Sam P De Visser

List of Publications by Year in Descending Order

271 papers	15,251 citations	66 h-index	114 g-index
292 ext. papers	16,717 ext. citations	7.9 avg, IF	7.03 L-index

#	Paper	IF	Citations
271	Cluster Model Study into the Catalytic Mechanism of □Ketoglutarate Biodegradation by the Ethylene-Forming Enzyme Reveals Structural Differences with Nonheme Iron Hydroxylases. *ACS Catalysis*, **2022**, 12, 3923-3937	13.1	0
270	Mechanism of substrate inhibition in cytochrome-c dependent NO reductases from denitrifying bacteria (cNORs).. *Journal of Inorganic Biochemistry*, **2022**, 231, 111781	4.2	1
269	Electrostatic perturbations in the substrate-binding pocket of taurine/□ketoglutarate dioxygenase determine its selectivity.. *Chemistry - A European Journal*, **2021**,	4.8	2
268	Mechanism of Oxidative Ring-Closure as Part of the Hygromycin Biosynthesis Step by a Nonheme Iron Dioxygenase. *ChemCatChem*, **2021**, 13, 3054-3066	5.2	6
267	A Noncanonical Tryptophan Analogue Reveals an Active Site Hydrogen Bond Controlling Ferryl Reactivity in a Heme Peroxidase. *Jacs Au*, **2021**, 1, 913-918		1
266	Substrate sulfoxidation by a biomimetic cytochrome P450 Compound I mimic: How do porphyrin and phthalocyanine equatorial ligands compare?. *Journal of Chemical Sciences*, **2021**, 133, 1	1.8	1
265	Electrostatic Perturbations from the Protein Affect C-H Bond Strengths of the Substrate and Enable Negative Catalysis in the TmpA Biosynthesis Enzyme. *Chemistry - A European Journal*, **2021**, 27, 8851-8864	4.8	8
264	pH Changes That Induce an Axial Ligand Effect on Nonheme Iron(IV) Oxo Complexes with an Appended Aminopropyl Functionality. *Inorganic Chemistry*, **2021**, 60, 13821-13832	5.1	
263	Energy-entropy method using multiscale cell correlation to calculate binding free energies in the SAMPL8 host-guest challenge. *Journal of Computer-Aided Molecular Design*, **2021**, 35, 911-921	4.2	3
262	A comprehensive insight into aldehyde deformylation: mechanistic implications from biology and chemistry. *Organic and Biomolecular Chemistry*, **2021**, 19, 1879-1899	3.9	9
261	What Determines the Selectivity of Arginine Dihydroxylation by the Nonheme Iron Enzyme OrfP?. *Chemistry - A European Journal*, **2021**, 27, 1795-1809	4.8	14
260	Theoretical studies unveil the unusual bonding in oxygenation reactions involving cobalt(ii)-iodylarene complexes. *Chemical Communications*, **2021**, 57, 3115-3118	5.8	1
259	How Do Electrostatic Perturbations of the Protein Affect the Bifurcation Pathways of Substrate Hydroxylation versus Desaturation in the Nonheme Iron-Dependent Viomycin Biosynthesis Enzyme?. *Journal of Physical Chemistry A*, **2021**, 125, 1720-1737	2.8	13
258	Glutarate Hydroxylation by the Carbon Starvation-Induced Protein D: A Computational Study into the Stereo- and Regioselectivities of the Reaction. *Inorganic Chemistry*, **2021**, 60, 4800-4815	5.1	7
257	Product Distributions of Cytochrome P450 OleT with Phenyl-Substituted Fatty Acids: A Computational Study. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	2
256	Inspiration from Nature: Influence of Engineered Ligand Scaffolds and Auxiliary Factors on the Reactivity of Biomimetic Oxidants. *ACS Catalysis*, **2021**, 11, 9761-9797	13.1	8
255	Negative catalysis / non-Bell-Evans-Polanyi reactivity by metalloenzymes: Examples from mononuclear heme and non-heme iron oxygenases. *Coordination Chemistry Reviews*, **2021**, 439, 213914	23.2	9

