Daniel Glossman-Mitnik

List of Publications by Year
in descending order

219	3,681	172386	233338
papers	citations	29 h-index	45 g-index

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

#	Article	IF	Citations
1	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, 2022, 40, 1930-1941.	2.0	4
2	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.	1.6	2
3	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
4	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
5	Virtual Prospection of Marine Cyclopeptides as Therapeutics by Means of Conceptual DFT and Computational ADMET. Pharmaceuticals, 2022, 15, 509.	1.7	4
6	Four-Coordinate Monoboron Complexes with 8-Hydroxyquinolin-5-Sulfonate: Synthesis, Crystal Structures, Theoretical Studies, and Luminescence Properties. Crystals, 2022, 12, 783.	1.0	4
7	An insight into reactivity and bioactivity properties of quorum sensing peptides against PDE10A: a computational peptidology approach. Journal of Molecular Modeling, 2022, 28, .	0.8	1
8	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
9	Revisiting the Validation of the KID Methodology through CDFT Descriptors of Fluorescent DNA Staining Dyes. , 2021, , 30-44.		1
10	The Reactivity Sites of Amyloid Î²-Peptides AÎ²40 and AÎ²42 in Alzheimer's Disease: Computational Prediction. , 2021, , 45-51.		0
11	A Short Update on Cheminformatics for Prompting the Process of Drug Design and Discovery. , 2021, , 23-29.		0
12	About the Computational Prediction of the Maximum Absorption Wavelengths of Indigo in Different Solvents with the Minnesota Family of Density Functionals. , 2021, , 70-77.		0
13	Study on the Computational Nutraceutics of a Citrus Flavonoid: An Approach Using Conceptual Density Functional Theory (CDFT). , 2021, , 88-101.		0
14	Determining the Informatics and Conceptual DFT Study of Pigments Derived from Carotenoids of Marine Origin. , 2021, , 102-121.		0
15	Study on the Molecular Reactivity of the Dansylglycine in Water and Dioxane Estimated through Conceptual DFT. , 2021, , 78-87.		0
16	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
17	Determination of Chemical Reactivities of Oxytocin and Vasopressin Peptide Hormones Studied through Conceptual Density Functional Theory (CDFT) and Molecular Electron Density Theory (MEDT). , 2021, , 21-30.		0
18	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.	0.9	3

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19	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.	1.8	4
20	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.	0.8	1
21	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
22	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
23	Virtual Screening for Potential Phytobioactives as Therapeutic Leads to Inhibit NQO1 for Selective Anticancer Therapy. Molecules, 2021, 26, 6863.	1.7	5
24	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
25	Virtual Screening of Marine Natural Compounds by Means of Chemoinformatics and CDFT-Based Computational Peptidology. Marine Drugs, 2020, 18, 478.	2.2	32
26	Conceptual DFT-Based Computational Peptidology of Marine Natural Compounds: Discodermins Aâ€“H. Molecules, 2020, 25, 4158.	1.7	30
27	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
28	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
29	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
30	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.	0.8	1
31	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.	1.3	4
32	Evaluation of Annona muricata Acetogenins as Potential Anti-SARS-CoV-2 Agents Through Computational Approaches. Frontiers in Chemistry, 2020, 8, 624716.	1.8	25
33	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.	1.8	4
34	Conceptual DFT as a Novel Chemoinformatics Tool for Studying the Chemical Reactivity Properties of the Amatoxin Family of Fungal Peptides. , 2020, , .		0
35	CDFT-Based Reactivity Descriptors as a Useful MEDT Chemoinformatics Tool for the Study of the Virotoxin Family of Fungal Peptides. , 2020, , .		0
36	Molecular Docking and Conceptual DFT-Based Study of Some Potential SARS-CoV-2 Inhibitors. Computational Molecular Bioscience, 2020, 10, 111-128.	0.6	0

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37	KID Procedure Applied on the [(PYMe)MoO] Complex. ACS Omega, 2020, 5, 30549-30555.	1.6	0
38	KID Procedure Applied on the [(PY₅Me₂)MoO]⁺ Complex. ACS Omega, 2020, 5, 30549-30555.	1.6	2
39	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
40	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
41	Conceptual DFT as a chemoinformatics tool for the study of the Taltobulin anticancer peptide. BMC Research Notes, 2019, 12, 442.	0.6	7
42	CDFT-Based Reactivity Descriptors as a Useful MEDT Chemoinformatics Tool for the Study of the Virotoxin Family of Fungal Peptides. Molecules, 2019, 24, 2707.	1.7	5
43	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
44	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
45	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
46	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.	1.8	5
47	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
48	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
49	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.	0.9	2
50	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
51	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.	1.0	4
52	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
53	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
54	Chemical Reactivity Properties, Drug-Likeness Features and Bioactivity Scores of the Cholecystokinin Peptide Hormone. Computational Molecular Bioscience, 2019, 09, 41-47.	0.6	12

