Daniel Glossman-Mitnik

List of Publications by Year in Descending Order

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	Conceptual DFT-Based Computational Peptidology, Pharmacokinetics Study and ADMET Report of the Veraguamides A-G Family of Marine Natural Drugs.. *Marine Drugs*, **2022**, 20,	6	1
198	Computational peptidology approach to the study of the chemical reactivity and bioactivity properties of Aspergillipeptide D, a cyclopentapeptide of marine origin.. *Scientific Reports*, **2022**, 12, 506	4.9	0
197	Virtual Prospection of Marine Cyclopeptides as Therapeutics by Means of Conceptual DFT and Computational ADMET. *Pharmaceuticals*, **2022**, 15, 509	5.2	0
196	Four-Coordinate Monoboron Complexes with 8-Hydroxyquinolin-5-Sulfonate: Synthesis, Crystal Structures, Theoretical Studies, and Luminescence Properties. *Crystals*, **2022**, 12, 783	2.3	1
195	Computational Pharmacokinetics Report, ADMET Study and Conceptual DFT-Based Estimation of the Chemical Reactivity Properties of Marine Cyclopeptides. *ChemistryOpen*, **2021**, 10, 1142-1149	2.3	0
194	An integrated molecular modeling protocol for drug screening based on conceptual density functional theory and chemoinformatics for the study of marine cyclopeptides. *Journal of Molecular Modeling*, **2021**, 27, 314	2	
193	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
192	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
191	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	5	1
190	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	2.3	2
189	Chemical synthesis, in vitro biological evaluation and theoretical investigations of transition metal complexes derived from 2-(((5-mercapto-1H-pyrrol-2-yl)imino) methyl)6-methoxyphenol. *Journal of Molecular Structure*, **2021**, 1244, 130920	3.4	1
188	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
187	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	2	1
186	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	1.8	0
185	KID Procedure Applied on the [(PY5Me2)MoO]+ Complex. *ACS Omega*, **2020**, 5, 30549-30555	3.9	0
184	KID Procedure Applied on the [(PYMe)MoO] Complex. *ACS Omega*, **2020**, 5, 30549-30555	3.9	
183	Molecular Docking and Conceptual DFT-Based Study of Some Potential SARS-CoV-2 Inhibitors. *Computational Molecular Bioscience*, **2020**, 10, 111-128	1.1	

182	Crystal structure, Hirshfeld surface, DFT calculations and photophysical properties of 2,4,5-tris(4-pyridyl)imidazole hydrogen chloride. *Journal of Molecular Structure*, **2020**, 1213, 128175	3.4	1
181	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
180	Oxidation degree of a cell membrane model and its response to structural changes, a coarse-grained molecular dynamics approach. *Journal of Biomolecular Structure and Dynamics*, **2020**, 1-12	3.6	1
179	Chemical Reactivity Properties and Bioactivity Scores of the Angiotensin II Vasoconstrictor Octapeptide **2020**,		3
178	Virtual Screening of Marine Natural Compounds by Means of Chemoinformatics and CDFT-Based Computational Peptidology. *Marine Drugs*, **2020**, 18,	6	14
177	Conceptual DFT-Based Computational Peptidology of Marine Natural Compounds: Discodermins A-H. *Molecules*, **2020**, 25,	4.8	14
176	Theoretical Study of the Effect of Bridge on Optical and Electronic Properties of Carbazole-Based Sensitizers for DSSCs. *Molecules*, **2020**, 25,	4.8	9
175	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
174	Evaluation of Acetogenins as Potential Anti-SARS-CoV-2 Agents Through Computational Approaches. *Frontiers in Chemistry*, **2020**, 8, 624716	5	9
173	Chemical-Reactivity Properties, Drug Likeness, and Bioactivity Scores of Seragamides A Anticancer Marine Peptides: Conceptual Density Functional Theory Viewpoint. *Computation*, **2019**, 7, 52	2.2	10
172	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
171	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
170	Preparation, spectroscopic investigations and chemical reactivity properties of a new schiff base ligand and its copper (II) complexes. *Journal of Molecular Structure*, **2019**, 1191, 17-23	3.4	1
169	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
168	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
167	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
166	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
165	Conceptual DFT as a chemoinformatics tool for the study of the Taltobulin anticancer peptide. *BMC Research Notes*, **2019**, 12, 442	2.3	4

