Sam P De Visser

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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	Mechanism of oxidation reactions catalyzed by cytochrome p450 enzymes. *Chemical Reviews*, **2004**, 104, 3947-80	68.1	1774
270	Theoretical perspective on the structure and mechanism of cytochrome P450 enzymes. *Chemical Reviews*, **2005**, 105, 2279-328	68.1	999
269	A Model Rebound Mechanism of Hydroxylation by Cytochrome P450: Stepwise and Effectively Concerted Pathways, and Their Reactivity Patterns. *Journal of the American Chemical Society*, **2000**, 122, 8977-8989	16.4	333
268	Two-state reactivity mechanisms of hydroxylation and epoxidation by cytochrome P-450 revealed by theory. *Current Opinion in Chemical Biology*, **2002**, 6, 556-67	9.7	299
267	A proton-shuttle mechanism mediated by the porphyrin in benzene hydroxylation by cytochrome p450 enzymes. *Journal of the American Chemical Society*, **2003**, 125, 7413-24	16.4	283
266	Searching for the second oxidant in the catalytic cycle of cytochrome P450: a theoretical investigation of the iron(III)-hydroperoxo species and its epoxidation pathways. *Journal of the American Chemical Society*, **2002**, 124, 2806-17	16.4	268
265	What factors affect the regioselectivity of oxidation by cytochrome p450? A DFT study of allylic hydroxylation and double bond epoxidation in a model reaction. *Journal of the American Chemical Society*, **2002**, 124, 11809-26	16.4	258
264	Photoactivation of the photoactive yellow protein: why photon absorption triggers a trans-to-cis Isomerization of the chromophore in the protein. *Journal of the American Chemical Society*, **2004**, 126, 4228-33	16.4	246
263	A valence bond modeling of trends in hydrogen abstraction barriers and transition states of hydroxylation reactions catalyzed by cytochrome P450 enzymes. *Journal of the American Chemical Society*, **2008**, 130, 10128-40	16.4	213
262	External electric field will control the selectivity of enzymatic-like bond activations. *Journal of the American Chemical Society*, **2004**, 126, 11746-9	16.4	201
261	Multi-state epoxidation of ethene by cytochrome P450: a quantum chemical study. *Journal of the American Chemical Society*, **2001**, 123, 3037-47	16.4	199
260	A predictive pattern of computed barriers for C-h hydroxylation by compound I of cytochrome p450. *Journal of the American Chemical Society*, **2004**, 126, 8362-3	16.4	195
259	Propene activation by the oxo-iron active species of taurine/alpha-ketoglutarate dioxygenase (TauD) enzyme. How does the catalysis compare to heme-enzymes?. *Journal of the American Chemical Society*, **2006**, 128, 9813-24	16.4	175
258	Theoretical study on the mechanism of the oxygen activation process in cysteine dioxygenase enzymes. *Journal of the American Chemical Society*, **2011**, 133, 3869-82	16.4	174
257	Combined experimental and theoretical study on aromatic hydroxylation by mononuclear nonheme iron(IV)-oxo complexes. *Inorganic Chemistry*, **2007**, 46, 4632-41	5.1	161
256	Trends in substrate hydroxylation reactions by heme and nonheme iron(IV)-oxo oxidants give correlations between intrinsic properties of the oxidant with barrier height. *Journal of the American Chemical Society*, **2010**, 132, 1087-97	16.4	159
255	Medium Polarization and Hydrogen Bonding Effects on Compound I of Cytochrome P450: What Kind of a Radical Is It Really?. *Journal of the American Chemical Society*, **2000**, 122, 12892-12893	16.4	158

