Daniel Glossman-Mitnik

List of Publications by Year
in descending order

219	3,681	172207	233125
papers	citations	29 h-index	45 g-index

228	228	228	2822
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Computational simulation of the molecular structure and properties of heterocyclic organic compounds with possible corrosion inhibition properties. Computational and Theoretical Chemistry, 2005, 713, 65-70.	1.5	164
2	Computational simulations of the molecular structure and corrosion properties of amidoethyl, aminoethyl and hydroxyethyl imidazolines inhibitors. Corrosion Science, 2006, 48, 4053-4064.	3.0	152
3	Title is missing!. Journal of Nanoparticle Research, 2002, 4, 167-174.	0.8	100
4	Fuel Gas Storage and Separations by Metalâ^'Organic Frameworks: Simulated Adsorption Isotherms for H₂ and CH₄ and Their Equimolar Mixture. Journal of Physical Chemistry C, 2009, 113, 6634-6642.	1.5	94
5	DFT studies of functionalized carbon nanotubes and fullerenes as nanovectors for drug delivery of antitubercular compounds. Chemical Physics Letters, 2007, 447, 105-109.	1.2	86
6	Theoretical study of the molecular properties and chemical reactivity of (+)-catechin and (â^')-epicatechin related to their antioxidant ability. Computational and Theoretical Chemistry, 2006, 761, 97-106.	1.5	81
7	CHIH-DFT study of the electronic properties and chemical reactivity of quercetin. Computational and Theoretical Chemistry, 2005, 716, 67-72.	1.5	67
8	CHIH-DFT theoretical study of isomeric thiatriazoles and their potential activity as corrosion inhibitors. Computational and Theoretical Chemistry, 2005, 716, 61-65.	1.5	65
9	Computational Study of the Chemical Reactivity Properties of the Rhodamine B Molecule. Procedia Computer Science, 2013, 18, 816-825.	1.2	63
10	Natural Carotenoids as Nanomaterial Precursors for Molecular Photovoltaics: A Computational DFT Study. Molecules, 2010, 15, 4490-4510.	1.7	59
11	Study of chemical reactivity in relation to experimental parameters of efficiency in coumarin derivatives for dye sensitized solar cells using DFT. Physical Chemistry Chemical Physics, 2015, 17, 14122-14129.	1.3	59
12	CHIH-DFT determination of the molecular structure, infrared and ultraviolet spectra of the flavonoid quercetin. Computational and Theoretical Chemistry, 2004, 681, 71-76.	1.5	55
13	Band structure, optical properties and infrared spectrum of glycineâ€“sodium nitrate crystal. Journal of Molecular Structure, 2008, 875, 295-301.	1.8	53
14	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.	2.2	49
15	CHIH-DFT determination of the molecular structure infrared spectra, UV spectra and chemical reactivity of three antitubercular compounds: Rifampicin, Isoniazid and Pyrazinamide. Journal of Molecular Modeling, 2007, 13, 505-518.	0.8	48
16	Conceptual DFT Study of the Local Chemical Reactivity of the Colored BISARG Melanoidin and Its Protonated Derivative. Frontiers in Chemistry, 2018, 6, 136.	1.8	45
17	Conceptual DFT study of the local chemical reactivity of the dilysyldipyrrolones A and B intermediate melanoidins. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	44
18	Molecular Reactivity and Absorption Properties of Melanoidin Blue-G1 through Conceptual DFT. Molecules, 2018, 23, 559.	1.7	41

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19	Computational study of the chemical reactivity of the Blue-M1 intermediate melanoidin. Computational and Theoretical Chemistry, 2018, 1134, 22-29.	1.1	39
20	A Molecular Electron Density Theory Study of the Chemical Reactivity of Cis- and Trans-Resveratrol. Molecules, 2016, 21, 1650.	1.7	38
21	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.	1.8	36
22	Computational prediction of the pKas of small peptides through Conceptual DFT descriptors. Chemical Physics Letters, 2017, 671, 138-141.	1.2	36
