Daniel Glossman-Mitnik

List of Publications by Citations

199 papers	2,714 citations	26 h-index	41 g-index
227 ext. papers	3,072 ext. citations	2.8 avg, IF	5.81 L-index

#	Paper	IF	Citations
199	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		121
198	Computational simulations of the molecular structure and corrosion properties of amidoethyl, aminoethyl and hydroxyethyl imidazolines inhibitors. *Corrosion Science*, **2006**, 48, 4053-4064	6.8	117
197	Degradation Studies of Polyolefins Incorporating Transparent Nanoparticulate Zinc Oxide UV Stabilizers. *Journal of Nanoparticle Research*, **2002**, 4, 167-174	2.3	90
196	Fuel Gas Storage and Separations by Metal□Organic Frameworks: Simulated Adsorption Isotherms for H2 and CH4 and Their Equimolar Mixture. *Journal of Physical Chemistry C*, **2009**, 113, 6634-6642	3.8	85
195	DFT studies of functionalized carbon nanotubes and fullerenes as nanovectors for drug delivery of antitubercular compounds. *Chemical Physics Letters*, **2007**, 447, 105-109	2.5	74
194	Theoretical study of the molecular properties and chemical reactivity of (+)-catechin and (□)epicatechin related to their antioxidant ability. *Computational and Theoretical Chemistry*, **2006**, 761, 97-106		74
193	CHIH-DFT study of the electronic properties and chemical reactivity of quercetin. *Computational and Theoretical Chemistry*, **2005**, 716, 67-72		61
192	CHIH-DFT theoretical study of isomeric thiatriazoles and their potential activity as corrosion inhibitors. *Computational and Theoretical Chemistry*, **2005**, 716, 61-65		55
191	CHIH-DFT determination of the molecular structure, infrared and ultraviolet spectra of the flavonoid quercetin. *Computational and Theoretical Chemistry*, **2004**, 681, 71-76		52
190	Natural carotenoids as nanomaterial precursors for molecular photovoltaics: a computational DFT study. *Molecules*, **2010**, 15, 4490-510	4.8	51
189	Band structure, optical properties and infrared spectrum of glycine□odium nitrate crystal. *Journal of Molecular Structure*, **2008**, 875, 295-301	3.4	44
188	Computational Study of the Chemical Reactivity Properties of the Rhodamine B Molecule. *Procedia Computer Science*, **2013**, 18, 816-825	1.6	41
187	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, 505-18	2	41
186	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, 14122-9	3.6	39
185	Conceptual DFT study of the local chemical reactivity of the dilysyldipyrrolones A and B intermediate melanoidins. *Theoretical Chemistry Accounts*, **2018**, 137, 1	1.9	35
184	Computational study of the chemical reactivity of the Blue-M1 intermediate melanoidin. *Computational and Theoretical Chemistry*, **2018**, 1134, 22-29	2	34
183	Chemical Reactivity Properties, p Values, AGEs Inhibitor Abilities and Bioactivity Scores of the Mirabamides A?H Peptides of Marine Origin Studied by Means of Conceptual DFT. *Marine Drugs*, **2018**, 16,	6	34