254	Structure and Functional Differences of Cysteine and 3-Mercaptopropionate Dioxygenases: A Computational Study. *Chemistry - A European Journal*, **2021**, 27, 13793-13806	4.8	3
253	Proton-coupled electron transfer reactivities of electronically divergent heme superoxide intermediates: a kinetic, thermodynamic, and theoretical study. *Chemical Science*, **2021**, 12, 8872-8883	9.4	3
252	How external perturbations affect the chemoselectivity of substrate activation by cytochrome P450 OleT. *Physical Chemistry Chemical Physics*, **2020**, 22, 27178-27190	3.6	7
251	Bioengineering of Cytochrome P450 OleT: How Does Substrate Positioning Affect the Product Distributions?. *Molecules*, **2020**, 25,	4.8	10
250	Computational Study on O□D Bond Formation on a Mononuclear Non-Heme Iron Center. *European Journal of Inorganic Chemistry*, **2020**, 2020, 2573-2581	2.3	1
249	Cross-linking of aromatic phenolate groups by cytochrome P450 enzymes: a model for the biosynthesis of vancomycin by OxyB. *Organic and Biomolecular Chemistry*, **2020**, 18, 4610-4618	3.9	5
248	Comparison of Free-Energy Methods to Calculate the Barriers for the Nucleophilic Substitution of Alkyl Halides by Hydroxide. *Journal of Physical Chemistry B*, **2020**, 124, 6835-6842	3.4	4
247	Lignin Biodegradation by a Cytochrome P450 Enzyme: A Computational Study into Syringol Activation by GcoA. *Chemistry - A European Journal*, **2020**, 26, 13093-13102	4.8	14
246	Computational studies of DNA base repair mechanisms by nonheme iron dioxygenases: selective epoxidation and hydroxylation pathways. *Dalton Transactions*, **2020**, 49, 4266-4276	4.3	13
245	O Activation by Non-Heme Thiolate-Based Dinuclear Fe Complexes. *Inorganic Chemistry*, **2020**, 59, 3249-3259	5.1	8
244	Sluggish reactivity by a nonheme iron(iv)-tosylimido complex as compared to its oxo analogue. *Dalton Transactions*, **2020**, 49, 5921-5931	4.3	8
243	How Does Replacement of the Axial Histidine Ligand in Cytochrome Peroxidase by N-Methyl Histidine Affect Its Properties and Functions? A Computational Study. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	2
242	Can a Mononuclear Iron(III)-Superoxo Active Site Catalyze the Decarboxylation of Dodecanoic Acid in UndA to Produce Biofuels?. *Chemistry - A European Journal*, **2020**, 26, 2233-2242	4.8	15
241	Computational Study on the Catalytic Reaction Mechanism of Heme Haloperoxidase Enzymes. *Israel Journal of Chemistry*, **2020**, 60, 963-972	3.4	2
240	Second-Coordination Sphere Effects on Selectivity and Specificity of Heme and Nonheme Iron Enzymes. *Chemistry - A European Journal*, **2020**, 26, 5308-5327	4.8	34
239	Hydroxyl Transfer to Carbon Radicals by Mn(OH) vs Fe(OH) Corrole Complexes. *Inorganic Chemistry*, **2020**, 59, 16053-16064	5.1	13
238	How Do Vanadium Chloroperoxidases Generate Hypochlorite from Hydrogen Peroxide and Chloride? A Computational Study. *ACS Catalysis*, **2020**, 10, 14067-14079	13.1	9
237	How Do Metal Ions Modulate the Rate-Determining Electron-Transfer Step in Cytochrome P450 Reactions?. *Chemistry - A European Journal*, **2020**, 26, 15270-15281	4.8	6

236	Fe-Catalyzed Aziridination Is Governed by the Electron Affinity of the Active Imido-Iron Species. *ACS Catalysis*, **2020**, 10, 10010-10020	13.1	22