23	A fast and simple evaluation of the chemical reactivity properties of the Pristinamycin family of antimicrobial peptides. Chemical Physics Letters, 2020, 739, 137021.	1.2	36
24	Chemical Reactivity Theory Applied to the Calculation of the Local Reactivity Descriptors of a Colored Maillard Reaction Product. Chemical Science International Journal, 2018, 22, 1-14.	0.3	36
25	CHIH-DFT determination of the molecular structure, infrared and ultraviolet spectra of potentially organic corrosion inhibitors. Computational and Theoretical Chemistry, 2004, 681, 83-88.	1.5	35
26	A comparison of the chemical reactivity of naringenin calculated with the M06 family of density functionals. Chemistry Central Journal, 2013, 7, 155.	2.6	35
27	Computational Nanochemistry Report on the Oxicamsâ€"Conceptual DFT Indices and Chemical Reactivity. Journal of Physical Chemistry B, 2013, 117, 6339-6351.	1.2	35
28	Conceptual DFT Descriptors of Amino Acids with Potential Corrosion Inhibition Properties Calculated with the Latest Minnesota Density Functionals. Frontiers in Chemistry, 2017, 5, 16.	1.8	34
29	Computational molecular characterization of the flavonoid rutin. Chemistry Central Journal, 2010, 4, 12.	2.6	33
30	Virtual Screening of Marine Natural Compounds by Means of Chemoinformatics and CDFT-Based Computational Peptidology. Marine Drugs, 2020, 18, 478.	2.2	32
31	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
32	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.	1.7	30
33	Conceptual DFT-Based Computational Peptidology of Marine Natural Compounds: Discodermins Aâ€"H. Molecules, 2020, 25, 4158.	1.7	30
34	Theoretical calculation of the maximum absorption wavelength for Cyanidin molecules with several methodologies. Computational and Theoretical Chemistry, 2015, 1067, 129-134.	1.1	29
35	Solvation Thermodynamic Properties of Hydrogen Sulfide in [C₄mim][PF₆], [C₄mim][BF₄], and [C₄mim][Cl] Ionic Liquids, Determined by Molecular Simulations. Journal of Physical Chemistry B, 2015, 119, 10727-10737.	1.2	28
36	Chemical-Reactivity Properties, Drug Likeness, and Bioactivity Scores of Seragamides Aâ€"F Anticancer Marine Peptides: Conceptual Density Functional Theory Viewpoint. Computation, 2019, 7, 52.	1.0	27

#	Article	IF	Citations
37	Theoretical Study of the Effect of Ï€-Bridge on Optical and Electronic Properties of Carbazole-Based Sensitizers for DSSCs. Molecules, 2020, 25, 3670.	1.7	27
38	Blue M2: an intermediate melanoidin studied via conceptual DFT. Journal of Molecular Modeling, 2018, 24, 138.	0.8	26
39	Application of density functional theory concepts to the study of the chemical reactivity of thiadiazoles. Computational and Theoretical Chemistry, 1995, 330, 385-388.	1.5	25
40	Local and nonlocal density functional calculations of the molecular structure of isomeric thiadiazoles. Computational and Theoretical Chemistry, 1997, 390, 67-78.	1.5	25
41	Computational Molecular Nanoscience Study of the Properties of Copper Complexes for Dye-Sensitized Solar Cells. International Journal of Molecular Sciences, 2012, 13, 16005-16019.	1.8	25
42	Chemical Reactivity Theory Study of Advanced Glycation Endproduct Inhibitors. Molecules, 2017, 22, 226.	1.7	25
43	Evaluation of Annona muricata Acetogenins as Potential Anti-SARS-CoV-2 Agents Through Computational Approaches. Frontiers in Chemistry, 2020, 8, 624716.	1.8	25
44	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
45	DFT Study of Polythiophene Energy Band Gap and Substitution Effects. Journal of Chemistry, 2015, 2015, 1-12.	0.9	24
46	Crystallographic study and molecular orbital calculations of 1,2,5-thiadiazole 1,1-dioxide derivatives. , 1998, 11, 91-100.		23
