

Liste des productions scientifiques(publications,communications,...)

Année 2023

Etablissement Universitaire: Université 8 Mai 1945 de Guelma  
 Faculté: Mathématiques, Informatique et Sciences de la Matière  
 Laboratoire: Chimie Computationnelle et Nanostructures(LCCN)

| Productions Scientifiques 2023 |  |  |                                 |       |  |        |        |   |
|--------------------------------|--|--|---------------------------------|-------|--|--------|--------|---|
| Publications                   |  |  |                                 |       |  |        |        |   |
|                                | Titre  | Auteurs  | Revue                           | Année | Catégorie de la revue:A+ , A , B-Scopus, B-non Scopus, non classée | Volume | Page   | URL   |
| Publications internationales   | Revealing the effect of Co/Cu (d7/d9) cationic doping on an electronic acceptor ZnO nanocage surface for the adsorption of citric acid, vinyl alcohol, and sulfamethoxazole ligands: DFT-D3, QTAIM, IGM-NCI, and MD analysis | B Gassoumi,<br>AM Ahmed Mahmoud,<br>A Karayel,<br>S Özkınalı,<br>ME Castro,<br>FJ Melendez,<br>M Mahdouani,<br>R Bourguiga,<br>R Ben Chaabane,<br>H Ghalla,<br>L Nouar,<br>F Madi,<br>S Nasr,<br>Y Zhou, | Materials Chemistry and Physics | 2023  | A  | 309    | 128364 | <a href="https://doi.org/10.1016/j.matchemphys.2023.128364">https://doi.org/10.1016/j.matchemphys.2023.128364</a> |

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|------------------------------|--|---|-------------------------------|------|---|----|-----------|---|
| Publications internationales | Structural Aspects and Stability of Interactions between Phenyl-3, 3'-Bis (Indolyl) Methanes and $\beta$ -Cyclodextrin from Density Functional Theory                            | A Antony Muthu Prabhu<br>K Sathiyaseelan<br>GS Suresh Kumar<br>Nouar Leila,<br>Fatiha Madi,   | Polycyclic Aromatic Compounds | 2023 | A | 43 | 5276-5298 | <a href="https://doi.org/10.1080/10406638.2022.2101490">https://doi.org/10.1080/10406638.2022.2101490</a>                               |
|                              | Computational investigation of dimethoate and $\beta$ -cyclodextrin inclusion complex: molecular structures, intermolecular interactions, and electronic analysis                | Abdelaziz Bouhadiba,<br>Amina Benaïssa,<br>Malika Khelfaoui,<br>Bachir Zouchoune,<br>Sulaiman Mogalli,<br>Ibtissem Bouras,<br>Noura Naili,<br>Leila Nouar,<br>Faiza Chekkal,<br>Najran Malfi,<br>Mohamed Salah Madjram<br>Fatiha Madi | Structural Chemistry          | 2023 | A | 34 | 1189-1204 | <a href="https://link.springer.com/article/10.1007/s11224-023-02162-8">https://link.springer.com/article/10.1007/s11224-023-02162-8</a> |
|                              | Host-Guest Inclusion Systems of Vanillic Acid into $\alpha$ -Cyclodextrin: Structures, Electronic Properties, QTAIM, NCI and IGM Analyses with Dispersion Corrected Calculations | Abdelaziz Bouhadiba<br>Abdelkrim Guendouzi<br>Imane Djellala,<br>Nora Merabet,<br>Fatiha Madi,<br>Leila Nouar,  | Polycyclic Aromatic Compounds | 2023 | A |    | 1-15      | <a href="https://doi.org/10.1080/10406638.2023.2202866">https://doi.org/10.1080/10406638.2023.2202866</a>                               |

