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	A SARS-CoV-2 protein interaction map reveals targets for drug repurposing. Nature, 2020, 583, 459-468.	13.7	3,542
2	A hierarchical approach to all-atom protein loop prediction. Proteins: Structure, Function and Bioinformatics, 2004, 55, 351-367.	1.5	1,874
3	Dysregulated pH: a perfect storm for cancer progression. Nature Reviews Cancer, 2011, 11, 671-677.	12.8	1,734
4	Novel Procedure for Modeling Ligand/Receptor Induced Fit Effects. Journal of Medicinal Chemistry, 2006, 49, 534-553.	2.9	1,671
5	On the Role of the Crystal Environment in Determining Protein Side-chain Conformations. Journal of Molecular Biology, 2002, 320, 597-608.	2.0	1,002
6	SIRT5 Regulates the Mitochondrial Lysine Succinylome and Metabolic Networks. Cell Metabolism, 2013, 18, 920-933.	7.2	549
7	SIRT3 Deacetylates Mitochondrial 3-Hydroxy-3-Methylglutaryl CoA Synthase 2 and Regulates Ketone Body Production. Cell Metabolism, 2010, 12, 654-661.	7.2	418
8	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
9	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
10	On-resin N-methylation of cyclic peptides for discovery of orally bioavailable scaffolds. Nature Chemical Biology, 2011, 7, 810-817.	3.9	318
11	Gasdermin D pore structure reveals preferential release of mature interleukin-1. Nature, 2021, 593, 607-611.	13.7	298
12	A kinematic view of loop closure. Journal of Computational Chemistry, 2004, 25, 510-528.	1.5	265
13	Transcriptional Control of a Plant Stem Cell Niche. Developmental Cell, 2010, 18, 841-853.	3.1	221
14	Intracellular pH Sensors: Design Principles and Functional Significance. Physiology, 2007, 22, 30-39.	1.6	212
15	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
16	Quantifying Correlations Between Allosteric Sites in Thermodynamic Ensembles. Journal of Chemical Theory and Computation, 2009, 5, 2486-2502.	2.3	203
17	Computer-aided antibody design. Protein Engineering, Design and Selection, 2012, 25, 507-522.	1.0	203
18	Molecular mechanics methods for predicting proteinâ€“ligand binding. Physical Chemistry Chemical Physics, 2006, 8, 5166-5177.	1.3	200

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19	Cell-Permeable Cyclic Peptides from Synthetic Libraries Inspired by Natural Products. Journal of the American Chemical Society, 2015, 137, 715-721.	6.6	186
20	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
21	The Enzyme Function Initiative. Biochemistry, 2011, 50, 9950-9962.	1.2	169
22	Rescoring Docking Hit Lists for Model Cavity Sites: Predictions and Experimental Testing. Journal of Molecular Biology, 2008, 377, 914-934.	2.0	168
23	Force Field Validation Using Protein Side Chain Prediction. Journal of Physical Chemistry B, 2002, 106, 11673-11680.	1.2	165
24	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
25	Beyond cyclosporine A: conformation-dependent passive membrane permeabilities of cyclic peptide natural products. Future Medicinal Chemistry, 2015, 7, 2121-2130.	1.1	140
26	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
27	Considering Protonation as a Posttranslational Modification Regulating Protein Structure and Function. Annual Review of Biophysics, 2013, 42, 289-314.	4.5	133
28	Discovery of GBT440, an Orally Bioavailable R-State Stabilizer of Sickle Cell Hemoglobin. ACS Medicinal Chemistry Letters, 2017, 8, 321-326.	1.3	129
29	Baseline subtraction using robust local regression estimation. Journal of Quantitative Spectroscopy and Radiative Transfer, 2001, 68, 179-193.	1.1	126
30	Discovery of new enzymes and metabolic pathways by using structure and genome context. Nature, 2013, 502, 698-702.	13.7	124
31	Conformational Changes in Protein Loops and Helices Induced by Post-Translational Phosphorylation. PLoS Computational Biology, 2006, 2, e32.	1.5	120
32	Optimizing PK properties of cyclic peptides: the effect of side chain substitutions on permeability and clearance. MedChemComm, 2012, 3, 1282-1289.	3.5	120
33	Strengths of Hydrogen Bonds Involving Phosphorylated Amino Acid Side Chains. Journal of the American Chemical Society, 2007, 129, 820-827.	6.6	119
