity of these EOs, assessed using the DPPH radical scavenging assay and expressed as $IC_{50}$ values, revealed that M. communis EO exhibited the highest antioxidant potential ($IC_{50}$ = 3.27 µL/mL), followed by M. piperita ($IC_{50}$ = 3.97 µL/mL) and M. pulegium ($IC_{50}$ = 4.31 µL/mL). These values were compared to the synthetic antioxidant butylated hydroxytoluene (BHT), which had an $IC_{50}$ of 2.66 µL/mL. The antifungal activity was evaluated against various foodborne fungi, including Aspergillus niger, A. ochraceus, A. terreus, A. carbonarius, A. fumigatus, Fusarium sp., Penicillium verrucosum, Alternaria sp., and Mucor sp., by determining the minimum inhibitory concentration (MIC) and minimum fungicidal concentration (MFC) using liquid PDB medium. M. pulegium EO demonstrated strong antifungal activity, with MIC values ranging from 2.00 to 3.83 µL/mL and MFC values from 2.33 to 3.83 µL/mL. M. communis EO showed MIC values between 2.00 and 4.00 µL/mL and MFC values from 2.33 to 4.00 µL/mL. M. piperita EO had MIC values ranging from 2.33 to 3.83 µL/mL and MFC values between 2.50 and 4.00 µL/mL. Notably, M. pulegium was particularly effective against A. terreus (MIC = 2.00 µL/mL, MFC = 2.50 µL/mL), while M. piperita demonstrated strong efficacy against A. carbonarius (MIC = 2.66 µL/mL, MFC = 2.83 µL/mL). These results highlight the potential of these EOs as natural antioxidants and antifungal agents, providing eco-friendly alternatives for food preservation.

**Keywords:** Essential oils, GC-MS analysis, antioxidant activity, antifungal activity.

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**Poster communication** **P-125**

# Etude phytochimique qualitative et quantitative Et analyse chimique Par chromatographie à haute performance des extraits d'Adiantum capillus-veneris (plante Algérienne)

Fadhela BOUKADA[1*], Sara SITAYEB[1], Fatima Zohra SOLTANI[1]

[1] *Laboratoire de Bioconversion Génie Microbiologie et Sécurité Sanitaire (LBGMSS), Faculté Science De La Nature Et De Vie, Université de Mustapha Stambouli, Mascara.*

**E-mail** : fadelaboukada6@gmail.com

**Résumé**

L'étude a été réalisée sur la partie aérienne d'Adiantum capillus-veneris (capillaire). Dans un premier temps, on a procédé à une étude phytochimique qualitative et quantitative afin de caractériser les grands groupes chimiques existés dans la plante par des tests de caractérisation chimiques puis on a réalisé une extraction des flavonoides suivie par une analyse chromatographique (HPLC). Les extraits soumis à l'étude phytochimique qualilative sont des extraits methanoliques, chloroformiques et aqueux. L'analyse phytochimique sommaire est réalisée sur la base des tests de coloration caractéristiques en vue de mettre en évidence les grands groupes chimiques. En plus, on a réalisé une étude phytochimique quantitatif des métabolites primaires et secondaires. Après extraction des flavonoides, 4 fractions obtenues qui sont soumises à une identification chimique par chromatographie à haute performance (HPLC-DAD-ESI-MS).

L'analyse phytochimique qualitative a révélé les alcaloïdes sels et bases, les polyterpènes, les flavones aglycones, les huiles volatils, les acides gras, les tanins catéchiques, les glycosides cardiaques, les flavonoïdes, les composés réducteurs, les hétérosides stéroliques et terpéniques, les acides aminés et les saponosides sont des classes de familles chimiques présentes dans la plante étudiées.

L'analyse phytochimique quantitative montre que le capillaire renferme plus d'eau, sa MS étant de 56.21±1.01 % et un taux relativement élevé en matière organique et minérale (77.44 ± 1.32 %, 22.86 ± 0.51 %). La plante présente un bon potentiel nutritif où le taux des protéines est de 19.01 ± 0.98 %. Le dosage des lipides et des sucres montre qu'A. iva présente des teneurs faibles. Les teneurs élevées des flavonoides, alcaloides, saponosides et en tanins révèlent que cette plante a des vertus thérapeutiques. Les principaux composants identifiés par HPLC sont Quercetine 3-O-glucoside (2322 µg/g), dérivé hydroxycinnamique (1413,0 µg/g) et dérivé d'acide ferulique (946,6 µg/g).

L'ensemble des résultats chimique obtenus confirment la valeur nutritionnelle et pharmaceutique d'Adiantum capillus-veneris.

**Mots-clés** : flavonoides, phytochimie, plantes médicinales, HPLC

**Poster communication** **P-126**

# The antibacterial and antioxidant activity of médicinal spieces Atractylis Caespitosa from The M'sila region

TURQUI Tarik [(1)], BENAICHE Ghania [(1)],DEBIH Elhadi [(1)],BENKOUIDER Imen

[1] *Chemistry Department, Research lab, Faculty of Science, University of M'sila.*
[1] *Chemistry Department, Faculty of Science, University M'Hamed Bouguara of Boumerdes, 35000, Algeria*

**E-mail** : tarik.turqui@univ-msila.dz

**Abstract**

The plant kingdom speaks to a critical source of a colossal assortment of bioactive atoms with nemerous benefets utilized within the nouishment industry, cosmetology and pharmacy. Among these compounds, we find comarins, alkaloids, phenolic acids, tannins, terpenes, and flavonoids. Indeed, polyphenols are endowed with multiple therapeutic virtues playing a very imortant role, mainly in thefight against cancer, cardiovascular diseases and lipid peroxidation. The Asteraceae is the large family of dicots and the second-largest family of blossoming plants (as it were, the Orchidaceae has more species). It contains 1,400-1,540 genera and aproximately 20,000-23,000 spacies and has a cosmopolitan distribution. One of these spacies is Atractyli caespitosa Desf. Algeria has one of the foremost diverse and unique greenery within the Mediterranean bowl where it has 3139 spaceies. We noticed the presence of this spacies in the semi-arid region of Hamam Dalaa in M'sila. In this work, we study an antioxidant and antibacterial activities of atractilys caespitosa extract produced by maceration with (methanol/woter) (70/30). Through this study, we have higher the total polyphenol contents are average in the extract of atractylis caespitosa. The antioxidant activity by the DPPH method was more important for the atractylis caespitosa extract, this extract is less active compared to ascorbic acid. The antimicrobial activitiy of the atractylis caespitosa extract were tested against a panel wich included three bacterial species selected as repesentative of *Staphylococcus aureus*, *Escherichia coli*, *Pseudomonas aeruginosas*. The results of the study of antimicrobial activity, carried out by the method of disc and that of dilution on, liquid medium

**Keywords**: Asteraceae, polyphenol, Antioxidant, Antimicrobial.

**Poster communication** **P-127**

# Date palm perianths and spiklets: cytotoxicity and the prebiotic properties in promoting probiotic growth

Nahla MEJRI[1] *, Hanen FALLEH[1], Mariem BEN JEMAA[1], Latifa ABDENNEBI-NAJAR[2], Wided MEGDICHE-KSOURI[1]

[1] *Laboratory of Aromatic and Medicinal Plants, Biotechnology Center of Borj-Cédria BP901 2050 Hammam-Lif, Tunisia*

[2]*Centre de Recherche Saint-Antoine (CRSA), Sorbonne University, INSERM UMR_S_938, 75020 Paris, France*

**E-mail** : nahlamejri@gmail.com

**Abstract**

Due to their prebiotic properties, which stimulate the growth and activity of gut bacteria, plant-derived polysaccharides have drawn a lot of interest recently from the food and pharmaceutical industries. In vitro biological efficiency and prebiotic effects of hydrophilic polysaccharides isolated from date palm perianths and spiklets were the focus of the current study. By employing only water and ethanol as solvents, an environmentally friendly approach was used to extract crude hydrophilic polysaccharides (CHP) from date palm perianths and spiklets. Following extraction crude polysaccharides, biological activity and cytotoxicity were evaluated. Lastly, Bacillus clausii growth was measured in vitro to examine the prebiotic effect of the produced polysaccharides. Different concentrations of crude hydrophilic polysaccharides from date palm by products (1, 2, 5% v/v) were used as carbohydrate source to assess the development of the studied bacteria using its selective but free carbohydrate medium. The growth promotion was assessed through the total viable cell count after 72h of incubation. Therefore, CHP showed no cytotoxicity to macrophages. Regarding the prebiotic effects of polysaccharides, the findings indicated that B. clausii growth was stimulated following a 72-hour incubation period at the three polysaccharide concentrations that were investigated, and that the bacterial population grew with increasing CHP concentrations. When CHP was used as a carbohydrate source by B. clausii, a significant growth effect was seen in the bacterium. According to these results, CHP that has been extracted from date palm by-products is a rich source of bioactive prebiotic that promotes the growth of good bacteria in the gut and has a number of positive effects on gut health.

**Keywords:** Perianth, spiklet, CHP, cytotoxicity and prebiotic effect.

*This work was elaborated under the framework of the PRIMA project “MEDGOAT”

**Poster communication** **P-128**

# Effet du solvant et de la méthode d'extraction sur la teneur en composés phénoliques d'une plante médicinale

Farida ZAKKAD[1], Nadia TOUDERT[2], Noureddine DADDA[1], Chaima ZERRAD[1] et Salah Eddine DJILANI[1]

[1]*LSBO, Université d'Annaba, BP.12, 2300. Annaba, Algérie.*
[2]*LPCM, Université d'El-Tarf , BP.76, 36000. El-Tarf, Algérie.*

**E-mail** : zeghadfarida@yahoo.fr

**Résumé**

L'objectif principal de ce travail est d'effectuer une étude phytochimique de Brassica insularis, une plante endémique Algérienne. Nous avons réalisé le dosage des composés phénoliques dans divers extraits des feuilles (eau distillée, éthanol, méthanol et un mélange méthanol-eau 7/3) par macération classique à froid, les valeurs trouvées ont montré la richesse de cette plante en polyphénols et en flavonoïdes.

En outre, nous avons évalué les teneurs en composés phénoliques et la capacité antioxydante des feuilles en utilisant une macération assistée par ultrasons, en jouant sur deux paramètres : le temps de sonication et le rapport entre la masse de la matière végétale et le volume de solvant. Les meilleurs résultats ont été obtenus avec un ratio de 1 g pour 30 ml de solvant, sur une durée de sonication de 30 minutes.

Les résultats ont démontré que la sonication est une technique très convenable pour extraire les composés phénoliques, avec des teneurs en polyphénols et une activité antioxydante nettement supérieures à celles obtenues par macération classique à froid.

Nous avons également conclu notre étude par une analyse in vivo de l'activité antibactérienne et antifongique de l'extrait méthanolique des feuilles, en utilisant la méthode de diffusion en milieu gélosé (méthode des disques). À l'exception de Staphylococcus aureus, qui a montré une sensibilité modérée, les autres germes se sont révélés résistants ou faiblement sensibles, avec des diamètres d'inhibition variant entre 7 et 13 mm.

**Mots clés :** Brassica insularis – polyphénols – Antibactérienne – DPPH – sonication.

**Poster communication** **P-131**

# Extraction, purification, characterization and antioxidant activity of peel pomegranate polysaccharides.

BERKOUD Moussa[1], LEFSIH Khalef[1,2], RADJA Lydia[1], KHETTAR Filicia[1], TEHARI Imane[1], MEDOUR Dyhia[1]; ACHAT Yasmine[2]

[1]*Laboratory of Ecology, Biotechnology and Health, Mouloud Mammeri University of Tizi ouzou*
[2]*Laboratory Biomathematics Biophysics Biochemistry and Scientometry, university of Bejaia*

**E-mail** : moussa.berkoud@ummto.dz.

**Abstract**

In this research, peels of Punica granatum polysaccharides (PPP) were extracted by the hot-water method and purified using a two-step three-phase partitioning (TPP) procedure. Thus, the recovered PPP is stored in a hermetically sealed bottle for further analyses. Two colorimetric methods were performed to measure the total carbohydrate and protein content of PPP, using phenol-sulfuric acid and Bradford assays, respectively. Thin layer chromatography (TLC) and FTIR spectroscopy are conducted to determine the preliminary structural characterization of PPP. In addition, the antioxidant activity has also been tested by the measurement of the residual DPPH, the ascorbic acid is used as the calibration curve for this purpose. As a result, 25.17% of PPP were collected from the raw material after the extraction and purification procedure. Also, about 96.5% of the total carbohydrates are found in the PPP extract, but only 0.06% represents the protein content. TLC analysis confirm the presence of two main sugars: galacturonic acid and rhamnose. Furthermore, FTIR analysis showed an intense peak at a wavelength of 1404, which can be attributed to symmetrical stretching vibration of (COO-) or deformation vibration of (C-OH) with symmetrical vibrational stretching contribution of the carboxylic acid (O-C-O). These two analytical techniques concluded that the most likely structure of the PPP is a rhamnogalacturonan. On the other hand, the purification efficiency of PPP performed by the TPP method has also been proved. Besides, the percentage of the residual DPPH is of the order of 1/3 of the initial concentration of the PPP extract. Comparing these results to the percentage of residual DPPH obtained for ascorbic acid which is 1/5, it can be concluded that the antioxidant activity of PPP is effective and that it could be an interesting and promising molecule for use in food and pharmaceutical purposes.

**Keywords:** Punica granatum; TPP; TLC; FTIR; Rhamnogalacturonan; Antioxidant activity

**Poster communication** **P-132**

# Phytochemical profile and antioxidant activity of ethyl acetate extract from an Erica plant.

Raounak Gouasmia[1], Fadila Khaldi[1], Noureddine Nasrallah[2].

[1]*Mohamed Cherif Messaadia University, Faculty of Natural and life science, Department of Biology, Laboratory of Sciences and Technology of Water and Environment, Souk Ahras, Algeria;* [2]*USTHB, Faculty of Mechanical Engineering and Process Engineering, Department of Process Engineering, Laboratory of Reaction Engineering, Algiers, Algeria.*

**E-mail** : ra.gouasmia@univ-soukahras.dz

**Abstract**

The aim of the present work is to screen the phytochemical profile of an Erica plant from souk Ahras (Northeastern of Algeria) known traditionally as diuretic, anti-inflammatory and hypolipidemic remedy. and to evaluate some biological activities of ethyl acetate (EtAOc) extract of leaves and flowers.

The phytochemical tests applied to the powders of the plant have shown the presence of some families of chemical compounds in particular: Flavonoids, Tannins, triterpenoids and sterols, and Anthraquinones.

The EtAOc extracts were obtained by Maceration and liquid/liquid extractions and the yields of extraction were given at 0.51% for leaves and 1% for the flowers.

The total phenolic content of the extracts was assessed by using Folin-ciocalteu colorimetric essay and it revealed a content of 184,058 ± 0.064 µg GAE/mg in leaves and a higher concentration in flowers with 223,913 ± 0.06 µg GAE/mg. Then, the antioxidant activity was measured using several methods: DPPH, FRAP and TAC (total antioxidant capacity). The following results reveal that the flowers have the highest antioxidant effect with: IC50 = 62.23 ± 0.71 µg/ml, A0.5 = 121.95 ± 0.035, TAC = 51.6 ± 0.0017 µg EAA/mg and for leaves: IC50 = 62.11 ± 1.002 µg/ml, A0.5 = 357.14 ± 0.0123, TAC = 18,66 ± 0.0014 µg EAA/mg (for DPPH, FRAP and TAC respectively).

**Keywords**: Antioxidant activity; DPPH; FRAP; Phytochemistry; TAC.

The 1st International Seminar on medicinal chemistry and green chemistry (1st IS MCGC - Annaba 2024)

**Poster communication** **P-133**

# Polyphenols from Pistacia Lentiscus L cake: A green valorization of a by-product with a proven bioactivity potential

Toufik OUATMANI[1,2], Leila REZIG[3], Samir HADJAL[2], Najla TRABELSI[4], Meriem MOKHTAR[5], Louiza KOUADRI[2], Rahma MAYOUF[1], Lila BOULEKBACHE-MAKHLOUF[1], Khodir MADANI[1,6], Hayate HADDADI-GUEMGHAR[1]

[1]*Laboratory of Biomathematics, Biophysics, Biochemistry and Scientometrics (L3BS), Faculty of Natural Sciences and Life, University of Bejaia, 06000 Bejaia, Algeria*

[2]*Laboratoiry of Analytical Development, Recherche and Development division, Cevital Agro-Industrie, BP 334 Nouveau Quai Port de Bejaia, 06000 Bejaia, Algeria*

[3]*Laboratory of Protein Engineering and Bioactive Molecules (LIP-MB), National Institute of Applied Sciences and Technology, University of Carthage, LR11ES26, Tunis 1080, Tunisia*

[4]*Laboratory of Olive Biotechnology, Center of Biotechnology of Borj-Cédria, Hammam-Lif, Tunisia*

[5]*Laboratory of Bioeconomy, Food Safety and Health, Faculty of Natural Sciences and Life, University of Abdelhamid Ibn Badis, 27000 Mostaganem, Algeria*

[6]*Research Center in Agri-Food Technology (CRTAA), route de Targa-Ouzemour, 06000 Bejaia, Algeria*

**E-mail**: toufik.ouatmani@univ-bejaia.dz

**Abstract**

Cold pressing of oil from Pistacia Lentiscus. L (Lentisk) berries is a common practice in the Mediterranean area, producing an undervalued by-product rich in bioactive compounds. This work aimed to optimize the green ultrasound-assisted extraction (UAE) of phenolic compounds from the lentisk berry cake (LBC). Box Behnken's design of experiments (BBD) was applied to evaluate the effect of the mixture of ethanol/water, temperature, and time extraction on yields in the LBC total phenolic content. HPLC-DAD was then used to determine the polyphenolic profile of the optimized extract. The latter has also been evaluated for its antioxidant and antidiabetic activities. The predicted conditions of extraction (50% ethanol, 60°C, and 86 min) were experimentally confirmed. Under these conditions, the optimized extract interestingly showed an IC50 of 61.79 ± 0.40 µg/ mL against the free radical ABTS versus Trolox as a positive control (IC50 = 50.67 ± 0.32 µg/mL). Moreover, a promising anti-α-amylase capacity has been shown by the sonicated LBC extract with an IC50 of 99,82 ± 2,03 µg/mL. These in vitro biological activities should be due to the bioactive phenolic composition of the LBC extract. Indeed, twelve phenolic compounds were identified and quantified in the optimized extract, comprising six flavonoids, five phenolic acids, and a phenylethanoid (Tyrosol).

**Keywords**: Pistacia Lentiscus L. cake, ultrasound-assisted extraction, Box Behnken design, phenolic compounds, HPLC-DAD, In vitro biological activities

**Poster communication** **P-134**

# Syzygium Aromaticum (Clove), a protective plant with beneficial effects on oxidative stress parameters in the liver in an experimental asthma model in rats.

Linda Sabrina Ounaceur, Mahfoud Messarah and Amel Boumendjel

*Laboratoire de biochimie et de toxicologie environnementale, Département de Biochimie, Faculté des Sciences, Université Badji Mokhtar Annaba (Algeria).*

**E-mail** : lynda.s.ounaceur@gmail.com

**Abstract**

Oxidative stress is thought to have a role in the development of human diseases such as cancer, cardiovascular disorders and respiratory diseases. Asthma is a disease resulting from chronic inflammation of the airways, and oxidative stress may be involved in its pathogenesis. Indeed, the pathogenesis of asthma involves complex interactions between several cell types and mediators, among the latter, endogenous and exogenous reactive oxygen and nitrogen species. The aim of this study was to confirm the antioxidant protective effect of the plant of the aqueous extract of Syzygium Aromaticum studied. For this purpose, male Wistar rats were sensitized to ovalbumin, in the context of experimental asthma, then treated with the aqueous extract of S.Aromaticum. The biological properties of oxidative stress were evaluated by measuring the non-enzymatic parameters of MDA, GSH, PC and AOPP in the liver. According to the results obtained, there was a statistically significant improvement in oxidative stress markers. In asthmatic rats treated with the aqueous extract of the plant, there was a very significant decrease ($p \leq 0.01$) in the level of MDA (1.07 ± 10.21 nmol/mg prot), a decrease significant ($p \leq 0.05$) of the PC level and the AOPP level compared to asthmatic rats. For the GSH level, there was a recovery evidenced by an increase (0.26 ± 10.15 µmol/mg prot) compared to OVA rats.

Taken as a whole, these results made it possible to highlight the strong anti-oxidant and therefore anti-asthmatic properties of the aqueous extract of clove.

**Keywords:** Aqueous extract, Oxidative stress , Syzygium Aromaticum, Asthma, Liver.

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**Poster communication** **P-135**

# Beneficial effects of crude extract of the Erodium plant on kidney tissue and various biochemical parameters in rats exposed to a triazole fungicide

OUNISSI Ismahan[1], SLIMANI Souheila[1], BOUNASS Jihane [1]

[1] *Laboratory of Interaction Research, Biodiversity, Ecosystems and Biotechnology, Faculty of Science University 20 Août 1955 of Skikda, Algeria.*

**E-mail** : ounissiismahan87@gmail.com

**Abstract**

The need to meet growing food demands has driven increased pesticide use, which can persist in fields and end up in our food due to reduced biodegradation capabilities. This study aims to evaluate, in vivo, the protective role of the crude extract from the aerial part of the Erodium plant against the harmful effects of the triazole fungicide on various biochemical parameters in rats. Triazole fungicide is a common agricultural fungicide known for its toxic and damaging environmental effects. For the experiment, 32 Wistar rats were divided into 4 groups and treated daily by gavage: the first was the control group, the second group received 50 mg/kg of fungicide, the third group received 70 mg/kg of crude extract; the fourth group received 50 mg/kg of fungicide and 70 mg/kg of crude extract. After eight weeks of treatment, the rats were sacrificed. Plasma levels of creatinine, urea, uric acid, blood glucose, cholesterol, triglyceride, and total bilirubin were observed and histopathological alteration in the kidneys was evaluated. Exposure to the fungicide increased the levels of all biochemical parameters, with no difference in blood glucose levels Histological analysis showed that treatment with the fungicide caused damage to kidney tissue. On the other hand, the Erodium plant reduced the undesirable effects induced by the fungicide improved the levels of biochemical parameters and significantly attenuated histopathological abnormalities. We conclude that the Erodium plant contains secondary metabolites that can be used as prophylactic substances against the harmful effects of the triazole.

**Keywords**: Erodium, Fungicide, Triazole, Cholesterol, Creatinine, toxicity.

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**Poster communication** **P-136**

# Biological activities of the medicinal plant Anastatica hierochuntica

Rahal Sarah*[1] , Djendi Manel Lina[1]

[1]*Laboratory of Microbiology and Molecular Biology, Badji Mokhtar University, Annaba*

**E-mail:** rhl_sara@yahoo.fr

**Abstract**

Antibiotic resistance is a serious global health issue, requiring new therapeutic alternatives. Medicinal plants, rich in bioactive compounds, emerge as a promising solution to combat resistant bacteria. They offer not only a potential alternative to synthetic antibiotics but also hope for diversifying treatments to better control infections. In this study, we evaluated the properties of the plant Anastatica hierochuntica and its biological activities, particularly its antimicrobial, anti-biofilm and antioxidant effects of aqueous and alcoholic extracts.

The antibacterial activity of both extracts was assessed first qualitatively using the solid medium diffusion method, then quantitatively by determining minimum inhibitory concentration (MIC) values. The anti-biofilm activity was tested using the 96-well microplate method. Microbial strains used for this study include bacterial species such as: Escherichia coli, Pseudomonas aeruginosa, Klebsiella pneumoniae, Staphylococcus aureus and Acinetobacter baumannii. The antioxidant activity was carried out by the 2,2-diphenyl-1-picrylhydrazyl (DPPH) free radical scavenging test.

Our results show that this plant exhibits high antibacterial effects, especially against Pseudomonas aeruginosa and Escherichia coli strains. Regarding anti-biofilm activity, the alcoholic extract showed a significant reduction in biofilm formation, with up to 85% inhibition of bacterial growth. Regarding antioxidant activity, our results show that the aqueous extract exhibited higher antioxidant effect in DPPH tests than the alcoholic extract.

In conclusion, our study suggests that Anastatica hierochuntica is a promising source of antibacterial and anti-biofilm agents, with potential therapeutic applications, particularly in the treatment of certain infections caused by multidrug-resistant bacteria.

**Keywords:** Antibacterial activity, Antibiofilm activity, Antioxidants activity, Anastatica hierochuntica, Green medicine.

**Poster communication** **P-137**

# Medicinal impact of Pistacia lentiscus oil from Tunisia and its antiplatelet activity with cytotoxicity evaluation

Raoudha Ben Ameur[1], Basma Hadjkacem[2], Ben Amor Ikram[3], Amira Feki[3], Jalel Gargouri[3], Ali Gargouri[2] and Noureddine Allouche[1]

[1]*Natural Substances Team (LR17ES08), Faculty of Sciences of Sfax, Laboratory of Organic Chemistry, University of Sfax, Sfax, Tunisia*

[2]*Laboratory of Molecular Biotechnology of Eucaryotes, Centre of Biotechnology of Sfax, University of Sfax, Sfax, Tunisia*

[3]*Medical Faculty of Sfax, Laboratory of Hematology (LR19SP04), University of Sfax, Sfax, Tunisia*

**E-mail :** mehdiraoudha@yahoo.fr

**Abstract**

Previous studies have highlighted the potential of Pistacia lentiscus fruit oil (PLFO) in the treatment of cardiovascular disease. Therefore, this study has been designed to examine, for the first time, the inhibitory effect on induced human platelet aggregation by the ADP, collagen and AA of PLFO as well as the evaluation of its cytotoxicity. The effect on platelet aggregation was evaluated on human platelet-rich plasma treated with various PLFO concentrations, dissolved in ethanol (named POE) and then induced by ADP, collagen, and arachidonic acid (AA). The outcome revealed that 8 µL $mL^{-1}$ of POE strongly inhibited ADP-induced platelet aggregation in humans. Additionally, the expression of CD63 and P-selectin as markers of platelet secretion, and αIIβ3 integrin activation were assessed by flow cytometry. It has been found that PLFO significantly reduced platelet activation as well as alpha and dense granule secretion. Moreover, the cytotoxicity assay on normal HEK-293 cells, the hemolysis test and the platelet viability confirmed that PLFO is a safe substance. The main tentatively identified triacylglycerols, which are in monounsaturated and polyunsaturated forms, were SLL + PLO (19.73%), OOL + LnPP (13.12%) and POO (10.57%). The primary sterol identified in PLFO was β-sitosterol (80.19%). These findings are veins. Furthermore, PLFO would prevent certain diseases such as phlebitis, and alleviates valuable for assessing the nutritional composition of PLFO within a preventive and/or therapeutic framework in a clinical context. PLFO is mainly used to alleviate problems related to poor blood circulation, especially for women but it is also employed to treat problems such as heavy legs and varicose various disorders, including cardiovascular problems.

**Keywords**: Pistacia lentiscus, antiplatelet activity, cytotoxicity, Triacylglycerol composition, Sterols analysis.

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**Poster communication** **P-138**

# Hemisynthesis of a α-aminophosphonate derivative by an eco-compatible process and theoretical study (DFT, ADMET)

Aicha RIZI [1,*], Ismahene GRIB[1], Anissa ACIDI [1], Khadidja OTMANE RACHEDI[1,2], Radia BOUASLA [1,3], Malika BERREDJEM[1].