182	Conceptual DFT Study of the Local Chemical Reactivity of the Colored BISARG Melanoidin and Its Protonated Derivative. *Frontiers in Chemistry*, **2018**, 6, 136	5	33
181	Molecular Reactivity and Absorption Properties of Melanoidin Blue-G1 through Conceptual DFT. *Molecules*, **2018**, 23,	4.8	32
180	Computational prediction of the pKas of small peptides through Conceptual DFT descriptors. *Chemical Physics Letters*, **2017**, 671, 138-141	2.5	31
179	CHIH-DFT determination of the molecular structure, infrared and ultraviolet spectra of potentially organic corrosion inhibitors. *Computational and Theoretical Chemistry*, **2004**, 681, 83-88		31
178	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	2	31
177	Density functional theory (DFT) study of triphenylamine-based dyes for their use as sensitizers in molecular photovoltaics. *International Journal of Molecular Sciences*, **2012**, 13, 4418-32	6.3	28
176	Computational molecular characterization of the flavonoid rutin. *Chemistry Central Journal*, **2010**, 4, 12		28
175	A comparison of the chemical reactivity of naringenin calculated with the M06 family of density functionals. *Chemistry Central Journal*, **2013**, 7, 155		27
174	Computational nanochemistry report on the oxicams--conceptual DFT indices and chemical reactivity. *Journal of Physical Chemistry B*, **2013**, 117, 6339-51	3.4	27
173	Theoretical study of chemical reactivity of the main species in the □-pinene isomerization reaction. *Computational and Theoretical Chemistry*, **2008**, 854, 81-88		25
172	A Molecular Electron Density Theory Study of the Chemical Reactivity of Cis- and Trans-Resveratrol. *Molecules*, **2016**, 21,	4.8	25
171	Application of density functional theory concepts to the study of the chemical reactivity of thiadiazoles. *Computational and Theoretical Chemistry*, **1995**, 330, 385-388		24
170	Conceptual DFT Descriptors of Amino Acids with Potential Corrosion Inhibition Properties Calculated with the Latest Minnesota Density Functionals. *Frontiers in Chemistry*, **2017**, 5, 16	5	23
169	Local and nonlocal density functional calculations of the molecular structure of isomeric thiadiazoles. *Computational and Theoretical Chemistry*, **1997**, 390, 67-78		23
168	Crystallographic study and molecular orbital calculations of 1,2,5-thiadiazole 1,1-dioxide derivatives **1998**, 11, 91-100		22
167	Influence of the basis set and correlation method on the calculation of molecular structures: thiadiazoles revisited. *Computational and Theoretical Chemistry*, **2001**, 548, 153-163		22
166	Computational molecular characterization of Coumarin-102. *Computational and Theoretical Chemistry*, **2009**, 911, 105-108		21
165	CHIH-DFT Determination of the Molecular Structure and Infrared and Ultraviolet Spectra of Azathiophenes. *Theoretical Chemistry Accounts*, **2006**, 117, 57-68	1.9	21

164	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, 10727-37	3.4	20
163	Optimized structure and thermochemical properties of flavonoids determined by the CHIH(medium)DFT model chemistry versus experimental techniques. *Journal of Molecular Structure*, **2007**, 871, 114-130	3.4	20
162	Thermal, mechanical, and electronic properties of glycine-sodium nitrate crystal. *Journal of Physics and Chemistry of Solids*, **2008**, 69, 1974-1979	3.9	20
161	Theoretical calculation of the maximum absorption wavelength for Cyanidin molecules with several methodologies. *Computational and Theoretical Chemistry*, **2015**, 1067, 129-134	2	19
160	Chemical Reactivity Theory Study of Advanced Glycation Endproduct Inhibitors. *Molecules*, **2017**, 22,	4.8	19
159	Theoretical analysis of anthracene and its carbonyl and carboxyl derivatives using DFT and TD-DFT. *Computational and Theoretical Chemistry*, **2009**, 894, 64-70		19
158	Theoretical calculations of molecular dipole moment, polarizability, and first hyperpolarizability of glycine sodium nitrate. *Computational and Theoretical Chemistry*, **2009**, 905, 76-80		19
157	CHIH-DFT determination of the molecular structure, infrared and ultraviolet spectra of the antiparasitic drug megazol. *Computational and Theoretical Chemistry*, **2004**, 681, 77-82		19
156	Blue M2: an intermediate melanoidin studied via conceptual DFT. *Journal of Molecular Modeling*, **2018**, 24, 138	2	19
155	Computational molecular nanoscience study of the properties of copper complexes for dye-sensitized solar cells. *International Journal of Molecular Sciences*, **2012**, 13, 16005-19	6.3	18
154	Nonlocal exchange and kinetic energy density functionals with correct asymptotic behavior for electronic systems. *International Journal of Quantum Chemistry*, **1994**, 49, 171-184	2.1	18
153	Theoretical study of electronic properties of organic photovoltaic materials. *Journal of Computational Chemistry*, **2009**, 30, 1027-37	3.5	17
152	Computational characterization of the carotene molecule. *Computational and Theoretical Chemistry*, **2009**, 913, 215-220		17
151	A theoretical study on the aromaticity of thiadiazoles and related compounds. *Computational and Theoretical Chemistry*, **2001**, 549, 285-288		17
150	Molecular design of copper complexes as sensitizers for efficient dye-sensitized solar cells. *Journal of Photochemistry and Photobiology A: Chemistry*, **2013**, 267, 1-5	4.7	16
149	DFT Study of Polythiophene Energy Band Gap and Substitution Effects. *Journal of Chemistry*, **2015**, 2015, 1-12	2.3	16
148	CHIH-DFT determination of the reactivity sites of the antiparasitic drug megazol. *Computational and Theoretical Chemistry*, **2005**, 723, 231-234		16
147	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,	4.8	15

