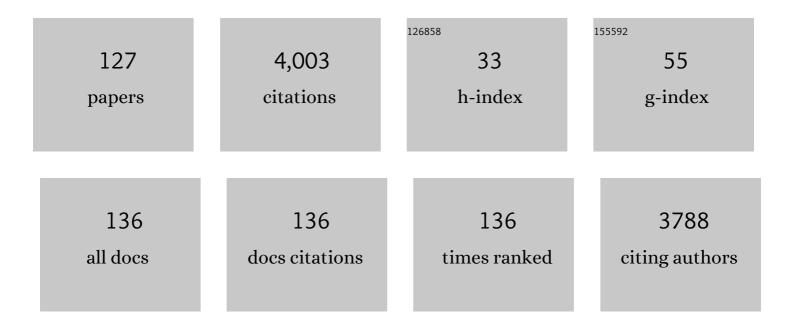
Sam Hay

List of Publications by Year in descending order

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SAM ΗΑΥ

#	Article	IF	CITATIONS
1	Molecular Determinants of Carbocation Cyclisation in Bacterial Monoterpene Synthases. ChemBioChem, 2022, 23, .	1.3	5
2	Chelator-Based Parameterization of the 12-6-4 Lennard-Jones Molecular Mechanics Potential for More Realistic Metal Ion–Protein Interactions. Journal of Chemical Theory and Computation, 2022, 18, 2367-2374.	2.3	3
3	How Photoactivation Triggers Protochlorophyllide Reduction: Computational Evidence of a Stepwise Hydride Transfer during Chlorophyll Biosynthesis. ACS Catalysis, 2022, 12, 4141-4148.	5.5	8
4	Engineering an efficient and enantioselective enzyme for the Morita–Baylis–Hillman reaction. Nature Chemistry, 2022, 14, 313-320.	6.6	34
5	Dual role of the active site â€~lid' regions of protochlorophyllide oxidoreductase in photocatalysis and plant development. FEBS Journal, 2021, 288, 175-189.	2.2	15
6	Interplay between chromophore binding and domain assembly by the B ₁₂ -dependent photoreceptor protein, CarH. Chemical Science, 2021, 12, 8333-8341.	3.7	10
7	Structure and Mechanism of <i>Pseudomonas aeruginosa</i> PA0254/HudA, a prFMN-Dependent Pyrrole-2-carboxylic Acid Decarboxylase Linked to Virulence. ACS Catalysis, 2021, 11, 2865-2878.	5.5	15
8	Photocatalysis as the â€~master switch' of photomorphogenesis in early plant development. Nature Plants, 2021, 7, 268-276.	4.7	22
9	Predicting new protein conformations from molecular dynamics simulation conformational landscapes and machine learning. Proteins: Structure, Function and Bioinformatics, 2021, 89, 915-921.	1.5	24
10	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
11	UbiD domain dynamics underpins aromatic decarboxylation. Nature Communications, 2021, 12, 5065.	5.8	14
12	Directed evolution of prenylated FMN-dependent Fdc supports efficient in vivo isobutene production. Nature Communications, 2021, 12, 5300.	5.8	11
13	Blood, sweat, and tears: extraterrestrial regolith biocomposites with in vivo binders. Materials Today Bio, 2021, 12, 100136.	2.6	12
14	Quantum Biology: An Update and Perspective. Quantum Reports, 2021, 3, 80-126.	0.6	74
15	Taming the Reactivity of Monoterpene Synthases To Guide Regioselective Product Hydroxylation. ChemBioChem, 2020, 21, 985-990.	1.3	13
16	Pressure and Temperature Effects on the Formation of Aminoacrylate Intermediates of Tyrosine Phenol-lyase Demonstrate Reaction Dynamics. ACS Catalysis, 2020, 10, 1692-1703.	5.5	6
17	Non-covalent protein-based adhesives for transparent substrates—bovine serum albumin vs. recombinant spider silk. Materials Today Bio, 2020, 7, 100068.	2.6	24
18	How Do Vanadium Chloroperoxidases Generate Hypochlorite from Hydrogen Peroxide and Chloride? A Computational Study. ACS Catalysis, 2020, 10, 14067-14079.	5.5	19

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19	Enzymatic C–H activation of aromatic compounds through CO2 fixation. Nature Chemical Biology, 2020, 16, 1255-1260.	3.9	29
20	Assessing the Covalent Attachment and Energy Transfer Capabilities of Upconverting Phosphors With Cofactor Containing Bioactive Enzymes. Frontiers in Chemistry, 2020, 8, 613334.	1.8	1
21	Covalent Attachment of Active Enzymes to Upconversion Phosphors Allows Ratiometric Detection of Substrates. Chemistry - A European Journal, 2020, 26, 14817-14822.	1.7	8
22	Ultrafast Vibrational Energy Transfer between Protein and Cofactor in a Flavoenzyme. Journal of Physical Chemistry B, 2020, 124, 5163-5168.	1.2	8
