Sam P De Visser

List of Publications by Year
in descending order

276 papers	18,167 citations	10351 72 h-index	16605 123 g-index
292 all docs	292 docs citations	292 times ranked	8619 citing authors

#	Article	IF	Citations
1	Density Functional Theory Study into the Reaction Mechanism of Isonitrile Biosynthesis by the Nonheme Iron Enzyme ScoE. Topics in Catalysis, 2022, 65, 528-543.	1.3	8
2	Oxidative dehalogenation of halophenols by high-valent nonheme iron(<scp>iv</scp>)-oxo intermediates. Faraday Discussions, 2022, 234, 58-69.	1.6	5
3	Biodegradation of Herbicides by a Plant Nonheme Iron Dioxygenase: Mechanism and Selectivity of Substrate Analogues. Chemistry - A European Journal, 2022, 28, .	1.7	6
4	Electrostatic Perturbations in the Substrateâ€Binding Pocket of Taurine/Î±â€Ketoglutarate Dioxygenase Determine its Selectivity. Chemistry - A European Journal, 2022, 28, .	1.7	32
5	Status report on the quantum chemical cluster approach for modeling enzyme reactions. Communications Chemistry, 2022, 5, .	2.0	40
6	Cluster Model Study into the Catalytic Mechanism of Î±-Ketoglutarate Biodegradation by the Ethylene-Forming Enzyme Reveals Structural Differences with Nonheme Iron Hydroxylases. ACS Catalysis, 2022, 12, 3923-3937.	5.5	17
7	Mechanism of substrate inhibition in cytochrome-c dependent NO reductases from denitrifying bacteria (cNORs). Journal of Inorganic Biochemistry, 2022, 231, 111781.	1.5	1
8	Local Charge Distributions, Electric Dipole Moments, and Local Electric Fields Influence Reactivity Patterns and Guide Regioselectivities in Î±-Ketoglutarate-Dependent Non-heme Iron Dioxygenases. Accounts of Chemical Research, 2022, 55, 65-74.	7.6	48
9	Second Coordination Sphere Effects on the Mechanistic Pathways for Dioxygen Activation by a Ferritin: Involvement of a Tyr Radical and the Identification of a Cation Binding Site. ChemBioChem, 2022, 23, .	1.3	12
10	What Drives Radical Halogenation versus Hydroxylation in Mononuclear Nonheme Iron Complexes? A Combined Experimental and Computational Study. Journal of the American Chemical Society, 2022, 144, 10752-10767.	6.6	27
11	A comprehensive insight into aldehyde deformylation: mechanistic implications from biology and chemistry. Organic and Biomolecular Chemistry, 2021, 19, 1879-1899.	1.5	25
12	What Determines the Selectivity of Arginine Dihydroxylation by the Nonheme Iron Enzyme OrfP?. Chemistry - A European Journal, 2021, 27, 1795-1809.	1.7	26
13	Theoretical studies unveil the unusual bonding in oxygenation reactions involving cobalt(<scp>ii</scp>)-iodylarene complexes. Chemical Communications, 2021, 57, 3115-3118.	2.2	4
14	Taurine/Alpha-Ketoglutarate Dioxygenase: Computational Studies. , 2021, , 1-4.		0
15	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.	1.1	33
16	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.	1.9	14
17	Mechanism of Oxidative Ringâ€Closure as Part of the Hygromycin Biosynthesis Step by a Nonheme Iron Dioxygenase. ChemCatChem, 2021, 13, 3054-3066.	1.8	13
18	A Noncanonical Tryptophan Analogue Reveals an Active Site Hydrogen Bond Controlling Ferryl Reactivity in a Heme Peroxidase. Jacs Au, 2021, 1, 913-918.	3.6	8

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19	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.	0.7	2
