Prasad Bharatam

List of Publications by Year
in descending order

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238 papers	5,175 citations	109321 35 h-index	175258 52 g-index
247 all docs	247 docs citations	247 times ranked	5850 citing authors

#	Article	IF	Citations
1	Thiazetidin-2-ylidenes as four membered N-heterocyclic carbenes: theoretical studies and the generation of complexes with N⁺ center. Physical Chemistry Chemical Physics, 2022, 24, 629-633.	2.8	6
2	Remdesivir: Mechanism of Metabolic Conversion from Prodrug to Drug. Current Drug Metabolism, 2022, 23, 73-81.	1.2	1
3	Understanding Poor Milling Behavior of Voriconazole from Crystal Structure and Intermolecular Interactions. Molecular Pharmaceutics, 2022, 19, 985-997.	4.6	6
4	NIS mediated dehydrogenative-cyclocondensation in aqueous medium towards the synthesis of 2-arylimidazo[1,2-a]pyridines and their 3-formylated derivatives. Tetrahedron, 2022, 112, 132715.	1.9	8
5	Nâ€heterocyclic carbene ligated oximes: Exploring the electronic structure and properties. International Journal of Quantum Chemistry, 2022, 122, .	2.0	4
6	Drug-dendrimer complexes and conjugates: Detailed furtherance through theory and experiments. Advances in Colloid and Interface Science, 2022, 303, 102639.	14.7	16
7	High dose nanocrystalline solid dispersion powder of voriconazole for inhalation. International Journal of Pharmaceutics, 2022, 622, 121827.	5.2	1
8	Design, synthesis, and biological evaluation of benzo[d]imidazole-2-carboxamides as new anti-TB agents. Bioorganic Chemistry, 2021, 107, 104538.	4.1	28
9	Visible light promoted tandem dehydrogenation-deaminative cyclocondensation under aerobic conditions for the synthesis of 2-aryl benzimidazoles/quinoxalines from ortho-phenylenediamines and arylmethyl/ethyl amines. New Journal of Chemistry, 2021, 45, 4569-4573.	2.8	10
10	Computer-Aided Drug Design. , 2021, , 137-210.		11
11	Quantum chemical study in exploring the role of donorâ†'acceptor interactions in 1,3-bis carbene-stabilized guanidinium cations. Journal of Molecular Modeling, 2021, 27, 87.	1.8	2
12	Selective lithiation of 2,4-lutidine: Role of transition states of lithium dialkylamides. Journal of Organometallic Chemistry, 2021, 936, 121691.	1.8	2
13	Reactive Metabolites from Thiazole-Containing Drugs: Quantum Chemical Insights into Biotransformation and Toxicity. Chemical Research in Toxicology, 2021, 34, 1503-1517.	3.3	13
14	Identification of selective LdDHFR inhibitors using quantum chemical and molecular modeling approach. Journal of Biomolecular Structure and Dynamics, 2021, , 1-9.	3.5	1
15	Iodine Catalyzed Oxidative Coupling of Diaminoazines and Amines for the Synthesis of 3,5-Disubstituted-1,2,4-Triazoles. Journal of Organic Chemistry, 2021, 86, 7659-7671.	3.2	11
16	Role of surface molecular environment and amorphous content in moisture sorption behavior of milled Terbutaline Sulphate. European Journal of Pharmaceutical Sciences, 2021, 161, 105782.	4.0	2
17	A novel copper-catalyzed, hydrazine-free synthesis of N-1 unsubstituted 1H-indazoles using stable guanylhydrazone salts as substrates. Tetrahedron, 2021, 91, 132192.	1.9	9
18	Biguanides: Species with versatile therapeutic applications. European Journal of Medicinal Chemistry, 2021, 219, 113378.	5.5	29