254	What factors influence the rate constant of substrate epoxidation by compound I of cytochrome P450 and analogous iron(IV)-oxo oxidants?. *Journal of the American Chemical Society*, **2010**, 132, 7656-67	16.4	155
253	Active species of horseradish peroxidase (HRP) and cytochrome P450: two electronic chameleons. *Journal of the American Chemical Society*, **2003**, 125, 15779-88	16.4	153
252	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
251	Intrinsic properties and reactivities of mononuclear nonheme iron-oxygen complexes bearing the tetramethylcyclam ligand. *Coordination Chemistry Reviews*, **2013**, 257, 381-393	23.2	140
250	The Rebound Controversy An Overview and Theoretical Modeling of the Rebound Step in C-H Hydroxylation by Cytochrome P450. *European Journal of Inorganic Chemistry*, **2004**, 2004, 207-226	2.3	138
249	Radical clock substrates, their C-H hydroxylation mechanism by cytochrome P450, and other reactivity patterns: what does theory reveal about the clocks' behavior?. *Journal of the American Chemical Society*, **2004**, 126, 1907-20	16.4	138
248	The 'push' effect of the thiolate ligand in cytochrome P450: a theoretical gauging. *Journal of Inorganic Biochemistry*, **2002**, 91, 554-67	4.2	127
247	What factors influence the ratio of C-H hydroxylation versus C=C epoxidation by a nonheme cytochrome P450 biomimetic?. *Journal of the American Chemical Society*, **2006**, 128, 15809-18	16.4	126
246	Unprecedented rate enhancements of hydrogen-atom transfer to a manganese(V)-oxo corrolazine complex. *Angewandte Chemie - International Edition*, **2010**, 49, 5091-5	16.4	125
245	The mechanism of cysteine oxygenation by cysteine dioxygenase enzymes. *Journal of the American Chemical Society*, **2007**, 129, 14846-7	16.4	111
244	Can a single oxidant with two spin states masquerade as two different oxidants? A study of the sulfoxidation mechanism by cytochrome p450. *Journal of the American Chemical Society*, **2003**, 125, 8698-9	16.4	111
243	Hydrogen Bonding Modulates the Selectivity of Enzymatic Oxidation by P450: Chameleon Oxidant Behavior by Compound I. *Angewandte Chemie - International Edition*, **2002**, 41, 1947	16.4	110
242	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
241	Chameleon States: High-Valent Metal-Oxo Species of Cytochrome P450 and Its Ruthenium Analogue. *Angewandte Chemie - International Edition*, **2001**, 40, 2874-2878	16.4	103
240	Structural characterization and remarkable axial ligand effect on the nucleophilic reactivity of a nonheme manganese(III)-peroxo complex. *Angewandte Chemie - International Edition*, **2009**, 48, 4150-3	16.4	101
239	Multistate reactivity in styrene epoxidation by compound I of cytochrome p450: mechanisms of products and side products formation. *Chemistry - A European Journal*, **2005**, 11, 2825-35	4.8	101
238	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
237	Quantum Mechanics/Molecular Mechanics Modeling of Enzymatic Processes: Caveats and Breakthroughs. *Chemistry - A European Journal*, **2016**, 22, 2562-81	4.8	100

236	Computational modelling of oxygenation processes in enzymes and biomimetic model complexes. *Chemical Communications*, **2014**, 50, 262-82	5.8	99
235	Nature of the Three-Electron Bond in H2S?SH2+ *Journal of Physical Chemistry A*, **1998**, 102, 9549-9553	2.8	96
234	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
233	Origin of the correlation of the rate constant of substrate hydroxylation by nonheme iron(IV)-oxo complexes with the bond-dissociation energy of the C-H bond of the substrate. *Chemistry - A European Journal*, **2009**, 15, 6651-62	4.8	90
232	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
231	Substitution of hydrogen by deuterium changes the regioselectivity of ethylbenzene hydroxylation by an oxo-iron-porphyrin catalyst. *Chemistry - A European Journal*, **2006**, 12, 8168-77	4.8	88
230	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
229	Differences in and comparison of the catalytic properties of heme and non-heme enzymes with a central oxo-iron group. *Angewandte Chemie - International Edition*, **2006**, 45, 1790-3	16.4	86
228	How does product isotope effect prove the operation of a two-state "rebound" mechanism in C-H hydroxylation by cytochrome P450?. *Journal of the American Chemical Society*, **2003**, 125, 13024-5	16.4	86
227	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
226	What is the difference between the manganese porphyrin and corrole analogues of cytochrome P450's compound I?. *Chemistry - A European Journal*, **2001**, 7, 4954-60	4.8	83
225	Is the bound substrate in nitric oxide synthase protonated or neutral and what is the active oxidant that performs substrate hydroxylation?. *Journal of the American Chemical Society*, **2008**, 130, 12961-74	16.4	82
224	How Does Ethene Inactivate Cytochrome P450 En Route to Its Epoxidation? A Density Functional Study. *Angewandte Chemie - International Edition*, **2001**, 40, 2871-2874	16.4	82
223	One oxidant, many pathways: a theoretical perspective of monooxygenation mechanisms by cytochrome P450 enzymes. *Journal of Biological Inorganic Chemistry*, **2004**, 9, 661-8	3.7	81
222	Electrophilic aromatic chlorination and haloperoxidation of chloride catalyzed by polyfluorinated alcohols: a new manifestation of template catalysis. *Journal of the American Chemical Society*, **2003**, 125, 12116-7	16.4	81
221	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
220	Effect of the axial ligand on substrate sulfoxidation mediated by iron(IV)-oxo porphyrin cation radical oxidants. *Chemistry - A European Journal*, **2011**, 17, 6196-205	4.8	79
219	Sulfoxide Synthase versus Cysteine Dioxygenase Reactivity in a Nonheme Iron Enzyme. *Journal of the American Chemical Society*, **2017**, 139, 9259-9270	16.4	75

