

# Kirsty J Mclean

## List of Publications by Year in descending order

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84  
papers

4,321  
citations

101543

36  
h-index

110387

64  
g-index

89  
all docs

89  
docs citations

89  
times ranked

4118  
citing authors

#	ARTICLE	IF	CITATIONS
1	P450 BM3: the very model of a modern flavocytochrome. Trends in Biochemical Sciences, 2002, 27, 250-257.	7.5	385
2	Variations on a (t)hemeâ€”novel mechanisms, redox partners and catalytic functions in the cytochrome P450 superfamily. Natural Product Reports, 2007, 24, 585-609.	10.3	256
3	What makes a P450 tick?. Trends in Biochemical Sciences, 2013, 38, 140-150.	7.5	181
4	Cytochrome P450â€™redox partner fusion enzymes. Biochimica Et Biophysica Acta - General Subjects, 2007, 1770, 345-359.	2.4	180
5	Azole antifungals are potent inhibitors of cytochrome P450 mono-oxygenases and bacterial growth in mycobacteria and streptomycetes. Microbiology (United Kingdom), 2002, 148, 2937-2949.	1.8	162
6	Structure and Biochemical Properties of the Alkene Producing Cytochrome P450 OleTJE (CYP152L1) from the Jeotgalicoccus sp. 8456 Bacterium. Journal of Biological Chemistry, 2014, 289, 6535-6550.	3.4	153
7	Structure and function of the cytochrome P450 peroxygenase enzymes. Biochemical Society Transactions, 2018, 46, 183-196.	3.4	138
8	P450-Catalyzed Regio- and Diastereoselective Steroid Hydroxylation: Efficient Directed Evolution Enabled by Mutability Landscaping. ACS Catalysis, 2018, 8, 3395-3410.	11.2	128
9	Atomic Structure of Mycobacterium tuberculosis CYP121 to 1.06 Å... Reveals Novel Features of Cytochrome P450. Journal of Biological Chemistry, 2003, 278, 5141-5147.	3.4	126
10	Characterization of Active Site Structure in CYP121: A Cytochrome P450 Essential for Viability of Mycobacterium Tuberculosis H37Rv*. Journal of Biological Chemistry, 2008, 283, 33406-33416.	3.4	114
11	Single-step fermentative production of the cholesterol-lowering drug pravastatin via reprogramming of <i>Penicillium chrysogenum</i> . Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 2847-2852.	7.1	112
12	Crystal Structure of the Mycobacterium tuberculosis P450 CYP121-Fluconazole Complex Reveals New Azole Drug-P450 Binding Mode. Journal of Biological Chemistry, 2006, 281, 39437-39443.	3.4	109
13	Structural and Biochemical Characterization of Mycobacterium tuberculosis CYP142. Journal of Biological Chemistry, 2010, 285, 38270-38282.	3.4	104
14	The Structure of Mycobacterium tuberculosis CYP125. Journal of Biological Chemistry, 2009, 284, 35524-35533.	3.4	102
15	Expression, purification and spectroscopic characterization of the cytochrome P450 CYP121 from Mycobacterium tuberculosis. Journal of Inorganic Biochemistry, 2002, 91, 527-541.	3.5	89
16	Biophysical Characterization of the Sterol Demethylase P450 from Mycobacterium tuberculosis, Its Cognate Ferredoxin, and Their Interactions. Biochemistry, 2006, 45, 8427-8443.	2.5	85
17	Redox and Spectroscopic Properties of Human Indoleamine 2,3-Dioxygenase and A His303Ala Variant:Â Implications for Catalysisâ€. Biochemistry, 2005, 44, 14318-14328.	2.5	79
18	How Do Azoles Inhibit Cytochrome P450 Enzymes? A Density Functional Study. Journal of Physical Chemistry A, 2008, 112, 12911-12918.	2.5	76

