

Liste des productions scientifiques (publication, communication,.....)

Année 2021

Etablissement Universitaire: Université 8 Mai 1945 Guelma

Faculté: Mathématiques, Informatique et Science de la matière

Laboratoire: Chimie Computationnelle et Nanostructures LCCN

Productions Scientifiques 2021							
Publications							
Titre	Auteurs	Revue	Année	Catégorie de la revue: A+, A, B- Scopus, B- non Scopus, non classée	Volume	Page	URL
Dopamine Family Complexes With $\beta$ -Cyclodextrin: Molecular Docking Studies	Mouna Cheriet Rayenne Djemil Ammar Khellaf Djameledine Khatmi	Journal of Polycyclic Aromatic Compounds	2021	A		110	<a href="https://doi.org/10.1080/10406638.2021.1970588">https://doi.org/10.1080/10406638.2021.1970588</a>
Computational investigation of vanillin@ $\beta$ -cyclodextrin inclusion complex: Electronic and intermolecular analysis	Gheribi Meryem Ksouri Rabah Madi Fatiha Nouar Leila Bouhadiba A Aziz Djellala Imane Merdes Rachid	Journal of Molecular Liquids	2021	A	321	114839	<a href="https://doi.org/10.1016/j.molliq.2020.114839">https://doi.org/10.1016/j.molliq.2020.114839</a>
In silico exploration of O-H...X <sup>2+</sup> (X = Cu, Ag, Hg) interaction, targeted adsorption zone, charge density iso-surface, O-H proton analysis and topographic parameters theory for calix[6]arene and calix[8]arene as model	B.Gassoumia F.E.Ben Mohamed M.E.Castrod F.J.Melendeze A.Karayelf L.Nouar F.Madig H.Ghallah S.Özknali V.I.Kovalenkoj R.Ben Chaabanea H.Ben Ouada	Journal of Molecular Liquids	2021	A	334	116127	<a href="https://doi.org/10.1016/j.molliq.2021.116127">https://doi.org/10.1016/j.molliq.2021.116127</a>
Effect of solvent on absorption and emission spectra of 2, 2'-Bipyridine and its inclusion complex into $\beta$ -cyclodextrin: DFT and TD-DFT study	Amrani Salma Madi Fatiha Nouar Leila	Computational and Theoretical Chemistry	2021	A	1206	113481	<a href="https://doi.org/10.1016/j.comptc.2021.113481">https://doi.org/10.1016/j.comptc.2021.113481</a>
Conformational Investigation of the Encapsulation of Nicotinic Acid Into $\beta$ Cyclodextrin	Guendouzi O. Nouar L Guendouzi A Madi F Boumediene M Yahia Cherif F Hendi A Djellala I Elkeurti	Journal of Organic & Supramolecular Chemistry	2021	A	68	1823	<a href="https://doi.org/10.1002/slct.202100197">https://doi.org/10.1002/slct.202100197</a>
Electrochemical and Theoretical Studies of Inula viscosa Extract as Green Corrosion Inhibitor for Mild Steel in Hydrochloric Acid Solution	Elhassasna Souhir Harkati Brahim Hadjar Samah	Journal of Defect and Diffusion Forum	2021	B	406	406-418	<a href="https://doi.org/10.4028/www.scientific.net/DDF.406.406">doi:10.4028/www.scientific.net/DDF.406.406</a>
Theoretical investigation of inclusion complex of 2-methyl mercapto phenothiazine with hydroxy propyl $\beta$ -cyclodextrin by DFT approaches	Y. Mezari L. Nouar F. Madi A. Guendouzi I. Djellala I. Lafifi R. Merdes A. Bouhadiba B. Houari	Bulgarian Chemical Communications	2021	B	53	196 - 210	DOI: 10.34049/bcc.53.2.5329

Publications Internationales

**Productions Scientifiques 2021**

**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>	Molecular docking of cyp3A4 inhibition by antiretroviral therapy	BENCHEIKH Bochra CHERJET Mouna DJEMIL Rayenne	2ème Séminaire National Sciences d'Interfaces Chimie-Biologie souk-ahras	2021				
	DFT investigation of host-guest interaction between two vitamins (Nicotinic, Ascorbic acid) and $\beta$ cyclodextrin	Yasmine MEZARI Leila NOUAR Fatih MADI Rachid MERDES	2ème séminaire National des sciences d'Interface Chimie-Biologie, Université Souk-Ahras	2021				
	Interactions in inclusion complexes pyroquilon with cucurbit [n] urils( N=7,8) using DFT-D3 correction dispersion	DJELLALA Imane Leila NOUAR Fatih MADI	2ème séminaire National des sciences d'Interface Chimie-Biologie, Université Souk-Ahras	2021				
	Theoretical investigation of host-guest interactions between pesticide pyroquilon with two different cucurbit[n]uril	DJELLALA Imane Leila NOUAR Fatih MADI	13 ème journée thésards sur la Chimie Appliquée et la Modélisation, Guelma	2021				
	Host-guest interaction between randomly methylated $\beta$ -cyclodextrin and indolinonic nitroxide radical	CHEKATTI leyla MADI Fatih NOUAR Leila OUMEDDOUR Rabah	13 ème journée thésards sur la Chimie Appliquée et la Modélisation, Guelma	2021				
	DFT and Molecular Docking Study of CYP 3A4 Inhibitors with anti-antiviral Therapy	BENCHEIKH Bochra	13 ème journée thésards sur la Chimie Appliquée et la Modélisation, Guelma	2021				
	DFT study of inclusion complex of 2-Methyl Mercapto Phenothiazine with Hydroxy Propyl $\beta$ -Cyclodextrin : EDA, NBO, QTAIM, and NCI analyses	Mezari Yasmine Nouar Leila Merdes Rachid Madi Fatih Djellala Imane	13 ème journée thésards sur la Chimie Appliquée et la Modélisation, Guelma	2021				
<b>Communications internationales</b>	molecular docking study of cyp3A4 with anti hiv	BENCHEIKH Bochra CHERJET Mouna DJEMIL Rayenne	2eme séminaire international sur les sciences de la matière (Oran)	2021				
	computational methode for antiretroviral therapy	BENCHEIKH Bochra CHERJET Mouna DJEMIL Rayenne	IC-SEAM21 Ouargla	2021				
	molecular docking of the inhibition of cyp 3A4 by grapefruit juice	BENCHEIKH Bochra CHERJET Mouna DJEMIL Rayenne	séminaire international sur la sciences de la matière (physique et chimie) Université USTO, Bir El Djir, Oran, 31000, Algeria	2021				
	Theoretical investigation of inclusion complex of 2-methyl mercapto phenothiazine with hydroxy propyl $\beta$ cyclodextrin by DFT approaches	Mezari Yasmine Nouar Leila Merdes Rachid Madi Fatih Djellala Imane	séminaire international sur la sciences de la matière (physique et chimie), Université USTO, Bir El Djir, Oran, 31000, Algeria	2021				
	Computational study of inclusion complex of nedaplatin with cucurbit[7]uril: Electronic and intermolecular interactions investigations	DJELLALA Imane Leila NOUAR Fatih MADI	1st International Conference on Sustainable Energy and Advanced Materials IC-SEAM'21 April 21-22, 2021, Ouargla, ALGERIA	2021				
	molecular docking of the inhibition of cyp 3A4 by grapefruit juice	Rayenne DJEMIL MESSAOUDI Boulouar CHERJET Mouna BENCHEIKH Bochra LACHI Nadia Khatmi Djameledine	Quatrième Colloque Maghrébin sur la Chimie des Hétérocycles CMCH Tunisie	2021				









