Kirsty J Mclean

List of Publications by Year
in descending order

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	A new strategy for hit generation: Novel in cellulo active inhibitors of CYP121A1 from Mycobacterium tuberculosis via a combined X-ray crystallographic and phenotypic screening approach (XP screen). European Journal of Medicinal Chemistry, 2022, 230, 114105.	5.5	4
2	A Promiscuous Bacterial P450: The Unparalleled Diversity of BM3 in Pharmaceutical Metabolism. International Journal of Molecular Sciences, 2021, 22, 11380.	4.1	12
3	Design and Synthesis of Imidazole and Triazole Pyrazoles as Mycobacterium Tuberculosis CYP121A1 Inhibitors. ChemistryOpen, 2019, 8, 995-1011.	1.9	19
4	Structureâ€“Activity Relationships of cyclo(<scp>l</scp>-Tyrosyl-<scp>l</scp>-tyrosine) Derivatives Binding to Mycobacterium tuberculosis CYP121: Iodinated Analogues Promote Shift to High-Spin Adduct. Journal of Medicinal Chemistry, 2019, 62, 9792-9805.	6.4	19
5	Novel insights into P450 BM3 interactions with FDA-approved antifungal azole drugs. Scientific Reports, 2019, 9, 1577.	3.3	17
6	Synthesis and biological evaluation of novel cYY analogues targeting Mycobacterium tuberculosis CYP121A1. Bioorganic and Medicinal Chemistry, 2019, 27, 1546-1561.	3.0	14
7	P450-Catalyzed Regio- and Diastereoselective Steroid Hydroxylation: Efficient Directed Evolution Enabled by Mutability Landscaping. ACS Catalysis, 2018, 8, 3395-3410.	11.2	128
8	Structure and function of the cytochrome P450 peroxygenase enzymes. Biochemical Society Transactions, 2018, 46, 183-196.	3.4	138
9	Design, synthesis and evaluation against Mycobacterium tuberculosis of azole piperazine derivatives as dicyclotyrosine (cYY) mimics. Bioorganic and Medicinal Chemistry, 2018, 26, 161-176.	3.0	13
10	Resonance Raman studies of Bacillus megaterium cytochrome P450 BM3 and biotechnologically important mutants. Journal of Raman Spectroscopy, 2018, 49, 287-297.	2.5	3
11	Structural and catalytic properties of the peroxygenase P450 enzyme CYP152K6 from Bacillus methanolicus. Journal of Inorganic Biochemistry, 2018, 188, 18-28.	3.5	18
12	Characterization of Cytochrome P450 Enzymes and Their Applications in Synthetic Biology. Methods in Enzymology, 2018, 608, 189-261.	1.0	14
13	Cytochrome P450 (cyp). , 2018, , 1288-1305.		0
14	Catalytic Determinants of Alkene Production by the Cytochrome P450 Peroxygenase OleTJE. Journal of Biological Chemistry, 2017, 292, 5128-5143.	3.4	73
15	Production of alkenes and novel secondary products by P450 Ole<scp>T_{JE}</scp> using novel H₂O₂â€generating fusion protein systems. FEBS Letters, 2017, 591, 737-750.	2.8	58
16	Fragment Profiling Approach to Inhibitors of the Orphan M. tuberculosis P450 CYP144A1. Biochemistry, 2017, 56, 1559-1572.	2.5	5
17	Structural Characterization and Ligand/Inhibitor Identification Provide Functional Insights into the Mycobacterium tuberculosis Cytochrome P450 CYP126A1. Journal of Biological Chemistry, 2017, 292, 1310-1329.	3.4	13
18	Effect of DMSO on Protein Structure and Interactions Assessed by Collision-Induced Dissociation and Unfolding. Analytical Chemistry, 2017, 89, 9976-9983.	6.5	34