20	Electrostatic Perturbations from the Protein Affect Câˆ'H Bond Strengths of the Substrate and Enable Negative Catalysis in the TmpA Biosynthesis Enzyme. Chemistry - A European Journal, 2021, 27, 8851-8864.	1.7	20
21	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.	1.9	0
22	Energyâ€"entropy method using multiscale cell correlation to calculate binding free energies in the SAMPL8 hostâ€"guest challenge. Journal of Computer-Aided Molecular Design, 2021, 35, 911-921.	1.3	11
23	Product Distributions of Cytochrome P450 OleTJE with Phenyl-Substituted Fatty Acids: A Computational Study. International Journal of Molecular Sciences, 2021, 22, 7172.	1.8	6
24	Inspiration from Nature: Influence of Engineered Ligand Scaffolds and Auxiliary Factors on the Reactivity of Biomimetic Oxidants. ACS Catalysis, 2021, 11, 9761-9797.	5.5	54
25	Negative catalysis / non-Bell-Evans-Polanyi reactivity by metalloenzymes: Examples from mononuclear heme and non-heme iron oxygenases. Coordination Chemistry Reviews, 2021, 439, 213914.	9.5	41
26	Structure and Functional Differences of Cysteine and 3â€Mercaptopropionate Dioxygenases: A Computational Study. Chemistry - A European Journal, 2021, 27, 13793-13806.	1.7	12
27	Proton-coupled electron transfer reactivities of electronically divergent heme superoxide intermediates: a kinetic, thermodynamic, and theoretical study. Chemical Science, 2021, 12, 8872-8883.	3.7	13
28	Can a Mononuclear Iron(III)â€Superoxo Active Site Catalyze the Decarboxylation of Dodecanoic Acid in UndA to Produce Biofuels?. Chemistry - A European Journal, 2020, 26, 2233-2242.	1.7	24
29	Computational Study on the Catalytic Reaction Mechanism of Heme Haloperoxidase Enzymes. Israel Journal of Chemistry, 2020, 60, 963-972.	1.0	5
30	Secondâ€Coordination Sphere Effects on Selectivity and Specificity of Heme and Nonheme Iron Enzymes. Chemistry - A European Journal, 2020, 26, 5308-5327.	1.7	75
31	Hydroxyl Transfer to Carbon Radicals by Mn(OH) vs Fe(OH) Corrole Complexes. Inorganic Chemistry, 2020, 59, 16053-16064.	1.9	24
32	How Do Vanadium Chloroperoxidases Generate Hypochlorite from Hydrogen Peroxide and Chloride? A Computational Study. ACS Catalysis, 2020, 10, 14067-14079.	5.5	19
33	How Do Metal Ions Modulate the Rateâ€Determining Electronâ€Transfer Step in Cytochrome P450 Reactions?. Chemistry - A European Journal, 2020, 26, 15270-15281.	1.7	15
34	Fe-Catalyzed Aziridination Is Governed by the Electron Affinity of the Active Imido-Iron Species. ACS Catalysis, 2020, 10, 10010-10020.	5.5	42
35	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.	6.6	55
36	How external perturbations affect the chemoselectivity of substrate activation by cytochrome P450 OleT_{JE}. Physical Chemistry Chemical Physics, 2020, 22, 27178-27190.	1.3	13

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37	Bioengineering of Cytochrome P450 OleTJE: How Does Substrate Positioning Affect the Product Distributions?. Molecules, 2020, 25, 2675.	1.7	21
38	Computational Study on Oâ€“O Bond Formation on a Mononuclear Nonâ€Heme Iron Center. European Journal of Inorganic Chemistry, 2020, 2020, 2573-2581.	1.0	2
39	Inorganic reaction mechanisms. Dalton Transactions, 2020, 49, 4597-4598.	1.6	0
40	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.	1.5	19