34	Divergent Evolution in Enolase Superfamily: Strategies for Assigning Functions. Journal of Biological Chemistry, 2012, 287, 29-34.	1.6	118
35	Acetylene at the Threshold of Isomerization. Journal of Physical Chemistry A, 2000, 104, 3073-3086.	1.1	115
36	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

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37	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
38	Pure bending dynamics in the acetylene XÌƒâ€‰1Î£g+ state up to 15â€‰000 cmâ^'1 of internal energy. Journal of Chemical Physics, 1998, 109, 121-133.	1.2	110
39	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
40	State-by-state assignment of the bending spectrum of acetylene at 15â€Š000 cmâ^'1: A case study of quantum-classical correspondence. Journal of Chemical Physics, 1999, 111, 600-618.	1.2	100
41	Testing Physical Models of Passive Membrane Permeation. Journal of Chemical Information and Modeling, 2012, 52, 1621-1636.	2.5	100
42	Prediction and assignment of function for a divergent N-succinyl amino acid racemase. Nature Chemical Biology, 2007, 3, 486-491.	3.9	98
43	Predicting and Improving the Membrane Permeability of Peptidic Small Molecules. Journal of Medicinal Chemistry, 2012, 55, 3163-3169.	2.9	96
44	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
45	Predicting Binding to P-Glycoprotein by Flexible Receptor Docking. PLoS Computational Biology, 2011, 7, e1002083.	1.5	90
46	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
47	Assessment of protein structure refinement in CASP9. Proteins: Structure, Function and Bioinformatics, 2011, 79, 74-90.	1.5	87
48	Structure-guided discovery of the metabolite carboxy-SAM that modulates tRNA function. Nature, 2013, 498, 123-126.	13.7	84
49	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
50	Novel Human Lipoxygenase Inhibitors Discovered Using Virtual Screening with Homology Models. Journal of Medicinal Chemistry, 2006, 49, 1356-1363.	2.9	81
51	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.	1.5	81
52	Prediction and characterization of enzymatic activities guided by sequence similarity and genome neighborhood networks. ELife, 2014, 3, .	2.8	81
53	Toward better refinement of comparative models: Predicting loops in inexact environments. Proteins: Structure, Function and Bioinformatics, 2008, 72, 959-971.	1.5	80
54	pH sensing by FAK-His58 regulates focal adhesion remodeling. Journal of Cell Biology, 2013, 202, 849-859.	2.3	79

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55	Computational Modeling of the Catalytic Reaction in Triosephosphate Isomerase. Journal of Molecular Biology, 2004, 337, 227-239.	2.0	78
56	Virtual Screening against Highly Charged Active Sites:â€‰ Identifying Substrates of Alphaâˆ’Beta Barrel Enzymes. Biochemistry, 2005, 44, 2059-2071.	1.2	78
57	Modeling Conformational Ensembles of Slow Functional Motions in Pin1-WW. PLoS Computational Biology, 2010, 6, e1001015.	1.5	76
58	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
59	Comparing Conformational Ensembles Using the Kullbackâ€“Leibler Divergence Expansion. Journal of Chemical Theory and Computation, 2012, 8, 2115-2126.	2.3	74
60	Local mode behavior in the acetylene bending system. Journal of Chemical Physics, 1999, 110, 845-859.	1.2	72
61	Computational studies of protein regulation by post-translational phosphorylation. Current Opinion in Structural Biology, 2009, 19, 156-163.	2.6	72
62	Conformation Switching of Clathrin Light Chain Regulates Clathrin Lattice Assembly. Developmental Cell, 2010, 18, 854-861.	3.1	72
63	Peptide to Peptoid Substitutions Increase Cell Permeability in Cyclic Hexapeptides. Organic Letters, 2015, 17, 2928-2931.	2.4	71
64	First-Shell Solvation of Ion Pairs:â€‰ Correction of Systematic Errors in Implicit Solvent Models. Journal of Physical Chemistry B, 2004, 108, 6643-6654.	1.2	69
65	Comparative Protein Structure Modeling and its Applications to Drug Discovery. Annual Reports in Medicinal Chemistry, 2004, 39, 259-276.	0.5	68
66	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