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19	Compound with possible NÂâ†'ÂN coordination bond: Synthesis, crystal structure and electronic structure analysis. Tetrahedron Letters, 2021, 77, 153246.	1.4	3
20	Mesoionic and Nâ€heterocyclic Carbenesâ€Coordinated N+ÂCenter: Experimental and Computational Analysis. ChemPlusChem, 2021, 86, 1416-1420.	2.8	10
21	3D QSAR studies on amphiphilic indoles for antimycobacterial activity. Journal of Biochemical and Molecular Toxicology, 2021, 35, e22675.	3.0	3
22	1,1-Diaminoazines as organocatalysts in phospha-Michael addition reactions. Chemical Communications, 2021, 57, 11717-11720.	4.1	9
23	LC-ESI-QTOF-MS analysis utilizing gas-phase fragmentation reactions subjected to ESI-IS-CID and ESI-CID-MS/MS conditions to study the degradation behaviour of sorafenib tosylate: NMR and in vitro cytotoxicity and apoptosis detection studies of hydrolytic degradation products. Journal of Pharmaceutical and Biomedical Analysis, 2020, 177, 112881.	2.8	8
24	Structural exploration of glutamine synthetase from Leishmania donovani: Insights from in silico and in vitro analysis. International Journal of Biological Macromolecules, 2020, 146, 860-874.	7.5	5
25	Divalent N I Compounds: Identifying new Carbocyclic Carbenes to Design Nitreones using Quantum Chemical Methods. Journal of Computational Chemistry, 2020, 41, 2624-2633.	3.3	7
26	Mechanistic studies on the drug metabolism and toxicity originating from cytochromes P450. Drug Metabolism Reviews, 2020, 52, 366-394.	3.6	18
27	Benzimidazoquinazolines as new potent anti-TB chemotypes: Design, synthesis, and biological evaluation. Bioorganic Chemistry, 2020, 99, 103774.	4.1	29
28	Characterization of Photodegradation Products of Bepotastine Besilate and In Silico Evaluation of Their Physicochemical, Absorption, Distribution, Metabolism, Excretion and Toxicity Properties. Journal of Pharmaceutical Sciences, 2020, 109, 1883-1895.	3.3	12
29	Oxone-DMSO Triggered Methylene Insertion and C(sp²)â^'C(sp³)-Hâ^'C(sp²) Bond Formation to Access Functional Bis-Heterocycles. Journal of Organic Chemistry, 2020, 85, 4951-4962.	3.2	23
30	Novel Furan-2-yl-1H-pyrazoles Possess Inhibitory Activity against Î±-Synuclein Aggregation. ACS Chemical Neuroscience, 2020, 11, 2303-2315.	3.5	9
31	Reaction behaviour of arylamines with nitroalkenes in the presence of bismuth(iii) triflate: an easy access to 2,3-dialkylquinolines. Organic and Biomolecular Chemistry, 2020, 18, 1785-1793.	2.8	6
32	Synthesis of Drugs and Biorelevant N-heterocycles Employing Recent Advances in C-N Bond Formation. Current Organic Chemistry, 2020, 24, 2293-2340.	1.6	1
33	Azines: synthesis, structure, electronic structure and their applications. Organic and Biomolecular Chemistry, 2019, 17, 8486-8521.	2.8	53
34	Singlet oxygen mediated one pot synthesis of N-pyridinylamides via oxidative amidation of aryl alkyl ketones. Tetrahedron, 2019, 75, 130536.	1.9	6
35	Tandem Oxidative Cyclocondensation towards 2,3â€Disubstituted Quinazolinones in the Presence of [Bmim][BF₄] and Iodine. European Journal of Organic Chemistry, 2019, 2019, 5887-5893.	2.4	11
36	Design, synthesis and biological evaluation of 4-aminoquinoline-guanylthiourea derivatives as antimalarial agents. Bioorganic Chemistry, 2019, 91, 103094.	4.1	22

