# Sam Hay

#### List of Publications by Citations

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129<br/>papers3,161<br/>citations30<br/>h-index50<br/>g-index136<br/>ext. papers3,590<br/>ext. citations9<br/>avg, IF5.31<br/>L-index

#	Paper	IF	Citations
129	Good vibrations in enzyme-catalysed reactions. <i>Nature Chemistry</i> , <b>2012</b> , 4, 161-8	17.6	216
128	Reductive dehalogenase structure suggests a mechanism for B12-dependent dehalogenation. <i>Nature</i> , <b>2015</b> , 517, 513-516	50.4	200
127	New cofactor supports Hunsaturated acid decarboxylation via 1,3-dipolar cycloaddition. <i>Nature</i> , <b>2015</b> , 522, 497-501	50.4	156
126	UbiX is a flavin prenyltransferase required for bacterial ubiquinone biosynthesis. <i>Nature</i> , <b>2015</b> , 522, 50	2- <b>6</b> 0.4	136
125	Promoting motions in enzyme catalysis probed by pressure studies of kinetic isotope effects.  Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 507-12	11.5	92
124	Fast protein motions are coupled to enzyme H-transfer reactions. <i>Journal of the American Chemical Society</i> , <b>2013</b> , 135, 2512-7	16.4	76
123	Direct analysis of donor-acceptor distance and relationship to isotope effects and the force constant for barrier compression in enzymatic H-tunneling reactions. <i>Journal of the American Chemical Society</i> , <b>2010</b> , 132, 11329-35	16.4	70
122	Evidence to support the hypothesis that promoting vibrations enhance the rate of an enzyme catalyzed H-tunneling reaction. <i>Journal of the American Chemical Society</i> , <b>2009</b> , 131, 17072-3	16.4	68
121	Deep tunneling dominates the biologically important hydride transfer reaction from NADH to FMN in morphinone reductase. <i>Journal of the American Chemical Society</i> , <b>2008</b> , 130, 7092-7	16.4	68
120	Alpha-secondary isotope effects as probes of "tunneling-ready" configurations in enzymatic H-tunneling: insight from environmentally coupled tunneling models. <i>Journal of the American Chemical Society</i> , <b>2006</b> , 128, 14053-8	16.4	65
119	Carboxylesterase converts Amplex red to resorufin: Implications for mitochondrial H2O2 release assays. <i>Free Radical Biology and Medicine</i> , <b>2016</b> , 90, 173-83	7.8	62
118	Proton tunneling in aromatic amine dehydrogenase is driven by a short-range sub-picosecond promoting vibration: consistency of simulation and theory with experiment. <i>Journal of Physical Chemistry B</i> , <b>2007</b> , 111, 2631-8	3.4	61
117	Nature of the energy landscape for gated electron transfer in a dynamic redox protein. <i>Journal of the American Chemical Society</i> , <b>2010</b> , 132, 9738-45	16.4	57
116	Barrier compression enhances an enzymatic hydrogen-transfer reaction. <i>Angewandte Chemie - International Edition</i> , <b>2009</b> , 48, 1452-4	16.4	51
115	Conformational and thermodynamic control of electron transfer in neuronal nitric oxide synthase. <i>Biochemistry</i> , <b>2007</b> , 46, 5018-29	3.2	50
114	Demonstration of proton-coupled electron transfer in the copper-containing nitrite reductases. Journal of Biological Chemistry, <b>2009</b> , 284, 25973-83	5.4	46
113	Are the catalytic properties of enzymes from piezophilic organisms pressure adapted?. <i>ChemBioChem</i> , <b>2009</b> , 10, 2348-53	3.8	45

## (2011-2007)

112	Mutagenesis of morphinone reductase induces multiple reactive configurations and identifies potential ambiguity in kinetic analysis of enzyme tunneling mechanisms. <i>Journal of the American Chemical Society</i> , <b>2007</b> , 129, 13949-56	16.4	45	