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55	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.	0.6	4
56	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
57	Assessment of ten density functionals through the use of local hyperâ€“softness to get insights about the catalytic activity. Journal of Molecular Modeling, 2018, 24, 42.	0.8	5
58	Computational study of the chemical reactivity of the Blue-M1 intermediate melanoidin. Computational and Theoretical Chemistry, 2018, 1134, 22-29.	1.1	39
59	Supramolecular arrangement and photophysical properties of a dinuclear cyanophenylboronic acid ester. Acta Crystallographica Section C, Structural Chemistry, 2018, 74, 452-459.	0.2	2
60	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.	0.8	3
61	Assessment of the Validity of Some Minnesota Density Functionals for the Prediction of the Chemical Reactivity of the SYBR Green I and Ethidium Bromide Nucleic Acid Stains. , 2018, , .		1
62	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
63	Blue M2: an intermediate melanoidin studied via conceptual DFT. Journal of Molecular Modeling, 2018, 24, 138.	0.8	26
64	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.	1.8	3
65	Molecular Reactivity and Absorption Properties of Melanoidin Blue-G1 through Conceptual DFT. Molecules, 2018, 23, 559.	1.7	41
66	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
67	Local Molecular Reactivity of the Colored Dansylglycine in Water and Dioxane Studied through Conceptual DFT. Journal of Chemistry, 2018, 2018, 1-7.	0.9	5
68	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
69	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
70	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
71	Computational prediction of the pKas of small peptides through Conceptual DFT descriptors. Chemical Physics Letters, 2017, 671, 138-141.	1.2	36
72	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

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73	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
74	A conceptual DFT study of the molecular properties of glycating carbonyl compounds. Chemistry Central Journal, 2017, 11, 8.	2.6	20
75	Theoretical investigation of the molecular structure and spectroscopic properties of oxicams. Journal of Structural Chemistry, 2017, 58, 261-267.	0.3	1
76	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
77	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
78	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
79	Chemical Reactivity Theory Study of Advanced Glycation Endproduct Inhibitors. Molecules, 2017, 22, 226.	1.7	25
80	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
81	New Methods of Esterification of Nanodiamonds in Fighting Breast Cancerâ€"A Density Functional Theory Approach. Molecules, 2017, 22, 1740.	1.7	4
82	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
83	A Brief Performance Test of the M06 Family of Density Functionals for the Prediction of the Maximum Absorption Wavelength of Thioindigo in Several Solvents. Journal of the Mexican Chemical Society, 2017, 57, .	0.2	2
84	Comparative Study of the Chemical Reactivity of Helical Peptide Models for Protein Glycation. Computational Chemistry, 2017, 05, 65-73.	0.2	5
85	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
86	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.	0.4	1
87	Molecular Modeling of the Structures, Properties and Glycating Power of Some Reducing Disaccharides. MOJ Drug Design Development & Therapy, 2017, 1, .	0.1	1
88	PREPARATION, IDENTIFICATION AND BIOLOGICAL PROPERTIES OF NEW FLUORIDE NANOCOMPOUNDS. Journal of the Chilean Chemical Society, 2016, 61, 3201-3205.	0.5	7
89	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
90	A Molecular Electron Density Theory Study of the Chemical Reactivity of Cis- and Trans-Resveratrol. Molecules, 2016, 21, 1650.	1.7	38

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91	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
92	Preparation and Characterization of Cerium (III) Doped Captopril Nanoparticles and Study of their Photoluminescence Properties. Open Chemistry, 2016, 14, 60-64.	1.0	13
93	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
94	Fractal Dimension Calculation of a Manganese-Chromium Bimetallic Nanocomposite Using Image Processing. Journal of Nanomaterials, 2015, 2015, 1-9.	1.5	4
95	Morphological Investigation and Fractal Properties of Realgar Nanoparticles. Journal of Nanomaterials, 2015, 2015, 1-8.	1.5	1
96	DFT Study of Polythiophene Energy Band Gap and Substitution Effects. Journal of Chemistry, 2015, 2015, 1-12.	0.9	24
97	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
98	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
99	Theoretical calculation of the maximum absorption wavelength for Cyanidin molecules with several methodologies. Computational and Theoretical Chemistry, 2015, 1067, 129-134.	1.1	29
100	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
101	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.	1.2	7
102	Geometric description and electronic properties of the principal photosynthetic pigments of higher plants: a DFT study. Journal of Molecular Modeling, 2015, 21, 256.	0.8	3
103	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
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.	0.8	4
105	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
106	Synthesis, structure, characterization and photophysical properties of copper(<scp>i</scp>) complexes containing polypyridyl ligands. RSC Advances, 2014, 4, 42624-42631.	1.7	17
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.	0.8	18
108	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