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37	Fabrication of a Hydrazone-Based Al(III)-Selective â€œTurn-Onâ€•Fluorescent Chemosensor and Ensuing Potential Recognition of Picric Acid. ACS Omega, 2019, 4, 18520-18529.	3.5	36
38	Formation of a Toxic Quinoneimine Metabolite from Diclofenac: A Quantum Chemical Study. Drug Metabolism Letters, 2019, 13, 64-76.	0.8	5
39	Donorâ†'acceptor coordination interactions in 1,3â€bis(NHC)triazenyl Cations: An electronic structure analysis. Journal of Computational Chemistry, 2019, 40, 2207-2215.	3.3	5
40	Molecular Basis of Water Sorption Behavior of Rivaroxaban-Malonic Acid Cocrystal. Molecular Pharmaceutics, 2019, 16, 2980-2991.	4.6	30
41	Geometrical Isomerism in Guanabenz Free Base: Synthesis, Characterization, Crystal Structure, and Theoretical Studies. Crystal Growth and Design, 2019, 19, 3183-3191.	3.0	8
42	Knoevenagel/Tandem Knoevenagel and Michael Adducts of Cyclohexane-1,3-dione and Aryl Aldehydes: Synthesis, DFT Studies, Xanthine Oxidase Inhibitory Potential, and Molecular Modeling. ACS Omega, 2019, 4, 4604-4614.	3.5	12
43	Enols, Diamino Enols, and Breslow Intermediates: A Comparative Quantum Chemical Analysis. European Journal of Organic Chemistry, 2019, 2019, 2481-2489.	2.4	4
44	An unprecedented intramolecular to intermolecular mechanistic switch in 1,1-diaminoazines leading to differential product formation during the I2-induced tandem oxidative transformation. Organic and Biomolecular Chemistry, 2019, 17, 4129-4138.	2.8	14
45	Bimetallic Cuâ€“Mn B spinel oxide catalyzed oxidative synthesis of 1,2-disubstituted benzimidazoles from benzyl bromides. New Journal of Chemistry, 2019, 43, 4013-4016.	2.8	10
46	An unprecedented N- to C-sulfonyl migration in the reaction of azomethine amine and allenoates: access to arylsulfonylmethyl substituted pyrazolo[1,5-c]quinazoline and mechanistic studies. Chemical Communications, 2019, 55, 14825-14828.	4.1	8
47	Exploring PfDHFR reaction surface: A combined molecular dynamics and QM/MM analysis. Journal of Molecular Graphics and Modelling, 2019, 87, 76-88.	2.4	4
48	Structure-Based Drug Design of PfDHODH Inhibitors as Antimalarial Agents. Challenges and Advances in Computational Chemistry and Physics, 2019, , 177-220.	0.6	2
49	Pharmacoinformatics analysis of merbarone binding site in human topoisomerase IIÎ±. Journal of Molecular Graphics and Modelling, 2019, 86, 1-18.	2.4	5
50	CÂâ†'ÂN coordination bonds in (CCC)Ââ†'ÂN + Ââ†Â(L) complexes. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	13
51	Can Remote Nâ€Heterocyclic Carbenes Coordinate with Main Group Elements? Synthesis, Structure, and Quantum Chemical Analysis of N⁺â€Centered Complexes. Chemistry - A European Journal, 2018, 24, 6418-6425.	3.3	21
52	Ring-chain isomerism in conjugated guanylhydrazones: Experimental and theoretical study. Tetrahedron, 2018, 74, 2857-2864.	1.9	13
53	Does Nâ€terminal huntingtin function as a â€˜holdaseâ€™ for inhibiting cellular protein aggregation?. FEBS Journal, 2018, 285, 1791-1811.	4.7	6
54	Additiveâ€Controlled Switchable Selectivity from Cyanobenzenes to 2â€Alkynylpyridines: Ruthenium(II)â€Catalyzed [2+2+2] Cycloadditions of Diynes and Alkynylnitriles. Advanced Synthesis and Catalysis, 2018, 360, 1876-1882.	4.3	30

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55	â€œWhat's in a structure?â€•The story of biguanides. Journal of Molecular Structure, 2018, 1152, 61-78.	3.6	48
