

Sam Hay

List of Publications by Year in descending order

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127
papers

4,003
citations

126858

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all docs

136
docs citations

136
times ranked

3788
citing authors

#	ARTICLE	IF	CITATIONS
1	Reductive dehalogenase structure suggests a mechanism for B12-dependent dehalogenation. <i>Nature</i> , 2015, 517, 513-516.	13.7	260
2	Good vibrations in enzyme-catalysed reactions. <i>Nature Chemistry</i> , 2012, 4, 161-168.	6.6	246
3	New cofactor supports $\hat{1}\pm, \hat{1}^2$ -unsaturated acid decarboxylation via 1,3-dipolar cycloaddition. <i>Nature</i> , 2015, 522, 497-501.	13.7	197
4	UbiX is a flavin prenyltransferase required for bacterial ubiquinone biosynthesis. <i>Nature</i> , 2015, 522, 502-506.	13.7	168
5	Promoting motions in enzyme catalysis probed by pressure studies of kinetic isotope effects. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007, 104, 507-512.	3.3	98
6	Structural basis for enzymatic photocatalysis in chlorophyll biosynthesis. <i>Nature</i> , 2019, 574, 722-725.	13.7	88
7	Fast Protein Motions Are Coupled to Enzyme H-Transfer Reactions. <i>Journal of the American Chemical Society</i> , 2013, 135, 2512-2517.	6.6	83
8	Carboxylesterase converts Amplex red to resorufin: Implications for mitochondrial H ₂ O ₂ release assays. <i>Free Radical Biology and Medicine</i> , 2016, 90, 173-183.	1.3	83
9	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> , 2009, 131, 17072-17073.	6.6	79
10	Deep Tunneling Dominates the Biologically Important Hydride Transfer Reaction from NADH to FMN in Morphinone Reductase. <i>Journal of the American Chemical Society</i> , 2008, 130, 7092-7097.	6.6	75
11	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> , 2010, 132, 11329-11335.	6.6	74
12	Quantum Biology: An Update and Perspective. <i>Quantum Reports</i> , 2021, 3, 80-126.	0.6	74
13	$\hat{1}\pm$ -Secondary Isotope Effects as Probes of $\hat{1}\pm$ -Tunneling-Ready Configurations in Enzymatic H-Tunneling: Insight from Environmentally Coupled Tunneling Models. <i>Journal of the American Chemical Society</i> , 2006, 128, 14053-14058.	6.6	66
14	Nature of the Energy Landscape for Gated Electron Transfer in a Dynamic Redox Protein. <i>Journal of the American Chemical Society</i> , 2010, 132, 9738-9745.	6.6	63
15	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> , 2007, 111, 2631-2638.	1.2	62
16	Decoupled Associative and Dissociative Processes in Strong yet Highly Dynamic Host-Guest Complexes. <i>Journal of the American Chemical Society</i> , 2017, 139, 12985-12993.	6.6	56
17	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> , 2007, 129, 13949-13956.	6.6	55
18	Conformational and Thermodynamic Control of Electron Transfer in Neuronal Nitric Oxide Synthase. <i>Biochemistry</i> , 2007, 46, 5018-5029.	1.2	53