218	Origin of the Enhanced Reactivity of µ-Nitrido-Bridged Diiron(IV)-Oxo Porphyrinoid Complexes over Cytochrome P450 Compound I. *ACS Catalysis*, **2016**, 6, 2230-2243	13.1	75
217	Nuclear quantum tunneling in the light-activated enzyme protochlorophyllide oxidoreductase. *Journal of Biological Chemistry*, **2009**, 284, 3762-7	5.4	75
216	How does the axial ligand of cytochrome P450 biomimetics influence the regioselectivity of aliphatic versus aromatic hydroxylation?. *Chemistry - A European Journal*, **2009**, 15, 5577-87	4.8	75
215	Fluorinated alcohols enable olefin epoxidation by H2O2: template catalysis. *Journal of Organic Chemistry*, **2003**, 68, 2903-12	4.2	75
214	The experimentally elusive oxidant of cytochrome P450: a theoretical "trapping" defining more closely the "real" species. *ChemBioChem*, **2001**, 2, 848-51	3.8	75
213	Theory favors a stepwise mechanism of porphyrin degradation by a ferric hydroperoxide model of the active species of heme oxygenase. *Journal of the American Chemical Society*, **2005**, 127, 8204-13	16.4	74
212	Comparative quantum mechanics/molecular mechanics (QM/MM) and density functional theory calculations on the oxo-iron species of taurine/alpha-ketoglutarate dioxygenase. *Journal of Physical Chemistry A*, **2008**, 112, 2464-8	2.8	73
211	Sulfoxidation mechanisms catalyzed by cytochrome P450 and horseradish peroxidase models: spin selection induced by the ligand. *Biochemistry*, **2005**, 44, 8148-58	3.2	68
210	Is the ruthenium analogue of compound I of cytochrome p450 an efficient oxidant? A theoretical investigation of the methane hydroxylation reaction. *Journal of the American Chemical Society*, **2003**, 125, 2291-300	16.4	68
209	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
208	Oxygen economy of cytochrome P450: what is the origin of the mixed functionality as a dehydrogenase-oxidase enzyme compared with its normal function?. *Journal of the American Chemical Society*, **2004**, 126, 5072-3	16.4	67
207	Hydrogen-bonding interactions trigger a spin-flip in iron(III) porphyrin complexes. *Angewandte Chemie - International Edition*, **2015**, 54, 4796-800	16.4	66
206	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
205	Effect of porphyrin ligands on the regioselective dehydrogenation versus epoxidation of olefins by oxoiron(IV) mimics of cytochrome P450. *Journal of Physical Chemistry A*, **2009**, 113, 11713-22	2.8	66
204	A manganese(V)-oxo π-cation radical complex: influence of one-electron oxidation on oxygen-atom transfer. *Journal of the American Chemical Society*, **2011**, 133, 15874-7	16.4	64
203	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
202	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
201	Nonheme ferric hydroperoxo intermediates are efficient oxidants of bromide oxidation. *Chemical Communications*, **2011**, 47, 11044-6	5.8	63

200	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?. *Angewandte Chemie - International Edition*, **2004**, 43, 5661-5	16.4	63
199	How do azoles inhibit cytochrome P450 enzymes? A density functional study. *Journal of Physical Chemistry A*, **2008**, 112, 12911-8	2.8	62
198	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
197	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
196	A biomimetic ferric hydroperoxo porphyrin intermediate. *Angewandte Chemie - International Edition* , **2010**, 49, 2099-101	16.4	58
195	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
194	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. *Journal of Inorganic Biochemistry*, **2004**, 98, 1183-93	4.2	57
193	Reactivity and Thermochemical Properties of the Water Dimer Radical Cation in the Gas Phase. *The Journal of Physical Chemistry*, **1995**, 99, 15444-15447		57
192	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
191	The intrinsic axial ligand effect on propene oxidation by horseradish peroxidase versus cytochrome P450 enzymes. *Journal of Biological Inorganic Chemistry*, **2005**, 10, 181-9	3.7	56
190	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
189	Axial ligand effect on the rate constant of aromatic hydroxylation by iron(IV)-oxo complexes mimicking cytochrome P450 enzymes. *Journal of Physical Chemistry B*, **2012**, 116, 718-30	3.4	55
188	Porphyrin traps its terminator! Concerted and stepwise porphyrin degradation mechanisms induced by heme-oxygenase and cytochrome p450. *Angewandte Chemie - International Edition*, **2004**, 43, 1129-32	16.4	55
187	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
186	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
185	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
184	Site-selective formation of an iron(iv)-oxo species at the more electron-rich iron atom of heteroleptic μ-nitrido diiron phthalocyanines. *Chemical Science*, **2015**, 6, 5063-5075	9.4	52
183	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

