

Debra Dunaway-Mariano

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L-index

#	Paper	IF	Citations
112	Evolutionary genomics of the HAD superfamily: understanding the structural adaptations and catalytic diversity in a superfamily of phosphoesterases and allied enzymes. <i>Journal of Molecular Biology</i> , 2006 , 361, 1003-34	6.5	315
111	The pentacovalent phosphorus intermediate of a phosphoryl transfer reaction. <i>Science</i> , 2003 , 299, 2067-71	31.3	291
110	Phosphoryl group transfer: evolution of a catalytic scaffold. <i>Trends in Biochemical Sciences</i> , 2004 , 29, 495-503	10.3	229
109	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. <i>Biochemistry</i> , 1992 , 31, 5594-604	3.2	190
108	Structure of 4-chlorobenzoyl coenzyme A dehalogenase determined to 1.8 Å resolution: an enzyme catalyst generated via adaptive mutation. <i>Biochemistry</i> , 1996 , 35, 8103-9	3.2	156
107	The crystal structure of bacillus cereus phosphonoacetaldehyde hydrolase: insight into catalysis of phosphorus bond cleavage and catalytic diversification within the HAD enzyme superfamily. <i>Biochemistry</i> , 2000 , 39, 10385-96	3.2	124
106	Acyl-adenylate motif of the acyl-adenylate/thioester-forming enzyme superfamily: a site-directed mutagenesis study with the <i>Pseudomonas</i> sp. strain CBS3 4-chlorobenzoate:coenzyme A ligase. <i>Biochemistry</i> , 1997 , 36, 15650-9	3.2	118
105	Enzyme promiscuity: engine of evolutionary innovation. <i>Journal of Biological Chemistry</i> , 2014 , 289, 30229-30236	10.7	107
104	Caught in the act: the structure of phosphorylated beta-phosphoglucomutase from <i>Lactococcus lactis</i> . <i>Biochemistry</i> , 2002 , 41, 8351-9	3.2	100
103	The three-dimensional structure of 4-hydroxybenzoyl-CoA thioesterase from <i>Pseudomonas</i> sp. Strain CBS-3. <i>Journal of Biological Chemistry</i> , 1998 , 273, 33572-9	5.4	98
102	Panoramic view of a superfamily of phosphatases through substrate profiling. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015 , 112, E1974-83	11.5	81
101	Analysis of the substrate specificity loop of the HAD superfamily cap domain. <i>Biochemistry</i> , 2004 , 43, 2812-20	3.2	78
100	Markers of fitness in a successful enzyme superfamily. <i>Current Opinion in Structural Biology</i> , 2009 , 19, 658-65	8.1	77
99	Oxaloacetate hydrolase, the C-C bond lyase of oxalate secreting fungi. <i>Journal of Biological Chemistry</i> , 2007 , 282, 9581-9590	5.4	77
98	Interchange of catalytic activity within the 2-enoyl-coenzyme A hydratase/isomerase superfamily based on a common active site template. <i>Biochemistry</i> , 1999 , 38, 7638-52	3.2	73
97	HAD superfamily phosphotransferase substrate diversification: structure and function analysis of HAD subclass IIB sugar phosphatase BT4131. <i>Biochemistry</i> , 2005 , 44, 8684-96	3.2	66
96	Insights into the mechanism of catalysis by the P-C bond-cleaving enzyme phosphonoacetaldehyde hydrolase derived from gene sequence analysis and mutagenesis. <i>Biochemistry</i> , 1998 , 37, 9305-15	3.2	63

95	On the origins and functions of the enzymes of the 4-chlorobenzoate to 4-hydroxybenzoate converting pathway. <i>Biodegradation</i> , 1994 , 5, 259-76	4.1	62
94	The X-ray crystal structures of human alpha-phosphomannomutase 1 reveal the structural basis of congenital disorder of glycosylation type 1a. <i>Journal of Biological Chemistry</i> , 2006 , 281, 14918-26	5.4	58