111	Magnetic field effect studies indicate reduced geminate recombination of the radical pair in substrate-bound adenosylcobalamin-dependent ethanolamine ammonia lyase. <i>Journal of the American Chemical Society</i> , <b>2007</b> , 129, 15718-27	16.4	44	
110	Protein engineering of cytochrome b562 for quinone binding and light-induced electron transfer. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2004</b> , 101, 17675-80	11.5	44	
109	Decoupled Associative and Dissociative Processes in Strong yet Highly Dynamic Host-Guest Complexes. <i>Journal of the American Chemical Society</i> , <b>2017</b> , 139, 12985-12993	16.4	43	
108	Barrier compression and its contribution to both classical and quantum mechanical aspects of enzyme catalysis. <i>Biophysical Journal</i> , <b>2010</b> , 98, 121-8	2.9	42	
107	Structural basis for enzymatic photocatalysis in chlorophyll biosynthesis. <i>Nature</i> , <b>2019</b> , 574, 722-725	50.4	38	
106	Inter-flavin electron transfer in cytochrome P450 reductase - effects of solvent and pH identify hidden complexity in mechanism. <i>FEBS Journal</i> , <b>2008</b> , 275, 4540-57	5.7	36	
105	Incorporation of hydrostatic pressure into models of hydrogen tunneling highlights a role for pressure-modulated promoting vibrations. <i>Biochemistry</i> , <b>2008</b> , 47, 9880-7	3.2	35	
104	A <b>9</b> lug and PlaySPlatform for the Production of Diverse Monoterpene Hydrocarbon Scaffolds in. <i>ChemistrySelect</i> , <b>2016</b> , 1, 1893-1896	1.8	32	
103	Structural Basis of Catalysis in the Bacterial Monoterpene Synthases Linalool Synthase and 1,8-Cineole Synthase. <i>ACS Catalysis</i> , <b>2017</b> , 7, 6268-6282	13.1	31	
102	Ultrafast infrared spectral fingerprints of vitamin B12 and related cobalamins. <i>Journal of Physical Chemistry A</i> , <b>2012</b> , 116, 5586-94	2.8	31	
101	Electrochemical and structural properties of a protein system designed to generate tyrosine Pourbaix diagrams. <i>Journal of the American Chemical Society</i> , <b>2011</b> , 133, 17786-95	16.4	31	
100	Are environmentally coupled enzymatic hydrogen tunneling reactions influenced by changes in solution viscosity?. <i>Angewandte Chemie - International Edition</i> , <b>2008</b> , 47, 537-40	16.4	31	
99	Donor-Acceptor Distance Sampling Enhances the Performance of "Better than Nature" Nicotinamide Coenzyme Biomimetics. <i>Journal of the American Chemical Society</i> , <b>2016</b> , 138, 11089-92	16.4	30	
98	Dual transcriptional-translational cascade permits cellular level tuneable expression control. <i>Nucleic Acids Research</i> , <b>2016</b> , 44, e21	20.1	29	
97	Gating mechanisms for biological electron transfer: integrating structure with biophysics reveals the nature of redox control in cytochrome P450 reductase and copper-dependent nitrite reductase. <i>FEBS Letters</i> , <b>2012</b> , 586, 578-84	3.8	29	
96	Epoxyqueuosine Reductase Structure Suggests a Mechanism for Cobalamin-dependent tRNA Modification. <i>Journal of Biological Chemistry</i> , <b>2015</b> , 290, 27572-81	5.4	28	
95	Is there a dynamic protein contribution to the substrate trigger in coenzyme B12-dependent ethanolamine ammonia lyase?. <i>Angewandte Chemie - International Edition</i> , <b>2011</b> , 50, 10843-6	16.4	28	

94	Structural and mechanistic aspects of flavoproteins: probes of hydrogen tunnelling. <i>FEBS Journal</i> , <b>2009</b> , 276, 3930-41	5.7	27
93	Quantum Biology: An Update and Perspective. <i>Quantum Reports</i> , <b>2021</b> , 3, 80-126	2.1	26
92	Convergence of theory and experiment on the role of preorganization, quantum tunneling and enzyme motions into flavoenzyme-catalyzed hydride transfer. <i>ACS Catalysis</i> , <b>2019</b> , 7, 3190-3198	13.1	25