23	Rewiring the "Push-Pull―Catalytic Machinery of a Heme Enzyme Using an Expanded Genetic Code. ACS Catalysis, 2020, 10, 2735-2746.	5.5	25
24	Evaluating spectral overlap with the degree of quenching in UCP luminescence energy transfer systems. Methods and Applications in Fluorescence, 2020, 8, 045003.	1.1	3
25	Isotopically labeled flavoenzymes and their uses in probing reaction mechanisms. Methods in Enzymology, 2019, 620, 145-166.	0.4	2
26	MhuD from <i>Mycobacterium tuberculosis</i> : Probing a Dual Role in Heme Storage and Degradation. ACS Infectious Diseases, 2019, 5, 1855-1866.	1.8	8
27	Enzymatic control of cycloadduct conformation ensures reversible 1,3-dipolar cycloaddition in a prFMN-dependent decarboxylase. Nature Chemistry, 2019, 11, 1049-1057.	6.6	28
28	Graphene–aramid nanocomposite fibres <i>via</i> superacid co-processing. Chemical Communications, 2019, 55, 11703-11706.	2.2	8
29	Unexpected Roles of a Tether Harboring a Tyrosine Gatekeeper Residue in Modular Nitrite Reductase Catalysis. ACS Catalysis, 2019, 9, 6087-6099.	5.5	17
30	Evaluating spectral overlap with the degree of quenching in UCP luminescence energy transfer systems. Methods and Applications in Fluorescence, 2019, 7, 034003.	1.1	2
31	Photochemical Spin Dynamics of the Vitamin B ₁₂ Derivative, Methylcobalamin. Journal of Physical Chemistry B, 2019, 123, 4663-4672.	1.2	9
32	Selectivity through discriminatory induced fit enables switching of <scp>NAD</scp> (P)H coenzyme specificity in Old Yellow Enzyme eneâ€reductases. FEBS Journal, 2019, 286, 3117-3128.	2.2	10
33	Synthetic biology for fibers, adhesives, and active camouflage materials in protection and aerospace. MRS Communications, 2019, 9, 486-504.	0.8	21
34	Equatorial Active Site Compaction and Electrostatic Reorganization in Catechol-O-methyltransferase. ACS Catalysis, 2019, 9, 4394-4401.	5.5	21
35	Structural basis for enzymatic photocatalysis in chlorophyll biosynthesis. Nature, 2019, 574, 722-725.	13.7	88
36	What are the signatures of tunnelling in enzyme-catalysed reactions?. Faraday Discussions, 2019, 221, 367-378.	1.6	7

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37	Zero-point energy and tunnelling: general discussion. Faraday Discussions, 2019, 221, 478-500.	1.6	4
38	Pressurized CO ₂ as a carboxylating agent for the biocatalytic <i>ortho</i> -carboxylation of resorcinol. Green Chemistry, 2018, 20, 1754-1759.	4.6	23
39	1H, 15N and 13C backbone resonance assignments of pentaerythritol tetranitrate reductase from Enterobacter cloacae PB2. Biomolecular NMR Assignments, 2018, 12, 79-83.	0.4	6
40	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. ACS Catalysis, 2018, 8, 11589-11599.	5.5	12
41	Trapping methods for probing functional intermediates in nitric oxide synthases and related enzymes. Frontiers in Bioscience - Landmark, 2018, 23, 1874-1888.	3.0	2
42	A common mechanism for coenzyme cobalamin-dependent reductive dehalogenases. Physical Chemistry Chemical Physics, 2017, 19, 6090-6094.	1.3	21
43	Liver microsomal lipid enhances the activity and redox coupling of colocalized cytochrome P450 reductaseâ€cytochrome P450 3A4 in nanodiscs. FEBS Journal, 2017, 284, 2302-2319.	2.2	14
44	Convergence of Theory and Experiment on the Role of Preorganization, Quantum Tunneling, and Enzyme Motions into Flavoenzyme-Catalyzed Hydride Transfer. ACS Catalysis, 2017, 7, 3190-3198.	5.5	31