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19	Catalytic Determinants of Alkene Production by the Cytochrome P450 Peroxygenase OleTJE. <i>Journal of Biological Chemistry</i> , 2017, 292, 5128-5143.	3.4	73
20	Application of Fragment Screening and Merging to the Discovery of Inhibitors of the <i>Mycobacterium tuberculosis</i> Cytochrome P450 CYP121. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 9311-9316.	13.8	69
21	The preponderance of P450s in the <i>Mycobacterium tuberculosis</i> genome. <i>Trends in Microbiology</i> , 2006, 14, 220-228.	7.7	67
22	The TB Structural Genomics Consortium: Providing a Structural Foundation for Drug Discovery. <i>Current Drug Targets Infectious Disorders</i> , 2002, 2, 121-141.	2.1	66
23	Structure, function and drug targeting in <i>Mycobacterium tuberculosis</i> cytochrome P450 systems. <i>Archives of Biochemistry and Biophysics</i> , 2007, 464, 228-240.	3.0	66
24	Production of alkenes and novel secondary products by P450 OleT <sub>JE</sub> using novel H <sub>2</sub> O <sub>2</sub> -generating fusion protein systems. <i>FEBS Letters</i> , 2017, 591, 737-750.	2.8	58
25	Identification and Characterization of a Novel Vitamin B12 (Cobalamin) Biosynthetic Enzyme (CobZ) from <i>Rhodobacter capsulatus</i> , Containing Flavin, Heme, and Fe-S Cofactors. <i>Journal of Biological Chemistry</i> , 2005, 280, 1086-1094.	3.4	52
26	Cholesterol, an essential molecule: diverse roles involving cytochrome P450 enzymes. <i>Biochemical Society Transactions</i> , 2012, 40, 587-593.	3.4	51
27	Rapid P450 Heme Iron Reduction by Laser Photoexcitation of <i>Mycobacterium tuberculosis</i> CYP121 and CYP51B1. <i>Journal of Biological Chemistry</i> , 2007, 282, 24816-24824.	3.4	50
28	Characterization of the Cobaltochelatase CbiXL. <i>Journal of Biological Chemistry</i> , 2003, 278, 41900-41907.	3.4	49
29	Biological Diversity of Cytochrome P450 Redox Partner Systems. <i>Advances in Experimental Medicine and Biology</i> , 2015, 851, 299-317.	1.6	49
30	FdC1, a Novel Ferredoxin Protein Capable of Alternative Electron Partitioning, Increases in Conditions of Acceptor Limitation at Photosystem I. <i>Journal of Biological Chemistry</i> , 2011, 286, 50-59.	3.4	47
31	Fragment-Based Approaches to the Development of <i>Mycobacterium tuberculosis</i> CYP121 Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2016, 59, 3272-3302.	6.4	47
32	Interaction of Nitric Oxide with Cytochrome P450 BM3. <i>Biochemistry</i> , 2004, 43, 16416-16431.	2.5	46
33	Kinetic, spectroscopic and thermodynamic characterization of the <i>Mycobacterium tuberculosis</i> adrenodoxin reductase homologue FprA. <i>Biochemical Journal</i> , 2003, 372, 317-327.	3.7	43
34	Identification and Characterization of the Terminal Enzyme of Siroheme Biosynthesis from <i>Arabidopsis thaliana</i> . <i>Journal of Biological Chemistry</i> , 2005, 280, 4713-4721.	3.4	42
35	Structural Biology and Biochemistry of Cytochrome P450 Systems in <i>Mycobacterium tuberculosis</i> . <i>Drug Metabolism Reviews</i> , 2008, 40, 427-446.	3.6	42
36	Characterization of <i>Cupriavidus metallidurans</i> CYP116B1 – A thiocarbamate herbicide oxygenating P450-phthalate dioxygenase reductase fusion protein. <i>FEBS Journal</i> , 2012, 279, 1675-1693.	4.7	37

