Matthew Jacobson

List of Publications by Year
in descending order

204	22,661	15466 65	9839 141
papers	citations	h-index	g-index

230	230	230	33398
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Modulating environmental signals to reveal mechanisms and vulnerabilities of cancer persisters. Science Advances, 2022, 8, eabi7711.	4.7	1
2	Synthesis and Screening of Î±-Xylosides in Human Glioblastoma Cells. Molecular Pharmaceutics, 2021, 18, 451-460.	2.3	5
3	The Synthesis and Structural Requirements for Measuring Glucocorticoid Receptor Expression In Vivo with (Â±)-¹¹C-YJH08 PET. Journal of Nuclear Medicine, 2021, 62, 723-731.	2.8	2
4	Mutagenesis, Hydrogenâ€“Deuterium Exchange, and Molecular Docking Investigations Establish the Dimeric Interface of Human Platelet-Type 12-Lipoxygenase. Biochemistry, 2021, 60, 802-812.	1.2	7
5	Matched Targeted Therapy for Pediatric Patients with Relapsed, Refractory, or High-Risk Leukemias: A Report from the LEAP Consortium. Cancer Discovery, 2021, 11, 1424-1439.	7.7	16
6	A Crowding Barrier to Protein Inhibition in Colloidal Aggregates. Journal of Medicinal Chemistry, 2021, 64, 4109-4116.	2.9	7
7	Gasdermin D pore structure reveals preferential release of mature interleukin-1. Nature, 2021, 593, 607-611.	13.7	298
8	Protomer alignment modulates specificity of RNA substrate recognition by Ire1. ELife, 2021, 10, .	2.8	7
9	In Vitro Biosynthetic Pathway Investigations of Neuroprotectin D1 (NPD1) and Protectin DX (PDX) by Human 12-Lipoxygenase, 15-Lipoxygenase-1, and 15-Lipoxygenase-2. Biochemistry, 2021, 60, 1741-1754.	1.2	20
10	Analogs of the Dopamine Metabolite 5,6-Dihydroxyindole Bind Directly to and Activate the Nuclear Receptor Nurr1. ACS Chemical Biology, 2021, 16, 1159-1163.	1.6	9
11	Kinetic and structural investigations of novel inhibitors of human epithelial 15-lipoxygenase-2. Bioorganic and Medicinal Chemistry, 2021, 46, 116349.	1.4	15
12	Docking and mutagenesis studies lead to improved inhibitor development of ML355 for human platelet 12-lipoxygenase. Bioorganic and Medicinal Chemistry, 2021, 46, 116347.	1.4	9
13	Curation of over 10â€‰000 transcriptomic studies to enable data reuse. Database: the Journal of Biological Databases and Curation, 2021, 2021, .	1.4	21
14	Role of Human 15-Lipoxygenase-2 in the Biosynthesis of the Lipoxin Intermediate, 5S,15S-diHpETE, Implicated with the Altered Positional Specificity of Human 15-Lipoxygenase-1. Biochemistry, 2020, 59, 4118-4130.	1.2	14
15	15-Lipoxygenase-1 biosynthesis of 7S,14S-diHDHA implicates 15-lipoxygenase-2 in biosynthesis of resolvin D5. Journal of Lipid Research, 2020, 61, 1087-1103.	2.0	35
16	Synthetic group A streptogramin antibiotics that overcome Vat resistance. Nature, 2020, 586, 145-150.	13.7	63
17	A SARS-CoV-2 protein interaction map reveals targets for drug repurposing. Nature, 2020, 583, 459-468.	13.7	3,542
18	Biosynthesis of the Maresin Intermediate, 13S,14S-Epoxy-DHA, by Human 15-Lipoxygenase and 12-Lipoxygenase and Its Regulation through Negative Allosteric Modulators. Biochemistry, 2020, 59, 1832-1844.	1.2	25

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19	Age- and stress-associated C. elegans granulins impair lysosomal function and induce a compensatory HLH-30/TFEB transcriptional response. PLoS Genetics, 2019, 15, e1008295.	1.5	23
20	ATP-Competitive Inhibitors Midostaurin and Avapritinib Have Distinct Resistance Profiles for Exon 17â€“Mutant KIT. Cancer Research, 2019, 79, 4283-4292.	0.4	21
21	VariCarta: A Comprehensive Database of Harmonized Genomic Variants Found in Autism Spectrum Disorder Sequencing Studies. Autism Research, 2019, 12, 1728-1736.	2.1	23
22	Progranulin Stimulates the In Vitro Maturation of Pro-Cathepsin D at Acidic pH. Journal of Molecular Biology, 2019, 431, 1038-1047.	2.0	52