235	Catalytic Mechanism of Aromatic Nitration by Cytochrome P450 TxtE: Involvement of a Ferric-Peroxynitrite Intermediate. *Journal of the American Chemical Society*, **2020**, 142, 15764-15779	16.4	25
234	Properties and reactivity of □-nitrido-bridged dimetal porphyrinoid complexes: how does ruthenium compare to iron?. *Journal of Biological Inorganic Chemistry*, **2019**, 24, 1127-1134	3.7	3
233	Interplay Between Steric and Electronic Effects: A Joint Spectroscopy and Computational Study of Nonheme Iron(IV)-Oxo Complexes. *Chemistry - A European Journal*, **2019**, 25, 5086-5098	4.8	25
232	Hydrogen by Deuterium Substitution in an Aldehyde Tunes the Regioselectivity by a Nonheme Manganese(III)-□-peroxo Complex. *Angewandte Chemie*, **2019**, 131, 10749-10753	3.6	13
231	Flavonol biosynthesis by nonheme iron dioxygenases: A computational study into the structure and mechanism. *Journal of Inorganic Biochemistry*, **2019**, 198, 110728	4.2	12
230	Hydrogen by Deuterium Substitution in an Aldehyde Tunes the Regioselectivity by a Nonheme Manganese(III)-Peroxo Complex. *Angewandte Chemie - International Edition*, **2019**, 58, 10639-10643	16.4	27
229	A Non-Heme Diiron Complex for (Electro)catalytic Reduction of Dioxygen: Tuning the Selectivity through Electron Delivery. *Journal of the American Chemical Society*, **2019**, 141, 8244-8253	16.4	30
228	The Quest for Accurate Theoretical Models of Metalloenzymes: An Aid to Experiment. *Challenges and Advances in Computational Chemistry and Physics*, **2019**, 439-462	0.7	
227	Regio- and Enantio-selective Chemo-enzymatic C-H-Lactonization of Decanoic Acid to (S)-□-Decalactone. *Angewandte Chemie - International Edition*, **2019**, 58, 5668-5671	16.4	35
226	Regio- and Enantio-selective Chemo-enzymatic C□H-Lactonization of Decanoic Acid to (S)-□-Decalactone. *Angewandte Chemie*, **2019**, 131, 5724-5727	3.6	5
225	The Equatorial Ligand Effect on the Properties and Reactivity of Iron(V) Oxo Intermediates. *Chemistry - A European Journal*, **2019**, 25, 8092-8104	4.8	13
224	Equatorial ligand plane perturbations lead to a spin-state change in an iron(iii) porphyrin dimer. *Dalton Transactions*, **2019**, 48, 6353-6357	4.3	13
223	The Hunt for the Closed Conformation of the Fruit-Ripening Enzyme 1-Aminocyclopropane-1-carboxylic Oxidase: A Combined Electron Paramagnetic Resonance and Molecular Dynamics Study. *Chemistry - A European Journal*, **2019**, 25, 13766-13776	4.8	1
222	Mechanistic Investigation of Oxygen Rebound in a Mononuclear Nonheme Iron Complex. *Inorganic Chemistry*, **2019**, 58, 9557-9561	5.1	11
221	CO Reduction on an Iron-Porphyrin Center: A Computational Study. *Journal of Physical Chemistry A*, **2019**, 123, 6527-6535	2.8	22
220	Mechanism of Oxidative Activation of Fluorinated Aromatic Compounds by N-Bridged Diiron-Phthalocyanine: What Determines the Reactivity?. *Chemistry - A European Journal*, **2019**, 25, 14320-14331	4.8	27
219	Second-Coordination Sphere Effect on the Reactivity of Vanadium-Peroxo Complexes: A Computational Study. *Inorganic Chemistry*, **2019**, 58, 15741-15750	5.1	6

218	Selective Hydrogen Atom Abstraction from Dihydroflavonol by a Nonheme Iron Center Is the Key Step in the Enzymatic Flavonol Synthesis and Avoids Byproducts. *Journal of the American Chemical Society*, **2019**, 141, 20278-20292	16.4	41