182	Elucidating enzyme mechanism and intrinsic chemical properties of short-lived intermediates in the catalytic cycles of cysteine dioxygenase and taurine/□ketoglutarate dioxygenase. *Coordination Chemistry Reviews*, **2009**, 253, 754-768	23.2	50
181	Can the peroxosuccinate complex in the catalytic cycle of taurine/alpha-ketoglutarate dioxygenase (TauD) act as an alternative oxidant?. *Chemical Communications*, **2007**, 171-3	5.8	50
180	New features in the catalytic cycle of cytochrome P450 during the formation of compound I from compound 0. *Journal of Physical Chemistry B*, **2005**, 109, 19946-51	3.4	50
179	Mechanistic Studies of Fatty Acid Activation by CYP152 Peroxygenases Reveal Unexpected Desaturase Activity. *ACS Catalysis*, **2019**, 9, 565-577	13.1	50
178	Generation of a high-valent iron imido corrolazine complex and NR group transfer reactivity. *Inorganic Chemistry*, **2013**, 52, 4668-82	5.1	49
177	Quantum mechanics/molecular mechanics studies on the sulfoxidation of dimethyl sulfide by compound I and compound 0 of cytochrome P450: which is the better oxidant?. *Journal of Physical Chemistry A*, **2009**, 113, 11635-42	2.8	49
176	The axial ligand effect of oxo-iron porphyrin catalysts. How does chloride compare to thiolate?. *Journal of Biological Inorganic Chemistry*, **2006**, 11, 168-78	3.7	49
175	What affects the quartet-doublet energy splitting in peroxidase enzymes?. *Journal of Physical Chemistry A*, **2005**, 109, 11050-7	2.8	48
174	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
173	Spin-state ordering in hydroxo-bridged diiron(III)bisporphyrin complexes. *Inorganic Chemistry*, **2015**, 54, 1919-30	5.1	45
172	Why do cysteine dioxygenase enzymes contain a 3-His ligand motif rather than a 2His/1Asp motif like most nonheme dioxygenases?. *Journal of Physical Chemistry A*, **2009**, 113, 1835-46	2.8	45
171	REKS calculations on ortho-, meta- and para-benzyne. *Physical Chemistry Chemical Physics*, **2000**, 2, 5046-5048	3.6	45
170	Carbon dioxide: a waste product in the catalytic cycle of alpha-ketoglutarate dependent halogenases prevents the formation of hydroxylated by-products. *Journal of Physical Chemistry B*, **2009**, 113, 12-4	3.4	44
169	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
168	The axial ligand effect on aliphatic and aromatic hydroxylation by non-heme iron(IV)-oxo biomimetic complexes. *Chemistry - an Asian Journal*, **2011**, 6, 493-504	4.5	40
167	Nonheme iron-oxo and -superoxo reactivities: O2 binding and spin inversion probability matter. *Chemical Communications*, **2012**, 48, 2189-91	5.8	39
166	Mechanistic insight into halide oxidation by non-heme iron complexes. Haloperoxidase versus halogenase activity. *Chemical Communications*, **2013**, 49, 10926-8	5.8	36
165	Steric factors override thermodynamic driving force in regioselectivity of proline hydroxylation by prolyl-4-hydroxylase enzymes. *Journal of Physical Chemistry A*, **2010**, 114, 13234-43	2.8	36

164	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
163	Fundamental differences of substrate hydroxylation by high-valent iron(IV)-oxo models of cytochrome P450. *Inorganic Chemistry*, **2009**, 48, 6661-9	5.1	35
162	Chemical and Thermodynamic Properties of Methyl Chloride Dimer Radical Cations in the Gas Phase. *Journal of the American Chemical Society*, **1998**, 120, 1517-1522	16.4	35
161	Identification and spectroscopic characterization of nonheme iron(III) hypochlorite intermediates. *Angewandte Chemie - International Edition*, **2015**, 54, 4357-61	16.4	34
160	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
159	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
158	Mechanism of S-oxygenation by a cysteine dioxygenase model complex. *Journal of Physical Chemistry A*, **2012**, 116, 582-91	2.8	33
157	Manganese substituted Compound I of cytochrome P450 biomimetics: a comparative reactivity study of Mn(V)-oxo versus Mn(IV)-oxo species. *Archives of Biochemistry and Biophysics*, **2011**, 507, 4-13	4.1	33
156	How does the push/pull effect of the axial ligand influence the catalytic properties of Compound I of catalase and cytochrome P450?. *Journal of Inorganic Biochemistry*, **2007**, 101, 1464-72	4.2	33
155	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
154	Ferromagnetic Bonding: Properties of High-Spin Lithium Clusters n+1Lin (n = 2□12) Devoid of Electron Pairs. *Journal of Physical Chemistry A*, **2002**, 106, 4961-4969	2.8	32
153	What external perturbations influence the electronic properties of catalase compound I?. *Inorganic Chemistry*, **2006**, 45, 9551-7	5.1	31
152	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
151	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
150	A Comparative Review on the Catalytic Mechanism of Nonheme Iron Hydroxylases and Halogenases. *Catalysts*, **2018**, 8, 314	4	30
149	□No-Pair Bonding□in High-Spin Lithium Clusters: n+1Lin (n = 2□6). *Journal of Physical Chemistry A*, **2000**, 104, 11223-11231	2.8	28
148	Does Substrate Positioning Affect the Selectivity and Reactivity in the Hectochlorin Biosynthesis Halogenase?. *Frontiers in Chemistry*, **2018**, 6, 513	5	28
147	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