[1] *Laboratory of Applied Organic Chemistry, Synthesis of Biomolecules and Molecular Modelling Group, Sciences Faculty, Chemistry Department, Badji-Mokhtar Annaba University, Box 12, 23000*
[2] *Chadli Bendjedid University, Faculty of Sciences and Technology, Bp 73; El-Taref, 36000 Algeria;*
[3]*National Higher School of Technology and Engineering, 23000 Annaba, Algeria;*

**E-mail:** aicha.rizi@univ-annaba.dz

**Abstract**

Aldehydes play a crucial role as starting reagents in organic synthesis; essential precursors for creating various types of substances with diverse biological effects such as anti-cancer, anti-viral and anti-microbial properties. Aromatic plants contain them in various parts, including seeds, flowers, leaves and bark, depending on the species. The cinnamic aldehyde in Ceylon cinnamon, from Cinnamomum zeylanicum, is a notable example. By hydrodistillation, the essential oil extracted from the bark of Cinnamomum zeylanicum gives a satisfactory yield of 5.46%. The most effective method for isolating Cinnamaldehyde is precipitation with sodium bisulphite (74%). Structural modification leads to the hemisynthesis product (89%), a α-aminophosphonate derivative by a multicomponent Kabachnik-fields reaction involving Cinnamaldehyde, 4-fluoroaniline and triethyl phosphite under ultrasonic irradiation in environmentally friendly conditions; at room temperature, without solvent or catalyst. A quick and easy method. Structural analysis is carried out using IR and NMR spectroscopy. DFT theory reveals that the α-aminophosphonate derivative is more reactive than Cinnamaldehyde. ADMET prediction indicates good bioavailability of these molecules with no significant risk of toxicity to human health.

**Keywords:** Cinnamaldehyde, Ultra sound, Kabachnik-fields reaction, α-aminophosphonate, DFT, ADMET

**Poster communication** **P-139**

# Hemisynthesis and theoritical study of α-sulfamidophosphonate via multi-component reaction under green conditions.

ACIDI Anissa[1]; RIZI Aicha[1] ; GRIB Ismahene[1] ; BOUASLA Radia[1 ; 2] ; OTMANE RACHEDI Khadidja [1 ;3]; BERREDJEM Malika[1]

[1] *Laboratory of Applied Organic Chemistry, Synthesis of Biomolecules and Molecular Modelling Group, Sciences Faculty, Chemistry Department, Badji-Mokhtar Annaba University, Box 12, 23000 Annaba; Algeria*

[2]*National Higher School of Technology and Engineering, 23000 Annaba, Algeria;*

[3] *Chadli Bendjedid University, Faculty of Sciences and Technology , Bp 73; El-Taref, 36000 Algeria*

**E-mail:** acidi.anissa@yahoo.com

**Abstract**

This study highlights the growing importance of aromatic and medicinal plants, particularly cinnamon (Cinnamomum zeylanicum), in pharmaceutical sciences and green chemistry.
Efficient extraction of cinnamaldehyde, a major bioactive compound, was achieved through column chromatography and precipitation with sodium bisulfite.

Additionally, multi-component reactions (MCRs) and hemisynthesis processes were explored to create new chemical derivatives, promoting environmentally friendly synthesis.

The synthesis of α-sulfamidophosphonate, characterized by various analytical methods, confirmed the formation of a pure and high-yield compound.

The theoretical study using DFT validated the chemical reactivity and stability of the synthesized product. These findings offer promising prospects for the development of new anticancer and antiviral therapies, underscoring the importance of in vivo studies and optimization of synthesis conditions to further this research.

**Keywords**:: Hemisynthesis, Cinammaldehyde, α-Sulfamidophosphonate , MCR, DFT, ADMET

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**Poster communication** **P-140**

# Synthesis of xanthene derivatives under ultrasound irradiation using zinc acetate as catalyst.

Rayene Sayad, Dounia Beldjezzia, Yousra Ouafa Bouone, Abdeslem Bouzina, Nour-Eddine Aouf, Zineb Aouf

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

**E-mail**: rayenesayad99@gmail.com

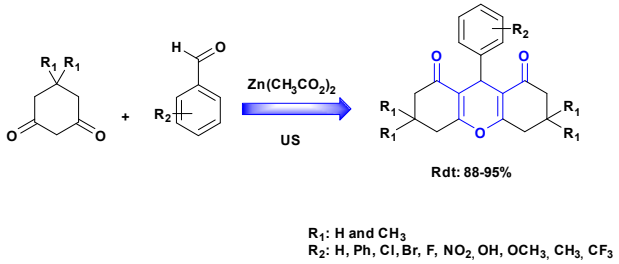
## Abstract

Xanthene derivatives have garnered considerable attention in the fields of medicinal chemistry and organic synthesis transformations over recent decades.[1] It is noted that many reviews focusing on the synthetic strategies and biological activities of xanthene derivatives have been published.[2]These molecules exhibit a range of biological activities, including anti-tumor, anticancer, antibacterial, antiviral, antifungal, analgesic and anti-inflammatory properties.[3]

In recent years, the combination of sonochemistry with catalytic systems has become a powerful strategy that integrates the advantages of ultrasound and catalysis to enhance chemical reactions. This synergistic approach has demonstrated significant benefits in various fields, including organic synthesis, pharmaceuticals industries, environmental chemistry, and materials sciences.[4] This combined system provides advantages that include reduced reaction duration, improved heat and mass transfer, resulting in increased chemical reaction rates, yields, and selectivity.[5]

In this context, our objective in this study was to develop an innovative method for the synthesis of xanthene compounds from Cyclohexandione or dimedone and aromatic aldehydes, using a combination of sonochemistry and catalytic system under various reaction conditions.

In this study, we conducted the synthesis of xanthene derivative By subjecting Cyclohexandione, or dimedone and various aromatic aldehydes via ultrasound irradiation, we successfully obtained the desired product with a good yield in just 15 minute. The resulting solid product was then filtered and recrystallized from ethanol. The synthesis procedure is depicted in **schema 1**.




**Schema 1.** $Zn(OAc)_2$/US as a combined system for the preparation of xanthene derivatives.

**Keywords**: Dimedone , Cyclohexandione , Aromatic aldehydes, Xanthene, Zinc acetate/US,

**Poster communication** **P-141**

# Etude des activités anti-oxydantes d'un nouveau N-sulfonylphtalimide : investigations in vivo dans un modèle d'asthme expérimental chez le rat wistar.

Silini Ilhem[1], Rouibah Zineb[1], Bouraoui Houda[1], Ahmida Meriem[1], Ismahene Grib[2], Malika Berredjem[2], Abdeslem Bouzina[2], Messarah Mahfoud[1] et Boumendjel Amel[1]

[1] *Laboratoire de Biochimie et de Toxicologie Environnementale, Faculté des Sciences, Université Badji Mokhtar, Annaba, Algérie*

[2] *Laboratoire de Chimie Organique Appliquée. Faculté des Sciences, Université Badji Mokhtar, Annaba, Algérie*

**E-mail** : siliilhem@gmail.com

**Abstract**

La diversité structurale et l'importance biologique des hétérocycles contenant de l'azote en ont fait des cibles attrayantes pour la synthèse chimique de nouvelles molécules et ce pendant de nombreuses années. Parmi ces molécules les dérivés phtalimides nouvellement synthétisés sont doués d'activités diverses et donc utilisés dans la chimie médicinale en raison de leur large éventail d'application.

Le but de ce travail est d'évaluer in vivo l'effet antioxydant et anti-inflammatoire et donc antiasthmatique d'une molécule nouvellement synthétisée, le N-sulfonylphtalimide (PHT), dans le cadre d'un protocole d'asthme induit expérimentalement. Pour ce faire, des rats mâles adultes de la souche Wistar ont été sensibilisés avec l'ovalbumine (OVA) et parallèlement traités par la molécule de N-sulfonyl phtalimide. Les paramètres de stress oxydant sont analysés dans Le foie.

Nos résultats montrent que la sensibilisation à l'OVA provoque une diminution significative ($p \leq 0,05$) de l'activité enzymatique de la catalase (CAT) dans le foie comparativement aux rats témoins. En revanche, on observe une augmentation significative ($p \leq 0,05$) de la CAT chez les rats sensibilisés par l'OVA et traités par le phtalimide (OVA + PHT) dans le foie par rapport au groupe sensibilisé (OVA).

La sensibilisation à l'ovalbumine chez les rats induit une augmentation très hautement significative ($p \leq 0,001$) du taux de malondialdéhyde (MDA) dans le foie comparativement au lot témoin. Par contre, il y a une diminution très hautement significative ($p \leq 0,001$) du MDA dans le foie chez les rats sensibilisés par l'OVA et traités par le phtalimide (OVA + PHT) comparativement au lot sensibilisé (OVA).

Pour conclure, la sensibilisation à l'OVA a induit un état d'inflammation avec une perturbation du système de défense antioxydant. Par contre, l'administration de la solution de N-sulfonylphtalimide a révélé les propriétés antioxydantes de cette molécule.

**Mots-clés** : asthme expérimental, rat Wistar, ovalbumine, stress oxydatif, N-sulfonyl phtalimide.

**Poster communication** **P-142**

# Microwave-assisted synthesis of Chromene-3-Carbonitrile: Studies on bioactivities

D. Siziani[1,2], Y. Abdi[1,2] , Z.Attou[2], M. Kelbouz[1] ;N. Bensouilah[2]

[1] *Applied sciences laboratory LSA, Ecole Nationale Supérieure des Technologies Avancées, Cité Diplomatique, ex. Centre biomédical, Dergana, Bordj El Kiffan, Algiers, Algeria*
[2] *Laboratory of Applied Organic Chemistry, Faculty of Chemistry (LAOC), University of Sciences and Technology Houari Boumediene, USTHB, PB 32, El-Alia, Bab-Ezzouar, 16111 Algiers, Algeria*

**E-mail :** Dhaouya.siziani@ensta.edu.dz

**Abstract**

Dehydroacetic acid (DHA) and derivatives are widely used in the synthesis of pharmacologically active heterocyclic compounds. Biologically, DHA and derivatives have been reported as antimicrobial, cytotoxic and antitumor compounds [1]. Structure-activity-relationship conclusions have stressed on the presence of a furano or pyrano ring fused with a polycyclic aromatic system. Besides, the 4 H -chromene compounds may exhibit a variety of biological activities depending on the nature of their substituents on the 4 H -pyran or adjacent rings [2]. Recently, the 2-amino- 4 H -chromenes have been used in technological areas, for instance, as laser dyes, optical brighteners, fluorescence markers, pigments, cosmetics and biodegradable agrochemicals. In addition, the 2-amino-4 H -chromene with a cyano group has been tested in the treatment of rheumatism, psoriasis and cancer [3].

Biological activities, such as the antioxidant DPPH radical scavenging and antibacterial/antifungal assays against ATCC strains have been evaluated in -vitro. Results showed that all compounds are capable to reduce DPPH with different IC 50 values. The germs sensitivity towards the synthesized compounds is variable with Staphylococcus aureus being the most sensitive bacteria.

**Keywords**: Dehydroacetic acid, Chromene-3-carbonitriles, Biological activity.

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**Poster communication** **P-143**

# Une nouvelle idée de Peridiniume para toluène sulfonate (PPTS) en tant que catalyseur efficace pour la synthèse de dérivés de 5-arylidène-2,4-thiazolidinediones

TAFER Radia

*Faculté des Sciences Exactes. Campus de Chaabat Ersas, Département De Chimie*
*Université Frère Mentouri-Constantine1. 25000. ALGERIE*

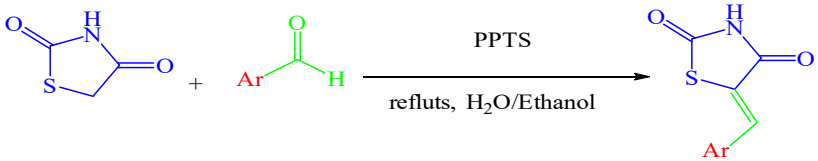
**E.mail:** taferradia@yahoo.fr // tafer-aris.radia@umc.edu.dz

**Resumé**

La thiazolidine-2,4-dione (TZD) a été découverte au 19ème siècle par Libermann et al.[(1)] bien que sa classe de médicaments ait commencé à être synthétisée en 1997.[(2)] La TZD est une substance intéressante dont les dérivés appartiennent à un groupe hétérocyclique important qui représente une source efficace et prolifique pour la synthèse d'un grand nombre d'agents actifs dans divers domaines tel que le domaine médicinal et thérapeutique comme anti-hyperglycémiques[(3)], anticancéreux[(4)], antiarthritiques[(5)], anti-inflammatoires[(6)] … etc.

La thiazolidine-2,4-dione TZD est constituée d'un anneau à 5 chaînons qui comporte un atome de soufre et un atome d'azote en position 1 et 3 respectivement, deux groupes carbonyle en position 2 et 4, et différents groupes chimiques peuvent se présenter comme substituants dans les positions 3 et 5.

La synthèse des dérivés d'arylidène-2,4-thiazolidinedione par une condensation de knoevenagel entre la thiazolidine-2,4-dione et une diversité d'aldéhydes (aromatiques, hétéroaromatiques…) catalysée pour la première fois par le peridinium para toluéne sulfonate (PPTS). La réaction a été effectuée dans des conditions exemptes de solvant.




Ar: Hétérocyclique Aromatique

**Mots-clés**: thiazolidine-2,4-dione, 5-arylidène-2,4-thiazolidinedione, Knoevenagel, peridinium para toluéne sulfonate (PPTS).

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**Poster communication** **P-144**

# Biosynthesis and characterization of silver nanoparticles using Hipochaeris radicata L.

Houria tarmoul[1*], Fatiha brahmi[2], Lila boulekbache-makhlouf[3]

[1,2,3] : *Département des sciences alimentaires, Faculté des sciences de la nature et de la vie, Université A.Mira de Bejaia, 06000, Béjaia, Algérie.*
*Laboratoire de Biochimie, Biophysique, Biomathématiques et Scientométrie « L3BS »*
*Université de Bejaia (06000, Algérie).*

**E-mail** : tarmoulhouria06@gmail.com.

**Abstract**

Nanotechnology concerns the design and manufacture of objects or materials smaller than 100 nanometers. These nanomaterials are composed of nanoparticles. Silver and its compounds have been used for their antibacterial and therapeutic applications for thousands of years. The aim of the present work is the biological biosynthesis and characterization of silver nanoparticles by the aqueous extract of Hypochaeris radicata.

Nanoparticles were synthesized using a biological method. Aqueous plant extract was added to a silver nitrate ($AgNO_3$) solution for $Ag^+$ ion reduction. The mixture was left under stirring with heating. Characterization by UV-visible spectroscopy, FTIR, DRX was carried out.

Biosynthesis was confirmed by color change. The synthesis of silver nanoparticles was successfully completed, and a very dark brown color was observed. The development of this coloration is an indication of the ability of H. radicata aqueous extracts to biochemically reduce silver nitrate. The formation of silver nanoparticles was monitored by measuring the UV-Vis absorption spectrum in the 190-700 nanometer wavelength range. The spectrum shows a clear absorbance band at around 419 nm. Fourier transform infrared spectroscopy affirmed the role of Hipochaeris radicata L. as a reducing and capping agent of silver ions. X ray diffraction revealed their crystalline nature.

Our experimental work has enabled us to validate the biosynthesis of silver nanoparticles by the aqueous extract of Hipochaeris radicata

**Key Words**: Biosynthesis, Nanoparticles, H. radicata, caracterisation.

**Poster communication** **P-145**

# Synthesis of some benzoxazolinonic Schiff base compounds under green conditions

Sourour Tliba[a], Yasmina Adjeroud[a,b], Karima Mellouk[a] and Messaoud Liacha[a]

[a] *Laboratory of Synthesis and Organic Biocatalysis (LSBO), Organic Synthesis and Medicinal Chemistry Group, BADJI Mokhtar-Annaba University, Annaba, 23000 Algeria.*

[b] *Department of Common Core in Sciences and Technology, Faculty of Technology, University of Amar TELIDJI-Laghouat, Laghouat, 03000 Algeria.*

**E-mail** : tlibasourour@hotmail.com

**Abstract**

Benzoxazolone scaffolds exhibit great versatility in organic synthesis, allowing for a wide variety of chemical modifications at different positions of the molecule. It has been the starting point for numerous studies, both in terms of chemistry and its pharmacodynamic properties, which indicate its growing interest in medicinal chemistry. Schiff bases are widely used in coordination and medicinal chemistry. Schiff bases are described as the result of a primary amine reacting with a ketone or an aldehyde and removing a water molecule. This work outlines the quick and easy synthesis of a new Schiff base. Therefore, 6-iminobenzoxazolone are synthesized by condensation of several substituted aldehyde derivatives with 6-aminobenzoxazolone and 6-amino-3-methylbenzoxazolone substrates in the presence of an ionic liquid under ultrasound irradiation. We created all of the synthesized compounds with quick reactions and good yields. The chemical structure of the synthesized compounds was ascertained by means of FT-IR, $^{1}H$, and $^{13}C$-NMR spectroscopic techniques.

**Keywords**: Benzoxazolone, Ionic liquid, Schiff base, Medicinal chemistry

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**Poster communication** **P-146**

# Synthesis, crystal structure, Hirshfeld surface analysis and DFT calculation of 4-amino -3,5- dichlorobenzene sulfonamide

Khouloud torche[(1)], salima samai[(2)], mhamed boudraa[(1)]

[(1)] *Unité de Recherche de Chimie de l'Environnement et Moléculaire Structurale (CHEMS), Université Constantine-1 25017, Algeria.*

[(2)] *Faculté de science depertement de science de la matiere université Abess Laghrour-Khenchela- Algerie*

**E-mail:** khouloud.torche@doc.umc.edu.dz

**Abstract**

4-amino-3, 5-dichlorobenzene sulfonamide was synthesized and characterized by single crystal X-ray diffraction. The compound crystallized in a centrosymmetric P21/C space group with a=8.0266 Å,
b =20.9859 Å, c = 5.3818 Å and β = 95.70°.

The molecules in the crystal structure are connected to one another by intermolecular C-H...O, N-H...Cl, C-H...Cl, N-H...O and N-H...N interactions forming and motifs. Through the examination of their Hirshfeld surfaces, these interactions with the molecular packing were carried out and compared to the 2D fingerprint plots.

Quantum-chemical calculations using the Density Functional Theory (DFT) approach for structural analysis are carried out using B3LYP methods with 6-311++G(d,p) basis set.

**Keywords**: Synthesis, crystal x-ray, intermolecular, interactions, Hirshfeld surfaces, DFT.

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**Poster communication** **P-147**

# Synthesis of novel rhodanine derivatives and evaluation of enzyme inhibitory potential using urease in vitro

Zadem Achwaq [1], Benzaim ahmed yasyne, Cheraiet Zinelaabidine [1,2], Bidjou-HaiourChahra [1]

[1] *Laboratoire de synthèse Organique,Modélisation et Optimisation des Procédés chimiques (LOMOP), Université Badji Mokhtar Annaba, Algérie.*

[2] *Laboratoire des Matériaux Organiques et Hétérochimie (LMOH), Département des sciences de la matière, Université Echahid-Larbi Tébessa, Algeria*

**E-mail** : achwaq.zadem@univ-annaba.dz

**Abstract**

The rhodanine motif has proved to be a promising framework for medicinal chemistry, displaying various biological properties and therapeutic potential[1]. Its polyfunctionality allows significant modifications, giving rise to various pharmacologically active compounds, notably in the anti-diabetic, anti-viral, anti-inflammatory, and anti-cancer fields[2]. Rhodanine-based structures have been central in developing new drugs and therapeutic agents.

Recently, urease inhibitors have attracted increasing interest as potential new anti-ulcer drugs that hydrolyze urea to ammonia and carbon dioxide in living organisms[3]. The aim of this study focuses on the synthesis of novel rhodanine Scaffolds Based on quinolones Moiety as a Urease Inhibitor, the strategy is achieved by a condensation reaction in the presence of a natural eutectic system as a catalyst, with acetic acid as a suitable solvent. Yields of the final products ranged from 30 to 47% and were achieved within a short timeframe.

To improve their biological activities Compounds a, b, and c were evaluated for testing in vitro the inhibition of the target enzymes like urease and were, and the results demonstrated that these new drugs have a moderate inhibitory capacity against urease, with an $IC_{50}$ value of 120-230 µM as compared with the standard thiourea, the compound a is the most active against compared to other members of the drugs. In conclusion, it can be concluded that the positions of substituents at the quinolone moiety and the radical of the rhodanine chain play vital roles in urease inhibitory activity.

**Keywords**: Knoevenagel reaction, Rhodanine, Quinolone, Green chemistry, urease, in vitro.

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**Poster communication** **P-148**

# L'évaluation in vitro des activités antioxydants d'une nouvelle molécule 1,3-dithole.

Chaima Aouachria[1], Khaled Aggoun[1], Abdelkrim Gouasmia[1], Lakhmissi Kaaboub[1].

[1] *Laboratoire des Matériaux Organiques et Hétérochimie, LMOH, Université Larbi Tebssi, Tébessa.*

**E-mail:** chaima.aouachria@univ-tebessa.dz

**Résumé**

Le stress oxydant peut être défini comme l'incapacité de l'organisme à se défendre contre l'agression des espèces réactives de l'oxygène (ROS) ou de l'azote (RNS), suite à un déséquilibre lié, soit à une production accrue en radicaux libres, ou une diminution de la capacité de défenses antioxydantes. Ce déséquilibre peut survenir suite à l'effet de certains stimuli pathologiques endogènes (hyper-LD Lémie, hypertension, diabète…) ou exogènes (polluants environnementaux, tabagisme…). Les antioxydants sont des composés capables à ralentir ou à empêche les processus d'oxydation qui se produisent sous l'influence d'une espèce réactive oxygénée. Ils préviennent l'oxydation des macromolécules en donnant de l'hydrogène, la désactivation des radicaux par création d'addition covalente, la réduction des métaux ou de peroxydes, la complexation d'ions et de métaux de transition et le captage de l'oxygène singlet.

Dans le cadre de l'activité antioxydant ce travail s'est orienté vers la synthèse d'une nouvelle molécule 1,3-dithiole (Schéma 1) par la méthode de couplage médie par le phosphite. Les compositions du produit synthétisé ont été confirmées par les méthodes spectroscopiques. De plus, le composé obtenu a été examiné pour leur potentiel antioxydant par les trois méthodes DPPH, FRAP et 1,10-phenanthroline. Nos résultats indiquent des activités antioxydants excellent, suggérant un certain pouvoir de neutralisation des radicaux libres, ainsi que la réduction de fer.

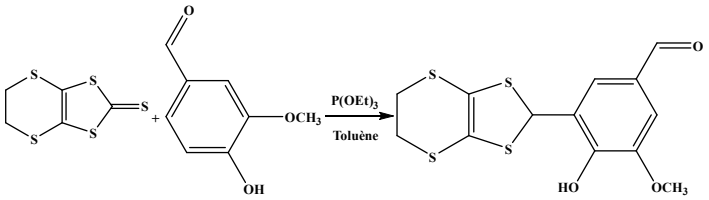


**Schéma 1.** La synthèse de la molécule 1,3-dithiole.

**Mots-clés** : 1,3-dithiole, antioxydant, DPPH, FRAP et 1,10-phenanthroline.

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**Poster communication** **P-149**

# Study of the effect of solution pH on the catalytic efficiency of an Eggshells@CuO biocatalyst used for the removal of basic fuchsin from aqueous media

Atef Ali Ahmed [1*], Zhour Hattab [2] and Yamina Berredjem [2]

[1] *Laboratory of Physics of matter and Radiation, Department of process engineering, Faculty of science and technology, University Mohammed Cherif Messaadia, 41000, Souk-Ahras, Algeria*
[2] *Laboratory of Water Treatment and Valorization of Industrial Wastes, Department of Chemistry, Faculty of Sciences, University Badji Mokhtar, 23000, Annaba, Algeria.*

**E-mail** : atef.aliahmed96@gmail.com

**Abstract**

Originally, for environmental and hygienic reasons, the treatment of polluted water has now become essential due to the growing pressure on the planet's freshwater reserves. Dyes are among the most persistent organic pollutants in wastewater. In recent years, photocatalysis has become the key to solving the problem of pollution by synthetic dyes. The efficiency of this technique is directly related to several factors, including temperature and pH. The aim of the present study is to investigate the effect of solution pH on the removal of basic fuchsin dye using a previously prepared biocatalyst (Eggshells@CuO), and thus understand the impact of photocatalytic experiments in a complex environment. The effect of pH was studied in batch mode, varying values from 2 to 12, while other parameters were kept constant.

**Keywords**: Water treatment, Photocatalysis, dyes, basic fuchsin.

**Poster communication** **P-150**

# Characterization of phenolic extracts from lemon peel by LC-MS/MS and evaluation of their antioxidant potentials

Rabha AYAD[1]; Abed ARABI[2]; Dyhia SADOU[1]; Naouel Kheyar-Kraouche[3]

[1] *Laboratoire de Biochimie, Biophysique, Biomathématiques et Scientométrie (L3BS), Faculté des Sciences de la Nature et de la Vie, Université de Bejaia, 06000 Bejaia, Algeria.*

[2] *Laboratoire de microbiologie et de biologie végétale, Faculté des Sciences de la Nature et de la vie, université de Mostaganem, 27000 Mostaganem, Algeria*

[3] *Laboratoire de biotechnologie végétale et d'ethnobotanique, Faculté des Sciences de la Nature et de la Vie, Université de Bejaia, 06000 Bejaia, Algeria.*

**E-mail:** ayad.rabha@gmail.com

**Abstract**

The zest is the outer, colored and fragrant part of the citrus fruit. The pericarp of these fruits is composed of two superimposed layers: the outer layer or epicarp, also known as “flavedo”, is the zest; the inner, white layer is the mesocarp, also known as “ziste”, or “albedo”. This fruit waste is a rich source of bioactive molecules, in particular polyphenols, which are beneficial metabolites for human health, as they reduce or inhibit oxidative stress and can be used in food or pharmaceutical products. This project therefore aims to study this acidic fruit for its polyphenols and antioxidant activities, and to support their symbiotic use as food, therapeutic and pharmaceutical products.

This research was started by preparing phenolic extracts and testing their antioxidant activities in-vitro using four different assays, and characterizing polyphenols by the LC-MS/MS method. Efficient extraction of phenolic compounds was achieved using 80% ethanol.

The results showed that lemon peel had a higher total phenolic content (TPC 8.35 ± 0.37 mg GAE/g). In addition, the antioxidant potential was higher when ripe, probably due to the presence of a greater quantity of favonoids, in particular anthocyanins, phenolic metabolites such as phenolic acids, favonoids, isofavonoids, chalcones, stilbenes, lignans and other compounds were identified by mass spectrometry.

In conclusion, these results support the use of this product in combination as a therapeutic ingredient in the food, biomedical and pharmaceutical industries.

**Keywords**: Lemon peel; Antioxidants; Phenolic acids; LC-MS/MS.

**Poster communication** **P-151**

# Investigating the anticancer properties of chloroform extract from a species of Cerinthe against AsPC-1 Pancreatic cancer cells.

Ayoub Nadji[1], Sabrina Bouguessa[1], Ercan Çaçan[3], Soumaya Menadi[3], Ramazan Erenler[2], Narimane Saigaa[1], Soraya Hioun[4], Abelkrim Gouasmia[1].

