Michael J Sutcliffe

List of Publications by Year
in descending order

140 papers	7,437 citations	36303 51 h-index	62596 80 g-index
143 all docs	143 docs citations	143 times ranked	6386 citing authors

#	Article	IF	Citations
1	An automated approach for clustering an ensemble of NMR-derived protein structures into conformationally related subfamilies. Protein Engineering, Design and Selection, 1996, 9, 1063-1065.	2.1	426
2	Crystal structure of a PDZ domain. Nature, 1996, 382, 649-652.	27.8	322
3	Atomic Description of an Enzyme Reaction Dominated by Proton Tunneling. Science, 2006, 312, 237-241.	12.6	304
4	Enzymatic H-Transfer Requires Vibration-Driven Extreme Tunneling. Biochemistry, 1999, 38, 3218-3222.	2.5	245
5	Cytochrome P450 6M2 from the malaria vector Anopheles gambiae metabolizes pyrethroids: Sequential metabolism of deltamethrin revealed. Insect Biochemistry and Molecular Biology, 2011, 41, 492-502.	2.7	217
6	Ligand Binding to Integrin Î±IIbÎ²3 Is Dependent on a MIDAS-like Domain in the Î²3 Subunit. Journal of Biological Chemistry, 1996, 271, 21978-21984.	3.4	161
7	TRAIL Receptor-Selective Mutants Signal to Apoptosis via TRAIL-R1 in Primary Lymphoid Malignancies. Cancer Research, 2005, 65, 11265-11270.	0.9	152
8	Structure of Hen Lysozyme in Solution. Journal of Molecular Biology, 1993, 229, 930-944.	4.2	147
9	A Single Mutation in Cytochrome P450 BM3 Changes Substrate Orientation in a Catalytic Intermediate and the Regiospecificity of Hydroxylationâ€. Biochemistry, 1997, 36, 1567-1572.	2.5	141
10	A new conceptual framework for enzyme catalysis. FEBS Journal, 2002, 269, 3096-3102.	0.2	132
11	The catalytic mechanism of cytochrome P450 BM3 involves a 6 Ã… movement of the bound substrate on reduction. Nature Structural Biology, 1996, 3, 414-417.	9.7	123
12	Extensive conformational sampling in a ternary electron transfer complex. Nature Structural and Molecular Biology, 2003, 10, 219-225.	8.2	112
13	Biodiversity of cytochrome P450 redox systems. Biochemical Society Transactions, 2005, 33, 796-801.	3.4	107
14	Molecular anatomy: Phyletic relationships derived from three-dimensional structures of proteins. Journal of Molecular Evolution, 1990, 30, 43-59.	1.8	103
15	Drug block of the hERG potassium channel: Insight from modeling. Proteins: Structure, Function and Bioinformatics, 2007, 68, 568-580.	2.6	100
16	Kinetic Studies of the Mechanism of Carbonâˆ'Hydrogen Bond Breakage by the Heterotetrameric Sarcosine Oxidase ofArthrobactersp. 1-INâ€. Biochemistry, 2000, 39, 1189-1198.	2.5	98
17	Importance of Barrier Shape in Enzyme-catalyzed Reactions. Journal of Biological Chemistry, 2001, 276, 6234-6242.	3.4	98
18	H-tunneling in the Multiple H-transfers of the Catalytic Cycle of Morphinone Reductase and in the Reductive Half-reaction of the Homologous Pentaerythritol Tetranitrate Reductase. Journal of Biological Chemistry, 2003, 278, 43973-43982.	3.4	98

#	Article	IF	Citations
19	Promoting motions in enzyme catalysis probed by pressure studies of kinetic isotope effects. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 507-512.	7.1	98
20	Definition of the Switch Surface in the Solution Structure of Cdc42Hsâ€,â€¡. Biochemistry, 1997, 36, 8755-8766.	2.5	95
21	Residues Glutamate 216 and Aspartate 301 Are Key Determinants of Substrate Specificity and Product Regioselectivity in Cytochrome P450 2D6. Journal of Biological Chemistry, 2003, 278, 4021-4027.	3.4	93