45	1H, 15N, 13C backbone resonance assignments of human soluble catechol O-methyltransferase in complex with S-adenosyl-l-methionine and 3,5-dinitrocatechol. Biomolecular NMR Assignments, 2017, 11, 57-61.	0.4	2
46	Structural Basis of Catalysis in the Bacterial Monoterpene Synthases Linalool Synthase and 1,8-Cineole Synthase. ACS Catalysis, 2017, 7, 6268-6282.	5.5	47
47	Extracting Kinetic Isotope Effects From a Global Analysis of Reaction Progress Curves. Methods in Enzymology, 2017, 596, 85-111.	0.4	1
48	Expanding the Scope of Biomolecule Monitoring with Ratiometric Signaling from Rareâ€Earth Upconverting Phosphors. European Journal of Inorganic Chemistry, 2017, 2017, 5176-5185.	1.0	7
49	Decoupled Associative and Dissociative Processes in Strong yet Highly Dynamic Host–Guest Complexes. Journal of the American Chemical Society, 2017, 139, 12985-12993.	6.6	56
50	A perspective on conformational control of electron transfer in nitric oxide synthases. Nitric Oxide - Biology and Chemistry, 2017, 63, 61-67.	1.2	19
51	Correlating Calmodulin Landscapes with Chemical Catalysis in Neuronal Nitric Oxide Synthase using Time-Resolved FRET and a 5-Deazaflavin Thermodynamic Trap. ACS Catalysis, 2016, 6, 5170-5180.	5.5	15
52	Time Course Analysis of Enzyme-Catalyzed DNA Polymerization. Biochemistry, 2016, 55, 5622-5634.	1.2	9
53	Untangling Heavy Protein and Cofactor Isotope Effects on Enzyme-Catalyzed Hydride Transfer. Journal of the American Chemical Society, 2016, 138, 13693-13699.	6.6	26
54	A â€~Plug and Play' Platform for the Production of Diverse Monoterpene Hydrocarbon Scaffolds in <i>Escherichia coli</i> ChemistrySelect, 2016, 1, 1893-1896.	0.7	42

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55	Donor–Acceptor Distance Sampling Enhances the Performance of "Better than Nature―Nicotinamide Coenzyme Biomimetics. Journal of the American Chemical Society, 2016, 138, 11089-11092.	6.6	38
56	Ground-State Destabilization by Phe-448 and Phe-449 Contributes to Tyrosine Phenol-Lyase Catalysis. ACS Catalysis, 2016, 6, 6770-6779.	5.5	20
57	An oxidative N-demethylase reveals PAS transition from ubiquitous sensor to enzyme. Nature, 2016, 539, 593-597.	13.7	21
58	Carboxylesterase converts Amplex red to resorufin: Implications for mitochondrial H2O2 release assays. Free Radical Biology and Medicine, 2016, 90, 173-183.	1.3	83
59	Dual transcriptional-translational cascade permits cellular level tuneable expression control. Nucleic Acids Research, 2016, 44, e21-e21.	6.5	39
60	Probing Reversible Chemistry in Coenzyme B ₁₂ â€Dependent Ethanolamine Ammonia Lyase with Kinetic Isotope Effects. Chemistry - A European Journal, 2015, 21, 8826-8831.	1.7	5
61	Towards the free energy landscape for catalysis in mammalian nitric oxide synthases. FEBS Journal, 2015, 282, 3016-3029.	2.2	23
62	Realâ€ŧime analysis of conformational control in electron transfer reactions of human cytochrome P450 reductase with cytochrome <i>c</i> . FEBS Journal, 2015, 282, 4357-4375.	2.2	27
63	Does the pressure dependence of kinetic isotope effects report usefully on dynamics in enzyme Hâ€ŧransfer reactions?. FEBS Journal, 2015, 282, 3243-3255.	2.2	8
64	UbiX is a flavin prenyltransferase required for bacterial ubiquinone biosynthesis. Nature, 2015, 522, 502-506.	13.7	168
65	New cofactor supports α,β-unsaturated acid decarboxylation via 1,3-dipolar cycloaddition. Nature, 2015, 522, 497-501.	13.7	197
66	Nuclear quantum tunnelling in enzymatic reactions – an enzymologist's perspective. Physical Chemistry Chemical Physics, 2015, 17, 30775-30782.	1.3	18