[1]*Laboratory of Organic Materials and Heterochemistry, Echahid Cheikh Larbi Tebessi University-Tebessa, Algeria.*

[2]*Iğdır University, Faculty of Health Sciences, Iğdır, Türkiye*

[3]*Department of Molecular Biology and Genetics, Tokat Gaziosmanpaşa University, 60250 Tokat, Turkey*

[4]*Department of Natural and Life Sciences FSESNV, Larbi Tebessi University, Tebessa-Algeria*

**E-mail:** ayoub.nadji@univ-tebessa.dz

**Abstract**

Pancreatic cancer remains a significant health challenge with limited treatment options, necessitating the exploration of novel therapeutic approaches. In this particular in vitro study, we focused on investigating the potential anticancer activity of a chloroform extract obtained from Cerinthe Genus: a medicinal plant renowned for its diverse pharmacological properties, against the AsPC-1 pancreatic cancer cell lines. To ensure consistency and reliability of the experimental results, we prepared the chloroform extract from Cerinthe using a standardized protocol. Subsequently, we treated AsPC-1 pancreatic cancer cell lines with various concentrations of the Cerinthe chloroform extract and evaluated the effects using the MTT assay, a method for assessing cell viability. The results of our study demonstrated an acceptable reduction in cell viability after treatment with the chloroform extract. Moreover, the extract exhibited acceptable effects on AsPC-1 cells. These findings underscore the potential of the Cerinthe chloroform extract as a promising anticancer agent against pancreatic cancer. The MTT assay results provide evidence of its effects on AsPC-1 cells, hinting at a potential mechanism of action that warrants further investigation.

**Keywords**: AsPC-1 cells, MTT assay, Cerinthe, Chloroform, Pancreatic Cancer.

**Poster communication** **P-152**

# Green synthesis and characterization of NiO nanoparticles using aqueous extract of Cynara Cardunculus

Azabi Warda , Gherraf Noureddine

*Exact sciences , laboratory of natural resources and management of sensitive environments , Oum El Bouaghi university*

**E-mail:** warda.azabi@univ-oeb.dz , ngherraf@yahoo.com

**Abstract**

Green synthesis of nanoparticles using plant extract is a novel development that has gained significant attention because of its nontoxicity, and environmental friendliness. In the present study nickel oxide nanoparticles was synthesized by an eco-friendly green synthesis method using Cynara Cardunculus plant extract. The green particles were synthesized by boiling the mixture of Cynara Cardunculus extract and 0.1M of nickel nitrate at $60^0$ C for 1 hour. The obtained nanoparticles were characterized using UV−vis spectra, Fourier transform infrared spectroscopy, and X-Ray diffraction techniques. The UV-visible spectrum indicated absorbance at 350 nm nanoparticles show a strong and broad absorption peak from FTIR spectral analysis revealed that the peak at 620.69 $cm^{-1}$ was assigned to Ni−O and O−Ni−O stretching vibration of NiO nanoparticles.

**Keywords**: green synthesis, nickel oxide , plant extract, nanoparticles, Cynara Cardunculus.

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**Poster communication** **P-155**

# Optimization of antibacterial syrups based on natural ingredients: improvement of preparation methods

BENCHIKH Imen[1], DEHBI Atallah[2], DJAFRI Fatiha[3]

[1]. *University, Laghouat Amar Telidji 03000, Faculty of Sciences, Laboratory of Materials for Application and Valorization of Renewable Energies, Algeria*

[2] *University Center, El-Bayadh Nour Bachir 32000, Department of Natural and Life Sciences, Institute of Sciences, Algeria*

[3]. *University Oran 1 Ahmed BENBELLA, Laboratory of Materials Chemistry, Algeria*

**E-mail :** i.benchikh@lagh-univ.dz

**Abstract**

This study aims to optimize the preparation of antibacterial syrups made from moringa, thyme, and sage by focusing on the interactions between their active compounds. Moringa, rich in isothiocyanates, flavonoids, and phenolic acids; thyme, containing thymol and carvacrol; and sage, with thujone and camphor, have each demonstrated notable antibacterial properties. The study revealed that combining these plant extracts produces a synergistic effect, enhancing the overall antibacterial effectiveness of the syrup. For instance, moringa's isothiocyanates enhance the action of thyme and sage compounds by making bacteria more vulnerable. Additionally, optimizing the proportions of the extracts and selecting appropriate extraction methods were found to be crucial for maximizing this effectiveness. The study also emphasized the importance of maceration duration and the quantities of plants used, highlighting their significant impact on antibacterial activity. The syrups, prepared hot with a density of 1.32 at 20°C and a sugar concentration of 65.01%, demonstrated good stability and extended shelf life due to the use of traditional techniques and natural preservatives. The study's results suggest that these syrups could serve as an effective alternative to traditional antibiotics, thereby reducing reliance on chemical medications and limiting bacterial resistance. In conclusion, this research encourages further investigations to refine the formulations and test the effectiveness of these syrups against a broader range of bacteria and medicinal plants, offering natural and promising solutions for human health.

**Keywords**: Antibacterial Syrups, Maceration Duration, Traditional Medicine, Bacterial Resistance, Herbal Medicine.

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**Poster communication** **P-157**

# Synthese d'un photostabilisant des materiaux polymeres

M. BOUTAMDJA[1], N. BENBELLAT[2]

*Département de Chimie, Faculté des Sciences de la matière, Université de Batna 1, Batna, Algérie*
*[1] Laboratoire de Chimie et Chimie de l'Environnement (LCCE)*
*[2] Laboratoire de Chimie des Matériaux et des Vivants : Activité et Réactivité (LCMVAR)*

**E-mail** : m.boutamdja@univ-batna2.dz

**Résumé**

Les matériaux polymères sont soumis à une dégradation photo oxydante pendant leur utilisation et déposition sous des conditions atmosphériques, surtout à l'exposition à la lumière du soleil. L'initiation de cette dégradation est causée par les impuretés et les groupements fonctionnels, présents dans la matrice polymère, capables d'absorber l'énergie de rayonnement ultraviolet. L'absorption de l'énergie est suivie par d'autres réactions photochimiques qui peut conduire ensuite à des changements de propriétés indésirables telles que la coloration, la déformation de la surface et la chute dans la résistance à la rupture, etc.

Ce problème reste un sujet important des recherches actuelles. Pour surmonter ce dernier, plusieurs approches ont été essayées. L'addition d'un UV-stabilisant est une des solutions largement employée avec les plastiques commerciaux afin de prolonger leur durée de vie. Le 2-hydroxybenzophénone et ses dérivés sont un genre de ses photostabilisants couramment utilisés pour la protection des plastiques contre le vieillissement. Ils ont la capacité d'absorber les radiations ultraviolettes endommageantes contenues dans le spectre solaire (radiations UV A et UV B) et sont capables de dissiper l'énergie absorbée sous forme d'énergie vibrationelle empêchant donc la dégradation de ces matériaux. Les recherches ont montré leur grande efficacité, mais malheureusement ils s'évaporent facilement après leur migration à la surface du polymère, qui est due certainement à la fois à la faible masse moléculaire et à l'incompatibilité avec les polymères.

Dans ce travail nous nous sommes intéressés à la synthèse de ce type de photostabilisants afin d'obtenir des monomères hydroxybenzophénoniques polymérisables qui peuvent être incorporés dans le squelette polymère, capables d'améliorer la durabilité des polymères. La synthèse du monomère et des composés intermédiaires a été caractérisée par les méthodes spectroscopiques IR et RMN $^{1}H$ et $^{13}C$.

**Mots-clés :** Photostabilisant, rayonnements ultraviolets, 2-hydroxybenzophénone, monomère polymérisable.

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# Recherche et évaluation in vitro du potentiel antifongique de l'extrait total d'une plante médicinale algérienne : salvia officinalis l., lamiaceae

DALIA Farid [(1)], BENTCHOUALA Chafia [(2)], BELKHIRI Abdelmalik [(1)]

[(1)] *Laboratoire d'Innovation et de Développement d'Actifs Pharmaceutiques (IDAP), Université de Constantine 3, Algérie*

[(2)] *Laboratoire de microbiologie médicale, Centre Hospitalo-universitaire de Constantine, Algerie*

**E-mail** : FARIDDALIA.21@GMAIL.COM

**Resumé**

Le traitement des mycoses cutanées bénéficie actuellement de nombreux antifongiques de synthèse efficaces. Malgré cela, les problèmes des récidives et des résistances aux antifongiques persistent. Ces différentes difficultés ont suscité notre intérêt pour la recherche d'autres substances naturelles bioactives à potentiel fongitoxiques pouvant être une solution alternative aux médicaments actuels.

Plusieurs espèces végétales sont connues depuis longtemps pour leurs effets antimicrobiens.

Dans cette étude ; nous nous sommes intéressés à une plante très répandue dans le bassin méditerranéen dont ses feuilles sont très utilisées en Algérie pour leurs nombreuses vertus thérapeutiques. Il s'agit de la sauge : Salvia officinalis L. de la famille des Lamiaceae.

Après l'identification botanique précise de notre matériel végétal, on a procédé à un travail expérimental où nous avons préparé un extrait hydro-éthanolique à partir des feuilles desséchées de la sauge. Ensuite, l'extrait a été testé sur la croissance in vitro de Candida albicans. Les résultats ont montré une activité antifongique évidente.

**Mots-clés :** Mycoses**, s**ubstances naturelles, bioactives, Salvia officinalis L., antifongique, Candida albicans.

**Poster communication** **P-159**

# A green synthesis of glyceryl trimethacrylate (gtma) catalyzed by a friendly and ecologic catalyst "maghnite h$^{+}$"

Derkaoui Samira[1,2*], Belbachir Mohammed[2]

[1]*University of Tissemsilt Ahmed Ben Yahia El Wancharissi*
[2]*Laboratory of Polymer Chemistry, Departmentof Chemistry, Faculty of Science, University Oran 1 Ahmed Benbella. BP N°1524 El'Menouer, 31000 Oran, Algeria.*

**E-mail:** s.derkaoui@univ-tissemsilt.dz / derkaoui.samira@gmail.com

**Abstract**

Green chemistry involves the development of chemical products and synthetic procedures, which are environment friendly and have reduced health risks with the search for more efficient methods to do chemistry. The development of materials with enhanced properties that can be understood and tailored at the molecular level is the premier challenge for materials chemists.

Usage of glycerol for the synthesis of value-added chemicals is of great industrial importance, not only because glycerol can be formed in large amounts during biodiesel process but also because it is a non-toxic, edible, bio-sustainable and biodegradable compound.

There are various studies on the synthesis of glyceryl triacrylate or methacrylate by using methacrylol chloride or methacrylic acid with alcohol and triethylamine in $CH_2Cl_2$ or Chloroform was cooled using an ice bath followed by stirring at room temperature for 60 min.

In the present work, we present a new approach to synthesis Glyceryl Trimethacrylate (GTMA) by reaction of glyceryl with methacrylic anhydride catalyzed by nontoxic catalysts "Maghnite $H^+$ " in one-pot in bulk (Without solvent) using an ice bath and at room temperature for 12 hours with a molar ratio of 3:1 of methacrylic anhydride to glyceryl, obtaining a better yield around 70% and selectivity to the product 100%.

The products were characterized and confirmed by Infrared Spectroscopy (FTIR), $^{1}H$ and $^{13}C$ nuclear magnetic resonance (NMR) spectroscopy;

**Keywords**: green chemistry; monomers; maghnite-$H^+$; Glyceryl Trimethacrylate; Methacrylic anhydride,one-pot.

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**Poster communication** **P-161**

# New eco-friendly procedure for the synthesis of (Z)-4-(2 methoxy benzylidene)-3-phenylisoxazol-5(4H)-one and its structural study and Hirshfeld surface analysis

Rima Laroum,[a,b] Assia Benouatas,[c] Noudjoud Hamdouni,[c] Wissame Zemamouche,[c] Ali Boudjada,[c] Abdelmadjid Debache[a]

[a)] *Laboratoire de Synthèse des Molécules d'Intérêts Biologiques, Université des Frères Mentouri-Constantine, 25000 Constantine, Algérie.*

[b)] *Département Sciences de la Matière, Faculté des Sciences Exactes et Sciences de la Nature et de la Vie, Université Larbi Ben M'Hidi, Oum El Bouaghi 04000, Algérie.*

[c)] *Laboratoire de Cristallographie, Departement de Physique, Université des Frères Mentouri Constantine, 25000, Constantine, Algérie.*

**E-mail**: laroum.rima@gmail.com

**Abstract**

Multi-component reactions (MCRs) have been proven a very powerful method for the synthesis of highly functionalized heterocyclic compounds in a single reaction vessel, showing high atom economy, high selectivity and higher yield as well. In addition, they contribute to the requirements of an environmentally friendly process by reducing the number of synthetic steps, energy consumption and waste production.

Among the wide variety of heterocyclic compounds that have been explored for developing pharmaceutically important molecules the isoxazolone derivatives.

Isoxazolone derivatives exhibit significant pharmaceutical and therapeutic properties. For these reasons, the synthesis of isoxazolone derivatives has aroused great interest in medicinal chemistry and organic synthesis.

Hence, in the context of multicomponent reactions we developed a new eco-friendly process for the synthesis of isoxazolone derivatives. The reaction has been carried out involving three components, an aromatic aldehyde and ethyl acetoacetate and hydroxylamine hydrochloride, catalyzed by an eco-friendly catalyst in aqueous media. We also report on the molecular and crystal structure together with a Hirshfeld surface analysis of (Z)-4-(2-methoxybenzylidene)-3-phenylisoxazol-5(4H)-one derivative.

**Keywords**: Multicomponent reactions, isoxazolone derivatives, green synthesis, crystal structure, eco-friendly catalyst, π–π interactions, hirshfeld surface.

**Poster communication** **P-162**

# Synthesis of Acetyl potato starch and characterization

Cherifa Mahieddine, Boubekeur Nadjemi

*Laboratoire d'Etude et de Développement des Techniques de Traitement et d'Epuration des Eaux et de Gestion Environnementale, Ecole Normale Supérieure de Kouba, B.P. 92, 16050 Vieux Kouba, Alger, Algérie.*

**E-mail:** mahieddinec@gmail.com

**Abstract**

Starch as an alcohol polymer assists to react with carboxylic acid and its derivatives to synthesize ester polymer or starch acetates [1], with using an alkaline catalyst [2] and in specific conditions of reaction. Hence, the acetylated potato starch was synthesized from reaction of native starch with anhydride acetic $(CH_3CO)_2O$ in water, which was catalysed with a weak alkaline at 25°C. The reaction efficiency (RE) [3] of the potato starch acetylation with anhydride acetic in water appears a significant correlation with degree of substitution (DS) depends on the reaction time, amount of reactive and water ratio. The change of starch function between native and acetylated starch was confirmed by spectroscopic techniques: ATR-FTIR, $^1$H-NMR and X-ray diffraction.

**Keywords**: Potato starch - Acetylation – degree of substitution – reaction efficiency.

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# Synthesis of cellulose Acetate from palm pollen sheath through chemical treatment

Neghmouche Nacer Salah [1*], Ben Amor Mohammed Larbi[2], Abadi Abderrezzak[1] and Fadila Louafi[3]

[1]*El Oued University, Faculty of Exact Sciences, Chemistry Department, P.O. Box 789, ElOued 39000, Algeria;*

[2]*El Oued university, Faculty of Technology, Process Engineering Department,P.O. Box 789, ElOued 39000, Algeria*

[3]*CHEMS Research Unit, University of the Mentouri Brothers of Constantine 1, Constantine, 25000, Algeria*

**E-mail:** neghmouchenacer-salah@univ-eloued.dz

**Abstract**

This study investigates the synthesis of cellulose acetate from palm pollen sheath, an abundant and underutilized local resource. The process involves a two-stage chemical treatment. In the first stage, cellulose was extracted from the palm pollen sheath using 2M sodium hydroxide (NaOH) and hydrochloric acid (HCl) solutions. The treatment revealed that the palm pollen sheath is rich in cellulose, making it a viable source for cellulose extraction. In the second stage, the extracted cellulose was subjected to esterification using a mixture of acetic anhydride and glacial acetic acid, with concentrated sulfuric acid serving as a catalyst. The cellulose acetate product was then characterized using infrared spectroscopy to confirm the successful acetylation and to analyze its chemical structure. This research demonstrates the potential of palm pollen sheath as a sustainable source for producing cellulose acetate and provides insights into the efficiency of the chemical treatment process.

**Keywords**: cellulose, cellulose acetate, palm pollen, esterification.

**Poster communication** **P-166**

# Adsorption of paracetamol on medical activated carbon

ABRANE RAHMA[1,2] , HAZOURLI Sabir[2]

[1]*Applied and Teorical Physics Laboratory, University Of Echahid Cheikh Larbi Tebessi,Tebessa 12002(Algeria)*

[2]*Laboratory of Water Treatment and Valorization of Industrial Waste,Faculty of Science, Department of Chemistry, Bp12, Annaba 23000 (Algeria), (11)*

**E-mail:** rahma.abrane@univ-tebessa.dz

**Abstract**

The adsorption of paracetamol in acidic (pH2) and basic (pH 8) media on medical charcoal (CAM) was studied. This pH option was aimed a purely medical purpose to test the adsorptive capacity of paracetamol on that coal. The results showed that a low concentration of CAM at 2 g/L, an initial paracetamol concentration of 50 mg/L, a contact or equilibrium time of 30 min and an ambient temperature at 20° C are sufficient to obtain a maximum adsorption capacity of 6 mg / g for tests at pH 2 and 7 mg/g for those at pH 8. Comparative adsorption tests of paracetamol by other commercial charcoals and natural biomaterials of agricultural origin, carried out under the same operating conditions, showed that microporous charcoals were the most competitive in terms of adsorptive power of paracetamol. For these coals, the adsorption capacities are around 20 mg / g for tests at pH 2 and 25 mg / g for tests at pH 8. Based on these results, it can be concluded that paracetamol could be adsorbed in acidic or basic medium and that the type of adsorbent played an important role in the concentration of all or part of this drug.

**Keywords**: Adsorption, Paracetamol, Carbon, Biomaterial, pH.

**Poster communication** **P-168**

# Organic synthesis, green, and medicinal chemistry with ZnO

REZGOUN SARRA [1], Ouchenane Sihem [2], Merzouki soraya[3] ,mayouf imane [4]

[1] *Centre Universitaire Abdelhafid Boulasouf, Mila.*
[2] *Laboratoire des Nanomatériaux -corrosion et Traitement des Surfaces,Badji Mokhtar University,BP.12 ,Annaba 23000,Algeria.*
[3] *Centre Universitaire Abdelhafid Boulasouf, Mila.*
[4] *Centre Universitaire Abdelhafid Boulasouf, Mila.*

**E-mail** : rezgoun.s@centre-univ-mila.dz

**Abstract**

Organic synthesis is a fundamental discipline in modern chemistry, serving as the backbone for creating complex molecules used in pharmaceuticals, agrochemicals, and materials science. My research focuses on integrating the principles of green chemistry into organic synthesis to create more sustainable and eco-friendly methods for chemical production. A central component of this work is the utilization of zinc oxide (ZnO) as a green catalyst. ZnO is an abundant, inexpensive, non-toxic, and recyclable material, making it an ideal candidate for sustainable catalytic processes. By leveraging ZnO's catalytic properties, we aim to facilitate organic reactions under milder conditions, reduce reliance on hazardous reagents, and minimize waste generation.

In the realm of medicinal chemistry, ZnO-catalyzed reactions are particularly promising for synthesizing bioactive molecules with therapeutic potential. This research explores the use of ZnO to create novel drug candidates targeting diseases such as cancer, infectious diseases, and neurodegenerative disorders. ZnO's ability to promote reactions with high efficiency, selectivity, and reduced energy consumption is critical to the development of greener synthetic pathways for drug discovery. Additionally, ZnO can be easily recovered and reused, further contributing to the sustainability of the process.

The combination of organic synthesis, green chemistry, and ZnO catalysis is not only an environmentally friendly approach but also enhances the efficiency of pharmaceutical development. By providing cleaner, more efficient routes for the synthesis of complex molecules, this research aims to contribute to both the advancement of medicinal chemistry and the reduction of the environmental footprint of chemical manufacturing.

Ultimately, the integration of ZnO in organic synthesis represents a significant step toward achieving the dual goals of sustainability and innovation in drug development, aligning with global efforts to create more environmentally responsible chemical processes.

**Keywords:** Organic synthesis, Green chemistry, Zinc oxide (ZnO) catalyst, Sustainable chemical processes, Eco-friendly catalysis

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**Poster communication** **P-169**

# Potential effect of Zinc oxide nanoparticles synthesized using Silybum marianum seeds extract on male reproduction: Focus on oxidative stress

Amina Talbi[1*], Kamel Khelili[1], Cherif Abdennour[1]

[1]*Laboratory of Animal Ecophysiology, Department of Biology, Faculty of Sciences, Badji Mokhtar-Annaba University 12, P.O.Box2300 Annaba, Algeria*

**E-mail:** amina.talbi@univ-annaba.dz // aminatalbi.bio@gmail.com

**Abstract**

This work examine the effect of three doses of zinc oxide nanoparticles (ZNP), extracted by Silybum marianum seeds using zinc acetate, on the sperm motility parameters of male Wistar rats. Animals were divided into 4 groups; the control received tap water, while ZNP1, ZNP2 and ZNP3 received respectively 10 mgZNP/kg bw, 50 mgZNP/kg bw and 100 mgZNP/kg bw by gavage every other day over a 30-day period. Testis were collected to analyze testicular malondialdehyde (MDA), glutathione (GSH) and glutathione peroxidase (GPx). According to the results, the ZnPs of the three doses did not affect testicular MDA level. Regarding GSH concentration and GPx activity, while the group receiving 50mg/kg of ZnPs exhibited significant improvement compared to the control group, groups receiving 10 mg/kg and 100mg/kg of ZnPs kept the same levels as the control group. To conclude, results indicated that exposure of ZnPs is relatively safe for male fertility and could be beneficial as well. Wherein, the synthesized ZnPs had improved sperm quality and increased the antioxidant parameters at 50 mg/kg.

**Keywords**: Green synthesis, zinc oxide nanoparticles, Silybum marianum, oxidative stress.

**Poster communication** **P-172**

# Synthèse d'un hydrogel à base de l'ULVA LACTUCA. Application dans la délivrance d'un antidiabétique

Zakia Zeffouni[1,2], Fatima M'Zyene[2], Faiza Zermane[1], Benamar Cheknane[1], Mohamed Elhattab[2]

[1]*Laboratoire de chimie- physique des interfaces des matériaux appliqués à l'environnement, Faculté de Technologie, Université Saad Dahleb Blida 1*

[2]*Laboratoire de Chimie des substances naturelles et des biomolécules LCSN-Biom, Faculté des Sciences, Universite Saad Dahleb Blida 1.*

**E-mail:** zzeffouni2@yahoo.fr

**Resumé**

Dans cette étude, nous avons valorisé un biopolymère L'Ulvane extrait à partir d'une algue marine L'Ulva Lactuca, récoltée le mois de mars 2022 à la plage de Fouka marine située à 39 km à l'ouest d'alger, Algerie. Après lavage, séchage et broyage de l'algue, la poudre est macérée dans un mélange de solvants (méthanol : dichlorométhane : eau) (8 :4 :2 en volume) pendant une semaine afin d'extraire tous les pigments. L'Ulvane a été extraite sous reflux dans l'eau à 90°C pendant 3 heures, avec un rendement de 13%.

La formation des hydrogels à base de l'ulvane et du chlorure de calcium, et l'encapsulation d'un principe actif antidiabétique 'la Metformine' ont été préparées à des proportions différentes (500 et 850 mg).

Les tests de libération sur les formulations comprenant le PA ont montré que :

- Les vitesses de libération des PA étaient assez courtes dans le milieu acide. Le temps pris pour la libération de plus de 90% de PA était de 1 heure et de 2 heures pour les hydrogels avec 850mg et 500 mg de PA respectivement.
- La vitesse de libération devient assez lente seulement quand les hydrogels qui ont été transférés dans le milieu neutre de pH 6,8. Le temps pris par la libération de plus de 90% de PA était de 3 heures.

**Mots-clés:** Hydrogel, Ulvane, ULVA Lactuca, Metformine, Libération du médicament

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**Poster communication** **P-173**

# Formulation des hydrogels à base des biomolécules pour la vectorisation de l'amoxicilline

Yamina Zouambia[1*], Khadidja Youcef-Ettoumi[1], Yousra Benkhaoua[2], Nesrine Ameri[2]

[1]*Faculté de Technologie-Laboratoire Matériaux et Environnement (LME)*
*Université Yahia Fares de Médéa, Algérie*
[2]*Faculté de Technologie, Université Yahia Fares de Médéa, Algérie*

**E-mail:** zouambia_y@yahoo.fr // zouambia.yamina@univ-medea.dz

**Abstract**

Les hydrogels à base des biopolymères connaissent aujourd'hui un intérêt croissant grâce à leur large potentiel d'application. Ces systèmes tridimensionnels à caractère hydrophile dont la particularité est de pouvoir retenir de grandes quantités d'eau, sont largement utilisés dans diverses industries notamment l'industrie pharmaceutique (administration des médicaments).

Cette étude porte principalement sur la formulation des hydrogels à base de deux biopolymères qui sont l'amidon et l'alginate de sodium et leur utilisation comme système de libération de l'amoxicilline. Les hydrogels obtenus ont été soumis à des analyses physicochimiques appropriés (FTIR, taux de gonflement…). Les résultats obtenus ont montré que l'aspect des hydrogels formulés dépend principalement de la concentration des polymères utilisés et que l'ajout de l'acide ascorbique (AA) mène à l'augmentation de la rigidité de ces hydrogels. Le meilleur taux de gonflement est enregistré dans le milieu alcalin à la température ambiante (≈25°C). L'étude de la cinétique de libération de l'amoxicilline à partir des hydrogels dans différents milieux (acide, neutre et basique) montre que l'équilibre est atteint après 15 mn de contact. De plus, la meilleure libération (3.53 g/L) est enregistrée dans le milieu neutre.

**Mots-clés**: Amidon, Alginate, Hydrogel, Principe actif, Libération.

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**Poster communication** **P-174**

# Synthesis and investigation of antioxidant and antibacterial activities of symmetrically triazinane derivatives

Zouchoune Soria [1*], Lefrada Leila[1], Bouchemma Ahcene[2]

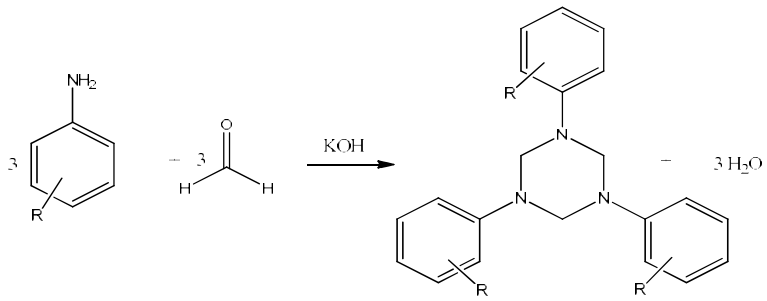
[1-] *Laboratory of Analytical Sciences Materials and Environment LSAME, Faculty of Exact Sciences and Sciences of Nature and Life, Larbi ben M'Hidi University, 04000 Oum El Bouaghi, Algeria*

[2-] *Laboratory of Applied Chemistry and Materials Technology LCATM, Faculty of Exact Sciences and Sciences of Nature and Life, Larbi ben M'Hidi University, 04000 Oum El Bouaghi, Algeria*

**E-mail :** soria.zouchoune@univ-oeb.dz

**Abstract**

Symmetrically triazinane derivatives are a family of nitrogen heterocyclic. They are well-known to possess various biological properties; they are also of considerable interest because of their synthetic utility as metal ligands in symmetric catalysts in organic synthesis. The primary goal is an efficient synthesis of symmetrically 1,3,5-triazinanes via a condensation reaction from three equivalents of primary amines and three equivalents of formaldehyde in a potassium hydroxide solution with good yields **(Scheme)**. The structure of these compounds has been characterized by ultraviolet-visible spectroscopy (UV-Vis), infrared spectroscopy (IR), thin-layer chromatography (TLC), nuclear magnetic resonance spectroscopy 1H and 13C, and melting point. The second object was these compounds' evaluated antibacterial and antioxidant activities. The antibacterial activity of these compounds was tested against four bacterial strains, including one Gram-positive bacteria and three Gram-negative bacteria, using the agar diffusion method. The antioxidant activity was also examined using ABTS and Phenanthroline assays.




