Thomas L Poulos

List of Publications by Year
in descending order

258 papers	18,922 citations	13099 68 h-index	14208 128 g-index
267 all docs	267 docs citations	267 times ranked	12032 citing authors

#	Article	IF	Citations
1	High-resolution crystal structure of cytochrome P450cam. Journal of Molecular Biology, 1987, 195, 687-700.	4.2	1,418
2	Heme Enzyme Structure and Function. Chemical Reviews, 2014, 114, 3919-3962.	47.7	1,049
3	Crystal structure of horseradish peroxidase C at 2.15 Ã… resolution. Nature Structural Biology, 1997, 4, 1032-1038.	9.7	642
4	Crystal Structure of Constitutive Endothelial Nitric Oxide Synthase. Cell, 1998, 95, 939-950.	28.9	636
5	Crystal structure of substrate-free Pseudomonas putida cytochrome P-450. Biochemistry, 1986, 25, 5314-5322.	2.5	608
6	Engineered ascorbate peroxidase as a genetically encoded reporter for electron microscopy. Nature Biotechnology, 2012, 30, 1143-1148.	17.5	584
7	The crystal structure of chloroperoxidase: a heme peroxidaseâ€"cytochrome P450 functional hybrid. Structure, 1995, 3, 1367-1378.	3.3	446
8	The structure of the cytochrome p450BM-3 haem domain complexed with the fatty acid substrate, palmitoleic acid. Nature Structural Biology, 1997, 4, 140-146.	9.7	433
9	Structure of cytochrome P450eryF involved in erythromycin biosynthesis. Nature Structural and Molecular Biology, 1995, 2, 144-153.	8.2	376
10	Crystal structure of human heme oxygenase-1. Nature Structural Biology, 1999, 6, 860-867.	9.7	282
11	Crystal structure of recombinant pea cytosolic ascorbate peroxidase. Biochemistry, 1995, 34, 4331-4341.	2.5	274
12	The crystal structure of peanut peroxidase. Structure, 1996, 4, 311-321.	3.3	270
13	Structure?function studies on nitric oxide synthases. Journal of Inorganic Biochemistry, 2005, 99, 293-305.	3.5	252
14	Understanding the Role of the Essential Asp251 in Cytochrome P450cam Using Site-Directed Mutagenesis, Crystallography, and Kinetic Solvent Isotope Effect. Biochemistry, 1998, 37, 9211-9219.	2.5	243
15	Structure and mechanism of the complex between cytochrome P4503A4 and ritonavir. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 18422-18427.	7.1	240
16	Crystal structure of the cytochrome P-450CAM active site mutant Thr252Ala. Biochemistry, 1991, 30, 11420-11429.	2.5	232
17	The role of the proximal ligand in heme enzymes. Journal of Biological Inorganic Chemistry, 1996, 1, 356-359.	2.6	219
18	Crystal structure of the carbon monoxide-substrate-cytochrome P-450CAM ternary complex. Biochemistry, 1989, 28, 7586-7592.	2.5	217

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19	A metal-mediated hydride shift mechanism for xylose isomerase based on the 1.6 Ã…Streptomycs rubiginosus structure with xylitol andD-xylose. Proteins: Structure, Function and Bioinformatics, 1991, 9, 153-173.	2.6	208
20	Structure of the CO sensing transcription activator CooA. Nature Structural Biology, 2000, 7, 876-880.	9.7	208
21	Crystal Structures of Zinc-free and -bound Heme Domain of Human Inducible Nitric-oxide Synthase. Journal of Biological Chemistry, 1999, 274, 21276-21284.	3.4	196
22	Evolutionary History of a Specialized P450 Propane Monooxygenase. Journal of Molecular Biology, 2008, 383, 1069-1080.	4.2	185
23	Crystallographic Study on the Dioxygen Complex of Wild-type and Mutant Cytochrome P450cam. Journal of Biological Chemistry, 2005, 280, 31659-31663.	3.4	182
24	Identification of a Porphyrin .pi. Cation Radical in Ascorbate Peroxidase Compound I. Biochemistry, 1995, 34, 4342-4345.	2.5	176
25	Crystal Structure of a Thermophilic Cytochrome P450 from the Archaeon Sulfolobus solfataricus. Journal of Biological Chemistry, 2000, 275, 31086-31092.	3.4	176
26	Cytochrome P450 _{cam} : crystallography, oxygen activation, and electron transfer ¹. FASEB Journal, 1992, 6, 674-679.	0.5	163
27	Structural Basis for Effector Control and Redox Partner Recognition in Cytochrome P450. Science, 2013, 340, 1227-1230.	12.6	160
28	Proteases of enhanced stability: Characteization of a thermostable variant of subtilisin. Proteins: Structure, Function and Bioinformatics, 1986, 1, 326-334.	2.6	154
29	Stereochemistry of the chloroperoxidase active site: crystallographic and molecular-modeling studies. Chemistry and Biology, 1998, 5, 461-473.	6.0	149
30	High-Resolution Crystal Structures and Spectroscopy of Native and Compound I CytochromecPeroxidaseâ€. Biochemistry, 2003, 42, 5600-5608.	2.5	140
31	Crystal Structure of Heme Oxygenase from the Gram-Negative PathogenNeisseria meningitidisand a Comparison with Mammalian Heme Oxygenase-1â€. Biochemistry, 2001, 40, 11552-11558.	2.5	136
32	Aspartate residue 7 in amyloid Î²-protein is critical for classical complement pathway activation: Implications for Alzheimer's disease pathogenesis. Nature Medicine, 1997, 3, 077-079.	30.7	134
33	Structural Basis for Novel Î´-Regioselective Heme Oxygenation in the Opportunistic PathogenPseudomonas aeruginosaâ€,â€¡. Biochemistry, 2004, 43, 5239-5245.	2.5	129
34	Structural insights into substrate and inhibitor binding sites in human indoleamine 2,3-dioxygenase 1. Nature Communications, 2017, 8, 1693.	12.8	129
35	The Novel Binding Mode of N-Alkyl-Nâ€˜-hydroxyguanidine to Neuronal Nitric Oxide Synthase Provides Mechanistic Insights into NO Biosynthesis. Biochemistry, 2002, 41, 13868-13875.	2.5	122
36	Soluble guanylate cyclase. Current Opinion in Structural Biology, 2006, 16, 736-743.	5.7	114

