Debra Dunaway-Mariano

List of Publications by Year in descending order

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112 papers

5,033 citations

38 h-index 98622 67 g-index

112 all docs

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times ranked

112

3950 citing authors

#	Article	IF	CITATIONS
1	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
2	The Pentacovalent Phosphorus Intermediate of a Phosphoryl Transfer Reaction. Science, 2003, 299, 2067-2071.	6.0	306
3	Phosphoryl group transfer: evolution of a catalytic scaffold. Trends in Biochemical Sciences, 2004, 29, 495-503.	3.7	249
4	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
5	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
6	The Crystal Structure ofBacillus cereusPhosphonoacetaldehyde Hydrolase: Insight into Catalysis of Phosphorus Bond Cleavage and Catalytic Diversification within the HAD Enzyme Superfamilyâ€,‡. Biochemistry, 2000, 39, 10385-10396.	1.2	136
7	Enzyme Promiscuity: Engine of Evolutionary Innovation. Journal of Biological Chemistry, 2014, 289, 30229-30236.	1.6	125
8	Acyl-Adenylate Motif of the Acyl-Adenylate/Thioester-Forming Enzyme Superfamily: A Site-Directed Mutagenesis Study with thePseudomonassp. Strain CBS3 4-Chlorobenzoate:Coenzyme A Ligaseâ€. Biochemistry, 1997, 36, 15650-15659.	1.2	120
9	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
10	Caught in the Act: The Structure of Phosphorylatedβ-Phosphoglucomutase fromLactococcus lactisâ€,‡. Biochemistry, 2002, 41, 8351-8359.	1.2	107
11	Oxaloacetate Hydrolase, the C–C Bond Lyase of Oxalate Secreting Fungi. Journal of Biological Chemistry, 2007, 282, 9581-9590.	1.6	102
12	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
13	Markers of fitness in a successful enzyme superfamily. Current Opinion in Structural Biology, 2009, 19, 658-665.	2.6	94
14	Analysis of the Substrate Specificity Loop of the HAD Superfamily Cap Domainâ€,‡. Biochemistry, 2004, 43, 2812-2820.	1.2	83
15	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
16	HAD Superfamily Phosphotransferase Substrate Diversification: Structure and Function Analysis of HAD Subclass IIB Sugar Phosphatase BT4131â€,‡. Biochemistry, 2005, 44, 8684-8696.	1.2	75
17	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
18	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

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19	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
20	Divergence of Function in the Hot Dog Fold Enzyme Superfamily: The Bacterial Thioesterase YciA. Biochemistry, 2008, 47, 2789-2796.	1.2	62
21	Structure, Function, and Mechanism of the Phenylacetate Pathway Hot Dog-fold Thioesterase Paal. Journal of Biological Chemistry, 2006, 281, 11028-11038.	1.6	60
22	The Structure of 4-Hydroxybenzoyl-CoA Thioesterase from Arthrobacter sp. strain SU. Journal of Biological Chemistry, 2003, 278, 43709-43716.	1.6	59
23	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
24	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
25	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
26	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
27	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
28	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
29	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
30	Catalytic Cycling in β-Phosphoglucomutase:  A Kinetic and Structural Analysis,. Biochemistry, 2005, 44, 9404-9416.	1.2	51
31	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
32	X-ray Crystal Structure of the Hypothetical Phosphotyrosine Phosphatase MDP-1 of the Haloacid Dehalogenase Superfamily,. Biochemistry, 2004, 43, 12770-12779.	1.2	47
33	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
34	Raman Study of the Polarizing Forces Promoting Catalysis in 4-Chlorobenzoate-CoA Dehalogenaseâ€. Biochemistry, 1997, 36, 10192-10199.	1.2	45
35	The Phosphonopyruvate Decarboxylase from Bacteroides fragilis. Journal of Biological Chemistry, 2003, 278, 41302-41308.	1.6	45
36	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