217	Hydrogen Atom Abstraction by High-Valent Fe(OH) versus Mn(OH) Porphyrinoid Complexes: Mechanistic Insights from Experimental and Computational Studies. *Inorganic Chemistry*, **2019**, 58, 16761-16770	5.1	13
216	Reactivity patterns of vanadium(iv/v)-oxo complexes with olefins in the presence of peroxides: a computational study. *Dalton Transactions*, **2019**, 48, 16899-16910	4.3	7
215	How Does the Oxidation State of Palladium Surfaces Affect the Reactivity and Selectivity of Direct Synthesis of Hydrogen Peroxide from Hydrogen and Oxygen Gases? A Density Functional Study. *Journal of the American Chemical Society*, **2019**, 141, 901-910	16.4	22
214	Selective Formation of an Fe O or an Fe OOH Intermediate From Iron(II) and H O : Controlled Heterolytic versus Homolytic Oxygen-Oxygen Bond Cleavage by the Second Coordination Sphere. *Angewandte Chemie - International Edition*, **2019**, 58, 854-858	16.4	30
213	Mechanistic Studies of Fatty Acid Activation by CYP152 Peroxygenases Reveal Unexpected Desaturase Activity. *ACS Catalysis*, **2019**, 9, 565-577	13.1	50
212	Selective Formation of an FeIVO or an FeIIIOOH Intermediate From Iron(II) and H2O2: Controlled Heterolytic versus Homolytic Oxygen–Oxygen Bond Cleavage by the Second Coordination Sphere. *Angewandte Chemie*, **2019**, 131, 864-868	3.6	16
211	Hydrogen Atom vs. Hydride Transfer in Cytochrome P450 Oxidations: A Combined Mass Spectrometry and Computational Study. *European Journal of Inorganic Chemistry*, **2018**, 2018, 1854-1865	2.3	7
210	Can Manganese(III)-Iodosylarene Act as an Oxidant Alongside High-Valent Manganese(V)-Oxo Complexes?. *ChemistrySelect*, **2018**, 3, 3208-3213	1.8	5
209	Group Transfer to an Aliphatic Bond: A Biomimetic Study Inspired by Nonheme Iron Halogenases. *ACS Catalysis*, **2018**, 8, 8685-8698	13.1	25
208	Quantum Mechanics/Molecular Mechanics Studies on the Relative Reactivities of Compound I and II in Cytochrome P450 Enzymes. *International Journal of Molecular Sciences*, **2018**, 19,	6.3	13
207	Solvent- and Halide-Induced (Inter)conversion between Iron(II)-Disulfide and Iron(III)-Thiolate Complexes. *Chemistry - A European Journal*, **2018**, 24, 11973-11982	4.8	15
206	Nitrogen Reduction to Ammonia on a Biomimetic Mononuclear Iron Centre: Insights into the Nitrogenase Enzyme. *Chemistry - A European Journal*, **2018**, 24, 5293-5302	4.8	34
205	Mechanistic Insight on the Activity and Substrate Selectivity of Nonheme Iron Dioxygenases. *Chemical Record*, **2018**, 18, 1501-1516	6.6	23
204	Does Substrate Positioning Affect the Selectivity and Reactivity in the Hectochlorin Biosynthesis Halogenase?. *Frontiers in Chemistry*, **2018**, 6, 513	5	28
203	Catalytic Mechanism of Nogalamycin Monoxygenase: How Does Nature Synthesize Antibiotics without a Metal Cofactor?. *Journal of Physical Chemistry B*, **2018**, 122, 10841-10854	3.4	6
202	Dramatic rate-enhancement of oxygen atom transfer by an iron(iv)-oxo species by equatorial ligand field perturbations. *Dalton Transactions*, **2018**, 47, 14945-14957	4.3	21
201	A Comparative Review on the Catalytic Mechanism of Nonheme Iron Hydroxylases and Halogenases. *Catalysts*, **2018**, 8, 314	4	30

200	Oxygen Atom Transfer Using an Iron(IV)-Oxo Embedded in a Tetracyclic N-Heterocyclic Carbene System: How Does the Reactivity Compare to Cytochrome P450 Compound I?. *Chemistry - A European Journal*, **2017**, 23, 2935-2944	4.8	32