91	Moving a phenol hydroxyl group from the surface to the interior of a protein: effects on the phenol potential and pK(A). <i>Biochemistry</i> , <b>2005</b> , 44, 11891-902	3.2	25
90	Protein motions are coupled to the reaction chemistry in coenzyme B12-dependent ethanolamine ammonia lyase. <i>Angewandte Chemie - International Edition</i> , <b>2012</b> , 51, 9306-10	16.4	24
89	Relating localized protein motions to the reaction coordinate in coenzyme BEdependent enzymes. <i>FEBS Journal</i> , <b>2013</b> , 280, 2997-3008	5.7	24
88	DNA binding suppresses human AIF-M2 activity and provides a connection between redox chemistry, reactive oxygen species, and apoptosis. <i>Journal of Biological Chemistry</i> , <b>2007</b> , 282, 30331-40	5.4	24
87	Untangling Heavy Protein and Cofactor Isotope Effects on Enzyme-Catalyzed Hydride Transfer. Journal of the American Chemical Society, <b>2016</b> , 138, 13693-13699	16.4	24
86	Pressure effects on enzyme-catalyzed quantum tunneling events arise from protein-specific structural and dynamic changes. <i>Journal of the American Chemical Society</i> , <b>2012</b> , 134, 9749-54	16.4	23
85	Conversion of the Escherichia coli cytochrome b562 to an archetype cytochrome b: a mutant with bis-histidine ligation of heme iron. <i>Biochemistry</i> , <b>2005</b> , 44, 431-9	3.2	23
84	Parallel pathways and free-energy landscapes for enzymatic hydride transfer probed by hydrostatic pressure. <i>ChemBioChem</i> , <b>2009</b> , 10, 1379-84	3.8	22
83	Bipartite recognition and conformational sampling mechanisms for hydride transfer from nicotinamide coenzyme to FMN in pentaerythritol tetranitrate reductase. <i>FEBS Journal</i> , <b>2009</b> , 276, 4780	). <b>5</b> 97	22
82	Energy landscapes and catalysis in nitric-oxide synthase. <i>Journal of Biological Chemistry</i> , <b>2014</b> , 289, 1172	2 <del>5</del> -417	<b>32</b> 1
81	Enzymatic control of cycloadduct conformation ensures reversible 1,3-dipolar cycloaddition in a prFMN-dependent decarboxylase. <i>Nature Chemistry</i> , <b>2019</b> , 11, 1049-1057	17.6	20
80	Real-time analysis of conformational control in electron transfer reactions of human cytochrome P450 reductase with cytochrome c. <i>FEBS Journal</i> , <b>2015</b> , 282, 4357-75	5.7	20
79	Atomistic insight into the origin of the temperature-dependence of kinetic isotope effects and H-tunnelling in enzyme systems is revealed through combined experimental studies and biomolecular simulation. <i>Biochemical Society Transactions</i> , <b>2008</b> , 36, 16-21	5.1	20
78	Towards the free energy landscape for catalysis in mammalian nitric oxide synthases. <i>FEBS Journal</i> , <b>2015</b> , 282, 3016-29	5.7	19
77	Redox characteristics of a de novo quinone protein. <i>Journal of Physical Chemistry B</i> , <b>2007</b> , 111, 3488-95	3.4	19

## (2015-2014)

76	Ratiometric detection of enzyme turnover and flavin reduction using rare-earth upconverting phosphors. <i>Dalton Transactions</i> , <b>2014</b> , 43, 5265-8	4.3	18
<i>75</i>	Enzymatic single-molecule kinetic isotope effects. <i>Journal of the American Chemical Society</i> , <b>2013</b> , 135, 3855-64	16.4	18
74	Driving force analysis of proton tunnelling across a reactivity series for an enzyme-substrate complex. <i>ChemBioChem</i> , <b>2008</b> , 9, 2839-45	3.8	18
73	Kinetic and spectroscopic probes of motions and catalysis in the cytochrome P450 reductase family of enzymes. <i>FEBS Journal</i> , <b>2012</b> , 279, 1534-44	5.7	17
72	Excited state dynamics can be used to probe donor-acceptor distances for H-tunneling reactions catalyzed by flavoproteins. <i>Biophysical Journal</i> , <b>2013</b> , 105, 2549-58	2.9	16