47	Influence of the basis set and correlation method on the calculation of molecular structures: thiadiazoles revisited. Computational and Theoretical Chemistry, 2001, 548, 153-163.	1.5	23
48	CHIH-DFT Determination of the Molecular Structure and Infrared and Ultraviolet Spectra of Azathiophenes. Theoretical Chemistry Accounts, 2006, 117, 57-68.	0.5	23
49	Computational molecular characterization of Coumarin-102. Computational and Theoretical Chemistry, 2009, 911, 105-108.	1.5	23
50	Theoretical analysis of anthracene and its carbonyl and carboxyl derivatives using DFT and TD-DFT. Computational and Theoretical Chemistry, 2009, 894, 64-70.	1.5	22
51	Computational prediction of bioactivity scores and chemical reactivity properties of the Parasin I therapeutic peptide of marine origin through the calculation of global and local conceptual DFT descriptors. Theoretical Chemistry Accounts, 2019, 138, 1.	0.5	22
52	Thermal, mechanical, and electronic properties of glycine-sodium nitrate crystal. Journal of Physics and Chemistry of Solids, 2008, 69, 1974-1979.	1.9	21
53	Computational characterization of the Î²,Î²-carotene molecule. Computational and Theoretical Chemistry, 2009, 913, 215-220.	1.5	21
54	Molecular design of copper complexes as sensitizers for efficient dye-sensitized solar cells. Journal of Photochemistry and Photobiology A: Chemistry, 2013, 267, 1-5.	2.0	21

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55	CHIH-DFT determination of the molecular structure, infrared and ultraviolet spectra of the antiparasitic drug megazol. Computational and Theoretical Chemistry, 2004, 681, 77-82.	1.5	20
56	Optimized structure and thermochemical properties of flavonoids determined by the CHIH(medium)â€“DFT model chemistry versus experimental techniques. Journal of Molecular Structure, 2007, 871, 114-130.	1.8	20
57	A conceptual DFT study of the molecular properties of glycating carbonyl compounds. Chemistry Central Journal, 2017, 11, 8.	2.6	20
58	Nonlocal exchange and kinetic energy density functionals with correct asymptotic behavior for electronic systems. International Journal of Quantum Chemistry, 1994, 49, 171-184.	1.0	19
59	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
60	Density functional theory study of indigo and its derivatives as photosensitizers for dye-sensitized solar cells. Journal of Photochemistry and Photobiology A: Chemistry, 2013, 255, 24-26.	2.0	19
61	Quantum chemical study of the effect of Ï€-bridge on the optical and electronic properties of sensitizers for DSSCs incorporating dioxythiophene and thiophene units. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	19
62	Unexpected production of 2,4,6-triphenyl-1,3,5-triazine in the electroreduction of 3,4-diphenyl-1,2,5-thiadiazole 1-oxide. Theoretical estimation of reactive sites for 1-oxide and 1,1-dioxide 1,2,5-thiadiazoles. Tetrahedron Letters, 2000, 41, 3531-3535.	0.7	18
63	A theoretical study on the aromaticity of thiadiazoles and related compounds. Computational and Theoretical Chemistry, 2001, 549, 285-288.	1.5	18
64	Theoretical study of electronic properties of organic photovoltaic materials. Journal of Computational Chemistry, 2009, 30, 1027-1037.	1.5	18
65	Comparison of several protocols for the computational prediction of the maximum absorption wavelength of chrysanthemin. Journal of Molecular Modeling, 2014, 20, 2378.	0.8	18
66	Computational chemistry of natural products: a comparison of the chemical reactivity of isonaringin calculated with the M06 family of density functionals. Journal of Molecular Modeling, 2014, 20, 2316.	0.8	18
67	Chemical synthesis, spectroscopic studies, chemical reactivity properties and bioactivity scores of an azepin-based molecule. Journal of Molecular Structure, 2019, 1180, 300-306.	1.8	18