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19	Barrier Compression Enhances an Enzymatic Hydrogenâ€”Transfer Reaction. <i>Angewandte Chemie - International Edition</i> , 2009, 48, 1452-1454.	7.2	52
20	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> , 2007, 129, 15718-15727.	6.6	51
21	Demonstration of Proton-coupled Electron Transfer in the Copper-containing Nitrite Reductases. <i>Journal of Biological Chemistry</i> , 2009, 284, 25973-25983.	1.6	50
22	Are the Catalytic Properties of Enzymes from Piezophilic Organisms Pressure Adapted?. <i>ChemBioChem</i> , 2009, 10, 2348-2353.	1.3	48
23	Structural Basis of Catalysis in the Bacterial Monoterpene Synthases Linalool Synthase and 1,8-Cineole Synthase. <i>ACS Catalysis</i> , 2017, 7, 6268-6282.	5.5	47
24	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> , 2004, 101, 17675-17680.	3.3	46
25	Barrier Compression and Its Contribution to Both Classical and Quantum Mechanical Aspects of Enzyme Catalysis. <i>Biophysical Journal</i> , 2010, 98, 121-128.	0.2	43
26	A â€”Plug and Playâ€” Platform for the Production of Diverse Monoterpene Hydrocarbon Scaffolds in <i>Escherichia coli</i> . <i>ChemistrySelect</i> , 2016, 1, 1893-1896.	0.7	42
27	Interâ€”flavin electron transfer in cytochrome P450 reductase â€” effects of solvent and pH identify hidden complexity in mechanism. <i>FEBS Journal</i> , 2008, 275, 4540-4557.	2.2	39
28	Dual transcriptional-translational cascade permits cellular level tuneable expression control. <i>Nucleic Acids Research</i> , 2016, 44, e21-e21.	6.5	39
29	Ultrafast Infrared Spectral Fingerprints of Vitamin B ₁₂ and Related Cobalamins. <i>Journal of Physical Chemistry A</i> , 2012, 116, 5586-5594.	1.1	38
30	Donorâ€”Acceptor Distance Sampling Enhances the Performance of â€”Better than Natureâ€”Nicotinamide Coenzyme Biomimetics. <i>Journal of the American Chemical Society</i> , 2016, 138, 11089-11092.	6.6	38
31	Electrochemical and Structural Properties of a Protein System Designed To Generate Tyrosine Pourbaix Diagrams. <i>Journal of the American Chemical Society</i> , 2011, 133, 17786-17795.	6.6	37
32	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> , 2007, 282, 30331-30340.	1.6	36
33	Incorporation of Hydrostatic Pressure into Models of Hydrogen Tunneling Highlights a Role for Pressure-Modulated Promoting Vibrations. <i>Biochemistry</i> , 2008, 47, 9880-9887.	1.2	36
34	Are Environmentally Coupled Enzymatic Hydrogen Tunneling Reactions Influenced by Changes in Solution Viscosity?. <i>Angewandte Chemie - International Edition</i> , 2008, 47, 537-540.	7.2	34
35	Epoxyqueuosine Reductase Structure Suggests a Mechanism for Cobalamin-dependent tRNA Modification. <i>Journal of Biological Chemistry</i> , 2015, 290, 27572-27581.	1.6	34
36	Engineering an efficient and enantioselective enzyme for the Moritaâ€”Baylisâ€”Hillman reaction. <i>Nature Chemistry</i> , 2022, 14, 313-320.	6.6	34

