

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

Année 2022

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 Scientifiques2022</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>Volume</i>	<i>Page</i>	<i>URL</i>
<i>Publications internationales</i>	Computational investigation of dimethoate and β -Cyclodextrin inclusion complex: molecular structures, intermolecular interactions and electronic analysis	Amina Benaissa Abdelaziz Bouhadiba Noura Naili Faiza Chekkal Malika Khelfaoui Bouras Ibtissem Mehri Karima Mohamed Salah Madjram Bachir Zouchoune Sulaiman Mogalli Najran Malfi Leila Nouar Fatiha Madi	Journal of Research square	2022	A	1-19	057187ca-a84e-4792-97528ab3ddb3b70.pdf (researchsquare.com)

Publications internationales	<p>Stability, spectroscopic, electrochemistry and QTAIM analysis of Cu-Znn-1On clusters for glucose sensing application: A study on theoretical and experimental insights</p>	<p>B.Gassoumi, N.Aouled Dlala, M.Echabaane, A.Karayel, S.Özkinalı, M E Castro, F.J Melendez, H Ghalla, L Nouar, F Madi, R. Ben Chaabane</p>	<p>Journal of Heliyon</p>	<p>2022</p>	<p>A</p>	<p>8</p>	<p>https://doi.org/10.1016/j.heliyon.2022.e12387</p>	
	<p>A novel and water-soluble material for coronavirus inactivation from oseltamivir in the cavity of methyl and sulfated-β-cyclodextrins through inclusion complexation</p>	<p>Rajaram Rajamohan, Sonaimuthu Mohandoss, Sekar Ashokkumar, Fatiha Madi, Nouar Leila, Kuppusamy Murugavel, Yong Rok Lee</p>	<p>Journal of pharmaceutical and biomedical analysis</p>	<p>2022</p>	<p>A</p>	<p>221</p>	<p>115057</p>	<p>https://doi.org/10.1016/j.jpba.2022.115057</p>
	<p>Water-soluble inclusion complexes for a novel anti-viral agent with low toxicity; Oseltamivir with the β-cyclodextrins</p>	<p>Rajaram Rajamohan, Sonaimuthu Mohandoss, Sekar Ashokkumar, Eun Ha Choi, Fatiha Madi, Nouar Leila, Yong Rok Lee</p>	<p>Journal of Molecular Liquids</p>	<p>2022</p>	<p>A</p>	<p>366</p>	<p>120297</p>	<p>https://doi.org/10.1016/j.molliq.2022.120297</p>

Publications internationales	<p>Adsorption of toxic and non-toxic metals with new model of CX [4]: Experimental and computational investigation, Spectroscopic, QTAIM, and Antibacterial activity analyses</p>	<p>Bouزيد Gassoumi, Najet Aouled Dlala, Mosaab Echabaane, Houcine Ghalla, Yang Zhou, Maria Eugenia Castro, Francisco Javier Melendez, Nouar Leila, Fatiha Madi, Rafik Ben Chaabane</p>	<p>Journal of Molecular Structure</p>	<p>2022</p>	<p>A</p>	<p>1268</p>	<p>133618</p>	<p>https://doi.org/10.1016/j.molstruc.2022.133618</p>
	<p>Interaction of chloroquine with 2-(hydroxypropyl)-β-cyclodextrin through the supramolecular assembly for cytotoxicity on breast cancer cell lines</p>	<p>Rajaram Rajamohan, Moorthiraman Murugan, Arumugam Anitha, Yong Rok Lee, Fatiha Madi, Nouar Leila, Muthusamy Viswalingam</p>	<p>Monatshefte für Chemie-Chemical Monthly,</p>	<p>2022</p>	<p>A</p>	<p>153</p>	<p>1171-184</p>	<p>https://link.springer.com/article/10.1007/s00706-022-02986-w</p>
	<p>Tetradentate square-planar acetylumbelliferone-nickel (II) complex formation: a DFT and TD-DFT study</p>	<p>Karima Belguidoum, Yamina Boulmouk, Fatima Zahra Hamamdia, Fatiha Madi, Leila Nouar, Habiba Amira-Guebailia</p>	<p>Journal of Theoretical Chemistry Accounts</p>	<p>2022</p>	<p>A</p>	<p>141</p>	<p>1-12</p>	<p>https://link.springer.com/article/10.1007/s00714-022-02903-8</p>

Publications internationales	<p>Structural Aspects and Stability of Interactions between Phenyl-3, 3'-Bis (Indolyl) Methanes and β-Cyclodextrin from Density Functional Theory</p>	<p>A Antony Muthu Prabhu, Fatiha Madi, Nouar Leila, GS Suresh Kumar, K Sathiyaseelan</p>	<p>Journal of Polycyclic Aromatic Compounds</p>	<p>2022</p>	<p>A</p>	<p>1-23</p>	<p>https://doi.org/10.1080/10406638.2022.2101490</p>	
	<p>Spectroscopic characterization, host-guest charge transfer, Hirshfeld surfaces, AIM-RDG and ELF study of adsorption and chemical sensing of heavy metals with new derivative of Calix [4]quinone: A DFT-D3 computation</p>	<p>B Gassoumi, A Mehri, H Hammami, ME Castro, A Karayel, S Özkınalı, FJ Melendez, L Nouar, F Madi, H Ghalla, R Ben Chaabane, H Ben Ouada</p>	<p>Journal of Materials Chemistry and Physics</p>	<p>2022</p>	<p>A</p>	<p>278</p>	<p>125555</p>	<p>https://doi.org/10.1016/j.matchemphys.2021.125555</p>
	<p>Molecular modeling study of structures, Hirshfeld surface, NBO, AIM, RDG, IGM and ¹HNMR of thymoquinone/hydroxypropyl-β-cyclodextrin inclusion complex from QM calculations</p>	<p>Kadri Rayene, Djellala Imane, Bouhadiba Abdelaziz, Nouar Leila, Madi Fatiha, Guendouzi Abdelkrim, Gassoumi Bouzid, Lafifi Ismahan, Houari Brahim, Oumeddour Rabah</p>	<p>Journal of Molecular Structure</p>	<p>2022</p>	<p>A</p>	<p>1249</p>	<p>131565</p>	<p>https://doi.org/10.1016/j.molstruc.2021.131565</p>