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109	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.	0.6	0
110	Experimental and quantum chemical studies of a novel synthetic prenylated chalcone. Chemistry Central Journal, 2013, 7, 17.	2.6	11
111	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
112	Computational nanochemistry study of the molecular structure and properties of ethambutol. Journal of Molecular Modeling, 2013, 19, 3507-3515.	0.8	10
113	Virtual Screening: Using Molecular Docking and 3Dâ€QSAR Analysis of Matrix Metalloproteinase Inhibitors. Journal of the Chinese Chemical Society, 2013, 60, 1212-1224.	0.8	2
114	Computational Study of the Chemical Reactivity Properties of the Rhodamine B Molecule. Procedia Computer Science, 2013, 18, 816-825.	1.2	63
115	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
116	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
117	Computational Nanochemistry Report on the Oxicamsâ€"Conceptual DFT Indices and Chemical Reactivity. Journal of Physical Chemistry B, 2013, 117, 6339-6351.	1.2	35
118	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.	0.9	3
119	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
120	Computational Nutraceutics: Chemical Reactivity Properties of the Flavonoid Naringin by Means of Conceptual DFT. Journal of Chemistry, 2013, 2013, 1-8.	0.9	16
121	Computational Nanochemistry Study of the Molecular Structure and Properties of Chlorophyll a. International Journal of Photoenergy, 2013, 2013, 1-8.	1.4	7
122	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
123	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
124	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
125	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
126	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

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127	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
128	Topics in quantum physics with origins in astronomy: Two examples. American Journal of Physics, 2012, 80, 406-416.	0.3	4
129	DFT study of the effect of substituents on the absorption and emission spectra of Indigo. Chemistry Central Journal, 2012, 6, 70.	2.6	16
130	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
131	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
132	Ab initio study of electron transport in 4-(3-nitro-4-tetrafluorophenylthiolate-ethynyl, phenylethynyl) benzenethiolate. Journal of Molecular Modeling, 2012, 18, 611-621.	0.8	4
133	Computational characterization of the molecular structure and properties of Dye 7 for organic photovoltaics. Journal of Molecular Modeling, 2012, 18, 835-842.	0.8	2
134	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
135	Computational characterization of sodium selenite using density functional theory. Journal of Molecular Modeling, 2011, 17, 701-708.	0.8	1
136	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
137	Electronic structure study using density functional theory in organic dendrimers. Journal of Molecular Modeling, 2011, 17, 1963-1972.	0.8	8
138	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
139	EFFECTS OF SULFUR SUBSTITUTIONAL IMPURITIES ON ZnO STRUCTURE USING DENSITY FUNCTIONAL THEORY. International Journal of Nanoscience, 2011, 10, 381-390.	0.4	1
140	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
141	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
142	TD-DFT/IEFPCM determination of the absorption and emission spectra of DABCYL. Computational and Theoretical Chemistry, 2010, 945, 101-103.	1.5	9
143	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
144	Computational molecular characterization of the flavonoid rutin. Chemistry Central Journal, 2010, 4, 12.	2.6	33

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145	Natural Carotenoids as Nanomaterial Precursors for Molecular Photovoltaics: A Computational DFT Study. Molecules, 2010, 15, 4490-4510.	1.7	59
146	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
147	Theoretical study of electronic properties of organic photovoltaic materials. Journal of Computational Chemistry, 2009, 30, 1027-1037.	1.5	18
148	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
149	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.	1.5	2
150	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
151	Molecular modeling of the melting temperature of a tuberculosis DNA nanobiosensor. New Biotechnology, 2009, 25, S30.	2.4	1
152	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
153	Characterization of the semiquinones and quinones of (âˆ’)-epicatechin by means of computational chemistry. Computational and Theoretical Chemistry, 2009, 897, 6-11.	1.5	8
154	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
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