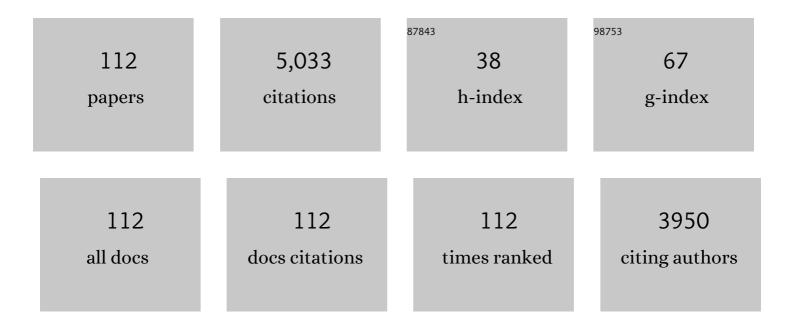
## Debra Dunaway-Mariano

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Structural Analysis of Binding Determinants of <i>Salmonella typhimurium</i> Trehalose-6-phosphate Phosphatase Using Ground-State Complexes. Biochemistry, 2020, 59, 3247-3257.	1.2	2
2	Structural Basis of the Molecular Switch between Phosphatase and Mutase Functions of Human Phosphomannomutase 1 under Ischemic Conditions. Biochemistry, 2018, 57, 3480-3492.	1.2	7
3	Mechanism of Substrate Recognition and Catalysis of the Haloalkanoic Acid Dehalogenase Family Member α-Phosphoglucomutase. Biochemistry, 2018, 57, 4504-4517.	1.2	8
4	Rational design of first generation inhibitors for trehalose 6-phosphate phosphatases. Tetrahedron, 2017, 73, 1324-1330.	1.0	12
5	Rational design of reversible inhibitors for trehalose 6-phosphate phosphatases. European Journal of Medicinal Chemistry, 2017, 128, 274-286.	2.6	16
6	Catalytic Mechanism of the Hotdogâ€Fold Thioesterase PA1618 Revealed by Xâ€ray Structure Determination of a Substrateâ€Bound Oxygen Ester Analogue Complex. ChemBioChem, 2017, 18, 1935-1943.	1.3	0
7	Catalytic scaffolds for phosphoryl group transfer. Current Opinion in Structural Biology, 2016, 41, 172-179.	2.6	17
8	Panoramic view of a superfamily of phosphatases through substrate profiling. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E1974-83.	3.3	118
9	Specificity and Promiscuity in Enzyme Superfamilies. FASEB Journal, 2015, 29, 237.1.	0.2	0
10	Structure of the Trehalose-6-phosphate Phosphatase from Brugia malayi Reveals Key Design Principles for Anthelmintic Drugs. PLoS Pathogens, 2014, 10, e1004245.	2.1	30
11	Structure-guided approach for detecting large domain inserts in protein sequences as illustrated using the haloacid dehalogenase superfamily. Proteins: Structure, Function and Bioinformatics, 2014, 82, 1896-1906.	1.5	3
12	Enzyme Promiscuity: Engine of Evolutionary Innovation. Journal of Biological Chemistry, 2014, 289, 30229-30236.	1.6	125
13	Structure and Catalysis in the <i>Escherichia coli</i> Hotdog-fold Thioesterase Paralogs Ydil and YbdB. Biochemistry, 2014, 53, 4788-4805.	1.2	12
14	Divergence of Substrate Specificity and Function in the <i>Escherichia coli</i> Hotdog-fold Thioesterase Paralogs Ydil and YbdB. Biochemistry, 2014, 53, 4775-4787.	1.2	14
15	Coâ€evolution of HAD phosphatase and hotdogâ€fold thioesterase domain function in the menaquinoneâ€pathway fusion proteins BF1314 and PG1653. FEBS Letters, 2013, 587, 2851-2859.	1.3	9
16	W. W. "Mo―Cleland: A Catalytic Life. Biochemistry, 2013, 52, 9092-9096.	1.2	6
17	Structural Basis for the Divergence of Substrate Specificity and Biological Function within HAD Phosphatases in Lipopolysaccharide and Sialic Acid Biosynthesis. Biochemistry, 2013, 52, 5372-5386.	1.2	20
18	Neutron diffraction studies towards deciphering the protonation state of catalytic residues in the bacterial KDN9P phosphatase. Acta Crystallographica Section F: Structural Biology Communications, 2013, 69, 1015-1019.	0.7	5

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19	Consequences of domain insertion on sequence-structure divergence in a superfold. Proceedings of the United States of America, 2013, 110, E3381-7.	3.3	25
20	Ligand Binding and Conformational Change Coupling in the HAD Superfamily. FASEB Journal, 2013, 27, 998.8.	0.2	0