71	A perspective on conformational control of electron transfer in nitric oxide synthases. <i>Nitric Oxide</i> - <i>Biology and Chemistry</i> , <b>2017</b> , 63, 61-67	5	16
70	Secondary kinetic isotope effects as probes of environmentally-coupled enzymatic hydrogen tunneling reactions. <i>ChemPhysChem</i> , <b>2008</b> , 9, 1536-9	3.2	16
69	Solvent as a probe of active site motion and chemistry during the hydrogen tunnelling reaction in morphinone reductase. <i>ChemPhysChem</i> , <b>2008</b> , 9, 1875-81	3.2	16
68	An oxidative N-demethylase reveals PAS transition from ubiquitous sensor to enzyme. <i>Nature</i> , <b>2016</b> , 539, 593-597	50.4	15
67	Probing active site geometry using high pressure and secondary isotope effects in an enzyme-catalysed Science Science Reaction. <i>Journal of Physical Organic Chemistry</i> , <b>2010</b> , 23, 696-701	2.1	15
66		3.4	15
	enzyme-catalysed SieepSH-tunnelling reaction. <i>Journal of Physical Organic Chemistry</i> , <b>2010</b> , 23, 696-701 Conformational dynamics of the cytochrome P450 BM3/N-palmitoylglycine complex: the proposed "proximal-distal" transition probed by temperature-jump spectroscopy. <i>Journal of Physical</i>		15
66	enzyme-catalysed SdeepSH-tunnelling reaction. <i>Journal of Physical Organic Chemistry</i> , <b>2010</b> , 23, 696-701 Conformational dynamics of the cytochrome P450 BM3/N-palmitoylglycine complex: the proposed "proximal-distal" transition probed by temperature-jump spectroscopy. <i>Journal of Physical Chemistry B</i> , <b>2007</b> , 111, 7879-86  Enzymatic C-H activation of aromatic compounds through CO fixation. <i>Nature Chemical Biology</i> ,	3.4	15
66	enzyme-catalysed SdeepSH-tunnelling reaction. <i>Journal of Physical Organic Chemistry</i> , <b>2010</b> , 23, 696-701 Conformational dynamics of the cytochrome P450 BM3/N-palmitoylglycine complex: the proposed "proximal-distal" transition probed by temperature-jump spectroscopy. <i>Journal of Physical Chemistry B</i> , <b>2007</b> , 111, 7879-86  Enzymatic C-H activation of aromatic compounds through CO fixation. <i>Nature Chemical Biology</i> , <b>2020</b> , 16, 1255-1260  Nuclear quantum tunnelling in enzymatic reactionsan enzymologistS perspective. <i>Physical</i>	3.4	15 15
66 65 64	enzyme-catalysed SdeepSH-tunnelling reaction. <i>Journal of Physical Organic Chemistry</i> , <b>2010</b> , 23, 696-701 Conformational dynamics of the cytochrome P450 BM3/N-palmitoylglycine complex: the proposed "proximal-distal" transition probed by temperature-jump spectroscopy. <i>Journal of Physical Chemistry B</i> , <b>2007</b> , 111, 7879-86  Enzymatic C-H activation of aromatic compounds through CO fixation. <i>Nature Chemical Biology</i> , <b>2020</b> , 16, 1255-1260  Nuclear quantum tunnelling in enzymatic reactionsan enzymologists perspective. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 30775-82  Rewiring the "Push-Pull" Catalytic Machinery of a Heme Enzyme Using an Expanded Genetic Code.	3.4 11.7 3.6	15 15 14
<ul><li>66</li><li>65</li><li>64</li><li>63</li></ul>	enzyme-catalysed SdeepSH-tunnelling reaction. <i>Journal of Physical Organic Chemistry</i> , <b>2010</b> , 23, 696-701 Conformational dynamics of the cytochrome P450 BM3/N-palmitoylglycine complex: the proposed "proximal-distal" transition probed by temperature-jump spectroscopy. <i>Journal of Physical Chemistry B</i> , <b>2007</b> , 111, 7879-86  Enzymatic C-H activation of aromatic compounds through CO fixation. <i>Nature Chemical Biology</i> , <b>2020</b> , 16, 1255-1260  Nuclear quantum tunnelling in enzymatic reactions—an enzymologistS perspective. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 30775-82  Rewiring the "Push-Pull" Catalytic Machinery of a Heme Enzyme Using an Expanded Genetic Code. <i>ACS Catalysis</i> , <b>2020</b> , 10, 2735-2746  Ground-State Destabilization by Phe-448 and Phe-449 Contributes to Tyrosine Phenol-Lyase	3.4 11.7 3.6	15 15 14