56	Cyclocondensation reactions of an electron deactivated 2-aminophenyl tethered imidazole with mono/1,2-biselectrophiles: synthesis and DFT studies on the rationalisation of imidazo[1,2-a]quinoxaline versus benzo[f]imidazo[1,5-a][1,3,5]triazepine selectivity switches. Organic Chemistry Frontiers, 2018, 5, 3526-3533.	4.5	12
57	Unanticipated Cleavage of 2-Nitrophenyl-Substituted N-Formyl Pyrazolines under Bechamp Conditions: Unveiling the Synthesis of 2-Aryl Quinolines and Their Mechanistic Exploration via DFT Studies. ACS Omega, 2018, 3, 18783-18790.	3.5	4
58	Electronic and ligating properties of carbocyclic carbenes: A theoretical investigation. Journal of Computational Chemistry, 2018, 40, 726.	3.3	7
59	N-(acridin-9-yl)arenesulfonamides: Synthesis, quantum chemical studies and crystal structure analysis to establish the tautomeric preferences. Tetrahedron, 2018, 74, 3634-3641.	1.9	3
60	Sulfoximine-Assisted One-Pot Unsymmetrical Multiple Annulation of Arenes: A Combined Experimental and Computational Study. Journal of Organic Chemistry, 2018, 83, 9667-9681.	3.2	39
61	NL₂⁺ Systems as New-Generation Phase-Transfer Catalysts. Chemical Reviews, 2018, 118, 8770-8785.	47.7	64
62	Guanylthiourea derivatives as potential antimalarial agents: Synthesis, inÂvivo and molecular modelling studies. European Journal of Medicinal Chemistry, 2017, 135, 339-348.	5.5	16
63	Cobalt-Catalyzed Regioselective Ortho C(sp²)-H Bond Nitration of Aromatics through Proton-Coupled Electron Transfer Assistance. Journal of Organic Chemistry, 2017, 82, 7234-7244.	3.2	32
64	Pharmacoinformatic Study on the Selective Inhibition of the Protozoan Dihydrofolate Reductase Enzymes. Molecular Informatics, 2017, 36, 1600156.	2.5	9
65	Biotransformation of Isoniazid by Cytochromes P450: Analyzing the Molecular Mechanism using Density Functional Theory. Chemical Research in Toxicology, 2017, 30, 2060-2073.	3.3	11
66	Rationalization of Benzazole-2-carboxylate versus Benzazine-3-one/Benzazine-2,3-dione Selectivity Switch during Cyclocondensation of 2-Aminothiophenols/Phenols/Anilines with 1,2-Biselectrophiles in Aqueous Medium. Journal of Organic Chemistry, 2017, 82, 10077-10091.	3.2	26
67	Geometry Driven Intramolecular Oxidative Cyclization of Enamides: An Umpolung Annulation of Primary Benzamides with Acrylates for the Synthesis of 3-Methyleneisoindolin-1-ones. Journal of Organic Chemistry, 2017, 82, 7346-7352.	3.2	25
68	Sulfonamide vs. sulfonimide: tautomerism and electronic structure analysis of N-heterocyclic arenesulfonamides. New Journal of Chemistry, 2017, 41, 8118-8129.	2.8	18
69	Integration of oxidative arylation with sulfonyl migration: one-pot tandem synthesis of densely functionalized (NH)-pyrroles. New Journal of Chemistry, 2017, 41, 8791-8803.	2.8	15
70	Mutational and Structural Analysis of Conserved Residues in Ribose-5-Phosphate Isomerase B from Leishmania donovani: Role in Substrate Recognition and Conformational Stability. PLoS ONE, 2016, 11, e0150764.	2.5	13
71	Atomic level insights into realistic molecular models of dendrimer-drug complexes through MD simulations. Journal of Chemical Physics, 2016, 145, 124902.	3.0	21
72	Ferulic acid amide derivatives as anticancer and antioxidant agents: synthesis, thermal, biological and computational studies. Medicinal Chemistry Research, 2016, 25, 1175-1192.	2.4	30