22	Characterization of inhibitors and substrates of Anopheles gambiae CYP6Z2. Insect Molecular Biology, 2008, 17, 125-135.	2.0	92
23	Drug Binding Interactions in the Inner Cavity of hERG Channels: Molecular Insights from Structure-Activity Relationships of Clofilium and Ibutilide Analogs. Molecular Pharmacology, 2006, 69, 509-519.	2.3	84
24	Extensive Domain Motion and Electron Transfer in the Human Electron Transferring FlavoproteinÂ·Medium Chain Acyl-CoA Dehydrogenase Complex. Journal of Biological Chemistry, 2004, 279, 32904-32912.	3.4	82
25	Evidence To Support the Hypothesis That Promoting Vibrations Enhance the Rate of an Enzyme Catalyzed H-Tunneling Reaction. Journal of the American Chemical Society, 2009, 131, 17072-17073.	13.7	79
26	New insights into enzyme catalysis. Ground state tunnelling driven by protein dynamics. FEBS Journal, 1999, 264, 666-671.	0.2	78
27	Validation of Model of Cytochrome P450 2D6:â€‰ An in Silico Tool for Predicting Metabolism and Inhibition. Journal of Medicinal Chemistry, 2004, 47, 5340-5346.	6.4	78
28	How Do Azoles Inhibit Cytochrome P450 Enzymes? A Density Functional Study. Journal of Physical Chemistry A, 2008, 112, 12911-12918.	2.5	76
29	[23] Protein-ligand interactions: Exchange processes and determination of ligand conformation and protein-ligand contacts. Methods in Enzymology, 1994, 239, 657-700.	1.0	75
30	Deep Tunneling Dominates the Biologically Important Hydride Transfer Reaction from NADH to FMN in Morphinone Reductase. Journal of the American Chemical Society, 2008, 130, 7092-7097.	13.7	75
31	Direct Analysis of Donorâˆ'Acceptor Distance and Relationship to Isotope Effects and the Force Constant for Barrier Compression in Enzymatic H-Tunneling Reactions. Journal of the American Chemical Society, 2010, 132, 11329-11335.	13.7	74
32	Deuterium Isotope Effects during Carbonâ€"Hydrogen Bond Cleavage by Trimethylamine Dehydrogenase. Journal of Biological Chemistry, 2001, 276, 24581-24587.	3.4	70
33	Determination of the solution structures of domains II and III of protein G from Streptococcus by 1H nuclear magnetic resonance. Journal of Molecular Biology, 1992, 228, 1219-1234.	4.2	69
34	Phe120 contributes to the regiospecificity of cytochrome P450 2D6: mutation leads to the formation of a novel dextromethorphan metabolite. Biochemical Journal, 2004, 380, 353-360.	3.7	69
35	Determinants of the substrate specificity of human cytochrome P-450 CYP2D6: design and construction of a mutant with testosterone hydroxylase activity. Biochemical Journal, 1998, 331, 783-792.	3.7	67
36	In Silico Methods for Predicting Ligand Binding Determinants of Cytochromes P450. Current Topics in Medicinal Chemistry, 2004, 4, 1803-1824.	2.1	67

#	Article	IF	Citations
37	The preponderance of P450s in the Mycobacterium tuberculosis genome. Trends in Microbiology, 2006, 14, 220-228.	7.7	67
38	Impact of incorporating the 2C5 crystal structure into comparative models of cytochrome P450 2D6. Proteins: Structure, Function and Bioinformatics, 2002, 49, 216-231.	2.6	66
39	Î±-Secondary Isotope Effects as Probes of â€œTunneling-Readyâ€•Configurations in Enzymatic H-Tunneling:Â Insight from Environmentally Coupled Tunneling Models. Journal of the American Chemical Society, 2006, 128, 14053-14058.	13.7	66
40	Why Is Quinidine an Inhibitor of Cytochrome P450 2D6?. Journal of Biological Chemistry, 2005, 280, 38617-38624.	3.4	63