23	Multi-Granulin Domain Peptides Bind to Pro-Cathepsin D and Stimulate Its Enzymatic Activity More Effectively Than Progranulin in Vitro. Biochemistry, 2019, 58, 2670-2674.	1.2	30
24	Tau repeat regions contain conserved histidine residues that modulate microtubule-binding in response to changes in pH. Journal of Biological Chemistry, 2019, 294, 8779-8790.	1.6	12
25	Crosstalk between RNA Pol II C-Terminal Domain Acetylation and Phosphorylation via RPRD Proteins. Molecular Cell, 2019, 74, 1164-1174.e4.	4.5	22
26	Covalent Modification and Regulation of the Nuclear Receptor Nurr1 by a Dopamine Metabolite. Cell Chemical Biology, 2019, 26, 674-685.e6.	2.5	41
27	Structure-based identification of novel CK2 inhibitors with a linear 2-propenone scaffold as anti-cancer agents. Biochemical and Biophysical Research Communications, 2019, 512, 208-212.	1.0	4
28	Conformational Dynamics of the HIV-Vif Protein Complex. Biophysical Journal, 2019, 116, 1432-1445.	0.2	8
29	Conformational Flexibility of the HIV VIF Protein Complex. Biophysical Journal, 2019, 116, 14a.	0.2	0
30	Probing the Electrostatic and Steric Requirements for Substrate Binding in Human Platelet-Type 12-Lipoxygenase. Biochemistry, 2019, 58, 848-857.	1.2	18
31	Structureâ€based Discovery of Novel CK2Î±â€Binding Cyclic Peptides with Antiâ€cancer Activity. Molecular Informatics, 2019, 38, e1800089.	1.4	5
32	A recurrent kinase domain mutation in PRKCA defines chordoid glioma of the third ventricle. Nature Communications, 2018, 9, 810.	5.8	56
33	High-throughput screen for inhibitors of proteinâ€“protein interactions in a reconstituted heat shock protein 70 (Hsp70) complex. Journal of Biological Chemistry, 2018, 293, 4014-4025.	1.6	28
34	Inhibitor binding mode and allosteric regulation of Na+-glucose symporters. Nature Communications, 2018, 9, 5245.	5.8	35
35	Prediction of enzymatic pathways by integrative pathway mapping. ELife, 2018, 7, .	2.8	30
36	Exploration of Benzothiazole Rhodacyanines as Allosteric Inhibitors of Proteinâ€“Protein Interactions with Heat Shock Protein 70 (Hsp70). Journal of Medicinal Chemistry, 2018, 61, 6163-6177.	2.9	84

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37	Structureâ€“Activity Relationship and Molecular Mechanics Reveal the Importance of Ring Entropy in the Biosynthesis and Activity of a Natural Product. Journal of the American Chemical Society, 2017, 139, 2541-2544.	6.6	43
38	Discovery of GBT440, an Orally Bioavailable R-State Stabilizer of Sickle Cell Hemoglobin. ACS Medicinal Chemistry Letters, 2017, 8, 321-326.	1.3	129
39	Synthesis of the Ca2+-mobilizing messengers NAADP and cADPR by intracellular CD38 enzyme in the mouse heart: Role in Î²-adrenoceptor signaling. Journal of Biological Chemistry, 2017, 292, 13243-13257.	1.6	44
40	Structural Insights into Sodium-Dependent Sugar Transporters and their Inhibition Mechanism. Biophysical Journal, 2017, 112, 128a.	0.2	2
41	Evolutionarily Conserved Roles for Blood-Brain Barrier Xenobiotic Transporters in Endogenous Steroid Partitioning and Behavior. Cell Reports, 2017, 21, 1304-1316.	2.9	48
42	Development of 5N-Bicalutamide, a High-Affinity Reversible Covalent Antiandrogen. ACS Chemical Biology, 2017, 12, 2934-2939.	1.6	11
43	Discovery of Potent and Orally Bioavailable Macrocyclic Peptideâ€“Peptoid Hybrid CXCR7 Modulators. Journal of Medicinal Chemistry, 2017, 60, 9653-9663.	2.9	54
44	Cancer-associated arginine-to-histidine mutations confer a gain in pH sensing to mutant proteins. Science Signaling, 2017, 10, .	1.6	54
45	Prominent features of the amino acid mutation landscape in cancer. PLoS ONE, 2017, 12, e0183273.	1.1	26
46	Structure-Bioactivity Relationship for Benzimidazole Thiophene Inhibitors of Polo-Like Kinase 1 (PLK1), a Potential Drug Target in Schistosoma mansoni. PLoS Neglected Tropical Diseases, 2016, 10, e0004356.	1.3	56
