Prasad Bharatam

List of Publications by Year
in descending order

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238	5,175	109264	175177
papers	citations	35 h-index	52 g-index

247	247	247	5850
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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.	2.9	248
2	Bonding Trends of Thiosemicarbazones in Mononuclear and Dinuclear Copper(I) Complexes: Syntheses, Structures, and Theoretical Aspects. Inorganic Chemistry, 2006, 45, 1535-1542.	1.9	126
3	Solid-state characterization of rifampicin samples and its biopharmaceutic relevance. European Journal of Pharmaceutical Sciences, 2004, 22, 127-144.	1.9	124
4	Pharmacophoric Features of Biguanide Derivatives:Â An Electronic and Structural Analysis. Journal of Medicinal Chemistry, 2005, 48, 7615-7622.	2.9	114
5	Dendrimer building toolkit: Model building and characterization of various dendrimer architectures. Journal of Computational Chemistry, 2012, 33, 1997-2011.	1.5	102
6	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.	1.3	84
7	Novel âŠ•N(â†Ł)2 species with two lone pairs on nitrogen: systems isoelectronic to carbodicarbenes. Chemical Communications, 2009, , 1064.	2.2	67
8	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.	2.6	66
9	NL₂⁺ Systems as New-Generation Phase-Transfer Catalysts. Chemical Reviews, 2018, 118, 8770-8785.	23.0	64
10	Divalent N(I) Compounds with Two Lone Pairs on Nitrogen. Journal of Physical Chemistry A, 2011, 115, 7645-7655.	1.1	62
11	Theoretical investigation on the conformational preferences of sulfinimines. Perkin Transactions II RSC, 2000, , 43-50.	1.1	58
12	Theoretical studies on Sâ€“N interactions in sulfonamides. Tetrahedron, 2002, 58, 1759-1764.	1.0	58
13	Keto â‡Œ Enol, Imine â‡Œ Enamine, and Nitro â‡Œaci-Nitro Tautomerism and Their Interrelationship in Substituted Nitroethylenes. Keto, Imine, Nitro, and Vinyl Substituent Effects and the Importance of H-bonding. Journal of Organic Chemistry, 2000, 65, 4662-4670.	1.7	55
14	TEMPO-Promoted Domino Heckâ€“Suzuki Arylation: Diastereoselective Cis-Diarylation of Glycals and Pseudoglycals. Organic Letters, 2015, 17, 3742-3745.	2.4	53
15	Azines: synthesis, structure, electronic structure and their applications. Organic and Biomolecular Chemistry, 2019, 17, 8486-8521.	1.5	53
16	Additivity of Molecular Fields:Â CoMFA Study on Dual Activators of PPARÎ± and PPARÎ³. Journal of Medicinal Chemistry, 2005, 48, 3015-3025.	2.9	51
17	To Bend or Not to Bend! The Dilemma of Allenes. Journal of Organic Chemistry, 2011, 76, 2558-2567.	1.7	49
18	Chiral Solvating Agents for Cyanohydrins and Carboxylic Acids. Journal of Organic Chemistry, 2010, 75, 5487-5498.	1.7	48