146	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
145	Electronic properties of pentacoordinated heme complexes in cytochrome P450 enzymes: search for an Fe(I) oxidation state. *Physical Chemistry Chemical Physics*, **2009**, 11, 10219-26	3.6	27
144	A Density Functional Study of the Factors That Influence the Regioselectivity of Toluene Hydroxylation by Cytochrome P450 Enzymes. *European Journal of Inorganic Chemistry*, **2007**, 2007, 2966-2974	2.2	27
143	Differences in and Comparison of the Catalytic Properties of Heme and Non-Heme Enzymes with a Central Oxo-Iron Group. *Angewandte Chemie*, **2006**, 118, 1822-1825	3.6	27
142	Ferromagnetic bonding in high-spin alkali-metal clusters. How does sodium compare to lithium?. *Physical Chemistry Chemical Physics*, **2003**, 5, 158-164	3.6	26
141	Myers-Saito and Schmittel cyclization of hepta-1,2,4-triene-6-yne: A theoretical REKS study. *Physical Chemistry Chemical Physics*, **2001**, 3, 1242-1245	3.6	26
140	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
139	Group Transfer to an Aliphatic Bond: A Biomimetic Study Inspired by Nonheme Iron Halogenases. *ACS Catalysis*, **2018**, 8, 8685-8698	13.1	25
138	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
137	Regioselectivity of substrate hydroxylation versus halogenation by a nonheme iron(IV)-oxo complex: possibility of rearrangement pathways. *Journal of Biological Inorganic Chemistry*, **2012**, 17, 841-52	3.7	25
136	Density functional theory (DFT) and combined quantum mechanical/molecular mechanics (QM/MM) studies on the oxygen activation step in nitric oxide synthase enzymes. *Biochemical Society Transactions*, **2009**, 37, 373-7	5.1	25
135	Activation of hydrocarbon C-H bonds by iodosylbenzene: how does it compare with iron(IV)-oxo oxidants?. *Chemical Communications*, **2009**, 1562-4	5.8	25
134	Stereospecific oxidation by compound I of cytochrome P450 does not proceed in a concerted synchronous manner. *Chemical Communications*, **2001**, 2322-3	5.8	25
133	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
132	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
131	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
130	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
129	Ferromagnetic bonding: high spin copper clusters (n+1)Cu(n); n = 2-14) devoid of electron pairs but possessing strong bonding. *Journal of Physical Chemistry A*, **2006**, 110, 8510-8	2.8	24

128	On the relationship between internal energy and both the polarizability volume and the diamagnetic susceptibility. *Physical Chemistry Chemical Physics*, **1999**, 1, 749-753	3.6	24
127	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
126	Mechanistic Insight on the Activity and Substrate Selectivity of Nonheme Iron Dioxygenases. *Chemical Record*, **2018**, 18, 1501-1516	6.6	23
125	CO Reduction on an Iron-Porphyrin Center: A Computational Study. *Journal of Physical Chemistry A*, **2019**, 123, 6527-6535	2.8	22
124	Oxidative properties of a nonheme Ni(II)(O2) complex: Reactivity patterns for C-H activation, aromatic hydroxylation and heteroatom oxidation. *Chemical Communications*, **2011**, 47, 10674-6	5.8	22
123	Fe-Catalyzed Aziridination Is Governed by the Electron Affinity of the Active Imido-Iron Species. *ACS Catalysis*, **2020**, 10, 10010-10020	13.1	22
122	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
121	Hydrogen-Bonding Interactions Trigger a Spin-Flip in Iron(III) Porphyrin Complexes. *Angewandte Chemie*, **2015**, 127, 4878-4882	3.6	21
120	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
119	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
118	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
117	Computational Approaches to Cytochrome P450 Function **2005**, 45-85		20
116	Challenging Density Functional Theory Calculations with Hemes and Porphyrins. *International Journal of Molecular Sciences*, **2016**, 17, 519	6.3	20
115	Hydrogen bonding modulates the selectivity of enzymatic oxidation by P450: chameleon oxidant behavior by compound I. *Angewandte Chemie - International Edition*, **2002**, 41, 1947-51	16.4	20
114	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
113	Preferential hydroxylation over epoxidation catalysis by a horseradish peroxidase mutant: a cytochrome P450 mimic. *Journal of Physical Chemistry B*, **2007**, 111, 12299-302	3.4	19
112	The effect and influence of cis-ligands on the electronic and oxidizing properties of nonheme oxoiron biomimetics. A density functional study. *Journal of Physical Chemistry A*, **2008**, 112, 12887-95	2.8	18
111	A REKS Assessment of the Face-Diagonal Bond in 1,3-Didehydrocubane and a Comparison with Benzyne Biradicals. *European Journal of Organic Chemistry*, **2003**, 2003, 4199-4204	3.2	18