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|------------------------------|---|--|---|-------------|----------|-----------|----------------------|--|
| Publications internationales | <p><i>Solubility and Antioxidant Activity of 1, 2-Dihydro-2-Methyl-2-Phenyl-3H-Indole-3-One-1-Oxyl Hosted at Randomly Methylated- Bétacyclodextrin: A Computational Investigation</i></p> | <p><i>Hekatti Leyla,<br/>Oumeddour Rabah<br/>Madi Fatiha,<br/>Nouar Leila,</i></p> | <p><i>Polycyclic Aromatic Compounds</i></p> | <p>2023</p> | <p>A</p> | <p>43</p> | <p>1-13</p>          | <p><a href="https://doi.org/10.1080/10406638.2022.2146148">https://doi.org/10.1080/10406638.2022.2146148</a></p>                               |
|                              | <p><i>Effect of cyclodextrins inclusion complexes into absorpction and emission spectra of P-methylaminobenzoate derivatives: A DFT and TD-DFT investigation</i></p>                      | <p><i>Sonia Badi,<br/>Leila Nouar,<br/>Fatiha Madi,<br/>abdelhak Gheid</i></p>     | <p><i>Journal of Fluorescence</i></p>       | <p>2023</p> | <p>A</p> | <p>33</p> | <p>457-14<br/>67</p> | <p><a href="https://link.springer.com/article/10.1007/s10895-023-03146-x">https://link.springer.com/article/10.1007/s10895-023-03146-x</a></p> |

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|------------------------------|---|--|---|------|---|----|-----------|---|
| Publications internationales | Theoretical investigation of inclusion complexes of 3-hydroxyflavone and quercetin as guests with native and modified $\beta$ -cyclodextrins as hosts | Fatiha Madi,<br>Arumugam Praveena,<br>Samikannu Prabu,<br>Rajaram Rajamohan        | Polycyclic Aromatic Compounds                   | 2023 | A | 43 | 141-153   | <a href="https://doi.org/10.1080/10406638.2021.2009526">https://doi.org/10.1080/10406638.2021.2009526</a> |
|                              | In Silico Study of Selected Natural Products as SARS-CoV-2 MPro Binder: Molecular Docking and Molecular Dynamics Simulation                           | Bochra Bencheikh,<br>Djameleddine Khatmi,<br>Rayenne Djemil,<br>Mouna Cheriet,     | Polycyclic Aromatic Compounds                   | 2023 | A | 43 | 5103-5115 | <a href="https://doi.org/10.1080/10406638.2022.2097279">https://doi.org/10.1080/10406638.2022.2097279</a> |
|                              | Quantum investigation of the reaction between triplet oxygen O ( $3P$ ) atom and butadiene  | Boulanouar MESSAOUDI,<br>Djameleddine KHATMI,<br>Rayenne DJEMIL,<br>Mouna CHERIET, | Turkish Computational and Theoretical Chemistry | 2023 | A | 7  | 1-11      | <a href="https://doi.org/10.33435/tcandtc.1144794">https://doi.org/10.33435/tcandtc.1144794</a>           |

**Productions Scientifiques 2023**

**Communications**

|                                  | <b>Titre</b>  | <b>Auteurs</b>  | <b>Intitulé de manifestation</b>   | <b>Année</b> | <b>Proceeding de la conférence indexé dans Scopus ( oui /non )</b> | <b>Volume</b> | <b>Page</b> | <b>URL</b> |
|----------------------------------|---|---|--|--------------|--|---------------|-------------|------------|
| <b>Communications nationales</b> | <i>Theoretical study of <math>\beta</math>-cyclodextrin inclusion complexes with chlorophane</i>                  | Rahim mohamed,<br>BOUHADIBA abdelaziz,<br>Bouneb wahiba ,<br>Nouar Leila ,<br>Madi fatiha | 2nd National Seminar on Molecular Modeling and Applied Chemistry December 19th, 2023 | 2023         |  |               |             |            |
|                                  | <i>Computational study of a novel synthesized azacyclohexane derivatives</i>                                      | ZABOUB Amal,<br>M. Hadjam ,<br>F. Madi,<br>R. Merdes                                      | 2nd National Seminar on Molecular Modeling and Applied Chemistry December 19th, 2023 | 2023         |  |               |             |            |
|                                  | <i>Investigation théorique des interaction hôte-invitée entre le MBDA et la <math>\beta</math>-Cyclodextrine.</i> | BOUCHEMELLA Houria,<br>Fatiha Madi,<br>Leila Nouar  | 2nd National Seminar on Molecular Modeling and Applied Chemistry December 19th, 2023 | 2023         |  |               |             |            |

