N Flores-HolguÃ-n

List of Publications by Year
in descending order

52	777	471509	610901
papers	citations	17	24
		h-index	g-index

54	54	54	683
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Natural Carotenoids as Nanomaterial Precursors for Molecular Photovoltaics: A Computational DFT Study. Molecules, 2010, 15, 4490-4510.	3.8	59
2	Chemical Reactivity Properties, pKa Values, AGEs Inhibitor Abilities and Bioactivity Scores of the Mirabamides Aâ€“H Peptides of Marine Origin Studied by Means of Conceptual DFT. Marine Drugs, 2018, 16, 302.	4.6	49
3	Density Functional Theory (DFT) Study of Triphenylamine-Based Dyes for Their Use as Sensitizers in Molecular Photovoltaics. International Journal of Molecular Sciences, 2012, 13, 4418-4432.	4.1	36
4	A fast and simple evaluation of the chemical reactivity properties of the Pristinamycin family of antimicrobial peptides. Chemical Physics Letters, 2020, 739, 137021.	2.6	36
5	Virtual Screening of Marine Natural Compounds by Means of Chemoinformatics and CDFT-Based Computational Peptidology. Marine Drugs, 2020, 18, 478.	4.6	32
6	Theoretical study of chemical reactivity of the main species in the Î±-pinene isomerization reaction. Computational and Theoretical Chemistry, 2008, 854, 81-88.	1.5	30
7	Chemical Reactivity Theory and Empirical Bioactivity Scores as Computational Peptidology Alternative Tools for the Study of Two Anticancer Peptides of Marine Origin. Molecules, 2019, 24, 1115.	3.8	30
8	Conceptual DFT-Based Computational Peptidology of Marine Natural Compounds: Discodermins Aâ€“H. Molecules, 2020, 25, 4158.	3.8	30
9	Theoretical calculation of the maximum absorption wavelength for Cyanidin molecules with several methodologies. Computational and Theoretical Chemistry, 2015, 1067, 129-134.	2.5	29
10	Chemical-Reactivity Properties, Drug Likeness, and Bioactivity Scores of Seragamides Aâ€“F Anticancer Marine Peptides: Conceptual Density Functional Theory Viewpoint. Computation, 2019, 7, 52.	2.0	27
11	Computational Molecular Nanoscience Study of the Properties of Copper Complexes for Dye-Sensitized Solar Cells. International Journal of Molecular Sciences, 2012, 13, 16005-16019.	4.1	25
12	Theoretical calculations of molecular dipole moment, polarizability, and first hyperpolarizability of glycineâ€“sodium nitrate. Computational and Theoretical Chemistry, 2009, 905, 76-80.	1.5	24
13	A proposal based on quantum phenomena for the ORR mechanism on nitrogen-doped carbon-based electrocatalysts. International Journal of Hydrogen Energy, 2019, 44, 12374-12380.	7.1	23
14	Structure-fluorescence relationship: interplay of non-covalent interactions in homologous 1,3,5-triaryl-2-pyrazolines. New Journal of Chemistry, 2015, 39, 4359-4367.	2.8	22
15	Molecular design of copper complexes as sensitizers for efficient dye-sensitized solar cells. Journal of Photochemistry and Photobiology A: Chemistry, 2013, 267, 1-5.	3.9	21
16	CHIH-DFT determination of the electrical, optical, and magnetic properties and NICS aromaticity of megazol. Computational and Theoretical Chemistry, 2005, 717, 1-3.	1.5	19
17	Theoretical study of electronic properties of organic photovoltaic materials. Journal of Computational Chemistry, 2009, 30, 1027-1037.	3.3	18
18	Investigation of Antifungal Properties of Synthetic Dimethyl-4-Bromo-1-(Substituted Benzoyl) Pyrrolo[1,2-a] Quinoline-2,3-Dicarboxylates Analogues: Molecular Docking Studies and Conceptual DFT-Based Chemical Reactivity Descriptors and Pharmacokinetics Evaluation. Molecules, 2021, 26, 2722.	3.8	18