<ul><li>66</li><li>65</li><li>64</li><li>63</li><li>62</li></ul>	enzyme-catalysed SdeepSH-tunnelling reaction. <i>Journal of Physical Organic Chemistry</i> , <b>2010</b> , 23, 696-701 Conformational dynamics of the cytochrome P450 BM3/N-palmitoylglycine complex: the proposed "proximal-distal" transition probed by temperature-jump spectroscopy. <i>Journal of Physical Chemistry B</i> , <b>2007</b> , 111, 7879-86  Enzymatic C-H activation of aromatic compounds through CO fixation. <i>Nature Chemical Biology</i> , <b>2020</b> , 16, 1255-1260  Nuclear quantum tunnelling in enzymatic reactionsan enzymologistS perspective. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 30775-82  Rewiring the "Push-Pull" Catalytic Machinery of a Heme Enzyme Using an Expanded Genetic Code. <i>ACS Catalysis</i> , <b>2020</b> , 10, 2735-2746  Ground-State Destabilization by Phe-448 and Phe-449 Contributes to Tyrosine Phenol-Lyase Catalysis. <i>ACS Catalysis</i> , <b>2016</b> , 6, 6770-6779  Synthetic biology for fibres, adhesives and active camouflage materials in protection and	3.4 11.7 3.6 13.1	15 15 14 14

58	A quantitative fluorescence-based steady-state assay of DNA polymerase. FEBS Journal, 2014, 281, 204	2550	13
57	Correlating Calmodulin Landscapes with Chemical Catalysis in Neuronal Nitric Oxide Synthase using Time-Resolved FRET and a 5-Deazaflavin Thermodynamic Trap. <i>ACS Catalysis</i> , <b>2016</b> , 6, 5170-5180	13.1	13
56	A common mechanism for coenzyme cobalamin-dependent reductive dehalogenases. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 6090-6094	3.6	12
55	Liver microsomal lipid enhances the activity and redox coupling of colocalized cytochrome P450 reductase-cytochrome P450 3A4 in nanodiscs. <i>FEBS Journal</i> , <b>2017</b> , 284, 2302-2319	5.7	12
54	Unexpected Roles of a Tether Harboring a Tyrosine Gatekeeper Residue in Modular Nitrite Reductase Catalysis. <i>ACS Catalysis</i> , <b>2019</b> , 9, 6087-6099	13.1	11
53	Non-covalent protein-based adhesives for transparent substrates-bovine serum albumin vs. recombinant spider silk. <i>Materials Today Bio</i> , <b>2020</b> , 7, 100068	9.9	11
52	Pressurized CO as a carboxylating agent for the biocatalytic -carboxylation of resorcinol. <i>Green Chemistry</i> , <b>2018</b> , 20, 1754-1759	10	10
51	Proton tunnelling and promoting vibrations during the oxidation of ascorbate by ferricyanide?. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 2256-9	3.6	10
50	Are Environmentally Coupled Enzymatic Hydrogen Tunneling Reactions Influenced by Changes in Solution Viscosity?. <i>Angewandte Chemie</i> , <b>2008</b> , 120, 547-550	3.6	10
49	Chapter 9:Probing Coupled Motions in Enzymatic Hydrogen Tunnelling Reactions: Beyond Temperature-Dependence Studies of Kinetic Isotope Effects. <i>RSC Biomolecular Sciences</i> , <b>2009</b> , 199-218		10
49		13.1	10
	Temperature-Dependence Studies of Kinetic Isotope Effects. <i>RSC Biomolecular Sciences</i> , <b>2009</b> , 199-218  Nonequivalence of Second Sphere "Noncatalytic" Residues in Pentaerythritol Tetranitrate  Reductase in Relation to Local Dynamics Linked to H-Transfer in Reactions with NADH and NADPH		
