

Devesh Kumar

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122
papers

7,637
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h-index

86
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131
ext. papers

8,184
ext. citations

7.8
avg, IF

5.88
L-index

#	Paper	IF	Citations
122	Theoretical perspective on the structure and mechanism of cytochrome P450 enzymes. <i>Chemical Reviews</i> , 2005 , 105, 2279-328	68.1	999
121	P450 enzymes: their structure, reactivity, and selectivity-modeled by QM/MM calculations. <i>Chemical Reviews</i> , 2010 , 110, 949-1017	68.1	791
120	Reactivity of high-valent iron-oxo species in enzymes and synthetic reagents: a tale of many states. <i>Accounts of Chemical Research</i> , 2007 , 40, 532-42	24.3	454
119	Two-state reactivity in alkane hydroxylation by non-heme iron-oxo complexes. <i>Journal of the American Chemical Society</i> , 2006 , 128, 8590-606	16.4	308
118	A valence bond modeling of trends in hydrogen abstraction barriers and transition states of hydroxylation reactions catalyzed by cytochrome P450 enzymes. <i>Journal of the American Chemical Society</i> , 2008 , 130, 10128-40	16.4	213
117	External electric field will control the selectivity of enzymatic-like bond activations. <i>Journal of the American Chemical Society</i> , 2004 , 126, 11746-9	16.4	201
116	A predictive pattern of computed barriers for C-h hydroxylation by compound I of cytochrome p450. <i>Journal of the American Chemical Society</i> , 2004 , 126, 8362-3	16.4	195
115	Theoretical study on the mechanism of the oxygen activation process in cysteine dioxygenase enzymes. <i>Journal of the American Chemical Society</i> , 2011 , 133, 3869-82	16.4	174
114	Theoretical investigation of C-H hydroxylation by (N4Py)Fe(IV)=O(2+): an oxidant more powerful than P450?. <i>Journal of the American Chemical Society</i> , 2005 , 127, 8026-7	16.4	172
113	What factors influence the rate constant of substrate epoxidation by compound I of cytochrome P450 and analogous iron(IV)-oxo oxidants?. <i>Journal of the American Chemical Society</i> , 2010 , 132, 7656-67	16.4	155
112	Active species of horseradish peroxidase (HRP) and cytochrome P450: two electronic chameleons. <i>Journal of the American Chemical Society</i> , 2003 , 125, 15779-88	16.4	153
111	Two states and two more in the mechanisms of hydroxylation and epoxidation by cytochrome P450. <i>Journal of the American Chemical Society</i> , 2005 , 127, 13007-18	16.4	146
110	The Rebound Controversy—An Overview and Theoretical Modeling of the Rebound Step in C _H Hydroxylation by Cytochrome P450. <i>European Journal of Inorganic Chemistry</i> , 2004 , 2004, 207-226	2.3	138
109	Radical clock substrates, their C-H hydroxylation mechanism by cytochrome P450, and other reactivity patterns: what does theory reveal about the clocks' behavior?. <i>Journal of the American Chemical Society</i> , 2004 , 126, 1907-20	16.4	138
108	Quantum mechanics/molecular mechanics study on the oxygen binding and substrate hydroxylation step in AlkB repair enzymes. <i>Chemistry - A European Journal</i> , 2014 , 20, 435-46	4.8	104
107	Theoretical study of N-demethylation of substituted N,N-dimethylanilines by cytochrome P450: the mechanistic significance of kinetic isotope effect profiles. <i>Journal of Physical Chemistry B</i> , 2007 , 111, 7700-10	3.4	103
106	Multistate reactivity in styrene epoxidation by compound I of cytochrome p450: mechanisms of products and side products formation. <i>Chemistry - A European Journal</i> , 2005 , 11, 2825-35	4.8	101