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37	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> , 2012, 586, 578-584.	1.3	31
38	Convergence of Theory and Experiment on the Role of Preorganization, Quantum Tunneling, and Enzyme Motions into Flavoenzyme-Catalyzed Hydride Transfer. <i>ACS Catalysis</i> , 2017, 7, 3190-3198.	5.5	31
39	Is There a Dynamic Protein Contribution to the Substrate Trigger in Coenzyme B ₁₂ -Dependent Ethanolamine Ammonia Lyase?. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 10843-10846.	7.2	30
40	Relating localized protein motions to the reaction coordinate in coenzyme-B ₁₂ -dependent enzymes. <i>FEBS Journal</i> , 2013, 280, 2997-3008.	2.2	29
41	Enzymatic C-H activation of aromatic compounds through CO ₂ fixation. <i>Nature Chemical Biology</i> , 2020, 16, 1255-1260.	3.9	29
42	Protein Motions Are Coupled to the Reaction Chemistry in Coenzyme B ₁₂ -Dependent Ethanolamine Ammonia Lyase. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 9306-9310.	7.2	28
43	Enzymatic control of cycloadduct conformation ensures reversible 1,3-dipolar cycloaddition in a prFMN-dependent decarboxylase. <i>Nature Chemistry</i> , 2019, 11, 1049-1057.	6.6	28
44	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> , 2005, 44, 11891-11902.	1.2	27
45	Structural and mechanistic aspects of flavoproteins: probes of hydrogen tunnelling. <i>FEBS Journal</i> , 2009, 276, 3930-3941.	2.2	27
46	Pressure Effects on Enzyme-Catalyzed Quantum Tunneling Events Arise from Protein-Specific Structural and Dynamic Changes. <i>Journal of the American Chemical Society</i> , 2012, 134, 9749-9754.	6.6	27
47	Real-time analysis of conformational control in electron transfer reactions of human cytochrome P450 reductase with cytochrome <i>c</i> . <i>FEBS Journal</i> , 2015, 282, 4357-4375.	2.2	27
48	Untangling Heavy Protein and Cofactor Isotope Effects on Enzyme-Catalyzed Hydride Transfer. <i>Journal of the American Chemical Society</i> , 2016, 138, 13693-13699.	6.6	26
49	Energy Landscapes and Catalysis in Nitric-oxide Synthase. <i>Journal of Biological Chemistry</i> , 2014, 289, 11725-11738.	1.6	25
50	Rewiring the "Push-Pull" Catalytic Machinery of a Heme Enzyme Using an Expanded Genetic Code. <i>ACS Catalysis</i> , 2020, 10, 2735-2746.	5.5	25
51	Conversion of the <i>Escherichia coli</i> Cytochrome b ₅₆₂ to an Archetype Cytochrome b ₅₆₂ A Mutant with Bis-Histidine Ligation of Heme Iron. <i>Biochemistry</i> , 2005, 44, 431-439.	1.2	24
52	Redox Characteristics of a de Novo Quinone Protein. <i>Journal of Physical Chemistry B</i> , 2007, 111, 3488-3495.	1.2	24
53	Bipartite recognition and conformational sampling mechanisms for hydride transfer from nicotinamide coenzyme to FMN in pentaerythritol tetranitrate reductase. <i>FEBS Journal</i> , 2009, 276, 4780-4789.	2.2	24
54	Non-covalent protein-based adhesives for transparent substrates: bovine serum albumin vs. recombinant spider silk. <i>Materials Today Bio</i> , 2020, 7, 100068.	2.6	24

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55	Predicting new protein conformations from molecular dynamics simulation conformational landscapes and machine learning. <i>Proteins: Structure, Function and Bioinformatics</i> , 2021, 89, 915-921.	1.5	24
56	Ratiometric detection of enzyme turnover and flavin reduction using rare-earth upconverting phosphors. <i>Dalton Transactions</i> , 2014, 43, 5265-5268.	1.6	23
57	Towards the free energy landscape for catalysis in mammalian nitric oxide synthases. <i>FEBS Journal</i> , 2015, 282, 3016-3029.	2.2	23
58	Pressurized CO ₂ as a carboxylating agent for the biocatalytic <i>ortho</i> -carboxylation of resorcinol. <i>Green Chemistry</i> , 2018, 20, 1754-1759.	4.6	23
59	Parallel Pathways and Free Energy Landscapes for Enzymatic Hydride Transfer Probed by Hydrostatic Pressure. <i>ChemBioChem</i> , 2009, 10, 1379-1384.	1.3	22
60	Photocatalysis as the "master switch" of photomorphogenesis in early plant development. <i>Nature Plants</i> , 2021, 7, 268-276.	4.7	22
61	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> , 2008, 36, 16-21.	1.6	21
62	Enzymatic Single-Molecule Kinetic Isotope Effects. <i>Journal of the American Chemical Society</i> , 2013, 135, 3855-3864.	6.6	21
63	An oxidative N-demethylase reveals PAS transition from ubiquitous sensor to enzyme. <i>Nature</i> , 2016, 539, 593-597.	13.7	21
64	A common mechanism for coenzyme cobalamin-dependent reductive dehalogenases. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 6090-6094.	1.3	21
65	Synthetic biology for fibers, adhesives, and active camouflage materials in protection and aerospace. <i>MRS Communications</i> , 2019, 9, 486-504.	0.8	21
66	Equatorial Active Site Compaction and Electrostatic Reorganization in Catechol-O-methyltransferase. <i>ACS Catalysis</i> , 2019, 9, 4394-4401.	5.5	21
67	Driving Force Analysis of Proton Tunnelling Across a Reactivity Series for an Enzyme-Substrate Complex. <i>ChemBioChem</i> , 2008, 9, 2839-2845.	1.3	20
68	Ground-State Destabilization by Phe-448 and Phe-449 Contributes to Tyrosine Phenol-Lyase Catalysis. <i>ACS Catalysis</i> , 2016, 6, 6770-6779.	5.5	20
69	Structure and Mechanism of a Viral Collagen Prolyl Hydroxylase. <i>Biochemistry</i> , 2015, 54, 6093-6105.	1.2	19
70	A perspective on conformational control of electron transfer in nitric oxide synthases. <i>Nitric Oxide - Biology and Chemistry</i> , 2017, 63, 61-67.	1.2	19
71	How Do Vanadium Chloroperoxidases Generate Hypochlorite from Hydrogen Peroxide and Chloride? A Computational Study. <i>ACS Catalysis</i> , 2020, 10, 14067-14079.	5.5	19
72	Kinetic and spectroscopic probes of motions and catalysis in the cytochrome P450 reductase family of enzymes. <i>FEBS Journal</i> , 2012, 279, 1534-1544.	2.2	18