146	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	2	15
145	CHIH-DFT determination of the electrical, optical, and magnetic properties and NICS aromaticity of megazol. *Computational and Theoretical Chemistry*, **2005**, 717, 1-3		15
144	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	4.7	14
143	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	2	14
142	A fast and simple evaluation of the chemical reactivity properties of the Pristinamycin family of antimicrobial peptides. *Chemical Physics Letters*, **2020**, 739, 137021	2.5	14
141	Virtual Screening of Marine Natural Compounds by Means of Chemoinformatics and CDFT-Based Computational Peptidology. *Marine Drugs*, **2020**, 18,	6	14
140	Conceptual DFT-Based Computational Peptidology of Marine Natural Compounds: Discodermins A-H. *Molecules*, **2020**, 25,	4.8	14
139	A conceptual DFT study of the molecular properties of glycating carbonyl compounds. *Chemistry Central Journal*, **2017**, 11, 8		13
138	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, 29764-75	3.6	13
137	Comparison of several protocols for the computational prediction of the maximum absorption wavelength of chrysanthemin. *Journal of Molecular Modeling*, **2014**, 20, 2378	2	13
136	Computational Nutraceutics: Chemical Reactivity Properties of the Flavonoid Naringin by Means of Conceptual DFT. *Journal of Chemistry*, **2013**, 2013, 1-8	2.3	13
135	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	3.4	13
134	Application of density functional theory concepts to the study of the chemical reactivity of isomeric thiadiazolines. *Computational and Theoretical Chemistry*, **2001**, 535, 39-47		13
133	HF and DFT calculations of the molecular structure of isomeric thiadiazole dioxides. *Computational and Theoretical Chemistry*, **2001**, 536, 41-51		13
132	Hartree□ock (HF) and local and nonlocal density functional (DFT) calculations of the molecular structure of isomeric thiadiazolidines. *Computational and Theoretical Chemistry*, **2001**, 538, 201-210		13
131	Nonlocal exchange- and kinetic-energy density functionals for electronic systems: Application to atoms and ions. *Physical Review A*, **1993**, 47, 1804-1810	2.6	13
130	Chemical synthesis, spectroscopic studies, chemical reactivity properties and bioactivity scores of an azepin-based molecule. *Journal of Molecular Structure*, **2019**, 1180, 300-306	3.4	13
129	Quantum chemical study of the effect of □bridge on the optical and electronic properties of sensitizers for DSSCs incorporating dioxythiophene and thiophene units. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	12