47	Disulfide-Trapping Identifies a New, Effective Chemical Probe for Activating the Nuclear Receptor Human LRH-1 (NR5A2). PLoS ONE, 2016, 11, e0159316.	1.1	12
48	Simple Predictive Models of Passive Membrane Permeability Incorporating Size-Dependent Membrane-Water Partition. Journal of Chemical Information and Modeling, 2016, 56, 924-929.	2.5	45
49	GluA1 signal peptide determines the spatial assembly of heteromeric AMPA receptors. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E5645-54.	3.3	13
50	Human 15-LOX-1 active site mutations alter inhibitor binding and decrease potency. Bioorganic and Medicinal Chemistry, 2016, 24, 5380-5387.	1.4	4
51	Exhaustive Conformational Sampling of Complex Fused Ring Macrocycles Using Inverse Kinematics. Journal of Chemical Theory and Computation, 2016, 12, 4674-4687.	2.3	54
52	Assignment of function to a domain of unknown function: DUF1537 is a new kinase family in catabolic pathways for acid sugars. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E4161-9.	3.3	46
53	Dihedral Angle-Based Sampling of Natural Product Polyketide Conformations: Application to Permeability Prediction. Journal of Chemical Information and Modeling, 2016, 56, 2194-2206.	2.5	12
54	Investigating HIV Vif Interactions with Host Proteins. Biophysical Journal, 2016, 110, 384a.	0.2	0

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55	A potent and selective inhibitor targeting human and murine 12/15-LOX. Bioorganic and Medicinal Chemistry, 2016, 24, 1183-1190.	1.4	15
56	Structure-Based Drug Design for Sodium-Dependent Glucose Transporters. Biophysical Journal, 2016, 110, 136a.	0.2	0
57	Non-degradative Ubiquitination of Protein Kinases. PLoS Computational Biology, 2016, 12, e1004898.	1.5	31
58	Defining the Product Chemical Space of Monoterpenoid Synthases. PLoS Computational Biology, 2016, 12, e1005053.	1.5	26
59	A Computational Model for E. coli Cytoplasm: Diffusion and Hydrodynamics. Biophysical Journal, 2015, 108, 116a-117a.	0.2	0
60	Probing the Physicochemical Boundaries of Cell Permeability and Oral Bioavailability in Lipophilic Macrocycles Inspired by Natural Products. Journal of Medicinal Chemistry, 2015, 58, 4581-4589.	2.9	112
61	Peptide to Peptoid Substitutions Increase Cell Permeability in Cyclic Hexapeptides. Organic Letters, 2015, 17, 2928-2931.	2.4	71
62	Cell-Permeable Cyclic Peptides from Synthetic Libraries Inspired by Natural Products. Journal of the American Chemical Society, 2015, 137, 715-721.	6.6	186
63	Experimental Strategies for Functional Annotation and Metabolism Discovery: Targeted Screening of Solute Binding Proteins and Unbiased Panning of Metabolomes. Biochemistry, 2015, 54, 909-931.	1.2	95
64	A Unique cis-3-Hydroxy-<scp>l</scp>-proline Dehydratase in the Enolase Superfamily. Journal of the American Chemical Society, 2015, 137, 1388-1391.	6.6	13
65	Computational-guided discovery and characterization of a sesquiterpene synthase from Streptomyces clavuligerus. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 5661-5666.	3.3	42
66	A Fragment-Based Ligand Screen Against Part of a Large Protein Machine: The ND1 Domains of the AAA+ ATPase p97/VCP. Journal of Biomolecular Screening, 2015, 20, 788-800.	2.6	14
67	Synthesis and Enzymatic Studies of Bisubstrate Analogues for Farnesyl Diphosphate Synthase. Journal of Organic Chemistry, 2015, 80, 3902-3913.	1.7	3
68	Beyond cyclosporine A: conformation-dependent passive membrane permeabilities of cyclic peptide natural products. Future Medicinal Chemistry, 2015, 7, 2121-2130.	1.1	140
69	A Structure-Based Model for Predicting Serum Albumin Binding. PLoS ONE, 2014, 9, e93323.	1.1	61
70	The Free Energy Profile of Tubulin Straight-Bent Conformational Changes, with Implications for Microtubule Assembly and Drug Discovery. PLoS Computational Biology, 2014, 10, e1003464.	1.5	35