93	Kinetic analysis of <i>Pseudomonas aeruginosa</i> arginine deiminase mutants and alternate substrates provides insight into structural determinants of function. <i>Biochemistry</i> , 2006 , 45, 1162-72	3.2	57
92	The structure of 4-hydroxybenzoyl-CoA thioesterase from <i>arthrobacter</i> sp. strain SU. <i>Journal of Biological Chemistry</i> , 2003 , 278, 43709-16	5.4	55
91	Crystal structures representing the Michaelis complex and the thiouronium reaction intermediate of <i>Pseudomonas aeruginosa</i> arginine deiminase. <i>Journal of Biological Chemistry</i> , 2005 , 280, 34080-7	5.4	55
90	Structure, function, and mechanism of the phenylacetate pathway hot dog-fold thioesterase Paal. <i>Journal of Biological Chemistry</i> , 2006 , 281, 11028-38	5.4	54
89	The catalytic scaffold of the haloalkanoic acid dehalogenase enzyme superfamily acts as a mold for the trigonal bipyramidal transition state. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008 , 105, 5687-92	11.5	52
88	Divergence of function in the hot dog fold enzyme superfamily: the bacterial thioesterase YciA. <i>Biochemistry</i> , 2008 , 47, 2789-96	3.2	51
87	Arginine deiminase uses an active-site cysteine in nucleophilic catalysis of L-arginine hydrolysis. <i>Journal of the American Chemical Society</i> , 2004 , 126, 5374-5	16.4	50
86	Catalytic cycling in beta-phosphoglucomutase: a kinetic and structural analysis. <i>Biochemistry</i> , 2005 , 44, 9404-16	3.2	49
85	X-ray crystallographic analyses of inhibitor and substrate complexes of wild-type and mutant 4-hydroxybenzoyl-CoA thioesterase. <i>Journal of Biological Chemistry</i> , 2002 , 277, 27468-76	5.4	49
84	The mechanisms of human hotdog-fold thioesterase 2 (hTHEM2) substrate recognition and catalysis illuminated by a structure and function based analysis. <i>Biochemistry</i> , 2009 , 48, 1293-304	3.2	48
83	Structure and activity analyses of <i>Escherichia coli</i> K-12 NagD provide insight into the evolution of biochemical function in the haloalkanoic acid dehalogenase superfamily. <i>Biochemistry</i> , 2006 , 45, 1183-93 ^{3.2}	3.2	48
82	Investigation of the <i>Bacillus cereus</i> phosphonoacetaldehyde hydrolase. Evidence for a Schiff base mechanism and sequence analysis of an active-site peptide containing the catalytic lysine residue. <i>Biochemistry</i> , 1988 , 27, 2229-34	3.2	44
81	X-ray crystal structure of the hypothetical phosphotyrosine phosphatase MDP-1 of the haloacid dehalogenase superfamily. <i>Biochemistry</i> , 2004 , 43, 12770-9	3.2	42
80	Raman study of the polarizing forces promoting catalysis in 4-chlorobenzoate-CoA dehalogenase. <i>Biochemistry</i> , 1997 , 36, 10192-9	3.2	41
79	Evidence for electrophilic catalysis in the 4-chlorobenzoyl-CoA dehalogenase reaction: UV, Raman, and ¹³ C-NMR spectral studies of dehalogenase complexes of benzoyl-CoA adducts. <i>Biochemistry</i> , 1995 , 34, 13881-8	3.2	41
78	Characterization, kinetics, and crystal structures of fructose-1,6-bisphosphate aldolase from the human parasite, <i>Giardia lamblia</i> . <i>Journal of Biological Chemistry</i> , 2007 , 282, 4859-4867	5.4	40

77	Role of active site binding interactions in 4-chlorobenzoyl-coenzyme A dehalogenase catalysis. <i>Biochemistry</i> , 2001 , 40, 15684-92	3.2	37
