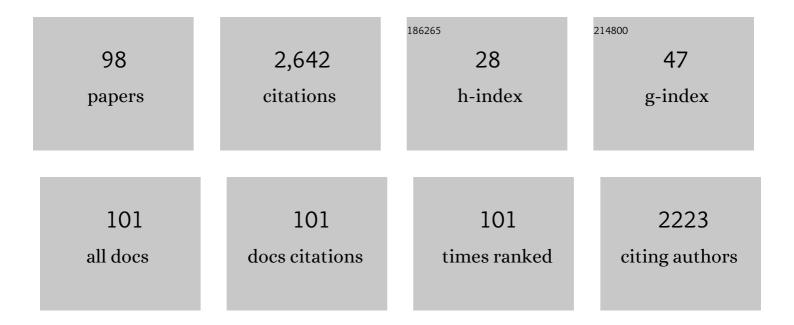
## Michael J Mcleish

List of Publications by Year in descending order

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| #  | Article  | IF  | CITATIONS |
|----|--|-----|-----------|
| 1  | The Crystal Structure of Benzoylformate Decarboxylase at 1.6 à Resolution:  Diversity of Catalytic<br>Residues in Thiamin Diphosphate-Dependent Enzymes,. Biochemistry, 1998, 37, 9918-9930.   | 2.5 | 180       |
| 2  | Relating Structure to Mechanism in Creatine Kinase. Critical Reviews in Biochemistry and Molecular Biology, 2005, 40, 1-20.  | 5.2 | 172       |
| 3  | The 2.1 Ã Structure of Torpedo californica Creatine Kinase Complexed with the<br>ADP-Mg2+â^'NO3-â^'Creatine Transition-State Analogue Complex,. Biochemistry, 2002, 41, 13861-13867.   | 2.5 | 129       |
| 4  | Involvement of Electrostatic Interactions in the Mechanism of Peptide Folding Induced by Sodium<br>Dodecyl Sulfate Bindingâ€,‡. Biochemistry, 2000, 39, 8362-8373.   | 2.5 | 123       |
| 5  | An Unusually Low pKafor Cys282 in the Active Site of Human Muscle Creatine Kinaseâ€. Biochemistry, 2001, 40, 11698-11705.  | 2.5 | 107       |
| 6  | Structural and Kinetic Analysis of Catalysis by a Thiamin Diphosphate-Dependent Enzyme,<br>Benzoylformate Decarboxylaseâ€. Biochemistry, 2003, 42, 1820-1830.  | 2.5 | 98        |
| 7  | Exchanging the substrate specificities of pyruvate decarboxylase from Zymomonas mobilis and<br>benzoylformate decarboxylase from Pseudomonas putida. Protein Engineering, Design and Selection,<br>2005, 18, 345-357.                              | 2.1 | 80        |
| 8  | Specific inhibitors of Plasmodium falciparum thioredoxin reductase as potential antimalarial agents.<br>Bioorganic and Medicinal Chemistry Letters, 2006, 16, 2283-2292.   | 2.2 | 66        |
| 9  | Characterization of benzaldehyde lyase from Pseudomonas fluorescens: A versatile enzyme for<br>asymmetric C–C bond formation. Bioorganic Chemistry, 2006, 34, 345-361.   | 4.1 | 66        |
| 10 | Getting the Adrenaline Going. Structure, 2001, 9, 977-985.   | 3.3 | 60        |
| 11 | Mechanism-Based Inactivation of Thioredoxin Reductase fromPlasmodium falciparumby Mannich Bases.<br>Implication for Cytotoxicityâ€. Biochemistry, 2003, 42, 13319-13330.   | 2.5 | 60        |
| 12 | High-performance liquid chromatographic determination of the alkaloids in betel nut. Journal of<br>Chromatography A, 1989, 475, 447-450.   | 3.7 | 54        |
| 13 | Elucidation of the Chemistry of Enzyme-Bound Thiamin Diphosphate Prior to Substrate Binding:<br>Defining Internal Equilibria among Tautomeric and Ionization States. Biochemistry, 2007, 46,<br>10739-10744.                                       | 2.5 | 54        |
| 14 | Spectroscopic Detection of Transient Thiamin Diphosphate-Bound Intermediates on Benzoylformate<br>Decarboxylaseâ€. Biochemistry, 2000, 39, 13862-13869.  | 2.5 | 50        |
| 15 | Conformational Analysis of LYS(11â~'36), a Peptide Derived from the β-Sheet Region of T4 Lysozyme, in TFE<br>and SDSâ€. Biochemistry, 1997, 36, 11525-11533.   | 2.5 | 46        |
| 16 | Characterization of a thiamin diphosphateâ€dependent phenylpyruvate decarboxylase from<br><i>Saccharomycesâ€∫cerevisiae</i> . FEBS Journal, 2011, 278, 1842-1853.  | 4.7 | 46        |