105	Drug metabolism by cytochrome p450 enzymes: what distinguishes the pathways leading to substrate hydroxylation over desaturation?. <i>Chemistry - A European Journal</i> , 2015 , 21, 9083-92	4.8	100
104	Long-range electron transfer triggers mechanistic differences between iron(IV)-oxo and iron(IV)-imido oxidants. <i>Journal of the American Chemical Society</i> , 2014 , 136, 17102-15	16.4	93
103	Reactivity patterns of cytochrome P450 enzymes: multifunctionality of the active species, and the two states-two oxidants conundrum. <i>Natural Product Reports</i> , 2007 , 24, 533-52	15.1	89
102	Characterization of manganese(V)-oxo polyoxometalate intermediates and their properties in oxygen-transfer reactions. <i>Journal of the American Chemical Society</i> , 2006 , 128, 15451-60	16.4	89
101	A comprehensive test set of epoxidation rate constants for iron(IV)-oxo porphyrin cation radical complexes. <i>Chemical Science</i> , 2015 , 6, 1516-1529	9.4	88
100	The high-valent iron-oxo species of polyoxometalate, if it can be made, will be a highly potent catalyst for C-H hydroxylation and double-bond epoxidation. <i>Journal of the American Chemical Society</i> , 2005 , 127, 17712-8	16.4	87
99	How does product isotope effect prove the operation of a two-state "rebound" mechanism in C-H hydroxylation by cytochrome P450?. <i>Journal of the American Chemical Society</i> , 2003 , 125, 13024-5	16.4	86
98	One oxidant, many pathways: a theoretical perspective of monooxygenation mechanisms by cytochrome P450 enzymes. <i>Journal of Biological Inorganic Chemistry</i> , 2004 , 9, 661-8	3.7	81
97	Comparison of the reactivity of nonheme iron(IV)-oxo versus iron(IV)-imido complexes: which is the better oxidant?. <i>Angewandte Chemie - International Edition</i> , 2013 , 52, 12288-92	16.4	79
96	Effect of the axial ligand on substrate sulfoxidation mediated by iron(IV)-oxo porphyrin cation radical oxidants. <i>Chemistry - A European Journal</i> , 2011 , 17, 6196-205	4.8	79
95	Origin of the Enhanced Reactivity of π -Nitrido-Bridged Diiron(IV)-Oxo Porphyrinoid Complexes over Cytochrome P450 Compound I. <i>ACS Catalysis</i> , 2016 , 6, 2230-2243	13.1	75
94	Kinetic isotope effect is a sensitive probe of spin state reactivity in C-H hydroxylation of N,N-dimethylaniline by cytochrome P450. <i>Journal of the American Chemical Society</i> , 2006 , 128, 394-5	16.4	75
93	Theory favors a stepwise mechanism of porphyrin degradation by a ferric hydroperoxide model of the active species of heme oxygenase. <i>Journal of the American Chemical Society</i> , 2005 , 127, 8204-13	16.4	74
92	Sulfoxidation mechanisms catalyzed by cytochrome P450 and horseradish peroxidase models: spin selection induced by the ligand. <i>Biochemistry</i> , 2005 , 44, 8148-58	3.2	68
91	Oxygen economy of cytochrome P450: what is the origin of the mixed functionality as a dehydrogenase-oxidase enzyme compared with its normal function?. <i>Journal of the American Chemical Society</i> , 2004 , 126, 5072-3	16.4	67
90	Effect of porphyrin ligands on the regioselective dehydrogenation versus epoxidation of olefins by oxoiron(IV) mimics of cytochrome P450. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 11713-22	2.8	66
89	Rationalization of the barrier height for p-Z-styrene epoxidation by iron(IV)-oxo porphyrin cation radicals with variable axial ligands. <i>Inorganic Chemistry</i> , 2013 , 52, 7968-79	5.1	63
88	Nonheme ferric hydroperoxo intermediates are efficient oxidants of bromide oxidation. <i>Chemical Communications</i> , 2011 , 47, 11044-6	5.8	63