68	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.	1.7	18
69	CHIH-DFT determination of the reactivity sites of the antiparasitic drug megazol. Computational and Theoretical Chemistry, 2005, 723, 231-234.	1.5	17
70	Synthesis, structure, characterization and photophysical properties of copper(<scp>i</scp>) complexes containing polypyridyl ligands. RSC Advances, 2014, 4, 42624-42631.	1.7	17
71	Towards the rationalization of catalytic activity values by means of local hyper-softness on the catalytic site: a criticism about the use of net electric charges. Physical Chemistry Chemical Physics, 2015, 17, 29764-29775.	1.3	17
72	Theoretical Study of the Effect of Different Ï€ Bridges Including an Azomethine Group in Triphenylamine-Based Dye for Dye-Sensitized Solar Cells. Molecules, 2019, 24, 3897.	1.7	17

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73	Crystallographic study and molecular orbital calculations of thiadiazole derivatives. 1. Phenanthro[9,10-c]-1,2,5-thiadiazole 1,1-dioxide and acenaphtho[1,2-c]-1,2,5-thiadiazole 1,1-dioxide. Journal of Molecular Structure, 2001, 562, 157-166.	1.8	16
74	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.	0.8	16
75	DFT study of the effect of substituents on the absorption and emission spectra of Indigo. Chemistry Central Journal, 2012, 6, 70.	2.6	16
76	Computational Nutraceutics: Chemical Reactivity Properties of the Flavonoid Naringin by Means of Conceptual DFT. Journal of Chemistry, 2013, 2013, 1-8.	0.9	16
77	Experimental and theoretical study on the molecular structure, covalent and non-covalent interactions of 2,4-dinitrodiphenylamine: X-ray diffraction and QTAIM approach. Journal of Molecular Structure, 2017, 1141, 53-63.	1.8	16
78	Local and nonlocal density functional calculations of the molecular structure of isomeric thiadiazole monoxides. International Journal of Quantum Chemistry, 2001, 81, 105-115.	1.0	15
79	Application of density functional theory concepts to the study of the chemical reactivity of isomeric thiadiazolines. Computational and Theoretical Chemistry, 2001, 535, 39-47.	1.5	15
80	HF and DFT calculations of the molecular structure of isomeric thiadiazole dioxides. Computational and Theoretical Chemistry, 2001, 536, 41-51.	1.5	15
81	Hartreeâ€“Fock (HF) and local and nonlocal density functional (DFT) calculations of the molecular structure of isomeric thiadiazolidines. Computational and Theoretical Chemistry, 2001, 538, 201-210.	1.5	15
82	CHIH-DFT determination of the molecular structure and infrared and ultraviolet spectra of -solanine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 66, 208-211.	2.0	15
83	Computational Peptidology Assisted by Conceptual Density Functional Theory for the Study of Five New Antifungal Tripeptides. ACS Omega, 2019, 4, 12555-12560.	1.6	15
84	In vitro anticancer activity of 4(3H)-quinazolinone derived Schiff base and its Cu(II), Zn(II) and Cd(II) complexes: Preparation, X-ray structural, spectral characterization and theoretical investigations. Inorganica Chimica Acta, 2020, 511, 119846.	1.2	15
85	Nonlocal exchange- and kinetic-energy density functionals for electronic systems: Application to atoms and ions. Physical Review A, 1993, 47, 1804-1810.	1.0	14
86	Crystallographic study and molecular orbital calculations of thiadiazole derivatives. Part 3: 3,4-diphenyl-1,2,5-thiadiazoline 1,1-dioxide, 3,4-diphenyl-1,2,5-thiadiazolidine 1,1-dioxide and 4-ethoxy-5-methyl-3,4-diphenyl-1,2,5-thiadiazoline 1,1-dioxide. Journal of Molecular Structure, 2001, 597, 163-175.	1.8	14
87	G3-B3 calculation of the molecular structure and descriptors of isomeric thiadiazoles. Computational and Theoretical Chemistry, 2005, 725, 27-30.	1.5	14
