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	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
2	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
3	Virtual Prospection of Marine Cyclopeptides as Therapeutics by Means of Conceptual DFT and Computational ADMET. Pharmaceuticals, 2022, 15, 509.	3.8	4
4	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
5	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
6	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
7	Virtual Screening for Potential Phytobioactives as Therapeutic Leads to Inhibit NQO1 for Selective Anticancer Therapy. Molecules, 2021, 26, 6863.	3.8	5
8	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
9	Virtual Screening of Marine Natural Compounds by Means of Chemoinformatics and CDFT-Based Computational Peptidology. Marine Drugs, 2020, 18, 478.	4.6	32
10	Conceptual DFT-Based Computational Peptidology of Marine Natural Compounds: Discodermins Aâ€“H. Molecules, 2020, 25, 4158.	3.8	30
11	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
12	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
13	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
14	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
15	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
16	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
17	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
18	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

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19	Theoretical analysis of the electronic properties in Zinc-porphyrins derivatives. Journal of Molecular Structure, 2019, 1191, 259-270.	3.6	9
20	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
21	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
22	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
23	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
24	New Methods of Esterification of Nanodiamonds in Fighting Breast Cancerâ€”A Density Functional Theory Approach. Molecules, 2017, 22, 1740.	3.8	4
25	Construction of a Nanodiamondâ€“Tamoxifen Complex as a Breast Cancer Drug Delivery Vehicle. Journal of Nanomaterials, 2016, 2016, 1-9.	2.7	14
26	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
27	Theoretical calculation of the maximum absorption wavelength for Cyanidin molecules with several methodologies. Computational and Theoretical Chemistry, 2015, 1067, 129-134.	2.5	29
28	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
29	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
30	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
31	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
32	DFT calculation of the electronic properties of fluorene-1,3,4-thiadiazole oligomers. Journal of Molecular Modeling, 2013, 19, 3537-3542.	1.8	9
33	Computational nanochemistry study of the molecular structure and properties of ethambutol. Journal of Molecular Modeling, 2013, 19, 3507-3515.	1.8	10
34	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
35	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
36	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

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37	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
38	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
39	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
40	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
41	Electronic structure study using density functional theory in organic dendrimers. Journal of Molecular Modeling, 2011, 17, 1963-1972.	1.8	8
42	TD-DFT/IEFPCM determination of the absorption and emission spectra of DABCYL. Computational and Theoretical Chemistry, 2010, 945, 101-103.	1.5	9
43	Natural Carotenoids as Nanomaterial Precursors for Molecular Photovoltaics: A Computational DFT Study. Molecules, 2010, 15, 4490-4510.	3.8	59
44	Theoretical study of electronic properties of organic photovoltaic materials. Journal of Computational Chemistry, 2009, 30, 1027-1037.	3.3	18
45	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
46	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
47	Computational note on the chemical reactivity of pyrrole derivatives. Computational and Theoretical Chemistry, 2009, 912, 119-120.	1.5	11
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	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
50	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
51	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
52	CHIH-DFT determination of the reactivity sites of the antiparasitic drug megazol. Computational and Theoretical Chemistry, 2005, 723, 231-234.	1.5	17