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37	Structural and Mechanistic Insights into the Interaction of Cytochrome P4503A4 with Bromoergocryptine, a Type I Ligand. Journal of Biological Chemistry, 2012, 287, 3510-3517.	3.4	106
38	Thirty years of heme peroxidase structural biology. Archives of Biochemistry and Biophysics, 2010, 500, 3-12.	3.0	105
39	Comparison of the Heme-free and -bound Crystal Structures of Human Heme Oxygenase-1. Journal of Biological Chemistry, 2003, 278, 7834-7843.	3.4	104
40	Minimal Pharmacophoric Elements and Fragment Hopping, an Approach Directed at Molecular Diversity and Isozyme Selectivity. Design of Selective Neuronal Nitric Oxide Synthase Inhibitors. Journal of the American Chemical Society, 2008, 130, 3900-3914.	13.7	101
41	Photoreduction of the active site of the metalloprotein putidaredoxin by synchrotron radiation. Acta Crystallographica Section D: Biological Crystallography, 2007, 63, 951-960.	2.5	97
42	Cytochrome P450 flexibility. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 13121-13122.	7.1	92
43	An Engineered Cation Site in Cytochrome c Peroxidase Alters the Reactivity of the Redox Active Tryptophan. Biochemistry, 1996, 35, 6107-6115.	2.5	91
44	Disruption of an Active Site Hydrogen Bond Converts Human Heme Oxygenase-1 into a Peroxidase. Journal of Biological Chemistry, 2001, 276, 10612-10619.	3.4	90
45	Structural basis for regiospecific midazolam oxidation by human cytochrome P450 3A4. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 486-491.	7.1	90
46	Structure-Based Inhibitor Design for Evaluation of a CYP3A4 Pharmacophore Model. Journal of Medicinal Chemistry, 2016, 59, 4210-4220.	6.4	88
47	Crystal Structure of Putidaredoxin, the [2Feâ€"2S] Component of the P450cam Monooxygenase System from Pseudomonas putida. Journal of Molecular Biology, 2003, 333, 377-392.	4.2	86
48	Discovery of Highly Potent and Selective Inhibitors of Neuronal Nitric Oxide Synthase by Fragment Hopping. Journal of Medicinal Chemistry, 2009, 52, 779-797.	6.4	86
49	Crystal Structure of <i>Nitrosomonas europaea</i> Cytochrome <i>c</i> Peroxidase and the Structural Basis for Ligand Switching in Bacterial Di-heme Peroxidases. Biochemistry, 2001, 40, 13483-13490.	2.5	83
50	Crystal Structures of the Ferrous Dioxygen Complex of Wild-type Cytochrome P450eryF and Its Mutants, A245S and A245T. Journal of Biological Chemistry, 2005, 280, 22102-22107.	3.4	83
51	Functional implications of interleukin-1Î² based on the three-dimensional structure. Proteins: Structure, Function and Bioinformatics, 1992, 12, 10-23.	2.6	79
52	Crystal Structure of Nitric Oxide Synthase Bound to Nitro Indazole Reveals a Novel Inactivation Mechanismâ€. Biochemistry, 2001, 40, 13448-13455.	2.5	78
53	Crystallographic Studies on Endothelial Nitric Oxide Synthase Complexed with Nitric Oxide and Mechanism-Based Inhibitors. Biochemistry, 2001, 40, 5399-5406.	2.5	78
54	New understandings of thermostable and peizostable enzymes. Current Opinion in Biotechnology, 2003, 14, 360-365.	6.6	78

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55	Selective neuronal nitric oxide synthase inhibitors and the prevention of cerebral palsy. Annals of Neurology, 2009, 65, 209-217.	5.3	78
56	Ultrahigh (0.93Ã…) resolution structure of manganese peroxidase from Phanerochaete chrysosporium: Implications for the catalytic mechanism. Journal of Inorganic Biochemistry, 2010, 104, 683-690.	3.5	78
57	Crystal Structures of Substrate Binding Site Mutants of Manganese Peroxidase. Journal of Biological Chemistry, 1997, 272, 17574-17580.	3.4	77
58	Crystal Structures of the Ferric, Ferrous, and Ferrousâ€"NO Forms of the Asp140Ala Mutant of Human Heme Oxygenase-1: Catalytic Implications. Journal of Molecular Biology, 2003, 330, 527-538.	4.2	77
59	Preliminary Characterization and Crystal Structure of a Thermostable Cytochrome P450 from Thermus thermophilus. Journal of Biological Chemistry, 2003, 278, 608-616.	3.4	76
60	Crystal Structures of Epothilone D-bound, Epothilone B-bound, and Substrate-free Forms of Cytochrome P450epoK. Journal of Biological Chemistry, 2003, 278, 44886-44893.	3.4	75
61	Structural basis for dipeptide amide isoform-selective inhibition of neuronal nitric oxide synthase. Nature Structural and Molecular Biology, 2004, 11, 54-59.	8.2	75
62	Crystallographic and Single-Crystal Spectral Analysis of the Peroxidase Ferryl Intermediate. Biochemistry, 2010, 49, 2984-2986.	2.5	75
63	Identification of Two Electron-Transfer Sites in Ascorbate Peroxidase Using Chemical Modification, Enzyme Kinetics, and Crystallography. Biochemistry, 1998, 37, 17610-17617.	2.5	74
64	Crystal Structure of Putidaredoxin Reductase from Pseudomonas putida, the Final Structural Component of the Cytochrome P450cam Monooxygenase. Journal of Molecular Biology, 2004, 336, 889-902.	4.2	74
65	Crystal Structure of Cytochrome P450cam Complexed with Its Catalytic Product, 5-exo-Hydroxycamphor. Journal of the American Chemical Society, 1995, 117, 6297-6299.	13.7	72
66	Structural biology of heme monooxygenases. Biochemical and Biophysical Research Communications, 2005, 338, 337-345.	2.1	70
67	Substrate-assisted catalysis in cytochrome P450eryF. Nature Structural Biology, 1996, 3, 632-637.	9.7	69
68	Computer Modeling of Selective Regions in the Active Site of Nitric Oxide Synthases:â€‰ Implication for the Design of Isoform-Selective Inhibitors. Journal of Medicinal Chemistry, 2003, 46, 5700-5711.	6.4	69
69	Holo- and Apo-bound Structures of Bacterial Periplasmic Heme-binding Proteins. Journal of Biological Chemistry, 2007, 282, 35796-35802.	3.4	69
70	Pyridine-Substituted Desoxyritonavir Is a More Potent Inhibitor of Cytochrome P450 3A4 than Ritonavir. Journal of Medicinal Chemistry, 2013, 56, 3733-3741.	6.4	68
71	The Janus nature of heme. Natural Product Reports, 2007, 24, 504.	10.3	66
72	Substrate recognition sites in 14Î±-sterol demethylase from comparative analysis of amino acid sequences and X-ray structure of Mycobacterium tuberculosis CYP51. Journal of Inorganic Biochemistry, 2001, 87, 227-235.	3.5	65

