Matthew Jacobson

List of Publications by Year in Descending Order

198 papers	16,919 citations	60 h-index	127 g-index
230 ext. papers	20,149 ext. citations	7.2 avg, IF	6.43 L-index

#	Paper	IF	Citations
198	Modulating environmental signals to reveal mechanisms and vulnerabilities of cancer persisters.. *Science Advances*, **2022**, 8, eabi7711	14.3	
197	Gasdermin D pore structure reveals preferential release of mature interleukin-1. *Nature*, **2021**, 593, 607-611	50.4	92
196	Protomer alignment modulates specificity of RNA substrate recognition by Ire1. *ELife*, **2021**, 10,	8.9	3
195	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	3.2	3
194	Analogs of the Dopamine Metabolite 5,6-Dihydroxyindole Bind Directly to and Activate the Nuclear Receptor Nurr1. *ACS Chemical Biology*, **2021**, 16, 1159-1163	4.9	3
193	Synthesis and Screening of □-Xylosides in Human Glioblastoma Cells. *Molecular Pharmaceutics*, **2021**, 18, 451-460	5.6	3
192	The Synthesis and Structural Requirements for Measuring Glucocorticoid Receptor Expression In Vivo with (□)-C-YJH08 PET. *Journal of Nuclear Medicine*, **2021**, 62, 723-731	8.9	1
191	Mutagenesis, Hydrogen-Deuterium Exchange, and Molecular Docking Investigations Establish the Dimeric Interface of Human Platelet-Type 12-Lipoxygenase. *Biochemistry*, **2021**, 60, 802-812	3.2	1
190	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	24.4	4
189	A Crowding Barrier to Protein Inhibition in Colloidal Aggregates. *Journal of Medicinal Chemistry*, **2021**, 64, 4109-4116	8.3	3
188	Kinetic and structural investigations of novel inhibitors of human epithelial 15-lipoxygenase-2. *Bioorganic and Medicinal Chemistry*, **2021**, 46, 116349	3.4	1
187	Docking and mutagenesis studies lead to improved inhibitor development of ML355 for human platelet 12-lipoxygenase. *Bioorganic and Medicinal Chemistry*, **2021**, 46, 116347	3.4	2
186	Curation of over 10 000 transcriptomic studies to enable data reuse. *Database: the Journal of Biological Databases and Curation*, **2021**, 2021,	5	7
185	A SARS-CoV-2 protein interaction map reveals targets for drug repurposing. *Nature*, **2020**, 583, 459-468	50.4	2142
184	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	3.2	13
183	A SARS-CoV-2-Human Protein-Protein Interaction Map Reveals Drug Targets and Potential Drug-Repurposing **2020**,		133
182	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	3.2	5

181	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	6.3	14
180	Synthetic group A streptogramin antibiotics that overcome Vat resistance. *Nature*, **2020**, 586, 145-150	50.4	27
179	Progranulin Stimulates the In Vitro Maturation of Pro-Cathepsin D at Acidic pH. *Journal of Molecular Biology*, **2019**, 431, 1038-1047	6.5	27
178	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	3.2	17
177	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	5.4	8
176	Crosstalk between RNA Pol II C-Terminal Domain Acetylation and Phosphorylation via RPRD Proteins. *Molecular Cell*, **2019**, 74, 1164-1174.e4	17.6	12
175	Covalent Modification and Regulation of the Nuclear Receptor Nurr1 by a Dopamine Metabolite. *Cell Chemical Biology*, **2019**, 26, 674-685.e6	8.2	23
174	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	3.4	3
173	Conformational Dynamics of the HIV-Vif Protein Complex. *Biophysical Journal*, **2019**, 116, 1432-1445	2.9	4
172	Age- and stress-associated C. elegans granulins impair lysosomal function and induce a compensatory HLH-30/TFEB transcriptional response. *PLoS Genetics*, **2019**, 15, e1008295	6	11
171	ATP-Competitive Inhibitors Midostaurin and Avapritinib Have Distinct Resistance Profiles in Exon 17-Mutant KIT. *Cancer Research*, **2019**, 79, 4283-4292	10.1	13
170	VariCarta: A Comprehensive Database of Harmonized Genomic Variants Found in Autism Spectrum Disorder Sequencing Studies. *Autism Research*, **2019**, 12, 1728-1736	5.1	11
169	Probing the Electrostatic and Steric Requirements for Substrate Binding in Human Platelet-Type 12-Lipoxygenase. *Biochemistry*, **2019**, 58, 848-857	3.2	9
168	Structure-based Discovery of Novel CK2-Binding Cyclic Peptides with Anti-cancer Activity. *Molecular Informatics*, **2019**, 38, e1800089	3.8	3
167	A recurrent kinase domain mutation in PRKCA defines chordoid glioma of the third ventricle. *Nature Communications*, **2018**, 9, 810	17.4	42
166	High-throughput screen for inhibitors of protein-protein interactions in a reconstituted heat shock protein 70 (Hsp70) complex. *Journal of Biological Chemistry*, **2018**, 293, 4014-4025	5.4	24
165	Inhibitor binding mode and allosteric regulation of Na-glucose symporters. *Nature Communications*, **2018**, 9, 5245	17.4	19
164	Prediction of enzymatic pathways by integrative pathway mapping. *ELife*, **2018**, 7,	8.9	22