164	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
163	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
162	Chemical Reactivity Properties, Drug-Likeness Features and Bioactivity Scores of the Cholecystokinin Peptide Hormone. *Computational Molecular Bioscience*, **2019**, 09, 41-47	1.1	11
161	Computational Study of the Chemical Reactivity and Bioactivity Rates of Marine Peptides Hemiasterlin and Its A and B Derivatives Used in the Cancer Treatment through Conceptual Density Functional Theory. *Computational Molecular Bioscience*, **2019**, 09, 95-107	1.1	1
160	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	2.3	1
159	Theoretical Study of the Effect of Different Bridges Including an Azomethine Group in Triphenylamine-Based Dye for Dye-Sensitized Solar Cells. *Molecules*, **2019**, 24,	4.8	11
158	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
157	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
156	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
155	Assessment of ten density functionals through the use of local hyper-softness to get insights about the catalytic activity : Iron-based organometallic compounds for ethylene polymerization as testing molecules. *Journal of Molecular Modeling*, **2018**, 24, 42	2	2
154	Computational study of the chemical reactivity of the Blue-M1 intermediate melanoidin. *Computational and Theoretical Chemistry*, **2018**, 1134, 22-29	2	34
153	Supramolecular arrangement and photophysical properties of a dinuclear cyanophenylboronic acid ester. *Acta Crystallographica Section C, Structural Chemistry*, **2018**, 74, 452-459	0.8	1
152	Interaction of Tamoxifen Analogs With the Pocket Site of Some Hormone Receptors. A Molecular Docking and Density Functional Theory Study. *Frontiers in Chemistry*, **2018**, 6, 293	5	2
151	Molecular Reactivity and Absorption Properties of Melanoidin Blue-G1 through Conceptual DFT. *Molecules*, **2018**, 23,	4.8	32
150	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
149	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
148	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
147	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

146	A Combined Molecular Docking and Electronic Structure Study for a Breast Cancer Drug Design **2018**,		1
145	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
144	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
143	Blue M2: an intermediate melanoidin studied via conceptual DFT. *Journal of Molecular Modeling*, **2018**, 24, 138	2	19
142	Application of DFT concepts to the study of the chemical reactivity of some resveratrol derivatives through the assessment of the validity of the Koopmans in DFT (KID) procedure. *Journal of Theoretical and Computational Chemistry*, **2017**, 16, 1750006	1.8	8
141	Computational prediction of the pKas of small peptides through Conceptual DFT descriptors. *Chemical Physics Letters*, **2017**, 671, 138-141	2.5	31
140	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
139	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
138	A conceptual DFT study of the molecular properties of glycating carbonyl compounds. *Chemistry Central Journal*, **2017**, 11, 8		13
137	Theoretical investigation of the molecular structure and spectroscopic properties of oxicams. *Journal of Structural Chemistry*, **2017**, 58, 261-267	0.9	
136	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
135	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
134	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
133	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
132	Chemical Reactivity Theory Study of Advanced Glycation Endproduct Inhibitors. *Molecules*, **2017**, 22,	4.8	19
131	Computational Prediction of the Protonation Sites of Ac-Lys-(Ala)n-Lys-NH2 Peptides through Conceptual DFT Descriptors. *Molecules*, **2017**, 22,	4.8	6
130	New Methods of Esterification of Nanodiamonds in Fighting Breast Cancer-A Density Functional Theory Approach. *Molecules*, **2017**, 22,	4.8	2
129	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