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19	CHIH-DFT determination of the reactivity sites of the antiparasitic drug megazol. Computational and Theoretical Chemistry, 2005, 723, 231-234.	1.5	17
20	Computational molecular characterization of the flavonoid Morin and its Pt(II), Pd(II) and Zn(II) complexes. Journal of Molecular Modeling, 2011, 17, 979-985.	1.8	16
21	Construction of a Nanodiamondâ€“Tamoxifen Complex as a Breast Cancer Drug Delivery Vehicle. Journal of Nanomaterials, 2016, 2016, 1-9.	2.7	14
22	Calculation of the Global and Local Conceptual DFT Indices for the Prediction of the Chemical Reactivity Properties of Papuamides Aâ€“F Marine Drugs. Molecules, 2019, 24, 3312.	3.8	14
23	Electron injection in anthocyanidin and betalain dyes for dye-sensitized solar cells: a DFT approach. Journal of Computational Electronics, 2019, 18, 396-406.	2.5	13
24	Preparation, Spectroscopic Characterization, Theoretical Investigations, and In Vitro Anticancer Activity of Cd(II), Ni(II), Zn(II), and Cu(II) Complexes of 4(3H)-Quinazolinone-Derived Schiff Base. Molecules, 2020, 25, 5973.	3.8	13
25	Computational Pharmacokinetics Report, ADMET Study and Conceptual DFTâ€Based Estimation of the Chemical Reactivity Properties of Marine Cyclopeptides. ChemistryOpen, 2021, 10, 1142-1149.	1.9	12
26	Computational note on the chemical reactivity of pyrrole derivatives. Computational and Theoretical Chemistry, 2009, 912, 119-120.	1.5	11
27	Computational nanochemistry study of the molecular structure and properties of ethambutol. Journal of Molecular Modeling, 2013, 19, 3507-3515.	1.8	10
28	Conceptual DFT-Based Computational Peptidology, Pharmacokinetics Study and ADMET Report of the Veraguamides Aâ€“G Family of Marine Natural Drugs. Marine Drugs, 2022, 20, 97.	4.6	10
29	TD-DFT/IEFPCM determination of the absorption and emission spectra of DABCYL. Computational and Theoretical Chemistry, 2010, 945, 101-103.	1.5	9
30	DFT study of the interaction between the conjugated fluorescein and dabcyl system, using fluorescene quenching method. Journal of Molecular Modeling, 2012, 18, 4113-4120.	1.8	9
31	DFT calculation of the electronic properties of fluorene-1,3,4-thiadiazole oligomers. Journal of Molecular Modeling, 2013, 19, 3537-3542.	1.8	9
32	Theoretical analysis of the electronic properties in Zinc-porphyrins derivatives. Journal of Molecular Structure, 2019, 1191, 259-270.	3.6	9
33	Electronic structure study using density functional theory in organic dendrimers. Journal of Molecular Modeling, 2011, 17, 1963-1972.	1.8	8
34	CHIH-DFT computational molecular characterization of phenanthro [9,10-c]-1,2,5-thiadiazole 1,1-dioxide. Computational and Theoretical Chemistry, 2008, 862, 60-65.	1.5	6
35	Comparative study of copper complexes with different anchoring groups by molecular modeling and its application to dye-sensitized solar cells. Polyhedron, 2014, 82, 33-36.	2.2	6
36	N-((1H-Pyrrol-2-yl)methylene)-6-methoxypyridin-3-amine and Its Co(II) and Cu(II) Complexes as Antimicrobial Agents: Chemical Preparation, In Vitro Antimicrobial Evaluation, In Silico Analysis and Computational and Theoretical Chemistry Investigations. Molecules, 2022, 27, 1436.	3.8	6

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37	A theoretical study of the carbocation formation energy involved in the isomerization of Î±-pinene. Chemical Physics Letters, 2012, 546, 168-170.	2.6	5
38	CDFT-Based Reactivity Descriptors as a Useful MEDT Chemoinformatics Tool for the Study of the Virotoxin Family of Fungal Peptides. Molecules, 2019, 24, 2707.	3.8	5
39	Virtual Screening for Potential Phytobioactives as Therapeutic Leads to Inhibit NQO1 for Selective Anticancer Therapy. Molecules, 2021, 26, 6863.	3.8	5
40	Computational prediction of the melting temperature of a DNA biosensor to detect Mycobacterium tuberculosis. Computational and Theoretical Chemistry, 2009, 912, 60-62.	1.5	4
41	Quantum chemical study of a new class of sensitisers: influence of the substitution of aromatic rings on the properties of copper complexes. Molecular Physics, 2014, 112, 987-994.	1.7	4
42	New Methods of Esterification of Nanodiamonds in Fighting Breast Cancerâ€"A Density Functional Theory Approach. Molecules, 2017, 22, 1740.	3.8	4
43	Analysis of the Molecular Interactions between Cytochromes P450 3A4 and 1A2 and Aflatoxins: A Docking Study. Applied Sciences (Switzerland), 2019, 9, 2467.	2.5	4
44	Theoretical modifications of the molecular structure of Aurantinidin and Betanidin dyes to improve their efficiency as dye-sensitized solar cells. Journal of Computational Electronics, 2020, 19, 507-515.	2.5	4
45	Virtual Prospection of Marine Cyclopeptides as Therapeutics by Means of Conceptual DFT and Computational ADMET. Pharmaceuticals, 2022, 15, 509.	3.8	4
46	Unexpected electron acceptor behavior of the 1,3,4-thiadiazole oligomer, a DFT study. Computational and Theoretical Chemistry, 2015, 1068, 109-116.	2.5	3
47	A CDFT-Based Computational Peptidology (CDFT-CP) Study of the Chemical Reactivity and Bioactivity of the Marine-Derived Alternaramide Cyclopentadepsipeptide. Journal of Chemistry, 2021, 2021, 1-11.	1.9	3
48	Computational note on the calculation of the dipole moment, polarizability and hyperpolarizability of solanidine. Computational and Theoretical Chemistry, 2008, 849, 122-123.	1.5	2
49	Computational characterization of the molecular structure and properties of Dye 7 for organic photovoltaics. Journal of Molecular Modeling, 2012, 18, 835-842.	1.8	2
50	Chemical Reactivity Properties, Solubilities, and Bioactivity Scores of Some Pigments Derived from Carotenoids of Marine Origin through Conceptual DFT Descriptors. Journal of Chemistry, 2019, 2019, 1-12.	1.9	2
51	Computational Study of 3,4-Diphenyl-4-(4-Metoxyphenyl)-1,2,5-Thiadiazoline 1,1-Dioxide for Molecular Photovoltaics. Journal of Computational and Theoretical Nanoscience, 2011, 8, 74-79.	0.4	1
52	Influence on the reactivity properties of the substitution by different halogens on the conjugated backbone of the 1,3,5-triaryl-2-pyrazoline skeleton in relation to the increasing alkyloxy chain length: a conceptual density functional theory study. Journal of Molecular Modeling, 2020, 26, 174.	1.8	1