| 17 | Saturation mutagenesis of putative catalytic residues of benzoylformate decarboxylase provides a<br>challenge to the accepted mechanism. Proceedings of the National Academy of Sciences of the United<br>States of America, 2008, 105, 5733-5738. | 7.1 | 44        |
| 18 | Determinants of substrate specificity in KdcA, a thiamin diphosphate-dependent decarboxylase.<br>Bioorganic Chemistry, 2006, 34, 325-336.  | 4.1 | 41        |

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|----|--|------|-----------|
| 19 | Fragment-based screening by X-ray crystallography, MS and isothermal titration calorimetry to<br>identify PNMT (phenylethanolamine N-methyltransferase) inhibitors. Biochemical Journal, 2010, 431,<br>51-61.    | 3.7  | 41        |
| 20 | Structural Relationship between the Active Sites of β-Lactam-Recognizing and Amidase Signature<br>Enzymes: Convergent Evolution?. Biochemistry, 2010, 49, 9688-9697.   | 2.5  | 36        |
| 21 | Conformation of a Peptide Corresponding to T4 Lysozyme Residues 59-81 by NMR and CD Spectroscopy.<br>Biochemistry, 1994, 33, 11174-11183.  | 2.5  | 35        |
| 22 | Mechanism-Based Inactivation of Benzoylformate Decarboxylase, A Thiamin Diphosphate-Dependent<br>Enzyme. Journal of the American Chemical Society, 2007, 129, 4120-4121.   | 13.7 | 34        |
| 23 | Probing the Active Center of Benzaldehyde Lyase with Substitutions and the Pseudosubstrate<br>Analogue Benzoylphosphonic Acid Methyl Ester. Biochemistry, 2008, 47, 7734-7743.                                   | 2.5  | 34        |
| 24 | Snapshot of a Reaction Intermediate: Analysis of Benzoylformate Decarboxylase in Complex with a Benzoylphosphonate Inhibitor. Biochemistry, 2009, 48, 3247-3257.   | 2.5  | 32        |
| 25 | Structural Analysis of the Heparin-Binding Site of the NC1 Domain of Collagen XIV by CD and NMR,.<br>Biochemistry, 1999, 38, 6479-6488.  | 2.5  | 31        |
| 26 | Mutagenesis of Two Acidic Active Site Residues in Human Muscle Creatine Kinase:  Implications for the<br>Catalytic Mechanism. Biochemistry, 2001, 40, 3056-3061.   | 2.5  | 31        |
| 27 | Identification and Characterization of a Mandelamide Hydrolase and an NAD(P) + -Dependent<br>Benzaldehyde Dehydrogenase from Pseudomonas putida ATCC 12633. Journal of Bacteriology, 2003, 185,<br>2451-2456.    | 2.2  | 31        |
| 28 | Molecular recognition of physiological substrate noradrenaline by the adrenaline-synthesizing<br>enzyme PNMT and factors influencing its methyltransferase activity. Biochemical Journal, 2009, 422,<br>463-471. | 3.7  | 30        |
| 29 | Substrate specificity in thiamin diphosphate-dependent decarboxylases. Bioorganic Chemistry, 2012, 43, 26-36.  | 4.1  | 29        |
| 30 | Exploring the active site of benzaldehyde lyase by modeling and mutagenesis. Biochimica Et Biophysica<br>Acta - Proteins and Proteomics, 2005, 1753, 263-271.  | 2.3  | 28        |
| 31 | Isoleucine 69 and Valine 325 Form a Specificity Pocket in Human Muscle Creatine Kinaseâ€. Biochemistry,<br>2004, 43, 13766-13774.  | 2.5  | 27        |
| 32 | Structural, Mutagenic, and Kinetic Analysis of the Binding of Substrates and Inhibitors of Human<br>Phenylethanolamine N-Methyltransferase. Journal of Medicinal Chemistry, 2005, 48, 7243-7252.                 | 6.4  | 26        |
| 33 | Enzyme Adaptation to Inhibitor Binding:  A Cryptic Binding Site in Phenylethanolamine<br><i>N</i> -Methyltransferase. Journal of Medicinal Chemistry, 2007, 50, 4845-4853.                                       | 6.4  | 26        |