67	Assessment of the proteinâ€structure refinement category in CASP8. Proteins: Structure, Function and Bioinformatics, 2009, 77, 66-80.	1.5	65
68	Structural and Kinetic Studies of a Cisplatin-modified DNA Icosamer Binding to HMG1 Domain B. Journal of Biological Chemistry, 1999, 274, 12346-12354.	1.6	63
69	Synthetic group A streptogramin antibiotics that overcome Vat resistance. Nature, 2020, 586, 145-150.	13.7	63
70	A Structure-Based Model for Predicting Serum Albumin Binding. PLoS ONE, 2014, 9, e93323.	1.1	61
71	Numerical pattern recognition analysis of acetylene dispersed fluorescence spectra. Journal of Chemical Physics, 1998, 108, 7100-7113.	1.2	59
72	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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73	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
74	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
75	A recurrent kinase domain mutation in PRKCA defines chordoid glioma of the third ventricle. Nature Communications, 2018, 9, 810.	5.8	56
76	Binding-Site Assessment by Virtual Fragment Screening. PLoS ONE, 2010, 5, e10109.	1.1	56
77	High-resolution prediction of protein helix positions and orientations. Proteins: Structure, Function and Bioinformatics, 2004, 55, 368-382.	1.5	55
78	Exhaustive Conformational Sampling of Complex Fused Ring Macrocycles Using Inverse Kinematics. Journal of Chemical Theory and Computation, 2016, 12, 4674-4687.	2.3	54
79	Discovery of Potent and Orally Bioavailable Macrocyclic Peptideâ€“Peptoid Hybrid CXCR7 Modulators. Journal of Medicinal Chemistry, 2017, 60, 9653-9663.	2.9	54
80	Cancer-associated arginine-to-histidine mutations confer a gain in pH sensing to mutant proteins. Science Signaling, 2017, 10, .	1.6	54
81	Surfaces Affect Ion Pairing. Journal of Physical Chemistry B, 2005, 109, 24056-24060.	1.2	52
82	Discovery of a Dipeptide Epimerase Enzymatic Function Guided by Homology Modeling and Virtual Screening. Structure, 2008, 16, 1668-1677.	1.6	52
83	A Cysteine Protease Inhibitor Rescues Mice from a Lethal Cryptosporidium parvum Infection. Antimicrobial Agents and Chemotherapy, 2013, 57, 6063-6073.	1.4	52
84	Progranulin Stimulates the In Vitro Maturation of Pro-Cathepsin D at Acidic pH. Journal of Molecular Biology, 2019, 431, 1038-1047.	2.0	52
85	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
86	Evolutionarily Conserved Roles for Blood-Brain Barrier Xenobiotic Transporters in Endogenous Steroid Partitioning and Behavior. Cell Reports, 2017, 21, 1304-1316.	2.9	48
87	Anomalously slow intramolecular vibrational redistribution in the acetylene XÌƒâ€‰1Î£g+ state above 10â€‰000 cmâ^'1 of internal energy. Journal of Chemical Physics, 1998, 109, 3831-3840.	1.2	46
88	Improving the species cross-reactivity of an antibody using computational design. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 3744-3747.	1.0	46
89	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
90	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

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91	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
92	Effects of somatic mutations on CDR loop flexibility during affinity maturation. Proteins: Structure, Function and Bioinformatics, 2011, 79, 821-829.	1.5	43
93	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
94	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
95	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
96	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
97	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
98	Covalent Modification and Regulation of the Nuclear Receptor Nurr1 by a Dopamine Metabolite. Cell Chemical Biology, 2019, 26, 674-685.e6.	2.5	41
99	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, 2006, 66, 824-837.	1.5	40
100	A New View of the Bacterial Cytosol Environment. PLoS Computational Biology, 2011, 7, e1002066.	1.5	39
101	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
102	The infrared-ultraviolet dispersed fluorescence spectrum of acetylene: New classes of bright states. Journal of Chemical Physics, 2001, 114, 7424-7442.	1.2	38