87	Computer-generated high-valent iron--oxo and manganese--oxo species with polyoxometalate ligands: how do they compare with the iron--oxo active species of heme enzymes?. <i>Angewandte Chemie - International Edition</i> , 2004 , 43, 5661-5	16.4	63
86	Gauging the relative oxidative powers of compound I, ferric-hydroperoxide, and the ferric-hydrogen peroxide species of cytochrome P450 toward C-H hydroxylation of a radical clock substrate. <i>Journal of the American Chemical Society</i> , 2006 , 128, 473-84	16.4	60
85	Comparison of computational methods to model DNA minor groove binders. <i>Journal of Chemical Information and Modeling</i> , 2011 , 51, 558-71	6.1	57
84	How do aldehyde side products occur during alkene epoxidation by cytochrome P450? Theory reveals a state-specific multi-state scenario where the high-spin component leads to all side products. <i>Journal of Inorganic Biochemistry</i> , 2004 , 98, 1183-93	4.2	57
83	The intrinsic axial ligand effect on propene oxidation by horseradish peroxidase versus cytochrome P450 enzymes. <i>Journal of Biological Inorganic Chemistry</i> , 2005 , 10, 181-9	3.7	56
82	Axial ligand effect on the rate constant of aromatic hydroxylation by iron(IV)-oxo complexes mimicking cytochrome P450 enzymes. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 718-30	3.4	55
81	Porphyrin traps its terminator! Concerted and stepwise porphyrin degradation mechanisms induced by heme-oxygenase and cytochrome p450. <i>Angewandte Chemie - International Edition</i> , 2004 , 43, 1129-32	16.4	55
80	Deformylation Reaction by a Nonheme Manganese(III)-Peroxo Complex via Initial Hydrogen-Atom Abstraction. <i>Angewandte Chemie - International Edition</i> , 2016 , 55, 11091-5	16.4	55
79	A Systematic Account on Aromatic Hydroxylation by a Cytochrome P450 Model Compound I: A Low-Pressure Mass Spectrometry and Computational Study. <i>Chemistry - A European Journal</i> , 2016 , 22, 18608-18619	4.8	54
78	Keto-Enol Tautomerization Triggers an Electrophilic Aldehyde Deformylation Reaction by a Nonheme Manganese(III)-Peroxo Complex. <i>Journal of the American Chemical Society</i> , 2017 , 139, 18328-18338	16.4	51
77	How is the reactivity of cytochrome P450cam affected by Thr252X mutation? A QM/MM study for X = serine, valine, alanine, glycine. <i>Journal of the American Chemical Society</i> , 2009 , 131, 4755-63	16.4	50
76	New features in the catalytic cycle of cytochrome P450 during the formation of compound I from compound 0. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 19946-51	3.4	50
75	Generation of a high-valent iron imido corrolazine complex and NR group transfer reactivity. <i>Inorganic Chemistry</i> , 2013 , 52, 4668-82	5.1	49
74	Inversion of enantioselectivity of a mononuclear non-heme iron(II)-dependent hydroxylase by tuning the interplay of metal-center geometry and protein structure. <i>Angewandte Chemie - International Edition</i> , 2013 , 52, 9677-81	16.4	45
73	Multireference ab initio quantum mechanics/molecular mechanics study on intermediates in the catalytic cycle of cytochrome P450(cam). <i>Journal of Physical Chemistry A</i> , 2008 , 112, 12904-10	2.8	42
72	Formation of the active species of cytochrome p450 by using iodosylbenzene: a case for spin-selective reactivity. <i>Chemistry - A European Journal</i> , 2007 , 13, 4103-15	4.8	42
71	Proton-shuffle mechanism of O-O activation for formation of a high-valent oxo-iron species of bleomycin. <i>Journal of the American Chemical Society</i> , 2006 , 128, 16148-58	16.4	41
70	Mechanistic insight into halide oxidation by non-heme iron complexes. Haloperoxidase versus halogenase activity. <i>Chemical Communications</i> , 2013 , 49, 10926-8	5.8	36