110	Metabolism of halogenated alkanes by cytochrome P450 enzymes. Aerobic oxidation versus anaerobic reduction. *Chemistry - an Asian Journal*, **2014**, 9, 1175-82	4.5	17
109	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
108	Cysteine protease inhibition by nitrile-based inhibitors: a computational study. *Frontiers in Chemistry*, **2013**, 1, 39	5	17
107	Deformylation Reaction by a Nonheme Manganese(III)-Peroxo Complex via Initial Hydrogen-Atom Abstraction. *Angewandte Chemie*, **2016**, 128, 11257-11261	3.6	17
106	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
105	Axial and equatorial ligand effects on biomimetic cysteine dioxygenase model complexes. *Organic and Biomolecular Chemistry*, **2012**, 10, 5401-9	3.9	16
104	Sulfur-sulfur three-electron bond dissociation enthalpies of dialkyl sulfide dimer radical cations. *International Journal of Mass Spectrometry*, **1998**, 179-180, 43-54	1.9	16
103	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
102	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
101	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
100	Hydrogen Bonding Modulates the Selectivity of Enzymatic Oxidation by P450: Chameleon Oxidant Behavior by Compound I. *Angewandte Chemie*, **2002**, 114, 2027	3.6	15
99	How Does Ethene Inactivate Cytochrome P450 En Route to Its Epoxidation? A Density Functional Study. *Angewandte Chemie*, **2001**, 113, 2955-2958	3.6	15
98	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
97	Chameleon States: High-Valent Metal-Oxo Species of Cytochrome P450 and Its Ruthenium Analogue The research in HU was sponsored by the Binational German Israeli Foundation (GIF) and by the Israeli Ministry of Science, Culture and Sport. Partial support by the US National Science Foundation (CHE-9814301) to J.T.G. is acknowledged. F.O. thanks the EU for a Marie Curie	16.4	15
96	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
95	Enzymatic Halogenases and Haloperoxidases: Computational Studies on Mechanism and Function. *Advances in Protein Chemistry and Structural Biology*, **2015**, 100, 113-51	5.3	14
94	Van der Waals equation of state revisited: importance of the dispersion correction. *Journal of Physical Chemistry B*, **2011**, 115, 4709-17	3.4	14
93	Reply to Comment on "Identity Hydrogen Abstraction Reactions, X• + H-X' → X-H + X'• (X = X' = CH3, SiH3, GeH3, SnH3, PbH3): A Valence Bond Modeling" *Journal of Physical Chemistry A*, **2002**, 106, 5043-5045	2.8	14

92	Bond dissociation energy of the radical cation dimers of diethyl sulfide, di-n-propyl sulfide and di-n-butyl sulfide. *International Journal of Mass Spectrometry and Ion Processes*, **1996**, 157-158, 283-291		14
91	Influence of cysteine 164 on active site structure in rat cysteine dioxygenase. *Journal of Biological Inorganic Chemistry*, **2016**, 21, 501-10	3.7	14
90	What Determines the Selectivity of Arginine Dihydroxylation by the Nonheme Iron Enzyme OrfP?. *Chemistry - A European Journal*, **2021**, 27, 1795-1809	4.8	14
89	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
88	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
87	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
86	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
85	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
84	Biodegradation of Cosmetics Products: A Computational Study of Cytochrome P450 Metabolism of Phthalates. *Inorganics*, **2017**, 5, 77	2.9	13
83	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
82	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
81	Can the replacement of a single atom in the enzyme horseradish peroxidase convert it into a monoxygenase? A density functional study. *Journal of Physical Chemistry B*, **2006**, 110, 20759-61	3.4	13
80	Hydroxyl Transfer to Carbon Radicals by Mn(OH) vs Fe(OH) Corrole Complexes. *Inorganic Chemistry*, **2020**, 59, 16053-16064	5.1	13
79	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
78	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
77	Flavonol biosynthesis by nonheme iron dioxygenases: A computational study into the structure and mechanism. *Journal of Inorganic Biochemistry*, **2019**, 198, 110728	4.2	12
76	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
75	High-Valent Iron-Oxo Porphyrins in Oxygenation Reactions. *Handbook of Porphyrin Science*, **2010**, 85-139	0.3	12