41	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.	1.2	8
42	Lignin Biodegradation by a Cytochrome P450 Enzyme: Aâ€‰Computational Study into Syringol Activation by GcoA. Chemistry - A European Journal, 2020, 26, 13093-13102.	1.7	34
43	Computational studies of DNA base repair mechanisms by nonheme iron dioxygenases: selective epoxidation and hydroxylation pathways. Dalton Transactions, 2020, 49, 4266-4276.	1.6	15
44	O₂ Activation by Non-Heme Thiolate-Based Dinuclear Fe Complexes. Inorganic Chemistry, 2020, 59, 3249-3259.	1.9	17
45	Sluggish reactivity by a nonheme iron(<scp>iv</scp>)-tosylimido complex as compared to its oxo analogue. Dalton Transactions, 2020, 49, 5921-5931.	1.6	17
46	Frontispiece: Secondâ€Coordination Sphere Effects on Selectivity and Specificity of Heme and Nonheme Iron Enzymes. Chemistry - A European Journal, 2020, 26, .	1.7	1
47	How Does Replacement of the Axial Histidine Ligand in Cytochrome c Peroxidase by NÎ´-Methyl Histidine Affect Its Properties and Functions? A Computational Study. International Journal of Molecular Sciences, 2020, 21, 7133.	1.8	5
48	Cysteine Dioxygenase â€“ Computational Studies. , 2020, , 1-3.		0
49	The Hunt for the Closed Conformation of the Fruitâ€Ripening Enzyme 1â€Aminocyclopropaneâ€1â€carboxylic Oxidase: A Combined Electron Paramagnetic Resonance and Molecular Dynamics Study. Chemistry - A European Journal, 2019, 25, 13766-13776.	1.7	4
50	Mechanistic Investigation of Oxygen Rebound in a Mononuclear Nonheme Iron Complex. Inorganic Chemistry, 2019, 58, 9557-9561.	1.9	14
51	CO₂ Reduction on an Iron-Porphyrin Center: A Computational Study. Journal of Physical Chemistry A, 2019, 123, 6527-6535.	1.1	45
52	Mechanism of Oxidative Activation of Fluorinated Aromatic Compounds by Nâ€Bridged Diironâ€Phthalocyanine: What Determines the Reactivity?. Chemistry - A European Journal, 2019, 25, 14320-14331.	1.7	43
53	Second-Coordination Sphere Effect on the Reactivity of Vanadiumâ€“Peroxo Complexes: A Computational Study. Inorganic Chemistry, 2019, 58, 15741-15750.	1.9	7
54	Properties and reactivity of Î¼-nitrido-bridged dimetal porphyrinoid complexes: how does ruthenium compare to iron?. Journal of Biological Inorganic Chemistry, 2019, 24, 1127-1134.	1.1	5

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55	Interplay Between Steric and Electronic Effects: A Joint Spectroscopy and Computational Study of Nonheme Iron(IV)â€Oxo Complexes. Chemistry - A European Journal, 2019, 25, 5086-5098.	1.7	44
56	Hydrogen by Deuterium Substitution in an Aldehyde Tunes the Regioselectivity by a Nonheme Manganese(III)â€"Peroxo Complex. Angewandte Chemie, 2019, 131, 10749-10753.	1.6	15
57	Flavonol biosynthesis by nonheme iron dioxygenases: A computational study into the structure and mechanism. Journal of Inorganic Biochemistry, 2019, 198, 110728.	1.5	17
58	Hydrogen by Deuterium Substitution in an Aldehyde Tunes the Regioselectivity by a Nonheme Manganese(III)â€"Peroxo Complex. Angewandte Chemie - International Edition, 2019, 58, 10639-10643.	7.2	37
59	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.	6.6	56
60	The Quest for Accurate Theoretical Models of Metalloenzymes: An Aid to Experiment. Challenges and Advances in Computational Chemistry and Physics, 2019, , 439-462.	0.6	0