41	QM/MM Studies Show Substantial Tunneling for the Hydrogen-Transfer Reaction in Methylamine Dehydrogenase. Journal of the American Chemical Society, 2001, 123, 8604-8605.	13.7	62
42	Proton Tunneling in Aromatic Amine Dehydrogenase is Driven by a Short-Range Sub-Picosecond Promoting Vibration:Â Consistency of Simulation and Theory with Experiment. Journal of Physical Chemistry B, 2007, 111, 2631-2638.	2.6	62
43	Hydrogen tunneling in quinoproteins. Archives of Biochemistry and Biophysics, 2004, 428, 41-51.	3.0	59
44	Hydrogen tunnelling in enzyme-catalysed H-transfer reactions: flavoprotein and quinoprotein systems. Philosophical Transactions of the Royal Society B: Biological Sciences, 2006, 361, 1375-1386.	4.0	59
45	IN SILICO AND IN VITRO SCREENING FOR INHIBITION OF CYTOCHROME P450 CYP3A4 BY COMEDICATIONS COMMONLY USED BY PATIENTS WITH CANCER. Drug Metabolism and Disposition, 2006, 34, 534-538.	3.3	58
46	Thermodynamic and Biophysical Characterization of Cytochrome P450 BioI fromBacillus subtilisâ€. Biochemistry, 2004, 43, 12410-12426.	2.5	57
47	Quantum Mechanics/Molecular Mechanics Studies on the Sulfoxidation of Dimethyl Sulfide by Compound I and Compound 0 of Cytochrome P450: Which Is the Better Oxidant?. Journal of Physical Chemistry A, 2009, 113, 11635-11642.	2.5	56
48	Mutagenesis of Morphinone Reductase Induces Multiple Reactive Configurations and Identifies Potential Ambiguity in Kinetic Analysis of Enzyme Tunneling Mechanisms. Journal of the American Chemical Society, 2007, 129, 13949-13956.	13.7	55
49	Enzyme catalysis: over-the-barrier or through-the-barrier?. Trends in Biochemical Sciences, 2000, 25, 405-408.	7.5	54
50	Tunneling and Classical Paths for Proton Transfer in an Enzyme Reaction Dominated by Tunneling:Â Oxidation of Tryptamine by Aromatic Amine Dehydrogenase. Journal of Physical Chemistry B, 2007, 111, 3032-3047.	2.6	53
51	OLDERADO: On-line database of ensemble representatives and domains. Protein Science, 2008, 6, 2628-2630.	7.6	53
52	Barrier Compression Enhances an Enzymatic Hydrogenâ€Transfer Reaction. Angewandte Chemie - International Edition, 2009, 48, 1452-1454.	13.8	52
53	Cysteine Substitution Mutagenesis and the Effects of Methanethiosulfonate Reagents at P2X2 and P2X4 Receptors Support a Core Common Mode of ATP Action at P2X Receptors. Journal of Biological Chemistry, 2008, 283, 20126-20136.	3.4	51
54	Insight into the Mechanism of Inactivation and pH Sensitivity in Potassium Channels from Molecular Dynamics Simulations. Biochemistry, 2008, 47, 7414-7422.	2.5	50

#	Article	IF	Citations
55	Multiple Substrate Binding by Cytochrome P450 3A4: Estimation of the Number of Bound Substrate Molecules. Drug Metabolism and Disposition, 2008, 36, 2136-2144.	3.3	50
56	Solution structure of neuronal bungarotoxin determined by two-dimensional NMR spectroscopy: sequence-specific assignments, secondary structure, and dimer formation. Biochemistry, 1991, 30, 4901-4909.	2.5	48
57	Three-dimensional structure of the RGD-containing neurotoxin homologue dendroaspin. Nature Structural Biology, 1994, 1, 802-807.	9.7	47
58	Comparative modelling of cytochromes P450. Advanced Drug Delivery Reviews, 2002, 54, 385-406.	13.7	47
59	Enzymology takes a quantum leap forward. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2000, 358, 367-386.	3.4	46
60	Proteinâ€“protein interactions. Biochemical Society Transactions, 2010, 38, 875-878.	3.4	45