76	Inactivation of microbial arginine deiminases by L-canavanine. <i>Journal of the American Chemical Society</i> , 2008 , 130, 1918-31	16.4	35
75	Crystal structures of 2-methylisocitrate lyase in complex with product and with isocitrate inhibitor provide insight into lyase substrate specificity, catalysis and evolution. <i>Biochemistry</i> , 2005 , 44, 2949-62	3.2	35
74	Investigations of the partial reactions catalyzed by pyruvate phosphate dikinase. <i>Biochemistry</i> , 1988 , 27, 625-33	3.2	35
73	Identification of active site residues essential to 4-chlorobenzoyl-coenzyme A dehalogenase catalysis by chemical modification and site directed mutagenesis. <i>Biochemistry</i> , 1996 , 35, 10879-85	3.2	33
72	Structural determinants of substrate recognition in the HAD superfamily member D-glycero-D-manno-heptose-1,7-bisphosphate phosphatase (GmhB). <i>Biochemistry</i> , 2010 , 49, 1082-92	3.2	32
71	Response to Comment on "The Pentacovalent Phosphorus Intermediate of a Phosphoryl Transfer Reaction". <i>Science</i> , 2003 , 301, 1184d-1184	33.3	32
70	Investigation of substrate activation by 4-chlorobenzoyl-coenzyme A dehalogenase. <i>Biochemistry</i> , 1997 , 36, 1349-61	3.2	31
69	The phosphonopyruvate decarboxylase from <i>Bacteroides fragilis</i> . <i>Journal of Biological Chemistry</i> , 2003 , 278, 41302-8	5.4	31
68	Investigation of metal ion binding in phosphonoacetaldehyde hydrolase identifies sequence markers for metal-activated enzymes of the HAD enzyme superfamily. <i>Biochemistry</i> , 2004 , 43, 4990-7	3.2	31
67	Characterization of the 4-hydroxybenzoyl-coenzyme A thioesterase from <i>Arthrobacter</i> sp. strain SU. <i>Applied and Environmental Microbiology</i> , 2003 , 69, 2707-11	4.8	31
66	The YbgC protein encoded by the ybgC gene of the tol-pal gene cluster of <i>Haemophilus influenzae</i> catalyzes acyl-coenzyme A thioester hydrolysis. <i>FEBS Letters</i> , 2002 , 516, 161-3	3.8	31
65	Helix swapping between two alpha/beta barrels: crystal structure of phosphoenolpyruvate mutase with bound Mg(2+)-oxalate. <i>Structure</i> , 1999 , 7, 539-48	5.2	31
64	Divergence of structure and function in the haloacid dehalogenase enzyme superfamily: <i>Bacteroides thetaiotaomicron</i> BT2127 is an inorganic pyrophosphatase. <i>Biochemistry</i> , 2011 , 50, 8937-49	3.2	30
63	Analysis of the structural determinants underlying discrimination between substrate and solvent in beta-phosphoglucomutase catalysis. <i>Biochemistry</i> , 2009 , 48, 1984-95	3.2	30
62	Conformational cycling in beta-phosphoglucomutase catalysis: reorientation of the beta-D-glucose 1,6-(Bis)phosphate intermediate. <i>Biochemistry</i> , 2006 , 45, 7818-24	3.2	30
61	Crystal structure of human thioesterase superfamily member 2. <i>Biochemical and Biophysical Research Communications</i> , 2006 , 349, 172-7	3.4	30
60	X-ray crystallographic and site-directed mutagenesis analysis of the mechanism of Schiff-base formation in phosphonoacetaldehyde hydrolase catalysis. <i>Journal of Biological Chemistry</i> , 2004 , 279, 9353-61	5.4	30

59	Stereochemical probe for the mechanism of phosphorus-carbon bond cleavage catalyzed by the <i>Bacillus cereus</i> phosphonoacetaldehyde hydrolase. <i>Journal of the American Chemical Society</i> , 1992 , 114, 7346-7354	16.4	30