| 34 | A Determination of the Solution Conformation of the Nonmammalian Tachykinin Eledoisin by NMR and<br>CD Spectroscopy. Biochemistry, 1994, 33, 6802-6811.  | 2.5  | 25        |
| 35 | Pharmacokinetics of Thiopental and Pentobarbital Enantiomers After Intravenous Administration of<br>Racemic Thiopental. Anesthesia and Analgesia, 1996, 83, 552-558.   | 2.2  | 25        |
| 36 | Molecular Recognition of Sub-micromolar Inhibitors by the Epinephrine-Synthesizing Enzyme<br>Phenylethanolamine N-Methyltransferase. Journal of Medicinal Chemistry, 2004, 47, 37-44.                            | 6.4  | 25        |

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|----|--|-------------------|-------------|
| 37 | Mode of Binding of Methyl Acceptor Substrates to the Adrenaline-Synthesizing Enzyme<br>Phenylethanolamine N-Methyltransferase:  Implications for Catalysis. Biochemistry, 2005, 44,<br>16875-16885.  | 2.5               | 24          |
| 38 | The reaction mechanism of phenylethanolamine N-methyltransferase: A density functional theory study. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2009, 1794, 1831-1837.   | 2.3               | 24          |
| 39 | Inhibitors of PhenylethanolamineN-Methyltransferase That Are Predicted To Penetrate the Bloodâ <sup>^</sup> Brain Barrier:Â Design, Synthesis, and Evaluation of 3-Fluoromethyl-7-(N-substituted) Tj ETQq1 1 0.7843  | 14 rgBT /(<br>6.4 | Overlock 10 |
| 40 | α2-Adrenoceptor1. Journal of Medicinal Chemistry. 2004. 47. 4483-4493.<br>Active-Site Engineering of Benzaldehyde Lyase Shows That a Point Mutation Can Confer Both New<br>Reactivity and Susceptibility to Mechanism-Based Inhibition. Journal of the American Chemical Society,<br>2010, 132, 438-439. | 13.7              | 23          |
| 41 | A comparative study of human muscle and brain creatine kinases expressed in Escherichia coli. The<br>Protein Journal, 2000, 19, 59-66.   | 1.1               | 22          |
| 42 | Pharmacokinetics of Thiopental and Pentobarbital Enantiomers After Intravenous Administration of<br>Racemic Thiopental. Anesthesia and Analgesia, 1996, 83, 552-558.   | 2.2               | 21          |
| 43 | Mandelamide Hydrolase from Pseudomonas putida:  Characterization of a New Member of the Amidase<br>Signature Family. Biochemistry, 2004, 43, 7725-7735.  | 2.5               | 21          |
| 44 | Exploring the Role of the Active Site Cysteine in Human Muscle Creatine Kinaseâ€. Biochemistry, 2006, 45, 11464-11472.   | 2.5               | 21          |
| 45 | Detection and Time Course of Formation of Major Thiamin Diphosphate-Bound Covalent Intermediates<br>Derived from a Chromophoric Substrate Analogue on Benzoylformate Decarboxylase. Biochemistry,<br>2009, 48, 981-994.  | 2.5               | 21          |
| 46 | Pharmacokinetics of intravenous clomiphene isomers British Journal of Clinical Pharmacology, 1989, 27, 639-640.  | 2.4               | 20          |
| 47 | Recombinant Human PhenylethanolamineN-Methyltransferase: Overproduction inEscherichia coli,Purification, and Characterization. Protein Expression and Purification, 1996, 8, 160-166.  | 1.3               | 20          |
| 48 | Mechanism of Benzaldehyde Lyase Studied via Thiamin Diphosphate-Bound Intermediates and Kinetic<br>Isotope Effectsâ€. Biochemistry, 2008, 47, 3800-3809.   | 2.5               | 20          |