61	Regioâ€•and Enantioâ€selective Chemoâ€enzymatic Câˆ'Hâ€Lactonization of Decanoic Acid to (<i>S</i>)â€Î´â€Decalactone. Angewandte Chemie - International Edition, 2019, 58, 5668-5671.	7.2	50
62	Regioâ€•and Enantioâ€selective Chemoâ€enzymatic Câˆ'Hâ€Lactonization of Decanoic Acid to (<i>S</i>)â€Î´â€Decalactone. Angewandte Chemie, 2019, 131, 5724-5727.	1.6	8
63	The Equatorial Ligand Effect on the Properties and Reactivity of Iron(V) Oxo Intermediates. Chemistry - A European Journal, 2019, 25, 8092-8104.	1.7	17
64	Equatorial ligand plane perturbations lead to a spin-state change in an iron(iii) porphyrin dimer. Dalton Transactions, 2019, 48, 6353-6357.	1.6	17
65	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.	6.6	66
66	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.	1.9	24
67	Reactivity patterns of vanadium(<scp>iv</scp>/<scp>v</scp>)-oxo complexes with olefins in the presence of peroxides: a computational study. Dalton Transactions, 2019, 48, 16899-16910.	1.6	12
68	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.	6.6	52
69	Selective Formation of an Fe^{IV}O or an Fe^{III}OOH Intermediate From Iron(II) and H₂O₂: Controlled Heterolytic versus Homolytic Oxygenâ€"Oxygen Bond Cleavage by the Second Coordination Sphere. Angewandte Chemie - International Edition, 2019, 58, 854-858.	7.2	54
70	Mechanistic Studies of Fatty Acid Activation by CYP152 Peroxygenases Reveal Unexpected Desaturase Activity. ACS Catalysis, 2019, 9, 565-577.	5.5	76
71	Selective Formation of an Fe^{IV}O or an Fe^{III}OOH Intermediate From Iron(II) and H₂O₂: Controlled Heterolytic versus Homolytic Oxygenâ€"Oxygen Bond Cleavage by the Second Coordination Sphere. Angewandte Chemie, 2019, 131, 864-868.	1.6	25
72	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.	1.0	7

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73	Can Manganese(III)â€Iodosylarene Act as an Oxidant Alongside Highâ€Valent Manganese(V)â€Oxo Complexes?. ChemistrySelect, 2018, 3, 3208-3213.	0.7	5
74	Nitrogen Reduction to Ammonia on a Biomimetic Mononuclear Iron Centre: Insights into the Nitrogenase Enzyme. Chemistry - A European Journal, 2018, 24, 5293-5302.	1.7	44
75	Mechanistic Insight on the Activity and Substrate Selectivity of Nonheme Iron Dioxygenases. Chemical Record, 2018, 18, 1501-1516.	2.9	30
76	Does Substrate Positioning Affect the Selectivity and Reactivity in the Hectochlorin Biosynthesis Halogenase?. Frontiers in Chemistry, 2018, 6, 513.	1.8	37
77	Editorial: Quantum Mechanical/Molecular Mechanical Approaches for the Investigation of Chemical Systems â€" Recent Developments and Advanced Applications. Frontiers in Chemistry, 2018, 6, 357.	1.8	32
78	Catalytic Mechanism of Nogalamycin Monoxygenase: How Does Nature Synthesize Antibiotics without a Metal Cofactor?. Journal of Physical Chemistry B, 2018, 122, 10841-10854.	1.2	11
79	Dramatic rate-enhancement of oxygen atom transfer by an iron(<scp>iv</scp>)-oxo species by equatorial ligand field perturbations. Dalton Transactions, 2018, 47, 14945-14957.	1.6	32
80	A Comparative Review on the Catalytic Mechanism of Nonheme Iron Hydroxylases and Halogenases. Catalysts, 2018, 8, 314.	1.6	50
81	Group Transfer to an Aliphatic Bond: A Biomimetic Study Inspired by Nonheme Iron Halogenases. ACS Catalysis, 2018, 8, 8685-8698.	5.5	32