58	Structure of the trehalose-6-phosphate phosphatase from <i>Brugia malayi</i> reveals key design principles for anthelmintic drugs. <i>PLoS Pathogens</i> , 2014 , 10, e1004245	7.6	29
57	Structure of YciA from <i>Haemophilus influenzae</i> (HI0827), a hexameric broad specificity acyl-coenzyme A thioesterase. <i>Biochemistry</i> , 2008 , 47, 2797-805	3.2	29
56	Diversification of function in the haloacid dehalogenase enzyme superfamily: The role of the cap domain in hydrolytic phosphorus-carbon bond cleavage. <i>Bioorganic Chemistry</i> , 2006 , 34, 394-409	5.1	29
55	Structure-function analysis of 2-keto-3-deoxy-D-glycero-D-galactonononate-9-phosphate phosphatase defines specificity elements in type C0 haloalkanoate dehalogenase family members. <i>Journal of Biological Chemistry</i> , 2009 , 284, 1224-33	5.4	27
54	Kinetic, Raman, NMR, and site-directed mutagenesis studies of the <i>Pseudomonas</i> sp. strain CBS3 4-hydroxybenzoyl-CoA thioesterase active site. <i>Biochemistry</i> , 2002 , 41, 11152-60	3.2	26
53	Investigation of the substrate binding and catalytic groups of the P-C bond cleaving enzyme, phosphonoacetaldehyde hydrolase. <i>Archives of Biochemistry and Biophysics</i> , 1992 , 296, 144-51	4.1	26
52	Kinetic evidence for a substrate-induced fit in phosphonoacetaldehyde hydrolase catalysis. <i>Biochemistry</i> , 2002 , 41, 13370-7	3.2	25
51	Modulating electron density in the bound product, 4-hydroxybenzoyl-CoA, by mutations in 4-chlorobenzoyl-CoA dehalogenase near the 4-hydroxy group. <i>Biochemistry</i> , 1999 , 38, 4198-206	3.2	25
50	Insight into the mechanism of phosphoenolpyruvate mutase catalysis derived from site-directed mutagenesis studies of active site residues. <i>Biochemistry</i> , 1999 , 38, 14165-73	3.2	25
49	Structure and kinetics of phosphonopyruvate hydrolase from <i>Variovorax</i> sp. Pal2: new insight into the divergence of catalysis within the PEP mutase/isocitrate lyase superfamily. <i>Biochemistry</i> , 2006 , 45, 11491-504	3.2	24
48	Mechanisms of catalysis and inhibition operative in the arginine deiminase from the human pathogen <i>Giardia lamblia</i> . <i>Bioorganic Chemistry</i> , 2009 , 37, 149-61	5.1	22
47	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. <i>Biochemistry</i> , 2009 , 48, 511-3	3.2	22
46	Phosphoenolpyruvate mutase catalysis of phosphoryl transfer in phosphoenolpyruvate: kinetics and mechanism of phosphorus-carbon bond formation. <i>Biochemistry</i> , 1996 , 35, 4628-35	3.2	22
45	The electrostatic driving force for nucleophilic catalysis in L-arginine deiminase: a combined experimental and theoretical study. <i>Biochemistry</i> , 2008 , 47, 4721-32	3.2	21
44	Location of the phosphate binding site within <i>Clostridium symbiosum</i> pyruvate phosphate dikinase. <i>Biochemistry</i> , 1998 , 37, 13463-74	3.2	21
43	The catalytic mechanism of the hotdog-fold enzyme superfamily 4-hydroxybenzoyl-CoA thioesterase from <i>Arthrobacter</i> sp. strain SU. <i>Biochemistry</i> , 2012 , 51, 7000-16	3.2	20
42	Consequences of domain insertion on sequence-structure divergence in a superfold. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013 , 110, E3381-7	11.5	19

41	The BH1999 protein of <i>Bacillus halodurans</i> C-125 is gentisyl-coenzyme A thioesterase. <i>Journal of Bacteriology</i> , 2004 , 186, 393-9	3.5	19