48	Temperature-Dependence Studies of Kinetic Isotope Effects. <i>RSC Biomolecular Sciences</i> , <b>2009</b> , 199-218  Nonequivalence of Second Sphere "Noncatalytic" Residues in Pentaerythritol Tetranitrate Reductase in Relation to Local Dynamics Linked to H-Transfer in Reactions with NADH and NADPH Coenzymes. <i>ACS Catalysis</i> , <b>2018</b> , 8, 11589-11599  Dynamic, electrostatic model for the generation and control of high-energy radical intermediates	13.1	10
48 47	Temperature-Dependence Studies of Kinetic Isotope Effects. <i>RSC Biomolecular Sciences</i> , <b>2009</b> , 199-218  Nonequivalence of Second Sphere "Noncatalytic" Residues in Pentaerythritol Tetranitrate Reductase in Relation to Local Dynamics Linked to H-Transfer in Reactions with NADH and NADPH Coenzymes. <i>ACS Catalysis</i> , <b>2018</b> , 8, 11589-11599  Dynamic, electrostatic model for the generation and control of high-energy radical intermediates by a coenzyme BEdependent enzyme. <i>ChemBioChem</i> , <b>2013</b> , 14, 1529-33  Correction of pre-steady-state KIEs for isotopic impurities and the consequences of kinetic isotope	<b>13.1 3.8</b>	10
48 47 46	Temperature-Dependence Studies of Kinetic Isotope Effects. <i>RSC Biomolecular Sciences</i> , <b>2009</b> , 199-218  Nonequivalence of Second Sphere "Noncatalytic" Residues in Pentaerythritol Tetranitrate Reductase in Relation to Local Dynamics Linked to H-Transfer in Reactions with NADH and NADPH Coenzymes. <i>ACS Catalysis</i> , <b>2018</b> , 8, 11589-11599  Dynamic, electrostatic model for the generation and control of high-energy radical intermediates by a coenzyme BEdependent enzyme. <i>ChemBioChem</i> , <b>2013</b> , 14, 1529-33  Correction of pre-steady-state KIEs for isotopic impurities and the consequences of kinetic isotope fractionation. <i>Journal of Physical Chemistry A</i> , <b>2008</b> , 112, 13109-15  How Do Vanadium Chloroperoxidases Generate Hypochlorite from Hydrogen Peroxide and	13.1 3.8 2.8	<ul><li>10</li><li>9</li><li>9</li></ul>
48 47 46 45	Temperature-Dependence Studies of Kinetic Isotope Effects. <i>RSC Biomolecular Sciences</i> , <b>2009</b> , 199-218  Nonequivalence of Second Sphere "Noncatalytic" Residues in Pentaerythritol Tetranitrate Reductase in Relation to Local Dynamics Linked to H-Transfer in Reactions with NADH and NADPH Coenzymes. <i>ACS Catalysis</i> , <b>2018</b> , 8, 11589-11599  Dynamic, electrostatic model for the generation and control of high-energy radical intermediates by a coenzyme BEberndent enzyme. <i>ChemBioChem</i> , <b>2013</b> , 14, 1529-33  Correction of pre-steady-state KIEs for isotopic impurities and the consequences of kinetic isotope fractionation. <i>Journal of Physical Chemistry A</i> , <b>2008</b> , 112, 13109-15  How Do Vanadium Chloroperoxidases Generate Hypochlorite from Hydrogen Peroxide and Chloride? A Computational Study. <i>ACS Catalysis</i> , <b>2020</b> , 10, 14067-14079  Preparation and photophysical properties of a caged kynurenine. <i>Bioorganic and Medicinal</i>	13.1 3.8 2.8	10 9 9
48 47 46 45 44	Temperature-Dependence Studies of Kinetic Isotope Effects. <i>RSC Biomolecular Sciences</i> , <b>2009</b> , 199-218  Nonequivalence of Second Sphere "Noncatalytic" Residues in Pentaerythritol Tetranitrate Reductase in Relation to Local Dynamics Linked to H-Transfer in Reactions with NADH and NADPH Coenzymes. <i>ACS Catalysis</i> , <b>2018</b> , 8, 11589-11599  Dynamic, electrostatic model for the generation and control of high-energy radical intermediates by a coenzyme BEdependent enzyme. <i>ChemBioChem</i> , <b>2013</b> , 14, 1529-33  Correction of pre-steady-state KIEs for isotopic impurities and the consequences of kinetic isotope fractionation. <i>Journal of Physical Chemistry A</i> , <b>2008</b> , 112, 13109-15  How Do Vanadium Chloroperoxidases Generate Hypochlorite from Hydrogen Peroxide and Chloride? A Computational Study. <i>ACS Catalysis</i> , <b>2020</b> , 10, 14067-14079  Preparation and photophysical properties of a caged kynurenine. <i>Bioorganic and Medicinal Chemistry Letters</i> , <b>2012</b> , 22, 2734-7  Taming the Reactivity of Monoterpene Synthases To Guide Regioselective Product Hydroxylation.	13.1 3.8 2.8 13.1	<ul><li>10</li><li>9</li><li>9</li><li>9</li><li>8</li></ul>