163	Exploration of Benzothiazole Rhodacyanines as Allosteric Inhibitors of Protein-Protein Interactions with Heat Shock Protein 70 (Hsp70). *Journal of Medicinal Chemistry*, **2018**, 61, 6163-6177	8.3	54
162	Structure-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	16.4	36
161	Discovery of GBT440, an Orally Bioavailable R-State Stabilizer of Sickle Cell Hemoglobin. *ACS Medicinal Chemistry Letters*, **2017**, 8, 321-326	4.3	76
160	Synthesis of the Ca-mobilizing messengers NAADP and cADPR by intracellular CD38 enzyme in the mouse heart: Role in β-adrenoceptor signaling. *Journal of Biological Chemistry*, **2017**, 292, 13243-13257	5.4	35
159	Evolutionarily Conserved Roles for Blood-Brain Barrier Xenobiotic Transporters in Endogenous Steroid Partitioning and Behavior. *Cell Reports*, **2017**, 21, 1304-1316	10.6	35
158	Development of 5N-Bicalutamide, a High-Affinity Reversible Covalent Antiandrogen. *ACS Chemical Biology*, **2017**, 12, 2934-2939	4.9	4
157	Discovery of Potent and Orally Bioavailable Macrocyclic Peptide-Peptoid Hybrid CXCR7 Modulators. *Journal of Medicinal Chemistry*, **2017**, 60, 9653-9663	8.3	41
156	Cancer-associated arginine-to-histidine mutations confer a gain in pH sensing to mutant proteins. *Science Signaling*, **2017**, 10,	8.8	28
155	Prominent features of the amino acid mutation landscape in cancer. *PLoS ONE*, **2017**, 12, e0183273	3.7	16
154	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	11.5	35
153	Dihedral Angle-Based Sampling of Natural Product Polyketide Conformations: Application to Permeability Prediction. *Journal of Chemical Information and Modeling*, **2016**, 56, 2194-2206	6.1	10
152	A potent and selective inhibitor targeting human and murine 12/15-LOX. *Bioorganic and Medicinal Chemistry*, **2016**, 24, 1183-90	3.4	13
151	Non-degradative Ubiquitination of Protein Kinases. *PLoS Computational Biology*, **2016**, 12, e1004898	5	23
150	Defining the Product Chemical Space of Monoterpenoid Synthases. *PLoS Computational Biology*, **2016**, 12, e1005053	5	15
149	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	4.8	40
148	Disulfide-Trapping Identifies a New, Effective Chemical Probe for Activating the Nuclear Receptor Human LRH-1 (NR5A2). *PLoS ONE*, **2016**, 11, e0159316	3.7	9
147	Simple Predictive Models of Passive Membrane Permeability Incorporating Size-Dependent Membrane-Water Partition. *Journal of Chemical Information and Modeling*, **2016**, 56, 924-9	6.1	31
146	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	11.5	10