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73	A Metal and Base-Free Chemoselective Primary Amination of Boronic Acids Using Cyanamidyl/Arylcyanamidyl Radical as Aminating Species: Synthesis and Mechanistic Studies by Density Functional Theory. Journal of Organic Chemistry, 2016, 81, 5120-5127.	3.2	26
74	Design, synthesis and biological evaluation of 5-benzylidene-2-iminothiazolidin-4-ones as selective GSK-3Î² inhibitors. European Journal of Medicinal Chemistry, 2016, 121, 727-736.	5.5	34
75	Carbene â†'N+ Coordination Bonds in Drugs: A Quantum Chemical Study. Journal of Chemical Sciences, 2016, 128, 1607-1614.	1.5	22
76	Azine-Hydrazone Tautomerism of Guanylhydrazones: Evidence for the Preference Toward the Azine Tautomer. Journal of Organic Chemistry, 2016, 81, 7574-7583.	3.2	35
77	Electronic structure and conformational analysis of P218: An antimalarial drug candidate. International Journal of Quantum Chemistry, 2016, 116, 1362-1369.	2.0	6
78	Design, Synthesis, and Structural Analysis of Divalent N^I Compounds and Identification of a New Electronâ€Donating Ligand. Chemistry - A European Journal, 2016, 22, 1088-1096.	3.3	33
79	Metalâ€free Intermolecular Hydrophenoxylation of Aryl Alkynes. Asian Journal of Organic Chemistry, 2016, 5, 213-221.	2.7	15
80	Design and synthesis of novel Y-shaped barbituric acid derivatives as PPARÎ³ activators. European Journal of Medicinal Chemistry, 2016, 108, 423-435.	5.5	21
81	Nucleophilic Addition versus S_NAr Study: Chemoâ€, Regioâ€and Stereoselective Hydrothiolation of Haloaryl Alkynes over Sâ€Arylation of Aryl Halides. Asian Journal of Organic Chemistry, 2015, 4, 894-898.	2.7	8
82	Azine or hydrazone? The dilemma in amidinohydrazones. RSC Advances, 2015, 5, 55938-55947.	3.6	27
83	Origins of the specificity of inhibitor P218 toward wild-type and mutantPfDHFR: a molecular dynamics analysis. Journal of Biomolecular Structure and Dynamics, 2015, 33, 1913-1928.	3.5	27
84	Mechanochemical click reaction as a tool for making carbohydrate-based triazole-linked self-assembling materials (CTSAMs). Carbohydrate Research, 2015, 407, 137-147.	2.3	11
85	Switch in Site of Inhibition: A Strategy for Structure-Based Discovery of Human Topoisomerase IIÎ± Catalytic Inhibitors. ACS Medicinal Chemistry Letters, 2015, 6, 481-485.	2.8	84
86	Molecular dynamics simulation studies of GSK-3Î² ATP competitive inhibitors: understanding the factors contributing to selectivity. Journal of Biomolecular Structure and Dynamics, 2015, 33, 2578-2593.	3.5	42
87	TEMPO-Promoted Domino Heckâ€"Suzuki Arylation: Diastereoselective Cis-Diarylation of Glycals and Pseudoglycals. Organic Letters, 2015, 17, 3742-3745.	4.6	53
88	Mechanism of the Paalâ€"Knorr reaction: the importance of water mediated hemialcohol pathway. RSC Advances, 2015, 5, 88353-88366.	3.6	32
89	Design, Synthesis, and Biological Evaluation of 1,2-Dihydroisoquinolines as HIV-1 Integrase Inhibitors. ACS Medicinal Chemistry Letters, 2015, 6, 1065-1070.	2.8	28
90	Design, synthesis and biological evaluation of novel unsymmetrical azines as quorum sensing inhibitors. RSC Advances, 2015, 5, 80027-80038.	3.6	21

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91	Toxicity Originating from Thiophene Containing Drugs: Exploring the Mechanism using Quantum Chemical Methods. Chemical Research in Toxicology, 2015, 28, 2364-2376.	3.3	35