| 49 | Engineering the Substrate Binding Site of Benzoylformate Decarboxylase. Biochemistry, 2009, 48, 8387-8395.   | 2.5               | 20          |
| 50 | Isolation and characterization of a benzoylformate decarboxylase and a NAD+/NADP+-dependent<br>benzaldehyde dehydrogenase involved in d-phenylglycine metabolism in Pseudomonas stutzeri ST-201.<br>Biochimica Et Biophysica Acta - General Subjects, 2007, 1770, 1585-1592.                             | 2.4               | 19          |
| 51 | Using site-saturation mutagenesis to explore mechanism and substrate specificity in thiamin diphosphate-dependent enzymes. FEBS Journal, 2013, 280, 6395-6411.   | 4.7               | 18          |
| 52 | Identification of Initiation Sites for T4 Lysozyme Folding Using CD and NMR Spectroscopy of Peptide<br>Fragmentsâ€. Biochemistry, 2000, 39, 5911-5920.   | 2.5               | 17          |
| 53 | A peptide corresponding to the N-terminal 13 residues of T4 lysozyme forms an α-helix. FEBS Letters,<br>1993, 315, 323-328.  | 2.8               | 16          |
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|----|---|------|-----------|
| 55 | Phenylethanolamine N-methyltransferase inhibition: re-evaluation of kinetic data. Bioorganic and<br>Medicinal Chemistry Letters, 2004, 14, 4217-4220.   | 2.2  | 15        |
| 56 | Kinetic and pH studies on human phenylethanolamine N-methyltransferase. Archives of Biochemistry and Biophysics, 2013, 539, 1-8.  | 3.0  | 15        |
| 57 | A Theoretical Study of the Benzoylformate Decarboxylase Reaction Mechanism. Frontiers in Chemistry, 2018, 6, 205.   | 3.6  | 15        |
| 58 | CD and NMR determination of the solution structure of a peptide corresponding to T4 lysozyme residues 38–51. BBA - Proteins and Proteomics, 1995, 1250, 163-170.  | 2.1  | 14        |
| 59 | Identification of Charge Transfer Transitions Related to Thiamin-Bound Intermediates on Enzymes<br>Provides a Plethora of Signatures Useful in Mechanistic Studies. Biochemistry, 2014, 53, 2145-2152.  | 2.5  | 14        |
| 60 | Computational Study of Enantioselective Carboligation Catalyzed by Benzoylformate Decarboxylase.<br>ACS Catalysis, 2019, 9, 5657-5667.  | 11.2 | 13        |
| 61 | Extended Reaction Scope of Thiamine Diphosphate Dependent Cyclohexaneâ€1,2â€dione Hydrolase: From<br>Cĭ£¿C Bond Cleavage to CC Bond Ligation. Angewandte Chemie - International Edition, 2014, 53,<br>14402-14406.   | 13.8 | 11        |
| 62 | Reactions of aryl diazonium salts and alkyl arylazo ethers. 9. Studies of the carbanionic and free<br>radical mechanisms of dediazoniation of substituted 2-chlorobenzenediazonium salts. Journal of<br>Organic Chemistry, 1983, 48, 191-195.   | 3.2  | 9         |
| 63 | Phosphonodifluoropyruvate is a mechanism-based inhibitor of phosphonopyruvate decarboxylase from Bacteroides fragilis. Bioorganic and Medicinal Chemistry, 2017, 25, 4368-4374.   | 3.0  | 9         |
| 64 | Gas chromatographic—mass spectroscopic characterisation of the psychotomimetic<br>indolealkylamines and their in vivo metabolites. Biomedical Applications, 1987, 422, 13-23.   | 1.7  | 8         |
| 65 | Expression of Torpedo californica creatine kinase in Escherichia coli and purification from inclusion bodies. Protein Expression and Purification, 2002, 26, 89-95.   | 1.3  | 8         |
| 66 | Loop Movement and Catalysis in Creatine Kinase. IUBMB Life, 2005, 57, 355-362.  | 3.4  | 8         |
