

# Michael J Mcleish

## List of Publications by Year in descending order

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98  
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186265

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101  
docs citations

101  
times ranked

2223  
citing authors

#	ARTICLE	IF	CITATIONS
1	Enzymatic Stetter Reaction: Computational Study of the Reaction Mechanism of MenD. <i>ACS Catalysis</i> , 2021, 11, 12355-12366.	11.2	6
2	Structure-Based Drug Design of Bisubstrate Inhibitors of Phenylethanolamine N-Methyltransferase Possessing Low Nanomolar Affinity at Both Substrate Binding Domains. <i>Journal of Medicinal Chemistry</i> , 2020, 63, 13878-13898.	6.4	2
3	Computational characterization of enzyme-bound thiamin diphosphate reveals a surprisingly stable tricyclic state: implications for catalysis. <i>Beilstein Journal of Organic Chemistry</i> , 2019, 15, 145-159.	2.2	7
4	Computational Study of Enantioselective Carbonylation Catalyzed by Benzoylformate Decarboxylase. <i>ACS Catalysis</i> , 2019, 9, 5657-5667.	11.2	13
5	A Theoretical Study of the Benzoylformate Decarboxylase Reaction Mechanism. <i>Frontiers in Chemistry</i> , 2018, 6, 205.	3.6	15
6	Specificity and mechanism of mandelamide hydrolase catalysis. <i>Archives of Biochemistry and Biophysics</i> , 2017, 618, 23-31.	3.0	0
7	Structure and mechanism of benzaldehyde dehydrogenase from <i>Pseudomonas putida</i> ATCC 12633, a member of the Class 3 aldehyde dehydrogenase superfamily. <i>Protein Engineering, Design and Selection</i> , 2017, 30, 273-280.	2.1	7
8	Phosphonodifluoropyruvate is a mechanism-based inhibitor of phosphonopyruvate decarboxylase from <i>Bacteroides fragilis</i> . <i>Bioorganic and Medicinal Chemistry</i> , 2017, 25, 4368-4374.	3.0	9
9	Mechanistic and Structural Insight to an Evolved Benzoylformate Decarboxylase with Enhanced Pyruvate Decarboxylase Activity. <i>Catalysts</i> , 2016, 6, 190.	3.5	3
10	The kinetic characterization and X-ray structure of a putative benzoylformate decarboxylase from <i>M. smegmatis</i> highlights the difficulties in the functional annotation of ThDP-dependent enzymes. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2015, 1854, 1001-1009.	2.3	8
11	Extended Reaction Scope of Thiamine Diphosphate Dependent Cyclohexane-1,2-dione Hydrolase: From C-C Bond Cleavage to C-C Bond Ligation. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 14402-14406.	13.8	11
12	Perturbation of the Monomer-Monomer Interfaces of the Benzoylformate Decarboxylase Tetramer. <i>Biochemistry</i> , 2014, 53, 4358-4367.	2.5	4
13	Identification of Charge Transfer Transitions Related to Thiamin-Bound Intermediates on Enzymes Provides a Plethora of Signatures Useful in Mechanistic Studies. <i>Biochemistry</i> , 2014, 53, 2145-2152.	2.5	14
14	Using site-saturation mutagenesis to explore mechanism and substrate specificity in thiamin diphosphate-dependent enzymes. <i>FEBS Journal</i> , 2013, 280, 6395-6411.	4.7	18
15	Kinetic and pH studies on human phenylethanolamine N-methyltransferase. <i>Archives of Biochemistry and Biophysics</i> , 2013, 539, 1-8.	3.0	15
16	A Bulky Hydrophobic Residue Is Not Required To Maintain the V-Conformation of Enzyme-Bound Thiamin Diphosphate. <i>Biochemistry</i> , 2013, 52, 3028-3030.	2.5	6
17	Substrate specificity in thiamin diphosphate-dependent decarboxylases. <i>Bioorganic Chemistry</i> , 2012, 43, 26-36.	4.1	29
18	Characterization of a thiamin diphosphate-dependent phenylpyruvate decarboxylase from <i>Saccharomyces cerevisiae</i> . <i>FEBS Journal</i> , 2011, 278, 1842-1853.	4.7	46