128	CHIH-DFT determination of the molecular structure and infrared and ultraviolet spectra of gamma-solanine. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2007**, 66, 208-11	4.4	12
127	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	3.4	11
126	DFT study of the effect of substituents on the absorption and emission spectra of Indigo. *Chemistry Central Journal*, **2012**, 6, 70		11
125	Computational Study of 3,4-Diphenyl-1,2,5-Thiadiazole 1-Oxide for Organic Photovoltaics. *International Journal of Photoenergy*, **2009**, 2009, 1-8	2.1	11
124	Theoretical evaluation of the order of reactivity of transfer agents utilized in RAFT polymerization: part 2: group R. *Journal of Molecular Modeling*, **2010**, 16, 95-105	2	11
123	Molecular structure and substitution effects on diphenylanthrazolines for organic semiconductors: A theoretical study. *Computational and Theoretical Chemistry*, **2008**, 863, 99-104		11
122	G3-B3 calculation of the molecular structure and descriptors of isomeric thiadiazoles. *Computational and Theoretical Chemistry*, **2005**, 725, 27-30		11
121	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	3.4	11
120	Local and nonlocal density functional calculations of the molecular structure of isomeric thiadiazole monoxides. *International Journal of Quantum Chemistry*, **2001**, 81, 105-115	2.1	11
119	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		11
118	Chemical Reactivity Properties, Drug-Likeness Features and Bioactivity Scores of the Cholecystokinin Peptide Hormone. *Computational Molecular Bioscience*, **2019**, 09, 41-47	1.1	11
117	Theoretical Study of the Effect of Different π-Bridges Including an Azomethine Group in Triphenylamine-Based Dye for Dye-Sensitized Solar Cells. *Molecules*, **2019**, 24,	4.8	11
116	Chemical-Reactivity Properties, Drug Likeness, and Bioactivity Scores of Seragamides A–F Anticancer Marine Peptides: Conceptual Density Functional Theory Viewpoint. *Computation*, **2019**, 7, 52	2.2	10
115	Chemical reactivity and bioactivity properties of the Phallotoxin family of fungal peptides based on Conceptual Peptidology and DFT study. *Heliyon*, **2019**, 5, e02335	3.6	10
114	Synthesis, structure, characterization and photophysical properties of copper(I) complexes containing polypyridyl ligands. *RSC Advances*, **2014**, 4, 42624-42631	3.7	10
113	Experimental and quantum chemical studies of a novel synthetic prenylated chalcone. *Chemistry Central Journal*, **2013**, 7, 17		10
112	Computational molecular characterization of the flavonoid Morin and its Pt(II), Pd(II) and Zn(II) complexes. *Journal of Molecular Modeling*, **2011**, 17, 979-85	2	10
111	Effects of sulfur substitutional impurities on (ZnO)n clusters (n=4–12) using density functional theory. *Computational and Theoretical Chemistry*, **2011**, 965, 154-162	2	10

110	Excited states analysis of sulfur substitutional impurities on (ZnO)6 clusters using DFT and TD-DFT. *Computational and Theoretical Chemistry*, **2010**, 957, 100-107		10
109	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	3.4	10
108	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	1.9	9
107	Preparation and Characterization of Cerium (III) Doped Captopril Nanoparticles and Study of their Photoluminescence Properties. *Open Chemistry*, **2016**, 14, 60-64	1.6	9
106	Computational Peptidology Assisted by Conceptual Density Functional Theory for the Study of Five New Antifungal Tripeptides. *ACS Omega*, **2019**, 4, 12555-12560	3.9	9
105	Exploration of the kinetic and thermochemical abilities for the free radical scavenging of two quercetin conformers. *Journal of Molecular Structure*, **2010**, 981, 187-193	3.4	9
104	Study of the effect of solvent induced swelling on the resistivity of butadiene based elastomers filled with carbon particles: Part I. Elucidating second order effects. *Sensors and Actuators A: Physical*, **2005**, 119, 157-168	3.9	9
103	Stabilities of large sodium clusters for different atomic arrangements. *Physical Review B*, **1993**, 47, 4747-4755	3.5	9
102	Nonlocal exchange and kinetic-energy density functionals for electronic systems. *International Journal of Quantum Chemistry*, **1992**, 44, 347-358	2.1	9
101	Nonlocal approximation to the exchange and kinetic energy functionals: Application to metallic clusters. *International Journal of Quantum Chemistry*, **1993**, 45, 333-347	2.1	9
100	Theoretical Study of the Effect of □Bridge on Optical and Electronic Properties of Carbazole-Based Sensitizers for DSSCs. *Molecules*, **2020**, 25,	4.8	9
99	Evaluation of Acetogenins as Potential Anti-SARS-CoV-2 Agents Through Computational Approaches. *Frontiers in Chemistry*, **2020**, 8, 624716	5	9
98	Application of DFT concepts to the study of the chemical reactivity of some resveratrol derivatives through the assessment of the validity of the □oopmans in DFT□(KID) procedure. *Journal of Theoretical and Computational Chemistry*, **2017**, 16, 1750006	1.8	8
97	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	3.4	8
96	Computational nanochemistry study of the molecular structure and properties of ethambutol. *Journal of Molecular Modeling*, **2013**, 19, 3507-15	2	8
95	CHIH-DFT determination of the molecular structure and IR and UV spectra of solanidine. *Journal of Molecular Modeling*, **2007**, 13, 43-6	2	8
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93	A Thomas-Fermi-Dirac Theory of an Atom in Strong Magnetic Fields. *Journal of the Physical Society of Japan*, **1990**, 59, 3571-3583	1.5	8