## (2019-2013)

40	Modulation of ligand-heme reactivity by binding pocket residues demonstrated in cytochrome cS over the femtosecond-second temporal range. <i>FEBS Journal</i> , <b>2013</b> , 280, 6070-82	5.7	7	
39	Predicting new protein conformations from molecular dynamics simulation conformational landscapes and machine learning. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2021</b> , 89, 915	4.2	7	
38	Time Course Analysis of Enzyme-Catalyzed DNA Polymerization. <i>Biochemistry</i> , <b>2016</b> , 55, 5622-5634	3.2	7	
37	Engineering an efficient and enantioselective enzyme for the Morita-Baylis-Hillman reaction <i>Nature Chemistry</i> , <b>2021</b> ,	17.6	7	
36	Photochemical Spin Dynamics of the Vitamin B Derivative, Methylcobalamin. <i>Journal of Physical Chemistry B</i> , <b>2019</b> , 123, 4663-4672	3.4	6	
35	Is There a Dynamic Protein Contribution to the Substrate Trigger in Coenzyme B12-Dependent Ethanolamine Ammonia Lyase?. <i>Angewandte Chemie</i> , <b>2011</b> , 123, 11035-11038	3.6	6	
34	Making a single-chain four-helix bundle for redox chemistry studies. <i>Protein Engineering, Design and Selection</i> , <b>2008</b> , 21, 645-52	1.9	6	
33	H-transfers in Photosystem II: what can we learn from recent lessons in the enzyme community?. <i>Photosynthesis Research</i> , <b>2008</b> , 98, 169-77	3.7	6	
32	Practical aspects on the use of kinetic isotope effects as probes of flavoprotein enzyme mechanisms. <i>Methods in Molecular Biology</i> , <b>2014</b> , 1146, 161-75	1.4	6	
31	Photocatalysis as the Snaster switchSof photomorphogenesis in early plant development. <i>Nature Plants</i> , <b>2021</b> , 7, 268-276	11.5	6	
30	MhuD from: Probing a Dual Role in Heme Storage and Degradation. <i>ACS Infectious Diseases</i> , <b>2019</b> , 5, 1855-1866	5.5	5	
29	Ultrafast Vibrational Energy Transfer between Protein and Cofactor in a Flavoenzyme. <i>Journal of Physical Chemistry B</i> , <b>2020</b> , 124, 5163-5168	3.4	5	
28	Probing reversible chemistry in coenzyme B12 -dependent ethanolamine ammonia lyase with kinetic isotope effects. <i>Chemistry - A European Journal</i> , <b>2015</b> , 21, 8826-31	4.8	5	
27	Evidence of preorganization in quinonoid intermediate formation from L-Trp in H463F mutant Escherichia coli tryptophan indole-lyase from effects of pressure and pH. <i>Biochemistry</i> , <b>2012</b> , 51, 6527-	-33 <sup>3.2</sup>	5	
26	Barrier Compression Enhances an Enzymatic Hydrogen-Transfer Reaction. <i>Angewandte Chemie</i> , <b>2009</b> , 121, 1480-1482	3.6	5	
25	What are the signatures of tunnelling in enzyme-catalysed reactions?. <i>Faraday Discussions</i> , <b>2019</b> , 221, 367-378	3.6	5	
24	Interplay between chromophore binding and domain assembly by the B-dependent photoreceptor protein, CarH. <i>Chemical Science</i> , <b>2021</b> , 12, 8333-8341	9.4	5	
23	Graphene-aramid nanocomposite fibres via superacid co-processing. <i>Chemical Communications</i> , <b>2019</b> , 55, 11703-11706	5.8	4	

22	Selectivity through discriminatory induced fit enables switching of NAD(P)H coenzyme specificity in Old Yellow Enzyme ene-reductases. <i>FEBS Journal</i> , <b>2019</b> , 286, 3117-3128	5.7	4
