

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

Année 2020

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

| <i>Productions Scientifiques2020</i> |  |   |  |              |   |                          |               |               |   |
|--------------------------------------|--|---|--|--------------|---|--------------------------|---------------|---------------|---|
| <i>Publications</i>                  |  |   |  |              |   |                          |               |               |   |
|                                      | <i>Titre</i>   | <i>Auteurs</i>  | <i>Revue</i>                           | <i>Année</i> | <i>Catégorie de la revue:A+ , A , B- Scopus, B- non Scopus, non classée</i> | <i>Micro Domaine</i>     | <i>Volume</i> | <i>Page</i>   | <i>URL</i>  |
| <i>Publications internationales</i>  | <i>Computational study of inclusion complex of L-Glutamine/betaCyclodextrin: Electronic and intermolecular interactions investigations</i> | <i>Lafifi Ismahan, Nouar Leila , Madi Fatiha Guendouzi Abdelkrim Cheriet Mouna Boulaha Nada , Houari Brahim</i> | <i>Journal of Molecular Structure</i>  | <i>2020</i>  | <i>A</i>  | <i>Chimie analytique</i> | <i>1206</i>   | <i>127740</i> | <a href="https://doi.org/10.1016/j.molstruc.2020.127740">https://doi.org/10.1016/j.molstruc.2020.127740</a> |
|                                      | <i>The inclusion behavior of 8-Anilino-1-naphthalene sulfonate into Cucurbit[7]uril: A DFT approach</i>                                    | <i>Himri Safia , Madi Fatiha , Bezzina Belgacem Nouar Leila</i>   | <i>Journal of Molecular Structure,</i> | <i>2020</i>  | <i>A</i>  | <i>Chimie analytique</i> | <i>1217</i>   | <i>128390</i> | <a href="https://doi.org/10.1016/j.molstruc.2020.128390">https://doi.org/10.1016/j.molstruc.2020.128390</a> |

|                              |  |  |  |      |   |                   |     |         |   |
|------------------------------|--|--|--|------|---|-------------------|-----|---------|---|
| Publications internationales | Investigation of intermolecular interactions in inclusion complexes of pyroquilon with cucurbit[n]urils (n = 7,8) using DFT-D3 correction dispersion | Djellala Imane ,<br>Nouar Leila,<br>Madi Fatiha<br>Guendouzi Abdelkrim<br>Cheriet Mouna<br>Lafifi Ismahan<br>Bouhadiba Abdelazize<br>Houari Brahim | Journal of Molecular Liquids,                            | 2020 | A | Chimie analytique | 309 | 113233  | <a href="https://doi.org/10.1016/j.molliq.2020.113233">https://doi.org/10.1016/j.molliq.2020.113233</a>   |
|                              | Binding kinetics calculations of the inclusion of some benzoic acid derivatives and paracetamol in $\beta$ CD  | Djamel Eddine Khatmi,<br>Belgacem Bezzina,<br>Stéphane Humbel  | Journal of Inclusion Phenomena and Macrocyclic Chemistry | 2020 | A | Chimie analytique | 96  | 373-379 | <a href="https://doi.org/10.1007/s10847-020-00976-1">https://doi.org/10.1007/s10847-020-00976-1</a>       |
|                              | Characterization of iron ore and scale for synthesizing vinyl paint  | Mohammed Tayeb ABEDGHARS<br>Mokhtar GHERS,<br>Salah BOUHOUCHE,<br>Belgacem BEZZINA   | Bulletin of the Mineral Research and Exploration         | 2020 | A | Chimie analytique | 162 | 01-sept | <a href="https://doi.org/10.19111/bulletinofmre.604081">https://doi.org/10.19111/bulletinofmre.604081</a> |

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| Publications internationales | <p><i>Non-Covalent Bonding Interaction between Primaquine as Guest and 2-(Hydroxypropyl)-<math>\beta</math>-Cyclodextrin as Host</i></p>   | <p>Moorthiraman Murugan<br/>Rajaram Rajamohan<br/>Arumugam Anitha<br/>Madi Fatiha</p>  | <p><i>Journal Polycyclic Aromatic Compounds</i></p> | <p>2020</p> | <p>A</p> | <p>Chimie analytique</p> | <p>janv-18</p> | <p><a href="https://doi.org/10.1080/10406638.2020.1813181">https://doi.org/10.1080/10406638.2020.1813181</a></p> |
|                              | <p><i>Structural and energetic investigation on the host/guest inclusion process of benzyl isothiocyanate into <math>\beta</math>-cyclodextrin using dispersion-corrected DFT calculations</i></p> | <p>Abdelaziz Bouhadiba,<br/>Seyfeddine Rahali,<br/>Youghourta Belhocine,<br/>Hamza Allal,<br/>Leila Nouar,<br/>Mohamed Rahim</p> | <p><i>Journal Carbohydrate Research</i></p>         | <p>2020</p> | <p>A</p> | <p>Chimie analytique</p> | <p>491</p>     | <p>107980</p>  |

*Productions Scientifiques 2020*

*Communications*

| <i>Titre</i>   | <i>Auteurs</i>  | <i>Intitulé de manifestation</i>   | <i>Année</i>       | <i>Proceeding de la conférence indexé dans Scopus ( oui /non )</i> | <i>Micro Domaine</i> | <i>Volume</i> | <i>Page</i> | <i>URL</i> |
|--|---|--|--------------------|--|----------------------|---------------|-------------|------------|
| <p><i>Biological and fungicidal activity of inclusion complexes of fungicide chlorothalonil with <math>\beta</math>-cyclodextrin and hydroxypropyl-<math>\beta</math>-cyclodextrin</i></p> | <p><i>IMANE DJELLA,<br/>FATIHA MADILA,<br/>LEILA NOUAR,</i></p> | <p><i>the Sixth MGIBR International Workshop of Aromatic, Medicinal and condiment plants Virtues and development prospects That was held in 21-22 December 2020, Tlemcen University, Algeria</i></p> | <p><i>2020</i></p> |  |                      |               |             |            |

*Communications internationales*

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|--------------------------------|---|---|--|------|--|--|--|--|--|
| Communications internationales | <p>Incapsulation of anti-tumoral drug imodin within cucurbit n uril (CB n, n=6,7 and 8): ADFT calculations</p>          | <p>IMANE DJELLA<br/>A. BOUHADIBA<br/>M.CHERIET<br/>L.NOUAR<br/>F.MADI</p> | <p>13<br/>International days of theoretical and computational chemistry, Biskra Algeria<br/>February 2<sup>nd</sup> and 3<sup>rd</sup>, 2020</p> | 2020 |  |  |  |  |  |
|                                | <p>Interactions in inclusion complex of anti-tumoral drug imodin within cucurbit n uril : DFT computational studies</p> | <p>IMANE DJELLA,<br/>Mouna CHERIET<br/>Leila NOUAR,<br/>Fatiha MADI</p>   | <p>Third International symposium medicinal plants and materials<br/>Tebessa Algeria<br/>February 25 to 27, 2020</p>                              | 2020 |  |  |  |  |  |