40	Structural basis for the divergence of substrate specificity and biological function within HAD phosphatases in lipopolysaccharide and sialic acid biosynthesis. <i>Biochemistry</i> , 2013 , 52, 5372-86	3.2	17
39	The Akt C-terminal modulator protein is an acyl-CoA thioesterase of the Hotdog-Fold family. <i>Biochemistry</i> , 2009 , 48, 5507-9	3.2	17
38	Structure and function of PA4872 from <i>Pseudomonas aeruginosa</i> , a novel class of oxaloacetate decarboxylase from the PEP mutase/isocitrate lyase superfamily. <i>Biochemistry</i> , 2008 , 47, 167-82	3.2	17
37	The strength of dehalogenase-substrate hydrogen bonding correlates with the rate of Meisenheimer intermediate formation. <i>Biochemistry</i> , 2003 , 42, 9482-90	3.2	16
36	Human symbiont <i>Bacteroides thetaiotaomicron</i> synthesizes 2-keto-3-deoxy-D-glycero-D-galacto-nononic acid (KDN). <i>Chemistry and Biology</i> , 2008 , 15, 893-7		15
35	Diversity of function in the isocitrate lyase enzyme superfamily: the <i>Dianthus caryophyllus</i> petal death protein cleaves alpha-keto and alpha-hydroxycarboxylic acids. <i>Biochemistry</i> , 2005 , 44, 16365-76	3.2	15
34	Crystal structure of the petal death protein from carnation flower. <i>Biochemistry</i> , 2005 , 44, 16377-84	3.2	14
33	Rational design of reversible inhibitors for trehalose 6-phosphate phosphatases. <i>European Journal of Medicinal Chemistry</i> , 2017 , 128, 274-286	6.8	13
32	Structure and catalysis in the <i>Escherichia coli</i> hotdog-fold thioesterase paralogs Ydil and Ybdb. <i>Biochemistry</i> , 2014 , 53, 4788-805	3.2	12
31	Divergence of substrate specificity and function in the <i>Escherichia coli</i> hotdog-fold thioesterase paralogs Ydil and Ybdb. <i>Biochemistry</i> , 2014 , 53, 4775-87	3.2	12
30	Crystallization and preliminary X-ray diffraction studies of beta-phosphoglucomutase from <i>Lactococcus lactus</i> . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2002 , 58, 324-6		12
29	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. <i>Journal of Raman Spectroscopy</i> , 2000 , 31, 365-371	2.3	12
28	Catalytic scaffolds for phosphoryl group transfer. <i>Current Opinion in Structural Biology</i> , 2016 , 41, 172-178	3.1	11
27	Investigation of the catalytic mechanism of the hotdog-fold enzyme superfamily <i>Pseudomonas</i> sp. strain CBS3 4-hydroxybenzoyl-CoA thioesterase. <i>Biochemistry</i> , 2012 , 51, 786-94	3.2	11
26	Structure and function of 2,3-dimethylmalate lyase, a PEP mutase/isocitrate lyase superfamily member. <i>Journal of Molecular Biology</i> , 2009 , 386, 486-503	6.5	11
25	Enzyme function discovery. <i>Structure</i> , 2008 , 16, 1599-600	5.2	11
24	Rational design of first generation inhibitors for trehalose 6-phosphate phosphatases. <i>Tetrahedron</i> , 2017 , 73, 1324-1330	2.4	9

23	The X-ray crystallographic structure and specificity profile of HAD superfamily phosphohydrolase BT1666: comparison of paralogous functions in <i>B. thetaiotaomicron</i> . <i>Proteins: Structure, Function and Bioinformatics</i> , 2011 , 79, 3099-107	4.2	9
22	X-ray structure and characterization of carbamate kinase from the human parasite <i>Giardia lamblia</i> . <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2010 , 66, 386-90		9
21	Investigation of the role of the substrate metal ion in the yeast inorganic pyrophosphatase reaction. <i>FEBS Letters</i> , 1984 , 165, 251-3	3.8	9