21	The nature of sequence and structure divergence in the Haloalkanoate Dehalogenase SuperFamily (HADSF). FASEB Journal, 2013, 27, 797.2.	0.2	Ο
22	The structural basis of the secondary function of PMM1 in the presence of IMP. FASEB Journal, 2013, 27, 998.5.	0.2	0
23	Ultra Highâ€ŧhroughput Screening Uncovers New Activities in Phosphatases of the Haloalkanoic Acid Dehalogenase Superfamily (HADSF). FASEB Journal, 2013, 27, 571.1.	0.2	Ο
24	Correlation of Structure and Function in the Human Hotdog-fold Enzyme hTHEM4. Biochemistry, 2012, 51, 6490-6492.	1.2	7
25	Investigation of the Catalytic Mechanism of the Hotdog-Fold Enzyme Superfamily <i>Pseudomonas</i> sp. Strain CBS3 4-Hydroxybenzoyl-CoA Thioesterase. Biochemistry, 2012, 51, 786-794.	1.2	11
26	The Catalytic Mechanism of the Hotdog-fold Enzyme Superfamily 4-Hydroxybenzoyl-CoA Thioesterase from <i>Arthrobacter </i> sp. Strain SU. Biochemistry, 2012, 51, 7000-7016.	1.2	22
27	A thioester substrate binds to the enzyme <i>Arthrobacter</i> thioesterase in two ionization states: evidence from Raman difference spectroscopy. Journal of Raman Spectroscopy, 2012, 43, 65-71.	1.2	8
28	Divergence of Structure and Function in the Haloacid Dehalogenase Enzyme Superfamily: <i>Bacteroides thetaiotaomicron</i> BT2127 Is an Inorganic Pyrophosphatase. Biochemistry, 2011, 50, 8937-8949.	1.2	36
29	The Xâ€ray crystallographic structure and specificity profile of HAD superfamily phosphohydrolase BT1666: Comparison of paralogous functions in <i>B. thetaiotaomicron</i> . Proteins: Structure, Function and Bioinformatics, 2011, 79, 3099-3107.	1.5	11
30	X-ray structure and characterization of carbamate kinase from the human parasite <i>Giardia lamblia</i> . Acta Crystallographica Section F: Structural Biology Communications, 2010, 66, 386-390.	0.7	11
31	Structural Determinants of Substrate Recognition in the HAD Superfamily Member d-glycero-d-manno-Heptose-1,7-bisphosphate Phosphatase (GmhB),. Biochemistry, 2010, 49, 1082-1092.	1.2	35
32	Structure-Function Analysis of 2-Keto-3-deoxy-D-glycero-D-galactonononate-9-phosphate Phosphatase Defines Specificity Elements in Type CO Haloalkanoate Dehalogenase Family Members. Journal of Biological Chemistry, 2009, 284, 1224-1233.	1.6	27
33	Markers of fitness in a successful enzyme superfamily. Current Opinion in Structural Biology, 2009, 19, 658-665.	2.6	94
34	Mechanisms of catalysis and inhibition operative in the arginine deiminase from the human pathogen Giardia lamblia. Bioorganic Chemistry, 2009, 37, 149-161.	2.0	30
35	The Akt C-Terminal Modulator Protein Is an Acyl-CoA Thioesterase of the Hotdog-Fold Family. Biochemistry, 2009, 48, 5507-5509.	1.2	17
36	Analysis of the Structural Determinants Underlying Discrimination between Substrate and Solvent in β-Phosphoglucomutase Catalysis. Biochemistry, 2009, 48, 1984-1995.	1.2	35

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37	The Mechanisms of Human Hotdog-fold Thioesterase 2 (hTHEM2) Substrate Recognition and Catalysis Illuminated by a Structure and Function Based Analysis <sup>,</sup> . Biochemistry, 2009, 48, 1293-1304.	1.2	54
38	In Vitro Kinetic Analysis of Substrate Specificity in Enterobactin Biosynthetic Lower Pathway Enzymes Provides Insight into the Biochemical Function of the Hot Dog-Fold Thioesterase EntH. Biochemistry, 2009, 48, 511-513.	1.2	22