21	Expanding the Scope of Biomolecule Monitoring with Ratiometric Signaling from Rare-Earth Upconverting Phosphors. <i>European Journal of Inorganic Chemistry</i> , <b>2017</b> , 2017, 5176-5185	2.3	4
20	Pressure and Temperature Effects on the Formation of Aminoacrylate Intermediates of Tyrosine Phenol-lyase Demonstrate Reaction Dynamics. <i>ACS Catalysis</i> , <b>2020</b> , 10, 1692-1703	13.1	4
19	Zero-point energy and tunnelling: general discussion. <i>Faraday Discussions</i> , <b>2019</b> , 221, 478-500	3.6	4
18	Dual role of the active site <b>\$</b> idSregions of protochlorophyllide oxidoreductase in photocatalysis and plant development. <i>FEBS Journal</i> , <b>2021</b> , 288, 175-189	5.7	4
17	H, N and C backbone resonance assignments of pentaerythritol tetranitrate reductase from Enterobacter cloacae PB2. <i>Biomolecular NMR Assignments</i> , <b>2018</b> , 12, 79-83	0.7	4
16	Protein Motions Are Coupled to the Reaction Chemistry in Coenzyme B12-Dependent Ethanolamine Ammonia Lyase. <i>Angewandte Chemie</i> , <b>2012</b> , 124, 9440-9444	3.6	3
15	UbiD domain dynamics underpins aromatic decarboxylation. <i>Nature Communications</i> , <b>2021</b> , 12, 5065	17.4	3
14	Covalent Attachment of Active Enzymes to Upconversion Phosphors Allows Ratiometric Detection of Substrates. <i>Chemistry - A European Journal</i> , <b>2020</b> , 26, 14817-14822	4.8	2
13	Trapping methods for probing functional intermediates in nitric oxide synthases and related enzymes. <i>Frontiers in Bioscience - Landmark</i> , <b>2018</b> , 23, 1874-1888	2.8	2
12	Isotopically labeled flavoenzymes and their uses in probing reaction mechanisms. <i>Methods in Enzymology</i> , <b>2019</b> , 620, 145-166	1.7	2
11	Directed evolution of prenylated FMN-dependent Fdc supports efficient in vivo isobutene production. <i>Nature Communications</i> , <b>2021</b> , 12, 5300	17.4	2
10	Blood, sweat, and tears: extraterrestrial regolith biocomposites with binders. <i>Materials Today Bio</i> , <b>2021</b> , 12, 100136	9.9	2
9	H, N, C backbone resonance assignments of human soluble catechol O-methyltransferase in complex with S-adenosyl-L-methionine and 3,5-dinitrocatechol. <i>Biomolecular NMR Assignments</i> , <b>2017</b> , 11, 57-61	0.7	1
8	Evaluating spectral overlap with the degree of quenching in UCP luminescence energy transfer systems. <i>Methods and Applications in Fluorescence</i> , <b>2019</b> , 7, 034003	3.1	1
7	Extracting Kinetic Isotope Effects From a Global Analysis of Reaction Progress Curves. <i>Methods in Enzymology</i> , <b>2017</b> , 596, 85-111	1.7	1
6	Examining the importance of dynamics, barrier compression and hydrogen tunnelling in enzyme catalysed reactions. <i>Procedia Chemistry</i> , <b>2011</b> , 3, 306-315		1
5	Evaluating spectral overlap with the degree of quenching in UCP luminescence energy transfer systems. <i>Methods and Applications in Fluorescence</i> , <b>2020</b> ,	3.1	1

#### LIST OF PUBLICATIONS

4	Reactivity in a Heme Peroxidase. <i>Jacs Au</i> , <b>2021</b> , 1, 913-918		1
3	How Photoactivation Triggers Protochlorophyllide Reduction: Computational Evidence of a Stepwise Hydride Transfer during Chlorophyll Biosynthesis <i>ACS Catalysis</i> , <b>2022</b> , 12, 4141-4148	13.1	O
2	Integrating Computational Methods with Experiment Uncovers the Role of Dynamics in Enzyme-Catalysed H-Tunnelling Reactions. <i>Challenges and Advances in Computational Chemistry and Physics</i> , <b>2010</b> , 501-519	0.7	
1	Assessing the Covalent Attachment and Energy Transfer Capabilities of Upconverting Phosphors With Cofactor Containing Bioactive Enzymes. <i>Frontiers in Chemistry</i> , <b>2020</b> , 8, 613334	5	