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73	Putidaredoxin-to-Cytochrome P450cam Electron Transfer:Â Differences between the Two Reductive Steps Required for Catalysisâ€. Biochemistry, 2006, 45, 11934-11944.	2.5	65
74	Crystal structure of the pristine peroxidase ferryl center and its relevance to proton-coupled electron transfer. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 1226-1231.	7.1	65
75	[2] Modeling of mammalian P450s on basis of P450cam x-ray structure. Methods in Enzymology, 1991, 206, 11-30.	1.0	64
76	Crystal Structures of the NO- and CO-bound Heme Oxygenase from Neisseriae meningitidis. Journal of Biological Chemistry, 2003, 278, 34654-34659.	3.4	64
77	Electrostatic Control of the Tryptophan Radical in CytochromecPeroxidaseâ€,â€¡. Biochemistry, 2004, 43, 8826-8834.	2.5	61
78	Crystal structure and characterization of a cytochrome c peroxidase-cytochrome c site-specific cross-link. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 5940-5945.	7.1	55
79	Potent, Highly Selective, and Orally Bioavailable <i>Gem</i>-Difluorinated Monocationic Inhibitors of Neuronal Nitric Oxide Synthase. Journal of the American Chemical Society, 2010, 132, 14229-14238.	13.7	55
80	Cytochrome P450: molecular architecture, mechanism, and prospects for rational inhibitor design. Pharmaceutical Research, 1988, 05, 67-75.	3.5	54
81	Preliminary Crystallographic Analysis of Manganese Peroxidase from Phanerochaete chrysosporium. Journal of Molecular Biology, 1994, 238, 845-848.	4.2	54
82	Crystal Structure of the Cytochrome P450cam Mutant That Exhibits the Same Spectral Perturbations Induced by Putidaredoxin Binding. Journal of Biological Chemistry, 2004, 279, 42844-42849.	3.4	54
83	Structures of Cytochrome P450 Enzymes. , 2005, , 87-114.		54
84	Structural studies of constitutive nitric oxide synthases with diatomic ligands bound. Journal of Biological Inorganic Chemistry, 2006, 11, 753-768.	2.6	54
85	Interaction of human cytochrome P4503A4 with ritonavir analogs. Archives of Biochemistry and Biophysics, 2012, 520, 108-116.	3.0	54
86	Crystal Structure of P450cin in a Complex with Its Substrate, 1,8-Cineole, a Close Structural Homologue to d-Camphor, the Substrate for P450cam,. Biochemistry, 2004, 43, 9487-9494.	2.5	53
87	Structural biology of redox partner interactions in P450cam monooxygenase: A fresh look at an old system. Archives of Biochemistry and Biophysics, 2011, 507, 66-74.	3.0	52
88	Structural variation in heme enzymes: a comparative analysis of peroxidase and P450 crystal structures. Structure, 1994, 2, 461-464.	3.3	51
89	Targeting Nitric Oxide Signaling with nNOS Inhibitors As a Novel Strategy for the Therapy and Prevention of Human Melanoma. Antioxidants and Redox Signaling, 2013, 19, 433-447.	5.4	51
90	Crystal Structure of Human Heme Oxygenase-1 in a Complex with Biliverdinâ€. Biochemistry, 2004, 43, 3793-3801.	2.5	50

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91	Unexpected Binding Modes of Nitric Oxide Synthase Inhibitors Effective in the Prevention of a Cerebral Palsy Phenotype in an Animal Model. Journal of the American Chemical Society, 2010, 132, 5437-5442.	13.7	50
92	STRUCTURAL AND FUNCTIONAL DIVERSITY IN HEME MONOOXYGENASES. Drug Metabolism and Disposition, 2005, 33, 10-18.	3.3	49
93	Crystallization of recombinant human heme oxygenaseâ€1. Protein Science, 1998, 7, 1836-1838.	7.6	48
94	Heme-mediated oxygen activation in biology: cytochrome c oxidase and nitric oxide synthase. Current Opinion in Chemical Biology, 1999, 3, 131-137.	6.1	47
95	Replacement of the Distal Glycine 139 Transforms Human Heme Oxygenase-1 into a Peroxidase. Journal of Biological Chemistry, 2000, 275, 34501-34507.	3.4	47
96	Crystal structure and preliminary functional analysis of the cytochrome c peroxidase His175Gln proximal ligand mutant. Journal of the American Chemical Society, 1991, 113, 7755-7757.	13.7	46
97	Probing the CytochromecPeroxidaseâ^'CytochromecElectron Transfer Reaction Using Site Specific Cross-Linkingâ€. Biochemistry, 1996, 35, 4837-4845.	2.5	46
98	The Putidaredoxin Reductase-Putidaredoxin Electron Transfer Complex. Journal of Biological Chemistry, 2005, 280, 16135-16142.	3.4	45
99	Exploration of the Active Site of Neuronal Nitric Oxide Synthase by the Design and Synthesis of Pyrrolidinomethyl 2-Aminopyridine Derivatives. Journal of Medicinal Chemistry, 2010, 53, 7804-7824.	6.4	45
100	Anion-Dependent Stimulation of CYP3A4 Monooxygenase. Biochemistry, 2015, 54, 4083-4096.	2.5	45
101	Conformational selectivity in cytochrome P450 redox partner interactions. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 8723-8728.	7.1	45
102	On the occurrence of cytochrome P450 in viruses. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 12343-12352.	7.1	45
103	The Domain Architecture of Cytochrome P450BM-3. Journal of Biological Chemistry, 1997, 272, 7915-7921.	3.4	43
104	The role of quaternary interactions on the stability and activity of ascorbate peroxidase. Protein Science, 1998, 7, 2089-2098.	7.6	43
105	The Effects of an Engineered Cation Site on the Structure, Activity, and EPR Properties of CytochromecPeroxidaseâ€. Biochemistry, 1999, 38, 5538-5545.	2.5	43
106	Structural and biological studies on bacterial nitric oxide synthase inhibitors. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 18127-18131.	7.1	43
107	Effect of Redox Partner Binding on Cytochrome P450 Conformational Dynamics. Journal of the American Chemical Society, 2017, 139, 13193-13199.	13.7	43
108	Crystallization of Cytochromes P450 and Substrate-Enzyme Interactions. Current Topics in Medicinal Chemistry, 2004, 4, 1789-1802.	2.1	43