128	Comparative Study of the Chemical Reactivity of Helical Peptide Models for Protein Glycation. *Computational Chemistry*, **2017**, 05, 65-73	0.2	1
127	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
126	A DFT study of the chemical reactivity of cimetidine A, C and D in the gas, H2O, MeOH and EtOH solvents. *Journal of the Serbian Chemical Society*, **2017**, 82, 25-37	0.9	
125	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
124	Preparation and Characterization of Cerium (III) Doped Captopril Nanoparticles and Study of their Photoluminescence Properties. *Open Chemistry*, **2016**, 14, 60-64	1.6	9
123	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
122	PREPARATION, IDENTIFICATION AND BIOLOGICAL PROPERTIES OF NEW FLUORIDE NANOCOMPOUNDS. *Journal of the Chilean Chemical Society*, **2016**, 61, 3201-3205	2.5	3
121	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
120	A Molecular Electron Density Theory Study of the Chemical Reactivity of Cis- and Trans-Resveratrol. *Molecules*, **2016**, 21,	4.8	25
119	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
118	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
117	Theoretical calculation of the maximum absorption wavelength for Cyanidin molecules with several methodologies. *Computational and Theoretical Chemistry*, **2015**, 1067, 129-134	2	19
116	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
115	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
114	Geometric description and electronic properties of the principal photosynthetic pigments of higher plants: a DFT study. *Journal of Molecular Modeling*, **2015**, 21, 256	2	2
113	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
112	Fractal Dimension Calculation of a Manganese-Chromium Bimetallic Nanocomposite Using Image Processing. *Journal of Nanomaterials*, **2015**, 2015, 1-9	3.2	3
111	Morphological Investigation and Fractal Properties of Realgar Nanoparticles. *Journal of Nanomaterials*, **2015**, 2015, 1-8	3.2	

110	DFT Study of Polythiophene Energy Band Gap and Substitution Effects. *Journal of Chemistry*, **2015**, 2015, 1-12	2.3	16
109	Comparison of several protocols for the computational prediction of the maximum absorption wavelength of chrysanthemin. *Journal of Molecular Modeling*, **2014**, 20, 2378	2	13
108	Synthesis, structure, characterization and photophysical properties of copper(I) complexes containing polypyridyl ligands. *RSC Advances*, **2014**, 4, 42624-42631	3.7	10
107	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
106	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	2.7	3
105	Computational Nanochemistry Study of the Molecular Structure, Spectra and Chemical Reactivity Properties of the BFPF Green Fluorescent Protein Chromophore **2014**, 199-238		
104	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	
103	Computational Nanochemistry Report of the Molecular Structure, Properties and Chemical Reactivity of Pheophorbide A. *Challenges and Advances in Computational Chemistry and Physics*, **2014**, 217-247	0.7	
102	Experimental and quantum chemical studies of a novel synthetic prenylated chalcone. *Chemistry Central Journal*, **2013**, 7, 17		10
101	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
100	Computational nanochemistry study of the molecular structure and properties of ethambutol. *Journal of Molecular Modeling*, **2013**, 19, 3507-15	2	8
99	Computational Study of the Chemical Reactivity Properties of the Rhodamine B Molecule. *Procedia Computer Science*, **2013**, 18, 816-825	1.6	41
98	A comparison of the chemical reactivity of naringenin calculated with the M06 family of density functionals. *Chemistry Central Journal*, **2013**, 7, 155		27
97	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
96	Computational nanochemistry report on the oxicams--conceptual DFT indices and chemical reactivity. *Journal of Physical Chemistry B*, **2013**, 117, 6339-51	3.4	27
95	The Indigo Molecule Revisited Again: Assessment of the Minnesota Family of Density Functionals for the Prediction of Its Maximum Absorption Wavelengths in Various Solvents. *Journal of Chemistry*, **2013**, 2013, 1-4	2.3	2
94	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
93	Computational Nutraceutics: Chemical Reactivity Properties of the Flavonoid Naringin by Means of Conceptual DFT. *Journal of Chemistry*, **2013**, 2013, 1-8	2.3	13

92	Computational Nanochemistry Study of the Molecular Structure and Properties of Chlorophyll a. *International Journal of Photoenergy*, **2013**, 2013, 1-8	2.1	5
91	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
90	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
89	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
88	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
87	Computational characterization of the molecular structure and properties of Dye 7 for organic photovoltaics. *Journal of Molecular Modeling*, **2012**, 18, 835-42	2	1
86	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
85	Computational study of Au_4 cluster on a carbon nanotube with and without defects using QM/MM methodology. *Journal of Molecular Modeling*, **2012**, 18, 4885-91	2	4
84	A theoretical study of the carbocation formation energy involved in the isomerization of □-pinene. *Chemical Physics Letters*, **2012**, 546, 168-170	2.5	3
83	Topics in quantum physics with origins in astronomy: Two examples. *American Journal of Physics*, **2012**, 80, 406-416	0.7	4
82	DFT study of the effect of substituents on the absorption and emission spectra of Indigo. *Chemistry Central Journal*, **2012**, 6, 70		11
81	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
80	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
79	Computational characterization of sodium selenite using density functional theory. *Journal of Molecular Modeling*, **2011**, 17, 701-8	2	
78	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
77	Electronic structure study using density functional theory in organic dendrimers. *Journal of Molecular Modeling*, **2011**, 17, 1963-72	2	7
76	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
75	EFFECTS OF SULFUR SUBSTITUTIONAL IMPURITIES ON ZnO STRUCTURE USING DENSITY FUNCTIONAL THEORY. *International Journal of Nanoscience*, **2011**, 10, 381-390	0.6	