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37	Investigations of the partial reactions catalyzed by pyruvate phosphate dikinase. Biochemistry, 1988, 27, 625-633.	1.2	40
38	Role of Active Site Binding Interactions in 4-Chlorobenzoyl-Coenzyme A Dehalogenase Catalysis. Biochemistry, 2001, 40, 15684-15692.	1.2	38
39	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
40	Inactivation of Microbial Arginine Deiminases by <scp>l</scp> -Canavanine. Journal of the American Chemical Society, 2008, 130, 1918-1931.	6.6	37
41	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
42	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
43	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
44	Helix swapping between two α/β barrels: crystal structure of phosphoenolpyruvate mutase with bound Mg2+–oxalate. Structure, 1999, 7, 539-548.	1.6	35
45	Crystal Structures of 2-Methylisocitrate Lyase in Complex with Product and with Isocitrate Inhibitor Provide Insight into Lyase Substrate Specificity, Catalysis and Evolutionâ€,‡. Biochemistry, 2005, 44, 2949-2962.	1.2	35
46	Analysis of the Structural Determinants Underlying Discrimination between Substrate and Solvent in β-Phosphoglucomutase Catalysis. Biochemistry, 2009, 48, 1984-1995.	1.2	35
47	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
48	Investigation of Substrate Activation by 4-Chlorobenzoyl-Coenzyme A Dehalogenase. Biochemistry, 1997, 36, 1349-1361.	1.2	34
49	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
50	Response to Comment on "The Pentacovalent Phosphorus Intermediate of a Phosphoryl Transfer Reaction". Science, 2003, 301, 1184d-1184.	6.0	33
51	Characterization of the 4-Hydroxybenzoyl-Coenzyme A Thioesterase from Arthrobacter sp. Strain SU. Applied and Environmental Microbiology, 2003, 69, 2707-2711.	1.4	33
52	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
53	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
54	Structure of YciA from Haemophilus influenzae (HI0827), a Hexameric Broad Specificity Acyl-Coenzyme A Thioesterase,. Biochemistry, 2008, 47, 2797-2805.	1,2	32

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55	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
56	Structure and Kinetics of Phosphonopyruvate Hydrolase fromVoriovoraxsp. Pal2: New Insight into the Divergence of Catalysis within the PEP Mutase/Isocitrate Lyase Superfamilyâ€,‡. Biochemistry, 2006, 45, 11491-11504.	1.2	31
57	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
58	Crystal structure of human thioesterase superfamily member 2. Biochemical and Biophysical Research Communications, 2006, 349, 172-177.	1.0	30
59	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
60	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
61	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
62	Kinetic Evidence for a Substrate-Induced Fit in Phosphonoacetaldehyde Hydrolase Catalysisâ€. Biochemistry, 2002, 41, 13370-13377.	1.2	28
63	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
64	Diversity of Function in the Isocitrate Lyase Enzyme Superfamily: TheDianthus caryophyllusPetal Death Protein Cleaves α-Keto and α-Hydroxycarboxylic Acidsâ€. Biochemistry, 2005, 44, 16365-16376.	1.2	28
65	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. Journal of Biological Chemistry, 2009, 284, 1224-1233.	1.6	27
66	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
67	Consequences of domain insertion on sequence-structure divergence in a superfold. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, E3381-7.	3.3	25
68	Phosphoenolpyruvate Mutase Catalysis of Phosphoryl Transfer in Phosphoenolpyruvate: Kinetics and Mechanism of Phosphorusâ°Carbon Bond Formationâ€. Biochemistry, 1996, 35, 4628-4635.	1.2	24
69	The Electrostatic Driving Force for Nucleophilic Catalysis in I-Arginine Deiminase: A Combined Experimental and Theoretical Study. Biochemistry, 2008, 47, 4721-4732.	1.2	22
70	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
71	The Catalytic Mechanism of the Hotdog-fold Enzyme Superfamily 4-Hydroxybenzoyl-CoA Thioesterase from <i>Arthrobacter </i> >p. Strain SU. Biochemistry, 2012, 51, 7000-7016.	1.2	22
72	Location of the Phosphate Binding Site within Clostridium symbiosum Pyruvate Phosphate Dikinase,. Biochemistry, 1998, 37, 13463-13474.	1.2	21