103	Competition between Intramolecular Hydrogen Bonds and Solvation in Phosphorylated Peptides:â€‰ Simulations with Explicit and Implicit Solvent. Journal of Physical Chemistry B, 2005, 109, 5249-5258.	1.2	38
104	Spectroscopic signatures of bond-breaking internal rotation. II. Rotation-vibration level structure and quantum monodromy in HCP. Journal of Chemical Physics, 2001, 114, 262.	1.2	37
105	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
106	Complete protein structure determination using backbone residual dipolar couplings and sidechain rotamer prediction. Journal of Structural and Functional Genomics, 2002, 2, 103-111.	1.2	36
107	Virtual Ligand Screening against Escherichia coli Dihydrofolate Reductase: Improving Docking Enrichment Using Physics-Based Methods. Journal of Biomolecular Screening, 2005, 10, 675-681.	2.6	35
108	Toward Deciphering the Code to Aminergic G Protein-Coupled Receptor Drug Design. Chemistry and Biology, 2008, 15, 343-353.	6.2	35

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109	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
110	Inhibitor binding mode and allosteric regulation of Na+-glucose symporters. Nature Communications, 2018, 9, 5245.	5.8	35
111	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
112	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
113	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
114	Tryptophan 500 and Arginine 707 Define Product and Substrate Active Site Binding in Soybean Lipoxygenase-1â€. Biochemistry, 2004, 43, 13063-13071.	1.2	32
115	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
116	Extended cross correlation: A technique for spectroscopic pattern recognition. Journal of Chemical Physics, 1997, 107, 8349-8356.	1.2	31
117	Prediction of side-chain conformations on protein surfaces. Proteins: Structure, Function and Bioinformatics, 2007, 66, 814-823.	1.5	31
118	Leveraging structure for enzyme function prediction: methods, opportunities, and challenges. Trends in Biochemical Sciences, 2014, 39, 363-371.	3.7	31
119	Non-degradative Ubiquitination of Protein Kinases. PLoS Computational Biology, 2016, 12, e1004898.	1.5	31
120	Prediction of enzymatic pathways by integrative pathway mapping. ELife, 2018, 7, .	2.8	30
121	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
122	Scaling Rules for Resonance Dynamics near a Saddle Point:Â The Pendulum as a Zero-Order Modelâ€. Journal of Physical Chemistry A, 2001, 105, 2834-2841.	1.1	29
123	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
124	Pharmacokinetics and Metabolism of 2-Aminothiazoles with Antiprion Activity in Mice. Pharmaceutical Research, 2013, 30, 932-950.	1.7	29
125	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
126	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

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127	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
128	The Acetylene Bending Spectrum at âˆ¼10000 cm-1:â€‰ Quantum Assignments in the Midst of Classical Chaos. Journal of Physical Chemistry A, 2001, 105, 681-693.	1.1	27
129	Defining the Product Chemical Space of Monoterpenoid Synthases. PLoS Computational Biology, 2016, 12, e1005053.	1.5	26
130	Prominent features of the amino acid mutation landscape in cancer. PLoS ONE, 2017, 12, e0183273.	1.1	26
131	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
132	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
133	Observation of Coriolis Coupling between Î½2 + 4Î½4 and 7Î½4 in Acetylene XÌƒ1Î£+g by Stimulated Emission Pumping Spectroscopy. Journal of Molecular Spectroscopy, 2000, 199, 265-274.	0.4	24
134	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
135	Spectroscopic signatures of bond-breaking internal rotation. I. Saddle point induced polyad breakdown. Journal of Chemical Physics, 2001, 114, 250.	1.2	23
136	Active Site Conformational Dynamics Are Coupled to Catalysis in the mRNA Decapping Enzyme Dcp2. Structure, 2013, 21, 1571-1580.	1.6	23