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19	Fragment-based screening by X-ray crystallography, MS and isothermal titration calorimetry to identify PNMT (phenylethanolamine N-methyltransferase) inhibitors. <i>Biochemical Journal</i> , 2010, 431, 51-61.	3.7	41
20	Active-Site Engineering of Benzaldehyde Lyase Shows That a Point Mutation Can Confer Both New Reactivity and Susceptibility to Mechanism-Based Inhibition. <i>Journal of the American Chemical Society</i> , 2010, 132, 438-439.	13.7	23
21	Structural Relationship between the Active Sites of $\hat{1}^2$ -Lactam-Recognizing and Amidase Signature Enzymes: Convergent Evolution?. <i>Biochemistry</i> , 2010, 49, 9688-9697.	2.5	36
22	Molecular recognition of physiological substrate noradrenaline by the adrenaline-synthesizing enzyme PNMT and factors influencing its methyltransferase activity. <i>Biochemical Journal</i> , 2009, 422, 463-471.	3.7	30
23	Using directed evolution to probe the substrate specificity of mandelamide hydrolase. <i>Protein Engineering, Design and Selection</i> , 2009, 22, 103-110.	2.1	6
24	The reaction mechanism of phenylethanolamine N-methyltransferase: A density functional theory study. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2009, 1794, 1831-1837.	2.3	24
25	Time-dependent inactivation of human phenylethanolamine N-methyltransferase by 7-isothiocyanatotetrahydroisoquinoline. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2009, 19, 1071-1074.	2.2	2
26	Snapshot of a Reaction Intermediate: Analysis of Benzoylformate Decarboxylase in Complex with a Benzoylphosphonate Inhibitor. <i>Biochemistry</i> , 2009, 48, 3247-3257.	2.5	32
27	Engineering the Substrate Binding Site of Benzoylformate Decarboxylase. <i>Biochemistry</i> , 2009, 48, 8387-8395.	2.5	20
28	Detection and Time Course of Formation of Major Thiamin Diphosphate-Bound Covalent Intermediates Derived from a Chromophoric Substrate Analogue on Benzoylformate Decarboxylase. <i>Biochemistry</i> , 2009, 48, 981-994.	2.5	21
29	Physical, kinetic and spectrophotometric studies of a NAD(P)-dependent benzaldehyde dehydrogenase from <i>Pseudomonas putida</i> ATCC 12633. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2008, 1784, 1248-1255.	2.3	8
30	Probing the Active Center of Benzaldehyde Lyase with Substitutions and the Pseudosubstrate Analogue Benzoylphosphonic Acid Methyl Ester. <i>Biochemistry</i> , 2008, 47, 7734-7743.	2.5	34
31	Mechanism of Benzaldehyde Lyase Studied via Thiamin Diphosphate-Bound Intermediates and Kinetic Isotope Effects. <i>Biochemistry</i> , 2008, 47, 3800-3809.	2.5	20
32	Saturation mutagenesis of putative catalytic residues of benzoylformate decarboxylase provides a challenge to the accepted mechanism. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 5733-5738.	7.1	44
33	Characterization of a benzoylformate decarboxylase and a NAD <sup>+</sup> /NADP <sup>+</sup> -dependent benzaldehyde dehydrogenase from <i>Pseudomonas stutzeri</i> ST-201. <i>FASEB Journal</i> , 2008, 22, 1008.4.	0.5	0
34	Isolation and characterization of a benzoylformate decarboxylase and a NAD <sup>+</sup> /NADP <sup>+</sup> -dependent benzaldehyde dehydrogenase involved in d-phenylglycine metabolism in <i>Pseudomonas stutzeri</i> ST-201. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2007, 1770, 1585-1592.	2.4	19
35	Enzyme Adaptation to Inhibitor Binding: A Cryptic Binding Site in Phenylethanolamine N-Methyltransferase. <i>Journal of Medicinal Chemistry</i> , 2007, 50, 4845-4853.	6.4	26
36	Elucidation of the Chemistry of Enzyme-Bound Thiamin Diphosphate Prior to Substrate Binding: Defining Internal Equilibria among Tautomeric and Ionization States. <i>Biochemistry</i> , 2007, 46, 10739-10744.	2.5	54