74	Density functional theory studies of oxygen and carbonate binding to a dicopper patellamide complex. *Journal of Inorganic Biochemistry*, **2008**, 102, 2171-8	4.2	12
73	Chameleon States: High-Valent Metal□xo Species of Cytochrome P450 and Its Ruthenium Analogue. *Angewandte Chemie*, **2001**, 113, 2958-2962	3.6	12
72	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
71	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
70	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
69	Mechanistic Investigation of Oxygen Rebound in a Mononuclear Nonheme Iron Complex. *Inorganic Chemistry*, **2019**, 58, 9557-9561	5.1	11
68	Features of reactive cysteines discovered through computation: from kinase inhibition to enrichment around protein degrons. *Scientific Reports*, **2017**, 7, 16338	4.9	11
67	Identification and Spectroscopic Characterization of Nonheme Iron(III) Hypochlorite Intermediates. *Angewandte Chemie*, **2015**, 127, 4431-4435	3.6	11
66	Bioengineering of Cytochrome P450 OleT: How Does Substrate Positioning Affect the Product Distributions?. *Molecules*, **2020**, 25,	4.8	10
65	Predictive studies of oxygen atom transfer reactions by Compound I of cytochrome P450: Aliphatic and aromatic hydroxylation, epoxidation, and sulfoxidation. *Advances in Inorganic Chemistry*, **2012**, 64, 1-31	2.1	10
64	New insights into the multi-step reaction pathway of the reductive half-reaction catalysed by aromatic amine dehydrogenase: a QM/MM study. *Chemical Communications*, **2010**, 46, 3104-6	5.8	10
63	Is the mu-oxo-mu-peroxodiiron intermediate of a ribonucleotide reductase biomimetic a possible oxidant of epoxidation reactions?. *Chemistry - A European Journal*, **2008**, 14, 4533-41	4.8	10
62	Porphyrin Traps Its Terminator! Concerted and Stepwise Porphyrin Degradation Mechanisms Induced by Heme-Oxygenase and Cytochrome P450. *Angewandte Chemie*, **2004**, 116, 1149-1152	3.6	10
61	How Does Ethene Inactivate Cytochrome P450 En Route to Its Epoxidation? A Density Functional Study The research is supported in part by the ISF and in part by the Ministry of Science, Culture, and Sport. F.O. acknowledges the European Union for a Marie Curie Fellowship.. *Angewandte Chemie - International Edition*, **2001**, 40, 2871-2874	16.4	10
60	Regioselectivity of aliphatic versus aromatic hydroxylation by a nonheme iron(II)-superoxo complex. *Physical Chemistry Chemical Physics*, **2012**, 14, 2518-24	3.6	9
59	Computer-Generated High-Valent Iron□xo and Manganese□xo Species with Polyoxometalate Ligands: How do they Compare with the Iron□xo Active Species of Heme Enzymes?. *Angewandte Chemie*, **2004**, 116, 5779-5783	3.6	9
58	How Do Vanadium Chloroperoxidases Generate Hypochlorite from Hydrogen Peroxide and Chloride? A Computational Study. *ACS Catalysis*, **2020**, 10, 14067-14079	13.1	9
57	A comprehensive insight into aldehyde deformylation: mechanistic implications from biology and chemistry. *Organic and Biomolecular Chemistry*, **2021**, 19, 1879-1899	3.9	9

56	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
55	O Activation by Non-Heme Thiolate-Based Dinuclear Fe Complexes. *Inorganic Chemistry*, **2020**, 59, 3249-3259	5.1	8
54	Sluggish reactivity by a nonheme iron(iv)-tosylimido complex as compared to its oxo analogue. *Dalton Transactions*, **2020**, 49, 5921-5931	4.3	8
53	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
52	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
51	How external perturbations affect the chemoselectivity of substrate activation by cytochrome P450 OleT. *Physical Chemistry Chemical Physics*, **2020**, 22, 27178-27190	3.6	7
50	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
49	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
48	Assignment of the vibrational spectra of enzyme-bound tryptophan tryptophyl quinones using a combined QM/MM approach. *Journal of Physical Chemistry A*, **2010**, 114, 1212-7	2.8	7
47	Theoretical Investigation on the Mechanism of Oxygen Atom Transfer between Two Non-Heme Iron Centres. *European Journal of Inorganic Chemistry*, **2008**, 2008, 1027-1030	2.3	7
46	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
45	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
44	Second-Coordination Sphere Effect on the Reactivity of Vanadium-Peroxo Complexes: A Computational Study. *Inorganic Chemistry*, **2019**, 58, 15741-15750	5.1	6
43	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
42	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
41	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
40	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
39	Regio- and Enantio-selective Chemo-enzymatic C-Lactonization of Decanoic Acid to (S)-Decalactone. *Angewandte Chemie*, **2019**, 131, 5724-5727	3.6	5