74	Natural carotenoids as nanomaterial precursors for molecular photovoltaics: a computational DFT study. *Molecules*, **2010**, 15, 4490-510	4.8	51
73	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
72	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
71	TD-DFT/IEFPCM determination of the absorption and emission spectra of DABCYL. *Computational and Theoretical Chemistry*, **2010**, 945, 101-103		6
70	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
69	Computational molecular characterization of the flavonoid rutin. *Chemistry Central Journal*, **2010**, 4, 12		28
68	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
67	Theoretical study of electronic properties of organic photovoltaic materials. *Journal of Computational Chemistry*, **2009**, 30, 1027-37	3.5	17
66	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
65	Computational note on the calculation of the molecular structure and properties of 3,4-diphenyl 1,2,5-thiadiazoline 1,1-dioxide derivatives for organic photovoltaics. *Computational and Theoretical Chemistry*, **2009**, 901, 258-259		1
64	Computational prediction of the melting temperature of a DNA biosensor to detect Mycobacterium tuberculosis. *Computational and Theoretical Chemistry*, **2009**, 912, 60-62		1
63	Theoretical analysis of anthracene and its carbonyl and carboxyl derivatives using DFT and TD-DFT. *Computational and Theoretical Chemistry*, **2009**, 894, 64-70		19
62	Characterization of the semiquinones and quinones of (−)-epicatechin by means of computational chemistry. *Computational and Theoretical Chemistry*, **2009**, 897, 6-11		6
61	Theoretical calculations of molecular dipole moment, polarizability, and first hyperpolarizability of glycine sodium nitrate. *Computational and Theoretical Chemistry*, **2009**, 905, 76-80		19
60	Computational molecular characterization of Coumarin-102. *Computational and Theoretical Chemistry*, **2009**, 911, 105-108		21
59	Computational note on the chemical reactivity of pyrrole derivatives. *Computational and Theoretical Chemistry*, **2009**, 912, 119-120		7
58	Computational characterization of the -carotene molecule. *Computational and Theoretical Chemistry*, **2009**, 913, 215-220		17
57	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

56	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		4
55	Thermal, mechanical, and electronic properties of glycine-sodium nitrate crystal. *Journal of Physics and Chemistry of Solids*, **2008**, 69, 1974-1979	3.9	20
54	Computational note on the calculation of the dipole moment, polarizability and hyperpolarizability of solanidine. *Computational and Theoretical Chemistry*, **2008**, 849, 122-123		
53	Theoretical study of chemical reactivity of the main species in the □-pinene isomerization reaction. *Computational and Theoretical Chemistry*, **2008**, 854, 81-88		25
52	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
51	Molecular structure and substitution effects on diphenylanthrazolines for organic semiconductors: A theoretical study. *Computational and Theoretical Chemistry*, **2008**, 863, 99-104		11
50	Computational note on the calculation of the pKa of fluorescein. *Computational and Theoretical Chemistry*, **2008**, 869, 105		4
49	Band structure, optical properties and infrared spectrum of glycine□odium nitrate crystal. *Journal of Molecular Structure*, **2008**, 875, 295-301	3.4	44
48	CHIH-DFT determination of the dipole moment, polarizability and hyperpolarizability of □solanine. *Computational and Theoretical Chemistry*, **2007**, 808, 81-84		2
47	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
46	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
45	Optimized structure and thermochemical properties of flavonoids determined by the CHIH(medium)□FT model chemistry versus experimental techniques. *Journal of Molecular Structure*, **2007**, 871, 114-130	3.4	20
44	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
43	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
42	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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