82	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, 1974.	1.8	14
83	Solventâ€and Halideâ€Induced (Inter)conversion between Iron(II)â€Disulfide and Iron(III)â€Thiolate Complexes. Chemistry - A European Journal, 2018, 24, 11973-11982.	1.7	19
84	Oxygen Atom Transfer Using an Iron(IV)â€Oxo Embedded in a Tetracyclic Nâ€Heterocyclic Carbene System: How Does the Reactivity Compare to Cytochrome P450 Compoundâ€…I?. Chemistry - A European Journal, 2017, 23, 2935-2944.	1.7	36
85	Modulation of Antimalarial Activity at a Putative Bisquinoline Receptor In Vivo Using Fluorinated Bisquinolines. Chemistry - A European Journal, 2017, 23, 6811-6828.	1.7	11
86	Reactivity Patterns of (Protonated) Compoundâ€…II and Compoundâ€…I of Cytochrome P450: Which is the Better Oxidant?. Chemistry - A European Journal, 2017, 23, 6406-6418.	1.7	71
87	Glutathione binding to dirhodium tetraacetate: a spectroscopic, mass spectral and computational study of an anti-tumour compound. Metallomics, 2017, 9, 501-516.	1.0	6
88	A Highâ€Valent Nonâ€Heme Î¼â€Oxo Manganese(IV) Dimer Generated from a Thiolateâ€Bound Manganese(II) Complex and Dioxygen. Angewandte Chemie - International Edition, 2017, 56, 8211-8215.	7.2	29
89	Sulfoxide Synthase versus Cysteine Dioxygenase Reactivity in a Nonheme Iron Enzyme. Journal of the American Chemical Society, 2017, 139, 9259-9270.	6.6	97
90	A Highâ€Valent Nonâ€Heme Î¼â€Oxo Manganese(IV) Dimer Generated from a Thiolateâ€Bound Manganese(II) Complex and Dioxygen. Angewandte Chemie, 2017, 129, 8323-8327.	1.6	10

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91	Prediction of Reduction Potentials of Copper Proteins with Continuum Electrostatics and Density Functional Theory. Chemistry - A European Journal, 2017, 23, 15436-15445.	1.7	20
92	Features of reactive cysteines discovered through computation: from kinase inhibition to enrichment around protein degrons. Scientific Reports, 2017, 7, 16338.	1.6	19
93	Ketoâ€“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.	6.6	66
94	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.	0.4	2
95	Understanding How Prolyl-4-hydroxylase Structure Steers a Ferryl Oxidant toward Scission of a Strong Câ€“H Bond. Journal of the American Chemical Society, 2017, 139, 9855-9866.	6.6	80
96	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.	3.3	23
97	Biodegradation of Cosmetics Products: A Computational Study of Cytochrome P450 Metabolism of Phthalates. Inorganics, 2017, 5, 77.	1.2	16
98	How Are Substrate Binding and Catalysis Affected by Mutating Glu127 and Arg161 in Prolyl-4-hydroxylase? A QM/MM and MD Study. Frontiers in Chemistry, 2017, 5, 94.	1.8	14
99	Challenging Density Functional Theory Calculations with Hemes and Porphyrins. International Journal of Molecular Sciences, 2016, 17, 519.	1.8	25
100	Influence of cysteine 164 on active site structure in rat cysteine dioxygenase. Journal of Biological Inorganic Chemistry, 2016, 21, 501-510.	1.1	18
101	Arene activation by a nonheme iron(III)â€“hydroperoxo complex: pathways leading to phenol and ketone products. Journal of Biological Inorganic Chemistry, 2016, 21, 453-462.	1.1	16
102	Deformylation Reaction by a Nonheme Manganese(III)â€“Peroxo Complex via Initial Hydrogenâ€Atom Abstraction. Angewandte Chemie, 2016, 128, 11257-11261.	1.6	23