39	Structure and Function of 2,3-Dimethylmalate Lyase, a PEP Mutase/Isocitrate Lyase Superfamily Member. Journal of Molecular Biology, 2009, 386, 486-503.	2.0	13
40	The Xâ€ray crystallographic structure and activity analysis of a <i>Pseudomonasâ€</i> specific subfamily of the HAD enzyme superfamily evidences a novel biochemical function. Proteins: Structure, Function and Bioinformatics, 2008, 70, 197-207.	1.5	5
41	Human Symbiont Bacteroides thetaiotaomicron Synthesizes 2-Keto-3-Deoxy-D-Glycero-D- Galacto-Nononic Acid (KDN). Chemistry and Biology, 2008, 15, 893-897.	6.2	16
42	Enzyme Function Discovery. Structure, 2008, 16, 1599-1600.	1.6	14
43	The Electrostatic Driving Force for Nucleophilic Catalysis in l-Arginine Deiminase: A Combined Experimental and Theoretical Study. Biochemistry, 2008, 47, 4721-4732.	1.2	22
44	Inactivation of Microbial Arginine Deiminases by <scp>l</scp> -Canavanine. Journal of the American Chemical Society, 2008, 130, 1918-1931.	6.6	37
45	Structure of YciA from Haemophilus influenzae (HI0827), a Hexameric Broad Specificity Acyl-Coenzyme A Thioesterase,. Biochemistry, 2008, 47, 2797-2805.	1.2	32
46	Divergence of Function in the Hot Dog Fold Enzyme Superfamily: The Bacterial Thioesterase YciA. Biochemistry, 2008, 47, 2789-2796.	1.2	62
47	Structure and Function of PA4872 from <i>Pseudomonas aeruginosa</i> , a Novel Class of Oxaloacetate Decarboxylase from the PEP Mutase/Isocitrate Lyase Superfamily <sup>,</sup> . Biochemistry, 2008, 47, 167-182.	1.2	20
48	The catalytic scaffold of the haloalkanoic acid dehalogenase enzyme superfamily acts as a mold for the trigonal bipyramidal transition state. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 5687-5692.	3.3	56
49	Characterization, Kinetics, and Crystal Structures of Fructose-1,6-bisphosphate Aldolase from the Human Parasite, Giardia lamblia. Journal of Biological Chemistry, 2007, 282, 4859-4867.	1.6	45
50	Oxaloacetate Hydrolase, the C–C Bond Lyase of Oxalate Secreting Fungi. Journal of Biological Chemistry, 2007, 282, 9581-9590.	1.6	102
51	Structure and Kinetics of Phosphonopyruvate Hydrolase fromVoriovoraxsp. Pal2:Â New Insight into the Divergence of Catalysis within the PEP Mutase/Isocitrate Lyase Superfamilyâ€,‡. Biochemistry, 2006, 45, 11491-11504.	1.2	31
52	Conformational Cycling in β-Phosphoglucomutase Catalysis: Reorientation of the β-d-Glucose 1,6-(Bis)phosphate Intermediateâ€. Biochemistry, 2006, 45, 7818-7824.	1.2	31
53	Crystal structure of human thioesterase superfamily member 2. Biochemical and Biophysical Research Communications, 2006, 349, 172-177.	1.0	30
54	Kinetic Analysis of Pseudomonas aeruginosa Arginine Deiminase Mutants and Alternate Substrates Provides Insight into Structural Determinants of Function. Biochemistry, 2006, 45, 1162-1172.	1.2	58

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55	Evolutionary Genomics of the HAD Superfamily: Understanding the Structural Adaptations and Catalytic Diversity in a Superfamily of Phosphoesterases and Allied Enzymes. Journal of Molecular Biology, 2006, 361, 1003-1034.	2.0	376
56	Diversification of function in the haloacid dehalogenase enzyme superfamily: The role of the cap domain in hydrolytic phosphoruscarbon bond cleavage. Bioorganic Chemistry, 2006, 34, 394-409.	2.0	32