145	Human 15-LOX-1 active site mutations alter inhibitor binding and decrease potency. *Bioorganic and Medicinal Chemistry*, **2016**, 24, 5380-5387	3.4	3
144	Exhaustive Conformational Sampling of Complex Fused Ring Macrocycles Using Inverse Kinematics. *Journal of Chemical Theory and Computation*, **2016**, 12, 4674-87	6.4	39
143	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, 5661-6	11.5	36
142	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		11
141	Synthesis and enzymatic studies of bisubstrate analogues for farnesyl diphosphate synthase. *Journal of Organic Chemistry*, **2015**, 80, 3902-13	4.2	2
140	Beyond cyclosporine A: conformation-dependent passive membrane permeabilities of cyclic peptide natural products. *Future Medicinal Chemistry*, **2015**, 7, 2121-30	4.1	100
139	Probing the Physicochemical Boundaries of Cell Permeability and Oral Bioavailability in Lipophilic Macrocycles Inspired by Natural Products. *Journal of Medicinal Chemistry*, **2015**, 58, 4581-9	8.3	91
138	Peptide to Peptoid Substitutions Increase Cell Permeability in Cyclic Hexapeptides. *Organic Letters*, **2015**, 17, 2928-31	6.2	59
137	Cell-permeable cyclic peptides from synthetic libraries inspired by natural products. *Journal of the American Chemical Society*, **2015**, 137, 715-21	16.4	152
136	Experimental strategies for functional annotation and metabolism discovery: targeted screening of solute binding proteins and unbiased panning of metabolomes. *Biochemistry*, **2015**, 54, 909-31	3.2	65
135	A unique cis-3-hydroxy-l-proline dehydratase in the enolase superfamily. *Journal of the American Chemical Society*, **2015**, 137, 1388-91	16.4	13
134	Novel compounds lowering the cellular isoform of the human prion protein in cultured human cells. *Bioorganic and Medicinal Chemistry*, **2014**, 22, 1960-72	3.4	16
133	Design of reversible, cysteine-targeted Michael acceptors guided by kinetic and computational analysis. *Journal of the American Chemical Society*, **2014**, 136, 12624-30	16.4	154
132	Leveraging structure for enzyme function prediction: methods, opportunities, and challenges. *Trends in Biochemical Sciences*, **2014**, 39, 363-71	10.3	26
131	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	2.5	4
130	Evolution of enzymatic activities in the enolase superfamily: galactarate dehydratase III from Agrobacterium tumefaciens C58. *Biochemistry*, **2014**, 53, 4192-203	3.2	15
129	Prediction of substrates for glutathione transferases by covalent docking. *Journal of Chemical Information and Modeling*, **2014**, 54, 1687-99	6.1	15
128	A structure-based model for predicting serum albumin binding. *PLoS ONE*, **2014**, 9, e93323	3.7	49

127	The free energy profile of tubulin straight-bent conformational changes, with implications for microtubule assembly and drug discovery. *PLoS Computational Biology*, **2014**, 10, e1003464	5	27
126	Correction to Design of Reversible, Cysteine-Targeted Michael Acceptors Guided by Kinetic and Computational Analysis *Journal of the American Chemical Society*, **2014**, 136, 17690-17690	16.4	1
125	Prediction and biochemical demonstration of a catabolic pathway for the osmoprotectant proline betaine. *MBio*, **2014**, 5, e00933-13	7.8	14
124	Predicting the functions and specificity of triterpenoid synthases: a mechanism-based multi-intermediate docking approach. *PLoS Computational Biology*, **2014**, 10, e1003874	5	19
123	A high throughput screen identifies potent and selective inhibitors to human epithelial 15-lipoxygenase-2. *PLoS ONE*, **2014**, 9, e104094	3.7	14
122	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	3.7	27
121	Prediction and characterization of enzymatic activities guided by sequence similarity and genome neighborhood networks. *ELife*, **2014**, 3,	8.9	64
120	Predicting enzyme-substrate specificity with QM/MM methods: a case study of the stereospecificity of (D)-glucarate dehydratase. *Biochemistry*, **2013**, 52, 5511-3	3.2	6
119	Design of a phosphorylatable PDZ domain with peptide-specific affinity changes. *Structure*, **2013**, 21, 54-64	5.2	14
118	A cysteine protease inhibitor rescues mice from a lethal Cryptosporidium parvum infection. *Antimicrobial Agents and Chemotherapy*, **2013**, 57, 6063-73	5.9	40
117	pH sensing by FAK-His58 regulates focal adhesion remodeling. *Journal of Cell Biology*, **2013**, 202, 849-59	7.3	59
116	SIRT5 regulates the mitochondrial lysine succinylome and metabolic networks. *Cell Metabolism*, **2013**, 18, 920-33	24.6	399
115	Discovery of new enzymes and metabolic pathways by using structure and genome context. *Nature*, **2013**, 502, 698-702	50.4	99
114	Active site conformational dynamics are coupled to catalysis in the mRNA decapping enzyme Dcp2. *Structure*, **2013**, 21, 1571-80	5.2	18
113	Pharmacokinetics and metabolism of 2-aminothiazoles with antiprion activity in mice. *Pharmaceutical Research*, **2013**, 30, 932-50	4.5	28
112	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, 361-7	5.7	22
111	2-Aminothiazoles with improved pharmacotherapeutic properties for treatment of prion disease. *ChemMedChem*, **2013**, 8, 847-57	3.7	20
110	Considering protonation as a posttranslational modification regulating protein structure and function. *Annual Review of Biophysics*, **2013**, 42, 289-314	21.1	93