88	Effects of sulfur substitutional impurities on (ZnO)n clusters (n=4â€“12) using density functional theory. Computational and Theoretical Chemistry, 2011, 965, 154-162.	1.1	14
89	Chemical reactivity and bioactivity properties of the Phallotoxin family of fungal peptides based on Conceptual Peptidology and DFT study. Heliyon, 2019, 5, e02335.	1.4	14
90	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.	1.7	14

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91	Crystallographic study and molecular orbital calculations of thiadiazole derivatives. 2. 3,4-diphenyl-1,2,5-thiadiazole 1-monoxide. Journal of Molecular Structure, 2002, 604, 195-203.	1.8	13
92	Molecular structure and substitution effects on diphenylanthrazolines for organic semiconductors: A theoretical study. Computational and Theoretical Chemistry, 2008, 863, 99-104.	1.5	13
93	Theoretical Study of theÏ€-Bridge Influence with Different Units of Thiophene and Thiazole in Coumarin Dye-Sensitized Solar Cells. International Journal of Photoenergy, 2016, 2016, 1-8.	1.4	13
94	Preparation and Characterization of Cerium (III) Doped Captopril Nanoparticles and Study of their Photoluminescence Properties. Open Chemistry, 2016, 14, 60-64.	1.0	13
95	Application of DFT concepts to the study of the chemical reactivity of some resveratrol derivatives through the assessment of the validity of the â€œKoopmans in DFTâ€•(KID) procedure. Journal of Theoretical and Computational Chemistry, 2017, 16, 1750006.	1.8	13
96	Electron injection in anthocyanidin and betalain dyes for dye-sensitized solar cells: a DFT approach. Journal of Computational Electronics, 2019, 18, 396-406.	1.3	13
97	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.	1.7	13
98	Atomic structure of metallic clusters of large size. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1994, 69, 1045-1050.	0.6	12
99	Computational Study of 3,4-Diphenyl-1,2,5-Thiadiazole 1-Oxide for Organic Photovoltaics. International Journal of Photoenergy, 2009, 2009, 1-8.	1.4	12
100	Theoretical evaluation of the order of reactivity of transfer agents utilized in RAFT polymerization. Journal of Molecular Modeling, 2010, 16, 95-105.	0.8	12
101	Theoretical Study of Copper Complexes: Molecular Structure, Properties, and Its Application to Solar Cells. International Journal of Photoenergy, 2013, 2013, 1-7.	1.4	12
102	Novel synthesis, structural analysis, photophysical properties and theoretical study of 2,4,5-tris(2-pyridyl)imidazole. Journal of Molecular Structure, 2015, 1099, 126-134.	1.8	12
103	Heteroleptic Cu(I) complexes containing polypyridyl ligands and triphenylphosphine: Synthesis, structure, photophysical properties, DFT studies and applications in co-sensitized solar cells. Inorganica Chimica Acta, 2017, 466, 486-496.	1.2	12
104	In Silico Pharmacokinetics, ADMET Study and Conceptual DFT Analysis of Two Plant Cyclopeptides Isolated From Rosaceae as a Computational Peptidology Approach. Frontiers in Chemistry, 2021, 9, 708364.	1.8	12
105	Chemical Reactivity Properties, Drug-Likeness Features and Bioactivity Scores of the Cholecystokinin Peptide Hormone. Computational Molecular Bioscience, 2019, 09, 41-47.	0.6	12
106	Computational Pharmacokinetics Report, ADMET Study and Conceptual DFTâ€Based Estimation of the Chemical Reactivity Properties of Marine Cyclopeptides. ChemistryOpen, 2021, 10, 1142-1149.	0.9	12
107	Nonlocal exchange and kinetic-energy density functionals for electronic systems. International Journal of Quantum Chemistry, 1992, 44, 347-358.	1.0	11
108	Stabilities of large sodium clusters for different atomic arrangements. Physical Review B, 1993, 47, 4747-4755.	1.1	11

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109	Study of the effect of solvent induced swelling on the resistivity of butadiene based elastomers filled with carbon particles. Sensors and Actuators A: Physical, 2005, 119, 157-168.	2.0	11