61	Structural and Biochemical Characterization of Recombinant Wild Type and a C30A Mutant of Trimethylamine Dehydrogenase fromMethylophilus methylotrophus(sp. W3A1)â€‚â€¡. Biochemistry, 2000, 39, 7678-7688.	2.5	44
62	The design and synthesis of novel 3-[2-indol-1-yl-ethyl]-1H-indole derivatives as selective inhibitors of CDK4. Tetrahedron Letters, 2005, 46, 1423-1425.	1.4	44
63	Structure of the Complex of Cdc42Hs with a Peptide Derived from P-21 Activated Kinase,. Biochemistry, 2000, 39, 3963-3971.	2.5	43
64	Barrier Compression and Its Contribution to Both Classical and Quantum Mechanical Aspects of Enzyme Catalysis. Biophysical Journal, 2010, 98, 121-128.	0.5	43
65	Design, synthesis and biological activity of new CDK4-specific inhibitors, based on fascaplysin. Organic and Biomolecular Chemistry, 2006, 4, 787.	2.8	42
66	Molecular mechanisms for drug interactions with hERG that cause long QT syndrome. Expert Opinion on Drug Metabolism and Toxicology, 2006, 2, 81-94.	3.3	41
67	IN SILICO PREDICTION OF DRUG BINDING TO CYP2D6: IDENTIFICATION OF A NEW METABOLITE OF METOCLOPRAMIDE. Drug Metabolism and Disposition, 2006, 34, 1386-1392.	3.3	41
68	Analysis of Classical and Quantum Paths for Deprotonation of Methylamine by Methylamine Dehydrogenase. ChemPhysChem, 2007, 8, 1816-1835.	2.1	41
69	Large-Scale Domain Conformational Change Is Coupled to the Activation of the Coâ€“C Bond in the B₁₂-Dependent Enzyme Ornithine 4,5-Aminomutase: A Computational Study. Journal of the American Chemical Society, 2012, 134, 2367-2377.	13.7	41
70	Representing an ensemble of NMRâ€derived protein structures by a single structure. Protein Science, 1993, 2, 936-944.	7.6	40
71	An Exposed Tyrosine on the Surface of Trimethylamine Dehydrogenase Facilitates Electron Transfer to Electron Transferring Flavoprotein:â€‰ Kinetics of Transfer in Wild-Type and Mutant Complexes. Biochemistry, 1997, 36, 41-48.	2.5	40
72	Activation Gating of hERG Potassium Channels. Journal of Biological Chemistry, 2007, 282, 31972-31981.	3.4	40

#	Article	IF	Citations
73	Identification of the Binding Surface on Cdc42Hs for p21-Activated Kinaseâ€. Biochemistry, 1998, 37, 14030-14037.	2.5	38
74	Amino Acid 305 Determines Catalytic Center Accessibility in CYP3A4â€. Biochemistry, 2000, 39, 4406-4414.	2.5	38
75	Are Environmentally Coupled Enzymatic Hydrogen Tunneling Reactions Influenced by Changes in Solution Viscosity?. Angewandte Chemie - International Edition, 2008, 47, 537-540.	13.8	34
76	Protein Dynamics Enhance Electronic Coupling in Electron Transfer Complexes. Journal of Biological Chemistry, 2001, 276, 34142-34147.	3.4	32
77	Cytochromes P450: novel drug targets in the war against multidrug-resistant Mycobacterium tuberculosis. Biochemical Society Transactions, 2003, 31, 625-630.	3.4	32
78	Î±Arg-237 in Methylophilus methylotrophus (sp. W3A1) Electron-transferring Flavoprotein Affords â^¼200-Millivolt Stabilization of the FAD Anionic Semiquinone and a Kinetic Block on Full Reduction to the Dihydroquinone. Journal of Biological Chemistry, 2001, 276, 20190-20196.	3.4	31
79	Role of conserved Asp293 of cytochrome P450 2C9 in substrate recognition and catalytic activity. Biochemical Journal, 2003, 370, 921-926.	3.7	31
80	New fascaplysin-based CDK4-specific inhibitors: design, synthesis and biological activity. Chemical Communications, 2004, , 1696-1697.	4.1	29