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109	Role of the Linker Region Connecting the Reductase and Heme Domains in Cytochrome P450BM-3. Biochemistry, 1995, 34, 11221-11226.	2.5	40
110	The FMN to Heme Electron Transfer in Cytochrome P450BM-3. Journal of Biological Chemistry, 1999, 274, 36097-36106.	3.4	40
111	Role of Zinc in Isoform-Selective Inhibitor Binding to Neuronal Nitric Oxide Synthase,. Biochemistry, 2010, 49, 10803-10810.	2.5	40
112	Simplified 2-Aminoquinoline-Based Scaffold for Potent and Selective Neuronal Nitric Oxide Synthase Inhibition. Journal of Medicinal Chemistry, 2014, 57, 1513-1530.	6.4	40
113	Resonance Raman spectroscopy shows different temperature-dependent coordination equilibria for native horseradish and cytochrome c peroxidase. FEBS Letters, 1985, 190, 221-226.	2.8	39
114	Preliminary crystallographic analysis of an enzyme involved in erythromycin biosynthesis: Cytochrome P450eryF. Proteins: Structure, Function and Bioinformatics, 1994, 20, 197-201.	2.6	39
115	A Novel Heme and Peroxide-dependent Tryptophanâ€“tyrosine Cross-link in a Mutant of Cytochrome c Peroxidase. Journal of Molecular Biology, 2003, 328, 157-166.	4.2	39
116	Crystal structures of ferrous and ferrousâ€“NO forms of verdoheme in a complex with human heme oxygenase-1: catalytic implications for heme cleavage. Journal of Inorganic Biochemistry, 2004, 98, 1686-1695.	3.5	39
117	Structural Basis for Isoform-Selective Inhibition in Nitric Oxide Synthase. Accounts of Chemical Research, 2013, 46, 390-398.	15.6	39
118	Electrostatic Control of Isoform Selective Inhibitor Binding in Nitric Oxide Synthase. Biochemistry, 2016, 55, 3702-3707.	2.5	39
119	Laser Flash Induced Electron Transfer in P450cam Monooxygenase:Â Putidaredoxin Reductaseâˆ'Putidaredoxin Interactionâ€. Biochemistry, 2001, 40, 10592-10600.	2.5	38
120	Symmetric Double-Headed Aminopyridines, a Novel Strategy for Potent and Membrane-Permeable Inhibitors of Neuronal Nitric Oxide Synthase. Journal of Medicinal Chemistry, 2011, 54, 2039-2048.	6.4	38
121	Nitric oxide synthase and structure-based inhibitor design. Nitric Oxide - Biology and Chemistry, 2017, 63, 68-77.	2.7	38
122	Isoform-Selective Substrates of Nitric Oxide Synthase. Journal of Medicinal Chemistry, 2003, 46, 2271-2274.	6.4	37
123	Role of Electrostatics and Salt Bridges in Stabilizing the Compound I Radical in Ascorbate Peroxidaseâ€. Biochemistry, 2005, 44, 14062-14068.	2.5	37
124	Potent and Selective Double-Headed Thiophene-2-carboximidamide Inhibitors of Neuronal Nitric Oxide Synthase for the Treatment of Melanoma. Journal of Medicinal Chemistry, 2014, 57, 686-700.	6.4	37
125	Electron Transfer between the FMN and Heme Domains of Cytochrome P450BM-3. Journal of Biological Chemistry, 1997, 272, 7922-7926.	3.4	35
126	The Critical Role of Substrate-Protein Hydrogen Bonding in the Control of Regioselective Hydroxylation in P450cin. Journal of Biological Chemistry, 2008, 283, 10804-10812.	3.4	35