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73	Nuclear quantum tunnelling in enzymatic reactions – an enzymologist's perspective. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 30775-30782.	1.3	18
74	Excited State Dynamics Can Be Used to Probe Donor-Acceptor Distances for H-Tunneling Reactions Catalyzed by Flavoproteins. <i>Biophysical Journal</i> , 2013, 105, 2549-2558.	0.2	17
75	Unexpected Roles of a Tether Harboring a Tyrosine Gatekeeper Residue in Modular Nitrite Reductase Catalysis. <i>ACS Catalysis</i> , 2019, 9, 6087-6099.	5.5	17
76	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> , 2007, 111, 7879-7886.	1.2	16
77	Secondary Kinetic Isotope Effects as Probes of Environmentally-Coupled Enzymatic Hydrogen Tunneling Reactions. <i>ChemPhysChem</i> , 2008, 9, 1536-1539.	1.0	16
78	Solvent as a Probe of Active Site Motion and Chemistry during the Hydrogen Tunnelling Reaction in Morphinone Reductase. <i>ChemPhysChem</i> , 2008, 9, 1875-1881.	1.0	16
79	Probing active site geometry using high pressure and secondary isotope effects in an enzyme-catalysed –deep– H-tunnelling reaction. <i>Journal of Physical Organic Chemistry</i> , 2010, 23, 696-701.	0.9	16
80	A quantitative fluorescence-based steady-state assay of <sc>DNA</sc> polymerase. <i>FEBS Journal</i> , 2014, 281, 2042-2050.	2.2	16
81	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> , 2016, 6, 5170-5180.	5.5	15
82	Dual role of the active site –lid– regions of protochlorophyllide oxidoreductase in photocatalysis and plant development. <i>FEBS Journal</i> , 2021, 288, 175-189.	2.2	15
83	Structure and Mechanism of <i>Pseudomonas aeruginosa</i> PA0254/HudA, a prFMN-Dependent Pyrrole-2-carboxylic Acid Decarboxylase Linked to Virulence. <i>ACS Catalysis</i> , 2021, 11, 2865-2878.	5.5	15
84	Liver microsomal lipid enhances the activity and redox coupling of colocalized cytochrome P450 reductase-cytochrome P450 3A4 in nanodiscs. <i>FEBS Journal</i> , 2017, 284, 2302-2319.	2.2	14
85	UbiD domain dynamics underpins aromatic decarboxylation. <i>Nature Communications</i> , 2021, 12, 5065.	5.8	14
86	Taming the Reactivity of Monoterpene Synthases To Guide Regioselective Product Hydroxylation. <i>ChemBioChem</i> , 2020, 21, 985-990.	1.3	13
87	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> , 2018, 8, 11589-11599.	5.5	12
88	Blood, sweat, and tears: extraterrestrial regolith biocomposites with in vivo binders. <i>Materials Today Bio</i> , 2021, 12, 100136.	2.6	12
89	Probing Coupled Motions in Enzymatic Hydrogen Tunnelling Reactions: Beyond Temperature-Dependence Studies of Kinetic Isotope Effects. <i>RSC Biomolecular Sciences</i> , 2009, , 199-218.	0.4	12
90	Dynamic, Electrostatic Model for the Generation and Control of High-Energy Radical Intermediates by a Coenzyme B ₁₂ -Dependent Enzyme. <i>ChemBioChem</i> , 2013, 14, 1529-1533.	1.3	11