109	Structure-guided discovery of the metabolite carboxy-SAM that modulates tRNA function. *Nature*, **2013**, 498, 123-6	50.4	62
108	Antiprion compounds that reduce PrP(Sc) levels in dividing and stationary-phase cells. *Bioorganic and Medicinal Chemistry*, **2013**, 21, 7999-8012	3.4	14
107	Substrate and inhibitor-induced dimerization and cooperativity in caspase-1 but not caspase-3. *Journal of Biological Chemistry*, **2013**, 288, 9971-9981	5.4	30
106	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	11.5	55
105	Biaryl amides and hydrazones as therapeutics for prion disease in transgenic mice. *Journal of Pharmacology and Experimental Therapeutics*, **2013**, 347, 325-38	4.7	34
104	Chemical-biological characterization of a cruzain inhibitor reveals a second target and a mammalian off-target. *Beilstein Journal of Organic Chemistry*, **2013**, 9, 15-25	2.5	31
103	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, 813-20	3	21
102	Optimizing PK properties of cyclic peptides: the effect of side chain substitutions on permeability and clearance(). *MedChemComm*, **2012**, 3, 1282-1289	5	102
101	Computer-aided antibody design. *Protein Engineering, Design and Selection*, **2012**, 25, 507-21	1.9	173
100	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, 4122-7	11.5	48
99	Predicting and improving the membrane permeability of peptidic small molecules. *Journal of Medicinal Chemistry*, **2012**, 55, 3163-9	8.3	83
98	Comparing Conformational Ensembles Using the Kullback-Leibler Divergence Expansion. *Journal of Chemical Theory and Computation*, **2012**, 8, 2115-2126	6.4	58
97	Testing physical models of passive membrane permeation. *Journal of Chemical Information and Modeling*, **2012**, 52, 1621-36	6.1	76
96	Investigation of the proteolytic functions of an expanded cercarial elastase gene family in Schistosoma mansoni. *PLoS Neglected Tropical Diseases*, **2012**, 6, e1589	4.8	29
95	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	5.4	59
94	Divergent evolution in enolase superfamily: strategies for assigning functions. *Journal of Biological Chemistry*, **2012**, 287, 29-34	5.4	106
93	A molecular mechanics approach to modeling protein-ligand interactions: relative binding affinities in congeneric series. *Journal of Chemical Information and Modeling*, **2011**, 51, 2082-9	6.1	39
92	Dysregulated pH: a perfect storm for cancer progression. *Nature Reviews Cancer*, **2011**, 11, 671-7	31.3	1283

91	On-resin N-methylation of cyclic peptides for discovery of orally bioavailable scaffolds. *Nature Chemical Biology*, **2011**, 7, 810-7	11.7	264
90	Effects of somatic mutations on CDR loop flexibility during affinity maturation. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 821-9	4.2	33
89	Assessment of protein structure refinement in CASP9. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79 Suppl 10, 74-90	4.2	79
88	Assessing protein loop flexibility by hierarchical Monte Carlo sampling. *Journal of Chemical Theory and Computation*, **2011**, 7, 1564-1574	6.4	22
87	The Enzyme Function Initiative. *Biochemistry*, **2011**, 50, 9950-62	3.2	140
86	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, 6056-61	11.5	108
85	Phosphorylation of the Arp2 subunit relieves auto-inhibitory interactions for Arp2/3 complex activation. *PLoS Computational Biology*, **2011**, 7, e1002226	5	14
84	A new view of the bacterial cytosol environment. *PLoS Computational Biology*, **2011**, 7, e1002066	5	34
83	Predicting binding to p-glycoprotein by flexible receptor docking. *PLoS Computational Biology*, **2011**, 7, e1002083	5	78
82	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	4.8	92
81	Modeling conformational ensembles of slow functional motions in Pin1-WW. *PLoS Computational Biology*, **2010**, 6, e1001015	5	60
80	A nonazole CYP51 inhibitor cures Chagas' disease in a mouse model of acute infection. *Antimicrobial Agents and Chemotherapy*, **2010**, 54, 2480-8	5.9	55
79	Studying enzyme-substrate specificity in silico: a case study of the Escherichia coli glycolysis pathway. *Biochemistry*, **2010**, 49, 4003-5	3.2	17
78	Transcriptional control of a plant stem cell niche. *Developmental Cell*, **2010**, 18, 849-61	10.2	190
77	Conformation switching of clathrin light chain regulates clathrin lattice assembly. *Developmental Cell*, **2010**, 18, 841-8	10.2	56
76	SIRT3 deacetylates mitochondrial 3-hydroxy-3-methylglutaryl CoA synthase 2 and regulates ketone body production. *Cell Metabolism*, **2010**, 12, 654-61	24.6	357
75	Antibodies as a model system for comparative model refinement. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 2490-505	4.2	15
74	Binding-site assessment by virtual fragment screening. *PLoS ONE*, **2010**, 5, e10109	3.7	48