81	The enzyme aromatic amine dehydrogenase induces a substrate conformation crucial for promoting vibration that significantly reduces the effective potential energy barrier to proton transfer. Journal of the Royal Society Interface, 2008, 5, 225-232.	3.4	29
82	CA224, a non-planar analogue of fascaplysin, inhibits Cdk4 but not Cdk2 and arrests cells at G0/G1 inhibiting pRB phosphorylation. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 4272-4278.	2.2	27
83	Pressure Effects on Enzyme-Catalyzed Quantum Tunneling Events Arise from Protein-Specific Structural and Dynamic Changes. Journal of the American Chemical Society, 2012, 134, 9749-9754.	13.7	27
84	Progress in cytochrome P450 active site modeling. Archives of Biochemistry and Biophysics, 2005, 433, 361-368.	3.0	26
85	Optimizing the Michaelis Complex of Trimethylamine Dehydrogenase. Journal of Biological Chemistry, 2001, 276, 42887-42892.	3.4	25
86	The response of the tandem pore potassium channel TASKâ€3 (K_{2P}9.1) to voltage: gating at the cytoplasmic mouth. Journal of Physiology, 2009, 587, 4769-4783.	2.9	25
87	How Does Pressure Affect Barrier Compression and Isotope Effects in an Enzymatic Hydrogen Tunneling Reaction?. Angewandte Chemie - International Edition, 2011, 50, 2129-2132.	13.8	25
88	Engineering the active site of ascorbate peroxidase. FEBS Journal, 2001, 268, 78-85.	0.2	24
89	Role of Active Site Residues and Solvent in Proton Transfer and the Modulation of Flavin Reduction Potential in Bacterial Morphinone Reductase. Journal of Biological Chemistry, 2005, 280, 27103-27110.	3.4	24
90	Chemical, Spectroscopic and Structural Investigation of the Substrate-Binding Site in Ascorbate Peroxidase. FEBS Journal, 1997, 248, 347-354.	0.2	23

#	Article	IF	Citations
91	Spermine Is Fit to Block Inward Rectifier (Kir) Channels. Journal of General Physiology, 2003, 122, 481-484.	1.9	22
92	Inhibition of CYP1A1 by Quassinoids Found in<i>Picrasma excelsa</i>. Planta Medica, 2009, 75, 137-141.	1.3	22
93	Parallel Pathways and Freeâ€Energy Landscapes for Enzymatic Hydride Transfer Probed by Hydrostatic Pressure. ChemBioChem, 2009, 10, 1379-1384.	2.6	22
94	The Role of Tyr-169 of Trimethylamine Dehydrogenase in Substrate Oxidation and Magnetic Interaction between FMN Cofactor and the 4Fe/4S Center. Journal of Biological Chemistry, 1999, 274, 13155-13161.	3.4	21
95	Differential Coupling through Val-344 and Tyr-442 of Trimethylamine Dehydrogenase in Electron Transfer Reactions with Ferricenium Ions and Electron Transferring Flavoproteinâ€. Biochemistry, 2000, 39, 9188-9200.	2.5	21
96	Electron Transfer and Conformational Change in Complexes of Trimethylamine Dehydrogenase and Electron Transferring Flavoprotein. Journal of Biological Chemistry, 2002, 277, 8457-8465.	3.4	21
97	Contribution of conserved glycine residues to ATP action at human P2X1 receptors: mutagenesis indicates that the glycine at position 250 is important for channel function. Journal of Neurochemistry, 2005, 95, 1746-1754.	3.9	21
98	Atomistic insight into the origin of the temperature-dependence of kinetic isotope effects and H-tunnelling in enzyme systems is revealed through combined experimental studies and biomolecular simulation. Biochemical Society Transactions, 2008, 36, 16-21.	3.4	21
99	Driving Force Analysis of Proton Tunnelling Across a Reactivity Series for an Enzymeâ€Substrate Complex. ChemBioChem, 2008, 9, 2839-2845.	2.6	20