**Scheme**

**Keywords**: synthesis, triazinane derivatives, antibacterial, ABTS assay, Phenanthroline assay.

**Poster communication** **P-175**

# Green Synthesis of zinc and silver nanoparticles for the degradation of organic pollutants in wastewater

Daoiya Zouied[1*] ; Malika Khefaoui[1]; Mohamed boubessil[2]

[1]*Laboratory of Chemical Engineering and Environment of Skikda (LGCES), University-20 Aout-1955-Skikda, Algeria.*
[2]*Laboratory of Stimulation and Biological and Environmental Processes, University-20 August-1955-Skikda, Algeria.*

**E-mail:** ch_hanine@yahoo.fr

**Abstract**

This work was devoted to the study of the synthesis method of three nanoparticles which are AgO, ZnO and a mixture Ag/ZnO based on CC plant extract followed by the application of these nanoparticles in the photodegradation of an aqueous solution of Crystal Violet (300 ppm). The results obtained show that the photodegradation efficiency of the dye in the presence of ZnO; Ag and Ag doped on Zn increases with time until reaching a value of 90.65% for 0.6 g of ZnO, for 0.3 g of Ag O reaches 95.33% while for 0.3 g of Ag/Zn O was 100% after a time of 90min. The use of mixture aims to minimize the use of Ag which is too expensive and increase the degradation efficiency.

**Keywords**: Green synthesis, CC plant extract, AgO, ZnO, mixture Ag/ZnO, Crystal Violet degradation.

**Poster communication** **P-176**

# A simple and eco-friendly method for the synthesis of new substituted benzothiazoles containing benzenesulfonamide

Chafika BOUGHELOUM [*1], Soumaya BOUSKIA [1]

[1] *Laboratory of Advanced Systems and Materials, Sciences Faculty, Badji Mokhtar-Annaba University, P.o.Box 12, Annaba. 23000, Algeria.*

**E-mail**: chafika.bougheloum@univ-annaba.dz

**Abstract**

A variety of biological activities, including antitumor, antimicrobial, and antiviral properties, are displayed by heterocyclic compounds, which frequently contain benzothiazoles and their derivatives. They can also be used as antioxidants, vulcanization accelerators in industry, and dopants in light-emitting organic electroluminescent devices. Due to the importance mentioned above, the synthesis of substituted benzothiazoles has attracted a lot of attention in recent years. Sulfonamide group may also change the bioactivity of organic molecules when they are added to them. Recently, there has been an ongoing effort to use supported catalysts or reagents. This is mainly due to their advantages, such as non-corrosivity, high selectivity, mild reactions conditions, and ease of work-up. Among of them, $FeCl_3$ supported on Montmorillonite K10 ($FeCl_3$/M K-10) has attracted considerable attention because of its desirable characteristics.

In this context and in continuation of our interest toward developing novel biologically important compounds, we report the $FeCl_3$/M K-10-catalyzed one-pot reaction between 2-aminobenzothiazole, cyclic anhydrides and various sulfonamides under ultrasound.

The synthesis of substituted benzothiazoles containing benzenesufonamide unit was completed with excellent yields and shorter reaction times, and their structures were systematically characterized by $^{1}$HNMR, $^{13}$C NMR and SM.

**Keywords:** Benzothiazoles, benzenesulfonamides, $FeCl_3$/M K-10, catalyst, ultrasound.

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**Poster communication** **P-177**

# Synthése et étude théorique d'un nouveau dérivé de sulfamide

Boussaker meriem*[1], Marminon Christelle[2], Berredjem malika[1]

[1]*Laboratoire de Chimie Organique Appliquée, Groupe de Synthèse de Biomolécules et Modélisation Moléculaire, Université Badji-Mokhtar. Annaba. BP 12, 23000 Annaba*

**E-mail:** Boussaker.m@gmail.com

**Resumé**

Les sulfamides sont des composés organiques les plus couramment utilisés, ils ont été utilisés pour exposer un large éventail d'activités biologiques, y compris des propriétés, antifongique, anticonvulsivant, agents hypoglycémiques, agents antipaludiques, Anti-VIH et comme inhibiteurs de protéase

Vu l'importance thérapeutique des deux motifs, notre travail a été orienté vers l'addition du sulfamide par la réaction de carbamoylation sulfamoylation sur l'amine 6-amino-2,3-dihydro-1H-inden-1-one (2) qui a été obtenue par la réduction de $NO_2$ afin d'obtenir un nouveau dérivé du sulfamide (3)

Une étude théorique par ADMET pour le nouveau dérivé a été effectuée.

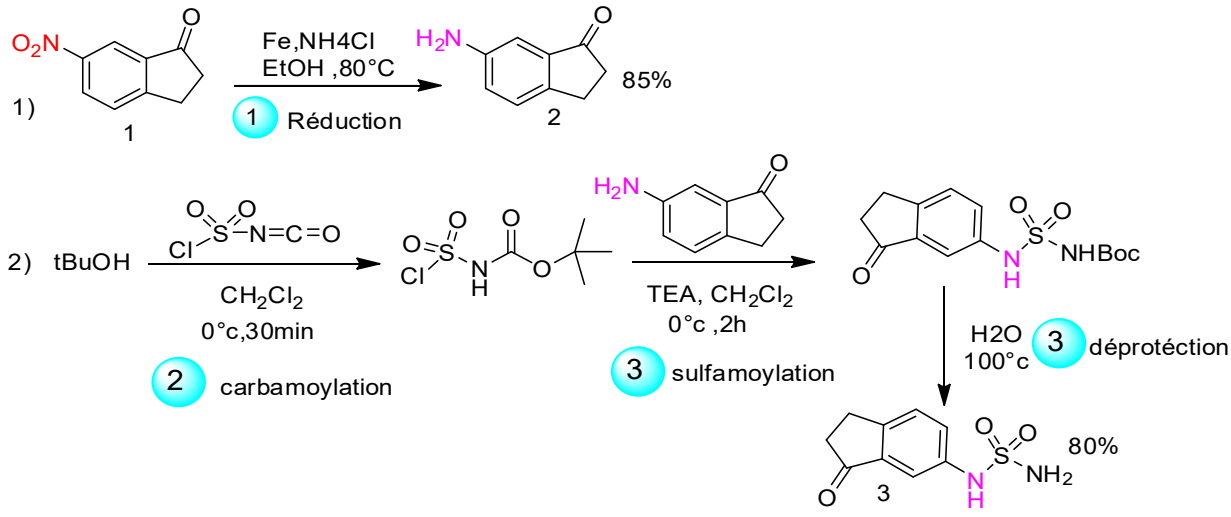


**Schéma 1**: Synthèse d'un nouveau dérivé de sulfamide.

**Mots-clés** : sulfamide, synthése, indenoindole, réduction, carbamoylation, sulfamoylation.

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# Efficient synthesis of magnetic activated carbon for improved adsorption of Rhodamine B dye from aqueous solutions

Amel RIAH [1], Salim BOUSBA [1], Dhirar BEN SALEM [2]

[1] *University of Constantine 03 Saleh Boubnider, Department of Chemical Engineering, Constantine, Algeria*

[2] *Research Laboratory in Subterranean and Surface Hydraulics, University of Biskra, PO Box 145, Biskra 07000, Algeria.*

**E-mail** : amel.riah@univ-constantine3.dz

**Abstract**

This study aimed to prepare a low-cost and efficient adsorbent for RhB removal from water. The adsorbent, labeled CAM, was designed through the one-step pyrolysis process of the olive pit waste at 600°C and then filled in the iron nanoparticle. Different techniques characterized the sample techniques and then subjected to the adsorption batch experiments. The effect of several key factors like solution pH, stirring time, and isothermal conditions on copper ions uptake has been investigated. Moreover, the adsorption behaviour and mechanism of the aqueous metal were discussed. From the results, the pHpzc of CAM is 5.8, kinetic data followed the pseudo-second-order perfectly. Isotherms study revealed that the Langmuir model was appropriate to simulate the adsorption data. The maximum adsorption capacity (Qmax) was calculated to be 267.4 mg/g. The absorption operation was affected by pH change. 50°C was chosen to be the suitable temperature to remove RhB from water. CAM adsorbent is eco-friendly and could be used for the future industrial scale.

**Keywords**: Magnetic Activated Carbon, Rhodamine B, Adsorption, Removal, adsorbent

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**Poster communication** **P-181**

# A novel, rapid and eco-sustainable approach for synthesis of malonamide derivatives as potent urease inhibitors

Billel BELHANI [a], Mohammed AISSAOUI [a], Salah Lakrout [a], Hacene K'TIR [b], Sofiane ALI RACHEDI [c].

[a] *Laboratory of Synthesis and Organic Biocatalysis, Department of Chemistry, Badji-Mokhtar-Annaba University, Algeria*

[b] *Laboratory of Applied Organic Chemistry, Department of Chemistry, Sciences Faculty, Badji-Mokhtar-Annaba University, Annaba, Algeria*

[c] *Environmental Research Center (CRE), Annaba 23000, Algeria*

**E-mail**: billelbelhani@yahoo.com

**Abstract**

Recently, malonamide derivatives have garnered significant attention in the research community due to their pharmaceutical and biological significance, particularly for their antimicrobial, enzyme inhibitory, and anticancer properties. Additionally, malonamide derivatives have been reported to exhibit significant inhibitory effects on urease activity.

Several methods for synthesizing malonamide derivatives have been developed; however, many of these approaches rely on expensive catalysts and solvents, require harsh acidic conditions and elevated temperatures, and involve lengthy reaction times. In response to these limitations, our research group is focused on discovering novel bioactive compounds using green chemistry approaches. In this study, we report the synthesis of malonamide analogs using a novel, eco-friendly method involving microwave irradiation. Furthermore, we assess the urease inhibitory activity of these analogs. The findings of this study may offer a safer and more sustainable route for the discovery of new scaffolds with potential applications in the pharmaceutical field.

The synthesized compounds were evaluated for their urease inhibitory potential. All analogs exhibited varied degrees of urease inhibitory potential with IC50 values ranging between 0.01 ± 0.001 and 0.08 ± 0.01 mM, when compared with thiourea as the standard urease inhibitor (IC50= 0.13 ± 0.02 mM). Among the tested derivatives, compound 3d (0.01 ± 0.001, 0.0µM) was identified as the most potent inhibitor of urease.

**Keywords**: Malonamide, Microwave Irradiations, Catalyst-free, Solvent-free, Urease inhibitor.

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**Poster communication** **P-183**

# Ultrasound-assisted synthesis and DFT sudies of novel Schiff Bases '(E)-6-{[(4-Methoxyphenyl)imino]methyl}-3- methyl-1,3-benzothiazol-2(3H)-one' in an ionic liquid medium

Yasser Bouchebcheb[1]*, Aya Alem[1], Dalila Fedaoui[1], Messaoud Liachaa[1]

[1]*Laboratory of Synthesis and Organic Biocatalysis (LSBO), Organic Synthesis and Medicinal Chemistry Group, Department Of Chemistry, Faculty of science, BADJI Mokhtar-Annaba University, P.O. Box 12, Annaba 23000, Algeria*

**E-mail:** bouchebchebyasser@gmail.com
yasser.bouchebcheb@univ-annaba.dz

**Abstract**

The benzothiazolinone heterocycle is included in many biologically-oriented molecule industries due to its diverse biological properties [1], adding to Schiff bases that have caught the attention of researchers since antiquity since it was first discovered by Hugo Schiff in 1864 [2], since when researchers have been interested in methods to obtain this imine function. With the emergence of a culture of respect for the environment during synthesis, known as green chemistry, researchers have developed their methods in this format using environmentally-friendly methods such as ultrasound and green solvents [3-5].

In this context, we have synthesized the imine benzothiazolinone derivative (E)-6-{[(4-Methoxyphenyl)imino]methyl}-3- methyl-1,3-benzothiazol-2(3H)-one following a green chemistry approach using ultrasound and ionic liquid [TEAA]. This method is effective in several respects: reduced time and high yield, not to mention easy and pure recovery of the final compound.

The structure of the newly synthesized derivative was established on the basis of IR, $^{1}$HNMR and $^{13}$C NMR spectroscopic techniques. In addition, the theoretical investigation of HUMO, LUMO, gap energy and reactivity indices for the molecule was carried out using the DFT method with B3LYP/6-31G (d,p) basis set.

**Keywords**: 3-methyl-1,3-benzothiazol-2(3H)-one, ionic liquid, green chemistry, ultrasonic irradiation, DFT.

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**Poster communication** **P-184**

# Synthese et evolution antibacterienne de nauveaux derives des n-acylhydrazones benzoxazinoniques

CHETTIBI Naouel, LIACHA Messaoud

*Laboratoire de Synthèse et Biocatalyse Organique (LSBO), Faculté des sciences, Département de chimie, Université BADJI Mokhtar-Annaba, B.P. 12, Annaba 23000, Algérie.*

**E-mail** : nawelchettibi23@yahoo.fr

**Résumé**

Les composés N-hétérocyclique présentent depuis longtemps une classe importante en raison de leurs diverses applications thérapeutiques et synthétique,[4] grâce à leurs propriétés particulières venant de la présence d'un atome d'azote. Les 2-H-benzoxazin-3(4H)-ones sont parmi les composés azotés les plus utilisés en synthèse organique, ce sont également des synthons utiles pour plusieurs produits naturels et de molécules bioactives. Ces propriétés particulières leurs ont donné une très grande importance dans l'industrie pharmaceutique et agrochimique, [5] et aussi pour leurs diverses applications telles que pesticides, bactéricides. [6] Dans ce contexte, nous rapportons dans cette étude de recherche, une méthode simple et efficace pour la synthèse de nouveaux dérivés N-acylhydrazones benzoxazinoniques. Les structures des dérivés synthétisés ont été élucidées et caractérisées sur la base de la spectroscopie FT-IR, 1H-RMN et 13C-RMN. De plus, une étude préliminaire sur l'activité antibactérienne et antifongique in vitro de ces composés a été réalisée. Tous ces composés présentaient une activité antibactérienne remarquable. Ils ont montré une activité antifongique modérée, la plupart d'entre eux ont été trouvés inactifs.

**Mots-clés** : 2-H-benzoxazin-3(4H)-ones, N-acylhydrazones, Activité antibactérienne, Activité antifongique.

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**Poster communication** **P-186**

# Marine-derived compounds as potential inhibitors of Hsp90 for anticancer and antimicrobial drug development

Nada Anede [1], Mebarka Ouassaf [1]

*Group of Computational and Medicinal Chemistry, LMCE Laboratory, University of Biskra*

**E-mail**: nada.anede@univ-biskra.dz

**Abstract**

Marine compounds constitute a diverse and invaluable resource for the discovery of bioactive substances with promising applications in the pharmaceutical development of anti-inflammatory and antibacterial agents. In this study, a comprehensive methodology was employed, encompassing pharmacophore modeling, virtual screening, in silico ADMET assessment (encompassing aspects of absorption, distribution, metabolism, excretion, and toxicity), and molecular dynamics simulations. These methods were applied to identify new inhibitors targeting the Hsp90 protein (heat shock protein 90), commencing with a diverse assembly of compounds sourced from marine origins. During the virtual screening phase, an extensive exploration was conducted on a dataset comprising 31,488 compounds sourced from the CMNPD database, characterized by a wide array of molecular structures. The principal objective was the development of structure-based pharmacophore models, a valuable approach when the pool of known ligands is limited. The pharmacophore model DDRRR was successfully constructed within the active sites of the Hsp90 crystal structure. Subsequent docking studies led to the identification of six compounds (CMNPD 22591, 9335, 10015, 360799, 15115, and 20988) demonstrating substantial binding affinities, each with values below −8.3 kcal/mol. In the realm of in silico ADMET predictions, five of these compounds exhibited favorable pharmacokinetic properties. Furthermore, molecular dynamics simulations indicated that these marine-derived compounds formed exceptionally stable complexes with the Hsp90 receptor over a 100-nanosecond simulation period. These findings underscore the considerable potential of these novel marine compounds as promising candidates for anticancer and antimicrobial drug development.

**Keywords**: anticancer; anti-bacterial agents; marine bioactive molecules; drug discovery; docking simulations; ADME; molecular dynamics simulat

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**Poster communication** **P-187**

# Contribution of molecular docking in the management of Herb/drug interactions in oncology

Saida Hanane ZITOUNI-NOURINE[1], Salim Bouchentouf [2], Fatima El-Houaria Zitouni-Haouar [3], Nesrine Zenai [1], Samira Boudia [1], Sarah Bouderbala [1] , Faiza Bereksi Reguig [4] , Houari Toumi [1]

[1]*Pharmaceutical Development Research Laboratory, Department of Pharmacy, Faculty of medicine, Oran 1 Ahmed Ben Bella University, Algeria*

.[2] *Moulay Taher University of Saida , algeria ,Laboratory of natural and bioactive substances-University of Tlemcen, Algeria*

[3] *Laboratory of Microorganism Biology and Biotechnology, Department of Biotechnology, Faculty of Natural Sciences and Life, Oran 1 Ahmed Ben Bella University, Algeria.*

[4] *Medical oncology department, university hospital 1 st November Oran.*

**E-mail** : zitounisaidahanane83@gmail.com

**Abstract**

**Introduction**

Cancer is one of the most complex and challenging diseases known to humankind and an inevitable public health concern. It was responsible for 8.2 million deaths in 2012. Herbal medicine has marked a comeback in the treatment of various diseases including cancer, the extent of this alternative medicine in patients under other conventional treatments poses a problem of interactions, causing toxicity or therapeutic failure.

**Materials and methods**

The first objective of this study is to identify the oral antineoplastics available in pharmacies and hospitals in the Oran region (Algeria). Secondly, the evaluation of the probable interactions between three of the most used medicinal plants in oncology in the region of Oran (Atriplex halimus L. Haloxylon scoparium pomel. and Prunus Persica L) and Cytochromes as well as the transporters implied in the metabolism of the oral antineoplasics,by using a computer simulation software MOE molecular docking, given that there are no data in the literature on the interactions that these plants can cause if taken concomitantly with these drugs.

**Results and discussion**

We found that theoretically there is an affinity between some cytochromes and the studied phytochemicals, the active complexes formed with CYP3A4, CYP3A7 and CYP2A6 were the most important when comparing their docking scores with the reference scores.

**Conclusion**

This work must absolutely be completed by in vitro and in vivo studies and even clinical trials, in order to adapt the dosage and the method of use of these plants for a safe and rational use.

**Keywords :** Cancer, medicinal chemistry, molecular docking, herb-drug interactions

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**Poster communication** **P-188**

# Inhibitive effect of bithiophene isomers on mild steel corrosion in 1M hydrochloric acid medium: theoretical approaches

Belgacem Bezzina[*1,2], Safia Himri[2], Mohamed Tayeb Abedghars[1],Amel Oulabbas[1],Hadria Ferdenache[1], Khedidja Bouhamla[1], Djameleddine Khatmi[3]

[1]*Research Center in Industrial Technologies (CRTI), Cheraga, P.O.BOX 64, 16014 Algiers, Algeria*

[2]*Laboratory of Computational Chemistry and Nanostructures, University of 08 May 1945, Guelma, Algeria*

[3]*CTOM, ISM2, Aix Marseille University, Marseille, France*

**E-mail**: b.bezzina@crti.dz

**Abstract**

The corrosion inhibition properties of three bithiophene isomers, namely 2,2-, 2,3- and 3,3-bithiophene, were investigated computationally on mild steel with Fe (110) in 1M HCl corrosive medium using Monte Carlo simulation and density functional theory (DFT) calculations**.** The three bithiophenes show high negative adsorption energies, which indicate that their adsorption on metal surface is stable and spontaneous, especially 3,3-bithiophene. All bithiophene molecules on the metal surface exhibit the most favorable adsorption configurations when positioned parallel to the steel surface, resulting in increased surface coverage and preventing direct contact with the acid medium, thereby achieving high inhibition efficiency. The inhibition efficiency of bithiophene isomers correlates well with some quantum chemical descriptors, and they follow the order 3,3-bithiophene > 2,2-bithiophene > 2,3-bithiophene. A radial distribution function study confirmed that bithiophene isomers could form protective layer by chemical adsorption on mild steel surface. The simulation data proved that all inhibitors could adsorb on metal surface through π electrons of the thiophene rings and lone pairs of electrons of S atoms.

**Keywords**: bithiophene, adsorption, Monte Carlo simulation, inhibition efficiency, DFT.

**Poster communication** **P-189**

# Docking studies of novel monovalent and bivalent Benzenesulfonamide incorporating 1,2,3-Triazole scaffold as potential carbonic anhydrase IX and XII inhibitors

Zeyneb Ourdjini, Achour Seridi *

*Laboratoire de Chimie physique, Université 8 Mai 1945, Guelma, 24000, Algérie*

**E-mail :** ourdjini.zeyneb@gmail.com

**Abstract**

Human carbonic anhydrase isoforms IX and XII have recently been identified as anticancer targets in solid hypoxic tumours. The selective inhibition of CA IX and XII isoenzymes by small-molecule CA inhibitors, such as sulfonamide derivative has been shown to inhibit many cancer models [1-3]. In this theoretical study, we performed the docking simulation by using Molegro Virtual Docker (MVD) program to investigate the inhibition of carbonic anhydrase IX and XII by a series of monovalent and bivalent benzenesulfonamide derivatives based on 1,2,3-triazole-pyridine in order to suggest its mode of inhibtion into the active site of hCA IX and hCA XII and to understand some structural observations about their binding modes and their binding interaction (**Figure 1**). Our data reveals that all of the compounds we tested have exhibited a favorable docking score against hCA IX and hCA XII, suggesting a strong affinity potential for these proteins.

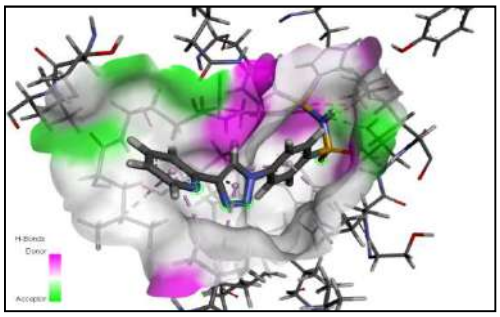

**Fig.1**: The docked pose of compound (1,2,3-triazole-pyridine based monovalent benzenesulfonamide) and the residues of Side chain in the cavity of the active site hCA IX. Hydrogen bonds are indicated in dashed green lines.

**Keywords :** hCA IX and hCA XII, Monovalent and bivalent benzenesulfonamide, DFT, Molecular docking.

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**Poster communication** **P-190**

# Identification de nouveaux composés, anticancéreux, phytochimiques marins par Docking moléculaire

Layachi. F[1], Ait kaki. S[1], Neghra.A[1], Kraim.K.E[2], Ferkous.F[2]

[1] *Laboratoire de Chimie Thérapeutique, Faculté de Médecine. Université Badji Mokhtar. Annaba*
[2]*Laboratory of Organic Chemistry Applied in the Organic Applied Synthesis and Bioconversion Group/University Badji Mokhtar-Annaba Faculty of Sciences Department of Chemistry*

**E-mail**: fay23th@yahoo.fr

**Résumé**

Les composés naturels phytochimiques d'origine marine constituent actuellement des points de départ précieux pour la chimie médicinale et la découverte de médicaments, du fait que l'écosystème marin abritent une biodiversité exceptionnelle avec une activité biologique prometteuse notamment contre le cancer sous des mécanismes d'action nouveaux et uniques.
En Algérie, le cancer du col de l'utérus représente 10.5 % des cancers féminins et occupe la 2e place après celui du sein. C'est une tumeur maligne développée à partir de la muqueuse du col utérin dont le facteur de risque principal est la présence prolongée du papillomavirus (HPV)

Les poly-(ADP-riboses) Polymérases (PARP1) sont des enzymes impliquées dans la réparation de l'ADN pour les cassures simple brin.

Pour les cellules tumorales, la régulation de la réparation des cassures simple brin par la voie de réparation par recombinaison homologue (HR) est inopérante du fait de l'inhibition de PARP1 ce qui entraîne un arrêt du cycle cellulaire conduisant à l'apoptose de la cellule.

Notre travail est une contribution au développement de nouveaux inhibiteurs de la PARP1 par criblage virtuel en prenant comme point de départ plusieurs chimiothèques marines a partir des banques de données Marines Seaweed Metabolite Database et Comprehensive Marine Products Database (CMNPD). Après docking moléculaire par le logiciel Molegro, nous avons sélectionné 17 molécules sur la base de leur énergie et après visualisation des interactions avec les acides aminés clés.

Enfin l'étude prédictive des propriétés, physico-chimiques, pharmacocinétiques et toxicologiques de ces molécules a fait ressortir les molécules RL326, RL514, RL125, RL079, RL372, et BS052 comme nouveaux inhibiteurs de cette enzyme.

En termes de perspectives d'avenir, ce travail pourra être complété et prolongé par une étude expérimentale in vitro et/ou in vivo afin de valider nos résultats et vérifier l'efficacité de l'approche in silico.

**Mots-clés:** Docking moléculaire, Molegro, inhibiteurs de la PARP-1, cancer du col de l'utérus.

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**Poster communication** **P-191**

# Conception d'une molécule à affect antibactérien issue d'origine naturelle par docking moléculaire

RAHMANI Amina[1]*, MERADI Laarem[1]

[1]*Université LARBI BEM MHIDI, département des sciences naturelles et de la vie - Laboratoire de biotechnologie des substances naturelles et applications*

**E-mail:** aminarahmani311@gmail.com

**Resumé**

Les plantes médicinales ont été utilisées pour soigner une très grande variété de maladies, elles sont aujourd'hui largement utilisées pour leurs propriétés thérapeutiques par des composés bioactifs ayant plusieurs activités telles qu'antimicrobiennes, antioxydantes, antiparasitaires, antifongiques et anticancérigènes. Il est donc impératif de rechercher des agents antimicrobiens naturels structurellement différents à ceux obtenus par synthèse chimique, capables de tuer les mutants résistants aux antibiotiques avec moins d'effets secondaires. Cependant, la découverte de médicaments est un processus difficile, Ainsi dans notre travail on a pu faire un docking moléculaire, qui est un criblage virtuel faisant partie des techniques de conception de médicaments assistée par ordinateur (CDAO). C'est l'outil de choix lorsque la structure tridimensionnelle (3D) de la protéine cible est disponible. L'affinité entre la protéine et l'enzyme a été réalisé avec le logiciel Autodock Vina, et nos résultats obtenus par le docking révèlent que les valeurs les plus négatives du ΔG (kcal/mol) des huiles essentielles présentent la meilleure activité d'inhibition de la production des beta lactamases à spectre étendu (BLSE) chez les bactéries résistantes testées, ces valeurs ont été obtenues pour les composés phénoliques de chaque huile essentielle. Finalement le docking moléculaire a permis de concevoir une interaction entre une petite molécule (ligand) et une macromolécule cible (protéine) en sachant exactement comment et où un ligand se lie, ce qui permet de concevoir rationnellement des changements pour optimiser l'interaction entre la protéine et le ligand. La propagation de la résistance aux antibiotiques constitue une menace imminente pour la santé animale et humaine et le développement de nouvelle molécule devient une nécessité afin de stopper l'apparition de souches bactériennes multirésistantes aux antibiotiques de synthèse chimique.