73	Computational studies of protein regulation by post-translational phosphorylation. *Current Opinion in Structural Biology*, **2009**, 19, 156-63	8.1	64
72	Target selection and annotation for the structural genomics of the amidohydrolase and enolase superfamilies. *Journal of Structural and Functional Genomics*, **2009**, 10, 107-25		24
71	Automated site preparation in physics-based rescoring of receptor ligand complexes. *Proteins: Structure, Function and Bioinformatics*, **2009**, 77, 52-61	4.2	17
70	Assessment of the protein-structure refinement category in CASP8. *Proteins: Structure, Function and Bioinformatics*, **2009**, 77 Suppl 9, 66-80	4.2	64
69	Improving the species cross-reactivity of an antibody using computational design. *Bioorganic and Medicinal Chemistry Letters*, **2009**, 19, 3744-7	2.9	40
68	Monte Carlo Sampling with Hierarchical Move Sets: POSH Monte Carlo. *Journal of Chemical Theory and Computation*, **2009**, 5, 1968-84	6.4	9
67	The molecular basis of species-specific ligand activation of trace amine-associated receptor 1 (TAAR(1)). *ACS Chemical Biology*, **2009**, 4, 209-20	4.9	34
66	Computation-facilitated assignment of the function in the enolase superfamily: a regiochemically distinct galactarate dehydratase from Oceanobacillus iheyensis. *Biochemistry*, **2009**, 48, 11546-58	3.2	31
65	Quantifying Correlations Between Allosteric Sites in Thermodynamic Ensembles. *Journal of Chemical Theory and Computation*, **2009**, 5, 2486-2502	6.4	172
64	Energy-based analysis and prediction of the orientation between light- and heavy-chain antibody variable domains. *Journal of Molecular Biology*, **2009**, 388, 941-53	6.5	37
63	The role of homology models in assigning enzyme function. *FASEB Journal*, **2009**, 23, 204.2	0.9	
62	Discovery of a dipeptide epimerase enzymatic function guided by homology modeling and virtual screening. *Structure*, **2008**, 16, 1668-77	5.2	49
61	Rescoring docking hit lists for model cavity sites: predictions and experimental testing. *Journal of Molecular Biology*, **2008**, 377, 914-34	6.5	149
60	Multiscale Monte Carlo Sampling of Protein Sidechains: Application to Binding Pocket Flexibility. *Journal of Chemical Theory and Computation*, **2008**, 4, 835-846	6.4	12
59	Structural model and functional significance of pH-dependent talin-actin binding for focal adhesion remodeling. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 14436-41	11.5	95
58	Cofilin is a pH sensor for actin free barbed end formation: role of phosphoinositide binding. *Journal of Cell Biology*, **2008**, 183, 865-79	7.3	147
57	Conformational selection in silico: loop latching motions and ligand binding in enzymes. *Proteins: Structure, Function and Bioinformatics*, **2008**, 71, 153-64	4.2	22
56	Toward better refinement of comparative models: predicting loops in inexact environments. *Proteins: Structure, Function and Bioinformatics*, **2008**, 72, 959-71	4.2	74