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19	â€œWhat's in a structure?â€•The story of biguanides. Journal of Molecular Structure, 2018, 1152, 61-78.	1.8	48
20	Molecular dynamics simulations of PPI dendrimerâ€“drug complexes. Soft Matter, 2013, 9, 6482.	1.2	46
21	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.	3.5	44
22	Electron Delocalization in Isocyanates, Formamides, and Ureas: Importance of Orbital Interactions. Journal of Physical Chemistry A, 2003, 107, 1627-1634.	1.1	43
23	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.	1.7	43
24	Pharmacoinformatic approaches to understand complexation of dendrimeric nanoparticles with drugs. Nanoscale, 2014, 6, 2476.	2.8	42
25	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.	2.0	42
26	3D-QSAR CoMFA study onÂindenopyrazole derivatives asÂcyclin dependent kinase 4 (CDK4) andÂcyclin dependent kinase 2 (CDK2) inhibitors. European Journal of Medicinal Chemistry, 2006, 41, 1310-1319.	2.6	41
27	3D-QSAR and molecular docking study on bisarylmaleimide series as glycogen synthase kinase 3, cyclin dependent kinase 2 and cyclin dependent kinase 4 inhibitors: An insight into the criteria for selectivity. European Journal of Medicinal Chemistry, 2007, 42, 1014-1027.	2.6	40
28	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.	1.7	40
29	Carbene Generation by Cytochromes and Electronic Structure of Heme-Iron-Porphyrin-Carbene Complex: A Quantum Chemical Study. Inorganic Chemistry, 2013, 52, 5097-5109.	1.9	40
30	Sulfoximine-Assisted One-Pot Unsymmetrical Multiple Annulation of Arenes: A Combined Experimental and Computational Study. Journal of Organic Chemistry, 2018, 83, 9667-9681.	1.7	39
31	3D-QSAR and molecular docking studies on pyrazolopyrimidine derivatives as glycogen synthase kinase-3Î² inhibitors. Journal of Molecular Graphics and Modelling, 2007, 25, 885-895.	1.3	38
32	Lewis Donor and Acceptor Interactions of Silylenes:Â A Theoretical Study. Organometallics, 2002, 21, 3683-3690.	1.1	37
33	Electron Delocalization in Aminoguanidine:Â A Computational Study. Journal of Physical Chemistry A, 2004, 108, 10509-10517.	1.1	37
34	Modeling and Informatics in Designing Anti-Diabetic Agents. Current Pharmaceutical Design, 2007, 13, 3518-3530.	0.9	37
35	Inclusion complexes of noscapine in Î²-cyclodextrin offer better solubility and improved pharmacokinetics. Cancer Chemotherapy and Pharmacology, 2010, 65, 537-548.	1.1	37
36	Design and synthesis of guanylthiourea derivatives as potential inhibitors of Plasmodium falciparum dihydrofolate reductase enzyme. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 613-617.	1.0	37

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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.	1.6	36
38	New PPARÎ³ ligands based on barbituric acid: Virtual screening, synthesis and receptor binding studies. Bioorganic and Medicinal Chemistry Letters, 2008, 18, 4959-4962.	1.0	35
39	Toxicity Originating from Thiophene Containing Drugs: Exploring the Mechanism using Quantum Chemical Methods. Chemical Research in Toxicology, 2015, 28, 2364-2376.	1.7	35
40	Azine-Hydrazone Tautomerism of Guanylhydrazones: Evidence for the Preference Toward the Azine Tautomer. Journal of Organic Chemistry, 2016, 81, 7574-7583.	1.7	35
41	A simple, mild, and regioselective method for the benzylation of carbohydrate derivatives promoted by silver carbonate. Carbohydrate Research, 2010, 345, 559-564.	1.1	34
42	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.	2.6	34
43	A Study of BF₃â€Promoted orthoâ€...Lithiation of Anilines and DFT Calculations on the Role of Fluorineâ€“Lithium Interactions. Angewandte Chemie - International Edition, 2008, 47, 4703-4706.	7.2	33
44	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.	0.8	33
45	Design of Glycogen Synthase Kinase-3 Inhibitors: An Overview on Recent Advancements. Current Pharmaceutical Design, 2013, 19, 4755-4775.	0.9	33
46	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.	1.7	33
47	Thiourea catalyzed aminolysis of epoxides under solvent free conditions. Electronic control of regioselective ring opening. Tetrahedron, 2010, 66, 3042-3049.	1.0	32
48	Mechanism of the Paalâ€“Knorr reaction: the importance of water mediated hemialcohol pathway. RSC Advances, 2015, 5, 88353-88366.	1.7	32
49	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.	1.7	32
50	Divalent N(I) Character in 2-(Thiazol-2-yl)guanidine: An Electronic Structure Analysis. Journal of Physical Chemistry A, 2012, 116, 9071-9079.	1.1	31
51	An Experimental and Computational Study of Stereoselectivity and Reactivity in Lewis Acid Promoted Lithiation-Substitution of Tertiary Amines. Journal of the American Chemical Society, 2007, 129, 4506-4507.	6.6	30
52	A new chiral shift reagent for the determination of enantiomeric excess and absolute configuration in cyanohydrins. Chemical Communications, 2009, , 1067.	2.2	30
53	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.	1.5	30
54	Ferulic acid amide derivatives as anticancer and antioxidant agents: synthesis, thermal, biological and computational studies. Medicinal Chemistry Research, 2016, 25, 1175-1192.	1.1	30