38	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
37	Can Manganese(III)-Iodosylarene Act as an Oxidant Alongside High-Valent Manganese(V)-Oxo Complexes?. *ChemistrySelect*, **2018**, 3, 3208-3213	1.8	5
36	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
35	A Trimetal Carbene with Reactivity Reminiscent of Fischer–Tropsch Catalysis. *Organometallics*, **2015** , 34, 1651-1660	3.8	4
34	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
33	Catalytic Function and Mechanism of Heme and Nonheme Iron(IV)–Oxo Complexes in Nature **2015**, 185-202		4
32	Modeling flexible pharmacophores with distance geometry, scoring, and bound stretching. *Journal of Chemical Information and Modeling*, **2012**, 52, 577-88	6.1	4
31	Polarizability-based equation of state: Application to CO, N2 and O2. *Chemical Physics Letters*, **2011**, 515, 170-172	2.5	4
30	Characterization of isomeric C4H5– anions in the gas phase; theory and experiment. *Journal of Mass Spectrometry*, **1999**, 34, 303-310	2.2	4
29	The Accuracy of Density Functional Theory Calculations in Biocatalysis **2012**, 1,		4
28	Properties and reactivity of μ-nitrido-bridged dimetal porphyrinoid complexes: how does ruthenium compare to iron?. *Journal of Biological Inorganic Chemistry*, **2019**, 24, 1127-1134	3.7	3
27	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
26	Chapter 1:Experimental and Computational Studies on the Catalytic Mechanism of Non-heme Iron Dioxygenases1-41		3
25	Chameleon States: High-Valent Metal–Oxo Species of Cytochrome P450 and Its Ruthenium Analogue. *Angewandte Chemie*, **2001**, 113, 3612-3612	3.6	3
24	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
23	Structure and Functional Differences of Cysteine and 3-Mercaptopropionate Dioxygenases: A Computational Study. *Chemistry - A European Journal*, **2021**, 27, 13793-13806	4.8	3
22	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
21	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

20	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
19	Theoretical Perspective on the Structure and Mechanism of Cytochrome P450 Enzymes. *ChemInform*, **2005**, 36, no		2
18	Electrostatic perturbations in the substrate-binding pocket of taurine/□ketoglutarate dioxygenase determine its selectivity.. *Chemistry - A European Journal*, **2021**,	4.8	2
17	Methane Hydroxylation by Axially Ligated Iron (IV)-oxo Porphyrin Cation Radical Models **2016**, 1,		2
16	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
15	Computational Study on the Catalytic Reaction Mechanism of Heme Haloperoxidase Enzymes. *Israel Journal of Chemistry*, **2020**, 60, 963-972	3.4	2
14	Density Functional Theory Study into the Reaction Mechanism of Isonitrile Biosynthesis by the Nonheme Iron Enzyme ScoE. *Topics in Catalysis*,1	2.3	2
13	Product Distributions of Cytochrome P450 OleT with Phenyl-Substituted Fatty Acids: A Computational Study. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	2
12	Computational Study on O□O Bond Formation on a Mononuclear Non-Heme Iron Center. *European Journal of Inorganic Chemistry*, **2020**, 2020, 2573-2581	2.3	1
11	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
10	Mechanism of Oxidation Reactions Catalyzed by Cytochrome P450 Enzyme. *ChemInform*, **2004**, 35, no		1
9	A Noncanonical Tryptophan Analogue Reveals an Active Site Hydrogen Bond Controlling Ferryl Reactivity in a Heme Peroxidase. *Jacs Au*, **2021**, 1, 913-918		1
8	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
7	Theoretical studies unveil the unusual bonding in oxygenation reactions involving cobalt(ii)-iodylarene complexes. *Chemical Communications*, **2021**, 57, 3115-3118	5.8	1
6	Mechanism of substrate inhibition in cytochrome-c dependent NO reductases from denitrifying bacteria (cNORs).. *Journal of Inorganic Biochemistry*, **2022**, 231, 111781	4.2	1
5	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
4	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	
3	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	

2	A tribute to Sason Shaik. *Journal of Physical Chemistry A*, **2008**, 112, 12721-3	2.8
1	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