137	Predicting the Functions and Specificity of Triterpenoid Synthases: A Mechanism-Based Multi-intermediate Docking Approach. PLoS Computational Biology, 2014, 10, e1003874.	1.5	23
138	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
139	VariCarta: A Comprehensive Database of Harmonized Genomic Variants Found in Autism Spectrum Disorder Sequencing Studies. Autism Research, 2019, 12, 1728-1736.	2.1	23
140	Physics-based methods for studying protein-ligand interactions. Current Opinion in Drug Discovery & Development, 2007, 10, 325-31.	1.9	23
141	Conformational selection in silico: Loop latching motions and ligand binding in enzymes. Proteins: Structure, Function and Bioinformatics, 2008, 71, 153-164.	1.5	22
142	Automated site preparation in physicsâ€based rescoring of receptor ligand complexes. Proteins: Structure, Function and Bioinformatics, 2009, 77, 52-61.	1.5	22
143	Assessing Protein Loop Flexibility by Hierarchical Monte Carlo Sampling. Journal of Chemical Theory and Computation, 2011, 7, 1564-1574.	2.3	22
144	Crosstalk between RNA Pol II C-Terminal Domain Acetylation and Phosphorylation via RPRD Proteins. Molecular Cell, 2019, 74, 1164-1174.e4.	4.5	22

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145	Phosphorylation of the Arp2 Subunit Relieves Auto-inhibitory Interactions for Arp2/3 Complex Activation. PLoS Computational Biology, 2011, 7, e1002226.	1.5	21
146	ATP-Competitive Inhibitors Midostaurin and Avapritinib Have Distinct Resistance Profiles in Exon 17â€“Mutant KIT. Cancer Research, 2019, 79, 4283-4292.	0.4	21
147	Curation of over 10â€‰000 transcriptomic studies to enable data reuse. Database: the Journal of Biological Databases and Curation, 2021, 2021, .	1.4	21
148	2â€Aminothiazoles with Improved Pharmacotherapeutic Properties for Treatment of Prion Disease. ChemMedChem, 2013, 8, 847-857.	1.6	20
149	Prediction of Substrates for Glutathione Transferases by Covalent Docking. Journal of Chemical Information and Modeling, 2014, 54, 1687-1699.	2.5	20
150	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
151	Prediction and Biochemical Demonstration of a Catabolic Pathway for the Osmoprotectant Proline Betaine. MBio, 2014, 5, e00933-13.	1.8	19
152	Identifying patterns in multicomponent signals by extended cross correlation. Journal of Chemical Physics, 1997, 107, 8357-8369.	1.2	18
153	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
154	Studying Enzymeâ”Substrate Specificity in Silico: A Case Study of the Escherichia coli Glycolysis Pathway. Biochemistry, 2010, 49, 4003-4005.	1.2	18
155	Probing the Electrostatic and Steric Requirements for Substrate Binding in Human Platelet-Type 12-Lipoxygenase. Biochemistry, 2019, 58, 848-857.	1.2	18
156	A High Throughput Screen Identifies Potent and Selective Inhibitors to Human Epithelial 15-Lipoxygenase-2. PLoS ONE, 2014, 9, e104094.	1.1	18
157	Design of a Phosphorylatable PDZ Domain with Peptide-Specific Affinity Changes. Structure, 2013, 21, 54-64.	1.6	17
158	Antiprion compounds that reduce PrPSc levels in dividing and stationary-phase cells. Bioorganic and Medicinal Chemistry, 2013, 21, 7999-8012.	1.4	17
159	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
160	Antibodies as a model system for comparative model refinement. Proteins: Structure, Function and Bioinformatics, 2010, 78, 2490-2505.	1.5	15
161	Evolution of Enzymatic Activities in the Enolase Superfamily: Galactarate Dehydratase III from Agrobacterium tumefaciens C58. Biochemistry, 2014, 53, 4192-4203.	1.2	15
162	A potent and selective inhibitor targeting human and murine 12/15-LOX. Bioorganic and Medicinal Chemistry, 2016, 24, 1183-1190.	1.4	15

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163	Kinetic and structural investigations of novel inhibitors of human epithelial 15-lipoxygenase-2. Bioorganic and Medicinal Chemistry, 2021, 46, 116349.	1.4	15
164	Visualizing intramolecular vibrational redistribution: expectation values of resonance operators. Chemical Physics Letters, 2000, 320, 553-560.	1.2	14
165	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
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