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55	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.	2.1	30
56	Molecular Basis of Water Sorption Behavior of Rivaroxaban-Malonic Acid Cocrystal. Molecular Pharmaceutics, 2019, 16, 2980-2991.	2.3	30
57	Rapid Racemization in Thiazolidinediones:â€‰ A Quantum Chemical Study. Journal of Physical Chemistry A, 2004, 108, 3784-3788.	1.1	29
58	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.	1.5	29
59	Benzimidazoquinazolines as new potent anti-TB chemotypes: Design, synthesis, and biological evaluation. Bioorganic Chemistry, 2020, 99, 103774.	2.0	29
60	Biguanides: Species with versatile therapeutic applications. European Journal of Medicinal Chemistry, 2021, 219, 113378.	2.6	29
61	Toxic Metabolite Formation from Troglitazone (TGZ): New Insights from a DFT Study. Chemical Research in Toxicology, 2011, 24, 1113-1122.	1.7	28
62	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
63	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.	1.5	28
64	Design, Synthesis, and Biological Evaluation of 1,2-Dihydroisoquinolines as HIV-1 Integrase Inhibitors. ACS Medicinal Chemistry Letters, 2015, 6, 1065-1070.	1.3	28
65	Design, synthesis, and biological evaluation of benzo[d]imidazole-2-carboxamides as new anti-TB agents. Bioorganic Chemistry, 2021, 107, 104538.	2.0	28
66	Theoretical studies on the S?N interaction in sulfinamides. Journal of Physical Organic Chemistry, 2002, 15, 197-203.	0.9	27
67	Azine or hydrazone? The dilemma in amidinohydrazones. RSC Advances, 2015, 5, 55938-55947.	1.7	27
68	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.	2.0	27
69	Substituent and solvent effects on the rotational barriers in selenoamides: A theoretical study. Computational and Theoretical Chemistry, 2006, 759, 41-49.	1.5	26
70	Structure-Based Approaches in the Design of GSK-3 Selective Inhibitors. Current Protein and Peptide Science, 2007, 8, 352-364.	0.7	26
71	Enhanced noscapine delivery using estrogen-receptor-targeted nanoparticles for breast cancer therapy. Anti-Cancer Drugs, 2014, 25, 704-716.	0.7	26
72	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.	1.7	26