67	Epoxyqueuosine Reductase Structure Suggests a Mechanism for Cobalamin-dependent tRNA Modification. Journal of Biological Chemistry, 2015, 290, 27572-27581.	1.6	34
68	Structure and Mechanism of a Viral Collagen Prolyl Hydroxylase. Biochemistry, 2015, 54, 6093-6105.	1.2	19
69	Reductive dehalogenase structure suggests a mechanism for B12-dependent dehalogenation. Nature, 2015, 517, 513-516.	13.7	260
70	Energy Landscapes and Catalysis in Nitric-oxide Synthase. Journal of Biological Chemistry, 2014, 289, 11725-11738.	1.6	25
71	Ratiometric detection of enzyme turnover and flavin reduction using rare-earth upconverting phosphors. Dalton Transactions, 2014, 43, 5265-5268.	1.6	23
72	Proton tunnelling and promoting vibrations during the oxidation of ascorbate by ferricyanide?. Physical Chemistry Chemical Physics, 2014, 16, 2256.	1.3	10

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73	A quantitative fluorescenceâ€based steadyâ€state assay of <scp>DNA</scp> polymerase. FEBS Journal, 2014, 281, 2042-2050.	2.2	16
74	Practical Aspects on the Use of Kinetic Isotope Effects as Probes of Flavoprotein Enzyme Mechanisms. Methods in Molecular Biology, 2014, 1146, 161-175.	0.4	6
75	Fast Protein Motions Are Coupled to Enzyme H-Transfer Reactions. Journal of the American Chemical Society, 2013, 135, 2512-2517.	6.6	83
76	Dynamic, Electrostatic Model for the Generation and Control of Highâ€Energy Radical Intermediates by a Coenzyme B ₁₂ â€Dependent Enzyme. ChemBioChem, 2013, 14, 1529-1533.	1.3	11
77	Excited State Dynamics Can Be Used to Probe Donor-Acceptor Distances for H-Tunneling Reactions Catalyzed by Flavoproteins. Biophysical Journal, 2013, 105, 2549-2558.	0.2	17
78	Enzymatic Single-Molecule Kinetic Isotope Effects. Journal of the American Chemical Society, 2013, 135, 3855-3864.	6.6	21
79	Modulation of ligand–heme reactivity by binding pocket residues demonstrated in cytochromeÂc' over the femtosecond–second temporal range. FEBS Journal, 2013, 280, 6070-6082.	2.2	7
80	Relating localized protein motions to the reaction coordinate in coenzymeÂ <scp>B</scp> ₁₂ â€dependent enzymes. FEBS Journal, 2013, 280, 2997-3008.	2.2	29
81	Ultrafast Infrared Spectral Fingerprints of Vitamin B ₁₂ and Related Cobalamins. Journal of Physical Chemistry A, 2012, 116, 5586-5594.	1.1	38
82	Evidence of Preorganization in Quinonoid Intermediate Formation from <scp>l</scp> -Trp in H463F Mutant <i>Escherichia coli</i> Tryptophan Indole-lyase from Effects of Pressure and pH. Biochemistry, 2012, 51, 6527-6533.	1.2	5
83	Protein Motions Are Coupled to the Reaction Chemistry in Coenzyme B ₁₂ â€Dependent Ethanolamine Ammonia Lyase. Angewandte Chemie - International Edition, 2012, 51, 9306-9310.	7.2	28
84	Pressure Effects on Enzyme-Catalyzed Quantum Tunneling Events Arise from Protein-Specific Structural and Dynamic Changes. Journal of the American Chemical Society, 2012, 134, 9749-9754.	6.6	27
85	Good vibrations in enzyme-catalysed reactions. Nature Chemistry, 2012, 4, 161-168.	6.6	246
86	Gating mechanisms for biological electron transfer: Integrating structure with biophysics reveals the nature of redox control in cytochrome P450 reductase and copperâ€dependent nitrite reductase. FEBS Letters, 2012, 586, 578-584.	1.3	31
87	Preparation and photophysical properties of a caged kynurenine. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 2734-2737.	1.0	9
88	Kinetic and spectroscopic probes of motions and catalysis in the cytochrome P450 reductase family of enzymes. FEBS Journal, 2012, 279, 1534-1544.	2.2	18