92	Theoretical Study of the Bridge Influence with Different Units of Thiophene and Thiazole in Coumarin Dye-Sensitized Solar Cells. *International Journal of Photoenergy*, **2016**, 2016, 1-8	2.1	8
91	Calculation of the Global and Local Conceptual DFT Indices for the Prediction of the Chemical Reactivity Properties of Papuamides A-F Marine Drugs. *Molecules*, **2019**, 24,	4.8	7
90	Electron injection in anthocyanidin and betalain dyes for dye-sensitized solar cells: a DFT approach. *Journal of Computational Electronics*, **2019**, 18, 396-406	1.8	7
89	Theoretical Study of Copper Complexes: Molecular Structure, Properties, and Its Application to Solar Cells. *International Journal of Photoenergy*, **2013**, 2013, 1-7	2.1	7
88	Docking Studies of Binding of Ethambutol to the C-Terminal Domain of the Arabinosyltransferase fromMycobacterium tuberculosis. *Journal of Chemistry*, **2013**, 2013, 1-5	2.3	7
87	Electronic structure study using density functional theory in organic dendrimers. *Journal of Molecular Modeling*, **2011**, 17, 1963-72	2	7
86	Computational note on the chemical reactivity of pyrrole derivatives. *Computational and Theoretical Chemistry*, **2009**, 912, 119-120		7
85	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	1.1	7
84	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,	4.8	7
83	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	1.9	6
82	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	2.7	6
81	Computational Prediction of the Protonation Sites of Ac-Lys-(Ala)n-Lys-NH2 Peptides through Conceptual DFT Descriptors. *Molecules*, **2017**, 22,	4.8	6
80	Theoretical evaluation of the order of reactivity of transfer agents utilized in RAFT polymerization: group Z. *Journal of Molecular Modeling*, **2009**, 15, 1133-43	2	6
79	Characterization of the semiquinones and quinones of (−)-epicatechin by means of computational chemistry. *Computational and Theoretical Chemistry*, **2009**, 897, 6-11		6
78	TD-DFT/IEFPCM determination of the absorption and emission spectra of DABCYL. *Computational and Theoretical Chemistry*, **2010**, 945, 101-103		6
77	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		6
76	Vibrational spectroscopic study, structural analysis, photophysical properties and theoretical calculations of cis-(±)-2,4,5-tris(pyridin-2-yl)imidazoline. *Journal of Molecular Structure*, **2017**, 1130, 951-962	3.4	5
75	DFT study of the interaction between the conjugated fluorescein and dabcyl system, using fluorescene quenching method. *Journal of Molecular Modeling*, **2012**, 18, 4113-20	2	5

74	Computational Nanochemistry Study of the Molecular Structure and Properties of Chlorophyll a. *International Journal of Photoenergy*, **2013**, 2013, 1-8	2.1	5
73	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	5
72	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		5
71	CBS-QB3 calculation of quantum chemical molecular descriptors of isomeric thiadiazoles. *Journal of Molecular Graphics and Modelling*, **2006**, 25, 455-8	2.8	5
70	Synthesis of TiO2nanorods in the presence of linear DNA plasmid pBR322 by a sol□gel process. *Nanotechnology*, **2005**, 16, 1272-1277	3.4	5
69	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		5
68	The substituent effect from the perspective of local hyper-softness. An example applied on normeloxicam, meloxicam and 4-meloxicam: Non-steroidal anti-inflammatory drugs. *Chemical Physics Letters*, **2015**, 618, 162-167	2.5	4
67	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	2.7	4
66	A Conceptual DFT Study of the Chemical Reactivity of Magnesium Octaethylporphyrin (MgOEP) as Predicted by the Minnesota Family of Density Functionals. *Quimica Nova*, **2017**,	1.6	4
65	Computational study of the influence of the □bridge conjugation order of novel molecular derivatives of coumarins for dye-sensitized solar cells using DFT. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	4
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62	Topics in quantum physics with origins in astronomy: Two examples. *American Journal of Physics*, **2012**, 80, 406-416	0.7	4
61	Computational Study of Cage Like (ZnO)12 Cluster Using Hybrid and Hybrid Meta Functionals. *Journal of the Chinese Chemical Society*, **2013**, 60, 1082-1091	1.5	4
60	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		4
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58	Computational note on the calculation of the pKa of fluorescein. *Computational and Theoretical Chemistry*, **2008**, 869, 105		4
57	Chemical Reactivity Theory (CRT) Study of the Melanoidin M8: Local Conceptual Density Functional Theory Descriptors. *Computational Molecular Bioscience*, **2018**, 08, 80-90	1.1	4