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73	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.	1.7	26
74	3D-QSAR studies of substituted 1-(3, 3-diphenylpropyl)-piperidinyl amides and ureas as CCR5 receptor antagonists. Journal of Molecular Modeling, 2007, 13, 519-529.	0.8	25
75	Modelling and Informatics in the Analysis of P. falciparum DHFR Enzyme Inhibitors. Current Medicinal Chemistry, 2008, 15, 1552-1569.	1.2	25
76	Possibility of the Existence of Donorâ€“Acceptor Interactions in Bis(azole)amines: An Electronic Structure Analysis. Journal of Organic Chemistry, 2014, 79, 4852-4862.	1.7	25
77	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.	1.7	25
78	Dienophilic Behavior of the Vinylic (CC) and the Carbonyl (CO) Bonds of Ketenes in Reactions with 1,3-Diazabuta-1,3-dienes. Organic Letters, 2000, 2, 2725-2728.	2.4	24
79	Drug metabolism. Resonance, 2014, 19, 259-282.	0.2	24
80	Regioselective [4+2] cycloaddition versus nucleophilic reactions of N-arylamino substituted 1,3-diaza-1,3-butadienes with ketenes: Synthesis of pyrimidinone and fused pyrimidinone derivatives. Part II. Tetrahedron, 1997, 53, 13829-13840.	1.0	23
81	New leads for selective GSK-3 inhibition: pharmacophore mapping and virtual screening studies. Journal of Computer-Aided Molecular Design, 2006, 20, 55-66.	1.3	23
82	Understanding selenocysteine through conformational analysis, proton affinities, acidities and bond dissociation energies. International Journal of Quantum Chemistry, 2008, 108, 983-991.	1.0	23
83	â€˜Sum of activitiesâ€™ as dependent parameter: A new CoMFA-based approach for the design of pan PPAR agonists. European Journal of Medicinal Chemistry, 2009, 44, 42-53.	2.6	23
84	Mechanism-Based Inactivation of Cytochromes by Furan Epoxide: Unraveling the Molecular Mechanism. Inorganic Chemistry, 2013, 52, 13496-13508.	1.9	23
85	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.	1.7	23
86	Shapeâ€•and Chemical Featureâ€Based 3Dâ€Pharmacophore Model Generation and Virtual Screening: Identification of Potential Leads for P.Âfalciparum DHFR Enzyme Inhibition. Chemical Biology and Drug Design, 2010, 75, 115-126.	1.5	22
87	S-Oxidation of Thiazolidinedione with Hydrogen Peroxide, Peroxynitrous Acid, and C4a-Hydroperoxyflavin: A Theoretical Study. Journal of Physical Chemistry A, 2011, 115, 891-898.	1.1	22
88	Tautomerism in drugs with benzimidazole carbamate moiety: an electronic structure analysis. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	22
89	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.	1.4	22
90	Carbene â†'N+ Coordination Bonds in Drugs: A Quantum Chemical Study. Journal of Chemical Sciences, 2016, 128, 1607-1614.	0.7	22

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91	Design, synthesis and biological evaluation of 4-aminoquinoline-guanylthiourea derivatives as antimalarial agents. Bioorganic Chemistry, 2019, 91, 103094.	2.0	22
92	3D-QSAR CoMFA Study on Oxindole Derivatives as Cyclin Dependent Kinase 1 (CDK1) and Cyclin Dependent Kinase 2 (CDK2) Inhibitors. Medicinal Chemistry, 2007, 3, 75-84.	0.7	21
93	A new colorimetric chemodosimeter for Hg2+ based on charge-transfer compound of N-methylpyrrole with TCNQ. Talanta, 2010, 83, 644-650.	2.9	21
94	A common feature-based 3D-pharmacophore model generation and virtual screening: identification of potential PfDHFR inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2010, 25, 635-645.	2.5	21
95	Design, synthesis and biological evaluation of novel unsymmetrical azines as quorum sensing inhibitors. RSC Advances, 2015, 5, 80027-80038.	1.7	21
96	Atomic level insights into realistic molecular models of dendrimer-drug complexes through MD simulations. Journal of Chemical Physics, 2016, 145, 124902.	1.2	21
97	Design and synthesis of novel Y-shaped barbituric acid derivatives as PPARÎ³ activators. European Journal of Medicinal Chemistry, 2016, 108, 423-435.	2.6	21
98	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.	1.7	21
99	Negative hyperconjugative interactions in S-nitrosothiols: a theoretical study. Tetrahedron Letters, 2002, 43, 8289-8291.	0.7	20
100	Electron Deficient Bridges Involving Silylenes:â€‰ A Theoretical Study. Inorganic Chemistry, 2003, 42, 4743-4749.	1.9	20
101	Identification of potential glycogen kinase-3 inhibitors by structure based virtual screening. Biophysical Chemistry, 2007, 128, 165-175.	1.5	20
102	Conformational Polymorphism in Sulfonylurea Drugs: Electronic Structure Analysis. Journal of Physical Chemistry B, 2010, 114, 11603-11611.	1.2	20
103	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.	1.1	20
104	Mechanistic insights into the bioactivation of phenacetin to reactive metabolites: A DFT study. Computational and Theoretical Chemistry, 2013, 1007, 48-56.	1.1	20
105	Theoretical studies on electron delocalisation in selenourea. Journal of Chemical Sciences, 2002, 114, 223-230.	0.7	19
106	Theoretical studies on the Sâ€“N interactions in sulfoximine. Tetrahedron, 2005, 61, 5633-5639.	1.0	19
107	A comparative study on the nature and strength of Oâ€“O, Sâ€“S, and Seâ€“Se bond. Computational and Theoretical Chemistry, 2007, 810, 31-37.	1.5	19
108	Minimum requirements of hydrophobic and hydrophilic features in cationic peptide antibiotics (CPAs): pharmacophore generation and validation with cationic steroid antibiotics (CSAs). Journal of Molecular Modeling, 2008, 14, 265-278.	0.8	19