**Mots-clés**: BLSE, composés phénoliques, docking moléculaire, huile essentielle, ligand, protéine.

**Poster communication** **P-192**

# Analyse QSAR de la toxicité des anilines et phénols substitués

HAMADA Hakim

*Materials and Environment Analytical Sciences Laboratory*
*Larbi Ben M'hidi* University - *Oum El Bouaghi*

**E-mail**:hakimannaba2178@yahoo.fr

**Abstract**

QSAR methodology was performed on literature data concerned with the toxicity of de 113 phenols and anilines , characterized by the 50 % inhibitory growth concentration (IGC50) of a population of Tetrahymena pyriformis. Hence, log of the inverse of the IGC50 (dependent variable) was correlated with two significant regressors: the square of the octanol / water partition of (GhoseCrippen (ALOGP)² and descriptors GETAWAY(REIG (first eigenvalue of matrix R)

The statistical parameters obtained for the calibration and validation sets (multiple determination and prediction coefficients, the roots of the mean square errors), ($R^2$ = 91.96% , $Q^2$ = 91.36%, SEDC = 0.177, SEDP = 0.184, $SEDP_{ext}$ = 0.200 et $Q^2_{ext}$ = 93.2%) highlight the quality and relevance of the calculated model

**Keywords**: toxicity; Tetrahymena pyriformis; methodology; statistics; validation; models

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**Poster communication** **P-194**

# Quantum mechanical study of complexation of 2-aminofluorene with β-cyclodextrin

Imene DJILANI [1]*, Leila NOUAR [2]

[1] *Lab. of Physical Chemistry and Biology of Materials. Higher Normal School of Technological Education – SKIKDA-B.P. Cité frères Bousseta Azzaba Skikda - Algeria.*
[2] *Lab. of computationel chemistry and nanostructure. University of 8 Mai 1945 Guelma- B.P. 401 GUELMA 24000 - ALGERIA*

**E-mail:** djilaniimene@gmail.com

**Abstract**

We simulated the docking of 2-aminofluorene in β-Cyclodextrin using two models. We considered in this study complexes formed by 1:1 host- guest stoichiometry in vacuum and aqueous phase, using PM6, DFT calculations.

The results obtained with PM6 method clearly indicate that the complexes formed are energetically favored with or without solvent,

Upon encapsulation, binding energy, thermodynamic parameters, structural parameters and electronic structures of complexes are investigated.

The structures show the presence of several intermolecular and hydrogen bond interactions between the host molecule and 2-aminofluorene

**Keywords**: 2-aminofluorene, β-Cyclodextrin, inclusion complex, PM6, DFT.

**Poster communication** **P-195**

# Approche de la pharmacologie computationnelle pour l'étude in silico des composés naturels qui ciblent sélectivement l'inhibition de l'acétylcholinestérase.

OTMANI Amar [a], ZAIDI Hicham [a], OUCHEMOUKH Salim [a]

[a] *Laboratoire de Biochimie Appliquée, Faculté des Sciences de la Nature et de la Vie, Université de Bejaia, 06000 Bejaia, Algeria.*

**E-mail:** amar.otmani@univ-bejaia.dz

**Resumé**

L'objectif de ce travail est d'étudier la capacité de certains composés naturels, comme les acides phénoliques, les flavonoïdes et les térpanoïdes, à inhiber l'activité de l'acétylcholinestérase. Cette enzyme est impliquée dans l'apparition des troubles de la mémoire et la démence chez les patients atteints de la maladie d'Alzheimer. Afin de déterminer l'énergie de liaison entre les ligands et la protéine, un docking moléculaire a été réalisé à l'aide du logiciel Autodock Vina. Les propriétés pharmacocinétiques, pharmacodynamiques et toxicologiques de ces composés ont également été étudiées à l'aide des méthodes in silico. Les résultats obtenus ont montré que la lutéoline, le kaempférol, la galanthamine et le gallate d'épigallocatéchine donnaient la plus faible énergie de liaison et la meilleure affinité, ce qui indique qu'ils sont les meilleurs inhibiteurs de l'acétylcholinestérase. Tous ces ligands sont situés dans la même poche de site actif de l'acétylcholinestérase et se lient à cette enzyme avec diverses interactions telles que des interactions hydrophobes et des liaisons hydrogène. Pour l'analyse in silico des propriétés pharmacocinétiques, la lutéoline et le kaempférol ont donné les meilleurs résultats par rapport à l'inhibiteur de référence, la galanthamine. Les deux composés répondaient aux critères ADME au terme de poids moléculaire, de lipophilie, de solubilité dans l'eau et des règles de Lipinski, Veber, Muegge, Egan et Ghose ainsi que de biodisponibilité et d'accessibilité synthétique. Les résultats ont également montré que les deux composés ne sont pas mutagènes et ne provoquent pas de toxicité hépatique et ni d'irritation cutanée. Cette étude a révélé que la lutéoline et le kaempférol sont des inhibiteurs fonctionnels de l'activité de l'acétylcholinestérase et peuvent être considérés comme des composés candidats à inclure dans les stratégies de traitement symptomatique de la maladie d'Alzheimer.

**Mots-clés** : Acétylcholinestérase, in silico, composés naturels, propriétés pharmacocinétique, toxicité.

**Poster communication** **P-196**

# Optimisation des additifs organiques pour l'électrodéposition des alliages Zn-Ni : Approche par modélisation moléculaire

Nazih RIBOUH [1], Kaddeche CHEMS EL ACIL [1], Alem SAMIA [2], Samia AMIRAT [1], Yassira BOUTALEB [3], Fatima GUETTARI [1],Rabah REHAMNIA[1]

[1] *Laboratory Nanomaterials for Corrosion and Surface treatment LNCTS, faculty of sciences, Badji Mokhtar University, Annaba*

[2] *Laboratory of Aquatic and Terrestrial Ecology, department of biology, faculty of sciences, Badji Mokhtar University, Annaba*

[3] *Laboratory for water treatment and industrial waste recovery (LTEVD), Faculty of Sciences, Badji Mokhtar University, Annaba*

**E-mail:** nazih.ribouh@univ-annaba.dz

**Resumé**

L'électrodéposition de l'alliage Zn-Ni à partir d'un électrolyte chloré en présence de substances organiques telles que le SDS, la saccharine, le 2-butyne-1,4-diol et le citrate de sodium a été étudiée. Les courbes de voltammétrie cyclique révèlent que ces additifs inhibent le processus d'électrodéposition de l'alliage Zn-Ni et influencent sélectivement sa composition de phases et son apparence extérieure. Trois phases ont été identifiées. Les revêtements obtenus avec ces additifs présentent une meilleure résistance à la corrosion. La modélisation moléculaire montre que les propriétés électriques calculées des additifs peuvent accélérer et faciliter la sélection des électrolytes les plus performants, augmentant ainsi l'efficacité du processus de revêtement tout en réduisant les coûts de production.

**Mots-clés**: Électrodéposition, Additifs organiques, Modélisation moléculaire.

The 1st International Seminar on medicinal chemistry and green chemistry (1st IS MCGC - Annaba 2024)

**Poster communication** **P-197**

# Phenolic profile and in silico anti-hemorrhoidal activity of flavonoids from Cytisus villosus

Khadidja Boudebaz*, Karima Boussafi

*Laboratory of Pharmacology and Phytochemistry, Department of Chemistry, Faculty of Exact Sciences and Informatics, University of Jijel, 18000 Jijel, Algeria.*

**E-mail** : khadidja.boudebaz@univ-jijel.dz

**Abstract**

Nowadays, in silico methods are increasingly being employed in strategies for the discovery of new molecules with therapeutic potential. In this study, we relied on molecular docking methods to evaluate the anti-inflammatory activity of C. villosus, a plant widely used in traditional medicine for the treatment and management of various inflammatory conditions, including hemorrhoids. Hemorrhoids are a common condition characterized by inflammation and dilation of veins in the anal and rectal region. The phytochemical profile obtained from the LC-ESI-MS analysis of the crude extract of C. villosus allowed for the identification of nine diverse flavonoid structures, which may exhibit the best affinities for the target of interest, inducible cyclooxygenase (COX-2) (PDB code: 4PH9). Based on the LC-ESI-MS results, molecular docking work was conducted on these flavonoid derivatives using Autodock Vina and Discovery Studio to predict the affinity of these substances and discover new COX-2 inhibitors. Four flavonoids demonstrated greater inhibitory efficacy than the reference with energies ranging from - 11 to - 8.4 kcal/mol. Inhibition of COX-2 blocks the production of prostaglandins by inhibiting the activity of the cyclooxygenase enzyme (COX). Specifically, prostaglandin E2 (PGE2) produced by rectal cells may be involved in the inflammatory processes and pain associated with hemorrhoids, contributing to hyperalgesia, increased vascular permeability, and vasodilation. COX-2 inhibitors can be used to treat inflammation and pain associated with rectal conditions.

**Keywords**: Cytisus villosus, Flavonoids, Hemorrhoids, Inflammation, COX-2.

**Poster communication** **P-198**

# Processuce d'inclusion du complexe Lidocaïne/β-cyclodextrine: Une étude d'analyse DFT, Hirshfeld et HOMO-LUMO

Amira Kadri[*a], Ouassila Attoui Yahia[a]

[(a)]*Laboratoire de chimie organique appliquée, groupe de synthèse de biomolécules et modélisation moléculaire, faculté des sciences, département de chimie, Université Badji Mokhtar-Annaba, BP :12, Annaba, 23000, Algérie.*

**E-mail** : amira.kadri07@gmail.com

**Résumé**

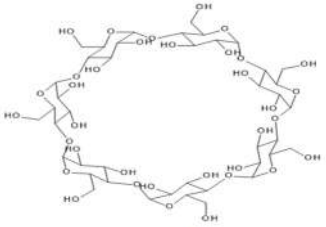
La chimie a pu s'enrichir d'outils informatiques spécialement conçus pour la représentation des molécules grâce à l'évolution significative des technologies informatiques ces dernières années. La modélisation moléculaire implique une description physique et tridimensionnelle des molécules, ce qui en fait désormais un élément quasiment indispensable dans toute étude en chimie, chimie médicale et biologie.

De nos jours, il est fréquent d'associer la recherche et la synthèse de nouveaux composés chimiques et biochimiques à une étude basée sur la modélisation moléculaire. Cela offre la possibilité de représenter non seulement les caractéristiques et les réactions chimiques, mais également de manipuler les modèles des structures en deux ou trois dimensions.

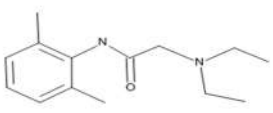
La création du complexe d'inclusion entraîne des changements dans les caractéristiques physico-chimiques des molécules invitées, notamment leur stabilité dans l'eau et leur stabilité en solution.

Dans ce travail, nous avons envisagé l'étude du processus d'encapsulation de l'anesthésique local la Lidocaïne, dans la cavité hydrophobe de la β-cyclodextrine par le docking moléculaire, pour envisager des différentes orientations possibles.

L'association moléculaire du complexe d'inclusion Lidocaïne/β-cyclodextrine donne des résultats satisfaisants, les deux conformations les plus efficaces identifiées ont démontré une bonne interaction avec la molécule invitée (lidocaïne), ses deux structures sont par la suite exposées à un calcul de mécanique quantique en utilisant l'approche ONIOM, qui permette d'analyses les diverses caractéristiques électroniques du complexe étudié, en se basant sur les méthodes hybrides QM/QM' mise en place dans le logiciel Gaussian. Étant données les résultats satisfaisants de la mécanique quantique, d'autres techniques de calcul seront mises en œuvre en utilisant les méthodes Hirshfield et HUMO-LUMO.



β-cyclodextrine



Lidocaine

**Mots-clés**: Modélisation moléculaire, Complexe d'inclusion, Docking moléculaire, Lidocaïne, β-cyclodextrine, ONIOM

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**Poster communication** **P-199**

# Theoretical study of Gallic and Rosmarinic acids as corrosion inhibitors for stainless steel in acidic environments

Sameh Athmani*[1, 2], Amel Sedik[1], Adel Saoudi[1], Belgacem Bezzina [3], Sihem Abderrahmane[2], Nabila Bouasla [2], Nawel Nadji[1], Djahida Lerari[1] and Khaldoun Bachari[1]

[1] *Centre de Recherche Scientifique et Technique en Analyses Physico-chimiques (CRAPC), Zone Industrielle, BP 384 Bou -Ismail, Tipaza, Algeria.*

[2] *Surface Engineering Laboratory (L.I.S); Department of chemistry; Faculty of Sciences; Badji Mokhtar -Annaba University. BP 12, 23000 Annaba, Algeria.*

[3] *Research Center in Industrial Technologies CRTI P.O. Box 64, Chéraga 16014 Algiers, Algeria.*

**E-mail**: samehathmani@yahoo.fr

**Abstract**

Recently, molecular dynamics simulations have proven to be an effective method for analyzing corrosion inhibition mechanisms. Numerous researchers have studied corrosion inhibition using molecular dynamics simulations. This study aims to evaluate the adsorption behavior of gallic acid (GA) and rosmarinic acid (RA), phytochemicals present in the Plectranthus amboinicus plant (PA), on a 304L stainless steel substrate in 1 M HCl. Density functional theory (DFT) calculations and Monte Carlo (MC) simulations were used in a focused modeling campaign to clarify the adsorption process. The computed quantum chemical parameters of GA and RA, such as total energy (ET), energy of the highest occupied molecular orbital ($E_{HOMO}$), energy of the lowest unoccupied molecular orbital ($E_{LUMO}$), dipole moment ($\mu$), ionization potential (I), electron affinity (A), electronegativity ($\chi$), global hardness ($\gamma$), and the fraction of electron transfer ($\Delta N$), were calculated. The results confirm that the GA and RA phytochemicals present in PA play an important role in corrosion inhibition. The majority of the HOMO orbital distribution for GA is located on the phenyl ring, whereas for RA, it is located over the benzyl-diol moieties, allowing these entities to act as electron acceptors with the metal surface. Conversely, the LUMO orbital distribution for GA is mainly found on the carboxylic group, while for RA, it is located on the hydroxy-phenyl-propanoate moieties, allowing these entities to act as electron donors. The adsorption energies of the inhibitors studied are significantly negative, confirming that the adsorption processes of GA and RA on the surface are spontaneous and thermodynamically favorable. The RA inhibitor shows relatively stronger adsorption compared to the GA inhibitor.

**Keywords**: Corrosion, Green inhibitor, Theoretical study, Environments.

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**Poster communication** **P-200**

# Organocatalyzed acylation of benzyl alcohol by an N-nucleophile: A combined experimental and theoretical study.

Khadidja Bougheloum[1]*, Mounia Merabet-Khelassi and Saoussen Zeror

[1]*Laboratory of Eco-compatible Asymmetric Catalysis (LCAE). Department of Chemistry, Faculty of Sciences, Badji Mokhtar Annaba University, BP12, 23000, Algeria.*

**E-mail:** khadidja.bougheloum@univ-annaba.dz

**Abstract**

Organocatalysts are considered an important development in green chemistry due to their ability to catalyze reactions without metals or metal ions. N-nucleophiles are easy-to-handle organocatalysts and are generally inexpensive. The activity of these organocatalysts largely depends on their nucleophilic character.

Transesterification is one of the classical organic reactions that have enjoyed many laboratory and industrial applications. Organic chemists often use this reaction as a convenient way to prepare esters.

The present study aims to undertake an experimental and theoretical study on a range of N-nucleophiles to observe the nucleophilicity effect and select the best catalyst.

For this, we have carried out an organocatalytic acylation of benzyl alcohol with acetic anhydride catalyzed by N-nucleophiles. We have shown the nucleophilicity effect at the theoretical level using DFT as a program.

**Keywords**: Organocatalysis, Catalysis, N-nucleophile, Acylation, DFT.

**Poster communication** **P-201**

# Spectroscopic and computational investigation of a novel charge transfer complex via hydrogen bonding between cyclomaltoheptaose and 2,3-dichloro-5,6-dicyano-1,4-benzoquinone

GHRIEB Hana[1], KADRI Mekki[2]

[1]*University of Algiers 1, Faculty of Medicine Algiers 16000*
[2]*Laboratory of Physical Chemistry (LCP), University of Guelma 24000*

**E-mail:** h.ghrieb@univ-alger.dz

**Abstract**

Charge transfer complex study remains of paramount importance in material science research. 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) as a famous and readily available π -acceptor, its charge transfer complexes have been the subject of extensive studies with different donors[1,2]. A novel charge transfer complex CTC including hydrogen bonding between cyclomaltoheptaose (β-cyclodextrin) as donor and 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) as π-acceptor has been synthesized and characterized experimentally and theoretically[3]. The solid complex was prepared and characterized by 1H NMR and FT-IR spectroscopies, the complex was formed in 1:1 ratio, with good evidences for existing both charge transfer and hydrogen bonding in its molecular structure. For supporting the experimental results, Density functional theory (DFT) computations were carried out using B3LYP/6-31G (d,p) method to compute the optimized structures of the reactant and complex. The analysis of DFT results strongly confirmed the high stability of the formed complex based on existing charge transfer beside proton transfer hydrogen bonding concordant with experimental results. Bader's atoms-in-molecule (AIM) and natural bonding orbital (NBO) calculations were analysed and discussed; they clearly demonstrate that a charge transfer was occurring between DDQ and cyclomaltoheptaose molecules. Theoretical studies propose that hydrophobic interaction and hydrogen bonding play significant role in determining the stability of the complexes.

**Keywords**: Cyclomaltoheptaose, DDQ, charge transfer, DFT, NBO, AIM.

**References:**

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[2] H. H. Eldaroti, S. A. Gadir, M. S. Refat, A. M. Adam, Int. J. Electrochem. Sci. 8 (2013) 5774-5800.

**[**3**]** H. Ghrieb, M. Kadri, Egypt. J. Chem. Vol. 65, No. 8, pp. (2022) 247 – 262.

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**Poster communication** **P-202**

# Prédiction par modélisation moléculaire la sélectivité de certaines réactions de cycloaddition

Chouit Hanifa, Messikh Samia, Sobhi Chafia

*Laboratory of Materials and Energetic Engineering, Faculty of Technology, University 20 August 1955 Skikda, BP 26, Road d'El Hadaiek -Skikda,21000, Algeria*

**E-mail:** hanifa2185@gmail.com

**Résumé**

Les réactions de cycloaddition constituent l'un des processus les plus importants en chimie organique qui ont été largement utilisées pour la synthèse des cycles et des hétérocycles. Les réactions de cycloaddition [3+2] des oxydes de benzonitrile sur les cyclopentènes β-substitués constituent une voie de synthèse élégante et efficace pour la préparation des agents peramivir. Ces composés ont trouvé une large utilisation dans le domaine médicinal comme médicament antigrippal. Récemment, Chien-Liang et al ont effectué expérimentalement des réactions de cycloaddition 32CA entre un oxyde de benzonitrile et une série de cyclopentènes β-substitués. Ils ont constaté que ces réactions 32CA procèdent via une 4-régiosélectivité complète avec des bons rendements de 76 à 87% (**Schéma 1**).

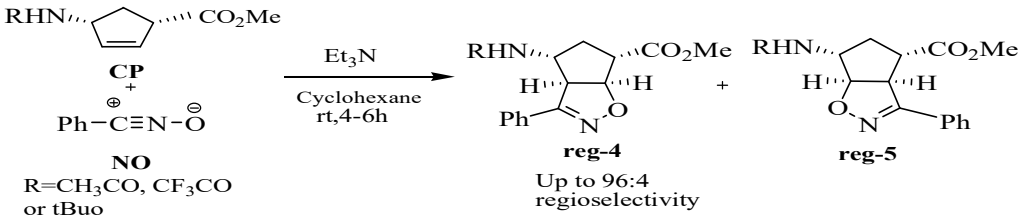


**Schéma 1.** Réaction de cycloaddition 32CA de NO avec cyclopentènes substitués

Pour comprendre l'origine de la sélectivité observée expérimentalement, nous avons utilisé la méthode théorique de la DFT dans la fonctionnelle ωB97XD avec la base standard 6-31G(d). Les énergies d'activation de ces réactions 32CA sont relativement élevées, en raison du faible pouvoir nucléophile des deux cycloalcènes CP et CP-f d'un côté et de la nature électrophile relativement modérée de l'oxyde de nitrile d'autre coté. La régiosélectivité complète obtenue le long du chemin 4-régioisomère a été expliquée par l'analyse des énergies relatives, dans laquelle la formation de cycloadduits 4-régioismères est toujours la plus favorisée cinétiquement. L'analyse topologique ELF a montré que les réactions 32CA étudiées procèdent selon un mécanisme non concerté en une seule étape et en deux paliers.

**Mots-clés**: Réactions 32CA, Oxyde de nitrile, Cyclopentène, Calculs DFT

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**Poster communication** **P-203**

# Design and in silico investigation of novel naphthalen-2-yl (2-oxoimidazolidine-1-carbonyl) sulfamate as urease inhibitor: molecular docking and ADMET prediction.

Dounia Beldjezzia[1*], Rayene sayad[1], Racha Ghodbane[1], Aicha Amira[1,2], Hacen k'tir[1,3]

[1]*Laboratory of Applied Organic Chemistry LCOA, Bio-Organic group, department of chemistry, sciences faculty, Badji-Mokhtar-Annaba University. Box12, 23000 Annaba Algeria*

[2]*Preparatory classes in sciences and technology department, national higher school of mining and metallurgy Amar Laskri-Annaba.*

[3]*Medical Sciences faculty, Badji-Mokhtar-Annaba University. Box 12, 23000 Annaba Algeria.*

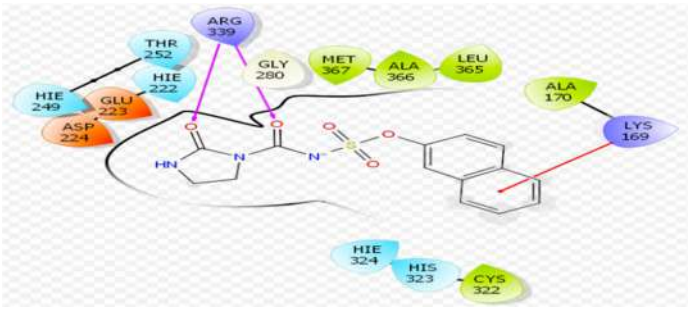
**E-mail**: beldjezzia.dounia96@gmail.com

**Abstract**

The importance of heterocyclic compounds has long been recognized in synthetic organic chemistry .Imidazolidines are five-membered heterocyclic scaffolds with two nitrogen atoms that are commonly used in drug discovery. sulfonyl urea derivatives are widely used to obtain compounds with different biological activities, including antimicrobial, anti-inflammatory, anticancer and anticoagulant, antihypertensive and antidiaetic agents.

The exceptional reactivity of these derivatives related to their structure made them very useful in organic synthesis as intermediates leading, to interesting compounds. Due to the importance of this type of pharmacophore, a new sulfonylurea derivative has been synthesized in high yields to explore the possibilities of some altered biological actions such as urease activity, in this work a docking simulation was performed to explore the binding mode of the prepared compound to the active site of main protease (PDB: 4UBP)

The synthesized molecule was also studied for evaluation of breast urease activity. Molecular docking was done with Acetohydroxamic Acid. An ADMET study was performed to predict the pharmacokinetic properties, toxicity of the compound. Our docking study was performed by using Maestro Schrödinger and we used the server SwissADME, PkCSM and PreADMET for the ADMET predictions.




**Keywords**: urea, urease activity, cyclic urea, molecular docking.

**Poster communication** **P-204**

# Etude computationnelle du mécanisme et de la régiosélectivité des réactions de cycloaddition

Samia Messikh, Hanifa Chouit, Chafia Sobhi

*Laboratory of Materials and Energetic Engineering, Faculty of Technology, University 20 August 1955 Skikda, BP 26, Road d'El Hadaiek -Skikda,21000, Algeria*

**E-mail:** sam_messikh@yahoo.fr

**Résumé**

Les réactions de cycloaddition [3 + 2] sont des procédures utiles pour la construction d'une variété de composés hétérocycliques à cinq membres, généralement avec un niveau élevé de régio- et de stéréosélectivité. Parmi les réactions de cycloaadition [3 + 2], les réactions des nitrones avec les allènes substitués offrent l'une des nouvelles méthodes pour la synthèse de dérivés d'isoxazolidines, qui sont présents dans de nombreuses molécules biologiques et produits naturels.

Notre étude a pour objectif d'étudier théoriquement la régiosélectivité et la stéréosélectivité de la réaction de cycloaddition [3+2] entre le N-méthyl-phénylnitrone et 1-sulfonyl-1-trifluorométhylallène. Cette étude a été réalisée dans le cadre de la théorie de la densité électronique moléculaire (MEDT) en utilisant les méthodes théoriques de la DFT au niveau théorique B3LYP/6-31G(d). Quatre voies compétitives ont été localisées et caractérisées, avec la formation du méta-exo comme isomère principal, se déroule via un mécanisme par étapes contrairement aux autres voies qui suivent un mécanisme en une seule étape. L'analyse des indices de réactivité explique le caractère polaire de cette réaction et l'analyse des fonctions de Parr locales nous permet d'expliquer la régiosélectivité observée expérimentalement. La présence du trifluorométhyle et du sulfonyle en tant que groupements électroattracteur augmente considérablement la réactivité de l'allène. L'inclusion de l'effet du solvant augmente légèrement les énergies d'activation et la stéréosélectivité de la voie méta-exo. L'analyse QTAIM révèle que la présence d'un nombre significatif d'interactions conventionnelles et non conventionnelles au niveau des deux TSs de la voie méta la plus favorable est responsable de la régiosélectivité observée expérimentalement.

**Mots-clés**: Cycloaddition [3 + 2], Nitrone, Allène, Sélectivité, Calculs DFT

**Poster communication** **P-205**

# The antioxidant properties and spectroscopic of novel heterocyclic compounds

Kaouther BAIRA[*1] and Fayçal BAIRA [1]

[1] *Department of Science and Technology, Faculty of Technology, University of BATNA2, Allées 53 rue Constantine. Fésdis, Batna 05078, Algeria.*

**E-mail:** kaouther.baira@univ-batna2.dz

**Abstract**

Our work is focused to perform quantum calculations using Density Functional Theory (DFT) to investigate the reactivity of three novel heterocyclic compounds: an azo dye (S1), an ester (S2), and a hydrazide (S3). The B3LYP method, paired with the 6-311 G (2d, 2p) basis set, has been utilized for this analysis. We have calculated the energies associated with three thermodynamic mechanisms: Hydrogen Atom Transfer (HAT), Single Electron Transfer followed by Proton Transfer (SET-PT), and Sequential Proton Loss Electron Transfer (SPLET). These calculations are intended to identify the most probable hydrogen atom transfer mechanism among the compounds studied. The DFT results indicate that the ester (S2) exhibits greater stability compared to both the azo dye (S1) and the hydrazide (S3).

**Keywords**: novel heterocyclic compounds, biological activity, DFT, TD-DFT.

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**Poster communication** **P-206**

# In silico targeting of the LasR Quorum sensing system: Towards new strategies to combat Pseudomonas aeruginosa virulence and biofilm formation

GRINE Nahla[1*], MNIF Sami[1], MENDIL Amina[2], GUENDOUZE Assia[3]

[1]*Laboratory of Molecular and Cellular Screening, Sfax Biotechnology Center, Tunisia*
[2]*Laboratory of Cellular and Molecular Biology, Faculty of Biological Sciences, Houari Boumédienne University of Science and Technology, BP 32 El-Alia Bab Ezzouar, 16111, Algiers, Algeria*
[3]*Laboratory of Applied Biochemistry, Department of Biochemistry and BCM, Faculty of Natural and Life Sciences, Mentouri Brothers Constantine 1 University..*

**E-mail**: grinenahla5@gmail.com

**Abstract**

Pseudomonas aeruginosa infections are becoming increasingly concerning due to the bacterium's growing antibiotic resistance and ability to form biofilms. Quorum sensing (QS), a chemical communication mechanism between bacteria, represents a promising target for new therapeutic strategies. Among these targets, the LasR protein, a key receptor involved in this bacterium's virulence, is particularly interesting. This study utilizes in silico approaches to identify novel LasR molecular inhibitors, aiming to reduce Pseudomonas aeruginosa virulence and biofilm formation, paving the way for more effective treatments.