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19	Expression, Purification, and Biochemical Characterization of the Flavocytochrome P450 CYP505A30 from Myceliophthora thermophila. ACS Omega, 2017, 2, 4705-4724.	3.5	21
20	Novel Aryl Substituted Pyrazoles as Small Molecule Inhibitors of Cytochrome P450 CYP121A1: Synthesis and Antimycobacterial Evaluation. Journal of Medicinal Chemistry, 2017, 60, 10257-10267.	6.4	26
21	Drug targeting of heme proteins in Mycobacterium tuberculosis. Drug Discovery Today, 2017, 22, 566-575.	6.4	20
22	Structural characterization of CYP144A1 â€“ a cytochrome P450 enzyme expressed from alternative transcripts in Mycobacterium tuberculosis. Scientific Reports, 2016, 6, 26628.	3.3	7
23	Substrate Fragmentation for the Design of M.â€…tuberculosis CYP121 Inhibitors. ChemMedChem, 2016, 11, 1924-1935.	3.2	15
24	Fragment-Based Approaches to the Development of Mycobacterium tuberculosis CYP121 Inhibitors. Journal of Medicinal Chemistry, 2016, 59, 3272-3302.	6.4	47
25	Cytochrome P450 (cyp). , 2016, , 1-18.		0
26	Biological Diversity of Cytochrome P450 Redox Partner Systems. Advances in Experimental Medicine and Biology, 2015, 851, 299-317.	1.6	49
27	Microbial Cytochromes P450. , 2015, , 261-407.		17
28	Single-step fermentative production of the cholesterol-lowering drug pravastatin via reprogramming of Penicillium chrysogenum. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 2847-2852.	7.1	112
29	Human P450-like oxidation of diverse proton pump inhibitor drugs by â€˜gatekeeperâ€™ mutants of flavocytochrome P450 BM3. Biochemical Journal, 2014, 460, 247-259.	3.7	31
30	Biofragments: An Approach towards Predicting Protein Function Using Biologically Related Fragments and its Application to Mycobacterium tuberculosis CYP126. ChemBioChem, 2014, 15, 549-555.	2.6	6
31	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
32	The structure, function and properties of sirohaem decarboxylase â€“ an enzyme with structural homology to a transcription factor family that is part of the alternative haem biosynthesis pathway. Molecular Microbiology, 2014, 93, 247-261.	2.5	14
33	Strength of Axial Water Ligation in Substrate-Free Cytochrome P450s Is Isoform Dependent. Biochemistry, 2014, 53, 1428-1434.	2.5	24
34	Electron Transfer Cofactors. , 2013, , 601-606.		7
35	Electron transfer reactions, cyanide and O2 binding of truncated hemoglobin from Bacillus subtilis. Electrochimica Acta, 2013, 110, 86-93.	5.2	16
36	What makes a P450 tick?. Trends in Biochemical Sciences, 2013, 38, 140-150.	7.5	181

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37	Nanoelectrospray Ionization Mass Spectrometric Study of Mycobacterium tuberculosis CYP121â€“Ligand Interactions. Analytical Chemistry, 2013, 85, 5707-5714.	6.5	12
38	Overcoming the Limitations of Fragment Merging: Rescuing a Strained Merged Fragment Series Targeting Mycobacterium tuberculosis CYP121. ChemMedChem, 2013, 8, 1451-1456.	3.2	28
39	Bacillus megaterium Has Both a Functional BluB Protein Required for DMB Synthesis and a Related Flavoprotein That Forms a Stable Radical Species. PLoS ONE, 2013, 8, e55708.	2.5	20
40	Application of Fragment Screening and Merging to the Discovery of Inhibitors of the Mycobacterium tuberculosis Cytochromeâ€…P450 CYP121. Angewandte Chemie - International Edition, 2012, 51, 9311-9316.	13.8	69
41	Cholesterol, an essential molecule: diverse roles involving cytochrome P450 enzymes. Biochemical Society Transactions, 2012, 40, 587-593.	3.4	51
42	Mycobacterium tuberculosis cytochrome P450 enzymes: a cohort of novel TB drug targets. Biochemical Society Transactions, 2012, 40, 573-579.	3.4	26
43	Unusual Spectroscopic and Ligand Binding Properties of the Cytochrome P450-Flavodoxin Fusion Enzyme XplA. Journal of Biological Chemistry, 2012, 287, 19699-19714.	3.4	27
44	Characterization of Cupriavidusâ€ƒmetallidurans CYP116B1 â€“ A thiocarbamate herbicide oxygenating P450â€“phthalate dioxygenase reductase fusion protein. FEBS Journal, 2012, 279, 1675-1693.	4.7	37
45	FdC1, a Novel Ferredoxin Protein Capable of Alternative Electron Partitioning, Increases in Conditions of Acceptor Limitation at Photosystem I. Journal of Biological Chemistry, 2011, 286, 50-59.	3.4	47
46	A Novel Intermediate in the Reaction of Seleno CYP119 with m-Chloroperbenzoic Acid. Biochemistry, 2011, 50, 3014-3024.	2.5	17
47	Expression and characterization of Mycobacterium tuberculosis CYP144: Common themes and lessons learned in the M. tuberculosis P450 enzyme family. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2011, 1814, 76-87.	2.3	23
48	Structural and Biochemical Characterization of Mycobacterium tuberculosis CYP142. Journal of Biological Chemistry, 2010, 285, 38270-38282.	3.4	104
49	The Mycobacterium tuberculosis cytochromes P450: physiology, biochemistry & molecular intervention. Future Medicinal Chemistry, 2010, 2, 1339-1353.	2.3	29
50	Characterisation of PduS, the pdu Metabolosome Corrin Reductase, and Evidence of Substructural Organisation within the Bacterial Microcompartment. PLoS ONE, 2010, 5, e14009.	2.5	36
51	The Structure of Mycobacterium tuberculosis CYP125. Journal of Biological Chemistry, 2009, 284, 35524-35533.	3.4	102
52	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. Journal of Biological Chemistry, 2009, 284, 4796-4805.	3.4	16
53	Characterization of coenzyme binding and selectivity determinants in Mycobacterium tuberculosis flavoprotein reductase A: analysis of Arg199 and Arg200 mutants at the NADP(H) 2â€²-phosphate binding site. Biochemical Journal, 2009, 417, 103-114.	3.7	9
54	Heme and Hemoproteins. , 2009, , 160-183.		21