69	Steric factors override thermodynamic driving force in regioselectivity of proline hydroxylation by prolyl-4-hydroxylase enzymes. <i>Journal of Physical Chemistry A</i> , 2010 , 114, 13234-43	2.8	36
68	In silico design of a mutant of cytochrome P450 containing selenocysteine. <i>Journal of the American Chemical Society</i> , 2006 , 128, 2649-53	16.4	35
67	Mechanism of S-oxygenation by a cysteine dioxygenase model complex. <i>Journal of Physical Chemistry A</i> , 2012 , 116, 582-91	2.8	33
66	Catalysts for monooxygenations made from polyoxometalate: an iron(V)-oxo derivative of the Lindqvist anion. <i>Inorganic Chemistry</i> , 2006 , 45, 8655-63	5.1	29
65	Hydrogen by Deuterium Substitution in an Aldehyde Tunes the Regioselectivity by a Nonheme Manganese(III)-Peroxo Complex. <i>Angewandte Chemie - International Edition</i> , 2019 , 58, 10639-10643	16.4	27
64	Water as biocatalyst in cytochrome P450. <i>Faraday Discussions</i> , 2011 , 148, 373-83; discussion 421-41	3.6	27
63	Electronic properties of pentacoordinated heme complexes in cytochrome P450 enzymes: search for an Fe(II) oxidation state. <i>Physical Chemistry Chemical Physics</i> , 2009 , 11, 10219-26	3.6	27
62	A Density Functional Study of the Factors That Influence the Regioselectivity of Toluene Hydroxylation by Cytochrome P450 Enzymes. <i>European Journal of Inorganic Chemistry</i> , 2007 , 2007, 2966-2974	2.3	27
61	On the identity and reactivity patterns of the "second oxidant" of the T252A mutant of cytochrome P450cam in the oxidation of 5-methylenenylcamphor. <i>Journal of Inorganic Biochemistry</i> , 2006 , 100, 2054-63	4.3	26
60	Interplay Between Steric and Electronic Effects: A Joint Spectroscopy and Computational Study of Nonheme Iron(IV)-Oxo Complexes. <i>Chemistry - A European Journal</i> , 2019 , 25, 5086-5098	4.8	25
59	Ferromagnetic bonding: high spin copper clusters (n+1)Cu(n); n = 2-14 devoid of electron pairs but possessing strong bonding. <i>Journal of Physical Chemistry A</i> , 2006 , 110, 8510-8	2.8	24
58	Comparison of the Reactivity of Nonheme Iron(IV)Oxo versus Iron(IV)Imido Complexes: Which is the Better Oxidant?. <i>Angewandte Chemie</i> , 2013 , 125, 12514-12518	3.6	23
57	Pyrazolo[3,4-d]pyrimidines as novel inhibitors of O-acetyl-L-serine sulfhydrylase of <i>Entamoeba histolytica</i> : an in silico study. <i>Journal of Molecular Modeling</i> , 2015 , 21, 96	2	22
56	Oxidative properties of a nonheme Ni(II)(O ₂) complex: Reactivity patterns for C-H activation, aromatic hydroxylation and heteroatom oxidation. <i>Chemical Communications</i> , 2011 , 47, 10674-6	5.8	22
55	Dramatic rate-enhancement of oxygen atom transfer by an iron(IV)-oxo species by equatorial ligand field perturbations. <i>Dalton Transactions</i> , 2018 , 47, 14945-14957	4.3	21
54	Synthesis and ligand non-innocence of thiolate-ligated (N4S) Iron(II) and nickel(II) bis(imino)pyridine complexes. <i>Inorganic Chemistry</i> , 2013 , 52, 10467-80	5.1	20
53	Singlet diradical character of an oxidized ruthenium trithiolate: electronic structure and reactivity. <i>Angewandte Chemie - International Edition</i> , 2007 , 46, 4085-8	16.4	20
52	Structure and mechanism leading to formation of the cysteine sulfinic acid product complex of a biomimetic cysteine dioxygenase model. <i>Chemistry - A European Journal</i> , 2015 , 21, 7470-9	4.8	19