Molecular docking, performed with the FlexX software, allowed the identification of potential LasR inhibitors from a library of 500 natural compounds, extracted from various essential oils of medicinal plants. The software's reliability was validated by an RMSD test and visual analysis. The results revealed that compounds 57 (CID: 11356918) and 4 (CID: 2345) exhibited the highest binding energies (-28.06 and -25.80 kJ/mol, respectively).

The study of ADMET (absorption, distribution, metabolism, excretion, toxicity) properties of compounds (57) and (4) yielded promising results, indicating their potential for development as therapeutic agents. These compounds exhibit pharmacokinetic and physicochemical characteristics favorable for medicinal use, with low toxicity.

**Keywords**: ADMET, molecular docking, drug discovery, LasR, quorum sensing, Pseudomonas aeruginosa.

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**Poster communication** **P-207**

# Study QSAR modeling to predict aquatic toxicity of benzene derivatives in Pimephales Promelas

[1]Ahmed bouaoune, [2]Nadia Ziani

[1]*Department, SM Alger 1 Benyoucef ben khada Algérie*
[2] *Département, de chimie Université Badji Mokhtar Annaba Algérie*

**E-mail** : a.bouaoune@univ-alger.dz

**Abstract**

The aquatic toxicity of 61 benzene derivatives have been subjected to quantitative structure-activity relationship studies. Optimization of 3D structures of the molecules carried out by Hyperhem using PM3 model. The molecular descriptors were obtained by Dragon software. The models were constructed using 49 molecules as training set and predictive ability tested using 12 compounds by Kennard and Stones Algorithm. The obtained model was chosen based on highest external predictive $Q^2$ values and lowest RMSEext values. The reliability of the proposed model was further illustrated using various evaluation techniques: leave-one-out cross-validation procedure, randomization tests, and validation through the test set. Modeling of log (1/LC50) of these compounds as a function of the theoretically derived descriptors was established by different approach (Multiple linear regression; Artificial Neural Networks; Support vector machine).

The statistical parameters obtained by three approaches are very similar, when confirmed that our model was stable, robust and significant. The values of Q2 and RMSE in internal validation are for MLR ($Q^2$ = **0.9222**, RMSE =**0.185**), SVM ($Q^2$ = **0.939**, RMSE = **0.167**) and NNA ($Q^2$ = **0.9294**, RMSE = **0.189**), while the values of $Q^2$ and RMSE in external validation are for MLR ($Q^2_{ext}$ = **0.8478**, $RMSE_{ext}$ = **0.2644**), SVM ($Q^2_{ext}$ = **0.896**, RMSEext = **0.205**) and NNA ($Q^2_{ext}$ = **0.89**, $RMSE_{ext}$ = **0.2176**).

**Keywords:** Aquatic toxicity**;** Pimephales Promelas; QSAR; MLR; ARN,

**Poster communication** **P-208**

# QSPR modeling for predicting vapor pressure of volatile organic compounds

ZINE Mounia

*Department of Science and Technology, Faculty of Technology, batna2 University, Algeria*

**E-mail:** mounia_zine@yahoo.com

**Abstract**

A theoretical QSPR model was developed using multiple linear regression analysis to predict the vapor pressure (pv) of volatile organic compounds (VOCs). The study involved analyzing a dataset of some compounds, which was divided into a training set of 39 chemicals and a test set of 12 chemicals for the purpose of external validation. A four-dimensional model was created by employing theoretical descriptors generated by Dragon software and applying the Genetic Algorithm (GA)–Variable Subset Selection (VSS) procedure to select the most relevant variables. The model successfully predicted the vapor pressure of compounds in the test set, demonstrating a high level of agreement with experimental data. The statistical significance of the model was confirmed with $R^2 = 0.9090$, $Q^2_{LOO} = 0.8748$, $Q^2_{ext} = 0.8307$, and standard deviation (s) = 0.24. This indicates that the model is robust and reliable for predicting the log pv values of other VOCs. The applicability domain of the multiple linear regression model was thoroughly evaluated using a Williams plot, which helped identify outliers and assess the model's performance on external compounds.

**Keywords**: QSPR, VOCs, applicability domain.

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**Poster communication** **P-209**

# Molecular modeling of α and β of octadecanoyl-D-xylopyranose using DFT method

LOULOU Fatma, BIDJOU-HAIOUR Chahra

*LOMOP. Organic Synthesis and Modeling group. Faculty of Sciences, Badji-Mokhtar University. BP 12 El-Hadjar. 23000 Annaba. Algeria.*

**E-mail** : lindabio18@yahoo.fr

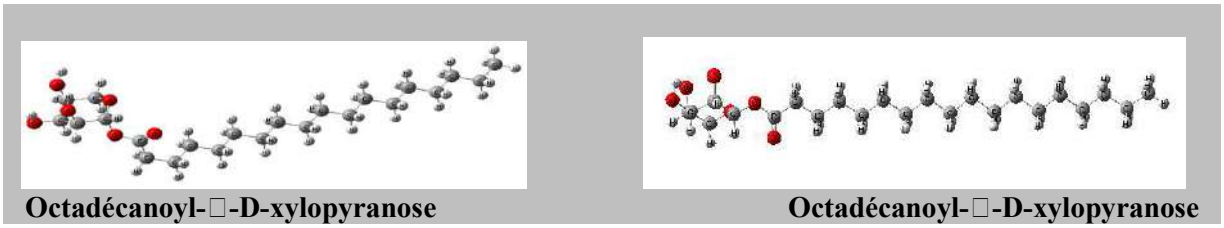
**Abstract**

Molecular modelling is an application of theoretical and computational methods to solve problems involving molecular structure and chemical reactivity. It is an important tool to aid the understanding of the fundamental concepts of structure activity relationships in modern chemistry, biochemistry, molecular biology, and other fields of knowledge of health sciences.

In this study we separated the anomers of fatty acid sugar esters, a green product from renewable resources obtained by enzymatic synthesis, then we optimized their structures to compare their reactivity using Gaussian 09 program package.

Geometry optimization was performed at density functional theory DFT level involving the well-known Becke three-parameter Lee-Yang-Parr function B3LYP/6-31G and 3.21G basis-sets for the synthesized compounds: α and β of octadecanoyl-D-xylopyranose (**figure 1**). The results of mediums of bond indicate that the most optimized structural parameters (bond length, bond angle) are calculated by B3LYP with 6-31G basis set.

The results presented in **table 1** of energy gap show that the anomer 1-O-octadecanoyl-α-D-xylopyranose is more reactive than the anomer **β.**



**Octadécanoyl-□-D-xylopyranose** **Octadécanoyl-□-D-xylopyranose**

**Figure 1.** Optimized structures of anomers α and β of octadecanoyl-D-xylopyranose.

**Table 2.** Energy gap of synthesized products

| Compound | **α 18(6.31G)** | **β 18(6.31G)** |
|---|---|---|
| $E_{HOMO}$ | -0,25866 | -0,25548 |
| $E_{LUMO}$ | 0,00371 | 0,00763 |
| Gap Energy, (ev) | 0,26237 | 0,26311 |

**Keywords**: Gaussian 9, fatty acid sugar ester, green product, reactivity, energy gap, basis-set.

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**Poster communication** **P-210**

# Theoretical study by DFT of the global and local reactivity descriptors of a TTF-Sulfonamide

Rachida Khammar[1], Amel Bendjeddou[1], Tahar Abbaz[1]

[1]*Organic Chemistry and Interdisciplinary Laboratory. University of Souk Ahras*

**E-mail:** r.khammar@univ-soukahras.dz

**Abstract**

The development of TTF derivatives has given rise to conductive organic materials that have a wide range of uses, particularly in macrocyclic and supramolecular chemistry as redox-active systems. In this work, we have studied the global and local reactivity descriptors of a TTF-Sulfonamide derivative, the synthesis protocol of which is described in a previous work. The theoretical study of this compound was carried out via the Gaussian programme using density functional theory (DFT) according to the B3LYP/6-31G (d,p) approach.

The physicochemical and energetic properties were determined by optimising the geometry of the molecule. Information on the charge density distribution and chemical reactivity of the molecules was obtained from global reactivity descriptors. Local reactivity descriptors, which describe the reactivity and selectivity of the site, are obtained using Fukui parameters. By interpreting the results of the chemical descriptors obtained, we were able to classify this compound according to its chemical reactivity using the DFT method, which has proved its reliability for characterising our electron donor compound.

**Keywords**: Tetrathiafulvalene, Density Functional Theory, Reactivity descriptors, Sulfonamide.

**Poster communication** **P-211**

# Determination of enantiopuirty and molecular modeling of some bioactive molecules via cellulose tris (3,5-dimethylphenylcarbamate as chiral selector

Mohamed Nadjib REBIZI*, Salah Eddin Rahmani

*Organic Chemistry and Natural Substances Laboratory, Faculty of Exact Sciences and Computer Science, University of Djelfa, PO Box 3117, Djelfa 17000, Algeria*

**E-mail**: mn.rebizi@univ-djelfa.dz

**Abstract**

Today in our pharmacies are a lot of developed drugs possess chiral centers, chirality has become increasingly important topic issue in drug research and has attracted increasing consideration in the pharmaceutical industry. The main objective of this work is to applied a simple direct isocratic high-performance liquid-chromatographic methods for chiral separation and determining the enantiomeric purity of some antibacterials drugs using (Chiralcel® OD-H) as chiral stationary phase, and online coupled with electronic circular dichroism (ECD) detector. The correlations of experimental ECD traces with quantum chemical ECD calculations with TD-DFT made it possible to elucidate the absolute configuration for each enantiomer, and establish the elution order. Furthermore, molecular docking was performed to confirm of absolute configuration, elution order and analyse the binding modes of R- and S-enantiomers. Moreover, the stereoselective and the chiral recognition mechanism of racemic bioactive molecules on Chiralcel® OD-H chiral stationary phase (CSP) has also been researched via modeling studies. It was observed that hydrogen bondings and π-π interactions are the major forces for chiral separation. The modeling studies indicated strong interactions of R-enantiomers with Chiralcel® OD-H chiral selector than S-enantiomers. This process was found to be suitable for rapid enantiomeric purity analysis and a quality control of quinolones in any matrices also racemic compounds.

**Keywords**: Bioactive Molecules, HPLC, Cellulose CSPs, Docking, chiral separation, TD-DFT.

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**Poster communication** **P-212**

# Synergistic effect between vitamin and KI corrosion inhibitors of copper in acidic medium using density functional and molecular dynamic

Sedik Amel[1,2], Athmani Sameh[1], Bezzina Belgacem[3] and Saoudi Adel[1]

[1] *Scientific and Technical Research Center in Physico-chemical Analysis, BP 384, Bou-ismail industrial zone, RP 42004, Tipaza, Algeria.*

[2] *Laboratory of Applied Organic Chemistry LCOA, Synthesis of Bimolecular and Molecular Modelling Group, Badji-Mokhtar- Annaba University, Box 12, 23000 Annaba, Algeria*

[3] *Research Center in Industrial Technologies CRTI P.O. Box 64, Chéraga 16014 Algiers, Algeria.*

**E-mail**: amelsedik2015@gmail.com

**Abstract**

Synergism is a widely studied phenomenon experimentally, a complete understanding of the underlying mechanisms such as inhibitor-inhibitor and the inhibitor-metal surface interactions, is still difficult to obtain through experiments alone. To better understand the inhibitor molecule's adsorption, orientation, inhibition activity, and adsorption mechanism, we have employed DFT-B3LYP and molecular dynamic (MC) to explain synergism between the vitamin B1 and KI molecules and their interaction with copper.

DFT computed HOMO-LUMO gaps (eV) follow the trend: VitB1-KI (176.05) < VitB1 (3693.39); while the interaction energy magnitudes, |Eint| (eV) for most stable configurations on Cu (111) surface follow the trend: VitB1-KI (9.55) > VitB1 (2.11) validating synergism. These simulations support the outcomes of the tests and give insight into how VitB1-KI inhibitor act as stronger inhibitor compared with VitB1 inhibitor.

**Keywords**: corrosion, copper, inhibitor, synergistic effect, DFT, molecular dynamic.

**Poster communication** **P-213**

# Discovery of novel anti-cancer inhibitors using the pharmacophore and 3D-QSAR approaches

MEZIANI Ouafa [1], AIT KAKI Samira [1,2], Khairedine Kraim [1.3], FERKOUS Fouad [1]

*(1) Laboratory of Applied Organic Chemistry, Department of Chemistry, Faculty of Science, Badji-Mokhtar-Annaba University, Algeria.*

*(2) Laboratory of Therapeutic Chemistry, Department of Pharmacy, Faculty of Medicine, Badji-Mokhtar-Annaba University, Algeria.*

*(3) Laboratory of Physical Chemistry and Biology of Materials, Department of Physics and Chemistry, Higher Normal School of Technological Education, Skikda, Algeria.*

**E-mail:** wafa97.dz@gmail.com

**Abstract**

Protein kinases form a large family of enzymes that regulate nearly all aspects of cell development and division [1]. Most of these promising therapeutic targets are receptor tyrosine kinase inhibitors, particularly the VEGFR2 enzyme [2]. Our main objective is to discover new molecules that act as VEGFR2 inhibitors using pharmacophore/3D-QSAR design followed by virtual screening.

In Discovery Studio, we generated 40 pharmacophore models and constructed 1440 3D-QSAR models from 101 known VEGFR2 inhibitors with available IC50 values from the ChEMBL database. One 3D-QSAR model,

**EQ 1**, was selected based on favorable statistical parameters, along with one pharmacophore model that was further validated using a ROC curve analysis [3-4].

**EQ 1**.

$$\text{Log}\,(1 / \text{IC}\,50) = -4.1578 - 0.96414 * \text{ES\_Count\_aaaC} + 0.13362 * \text{ES\_Count\_ssCH2} + 0.38644 * \text{ES\_Count\_ssO} - 0.28299 * \text{ES\_Sum\_dssC} - 12.334 * \text{LUMO\_Energy\_DMol3} - 0.00035927 * \text{Total\_Energy\_DMol3} + 0.044732 * \text{HypoA/8/05}$$

EQ 1 and the selected pharmacophore were satisfactory and will be used for the virtual screening of 399 similar to sorafenib, as sorafenib is used as a reference drug. Only 53 molecules have been selected by the pharmacophore; an inhibitory activity value will be predicted using the 3D QSAR equation. 2 molecules with a predicted IC50 of less than 0.16 nM (sorafenib IC50) were retained and underwent ADMET analysis using suisseADME, preADMET, and PkCSM.

Only 1 molecule was selected that could present a good characteristic for being a potential new active inhibitor of VEGFR2.

**Keywords** : VEGFR2, cancer, pharmacophore, 3D QSAR, ADMET.

**References**

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**Poster communication** **P-214**

# Application parallèle du criblage virtuel à la recherche de nouveaux inhibiteurs du MAPK14

Samira AIT KAKI[1,2], Fayçal LAYACHI[1,2], Houssem SEBOUI[4], Khair-Eddine KRAIM[1,3], Abdelhak NEGHRA[2] et Fouad FERKOUS[1]

*Laboratoire de recherche Chimie Organique Appliquée LCOA, UBMA*
*Laboratoire de Chimie Thérapeutique, département de Pharmacie, Faculté de Médecine, UBMA*
*Laboratoire Physicochimie et Biologie des matériaux, école supérieure normale de l'éducation technologique, Skikda, Algérie*
*EHS Souk-Ahras*

**E-mail:** kaki_samira@yahoo.fr

**Résumé**

Le cancer constitue un problème de santé publique pour lequel l'humanité paye un très lourd tribut. Malgré l'arsenal thérapeutique disponible, les résistances et les effets secondaires constituent une source de motivation sans limite pour la recherche de nouveaux anticancéreux.

Outre les méthodes de recherche classiques, la modélisation moléculaire dont le criblage virtuel qui est une des méthodes les plus utilisées, a permis la commercialisation d'un nombre important de médicaments notamment dans le domaine du cancer tels que le sorafenib, sunitinib et pazopanib.

Dans l'application parallèle du criblage virtuel, plusieurs méthodes sont utilisées : criblage virtuel basé sur les ligands, criblage virtuel basé sur la structure, recherche de similarité et les méthodes de modélisation moléculaire. Les résultats sont ensuite combinés. Les méthodes sont complémentaires et leur fusion améliore le rendement global en augmentant le nombre de vrais positifs et diminuant le nombre de faux positifs dans la sélection.

Les protéines kinases activées par les mitogènes p38 (MAPK) jouent un rôle essentiel dans les réponses cellulaires, la prolifération, la survie, le cycle cellulaire et la migration dans le cancer.

Dans ce contexte, nous rapportons les résultats d'un criblage virtuel de la base de données du National Cancer Institute (NCI), basé sur le docking et sur le 3DQSAR pour l'identification d'inhibiteurs potentiels du MAPK p38 à visée anticancéreuse. Une étude des propriétés ADMET a suivi pour proposer des hits avec un bon profil pharmacocinétique.

Les hits prometteurs obtenus doivent faire l'objet de tests d'inhibition enzymatique et d'activité sur cellules cancéreuses pour valider les résultats obtenus in silico.

**Mots-clés**: 3DQSAR, Pharmacophore, Docking, Cancer, MAPK, ADMET

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**Poster communication** **P-215**

# PES and theoretical studies on electronic structure and intermolecular interactions between edaravone and cucurbit[7]uril.

Ismahan. Lafifi [1], Noura. Merabet[1] , Imane. Djillala , Imane. Djilani[2] ,Fatiha. Madi[1], Leila. Nouar[1]

[1] *Laboratory of computational chemistry and nanostructures, University ofMay 8th 1945- Guelma- Algeria,*

[2] *Higher Normal School of Technological Education.*

**E-mail:** lafifiismahane@gmail.com

**Abstract**

Potential energy surface (PES) analyzes using density functional theory were performed to theoreticallyinvestigate the structural and electronic properties of cucurbit [7]uril (CB[7]) inclusion complexes with edaravone using a Gaussian. The results obtained with the hybrid functional B3LYP/6-31G(d) clearly indicate that the complexes formed are thermodynamically favorable. The results indicate that edv@CB[7] is the most favorable complex in the gas phases. The calculations of the UV by the methodTD-DFT were analyzed and discussed. To quantify host-guest interactions, topological parameters derived from the AIM approach and the Reduced Density Gradient (RDG) method of non-covalent interactions (NCI) were calculated and interpreted.

**Keywords**: Cucurbit[n]uril (CBn), inclusion complexes, PES , DFT, AIM, RDG, NCI.

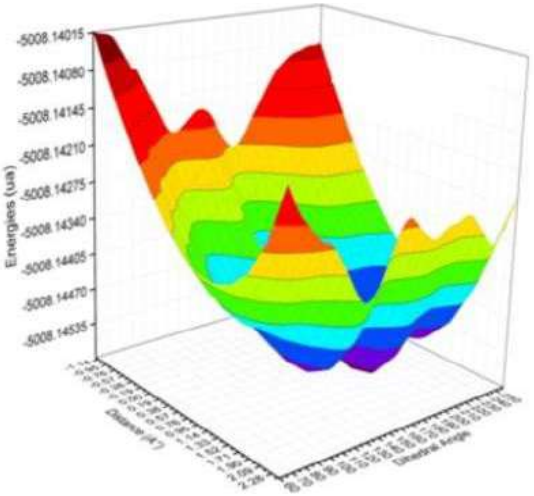



**Fig. 1**: The generated conformational iso-energetic maps for edv@CB[7]

**Poster communication** **P-216**

# Molecular modeling, atomic force analysis and electrochemical insights of carbazole polymerization by chemical bath method

Houssem Eddine El Yamine SAKHRAOUI [1,2] and Ali ZERRIOUH [3]

[1] *Laboratoire d'Electrochimie et Matériaux, Département de Génie des Procédés, Faculté de Technologie, Université Ferhat Abbas Sétif, Sétif 19000, Algeria.*

[2] *Département de Chimie, Faculté des Sciences, Université Badji Mokhtar Annaba, Annaba 23000, Algeria.*

[3] *University of Genoa, Department of Chemistry and Industrial Chemistry, Via Dodecaneso 31, Genova 16146, Italy.*

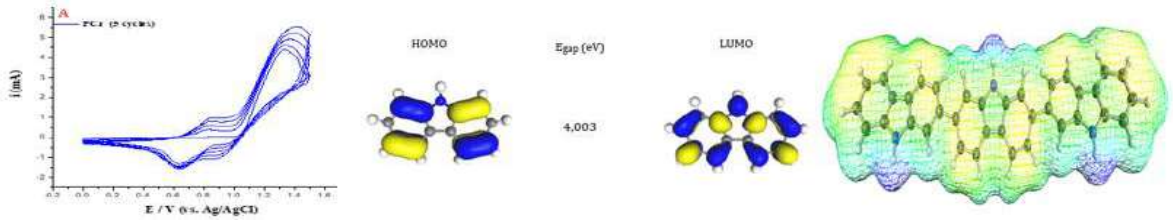
**E-mail**: H_Sakhraoui@hotmail.com

**Abstract**

Redox active polymer-based materials as supercapacitors (SC), have significantly attracted scientists' interest due to their irreplaceable merits of high power density, fast charge/discharge rate, and the ability for modifying functions for the power/energy gap between traditional dielectric capacitors with high power output and batteries/fuel cells with high energy storage [1]. Polycarbazole (PCz) is one of the largest studied polymers in energy storage applications [2]. Because of its electron-rich conjugated system, (PCz) has an interesting electrochemical activity [3], thermal stability [4], physical property [5] and electrochromatic characteristic [6].

In this conference, we highlight the effect of surface thickness of polymeric matrix on the computational, COSMO, theoretical and electrochemical performance for energetic applications.

PCz films were electrochemically deposited by bath deposition method on Indium Tin Oxid (ITO) substrates and then subsequently analyzed by different physical and physico-chemical techniques such, Cyclic Voltammetry (CV) and Atomic Force Microscopy (AFM). The PCz films have an interesting super-capacitive behavior, in matter of fact, the specific capacitance found to be 117 F/g and 331 F/g for 5 and 10 cycles respectively. computational studies show that increasing the electropolymerization of carbazole increases its electrical properties, making the polymer easier to be oxidized, which is confirmed by DFT calculations by increasing the π-conjunction sites.




**Keywords**: Polymers, AFM, DFT, COSMO.

**References:**

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**Poster communication** **P-218**

# Thymol attenuates oxidative stress in respiratory infection by targeting the HO-1 pathway: An experimental and in silico approach

AMARNI Meriem[1], LADJEL-MENDIL Amina[1], AHRAS-SIFI Nesrine[1], CHAFAA Imene[2], MOUSSAOUI Hadjila[1], MERZOUAGUI Rania[1], and LARABA-DJEBEBARI Fatima[1]

[1] *Department of Cellular and Molecular Biology, Faculty of Biological Sciences, University of Sciences and Technology Houari Boumediene "USTHB", BP 32, El–Alia Bab Ezzouar, 16111, Algiers, Algeria*

[2] *Laboratory of Veterinary Pathological Anatomy and Cytology, Pasteur Institute of Algiers, Rue du Dr Laveran, Mohamed Belouizdad, El Hamma, Algiers, Algeria*

**E-mail**: amarnimeriem@outlook.fr

## Abstract

**Introduction**: Respiratory infections are a leading cause of morbidity and mortality worldwide, largely due to the imbalance between reactive oxygen species (ROS) production and the body's capacity to neutralize or repair their damaging effects. This oxidative stress, triggered by the immune response, can harm lung tissues and compromise respiratory function. Thus, there is a need for antimicrobial agents with antioxidant properties.
**Objectives**: This study aims to evaluate the antioxidant effects of Thymol, a natural phenol found in various Mediterranean aromatic plants, on oxidative stress induced in an experimental pneumonia model. The mechanistic pathways involved were explored through molecular docking. **Materials and Methods**: An animal model of pneumonia was established by intranasal inoculation of Klebsiella pneumoniae in mice. Following infection, mice were treated with Thymol via oral gavage to assess its therapeutic potential. Molecular docking studies targeting the human Heme Oxygenase-1 (HO-1) were conducted using Autodock 1.5.7 software to predict Thymol's binding affinity and interactions with the enzyme. The best-docked conformations were selected based on binding energy scores and were further analyzed and visualized using Biovia Discovery Studio 2021 for detailed interaction mapping. **Results**: Thymol administration reduced pro-oxidant parameters in the treated group, significantly lowering levels of NO and $H_2O_2$. Additionally, Thymol enhanced catalase activity compared to the untreated group. In silico analysis revealed strong binding affinity of Thymol to HO-1, with a docking energy of -5.29 kcal/mol. Thymol exhibited non-covalent interactions with residues P72, E127, E190, T192, and covalent interactions with V73, V130, L189, M191, and V195. **Conclusion**: These findings suggest that Thymol exerts a protective effect during respiratory infection by modulating oxidative stress, likely through activation of the HO-1 antioxidant pathway.

**Keywords:** Thymol; Molecular docking; Respiratory infection; Oxidative stress; Heme Oxygenase-1.

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**Poster communication** **P-221**

# Etude par modélisation moléculaire d'un complexe d'inclusion à base de β-cyclodextrine et de 5,10,15,20-tétrakis(4-hydroxyphényl)porphyrine

Fatima M'zyene[1], Zakia Zeffouni[1], Sâad Moulay, Fatiha Madi[2], Mohammed El Hattab [1]

[1] *Laboratoire LSN-Biom, Département de chimie, Faculté des sciences, Université de Blida 1, Algeria*

[2.] *Laboratory of Computational Chemistry and Nanostructures, Department of Material Sciences, Faculty of Mathematical, Informatics and Material Sciences, University of 08 Mai 1945, Guelma, Algeria*

**E-mail**: mzyene_f@yahoo.fr

**Résumé**

Le but de notre travail est l'étude théorique d'un complexe d'inclusion à base de β-cyclodextrine (β-CD) et de 5,10,15,20-tétrakis(4-hydroxyphényl)porphyrine (p-THPP), un photosensibilisateur pour les médicaments anticancéreux, par modélisation moléculaire afin de déterminer la structure la plus favorable et les interactions intermoléculaires stabilisantes. La principale performance de la β-cyclodextrine est étroitement liée à sa capacité à former des complexes d'inclusion (CI) avec des molécules organiques (substances biologiquement et pharmaceutiquement importantes), améliorant la solubilité, la stabilité et la biodisponibilité de ces derniers.

En premier, le complexe d'inclusion β-CD : p-THPP est formé par l'introduction de la molécule invitée dans la cavité de la β-CD selon deux orientations proposées (orientations A et B). Ensuite, l'optimisation de géométrie a été réalisé en utilisant le logiciel MOPAC, par la méthode semi empirique PM7 et la méthode de la fonctionnelle de densité (DFT/CAM-B3LYP) successivement, via la base 6-31G. Après l'obtention des structures du complexe d'inclusion les plus favorables (orientations A et B), les interactions intermoléculaires ont été déterminées par les deux techniques : natural bond orbital (NBO) et quantum theory of atoms in molecules (QTAIM).

Les résultats de l'énergie d'interaction de la p-THPP avec la β-cyclodextrine obtenus par la méthode semi-empirique PM7, prouvent la formation d'un complexe stable avec une énergie de complexation négative de l'ordre de -27 kcal/mol, due à l'insertion totale du noyau phényle dans la cavité de la β-cyclodextrine.

L'inclusion de la molécule invitée dans la cavité de la β-CD est favorisée à l'extrémité la plus large. La raison est que cette région offre une surface plus importante pour que l'invité, quel que soit son mode d'inclusion, puisse se positionner à l'intérieur de la cavité.