199	Modulation of Antimalarial Activity at a Putative Bisquinoline Receptor In Vivo Using Fluorinated Bisquinolines. *Chemistry - A European Journal*, **2017**, 23, 6811-6828	4.8	11
198	Reactivity Patterns of (Protonated) Compound II and Compound I of Cytochrome P450: Which is the Better Oxidant?. *Chemistry - A European Journal*, **2017**, 23, 6406-6418	4.8	55
197	Glutathione binding to dirhodium tetraacetate: a spectroscopic, mass spectral and computational study of an anti-tumour compound. *Metallomics*, **2017**, 9, 501-516	4.5	5
196	A High-Valent Non-Heme □Oxo Manganese(IV) Dimer Generated from a Thiolate-Bound Manganese(II) Complex and Dioxygen. *Angewandte Chemie - International Edition*, **2017**, 56, 8211-8215	16.4	24
195	Sulfoxide Synthase versus Cysteine Dioxygenase Reactivity in a Nonheme Iron Enzyme. *Journal of the American Chemical Society*, **2017**, 139, 9259-9270	16.4	75
194	A High-Valent Non-Heme □Oxo Manganese(IV) Dimer Generated from a Thiolate-Bound Manganese(II) Complex and Dioxygen. *Angewandte Chemie*, **2017**, 129, 8323-8327	3.6	7
193	Prediction of Reduction Potentials of Copper Proteins with Continuum Electrostatics and Density Functional Theory. *Chemistry - A European Journal*, **2017**, 23, 15436-15445	4.8	15
192	Features of reactive cysteines discovered through computation: from kinase inhibition to enrichment around protein degrons. *Scientific Reports*, **2017**, 7, 16338	4.9	11
191	Keto-Enol Tautomerization Triggers an Electrophilic Aldehyde Deformylation Reaction by a Nonheme Manganese(III)-Peroxo Complex. *Journal of the American Chemical Society*, **2017**, 139, 18328-18338	16.4	51
190	The Role of Nonheme Transition Metal-Oxo, -Peroxo, and -Superoxo Intermediates in Enzyme Catalysis and Reactions of Bioinspired Complexes. *Advances in Inorganic Chemistry*, **2017**, 70, 167-194	2.1	2
189	Understanding How Prolyl-4-hydroxylase Structure Steers a Ferryl Oxidant toward Scission of a Strong C-H Bond. *Journal of the American Chemical Society*, **2017**, 139, 9855-9866	16.4	60
188	Recombinant silicateins as model biocatalysts in organosiloxane chemistry. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, E5285-E5291	11.5	16
187	Biodegradation of Cosmetics Products: A Computational Study of Cytochrome P450 Metabolism of Phthalates. *Inorganics*, **2017**, 5, 77	2.9	13
186	How Are Substrate Binding and Catalysis Affected by Mutating Glu and Arg in Prolyl-4-hydroxylase? A QM/MM and MD Study. *Frontiers in Chemistry*, **2017**, 5, 94	5	12
185	Singlet versus Triplet Reactivity in an Mn(V)-Oxo Species: Testing Theoretical Predictions Against Experimental Evidence. *Journal of the American Chemical Society*, **2016**, 138, 12375-86	16.4	67
184	Substrate Sulfoxidation by an Iron(IV)-Oxo Complex: Benchmarking Computationally Calculated Barrier Heights to Experiment. *Journal of Physical Chemistry A*, **2016**, 120, 9805-9814	2.8	63
183	Quantum Mechanics/Molecular Mechanics Modeling of Enzymatic Processes: Caveats and Breakthroughs. *Chemistry - A European Journal*, **2016**, 22, 2562-81	4.8	100

182	Origin of the Regioselective Fatty-Acid Hydroxylation versus Decarboxylation by a Cytochrome P450 Peroxygenase: What Drives the Reaction to Biofuel Production?. *Chemistry - A European Journal*, **2016**, 22, 5478-83	4.8	86