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127	Intramolecular hydrogen bonding: A potential strategy for more bioavailable inhibitors of neuronal nitric oxide synthase. Bioorganic and Medicinal Chemistry, 2012, 20, 2435-2443.	3.0	35
128	Heme Binding Biguanides Target Cytochrome P450-Dependent Cancer Cell Mitochondria. Cell Chemical Biology, 2017, 24, 1259-1275.e6.	5.2	35
129	Inhibition Mechanisms of Human Indoleamine 2,3 Dioxygenase 1. Journal of the American Chemical Society, 2018, 140, 8518-8525.	13.7	35
130	The homologous tryptophan critical for cytochrome c peroxidase function is not essential for ascorbate peroxidase activity. Journal of Biological Inorganic Chemistry, 1996, 1, 61-66.	2.6	34
131	A study of the K+-site mutant of ascorbate peroxidase: mutations of protein residues on the proximal side of the heme cause changes in iron ligation on the distal side. Journal of Biological Inorganic Chemistry, 1999, 4, 64-72.	2.6	34
132	Electron Transfer between Cytochrome P450cin and Its FMN-containing Redox Partner, Cindoxin. Journal of Biological Chemistry, 2007, 282, 27006-27011.	3.4	34
133	Structural Characterization and Kinetics of Nitric-oxide Synthase Inhibition by Novel N5-(Iminoalkyl)- and N5-(Iminoalkenyl)-ornithines. Journal of Biological Chemistry, 2003, 278, 46789-46797.	3.4	33
134	Intermediates in P450 catalysis. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2005, 363, 793-806.	3.4	33
135	Structures of human constitutive nitric oxide synthases. Acta Crystallographica Section D: Biological Crystallography, 2014, 70, 2667-2674.	2.5	33
136	Structure-based hypothesis on the activation of the CO-sensing transcription factor CooA. Acta Crystallographica Section D: Biological Crystallography, 2007, 63, 282-287.	2.5	32
137	Crystal Structure of Leishmania major Peroxidase and Characterization of the Compound I Tryptophan Radical. Journal of Biological Chemistry, 2011, 286, 24608-24615.	3.4	32
138	Calmodulin activates neuronal nitric oxide synthase by enabling transitions between conformational states. FEBS Letters, 2013, 587, 44-47.	2.8	32
139	Substrate-Dependent Allosteric Regulation in Cytochrome P450cam (CYP101A1). Journal of the American Chemical Society, 2018, 140, 16222-16228.	13.7	32
140	Conversion of an Engineered Potassium-binding Site into a Calcium-selective Site in Cytochrome c Peroxidase. Journal of Biological Chemistry, 1999, 274, 37827-37833.	3.4	31
141	Exploring the Electron Transfer Properties of Neuronal Nitric-oxide Synthase by Reversal of the FMN Redox Potential. Journal of Biological Chemistry, 2008, 283, 34762-34772.	3.4	31
142	Crystal Structure of the Putidaredoxin ReductaseÂ·Putidaredoxin Electron Transfer Complex. Journal of Biological Chemistry, 2010, 285, 13616-13620.	3.4	30
143	Structures of the Neuronal and Endothelial Nitric Oxide Synthase Heme Domain withd-Nitroarginine-Containing Dipeptide Inhibitors Boundâ€. Biochemistry, 2004, 43, 5181-5187.	2.5	29
144	Structure-Based Design and Synthesis ofNÏ‰-Nitro-l-Arginine-Containing Peptidomimetics as Selective Inhibitors of Neuronal Nitric Oxide Synthase. Displacement of the Heme Structural Water. Journal of Medicinal Chemistry, 2007, 50, 2089-2099.	6.4	29

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145	Optimization of Bloodâ€"Brain Barrier Permeability with Potent and Selective Human Neuronal Nitric Oxide Synthase Inhibitors Having a 2-Aminopyridine Scaffold. Journal of Medicinal Chemistry, 2019, 62, 2690-2707.	6.4	29
146	Probing the structure of the linker connecting the reductase and heme domains of cytochrome P450BMâ€3 using siteâ€directed mutagenesis. Protein Science, 1996, 5, 1389-1393.	7.6	28
147	Mapping the active site polarity in structures of endothelial nitric oxide synthase heme domain complexed with isothioureas. Journal of Inorganic Biochemistry, 2000, 81, 133-139.	3.5	28
148	Putidaredoxin Reductase, a New Function for an Old Protein. Journal of Biological Chemistry, 2002, 277, 25831-25839.	3.4	28
149	Nitrile in the Hole: Discovery of a Small Auxiliary Pocket in Neuronal Nitric Oxide Synthase Leading to the Development of Potent and Selective 2-Aminoquinoline Inhibitors. Journal of Medicinal Chemistry, 2017, 60, 3958-3978.	6.4	28
150	Ritonavir Analogues as a Probe for Deciphering the Cytochrome P450 3A4 Inhibitory Mechanism. Current Topics in Medicinal Chemistry, 2014, 14, 1348-1355.	2.1	28
151	Electron transfer in the ruthenated heme domain of cytochrome P450BM-3. Israel Journal of Chemistry, 2000, 40, 47-53.	2.3	27
152	Novel 2,4-Disubstituted Pyrimidines as Potent, Selective, and Cell-Permeable Inhibitors of Neuronal Nitric Oxide Synthase. Journal of Medicinal Chemistry, 2015, 58, 1067-1088.	6.4	27
153	Engineering proteins, subcloning and hyperexpressing oxidoreductase genes. Protein Engineering, Design and Selection, 1991, 4, 701-708.	2.1	26
154	Using Molecular Dynamics To Probe the Structural Basis for Enhanced Stability in Thermal Stable Cytochromes P450. Biochemistry, 2010, 49, 6680-6686.	2.5	26
155	Structures of Cytochrome P450 Enzymes. , 2015, , 3-32.		26
156	Implications for Isoform-selective Inhibitor Design Derived from the Binding Mode of Bulky Isothioureas to the Heme Domain of Endothelial Nitric-oxide Synthase. Journal of Biological Chemistry, 2001, 276, 26486-26491.	3.4	25
157	Structural Basis for Pterin Antagonism in Nitric-oxide Synthase. Journal of Biological Chemistry, 2001, 276, 49133-49141.	3.4	25
158	Structure-Guided Design of Selective Inhibitors of Neuronal Nitric Oxide Synthase. Journal of Medicinal Chemistry, 2013, 56, 3024-3032.	6.4	25
159	Double Barrel Shotgun Scanning of the Caveolin-1 Scaffolding Domain. ACS Chemical Biology, 2007, 2, 493-500.	3.4	24
160	<i>Leishmania major</i> Peroxidase Is a Cytochrome <i>c</i> Peroxidase. Biochemistry, 2012, 51, 2453-2460.	2.5	24
161	Pulsed Electron Paramagnetic Resonance Study of Domain Docking in Neuronal Nitric Oxide Synthase: The Calmodulin and Output State Perspective. Journal of Physical Chemistry A, 2014, 118, 6864-6872.	2.5	24
162	2-Aminopyridines with a Truncated Side Chain To Improve Human Neuronal Nitric Oxide Synthase Inhibitory Potency and Selectivity. Journal of Medicinal Chemistry, 2015, 58, 5548-5560.	6.4	23