71	Correction to â€œDesign of Reversible, Cysteine-Targeted Michael Acceptors Guided by Kinetic and Computational Analysisâ€. Journal of the American Chemical Society, 2014, 136, 17690-17690.	6.6	1
72	Prediction and Biochemical Demonstration of a Catabolic Pathway for the Osmoprotectant Proline Betaine. MBio, 2014, 5, e00933-13.	1.8	19

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73	Predicting the Functions and Specificity of Triterpenoid Synthases: A Mechanism-Based Multi-intermediate Docking Approach. PLoS Computational Biology, 2014, 10, e1003874.	1.5	23
74	Novel compounds lowering the cellular isoform of the human prion protein in cultured human cells. Bioorganic and Medicinal Chemistry, 2014, 22, 1960-1972.	1.4	24
75	Design of Reversible, Cysteine-Targeted Michael Acceptors Guided by Kinetic and Computational Analysis. Journal of the American Chemical Society, 2014, 136, 12624-12630.	6.6	204
76	Leveraging structure for enzyme function prediction: methods, opportunities, and challenges. Trends in Biochemical Sciences, 2014, 39, 363-371.	3.7	31
77	A comparative Brownian dynamics investigation between small linear and circular DNA: Scaling of diffusion coefficient with size and topology of DNA. Chemical Physics Letters, 2014, 591, 253-258.	1.2	4
78	Evolution of Enzymatic Activities in the Enolase Superfamily: Galactarate Dehydratase III from Agrobacterium tumefaciens C58. Biochemistry, 2014, 53, 4192-4203.	1.2	15
79	Prediction of Substrates for Glutathione Transferases by Covalent Docking. Journal of Chemical Information and Modeling, 2014, 54, 1687-1699.	2.5	20
80	A High Throughput Screen Identifies Potent and Selective Inhibitors to Human Epithelial 15-Lipoxygenase-2. PLoS ONE, 2014, 9, e104094.	1.1	18
81	A New Coarse-Grained Model for E. coli Cytoplasm: Accurate Calculation of the Diffusion Coefficient of Proteins and Observation of Anomalous Diffusion. PLoS ONE, 2014, 9, e106466.	1.1	34
82	Prediction and characterization of enzymatic activities guided by sequence similarity and genome neighborhood networks. ELife, 2014, 3, .	2.8	81
83	Predicting Enzymeâ€“Substrate Specificity with QM/MM Methods: A Case Study of the Stereospecificity of <scp>d</scp>-Glucarate Dehydratase. Biochemistry, 2013, 52, 5511-5513.	1.2	6
84	Design of a Phosphorylatable PDZ Domain with Peptide-Specific Affinity Changes. Structure, 2013, 21, 54-64.	1.6	17
85	A Cysteine Protease Inhibitor Rescues Mice from a Lethal Cryptosporidium parvum Infection. Antimicrobial Agents and Chemotherapy, 2013, 57, 6063-6073.	1.4	52
86	pH sensing by FAK-His58 regulates focal adhesion remodeling. Journal of Cell Biology, 2013, 202, 849-859.	2.3	79
87	SIRT5 Regulates the Mitochondrial Lysine Succinylome and Metabolic Networks. Cell Metabolism, 2013, 18, 920-933.	7.2	549
88	Discovery of new enzymes and metabolic pathways by using structure and genome context. Nature, 2013, 502, 698-702.	13.7	124
89	Active Site Conformational Dynamics Are Coupled to Catalysis in the mRNA Decapping Enzyme Dcp2. Structure, 2013, 21, 1571-1580.	1.6	23
90	Pharmacokinetics and Metabolism of 2-Aminothiazoles with Antiprion Activity in Mice. Pharmaceutical Research, 2013, 30, 932-950.	1.7	29

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91	Predicting Efflux Ratios and Blood-Brain Barrier Penetration from Chemical Structure: Combining Passive Permeability with Active Efflux by P-Glycoprotein. ACS Chemical Neuroscience, 2013, 4, 361-367.	1.7	29
92	2â€Aminothiazoles with Improved Pharmacotherapeutic Properties for Treatment of Prion Disease. ChemMedChem, 2013, 8, 847-857.	1.6	20
93	Considering Protonation as a Posttranslational Modification Regulating Protein Structure and Function. Annual Review of Biophysics, 2013, 42, 289-314.	4.5	133