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37	Characterisation of PduS, the pdu Metabolosome Corrin Reductase, and Evidence of Substructural Organisation within the Bacterial Microcompartment. <i>PLoS ONE</i> , 2010, 5, e14009.	2.5	36
38	Effect of DMSO on Protein Structure and Interactions Assessed by Collision-Induced Dissociation and Unfolding. <i>Analytical Chemistry</i> , 2017, 89, 9976-9983.	6.5	34
39	The Redox Properties of Ascorbate Peroxidase. <i>Biochemistry</i> , 2007, 46, 8017-8023.	2.5	33
40	Human P450-like oxidation of diverse proton pump inhibitor drugs by "gatekeeper"™ mutants of flavocytochrome P450 BM3. <i>Biochemical Journal</i> , 2014, 460, 247-259.	3.7	31
41	Cytochrome P450/redox partner fusion enzymes: biotechnological and toxicological prospects. <i>Expert Opinion on Drug Metabolism and Toxicology</i> , 2007, 3, 847-863.	3.3	29
42	Identification, Characterization, and Structure/Function Analysis of a Corrin Reductase Involved in Adenosylcobalamin Biosynthesis. <i>Journal of Biological Chemistry</i> , 2008, 283, 10813-10821.	3.4	29
43	The <i>Mycobacterium tuberculosis</i> cytochromes P450: physiology, biochemistry & molecular intervention. <i>Future Medicinal Chemistry</i> , 2010, 2, 1339-1353.	2.3	29
44	Overcoming the Limitations of Fragment Merging: Rescuing a Strained Merged Fragment Series Targeting <i>Mycobacterium tuberculosis</i> CYP121. <i>ChemMedChem</i> , 2013, 8, 1451-1456.	3.2	28
45	Unusual Spectroscopic and Ligand Binding Properties of the Cytochrome P450-Flavodoxin Fusion Enzyme XplA. <i>Journal of Biological Chemistry</i> , 2012, 287, 19699-19714.	3.4	27
46	<i>Mycobacterium tuberculosis</i> cytochrome P450 enzymes: a cohort of novel TB drug targets. <i>Biochemical Society Transactions</i> , 2012, 40, 573-579.	3.4	26
47	Novel Aryl Substituted Pyrazoles as Small Molecule Inhibitors of Cytochrome P450 CYP121A1: Synthesis and Antimycobacterial Evaluation. <i>Journal of Medicinal Chemistry</i> , 2017, 60, 10257-10267.	6.4	26
48	Strength of Axial Water Ligation in Substrate-Free Cytochrome P450s Is Isoform Dependent. <i>Biochemistry</i> , 2014, 53, 1428-1434.	2.5	24
49	Expression and characterization of <i>Mycobacterium tuberculosis</i> CYP144: Common themes and lessons learned in the <i>M. tuberculosis</i> P450 enzyme family. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2011, 1814, 76-87.	2.3	23
50	Expression, Purification, and Biochemical Characterization of the Flavocytochrome P450 CYP505A30 from <i>Myceliophthora thermophila</i> . <i>ACS Omega</i> , 2017, 2, 4705-4724.	3.5	21
51	Heme and Hemoproteins. , 2009, , 160-183.		21
52	Drug targeting of heme proteins in <i>Mycobacterium tuberculosis</i> . <i>Drug Discovery Today</i> , 2017, 22, 566-575.	6.4	20
53	<i>Bacillus megaterium</i> Has Both a Functional BluB Protein Required for DMB Synthesis and a Related Flavoprotein That Forms a Stable Radical Species. <i>PLoS ONE</i> , 2013, 8, e55708.	2.5	20
54	Design and Synthesis of Imidazole and Triazole Pyrazoles as <i>Mycobacterium Tuberculosis</i> CYP121A1 Inhibitors. <i>ChemistryOpen</i> , 2019, 8, 995-1011.	1.9	19