56	Synthesis, crystal structure, DFT studies and photophysical properties of a copper(I)-triphenylphosphane complex based on trans-(±)-2,4,5-tris(pyridin-2-yl)-2-imidazoline. *Acta Crystallographica Section C, Structural Chemistry*, **2017**, 73, 280-286	0.8	3
55	Local Molecular Reactivity of the Colored Dansylglycine in Water and Dioxane Studied through Conceptual DFT. *Journal of Chemistry*, **2018**, 2018, 1-7	2.3	3
54	CDFT-Based Reactivity Descriptors as a Useful MEDT Chemoinformatics Tool for the Study of the Virotoxin Family of Fungal Peptides. *Molecules*, **2019**, 24,	4.8	3
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52	Ab initio study of electron transport in 4-(3-nitro-4-tetrafluorophenylthiolate-ethynyl, phenylethynyl) benzenethiolate. *Journal of Molecular Modeling*, **2012**, 18, 611-21	2	3
51	Fractal Dimension Calculation of a Manganese-Chromium Bimetallic Nanocomposite Using Image Processing. *Journal of Nanomaterials*, **2015**, 2015, 1-9	3.2	3
50	A theoretical study of the carbocation formation energy involved in the isomerization of α-pinene. *Chemical Physics Letters*, **2012**, 546, 168-170	2.5	3
49	Ab initio study of the additivity concept applied for the effects of one substituent within cyclic compounds. *Computational and Theoretical Chemistry*, **2001**, 538, 267-285		3
48	Synthesis, Computational Pharmacokinetics Report, Conceptual DFT-Based Calculations and Anti-Acetylcholinesterase Activity of Hydroxyapatite Nanoparticles Derived From Plant Extract. *Frontiers in Chemistry*, **2021**, 9, 741037	5	3
47	Chemical Reactivity Properties and Bioactivity Scores of the Angiotensin II Vasoconstrictor Octapeptide **2020**,		3
46	Preparation, Spectroscopic Characterization, Theoretical Investigations, and In Vitro Anticancer Activity of Cd(II), Ni(II), Zn(II), and Cu(II) Complexes of 4(3)-Quinazolinone-Derived Schiff Base. *Molecules*, **2020**, 25,	4.8	3
45	PREPARATION, IDENTIFICATION AND BIOLOGICAL PROPERTIES OF NEW FLUORIDE NANOCOMPOUNDS. *Journal of the Chilean Chemical Society*, **2016**, 61, 3201-3205	2.5	3
44	Conceptual DFT as a Novel Chemoinformatics Tool for Studying the Chemical Reactivity Properties of the Amatoxin Family of Fungal Peptides. *Open Chemistry*, **2019**, 17, 1133-1139	1.6	3
43	Conceptual DFT as a Helpful Chemoinformatics Tool for the Study of the Clavanin Family of Antimicrobial Marine Peptides		3
42	Studying the chemical reactivity properties of the target tumor-environment tripeptides NGR (asparagine-glycine-arginine) and RGD (arginine-glycine-aspartic acid) in their interactions with tamoxifen through conceptual density functional theory. *Journal of Molecular Modeling*, **2018**, 24, 336	2	3
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