94	Structure-guided discovery of the metabolite carboxy-SAM that modulates tRNA function. Nature, 2013, 498, 123-126.	13.7	84
95	Antiprion compounds that reduce PrPSc levels in dividing and stationary-phase cells. Bioorganic and Medicinal Chemistry, 2013, 21, 7999-8012.	1.4	17
96	Substrate and Inhibitor-induced Dimerization and Cooperativity in Caspase-1 but Not Caspase-3. Journal of Biological Chemistry, 2013, 288, 9971-9981.	1.6	39
97	Prediction of function for the polyprenyl transferase subgroup in the isoprenoid synthase superfamily. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, E1196-202.	3.3	75
98	Biaryl Amides and Hydrazones as Therapeutics for Prion Disease in Transgenic Mice. Journal of Pharmacology and Experimental Therapeutics, 2013, 347, 325-338.	1.3	41
99	Chemicalâ€“biological characterization of a cruzain inhibitor reveals a second target and a mammalian off-target. Beilstein Journal of Organic Chemistry, 2013, 9, 15-25.	1.3	34
100	Editorial (Hot Topic:Designing Molecules to Cross Biological Membranes). Current Topics in Medicinal Chemistry, 2013, 13, 775-775.	1.0	3
101	In Silico Prediction of Brain Exposure: Drug Free Fraction, Unbound Brain to Plasma Concentration Ratio and Equilibrium Half-Life. Current Topics in Medicinal Chemistry, 2013, 13, 813-820.	1.0	28
102	Investigation of the Proteolytic Functions of an Expanded Cercarial Elastase Gene Family in Schistosoma mansoni. PLoS Neglected Tropical Diseases, 2012, 6, e1589.	1.3	37
103	Multisite Phosphorylation Disrupts Arginine-Glutamate Salt Bridge Networks Required for Binding of Cytoplasmic Linker-associated Protein 2 (CLASP2) to End-binding Protein 1 (EB1). Journal of Biological Chemistry, 2012, 287, 17050-17064.	1.6	89
104	Divergent Evolution in Enolase Superfamily: Strategies for Assigning Functions. Journal of Biological Chemistry, 2012, 287, 29-34.	1.6	118
105	Optimizing PK properties of cyclic peptides: the effect of side chain substitutions on permeability and clearance. MedChemComm, 2012, 3, 1282-1289.	3.5	120
106	Computer-aided antibody design. Protein Engineering, Design and Selection, 2012, 25, 507-522.	1.0	203
107	Homology models guide discovery of diverse enzyme specificities among dipeptide epimerases in the enolase superfamily. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 4122-4127.	3.3	56
108	Predicting and Improving the Membrane Permeability of Peptidic Small Molecules. Journal of Medicinal Chemistry, 2012, 55, 3163-3169.	2.9	96

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109	Comparing Conformational Ensembles Using the Kullbackâ€“Leibler Divergence Expansion. Journal of Chemical Theory and Computation, 2012, 8, 2115-2126.	2.3	74
110	Testing Physical Models of Passive Membrane Permeation. Journal of Chemical Information and Modeling, 2012, 52, 1621-1636.	2.5	100
111	Assessing Protein Loop Flexibility by Hierarchical Monte Carlo Sampling. Journal of Chemical Theory and Computation, 2011, 7, 1564-1574.	2.3	22
112	The Enzyme Function Initiative. Biochemistry, 2011, 50, 9950-9962.	1.2	169
113	A Molecular Mechanics Approach to Modeling Proteinâ€“Ligand Interactions: Relative Binding Affinities in Congeneric Series. Journal of Chemical Information and Modeling, 2011, 51, 2082-2089.	2.5	50
114	Dysregulated pH: a perfect storm for cancer progression. Nature Reviews Cancer, 2011, 11, 671-677.	12.8	1,734
115	On-resin N-methylation of cyclic peptides for discovery of orally bioavailable scaffolds. Nature Chemical Biology, 2011, 7, 810-817.	3.9	318
116	Effects of somatic mutations on CDR loop flexibility during affinity maturation. Proteins: Structure, Function and Bioinformatics, 2011, 79, 821-829.	1.5	43
117	Assessment of protein structure refinement in CASP9. Proteins: Structure, Function and Bioinformatics, 2011, 79, 74-90.	1.5	87