103	A Systematic Account on Aromatic Hydroxylation by a Cytochrome P450 Model Compound I: A Lowâ€Pressure Mass Spectrometry and Computational Study. Chemistry - A European Journal, 2016, 22, 18608-18619.	1.7	74
104	Influence of Ligand Architecture in Tuning Reaction Bifurcation Pathways for Chlorite Oxidation by Non-Heme Iron Complexes. Inorganic Chemistry, 2016, 55, 10170-10181.	1.9	17
105	Deformylation Reaction by a Nonheme Manganese(III)â€“Peroxo Complex via Initial Hydrogenâ€Atom Abstraction. Angewandte Chemie - International Edition, 2016, 55, 11091-11095.	7.2	73
106	Singlet versus Triplet Reactivity in an Mn(V)â€“Oxo Species: Testing Theoretical Predictions Against Experimental Evidence. Journal of the American Chemical Society, 2016, 138, 12375-12386.	6.6	88
107	Substrate Sulfoxidation by an Iron(IV)-Oxo Complex: Benchmarking Computationally Calculated Barrier Heights to Experiment. Journal of Physical Chemistry A, 2016, 120, 9805-9814.	1.1	80
108	Quantum Mechanics/Molecular Mechanics Modeling of Enzymatic Processes: Caveats and Breakthroughs. Chemistry - A European Journal, 2016, 22, 2562-2581.	1.7	133

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109	Frontispiece: 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, .	1.7	0
110	Origin of the Regioselective Fattyâ€Acid Hydroxylation versus Decarboxylation by a Cytochrome P450 Peroxygenase: What Drives the Reaction to Biofuel Production?. Chemistry - A European Journal, 2016, 22, 5478-5483.	1.7	102
111	Origin of the Enhanced Reactivity of Î¼-Nitrido-Bridged Diiron(IV)-Oxo Porphyrinoid Complexes over Cytochrome P450 Compound I. ACS Catalysis, 2016, 6, 2230-2243.	5.5	98
112	Methane Hydroxylation by Axially Ligated Iron (IV)-oxo Porphyrin Cation Radical Models. International Journal of Science, Technology and Society, 2016, 1, .	0.2	2
113	Drug Metabolism by Cytochrome P450 Enzymes: What Distinguishes the Pathways Leading to Substrate Hydroxylation Over Desaturation?. Chemistry - A European Journal, 2015, 21, 8973-8973.	1.7	3
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, 7470-7479.	1.7	20
115	Alkyl Chain Growth on a Transition Metal Center: How Does Iron Compare to Ruthenium and Osmium?. International Journal of Molecular Sciences, 2015, 16, 23369-23381.	1.8	0
116	Enzymatic Halogenases and Haloperoxidases. Advances in Protein Chemistry and Structural Biology, 2015, 100, 113-151.	1.0	17
117	Catalytic Mechanism of Cofactor-Free Dioxygenases and How They Circumvent Spin-Forbidden Oxygenation of Their Substrates. Journal of the American Chemical Society, 2015, 137, 7474-7487.	6.6	70
118	A comprehensive test set of epoxidation rate constants for iron(<scp>iv</scp>)â€“oxo porphyrin cation radical complexes. Chemical Science, 2015, 6, 1516-1529.	3.7	96
119	Identification and Spectroscopic Characterization of Nonheme Iron(III) Hypochlorite Intermediates. Angewandte Chemie, 2015, 127, 4431-4435.	1.6	13
120	Identification and Spectroscopic Characterization of Nonheme Iron(III) Hypochlorite Intermediates. Angewandte Chemie - International Edition, 2015, 54, 4357-4361.	7.2	38
121	Spin-State Ordering in Hydroxo-Bridged Diiron(III)bisporphyrin Complexes. Inorganic Chemistry, 2015, 54, 1919-1930.	1.9	49