51	The Electronic Structure of Reduced Phosphovanadomolybdates and the Implications on Their Use in Catalytic Oxidation Initiated by Electron Transfer. <i>Journal of Physical Chemistry C</i> , 2007 , 111, 7711-7719	3.8	19
50	Deformylation Reaction by a Nonheme Manganese(III) Peroxo Complex via Initial Hydrogen-Atom Abstraction. <i>Angewandte Chemie</i> , 2016 , 128, 11257-11261	3.6	17
49	Adsorption of small gas molecules on pure and Al-doped graphene sheet: a quantum mechanical study. <i>Bulletin of Materials Science</i> , 2017 , 40, 1263-1271	1.7	16
48	Axial and equatorial ligand effects on biomimetic cysteine dioxygenase model complexes. <i>Organic and Biomolecular Chemistry</i> , 2012 , 10, 5401-9	3.9	16
47	Diheme Cytochrome c: Structure-Function Correlation and Effect of Heme-Heme Interactions. <i>Inorganic Chemistry</i> , 2018 , 57, 11498-11510	5.1	15
46	Hydrogen by Deuterium Substitution in an Aldehyde Tunes the Regioselectivity by a Nonheme Manganese(III) Peroxo Complex. <i>Angewandte Chemie</i> , 2019 , 131, 10749-10753	3.6	13
45	A Hemilabile Palladium-Carbon Bond: Characterization and Its Implication in Catalysis. <i>Organometallics</i> , 2014 , 33, 3243-3246	3.8	13
44	Inversion of Enantioselectivity of a Mononuclear Non-Heme Iron(II)-dependent Hydroxylase by Tuning the Interplay of Metal-Center Geometry and Protein Structure. <i>Angewandte Chemie</i> , 2013 , 125, 9859-9863	3.6	13
43	QM/MM study of the second proton transfer in the catalytic cycle of the D251N mutant of cytochrome P450cam. <i>Journal of Physical Chemistry B</i> , 2009 , 113, 9577-88	3.4	13
42	Assessing therapeutic potential of molecules: molecular property diagnostic suite for tuberculosis (MPDS^{TB}). <i>Journal of Chemical Sciences</i> , 2017 , 129, 515-531	1.8	12
41	An antimony(V) substituted Keggin heteropolyacid, H ₄ PSbMo ₁₁ O ₄₀ : Why is its catalytic activity in oxidation reactions so different from that of H ₄ PVMO ₁₁ O ₄₀ ?. <i>Journal of Molecular Catalysis A</i> , 2012 , 356, 152-157		12
40	Coupling and uncoupling mechanisms in the methoxythreonine mutant of cytochrome P450cam: a quantum mechanical/molecular mechanical study. <i>Journal of Biological Inorganic Chemistry</i> , 2010 , 15, 361-72	3.7	12
39	On copper-copper bond in hydrated cupric acetate. <i>Computational and Theoretical Chemistry</i> , 2015 , 1061, 1-5	2	10
38	Porphyrim Traps Its Terminator! Concerted and Stepwise Porphyrim Degradation Mechanisms Induced by Heme-Oxygenase and Cytochrome P450. <i>Angewandte Chemie</i> , 2004 , 116, 1149-1152	3.6	10
37	Computer-Generated High-Valent Iron-Oxo and Manganese-Oxo Species with Polyoxometalate Ligands: How do they Compare with the Iron-Oxo Active Species of Heme Enzymes?. <i>Angewandte Chemie</i> , 2004 , 116, 5779-5783	3.6	9
36	Polarizability study of nematic liquid crystal 4-cyano-4'-pentylbiphenyl (5CB) and its nitrogen derivatives. <i>Chemical Physics</i> , 2015 , 456, 41-46	2.3	8
35	Molecular spectroscopy and adverse optical properties of N-(p-hexyloxy-benzylidene)- β -toluidine (HBT) liquid crystal molecule studied by DFT methodology. <i>IOP SciNotes</i> , 2020 , 1, 015202	1.2	6
34	Even-odd effect of the homologous series of nCHBT liquid crystal molecules under the influence of an electric field: A theoretical approach 2020 , 94, 1		6

33	A copper(II) complex with a Cu-S bond. Attenuated total reflectance, electron paramagnetic resonance, resonance Raman and atoms-in-molecule calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015 , 151, 96-9	4.4	5
32	Odd-even effect of 70 nm liquid crystal compound series studied under the effect of the electric field by density functional theory (DFT) methods. <i>European Physical Journal Plus</i> , 2020 , 135, 1	3.1	5
31	Properties and reactivities of nonheme iron(IV)-oxo versus iron(V)-oxo: long-range electron transfer versus hydrogen atom abstraction. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 22611-22	3.6	5
30	Odd-even Effect in a Homologous Series of 4-n-Alkylbenzoic Acids: Role of Anisotropic Pair Potential. <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , 2002 , 57, 189-193	1.4	5
29	A Trimetal Carbene with Reactivity Reminiscent of Fischer-Tropsch Catalysis. <i>Organometallics</i> , 2015 , 34, 1651-1660	3.8	4
28	Effective optical properties of the one-dimensional periodic structure of (hbox {TiO}_{2}) and (hbox {SiO}_{2}) layers with a defect layer of nanocomposite consisting of silver nanoparticle and E7 liquid crystal 2019 , 93, 1		4
27	Singlet Diradical Character of an Oxidized Ruthenium Trithiolate: Electronic Structure and Reactivity. <i>Angewandte Chemie</i> , 2007 , 119, 4163-4166	3.6	4
26	Drug Metabolism by Cytochrome P450 Enzymes: What Distinguishes the Pathways Leading to Substrate Hydroxylation Over Desaturation?. <i>Chemistry - A European Journal</i> , 2015 , 21, 8973-8973	4.8	3
25	Order of a Thermotropic Mesogen: HCCPP-A Statistical Study Based on Quantum Mechanics and Computer Simulation. <i>Molecular Crystals and Liquid Crystals</i> , 2002 , 378, 65-75	0.5	3
24	A comparative ab initio study on structural evolution, stability and electronic properties of undoped and Al-doped GaN _x (x + y = 4-25 clusters. <i>European Physical Journal Plus</i> , 2017 , 132, 1	3.1	2
23	Theoretical Perspective on the Structure and Mechanism of Cytochrome P450 Enzymes. <i>ChemInform</i> , 2005 , 36, no		2
22	Molecular Organization in a Nematogen: PBPCN -A Computational Analysis Based on Quantum Mechanics. <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , 2001 , 56, 730-734	1.4	2
21	Effect of Reaction Temperature on Shape Evolution of Palladium Nanoparticles and Their Cytotoxicity against A-549 Lung Cancer Cells. <i>ACS Omega</i> , 2019 , 4, 21839-21847	3.9	2
20	Tunable transmission of a nematic liquid crystal as defect in a 1D periodic structure of dielectric materials by orientation and re-orientation of liquid crystal molecules. <i>European Physical Journal E</i> , 2018 , 41, 100	1.5	2
19	Electro-optical odd-even effect of APAPA liquid crystal molecules studied under the influence of an extraneous electric field (THz): A theoretical approach. <i>Journal of Molecular Liquids</i> , 2020 , 318, 114254	6	1
18	Interplay between two spin states determines the hydroxylation catalyzed by P monooxygenase from <i>Trichoderma brevicompactum</i> . <i>Journal of Computational Chemistry</i> , 2020 , 41, 1330-1336	3.5	1
17	Correlation of mesogenic properties with intermolecular interaction energy for homologous series of HnCBP. <i>Molecular Crystals and Liquid Crystals</i> , 2017 , 652, 51-66	0.5	1
16	Molecular spectroscopy and electro-optical effect of I52 liquid crystal molecules studied under the influence of an external electric field (THz): a theoretical approach. <i>Journal of Molecular Modeling</i> , 2021 , 27, 11	2	1