100	Introduction. Quantum catalysis in enzymes: beyond the transition state theory paradigm. Philosophical Transactions of the Royal Society B: Biological Sciences, 2006, 361, 1293-1294.	4.0	19
101	Inhibition of cancer cell growth by cyclin dependent kinase 4 inhibitors synthesized based on the structure of fascaplysin. Bioorganic Chemistry, 2006, 34, 287-297.	4.1	18
102	Steroid Recognition by Chloramphenicol Acetyltransferase: Engineering and Structural Analysis of a High Affinity Fusidic Acid Binding Site. Journal of Molecular Biology, 1995, 254, 993-1005.	4.2	17
103	[32] Molecular modeling of ligand-gated ion channels. Methods in Enzymology, 1998, 293, 589-620.	1.0	17
104	Effects of Multiple Ligand Binding on Kinetic Isotope Effects in PQQ-Dependent Methanol Dehydrogenase. Biochemistry, 2003, 42, 3966-3978.	2.5	17
105	Calculating Chemically Accurate Redox Potentials for Engineered Flavoproteins from Classical Molecular Dynamics Free Energy Simulations. Journal of Physical Chemistry A, 2008, 112, 13053-13057.	2.5	17
106	To what extent is capital expenditure in UK higher education meeting the pedagogical needs of staff and students?. Journal of Higher Education Policy and Management, 2016, 38, 477-489.	2.3	17
107	Flavoenzyme catalysed oxidation of amines: roles for flavin and protein-based radicals. Biochemical Society Transactions, 2005, 33, 754-757.	3.4	16
108	New Insights into the Reductive Half-reaction Mechanism of Aromatic Amine Dehydrogenase Revealed by Reaction with Carbinolamine Substrates*. Journal of Biological Chemistry, 2007, 282, 23766-23777.	3.4	16

#	Article	IF	Citations
109	Secondary Kinetic Isotope Effects as Probes of Environmentallyâ€Coupled Enzymatic Hydrogen Tunneling Reactions. ChemPhysChem, 2008, 9, 1536-1539.	2.1	16
110	Solvent as a Probe of Active Site Motion and Chemistry during the Hydrogen Tunnelling Reaction in Morphinone Reductase. ChemPhysChem, 2008, 9, 1875-1881.	2.1	16
111	Probing active site geometry using high pressure and secondary isotope effects in an enzymeâ€catalysed â€˜deepâ€™ Hâ€tunnelling reaction. Journal of Physical Organic Chemistry, 2010, 23, 696-701.	1.9	16
112	Steady-State and Picosecond-Time-Resolved Fluorenscence Studies on the Recombinant Heme Domain of Bacillus megaterium Cytochrome P-450. FEBS Journal, 1997, 244, 361-370.	0.2	15
113	X-ray Scattering Studies of Methylophilus methylotrophus (sp. W3A1) Electron-transferring Flavoprotein. Journal of Biological Chemistry, 2000, 275, 21349-21354.	3.4	15
114	Reductive half-reaction of the H172Q mutant of trimethylamine dehydrogenase: evidence against a carbanion mechanism and assignment of kinetically influential ionizations in the enzymeâ€"substrate complex. Biochemical Journal, 1999, 341, 307-314.	3.7	14
115	Computational studies of enzyme mechanism: linking theory with experiment in the analysis of enzymic H-tunnelling. Physical Chemistry Chemical Physics, 2006, 8, 4510.	2.8	14
116	1H-NMR Assignments and Secondary Structure of Dendroaspin, an RGD-Containing Glycoprotein IIb-IIIa (alphaIIb-beta3) Antagonist with a Neurotoxin Fold. FEBS Journal, 1994, 226, 861-868.	0.2	13
117	Kinetic isotope effects and ligand binding in PQQ-dependent methanol dehydrogenase. Biochemical Journal, 2005, 388, 123-133.	3.7	11
118	NMR Studies of the Mode of Binding of Corepressors and Inducers to Escherichia coli Trp Repressor. FEBS Journal, 1996, 235, 804-813.	0.2	10