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163	Phenyl Ether- and Aniline-Containing 2-Aminoquinolines as Potent and Selective Inhibitors of Neuronal Nitric Oxide Synthase. Journal of Medicinal Chemistry, 2015, 58, 8694-8712.	6.4	23
164	Potent and Selective Human Neuronal Nitric Oxide Synthase Inhibition by Optimization of the 2-Aminopyridine-Based Scaffold with a Pyridine Linker. Journal of Medicinal Chemistry, 2016, 59, 4913-4925.	6.4	23
165	Ligand and Redox Partner Binding Generates a New Conformational State in Cytochrome P450cam (CYP101A1). Journal of the American Chemical Society, 2019, 141, 2678-2683.	13.7	23
166	Reversing enzyme specificity. Nature, 1989, 339, 580-581.	27.8	22
167	Engineering Ascorbate Peroxidase Activity into Cytochrome <i>c</i> Peroxidase. Biochemistry, 2008, 47, 10324-10332.	2.5	22
168	Single Crystal Structural and Absorption Spectral Characterizations of Nitric Oxide Synthase Complexed with <i>N</i>^{Ï‰}-Hydroxy-<scp>l</scp>-arginine and Diatomic Ligands[,]. Biochemistry, 2009, 48, 10246-10254.	2.5	22
169	Crystal Structures and Functional Characterization of Wild-Type CYP101D1 and Its Active Site Mutants. Biochemistry, 2013, 52, 8898-8906.	2.5	22
170	Helping copper find a home. , 1999, 6, 709-711.		21
171	Crystal structure of the <i>Leishmania major</i> peroxidaseâ€"cytochrome <i>c</i> complex. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 18390-18394.	7.1	21
172	Selective Monocationic Inhibitors of Neuronal Nitric Oxide Synthase. Binding Mode Insights from Molecular Dynamics Simulations. Journal of the American Chemical Society, 2012, 134, 11559-11572.	13.7	21
173	Nitric Oxide Synthase Inhibitors That Interact with Both Heme Propionate and Tetrahydrobiopterin Show High Isoform Selectivity. Journal of Medicinal Chemistry, 2014, 57, 4382-4396.	6.4	21
174	Heme-Coordinating Inhibitors of Neuronal Nitric Oxide Synthase. Ironâˆ'Thioether Coordination Is Stabilized by Hydrophobic Contacts without Increased Inhibitor Potency. Journal of the American Chemical Society, 2010, 132, 798-806.	13.7	20
175	Geometric and electronic structures of the Hisâ€"Fe(IV)=O and Hisâ€"Fe(IV)â€"Tyr hemes of MauG. Journal of Biological Inorganic Chemistry, 2012, 17, 1241-1255.	2.6	20
176	Cation-Induced Stabilization of the Engineered Cation-Binding Loop in CytochromecPeroxidase (CcP)â€. Biochemistry, 2002, 41, 2684-2693.	2.5	19
177	Crystal Structures of Constitutive Nitric Oxide Synthases in Complex with De Novo Designed Inhibitors. Journal of Medicinal Chemistry, 2009, 52, 2060-2066.	6.4	19
178	Structure-based design, synthesis, and biological evaluation of lipophilic-tailed monocationic inhibitors of neuronal nitric oxide synthase. Bioorganic and Medicinal Chemistry, 2010, 18, 6526-6537.	3.0	19
179	Crystal Structure of Cindoxin, the P450cin Redox Partner. Biochemistry, 2014, 53, 1435-1446.	2.5	19
180	The Mobility of a Conserved Tyrosine Residue Controls Isoform-Dependent Enzymeâ€"Inhibitor Interactions in Nitric Oxide Synthases. Biochemistry, 2014, 53, 5272-5279.	2.5	19

#	Article	IF	Citations
181	Communication between the Zinc and Tetrahydrobiopterin Binding Sites in Nitric Oxide Synthase. Biochemistry, 2014, 53, 4216-4223.	2.5	19
182	Molecular dynamics of the <scp>P</scp>450camâ€“<scp>P</scp>dx complex reveals complex stability and novel interface contacts. Protein Science, 2015, 24, 49-57.	7.6	19
183	Updating the Paradigm: Redox Partner Binding and Conformational Dynamics in Cytochromes P450. Accounts of Chemical Research, 2022, 55, 373-380.	15.6	19
184	The Effect of the Asn82Asp Mutation in Yeast Cytochrome c Peroxidase Studied by Proton NMR Spectroscopy. FEBS Journal, 1994, 224, 81-87.	0.2	18
185	Regiospecificity Determinants of Human Heme Oxygenase. Journal of Biological Chemistry, 2005, 280, 2797-2806.	3.4	18
186	Exploring the Binding Conformations of Bulkier Dipeptide Amide Inhibitors in Constitutive Nitric Oxide Synthasesâ€. Biochemistry, 2005, 44, 15222-15229.	2.5	18
187	Mechanism of the CO-sensing heme protein CooA: New insights from the truncated heme domain and UVRR spectroscopy. Journal of Inorganic Biochemistry, 2007, 101, 1776-1785.	3.5	18
188	Peripheral but crucial: A hydrophobic pocket (Tyr706, Leu337, and Met336) for potent and selective inhibition of neuronal nitric oxide synthase. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 6258-6261.	2.2	18
189	Effect of DNA Binding on Geminate CO Recombination Kinetics in CO-sensing Transcription Factor CooA. Journal of Biological Chemistry, 2012, 287, 21729-21740.	3.4	18
190	Hydrophilic, Potent, and Selective 7-Substituted 2-Aminoquinolines as Improved Human Neuronal Nitric Oxide Synthase Inhibitors. Journal of Medicinal Chemistry, 2017, 60, 7146-7165.	6.4	18
191	NO news is good news. Structure, 1998, 6, 255-258.	3.3	17
192	Structural Biology of P450-Oxy Complexes. Drug Metabolism Reviews, 2007, 39, 557-566.	3.6	17
193	Synergistic Effects of Mutations in Cytochrome P450cam Designed To Mimic CYP101D1. Biochemistry, 2013, 52, 5396-5402.	2.5	17
194	Elucidating nitric oxide synthase domain interactions by molecular dynamics. Protein Science, 2016, 25, 374-382.	7.6	17
195	The past and present of P450cam structural biology. Biochemical and Biophysical Research Communications, 2003, 312, 35-39.	2.1	16
196	Temperature-Dependent Spin Crossover in Neuronal Nitric Oxide Synthase Bound with the Heme-Coordinating Thioether Inhibitors. Journal of the American Chemical Society, 2011, 133, 8326-8334.	13.7	16
197	Targeting Bacterial Nitric Oxide Synthase with Aminoquinoline-Based Inhibitors. Biochemistry, 2016, 55, 5587-5594.	2.5	16
198	Crystal Structures of Substrate-Free and Nitrosyl Cytochrome P450cin: Implications for O2 Activation. Biochemistry, 2012, 51, 6623-6631.	2.5	15