| 67 | Physical, kinetic and spectrophotometric studies of a NAD(P)-dependent benzaldehyde dehydrogenase<br>from Pseudomonas putida ATCC 12633. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2008,<br>1784, 1248-1255.   | 2.3  | 8         |
| 68 | The kinetic characterization and X-ray structure of a putative benzoylformate decarboxylase from M.<br>smegmatis highlights the difficulties in the functional annotation of ThDP-dependent enzymes.<br>Biochimica Et Biophysica Acta - Proteins and Proteomics, 2015, 1854, 1001-1009. | 2.3  | 8         |
| 69 | Aspartate aminotransferase catalyzed oxygen exchange with solvent from oxygen-18-enriched<br>.alphaketoglutarate: evidence for slow exchange of enzyme-bound water. Biochemistry, 1989, 28,<br>3821-3825.   | 2.5  | 7         |
| 70 | Phenylethanolamine N-methyltransferase kinetics: bovine versus recombinant human enzyme.<br>Bioorganic and Medicinal Chemistry Letters, 2001, 11, 1579-1582.  | 2.2  | 7         |
| 71 | Structure and mechanism of benzaldehyde dehydrogenase from Pseudomonas putida ATCC 12633, a member of the Class 3 aldehyde dehydrogenase superfamily. Protein Engineering, Design and Selection, 2017, 30, 273-280.   | 2.1  | 7         |
| 72 | Computational characterization of enzyme-bound thiamin diphosphate reveals a surprisingly stable tricyclic state: implications for catalysis. Beilstein Journal of Organic Chemistry, 2019, 15, 145-159.  | 2.2  | 7         |

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|----|--|------|-----------|
| 73 | Thiopental Sodium. Analytical Profiles of Drug Substances and Excipients, 1992, 21, 535-572.   | 0.0  | 6         |
| 74 | Crystallization of PNMT, the adrenaline-synthesizing enzyme, is critically dependent on a high protein concentration. Acta Crystallographica Section D: Biological Crystallography, 2002, 58, 314-315.   | 2.5  | 6         |
| 75 | Using directed evolution to probe the substrate specificity of mandelamide hydrolase. Protein Engineering, Design and Selection, 2009, 22, 103-110.  | 2.1  | 6         |
| 76 | A Bulky Hydrophobic Residue Is Not Required To Maintain the V-Conformation of Enzyme-Bound<br>Thiamin Diphosphate. Biochemistry, 2013, 52, 3028-3030.  | 2.5  | 6         |
| 77 | Enzymatic Stetter Reaction: Computational Study of the Reaction Mechanism of MenD. ACS Catalysis, 2021, 11, 12355-12366.   | 11.2 | 6         |
| 78 | Reactions of aryl diazonium salts and arylazo alkyl ethers. 7. Kinetic studies of the decomposition of Z<br>ethers derived from some substituted 2-nitrobenzenediazonium salts. Journal of Organic Chemistry,<br>1982, 47, 3673-3679.                                | 3.2  | 5         |
| 79 | Synthesis and conformational analysis of an O-phosphotyrosine-containing α-helical peptide.<br>International Journal of Peptide Research and Therapeutics, 1995, 2, 71-76.   | 0.1  | 5         |
| 80 | Disulfide-linked dimers of human adrenaline synthesizing enzyme PNMT are catalytically active.<br>Biochimica Et Biophysica Acta - Proteins and Proteomics, 2005, 1750, 82-92.  | 2.3  | 4         |
| 81 | Perturbation of the Monomer–Monomer Interfaces of the Benzoylformate Decarboxylase Tetramer.<br>Biochemistry, 2014, 53, 4358-4367.   | 2.5  | 4         |
| 82 | Reactions of aryl diazonium salts and alkyl arylazo ethers. XI. Further evidence for the mechanism of dediazoniation in basic alcoholic solution. Australian Journal of Chemistry, 1983, 36, 1031.   | 0.9  | 3         |