181	Origin of the Enhanced Reactivity of Nitrido-Bridged Diiron(IV)-Oxo Porphyrinoid Complexes over Cytochrome P450 Compound I. *ACS Catalysis*, **2016**, 6, 2230-2243	13.1	75
180	Methane Hydroxylation by Axially Ligated Iron (IV)-oxo Porphyrin Cation Radical Models **2016**, 1,		2
179	Challenging Density Functional Theory Calculations with Hemes and Porphyrins. *International Journal of Molecular Sciences*, **2016**, 17, 519	6.3	20
178	Influence of cysteine 164 on active site structure in rat cysteine dioxygenase. *Journal of Biological Inorganic Chemistry*, **2016**, 21, 501-10	3.7	14
177	Arene activation by a nonheme iron(III)-hydroperoxo complex: pathways leading to phenol and ketone products. *Journal of Biological Inorganic Chemistry*, **2016**, 21, 453-62	3.7	12
176	Deformylation Reaction by a Nonheme Manganese(III) Peroxo Complex via Initial Hydrogen-Atom Abstraction. *Angewandte Chemie*, **2016**, 128, 11257-11261	3.6	17
175	A Systematic Account on Aromatic Hydroxylation by a Cytochrome P450 Model Compound I: A Low-Pressure Mass Spectrometry and Computational Study. *Chemistry - A European Journal*, **2016**, 22, 18608-18619	4.8	54
174	Influence of Ligand Architecture in Tuning Reaction Bifurcation Pathways for Chlorite Oxidation by Non-Heme Iron Complexes. *Inorganic Chemistry*, **2016**, 55, 10170-10181	5.1	12
173	Deformylation Reaction by a Nonheme Manganese(III)-Peroxo Complex via Initial Hydrogen-Atom Abstraction. *Angewandte Chemie - International Edition*, **2016**, 55, 11091-5	16.4	55
172	Site-selective formation of an iron(iv)-oxo species at the more electron-rich iron atom of heteroleptic nitrido diiron phthalocyanines. *Chemical Science*, **2015**, 6, 5063-5075	9.4	52
171	Drug metabolism by cytochrome p450 enzymes: what distinguishes the pathways leading to substrate hydroxylation over desaturation?. *Chemistry - A European Journal*, **2015**, 21, 9083-92	4.8	100
170	A Trimetal Carbene with Reactivity Reminiscent of Fischer Tropsch Catalysis. *Organometallics*, **2015**, 34, 1651-1660	3.8	4
169	Hydrogen-bonding interactions trigger a spin-flip in iron(III) porphyrin complexes. *Angewandte Chemie - International Edition*, **2015**, 54, 4796-800	16.4	66
168	Differences and comparisons of the properties and reactivities of iron(III)-hydroperoxo complexes with saturated coordination sphere. *Chemistry - A European Journal*, **2015**, 21, 1221-36	4.8	56
167	Drug Metabolism by Cytochrome P450 Enzymes: What Distinguishes the Pathways Leading to Substrate Hydroxylation Over Desaturation?. *Chemistry - A European Journal*, **2015**, 21, 8973-8973	4.8	3
166	Catalytic Function and Mechanism of Heme and Nonheme Iron(IV) Oxo Complexes in Nature **2015**, 185-202		4
165	Structure and mechanism leading to formation of the cysteine sulfinate product complex of a biomimetic cysteine dioxygenase model. *Chemistry - A European Journal*, **2015**, 21, 7470-9	4.8	19

164	Alkyl Chain Growth on a Transition Metal Center: How Does Iron Compare to Ruthenium and Osmium?. *International Journal of Molecular Sciences*, **2015**, 16, 23369-81	6.3	
163	Enzymatic Halogenases and Haloperoxidases: Computational Studies on Mechanism and Function. *Advances in Protein Chemistry and Structural Biology*, **2015**, 100, 113-51	5.3	14