57	Structure and Activity Analyses of Escherichia coli K-12 NagD Provide Insight into the Evolution of Biochemical Function in the Haloalkanoic Acid Dehalogenase Superfamily,. Biochemistry, 2006, 45, 1183-1193.	1.2	57
58	Structure, Function, and Mechanism of the Phenylacetate Pathway Hot Dog-fold Thioesterase Paal. Journal of Biological Chemistry, 2006, 281, 11028-11038.	1.6	60
59	The X-ray Crystal Structures of Human α-Phosphomannomutase 1 Reveal the Structural Basis of Congenital Disorder of Glycosylation Type 1a. Journal of Biological Chemistry, 2006, 281, 14918-14926.	1.6	66
60	Raman evidence for product binding to the enzyme W137F 4-chlorobenzoyl-CoA dehalogenase in two conformational states. Journal of Raman Spectroscopy, 2005, 36, 320-325.	1.2	2
61	Crystal Structures Representing the Michaelis Complex and the Thiouronium Reaction Intermediate of Pseudomonas aeruginosa Arginine Deiminase. Journal of Biological Chemistry, 2005, 280, 34080-34087.	1.6	58
62	Crystal Structure of the Petal Death Protein from Carnation Flowerâ€,‡. Biochemistry, 2005, 44, 16377-16384.	1.2	14
63	Catalytic Cycling in β-Phosphoglucomutase:  A Kinetic and Structural Analysis,. Biochemistry, 2005, 44, 9404-9416.	1.2	51
64	Diversity of Function in the Isocitrate Lyase Enzyme Superfamily:Â TheDianthus caryophyllusPetal Death Protein Cleaves α-Keto and α-Hydroxycarboxylic Acidsâ€. Biochemistry, 2005, 44, 16365-16376.	1.2	28
65	HAD Superfamily Phosphotransferase Substrate Diversification:Â Structure and Function Analysis of HAD Subclass IIB Sugar Phosphatase BT4131â€,‡. Biochemistry, 2005, 44, 8684-8696.	1.2	75
66	Crystal Structures of 2-Methylisocitrate Lyase in Complex with Product and with Isocitrate Inhibitor Provide Insight into Lyase Substrate Specificity, Catalysis and Evolutionâ€,â€j. Biochemistry, 2005, 44, 2949-2962.	1.2	35
67	The BH1999 Protein of Bacillus halodurans C-125 Is Gentisyl-Coenzyme A Thioesterase. Journal of Bacteriology, 2004, 186, 393-399.	1.0	19
68	X-ray Crystallographic and Site-directed Mutagenesis Analysis of the Mechanism of Schiff-base Formation in Phosphonoacetaldehyde Hydrolase Catalysis. Journal of Biological Chemistry, 2004, 279, 9353-9361.	1.6	34
69	Phosphoryl group transfer: evolution of a catalytic scaffold. Trends in Biochemical Sciences, 2004, 29, 495-503.	3.7	249
70	Analysis of the Substrate Specificity Loop of the HAD Superfamily Cap Domainâ€,‡. Biochemistry, 2004, 43, 2812-2820.	1.2	83
71	Investigation of Metal Ion Binding in Phosphonoacetaldehyde Hydrolase Identifies Sequence Markers for Metal-Activated Enzymes of the HAD Enzyme Superfamily,. Biochemistry, 2004, 43, 4990-4997.	1.2	33
72	X-ray Crystal Structure of the Hypothetical Phosphotyrosine Phosphatase MDP-1 of the Haloacid Dehalogenase Superfamily,. Biochemistry, 2004, 43, 12770-12779.	1.2	47

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73	Arginine Deiminase Uses an Active-Site Cysteine in Nucleophilic Catalysis ofl-Arginine Hydrolysis. Journal of the American Chemical Society, 2004, 126, 5374-5375.	6.6	56
74	Enzymatic synthesis of radiolabeled phosphonoacetaldehyde. Analytical Biochemistry, 2003, 322, 233-237.	1.1	6
75	The Pentacovalent Phosphorus Intermediate of a Phosphoryl Transfer Reaction. Science, 2003, 299, 2067-2071.	6.0	306
76	The Strength of Dehalogenaseâ^'Substrate Hydrogen Bonding Correlates with the Rate of Meisenheimer Intermediate Formationâ€. Biochemistry, 2003, 42, 9482-9490.	1.2	18