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91	Directed evolution of prenylated FMN-dependent Fdc supports efficient in vivo isobutene production. <i>Nature Communications</i> , 2021, 12, 5300.	5.8	11
92	Proton tunnelling and promoting vibrations during the oxidation of ascorbate by ferricyanide?. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 2256.	1.3	10
93	Selectivity through discriminatory induced fit enables switching of <sc>NAD</sc>(P)H coenzyme specificity in Old Yellow Enzyme eneâ€reductases. <i>FEBS Journal</i> , 2019, 286, 3117-3128.	2.2	10
94	Interplay between chromophore binding and domain assembly by the B₁₂-dependent photoreceptor protein, CarH. <i>Chemical Science</i> , 2021, 12, 8333-8341.	3.7	10
95	Correction of Pre-Steady-State KIEs for Isotopic Impurities and the Consequences of Kinetic Isotope Fractionation. <i>Journal of Physical Chemistry A</i> , 2008, 112, 13109-13115.	1.1	9
96	Making a single-chain four-helix bundle for redox chemistry studies. <i>Protein Engineering, Design and Selection</i> , 2008, 21, 645-652.	1.0	9
97	Preparation and photophysical properties of a caged kynurenine. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2012, 22, 2734-2737.	1.0	9
98	Time Course Analysis of Enzyme-Catalyzed DNA Polymerization. <i>Biochemistry</i> , 2016, 55, 5622-5634.	1.2	9
99	Photochemical Spin Dynamics of the Vitamin B₁₂ Derivative, Methylcobalamin. <i>Journal of Physical Chemistry B</i> , 2019, 123, 4663-4672.	1.2	9
100	Does the pressure dependence of kinetic isotope effects report usefully on dynamics in enzyme Hâ€transfer reactions?. <i>FEBS Journal</i> , 2015, 282, 3243-3255.	2.2	8
101	MhuD from <i>Mycobacterium tuberculosis</i>: Probing a Dual Role in Heme Storage and Degradation. <i>ACS Infectious Diseases</i> , 2019, 5, 1855-1866.	1.8	8
102	Grapheneâ€aramid nanocomposite fibres <i>via</i> superacid co-processing. <i>Chemical Communications</i> , 2019, 55, 11703-11706.	2.2	8
103	Covalent Attachment of Active Enzymes to Upconversion Phosphors Allows Ratiometric Detection of Substrates. <i>Chemistry - A European Journal</i> , 2020, 26, 14817-14822.	1.7	8
104	Ultrafast Vibrational Energy Transfer between Protein and Cofactor in a Flavoenzyme. <i>Journal of Physical Chemistry B</i> , 2020, 124, 5163-5168.	1.2	8
105	A Noncanonical Tryptophan Analogue Reveals an Active Site Hydrogen Bond Controlling Ferryl Reactivity in a Heme Peroxidase. <i>Jacs Au</i> , 2021, 1, 913-918.	3.6	8
106	How Photoactivation Triggers Protochlorophyllide Reduction: Computational Evidence of a Stepwise Hydride Transfer during Chlorophyll Biosynthesis. <i>ACS Catalysis</i> , 2022, 12, 4141-4148.	5.5	8
107	Modulation of ligandâ€heme reactivity by binding pocket residues demonstrated in cytochromeâ€' over the femtosecondâ€second temporal range. <i>FEBS Journal</i> , 2013, 280, 6070-6082.	2.2	7
108	Expanding the Scope of Biomolecule Monitoring with Ratiometric Signaling from Rareâ€Earth Upconverting Phosphors. <i>European Journal of Inorganic Chemistry</i> , 2017, 2017, 5176-5185.	1.0	7