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37	Mechanism-Based Inactivation of Benzoylformate Decarboxylase, A Thiamin Diphosphate-Dependent Enzyme. <i>Journal of the American Chemical Society</i> , 2007, 129, 4120-4121.	13.7	34
38	Identification of the Ionization State and pKa for Protonation of the 4-aminopyrimidine Ring on Enzymes Utilizing Thiamin Diphosphate by Circular Dichroism Spectroscopy. <i>FASEB Journal</i> , 2007, 21, A1016.	0.5	0
39	Using saturation mutagenesis to replace putative catalytic residues in thiamin diphosphate dependent enzymes. <i>FASEB Journal</i> , 2007, 21, A1016.	0.5	0
40	Exploring the Role of the Active Site Cysteine in Human Muscle Creatine Kinase. <i>Biochemistry</i> , 2006, 45, 11464-11472.	2.5	21
41	Specific inhibitors of Plasmodium falciparum thioredoxin reductase as potential antimalarial agents. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2006, 16, 2283-2292.	2.2	66
42	Determinants of substrate specificity in KdcA, a thiamin diphosphate-dependent decarboxylase. <i>Bioorganic Chemistry</i> , 2006, 34, 325-336.	4.1	41
43	Characterization of benzaldehyde lyase from Pseudomonas fluorescens: A versatile enzyme for asymmetric C-C bond formation. <i>Bioorganic Chemistry</i> , 2006, 34, 345-361.	4.1	66
44	Heterogeneity of Escherichia coli -expressed human muscle creatine kinase. <i>IUBMB Life</i> , 2006, 58, 421-428.	3.4	1
45	Structural basis of substrate specificity in thiamin diphosphate dependent decarboxylases. <i>FASEB Journal</i> , 2006, 20, A471.	0.5	0
46	Observation and time resolution of chiral thiamin diphosphate-bound intermediates in the catalytic cycle of pyruvate decarboxylase and benzoylformate decarboxylase by stopped-flow circular dichroism. <i>FASEB Journal</i> , 2006, 20, A40.	0.5	0
47	Disulfide-linked dimers of human adrenaline synthesizing enzyme PNMT are catalytically active. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2005, 1750, 82-92.	2.3	4
48	Exploring the active site of benzaldehyde lyase by modeling and mutagenesis. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2005, 1753, 263-271.	2.3	28
49	Loop Movement and Catalysis in Creatine Kinase. <i>IUBMB Life</i> , 2005, 57, 355-362.	3.4	8
50	Exchanging the substrate specificities of pyruvate decarboxylase from Zymomonas mobilis and benzoylformate decarboxylase from Pseudomonas putida. <i>Protein Engineering, Design and Selection</i> , 2005, 18, 345-357.	2.1	80
51	Relating Structure to Mechanism in Creatine Kinase. <i>Critical Reviews in Biochemistry and Molecular Biology</i> , 2005, 40, 1-20.	5.2	172
52	Mode of Binding of Methyl Acceptor Substrates to the Adrenaline-Synthesizing Enzyme Phenylethanolamine N-Methyltransferase: Implications for Catalysis. <i>Biochemistry</i> , 2005, 44, 16875-16885.	2.5	24
53	Structural, Mutagenic, and Kinetic Analysis of the Binding of Substrates and Inhibitors of Human Phenylethanolamine N-Methyltransferase. <i>Journal of Medicinal Chemistry</i> , 2005, 48, 7243-7252.	6.4	26
54	Phenylethanolamine N-methyltransferase inhibition: re-evaluation of kinetic data. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2004, 14, 4217-4220.	2.2	15