162	Catalytic mechanism of cofactor-free dioxygenases and how they circumvent spin-forbidden oxygenation of their substrates. *Journal of the American Chemical Society*, **2015**, 137, 7474-87	16.4	57
161	A comprehensive test set of epoxidation rate constants for iron(iv)-oxo porphyrin cation radical complexes. *Chemical Science*, **2015**, 6, 1516-1529	9.4	88
160	Identification and Spectroscopic Characterization of Nonheme Iron(III) Hypochlorite Intermediates. *Angewandte Chemie*, **2015**, 127, 4431-4435	3.6	11
159	Identification and spectroscopic characterization of nonheme iron(III) hypochlorite intermediates. *Angewandte Chemie - International Edition*, **2015**, 54, 4357-61	16.4	34
158	Spin-state ordering in hydroxo-bridged diiron(III)bisporphyrin complexes. *Inorganic Chemistry*, **2015**, 54, 1919-30	5.1	45
157	Hydrogen-Bonding Interactions Trigger a Spin-Flip in Iron(III) Porphyrin Complexes. *Angewandte Chemie*, **2015**, 127, 4878-4882	3.6	21
156	Origin of the proton-transfer step in the cofactor-free (1H)-3-hydroxy-4-oxoquinaldine 2,4-dioxygenase: effect of the basicity of an active site His residue. *Journal of Biological Chemistry*, **2014**, 289, 8620-32	5.4	25
155	Metabolism of halogenated alkanes by cytochrome P450 enzymes. Aerobic oxidation versus anaerobic reduction. *Chemistry - an Asian Journal*, **2014**, 9, 1175-82	4.5	17
154	Computational modelling of oxygenation processes in enzymes and biomimetic model complexes. *Chemical Communications*, **2014**, 50, 262-82	5.8	99
153	Direct observation of a nonheme iron(IV)-oxo complex that mediates aromatic C-F hydroxylation. *Journal of the American Chemical Society*, **2014**, 136, 13542-5	16.4	58
152	Oxygen-atom transfer reactivity of axially ligated Mn(V)-oxo complexes: evidence for enhanced electrophilic and nucleophilic pathways. *Journal of the American Chemical Society*, **2014**, 136, 13845-52	16.4	53
151	Properties and reactivities of nonheme iron(IV)-oxo versus iron(V)-oxo: long-range electron transfer versus hydrogen atom abstraction. *Physical Chemistry Chemical Physics*, **2014**, 16, 22611-22	3.6	5
150	Dramatic influence of an anionic donor on the oxygen-atom transfer reactivity of a Mn(V) -oxo complex. *Chemistry - A European Journal*, **2014**, 20, 14584-8	4.8	24
149	Quantum mechanics/molecular mechanics study on the oxygen binding and substrate hydroxylation step in AlkB repair enzymes. *Chemistry - A European Journal*, **2014**, 20, 435-46	4.8	104
148	Thioether-ligated iron(II) and iron(III)-hydroperoxo/alkylperoxo complexes with an H-bond donor in the second coordination sphere. *Dalton Transactions*, **2014**, 43, 7522-32	4.3	24
147	Long-range electron transfer triggers mechanistic differences between iron(IV)-oxo and iron(IV)-imido oxidants. *Journal of the American Chemical Society*, **2014**, 136, 17102-15	16.4	93

146	Experimental and computational evidence for the mechanism of intradiol catechol dioxygenation by non-heme iron(III) complexes. *Chemistry - A European Journal*, **2014**, 20, 15686-91	4.8	20
145	Secondary coordination sphere influence on the reactivity of nonheme iron(II) complexes: an experimental and DFT approach. *Journal of the American Chemical Society*, **2013**, 135, 10590-3	16.4	85
144	Synthesis and ligand non-innocence of thiolate-ligated (N4S) Iron(II) and nickel(II) bis(imino)pyridine complexes. *Inorganic Chemistry*, **2013**, 52, 10467-80	5.1	20