20	A Thioester Substrate Binds to the Enzyme <i>Arthrobacter</i> Thioesterase in Two Ionization States; Evidence from Raman Difference Spectroscopy. <i>Journal of Raman Spectroscopy</i> , 2012 , 43, 65-71	2.3	8
19	Co-evolution of HAD phosphatase and hotdog-fold thioesterase domain function in the menaquinone-pathway fusion proteins BF1314 and PG1653. <i>FEBS Letters</i> , 2013 , 587, 2851-9	3.8	8
18	Correlation of structure and function in the human hotdog-fold enzyme hTHEM4. <i>Biochemistry</i> , 2012 , 51, 6490-2	3.2	6
17	W. W. "Mo" Cleland: a catalytic life. <i>Biochemistry</i> , 2013 , 52, 9092-6	3.2	6
16	Enzymatic synthesis of radiolabeled phosphonoacetaldehyde. <i>Analytical Biochemistry</i> , 2003 , 322, 233-7	3.1	6
15	Neutron diffraction studies towards deciphering the protonation state of catalytic residues in the bacterial KDN9P phosphatase. <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2013 , 69, 1015-9		5
14	The X-ray crystallographic structure and activity analysis of a <i>Pseudomonas</i> -specific subfamily of the HAD enzyme superfamily evidences a novel biochemical function. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008 , 70, 197-207	4.2	5
13	Investigation of the role of the domain linkers in separate site catalysis by <i>Clostridium symbiosum</i> pyruvate phosphate dikinase. <i>Biochemistry</i> , 2001 , 40, 13466-73	3.2	5
12	Structural Basis of the Molecular Switch between Phosphatase and Mutase Functions of Human Phosphomannomutase 1 under Ischemic Conditions. <i>Biochemistry</i> , 2018 , 57, 3480-3492	3.2	4
11	Mechanism of Substrate Recognition and Catalysis of the Haloalkanoic Acid Dehalogenase Family Member ϵ Phosphoglucomutase. <i>Biochemistry</i> , 2018 , 57, 4504-4517	3.2	4
10	Structure-guided approach for detecting large domain inserts in protein sequences as illustrated using the haloacid dehalogenase superfamily. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014 , 82, 1896-906	4.2	3
9	Raman evidence for product binding to the enzyme W137F 4-chlorobenzoyl-CoA dehalogenase in two conformational states. <i>Journal of Raman Spectroscopy</i> , 2005 , 36, 320-325	2.3	2
8	Inhibition and inactivation of pyruvate phosphate dikinase with Cr(III) complexes of adenosine 5Rtriphosphate and inorganic pyrophosphate. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 1986 , 1, 113-25		1
7	Structural Analysis of Binding Determinants of Trehalose-6-phosphate Phosphatase Using Ground-State Complexes. <i>Biochemistry</i> , 2020 , 59, 3247-3257	3.2	1
6	Catalytic Mechanism of the Hotdog-Fold Thioesterase PA1618 Revealed by X-ray Structure Determination of a Substrate-Bound Oxygen Ester Analogue Complex. <i>ChemBioChem</i> , 2017 , 18, 1935-1943	3.8	1

- 5 Specificity and Promiscuity in Enzyme Superfamilies. *FASEB Journal*, **2015**, 29, 237.1 0.9
- 4 Ligand Binding and Conformational Change Coupling in the HAD Superfamily. *FASEB Journal*, **2013**, 27, 998.8 0.9
- 3 The nature of sequence and structure divergence in the Haloalkanoate Dehalogenase SuperFamily (HADSf). *FASEB Journal*, **2013**, 27, 797.2 0.9
- 2 The structural basis of the secondary function of PMM1 in the presence of IMP. *FASEB Journal*, **2013**, 27, 998.5 0.9
- 1 Ultra High-throughput Screening Uncovers New Activities in Phosphatases of the Haloalkanoic Acid Dehalogenase Superfamily (HADSf). *FASEB Journal*, **2013**, 27, 571.1 0.9