119	New insights into the multi-step reaction pathway of the reductive half-reaction catalysed by aromatic amine dehydrogenase: a QM/MM study. Chemical Communications, 2010, 46, 3104.	4.1	10
120	Cysteine Mutagenesis and Homology Modeling of the Ligand-binding Site of a Kainate-binding Protein. Journal of Biological Chemistry, 1999, 274, 37210-37218.	3.4	9
121	Reductive half-reaction of the H172Q mutant of trimethylamine dehydrogenase: evidence against a carbanion mechanism and assignment of kinetically influential ionizations in the enzymeâ€'substrate complex. Biochemical Journal, 1999, 341, 307.	3.7	8
122	Structural Insights Into NMDA Ionotropic Glutamate Receptors via Molecular Modelling. Journal of Molecular Modeling, 2000, 6, 16-25.	1.8	8
123	Quantum Mechanics/Molecular Mechanics Studies on the Mechanism of Action of Cofactor Pyridoxal 5â€²â€Phosphate in Ornithine 4,5â€Aminomutase. Chemistry - A European Journal, 2014, 20, 11390-11401.	3.3	8
124	Relaxation data in NMR structure determination: Model calculations for the lysozyme-Gd3+ complex. Proteins: Structure, Function and Bioinformatics, 1991, 10, 117-129.	2.6	7
125	Assignment of the Vibrational Spectra of Enzyme-Bound Tryptophan Tryptophyl Quinones Using a Combined QM/MM Approach. Journal of Physical Chemistry A, 2010, 114, 1212-1217.	2.5	7
126	Trimethylamine Dehydrogenase and Electron Transferring Flavoprotein. Sub-Cellular Biochemistry, 2000, 35, 145-181.	2.4	6

#	Article	IF	Citations
127	Insights into Drug Metabolism from Modelling Studies of Cytochrome P450-Drug Interactions. Current Topics in Medicinal Chemistry, 2006, 6, 1619-1626.	2.1	6
128	Temperatureâ€dependent study reveals that dynamics of hydrophobic residues plays an important functional role in the mitochondrial Tim9â€"Tim10 complex. Proteins: Structure, Function and Bioinformatics, 2012, 80, 602-615.	2.6	6
129	Model Building Predicts an Additional Conformational Switch when GTP Binds to the CDC42HS Protein. Protein and Peptide Letters, 1994, 1, 84-91.	0.9	6
130	Another turn for Eâ€"F hands. Nature Structural and Molecular Biology, 1994, 1, 209-212.	8.2	4
131	Structure and mechanism of Streptococcal protein G. Biochemical Society Transactions, 1993, 21, 333S-333S.	3.4	3
132	Three-dimensional models of glutamate receptors. Faraday Discussions, 1999, 111, 259-272.	3.2	3
133	In-silico characterization of the effects of phosphorylated tyrosines 86 and 106 on structure and binding of MAL: insight into hyperinflammatory response to infection by the human malaria parasites. Journal of Receptor and Signal Transduction Research, 2011, 31, 53-65.	2.5	2
134	A Copper-Bottomed Trafficking Solution. Structure, 2004, 12, 517-518.	3.3	1
135	Engineering the active site of ascorbate peroxidase. Biochemical Society Transactions, 2001, 29, 105.	3.4	1
136	Topology of the Pore Region of an Inward Rectifier K+ Channel, Kir2.1. Annals of the New York Academy of Sciences, 1999, 868, 414-417.	3.8	0
137	The Design and Synthesis of Novel 3-[2-Indol-1-yl-ethyl]-1H-indole Derivatives as Selective Inhibitors of CDK4.. ChemInform, 2005, 36, no.	0.0	0
138	Hydrogen Tunneling in Enzyme-Catalyzed Hydrogen Transfer: Aspects from Flavoprotein Catalysed Reactions. , 0, , 1341-1359.		0
139	Homology Models Applied to Toxicology. , 0, , 433-468.		0
140	Relationship between protein structure and function: Valuable insight from computational studies. Biochemist, 2004, 26, 13-16.	0.5	0