92	DFT study on the oxygen transfer mechanism in nitroethenediamine based H2-receptor antagonists using the bis-dithiolene complex as the model catalyst for N-oxide reductase enzyme. Journal of Inorganic Biochemistry, 2015, 142, 84-91.	3.5	7
93	Design, synthesis, biological evaluation and toxicity studies of N,N-disubstituted biguanides as quorum sensing inhibitors. Medicinal Chemistry Research, 2015, 24, 1974-1987.	2.4	17
94	Importance of cytochromes in cyclization reactions: Quantum chemical study on a model reaction of proguanil to cycloguanil. Journal of Computational Chemistry, 2014, 35, 2047-2055.	3.3	28
95	Enhanced noscapine delivery using estrogen-receptor-targeted nanoparticles for breast cancer therapy. Anti-Cancer Drugs, 2014, 25, 704-716.	1.4	26
96	Comparative modeling of pivotal enzymes, MurA and MurZ, of Enterococcus faecalis and identification of potential inhibitors by computational methods. Medicinal Chemistry Research, 2014, 23, 1819-1828.	2.4	2
97	Combretastatin A-4 inspired novel 2-aryl-3-arylamino-imidazo-pyridines/pyrazines as tubulin polymerization inhibitors, antimitotic and anticancer agents. MedChemComm, 2014, 5, 766-782.	3.4	44
98	Possibility of the Existence of Donorâ€“Acceptor Interactions in Bis(azole)amines: An Electronic Structure Analysis. Journal of Organic Chemistry, 2014, 79, 4852-4862.	3.2	25
99	Design and synthesis of guanylthiourea derivatives as potential inhibitors of Plasmodium falciparum dihydrofolate reductase enzyme. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 613-617.	2.2	37
100	On the Stability of Zwitterions of Pyridine Sulfonylureas: The Effect of Isosterism, Acidity, and Microsolvation. Journal of Physical Chemistry A, 2014, 118, 187-196.	2.5	6
101	Pharmacoinformatic approaches to understand complexation of dendrimeric nanoparticles with drugs. Nanoscale, 2014, 6, 2476.	5.6	42
102	Relative Eccentric Distance Sum/Product Indices for QSAR/QSPR: Development, Evaluation, and Application. ACS Combinatorial Science, 2014, 16, 101-112.	3.8	0
103	Drug metabolism. Resonance, 2014, 19, 259-282.	0.3	24
104	Self-Association Behavior of aNovelNonproteinogenic Î²-Strand-Mimicin an Organic Solvent. Journal of Physical Chemistry B, 2014, 118, 9199-9208.	2.6	5
105	Importance of hydrophobic parameters in identifying appropriate pose of CYP substrates in cytochromes. European Journal of Medicinal Chemistry, 2014, 71, 15-23.	5.5	13
106	Detour matrix-based adjacent path eccentric distance sum indices for QSAR/QSPR. Part I: development and evaluation. International Journal of Computational Biology and Drug Design, 2014, 7, 295.	0.3	1
107	3-Formylchromone based topoisomerase IIÎ± inhibitors: discovery of potent leads. MedChemComm, 2013, 4, 1257.	3.4	11
108	Identification of Druggable Targets for Acinetobacter baumannii Via Subtractive Genomics and Plausible Inhibitors for MurA and MurB. Applied Biochemistry and Biotechnology, 2013, 171, 417-436.	2.9	22

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109	Structural Elaboration of a Natural Product: Identification of 3,3â€²â€Ðiindolylmethane Aminophosphonate and Urea Derivatives as Potent Anticancer Agents. ChemMedChem, 2013, 8, 1873-1884.	3.2	11