15	A theoretical investigation of nonlinear optical and electronic molecular parameters of hexabutyloxytryphenylene and halogenated hexabutyloxytryphenylene molecules using density functional theory (DFT) for nonlinear device applications. <i>Physica Scripta</i> , 2022 , 97, 065808	2.6	1
14	Ferromagnetic Coupling in Oxidovanadium(IV)-Porphyrin Radical Dimers. <i>Inorganic Chemistry</i> , 2021 , 60, 16492-16506	5.1	0
13	Metabolism of 8-aminoquinoline (8AQ) Primaquine via aromatic hydroxylation step mediated by Cytochrome P450 enzyme using Density Functional Theory. <i>Journal of Organometallic Chemistry</i> , 2021 , 957, 122154	2.3	0
12	Interaction of modified nucleic bases with graphene and doped graphenes: a DFT study. <i>Bulletin of Materials Science</i> , 2020 , 43, 1	1.7	0
11	Interplay between two degenerate spin state determines the hydroxylation of 4-nitrophenol catalyzed via Cytochrome P450. <i>Inorganic Chemistry Communication</i> , 2021 , 132, 108857	3.1	0
10	Biotransformation of BPA via epoxidation catalyzed by Cytochrome P450. <i>Inorganic Chemistry Communication</i> , 2022 , 139, 109321	3.1	0
9	A tribute to Sason Shaik. <i>Journal of Physical Chemistry A</i> , 2008 , 112, 12721-3	2.8	
8	Molecular Ordering of a Nematogen at Phase Transition Temperature - A Theoretical Study. <i>Phase Transitions</i> , 2002 , 75, 621-629	1.3	
7	Smectogenic Behaviour of 7O.6 at it's Phase Transition Temperature: A Computational Analysis Reprint request to. <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , 2001 , 56, 873-878	1.4	
6	A comparative study of crystal packing vs. conformational energy of N-acetyl-2,3-didehydroproline. <i>International Journal of Quantum Chemistry</i> , 1995 , 55, 71-74	2.1	
5	Effect of annealing temperature on the spectroscopic and photoluminescence properties of CdO-ZnO nanocomposites. <i>Journal of Modern Optics</i> , 2020 , 67, 1410-1415	1.1	
4	Scavenging of OH and OOH radicals by polyradicals of small polycyclic aromatic hydrocarbons. <i>Journal of Molecular Modeling</i> , 2021 , 27, 112	2	
3	DFT-based numerical study of the re-entrant phase and optical parameters of the homologous series of MBC liquid crystal molecules studied under the influence of an electric field. <i>Bulletin of Materials Science</i> , 2021 , 44, 1	1.7	
2	Modeling the hydroxylation of estragole via human liver cytochrome P450. <i>Journal of Molecular Modeling</i> , 2021 , 27, 199	2	
1	Interplay Between Theory and Experiment: A Future Approach for Biomedical Research 2022 , 41-67		