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109	Tautomeric preferences and electron delocalization in biurets, thiobiurets, and dithiobiurets: Anab initiostudy. International Journal of Quantum Chemistry, 2008, 108, 1277-1286.	1.0	19
110	New PPARÎ³ ligands based on 2-hydroxy-1,4-naphthoquinone: Computer-aided design, synthesis, and receptor-binding studies. Bioorganic and Medicinal Chemistry Letters, 2008, 18, 3192-3195.	1.0	19
111	Electronic structure and reactivity of guanylthiourea: A quantum chemical study. Journal of Computational Chemistry, 2010, 31, 1259-1267.	1.5	18
112	Sulfonamide vs. sulfonimide: tautomerism and electronic structure analysis of N-heterocyclic arenesulfonamides. New Journal of Chemistry, 2017, 41, 8118-8129.	1.4	18
113	Mechanistic studies on the drug metabolism and toxicity originating from cytochromes P450. Drug Metabolism Reviews, 2020, 52, 366-394.	1.5	18
114	3D-QSAR studies of pyruvate dehydrogenase kinase inhibitors based on a divide and conquer strategy. Bioorganic and Medicinal Chemistry, 2004, 12, 2709-2715.	1.4	17
115	Amide resonance in thio- and seleno- carbamates: A theoretical study. Computational and Theoretical Chemistry, 2005, 757, 149-153.	1.5	17
116	Design, synthesis, biological evaluation and toxicity studies of N,N-disubstituted biguanides as quorum sensing inhibitors. Medicinal Chemistry Research, 2015, 24, 1974-1987.	1.1	17
117	Studies on some glitazones having pyridine as the linker unit. Bioorganic and Medicinal Chemistry, 2004, 12, 655-662.	1.4	16
118	3D-QSAR analysis of cycloguanil derivatives as inhibitors of A16V+S108T mutant Plasmodium falciparum dihydrofolate reductase enzyme. Journal of Molecular Graphics and Modelling, 2009, 28, 357-367.	1.3	16
119	Guanylthiourea derivatives as potential antimalarial agents: Synthesis, inÂvivo and molecular modelling studies. European Journal of Medicinal Chemistry, 2017, 135, 339-348.	2.6	16
120	Drug-dendrimer complexes and conjugates: Detailed furtherance through theory and experiments. Advances in Colloid and Interface Science, 2022, 303, 102639.	7.0	16
121	Metformin and glitazones: does similarity in biomolecular mechanism originate from tautomerism in these drugs?. Journal of Physical Organic Chemistry, 2008, 21, 30-33.	0.9	15
122	Important pharmacophoric features of pan PPAR agonists: Common chemical feature analysis and virtual screening. European Journal of Medicinal Chemistry, 2009, 44, 3488-3495.	2.6	15
123	Metalâ€free Intermolecular Hydrophenoxylation of Aryl Alkynes. Asian Journal of Organic Chemistry, 2016, 5, 213-221.	1.3	15
124	Integration of oxidative arylation with sulfonyl migration: one-pot tandem synthesis of densely functionalized (NH)-pyrroles. New Journal of Chemistry, 2017, 41, 8791-8803.	1.4	15
125	Comparative molecular similarity indices analysis (CoMSIA) studies of 1,2-naphthoquinone derivatives as PTP1B inhibitors. Bioorganic and Medicinal Chemistry, 2005, 13, 2331-2338.	1.4	14
126	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.	1.5	14