55	Toward deciphering the code to aminergic G protein-coupled receptor drug design. *Chemistry and Biology*, **2008**, 15, 343-53		32
54	Multiscale Optimization of a Truncated Newton Minimization Algorithm and Application to Proteins and Protein-Ligand Complexes. *Journal of Chemical Theory and Computation*, **2007**, 3, 640-8	6.4	27
53	Strengths of hydrogen bonds involving phosphorylated amino acid side chains. *Journal of the American Chemical Society*, **2007**, 129, 820-7	16.4	94
52	Intramolecular Dynamics in the Frequency Domain. *Advances in Chemical Physics*, **2007**, 463-490		7
51	Prediction of side-chain conformations on protein surfaces. *Proteins: Structure, Function and Bioinformatics*, **2007**, 66, 814-23	4.2	27
50	Prediction and assignment of function for a divergent N-succinyl amino acid racemase. *Nature Chemical Biology*, **2007**, 3, 486-91	11.7	87
49	An atomistic model of passive membrane permeability: application to a series of FDA approved drugs. *Journal of Computer-Aided Molecular Design*, **2007**, 21, 675-9	4.2	17
48	Intracellular pH sensors: design principles and functional significance. *Physiology*, **2007**, 22, 30-9	9.8	189
47	Assignment of polar states for protein amino acid residues using an interaction cluster decomposition algorithm and its application to high resolution protein structure modeling. *Proteins: Structure, Function and Bioinformatics*, **2007**, 66, 824-37	4.2	37
46	Physics-based methods for studying protein-ligand interactions. *Current Opinion in Drug Discovery & Development*, **2007**, 10, 325-31		22
45	What role do surfaces play in GB models? A new-generation of surface-generalized born model based on a novel gaussian surface for biomolecules. *Journal of Computational Chemistry*, **2006**, 27, 72-89	3.5	72
44	Conformational changes in protein loops and helices induced by post-translational phosphorylation. *PLoS Computational Biology*, **2006**, 2, e32	5	98
43	Testing the conformational hypothesis of passive membrane permeability using synthetic cyclic peptide diastereomers. *Journal of the American Chemical Society*, **2006**, 128, 2510-1	16.4	340
42	Physics-based scoring of protein-ligand complexes: enrichment of known inhibitors in large-scale virtual screening. *Journal of Chemical Information and Modeling*, **2006**, 46, 243-53	6.1	127
41	Molecular mechanics methods for predicting protein-ligand binding. *Physical Chemistry Chemical Physics*, **2006**, 8, 5166-77	3.6	163
40	Novel procedure for modeling ligand/receptor induced fit effects. *Journal of Medicinal Chemistry*, **2006**, 49, 534-53	8.3	1320
39	Conformational flexibility, internal hydrogen bonding, and passive membrane permeability: successful in silico prediction of the relative permeabilities of cyclic peptides. *Journal of the American Chemical Society*, **2006**, 128, 14073-80	16.4	280
38	Novel human lipoxygenase inhibitors discovered using virtual screening with homology models. *Journal of Medicinal Chemistry*, **2006**, 49, 1356-63	8.3	72

37	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, 228-50	6.5	60
36	Surfaces affect ion pairing. *Journal of Physical Chemistry B*, **2005**, 109, 24056-60	3.4	50
35	Competition between intramolecular hydrogen bonds and solvation in phosphorylated peptides: simulations with explicit and implicit solvent. *Journal of Physical Chemistry B*, **2005**, 109, 5249-58	3.4	36
34	Virtual screening against highly charged active sites: identifying substrates of alpha-beta barrel enzymes. *Biochemistry*, **2005**, 44, 2059-71	3.2	74
33	Virtual ligand screening against Escherichia coli dihydrofolate reductase: improving docking enrichment using physics-based methods. *Journal of Biomolecular Screening*, **2005**, 10, 675-81		29
32	High-resolution prediction of protein helix positions and orientations. *Proteins: Structure, Function and Bioinformatics*, **2004**, 55, 368-82	4.2	51
31	A hierarchical approach to all-atom protein loop prediction. *Proteins: Structure, Function and Bioinformatics*, **2004**, 55, 351-67	4.2	1329
30	A kinematic view of loop closure. *Journal of Computational Chemistry*, **2004**, 25, 510-28	3.5	206
29	Comparative Protein Structure Modeling and its Applications to Drug Discovery. *Annual Reports in Medicinal Chemistry*, **2004**, 39, 259-276	1.6	56
28	Tryptophan 500 and arginine 707 define product and substrate active site binding in soybean lipoxygenase-1. *Biochemistry*, **2004**, 43, 13063-71	3.2	28
27	First-Shell Solvation of Ion Pairs: Correction of Systematic Errors in Implicit Solvent Models *Journal of Physical Chemistry B*, **2004**, 108, 6643-6654	3.4	62
26	Computational modeling of the catalytic reaction in triosephosphate isomerase. *Journal of Molecular Biology*, **2004**, 337, 227-39	6.5	69
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