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109	What are the signatures of tunnelling in enzyme-catalysed reactions?. <i>Faraday Discussions</i> , 2019, 221, 367-378.	1.6	7
110	H-transfers in Photosystem II: what can we learn from recent lessons in the enzyme community?. <i>Photosynthesis Research</i> , 2008, 98, 169-177.	1.6	6
111	¹ H, ¹⁵ N and ¹³ C backbone resonance assignments of pentaerythritol tetranitrate reductase from <i>Enterobacter cloacae</i> PB2. <i>Biomolecular NMR Assignments</i> , 2018, 12, 79-83.	0.4	6
112	Pressure and Temperature Effects on the Formation of Aminoacrylate Intermediates of Tyrosine Phenol-lyase Demonstrate Reaction Dynamics. <i>ACS Catalysis</i> , 2020, 10, 1692-1703.	5.5	6
113	Practical Aspects on the Use of Kinetic Isotope Effects as Probes of Flavoprotein Enzyme Mechanisms. <i>Methods in Molecular Biology</i> , 2014, 1146, 161-175.	0.4	6
114	Evidence of Preorganization in Quinonoid Intermediate Formation from Trp in H463F Mutant <i>Escherichia coli</i> Tryptophan Indole-lyase from Effects of Pressure and pH. <i>Biochemistry</i> , 2012, 51, 6527-6533.	1.2	5
115	Probing Reversible Chemistry in Coenzyme B ₁₂ -Dependent Ethanolamine Ammonia Lyase with Kinetic Isotope Effects. <i>Chemistry - A European Journal</i> , 2015, 21, 8826-8831.	1.7	5
116	Molecular Determinants of Carbocation Cyclisation in Bacterial Monoterpene Synthases. <i>ChemBioChem</i> , 2022, 23, .	1.3	5
117	Zero-point energy and tunnelling: general discussion. <i>Faraday Discussions</i> , 2019, 221, 478-500.	1.6	4
118	Evaluating spectral overlap with the degree of quenching in UCP luminescence energy transfer systems. <i>Methods and Applications in Fluorescence</i> , 2020, 8, 045003.	1.1	3
119	Chelator-Based Parameterization of the 12-6-4 Lennard-Jones Molecular Mechanics Potential for More Realistic Metal Ion-Protein Interactions. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 2367-2374.	2.3	3
120	Examining the importance of dynamics, barrier compression and hydrogen tunnelling in enzyme catalysed reactions. <i>Procedia Chemistry</i> , 2011, 3, 306-315.	0.7	2
121	¹ H, ¹⁵ N, ¹³ 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> , 2017, 11, 57-61.	0.4	2
122	Trapping methods for probing functional intermediates in nitric oxide synthases and related enzymes. <i>Frontiers in Bioscience - Landmark</i> , 2018, 23, 1874-1888.	3.0	2
123	Isotopically labeled flavoenzymes and their uses in probing reaction mechanisms. <i>Methods in Enzymology</i> , 2019, 620, 145-166.	0.4	2
124	Evaluating spectral overlap with the degree of quenching in UCP luminescence energy transfer systems. <i>Methods and Applications in Fluorescence</i> , 2019, 7, 034003.	1.1	2
125	Chapter 3. Experimental Approaches Towards Proton-Coupled Electron Transfer Reactions in Biological Redox Systems. <i>RSC Catalysis Series</i> , 2011, , 57-88.	0.1	1
126	Extracting Kinetic Isotope Effects From a Global Analysis of Reaction Progress Curves. <i>Methods in Enzymology</i> , 2017, 596, 85-111.	0.4	1

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127	Assessing the Covalent Attachment and Energy Transfer Capabilities of Upconverting Phosphors With Cofactor Containing Bioactive Enzymes. <i>Frontiers in Chemistry</i> , 2020, 8, 613334.	1.8	1