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73	Structure and Function of PA4872 from <i>Pseudomonas aeruginosa</i> , a Novel Class of Oxaloacetate Decarboxylase from the PEP Mutase/Isocitrate Lyase Superfamily [,] . Biochemistry, 2008, 47, 167-182.	1.2	20
74	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
75	The BH1999 Protein of Bacillus halodurans C-125 Is Gentisyl-Coenzyme A Thioesterase. Journal of Bacteriology, 2004, 186, 393-399.	1.0	19
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	The Akt C-Terminal Modulator Protein Is an Acyl-CoA Thioesterase of the Hotdog-Fold Family. Biochemistry, 2009, 48, 5507-5509.	1.2	17
78	Catalytic scaffolds for phosphoryl group transfer. Current Opinion in Structural Biology, 2016, 41, 172-179.	2.6	17
79	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
80	Rational design of reversible inhibitors for trehalose 6-phosphate phosphatases. European Journal of Medicinal Chemistry, 2017, 128, 274-286.	2.6	16
81	Crystal Structure of the Petal Death Protein from Carnation Flowerâ€,‡. Biochemistry, 2005, 44, 16377-16384.	1.2	14
82	Enzyme Function Discovery. Structure, 2008, 16, 1599-1600.	1.6	14
83	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
84	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
85	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
86	Crystallization and preliminary X-ray diffraction studies of \hat{l}^2 -phosphoglucomutase fromLactococcus lactus. Acta Crystallographica Section D: Biological Crystallography, 2002, 58, 324-326.	2.5	12
87	Structure and Catalysis in the <i>Escherichia coli</i> Hotdog-fold Thioesterase Paralogs Ydil and YbdB. Biochemistry, 2014, 53, 4788-4805.	1.2	12
88	Rational design of first generation inhibitors for trehalose 6-phosphate phosphatases. Tetrahedron, 2017, 73, 1324-1330.	1.0	12
89	Investigation of the role of the substrate metal ion in the yeast inorganic pyrophosphatase reaction. FEBS Letters, 1984, 165, 251-253.	1.3	11
90	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

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91	The Xâ€ray crystallographic structure and specificity profile of HAD superfamily phosphohydrolase BT1666: Comparison of paralogous functions in ⟨i⟩B. thetaiotaomicron⟨li⟩. Proteins: Structure, Function and Bioinformatics, 2011, 79, 3099-3107.	1.5	11
92	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
93	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
94	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
95	Mechanism of Substrate Recognition and Catalysis of the Haloalkanoic Acid Dehalogenase Family Member α-Phosphoglucomutase. Biochemistry, 2018, 57, 4504-4517.	1.2	8
96	Correlation of Structure and Function in the Human Hotdog-fold Enzyme hTHEM4. Biochemistry, 2012, 51, 6490-6492.	1.2	7
97	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
98	Enzymatic synthesis of radiolabeled phosphonoacetaldehyde. Analytical Biochemistry, 2003, 322, 233-237.	1.1	6
99	W. W. "Mo―Cleland: A Catalytic Life. Biochemistry, 2013, 52, 9092-9096.	1.2	6
100	Investigation of the Role of the Domain Linkers in Separate Site Catalysis byClostridium symbiosumPyruvate Phosphate Dikinaseâ€. Biochemistry, 2001, 40, 13466-13473.	1.2	5
101	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
102	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
103	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
104	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
105	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
106	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
107	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	O
108	Ligand Binding and Conformational Change Coupling in the HAD Superfamily. FASEB Journal, 2013, 27, 998.8.	0.2	0

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109	The nature of sequence and structure divergence in the Haloalkanoate Dehalogenase SuperFamily (HADSF). FASEB Journal, 2013, 27, 797.2.	0.2	O
110	The structural basis of the secondary function of PMM1 in the presence of IMP. FASEB Journal, 2013, 27, 998.5.	0.2	0
111	Ultra Highâ€throughput Screening Uncovers New Activities in Phosphatases of the Haloalkanoic Acid Dehalogenase Superfamily (HADSF). FASEB Journal, 2013, 27, 571.1.	0.2	O
112	Specificity and Promiscuity in Enzyme Superfamilies. FASEB Journal, 2015, 29, 237.1.	0.2	0