#	Article	IF	Citations
199	Structure-Based Design of Bacterial Nitric Oxide Synthase Inhibitors. Journal of Medicinal Chemistry, 2015, 58, 994-1004.	6.4	15
200	Nitric Oxide Synthase as a Target for Methicillin-Resistant Staphylococcus aureus. Chemistry and Biology, 2015, 22, 785-792.	6.0	15
201	Structures of gas-generating heme enzymes: Nitric oxide synthase and heme oxygenase. Advances in Inorganic Chemistry, 2000, 51, 243-294.	1.0	14
202	Human Heme Oxygenase Oxidation of 5- and 15-Phenylhemes. Journal of Biological Chemistry, 2004, 279, 42593-42604.	3.4	14
203	Production and Characterization of a Functional Putidaredoxin Reductaseâˆ'Putidaredoxin Covalent Complex. Biochemistry, 2010, 49, 58-67.	2.5	14
204	Cyclopropyl- and methyl-containing inhibitors of neuronal nitric oxide synthase. Bioorganic and Medicinal Chemistry, 2013, 21, 1333-1343.	3.0	14
205	Crystal structure of the Pseudomonas aeruginosa cytoplasmic heme binding protein, Apo-PhuS. Journal of Inorganic Biochemistry, 2013, 128, 131-136.	3.5	14
206	P450cin Active Site Water: Implications for Substrate Binding and Solvent Accessibility. Biochemistry, 2013, 52, 5039-5050.	2.5	14
207	First Contact: 7-Phenyl-2-Aminoquinolines, Potent and Selective Neuronal Nitric Oxide Synthase Inhibitors That Target an Isoform-Specific Aspartate. Journal of Medicinal Chemistry, 2020, 63, 4528-4554.	6.4	14
208	Crystal structures of the G139A, G139A?NO and G143H mutants of human heme oxygenase-1. A finely tuned hydrogen-bonding network controls oxygenase versus peroxidase activity. Journal of Biological Inorganic Chemistry, 2005, 10, 138-146.	2.6	13
209	Accessible Chiral Linker to Enhance Potency and Selectivity of Neuronal Nitric Oxide Synthase Inhibitors. ACS Medicinal Chemistry Letters, 2014, 5, 56-60.	2.8	13
210	Rate of intramolecular reduction of ferryl iron in compound I of cytochrome c peroxidase. Journal of the American Chemical Society, 1990, 112, 7426-7428.	13.7	12
211	Methylated <i>N</i>^{Ï‰}-Hydroxy-<scp>l</scp>-arginine Analogues as Mechanistic Probes for the Second Step of the Nitric Oxide Synthase-Catalyzed Reaction. Biochemistry, 2013, 52, 3062-3073.	2.5	12
212	â€œBind and Crawlâ€•Association Mechanism of <i>Leishmania major</i> Peroxidase and Cytochrome <i>c</i> Revealed by Brownian and Molecular Dynamics Simulations. Biochemistry, 2015, 54, 7272-7282.	2.5	12
213	Conformational Response of N-Terminally Truncated Cytochrome P450 3A4 to Ligand Binding in Solution. Biochemistry, 2019, 58, 3903-3910.	2.5	12
214	Diatomic Ligand Discrimination by the Heme Oxygenases from Neisseria meningitidis and Pseudomonas aeruginosa. Journal of Biological Chemistry, 2007, 282, 1066-1071.	3.4	11
215	Identification of Redox Partners and Development of a Novel Chimeric Bacterial Nitric Oxide Synthase for Structure Activity Analyses. Journal of Biological Chemistry, 2014, 289, 29437-29445.	3.4	11
216	A Comparative Analysis of the Effector Role of Redox Partner Binding in Bacterial P450s. Biochemistry, 2016, 55, 6517-6523.	2.5	11

#	Article	IF	Citations
217	Improvement of Cell Permeability of Human Neuronal Nitric Oxide Synthase Inhibitors Using Potent and Selective 2-Aminopyridine-Based Scaffolds with a Fluorobenzene Linker. Journal of Medicinal Chemistry, 2017, 60, 9360-9375.	6.4	11
218	Chiral linkers to improve selectivity of double-headed neuronal nitric oxide synthase inhibitors. Bioorganic and Medicinal Chemistry Letters, 2013, 23, 5674-5679.	2.2	10
219	The Role of the DNA-Binding Domains in CooA Activationâ€. Biochemistry, 2006, 45, 7148-7153.	2.5	9
220	Structures of P450 Proteins and Their Molecular Phylogeny. , 2007, , 57-96.		9
221	Enzymatic Mechanism of <i>Leishmania major</i> Peroxidase and the Critical Role of Specific Ionic Interactions. Biochemistry, 2015, 54, 3328-3336.	2.5	9
222	Inhibitor Bound Crystal Structures of Bacterial Nitric Oxide Synthase. Biochemistry, 2015, 54, 4075-4082.	2.5	9
223	Mechanistic Studies of Inactivation of Inducible Nitric Oxide Synthase by Amidines. Biochemistry, 2015, 54, 2530-2538.	2.5	9
224	Improved Synthesis of Chiral Pyrrolidine Inhibitors and Their Binding Properties to Neuronal Nitric Oxide Synthase. Journal of Medicinal Chemistry, 2011, 54, 6399-6403.	6.4	8
225	Proton Relay Network in the Bacterial P450s: CYP101A1 and CYP101D1. Biochemistry, 2020, 59, 2896-2902.	2.5	8
226	In search of potent and selective inhibitors of neuronal nitric oxide synthase with more simple structures. Bioorganic and Medicinal Chemistry, 2013, 21, 5323-5331.	3.0	7
227	Combination of chiral linkers with thiophenecarboximidamide heads to improve the selectivity of inhibitors of neuronal nitric oxide synthase. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 4504-4510.	2.2	7
228	The 1.13-Ã… structure of iron-free cytochrome c peroxidase. Journal of Biological Inorganic Chemistry, 2005, 10, 425-430.	2.6	6
229	Hydroxyl-terminated peptidomimetic inhibitors of neuronal nitric oxide synthase. Bioorganic and Medicinal Chemistry, 2006, 14, 3681-3690.	3.0	6
230	Oxygen activation and redox partner binding in cytochromes P450. Biotechnology and Applied Biochemistry, 2013, 60, 128-133.	3.1	6
231	Probing the Hydrogen Bonding of the Ferrousâ€"NO Heme Center of nNOS by Pulsed Electron Paramagnetic Resonance. Journal of Physical Chemistry A, 2015, 119, 6641-6649.	2.5	6
232	Mechanism of Inactivation of Neuronal Nitric Oxide Synthase by (S)-2-Amino-5-(2-(methylthio)acetimidamido)pentanoic Acid. Journal of the American Chemical Society, 2015, 137, 5980-5989.	13.7	6
233	Ultrafast CO Kinetics in Heme Proteins: Adiabatic Ligand Binding and Heavy Atom Tunneling. Journal of the American Chemical Society, 2017, 139, 15738-15747.	13.7	6
234	Insights into the Dynamics and Dissociation Mechanism of a Protein Redox Complex Using Molecular Dynamics. Journal of Chemical Information and Modeling, 2017, 57, 2344-2350.	5.4	6