110	Importance of Câ€“HÂ·Â·Â·O Intramolecular Hydrogen Bonding Across a Nonproteinogenic Î³-Aminobenzoic Acid Residue: Stabilization of a Flat Î²-Strand-like Template. Crystal Growth and Design, 2013, 13, 2004-2012.	3.0	9
111	Electronic structure analysis of isomeric preferences of canonical and zwitterionic forms of lornoxicam. Computational and Theoretical Chemistry, 2013, 1023, 51-58.	2.5	4
112	Nitro â‡Œ aci-nitro tautomerism and E/Z isomeric preferences of nitroethenediamine derivatives: a quantum chemical study. RSC Advances, 2013, 3, 25268.	3.6	12
113	Mechanism-Based Inactivation of Cytochromes by Furan Epoxide: Unraveling the Molecular Mechanism. Inorganic Chemistry, 2013, 52, 13496-13508.	4.0	23
114	Pharmacophoric features of drugs with guanylurea moiety: an electronic structure analysis. Journal of Molecular Modeling, 2013, 19, 1865-1874.	1.8	5
115	Mechanistic insights into the bioactivation of phenacetin to reactive metabolites: A DFT study. Computational and Theoretical Chemistry, 2013, 1007, 48-56.	2.5	20
116	Synthesis, biological evaluation, and molecular modeling studies of novel heterocyclic compounds as anti-proliferative agents. Medicinal Chemistry Research, 2013, 22, 5654-5669.	2.4	12
117	Carbene Generation by Cytochromes and Electronic Structure of Heme-Iron-Porphyrin-Carbene Complex: A Quantum Chemical Study. Inorganic Chemistry, 2013, 52, 5097-5109.	4.0	40
118	Existence of dynamic tautomerism and divalent N(I) character in Nâ€(pyridinâ€2â€yl)thiazolâ€2â€amine. Journal of Computational Chemistry, 2013, 34, 1577-1588.	3.3	29
119	Molecular dynamics simulations of PPI dendrimerâ€“drug complexes. Soft Matter, 2013, 9, 6482.	2.7	46
120	Design of Glycogen Synthase Kinase-3 Inhibitors: An Overview on Recent Advancements. Current Pharmaceutical Design, 2013, 19, 4755-4775.	1.9	33
121	SAR and Computer-Aided Drug Design Approaches in the Discovery of Peroxisome Proliferator-Activated Receptor Î³ Activators: A Perspective. Journal of Computational Medicine, 2013, 2013, 1-38.	0.3	28
122	Formation/Fate of Reactive Metabolites from General Anesthetics and A Comparison of Toxic and Non-Toxic Analogues: A DFT Study. Drug Metabolism Letters, 2013, 6, 221-234.	0.8	2
123	2D QSAR Study for Gemfibrozil Glucuronide as the Mechanism-based Inhibitor of CYP2C8. Indian Journal of Pharmaceutical Sciences, 2013, 75, 680-7.	1.0	4
124	Fourth generation detour matrix-based topological indices for QSAR/QSPR - Part-1: development and evaluation. International Journal of Computational Biology and Drug Design, 2012, 5, 335.	0.3	3
125	CytochromeP450 isoenzyme specificity in the metabolism of anti-malarial biguanides: molecular docking and molecular dynamics analyses. Medicinal Chemistry Research, 2012, 21, 4274-4289.	2.4	7
126	Câ€“H Bond Functionalization Under Metalationâ€“Deprotonation Process: Regioselective Direct Arylation of 3-Aminoimidazo[1,2-a]pyrazine. Journal of Organic Chemistry, 2012, 77, 8321-8328.	3.2	40

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127	Synthesis of self-assembling glycerotriazolophanes. RSC Advances, 2012, 2, 11366.	3.6	6
128	Site-Selective Electrophilic Cyclization and Subsequent Ring-Opening: A Synthetic Route to Pyrrolo[1,2-a]quinolines and Indolizines. Journal of Organic Chemistry, 2012, 77, 8562-8573.	3.2	43
129	Divalent N(I) Character in 2-(Thiazol-2-yl)guanidine: An Electronic Structure Analysis. Journal of Physical Chemistry A, 2012, 116, 9071-9079.	2.5	31