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55	Isoleucine 69 and Valine 325 Form a Specificity Pocket in Human Muscle Creatine Kinase. <i>Biochemistry</i> , 2004, 43, 13766-13774.	2.5	27
56	Mandelamide Hydrolase from <i>Pseudomonas putida</i> : Characterization of a New Member of the Amidase Signature Family. <i>Biochemistry</i> , 2004, 43, 7725-7735.	2.5	21
57	Molecular Recognition of Sub-micromolar Inhibitors by the Epinephrine-Synthesizing Enzyme Phenylethanolamine N-Methyltransferase. <i>Journal of Medicinal Chemistry</i> , 2004, 47, 37-44.	6.4	25
58	Inhibitors of Phenylethanolamine N-Methyltransferase That Are Predicted To Penetrate the Blood-Brain Barrier: Design, Synthesis, and Evaluation of 3-Fluoromethyl-7-(N-substituted) Î±2-Adrenoceptor1. <i>Journal of Medicinal Chemistry</i> , 2004, 47, 4483-4493.	6.4	23
59	Mechanism-Based Inactivation of Thioredoxin Reductase from <i>Plasmodium falciparum</i> by Mannich Bases. Implication for Cytotoxicity. <i>Biochemistry</i> , 2003, 42, 13319-13330.	2.5	60
60	Structural and Kinetic Analysis of Catalysis by a Thiamin Diphosphate-Dependent Enzyme, Benzoylformate Decarboxylase. <i>Biochemistry</i> , 2003, 42, 1820-1830.	2.5	98
61	Identification and Characterization of a Mandelamide Hydrolase and an NAD(P) + -Dependent Benzaldehyde Dehydrogenase from <i>Pseudomonas putida</i> ATCC 12633. <i>Journal of Bacteriology</i> , 2003, 185, 2451-2456.	2.2	31
62	Exploring the Substrate Specificity of Benzoylformate Decarboxylase, Pyruvate Decarboxylase, and Benzaldehyde Lyase. <i>Oxidative Stress and Disease</i> , 2003, , .	0.3	1
63	Benzoylformate Decarboxylase. <i>Oxidative Stress and Disease</i> , 2003, , .	0.3	0
64	The 2.1 Å... Structure of <i>Torpedo californica</i> Creatine Kinase Complexed with the ADP-Mg <sup>2+</sup> -NO <sub>3</sub> <sup>-</sup> Creatine Transition-State Analogue Complex. <i>Biochemistry</i> , 2002, 41, 13861-13867.	2.5	129
65	Expression of <i>Torpedo californica</i> creatine kinase in <i>Escherichia coli</i> and purification from inclusion bodies. <i>Protein Expression and Purification</i> , 2002, 26, 89-95.	1.3	8
66	Crystallization of PNMT, the adrenaline-synthesizing enzyme, is critically dependent on a high protein concentration. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2002, 58, 314-315.	2.5	6
67	An Unusually Low pKa for Cys282 in the Active Site of Human Muscle Creatine Kinase. <i>Biochemistry</i> , 2001, 40, 11698-11705.	2.5	107
68	Mutagenesis of Two Acidic Active Site Residues in Human Muscle Creatine Kinase: Implications for the Catalytic Mechanism. <i>Biochemistry</i> , 2001, 40, 3056-3061.	2.5	31
69	Phenylethanolamine N-methyltransferase kinetics: bovine versus recombinant human enzyme. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2001, 11, 1579-1582.	2.2	7
70	Getting the Adrenaline Going. <i>Structure</i> , 2001, 9, 977-985.	3.3	60
71	Studies on the conformational properties of CP-1042 <sup>55</sup> , the hinge region of CP-10, using circular dichroism and RP-HPLC. <i>Chemical Biology and Drug Design</i> , 2000, 55, 411-418.	1.1	2
72	A comparative study of human muscle and brain creatine kinases expressed in <i>Escherichia coli</i> . <i>The Protein Journal</i> , 2000, 19, 59-66.	1.1	22