89	Electrochemical and Structural Properties of a Protein System Designed To Generate Tyrosine Pourbaix Diagrams. Journal of the American Chemical Society, 2011, 133, 17786-17795.	6.6	37
90	Chapter 3. Experimental Approaches Towards Proton-Coupled Electron Transfer Reactions in Biological Redox Systems. RSC Catalysis Series, 2011, , 57-88.	0.1	1

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91	Examining the importance of dynamics, barrier compression and hydrogen tunnelling in enzyme catalysed reactions. Procedia Chemistry, 2011, 3, 306-315.	0.7	2
92	ls There a Dynamic Protein Contribution to the Substrate Trigger in Coenzyme B ₁₂ â€Dependent Ethanolamine Ammonia Lyase?. Angewandte Chemie - International Edition, 2011, 50, 10843-10846.	7.2	30
93	Probing active site geometry using high pressure and secondary isotope effects in an enzymeâ€catalysed â€`deep' Hâ€tunnelling reaction. Journal of Physical Organic Chemistry, 2010, 23, 696-701.	0.9	16
94	Barrier Compression and Its Contribution to Both Classical and Quantum Mechanical Aspects of Enzyme Catalysis. Biophysical Journal, 2010, 98, 121-128.	0.2	43
95	Nature of the Energy Landscape for Gated Electron Transfer in a Dynamic Redox Protein. Journal of the American Chemical Society, 2010, 132, 9738-9745.	6.6	63
96	Direct Analysis of Donorâ^'Acceptor Distance and Relationship to Isotope Effects and the Force Constant for Barrier Compression in Enzymatic H-Tunneling Reactions. Journal of the American Chemical Society, 2010, 132, 11329-11335.	6.6	74
97	Demonstration of Proton-coupled Electron Transfer in the Copper-containing Nitrite Reductases. Journal of Biological Chemistry, 2009, 284, 25973-25983.	1.6	50
98	Parallel Pathways and Freeâ€Energy Landscapes for Enzymatic Hydride Transfer Probed by Hydrostatic Pressure. ChemBioChem, 2009, 10, 1379-1384.	1.3	22
99	Are the Catalytic Properties of Enzymes from Piezophilic Organisms Pressure Adapted?. ChemBioChem, 2009, 10, 2348-2353.	1.3	48
100	Barrier Compression Enhances an Enzymatic Hydrogenâ€Transfer Reaction. Angewandte Chemie - International Edition, 2009, 48, 1452-1454.	7.2	52
101	Structural and mechanistic aspects of flavoproteins: probes of hydrogen tunnelling. FEBS Journal, 2009, 276, 3930-3941.	2.2	27
102	Bipartite recognition and conformational sampling mechanisms for hydride transfer from nicotinamide coenzyme to FMN in pentaerythritol tetranitrate reductase. FEBS Journal, 2009, 276, 4780-4789.	2.2	24
103	Evidence To Support the Hypothesis That Promoting Vibrations Enhance the Rate of an Enzyme Catalyzed H-Tunneling Reaction. Journal of the American Chemical Society, 2009, 131, 17072-17073.	6.6	79
104	Probing Coupled Motions in Enzymatic Hydrogen Tunnelling Reactions: Beyond Temperature-Dependence Studies of Kinetic Isotope Effects. RSC Biomolecular Sciences, 2009, , 199-218.	0.4	12
105	H-transfers in Photosystem II: what can we learn from recent lessons in the enzyme community?. Photosynthesis Research, 2008, 98, 169-177.	1.6	6
106	Driving Force Analysis of Proton Tunnelling Across a Reactivity Series for an Enzymeâ€Substrate Complex. ChemBioChem, 2008, 9, 2839-2845.	1.3	20
107	Secondary Kinetic Isotope Effects as Probes of Environmentallyâ€Coupled Enzymatic Hydrogen Tunneling Reactions. ChemPhysChem, 2008, 9, 1536-1539.	1.0	16
108	Solvent as a Probe of Active Site Motion and Chemistry during the Hydrogen Tunnelling Reaction in Morphinone Reductase. ChemPhysChem, 2008, 9, 1875-1881.	1.0	16