Publications internationales	<p>Azo-methoxy-calix[4]arene complexes with metal cations for chemical sensor applications: Characterization, QTAIM analyses and dispersion-corrected DFT- computations</p>	<p>B Gassoumi, M Echabaane, FE Ben Mohamed, L Nouar, F Madi, A Karayel, H Ghalla, ME Castro, FJ Melendez, S Özkınalı, A Rouis, R Ben Chaabane</p>	<p>Journal of Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy</p>	2022	A	264	120242	<p>https://doi.org/10.1016/j.saa.2021.120242</p>
	<p>In Silico Study of Selected Natural Products as SARS-CoV-2 MPro Binder: Molecular Docking and Molecular Dynamics Simulation</p>	<p>Bochra Bencheikh, Mouna Cheriet, Rayenne Djemil, Djameleddine Khatmi</p>	<p>Journal of Polycyclic Aromatic Compounds</p>	2022	A		1-13	<p>https://doi.org/10.1080/10406638.2022.2097279</p>

Publications internationales	<p>Adsorption of toxic and non-toxic metals with new model of CX [4]: Experimental and computational investigation, Spectroscopic, QTAIM, and Antibacterial activity analyses</p>	<p>Bouzid Gassoumi, Najet Aouled Dlala, Mosaab Echabaane, Houcine Ghalla, Yang Zhou, María Eugenia Castro, Francisco Javier Melendez, Nouar Leila, Fatiha Madi, Rafik Ben Chaabane</p>	<p>Journal of Molecular Structure</p>	<p>2022</p>	<p>A</p>	<p>1268</p>	<p>133618</p>	<p>https://doi.org/10.1016/j.molstruc.2022.133618</p>
	<p>Synthesis of thiazolyldenethiazolo quinazolinone hybrids from monocarbonyl curcumin analogues. Characterization, bio-evaluation and DFT study</p>	<p>Soufiane Benreka, Fatima-Zohra Zradni, Fatiha Madi, Gilbert Kirsch, Souad Kasmi-Mir</p>	<p>Journal of Sulfur Chemistry</p>	<p>2022</p>	<p>A</p>	<p>43</p>	<p>53-77</p>	<p>https://doi.org/10.1080/17415993.2021.1971669</p>

<i>Productions Scientifiques2022</i>							
<i>Communications</i>							
<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>Volume</i>	<i>Page</i>	<i>URL</i>
<i>Doking Moleculaire</i>	<i>DJELLALA Imane</i>	<i>Au webinaire formation</i>	<i>2022</i>				
<i>Computational study of inclusion complex of nedaplatin with cucurbit[7]uril: Electronic and intermolecular interactions investigations</i>	<i>DJELLALA Imane</i>	<i>Qsar workshop</i>	<i>2022</i>				

Communications nationales

Communications internationales	<p>Moleculaire modeling study of inclusion complex "β-cyclodextrin/ Eucalyptol"</p>	<p>DJELLALA Imane, NOUAR Leila</p>	<p>the 5th international days on organic chemistry of annaba-JICOA'22</p>	2022				University of ANNABA
	<p>Density functional theories study of the interactions between hostrandomly methylated β-cyclodextrin and guestindolinonicntroxi de radical : moléculaire structure, HOMO, LUMO, NCI, QTAIM, analyse</p>	<p>CHEKATTI Leyla, MADI Fatiha, NOUAR Leila, OUMEDDOUR Rabah</p>	<p>6th international chemistry symposium (CIC-6)</p>	2022				
	<p>Computational investigation of indolinonic nitroxide radical @ randomly β-cyclodextrin inclusion complex electronic and intermolecular analysis</p>	<p>CHEKATTI Leyla, MADI Fatiha, NOUAR Leila, OUMEDDOUR Rabah</p>	<p>the 5th international days on organic chemistry of annaba-JICOA'22</p>	2022				University of ANNABA

<i>Communications internationales</i>	<i>Decouverte d'inhibiteurs flavonoides potentiels contr le SARS-COV2 bassee sur une strategie du docking moleculaire</i>	<i>BENCHEIKH Bochra, DJEMIL Rayenne</i>	<i>the first international congress of innovations in chemistry for therapeutic amis</i>	<i>2022</i>				<i>University of oum elbouaghi , algeria</i>
	<i>Etude des structures , propriétés électroniques et les interctions du complexe d'inclusion par la méthode DFT</i>	<i>HAYAHEM Sakina, NOUAR Leila</i>	<i>the 5th international days on organic chemistry of annaba-JICOA'22</i>	<i>2022</i>				<i>University of ANNABA</i>