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73	Involvement of Electrostatic Interactions in the Mechanism of Peptide Folding Induced by Sodium Dodecyl Sulfate Binding. <i>Biochemistry</i> , 2000, 39, 8362-8373.	2.5	123
74	Spectroscopic Detection of Transient Thiamin Diphosphate-Bound Intermediates on Benzoylformate Decarboxylase. <i>Biochemistry</i> , 2000, 39, 13862-13869.	2.5	50
75	Identification of Initiation Sites for T4 Lysozyme Folding Using CD and NMR Spectroscopy of Peptide Fragments. <i>Biochemistry</i> , 2000, 39, 5911-5920.	2.5	17
76	Structural Analysis of the Heparin-Binding Site of the NC1 Domain of Collagen XIV by CD and NMR. <i>Biochemistry</i> , 1999, 38, 6479-6488.	2.5	31
77	The Crystal Structure of Benzoylformate Decarboxylase at 1.6 Å... Resolution: Diversity of Catalytic Residues in Thiamin Diphosphate-Dependent Enzymes. <i>Biochemistry</i> , 1998, 37, 9918-9930.	2.5	180
78	Clomiphene Citrate. <i>Analytical Profiles of Drug Substances and Excipients</i> , 1998, 25, 85-120.	0.0	3
79	Conformational Analysis of LYS(11-36), a Peptide Derived from the $\beta$ -Sheet Region of T4 Lysozyme, in TFE and SDS. <i>Biochemistry</i> , 1997, 36, 11525-11533.	2.5	46
80	Recombinant Human Phenylethanolamine N-Methyltransferase: Overproduction in <i>Escherichia coli</i> , Purification, and Characterization. <i>Protein Expression and Purification</i> , 1996, 8, 160-166.	1.3	20
81	Pharmacokinetics of Thiopental and Pentobarbital Enantiomers After Intravenous Administration of Racemic Thiopental. <i>Anesthesia and Analgesia</i> , 1996, 83, 552-558.	2.2	21
82	Pharmacokinetics of Thiopental and Pentobarbital Enantiomers After Intravenous Administration of Racemic Thiopental. <i>Anesthesia and Analgesia</i> , 1996, 83, 552-558.	2.2	25
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91	Aspartate aminotransferase catalyzed oxygen exchange with solvent from oxygen-18-enriched .alpha.-ketoglutarate: evidence for slow exchange of enzyme-bound water. <i>Biochemistry</i> , 1989, 28, 3821-3825.	2.5	7
92	Pharmacokinetics of intravenous clomiphene isomers.. <i>British Journal of Clinical Pharmacology</i> , 1989, 27, 639-640.	2.4	20
93	Gas chromatographic mass spectroscopic characterisation of the psychotomimetic indolealkylamines and their in vivo metabolites. <i>Biomedical Applications</i> , 1987, 422, 13-23.	1.7	8
94	Reactions of aryl diazonium salts and alkyl arylazo ethers. 9. Studies of the carbanionic and free radical mechanisms of dediazonation of substituted 2-chlorobenzenediazonium salts. <i>Journal of Organic Chemistry</i> , 1983, 48, 191-195.	3.2	9
95	Reactions of aryl diazonium salts and alkyl arylazo ethers. XI. Further evidence for the mechanism of dediazonation in basic alcoholic solution. <i>Australian Journal of Chemistry</i> , 1983, 36, 1031.	0.9	3
96	Reactions of aryl diazonium salts and alkyl arylazo ethers. X. General acid and intramolecular electrostatic catalysis in the ionization of methyl (E)-2-Organyl-5-nitrophenylazo ethers in alcoholic solvents. <i>Australian Journal of Chemistry</i> , 1983, 36, 55.	0.9	1
97	Reactions of aryl diazonium salts and arylazo alkyl ethers. 7. Kinetic studies of the decomposition of Z ethers derived from some substituted 2-nitrobenzenediazonium salts. <i>Journal of Organic Chemistry</i> , 1982, 47, 3673-3679.	3.2	5
98	Reactions of aryl diazonium salts and arylazo alkyl ethers. VI. A comparison of the available methods for the measurement of the rate of ionization of (Z)-arylazo alkyl ethers in alcoholic solvents. <i>Australian Journal of Chemistry</i> , 1982, 35, 319.	0.9	2