110	Computational note on the chemical reactivity of pyrrole derivatives. Computational and Theoretical Chemistry, 2009, 912, 119-120.	1.5	11
111	Exploration of the kinetic and thermochemical abilities for the free radical scavenging of two quercetin conformers. Journal of Molecular Structure, 2010, 981, 187-193.	1.8	11
112	Excited states analysis of sulfur substitutional impurities on (ZnO)6 clusters using DFT and TD-DFT. Computational and Theoretical Chemistry, 2010, 957, 100-107.	1.5	11
113	Experimental and quantum chemical studies of a novel synthetic prenylated chalcone. Chemistry Central Journal, 2013, 7, 17.	2.6	11
114	Conceptual Density Functional Theory Study of the Chemical Reactivity Properties and Bioactivity Scores of the Leu-Enkephalin Opioid Peptide Neurotransmitter. Computational Molecular Bioscience, 2019, 09, 13-26.	0.6	11
115	Synthesis, Computational Pharmacokinetics Report, Conceptual DFT-Based Calculations and Anti-Acetylcholinesterase Activity of Hydroxyapatite Nanoparticles Derived From Acorus Calamus Plant Extract. Frontiers in Chemistry, 2021, 9, 741037.	1.8	11
116	Nonlocal approximation to the exchange and kinetic energy functionals: Application to metallic clusters. International Journal of Quantum Chemistry, 1993, 45, 333-347.	1.0	10
117	Computational nanochemistry study of the molecular structure and properties of ethambutol. Journal of Molecular Modeling, 2013, 19, 3507-3515.	0.8	10
118	Computational prediction of the preferred glycation sites of model helical peptides derived from human serum albumin (HSA) and lysozyme helix 4 (LH4). Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	10
119	Computational Prediction of the Protonation Sites of Ac-Lys-(Ala)n-Lys-NH2 Peptides through Conceptual DFT Descriptors. Molecules, 2017, 22, 458.	1.7	10
120	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.	2.2	10
121	An introductory study of the molecular structure and properties of oligothiadiazoles. Computational and Theoretical Chemistry, 2003, 634, 67-76.	1.5	9
122	CHIH-DFT determination of the molecular structure and IR and UV spectra of solanidine. Journal of Molecular Modeling, 2006, 13, 43-46.	0.8	9
123	TD-DFT/IEFPCM determination of the absorption and emission spectra of DABCYL. Computational and Theoretical Chemistry, 2010, 945, 101-103.	1.5	9
124	DFT study of the interaction between the conjugated fluorescein and dabcyl system, using fluorescene quenching method. Journal of Molecular Modeling, 2012, 18, 4113-4120.	0.8	9
125	Docking Studies of Binding of Ethambutol to the C-Terminal Domain of the Arabinosyltransferase fromMycobacterium tuberculosis. Journal of Chemistry, 2013, 2013, 1-5.	0.9	9
126	Conceptual DFT as a Helpful Chemoinformatics Tool for the Study of the Clavanin Family of Antimicrobial Marine Peptides. , 0, , .		9

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127	A Thomas-Fermi-Dirac Theory of an Atom in Strong Magnetic Fields. Journal of the Physical Society of Japan, 1990, 59, 3571-3583.	0.7	8
128	Characterization of the semiquinones and quinones of (â˜')-epicatechin by means of computational chemistry. Computational and Theoretical Chemistry, 2009, 897, 6-11.	1.5	8
129	Electronic structure study using density functional theory in organic dendrimers. Journal of Molecular Modeling, 2011, 17, 1963-1972.	0.8	8
130	DENSITY FUNCTIONAL STUDY OF THE EFFECTS OF THE SUBSTITUENTS ON THE CHEMICAL REACTIVITY OF THE INDIGO MOLECULE. Journal of Theoretical and Computational Chemistry, 2013, 12, 1350013.	1.8	8
131	Influence of the basis set and correlation method on the calculation of the dipole moments of isomeric thiadiazoles. Computational and Theoretical Chemistry, 2003, 634, 77-81.	1.5	7