118	Turning a protein kinase on or off from a single allosteric site via disulfide trapping. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 6056-6061.	3.3	134
119	Phosphorylation of the Arp2 Subunit Relieves Auto-inhibitory Interactions for Arp2/3 Complex Activation. PLoS Computational Biology, 2011, 7, e1002226.	1.5	21
120	A New View of the Bacterial Cytosol Environment. PLoS Computational Biology, 2011, 7, e1002066.	1.5	39
121	Predicting Binding to P-Glycoprotein by Flexible Receptor Docking. PLoS Computational Biology, 2011, 7, e1002083.	1.5	90
122	Antibodies as a model system for comparative model refinement. Proteins: Structure, Function and Bioinformatics, 2010, 78, 2490-2505.	1.5	15
123	Structural Characterization of CYP51 from Trypanosoma cruzi and Trypanosoma brucei Bound to the Antifungal Drugs Posaconazole and Fluconazole. PLoS Neglected Tropical Diseases, 2010, 4, e651.	1.3	106
124	Modeling Conformational Ensembles of Slow Functional Motions in Pin1-WW. PLoS Computational Biology, 2010, 6, e1001015.	1.5	76
125	Molecular Dynamics Simulations Predict A pH-Dependent Conformational Change in the C-Helix of Cell Cycle Checkpoint Kinase Wee1. Biophysical Journal, 2010, 98, 232a.	0.2	0
126	A Nonazole CYP51 Inhibitor Cures Chagasâ€™ Disease in a Mouse Model of Acute Infection. Antimicrobial Agents and Chemotherapy, 2010, 54, 2480-2488.	1.4	56

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127	Studying Enzymeâ"Substrate Specificity in Silico: A Case Study of the Escherichia coli Glycolysis Pathway. Biochemistry, 2010, 49, 4003-4005.	1.2	18
128	Transcriptional Control of a Plant Stem Cell Niche. Developmental Cell, 2010, 18, 841-853.	3.1	221
129	Conformation Switching of Clathrin Light Chain Regulates Clathrin Lattice Assembly. Developmental Cell, 2010, 18, 854-861.	3.1	72
130	SIRT3 Deacetylates Mitochondrial 3-Hydroxy-3-Methylglutaryl CoA Synthase 2 and Regulates Ketone Body Production. Cell Metabolism, 2010, 12, 654-661.	7.2	418
131	Binding-Site Assessment by Virtual Fragment Screening. PLoS ONE, 2010, 5, e10109.	1.1	56
132	Computational studies of protein regulation by post-translational phosphorylation. Current Opinion in Structural Biology, 2009, 19, 156-163.	2.6	72
133	Target selection and annotation for the structural genomics of the amidohydrolase and enolase superfamilies. Journal of Structural and Functional Genomics, 2009, 10, 107-125.	1.2	25
134	Automated site preparation in physicsâ€based rescoring of receptor ligand complexes. Proteins: Structure, Function and Bioinformatics, 2009, 77, 52-61.	1.5	22
135	Assessment of the proteinâ€structure refinement category in CASP8. Proteins: Structure, Function and Bioinformatics, 2009, 77, 66-80.	1.5	65
136	Improving the species cross-reactivity of an antibody using computational design. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 3744-3747.	1.0	46
137	Monte Carlo Sampling with Hierarchical Move Sets: POSH Monte Carlo. Journal of Chemical Theory and Computation, 2009, 5, 1968-1984.	2.3	10
138	The Molecular Basis of Species-Specific Ligand Activation of Trace Amine-Associated Receptor 1 (TAAR₁). ACS Chemical Biology, 2009, 4, 209-220.	1.6	41
139	Computation-Facilitated Assignment of the Function in the Enolase Superfamily: A Regiochemically Distinct Galactarate Dehydratase from Oceanobacillus iheyensis,. Biochemistry, 2009, 48, 11546-11558.	1.2	32
140	Quantifying Correlations Between Allosteric Sites in Thermodynamic Ensembles. Journal of Chemical Theory and Computation, 2009, 5, 2486-2502.	2.3	203
141	Energy-Based Analysis and Prediction of the Orientation between Light- and Heavy-Chain Antibody Variable Domains. Journal of Molecular Biology, 2009, 388, 941-953.	2.0	41
142	The role of homology models in assigning enzyme function. FASEB Journal, 2009, 23, 204.2.	0.2	0