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55	Structure-Activity Relationships of <i>cyclo</i> -( <i>scp</i> )-Tyrosyl- <i>scp</i> -tyrosine) Derivatives Binding to <i>Mycobacterium tuberculosis</i> CYP121: Iodinated Analogues Promote Shift to High-Spin Adduct. <i>Journal of Medicinal Chemistry</i> , 2019, 62, 9792-9805.	6.4	19
56	Structural and catalytic properties of the peroxygenase P450 enzyme CYP152K6 from <i>Bacillus methanolicus</i> . <i>Journal of Inorganic Biochemistry</i> , 2018, 188, 18-28.	3.5	18
57	The genome sequence of <i>Mycobacterium tuberculosis</i> reveals cytochromes P450 as novel anti-TB drug targets. <i>Journal of Chemical Technology and Biotechnology</i> , 2000, 75, 933-941.	3.2	17
58	A Novel Intermediate in the Reaction of Seleno CYP119 with <i>m</i> -Chloroperbenzoic Acid. <i>Biochemistry</i> , 2011, 50, 3014-3024.	2.5	17
59	Microbial Cytochromes P450. , 2015, , 261-407.		17
60	Novel insights into P450 BM3 interactions with FDA-approved antifungal azole drugs. <i>Scientific Reports</i> , 2019, 9, 1577.	3.3	17
61	Demonstration That CobG, the Monooxygenase Associated with the Ring Contraction Process of the Aerobic Cobalamin (Vitamin B12) Biosynthetic Pathway, Contains an Fe-S Center and a Mononuclear Non-heme Iron Center. <i>Journal of Biological Chemistry</i> , 2009, 284, 4796-4805.	3.4	16
62	Electron transfer reactions, cyanide and O <sub>2</sub> binding of truncated hemoglobin from <i>Bacillus subtilis</i> . <i>Electrochimica Acta</i> , 2013, 110, 86-93.	5.2	16
63	Substrate Fragmentation for the Design of <i>M. tuberculosis</i> CYP121 Inhibitors. <i>ChemMedChem</i> , 2016, 11, 1924-1935.	3.2	15
64	The structure, function and properties of sirohaem decarboxylase – an enzyme with structural homology to a transcription factor family that is part of the alternative haem biosynthesis pathway. <i>Molecular Microbiology</i> , 2014, 93, 247-261.	2.5	14
65	Characterization of Cytochrome P450 Enzymes and Their Applications in Synthetic Biology. <i>Methods in Enzymology</i> , 2018, 608, 189-261.	1.0	14
66	Synthesis and biological evaluation of novel cYY analogues targeting <i>Mycobacterium tuberculosis</i> CYP121A1. <i>Bioorganic and Medicinal Chemistry</i> , 2019, 27, 1546-1561.	3.0	14
67	Structural Characterization and Ligand/Inhibitor Identification Provide Functional Insights into the <i>Mycobacterium tuberculosis</i> Cytochrome P450 CYP126A1. <i>Journal of Biological Chemistry</i> , 2017, 292, 1310-1329.	3.4	13
68	Design, synthesis and evaluation against <i>Mycobacterium tuberculosis</i> of azole piperazine derivatives as dicycloyrosine (cYY) mimics. <i>Bioorganic and Medicinal Chemistry</i> , 2018, 26, 161-176.	3.0	13
69	Nanoelectrospray Ionization Mass Spectrometric Study of <i>Mycobacterium tuberculosis</i> CYP121 – Ligand Interactions. <i>Analytical Chemistry</i> , 2013, 85, 5707-5714.	6.5	12
70	A Promiscuous Bacterial P450: The Unparalleled Diversity of BM3 in Pharmaceutical Metabolism. <i>International Journal of Molecular Sciences</i> , 2021, 22, 11380.	4.1	12
71	Characterization of coenzyme binding and selectivity determinants in <i>Mycobacterium tuberculosis</i> flavoprotein reductase A: analysis of Arg199 and Arg200 mutants at the NADP(H) 2- $\epsilon^2$ -phosphate binding site. <i>Biochemical Journal</i> , 2009, 417, 103-114.	3.7	9
72	Electron Transfer Cofactors. , 2013, , 601-606.		7

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73	Structural characterization of CYP144A1 – a cytochrome P450 enzyme expressed from alternative transcripts in <i>Mycobacterium tuberculosis</i> . <i>Scientific Reports</i> , 2016, 6, 26628.	3.3	7
74	Biofragments: An Approach towards Predicting Protein Function Using Biologically Related Fragments and its Application to <i>Mycobacterium tuberculosis</i> CYP126. <i>ChemBioChem</i> , 2014, 15, 549-555.	2.6	6
75	Crystallization and preliminary crystallographic analysis of a novel cytochrome P450 from <i>Mycobacterium tuberculosis</i> . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2002, 58, 704-705.	2.5	5
76	Fragment Profiling Approach to Inhibitors of the Orphan <i>M. tuberculosis</i> P450 CYP144A1. <i>Biochemistry</i> , 2017, 56, 1559-1572.	2.5	5
77	Trp359 regulates flavin thermodynamics and coenzyme selectivity in <i>Mycobacterium tuberculosis</i> FprA. <i>Biochemical Journal</i> , 2008, 411, 563-570.	3.7	4
78	The genome sequence of <i>Mycobacterium tuberculosis</i> reveals cytochromes P450 as novel anti-TB drug targets. <i>Journal of Chemical Technology and Biotechnology</i> , 2000, 75, 933-941.	3.2	4
79	A new strategy for hit generation: Novel in cellulo active inhibitors of CYP121A1 from <i>Mycobacterium tuberculosis</i> via a combined X-ray crystallographic and phenotypic screening approach (XP screen). <i>European Journal of Medicinal Chemistry</i> , 2022, 230, 114105.	5.5	4
80	Resonance Raman studies of <i>Bacillus megaterium</i> cytochrome P450 BM3 and biotechnologically important mutants. <i>Journal of Raman Spectroscopy</i> , 2018, 49, 287-297.	2.5	3
81	Cytochromes P450 as drug targets in <i>Mycobacterium tuberculosis</i> . <i>Biochemical Society Transactions</i> , 2001, 29, A33-A33.	3.4	0
82	Interactions of Cytochrome P450 with Nitric Oxide and Related Ligands. , 2007, , 285-317.		0
83	Cytochrome P450 (cyp). , 2016, , 1-18.		0
84	Cytochrome P450 (cyp). , 2018, , 1288-1305.		0