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127	Theoretical investigations on R(O)nSâ€“NO (n=0,1,2) systems. Tetrahedron, 2004, 60, 4801-4805.	1.0	13
128	Selectivity criterion for pyrazolo[3,4-b]pyrid[az]ine derivatives as GSK-3 inhibitors: CoMFA and molecular docking studies. European Journal of Medicinal Chemistry, 2008, 43, 949-957.	2.6	13
129	Complexâ€Induced Proximity Effect in the Regioselective Lithiation of Pyridine Derivatives. European Journal of Organic Chemistry, 2012, 2012, 1746-1752.	1.2	13
130	Importance of hydrophobic parameters in identifying appropriate pose of CYP substrates in cytochromes. European Journal of Medicinal Chemistry, 2014, 71, 15-23.	2.6	13
131	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.	1.1	13
132	CÂâ†'ÂN coordination bonds in (CCC)Ââ†'ÂN + Ââ†Â(L) complexes. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	13
133	Ring-chain isomerism in conjugated guanylhydrazones: Experimental and theoretical study. Tetrahedron, 2018, 74, 2857-2864.	1.0	13
134	Reactive Metabolites from Thiazole-Containing Drugs: Quantum Chemical Insights into Biotransformation and Toxicity. Chemical Research in Toxicology, 2021, 34, 1503-1517.	1.7	13
135	3D-QSAR CoMFA Study on Aminothiazole Derivatives as Cyclin-Dependent Kinase 2 Inhibitors. QSAR and Combinatorial Science, 2007, 26, 85-91.	1.5	12
136	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.	1.5	12
137	Nitro â‡Œ aci-nitro tautomerism and E/Z isomeric preferences of nitroethenediamine derivatives: a quantum chemical study. RSC Advances, 2013, 3, 25268.	1.7	12
138	Synthesis, biological evaluation, and molecular modeling studies of novel heterocyclic compounds as anti-proliferative agents. Medicinal Chemistry Research, 2013, 22, 5654-5669.	1.1	12
139	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.	2.3	12
140	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.	1.6	12
141	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.	1.6	12
142	Seâ€“N interactions in selenohydroxylamine: a theoretical study. Perkin Transactions II RSC, 2000, , 2469-2474.	1.1	11
143	Theoretical studies on the conformational preferences of 1,3-diazabuta-1,3-dienes. Computational and Theoretical Chemistry, 2003, 640, 1-12.	1.5	11
144	Electronic structure ofN-sulfenylimines. Journal of Physical Organic Chemistry, 2003, 16, 183-188.	0.9	11

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145	Potential energy surface of thionylimide. International Journal of Quantum Chemistry, 2006, 106, 1237-1249.	1.0	11
146	Investigation of Potential Glycogen Synthase Kinase 3 Inhibitors Using Pharmacophore Mapping and Virtual Screening. Chemical Biology and Drug Design, 2006, 68, 154-165.	1.5	11
147	Synthesis, in vitro and in silico evaluation of l-tyrosine containing PPARÎ±/Î³ dual agonists. Bioorganic and Medicinal Chemistry, 2007, 15, 1547-1555.	1.4	11
148	CoMFA analysis of dual/multiple PPAR activators. European Journal of Medicinal Chemistry, 2008, 43, 2784-2791.	2.6	11
149	3-Formylchromone based topoisomerase IIÎ± inhibitors: discovery of potent leads. MedChemComm, 2013, 4, 1257.	3.5	11
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