**Mots-clés** : β-cyclodextrine, 5,10,15,20-tétrakis(4-hydroxyphényl)porphyrine , complexe d'inclusion, modélisation moléculaire.

**Poster communication** **P-223**

# Green chemistry and QSPR: Pioneering sustainable petrochemical derivatives

Imen TOUHAMI[1*], Mourad CHAOUKI[2], Zine Alabidine CHINI[3], Fatiha BENAMIA[4]

[1]*ensti-annaba*
[2] *kasdi merbah university*
[3] *saad dahleb university*
[4]*badji mokhtar university*

**Abstract**

The relationship between Quantitative Structure-Activity Relationship (QSAR) and Quantitative Structure-Property Relationship (QSPR) methods and green chemistry in the context of hydrocarbons lies at the heart of efforts to make chemistry and the petrochemical industry more sustainable. QSAR/QSPR methods enable the prediction of the physicochemical, biological, and environmental properties of chemical compounds based on their molecular structure. This has direct implications for green chemistry, which aims to design chemical products and processes that reduce or eliminate the use and generation of hazardous substances.

In summary, integrating QSPR methods into green chemistry offers a powerful approach to accelerate the development of sustainable petrochemical solutions. By allowing for a rapid and predictive evaluation of chemical properties, these methods support innovation in the design of compounds that are safer and less harmful to the environment, while meeting the performance and efficiency needs of the industry.

**Keywords:** QSAR, QSPR, Phenol, PLS, SD.

**Poster communication** **P-224**

# Molecular docking of novel sulfamidophosphonates. Interaction with CHK2

REDJEMIA Rayenne[1]*, DJOUAD Seif-Eddine[1,2], GRIB Ismahene[1], BERREDJEM Malika[1]

*Laboratory of applied organic chemistry, synthesis of biomolecules and molecular modelling group, department of chemistry, sciences faculty, badji-mokhtar-Annaba-*

**E-mail:** Flower-95@live.fr

## Abstract

The combination of two pharmacophores, sulfonamide and phosphonate, is still the subject of research today in the medical field to synthesize the sulfamidophosphonates. A one-pot synthetic strategy was developed for the synthesis of these derivatives via a three-component Kabachnik-Fields reaction of sulfanilamide, triethyl phosphite and benzaldehyde using ultrasonic irradiation.

The enzyme Checkpoint kinase 2 (CHK2) is indeed a crucial biological target in the development of anticancer agents. Its pivotal role in regulating the cellular response to genetic and cellular stress makes it an attractive target for cancer treatment.

As a component of our research aimed at clarifying the binding mode and mechanism of action of our sulfamidophosphonate molecules, our primary focus was directed toward understanding their interactions with the ATP pocket of the biological target, the CHK2 enzyme.

**Keywords:** sulfamidophosphonate, molecular docking, Checkpoint kinase 2, anticancer agents.

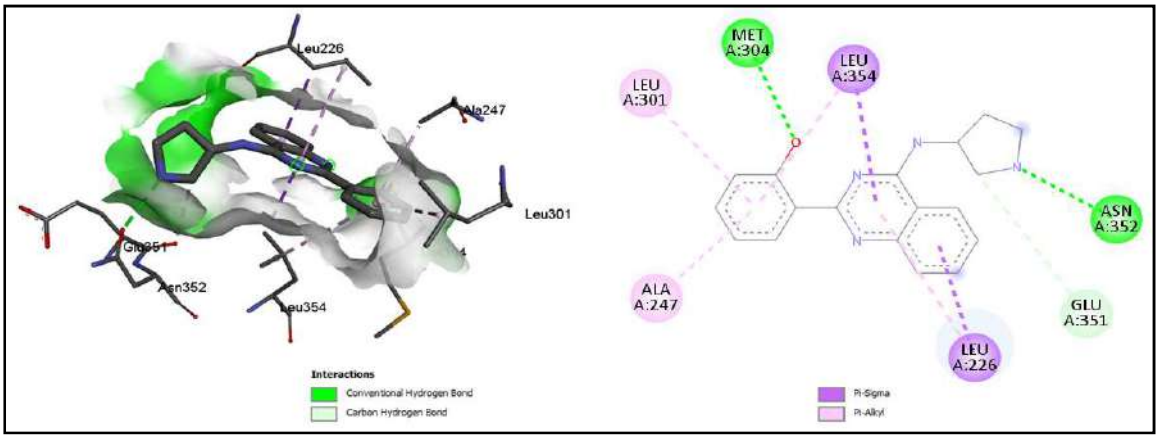


**Figure . Cocrystal structure of co-crystallized ligand (B4W) in complex with CHK2 (PDB: 2XM8).**

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**Poster communication** **P-225**

# Molecular docking investigation of N-Diphenylpiperazinyl-sulfonylamide compound as an acetylcholinesterase inhibitor against Alzheimer's disease

Mohamed Yazid BELGHIT[1] and Malika BERREDJEM[2]

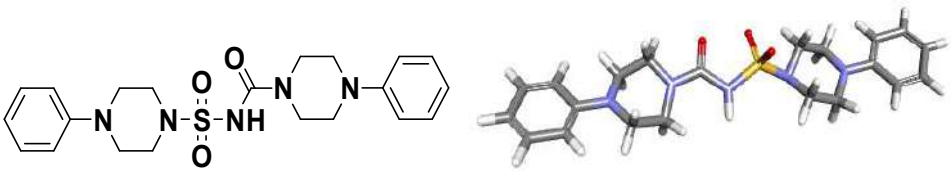
[1]*Department of Process Engineering and Petrochemicals, Faculty of Technology, University of Echahid Hamma Lakhdar, P.O.Box: 789, El-Oued 39000, Algeria.*

[2] *Laboratory of Applied Organic Chemistry, Synthesis of Biomolecules and Molecular Modelling Group, Department of Chemistry, Badji-Mokhtar-Annaba University, Box 12, 23000 Annaba, Algeria.*

**E-mail:** Belghit.yazid07@gmail.com

**Abstract**

Cholinesterase inhibitors are promising drugs for the symptomatic treatment of mild to moderate forms of Alzheimer's disease. In our study, we exploited the inhibitory effect of the N-Diphenylpiperazinyl-sulfonylamide compound on anti-acetylcholinesterase activity. A molecular docking simulation method was applied to this compound to create stable complexes with protein targets (PDB ID: 7E3H) and (PDB ID: 6O4W). The result obtained highlighted interesting hydrophobic and hydrogen interactions of N-Diphenylpiperazinyl-sulfonylamide in comparison with the drug DONEPEZIL. These interactions cluster in the active pocket binding site of human acetylcholinesterase (AChE) 7E3H and 6O4W with residues Phe295, Tyr337 and Glu202 at interaction energies equal to -180.175 and -191.178 Kcal/mol, respectively. In addition, the pharmacokinetic parameters presenting to the invented compound were determined. As a result, the N-diphenylpiperazinyl-sulfonylamide compounds were found to have better pharmacokinetic properties and to form stable complexes with the acetylcholinesterase protein, which supports their use as drug candidates for Alzheimer's disease.




2D 3D

N-Diphenylpiperazinyl-sulfonylamide

**Keywords**: Molecular docking, sulfonylamide, human acetylcholinesterase (AChE), Alzheimer's disease, cholinesterase inhibitors.

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**Poster communication** **P-226**

# 3D-QSAR Structure Based Virtual Screening Studies on Monoacylglycerol Lipase Selective Inhibitors

Mohamed AISSAOUI[a]; Billel BELHANI[a]; Saleh LAKROUT[a]; Sofiane ALI RACHEDI[b]; Hacene Ktir[c]; Noureddine DADDA[a]; Salah Eddine DJILANI[a].

[a] *Laboratory of Synthesis and Organic Biocatalysis, Department of Chemistry, Badji-Mokhtar-Annaba University, Algeria*

[b] *Environmental Research Center (CRE, Annaba 23000, Algeria*

[c] *Laboratory of Applied Organic Chemistry, Department Of Chemistry, Sciences faculty, Badji-Mokhtar-Annaba University, Algeria*

**E-mail**: aissaouimohamed.chem@gmail.com

**Abstract**

Monoacylglycerol lipase is a serine hydrolase that plays a crucial role in breaking down 2-arachidonoylglycerol, an endocannabinoid neurotransmitter involved in various physiological processes. Recent research has suggested that MAGL inhibitors may serve as anti-inflammatory, anti-nociceptive, and anti-cancer agents. Hit identification and hit-to-lead optimization are key steps of the early drug discovery program. In this study, we reported a 3D-QSAR receptor-based virtual screening method for the identification of reversible MAGL inhibitors. Starting from the X-ray crystal structure of the human monoacylglycerol lipase (hMAGL), we herein develop a 3D-QSAR model by means of pharmacophore mapping. Then a dataset of MAGL inhibitors was generated through the developed 3D-QSAR model, and 50.000 ligands were suggested. All ligands were docked and their MM-GBSA free binding energy were calculated. Next, ADME descriptors were calculated, and only ligands with ADME properties better than the most potent inhibitors were identified. The resulting molecules were subjected to molecular dynamics (MD) simulation for 100 ns. The results of MD simulations indicate that only two ligands could be promising as MAGL inhibitors as showing an interesting stability inside the active site.

**Keywords**: Monoacylglycerol lipase, QSAR-3D, Docking, Virtual screening, Keyword5, Keyword6.

**Poster communication** **P-227**

# Modeling of the synthesis of biologically active alcohols

Sofiane ALI RACHEDI, Zahra MELLOUK, linda SAILI, fares HAMOUD, yazid BEDOUH, takai eddine YAHI

*Author's environmental research center, annaba, algeria*

**E-mail**: sofianealirachedi@yahoo.com

**Abstract**

The asymmetric reduction of ketones, catalyzed by the coenzyme NADPH, is crucial for synthesizing chiral molecules in organic chemistry. We use Density Functional Theory (DFT) with Gaussian software to model this reaction. The process begins with the geometric optimization of the structures of reactants, catalytic complexes, and products. We model the ketones and NADPH, then optimize their geometries to achieve energy-minimized states.

Next, we construct and optimize the catalytic complexes formed by the ketone and NADPH to simulate the reduction mechanism. Transition state search helps identify the critical configuration during the reaction, providing insights into the energy barrier and the feasibility of the reaction. DFT calculations also evaluate chiral selectivity by analyzing the chiroptical properties of the final products.

This DFT approach offers detailed insights into the mechanisms of asymmetric reduction, aiding in the design of more effective reactions for the controlled synthesis of chiral compounds.

**Keywords**: asymmetric reduction, ketones, NADPH, DFT, Gaussian, geometric optimization.

The 1st International Seminar on medicinal chemistry and green chemistry (1st IS MCGC - Annaba 2024)

**Poster communication** **P-228**

# Theoretical and biological activity of a new α-sulfamidophosphonate derivative

Racha GHODBANE[1], Dounia BELDJEZZIA[1*], Hacen K'TIR[1,2], Noureddine AOUF[1]

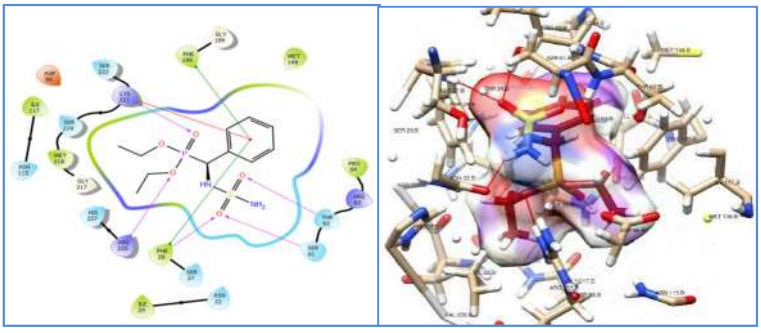
[1] *Laboratory of Applied Organic Chemistry LCOA, Bio-Organic group, department of chemistry, sciences faculty, Badji-Mokhtar-Annaba University. Box12, 23000 Annaba Algeria*

[2] *Medical Sciences faculty, Badji-Mokhtar-Annaba University. Box 12, 23000 Annaba Algeria.*

**E-mail**: rachagh2022@gmail.com

**Abstract**

Antibiotic resistance occurs when one or more antibiotics become ineffective against a bacterial infection. This condition can make it difficult, or even impossible, to treat certain infections. Pharmaceutical research is constantly seeking ways to avoid natural resistance and expand the range of antibiotics by modifying their chemical structure or inventing new molecules. The literature reports that α-sulfamidophosphonate can serve as potential medicinal molecules in drug discovery and development. They have shown several significant activities, such as antihypertensive, anti-inflammatory, anticonvulsant, antibacterial, and antifungal. All these findings suggest that α-sulfamidophosphonate provide a suitable framework for the development of effective bactericidal agents. in this work a docking simulation was performed to explore the binding mode of the prepared compound to the active site of main protease (PDB: 3TZF). The synthesized molecule was also studied for evaluation of breast antibacterial activity to inhibit the activity of three different types of carbapenemases: VIM, OXA-48, and KPC-3. Our docking study was performed by using Maestro Schrödinger.



**Keywords**: sulfamidophosphonate, antibacterial activity, molecular docking.

**Poster communication** **P-231**

# Prediction of octanol/organic carbon partition coefficient of organic compounds

A. Bouakkadia [1,2*], M A. Boudraa [1], A. Gaagai [1]

[1] *Department of Sciences of Matters, Faculty of Sciences and Technologies, Abbes Laghrour University, Khenchela 40000, Algeria;*

[2] *Laboratory of Synthesis and Organic biocatalysis, Department of Chemistry, Faculty of Sciences, Badji Mokhtar University, Annaba 23000, Algeria*

**E-mail**: amel.bouakkadia@univ-khenchela.dz

**Abstract**

Pesticides pose a significant concern in environmental contamination due to their persistence, bioaccumulation, and potential adverse effects on human health and ecosystems. The physicochemical properties of pesticides play a crucial role in determining their distribution and fate in the environment. Chemometric methods can describe how these properties vary based on molecular structure characteristics expressed through appropriate molecular descriptors. Quantitative Structure-Property Relationship (QSPR) models can offer a comprehensive understanding of the molecular structure's influence on these properties.

The octanol/carbon partition coefficient (Koc) is a vital property for predicting the mobility and bioavailability of pesticides in the environment. We optimized and computed molecular descriptors using specific molecular modeling software (HyperChem, Dragon). The resulting QSPR model was developed using the Multiple Linear Regression (MLR) stepwise method with Minitab software.

The dataset of 34 compounds randomly divided into two subsets: a training set of 22 compounds for model construction and a test set of 12 compounds for validation. The values of statistical parameters (coefficient of determination and prediction: $R^2$, $Q^2_{EXT}$, , standard deviation s, SDEPext and SDEC) highlight the quality and relevance of the obtained model.
The applicability domain was discussed using Williams plots.

**Keywords**: QSPR methods, Pesticides, Octanol/Carbon Partition Coefficient (Koc), Multiple Linear Regression (MLR), Molecular Descriptors.

**Poster communication** **P-232**

# QSPR approach for flash point of esters prediction

H. HADDAG[1]; N. KERTIOU[1,2];A. BOUAKKADIA[1,2], N. DADDA[1]; S. E. DJILANI[1]

[1]*Organic Synthesis and Biocatalysis Laboratory, BADJI Mokhtar - Annaba University. Algeria*
[2]*Abbès Laghrour Khenchela University, Algeria*

**E-mail**: hamza.haddag@univ-annaba.dz

**Abstract**

All over the world, thousands of chemicals pose a risk to people and ecosystems. Among these compounds are carboxylic esters, which are derivatives of carboxylic acids, usually resulting from the action of an alcohol on these acids, with the elimination of water. Ester functions are found in many biological molecules, notably triglycerides. Carboxylic esters often have a pleasant odor and are often the source of the natural aroma of fruit.

Over the past decades, Quantitative Structure-Activity/Property Relationships (QSAR/QSPR) become a powerful theoretical tool, as an alternative to quantum mechanics, for describing and predicting the properties of complex molecular systems in different environments. The QSAR/QSPR approach is based on the assumption of a correspondence between any physical property, chemical affinity or biological activity of a chemical compound and its molecular structure.

In this work, we tried to model the flash point (Fp) by linking it to molecular descriptors calculated with specialized software, using the QSPR methodology.
The three molecular descriptors (ATS1m, ATS5v and X0Av), linked to Fp by multiple linear regression, were selected using a genetic algorithm.

The statistical parameter values obtained highlight the quality of the model developed. The model's field of applicability has been defined, and rigorous tests for its predictive validity have been carried out.

**Keywords**: Esters, Flash point, Theoretical molecular descriptors, Quantitative structure/property relationship.

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**Poster communication** **P-233**

# DFT and experimental studies on copper (II) and iron metallic (II) ions with Adriblastina ligand

Rayene KADRI[*1], Nour HASNI[2], Mekki KADRI[2].

[1]*Pharmaceutical sciences research center (CRSP), Constantine, Algeria.*
[2]*Laboratory of physical chemistry, University 8 May 1945, Guelma, Algeria.*

**E-mail**: kadri.rayenee94@gmail.com

**Abstract**

Adriblastina (ADR) is an anticancer agent, that has been used succefully in chemotherapy since1963. Nevertheless, this molecule displays a cardiotoxicity as a side effect which is caused by the radical reactions in which the DOX molecule is involved.Also, it has been reported also that the presence of Fe (II) and Cu (II) ions catalyzes the reaction of DOX with free radicals. This finding prompted researchers to investigate the interaction of these ions with DOX and its role in radical reactions.

The objective of the present work is to carry out a spectroscopic and thermodynamic study of Fe (II) and Cu (II)–DOX interactions. Distribution diagrams of different formed chemical species were plotted, stability constants of 1:1 and 1:2 complexes then the thermodynamic quantities ($\Delta H^0$, $\Delta S^0$, $\Delta G^0$) were computed.The solid-state complexes were prepared in methanol solution under ultrasonic conditions at 20 kHz frequency, and characterized.On the other hand, theses ion-DOX interactions were investigated by molecular modeling studies using DFT / B3LYP /6.311++g (d, p) and DFT/B3LYP /6.311++g(d,p) Empirical Dispersion = GD3BJ ( taking into account the Grimme dispersion).The obtained results were compared and discussed with respect to bonds lengths, angles and dihedrals.

The FTIR (DFT) and UV-vis spectra (TD-DFT) obtained theoretically are in good agreement with those obtained experimentally. Also, the TD-DFT allowed to acquire the description of the frontier orbitals properties namely the Highest Occupied Molecular Orbital (HOMO) and the Lowest Unoccupied Molecular Orbital (LUMO), and to compute the corresponding electronic properties.

The NBO analysis were carried out to elucidate intermolecular interactions between DOX molecules and metallic ions.

**Keywords**: Adriblastina, organometallic complexes, non-covalent interactions, DFT.

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**Poster communication** **P-234**

# The various strategies for enantioselective hydrolysis using CAL-B

Samra RAZI, Saoussen ZEROR, Mounia MERABET-KHELASSİ.

*Badji Mokhtar Annaba University Faculty of Science. Department of Chemistry L.C.A.E.*
*Ecocompatible Asymmetric Catalysis Laboratory*

**E-mail**: samrarazi23@gmail.com

**Abstract**

The enzymatic hydrolysis resolution is a crucial and practical reaction for obtaining optically enriched compounds that can be modified with various functionalities. In this study, we demonstrate an efficient enantioselective cleavage of the acyl group from a series of α-phenylethyl esters with varying chain lengths, catalyzed by Candida antarctica lipase B (**CAL-B**). We compare two reaction methods: one in an anhydrous medium with sodium carbonate and the other in a microaqueous medium. The deacylation occurs in an organic solvent, using $Na_2CO_3$ in the first method and a drop of water in the second.

Our findings reveal a significant impact of the acyl donor's leaving group, with notable differences in CAL-B reactivity and selectivity based on the acyl group's structure. The results indicate that deacylation with sodium carbonate is particularly effective for enzymatic resolution, especially for fatty esters (E >> 200). For conventional hydrolysis in biphasic systems, we optimized the minimum water requirement and highlighted the limitations of microaqueous conditions for ester hydrolysis. Consequently, the alkaline enzymatic hydrolysis method proves to be the most effective approach for cleaving long-chain aliphatic acyl esters, making it highly suitable for the enantioselective hydrolysis of fatty esters. In contrast, microaqueous conditions are less effective and only work well with esters that have short-chain leaving groups.

**Keywords:** CAL-B - Ethyl α-phenyl esters - Deacylation - Anhydrous medium - Micro-aqueous medium

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**Poster communication** **P-235**

# Efficient synthesis of a new complex derived from (E)-4-((2-benzylideneamino)benzenesulfonamide

MANSOURI ACHRAF[a, b*], BERREDJEM MALIKA[a], BOUCHAREB FOUZIA [a,b]

[a]*Applied Organic Chemistry Laboratory (LCOA). Synthesis of biomolecules and molecular modeling group. Faculty of Sciences. Badji Mokhtar University. BP.12.23000 Annaba-Algeria*

[b]*Department of Chemistry. Faculty of Science and Technology. Chadli Bendjedid University. BP: 73, El Tarf 36000 Algeria*

**Abstract**

The chemistry of complexes has been the focus of numerous research endeavors, particularly regarding the complexation of metal ions by organic molecules known as Schiff bases. These versatile ligands exist in various forms with coordinated sites of diverse nature, defined as a group of chemical compounds comprising one or more imine groups. They find extensive applications in medicine for treating various diseases [1-2], as well as in biology and industry for combating corrosion [3-4].
In this study, we have developed a novel one-step method for synthesizing Schiff bases by employing sulfanilamide and salicylaldehyde under microwave irradiation. These Schiff bases were subsequently utilized as ligands for the synthesis of new copper(II) complexes with metal ions. The synthesis of these complexes was achieved through an innovative and environmentally friendly approach using microwave irradiation. The resulting complex was obtained as a black powder with a high yield.

**Keywords :** Schiff base, complex, CuCl2 , microwave irradiation.

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**Poster communication** **P-237**

# Etude phytochimique et pharmacologique de Linaria pinifolia (Poir.) plante du Nord-Est Algérien.

DADDA Noureddine[1], SAMAI Zakaria[1], TOUDERT Nadia[2], DJILANI Salah Eddine[1]

[1] *Laboratoire de Synthèse et Biocatalyse Organique (LSBO), Département de Chimie, Université Badji Mokhtar Annaba, B.P. 12, Annaba 23000, Algérie*

[2] *Laboratoire de physicochimie des matériaux (LPCM), Département de Chimie, Faculté des Sciences et de la Technologie, Université Chadli Bendjedid, El Tarf, Algérie.*

**E-mail**: naouridadda2@gmail.com

**Abstract**

Le but de ce travail est de mettre en évidence l'effet des méthodes d'extraction sur le rendement et les activités biologiques d'extrait alcoolique d'une plante endémique du nord-est algérien Linaria pinifolia (Poir.) [1, 2].

Nous avons procédé à des extractions par sonication et macération en utilisant des solutions hydro-alcooliques, puis nous avons évalué quelques activités biologiques des extraits de différents organes (fleurs, feuilles, racines). Nous avons étudié également l'effet du solvant (éthanol 70% et méthanol 70%) sur ces activités. Les résultats ont montré une forte capacité inhibitrice contre la cholinestérase, l'anti-α-amylase, l'α-glucosidase, et l'antimicrobiens.

On n'a évalué l'activité anti-oxydante (ABTS). Les résultats sont très encourageants. Sur la base de ces résultats, on peut dire que la plante étudiée à des activités biologiques importantes, elles peuvent être utilisées dans le secteur alimentaire, pharmaceutique ou en phytothérapie.

**Key words:** Plante endémique, ultrason, Activité antimicrobien, Activité anti-oxydante.

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**Poster communication** **P-238**

# Synthesis and antifungal activity of some bicylic $\delta^2$-1,2,3-triazolines.

Y.R. HACHEMI[1*], M. DAHOUI KHALFA[1], S. DIB[2], M. HAMADOUCHE[1].

[1] *Laboratoire de Chimie Fine, Département de Chimie, Faculté des Sciences Exactes et Appliquées.*

[2] *Laboratoire de Biologie des Micro-organismes et de Biotechnologie, Département de Biotechnologie, Faculté des Sciences de la Nature et de la vie.*

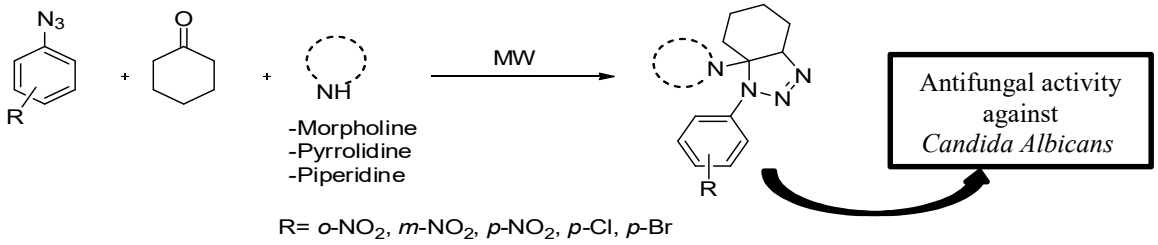
[1,2] *Université Oran1 Ahmed Ben Bella, BP 1524 El M'naouer, Oran 31000, Algérie*

**E-mail**: hachemi.yasmine@univ-oran1.dz

**Abstract**

Representing an important part of organic chemistry, aza-heterocycles are widely studied because of their various biological activities[1]. In addition, (1,2,3)-triazolines have also long been explored for their many synthesis routes and biological properties[2].

Our study aims to perform a green synthesis of some (1,2,3)-bicyclic triazolines by one-pot reaction and microwave activation, and then to demonstrate their antifungal potential against Candida Albicans.




R= *o*-$NO_2$, *m*-$NO_2$, *p*-$NO_2$, *p*-Cl, *p*-Br

**Keywords**: organic azids, enamines, one-pot reaction, 1,3-dipolar cycloaddition, (1,2,3)-triazolines, biological activity.

**References:**

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**Poster communication** **P-239**

# Étude de la dégradation des polluants organiques par différents procédés

BOUTALEB Yassira[1], BENSID Nadia[1], Yamina BERREDJEM[1], HATTAB Zhour[1]

[1]*Laboratoire de traitement des eaux et valorisation de déchets industrielle, Département de chimie, Faculté des sciences, Université Badji Mokhtar –Annaba*

**E-mail**: yassibout@gmail.com

**Résumé**

De par son activité, l'industrie textile qui est une très grande consommatrice génère une pollution très importante du milieu aqueux avec des rejets fortement contaminés par des colorants. Le traitement de ces eaux reste un défi majeur surtout pour les pays en voie de développement qui n'ont pas encore toutes les possibilités d'intégrer les concepts de développement durable. Cette étude décrit un procédé de traitement, de rejet textile la fuchsine basique, (FB), qui est l'adsorption et une étude comparative avec un notre procédé c'est la photochimie cette combinaison se fait avec une source de lumière (Lampe). Ces traitements ont été effectués par un adsorbant d'une plante naturelle, l'Avogado. L'influence des différents paramètres d'adsorption de ce colorant par cet adsorbant tels que : le temps de contact, le pH de la solution, la dose d'adsorbant et la concentration initiale ont été étudiés. Le modèle deuxième ordre est le plus appropriée. Les paramètres thermodynamiques obtenus révèlent que l'adsorption est spontanée et endothermique pour simuler la cinétique d'adsorption de ce colorant Les isothermes d'adsorption ont été modélisées par le modèle Freundlich.