#	Article	IF	Citations
235	Testing the N-Terminal Velcro Model of CooA Carbon Monoxide Activation. Biochemistry, 2018, 57, 3059-3064.	2.5	6
236	Unexpected Differences between Two Closely Related Bacterial P450 Camphor Monooxygenases. Biochemistry, 2020, 59, 2743-2750.	2.5	6
237	Partial Opening of Cytochrome P450cam (CYP101A1) Is Driven by Allostery and Putidaredoxin Binding. Biochemistry, 2021, 60, 2932-2942.	2.5	6
238	2-Aminopyridines with a shortened amino sidechain as potent, selective, and highly permeable human neuronal nitric oxide synthase inhibitors. Bioorganic and Medicinal Chemistry, 2022, 69, 116878.	3.0	6
239	Coupling crystallography and computational biochemistry in understanding heme enzyme structure and function. International Journal of Quantum Chemistry, 2002, 88, 211-219.	2.0	5
240	Temperature, pH, and solvent isotope effects on cytochrome c peroxidase mutant N82A studied by proton NMR. The Protein Journal, 2000, 19, 535-542.	1.1	4
241	The crystal structure of chloroperoxidase: A heme peroxidase-cytochrome P450 functional hybrid. Journal of Inorganic Biochemistry, 1995, 59, 427.	3.5	3
242	[39] Approaches to crystallizing P450s. Methods in Enzymology, 1996, 272, 358-368.	1.0	3
243	Loop Stability in the Engineered Potassium Binding Site of Cytochrome c Peroxidase. Tetrahedron, 2000, 56, 9471-9475.	1.9	3
244	Polymerase Translocation with Respect to Single-Stranded Nucleic Acid: Looping or Wrapping of Primer around a Poly(A) Polymerase. Structure, 2009, 17, 680-689.	3.3	3
245	Cytochrome P450 Dynamics. , 2014, , 75-94.		3
246	Effect of redox partner binding on CYP101D1 conformational dynamics. Journal of Inorganic Biochemistry, 2018, 183, 179-183.	3.5	3
247	Structural Basis for Isoform Selective Nitric Oxide Synthase Inhibition by Thiophene-2-carboximidamides. Biochemistry, 2018, 57, 6319-6325.	2.5	3
248	Structural Insights on the Conversion of Cytochrome P450 to P420. ACS Omega, 2022, 7, 18481-18485.	3.5	3
249	Dissecting binding of a Î²-barrel membrane protein by phage display. Molecular BioSystems, 2017, 13, 1438-1447.	2.9	2
250	Crystal structure and functional analysis of Leishmania major pseudoperoxidase. Journal of Biological Inorganic Chemistry, 2017, 22, 919-927.	2.6	2
251	Dissecting the kinetics of the NADP+â€"FADH2 charge transfer complex and flavin semiquinones in neuronal nitric oxide synthase. Journal of Inorganic Biochemistry, 2013, 124, 1-10.	3.5	1
252	Domain-level rocking motion within a polymerase that translocates on single-stranded nucleic acid. Acta Crystallographica Section D: Biological Crystallography, 2013, 69, 617-624.	2.5	1

#	Article	IF	Citations
253	Structural analysis of P450 AmphL from Streptomyces nodosus provides insights into substrate selectivity of polyene macrolide antibiotic biosynthetic P450s. Journal of Biological Chemistry, 2022, 298, 101746.	3.4	1
254	1P157 Exploring the Binding Conformations of Bulkier Dipeptide Amide Inhibitors in Constitutive Nitric Oxide Synthases(5. Heme protein,Poster Session,Abstract,Meeting Program of EABS & BSJ 2006). Seibutsu Butsuri, 2006, 46, S186.	0.1	0
255	Neuronal Nitric Oxide Synthase (nNOS)/NO, An Accelerator of Melanoma Progression, is a Potential Target for Chemoprevention. Free Radical Biology and Medicine, 2011, 51, S91-S92.	2.9	0
256	Association Mechanism of Leishmania major Peroxidase and cytochrome c revealed through Brownian and Molecular Dynamics. Biophysical Journal, 2016, 110, 42a.	0.5	0
257	Structureâ€Based Hypothesis on the Activation of the COâ€sensing Transcription Factor CooA. FASEB Journal, 2007, 21, A670.	0.5	0
258	Computational analysis of the tryptophan cation radical energetics in peroxidase Compound I. Journal of Biological Inorganic Chemistry, 2022, 27, 229-237.	2.6	0