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|---------------------------|---|--|--|------|--|--|--|--|
| Communications nationales | Reactivity and intermolecular interactions in the inclusion complex of eugenol@ $\beta$ -cyclodextrin.  | MERABET Nora,<br>Fatiha Madi,<br>Leila Nouar<br>Lafifi Ismahan                 | 2nd National Seminar on Molecular Modeling and Applied Chemistry December 19th, 2023 | 2023 |  |  |  |  |
|                           | Contribution to the study of the inclusion complex of 3-AC @ B-cyclodextrin by quantum methods.         | MERABET Nora,<br>Fatiha Madi,<br>Leila Nouar                                   | 2nd National Seminar on Molecular Modeling and Applied Chemistry December 19th, 2023 | 2023 |  |  |  |  |
|                           | Encapsulation of menthol in $\beta$ -cyclodextrin and release characteristics of the inclusion complex. | Bouchemela Houria<br>BAHLOUL Abida<br>Fatiha Madi<br>Leila Nouar<br>Badi Sonia | 2nd National Seminar on Molecular Modeling and Applied Chemistry December 19th, 2023 | 2023 |  |  |  |  |

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|---------------------------|---|--|---|------|--|--|--|--|
| Communications nationales | <p>Theoretical modeling and experimental studies of commercially pure titanium (cp-ti) in 3.0 wt.% NaCl solution containing a green corrosion inhibitor</p> | <p>BAHLOUL Abida<br/>Fatiha Madi<br/>Leila Nouar<br/>Badi Sonia<br/>Chouarfa Fella</p> | <p>2nd National Seminar on Molecular Modeling and Applied Chemistry December 19th, 2023</p> | 2023 |  |  |  |  |
|                           | <p>Molecular modelling studies the interactions of non-steroidal anti inflammatory drugs with <math>\beta</math>-cyclodextrin.</p>                          | <p>LACHI Nadia</p>   | <p>2nd National Seminar on Molecular Modeling and Applied Chemistry December 19th, 2023</p> | 2023 |  |  |  |  |
|                           | <p>Etude par modelisation moleculaire du complexe d'inclusion antiasthmatisque 2-hp-<math>\beta</math>-cyclodextrine.</p>                                   | <p>HAYAHM SAKINA,<br/>Fatiha Madi<br/>Leila Nouar</p>                                  | <p>2nd National Seminar on Molecular Modeling and Applied Chemistry December 19th, 2023</p> | 2023 |  |  |  |  |

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|---------------------------|--|---|--|------|--|--|--|--|
| Communications nationales | Theoretical Study of chemical reactivity of Pyrrithione and its Complexation with Zinc.  | LAFIFI Ismahan,<br>Fatiha Madi<br>Leila Nouar<br>Merabet Nora                         | 2nd National Seminar on Molecular Modeling and Applied Chemistry December 19th, 2023 | 2023 |  |  |  |  |
|                           | Solubility of 1,2-dihydro-2-methyl-2-phenyl-3H-indole-3-one-1-oxyl hosted at randomly methylated- $\beta$ -tacyclodextrin : A computational investigation. | CHEKATTI leyla<br>Nouar Leila<br>Oumeddour Rabah<br>Madi Fatiha                       | 2nd National Seminar on Molecular Modeling and Applied Chemistry December 19th, 2023 | 2023 |  |  |  |  |
|                           | Study of the stability of $si\ 2\ h\ 2$ : a computational investigation.   | AMIRAT Samia,<br>Gheid Abdelhak,<br>Madi Fatiha ,<br>Nouar Leila,<br>Benguerba Yacine | 2nd National Seminar on Molecular Modeling and Applied Chemistry December 19th, 2023 | 2023 |  |  |  |  |