143	Inversion of enantioselectivity of a mononuclear non-heme iron(II)-dependent hydroxylase by tuning the interplay of metal-center geometry and protein structure. *Angewandte Chemie - International Edition*, **2013**, 52, 9677-81	16.4	45
142	Mechanistic insight into halide oxidation by non-heme iron complexes. Haloperoxidase versus halogenase activity. *Chemical Communications*, **2013**, 49, 10926-8	5.8	36
141	Does hydrogen-bonding donation to manganese(IV)-oxo and iron(IV)-oxo oxidants affect the oxygen-atom transfer ability? A computational study. *Chemistry - A European Journal*, **2013**, 19, 4058-68	4.8	66
140	Comparison of the reactivity of nonheme iron(IV)-oxo versus iron(IV)-imido complexes: which is the better oxidant?. *Angewandte Chemie - International Edition*, **2013**, 52, 12288-92	16.4	79
139	Intrinsic properties and reactivities of mononuclear nonheme iron□oxygen complexes bearing the tetramethylcyclam ligand. *Coordination Chemistry Reviews*, **2013**, 257, 381-393	23.2	140
138	Rationalization of the barrier height for p-Z-styrene epoxidation by iron(IV)-oxo porphyrin cation radicals with variable axial ligands. *Inorganic Chemistry*, **2013**, 52, 7968-79	5.1	63
137	Generation of a high-valent iron imido corrolazine complex and NR group transfer reactivity. *Inorganic Chemistry*, **2013**, 52, 4668-82	5.1	49
136	Inversion of Enantioselectivity of a Mononuclear Non-Heme Iron(II)-dependent Hydroxylase by Tuning the Interplay of Metal-Center Geometry and Protein Structure. *Angewandte Chemie*, **2013**, 125, 9859-9863	3.6	13
135	Differences in chemical properties and reactivity patterns of mono- and dioxomanganese(V) porphyrins as revealed by density functional theory. *Journal of Porphyrins and Phthalocyanines*, **2013**, 17, 954-963	1.8	2
134	Comparison of the Reactivity of Nonheme Iron(IV)□Oxo versus Iron(IV)□Imido Complexes: Which is the Better Oxidant?. *Angewandte Chemie*, **2013**, 125, 12514-12518	3.6	23
133	Overview on theoretical studies discriminating the two-oxidant versus two-state-reactivity models for substrate monoxygenation by cytochrome P450 enzymes. *Current Topics in Medicinal Chemistry*, **2013**, 13, 2218-32	3	13
132	Cysteine protease inhibition by nitrile-based inhibitors: a computational study. *Frontiers in Chemistry*, **2013**, 1, 39	5	17
131	Nonheme iron-oxo and -superoxo reactivities: O2 binding and spin inversion probability matter. *Chemical Communications*, **2012**, 48, 2189-91	5.8	39
130	Predictive studies of H-atom abstraction reactions by an iron(IV)-oxo corrole cation radical oxidant. *Chemical Communications*, **2012**, 48, 3491-3	5.8	17
129	Valence tautomerism in a high-valent manganese-oxo porphyrinoid complex induced by a Lewis acid. *Journal of the American Chemical Society*, **2012**, 134, 10397-400	16.4	144

128	Modeling flexible pharmacophores with distance geometry, scoring, and bound stretching. *Journal of Chemical Information and Modeling*, **2012**, 52, 577-88	6.1	4
127	Mechanism of S-oxygenation by a cysteine dioxygenase model complex. *Journal of Physical Chemistry A*, **2012**, 116, 582-91	2.8	33
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2	Chapter 1:Experimental and Computational Studies on the Catalytic Mechanism of Non-heme Iron Dioxygenases	1-41	3
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