122	Hydrogenâ€Bonding Interactions Trigger a Spinâ€Flip in Iron(III) Porphyrin Complexes. Angewandte Chemie, 2015, 127, 4878-4882.	1.6	33
123	Site-selective formation of an iron(<scp>iv</scp>)â€“oxo species at the more electron-rich iron atom of heteroleptic Î¼-nitrido diiron phthalocyanines. Chemical Science, 2015, 6, 5063-5075.	3.7	70
124	Drug Metabolism by Cytochrome P450 Enzymes: What Distinguishes the Pathways Leading to Substrate Hydroxylation Over Desaturation?. Chemistry - A European Journal, 2015, 21, 9083-9092.	1.7	116
125	A Trimetal Carbene with Reactivity Reminiscent of Fischerâ€“Tropsch Catalysis. Organometallics, 2015, 34, 1651-1660.	1.1	5
126	Hydrogenâ€Bonding Interactions Trigger a Spinâ€Flip in Iron(III) Porphyrin Complexes. Angewandte Chemie - International Edition, 2015, 54, 4796-4800.	7.2	83

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127	Differences and Comparisons of the Properties and Reactivities of Iron(III)â€“hydroperoxo Complexes with Saturated Coordination Sphere. Chemistry - A European Journal, 2015, 21, 1221-1236.	1.7	67
128	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.	1.6	30
129	Long-Range Electron Transfer Triggers Mechanistic Differences between Iron(IV)-Oxo and Iron(IV)-Imido Oxidants. Journal of the American Chemical Society, 2014, 136, 17102-17115.	6.6	106
130	Experimental and Computational Evidence for the Mechanism of Intradiol Catechol Dioxygenation by Nonâ€Heme Iron(III) Complexes. Chemistry - A European Journal, 2014, 20, 15686-15691.	1.7	22
131	Origin of the Proton-transfer Step in the Cofactor-free (1H)-3-Hydroxy-4-oxoquinaldine 2,4-Dioxygenase. Journal of Biological Chemistry, 2014, 289, 8620-8632.	1.6	31
132	Metabolism of Halogenated Alkanes by Cytochrome P450 enzymes. Aerobic Oxidation versus Anaerobic Reduction. Chemistry - an Asian Journal, 2014, 9, 1175-1182.	1.7	19
133	Computational modelling of oxygenation processes in enzymes and biomimetic model complexes. Chemical Communications, 2014, 50, 262-282.	2.2	110
134	Direct Observation of a Nonheme Iron(IV)â€“Oxo Complex That Mediates Aromatic Câ€“F Hydroxylation. Journal of the American Chemical Society, 2014, 136, 13542-13545.	6.6	66
135	Oxygen-Atom Transfer Reactivity of Axially Ligated Mn(V)â€“Oxo Complexes: Evidence for Enhanced Electrophilic and Nucleophilic Pathways. Journal of the American Chemical Society, 2014, 136, 13845-13852.	6.6	68
136	Properties and reactivities of nonheme iron(<scp>iv</scp>)â€“oxo versus iron(<scp>v</scp>)â€“oxo: long-range electron transfer versus hydrogen atom abstraction. Physical Chemistry Chemical Physics, 2014, 16, 22611-22622.	1.3	7
137	Frontispiece: Experimental and Computational Evidence for the Mechanism of Intradiol Catechol Dioxygenation by Non-Heme Iron(III) Complexes. Chemistry - A European Journal, 2014, 20, n/a-n/a.	1.7	0
138	Dramatic Influence of an Anionic Donor on the Oxygenâ€Atom Transfer Reactivity of a Mn^Vâ€“Oxo Complex. Chemistry - A European Journal, 2014, 20, 14584-14588.	1.7	26
139	Quantum Mechanics/Molecular Mechanics Study on the Oxygen Binding and Substrate Hydroxylation Step in AlkB Repair Enzymes. Chemistry - A European Journal, 2014, 20, 435-446.	1.7	122
140	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, 10590-10593.	6.6	102
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