130	Density Functional Study on the Cytochrome-Mediated S-Oxidation: Identification of Crucial Reactive Intermediate on the Metabolic Path of Thiazolidinediones. Journal of Physical Chemistry A, 2012, 116, 10441-10450.	2.5	20
131	Conformational polymorphism in bicalutamide: a quantum chemical study. Structural Chemistry, 2012, 23, 1857-1866.	2.0	10
132	Computational study on the conformational preferences in nateglinide. Journal of Physical Organic Chemistry, 2012, 25, 649-657.	1.9	8
133	Metabolicâ€intermediate complex formation with cytochrome P450: Theoretical studies in elucidating the reaction pathway for the generation of reactive nitroso intermediate. Journal of Computational Chemistry, 2012, 33, 1740-1747.	3.3	30
134	Dendrimer building toolkit: Model building and characterization of various dendrimer architectures. Journal of Computational Chemistry, 2012, 33, 1997-2011.	3.3	102
135	Complexâ€induced Proximity Effect in the Regioselective Lithiation of Pyridine Derivatives. European Journal of Organic Chemistry, 2012, 2012, 1746-1752.	2.4	13
136	Tautomerism in drugs with benzimidazole carbamate moiety: an electronic structure analysis. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	22
137	Research expedition of Prof. Eluvathingal D. Jemmis. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	0
138	2-Aminopyrimidine based 4-aminoquinoline anti-plasmodial agents. Synthesis, biological activity, structureâ€“activity relationship and mode of action studies. European Journal of Medicinal Chemistry, 2012, 52, 82-97.	5.5	66
139	3Dâ€QSAR and Molecular Docking Studies on 3â€Anilinoâ€4â€Arylmaleimide Derivatives as Glycogen Synthase Kinaseâ€3Î² Inhibitors. Chemical Biology and Drug Design, 2012, 79, 560-571.	3.2	12
140	CYP isoform specificity toward drug metabolism: analysis using common feature hypothesis. Journal of Molecular Modeling, 2012, 18, 709-720.	1.8	9
141	Entrapment and Kinetic Resolution of Stabilized Axial and Equatorial Conformers of Spiro-Î²-lactams. Journal of Organic Chemistry, 2011, 76, 5999-6006.	3.2	7
142	To Bend or Not to Bend! The Dilemma of Allenes. Journal of Organic Chemistry, 2011, 76, 2558-2567.	3.2	49
143	N-Fused Imidazoles As Novel Anticancer Agents That Inhibit Catalytic Activity of Topoisomerase IIÎ± and Induce Apoptosis in G1/S Phase. Journal of Medicinal Chemistry, 2011, 54, 5013-5030.	6.4	248
144	S-Oxidation of Thiazolidinedione with Hydrogen Peroxide, Peroxynitrous Acid, and C4a-Hydroperoxyflavin: A Theoretical Study. Journal of Physical Chemistry A, 2011, 115, 891-898.	2.5	22

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145	Toxic Metabolite Formation from Troglitazone (TGZ): New Insights from a DFT Study. Chemical Research in Toxicology, 2011, 24, 1113-1122.	3.3	28
146	Divalent N(I) Compounds with Two Lone Pairs on Nitrogen. Journal of Physical Chemistry A, 2011, 115, 7645-7655.	2.5	62
147	Computer-aided molecular design of 1H-imidazole-2,4-diamine derivatives as potential inhibitors of Plasmodium falciparum DHFR enzyme. Journal of Molecular Modeling, 2011, 17, 657-667.	1.8	33
148	Electronic structure and reactivity of guanylthiourea: A quantum chemical study. Journal of Computational Chemistry, 2010, 31, 1259-1267.	3.3	18
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