**Mots-clés :** photochimie, Valorisation, Adsorption, Fuchsine Basique, cinétique, modélisation.

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**Poster communication** **P-241**

# Etude in Silico d'un nouveau gène codant pour une métalloprotéase de type « inhA3 » secrété par BLB30AF

Ameny FARHAT*, Fatma DRISS, Slim TOUNSI

*Laboratoire des Biopesticides, Centre de Biotechnologie de Sfax, Université de Sfax, Route Sidi Mansour km 6 Bp "1177" 3018 Sfax, Tunisie*

**E-mail**: ameny2908@gmail.com // ameny.farhat@cbs.rnrt.tn

**Resumé**

Les métalloprotéases de type inhibiteur immunitaire A (InhA) sont des facteurs de virulence potentiels sécrétés par les membres du groupe Bacillus cereus et Bacillus thuringiensis. L'analyse du Whole génome de Bacillus thuringiensis BLB30AF, nouvellement isolée, a montré la présence de quatre gènes de virulence dont un code pour une métalloprotéase de type « inhA3 ». Ce gène de taille 2388 pb code pour une protéine de 795 aa. La comparaison de la séquence nucléotidique du gène montre une identité de 98% par rapport au gène inhA3 de Bacillus thuringiensis strain 407. L'analyse bioinformatique de la séquence montre que cette protéine contient une séquence signal de 32aa (clivage entre Ala32-Glu33). Une modélisation a été réalisée en se basant sur la structure cristalline de la protéine de Bacillus anthracis inhA2 peptidase zymogen (pdb: 4yu6) avec un pourcentage d'identité de 71%. Le modèle obtenu montre une superposition quasi-parfaite avec une GMQE de 0.88. Cette protéine possède une structure en quatre domaines comprenant un propeptide, un domaine catalytique, un domaine VEG et un domaine MAM greffé dans ce dernier. Pour la famille des métzincines, dont InhA3 est membre, cette protéine possède un domaine N-terminal et un domaine C-terminal qui sont séparés par une crevasse contenant le site actif. Le domaine N-terminal est formé par un domaine catalytique globulaire et formé par 5 feuillets  standards, une hélice α de support et une hélice α qui contient le motif de liaison au zinc HEXXHXX (G, N) XX (H, D). Ce dernier englobe les trois résidus de liaison au zinc (His) et un résidu glutamate (Glu), qui est l'acide aminé catalytique. En aval du domaine C-terminal, formé par une seule hélice, nous remarquons la présence d'une partie conservée contenant un résidu méthionine (Met-tour) central qui fournit une base hydrophobe nécessaire pour le fonctionnement du site actif.

**Mots-clés**: inhA3; Bacillus thuringiensis; structure cristalline; métalloprotease.

**Poster communication** **P-242**

# Chemical composition and biological activity of essential oil from origanum majorana L. in El Oued

Hammadi Maroua*

*University of El Oued, B.P. 789 RP El-Oued, 39000, El-Oued, Algeria*

**E-mail**: hammadimaroua90@gmail.com

**Abstract**

Origanum majorana L., or marjoram, is a Mediterranean aromatic plant valued for its culinary and medicinal uses. This study focused on the extraction of essential oil from Origanum majorana L. using hydro distillation, yielding 1.5%. Gas chromatography-mass spectrometry (GC/MS) analysis identified 42 compounds, with oxygenated monoterpenes dominating (over 57%), notably trans-thujone (33.3%), along with α-thujene (1.44%), α-pinene (1.19%), and β-pinene oxide (4.42%). The essential oil from the El Oued region displayed distinct chemical compositions compared to other regions, likely influenced by soil quality, climate, and harvest timing. A molecular docking study indicated that major compounds in the essential oil interact with human glutathione reductase, potentially decreasing its activity.

**Keywords**: Origanum Majorana L, plant, medecinal, GC/MS, El Oued.

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**Poster communication** **P-243**

# Theoretical study of the regioselectivity in 1,3-dipolar cycloadditions of N-benzoyliminoquinolinium with propene and Acrolein using FMO theory

BELKADI Anis*[1], Abdelhafid Djerourou*[2], Abdelmalek Khorief Nacereddine*[3]

[1]*Department of Chemistry, University of Annaba-Algeria*
[2]*Department of Chemistry, University of Annaba-Algeria*
[3]*Department of Physics and Chemistry, Higher Normal School of Technological Education-Skikda, Azzaba, Skikda, Algeria*

**E-mail** : anis.belkadi@univ-annaba.dz

**Abstract**

This study explores the theoretical aspects of cycloaddition reactions, building upon the computational research conducted by Abdul Rashid Umar, Richard Tia, and Evans Adei. These researchers examined the regio-, stereo-, and enantioselectivity of azomethine imine reactions with olefins, maleimides, and benzynes—reactions critical to the synthesis of spirocyclic heteropolycyclic (N,N) systems, which serve as pivotal intermediates in the development of pharmaceutical, agrochemical, and biologically active compounds. Our research extends this work by investigating the 1,3-dipolar cycloaddition of N-benzoyliminoquinolinium with propene and acrolein, focusing on its regioselectivity using Frontier Molecular Orbital (FMO) theory.

In this study, we selected a methyl group ($CH_3$) as the R substituent on the imine to assess its effect on both the selectivity and reactivity of the system. Using quantum mechanical calculations, we will evaluate how interactions between the HOMO (highest occupied molecular orbital) and LUMO (lowest unoccupied molecular orbital) dictate the regioselectivity and stereoselectivity of the reaction. By mapping the transition states and potential energy surfaces, we aim to provide a comprehensive analysis of the reaction mechanism.

The findings of this theoretical investigation are anticipated to offer significant insights into the electronic factors influencing the regioselectivity of cycloaddition reactions. Additionally, the results could inform the design of more selective and efficient catalysts for organic synthesis, with potential applications in the synthesis of complex chemical systems and drug discovery.

**Keywords**: FMO ; Cycloaddition ; computational methods ; regeoselectivity ; Gaussian.

**Poster communication** **P-244**

# Évaluation in vitro et in silico du pouvoir antibactérien d'une molécule bioactive d'origine végétale

Sara GRINE [a,b]., Malika BERREDJEM [b]., Faiza TAIBI [a].

[a] *Laboratoire de Biologie Animale Appliquée*
[b] *Laboratoire de Chimie Organique Appliquée*

**E-mail**: grinesarah21@gmail.com

**Résumé**

Les plantes aromatiques sont une ressource inépuisable de substances naturelles douées de propriétés chimiques et activités biologiques. Présentant alors un intérêt réel en industrie et en pharmacologie. D'une autre part, les méthodes in silico ont trouvé leur place dans le domaine du Drug design. Le docking ou l'amarrage moléculaire est l'un des approches numériques de modélisation moléculaire, le plus couramment utilisé actuellement, grâce aux avantages qui en découlent de celui-ci. Il permet la prédiction in silico de la conformation (position et orientation relative) la plus favorable d'un ligand au sein de son récepteur.

C'est dans ce contexte que l'intérêt actuel s'est porté sur l'étude in vitro de l'huile essentielle d'une plante aromatique et médicinale, Salvia officinalis contre une souche bactérienne Klebsiella pneumoniae. Puis, l'étude vise à prouver in silico par docking moléculaire ; le pouvoir antibactérien d'une molécule bioactive majoritaire issue de cette plante, le camphor, contre la cible biologique '5KUN' téléchargé de la base de données PDB, de la même espèce, K. pneumoniae.

L'étude in vitro a montré que l'huile essentielle a exercé un fort pouvoir antibactérien contre la souche bactérienne. De même, le protocole de docking a montré que la molécule bioactive a bien interagit avec la cible biologique, en faisant intervenir des liaisons d'hydrogènes et Van der Walls.

En conclusion, les résultats de l'étude in silico prouve les résultats obtenus de l'étude in vitro et confirme que l'huile essentielle de S. officinalis et le camphor peuvent être à l'origine de nouveaux produits antibactériens.

**Mots-clés** : molécule bioactive, docking moléculaire, étude in silico, étude in vitro.

**Poster communication** **P-245**

# Investigation à l'utilisation des plantes pour la protection des eaux usée

BENSID Nadia[1], BOUTALEB Yassira[1], Yamina BERREDJEM[1], HATTAB Zhour[1]

*Laboratoire de traitement des eaux et valorisation de déchets industrielle, Département de chimie, Faculté des sciences, Université Badji Mokhtar –Annaba*

**E-mail**: nadinadibensi@gmail.com

**Résumé**

La demande croissante des adsorbants utilisés dans les procédés de protection de l'environnement a fait que leur prix coûte de plus en plus cher ce qui suscite une recherche complémentaire pour la fabrication de nouveaux matériaux adsorbant moins coûteux à partir de matières qui ne sont pas classiques, concrètement à partir de la biomasse. L'objectif principal de ce travail est d'étudier le phénomène d'adsorption de l'élimination d'un colorant cationique (Le vert de malachite, (VM) des eaux usées par une plante naturelle locale, les déchets des écorces de petit pois. Une étude comparative a été effectuée par le procédé photochimique. L'influence des différents paramètres tels que la température, le pH, la masse et le temps de contact ont été étudiés. L'effet de certains paramètres sur la vitesse de dégradation de ce colorant par photochimie directe a été étudié (l'intensité de la lumière). L'interaction du petit pois avec les cations du VM est rapide et sa cinétique suit l'équation de vitesse de sorption réversible de Langmuir. Les valeurs de ΔG° et ΔH° montrent que le processus d'adsorption étudié est spontané et endothermique.

**Mots-clés :** Plante, Photochimie, Valorisation, Adsorption, Vert de Malachite, cinétique, modélisation

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**Poster communication** **P-246**

# Ammodaucus Leucotrichus plant extract as sustainable and green corrosion inhibitor for protection XC38 steel in corrosive medium: experimental and quantum chemical investigations

Houssem-Eddine Ammouchi[2], Hana FERKOUS[1], Malika Berredjem, Delimi Amel[1], Imane GHOUAFRIA[2]

[1]*Laboratoire de Génie mécanique et Matériaux, Faculté de Technologie, Université de Skikda, 21000, Algeria*

[2]*Laboratory of Industrial Analysis and Materials Engineering, Department of Process Engineering, Faculty of Science and Technology, University 8 May 1945, Guelma, Algeria*

**E-mail**: h.ammouchi@univ-skikda.dz

**Abstract**

This research examines how well polyphenols extracted from Ammodaucus Leucotrichus prevent mild steel corrosion in a 1 M HCl solution. Inhibitory performance is determined using electrochemical impedance spectroscopy (EIS), potentiodynamic polarization, and weight loss tests. The shape and chemical content of the mild steel sample surface are evaluated by atomic force microscopy (AFM), scanning electron microscopy (SEM), X-ray diffraction (XRD), and X-ray photoelectron spectroscopy (XPS) after contact with Ammodaucus Leucotrichus secondary metabolites in the acidic solution. According to the results of polarization curves, Ammodaucus Leucotrichus extract works as a mixed-type inhibitor. For all Ammodaucus Leucotrichus concentrations tested, the Nyquist plots show a semi-circular capacitive loop. On metal surfaces, the Langmuir isotherm regulates inhibitor adsorption. The effectiveness of inhibition is proportional to the extract concentration, reaching 92.9% at 900 ppm. On metal surfaces, the Langmuir isotherm governs inhibitor adsorption. The effectiveness of inhibition is proportional to the extract concentration, reaching 92.9% at 900 ppm. These findings are supported by metal surface experiments, which show that the deposited inhibitor molecules successfully prevent HCl attacks at steel grain boundaries. Finally, quantum chemistry simulations show that dicaffeoylquinic acids, which were found to be the most prevalent Ammodaucus Leucotrichus extract components, are effective corrosion inhibitors.

**Keywords**: Green Corrosion Inhibitor, Polyphenols, Ammodaucus Leucotrichus, DFT calculations Monte Carlo simulations.

**Poster communication** **P-247**

# New heterocyclic derivative based on vanillin: Synthesis, structural characterization, and electrochemical behavior Study.

Takoua Belghit, Chaima Aouachria , Abdelkrim Gouasmia, Fabrice Pointillart

*Laboratory of Organic Materials and Heterochemistry (LOMH), Echahid Cheikh Larbi Tebessi University, Constantine Road, 12002, Tebessa-Algeria.*

**E-mail:** takoua.belghit@univ-tebessa.dz

## Abstract

Heterocyclic compounds form an essential category of organic molecules that attract the attention of organic chemists **[1]**. Among them, sulfur-containing heterocycles bring significant bioactivity in many natural and synthetic molecules.

Vanillin, an exemplary oxygenated aromatic product, exhibits several biological activities **[2-4]**, and numerous structural modifications carried out on its heterocycle have led to the improvement of its biological properties.

This work focuses on the synthesis, characterization, and study of the electrochemical properties of a new vanillin derivative incorporating the 4,5,6,7-tetrahydrobenzo[d][1,3]dithiole-2-yl group by condensing vanillin with an aromatic selenone in a trialkyl phosphite medium under ultrasonic irradiation.

Various spectroscopic methods, including infrared, $^{1}$H NMR, $^{13}$C NMR, mass spectrometry, and X-ray diffraction, were used to establish the structural characteristics of the synthesized compound.

**Keywords**: Vanillin, 1,3-dithiol-2-selenone, Functionalization, Ultrasonic Irradiation, X-ray.

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**Poster communication** **P-248**

# Design, molecular docking and dynamic simulations of 1,3-thiazoline derivatives as potential antiviral agents

Bahaz Farial[*1], Bourougaa Lotfi [2] , Belghit Takoua [1] , Gouasmia Abdelkrim [1]

[1] *Laboratory of Organic Materials and Heterochemistry, Echahid Cheikh Larbi Tebessi University, Tebessa, Algeria*

[2]*Group of Computational and Medicinal Chemistry, LMCE Laboratory, University of Biskra, BP 145, Biskra 70700, Algeria*

**E-mail:** farial.bahaz@univ-tebessa.dz

**Abstract**

The current study focused on the in-silico assessment of1,3-thiazoline, as neuraminidase inhibitors. Initially, molecular docking studies were performed on the 1,3-thiazoline derivatives, revealing that they possess better binding energies compared to the reference molecule (clinical inhibitor), enabling them to form highly stable complexes with the neuraminidase receptor. Furthermore, the pharmacokinetic analysis of all 1,3-thiazoline derivatives revealed promising results, indicating that these compounds not only possess favorable absorption, distribution, metabolism, and excretion (ADME) properties but also align well with drug-likeness criteria, enhancing their potential as effective antiviral agents. Furthermore, the potential toxicity of the proposed inhibitors was assessed using basic toxicity filters and PASS, showing no significant concerns regarding their toxicity and metabolism. Additionally, a synthesis mechanism for the suggested compounds was developed through machine learning and artificial intelligence algorithms, enhancing the efficiency and feasibility of their production. At the biomolecular level, molecular dynamics simulations (100 ns) were conducted for all studied systems using the Gromacs package. Analysis of the molecular dynamics trajectories and the evaluation of dynamic changes in neuraminidase, following its interaction with the proposed compounds, were performed through dynamic cross-correlation matrix, free energy landscape, and MM-PBSA calculations. The results indicate that the 1,3-thiazoline derivatives form highly stable complexes compared to clinical neuraminidase inhibitors. Ultimately, the findings of this study could significantly contribute to the development of novel, potent neuraminidase inhibitors and aid in the search for new antiviral drugs.

**Keywords**: 1,3-thiazoline Molecular docking, ADME, Molecular dynamic simulations, free energy landscape, MM-PBSA calculations.

**Poster communication** **P-249**

# Propriétés antimicrobiennes, antioxydantes et anti-inflammatoires de la nouvelle synthèse de la 3-(2-chloroacétyl) oxazolidin-2-one

Djendi Manel Lina*[1], Benzaid Chahrazed[1]

[1]*Laboratoire de microbiologie et biologie moléculaire, université Badji Mokhtar Annaba*

**E-mail:** linadjendi23@gmail.com

**Resumé**

La résistance aux antibiotiques reste aujourd'hui un problème majeur de santé publique. L'augmentation de la résistance aux antibiotiques se traduit dans la pratique hospitalière par une augmentation de la morbidité et de la mortalité et par l'apparition de microorganismes résistants à l'ensemble des antibiotiques disponibles, par création d'un mécanisme de protection.

Les causes de l'émergence de l'antibiorésistance sont multiples, mais l'utilisation excessive et/ou inappropriée des antibiotiques est, sans conteste, la principale raison de cette évolution.

La recherche de nouvelles molécules est devenue une nécessité afin de palier à ce phénomène qui engendre des répercussions sur la santé publique et l'économie.

Cette étude vise l'évaluation de l'effet antimicrobien, antioxydant et anti inflammatoire d'une molécule chimique nouvellement synthétisée analogues de la famille des oxazolidinones

L'évaluation de l'activité antimicrobienne de cette molécule néo est déterminée d'abord qualitativement par la méthode des puits, puis quantitativement par la détermination des valeurs de CMI avec le test en milieu liquide sur microplaque, les résultats sont ensuite complétés par la détermination de l'activité antibiofilm, anti oxydante et anti inflammatoire. On a utilisé pour cette étude des souches microbiennes qui comprennent des espèces bactériennes comme : Escherichia coli, Pseudomonas aeruginosa, Klebsiella pneumoniae, Staphylococcus aureus et des espèces fongiques: Candida albicans, Candida tropicalis.

On constate que la molécule présente une activité antimicrobienne notable contre les souches bactériennes, tandis qu'elle manifeste un effet particulièrement prononcé contre les souches fongiques. De plus, elle montre une efficacité significative en tant qu'agent antibiofilm vis-à-vis des souches testées, ainsi qu'une activité antioxydante et anti-inflammatoire remarquable.

Nos résultats montrent que les sulfamides présentent un remarquable pouvoir antimicrobien et antibiofilm, ces molécules pourraient être utilisées comme agents antimicrobiens dans certaines maladies infectieuses.

**Mots-clés** : Synthèse chimique, antibactériens, antifongiques, anti-biofilms.

**Poster communication** **P-250**

# Synergistic combination of Myristica fragrans and Illicium verum essential oils against food-related microorganisms

Mohamed Reda Zahi*, Rania Larouci, Smain Sabour, Abdelraouf Bounaim, Racha Insaf Joucdar, Mohamed EL Hattab

*Laboratory of Natural Products Chemistry and Biomolecules, University Blida 1, Faculty of Science, Chemistry Department, BP 270 09000 Blida, Algeria*

**E-mail**: z-reda@hotmail.com // reda.zahi@univ-blida.dz

**Abstract**

Essential oils (EOs) are a naturally occurring mixture of secondary metabolites[1]. EOs are well-known for their vast range of biological activities[2], and are widely used by the cosmetic, agriculture, pharmaceutical and food industries. Regrettably, a number of issues with these natural preservatives, including volatility, instability, polymerization, degradation and oxidation compromise their effectiveness and quality[3]. In this case, a greater concentration is required to achieve a desired biological impact. Nevertheless, the use of such elevated concentrations could have a negative sensory effect of the materials in which these EOs are incorporated. To overcome this problem, smart combination of EOs with a high synergistic effect could be a suitable solution to facilitate their application and enhance their activities. In the present investigation, EOs of Myristica fragrans and Illicuim verum were extracted using a Clevenger Type apparatus, their organoleptic, physico-chemical properties were determined. And then, the antimicrobial activity of these two EOs was tested singly or in combination against six food-related microorganisms. The antimicrobial test revealed that both EOs had an interesting inhibitory effect against the tested strains, where the MICs values were in the range 0.493-1.975 mg/ml for Illicuim verum and from 1.1 to 4.4 mg/ml for Myristcia fragrans. Regarding the synergism test, non-indifference neither antagonism effects were obtained following the combination of this two EOs. In contrast, a strong synergism was shown against Bacillus subtilis, Listeria monocytogenes and Escherichia coli followed by a considerable additive effect against Pseudomonas aeruginosa, Staphylococcus aureus and Candida albicans with a substantial decrease in their individual MICs. These results could have a valuable utility for the food industry to control undesired food-borne pathogens at lower amounts.

**Keywords**: Synergism, antimicrobial activity, Essential oils, Myristica fragrans, Illicuim verum

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**Poster communication** **P-251**

# In-silico study for investigating novel hepatitis B virus inhibitors

Salah Lakrout[1*], Hacen K'tir[2], Mohamed Aissaoui[1], Billel Belhani[1]

[1] *Laboratoire de Synthèse et Biocatalyse Organique, Université Badji Mokhtar - Annaba.*

[2] *Laboratoire de chimie organique appliquée, Université Badji Mokhtar - Annaba.*

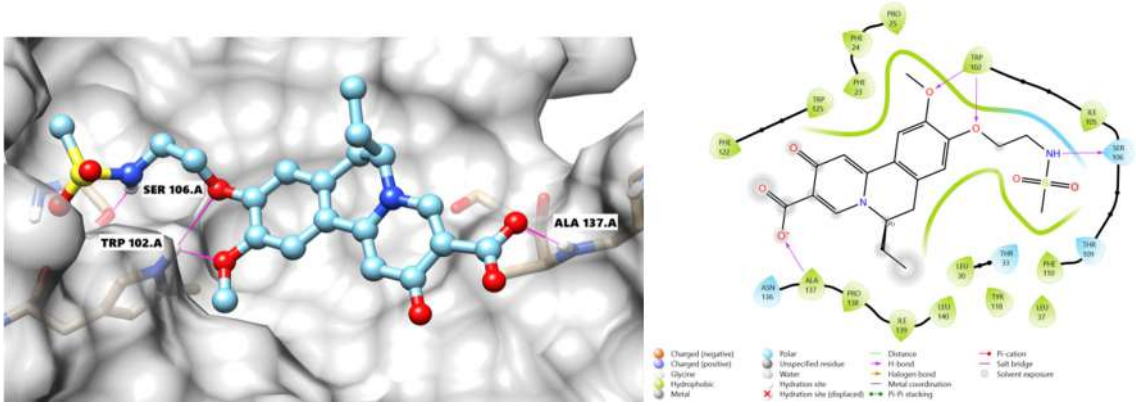
**E-mail:** salah.akroot@yahoo.fr

## Abstract

Chemical and Biological research requires more and more computer tools to process the data produced and optimize its results. One of these tools is the molecular modeling and, more specifically, molecular docking.

Molecular docking is mainly used to predict and reproduce protein-ligand complexes by recognizing the types of interactions, which is proved to be a key factor in the construction of new drugs.

The work presented here, is part of a research for the discovery of new selective and efficient inhibitors of hepatitis B virus. We used molecular docking approach to study and check the anti-HBV activity of a dataset of 77 molecules (DHQ derivatives) using Gilde docking software.




In agreement with the experimental results, the docking results proved that RG7834 and its derivatives have good affinity with a few HBV-related proteins (PDB ID: 5E0I, 5TP2, 5WRE, 5GMZ). We were able to explain the interaction modes of the co-crystalized ligands as well as the RG7834 derivatives.
Our in-silico approach, using Glide, is therefore proven as a reliable method that can make an effective contribution to the development of new HBV inhibitors by expanding the ligands dataset.

**Keywords**: Molecular docking, Glide, DHQ, Hepatitis B, RG7834, Inhibitors.

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**Poster communication** **P-252**

# Development of a new method for the determination of phenolic compounds in brown seaweed by FTIR spectrometry

M. Gasmi, M. Fekhar, Y. Daghbouche, S. Mounier, N. Bouzidi*, M. El Hattab

*Laboratory of Chemistry of Natural Substances and BioMolecules, University of Blida 1, Algeria (LCSN-BIOM)*

**E-mail**: bouzna@yahoo.fr // Bouzidi_naima@univ-blida.dz

**Abstract**

Brown marine algae are among plants rich in phenolic compounds with different physiological effects on human health. These secondary metabolites, not essential to the body, are present in variable quantities in vascular plants (known as tannins) and in brown algae (known as phlorotannins).

In recent years, work concerning the extraction of phenolic compounds has attracted special interest. Extraction is a very important step in the isolation, identification and utilization of phenolic compounds and there is no single, standard extraction method.

This study is devoted to the development of an analytical method for the determination of phenols in the brown alga Cystoseira tamariscifolia by FTIR spectrometry, using liquid-liquid extraction and solid phase extraction (SPE). Phloroglucinol was considered as a standard to carry out this study.

The phloroglucinol content was obtained by FTIR spectrometry in the brown alga Cystoseira tamariscifolia, previously treated using the absorbance bands at 827, 1150, 1159 and 1611 $cm^{-1}$ corrected with the appropriate baselines.

**Keywords**: Cystoseira tamariscifolia, phloroglucinol, liquid-liquid extraction, solid-phase extraction, FTIR spectrometry.

**Poster communication** **P-253**

# The anti-epstein barr virus activity of Tunisian Olea europaea L. Leaf extracts

Bochra Gargouri [1], Ichrak Ben-Amor [1,2], Rosamaria Pennisi [2], Hamadi Attia [1]

[2] *Unit of Biotechnology and Pathologies, Higher Institute of Biotechnology of Sfax, University of Sfax, Sfax 3029, Tunisia; bochragargouri@yahoo.fr (B.G.); hamadi.attia@gmail.com (H.A.);*

[1] *Department of Chemical, Biological, Pharmaceutical and Environmental Sciences, University of Messina,*

**E-mail**: Hamza.elrobrini@hotmail.fr

**Abstract**

Olea europaea L. var. sativa (OESA) preparations are widely used in traditional medicine in the Mediterranean region to prevent and treat different diseases. In this research, olive extracts derived from the leaves of the OESA tree have been screened for antioxidant activity by two methods: the DPPH free radical scavenging assay (DPPH) and the Ferric reducing antioxidant power (FRAP) assay. The DPPH assay showed that OESA possesses a stronger antioxidant activity (84%) at 1 mg/mL while the FRAP method showed a strong metal ion chelating activity (90%) at 1 mg/mL. The low IC50 values, obtained by two different methods, implies that OESA has a noticeable effect on scavenging free radicals comparable to standards. During EBV infection, the free radicals increased triggering lipid oxidation. Therefore, the monitoring of the secondary lipid peroxidation products was done by measuring malonaldehyde (MDA) and conjugated dienes (DC). The simultaneous treatment of Raji cells with OESA and TPA, as an inductorof the lytic cycle, generated a significant decrease in MDA levels and DC ($p < 0.05$). Besides, Raji cells simultaneously exposed to TPA and OESA exhibited a percentage of EBV-positive fluorescence cells lower than TPA treated cells (**** $p < 0.0001$). This suggests that OESA treatment has a protective effect against EBV lytic cycle induction.

**Keywords:** Olea europaea leaves; antivirals; antioxidant; plants bioactive compounds.

**Poster communication** **P-254**

# Antimicrobial activity of new acid anhydride from Phalaris canariensis : An in vitro and in silico study

Mona Kchaou[1], Siwar Soltani[1], Allouche Noureddine[1] and Ben Salah Hichem[1]*

[1]*Organic Chemistry Laboratory LR17-ES08 (Natural Substances Team), Faculty of Sciences of Sfax, PB 1171, 3000 Sfax, University of Sfax, Tunisia*

**E-mail:** hichembensalah9@gmail.com

**Abstract**

In this study, a novel fatty acid anhydride, named phalarisin **1**, was successfully isolated from the ethyl acetate extract of Phalaris canariensis growing in Tunisia. The structural characterization of the compound was achieved through various spectroscopic techniques including FT-IR, 1D and 2D-NMR spectroscopy, as well as acidic hydrolysis analyses. Remarkably, phalarisin exhibited potent antimicrobial properties against a range of pathogens including Micrococcus luteus, Bacillus subtilis, Fusarium oxysporum, and Fusarium phylophylum, with minimum inhibitory concentrations (MIC) ranging from 31.25 to 62.5 µg/mL. Molecular docking studies were carried out to understand the antimicrobial potential of compound **1**, and provided evidence of its ability to bind to proteins in bacteria and fungi that are key to drug resistance.

**Keywords:** Antimicrobial activity, Fatty acid anhydride, Molecular docking study, Phalaris canariensis