132	CBS-QB3 calculation of quantum chemical molecular descriptors of isomeric thiadiazoles. Journal of Molecular Graphics and Modelling, 2006, 25, 455-458.	1.3	7
133	Theoretical evaluation of the order of reactivity of transfer agents utilized in RAFT polymerization: group Z. Journal of Molecular Modeling, 2009, 15, 1133-1143.	0.8	7
134	Computational Nanochemistry Study of the Molecular Structure and Properties of Chlorophyll a. International Journal of Photoenergy, 2013, 2013, 1-8.	1.4	7
135	The substituent effect from the perspective of local hyper-softness. An example applied on norneloxicam, meloxicam and 4-meloxicam: Non-steroidal anti-inflammatory drugs. Chemical Physics Letters, 2015, 618, 162-167.	1.2	7
136	PREPARATION, IDENTIFICATION AND BIOLOGICAL PROPERTIES OF NEW FLUORIDE NANOCOMPOUNDS. Journal of the Chilean Chemical Society, 2016, 61, 3201-3205.	0.5	7
137	Synthesis, crystal structure, DFT studies and photophysical properties of a copper(I)â€“triphenylphosphane complex based on trans-(Â±)-2,4,5-tris(pyridin-2-yl)-2-imidazoline. Acta Crystallographica Section C, Structural Chemistry, 2017, 73, 280-286.	0.2	7
138	Vibrational spectroscopic study, structural analysis, photophysical properties and theoretical calculations of cis-(Â±)-2,4,5-tris(pyridin-2-yl)imidazoline. Journal of Molecular Structure, 2017, 1130, 951-962.	1.8	7
139	A Conceptual DFT Study of the Chemical Reactivity of Magnesium Octaethylporphyrin (MgOEP) as Predicted by the Minnesota Family of Density Functionals. Quimica Nova, 0, , .	0.3	7
140	Conceptual DFT as a chemoinformatics tool for the study of the Taltobulin anticancer peptide. BMC Research Notes, 2019, 12, 442.	0.6	7
141	Chemical Reactivity Theory (CRT) Study of the Melanoidin M8: Local Conceptual Density Functional Theory Descriptors. Computational Molecular Bioscience, 2018, 08, 80-90.	0.6	7
142	A Comparative Study of the Glycating Power of Simple Carbohydrates in the Maillard Reaction by Means of Conceptual DFT Descriptors. British Journal of Applied Science & Technology, 2017, 21, 1-12.	0.2	7
143	Synthesis of TiO2nanorods in the presence of linear DNA plasmid pBR322 by a solâ€“gel process. Nanotechnology, 2005, 16, 1272-1277.	1.3	6
144	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

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145	Computational Study of Cage Like (ZnO)₁₂ Cluster Using Hybrid and Hybrid Meta Functionals. Journal of the Chinese Chemical Society, 2013, 60, 1082-1091.	0.8	6
146	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.	1.0	6
147	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.	1.7	6
148	CHIH-DFT computational molecular characterization of acenaphto[1,2-c]-1,2,5-thiadiazole 1,1-dioxide. Computational and Theoretical Chemistry, 2007, 811, 373-378.	1.5	5
149	Computational study of the molecular structure and reactive sites of the R and S isomers of persin diene. Computational and Theoretical Chemistry, 2008, 869, 67-74.	1.5	5
150	Computational note on the calculation of the pKa of fluorescein. Computational and Theoretical Chemistry, 2008, 869, 105.	1.5	5
151	Computational study of Au_4 cluster on a carbon nanotube with and without defects using QM/MM methodology. Journal of Molecular Modeling, 2012, 18, 4885-4891.	0.8	5
152	A theoretical study of the carbocation formation energy involved in the isomerization of Î±-pinene. Chemical Physics Letters, 2012, 546, 168-170.	1.2	5
153	Computational study of the influence of the Ï€-bridge conjugation order of novel molecular derivatives of coumarins for dye-sensitized solar cells using DFT. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	5
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