| 83 | Clomiphene Citrate. Analytical Profiles of Drug Substances and Excipients, 1998, 25, 85-120.   | 0.0  | 3         |
| 84 | Mechanistic and Structural Insight to an Evolved Benzoylformate Decarboxylase with Enhanced<br>Pyruvate Decarboxylase Activity. Catalysts, 2016, 6, 190.   | 3.5  | 3         |
| 85 | Reactions of aryl diazonium salts and arylazo alkyl ethers. VI. A comparison of the available methods<br>for the measurement of the rate of ionization of (Z)-arylazo alkyl ethers in alcoholic solvents.<br>Australian Journal of Chemistry, 1982, 35, 319.         | 0.9  | 2         |
| 86 | Studies on the conformational properties of CP-1042â^'55, the hinge region of CP-10, using circular dichroism and RP-HPLC. Chemical Biology and Drug Design, 2000, 55, 411-418.  | 1.1  | 2         |
| 87 | Time-dependent inactivation of human phenylethanolamine N-methyltransferase by<br>7-isothiocyanatotetrahydroisoquinoline. Bioorganic and Medicinal Chemistry Letters, 2009, 19,<br>1071-1074.  | 2.2  | 2         |
| 88 | Structure-Based Drug Design of Bisubstrate Inhibitors of Phenylethanolamine<br><i>N</i> -Methyltransferase Possessing Low Nanomolar Affinity at Both Substrate Binding<br>Domains <sup>1</sup> . Journal of Medicinal Chemistry, 2020, 63, 13878-13898.              | 6.4  | 2         |
| 89 | Reactions of aryl diazonium salts and alkyl arylazo ethers. X. General acid and intramolecular<br>electrostatic catalysis in the ionization of methyl (E)-2-Organyl-5-nitrophenylazo ethers in alcoholic<br>solvents. Australian Journal of Chemistry, 1983, 36, 55. | 0.9  | 1         |
| 90 | Heterogeneity of Escherichia coli -expressed human muscle creatine kinase. IUBMB Life, 2006, 58, 421-428.  | 3.4  | 1         |

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|----|--|-----|-----------|
| 91 | Exploring the Substrate Specificity of Benzoylformate Decarboxylase, Pyruvate Decarboxylase, and<br>Benzaldehyde Lyase. Oxidative Stress and Disease, 2003, , .  | 0.3 | 1         |
| 92 | Specificity and mechanism of mandelamide hydrolase catalysis. Archives of Biochemistry and Biophysics, 2017, 618, 23-31.   | 3.0 | 0         |
| 93 | Benzoylformate Decarboxylase. Oxidative Stress and Disease, 2003, , .  | 0.3 | 0         |
| 94 | Structural basis of substrate specificity in thiamin diphosphate dependent decarboxylases. FASEB<br>Journal, 2006, 20, A471.   | 0.5 | 0         |
| 95 | Observation and time resolution of chiral thiamin diphosphateâ€bound intermediates in the catalytic cycle of pyruvate decarboxylase and benzoylformate decarboxylase by stoppedâ€flow circular dichroism FASEB Journal, 2006, 20, A40. | 0.5 | 0         |
| 96 | Identification of the Ionization State and pKa for Protonation of the 4′â€Aminopyrimidine Ring on<br>Enzymes Utilizing Thiamin Diphosphate by Circular Dichroism Spectroscopy. FASEB Journal, 2007, 21,<br>A1016.                      | 0.5 | 0         |
| 97 | Using saturation mutagenesis to replace putative catalytic residues in thiamin diphosphate dependent enzymes. FASEB Journal, 2007, 21, A1016.  | 0.5 | 0         |
| 98 | Characterization of a benzoylformate decarboxylase and a NAD+/NADP+â€dependent benzaldehyde  | 0.5 | 0         |

dehydrogenase from Pseudomonas stutzeri STâ€201. FASEB Journal, 2008, 22, 1008.4. 98