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109	Are Environmentally Coupled Enzymatic Hydrogen Tunneling Reactions Influenced by Changes in Solution Viscosity?. Angewandte Chemie - International Edition, 2008, 47, 537-540.	7.2	34
110	Interâ€flavin electron transfer in cytochrome P450 reductase – effects of solvent and pH identify hidden complexity in mechanism. FEBS Journal, 2008, 275, 4540-4557.	2.2	39
111	Deep Tunneling Dominates the Biologically Important Hydride Transfer Reaction from NADH to FMN in Morphinone Reductase. Journal of the American Chemical Society, 2008, 130, 7092-7097.	6.6	75
112	Incorporation of Hydrostatic Pressure into Models of Hydrogen Tunneling Highlights a Role for Pressure-Modulated Promoting Vibrations. Biochemistry, 2008, 47, 9880-9887.	1.2	36
113	Correction of Pre-Steady-State KIEs for Isotopic Impurities and the Consequences of Kinetic Isotope Fractionation. Journal of Physical Chemistry A, 2008, 112, 13109-13115.	1.1	9
114	Making a single-chain four-helix bundle for redox chemistry studies. Protein Engineering, Design and Selection, 2008, 21, 645-652.	1.0	9
115	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. Biochemical Society Transactions, 2008, 36, 16-21.	1.6	21
116	DNA Binding Suppresses Human AIF-M2 Activity and Provides a Connection between Redox Chemistry, Reactive Oxygen Species, and Apoptosis. Journal of Biological Chemistry, 2007, 282, 30331-30340.	1.6	36
117	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, 507-512.	3.3	98
118	Redox Characteristics of a de Novo Quinone Protein. Journal of Physical Chemistry B, 2007, 111, 3488-3495.	1.2	24
119	Conformational Dynamics of the Cytochrome P450 BM3/N-Palmitoylglycine Complex:  The Proposed "ProximalⰒDistal―Transition Probed by Temperature-Jump Spectroscopy. Journal of Physical Chemistry B, 2007, 111, 7879-7886.	1.2	16
120	Conformational and Thermodynamic Control of Electron Transfer in Neuronal Nitric Oxide Synthase. Biochemistry, 2007, 46, 5018-5029.	1.2	53
121	Mutagenesis of Morphinone Reductase Induces Multiple Reactive Configurations and Identifies Potential Ambiguity in Kinetic Analysis of Enzyme Tunneling Mechanisms. Journal of the American Chemical Society, 2007, 129, 13949-13956.	6.6	55
122	Proton Tunneling in Aromatic Amine Dehydrogenase is Driven by a Short-Range Sub-Picosecond Promoting Vibration:Â Consistency of Simulation and Theory with Experiment. Journal of Physical Chemistry B, 2007, 111, 2631-2638.	1.2	62
123	Magnetic Field Effect Studies Indicate Reduced Geminate Recombination of the Radical Pair in Substrate-Bound Adenosylcobalamin-Dependent Ethanolamine Ammonia Lyase. Journal of the American Chemical Society, 2007, 129, 15718-15727.	6.6	51
124	α-Secondary Isotope Effects as Probes of "Tunneling-Ready―Configurations in Enzymatic H-Tunneling:Â Insight from Environmentally Coupled Tunneling Models. Journal of the American Chemical Society, 2006, 128, 14053-14058.	6.6	66
125	Moving a Phenol Hydroxyl Group from the Surface to the Interior of a Protein:  Effects on the Phenol Potential and pKA. Biochemistry, 2005, 44, 11891-11902.	1.2	27
126	Conversion of theEscherichia coliCytochromeb562to an Archetype Cytochromeb:Â A Mutant with Bis-Histidine Ligation of Heme Ironâ€. Biochemistry, 2005, 44, 431-439.	1.2	24

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127	Protein engineering of cytochrome b562 for quinone binding and light-induced electron transfer. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 17675-17680.	3.3	46