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55	How Do Azoles Inhibit Cytochrome P450 Enzymes? A Density Functional Study. Journal of Physical Chemistry A, 2008, 112, 12911-12918.	2.5	76
56	Structural Biology and Biochemistry of Cytochrome P450 Systems inMycobacterium tuberculosis. Drug Metabolism Reviews, 2008, 40, 427-446.	3.6	42
57	Identification, Characterization, and Structure/Function Analysis of a Corrin Reductase Involved in Adenosylcobalamin Biosynthesis. Journal of Biological Chemistry, 2008, 283, 10813-10821.	3.4	29
58	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
59	Trp359 regulates flavin thermodynamics and coenzyme selectivity in Mycobacterium tuberculosis FprA. Biochemical Journal, 2008, 411, 563-570.	3.7	4
60	Rapid P450 Heme Iron Reduction by Laser Photoexcitation of Mycobacterium tuberculosis CYP121 and CYP51B1. Journal of Biological Chemistry, 2007, 282, 24816-24824.	3.4	50
61	Cytochrome P450/redox partner fusion enzymes: biotechnological and toxicological prospects. Expert Opinion on Drug Metabolism and Toxicology, 2007, 3, 847-863.	3.3	29
62	Structure, function and drug targeting in Mycobacterium tuberculosis cytochrome P450 systems. Archives of Biochemistry and Biophysics, 2007, 464, 228-240.	3.0	66
63	Cytochrome P450â€“redox partner fusion enzymes. Biochimica Et Biophysica Acta - General Subjects, 2007, 1770, 345-359.	2.4	180
64	The Redox Properties of Ascorbate Peroxidase. Biochemistry, 2007, 46, 8017-8023.	2.5	33
65	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
66	Interactions of Cytochrome P450 with Nitric Oxide and Related Ligands. , 2007, , 285-317.		0
67	Biophysical Characterization of the Sterol Demethylase P450 from Mycobacterium tuberculosis, Its Cognate Ferredoxin, and Their Interactions. Biochemistry, 2006, 45, 8427-8443.	2.5	85
68	The preponderance of P450s in the Mycobacterium tuberculosis genome. Trends in Microbiology, 2006, 14, 220-228.	7.7	67
69	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
70	Identification and Characterization of the Terminal Enzyme of Siroheme Biosynthesis from Arabidopsis thaliana. Journal of Biological Chemistry, 2005, 280, 4713-4721.	3.4	42
71	Identification and Characterization of a Novel Vitamin B12 (Cobalamin) Biosynthetic Enzyme (CobZ) from Rhodobacter capsulatus, Containing Flavin, Heme, and Fe-S Cofactors. Journal of Biological Chemistry, 2005, 280, 1086-1094.	3.4	52
72	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

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73	Interaction of Nitric Oxide with Cytochrome P450 BM3â€. Biochemistry, 2004, 43, 16416-16431.	2.5	46
74	Atomic Structure of Mycobacterium tuberculosis CYP121 to 1.06 Ã... Reveals Novel Features of Cytochrome P450. Journal of Biological Chemistry, 2003, 278, 5141-5147.	3.4	126
75	Characterization of the Cobaltochelatase CbiXL. Journal of Biological Chemistry, 2003, 278, 41900-41907.	3.4	49
76	Kinetic, spectroscopic and thermodynamic characterization of the Mycobacterium tuberculosis adrenodoxin reductase homologue FprA. Biochemical Journal, 2003, 372, 317-327.	3.7	43
77	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
78	The TB Structural Genomics Consortium: Providing a Structural Foundation for Drug Discovery. Current Drug Targets Infectious Disorders, 2002, 2, 121-141.	2.1	66
79	P450 BM3: the very model of a modern flavocytochrome. Trends in Biochemical Sciences, 2002, 27, 250-257.	7.5	385
80	Crystallization and preliminary crystallographic analysis of a novel cytochrome P450 fromMycobacterium tuberculosis. Acta Crystallographica Section D: Biological Crystallography, 2002, 58, 704-705.	2.5	5
81	Expression, purification and spectroscopic characterization of the cytochrome P450 CYP121 from Mycobacterium tuberculosis. Journal of Inorganic Biochemistry, 2002, 91, 527-541.	3.5	89
82	Cytochromes P450 as drug targets in Mycobacterium tuberculosis. Biochemical Society Transactions, 2001, 29, A33-A33.	3.4	0
83	The genome sequence ofMycobacterium tuberculosis reveals cytochromes P450 as novel anti-TB drug targets. Journal of Chemical Technology and Biotechnology, 2000, 75, 933-941.	3.2	17
84	The genome sequence of Mycobacterium tuberculosis reveals cytochromes P450 as novel antiâ€TB drug targets. Journal of Chemical Technology and Biotechnology, 2000, 75, 933-941.	3.2	4