77	Response to Comment on "The Pentacovalent Phosphorus Intermediate of a Phosphoryl Transfer Reaction". Science, 2003, 301, 1184d-1184.	6.0	33
78	Characterization of the 4-Hydroxybenzoyl-Coenzyme A Thioesterase from Arthrobacter sp. Strain SU. Applied and Environmental Microbiology, 2003, 69, 2707-2711.	1.4	33
79	The Structure of 4-Hydroxybenzoyl-CoA Thioesterase from Arthrobacter sp. strain SU. Journal of Biological Chemistry, 2003, 278, 43709-43716.	1.6	59
80	The Phosphonopyruvate Decarboxylase from Bacteroides fragilis. Journal of Biological Chemistry, 2003, 278, 41302-41308.	1.6	45
81	X-ray Crystallographic Analyses of Inhibitor and Substrate Complexes of Wild-type and Mutant 4-Hydroxybenzoyl-CoA Thioesterase. Journal of Biological Chemistry, 2002, 277, 27468-27476.	1.6	53
82	Caught in the Act: The Structure of Phosphorylatedβ-Phosphoglucomutase fromLactococcus lactisâ€,‡. Biochemistry, 2002, 41, 8351-8359.	1.2	107
83	Kinetic Evidence for a Substrate-Induced Fit in Phosphonoacetaldehyde Hydrolase Catalysisâ€. Biochemistry, 2002, 41, 13370-13377.	1.2	28
84	The YbgC protein encoded by theybgCgene of thetol-palgene cluster ofHaemophilus influenzaecatalyzes acyl-coenzyme A thioester hydrolysis. FEBS Letters, 2002, 516, 161-163.	1.3	36
85	Kinetic, Raman, NMR, and Site-Directed Mutagenesis Studies of the Pseudomonas Sp. Strain CBS3 4-Hydroxybenzoyl-CoA Thioesterase Active Site. Biochemistry, 2002, 41, 11152-11160.	1.2	28
86	Crystallization and preliminary X-ray diffraction studies of β-phosphoglucomutase fromLactococcus lactus. Acta Crystallographica Section D: Biological Crystallography, 2002, 58, 324-326.	2.5	12
87	Investigation of the Role of the Domain Linkers in Separate Site Catalysis byClostridium symbiosumPyruvate Phosphate Dikinaseâ€. Biochemistry, 2001, 40, 13466-13473.	1.2	5
88	Role of Active Site Binding Interactions in 4-Chlorobenzoyl-Coenzyme A Dehalogenase Catalysis. Biochemistry, 2001, 40, 15684-15692.	1.2	38
89	Raman difference spectroscopic studies of dithiobenzoyl substrate and product analogs binding to the enzyme dehalogenase: ?-electron polarization is prevented by the C?O to C?S substitution. Journal of Raman Spectroscopy, 2000, 31, 365-371.	1.2	12
90	The Crystal Structure ofBacillus cereusPhosphonoacetaldehyde Hydrolase:Â Insight into Catalysis of Phosphorus Bond Cleavage and Catalytic Diversification within the HAD Enzyme Superfamilyâ€,‡. Biochemistry, 2000, 39, 10385-10396.	1.2	136

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91	Helix swapping between two α/β barrels: crystal structure of phosphoenolpyruvate mutase with bound Mg2+–oxalate. Structure, 1999, 7, 539-548.	1.6	35
92	Modulating Electron Density in the Bound Product, 4-Hydroxybenzoyl-CoA, by Mutations in 4-Chlorobenzoyl-CoA Dehalogenase Near the 4-Hydroxy Groupâ€. Biochemistry, 1999, 38, 4198-4206.	1.2	26
93	Interchange of Catalytic Activity within the 2-Enoyl-Coenzyme A Hydratase/Isomerase Superfamily Based on a Common Active Site Templateâ€. Biochemistry, 1999, 38, 7638-7652.	1.2	78
94	Insight into the Mechanism of Phosphoenolpyruvate Mutase Catalysis Derived from Site-Directed Mutagenesis Studies of Active Site Residuesâ€. Biochemistry, 1999, 38, 14165-14173.	1.2	28