143	Conformational selection in silico: Loop latching motions and ligand binding in enzymes. Proteins: Structure, Function and Bioinformatics, 2008, 71, 153-164.	1.5	22
144	Toward better refinement of comparative models: Predicting loops in inexact environments. Proteins: Structure, Function and Bioinformatics, 2008, 72, 959-971.	1.5	80

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145	Toward Deciphering the Code to Aminergic G Protein-Coupled Receptor Drug Design. Chemistry and Biology, 2008, 15, 343-353.	6.2	35
146	Discovery of a Dipeptide Epimerase Enzymatic Function Guided by Homology Modeling and Virtual Screening. Structure, 2008, 16, 1668-1677.	1.6	52
147	Rescoring Docking Hit Lists for Model Cavity Sites: Predictions and Experimental Testing. Journal of Molecular Biology, 2008, 377, 914-934.	2.0	168
148	Multiscale Monte Carlo Sampling of Protein Sidechains: Application to Binding Pocket Flexibility. Journal of Chemical Theory and Computation, 2008, 4, 835-846.	2.3	14
149	Structural model and functional significance of pH-dependent talinâ€“actin binding for focal adhesion remodeling. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 14436-14441.	3.3	115
150	Cofilin is a pH sensor for actin free barbed end formation: role of phosphoinositide binding. Journal of Cell Biology, 2008, 183, 865-879.	2.3	169
151	Intracellular pH Sensors: Design Principles and Functional Significance. Physiology, 2007, 22, 30-39.	1.6	212
152	Multiscale Optimization of a Truncated Newton Minimization Algorithm and Application to Proteins and Proteinâ^'Ligand Complexes. Journal of Chemical Theory and Computation, 2007, 3, 640-648.	2.3	29
153	Strengths of Hydrogen Bonds Involving Phosphorylated Amino Acid Side Chains. Journal of the American Chemical Society, 2007, 129, 820-827.	6.6	119
154	Intramolecular Dynamics in the Frequency Domain. Advances in Chemical Physics, 2007, , 463-490.	0.3	7
155	Prediction of side-chain conformations on protein surfaces. Proteins: Structure, Function and Bioinformatics, 2007, 66, 814-823.	1.5	31
156	Prediction and assignment of function for a divergent N-succinyl amino acid racemase. Nature Chemical Biology, 2007, 3, 486-491.	3.9	98
157	An atomistic model of passive membrane permeability: application to a series of FDA approved drugs. Journal of Computer-Aided Molecular Design, 2007, 21, 675-679.	1.3	18
158	Physics-based methods for studying protein-ligand interactions. Current Opinion in Drug Discovery & Development, 2007, 10, 325-31.	1.9	23
159	Testing the Conformational Hypothesis of Passive Membrane Permeability Using Synthetic Cyclic Peptide Diastereomers. Journal of the American Chemical Society, 2006, 128, 2510-2511.	6.6	415
160	Physics-Based Scoring of Proteinâ^'Ligand Complexes:Â Enrichment of Known Inhibitors in Large-Scale Virtual Screening. Journal of Chemical Information and Modeling, 2006, 46, 243-253.	2.5	149
161	Molecular mechanics methods for predicting proteinâ€“ligand binding. Physical Chemistry Chemical Physics, 2006, 8, 5166-5177.	1.3	200
162	Novel Procedure for Modeling Ligand/Receptor Induced Fit Effects. Journal of Medicinal Chemistry, 2006, 49, 534-553.	2.9	1,671

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163	Conformational Flexibility, Internal Hydrogen Bonding, and Passive Membrane Permeability:Â Successful in Silico Prediction of the Relative Permeabilities of Cyclic Peptides. Journal of the American Chemical Society, 2006, 128, 14073-14080.	6.6	342
164	Novel Human Lipoxygenase Inhibitors Discovered Using Virtual Screening with Homology Models. Journal of Medicinal Chemistry, 2006, 49, 1356-1363.	2.9	81
165	Evolution of Structure and Function in the o-Succinylbenzoate Synthase/N-Acylamino Acid Racemase Family of the Enolase Superfamily. Journal of Molecular Biology, 2006, 360, 228-250.	2.0	65
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