95	Insights into the Mechanism of Catalysis by the Pâ^'C Bond-Cleaving Enzyme Phosphonoacetaldehyde Hydrolase Derived from Gene Sequence Analysis and Mutagenesis. Biochemistry, 1998, 37, 9305-9315.	1.2	71
96	Location of the Phosphate Binding Site within Clostridium symbiosum Pyruvate Phosphate Dikinase,. Biochemistry, 1998, 37, 13463-13474.	1.2	21
97	The Three-dimensional Structure of 4-Hydroxybenzoyl-CoA Thioesterase from Pseudomonas sp. Strain CBS-3. Journal of Biological Chemistry, 1998, 273, 33572-33579.	1.6	101
98	Investigation of Substrate Activation by 4-Chlorobenzoyl-Coenzyme A Dehalogenase. Biochemistry, 1997, 36, 1349-1361.	1.2	34
99	Raman Study of the Polarizing Forces Promoting Catalysis in 4-Chlorobenzoate-CoA Dehalogenaseâ€. Biochemistry, 1997, 36, 10192-10199.	1.2	45
100	Acyl-Adenylate Motif of the Acyl-Adenylate/Thioester-Forming Enzyme Superfamily:Â A Site-Directed Mutagenesis Study with thePseudomonassp. Strain CBS3 4-Chlorobenzoate:Coenzyme A Ligaseâ€. Biochemistry, 1997, 36, 15650-15659.	1.2	120
101	Phosphoenolpyruvate Mutase Catalysis of Phosphoryl Transfer in Phosphoenolpyruvate:Â Kinetics and Mechanism of Phosphorusâ°'Carbon Bond Formationâ€. Biochemistry, 1996, 35, 4628-4635.	1.2	24
102	Structure of 4-Chlorobenzoyl Coenzyme A Dehalogenase Determined to 1.8 Ã Resolution:Â An Enzyme Catalyst Generated via Adaptive Mutationâ€,‡. Biochemistry, 1996, 35, 8103-8109.	1.2	169
103	Identification of Active Site Residues Essential to 4-Chlorobenzoylâ^'Coenzyme A Dehalogenase Catalysis by Chemical Modification and Site Directed Mutagenesisâ€. Biochemistry, 1996, 35, 10879-10885.	1.2	37
104	Evidence for electrophilic catalysis in the 4-chlorobenzoyl-CoA dehalogenase reaction: UV, Raman, and 13C-NMR spectral studies of dehalogenase complexes of benzoyl-CoA adducts. Biochemistry, 1995, 34, 13881-13888.	1.2	45
105	On the origins and functions of the enzymes of the 4-chlorobenzoate to 4-hydroxybenzoate converting pathway. Biodegradation, 1994, 5, 259-276.	1.5	68
106	Ancestry of the 4-chlorobenzoate dehalogenase: analysis of amino acid sequence identities among families of acyl:adenyl ligases, enoyl-CoA hydratases/isomerases, and acyl-CoA thioesterases. Biochemistry, 1992, 31, 5594-5604.	1.2	212
107	Stereochemical probe for the mechanism of phosphorus-carbon bond cleavage catalyzed by the Bacillus cereus phosphonoacetaldehyde hydrolase. Journal of the American Chemical Society, 1992, 114, 7346-7354.	6.6	35
108	Investigation of the substrate binding and catalytic groups of the Pî—,C bond cleaving enzyme, phosphonoacetaldehyde hydrolase. Archives of Biochemistry and Biophysics, 1992, 296, 144-151.	1.4	31

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109	Investigations of the partial reactions catalyzed by pyruvate phosphate dikinase. Biochemistry, 1988, 27, 625-633.	1.2	40
110	Investigation of the Bacillus cereus phosphonoacetaldehyde hydrolase. Evidence for a Schiff base mechanism and sequence analysis of an active-site peptide containing the catalytic lysine residue. Biochemistry, 1988, 27, 2229-2234.	1.2	48
111	Inhibition and Inactivation of Pyruvate Phosphate Dikinase with Cr(III) Complexes of Adenosine 5′-Triphosphate and Inorganic Pyrophosphate. Journal of Enzyme Inhibition and Medicinal Chemistry, 1986, 1, 113-125.	0.5	1
112	Investigation of the role of the substrate metal ion in the yeast inorganic pyrophosphatase reaction. FEBS Letters, 1984, 165, 251-253.	1.3	11